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SAS/STAT[®] 12.3

User's Guide

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Chapter 1

What's New in SAS/STAT 12.1 and 12.3

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Overview

SAS/STAT 12.1 includes four new procedures and many enhancements.

In previous years, SAS/STAT software was updated only with new releases of Base SAS software, but this is no longer the case. This means that SAS/STAT software can be released to customers when enhancements are ready, and the goal is to update SAS/STAT every 12 to 18 months. To mark this newfound independence, the release numbering scheme for SAS/STAT changed starting with SAS/STAT 12.1. This new numbering scheme will be maintained when new versions of Base SAS and SAS/STAT are shipped at the same time.

SAS/STAT 12.3 is a maintenance release. No new features have been added. The information in this book applies to SAS/STAT 12.1 and SAS/STAT 12.3.

New Procedures

New Experimental ADAPTIVEREG Procedure

The ADAPTIVEREG procedure fits multivariate adaptive regression splines. The method is a nonparametric regression technique that combines both regression splines and model selection methods. It constructs spline basis functions in an adaptive way by automatically selecting appropriate knot values for different variables. The procedure performs model reduction by applying model selection techniques. Thus, the ADAPTIVEREG procedure is both a nonparametric regression procedure and a predictive modeling procedure.

The ADAPTIVEREG procedure supports models with classification variables, and it provides options for improving modeling speed. PROC ADAPTIVEREG extends the method to data with response variables that are distributed in the exponential family, including the binomial, Poisson, negative binomial, gamma, and inverse Gaussian distributions. PROC ADAPTIVEREG is multithreaded, enabling it to take advantage of multiple processors.

New Experimental QUANTLIFE Procedure

The QUANTLIFE procedure implements two quantile regression approaches that have been developed to account for right-censoring and provide valid estimates. Portnoy (2003) proposed a method to estimate conditional quantile functions from survival data by generalizing the idea of the Kaplan-Meier estimator of the survival function, and Peng and Huang (2008) developed a quantile regression approach motivated by the Nelson-Aalen estimator of the cumulative hazard function. Both methods are implemented with linear programming algorithms in the QUANTLIFE procedure. Like the standard quantile regression method for uncensored data, these two methods are distribution-free and are applicable to heteroscedastic data.

The QUANTLIFE procedure produces survival plots, conditional quantile plots, and quantile process plots. It performs semiparametric quantile regression when you specify spline effects. PROC QUANTLIFE takes advantage of parallel computing when multiple processors are available.

New Experimental QUANTSELECT Procedure

The QUANTSELECT procedure performs model selection for linear quantile regression. It provides capabilities similar to those offered by the GLMSELECT procedure (provides model selection for univariate linear models) including forward, backward, stepwise, LASSO, and adaptive LASSO selection methods.

You can specify criteria such as AIC, SBC, AICC, adjusted R1, and significance levels to compare the fit of models, to determine when to stop the model selection process, and to choose the final selection model. The QUANTSELECT procedure supports constructed effects (such as smoothing splines and polynomials) and the SPLIT option for its CLASS statement. PROC QUANTREG produces parameter estimates progression plots and a variety of criterion progression plots.

PROC QUANTSELECT supports constructed effects such as regression spline, and it enables you to partition your data into training, validation, and testing roles. It is also multithreaded so that it can take advantage of multiple processors.

PROC QUANTSELECT is very efficient and can handle hundreds of variables and thousands of observations.

New STDRA TE Procedure

The STDRA TE procedure computes direct and indirect standardized rates and risks for study populations. With direct standardization, you compute the weighted average of stratum-specific estimates in the study population, using weights such as population-time from a standard or reference population. With indirect standardization, you compute the weighted average of stratum-specific estimates in the reference population by using weights from the study population. The procedure provides summary statistics such as rate and risk estimates (and their confidence limits) for each stratum, as well as graphs.

Highlights of Enhancements

The following are highlights of other enhancements in SAS/STAT 12.1:

- The MCMC procedure now models missing values by default. The RANDOM statement supports multilevel hierarchy to an arbitrary depth. The procedure also implements faster and more efficient sampling algorithms.
- The PHREG procedure supports Bayesian frailty models.
- The FMM procedure for finite mixture models is now production and adds several truncated distributions.
- The LIFEREG and PROBIT procedures include additional postprocessing statements. They now support the TEST, LSMEANS, LSMESTIMATE, ESTIMATE, SLICE, and EFFECTPLOT statements.
- The FREQ procedure produces mosaic plots.
- The SURVEYSELECT procedure provides Poisson sampling.
- The SURVEYMEANS procedure now performs poststratification estimation.
- The GLM, MIXED, GLIMMIX, and ORTHOREG procedures support the REF= option in the CLASS statement.

More information about the changes and enhancements follows. Details can be found in the documentation for the individual procedures in the *SAS/STAT 12.1 User's Guide*.

Highlights of Enhancements in SAS/STAT 9.3

Some users might be unfamiliar with updates made in SAS/STAT 9.3. The following are some of the major enhancements that were introduced in SAS/STAT 9.3:

- The experimental FMM procedure fits statistical models to data where the distribution of the response is a finite mixture of univariate distributions. These models are useful for applications such as estimating multimodal or heavy-tailed densities, fitting zero-inflated or hurdle models to count data with excess zeros, modeling overdispersed data, and fitting regression models with complex error distributions.
- The EFFECT statement became production. This statement is available in the HPMIXED, GLIMMIX, GLMSELECT, LOGISTIC, ORTHOREG, PHREG, PLS, QUANTREG, ROBUSTREG, SURVEYLOGISTIC, and SURVEYREG procedures.
- The MCMC procedure added a RANDOM statement, which simplifies the specification of hierarchical random-effects models and significantly reduces simulation time while improving convergence.
- The METHOD=FIML option in the CALIS procedure became production. This option specifies the full information maximum likelihood method.
- The SURVEYPHREG procedure became production and handles time-dependent covariates.
- The HPMIXED procedure added a REPEATED statement and additional covariance structures.
- The MI procedure added fully conditional specification methods for multiple imputation.
- The NLIN procedure was updated with features for diagnosing the nonlinear model fit.

New Macros

Bayesian Analysis Postprocessing Macros

Postprocessing macros are now available in the SAS autocall library. These macros duplicate the corresponding summary and diagnostic capabilities provided by the MCMC procedure and can be used with any SAS data set that contains posterior samples. These macros are documented with the MCMC procedure.

%CIF Macro

The %CIF macro implements nonparametric methods for estimating cumulative incidence functions with competing risks data. The macro can also be used to test the hypothesis that cumulative incidence functions are identical across groups. The %CIF macro is available from the SAS autocall library.

Enhancements

CALIS Procedure

The CALIS procedure now provides the following features:

- Residual analysis at the case level or observation level is provided when you input raw data.
- Robust estimation is now available. You can request either direct robust estimation based on residual weighting or two-stage robust estimation based on analyzing the robust mean and covariance matrices.
- The BASEFUNC= and BASEFIT= options enable you to input the model fit information of the customized baseline model of your choice. With this input information, PROC CALIS computes various fit indices (mainly the incremental fit indices) based on your customized model fit rather than the fit of the default uncorrelatedness model.

EFFECTPLOT Statement

The CLUSTER option in the EFFECTPLOT statement modifies the INTERACTION plot-type by displaying the levels of the SLICEBY= effect in a side-by-side fashion. The CONNECT option in the EFFECTPLOT statement modifies the BOX and INTERACTION plot-types by connecting the predicted values with a line.

FMM Procedure

The FMM procedure is now production and adds the truncated exponential, truncated lognormal, truncated negative binomial, and truncated normal distributions.

FREQ Procedure

The Agresti-Caffo and Miettinen-Nurminen confidence limits for the risk (proportion) difference are now available, and any confidence limit type can now be displayed in the risk difference plot. You can also request a continuity correction for the Wilson confidence limits for a binomial proportion.

The PLCORR option in the TEST statement produces Wald and likelihood ratio tests for the polychoric correlation coefficient.

The new DF= chi-square option specifies or adjusts the degrees of freedom for chi-square tests. The TESTF= chi-square option now permits you to provide null frequencies for a one-way chi-square test by using a secondary input data set. Similarly, the TESTP= chi-square option now permits you to provide null proportions by using a secondary input data set.

The LRCHISQ chi-square option in the TABLES statement produces a likelihood ratio chi-square test for one-way tables. This test can be based on a null hypothesis of equal proportions, specified proportions, or specified frequencies. The LRCHISQ option in the EXACT statement produces an exact likelihood ratio chi-square test for one-way tables.

The EXACT statement can now produce Barnard's exact unconditional test for the risk difference as well as an exact likelihood ratio goodness-of-fit test.

The MAXLEVELS=*n* option in the TABLES statement specifies the maximum number of variable levels to display in one-way frequency tables; it also applies to one-way frequency plots.

The CROSSLIST(STDRES) option in the TABLES statement displays standardized residuals in the CROSSLIST table for two-way crosstabulation.

Mosaic plots are now produced with the PLOTS=MOSAICPLOT option. The GROUPBY= plot option specifies the primary grouping for two-way frequency plots. The new TWOWAY=CLUSTER plot option provides a cluster layout for two-way frequency plots that are displayed as bar charts.

GLIMMIX Procedure

The new DDFM=KENWARDROGER2 option applies the (prediction) standard error and degrees-of-freedom correction that are detailed by Kenward and Roger (2009). This correction further reduces the precision estimator bias for the fixed and random effects under nonlinear covariance structures.

The odds ratio, relative risk, and kappa plots now display the common (overall) statistic in addition to the statistics for each two-way table (stratum).

LIFEREG Procedure

The LIFEREG procedure now supports numerous postprocessing statements including the ESTIMATE, EFFECTPLOT, LSMEANS, LSMESTIMATE, SLICE, STORE, and TEST statements.

LIFETEST Procedure

The LIFETEST procedure now supports a WEIGHT statement. For survival plot enhancements, the MAXLEN= option of the ATRISK option specifies a maximum number of characters that can be used in displaying stratum labels, and the OUTSIDE option of the ATRISK option specifies that the at-risk table be drawn outside the plot area. If you assign a label to a strata variable, that label is used in all tables and graphs.

LOESS Procedure

The LOESS procedure now supports an OUTPUT statement.

LOGISTIC Procedure

PROC LOGISTIC provides partial proportional odds logistic regression with the UNEQUALSLOPES option in the MODEL statement. The ESTIMATE, LSMEANS, LSMESTIMATE, SLICE, and STORE statements

can now be used for a stratified analysis. The PCORR option in the MODEL statement computes the partial correlation statistic for each model parameter (excluding the intercept).

The ID statement specifies variables in the DATA= data set that are used for labeling ROC curves and influence diagnostic plots.

The NLOPTIONS statement controls the optimization process for conditional analyses (specified with a STRATA statement) and for constrained optimization (specified with the UNEQUALSLOPES option in the MODEL statement).

The EFFECTPLOT statement and the PLOTS=EFFECT option have two new options for displaying plots with a CLASS effect on the X axis. The CLUSTER option displays the levels of the SLICEBY= effect in a side-by-side fashion. The CONNECT option connects the predicted values with a line.

MCMC Procedure

The MCMC procedure provides the following new capabilities:

- The MODEL statement augments missing values in the response variable by default. PROC MCMC treats missing values as unknown parameters and incorporates the sampling of the missing data as part of the Markov chain.
- The RANDOM statement supports multilevel hierarchical modeling to an arbitrary depth; a random effect can appear in the distributional hierarchy of other random effects.
- More distributions, such as multivariate normal distribution with autoregressive structure, Poisson distribution, and general distribution (for the construction of nonstandard distributions), are made available for the RANDOM statement.
- Direct sampling and more conjugate sampling algorithms are available for all parameters in the model (including model parameters, random-effects parameters, and missing data variables) when appropriate.
- A slice sampler is an alternative sampling algorithm for both the model parameters and random-effects parameters.

MULTTEST Procedure

The ID statement names one or more variables for identifying observations in the output and in the plots. In addition, the MANHATTAN plot option generates a Manhattan plot.

NLIN Procedure

The PROFILE statement selects parameters for profiling for the assessment of their nonlinear characteristics. It can also gauge the influence of each observation on the selected parameters.

NPARIWAY Procedure

The following options are added to the PROC NPARIWAY statement:

- The DSCF option requests the Dwass, Steel, Critchlow-Fligner multiple comparison procedure, which is based on pairwise two-sample rankings.
- The FP option requests the Fligner-Policello test for two-sample data.
- The ADJUST option adjusts for location differences among classes before tests for scale differences are performed.
- The REFCLASS= option of the HL option specifies which of the two CLASS variable levels (samples) to use as the reference class X for the location shift, Y-X.

ODS Graphics

You can use the new ODS GRAPHICS statement option BYLINE=FOOTNOTE or BYLINE=TITLE to display BY-group lines in a footnote or title in graphs.

PHREG Procedure

The DIST= option in the RANDOM statement enables you to specify either a gamma or lognormal distribution for the shared frailty. Bayesian frailty models are now supported. The DISPERSIONPRIOR= option in the BAYES statement specifies the prior distribution of the dispersion parameter.

Fleming-Harrington estimates can be requested with the METHOD=FM option in the BASELINE statement and in the OUTPUT statement. The DIRADJ option in the BASELINE statement specifies direct adjusted survival curves.

POWER Procedure

You can specify the multiple correlation between the tested predictor and the covariates with the CORR= option in the LOGISTIC statement.

PROBIT Procedure

The PROBIT procedure now supports numerous postprocessing statements including the ESTIMATE, EFFECTPLOT, LSMEANS, LSMESTIMATE, SLICE, STORE, and TEST statements.

QUANTREG Procedure

The QUANTREG procedure now supports the ESTIMATE statement. The EFFECT statement now supports the effect-types COLLECTION, LAG, MULTIMEMBER, and POLYNOMIAL in addition to SPLINE.

REG Procedure

The REG procedure creates heat maps for residual and fit plots when the MAXPOINTS= threshold is exceeded.

ROBUSTREG Procedure

The STDI= option in the OUTPUT statement specifies a variable to contain the estimates of the standard errors of the individual predicted values.

SEQDESIGN Procedure

The MODEL=INPUTNEVENTS option in the SAMPLESIZE statement specifies the number of events from a fixed-sample study of survival data. There are two new INPUTEVENTS options for the sample size computation: ACCRUAL= and LOSS=. The ACCRUAL= option specifies the method for individual accrual. The LOSS= option specifies the individual loss to follow-up in the sample size computation.

The STOP=BOTH option in the DESIGN statement specifies the condition of early stopping for the design. The new BETABOUNDARY=BINDING suboption computes the Type I error probability with the acceptance boundary, and the new BETABOUNDARY=NONBINDING suboption computes the Type I error probability without the acceptance boundary.

SEQTEST Procedure

The BETABOUNDARY option in the PROC SEQTEST statement specifies whether the β boundary is used in the computation of the Type I error level α . The BETABOUNDARY=BINDING option computes the Type I error probability with the β (acceptance) boundary, and the BETABOUNDARY=NONBINDING suboption computes the Type I error probability without the β boundary.

SURVEYFREQ Procedure

The SURVEYFREQ procedure now produces mosaic plots for crosstabulation tables. The GROUPBY= plot option specifies the primary grouping for two-way weighted frequency plots.

SURVEYMEANS Procedure

You can now estimate geometric means for finite populations with the GEOMEAN keyword in the PROC SURVEYMEANS statement. The new POSTSTRATA statement provides poststratification analysis.

SURVEYPHREG Procedure

The SERATIO and VARRATIO options in the MODEL statement compute the ratio of two standard errors for the regression coefficients and the ratio of two variances for the regression coefficients, respectively.

SURVEYREG Procedure

The STB option in the MODEL statement produces standardized regression coefficients.

SURVEYSELECT Procedure

The SURVEYSELECT procedure now provides Bernoulli and Poisson sampling.

What's Changed

What follows are changes in software behavior from SAS/STAT 9.3 to SAS/STAT 12.1.

LIFETEST Procedure

If you assign a label to a strata variable, the procedure now uses the label instead of the variable name in all tables and graphs.

FREQ Procedure

The appearance of the default bar chart for two-way frequency plots has changed. The row level labels have been moved outside the plot so that the row grouping appears less dominant.

For two-way dot plots (TYPE=DOTPLOT) in nonstacked layouts, the default positions of the row and column variables are reversed to group graph cells by the column variable. You can specify GROUPBY=ROW to group graph cells by the row variable.

MCMC Procedure

Random-effects parameter names are constructed using the formatted values rather than the unformatted values.

If the MISSING= option is not specified, PROC MCMC samples all missing values (including partial missing in some cases) by default. Observations for which the procedure failed to identify proper sampling algorithms

are discarded prior to the simulation. If the MISSING= option is explicitly specified (AC or CC), the option is honored.

PROC MCMC avoids performing an optimization prior to the start of the simulation if the only sampling algorithms used in the program are conjugate or direct.

PROC MCMC now permits a model specification that has only RANDOM and MODEL statements; PRIOR and PARMs statements are no longer required in that case.

MULTTEST Procedure

By default, the AFDR and PFDR are constrained to be greater than or equal to the raw p -value. The UNRESTRICT option of the PROC MULTTEST statement's AFDR and PFDR options estimates the AFDR and PFDR as defined in Benjamini and Hochberg (2000), which allows the adjustment to reduce the raw p -value.

SURVEYSELECT Procedure

PROC SURVEYSELECT now uses the Mersenne-Twister random number generator by default. In previous releases, PROC SURVEYSELECT used the RANUNI random number generator. To reproduce samples that PROC SURVEYSELECT selected in releases prior to SAS/STAT 12.1, you can use the RANUNI option with the SEED= option (for the same input data set and selection parameters).

GLIMMIX, GLM, HPMIXED, and MIXED Procedures

PCs running Windows 64-bit operating systems can now allocate more than 2Gb of memory to fit a model. This change affects the GLIMMIX, GLM, HPMIXED, and MIXED procedures.

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Chapter 2

Introduction

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Overview of SAS/STAT Software

SAS/STAT software provides comprehensive statistical tools for a wide range of statistical analyses, including analysis of variance, categorical data analysis, cluster analysis, multiple imputation, multivariate analysis, nonparametric analysis, power and sample size computations, psychometric analysis, regression, survey data analysis, and survival analysis. A few examples include nonlinear mixed models, generalized linear models, correspondence analysis, and robust regression. The software is constantly being updated to reflect new methodology. In addition to more than 75 procedures for statistical analysis, SAS/STAT software also includes the Power and Sample Size Application (PSS), an interface to power and sample size computations.

Experimental Software

Experimental software is sometimes included as part of a production-release product. It is provided to (sometimes targeted) customers in order to obtain feedback. All experimental uses are marked Experimental in this document. Whenever an experimental procedure, statement, or option is used, a message is printed to the SAS log to indicate that it is experimental.

The design and syntax of experimental software might change before any production release. Experimental software has been tested prior to release, but it has not necessarily been tested to production-quality standards, and so should be used with care.

About This Book

Since SAS/STAT software is a part of the SAS System, this book assumes that you are familiar with Base SAS software and with the books *SAS Language Reference: Concepts* and the *Base SAS Procedures Guide*. It also assumes that you are familiar with basic SAS System concepts such as creating SAS data sets with the DATA step and manipulating SAS data sets with the procedures in Base SAS software (for example, the PRINT and SORT procedures).

Chapter Organization

This book is organized as follows.

Chapter 1, “[What’s New in SAS/STAT 12.1](#),” provides information about the changes and enhancements to SAS/STAT software in SAS 9.3.

Chapter 2, this chapter, provides an overview of SAS/STAT software and summarizes related information, products, and services. The remaining introductory chapters (Chapter 3, “[Introduction to Statistical Modeling with SAS/STAT Software](#),” through Chapter 17, “[Introduction to Structural Equation Modeling with Latent Variables](#),”) provide an introduction to the broad areas covered by SAS/STAT software.

Chapter 18, “[Introduction to Power and Sample Size Analysis](#),” provides documentation for the Power and Sample Size Application (PSS).

Chapter 19, “[Shared Concepts and Topics](#),” provides information about topics that are common to multiple procedures. Topics include parameterization of model effects, the EFFECT statement, and the NLOPTIONS statement. Starting in SAS/STAT 9.22, this chapter also documents the following statements that are used for postfitting analysis and are common across many modeling procedures: EFFECTPLOT, ESTIMATE, LSMEANS, LSMESTIMATE, SLICE, STORE, and TEST.

Chapter 20, “[Using the Output Delivery System](#),” explains the fundamentals of using the Output Delivery System (ODS) to manage your SAS output.

Chapter 21, “[Statistical Graphics Using ODS](#),” describes the extension to ODS that enables many statistical procedures to create statistical graphics as easily as they create tables.

Subsequent chapters describe the SAS procedures that make up SAS/STAT software. These chapters appear in alphabetical order by procedure name and are organized as follows:

- The “Overview” section provides a brief description of the analysis provided by the procedure.
- The “Getting Started” section provides a quick introduction to the procedure through a simple example.
- The “Syntax” section describes the SAS statements and options that control the procedure.
- The “Details” section discusses methodology and miscellaneous details, such as ODS tables and ODS graphics.
- The “Examples” section contains examples that use the procedure.
- The “References” section contains references for the methodology and for examples of the procedure.

Following the chapters on the SAS/STAT procedures, Chapter A, “[Special SAS Data Sets](#),” documents the special SAS data sets that are associated with SAS/STAT procedures.

Typographical Conventions

This book uses several type styles for presenting information. The following list explains the meaning of the typographical conventions used in this book:

roman	is the standard type style used for most text.
UPPERCASE ROMAN	is used for SAS statements, options, and other SAS language elements when they appear in the text. However, you can enter these elements in your own SAS programs in lowercase, uppercase, or a mixture of the two.
UPPERCASE BOLD	is used in the “Syntax” sections’ initial lists of SAS statements and options.
<i>oblique</i>	is used for user-supplied values for options in the syntax definitions. In the text, these values are written in <i>italic</i> .
VariableName	is used for the names of variables and data sets when they appear in the text.
bold	is used to refer to matrices and vectors.
<i>italic</i>	is used for terms that are defined in the text, for emphasis, and for references to publications.
monospace	is used for example code. In most cases, this book uses lowercase type for SAS code.

Options Used in Examples

Output of Examples

Most of the output shown in this book is produced with the following SAS System options:

```
options linesize=80 pagesize=500 nonumber nodate;
```

The HTMLBLUE style is used to create the HTML output and graphs that appear in the online documentation. A style template controls stylistic elements such as colors, fonts, and presentation attributes. The style template is specified in the ODS HTML statement as follows:

```
ods html style=HTMLBlue;
```

See Chapter 21, “Statistical Graphics Using ODS,” for more information about styles.

If you run the examples, you might get slightly different output. This is a function of the SAS System options used and the precision used by your computer for floating-point calculations.

Where to Turn for More Information

This section describes other sources of information about SAS/STAT software.

Accessing the SAS/STAT Sample Library

The SAS/STAT sample library includes many examples that illustrate the use of SAS/STAT software, including the examples used in this documentation. To access these sample programs from the SAS windowing environment, select **Help** from the main menu and then select **Getting Started with SAS Software**. On the **Contents** tab, expand the **Learning to Use SAS, Sample SAS Programs**, and **SAS/STAT** items. Then click **Samples**.

Sashelp Data Sets

SAS provides over 200 data sets in the Sashelp library. These data sets are available for you to use for examples and for testing code. For example, the following step uses the Sashelp.Class data set:

```
proc reg data=sashelp.class;  
    model weight = height;  
run; quit;
```

You do not need to provide a DATA step to use Sashelp data sets.

The following steps list all of the data sets that are available in Sashelp:

```
ods listing close;
proc contents data=sashelp._all_;
  ods output members=m;
run;
ods listing;

proc print;
  where memtype = 'DATA';
run;
```

The results of these steps (over 200 data set names) are not displayed.

The following steps provide detailed information about the Sashelp data sets:

```
proc contents data=sashelp._all_;
run;
```

The results of this step (hundreds of pages of PROC CONTENTS information) are not displayed. See Chapter B, “Sashelp Data Sets,” for more information about Sashelp data sets.

Online Documentation

This documentation is available online with the SAS System. To access SAS/STAT documentation from the SAS windowing environment, select **Help** from the main menu and then select **SAS Help and Documentation**. (Alternatively, you can type **help STAT** in the command line.) On the **Contents** tab, expand the **SAS Products**, **SAS/STAT**, and **SAS/STAT User’s Guide** items. Then expand chapters and click on sections. You can search the documentation by using the **Search** tab.

You can also access the documentation by going to <http://support.sas.com/documentation>.

SAS Technical Support Services

As with all SAS products, the SAS Technical Support staff is available to respond to problems and answer technical questions regarding the use of SAS/STAT software. Go to <http://support.sas.com/techsup> for more information.

Related SAS Software

Many features not found in SAS/STAT software are available in other parts of the SAS System. If you do not find something you need in SAS/STAT software, try looking for the feature in the following SAS software products.

SAS/IML Software

SAS/IML software gives you access to a powerful and flexible programming language (Interactive Matrix Language) in a dynamic, interactive environment. The fundamental object of the language is a data matrix. You can use SAS/IML software interactively (at the statement level) to see results immediately, or you can store statements in a module and execute them later. The programming is dynamic because necessary activities such as memory allocation and dimensioning of matrices are done automatically. SAS/IML software is of interest to users of SAS/STAT software because it enables you to program your methods in the SAS System.

Base SAS Software

The features provided by SAS/STAT software are in addition to the features provided by Base SAS software. Many data management and reporting capabilities you will need are part of Base SAS software. See *SAS Language Reference: Concepts*, *SAS Language Reference: Dictionary*, and the *Base SAS Procedures Guide* for documentation of Base SAS software.

ODS Graphics

Base SAS software provides the following:

- The SG family of procedures provides a simple syntax for creating stand-alone statistical graphics. These procedures include SGPLOT, SGSCATTER, and SGPANEL, which provide a simple and convenient syntax for producing many types of displays. They are particularly convenient for exploring and presenting data. See the *SAS/GRAPH: Statistical Graphics Procedures Guide* for more information.
- The GTL (Graph Template Language) and the SGRENDER procedure provide a powerful syntax for creating customized graphs. See the *SAS/GRAPH: Graph Template Language User's Guide* and the *SAS/GRAPH: Graph Template Language Reference* for more information. You can also use the GTL to modify the SAS templates that are provided for use with SAS/STAT procedures. See Chapter 22, “ODS Graphics Template Modification,” for more information about template modification.
- The ODS Graphics Editor enables you to make immediate changes to ODS Graphics by using a point-and-click interface. See the *SAS/GRAPH: ODS Graphics Editor User's Guide* for more information.

See Chapter 21, “Statistical Graphics Using ODS,” for more information about ODS Graphics.

SAS DATA Step

The DATA step is your primary tool for reading and processing data in the SAS System. The DATA step provides a powerful general purpose programming language that enables you to perform all kinds of data processing tasks. The DATA step is documented in *SAS Language Reference: Concepts*.

Base SAS Procedures

Base SAS software includes many useful SAS procedures. Base SAS procedures are documented in the *Base SAS Procedures Guide*. The following is a list of Base SAS procedures you might find useful:

CORR	computes correlations.
RANK	computes rankings or order statistics.
STANDARD	standardizes variables to a fixed mean and variance.
MEANS	computes descriptive statistics and summarizes or collapses data over cross sections.
TABULATE	prints descriptive statistics in tabular format.
UNIVARIATE	computes descriptive statistics.

SAS/ETS Software

SAS/ETS software provides SAS procedures for econometrics and time series analysis. It includes capabilities for forecasting, systems modeling and simulation, seasonal adjustment, and financial analysis and reporting. In addition, SAS/ETS software includes an interactive time series forecasting system.

SAS/GRAPH Software

SAS/GRAPH software includes procedures that create two- and three-dimensional plots and charts.

SAS/INSIGHT Software

SAS/INSIGHT software is a highly interactive tool for data analysis. You can explore data through a variety of interactive graphs including bar charts, scatter plots, box plots, and three-dimensional rotating plots. You can examine distributions and perform parametric and nonparametric regression, analyze general linear models and generalized linear models, examine correlation matrices, and perform principal component analyses. Any changes you make to your data show immediately in all graphs and analyses. You can also configure SAS/INSIGHT software to produce graphs and analyses tailored to the way you work.

SAS/INSIGHT software might be of interest to users of SAS/STAT software for interactive graphical viewing of data, editing data, exploratory data analysis, and checking distributional assumptions.

SAS/OR Software

SAS/OR software provides SAS procedures for operations research and project planning and includes a point-and-click interface to project management. Its capabilities include the following:

- solving transportation problems
- linear, integer, and mixed-integer programming

- nonlinear programming
- scheduling projects
- plotting Gantt charts
- drawing network diagrams
- solving optimal assignment problems
- network flow programming

SAS/OR software might be of interest to users of SAS/STAT software for its mathematical programming features. In particular, the NLP procedure in SAS/OR software solves nonlinear programming problems, and it can be used for constrained and unconstrained maximization of user-defined likelihood functions.

SAS/QC Software

SAS/QC software provides a variety of procedures for statistical quality control and quality improvement. SAS/QC software includes procedures for the following:

- Shewhart control charts
- cumulative sum control charts
- moving average control charts
- process capability analysis
- Ishikawa diagrams
- Pareto charts
- experimental design

SAS/QC software also includes the ADX interface for experimental design.

SAS/IML Studio

Many users of SAS/STAT software will be interested in SAS/IML Studio, which is new in SAS 9.2 software. Formerly known as SAS Stat Studio, SAS/IML Studio is a tool for data exploration and analysis; it provides a highly flexible programming environment in which you can run SAS/STAT or SAS/IML analyses and display the results with dynamically linked graphics and data tables. You can also move seamlessly between interactive analysis and programmatically driven analysis. SAS/IML Studio is intended for data analysts who write SAS programs to solve statistical problems but need more versatility for data exploration and model building.

The programming language in SAS/IML Studio, which is called *IMLPlus*, is an enhanced version of the SAS/IML programming language. IMLPlus extends SAS/IML by providing features such as the ability to create and manipulate dynamically linked graphs and the ability to call SAS procedures.

SAS/IML Studio also includes an interface to the R language. The IMLPlus language provides functions that transfer data between SAS data sets and R data frames, and between SAS/IML matrices and R matrices.

SAS/IML Studio runs on a PC in the Microsoft Windows operating environment. For more information about SAS/IML Studio, see the *SAS/IML Studio User's Guide* and *SAS/IML Studio for SAS/STAT Users*.

Chapter 3

Introduction to Statistical Modeling with SAS/STAT Software

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Overview: Statistical Modeling

There are more than 70 procedures in SAS/STAT software, and the majority of them are dedicated to solving problems in statistical modeling. The goal of this chapter is to provide a roadmap to statistical models and to modeling tasks, enabling you to make informed choices about the appropriate modeling context and tool. This chapter also introduces important terminology, notation, and concepts used throughout this documentation. Subsequent introductory chapters discuss model families and related procedures.

It is difficult to capture the complexity of statistical models in a simple scheme, so the classification used here is necessarily incomplete. It is most practical to classify models in terms of simple criteria, such as the presence of random effects, the presence of nonlinearity, characteristics of the data, and so on. That is the approach used here. After a brief introduction to statistical modeling in general terms, the chapter describes a number of model classifications and relates them to modeling tools in SAS/STAT software.

Statistical Models

Deterministic and Stochastic Models

Purely mathematical models, in which the relationships between inputs and outputs are captured entirely in deterministic fashion, can be important theoretical tools but are impractical for describing observational, experimental, or survey data. For such phenomena, researchers usually allow the model to draw on stochastic as well as deterministic elements. When the uncertainty of realizations leads to the inclusion of random components, the resulting models are called *stochastic* models. A *statistical* model, finally, is a stochastic model that contains *parameters*, which are unknown constants that need to be estimated based on assumptions about the model and the observed data.

There are many reasons why statistical models are preferred over deterministic models. For example:

- Randomness is often introduced into a system in order to achieve a certain balance or representativeness. For example, random assignment of treatments to experimental units allows unbiased inferences about treatment effects. As another example, selecting individuals for a survey sample by random mechanisms ensures a representative sample.
- Even if a deterministic model can be formulated for the phenomenon under study, a stochastic model can provide a more parsimonious and more easily comprehended description. For example, it is possible in principle to capture the result of a coin toss with a deterministic model, taking into account the properties of the coin, the method of tossing, conditions of the medium through which the coin travels and of the surface on which it lands, and so on. A very complex model is required to describe the simple outcome—heads or tails. Alternatively, you can describe the outcome quite simply as the result of a stochastic process, a Bernoulli variable that results in heads with a certain probability.
- It is often sufficient to describe the average behavior of a process, rather than each particular realization. For example, a regression model might be developed to relate plant growth to nutrient availability. The explicit aim of the model might be to describe how the average growth changes with nutrient availability, not to predict the growth of an individual plant. The support for the notion of averaging in a model lies in the nature of expected values, describing typical behavior in the presence of randomness. This, in turn, requires that the model contain stochastic components.

The defining characteristic of statistical models is their dependence on parameters and the incorporation of stochastic terms. The properties of the model and the properties of quantities derived from it must be studied in a long-run, average sense through expectations, variances, and covariances. The fact that the parameters of the model must be estimated from the data introduces a stochastic element in applying a statistical model: because the model is not deterministic but includes randomness, parameters and related quantities derived from the model are likewise random. The properties of parameter estimators can often be described only in an asymptotic sense, imagining that some aspect of the data increases without bound (for example, the number of observations or the number of groups).

The process of estimating the parameters in a statistical model based on your data is called *fitting* the model. For many classes of statistical models there are a number of procedures in SAS/STAT software that can perform the fitting. In many cases, different procedures solve identical estimation problems—that is, their parameter estimates are identical. In some cases, the same model parameters are estimated by different statistical principles, such as least squares versus maximum likelihood estimation. Parameter estimates obtained by different methods typically have different statistical properties—distribution, variance, bias, and so on. The choice between competing estimation principles is often made on the basis of properties of the estimators. Distinguishing properties might include (but are not necessarily limited to) computational ease, interpretive ease, bias, variance, mean squared error, and consistency.

Model-Based and Design-Based Randomness

A statistical model is a description of the data-generating mechanism, not a description of the specific data to which it is applied. The aim of a model is to capture those aspects of a phenomenon that are relevant to inquiry and to explain how the data could have come about as a realization of a random experiment. These relevant aspects might include the genesis of the randomness and the stochastic effects in the phenomenon under study. Different schools of thought can lead to different model formulations, different analytic strategies, and different results. Coarsely, you can distinguish between a viewpoint of *innate* randomness and one of *induced* randomness. This distinction leads to model-based and design-based inference approaches.

In a design-based inference framework, the random variation in the observed data is induced by random *selection* or random *assignment*. Consider the case of a survey sample from a finite population of size N ; suppose that $\mathcal{F}_N = \{y_i : i \in U_N\}$ denotes the finite set of possible values and U_N is the index set $U_N = \{1, 2, \dots, N\}$. Then a sample S , a subset of U_N , is selected by probability rules. The realization of the random experiment is the selection of a particular set S ; the associated values selected from \mathcal{F}_N are considered fixed. If properties of a design-based sampling estimator are evaluated, such as bias, variance, and mean squared error, they are evaluated with respect to the distribution induced by the sampling mechanism.

Design-based approaches also play an important role in the analysis of data from controlled experiments by randomization tests. Suppose that k treatments are to be assigned to kr homogeneous experimental units. If you form k sets of r units with equal probability, and you assign the j th treatment to the t th set, a completely randomized experimental design (CRD) results. A design-based view treats the potential response of a particular treatment for a particular experimental unit as a constant. The stochastic nature of the error-control design is induced by randomly selecting one of the potential responses.

Statistical models are often used in the design-based framework. In a survey sample the model is used to motivate the choice of the finite population parameters and their sample-based estimators. In an experimental design, an assumption of additivity of the contributions from treatments, experimental units, observational errors, and experimental errors leads to a linear statistical model. The approach to statistical inference where statistical models are used to construct estimators and their properties are evaluated with respect to

the distribution induced by the sample selection mechanism is known as *model-assisted inference* (Särndal, Swensson, and Wretman 1992).

In a purely model-based framework, the only source of random variation for inference comes from the unknown variation in the responses. Finite population values are thought of as a realization of a superpopulation model that describes random variables Y_1, Y_2, \dots . The observed values y_1, y_2, \dots are realizations of these random variables. A model-based framework does not imply that there is only one source of random variation in the data. For example, mixed models might contain random terms that represent selection of effects from hierarchical (super-) populations at different granularity. The analysis takes into account the hierarchical structure of the random variation, but it continues to be model based.

A design-based approach is implicit in SAS/STAT procedures whose name commences with SURVEY, such as the SURVEYFREQ, SURVEYMEANS, SURVEYREG, SURVEYLOGISTIC, and SURVEYPHREG procedures. Inferential approaches are model based in other SAS/STAT procedures. For more information about analyzing survey data with SAS/STAT software, see Chapter 14, “Introduction to Survey Procedures.”

Model Specification

If the model is accepted as a description of the data-generating mechanism, then its parameters are estimated using the data at hand. Once the parameter estimates are available, you can apply the model to answer questions of interest about the study population. In other words, the model becomes the lens through which you view the problem itself, in order to ask and answer questions of interest. For example, you might use the estimated model to derive new predictions or forecasts, to test hypotheses, to derive confidence intervals, and so on.

Obviously, the model must be “correct” to the extent that it sufficiently describes the data-generating mechanism. Model selection, diagnosis, and discrimination are important steps in the model-building process. This is typically an iterative process, starting with an initial model and refining it. The first important step is thus to formulate your knowledge about the data-generating process and to express the real observed phenomenon in terms of a statistical model. A statistical model describes the distributional properties of one or more variables, the *response* variables. The extent of the required distributional specification depends on the model, estimation technique, and inferential goals. This description often takes the simple form of a model with additive error structure:

$$\text{response} = \text{mean} + \text{error}$$

In mathematical notation this simple model equation becomes

$$Y = f(x_1, \dots, x_k; \beta_1, \dots, \beta_p) + \epsilon$$

In this equation Y is the *response* variable, often also called the *dependent* variable or the *outcome* variable. The terms x_1, \dots, x_k denote the values of k regressor variables, often termed the *covariates* or the “independent” variables. The terms β_1, \dots, β_p denote parameters of the model, unknown constants that are to be estimated. The term ϵ denotes the random disturbance of the model; it is also called the residual term or the error term of the model.

In this simple model formulation, stochastic properties are usually associated only with the ϵ term. The covariates x_1, \dots, x_k are usually known values, not subject to random variation. Even if the covariates are measured with error, so that their values are in principle random, they are considered fixed in most models fit by SAS/STAT software. In other words, stochastic properties under the model are derived conditional on

the x s. If ϵ is the only stochastic term in the model, and if the errors have a mean of zero, then the function $f(\cdot)$ is the *mean function* of the statistical model. More formally,

$$E[Y] = f(x_1, \dots, x_k; \beta_1, \dots, \beta_p)$$

where $E[\cdot]$ denotes the expectation operator.

In many applications, a simple model formulation is inadequate. It might be necessary to specify not only the stochastic properties of a single error term, but also how model errors associated with different observations relate to each other. A simple additive error model is typically inappropriate to describe the data-generating mechanism if the errors do not have zero mean or if the variance of observations depends on their means. For example, if Y is a Bernoulli random variable that takes on the values 0 and 1 only, a regression model with additive error is not meaningful. Models for such data require more elaborate formulations involving probability distributions.

Classes of Statistical Models

Linear and Nonlinear Models

A statistical estimation problem is nonlinear if the estimating equations—the equations whose solution yields the parameter estimates—depend on the parameters in a nonlinear fashion. Such estimation problems typically have no closed-form solution and must be solved by iterative, numerical techniques.

Nonlinearity in the mean function is often used to distinguish between linear and nonlinear models. A model has a nonlinear mean function if the derivative of the mean function with respect to the parameters depends on at least one other parameter. Consider, for example, the following models that relate a response variable Y to a single regressor variable x :

$$E[Y|x] = \beta_0 + \beta_1 x$$

$$E[Y|x] = \beta_0 + \beta_1 x + \beta_2 x^2$$

$$E[Y|x] = \beta + x/\alpha$$

In these expressions, $E[Y|x]$ denotes the expected value of the response variable Y at the fixed value of x . (The conditioning on x simply indicates that the predictor variables are assumed to be non-random. Conditioning is often omitted for brevity in this and subsequent chapters.)

The first model in the previous list is a simple linear regression (SLR) model. It is linear in the parameters β_0 and β_1 since the model derivatives do not depend on unknowns:

$$\frac{\partial}{\partial \beta_0} (\beta_0 + \beta_1 x) = 1$$

$$\frac{\partial}{\partial \beta_1} (\beta_0 + \beta_1 x) = x$$

The model is also linear in its relationship with x (a straight line). The second model is also linear in the parameters, since

$$\begin{aligned}\frac{\partial}{\partial \beta_0} (\beta_0 + \beta_1 x + \beta_2 x^2) &= 1 \\ \frac{\partial}{\partial \beta_1} (\beta_0 + \beta_1 x + \beta_2 x^2) &= x \\ \frac{\partial}{\partial \beta_2} (\beta_0 + \beta_1 x + \beta_2 x^2) &= x^2\end{aligned}$$

However, this second model is *curvilinear*, since it exhibits a curved relationship when plotted against x . The third model, finally, is a nonlinear model since

$$\begin{aligned}\frac{\partial}{\partial \beta} (\beta + x/\alpha) &= 1 \\ \frac{\partial}{\partial \alpha} (\beta + x/\alpha) &= -\frac{x}{\alpha^2}\end{aligned}$$

The second of these derivatives depends on a parameter α . A model is nonlinear if it is not linear in at least one parameter. Only the third model is a nonlinear model. A graph of $E[Y]$ versus the regressor variable thus does not indicate whether a model is nonlinear. A curvilinear relationship in this graph can be achieved by a model that is linear in the parameters.

Nonlinear mean functions lead to nonlinear estimation. It is important to note, however, that nonlinear estimation arises also because of the estimation principle or because the model structure contains nonlinearity in other parts, such as the covariance structure. For example, fitting a simple linear regression model by minimizing the sum of the absolute residuals leads to a nonlinear estimation problem despite the fact that the mean function is linear.

Regression Models and Models with Classification Effects

A linear regression model in the broad sense has the form

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

where \mathbf{Y} is the vector of response values, \mathbf{X} is the matrix of regressor effects, $\boldsymbol{\beta}$ is the vector of regression parameters, and $\boldsymbol{\epsilon}$ is the vector of errors or residuals. A regression model in the narrow sense—as compared to a classification model—is a linear model in which all regressor effects are continuous variables. In other words, each effect in the model contributes a single column to the \mathbf{X} matrix and a single parameter to the overall model. For example, a regression of subjects' weight (Y) on the regressors age (x_1) and body mass index (bmi, x_2) is a regression model in this narrow sense. In symbolic notation you can write this regression model as

$$\text{weight} = \text{age} + \text{bmi} + \text{error}$$

This symbolic notation expands into the statistical model

$$Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \epsilon_i$$

Single parameters are used to model the effects of age (β_1) and bmi (β_2), respectively.

A classification effect, on the other hand, is associated with possibly more than one column of the \mathbf{X} matrix. Classification with respect to a variable is the process by which each observation is associated with one of k levels; the process of determining these k levels is referred to as *levelization* of the variable. Classification variables are used in models to identify experimental conditions, group membership, treatments, and so on. The actual values of the classification variable are not important, and the variable can be a numeric or a character variable. What is important is the association of discrete values or levels of the classification variable with groups of observations. For example, in the previous illustration, if the regression also takes into account the subjects' gender, this can be incorporated in the model with a two-level classification variable. Suppose that the values of the gender variable are coded as 'F' and 'M', respectively. In symbolic notation the model

$$\text{weight} = \text{age} + \text{bmi} + \text{gender} + \text{error}$$

expands into the statistical model

$$Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \tau_1 I(\text{gender} = 'F') + \tau_2 I(\text{gender} = 'M') + \epsilon_i$$

where $I(\text{gender}='F')$ is the indicator function that returns 1 if the value of the gender variable is 'F' and 0 otherwise. Parameters τ_1 and τ_2 are associated with the gender classification effect. This form of parameterizing the gender effect in the model is only one of several different methods of incorporating the levels of a classification variable in the model. This form, the so-called singular parameterization, is the most general approach, and it is used in the GLM, MIXED, and GLIMMIX procedures. Alternatively, classification effects with various forms of nonsingular parameterizations are available in such procedures as GENMOD and LOGISTIC. See the documentation for the individual SAS/STAT procedures on their respective facilities for parameterizing classification variables and the section "[Parameterization of Model Effects](#)" on page 383 in Chapter 19, "[Shared Concepts and Topics](#)," for general details.

Models that contain only classification effects are often identified with *analysis of variance* (ANOVA) models, because ANOVA methods are frequently used in their analysis. This is particularly true for experimental data where the model effects comprise effects of the treatment and error-control design. However, classification effects appear more widely than in models to which analysis of variance methods are applied. For example, many mixed models, where parameters are estimated by restricted maximum likelihood, consist entirely of classification effects but do not permit the sum of squares decomposition typical for ANOVA techniques.

Many models contain both continuous and classification effects. For example, a continuous-by-class effect consists of at least one continuous variable and at least one classification variable. Such effects are convenient, for example, to vary slopes in a regression model by the levels of a classification variable. Also, recent enhancements to linear modeling syntax in some SAS/STAT procedures (including GLIMMIX and GLMSELECT) enable you to construct sets of columns in \mathbf{X} matrices from a single continuous variable. An example is modeling with splines where the values of a continuous variable x are expanded into a spline basis that occupies multiple columns in the \mathbf{X} matrix. For purposes of the analysis you can treat these columns as a single unit or as individual, unrelated columns. For more details, see the section "[EFFECT Statement](#)" on page 393 in Chapter 19, "[Shared Concepts and Topics](#)."

Univariate and Multivariate Models

A multivariate statistical model is a model in which multiple response variables are modeled jointly. Suppose, for example, that your data consist of heights (h_i) and weights (w_i) of children, collected over several years (t_i). The following separate regressions represent two univariate models:

$$\begin{aligned}w_i &= \beta_{w0} + \beta_{w1}t_i + \epsilon_{wi} \\h_i &= \beta_{h0} + \beta_{h1}t_i + \epsilon_{hi}\end{aligned}$$

In the univariate setting, no information about the children’s heights “flows” to the model about their weights and vice versa. In a multivariate setting, the heights and weights would be modeled jointly. For example:

$$\begin{aligned}\mathbf{Y}_i &= \begin{bmatrix} w_i \\ h_i \end{bmatrix} = \mathbf{X}\boldsymbol{\beta} + \begin{bmatrix} \epsilon_{wi} \\ \epsilon_{hi} \end{bmatrix} \\ &= \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}_i \\ \boldsymbol{\epsilon}_i &\sim \left(\mathbf{0}, \begin{bmatrix} \sigma_1^2 & \sigma_{12} \\ \sigma_{12} & \sigma_2^2 \end{bmatrix} \right)\end{aligned}$$

The vectors \mathbf{Y}_i and $\boldsymbol{\epsilon}_i$ collect the responses and errors for the two observation that belong to the same subject. The errors from the same child now have the correlation

$$\text{Corr}[\epsilon_{wi}, \epsilon_{hi}] = \frac{\sigma_{12}}{\sqrt{\sigma_1^2 \sigma_2^2}}$$

and it is through this correlation that information about heights “flows” to the weights and vice versa. This simple example shows only one approach to modeling multivariate data, through the use of covariance structures. Other techniques involve seemingly unrelated regressions, systems of linear equations, and so on.

Multivariate data can be coarsely classified into three types. The response vectors of *homogeneous multivariate data* consist of observations of the same attribute. Such data are common in repeated measures experiments and longitudinal studies, where the same attribute is measured repeatedly over time. Homogeneous multivariate data also arise in spatial statistics where a set of geostatistical data is the incomplete observation of a single realization of a random experiment that generates a two-dimensional surface. One hundred measurements of soil electrical conductivity collected in a forest stand compose a single observation of a 100-dimensional homogeneous multivariate vector. *Heterogeneous multivariate* observations arise when the responses that are modeled jointly refer to different attributes, such as in the previous example of children’s weights and heights. There are two important subtypes of heterogeneous multivariate data. In *homocatanomic multivariate data* the observations come from the same distributional family. For example, the weights and heights might both be assumed to be normally distributed. With *heterocatanomic multivariate data* the observations can come from different distributional families. The following are examples of heterocatanomic multivariate data:

- For each patient you observe blood pressure (a continuous outcome), the number of prior episodes of an illness (a count variable), and whether the patient has a history of diabetes in the family (a binary outcome). A multivariate model that models the three attributes jointly might assume a lognormal distribution for the blood pressure measurements, a Poisson distribution for the count variable and a Bernoulli distribution for the family history.
- In a study of HIV/AIDS survival, you model jointly a patient’s CD4 cell count over time—itsself a homogeneous multivariate outcome—and the survival of the patient (event-time data).

Fixed, Random, and Mixed Models

Each term in a statistical model represents either a *fixed effect* or a *random effect*. Models in which all effects are fixed are called fixed-effects models. Similarly, models in which all effects are random—apart from possibly an overall intercept term—are called random-effects models. Mixed models, then, are those models that have fixed-effects and random-effects terms. In matrix notation, the linear fixed, linear random, and linear mixed model are represented by the following model equations, respectively:

$$\begin{aligned} \mathbf{Y} &= \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon} \\ \mathbf{Y} &= \mathbf{Z}\boldsymbol{\gamma} + \boldsymbol{\epsilon} \\ \mathbf{Y} &= \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\boldsymbol{\gamma} + \boldsymbol{\epsilon} \end{aligned}$$

In these expressions, \mathbf{X} and \mathbf{Z} are design or regressor matrices associated with the fixed and random effects, respectively. The vector $\boldsymbol{\beta}$ is a vector of fixed-effects parameters, and the vector $\boldsymbol{\gamma}$ represents the random effects. The mixed modeling procedures in SAS/STAT software assume that the random effects $\boldsymbol{\gamma}$ follow a normal distribution with variance-covariance matrix \mathbf{G} and, in most cases, that the random effects have mean zero.

Random effects are often associated with classification effects, but this is not necessary. As an example of random regression effects, you might want to model the slopes in a growth model as consisting of two components: an overall (fixed-effects) slope that represents the slope of the average individual, and individual-specific random deviations from the overall slope. The \mathbf{X} and \mathbf{Z} matrix would then have column entries for the regressor variable associated with the slope. You are modeling fixed and randomly varying regression coefficients.

Having random effects in your model has a number of important consequences:

- Some observations are no longer uncorrelated but instead have a covariance that depends on the variance of the random effects.
- You can and should distinguish between the inference spaces; inferences can be drawn in a broad, intermediate, and narrow inference space. In the narrow inference space, conclusions are drawn about the particular values of the random effects selected in the study. The broad inference space applies if inferences are drawn with respect to all possible levels of the random effects. The intermediate inference space can be applied for effects consisting of more than one random term, when inferences are broad with respect to some factors and narrow with respect to others. In fixed-effects models, there is no corresponding concept to the broad and intermediate inference spaces.
- Depending on the structure of \mathbf{G} and $\text{Var}[\boldsymbol{\epsilon}]$ and also subject to the balance in your data, there might be no closed-form solution for the parameter estimates. Although the model is linear in $\boldsymbol{\beta}$, iterative estimation methods might be required to estimate all parameters of the model.
- Certain concepts, such as least squares means and Type III estimable functions, are meaningful only for fixed effects.
- By using random effects, you are modeling variation through variance. Variation in data simply implies that things are not equal. Variance, on the other hand, describes a feature of a random variable. Random effects in your model are random variables: they model variation through variance.

It is important to properly determine the nature of the model effects as fixed or random. An effect is either fixed or random by its very nature; it is improper to consider it fixed in one analysis and random in another

depending on what type of results you want to produce. If, for example, a treatment effect is random and you are interested in comparing treatment means, and only the levels selected in the study are of interest, then it is not appropriate to model the treatment effect as fixed so that you can draw on least squares mean analysis. The appropriate strategy is to model the treatment effect as random and to compare the solutions for the treatment effects in the narrow inference space.

In determining whether an effect is fixed or random, it is helpful to inquire about the *genesis* of the effect. If the levels of an effect are randomly sampled, then the effect is a random effect. The following are examples:

- In a large clinical trial, drugs A, B, and C are applied to patients in various clinical centers. If the clinical centers are selected at random from a population of possible clinics, their effect on the response is modeled with a random effect.
- In repeated measures experiments with people or animals as subjects, subjects are declared to be random because they are selected from the larger population to which you want to generalize.
- Fertilizers could be applied at a number of levels. Three levels are randomly selected for an experiment to represent the population of possible levels. The fertilizer effects are random effects.

Quite often it is not possible to select effects at random, or it is not known how the values in the data became part of the study. For example, suppose you are presented with a data set consisting of student scores in three school districts, with four to ten schools in each district and two to three classrooms in each school. How do you decide which effects are fixed and which are random? As another example, in an agricultural experiment conducted in successive years at two locations, how do you decide whether location and year effects are fixed or random? In these situations, the fixed or random nature of the effect might be debatable, bearing out the adage that “one modeler’s fixed effect is another modeler’s random effect.” However, this fact does not constitute license to treat as random those effects that are clearly fixed, or vice versa.

When an effect cannot be randomized or it is not known whether its levels have been randomly selected, it can be a random effect if its impact on the outcome variable is of a stochastic nature—that is, if it is the realization of a random process. Again, this line of thinking relates to the genesis of the effect. A random year, location, or school district effect is a placeholder for different environments that cannot be selected at random but whose effects are the cumulative result of many individual random processes. Note that this argument does not imply that effects are random because the experimenter does not know much about them. The key notion is that effects represent something, whether or not that something is known to the modeler. Broadening the inference space beyond the observed levels is thus possible, although you might not be able to articulate what the realizations of the random effects represent.

A consequence of having random effects in your model is that some observations are no longer uncorrelated but instead have a covariance that depends on the variance of the random effect. In fact, in some modeling applications random effects might be used not only to model heterogeneity in the parameters of a model, but also to induce correlations among observations. The typical assumption about random effects in SAS/STAT software is that the effects are normally distributed.

For more information about mixed modeling tools in SAS/STAT software, see Chapter 6, “[Introduction to Mixed Modeling Procedures](#).”

Generalized Linear Models

A class of models that has gained increasing importance in the past several decades is the class of generalized linear models. The theory of generalized linear models originated with Nelder and Wedderburn (1972); Wedderburn (1974), and was subsequently made popular in the monograph by McCullagh and Nelder (1989). This class of models extends the theory and methods of linear models to data with nonnormal responses. Before this theory was developed, modeling of nonnormal data typically relied on transformations of the data, and the transformations were chosen to improve symmetry, homogeneity of variance, or normality. Such transformations have to be performed with care because they also have implications for the error structure of the model. Also, back-transforming estimates or predicted values can introduce bias.

Generalized linear models also apply a transformation, known as the *link function*, but it is applied to a deterministic component, the mean of the data. Furthermore, generalized linear models take the distribution of the data into account, rather than assuming that a transformation of the data leads to normally distributed data to which standard linear modeling techniques can be applied.

To put this generalization in place requires a slightly more sophisticated model setup than that required for linear models for normal data:

- The *systematic* component is a linear predictor similar to that in linear models, $\eta = \mathbf{x}'\boldsymbol{\beta}$. The linear predictor is a linear function in the parameters. In contrast to the linear model, η does not represent the mean function of the data.
- The *link function* $g(\cdot)$ relates the linear predictor to the mean, $g(\mu) = \eta$. The link function is a monotonic, invertible function. The mean can thus be expressed as the inversely linked linear predictor, $\mu = g^{-1}(\eta)$. For example, a common link function for binary and binomial data is the logit link, $g(t) = \log\{t/(1-t)\}$. The mean function of a generalized linear model with logit link and a single regressor can thus be written as

$$\log \left\{ \frac{\mu}{1-\mu} \right\} = \beta_0 + \beta_1 x$$

$$\mu = \frac{1}{1 + \exp\{-\beta_0 - \beta_1 x\}}$$

This is known as a logistic regression model.

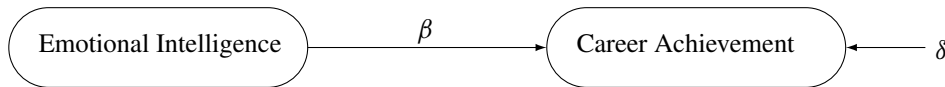
- The *random component* of a generalized linear model is the distribution of the data, assumed to be a member of the exponential family of distributions. Discrete members of this family include the Bernoulli (binary), binomial, Poisson, geometric, and negative binomial (for a given value of the scale parameter) distribution. Continuous members include the normal (Gaussian), beta, gamma, inverse Gaussian, and exponential distribution.

The standard linear model with normally distributed error is a special case of a generalized linear model; the link function is the identity function and the distribution is normal.

Latent Variable Models

Latent variable modeling involves variables that are not observed directly in your research. It has a relatively long history, dating back from the measure of general intelligence by common factor analysis (Spearman 1904) to the emergence of modern-day structural equation modeling (Jöreskog 1973; Keesling 1972; Wiley 1973).

Latent variables are involved in almost all kinds of regression models. In a broad sense, all additive error terms in regression models are latent variables simply because they are not measured in research. Hereafter, however, a narrower sense of latent variables is used when referring to latent variable models. Latent variables are *systematic* unmeasured variables that are also referred to as *factors*. For example, in the following diagram a simple relation between Emotional Intelligence and Career Achievement is shown:



In the diagram, both Emotional Intelligence and Career Achievement are treated as latent factors. They are hypothetical constructs in your model. You hypothesize that Emotional Intelligence is a “causal factor” or predictor of Career Achievement. The symbol β represents the regression coefficient or the effect of Emotional Intelligence on Career Achievement. However, the “causal relationship” or prediction is not perfect. There is an error term δ , which accounts for the unsystematic part of the prediction. You can represent the preceding diagram by using the following linear equation:

$$CA = \beta EI + \delta$$

where CA represents Career Achievement and EI represents Emotional Intelligence. The means of the latent factors in the linear model are arbitrary, and so they are assumed to be zero. The error variable δ also has a zero mean with an unknown variance. This equation represents the so-called “structural model,” where the “true” relationships among latent factors are theorized.

In order to model this theoretical model with latent factors, some observed variables must somehow relate to these factors. This calls for the measurement models for latent factors. For example, Emotional Intelligence could be measured by some established tests. In these tests, individuals are asked to respond to certain special situations that involve stressful decision making, personal confrontations, and so on. Their responses to these situations are then rated by experts or a standardized scoring system. Suppose there are three such tests and the test scores are labeled as X1, X2 and X3, respectively. The measurement model for the latent factor Emotional Intelligence is specified as follows:

$$X1 = a_1 EI + e_1$$

$$X2 = a_2 EI + e_2$$

$$X3 = a_3 EI + e_3$$

where a_1 , a_2 , and a_3 are regression coefficients and e_1 , e_2 , and e_3 are measurement errors. Measurement errors are assumed to be independent of the latent factors EI and CA. In the measurement model, X1, X2, and X3 are called the indicators of the latent variable EI. These observed variables are assumed to be centered in the model, and therefore no intercept terms are needed. Each of the indicators is a scaled measurement of the latent factor EI plus a unique error term.

Similarly, you need to have a measurement model for the latent factor CA. Suppose that there are four observed indicators Y1, Y2, Y3, and Y4 (for example, Job Status) for this latent factor. The measurement model for CA is specified as follows:

$$Y1 = a_4 CA + e_4$$

$$Y2 = a_5 CA + e_5$$

$$Y3 = a_6 CA + e_6$$

$$Y4 = a_7 CA + e_7$$

where $a_4, a_5, a_6,$ and a_7 are regression coefficients and $e_4, e_5, e_6,$ and e_7 are error terms. Again, the error terms are assumed to be independent of the latent variables EI and CA, and Y1, Y2, Y3, and Y4 are centered in the equations.

Given the data for the measured variables, you analyze the structural and measurement models simultaneously by the structural equation modeling techniques. In other words, estimation of β, a_1 – $a_7,$ and other parameters in the model are carried out simultaneously in the modeling.

Modeling involving the use of latent factors is quite common in social and behavioral sciences, personality assessment, and marketing research. Hypothetical constructs, although not observable, are very important in building theories in these areas.

Another use of latent factors in modeling is to “purify” the predictors in regression analysis. A common assumption in linear regression models is that predictors are measured without errors. That is, in the following linear equation x is assumed to have been measured without errors:

$$y = \alpha + \beta x + \epsilon$$

However, if x has been contaminated with measurement errors that cannot be ignored, the estimate of β might be biased severely so that the true relationship between x and y would be masked.

A measurement model for x provides a solution to such a problem. Let F_x be a “purified” version of x . That is, F_x is the “true” measure of x without measurement errors, as described in the following equation:

$$x = F_x + \delta$$

where δ represents a random measurement error term. Now, the linear relationship of interest is specified in the following new linear regression equation:

$$y = \alpha + \beta F_x + \epsilon$$

In this equation, F_x , which is now free from measurement errors, replaces x in the original equation. With measurement errors taken into account in the simultaneous fitting of the measurement and the new regression equations, estimation of β is unbiased; hence it reflects the true relationship much better.

Certainly, introducing latent factors in models is not a “free lunch.” You must pay attention to the identification issues induced by the latent variable methodology. That is, in order to estimate the parameters in structural equation models with latent variables, you must set some identification constraints in these models. There are some established rules or conventions that would lead to proper model identification and estimation. See Chapter 17, “[Introduction to Structural Equation Modeling with Latent Variables](#),” for examples and general details.

In addition, because of the nature of latent variables, estimation in structural equation modeling with latent variables does not follow the same form as that of linear regression analysis. Instead of defining the estimators in terms of the data matrices, most estimation methods in structural equation modeling use the fitting of the first- and second- order moments. Hence, estimation principles described in the section “[Classical Estimation Principles](#)” on page 37 do not apply to structural equation modeling. However, you can see the section “[Estimation Criteria](#)” on page 1309 in Chapter 27, “[The CALIS Procedure](#),” for details about estimation in structural equation modeling with latent variables.

Bayesian Models

Statistical models based on the classical (or *frequentist*) paradigm treat the parameters of the model as fixed, unknown constants. They are not random variables, and the notion of probability is derived in an objective sense as a limiting relative frequency. The Bayesian paradigm takes a different approach. Model parameters are random variables, and the probability of an event is defined in a subjective sense as the degree to which you believe that the event is true. This fundamental difference in philosophy leads to profound differences in the statistical content of estimation and inference. In the frequentist framework, you use the data to best estimate the unknown value of a parameter; you are trying to pinpoint a value in the parameter space as well as possible. In the Bayesian framework, you use the data to update your beliefs about the *behavior* of the parameter to assess its distributional properties as well as possible.

Suppose you are interested in estimating θ from data $\mathbf{Y} = [Y_1, \dots, Y_n]$ by using a statistical model described by a density $p(\mathbf{y}|\theta)$. Bayesian philosophy states that θ cannot be determined exactly, and uncertainty about the parameter is expressed through probability statements and distributions. You can say, for example, that θ follows a normal distribution with mean 0 and variance 1, if you believe that this distribution best describes the uncertainty associated with the parameter.

The following steps describe the essential elements of Bayesian inference:

1. A probability distribution for θ is formulated as $\pi(\theta)$, which is known as the *prior* distribution, or just the prior. The prior distribution expresses your beliefs, for example, on the mean, the spread, the skewness, and so forth, about the parameter prior to examining the data.
2. Given the observed data \mathbf{Y} , you choose a statistical model $p(\mathbf{y}|\theta)$ to describe the distribution of \mathbf{Y} given θ .
3. You update your beliefs about θ by combining information from the prior distribution and the data through the calculation of the *posterior* distribution, $p(\theta|\mathbf{y})$.

The third step is carried out by using Bayes' theorem, from which this branch of statistical philosophy derives its name. The theorem enables you to combine the prior distribution and the model in the following way:

$$p(\theta|\mathbf{y}) = \frac{p(\theta, \mathbf{y})}{p(\mathbf{y})} = \frac{p(\mathbf{y}|\theta)\pi(\theta)}{p(\mathbf{y})} = \frac{p(\mathbf{y}|\theta)\pi(\theta)}{\int p(\mathbf{y}|\theta)\pi(\theta)d\theta}$$

The quantity $p(\mathbf{y}) = \int p(\mathbf{y}|\theta)\pi(\theta) d\theta$ is the normalizing constant of the posterior distribution. It is also the marginal distribution of \mathbf{Y} , and it is sometimes called the marginal distribution of the data.

The likelihood function of θ is any function proportional to $p(\mathbf{y}|\theta)$ —that is, $L(\theta) \propto p(\mathbf{y}|\theta)$. Another way of writing Bayes' theorem is

$$p(\theta|\mathbf{y}) = \frac{L(\theta)\pi(\theta)}{\int L(\theta)\pi(\theta) d\theta}$$

The marginal distribution $p(\mathbf{y})$ is an integral; therefore, provided that it is finite, the particular value of the integral does not yield any additional information about the posterior distribution. Hence, $p(\theta|\mathbf{y})$ can be written up to an arbitrary constant, presented here in proportional form, as

$$p(\theta|\mathbf{y}) \propto L(\theta)\pi(\theta)$$

Bayes' theorem instructs you how to update existing knowledge with new information. You start from a prior belief $\pi(\theta)$, and, after learning information from data \mathbf{y} , you change or update the belief on θ and obtain $p(\theta|\mathbf{y})$. These are the essential elements of the Bayesian approach to data analysis.

In theory, Bayesian methods offer a very simple alternative to statistical inference—all inferences follow from the posterior distribution $p(\theta|\mathbf{y})$. However, in practice, only the most elementary problems enable you to obtain the posterior distribution analytically. Most Bayesian analyses require sophisticated computations, including the use of simulation methods. You generate samples from the posterior distribution and use these samples to estimate the quantities of interest.

Both Bayesian and classical analysis methods have their advantages and disadvantages. Your choice of method might depend on the goals of your data analysis. If prior information is available, such as in the form of expert opinion or historical knowledge, and you want to incorporate this information into the analysis, then you might consider Bayesian methods. In addition, if you want to communicate your findings in terms of probability notions that can be more easily understood by nonstatisticians, Bayesian methods might be appropriate. The Bayesian paradigm can provide a framework for answering specific scientific questions that a single point estimate cannot sufficiently address. On the other hand, if you are interested in estimating parameters and in formulating inferences based on the properties of the parameter estimators, then there is no need to use Bayesian analysis. When the sample size is large, Bayesian inference often provides results for parametric models that are very similar to the results produced by classical, frequentist methods.

For more information, see Chapter 7, “[Introduction to Bayesian Analysis Procedures](#).”

Classical Estimation Principles

An estimation principle captures the set of rules and procedures by which parameter estimates are derived. When an estimation principle “meets” a statistical model, the result is an *estimation problem*, the solution of which are the parameter estimates. For example, if you apply the estimation principle of least squares to the SLR model $Y_i = \beta_0 + \beta_1 x_i + \epsilon_i$, the estimation problem is to find those values $\hat{\beta}_0$ and $\hat{\beta}_1$ that minimize

$$\sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2$$

The solutions are the least squares estimators.

The two most important classes of estimation principles in statistical modeling are the least squares principle and the likelihood principle. All principles have in common that they provide a metric by which you measure the distance between the data and the model. They differ in the nature of the metric; least squares relies on a geometric measure of distance, while likelihood inference is based on a distance that measures plausability.

Least Squares

The idea of the ordinary least squares (OLS) principle is to choose parameter estimates that minimize the squared distance between the data and the model. In terms of the general, additive model,

$$Y_i = f(x_{i1}, \dots, x_{ik}; \beta_1, \dots, \beta_p) + \epsilon_i$$

the OLS principle minimizes

$$\text{SSE} = \sum_{i=1}^n (y_i - f(x_{i1}, \dots, x_{ik}; \beta_1, \dots, \beta_p))^2$$

The least squares principle is sometimes called “nonparametric” in the sense that it does not require the distributional specification of the response or the error term, but it might be better termed “distributionally agnostic.” In an additive-error model it is only required that the model errors have zero mean. For example, the specification

$$Y_i = \beta_0 + \beta_1 x_i + \epsilon_i$$

$$E[\epsilon_i] = 0$$

is sufficient to derive ordinary least squares (OLS) estimators for β_0 and β_1 and to study a number of their properties. It is easy to show that the OLS estimators in this SLR model are

$$\hat{\beta}_1 = \left(\sum_{i=1}^n (Y_i - \bar{Y}) \sum_{i=1}^n (x_i - \bar{x}) \right) / \sum_{i=1}^n (x_i - \bar{x})^2$$

$$\hat{\beta}_0 = \bar{Y} - \hat{\beta}_1 \bar{x}$$

Based on the assumption of a zero mean of the model errors, you can show that these estimators are unbiased, $E[\hat{\beta}_1] = \beta_1$, $E[\hat{\beta}_0] = \beta_0$. However, without further assumptions about the distribution of the ϵ_i , you cannot derive the variability of the least squares estimators or perform statistical inferences such as hypothesis tests or confidence intervals. In addition, depending on the distribution of the ϵ_i , other forms of least squares estimation can be more efficient than OLS estimation.

The conditions for which ordinary least squares estimation is efficient are zero mean, homoscedastic, uncorrelated model errors. Mathematically,

$$E[\epsilon_i] = 0$$

$$\text{Var}[\epsilon_i] = \sigma^2$$

$$\text{Cov}[\epsilon_i, \epsilon_j] = 0 \text{ if } i \neq j$$

The second and third assumption are met if the errors have an *iid* distribution—that is, if they are independent and identically distributed. Note, however, that the notion of stochastic independence is stronger than that of absence of correlation. Only if the data are normally distributed does the latter implies the former.

The various other forms of the least squares principle are motivated by different extensions of these assumptions in order to find more efficient estimators.

Weighted Least Squares

The objective function in weighted least squares (WLS) estimation is

$$\text{SSE}_w = \sum_{i=1}^n w_i (Y_i - f(x_{i1}, \dots, x_{ik}; \beta_1, \dots, \beta_p))^2$$

where w_i is a weight associated with the i th observation. A situation where WLS estimation is appropriate is when the errors are uncorrelated but not homoscedastic. If the weights for the observations are proportional to the reciprocals of the error variances, $\text{Var}[\epsilon_i] = \sigma^2/w_i$, then the weighted least squares estimates are best linear unbiased estimators (BLUE). Suppose that the weights w_i are collected in the diagonal matrix \mathbf{W} and that the mean function has the form of a linear model. The weighted sum of squares criterion then can be written as

$$\text{SSE}_w = (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})' \mathbf{W} (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})$$

which gives rise to the weighted normal equations

$$(\mathbf{X}'\mathbf{W}\mathbf{X})\boldsymbol{\beta} = \mathbf{X}'\mathbf{W}\mathbf{Y}$$

The resulting WLS estimator of $\boldsymbol{\beta}$ is

$$\widehat{\boldsymbol{\beta}}_w = (\mathbf{X}'\mathbf{W}\mathbf{X})^{-1} \mathbf{X}'\mathbf{W}\mathbf{Y}$$

Iteratively Reweighted Least Squares

If the weights in a least squares problem depend on the parameters, then a change in the parameters also changes the weight structure of the model. Iteratively reweighted least squares (IRLS) estimation is an iterative technique that solves a series of weighted least squares problems, where the weights are recomputed between iterations. IRLS estimation can be used, for example, to derive maximum likelihood estimates in generalized linear models.

Generalized Least Squares

The previously discussed least squares methods have in common that the observations are assumed to be uncorrelated—that is, $\text{Cov}[\epsilon_i, \epsilon_j] = 0$, whenever $i \neq j$. The weighted least squares estimation problem is a special case of a more general least squares problem, where the model errors have a general covariance matrix, $\text{Var}[\boldsymbol{\epsilon}] = \boldsymbol{\Sigma}$. Suppose again that the mean function is linear, so that the model becomes

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon} \quad \boldsymbol{\epsilon} \sim (\mathbf{0}, \boldsymbol{\Sigma})$$

The generalized least squares (GLS) principle is to minimize the generalized error sum of squares

$$\text{SSE}_g = (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})' \boldsymbol{\Sigma}^{-1} (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})$$

This leads to the generalized normal equations

$$(\mathbf{X}'\boldsymbol{\Sigma}^{-1}\mathbf{X})\boldsymbol{\beta} = \mathbf{X}'\boldsymbol{\Sigma}^{-1}\mathbf{Y}$$

and the GLS estimator

$$\widehat{\boldsymbol{\beta}}_g = (\mathbf{X}'\boldsymbol{\Sigma}^{-1}\mathbf{X})^{-1} \mathbf{X}'\boldsymbol{\Sigma}^{-1}\mathbf{Y}$$

Obviously, WLS estimation is a special case of GLS estimation, where $\boldsymbol{\Sigma} = \sigma^2\mathbf{W}^{-1}$ —that is, the model is

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon} \quad \boldsymbol{\epsilon} \sim (\mathbf{0}, \sigma^2\mathbf{W}^{-1})$$

Likelihood

There are several forms of likelihood estimation and a large number of offshoot principles derived from it, such as pseudo-likelihood, quasi-likelihood, composite likelihood, etc. The basic likelihood principle is *maximum likelihood*, which asks to estimate the model parameters by those quantities that maximize the likelihood function of the data. The likelihood function is the joint distribution of the data, but in contrast to a probability mass or density function, it is thought of as a function of the parameters, given the data. The heuristic appeal of the maximum likelihood estimates (MLE) is that these are the values that make the observed data “most likely.” Especially for discrete response data, the value of the likelihood function is the ordinate of a probability mass function, even if the likelihood is not a probability function. Since a statistical

model is thought of as a representation of the data-generating mechanism, what could be more preferable as parameter estimates than those values that make it most likely that the data at hand will be observed?

Maximum likelihood estimates, if they exist, have appealing statistical properties. Under fairly mild conditions, they are best-asymptotic-normal (BAN) estimates—that is, their asymptotic distribution is normal, and no other estimator has a smaller asymptotic variance. However, their statistical behavior in finite samples is often difficult to establish, and you have to appeal to the asymptotic results that hold as the sample size tends to infinity. For example, maximum likelihood estimates are often biased estimates and the bias disappears as the sample size grows. A famous example is random sampling from a normal distribution. The corresponding statistical model is

$$Y_i = \mu + \epsilon_i$$

$$\epsilon_i \sim iid N(0, \sigma^2)$$

where the symbol \sim is read as “is distributed as” and *iid* is read as “independent and identically distributed.” Under the normality assumption, the density function of y_i is

$$f(y_i; \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left\{ -\frac{1}{2} \left(\frac{y_i - \mu}{\sigma} \right)^2 \right\}$$

and the likelihood for a random sample of size n is

$$L(\mu, \sigma^2; \mathbf{y}) = \prod_{i=1}^n \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left\{ -\frac{1}{2} \left(\frac{y_i - \mu}{\sigma} \right)^2 \right\}$$

Maximizing the likelihood function $L(\mu, \sigma^2; \mathbf{y})$ is equivalent to maximizing the log-likelihood function $\log L = l(\mu, \sigma^2; \mathbf{y})$,

$$l(\mu, \sigma^2; \mathbf{y}) = \sum_{i=1}^n -\frac{1}{2} \left(\log\{2\pi\} + \frac{(y_i - \mu)^2}{\sigma^2} + \log\{\sigma^2\} \right)$$

$$= -\frac{1}{2} \left(n \log\{2\pi\} + n \log\{\sigma^2\} + \sum_{i=1}^n (y_i - \mu)^2 / \sigma^2 \right)$$

The maximum likelihood estimators of μ and σ^2 are thus

$$\hat{\mu} = \frac{1}{n} \sum_{i=1}^n Y_i = \bar{Y} \quad \hat{\sigma}^2 = \frac{1}{n} \sum_{i=1}^n (Y_i - \hat{\mu})^2$$

The MLE of the mean μ is the sample mean, and it is an unbiased estimator of μ . However, the MLE of the variance σ^2 is not an unbiased estimator. It has bias

$$E[\hat{\sigma}^2 - \sigma^2] = -\frac{1}{n}\sigma^2$$

As the sample size n increases, the bias vanishes.

For certain classes of models, special forms of likelihood estimation have been developed to maintain the appeal of likelihood-based statistical inference and to address specific properties that are believed to be shortcomings:

- The bias in maximum likelihood parameter estimators of variances and covariances has led to the development of restricted (or residual) maximum likelihood (REML) estimators that play an important role in mixed models.
- Quasi-likelihood methods do not require that the joint distribution of the data be specified. These methods derive estimators based on only the first two moments (mean and variance) of the joint distributions and play an important role in the analysis of correlated data.
- The idea of composite likelihood is applied in situations where the likelihood of the vector of responses is intractable but the likelihood of components or functions of the full-data likelihood are tractable. For example, instead of the likelihood of \mathbf{Y} , you might consider the likelihood of pairwise differences $Y_i - Y_j$.
- The pseudo-likelihood concept is also applied when the likelihood function is intractable, but the likelihood of a related, simpler model is available. An important difference between quasi-likelihood and pseudo-likelihood techniques is that the latter make distributional assumptions to obtain a likelihood function in the pseudo-model. Quasi-likelihood methods do not specify the distributional family.
- The penalized likelihood principle is applied when additional constraints and conditions need to be imposed on the parameter estimates or the resulting model fit. For example, you might augment the likelihood with conditions that govern the smoothness of the predictions or that prevent overfitting of the model.

Least Squares or Likelihood

For many statistical modeling problems, you have a choice between a least squares principle and the maximum likelihood principle. Table 3.1 compares these two basic principles.

Table 3.1 Least Squares and Maximum Likelihood

Criterion	Least Squares	Maximum Likelihood
Requires specification of joint distribution of data	No, but in order to perform confirmatory inference (tests, confidence intervals), a distributional assumption is needed, or an appeal to asymptotics.	Yes, no progress can be made with the genuine likelihood principle without knowing the distribution of the data.
All parameters of the model are estimated	No. In the additive-error type models, least squares provides estimates of only the parameters in the mean function. The residual variance, for example, must be estimated by some other method—typically by using the mean squared error of the model.	Yes
Estimates always exist	Yes, but they might not be unique, such as when the \mathbf{X} matrix is singular.	No, maximum likelihood estimates do not exist for all estimation problems.
Estimators are biased	Unbiased, provided that the model is correct—that is, the errors have zero mean.	Often biased, but asymptotically unbiased

Table 3.1 continued

Criterion	Least Squares	Maximum Likelihood
Estimators are consistent	Not necessarily, but often true. Sometimes estimators are consistent even in a misspecified model, such as when misspecification is in the covariance structure.	Almost always
Estimators are best linear unbiased estimates (BLUE)	Typically, if the least squares assumptions are met.	Not necessarily: estimators are often non-linear in the data and are often biased.
Asymptotically most efficient	Not necessarily	Typically
Easy to compute	Yes	No

Inference Principles for Survey Data

Design-based and model-assisted statistical inference for survey data requires that the randomness due to the selection mechanism be taken into account. This can require special estimation principles and techniques.

The SURVEYMEANS, SURVEYFREQ, SURVEYREG, SURVEYLOGISTIC, and SURVEYPHREG procedures support design-based and/or model-assisted inference for sample surveys. Suppose π_i is the selection probability for unit i in sample S . The inverse of the inclusion probability is known as sampling weight and is denoted by w_i . Briefly, the idea is to apply a relationship that exists in the population to the sample and to take into account the sampling weights. For example, to estimate the finite population total $T_N = \sum_{i \in U_N} y_i$ based on the sample S , you can accumulate the sampled values while properly weighting: $\hat{T}_\pi = \sum_{i \in S} w_i y_i$. It is easy to verify that \hat{T}_π is design-unbiased in the sense that $E[\hat{T}_\pi | \mathcal{F}_N] = T_N$ (see Cochran 1977).

When a statistical model is present, similar ideas apply. For example, if β_{N0} and β_{N1} are finite population quantities for a simple linear regression working model that minimize the sum of squares

$$\sum_{i \in U_N} (y_i - \beta_{0N} - \beta_{1N} x_i)^2$$

in the population, then the sample-based estimators $\hat{\beta}_{0S}$ and $\hat{\beta}_{1S}$ are obtained by minimizing the weighted sum of squares

$$\sum_{i \in S} w_i (y_i - \hat{\beta}_{0S} - \hat{\beta}_{1S} x_i)^2$$

in the sample, taking into account the inclusion probabilities.

In model-assisted inference, weighted least squares or pseudo-maximum likelihood estimators are commonly used to solve such estimation problems. Maximum pseudo-likelihood or weighted maximum likelihood estimators for survey data maximize a sample-based estimator of the population likelihood. Assume a

working model with uncorrelated responses such that the finite population log-likelihood is

$$\sum_{i \in U_N} l(\theta_{1N}, \dots, \theta_{pN}; y_i),$$

where $\theta_{1N}, \dots, \theta_{pN}$ are finite population quantities. For independent sampling, one possible sample-based estimator of the population log likelihood is

$$\sum_{i \in S} w_i l(\theta_{1N}, \dots, \theta_{pN}; y_i)$$

Sample-based estimators $\hat{\theta}_{1S}, \dots, \hat{\theta}_{pS}$ are obtained by maximizing this expression.

Design-based and model-based statistical analysis might employ the same statistical model (for example, a linear regression) and the same estimation principle (for example, weighted least squares), and arrive at the same estimates. The design-based estimation of the precision of the estimators differs from the model-based estimation, however. For complex surveys, design-based variance estimates are in general different from their model-based counterpart. The SAS/STAT procedures for survey data (SURVEYMEANS, SURVEYFREQ, SURVEYREG, SURVEYLOGISTIC, and SURVEYPHREG procedures) compute design-based variance estimates for complex survey data. See the section “Variance Estimation” on page 247, in Chapter 14, “Introduction to Survey Procedures,” for details about design-based variance estimation.

Statistical Background

Hypothesis Testing and Power

In statistical hypothesis testing, you typically express the belief that some effect exists in a population by specifying an alternative hypothesis H_1 . You state a null hypothesis H_0 as the assertion that the effect does *not* exist and attempt to gather evidence to reject H_0 in favor of H_1 . Evidence is gathered in the form of sample data, and a statistical test is used to assess H_0 . If H_0 is rejected but there really is *no* effect, this is called a *Type I error*. The probability of a Type I error is usually designated “alpha” or α , and statistical tests are designed to ensure that α is suitably small (for example, less than 0.05).

If there is an effect in the population but H_0 is *not* rejected in the statistical test, then a *Type II error* has been committed. The probability of a Type II error is usually designated “beta” or β . The probability $1 - \beta$ of avoiding a Type II error—that is, correctly rejecting H_0 and achieving statistical significance, is called the *power* of the test.

An important goal in study planning is to ensure an acceptably high level of power. Sample size plays a prominent role in power computations because the focus is often on determining a sufficient sample size to achieve a certain power, or assessing the power for a range of different sample sizes.

There are several tools available in SAS/STAT software for power and sample size analysis. PROC POWER covers a variety of analyses such as t tests, equivalence tests, confidence intervals, binomial proportions, multiple regression, one-way ANOVA, survival analysis, logistic regression, and the Wilcoxon rank-sum test. PROC GLMPower supports more complex linear models. The Power and Sample Size application provides a user interface and implements many of the analyses supported in the procedures.

Important Linear Algebra Concepts

A *matrix* \mathbf{A} is a rectangular array of numbers. The *order* of a matrix with n rows and k columns is $(n \times k)$. The element in row i , column j of \mathbf{A} is denoted as a_{ij} , and the notation $[a_{ij}]$ is sometimes used to refer to the two-dimensional row-column array

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1k} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2k} \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3k} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nk} \end{bmatrix} = [a_{ij}]$$

A *vector* is a one-dimensional array of numbers. A *column vector* has a single column ($k = 1$). A *row vector* has a single row ($n = 1$). A *scalar* is a matrix of order (1×1) —that is, a single number. A *square matrix* has the same row and column order, $n = k$. A *diagonal matrix* is a square matrix where all off-diagonal elements are zero, $a_{ij} = 0$ if $i \neq j$. The *identity matrix* \mathbf{I} is a diagonal matrix with $a_{ii} = 1$ for all i . The *unit vector* $\mathbf{1}$ is a vector where all elements are 1. The *unit matrix* \mathbf{J} is a matrix of all 1s. Similarly, the elements of the null vector and the null matrix are all 0.

Basic matrix operations are as follows:

Addition If \mathbf{A} and \mathbf{B} are of the same order, then $\mathbf{A} + \mathbf{B}$ is the matrix of elementwise sums,

$$\mathbf{A} + \mathbf{B} = [a_{ij} + b_{ij}]$$

Subtraction If \mathbf{A} and \mathbf{B} are of the same order, then $\mathbf{A} - \mathbf{B}$ is the matrix of elementwise differences,

$$\mathbf{A} - \mathbf{B} = [a_{ij} - b_{ij}]$$

Dot product The dot product of two n -vectors \mathbf{a} and \mathbf{b} is the sum of their elementwise products,

$$\mathbf{a} \cdot \mathbf{b} = \sum_{i=1}^n a_i b_i$$

The dot product is also known as the *inner product* of \mathbf{a} and \mathbf{b} . Two vectors are said to be *orthogonal* if their dot product is zero.

Multiplication Matrices \mathbf{A} and \mathbf{B} are said to be conformable for \mathbf{AB} multiplication if the number of columns in \mathbf{A} equals the number of rows in \mathbf{B} . Suppose that \mathbf{A} is of order $(n \times k)$ and that \mathbf{B} is of order $(k \times p)$. The product \mathbf{AB} is then defined as the $(n \times p)$ matrix of the dot products of the i th row of \mathbf{A} and the j th column of \mathbf{B} ,

$$\mathbf{AB} = [\mathbf{a}_i \cdot \mathbf{b}_j]_{n \times p}$$

Transposition The transpose of the $(n \times k)$ matrix \mathbf{A} is denoted as \mathbf{A}' and is obtained by interchanging the rows and columns,

$$\mathbf{A}' = \begin{bmatrix} a_{11} & a_{21} & a_{31} & \cdots & a_{n1} \\ a_{12} & a_{22} & a_{32} & \cdots & a_{n2} \\ a_{13} & a_{23} & a_{33} & \cdots & a_{n3} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{1k} & a_{2k} & a_{3k} & \cdots & a_{nk} \end{bmatrix} = [a_{ji}]$$

A *symmetric* matrix is equal to its transpose, $\mathbf{A} = \mathbf{A}'$. The inner product of two $(n \times 1)$ column vectors \mathbf{a} and \mathbf{b} is $\mathbf{a} \cdot \mathbf{b} = \mathbf{a}'\mathbf{b}$.

Matrix Inversion

Regular Inverses

The right inverse of a matrix \mathbf{A} is the matrix that yields the identity when \mathbf{A} is postmultiplied by it. Similarly, the left inverse of \mathbf{A} yields the identity if \mathbf{A} is premultiplied by it. \mathbf{A} is said to be invertible and \mathbf{B} is said to be the inverse of \mathbf{A} , if \mathbf{B} is its right and left inverse, $\mathbf{BA} = \mathbf{AB} = \mathbf{I}$. This requires \mathbf{A} to be square and nonsingular. The inverse of a matrix \mathbf{A} is commonly denoted as \mathbf{A}^{-1} . The following results are useful in manipulating inverse matrices (assuming both \mathbf{A} and \mathbf{C} are invertible):

$$\begin{aligned}\mathbf{AA}^{-1} &= \mathbf{A}^{-1}\mathbf{A} = \mathbf{I} \\ (\mathbf{A}')^{-1} &= (\mathbf{A}^{-1})' \\ (\mathbf{A}^{-1})^{-1} &= \mathbf{A} \\ (\mathbf{AC})^{-1} &= \mathbf{C}^{-1}\mathbf{A}^{-1} \\ \text{rank}(\mathbf{A}) &= \text{rank}(\mathbf{A}^{-1})\end{aligned}$$

If \mathbf{D} is a diagonal matrix with nonzero entries on the diagonal—that is, $\mathbf{D} = \text{diag}(d_1, \dots, d_n)$ —then $\mathbf{D}^{-1} = \text{diag}(1/d_1, \dots, 1/d_n)$. If \mathbf{D} is a block-diagonal matrix whose blocks are invertible, then

$$\mathbf{D} = \begin{bmatrix} \mathbf{D}_1 & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \mathbf{D}_2 & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{D}_3 & \cdots & \mathbf{0} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{D}_n \end{bmatrix} \quad \mathbf{D}^{-1} = \begin{bmatrix} \mathbf{D}_1^{-1} & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \mathbf{D}_2^{-1} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{D}_3^{-1} & \cdots & \mathbf{0} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{D}_n^{-1} \end{bmatrix}$$

In statistical applications the following two results are particularly important, because they can significantly reduce the computational burden in working with inverse matrices.

Partitioned Matrix Suppose \mathbf{A} is a nonsingular matrix that is partitioned as

$$\mathbf{A} = \begin{bmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{bmatrix}$$

Then, provided that all the inverses exist, the inverse of \mathbf{A} is given by

$$\mathbf{A}^{-1} = \begin{bmatrix} \mathbf{B}_{11} & \mathbf{B}_{12} \\ \mathbf{B}_{21} & \mathbf{B}_{22} \end{bmatrix}$$

where $\mathbf{B}_{11} = (\mathbf{A}_{11} - \mathbf{A}_{12}\mathbf{A}_{22}^{-1}\mathbf{A}_{21})^{-1}$, $\mathbf{B}_{12} = -\mathbf{B}_{11}\mathbf{A}_{12}\mathbf{A}_{22}^{-1}$, $\mathbf{B}_{21} = -\mathbf{A}_{22}^{-1}\mathbf{A}_{21}\mathbf{B}_{11}$, and $\mathbf{B}_{22} = (\mathbf{A}_{22} - \mathbf{A}_{21}\mathbf{A}_{11}^{-1}\mathbf{A}_{12})^{-1}$.

Patterned Sum Suppose \mathbf{R} is $(n \times n)$ nonsingular, \mathbf{G} is $(k \times k)$ nonsingular, and \mathbf{B} and \mathbf{C} are $(n \times k)$ and $(k \times n)$ matrices, respectively. Then the inverse of $\mathbf{R} + \mathbf{BGC}$ is given by

$$(\mathbf{R} + \mathbf{BGC})^{-1} = \mathbf{R}^{-1} - \mathbf{R}^{-1}\mathbf{B}(\mathbf{G}^{-1} + \mathbf{CR}^{-1}\mathbf{B})^{-1}\mathbf{CR}^{-1}$$

This formula is particularly useful if $k \ll n$ and \mathbf{R} has a simple form that is easy to invert. This case arises, for example, in mixed models where \mathbf{R} might be a diagonal or block-diagonal matrix, and $\mathbf{B} = \mathbf{C}'$.

Another situation where this formula plays a critical role is in the computation of regression diagnostics, such as in determining the effect of removing an observation from the analysis. Suppose that $\mathbf{A} = \mathbf{X}'\mathbf{X}$ represents the crossproduct matrix in the linear model $E[\mathbf{Y}] = \mathbf{X}\boldsymbol{\beta}$. If \mathbf{x}'_i is the i th row of the \mathbf{X} matrix, then $(\mathbf{X}'\mathbf{X} - \mathbf{x}_i\mathbf{x}'_i)$ is the crossproduct matrix in the same model with the i th observation removed. Identifying $\mathbf{B} = -\mathbf{x}_i$, $\mathbf{C} = \mathbf{x}'_i$, and $\mathbf{G} = \mathbf{I}$ in the preceding inversion formula, you can obtain the expression for the inverse of the crossproduct matrix:

$$(\mathbf{X}'\mathbf{X} - \mathbf{x}_i\mathbf{x}'_i)^{-1} = \mathbf{X}'\mathbf{X} + \frac{(\mathbf{X}'\mathbf{X})^{-1} \mathbf{x}_i\mathbf{x}'_i (\mathbf{X}'\mathbf{X})^{-1}}{1 - \mathbf{x}'_i (\mathbf{X}'\mathbf{X})^{-1} \mathbf{x}_i}$$

This expression for the inverse of the reduced data crossproduct matrix enables you to compute “leave-one-out” deletion diagnostics in linear models without refitting the model.

Generalized Inverse Matrices

If \mathbf{A} is rectangular (not square) or singular, then it is not invertible and the matrix \mathbf{A}^{-1} does not exist. Suppose you want to find a solution to simultaneous linear equations of the form

$$\mathbf{A}\mathbf{b} = \mathbf{c}$$

If \mathbf{A} is square and nonsingular, then the unique solution is $\mathbf{b} = \mathbf{A}^{-1}\mathbf{c}$. In statistical applications, the case where \mathbf{A} is $(n \times k)$ rectangular is less important than the case where \mathbf{A} is a $(k \times k)$ square matrix of rank less than k . For example, the normal equations in ordinary least squares (OLS) estimation in the model $\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$ are

$$(\mathbf{X}'\mathbf{X})\boldsymbol{\beta} = \mathbf{X}'\mathbf{Y}$$

A *generalized inverse* matrix is a matrix \mathbf{A}^- such that $\mathbf{A}^-\mathbf{c}$ is a solution to the linear system. In the OLS example, a solution can be found as $(\mathbf{X}'\mathbf{X})^- \mathbf{X}'\mathbf{Y}$, where $(\mathbf{X}'\mathbf{X})^-$ is a generalized inverse of $\mathbf{X}'\mathbf{X}$.

The following four conditions are often associated with generalized inverses. For the square or rectangular matrix \mathbf{A} there exist matrices \mathbf{G} that satisfy

- (i) $\mathbf{AGA} = \mathbf{A}$
- (ii) $\mathbf{GAG} = \mathbf{G}$
- (iii) $(\mathbf{AG})' = \mathbf{AG}$
- (iv) $(\mathbf{GA})' = \mathbf{GA}$

The matrix \mathbf{G} that satisfies all four conditions is unique and is called the Moore-Penrose inverse, after the first published work on generalized inverses by Moore (1920) and the subsequent definition by Penrose (1955). Only the first condition is required, however, to provide a solution to the linear system above.

Pringle and Rayner (1971) introduced a numbering system to distinguish between different types of generalized inverses. A matrix that satisfies only condition (i) is a g_1 -inverse. The g_2 -inverse satisfies conditions (i) and (ii). It is also called a *reflexive* generalized inverse. Matrices satisfying conditions (i)–(iii) or conditions (i), (ii), and (iv) are g_3 -inverses. Note that a matrix that satisfies the first three conditions is a right generalized inverse, and a matrix that satisfies conditions (i), (ii), and (iv) is a left generalized inverse. For example, if \mathbf{B} is $(n \times k)$ of rank k , then $(\mathbf{B}'\mathbf{B})^{-1}\mathbf{B}'$ is a left generalized inverse of \mathbf{B} . The notation g_4 -inverse for the Moore-Penrose inverse, satisfying conditions (i)–(iv), is often used by extension, but note that Pringle and Rayner (1971) do not use it; rather, they call such a matrix “the” generalized inverse.

If the $(n \times k)$ matrix \mathbf{X} is rank-deficient—that is, $\text{rank}(\mathbf{X}) < \min\{n, k\}$ —then the system of equations

$$(\mathbf{X}'\mathbf{X})\boldsymbol{\beta} = \mathbf{X}'\mathbf{Y}$$

does not have a unique solution. A particular solution depends on the choice of the generalized inverse. However, some aspects of the statistical inference are invariant to the choice of the generalized inverse. If \mathbf{G} is a generalized inverse of $\mathbf{X}'\mathbf{X}$, then \mathbf{XGX}' is invariant to the choice of \mathbf{G} . This result comes into play, for example, when you are computing predictions in an OLS model with a rank-deficient \mathbf{X} matrix, since it implies that the predicted values

$$\mathbf{X}\widehat{\boldsymbol{\beta}} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'\mathbf{y}$$

are invariant to the choice of $(\mathbf{X}'\mathbf{X})^{-}$.

Matrix Differentiation

Taking the derivative of expressions involving matrices is a frequent task in statistical estimation. Objective functions that are to be minimized or maximized are usually written in terms of model matrices and/or vectors whose elements depend on the unknowns of the estimation problem. Suppose that \mathbf{A} and \mathbf{B} are real matrices whose elements depend on the scalar quantities β and θ —that is, $\mathbf{A} = [a_{ij}(\beta, \theta)]$, and similarly for \mathbf{B} .

The following are useful results in finding the derivative of elements of a matrix and of functions involving a matrix. For more in-depth discussion of matrix differentiation and matrix calculus, see, for example, Magnus and Neudecker (1999) and Harville (1997).

The derivative of \mathbf{A} with respect to β is denoted $\dot{\mathbf{A}}_{\beta}$ and is the matrix of the first derivatives of the elements of \mathbf{A} :

$$\dot{\mathbf{A}}_{\beta} = \frac{\partial}{\partial \beta} \mathbf{A} = \left[\frac{\partial a_{ij}(\beta, \theta)}{\partial \beta} \right]$$

Similarly, the second derivative of \mathbf{A} with respect to β and θ is the matrix of the second derivatives

$$\ddot{\mathbf{A}}_{\beta\theta} = \frac{\partial^2}{\partial \beta \partial \theta} \mathbf{A} = \left[\frac{\partial^2 a_{ij}(\beta, \theta)}{\partial \beta \partial \theta} \right]$$

The following are some basic results involving sums, products, and traces of matrices:

$$\begin{aligned}\frac{\partial}{\partial \beta} c_1 \mathbf{A} &= c_1 \dot{\mathbf{A}}_{\beta} \\ \frac{\partial}{\partial \beta} (\mathbf{A} + \mathbf{B}) &= \dot{\mathbf{A}}_{\beta} + \dot{\mathbf{B}}_{\beta} \\ \frac{\partial}{\partial \beta} (c_1 \mathbf{A} + c_2 \mathbf{B}) &= c_1 \dot{\mathbf{A}}_{\beta} + c_2 \dot{\mathbf{B}}_{\beta} \\ \frac{\partial}{\partial \beta} \mathbf{AB} &= \mathbf{A} \dot{\mathbf{B}}_{\beta} + \dot{\mathbf{A}}_{\beta} \mathbf{B} \\ \frac{\partial}{\partial \beta} \text{trace}(\mathbf{A}) &= \text{trace}(\dot{\mathbf{A}}_{\beta}) \\ \frac{\partial}{\partial \beta} \text{trace}(\mathbf{AB}) &= \text{trace}(\mathbf{A} \dot{\mathbf{B}}_{\beta}) + \text{trace}(\dot{\mathbf{A}}_{\beta} \mathbf{B})\end{aligned}$$

The next set of results is useful in finding the derivative of elements of \mathbf{A} and of functions of \mathbf{A} , if \mathbf{A} is a nonsingular matrix:

$$\begin{aligned}\frac{\partial}{\partial \beta} \mathbf{x}' \mathbf{A}^{-1} \mathbf{x} &= -\mathbf{x}' \mathbf{A}^{-1} \dot{\mathbf{A}}_{\beta} \mathbf{A}^{-1} \mathbf{x} \\ \frac{\partial}{\partial \beta} \mathbf{A}^{-1} &= -\mathbf{A}^{-1} \dot{\mathbf{A}}_{\beta} \mathbf{A}^{-1} \\ \frac{\partial}{\partial \beta} |\mathbf{A}| &= |\mathbf{A}| \text{trace}(\mathbf{A}^{-1} \dot{\mathbf{A}}_{\beta}) \\ \frac{\partial}{\partial \beta} \log \{|\mathbf{A}|\} &= \frac{1}{|\mathbf{A}|} \frac{\partial}{\partial \beta} |\mathbf{A}| = \text{trace}(\mathbf{A}^{-1} \dot{\mathbf{A}}_{\beta}) \\ \frac{\partial^2}{\partial \beta \partial \theta} \mathbf{A}^{-1} &= -\mathbf{A}^{-1} \ddot{\mathbf{A}}_{\beta \theta} \mathbf{A}^{-1} + \mathbf{A}^{-1} \dot{\mathbf{A}}_{\beta} \mathbf{A}^{-1} \dot{\mathbf{A}}_{\theta} \mathbf{A}^{-1} + \mathbf{A}^{-1} \dot{\mathbf{A}}_{\theta} \mathbf{A}^{-1} \dot{\mathbf{A}}_{\beta} \mathbf{A}^{-1} \\ \frac{\partial^2}{\partial \beta \partial \theta} \log \{|\mathbf{A}|\} &= \text{trace}(\mathbf{A}^{-1} \ddot{\mathbf{A}}_{\beta \theta}) - \text{trace}(\mathbf{A}^{-1} \dot{\mathbf{A}}_{\beta} \mathbf{A}^{-1} \dot{\mathbf{A}}_{\theta})\end{aligned}$$

Now suppose that \mathbf{a} and \mathbf{b} are column vectors that depend on β and/or θ and that \mathbf{x} is a vector of constants. The following results are useful for manipulating derivatives of linear and quadratic forms:

$$\begin{aligned}\frac{\partial}{\partial \mathbf{x}} \mathbf{a}' \mathbf{x} &= \mathbf{a} \\ \frac{\partial}{\partial \mathbf{x}'} \mathbf{B} \mathbf{x} &= \mathbf{B} \\ \frac{\partial}{\partial \mathbf{x}} \mathbf{x}' \mathbf{B} \mathbf{x} &= (\mathbf{B} + \mathbf{B}') \mathbf{x} \\ \frac{\partial^2}{\partial \mathbf{x} \partial \mathbf{x}'} \mathbf{x}' \mathbf{B} \mathbf{x} &= \mathbf{B} + \mathbf{B}'\end{aligned}$$

Matrix Decompositions

To decompose a matrix is to express it as a function—typically a product—of other matrices that have particular properties such as orthogonality, diagonality, triangularity. For example, the Cholesky decomposition of a symmetric positive definite matrix \mathbf{A} is $\mathbf{C}\mathbf{C}' = \mathbf{A}$, where \mathbf{C} is a lower-triangular matrix. The spectral decomposition of a symmetric matrix is $\mathbf{A} = \mathbf{P}\mathbf{D}\mathbf{P}'$, where \mathbf{D} is a diagonal matrix and \mathbf{P} is an orthogonal matrix.

Matrix decomposition play an important role in statistical theory as well as in statistical computations. Calculations in terms of decompositions can have greater numerical stability. Decompositions are often necessary to extract information about matrices, such as matrix rank, eigenvalues, or eigenvectors. Decompositions are also used to form special transformations of matrices, such as to form a “square-root” matrix. This section briefly mentions several decompositions that are particularly prevalent and important.

LDU, LU, and Cholesky Decomposition

Every square matrix \mathbf{A} , whether it is positive definite or not, can be expressed in the form $\mathbf{A} = \mathbf{L}\mathbf{D}\mathbf{U}$, where \mathbf{L} is a unit lower-triangular matrix, \mathbf{D} is a diagonal matrix, and \mathbf{U} is a unit upper-triangular matrix. (The diagonal elements of a unit triangular matrix are 1.) Because of the arrangement of the matrices, the decomposition is called the LDU decomposition. Since you can absorb the diagonal matrix into the triangular matrices, the decomposition

$$\mathbf{A} = \mathbf{L}\mathbf{D}^{1/2}\mathbf{D}^{1/2}\mathbf{U} = \mathbf{L}^*\mathbf{U}^*$$

is also referred to as the LU decomposition of \mathbf{A} .

If the matrix \mathbf{A} is positive definite, then the diagonal elements of \mathbf{D} are positive and the LDU decomposition is unique. Furthermore, we can add more specificity to this result in that for a symmetric, positive definite matrix, there is a unique decomposition $\mathbf{A} = \mathbf{U}'\mathbf{D}\mathbf{U}$, where \mathbf{U} is unit upper-triangular and \mathbf{D} is diagonal with positive elements. Absorbing the square root of \mathbf{D} into \mathbf{U} , $\mathbf{C} = \mathbf{D}^{1/2}\mathbf{U}$, the decomposition is known as the *Cholesky* decomposition of a positive-definite matrix:

$$\mathbf{B} = \mathbf{U}'\mathbf{D}^{1/2}\mathbf{D}^{1/2}\mathbf{U} = \mathbf{C}'\mathbf{C}$$

where \mathbf{C} is upper triangular.

If \mathbf{B} is $(n \times n)$ symmetric nonnegative definite of rank k , then we can extend the Cholesky decomposition as follows. Let \mathbf{C}^* denote the lower-triangular matrix such that

$$\mathbf{C}^* = \begin{bmatrix} \mathbf{C}_{k \times k} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}$$

Then $\mathbf{B} = \mathbf{C}\mathbf{C}'$.

Spectral Decomposition

Suppose that \mathbf{A} is an $(n \times n)$ symmetric matrix. Then there exists an orthogonal matrix \mathbf{Q} and a diagonal matrix \mathbf{D} such that $\mathbf{A} = \mathbf{Q}\mathbf{D}\mathbf{Q}'$. Of particular importance is the case where the orthogonal matrix is also orthonormal—that is, its column vectors have unit norm. Denote this orthonormal matrix as \mathbf{P} . Then the corresponding diagonal matrix— $\mathbf{\Lambda} = \text{diag}(\lambda_1, \dots, \lambda_n)$, say—contains the eigenvalues of \mathbf{A} . The spectral decomposition of \mathbf{A} can be written as

$$\mathbf{A} = \mathbf{P}\mathbf{\Lambda}\mathbf{P}' = \sum_{i=1}^n \lambda_i \mathbf{p}_i \mathbf{p}_i'$$

where \mathbf{p}_i denotes the i th column vector of \mathbf{P} . The right-side expression decomposes \mathbf{A} into a sum of rank-1 matrices, and the weight of each contribution is equal to the eigenvalue associated with the i th eigenvector. The sum furthermore emphasizes that the rank of \mathbf{A} is equal to the number of nonzero eigenvalues.

Harville (1997, p. 538) refers to the spectral decomposition of \mathbf{A} as the decomposition that takes the previous sum one step further and accumulates contributions associated with the distinct eigenvalues. If $\lambda_1^*, \dots, \lambda_k^*$ are the distinct eigenvalues and $\mathbf{E}_j = \sum \mathbf{p}_i \mathbf{p}_i'$, where the sum is taken over the set of columns for which $\lambda_i = \lambda_j^*$, then

$$\mathbf{A} = \sum_{i=1}^k \lambda_i^* \mathbf{E}_i$$

You can employ the spectral decomposition of a nonnegative definite symmetric matrix to form a “square-root” matrix of \mathbf{A} . Suppose that $\mathbf{\Lambda}^{1/2}$ is the diagonal matrix containing the square roots of the λ_i . Then $\mathbf{B} = \mathbf{P}\mathbf{\Lambda}^{1/2}\mathbf{P}'$ is a square-root matrix of \mathbf{A} in the sense that $\mathbf{B}\mathbf{B} = \mathbf{A}$, because

$$\mathbf{B}\mathbf{B} = \mathbf{P}\mathbf{\Lambda}^{1/2}\mathbf{P}'\mathbf{P}\mathbf{\Lambda}^{1/2}\mathbf{P}' = \mathbf{P}\mathbf{\Lambda}^{1/2}\mathbf{\Lambda}^{1/2}\mathbf{P}' = \mathbf{P}\mathbf{A}\mathbf{P}'$$

Generating the Moore-Penrose inverse of a matrix based on the spectral decomposition is also simple. Denote as $\mathbf{\Delta}$ the diagonal matrix with typical element

$$\delta_i = \begin{cases} 1/\lambda_i & \lambda_i \neq 0 \\ 0 & \lambda_i = 0 \end{cases}$$

Then the matrix $\mathbf{P}\mathbf{\Delta}\mathbf{P}' = \sum \delta_i \mathbf{p}_i \mathbf{p}_i'$ is the Moore-Penrose (g_4 -generalized) inverse of \mathbf{A} .

Singular-Value Decomposition

The singular-value decomposition is related to the spectral decomposition of a matrix, but it is more general. The singular-value decomposition can be applied to any matrix. Let \mathbf{B} be an $(n \times p)$ matrix of rank k . Then there exist orthogonal matrices \mathbf{P} and \mathbf{Q} of order $(n \times n)$ and $(p \times p)$, respectively, and a diagonal matrix \mathbf{D} such that

$$\mathbf{P}'\mathbf{B}\mathbf{Q} = \mathbf{D} = \begin{bmatrix} \mathbf{D}_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}$$

where \mathbf{D}_1 is a diagonal matrix of order k . The diagonal elements of \mathbf{D}_1 are strictly positive. As with the spectral decomposition, this result can be written as a decomposition of \mathbf{B} into a weighted sum of rank-1 matrices

$$\mathbf{B} = \mathbf{P}\mathbf{D}\mathbf{Q}' = \sum_{i=1}^n d_i \mathbf{p}_i \mathbf{q}_i'$$

The scalars d_1, \dots, d_k are called the *singular values* of the matrix \mathbf{B} . They are the positive square roots of the nonzero eigenvalues of the matrix $\mathbf{B}'\mathbf{B}$. If the singular-value decomposition is applied to a symmetric, nonnegative definite matrix \mathbf{A} , then the singular values d_1, \dots, d_n are the nonzero eigenvalues of \mathbf{A} and the singular-value decomposition is the same as the spectral decomposition.

As with the spectral decomposition, you can use the results of the singular-value decomposition to generate the Moore-Penrose inverse of a matrix. If \mathbf{B} is $(n \times p)$ with singular-value decomposition $\mathbf{P}\mathbf{D}\mathbf{Q}'$, and if $\mathbf{\Delta}$ is a diagonal matrix with typical element

$$\delta_i = \begin{cases} 1/d_i & |d_i| \neq 0 \\ 0 & d_i = 0 \end{cases}$$

then $\mathbf{Q}\mathbf{\Delta}\mathbf{P}'$ is the g_4 -generalized inverse of \mathbf{B} .

Expectations of Random Variables and Vectors

If Y is a discrete random variable with mass function $p(y)$ and support (possible values) y_1, y_2, \dots , then the expectation (expected value) of Y is defined as

$$E[Y] = \sum_{j=1}^{\infty} y_j p(y_j)$$

provided that $\sum |y_j| p(y_j) < \infty$, otherwise the sum in the definition is not well-defined. The expected value of a function $h(y)$ is similarly defined: provided that $\sum |h(y_j)| p(y_j) < \infty$,

$$E[h(Y)] = \sum_{j=1}^{\infty} h(y_j) p(y_j)$$

For continuous random variables, similar definitions apply, but summation is replaced by integration over the support of the random variable. If X is a continuous random variable with density function $f(x)$, and $\int |x| f(x) dx < \infty$, then the expectation of X is defined as

$$E[X] = \int_{-\infty}^{\infty} x f(x) dx$$

The expected value of a random variable is also called its *mean* or its first moment. A particularly important function of a random variable is $h(Y) = (Y - E[Y])^2$. The expectation of $h(Y)$ is called the *variance* of Y or the second central moment of Y . When you study the properties of multiple random variables, then you might be interested in aspects of their joint distribution. The covariance between random variables Y and X is defined as the expected value of the function $(Y - E[Y])(X - E[X])$, where the expectation is taken under the bivariate joint distribution of Y and X :

$$\text{Cov}[Y, X] = E[(Y - E[Y])(X - E[X])] = E[XY] - E[Y]E[X] = \int \int x y f(x, y) dx dy - E[Y]E[X]$$

The *covariance* between a random variable and itself is the variance, $\text{Cov}[Y, Y] = \text{Var}[Y]$.

In statistical applications and formulas, random variables are often collected into vectors. For example, a random sample of size n from the distribution of Y generates a random vector of order $(n \times 1)$,

$$\mathbf{Y} = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix}$$

The expected value of the $(n \times 1)$ random vector \mathbf{Y} is the vector of the means of the elements of \mathbf{Y} :

$$E[\mathbf{Y}] = [E[Y_i]] = \begin{bmatrix} E[Y_1] \\ E[Y_2] \\ \vdots \\ E[Y_n] \end{bmatrix}$$

It is often useful to directly apply rules about working with means, variances, and covariances of random vectors. To develop these rules, suppose that \mathbf{Y} and \mathbf{U} denote two random vectors with typical elements

Y_1, \dots, Y_n and U_1, \dots, U_k . Further suppose that \mathbf{A} and \mathbf{B} are constant (nonstochastic) matrices, that \mathbf{a} is a constant vector, and that the c_i are scalar constants.

The following rules enable you to derive the mean of a linear function of a random vector:

$$\begin{aligned} E[\mathbf{A}] &= \mathbf{A} \\ E[\mathbf{Y} + \mathbf{a}] &= E[\mathbf{Y}] \\ E[\mathbf{A}\mathbf{Y} + \mathbf{a}] &= \mathbf{A}E[\mathbf{Y}] + \mathbf{a} \\ E[\mathbf{Y} + \mathbf{U}] &= E[\mathbf{Y}] + E[\mathbf{U}] \end{aligned}$$

The *covariance matrix* of \mathbf{Y} and \mathbf{U} is the $(n \times k)$ matrix whose typical element in row i , column j is the covariance between Y_i and U_j . The covariance matrix between two random vectors is frequently denoted with the Cov “operator.”

$$\begin{aligned} \text{Cov}[\mathbf{Y}, \mathbf{U}] &= [\text{Cov}[Y_i, U_j]] \\ &= E[(\mathbf{Y} - E[\mathbf{Y}])(\mathbf{U} - E[\mathbf{U}])'] = E[\mathbf{Y}\mathbf{U}'] - E[\mathbf{Y}]E[\mathbf{U}]' \\ &= \begin{bmatrix} \text{Cov}[Y_1, U_1] & \text{Cov}[Y_1, U_2] & \text{Cov}[Y_1, U_3] & \cdots & \text{Cov}[Y_1, U_k] \\ \text{Cov}[Y_2, U_1] & \text{Cov}[Y_2, U_2] & \text{Cov}[Y_2, U_3] & \cdots & \text{Cov}[Y_2, U_k] \\ \text{Cov}[Y_3, U_1] & \text{Cov}[Y_3, U_2] & \text{Cov}[Y_3, U_3] & \cdots & \text{Cov}[Y_3, U_k] \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \text{Cov}[Y_n, U_1] & \text{Cov}[Y_n, U_2] & \text{Cov}[Y_n, U_3] & \cdots & \text{Cov}[Y_n, U_k] \end{bmatrix} \end{aligned}$$

The *variance matrix* of a random vector \mathbf{Y} is the covariance matrix between \mathbf{Y} and itself. The variance matrix is frequently denoted with the Var “operator.”

$$\begin{aligned} \text{Var}[\mathbf{Y}] &= \text{Cov}[\mathbf{Y}, \mathbf{Y}] = [\text{Cov}[Y_i, Y_j]] \\ &= E[(\mathbf{Y} - E[\mathbf{Y}])(\mathbf{Y} - E[\mathbf{Y}])'] = E[\mathbf{Y}\mathbf{Y}'] - E[\mathbf{Y}]E[\mathbf{Y}]' \\ &= \begin{bmatrix} \text{Cov}[Y_1, Y_1] & \text{Cov}[Y_1, Y_2] & \text{Cov}[Y_1, Y_3] & \cdots & \text{Cov}[Y_1, Y_n] \\ \text{Cov}[Y_2, Y_1] & \text{Cov}[Y_2, Y_2] & \text{Cov}[Y_2, Y_3] & \cdots & \text{Cov}[Y_2, Y_n] \\ \text{Cov}[Y_3, Y_1] & \text{Cov}[Y_3, Y_2] & \text{Cov}[Y_3, Y_3] & \cdots & \text{Cov}[Y_3, Y_n] \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \text{Cov}[Y_n, Y_1] & \text{Cov}[Y_n, Y_2] & \text{Cov}[Y_n, Y_3] & \cdots & \text{Cov}[Y_n, Y_n] \end{bmatrix} \\ &= \begin{bmatrix} \text{Var}[Y_1] & \text{Cov}[Y_1, Y_2] & \text{Cov}[Y_1, Y_3] & \cdots & \text{Cov}[Y_1, Y_n] \\ \text{Cov}[Y_2, Y_1] & \text{Var}[Y_2] & \text{Cov}[Y_2, Y_3] & \cdots & \text{Cov}[Y_2, Y_n] \\ \text{Cov}[Y_3, Y_1] & \text{Cov}[Y_3, Y_2] & \text{Var}[Y_3] & \cdots & \text{Cov}[Y_3, Y_n] \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \text{Cov}[Y_n, Y_1] & \text{Cov}[Y_n, Y_2] & \text{Cov}[Y_n, Y_3] & \cdots & \text{Var}[Y_n] \end{bmatrix} \end{aligned}$$

Because the variance matrix contains variances on the diagonal and covariances in the off-diagonal positions, it is also referred to as the *variance-covariance matrix* of the random vector \mathbf{Y} .

If the elements of the covariance matrix $\text{Cov}[\mathbf{Y}, \mathbf{U}]$ are zero, the random vectors are uncorrelated. If \mathbf{Y} and \mathbf{U} are normally distributed, then a zero covariance matrix implies that the vectors are stochastically independent. If the off-diagonal elements of the variance matrix $\text{Var}[\mathbf{Y}]$ are zero, the elements of the random vector \mathbf{Y} are uncorrelated. If \mathbf{Y} is normally distributed, then a diagonal variance matrix implies that its elements are stochastically independent.

Suppose that \mathbf{A} and \mathbf{B} are constant (nonstochastic) matrices and that c_i denotes a scalar constant. The following results are useful in manipulating covariance matrices:

$$\begin{aligned}\text{Cov}[\mathbf{AY}, \mathbf{U}] &= \mathbf{A}\text{Cov}[\mathbf{Y}, \mathbf{U}] \\ \text{Cov}[\mathbf{Y}, \mathbf{BU}] &= \text{Cov}[\mathbf{Y}, \mathbf{U}]\mathbf{B}' \\ \text{Cov}[\mathbf{AY}, \mathbf{BU}] &= \mathbf{A}\text{Cov}[\mathbf{Y}, \mathbf{U}]\mathbf{B}' \\ \text{Cov}[c_1\mathbf{Y}_1 + c_2\mathbf{U}_1, c_3\mathbf{Y}_2 + c_4\mathbf{U}_2] &= c_1c_3\text{Cov}[\mathbf{Y}_1, \mathbf{Y}_2] + c_1c_4\text{Cov}[\mathbf{Y}_1, \mathbf{U}_2] \\ &\quad + c_2c_3\text{Cov}[\mathbf{U}_1, \mathbf{Y}_2] + c_2c_4\text{Cov}[\mathbf{U}_1, \mathbf{U}_2]\end{aligned}$$

Since $\text{Cov}[\mathbf{Y}, \mathbf{Y}] = \text{Var}[\mathbf{Y}]$, these results can be applied to produce the following results, useful in manipulating variances of random vectors:

$$\begin{aligned}\text{Var}[\mathbf{A}] &= \mathbf{0} \\ \text{Var}[\mathbf{AY}] &= \mathbf{A}\text{Var}[\mathbf{Y}]\mathbf{A}' \\ \text{Var}[\mathbf{Y} + \mathbf{x}] &= \text{Var}[\mathbf{Y}] \\ \text{Var}[\mathbf{x}'\mathbf{Y}] &= \mathbf{x}'\text{Var}[\mathbf{Y}]\mathbf{x} \\ \text{Var}[c_1\mathbf{Y}] &= c_1^2\text{Var}[\mathbf{Y}] \\ \text{Var}[c_1\mathbf{Y} + c_2\mathbf{U}] &= c_1^2\text{Var}[\mathbf{Y}] + c_2^2\text{Var}[\mathbf{U}] + 2c_1c_2\text{Cov}[\mathbf{Y}, \mathbf{U}]\end{aligned}$$

Another area where expectation rules are helpful is quadratic forms in random variables. These forms arise particularly in the study of linear statistical models and in linear statistical inference. Linear inference is statistical inference about linear function of random variables, even if those random variables are defined through nonlinear models. For example, the parameter estimator $\hat{\boldsymbol{\theta}}$ might be derived in a nonlinear model, but this does not prevent statistical questions from being raised that can be expressed through linear functions of $\boldsymbol{\theta}$; for example,

$$H_0: \begin{cases} \theta_1 - 2\theta_2 = 0 \\ \theta_2 - \theta_3 = 0 \end{cases}$$

if \mathbf{A} is a matrix of constants and \mathbf{Y} is a random vector, then

$$E[\mathbf{Y}'\mathbf{AY}] = \text{trace}(\mathbf{A}\text{Var}[\mathbf{Y}]) + E[\mathbf{Y}]'\mathbf{A}E[\mathbf{Y}]$$

Mean Squared Error

The mean squared error is arguably the most important criterion used to evaluate the performance of a predictor or an estimator. (The subtle distinction between predictors and estimators is that random variables are predicted and constants are estimated.) The mean squared error is also useful to relay the concepts of bias, precision, and accuracy in statistical estimation. In order to examine a mean squared error, you need a

target of estimation or prediction, and a predictor or estimator that is a function of the data. Suppose that the target, whether a constant or a random variable, is denoted as U . The mean squared error of the estimator or predictor $T(\mathbf{Y})$ for U is

$$\text{MSE}[T(\mathbf{Y}); U] = \text{E} \left[(T(\mathbf{Y}) - U)^2 \right]$$

The reason for using a squared difference to measure the “loss” between $T(\mathbf{Y})$ and U is mostly convenience; properties of squared differences involving random variables are more easily examined than, say, absolute differences. The reason for taking an expectation is to remove the randomness of the squared difference by averaging over the distribution of the data.

Consider first the case where the target U is a constant—say, the parameter β —and denote the mean of the estimator $T(\mathbf{Y})$ as μ_T . The mean squared error can then be decomposed as

$$\begin{aligned} \text{MSE}[T(\mathbf{Y}); \beta] &= \text{E} \left[(T(\mathbf{Y}) - \beta)^2 \right] \\ &= \text{E} \left[(T(\mathbf{Y}) - \mu_T)^2 \right] - \text{E} \left[(\beta - \mu_T)^2 \right] \\ &= \text{Var}[T(\mathbf{Y})] + (\beta - \mu_T)^2 \end{aligned}$$

The mean squared error thus comprises the variance of the estimator and the squared bias. The two components can be associated with an estimator’s precision (small variance) and its accuracy (small bias).

If $T(\mathbf{Y})$ is an unbiased estimator of β —that is, if $\text{E}[T(\mathbf{Y})] = \beta$ —then the mean squared error is simply the variance of the estimator. By choosing an estimator that has minimum variance, you also choose an estimator that has minimum mean squared error among all unbiased estimators. However, as you can see from the previous expression, bias is also an “average” property; it is defined as an expectation. It is quite possible to find estimators in some statistical modeling problems that have smaller mean squared error than a minimum variance unbiased estimator; these are estimators that permit a certain amount of bias but improve on the variance. For example, in models where regressors are highly collinear, the ordinary least squares estimator continues to be unbiased. However, the presence of collinearity can induce poor precision and lead to an erratic estimator. Ridge regression stabilizes the regression estimates in this situation, and the coefficient estimates are somewhat biased, but the bias is more than offset by the gains in precision.

When the target U is a random variable, you need to carefully define what an unbiased prediction means. If the statistic and the target have the same expectation, $\text{E}[U] = \text{E}[T(\mathbf{Y})]$, then

$$\text{MSE}[T(\mathbf{Y}); U] = \text{Var}[T(\mathbf{Y})] + \text{Var}[U] - 2\text{Cov}[T(\mathbf{Y}), U]$$

In many instances the target U is a new observation that was not part of the analysis. If the data are uncorrelated, then it is reasonable to assume in that instance that the new observation is also not correlated with the data. The mean squared error then reduces to the sum of the two variances. For example, in a linear regression model where U is a new observation Y_0 and $T(\mathbf{Y})$ is the regression estimator

$$\hat{Y}_0 = \mathbf{x}'_0 (\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}'\mathbf{Y}$$

with variance $\text{Var}[Y_0] = \sigma^2 \mathbf{x}'_0 (\mathbf{X}'\mathbf{X})^{-1} \mathbf{x}_0$, the mean squared prediction error for Y_0 is

$$\text{MSE}[\hat{Y}_0; Y_0] = \sigma^2 \left(\mathbf{x}'_0 (\mathbf{X}'\mathbf{X})^{-1} \mathbf{x}_0 + 1 \right)$$

and the mean squared prediction error for predicting the mean $\text{E}[Y_0]$ is

$$\text{MSE}[\hat{Y}_0; \text{E}[Y_0]] = \sigma^2 \mathbf{x}'_0 (\mathbf{X}'\mathbf{X})^{-1} \mathbf{x}_0$$

Linear Model Theory

This section presents some basic statistical concepts and results for the linear model with homoscedastic, uncorrelated errors in which the parameters are estimated by ordinary least squares. The model can be written as

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon} \quad \boldsymbol{\epsilon} \sim (0, \sigma^2\mathbf{I})$$

where \mathbf{Y} is an $(n \times 1)$ vector and \mathbf{X} is an $(n \times k)$ matrix of known constants. The model equation implies the following expected values:

$$\begin{aligned} E[\mathbf{Y}] &= \mathbf{X}\boldsymbol{\beta} \\ \text{Var}[\mathbf{Y}] = \sigma^2\mathbf{I} &\Leftrightarrow \text{Cov}[Y_i, Y_j] = \begin{cases} \sigma^2 & i = j \\ 0 & \text{otherwise} \end{cases} \end{aligned}$$

Finding the Least Squares Estimators

Finding the least squares estimator of $\boldsymbol{\beta}$ can be motivated as a calculus problem or by considering the geometry of least squares. The former approach simply states that the OLS estimator is the vector $\hat{\boldsymbol{\beta}}$ that minimizes the objective function

$$\text{SSE} = (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})'(\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})$$

Applying the differentiation rules from the section “Matrix Differentiation” on page 47 leads to

$$\begin{aligned} \frac{\partial}{\partial \boldsymbol{\beta}} \text{SSE} &= \frac{\partial}{\partial \boldsymbol{\beta}} (\mathbf{Y}'\mathbf{Y} - 2\mathbf{Y}'\mathbf{X}\boldsymbol{\beta} + \boldsymbol{\beta}'\mathbf{X}'\mathbf{X}\boldsymbol{\beta}) \\ &= \mathbf{0} - 2\mathbf{X}'\mathbf{Y} + 2\mathbf{X}'\mathbf{X}\boldsymbol{\beta} \\ \frac{\partial^2}{\partial \boldsymbol{\beta} \partial \boldsymbol{\beta}} \text{SSE} &= \mathbf{X}'\mathbf{X} \end{aligned}$$

Consequently, the solution to the *normal equations*, $\mathbf{X}'\mathbf{X}\boldsymbol{\beta} = \mathbf{X}'\mathbf{Y}$, solves $\frac{\partial}{\partial \boldsymbol{\beta}} \text{SSE} = 0$, and the fact that the second derivative is nonnegative definite guarantees that this solution minimizes SSE. The geometric argument to motivate ordinary least squares estimation is as follows. Assume that \mathbf{X} is of rank k . For any value of $\boldsymbol{\beta}$, such as $\tilde{\boldsymbol{\beta}}$, the following identity holds:

$$\mathbf{Y} = \mathbf{X}\tilde{\boldsymbol{\beta}} + (\mathbf{Y} - \mathbf{X}\tilde{\boldsymbol{\beta}})$$

The vector $\mathbf{X}\tilde{\boldsymbol{\beta}}$ is a point in a k -dimensional subspace of R^n , and the residual $(\mathbf{Y} - \mathbf{X}\tilde{\boldsymbol{\beta}})$ is a point in an $(n - k)$ -dimensional subspace. The OLS estimator is the value $\hat{\boldsymbol{\beta}}$ that minimizes the distance of $\mathbf{X}\tilde{\boldsymbol{\beta}}$ from \mathbf{Y} , implying that $\mathbf{X}\hat{\boldsymbol{\beta}}$ and $(\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}})$ are orthogonal to each other; that is,

$(\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}})' \mathbf{X}\hat{\boldsymbol{\beta}} = 0$. This in turn implies that $\hat{\boldsymbol{\beta}}$ satisfies the normal equations, since

$$\hat{\boldsymbol{\beta}}' \mathbf{X}' \mathbf{Y} = \hat{\boldsymbol{\beta}}' \mathbf{X}' \mathbf{X} \hat{\boldsymbol{\beta}} \Leftrightarrow \mathbf{X}' \mathbf{X} \hat{\boldsymbol{\beta}} = \mathbf{X}' \mathbf{Y}$$

Full-Rank Case

If \mathbf{X} is of full column rank, the OLS estimator is unique and given by

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}'\mathbf{Y}$$

The OLS estimator is an unbiased estimator of $\boldsymbol{\beta}$ —that is,

$$\begin{aligned} E[\hat{\boldsymbol{\beta}}] &= E\left[(\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}'\mathbf{Y}\right] \\ &= (\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}'E[\mathbf{Y}] = (\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}'\mathbf{X}\boldsymbol{\beta} = \boldsymbol{\beta} \end{aligned}$$

Note that this result holds if $E[\mathbf{Y}] = \mathbf{X}\boldsymbol{\beta}$; in other words, the condition that the model errors have mean zero is sufficient for the OLS estimator to be unbiased. If the errors are homoscedastic and uncorrelated, the OLS estimator is indeed the *best* linear unbiased estimator (BLUE) of $\boldsymbol{\beta}$ —that is, no other estimator that is a linear function of \mathbf{Y} has a smaller mean squared error. The fact that the estimator is unbiased implies that no other linear estimator has a smaller variance. If, furthermore, the model errors are normally distributed, then the OLS estimator has minimum variance among all unbiased estimators of $\boldsymbol{\beta}$, whether they are linear or not. Such an estimator is called a *uniformly minimum variance unbiased estimator*, or UMVUE.

Rank-Deficient Case

In the case of a rank-deficient \mathbf{X} matrix, a generalized inverse is used to solve the normal equations:

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^- \mathbf{X}'\mathbf{Y}$$

Although a g_1 -inverse is sufficient to solve a linear system, computational expedience and interpretation of the results often dictate the use of a generalized inverse with reflexive properties (that is, a g_2 -inverse; see the section “Generalized Inverse Matrices” on page 46 for details). Suppose, for example, that the \mathbf{X} matrix is partitioned as $\mathbf{X} = [\mathbf{X}_1 \ \mathbf{X}_2]$, where \mathbf{X}_1 is of full column rank and each column in \mathbf{X}_2 is a linear combination of the columns of \mathbf{X}_1 . The matrix

$$\mathbf{G}_1 = \begin{bmatrix} (\mathbf{X}'_1\mathbf{X}_1)^{-1} & (\mathbf{X}'_1\mathbf{X}_1)^{-1} \mathbf{X}'_1\mathbf{X}_2 \\ -\mathbf{X}'_2\mathbf{X}_1 (\mathbf{X}'_1\mathbf{X}_1)^{-1} & \mathbf{0} \end{bmatrix}$$

is a g_1 -inverse of $\mathbf{X}'\mathbf{X}$ and

$$\mathbf{G}_2 = \begin{bmatrix} (\mathbf{X}'_1\mathbf{X}_1)^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}$$

is a g_2 -inverse. If the least squares solution is computed with the g_1 -inverse, then computing the variance of the estimator requires additional matrix operations and storage. On the other hand, the variance of the solution that uses a g_2 -inverse is proportional to \mathbf{G}_2 .

$$\begin{aligned} \text{Var}[\mathbf{G}_1\mathbf{X}'\mathbf{Y}] &= \sigma^2 \mathbf{G}_1\mathbf{X}'\mathbf{X}\mathbf{G}_1 \\ \text{Var}[\mathbf{G}_2\mathbf{X}'\mathbf{Y}] &= \sigma^2 \mathbf{G}_2\mathbf{X}'\mathbf{X}\mathbf{G}_2 = \sigma^2 \mathbf{G}_2 \end{aligned}$$

If a generalized inverse \mathbf{G} of $\mathbf{X}'\mathbf{X}$ is used to solve the normal equations, then the resulting solution is a biased estimator of $\boldsymbol{\beta}$ (unless $\mathbf{X}'\mathbf{X}$ is of full rank, in which case the generalized inverse is “the” inverse), since $E[\hat{\boldsymbol{\beta}}] = \mathbf{G}\mathbf{X}'\mathbf{X}\boldsymbol{\beta}$, which is not in general equal to $\boldsymbol{\beta}$.

If you think of estimation as “estimation without bias,” then $\hat{\boldsymbol{\beta}}$ is the estimator of something, namely $\mathbf{G}\mathbf{X}\boldsymbol{\beta}$. Since this is not a quantity of interest and since it is not unique—it depends on your choice of \mathbf{G} —Searle (1971, p. 169) cautions that in the less-than-full-rank case, $\hat{\boldsymbol{\beta}}$ is a solution to the normal equations and “nothing more.”

Analysis of Variance

The identity

$$\mathbf{Y} = \mathbf{X}\tilde{\boldsymbol{\beta}} + (\mathbf{Y} - \mathbf{X}\tilde{\boldsymbol{\beta}})$$

holds for all vectors $\tilde{\boldsymbol{\beta}}$, but only for the least squares solution is the residual $(\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}})$ orthogonal to the predicted value $\mathbf{X}\hat{\boldsymbol{\beta}}$. Because of this orthogonality, the additive identity holds not only for the vectors themselves, but also for their lengths (Pythagorean theorem):

$$\|\mathbf{Y}\|^2 = \|\mathbf{X}\hat{\boldsymbol{\beta}}\|^2 + \|(\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}})\|^2$$

Note that $\mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y} = \mathbf{H}\mathbf{Y}$ and note that $\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}} = (\mathbf{I} - \mathbf{H})\mathbf{Y} = \mathbf{M}\mathbf{Y}$. The matrices \mathbf{H} and $\mathbf{M} = \mathbf{I} - \mathbf{H}$ play an important role in the theory of linear models and in statistical computations. Both are *projection* matrices—that is, they are symmetric and idempotent. (An idempotent matrix \mathbf{A} is a square matrix that satisfies $\mathbf{A}\mathbf{A} = \mathbf{A}$. The eigenvalues of an idempotent matrix take on the values 1 and 0 only.) The matrix \mathbf{H} projects onto the subspace of R^n that is spanned by the columns of \mathbf{X} . The matrix \mathbf{M} projects onto the orthogonal complement of that space. Because of these properties you have $\mathbf{H}' = \mathbf{H}$, $\mathbf{H}\mathbf{H} = \mathbf{H}$, $\mathbf{M}' = \mathbf{M}$, $\mathbf{M}\mathbf{M} = \mathbf{M}$, $\mathbf{H}\mathbf{M} = \mathbf{0}$.

The Pythagorean relationship now can be written in terms of \mathbf{H} and \mathbf{M} as follows:

$$\|\mathbf{Y}\|^2 = \mathbf{Y}'\mathbf{Y} = \|\mathbf{H}\mathbf{Y}\|^2 + \|\mathbf{M}\mathbf{Y}\|^2 = \mathbf{Y}'\mathbf{H}'\mathbf{H}\mathbf{Y} + \mathbf{Y}'\mathbf{M}'\mathbf{M}\mathbf{Y} = \mathbf{Y}'\mathbf{H}\mathbf{Y} + \mathbf{Y}'\mathbf{M}\mathbf{Y}$$

If $\mathbf{X}'\mathbf{X}$ is deficient in rank and a generalized inverse is used to solve the normal equations, then you work instead with the projection matrices $\mathbf{H} = \mathbf{X}(\mathbf{X}'\mathbf{X})^- \mathbf{X}'$. Note that if \mathbf{G} is a generalized inverse of $\mathbf{X}'\mathbf{X}$, then $\mathbf{X}\mathbf{G}\mathbf{X}'$, and hence also \mathbf{H} and \mathbf{M} , are invariant to the choice of \mathbf{G} .

The matrix \mathbf{H} is sometimes referred to as the “hat” matrix because when you premultiply the vector of observations with \mathbf{H} , you produce the fitted values, which are commonly denoted by placing a “hat” over the \mathbf{Y} vector, $\hat{\mathbf{Y}} = \mathbf{H}\mathbf{Y}$.

The term $\mathbf{Y}'\mathbf{Y}$ is the uncorrected total sum of squares (SST) of the linear model, $\mathbf{Y}'\mathbf{M}\mathbf{Y}$ is the error (residual) sum of squares (SSR), and $\mathbf{Y}'\mathbf{H}\mathbf{Y}$ is the uncorrected model sum of squares. This leads to the analysis of variance table shown in Table 3.2.

Table 3.2 Analysis of Variance with Uncorrected Sums of Squares

Source	df	Sum of Squares
Model	rank(\mathbf{X})	SSM = $\mathbf{Y}'\mathbf{H}\mathbf{Y} = \hat{\boldsymbol{\beta}}'\mathbf{X}'\mathbf{Y}$
Residual	$n - \text{rank}(\mathbf{X})$	SSR = $\mathbf{Y}'\mathbf{M}\mathbf{Y} = \mathbf{Y}'\mathbf{Y} - \hat{\boldsymbol{\beta}}'\mathbf{X}'\mathbf{Y} = \sum_{i=1}^n (Y_i - \hat{Y}_i)^2$
Uncorr. Total	n	SST = $\mathbf{Y}'\mathbf{Y} = \sum_{i=1}^n Y_i^2$

When the model contains an intercept term, then the analysis of variance is usually corrected for the mean, as shown in Table 3.3.

Table 3.3 Analysis of Variance with Corrected Sums of Squares

Source	df	Sum of Squares
Model	$\text{rank}(\mathbf{X}) - 1$	$\text{SSM}_c = \hat{\boldsymbol{\beta}}' \mathbf{X}' \mathbf{Y} - n \bar{Y}^2 = \sum_{i=1}^n (\hat{Y}_i - \bar{Y})^2$
Residual	$n - \text{rank}(\mathbf{X})$	$\text{SSR} = \mathbf{Y}' \mathbf{M} \mathbf{Y} = \mathbf{Y}' \mathbf{Y} - \hat{\boldsymbol{\beta}}' \mathbf{X}' \mathbf{Y} = \sum_{i=1}^n (Y_i - \hat{Y}_i)^2$
Corrected Total	$n - 1$	$\text{SST}_c = \mathbf{Y}' \mathbf{Y} - n \bar{Y}^2 = \sum_{i=1}^n (Y_i - \bar{Y})^2$

The *coefficient of determination*, also called the R-square statistic, measures the proportion of the total variation explained by the linear model. In models with intercept, it is defined as the ratio

$$R^2 = 1 - \frac{\text{SSR}}{\text{SST}_c} = 1 - \frac{\sum_{i=1}^n (Y_i - \hat{Y}_i)^2}{\sum_{i=1}^n (Y_i - \bar{Y})^2}$$

In models without intercept, the R-square statistic is a ratio of the uncorrected sums of squares

$$R^2 = 1 - \frac{\text{SSR}}{\text{SST}} = 1 - \frac{\sum_{i=1}^n (Y_i - \hat{Y}_i)^2}{\sum_{i=1}^n Y_i^2}$$

Estimating the Error Variance

The least squares principle does not provide for a parameter estimator for σ^2 . The usual approach is to use a method-of-moments estimator that is based on the sum of squared residuals. If the model is correct, then the mean square for error, defined to be SSR divided by its degrees of freedom,

$$\begin{aligned} \hat{\sigma}^2 &= \frac{1}{n - \text{rank}(\mathbf{X})} (\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}})' (\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}}) \\ &= \text{SSR} / (n - \text{rank}(\mathbf{X})) \end{aligned}$$

is an unbiased estimator of σ^2 .

Maximum Likelihood Estimation

To estimate the parameters in a linear model with mean function $E[\mathbf{Y}] = \mathbf{X}\boldsymbol{\beta}$ by maximum likelihood, you need to specify the distribution of the response vector \mathbf{Y} . In the linear model with a continuous response variable, it is commonly assumed that the response is normally distributed. In that case, the estimation problem is completely defined by specifying the mean and variance of \mathbf{Y} in addition to the normality assumption. The model can be written as $\mathbf{Y} \sim N(\mathbf{X}\boldsymbol{\beta}, \sigma^2 \mathbf{I})$, where the notation $N(\mathbf{a}, \mathbf{V})$ indicates a multivariate normal distribution with mean vector \mathbf{a} and variance matrix \mathbf{V} . The log likelihood for \mathbf{Y} then can be written as

$$l(\boldsymbol{\beta}, \sigma^2; \mathbf{y}) = -\frac{n}{2} \log\{2\pi\} - \frac{n}{2} \log\{\sigma^2\} - \frac{1}{2\sigma^2} (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})' (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$$

This function is maximized in $\boldsymbol{\beta}$ when the sum of squares $(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})' (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$ is minimized. The maximum likelihood estimator of $\boldsymbol{\beta}$ is thus identical to the ordinary least squares estimator. To maximize $l(\boldsymbol{\beta}, \sigma^2; \mathbf{y})$ with respect to σ^2 , note that

$$\frac{\partial l(\boldsymbol{\beta}, \sigma^2; \mathbf{y})}{\partial \sigma^2} = -\frac{n}{2\sigma^2} + \frac{1}{2\sigma^4} (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})' (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$$

Hence the MLE of σ^2 is the estimator

$$\begin{aligned}\hat{\sigma}_M^2 &= \frac{1}{n} (\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}})' (\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}}) \\ &= \text{SSR}/n\end{aligned}$$

This is a biased estimator of σ^2 , with a bias that decreases with n .

Estimable Functions

A function $\mathbf{L}\boldsymbol{\beta}$ is said to be estimable if there exists a linear combination of the expected value of \mathbf{Y} , such as $\mathbf{K}E[\mathbf{Y}]$, that equals $\mathbf{L}\boldsymbol{\beta}$. Since $E[\mathbf{Y}] = \mathbf{X}\boldsymbol{\beta}$, the definition of estimability implies that $\mathbf{L}\boldsymbol{\beta}$ is estimable if there is a matrix \mathbf{K} such that $\mathbf{L} = \mathbf{K}\mathbf{X}$. Another way of looking at this result is that the rows of \mathbf{X} form a generating set from which all estimable functions can be constructed.

The concept of estimability of functions is important in the theory and application of linear models because hypotheses of interest are often expressed as linear combinations of the parameter estimates (for example, hypotheses of equality between parameters, $\beta_1 = \beta_2 \Leftrightarrow \beta_1 - \beta_2 = 0$). Since estimability is not related to the particular value of the parameter estimate, but to the row space of \mathbf{X} , you can test only hypotheses that consist of estimable functions. Further, because estimability is not related to the value of $\boldsymbol{\beta}$ (Searle 1971, p. 181), the choice of the generalized inverse in a situation with rank-deficient $\mathbf{X}'\mathbf{X}$ matrix is immaterial, since

$$\mathbf{L}\hat{\boldsymbol{\beta}} = \mathbf{K}\mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{K}\mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'\mathbf{Y}$$

where $\mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}$ is invariant to the choice of generalized inverse.

$\mathbf{L}\boldsymbol{\beta}$ is estimable if and only if $\mathbf{L}(\mathbf{X}'\mathbf{X})^{-}(\mathbf{X}'\mathbf{X}) = \mathbf{L}$ (see, for example, Searle 1971, p. 185). If \mathbf{X} is of full rank, then the *Hermite* matrix $(\mathbf{X}'\mathbf{X})^{-}(\mathbf{X}'\mathbf{X})$ is the identity, which implies that all linear functions are estimable in the full-rank case.

See Chapter 15, “The Four Types of Estimable Functions,” for many details about the various forms of estimable functions in SAS/STAT.

Test of Hypotheses

Consider a general linear hypothesis of the form $H: \mathbf{L}\boldsymbol{\beta} = \mathbf{d}$, where \mathbf{L} is a $(k \times p)$ matrix. It is assumed that \mathbf{d} is such that this hypothesis is linearly consistent—that is, that there exists *some* $\boldsymbol{\beta}$ for which $\mathbf{L}\boldsymbol{\beta} = \mathbf{d}$. This is always the case if \mathbf{d} is in the column space of \mathbf{L} , if \mathbf{L} has full row rank, or if $\mathbf{d} = \mathbf{0}$; the latter is the most common case. Since many linear models have a rank-deficient \mathbf{X} matrix, the question arises whether the hypothesis is testable. The idea of testability of a hypothesis is—not surprisingly—connected to the concept of estimability as introduced previously. The hypothesis $H: \mathbf{L}\boldsymbol{\beta} = \mathbf{d}$ is testable if it consists of estimable functions.

There are two important approaches to testing hypotheses in statistical applications—the reduction principle and the linear inference approach. The reduction principle states that the validity of the hypothesis can be inferred by comparing a suitably chosen summary statistic between the model at hand and a reduced model in which the constraint $\mathbf{L}\boldsymbol{\beta} = \mathbf{d}$ is imposed. The linear inference approach relies on the fact that $\hat{\boldsymbol{\beta}}$ is an estimator of $\boldsymbol{\beta}$ and its stochastic properties are known, at least approximately. A test statistic can then be formed using $\hat{\boldsymbol{\beta}}$, and its behavior under the restriction $\mathbf{L}\boldsymbol{\beta} = \mathbf{d}$ can be ascertained.

The two principles lead to identical results in certain—for example, least squares estimation in the classical linear model. In more complex situations the two approaches lead to similar but not identical results. This is the case, for example, when weights or unequal variances are involved, or when $\hat{\boldsymbol{\beta}}$ is a nonlinear estimator.

Reduction Tests

The two main reduction principles are the sum of squares reduction test and the likelihood ratio test. The test statistic in the former is proportional to the difference of the residual sum of squares between the reduced model and the full model. The test statistic in the likelihood ratio test is proportional to the difference of the log likelihoods between the full and reduced models. To fix these ideas, suppose that you are fitting the model $\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$, where $\boldsymbol{\epsilon} \sim N(\mathbf{0}, \sigma^2\mathbf{I})$. Suppose that SSR denotes the residual sum of squares in this model and that SSR_H is the residual sum of squares in the model for which $\mathbf{L}\boldsymbol{\beta} = \mathbf{d}$ holds. Then under the hypothesis the ratio

$$(SSR_H - SSR)/\sigma^2$$

follows a chi-square distribution with degrees of freedom equal to the rank of \mathbf{L} . Maybe surprisingly, the residual sum of squares in the full model is distributed independently of this quantity, so that under the hypothesis,

$$F = \frac{(SSR_H - SSR)/\text{rank}(\mathbf{L})}{SSR/(n - \text{rank}(\mathbf{X}))}$$

follows an F distribution with $\text{rank}(\mathbf{L})$ numerator and $n - \text{rank}(\mathbf{X})$ denominator degrees of freedom. Note that the quantity in the denominator of the F statistic is a particular estimator of σ^2 —namely, the unbiased moment-based estimator that is customarily associated with least squares estimation. It is also the restricted maximum likelihood estimator of σ^2 if \mathbf{Y} is normally distributed.

In the case of the likelihood ratio test, suppose that $l(\widehat{\boldsymbol{\beta}}, \widehat{\sigma}^2; \mathbf{y})$ denotes the log likelihood evaluated at the ML estimators. Also suppose that $l(\widehat{\boldsymbol{\beta}}_H, \widehat{\sigma}_H^2; \mathbf{y})$ denotes the log likelihood in the model for which $\mathbf{L}\boldsymbol{\beta} = \mathbf{d}$ holds. Then under the hypothesis the statistic

$$\lambda = 2 \left(l(\widehat{\boldsymbol{\beta}}, \widehat{\sigma}^2; \mathbf{y}) - l(\widehat{\boldsymbol{\beta}}_H, \widehat{\sigma}_H^2; \mathbf{y}) \right)$$

follows approximately a chi-square distribution with degrees of freedom equal to the rank of \mathbf{L} . In the case of a normally distributed response, the log-likelihood function can be profiled with respect to $\boldsymbol{\beta}$. The resulting profile log likelihood is

$$l(\widehat{\sigma}^2; \mathbf{y}) = -\frac{n}{2} \log\{2\pi\} - \frac{n}{2} (\log\{\widehat{\sigma}^2\})$$

and the likelihood ratio test statistic becomes

$$\lambda = n (\log\{\widehat{\sigma}_H^2\} - \log\{\widehat{\sigma}^2\}) = n (\log\{SSR_H\} - \log\{SSR\}) = n (\log\{SSR_H/SSR\})$$

The preceding expressions show that, in the case of normally distributed data, both reduction principles lead to simple functions of the residual sums of squares in two models. As Pawitan (2001, p. 151) puts it, there is, however, an important difference not in the computations but in the statistical content. The least squares principle, where sum of squares reduction tests are widely used, does not require a distributional specification. Assumptions about the distribution of the data are added to provide a framework for confirmatory inferences, such as the testing of hypotheses. This framework stems directly from the assumption about the data's distribution, or from the sampling distribution of the least squares estimators. The likelihood principle, on the other hand, requires a distributional specification at the outset. Inference about the parameters is implicit in the model; it is the result of further *computations* following the estimation of the parameters. In the least squares framework, inference about the parameters is the result of further *assumptions*.

Linear Inference

The principle of linear inference is to formulate a test statistic for $H: \mathbf{L}\boldsymbol{\beta} = \mathbf{d}$ that builds on the linearity of the hypothesis about $\boldsymbol{\beta}$. For many models that have linear components, the estimator $\mathbf{L}\widehat{\boldsymbol{\beta}}$ is also linear in \mathbf{Y} . It is then simple to establish the distributional properties of $\mathbf{L}\widehat{\boldsymbol{\beta}}$ based on the distributional assumptions about \mathbf{Y} or based on large-sample arguments. For example, $\widehat{\boldsymbol{\beta}}$ might be a nonlinear estimator, but it is known to asymptotically follow a normal distribution; this is the case in many nonlinear and generalized linear models.

If the sampling distribution or the asymptotic distribution of $\widehat{\boldsymbol{\beta}}$ is normal, then one can easily derive quadratic forms with known distributional properties. For example, if the random vector \mathbf{U} is distributed as $N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, then $\mathbf{U}'\mathbf{A}\mathbf{U}$ follows a chi-square distribution with $\text{rank}(\mathbf{A})$ degrees of freedom and noncentrality parameter $1/2\boldsymbol{\mu}'\mathbf{A}\boldsymbol{\mu}$, provided that $\mathbf{A}\boldsymbol{\Sigma}\mathbf{A}\boldsymbol{\Sigma} = \mathbf{A}\boldsymbol{\Sigma}$.

In the classical linear model, suppose that \mathbf{X} is deficient in rank and that $\widehat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'\mathbf{Y}$ is a solution to the normal equations. Then, if the errors are normally distributed,

$$\widehat{\boldsymbol{\beta}} \sim N((\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'\mathbf{X}\boldsymbol{\beta}, \sigma^2(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'\mathbf{X}(\mathbf{X}'\mathbf{X})^{-})$$

Because $H: \mathbf{L}\boldsymbol{\beta} = \mathbf{d}$ is testable, $\mathbf{L}\boldsymbol{\beta}$ is estimable, and thus $\mathbf{L}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'\mathbf{X} = \mathbf{L}$, as established in the previous section. Hence,

$$\mathbf{L}\widehat{\boldsymbol{\beta}} \sim N(\mathbf{L}\boldsymbol{\beta}, \sigma^2\mathbf{L}(\mathbf{X}'\mathbf{X})^{-}\mathbf{L}')$$

The conditions for a chi-square distribution of the quadratic form

$$(\mathbf{L}\widehat{\boldsymbol{\beta}} - \mathbf{d})'(\mathbf{L}(\mathbf{X}'\mathbf{X})^{-}\mathbf{L}')^{-}(\mathbf{L}\widehat{\boldsymbol{\beta}} - \mathbf{d})$$

are thus met, provided that

$$(\mathbf{L}(\mathbf{X}'\mathbf{X})^{-}\mathbf{L}')^{-}\mathbf{L}(\mathbf{X}'\mathbf{X})^{-}\mathbf{L}'(\mathbf{L}(\mathbf{X}'\mathbf{X})^{-}\mathbf{L}')^{-}\mathbf{L}(\mathbf{X}'\mathbf{X})^{-}\mathbf{L}' = (\mathbf{L}(\mathbf{X}'\mathbf{X})^{-}\mathbf{L}')^{-}\mathbf{L}(\mathbf{X}'\mathbf{X})^{-}\mathbf{L}'$$

This condition is obviously met if $\mathbf{L}(\mathbf{X}'\mathbf{X})^{-}\mathbf{L}'$ is of full rank. The condition is also met if $\mathbf{L}(\mathbf{X}'\mathbf{X})^{-}\mathbf{L}'^{-}$ is a reflexive inverse (a g_2 -inverse) of $\mathbf{L}(\mathbf{X}'\mathbf{X})^{-}\mathbf{L}'$.

The test statistic to test the linear hypothesis $H: \mathbf{L}\boldsymbol{\beta} = \mathbf{d}$ is thus

$$F = \frac{(\mathbf{L}\widehat{\boldsymbol{\beta}} - \mathbf{d})'(\mathbf{L}(\mathbf{X}'\mathbf{X})^{-}\mathbf{L}')^{-}(\mathbf{L}\widehat{\boldsymbol{\beta}} - \mathbf{d})/\text{rank}(\mathbf{L})}{\text{SSR}/(n - \text{rank}(\mathbf{X}))}$$

and it follows an F distribution with $\text{rank}(\mathbf{L})$ numerator and $n - \text{rank}(\mathbf{X})$ denominator degrees of freedom under the hypothesis.

This test statistic looks very similar to the F statistic for the sum of squares reduction test. This is no accident. If the model is linear and parameters are estimated by ordinary least squares, then you can show that the quadratic form $(\mathbf{L}\widehat{\boldsymbol{\beta}} - \mathbf{d})'(\mathbf{L}(\mathbf{X}'\mathbf{X})^{-}\mathbf{L}')^{-}(\mathbf{L}\widehat{\boldsymbol{\beta}} - \mathbf{d})$ equals the differences in the residual sum of squares, $\text{SSR}_H - \text{SSR}$, where SSR_H is obtained as the residual sum of squares from OLS estimation in a model that satisfies $\mathbf{L}\boldsymbol{\beta} = \mathbf{d}$. However, this correspondence between the two test formulations does not apply when a different estimation principle is used. For example, assume that $\boldsymbol{\epsilon} \sim N(\mathbf{0}, \mathbf{V})$ and that $\boldsymbol{\beta}$ is estimated by generalized least squares:

$$\widehat{\boldsymbol{\beta}}_g = (\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-}\mathbf{X}'\mathbf{V}^{-1}\mathbf{Y}$$

The construction of \mathbf{L} matrices associated with hypotheses in SAS/STAT software is frequently based on the properties of the \mathbf{X} matrix, not of $\mathbf{X}'\mathbf{V}^{-1}\mathbf{X}$. In other words, the construction of the \mathbf{L} matrix is governed

only by the design. A sum of squares reduction test for $H: \mathbf{L}\boldsymbol{\beta} = \mathbf{0}$ that uses the generalized residual sum of squares $(\mathbf{Y} - \widehat{\boldsymbol{\beta}}_g)' \mathbf{V}^{-1} (\mathbf{Y} - \widehat{\boldsymbol{\beta}}_g)$ is not identical to a linear hypothesis test with the statistic

$$F^* = \frac{\widehat{\boldsymbol{\beta}}_g' \mathbf{L}' (\mathbf{L} (\mathbf{X}' \mathbf{V}^{-1} \mathbf{X})^{-1} \mathbf{L}')^{-1} \mathbf{L} \widehat{\boldsymbol{\beta}}_g}{\text{rank}(\mathbf{L})}$$

Furthermore, \mathbf{V} is usually unknown and must be estimated as well. The estimate for \mathbf{V} depends on the model, and imposing a constraint on the model would change the estimate. The asymptotic distribution of the statistic F^* is a chi-square distribution. However, in practical applications the F distribution with $\text{rank}(\mathbf{L})$ numerator and ν denominator degrees of freedom is often used because it provides a better approximation to the sampling distribution of F^* in finite samples. The computation of the denominator degrees of freedom ν , however, is a matter of considerable discussion. A number of methods have been proposed and are implemented in various forms in SAS/STAT (see, for example, the degrees-of-freedom methods in the MIXED and GLIMMIX procedures).

Residual Analysis

The model errors $\boldsymbol{\epsilon} = \mathbf{Y} - \mathbf{X}\boldsymbol{\beta}$ are unobservable. Yet important features of the statistical model are connected to them, such as the distribution of the data, the correlation among observations, and the constancy of variance. It is customary to diagnose and investigate features of the model errors through the fitted residuals $\widehat{\boldsymbol{\epsilon}} = \mathbf{Y} - \widehat{\mathbf{Y}} = \mathbf{Y} - \mathbf{H}\mathbf{Y} = \mathbf{M}\mathbf{Y}$. These residuals are projections of the data onto the null space of \mathbf{X} and are also referred to as the “raw” residuals to contrast them with other forms of residuals that are transformations of $\widehat{\boldsymbol{\epsilon}}$. For the classical linear model, the statistical properties of $\widehat{\boldsymbol{\epsilon}}$ are affected by the features of that projection and can be summarized as follows:

$$\begin{aligned} E[\widehat{\boldsymbol{\epsilon}}] &= \mathbf{0} \\ \text{Var}[\widehat{\boldsymbol{\epsilon}}] &= \sigma^2 \mathbf{M} \\ \text{rank}(\mathbf{M}) &= n - \text{rank}(\mathbf{X}) \end{aligned}$$

Furthermore, if $\boldsymbol{\epsilon} \sim N(\mathbf{0}, \sigma^2 \mathbf{I})$, then $\widehat{\boldsymbol{\epsilon}} \sim N(\mathbf{0}, \sigma^2 \mathbf{M})$.

Because $\mathbf{M} = \mathbf{I} - \mathbf{H}$, and the “hat” matrix \mathbf{H} satisfies $\partial \widehat{\mathbf{Y}} / \partial \mathbf{Y}$, the hat matrix is also the leverage matrix of the model. If h_{ii} denotes the i th diagonal element of \mathbf{H} (the leverage of observation i), then the leverages are bounded in a model with intercept, $1/n \leq h_{ii} \leq 1$. Consequently, the variance of a raw residual is less than that of an observation: $\text{Var}[\widehat{\epsilon}_i] = \sigma^2(1 - h_{ii}) < \sigma^2$. In applications where the variability of the data is estimated from fitted residuals, the estimate is invariably biased low. An example is the computation of an empirical semivariogram based on fitted (detrended) residuals.

More important, the diagonal entries of \mathbf{H} are not necessarily identical; the residuals are heteroscedastic. The “hat” matrix is also not a diagonal matrix; the residuals are correlated. In summary, the only property that the fitted residuals $\widehat{\boldsymbol{\epsilon}}$ share with the model errors is a zero mean. It is thus commonplace to use transformations of the fitted residuals for diagnostic purposes.

Raw and Studentized Residuals

A *standardized* residual is a raw residual that is divided by its standard deviation:

$$\widehat{\epsilon}_i^* = \frac{Y_i - \widehat{Y}_i}{\sqrt{\text{Var}[Y_i - \widehat{Y}_i]}} = \frac{\widehat{\epsilon}_i}{\sqrt{\sigma^2(1 - h_{ii})}}$$

Because σ^2 is unknown, residual standardization is usually not practical. A *studentized* residual is a raw residual that is divided by its estimated standard deviation. If the estimate of the standard deviation is based on the same data that were used in fitting the model, the residual is also called an *internally studentized* residual:

$$\hat{\epsilon}_{is} = \frac{Y_i - \hat{Y}_i}{\sqrt{\widehat{\text{Var}}[Y_i - \hat{Y}_i]}} = \frac{\hat{\epsilon}_i}{\sqrt{\hat{\sigma}^2(1 - h_{ii})}}$$

If the estimate of the residual's variance does not involve the i th observation, it is called an *externally studentized* residual. Suppose that $\hat{\sigma}_{-i}^2$ denotes the estimate of the residual variance obtained without the i th observation; then the externally studentized residual is

$$\hat{\epsilon}_{ir} = \frac{\hat{\epsilon}_i}{\sqrt{\hat{\sigma}_{-i}^2(1 - h_{ii})}}$$

Scaled Residuals

A scaled residual is simply a raw residual divided by a scalar quantity that is not an estimate of the variance of the residual. For example, residuals divided by the standard deviation of the response variable are scaled and referred to as Pearson or Pearson-type residuals:

$$\hat{\epsilon}_{ic} = \frac{Y_i - \hat{Y}_i}{\sqrt{\widehat{\text{Var}}[Y_i]}}$$

In generalized linear models, where the variance of an observation is a function of the mean μ and possibly of an extra scale parameter, $\text{Var}[Y] = a(\mu)\phi$, the Pearson residual is

$$\hat{\epsilon}_{iP} = \frac{Y_i - \hat{\mu}_i}{\sqrt{a(\hat{\mu}_i)}}$$

because the sum of the squared Pearson residuals equals the Pearson X^2 statistic:

$$X^2 = \sum_{i=1}^n \hat{\epsilon}_{iP}^2$$

When the scale parameter ϕ participates in the scaling, the residual is also referred to as a Pearson-type residual:

$$\hat{\epsilon}_{iP} = \frac{Y_i - \hat{\mu}_i}{\sqrt{a(\hat{\mu}_i)\phi}}$$

Other Residuals

You might encounter other residuals in SAS/STAT software. A “leave-one-out” residual is the difference between the observed value and the residual obtained from fitting a model in which the observation in question did not participate. If \hat{Y}_i is the predicted value of the i th observation and $\hat{Y}_{i,-i}$ is the predicted value if Y_i is removed from the analysis, then the “leave-one-out” residual is

$$\hat{\epsilon}_{i,-i} = Y_i - \hat{Y}_{i,-i}$$

Since the sum of the squared “leave-one-out” residuals is the PRESS statistic (prediction sum of squares; Allen 1974), $\widehat{\epsilon}_{i,-i}$ is also called the PRESS residual. The concept of the PRESS residual can be generalized if the deletion residual can be based on the removal of sets of observations. In the classical linear model, the PRESS residual for case deletion has a particularly simple form:

$$\widehat{\epsilon}_{i,-i} = Y_i - \widehat{Y}_{i,-i} = \frac{\widehat{\epsilon}_i}{1 - h_{ii}}$$

That is, the PRESS residual is simply a scaled form of the raw residual, where the scaling factor is a function of the leverage of the observation.

When data are correlated, $\text{Var}[\mathbf{Y}] = \mathbf{V}$, you can scale the vector of residuals rather than scale each residual separately. This takes the covariances among the observations into account. This form of scaling is accomplished by forming the Cholesky root $\mathbf{C}'\mathbf{C} = \mathbf{V}$, where \mathbf{C}' is a lower-triangular matrix. Then $\mathbf{C}'^{-1}\mathbf{Y}$ is a vector of uncorrelated variables with unit variance. The Cholesky residuals in the model $\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$ are

$$\widehat{\boldsymbol{\epsilon}}_{\mathbf{C}} = \mathbf{C}'^{-1}(\mathbf{Y} - \mathbf{X}\widehat{\boldsymbol{\beta}})$$

In generalized linear models, the fit of a model can be measured by the scaled deviance statistic D^* . It measures the difference between the log likelihood under the model and the maximum log likelihood that is achievable. In models with a scale parameter ϕ , the deviance is $D = \phi \times D^* = \sum_{i=1}^n d_i$. The deviance residuals are the signed square roots of the contributions to the deviance statistic:

$$\widehat{\epsilon}_{id} = \text{sign}\{y_i - \widehat{\mu}_i\} \sqrt{d_i}$$

Sweep Operator

The sweep operator (Goodnight 1979) is closely related to Gauss-Jordan elimination and the Forward Doolittle procedure. The fact that a sweep operation can produce a generalized inverse by in-place mapping with minimal storage and that its application invariably leads to some form of matrix inversion is important, but this observation does not do justice to the pervasive relevance of sweeping to statistical computing. In this section the sweep operator is discussed as a conceptual tool for further insight into linear model operations. Consider the nonnegative definite, symmetric, partitioned matrix

$$\mathbf{A} = \begin{bmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}'_{12} & \mathbf{A}_{22} \end{bmatrix}$$

Sweeping a matrix consists of performing a series of row operations akin to Gauss-Jordan elimination. Basic row operations are the multiplication of a row by a constant and the addition of a multiple of one row to another. The sweep operator restricts row operations to pivots on the diagonal elements of a matrix; further details about the elementary operations can be found in Goodnight (1979). The process of sweeping the matrix \mathbf{A} on its leading partition is denoted as $\text{Sweep}(\mathbf{A}, \mathbf{A}_{11})$ and leads to

$$\text{Sweep}(\mathbf{A}, \mathbf{A}_{11}) = \begin{bmatrix} \mathbf{A}_{11}^- & \mathbf{A}_{11}^- \mathbf{A}_{12} \\ -\mathbf{A}'_{12} \mathbf{A}_{11}^- & \mathbf{A}_{22} - \mathbf{A}'_{12} \mathbf{A}_{11}^- \mathbf{A}_{12} \end{bmatrix}$$

If the k th row and column are set to zero when the pivot is zero (or in practice, less than some singularity tolerance), the generalized inverse in the leading position of the swept matrix is a reflexive, g_2 -inverse. Suppose that the crossproduct matrix of the linear model is augmented with a “Y-border” as follows:

$$\mathbf{C} = \begin{bmatrix} \mathbf{X}'\mathbf{X} & \mathbf{X}'\mathbf{Y} \\ \mathbf{Y}'\mathbf{X} & \mathbf{Y}'\mathbf{Y} \end{bmatrix}$$

Then the result of sweeping on the rows of \mathbf{X} is

$$\begin{aligned} \text{Sweep}(\mathbf{C}, \mathbf{X}) &= \begin{bmatrix} (\mathbf{X}'\mathbf{X})^{-} & (\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'\mathbf{Y} \\ -\mathbf{Y}'\mathbf{X}(\mathbf{X}'\mathbf{X})^{-} & \mathbf{Y}'\mathbf{Y} - \mathbf{Y}'\mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'\mathbf{Y} \end{bmatrix} \\ &= \begin{bmatrix} (\mathbf{X}'\mathbf{X})^{-} & \hat{\boldsymbol{\beta}} \\ -\hat{\boldsymbol{\beta}} & \mathbf{Y}'\mathbf{M}\mathbf{Y} \end{bmatrix} = \begin{bmatrix} (\mathbf{X}'\mathbf{X})^{-} & \hat{\boldsymbol{\beta}} \\ -\hat{\boldsymbol{\beta}} & \text{SSR} \end{bmatrix} \end{aligned}$$

The “Y-border” has been transformed into the least squares solution and the residual sum of squares.

Partial sweeps are common in model selection. Suppose that the \mathbf{X} matrix is partitioned as $[\mathbf{X}_1 \ \mathbf{X}_2]$, and consider the augmented crossproduct matrix

$$\mathbf{C} = \begin{bmatrix} \mathbf{X}'_1\mathbf{X}_1 & \mathbf{X}'_1\mathbf{X}_2 & \mathbf{X}'_1\mathbf{Y} \\ \mathbf{X}'_2\mathbf{X}_1 & \mathbf{X}'_2\mathbf{X}_2 & \mathbf{X}'_2\mathbf{Y} \\ \mathbf{Y}'\mathbf{X}_1 & \mathbf{Y}'\mathbf{X}_2 & \mathbf{Y}'\mathbf{Y} \end{bmatrix}$$

Sweeping on the \mathbf{X}_1 partition yields

$$\text{Sweep}(\mathbf{C}, \mathbf{X}_1) = \begin{bmatrix} (\mathbf{X}'_1\mathbf{X}_1)^{-} & (\mathbf{X}'_1\mathbf{X}_1)^{-}\mathbf{X}'_1\mathbf{X}_2 & (\mathbf{X}'_1\mathbf{X}_1)^{-}\mathbf{X}'_1\mathbf{Y} \\ -\mathbf{X}'_2\mathbf{X}_1(\mathbf{X}'_1\mathbf{X}_1)^{-} & \mathbf{X}'_2\mathbf{M}_1\mathbf{X}_2 & \mathbf{X}'_2\mathbf{M}_1\mathbf{Y} \\ \mathbf{Y}'\mathbf{X}_1(\mathbf{X}'_1\mathbf{X}_1)^{-} & \mathbf{Y}'\mathbf{M}_1\mathbf{X}_2 & \mathbf{Y}'\mathbf{M}_1\mathbf{Y} \end{bmatrix}$$

where $\mathbf{M}_1 = \mathbf{I} - \mathbf{X}_1(\mathbf{X}'_1\mathbf{X}_1)^{-}\mathbf{X}'_1$. The entries in the first row of this partition are the generalized inverse of $\mathbf{X}'_1\mathbf{X}_1$, the coefficients for regressing \mathbf{X}_2 on \mathbf{X}_1 , and the coefficients for regressing \mathbf{Y} on \mathbf{X}_1 . The diagonal entries $\mathbf{X}'_2\mathbf{M}_1\mathbf{X}_2$ and $\mathbf{Y}'\mathbf{M}_1\mathbf{Y}$ are the sum of squares and crossproduct matrices for regressing \mathbf{X}_2 on \mathbf{X}_1 and for regressing \mathbf{Y} on \mathbf{X}_1 , respectively. As you continue to sweep the matrix, the last cell in the partition contains the residual sum of square of a model in which \mathbf{Y} is regressed on all columns swept up to that point.

The sweep operator is not only useful to conceptualize the computation of least squares solutions, Type I and Type II sums of squares, and generalized inverses. It can also be used to obtain other statistical information. For example, adding the logarithms of the pivots of the rows that are swept yields the log determinant of the matrix.

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Chapter 4

Introduction to Regression Procedures

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Overview: Regression Procedures

This chapter provides an overview of procedures in SAS/STAT software that perform regression analysis. The REG procedure provides the most extensive analysis capabilities for linear regression models involving individual numeric independent variables. Many other procedures can fit such models, but they are designed

for more general models, such as robust regression, generalized linear regression, nonlinear regression, nonparametric regression, regression modeling of survey data, regression modeling of survival data, and regression modeling of transformed variables.

The aim of this chapter is to provide a brief road map and delineation of the various SAS/STAT procedures that can fit regression models. Some of the procedures that fall into this category are the CATMOD, GAM, GENMOD, GLIMMIX, GLM, LIFEREG, LOESS, LOGISTIC, MIXED, NLIN, NLMIXED, ORTHOREG, PHREG, PLS, PROBIT, REG, ROBUSTREG, RSREG, SURVEYLOGISTIC, SURVEYPHREG, SURVEYREG, and TRANSREG procedures.

This chapter also briefly mentions several procedures in SAS/ETS software.

Introduction

Recall from Chapter 3, “[Introduction to Statistical Modeling with SAS/STAT Software](#),” that the general regression problem is to model the mean of a random vector \mathbf{Y} as a function of a parameters and covariates in a statistical model. The many forms of regression models have their origin in the characteristics of the response variable (discrete or continuous, normal or nonnormal distributed), assumptions about the form of the model (linear, nonlinear, or generalized linear), assumptions about the data-generating mechanism (survey, observational, or experimental data), and estimation principles. The following procedures, listed in alphabetical order, perform at least one type of regression analysis.

CATMOD	analyzes data that can be represented by a contingency table. PROC CATMOD fits linear models to functions of response frequencies, and it can be used for linear and logistic regression. See Chapter 8, “ Introduction to Categorical Data Analysis Procedures ,” and Chapter 30, “ The CATMOD Procedure ,” for more information.
GAM	fits generalized additive models. The models fitted with the GAM procedure are nonparametric in that the usual assumption of a linear predictor is relaxed. The name stems from the fact that the models consist of additive, smooth functions in the regression variables. The GAM procedure can fit additive models to nonnormal data. See Chapter 39, “ The GAM Procedure ,” for more information.
GENMOD	fits generalized linear models. PROC GENMOD is especially suited for responses with discrete outcomes, and it performs logistic regression and Poisson regression in addition to fitting generalized estimating equations for repeated measures data. Bayesian analysis capabilities for generalized linear models are also available with the GENMOD procedure. See Chapter 8, “ Introduction to Categorical Data Analysis Procedures ,” and Chapter 40, “ The GENMOD Procedure ,” for more information.
GLIMMIX	fits generalized linear mixed models by likelihood-based methods. In addition to many other analyses, PROC GLIMMIX can perform simple, multiple, polynomial, and weighted regression. The GLIMMIX procedure can also fit linear mixed models and models without random effects. See Chapter 41, “ The GLIMMIX Procedure ,” for more information.
GLM	uses the method of least squares to fit general linear models. In addition to many other analyses, PROC GLM can perform simple, multiple, polynomial, and weighted regression. PROC GLM has many of the same input/output capabilities as PROC REG, but it does not provide as many diagnostic tools or allow interactive changes in the model or

data. See Chapter 5, “[Introduction to Analysis of Variance Procedures](#),” and Chapter 42, “[The GLM Procedure](#),” for more information.

LIFEREG	fits parametric models to failure-time data that might be right-censored. These types of models are commonly used in survival analysis. See Chapter 14, “ Introduction to Survey Procedures ,” and Chapter 51, “ The LIFEREG Procedure ,” for more information.
LOESS	fits nonparametric models by using a local regression method. PROC LOESS is suitable for modeling regression surfaces where the underlying parametric form is unknown and where robustness in the presence of outliers is required. See Chapter 53, “ The LOESS Procedure ,” for more information.
LOGISTIC	fits logistic models for binomial and ordinal outcomes. PROC LOGISTIC provides a wide variety of model-building methods and computes numerous regression diagnostics. See Chapter 8, “ Introduction to Categorical Data Analysis Procedures ,” and Chapter 54, “ The LOGISTIC Procedure ,” for more information.
MIXED	fits linear mixed models by likelihood-based techniques. In addition to many other analyses, PROC MIXED can fit models without random effects; hence, the procedure can perform simple, multiple, polynomial, and weighted regression. See Chapter 59, “ The MIXED Procedure ,” for more information.
NLIN	fits general nonlinear regression models by the method of nonlinear least squares. Several different iterative methods are available. See Chapter 63, “ The NLIN Procedure ,” for more information.
NLMIXED	fits general nonlinear mixed regression models by the method of maximum likelihood. With the NLMIXED procedure you can specify a custom objective function for parameter estimation and fit models with or without random effects. See Chapter 64, “ The NLMIXED Procedure ,” for more information.
ORTHOREG	performs regression by using the Gentleman-Givens computational method. For ill-conditioned data, PROC ORTHOREG can produce more accurate parameter estimates than other procedures such as PROC GLM and PROC REG. See Chapter 66, “ The ORTHOREG Procedure ,” for more information.
PHREG	fits Cox proportional hazards regression models to survival data. See Chapter 67, “ The PHREG Procedure ,” for more information.
PLS	performs partial least squares regression, principal components regression, and reduced rank regression, with cross validation for the number of components. See Chapter 70, “ The PLS Procedure ,” for more information.
PROBIT	performs probit regression in addition to logistic regression and ordinal logistic regression. The PROBIT procedure is useful when the dependent variable is either dichotomous or polychotomous and the independent variables are continuous. See Chapter 75, “ The PROBIT Procedure ,” for more information.
QUANTREG	models the effects of covariates on the conditional quantiles of a response variable by means of quantile regression. See Chapter 77, “ The QUANTREG Procedure ,” for more information.
REG	performs linear regression with many diagnostic capabilities, selects models by using one of nine methods, produces scatter plots of raw data and statistics, highlights scatter plots to identify particular observations, and allows interactive changes in both the regression

model and the data that are used to fit the model. See Chapter 79, “The REG Procedure,” for more information.

- ROBUSTREG** performs robust regression by using Huber M estimation and high breakdown value estimation. PROC ROBUSTREG is suitable for detecting outliers and providing resistant (stable) results in the presence of outliers. See Chapter 80, “The ROBUSTREG Procedure,” for more information.
- RSREG** builds quadratic response-surface regression models. PROC RSREG analyzes the fitted response surface to determine the factor levels of optimum response and performs a ridge analysis to search for the region of optimum response. See Chapter 81, “The RSREG Procedure,” for more information.
- SURVEYLOGISTIC** fits logistic models for binary and ordinal outcomes to survey data by maximum likelihood. See Chapter 91, “The SURVEYLOGISTIC Procedure,” for more information.
- SURVEYPHREG** fits proportional hazards models for survey data by maximizing a partial pseudo-likelihood function that incorporates the sampling weights. The procedure provides design-based variance estimates, confidence intervals, and tests for the estimated proportional hazards regression coefficients. See Chapter 93, “The SURVEYPHREG Procedure,” for more information.
- SURVEYREG** fits linear regression models to survey data by generalized least squares by using elementwise regression. See Chapter 94, “The SURVEYREG Procedure,” for more information.
- TRANSREG** fits univariate and multivariate linear models, optionally with spline and other nonlinear transformations. Models include ordinary regression and ANOVA, multiple and multivariate regression, metric and nonmetric conjoint analysis, metric and nonmetric vector and ideal point preference mapping, redundancy analysis, canonical correlation, and response surface regression. See Chapter 97, “The TRANSREG Procedure,” for more information.

Several SAS/ETS procedures also perform regression. The following procedures are documented in the *SAS/ETS User's Guide*.

- AUTOREG** implements regression models that use time series data where the errors are autocorrelated. See Chapter 8, “The AUTOREG Procedure” (*SAS/ETS User's Guide*), for more details.
- COUNTREG** analyzes regression models in which the dependent variable takes nonnegative integer or count values. See Chapter 11, “The COUNTREG Procedure” (*SAS/ETS User's Guide*), for more details.
- MODEL** handles nonlinear simultaneous systems of equations, such as econometric models. See Chapter 19, “The MODEL Procedure” (*SAS/ETS User's Guide*), for more details.
- PANEL** analyzes a class of linear econometric models that commonly arise when time series and cross-sectional data are combined. See Chapter 20, “The PANEL Procedure” (*SAS/ETS User's Guide*), for more details.
- PDLREG** performs regression analysis with polynomial distributed lags. See Chapter 21, “The PDLREG Procedure” (*SAS/ETS User's Guide*), for more details.

SYSLIN handles linear simultaneous systems of equations, such as econometric models. See Chapter 29, “The SYSLIN Procedure” (*SAS/ETS User’s Guide*), for more details.

Introductory Example: Linear Regression

Regression analysis is the analysis of the relationship between a response or outcome variable and another set of variables. The relationship is expressed through a statistical model equation that predicts a *response variable* (also called a *dependent variable* or *criterion*) from a function of *regressor variables* (also called *independent variables*, *predictors*, *explanatory variables*, *factors*, or *carriers*) and *parameters*. In a linear regression model the predictor function is linear in the parameters (but not necessarily linear in the regressor variables). The parameters are estimated so that a measure of fit is optimized. For example, the equation for the i th observation might be

$$Y_i = \beta_0 + \beta_1 x_i + \epsilon_i$$

where Y_i is the response variable, x_i is a regressor variable, β_0 and β_1 are unknown parameters to be estimated, and ϵ_i is an error term. This model is termed the simple linear regression (SLR) model, because it is linear in β_0 and β_1 and contains only a single regressor variable.

Suppose you are using regression analysis to relate a child’s weight to a child’s height. One application of a regression model with the response variable Weight is to predict a child’s weight for a known height. Suppose you collect data by measuring heights and weights of 19 randomly selected schoolchildren. A simple linear regression model with the response variable weight and the regressor variable height can be written as

$$\text{Weight}_i = \beta_0 + \beta_1 \text{Height}_i + \epsilon_i$$

where

Weight _{<i>i</i>}	is the response variable for the <i>i</i> th child
Height _{<i>i</i>}	is the regressor variable for the <i>i</i> th child
β_0, β_1	are the unknown regression parameters
ϵ_i	is the unobservable random error associated with the <i>i</i> th observation

The data set `sashelp.class`, which is available in the `Sashelp` library, identifies the children and their observed heights (variable `Height`) and weights (variable `Weight`). The following statements perform the regression analysis:

```
ods graphics on;
proc reg data=sashelp.class;
  model Weight = Height;
run;
```

Figure 4.1 displays the default tabular output of the REG procedure for this model. Nineteen observations are read from the data set and all observations are used in the analysis. The estimates of the two regression parameters are $\hat{\beta}_0 = -143.02692$ and $\hat{\beta}_1 = 3.89903$. These estimates are obtained by the least squares principle. See the sections “Classical Estimation Principles” and “Linear Model Theory” in Chapter 3,

“Introduction to Statistical Modeling with SAS/STAT Software,” for details about the principle of least squares estimation and its role in linear model analysis. For a general discussion of the theory of least squares estimation of linear models and its application to regression and analysis of variance, refer to one of the applied regression texts, including Draper and Smith (1981); Daniel and Wood (1980); Johnston (1972); Weisberg (1985).

Figure 4.1 Regression for Weight and Height Data

The REG Procedure					
Model: MODEL1					
Dependent Variable: Weight					
Number of Observations Read		19			
Number of Observations Used		19			
Analysis of Variance					
Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	1	7193.24912	7193.24912	57.08	<.0001
Error	17	2142.48772	126.02869		
Corrected Total	18	9335.73684			
Root MSE		11.22625	R-Square	0.7705	
Dependent Mean		100.02632	Adj R-Sq	0.7570	
Coeff Var		11.22330			
Parameter Estimates					
Variable	DF	Parameter Estimate	Standard Error	t Value	Pr > t
Intercept	1	-143.02692	32.27459	-4.43	0.0004
Height	1	3.89903	0.51609	7.55	<.0001

Based on the least squares estimates shown in Figure 4.1, the fitted regression line relating height to weight is described by the equation

$$\widehat{\text{Weight}} = -143.02692 + 3.89903 \times \text{Height}$$

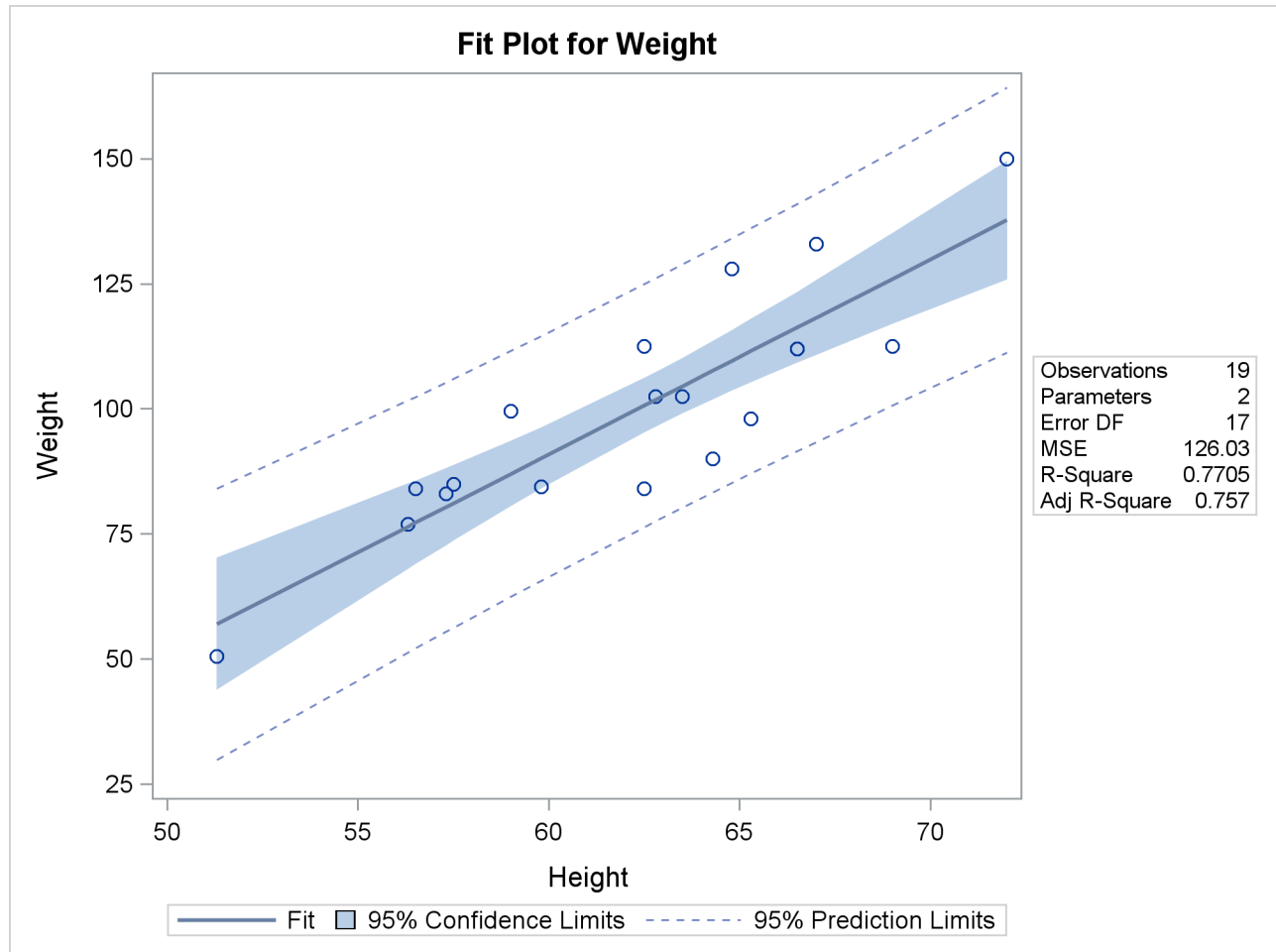
The “hat” notation is used to emphasize that $\widehat{\text{Weight}}$ is not one of the original observations but a value predicted under the regression model that has been fit to the data. At the least squares solution the residual sum of squares

$$\text{SSE} = \sum_{i=1}^{19} (\text{Weight}_i - \beta_0 - \beta_1 \text{Height}_i)^2$$

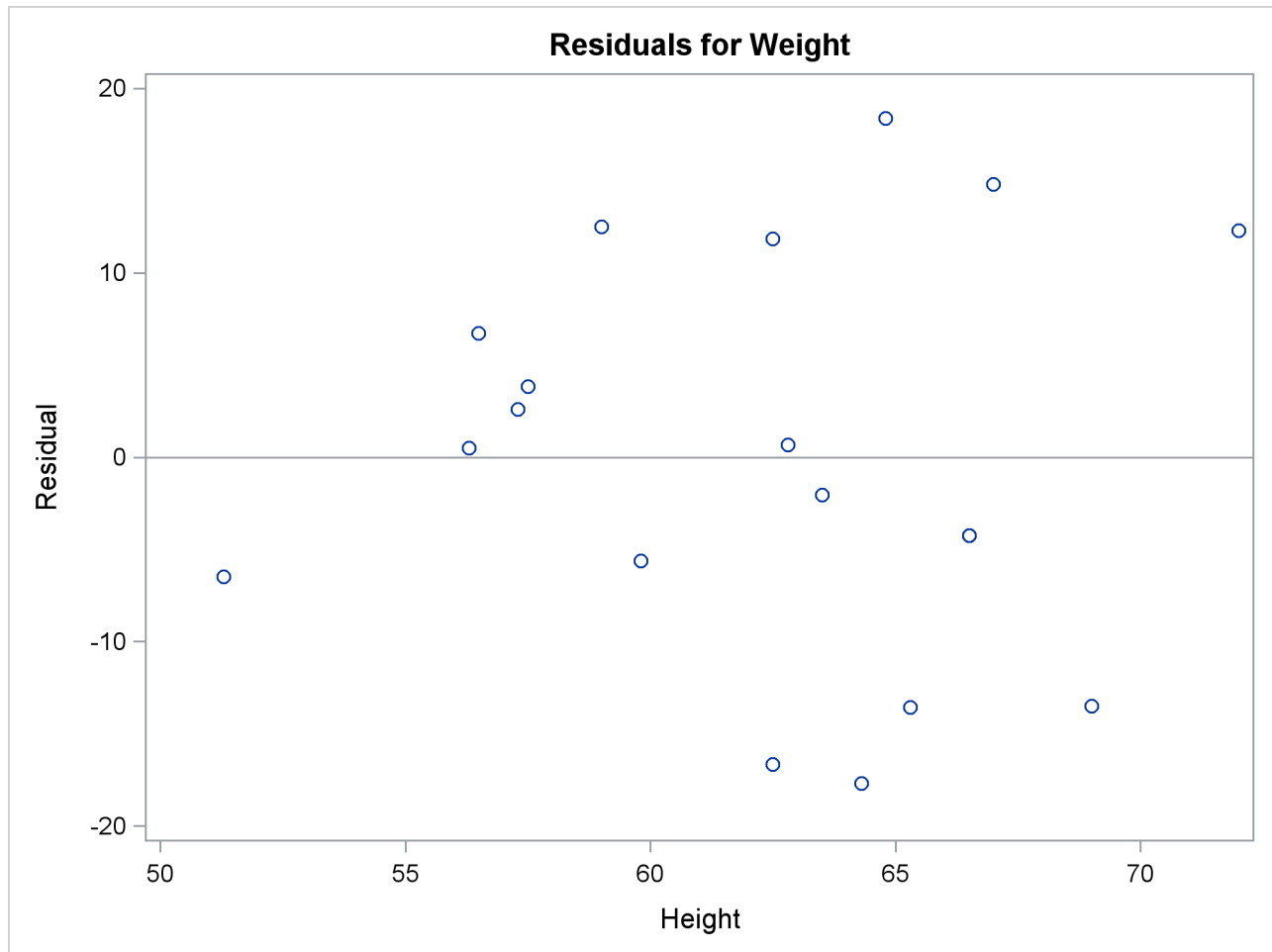
is minimized and the achieved criterion value is displayed in the analysis of variance table as the error sum of squares (2142.48772).

Figure 4.2 displays the fit plot produced by ODS Graphics. The fit plot shows the positive slope of the fitted line. The average weight of a child changes by $\hat{\beta}_1 = 3.89903$ units for each unit change in height. The 95% confidence limits in the fit plot are pointwise limits that cover the mean weight for a particular height with probability 0.95. The prediction limits, which are wider than the confidence limits, show the pointwise limits that cover a new observation for a given height with probability 0.95.

Figure 4.2 Fit Plot for Regression of Weight on Height

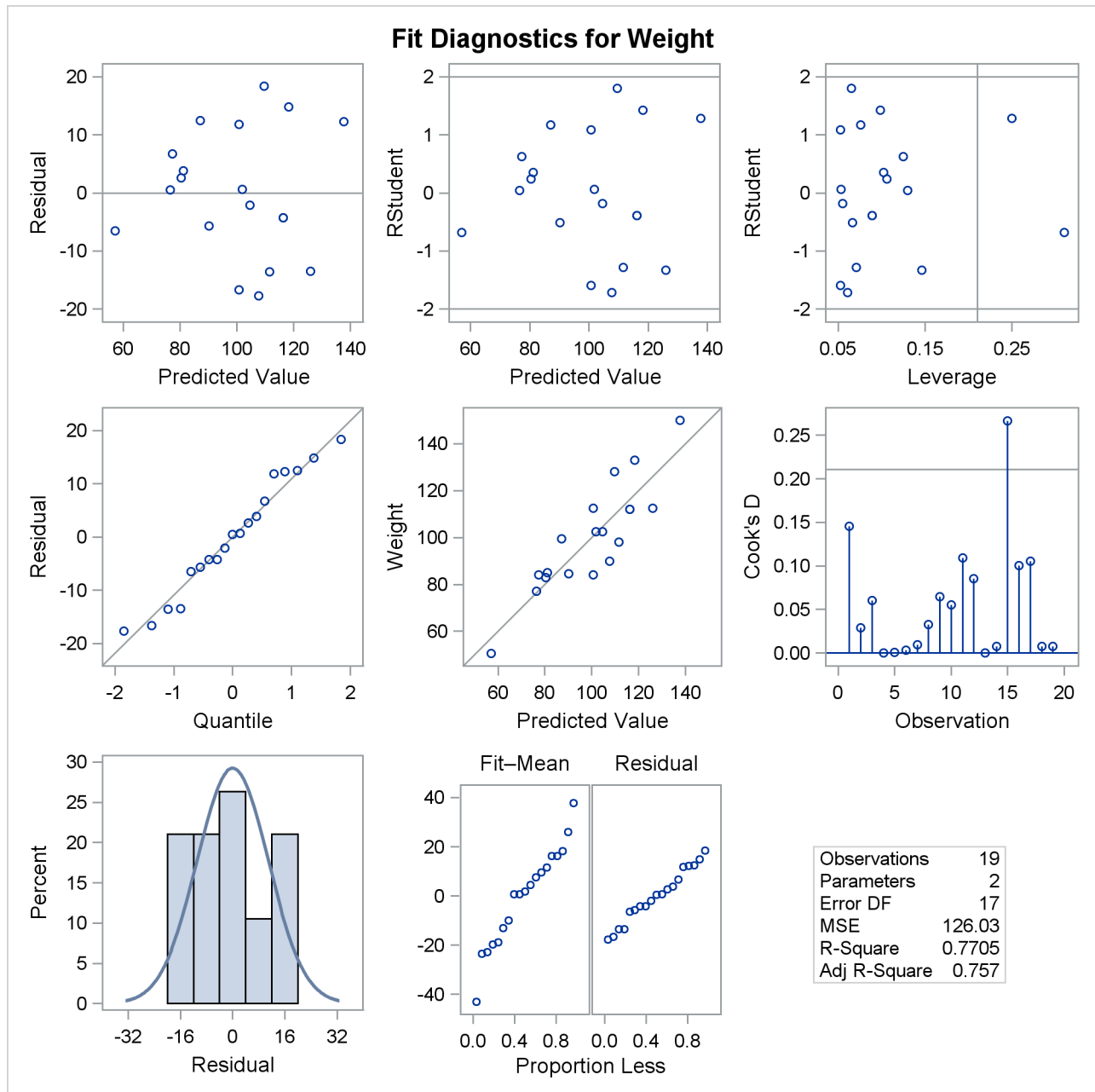


Regression is often used in an exploratory fashion to look for empirical relationships, such as the relationship between Height and Weight. In this example, Height is not the cause of Weight. You would need a controlled experiment to confirm the relationship scientifically. See the section “[Comments on Interpreting Regression Statistics](#)” on page 97 for more information. A separate question from a possible cause-and-effect relationship between the two variables involved in this regression is whether the simple linear regression model adequately describes the relationship in these data. If the usual assumptions about the model errors ϵ_i are met in the SLR model, then the errors should have zero mean and equal variance and be uncorrelated. Because the children were randomly selected, the observations from different children are not correlated. If the mean function of the model is correctly specified, the fitted residuals $\text{Weight}_i - \widehat{\text{Weight}}_i$ should scatter about the zero reference line without discernible structure. The residual plot in [Figure 4.3](#) confirms this behavior.

Figure 4.3 Residual Plot for Regression of Weight on Height

An even more detailed look at the model-data agreement is gained with the panel of regression diagnostics in Figure 4.4. The graph in the upper left panel repeats the raw residual plot in Figure 4.3. The plot of the RSTUDENT residuals shows externally studentized residuals that take into account heterogeneity in the variability of the residuals. RSTUDENT residuals that exceed the threshold values of ± 2 often indicate outlying observations. The residual-by-leverage plot shows that two observations have high leverage—that is, they are unusual in their height values relative to the other children. The normal-probability Q-Q plot in the second row of the panel shows that the normality assumption for the residuals is reasonable. The plot of the Cook's D statistic shows that observation 15 exceeds the threshold value; this indicates that the observation for this child is influential on the regression parameter estimates.

Figure 4.4 Panel of Regression Diagnostics



For detailed information about the interpretation of regression diagnostics and about ODS statistical graphics with the REG procedure, see Chapter 79, “The REG Procedure.”

SAS/STAT regression procedures produce the following information for a typical regression analysis:

- parameter estimates derived by using the least squares criterion
- estimates of the variance of the error term
- estimates of the variance or standard deviation of the sampling distribution of the parameter estimates
- tests of hypotheses about the parameters

SAS/STAT regression procedures can produce many other specialized diagnostic statistics, including the following:

- collinearity diagnostics to measure how strongly regressors are related to other regressors and how this affects the stability and variance of the estimates (REG)
- influence diagnostics to measure how each individual observation contributes to determining the parameter estimates, the SSE, and the fitted values (LOGISTIC, MIXED, REG, RSREG)
- lack-of-fit diagnostics that measure the lack of fit of the regression model by comparing the error variance estimate to another pure error variance that is not dependent on the form of the model (CATMOD, PROBIT, RSREG)
- diagnostic scatter plots that check the fit of the model and highlighted scatter plots that identify particular observations or groups of observations (REG)
- predicted and residual values, and confidence intervals for the mean and for an individual value (GLM, LOGISTIC, REG)
- time series diagnostics for equally spaced time series data that measure how much errors might be related across neighboring observations. These diagnostics can also measure functional goodness of fit for data that are sorted by regressor or response variables (REG, SAS/ETS procedures).

Many SAS/STAT procedures produce general and specialized statistical graphics through ODS Graphics to diagnose the fit of the model and the model-data agreement, and to highlight observations that are influential on the analysis. Figure 4.2 and Figure 4.3, for example, are two of the ODS statistical graphs produced by the REG procedure by default for the simple linear regression model. For general information about ODS Graphics, see Chapter 21, “Statistical Graphics Using ODS.” For specific information about the ODS statistical graphs available with a SAS/STAT procedure, see the PLOTS option in the “Syntax” section for the PROC statement and the “ODS Table Names” section in the “Details” section of the individual procedure documentation.

Linear Regression: The REG Procedure

The REG procedure is a general-purpose procedure for linear regression that does the following:

- handles multiple regression models
- provides nine model-selection methods
- allows interactive changes both in the model and in the data used to fit the model
- allows linear equality restrictions on parameters
- tests linear hypotheses and multivariate hypotheses
- produces collinearity diagnostics, influence diagnostics, and partial regression leverage plots
- saves estimates, predicted values, residuals, confidence limits, and other diagnostic statistics in output SAS data sets

- generates plots of data and of various statistics
- “paints” or highlights scatter plots to identify particular observations or groups of observations
- uses, optionally, correlations or crossproducts for input

Model-Selection Methods in Linear Regression Models

An important step in building statistical models is to determine which effects and variables affect the response variable and to form a model that fits the data well without incurring the negative effects of overfitting the model. Models that are overfit—that is, contain too many regressor variables and unimportant regressor variables—have a tendency to be too closely molded to a particular set of data, have unstable regression coefficients, and possibly have poor predictive precision. In situations where many potential regressor variables are available for inclusion in a regression model, guided, numerical variable-selection methods offer one approach to model building.

The model-selection techniques for linear regression models implemented in the REG procedure are as follows:

NONE	specifies that no selection be made. This method is the default and uses the full model given in the MODEL statement to fit the linear regression.
FORWARD	specifies that variables be selected based on a forward-selection algorithm. This method starts with no variables in the model and adds variables one by one to the model. At each step, the variable added is the one that most improves the fit of the model. You can also specify groups of variables to treat as a unit during the selection process. An option enables you to specify the criterion for inclusion.
BACKWARD	specifies that variables be selected based on a backward-elimination algorithm. This method starts with a full model and eliminates variables one by one from the model. At each step, the variable with the smallest contribution to the model is deleted. You can also specify groups of variables to treat as a unit during the selection process. An option enables you to specify the criterion for exclusion.
STEPWISE	specifies that variables be selected for the model based on a stepwise-regression algorithm, which combines forward-selection and backward-elimination steps. This method is a modification of the forward-selection method in that variables already in the model do not necessarily stay there. You can also specify groups of variables to treat as a unit during the selection process. Again, options enable you to specify criteria for entry into the model and for remaining in the model.
MAXR	specifies that model formation be based on the maximum R square improvement. This method tries to find the best one-variable model, the best two-variable model, and so on. The MAXR method differs from the STEPWISE method in that many more models are evaluated. The MAXR method considers all possible variable exchanges before making any exchange. The STEPWISE method might remove the “worst” variable without considering what the “best” remaining variable might accomplish, whereas MAXR would consider what the “best” remaining variable might accomplish. Consequently, model building based on the maximum R square improvement typically takes much longer to run than stepwise model building.

MINR	specifies that model formation be based on the minimum R square improvement. This method closely resembles MAXR, but the switch chosen is the one that produces the smallest increase in R square.
RSQUARE	finds a specified number of models having the highest R square in each of a range of model sizes.
CP	finds a specified number of models with the lowest C_p within a range of model sizes.
ADJRSQ	finds a specified number of models having the highest adjusted R square within a range of model sizes.

The GLMSELECT procedure has been specifically designed for the purpose of model building in linear models. In addition to having a wider array of selection methods and criteria compared to the REG procedure, the GLMSELECT procedure also supports classification variables. See Chapter 45, “The GLMSELECT Procedure,” for more information.

Regression with the REG and GLM Procedures

In terms of the assumptions about the basic model and the estimation principles, the REG and GLM procedures are very closely related. Both procedures estimate parameters by ordinary or weighted least squares and assume homoscedastic, uncorrelated model errors with zero mean. An assumption of normality of the model errors is not necessary for parameter estimation, but it is implied in confirmatory inference based on the parameter estimates—that is, the computation of tests, p -values, and confidence and prediction intervals.

The GLM procedure supports a CLASS statement for the levelization of classification variables; see the section “Parameterization of Model Effects” on page 383 in Chapter 19, “Shared Concepts and Topics,” on the parameterization of classification variables in statistical models. Classification variables are accommodated in the REG procedure by the inclusion of the necessary dummy regressor variables.

Most of the statistics based on predicted and residual values that are available in PROC REG are also available in PROC GLM. However, PROC GLM does not produce collinearity diagnostics, influence diagnostics, or scatter plots. In addition, PROC GLM allows only one model and fits the full model.

Both procedures are interactive, in that they do not stop after processing a RUN statement. The procedures accept statements until a QUIT statement is submitted.

Response Surface Regression: The RSREG Procedure

The RSREG procedure fits a quadratic response-surface model, which is useful in searching for factor values that optimize a response. The following features in PROC RSREG make it preferable to other regression procedures for analyzing response surfaces:

- automatic generation of quadratic effects
- a lack-of-fit test
- solutions for critical values of the surface
- eigenvalues of the associated quadratic form
- a ridge analysis to search for the direction of optimum response

Partial Least Squares Regression: The PLS Procedure

The PLS procedure fits models by using any of a number of linear predictive methods, including *partial least squares* (PLS). Ordinary least squares regression, as implemented in the GLM or REG procedure, has the single goal of minimizing sample response prediction error by seeking linear functions of the predictors that explain as much variation in each response as possible. The techniques implemented in the PLS procedure have the additional goal of accounting for variation in the predictors under the assumption that directions in the predictor space that are well sampled should provide better prediction for *new* observations when the predictors are highly correlated. All of the techniques implemented in the PLS procedure work by extracting successive linear combinations of the predictors, called *factors* (also called *components* or *latent vectors*), which optimally address one or both of these two goals—explaining response variation and explaining predictor variation. In particular, the method of partial least squares balances the two objectives, seeking factors that explain both response and predictor variation.

Generalized Linear Regression

As outlined in the section “Generalized Linear Models” on page 33 of Chapter 3, “Introduction to Statistical Modeling with SAS/STAT Software,” the class of generalized linear model generalizes the linear regression model in two ways:

- by allowing the data to come from a distribution that is a member of the exponential family of distributions
- by introducing a link function $g(\cdot)$ that provides a mapping between the linear predictor $\eta = \mathbf{x}'\boldsymbol{\beta}$ and the mean of the data, $g(E[Y]) = \eta$. The link function is monotonic, so that $E[Y] = g^{-1}(\eta)$ and $g^{-1}(\cdot)$ is called the inverse link function.

One of the most commonly used generalized linear regression models is the logistic model for binary or binomial data. Suppose that Y denotes a binary outcome variable that takes on the values 1 and 0 with probabilities π and $1 - \pi$, respectively. The probability π is also referred to as the “success probability,” supposing that the coding $Y = 1$ corresponds to a success in a Bernoulli experiment. The success probability is also the mean of Y , and one of the aims of logistic regression analysis is to study how regressor variables affect the outcome probabilities or functions thereof, such as odds ratios.

The logistic regression model for π is defined by a linear predictor $\eta = \mathbf{x}'\boldsymbol{\beta}$ and the logit link function:

$$\text{logit}\{\Pr(Y = 0)\} = \log\left\{\frac{\pi}{1 - \pi}\right\} = \mathbf{x}'\boldsymbol{\beta}$$

The inversely linked linear predictor function in this model is

$$\Pr(Y = 0) = \frac{1}{1 + \exp\{-\eta\}}$$

An extension of the dichotomous logistic regression model is models for multinomial (polychotomous) data. Two classes of models for multinomial data can be fit with procedures in SAS/STAT software: models for ordinal data that rely on cumulative link functions and models for nominal (unordered) outcomes that rely on generalized logits. The next section briefly discusses SAS/STAT procedures for logistic regression. See Chapter 8, “Introduction to Categorical Data Analysis Procedures,” for more information about the comparison of the procedures mentioned there with respect to analysis of categorical responses.

Logistic Regression

The SAS/STAT procedures CATMOD, GENMOD, GLIMMIX, LOGISTIC, and PROBIT can fit generalized linear models for binary, binomial, and multinomial outcomes.

CATMOD	provides maximum likelihood estimation for logistic regression, including the analysis of logits for dichotomous outcomes and the analysis of generalized logits for polychotomous outcomes. The CATMOD procedure can analyze data represented by a contingency table.
GENMOD	is a general modeling procedure for generalized linear models. It estimates parameters by maximum likelihood. Like the LOGISTIC procedure, it uses CLASS and MODEL statements in SAS/STAT procedures to form the statistical model and can fit models to binary and ordinal outcomes. The GENMOD procedure does not fit generalized logit models for nominal outcomes. However, the procedure also provides the capability of solving generalized estimating equations (GEE) to model correlated data and can perform a Bayesian analysis.
GLIMMIX	is a general modeling procedure for generalized linear mixed models. If the model does not contain random effects, the GLIMMIX procedure fits generalized linear models by the method of maximum likelihood. In the class of logistic regression models, the procedure can fit models to binary, binomial, ordinal, and nominal outcomes.
LOGISTIC	is specifically designed for logistic regression and estimates parameters by maximum likelihood. The procedure fits the usual logistic regression model for binary data as well as models with cumulative link function for ordinal data (such as the proportional odds model) and the generalized logit model for nominal data. The LOGISTIC procedure offers a number of variable selection methods and can perform conditional and exact conditional logistic regression analysis.
PROBIT	calculates maximum likelihood estimates of regression parameters and the natural (or threshold) response rate for quantal response data from biological assays or other discrete event data. This includes probit, logit, ordinal logistic, and extreme value (or gompit) regression models.
SURVEYLOGISTIC	is designed for logistic regression and estimates parameters by maximum likelihood. The procedure incorporates complex survey sample designs, including designs with stratification, clustering, and unequal weighting.

Other Generalized Linear Models

When a generalized linear model is formed with distributions other than the binary, binomial, or multinomial, you can use the GENMOD and GLIMMIX procedures for parameter estimation and inference.

Both procedures can accommodate correlated observations, but they use different techniques to accomplish this goal. The GENMOD procedure can fit correlated data models via generalized estimating equations that rely on a first- and second-moment specification for the response data and a working correlation assumption. With the GLIMMIX procedure, you can model correlations between the observations by (1) specifying random effects in the conditional distribution that induce a marginal correlation structure or (2) direct modeling of the marginal dependence. The GLIMMIX procedure employs likelihood-based techniques in parameter estimation.

The GENMOD procedure supports a Bayesian analysis through its BAYES statement.

With the GLIMMIX procedure you can vary the distribution or link function on an observation-by-observation basis.

To fit a generalized linear model with a distribution that is not available in the GENMOD or GLIMMIX procedure, you can use the NLMIXED procedure and code the log-likelihood function of an observation with SAS programming statements.

Regression for Ill-Conditioned Data: The ORTHOREG Procedure

The ORTHOREG procedure performs linear least squares regression by using the Gentleman-Givens computational method, and it can produce more accurate parameter estimates for ill-conditioned data. PROC GLM and PROC REG produce very accurate estimates for most problems. However, if you have very ill-conditioned data, consider using the ORTHOREG procedure. The collinearity diagnostics in PROC REG can help you to determine whether PROC ORTHOREG would be useful.

Quantile Regression: The QUANTREG Procedure

The QUANTREG procedure models the effects of covariates on the conditional quantiles of a response variable by means of quantile regression.

Ordinary least squares regression models the relationship between one or more covariates X and the conditional mean of the response variable $E[Y|X = x]$. Quantile regression extends the regression model to conditional quantiles of the response variable, such as the 90th percentile. Quantile regression is particularly useful when the rate of change in the conditional quantile, expressed by the regression coefficients, depends on the quantile. An advantage of quantile regression over least squares regression is its flexibility for modeling data with heterogeneous conditional distributions. Data of this type occur in many fields, including biomedicine, econometrics, and ecology.

Features that you will find in the QUANTREG procedure include the following:

- simplex, interior point, and smoothing algorithms for estimation
- sparsity, rank, and resampling methods for confidence intervals
- asymptotic and bootstrap methods to estimate covariance and correlation matrices of the parameter estimates
- Wald and likelihood ratio tests for the regression parameter estimates
- regression quantile spline fits

Nonlinear Regression

Recall from Chapter 3, “Introduction to Statistical Modeling with SAS/STAT Software,” that a nonlinear regression model is a statistical model in which the mean function depends on the model parameters in a nonlinear function. The SAS/STAT procedures that can fit general, nonlinear models are the NLIN and NLMIXED procedures. The procedures have the following in common:

- Nonlinear models are fit by iterative methods.
- You must provide an expression for the model through programming statements.
- Analytic derivatives of the objective function with respect to the parameters are calculated automatically.
- A grid search is available to select the best starting values for the parameters from a set of starting points that you provide.

The following items reflect some important differences between the NLIN and NLMIXED procedures:

- Parameters are estimated by nonlinear least squares with the NLIN procedure and by maximum likelihood with the NLMIXED procedure.
- The NLMIXED procedure enables you to construct nonlinear models that contain normally distributed random effects.
- The NLIN procedure requires that you declare all model parameters in the PARAMETERS statement and assign starting values. The NLMIXED procedure determines the parameters in your model based on the PARAMETER statement and the other modeling statements. It is not necessary to supply starting values for all parameters in the NLMIXED procedure, but it is highly recommended.
- The residual variance is not a parameter in models fit with the NLIN procedure, but it is in models fit with the NLMIXED procedure.
- The default iterative optimization method in the NLIN procedure is the Gauss-Newton method; the default method in the NLMIXED procedure is the quasi-Newton method. Other optimization techniques are available in both procedures.

Nonlinear models are fit with iterative techniques that begin from starting values and attempt to iteratively improve on the estimates by updating the estimates. There is no guarantee that the solution achieved when the iterative algorithm converges will correspond to a global optimum.

Nonparametric Regression

Regression models that suppose a parametric form express the mean of an observation as a function of regressor variables x_1, \dots, x_k and parameters β_1, \dots, β_p :

$$E[Y] = f(x_1, \dots, x_k; \beta_1, \dots, \beta_p)$$

Nonparametric regression techniques not only relax the assumption of linearity in the regression parameters, but they also do not require that you specify a precise functional form for the relationship between response and regressor variables. Consider a regression problem where the relationship between response Y and regressor X is to be modeled. It is assumed that $E[Y_i] = g(x_i) + \epsilon_i$, where $g(\cdot)$ is an unspecified regression function. Two primary approaches in nonparametric regression modeling are as follows:

- approximate $g(x_i)$ locally by a parametric function constructed from information in a local neighborhood of x_i
- approximate the unknown function $g(x_i)$ by a smooth, flexible function and determine the necessary smoothness and continuity properties from the data

The SAS/STAT procedures LOESS, GAM, and TPSPLINE fit nonparametric regression models by one of these methods.

Local Regression: The LOESS Procedure

The LOESS procedure implements a local regression approach for estimating regression surfaces pioneered by Cleveland, Devlin, and Grosse (1988). No assumptions about the parametric form of the entire regression surface are made with the LOESS procedure. Only a parametric form of the local approximation is specified by the user. Furthermore, the LOESS procedure is suitable when there are outliers in the data and a robust fitting method is necessary.

Smooth Function Approximation: The TPSPLINE Procedure

The TPSPLINE procedure decomposes the regressor contributions to the mean function into parametric components and into smooth functional components. Suppose that the regressor variables are collected into the vector \mathbf{x} and that this vector is partitioned as $\mathbf{x} = [\mathbf{x}'_1 \ \mathbf{x}'_2]'$. The relationship between Y and \mathbf{x}_2 is linear (parametric) and the relationship between Y and \mathbf{x}_1 is nonparametric. The TPSPLINE procedure fits models of the form

$$E[Y] = g(\mathbf{x}_1) + \mathbf{x}'_2 \boldsymbol{\beta}$$

The function $g(\cdot)$ can be represented as a sequence of spline basis functions.

The parameters are estimated by a penalized least squares method. The penalty is applied to the usual least squares criterion to obtain a regression estimate that fits the data well and to prevent the fit from attempting to interpolate the data (fit the data too closely).

Generalized Additive Models: The GAM Procedure

Generalized additive models are nonparametric models in which one or more regressor variables are present and can make different smooth contributions to the mean function. For example, if $\mathbf{x}_i = [x_{i1}, x_{i2}, \dots, x_{ik}]$ is a vector of k regressor for the i th observation, then an additive model represents the mean function as

$$E[Y] = f_0 + f_1(x_{i1}) + f_2(x_{i2}) + \dots + f_3(x_{i3})$$

The individual functions f_j can have a parametric or nonparametric form. If all f_j are parametric, the GAM procedure fits a fully parametric model. If some f_j are nonparametric, the GAM procedure fits a semiparametric model. Otherwise, the models are fully nonparametric.

The generalization of additive models is akin to the generalization for linear models: nonnormal data are accommodated by explicitly modeling the distribution of the data as a member of the exponential family and by applying a monotonic link function that provides a mapping between the predictor and the mean of the data.

Robust Regression: The ROBUSTREG Procedure

The ROBUSTREG procedure implements algorithms to detect outliers and provide resistant (stable) results in the presence of outliers. The ROBUSTREG procedure provides four such methods: M estimation, LTS estimation, S estimation, and MM estimation.

- M estimation was introduced by Huber (1973), and it is the simplest approach both computationally and theoretically. Although it is not robust with respect to leverage points, it is still used extensively in analyzing data for which it can be assumed that the contamination is mainly in the response direction.
- Least trimmed squares (LTS) estimation is a high breakdown value method introduced by Rousseeuw (1984). The breakdown value is a measure of the proportion of contamination that an estimation method can withstand and still maintain its robustness.
- S estimation is a high breakdown value method introduced by Rousseeuw and Yohai (1984). With the same breakdown value, it has a higher statistical efficiency than LTS estimation.
- MM estimation, introduced by Yohai (1987), combines high breakdown value estimation and M estimation. It has both the high breakdown property and a higher statistical efficiency than S estimation.

For diagnostic purposes, the ROBUSTREG procedure also implements robust leverage-point detection based on the robust Mahalanobis distance. The robust distance is computed by using a generalized minimum covariance determinant (MCD) algorithm.

Regression with Transformations: The TRANSREG Procedure

The TRANSREG procedure can fit many standard linear models. In addition, PROC TRANSREG can find nonlinear transformations of the data and fit a linear model to the transformed variables. This is in contrast to PROC REG and PROC GLM, which fit linear models to data, or PROC NLIN, which fits nonlinear models to data. The TRANSREG procedure fits many types of linear models, including the following:

- ordinary regression and ANOVA
- metric and nonmetric conjoint analysis
- metric and nonmetric vector and ideal point preference mapping
- simple, multiple, and multivariate regression with variable transformations
- redundancy analysis with variable transformations
- canonical correlation analysis with variable transformations
- response surface regression with variable transformations

Interactive Features in the CATMOD, GLM, and REG Procedures

The CATMOD, GLM, and REG procedures do not stop after processing a RUN statement. More statements can be submitted as a continuation of the previous statements. Many new features in these procedures are useful to request after you have reviewed the results from previous statements. The procedures stop if a DATA step or another procedure is requested or if a QUIT statement is submitted.

Statistical Background in Linear Regression

The remainder of this chapter outlines the way in which many SAS/STAT regression procedures calculate various regression quantities. The discussion focuses on the linear regression models. General statistical background about linear statistical models can be found in the section “[Linear Model Theory](#)” of Chapter 3, “[Introduction to Statistical Modeling with SAS/STAT Software](#).”

Exceptions and further details are documented with individual procedures.

Linear Regression Models

In matrix notation, a linear model is written as

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

where \mathbf{X} is the $(n \times k)$ design matrix (rows are observations and columns are the regressors), $\boldsymbol{\beta}$ is the $(k \times 1)$ vector of unknown parameters, and $\boldsymbol{\epsilon}$ is the $(n \times 1)$ vector of unobservable model errors. The first column of \mathbf{X} is usually a vector of 1s and is used to estimate the intercept term.

The statistical theory of linear models is based on strict classical assumptions. Ideally, the response is measured with all the factors controlled in an experimentally determined environment. If you cannot control the factors experimentally, some tests must be interpreted as being conditional on the observed values of the regressors.

Other assumptions are as follows:

- The form of the model is correct (all important explanatory variables have been included). This assumption is reflected mathematically in the assumption of a zero mean of the model errors, $E[\boldsymbol{\epsilon}] = \mathbf{0}$.
- Regressor variables are measured without error.
- The expected value of the errors is zero.
- The variance of the error (and thus the dependent variable) for the i th observation is σ^2/w_i , where w_i is a known weight factor. Usually, $w_i = 1$ for all i and thus σ^2 is the common, constant variance.
- The errors are uncorrelated across observations.

When hypotheses are tested, or when confidence and prediction intervals are computed, an additional assumption is made that the errors are normally distributed.

Parameter Estimates and Associated Statistics

The Least Squares Estimators

Least squares estimators of the regression parameters are found by solving the normal equations

$$(\mathbf{X}'\mathbf{W}\mathbf{X})\boldsymbol{\beta} = \mathbf{X}'\mathbf{W}\mathbf{Y}$$

for the vector $\boldsymbol{\beta}$, where \mathbf{W} is a diagonal matrix with the observed weights on the diagonal. The resulting estimator of the parameter vector is

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{W}\mathbf{X})^{-1} \mathbf{X}'\mathbf{W}\mathbf{Y}$$

This is an unbiased estimator, since

$$\begin{aligned} E[\hat{\boldsymbol{\beta}}] &= (\mathbf{X}'\mathbf{W}\mathbf{X})^{-1} \mathbf{X}'\mathbf{W}E[\mathbf{Y}] \\ &= (\mathbf{X}'\mathbf{W}\mathbf{X})^{-1} \mathbf{X}'\mathbf{W}\mathbf{X}\boldsymbol{\beta} = \boldsymbol{\beta} \end{aligned}$$

Notice that the only assumption necessary in order for the least squares estimators to be unbiased is that of a zero mean of the model errors. If the estimator is evaluated at the observed data, it is referred to as the least squares estimate (Introduction to Regression) as the least squares estimate,

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{W}\mathbf{X})^{-1} \mathbf{X}'\mathbf{W}\mathbf{y}$$

If the standard classical assumptions are met, the least squares estimators of the regression parameters are the best linear unbiased estimators (BLUE). In other words, the estimators have minimum variance in the class of estimators that are unbiased and that are linear functions of the responses. If the additional assumption of normally distributed errors is satisfied, then the following are true:

- The statistics that are computed have the proper sampling distributions for hypothesis testing.
- Parameter estimators are normally distributed.
- Various sums of squares are distributed proportional to chi-square, at least under proper hypotheses.
- Ratios of estimators to standard errors follow the Student's t distribution under certain hypotheses.
- Appropriate ratios of sums of squares follow an F distribution for certain hypotheses.

When regression analysis is used to model data that do not meet the assumptions, the results should be interpreted in a cautious, exploratory fashion. The significance probabilities under these circumstances are unreliable.

Box (1966) and Mosteller and Tukey (1977, Chapters 12 and 13) discuss the problems that are encountered with regression data, especially when the data are not under experimental control.

Estimating the Precision

Assume for the present that $\mathbf{X}'\mathbf{W}\mathbf{X}$ has full column rank k (this assumption is relaxed later). The variance of the error terms, $\text{Var}[\epsilon_i] = \sigma^2$, is then estimated by the mean square error

$$s^2 = \text{MSE} = \frac{\text{SSE}}{n - k} = \frac{1}{n - k} \sum_{i=1}^n w_i (y_i - \mathbf{x}'_i \boldsymbol{\beta})^2$$

where \mathbf{x}'_i is the i th row of the design matrix \mathbf{X} . The residual variance estimate is also unbiased: $E[s^2] = \sigma^2$.

The covariance matrix of the least squares estimators is

$$\text{Var}[\hat{\boldsymbol{\beta}}] = \sigma^2 (\mathbf{X}'\mathbf{W}\mathbf{X})^{-1}$$

An estimate of the covariance matrix is obtained by replacing σ^2 with its estimate, s^2 in the preceding formula. This estimate is often referred to as COVB in SAS/STAT modeling procedures:

$$\text{COVB} = \widehat{\text{Var}}[\hat{\boldsymbol{\beta}}] = s^2 (\mathbf{X}'\mathbf{W}\mathbf{X})^{-1}$$

The correlation matrix of the estimates, often referred to as CORRB, is derived by scaling the covariance matrix: Let $\mathbf{S} = \text{diag} \left((\mathbf{X}'\mathbf{W}\mathbf{X})^{-1} \right)^{-\frac{1}{2}}$. Then the correlation matrix of the estimates is

$$\text{CORRB} = \mathbf{S} (\mathbf{X}'\mathbf{W}\mathbf{X})^{-1} \mathbf{S}$$

The estimated standard error of the i th parameter estimator is obtained as the square root of the i th diagonal element of the COVB matrix. Formally,

$$\text{STDERR}(\hat{\beta}_i) = \sqrt{[s^2 (\mathbf{X}'\mathbf{W}\mathbf{X})^{-1}]_{ii}}$$

The ratio

$$t = \frac{\hat{\beta}_i}{\text{STDERR}(\hat{\beta}_i)}$$

follows a Student's t distribution with $(n - k)$ degrees of freedom under the hypothesis that β_i is zero and provided that the model errors are normally distributed.

Regression procedures display the t ratio and the significance probability, which is the probability under the hypothesis $H: \beta_i = 0$ of a larger absolute t value than was actually obtained. When the probability is less than some small level, the event is considered so unlikely that the hypothesis is rejected.

Type I SS and Type II SS measure the contribution of a variable to the reduction in SSE. Type I SS measure the reduction in SSE as that variable is entered into the model in sequence. Type II SS are the increment in SSE that results from removing the variable from the full model. Type II SS are equivalent to the Type III and Type IV SS reported in the GLM procedure. If Type II SS are used in the numerator of an F test, the test is equivalent to the t test for the hypothesis that the parameter is zero. In polynomial models, Type I SS measure the contribution of each polynomial term after it is orthogonalized to the previous terms in the model. The four types of SS are described in Chapter 15, “[The Four Types of Estimable Functions](#).”

Coefficient of Determination

The coefficient of determination in a regression model, also known as the R-square statistic (R^2), measures the proportion of variability in the response that is explained by the regressor variables. In a linear regression model with intercept, R square is defined as

$$R^2 = 1 - \frac{SSE}{SST}$$

where SSE is the residual (error) sum of squares and SST is the total sum of squares corrected for the mean. The adjusted R square statistic is an alternative to R square that takes into account the number of parameters in the model. This statistic is calculated as

$$ADJRSQ = 1 - \frac{n - i}{n - p} (1 - R^2)$$

where n is the number of observations used to fit the model, p is the number of parameters in the model (including the intercept), and i is 1 if the model includes an intercept term, and 0 otherwise.

R square statistics also play an important indirect role in regression calculations. For example, the proportion of variability explained by regressing all other variables in a model on a particular regressor can provide insights into the interrelationship among the regressors.

Tolerances and variance inflation factors measure the strength of interrelationships among the regressor variables in the model. If all variables are orthogonal to each other, both tolerance and variance inflation are 1. If a variable is very closely related to other variables, the tolerance approaches 0 and the variance inflation gets very large. Tolerance (TOL) is 1 minus the R square that results from the regression of the other variables in the model on that regressor. Variance inflation (VIF) is the diagonal of $(\mathbf{X}'\mathbf{W}\mathbf{X})^{-1}$, if $(\mathbf{X}'\mathbf{W}\mathbf{X})$ is scaled to correlation form. The statistics are related as

$$VIF = \frac{1}{TOL}$$

Explicit and Implicit Intercepts

A linear model contains an *explicit* intercept if the \mathbf{X} matrix contains a column whose nonzero values do not vary, typically a column of ones. Many SAS/STAT procedures automatically add this column of ones as the first column in the \mathbf{X} matrix. Procedures that support a NOINT option in the MODEL statement provide the capability to suppress the automatic addition of the intercept column.

In general, models without intercept should be the exception, especially if your model does not contain classification variables. An overall intercept is provided in many models to adjust for the grand total or overall mean in your data. A simple linear regression without intercept, such as

$$E[Y_i] = \beta_1 x_i + \epsilon_i$$

assumes that Y has mean zero if X takes on the value zero. This might not be a reasonable assumption.

If you explicitly suppress the intercept in a statistical model, the calculation and interpretation of your results can change. For example, the exclusion of the intercept in the following PROC REG statements leads to a different calculation of the R-square statistic. It also affects the calculation of the sum of squares in the analysis of variance for the model. For example, the model and error sum of squares add up to the uncorrected total sum of squares in the absence of an intercept.

```
proc reg;
  model y = x / noint;
quit;
```

Many statistical models contain an *implicit* intercept. This occurs when a linear function of one or more columns in the \mathbf{X} matrix produces a column of constant, nonzero values. For example, the presence of a CLASS variable in the GLM parameterization always implies an intercept in the model. If a model contains an implicit intercept, adding an intercept to the model does not alter the quality of the model fit, but it changes the interpretation (and number) of the parameter estimates.

The way in which the implicit intercept is detected and accounted for in the analysis depends on the procedure. For example, the following statements in the GLM procedure lead to an implied intercept:

```
proc glm;
  class a;
  model y = a / solution noint;
run;
```

Whereas the analysis of variance table uses the uncorrected total sum of squares (due to the NOINT option), the implied intercept does not lead to a redefinition or recalculation of the R-square statistic (compared to the model without the NOINT option). Also, because the intercept is implied by the presence of the CLASS variable a in the model, the same error sum of squares results whether the NOINT option is specified or not.

A different approach is taken, for example, by the TRANSREG procedure. The ZERO=NONE option in the CLASS parameterization of the following statements leads to an implicit intercept model:

```
proc transreg;
  model ide(y) = class(a / zero=none) / ss2;
run;
```

The analysis of variance table or the regression fit statistics are not affected in the TRANSREG procedure. Only the interpretation of the parameter estimates changes because of the way in which the intercept is accounted for in the model.

Implied intercepts not only occur when classification effects are present in the model. They also occur with B-splines and other sets of constructed columns.

Models Not of Full Rank

If the \mathbf{X} matrix is not of full rank, then a generalized inverse can be used to solve the normal equations to minimize the SSE:

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{W}\mathbf{X})^{-} \mathbf{X}'\mathbf{W}\mathbf{y}$$

However, these estimates are not unique since there are an infinite number of solutions corresponding to different generalized inverses. PROC REG and other regression procedures choose a nonzero solution for all variables that are linearly independent of previous variables and a zero solution for other variables. This corresponds to using a generalized inverse in the normal equations, and the expected values of the estimates are the Hermite normal form of $\mathbf{X}'\mathbf{W}\mathbf{X}$ multiplied by the true parameters:

$$E[\hat{\boldsymbol{\beta}}] = (\mathbf{X}'\mathbf{W}\mathbf{X})^{-} (\mathbf{X}'\mathbf{W}\mathbf{X})\boldsymbol{\beta}$$

Degrees of freedom for the estimates that correspond to singularities are not counted (reported as zero). The hypotheses that are not testable have t tests displayed as missing. The message that the model is not of full rank includes a display of the relations that exist in the matrix.

See the sections “Generalized Inverse Matrices” and “Linear Model Theory” in Chapter 3, “Introduction to Statistical Modeling with SAS/STAT Software,” on the nature and construction of generalized inverses and their importance for statistical inference in linear models.

Predicted and Residual Values

After the model has been fit, predicted and residual values are usually calculated, graphed, and output. The predicted values are calculated from the estimated regression equation; the raw residuals are calculated as the observed minus the predicted value. Often other forms of residuals are used for model diagnostics, such as studentized or cumulative residuals. Some procedures can calculate standard errors of residuals, predicted mean values, and individual predicted values.

Consider the i th observation where \mathbf{x}'_i is the row of regressors, $\hat{\boldsymbol{\beta}}$ is the vector of parameter estimates, and s^2 is the estimate of the residual variance (the mean squared error). The *leverage* value of the i th observation is defined as

$$h_i = w_i \mathbf{x}'_i (\mathbf{X}' \mathbf{W} \mathbf{X})^{-1} \mathbf{x}_i$$

where \mathbf{X} is the design matrix for the observed data, \mathbf{x}'_i is an arbitrary regressor vector (possibly but not necessarily a row of \mathbf{X}), \mathbf{W} is a diagonal matrix with the observed weights on the diagonal, and w_i is the weight corresponding to \mathbf{x}'_i .

Then the predicted mean and the standard error of the predicted mean are

$$\hat{y}_i = \mathbf{x}'_i \hat{\boldsymbol{\beta}}$$

$$\text{STDERR}(\hat{y}_i) = \sqrt{s^2 h_i / w_i}$$

The standard error of the individual (future) predicted value y_i is

$$\text{STDERR}(y_i) = \sqrt{s^2 (1 + h_i) / w_i}$$

If the predictor vector \mathbf{x}_i corresponds to an observation in the analysis data, then the raw residual for that observation and the standard error of the raw residual are defined as

$$\text{RESID}_i = y_i - \mathbf{x}'_i \hat{\boldsymbol{\beta}}$$

$$\text{STDERR}(\text{RESID}_i) = \sqrt{s^2 (1 - h_i) / w_i}$$

The *studentized residual* is the ratio of the raw residual and its estimated standard error. Symbolically,

$$\text{STUDENT}_i = \frac{\text{RESID}_i}{\text{STDERR}(\text{RESID}_i)}$$

There are two kinds of intervals involving predicted values that are associated with a measure of confidence: the *confidence* interval for the mean value of the response and the *prediction* (or *forecasting*) interval for an individual observation. As discussed in the section “Mean Squared Error” in Chapter 3, “Introduction

to *Statistical Modeling with SAS/STAT Software*,” both intervals are based on the mean squared error of predicting a target based on the result of the model fit. The difference in the expressions for the confidence interval and the prediction interval comes about because the target of estimation is a constant in the case of the confidence interval (the mean of an observation) and the target is a random variable in the case of the prediction interval (a new observation).

For example, you can construct a confidence interval for the i th observation that contains the true mean value of the response with probability $1 - \alpha$. The upper and lower limits of the confidence interval for the mean value are

$$\begin{aligned}\text{LowerM} &= \mathbf{x}'_i \hat{\boldsymbol{\beta}} - t_{\alpha/2, \nu} \sqrt{s^2 h_i / w_i} \\ \text{UpperM} &= \mathbf{x}'_i \hat{\boldsymbol{\beta}} + t_{\alpha/2, \nu} \sqrt{s^2 h_i / w_i}\end{aligned}$$

where $t_{\alpha/2, \nu}$ is the tabulated t quantile with degrees of freedom equal to the degrees of freedom for the mean squared error, $\nu = n - \text{rank}(\mathbf{X})$.

The limits for the prediction interval for an individual response are

$$\begin{aligned}\text{LowerI} &= \mathbf{x}'_i \hat{\boldsymbol{\beta}} - t_{\alpha/2, \nu} \sqrt{s^2(1 + h_i) / w_i} \\ \text{UpperI} &= \mathbf{x}'_i \hat{\boldsymbol{\beta}} + t_{\alpha/2, \nu} \sqrt{s^2(1 + h_i) / w_i}\end{aligned}$$

Influential observations are those that, according to various criteria, appear to have a large influence on the analysis. One measure of influence, Cook's D , measures the change to the estimates that results from deleting an observation:

$$\text{COOKD}_i = \frac{1}{k} \text{STUDENT}_i^2 \left(\frac{\text{STDERR}(\hat{y}_i)}{\text{STDERR}(\text{RESID}_i)} \right)^2$$

where k is the number of parameters in the model (including the intercept). For more information, see Cook (1977, 1979).

The *predicted residual* for observation i is defined as the residual for the i th observation that results from dropping the i th observation from the parameter estimates. The sum of squares of predicted residual errors is called the *PRESS statistic*:

$$\begin{aligned}\text{PRESID}_i &= \frac{\text{RESID}_i}{1 - h_i} \\ \text{PRESS} &= \sum_{i=1}^n w_i \text{PRESID}_i^2\end{aligned}$$

Testing Linear Hypotheses

Testing of linear hypothesis based on estimable functions is discussed in the section “Test of Hypotheses” on page 59 in Chapter 3, “Introduction to Statistical Modeling with SAS/STAT Software,” and the construction of special sets of estimable functions corresponding to Type I–Type IV hypotheses is discussed in Chapter 15, “The Four Types of Estimable Functions.” In linear regression models, testing of general

linear hypotheses follows along the same lines. Test statistics are usually formed based on sums of squares associated with the hypothesis in question. Furthermore, when \mathbf{X} is of full rank—as is the case in many regression models—the consistency of the linear hypothesis is guaranteed.

Recall from Chapter 3, “Introduction to Statistical Modeling with SAS/STAT Software,” that the general form of a linear hypothesis for the parameters is $H: \mathbf{L}\boldsymbol{\beta} = \mathbf{d}$, where \mathbf{L} is $(q \times k)$, $\boldsymbol{\beta}$ is $(k \times 1)$, and \mathbf{d} is $(q \times 1)$. To test this hypothesis, the linear function is taken with respect to the parameter estimates: $\mathbf{L}\widehat{\boldsymbol{\beta}} - \mathbf{d}$. This linear function in $\widehat{\boldsymbol{\beta}}$ has variance

$$\text{Var}[\mathbf{L}\widehat{\boldsymbol{\beta}}] = \mathbf{L}\text{Var}[\widehat{\boldsymbol{\beta}}]\mathbf{L}' = \sigma^2\mathbf{L}(\mathbf{X}'\mathbf{W}\mathbf{X})^{-1}\mathbf{L}'$$

The *sum of squares due to the hypothesis* is a simple quadratic form:

$$SS(H) = SS(\mathbf{L}\widehat{\boldsymbol{\beta}} - \mathbf{d}) = (\mathbf{L}\widehat{\boldsymbol{\beta}} - \mathbf{d})' (\mathbf{L}(\mathbf{X}'\mathbf{W}\mathbf{X})^{-1}\mathbf{L}')^{-1} (\mathbf{L}\widehat{\boldsymbol{\beta}} - \mathbf{d})$$

If this hypothesis is testable, then $SS(H)$ can be used in the numerator of an F statistic:

$$F = \frac{SS(H)/q}{s^2} = \frac{SS(\mathbf{L}\widehat{\boldsymbol{\beta}} - \mathbf{d})/q}{s^2}$$

If $\widehat{\boldsymbol{\beta}}$ is normally distributed, which follows as a consequence of normally distributed model errors, then this statistic follows an F distribution with q numerator degrees of freedom and $n - \text{rank}(\mathbf{X})$ denominator degrees of freedom. Note that it was assumed in this derivation that \mathbf{L} is of full row rank q .

Multivariate Tests

Multivariate hypotheses involve several dependent variables in the form

$$H: \mathbf{L}\boldsymbol{\beta}\mathbf{M} = \mathbf{d}$$

where \mathbf{L} is a linear function on the regressor side, $\boldsymbol{\beta}$ is a matrix of parameters, \mathbf{M} is a linear function on the dependent side, and \mathbf{d} is a matrix of constants. The special case (handled by PROC REG) in which the constants are the same for each dependent variable is expressed as

$$(\mathbf{L}\boldsymbol{\beta} - \mathbf{c}\mathbf{j})\mathbf{M} = \mathbf{0}$$

where \mathbf{c} is a column vector of constants and \mathbf{j} is a row vector of 1s. The special case in which the constants are 0 is then

$$\mathbf{L}\boldsymbol{\beta}\mathbf{M} = \mathbf{0}$$

These multivariate tests are covered in detail in Morrison (1976); Timm (1975); Mardia, Kent, and Bibby (1979); Bock (1975) and other works cited in Chapter 9, “Introduction to Multivariate Procedures.”

Notice that in contrast to the tests discussed in the preceding section, $\boldsymbol{\beta}$ here is a matrix of parameter estimates. Suppose that the matrix of estimates is denoted as \mathbf{B} . To test the multivariate hypothesis, construct two matrices, \mathbf{H} and \mathbf{E} , that correspond to the numerator and denominator of a univariate F test:

$$\begin{aligned} \mathbf{H} &= \mathbf{M}'(\mathbf{L}\mathbf{B} - \mathbf{c}\mathbf{j})'(\mathbf{L}(\mathbf{X}'\mathbf{W}\mathbf{X})^{-1}\mathbf{L}')^{-1}(\mathbf{L}\mathbf{B} - \mathbf{c}\mathbf{j})\mathbf{M} \\ \mathbf{E} &= \mathbf{M}'(\mathbf{Y}'\mathbf{W}\mathbf{Y} - \mathbf{B}'(\mathbf{X}'\mathbf{W}\mathbf{X})\mathbf{B})\mathbf{M} \end{aligned}$$

Four test statistics, based on the eigenvalues of $\mathbf{E}^{-1}\mathbf{H}$ or $(\mathbf{E} + \mathbf{H})^{-1}\mathbf{H}$, are formed. Let λ_i be the ordered eigenvalues of $\mathbf{E}^{-1}\mathbf{H}$ (if the inverse exists), and let ξ_i be the ordered eigenvalues of $(\mathbf{E} + \mathbf{H})^{-1}\mathbf{H}$. It happens that $\xi_i = \lambda_i / (1 + \lambda_i)$ and $\lambda_i = \xi_i / (1 - \xi_i)$, and it turns out that $\rho_i = \sqrt{\xi_i}$ is the i th canonical correlation.

Let p be the rank of $(\mathbf{H} + \mathbf{E})$, which is less than or equal to the number of columns of \mathbf{M} . Let q be the rank of $\mathbf{L}(\mathbf{X}'\mathbf{W}\mathbf{X})^{-1}\mathbf{L}'$. Let v be the error degrees of freedom and $s = \min(p, q)$. Let $m = (|p - q| - 1)/2$, and let $n = (v - p - 1)/2$. Then the following statistics test the multivariate hypothesis in various ways, and their p -values can be approximated by F distributions. Note that in the special case that the rank of \mathbf{H} is 1, all of these F statistics will be the same and the corresponding p -values will in fact be exact, since in this case the hypothesis is really univariate.

Wilks' Lambda

If

$$\Lambda = \frac{\det(\mathbf{E})}{\det(\mathbf{H} + \mathbf{E})} = \prod_{i=1}^n \frac{1}{1 + \lambda_i} = \prod_{i=1}^n (1 - \xi_i)$$

then

$$F = \frac{1 - \Lambda^{1/t}}{\Lambda^{1/t}} \cdot \frac{rt - 2u}{pq}$$

is approximately F distributed, where

$$\begin{aligned} r &= v - \frac{p - q + 1}{2} \\ u &= \frac{pq - 2}{4} \\ t &= \begin{cases} \sqrt{\frac{p^2q^2 - 4}{p^2 + q^2 - 5}} & \text{if } p^2 + q^2 - 5 > 0 \\ 1 & \text{otherwise} \end{cases} \end{aligned}$$

The degrees of freedom are pq and $rt - 2u$. The distribution is exact if $\min(p, q) \leq 2$. (See Rao 1973, p. 556.)

Pillai's Trace

If

$$\mathbf{V} = \text{trace}(\mathbf{H}(\mathbf{H} + \mathbf{E})^{-1}) = \sum_{i=1}^n \frac{\lambda_i}{1 + \lambda_i} = \sum_{i=1}^n \xi_i$$

then

$$F = \frac{2n + s + 1}{2m + s + 1} \cdot \frac{\mathbf{V}}{s - \mathbf{V}}$$

is approximately F distributed with $s(2m + s + 1)$ and $s(2n + s + 1)$ degrees of freedom.

Hotelling-Lawley Trace

If

$$U = \text{trace}(\mathbf{E}^{-1}\mathbf{H}) = \sum_{i=1}^n \lambda_i = \sum_{i=1}^n \frac{\xi_i}{1 - \xi_i}$$

then for $n > 0$

$$F = (U/c)((4 + (pq + 2)/(b - 1))/(pq))$$

is approximately F distributed with pq and $4 + (pq + 2)/(b - 1)$ degrees of freedom, where $b = (p + 2n)(q + 2n)/(2(2n + 1)(n - 1))$ and $c = (2 + (pq + 2)/(b - 1))/(2n)$; while for $n \leq 0$

$$F = \frac{2(sn + 1)\mathbf{U}}{s^2(2m + s + 1)}$$

is approximately F with $s(2m + s + 1)$ and $2(sn + 1)$ degrees of freedom.

Roy's Maximum Root

If $\Theta = \lambda_1$, then

$$F = \Theta \frac{v - r + q}{r}$$

where $r = \max(p, q)$ is an upper bound on F that yields a lower bound on the significance level. Degrees of freedom are r for the numerator and $v - r + q$ for the denominator.

Tables of critical values for these statistics are found in Pillai (1960).

Exact Multivariate Tests

Beginning with SAS 9, if you specify the `MSTAT=EXACT` option in the appropriate statement, p -values for three of the four tests are computed exactly (Wilks' lambda, the Hotelling-Lawley trace, and Roy's greatest root), and the p -values for the fourth (Pillai's trace) are based on an F approximation that is more accurate (but occasionally slightly more liberal) than the default. The exact p -values for Roy's greatest root benefit the most, since in this case the F approximation provides only a lower bound for the p -value. If you use the F -based p -value for this test in the usual way, declaring a test significant if $p < 0.05$, then your decisions might be very liberal. For example, instead of the nominal 5% Type I error rate, such a procedure can easily have an actual Type I error rate in excess of 30%. By contrast, basing such a procedure on the exact p -values will result in the appropriate 5% Type I error rate, under the usual regression assumptions.

The `MSTAT=EXACT` option is supported in the ANOVA, CANCELL, CANDISC, GLM, and REG procedures.

The exact p -values are based on the following sources:

- **Wilks' lambda:** Lee (1972); Davis (1979)
- **Pillai's trace:** Muller (1998)
- **Hotelling-Lawley trace:** Davis (1970, 1980)
- **Roy's greatest root:** Davis (1972); Pillai and Flury (1984)

Note that, although the MSTAT=EXACT p -value for Pillai's trace is still approximate, it has “substantially greater accuracy” than the default approximation (Muller 1998).

Since most of the MSTAT=EXACT p -values are not based on the F distribution, the columns in the multivariate tests table corresponding to this approximation—in particular, the F value and the numerator and denominator degrees of freedom—are no longer displayed, and the column containing the p -values is labeled “P Value” instead of “Pr > F.” Suppose, for example, you use the following PROC ANOVA statements to perform a multivariate analysis of an archaeological data set:

```
data Skulls;
  input Loc $20. Basal Occ Max;
  datalines;
Minas Graes, Brazil  2.068 2.070 1.580
Minas Graes, Brazil  2.068 2.074 1.602
Minas Graes, Brazil  2.090 2.090 1.613
Minas Graes, Brazil  2.097 2.093 1.613
Minas Graes, Brazil  2.117 2.125 1.663
Minas Graes, Brazil  2.140 2.146 1.681
Matto Grosso, Brazil 2.045 2.054 1.580
Matto Grosso, Brazil 2.076 2.088 1.602
Matto Grosso, Brazil 2.090 2.093 1.643
Matto Grosso, Brazil 2.111 2.114 1.643
Santa Cruz, Bolivia  2.093 2.098 1.653
Santa Cruz, Bolivia  2.100 2.106 1.623
Santa Cruz, Bolivia  2.104 2.101 1.653
;

proc anova data=Skulls;
  class Loc;
  model Basal Occ Max = Loc / nouni;
  manova h=Loc;
  ods select MultStat;
run;
```

The default multivariate tests, based on the F approximations, are shown in [Figure 4.5](#).

Figure 4.5 Default Multivariate Tests

```

The ANOVA Procedure
Multivariate Analysis of Variance

MANOVA Test Criteria and F Approximations for
the Hypothesis of No Overall Loc Effect
H = Anova SSCP Matrix for Loc
E = Error SSCP Matrix

S=2    M=0    N=3

Statistic                Value      F Value    Num DF    Den DF    Pr > F

Wilks' Lambda            0.60143661    0.77        6         16       0.6032
Pillai's Trace           0.44702843    0.86        6         18       0.5397
Hotelling-Lawley Trace   0.58210348    0.75        6         9.0909   0.6272
Roy's Greatest Root      0.35530890    1.07        3          9       0.4109

NOTE: F Statistic for Roy's Greatest Root is an upper bound.
NOTE: F Statistic for Wilks' Lambda is exact.
    
```

If you specify `MSTAT=EXACT` in the MANOVA statement, as in the following statements, then the displayed output is the much simpler table shown in [Figure 4.6](#).

```

proc anova data=Skulls;
  class Loc;
  model Basal Occ Max = Loc / nouni;
  manova h=Loc / mstat=exact;
  ods select MultStat;
run;
    
```

Figure 4.6 Multivariate Tests with `MSTAT=EXACT`

```

The ANOVA Procedure
Multivariate Analysis of Variance

MANOVA Tests for the Hypothesis of No Overall Loc Effect
H = Anova SSCP Matrix for Loc
E = Error SSCP Matrix

S=2    M=0    N=3

Statistic                Value      P-Value

Wilks' Lambda            0.60143661    0.6032
Pillai's Trace           0.44702843    0.5521
Hotelling-Lawley Trace   0.58210348    0.6337
Roy's Greatest Root      0.35530890    0.7641
    
```

Notice that the *p*-value for Roy’s greatest root is substantially larger in the new table, and correspondingly more in line with the *p*-values for the other tests.

If you reference the underlying ODS output object for the table of multivariate statistics, it is important to note that its structure does not depend on the value of the MSTAT= specification. In particular, it always contains columns corresponding to both the default MSTAT=FAPPROX and the MSTAT=EXACT tests. Moreover, since the MSTAT=FAPPROX tests are relatively cheap to compute, the columns corresponding to them are always filled in, even though they are not displayed when you specify MSTAT=EXACT. On the other hand, for MSTAT=FAPPROX (which is the default), the column of exact p -values contains missing values, and is not displayed.

Comments on Interpreting Regression Statistics

In most applications, regression models are merely useful approximations. Reality is often so complicated that you cannot know what the true model is. You might have to choose a model more on the basis of what variables can be measured and what kinds of models can be estimated than on a rigorous theory that explains how the universe really works. However, even in cases where theory is lacking, a regression model can be an excellent predictor of the response if the model is carefully formulated from a large sample. The interpretation of statistics such as parameter estimates might nevertheless be highly problematic.

Statisticians usually use the word “prediction” in a technical sense. *Prediction* in this sense does not refer to “predicting the future” (statisticians call that *forecasting*) but rather to guessing the response from the values of the regressors in an observation taken under the same circumstances as the sample from which the regression equation was estimated. If you developed a regression model for predicting consumer preferences in 1977, it might not give very good predictions in 2007 no matter how well it did in 1977. If it is the future you want to predict, your model must include whatever relevant factors might change over time. If the process you are studying does in fact change over time, you must take observations at several, perhaps many, different times. Analysis of such data is the province of SAS/STAT procedures such as MIXED and GLIMMIX and SAS/ETS procedures such as AUTOREG and STATESPACE. See Chapter 41, “[The GLIMMIX Procedure](#),” and Chapter 59, “[The MIXED Procedure](#),” for more information about modeling serial correlation in longitudinal, repeated measures, or time series data with SAS/STAT mixed modeling procedures. See the *SAS/ETS User’s Guide* for more information about the AUTOREG and STATESPACE procedures.

The comments in the rest of this section are directed toward linear least squares regression. For more detailed discussions of the interpretation of regression statistics, see Darlington (1968); Mosteller and Tukey (1977); Weisberg (1985); Younger (1979).

Interpreting Parameter Estimates from a Controlled Experiment

Parameter estimates are easiest to interpret in a controlled experiment in which the regressors are manipulated independently of each other. In a well-designed experiment, such as a randomized factorial design with replications in each cell, you can use lack-of-fit tests and estimates of the standard error of prediction to determine whether the model describes the experimental process with adequate precision. If so, a regression coefficient estimates the amount by which the mean response changes when the regressor is changed by one unit while all the other regressors are unchanged. However, if the model involves interactions or polynomial terms, it might not be possible to interpret individual regression coefficients. For example, if the equation includes both linear and quadratic terms for a given variable, you cannot physically change the value of the linear term without also changing the value of the quadratic term. Sometimes it might be possible to recode the regressors, such as by using orthogonal polynomials, to simplify the interpretation.

If the nonstatistical aspects of the experiment are also treated with sufficient care (such as the use of placebos and double blinds), then you can state conclusions in causal terms; that is, this change in a regressor causes that change in the response. Causality can never be inferred from statistical results alone or from an observational study.

If the model you fit is not the true model, then the parameter estimates can depend strongly on the particular values of the regressors used in the experiment. For example, if the response is actually a quadratic function of a regressor but you fit a linear function, the estimated slope can be a large negative value if you use only small values of the regressor, a large positive value if you use only large values of the regressor, or near zero if you use both large and small regressor values. When you report the results of an experiment, it is important to include the values of the regressors. It is also important to avoid extrapolating the regression equation outside the range of regressors in the sample.

Interpreting Parameter Estimates from an Observational Study

In an observational study, parameter estimates can be interpreted as the expected difference in response of two observations that differ by one unit on the regressor in question and that have the same values for all other regressors. You cannot make inferences about “changes” in an observational study since you have not actually changed anything. It might not be possible even in principle to change one regressor independently of all the others. Neither can you draw conclusions about causality without experimental manipulation.

If you conduct an observational study and you do not know the true form of the model, interpretation of parameter estimates becomes even more convoluted. A coefficient must then be interpreted as an average over the sampled population of expected differences in response of observations that differ by one unit on only one regressor. The considerations that are discussed under controlled experiments for which the true model is not known also apply.

Comparing Parameter Estimates

Two coefficients in the same model can be directly compared only if the regressors are measured in the same units. You can make any coefficient large or small just by changing the units. If you convert a regressor from feet to miles, the parameter estimate is multiplied by 5280.

Sometimes standardized regression coefficients are used to compare the effects of regressors measured in different units. Standardized estimates are defined as the estimates that result when all variables are standardized to a mean of 0 and a variance of 1. Standardized estimates are computed by multiplying the original estimates by the sample standard deviation of the regressor variable and dividing by the sample standard deviation of the dependent variable.

Standardizing the variables effectively makes the standard deviation the unit of measurement. This makes sense only if the standard deviation is a meaningful quantity, which usually is the case only if the observations are sampled from a well-defined population. In a controlled experiment, the standard deviation of a regressor depends on the values of the regressor selected by the experimenter. Thus, you can make a standardized regression coefficient large by using a large range of values for the regressor.

In some applications you might be able to compare regression coefficients in terms of the practical range of variation of a regressor. Suppose that each independent variable in an industrial process can be set to values only within a certain range. You can rescale the variables so that the smallest possible value is zero and the largest possible value is one. Then the unit of measurement for each regressor is the maximum possible range of the regressor, and the parameter estimates are comparable in that sense. Another possibility is to

scale the regressors in terms of the cost of setting a regressor to a particular value, so comparisons can be made in monetary terms.

Correlated Regressors

In an experiment, you can often select values for the regressors such that the regressors are orthogonal (not correlated with each other). Orthogonal designs have enormous advantages in interpretation. With orthogonal regressors, the parameter estimate for a given regressor does not depend on which other regressors are included in the model, although other statistics such as standard errors and p -values might change.

If the regressors are correlated, it becomes difficult to disentangle the effects of one regressor from another, and the parameter estimates can be highly dependent on which regressors are used in the model. Two correlated regressors might be nonsignificant when tested separately but highly significant when considered together. If two regressors have a correlation of 1.0, it is impossible to separate their effects.

It might be possible to recode correlated regressors to make interpretation easier. For example, if X and Y are highly correlated, they could be replaced in a linear regression by $X + Y$ and $X - Y$ without changing the fit of the model or statistics for other regressors.

Errors in the Regressors

If there is error in the measurements of the regressors, the parameter estimates must be interpreted with respect to the measured values of the regressors, not the true values. A regressor might be statistically nonsignificant when measured with error even though it would have been highly significant if measured accurately.

Probability Values (p -Values)

Probability values (p -values) do not necessarily measure the importance of a regressor. An important regressor can have a large (nonsignificant) p -value if the sample is small, if the regressor is measured over a narrow range, if there are large measurement errors, or if another closely related regressor is included in the equation. An unimportant regressor can have a very small p -value in a large sample. Computing a confidence interval for a parameter estimate gives you more useful information than just looking at the p -value, but confidence intervals do not solve problems of measurement errors in the regressors or highly correlated regressors.

Interpreting R^2

R square is usually defined as the proportion of variance of the response that is predictable from (can be explained by) the regressor variables. It might be easier to interpret $\sqrt{1 - R^2}$, which is approximately the factor by which the standard error of prediction is reduced by the introduction of the regressor variables.

R square is easiest to interpret when the observations, including the values of both the regressors and response, are randomly sampled from a well-defined population. Nonrandom sampling can greatly distort R square. For example, excessively large values of R square can be obtained by omitting from the sample observations with regressor values near the mean.

In a controlled experiment, R square depends on the values chosen for the regressors. A wide range of regressor values generally yields a larger R square than a narrow range. In comparing the results of two experiments on the same variables but with different ranges for the regressors, you should look at the standard error of prediction (root mean square error) rather than R square.

Whether a given R square value is considered to be large or small depends on the context of the particular study. A social scientist might consider an R square of 0.30 to be large, while a physicist might consider 0.98 to be small.

You can always get an R square arbitrarily close to 1.0 by including a large number of completely unrelated regressors in the equation. If the number of regressors is close to the sample size, R square is very biased. In such cases, the adjusted R square and related statistics discussed by Darlington (1968) are less misleading.

If you fit many different models and choose the model with the largest R square, all the statistics are biased and the p -values for the parameter estimates are not valid. Caution must be taken with the interpretation of R square for models with no intercept term. As a general rule, no-intercept models should be fit only when theoretical justification exists and the data appear to fit a no-intercept framework. The R square in those cases is measuring something different (see Kvalseth 1985).

Incorrect Data Values

All regression statistics can be seriously distorted by a single incorrect data value. A decimal point in the wrong place can completely change the parameter estimates, R square, and other statistics. It is important to check your data for outliers and influential observations. Residual and influence diagnostics are particularly useful in this regard.

When a data point is declared as influential or as outlying as measured by a particular model diagnostic, this does not imply that the case should be excluded from the analysis. The label “outlier” does not have a negative connotation. It means that a data point is unusual with respect to the model at hand. If your data follow a strong curved trend and you fit a linear regression, then many data points might be labeled as outliers not because they are “bad” or incorrect data values, but because your model is not appropriate.

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Chapter 5

Introduction to Analysis of Variance Procedures

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Overview: Analysis of Variance Procedures

The statistical term “analysis of variance” is used in a variety of circumstances in statistical theory and applications. In the *narrowest* sense, and the original sense of the phrase, it signifies a decomposition of a variance into contributing components. This was the sense used by R. A. Fisher when he defined the term to mean the expression of genetic variance as a sum of variance components due to environment, heredity, and so forth:

$$\sigma^2 = \sigma_1^2 + \sigma_2^2 + \cdots + \sigma_p^2$$

In this sense of the term, the SAS/STAT procedures that fit variance component models, such as the GLIMMIX, HPMIXED, MIXED, NESTED, and VARCOMP procedures, are “true” analysis of variance procedures.

Analysis of variance methodology in a slightly broader sense—and the sense most frequently understood today—applies the idea of an additive decomposition of variance to an additive decomposition of *sums of*

squares, whose expected values are functionally related to components of variation. A collection of sums of squares that measure and can be used for inference about meaningful features of a model is called a *sum of squares analysis of variance*, whether or not such a collection is an additive decomposition. In a linear model, the decomposition of sums of squares can be expressed in terms of projections onto orthogonal subspaces spanned by the columns of the design matrix \mathbf{X} . This is the general approach followed in the section “Analysis of Variance” on page 57 in Chapter 3, “Introduction to Statistical Modeling with SAS/STAT Software.” Depending on the statistical question at hand, the projections can be formulated based on estimable functions, with different types of estimable functions giving rise to different types of sums of squares. Note that not all sum of squares analyses necessarily correspond to additive decompositions. For example, the Type III sums of squares often test hypotheses about the model that are more meaningful than those corresponding to the Type I sums of squares. But while the Type I sums of squares additively decompose the sum of squares due to all model contributions, the Type III sums of squares do not necessarily add up to any useful quantity. The four types of estimable functions in SAS/STAT software, their interpretation, and their construction are discussed in Chapter 15, “The Four Types of Estimable Functions.” The application of sum of squares analyses is not necessarily limited to models with classification effects (factors). The methodology also applies to linear regression models that contain only continuous regressor variables.

An even broader sense of the term “analysis of variance” pertains to statistical models that contain classification effects (factors), and in particular, to models that contain *only* classification effects. Any statistical approach that measures features of such a model and can be used for inference is called a *general analysis of variance*. Thus the procedures for general analysis of variance in SAS/STAT are considered to be those that can fit statistical models containing factors, whether the data are experimental or observational. Some procedures for general analysis of variance have a statistical estimation principle that gives rise to a sum of squares analysis as discussed previously; others express a factor’s contribution to the model fit in some other form. Note that this view of analysis of variance includes, for example, maximum likelihood estimation in generalized linear models with the GENMOD procedure, restricted maximum likelihood estimation in linear mixed models with the MIXED procedure, the estimation of variance components with the VARCOMP procedure, the comparison of means of groups with the TTEST procedure, and the nonparametric analysis of rank scores with the NPAR1WAY procedure, and so on.

In summary, analysis of variance in the contemporary sense of statistical modeling and analysis is more aptly described as *analysis of variation*, the study of the influences on the variation of a phenomenon. This can take, for example, the following forms:

- an analysis of variance table based on sums of squares followed by more specific inquiries into the relationship among factors and their levels
- a deviance decomposition in a generalized linear model
- a series of Type III tests followed by comparisons of least squares means in a mixed model

Procedures That Perform Sum of Squares Analysis of Variance

The flagship procedure in SAS/STAT software for linear modeling with sum of squares analysis techniques is the GLM procedure. It handles most standard analysis of variance problems. The following list provides descriptions of PROC GLM and other procedures that are used for more specialized situations:

ANOVA	performs analysis of variance, multivariate analysis of variance, and repeated measures analysis of variance for <i>balanced</i> designs. PROC ANOVA also performs multiple comparison tests on arithmetic means.
GLM	performs analysis of variance, regression, analysis of covariance, repeated measures analysis, and multivariate analysis of variance. PROC GLM produces several diagnostic measures, performs tests for random effects, provides contrasts and estimates for customized hypothesis tests, provides tests for means adjusted for covariates, and performs multiple-comparison tests on both arithmetic and adjusted means.
LATTICE	computes the analysis of variance and analysis of simple covariance for data from an experiment with a lattice design. PROC LATTICE analyzes balanced square lattices, partially balanced square lattices, and some rectangular lattices.
MIXED	performs mixed model analysis of variance and repeated measures analysis of variance via covariance structure modeling. When you choose one of the method-of-moment estimation techniques, the MIXED procedure produces an analysis of variance table with sums of squares, mean squares, and expected mean squares. PROC MIXED constructs statistical tests and intervals, enables customized contrasts and estimates, and computes empirical Bayes predictions.
NESTED	performs analysis of variance and analysis of covariance for purely nested random models.
ORTHOREG	performs regression by using the Gentleman-Givens computational method. For ill-conditioned data, PROC ORTHOREG can produce more accurate parameter estimates than other procedures, such as PROC GLM. See Chapter 66, “ The ORTHOREG Procedure ,” for more information.
VARCOMP	estimates variance components for random or mixed models. If you choose the METHOD=TYPE1 or METHOD=GRR option, the VARCOMP procedure produces an analysis of variance table with sums of squares that correspond to the random effects in your models.
TRANSREG	fits univariate and multivariate linear models, optionally with spline and other nonlinear transformations. Models include ordinary regression and ANOVA, multiple and multivariate regression, metric and nonmetric conjoint analysis, metric and nonmetric vector and ideal point preference mapping, redundancy analysis, canonical correlation, and response surface regression. See Chapter 97, “ The TRANSREG Procedure ,” for more information.

Procedures That Perform General Analysis of Variance

Many procedures in SAS/STAT enable you to incorporate classification effects into your model and to perform statistical inferences for experimental factors and their interactions. These procedures do not necessarily rely on sums of squares decompositions to perform these inferences. Examples of such procedures are the CATMOD, GENMOD, GLIMMIX, LOGISTIC, NPARIWAY, and TTEST procedures. In fact, any one of the more than two dozen SAS/STAT modeling procedures that include a CLASS statement can be said to perform analysis of variance in this general sense. For more information about individual procedures, refer to their corresponding chapters in this documentation.

The following section discusses procedures in SAS/STAT that compute analysis of variance in models with classification factors in the narrow sense—that is, they produce analysis of variance tables and form F tests based on sums of squares, mean squares, and expected mean squares.

The subsequent sections discuss procedures that perform statistical inference in models with classification effects in the broader sense.

The following section also presents an overview of some of the fundamental features of analysis of variance. Subsequent sections describe how this analysis is performed with procedures in SAS/STAT software. For more detail, see the chapters for the individual procedures. Additional sources are described in the section References.

Statistical Details for Analysis of Variance

From Sums of Squares to Linear Hypotheses

Analysis of variance (ANOVA) is a technique for analyzing data in which one or more *response* (or *dependent* or simply Y) variables are measured under various conditions identified by one or more classification variables. The combinations of levels for the classification variables form the cells of the design for the data. This design can be the result of a controlled experiment or the result of an observational study in which you observe factors and factor level combinations in an uncontrolled environment. For example, an experiment might measure weight change (the dependent variable) for men and women who participated in three different weight-loss programs. The six cells of the design are formed by the six combinations of gender (men, women) and program (A, B, C).

In an analysis of variance, the variation in the response is separated into variation attributable to differences between the classification variables and variation attributable to random error. An analysis of variance constructs tests to determine the significance of the classification effects. A typical goal in such an analysis is to compare means of the response variable for various combinations of the classification variables.

The least squares principle is central to computing sums of squares in analysis of variance models. Suppose that you are fitting the linear model $\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$ and that the error terms satisfy the usual assumptions (uncorrelated, zero mean, homogeneous variance). Further, suppose that \mathbf{X} is partitioned according to several model effects, $\mathbf{X} = [\mathbf{X}_1 \ \mathbf{X}_2 \ \cdots \ \mathbf{X}_k]$. If $\hat{\boldsymbol{\beta}}$ denotes the ordinary least squares solution for this model, then the sum of squares attributable to the overall model can be written as

$$\text{SSM} = \hat{\boldsymbol{\beta}}' \mathbf{X}' \mathbf{Y} = \mathbf{Y}' \mathbf{H} \mathbf{Y}$$

where \mathbf{H} is the “hat” matrix $\mathbf{H} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'$. (This model sum of squares is not yet corrected for the presence of an explicit or implied intercept. This adjustment would consist of subtracting $n\bar{Y}^2$ from SSM.) Because of the properties of the hat matrix \mathbf{H} , you can write $\mathbf{X}' = \mathbf{X}'\mathbf{H}$ and $\mathbf{H}\mathbf{X} = \mathbf{X}$. The (uncorrected) model sum of squares thus can also be written as

$$\text{SSM} = \hat{\boldsymbol{\beta}}' (\mathbf{X}'\mathbf{X}) \hat{\boldsymbol{\beta}}$$

This step is significant, because it demonstrates that sums of squares can be identified with quadratic functions in the least squares coefficients. The generalization of this idea is to do the following:

- consider hypotheses of interest in an analysis of variance model
- express the hypotheses in terms of linear estimable functions of the parameters
- compute the sums of squares associated with the estimable function
- construct statistical tests based on the sums of squares

Decomposing a model sum of squares into sequential, additive components, testing the significance of experimental factors, comparing factor levels, and performing other statistical inferences fall within this generalization. Suppose that $\mathbf{L}\boldsymbol{\beta}$ is an estimable function (see the section “Estimable Functions” on page 59 in Chapter 3, “Introduction to Statistical Modeling with SAS/STAT Software,” and Chapter 15, “The Four Types of Estimable Functions,” for details). The sum of squares associated with the hypothesis $H: \mathbf{L}\boldsymbol{\beta} = \mathbf{0}$ is

$$SS(H) = SS(\mathbf{L}\boldsymbol{\beta} = \mathbf{0}) = \widehat{\boldsymbol{\beta}}' \mathbf{L}' (\mathbf{L}(\mathbf{X}'\mathbf{X})^{-1} \mathbf{L}')^{-1} \mathbf{L} \widehat{\boldsymbol{\beta}}$$

One application would be to form sums of squares associated with the different components of \mathbf{X} . For example, you can form a matrix \mathbf{L}_2 matrix such that $\mathbf{L}_2\boldsymbol{\beta} = \mathbf{0}$ tests the effect of adding the columns for \mathbf{X}_2 to an empty model or to test the effect of adding \mathbf{X}_2 to a model that already contains \mathbf{X}_1 .

These sums of squares can also be expressed as the difference between two residual sums of squares, since $\mathbf{L}\boldsymbol{\beta} = \mathbf{0}$ can be thought of as a (linear) restriction on the parameter estimates in the model:

$$SS(H) = SSR(\text{constrained model}) - SSR(\text{full model})$$

If, in addition to the usual assumptions mentioned previously, the model errors are assumed to be normally distributed, then $SS(H)$ follows a distribution that is proportional to a chi-square distribution. This fact, and the independence of $SS(H)$ from the residual sum of squares, enables you to construct F tests based on sums of squares in least squares models.

The extension of sum of squares analysis of variance to general analysis of variance for classification effects depends on the fact that the distributional properties of quadratic forms in normal random variables are well understood. It is not necessary to first formulate a sum of squares to arrive at an exact or even approximate F test. The generalization of the expression for $SS(H)$ is to form test statistics based on quadratic forms

$$\widehat{\boldsymbol{\beta}}' \mathbf{L}' \text{Var} [\mathbf{L} \widehat{\boldsymbol{\beta}}]^{-1} \mathbf{L} \widehat{\boldsymbol{\beta}}$$

that follow a chi-square distribution if $\widehat{\boldsymbol{\beta}}$ is normally distributed.

Tests of Effects Based on Expected Mean Squares

Statistical tests in analysis of variance models can be constructed by comparing independent mean squares. To test a particular null hypothesis, you compute the ratio of two mean squares that have the same expected value under that hypothesis; if the ratio is much larger than 1, then that constitutes significant evidence against the null. In particular, in an analysis of variance model with fixed effects only, the expected value of each mean square has two components: quadratic functions of fixed parameters and random variation. For example, for a fixed effect called A, the expected value of its mean square is

$$E[\text{MS}(A)] = Q(\boldsymbol{\beta}) + \sigma^2$$

where σ^2 is the common variance of the ϵ_i .

Under the null hypothesis of no A effect, the fixed portion $Q(\beta)$ of the expected mean square is zero. This mean square is then compared to another mean square—say, $MS(E)$ —that is independent of the first and has the expected value σ^2 . The ratio of the two mean squares

$$F = \frac{MS(A)}{MS(E)}$$

has an F distribution under the null hypothesis.

When the null hypothesis is false, the numerator term has a larger expected value, but the expected value of the denominator remains the same. Thus, large F values lead to rejection of the null hypothesis. The probability of getting an F value at least as large as the one observed given that the null hypothesis is true is called the *significance probability value* (or the p -value). A p -value of less than 0.05, for example, indicates that data with *no* A effect will yield F values as large as the one observed less than 5% of the time. This is usually considered moderate evidence that there *is* a real A effect. Smaller p -values constitute even stronger evidence. Larger p -values indicate that the effect of interest is less than random noise. In this case, you can conclude either that there is no effect at all or that you do not have enough data to detect the differences being tested.

The actual pattern in expected mean squares of terms related to fixed quantities ($Q(\beta)$) and functions of variance components depends on which terms in your model are fixed effects and which terms are random effects. This has bearing on how F statistics can be constructed. In some instances, exact tests are not available, such as when a linear combination of expected mean squares is necessary to form a proper denominator for an F test and a Satterthwaite approximation is used to determine the degrees of freedom of the approximation. The GLM and MIXED procedures can generate tables of expected mean squares and compute degrees of freedom by Satterthwaite's method. The MIXED and GLIMMIX procedures can apply Satterthwaite approximations and other degrees-of-freedom computations more widely than in analysis of variance models. See the section “Fixed, Random, and Mixed Models” on page 31 in Chapter 3, “Introduction to Statistical Modeling with SAS/STAT Software,” for a discussion of fixed versus random effects in statistical models.

Analysis of Variance for Fixed-Effect Models

PROC GLM for General Linear Models

The GLM procedure is the flagship tool for classical analysis of variance in SAS/STAT software. It performs analysis of variance by using least squares regression to fit general linear models. Among the statistical methods available in PROC GLM are regression, analysis of variance, analysis of covariance, multivariate analysis of variance, repeated measures analysis, and partial correlation analysis.

While PROC GLM can handle most common analysis of variance problems, other procedures are more efficient or have more features than PROC GLM for certain specialized analyses, or they can handle specialized models that PROC GLM cannot. Much of the rest of this chapter is concerned with comparing PROC GLM to other procedures.

PROC ANOVA for Balanced Designs

When you design an experiment, you choose how many experimental units to assign to each combination of levels (or cells) in the classification. In order to achieve good statistical properties and simplify the computations, you typically attempt to assign the same number of units to every cell in the design. Such designs are called *balanced designs*.

In SAS/STAT software, you can use the ANOVA procedure to perform analysis of variance for balanced data. The ANOVA procedure performs computations for analysis of variance that assume the balanced nature of the data. These computations are simpler and more efficient than the corresponding general computations performed by PROC GLM. Note that PROC ANOVA can be applied to certain designs that are not balanced in the strict sense of equal numbers of observations for all cells. These additional designs include all one-way models, regardless of how unbalanced the cell counts are, as well as Latin squares, which do not have data in all cells. In general, however, the ANOVA procedure is recommended only for balanced data. **If you use ANOVA to analyze a design that is not balanced, you must assume responsibility for the validity of the output.** You are responsible for recognizing incorrect results, which might include negative values reported for the sums of squares. If you are not certain that your data fit into a balanced design, then you probably need the framework of general linear models in the GLM procedure.

Comparing Group Means

The F test for a classification factor that has more than two levels tells you whether the level effects are significantly different from each other, but it does not tell you which levels differ from which other levels.

If the level comparisons are expressed through differences of the arithmetic cell means, you can use the MEANS statement in the GLM and ANOVA procedure for comparison. If arithmetic means are not appropriate for comparison, for example, because your data are unbalanced or means need to be adjusted for other model effects, then you can use the LSMEANS statement in the GLIMMIX, GLM, and MIXED procedures for level comparisons.

If you have specific comparisons in mind, you can use the CONTRAST statement in these procedures to make these comparisons. However, if you make many comparisons that use some given significance level (0.05, for example), you are more likely to make a type 1 error (incorrectly rejecting a hypothesis that the means are equal) simply because you have more chances to make the error.

Multiple-comparison methods give you more detailed information about the differences among the means and enable you to control error rates for a multitude of comparisons. A variety of multiple-comparison methods are available with the MEANS statement in both the ANOVA and GLM procedures, as well as the LSMEANS statement in the GLIMMIX, GLM, and MIXED procedures. These are described in detail in the section “Multiple Comparisons” on page 3349 in Chapter 42, “The GLM Procedure,” and in Chapter 41, “The GLIMMIX Procedure,” and Chapter 59, “The MIXED Procedure.”

PROC TTEST for Comparing Two Groups

If you want to perform an analysis of variance and have only one classification variable with two levels, you can use PROC TTEST. In this special case, the results generated by PROC TTEST are equivalent to the results generated by PROC ANOVA or PROC GLM.

You can use PROC TTEST with balanced or unbalanced groups. In addition to the test assuming equal variances, PROC TTEST also performs a Satterthwaite test assuming unequal variances.

The TTEST procedure also performs equivalence tests, computes confidence limits, and supports both normal and lognormal data. If you have an AB/BA crossover design with no carryover effects, then you can use the TTEST procedure to analyze the treatment and period effects.

The PROC NPAR1WAY procedure performs nonparametric analogues to t tests. See Chapter 16, “Introduction to Nonparametric Analysis,” for an overview and Chapter 65, “The NPAR1WAY Procedure,” for details on PROC NPAR1WAY.

Analysis of Variance for Categorical Data and Generalized Linear Models

A *categorical variable* is defined as one that can assume only a limited number of values. For example, a person’s gender is a categorical variable that can assume one of two values. Variables with levels that simply name a group are said to be measured on a *nominal scale*. Categorical variables can also be measured using an *ordinal scale*, which means that the levels of the variable are ordered in some way. For example, responses to an opinion poll are usually measured on an ordinal scale, with levels ranging from “strongly disagree” to “no opinion” to “strongly agree.”

For two categorical variables, one measured on an ordinal scale and one measured on a nominal scale, you can assign scores to the levels of the ordinal variable and test whether the mean scores for the different levels of the nominal variable are significantly different. This process is analogous to performing an analysis of variance on continuous data, which can be performed by PROC CATMOD. If there are n nominal variables, rather than 1, then PROC CATMOD can perform an n -way analysis of variance of the mean scores.

For two categorical variables measured on a nominal scale, you can test whether the distribution of the first variable is significantly different for the levels of the second variable. This process is an analysis of variance of proportions, rather than means, and can be performed by PROC CATMOD. The corresponding n -way analysis of variance can also be performed by PROC CATMOD.

See Chapter 8, “Introduction to Categorical Data Analysis Procedures,” and Chapter 30, “The CATMOD Procedure,” for more information.

The GENMOD procedure uses maximum likelihood estimation to fit generalized linear models. This family includes models for categorical data such as logistic, probit, and complementary log-log regression for binomial data and Poisson regression for count data, as well as continuous models such as ordinary linear regression, gamma, and inverse Gaussian regression models. PROC GENMOD performs analysis of variance through likelihood ratio and Wald tests of fixed effects in generalized linear models, and provides contrasts and estimates for customized hypothesis tests. It performs analysis of repeated measures data with generalized estimating equation (GEE) methods.

See Chapter 8, “Introduction to Categorical Data Analysis Procedures,” and Chapter 40, “The GENMOD Procedure,” for more information.

Nonparametric Analysis of Variance

Analysis of variance is sensitive to the distribution of the error term. If the error term is not normally distributed, the statistics based on normality can be misleading. The traditional test statistics are called *parametric tests* because they depend on the specification of a certain probability distribution except for a set of free parameters. Parametric tests are said to depend on distributional assumptions. Nonparametric methods perform the tests without making any strict distributional assumptions. Even if the data are distributed normally, nonparametric methods are often almost as powerful as parametric methods.

Most nonparametric methods are based on taking the ranks of a variable and analyzing these ranks (or transformations of them) instead of the original values. The NPAR1WAY procedure performs a nonparametric one-way analysis of variance. Other nonparametric tests can be performed by taking ranks of the data (using the RANK procedure) and using a regular parametric procedure (such as GLM or ANOVA) to perform the analysis. Some of these techniques are outlined in the description of PROC RANK in *SAS Language Reference: Concepts* and in Conover and Iman (1981).

Constructing Analysis of Variance Designs

Analysis of variance is most often used for data from designed experiments. You can use the PLAN procedure to construct designs for many experiments. For example, PROC PLAN constructs designs for completely randomized experiments, randomized blocks, Latin squares, factorial experiments, certain balanced incomplete block designs, and balanced crossover designs.

Randomization, or randomly assigning experimental units to cells in a design and to treatments within a cell, is another important aspect of experimental design. For either a new or an existing design, you can use PROC PLAN to randomize the experimental plan.

Additional features for design of experiments are available in SAS/QC software. The FACTEX and OPTEX procedures can construct a wide variety of designs, including factorials, fractional factorials, and D-optimal or A-optimal designs. These procedures, as well as the ADX Interface, provide features for randomizing and replicating designs; saving the design in an output data set; and interactively changing the design by changing its size, use of blocking, or the search strategies used. For more information, see the *SAS/QC User's Guide*.

For More Information

Analysis of variance was pioneered by Fisher (1925). For a general introduction to analysis of variance, see an intermediate statistical methods textbook such as Steel and Torrie (1980); Snedecor and Cochran (1980); Milliken and Johnson (1984); Mendenhall (1968); John (1971); Ott (1977); Kirk (1968). A classic source is Scheffé (1959). Freund, Littell, and Spector (1991) bring together a treatment of these statistical methods and SAS/STAT software procedures. Schlotzhauer and Littell (1997) cover how to perform *t* tests and one-way analysis of variance with SAS/STAT procedures. Texts on linear models include Searle (1971); Graybill (1976); Hocking (1984). Kennedy and Gentle (1980) survey the computing aspects. Other references appear in the reference section.

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Chapter 6

Introduction to Mixed Modeling Procedures

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Overview: Mixed Modeling Procedures

A mixed model is a model that contains fixed and random effects. Since all statistical models contain some stochastic component and many models contain a residual error term, the preceding sentence deserves some clarification. The classical linear model $\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$ contains the parameters $\boldsymbol{\beta}$ and the random vector $\boldsymbol{\epsilon}$. The vector $\boldsymbol{\beta}$ is a vector of fixed-effects parameters; its elements are unknown constants to be estimated from the data. A mixed model in the narrow sense also contains random effects, which are unobservable random variables. If the vector of random effects is denoted by $\boldsymbol{\gamma}$, then a linear mixed model can be written as

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\boldsymbol{\gamma} + \boldsymbol{\epsilon}$$

In a broader sense, mixed modeling and mixed model software is applied to special cases and generalizations of this model. For example, a purely random effects model, $\mathbf{Y} = \mathbf{Z}\boldsymbol{\gamma} + \boldsymbol{\epsilon}$, or a correlated-error model, $\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$, is subsumed by mixed modeling methodology.

Over the last few decades virtually every form of classical statistical model has been enhanced to accommodate random effects. The linear model has been extended to the linear mixed model, generalized linear models have been extended to generalized linear mixed models, and so on. In parallel with this trend,

SAS/STAT software offers a number of classical and contemporary mixed modeling tools. The aim of this chapter is to provide a brief introduction and comparison of the procedures for mixed model analysis (in the broad sense) in SAS/STAT software. The theory and application of mixed models are discussed at length in many monographs, including Milliken and Johnson (1992); Diggle, Liang, and Zeger (1994); Davidian and Giltinan (1995); Verbeke and Molenberghs (1997, 2000); Vonesh and Chinchilli (1997); Demidenko (2004); Molenberghs and Verbeke (2005); and Littell et al. (2006).

The following procedures in SAS/STAT software can perform mixed and random effects analysis to various degrees:

GLM	is primarily a tool for fitting linear models by least squares. The GLM procedure has some capabilities for including random effects in a statistical model and for performing statistical tests in mixed models. Repeated measures analysis is also possible with the GLM procedure, assuming unstructured covariance modeling. Estimation methods for covariance parameters in PROC GLM are based on the method of moments, and a portion of its output applies only to the fixed-effects model.
GLIMMIX	fits generalized linear mixed models by likelihood-based techniques. As in the MIXED procedure, covariance structures are modeled parametrically. The GLIMMIX procedure also has built-in capabilities for mixed model smoothing and joint modeling of heterocategorical multivariate data.
HPMIXED	fits linear mixed models by sparse-matrix techniques. The HPMIXED procedure is designed to handle large mixed model problems, such as the solution of mixed model equations with thousands of fixed-effects parameters and random-effects solutions.
LATTICE	computes the analysis of variance and analysis of simple covariance for data from an experiment with a lattice design. PROC LATTICE analyzes balanced square lattices, partially balanced square lattices, and some rectangular lattices. Analyses performed with the LATTICE procedure can also be performed as mixed models for complete or incomplete block designs with the MIXED procedure.
MIXED	performs mixed model analysis and repeated measures analysis by way of structured covariance models. The MIXED procedure estimates parameters by likelihood or moment-based techniques. You can compute mixed model diagnostics and influence analysis for observations and groups of observations. The default fitting method maximizes the restricted likelihood of the data under the assumption that the data are normally distributed and any missing data are missing at random. This general framework accommodates many common correlated-data methods, including variance component models and repeated measures analyses.
NESTED	performs analysis of variance and analysis of covariance for purely nested random-effects models. Because of its customized algorithms, PROC NESTED can be useful for large data sets with nested random effects.
NLMIXED	fits mixed models in which the fixed or random effects enter nonlinearly. The NLMIXED procedure requires that you specify components of your mixed model via programming statements. Some built-in distributions enable you to easily specify the conditional distribution of the data, given the random effects.
VARCOMP	estimates variance components for random or mixed models.

The focus in the remainder of this chapter is on procedures designed for random effects and mixed model analysis: the GLIMMIX, HPMIXED, MIXED, NESTED, NLMIXED, and VARCOMP procedures. The

important distinction between fixed and random effects in statistical models is addressed in the section “Fixed, Random, and Mixed Models” on page 31, in Chapter 3, “Introduction to Statistical Modeling with SAS/STAT Software.”

Types of Mixed Models

Linear, Generalized Linear, and Nonlinear Mixed Models

The linear model shown at the beginning of this chapter was incomplete because the distributional properties of the random variables and their relationship were not specified. In this section the specification of the models is completed and the three model classes, linear mixed models (LMM), generalized linear mixed models (GLMM), and nonlinear mixed models (NLMM), are delineated.

Linear Mixed Model

It is a defining characteristic of the class of linear mixed models (LMM), the class of generalized linear mixed models (GLMM), and the class of nonlinear mixed models (NLMM) that the random effects are normally distributed. In the linear mixed model, this also applies to the error term; furthermore, the errors and random effects are uncorrelated. The standard linear mixed model (LMM) is thus represented by the following assumptions:

$$\begin{aligned} \mathbf{Y} &= \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\boldsymbol{\gamma} + \boldsymbol{\epsilon} \\ \boldsymbol{\gamma} &\sim N(\mathbf{0}, \mathbf{G}) \\ \boldsymbol{\epsilon} &\sim N(\mathbf{0}, \mathbf{R}) \\ \text{Cov}[\boldsymbol{\gamma}, \boldsymbol{\epsilon}] &= \mathbf{0} \end{aligned}$$

The matrices \mathbf{G} and \mathbf{R} are covariance matrices for the random effects and the random errors, respectively. A *G-side* random effect in a linear mixed model is an element of $\boldsymbol{\gamma}$, and its variance is expressed through an element in \mathbf{G} . An *R-side* random variable is an element of $\boldsymbol{\epsilon}$, and its variance is an element of \mathbf{R} . The GLIMMIX, HPMIXED, and MIXED procedures express the \mathbf{G} and \mathbf{R} matrices in parametric form—that is, you structure the covariance matrix, and its elements are expressed as functions of some parameters, known as the *covariance parameters* of the mixed models. The NLMIXED procedure also parameterizes the covariance structure, but you accomplish this with programming statements rather than with predefined syntax.

Since the right side of the model equation contains multiple random variables, the stochastic properties of \mathbf{Y} can be examined by conditioning on the random effects, or through the marginal distribution. Because of the linearity of the G-side random effects and the normality of the random variables, the conditional and the marginal distribution of the data are also normal with the following mean and variance matrices:

$$\begin{aligned} \mathbf{Y}|\boldsymbol{\gamma} &\sim N(\mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\boldsymbol{\gamma}, \mathbf{R}) \\ \mathbf{Y} &\sim N(\mathbf{X}\boldsymbol{\beta}, \mathbf{V}) \\ \mathbf{V} &= \mathbf{Z}\mathbf{G}\mathbf{Z}' + \mathbf{R} \end{aligned}$$

Parameter estimation in linear mixed models is based on likelihood or method-of-moment techniques. The default estimation method in PROC MIXED, and the only method available in PROC HP MIXED, is restricted (residual) maximum likelihood, a form of likelihood estimation that accounts for the parameters in the fixed-effects structure of the model to reduce the bias in the covariance parameter estimates. Moment-based estimation of the covariance parameters is available in the MIXED procedure through the METHOD= option in the PROC MIXED statement. The moment-based estimators are associated with sums of squares, expected mean squares (EMS), and the solution of EMS equations.

Parameter estimation by likelihood-based techniques in linear mixed models maximizes the marginal (restricted) log likelihood of the data—that is, the log likelihood is formed from $\mathbf{Y} \sim N(\mathbf{X}\boldsymbol{\beta}, \mathbf{V})$. This is a model for \mathbf{Y} with mean $\mathbf{X}\boldsymbol{\beta}$ and covariance matrix \mathbf{V} , a correlated-error model. Such *marginal models* arise, for example, in the analysis of time series data, repeated measures, or spatial data, and are naturally subsumed into the linear mixed model family. Furthermore, some mixed models have an equivalent formulation as a correlated-error model, when both give rise to the same marginal mean and covariance matrix. For example, a mixed model with a single variance component is identical to a correlated-error model with compound-symmetric covariance structure, provided that the common correlation is positive.

Generalized Linear Mixed Model

In a generalized linear mixed model (GLMM) the G-side random effects are part of the linear predictor, $\boldsymbol{\eta} = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\boldsymbol{\gamma}$, and the predictor is related nonlinearly to the conditional mean of the data

$$E[\mathbf{Y}|\boldsymbol{\gamma}] = g^{-1}(\boldsymbol{\eta}) = g^{-1}(\mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\boldsymbol{\gamma})$$

where $g^{-1}(\cdot)$ is the inverse link function. The conditional distribution of the data, given the random effects, is a member of the exponential family of distributions, such as the binary, binomial, Poisson, gamma, beta, or chi-square distribution. Because the normal distribution is also a member of the exponential family, the class of the linear mixed models is a subset of the generalized linear mixed models. In order to completely specify a GLMM, you need to do the following:

1. Formulate the linear predictor, including fixed and random effects.
2. Choose a link function.
3. Choose the distribution of the response, conditional on the random effects, from the exponential family.

As an example, suppose that s pairs of twins are randomly selected in a matched-pair design. One of the twins in each pair receives a treatment and the outcome variable is some binary measure. This is a study with s clusters (subjects) and each cluster is of size 2. If Y_{ij} denotes the binary response of twin $j = 1, 2$ in cluster i , then a linear predictor for this experiment could be

$$\eta_{ij} = \beta_0 + \tau x_{ij} + \gamma_i$$

where x_{ij} denotes a regressor variable that takes on the value 1 for the treated observation in each pair, and 0 otherwise. The γ_i are pair-specific random effects that model heterogeneity across sets of twins and that induce a correlation between the members of each pair. By virtue of random sampling the sets of twins,

it is reasonable to assume that the γ_i are independent and have equal variance. This leads to a diagonal \mathbf{G} matrix,

$$\text{Var}[\boldsymbol{\gamma}] = \text{Var} \begin{bmatrix} \gamma_1 \\ \gamma_2 \\ \gamma_3 \\ \vdots \\ \gamma_s \end{bmatrix} = \begin{bmatrix} \sigma_\gamma^2 & 0 & 0 & \cdots & 0 \\ 0 & \sigma_\gamma^2 & 0 & \cdots & 0 \\ 0 & 0 & \sigma_\gamma^2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \sigma_\gamma^2 \end{bmatrix}$$

A common link function for binary data is the logit link, which leads in the second step of model formulation to

$$E[Y_{ij}|\gamma_i] = \mu_{ij}|\gamma_i = \frac{1}{1 + \exp\{-\eta_{ij}\}}$$

$$\text{logit} \left\{ \frac{\mu_{ij}|\gamma_i}{1 - \mu_{ij}|\gamma_i} \right\} = \eta_{ij}$$

The final step, choosing a distribution from the exponential family, is automatic in this example; only the binary distribution comes into play to model the distribution of $Y_{ij}|\gamma_i$.

As for the linear mixed model, there is a marginal model in the case of a generalized linear mixed model that results from integrating the joint distribution over the random effects. This marginal distribution is elusive for many GLMMs, and parameter estimation proceeds by either approximating the model or by approximating the marginal integral. Details of these approaches are described in the section “[Generalized Linear Mixed Models Theory](#)” on page 3052, in Chapter 41, “[The GLIMMIX Procedure](#).”

A marginal model, one that models correlation through the \mathbf{R} matrix and does not involve G-side random effects, can also be formulated in the GLMM family; such models are the extension of the correlated-error models in the linear mixed model family. Because nonnormal distributions in the exponential family exhibit a functional mean-variance relationship, fully parametric estimation is not possible in such models. Instead, estimating equations are formed based on first-moment (mean) and second-moment (covariance) assumptions for the marginal data. The approaches for modeling correlated nonnormal data via generalized estimating equations (GEE) fall into this category (see, for example, Liang and Zeger 1986; Zeger and Liang 1986).

Nonlinear Mixed Model

In a nonlinear mixed model (NLMM), the fixed and/or random effects enter the conditional mean function nonlinearly. If the mean function is a general, nonlinear function, then it is customary to assume that the conditional distribution is normal, such as in modeling growth curves or pharmacokinetic response. This is not a requirement, however.

An example of a nonlinear mixed model is the following logistic growth curve model for the j th observation of the i th subject (cluster):

$$f(\boldsymbol{\beta}, \boldsymbol{\gamma}_i, x_{ij}) = \frac{\beta_1 + \gamma_{i1}}{1 + \exp[-(x_{ij} - \beta_2)/(\beta_3 + \gamma_{i2})]}$$

$$Y_{ij} = f(\boldsymbol{\beta}, \boldsymbol{\gamma}_i, x_{ij}) + \epsilon_{ij}$$

$$\begin{bmatrix} \gamma_{i1} \\ \gamma_{i2} \end{bmatrix} \sim N \left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} \sigma_1^2 & \sigma_{12} \\ \sigma_{21} & \sigma_2^2 \end{bmatrix} \right)$$

$$Y_{ij} | \gamma_{i1}, \gamma_{i2} \sim N(0, \sigma_\epsilon^2)$$

The inclusion of R-side covariance structures in GLMM and NLMM models is not as straightforward as in linear mixed models for the following reasons:

- The normality of the conditional distribution in the LMM enables straightforward modeling of the covariance structure because the mean structure and covariance structure are not functionally related.
- The linearity of the random effects in the LMM leads to a marginal distribution that incorporates the \mathbf{R} matrix in a natural and meaningful way.

To incorporate R-side covariance structures when random effects enter nonlinearly or when the data are not normally distributed requires estimation approaches that rely on linearizations of the mixed model. Among such estimation methods are the pseudo-likelihood methods that are available with the GLIMMIX procedure. Generalized estimating equations also solve this marginal estimation problem for nonnormal data; these are available with the GENMOD procedure.

Models for Clustered and Hierarchical Data

Mixed models are often applied in situations where data are clustered, grouped, or otherwise hierarchically organized. For example, observations might be collected by randomly selecting schools in a school district, then randomly selecting classrooms within schools, followed by selecting students within the classroom. A longitudinal study might randomly select individuals and take repeatedly measurements on them. In the first example, a school is a cluster of observations, which consists of smaller clusters (classrooms) and so on. In the longitudinal example the observations for a particular individual form a cluster. Mixed models are popular analysis tools for hierarchically organized data for the following reasons:

- The selection of groups is often performed randomly, so that the associated effects are random effects.
- The data from different clusters are independent by virtue of the random selection or by assumption.
- The observations from the same cluster are often correlated, such as the repeated observations in a repeated measures or longitudinal study.
- It is often believed that there is heterogeneity in model parameters across subjects; for example, slopes and intercepts might differ across individuals in a longitudinal growth study. This heterogeneity, if due to stochastic sources, can be modeled with random effects.

A linear mixed models with clustered, hierarchical structure can be written as a special case of the general linear mixed model by introducing appropriate subscripts. For example, a mixed model with one type of clustering and s clusters can be written as

$$\mathbf{Y}_i = \mathbf{X}_i\boldsymbol{\beta} + \mathbf{Z}_i\boldsymbol{\gamma}_i + \boldsymbol{\epsilon}_i \quad i = 1, \dots, s$$

In SAS/STAT software, the clusters are referred to as *subjects*, and the effects that define clusters in your data can be specified with the SUBJECT= option in the GLIMMIX, HPMIXED, MIXED, and NLMIXED procedures. The vector \mathbf{Y}_i collects the n_i observations for the i th subject. In certain disciplines, the organization of a hierarchical model is viewed in a *bottom-up* form, where the measured observations represent the first level, these are collected into units at the second level, and so forth. In the school data example, the bottom-up approach considers a student's score as the level-1 observation, the classroom as the level-2 unit, and the school district as the level-3 unit (if these were also selected from a population of districts).

The following points are noteworthy about mixed models with SUBJECT= specification:

- A SUBJECT= option is available in the RANDOM statements of the GLIMMIX, HPMIXED, MIXED, and NLMIXED procedures and in the REPEATED statement of the MIXED and HPMIXED procedures.
- A SUBJECT= specification is required in the NLMIXED and HPMIXED procedures. It is not required with any other mixed modeling procedure in SAS/STAT software.
- Specifying models with subjects is usually more computationally efficient in the MIXED and GLIMMIX procedures, especially if the SUBJECT= effects are identical or contained within each other. The computational efficiency of the HPMIXED procedure is not dependent on SUBJECT= effects in the manner in which the MIXED and GLIMMIX procedures are affected.
- There is no limit to the number of SUBJECT= effects with the MIXED, HPMIXED, and GLIMMIX procedures—that is, you can achieve an arbitrary depth of the nesting.

Models with Subjects and Groups

The concept of a subject as a unit of clustering observations in a mixed model has been described in the preceding section. This concept is important for mixed modeling with the GLIMMIX, HPMIXED, MIXED, and NLMIXED procedures. Observations from two subjects are considered uncorrelated in the analysis. Observations from the same subject are potentially correlated, depending on your specification of the covariance structure. Random effects at the subject level always lead to correlation in the marginal distribution of the observations that belong to the subject.

The GLIMMIX, HPMIXED, and MIXED procedures also support the notion of a GROUP= effect in the specification of the covariance structure. Like a subject effect, a G-side group effect identifies independent random effects. In addition to a subject effect, the group effect assumes that the realizations of the random effects correspond to draws from different distributions; in other words, each level of the group effect is associated with a different set of covariance parameters. For example, the following statements in any of these procedures fit a random coefficient model with fixed intercept and slope and subject-specific random intercept and slope:

```
class id;
model y = x;
random intercept x / subject=id;
```

The interpretation of the RANDOM statement is that for each ID an independent draw is made from a bivariate normal distribution with zero mean and a diagonal covariance matrix. In the following statements (in any of these procedures) these independent draws come from different bivariate normal distributions depending on the value of the grp variable.

```
class id grp;
model y = x;
random intercept x / subject=id group=grp;
```

Adding GROUP= effects in your model increases the flexibility to model heterogeneity in the covariance parameters, but it can add numerical complexity to the estimation process.

Linear Mixed Models

You can fit linear mixed models in SAS/STAT software with the GLM, GLIMMIX, HPMIXED, LATTICE, MIXED, NESTED, and VARCOMP procedures.

The procedure specifically designed for statistical estimation in linear mixed models is the MIXED procedure. To fit the linear mixed model

$$\begin{aligned} \mathbf{Y} &= \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\boldsymbol{\gamma} + \boldsymbol{\epsilon} \\ \boldsymbol{\gamma} &\sim N(\mathbf{0}, \mathbf{G}) \\ \boldsymbol{\epsilon} &\sim N(\mathbf{0}, \mathbf{R}) \\ \text{Cov}[\boldsymbol{\gamma}, \boldsymbol{\epsilon}] &= \mathbf{0} \end{aligned}$$

with the MIXED procedure, you specify the fixed-effects design matrix \mathbf{X} in the MODEL statement, the random-effects design matrix \mathbf{Z} in the RANDOM statement, the covariance matrix of the random effects \mathbf{G} with options (SUBJECT=, GROUP=, TYPE=) in the RANDOM statement, and the \mathbf{R} matrix in the REPEATED statement.

By default, covariance parameters are estimated by restricted (residual) maximum likelihood. In supported models, the METHOD=TYPE1, METHOD=TYPE2, and METHOD=TYPE3 options lead to method-of-moment-based estimators and analysis of variance. The MIXED procedure provides an extensive list of diagnostics for mixed models, from various residual graphics to observationwise and groupwise influence diagnostics.

The NESTED procedure performs an analysis of variance in nested random effects models. The VARCOMP procedure can be used to estimate variance components associated with random effects in random and mixed models. The LATTICE procedure computes analysis of variance for balanced and partially balanced square lattices. You can fit the random and mixed models supported by these procedures with the MIXED procedure as well. Some specific analyses, such as the analysis of Gauge R & R studies in the VARCOMP procedure (Burdick, Borror, and Montgomery 2005), are unique to the specialized procedures.

The GLIMMIX procedure can fit most of the models that you can fit with the MIXED procedure, but it does not offer method-of-moment-based estimation and analysis of variance in the narrow sense. Also, PROC

GLIMMIX does not support the same array of covariance structures as the MIXED procedure and does not support a sampling-based Bayesian analysis. An in-depth comparison of the GLIMMIX and MIXED procedures can be found in the section “Comparing the GLIMMIX and MIXED Procedures” on page 3101, in Chapter 41, “The GLIMMIX Procedure.”

Comparing the MIXED and GLM Procedures

Random- and mixed-effects models can also be fitted with the GLM procedure, but the philosophy is different from that of PROC MIXED and other dedicated mixed modeling procedures. The following lists important differences between the GLM and MIXED procedures in fitting random and mixed models:

- The default estimation method for covariance parameters in the MIXED procedure is restricted maximum likelihood. Covariance parameters are estimated by the method of moments by solving expressions for expected mean squares.
- In the GLM procedure, fixed and random effects are listed in the MODEL statement. Only fixed effects are listed in the MODEL statement of the MIXED procedure. In the GLM procedure, random effects must be repeated in the RANDOM statement.
- You can request tests for model effects by adding the TEST option in the RANDOM statement of the GLM procedure. PROC GLM then constructs exact tests for random effects if possible and constructs approximate tests if exact tests are not possible. For details on how the GLM procedure constructs tests for random effects, see the section “Computation of Expected Mean Squares for Random Effects” on page 3376, in Chapter 42, “The GLM Procedure.” Tests for fixed effects are constructed by the MIXED procedure as Wald-type F tests, and the degrees of freedom for these tests can be determined by a variety of methods.
- Some of the output of the GLM procedure applies only to the fixed effects part of the model, whether a RANDOM statement is specified or not.
- Variance components are independent in the GLM procedure and covariance matrices are generally unstructured. The default covariance structure for variance components in the MIXED procedure is also a variance component structure, but the procedure offers a large number of parametric structures to model covariation among random effects and observations.

Comparing the MIXED and HPMIXED Procedures

The HPMIXED procedure is designed to solve large mixed model problems by using sparse matrix techniques. The largeness of a mixed model can take many forms: a large number of observations, large number of columns in the \mathbf{X} matrix, a large number of random effects, or a large number of covariance parameters. The province of the HPMIXED procedure is parameter estimation, inference, and prediction in mixed models with large \mathbf{X} and/or \mathbf{Z} matrices, many observations, but relatively few covariance parameters.

The models that you can fit with the HPMIXED procedure are a subset of the models available with the MIXED procedure. The HPMIXED procedure supports only a limited number of types of covariance structure in the RANDOM and REPEATED statements in order to balance performance and generality.

To some extent, the generality of the MIXED procedure precludes it from serving as a high-performance computing tool for all the model-data scenarios that the procedure can potentially estimate parameters for. For example, although efficient sparse algorithms are available to estimate variance components in large mixed models, the computational configuration changes profoundly when, for example, standard error adjustments and degrees of freedom by the Kenward-Roger method are requested.

Generalized Linear Mixed Models

Generalized linear mixed models can be fit with the GLIMMIX and NLMIXED procedures in SAS/STAT software. The GLIMMIX procedure is specifically designed to fit this class of models and offers syntax very similar to the syntax of other linear modeling procedures, such as the MIXED procedure. Consider a generalized linear model with linear predictor and link function

$$E[\mathbf{Y}|\boldsymbol{\gamma}] = g^{-1}(\boldsymbol{\eta}) = g^{-1}(\mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\boldsymbol{\gamma})$$

and distribution in the exponential family. The fixed-effects design matrix \mathbf{X} is specified in the MODEL statement of the GLIMMIX procedure, and the random-effects design matrix \mathbf{Z} is specified in the RANDOM statement, along with the covariance matrix of the random effects and the covariance matrix of R-side random variables. The link function and (conditional) distribution are determined by defaults or through options in the MODEL statement.

The GLIMMIX procedure can fit heterocatanomic multivariate data—that is, data that stem from different distributions. For example, one measurement taken on a patient might be a continuous, normally distributed outcome, whereas another measurement might be a binary indicator of medical history. The GLIMMIX procedure also provides capabilities for mixed model smoothing and mixed model splines.

The GLIMMIX procedure offers an extensive array of postprocessing features to produce output statistics and to perform linear inference. The ESTIMATE and LSMESTIMATE statements support multiplicity-adjusted p -values for the protection of the familywise Type-I error rate. The LSMEANS statement supports the slicing of interactions, simple effect differences, and ODS statistical graphs for group comparisons.

The default estimation technique in the GLIMMIX procedure depends on the class of models fit. For linear mixed models, the default technique is restricted maximum likelihood, as in the MIXED procedure. For generalized linear mixed models, the estimation is based on linearization methods (pseudo-likelihood) or on integral approximation by adaptive quadrature or Laplace methods.

The NLMIXED procedure facilitates the fitting of generalized linear mixed models through several built-in distributions from the exponential family (binary, binomial, gamma, negative binomial, and Poisson). You have to code the linear predictor and link function with SAS programming statements and assign starting values to all parameters, including the covariance parameters. Although you are not required to specify starting values with the NLMIXED procedure (because the procedure assigns a default value of 1.0 to every parameter not explicitly given a starting value), it is highly recommended that you specify good starting values. The default estimation technique of the NLMIXED procedure, an adaptive Gauss-Hermite quadrature, is also available in the GLIMMIX procedure through the METHOD=QUAD option in the PROC GLIMMIX statement. The Laplace approximation that is available in the NLMIXED procedure by setting QPOINTS=1 is available in the GLIMMIX procedure through the METHOD=LAPLACE option.

Comparing the GENMOD and GLIMMIX Procedures

The GENMOD and GLIMMIX procedures can fit generalized linear models and estimate the parameters by maximum likelihood. For multinomial data, the GENMOD procedure fits cumulative link models for ordinal data. The GLIMMIX procedure fits these models and generalized logit models for nominal data.

When data are correlated, you can use the REPEATED statement in the GENMOD procedure to fit marginal models via generalized estimating equations. A working covariance structure is assumed, and the standard errors of the parameter estimates are computed according to an empirical (“sandwich”) estimator that is robust to the misspecification of the covariance structure. Marginal generalized linear models for correlated data can also be fit with the GLIMMIX procedure by specifying the random effects as R-side effects. The empirical covariance estimators are available through the EMPIRICAL= option in the PROC GLIMMIX statement. The essential difference between the estimation approaches taken by the GLIMMIX procedure and generalized estimating equations is that the latter approach estimates the covariance parameters by the method of moments, whereas the GLIMMIX procedure uses likelihood-based techniques.

The GENMOD procedure supports nonsingular parameterizations of classification variables through its CLASS statement. The GLIMMIX procedure supports only the standard, GLM-type singular parameterization of CLASS variables. For the differences between these parameterizations, see the section “Parameterization of Model Effects” on page 383, in Chapter 19, “Shared Concepts and Topics.”

Nonlinear Mixed Models: The NLMIXED Procedure

PROC NLMIXED handles models in which the fixed or random effects enter nonlinearly. It requires that you specify a conditional distribution of the data given the random effects, with available distributions including the normal, binomial, and Poisson. You can alternatively code your own distribution with SAS programming statements. Under a normality assumption for the random effects, PROC NLMIXED performs maximum likelihood estimation via adaptive Gaussian quadrature and a dual quasi-Newton optimization algorithm. Besides standard maximum likelihood results, you can obtain empirical Bayes predictions of the random effects and estimates of arbitrary functions of the parameters with delta-method standard errors. PROC NLMIXED has a wide variety of applications; two of the most common applications are nonlinear growth curves and overdispersed binomial data.

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Chapter 7

Introduction to Bayesian Analysis Procedures

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Overview

SAS/STAT software provides Bayesian capabilities in four procedures: GENMOD, LIFEREG, MCMC, and PHREG. The GENMOD, LIFEREG, and PHREG procedures provide Bayesian analysis in addition to the standard frequentist analyses they have always performed. Thus, these procedures provide convenient access to Bayesian modeling and inference for generalized linear models, accelerated life failure models, Cox regression models, and piecewise constant baseline hazard models (also known as piecewise exponential models). The MCMC procedure is a general procedure that fits Bayesian models with arbitrary priors and likelihood functions.

This chapter provides an overview of Bayesian statistics; describes specific sampling algorithms used in these four procedures; and discusses posterior inference and convergence diagnostics computations. Sources that provide in-depth treatment of Bayesian statistics can be found at the end of this chapter, in the section “A Bayesian Reading List” on page 156. Additional chapters contain syntax, details, and examples for the individual procedures GENMOD (see Chapter 40, “The GENMOD Procedure”), LIFEREG (see Chapter 51, “The LIFEREG Procedure”), MCMC (see Chapter 55, “The MCMC Procedure”), and PHREG (see Chapter 67, “The PHREG Procedure”).

Introduction

The most frequently used statistical methods are known as *frequentist* (or *classical*) methods. These methods assume that unknown parameters are fixed constants, and they define probability by using limiting relative frequencies. It follows from these assumptions that probabilities are objective and that you cannot make probabilistic statements about parameters because they are fixed. Bayesian methods offer an alternative approach; they treat parameters as random variables and define probability as “degrees of belief” (that is, the probability of an event is the degree to which you believe the event is true). It follows from these postulates that probabilities are subjective and that you can make probability statements about parameters. The term “Bayesian” comes from the prevalent usage of Bayes’ theorem, which was named after the Reverend Thomas Bayes, an eighteenth century Presbyterian minister. Bayes was interested in solving the question of inverse probability: after observing a collection of events, what is the probability of one event?

Suppose you are interested in estimating θ from data $\mathbf{y} = \{y_1, \dots, y_n\}$ by using a statistical model described by a density $p(\mathbf{y}|\theta)$. Bayesian philosophy states that θ cannot be determined exactly, and uncertainty about the parameter is expressed through probability statements and distributions. You can say that θ follows a normal distribution with mean 0 and variance 1, if it is believed that this distribution best describes the uncertainty associated with the parameter. The following steps describe the essential elements of Bayesian inference:

1. A probability distribution for θ is formulated as $\pi(\theta)$, which is known as the *prior* distribution, or just the prior. The prior distribution expresses your beliefs (for example, on the mean, the spread, the skewness, and so forth) about the parameter before you examine the data.
2. Given the observed data \mathbf{y} , you choose a statistical model $p(\mathbf{y}|\theta)$ to describe the distribution of \mathbf{y} given θ .
3. You update your beliefs about θ by combining information from the prior distribution and the data through the calculation of the *posterior* distribution, $p(\theta|\mathbf{y})$.

The third step is carried out by using Bayes’ theorem, which enables you to combine the prior distribution and the model in the following way:

$$p(\theta|\mathbf{y}) = \frac{p(\theta, \mathbf{y})}{p(\mathbf{y})} = \frac{p(\mathbf{y}|\theta)\pi(\theta)}{p(\mathbf{y})} = \frac{p(\mathbf{y}|\theta)\pi(\theta)}{\int p(\mathbf{y}|\theta)\pi(\theta)d\theta}$$

The quantity

$$p(\mathbf{y}) = \int p(\mathbf{y}|\theta)\pi(\theta)d\theta$$

is the normalizing constant of the posterior distribution. This quantity $p(\mathbf{y})$ is also the marginal distribution of \mathbf{y} , and it is sometimes called the marginal distribution of the data. The likelihood function of θ is any function proportional to $p(\mathbf{y}|\theta)$; that is, $L(\theta) \propto p(\mathbf{y}|\theta)$. Another way of writing Bayes’ theorem is as follows:

$$p(\theta|\mathbf{y}) = \frac{L(\theta)\pi(\theta)}{\int L(\theta)\pi(\theta)d\theta}$$

The marginal distribution $p(\mathbf{y})$ is an integral. As long as the integral is finite, the particular value of the integral does not provide any additional information about the posterior distribution. Hence, $p(\theta|\mathbf{y})$ can be written up to an arbitrary constant, presented here in proportional form as:

$$p(\theta|\mathbf{y}) \propto L(\theta)\pi(\theta)$$

Simply put, Bayes' theorem tells you how to update existing knowledge with new information. You begin with a prior belief $\pi(\theta)$, and after learning information from data \mathbf{y} , you change or update your belief about θ and obtain $p(\theta|\mathbf{y})$. These are the essential elements of the Bayesian approach to data analysis.

In theory, Bayesian methods offer simple alternatives to statistical inference—all inferences follow from the posterior distribution $p(\theta|\mathbf{y})$. In practice, however, you can obtain the posterior distribution with straightforward analytical solutions only in the most rudimentary problems. Most Bayesian analyses require sophisticated computations, including the use of simulation methods. You generate samples from the posterior distribution and use these samples to estimate the quantities of interest. PROC MCMC uses a self-tuning Metropolis algorithm (see the section “[Metropolis and Metropolis-Hastings Algorithms](#)” on page 134). The GENMOD, LIFEREG, and PHREG procedures use the Gibbs sampler (see the section “[Gibbs Sampler](#)” on page 135). An important aspect of any analysis is assessing the convergence of the Markov chains. Inferences based on nonconverged Markov chains can be both inaccurate and misleading.

Both Bayesian and classical methods have their advantages and disadvantages. From a practical point of view, your choice of method depends on what you want to accomplish with your data analysis. If you have prior information (either expert opinion or historical knowledge) that you want to incorporate into the analysis, then you should consider Bayesian methods. In addition, if you want to communicate your findings in terms of probability notions that can be more easily understood by nonstatisticians, Bayesian methods might be appropriate. The Bayesian paradigm can often provide a framework for answering specific scientific questions that a single point estimate cannot sufficiently address. Alternatively, if you are interested only in estimating parameters based on the likelihood, then numerical optimization methods, such as the Newton-Raphson method, can give you very precise estimates and there is no need to use a Bayesian analysis. For further discussions of the relative advantages and disadvantages of Bayesian analysis, see the section “[Bayesian Analysis: Advantages and Disadvantages](#)” on page 132.

Background in Bayesian Statistics

Prior Distributions

A prior distribution of a parameter is the probability distribution that represents your uncertainty about the parameter before the current data are examined. Multiplying the prior distribution and the likelihood function together leads to the posterior distribution of the parameter. You use the posterior distribution to carry out all inferences. You cannot carry out any Bayesian inference or perform any modeling without using a prior distribution.

Objective Priors versus Subjective Priors

Bayesian probability measures the degree of belief that you have in a random event. By this definition, probability is highly subjective. It follows that all priors are *subjective priors*. Not everyone agrees with this notion of subjectivity when it comes to specifying prior distributions. There has long been a desire to obtain results that are objectively valid. Within the Bayesian paradigm, this can be somewhat achieved by using prior distributions that are “objective” (that is, that have a minimal impact on the posterior distribution). Such distributions are called *objective* or *noninformative* priors (see the next section). However, while noninformative priors are very popular in some applications, they are not always easy to construct. See DeGroot and Schervish (2002, Section 1.2) and Press (2003, Section 2.2) for more information about interpretations of probability. See Berger (2006) and Goldstein (2006) for discussions about objective Bayesian versus subjective Bayesian analysis.

Noninformative Priors

Roughly speaking, a prior distribution is noninformative if the prior is “flat” relative to the likelihood function. Thus, a prior $\pi(\theta)$ is noninformative if it has minimal impact on the posterior distribution of θ . Other names for the noninformative prior are *vague*, *diffuse*, and *flat* prior. Many statisticians favor noninformative priors because they appear to be more objective. However, it is unrealistic to expect that noninformative priors represent total ignorance about the parameter of interest. In some cases, noninformative priors can lead to *improper posteriors* (nonintegrable posterior density). You cannot make inferences with improper posterior distributions. In addition, noninformative priors are often not invariant under transformation; that is, a prior might be noninformative in one parameterization but not necessarily noninformative if a transformation is applied.

See Box and Tiao (1973) for a more formal development of noninformative priors. See Kass and Wasserman (1996) for techniques for deriving noninformative priors.

Improper Priors

A prior $\pi(\theta)$ is said to be improper if

$$\int \pi(\theta) d\theta = \infty$$

For example, a uniform prior distribution on the real line, $\pi(\theta) \propto 1$, for $-\infty < \theta < \infty$, is an improper prior. Improper priors are often used in Bayesian inference since they usually yield noninformative priors and proper posterior distributions. Improper prior distributions can lead to posterior impropriety (improper posterior distribution). To determine whether a posterior distribution is proper, you need to make sure that the normalizing constant $\int p(y|\theta)p(\theta)d\theta$ is finite for all y . If an improper prior distribution leads to an improper posterior distribution, inference based on the improper posterior distribution is invalid.

The GENMOD, LIFEREG, and PHREG procedures allow the use of improper priors—that is, the flat prior on the real line—for regression coefficients. These improper priors do not lead to any improper posterior distributions in the models that these procedures fit. PROC MCMC allows the use of any prior, as long as the distribution is programmable using DATA step functions. However, the procedure does not verify whether the posterior distribution is integrable. You must ensure this yourself.

Informative Priors

An informative prior is a prior that is not dominated by the likelihood and that has an impact on the posterior distribution. If a prior distribution dominates the likelihood, it is clearly an informative prior. These types of distributions must be specified with care in actual practice. On the other hand, the proper use of prior distributions illustrates the power of the Bayesian method: information gathered from the previous study, past experience, or expert opinion can be combined with current information in a natural way. See the “Examples” sections of the GENMOD and PHREG procedure chapters for instructions about constructing informative prior distributions.

Conjugate Priors

A prior is said to be a conjugate prior for a family of distributions if the prior and posterior distributions are from the same family, which means that the form of the posterior has the same distributional form as the prior distribution. For example, if the likelihood is binomial, $y \sim \text{Bin}(n, \theta)$, a conjugate prior on θ is the beta distribution; it follows that the posterior distribution of θ is also a beta distribution. Other commonly used conjugate prior/likelihood combinations include the normal/normal, gamma/Poisson, gamma/gamma, and gamma/beta cases. The development of conjugate priors was partially driven by a desire for computational convenience—conjugacy provides a practical way to obtain the posterior distributions. The Bayesian procedures do not use conjugacy in posterior sampling.

Jeffreys’ Prior

A very useful prior is Jeffreys’ prior (Jeffreys 1961). It satisfies the local uniformity property: a prior that does not change much over the region in which the likelihood is significant and does not assume large values outside that range. It is based on the Fisher information matrix. Jeffreys’ prior is defined as

$$\pi(\theta) \propto |I(\theta)|^{1/2}$$

where $||$ denotes the determinant and $I(\theta)$ is the Fisher information matrix based on the likelihood function $p(\mathbf{y}|\theta)$:

$$I(\theta) = -E \left[\frac{\partial^2 \log p(\mathbf{y}|\theta)}{\partial \theta^2} \right]$$

Jeffreys’ prior is locally uniform and hence noninformative. It provides an automated scheme for finding a noninformative prior for any parametric model $p(\mathbf{y}|\theta)$. Another appealing property of Jeffreys’ prior is that it is invariant with respect to one-to-one transformations. The invariance property means that if you have a locally uniform prior on θ and $\phi(\theta)$ is a one-to-one function of θ , then $p(\phi(\theta)) = \pi(\theta) \cdot |\phi'(\theta)|^{-1}$ is a locally uniform prior for $\phi(\theta)$. This invariance principle carries through to multidimensional parameters as well. While Jeffreys’ prior provides a general recipe for obtaining noninformative priors, it has some shortcomings: the prior is improper for many models, and it can lead to improper posterior in some cases; and the prior can be cumbersome to use in high dimensions. PROC GENMOD calculates Jeffreys’ prior automatically for any generalized linear model. You can set it as your prior density for the coefficient parameters, and it does not lead to improper posteriors. You can construct Jeffreys’ prior for a variety of statistical models in the MCMC procedure. See the section “[Example 55.4: Logistic Regression Model with Jeffreys’ Prior](#)” on page 4563 for an example. PROC MCMC does not guarantee that the corresponding posterior distribution is proper, and you need to exercise extra caution in this case.

Bayesian Inference

Bayesian inference about θ is primarily based on the posterior distribution of θ . There are various ways in which you can summarize this distribution. For example, you can report your findings through point estimates. You can also use the posterior distribution to construct hypothesis tests or probability statements.

Point Estimation and Estimation Error

Classical methods often report the maximum likelihood estimator (MLE) or the method of moments estimator (MOME) of a parameter. In contrast, Bayesian approaches often use the posterior mean. The definition of the posterior mean is given by

$$E(\theta|\mathbf{y}) = \int \theta p(\theta|\mathbf{y}) d\theta$$

Other commonly used posterior estimators include the posterior median, defined as

$$\theta: P(\theta \geq \text{median}|\mathbf{y}) = P(\text{median} \leq \theta|\mathbf{y}) = \frac{1}{2}$$

and the posterior mode, defined as the value of θ that maximizes $p(\theta|\mathbf{y})$.

The variance of the posterior density (simply referred to as the *posterior variance*) describes the uncertainty in the parameter, which is a random variable in the Bayesian paradigm. A Bayesian analysis typically uses the posterior variance, or the posterior standard deviation, to characterize the dispersion of the parameter. In multidimensional models, covariance or correlation matrices are used.

If you know the distributional form of the posterior density of interest, you can report the exact posterior point estimates. When models become too difficult to analyze analytically, you have to use simulation algorithms, such as the Markov chain Monte Carlo (MCMC) method to obtain posterior estimates (see the section “[Markov Chain Monte Carlo Method](#)” on page 133). All of the Bayesian procedures rely on MCMC to obtain all posterior estimates. Using only a finite number of samples, simulations introduce an additional level of uncertainty to the accuracy of the estimates. *Monte Carlo standard error (MCSE)*, which is the standard error of the posterior mean estimate, measures the simulation accuracy. See the section “[Standard Error of the Mean Estimate](#)” on page 153 for more information.

The posterior standard deviation and the MCSE are two completely different concepts: the posterior standard deviation describes the uncertainty in the parameter, while the MCSE describes only the uncertainty in the parameter estimate as a result of MCMC simulation. The posterior standard deviation is a function of the sample size in the data set, and the MCSE is a function of the number of iterations in the simulation.

Hypothesis Testing

Suppose you have the following null and alternative hypotheses: H_0 is $\theta \in \Theta_0$ and H_1 is $\theta \in \Theta_0^c$, where Θ_0 is a subset of the parameter space and Θ_0^c is its complement. Using the posterior distribution $\pi(\theta|\mathbf{y})$, you can compute the posterior probabilities $P(\theta \in \Theta_0|\mathbf{y})$ and $P(\theta \in \Theta_0^c|\mathbf{y})$, or the probabilities that H_0 and H_1 are true, respectively. One way to perform a Bayesian hypothesis test is to accept the null hypothesis

if $P(\theta \in \Theta_0|\mathbf{y}) \geq P(\theta \in \Theta_0^c|\mathbf{y})$ and vice versa, or to accept the null hypothesis if $P(\theta \in \Theta_0|\mathbf{y})$ is greater than a predefined threshold, such as 0.75, to guard against falsely accepted null distribution.

It is more difficult to carry out a point null hypothesis test in a Bayesian analysis. A point null hypothesis is a test of $H_0: \theta = \theta_0$ versus $H_1: \theta \neq \theta_0$. If the prior distribution $\pi(\theta)$ is a continuous density, then the posterior probability of the null hypothesis being true is 0, and there is no point in carrying out the test. One alternative is to restate the null to be a small interval hypothesis: $\theta \in \Theta_0 = (\theta_0 - a, \theta_0 + a)$, where a is a very small constant. The Bayesian paradigm can deal with an interval hypothesis more easily. Another approach is to give a mixture prior distribution to θ with a positive probability of p_0 on θ_0 and the density $(1 - p_0)\pi(\theta)$ on $\theta \neq \theta_0$. This prior ensures a nonzero posterior probability on θ_0 , and you can then make realistic probabilistic comparisons. For more detailed treatment of Bayesian hypothesis testing, see Berger (1985).

Interval Estimation

The Bayesian set estimates are called *credible sets*, which is also known as *credible intervals*. This is analogous to the concept of confidence intervals used in classical statistics. Given a posterior distribution $p(\theta|\mathbf{y})$, A is a credible set for θ if

$$P(\theta \in A|\mathbf{y}) = \int_A p(\theta|\mathbf{y})d\theta$$

For example, you can construct a 95% credible set for θ by finding an interval, A , over which $\int_A p(\theta|\mathbf{y}) = 0.95$.

You can construct credible sets that have equal tails. A $100(1 - \alpha)\%$ equal-tail interval corresponds to the $100(\alpha/2)$ and $100(1 - \alpha/2)$ percentiles of the posterior distribution. Some statisticians prefer this interval because it is invariant under transformations. Another frequently used Bayesian credible set is called the *highest posterior density* (HPD) interval.

A $100(1 - \alpha)\%$ HPD interval is a region that satisfies the following two conditions:

1. The posterior probability of that region is $100(1 - \alpha)\%$.
2. The minimum density of any point within that region is equal to or larger than the density of any point outside that region.

The HPD is an interval in which most of the distribution lies. Some statisticians prefer this interval because it is the smallest interval.

One major distinction between Bayesian and classical sets is their interpretation. The Bayesian probability reflects a person's subjective beliefs. Following this approach, a statistician can make the claim that θ is inside a credible interval with measurable probability. This property is appealing because it enables you to make a direct probability statement about parameters. Many people find this concept to be a more natural way of understanding a probability interval, which is also easier to explain to nonstatisticians. A confidence interval, on the other hand, enables you to make a claim that the interval covers the true parameter. The interpretation reflects the uncertainty in the sampling procedure; a confidence interval of $100(1 - \alpha)\%$ asserts that, in the long run, $100(1 - \alpha)\%$ of the realized confidence intervals cover the true parameter.

Bayesian Analysis: Advantages and Disadvantages

Bayesian methods and classical methods both have advantages and disadvantages, and there are some similarities. When the sample size is large, Bayesian inference often provides results for parametric models that are very similar to the results produced by frequentist methods. Some advantages to using Bayesian analysis include the following:

- It provides a natural and principled way of combining prior information with data, within a solid decision theoretical framework. You can incorporate past information about a parameter and form a prior distribution for future analysis. When new observations become available, the previous posterior distribution can be used as a prior. All inferences logically follow from Bayes' theorem.
- It provides inferences that are conditional on the data and are exact, without reliance on asymptotic approximation. Small sample inference proceeds in the same manner as if one had a large sample. Bayesian analysis also can estimate any functions of parameters directly, without using the “plug-in” method (a way to estimate functionals by plugging the estimated parameters in the functionals).
- It obeys the likelihood principle. If two distinct sampling designs yield proportional likelihood functions for θ , then all inferences about θ should be identical from these two designs. Classical inference does not in general obey the likelihood principle.
- It provides interpretable answers, such as “the true parameter θ has a probability of 0.95 of falling in a 95% credible interval.”
- It provides a convenient setting for a wide range of models, such as hierarchical models and missing data problems. MCMC, along with other numerical methods, makes computations tractable for virtually all parametric models.

There are also disadvantages to using Bayesian analysis:

- It does not tell you how to select a prior. There is no correct way to choose a prior. Bayesian inferences require skills to translate subjective prior beliefs into a mathematically formulated prior. If you do not proceed with caution, you can generate misleading results.
- It can produce posterior distributions that are heavily influenced by the priors. From a practical point of view, it might sometimes be difficult to convince subject matter experts who do not agree with the validity of the chosen prior.
- It often comes with a high computational cost, especially in models with a large number of parameters. In addition, simulations provide slightly different answers unless the same random seed is used. Note that slight variations in simulation results do not contradict the early claim that Bayesian inferences are exact. The posterior distribution of a parameter is exact, given the likelihood function and the priors, while simulation-based estimates of posterior quantities can vary due to the random number generator used in the procedures.

For more in-depth treatments of the pros and cons of Bayesian analysis, see Berger (1985, Sections 4.1 and 4.12), Berger and Wolpert (1988), Bernardo and Smith (1994, with a new edition coming out), Carlin and Louis (2000, Section 1.4), Robert (2001, Chapter 11), and Wasserman (2004, Section 11.9).

The following sections provide detailed information about the Bayesian methods provided in SAS.

Markov Chain Monte Carlo Method

The Markov chain Monte Carlo (MCMC) method is a general simulation method for sampling from posterior distributions and computing posterior quantities of interest. MCMC methods sample successively from a target distribution. Each sample depends on the previous one, hence the notion of the Markov chain. A Markov chain is a sequence of random variables, $\theta^1, \theta^2, \dots$, for which the random variable θ^t depends on all previous θ s only through its immediate predecessor θ^{t-1} . You can think of a Markov chain applied to sampling as a mechanism that traverses randomly through a target distribution without having any memory of where it has been. Where it moves next is entirely dependent on where it is now.

Monte Carlo, as in Monte Carlo integration, is mainly used to approximate an expectation by using the Markov chain samples. In the simplest version

$$\int_S g(\theta) p(\theta) d\theta \cong \frac{1}{n} \sum_{t=1}^n g(\theta^t)$$

where $g(\cdot)$ is a function of interest and θ^t are samples from $p(\theta)$ on its support S . This approximates the expected value of $g(\theta)$. The earliest reference to MCMC simulation occurs in the physics literature. Metropolis and Ulam (1949) and Metropolis et al. (1953) describe what is known as the Metropolis algorithm (see the section “[Metropolis and Metropolis-Hastings Algorithms](#)” on page 134). The algorithm can be used to generate sequences of samples from the joint distribution of multiple variables, and it is the foundation of MCMC. Hastings (1970) generalized their work, resulting in the Metropolis-Hastings algorithm.

Geman and Geman (1984) analyzed image data by using what is now called Gibbs sampling (see the section “[Gibbs Sampler](#)” on page 135). These MCMC methods first appeared in the mainstream statistical literature in Tanner and Wong (1987).

The Markov chain method has been quite successful in modern Bayesian computing. Only in the simplest Bayesian models can you recognize the analytical forms of the posterior distributions and summarize inferences directly. In moderately complex models, posterior densities are too difficult to work with directly. With the MCMC method, it is possible to generate samples from an arbitrary posterior density $p(\theta|\mathbf{y})$ and to use these samples to approximate expectations of quantities of interest. Several other aspects of the Markov chain method also contributed to its success. Most importantly, if the simulation algorithm is implemented correctly, the Markov chain is guaranteed to converge to the target distribution $p(\theta|\mathbf{y})$ under rather broad conditions, regardless of where the chain was initialized. In other words, a Markov chain is able to improve its approximation to the true distribution at each step in the simulation. Furthermore, if the chain is run for a very long time (often required), you can recover $p(\theta|\mathbf{y})$ to any precision. Also, the simulation algorithm is easily extensible to models with a large number of parameters or high complexity, although the “curse of dimensionality” often causes problems in practice.

Properties of Markov chains are discussed in Feller (1968), Breiman (1968), and Meyn and Tweedie (1993). Ross (1997) and Karlin and Taylor (1975) give a non-measure-theoretic treatment of stochastic processes, including Markov chains. For conditions that govern Markov chain convergence and rates of convergence, see Amit (1991), Applegate, Kannan, and Polson (1990), Chan (1993), Geman and Geman (1984), Liu, Wong, and Kong (1991a, b), Rosenthal (1991a, b), Tierney (1994), and Schervish and Carlin (1992). Besag (1974) describes conditions under which a set of conditional distributions gives a unique joint distribution. Tanner (1993), Gilks, Richardson, and Spiegelhalter (1996), Chen, Shao, and Ibrahim (2000), Liu (2001), Gelman et al. (2004), Robert and Casella (2004), and Congdon (2001, 2003, 2005) provide both theoretical

and applied treatments of MCMC methods. You can also see the section “A Bayesian Reading List” on page 156 for a list of books with varying levels of difficulty of treatment of the subject and its application to Bayesian statistics.

Metropolis and Metropolis-Hastings Algorithms

The Metropolis algorithm is named after its inventor, the American physicist and computer scientist Nicholas C. Metropolis. The algorithm is simple but practical, and it can be used to obtain random samples from any arbitrarily complicated target distribution of any dimension that is known up to a normalizing constant.

Suppose you want to obtain T samples from a univariate distribution with probability density function $f(\theta|\mathbf{y})$. Suppose θ^t is the t th sample from f . To use the Metropolis algorithm, you need to have an initial value θ^0 and a symmetric *proposal* density $q(\theta^{t+1}|\theta^t)$. For the $(t + 1)$ iteration, the algorithm generates a sample from $q(\cdot|\cdot)$ based on the current sample θ^t , and it makes a decision to either accept or reject the new sample. If the new sample is accepted, the algorithm repeats itself by starting at the new sample. If the new sample is rejected, the algorithm starts at the current point and repeats. The algorithm is self-repeating, so it can be carried out as long as required. In practice, you have to decide the total number of samples needed in advance and stop the sampler after that many iterations have been completed.

Suppose $q(\theta_{\text{new}}|\theta^t)$ is a symmetric distribution. The proposal distribution should be an easy distribution from which to sample, and it must be such that $q(\theta_{\text{new}}|\theta^t) = q(\theta^t|\theta_{\text{new}})$, meaning that the likelihood of jumping to θ_{new} from θ^t is the same as the likelihood of jumping back to θ^t from θ_{new} . The most common choice of the proposal distribution is the normal distribution $N(\theta^t, \sigma)$ with a fixed σ . The Metropolis algorithm can be summarized as follows:

1. Set $t = 0$. Choose a starting point θ^0 . This can be an arbitrary point as long as $f(\theta^0|\mathbf{y}) > 0$.
2. Generate a new sample, θ_{new} , by using the proposal distribution $q(\cdot|\theta^t)$.
3. Calculate the following quantity:

$$r = \min \left\{ \frac{f(\theta_{\text{new}}|\mathbf{y})}{f(\theta^t|\mathbf{y})}, 1 \right\}$$

4. Sample u from the uniform distribution $U(0, 1)$.
5. Set $\theta^{t+1} = \theta_{\text{new}}$ if $u < r$; otherwise set $\theta^{t+1} = \theta^t$.
6. Set $t = t + 1$. If $t < T$, the number of desired samples, return to step 2. Otherwise, stop.

Note that the number of iteration keeps increasing regardless of whether a proposed sample is accepted.

This algorithm defines a chain of random variates whose distribution will converge to the desired distribution $f(\theta|\mathbf{y})$, and so from some point forward, the chain of samples is a sample from the distribution of interest. In Markov chain terminology, this distribution is called the *stationary distribution* of the chain, and in Bayesian statistics, it is the posterior distribution of the model parameters. The reason that the Metropolis algorithm works is beyond the scope of this documentation, but you can find more detailed descriptions and proofs in many standard textbooks, including Roberts (1996) and Liu (2001). The random-walk Metropolis algorithm is used in the MCMC procedure.

You are not limited to a symmetric random-walk proposal distribution in establishing a valid sampling algorithm. A more general form, the Metropolis-Hastings (MH) algorithm, was proposed by Hastings (1970). The MH algorithm uses an asymmetric proposal distribution: $q(\theta_{\text{new}}|\theta^t) \neq q(\theta^t|\theta_{\text{new}})$. The difference in its implementation comes in calculating the ratio of densities:

$$r = \min \left\{ \frac{f(\theta_{\text{new}}|\mathbf{y})q(\theta^t|\theta_{\text{new}})}{f(\theta^t|\mathbf{y})q(\theta_{\text{new}}|\theta^t)}, 1 \right\}$$

Other steps remain the same.

The extension of the Metropolis algorithm to a higher-dimensional $\boldsymbol{\theta}$ is straightforward. Suppose $\boldsymbol{\theta} = (\theta_1, \theta_2, \dots, \theta_k)'$ is the parameter vector. To start the Metropolis algorithm, select an initial value for each θ_k and use a multivariate version of proposal distribution $q(\cdot|\cdot)$, such as a multivariate normal distribution, to select a k -dimensional new parameter. Other steps remain the same as those previously described, and this Markov chain eventually converges to the target distribution of $f(\boldsymbol{\theta}|\mathbf{y})$. Chib and Greenberg (1995) provide a useful tutorial on the algorithm.

Gibbs Sampler

The Gibbs sampler, named by Geman and Geman (1984) after the American physicist Josiah W. Gibbs, is a special case of the “Metropolis and Metropolis-Hastings Algorithms” on page 134 in which the proposal distributions exactly match the posterior conditional distributions and proposals are accepted 100% of the time. Gibbs sampling requires you to decompose the joint posterior distribution into full conditional distributions for each parameter in the model and then sample from them. The sampler can be efficient when the parameters are not highly dependent on each other and the full conditional distributions are easy to sample from. Some researchers favor this algorithm because it does not require an instrumental proposal distribution as Metropolis methods do. However, while deriving the conditional distributions can be relatively easy, it is not always possible to find an efficient way to sample from these conditional distributions.

Suppose $\boldsymbol{\theta} = (\theta_1, \dots, \theta_k)'$ is the parameter vector, $p(\mathbf{y}|\boldsymbol{\theta})$ is the likelihood, and $\pi(\boldsymbol{\theta})$ is the prior distribution. The full posterior conditional distribution of $\pi(\theta_i|\theta_j, i \neq j, \mathbf{y})$ is proportional to the joint posterior density; that is,

$$\pi(\theta_i|\theta_j, i \neq j, \mathbf{y}) \propto p(\mathbf{y}|\boldsymbol{\theta})\pi(\boldsymbol{\theta})$$

For instance, the one-dimensional conditional distribution of θ_1 given $\theta_j = \theta_j^*, 2 \leq j \leq k$, is computed as the following:

$$\pi(\theta_1|\theta_j = \theta_j^*, 2 \leq j \leq k, \mathbf{y}) = p(\mathbf{y}|\boldsymbol{\theta} = (\theta_1, \theta_2^*, \dots, \theta_k^*)')\pi(\boldsymbol{\theta} = (\theta_1, \theta_2^*, \dots, \theta_k^*)')$$

The Gibbs sampler works as follows:

1. Set $t = 0$, and choose an arbitrary initial value of $\boldsymbol{\theta}^{(0)} = \{\theta_1^{(0)}, \dots, \theta_k^{(0)}\}$.
2. Generate each component of $\boldsymbol{\theta}$ as follows:

- draw $\theta_1^{(t+1)}$ from $\pi(\theta_1|\theta_2^{(t)}, \dots, \theta_k^{(t)}, \mathbf{y})$
 - draw $\theta_2^{(t+1)}$ from $\pi(\theta_2|\theta_1^{(t+1)}, \theta_3^{(t)}, \dots, \theta_k^{(t)}, \mathbf{y})$
 - ...
 - draw $\theta_k^{(t+1)}$ from $\pi(\theta_k|\theta_1^{(t+1)}, \dots, \theta_{k-1}^{(t+1)}, \mathbf{y})$
3. Set $t = t + 1$. If $t < T$, the number of desired samples, return to step 2. Otherwise, stop.

The name “Gibbs” was introduced by Geman and Geman (1984). Gelfand et al. (1990) first used Gibbs sampling to solve problems in Bayesian inference. See Casella and George (1992) for a tutorial on the sampler. The GENMOD, LIFEREG, and PHREG procedures update parameters using the Gibbs sampler.

Adaptive Rejection Sampling Algorithm

The GENMOD, LIFEREG, and PHREG procedures use the adaptive rejection sampling (ARS) algorithm to sample parameters sequentially from their univariate full conditional distributions. The ARS algorithm is a rejection algorithm that was originally proposed by Gilks and Wild (1992). Given a log-concave density (the log of the density is concave), you can construct an envelope for the density by using linear segments. You then use the linear segment envelope as a proposal density (it becomes a piecewise exponential density on the original scale and is easy to generate samplers from) in the rejection sampling.

The log-concavity condition is met in some of the models that are fit by the procedures. For example, the posterior densities for the regression parameters in the generalized linear models are log-concave under flat priors. When this condition fails, the ARS algorithm calls for an additional Metropolis-Hastings step (Gilks, Best, and Tan 1995), and the modified algorithm becomes the adaptive rejection Metropolis sampling (ARMS) algorithm. The GENMOD, LIFEREG, and PHREG procedures can recognize whether a model is log-concave and select the appropriate sampler for the problem at hand.

Although samples obtained from the ARMS algorithm often exhibit less dependence with lower autocorrelations, the algorithm could have a high computational cost because it requires repeated evaluations of the objective function (usually five to seven repetitions) at each iteration for each univariate parameter.¹

Implementation the ARMS algorithm in the GENMOD, LIFEREG, and PHREG procedures is based on code that is provided by Walter R. Gilks, University of Leeds (Gilks 2003). For a detailed description and explanation of the algorithm, see Gilks and Wild (1992); Gilks, Best, and Tan (1995).

Slice Sampler

The slice sampler (Neal 2003), like the ARMS algorithm, is a general algorithm that can be used to sample parameters from their target distribution. As with the ARMS algorithm, the only requirement of the slice sampler is the ability to evaluate the objective function (the unnormalized conditional distribution in a Gibbs step, for example) at a given parameter value. In theory, you can draw a random number from any given distribution as long as you can first obtain a random number uniformly under the curve of that distribution. Treat the area under the curve of $p(\theta)$ as a two-dimensional space that is defined by the θ -axis and the Y-axis, the latter being the axis for the density function. You draw uniformly in that area, obtain a two-dimensional vector of (θ_i, y_i) , ignore the y_i , and keep the θ_i . The θ_i 's are distributed according to the right density.

¹The extension to the multivariate ARMS algorithm is possible in theory but problematic in practice because the computational cost associated with constructing a multidimensional hyperbola envelop is often prohibitive.

To solve the problem of sampling uniformly under the curve, Neal (2003) proposed the idea of slices (hence the name of the sampler), which can be explained as follows:

1. Start the algorithm at θ_0 .
2. Calculate the objective function $p(\theta_0)$ and draw a line between $y = 0$ and $y = p(\theta_0)$, which defines a vertical slice. You draw a uniform number, y_1 , on this slice, between $(0, p(\theta_0))$.
3. Draw a horizontal line at y_1 and find the two points where the line intercepts with the curve, (L_1, R_1) . These two points define a horizontal slice. Draw a uniform number, x_1 , on this slice, between (L_1, R_1) .
4. Repeat steps 2 and 3 many times.

The challenging part of the algorithm is finding the horizontal slice (L_i, R_i) at each iteration. The closed form expressions of $p_L^{-1}(y_i)$ and $p_R^{-1}(y_i)$ are virtually impossible to obtain analytically in most problems. Neal (2003) proved that although exact solutions would be nice, devising a search algorithm that finds portions of this horizontal slice is sufficient for the sampler to work. The search algorithm is based on the rejection method to expand and contract, when needed.

The sampler is implemented as an optional algorithm in the MCMC procedure, where you can use it to draw either model parameters or random-effects parameters. As with the ARMS algorithm, only the univariate version of the slice sampler is implemented. The slice sampler requires repeated evaluations of the objective function; this happens in the search algorithm to identify each horizontal slice at every iteration. Hence, the computational cost could be high if each evaluation of the objective function requires one pass through the entire data set.

Independence Sampler

Another type of Metropolis algorithm is the “independence” sampler. It is called the independence sampler because the proposal distribution in the algorithm does not depend on the current point as it does with the random-walk Metropolis algorithm. For this sampler to work well, you want to have a proposal distribution that mimics the target distribution and have the acceptance rate be as high as possible.

1. Set $t = 0$. Choose a starting point θ^0 . This can be an arbitrary point as long as $f(\theta^0|\mathbf{y}) > 0$.
2. Generate a new sample, θ_{new} , by using the proposal distribution $q(\cdot)$. The proposal distribution does not depend on the current value of θ^t .
3. Calculate the following quantity:

$$r = \min \left\{ \frac{f(\theta_{\text{new}}|\mathbf{y})/q(\theta_{\text{new}})}{f(\theta^t|\mathbf{y})/q(\theta^t)}, 1 \right\}$$

4. Sample u from the uniform distribution $U(0, 1)$.
5. Set $\theta^{t+1} = \theta_{\text{new}}$ if $u < r$; otherwise set $\theta^{t+1} = \theta^t$.
6. Set $t = t + 1$. If $t < T$, the number of desired samples, return to step 2. Otherwise, stop.

A good proposal density should have thicker tails than those of the target distribution. This requirement sometimes can be difficult to satisfy especially in cases where you do not know what the target posterior distributions are like. In addition, this sampler does not produce independent samples as the name seems to imply, and sample chains from independence samplers can get stuck in the tails of the posterior distribution if the proposal distribution is not chosen carefully. The MCMC procedure uses the independence sampler.

Gamerman Algorithm

The Gamerman algorithm, named after the inventor Dani Gamerman is a special case of the “[Metropolis and Metropolis-Hastings Algorithms](#)” on page 134 in which the proposal distribution is derived from one iteration of the iterative weighted least squares (IWLS) algorithm. As the name suggests, a weighted least squares algorithm is carried out inside an iteration loop. For each iteration, a set of weights for the observations is used in the least squares fit. The weights are constructed by applying a weight function to the current residuals. The proposal distribution uses the current iteration’s values of the parameters to form the proposal distribution from which to generate a proposed random value (Gamerman 1997).

The multivariate sampling algorithm is simple but practical, and can be used to obtain random samples from the posterior distribution of the regression parameters in a generalized linear model (GLM). See “[Generalized Linear Regression](#)” on page 79 for further details on generalized linear regression models. See McCullagh and Nelder (1989) for a discussion of transformed observations and diagonal matrix of weights pertaining to IWLS.

The GENMOD procedure uses the Gamerman algorithm to sample parameters from their multivariate posterior conditional distributions. For a detailed description and explanation of the algorithm, see Gamerman (1997).

Burn-in, Thinning, and Markov Chain Samples

Burn-in refers to the practice of discarding an initial portion of a Markov chain sample so that the effect of initial values on the posterior inference is minimized. For example, suppose the target distribution is $N(0, 1)$ and the Markov chain was started at the value 10^6 . The chain might quickly travel to regions around 0 in a few iterations. However, including samples around the value 10^6 in the posterior mean calculation can produce substantial bias in the mean estimate. In theory, if the Markov chain is run for an infinite amount of time, the effect of the initial values decreases to zero. In practice, you do not have the luxury of infinite samples. In practice, you assume that after t iterations, the chain has reached its target distribution and you can throw away the early portion and use the good samples for posterior inference. The value of t is the burn-in number.

With some models you might experience poor mixing (or slow convergence) of the Markov chain. This can happen, for example, when parameters are highly correlated with each other. Poor mixing means that the Markov chain slowly traverses the parameter space (see the section “[Visual Analysis via Trace Plots](#)” on page 139 for examples of poorly mixed chains) and the chain has high dependence. High sample autocorrelation can result in biased Monte Carlo standard errors. A common strategy is to *thin* the Markov chain in order to reduce sample autocorrelations. You thin a chain by keeping every k th simulated draw from each sequence. You can safely use a thinned Markov chain for posterior inference as long as the chain converges. It is important to note that thinning a Markov chain can be wasteful because you are throwing away a $\frac{k-1}{k}$ fraction of all the posterior samples generated. MacEachern and Berliner (1994) show that you always get more precise posterior estimates if the entire Markov chain is used. However, other factors, such as computer storage or plotting time, might prevent you from keeping all samples.

To use the GENMOD, LIFEREG, MCMC, and PHREG procedures, you need to determine the total number of samples to keep ahead of time. This number is not obvious and often depends on the type of inference you want to make. Mean estimates do not require nearly as many samples as small-tail percentile estimates. In most applications, you might find that keeping a few thousand iterations is sufficient for reasonably accurate posterior inference. In all four procedures, the relationship between the number of iterations requested, the number of iterations kept, and the amount of thinning is as follows:

$$\text{kept} = \left[\frac{\text{requested}}{\text{thinning}} \right]$$

where $[]$ is the rounding operator.

Assessing Markov Chain Convergence

Simulation-based Bayesian inference requires using simulated draws to summarize the posterior distribution or calculate any relevant quantities of interest. You need to treat the simulation draws with care. There are usually two issues. First, you have to decide whether the Markov chain has reached its stationary, or the desired posterior, distribution. Second, you have to determine the number of iterations to keep after the Markov chain has reached stationarity. Convergence diagnostics help to resolve these issues. Note that many diagnostic tools are designed to verify a necessary but not sufficient condition for convergence. There are no conclusive tests that can tell you when the Markov chain has converged to its stationary distribution. You should proceed with caution. Also, note that you should check the convergence of *all* parameters, and not just those of interest, before proceeding to make any inference. With some models, certain parameters can appear to have very good convergence behavior, but that could be misleading due to the slow convergence of other parameters. If some of the parameters have bad mixing, you cannot get accurate posterior inference for parameters that appear to have good mixing. See Cowles and Carlin (1996) and Brooks and Roberts (1998) for discussions about convergence diagnostics.

Visual Analysis via Trace Plots

Trace plots of samples versus the simulation index can be very useful in assessing convergence. The trace tells you if the chain has not yet converged to its stationary distribution—that is, if it needs a longer burn-in period. A trace can also tell you whether the chain is mixing well. A chain might have reached stationarity if the distribution of points is not changing as the chain progresses. The aspects of stationarity that are most recognizable from a trace plot are a relatively constant mean and variance. A chain that mixes well traverses its posterior space rapidly, and it can jump from one remote region of the posterior to another in relatively few steps. [Figure 7.1](#) through [Figure 7.4](#) display some typical features that you might see in trace plots. The traces are for a parameter called γ .

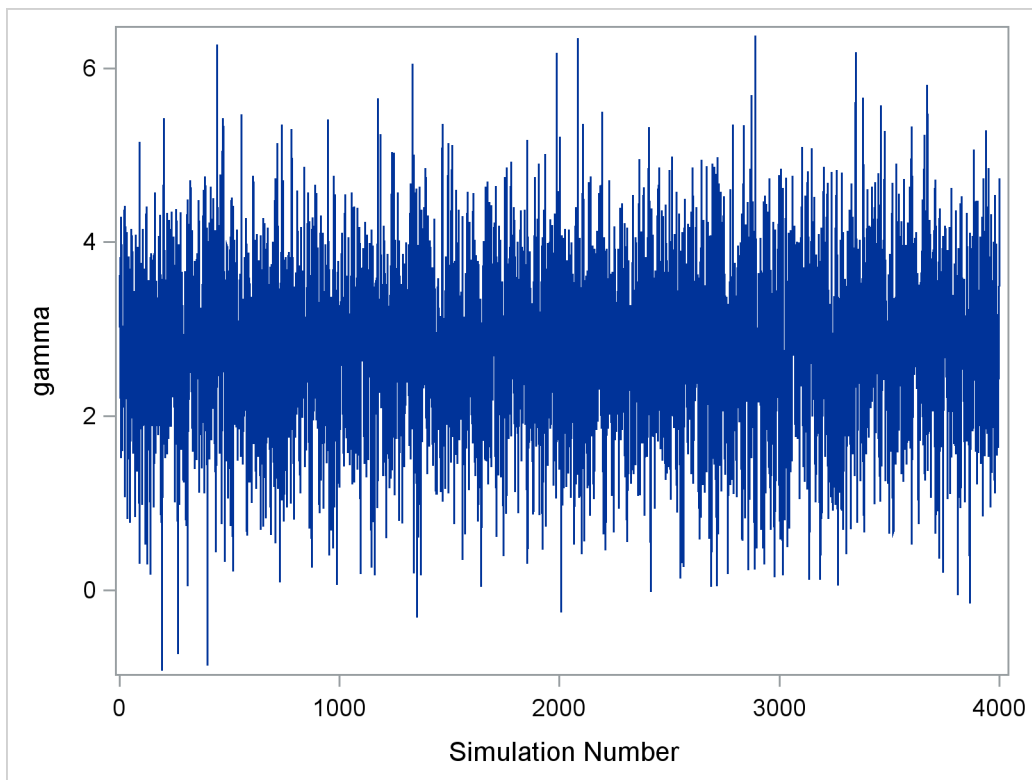
Figure 7.1 Essentially Perfect Trace for γ 

Figure 7.1 displays a “perfect” trace plot. Note that the center of the chain appears to be around the value 3, with very small fluctuations. This indicates that the chain could have reached the right distribution. The chain is mixing well; it is exploring the distribution by traversing to areas where its density is very low. You can conclude that the mixing is quite good here.

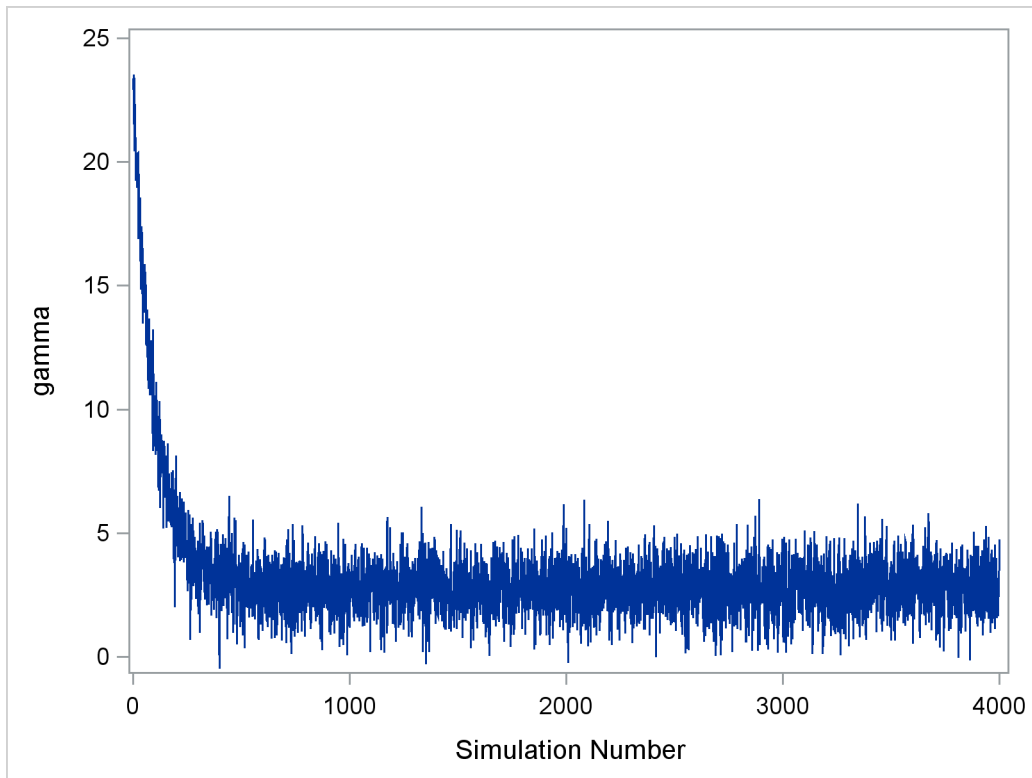
Figure 7.2 Initial Samples of γ Need to be Discarded

Figure 7.2 displays a trace plot for a chain that starts at a very remote initial value and makes its way to the targeting distribution. The first few hundred observations should be discarded. This chain appears to be mixing very well locally. It travels relatively quickly to the target distribution, reaching it in a few hundred iterations. If you have a chain that looks like this, you would want to increase the burn-in sample size. If you need to use this sample to make inferences, you would want to use only the samples toward the end of the chain.

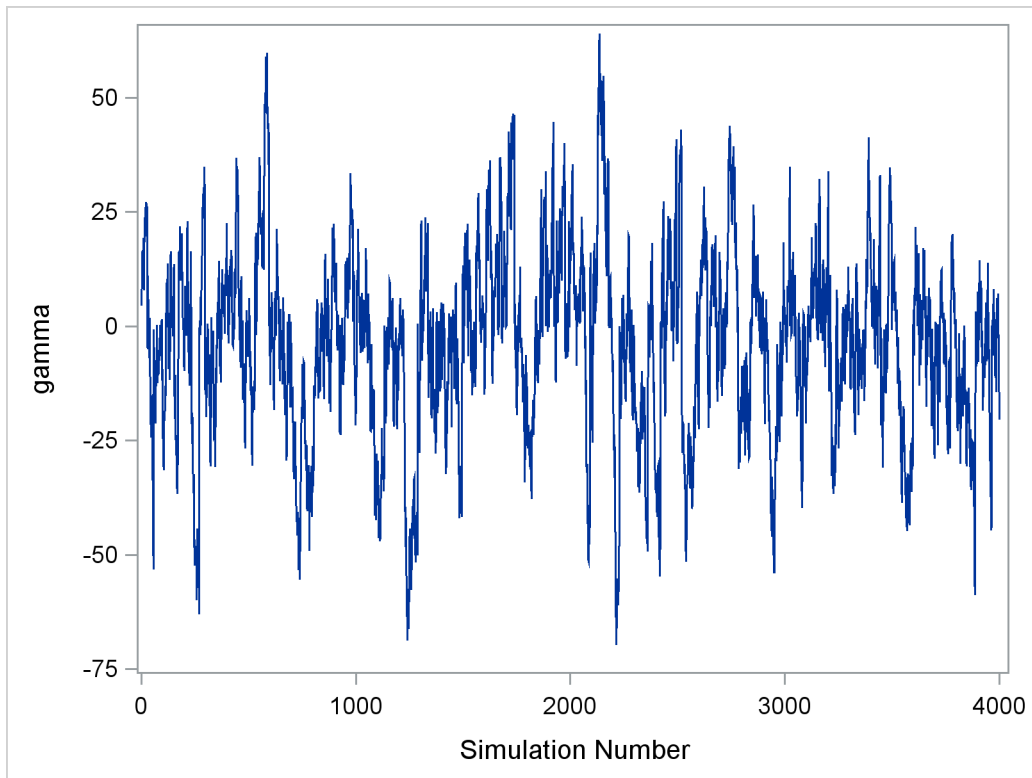
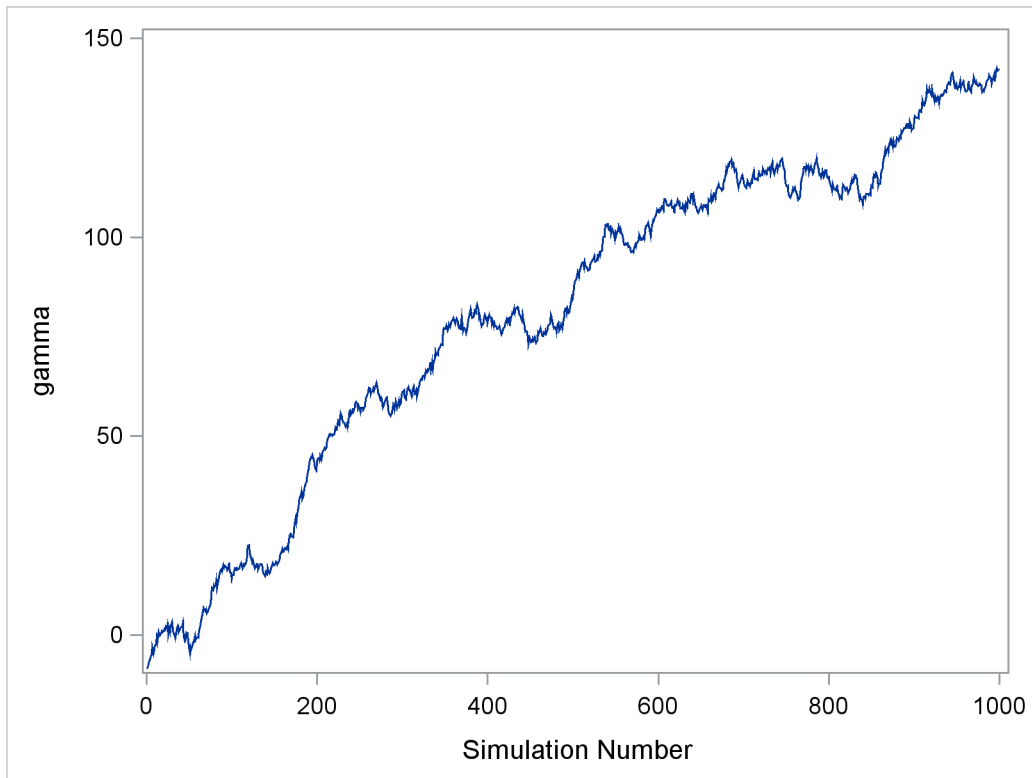
Figure 7.3 Marginal Mixing for γ 

Figure 7.3 demonstrates marginal mixing. The chain is taking only small steps and does not traverse its distribution quickly. This type of trace plot is typically associated with high autocorrelation among the samples. To obtain a few thousand independent samples, you need to run the chain for much longer.

Figure 7.4 Bad Mixing, Nonconvergence of γ 

The trace plot shown in [Figure 7.4](#) depicts a chain with serious problems. It is mixing very slowly, and it offers no evidence of convergence. You would want to try to improve the mixing of this chain. For example, you might consider reparameterizing your model on the log scale. Run the Markov chain for a long time to see where it goes. This type of chain is entirely unsuitable for making parameter inferences.

Statistical Diagnostic Tests

The Bayesian procedures include several statistical diagnostic tests that can help you assess Markov chain convergence. For a detailed description of each of the diagnostic tests, see the following subsections. Table 7.1 provides a summary of the diagnostic tests and their interpretations.

Table 7.1 Convergence Diagnostic Tests Available in the Bayesian Procedures

Name	Description	Interpretation of the Test
Gelman-Rubin	Uses parallel chains with dispersed initial values to test whether they all converge to the same target distribution. Failure could indicate the presence of a multi-mode posterior distribution (different chains converge to different local modes) or the need to run a longer chain (burn-in is yet to be completed).	One-sided test based on a variance ratio test statistic. Large \hat{R}_c values indicate rejection.
Geweke	Tests whether the mean estimates have converged by comparing means from the early and latter part of the Markov chain.	Two-sided test based on a z-score statistic. Large absolute z values indicate rejection.
Heidelberger-Welch (stationarity test)	Tests whether the Markov chain is a covariance (or weakly) stationary process. Failure could indicate that a longer Markov chain is needed.	One-sided test based on a Cramer-von Mises statistic. Small p -values indicate rejection.
Heidelberger-Welch (half-width test)	Reports whether the sample size is adequate to meet the required accuracy for the mean estimate. Failure could indicate that a longer Markov chain is needed.	If a relative half-width statistic is greater than a predetermined accuracy measure, this indicates rejection.
Raftery-Lewis	Evaluates the accuracy of the estimated (desired) percentiles by reporting the number of samples needed to reach the desired accuracy of the percentiles. Failure could indicate that a longer Markov chain is needed.	If the total samples needed are fewer than the Markov chain sample, this indicates rejection.
autocorrelation	Measures dependency among Markov chain samples.	High correlations between long lags indicate poor mixing.
effective sample size	Relates to autocorrelation; measures mixing of the Markov chain.	Large discrepancy between the effective sample size and the simulation sample size indicates poor mixing.

Gelman and Rubin Diagnostics

Gelman and Rubin diagnostics (Gelman and Rubin 1992; Brooks and Gelman 1997) are based on analyzing multiple simulated MCMC chains by comparing the variances within each chain and the variance between chains. Large deviation between these two variances indicates nonconvergence.

Define $\{\theta^t\}$, where $t = 1, \dots, n$, to be the collection of a single Markov chain output. The parameter θ^t is the t th sample of the Markov chain. For notational simplicity, θ is assumed to be single dimensional in this section.

Suppose you have M parallel MCMC chains that were initialized from various parts of the target distribution. Each chain is of length n (after discarding the burn-in). For each θ^t , the simulations are labeled as θ_m^t , where $t = 1, \dots, n$ and $m = 1, \dots, M$. The between-chain variance B and the within-chain variance W are calculated as

$$B = \frac{n}{M-1} \sum_{m=1}^M (\bar{\theta}_m - \bar{\theta})^2, \quad \text{where } \bar{\theta}_m = \frac{1}{n} \sum_{t=1}^n \theta_m^t, \quad \bar{\theta} = \frac{1}{M} \sum_{m=1}^M \bar{\theta}_m$$

$$W = \frac{1}{M} \sum_{m=1}^M s_m^2, \quad \text{where } s_m^2 = \frac{1}{n-1} \sum_{t=1}^n (\theta_m^t - \bar{\theta}_m)^2$$

The posterior marginal variance, $\text{var}(\theta|\mathbf{y})$, is a weighted average of W and B . The estimate of the variance is

$$\hat{V} = \frac{n-1}{n} W + \frac{M+1}{nM} B$$

If all M chains have reached the target distribution, this posterior variance estimate should be very close to the within-chain variance W . Therefore, you would expect to see the ratio \hat{V}/W be close to 1. The square root of this ratio is referred to as the *potential scale reduction factor* (PSRF). A large PSRF indicates that the between-chain variance is substantially greater than the within-chain variance, so that longer simulation is needed. If the PSRF is close to 1, you can conclude that each of the M chains has stabilized, and they are likely to have reached the target distribution.

A refined version of PSRF is calculated, as suggested by Brooks and Gelman (1997), as

$$\hat{R}_c = \sqrt{\frac{\hat{d}+3}{\hat{d}+1} \cdot \frac{\hat{V}}{W}} = \sqrt{\frac{\hat{d}+3}{\hat{d}+1} \left(\frac{n-1}{n} + \frac{M+1}{nM} \frac{B}{W} \right)}$$

where

$$\hat{d} = \frac{2\hat{V}^2}{\widehat{\text{Var}}(\hat{V})}$$

and

$$\widehat{\text{Var}}(\widehat{V}) = \left(\frac{n-1}{n}\right)^2 \frac{1}{M} \widehat{\text{Var}}(s_m^2) + \left(\frac{M+1}{nM}\right)^2 \frac{2}{M-1} B^2 + 2 \frac{(M+1)(n-1)}{n^2 M} \frac{n}{M} (\widehat{\text{cov}}(s_m^2, \bar{\theta}_m^2) - 2\bar{\theta}_m \widehat{\text{cov}}(s_m^2, \bar{\theta}_m))$$

All the Bayesian procedures also produce an upper $100(1 - \alpha/2)\%$ confidence limit of \widehat{R}_c . Gelman and Rubin (1992) showed that the ratio B/W in \widehat{R}_c has an F distribution with degrees of freedom $M - 1$ and $2W^2 M / \widehat{\text{Var}}(s_m^2)$. Because you are concerned only if the scale is large, not small, only the upper $100(1 - \alpha/2)\%$ confidence limit is reported. This is written as

$$\sqrt{\left(\frac{n-1}{n} + \frac{M+1}{nM} \cdot F_{1-\alpha/2}\left(M-1, \frac{2W^2}{\widehat{\text{Var}}(s_m^2)/M}\right)\right) \cdot \frac{\hat{d} + 3}{\hat{d} + 1}}$$

In the Bayesian procedures, you can specify the number of chains that you want to run. Typically three chains are sufficient. The first chain is used for posterior inference, such as mean and standard deviation; the other $M - 1$ chains are used for computing the diagnostics and are discarded afterward. This test can be computationally costly, because it prolongs the simulation M -fold.

It is best to choose different initial values for all M chains. The initial values should be as dispersed from each other as possible so that the Markov chains can fully explore different parts of the distribution before they converge to the target. Similar initial values can be risky because all of the chains can get stuck in a local maximum; that is something this convergence test cannot detect. If you do not supply initial values for all the different chains, the procedures generate them for you.

Geweke Diagnostics

The Geweke test (Geweke 1992) compares values in the early part of the Markov chain to those in the latter part of the chain in order to detect failure of convergence. The statistic is constructed as follows. Two subsequences of the Markov chain $\{\theta^t\}$ are taken out, with $\{\theta_1^t : t = 1, \dots, n_1\}$ and $\{\theta_2^t : t = n_a, \dots, n\}$, where $1 < n_1 < n_a < n$. Let $n_2 = n - n_a + 1$, and define

$$\bar{\theta}_1 = \frac{1}{n_1} \sum_{t=1}^{n_1} \theta^t \quad \text{and} \quad \bar{\theta}_2 = \frac{1}{n_2} \sum_{t=n_a}^n \theta^t$$

Let $\hat{s}_1(0)$ and $\hat{s}_2(0)$ denote consistent spectral density estimates at zero frequency (see the subsection “Spectral Density Estimate at Zero Frequency” on page 147 for estimation details) for the two MCMC chains, respectively. If the ratios n_1/n and n_2/n are fixed, $(n_1 + n_2)/n < 1$, and the chain is stationary, then the following statistic converges to a standard normal distribution as $n \rightarrow \infty$:

$$Z_n = \frac{\bar{\theta}_1 - \bar{\theta}_2}{\sqrt{\frac{\hat{s}_1(0)}{n_1} + \frac{\hat{s}_2(0)}{n_2}}}$$

This is a two-sided test, and large absolute z -scores indicate rejection.

Spectral Density Estimate at Zero Frequency

For one sequence of the Markov chain $\{\theta_t\}$, the relationship between the h -lag covariance sequence of a time series and the spectral density, f , is

$$s_h = \frac{1}{2\pi} \int_{-\pi}^{\pi} \exp(i\omega h) f(\omega) d\omega$$

where i indicates that ωh is the complex argument. Inverting this Fourier integral,

$$f(\omega) = \sum_{h=-\infty}^{\infty} s_h \exp(-i\omega h) = s_0 \left(1 + 2 \sum_{h=1}^{\infty} \rho_h \cos(\omega h) \right)$$

It follows that

$$f(0) = \sigma^2 \left(1 + 2 \sum_{h=1}^{\infty} \rho_h \right)$$

which gives an autocorrelation adjusted estimate of the variance. In this equation, σ^2 is the naive variance estimate of the sequence $\{\theta_t\}$ and ρ_h is the lag h autocorrelation. Due to obvious computational difficulties, such as calculation of autocorrelation at infinity, you cannot effectively estimate $f(0)$ by using the preceding formula. The usual route is to first obtain the *periodogram* $p(\omega)$ of the sequence, and then estimate $f(0)$ by smoothing the estimated periodogram. The periodogram is defined to be

$$p(\omega) = \frac{1}{n} \left[\left(\sum_{t=1}^n \theta_t \sin(\omega t) \right)^2 + \left(\sum_{t=1}^n \theta_t \cos(\omega t) \right)^2 \right]$$

The procedures use the following way to estimate $\hat{f}(0)$ from p (Heidelberger and Welch 1981). In $p(\omega)$, let $\omega = \omega_k = 2\pi k/n$ and $k = 1, \dots, \lfloor \frac{n}{2} \rfloor$.² A smooth spectral density in the domain of $(0, \pi]$ is obtained by fitting a gamma model with the log link function, using $p(\omega_k)$ as response and $x_1(\omega_k) = \sqrt{3}(4\omega_k/(2\pi) - 1)$ as the only regressor. The predicted value $\hat{f}(0)$ is given by

$$\hat{f}(0) = \exp(\hat{\beta}_0 - \sqrt{3}\hat{\beta}_1)$$

where $\hat{\beta}_0$ and $\hat{\beta}_1$ are the estimates of the intercept and slope parameters, respectively.

²This is equivalent to the fast Fourier transformation of the original time series θ_t .

Heidelberger and Welch Diagnostics

The Heidelberger and Welch test (Heidelberger and Welch 1981, 1983) consists of two parts: a stationary portion test and a half-width test. The stationarity test assesses the stationarity of a Markov chain by testing the hypothesis that the chain comes from a covariance stationary process. The half-width test checks whether the Markov chain sample size is adequate to estimate the mean values accurately.

Given $\{\theta^t\}$, set $S_0 = 0$, $S_n = \sum_{t=1}^n \theta^t$, and $\bar{\theta} = (1/n) \sum_{t=1}^n \theta^t$. You can construct the following sequence with s coordinates on values from $\frac{1}{n}, \frac{2}{n}, \dots, 1$:

$$B_n(s) = (S_{[ns]} - [ns]\bar{\theta}) / (n\hat{p}(0))^{1/2}$$

where $[]$ is the rounding operator, and $\hat{p}(0)$ is an estimate of the spectral density at zero frequency that uses the second half of the sequence (see the section “Spectral Density Estimate at Zero Frequency” on page 147 for estimation details). For large n , B_n converges in distribution to a Brownian bridge (Billingsley 1986). So you can construct a test statistic by using B_n . The statistic used in these procedures is the Cramer–von Mises statistic³; that is $\int_0^1 B_n(s)^2 ds = \text{CVM}(B_n)$. As $n \rightarrow \infty$, the statistic converges in distribution to a standard Cramer–von Mises distribution. The integral $\int_0^1 B_n(s)^2 ds$ is numerically approximated using Simpson’s rule.

Let $y_i = B_n(s)^2$, where $s = 0, \frac{1}{n}, \dots, \frac{n-1}{n}, 1$, and $i = ns = 0, 1, \dots, n$. If n is even, let $m = n/2$; otherwise, let $m = (n - 1)/2$. The Simpson’s approximation to the integral is

$$\int_0^1 B_n(s)^2 ds \approx \frac{1}{3n} [y_0 + 4(y_1 + \dots + y_{2m-1}) + 2(y_2 + \dots + y_{2m-2}) + y_{2m}]$$

Note that Simpson’s rule requires an even number of intervals. When n is odd, y_n is set to be 0 and the value does not contribute to the approximation.

This test can be performed repeatedly on the same chain, and it helps you identify a time t when the chain has reached stationarity. The whole chain, $\{\theta^t\}$, is first used to construct the Cramer–von Mises statistic. If it passes the test, you can conclude that the entire chain is stationary. If it fails the test, you drop the initial 10% of the chain and redo the test by using the remaining 90%. This process is repeated until either a time t is selected or it reaches a point where there are not enough data remaining to construct a confidence interval (the cutoff proportion is set to be 50%).

The part of the chain that is deemed stationary is put through a half-width test, which reports whether the sample size is adequate to meet certain accuracy requirements for the mean estimates. Running the simulation less than this length of time would not meet the requirement, while running it longer would not provide any additional information that is needed. The statistic calculated here is the *relative half-width* (RHW) of the confidence interval. The RHW for a confidence interval of level $1 - \alpha$ is

$$\text{RHW} = \frac{z_{(1-\alpha/2)} \cdot (\hat{s}_n/n)^{1/2}}{\hat{\theta}}$$

³ The von Mises distribution was first introduced by von Mises (1918). The density function is $p(\theta|\mu\kappa) \sim M(\mu, \kappa) = [2\pi I_0(\kappa)]^{-1} \exp(\kappa \cos(\theta - \mu))$ ($0 \leq \theta \leq 2\pi$), where the function $I_0(\kappa)$ is the modified Bessel function of the first kind and order zero, defined by $I_0(\kappa) = (2\pi)^{-1} \int_0^{2\pi} \exp(\kappa \cos(\theta - \mu)) d\theta$.

where $z_{(1-\alpha/2)}$ is the z -score of the $100(1 - \alpha/2)$ percentile (for example, $z_{(1-\alpha/2)} = 1.96$ if $\alpha = 0.05$), \hat{s}_n is the variance of the chain estimated using the spectral density method (see explanation in the section “Spectral Density Estimate at Zero Frequency” on page 147), n is the length, and $\hat{\theta}$ is the estimated mean. The RHW quantifies accuracy of the $1 - \alpha$ level confidence interval of the mean estimate by measuring the ratio between the sample standard error of the mean and the mean itself. In other words, you can stop the Markov chain if the variability of the mean stabilizes with respect to the mean. An implicit assumption is that large means are often accompanied by large variances. If this assumption is not met, then this test can produce false rejections (such as a small mean around 0 and large standard deviation) or false acceptance (such as a very large mean with relative small variance). As with any other convergence diagnostics, you might want to exercise caution in interpreting the results.

The stationarity test is one-sided; rejection occurs when the p -value is greater than $1 - \alpha$. To perform the half-width test, you need to select an α level (the default of which is 0.05) and a predetermined tolerance value ϵ (the default of which is 0.1). If the calculated RHW is greater than ϵ , you conclude that there are not enough data to accurately estimate the mean with $1 - \alpha$ confidence under tolerance of ϵ .

Raftery and Lewis Diagnostics

If your interest lies in posterior percentiles, you want a diagnostic test that evaluates the accuracy of the estimated percentiles. The Raftery-Lewis test (Raftery and Lewis 1992, 1996) is designed for this purpose. Notation and deductions here closely resemble those in Raftery and Lewis (1996).

Suppose you are interested in a quantity θ_q such that $P(\theta \leq \theta_q | \mathbf{y}) = q$, where q can be an arbitrary cumulative probability, such as 0.025. This θ_q can be empirically estimated by finding the $[n \cdot 100 \cdot q]$ th number of the sorted $\{\theta^t\}$. Let $\hat{\theta}_q$ denote the estimand, which corresponds to an estimated probability $P(\theta \leq \hat{\theta}_q) = \hat{P}_q$. Because the simulated posterior distribution converges to the true distribution as the simulation sample size grows, $\hat{\theta}_q$ can achieve any degree of accuracy if the simulator is run for a very long time. However, running too long a simulation can be wasteful. Alternatively, you can use coverage probability to measure accuracy and stop the chain when a certain accuracy is reached.

A stopping criterion is reached when the estimated probability is within $\pm r$ of the true cumulative probability q , with probability s , such as $P(\hat{P}_q \in (q - r, q + r)) = s$. For example, suppose you want the coverage probability s to be 0.95 and the amount of tolerance r to be 0.005. This corresponds to requiring that the estimate of the cumulative distribution function of the 2.5th percentile be estimated to within ± 0.5 percentage points with probability 0.95.

The Raftery-Lewis diagnostics test finds the number of iterations, M , that need to be discarded (burn-ins) and the number of iterations needed, N , to achieve a desired precision. Given a predefined cumulative probability q , these procedures first find $\hat{\theta}_q$, and then they construct a binary 0 – 1 process $\{Z_t\}$ by setting $Z_t = 1$ if $\theta^t \leq \hat{\theta}_q$ and 0 otherwise for all t . The sequence $\{Z_t\}$ is itself not a Markov chain, but you can construct a subsequence of $\{Z_t\}$ that is approximately Markovian if it is sufficiently k -thinned. When k becomes reasonably large, $\{Z_t^{(k)}\}$ starts to behave like a Markov chain.

Next, the procedures find this thinning parameter k . The number k is estimated by comparing the Bayesian information criterion (BIC) between two Markov models: a first-order and a second-order Markov model. A j th-order Markov model is one in which the current value of $\{Z_t^{(k)}\}$ depends on the previous j values. For example, in a second-order Markov model,

$$\begin{aligned}
 p \left(Z_t^{(k)} = z_t \mid Z_{t-1}^{(k)} = z_{t-1}, Z_{t-2}^{(k)} = z_{t-2}, \dots, Z_0^{(k)} = z_0 \right) \\
 = p \left(Z_t^{(k)} = z_t \mid Z_{t-1}^{(k)} = z_{t-1}, Z_{t-2}^{(k)} = z_{t-2} \right)
 \end{aligned}$$

where $z_i = \{0, 1\}, i = 0, \dots, t$. Given $\{Z_t^{(k)}\}$, you can construct two transition count matrices for a second-order Markov model:

$$\begin{array}{cc|cc}
 & & z_t = 0 & z_t = 1 \\
 & & z_{t-1} = 0 & z_{t-1} = 1 \\
 z_{t-2} = 0 & w_{000} & w_{010} & \\
 z_{t-2} = 1 & w_{100} & w_{110} & \\
 \hline
 z_{t-2} = 0 & w_{001} & w_{011} & \\
 z_{t-2} = 1 & w_{101} & w_{111} &
 \end{array}$$

For each k , the procedures calculate the BIC that compares the two Markov models. The BIC is based on a likelihood ratio test statistic that is defined as

$$G_k^2 = 2 \sum_{i=0}^1 \sum_{j=0}^1 \sum_{l=0}^1 w_{ijl} \log \frac{w_{ijl}}{\hat{w}_{ijl}}$$

where \hat{w}_{ijl} is the expected cell count of w_{ijl} under the null model, the first-order Markov model, where the assumption $(Z_t^{(k)} \perp Z_{t-2}^{(k)}) \mid Z_{t-1}^{(k)}$ holds. The formula for the expected cell count is

$$\hat{w}_{ijl} = \frac{\sum_i w_{ijl} \cdot \sum_l w_{ijl}}{\sum_i \sum_l w_{ijl}}$$

The BIC is $G_k^2 - 2 \log(n_k - 2)$, where n_k is the k -thinned sample size (every k th sample starting with the first), with the last two data points discarded due to the construction of the second-order Markov model. The thinning parameter k is the smallest k for which the BIC is negative. When k is found, you can estimate a transition probability matrix between state 0 and state 1 for $\{Z_t^{(k)}\}$:

$$Q = \begin{pmatrix} 1 - \alpha & \alpha \\ \beta & 1 - \beta \end{pmatrix}$$

Because $\{Z_t^{(k)}\}$ is a Markov chain, its equilibrium distribution exists and is estimated by

$$\pi = (\pi_0, \pi_1) = \frac{(\beta, \alpha)}{\alpha + \beta}$$

where $\pi_0 = P(\theta \leq \theta_q | y)$ and $\pi_1 = 1 - \pi_0$. The goal is to find an iteration number m such that after m steps, the estimated transition probability $P(Z_m^{(k)} = i | Z_0^{(k)} = j)$ is within ϵ of equilibrium π_i for $i, j = 0, 1$. Let $e_0 = (1, 0)$ and $e_1 = 1 - e_0$. The estimated transition probability after step m is

$$P(Z_m^{(k)} = i | Z_0^{(k)} = j) = e_j \left[\begin{pmatrix} \pi_0 & \pi_1 \\ \pi_0 & \pi_1 \end{pmatrix} + \frac{(1 - \alpha - \beta)^m}{\alpha + \beta} \begin{pmatrix} \alpha & -\alpha \\ -\beta & \beta \end{pmatrix} \right] e_j'$$

which holds when

$$m = \frac{\log\left(\frac{(\alpha + \beta)\epsilon}{\max(\alpha, \beta)}\right)}{\log(1 - \alpha - \beta)}$$

assuming $1 - \alpha - \beta > 0$.

Therefore, by time m , $\{Z_t^{(k)}\}$ is sufficiently close to its equilibrium distribution, and you know that a total size of $M = mk$ should be discarded as the burn-in.

Next, the procedures estimate N , the number of simulations needed to achieve desired accuracy on percentile estimation. The estimate of $P(\theta \leq \theta_q | y)$ is $\bar{Z}_n^{(k)} = \frac{1}{n} \sum_{t=1}^n Z_t^{(k)}$. For large n , $\bar{Z}_n^{(k)}$ is normally distributed with mean q , the true cumulative probability, and variance

$$\frac{1}{n} \frac{(2 - \alpha - \beta)\alpha\beta}{(\alpha + \beta)^3}$$

$P(q - r \leq \bar{Z}_n^{(k)} \leq q + r) = s$ is satisfied if

$$n = \frac{(2 - \alpha - \beta)\alpha\beta}{(\alpha + \beta)^3} \left\{ \frac{\Phi^{-1}\left(\frac{s+1}{2}\right)}{r} \right\}^2$$

Therefore, $N = nk$.

By using similar reasoning, the procedures first calculate the minimal number of iterations needed to achieve the desired accuracy, assuming the samples are independent:

$$N_{min} = \left\{ \Phi^{-1}\left(\frac{s+1}{2}\right) \right\}^2 \frac{q(1-q)}{r^2}$$

If $\{\theta^t\}$ does not have that required sample size, the Raftery-Lewis test is not carried out. If you still want to carry out the test, increase the number of Markov chain iterations.

The ratio N/N_{min} is sometimes referred to as the *dependence factor*. It measures deviation from posterior sample independence: the closer it is to 1, the less correlated are the samples. There are a few things to keep

in mind when you use this test. This diagnostic tool is specifically designed for the percentile of interest and does not provide information about convergence of the chain as a whole (Brooks and Roberts 1999). In addition, the test can be very sensitive to small changes. Both N and N_{min} are inversely proportional to r^2 , so you can expect to see large variations in these numbers with small changes to input variables, such as the desired coverage probability or the cumulative probability of interest. Last, the time until convergence for a parameter can differ substantially for different cumulative probabilities.

Autocorrelations

The sample autocorrelation of lag h for a parameter θ is defined in terms of the sample autocovariance function:

$$\hat{\rho}_h(\theta) = \frac{\hat{\gamma}_h(\theta)}{\hat{\gamma}_0(\theta)}, \quad |h| < n$$

The sample autocovariance function of lag h of θ is defined by

$$\hat{\gamma}_h(\theta) = \frac{1}{n-h} \sum_{t=1}^{n-h} (\theta^{t+h} - \bar{\theta})(\theta^t - \bar{\theta}), \quad 0 \leq h < n$$

Effective Sample Size

You can use autocorrelation and trace plots to examine the mixing of a Markov chain. A closely related measure of mixing is the effective sample size (ESS) (Kass et al. 1998).

ESS is defined as follows:

$$\text{ESS} = \frac{n}{\tau} = \frac{n}{1 + 2 \sum_{k=1}^{\infty} \rho_k(\theta)}$$

where n is the total sample size and $\rho_k(\theta)$ is the autocorrelation of lag k for θ . The quantity τ is referred to as the autocorrelation time. To estimate τ , the Bayesian procedures first find a cutoff point k after which the autocorrelations are very close to zero, and then sum all the ρ_k up to that point. The cutoff point k is such that $|\rho_k| < \min\{0.01, 2s_k\}$, where s_k is the estimated standard deviation:

$$s_k = \sqrt{\left(\frac{1}{n} \left(1 + 2 \sum_{j=1}^{k-1} \hat{\rho}_j^2(\theta) \right) \right)}$$

ESS and τ are inversely proportional to each other, and low ESS or high τ indicates bad mixing of the Markov chain.

Summary Statistics

Let θ be a p -dimensional parameter vector of interest: $\theta = \{\theta_1, \dots, \theta_p\}$. For each $i \in \{1, \dots, p\}$, there are n observations: $\theta_i = \{\theta_i^t, t = 1, \dots, n\}$.

Mean

The posterior mean is calculated by using the following formula:

$$E(\theta_i | \mathbf{y}) \approx \bar{\theta}_i = \frac{1}{n} \sum_{t=1}^n \theta_i^t, \text{ for } i = 1, \dots, p$$

Standard Deviation

Sample standard deviation (expressed in variance term) is calculated by using the following formula:

$$\text{Var}(\theta_i | \mathbf{y}) \approx s_i^2 = \frac{1}{n-1} \sum_{t=1}^n (\theta_i^t - \bar{\theta}_i)^2$$

Standard Error of the Mean Estimate

Suppose you have n iid samples, the mean estimate is $\bar{\theta}_i$, and the sample standard deviation is s_i . The standard error of the estimate is $\hat{\sigma}_i / \sqrt{n}$. However, positive autocorrelation (see the section “Autocorrelations” on page 152 for a definition) in the MCMC samples makes this an underestimate. To take account of the autocorrelation, the Bayesian procedures correct the standard error by using effective sample size (see the section “Effective Sample Size” on page 152).

Given an effective sample size of m , the standard error for $\bar{\theta}_i$ is $\hat{\sigma}_i / \sqrt{m}$. The procedures use the following formula (expressed in variance term):

$$\widehat{\text{Var}}(\bar{\theta}_i) = \frac{1 + 2 \sum_{k=1}^{\infty} \rho_k(\theta_i)}{n} \cdot \frac{\sum_{t=1}^n (\theta_i^t - \bar{\theta}_i)^2}{(n-1)}$$

The standard error of the mean is also known as the Monte Carlo standard error (MCSE). The MCSE provides a measurement of the accuracy of the posterior estimates, and small values do not necessarily indicate that you have recovered the true posterior mean.

Percentiles

Sample percentiles are calculated using Definition 5 (see Chapter 4, “The UNIVARIATE Procedure” (*Base SAS Procedures Guide: Statistical Procedures*)).

Correlation

Correlation between θ_i and θ_j is calculated as

$$r_{ij} = \frac{\sum_{t=1}^n (\theta_i^t - \bar{\theta}_i) (\theta_j^t - \bar{\theta}_j)}{\sqrt{\sum_{t=1}^n (\theta_i^t - \bar{\theta}_i)^2 \sum_{t=1}^n (\theta_j^t - \bar{\theta}_j)^2}}$$

Covariance

Covariance θ_i and θ_j is calculated as

$$s_{ij} = \sum_{t=1}^n (\theta_i^t - \bar{\theta}_i) (\theta_j^t - \bar{\theta}_j) / (n - 1)$$

Equal-Tail Credible Interval

Let $\pi(\theta_i | \mathbf{y})$ denote the marginal posterior cumulative distribution function of θ_i . A $100(1 - \alpha)\%$ Bayesian equal-tail credible interval for θ_i is $(\theta_i^{\alpha/2}, \theta_i^{1-\alpha/2})$, where $\pi(\theta_i^{\alpha/2} | \mathbf{y}) = \frac{\alpha}{2}$, and $\pi(\theta_i^{1-\alpha/2} | \mathbf{y}) = 1 - \frac{\alpha}{2}$. The interval is obtained using the empirical $\frac{\alpha}{2}$ and $(1 - \frac{\alpha}{2})$ percentiles of $\{\theta_i^t\}$.

Highest Posterior Density (HPD) Interval

For a definition of an HPD interval, see the section “[Interval Estimation](#)” on page 131. The procedures use the Chen-Shao algorithm (Chen and Shao 1999; Chen, Shao, and Ibrahim 2000) to estimate an empirical HPD interval of θ_i :

1. Sort $\{\theta_i^t\}$ to obtain the ordered values:

$$\theta_{i(1)} \leq \theta_{i(2)} \leq \dots \leq \theta_{i(n)}$$

2. Compute the $100(1 - \alpha)\%$ credible intervals:

$$R_j(n) = (\theta_{i(j)}, \theta_{i(j+[1-\alpha)n]})$$

for $j = 1, 2, \dots, n - [(1 - \alpha)n]$.

3. The $100(1 - \alpha)\%$ HPD interval, denoted by $R_{j^*}(n)$, is the one with the smallest interval width among all credible intervals.

Deviance Information Criterion (DIC)

The deviance information criterion (DIC) (Spiegelhalter et al. 2002) is a model assessment tool, and it is a Bayesian alternative to Akaike's information criterion (AIC) and the Bayesian information criterion (BIC, also known as the Schwarz criterion). The DIC uses the posterior densities, which means that it takes the prior information into account. The criterion can be applied to nonnested models and models that have non-iid data. Calculation of the DIC in MCMC is trivial—it does not require maximization over the parameter space, like the AIC and BIC. A smaller DIC indicates a better fit to the data set.

Letting θ be the parameters of the model, the deviance information formula is

$$\text{DIC} = \overline{D(\theta)} + p_D = D(\bar{\theta}) + 2p_D$$

where

$$D(\theta) = 2 (\log(f(\mathbf{y})) - \log(p(\mathbf{y}|\theta))) : \text{deviance}$$

where

$p(\mathbf{y}|\theta)$: likelihood function with the normalizing constants.

$f(\mathbf{y})$: a standardizing term that is a function of the data alone. This term is constant with respect to the parameter and is irrelevant when you compare different models that have the same likelihood function. Since the term cancels out in DIC comparisons, its calculation is often omitted.

NOTE: You can think of the deviance as the difference in twice the log likelihood between the saturated, $f(\mathbf{y})$, and fitted, $p(\mathbf{y}|\theta)$, models.

$\bar{\theta}$: posterior mean, approximated by $\frac{1}{n} \sum_{t=1}^n \theta^t$

$\overline{D(\theta)}$: posterior mean of the deviance, approximated by $\frac{1}{n} \sum_{t=1}^n D(\theta^t)$. The expected deviation measures how well the model fits the data.

$D(\bar{\theta})$: deviance evaluated at $\bar{\theta}$, equal to $-2 \log(p(\mathbf{y}|\bar{\theta}))$. It is the deviance evaluated at your “best” posterior estimate.

p_D : effective number of parameters. It is the difference between the measure of fit and the deviance at the estimates: $\overline{D(\theta)} - D(\bar{\theta})$. This term describes the complexity of the model, and it serves as a penalization term that corrects deviance's propensity toward models with more parameters.

A Bayesian Reading List

This section lists a number of Bayesian textbooks of varying difficulty degrees and a few tutorial/review papers.

Textbooks

Introductory Books

- Berry, D. A. (1996), *Statistics: A Bayesian Perspective*, London: Duxbury Press.
- Bolstad, W. M. (2007), *Introduction to Bayesian Statistics*, 2nd ed. New York: John Wiley & Sons.
- DeGroot, M. H. and Schervish, M. J. (2002), *Probability and Statistics*, Reading, MA: Addison Wesley.
- Gamerman, D. and Lopes, H. F. (2006), *Markov Chain Monte Carlo: Stochastic Simulation for Bayesian Inference*, 2nd ed. London: Chapman & Hall/CRC.
- Ghosh, J. K., Delampady, M., and Samanta, T. (2006), *An Introduction to Bayesian Analysis*, New York: Springer-Verlag.
- Lee, P. M. (2004), *Bayesian Statistics: An Introduction*, 3rd ed. London: Arnold.
- Sivia, D. S. (1996), *Data Analysis: A Bayesian Tutorial*, Oxford: Oxford University Press.

Intermediate-Level Books

- Box, G. E. P., and Tiao, G. C. (1992), *Bayesian Inference in Statistical Analysis*, New York: John Wiley & Sons.
- Chen, M. H., Shao Q. M., and Ibrahim, J. G. (2000), *Monte Carlo Methods in Bayesian Computation*, New York: Springer-Verlag.
- Gelman, A. and Hill, J. (2006), *Data Analysis Using Regression and Multilevel/Hierarchical Models*, Cambridge: Cambridge University Press.
- Goldstein, M. and Woof, D. A. (2007), *Bayes Linear Statistics: Theory and Methods*, New York: John Wiley & Sons.
- Harney, H. L. (2003), *Bayesian Inference: Parameter Estimation and Decisions*, New York: Springer-Verlag.
- Leonard, T. and Hsu, J. S. (1999), *Bayesian Methods: An Analysis for Statisticians and Interdisciplinary Researchers*, Cambridge: Cambridge University Press.
- Liu, J. S. (2001), *Monte Carlo Strategies in Scientific Computing*, New York: Springer-Verlag.
- Marin, J. M. and Robert, C. P. (2007), *Bayesian Core: a Practical Approach to Computational Bayesian Statistics*, New York: Springer-Verlag.
- Press, S. J. (2002), *Subjective and Objective Bayesian Statistics: Principles, Models, and Applications*, 2nd ed. New York: Wiley-Interscience.
- Robert, C. P. (2001), *The Bayesian Choice*, 2nd ed. New York: Springer-Verlag.

- Robert, C. P. and Casella, G. (2004), *Monte Carlo Statistical Methods*, 2nd ed. New York: Springer-Verlag.
- Tanner, M. A. (1993), *Tools for Statistical Inference: Methods for the Exploration of Posterior Distributions and Likelihood Functions*, New York: Springer-Verlag.

Advanced Titles

- Berger, J. O. (1985), *Statistical Decision Theory and Bayesian Analysis*, New York: Springer-Verlag.
- Bernardo, J. M. and Smith, A. F. M. (2007), *Bayesian Theory*, 2nd ed. New York: John Wiley & Sons.
- de Finetti, B. (1992), *Theory of Probability*, New York: John Wiley & Sons.
- Jeffreys, H. (1998), *Theory of Probability*, Oxford: Oxford University Press.
- O'Hagan, A. (1994), *Bayesian Inference*, volume 2B of *Kendall's Advanced Theory of Statistics*, London: Arnold.
- Savage, L. J. (1954), *The Foundations of Statistics*, New York: John Wiley & Sons.

Books Motivated by Statistical Applications and Data Analysis

- Carlin, B. and Louis, T. A. (2000), *Bayes and Empirical Bayes Methods for Data Analysis*, 2nd ed. London: Chapman & Hall.
- Congdon, P. (2006), *Bayesian Statistical Modeling*, 2nd ed. New York: John Wiley & Sons.
- Congdon, P. (2003), *Applied Bayesian Modeling*, New York: John Wiley & Sons.
- Congdon, P. (2005), *Bayesian Models for Categorical Data*, New York: John Wiley & Sons.
- Gelman, A., Carlin, J. B., Stern, H. S., and Rubin, D. B. (2004), *Bayesian Data Analysis*, 3rd ed. London: Chapman & Hall.
- Gilks, W. R., Richardson, S., and Spiegelhalter, D. J. (1996), *Markov Chain Monte Carlo in Practice*, London: Chapman & Hall.

Tutorial and Review Papers on MCMC

- Besag, J., Green, P., Higdon, D., and Mengersen, K. (1995), "Bayesian Computation and Stochastic Systems," *Statistical Science*, 10(1), 3–66.
- Casella, G. and George, E. (1992), "Explaining the Gibbs Sampler," *The American Statistician*, 46, 167–174.
- Chib, S. and Greenberg, E. (1995), "Understanding the Metropolis-Hastings Algorithm," *The American Statistician*, 49, 327–335.
- Chib, S. and Greenberg, E. (1996), "Markov Chain Monte Carlo Simulation Methods in Econometrics," *Econometric Theory*, 12, 409–431.
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Chapter 8

Introduction to Categorical Data Analysis Procedures

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Overview: Categorical Data Analysis Procedures

There are two approaches to performing categorical data analyses. The first computes statistics based on tables defined by *categorical variables* (variables that assume only a limited number of discrete values), performs hypothesis tests about the association between these variables, and requires the assumption of a randomized process; following Stokes, Davis, and Koch (2000), call these methods *randomization procedures*. The other approach investigates the association by modeling a categorical response variable, regardless of whether the explanatory variables are continuous or categorical; call these methods *modeling procedures*. Several procedures in SAS/STAT software can be used for the analysis of categorical data.

The randomization procedures are:

FREQ builds frequency tables or contingency tables and can produce numerous statistics. For one-way frequency tables, it can perform tests for equal proportions, specified proportions, or the binomial proportion. For contingency tables, it can compute various tests and measures of association and agreement including chi-square statistics, odds ratios, correlation statistics, Fisher's exact test for any size two-way table, kappa, and trend tests. In addition, it performs stratified analysis, computing Cochran-Mantel-Haenszel statistics and estimates of the common relative risk. Exact *p*-values and confidence intervals are available for various test statistics and measures. See Chapter 38, "The FREQ Procedure," for more information.

SURVEYFREQ incorporates complex sample designs to analyze one-way, two-way, and multiway crosstabulation tables. Estimates population totals and proportions and performs tests of goodness-of-fit and independence. See Chapter 14, “Introduction to Survey Procedures,” and Chapter 90, “The SURVEYFREQ Procedure,” for more information.

The modeling procedures, which require a categorical response variable, are:

CATMOD fits linear models to functions of categorical data, facilitating such analyses as regression, analysis of variance, linear modeling, log-linear modeling, logistic regression, and repeated measures analysis. Maximum likelihood estimation is used for the analysis of logits and generalized logits, and weighted least squares analysis is used for fitting models to other response functions. Iterative proportional fitting (IPF), which avoids the need for parameter estimation, is available for fitting hierarchical log-linear models when there is a single population. See Chapter 30, “The CATMOD Procedure,” for more information.

GENMOD fits generalized linear models with maximum-likelihood methods. This family includes logistic, probit, and complementary log-log regression models for binomial data, Poisson and negative binomial regression models for count data, and multinomial models for ordinal response data. It performs likelihood ratio and Wald tests for Type I, Type III, and user-defined contrasts. It analyzes repeated measures data with generalized estimating equation (GEE) methods. Bayesian analysis capabilities for generalized linear models are also available. See Chapter 40, “The GENMOD Procedure,” for more information.

GLIMMIX fits generalized linear mixed models with maximum-likelihood methods. If the model does not contain random effects, the GLIMMIX procedure fits generalized linear models by the method of maximum likelihood. This family includes logistic, probit, and complementary log-log regression models for binomial data, Poisson and negative binomial regression models for count data, and multinomial models for ordinal response data. See Chapter 41, “The GLIMMIX Procedure,” for more information.

LOGISTIC fits linear logistic regression models for discrete response data with maximum-likelihood methods. It provides four variable selection methods, computes regression diagnostics, and compares and outputs receiver operating characteristic curves. It can also perform stratified conditional logistic regression analysis for binary response data and exact conditional regression analysis for binary and nominal response data. The logit link function in the logistic regression models can be replaced by the probit function or the complementary log-log function. See Chapter 54, “The LOGISTIC Procedure,” for more information.

PROBIT fits models with probit, logit, or complementary log-log links for quantal assay or other discrete event data. It is mainly designed for dose-response analysis with a natural response rate. It computes the fiducial limits for the dose variable and provides various graphical displays for the analysis. See Chapter 75, “The PROBIT Procedure,” for more information.

SURVEYLOGISTIC fits logistic models for binary and ordinal outcomes to survey data by maximum likelihood, incorporating complex survey sample designs. See Chapter 91, “The SURVEYLOGISTIC Procedure,” for more information.

Also see Chapter 3, “Introduction to Statistical Modeling with SAS/STAT Software,” and Chapter 4, “Introduction to Regression Procedures,” for more information about all the modeling and regression procedures.

Other procedures that can be used for categorical data analysis and modeling are:

- CORRESP** performs simple and multiple correspondence analyses, using a contingency table, Burt table, binary table, or raw categorical data as input. See Chapter 9, “Introduction to Multivariate Procedures,” and Chapter 32, “The CORRESP Procedure,” for more information.
- PRINQUAL** performs a principal component analysis of qualitative and/or quantitative data, and multidimensional preference analysis. See Chapter 9, “Introduction to Multivariate Procedures,” and Chapter 74, “The PRINQUAL Procedure,” for more information.
- TRANSREG** fits univariate and multivariate linear models, optionally with spline and other nonlinear transformations. Models include ordinary regression and ANOVA, multiple and multivariate regression, metric and nonmetric conjoint analysis, metric and nonmetric vector and ideal point preference mapping, redundancy analysis, canonical correlation, and response surface regression. See Chapter 4, “Introduction to Regression Procedures,” and Chapter 97, “The TRANSREG Procedure,” for more information.

Introduction

A *categorical variable* is a variable that assumes only a limited number of discrete values. The measurement scale for a categorical variable is unrestricted. It can be *nominal*, which means that the observed levels are not ordered. It can be *ordinal*, which means that the observed levels are ordered in some way. Or it can be *interval*, which means that the observed levels are ordered and numeric and that any interval of one unit on the scale of measurement represents the same amount, regardless of its location on the scale. One example of a categorical variable is litter size; another is the number of times a subject has been married. A variable that lies on a nominal scale is sometimes called a *qualitative* or *classification variable*.

Categorical data result from observations on multiple subjects where one or more categorical variables are observed for each subject. If there is only one categorical variable, then the data are generally represented by a *frequency table*, which lists each observed value of the variable and its frequency of occurrence.

If there are two or more categorical variables, then a subject’s *profile* is defined as the subject’s observed values for each of the variables. Such categorical data can be represented by a frequency table that lists each observed profile and its frequency of occurrence.

If there are exactly two categorical variables, then the data are often represented by a two-dimensional *contingency table*, which has one row for each level of variable 1 and one column for each level of variable 2. The intersections of rows and columns, called *cells*, correspond to variable profiles, and each cell contains the frequency of occurrence of the corresponding profile.

If there are more than two categorical variables, then the data can be represented by a *multidimensional contingency table*. There are two commonly used methods for displaying such tables, and both require that the variables be divided into two sets.

- In the first method, one set contains a row variable and a column variable for a two-dimensional contingency table, and the second set contains all of the other variables. The variables in the second set are used to form a set of profiles. Thus, the data are represented as a series of two-dimensional

contingency tables, one for each profile. This is the data representation used by PROC FREQ. For example, if you request tables for RACE*SEX*AGE*INCOME, the FREQ procedure represents the data as a series of contingency tables: the row variable is AGE, the column variable is INCOME, and the combinations of levels of RACE and SEX form a set of profiles.

- In the second method, one set contains the independent variables, and the other set contains the dependent variables. Profiles based on the independent variables are called *population profiles*, whereas those based on the dependent variables are called *response profiles*. A two-dimensional contingency table is then formed, with one row for each population profile and one column for each response profile. Since any subject can have only one population profile and one response profile, the contingency table is uniquely defined. This is the data representation used by the modeling procedures.

NOTE: Modeling procedures for categorical data analysis only require that the response variable be categorical—the explanatory variables are allowed to be continuous or categorical. However, note that PROC CATMOD was designed to handle contingency table data, and it does not efficiently handle continuous covariates.

Sampling Frameworks and Distribution Assumptions

This section discusses the sampling frameworks and distribution assumptions for the modeling and randomization procedures.

Simple Random Sampling: One Population

Suppose you take a simple random sample of 100 people and ask each person the following question, “Of the three colors red, blue, and green, which is your favorite?” You then tabulate the results in a frequency table as shown in Table 8.1.

Table 8.1 One-Way Frequency Table

	Favorite Color			Total
	Red	Blue	Green	
Frequency	52	31	17	100
Proportion	0.52	0.31	0.17	1.00

In the population you are sampling, you assume there is an unknown probability that a population member, selected at random, would choose any given color. In order to estimate that probability, you use the sample proportion

$$p_j = \frac{n_j}{n}$$

where n_j is the frequency of the j th response and n is the total frequency.

Because of the random variation inherent in any random sample, the frequencies have a probability distribution representing their relative frequency of occurrence in a hypothetical series of samples. For a simple

random sample, the distribution of frequencies for a frequency table with three levels is as follows. The probability that the first frequency is n_1 , the second frequency is n_2 , and the third is $n_3 = n - n_1 - n_2$, is given by

$$\Pr(n_1, n_2, n_3) = \frac{n!}{n_1!n_2!n_3!} \pi_1^{n_1} \pi_2^{n_2} \pi_3^{n_3}$$

where π_j is the true probability of observing the j th response level in the population.

This distribution, called the *multinomial distribution*, can be generalized to any number of response levels. The special case of two response levels is called the *binomial distribution*.

Simple random sampling is the type of sampling required by the (non-survey) modeling procedures when there is one population. The modeling procedures use the multinomial distribution to estimate a probability vector and its covariance matrix. If the sample size is sufficiently large, then the probability vector is approximately normally distributed as a result of central limit theory. This result is used to compute appropriate test statistics for the specified statistical model.

Stratified Simple Random Sampling: Multiple Populations

Suppose you take two simple random samples, 50 men and 50 women, and ask the same question as before. You are now sampling two different populations that may have different response probabilities. The data can be tabulated as shown in Table 8.2.

Table 8.2 Two-Way Contingency Table: Sex by Color

Sex	Favorite Color			Total
	Red	Blue	Green	
Male	30	10	10	50
Female	20	10	20	50
Total	50	20	30	100

Note that the row marginal totals (50, 50) of the contingency table are fixed by the sampling design, but the column marginal totals (50, 20, 30) are random. There are six probabilities of interest for this table, and they are estimated by the sample proportions

$$p_{ij} = \frac{n_{ij}}{n_i}$$

where n_{ij} denotes the frequency for the i th population and the j th response and n_i is the total frequency for the i th population. For this contingency table, the sample proportions are shown in Table 8.3.

Table 8.3 Table of Sample Proportions by Sex

Sex	Favorite Color			Total
	Red	Blue	Green	
Male	0.60	0.20	0.20	1.00
Female	0.40	0.20	0.40	1.00

The probability distribution of the six frequencies is the *product multinomial distribution*

$$\Pr(n_{11}, n_{12}, n_{13}, n_{21}, n_{22}, n_{23}) = \frac{n_1!n_2!\pi_{11}^{n_{11}}\pi_{12}^{n_{12}}\pi_{13}^{n_{13}}\pi_{21}^{n_{21}}\pi_{22}^{n_{22}}\pi_{23}^{n_{23}}}{n_{11}!n_{12}!n_{13}!n_{21}!n_{22}!n_{23}!}$$

where π_{ij} is the true probability of observing the j th response level in the i th population. The product multinomial distribution is simply the product of two or more individual multinomial distributions since the populations are independent. This distribution can be generalized to any number of populations and response levels.

Stratified simple random sampling is the type of sampling required by the modeling procedures when there is more than one population. The product multinomial distribution is used to estimate a probability vector and its covariance matrix. If the sample sizes are sufficiently large, then the probability vector is approximately normally distributed as a result of central limit theory, and this result is used to compute appropriate test statistics for the specified statistical model. The statistics are known as Wald statistics, and they are approximately distributed as chi-square when the null hypothesis is true.

Observational Data: Analyzing the Entire Population

Sometimes the observed data do not come from a random sample but instead represent a complete set of observations on some population. For example, suppose a class of 100 students is classified according to sex and favorite color. The results are shown in Table 8.4.

In this case, you could argue that all of the frequencies are fixed since the entire population is observed; therefore, there is no sampling error. On the other hand, you could hypothesize that the observed table has only fixed marginals and that the cell frequencies represent one realization of a conceptual process of assigning color preferences to individuals. The assignment process is open to hypothesis, which means that you can hypothesize restrictions on the joint probabilities.

Table 8.4 Two-Way Contingency Table: Sex by Color

Sex	Favorite Color			Total
	Red	Blue	Green	
Male	16	21	20	57
Female	12	20	11	43
Total	28	41	31	100

The usual hypothesis (sometimes called *randomness*) is that the distribution of the column variable (Favorite Color) does not depend on the row variable (Sex). This implies that, for each row of the table, the assignment process corresponds to a simple random sample (without replacement) from the finite population represented by the column marginal totals (or by the column marginal subtotals that remain after sampling other rows). The hypothesis of randomness implies that the probability distribution on the frequencies in the table is the *hypergeometric distribution*.

If the same row and column variables are observed for each of several populations, then the probability distribution of all the frequencies can be called the *multiple hypergeometric distribution*. Each population is called a *stratum*, and an analysis that draws information from each stratum and then summarizes across

them is called a *stratified analysis* (or a *blocked analysis* or a *matched analysis*). PROC FREQ does such a stratified analysis, computing test statistics and measures of association.

In general, the populations are formed on the basis of cross-classifications of independent variables. Stratified analysis is a method of adjusting for the effect of these variables without being forced to estimate parameters for them. Note that PROC LOGISTIC can perform analyses on stratified tables as well, using the usual modeling procedure assumptions, by using conditional or exact conditional logistic regression.

The multiple hypergeometric distribution is the one used by PROC FREQ for the computation of Cochran-Mantel-Haenszel statistics. These statistics are in the class of *randomization model test statistics*, which require minimal assumptions for their validity. PROC FREQ uses the multiple hypergeometric distribution to compute the mean and the covariance matrix of a function vector in order to measure the deviation between the observed and expected frequencies with respect to a particular type of alternative hypothesis. If the cell frequencies are sufficiently large, then the function vector is approximately normally distributed as a result of central limit theory, and PROC FREQ uses this result to compute a quadratic form that has a chi-square distribution when the null hypothesis is true.

Randomized Experiments

Consider a *randomized experiment* in which patients are assigned to one of two treatment groups according to a randomization process that allocates 50 patients to each group. After a specified period of time, each patient's status (cured or not cured) is recorded. Suppose the data shown in Table 8.5 give the results of the experiment. The null hypothesis is that the two treatments are equally effective. Under this hypothesis, treatment is a randomly assigned label that has no effect on the cure rate of the patients. But this implies that each row of the table represents a simple random sample from the finite population whose cure rate is described by the column marginal totals. Therefore, the column marginals (58, 42) are fixed under the hypothesis. Since the row marginals (50, 50) are fixed by the allocation process, the hypergeometric distribution is induced on the cell frequencies. Randomized experiments can also be specified in a stratified framework, and Cochran-Mantel-Haenszel statistics can be computed relative to the corresponding multiple hypergeometric distribution.

Table 8.5 Two-Way Contingency Table: Treatment by Status

Treatment	Status		Total
	Cured	Not Cured	
1	36	14	50
2	22	28	50
Total	58	42	100

Relaxation of Sampling Assumptions

As indicated previously, the modeling procedures assume that the data are from a stratified simple random sample, so they use the product multinomial distribution. If the data are not from such a sample, then in many cases it is still possible to use a modeling procedure by arguing that each row of the contingency table *does* represent a simple random sample from some hypothetical population. The extent to which the inferences are generalizable depends on the extent to which the hypothetical population is perceived to resemble the target population.

Similarly, the Cochran-Mantel-Haenszel statistics use the multiple hypergeometric distribution, which requires fixed row and column marginal totals in each contingency table. If the sampling process does not yield a table with fixed margins, then it is usually possible to fix the margins through conditioning arguments similar to the ones used by Fisher when he developed the Exact Test for 2×2 tables. In other words, if you want fixed marginal totals, you can generally make your analysis conditional on those observed totals.

For more information on sampling models for categorical data, see Bishop, Fienberg, and Holland (1975, Chapter 13) and Agresti (2002, Chapter 1.2).

Comparison of PROC FREQ and the Modeling Procedures

PROC FREQ is used primarily to investigate the relationship between two variables; any confounding variables are taken into account by stratification rather than by parameter estimation. Modeling procedures are used to investigate the relationship among many variables, all of which are integrated into a parametric model.

When a modeling procedure estimates the covariance matrix of the frequencies, it assumes that the frequencies were obtained by a stratified simple random-sampling procedure. However, some modeling procedures can handle different sampling methods. PROC CATMOD can analyze input data that consists of a function vector and a covariance matrix, so you can estimate the covariance matrix of the frequencies in the appropriate manner before modeling the data. PROC SURVEYLOGISTIC can analyze data from a completely different, but known, sampling scheme.

For the FREQ procedure, Fisher's Exact Test and Cochran-Mantel-Haenszel (CMH) statistics are based on the hypergeometric distribution, which corresponds to fixed marginal totals. However, by conditioning arguments, these tests are generally applicable to a wide range of sampling procedures. Similarly, the Pearson and likelihood-ratio chi-square statistics can be derived under a variety of sampling situations.

PROC FREQ can do some traditional nonparametric analysis (such as the Kruskal-Wallis test and Spearman's correlation) since it can generate rank scores internally. Fisher's Exact Test and the CMH statistics are also inherently nonparametric. However, the main vehicle for nonparametric analyses in the SAS System is the NPAR1WAY procedure.

A large sample size is required for the validity of the chi-square distributions, the standard errors, and the covariance matrices for PROC FREQ and the modeling procedures. If sample size is a problem, then PROC FREQ has the advantage with its CMH statistics because it does not use any degrees of freedom to estimate parameters for confounding variables. In addition, PROC FREQ can compute exact p -values for any two-way table, provided that the sample size is sufficiently small in relation to the size of the table. It can also produce exact p -values for many tests, including the test of binomial proportions, the Cochran-Armitage test for trend, and the Jonckheere-Terpstra test for ordered differences among classes. PROC LOGISTIC can perform exact conditional logistic regression and Firth's penalized-likelihood regression to compensate for small sample sizes.

See the procedure chapters for more information. In addition, some well-known texts that deal with analyzing categorical data are listed in the "References" section of this chapter.

Comparison of Modeling Procedures

The CATMOD, GENMOD, GLIMMIX, LOGISTIC, PROBIT, and SURVEYLOGISTIC procedures can all be used for statistical modeling of categorical data.

The CATMOD procedure treats all explanatory (independent) variables as classification variables by default, and you specify continuous covariates in the DIRECT statement. The other procedures treat covariates as continuous by default, and you specify the classification variables in the CLASS statement.

The CATMOD procedure provides weighted least squares estimation of many response functions, such as means, cumulative logits, and proportions, and you can also compute and analyze other response functions that can be formed from the proportions corresponding to the rows of a contingency table. In addition, a user can input and analyze a set of response functions and user-supplied covariance matrix with weighted least squares. PROC CATMOD also provides maximum likelihood estimation for binary and polytomous logistic regression.

The GENMOD procedure is also a general statistical modeling tool which fits generalized linear models to data; it fits several useful models to categorical data including logistic regression, the proportional odds model, and Poisson and negative binomial regression for count data. The GENMOD procedure also provides a facility for fitting generalized estimating equations to correlated response data that are categorical, such as repeated dichotomous outcomes. The GENMOD procedure fits models using maximum likelihood estimation. PROC GENMOD can perform Type I and Type III tests, and it provides predicted values and residuals. Bayesian analysis capabilities for generalized linear models are also available.

The GLIMMIX procedure fits many of the same models as the GENMOD procedure but also allows the inclusion of random effects. The GLIMMIX procedure fits models using maximum likelihood estimation.

The LOGISTIC procedure is specifically designed for logistic regression. It performs the usual logistic regression analysis for dichotomous outcomes and it fits the proportional odds model and the generalized logit model for ordinal and nominal outcomes, respectively, by the method of maximum likelihood. This procedure has capabilities for a variety of model-building techniques, including stepwise, forward, and backward selection. It computes predicted values, the receiver operating characteristics (ROC) curve and the area beneath the curve, and a number of regression diagnostics. It can create output data sets containing these values and other statistics. PROC LOGISTIC can perform a conditional logistic regression analysis (matched-set and case-controlled) for binary response data. For small data sets, PROC LOGISTIC can perform exact conditional logistic regression. Firth's bias-reducing penalized-likelihood method can also be used in place of conditional and exact conditional logistic regression.

The PROBIT procedure is designed for quantal assay or other discrete event data. In addition to performing the logistic regression analysis, it can estimate the threshold response rate. PROC PROBIT can also estimate the values of independent variables that yield a desired response.

The SURVEYLOGISTIC procedure performs logistic regression for binary, ordinal, and nominal responses under a specified complex sampling scheme, instead of the usual stratified simple random sampling.

Stokes, Davis, and Koch (2012) provide substantial discussion of these procedures, particularly the use of the FREQ, LOGISTIC, GENMOD, and CATMOD procedures for statistical modeling.

Logistic Regression

Dichotomous Response

You have many choices of performing logistic regression in the SAS System. The CATMOD, GENMOD, GLIMMIX, LOGISTIC, PROBIT, and SURVEYLOGISTIC procedures fit the usual logistic regression model.

PROC CATMOD might not be efficient when there are continuous independent variables with large numbers of different values. For a continuous variable with a very limited number of values, PROC CATMOD might still be useful.

PROC GLIMMIX enables you to specify random effects in the models; in particular, you can fit a random-intercept logistic regression model.

PROC LOGISTIC provides the capability of model-building and performs conditional and exact conditional logistic regression. It can also use Firth's bias-reducing penalized likelihood method.

PROC PROBIT enables you to estimate the natural response rate and compute fiducial limits for the dose variable.

The LOGISTIC, GENMOD, GLIMMIX, PROBIT, and SURVEYLOGISTIC procedures can analyze summarized data by enabling you to input the numbers of events and trials; the ratio of events to trials must be between 0 and 1.

Ordinal Response

PROC LOGISTIC fits the proportional odds model to the ordinal response data by default, PROC PROBIT fits this model if you specify the logistic distribution, and PROC GENMOD and PROC GLIMMIX fit this model if you specify the CLOGIT link and the multinomial distribution. PROC CATMOD fits the cumulative logit or adjacent-category logit response functions.

Nominal Response

When the response variable is nominal, there is no concept of ordering of the response values. Response functions called *generalized logits* can be fit by the CATMOD, GLIMMIX, and LOGISTIC procedures. PROC CATMOD fits this model by default; PROC GLIMMIX and PROC LOGISTIC require you to specify the GLOGIT link.

Numerical Differences

Differences in the way the models are parameterized and fit might result in different parameter estimates if you perform logistic regression in each of these procedures.

- Parameter estimates from the procedures can differ in sign depending on the ordering of response levels, which you can change if you want.
- The parameter estimates associated with a categorical independent variable might differ among the procedures, since the estimates depend on the coding of the indicator variables in the design matrix. By default, the design matrix column produced by PROC CATMOD and PROC LOGISTIC

for a binary independent variable is coded using the values 1 and -1 (deviation from the mean coding, which is a full-rank parameterization). The same column produced by the CLASS statement of PROC GENMOD, PROC GLIMMIX, and PROC PROBIT is coded using 1 and 0 (GLM coding, which is less-than-full-rank parameterization). As a result, the parameter estimate printed by PROC LOGISTIC is one-half of the estimate produced by PROC GENMOD. Both PROC GENMOD and PROC LOGISTIC allow you to select either a full-rank parameterization or the less-than-full-rank parameterization. The GLIMMIX and PROBIT procedures allow only the less-than-full-rank parameterization for the CLASS variables. The CATMOD procedure allows only full-rank parameterizations. See the “Details” sections in the chapters on the CATMOD, GENMOD, GLIMMIX, LOGISTIC, and PROBIT procedures for more information on the generation of the design matrices used by these procedures. See Chapter 19, “[Shared Concepts and Topics](#),” for a general discussion of the various parameterizations.

- The maximum-likelihood algorithm used differs among the procedures. PROC LOGISTIC uses the Fisher’s scoring method by default, while PROC PROBIT, PROC GENMOD, PROC GLIMMIX, and PROC CATMOD use the Newton-Raphson method. The parameter estimates should be the same for all three procedures, and the standard errors should be the same for the logistic model. For the normal and extreme-value (Gompertz) distributions in PROC PROBIT, which correspond to the probit and cloglog links, respectively, in PROC GENMOD and PROC LOGISTIC, the standard errors might differ. In general, tests computed using the standard errors from the Newton-Raphson method are more conservative.
- The LOGISTIC, GENMOD, GLIMMIX, and PROBIT procedures can fit a cumulative regression model for ordinal response data by using maximum-likelihood estimation. PROC LOGISTIC and PROC GENMOD use a different parameterization from that of PROC PROBIT, which results in different intercept parameters. Estimates of the slope parameters, however, should be the same for both procedures. The estimated standard errors of the slope estimates are slightly different between the procedures because of the different computational algorithms used as default.

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Chapter 9

Introduction to Multivariate Procedures

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Overview: Multivariate Procedures

The procedures discussed in this chapter investigate relationships among variables without designating some as independent and others as dependent. Principal component analysis and common factor analysis examine relationships within a single set of variables, whereas canonical correlation looks at the relationship between two sets of variables. The following is a brief description of SAS/STAT multivariate procedures:

- CORRESP** performs simple and multiple correspondence analyses, with a contingency table, Burt table, binary table, or raw categorical data as input. Correspondence analysis is a weighted form of principal component analysis that is appropriate for frequency data. The results are displayed in plots and tables and are also available in output data sets.
- PRINCOMP** performs a principal component analysis and outputs standardized or unstandardized principal component scores. The results are displayed in plots and tables and are also available in output data sets.
- PRINQUAL** performs a principal component analysis of qualitative data and multidimensional preference analysis. The results are displayed in plots and are also available in output data sets.
- FACTOR** performs principal component and common factor analyses with rotations and outputs component scores or estimates of common factor scores. The results are displayed in plots and tables and are also available in output data sets.
- CANCORR** performs a canonical correlation analysis and outputs canonical variable scores. The results are displayed in tables and are also available in output data sets for plotting.

Many other SAS/STAT procedures can also analyze multivariate data—for example, the CATMOD, GLM, REG, CALIS, and TRANSREG procedures as well as the procedures for clustering and discriminant analysis.

The purpose of *principal component analysis* (Rao 1964) is to derive a small number of linear combinations (principal components) of a set of variables that retain as much of the information in the original variables as possible. Often a small number of principal components can be used in place of the original variables for plotting, regression, clustering, and so on. Principal component analysis can also be viewed as an attempt to uncover approximate linear dependencies among variables.

The purpose of *common factor analysis* (Mulaik 1972) is to explain the correlations or covariances among a set of variables in terms of a limited number of unobservable, latent variables. The latent variables are not generally computable as linear combinations of the original variables. In common factor analysis, it is assumed that the variables are linearly related if not for uncorrelated random error or *unique variation* in each variable; both the linear relations and the amount of unique variation can be estimated.

Principal component and common factor analysis are often followed by rotation of the components or factors. *Rotation* is the application of a nonsingular linear transformation to components or common factors to aid interpretation.

The purpose of *canonical correlation analysis* (Mardia, Kent, and Bibby 1979) is to explain or summarize the relationship between two sets of variables by finding a small number of linear combinations from each set of variables that have the highest possible between-set correlations. Plots of the canonical variables can be useful in examining multivariate dependencies. If one of the two sets of variables consists of dummy variables generated from a classification variable, the canonical correlation is equivalent to canonical discriminant analysis (see Chapter 29, “The CANDISC Procedure”). If both sets of variables are dummy variables, canonical correlation is equivalent to simple correspondence analysis.

The purpose of *correspondence analysis* (Lebart, Morineau, and Warwick 1984; Greenacre 1984; Nishisato 1980) is to summarize the associations between a set of categorical variables in a small number of dimensions. Correspondence analysis computes scores on each dimension for each row and column category in a contingency table. Plots of these scores show the relationships among the categories.

The PRINQUAL procedure obtains linear and nonlinear transformations of variables by using the method of alternating least squares (Young 1981) to optimize properties of the transformed variables’ covariance or correlation matrix. PROC PRINQUAL nonlinearly transforms variables, improving their fit to a principal component model. The name, PRINQUAL, for principal components of qualitative data, comes from the special case analysis of fitting a principal component model to nominal and ordinal scale of measurement variables (Young, Takane, and de Leeuw 1978). However, PROC PRINQUAL also has facilities for smoothly transforming continuous variables. All of PROC PRINQUAL’s transformations are also available in the TRANSREG procedure, which fits regression models with nonlinear transformations. PROC PRINQUAL can also perform metric and nonmetric multidimensional preference (MDPREF) analyses (Carroll 1972) and produce plots of the results.

Comparison of the PRINCOMP and FACTOR Procedures

Although PROC FACTOR can be used for common factor analysis, the default method is principal components. PROC FACTOR produces the same results as PROC PRINCOMP except that scoring coefficients from PROC FACTOR are normalized to give principal component scores with unit variance, whereas PROC PRINCOMP by default produces principal component scores with variance equal to the corresponding eigenvalue. PROC PRINCOMP can also compute scores standardized to unit variance. Both procedures produce graphical results through ODS Graphics.

PROC PRINCOMP has the following advantages over PROC FACTOR:

- PROC PRINCOMP is slightly faster if a small number of components is requested.
- PROC PRINCOMP can analyze somewhat larger problems in a fixed amount of memory.
- PROC PRINCOMP can output scores from an analysis of a partial correlation or covariance matrix.
- PROC PRINCOMP is simpler to use.

PROC FACTOR has the following advantages over PROC PRINCOMP for principal component analysis:

- PROC FACTOR produces more output.
- PROC FACTOR does rotations.

If you want to perform a common factor analysis, you must use PROC FACTOR instead of PROC PRINCOMP. Principal component analysis should never be used if a common factor solution is desired (Dziuban and Harris 1973; Lee and Comrey 1979).

Comparison of the PRINCOMP and PRINQUAL Procedures

The PRINCOMP procedure performs principal component analysis. The PRINQUAL procedure finds linear and nonlinear transformations of variables to optimize properties of the transformed variables' covariance or correlation matrix. One property is the sum of the first n eigenvalues, which is a measure of the fit of a principal component model with n components. Use PROC PRINQUAL to find nonlinear transformations of your variables or to perform a multidimensional preference analysis. Use PROC PRINCOMP to fit a principal component model to your data or to PROC PRINQUAL's output data set. PROC PRINCOMP produces a report of the principal component analysis, a number of graphical displays, and output data sets. PROC PRINQUAL produces only a few graphs and an output data set.

Comparison of the PRINCOMP and CORRESP Procedures

As summarized previously, PROC PRINCOMP performs a principal component analysis of interval-scaled data. PROC CORRESP performs correspondence analysis, which is a weighted form of principal component analysis that is appropriate for frequency data. If your data are categorical, use PROC CORRESP instead of PROC PRINCOMP. Both procedures produce graphical displays of the results with ODS Graphics. The plots produced by PROC CORRESP graphically show relationships among the categories of the categorical variables.

Comparison of the PRINQUAL and CORRESP Procedures

Both PROC PRINQUAL and PROC CORRESP can be used to summarize associations among variables measured on a nominal scale. PROC PRINQUAL searches for a single nonlinear transformation of the original scoring of each nominal variable that optimizes some aspect of the covariance matrix of the transformed variables. For example, PROC PRINQUAL could be used to find scorings that maximize the fit of a principal component model with one component. PROC CORRESP uses the crosstabulations of nominal variables, not covariances, and produces multiple scores for each category of each nominal variable. The main conceptual difference between PROC PRINQUAL and PROC CORRESP is that PROC PRINQUAL assumes that the categories of a nominal variable correspond to values of a single underlying interval variable, whereas PROC CORRESP assumes that there are multiple underlying interval variables and therefore uses different category scores for each dimension of the correspondence analysis. Scores from PROC CORRESP on the first dimension match the single set of PROC PRINQUAL scores (with appropriate standardizations for both analyses).

Comparison of the TRANSREG and PRINQUAL Procedures

Both the TRANSREG and PRINQUAL procedures are data transformation procedures that have many of the same transformations. These procedures can either directly perform the specified transformation (such as taking the logarithm of the variable) or search for an optimal transformation (such as a spline with a specified number of knots). Both procedures can use an iterative, alternating least squares analysis. Both procedures create an output data set that can be used as input to other procedures. PROC PRINQUAL displays relatively little output, whereas PROC TRANSREG displays many results. PROC TRANSREG has two sets of variables, usually dependent and independent, and it fits linear models such as ordinary regression and ANOVA, multiple and multivariate regression, metric and nonmetric conjoint analysis, metric and nonmetric vector and ideal point preference mapping, redundancy analysis, canonical correlation, and response surface regression. In contrast, PROC PRINQUAL has one set of variables, fits a principal component model or multidimensional preference analysis, and can also optimize other properties of a correlation or covariance matrix. PROC TRANSREG performs hypothesis testing and can be used to code experimental designs prior to their use in other analyses. PROC TRANSREG can also perform Box-Cox transformations and fit models with smoothing spline and penalized B-spline transformations.

See Chapter 4, “Introduction to Regression Procedures,” for comparisons of the TRANSREG and REG procedures.

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Chapter 10

Introduction to Discriminant Procedures

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Overview: Discriminant Procedures

The SAS procedures for discriminant analysis fit data with one classification variable and several quantitative variables. The purpose of discriminant analysis can be to find one or more of the following:

- a mathematical rule, or *discriminant function*, for guessing to which class an observation belongs, based on knowledge of the quantitative variables only
- a set of linear combinations of the quantitative variables that best reveals the differences among the classes
- a subset of the quantitative variables that best reveals the differences among the classes

The SAS discriminant procedures are as follows:

DISCRIM	computes various discriminant functions for classifying observations. Linear or quadratic discriminant functions can be used for data with approximately multivariate normal within-class distributions. Nonparametric methods can be used without making any assumptions about these distributions.
CANDISC	performs a canonical analysis to find linear combinations of the quantitative variables that best summarize the differences among the classes.
STEPDISC	uses forward selection, backward elimination, or stepwise selection to try to find a subset of quantitative variables that best reveals differences among the classes.

Background: Discriminant Procedures

The term *discriminant analysis* (Fisher 1936; Cooley and Lohnes 1971; Tatsuoka 1971; Kshirsagar 1972; Lachenbruch 1975, 1979; Gnanadesikan 1977; Klecka 1980; Hand 1981, 1982; Silverman 1986) refers to

several different types of analyses. Classificatory discriminant analysis is used to classify observations into two or more known groups on the basis of one or more quantitative variables. Classification can be done by either a parametric method or a nonparametric method in the DISCRIM procedure. A parametric method is appropriate only for approximately normal within-class distributions. The method generates either a linear discriminant function (the within-class covariance matrices are assumed to be equal) or a quadratic discriminant function (the within-class covariance matrices are assumed to be unequal).

When the distribution within each group is not assumed to have any specific distribution or is assumed to have a distribution different from the multivariate normal distribution, nonparametric methods can be used to derive classification criteria. These methods include the kernel method and nearest-neighbor methods. The kernel method uses uniform, normal, Epanechnikov, biweight, or triweight kernels in estimating the group-specific density at each observation. The within-group covariance matrices or the pooled covariance matrix can be used to scale the data.

The performance of a discriminant function can be evaluated by estimating error rates (probabilities of misclassification). Error count estimates and posterior probability error rate estimates can be evaluated with PROC DISCRIM. When the input data set is an ordinary SAS data set, the error rates can also be estimated by cross validation.

In multivariate statistical applications, the data collected are largely from distributions different from the normal distribution. Various forms of nonnormality can arise, such as qualitative variables or variables with underlying continuous but nonnormal distributions. If the multivariate normality assumption is violated, the use of parametric discriminant analysis might not be appropriate. When a parametric classification criterion (linear or quadratic discriminant function) is derived from a nonnormal population, the resulting error rate estimates might be biased.

If your quantitative variables are not normally distributed, or if you want to classify observations on the basis of categorical variables, you should consider using the CATMOD or LOGISTIC procedure to fit a categorical linear model with the classification variable as the dependent variable. Press and Wilson (1978) compare logistic regression and parametric discriminant analysis and conclude that logistic regression is preferable to parametric discriminant analysis in cases for which the variables do not have multivariate normal distributions within classes. However, if you do have normal within-class distributions, logistic regression is less efficient than parametric discriminant analysis. Efron (1975) shows that with two normal populations having a common covariance matrix, logistic regression is between one-half and two-thirds as effective as the linear discriminant function in achieving asymptotically the same error rate.

Do not confuse discriminant analysis with cluster analysis. All varieties of discriminant analysis require prior knowledge of the classes, usually in the form of a sample from each class. In cluster analysis, the data do not include information about class membership; the purpose is to construct a classification. See Chapter 11, “[Introduction to Clustering Procedures](#).”

Canonical discriminant analysis is a dimension-reduction technique related to principal components and canonical correlation, and it can be performed by both the CANDISC and DISCRIM procedures. A discriminant criterion is always derived in PROC DISCRIM. If you want canonical discriminant analysis without the use of a discriminant criterion, you should use PROC CANDISC. Stepwise discriminant analysis is a variable-selection technique implemented by the STEPDISC procedure. After selecting a subset of variables with PROC STEPDISC, use any of the other discriminant procedures to obtain more detailed analyses. PROC CANDISC and PROC STEPDISC perform hypothesis tests that require the within-class distributions to be approximately normal, but these procedures can be used descriptively with nonnormal data.

Another alternative to discriminant analysis is to perform a series of univariate one-way ANOVAs. All three discriminant procedures provide summaries of the univariate ANOVAs. The advantage of the multivariate approach is that two or more classes that overlap considerably when each variable is viewed separately might be more distinct when examined from a multivariate point of view.

Example: Contrasting Univariate and Multivariate Analyses

Consider an artificial data set with two classes of observations indicated by 'H' and 'O'. The following statements generate and plot the data:

```
data random;
  drop n;

  Group = 'H';
  do n = 1 to 20;
    x = 4.5 + 2 * normal(57391);
    y = x + .5 + normal(57391);
    output;
  end;

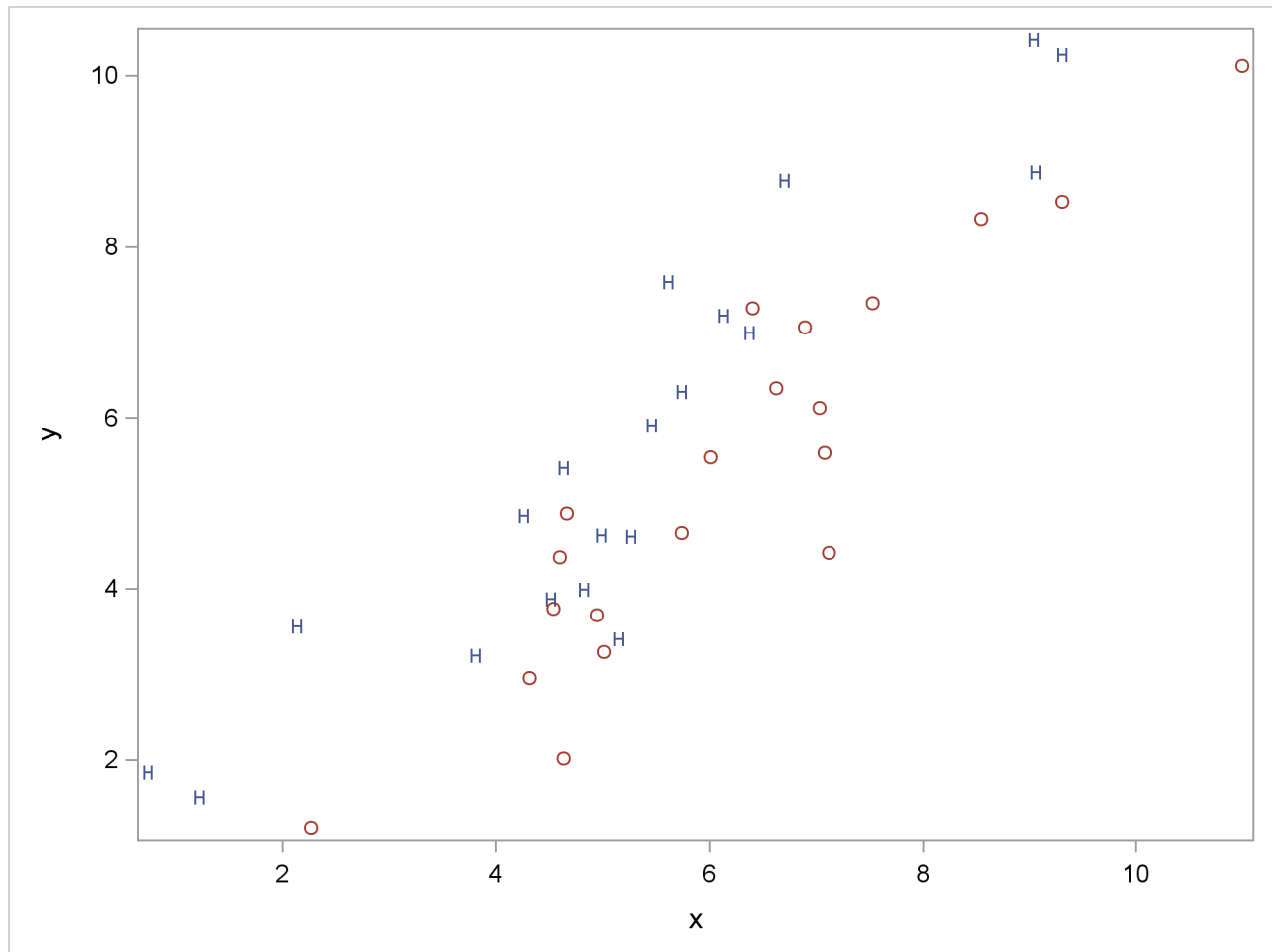
  Group = 'O';
  do n = 1 to 20;
    x = 6.25 + 2 * normal(57391);
    y = x - 1 + normal(57391);
    output;
  end;

run;

proc sgplot noautolegend;
  scatter y=y x=x / markerchar=group group=group;
run;
```

The plot is shown in [Figure 10.1](#).

Figure 10.1 Groups for Contrasting Univariate and Multivariate Analyses



The following statements perform a canonical discriminant analysis and display the results in Figure 10.2:

```
proc candisc anova;
  class Group;
  var x y;
run;
```

Figure 10.2 Contrasting Univariate and Multivariate Analyses

The CANDISC Procedure			
Total Sample Size	40	DF Total	39
Variables	2	DF Within Classes	38
Classes	2	DF Between Classes	1
Number of Observations Read		40	
Number of Observations Used		40	

Figure 10.2 continued

Class Level Information							
Group	Variable Name	Frequency	Weight	Proportion			
H	H	20	20.0000	0.500000			
O	O	20	20.0000	0.500000			

The CANDISC Procedure							
Univariate Test Statistics							
F Statistics, Num DF=1, Den DF=38							
Variable	Total Standard Deviation	Pooled Standard Deviation	Between Standard Deviation	R-Square	R-Square / (1-RSq)	F Value	Pr > F
x	2.1776	2.1498	0.6820	0.0503	0.0530	2.01	0.1641
y	2.4215	2.4486	0.2047	0.0037	0.0037	0.14	0.7105

Average R-Square	
Unweighted	0.0269868
Weighted by Variance	0.0245201

Multivariate Statistics and Exact F Statistics						
S=1 M=0 N=17.5						
Statistic	Value	F Value	Num DF	Den DF	Pr > F	
Wilks' Lambda	0.64203704	10.31	2	37	0.0003	
Pillai's Trace	0.35796296	10.31	2	37	0.0003	
Hotelling-Lawley Trace	0.55754252	10.31	2	37	0.0003	
Roy's Greatest Root	0.55754252	10.31	2	37	0.0003	

Figure 10.2 continued

The CANDISC Procedure					
	Canonical Correlation	Adjusted Canonical Correlation	Approximate Standard Error	Squared Canonical Correlation	
1	0.598300	0.589467	0.102808	0.357963	
Eigenvalues of Inv(E)*H = CanRsq/(1-CanRsq)					
	Eigenvalue	Difference	Proportion	Cumulative	
1	0.5575		1.0000	1.0000	
Test of H0: The canonical correlations in the current row and all that follow are zero					
	Likelihood Ratio	Approximate F Value	Num DF	Den DF	Pr > F
1	0.64203704	10.31	2	37	0.0003
NOTE: The F statistic is exact.					
The CANDISC Procedure					
Total Canonical Structure					
Variable	Can1				
x	-0.374883				
y	0.101206				
Between Canonical Structure					
Variable	Can1				
x	-1.000000				
y	1.000000				
Pooled Within Canonical Structure					
Variable	Can1				
x	-0.308237				
y	0.081243				

Figure 10.2 continued

The CANDISC Procedure	
Total-Sample Standardized Canonical Coefficients	
Variable	Can1
x	-2.625596855
y	2.446680169
Pooled Within-Class Standardized Canonical Coefficients	
Variable	Can1
x	-2.592150014
y	2.474116072
Raw Canonical Coefficients	
Variable	Can1
x	-1.205756217
y	1.010412967
Class Means on Canonical Variables	
Group	Can1
H	0.7277811475
O	-.7277811475

The univariate R squares are very small, 0.0503 for x and 0.0037 for y, and neither variable shows a significant difference between the classes at the 0.10 level.

The multivariate test for differences between the classes is significant at the 0.0003 level. Thus, the multivariate analysis has found a highly significant difference, whereas the univariate analyses failed to achieve even the 0.10 level. The raw canonical coefficients for the first canonical variable, Can1, show that the classes differ most widely on the linear combination $-1.205756217x + 1.010412967y$ or approximately $y - 1.2x$. The R square between Can1 and the class variable is 0.357963 as given by the squared canonical correlation, which is much higher than either univariate R square.

In this example, the variables are highly correlated within classes. If the within-class correlation were smaller, there would be greater agreement between the univariate and multivariate analyses.

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Chapter 11

Introduction to Clustering Procedures

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Overview: Clustering Procedures

You can use SAS clustering procedures to cluster the observations or the variables in a SAS data set. Both hierarchical and disjoint clusters can be obtained. Only numeric variables can be analyzed directly by the procedures, although the DISTANCE procedure can compute a distance matrix that uses character or numeric variables.

The purpose of cluster analysis is to place objects into groups, or clusters, suggested by the data, not defined a priori, such that objects in a given cluster tend to be similar to each other in some sense, and objects in different clusters tend to be dissimilar. You can also use cluster analysis to summarize data rather than to find “natural” or “real” clusters; this use of clustering is sometimes called *dissection* (Everitt 1980).

Any generalization about cluster analysis must be vague because a vast number of clustering methods have been developed in several different fields, with different definitions of clusters and similarity among objects. The variety of clustering techniques is reflected by the variety of terms used for cluster analysis: botryology, classification, clumping, competitive learning, morphometrics, nosography, nosology, numerical taxonomy, partitioning, Q-analysis, systematics, taximetrics, taxonrics, typology, unsupervised pattern recognition, vector quantization, and winner-take-all learning. Good (1977) has also suggested aciniformics and agminatics.

Several types of clusters are possible:

- Disjoint clusters place each object in one and only one cluster.
- Hierarchical clusters are organized so that one cluster can be entirely contained within another cluster, but no other kind of overlap between clusters is allowed.
- Overlapping clusters can be constrained to limit the number of objects that belong simultaneously to two clusters, or they can be unconstrained, allowing any degree of overlap in cluster membership.
- Fuzzy clusters are defined by a probability or grade of membership of each object in each cluster. Fuzzy clusters can be disjoint, hierarchical, or overlapping.

The data representations of objects to be clustered also take many forms. The most common are as follows:

- a square distance or similarity matrix, in which both rows and columns correspond to the objects to be clustered. A correlation matrix is an example of a similarity matrix.
- a coordinate matrix, in which the rows are observations and the columns are variables, as in the usual SAS multivariate data set. The observations, the variables, or both can be clustered.

The SAS procedures for clustering are oriented toward disjoint or hierarchical clusters from coordinate data, distance data, or a correlation or covariance matrix. The following procedures are used for clustering:

CLUSTER	performs hierarchical clustering of observations by using eleven agglomerative methods applied to coordinate data or distance data and draws tree diagrams, which are also called <i>dendrograms</i> or <i>phenograms</i> .
FASTCLUS	finds disjoint clusters of observations by using a k -means method applied to coordinate data. PROC FASTCLUS is especially suitable for large data sets.
MODECLUS	finds disjoint clusters of observations with coordinate or distance data by using nonparametric density estimation. It can also perform approximate nonparametric significance tests for the number of clusters.
VARCLUS	performs both hierarchical and disjoint clustering of variables by using oblique multiple-group component analysis and draws tree diagrams, which are also called <i>dendrograms</i> or <i>phenograms</i> .
TREE	draws tree diagrams, also called <i>dendrograms</i> or <i>phenograms</i> , by using output from the CLUSTER or VARCLUS procedure. PROC TREE can also create a data set indicating cluster membership at any specified level of the cluster tree.

The following procedures are useful for processing data prior to the actual cluster analysis:

ACECLUS	attempts to estimate the pooled within-cluster covariance matrix from coordinate data without knowledge of the number or the membership of the clusters (Art, Gnanadesikan, and Kettenring 1982). PROC ACECLUS outputs a data set containing canonical variable scores to be used in the cluster analysis proper.
---------	---

DISTANCE	computes various measures of distance, dissimilarity, or similarity between the observations (rows) of a SAS data set. PROC DISTANCE also provides various nonparametric and parametric methods for standardizing variables. Different variables can be standardized with different methods.
PRINCOMP	performs a principal component analysis and outputs principal component scores.
STDIZE	standardizes variables by using any of a variety of location and scale measures, including mean and standard deviation, minimum and range, median and absolute deviation from the median, various M-estimators and A-estimators, and some scale estimators designed specifically for cluster analysis.

Massart and Kaufman (1983) is the best elementary introduction to cluster analysis. Other important texts are Anderberg (1973); Sneath and Sokal (1973); Duran and Odell (1974); Hartigan (1975); Titterton, Smith, and Makov (1985); McLachlan and Basford (1988); Kaufman and Rousseeuw (1990). Hartigan (1975); Spath (1980) give numerous FORTRAN programs for clustering. Any prospective user of cluster analysis should study the Monte Carlo results of Milligan (1980); Milligan and Cooper (1985); Cooper and Milligan (1988). Important references on the statistical aspects of clustering include MacQueen (1967); Wolfe (1970); Scott and Symons (1971); Hartigan (1977, 1978, 1981, 1985a); Symons (1981); Everitt (1981); Sarle (1983); Bock (1985); Thode, Mendell, and Finch (1988). Bayesian methods have important advantages over maximum likelihood; see Binder (1978, 1981); Banfield and Raftery (1993); Bensmail et al. (1997). For fuzzy clustering, see Bezdek (1981); Bezdek and Pal (1992). The signal-processing perspective is provided by Gersho and Gray (1992). For a discussion of the fragmented state of the literature on cluster analysis, see Blashfield and Aldenderfer (1978).

Clustering Variables

Factor rotation is often used to cluster variables, but the resulting clusters are fuzzy. It is preferable to use PROC VARCLUS if you want hard (nonfuzzy), disjoint clusters. Factor rotation is better if you want to be able to find overlapping clusters. It is often a good idea to try both PROC VARCLUS and PROC FACTOR with an oblique rotation, compare the amount of variance explained by each, and see how fuzzy the factor loadings are and whether there seem to be overlapping clusters.

You can use PROC VARCLUS to harden a fuzzy factor rotation; use PROC FACTOR to create an output data set containing scoring coefficients and initialize PROC VARCLUS with this data set as follows:

```
proc factor rotate=promax score outstat=fact;
run;

proc varclus initial=input proportion=0;
run;
```

You can use any rotation method instead of the PROMAX method. The SCORE and OUTSTAT= options are necessary in the PROC FACTOR statement. PROC VARCLUS reads the correlation matrix from the data set created by PROC FACTOR. The INITIAL=INPUT option tells PROC VARCLUS to read initial scoring coefficients from the data set. The option PROPORTION=0 keeps PROC VARCLUS from splitting any of the clusters.

Clustering Observations

PROC CLUSTER is easier to use than PROC FASTCLUS because one run produces results from one cluster up to as many as you like. You must run PROC FASTCLUS once for each number of clusters.

The time required by PROC FASTCLUS is roughly proportional to the number of observations, whereas the time required by PROC CLUSTER with most methods varies with the square or cube of the number of observations. Therefore, you can use PROC FASTCLUS with much larger data sets than PROC CLUSTER.

If you want to hierarchically cluster a data set that is too large to use with PROC CLUSTER directly, you can have PROC FASTCLUS produce, for example, 50 clusters, and let PROC CLUSTER analyze these 50 clusters instead of the entire data set. The MEAN= data set produced by PROC FASTCLUS contains two special variables:

- The variable `_FREQ_` gives the number of observations in the cluster.
- The variable `_RMSSTD_` gives the root mean square across variables of the cluster standard deviations.

These variables are automatically used by PROC CLUSTER to give the correct results when clustering clusters. For example, you could specify Ward's minimum variance method Ward (1963):

```
proc fastclus maxclusters=50 mean=temp;
  var x y z;
run;

ods graphics on;
proc cluster method=ward outtree=tree;
  var x y z;
run;
```

Or you could specify Wong's hybrid method (Wong 1982):

```
proc fastclus maxclusters=50 mean=temp;
  var x y z;
run;

ods graphics on;
proc cluster method=density hybrid outtree=tree;
  var x y z;
run;
```

More detailed examples are given in Chapter 31, "The CLUSTER Procedure."

Characteristics of Methods for Clustering Observations

Many simulation studies comparing various methods of cluster analysis have been performed. In these studies, artificial data sets containing known clusters are produced using pseudo-random-number generators. The data sets are analyzed by a variety of clustering methods, and the degree to which each clustering method recovers the known cluster structure is evaluated. See Milligan (1981) for a review of such studies. In most of these studies, the clustering method with the best overall performance has been either average linkage or Ward's minimum variance method. The method with the poorest overall performance has almost invariably been single linkage. However, in many respects, the results of simulation studies are inconsistent and confusing.

When you attempt to evaluate clustering methods, it is essential to realize that most methods are biased toward finding clusters possessing certain characteristics related to size (number of members), shape, or dispersion. Methods based on the least squares criterion (Sarle 1982), such as k -means and Ward's minimum variance method, tend to find clusters with roughly the same number of observations in each cluster. Average linkage is somewhat biased toward finding clusters of equal variance. Many clustering methods tend to produce compact, roughly hyperspherical clusters and are incapable of detecting clusters with highly elongated or irregular shapes. The methods with the least bias are those based on nonparametric density estimation such as single linkage and density linkage.

Most simulation studies have generated compact (often multivariate normal) clusters of roughly equal size or dispersion. Such studies naturally favor average linkage and Ward's method over most other hierarchical methods, especially single linkage. It would be easy, however, to design a study that uses elongated or irregular clusters in which single linkage would perform much better than average linkage or Ward's method (see some of the following examples). Even studies that compare clustering methods that use "realistic" data might unfairly favor particular methods. For example, in all the data sets used by Mezzich and Solomon (1980), the clusters established by field experts are of equal size. When interpreting simulation or other comparative studies, you must, therefore, decide whether the artificially generated clusters in the study resemble the clusters you suspect might exist in your data in terms of size, shape, and dispersion. If, like many people doing exploratory cluster analysis, you have no idea what kinds of clusters to expect, you should include at least one of the relatively unbiased methods, such as density linkage, in your analysis.

The rest of this section consists of a series of examples that illustrate the performance of various clustering methods under various conditions. The first, and simplest, example shows a case of well-separated clusters. The other examples show cases of poorly separated clusters, clusters of unequal size, parallel elongated clusters, and nonconvex clusters.

Well-Separated Clusters

If the population clusters are sufficiently well separated, almost any clustering method performs well, as demonstrated in the following example, which uses single linkage. In this and subsequent examples, the output from the clustering procedures is not shown, but cluster membership is displayed in scatter plots. The SAS autocall macro MODSTYLE is specified to change the default marker symbols for the plot. For more information about autocall libraries, see *SAS Macro Language: Reference*. The following SAS statements produce Figure 11.1:

```
data compact;
  keep x y;
  n=50; scale=1;
  mx=0; my=0; link generate;
  mx=8; my=0; link generate;
  mx=4; my=8; link generate;
  stop;
generate:
  do i=1 to n;
    x=rannor(1)*scale+mx;
    y=rannor(1)*scale+my;
    output;
  end;
  return;
run;

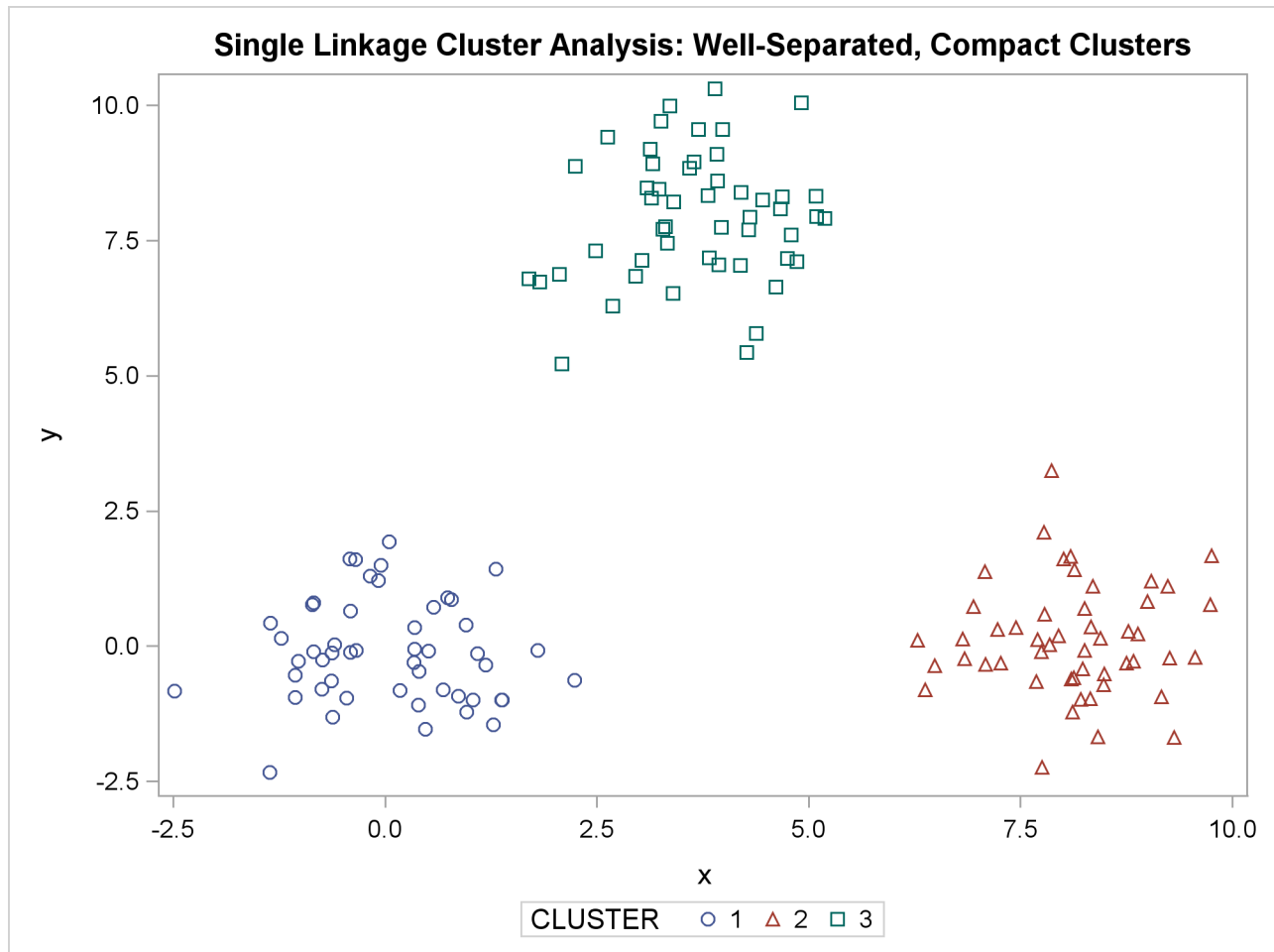
proc cluster data=compact outtree=tree method=single noprint;
run;

proc tree noprint out=out n=3;
  copy x y;
run;

%modstyle(name=ClusterStyle,parent=Statistical,type=CLM,
markers=Circle Triangle Square circlefilled);
ods listing style=ClusterStyle;

proc sgplot;
  scatter y=y x=x / group=cluster;
  title 'Single Linkage Cluster Analysis: '
        'Well-Separated, Compact Clusters';
run;
```

Figure 11.1 Well-Separated, Compact Clusters: PROC CLUSTER METHOD=SINGLE



Poorly Separated Clusters

To see how various clustering methods differ, you must examine a more difficult problem than that of the previous example.

The following data set is similar to the first except that the three clusters are much closer together. This example demonstrates the use of PROC FASTCLUS and five hierarchical methods available in PROC CLUSTER. To help you compare methods, this example plots true, generated clusters. Also included is a bubble plot of the density estimates obtained in conjunction with two-stage density linkage in PROC CLUSTER.

The following SAS statements produce Figure 11.2:

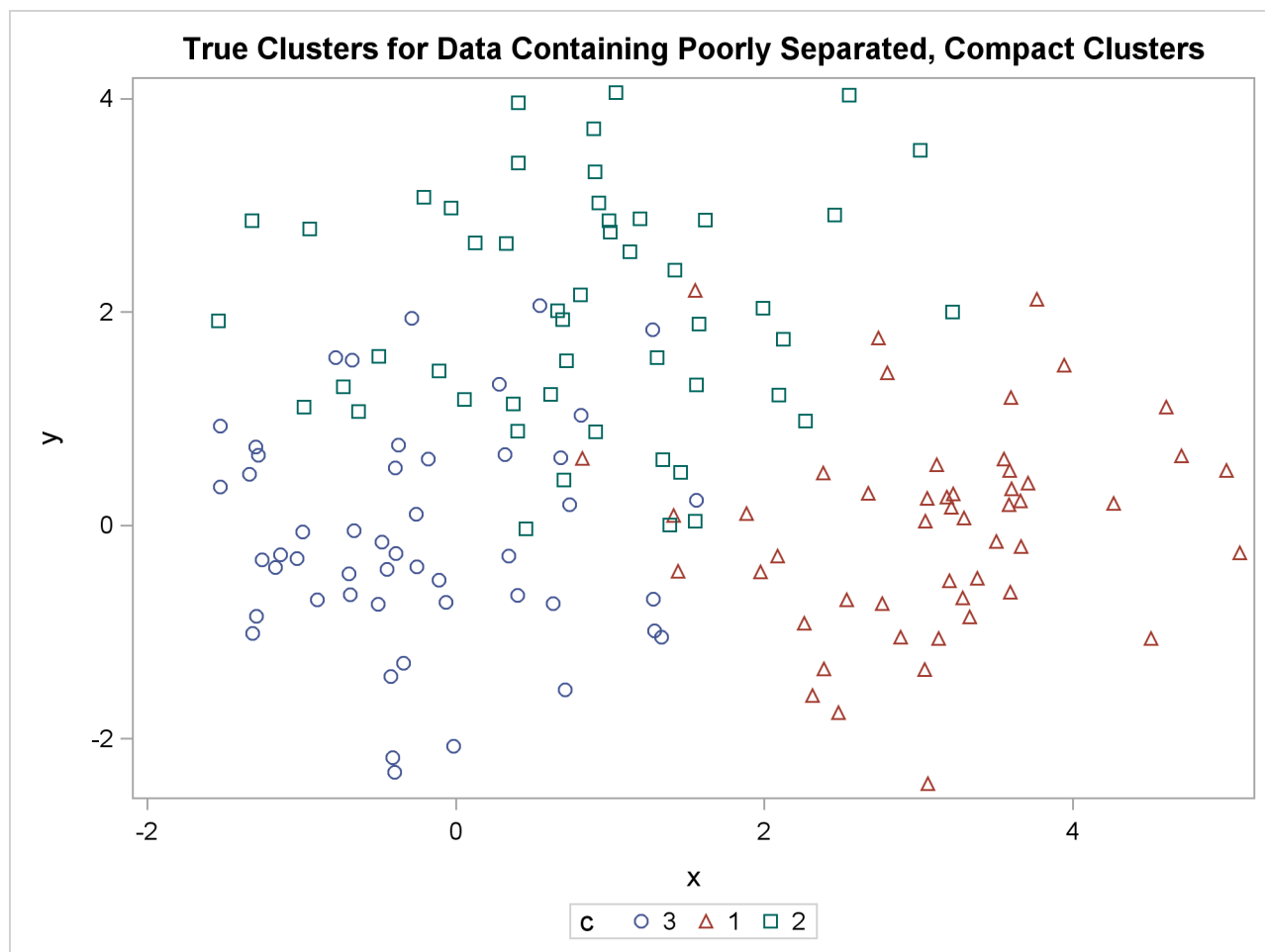
```

data closer;
  keep x y c;
  n=50; scale=1;
  mx=0; my=0; c=3; link generate;
  mx=3; my=0; c=1; link generate;
  mx=1; my=2; c=2; link generate;
  stop;
generate:
  do i=1 to n;
    x=rannor(9)*scale+mx;
    y=rannor(9)*scale+my;
    output;
  end;
  return;
run;

title 'True Clusters for Data Containing Poorly Separated, Compact Clusters';
proc sgplot;
  scatter y=y x=x / group=c ;
run;

```

Figure 11.2 Poorly Separated, Compact Clusters: Plot of True Clusters

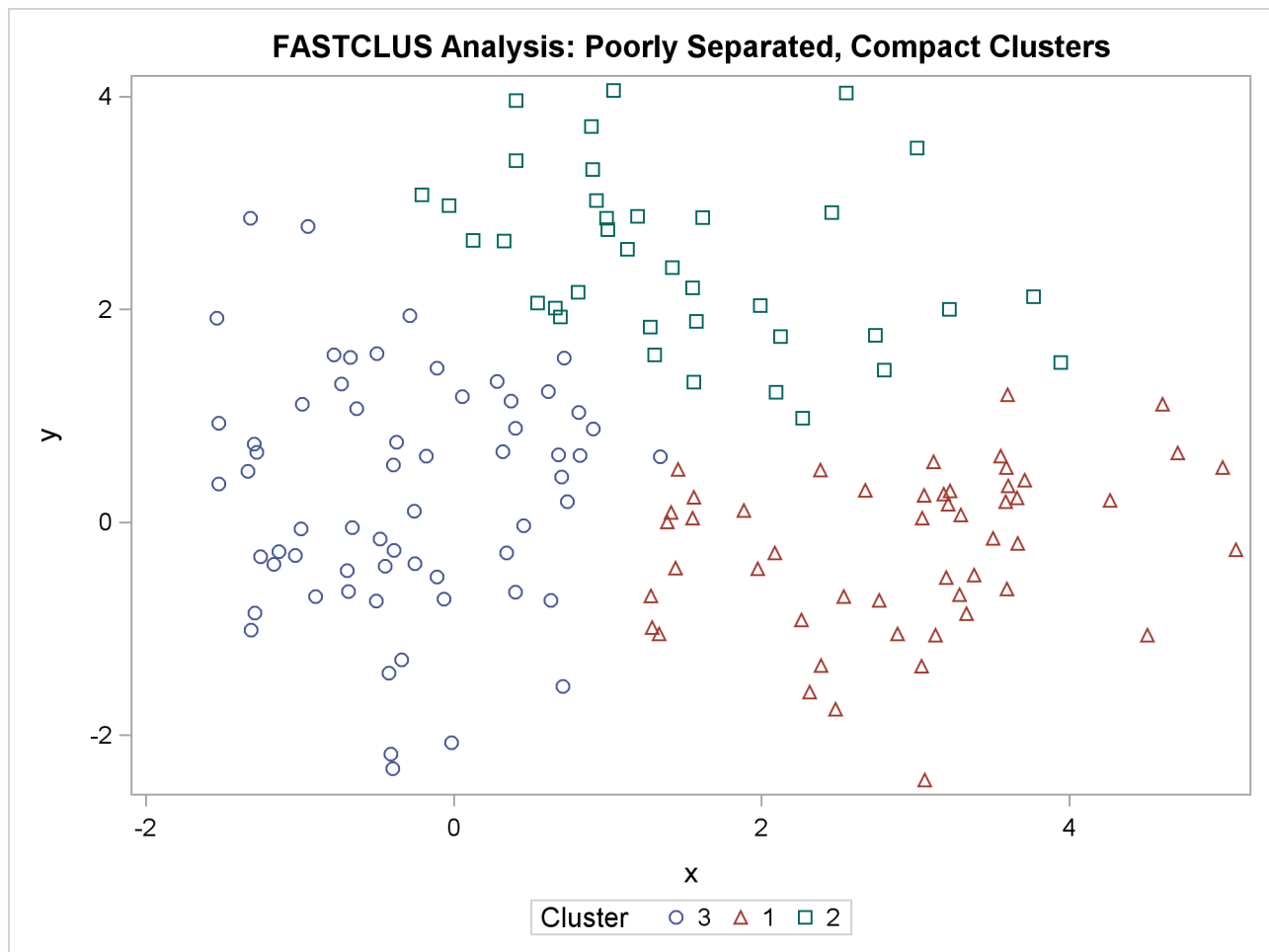


The following statements use the FASTCLUS procedure to find three clusters and then use the SGPLOT procedure to plot the clusters. The following statements produce Figure 11.3:

```
proc fastclus data=closer out=out maxc=3 noprint;
  var x y;
  title 'FASTCLUS Analysis: '
        'Poorly Separated, Compact Clusters';
run;

proc sgplot;
  scatter y=y x=x / group=cluster;
run;
```

Figure 11.3 Poorly Separated, Compact Clusters: PROC FASTCLUS



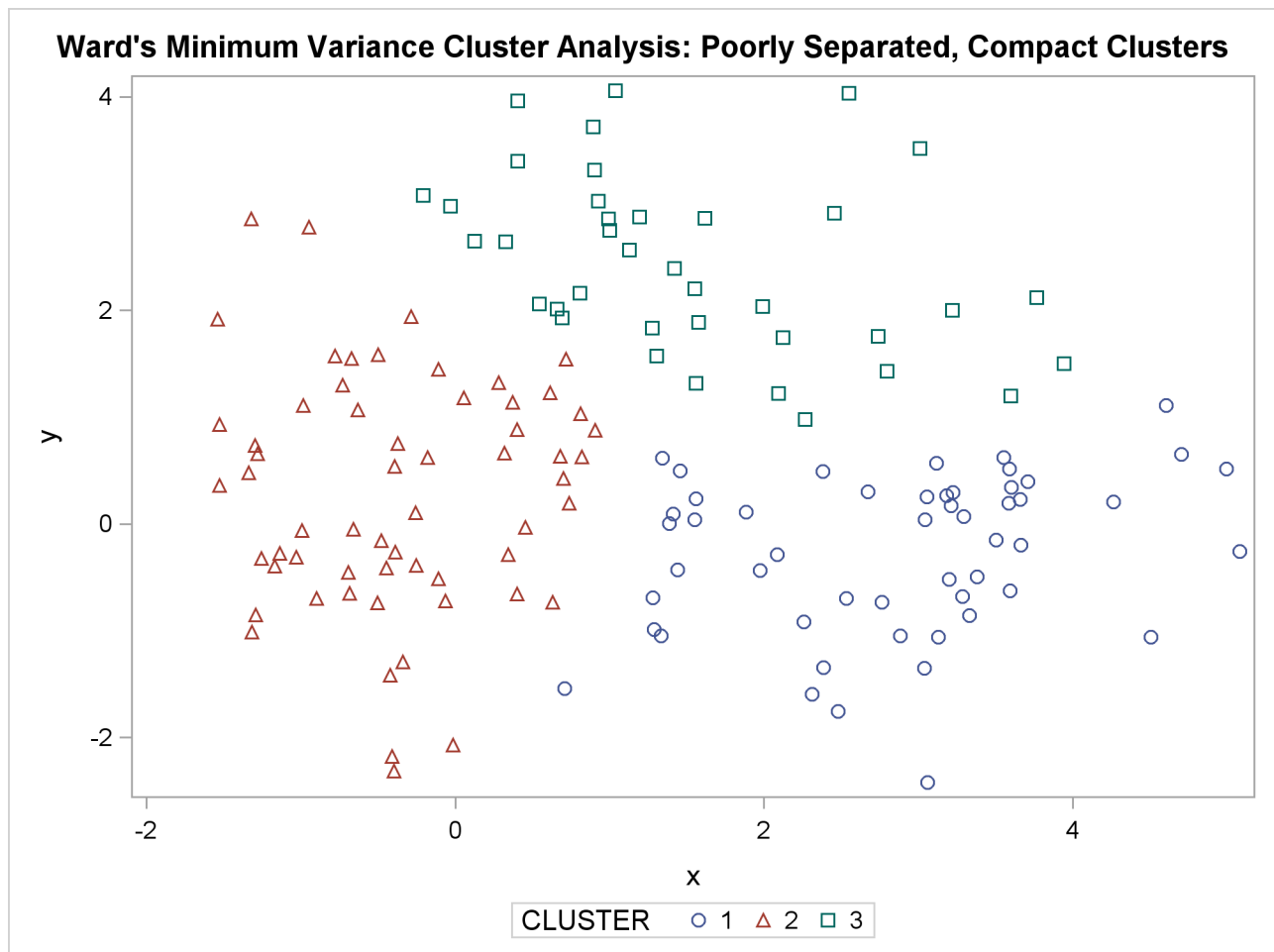
The following SAS statements produce Figure 11.4:

```
proc cluster data=closer outtree=tree method=ward noprint;
  var x y;
run;

proc tree noprint out=out n=3;
  copy x y;
  title 'Ward's Minimum Variance Cluster Analysis: '
        'Poorly Separated, Compact Clusters';
run;

proc sgplot;
  scatter y=y x=x / group=cluster;
run;
```

Figure 11.4 Poorly Separated, Compact Clusters: PROC CLUSTER METHOD=WARD



The following SAS statements produce Figure 11.5:

```

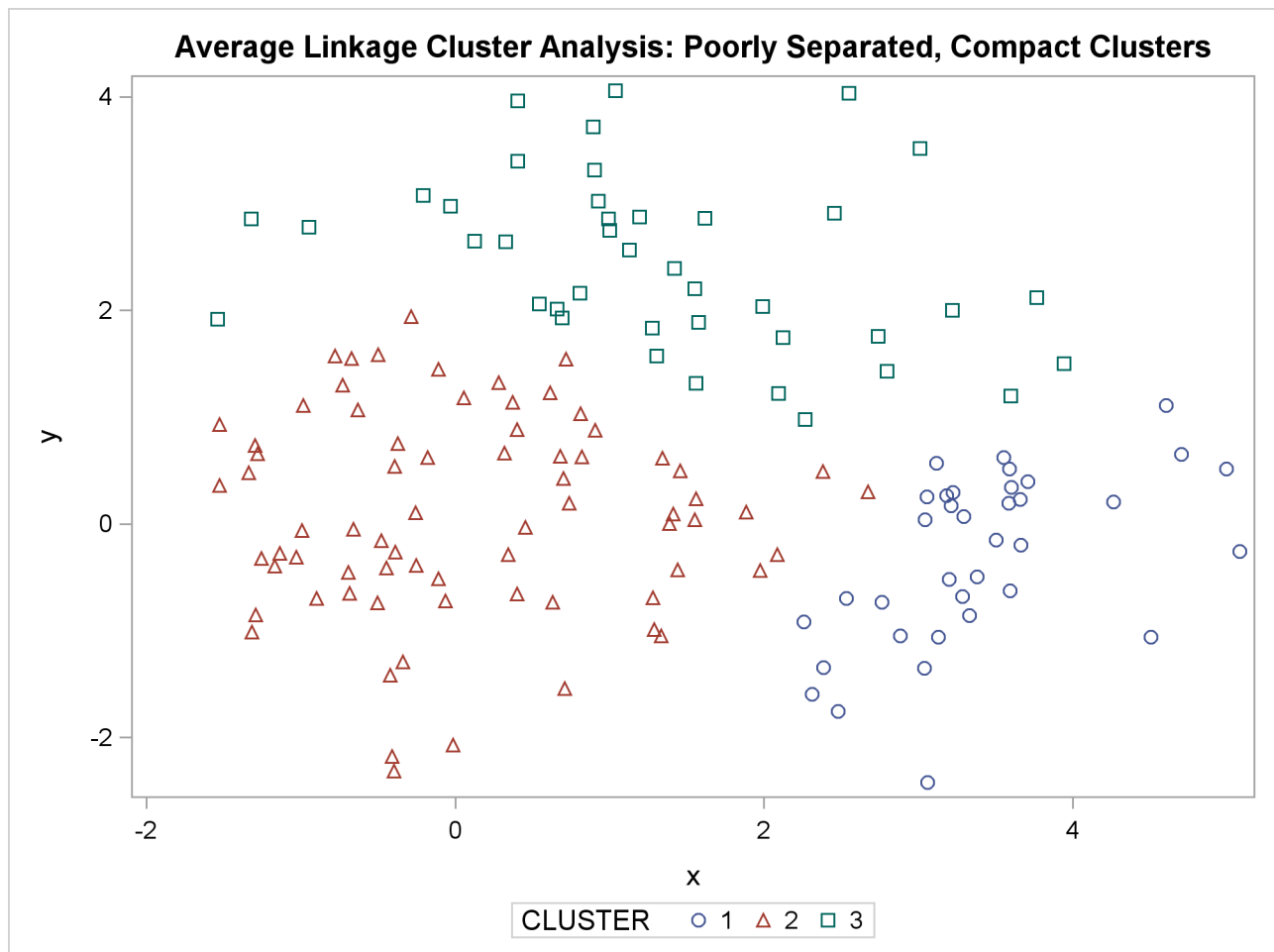
proc cluster data=closer outtree=tree method=average noprint;
  var x y;
run;

proc tree noprint out=out n=3 dock=5;
  copy x y;
  title 'Average Linkage Cluster Analysis: '
        'Poorly Separated, Compact Clusters';
run;

proc sgplot;
  scatter y=y x=x / group=cluster;
run;

```

Figure 11.5 Poorly Separated, Compact Clusters: PROC CLUSTER METHOD=AVERAGE



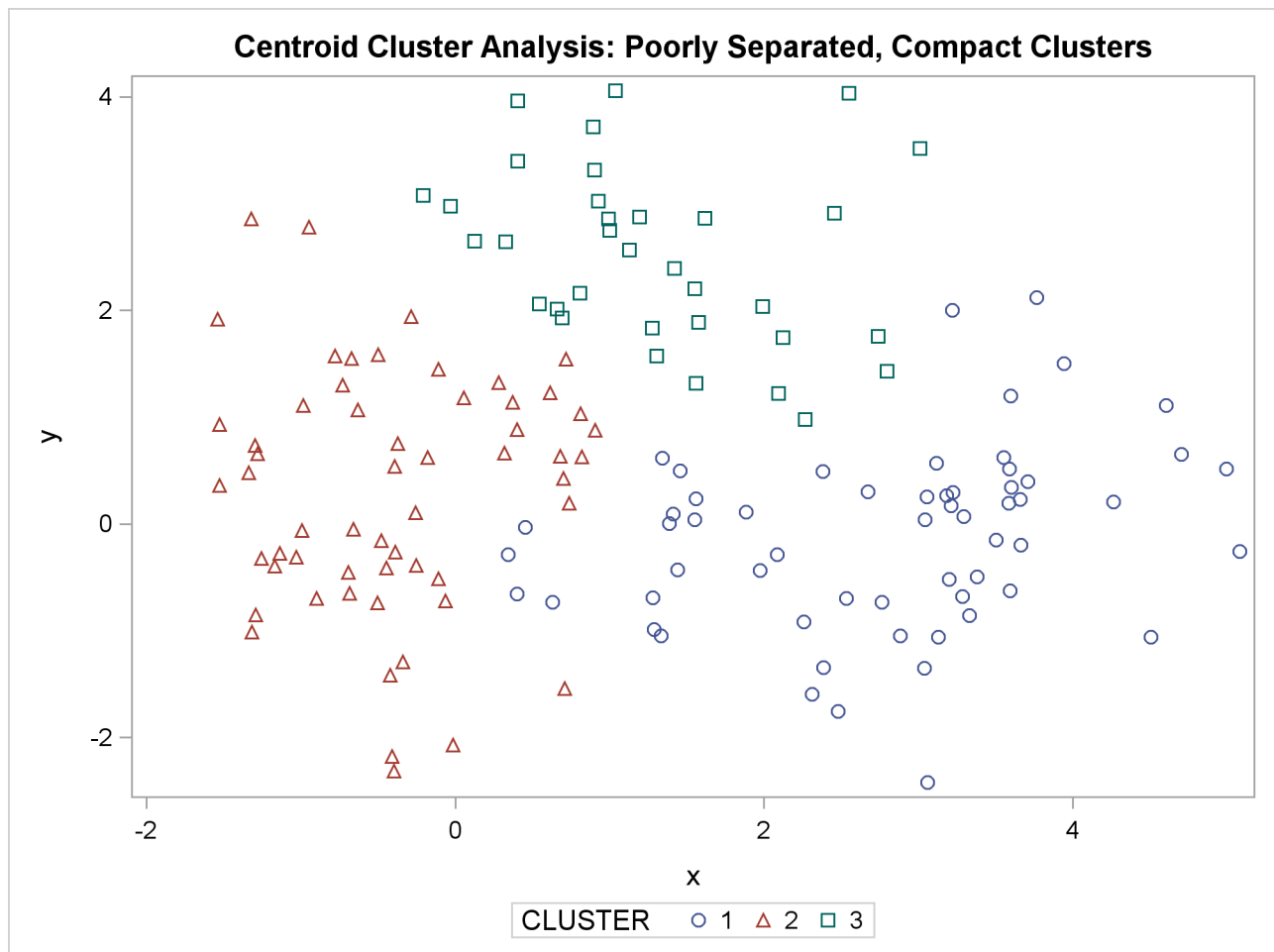
The following SAS statements produce [Figure 11.6](#):

```
proc cluster data=closer outtree=tree method=centroid noprint;
  var x y;
run;

proc tree noprint out=out n=3 dock=5;
  copy x y;
  title 'Centroid Cluster Analysis: '
        'Poorly Separated, Compact Clusters';
run;

proc sgplot;
  scatter y=y x=x / group=cluster;
run;
```

Figure 11.6 Poorly Separated, Compact Clusters: PROC CLUSTER METHOD=CENTROID



The following SAS statements produce Figure 11.7 and Figure 11.8:

```

proc cluster data=closer outtree=tree method=twostage k=10 noprint;
  var x y;
run;

proc tree noprint out=out n=3;
  copy x y _dens_;
  title 'Two-Stage Density Linkage Cluster Analysis: '
        'Poorly Separated, Compact Clusters';
run;

proc sgplot;
  scatter y=y x=x / group=cluster;
run;

proc sgplot;
  bubble y=y x=x size=_dens_ / nofill lineattrs=graphdatadefault;
  title 'Estimated Densities for Data Containing Poorly Separated, '
        'Compact Clusters';
run;

```

Figure 11.7 Poorly Separated, Compact Clusters: PROC CLUSTER METHOD=TWOSTAGE

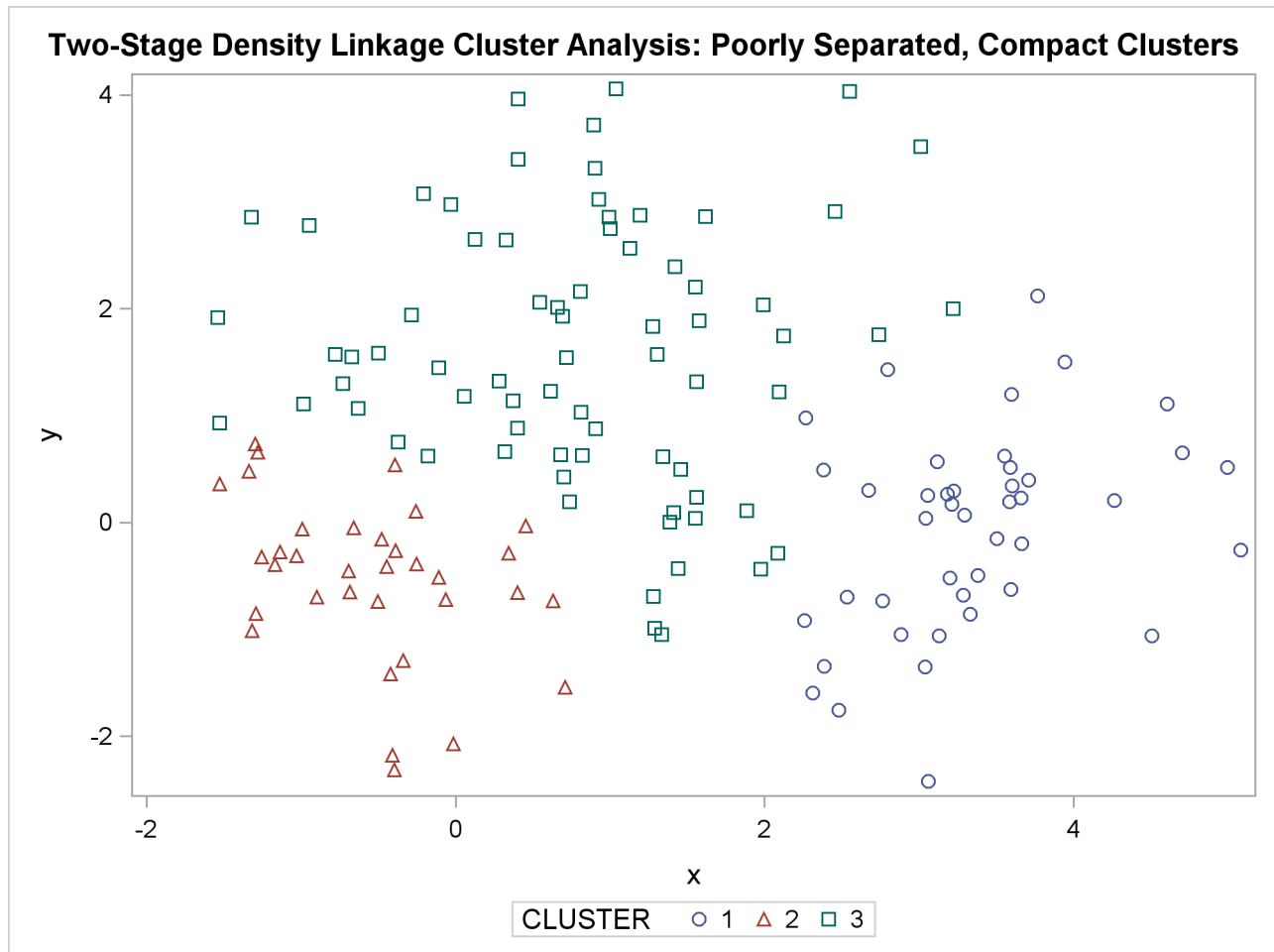
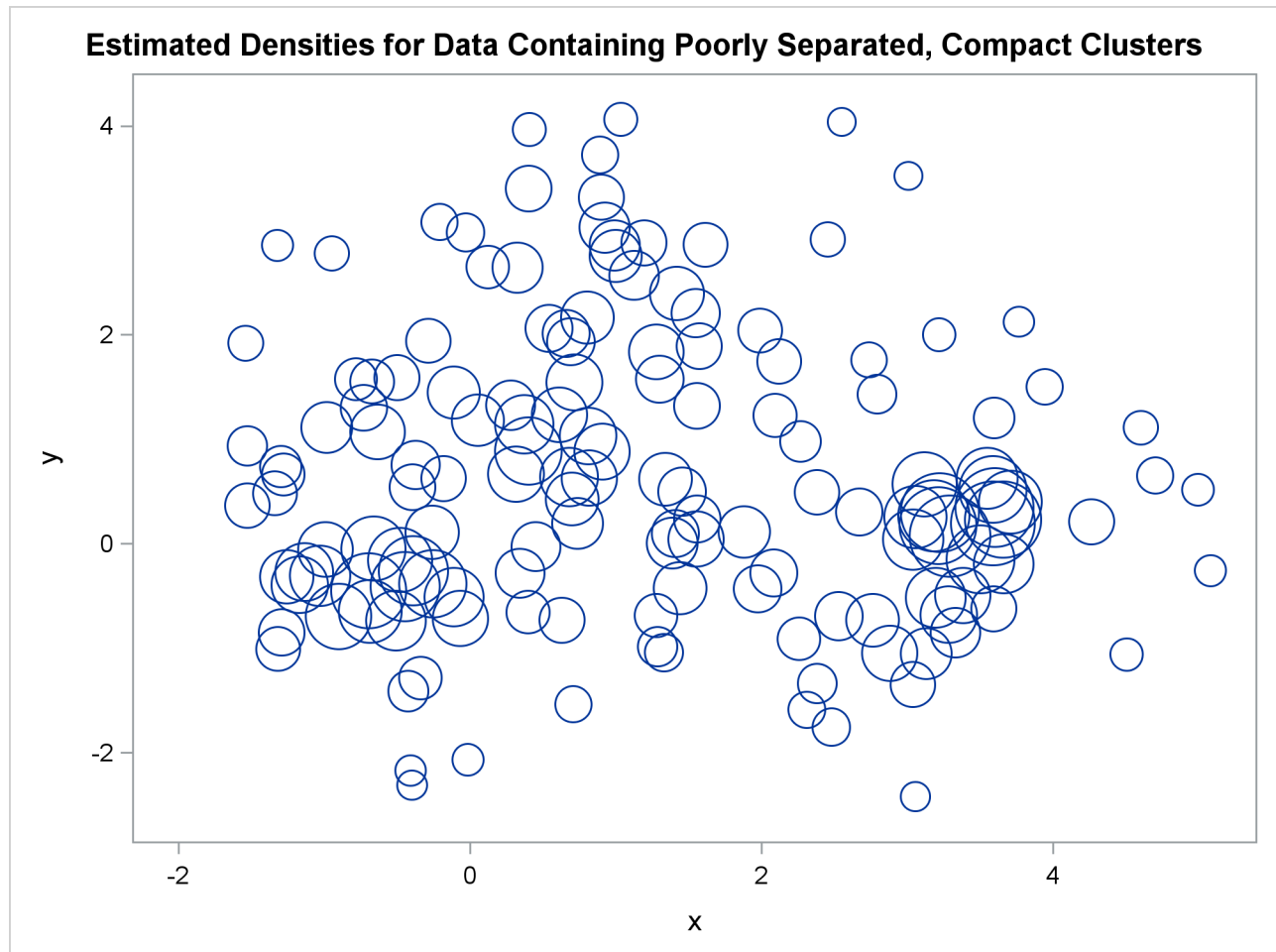


Figure 11.8 Poorly Separated, Compact Clusters: PROC CLUSTER METHOD=TWOSTAGE

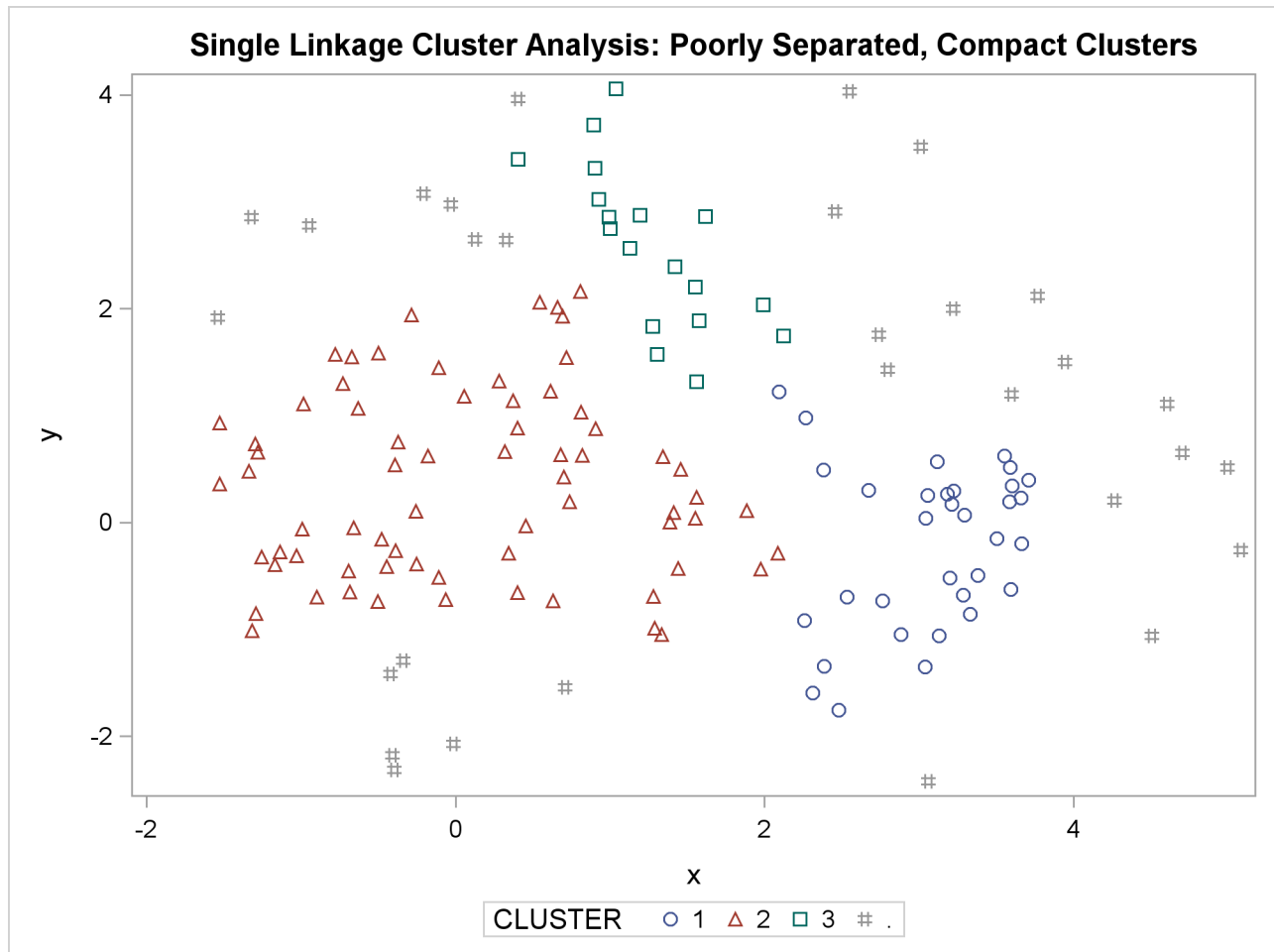
In two-stage density linkage, each cluster is a region surrounding a local maximum of the estimated probability density function. If you think of the estimated density function as a landscape with mountains and valleys, each mountain is a cluster, and the boundaries between clusters are placed near the bottoms of the valleys.

The following SAS statements produce [Figure 11.9](#):

```
proc cluster data=closer outtree=tree method=single noprint;
  var x y;
run;

proc tree data=tree noprint out=out n=3 dock=5;
  copy x y;
  title 'Single Linkage Cluster Analysis: '
        'Poorly Separated, Compact Clusters';
run;

proc sgplot;
  scatter y=y x=x / group=cluster;
run;
```

Figure 11.9 Poorly Separated, Compact Clusters: PROC CLUSTER METHOD=SINGLE

The two least squares methods, PROC FASTCLUS and Ward's, yield the most uniform cluster sizes and the best recovery of the true clusters. This result is expected since these two methods are biased toward recovering compact clusters of equal size. With average linkage, the lower-left cluster is too large; with the centroid method, the lower-right cluster is too large; and with two-stage density linkage, the top cluster is too large. The single linkage analysis resembles average linkage except for the large number of outliers resulting from the DOCK= option in the PROC TREE statement; the outliers are plotted as filled circles (missing values).

Multinormal Clusters of Unequal Size and Dispersion

In this example, there are three multinormal clusters that differ in size and dispersion. PROC FASTCLUS and five of the hierarchical methods available in PROC CLUSTER are used. To help you compare methods, the true, generated clusters are plotted.

The following SAS statements produce Figure 11.10:

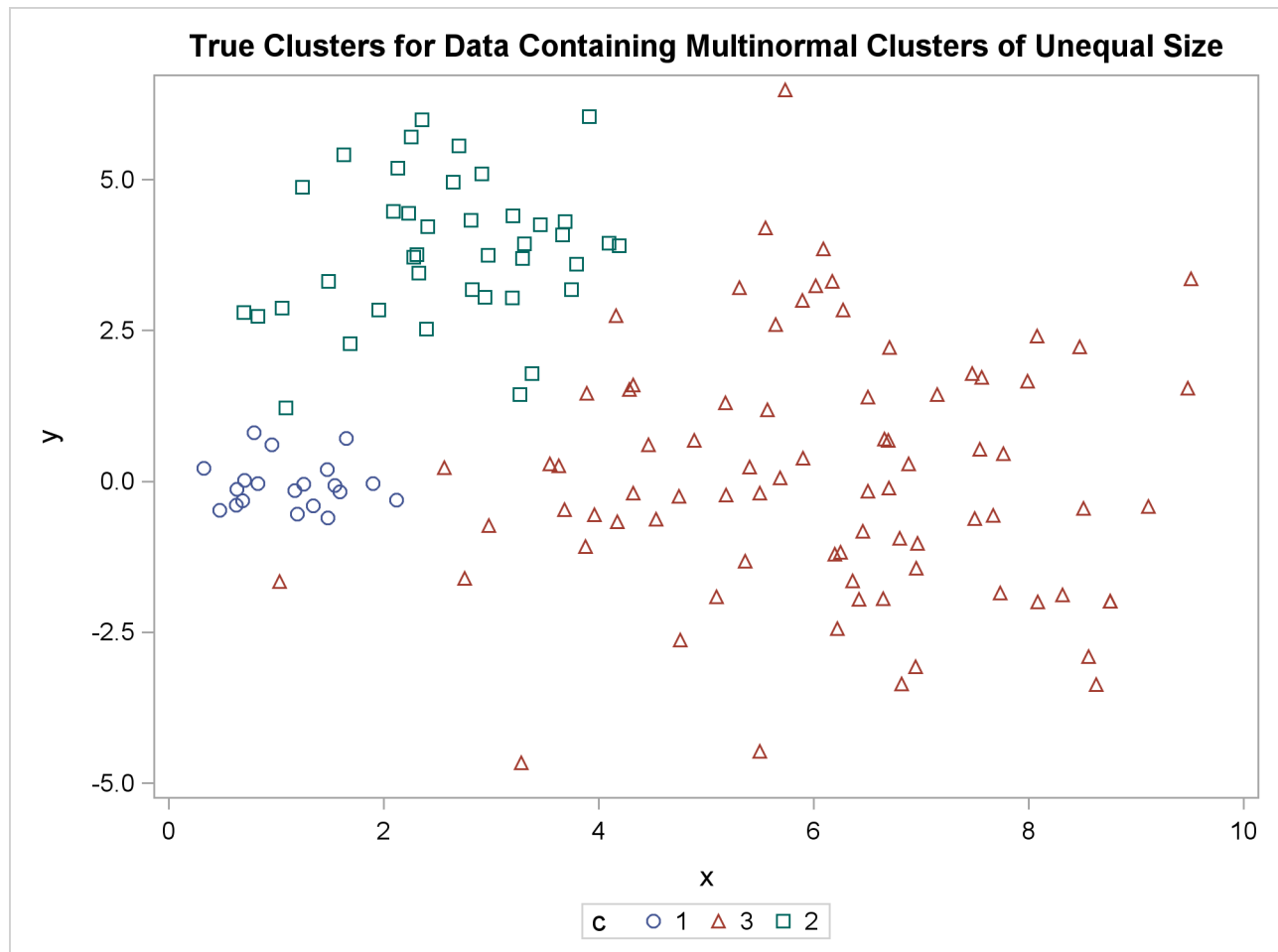
```

data unequal;
  keep x y c;
  mx=1; my=0; n=20; scale=.5; c=1; link generate;
  mx=6; my=0; n=80; scale=2.; c=3; link generate;
  mx=3; my=4; n=40; scale=1.; c=2; link generate;
  stop;
generate:
  do i=1 to n;
    x=rannor(1)*scale+mx;
    y=rannor(1)*scale+my;
    output;
  end;
  return;
run;

title 'True Clusters for Data Containing Multinormal Clusters of Unequal Size';
proc sgplot;
  scatter y=y x=x / group=c;
run;

```

Figure 11.10 Generated Clusters of Unequal Size

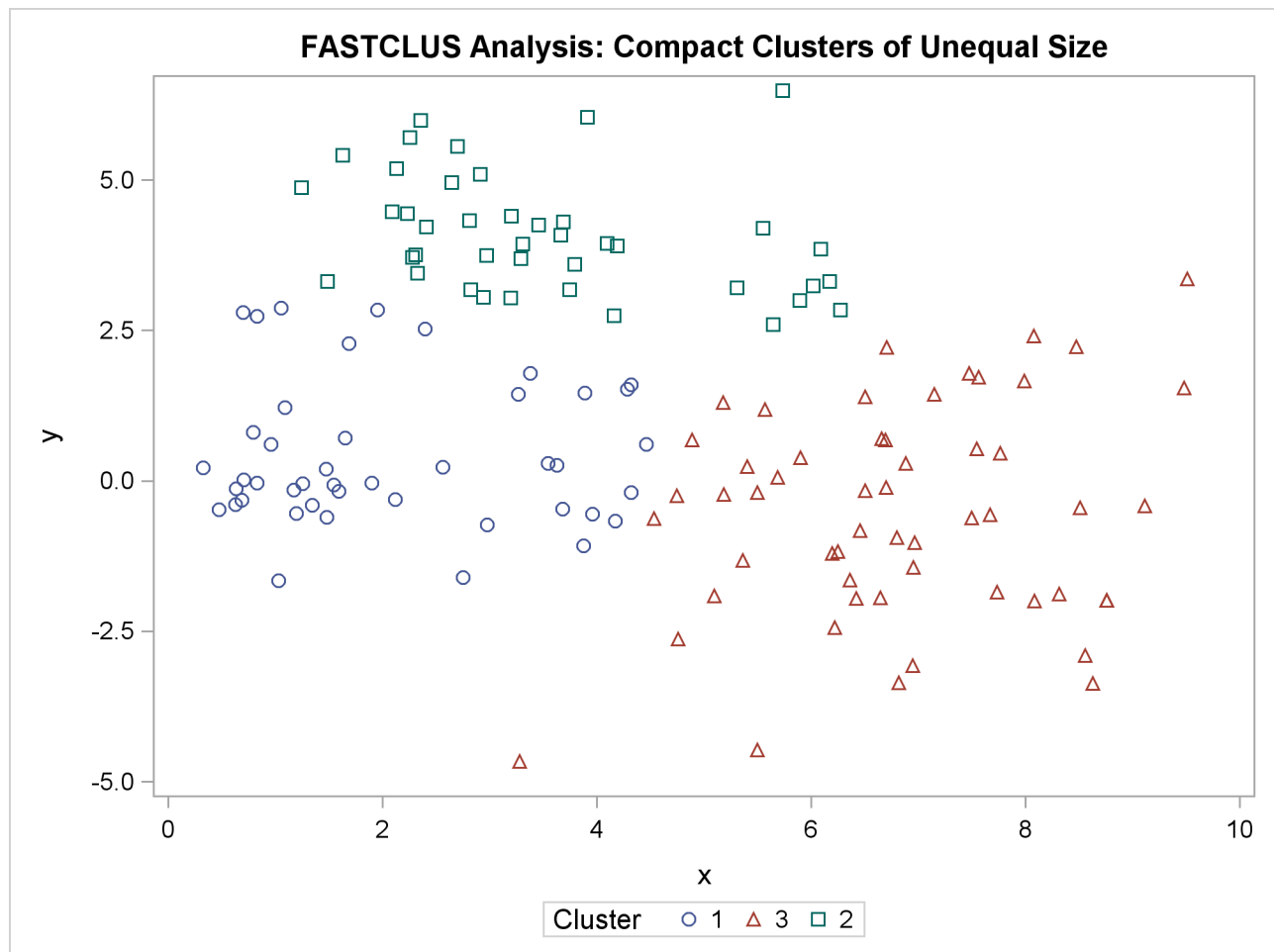


The following statements use the FASTCLUS procedure to find three clusters and then use the SGPLOT procedure to plot the clusters. The following statements produce [Figure 11.11](#):

```
proc fastclus data=unequal out=out maxc=3 noprint;
  var x y;
  title 'FASTCLUS Analysis: Compact Clusters of Unequal Size';
run;

proc sgplot;
  scatter y=y x=x / group=cluster;
run;
```

Figure 11.11 Compact Clusters of Unequal Size: PROC FASTCLUS



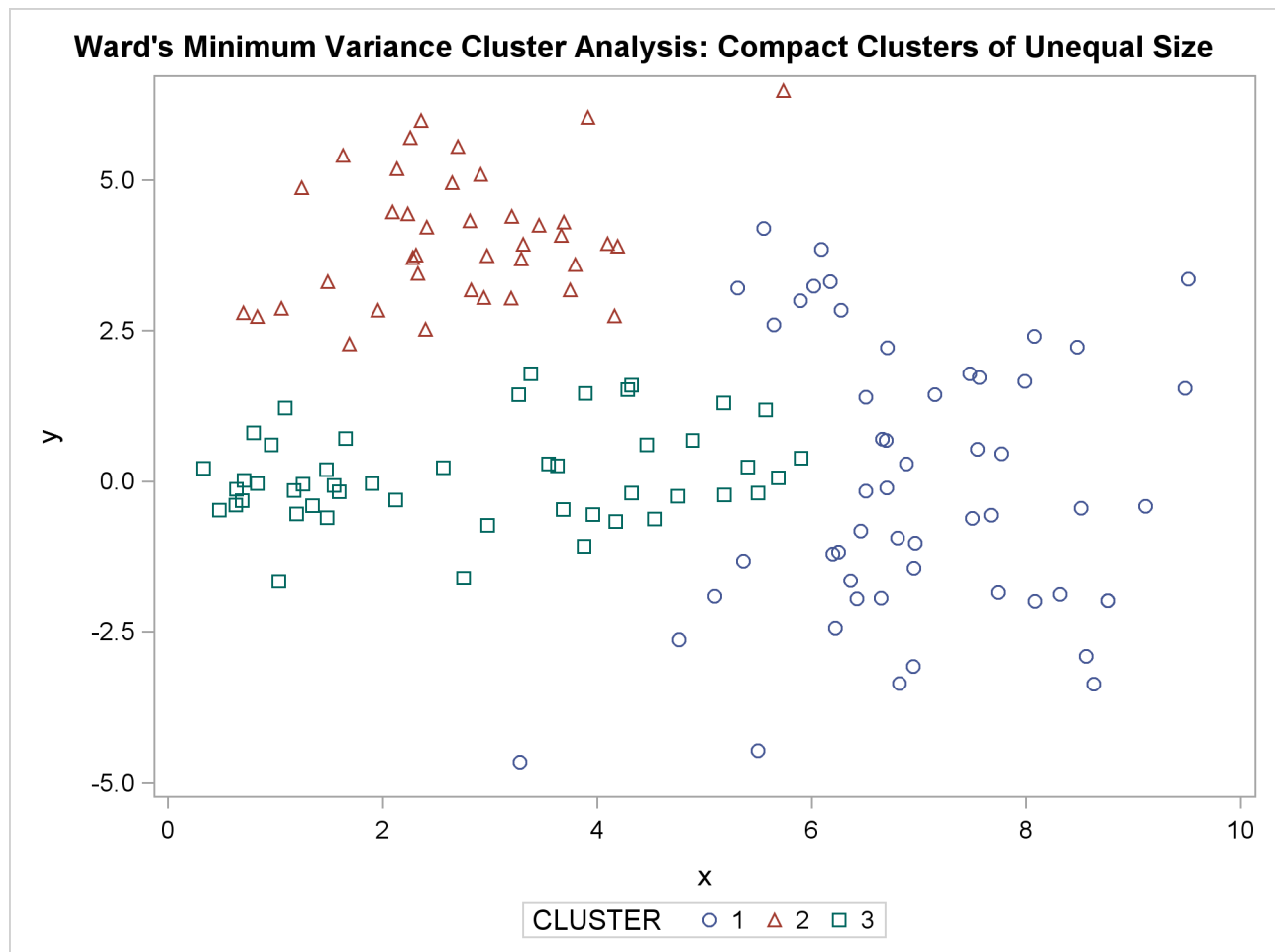
The following SAS statements produce Figure 11.12:

```
proc cluster data=unequal outtree=tree method=ward noprint;
  var x y;
run;

proc tree noprint out=out n=3;
  copy x y;
  title 'Ward''s Minimum Variance Cluster Analysis: '
        'Compact Clusters of Unequal Size';
run;

proc sgplot;
  scatter y=y x=x / group=cluster;
run;
```

Figure 11.12 Compact Clusters of Unequal Size: PROC CLUSTER METHOD=WARD



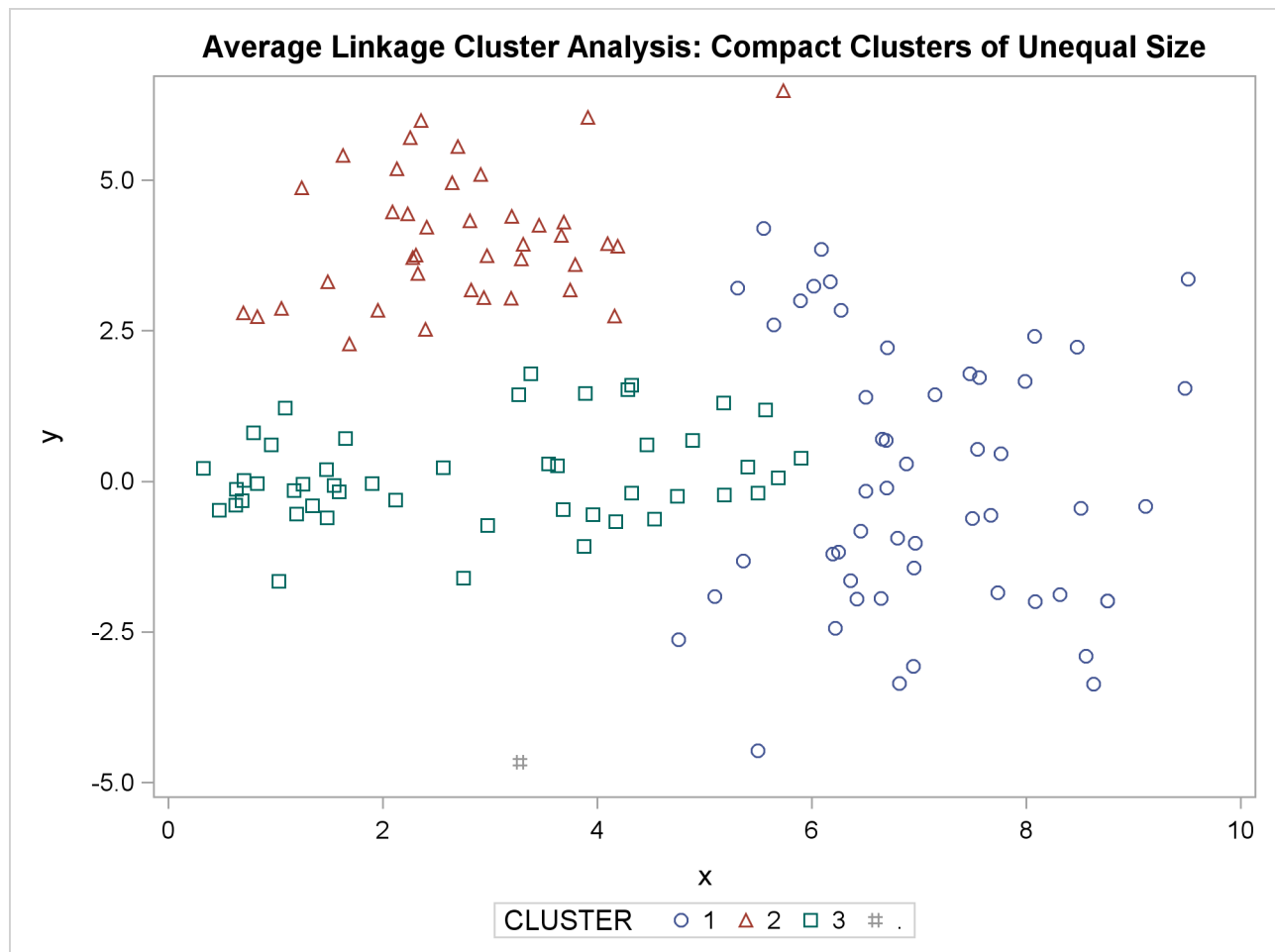
The following SAS statements produce Figure 11.13:

```
proc cluster data=unequal outtree=tree method=average noprint;
  var x y;
run;

proc tree noprint out=out n=3 dock=5;
  copy x y;
  title 'Average Linkage Cluster Analysis: '
        'Compact Clusters of Unequal Size';
run;

proc sgplot;
  scatter y=y x=x / group=cluster;
run;
```

Figure 11.13 Compact Clusters of Unequal Size: PROC CLUSTER METHOD=AVERAGE



The following SAS statements produce Figure 11.14:

```

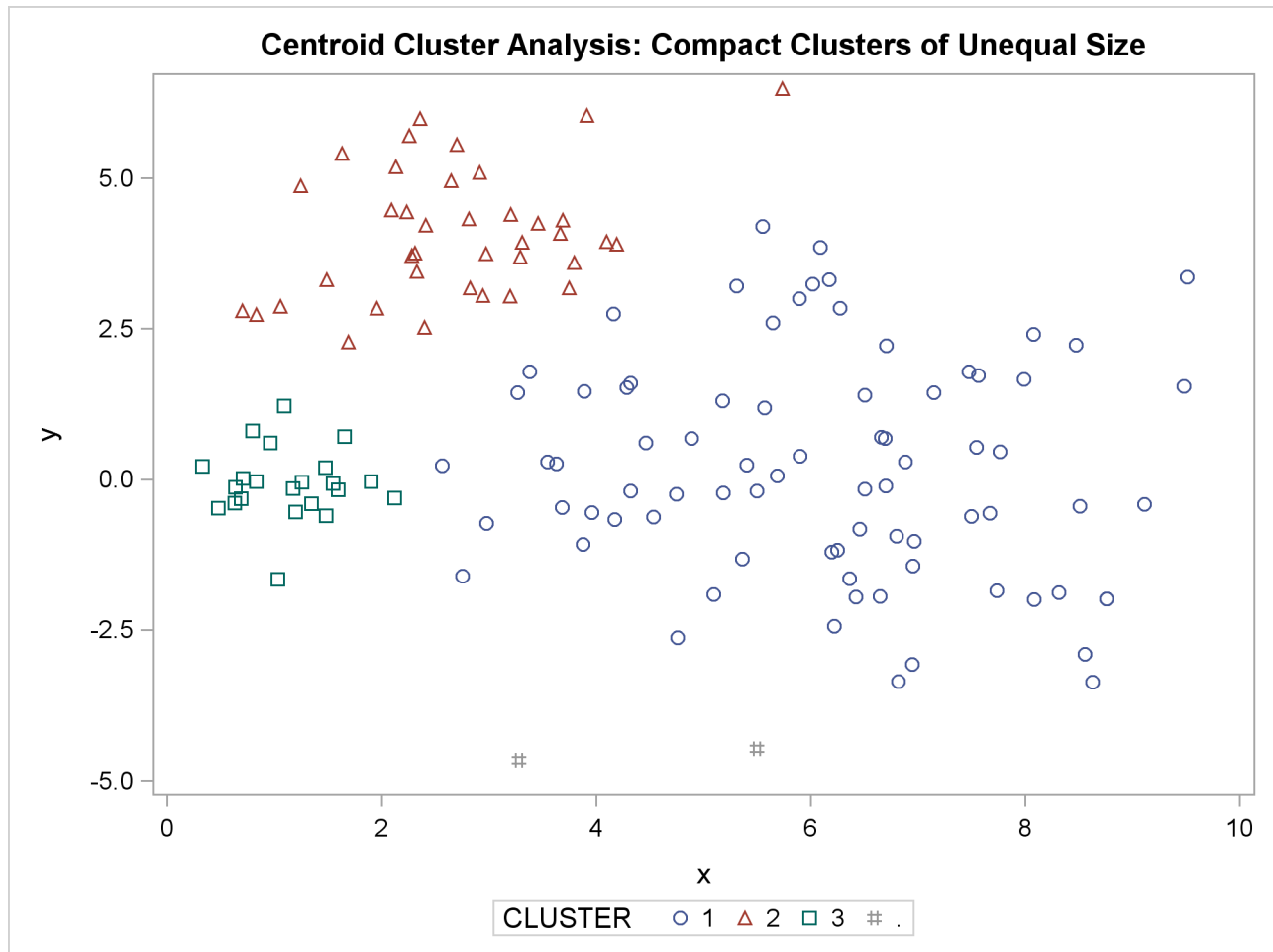
proc cluster data=unequal outtree=tree method=centroid noprint;
  var x y;
run;

proc tree noprint out=out n=3 dock=5;
  copy x y;
  title 'Centroid Cluster Analysis: '
        'Compact Clusters of Unequal Size';
run;

proc sgplot;
  scatter y=y x=x / group=cluster;
run;

```

Figure 11.14 Compact Clusters of Unequal Size: PROC CLUSTER METHOD=CENTROID



The following SAS statements produce Figure 11.15 and Figure 11.16:

```
proc cluster data=unequal outtree=tree method=twostage k=10 noprint;
  var x y;
run;

proc tree noprint out=out n=3;
  copy x y _dens_;
  title 'Two-Stage Density Linkage Cluster Analysis: '
        'Compact Clusters of Unequal Size';
run;

proc sgplot;
  scatter y=y x=x / group=cluster;
run;

proc sgplot;
  bubble y=y x=x size=_dens_ / nofill lineattrs=graphdatadefault;
  title 'Estimated Densities for Data Containing '
        'Compact Clusters of Unequal Size';
run;
```

Figure 11.15 Compact Clusters of Unequal Size: PROC CLUSTER METHOD=TWOSTAGE

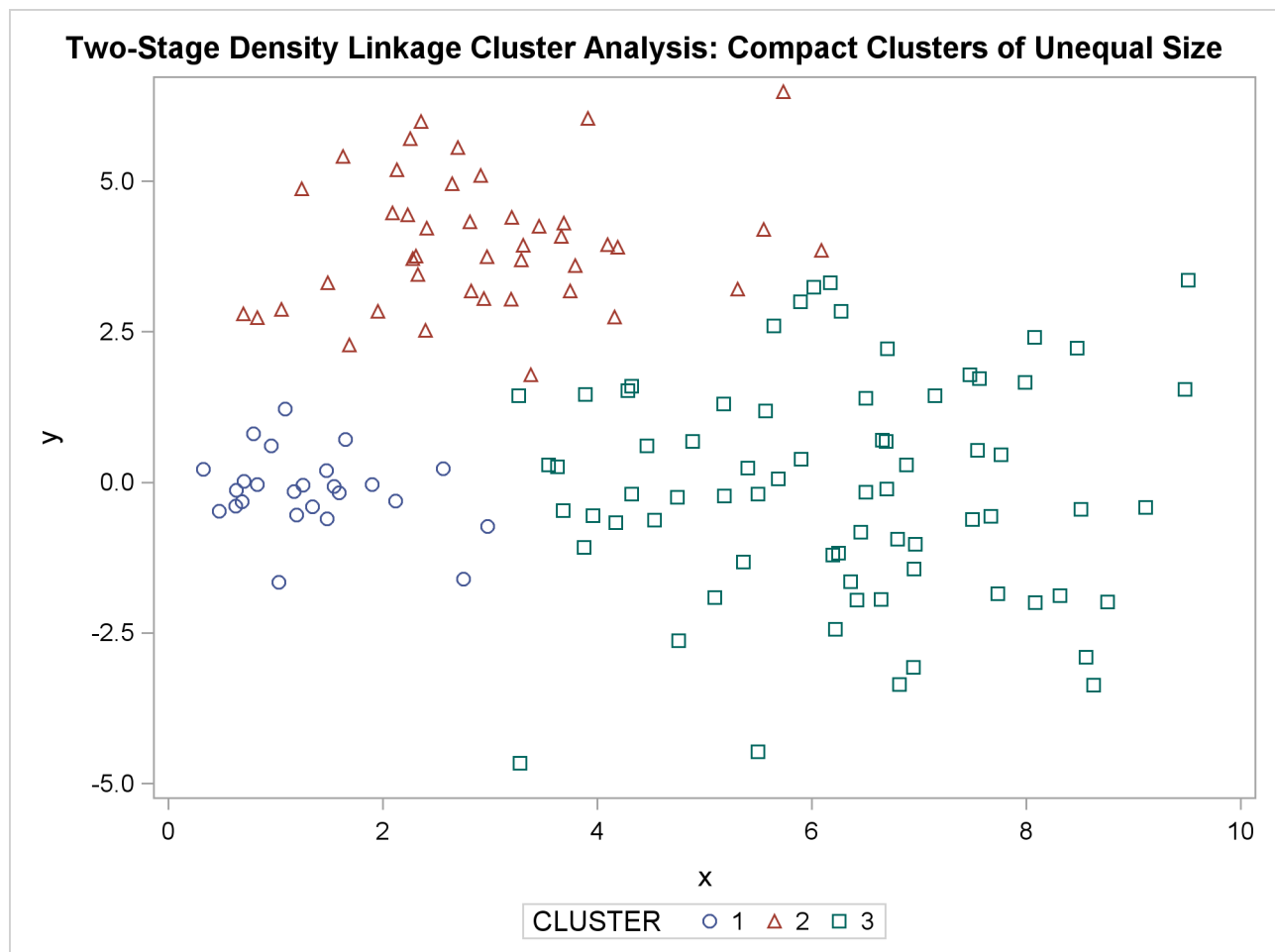
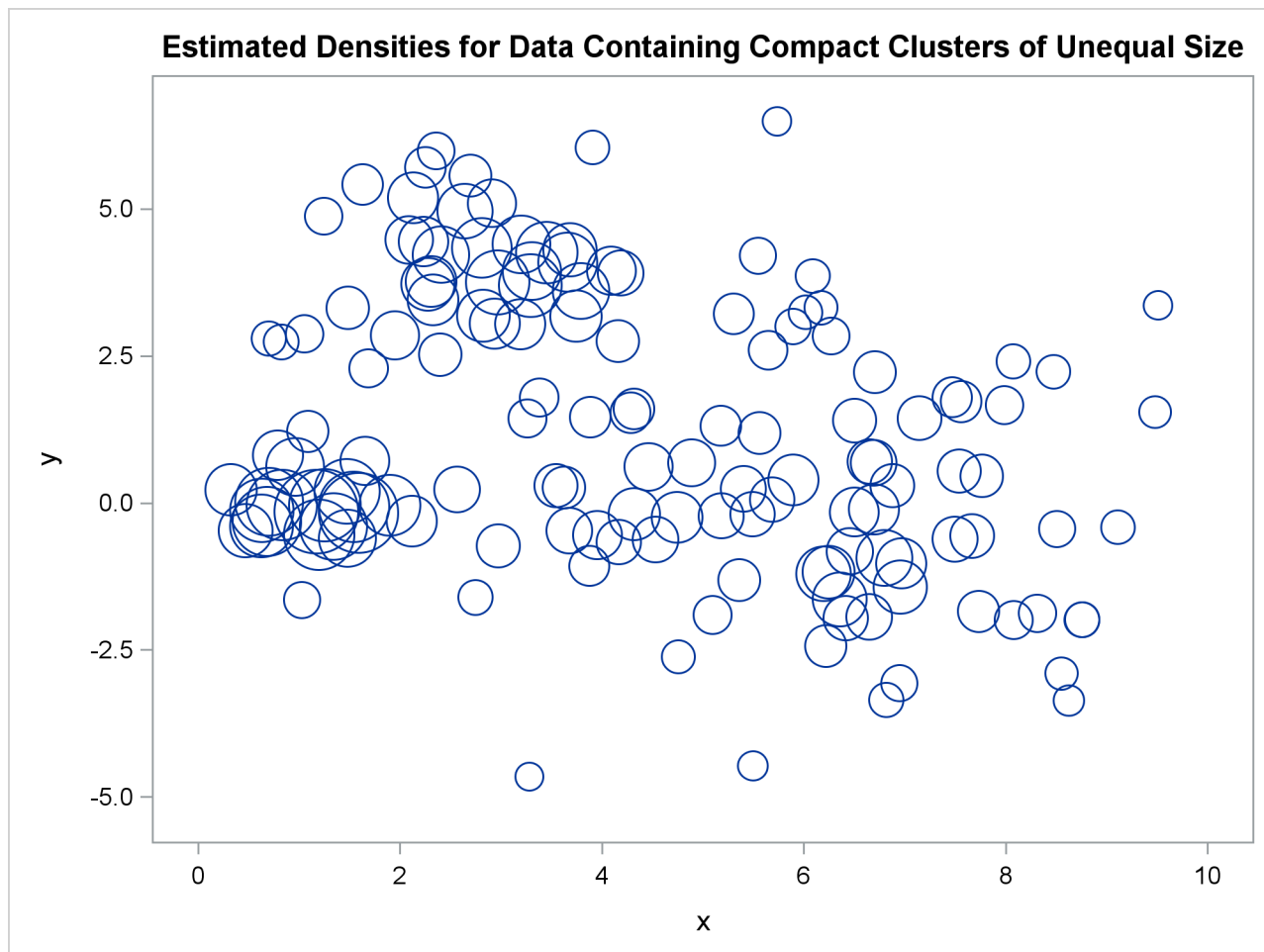


Figure 11.16 Compact Clusters of Unequal Size: PROC CLUSTER METHOD=TWOSTAGE



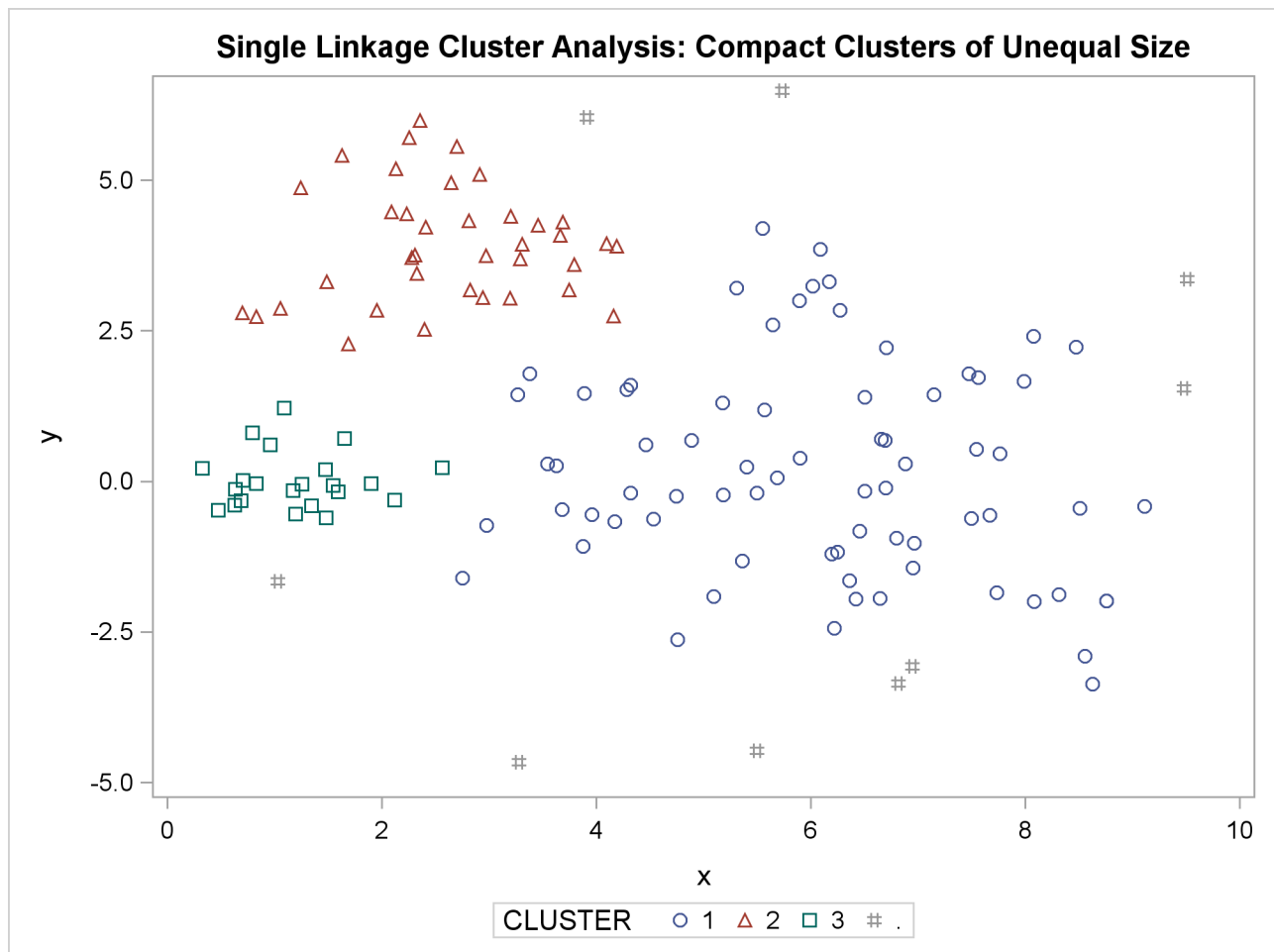
The following SAS statements produce Figure 11.17:

```
proc cluster data=unequal outtree=tree method=single noprint;
  var x y;
run;

proc tree data=tree noprint out=out n=3 dock=5;
  copy x y;
  title 'Single Linkage Cluster Analysis: '
        'Compact Clusters of Unequal Size';
run;

proc sgplot;
  scatter y=y x=x / group=cluster;
run;
```

Figure 11.17 Compact Clusters of Unequal Size: PROC CLUSTER METHOD=SINGLE



In the PROC FASTCLUS analysis, the smallest cluster, in the bottom-left portion of the plot, has stolen members from the other two clusters, and the upper-left cluster has also acquired some observations that rightfully belong to the larger, lower-right cluster. With Ward's method, the upper-left cluster is separated correctly, but the lower-left cluster has taken a large bite out of the lower-right cluster. For both of these methods, the clustering errors are in accord with the biases of the methods to produce clusters of equal size. In the average linkage analysis, both the upper-left and lower-left clusters have encroached on the lower-right cluster, thereby making the variances more nearly equal than in the true clusters. The centroid method, which lacks the size and dispersion biases of the previous methods, obtains an essentially correct partition.

Two-stage density linkage does almost as well, even though the compact shapes of these clusters favor the traditional methods. Single linkage also produces excellent results.

Elongated Multinormal Clusters

In this example, the data are sampled from two highly elongated multinormal distributions with equal covariance matrices. The following SAS statements produce [Figure 11.18](#):

```

data elongate;
  keep x y;
  ma=8; mb=0; link generate;
  ma=6; mb=8; link generate;
  stop;
generate:
  do i=1 to 50;
    a=rannor(7)*6+ma;
    b=rannor(7)+mb;
    x=a-b;
    y=a+b;
    output;
  end;
  return;
run;

proc fastclus data=elongate out=out maxc=2 noprint;
run;

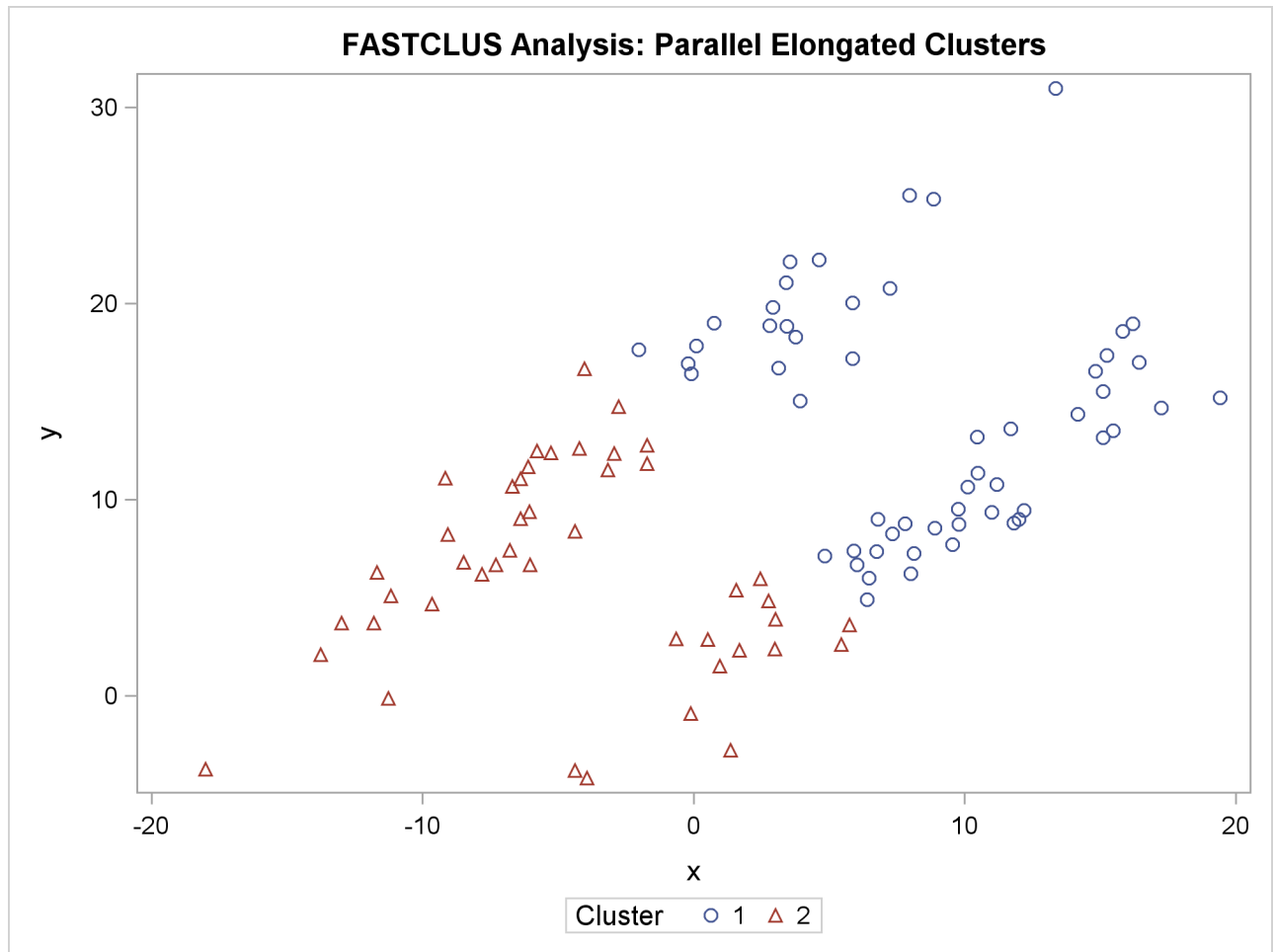
%modstyle(name=ClusterStyle2,parent=Statistical,type=CLM,
markers=Circle Triangle circlefilled);
ods listing style=ClusterStyle2;

proc sgplot;
  scatter y=y x=x / group=cluster;
  title 'FASTCLUS Analysis: Parallel Elongated Clusters';
run;

```

Notice that PROC FASTCLUS found two clusters, as requested by the MAXC= option. However, it attempted to form spherical clusters, which are obviously inappropriate for these data.

Figure 11.18 Parallel Elongated Clusters: PROC FASTCLUS



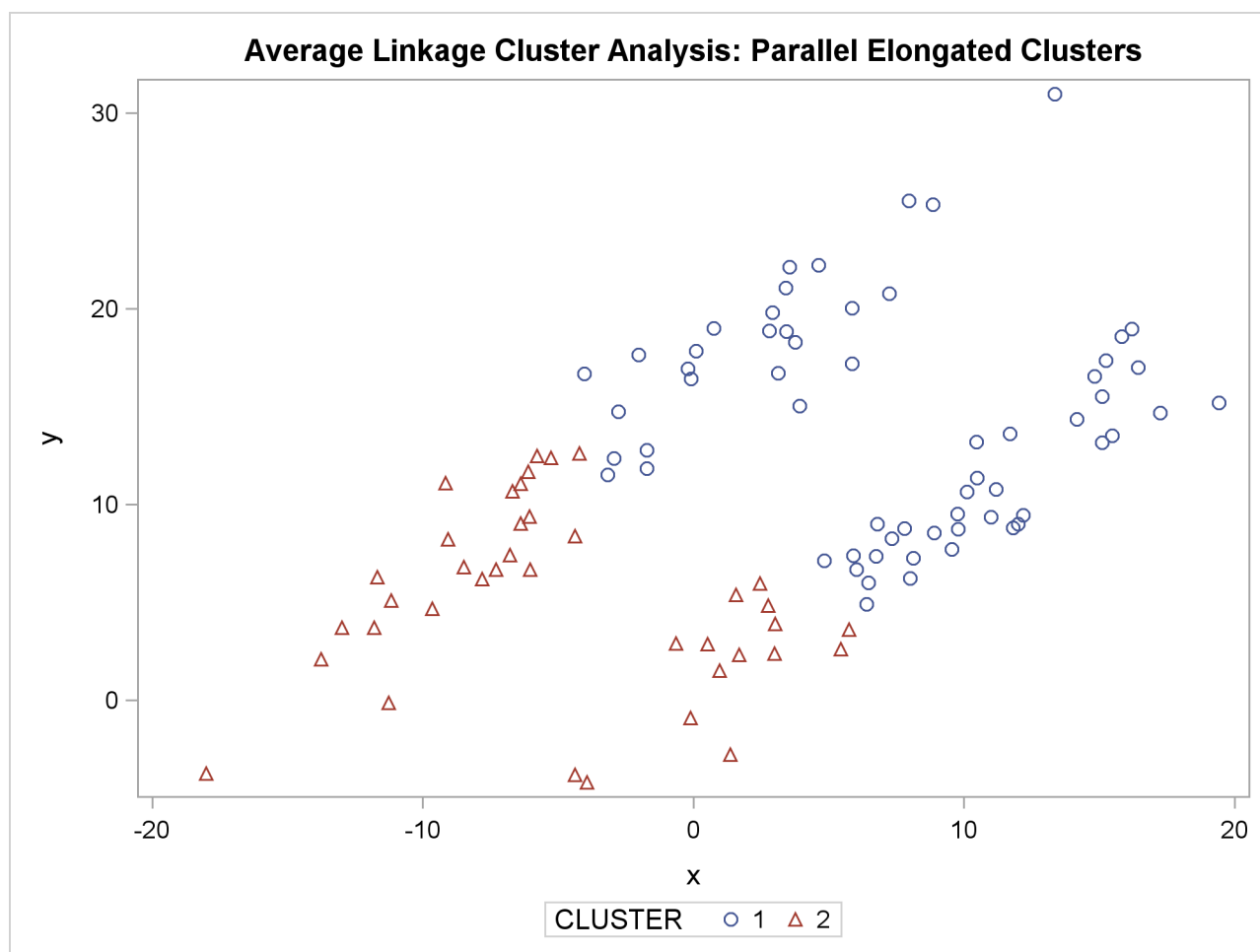
The following SAS statements produce Figure 11.19:

```
proc cluster data=elongate outtree=tree method=average noprint;
run;

proc tree noprint out=out n=2 dock=5;
  copy x y;
run;

proc sgplot;
  scatter y=y x=x / group=cluster;
  title 'Average Linkage Cluster Analysis: '
        'Parallel Elongated Clusters';
run;
```

Figure 11.19 Parallel Elongated Clusters: PROC CLUSTER METHOD=AVERAGE



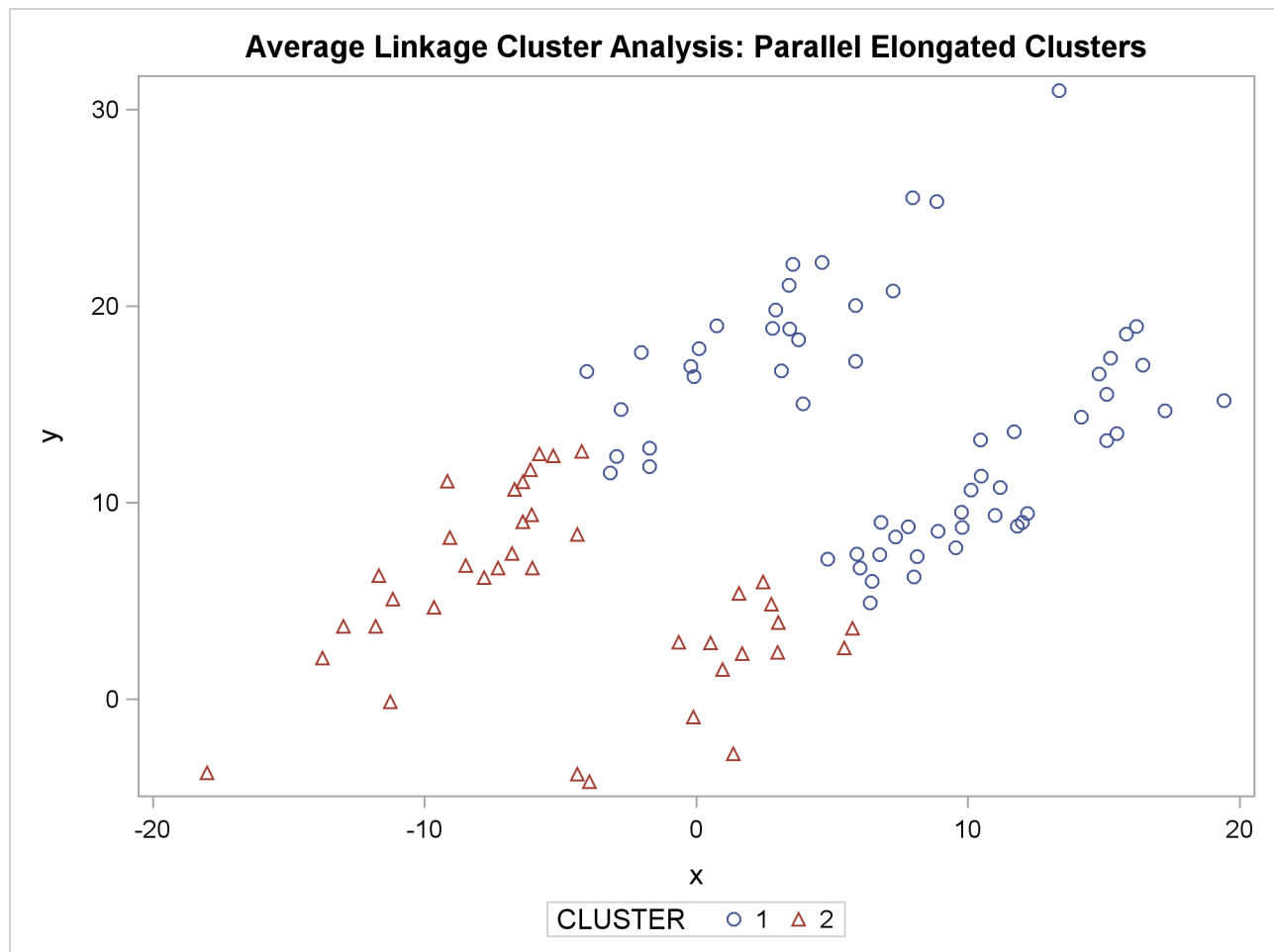
The following SAS statements produce Figure 11.20:

```
proc cluster data=elongate outtree=tree method=twostage k=10 noprint;
run;

proc tree noprint out=out n=2;
  copy x y;
run;

proc sgplot;
  scatter y=y x=x / group=cluster;
  title 'Two-Stage Density Linkage Cluster Analysis: '
        'Parallel Elongated Clusters';
run;
```

Figure 11.20 Parallel Elongated Clusters: PROC CLUSTER METHOD=TWOSTAGE



PROC FASTCLUS and average linkage fail miserably. Ward's method and the centroid method (not shown) produce almost the same results. Two-stage density linkage, however, recovers the correct clusters. Single linkage (not shown) finds the same clusters as two-stage density linkage except for some outliers.

In this example, the population clusters have equal covariance matrices. If the within-cluster covariances are known, the data can be transformed to make the clusters spherical so that any of the clustering methods

can find the correct clusters. But when you are doing a cluster analysis, you do not know what the true clusters are, so you cannot calculate the within-cluster covariance matrix. Nevertheless, it is sometimes possible to estimate the within-cluster covariance matrix without knowing the cluster membership or even the number of clusters, using an approach invented by Art, Gnanadesikan, and Kettenring (1982). A method for obtaining such an estimate is available in the ACECLUS procedure.

In the following analysis, PROC ACECLUS transforms the variables X and Y into the canonical variables Can1 and Can2. The latter are plotted and then used in a cluster analysis by Ward's method. The clusters are then plotted with the original variables X and Y.

The following SAS statements produce [Figure 11.21](#) and [Figure 11.22](#):

```
proc aceclus data=elongate out=ace p=.1;
  var x y;
  title 'ACECLUS Analysis: Parallel Elongated Clusters';
run;

proc sgplot;
  scatter y=can2 x=can1;
  title 'Data Containing Parallel Elongated Clusters';
  title2 'After Transformation by PROC ACECLUS';
run;
```

Figure 11.21 Parallel Elongated Clusters: PROC ACECLUS

ACECLUS Analysis: Parallel Elongated Clusters			
The ACECLUS Procedure			
Approximate Covariance Estimation for Cluster Analysis			
Observations	100	Proportion	0.1000
Variables	2	Converge	0.00100
Means and Standard Deviations			
Variable	Mean	Standard Deviation	
x	2.6406	8.3494	
y	10.6488	6.8420	
COV: Total Sample Covariances			
	x	y	
x	69.71314819	24.24268934	
y	24.24268934	46.81324861	
Initial Within-Cluster Covariance Estimate = Full Covariance Matrix			
Threshold =		0.328478	

Figure 11.21 continued

Iteration History				
Iteration	RMS Distance	Distance Cutoff	Pairs Within Cutoff	Convergence Measure
1	2.000	0.657	672.0	0.673685
2	9.382	3.082	716.0	0.006963
3	9.339	3.068	760.0	0.008362
4	9.437	3.100	824.0	0.009656
5	9.359	3.074	889.0	0.010269
6	9.267	3.044	955.0	0.011276
7	9.208	3.025	999.0	0.009230
8	9.230	3.032	1052.0	0.011394
9	9.226	3.030	1091.0	0.007924
10	9.173	3.013	1121.0	0.007993

WARNING: Iteration limit exceeded.

ACE: Approximate Covariance Estimate Within Clusters

	x	y
x	9.299329632	8.215362614
y	8.215362614	8.937753936

Eigenvalues of $\text{Inv}(\text{ACE}) * (\text{COV} - \text{ACE})$

	Eigenvalue	Difference	Proportion	Cumulative
1	36.7091	33.1672	0.9120	0.9120
2	3.5420		0.0880	1.0000

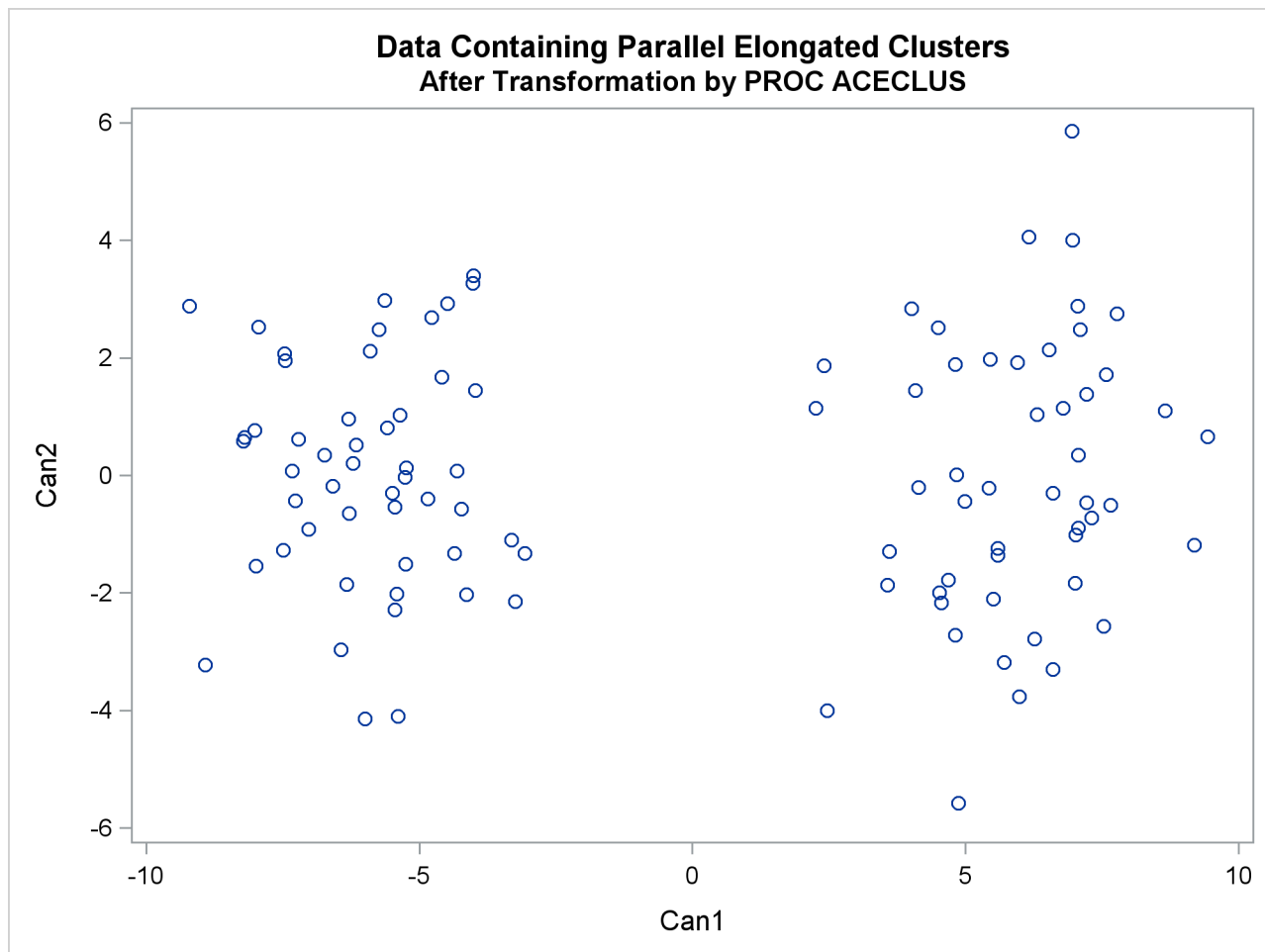
Eigenvectors (Raw Canonical Coefficients)

	Can1	Can2
x	-0.748392	0.109547
y	0.736349	0.230272

Standardized Canonical Coefficients

	Can1	Can2
x	-6.24866	0.91466
y	5.03812	1.57553

Figure 11.22 Parallel Elongated Clusters after Transformation by PROC ACECLUS



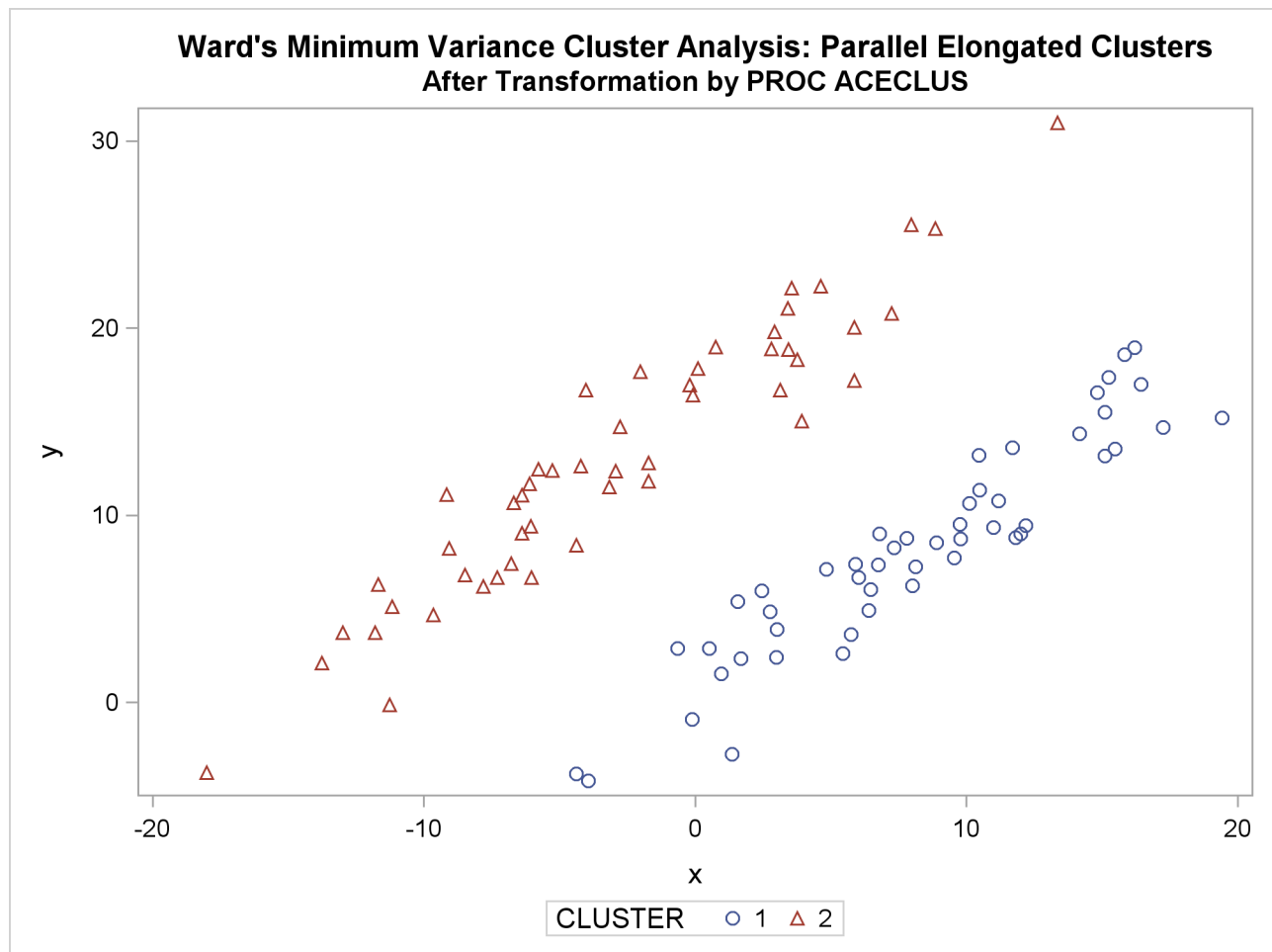
The following SAS statements produce Figure 11.23:

```
proc cluster data=ace outtree=tree method=ward noprint;
  var can1 can2;
  copy x y;
run;

proc tree noprint out=out n=2;
  copy x y;
run;

proc sgplot;
  scatter y=y x=x / group=cluster;
  title 'Ward's Minimum Variance Cluster Analysis: '
        'Parallel Elongated Clusters';
  title2 'After Transformation by PROC ACECLUS';
run;
```

Figure 11.23 Transformed Data Containing Parallel Elongated Clusters: PROC CLUSTER METHOD=WARD



Nonconvex Clusters

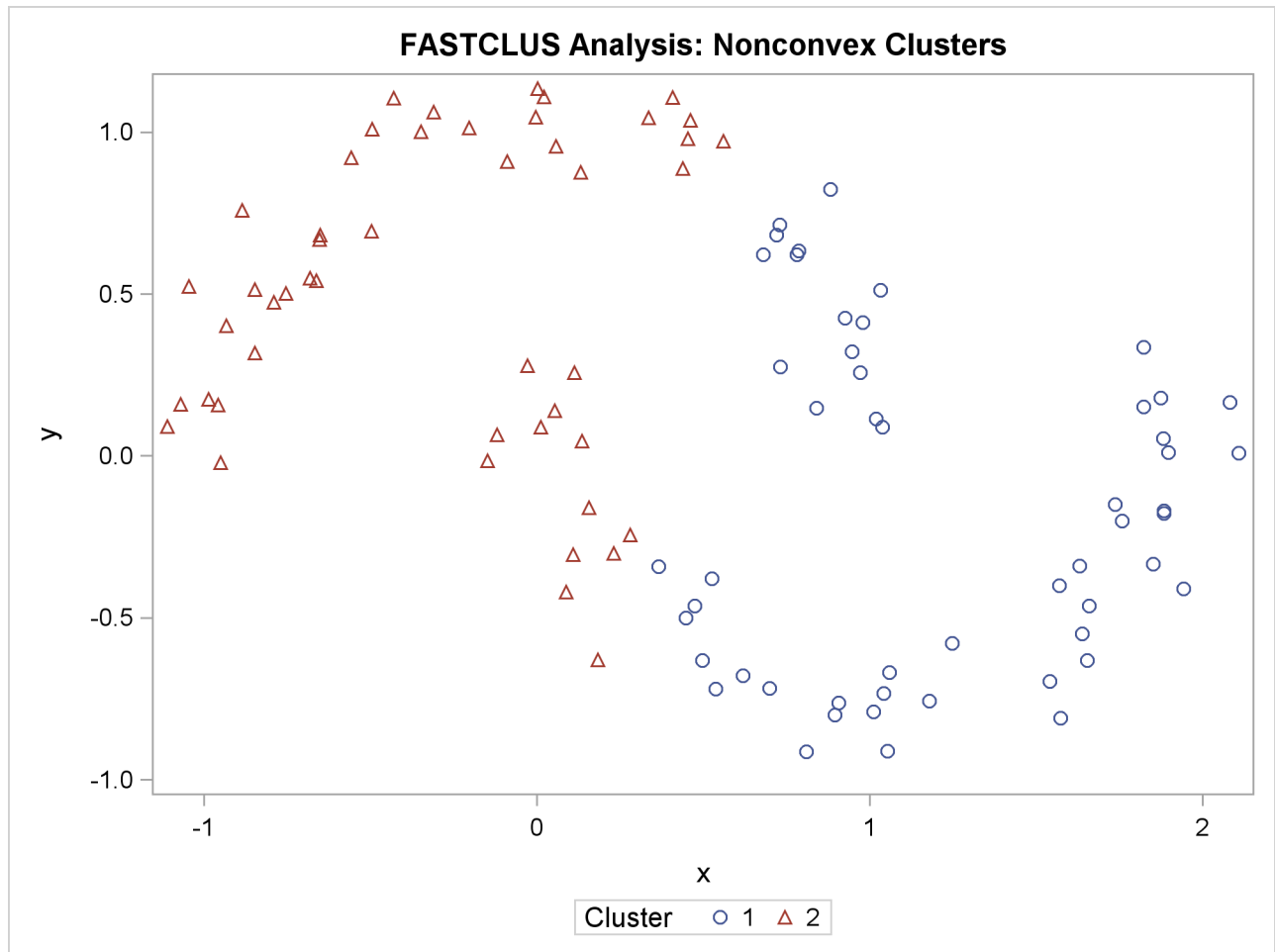
If the population clusters have very different covariance matrices, using PROC ACECLUS is of no avail. Although methods exist for estimating multinormal clusters with unequal covariance matrices (Wolfe 1970; Symons 1981; Everitt and Hand 1981; Titterton, Smith, and Makov 1985; McLachlan and Basford 1988), these methods tend to have serious problems with initialization and might converge to degenerate solutions. For unequal covariance matrices or radically nonnormal distributions, the best approach to cluster analysis is through nonparametric density estimation, as in density linkage. The next example illustrates population clusters with nonconvex density contours. The following SAS statements produce [Figure 11.24](#):

```
data noncon;
  keep x y;
  do i=1 to 100;
    a=i*.0628319;
    x=cos(a)+(i>50)+rannor(7)*.1;
    y=sin(a)+(i>50)*.3+rannor(7)*.1;
    output;
  end;
run;

proc fastclus data=noncon out=out maxc=2 noprint;
run;

proc sgplot;
  scatter y=y x=x / group=cluster;
  title 'FASTCLUS Analysis: Nonconvex Clusters';
run;
```

Figure 11.24 Nonconvex Clusters: PROC FASTCLUS



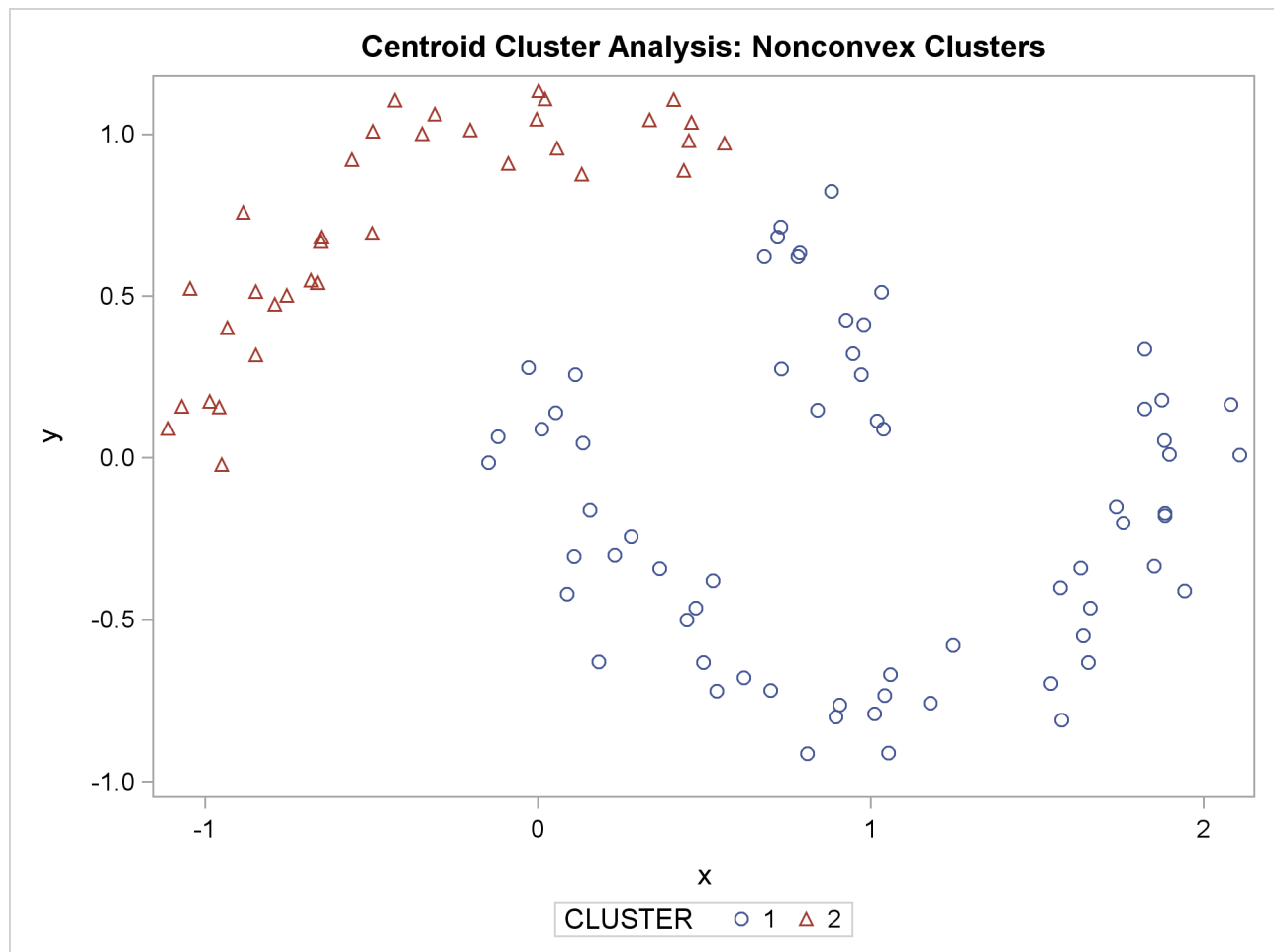
The following SAS statements produce Figure 11.25:

```
proc cluster data=noncon outtree=tree method=centroid noprint;
run;

proc tree noprint out=out n=2 dock=5;
  copy x y;
run;

proc sgplot;
  scatter y=y x=x / group=cluster;
  title 'Centroid Cluster Analysis: Nonconvex Clusters';
run;
```

Figure 11.25 Nonconvex Clusters: PROC CLUSTER METHOD=CENTROID



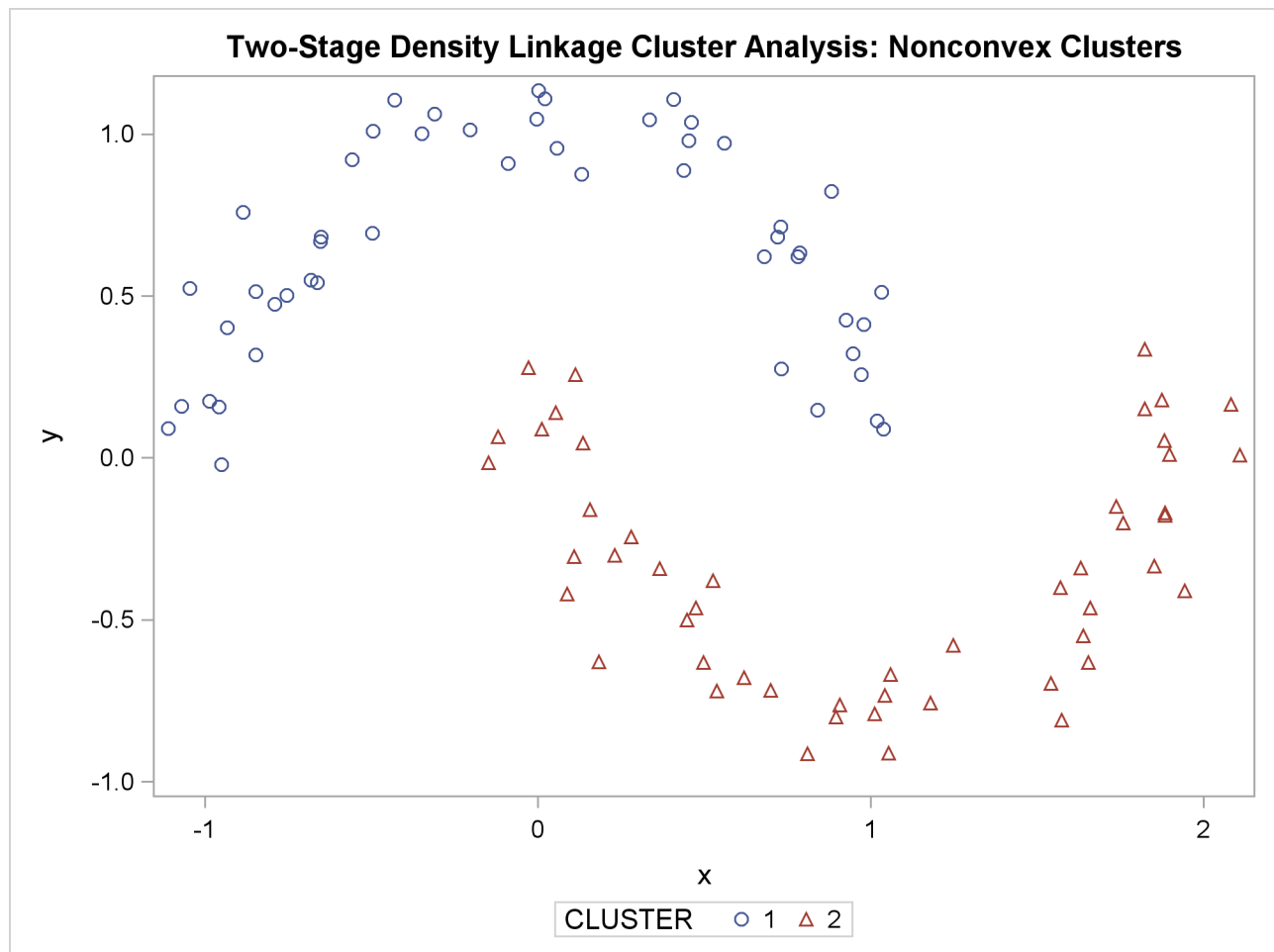
The following SAS statements produce Figure 11.26:

```
proc cluster data=noncon outtree=tree method=twostage k=10 noprint;
run;

proc tree noprint out=out n=2;
  copy x y;
run;

proc sgplot;
  scatter y=y x=x / group=cluster;
  title 'Two-Stage Density Linkage Cluster Analysis: Nonconvex Clusters';
run;
```

Figure 11.26 Nonconvex Clusters: PROC CLUSTER METHOD=TWOSTAGE



Ward's method and average linkage (not shown) do better than PROC FASTCLUS but not as well as the centroid method. Two-stage density linkage recovers the correct clusters, as does single linkage (not shown).

The preceding examples are intended merely to illustrate some of the properties of clustering methods in common use. If you intend to perform a cluster analysis, you should consult more systematic and rigorous studies of the properties of clustering methods, such as Milligan (1980).

The Number of Clusters

There are no completely satisfactory methods that can be used for determining the number of population clusters for any type of cluster analysis (Everitt 1979; Hartigan 1985a; Bock 1985).

If your purpose in clustering is dissection—that is, to summarize the data without trying to uncover real clusters—it might suffice to look at R square for each variable and pooled over all variables. Plots of R square against the number of clusters are useful.

It is always a good idea to look at your data graphically. If you have only two or three variables, use PROC SGPLOT to make scatter plots identifying the clusters. With more variables, use PROC CANDISC to compute canonical variables for plotting.

Ordinary significance tests, such as analysis of variance F tests, are not valid for testing differences between clusters. Since clustering methods attempt to maximize the separation between clusters, the assumptions of the usual significance tests, parametric or nonparametric, are drastically violated. For example, if you take a sample of 100 observations from a single univariate normal distribution, have PROC FASTCLUS divide it into two clusters, and run a t test between the clusters, you usually obtain a p -value of less than 0.0001. For the same reason, methods that purport to test for clusters against the null hypothesis that objects are assigned randomly to clusters (such as McClain and Rao 1975 and Klastorin 1983) are useless.

Most valid tests for clusters either have intractable sampling distributions or involve null hypotheses for which rejection is uninformative. For clustering methods based on distance matrices, a popular null hypothesis is that all permutations of the values in the distance matrix are equally likely (Ling 1973; Hubert 1974). Using this null hypothesis, you can do a permutation test or a rank test. The trouble with the permutation hypothesis is that, with any real data, the null hypothesis is implausible even if the data do not contain clusters. Rejecting the null hypothesis does not provide any useful information (Hubert and Baker 1977).

Another common null hypothesis is that the data are a random sample from a multivariate normal distribution (Wolfe 1970, 1978; Duda and Hart 1973; Lee 1979). The multivariate normal null hypothesis arises naturally in normal mixture models (Titterton, Smith, and Makov 1985; McLachlan and Basford 1988). Unfortunately, the likelihood ratio test statistic does not have the usual asymptotic χ^2 distribution because the regularity conditions do not hold. Approximations to the asymptotic distribution of the likelihood ratio have been suggested Wolfe (1978), but the adequacy of these approximations is debatable (Everitt 1981; Thode, Mendell, and Finch 1988). For small samples, bootstrapping seems preferable (McLachlan and Basford 1988). Bayesian inference provides a promising alternative to likelihood ratio tests for the number of mixture components for both normal mixtures and other types of distributions (Binder 1978, 1981; Banfield and Raftery 1993; Bensmail et al. 1997).

The multivariate normal null hypothesis is better than the permutation null hypothesis, but it is not satisfactory because there is typically a high probability of rejection if the data are sampled from a distribution with lower kurtosis than a normal distribution, such as a uniform distribution. The tables in Englemann and Hartigan (1969), for example, generally lead to rejection of the null hypothesis when the data are sampled from a uniform distribution. Hawkins, Muller, and ten Krooden (1982, pp. 337–340) discuss a highly conservative Bonferroni method for the use of hypothesis testing. The conservativeness of this approach might compensate to some extent for the liberalness exhibited by tests based on normal distributions when the population is uniform.

Perhaps a better null hypothesis is that the data are sampled from a uniform distribution (Hartigan 1978; Arnold 1979; Sarle 1983). The uniform null hypothesis leads to conservative error rates when the data are sampled from a strongly unimodal distribution such as the normal. However, in two or more dimensions and depending on the test statistic, the results can be very sensitive to the shape of the region of support of the uniform distribution. Sarle (1983) suggests using a hyperbox with sides proportional in length to the singular values of the centered coordinate matrix.

Given that the uniform distribution provides an appropriate null hypothesis, there are still serious difficulties in obtaining sampling distributions. Some asymptotic results are available (Hartigan 1978, 1985a; Pollard 1981; Bock 1985) for the within-cluster sum of squares, the criterion that PROC FASTCLUS and Ward's minimum variance method attempt to optimize. No distributional theory for finite sample sizes has yet appeared. Currently, the only practical way to obtain sampling distributions for realistic sample sizes is by computer simulation.

Arnold (1979) used simulation to derive tables of the distribution of a criterion based on the determinant of the within-cluster sum of squares matrix $|\mathbf{W}|$. Both normal and uniform null distributions were used. Having obtained clusters with either PROC FASTCLUS or PROC CLUSTER, you can compute Arnold's criterion with the ANOVA or CANDISC procedure. Arnold's tables provide a conservative test because PROC FASTCLUS and PROC CLUSTER attempt to minimize the trace of \mathbf{W} rather than the determinant. Marriott (1971, 1975) also provides useful information about $|\mathbf{W}|$ as a criterion for the number of clusters.

Sarle (1983) used extensive simulations to develop the cubic clustering criterion (CCC), which can be used for crude hypothesis testing and estimating the number of population clusters. The CCC is based on the assumption that a uniform distribution on a hyperrectangle will be divided into clusters shaped roughly like hypercubes. In large samples that can be divided into the appropriate number of hypercubes, this assumption gives very accurate results. In other cases the approximation is generally conservative. For details about the interpretation of the CCC, consult Sarle (1983).

Milligan and Cooper (1985) and Cooper and Milligan (1988) compared 30 methods of estimating the number of population clusters by using four hierarchical clustering methods. The three criteria that performed best in these simulation studies with a high degree of error in the data were a pseudo F statistic developed by Calinski and Harabasz (1974), a statistic referred to as $J_e(2)/J_e(1)$ by Duda and Hart (1973) that can be transformed into a pseudo t^2 statistic, and the cubic clustering criterion. The pseudo F statistic and the CCC are displayed by PROC FASTCLUS; these two statistics and the pseudo t^2 statistic, which can be applied only to hierarchical methods, are displayed by PROC CLUSTER. It might be advisable to look for consensus among the three statistics—that is, local peaks of the CCC and pseudo F statistic combined with a small value of the pseudo t^2 statistic and a larger pseudo t^2 for the next cluster fusion. It must be emphasized that these criteria are appropriate only for compact or slightly elongated clusters, preferably clusters that are roughly multivariate normal.

Recent research has tended to deemphasize mixture models in favor of nonparametric models in which clusters correspond to modes in the probability density function. Hartigan and Hartigan (1985) and Hartigan (1985b) developed a test of unimodality versus bimodality in the univariate case.

Nonparametric tests for the number of clusters can also be based on nonparametric density estimates. This approach requires much weaker assumptions than mixture models, namely, that the observations are sampled independently and that the distribution can be estimated nonparametrically. Silverman (1986) describes a bootstrap test for the number of modes using a Gaussian kernel density estimate, but problems have been reported with this method under the uniform null distribution. Further developments in nonparametric methods are given by Müller and Sawitzki (1991); Minnotte (1992); Polonik (1993). All of these methods suffer from heavy computational requirements.

One useful descriptive approach to the number-of-clusters problem is provided by Wong and Schaack (1982) based on a k th-nearest-neighbor density estimate. The k th-nearest-neighbor clustering method developed by Wong and Lane (1983) is applied with varying values of k . Each value of k yields an estimate of the number of modal clusters. If the estimated number of modal clusters is constant for a wide range of k values, there is strong evidence of at least that many modes in the population. A plot of the estimated number of modes against k can be highly informative. Attempts to derive a formal hypothesis test from this diagnostic plot have met with difficulties, but a simulation approach similar to Silverman (1986) does seem to work Girman (1994). The simulation, of course, requires considerable computer time.

PROC MODECLUS uses a less expensive approximate nonparametric test for the number of clusters. This test sacrifices statistical efficiency for computational efficiency. The method for conducting significance tests is described in the chapter on the MODECLUS procedure. This method has the following useful features:

- No distributional assumptions are required.
- The choice of smoothing parameter is not critical since you can try any number of different values.
- The data can be coordinates or distances.
- Time and space requirements for the significance tests are no worse than those for obtaining the clusters.
- The power is high enough to be useful for practical purposes.

The method for computing the p -values is based on a series of plausible approximations. There are as yet no rigorous proofs that the method is infallible. Neither are there any asymptotic results. However, simulations for sample sizes ranging from 20 to 2000 indicate that the p -values are almost always conservative. The only case discovered so far in which the p -values are liberal is a uniform distribution in one dimension for which the simulated error rates exceed the nominal significance level only slightly for a limited range of sample sizes.

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Chapter 12

Introduction to Scoring, Standardization, and Ranking Procedures

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Overview: Scoring, Standardization, and Ranking Procedures

Several SAS/STAT procedures are utilities that produce an output data set with new variables that are transformations of data in the input data set. SAS/STAT software includes four of these procedures. The RANK procedure produces rank scores across observations, the SCORE procedure constructs functions across the variables, and the STANDARD and STDIZE procedures transform each variable individually.

RANK	ranks the observations of each numeric variable and outputs ranks or rank scores. For a complete discussion of the RANK procedure, see the <i>Base SAS Procedures Guide: Statistical Procedures</i> .
SCORE	constructs new variables that are linear combinations of old variables according to a scoring data set. This procedure is used with the FACTOR procedure and other procedures that output scoring coefficients.
STANDARD	standardizes variables to a given mean and standard deviation. For a complete discussion of PROC STANDARD, see the <i>Base SAS Procedures Guide: Statistical Procedures</i> .
STDIZE	standardizes variables by subtracting a location measure and dividing by a scale measure. A variety of location and scale measures are provided. Such measures include the mean, median, Huber's estimate, Tukey's biweight estimate, and Andrew's wave estimate.

Chapter 13

Introduction to Survival Analysis Procedures

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Overview

Data that measure lifetime or the length of time until the occurrence of an event are called *lifetime*, *failure time*, or *survival* data. For example, variables of interest might be the lifetime of diesel engines, the length of time a person stay on a job, or the survival time for heart transplant patients. Such data have special considerations that must be incorporated into any analysis.

Survival data consist of a response (event time, failure time, or survival time) variable that measures the duration of time until a specified event occurs and possibly a set of independent variables thought to be associated with the failure time variable. These independent variables (concomitant variables, covariates, or prognostic factors) can be either discrete, such as sex or race, or continuous, such as age or temperature. The system that gives rise to the event of interest can be biological (as for most medical data) or physical (as for engineering data). The purpose of survival analysis is to model the underlying distribution of the failure time variable and to assess the dependence of the failure time variable on the independent variables.

An intrinsic characteristic of survival data is the possibility for censoring of observations (that is, the actual time until the event is not observed). Such censoring can arise from withdrawal from the experiment or termination of the experiment. Because the response is usually a duration, some of the possible events may not yet have occurred when the period for data collection has terminated. For example, clinical trials are conducted over a finite period of time with staggered entry of patients. That is, patients enter a clinical trial over time, and thus the length of follow-up varies by individuals; consequently, the time to the event may not be ascertained on all patients in the study. Additionally, some of the responses may be lost to follow-up (for example, a participant may move or refuse to continue to participate) before termination of data collection. In either case, only a lower bound on the failure time of the censored observations is known. These observations are said to be *right censored*. Thus, an additional variable is incorporated into the analysis to indicate which failure times are observed event times and which are censored times. More

generally, the failure time might only be known to be smaller than a given value (*left censored*) or known to be within a given interval (*interval censored*). There are numerous possible censoring schemes that arise in survival analysis. The monograph by Maddala (1983) discusses several related types of censoring situations, and the text by Kalbfleisch and Prentice (1980) also discusses several censoring schemes. Data with censored observations cannot be analyzed by ignoring the censored observations because, among other considerations, the longer-lived individuals are generally more likely to be right censored. The method of analysis must take the censoring into account and correctly use the censored observations as well as the uncensored observations.

Another characteristic of survival data is that the response cannot be negative. This suggests that a transformation of the survival time such as a log transformation might be necessary or that specialized methods might be more appropriate than those that assume a normal distribution for the error term. It is especially important to check any underlying assumptions as a part of the analysis because some of the models used are very sensitive to these assumptions.

Survival Analysis Procedures

There are four SAS procedures for analyzing survival data:

- The LIFEREG procedure is a parametric regression procedure for modeling the distribution of survival time with a set of concomitant variables.
- The LIFETEST procedure is a nonparametric procedure for estimating the survivor function, comparing the underlying survival curves of two or more samples, and testing the association of survival time with other variables.
- The PHREG procedure is a semiparametric procedure that fits the Cox proportional hazards model and its extensions.
- The SURVEYPHREG procedure is a Cox modeling procedure similar to PROC PHREG, appropriate for data collected from a survey sample.

The LIFEREG Procedure

The LIFEREG procedure fits parametric accelerated failure time models to survival data that may be left, right, or interval censored. The parametric model is of the form

$$y = \mathbf{x}'\boldsymbol{\beta} + \sigma\epsilon$$

where y is usually the log of the failure time variable, \mathbf{x} is a vector of covariate values, $\boldsymbol{\beta}$ is a vector of unknown regression parameters, σ is an unknown scale parameter, and ϵ is an error term. The baseline distribution of the error term can be specified as one of several possible distributions including (but not limited to) the log normal, log logistic, and Weibull distributions. Several texts that discuss these parametric models are Kalbfleisch and Prentice (1980); Lawless (1982); Nelson (1990); Meeker and Escobar (1998). For more information about PROC LIFEREG, see Chapter 51, “[The LIFEREG Procedure](#).”

The LIFETEST Procedure

The LIFETEST procedure computes nonparametric estimates of the survival distribution function. You can request either the product-limit (Kaplan and Meier 1958) or the life-table (actuarial) estimate of the distribution. The texts by Cox and Oakes (1984) and Kalbfleisch and Prentice (1980) provide good discussions of the product-limit estimator, and the texts by Lee (1992) and Elandt-Johnson and Johnson (1980) include detailed discussions of the life-table estimator. PROC LIFETEST computes nonparametric tests to compare the survival curves of two or more groups. The procedure also computes rank tests of association of the survival time variable with other concomitant variables as given in Kalbfleisch and Prentice (1980, Chapter 6). For more information about PROC LIFETEST, see Chapter 52, “[The LIFETEST Procedure](#).”

The PHREG Procedure

The PHREG procedure fits the proportional hazards model of Cox (1972, 1975) to survival data that might be right censored. The Cox model is a semiparametric model in which the hazard function of the survival time is given by

$$\lambda(t; \mathbf{x}) = \lambda_0(t)e^{\boldsymbol{\beta}'\mathbf{x}(t)}$$

where $\lambda_0(t)$ is an unspecified baseline hazard function, $\mathbf{x}(t)$ is a vector of covariate values (possibly time-dependent), and $\boldsymbol{\beta}$ is a vector of unknown regression parameters. The model is referred to as a semiparametric model because part of the model involves the unspecified baseline function over time (which has an infinite dimension) and the other part involves a finite number of regression parameters. Several texts that discuss the Cox regression models are Collett (1994); Cox and Oakes (1984); Kalbfleisch and Prentice (1980); Lawless (1982). Extensions of the Cox model are discussed in Therneau and Grambsch (2000); Andersen et al. (1992); Fleming and Harrington (1991). For more information about PROC PHREG, see Chapter 67, “[The PHREG Procedure](#).”

The SURVEYPHREG Procedure

The SURVEYPHREG procedure fits the Cox proportional hazards model for sample survey data. The procedure is similar to [the PHREG procedure](#), except that it incorporates complex sample design information in the analysis. The proportional hazards regression coefficients are estimated by maximizing a partial pseudo-log-likelihood function that incorporates the sampling weights. PROC SURVEYPHREG provides design-based variance estimates, confidence intervals, and tests for the estimated regression coefficients. For more information about PROC SURVEYPHREG, see Chapter 93, “[The SURVEYPHREG Procedure](#).”

Survival Analysis with SAS/STAT Procedures

The typical goal in survival analysis is to characterize the distribution of the survival time for a given population, to compare the survival distributions among different groups, or to study the relationship between the survival time and some concomitant variables.

A first step in the analysis of a set of survival data is to use PROC LIFETEST to compute and plot the estimate of the distribution of the survival time. In many applications, there are often several survival curves to compare. For example, you want to compare the survival experiences of patients who receive different treatments for their disease. The association between covariates and the survival time variable can be investigated by computing estimates of the survival distribution function within strata defined by the covariates. In particular, if the proportional hazards model is appropriate, the estimates of the log(-log(SURVIVAL)) plotted against the log(TIME) variable should give approximately parallel lines, where SURVIVAL is the survival distribution estimate and TIME is the failure time variable. Additionally, these lines should be approximately straight if the Weibull model is appropriate.

Statistics that test for association between failure time and covariates can be used to select covariates for further investigation. The LIFETEST procedure computes linear rank statistics using either Wilcoxon or log-rank scores. These statistics and their estimated covariance matrix can be used with the REG procedure with the option METHOD=RSQUARE to find the subset of variables that produce the largest joint test statistic for association. An illustration of this methodology is given in [Example 52.1](#) of Chapter 52, “The LIFETEST Procedure.”

Another approach to examining the relationship between the concomitant variables and survival time is through a regression model in which the survival time has a distribution that depends on the concomitant variables. The regression coefficients can be interpreted as describing the direction and strength of the relationship of each explanatory variable on the effect of the survival time.

In many biological systems, the Cox model might be a reasonable description of the relationship between the distribution of the survival time and the prognostic factors. You use PROC PHREG to fit the Cox regression model. The regression coefficient is interpreted as the increase of the log-hazard ratio resulting in the increase of one unit in the covariate. However, the underlying hazard function is left unspecified and, as in any other model, the results can be misleading if the proportional hazards assumptions do not hold.

Accelerated failure time models are popular for survival data of physical systems. In many cases, the underlying survival distribution is known empirically. You use PROC LIFEREG to fit these parametric models. Also, PROC LIFEREG can accommodate data with left-censored or interval-censored observations, which are not allowed in PROC PHREG.

A common technique for checking the validity of a regression model is to embed it in a larger model and use the likelihood ratio test to check whether the reduction to the actual model is valid. Other techniques include examining the residuals. Both PROC LIFEREG and PROC PHREG produce predicted values, residuals, and other computed values that can be used to assess the model adequacy.

Bayesian Survival Analysis with SAS/STAT Procedures

Bayesian analysis of survival models can be requested in the LIFEREG and PHREG procedures. In addition to the Cox model, PROC PHREG also allow you to fit a piecewise exponential model. In Bayesian analysis, the model parameters are treated as random variables, and inference about parameters is based on the posterior distribution of the parameters. A posterior distribution is a weighted likelihood function of the data with a prior distribution of the parameters using the Bayes theorem. The prior distribution enables you to incorporate into the analysis knowledge or experience of the likely range of values of the parameters of interest. You can specify normal or uniform prior distributions for the model regression coefficients in both LIFEREG and PHREG procedures. In addition, you can specify a gamma or improper prior distribution for

the scale or variance parameter in PROC LIFEREG. For the piecewise exponential model in PROC PHREG, you can specify normal or uniform prior distributions for the log-hazard parameters; alternatively, you can specify gamma or improper prior distributions for the hazards parameters. If you have no prior knowledge of the parameter values, you can use a noninformative prior distribution, and the results of a Bayesian analysis will be very similar to a classical analysis based on maximum likelihood.

A closed form of the posterior distribution is often not feasible, and a Markov chain Monte Carlo method by Gibbs sampling is used to simulate samples from the posterior distribution. You can perform inference by using the simulated samples, for example, to estimate the probability that a function of the parameters of interest lies within a specified range of values.

See Chapter 7, “[Introduction to Bayesian Analysis Procedures](#),” for an introduction to the basic concepts of Bayesian statistics. Also see “[Bayesian Analysis: Advantages and Disadvantages](#)” on page 132 for a discussion of the advantages and disadvantages of Bayesian analysis. See Ibrahim, Chen, and Sinha (2001); Gelman et al. (2004); Gilks, Richardson, and Spiegelhalter (1996) for more information about Bayesian analysis, including guidance about choosing prior distributions.

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Chapter 14

Introduction to Survey Sampling and Analysis Procedures

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Overview: Survey Sampling and Analysis Procedures

This chapter introduces the SAS/STAT procedures for survey sampling and describes how you can use these procedures to analyze survey data.

Researchers often use sample survey methodology to obtain information about a large population by selecting and measuring a sample from that population. Because of variability among items, researchers apply probability-based scientific designs to select the sample. This reduces the risk of a distorted view of the population and enables statistically valid inferences to be made from the sample. For more information about statistical sampling and analysis of complex survey data, see Lohr (2010); Kalton (1983); Cochran (1977); Kish (1965). To select probability-based random samples from a study population, you can use the SURVEYSELECT procedure, which provides a variety of methods for probability sampling. To analyze sample survey data, you can use the SURVEYMEANS, SURVEYFREQ, SURVEYREG, SURVEYLOGISTIC, and SURVEYPHREG procedures, which incorporate the sample design into the analyses.

Many SAS/STAT procedures, such as the MEANS, FREQ, GLM, LOGISTIC, and PHREG procedures, can compute sample means, produce crosstabulation tables, and estimate regression relationships. However, in most of these procedures, statistical inference is based on the assumption that the sample is drawn from an infinite population by simple random sampling. If the sample is in fact selected from a finite population by using a complex survey design, these procedures generally do not calculate the estimates and their variances according to the design actually used. Using analyses that are not appropriate for your sample design can lead to incorrect statistical inferences.

The SURVEYMEANS, SURVEYFREQ, SURVEYREG, SURVEYLOGISTIC, and SURVEYPHREG procedures properly analyze complex survey data by taking into account the sample design. These procedures can be used for multistage or single-stage designs, with or without stratification, and with or without unequal weighting. The survey analysis procedures provide a choice of variance estimation methods, which include Taylor series linearization, balanced repeated replication (BRR), and the jackknife.

Table 14.1 briefly describes the SAS/STAT sampling and analysis procedures.

Table 14.1 Survey Sampling and Analysis Procedures in SAS/STAT Software

PROC SURVEYSELECT	
<i>Selection Methods</i>	Simple random sampling (without replacement) Unrestricted random sampling (with replacement) Systematic Sequential Bernoulli Poisson Probability proportional to size (PPS) sampling, with and without replacement PPS systematic PPS for two units per stratum PPS sequential with minimum replacement
<i>Allocation Methods</i>	Proportional Optimal Neyman
<i>Sampling Tools</i>	Cluster sampling Replicated sampling Serpentine sorting
PROC SURVEYMEANS	
<i>Statistics</i>	Means and totals Proportions Quantiles Geometric means Ratios Standard errors Confidence limits
<i>Analyses</i>	Hypothesis tests Domain analysis Poststratification

Table 14.1 *continued*

PROC SURVEYFREQ	
<i>Tables</i>	One-way frequency tables Two-way and multiway crosstabulation tables Estimates of population totals and proportions Standard errors Confidence limits
<i>Analyses</i>	Tests of goodness of fit Tests of independence Risks and risk differences Odds ratios and relative risks
<i>Graphics</i>	Weighted frequency and percent plots Mosaic plots Odds ratio, relative risk, and risk difference plots
PROC SURVEYREG	
<i>Analyses</i>	Linear regression model fitting Regression coefficients Covariance matrices Confidence limits Hypothesis tests Estimable functions Contrasts Least squares means (LS-means) of effects Custom hypothesis tests among LS-means Regression with constructed effects Predicted values and residuals Domain analysis
PROC SURVEYLOGISTIC	
<i>Analyses</i>	Cumulative logit regression model fitting Logit, probit, and complementary log-log link functions Generalized logit regression model fitting Regression coefficients Covariance matrices Confidence limits Hypothesis tests Odds ratios Estimable functions Contrasts Least squares means (LS-means) of effects Custom hypothesis tests among LS-means Regression with constructed effects Model diagnostics Domain analysis

Table 14.1 *continued*

PROC SURVEYPHREG	
<i>Analyses</i>	Proportional hazards regression model fitting Breslow and Efron likelihoods Regression coefficients Covariance matrices Confidence limits Hypothesis tests Hazard ratios Contrasts Predicted values and standard errors Martingale, Schoenfeld, score, and deviance residuals Domain analysis

The Survey Procedures

The SURVEYSELECT procedure provides methods for probability sample selection. The SURVEYMEANS, SURVEYFREQ, SURVEYREG, SURVEYLOGISTIC, and SURVEYPHREG procedures provide statistical analyses for sample survey data. The following sections contain brief descriptions of these procedures. See the chapters on these procedures for more detailed information.

PROC SURVEYSELECT

The SURVEYSELECT procedure provides a variety of methods for selecting probability-based random samples. The procedure can select a simple random sample or can sample according to a complex multistage sample design that includes stratification, clustering, and unequal probabilities of selection. With probability sampling, each unit in the survey population has a known, positive probability of selection. This property of probability sampling avoids selection bias and enables you to use statistical theory to make valid inferences from the sample to the survey population.

PROC SURVEYSELECT provides methods for both equal probability sampling and probability proportional to size (PPS) sampling. In PPS sampling, a unit's selection probability is proportional to its size measure. PPS sampling is often used in cluster sampling, where you select clusters (groups of sampling units) of varying size in the first stage of selection. Available PPS methods include without replacement, with replacement, systematic, and sequential with minimum replacement. The procedure can apply these methods for stratified and replicated sample designs.

For stratified sampling, PROC SURVEYSELECT provides survey design methods to allocate the total sample size among the strata. Available allocation methods include proportional, Neyman, and optimal allocation. Optimal allocation maximizes the estimation precision within the available resources, taking into account stratum sizes, costs, and variances.

See Chapter 95, “The SURVEYSELECT Procedure,” for more information.

PROC SURVEYMEANS

The SURVEYMEANS procedure produces estimates of population means and totals from sample survey data. The procedure also computes estimates of proportions for categorical variables, estimates of quantiles for continuous variables, estimates of geometric means for positive continuous variables, and ratio estimates of means and proportions. For all these statistics, PROC SURVEYMEANS provides standard errors, confidence limits, and *t* tests when appropriate.

PROC SURVEYMEANS provides domain analysis, which computes estimates for domains (subpopulations), in addition to analysis for the entire study population. Formation of subpopulations can be unrelated to the sample design, and so the domain sample sizes can actually be random variables. Domain analysis takes this variability into account by using the entire sample to estimate the variance of domain estimates. Domain analysis is also known as subgroup analysis, subpopulation analysis, and subdomain analysis.

The SURVEYMEANS procedure can also apply poststratification for these analyses.

See Chapter 92, “The SURVEYMEANS Procedure,” for more information.

PROC SURVEYFREQ

The SURVEYFREQ procedure produces one-way to *n*-way frequency and crosstabulation tables from sample survey data. These tables include estimates of population totals, population proportions (overall proportions, and also row and column proportions), and corresponding standard errors. Confidence limits, coefficients of variation, and design effects are also available. The procedure provides the following types of design-adjusted confidence limits for proportions: Wald, logit, modified Wilson (score), and modified Clopper-Pearson (exact).

For one-way frequency tables, PROC SURVEYFREQ provides Rao-Scott chi-square goodness-of-fit tests, which are adjusted for the sample design. You can test a null hypothesis of equal proportions for a one-way frequency table, or you can input custom null hypothesis proportions for the test. For two-way frequency tables, PROC SURVEYFREQ provides design-adjusted tests of independence, or no association, between the row and column variables. These tests include the Rao-Scott chi-square test, the Rao-Scott likelihood ratio test, the Wald chi-square test, and the Wald log-linear chi-square test.

For 2×2 tables, PROC SURVEYFREQ computes estimates and confidence limits for risks (or row proportions), the risk difference, the odds ratio, and relative risks.

PROC SURVEYFREQ uses ODS Graphics to create graphs as part of its output. Available statistical graphics include weighted frequency and percent plots, mosaic plots, and odds ratio plots.

See Chapter 90, “The SURVEYFREQ Procedure,” for more information.

PROC SURVEYREG

The SURVEYREG procedure performs regression analysis for sample survey data. The procedure fits linear models and computes regression coefficients and their variance-covariance matrix. The procedure enables you to specify classification effects by using the same syntax as in the GLM procedure.

PROC SURVEYREG provides hypothesis tests for the model effects. The procedure also provides custom hypothesis tests for linear combinations of the regression parameters. The procedure computes confidence limits for the parameter estimates, and also for any specified linear functions of the regression parameters. The procedure can produce an output data set that contains the predicted values from the linear regression, their standard errors and confidence limits, and the residuals.

PROC SURVEYREG also performs regression analysis for domains (subpopulations).

See Chapter 94, “[The SURVEYREG Procedure](#),” for more information.

PROC SURVEYLOGISTIC

The SURVEYLOGISTIC procedure provides logistic regression analysis for sample survey data. Logistic regression analysis investigates the relationship between discrete responses and a set of explanatory variables. PROC SURVEYLOGISTIC fits linear logistic regression models for discrete response survey data by the method of maximum likelihood and incorporates the sample design into the analysis. The SURVEYLOGISTIC procedure enables you to specify categorical classification variables (also known as CLASS variables) as explanatory variables in the model by using the same syntax for main effects and interactions as in the GLM and LOGISTIC procedures.

The following link functions are available for regression in PROC SURVEYLOGISTIC: the cumulative logit function (CLOGIT), the generalized logit function (GLOGIT), the probit function (PROBIT), and the complementary log-log function (CLOGLOG). The procedure performs maximum likelihood estimation of the regression coefficients with either the Fisher scoring algorithm or the Newton-Raphson algorithm.

PROC SURVEYLOGISTIC also performs logistic regression analysis for domains (subpopulations).

See Chapter 91, “[The SURVEYLOGISTIC Procedure](#),” for more information.

PROC SURVEYPHREG

The SURVEYPHREG procedure performs regression analysis based on the Cox proportional hazards model for sample survey data. Cox’s semiparametric model is widely used in the analysis of survival data to estimate hazard rates when explanatory variables are available. The regression coefficients are estimated by maximizing a pseudo-partial-likelihood function that incorporates the sampling weights. The procedure provides design-based variance estimates, confidence intervals, and tests for the estimated regression coefficients.

PROC SURVEYPHREG provides hypothesis tests for the model effects. The procedure also provides custom hypothesis tests for linear combinations of the regression parameters. The procedure computes hazard ratios and their confidence limits. The procedure can produce several observation-level output statistics, such as predicted values and their standard errors, martingale residuals, Schoenfeld residuals, score residuals, and deviance residuals.

PROC SURVEYPHREG also performs proportional hazards regressions for domains (subpopulations).

See Chapter 93, “[The SURVEYPHREG Procedure](#),” for more information.

Survey Design Specification

Survey sampling is the process of selecting a probability-based sample from a finite population according to a sample design. You then collect data from these selected units and use them to estimate characteristics of the entire population.

A *sample design* encompasses the rules and operations by which you select sampling units from the population and the computation of sample statistics, which are estimates of the population values of interest. The objective of your survey often determines appropriate sample designs and valid data collection methodology. A complex sample design can include stratification, clustering, multiple stages of selection, and unequal weighting. The survey procedures can be used for single-stage designs or for multistage designs, with or without stratification, and with or without unequal weighting.

To analyze your survey data with the SURVEYMEANS, SURVEYFREQ, SURVEYREG, SURVEYLOGISTIC, and SURVEYPHREG procedures, you need to specify sample design information for the procedures. This information can include design strata, clusters, and sampling weights. All the survey analysis procedures use the same syntax for specifying sample design information. You provide sample design information with the STRATA, CLUSTER, and WEIGHT statements, and with the RATE= or TOTAL= option in the PROC statement.

If you provide replicate weights for BRR or jackknife variance estimation, you do not need to specify a STRATA or CLUSTER statement. Otherwise, you should specify STRATA and CLUSTER statements whenever your design includes stratification and clustering.

When there are clusters (PSUs) in the sample design, the procedures estimate variance by using the PSUs, as described in the section “[Variance Estimation](#)” on page 247. For a multistage sample design, the procedures use only the first stage of the sample design for variance estimation. Therefore, the required input includes only first-stage cluster (PSU) and first-stage stratum identification. You do not need to input design information about any additional stages of sampling.

The following sections provide brief descriptions of basic sample design concepts and terminology used in the survey procedures. For more detailed information, see Lohr (2010); Kalton (1983); Cochran (1977); Kish (1965).

Population

Population refers to the target population, which is the group of units (individuals or elements) of interest for study. Often, the primary objective is to estimate certain characteristics of this population, which are called *population values*. A *sampling unit* is an individual or element in the target population. A *sample* is a subset of the population that is selected for the study.

Before you use the survey procedures, you should have a well-defined target population, sampling units, and an appropriate sample design.

In order to select a sample according to your sample design, you need to have a list of sampling units in the population. This is called a *sampling frame*. PROC SURVEYSELECT uses probability-based selection methods to select a sample from a sampling frame.

Stratification

Stratified sampling involves selecting samples independently within strata, which are nonoverlapping subgroups of the survey population. Stratification controls the distribution of the sample size in the strata. It is widely used to meet a variety of survey objectives. For example, with stratification you can ensure adequate sample sizes for subgroups of interest, including small subgroups, or you can use stratification to improve the precision of overall estimates. To improve precision, units within strata should be as homogeneous as possible for the characteristics of interest.

Clustering

Cluster sampling involves selecting clusters, which are groups of sampling units. For example, clusters might be schools, hospitals, or geographical areas, and sampling units might be students, patients, or citizens. Cluster sampling can provide efficiency in frame construction and other survey operations. However, it can also result in a loss in precision of your estimates, compared to a nonclustered sample of the same size. To minimize this effect, units within clusters should be as heterogeneous as possible for the characteristics of interest.

Multistage Sampling

In *multistage sampling*, you select an initial (first-stage) sample that is based on groups of elements in the population, which are called *primary sampling units (PSUs)*.

Then you create a second-stage sample by drawing a subsample from each selected PSU in the first-stage sample. By repeating this operation, you can select a higher-stage sample. If you include all the elements from the selected primary sampling units, then the two-stage sample is a cluster sample.

Sampling Weights

Sampling weights, which are also known as *survey weights*, are positive values associated with the units in your sample. Ideally, the weight of a sampling unit should be the “frequency” that the sampling unit represents in the target population.

Often, sampling weights are the reciprocals of the selection probabilities for the sampling units. When you use PROC SURVEYSELECT, the procedure generates the sampling weight component for each stage of the design, and you can multiply these sampling weight components to obtain the final sampling weights. Sometimes, sampling weights also include nonresponse adjustments, poststratification, or regression adjustments by using supplemental information.

When the sampling units have unequal weights, you must provide the weights to the survey analysis procedures. If you do not specify sampling weights, the procedures use equal weights in the analyses.

Population Totals and Sampling Rates

If you use Taylor series variance estimation, the survey procedures include a finite population correction factor in the analysis if you input either the sampling rate or the population total.

The sampling rate is the ratio of the sample size (the number of sampling units in the sample) n to the population size (the total number of sampling units in the target population) N , $f = n/N$. This ratio is also called the *sampling fraction*. If you select a sample without replacement, the extra efficiency compared to selecting a sample with replacement can be measured by the *finite population correction* (*fpc*) factor, $(1-f)$.

To include a finite population correction factor in your analysis, you can input either the sampling rate or the population total. Otherwise, the procedures do not use the *fpc* in computing variance estimates. For fairly small sampling fractions, it is appropriate to ignore this correction. See Cochran (1977) and Kish (1965) for details.

As discussed in the section “[Variance Estimation](#)” on page 247, for a multistage sample design, the procedures use only the first stage of the sample design for variance estimation. Therefore, if you are specifying the sampling rate, you should input the *first-stage sampling rate*, which is the ratio of the number of PSUs in the sample to the total number of PSUs in the target population.

If you use BRR or jackknife variance estimate, the procedures do not include a finite population correction in the analysis, and you do not need to input the sampling rate or the population total.

Variance Estimation

The survey analysis procedures provide a choice of variance estimation methods for complex survey designs. In addition to the Taylor series linearization method, the procedures offer two replication-based (resampling) methods—balanced repeated replication (BRR) and the delete-1 jackknife. These variance estimation methods usually give similar, satisfactory results (Lohr 2010; Särndal, Swensson, and Wretman 1992; Wolter 2007). The choice of a variance estimation method can depend on the sample design used, the sample design information available, the parameters to be estimated, and computational issues. See Lohr (2010) for more details.

The Taylor series linearization method is appropriate for all designs where the first-stage sample is selected with replacement, or where the first-stage sampling fraction is small, as it often is in practice. The Taylor series method obtains a linear approximation for the estimator and then uses the variance estimate for this approximation to estimate the variance of the estimate itself (Fuller 1975; Woodruff 1971). When there are clusters (PSUs) in the sample design, the procedures estimate the variance from the variation among the PSUs. When the design is stratified, the procedures pool stratum variance estimates to compute the overall variance estimate.

For a multistage sample design, the Taylor series method uses only the first stage of the sample design. Therefore, the required input includes only first-stage cluster (PSU) and first-stage stratum identification. You do not need to input design information about any additional stages of sampling.

Replication methods for variance estimation draw multiple replicates (or subsamples) from the full sample by following a specific resampling scheme. Commonly used resampling schemes include *balanced repeated*

replication (BRR) and the *jackknife*. The parameter of interest is estimated from each replicate, and the variability among the replicate estimates is used to estimate the overall variance of the parameter estimate.

The BRR variance estimation method requires a stratified sample design with two PSUs in each stratum. Each replicate is obtained by deleting one PSU per stratum according to the corresponding Hadamard matrix and adjusting the original weights for the remaining PSUs. The adjusted weights are called *replicate weights*. The survey procedures also provide Fay's method, which is a modification of the BRR method.

The jackknife method deletes one PSU at a time from the full sample to create replicates, and modifies the original weights to obtain replicate weights. The total number of replicates equals the number of PSUs. If the sample design is stratified, each stratum must contain at least two PSUs, and the jackknife is applied separately within each stratum.

Instead of having the survey procedures generate replicate weights for the analysis, you can directly input your own replicate weights. This can be useful if you need to do multiple analyses with the same set of replicate weights, or if you have access to replicate weights without complete design information.

See the chapters on the survey procedures for complete details. For more information about variance estimation for sample survey data, see Lohr (2010); Wolter (2007); Särndal, Swensson, and Wretman (1992); Lee, Forthoffer, and Lorimor (1989); Cochran (1977); Kish (1965); Hansen, Hurwitz, and Madow (1953).

Example: Survey Sampling and Analysis Procedures

This section demonstrates how you can use the survey procedures to select a probability-based sample and then analyze the survey data to make inferences about the population. The analyses include descriptive statistics and regression analysis. This example is a survey of income and expenditures for a group of households in North Carolina and South Carolina. The goals of the survey are as follows:

- Estimate total income and total living expenses
- Estimate the median income and the median living expenses
- Investigate the linear relationship between income and living expenses

Sample Selection

To select a sample with PROC SURVEYSELECT, you input a SAS data set that contains the sampling frame (the list of units from which the sample is to be selected). You also specify the selection method, the desired sample size or sampling rate, and other selection parameters. PROC SURVEYSELECT selects the sample and produces an output data set that contains the selected units, their selection probabilities, and their sampling weights. See Chapter 95, “[The SURVEYSELECT Procedure](#),” for more information about PROC SURVEYSELECT.

In this example, the sample design is a stratified sample design, with households as the sampling units and selection by simple random sampling. The SAS data set HHFrame contains the sampling frame, which is the list of households in the survey population. The sampling frame is stratified by the variables State

and Region. Within strata, households are selected by simple random sampling. The following PROC SURVEYSELECT statements select a probability sample of households according to this sample design:

```
proc surveyselect data=HHFrame out=HHSample
                 method=srs n=(3, 5, 3, 6, 2);
  strata State Region;
run;
```

The STRATA statement names the stratification variables State and Region. In the PROC SURVEYSELECT statement, the DATA= option names the SAS data set HHFrame as the input data set (or sampling frame) from which to select the sample. The OUT= option stores the sample in the SAS data set named HHSample. The METHOD=SRS option specifies simple random sampling as the sample selection method. The N= option specifies the stratum sample sizes.

The SURVEYSELECT procedure then selects a stratified random sample of households and produces the output data set HHSample, which contains the selected households together with their selection probabilities and sampling weights. The data set HHSample also contains the sampling unit identification variable Id and the stratification variables State and Region from the input data set HHFrame.

Survey Data Analysis

You can use the SURVEYMEANS and SURVEYREG procedures to estimate population values and perform regression analyses for survey data. The following example briefly shows the capabilities of these procedures. See Chapter 92, “The SURVEYMEANS Procedure,” and Chapter 94, “The SURVEYREG Procedure,” for more information.

The following PROC SURVEYMEANS statements estimate the total income and living expenses for the survey population based on the data from the stratified sample design:

```
proc surveymeans data=HHSample sum median;
  var Income Expense;
  strata State Region;
  weight Weight;
run;
```

The PROC SURVEYMEANS statement invokes the procedure, and the DATA= option names the SAS data set HHSample as the input data set to be analyzed. The keywords SUM and MEDIAN request estimates of population totals and medians.

The VAR statement specifies the two analysis variables Income and Expense. The STRATA statement names the stratification variables State and Region. The WEIGHT statement specifies the sampling weight variable Weight.

You can use PROC SURVEYREG to perform regression analysis for survey data. Suppose that, in order to explore the relationship between household income and living expenses in the survey population, you choose the following linear model:

$$\text{Expense} = \alpha + \beta * \text{Income} + \text{error}$$

The following PROC SURVEYREG statements fit this linear model for the survey population based on the data from the stratified sample design:

```
proc surveyreg data=HHSample;
  strata State Region ;
  model Expense = Income;
  weight Weight;
run;
```

The STRATA statement names the stratification variables State and Region. The MODEL statement specifies the model, with Expense as the dependent variable and Income as the independent variable. The WEIGHT statement specifies the sampling weight variable Weight.

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Chapter 15

The Four Types of Estimable Functions

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Overview

Many regression and analysis of variance procedures in SAS/STAT label tests for various effects in the model as Type I, Type II, Type III, or Type IV. These four types of hypotheses might not always be sufficient for a statistician to perform all desired inferences, but they should suffice for the vast majority of analyses. This chapter explains the hypotheses involved in each of the four test types. For additional discussion, see Freund, Littell, and Spector (1991) or Milliken and Johnson (1984).

The primary context of the discussion is testing linear hypotheses in least squares regression and analysis of variance, such as with PROC GLM. In this context, tests correspond to hypotheses about linear functions of the true parameters and are evaluated using sums of squares of the estimated parameters. Thus, there will be frequent references to Type I, II, III, and IV (estimable) functions and corresponding Type I, II, III, and IV sums of squares, or simply SS.

Estimability

Given a response or dependent variable Y , predictors or independent variables X , and a linear expectation model $E[Y] = X\beta$ relating the two, a primary analytical goal is to estimate or test for the significance of certain linear combinations of the elements of β . For least squares regression and analysis of variance, this is accomplished by computing linear combinations of the observed Y s. An unbiased linear estimate of a specific linear function of the individual β s, say $L\beta$, is a linear combination of the Y s that has an expected value of $L\beta$. Hence, the following definition:

A linear combination of the parameters $\mathbf{L}\boldsymbol{\beta}$ is estimable if and only if a linear combination of the \mathbf{Y} s exists that has expected value $\mathbf{L}\boldsymbol{\beta}$.

Any linear combination of the \mathbf{Y} s, for instance \mathbf{KY} , will have expectation $E[\mathbf{KY}] = \mathbf{KX}\boldsymbol{\beta}$. Thus, the expected value of any linear combination of the \mathbf{Y} s is equal to that same linear combination of the rows of \mathbf{X} multiplied by $\boldsymbol{\beta}$. Therefore,

$\mathbf{L}\boldsymbol{\beta}$ is estimable if and only if there is a linear combination of the rows of \mathbf{X} that is equal to \mathbf{L} —that is, if and only if there is a \mathbf{K} such that $\mathbf{L} = \mathbf{KX}$.

Thus, the rows of \mathbf{X} form a generating set from which any estimable \mathbf{L} can be constructed. Since the row space of \mathbf{X} is the same as the row space of $\mathbf{X}'\mathbf{X}$, the rows of $\mathbf{X}'\mathbf{X}$ also form a generating set from which all estimable \mathbf{L} s can be constructed. Similarly, the rows of $(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{X}$ also form a generating set for \mathbf{L} .

Therefore, if \mathbf{L} can be written as a linear combination of the rows of \mathbf{X} , $\mathbf{X}'\mathbf{X}$, or $(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{X}$, then $\mathbf{L}\boldsymbol{\beta}$ is estimable.

In the context of least squares regression and analysis of variance, an estimable linear function $\mathbf{L}\boldsymbol{\beta}$ can be estimated by $\mathbf{L}\hat{\boldsymbol{\beta}}$, where $\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$. From the general theory of linear models, the unbiased estimator $\mathbf{L}\hat{\boldsymbol{\beta}}$ is, in fact, the *best* linear unbiased estimator of $\mathbf{L}\boldsymbol{\beta}$, in the sense of having minimum variance as well as maximum likelihood when the residuals are normal. To test the hypothesis that $\mathbf{L}\boldsymbol{\beta} = \mathbf{0}$, compute the sum of squares

$$SS(H_0: \mathbf{L}\boldsymbol{\beta} = \mathbf{0}) = (\mathbf{L}\hat{\boldsymbol{\beta}})'(\mathbf{L}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{L}')^{-1}\mathbf{L}\hat{\boldsymbol{\beta}}$$

and form an F test with the appropriate error term. Note that in contexts more general than least squares regression (for example, generalized and/or mixed linear models), linear hypotheses are often tested by analogous sums of squares of the estimated linear parameters $(\mathbf{L}\hat{\boldsymbol{\beta}})'(\text{Var}[\mathbf{L}\hat{\boldsymbol{\beta}}])^{-1}\mathbf{L}\hat{\boldsymbol{\beta}}$.

General Form of an Estimable Function

This section demonstrates a shorthand technique for displaying the generating set for any estimable \mathbf{L} . Suppose

$$\mathbf{X} = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \end{bmatrix} \quad \text{and} \quad \boldsymbol{\beta} = \begin{bmatrix} \mu \\ A_1 \\ A_2 \\ A_3 \end{bmatrix}$$

\mathbf{X} is a generating set for \mathbf{L} , but so is the smaller set

$$\mathbf{X}^* = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix}$$

\mathbf{X}^* is formed from \mathbf{X} by deleting duplicate rows.

Since all estimable \mathbf{L} s must be linear functions of the rows of \mathbf{X}^* for $\mathbf{L}\boldsymbol{\beta}$ to be estimable, an \mathbf{L} for a single-degree-of-freedom estimate can be represented symbolically as

$$L1 \times (1 \ 1 \ 0 \ 0) + L2 \times (1 \ 0 \ 1 \ 0) + L3 \times (1 \ 0 \ 0 \ 1)$$

or

$$\mathbf{L} = (L1 + L2 + L3, L1, L2, L3)$$

For this example, $\mathbf{L}\boldsymbol{\beta}$ is estimable if and only if the first element of \mathbf{L} is equal to the sum of the other elements of \mathbf{L} or if

$$\mathbf{L}\boldsymbol{\beta} = (L1 + L2 + L3) \times \mu + L1 \times A_1 + L2 \times A_2 + L3 \times A_3$$

is estimable for any values of $L1$, $L2$, and $L3$.

If other generating sets for \mathbf{L} are represented symbolically, the symbolic notation looks different. However, the inherent nature of the rules is the same. For example, if row operations are performed on \mathbf{X}^* to produce an identity matrix in the first 3×3 submatrix of the resulting matrix

$$\mathbf{X}^{**} = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & -1 \\ 0 & 0 & 1 & -1 \end{bmatrix}$$

then \mathbf{X}^{**} is also a generating set for \mathbf{L} . An estimable \mathbf{L} generated from \mathbf{X}^{**} can be represented symbolically as

$$\mathbf{L} = (L1, L2, L3, L1 - L2 - L3)$$

Note that, again, the first element of \mathbf{L} is equal to the sum of the other elements.

With multiple generating sets available, the question arises as to which one is the best to represent \mathbf{L} symbolically. Clearly, a generating set containing a minimum of rows (of full row rank) and a maximum of zero elements is desirable.

The generalized g_2 -inverse $(\mathbf{X}'\mathbf{X})^-$ of $\mathbf{X}'\mathbf{X}$ computed by the modified sweep operation (Goodnight 1979) has the property that $(\mathbf{X}'\mathbf{X})^- \mathbf{X}'\mathbf{X}$ usually contains numerous zeros. For this reason, in PROC GLM the nonzero rows of $(\mathbf{X}'\mathbf{X})^- \mathbf{X}'\mathbf{X}$ are used to represent \mathbf{L} symbolically.

If the generating set represented symbolically is of full row rank, the number of symbols ($L1, L2, \dots$) represents the maximum rank of any testable hypothesis (in other words, the maximum number of linearly independent rows for any \mathbf{L} matrix that can be constructed). By letting each symbol in turn take on the value of 1 while the others are set to 0, the original generating set can be reconstructed.

Introduction to Reduction Notation

Reduction notation can be used to represent differences in sums of squares (SS) for two models. The notation $R(\mu, A, B, C)$ denotes the complete main-effects model for effects A , B , and C . The notation

$$R(A \mid \mu, B, C)$$

denotes the difference between the model SS for the complete main-effects model containing A , B , and C and the model SS for the reduced model containing only B and C .

In other words, this notation represents the differences in model SS produced by


```
proc glm;
  class a b c;
  model y = a b c;
run;
```

and

```
proc glm;
  class b c;
  model y = b c;
run;
```

As another example, consider a regression equation with four independent variables. The notation $R(\beta_3, \beta_4 | \beta_1, \beta_2)$ denotes the differences in model SS between

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \epsilon$$

and

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \epsilon$$

This is the difference in the model SS for the models produced, respectively, by

```
model y = x1 x2 x3 x4;
```

and

```
model y = x1 x2;
```

The following examples demonstrate the ability to manipulate the symbolic representation of a generating set. Note that any operations performed on the symbolic notation have corresponding row operations that are performed on the generating set itself.

Examples

A One-Way Classification Model

For the model

$$Y = \mu + A_i + \epsilon \quad i = 1, 2, 3$$

the general form of estimable functions $\mathbf{L}\boldsymbol{\beta}$ is (from the previous example)

$$\mathbf{L}\boldsymbol{\beta} = L1 \times \mu + L2 \times A_1 + L3 \times A_2 + (L1 - L2 - L3) \times A_3$$

Thus,

$$\mathbf{L} = (L1, L2, L3, L1 - L2 - L3)$$

Tests involving only the parameters A_1 , A_2 , and A_3 must have an \mathbf{L} of the form

$$\mathbf{L} = (0, L2, L3, -L2 - L3)$$

Since this \mathbf{L} for the A parameters involves only two symbols, hypotheses with at most two degrees of freedom can be constructed. For example, letting $(L2, L3)$ be $(1, 0)$ and $(0, 1)$, respectively, yields

$$\mathbf{L} = \begin{bmatrix} 0 & 1 & 0 & -1 \\ 0 & 0 & 1 & -1 \end{bmatrix}$$

The preceding \mathbf{L} can be used to test the hypothesis that $A_1 = A_2 = A_3$. For this example, any \mathbf{L} with two linearly independent rows with column 1 equal to zero produces the same sum of squares. For example, a joint test for linear and quadratic effects of A

$$\mathbf{L} = \begin{bmatrix} 0 & 1 & 0 & -1 \\ 0 & 1 & -2 & 1 \end{bmatrix}$$

gives the same SS. In fact, for any \mathbf{L} of full row rank and any nonsingular matrix \mathbf{K} of conformable dimensions,

$$SS(H_0: \mathbf{L}\boldsymbol{\beta} = 0) = SS(H_0: \mathbf{KL}\boldsymbol{\beta} = 0)$$

A Three-Factor Main-Effects Model

Consider a three-factor main-effects model involving the CLASS variables A , B , and C , as shown in Table 15.1.

Table 15.1 Three-Factor Main-Effects Model

Obs	A	B	C
1	1	2	1
2	1	1	2
3	2	1	3
4	2	2	2
5	2	2	2

The general form of an estimable function is shown in Table 15.2.

Table 15.2 General Form of an Estimable Function for Three-Factor Main-Effects Model

Parameter	Coefficient
μ (Intercept)	$L1$
$A1$	$L2$
$A2$	$L1 - L2$
$B1$	$L4$
$B2$	$L1 - L4$
$C1$	$L6$
$C2$	$L1 + L2 - L4 - 2 \times L6$
$C3$	$-L2 + L4 + L6$

Since only four symbols ($L1$, $L2$, $L4$, and $L6$) are involved, any testable hypothesis will have at most four degrees of freedom. If you form an \mathbf{L} matrix with four linearly independent rows according to the preceding

rules, then testing $L\beta = 0$ is equivalent to testing that $E[Y]$ is uniformly 0. Symbolically,

$$SS(H_0: L\beta = 0) = R(\mu, A, B, C)$$

In a main-effects model, the usual hypothesis of interest for a main effect is the equality of all the parameters. In this example, it is not possible to unambiguously test such a hypothesis because of confounding: any test for the equality of the parameters for any one of A , B , or C will necessarily involve the parameters for the other two effects. One way to proceed is to construct a maximum rank hypothesis (MRH) involving only the parameters of the main effect in question. This can be done using the general form of estimable functions. Note the following:

- To get an MRH involving only the parameters of A , the coefficients of L associated with μ , $B1$, $B2$, $C1$, $C2$, and $C3$ must be equated to zero. Starting at the top of the general form, let $L1 = 0$, then $L4 = 0$, then $L6 = 0$. If $C2$ and $C3$ are not to be involved, then $L2$ must also be zero. Thus, $A1 - A2$ is not estimable; that is, the MRH involving only the A parameters has zero rank and $R(A | \mu, B, C) = 0$.
- To obtain the MRH involving only the B parameters, let $L1 = L2 = L6 = 0$. But then to remove $C2$ and $C3$ from the comparison, $L4$ must also be set to 0. Thus, $B1 - B2$ is not estimable and $R(B | \mu, A, C) = 0$.
- To obtain the MRH involving only the C parameters, let $L1 = L2 = L4 = 0$. Thus, the MRH involving only C parameters is

$$C1 - 2 \times C2 + C3 = K \quad (\text{for any } K)$$

or any multiple of the left-hand side equal to K . Furthermore,

$$SS(H_0: C1 - 2 \times C2 + C3 = 0) = R(C | \mu, A, B)$$

A Multiple Regression Model

Suppose

$$E[Y] = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3$$

where the $X'X$ matrix has full rank. The general form of estimable functions is as shown in Table 15.3.

Table 15.3 General Form of Estimable Functions for a Multiple Regression Model When $X'X$ Matrix Is of Full Rank

Parameter	Coefficient
β_0	$L1$
β_1	$L2$
β_2	$L3$
β_3	$L4$

For example, to test the hypothesis that $\beta_2 = 0$, let $L1 = L2 = L4 = 0$ and let $L3 = 1$. Then $SS(L\beta = 0) = R(\beta_2 | \beta_0, \beta_1, \beta_3)$. In this full-rank case, all parameters, as well as any linear combination of parameters, are estimable.

Suppose, however, that $X3 = 2x_1 + 3x_2$. The general form of estimable functions is shown in Table 15.4.

Table 15.4 General Form of Estimable Functions for a Multiple Regression Model When $\mathbf{X}'\mathbf{X}$ Matrix Is Not of Full Rank

Parameter	Coefficient
β_0	$L1$
β_1	$L2$
β_2	$L3$
β_3	$2 \times L2 + 3 \times L3$

For this example, it is possible to test $H_0: \beta_0 = 0$. However, β_1 , β_2 , and β_3 are not jointly estimable; that is,

$$R(\beta_1 | \beta_0, \beta_2, \beta_3) = 0$$

$$R(\beta_2 | \beta_0, \beta_1, \beta_3) = 0$$

$$R(\beta_3 | \beta_0, \beta_1, \beta_2) = 0$$

Estimable Functions

Type I SS and Estimable Functions

In PROC GLM, the Type I SS and the associated hypotheses they test are byproducts of the modified sweep operator used to compute a generalized g_2 -inverse of $\mathbf{X}'\mathbf{X}$ and a solution to the normal equations. For the model $E[Y] = x_1\beta_1 + x_2\beta_2 + x_3\beta_3$, the Type I SS for each effect are as follows:

Effect	Type I SS
x_1	$R(\beta_1)$
x_2	$R(\beta_2 \beta_1)$
x_3	$R(\beta_3 \beta_1, \beta_2)$

Note that some other SAS/STAT procedures compute Type I hypotheses by sweeping $\mathbf{X}'\mathbf{X}$ (for example, PROC MIXED and PROC GLIMMIX), but their test statistics are not necessarily equivalent to the results of using those procedures to fit models that contain successively more effects.

The Type I SS are model-order dependent; each effect is adjusted only for the preceding effects in the model.

There are numerous ways to obtain a Type I hypothesis matrix \mathbf{L} for each effect. One way is to form the $\mathbf{X}'\mathbf{X}$ matrix and then reduce $\mathbf{X}'\mathbf{X}$ to an upper triangular matrix by row operations, skipping over any rows with a zero diagonal. The nonzero rows of the resulting matrix associated with x_1 provide an \mathbf{L} such that

$$SS(H_0: \mathbf{L}\boldsymbol{\beta} = \mathbf{0}) = R(\beta_1)$$

The nonzero rows of the resulting matrix associated with x_2 provide an \mathbf{L} such that

$$SS(H_0: \mathbf{L}\boldsymbol{\beta} = \mathbf{0}) = R(\beta_2 | \beta_1)$$

The last set of nonzero rows (associated with x_3) provide an \mathbf{L} such that

$$SS(H_0: \mathbf{L}\boldsymbol{\beta} = \mathbf{0}) = R(\beta_3 | \beta_1, \beta_2)$$

Another more formalized representation of Type I generating sets for x_1 , x_2 , and x_3 , respectively, is

$$\begin{aligned} \mathbf{G}_1 &= (\mathbf{X}'_1\mathbf{X}_1 \mid \mathbf{X}'_1\mathbf{X}_2 \mid \mathbf{X}'_1\mathbf{X}_3) \\ \mathbf{G}_2 &= (\quad 0 \mid \mathbf{X}'_2\mathbf{M}_1\mathbf{X}_2 \mid \mathbf{X}'_2\mathbf{M}_1\mathbf{X}_3) \\ \mathbf{G}_3 &= (\quad 0 \mid \quad 0 \mid \mathbf{X}'_3\mathbf{M}_2\mathbf{X}_3) \end{aligned}$$

where

$$\mathbf{M}_1 = \mathbf{I} - \mathbf{X}_1(\mathbf{X}'_1\mathbf{X}_1)^{-1}\mathbf{X}'_1$$

and

$$\mathbf{M}_2 = \mathbf{M}_1 - \mathbf{M}_1\mathbf{X}_2(\mathbf{X}'_2\mathbf{M}_1\mathbf{X}_2)^{-1}\mathbf{X}'_2\mathbf{M}_1$$

Using the Type I generating set \mathbf{G}_2 (for example), if an \mathbf{L} is formed from linear combinations of the rows of \mathbf{G}_2 such that \mathbf{L} is of full row rank and of the same row rank as \mathbf{G}_2 , then $SS(H_0: \mathbf{L}\boldsymbol{\beta} = \mathbf{0}) = R(\beta_2 | \beta_1)$.

In the GLM procedure, the Type I estimable functions displayed symbolically when the E1 option is requested are

$$\begin{aligned} \mathbf{G}_1^* &= (\mathbf{X}'_1\mathbf{X}_1)^{-1}\mathbf{G}_1 \\ \mathbf{G}_2^* &= (\mathbf{X}'_2\mathbf{M}_1\mathbf{X}_2)^{-1}\mathbf{G}_2 \\ \mathbf{G}_3^* &= (\mathbf{X}'_3\mathbf{M}_2\mathbf{X}_3)^{-1}\mathbf{G}_3 \end{aligned}$$

As can be seen from the nature of the generating sets \mathbf{G}_1 , \mathbf{G}_2 , and \mathbf{G}_3 , only the Type I estimable functions for β_3 are guaranteed not to involve the β_1 and β_2 parameters. The Type I hypothesis for β_2 can (and often does) involve β_3 parameters, and likewise the Type I hypothesis for β_1 often involves β_2 and β_3 parameters.

There are, however, a number of models for which the Type I hypotheses are considered appropriate. These are as follows:

- balanced ANOVA models specified in proper sequence (that is, interactions do not precede main effects in the MODEL statement and so forth)
- purely nested models (specified in the proper sequence)
- polynomial regression models (in the proper sequence)

Type II SS and Estimable Functions

For main-effects models and regression models, the general form of estimable functions can be manipulated to provide tests of hypotheses involving only the parameters of the effect in question. The same result can also be obtained by entering each effect in turn as the last effect in the model and obtaining the Type I SS for that effect. These are the *Type II SS*. Using a modified reversible sweep operator, it is possible to obtain the Type II SS without actually refitting the model.

Thus, the **Type II SS correspond to the R notation in which each effect is adjusted for all other appropriate effects**. For a regression model such as

$$E[Y] = x_1\beta_1 + x_2\beta_2 + x_3\beta_3$$

the Type II SS correspond to

Effect	Type II SS
x_1	$R(\beta_1 \mid \beta_2, \beta_3)$
x_2	$R(\beta_2 \mid \beta_1, \beta_3)$
x_3	$R(\beta_3 \mid \beta_1, \beta_2)$

For a main-effects model (A , B , and C as classification variables), the Type II SS correspond to

Effect	Type II SS
A	$R(A \mid B, C)$
B	$R(B \mid A, C)$
C	$R(C \mid A, B)$

As the discussion in the section “[A Three-Factor Main-Effects Model](#)” on page 255 indicates, for regression and main-effects models the Type II SS provide an MRH for each effect that does not involve the parameters of the other effects.

In order to see what effects are appropriate to adjust for in computing Type II estimable functions, note that for models involving interactions and nested effects, in the absence of a priori parametric restrictions, it is not possible to obtain a test of a hypothesis for a main effect free of parameters of higher-level interactions effects with which the main effect is involved. It is reasonable to assume, then, that any test of a hypothesis concerning an effect should involve the parameters of that effect and only those other parameters with which that effect is involved. The concept of effect containment helps to define this involvement.

Contained Effect

Given two effects $F1$ and $F2$, $F1$ is said to be *contained in* $F2$ provided that the following two conditions are met:

- Both effects involve the same continuous variables (if any).
- $F2$ has more CLASS variables than $F1$ does, and if $F1$ has CLASS variables, they all appear in $F2$.

Note that the intercept effect μ is contained in all pure CLASS effects, but it is not contained in any effect involving a continuous variable. No effect is contained by μ .

Type II, Type III, and Type IV estimable functions rely on this definition, and they all have one thing in common: the estimable functions involving an effect FI also involve the parameters of all effects that contain FI , and they do not involve the parameters of effects that do not contain FI (other than FI).

Hypothesis Matrix for Type II Estimable Functions

The Type II estimable functions for an effect FI have an \mathbf{L} (before reduction to full row rank) of the following form:

- All columns of \mathbf{L} associated with effects not containing FI (except FI) are zero.
- The submatrix of \mathbf{L} associated with effect FI is $(\mathbf{X}'_1\mathbf{M}\mathbf{X}_1)^-(\mathbf{X}'_1\mathbf{M}\mathbf{X}_1)$.
- Each of the remaining submatrices of \mathbf{L} associated with an effect $F2$ that contains FI is $(\mathbf{X}'_1\mathbf{M}\mathbf{X}_1)^-(\mathbf{X}'_1\mathbf{M}\mathbf{X}_2)$.

In these submatrices,

$$\begin{aligned} \mathbf{X}_0 &= \text{the columns of } \mathbf{X} \text{ whose associated effects do not contain } FI \\ \mathbf{X}_1 &= \text{the columns of } \mathbf{X} \text{ associated with } FI \\ \mathbf{X}_2 &= \text{the columns of } \mathbf{X} \text{ associated with an } F2 \text{ effect that contains } FI \\ \mathbf{M} &= \mathbf{I} - \mathbf{X}_0(\mathbf{X}'_0\mathbf{X}_0)^-\mathbf{X}'_0 \end{aligned}$$

For the model

```
class A B;
model Y = A B A*B;
```

the Type II SS correspond to

$$R(A \mid \mu, B), \quad R(B \mid \mu, A), \quad R(A * B \mid \mu, A, B)$$

for effects A , B , and $A * B$, respectively. For the model

```
class A B C;
model Y = A B(A) C(A B);
```

the Type II SS correspond to

$$R(A \mid \mu), \quad R(B(A) \mid \mu, A), \quad R(C(AB) \mid \mu, A, B(A))$$

for effects A , $B(A)$ and $C(A B)$, respectively. For the model

```
model Y = x x*x;
```

the Type II SS correspond to

$$R(X \mid \mu, X * X) \text{ and } R(X * X \mid \mu, X)$$

for x and $x * x$, respectively.

Note that, as in the situation for Type I tests, PROC MIXED and PROC GLIMMIX compute Type I hypotheses by sweeping $X'X$, but their test statistics are not necessarily equivalent to the results of sequentially fitting with those procedures models that contain successively more effects; while PROC TRANSREG computes tests labeled as being Type II by leaving out each effect in turn, but the specific linear hypotheses associated with these tests might not be precisely the same as the ones derived from successively sweeping $X'X$.

Example of Type II Estimable Functions

For a 2×2 factorial with w observations per cell, the general form of estimable functions is shown in Table 15.5. Any nonzero values for $L2$, $L4$, and $L6$ can be used to construct L vectors for computing the Type II SS for A , B , and $A * B$, respectively.

Table 15.5 General Form of Estimable Functions for 2×2 Factorial

Effect	Coefficient
μ	$L1$
$A1$	$L2$
$A2$	$L1 - L2$
$B1$	$L4$
$B2$	$L1 - L4$
$AB11$	$L6$
$AB12$	$L2 - L6$
$AB21$	$L4 - L6$
$AB22$	$L1 - L2 - L4 + L6$

For a balanced 2×2 factorial with the same number of observations in every cell, the Type II estimable functions are shown in Table 15.6.

Table 15.6 Type II Estimable Functions for Balanced 2×2 Factorial

Effect	Coefficients for Effect		
	A	B	$A * B$
μ	0	0	0
$A1$	$L2$	0	0
$A2$	$-L2$	0	0
$B1$	0	$L4$	0
$B2$	0	$-L4$	0
$AB11$	$0.5 \times L2$	$0.5 \times L4$	$L6$
$AB12$	$0.5 \times L2$	$-0.5 \times L4$	$-L6$
$AB21$	$-0.5 \times L2$	$0.5 \times L4$	$-L6$
$AB22$	$-0.5 \times L2$	$-0.5 \times L4$	$L6$

Now consider an unbalanced 2×2 factorial with two observations in every cell except the $AB22$ cell, which contains only one observation. The general form of estimable functions is the same as if it were balanced, since the same effects are still estimable. However, the Type II estimable functions for A and B are not the same as they were for the balanced design. The Type II estimable functions for this unbalanced 2×2 factorial are shown in Table 15.7.

Table 15.7 Type II Estimable Functions for Unbalanced 2×2 Factorial

Effect	Coefficients for Effect		
	A	B	$A * B$
μ	0	0	0
$A1$	$L2$	0	0
$A2$	$-L2$	0	0
$B1$	0	$L4$	0
$B2$	0	$-L4$	0
$AB11$	$0.6 \times L2$	$0.6 \times L4$	$L6$
$AB12$	$0.4 \times L2$	$-0.6 \times L4$	$-L6$
$AB21$	$-0.6 \times L2$	$0.4 \times L4$	$-L6$
$AB22$	$-0.4 \times L2$	$-0.4 \times L4$	$L6$

By comparing the hypothesis being tested in the balanced case to the hypothesis being tested in the unbalanced case for effects A and B , you can note that the Type II hypotheses for A and B are dependent on the cell frequencies in the design. For unbalanced designs in which the cell frequencies are not proportional to the background population, the Type II hypotheses for effects that are contained in other effects are of questionable value.

However, if an effect is not contained in any other effect, the Type II hypothesis for that effect is an MRH that does not involve any parameters except those associated with the effect in question.

Thus, Type II SS are appropriate for the following models:

- any balanced model
- any main-effects model
- any pure regression model
- an effect not contained in any other effect (regardless of the model)

In addition to the preceding models, Type II SS are generally accepted by most statisticians for purely nested models.

Type III and IV SS and Estimable Functions

When an effect is contained in another effect, the Type II hypotheses for that effect are dependent on the cell frequencies. The philosophy behind both the Type III and Type IV hypotheses is that the hypotheses tested for any given effect should be the same for all designs with the same general form of estimable functions.

To demonstrate this concept, recall the hypotheses being tested by the Type II SS in the balanced 2×2 factorial shown in Table 15.6. Those hypotheses are precisely the ones that the Type III and Type IV hypotheses employ for all 2×2 factorials that have at least one observation per cell. The Type III and Type IV hypotheses for a design without missing cells usually differ from the hypothesis employed for the same design with missing cells since the general form of estimable functions usually differs.

Many SAS/STAT procedures can perform tests of Type III hypotheses, but only PROC GLM offers Type IV tests as well.

Type III Estimable Functions

Type III hypotheses are constructed by working directly with the general form of estimable functions. The following steps are used to construct a hypothesis for an effect FI :

1. For every effect in the model except FI and those effects that contain FI , equate the coefficients in the general form of estimable functions to zero.
If FI is not contained in any other effect, this step defines the Type III hypothesis (as well as the Type II and Type IV hypotheses). If FI is contained in other effects, go on to step 2. (See the section “Type II SS and Estimable Functions” on page 259 for a definition of when effect FI is contained in another effect.)
2. If necessary, equate new symbols to compound expressions in the FI block in order to obtain the simplest form for the FI coefficients.
3. Equate all symbolic coefficients outside the FI block to a linear function of the symbols in the FI block in order to make the FI hypothesis orthogonal to hypotheses associated with effects that contain FI .

By once again observing the Type II hypotheses being tested in the balanced 2×2 factorial, it is possible to verify that the A and $A * B$ hypotheses are orthogonal and also that the B and $A * B$ hypotheses are orthogonal. This principle of orthogonality between an effect and any effect that contains it holds for all balanced designs. Thus, construction of Type III hypotheses for any design is a logical extension of a process that is used for balanced designs.

The Type III hypotheses are precisely the hypotheses being tested by programs that reparameterize using the usual assumptions (for example, constraining all parameters for an effect to sum to zero). When no missing cells exist in a factorial model, Type III SS coincide with Yates’ weighted squares-of-means technique. When cells are missing in factorial models, the Type III SS coincide with those discussed in Harvey (1960) and Henderson (1953).

The following discussion illustrates the construction of Type III estimable functions for a 2×2 factorial with no missing cells.

To obtain the $A * B$ interaction hypothesis, start with the general form and equate the coefficients for effects μ , A , and B to zero, as shown in Table 15.8.

Table 15.8 Type III Hypothesis for $A * B$ Interaction

Effect	General Form	$L1 = L2 = L4 = 0$
μ	$L1$	0
$A1$	$L2$	0
$A2$	$L1 - L2$	0
$B1$	$L4$	0
$B2$	$L1 - L4$	0
$AB11$	$L6$	$L6$
$AB12$	$L2 - L6$	$-L6$
$AB21$	$L4 - L6$	$-L6$
$AB22$	$L1 - L2 - L4 + L6$	$L6$

The last column in Table 15.8 represents the form of the MRH for $A * B$.

To obtain the Type III hypothesis for A , first start with the general form and equate the coefficients for effects μ and B to zero (let $L1 = L4 = 0$). Next let $L6 = K \times L2$, and find the value of K that makes the A hypothesis orthogonal to the $A * B$ hypothesis. In this case, $K = 0.5$. Each of these steps is shown in Table 15.9.

In Table 15.9, the fourth column (under $L6 = K \times L2$) represents the form of all estimable functions not involving μ , $B1$, or $B2$. The prime difference between the Type II and Type III hypotheses for A is the way K is determined. Type II chooses K as a function of the cell frequencies, whereas Type III chooses K such that the estimable functions for A are orthogonal to the estimable functions for $A * B$.

Table 15.9 Type III Hypothesis for A

Effect	General Form	$L1 = L4 = 0$	$L6 = K \times L2$	$K = 0.5$
μ	$L1$	0	0	0
$A1$	$L2$	$L2$	$L2$	$L2$
$A2$	$L1 - L2$	$-L2$	$-L2$	$-L2$
$B1$	$L4$	0	0	0
$B2$	$L1 - L4$	0	0	0
$AB11$	$L6$	$L6$	$K \times L2$	$0.5 \times L2$
$AB12$	$L2 - L6$	$L2 - L6$	$(1 - K) \times L2$	$0.5 \times L2$
$AB21$	$L4 - L6$	$-L6$	$-K \times L2$	$-0.5 \times L2$
$AB22$	$L1 - L2 - L4 + L6$	$-L2 + L6$	$-(1 - K) \times L2$	$-0.5 \times L2$

An example of Type III estimable functions in a 3×3 factorial with unequal cell frequencies and missing diagonals is given in Table 15.10 (N_1 through N_6 represent the nonzero cell frequencies).

Table 15.10 3×3 Factorial Design with Unequal Cell Frequencies and Missing Diagonals

		B		
		1	2	3
A	1		N_1	N_2
	2	N_3		N_4
	3	N_5	N_6	

For any nonzero values of N_1 through N_6 , the Type III estimable functions for each effect are shown in Table 15.11.

Table 15.11 Type III Estimable Functions for 3×3 Factorial Design with Unequal Cell Frequencies and Missing Diagonals

Effect	A	B	A * B
μ	0	0	0
A1	L2	0	0
A2	L3	0	0
A3	$-L2 - L3$	0	0
B1	0	L5	0
B2	0	L6	0
B3	0	$-L5 - L6$	0
AB12	$0.667 \times L2 + 0.333 \times L3$	$0.333 \times L5 + 0.667 \times L6$	L8
AB13	$0.333 \times L2 - 0.333 \times L3$	$-0.333 \times L5 - 0.667 \times L6$	$-L8$
AB21	$0.333 \times L2 + 0.667 \times L3$	$0.667 \times L5 + 0.333 \times L6$	$-L8$
AB23	$-0.333 \times L2 + 0.333 \times L3$	$-0.667 \times L5 - 0.333 \times L6$	L8
AB31	$-0.333 \times L2 - 0.667 \times L3$	$0.333 \times L5 - 0.333 \times L6$	L8
AB32	$-0.667 \times L2 - 0.333 \times L3$	$-0.333 \times L5 + 0.333 \times L6$	$-L8$

Type IV Estimable Functions

By once again looking at the Type II hypotheses being tested in the balanced 2×2 factorial (see Table 15.6), you can see another characteristic of the hypotheses employed for balanced designs: the coefficients of lower-order effects are averaged across each higher-level effect involving the same subscripts. For example, in the A hypothesis, the coefficients of AB11 and AB12 are equal to one-half the coefficient of A1, and the coefficients of AB21 and AB22 are equal to one-half the coefficient of A2. With this in mind, the basic concept used to construct Type IV hypotheses is that the coefficients of any effect, say FI, are distributed equitably across higher-level effects that contain FI. When missing cells occur, this same general philosophy is adhered to, but care must be taken in the way the distributive concept is applied.

Construction of Type IV hypotheses begins as does the construction of the Type III hypotheses. That is, for an effect FI, equate to zero all coefficients in the general form that do not belong to FI or to any other effect containing FI. If FI is not contained in any other effect, then the Type IV hypothesis (and Type II and III) has been found. If FI is contained in other effects, then simplify, if necessary, the coefficients associated with FI so that they are all free coefficients or functions of other free coefficients in the FI block.

To illustrate the method of resolving the free coefficients outside the FI block, suppose that you are interested in the estimable functions for an effect A and that A is contained in AB, AC, and ABC. (In other words, the main effects in the model are A, B, and C.)

With missing cells, the coefficients of intermediate effects (here they are AB and AC) do not always have an equal distribution of the lower-order coefficients, so the coefficients of the highest-order effects are determined first (here it is ABC). Once the highest-order coefficients are determined, the coefficients of intermediate effects are automatically determined.

The following process is performed for each free coefficient of A in turn. The resulting symbolic vectors are then added together to give the Type IV estimable functions for A.

1. Select a free coefficient of A , and set all other free coefficients of A to zero.
2. If any of the levels of A have zero as a coefficient, equate all of the coefficients of higher-level effects involving that level of A to zero. This step alone usually resolves most of the free coefficients remaining.
3. Check to see if any higher-level coefficients are now zero when the coefficient of the associated level of A is not zero. If this situation occurs, the Type IV estimable functions for A are not unique.
4. For each level of A in turn, if the A coefficient for that level is nonzero, count the number of times that level occurs in the higher-level effect. Then equate each of the higher-level coefficients to the coefficient of that level of A divided by the count.

An example of a 3×3 factorial with four missing cells (N_1 through N_5 represent positive cell frequencies) is shown in Table 15.12.

Table 15.12 3×3 Factorial Design with Four Missing Cells

		B		
		1	2	3
A	1	N_1	N_2	
	2	N_3	N_4	
	3			N_5

The Type IV estimable functions are shown in Table 15.13.

Table 15.13 Type IV Estimable Functions for 3×3 Factorial Design with Four Missing Cells

Effect	A	B	$A * B$
μ	0	0	0
$A1$	$-L3$	0	0
$A2$	$L3$	0	0
$A3$	0	0	0
$B1$	0	$L5$	0
$B2$	0	$-L5$	0
$B3$	0	0	0
$AB11$	$-0.5 \times L3$	$0.5 \times L5$	$L8$
$AB12$	$-0.5 \times L3$	$-0.5 \times L5$	$-L8$
$AB21$	$0.5 \times L3$	$0.5 \times L5$	$-L8$
$AB22$	$0.5 \times L3$	$-0.5 \times L5$	$L8$
$AB33$	0	0	0

A Comparison of Type III and Type IV Hypotheses

For the vast majority of designs, Type III and Type IV hypotheses for a given effect are the same. Specifically, they are the same for any effect $F1$ that is not contained in other effects for any design (with or without missing cells). For factorial designs with no missing cells, the Type III and Type IV hypotheses coincide for all effects. When there are missing cells, the hypotheses can differ. By using the GLM procedure, you

can study the differences in the hypotheses and then decide on the appropriateness of the hypotheses for a particular model.

The Type III hypotheses for three-factor and higher completely nested designs with unequal N s in the lowest level differ from the Type II hypotheses; however, the Type IV hypotheses do correspond to the Type II hypotheses in this case.

When missing cells occur in a design, the Type IV hypotheses might not be unique. If this occurs in PROC GLM, you are notified, and you might need to consider defining your own specific comparisons.

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Chapter 16

Introduction to Nonparametric Analysis

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Overview: Nonparametric Analysis

In statistical inference, or hypothesis testing, the traditional tests are called *parametric tests* because they depend on the specification of a probability distribution (such as the normal) except for a set of free parameters. Parametric tests are said to depend on distributional assumptions. *Nonparametric tests*, on the other hand, do not require any strict distributional assumptions. Even if the data are distributed normally, nonparametric methods are often almost as powerful as parametric methods.

Many nonparametric methods analyze the ranks of a variable rather than the original values. Procedures such as PROC NPAR1WAY calculate the ranks for you and then perform appropriate nonparametric tests. However, there are some situations in which you use a procedure such as PROC RANK to calculate ranks and then use another procedure to perform the appropriate test. See the section “[Obtaining Ranks](#)” on page 274 for details.

Although the NPAR1WAY procedure is specifically targeted for nonparametric analysis, many other procedures also perform nonparametric analyses. Some general references on nonparametrics include Hollander and Wolfe (1999); Conover (1999); Gibbons and Chakraborti (2010); Hettmansperger (1984); Randles and Wolfe (1979); Lehmann (2006).

Testing for Normality

Many parametric tests assume an underlying normal distribution for the population. If your data do not meet this assumption, you might prefer to use a nonparametric analysis.

Base SAS software provides several tests for normality in the UNIVARIATE procedure. Depending on your sample size, PROC UNIVARIATE performs the Kolmogorov-Smirnov, Shapiro-Wilk, Anderson-Darling, and Cramér-von Mises tests. For more information, see the chapter “The UNIVARIATE Procedure” in the *Base SAS Procedures Guide*.

Comparing Distributions

To test the hypothesis that two or more groups of observations have identical distributions, use the NPAR1WAY procedure, which provides empirical distribution function (EDF) statistics. The procedure calculates the Kolmogorov-Smirnov test, the Cramér-von Mises test, and, when the data are classified into only two samples, the Kuiper test. Exact p -values are available for the two-sample Kolmogorov-Smirnov test. To obtain these tests, use the EDF option in the PROC NPAR1WAY statement. See Chapter 65, “The NPAR1WAY Procedure,” for details.

One-Sample Tests

Base SAS software provides two one-sample tests in the UNIVARIATE procedure: a sign test and the Wilcoxon signed rank test. Both tests are designed for situations where you want to make an inference about the location (median) of a population. For example, suppose you want to test whether the median resting pulse rate of marathon runners differs from a specified value.

By default, both of these tests examine the hypothesis that the median of the population from which the sample is drawn is equal to a specified value, which is zero by default. The Wilcoxon signed rank test requires that the distribution be symmetric; the sign test does not require this assumption. These tests can also be used for the case of two related samples; see the section “Comparing Two Independent Samples” on page 271 for more information.

These two tests are automatically provided by the UNIVARIATE procedure. For details, formulas, and examples, see the chapter “The UNIVARIATE Procedure” in the *Base SAS Procedures Guide*.

Two-Sample Tests

This section describes tests appropriate for two independent samples (for example, two groups of subjects given different treatments) and for two related samples (for example, before-and-after measurements on a single group of subjects). Related samples are also referred to as paired samples or matched pairs.

Comparing Two Independent Samples

SAS/STAT software provides several nonparametric tests for location and scale differences for two independent samples.

When you perform these tests, your data should consist of a random sample of observations from two different populations. Your goal is to compare either the location parameters (medians) or the scale parameters of the two populations. For example, suppose your data consist of the number of days in the hospital for two groups of patients: those who received a standard surgical procedure and those who received a new, experimental surgical procedure. These patients are a random sample from the population of patients who have received the two types of surgery. Your goal is to decide whether the median hospital stays differ for the two populations.

Tests in the NPAR1WAY Procedure

The NPAR1WAY procedure provides the following location tests: Wilcoxon rank sum test (Mann-Whitney U test), median test, Savage test, and Van der Waerden (normal scores) test. Note that the Wilcoxon rank sum test can also be obtained from the FREQ procedure. PROC NPAR1WAY provides Hodges-Lehmann estimation of the location shift between two samples, including asymptotic (Moses) and exact confidence limits.

In addition, PROC NPAR1WAY produces the following tests for scale differences: Siegel-Tukey test, Ansari-Bradley test, Klotz test, and Mood test. PROC NPAR1WAY also provides the Conover test, which can be used to test for differences in both location and scale.

Additionally, PROC NPAR1WAY provides tests that use the input data observations as scores, enabling you to produce a wide variety of tests. You can construct any scores for your data with the DATA step, and then PROC NPAR1WAY computes the corresponding linear rank test. You can directly analyze the raw data this way, producing the permutation test known as Pitman's test.

When data are sparse, skewed, or heavily tied, the usual asymptotic tests might not be appropriate. In these situations, exact tests might be suitable for analyzing your data. The NPAR1WAY procedure can produce exact p -values for all of the two-sample tests for location and scale differences.

See Chapter 65, “The NPAR1WAY Procedure,” for details, formulas, and examples of these tests.

Tests in the FREQ Procedure

The FREQ procedure provides nonparametric tests that compare the location of two groups and that test for independence between two variables.

The situation in which you want to compare the location of two groups of observations corresponds to a table with two rows. In this case, the asymptotic Wilcoxon rank sum test can be obtained by using SCORES=RANK in the TABLES statement and by looking at either of the following:

- the Mantel-Haenszel statistic in the list of tests for no association. This is labeled as “Mantel Haenszel Chi-Square,” and PROC FREQ displays the statistic, the degrees of freedom, and the p -value. To obtain this statistic, specify the CHISQ option in the TABLES statement.
- the CMH statistic 2 in the section on Cochran-Mantel-Haenszel statistics. PROC FREQ displays the statistic, the degrees of freedom, and the p -value. To obtain this statistic, specify the CMH2 option in the TABLES statement.

When you test for independence, the question being answered is whether the two variables of interest are related in some way. For example, you might want to know if student scores on a standard test are related to whether students attended a public or private school. One way to think of this situation is to consider the data as a two-way table; the hypothesis of interest is whether the rows and columns are independent. In the preceding example, the groups of students would form the two rows, and the scores would form the columns. The special case of a two-category response (Pass/Fail) leads to a 2×2 table; the case of more than two categories for the response (A/B/C/D/F) leads to a $2 \times c$ table, where c is the number of response categories.

For testing whether two variables are independent, PROC FREQ provides Fisher's exact test. For a 2×2 table, PROC FREQ automatically provides Fisher's exact test when you specify the CHISQ option in the TABLES statement. For a $2 \times c$ table, use the FISHER option in the EXACT statement to obtain the test.

See Chapter 38, "The FREQ Procedure," for details, formulas, and examples of these tests.

Comparing Two Related Samples

SAS/STAT software provides the following nonparametric tests for comparing the locations of two related samples:

- Wilcoxon signed rank test
- sign test
- McNemar's test

The first two tests are available in the UNIVARIATE procedure, and the last test is available in the FREQ procedure. When you perform these tests, your data should consist of pairs of measurements for a random sample from a single population. For example, suppose your data consist of SAT scores for students before and after attending a course on how to prepare for the SAT. The pairs of measurements are the scores before and after the course, and the students should be a random sample of students who attended the course. Your goal in analysis is to decide whether the median change in scores is significantly different from zero.

Tests in the UNIVARIATE Procedure

By default, PROC UNIVARIATE performs a Wilcoxon signed rank test and a sign test. To use these tests on two related samples, perform the following steps:

1. In the DATA step, create a new variable that contains the differences between the two related variables.
2. Run PROC UNIVARIATE, using the new variable in the VAR statement.

See the chapter "The UNIVARIATE Procedure" in the *Base SAS Procedures Guide* for details and examples of these tests.

Tests in the FREQ Procedure

The FREQ procedure can be used to obtain McNemar's test, which is simply another special case of a Cochran-Mantel-Haenszel statistic (and also of the sign test). The AGREE option in the TABLES statement produces this test for 2×2 tables, and exact p -values are also available for this test. See Chapter 38, "The FREQ Procedure," for more information.

Tests for k Samples

Comparing k Independent Samples

One goal in comparing k independent samples is to determine whether the location parameters (medians) of the populations are different. Another goal is to determine whether the scale parameters for the populations are different. For example, suppose new employees are randomly assigned to one of three training programs. At the end of the program, the employees are given a standard test that provides a rating score of their job ability. The goal of analysis is to compare the median scores for the three groups and decide whether the differences are real or due to chance alone.

To compare k independent samples, either the `NPARIWAY` or the `FREQ` procedure provides a Kruskal-Wallis test. `PROC NPARIWAY` also provides the Savage, median, and Van der Waerden (normal scores) tests. In addition, `PROC NPARIWAY` produces the following tests for scale differences: Siegel-Tukey test, Ansari-Bradley test, Klotz test, and Mood test. `PROC NPARIWAY` also provides the Conover test, which can be used to test for differences in both location and scale. Note that you can obtain exact p -values for all of these tests.

Additionally, you can specify the `SCORES=DATA` option to use the input data observations as scores. This enables you to produce a very wide variety of tests. You can construct any scores for your data with the `DATA` step, and then `PROC NPARIWAY` computes the corresponding linear rank and one-way ANOVA tests. You can also analyze the raw data with the `SCORES=DATA` option; for two-sample data, this permutation test is known as Pitman's test.

See Chapter 65, “[The NPARIWAY Procedure](#),” for details, formulas, and examples.

To produce a Kruskal-Wallis test in the `FREQ` procedure, use `SCORES=RANK` and the `CMH2` option in the `TABLES` statement. Then, look at the second Cochran-Mantel-Haenszel statistic (labeled “Row Mean Scores Differ”) to obtain the Kruskal-Wallis test. The `FREQ` procedure also provides the Jonckheere-Terpstra test, which is more powerful than the Kruskal-Wallis test for comparing k samples against ordered alternatives. The exact test is also available. In addition, you can obtain a riddit analysis, developed by Bross (1958), by specifying `SCORES=RIDIT` or `SCORES=MODRIDIT` in the `TABLES` statement in the `FREQ` procedure. See Chapter 38, “[The FREQ Procedure](#),” for more information.

Comparing k Dependent Samples

Friedman's test enables you to compare the locations of three or more dependent samples. You can obtain Friedman's chi-square with the `FREQ` procedure by using the `CMH2` option with `SCORES=RANK` and by looking at the second `CMH` statistic in the output. For an example, see Chapter 38, “[The FREQ Procedure](#),” which also contains formulas and other details about the `CMH` statistics. For a discussion of how to use the `RANK` and `GLM` procedures to obtain Friedman's test, see Ipe (1987).

Measures of Correlation and Associated Tests

The CORR procedure in Base SAS software provides several nonparametric measures of association and associated tests. It computes Spearman's rank-order correlation, Kendall's tau-*b*, and Hoeffding's measure of dependence, and it provides tests for each of these statistics. PROC CORR also computes Spearman's partial rank-order correlation and Kendall's partial tau-*b*. Finally, PROC CORR computes Cronbach's coefficient alpha for raw and standardized variables. This statistic can be used to estimate the reliability coefficient. For a general discussion of correlations, formulas, interpretation, and examples, see the chapter "The CORR Procedure" in the *Base SAS Procedures Guide*.

The FREQ procedure also provides some nonparametric measures of association: gamma, Kendall's tau-*b*, Stuart's tau-*c*, Somers' *D*, and the Spearman rank correlation. The output includes the measure, the asymptotic standard error, confidence limits, and the asymptotic test that the measure equals zero. Exact tests are also available for some of these measures. For more information, see Chapter 38, "The FREQ Procedure."

Obtaining Ranks

The primary procedure for obtaining ranks is the RANK procedure in Base SAS software. Note that the PRINQUAL and TRANSREG procedures also provide rank transformations. With all three of these procedures, you can create an output data set and use it as input to another SAS/STAT procedure or to the IML procedure. For more information, see the chapter "The RANK Procedure" in the *Base SAS Procedures Guide*. Also see Chapter 74, "The PRINQUAL Procedure," and Chapter 97, "The TRANSREG Procedure."

In addition, you can specify SCORES=RANK in the TABLES statement in the FREQ procedure. PROC FREQ then uses ranks to perform the analyses requested and generates nonparametric analyses.

For more discussion of the rank transform, see Iman and Conover (1979); Conover and Iman (1981); Hora and Conover (1984); Iman, Hora, and Conover (1984); Hora and Iman (1988); Iman (1988).

Kernel Density Estimation

The KDE procedure performs either univariate or bivariate kernel density estimation. Statistical *density estimation* involves approximating a hypothesized probability density function from observed data. *Kernel density estimation* is a nonparametric technique for density estimation in which a known density function (the kernel) is averaged across the observed data points to create a smooth approximation.

PROC KDE uses a Gaussian density as the kernel, and its assumed variance determines the smoothness of the resulting estimate. PROC KDE outputs the kernel density estimate to a SAS data set, which you can then use with other procedures for plotting or analysis. PROC KDE also computes a variety of common statistics, including estimates of the percentiles of the hypothesized probability density function.

For more information, see Chapter 48, "The KDE Procedure."

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Chapter 17

Introduction to Structural Equation Modeling with Latent Variables

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Overview of Structural Equation Modeling with Latent Variables

Structural equation modeling includes analysis of covariance structures and mean structures, fitting systems of linear structural equations, factor analysis, and path analysis. In terms of the mathematical and statistical techniques involved, these various types of analyses are more or less interchangeable because the underlying methodology is based on analyzing the mean and covariance structures. However, the different analysis types emphasize different aspects of the analysis.

The analysis of covariance structures refers to the formulation of a model for the observed variances and covariances among a set of variables. The model expresses the variances and covariances as functions of some basic parameters. Similarly, the analysis of mean structures refers to the formulation of a model for the observed means. The model expresses the means as functions of some basic parameters. Usually, the covariance structures are of primary interest. However, sometimes the mean structures are analyzed simultaneously with the covariance structures in a model.

Corresponding to this kind of abstract formulation of mean and covariance structure analysis, PROC CALIS offers you two matrix-based modeling languages for specifying your model:

- **MSTRUCT**: a matrix-based model specification language that enables you to directly specify the parameters in the covariance and mean model matrices
- **COSAN**: a general matrix-based model specification language that enables you to specify a very wide class of mean and covariance structure models in terms of matrix expressions

Instead of focusing directly on the mean and covariance structures, other generic types of structural equation modeling emphasize more about the functional relationships among variables. Mean and covariance structures are still the means of these analyses, but they are usually implied from the structural relationships, rather than being directly specified as in the COSAN or MSTRUCT modeling languages.

In linear structural equations, the model is formulated as a system of equations that relates several random variables with assumptions about the variances and covariances of the random variables. The variables involved in the system of linear structural equations could be observed (manifest) or latent. Causal relationships between variables are hypothesized in the model.

When all observed variables in the model are hypothesized as indicator measures of underlying latent factors and the main interest is about studying the structural relations among the latent factors, it is a modeling scenario for factor-analysis or LISREL (Keesling 1972; Wiley 1973; Jöreskog 1973). PROC CALIS provides you two modeling languages that are closely related to this type of modeling scenario:

- **FACTOR:** a non-matrix-based model specification language that supports both exploratory and confirmatory factor analysis, including orthogonal and oblique factor rotations
- **LISMOD:** a matrix-based model specification language that enables you to specify the parameters in the LISREL model matrices

When causal relationships among observed and latent variables are freely hypothesized so that the observed variables are not limited to the roles of being measured indicators of latent factors, it is a modeling scenario for general path modeling (path analysis). In general path modeling, the model is formulated as a path diagram, in which arrows that connect variables represent variances, covariances, and path coefficients (effects). Depending on the way you represent the path diagram, you can use any of the following three different modeling languages in PROC CALIS:

- **PATH:** a non-matrix-based language that enables you to specify path-like relationships among variables
- **RAM:** a matrix-based language that enables you to specify the paths, variances, and covariance parameters in terms of the RAM model matrices (McArdle and McDonald 1984)
- **LINEQS:** an equation-based language that uses linear equations to specify functional or path relationships among variables (for example, the EQS model by Bentler 1995)

Although various types of analyses are put into distinct classes (with distinct modeling languages), with careful parameterization and model specification, it is possible to apply any of these modeling languages to the same analysis. For example, you can use the PATH modeling language to specify a confirmatory factor-analysis model, or you can use the LISMOD modeling language to specify a general path model. However, for some situations some modeling languages are easier to use than others. See the section “[Which Modeling Language?](#)” on page 1077 of Chapter 27, “[The CALIS Procedure](#),” for a detailed discussion of the modeling languages supported in PROC CALIS.

Loehlin (1987) provides an excellent introduction to latent variable models by using path diagrams and structural equations. A more advanced treatment of structural equation models with latent variables is given by Bollen (1989). Fuller (1987) provides a highly technical statistical treatment of measurement-error models.

This chapter illustrates applications of PROC CALIS, describes some of the main modeling features of PROC CALIS, and compares the CALIS procedure with the FACTOR and the SYSLIN procedures.

Testing Covariance Patterns

The most basic use of PROC CALIS is testing covariance patterns. Consider a repeated-measures experiment where individuals are tested for their motor skills at three different time points. No treatments are introduced between these tests. The three test scores are denoted as X_1 , X_2 , and X_3 , respectively. These test scores are likely correlated because the same set of individuals has been used. More specifically, the researcher wants to test the following pattern of the population covariance matrix Σ :

$$\Sigma = \begin{pmatrix} \phi & \theta & \theta \\ \theta & \phi & \theta \\ \theta & \theta & \phi \end{pmatrix}$$

Because there are no treatments between the tests, this pattern assumes that the distribution of motor skills stays more or less the same over time, as represented by the same ϕ for the diagonal elements of Σ . The covariances between the test scores for motor skills also stay the same, as represented by the same θ for all the off-diagonal elements of Σ .

Suppose you summarize your data in a covariance matrix, which is stored in the following SAS data set:

```
data motor(type=cov);
  input _type_ $ _name_ $ x1 x2 x3;
  datalines;
COV   x1      3.566   1.342   1.114
COV   x2      1.342   4.012   1.056
COV   x3      1.114   1.056   3.776
N     .         36     36     36
;
```

The diagonal elements are somewhat close to each other but are not the same. The off-diagonal elements are also very close to each other but are not the same. Could these observed differences be due to chance? Given the sample covariance matrix, can you test the hypothesized patterned covariance matrix in the population?

Setting up this patterned covariance model in PROC CALIS is straightforward with the MSTRUCT modeling language:

```
proc calis data=motor;
  mstruct var = x1-x3;
  matrix _cov_ = phi
              theta phi
              theta theta phi;
run;
```

In the VAR= option in the MSTRUCT statement, you specify that x1–x3 are the variables in the covariance matrix. Next, you specify the elements of the patterned covariance matrix in the MATRIX statement with the _COV_ keyword. Because the covariance matrix is symmetric, you need to specify only the lower triangular elements in the MATRIX statement. You use phi for the parameters of all diagonal elements and theta for the parameters of all off-diagonal elements. Matrix elements with the same parameter name are implicitly constrained to be equal. Hence, this is the patterned covariance matrix that you want to test. Some output results from PROC CALIS are shown in Figure 17.1.

Figure 17.1 Fit Summary

Fit Summary			
Chi-Square	0.3656		
Chi-Square DF	4		
Pr > Chi-Square	0.9852		
MSTRUCT _COV_ Matrix: Estimate/StdErr/t-value			
	x1	x2	x3
x1	3.7847	1.1707	1.1707
	0.5701	0.5099	0.5099
	6.6383	2.2960	2.2960
	[phi]	[theta]	[theta]
x2	1.1707	3.7847	1.1707
	0.5099	0.5701	0.5099
	2.2960	6.6383	2.2960
	[theta]	[phi]	[theta]
x3	1.1707	1.1707	3.7847
	0.5099	0.5099	0.5701
	2.2960	2.2960	6.6383
	[theta]	[theta]	[phi]

First, PROC CALIS shows that the chi-square test for the model fit is 0.3656 ($df = 4$, $p=0.9852$). Because the chi-square test is not significant, it supports the hypothesized patterned covariance model. Next, PROC CALIS shows the estimates in the covariance matrix under the hypothesized model. The estimates for the diagonal elements are all 3.7847, and the estimates for off-diagonal elements are all 1.1707. Estimates of standard errors and t values for these covariance and variance parameters are also shown.

The MSTRUCT modeling language in PROC CALIS enables you to test various kinds of covariance and mean patterns, including matrices with fixed or constrained values. For example, consider a population covariance model in which correlations among the motor test scores are hypothesized to be zero. In other words, the covariance pattern is:

$$\Sigma = \begin{pmatrix} \phi_1 & 0 & 0 \\ 0 & \phi_2 & 0 \\ 0 & 0 & \phi_3 \end{pmatrix}$$

Essentially, this diagonally-patterned covariance model means that the data are randomly and independently generated for x_1 – x_3 under the multivariate normal distribution. Only the variances of the variables are parameters in the model, and the variables are not correlated at all.

You can use the MSTRUCT modeling language of PROC CALIS to fit this diagonally-patterned covariance matrix to the data for motor skills, as shown in the following statements:

```

proc calis data=motor;
  mstruct var = x1-x3;
  matrix _cov_ = phi1
                0.   phi2
                0.   0.   phi3;
run;

```

Some of the output is shown in Figure 17.2.

Figure 17.2 Fit Summary: Testing Uncorrelatedness

Fit Summary			
Chi-Square		9.2939	
Chi-Square DF		3	
Pr > Chi-Square		0.0256	
MSTRUCT _COV_ Matrix: Estimate/StdErr/t-value			
	x1	x2	x3
x1	3.5660 0.8524 4.1833 [phi1]	0	0
x2	0	4.0120 0.9591 4.1833 [phi2]	0
x3	0	0	3.7760 0.9026 4.1833 [phi3]

PROC CALIS shows that the chi-square test for the model fit is 9.2939 ($df=3$, $p=0.0256$). Because the chi-square test is significant, it does not support the patterned covariance model that postulates zero correlations among the variables. This conclusion is consistent with what is already known—the motor test scores should be somewhat correlated because they are measurements over time for the same group of individuals.

The output also shows the estimates of variances under the model. Each diagonal element of the covariance matrix has a distinct estimate because different parameters have been hypothesized under the patterned covariance model.

Testing Built-In Covariance Patterns in PROC CALIS

Some covariance patterns are well-known in multivariate statistics. For example, testing the diagonal pattern for a covariance matrix in the preceding section is a test of uncorrelatedness between the observed variables.

Under the multivariate normal assumption, this test is also a test of independence between the observed variables. This test of independence is routinely applied in maximum likelihood factor analysis for testing the zero common factor hypothesis for the observed variables. For testing such a well-known covariance pattern, PROC CALIS provides an efficient way of specifying a model. With the `COVPATTERN=` option, you can invoke the built-in covariance patterns in PROC CALIS without the MSTRUCT model specifications, which could become laborious when the number of variables are large.

For example, to test the diagonal pattern (uncorrelatedness) of the motor skills, you can simply use the following specification:

```
proc calis data=motor covpattern=uncorr;
run;
```

The `COVPATTERN=UNCORR` option in the PROC CALIS statement invokes the diagonally patterned covariance matrix for the motor skills. PROC CALIS then generates the appropriate free parameters for this built-in covariance pattern. As a result, the `MATRIX` statement is not needed for specifying the free parameters, as it is if you use explicit MSTRUCT model specifications. Some of the output for using the `COVPATTERN=` option is shown in Figure 17.3.

Figure 17.3 Fit Summary: Testing Uncorrelatedness with the `COVPATTERN=` Option

Fit Summary			
Chi-Square		8.8071	
Chi-Square DF		3	
Pr > Chi-Square		0.0320	
MSTRUCT _COV_ Matrix: Estimate/StdErr/t-value			
	x1	x2	x3
x1	3.5660 0.8524 4.1833 [_varparm_1]	0	0
x2	0	4.0120 0.9591 4.1833 [_varparm_2]	0
x3	0	0	3.7760 0.9026 4.1833 [_varparm_3]

In the second table of Figure 17.3, the estimates of variances and their standard errors are the same as those shown in Figure 17.2. The only difference is that the parameter names (for example, `_varparm_1`) for the variances in Figure 17.3 are generated by PROC CALIS, instead of being specified as those in Figure 17.2.

However, the current chi-square test for the model fit is 8.8071 ($df=3$, $p=0.0320$), which is different from that in Figure 17.2 for testing the same covariance pattern. The reason is that the chi-square correction

due to Bartlett (1950) has been applied automatically to the current built-in covariance pattern testing. Theoretically, this corrected chi-square value is more accurate. Therefore, in addition to its efficiency in specification, the built-in covariance pattern with the `COVPATTERN=` option offers an extra advantage in the automatic chi-square correction.

The `COVPATTERN=` option supports many other built-in covariance patterns. For details, see the `COVPATTERN=` option. See also the `MEANPATTERN=` option for testing built-in mean patterns.

Direct and Implied Covariance Patterns

You have seen how you can use PROC CALIS to test covariance patterns directly. Basically, you can specify the parameters in the covariance and mean matrices directly by using the MSTRUCT modeling language, which is invoked by the MSTRUCT statement. You can also use the `COVPATTERN=` option to test some built-in covariance patterns in PROC CALIS. To handle more complicated covariance and mean structures that are products of several model matrices, you can use the COSAN modeling language. The COSAN modeling language is too powerful to consider in this introductory chapter, but see the `COSAN` statement and the section “The COSAN Model” on page 1259 of Chapter 27, “The CALIS Procedure.”

This section considers the fitting of patterned covariances matrix directly by using the MSTRUCT and the MATRIX statements or by the `COVPATTERN=` option. However, in most applications of structural equation modeling, the covariance patterns are not specified directly but are implied from the linear structural relationships among variables. The next few sections show how you can use other modeling languages in PROC CALIS to specify structural equation models with implied mean and covariance structures.

Regression with Measurement Errors

In this section, you start with a linear regression model and learn how the regression equation can be specified in PROC CALIS. The regression model is then extended to include measurement errors in the predictors and in the outcome variables. Problems with model identification are introduced.

Simple Linear Regression

Consider fitting a linear equation to two observed variables, Y and X . Simple linear regression uses the following model form:

$$Y = \alpha + \beta X + E_Y$$

The model makes the following assumption:

$$\text{Cov}(X, E_Y) = 0$$

The parameters α and β are the intercept and regression coefficient, respectively, and E_Y is an error term. If the values of X are fixed, the values of E_Y are assumed to be independent and identically distributed realizations of a normally distributed random variable with mean zero and variance $\text{Var}(E_Y)$. If X is a random variable, X and E_Y are assumed to have a bivariate normal distribution with zero correlation and

variances $\text{Var}(X)$ and $\text{Var}(E_Y)$, respectively. Under either set of assumptions, the usual formulas hold for the estimates of the intercept and regression coefficient and their standard errors. (See Chapter 4, “Introduction to Regression Procedures.”)

In the REG procedure, you can fit a simple linear regression model with a MODEL statement that lists only the names of the manifest variables, as shown in the following statements:

```
proc reg;
  model Y = X;
run;
```

You can also fit this model with PROC CALIS, but the syntax is different. You can specify the simple linear regression model in PROC CALIS by using the LINEQS modeling language, as shown in the following statements:

```
proc calis;
  lineqs
    Y = beta * X + Ey;
run;
```

LINEQS stands for “LINEar EQUationS.” You invoke the LINEQS modeling language by using the LINEQS statement in PROC CALIS. In the LINEQS statement, you specify the linear equations of your model. The LINEQS statement syntax is similar to the mathematical equation that you would write for the model. An obvious difference between the LINEQS and the PROC REG model specification is that in LINEQS you can name the parameter involved (for example, beta) and you also specify the error term explicitly. The additional syntax required by the LINEQS statement seems to make the model specification more time-consuming and cumbersome. However, this inconvenience is minor and is offset by the modeling flexibility of the LINEQS modeling language (and of PROC CALIS, generally). As you proceed to more examples in this chapter, you will find the benefits of specifying parameter names for more complicated models with constraints. You will also find that specifying parameter names for unconstrained parameters is optional. Using parameter names in the current example is for the ease of reference in the current discussion.

You might wonder whether an intercept term is missing in the LINEQS statement and where you should put the intercept term if you want to specify it. The intercept term, which is considered as a mean structure parameter in the context of structural equation modeling, is usually omitted when statistical inferences can be drawn from analyzing the covariance structures alone. However, this does not mean that the regression equation has a default fixed-zero intercept in the LINEQS specification. Rather, it means only that the mean structures are saturated and are not estimated in the covariance structure model. Therefore, in the preceding LINEQS specification, the intercept term α is implicitly assumed in the model. It is not of primary interest and is not estimated.

However, if you want to estimate the intercept, you can specify it in the LINEQS equations, as shown in the following specification:

```
proc calis;
  lineqs
    Y = alpha * Intercept + beta * X + Ey;
run;
```

In this LINEQS statement, alpha represents the intercept parameter α and intercept represents an internal “variable” that has a fixed value of 1 for each observation. With this specification, an estimate of α is displayed in the PROC CALIS output results. However, estimation results for other parameters are the same

as those from the specification without the intercept term. For this reason the intercept term is not specified in the examples of this section.

Errors-in-Variables Regression

For ordinary unconstrained regression models, there is no reason to use PROC CALIS instead of PROC REG. But suppose that the predictor variable X is a random variable that is contaminated by errors (especially measurement errors), and you want to estimate the linear relationship between the true, error-free scores. The following model takes this kind of measurement errors into account:

$$\begin{aligned} Y &= \alpha + \beta F_X + E_Y \\ X &= F_X + E_X \end{aligned}$$

The model assumes the following:

$$\text{Cov}(F_X, E_Y) = \text{Cov}(F_X, E_X) = \text{Cov}(E_X, E_Y) = 0$$

There are two equations in the model. The first one is the so-called structural model, which describes the relationships between Y and the true score predictor F_X . This equation is your main interest. However, F_X is a latent variable that has not been observed. Instead, what you have observed for this predictor is X , which is the contaminated version of F_X with measurement error or other errors, denoted by E_X , added. This measurement process is described in the second equation, or the so-called measurement model. By analyzing the structural and measurement models (or the two linear equations) simultaneously, you want to estimate the true score effect β .

The assumption that the error terms E_X and E_Y and the latent variable F_X are jointly uncorrelated is of critical importance in the model. This assumption must be justified on substantive grounds such as the physical properties of the measurement process. If this assumption is violated, the estimators might be severely biased and inconsistent.

You can express the current errors-in-variables model by the LINEQS modeling language as shown in the following statements:

```
proc calis;
  lineqs
    Y = beta * Fx + Ey,
    X = 1. * Fx + Ex;
run;
```

In this specification, you need to specify only the equations involved without specifying the assumptions about the correlations among F_X , E_Y , and E_X . In the LINEQS modeling language, you should always name latent factors with the 'F' or 'f' prefix (for example, F_X) and error terms with the 'E' or 'e' prefix (for example, E_Y and E_X). Given this LINEQS notation, latent factors and error terms, by default, are uncorrelated in the model.

Consider an example of an errors-in-variables regression model. Fuller (1987, pp. 18–19) analyzes a data set from Voss (1969) that involves corn yields (Y) and available soil nitrogen (X) for which there is a prior estimate of the measurement error for soil nitrogen $\text{Var}(E_X)$ of 57. The scientific question is: how does nitrogen affect corn yields? The linear prediction of corn yields by nitrogen should be based on a measure of nitrogen that is not contaminated with measurement error. Hence, the errors-in-variables model is applied. F_X in the model represents the “true” nitrogen measure, X represents the observed measure of nitrogen, which has a true score component F_X and an error component E_X . Given that the measurement error for soil nitrogen $\text{Var}(E_X)$ is 57, you can specify the errors-in-variables regression model with the following statements in PROC CALIS:

```
data corn(type=cov);
  input _type_ $ _name_ $ y x;
  datalines;
cov   y      87.6727      .
cov   x      104.8818    304.8545
mean  .       97.4545     70.6364
n     .       11          11
;

proc calis data=corn;
  lineqs
    Y = beta * Fx + Ey,
    X = 1.   * Fx + Ex;
  variance
    Ex = 57.;
run;
```

In the VARIANCE statement, the variance of E_x (measurement error for X) is given as the constant value 57. PROC CALIS produces the estimates shown in Figure 17.4.

Figure 17.4 Errors-in-Variables Model for Corn Data

Linear Equations					
	y	=	0.4232*Fx	+	1.0000 Ey
	Std Err		0.1658 beta		
	t Value		2.5520		
	x	=	1.0000 Fx	+	1.0000 Ex
Estimates for Variances of Exogenous Variables					
Variable Type	Variable	Parameter	Estimate	Standard Error	t Value
Error	Ex		57.00000		
Latent	Fx	_Add1	247.85450	136.33508	1.81798
Error	Ey	_Add2	43.29105	23.92488	1.80946

In Figure 17.4, the estimate of beta is 0.4232 with a standard error estimate of 0.1658. The t value is 2.552. It is significant at the 0.05 α -level when compared to the critical value of the standard normal variate (that is, the z table). Also shown in Figure 17.4 are the estimated variances of F_x , E_y , and their estimated standard errors. The names of these parameters have the prefix ‘_Add’. They are added by PROC CALIS as default parameters. By employing some conventional rules for setting default parameters, PROC CALIS makes your model specification much easier and concise. For example, you do not need to specify each error variance parameter manually if it is not constrained in the model. However, you can specify these parameters explicitly if you desire. Note that in Figure 17.4, the variance of E_x is shown to be 57 without a standard error estimate because it is a fixed constant in the model.

What if you did not model the measurement error in the predictor X ? That is, what is the estimate of beta if you use ordinary regression of Y on X , as described by the equation in the section “Simple Linear Regression” on page 284? You can specify such a linear regression model easily by the LINEQS modeling language. Here, you specify this linear regression model as a special case of the errors-in-variables model. That is, you constrain the variance of measurement error E_x to 0 in the preceding LINEQS model specification to form the linear regression model, as shown in the following statements:

```
proc calis data=corn;
  lineqs
    Y = beta * Fx + Ey,
    X = 1. * Fx + Ex;
  variance
    Ex = 0.;
run;
```

Fixing the variance of E_x to zero forces the equality of X and F_x in the measurement model so that this “new” errors-in-variables model is in fact an ordinary regression model. PROC CALIS produces the estimation results in Figure 17.5.

Figure 17.5 Ordinary Regression Model for Corn Data: Zero Measurement Error in X

Linear Equations					
y	=	0.3440*Fx	+	1.0000 Ey	
Std Err		0.1301 beta			
t Value		2.6447			
x	=	1.0000 Fx	+	1.0000 Ex	
Estimates for Variances of Exogenous Variables					
Variable Type	Variable	Parameter	Estimate	Standard Error	t Value
Error	Ex		0		
Latent	Fx	_Add1	304.85450	136.33508	2.23607
Error	Ey	_Add2	51.58928	23.07143	2.23607

The estimate of beta is now 0.3440, which is an underestimate of the effect of nitrogen on corn yields given the presence of nonzero measurement error in X , where the estimate of beta is 0.4232.

Regression with Measurement Errors in X and Y

What if there are also measurement errors in the outcome variable Y ? How can you write such an extended model? The following model would take measurement errors in both X and Y into account:

$$\begin{aligned} F_Y &= \alpha + \beta F_X + D_{F_y} \\ Y &= F_Y + E_Y \\ X &= F_X + E_X \end{aligned}$$

with the following assumption:

$$\begin{aligned} \text{Cov}(F_X, D_{F_y}) &= \text{Cov}(F_X, E_Y) = \text{Cov}(F_X, E_X) = \text{Cov}(F_Y, E_Y) \\ &= \text{Cov}(F_Y, E_X) = \text{Cov}(E_X, E_Y) = \text{Cov}(E_X, D_{F_y}) \\ &= \text{Cov}(E_Y, D_{F_y}) = 0 \end{aligned}$$

Again, the first equation, expressing the relationship between two latent true-score variables, defines the structural or causal model. The next two equations express the observed variables in terms of a true score plus error; these two equations define the measurement model. This is essentially the same form as the so-called LISREL model (Keesling 1972; Wiley 1973; Jöreskog 1973), which has been popularized by the LISREL program (Jöreskog and Sörbom 1988). Typically, there are several X and Y variables in a LISREL model. For the moment, however, the focus is on the current regression form in which there is only a single predictor and a single outcome variable. The LISREL model is considered in the section “Fitting LISREL Models by the LISMOD Modeling Language” on page 336.

With the intercept term left out for modeling, you can use the following statements for fitting the regression model with measurement errors in both X and Y :

```
proc calis data=corn;
  lineqs
    Fy = beta * Fx + DFy,
    Y  = 1.   * Fy + Ey,
    X  = 1.   * Fx + Ex;
run;
```

Again, you do not need to specify the zero-correlation assumptions in the LINEQS model because they are set by default given the latent factors and errors in the LINEQS modeling language. When you run this model, PROC CALIS issues the following warning:

```
WARNING: Estimation problem not identified: More parameters to
estimate ( 5 ) than the total number of mean and
covariance elements ( 3 ).
```

The five parameters in the model include β and the variances for the exogenous variables: F_x , D_{F_y} , E_y , and E_x . These variance parameters are treated as free parameters by default in PROC CALIS. You have five parameters to estimate, but the information for estimating these five parameters comes from the three

unique elements in the sample covariance matrix for X and Y . Hence, your model is in the so-called underidentification situation. Model identification is discussed in more detail in the section “[Model Identification](#)” on page 291.

To make the current model identified, you can put constraints on some parameters. This reduces the number of independent parameters to estimate in the model. In the errors-in-variables model for the corn data, the variance of Ex (measurement error for X) is given as the constant value 57, which was obtained from a previous study. This could still be applied in the current model with measurement errors in both X and Y . In addition, if you are willing to accept the assumption that the structural equation model is (almost) deterministic, then the variance of Dfy could be set to 0. With these two parameter constraints, the current model is just-identified. That is, you can now estimate three free parameters from three distinct covariance elements in the data. The following statements show the LINEQS model specification for this just-identified model:

```
proc calis data=corn;
  lineqs
    Fy = beta * Fx + Dfy,
    Y  = 1.   * Fy + Ey,
    X  = 1.   * Fx + Ex;
  variance
    Ex = 57.,
    Dfy = 0.;
run;
```

Figure 17.6 shows the estimation results.

Figure 17.6 Regression Model With Measurement Errors in X and Y for Corn Data

Linear Equations					
	Fy	=	0.4232*Fx	+	1.0000 Dfy
	Std Err		0.1658 beta		
	t Value		2.5520		
	y	=	1.0000 Fy	+	1.0000 Ey
	x	=	1.0000 Fx	+	1.0000 Ex
Estimates for Variances of Exogenous Variables					
Variable Type	Variable	Parameter	Estimate	Standard Error	t Value
Error	Ex		57.00000		
Disturbance	Dfy		0		
Latent	Fx	_Add1	247.85450	136.33508	1.81798
Error	Ey	_Add2	43.29105	23.92488	1.80946

In Figure 17.6, the estimate of beta is 0.4232, which is basically the same as the estimate for beta in the errors-in-variables model shown in Figure 17.4. The estimated variances for Fx and Ey match for the two models too. In fact, it is not difficult to show mathematically that the current constrained model with measurements errors in both Y and X is equivalent to the errors-in-variables model for the corn data. The numerical results merely confirm this fact.

It is important to emphasize that the equivalence shown here is not a general statement about the current model with measurement errors in X and Y and the errors-in-variables model. Essentially, the equivalence of the two models as applied to the corn data is due to those constraints imposed on the measurement error variances for Df_y and Ex . The more important implication from these two analyses is that for the model with measurement errors in both X and Y , you need to set more parameter constraints to make the model identified. Some constraints might be substantively meaningful, while others might need strong or risky assumptions.

For example, setting the variance of Ex to 57 is substantively meaningful because it is based on a prior study. However, setting the variance of Df_y to 0 implies the acceptance of the deterministic structural model, which could be a rather risky assumption in most practical situations. It turns out that using these two constraints together for the model identification of the regression with measurement errors in both X and Y does not give you more substantively important information than what the errors-in-variables model has already given you (compare [Figure 17.6](#) with [Figure 17.4](#)). Therefore, the set of identification constraints you use might be important in at least two aspects. First, it might lead to an identified model if you set them properly. Second, given that the model is identified, the meaningfulness of your model depends on how reasonable your identification constraints are.

The two identification constraints set on the regression model with measurement errors in both X and Y make the model identified. But they do not lead to model estimates that are more informative than that of the errors-in-variables regression. Some other sets of identification constraints, if available, might have been more informative. For example, if there were a prior study about the measurement error variance of corn yields (Y), a fixed constant for the variance of Ey could have been set, instead of the unrealistic zero variance constraint of Df_y . This way the estimation results of the regression model with measurement errors in both X and Y would offer you something different from the errors-in-variables regression.

Setting identification constraints could be based on convention or other arguments. See the section “[Illustration of Model Identification: Spleen Data](#)” on page 292 for an example where model identification is attained by setting constant error variances for X and Y in the model. For the corn data, you have seen that fixing the error variance of the predictor variable led to model identification of the errors-in-variables model. In this case, prior knowledge about the measurement error variance is necessary. This necessity is partly due to the fact that each latent true score variable has only one observed variable as its indicator measure. When you have more measurement indicators for the same latent factor, fixing the measurement error variances to constants for model identification would not be necessary. This is the modeling scenario assumed by the LISREL model (see the section “[Fitting LISREL Models by the LISMOD Modeling Language](#)” on page 336), of which the confirmatory factor model is a special case. The confirmatory factor model is described and illustrated in the section “[The FACTOR and RAM Modeling Languages](#)” on page 313.

Model Identification

As discussed in the preceding section, if you try to fit the errors-in-variables model with measurement errors in both X and Y without applying certain constraints, the model is not identified and you cannot obtain unique estimates of the parameters. For example, the errors-in-variables model with measurement errors in both X and Y has five parameters (one coefficient β and four variances). The covariance matrix of the observed variables Y and X has only three elements that are free to vary, since $\text{Cov}(Y,X)=\text{Cov}(X,Y)$. Therefore, the covariance structure can be expressed as three equations in five unknown parameters. Since

there are fewer equations than unknowns, there are many different sets of values for the parameters that provide a solution for the equations. Such a model is said to be underidentified.

If the number of parameters equals the number of free elements in the covariance matrix, then there might exist a unique set of parameter estimates that exactly reproduce the observed covariance matrix. In this case, the model is said to be just-identified or saturated.

If the number of parameters is less than the number of free elements in the covariance matrix, there might exist no set of parameter estimates that reproduces the observed covariance matrix exactly. In this case, the model is said to be overidentified. Various statistical criteria, such as maximum likelihood, can be used to choose parameter estimates that approximately reproduce the observed covariance matrix. If you use ML, FIML, GLS, or WLS estimation, PROC CALIS can perform a statistical test of the goodness of fit of the model under the certain statistical assumptions.

If the model is just-identified or overidentified, it is said to be identified. If you use ML, FIML, GLS, or WLS estimation for an identified model, PROC CALIS can compute approximate standard errors for the parameter estimates. For underidentified models, PROC CALIS obtains approximate standard errors by imposing additional constraints resulting from the use of a generalized inverse of the Hessian matrix.

You cannot guarantee that a model is identified simply by counting the parameters. For example, for any latent variable, you must specify a numeric value for the variance, or for some covariance involving the variable, or for a coefficient of an indicator variable. Otherwise, the scale of the latent variable is indeterminate, and the model is underidentified regardless of the number of parameters and the size of the covariance matrix. As another example, an exploratory factor analysis with two or more common factors is always underidentified because you can rotate the common factors without affecting the fit of the model.

PROC CALIS can usually detect an underidentified model by computing the approximate covariance matrix of the parameter estimates and checking whether any estimate is linearly related to other estimates (Bollen 1989, pp. 248–250), in which case PROC CALIS displays equations showing the linear relationships among the estimates. Another way to obtain empirical evidence regarding the identification of a model is to run the analysis several times with different initial estimates to see whether the same final estimates are obtained. Bollen (1989) provides detailed discussions of conditions for identification in a variety of models.

Illustration of Model Identification: Spleen Data

When your model involves measurement errors in variables and you need to use latent true scores in the regression or structural equation, you might encounter some model identification problems in estimation if you do not put certain identification constraints in the model. An example is shown in the section “[Regression with Measurement Errors in \$X\$ and \$Y\$](#) ” on page 289 for the corn data. You “solved” the problem by assuming a deterministic model with perfect prediction in the structural model. However, this assumption could be very risky and does not lead to estimation results that are substantively different from the model with measurement error only in X .

This section shows how you can apply another set of constraints to make the measurement model with errors in both X and Y identified without assuming the deterministic structural model. First, the identification problem is illustrated here again in light of the PROC CALIS diagnostics.

The following example is inspired by Fuller (1987, pp. 40–41). The hypothetical data are counts of two types of cells in spleen samples: cells that form rosettes and nucleated cells. It is reasonable to assume that counts have a Poisson distribution; hence, the square roots of the counts should have a constant error

variance of 0.25. You can use PROC CALIS to fit this regression model with measurement errors in X and Y to the data. (See the section “Regression with Measurement Errors in X and Y ” on page 289 for model definitions.) However, before fitting this target model, it is illustrative to see what would happen if you do not assume the constant error variance.

The following statements show the LINEQS specification of an errors-in-variables regression model for the square roots of the counts without constraints on the parameters:

```

data spleen;
  input rosette nucleate;
  sqrtrose=sqrt(rosette);
  sqrtnucl=sqrt(nucleate);
  datalines;
4 62
5 87
5 117
6 142
8 212
9 120
12 254
13 179
15 125
19 182
28 301
51 357
;

proc calis data=spleen;
  lineqs factrose = beta * factnucl + disturb,
         sqrtrose =          factrose + err_rose,
         sqrtnucl =          factnucl + err_nucl;
  variance
         factnucl = v_factnucl,
         disturb  = v_disturb,
         err_rose = v_rose,
         err_nucl = v_nucl;
run;

```

This model is underidentified. You have five parameters to estimate in the model, but the number of distinct covariance elements is only three.

In the LINEQS statement, you specify the structural equation and then two measurement equations. In the structural equation, the variables `factrose` and `factnucl` are latent true scores for the corresponding measurements in `sqrtrose` and `sqrtnucl`, respectively. The structural equation represents the true variable relationship of interest. You name the regression coefficient parameter as `beta` and the error term as `disturb` in the structural model. (For structural equations, you can use names with prefix ‘D’ or ‘d’ to denote error terms.) The variance of `factnucl` and the variance of `disturb` are also parameters in the model. You name these variance parameters as `v_factnucl` and `v_disturb` in the VARIANCE statement. Therefore, you have three parameters in the structural equation.

In the measurement equations, the observed variables `sqrtrose` and `sqrtnucl` are specified as the sums of their corresponding true latent scores and error terms, respectively. The error variances are also parameters in the model. You name them as `v_rose` and `v_nucl` in the VARIANCE statement. Now, together with the three parameters in the structural equation, you have a total of five parameters in your model.

All variance specifications in the VARIANCE statement are actually optional in PROC CALIS. They are free parameters by default. In this example, it is useful to name these parameters so that explicit references to these parameters can be made in the following discussion.

PROC CALIS displays the following warning when you fit this underidentified model:

```
WARNING: Estimation problem not identified: More parameters to
estimate ( 5 ) than the total number of mean and
covariance elements ( 3 ).
```

In this warning, the three covariance elements refer to the sample variances of `sqrtrose` and `sqrtnucl` and their covariance. PROC CALIS diagnoses the parameter indeterminacy as follows:

```
NOTE: Covariance matrix for the estimates is not full rank.
NOTE: The variance of some parameter estimates is zero or
some parameter estimates are linearly related to other
parameter estimates as shown in the following equations:
```

```
v_rose      =      -0.147856  +      0.447307  *  v_disturb
v_nucl      =     -110.923690  -      0.374367  *  beta      +
              10.353896  *  v_factnucl  +  1.536613  *  v_disturb
```

With the warning and the notes, you are now certain that the model is underidentified and you cannot interpret your parameter estimates meaningfully.

Now, to make the model identified, you set the error variances to 0.25 in the VARIANCE statement, as shown in the following specification:

```
proc calis data=spleen residual;
  lineqs factrose = beta * factnucl + disturb,
  sqrtrose = factrose + err_rose,
  sqrtnucl = factnucl + err_nucl;
  variance
    factnucl = v_factnucl,
    disturb = v_disturb,
    err_rose = 0.25,
    err_nucl = 0.25;
run;
```

In the specification, you use the RESIDUAL option in the PROC CALIS statement to request the residual analysis. An annotated fit summary is shown in Figure 17.7.

Figure 17.7 Spleen Data: Annotated Fit Summary for the Just-Identified Model

Fit Summary	
Chi-Square	0.0000
Chi-Square DF	0
Pr > Chi-Square	.

You notice that the model fit chi-square is 0 and the corresponding degrees of freedom is also 0. This indicates that your model is “just” identified, or your model is saturated—you have three distinct elements in the sample covariance matrix for the estimation of three parameters in the model. In the PROC CALIS results, you no longer see the warning message about underidentification or any notes about linear dependence in parameters.

For just-identified or saturated models like the current case, you expect to get zero residuals in the covariance matrix, as shown in Figure 17.8:

Figure 17.8 Spleen Data: Residuals for the Just-identified Model

Raw Residual Matrix		
	sqrtrose	sqrtnucl
sqrtrose	0.00000	0.00000
sqrtnucl	0.00000	0.00000

Residuals are the differences between the fitted covariance matrix and the sample covariance matrix. When the residuals are all zero, the fitted covariance matrix matches the sample covariance matrix perfectly (the parameter estimates reproduce the sample covariance matrix exactly).

You can now interpret the estimation results of this just-identified model, as shown in Figure 17.9:

Figure 17.9 Spleen Data: Parameter Estimated for the Just-Identified Model

Linear Equations					
factrose =	0.3907*factnucl +	1.0000	disturb		
Std Err	0.0771	beta			
t Value	5.0692				
sqrtrose =	1.0000	factrose +	1.0000	err_rose	
sqrtnucl =	1.0000	factnucl +	1.0000	err_nucl	
Estimates for Variances of Exogenous Variables					
Variable Type	Variable	Parameter	Estimate	Standard Error	t Value
Latent	factnucl	v_factnucl	10.50458	4.58577	2.29069
Disturbance	disturb	v_disturb	0.38153	0.28556	1.33607
Error	err_rose		0.25000		
	err_nucl		0.25000		

Notice that because the error variance parameters for variables `err_rose` and `err_nucl` are fixed constants in the model, there are no standard error estimates for them in Figure 17.9. For the current application, the estimation results of the just-identified model are those you would interpret and report. However, to completely illustrate model identification, an additional constraint is imposed to show an overidentified model. In the section “Regression with Measurement Errors in X and Y” on page 289, you impose a zero-

variance constraint on the disturbance variable Dfy for the model identification. Would this constraint be necessary here for the spleen data too? The answer is no because with the two constraints on the variances of `err_rose` and `err_nucl`, the model has already been meaningfully specified and identified. Adding more constraints such as a zero variance for `disturb` would make the model overidentified unnecessarily. The following statements show the specification of such an overidentified model for the spleen data:

```
proc calis data=spleen residual;
  lineqs factrose = beta * factnucl + disturb,
        sqrtrose =      factrose + err_rose,
        sqrtnucl =      factnucl + err_nucl;
  variance
    factnucl = v_factnucl,
    disturb  = 0.,
    err_rose = 0.25,
    err_nucl = 0.25;
run;
```

An annotated fit summary table for the overidentified model is shown in Figure 17.10.

Figure 17.10 Spleen Data: Annotated Fit Summary for the Overidentified Model

Fit Summary	
Chi-Square	5.2522
Chi-Square DF	1
Pr > Chi-Square	0.0219
Standardized RMR (SRMR)	0.0745
Adjusted GFI (AGFI)	0.1821
RMSEA Estimate	0.6217
Bentler Comparative Fit Index	0.6535

The chi-square is 5.2522 ($df=1$, $p=0.0219$). Overall, the model does not provide a good fit. The sample size is so small that the p -value of the chi-square test should not be taken to be accurate, but to get a small p -value with such a small sample indicates that it is possible that the model is seriously deficient.

This same conclusion can be drawn by looking at other fit indices in the table. In Figure 17.10, several fit indices are computed for the model. For example, the standardized root mean square residual (SRMSR) is 0.0745 and the adjusted goodness of fit (AGFI) is 0.1821. By conventions, a good model should have an SRMSR smaller than 0.05 and an AGFI larger than 0.90. The root mean square error of approximation (RMSEA) (Steiger and Lind 1980) is 0.6217, but an RMSEA below 0.05 is recommended for a good model fit (Browne and Cudeck 1993). The comparative fit index (CFI) is 0.6535, which is also low as compared to the acceptable level at 0.90.

When you fit an overidentified model, usually you do not find estimates that match the sample covariance matrix exactly. The discrepancies between the fitted covariance matrix and the sample covariance matrix are shown as residuals in the covariance matrix, as shown in Figure 17.11.

Figure 17.11 Spleen Data: Residuals for the Overidentified Model

Raw Residual Matrix		
	sqrtrose	sqrtnucl
sqrtrose	0.28345	-0.11434
sqrtnucl	-0.11434	0.04613

As you can see in Figure 17.11, the residuals are nonzero. This indicates that the parameter estimates do not reproduce the sample covariance matrix exactly. For overidentified models, nonzero residuals would be the norm rather than exception, but the general goal is to find the “best” set of estimates so that the residuals are as small as possible.

The parameter estimates are shown in Figure 17.12.

Figure 17.12 Spleen Data: Parameter Estimated for the Overidentified Model

Linear Equations					
	factrose =	0.4034*factnucl +	1.0000	disturb	
	Std Err	0.0508	beta		
	t Value	7.9439			
	sqrtrose =	1.0000	factrose +	1.0000	err_rose
	sqrtnucl =	1.0000	factnucl +	1.0000	err_nucl
Estimates for Variances of Exogenous Variables					
Variable Type	Variable	Parameter	Estimate	Standard Error	t Value
Latent	factnucl	v_factnucl	10.45846	4.56608	2.29047
Disturbance	disturb		0		
Error	err_rose		0.25000		
	err_nucl		0.25000		

The estimate of beta in this model is 0.4034. Given that the model fit is bad and the zero variance for the error term disturb is unreasonable, beta could have been overestimated in the current overidentified model, as compared with the just-identified model, where the estimate of beta is only 0.3907. In summary, both the fit summary and the estimation results indicate that the zero variance for disturb in the overidentified model for the spleen data has been imposed unreasonably.

The purpose of the current illustration is not that you should not consider an overidentified model for your data in general. Quite the opposite, in practical structural equation modeling it is usually the overidentified models that are of the paramount interest. You can test or gauge the model fit of overidentified models. Good overidentified models enable you to establish scientific theories that are precise and general. However, most fit indices are not meaningful when applied to just-identified saturated models. Also, even though you always get zero residuals for just-identified saturated models, those models usually are not precise enough to be a scientific theory.

The overidentified model for the spleen data highlights the importance of setting meaningful identification constraints. Whether your resulting model is just-identified or overidentified, it is recommended that you do the following:

- Give priorities to those identification constraints that are derived from prior studies, substantive grounds, or mathematical basis.
- Avoid making unnecessary identification constraints that might bias your model estimation.

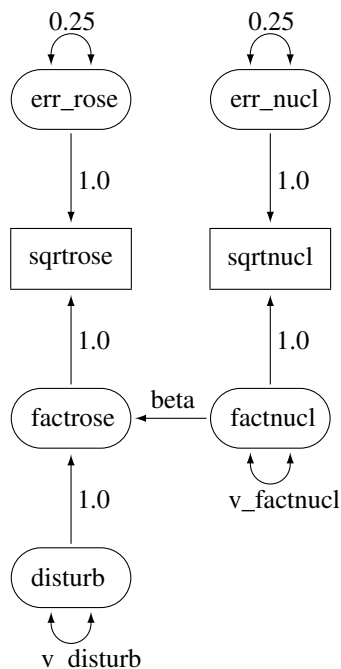
Path Diagrams and Path Analysis

Sections “Errors-in-Variables Regression” on page 286, “Regression with Measurement Errors in X and Y ” on page 289, and “Illustration of Model Identification: Spleen Data” on page 292 show how you can specify models by means of equations in the LINEQS modeling language. This section shows you how to specify models that are represented by path diagrams. The PATH modeling language of PROC CALIS is the main tool for this purpose.

Complicated models are often easier to understand when they are expressed as path diagrams. One advantage of path diagrams over equations is that variances and covariances can be shown directly in the path diagram. Loehlin (1987) provides a detailed discussion of path diagrams. Another advantage is that the path diagram can be transcribed easily into the PATH modeling language supported by PROC CALIS.

A path diagram for the spleen data is shown in Figure 17.13. It explicitly shows all latent variables (including error terms) and variances of exogenous variables.

Figure 17.13 Path Diagram: Spleen Data



The path diagram shown in [Figure 17.13](#) is essentially a graphical representation of the same just-identified model for the spleen data that is described in the section “[Illustration of Model Identification: Spleen Data](#)” on page 292. In path diagrams, it is customary to write the names of manifest or observed variables in rectangles and the names of latent variables in ovals. For example, `sqrtrose` and `sqrtnucl` are observed variables in the path diagram, while all others are latent variables.

The effects (the regression coefficients) in each equation are indicated by drawing arrows from the predictor variables to the outcome variable. For example, the path from `factnucl` to `factrose` is labeled with the regression coefficient β in the path diagram shown in [Figure 17.13](#). Other paths are labeled with fixed coefficients (or effects) of 1.

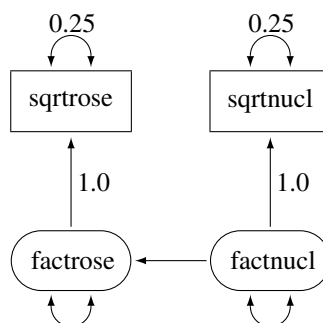
Variances of exogenous variables are drawn as double-headed arrows in [Figure 17.13](#). For example, the variance of `disturb` is shown as a double-headed arrow pointing to the variable itself and is named `v_disturb`. Variances of the `err_nucl` and `err_rose` are also drawn as double-headed arrows but are labeled with fixed constants 0.25.

The path diagram shown in [Figure 17.13](#) matches the features in the LINEQS model closely. For example, the error terms are depicted explicitly and their paths (regression coefficients) that connect to the associated endogenous variables are marked with fixed constants 1, reflecting the same specification in the equations of the LINEQS model. However, you can simplify the path diagram by using McArdle’s RAM (reticular action model) notation (McArdle and McDonald 1984), as described in the following section.

A Simplified Path Diagram for the Spleen Data

The main simplification in the path diagram is to drop all the error terms in the model. Instead, error variances are treated as residual (or partial) variances for the endogenous variables in the model or path diagram. Hence, in the path diagrams for RAM models, error variances are also represented by double-headed arrows directly attached to the endogenous variables, which is the same way you represent variances for the exogenous variables. The RAM model convention leads to a simplified representation of the path diagram for the spleen data, as shown in [Figure 17.14](#).

Figure 17.14 Simplified Path Diagram: Spleen



Another simplification done in [Figure 17.14](#) is the omission of the parameter labeling in the path diagram. This simplification is not a part of the RAM notation. It is just a convention in PROC CALIS that you can omit the unconstrained parameter names without affecting the meaning of the model. Hence, the parameter

names `beta`, `v_disturb`, and `v_factnucl` are no longer necessary in the simplified path diagram [Figure 17.14](#). As you can see, this convention makes the task of model specification considerably simpler and easier.

The following statements show the specification of the simplified path diagram in [Figure 17.14](#):

```
proc calis data=spleen;
  path
    sqrtrose <=== factrose   = 1.0,
    sqrtnucl  <=== factnucl  = 1.0,
    factrose  <=== factnucl  ;
  pvar
    sqrtrose = 0.25,      /* error variance for sqrtrose */
    sqrtnucl = 0.25,      /* error variance for sqrtnucl */
    factrose,              /* disturbance/error variance for factrose */
    factnucl;              /* variance of factnucl */
run;
```

The PATH statement invokes the PATH modeling language of PROC CALIS. In the PATH modeling language, each entry of specification corresponds to either a single- or double-headed arrow specification in the path diagram shown in [Figure 17.14](#), as explained in the following:

- The PATH statement enables you to specify each of the single-headed arrows (paths) as path entries, which are separated by commas. You have three single-headed arrows in the path diagram and therefore you have three path entries in the PATH statement. The path entries “`sqrtrose <=== factrose`” and “`sqrtnucl <=== factnucl`” are followed by the constant 1, indicating fixed path coefficients. The path “`factrose <=== factnucl`” is also specified, but without giving a fixed value or a parameter name. By default, this path entry is associated with a free parameter for the effect or path coefficient.
- The PVAR statement enables you to specify each of the double-headed arrows with both heads pointing to the *same* variable, exogenous or endogenous. This type of arrows represents variances or error variances. You have four such double-headed arrows in the path diagram, and therefore there are four corresponding entries under the PVAR statement. Two of them are assigned with fixed constants (0.25), and the remaining two (error variance of `factrose` and variance of `factnucl`) are free variance parameters.
- The PCOV statement enables you to specify each of the double-headed arrows with its heads pointing to *different* variables, exogenous or endogenous. This type of arrows represents covariances between variables or their error terms. You do not have this type of double-headed arrows in the current path diagram, and therefore you do not need a PCOV statement for the corresponding model specification.

The estimation results are shown in [Figure 17.15](#). Essentially, these are exactly the same estimation results as those that result from the LINEQS modeling language for the just-identified model in section “[Illustration of Model Identification: Spleen Data](#)” on page 292.

Figure 17.15 Spleen Data: RAM Model

PATH List					
-----Path-----	Parameter	Estimate	Standard Error	t Value	
sqrtrose <=== factrose		1.00000			
sqrtnucl <=== factnucl		1.00000			
factrose <=== factnucl	_Parm1	0.39074	0.07708	5.06920	
Variance Parameters					
Variance Type	Variable	Parameter	Estimate	Standard Error	t Value
Error	sqrtrose		0.25000		
	sqrtnucl		0.25000		
	factrose	_Parm2	0.38153	0.28556	1.33607
Exogenous	factnucl	_Parm3	10.50458	4.58577	2.29069

Notice in Figure 17.15 that the path coefficient for path “factrose <=== factnucl” is given a parameter name `_Parm1`, which is generated automatically by PROC CALIS. This is the same beta parameter of the LINEQS model in the section “Illustration of Model Identification: Spleen Data” on page 292. Also, the variance parameters `_Parm2` and `_Parm3` in Figure 17.15 are the same `v_disturb` and `v_factnucl` parameters, respectively, in the preceding LINEQS model.

In PROC CALIS, using parameter names to specify free parameters is optional. Parameter names are generated for free parameters by default. Or, if you choose parameter names for your own convenience, you can do so without changing the model specification. For example, you can specify the preceding PATH model equivalently by adding the desired parameter names, as shown in the following statements:

```
proc calis data=spleen;
  path
    sqrtrose <=== factrose = 1.0,
    sqrtnucl <=== factnucl = 1.0,
    factrose <=== factnucl = beta;
  pvar
    sqrtrose = 0.25,          /* error variance for sqrtrose */
    sqrtnucl = 0.25,          /* error variance for sqrtnucl */
    factrose = v_disturb,     /* disturbance/error variance for factrose */
    factnucl = v_factnucl;    /* variance of factnucl */
run;
```


A path diagram provides you an easy and conceptual way to represent your model, while the PATH modeling language in PROC CALIS offers you an easy way to input your path diagram in a non-graphical fashion. This is especially useful for models with more complicated path structures. See the section “A Combined Measurement-Structural Model” on page 320 for a more elaborated example of the PATH model application.

The next section provides examples of the PATH model applied to classical test theory.

Some Measurement Models

In the section “Regression with Measurement Errors in X and Y ” on page 289, outcome variables and predictor variables are assumed to have been measured with errors. In order to study the true relationships among the true scores variables, models for measurement errors are also incorporated into the estimation. The context of applications is that of regression or econometric analysis.

In the social and behavioral sciences, the same kind of model is developed in the context of test theory or item construction for measuring cognitive abilities, personality traits, or other latent variables. This kind of modeling is better-known as measurement models or confirmatory factor analysis (these two terms are interchangeable) in the psychometric field. Usually, applications in the social and behavioral sciences involve a much larger number of observed variables. This section considers some of these measurement or confirmatory factor-analytic models. For illustration purposes, only a handful of variables are used in the examples. Applications that use the PATH modeling language in PROC CALIS are described.

H4: Full Measurement Model for Lord Data

Psychometric test theory involves many kinds of models that relate scores on psychological and educational tests to latent variables that represent intelligence or various underlying abilities. The following example uses data on four vocabulary tests from Lord (1957). Tests W and X have 15 items each and are administered with very liberal time limits. Tests Y and Z have 75 items and are administered under time pressure. The covariance matrix is read by the following DATA step:

```
data lord(type=cov);
  input _type_ $ _name_ $ W X Y Z;
  datalines;
n      . 649      .      .      .
cov W  86.3979   .      .      .
cov X  57.7751  86.2632   .      .
cov Y  56.8651  59.3177  97.2850   .
cov Z  58.8986  59.6683  73.8201  97.8192
;
```

The psychometric model of interest states that W and X are determined by a single common factor F_1 , and Y and Z are determined by a single common factor F_2 . The two common factors are expected to have a positive correlation, and it is desired to estimate this correlation. It is convenient to assume that the common factors have unit variance, so their correlation will be equal to their covariance. The error terms for all the manifest variables are assumed to be uncorrelated with each other and with the common factors. The model equations are

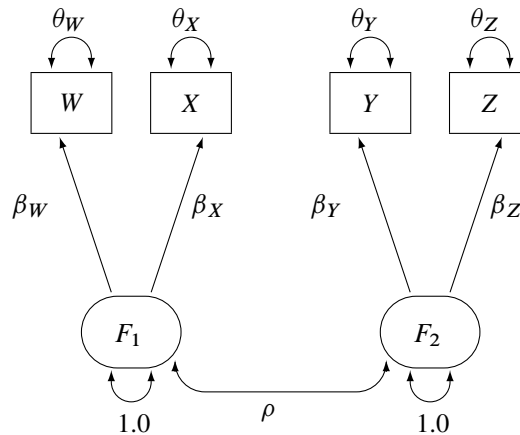
$$\begin{aligned}
 W &= \beta_W F_1 + E_W \\
 X &= \beta_X F_1 + E_X \\
 Y &= \beta_Y F_2 + E_Y \\
 Z &= \beta_Z F_2 + E_Z
 \end{aligned}$$

with the following assumptions:

$$\begin{aligned}
 \text{Var}(F_1) &= \text{Var}(F_2) = 1 \\
 \text{Cov}(F_1, F_2) &= \rho \\
 \text{Cov}(E_W, E_X) &= \text{Cov}(E_W, E_Y) = \text{Cov}(E_W, E_Z) = \text{Cov}(E_X, E_Y) \\
 &= \text{Cov}(E_X, E_Z) = \text{Cov}(E_Y, E_Z) = \text{Cov}(E_W, F_1) \\
 &= \text{Cov}(E_W, F_2) = \text{Cov}(E_X, F_1) = \text{Cov}(E_X, F_2) \\
 &= \text{Cov}(E_Y, F_1) = \text{Cov}(E_Y, F_2) = \text{Cov}(E_Z, F_1) \\
 &= \text{Cov}(E_Z, F_2) = 0
 \end{aligned}$$

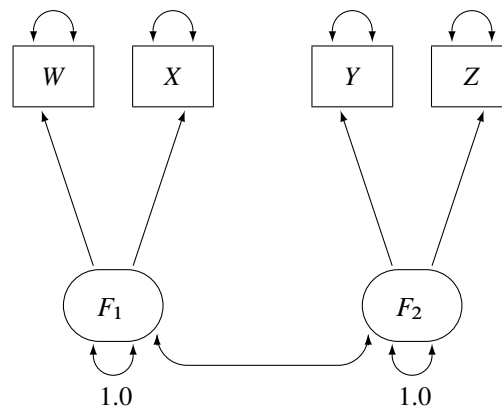
The corresponding path diagram is shown in Figure 17.16.

Figure 17.16 Path Diagram: Lord Data



In Figure 17.16, error terms are not explicitly represented, but error variances for the observed variables are represented by double-headed arrows that point to the variables. The error variance parameters in the model are labeled with θ_W , θ_X , θ_Y , and θ_Z , respectively, for the four observed variables. In the terminology of confirmatory factor analysis, these four variables are called indicators of the corresponding latent factors F_1 and F_2 .

Figure 17.16 represents the model equations clearly. It includes all the variables and the parameters in the diagram. However, sometimes researchers represent the same model with a simplified path diagram in which unconstrained parameters are not labeled, as shown in Figure 17.17.

Figure 17.17 Simplified Path Diagram: Lord Data

This simplified representation is also compatible with the PATH modeling language of PROC CALIS. In fact, this might be an easier starting point for modelers. With the following rules, the conversion from the path diagram to the PATH model specification is very straightforward:

- Each single-headed arrow in the path diagram is specified in the PATH statement.
- Each double-headed arrow that points to a single variable is specified in the PVAR statement.
- Each double-headed arrow that points to two distinct variables is specified in the PCOV statement.

Hence, you can convert the simplified path diagram in [Figure 17.17](#) easily to the following PATH model specification:

```
proc calis data=lord;
  path
    W <=== F1,
    X <=== F1,
    Y <=== F2,
    Z <=== F2;
  pvar
    F1 = 1.0,
    F2 = 1.0,
    W X Y Z;
  pcov
    F1 F2;
run;
```

In this specification, you do not need to specify the parameter names. However, you do need to specify fixed values specified in the path diagram. For example, the variances of F1 and F2 are both fixed at 1 in the PVAR statement.

These fixed variances are applied solely for the purpose of model identification. Because F1 and F2 are latent variables and their scales are arbitrary, fixing their scales are necessary for model identification. Beyond these two identification constraints, none of the parameters in the model is constrained. Therefore, this is referred to as the “full” measurement model for the Lord data.

An annotated fit summary is displayed in Figure 17.18.

Figure 17.18 Fit Summary, H4: Full Model With Two Factors for Lord Data

Fit Summary	
Chi-Square	0.7030
Chi-Square DF	1
Pr > Chi-Square	0.4018
Standardized RMR (SRMR)	0.0030
Adjusted GFI (AGFI)	0.9946
RMSEA Estimate	0.0000
Bentler Comparative Fit Index	1.0000

The chi-square value is 0.7030 ($df=1$, $p=0.4018$). This indicates that you cannot reject the hypothesized model. The standardized root mean square error (SRMSR) is 0.003, which is much smaller than the conventional 0.05 value for accepting good model fit. Similarly, the RMSEA value is virtually zero, indicating an excellent fit. The adjusted GFI (AGFI) and Bentler comparative fit index are close to 1, which also indicate an excellent model fit.

The estimation results are displayed in Figure 17.19.

Figure 17.19 Estimation Results, H4: Full Model With Two Factors for Lord Data

PATH List						
-----Path-----	Parameter	Estimate	Standard Error	t Value		
W <=== F1	_Parm1	7.50066	0.32339	23.19390		
X <=== F1	_Parm2	7.70266	0.32063	24.02354		
Y <=== F2	_Parm3	8.50947	0.32694	26.02730		
Z <=== F2	_Parm4	8.67505	0.32560	26.64301		
Variance Parameters						
Variance Type	Variable	Parameter	Estimate	Standard Error	t Value	
Exogenous	F1		1.00000			
	F2		1.00000			
Error	W	_Parm5	30.13796	2.47037	12.19979	
	X	_Parm6	26.93217	2.43065	11.08021	
	Y	_Parm7	24.87396	2.35986	10.54044	
	Z	_Parm8	22.56264	2.35028	9.60000	
Covariances Among Exogenous Variables						
Var1	Var2	Parameter	Estimate	Standard Error	t Value	
F1	F2	_Parm9	0.89855	0.01865	48.17998	

All estimates are shown with estimates of standard errors in Figure 17.19. They are all statistically significant, supporting nontrivial relationships between the observed variables and the latent factors. Notice that each free parameter in the model has been named automatically in the output. For example, the path coefficient from F1 to W is named `_Parm1`.

Two results in Figure 17.19 are particularly interesting. First, in the table for estimates of the path coefficients, `_Parm1` and `_Parm2` values form one cluster, while `_Parm3` and `_Parm4` values form another cluster. This seems to indicate that the effects from F1 on the indicators W and X could have been the same in the population and the effects from F2 on the indicators Y and Z could also have been the same in the population. Another interesting result is the estimate for the correlation between F1 and F2 (both were set to have variance 1). The correlation estimate (`_Parm9` in Figure 17.19) is 0.8986. It is so close to 1 that you wonder whether F1 and F2 could have been the same factor in the population. These estimation results can be used to motivate additional analyses for testing the suggested constrained models against new data sets. However, for illustration purposes, the same data set is used to demonstrate the additional model fitting in the subsequent sections.

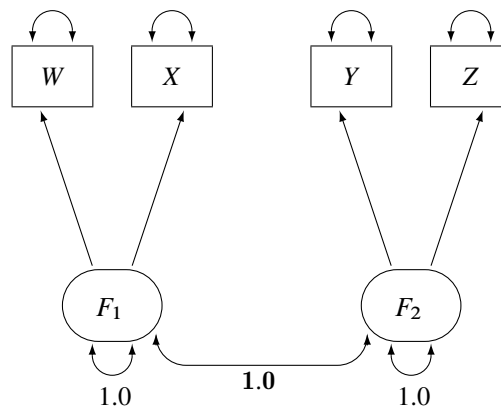
In an analysis of these data by Jöreskog and Sörbom (1979, pp. 54–56) (see also Loehlin 1987, pp. 84–87), four hypotheses are considered:

- H_1 : One-factor model with parallel tests
 $\rho = 1$
 $\beta_W = \beta_X$ and $\text{Var}(E_W) = \text{Var}(E_X)$
 $\beta_Y = \beta_Z$ and $\text{Var}(E_Y) = \text{Var}(E_Z)$
- H_2 : Two-factor model with parallel tests
 $\beta_W = \beta_X$ and $\text{Var}(E_W) = \text{Var}(E_X)$
 $\beta_Y = \beta_Z$ and $\text{Var}(E_Y) = \text{Var}(E_Z)$
- H_3 : Congeneric model: One factor without assuming parallel tests
 $\rho = 1$
- H_4 : Full model: Two factors without assuming parallel tests

These hypotheses are ordered such that the latter models are less constrained. The hypothesis H_4 is the full model that has been considered in this section. The hypothesis H_3 specifies that there is really just one common factor instead of two; in the terminology of test theory, W, X, Y, and Z are said to be congeneric. Setting the correlation ρ between F1 and F2 to 1 makes the two factors indistinguishable. The hypothesis H_2 specifies that W and X have the same true scores and have equal error variance; such tests are said to be parallel. The hypothesis H_2 also requires Y and Z to be parallel. Because ρ is not constrained to 1 in H_2 , two factors are assumed for this model. The hypothesis H_1 says that W and X are parallel tests, Y and Z are parallel tests, and all four tests are congeneric (with ρ also set to 1).

H3: Congeneric (One-Factor) Model for Lord Data

The path diagram for this congeneric (one-factor) model is shown in Figure 17.20.

Figure 17.20 H3: Congeneric (One-Factor) Model for Lord Data

The only difference between the current path diagram in [Figure 17.20](#) for the congeneric (one-factor) model and the preceding path diagram in [Figure 17.17](#) for the full (two-factor) model is that the double-headed path that connects F1 and F2 is fixed to 1 in the current path diagram. Accordingly, you need to modify only slightly the preceding PROC CALIS specification to form the new model specification, as shown in the following statements:

```
proc calis data=lord;
  path
    W <=== F1,
    X <=== F1,
    Y <=== F2,
    Z <=== F2;
  pvar
    F1 = 1.0,
    F2 = 1.0,
    W X Y Z;
  pcov
    F1 F2 = 1.0;
run;
```

This specification sets the covariance between F1 and F2 to 1.0 in the PCOV statement. An annotated fit summary is displayed in [Figure 17.21](#).

Figure 17.21 Fit Summary, H3: Congeneric (One-Factor) Model for Lord Data

Fit Summary	
Chi-Square	36.2095
Chi-Square DF	2
Pr > Chi-Square	<.0001
Standardized RMR (SRMR)	0.0277
Adjusted GFI (AGFI)	0.8570
RMSEA Estimate	0.1625
Bentler Comparative Fit Index	0.9766

The chi-square value is 36.2095 ($df = 2, p < 0.0001$). This indicates that you can reject the hypothesized model at the 0.01 α -level. The standardized root mean square error (SRMSR) is 0.0277, which indicates a good fit. Bentler's comparative fit index is 0.9766, which is also a good model fit. However, the adjusted GFI (AGFI) is 0.8570, which is not very impressive. Also, the RMSEA value is 0.1625, which is too large to be an acceptable model. Therefore, the congeneric model might not be the one you want to use.

The estimation results are displayed in Figure 17.22. Because the model does not fit well, the corresponding estimation results are not interpreted.

Figure 17.22 Estimation Results, H3: Congeneric (One-Factor) Model for Lord Data

PATH List					
-----Path-----	Parameter	Estimate	Standard Error	t Value	
W <==== F1	_Parm1	7.10470	0.32177	22.08012	
X <==== F1	_Parm2	7.26908	0.31826	22.83973	
Y <==== F2	_Parm3	8.37344	0.32542	25.73143	
Z <==== F2	_Parm4	8.51060	0.32409	26.26002	
Variance Parameters					
Variance Type	Variable	Parameter	Estimate	Standard Error	t Value
Exogenous	F1		1.00000		
	F2		1.00000		
Error	W	_Parm5	35.92111	2.41467	14.87619
	X	_Parm6	33.42373	2.31037	14.46684
	Y	_Parm7	27.17043	2.24621	12.09613
	Z	_Parm8	25.38887	2.20837	11.49664
Covariances Among Exogenous Variables					
Var1	Var2	Estimate	Standard Error	t Value	
F1	F2	1.00000			

Perhaps a more natural way to specify the model under hypothesis H_3 is to use only one factor in the PATH model, as shown in the following statements:

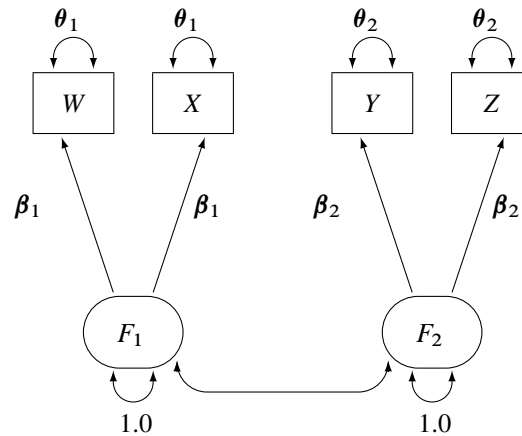
```
proc calis data=lord;
  path
    W <==== F1,
    X <==== F1,
    Y <==== F1,
    Z <==== F1;
  pvar
    F1 = 1.0,
    W X Y Z;
run;
```

This produces essentially the same results as the specification with two factors that have perfect correlation.

H2: Two-Factor Model with Parallel Tests for Lord Data

The path diagram for the two-factor model with parallel tests is shown in Figure 17.23.

Figure 17.23 H2: Two-Factor Model with Parallel Tests for Lord Data



The hypothesis H_2 requires that variables or tests under each factor are “interchangeable.” In terms of the measurement model, several pairs of parameters must be constrained to have equal estimates. That is, under the parallel-test model W and X should have the same effect or path coefficient β_1 from their common factor F_1 , and they should also have the same measurement error variance θ_1 . Similarly, Y and Z should have the same effect or path coefficient β_2 from their common factor F_2 , and they should also have the same measurement error variance θ_2 . These constraints are labeled in Figure 17.23.

You can impose each of these equality constraints by giving the same name for the parameters involved in the PATH model specification. The following statements specify the path diagram in Figure 17.23:

```
proc calis data=lord;
  path
    W <=== F1   = beta1,
    X <=== F1   = beta1,
    Y <=== F2   = beta2,
    Z <=== F2   = beta2;
  pvar
    F1 = 1.0,
    F2 = 1.0,
    W X = 2 * theta1,
    Y Z = 2 * theta2;
  pcov
    F1 F2;
run;
```

Note that the specification $2*\theta_1$ in the PVAR statement means that θ_1 is specified twice for the error variances of the two variables W and X . Similarly for the specification $2*\theta_2$. An annotated fit summary is displayed in Figure 17.24.

Figure 17.24 Fit Summary, H2: Two-Factor Model with Parallel Tests for Lord Data

Fit Summary	
Chi-Square	1.9335
Chi-Square DF	5
Pr > Chi-Square	0.8583
Standardized RMR (SRMR)	0.0076
Adjusted GFI (AGFI)	0.9970
RMSEA Estimate	0.0000
Bentler Comparative Fit Index	1.0000

The chi-square value is 1.9335 ($df=5, p=0.8583$). This indicates that you cannot reject the hypothesized model H2. The standardized root mean square error (SRMSR) is 0.0076, which indicates a very good fit. Bentler’s comparative fit index is 1.0000. The adjusted GFI (AGFI) is 0.9970, and the RMSEA is close to zero. All results indicate that this is a good model for the data.

The estimation results are displayed in Figure 17.25.

Figure 17.25 Estimation Results, H2: Two-Factor Model with Parallel Tests for Lord Data

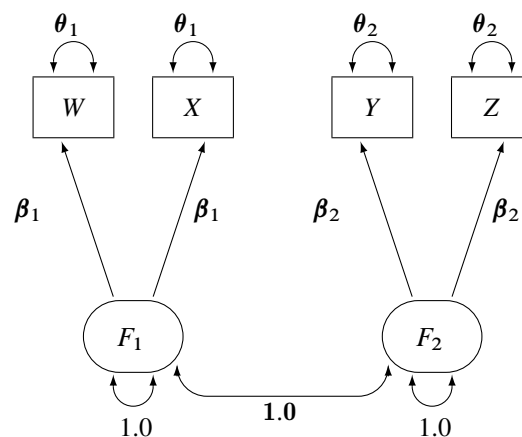
PATH List						
-----Path-----	Parameter	Estimate	Standard Error	t Value		
W <=== F1	beta1	7.60099	0.26844	28.31580		
X <=== F1	beta1	7.60099	0.26844	28.31580		
Y <=== F2	beta2	8.59186	0.27967	30.72146		
Z <=== F2	beta2	8.59186	0.27967	30.72146		
Variance Parameters						
Variance Type	Variable	Parameter	Estimate	Standard Error	t Value	
Exogenous	F1		1.00000			
	F2		1.00000			
Error	W	theta1	28.55545	1.58641	18.00000	
	X	theta1	28.55545	1.58641	18.00000	
	Y	theta2	23.73200	1.31844	18.00000	
	Z	theta2	23.73200	1.31844	18.00000	
Covariances Among Exogenous Variables						
Var1	Var2	Parameter	Estimate	Standard Error	t Value	
F1	F2	_Parm1	0.89864	0.01865	48.18011	

Notice that because you explicitly specify the parameter names for the path coefficients (that is, β_1 and β_2), they are used in the output shown in Figure 17.25. The correlation between F_1 and F_2 is 0.8987, which is a very high correlation that suggests F_1 and F_2 might have been the same factor in the population. The next section sets this value to one so that the current model becomes a one-factor model with parallel tests.

H1: One-Factor Model with Parallel Tests for Lord Data

The path diagram for the one-factor model with parallel tests is shown in Figure 17.26.

Figure 17.26 H1: One-Factor Model with Parallel Tests for Lord Data



The hypothesis H_1 differs from H_2 in that F_1 and F_2 have a perfect correlation in H_1 . This is indicated by the fixed value 1.0 for the double-headed path that connects F_1 and F_2 in Figure 17.26. Again, you need only minimal modification of the preceding specification for H_2 to specify the path diagram in Figure 17.26, as shown in the following statements:

```
proc calis data=lord;
  path
    W <=== F1   = beta1,
    X <=== F1   = beta1,
    Y <=== F2   = beta2,
    Z <=== F2   = beta2;
  pvar
    F1 = 1.0,
    F2 = 1.0,
    W X = 2 * theta1,
    Y Z = 2 * theta2;
  pcov
    F1 F2 = 1.0;
run;
```

The only modification of the preceding specification is in the PCOV statement, where you put a constant 1 for the covariance between F_1 and F_2 . An annotated fit summary is displayed in Figure 17.27.

Figure 17.27 Fit Summary, H1: One-Factor Model with Parallel Tests for Lord Data

Fit Summary	
Chi-Square	37.3337
Chi-Square DF	6
Pr > Chi-Square	<.0001
Standardized RMR (SRMR)	0.0286
Adjusted GFI (AGFI)	0.9509
RMSEA Estimate	0.0898
Bentler Comparative Fit Index	0.9785

The chi-square value is 37.3337 ($df=6, p<0.0001$). This indicates that you can reject the hypothesized model H1 at the 0.01 α -level. The standardized root mean square error (SRMSR) is 0.0286, the adjusted GFI (AGFI) is 0.9509, and Bentler’s comparative fit index is 0.9785. All these indicate good model fit. However, the RMSEA is 0.0898, which does not support an acceptable model for the data.

The estimation results are displayed in Figure 17.28.

Figure 17.28 Estimation Results, H1: One-Factor Model with Parallel Tests for Lord Data

PATH List						
-----Path-----	Parameter	Estimate	Standard Error	t Value		
W <=== F1	beta1	7.18623	0.26598	27.01802		
X <=== F1	beta1	7.18623	0.26598	27.01802		
Y <=== F2	beta2	8.44198	0.28000	30.14943		
Z <=== F2	beta2	8.44198	0.28000	30.14943		
Variance Parameters						
Variance Type	Variable	Parameter	Estimate	Standard Error	t Value	
Exogenous	F1		1.00000			
	F2		1.00000			
Error	W	theta1	34.68865	1.64634	21.07010	
	X	theta1	34.68865	1.64634	21.07010	
	Y	theta2	26.28513	1.39955	18.78119	
	Z	theta2	26.28513	1.39955	18.78119	
Covariances Among Exogenous Variables						
Var1	Var2	Estimate	Standard Error	t Value		
F1	F2	1.00000				

The goodness-of-fit tests for the four hypotheses are summarized in the following table.

Hypothesis	Number of Parameters	χ^2	Degrees of Freedom	<i>p</i> -value	$\hat{\rho}$
H_1	4	37.33	6	< .0001	1.0
H_2	5	1.93	5	0.8583	0.8986
H_3	8	36.21	2	< .0001	1.0
H_4	9	0.70	1	0.4018	0.8986

Recall that the estimates of ρ for H_2 and H_4 are almost identical, about 0.90, indicating that the speeded and unspeeded tests are measuring almost the same latent variable. However, when ρ was set to 1 in H_1 and H_3 (both one-factor models), both hypotheses were rejected. Hypotheses H_2 and H_4 (both two-factor models) seem to be consistent with the data. Since H_2 is obtained by adding four constraints (for the requirement of parallel tests) to H_4 (the full model), you can test H_2 versus H_4 by computing the differences of the chi-square statistics and their degrees of freedom, yielding a chi-square of 1.23 with four degrees of freedom, which is obviously not significant. In a sense, the chi-square difference test means that representing the data by H_2 would not be significantly worse than representing the data by H_4 . In addition, because H_2 offers a more precise description of the data (with the assumption of parallel tests) than H_4 , it should be chosen because of its simplicity. In conclusion, the two-factor model with parallel tests provides the best explanation of the data.

The FACTOR and RAM Modeling Languages

In the section “Some Measurement Models” on page 302, you use the path diagram to represent the measurement models for data with cognitive tests and then you use the PATH modeling language to specify the model in PROC CALIS. You could have used other types of modeling languages for specifying the same model. In this section, the FACTOR and the RAM modeling languages are illustrated.

Specifying the Full Measurement Model (H4) by the FACTOR Modeling Language: Lord Data

The measurement models described in the section “Some Measurement Models” on page 302 are also known as confirmatory factor models. PROC CALIS has a specific modeling language, called FACTOR, for confirmatory factor models. You can use this modeling language for both exploratory and confirmatory factor analysis.

For example, the full measurement model H4 in the section “H4: Full Measurement Model for Lord Data” on page 302 can be specified equivalently by the FACTOR modeling language with the following statements:

```

proc calis data=lord;
  factor
    F1 ==> W X,
    F2 ==> Y Z;
  pvar
    F1 = 1.0,
    F2 = 1.0,
    W X Y Z;
  cov
    F1 F2;
run;

```

In the specification, you use the FACTOR statement to invoke the FACTOR modeling language. In the FACTOR statement, you specify the paths from the latent factors to the measurement indicators. For example, F1 has two paths to its indicators, W and X. Similarly, F2 has two paths to its indicators, Y and Z. Next, you use the PVAR statement to specify the variances, which is exactly the same way you use the PATH model specification in the section “H4: Full Measurement Model for Lord Data” on page 302. Lastly, you use the COV statement to specify the covariance among the factors, much like you use the PCOV statement to specify the same covariance in the PATH model specification.

Given the same confirmatory factor model, there is a major difference between the paths specified by the PATH statement and the paths specified by the FACTOR statement. In the FACTOR statement, each path must start with a latent factor followed by a right arrow and the variable list. In the PATH statement, each path can start or end with an observed or latent variable, and the direction of the arrow can be left or right.

The fit summary table for the FACTOR model is shown in [Figure 17.29](#):

Figure 17.29 Fit Summary of the Full Confirmatory Factor Model for Lord Data

Fit Summary	
Chi-Square	0.7030
Chi-Square DF	1
Pr > Chi-Square	0.4018
Standardized RMR (SRMR)	0.0030
Adjusted GFI (AGFI)	0.9946
RMSEA Estimate	0.0000
Bentler Comparative Fit Index	1.0000

This is exactly the same fit summary as shown in [Figure 17.18](#), which is for the PATH model specification. Therefore, this confirms that the same model is being fit by the FACTOR model specification.

The estimation results are shown in [Figure 17.30](#).

Figure 17.30 Estimation Results of Full Confirmatory Factor Model for Lord Data

Factor Loading Matrix: Estimate/StdErr/t-value				
		F1	F2	
W		7.5007	0	
		0.3234		
		23.1939		
		[_Parm1]		
X		7.7027	0	
		0.3206		
		24.0235		
		[_Parm2]		
Y		0	8.5095	
			0.3269	
			26.0273	
			[_Parm3]	
Z		0	8.6751	
			0.3256	
			26.6430	
			[_Parm4]	
Factor Covariance Matrix: Estimate/StdErr/t-value				
		F1	F2	
F1		1.0000	0.8986	
			0.0186	
			48.1800	
			[_Parm9]	
F2		0.8986	1.0000	
		0.0186		
		48.1800		
		[_Parm9]		
Error Variances				
Variable	Parameter	Estimate	Standard Error	t Value
W	_Parm5	30.13796	2.47037	12.19979
X	_Parm6	26.93217	2.43065	11.08021
Y	_Parm7	24.87396	2.35986	10.54044
Z	_Parm8	22.56264	2.35028	9.60000

Again, these are the same estimates as those shown in Figure 17.19, which is for the PATH model specification. The FACTOR results displayed in Figure 17.30 are arranged differently though. No paths are shown there. The relationships between the latent factors and its indicators are shown in matrix form. The factor variance and covariances are also shown in matrix form.

Specifying the Parallel Tests Model (H2) by the FACTOR Modeling Language: Lord Data

In the section “H2: Two-Factor Model with Parallel Tests for Lord Data” on page 309, you fit a two-factor model with parallel tests for the Lord data by the PATH modeling language in PROC CALIS. Some paths and error variance are constrained under the PATH model. You can also specify this parallel tests model by the FACTOR modeling language, as shown in the following statements:

```
proc calis data=lord;
  factor
    F1 ==> W X = 2 * beta1,
    F2 ==> Y Z = 2 * beta2;
  pvar
    F1 = 1.0,
    F2 = 1.0,
    W X = 2 * theta1,
    Y Z = 2 * theta2;
  cov
    F1 F2;
run;
```

In this specification, you specify some parameters explicitly. You apply the parameter beta1 to the loadings of both W and X on F1. This means that F1 has the same amount of effect on W and X. Similarly, you apply the parameter beta2 to the loadings of Y and Z on F2. The constraints on the error variances for W, X, Y, and Z in this FACTOR model specification are done in the same way as in the PATH model specification in the section “H2: Two-Factor Model with Parallel Tests for Lord Data” on page 309.

The fit summary table for this parallel tests model is shown in Figure 17.31.

Figure 17.31 Fit Summary of the Confirmatory Factor Model with Parallel Tests for Lord Data

Fit Summary	
Chi-Square	1.9335
Chi-Square DF	5
Pr > Chi-Square	0.8583
Standardized RMR (SRMR)	0.0076
Adjusted GFI (AGFI)	0.9970
RMSEA Estimate	0.0000
Bentler Comparative Fit Index	1.0000

All the fit indices shown in Figure 17.31 for the FACTOR model match the corresponding PATH model results displayed in Figure 17.24. All the estimation results in Figure 17.32 for the FACTOR model are the same as those for the corresponding PATH model in Figure 17.25.

Figure 17.32 Estimation Results of the Confirmatory Factor Model with Parallel Tests for Lord Data

Factor Loading Matrix: Estimate/StdErr/t-value				
		F1	F2	
W		7.6010	0	
		0.2684		
		28.3158		
		[beta1]		
X		7.6010	0	
		0.2684		
		28.3158		
		[beta1]		
Y		0	8.5919	
			0.2797	
			30.7215	
			[beta2]	
Z		0	8.5919	
			0.2797	
			30.7215	
			[beta2]	
Factor Covariance Matrix: Estimate/StdErr/t-value				
		F1	F2	
F1		1.0000	0.8986	
			0.0187	
			48.1801	
			[_Parm1]	
F2		0.8986	1.0000	
		0.0187		
		48.1801		
		[_Parm1]		
Error Variances				
Variable	Parameter	Estimate	Standard Error	t Value
W	theta1	28.55545	1.58641	18.00000
X	theta1	28.55545	1.58641	18.00000
Y	theta2	23.73200	1.31844	18.00000
Z	theta2	23.73200	1.31844	18.00000

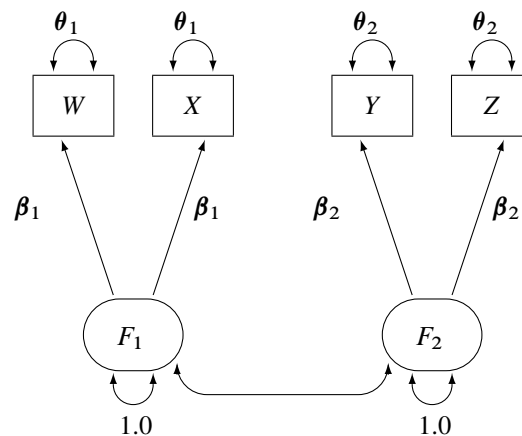
Specifying the Parallel Tests Model (H2) by the RAM Modeling Language: Lord Data

In the preceding section, you use the FACTOR modeling language of PROC CALIS to specify the parallel tests model. This model has also been specified by the PATH modeling language in the section “H2: Two-Factor Model with Parallel Tests for Lord Data” on page 309. The two specifications are equivalent; they lead to the same model fitting and estimation results. The main reason for providing two different types of modeling languages in PROC CALIS is that different researchers come from different fields of applications. Some researchers might be more comfortable with the confirmatory factor tradition, and some might equate structural equation models with path diagrams for variables.

PROC CALIS has still another modeling language that is closely related to the path diagram representation: the RAM model specification. In this section, the parallel tests model (H2) described in “H2: Two-Factor Model with Parallel Tests for Lord Data” on page 309 is used to illustrate the RAM model specification in PROC CALIS.

The path diagram for this model is reproduced in Figure 17.33.

Figure 17.33 H2: Two-Factor Model with Parallel Tests for Lord Data



The path diagram in Figure 17.33 can be readily transcribed into the RAM model specification by following these simple rules:

- Each single- or double-headed path corresponds to an entry in the RAM model specification.
- The single-headed paths are specified with the `_A_` path type or matrix keyword.
- The double-headed paths are specified with the `_P_` path type or matrix keyword.

At this point, you do not need to define the RAM model matrices `_A_` and `_P_`, as long as you recognize that they are used as keywords to distinguish different path types. There are 11 single- or double-headed paths in Figure 17.33, and therefore you expect to specify these 11 elements in the RAM model, as shown in the following statements:

```

proc calis data=lord;
  ram var = W X Y Z F1 F2, /* W=1, X=2, Y=3, Z=4, F1=5, F2=6*/
    _A_ 1 5 beta1,
    _A_ 2 5 beta1,
    _A_ 3 6 beta2,
    _A_ 4 6 beta2,
    _P_ 5 5 1.0,
    _P_ 6 6 1.0,
    _P_ 1 1 theta1,
    _P_ 2 2 theta1,
    _P_ 3 3 theta2,
    _P_ 4 4 theta2,
    _P_ 5 6 ;
run;

```

In this specification, the RAM statement invokes the RAM modeling language. The first option is the VAR= option where you specify the variables, observed and latent, in the model. The order in the VAR= variable list represents the order of these variables in the RAM model matrices. For this example, W is 1, X is 2, and so on. Next, you specify 11 RAM entries for the 11 path elements in the path diagram shown in [Figure 17.33](#).

The first four entries are for the single-headed paths. They all begin with the `_A_` keyword. In each of these `_A_` entries, you specify the variable number of the outcome variable (being pointed at), and then the variable number of the predictor variable. At the end of the entry, you can specify a parameter name, a fixed value, an initial value, or nothing. In this example, all the `_A_` entries are specified with parameter names. The first two paths are constrained because they use the same parameter name `beta1`. The next two paths are constrained because they use the same parameter name `beta2`.

The rest of the RAM entries in the example are of the `_P_` type, which is for the specification of variances or covariances in the RAM model (the double-headed arrows in the path diagram). The `_P_` entry with [5,5] is for the variance of the fifth variable, F1, on the VAR= list. This variance is fixed at 1.0 in the model, and so is the variance of the sixth variable, F2, in the next `_P_` entry.

The next four `_P_` entries are for the specification of error variances of the observed variables W, X, Y, and Z. You use the desired parameter names for constraining these parameters, as required in the parallel test model.

The last `_P_` entry in the RAM statement is for the covariance between the fifth variable (F1) and the sixth variable (F2). You specify neither a parameter name nor a fixed value at the end of this entry. By default, this empty parameter specification is treated as a free parameter in the model. A parameter name for this entry is generated by PROC CALIS.

The fit summary for this RAM model is shown in [Figure 17.34](#), and the estimation results are shown in [Figure 17.35](#).

Figure 17.34 Fit Summary of RAM Model with Parallel Tests for Lord Data

Fit Summary	
Chi-Square	1.9335
Chi-Square DF	5
Pr > Chi-Square	0.8583
Standardized RMR (SRMR)	0.0076
Adjusted GFI (AGFI)	0.9970
RMSEA Estimate	0.0000
Bentler Comparative Fit Index	1.0000

Figure 17.35 Estimation Results of RAM Model with Parallel Tests for Lord Data

RAM Pattern and Estimates								
Matrix	--Row--	-Column-	Parameter	Estimate	Standard Error	t Value		
A (1)	W	1 F1	5 beta1	7.60099	0.26844	28.31580		
	X	2 F1	5 beta1	7.60099	0.26844	28.31580		
	Y	3 F2	6 beta2	8.59186	0.27967	30.72146		
	Z	4 F2	6 beta2	8.59186	0.27967	30.72146		
P (2)	F1	5 F1	5	1.00000				
	F2	6 F2	6	1.00000				
	W	1 W	1 theta1	28.55545	1.58641	18.00000		
	X	2 X	2 theta1	28.55545	1.58641	18.00000		
	Y	3 Y	3 theta2	23.73200	1.31844	18.00000		
	Z	4 Z	4 theta2	23.73200	1.31844	18.00000		
	F1	5 F2	6 _Parm1	0.89864	0.01865	48.18011		

Again, the model fit and the estimation results match those from the PATH model specification in Figure 17.24 and Figure 17.25, and those from the FACTOR model specification in Figure 17.31 and Figure 17.32.

A Combined Measurement-Structural Model

To illustrate a more complex model, this example uses some well-known data from Haller and Butterworth (1960). Various models and analyses of these data are given by Duncan, Haller, and Portes (1968); Jöreskog and Sörbom (1988); Loehlin (1987).

The study concerns the career aspirations of high school students and how these aspirations are affected by close friends. The data are collected from 442 seventeen-year-old boys in Michigan. There are 329 boys in the sample who named another boy in the sample as a best friend. The data from these 329 boys paired with the data from their best friends are analyzed.

The method of data collection introduces two statistical problems. First, restricting the analysis to boys whose best friends are in the original sample causes the reduced sample to be biased. Second, since the data from a given boy might appear in two or more observations, the observations are not independent. Therefore, any statistical conclusions should be considered tentative. It is difficult to accurately assess the effects of the dependence of the observations on the analysis, but it could be argued on intuitive grounds that since each observation has data from two boys and since it seems likely that many of the boys appear in the data set at least twice, the effective sample size might be as small as half of the reported 329 observations.

The correlation matrix, taken from Jöreskog and Sörbom (1988), is shown in the following DATA step:

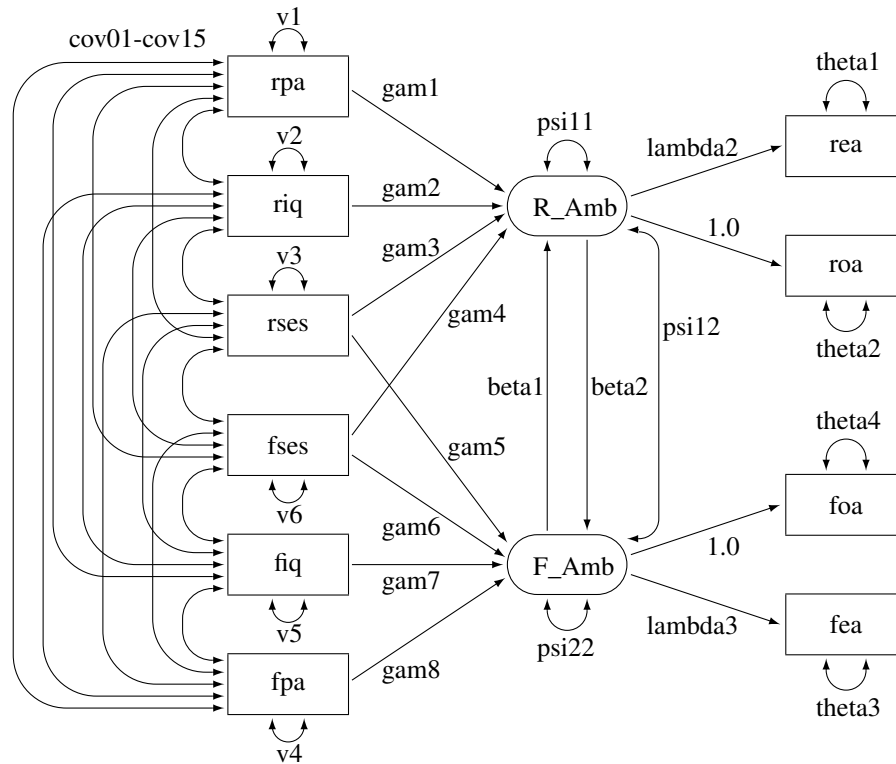
```

title 'Peer Influences on Aspiration: Haller & Butterworth (1960)';
data aspire(type=corr);
  _type_='corr';
  input _name_ $ riq rpa rses roa rea fiq fpa fses foa fea;
  label riq='Respondent: Intelligence'
        rpa='Respondent: Parental Aspiration'
        rses='Respondent: Family SES'
        roa='Respondent: Occupational Aspiration'
        rea='Respondent: Educational Aspiration'
        fiq='Friend: Intelligence'
        fpa='Friend: Parental Aspiration'
        fses='Friend: Family SES'
        foa='Friend: Occupational Aspiration'
        fea='Friend: Educational Aspiration';
  datalines;
riq  1.      .      .      .      .      .      .      .      .      .
rpa  .1839   1.      .      .      .      .      .      .      .      .
rses .2220   .0489   1.      .      .      .      .      .      .      .
roa  .4105   .2137   .3240   1.      .      .      .      .      .      .
rea  .4043   .2742   .4047   .6247   1.      .      .      .      .      .
fiq  .3355   .0782   .2302   .2995   .2863   1.      .      .      .      .
fpa  .1021   .1147   .0931   .0760   .0702   .2087   1.      .      .      .
fses .1861   .0186   .2707   .2930   .2407   .2950  -.0438   1.      .      .
foa  .2598   .0839   .2786   .4216   .3275   .5007   .1988   .3607   1.      .
fea  .2903   .1124   .3054   .3269   .3669   .5191   .2784   .4105   .6404   1.
;

```

Career Aspiration: Analysis 1

The model analyzed by Jöreskog and Sörbom (1988) is displayed in the path diagram in [Figure 17.36](#).

Figure 17.36 Path Diagram: Career Aspiration – Jöreskog and Sörbom (1988)

Two latent variables, R_Amb and F_Amb , represent the respondent's level of ambition and his best friend's level of ambition, respectively. The model states that the respondent's ambition (R_Amb) is determined by his intelligence (riq) and socioeconomic status ($rses$), his perception of his parents' aspiration for him (rpa), and his friend's socioeconomic status ($fses$) and ambition (F_Amb). It is assumed that his friend's intelligence (fiq) and parental aspiration (fpa) affect the respondent's ambition only indirectly through the friend's ambition (F_Amb). Ambition is indicated by the manifest variables of occupational (roa) and educational aspiration (rea), which are assumed to have uncorrelated residuals. The path coefficient from ambition to occupational aspiration is set to 1.0 to determine the scale of the ambition latent variable.

The path diagram shown in Figure 17.36 appears to be very complicated. Sometimes when researchers draw their path diagram with a lot of variables, they omit the covariances among exogenous variables for overall clarity. For example, the double-headed paths that represent $cov01-cov15$ in Figure 17.36 can be omitted. In addition, unconstrained variance and error variance parameters in the path diagram could be omitted without losing the pertinent information in the path diagram. For example, variance parameters $v1-v6$ and error variance parameters $theta1-theta4$ in Figure 17.36 detract from the main focus on the functional relationships of the model.

These omissions in the path diagram are in fact inconsequential when you transcribe them into the PATH model in PROC CALIS. The reason is that PROC CALIS employs several useful default parameterization rules that make the model specification process much easier and more intuitive. Here are the sets of default covariance structure parameters in the PATH modeling language:

- variances for all exogenous (observed or latent) variables

- error variances of all endogenous (observed or latent) variables
- covariances among all exogenous (observed or latent, excluding error) variables

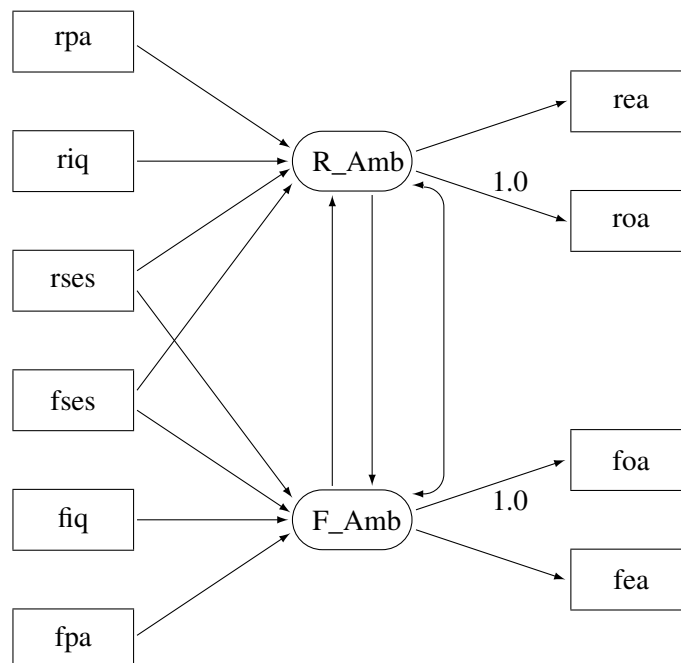
For example, these rules for setting default covariance structure parameters mean that the following sets of parameters in Figure 17.36 are optional in the path diagram representation and in the corresponding PATH model specification:

- v1–v6
- theta1–theta4, psi11, and psi22
- cov01–cov15

Note that the double-headed path labeled with psi12, which is a covariance parameter among error terms for R_Amb and F_Amb, is not a default parameter. As a result, it must be represented in the path diagram and in the PATH model specification.

Another simplification is to omit the unconstrained parameter names in the path diagram. In the PATH model specification, an “unnamed” parameter is a free parameter by default—there is no need to give unique names to denote free parameters. With all the mentioned simplifications, you can depict your path diagram simply as the one in Figure 17.37.

Figure 17.37 Simplified Path Diagram for Career Aspiration : Analysis 1



The simplified path diagram in Figure 17.37 is readily transcribed into the PATH model as shown in the following statements:

```

proc calis data=aspire nobs=329;
  path
    /* structural model of influences */
    R_Amb <=== rpa      ,
    R_Amb <=== riq      ,
    R_Amb <=== rses     ,
    R_Amb <=== fses     ,
    F_Amb <=== rses     ,
    F_Amb <=== fses     ,
    F_Amb <=== fiq      ,
    F_Amb <=== fpa      ,
    R_Amb <=== F_Amb    ,
    F_Amb <=== R_Amb    ,

    /* measurement model for aspiration */
    rea <=== R_Amb      ,
    roa <=== R_Amb = 1.,
    foa <=== F_Amb = 1.,
    fea <=== F_Amb      ;
  pcov
    R_Amb F_Amb;
run;

```

Again, because you have 15 paths (single- or double- headed) in the path diagram, you expect that there are 15 entries in the PATH and the PCOV statements. Essentially, in this PATH model specification you specify all the functional relationships (single-headed arrows) in the path diagram and the covariance of error terms (double-headed arrows) for R_Amb and F_Amb.

Since this TYPE=CORR data set does not contain an observation with _TYPE_=N giving the sample size, it is necessary to specify the NOBS= option in the PROC CALIS statement.

The fit summary is displayed in Figure 17.38, and the estimation results are displayed in Figure 17.39.

Figure 17.38 Career Aspiration Data: Fit Summary for Analysis 1

Fit Summary	
Chi-Square	26.6972
Chi-Square DF	15
Pr > Chi-Square	0.0313
Standardized RMR (SRMR)	0.0202
Adjusted GFI (AGFI)	0.9428
RMSEA Estimate	0.0488
Akaike Information Criterion	106.6972
Schwarz Bayesian Criterion	258.5395
Bentler Comparative Fit Index	0.9859

The model fit chi-square value is 26.6972 ($df=15$, $p=0.0313$). From the hypothesis testing point of view, this result says that this is an extreme sample given the model is true; therefore, the model should be rejected. But in social and behavioral sciences, you rarely abandon a model purely on the ground of chi-square significance test. The main reason is that you might only need to find a model that is approximately true, but

the hypothesis testing framework is for testing exact model representation in the population. To determine whether a model is good or bad, you usually consult other fit indices. Several fit indices are shown in Figure 17.38.

The standardized RMSR is 0.0202. The RMSEA value is 0.0488. Both of these indices are smaller than 0.05, which indicate good model fit by convention. The adjusted GFI is 0.9428, and the comparative fit index is 0.9859. Again, values greater than 0.9 for these indices indicate good model fit by convention. Therefore, you can conclude that this is a good model for the data. Akaike’s information criterion (AIC) and the Schwarz Bayesian criterion are also shown. You cannot interpret these values directly, but they are useful for model comparison given the same data, as shown in later sections.

Figure 17.39 Career Aspiration Data: Estimation Results for Analysis 1

PATH List					
-----Path-----	Parameter	Estimate	Standard Error	t Value	
R_Amb <=== rpa	_Parm01	0.16122	0.03879	4.15602	
R_Amb <=== riq	_Parm02	0.24965	0.04398	5.67631	
R_Amb <=== rses	_Parm03	0.21840	0.04420	4.94151	
R_Amb <=== fses	_Parm04	0.07184	0.04971	1.44527	
F_Amb <=== rses	_Parm05	0.05754	0.04812	1.19561	
F_Amb <=== fses	_Parm06	0.21278	0.04169	5.10416	
F_Amb <=== fiq	_Parm07	0.32451	0.04352	7.45618	
F_Amb <=== fpa	_Parm08	0.14832	0.03645	4.06964	
R_Amb <=== F_Amb	_Parm09	0.19816	0.10228	1.93741	
F_Amb <=== R_Amb	_Parm10	0.21893	0.11125	1.96795	
rea <=== R_Amb	_Parm11	1.06268	0.09014	11.78936	
roa <=== R_Amb		1.00000			
foa <=== F_Amb		1.00000			
fea <=== F_Amb	_Parm12	1.07558	0.08131	13.22868	

Variance Parameters					
Variance Type	Variable	Parameter	Estimate	Standard Error	t Value
Exogenous	riq	_Add01	1.00000	0.07809	12.80625
	rpa	_Add02	1.00000	0.07809	12.80625
	rses	_Add03	1.00000	0.07809	12.80625
	fiq	_Add04	1.00000	0.07809	12.80625
	fpa	_Add05	1.00000	0.07809	12.80625
	fses	_Add06	1.00000	0.07809	12.80625
Error	roa	_Add07	0.41215	0.05122	8.04585
	rea	_Add08	0.33614	0.05210	6.45192
	foa	_Add09	0.40460	0.04618	8.76059
	fea	_Add10	0.31120	0.04593	6.77588
	R_Amb	_Add11	0.28099	0.04623	6.07782
	F_Amb	_Add12	0.22806	0.03850	5.92335

Figure 17.39 continued

Covariances Among Exogenous Variables					
Var1	Var2	Parameter	Estimate	Standard Error	t Value
rpa	riq	_Add13	0.18390	0.05614	3.27564
rses	riq	_Add14	0.22200	0.05656	3.92503
rses	rpa	_Add15	0.04890	0.05528	0.88456
fiq	riq	_Add16	0.33550	0.05824	5.76060
fiq	rpa	_Add17	0.07820	0.05538	1.41195
fiq	rses	_Add18	0.23020	0.05666	4.06284
fpa	riq	_Add19	0.10210	0.05550	1.83955
fpa	rpa	_Add20	0.11470	0.05558	2.06377
fpa	rses	_Add21	0.09310	0.05545	1.67885
fpa	fiq	_Add22	0.20870	0.05641	3.70000
fses	riq	_Add23	0.18610	0.05616	3.31352
fses	rpa	_Add24	0.01860	0.05523	0.33680
fses	rses	_Add25	0.27070	0.05720	4.73226
fses	fiq	_Add26	0.29500	0.05757	5.12435
fses	fpa	_Add27	-0.04380	0.05527	-0.79249

In Figure 17.39, some of the paths do not show significance. That is, *fses* does not seem to be a good indicator of a respondent's ambition *R_Amb* and *rses* does not seem to be a good indicator of a friend's ambition *F_Amb*. The *t* values are 1.445 and 1.195, respectively, which are much smaller than the nominal 1.96 value at the 0.05 α -level of significance. Other paths are either significant or marginally significant.

You should be very cautious about interpreting the current analysis results for two reasons. First, as mentioned previously the data consist of dependent observations, and it was not certain how the issue could have been addressed beyond setting the sample size to half of the actual size. Second, structural equation modeling methodology is mainly applicable when you analyze covariance structures. When you input a correlation matrix for analysis, there is no guarantee that the statistical tests and standard error estimates are applicable. You should view the interpretations made here just as an exercise of applying structural equation modeling.

In Output 17.39, all parameter names are generated by PROC CALIS. Alternatively, you can also name these parameters in your PATH model specification. The following shows a PATH model specification that corresponds to the complete path diagram shown in Figure 17.36:

```
proc calis data=aspire nobs=329;
  path
    /* structural model of influences */
    rpa    ==> R_Amb    = gam1,
    riq    ==> R_Amb    = gam2,
    rses   ==> R_Amb    = gam3,
    fses   ==> R_Amb    = gam4,
    rses   ==> F_Amb    = gam5,
    fses   ==> F_Amb    = gam6,
    fiq    ==> F_Amb    = gam7,
    fpa    ==> F_Amb    = gam8,
    F_Amb  ==> R_Amb    = beta1,
    R_Amb  ==> F_Amb    = beta2,
```

```

/* measurement model for aspiration */
R_Amb ==> rea      = lambda2,
R_Amb ==> roa      = 1.,
F_Amb ==> foa      = 1.,
F_Amb ==> fea      = lambda3;
pvar
R_Amb = psi11,
F_Amb = psi22,
rpa riq rses fpa fiq fses = v1-v6,
rea roa fea foa = theta1-theta4;
pcov
R_Amb F_Amb = psi12,
rpa riq rses fpa fiq fses = cov01-cov15;
run;

```

In this specification, the names of the parameters correspond to those used by Jöreskog and Sörbom (1988). Compared with the simplified version of the same model specification, you name 27 more parameters in the current specification. You have to be careful with this many parameters. If you inadvertently repeat the use of some parameter names, you will have unexpected constraints in the model.

The results from this analysis are displayed in [Figure 17.40](#).

Figure 17.40 Career Aspiration Data: Estimation Results with Designated Parameter Names (Analysis 1)

PATH List						
-----Path-----	Parameter	Estimate	Standard Error	t Value		
rpa ==>	R_Amb gam1	0.16122	0.03879	4.15602		
riq ==>	R_Amb gam2	0.24965	0.04398	5.67631		
rses ==>	R_Amb gam3	0.21840	0.04420	4.94151		
fses ==>	R_Amb gam4	0.07184	0.04971	1.44527		
rses ==>	F_Amb gam5	0.05754	0.04812	1.19561		
fses ==>	F_Amb gam6	0.21278	0.04169	5.10416		
fiq ==>	F_Amb gam7	0.32451	0.04352	7.45618		
fpa ==>	F_Amb gam8	0.14832	0.03645	4.06964		
F_Amb ==>	R_Amb beta1	0.19816	0.10228	1.93741		
R_Amb ==>	F_Amb beta2	0.21893	0.11125	1.96795		
R_Amb ==>	rea lambda2	1.06268	0.09014	11.78936		
R_Amb ==>	roa	1.00000				
F_Amb ==>	foa	1.00000				
F_Amb ==>	fea lambda3	1.07558	0.08131	13.22868		

Figure 17.40 continued

Variance Parameters					
Variance Type	Variable	Parameter	Estimate	Standard Error	t Value
Error	R_Amb	psi11	0.28099	0.04623	6.07782
	F_Amb	psi22	0.22806	0.03850	5.92335
Exogenous	rpa	v1	1.00000	0.07809	12.80625
	riq	v2	1.00000	0.07809	12.80625
	rses	v3	1.00000	0.07809	12.80625
	fpa	v4	1.00000	0.07809	12.80625
	fiq	v5	1.00000	0.07809	12.80625
	fses	v6	1.00000	0.07809	12.80625
Error	rea	theta1	0.33614	0.05210	6.45192
	roa	theta2	0.41215	0.05122	8.04585
	fea	theta3	0.31120	0.04593	6.77588
	foa	theta4	0.40460	0.04618	8.76059

Covariances Among Exogenous Variables					
Var1	Var2	Parameter	Estimate	Standard Error	t Value
rpa	riq	cov01	0.18390	0.05614	3.27564
rpa	rses	cov02	0.04890	0.05528	0.88456
riq	rses	cov03	0.22200	0.05656	3.92503
rpa	fpa	cov04	0.11470	0.05558	2.06377
riq	fpa	cov05	0.10210	0.05550	1.83955
rses	fpa	cov06	0.09310	0.05545	1.67885
rpa	fiq	cov07	0.07820	0.05538	1.41195
riq	fiq	cov08	0.33550	0.05824	5.76060
rses	fiq	cov09	0.23020	0.05666	4.06284
fpa	fiq	cov10	0.20870	0.05641	3.70000
rpa	fses	cov11	0.01860	0.05523	0.33680
riq	fses	cov12	0.18610	0.05616	3.31352
rses	fses	cov13	0.27070	0.05720	4.73226
fpa	fses	cov14	-0.04380	0.05527	-0.79249
fiq	fses	cov15	0.29500	0.05757	5.12435

These are the same results as displayed in Figure 17.39 for the simplified PATH model specification. The only differences are the arrangement of estimation results and the naming of the parameters.

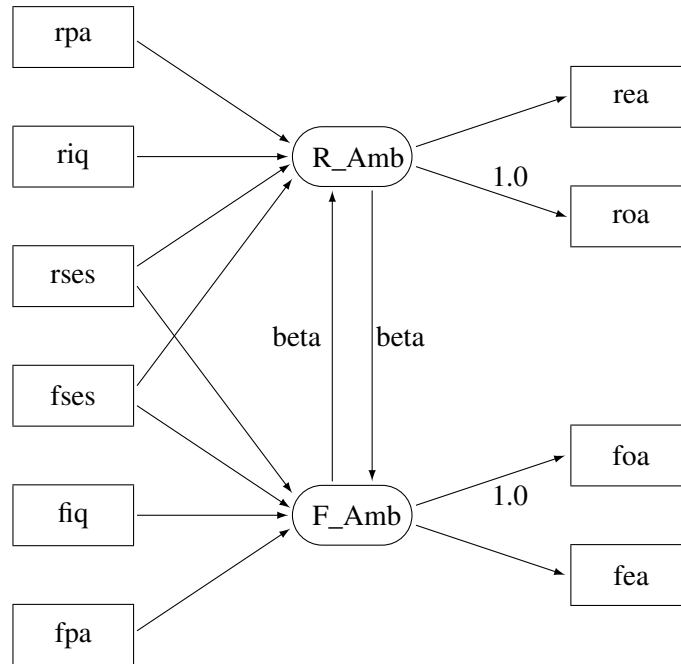
Career Aspiration: Analysis 2

Jöreskog and Sörbom (1988) present more detailed results from a second analysis in which two constraints are imposed:

- The coefficients that connect the latent ambition variables are equal.
- The covariance of the disturbances of the ambition variables is zero.

Applying these constraints to Figure 17.37, you get the path diagram displayed in Figure 17.41.

Figure 17.41 Path Diagram for Career Aspiration : Analysis 2



In Figure 17.41, the double-headed path that connected R_Amb and F_Amb no longer exists. Also, the single-headed paths between R_Amb and F_Amb are both labeled with beta, indicating the required constrained effects in the model. The path diagram in Figure 17.41 is transcribed into the PATH model in the following statements:

```
proc calis data=aspire nobs=329;
  path
    /* structural model of influences */
    rpa    ==> R_Amb      ,
    riq    ==> R_Amb      ,
    rses    ==> R_Amb      ,
    fses    ==> R_Amb      ,
    rses    ==> F_Amb      ,
    fses    ==> F_Amb      ,
    fiq    ==> F_Amb      ,
    fpa    ==> F_Amb      ,
    F_Amb  ==> R_Amb    = beta,
    R_Amb  ==> F_Amb    = beta,

    /* measurement model for aspiration */
    R_Amb  ==> rea        ,
    R_Amb  ==> roa        = 1.,
    F_Amb  ==> foa        = 1.,
    F_Amb  ==> fea        ;
run;
```

The only differences between the current specification and the preceding specification for Analysis 1 are the labeling of two paths with the same parameter beta and the deletion of PCOV statement where the covariance of R_Amb and F_Amb was specified in Analysis 1. The fit summary of the current model is displayed in Figure 17.42, and the estimation results are displayed in Figure 17.43.

Figure 17.42 Career Aspiration Data: Fit Summary for Analysis 2

Fit Summary	
Chi-Square	26.8987
Chi-Square DF	17
Pr > Chi-Square	0.0596
Standardized RMR (SRMR)	0.0203
Adjusted GFI (AGFI)	0.9492
RMSEA Estimate	0.0421
Akaike Information Criterion	102.8987
Schwarz Bayesian Criterion	247.1489
Bentler Comparative Fit Index	0.9880

The model fit chi-square value is 26.8987 ($df=17, p=0.0596$). The standardized RMSR and the RMSEA are both less than 0.05, while the adjusted GFI and comparative fit index are both bigger than 0.9. All these indicate a good model fit, but how does this model (Analysis 2) compare with that in Analysis 1?

The difference between the chi-square values for Analyses 1 and 2 is $26.8987 - 26.6972 = 0.2015$ with two degrees of freedom, which is far from significant. This indicates that the restricted model (Analysis 2) fits as well as the unrestricted model (Analysis 1). The AIC is 102.8987, and the SBC is 247.149. Both of these values are smaller than that of Analysis 1 (106.697 for AIC and 258.540 for SBC), and hence they indicate that the current model is a better one.

Figure 17.43 Career Aspiration Data: Estimation Results for Analysis 2

PATH List						
-----Path-----	Parameter	Estimate	Standard Error	t Value		
rpa ==>	R_Amb _Parm01	0.16367	0.03872	4.22740		
riq ==>	R_Amb _Parm02	0.25395	0.04186	6.06726		
rses ==>	R_Amb _Parm03	0.22115	0.04187	5.28218		
fses ==>	R_Amb _Parm04	0.07728	0.04149	1.86264		
rses ==>	F_Amb _Parm05	0.06840	0.03868	1.76809		
fses ==>	F_Amb _Parm06	0.21839	0.03948	5.53198		
fiq ==>	F_Amb _Parm07	0.33063	0.04116	8.03314		
fpa ==>	F_Amb _Parm08	0.15204	0.03636	4.18169		
F_Amb ==>	R_Amb beta	0.18007	0.03912	4.60305		
R_Amb ==>	F_Amb beta	0.18007	0.03912	4.60305		
R_Amb ==>	rea _Parm09	1.06097	0.08921	11.89233		
R_Amb ==>	roa	1.00000				
F_Amb ==>	foa	1.00000				
F_Amb ==>	fea _Parm10	1.07359	0.08063	13.31498		

Figure 17.43 continued

Variance Parameters					
Variance Type	Variable	Parameter	Estimate	Standard Error	t Value
Exogenous	riq	_Add01	1.00000	0.07809	12.80625
	rpa	_Add02	1.00000	0.07809	12.80625
	rses	_Add03	1.00000	0.07809	12.80625
	fiq	_Add04	1.00000	0.07809	12.80625
	fpa	_Add05	1.00000	0.07809	12.80625
	fses	_Add06	1.00000	0.07809	12.80625
Error	roa	_Add07	0.41205	0.05103	8.07403
	rea	_Add08	0.33764	0.05178	6.52039
	foa	_Add09	0.40381	0.04608	8.76427
	fea	_Add10	0.31337	0.04574	6.85166
	R_Amb	_Add11	0.28113	0.04640	6.05867
	F_Amb	_Add12	0.22924	0.03889	5.89393

Covariances Among Exogenous Variables					
Var1	Var2	Parameter	Estimate	Standard Error	t Value
rpa	riq	_Add13	0.18390	0.05614	3.27564
rses	riq	_Add14	0.22200	0.05656	3.92503
rses	rpa	_Add15	0.04890	0.05528	0.88456
fiq	riq	_Add16	0.33550	0.05824	5.76060
fiq	rpa	_Add17	0.07820	0.05538	1.41195
fiq	rses	_Add18	0.23020	0.05666	4.06284
fpa	riq	_Add19	0.10210	0.05550	1.83955
fpa	rpa	_Add20	0.11470	0.05558	2.06377
fpa	rses	_Add21	0.09310	0.05545	1.67885
fpa	fiq	_Add22	0.20870	0.05641	3.70000
fses	riq	_Add23	0.18610	0.05616	3.31352
fses	rpa	_Add24	0.01860	0.05523	0.33680
fses	rses	_Add25	0.27070	0.05720	4.73226
fses	fiq	_Add26	0.29500	0.05757	5.12435
fses	fpa	_Add27	-0.04380	0.05527	-0.79249

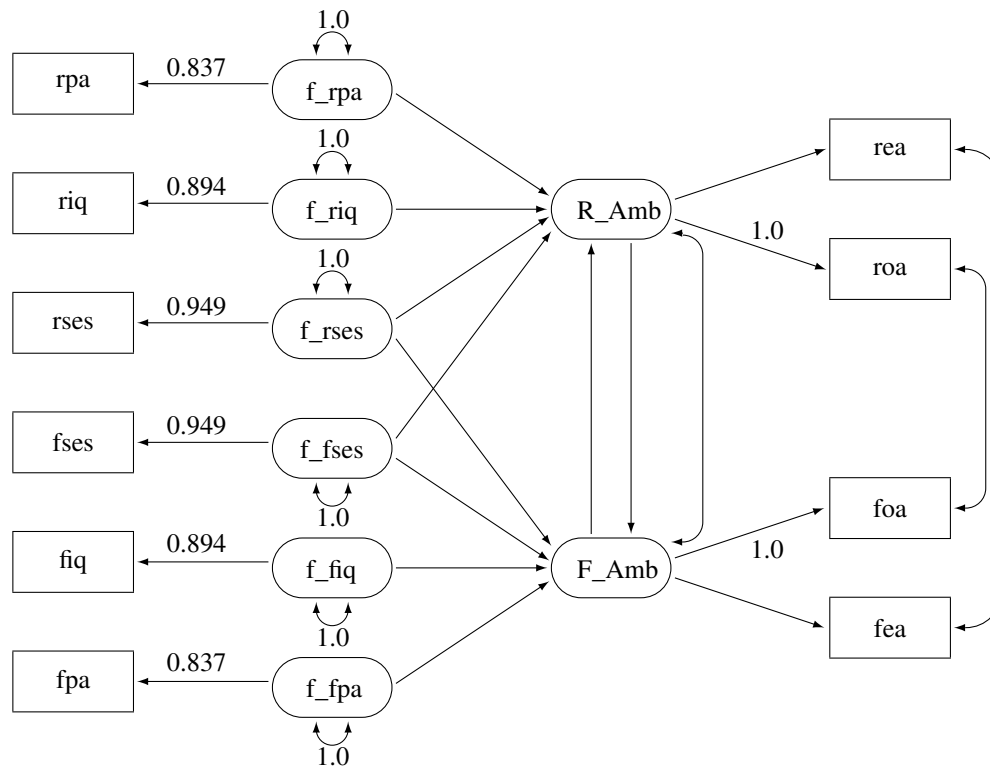
Like Analysis 1, the same two paths in the current analysis are not significant. That is, *fses* does not seem to be a good indicator of a respondent's ambition *R_Amb*, and *rses* does not seem to be a good indicator of a friend's ambition *F_Amb*. The *t* values are 1.862 and 1.768, respectively.

Career Aspiration: Analysis 3

Loehlin (1987) points out that the models considered are unrealistic in at least two respects. First, the variables of parental aspiration, intelligence, and socioeconomic status are assumed to be measured without error. Loehlin adds uncorrelated measurement errors to the model and assumes, for illustrative purposes, that the reliabilities of these variables are known to be 0.7, 0.8, and 0.9, respectively. In practice, these

reliabilities would need to be obtained from a separate study of the same or a very similar population. If these constraints are omitted, the model is not identified. However, constraining parameters to a constant in an analysis of a correlation matrix might make the chi-square goodness-of-fit test inaccurate, so there is more reason to be skeptical of the p -values. Second, the error terms for the respondent's aspiration are assumed to be uncorrelated with the corresponding terms for his friend. Loehlin introduces a correlation between the two educational aspiration error terms and between the two occupational aspiration error terms. These additions produce the path diagram for Loehlin's model shown in Figure 17.44.

Figure 17.44 Path Diagram for Career Aspiration: Analysis 3



In Figure 17.44, the observed variables rpa , riq , $rses$, $fses$, fiq , and fpa are all measured with measurement errors. Their true scores counterparts f_rpa , f_riq , f_rses , f_fses , f_fiq , and f_fpa are latent variables in the model. Path coefficients from these latent variables to the observed variables are fixed coefficients, indicating the square roots of the theoretical reliabilities in the model. These latent variables, rather than the observed counterparts, serve as predictors of the ambition factors R_Amb and F_Amb in the current model (Analysis 3). The error terms for these two latent factors are correlated, as indicated by a double-headed path (arrow) that connects the two factors. Correlated errors for the occupational aspiration variables (roa and foa) and the educational aspiration variables (rea and fea) are also shown in Figure 17.44. Again, these correlated errors are represented by two double-headed paths (arrows) in the path diagram.

You use the following statements to specify the path model for Analysis 3:

```
proc calis data=aspire nobs=329;
  path
    /* measurement model for intelligence and environment */
    rpa    <=== f_rpa    = 0.837,
    riq    <=== f_riq    = 0.894,
    rses    <=== f_rses   = 0.949,
    fses    <=== f_fses   = 0.949,
    fiq    <=== f_fiq    = 0.894,
    fpa    <=== f_fpa    = 0.837,

    /* structural model of influences */
    f_rpa   <===> R_Amb,
    f_riq   <===> R_Amb,
    f_rses  <===> R_Amb,
    f_fses  <===> R_Amb,
    f_rses  <===> F_Amb,
    f_fses  <===> F_Amb,
    f_fiq   <===> F_Amb,
    f_fpa   <===> F_Amb,
    F_Amb   <===> R_Amb,
    R_Amb   <===> F_Amb,

    /* measurement model for aspiration */
    R_Amb   <===> rea      ,
    R_Amb   <===> roa     = 1.,
    F_Amb   <===> foa     = 1.,
    F_Amb   <===> fea     ;
  pvar
    f_rpa f_riq f_rses f_fses f_fiq f_fpa = 6 * 1.0;
  pcov
    R_Amb F_Amb  ,
    rea fea      ,
    roa foa      ;
run;
```

In this specification, the measurement model for the six intelligence and environment variables are added. They are the first six paths in the PATH statement. Fixed constants are set for these path coefficients so as to make the measurement model identified and to set the required reliabilities of these measurement indicators. The structural model of influences and the measurement model for aspiration are the same as specified in Analysis 1. (See the section “Career Aspiration: Analysis 1” on page 321.) All the correlated errors are specified in the PCOV statement.

The fit summary of the current model is displayed in [Figure 17.45](#).

Figure 17.45 Career Aspiration Data: Fit Summary for Analysis 3

Fit Summary	
Chi-Square	12.0132
Chi-Square DF	13
Pr > Chi-Square	0.5266
Standardized RMR (SRMR)	0.0149
Adjusted GFI (AGFI)	0.9692
RMSEA Estimate	0.0000
Akaike Information Criterion	96.0132
Schwarz Bayesian Criterion	255.4476
Bentler Comparative Fit Index	1.0000

Since the *p*-value for the chi-square test is 0.5266, this model clearly cannot be rejected. Both the standardized RMSR and the RMSEA are very small, and both the adjusted GFI and the comparative fit index are high. All these point to an excellent model fit. However, Schwarz’s Bayesian criterion for this model (SBC = 255.4476) is somewhat larger than for Jöreskog and Sörbom (1988) Analysis 2 in Figure 17.42 (SBC = 247.1489), suggesting that a more parsimonious model would be desirable.

The estimation results are displayed in Figure 17.46.

Figure 17.46 Career Aspiration Data: Estimation Results for Analysis 3

PATH List					
-----Path-----	Parameter	Estimate	Standard Error	t Value	
rpa <=== f_rpa		0.83700			
riq <=== f_riq		0.89400			
rses <=== f_rses		0.94900			
fses <=== f_fses		0.94900			
fiq <=== f_fiq		0.89400			
fpa <=== f_fpa		0.83700			
f_rpa ==> R_Amb	_Parm01	0.18370	0.05044	3.64197	
f_riq ==> R_Amb	_Parm02	0.28004	0.06139	4.56182	
f_rses ==> R_Amb	_Parm03	0.22616	0.05223	4.32999	
f_fses ==> R_Amb	_Parm04	0.08698	0.05476	1.58829	
f_rses ==> F_Amb	_Parm05	0.06327	0.05219	1.21242	
f_fses ==> F_Amb	_Parm06	0.21539	0.05121	4.20597	
f_fiq ==> F_Amb	_Parm07	0.35387	0.06741	5.24970	
f_fpa ==> F_Amb	_Parm08	0.16876	0.04934	3.42048	
F_Amb ==> R_Amb	_Parm09	0.11898	0.11396	1.04412	
R_Amb ==> F_Amb	_Parm10	0.13022	0.12067	1.07912	
R_Amb ==> rea	_Parm11	1.08399	0.09417	11.51051	
R_Amb ==> roa		1.00000			
F_Amb ==> foa		1.00000			
F_Amb ==> fea	_Parm12	1.11630	0.08627	12.93945	

Figure 17.46 continued

Variance Parameters					
Variance Type	Variable	Parameter	Estimate	Standard Error	t Value
Exogenous	f_rpa		1.00000		
	f_riq		1.00000		
	f_rses		1.00000		
	f_fses		1.00000		
	f_fiq		1.00000		
	f_fpa		1.00000		
Error	riq	_Add01	0.20874	0.07832	2.66518
	rpa	_Add02	0.29584	0.07774	3.80572
	rses	_Add03	0.09887	0.07803	1.26712
	roa	_Add04	0.42307	0.05243	8.06949
	rea	_Add05	0.32707	0.05452	5.99881
	fiq	_Add06	0.19989	0.07674	2.60483
	fpa	_Add07	0.29988	0.07807	3.84092
	fses	_Add08	0.10324	0.07824	1.31952
	foa	_Add09	0.42240	0.04730	8.93099
	fea	_Add10	0.28716	0.04804	5.97756
	R_Amb	_Add11	0.25418	0.04469	5.68740
	F_Amb	_Add12	0.19698	0.03814	5.16528

Covariances Among Exogenous Variables					
Var1	Var2	Parameter	Estimate	Standard Error	t Value
f_riq	f_rpa	_Add13	0.24677	0.07519	3.28202
f_rses	f_rpa	_Add14	0.06183	0.06945	0.89030
f_rses	f_riq	_Add15	0.26351	0.06687	3.94078
f_fses	f_rpa	_Add16	0.02382	0.06952	0.34267
f_fses	f_riq	_Add17	0.22136	0.06648	3.32983
f_fses	f_rses	_Add18	0.30156	0.06359	4.74210
f_fiq	f_rpa	_Add19	0.10853	0.07362	1.47416
f_fiq	f_riq	_Add20	0.42476	0.07219	5.88372
f_fiq	f_rses	_Add21	0.27250	0.06660	4.09143
f_fiq	f_fses	_Add22	0.34922	0.06771	5.15762
f_fpa	f_rpa	_Add23	0.15789	0.07873	2.00555
f_fpa	f_riq	_Add24	0.13084	0.07418	1.76387
f_fpa	f_rses	_Add25	0.11516	0.06978	1.65050
f_fpa	f_fses	_Add26	-0.05622	0.06971	-0.80648
f_fpa	f_fiq	_Add27	0.27867	0.07530	3.70082

Covariances Among Errors					
Error of	Error of	Parameter	Estimate	Standard Error	t Value
R_Amb	F_Amb	_Parm13	-0.00936	0.05010	-0.18673
rea	fea	_Parm14	0.02308	0.03139	0.73545
roa	foa	_Parm15	0.11206	0.03258	3.43988

Like Analyses 1 and 2, two paths that concern the validity of the indicators in the current analysis do not show significance. That is, f_fses does not seem to be a good indicator of a respondent's ambition R_Amb , and f_rses does not seem to be a good indicator of a friend's ambition F_Amb . The t values are 1.588 and 1.212, respectively. In addition, in the current model (Analysis 3), the structural relationships between the ambition factors do not show significance. The t value for the path from the friend's ambition factor F_Amb on the respondent's ambition factor R_Amb is only 1.044, while the t value for the path from the respondent's ambition factor R_Amb on the friend's ambition factor F_Amb is only 1.079. These cast doubts on the validity of the structural model and perhaps even the entire model.

Fitting LISREL Models by the LISMOD Modeling Language

The model described in the section “Career Aspiration: Analysis 3” on page 331 provides a good example of the LISREL model. In PROC CALIS, the LISREL model specifications are supported by a matrix-based language called LISMOD (LISREL model). In this section, the path diagram in Figure 17.44 is specified by the LISMOD modeling language of PROC CALIS. See the section “Career Aspiration: Analysis 3” on page 331 for detailed descriptions of the model.

In order to understand the LISMOD modeling language of PROC CALIS, some basic understanding of the LISREL model is necessary. In a LISREL model, variables are classified into four distinct classes:

- ξ is a vector of exogenous (independent) latent variables in the model. They are specified in `XI=` variable list in the LISMOD statement.
- η is a vector of endogenous (dependent) latent variables in the model. They are specified in `ETA=` variable list in the LISMOD statement.
- x is a vector of observed indicator variables for ξ in the model. They are specified in `XVAR=` variable list in the LISMOD statement.
- y is a vector of observed indicator variables for η in the model. They are specified in `YVAR=` variable list in the LISMOD statement.

For detailed descriptions of the LISMOD modeling language, see the LISMOD statement and the section “The LISMOD Model and Submodels” on page 1277. To successfully set up a LISMOD model in PROC CALIS, you first need to recognize these classes of variables in your model. For the path diagram in Figure 17.44, it is not difficult to see the following:

- ξ is the vector of the intelligence and environmental factors: f_rpa , f_riq , f_rses , f_fses , f_fiq , and f_fpa . These variables are exogenous because no single-headed arrows point to them.
- η is the vector of the ambition factors: R_Amb , and F_Amb . They are endogenous because each of them has at least one single-headed arrow pointing to it.
- x is the vector of the observed indicator variables for the intelligence and environmental factors ξ . These indicators are rpa , riq , $rses$, $fses$, fiq , and fpa .
- y is the vector of observed indicator variables for the ambition factors η . These indicators are rea , roa , foa , and fea .

In LISMOD, you do not need to define error terms explicitly as latent variables. The parameters in LISMOD are defined as entries in various model matrices. The following statements specify the LISMOD model for the diagram in Figure 17.44:

```
proc calis data=aspire nobs=329;
  lismod
    xi   = f_rpa f_riq f_rses f_fses f_fiq f_fpa,
    eta  = R_Amb F_Amb,
    xvar = rpa riq rses fses fiq fpa,
    yvar = rea roa foa fea;

  /* measurement model for aspiration */
  matrix _lambday_ [1,1], [2,1] = 1.0, [3,2] = 1.0, [4,2];
  matrix _thetay_  [4,1], [3,2];

  /* measurement model for intelligence and environment */
  matrix _lambdax_ [1,1] = 0.837 0.894 0.949 0.949 0.894 0.837;

  /* structural model of influences */
  matrix _beta_ [2,1], [1,2];
  matrix _gamma_ [1,1 to 4], [2,3 to 6];

  /* Covariances among Eta-variables */
  matrix _psi_ [2,1];

  /* Fixed variances for Xi-variables */
  matrix _phi_ [1,1] = 6 * 1.0;
run;
```

The LISMOD statement invokes the LISMOD modeling language of PROC CALIS. In the LISMOD statement, you list the four classes of variables in the model in the XI=, ETA=, XVAR=, and YVAR= variable lists, respectively. After you define the four classes of variables, you use several MATRIX statements to specify the model matrices and the parameters in the model.

Basically, there are three model components in the LISMOD specification: two measurement models and one structural model. The first measurement model specifies the functional relationships between observed variables y (YVAR= variables) and the endogenous (dependent) latent factors η (ETA= variables). The second measurement model specifies the functional relationships between observed variables x and (XVAR= variables) and the exogenous (independent) latent factors ξ (XI= variables). The structural model specifies the relationships between the endogenous and exogenous latent variables η and ξ . To facilitate the discussion of these model components and the corresponding LISMOD model specification, some initial model output from PROC CALIS are shown.

The Measurement Model for y

The first component of the LISMOD specification is the measurement model for y , as shown in the following equation:

$$y = \Lambda_y \eta + \epsilon$$

In the context of covariance structure analysis, without loss of generality, it is assumed that y and η are centered so that there is no intercept term in the equation. This equation essentially states that y is a function

of the true scores vector η plus the error term ϵ , which is independent of η . The model matrices involved in this measurement model are Λ_y (effects of η on y) and Θ_y , which is the covariance matrix of ϵ .

For the career aspiration data, you specify the following two MATRIX statements for this measurement model:

```
matrix _lambday_ [1,1], [2,1] = 1.0, [3,2] = 1.0, [4,2];
matrix _thetay_ [4,1], [3,2];
```

The first matrix statement is for matrix Λ_y . You specify four parameters in this matrix. The [1,1] and [4,2] elements are free parameters, and the [2,1] and [3,2] elements have fixed values of 1. You do not specify other elements in this matrix. By default, unspecified elements in the Λ_y matrix are fixed zeros. You can check your initial model specification of this matrix, as shown in the Figure 17.47.

Figure 17.47 Career Aspiration Analysis 3: Initial Measurement Model for y

Initial _LAMBDAY_ Matrix				
		R_Amb	F_Amb	
rea		.	0	
	[_Parm01]			
roa		1.0000	0	
foa		0	1.0000	
fea		0	.	
			[_Parm02]	
Initial _THETAY_ Matrix				
	rea	roa	foa	fea
rea	.	0	0	.
	[_Add07]			[_Parm13]
roa	0	.	.	0
		[_Add08]	[_Parm14]	
foa	0	.	.	0
		[_Parm14]	[_Add09]	
fea	.	0	0	.
	[_Parm13]			[_Add10]

NOTE: Parameters with prefix '_Add' are added by PROC CALIS.

In Figure 17.47, the initial `_LAMBDAY_` matrix is a 4×2 matrix. The `_LAMBDAY_` matrix contains information about the relationships between the row indicator variables y (YVAR= variables) and the column factors η (ETA= variables). As specified in the MATRIX statement for `_LAMBDAY_`, the [1,1] and [4,2]

are free parameters named `_Parm01` and `_Parm02`, respectively. These parameter names are generated by PROC CALIS. Fixed values 1.0 appear in the [2,1] and [3,2] elements. These fixed values are used to identify the scales of the latent variables `R_Amb` and `F_Amb`.

The `_THETAY_` matrix in Figure 17.47 is the covariance matrix among the error terms for the y -variables (YVAR= variables). This is a 4×4 matrix for the four measured indicators. As specified in the MATRIX statement for `_THETAY_`, the [4,1] and [3,2] elements are free parameters named `_Parm13` and `_Parm14`, respectively. Because `_THETAY_` is a symmetric matrix, elements [1,4] and [2,3] are also implicitly specified as parameters in this model matrix.

As shown in Figure 17.47, PROC CALIS adds four default free parameters to the `_THETAY_` matrix. On the diagonal of the `_THETAY_` matrix, parameters `_Add07`, `_Add08`, `_Add09`, and `_Add10` are added as default free parameters by PROC CALIS automatically. In general, error variances are default free parameters in PROC CALIS. You do not have to specify them but you can specify them if you want to, especially when you need to set fixed values or other constraints on them.

The Measurement Model for x

The second component of the LISMOD specification is the measurement model for x , as shown in the following equation:

$$x = \Lambda_x \xi + \delta$$

The measurement model for x is similar to that for y . Assuming that x and ξ are centered, this equation states that x is a function of the true scores vector ξ plus the error term δ , which is independent of ξ . The model matrices involved in this measurement model are Λ_x (effects of ξ on x) and Θ_x , which is the covariance matrix of δ .

For the career aspiration data, you specify the following MATRIX statement for this measurement model:

```
matrix _lambdax_ [1,1] = 0.837 0.894 0.949 0.949 0.894 0.837;
```

Figure 17.48 shows the output related to the specification of the measurement model for x .

Figure 17.48 Career Aspiration Analysis 3: Initial Measurement Model for x

Initial <code>_LAMBDA_X_</code> Matrix						
	<code>f_rpa</code>	<code>f_riq</code>	<code>f_rses</code>	<code>f_fses</code>	<code>f_fiq</code>	<code>f_fpa</code>
<code>rpa</code>	0.8370	0	0	0	0	0
<code>riq</code>	0	0.8940	0	0	0	0
<code>rses</code>	0	0	0.9490	0	0	0
<code>fses</code>	0	0	0	0.9490	0	0
<code>fiq</code>	0	0	0	0	0.8940	0
<code>fpa</code>	0	0	0	0	0	0.8370

Figure 17.48 continued

Initial _THETAX_ Matrix						
	rpa	riq	rses	fses	fiq	fpa
rpa	.	0	0	0	0	0
	[_Add01]					
riq	0	.	0	0	0	0
		[_Add02]				
rses	0	0	.	0	0	0
			[_Add03]			
fses	0	0	0	.	0	0
				[_Add04]		
fiq	0	0	0	0	.	0
					[_Add05]	
fpa	0	0	0	0	0	.
						[_Add06]

NOTE: Parameters with prefix '_Add' are added by PROC CALIS.

In Figure 17.48, the initial `_LAMBDA_X_` matrix is a 6×6 matrix. The `_LAMBDA_X_` matrix contains information about the relationships between the row indicator variables x (`XVAR=` variables) and the column factors ξ (`XI=` variables). As specified in the `MATRIX` statement for `_LAMBDA_X_`, the diagonal elements are filled with the fixed values provided. The `[1,1]` specification in the `MATRIX` statement for `_LAMBDA_X_` provides the starting element for the subsequent parameter list to fill in. In this case, the list contains six fixed values, and PROC CALIS proceeds from `[1,1]` to `[2,2]`, `[3,3]` and so on until the entire list of parameters is consumed. This kind of notation is a shortcut of the following equivalent specification:

```
matrix _lambdax_ [1,1]=0.837, [2,2]=0.894, [3,3]=0.949,
                 [4,4]=0.949, [5,5]=0.894, [6,6]=0.837;
```

PROC CALIS provides many different kinds of shortcuts in specifying matrix elements. See the `MATRIX` statement of Chapter 27, “The CALIS Procedure,” for details.

At the bottom of Figure 17.48, the initial `_THETA_X_` matrix is shown. Even though you did not specify any elements of this matrix in any `MATRIX` statements, the diagonal elements of this matrix are set as default parameters by PROC CALIS. Default parameters added by PROC CALIS are all denoted by names with the prefix ‘_Add’.

The Structural Model

The last component of the LISMOD specification is the structural model that describes the relationship between η and ξ , as shown in the following equation:

$$\eta = \beta\eta + \Gamma\xi + \zeta$$

In this equation, η is endogenous (dependent) and ξ is exogenous (independent). Variables in η can have effects among themselves. Their effects are specified in the β matrix. The effects of ξ on η are specified in the Γ matrix. Finally, the error term for the structural relationships is denoted by ζ , which is independent of ξ .

There are four model matrices assumed in the structural model. β and Γ are matrices for the effects of variables. In addition, matrix Ψ denotes the covariance matrix for the error term ζ , and matrix Φ denotes the covariance matrix of ξ .

For the career aspiration data, you use the following MATRIX statements for the structural model:

```
matrix _beta_ [2,1], [1,2];
matrix _gamma_ [1,1 to 4], [2,3 to 6];
matrix _psi_ [2,1];
matrix _phi_ [1,1] = 6 * 1.0;
```

In Figure 17.49, initial `_BETA_` and `_GAMMA_` matrices are shown.

Figure 17.49 Career Aspiration Analysis 3: Initial Structural Equations

Initial <code>_BETA_</code> Matrix						
	R_Amb	F_Amb				
R_Amb	0	.				
F_Amb	.	0				
			[_Parm12]			
			[_Parm11]			
Initial <code>_GAMMA_</code> Matrix						
	f_rpa	f_riq	f_rses	f_fses	f_fiq	f_fpa
R_Amb	0	0
	[_Parm03]	[_Parm04]	[_Parm05]	[_Parm06]		
F_Amb	0	0
			[_Parm07]	[_Parm08]	[_Parm09]	[_Parm10]

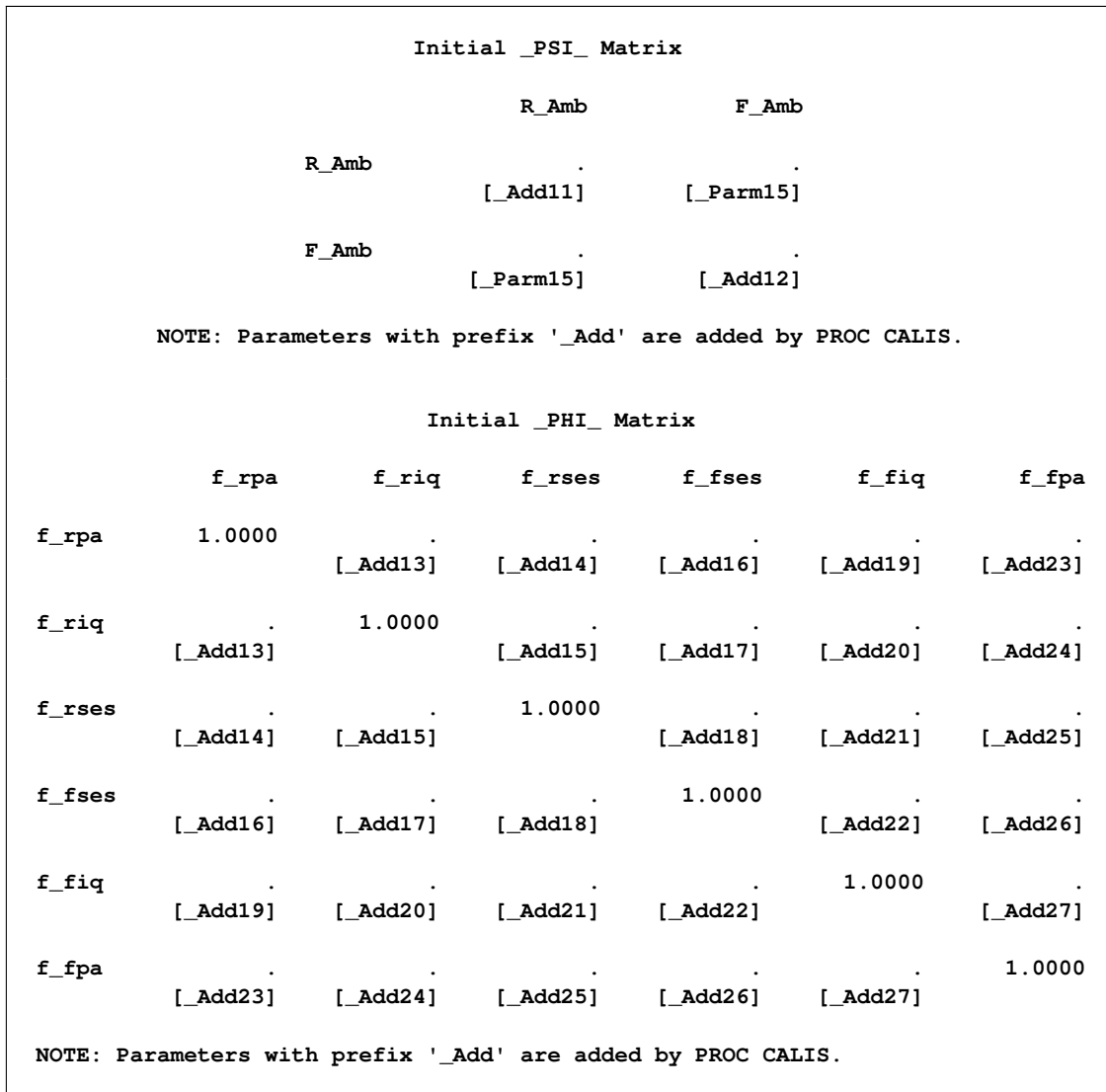
In Figure 17.49, the `_BETA_` matrix contains information about the relationships among the η -variables (ETA= variables). Both the row and column variables of the `_BETA_` matrix refer to the list of η -variables. The row variables receive effects from the column variables. You specify two parameters in the `_BETA_` matrix: element [2,1] is the effect of R_Amb on F_Amb, and element [1,2] is the effect of F_Amb on R_Amb. Other effects are fixed zeros in this matrix.

The `_GAMMA_` matrix contains information about the relationships between the η -variables (ETA= variables) and the ξ -variables (XI= variables). The row variables are the η -variables, which receive effects from the column ξ -variables. You specify eight free parameters in this matrix. These eight parameters represent the eight path coefficients from ξ (the intelligence and environment factors) to the η variables (the ambition factors), as shown in the path diagram in Figure 17.44. A shortcut in the MATRIX statement syntax for the `_GAMMA_` matrix has been used. That is, [1, 1 to 4] means the [1,1], [1,2], [1,3], and [1,4] elements,

and [2, 3 to 6] means the [2,3], [2,4], [2,5], and [2,6] elements. All these elements are free parameters in the model and free parameter names are generated for these elements.

Figure 17.50 shows the initial `_PSI_` and `_PHI_` matrices.

Figure 17.50 Career Aspiration Analysis 3: Initial Variances and Covariances



The `_PSI_` matrix contains information about the covariances of error terms for the η -variables, which are endogenous in the structural model. There are two η -variables in the model—the two ambition factors `R_Amb` and `F_Amb`. You specify the [2,1] element as a free parameter in the `MATRIX` statement for `_PSI_`. This means that the error covariance between `R_Amb` and `F_Amb` is a free parameter to estimate in the model. In [Figure 17.50](#), both [2,1] and [1,2] elements are named as `_Parm15` because `_PSI_` is a symmetric matrix. Again, the diagonal elements of this covariance matrix, which are for the error variances of the ambition factors, are default free parameters in `PROC CALIS`. These parameters are named with the prefix `_Add`.

Finally, the `_PHI_` matrix contains information about the covariances among the exogenous latent factors in the structural model. For the `_PHI_` matrix, you fix all the diagonal elements to 1 in the `MATRIX` statement for `_PHI_`. This makes the latent variable scales identified. These fixed values are echoed in the output of the initial `_PHI_` matrix shown in [Figure 17.50](#). In addition, all covariances among latent exogenous variables are set to be free parameters by default.

Fit Summary of the LISMOD Model for Career Aspiration Analysis 3

[Figure 17.51](#) shows the fit summary of the LISMOD model. All these fit index values match those from using the `PATH` model specification of the same model, as shown in [Figure 17.45](#). Therefore, you are confident that the current LISMOD model specification is equivalent to the `PATH` model specification shown in the section “Career Aspiration: Analysis 3” on page 331.

Figure 17.51 Career Aspiration Analysis 3: Fit Summary of the LISMOD Model

Fit Summary	
Chi-Square	12.0132
Chi-Square DF	13
Pr > Chi-Square	0.5266
Standardized RMR (SRMR)	0.0149
Adjusted GFI (AGFI)	0.9692
RMSEA Estimate	0.0000
Akaike Information Criterion	96.0132
Schwarz Bayesian Criterion	255.4476
Bentler Comparative Fit Index	1.0000

Estimation results are shown in [Figure 17.52](#), [Figure 17.53](#), and [Figure 17.54](#), respectively for the measurement model for y , measurement model for x , and the structural model. These are the same estimation results as those from the equivalent `PATH` model specification in [Figure 17.46](#). However, estimates in the LISMOD model are now arranged in the matrix form, with standard error estimates and t values shown.

Figure 17.52 Career Aspiration Analysis 3: Estimation of Measurement Model for y

<u>_LAMBDA_</u> Matrix: Estimate/StdErr/t-value				
		R_Amb	F_Amb	
rea		1.0840	0	
		0.0942		
		11.5105		
		[_Parm01]		
roa		1.0000	0	
foa		0	1.0000	
fea		0	1.1163	
			0.0863	
			12.9394	
			[_Parm02]	
<u>_THETA_</u> Matrix: Estimate/StdErr/t-value				
	rea	roa	foa	fea
rea	0.3271	0	0	0.0231
	0.0545			0.0314
	5.9988			0.7355
	[_Add07]			[_Parm13]
roa	0	0.4231	0.1121	0
		0.0524	0.0326	
		8.0695	3.4399	
		[_Add08]	[_Parm14]	
foa	0	0.1121	0.4224	0
		0.0326	0.0473	
		3.4399	8.9310	
		[_Parm14]	[_Add09]	
fea	0.0231	0	0	0.2872
	0.0314			0.0480
	0.7355			5.9776
	[_Parm13]			[_Add10]

Figure 17.53 Career Aspiration Analysis 3: Estimation of Measurement Model for x

<u>LAMBDA</u> Matrix: Estimate/StdErr/t-value						
	f_rpa	f_riq	f_rses	f_fses	f_fiq	f_fpa
rpa	0.8370	0	0	0	0	0
riq	0	0.8940	0	0	0	0
rses	0	0	0.9490	0	0	0
fses	0	0	0	0.9490	0	0
fiq	0	0	0	0	0.8940	0
fpa	0	0	0	0	0	0.8370

Figure 17.53 continued

THETAX Matrix: Estimate/StdErr/t-value						
	rpa	riq	rses	fses	fiq	fpa
rpa	0.2958 0.0777 3.8057 [_Add01]	0	0	0	0	0
riq	0	0.2087 0.0783 2.6652 [_Add02]	0	0	0	0
rses	0	0	0.0989 0.0780 1.2671 [_Add03]	0	0	0
fses	0	0	0	0.1032 0.0782 1.3195 [_Add04]	0	0
fiq	0	0	0	0	0.1999 0.0767 2.6048 [_Add05]	0
fpa	0	0	0	0	0	0.2999 0.0781 3.8409 [_Add06]

Figure 17.54 Career Aspiration Analysis 3: Estimation of Structural Model

<u>BETA</u> Matrix: Estimate/StdErr/t-value						
	R_Amb	F_Amb				
R_Amb	0	0.1190				
		0.1140				
		1.0441				
		[_Parm12]				
F_Amb	0.1302	0				
	0.1207					
	1.0791					
	[_Parm11]					
<u>GAMMA</u> Matrix: Estimate/StdErr/t-value						
	f_rpa	f_riq	f_rses	f_fses	f_fiq	f_fpa
R_Amb	0.1837	0.2800	0.2262	0.0870	0	0
	0.0504	0.0614	0.0522	0.0548		
	3.6420	4.5618	4.3300	1.5883		
	[_Parm03]	[_Parm04]	[_Parm05]	[_Parm06]		
F_Amb	0	0	0.0633	0.2154	0.3539	0.1688
			0.0522	0.0512	0.0674	0.0493
			1.2124	4.2060	5.2497	3.4205
			[_Parm07]	[_Parm08]	[_Parm09]	[_Parm10]
<u>PSI</u> Matrix: Estimate/StdErr/t-value						
	R_Amb	F_Amb				
R_Amb	0.2542	-0.009355				
	0.0447	0.0501				
	5.6874	-0.1867				
	[_Add11]	[_Parm15]				
F_Amb	-0.009355	0.1970				
	0.0501	0.0381				
	-0.1867	5.1653				
	[_Parm15]	[_Add12]				

Figure 17.54 continued

<u>_PHI_ Matrix: Estimate/StdErr/t-value</u>						
	f_rpa	f_riq	f_rses	f_fses	f_fiq	f_fpa
f_rpa	1.0000	0.2468	0.0618	0.0238	0.1085	0.1579
		0.0752	0.0695	0.0695	0.0736	0.0787
		3.2820	0.8903	0.3427	1.4742	2.0056
		[_Add13]	[_Add14]	[_Add16]	[_Add19]	[_Add23]
f_riq	0.2468	1.0000	0.2635	0.2214	0.4248	0.1308
	0.0752		0.0669	0.0665	0.0722	0.0742
	3.2820		3.9408	3.3298	5.8837	1.7639
	[_Add13]		[_Add15]	[_Add17]	[_Add20]	[_Add24]
f_rses	0.0618	0.2635	1.0000	0.3016	0.2725	0.1152
	0.0695	0.0669		0.0636	0.0666	0.0698
	0.8903	3.9408		4.7421	4.0914	1.6505
	[_Add14]	[_Add15]		[_Add18]	[_Add21]	[_Add25]
f_fses	0.0238	0.2214	0.3016	1.0000	0.3492	-0.0562
	0.0695	0.0665	0.0636		0.0677	0.0697
	0.3427	3.3298	4.7421		5.1576	-0.8065
	[_Add16]	[_Add17]	[_Add18]		[_Add22]	[_Add26]
f_fiq	0.1085	0.4248	0.2725	0.3492	1.0000	0.2787
	0.0736	0.0722	0.0666	0.0677		0.0753
	1.4742	5.8837	4.0914	5.1576		3.7008
	[_Add19]	[_Add20]	[_Add21]	[_Add22]		[_Add27]
f_fpa	0.1579	0.1308	0.1152	-0.0562	0.2787	1.0000
	0.0787	0.0742	0.0698	0.0697	0.0753	
	2.0056	1.7639	1.6505	-0.8065	3.7008	
	[_Add23]	[_Add24]	[_Add25]	[_Add26]	[_Add27]	

Some Important PROC CALIS Features

In this section, some of the main features of PROC CALIS are introduced. Emphasis is placed on showing how these features are useful in practical structural equation modeling.

Modeling Languages for Specifying Models

PROC CALIS provides several modeling languages to specify a model. Different modeling languages in PROC CALIS are signified by the main model specification statement used. In this chapter, you have seen examples of the FACTOR, LINEQS, LISMOD, MSTRUCT, PATH, and RAM modeling languages. Depending on your modeling philosophy and the type of the model, you can choose a modeling language that is most suitable for your application. For example, models specified using structural equations can be

transcribed directly into the LINEQS statement. Models that are hypothesized using path diagrams can be described easily in the PATH or RAM statement. First-order confirmatory or exploratory factor models are most conveniently specified by using the FACTOR and MATRIX statements. Traditional LISREL models are supported through the LISMOD and MATRIX statements. Finally, patterned covariance and mean models can be specified directly by the MSTRUCT and MATRIX statements, or by the `COVPATTERN=` and `MEANPATTERN=` options.

For most applications in structural equation modeling, the PATH and LINEQS statements are the easiest to use. For testing the built-in covariance and mean patterns of PROC CALIS, the use of the `COVPATTERN=` and the `MEANPATTERN=` options are the most efficient. In other cases, the FACTOR, LISMOD, MSTRUCT, or RAM statement might be more suitable. For very general matrix model specifications, you can use the COSAN modeling language. See the `COSAN` statement and the section “The COSAN Model” on page 1259 of Chapter 27, “The CALIS Procedure,” for details about the COSAN modeling language. See also the section “Which Modeling Language?” on page 1077 in Chapter 27, “The CALIS Procedure,” for a more detailed discussion about the use of different modeling languages.

Estimation Methods

The CALIS procedure provides six methods of estimation specified by the `METHOD=` option:

DWLS	diagonally weighted least squares
FIML	full-information maximum likelihood
GLS	normal theory generalized least squares
ML	maximum likelihood for multivariate normal distributions
ULS	unweighted least squares
WLS	weighted least squares for arbitrary distributions

Each estimation method is based on finding parameter estimates that minimize a discrepancy (badness-of-fit) function, which measures the difference between the observed sample covariance matrix and the fitted (predicted) covariance matrix, given the model and the parameter estimates. The difference between the observed sample mean vector and the fitted (predicted) mean vector is also taken into account when the mean structures are modeled. See the section “Estimation Criteria” on page 1309 in Chapter 27, “The CALIS Procedure,” for formulas, or see Loehlin (1987, pp. 54–62) and Bollen (1989, pp. 104–123) for further discussion. For the ML method, robust estimation with the `ROBUST` option is also available.

The default estimation is `METHOD=ML`, which is the most popular method for applications. The option `METHOD=GLS` usually produces very similar results to those produced by `METHOD=ML`. If your data contain random missing values and it is important to use the information from those incomplete observations, you might want to use the FIML method, which provides a sound treatment of missing values in data. `METHOD=ML` and `METHOD=FIML` are essentially the same method when you do not have missing values (see Example 27.16 of Chapter 27, “The CALIS Procedure,”). Asymptotically, ML and GLS are the same. Both methods assume a multivariate normal distribution in the population. The WLS method with the default weight matrix is equivalent to the asymptotically distribution free (ADF) method, which yields asymptotically normal estimates regardless of the distribution in the population. When the multivariate normal assumption is in doubt, especially if the variables have high kurtosis, you should seriously consider the WLS method. When a correlation matrix is analyzed, only WLS can produce correct standard error

estimates. However, in order to use the WLS method with the expected statistical properties, the sample size must be large. Several thousand might be a minimum requirement.

The ULS and DWLS methods yield reasonable estimates under less restrictive assumptions. You can apply these methods to normal or nonnormal situations or to covariance or correlation matrices. The drawback is that the statistical qualities of the estimates seem to be unknown. For this reason, PROC CALIS does not provide standard errors or test statistics with these two methods.

You cannot use METHOD=ML or METHOD=GLS if the observed covariance matrix is singular. You can either remove variables involved in the linear dependencies or use less restrictive estimation methods such as ULS. Specifying METHOD=ML assumes that the predicted covariance matrix is nonsingular. If ML fails because of a singular predicted covariance matrix, you need to examine whether the model specification leads to the singularity. If so, modify the model specification to eliminate the problem. If not, you probably need to use other estimation methods.

You should remove outliers and try to transform variables that are skewed or heavy-tailed. This applies to all estimation methods, since all the estimation methods depend on the sample covariance matrix, and the sample covariance matrix is a poor estimator for distributions with high kurtosis (Bollen 1989, pp. 415–418; Huber 1981; Hampel et al. 1986). PROC CALIS displays estimates of univariate and multivariate kurtosis (Bollen 1989, pp. 418–425) if you specify the KURTOSIS option in the PROC CALIS statement.

See the section “[Estimation Methods](#)” on page 349 for the general use of these methods. See the section “[Estimation Criteria](#)” on page 1309 of Chapter 27, “[The CALIS Procedure](#),” for details about these estimation criteria.

Statistical Inference

When you specify the ML, FIML, GLS, or WLS estimation with appropriate models, PROC CALIS can compute the following:

- a chi-square goodness-of-fit test of the specified model versus the alternative that the data are from a population with unconstrained covariance matrix (Loehlin 1987, pp. 62–64; Bollen 1989, pp. 110, 115, 263–269)
- approximate standard errors of the parameter estimates (Bollen 1989, pp. 109, 114, 286), displayed with the STDERR option
- various modification indices, requested via the MODIFICATION or MOD option, that give the approximate change in the chi-square statistic that would result from removing constraints on the parameters or constraining additional parameters to zero (Bollen 1989, pp. 293–303)

If you have two models such that one model results from imposing constraints on the parameters of the other, you can test the constrained model against the more general model by fitting both models with PROC CALIS. If the constrained model is correct, the difference between the chi-square goodness of fit statistics for the two models has an approximate chi-square distribution with degrees of freedom equal to the difference between the degrees of freedom for the two models (Loehlin 1987, pp. 62–67; Bollen 1989, pp. 291–292).

All of the test statistics and standard errors computed under ML and GLS depend on the assumption of multivariate normality. Normality is a much more important requirement for data with random independent

variables than it is for fixed independent variables. If the independent variables are random, distributions with high kurtosis tend to give liberal tests and excessively small standard errors, while low kurtosis tends to produce the opposite effects (Bollen 1989, pp. 266–267, 415–432).

All test statistics and standard errors computed by PROC CALIS are based on asymptotic theory and should not be trusted in small samples. There are no firm guidelines on how large a sample must be for the asymptotic theory to apply with reasonable accuracy. Some simulation studies have indicated that problems are likely to occur with sample sizes less than 100 (Loehlin 1987, pp. 60–61; Bollen 1989, pp. 267–268). Extrapolating from experience with multiple regression would suggest that the sample size should be at least 5 to 20 times the number of parameters to be estimated in order to get reliable and interpretable results. The WLS method might even require that the sample size be over several thousand.

The asymptotic theory requires the parameter estimates to be in the interior of the parameter space. If you do an analysis with inequality constraints and one or more constraints are active at the solution (for example, if you constrain a variance to be nonnegative and the estimate turns out to be zero), the chi-square test and standard errors might not provide good approximations to the actual sampling distributions.

For modeling correlation structures, the only theoretically correct method is the WLS method with the default `ASYCOV=CORR` option. For other methods, standard error estimates for modeling correlation structures might be inaccurate even for sample sizes as large as 400. The chi-square statistic is generally the same regardless of which matrix is analyzed, provided that the model involves no scale-dependent constraints. However, if the purpose is to obtain reasonable parameter estimates for the correlation structures only, then you might also find other estimation methods useful.

If you fit a model to a correlation matrix and the model constrains one or more elements of the predicted matrix to equal 1.0, the degrees of freedom of the chi-square statistic must be reduced by the number of such constraints. PROC CALIS attempts to determine which diagonal elements of the predicted correlation matrix are constrained to a constant, but it might fail to detect such constraints in complicated models, particularly when programming statements are used. If this happens, you should add parameters to the model to release the constraints on the diagonal elements.

Multiple-Group Analysis

PROC CALIS supports multiple-group multiple-model analysis. You can fit the same covariance (and mean) structure model to several independent groups (data sets). Or, you can fit several different but constrained models to the independent groups (data sets). In PROC CALIS, you can use the `GROUP` statements to define several independent groups and the `MODEL` statements to define several different models. For example, the following statements show a multiple-group analysis by PROC CALIS:

```
proc calis;
  group 1 / data=set1;
  group 2 / data=set2;
  group 3 / data=set3;
  model 1 / group=1,2;
    path
      y <=== x   = beta ,
      x <=== z   = gamma;
  model 2 / group=3;
    path
      y <=== x   = beta,
      x <=== z   = alpha;
run;
```

In this specification, you conduct a three-group analysis. You define two PATH models. You fit Model 1 to Groups 1 and 2 and Model 2 to Group 3. The two models are constrained for the $y \leftarrow x$ path because they use the same path coefficient parameter β . Other parameters in the models are not constrained.

To facilitate model specification by model referencing, you can use the `REFMODEL` statement to specify models based on model referencing. For example, the previous example can be specified equivalently as the following statements:

```
proc calis;
  group 1 / data=set1;
  group 2 / data=set2;
  group 3 / data=set3;
  model 1 / group=1,2;
    path
      y <=== x = beta ,
      x <=== z = gamma;
  model 2 / group=3;
    refmodel 1;
    renameparm gamma=alpha;
run;
```

The current specification differs from the preceding specification in the definition of Model 2. In the current specification, Model 2 is making reference to Model 1. Basically, this means that the *explicit* specification in Model 1 is transferred to Model 2. However, the `RENAMEPARM` statement requests a name change for gamma, which becomes a new parameter named alpha in Model 2. Hence, Model 2 and Model 1 are not the same. They are constrained by the same path coefficient β for the $y \leftarrow x$ path, but they have different path coefficients for the $x \leftarrow z$ path.

Model referencing by the `REFMODEL` statement offers you an efficient and concise way to define models based on the similarities and differences between models. The advantages become more obvious when you have several large models in multiple-group analysis and each model differs just a little bit from each other.

Goodness-of-Fit Statistics

In addition to the chi-square test, there are many other statistics for assessing the goodness of fit of the predicted correlation or covariance matrix to the observed matrix.

Akaike's information criterion (AIC, Akaike 1987) and Schwarz's Bayesian criterion (SBC, Schwarz 1978) are useful for comparing models with different numbers of parameters—the model with the smallest value of AIC or SBC is considered best. Based on both theoretical considerations and various simulation studies, SBC seems to work better, since AIC tends to select models with too many parameters when the sample size is large.

There are many descriptive measures of goodness of fit that are scaled to range approximately from zero to one: the goodness-of-fit index (GFI) and GFI adjusted for degrees of freedom (AGFI) (Jöreskog and Sörbom 1988), centrality (McDonald 1989), and the parsimonious fit index (James, Mulaik, and Brett 1982). Bentler and Bonett (1980) and Bollen (1986) have proposed measures for comparing the goodness of fit of one model with another in a descriptive rather than inferential sense.

The root mean squared error approximation (RMSEA) proposed by Steiger and Lind (1980) does not assume a true model being fitted to the data. It measures the discrepancy between the fitted model and the covariance matrix in the population. For samples, RMSEA and confidence intervals can be estimated. Statistical tests

for determining whether the population RMSEAs fall below certain specified values are available (Browne and Cudeck 1993). In the same vein, Browne and Cudeck (1993) propose the expected cross validation index (ECVI), which measures how good a model is for predicting future sample covariances. Point estimate and confidence intervals for ECVI are also developed.

None of these measures of goodness of fit are related to the goodness of prediction of the structural equations. Goodness of fit is assessed by comparing the observed correlation or covariance and mean matrices with the matrices computed from the model and parameter estimates. Goodness of prediction is assessed by comparing the actual values of the endogenous variables with their predicted values, usually in terms of root mean squared error or proportion of variance accounted for (R square). For latent endogenous variables, root mean squared error and R square can be estimated from the fitted model.

Customizable Fit Summary Table

Because there are so many fit indices that PROC CALIS can display and researchers prefer certain sets of fit indices, PROC CALIS enables you to customize the set of fit indices to display. For example, you can use the following statement to limit the set of fit indices to display:

```
fitindex on(only) = [chisq SRMSR RMSEA AIC];
```

With this statement, only the model-fit chi-square, standardized root mean square residual, root mean square error of approximation, and Akaiki's information criterion are displayed in your output. You can also save all your fit index values in an output data file by adding the `OUTFIT=` option in the `FITINDEX` statement. This output data file contains all available fit index values even if you have limited the set of fit indices to display in the listing output.

Standardized Solution

In many applications in social and behavioral sciences, measurement scales of variables are arbitrary. Although it should not be viewed as a universal solution, some researchers resort to the standardized solution for interpreting estimation results. PROC CALIS computes the standardized solutions for all models (except for COSAN) automatically. Standard error estimates are also produced for standardized solutions so that you can examine the statistical significance of the standardized estimates too.

However, equality or linear constraints on parameters are almost always set on the unstandardized variables. These parameter constraints are not preserved when the estimation solution is standardized. This would add difficulties in interpreting standardized estimates when your model is defined meaningfully with constraints on the unstandardized variables.

A general recommendation is to make sure your variables are measured on “comparable” scales (it does not necessarily mean that they are mean- and variance-standardized) for the analysis. But what makes different kinds of variables “comparable” is an ongoing philosophical issue.

Some researchers might totally abandon the concept of standardized solutions in structural equation modeling. If you prefer to turn off the standardized solutions in PROC CALIS, you can use the `NOSTAND` option in the PROC CALIS statement.

Testing Parametric Functions

Oftentimes, researchers might have a priori hypotheses about the parameters in their models. After knowing the model fit is satisfactory, they want to test those hypotheses under the model. PROC CALIS provides two statements for testing these kinds of hypotheses. The **TESTFUNC** statement enables you to test each parametric function separately, and the **SIMTESTS** statement enables you to test parametric functions jointly (and separately). For example, assuming that `effect1`, `effect2`, `effect3`, and `effect4` are parameters in your model, the following **SIMTESTS** statement tests the joint hypothesis `test1`, which consists of two component hypotheses `diff_effect` and `sum_effect`:

```
SIMTESTS test1 = (diff_effect sum_ffect);
diff_effect = effect1 - effect2;
sum_effect  = effect3 + effect4;
```

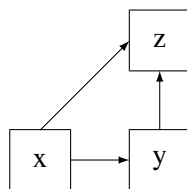
To make `test1` well-defined, each of the component hypotheses `diff_effect` and `sum_effect` is assumed to be defined as a parametric function by some SAS programming statements. In the specification, `diff_effect` represents the difference between `effect1` and `effect2`, and `sum_effect` represents the sum of `effect3` and `effect4`. Hence, the component hypotheses being tested are:

$$H_1: \quad \text{diff_effect} = \text{effect1} - \text{effect2} = 0$$

$$H_2: \quad \text{sum_effect} = \text{effect3} + \text{effect4} = 0$$

Effect Analysis

In structural equation modeling, effects from one variable to other variables can be direct or indirect. For example, in the following path diagram `x` has a direct effect on `z` in addition to an indirect effect on `z` via `y`:



However, `y` has only a direct effect (but no indirect effect) on `z`. In cases like this, researchers are interested in computing the total, direct, and indirect effects from `x` and `y` to `z`. You can use the **EFFPART** option in the PROC CALIS statement to request this kind of effect partitioning in your model. Total, direct, and indirect effects are displayed, together with their standard error estimates. If your output contains standardized results (default), the standardized total, direct, and indirect effects and their standard error estimates are also displayed. With the **EFFPART** option, effects analysis is applied to all variables (excluding error terms) in your model.

In large models with many variables, researchers might want to analyze the effects only for a handful of variables. In this regard, PROC CALIS provides you a way to do a customized version of effect analysis.

For example, the following EFFPART statement requests the effect partitioning of x1 and x2 on y1 and y2, even though there might be many more variables in the model:

```
effpart    x1 x2 ===> y1 y2;
```

See the EFFPART statement of Chapter 27, “The CALIS Procedure,” for details.

Model Modifications

When you fit a model and the model fit is not satisfactory, you might want to know what you could do to improve the model. The LM (Lagrange multiplier) tests in PROC CALIS can help you improve the model fit by testing the potential free parameters in the model. To request the LM tests, you can use the MODIFICATION option in the PROC CALIS statement.

The LM test results contain lists of parameters, organized according to their types. In each list, the potential parameter with the greatest model improvement is shown first. Adding these new parameters improves the model fit approximately by the amount of the corresponding LM statistic.

Sometimes, researchers might have a target set of parameters they want to test in the LM tests. PROC CALIS offers a flexible way that you can customize the set the parameters for the LM tests. See the LMTESTS statement for details.

In addition, the Wald statistics produced by PROC CALIS suggest whether any parameters in your model can be dropped (or fixed to zero) without significantly affecting the model fit. You can request the Wald statistics with the MODIFICATION option in the PROC CALIS statement.

Optimization Methods

PROC CALIS uses a variety of nonlinear optimization algorithms for computing parameter estimates. These algorithms are very complicated and do not always work for every data set. PROC CALIS generally informs you when the computations fail, usually by displaying an error message about the iteration limit being exceeded. When this happens, you might be able to correct the problem simply by increasing the iteration limit (MAXITER= and MAXFUNC=). However, it is often more effective to change the optimization method (OMETHOD=) or initial values. For more details, see the section “Use of Optimization Techniques” on page 1352 in Chapter 27, “The CALIS Procedure,” and see Bollen (1989, pp. 254–256).

PROC CALIS might sometimes converge to a local optimum rather than the global optimum. To gain some protection against local optima, you can run the analysis several times with different initial estimates. The RANDOM= option in the PROC CALIS statement is useful for generating a variety of initial estimates.

Other Commonly Used Options

Other commonly used options in the PROC CALIS statement include the following:

- **INMODEL=** to input model specification from a data set, usually created by the **OUTMODEL=** option

- **MEANSTR** to analyze the mean structures
- **NOBS** to specify the number of observations
- **NOPARMNAME** to suppress the printing of parameter names
- **NOSE** to suppress the display of approximate standard errors
- **OUTMODEL=** to output model specification and estimation results to an external file for later use (for example, fitting the same model to other data sets)
- **RESIDUAL** to display residual correlations or covariances

Comparison of the CALIS and FACTOR Procedures for Exploratory Factor Analysis

Both the CALIS and the FACTOR procedures can fit exploratory factor models. However, there are several notable differences:

- By default, PROC FACTOR analyzes the correlation matrix, while PROC CALIS analyzes the covariance matrix.
- PROC FACTOR and PROC CALIS use different parameterizations in the initial factor solution. PROC CALIS uses a lower triangle pattern on the factor loading matrix (a confirmatory factor pattern) in the initial unrotated solution, while PROC FACTOR use certain matrix constraints in the initial unrotated solution. All other things being equal, PROC CALIS and PROC FACTOR might give the same solution after the same factor rotation.
- Because of the way it parameterizes, PROC FACTOR is usually more efficient computationally. PROC CALIS uses a more general algorithm that might not be computationally optimal for exploratory factor analysis.

Comparison of the CALIS and SYSLIN Procedures

The SYSLIN procedure in SAS/ETS software can fit certain kinds of path models and linear structural equation models. PROC CALIS differs from PROC SYSLIN in that PROC CALIS is more general in the use of latent variables in the models. Latent variables are unobserved, hypothetical variables, as distinct from manifest variables, which are the observed data. PROC SYSLIN allows at most one latent variable, the error term, in each equation. PROC CALIS allows several latent variables to appear in an equation—in fact, all the variables in an equation can be latent as long as there are other equations that relate the latent variables to manifest variables.

Both the CALIS and SYSLIN procedures enable you to specify a model as a system of linear equations. When there are several equations, a given variable might be a dependent variable in one equation and an

independent variable in other equations. Therefore, additional terminology is needed to describe unambiguously the roles of variables in the system. Variables with values that are determined jointly and simultaneously by the system of equations are called *endogenous variables*. Variables with values that are determined outside the system—that is, in a manner separate from the process described by the system of equations—are called exogenous variables. The purpose of the system of equations is to explain the variation of each endogenous variable in terms of exogenous variables or other endogenous variables or both. See Loehlin (1987, p. 4) for further discussion of endogenous and exogenous variables. In the econometric literature, error and disturbance terms are usually distinguished from exogenous variables, but in systems with more than one latent variable in an equation, the distinction is not always clear.

In PROC SYSLIN, endogenous variables are identified by the ENDOGENOUS statement. In PROC CALIS, endogenous variables are identified by the procedure automatically after you specify the model. With different modeling languages, the identification of endogenous variables by PROC CALIS is done by different sets of rules. For example, when you specify structural equations by using the LINEQS modeling language in PROC CALIS, endogenous variables are assumed to be those that appear on the left-hand sides of the equations; a given variable can appear on the left-hand side of at most one equation. When you specify your model by using the PATH modeling language in PROC CALIS, endogenous variables are those variables pointed to by arrows at least once in the path specifications.

PROC SYSLIN provides many methods of estimation, some of which are applicable only in special cases. For example, ordinary least squares estimates are suitable in certain kinds of systems but might be statistically biased and inconsistent in other kinds. PROC CALIS provides three major methods of estimation that can be used with most models. Both the CALIS and SYSLIN procedures can do maximum likelihood estimation, which PROC CALIS calls ML and PROC SYSLIN calls FIML. PROC SYSLIN can be much faster than PROC CALIS in those special cases for which it provides computationally efficient estimation methods. However, PROC CALIS has a variety of sophisticated algorithms for maximum likelihood estimation that might be much faster than FIML in PROC SYSLIN.

PROC CALIS can impose a wider variety of constraints on the parameters, including nonlinear constraints, than can PROC SYSLIN. For example, PROC CALIS can constrain error variances or covariances to equal specified constants, or it can constrain two error variances to have a specified ratio.

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Chapter 18

Introduction to Power and Sample Size Analysis

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Overview

Power and sample size analysis optimizes the resource usage and design of a study, improving chances of conclusive results with maximum efficiency. The standard statistical testing paradigm implicitly assumes that Type I errors (mistakenly concluding significance when there is no true effect) are more costly than Type II errors (missing a truly significant result). This may be appropriate for your situation, or the relative costs of the two types of error may be reversed. For example, in screening experiments for drug development, it is often less damaging to carry a few false positives forward for follow-up testing than to miss potential leads. Power and sample size analysis can help you achieve your desired balance between Type I and Type II errors. With optimal designs and sample sizes, you can improve your chances of detecting effects that might otherwise have been ignored, save money and time, and perhaps minimize risks to subjects.

Relevant tools in SAS/STAT software for power and sample size analysis include the following:

- the GLMPOWER procedure
- the POWER procedure
- the Power and Sample Size application
- the %POWTABLE macro
- various procedures, statements, and functions in Base SAS and SAS/STAT for developing customized formulas and simulations

These tools, discussed in detail in the section “[SAS/STAT Tools for Power and Sample Size Analysis](#)” on page 365, deal exclusively with *prospective* analysis—that is, planning for a future study. This is in contrast to *retrospective* analysis for a past study, which is not supported by the main tools. Although retrospective analysis is more convenient to perform, it is often uninformative or misleading, especially when power is computed directly based on observed data.

The goals of prospective power and sample size analysis include the following:

- determining the sample size required to get a significant result with adequate probability (power)
- characterizing the power of a study to detect a meaningful effect
- computing the probability of achieving the desired precision of a confidence interval, or the sample size required to ensure this probability
- conducting what-if analyses to assess how sensitive the power or required sample size is to other factors

The phrase *power analysis* is used for the remainder of this document as a shorthand to represent any or all of these goals. For more information about the GLMPOWER procedure, see Chapter 44, “[The GLMPOWER Procedure](#).” For more information about the POWER procedure, see Chapter 71, “[The POWER Procedure](#).” For more information about the Power and Sample Size application, see Chapter 72, “[The Power and Sample Size Application](#).”

Coverage of Statistical Analyses

The GLMPOWER procedure covers power analysis for Type III tests and contrasts of fixed effects in univariate linear models, optionally with covariates. The covariates can be continuous or categorical. Tests and contrasts involving random effects are not supported.

The POWER procedure covers power analysis for the following:

- *t* tests, equivalence tests, and confidence intervals for means
- tests, equivalence tests, and confidence intervals for binomial proportions
- multiple regression

- tests of correlation and partial correlation
- one-way analysis of variance
- rank tests for comparing two survival curves
- logistic regression with binary response
- Wilcoxon Mann-Whitney rank-sum test

The Power and Sample Size application covers a large subset of the analyses in the GLMPOWER and POWER procedures.

Statistical Background

Hypothesis Testing, Power, and Confidence Interval Precision

Standard Hypothesis Tests

In statistical hypothesis testing, you typically express the belief that some effect exists in a population by specifying an alternative hypothesis H_1 . You state a null hypothesis H_0 as the assertion that the effect does *not* exist and attempt to gather evidence to reject H_0 in favor of H_1 . Evidence is gathered in the form of sample data, and a statistical test is used to assess H_0 . If H_0 is rejected but there really is *no* effect, this is called a *Type I error*. The probability of a Type I error is usually designated “alpha” or α , and statistical tests are designed to ensure that α is suitably small (for example, less than 0.05).

If there is an effect in the population but H_0 is *not* rejected in the statistical test, then a *Type II error* has been committed. The probability of a Type II error is usually designated “beta” or β . The probability $1 - \beta$ of avoiding a Type II error (that is, correctly rejecting H_0 and achieving statistical significance) is called the *power* of the test.

Most, but not all, of the power analyses in the GLMPOWER and POWER procedures are based on such standard hypothesis tests.

Equivalence and Noninferiority

Whereas the standard two-sided hypothesis test for a parameter μ (such as a mean difference) aims to demonstrate that it is significantly different than a null value μ_0 :

$$H_0: \mu = \mu_0$$

$$H_1: \mu \neq \mu_0$$

an equivalence test instead aims to demonstrate that it is *significantly similar* to some value, expressed in terms of a range θ_L, θ_U around that value:

$$H_0: \mu < \theta_L \quad \text{or} \quad \mu > \theta_U$$

$$H_1: \theta_L \leq \mu \leq \theta_U$$

Whereas the standard one-sided hypothesis test for μ (say, the upper one-sided test) aims to demonstrate that it is significantly greater than μ_0 :

$$H_0: \mu \leq \mu_0$$

$$H_1: \mu > \mu_0$$

a corresponding noninferiority test aims to demonstrate that it is *not significantly less* than μ_0 , expressed in terms of a margin $\delta > 0$:

$$H_0: \mu \leq \mu_0 - \delta$$

$$H_1: \mu > \mu_0 - \delta$$

Corresponding forms of these hypotheses with the inequalities reversed apply to lower one-sided noninferiority tests (sometimes called *nonsuperiority* tests).

The POWER procedure performs power analyses for equivalence tests for one-sample, paired, and two-sample tests of normal and lognormal mean differences and ratios. It also supports noninferiority tests for a variety of analyses of means, proportions, and correlation, both directly (with a MARGIN= option representing δ) and indirectly (with an option for a custom null value representing the sum or difference of μ_0 and δ).

Confidence Interval Precision

An analysis of confidence interval precision is analogous to a traditional power analysis, with *CI Half-Width* taking the place of effect size and *Prob(Width)* taking the place of power. The *CI Half-Width* is the margin of error associated with the confidence interval, the distance between the point estimate and an endpoint. The *Prob(Width)* is the probability of obtaining a confidence interval with *at most* a target half-width.

The POWER procedure performs confidence interval precision analyses for *t*-based confidence intervals for one-sample, paired, and two-sample designs, and for several varieties of confidence intervals for a binomial proportion.

Computing Power and Sample Size

For some statistical models and tests, power analysis calculations are exact—that is, they are based on a mathematically accurate formula that expresses power in terms of the other components. Such formulas typically involve either enumeration or noncentral versions of the distribution of the test statistic.

When a power computation is based on a noncentral *t*, *F*, or chi-square distribution, the noncentrality parameter generally has the same form as the test statistic, with the conjectured population parameters in place of their corresponding estimators.

For example, the test statistic for a two-sample *t* test is computed as follows:

$$t = N^{\frac{1}{2}}(w_1 w_2)^{\frac{1}{2}} \left(\frac{\bar{x}_2 - \bar{x}_1 - \mu_0}{s_p} \right)$$

where N is the total sample size, w_1 and w_2 are the group allocation weights, \bar{x}_1 and \bar{x}_2 are the sample means, μ_0 is the null mean difference, and s_p is the pooled standard deviation. Under the null hypothesis, the

statistic $F = t^2$ is distributed as $F(1, N - 2)$. In general, F has a noncentral F distribution $F(1, N - 2, \delta^2)$ where

$$\delta = N^{\frac{1}{2}}(w_1 w_2)^{\frac{1}{2}} \left(\frac{\mu_{\text{diff}} - \mu_0}{\sigma} \right)$$

and μ_{diff} and σ are the (unknown) true mean difference and common group standard deviation, respectively. Note that the square-root noncentrality δ is exactly the same as the t statistic except that the estimators of mean difference and standard deviation are replaced by their corresponding true population values.

The power for the two-sided two-sample t test with significance level α is computed as

$$P(F \geq F_{1-\alpha}(1, N - 2))$$

where F is distributed as $F(1, N - 2, \delta^2)$ and $F_{1-\alpha}(1, N - 2)$ is the $100(1 - \alpha)\%$ quantile of the central F distribution with 1 and $N - 2$ degrees of freedom. See the section “[Customized Power Formulas \(DATA Step\)](#)” on page 374 for an example of the implementation of this formula in the DATA step.

In the absence of exact mathematical results, approximate formulas can sometimes be used. When neither exact power computations nor reasonable approximations are possible, simulation provides an increasingly viable alternative. You specify values for model parameters and use them to randomly generate a large number of hypothetical data sets. Applying the statistical test to each data set, you estimate power with the percentage of times the null hypothesis is rejected. While the simulation approach is computationally intensive, faster computing makes this less of an issue. A simulation-based power analysis is always a valid option, and, with a large number of data set replications, it can often be more accurate than approximations. See the section “[Empirical Power Simulation \(DATA Step, SAS/STAT Software\)](#)” on page 375 for an example of an empirical power simulation.

Sample size is usually computed by iterative numerical methods because it often cannot be expressed in closed form as a function of the other parameters. Sample size tends to appear in both a noncentrality parameter and a degrees of freedom term for the critical value.

Power and Study Planning

Power analysis is most effective when performed at the study planning stage, and as such it encourages early collaboration between researcher and statistician. It also focuses attention on effect sizes and variability in the underlying scientific process, concepts that both researcher and statistician should consider carefully at this stage.

There are many factors involved in a power analysis, such as the research objective, design, data analysis method, power, sample size, Type I error, variability, and effect size. By performing a power analysis, you can learn about the relationships between these factors, optimizing those that are under your control and exploring the implications of those that are fixed or unknown.

Components of Study Planning

Even when the research questions and study design seem straightforward, the ensuing power analysis can seem technically daunting. It is often helpful to break the process down into five components:

- **Study Design:** What is the structure of the planned design? This must be clearly and completely specified. What groups and treatments (“cells” and “factors” of the design) are going to be assessed, and what will be the relative sizes of those cells? How is each case going to be studied—that is, what is the primary outcome measure (“dependent variable”)? Will covariates be measured and included in the statistical model?
- **Scenario Model:** What are your beliefs about patterns in the data? Imagine that you had unlimited time and resources to execute the study design, so that you could gather an “infinite data set.” Characterize that infinite data set as best you can using a mathematical model, realizing that it will be a simplification of reality. Alternatively, as is common with complex linear models, you may decide to construct an “exemplary” data set that mimics the infinite data set. However you do this, your scenario model should capture the key features of the study design and the main relationships among the primary outcome variables and study factors.
- **Effects and Variability:** What exactly are the “signals and noises” in the patterns you suspect? Set specific values for the parameters of your scenario model, keeping at most one unspecified. It is often enlightening to consider a variety of realistic possibilities for the key values by performing a sensitivity analysis, to explore the consequences of competing views on what the infinite data set might look like.
- **Statistical Method:** How will you cast your model in statistical terms and conduct the eventual data analysis? Define the statistical models and procedures that will be used to embody the study design and estimate and/or test the effects central to the research question. What significance levels will be used? Will one- or two-sided tests be used?
- **Aim of Assessment:** Finally, what needs to be determined in the power analysis? Most often you want to examine the statistical powers obtained across the various scenarios for the effects, variability, alternative varieties of the statistical procedures to be used, and the feasible total sample sizes. Sometimes the goal is to find sample size values that provide given levels of power, say 85%, 90%, or 95%.

Effect Size

There is some confusion in practice about how to postulate the effect size. One alternative is to specify the effect size that represents minimal clinical significance; then the result of the power analysis reveals the chances of detecting a minimally meaningful effect size. Often this minimal effect size is so small that it requires excessive resources to detect. Another alternative is to make an educated guess of the true underlying effect size. Then the power analysis determines the chance of detecting the effect size that is believed to be true. The choice is ultimately determined by the research goals. Finally, you can specify a collection of possible values, perhaps spanning the range between minimally meaningful effects and larger surmised effects.

You can arrive at values for required quantities in a power analysis, such as effect sizes and measures of variability, in many different ways. For example, you can use pilot data, results of previous studies reported in literature, educated guesses derived from theory, or educated guesses derived from partial data (a small sample or even just quantiles).

Uncertainty and Sensitivity Analysis

Uncertainty is a fact of life in any power analysis, because at least some of the numbers used are best guesses of unknown values. The result of a power calculation, whether it be achieved power or required sample size or something else, serves only as a point estimate, conditional on the conjectured values of the other components. It is not feasible in general to quantify the variability involved in using educated guesses or undocumented results to specify these components. If observed data are used, relevant adjustments for variability in the data tend to be problematic in the sense of producing confidence intervals for power that are too wide for practical use. But there is a useful way for you to characterize the uncertainty in your power analysis, and also discover the extent to which statistical power is affected by each component. You can posit a reasonable range for each input component, vary each one within its range, and observe the variety of results in the form of tables or graphs.

SAS/STAT Tools for Power and Sample Size Analysis

This section demonstrates how you can use the different SAS power analysis tools mentioned in the section “Overview” on page 359 to generate graphs, tables, and narratives; implement your own power formulas; and simulate empirical power.

Suppose you want to compute the power of a two-sample t test. You conjecture that the mean difference is between 5 and 6 and that the common group standard deviation is between 12 and 18. You plan to use a significance level between 0.05 and 0.1 and a sample size between 100 and 200. The following SAS statements use the POWER procedure to compute the power for these scenarios:

```
proc power;  
  twosamplemeans test=diff  
    meandiff = 5 6  
    stddev = 12 18  
    alpha = 0.05 0.1  
    ntotal = 100 200  
    power = .;  
run;
```

Figure 18.1 shows the results. Depending on the plausibility of the various combinations of input parameter values, the power ranges between 0.379 and 0.970.

Figure 18.1 PROC POWER Tabular Output

The POWER Procedure					
Two-Sample t Test for Mean Difference					
Computed Power					
Index	Alpha	Mean Diff	Std Dev	N Total	Power
1	0.05	5	12	100	0.541
2	0.05	5	12	200	0.834
3	0.05	5	18	100	0.280
4	0.05	5	18	200	0.498
5	0.05	6	12	100	0.697
6	0.05	6	12	200	0.940
7	0.05	6	18	100	0.379
8	0.05	6	18	200	0.650
9	0.10	5	12	100	0.664
10	0.10	5	12	200	0.902
11	0.10	5	18	100	0.397
12	0.10	5	18	200	0.623
13	0.10	6	12	100	0.799
14	0.10	6	12	200	0.970
15	0.10	6	18	100	0.505
16	0.10	6	18	200	0.759

The following seven sections illustrate additional ways of displaying these results using the different SAS tools.

Basic Graphs (POWER, GLMPOWER, Power and Sample Size Application)

If you include a PLOT statement, the GLMPOWER and POWER procedures produce standard power curves, which represent any multivalued input parameters with varying line styles, symbols, colors, and/or panels. The Power and Sample Size application also has an option to produce power curves. If ODS Graphics is enabled, then graphs are created using ODS Graphics; otherwise, traditional graphs are produced.

To display default power curves for the preceding PROC POWER call, add the PLOT statement with no arguments as follows:

```
ods listing style=htmlbluecml;
ods graphics on;

proc power plotonly;
  twosamplemeans test=diff
    meandiff = 5 6
    stddev = 12 18
    alpha = 0.05 0.1
    ntotal = 100 200
    power = .;
  plot;
run;

ods graphics off;
```

The ODS GRAPHICS ON statement enables ODS Graphics. The ODS LISTING STYLE=HTMLBLUECML statement specifies the HTMLBLUECML style, which is suitable for use with PROC POWER because it allows both marker symbols and line styles to vary.

Figure 18.2 shows the results. Note that the line style varies by the significance level α , the symbol varies by the mean difference, and the panel varies by standard deviation.

Figure 18.2 PROC POWER Default Graphical Output

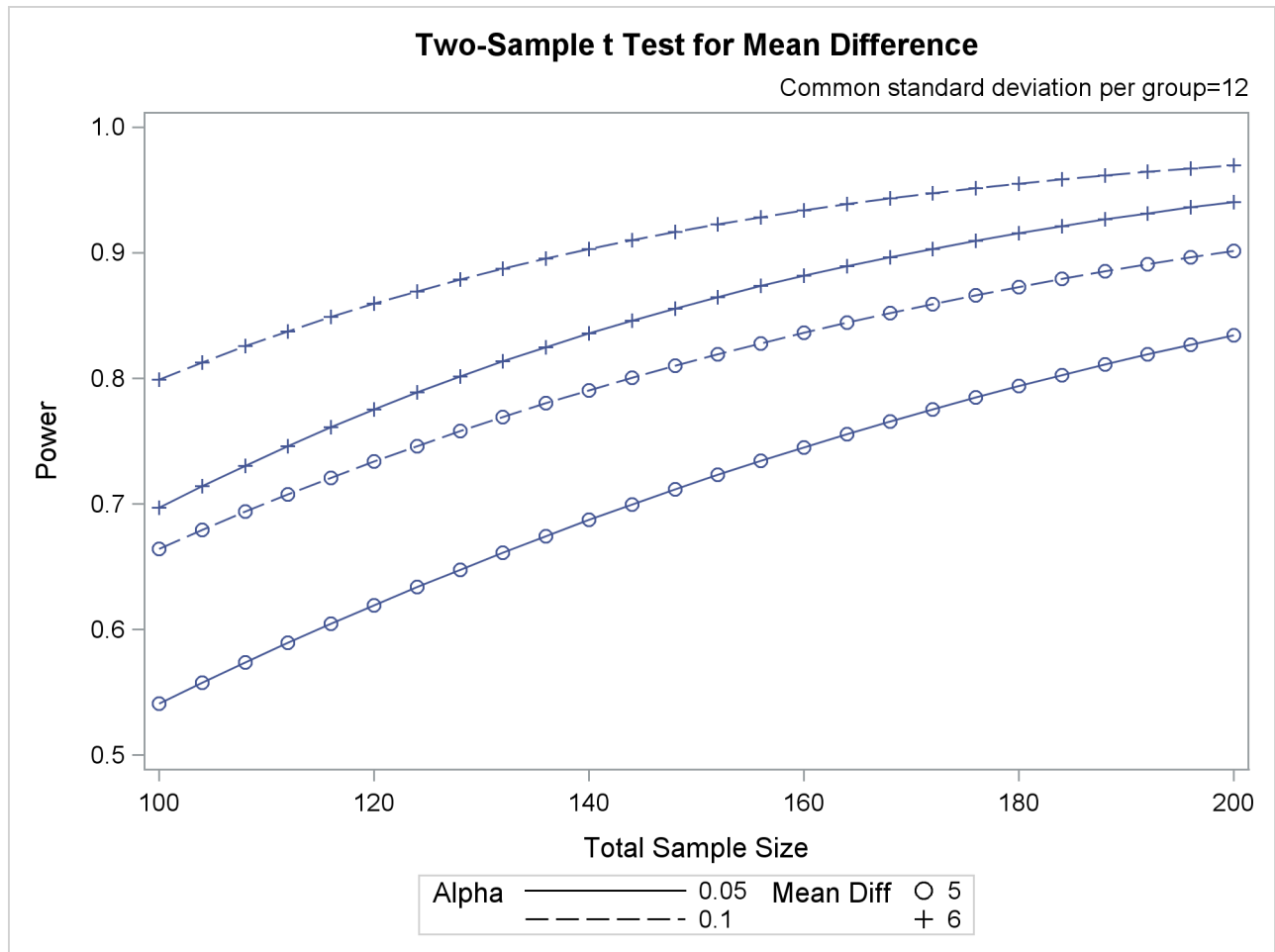
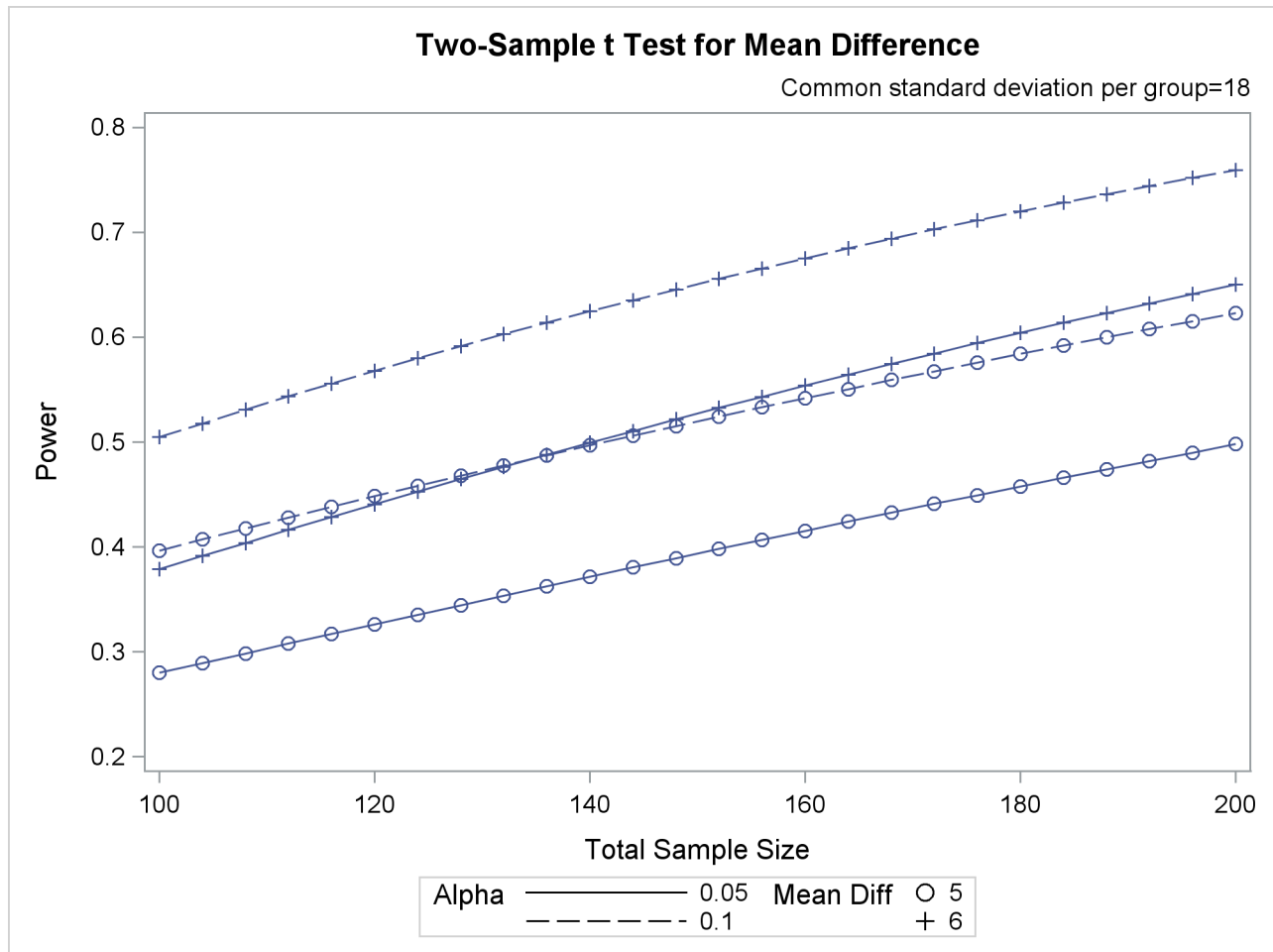


Figure 18.2 continued



Highly Customized Graphs (POWER, GLMPOWER)

Example 71.8 of Chapter 71, “The POWER Procedure,” demonstrates various ways you can modify and enhance plots created in the GLMPOWER or POWER procedures:

- assigning analysis parameters to axes
- fine-tuning a sample size axis
- adding reference lines
- linking plot features to analysis parameters
- choosing key (legend) styles
- modifying symbol locations

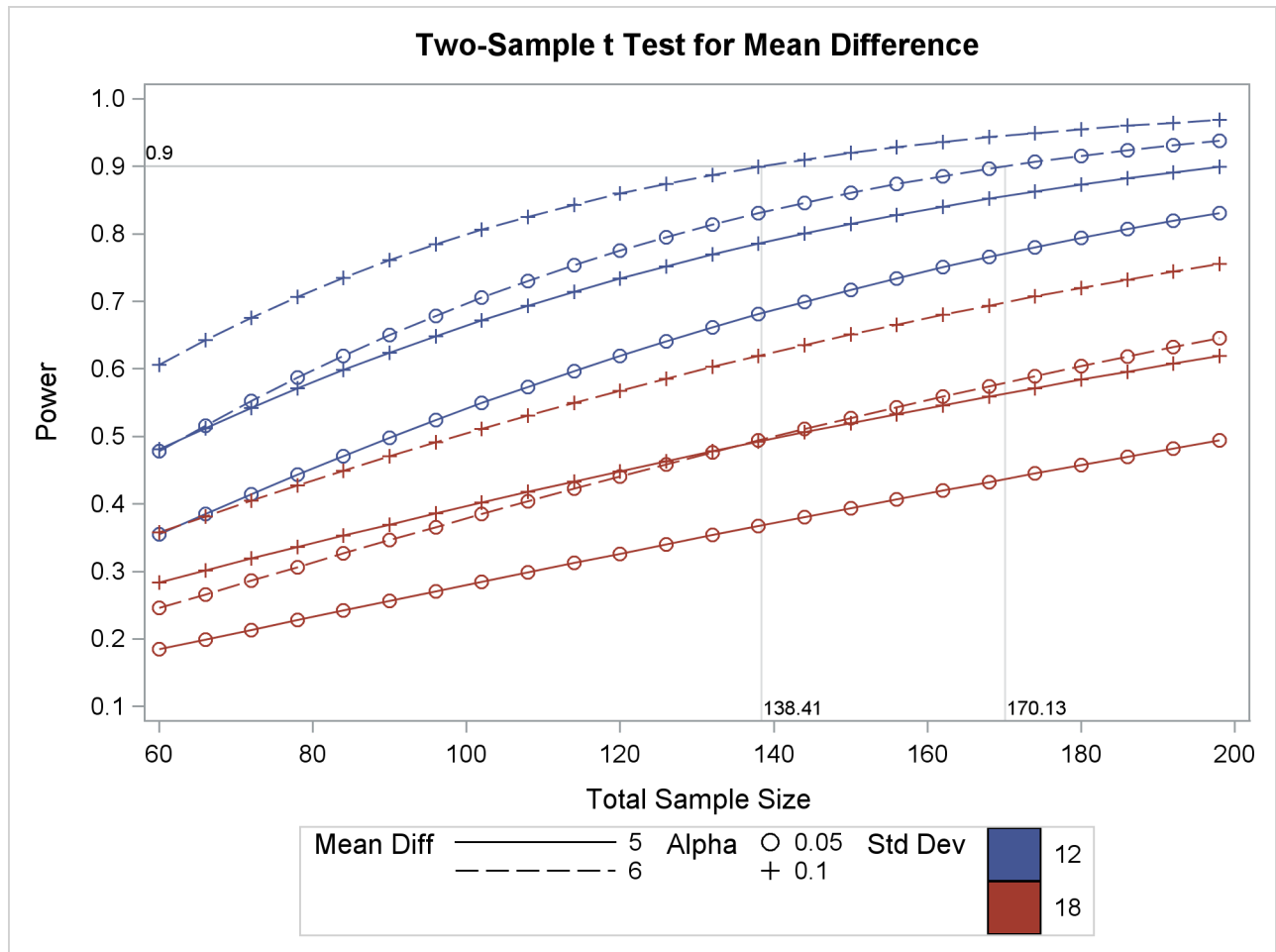
For example, replace the default PLOT statement with the following statement to modify the graphical results in Figure 18.2 to lower the minimum sample size to 60, show a reference line at power=0.9 with

corresponding sample size values, distinguish standard deviation by color instead of panel, and swap the roles of α and mean difference:

```
plot
  min=60
  yopts=(ref=0.9 crossref=yes)
  vary(color by stddev, linestyle by meandiff, symbol by alpha);
```

Figure 18.3 shows the results. The plot reveals that only the scenarios with the largest mean difference and smallest standard deviation achieve a power of at least 0.9 for this sample size range.

Figure 18.3 PROC POWER Customized Graphical Output



Formatted Tables (%POWTABLE Macro)

The %POWTABLE macro renders the output of the POWER and GLMPOWER procedures in rectangular form, and it optionally produces simplified results using weighted means across chosen variables. PROC REPORT and the Output Delivery System (ODS) are used to generate the tables. Base SAS and SAS/STAT 9.1 or higher versions are required.

You can run the %POWTABLE macro for the output in Figure 18.1 to display the results in a form more suitable for quickly discerning relationships among parameters. First use the ODS OUTPUT statement to assign the “Output” table produced by the POWER procedure to a data set as follows:

```
ods output output=powdata;
```

Next, specify the same PROC POWER statements that generate Figure 18.1. Finally, use the %POWTABLE macro to assign analysis parameters to table dimensions. To create a table of computed power values with mean difference assigned to rows, sample size and α assigned to columns, and standard deviation assigned to “panels” (rendered by default as rows separated by blank lines), specify the following statements:

```
%powtable ( Data = powdata,
            Entries = power,
            Rows = meandiff,
            Cols = ntotal alpha,
            Panels = stddev )
```

Figure 18.4 shows the results.

Figure 18.4 %POWTABLE Macro Output

The POWTABLE Macro						
Entries are Power						
Std Dev	Mean Diff	----- N Total -----				
		100		200		
		-- Alpha	---	-- Alpha	---	
		0.05	0.10	0.05	0.10	
12	5	0.541	0.664	0.834	0.902	
	6	0.697	0.799	0.940	0.970	
18	5	0.280	0.397	0.498	0.623	
	6	0.379	0.505	0.650	0.759	

Narratives and Graphical User Interface (Power and Sample Size Application)

The Power and Sample Size application produces narratives for the results. Narratives are descriptions of the input parameters and a statement about the computed power or sample size.

For example, the Power and Sample Size application creates the following narrative for the scenario corresponding to the first row in [Figure 18.1](#):

“For a two-sample pooled t test of a normal mean difference with a two-sided significance level of 0.05, assuming a common standard deviation of 12, a total sample size of 100 assuming a balanced design has a power of 0.541 to detect a mean difference of 5.”

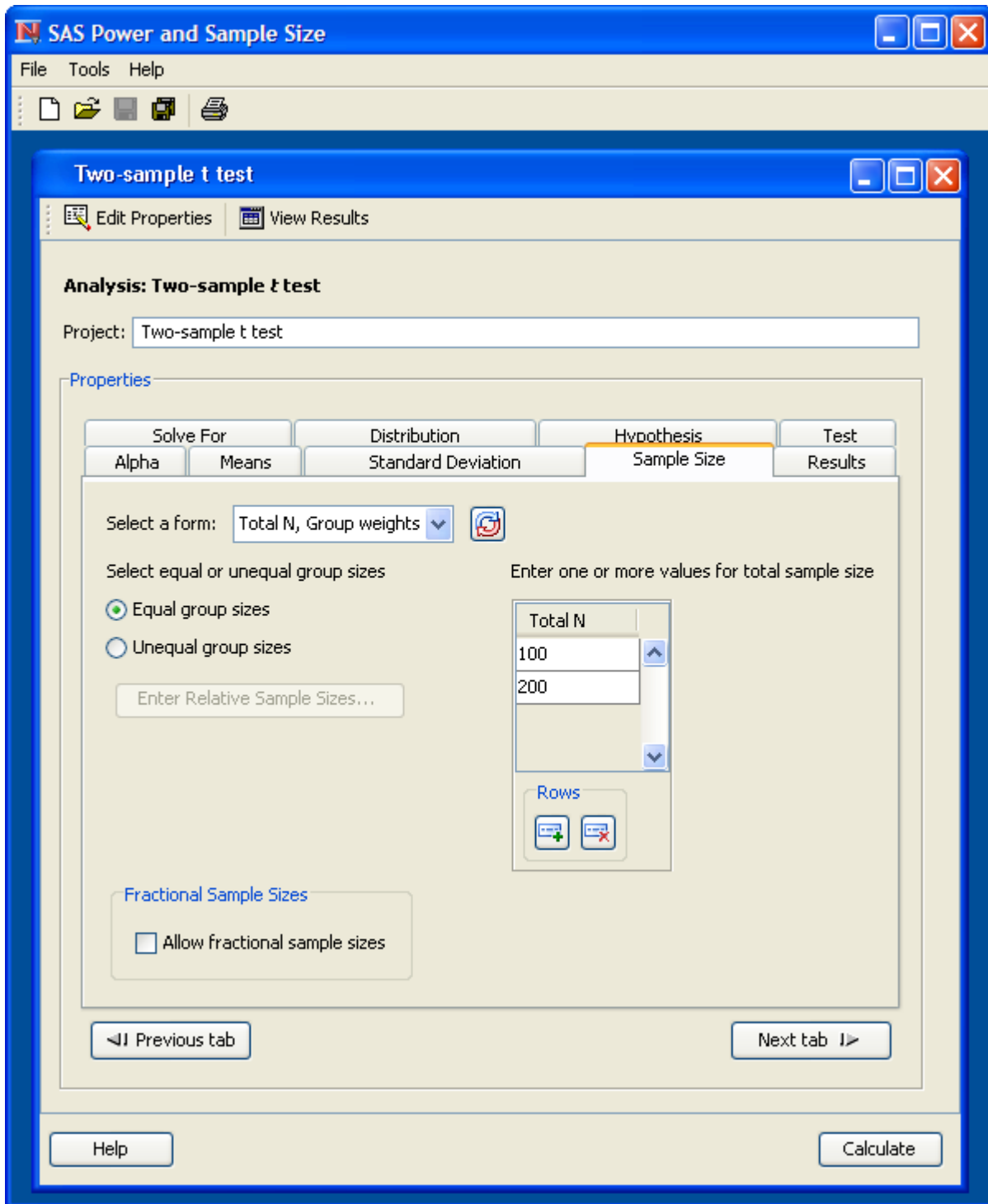
The Power and Sample Size application also provides multiple input parameter options, stores the results in a project format, displays power curves, and shows the SAS log and SAS code. You can access each project to review the results or to edit your input parameters and produce another analysis.

Where appropriate, several alternate ways of entering values for certain parameters are offered. For example, in the two-sample t test analysis, sample sizes can be entered in any of several parameterizations:

- total sample size in a balanced design
- sample size per group in a balanced design
- total sample size and group allocation weights
- groupwise sample sizes

See [Figure 18.5](#) for an illustration of the application, showing the sample size input page for a two-sample t test.

Figure 18.5 Power and Sample Size Application



Customized Power Formulas (DATA Step)

If you want to perform a power computation for an analysis that is not currently supported directly in SAS/STAT tools, and you have a power formula, then you can program the formula in the DATA step.

For purposes of illustration, here is the power formula in the section “Computing Power and Sample Size” on page 362 implemented in the DATA step to compute power for the t test example:

```
data tpow;
  do meandiff = 5, 6;
    do stddev = 12, 18;
      do alpha = 0.05, 0.1;
        do ntotal = 100, 200;
          ncp = ntotal * 0.5 * 0.5 * meandiff**2 / stddev**2;
          critval = finv(1-alpha, 1, ntotal-2, 0);
          power = sdf('f', critval, 1, ntotal-2, ncp);
          output;
        end;
      end;
    end;
  end;
run;

proc print data=tpow;
run;
```

The output is shown in Figure 18.6.

Figure 18.6 Customized Power Formula (DATA Step)

Obs	meandiff	stddev	alpha	ntotal	ncp	critval	power
1	5	12	0.05	100	4.3403	3.93811	0.54102
2	5	12	0.05	200	8.6806	3.88885	0.83447
3	5	12	0.10	100	4.3403	2.75743	0.66434
4	5	12	0.10	200	8.6806	2.73104	0.90171
5	5	18	0.05	100	1.9290	3.93811	0.27981
6	5	18	0.05	200	3.8580	3.88885	0.49793
7	5	18	0.10	100	1.9290	2.75743	0.39654
8	5	18	0.10	200	3.8580	2.73104	0.62287
9	6	12	0.05	100	6.2500	3.93811	0.69689
10	6	12	0.05	200	12.5000	3.88885	0.94043
11	6	12	0.10	100	6.2500	2.75743	0.79895
12	6	12	0.10	200	12.5000	2.73104	0.96985
13	6	18	0.05	100	2.7778	3.93811	0.37857
14	6	18	0.05	200	5.5556	3.88885	0.65012
15	6	18	0.10	100	2.7778	2.75743	0.50459
16	6	18	0.10	200	5.5556	2.73104	0.75935

Empirical Power Simulation (DATA Step, SAS/STAT Software)

You can obtain a highly accurate power estimate by simulating the power empirically. You need to use this approach for analyses that are not supported directly in SAS/STAT tools and for which you lack a power formula. But the simulation approach is also a viable alternative to existing power approximations. A high number of simulations will yield a more accurate estimate than a non-exact power approximation.

Although exact power computations for the two-sample t test are supported in several of the SAS/STAT tools, suppose for purposes of illustration that you want to simulate power for the continuing t test example. This section describes how you can use the DATA step and SAS/STAT software to do this.

The simulation involves generating a large number of data sets according to the distributions defined by the power analysis input parameters, computing the relevant p -value for each data set, and then estimating the power as the proportion of times that the p -value is significant.

The following statements compute a power estimate along with a 95% confidence interval for power for the first scenario in the two-sample t test example, with 10,000 simulations:

```
%let meandiff = 5;
%let stddev = 12;
%let alpha = 0.05;
%let ntotal = 100;
%let nsim = 10000;

data simdata;
  call streaminit(123);
  do isim = 1 to &nsim;
    do i = 1 to floor(&ntotal/2);
      group = 1;
      y = rand('normal', 0, &stddev);
      output;
      group = 2;
      y = rand('normal', &meandiff, &stddev);
      output;
    end;
  end;
run;

ods listing close;
proc ttest data=simdata;
  ods output ttests=tests;
  by isim;
  class group;
  var y;
run;
ods listing;

data tests;
  set tests;
  where method="Pooled";
  issig = probt < &alpha;
run;
```

```

proc freq data=tests;
  ods select binomialprop;
  tables issig / binomial(level='1');
run;

```

First the DATA step is used to randomly generate $nsim = 10,000$ data sets based on the *meandiff*, *stddev*, and *ntotal* parameters and the normal distribution, consistent with the assumptions underlying the two-sample *t* test. These data sets are contained in a large SAS data set called *simdata* indexed by the variable *isim*.

The CALL STREAMINIT(123) statement initializes the random number generator with a specific sequence and ensures repeatable results for purposes of this example. (NOTE: Skip this step when you are performing actual power simulations.)

The TTEST procedure is run using *isim* as a BY variable, with the ODS LISTING CLOSE statement to suppress output. The ODS OUTPUT statement saves the “TTests” table to a data set called *tests*. The *p*-values are contained in a column called *probt*.

The subsequent DATA step defines a variable called *issig* to flag the significant *p*-values.

Finally, the FREQ procedure computes the empirical power estimate as the estimate of $P(\text{issig} = 1)$ and provides approximate and exact confidence intervals for this estimate.

Figure 18.7 shows the results. The estimated power is 0.5388 with 95% confidence interval (0.5290, 0.5486). Note that the exact power of 0.541 shown in the first row in Figure 18.1 is contained within this tight confidence interval.

Figure 18.7 Simulated Power (DATA Step, SAS/STAT Software)

The FREQ Procedure	
Binomial Proportion	
issig = 1	
Proportion	0.5388
ASE	0.0050
95% Lower Conf Limit	0.5290
95% Upper Conf Limit	0.5486
Exact Conf Limits	
95% Lower Conf Limit	0.5290
95% Upper Conf Limit	0.5486

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Chapter 19

Shared Concepts and Topics

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This chapter introduces a number of concepts that are common to two or more SAS/STAT procedures. Most sections display a listing of the procedures for which the shared topic is relevant.

Levelization of Classification Variables

A classification variable is a variable that enters the statistical analysis or model not through its values, but through its levels. The process of associating values of a variable with levels is termed *levelization*.

This section covers in particular procedures that support a CLASS statement for specifying classification variables. Some of the concepts discussed also apply to procedures that use different syntax to request levelization of variables (for example, the CLASS() transformation in the TRANSREG procedure).

During the process of levelization, observations that share the same value are assigned to the same level. The manner in which values are grouped can be affected by the inclusion of formats. The sort order of the levels can be determined with the ORDER= option in the procedure statement. With the GENMOD, GLMSELECT, and LOGISTIC procedures, you can also control the sort order separately for each variable in the CLASS statement.

Consider the data on nine observations in [Table 19.1](#). The variable A is integer valued, and the variable X is a continuous variable with a missing value for the fourth observations. The fourth and fifth columns of [Table 19.1](#) apply two different formats to the variable X.

Table 19.1 Example Data for Levelization

Obs	A	x	FORMAT x 3.0	FORMAT x 3.1
1	2	1.09	1	1.1
2	2	1.13	1	1.1
3	2	1.27	1	1.3
4	3	.	.	.
5	3	2.26	2	2.3
6	3	2.48	2	2.5
7	4	3.34	3	3.3
8	4	3.34	3	3.3
9	4	3.14	3	3.1

By default, levelization of the variables groups observations by the formatted value of the variable, except for numerical variables for which no explicit format is provided. Numerical variables for which no explicit format is provided are sorted by their internal value. The levelization of the four columns in [Table 19.1](#) leads to the level assignment in [Table 19.2](#).

Table 19.2 Values and Levels

Obs	A		X		FORMAT x 3.0		FORMAT x 3.1	
	Value	Level	Value	Level	Value	Level	Value	Level
1	2	1	1.09	1	1	1	1.1	1
2	2	1	1.13	2	1	1	1.1	1
3	2	1	1.27	3	1	1	1.3	2
4	3	2
5	3	2	2.26	4	2	2	2.3	3
6	3	2	2.48	5	2	2	2.5	4
7	4	3	3.34	7	3	3	3.3	6
8	4	3	3.34	7	3	3	3.3	6
9	4	3	3.14	6	3	3	3.1	5

The ORDER= option in the PROC statement specifies the sort order for the levels of CLASS variables. When ORDER=FORMATTED (which is the default) is in effect for numeric variables for which you have supplied no explicit format, the levels are ordered by their internal values. To order numeric class levels with no explicit format by their BEST12. formatted values, you can specify the BEST12. format explicitly for the CLASS variables.

The following table shows how values of the ORDER= option are interpreted.

Value of ORDER=	Levels Sorted By
DATA	Order of appearance in the input data set
FORMATTED	External formatted value, except for numeric variables with no explicit format, which are sorted by their unformatted (internal) value
FREQ	Descending frequency count; levels with the most observations come first in the order
INTERNAL	Unformatted value

For FORMATTED and INTERNAL values, the sort order is machine dependent. For more information about sort order, see the chapter on the SORT procedure in the *Base SAS Procedures Guide* and the discussion of BY-group processing in *SAS Language Reference: Concepts*.

The GLMSELECT, LOGISTIC, and GENMOD procedures support a MISSING option in the CLASS statement. When this option is in effect, missing values (‘.’ for a numeric variable and blanks for a character variable) are included in the levelization and are assigned a level. Table 19.3 displays the results of levelizing the values in Table 19.1 when the MISSING option is in effect.

Table 19.3 Values and Levels with MISSING Option

Obs	A		X		FORMAT x 3.0		FORMAT x 3.1	
	Value	Level	Value	Level	Value	Level	Value	Level
1	2	1	1.09	2	1	2	1.1	2
2	2	1	1.13	3	1	2	1.1	2
3	2	1	1.27	4	1	2	1.3	3
4	3	2	.	1	.	1	.	1
5	3	2	2.26	5	2	3	2.3	4
6	3	2	2.48	6	2	3	2.5	5
7	4	3	3.34	8	3	4	3.3	7
8	4	3	3.34	8	3	4	3.3	7
9	4	3	3.14	7	3	4	3.1	6

When the MISSING option is not specified, or for procedures whose CLASS statement does not support this option, it is important to understand the implications of missing values for your statistical analysis. When a SAS/STAT procedure levelizes the CLASS variables, an observation for which a CLASS variable has a missing value is excluded from the analysis. This is true regardless of whether the variable is used to form the statistical model. Consider, for example, the case where some observations contain missing values for variable A but the records for these observations are otherwise complete with respect to all other variables in the statistical models. The analysis results from the following statements do not include any observations for which variable A contains missing values, even though A is not specified in the MODEL statement:

```
class A B;
model y = B x B*x;
```

Many statistical procedures print a “Number of Observations” table that shows the number of observations read from the data set and the number of observations used in the analysis. Pay careful attention to this

table—especially when your data set contains missing values—to ensure that no observations are unintentionally excluded from the analysis.

Parameterization of Model Effects

The general form of a linear regression model is defined in Chapter 3, “Regression Models and Models with Classification Effects” as

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

This section describes how matrices of regressor effects such as \mathbf{X} are constructed in SAS/STAT software. These constructions (*parameterization* rules) apply to regression models, models with classification effects, generalized linear models, and mixed models. The simplest and most general parameterization rules are the ones used in the GLM procedure, and they are discussed first. Several procedures also support alternate parameterizations of classification variables, including the CATMOD, GENMOD, GLMSELECT, LOGISTIC, PHREG, SURVEYLOGISTIC, and SURVEYPHREG procedures. These are discussed after the GLM parameterization of classification variables and model effects.

All modeling procedures that have a CLASS statement support classification variables and effects, and those procedures that additionally support the supplemental parameterizations have a PARAM= option in the CLASS statement.

GLM Parameterization of Classification Variables and Effects

This section applies to the following procedures:

GAM, GENMOD, GLIMMIX, GLM, GLMPOWER, GLMSELECT, LIFEREG, LOGISTIC, MI, MIXED, MULLTEST, ORTHOREG, PHREG, PLS, QUANTREG, ROBUSTREG, SURVEYLOGISTIC, and SURVEYPHREG.

Intercept

By default, SAS/STAT linear models automatically include a column of 1s in \mathbf{X} which corresponds to an intercept parameter. In many procedures you can use the NOINT option in the MODEL statement to suppress this intercept. For example, the NOINT option is useful when the MODEL statement contains a classification effect and you want the parameter estimates to be in terms of the mean response for each level of that effect.

Regression Effects

Numeric variables or polynomial terms that involve them can be included in the model as regression effects (covariates). The actual values of such terms are included as columns of the relevant model matrices. You can use the bar operator with a regression effect to generate polynomial effects. For example, XIXIX expands to $X X^*X X^*X^*X$, which is a cubic model.

Main Effects

If a classification variable has m levels, the GLM parameterization generates m columns for its main effect in the model matrix. Each column is an indicator variable for a given level. The order of the columns is the sort order of the values of their levels and frequently can be controlled with the `ORDER=` option in the procedure or `CLASS` statement.

Table 19.4 is an example where β_0 denotes the intercept and A and B are classification variables with two and three levels, respectively.

Table 19.4 Example of Main Effects

Data		I	A			B		
A	B	β_0	A1	A2	B1	B2	B3	
1	1	1	1	0	1	0	0	
1	2	1	1	0	0	1	0	
1	3	1	1	0	0	0	1	
2	1	1	0	1	1	0	0	
2	2	1	0	1	0	1	0	
2	3	1	0	1	0	0	1	

Typically, there are more columns for these effects than there are degrees of freedom to estimate them. In other words, the GLM parameterization of main effects is *singular*.

Interaction Effects

Often a model includes interaction (crossed) effects to account for how the effect of a variable changes with the values of other variables. With an interaction, the terms are first reordered to correspond to the order of the variables in the `CLASS` statement. Thus, `B*A` becomes `A*B` if A precedes B in the `CLASS` statement. Then, the GLM parameterization generates columns for all combinations of levels that occur in the data. The order of the columns is such that the rightmost variables in the interaction change faster than the leftmost variables (Table 19.5). In the `MIXED` and `GLIMMIX` procedures, which support both fixed- and random-effects models, empty columns (that is, columns that would contain all 0s) are not generated for fixed effects, but they are generated for random effects.

Table 19.5 Example of Interaction Effects

Data		I	A			B			A*B					
A	B	β_0	A1	A2	B1	B2	B3	A1B1	A1B2	A1B3	A2B1	A2B2	A2B3	
1	1	1	1	0	1	0	0	1	0	0	0	0	0	
1	2	1	1	0	0	1	0	0	1	0	0	0	0	
1	3	1	1	0	0	0	1	0	0	1	0	0	0	
2	1	1	0	1	1	0	0	0	0	0	1	0	0	
2	2	1	0	1	0	1	0	0	0	0	0	1	0	
2	3	1	0	1	0	0	1	0	0	0	0	0	1	

In the preceding matrix, main-effects columns are not linearly independent of crossed-effects columns; in fact, the column space for the crossed effects contains the space of the main effect.

When your model contains many interaction effects, you might be able to code them more parsimoniously by using the bar operator ($|$). The bar operator generates all possible interaction effects. For example, $A|B|C$ expands to $A B A*B C A*C B*C A*B*C$. To eliminate higher-order interaction effects, use the at sign ($@$) in conjunction with the bar operator. For instance, $A|B|C|D@2$ expands to $A B A*B C A*C B*C D A*D B*D C*D$.

Nested Effects

Nested effects are generated in the same manner as crossed effects. Hence, the design columns generated by the following two statements are the same (but the ordering of the columns is different):

```
model Y=A B(A);
```

```
model Y=A A*B;
```

The nesting operator in SAS/STAT software is more of a notational convenience than an operation distinct from crossing. Nested effects are typically characterized by the property that the nested variables never appear as main effects. The order of the variables within nesting parentheses is made to correspond to the order of these variables in the CLASS statement. The order of the columns is such that variables outside the parentheses index faster than those inside the parentheses, and the rightmost nested variables index faster than the leftmost variables (Table 19.6).

Table 19.6 Example of Nested Effects

Data		I	A		B(A)					
A	B	β_0	A1	A2	B1A1	B2A1	B3A1	B1A2	B2A2	B3A2
1	1	1	1	0	1	0	0	0	0	0
1	2	1	1	0	0	1	0	0	0	0
1	3	1	1	0	0	0	1	0	0	0
2	1	1	0	1	0	0	0	1	0	0
2	2	1	0	1	0	0	0	0	1	0
2	3	1	0	1	0	0	0	0	0	1

Continuous-Nesting-Class Effects

When a continuous variable nests or crosses with a classification variable, the design columns are constructed by multiplying the continuous values into the design columns for the classification effect (Table 19.7).

Table 19.7 Example of Continuous-Nesting-Class Effects

Data		I	A		X(A)	
X	A	β_0	A1	A2	X(A1)	X(A2)
21	1	1	1	0	21	0
24	1	1	1	0	24	0
22	1	1	1	0	22	0
28	2	1	0	1	0	28
19	2	1	0	1	0	19
23	2	1	0	1	0	23

This model estimates a separate intercept and a separate slope for X within each level of A.

Continuous-by-Class Effects

Continuous-by-class effects generate the same design columns as continuous-nesting-class effects. Table 19.8 shows the construction of the X*A effect. The two columns for this effect are the same as the columns for the X(A) effect in Table 19.7.

Table 19.8 Example of Continuous-by-Class Effects

Data		I	X	A		X*A	
X	A	β_0	X	A1	A2	X*A1	X*A2
21	1	1	21	1	0	21	0
24	1	1	24	1	0	24	0
22	1	1	22	1	0	22	0
28	2	1	28	0	1	0	28
19	2	1	19	0	1	0	19
23	2	1	23	0	1	0	23

You can use continuous-by-class effects together with pure continuous effects to test for homogeneity of slopes.

General Effects

An example that combines all the effects is X1*X2*A*B*(D E). The continuous list comes first, followed by the crossed list, followed by the nested list in parentheses. You should be aware of the sequencing of parameters when you use statements that depend on the ordering of parameters. Such statements include CONTRAST and ESTIMATE statements, which are used in a number of procedures to estimate and test functions of the parameters.

Effects might be renamed by the procedure to correspond to ordering rules. For example, B*A(E D) might be renamed A*B(D E) to satisfy the following:

- Classification variables that occur outside parentheses (crossed effects) are sorted in the order in which they appear in the CLASS statement.
- Variables within parentheses (nested effects) are sorted in the order in which they appear in the CLASS statement.

The sequencing of the parameters generated by an effect can be described by which variables have their levels indexed faster:

- Variables in the crossed list index faster than variables in the nested list.
- Within a crossed or nested list, variables to the right index faster than variables to the left.

For example, suppose a model includes four effects—A, B, C, and D—each having two levels, 1 and 2. If the CLASS statement is

```
class A B C D;
```

then the order of the parameters for the effect B*A(C D), which is renamed A*B(C D), is

$$\begin{aligned}
 &A_1 B_1 C_1 D_1 \rightarrow A_1 B_2 C_1 D_1 \rightarrow A_2 B_1 C_1 D_1 \rightarrow A_2 B_2 C_1 D_1 \rightarrow \\
 &A_1 B_1 C_1 D_2 \rightarrow A_1 B_2 C_1 D_2 \rightarrow A_2 B_1 C_1 D_2 \rightarrow A_2 B_2 C_1 D_2 \rightarrow \\
 &A_1 B_1 C_2 D_1 \rightarrow A_1 B_2 C_2 D_1 \rightarrow A_2 B_1 C_2 D_1 \rightarrow A_2 B_2 C_2 D_1 \rightarrow \\
 &A_1 B_1 C_2 D_2 \rightarrow A_1 B_2 C_2 D_2 \rightarrow A_2 B_1 C_2 D_2 \rightarrow A_2 B_2 C_2 D_2
 \end{aligned}$$

Note that first the crossed effects B and A are sorted in the order in which they appear in the CLASS statement so that A precedes B in the parameter list. Then, for each combination of the nested effects in turn, combinations of A and B appear. The B effect changes fastest because it is rightmost in the cross list. Then A changes next fastest, and D changes next fastest. The C effect changes most slowly because it is leftmost in the nested list.

Other Parameterizations

This section applies to the following procedures:

CATMOD, GENMOD, GLMSELECT, LOGISTIC, PHREG, and SURVEYPHREG.

Some SAS/STAT procedures, including GENMOD, GLMSELECT, and LOGISTIC, support nonsingular parameterizations for classification effects. A variety of these nonsingular parameterizations are available. In most of these procedures you use the PARAM= option in the CLASS statement to specify the parameterization.

Consider a model with one CLASS variable A that has four levels, 1, 2, 5, and 7. Details of the possible choices for the PARAM= option follow.

EFFECT Three columns are created to indicate group membership of the nonreference levels. For the reference level, all three dummy variables have a value of -1 . For example, if the reference level is 7 (REF=7), the design matrix columns for A are as follows.

Effect Coding			
Design Matrix			
A	A1	A2	A5
1	1	0	0
2	0	1	0
5	0	0	1
7	-1	-1	-1

Parameter estimates of CLASS main effects that use the effect coding scheme estimate the difference in the effect of each nonreference level compared to the average effect over all four levels.

The EFFECT parameterization is the default parameterization in the CATMOD procedure. See the section “[Generation of the Design Matrix](#)” on page 1832, in Chapter 30, “[The CATMOD Procedure](#),” for further details about parameterization of model effects with the CATMOD procedure.

GLM

As in the GLM procedure, four columns are created to indicate group membership. The design matrix columns for A are as follows.

GLM Coding				
Design Matrix				
A	A1	A2	A5	A7
1	1	0	0	0
2	0	1	0	0
5	0	0	1	0
7	0	0	0	1

Parameter estimates of CLASS main effects that use the GLM coding scheme estimate the difference in the effects of each level compared to the last level. See the previous section for details about the GLM parameterization of model effects.

ORDINAL | THERMOMETER Three columns are created to indicate group membership of the higher levels of the effect. For the first level of the effect (which for A is 1), all three dummy variables have a value of 0. The design matrix columns for A are as follows.

Ordinal Coding			
Design Matrix			
A	A2	A5	A7
1	0	0	0
2	1	0	0
5	1	1	0
7	1	1	1

The first level of the effect is a control or baseline level. Parameter estimates of CLASS main effects, using the ORDINAL coding scheme, estimate the differences between effects of successive levels. When the parameters have the same sign, the effect is monotonic across the levels.

POLYNOMIAL | POLY Three columns are created. The first represents the linear term (x), the second represents the quadratic term (x^2), and the third represents the cubic term (x^3), where x is the level value. If the CLASS levels are not numeric, they are translated into 1, 2, 3, . . . according to their sort order. The design matrix columns for A are as follows.

Polynomial Coding			
Design Matrix			
A	APOLY1	APOLY2	APOLY3
1	1	1	1
2	2	4	8
5	5	25	125
7	7	49	343

REFERENCE | REF Three columns are created to indicate group membership of the nonreference levels. For the reference level, all three dummy variables have a value of 0. For example, if the reference level is 7 (REF=7), the design matrix columns for A are as follows.

Reference Coding			
Design Matrix			
A	A1	A2	A5
1	1	0	0
2	0	1	0
5	0	0	1
7	0	0	0

Parameter estimates of CLASS main effects that use the reference coding scheme estimate the difference in the effect of each nonreference level compared to the effect of the reference level.

The REFERENCE parameterization is also available through the MODEL statement in the CATMOD procedure. See the section “[Generation of the Design Matrix](#)” on page 1832, in Chapter 30, “[The CATMOD Procedure](#),” for further details about parameterization of model effects with the CATMOD procedure.

ORTHEFFECT The columns are obtained by applying the Gram-Schmidt orthogonalization to the columns for PARAM=EFFECT. The design matrix columns for A are as follows.

Orthogonal Effect Coding			
Design Matrix			
A	AOEFF1	AOEFF2	AOEFF3
1	1.41421	-0.81650	-0.57735
2	0	1.63299	-0.57735
5	0	0	1.73205
7	-1.41421	-0.81649	-0.57735

ORTHORDINAL | ORTHOTHERM The columns are obtained by applying the Gram-Schmidt orthogonalization to the columns for PARAM=ORDINAL. The design matrix columns for A are as follows.

Orthogonal Ordinal Coding			
Design Matrix			
A	AOORD1	AOORD2	AOORD3
1	-1.73205	0	0
2	0.57735	-1.63299	0
5	0.57735	0.81650	-1.41421
7	0.57735	0.81650	1.41421

ORTHPOLY

The columns are obtained by applying the Gram-Schmidt orthogonalization to the columns for PARAM=POLY. The design matrix columns for A are as follows.

Orthogonal Polynomial Coding			
Design Matrix			
A	AOPOLY1	AOPOLY2	AOPOLY5
1	-1.15311	0.90712	-0.92058
2	-0.73380	-0.54041	1.47292
5	0.52414	-1.37034	-0.92058
7	1.36277	1.00363	0.36823

ORTHREF

The columns are obtained by applying the Gram-Schmidt orthogonalization to the columns for PARAM=REFERENCE. The design matrix columns for A are as follows.

Orthogonal Reference Coding			
Design Matrix			
A	AOREF1	AOREF2	AOREF3
1	1.73205	0	0
2	-0.57735	1.63299	0
5	-0.57735	-0.81650	1.41421
7	-0.57735	-0.81650	-1.41421

CODE Statement

This statement documentation applies to the following procedures: GENMOD, GLIMMIX, GLM, GLMSELECT, LOGISTIC, MIXED, PLM, and REG. It also applies to the HPLOGISTIC and HPREG procedures in SAS High-Performance Analytics software.

The CODE statement enables you to write SAS DATA step code to a file or catalog entry for computing predicted values of the fitted model. This code can then be included in a DATA step to score new data. For example, in the following program, the CODE statement writes the code for predicting the outcome of a logistic model to the file *mycode.sas*. The file is subsequently included in a DATA step to score the sashelp.Bmt data.

```

proc logistic data=sashelp.Bmt;
  class Group;
  model Status=Group;
  code file='mycode.sas';
run;

data Score;
  set sashelp.Bmt;
  %include mycode;
run;

```

Syntax: CODE Statement

CODE < options > ;

Table 19.9 summarizes the *options* you can specify in the CODE statement.

Table 19.9 CODE Statement Options

Option	Description
CATALOG=	Names the catalog entry where the generated code is saved
DUMMIES	Retains the dummy variables in the data set
ERROR	Computes the error function
FILE=	Names the file where the generated code is saved
FORMAT=	Specifies the numeric format for the regression coefficients
GROUP=	Specifies the group identifier for array names and statement labels
IMPUTE	Imputes predicted values for observations with missing or invalid covariates
LINESIZE=	Specifies the line size of the generated code
LOOKUP=	Specifies the algorithm for looking up CLASS levels
RESIDUAL	Computes residuals

You cannot specify both the FILE= and CATALOG= options. If you specify neither, the SAS scoring code is written to the SAS log. You can specify the following *options* in the CODE statement.

CATALOG=*library.catalog.entry.type*

CAT=*library.catalog.entry.type*

specifies where to write the generated code in the form of *library.catalog.entry.type*. The compound name can have from one to four levels. The default library is determined by the USER= SAS system option, which by default is WORK. The default *entry* is SASCODE, and the default *type* is SOURCE.

DUMMIES | NODUMMIES

specifies whether to keep dummy variables that represent the CLASS levels in the data set. The default is NODUMMIES, which specifies that dummy variables not be retained.

ERROR | NOERROR

specifies whether to generate code to compute the error function. The default is NOERROR, which specifies that the error function not be generated.

FILE=*filename*

names the external file that saves the generated code. When enclosed in a quoted string (for example, FILE="c:\mydir\scorecode.sas"), this option specifies the path for writing the code to an external file. You can also specify unquoted SAS filenames of no more than eight characters for *filename*. If the *filename* is assigned as a *fileref* in a Base SAS FILENAME statement, the file specified in the FILENAME statement is opened. The special *filerrefs* LOG and PRINT are always assigned. If the specified *filename* is not an assigned *fileref*, the specified value for *filename* is concatenated with a .txt extension before the file is opened. For example, if FOO is not an assigned *fileref*, FILE=FOO causes FOO.txt to be opened. If *filename* has more than eight characters, an error message is printed.

FORMAT=*format*

specifies the format for the regression coefficients and other numerical values that do not have a format from the input data set. The default *format* is BEST20.

GROUP=*group-name*

specifies the group identifier for group processing. The *group-name* should be a valid SAS name of no more than 16 characters. It is used to construct array names and statement labels in the generated code.

IMPUTE

imputes the predicted values according to an intercept-only model for observations with missing or invalid covariate values. For a continuous response, the predicted value is the mean of the response variable; for a categorical response, the predicted values are the proportions of the response categories. When the IMPUTE option is specified, the scoring code also creates a variable named _WARN_ that contains one or more single-character codes that indicate problems in computing predicted values. The character codes used in _WARN_ go in the following positions:

Table 19.10 _WARN_ Variable Codes

Code	Column	Meaning
M	1	Missing covariate value
U	2	Unrecognized covariate category

LINESIZE=*value***LS=*value***

specifies the line size for the generated code. The default is 72. The permissible range is 64 to 254.

LOOKUP=*lookup-method*

specifies the algorithm for looking up CLASS levels. You can specify the following *lookup-methods*:

AUTO

selects the LINEAR algorithm if a CLASS variable has fewer than five categories; otherwise, the BINARY algorithm is used. This is the default.

BINARY

uses a binary search. This method is fast, but might produce incorrect results and the normalized category values might contain characters that collate in different orders in ASCII and EBCDIC, if you generate the code on an ASCII machine and execute the code on an EBCDIC machine or vice versa.

LINEAR

uses a linear search with IF statements that have categories in the order of the class levels. This method is slow if there are many categories.

SELECT

uses a SELECT statement.

The default is LOOKUP=AUTO.

RESIDUAL | NORESIDUAL

specifies whether to generate code to compute residual values. If you request code for residuals and then score a data set that does not contain target values, the residuals will have missing values. The default is NORESIDUAL, which specifies that the code for residuals not be generated.

EFFECT Statement

This section applies to the following procedures:

GLIMMIX, GLMSELECT, HPMIXED, LOGISTIC, ORTHOREG, PHREG, PLS, QUANTLIFE, QUANTREG, QUANTSELECT, ROBUSTREG, SURVEYLOGISTIC, and SURVEYREG.

The EFFECT statement enables you to construct special collections of columns for design matrices. These collections are referred to as *constructed effects* to distinguish them from the usual model effects that are formed from continuous or classification variables, as discussed in the section “[GLM Parameterization of Classification Variables and Effects](#)” on page 383. For example, the terms A, B, x, A*x, A*B, and sub in the following statements define fixed, random, and subject effects of the usual type in a mixed model:

```
proc glimmix;
  class A B sub;
  model y = A B x A*x;
  random A*B / subject=sub;
run;
```

A constructed effect, on the other hand, is assigned through the EFFECT statement. For example, in the following program, the EFFECT statement defines a constructed effect named spl:

```
proc glimmix;
  class A B SUB;
  effect spl = spline(x);
  model y = A B A*spl;
  random A*B / subject=sub;
run;
```

The columns of `spl` are formed from the data set variable `x` as a cubic B-spline basis with three equally spaced interior knots.

Each constructed effect corresponds to a collection of columns that are referred to by using the name you supply. You can specify multiple `EFFECT` statements, and all `EFFECT` statements must precede the `MODEL` statement.

The general syntax for the `EFFECT` statement with *effect-specification* is

```
EFFECT effect-name = effect-type (var-list < / effect-options > ) ;
```

The name of the effect is specified after the `EFFECT` keyword. This name can appear in only one `EFFECT` statement and cannot be the name of a variable in the input data set. The *effect-type* is specified after an equal sign, followed by a list of variables within parentheses which are used in constructing the effect. *Effect-options* that are specific to an *effect-type* can be specified after a slash (/) following the variable list. The following *effect-types* are available and are discussed in the following sections:

COLLECTION	is a collection effect that defines one or more variables as a single effect with multiple degrees of freedom. The variables in a collection are considered as a unit for estimation and inference.
LAG	is a classification effect in which the level that is used for a given period corresponds to the level in the preceding period.
MULTIMEMBER MM	is a multimember classification effect whose levels are determined by one or more variables that appear in a <code>CLASS</code> statement.
POLYNOMIAL POLY	is a multivariate polynomial effect in the specified numeric variables.
SPLINE	is a regression spline effect whose columns are univariate spline expansions of one or more variables. A spline expansion replaces the original variable with an expanded or larger set of new variables.

Table 19.11 summarizes the *options* available in the `EFFECT` statement.

Table 19.11 EFFECT Statement Options

Option	Description
Collection Effects Options	
<code>DETAILS</code>	Displays the constituents of the collection effect
Lag Effects Options	
<code>DESIGNROLE=</code>	Names a variable that controls to which lag design an observation is assigned
<code>DETAILS</code>	Displays the lag design of the lag effect
<code>NLAG=</code>	Specifies the number of periods in the lag
<code>PERIOD=</code>	Names the variable that defines the period
<code>WITHIN=</code>	Names the variable or variables that define the group within which each period is defined

Table 19.11 *continued*

Option	Description
Multimember Effects Options	
NOEFFECT	Specifies that observations with all missing levels for the multimember variables should have zero values in the corresponding design matrix columns
WEIGHT=	Specifies the weight variable for the contributions of each of the classification effects
Polynomial Effects Options	
DEGREE=	Specifies the degree of the polynomial
MDEGREE=	Specifies the maximum degree of any variable in a term of the polynomial
STANDARDIZE=	Specifies centering and scaling suboptions for the variables that define the polynomial
Spline Effects Options	
BASIS=	Specifies the type of basis (B-spline basis or truncated power function basis) for the spline expansion
DEGREE=	Specifies the degree of the spline transformation
KNOTMETHOD=	Specifies how to construct the knots for spline effects

Collection Effects

EFFECT *name*=COLLECTION (*var-list* </ DETAILS >) ;

You use a collection effect to define a set of variables that are treated as a single effect with multiple degrees of freedom. The variables in *var-list* can be continuous or classification variables. The columns in the design matrix that are contributed by a collection effect are the design columns of its constituent variables in the order in which they appear in the definition of the collection effect. If you specify the DETAILS option, then a table that shows the constituents of the collection effect is displayed.

Lag Effects

EFFECT *name*=LAG (*variable* / *lag-options*) ;

A lag effect is a classification effect for the CLASS variable that is given after the keyword LAG. A lag effect is used to represent the effect of a previous value of the lagged variable when there is some inherent ordering of the observations of this variable. A typical example where lag effects are useful is a study in which different subjects are given sequences of treatments and you want to investigate whether the treatment in the previous period is important in understanding the outcome in the current period. You can do this by including a lagged treatment effect in your model.

The precise definition of a LAG effect depends on a subdivision of the data into disjoint subsets, often referred to as “subjects,” and an ordering into units called “periods” of the observations within a subject.

For an observation that belongs to a given subject and at a given period, the design matrix columns of the lagged variable are the usual design matrix columns of that variable except for the observation at the preceding period for that subject. Observations at the initial period do not have a preceding value, and so the design matrix columns of the lag effect for these observations are set to zero. You can also define lag effects where the number of periods that are lagged is greater than one. If the number of periods that are lagged is n , then the design matrix columns of observations in periods less than or equal to n are set to zero. The design matrix columns that correspond to a subject at period p , where $p > n$, are the usual design matrix columns of the lagged variable for that subject at period $p - n$.

A convenient way to represent the organization of observations into subjects and periods is to form the lag design matrix. The rows and columns of this matrix correspond to the subjects and periods respectively. The lag design matrix entry is the treatment for the corresponding subject and period. In a valid lag design there is at most one observation for a given period and subject. For example, the following set of treatments by subject and period form a valid lag design:

Subject	Period	Treatment
Sheila	1	B
Joey	1	A
Athena	1	A
Gelindo	1	A
Sheila	2	C
Joey	2	A
Athena	2	.
Gelindo	2	B
Sheila	3	B
Joey	3	C
Athena	3	A
Gelindo	3	B

The associated lag design matrix is

Subject	--Period--		
	1	2	3
Athena	A		A
Gelindo	A	B	B
Joey	A	A	C
Sheila	B	C	B

Note that the subject Athena did not receive a treatment at period 2, and so the corresponding entry in the lag design matrix is missing. You can define a lag effect for this lag design with the following statements:

```
CLASS treatment;
EFFECT Lag = LAG( treatment / WITHIN=subject PERIOD=period);
```

When GLM coding is used for the CLASS variable treatment, the design matrix columns Lag_A, Lag_B, and Lag_C for the constructed effect Lag are as follows:

Subject	period	treatment	Lag_A	Lag_B	Lag_C
Athena	1	A	0	0	0
Athena	2		1	0	0
Athena	3	A	.	.	.
Gelindo	1	A	0	0	0
Gelindo	2	B	1	0	0
Gelindo	3	B	0	1	0
Joey	1	A	0	0	0
Joey	2	A	1	0	0
Joey	3	C	1	0	0
Sheila	1	B	0	0	0
Sheila	2	C	0	1	0
Sheila	3	B	0	0	1

The design matrix columns for each subject at period 1 are all zero because there are no lagged observations for period 1. You can also see that the design matrix columns at period 3 for subject Athena are missing because Athena did not receive a treatment at period 2. Nevertheless, the design matrix columns for Athena at period 2 are nonmissing and correspond to the treatment “A” that she received in period 1.

The following *lag-options* are required:

PERIOD=*variable*

specifies the period variable of the LAG design. The number of periods is the number of unique formatted values of the PERIOD= variable, and the ordering of the period is formed by sorting these formatted values in ascending order. You must specify a PERIOD= variable.

WITHIN=*(variables)*

WITHIN=*variable*

specifies a variable (or a list of variables within parentheses) that defines the subject grouping of the lag design. If there is only one WITHIN= *variable*, then the parentheses are not required. Each *subject* is defined by the unique set of formatted values of the *variables* in the WITHIN= list. The subjects are sorted in ascending lexicographic order. You must specify a WITHIN= variable.

You can also specify the following *lag-options*:

DESIGNROLE=*variable*

specifies a numeric variable that is used to subset observations into a fitting group in which the value of the DESIGNROLE= variable is nonzero and a second group in which the value of the specified *variable* is zero. The observations in the fitting group are used to form the LAG design matrix that is used in fitting the model. The LAG design that corresponds to the non-fitting group is used when scoring observations in the input data set that do not belong to the fitting group. This option is useful when you want to obtain predicted values in an output data set for observations that are not used in fitting the model. If you do not specify a DESIGNROLE= *variable*, then all observations are assigned to the fitting group.

DETAILS

requests a table that shows the lag design matrix of the lag effect.

NLAG= *n*

specifies the number of lags. By default NLAG=1.

Multimember Effects

EFFECT *name*=MULTIMEMBER (*var-list* </ *mm-options*>);

EFFECT *name*=MM (*var-list* </ *mm-options*>);

A multimember effect is formed from one or more classification variables in such a way that each observation can be associated with one or more levels of the union of the levels of the classification variables. In other words, a multimember effect is a classification-type effect with possibly more than one nonzero column entry for each observation. Multimember effects are useful, for example, in modeling the following:

- nurses' effects on patient recovery in hospitals
- teachers' effects on student scores
- lineage effects in genetic studies. See [Example 41.16](#) in Chapter 41, “The GLIMMIX Procedure,” for an application with random multimember effects in a genetic diallel experiment.

The levels of a multimember effect consist of the union of formatted values of the variables that define this effect. Each such level contributes one column to the design matrix. For each observation, the value that corresponds to each level of the multimember effect in the design matrix is the number of times that this level occurs for the observation.

For example, the following data provide teacher information and end-of-year test scores for students after two semesters:

Student	Score	Teacher1	Teacher2
Mary	87	Tobias	Cohen
Tom	89	Rodriguez	Tobias
Fred	82	Cohen	Cohen
Jane	88	Tobias	.
Jack	99	.	.

For example, Mary had different teachers in the two semesters, Fred had the same teacher in both semesters, and Jane received instruction only in the first semester.

You can model the effect of the teachers on student performance by using a multimember effect specified as follows:

```
CLASS teacher1 teacher2;
EFFECT teacher = MM(teacher1 teacher2);
```

The levels of the teacher effect are Cohen, Rodriguez, and Tobias, and the associated design matrix columns are as follows:

Student	Cohen	Rodriguez	Tobias
Mary	1	0	1
Tom	0	1	1
Fred	2	0	0
Jane	0	0	1
Jack	.	.	.

You can specify the following *mm-options* after a slash (/):

DETAILS

requests a table that shows the levels of the multimember effect.

NOEFFECT

specifies that, for observations with all missing levels of the multimember variables, the values in the corresponding design matrix columns be set to zero. If, in the preceding example, the teacher effect is defined by

```
EFFECT teacher = MM(teacher1 teacher2 / noeffect);
```

then the associated design matrix columns values for Jack are all zero. This enables you to include Jack in the analysis even though there is no effect of teachers on his performance.

A situation where it is important to designate observations as having no effect due to a classification variable is the analysis of crossover designs, where lagged treatment levels are used to model the carryover effects of treatments between periods. Since there is no carryover effect for the first period, the treatment lag effect in a crossover design can be modeled with a multimember effect that consists of a single classification variable and the NOEFFECT option, as in the following statements:

```
CLASS Treatment lagTreatment;  
EFFECT Carryover = MM(lagTreatment / noeffect);
```

The lagTreatment variable contains a missing value for the first period. Otherwise, it contains the value of the treatment variable for the preceding period.

STDIZE

specifies that for each observation, the entries in the design matrix that corresponds to the multimember effect be scaled to have a sum of one.

WEIGHT=*wght-list*

specifies numeric variables used to weigh the contributions of each of the classification effects that define the constructed multimember effect. The number of variables in *wght-list* must match the number of classification variables that define the effect.

Polynomial Effects

```
EFFECT name=POLYNOMIAL (var-list </ polynomial-options>);
```

```
EFFECT name=POLY (var-list </ polynomial-options>);
```

The variables in *var-list* must be numeric. A design matrix column is generated for each term of the specified polynomial. By default, each of these terms is treated as a separate effect for the purpose of model building. For example, the statements

```
proc glmselect;
  effect MyPoly = polynomial(x1-x3/degree=2);
  model y = MyPoly;
run;
```

yield the identical analysis to the statements

```
proc glmselect;
  model y = x1 x2 x3 x1*x1 x1*x2 x1*x3 x2*x2 x2*x3 x3*x3;
run;
```

You can specify the following *polynomial-options* after a slash (/):

DEGREE=*n*

specifies the degree of the polynomial. The degree must be a positive integer. The degree is typically a small integer, such as 1, 2, or 3. The default is DEGREE=1.

DETAILS

requests a table that shows the details of the specified polynomial, including the number of terms generated. If you also specify the [STANDARDIZE](#) option, then a table that shows the standardization details is also produced.

LABELSTYLE=(*style-opts*)

LABELSTYLE=*style-opt*

specifies how the terms in the polynomial are labeled. By default, powers are shown with ^ as the exponentiation operator and * as the multiplication operator. For example, a polynomial term such as $x_1^3 x_2 x_3^2$ is labeled $x1^3*x2*x3^2$. You can change the style of the label by using the following *style-opts* within parentheses. If you specify a single *style-opt*, then you can omit the enclosing parentheses.

EXPAND

specifies that each variable with an exponent greater than 1 be written as products of that variable. For example, the term $x_1^3 x_2 x_3^2$ receives the label $x1*x1*x1*x2*x3*x3$.

EXPONENT <=*quoted string*>

specifies that each variable with an exponent greater than 1 be written using exponential notation. By default, the symbol ^ is used as the exponentiation operator. If you supply the optional quoted string after an equal sign, then that string is used as the exponentiation operator. For example, if you specify

```
LABELSTYLE= (EXPONENT="**")
```

then the term $x_1^3 x_2 x_3^2$ receives the label $x1**3*x2*x3**2$.

INCLUDENAME

specifies that the name of the effect followed by an underscore be used as a prefix for term labels. For example, the following statement generates terms with labels MyPoly_x1 and MyPoly_x1^2:

```
EFFECT MyPoly=POLYNOMIAL(x1/degree=2 labelstyle=INCLUDENAME)
```

The INCLUDENAME option is ignored if you also specify the NOSEPARATE option in the EFFECT=POLYNOMIAL statement.

PRODUCTSYMBOL=NONE | *quoted string*

specifies that the supplied string be used as the product symbol. For example, the following statement generates terms with labels x_1 , x_2 , and $x_1 x_2$:

```
EFFECT MyPoly=POLYNOMIAL(x1 x2 / degree=2 mdegree=1  
labelstyle=(PRODUCTSYMBOL=" "))
```

If you specify PRODUCTSYMBOL=NONE, then the labels are formed by juxtaposing the constituent variable names.

MDEGREE=*n*

specifies the maximum degree of any variable in a term of the polynomial. This degree must be a positive integer. The default is the degree of the specified polynomial. For example, the following statement generates the terms x_1 , x_2 , x_1^2 , $x_1 x_2$, x_2^2 , $x_1^2 x_2$, $x_1 x_2^2$ and $x_1^2 x_2^2$:

```
EFFECT MyPoly=POLYNOMIAL(x1 x2/degree=4 MDEGREE=2);
```

NOSEPARATE

specifies that the polynomial be treated as a single effect with multiple degrees of freedom. The effect name that you specify is used as the constructed effect name, and the labels of the terms are used as labels of the corresponding parameters.

STANDARDIZE < (*centerscale-opts*) > < = *standardize-opt* >

specifies that the variables that define the polynomial be standardized. By default, the standardized variables receive prefix “s_” in the variable names.

You can use the following *centerscale-opts* to specify how the center and scale are estimated:

METHOD=MOMENTS

specifies that the center be estimated by the variable mean and the scale be estimated by the standard deviation. If a weight variable is specified using a WEIGHT statement, the observations with invalid weights are ignored when forming the mean and standard deviation, but the weights are otherwise not used. Only observations that are used in performing the analysis are used for the standardization.

METHOD=RANGE

specifies that the center be estimated by the midpoint of the variable range and the scale be estimated as half the variable range. Any observation that has a missing value for any regressor used in the model is ignored when computing the range of variables in a polynomial effect. Observations with valid regressor values but missing or invalid values of frequency variables, weight variables, or dependent variables are used in computing variable ranges. The default (if you do not specify the METHOD= suboption) is METHOD=RANGE.

METHOD=WMOMENTS

is the same as METHOD=MOMENTS except that weighted means and weighted standard deviations are used.

Let

- n = number of observations used in the analysis
- w = weight variable
- f = frequency variable
- x = variable to be standardized
- $x_{(n)}$ = $\text{Max}_{i=1}^n(x_i)$
- $x_{(1)}$ = $\text{Min}_{i=1}^n(x_i)$
- F = sum of frequencies
= $\sum_{i=1}^n f_i$
- WF = sum of weighted frequencies
= $\sum_{i=1}^n w_i f_i$

Table 19.12 shows how the center and scale are computed for each of the supported methods.

Table 19.12 Center and Scale Estimates by Method

Method	Center	Scale
Range	$(x_{(n)} + x_{(1)})/2$	$(x_{(n)} - x_{(1)})/2$
Moments	$\bar{x} = \sum_{i=1}^n f_i x_i / F$	$\sqrt{\sum_{i=1}^n f_i (x_i - \bar{x})^2 / (F - 1)}$
WMoments	$\bar{x}_w = \sum_{i=1}^n w_i f_i x_i / \text{WF}$	$\sqrt{\sum_{i=1}^n w_i f_i (x_i - \bar{x}_w)^2 / (F - 1)}$

PREFIX=NONE | *quoted-string*

specifies the prefix that is appended to standardized variables when forming the term labels. If you omit this option, the default prefix is “s_”. If you specify PREFIX=NONE, then standardized variables are not prefixed.

You can control whether the standardization is to center, scale, or both center and scale by specifying a *standardize-opt*:

CENTER

specifies that variables be centered but not scaled. For a variable x ,

$$s_x = x - \text{center}$$

CENTERSCALE

specifies that variables be centered and scaled. This is the default if you do not specify a *standardization-opt*. For a variable x ,

$$s_x = \frac{x - \text{center}}{\text{scale}}$$

NONE

specifies that no standardization be performed.

SCALE

specifies that variables be scaled but not centered. For a variable x ,

$$s_x = \frac{x}{\text{scale}}$$

Spline Effects

This section discusses the construction of spline effects through the EFFECT statement. You can also include spline effects in statistical models by other means. The TRANSREG procedure has dedicated facilities for including regression splines in your model and controlling the construction of the splines. For example, you can use the TRANSREG procedure to fit a spline function but restrict the function to be always increasing or decreasing (monotone). See the section “Using Splines and Knots” on page 8233 in Chapter 97, “The TRANSREG Procedure,” for more information about using splines with the TRANSREG procedure. The GAM and TPSPLINE procedures also can model the effects of regressor variables in terms of smooth functions that are generated from spline bases. For more information see Chapter 39, “The GAM Procedure,” and Chapter 96, “The TPSPLINE Procedure.”

A spline effect expands variables into spline bases whose form depends on the options that you specify. You can find details about regression splines and spline bases in the section “Splines and Spline Bases” on page 406. You request a spline effect with the syntax

```
EFFECT name=SPLINE (var-list </ spline-options>);
```

The variables in *var-list* must be numeric. Design matrix columns are generated separately for each of these variables, and the set of columns is collectively referred to with the specified name. By default, the spline basis that is generated for each variable is a cubic B-spline basis with three equally spaced knots positioned between the minimum and maximum values of that variable. This yields by default seven design matrix columns for each of the variables in the SPLINE effect.

You can specify the following *spline-options* after a slash (/):

BASIS=BSPLINE

specifies a B-spline basis for the spline expansion. For splines of degree d defined with n knots, this basis consists of $n + d + 1$ columns. In order to completely specify the B-spline basis, d left-side boundary knots and $\max\{d, 1\}$ right-side boundary knots are also required. See the suboptions **KNOTMETHOD=**, **DATABOUNDARY**, **KNOTMIN=**, and **KNOTMAX=** for details about how to specify the positions of both the internal and boundary knots. This is the default if you do not specify the **BASIS=** suboption.

BASIS=TPF(*options*)

specifies a truncated power function basis for the spline expansion. For splines of degree d defined with n knots for a variable x , this basis consists of an intercept, polynomials x, x^2, \dots, x^d and one truncated power function for each of the n knots. Unlike the B-spline basis, no boundary knots are required. See the suboption **KNOTMETHOD=** for details about how you can specify the position of the internal knots.

You can modify the number of columns when you request **BASIS=TPF** with the following *options*:

NOINT

excludes the intercept column.

NOPOWERS

excludes the intercept and polynomial columns.

DATABOUNDARY

specifies that the extremes of the data be used as boundary knots when building a B-spline basis.

DEGREE= n

specifies the degree of the spline transformation. The degree must be a nonnegative integer. The degree is typically a small integer, such as 0, 1, 2, or 3. The default is **DEGREE=3**.

DETAILS

requests tables that show the knot locations and the knots associated with each spline basis function.

KNOTMAX=*value*

specifies that, for each variable in the **EFFECT** statement, the right-side boundary knots be equally spaced starting at the maximum of the variable and ending at the specified value. This option is ignored for variables whose maximum value is greater than the specified value or if the **DATABOUNDARY** option is also specified.

KNOTMETHOD=*knot-method*< (*knot-options*) >

specifies how to construct the knots for spline effects. You can choose from the following *knot-methods* and affect the knot construction further with the method-specific *knot-options*:

EQUAL< (n) >

specifies that n equally spaced knots be positioned between the extremes of the data. The default is $n = 3$. For a B-spline basis, any needed boundary knots continue to be equally spaced unless the **DATABOUNDARY** option has also been specified. **KNOTMETHOD=EQUAL** is the default if no *knot-method* is specified.

LIST(*number-list*)

specifies the list of internal knots to be used in forming the spline basis columns. For a B-spline basis, the data extremes are used as boundary knots.

LISTWITHBOUNDARY(*number-list*)

specifies the list of all knots that are used in forming the spline basis columns. When you use a truncated power function basis, this list is interpreted as the list of internal knots. When you use a B-spline basis of degree d , then the first d entries are used as left-side boundary knots and the last $\text{MAX}(d, 1)$ entries in the list are used as right-side boundary knots.

MULTISCALE< (*multiscale-options*)>

specifies that multiple B-spline bases be generated, corresponding to sets with an increasing number of internal knots. As you increase the number of internal knots, the spline basis you generate is able to approximate features of the data at finer scales. So, by generating bases at multiple scales, you facilitate the modeling of both coarse- and fine-grained features of the data. For scale i , the spline basis corresponds to 2^i equally spaced internal knots. By default, the bases for scales 0–7 are generated. For each scale, a separate spline effect is generated. The name of the constructed spline effect at scale i is formed by appending $_Si$ to the effect name that you specify in the EFFECT statement. If you specify multiple variables in the EFFECT statement, then spline bases are generated separately for each variable at each scale and the name of the corresponding effect is obtained by appending the variable name followed by $_Si$ to the name in the EFFECT statement. For example, the following statement generates effects named `spl_x1_S0`, `spl_x1_S1`, `spl_x1_S2`, . . . , `spl_x1_S7` and `spl_x2_S1`, `spl_x2_S2`, . . . , `spl_x2_S7`:

```
EFFECT spl = spline(x1 x2 / knotmethod=multiscale);
```

The MULTISCALE option is ignored if you specify the BASIS=TPF *spline-option*. The MULTISCALE option is not available for spline effects that are specified in the RANDOM statement of the GLIMMIX procedure.

You can control which scales are included with the following *multiscale-options*:

STARTSCALE= n

specifies the start scale, where n is a positive integer. The default is STARTSCALE=0.

ENDSCALE= n

specifies the end scale, where n is a positive integer. The default is ENDSCALE=7.

PERCENTILES(n)

requests that internal knots be placed at n equally spaced percentiles of the variable or variables named in the EFFECT statement. For example, the following statement positions internal knots at the deciles of the variable x . For a B-spline basis, the extremes of the data are used as boundary knots:

```
EFFECT spl = spline(x / knotmethod=percentiles(9));
```

RANGEFRACTIONS(*fraction-list*)

requests that internal knots be placed at each fraction of the ranges of the variables in the EFFECT statement. For example, if variable $x1$ ranges between 1 and 3, and variable $x2$ ranges between 0 and 20, then the following EFFECT statement uses internal knots 1.2, 2, and 2.5 for variable $x1$ and internal knots 2, 10, and 15 for variable $x2$:

```
EFFECT spl = spline(x1 x2 / knotmethod=rangefractions(.1 .5 .75));
```

For a B-spline basis, the data extremes are used as boundary knots.

KNOTMIN=value

specifies that for each variable in the EFFECT statement, the left-side boundary knots be equally spaced starting at the specified value and ending at the minimum of the variable. This option is ignored for variables whose minimum value is less than the specified value or if the DATABOUNDARY option is also specified.

NATURALCUBIC

specifies a natural cubic spline basis for the spline expansion. Natural cubic splines, also known as restricted cubic splines, are cubic splines that are constrained to be linear beyond the extreme knots. The natural cubic spline basis that is produced by the EFFECT statement is obtained by starting from the unrestricted truncated power function cubic spline basis that is defined with n distinct knots and imposes the linearity constraints beyond the extreme knots. This basis consists of an intercept, the polynomial x , and $n - 2$ functions that are all linear beyond the largest knot. The i th function, $i = 1, 2, \dots, n - 2$, is zero to the left of the i th knot, which is called the “break knot.” See the section “Splines and Spline Bases” on page 406 for details of this basis. You can use the NOINT and NOPOWERS suboptions of the BASIS=TPF option to suppress the intercept and polynomial x when forming the columns of the natural cubic spline basis. When you specify the NATURALCUBIC option, the options BASIS=BSPLINE, DATABOUNDARY, DEGREE=, and KNOTMETHOD=MULTISCALE are not applicable.

SEPARATE

specifies that when multiple variables are specified in the EFFECT statement, the spline basis for each variable be treated as a separate effect. The names of these separated effects are formed by appending an underscore followed by the name of the variable to the name that you specify in the EFFECT statement. For example, the effect names generated with the following statement are spl_x1 and spl_x2:

```
EFFECT spl = spline(x1 x2 / separate);
```

In procedures that support variable selection, such as the GLMSELECT procedure, these two effects can enter or leave the model independently during the selection process. Separated effects are not supported in the RANDOM statement of the GLIMMIX procedure.

SPLIT

specifies that each individual column in the design matrix that corresponds to the spline effect be treated as a separate effect that can enter or leave the model independently. Names for these split effects are generated by appending the variable name and an index for each column to the name that you specify in the EFFECT statement. For example, the effects generated for the spline effect in the following statement are spl_x1:1, spl_x1:2, ..., spl_x1:7 and spl_x2:1, spl_x2:2, ..., spl_x2:7:

```
EFFECT spl = spline(x1 x2 / split);
```

The SPLIT option is not supported in the GLIMMIX procedure.

Splines and Spline Bases

This section provides details about the construction of spline bases with the EFFECT statement. A spline function is a piecewise polynomial function in which the individual polynomials have the same degree and

connect smoothly at join points whose abscissa values, referred to as knots, are prespecified. You can use spline functions to fit curves to a wide variety of data.

A spline of degree 0 is a step function with steps located at the knots. A spline of degree 1 is a piecewise linear function where the lines connect at the knots. A spline of degree 2 is a piecewise quadratic curve whose values and slopes coincide at the knots. A spline of degree 3 is a piecewise cubic curve whose values, slopes, and curvature coincide at the knots. Visually, a cubic spline is a smooth curve, and it is the most commonly used spline when a smooth fit is desired. Note that when no knots are used, splines of degree d are simply polynomials of degree d .

More formally, suppose you specify knots $k_1 < k_2 < k_3 < \dots < k_n$. Then a spline of degree $d \geq 0$ is a function $S(x)$ with $d - 1$ continuous derivatives such that

$$S(x) = \begin{cases} P_0(x) & x < k_1 \\ P_i(x) & k_i \leq x < k_{i+1}; i = 1, 2, \dots, n - 1 \\ P_n(x) & x \geq k_n \end{cases}$$

where each $P_i(x)$ is a polynomial of degree d . The requirement that $S(x)$ has $d - 1$ continuous derivatives is satisfied by requiring that the function values and all derivatives up to order $d - 1$ of the adjacent polynomials at each knot match.

A counting argument yields the number of parameters that define a spline with n knots. There are $n + 1$ polynomials of degree d , giving $(n + 1)(d + 1)$ coefficients. However, there are d restrictions at each of the n knots, so the number of free parameters is $(n + 1)(d + 1) - nd = n + d + 1$. In mathematical terminology this says that the dimension of the vector space of splines of degree d on n distinct knots is $n + d + 1$. If you have $n + d + 1$ basis vectors, then you can fit a curve to your data by regressing your dependent variable by using this basis for the corresponding design matrix columns. In this context, such a spline is known as a regression spline. The EFFECT statement provides a simple mechanism for obtaining such a basis.

If you remove the restriction that the knots of a spline must be distinct and allow repeated knots, then you can obtain functions with less smoothness and even discontinuities at the repeated knot location. For a spline of degree d and a repeated knot with multiplicity $m \leq d$, the piecewise polynomials that join such a knot are required to have only $d - m$ matching derivatives. Note that this increases the number of free parameters by $m - 1$ but also decreases the number of distinct knots by $m - 1$. Hence the dimension of the vector space of splines of degree d with n knots is still $n + d + 1$, provided that any repeated knot has a multiplicity less than or equal to d .

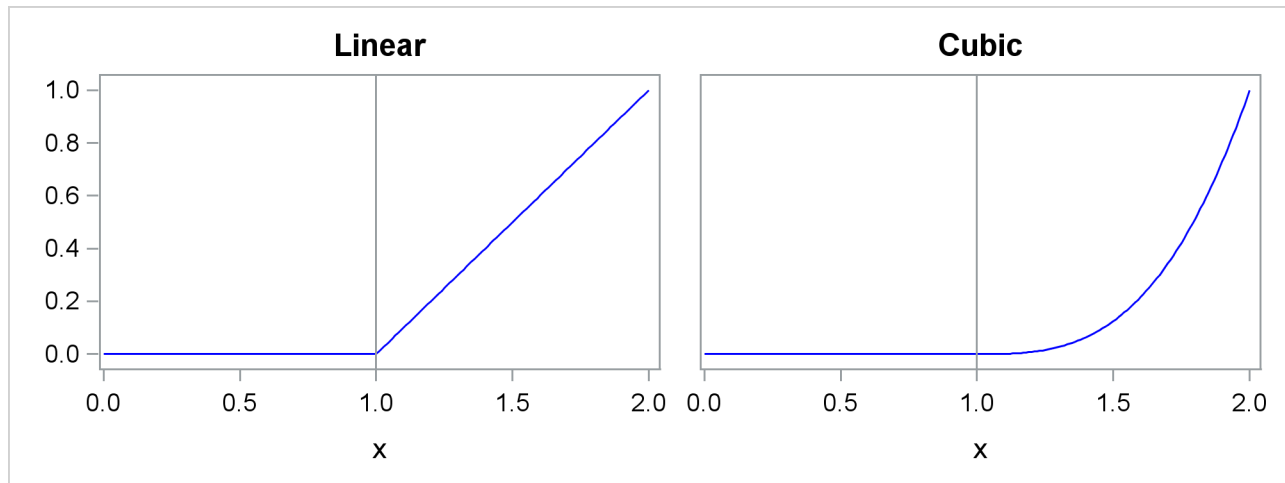
The EFFECT statement provides support for the commonly used *truncated power function* basis and *B-spline* basis. With exact arithmetic and by using the complete basis, you obtain the same fit with either of these bases. The following sections provide details about constructing spline bases for the space of splines of degree d with n knots that satisfies $k_1 \leq k_2 \leq k_3 < \dots \leq k_n$.

Truncated Power Function Basis

A truncated power function for a knot k_i is a function defined by

$$t_i(x) = \begin{cases} 0 & x < k_i \\ (x - k_i)^d & x \geq k_i \end{cases}$$

Figure 19.1 shows such functions for $d = 1$ and $d = 3$ with a knot at $x = 1$.

Figure 19.1 Truncated Power Functions with Knot at $x = 1$ 

The name is derived from the fact that these functions are shifted power functions that get truncated to zero to the left of the knot. These functions are piecewise polynomial functions with two pieces whose function values and derivatives of all orders up to $d - 1$ are zero at the defining knot. Hence these functions are splines of degree d . It is easy to see that these n functions are linearly independent. However, they do not form a basis, because such a basis requires $n + d + 1$ functions. The usual way to add $d + 1$ additional basis functions is to use the polynomials $1, x, x^2, \dots, x^d$. These $d + 1$ functions together with the n truncated power functions $t_i(x), i = 1, 2, \dots, n$ form the truncated power basis.

Note that each time a knot is repeated, the associated exponent used in the corresponding basis function is reduced by 1. For example, for splines of degree d with three repeated knots $k_i = k_{i+1} = k_{i+2}$ the corresponding basis functions are $t_i(x) = (x - k_i)_+^d$, $t_{i+1}(x) = (x - k_i)_+^{d-1}$, and $t_{i+2}(x) = (x - k_i)_+^{d-2}$. Provided that the multiplicity of each repeated knot is less than or equal to the degree, this construction continues to yield a basis for the associated space of splines.

The main advantage of the truncated power function basis is the simplicity of its construction and the ease of interpreting the parameters in a model that corresponds to these basis functions. However, there are two weaknesses when you use this basis for regression. These functions grow rapidly without bound as x increases, resulting in numerical precision problems when the x data span a wide range. Furthermore, many or even all of these basis functions can be nonzero when evaluated at some x value, resulting in a design matrix with few zeros that precludes the use of sparse matrix technology to speed up computation. This weakness can be addressed by using a B-spline basis.

B-Spline Basis

A B-spline basis can be built by starting with a set of Haar basis functions, which are functions that are 1 between adjacent knots and 0 elsewhere, and then applying a simple linear recursion relationship d times, yielding the $n + d + 1$ needed basis functions. For the purpose of building the B-spline basis, the n prespecified knots are referred to as internal knots. This construction requires d additional knots, known as boundary knots, to be positioned to the left of the internal knots, and $\text{MAX}(d, 1)$ boundary knots to be positioned to the right of the internal knots. The actual values of these boundary knots can be arbitrary. The EFFECT statement provides several methods for placing the needed boundary knots, including the common method of using repeated values of the data extremes as the boundary knots. The boundary knot placement

affects the precise form of the basis functions that are generated, but it does not affect the following two desirable properties:

1. The B-spline basis functions are nonzero over an interval that spans at most $d + 2$ knots. This yields design matrix columns each of whose rows contain at most $d + 2$ adjacent nonzero entries.
2. The computation of the basis functions at any x value is numerically stable and does not require evaluating powers of this value.

The following figures show the B-spline bases defined on $[0, 1]$ with four equally spaced internal knots at 0.2, 0.4, 0.6, and 0.8.

Figure 19.2 shows a linear B-spline basis. Note that this basis consists of six functions each of which is nonzero over an interval that spans at most three knots.

Figure 19.2 Linear B-Spline Basis with Four Equally Spaced Interior Knots

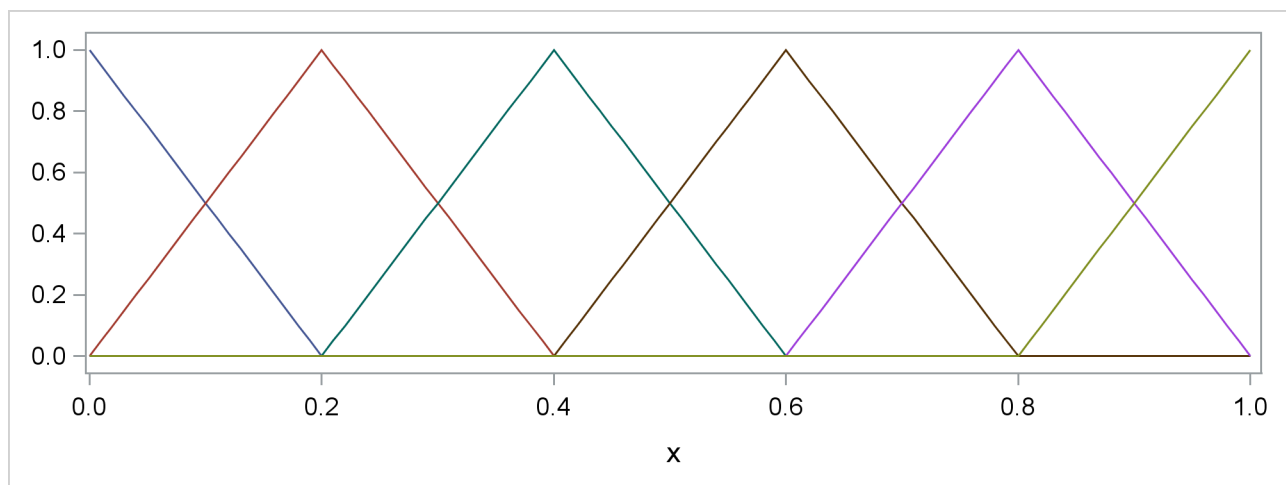


Figure 19.3 shows a cubic B-spline basis where the needed boundary knots are positioned at $x = 0$ and $x = 1$. Note that this basis consists of eight functions, each of which is nonzero over an interval spanning at most five knots.

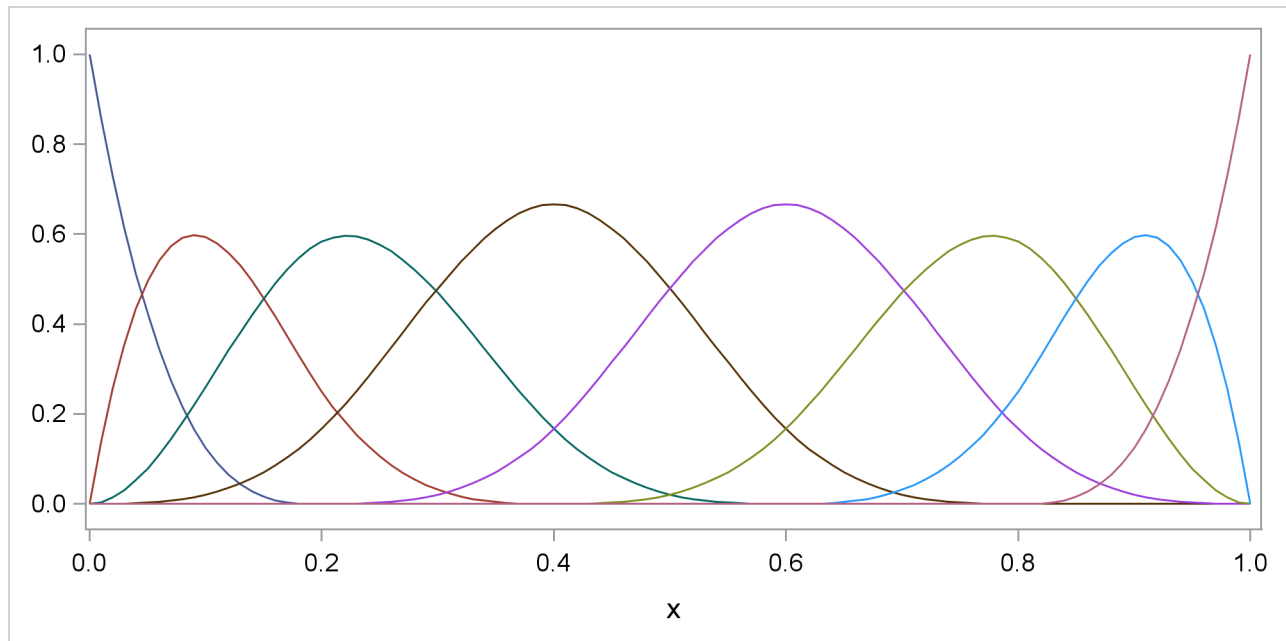
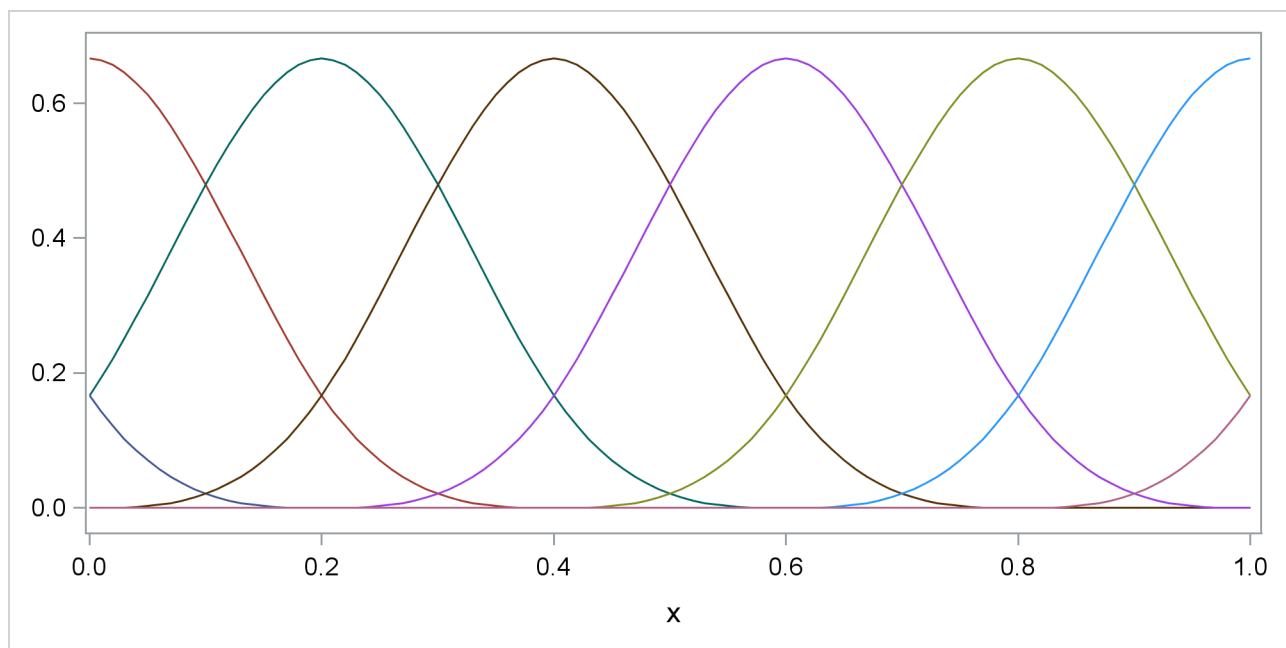
Figure 19.3 Cubic B-Spline Basis with Four Equally Spaced Interior Knots

Figure 19.4 shows a different cubic B-spline basis where the needed left-side boundary knots are positioned at -0.6 , -0.4 , -0.2 , and 0 . The right-side boundary knots are positioned at 1 , 1.2 , 1.4 , and 1.6 . Note that, as in the basis shown in Figure 19.3, this basis consists of eight functions, each of which is nonzero over an interval spanning at most five knots. The different positioning of the boundary knots has merely changed the shape of the individual basis functions.

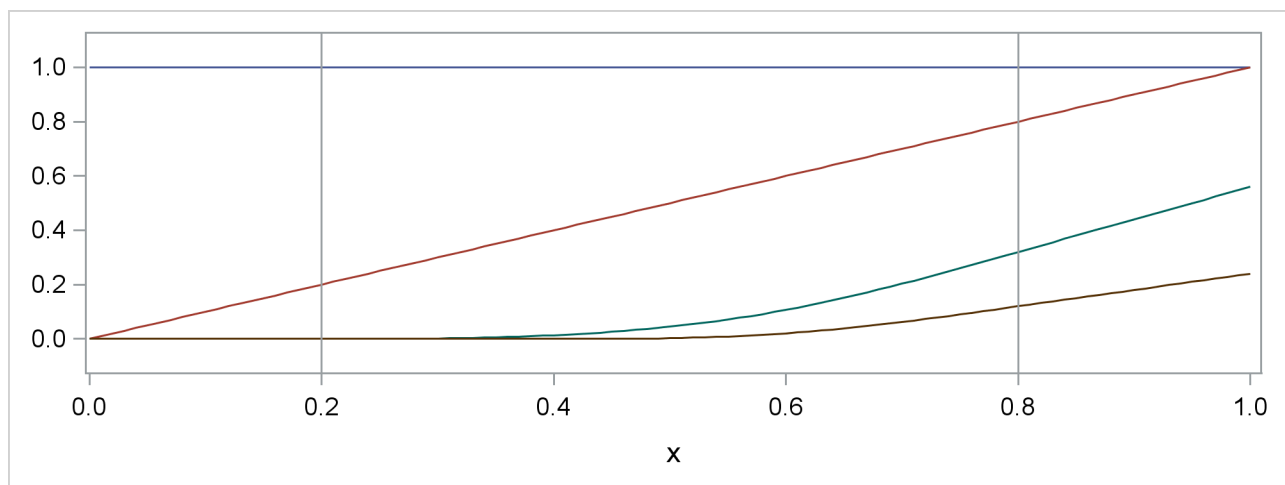
Figure 19.4 Cubic B-Spline Basis with Equally Spaced Boundary and Interior Knots

You can find details about this construction in Hastie, Tibshirani, and Friedman (2001).

Natural Cubic Spline Basis

Natural cubic splines are cubic splines with the additional restriction that the splines are required to be linear beyond the extreme knots. Some authors use the terminology “restricted cubic splines” in preference to the terminology “natural cubic splines.” The space of unrestricted cubic splines on n knots has dimension $n + 4$. Imposing the restrictions that the cubic polynomials beyond the first and last knot reduce to linear polynomials reduces the number of degrees of freedom by 4, and so a basis for the natural cubic splines consists of n functions. Starting from the truncated power function basis for the unrestricted cubic splines, you can obtain a reduced basis by imposing linearity constraints. You can find details about this construction in Hastie, Tibshirani, and Friedman (2001). Figure 19.5 shows this natural cubic spline basis defined on $[0, 1]$ with four equally spaced internal knots at 0.2, 0.4, 0.6, and 0.8. Note that this basis consists of four basis functions that are all linear beyond the extreme knots at 0.2 and 0.8.

Figure 19.5 Natural Cubic Spline Basis with Four Equally Spaced Knots



EFFECTPLOT Statement

This statement applies to the following procedures:
GENMOD, LOGISTIC, ORTHOREG, and PLM.

The EFFECTPLOT statement produces a display (*effect plot*) of a complex fitted model and provides options for changing and enhancing the displays. One simple effect plot is the display for a linear regression of the response Y on a single predictor X : the regression line is drawn with the predicted response on the Y axis and the covariate on the X axis. The regression line can be enhanced by displaying the observations and adding confidence and prediction limits. When your model is more complicated—with more continuous and categorical covariates, nestings and interactions, and link functions—the effect plots display the behavior of some covariates over their ranges while fixing other covariates at some fixed values; this can enable easier interpretation and explanation of the resulting model.

By default, a single plot is produced based on the type of response variable and the number of continuous and classification covariates in the model. You can also specify options to do the following:

- select the variables to display on the plots
- produce multiple plots based on the following: the levels of classification covariates; the minimum, maximum, mean or middle (midrange) value of continuous covariates; and specified values of the covariates
- specify different fixed values for continuous and classification covariates that are not displayed on the plot
- panel and unpanel plots
- select variables to slice or group by
- display (or remove from display) observations and confidence limits

Syntax: EFFECTPLOT Statement

EFFECTPLOT < *plot-type* < (*plot-definition-options*) > > < / *options* > ;

The available *plot-types* and their *plot-definition-options* are described in Table 19.13. Table 19.15 lists the *options* that can be specified after a slash (/) for any *plot-type*, and Table 19.16 lists additional *options* that enhance specific *plot-types*. Full descriptions of the *plot-definition-options* and the other *options* are provided in the section “Dictionary of Options” on page 414.

Table 19.13 *Plot-Types and Plot-Definition-Options*

Plot-Type and Description	Plot-Definition-Options
<p>BOX</p> <p>Displays a box plot of continuous response data at each level of a CLASS effect, with predicted values superimposed and connected by a line. This is an alternative to the INTERACTION <i>plot-type</i>.</p>	<p>PLOTBY= variable or CLASS effect X= CLASS variable or effect</p>
<p>CONTOUR</p> <p>Displays a contour plot of predicted values against two continuous covariates.</p>	<p>PLOTBY= variable or CLASS effect X= continuous variable Y= continuous variable</p>
<p>FIT</p> <p>Displays a curve of predicted values versus a continuous variable.</p>	<p>PLOTBY= variable or CLASS effect X= continuous variable</p>
<p>INTERACTION</p> <p>Displays a plot of predicted values (possibly with error bars) versus the levels of a CLASS effect. The predicted values are connected with lines and can be grouped by the levels of another CLASS effect.</p>	<p>PLOTBY= variable or CLASS effect SLICEBY= variable or CLASS effect X= CLASS variable or effect</p>

Table 19.13 continued

Plot-Type and Description	Plot-Definition-Options
SLICEFIT Displays a curve of predicted values versus a continuous variable grouped by the levels of a CLASS effect.	PLOTBY= variable or CLASS effect SLICEBY= variable or CLASS effect X= continuous variable

By default, a single plot is produced based on the type of response variable and the number of continuous and classification covariates in the model as shown in Table 19.14. If you have a polytomous response model, then the response variable is treated as the grouping classification variable in this table. If your model does not fit into Table 19.14, then a default plot is not produced; however, specifying the *plot-type* argument displays a plot with the extra continuous covariates fixed at their mean values and the extra classification covariates fixed at their reference levels.

Table 19.14 Default Plot-Types

Number of Covariates		Type of Response Variable	
Classification	Continuous	Continuous or Binary	Polytomous
1	0	INTERACTION	INTERACTION with groups
2	0	INTERACTION with groups	None
0	1	FIT	SLICEFIT
0	2	CONTOUR	None
1	1	SLICEFIT	None

Table 19.15 and Table 19.16 list the *options* that can be specified after a slash (/) to enhance the effect plots.

Table 19.15 Available Options for All Plot-Types

AT< args >	ATLEN=	ATORORDER=	ILINK	INDIVIDUAL*
LINK	MOFF	NCOLS=*	NOOBS*	NROWS=*
OBS< (options) >	PLOTBYLEN=	PREDLABEL=	UNPACK	

* Not available for the BOX *plot-type*

NOTE: If your model contains an offset variable and the MOFF option is not specified or not valid, then the predicted values are computed only at the observations. In this case, the FIT and SLICEFIT *plot-types* display scatter plots of the predicted values, the CONTOUR *plot-type* displays the residuals against two continuous covariates but with no fitted surface, the INTERACTION *plot-type* does not connect the predicted values with lines, and the BOX *plot-type* is unchanged.

Table 19.16 Additional Options for Each Plot-Type

Plot-Type	Options			
BOX	CLUSTER YRANGE=	CONNECT	NOCLUSTER	NOCONNECT
CONTOUR	EXTEND=	GRIDSIZE=		
FIT	ALPHA= NOCLM	EXTEND= NOLIMITS	GRIDSIZE= SMOOTH	NOCLI YRANGE=
INTERACTION	ALPHA= CONNECT POLYBAR	CLI LIMITS YRANGE=	CLM NOCLUSTER	CLUSTER NOCONNECT
SLICEFIT	ALPHA= GRIDSIZE=	CLI LIMITS	CLM YRANGE=	EXTEND=

Dictionary of Options

This section describes the EFFECTPLOT *options* in alphabetical order.

ALPHA=*value*

specifies the significance level, $0 \leq \text{value} \leq 1$, for producing $100(1 - \text{value}/2)\%$ prediction and confidence limits. By default, *value*=0.05.

AT < *contopt* > < *classopt* > < *variable1=varopt* < *variable2=varopt... >* >

where *contopt*= **MEAN** | **MIN** | **MAX** | **MIDRANGE**

classopt= **ALL** | **REF**

varopt= *contopts* | *number-list* | *classopts* | '*class-level*'... '*class-level*'

specifies values at which to fix continuous and class variables when they are not used in **X=**, **Y=**, **SLICEBY=**, or **PLOTBY=** effects. The *contopt* keyword fixes continuous variables at their mean, minimum, maximum, or midrange = $\frac{1}{2}(\text{minimum} + \text{maximum})$; the default is to use the mean. The *classopt* keyword either fixes a CLASS variable at its reference (last) level or indicates that all levels of the CLASS variable should be processed; the default is to use the reference level. The *varopt* values enable you to specify *contopt* and *classopt* keywords, or to specify lists of numbers or class levels. You can specify a CLASS variable only once in the AT specification, but you can specify a continuous variable multiple times; for example, the following syntax is valid when X is a continuous variable:

```
effectplot / at(x=min max x=0 to 2 by 1 x=2 5 7);
```

Duplicate AT values are suppressed, so the last X=2 value is ignored.

You can also specify *plug-in values* for CLASS variable levels when computing the predicted values $\mathbf{x}'\boldsymbol{\beta}$. For example, suppose a CLASS variable A with two levels={0,1} is in the model. Then instead of using the coding for A in the x vector by specifying **AT (A=all)**, **AT (A=ref)** or **AT (A='0' '1')**, you can specify a numeric list to plug in. For example, if the proportion of A's that equal 0 in the data set is 0.3, then you can input the proportions for all levels of the variable by specifying **AT (A=0 .3 0 .7)**. Under GLM coding, A=0 is coded as "1 0" and A=1 is coded as "0 1", so the plug-in specification

replaces both of these codings with “0.3 0.7”. Under REFERENCE coding A=0 is coded as “1” and A=1 is coded as “0”, so this specification replaces both of these codings with “0.3” followed by “0.7”; however, if another variable is nested within A, then only “0.3” is used. To plug in values, you must specify a multiple of the number of parameters used for the CLASS variable or, if a variable is nested within the CLASS variable, a multiple of the number of levels of the CLASS variable.

The plug-in values are distributed through the rest of the model effects in the following fashion. If a variable is nested within a plug-in variable, then its coding is multiplied by the plug-in value for the level it is nested in. If a variable interacts with a plug-in variable, its coding is multiplied by the appropriate plug-in value for the level it is interacting with. Lag, multimember, polynomial, and spline constructed effects are affected only by interactions and nestings. If the plug-in variable is part of a collection effect, then its values are replaced by the plug-in values; collection effects are also affected by interactions and nestings.

The AT levels are used for computing the predicted values. If the OBS option is also specified, then all observations are still displayed on all of the plots. For example, if you specify the options **AT (A=' 1')** **OBS**, then the fitted values are computed with A=1, but all of the observations are displayed with their predicted values computed at their observed level of A. If you want to display only a subset of the observations based on the levels of a CLASS variable, then you must specify either the **PLOTBY=** option or the **OBS(BYAT)** option.

ATLEN=*n*

specifies the maximum length ($1 \leq n \leq 256$) of the levels of the AT variables that are displayed in footnotes and headers. By default, up to 256 characters of the CLASS levels are displayed, and the continuous AT levels are displayed with a BEST format that has a width greater than or equal to 5, which distinguishes each level. **CAUTION:** If the levels of your AT variables are not unique when the first *n* characters are displayed, then the levels are combined in the plots but not in the underlying computations. Also, at most *n* characters for continuous AT variables are displayed.

ATORORDER=ASCENDING | DESCENDING

uses the AT values for continuous variables in ascending or descending order as specified. By default, values are used in the order of their first appearance in the AT option.

CLI

displays normal (Wald) prediction limits. This option is available only for normal distributions with identity links. If your model is from a Bayesian analysis, then sampling-based intervals are computed; see the section “Analysis Based on Posterior Estimates” on page 5833 in Chapter 69, “The PLM Procedure,” for more information.

CLM

displays confidence limits. These are computed as the normal (Wald) confidence limits for the linear predictor, and if the ILINK option is specified, the limits are also back-transformed by the inverse link function. If your model is from a Bayesian analysis, then sampling-based intervals are computed; see the section “Analysis Based on Posterior Estimates” on page 5833 in Chapter 69, “The PLM Procedure,” for more information.

CLUSTER<=*percent*>

modifies the BOX and INTERACTION *plot-types* by displaying the levels of the SLICEBY= effect in a side-by-side fashion. You can specify *percent* as a percentage of half the distance between X levels. The *percent* value must be between 0.1 and 1; the default *percent* depends on the number

of X levels, the number of SLICEBY levels, and the number of PLOTBY levels for **INTERACTION** *plot-types*. Default clustering can be removed by specifying the **NOCLUSTER** option.

CONNECT

modifies the **BOX** and **INTERACTION** *plot-types* by connecting the predicted values with a line. Default connecting lines can be removed by specifying the **NOCONNECT** option.

EXTEND=DATA | *value*

extends continuous covariate axes by $value \times \frac{1}{2}range$ in both directions, where *range* is the range of the X axis. Specifying the **DATA** keyword displays curves to the range of the data within the appropriate **SLICEBY=**, **PLOTBY=**, and **AT** level. For the **CONTOUR** *plot-type*, *value*=0.05 by default; other *plot-types* set the default value to 0. When constructed effects are present, only the **EXTEND=DATA** option is available.

GRIDSIZE=*n*

specifies the resolution of curves by computing the predicted values at *n* equally spaced x-values and specifies the resolution of surfaces by computing the predicted values on an $n \times n$ grid of points. Default values are $n = 200$ for curves and bands, $n = 50$ for surfaces, and $n = 2$ for lines. If results of a Bayesian or bootstrap analysis are being displayed, then the defaults are $n = 500000/B$, where *B* is the number of samples, the upper limit is equal to the usual defaults, and the lower limit equal to 20.

ILINK

displays the fit on the scale of the inverse link function. In particular, the results are displayed on the probability scale for logistic regression. By default, a procedure displays the fit on either the **link** or inverse link scale.

INDIVIDUAL

displays individual probabilities for polytomous response models with cumulative links on the scale of the inverse link function. This option is not available when the **LINK** option is specified, and confidence limits are not available with this option.

LIMITS

invokes the **CLI** and **CLM** options.

LINK

displays the fit on the scale of the link function; that is, the linear predictor. Note that probabilities or observed proportions near 0 and 1 are transformed to ± 20 . By default, a procedure displays the fit on either the **link** or **inverse link** scale.

MOFF

moves the offset for a Poisson regression model to the response side of the equation. If the **ILINK** option is also in effect, then the rate is displayed on the Y axis, while the **LINK** option displays the log of the rate on the Y axis. Without this option, the predicted values are computed and displayed only for the observations.

NCOLS=*n*

specifies the maximum number of columns in a paneled plot. This option is not available with the **BOX** *plot-type*.

The default choice of **NROWS=** and **NCOLS=** is based on the number of **PLOTBY=** and **AT** levels. If there is only one plot being displayed in a panel, then **NROWS=1** and **NCOLS=1** and the plots are

produced as if you specified only the **UNPACK** option. If only two plots are displayed in a panel, then **NROWS=1** and **NCOLS=2**. For all other cases, a 2x2, 2x3, or 3x3 panel is chosen based on how much of the last panel is used, with ties going to the larger panels. For example, if 14 plots are being created, then this requires either four 2x2 panels with 50% of the last panel filled, three 2x3 panels with 33% of the last panel filled, or two 3x3 panels with 55% of the last panel filled; in this case, the 3x3 panels are chosen.

If you specify both of the **NROWS=** and **NCOLS=** options, then those are the values used. However, if you only specify one of the options but have fewer plots, then the panel size is reduced; for example, if you specify **NROWS=6** but only have four plots, then a plot with four rows and one column is produced.

NOCLI

suppresses the prediction limits.

NOCLM

suppresses the confidence limits.

NOCLUSTER

modifies the **BOX** and **INTERACTION** *plot-types* by preventing the side-by-side display of the levels of the **SLICEBY=** effect.

NOCONNECT

modifies the **BOX** and **INTERACTION** *plot-types* by suppressing the line that connects the predicted values.

NOLIMITS

invokes the **NOCLI** and **NOCLM** options.

NOOBS

suppresses the display of observations and overrides the specification of the **OBS=** option.

NROWS=*n*

specifies the maximum number of rows in a paneled plot. This option is not available with the **BOX** *plot-type*. See the **NCOLS=** option for more details.

OBS<(obs-options)>

displays observations on the effect plots. An input data set is required; hence the **OBS** option is not available with **PROC PLM**. The **OBS** option is overridden by the **NOOBS** option. When the **ILINK** option is specified with binary response variables, then either the observed proportions or a coded value of the response is displayed. For polytomous response variables, the observed values are overlaid onto the fitted curves unless the **LOCATION=** option is specified. Whether observations are displayed by default or not depends upon the procedure. If the **PLOTBY=** option is specified, then the observations displayed on each plot are from the corresponding **PLOTBY=** level for classification effects; for continuous effects, all observations are displayed on every plot.

The following *obs-options* are available:

BYAT

subsets the observations by **AT** level and by the **PLOTBY=** level. If you specify the **PLOTBY=** option without specifying this option, the observations are displayed on the plots that correspond to their **PLOTBY=** level without regard to any classification variables specified in the **AT** option.

However, for `FIT` *plot-types* a distance can be computed and displayed (see the `DISTANCE` option for more information). This option is ignored when there are no `AT` variables.

CDISPLAY=NONE | OUTLINE | GRADIENT | OUTLINEGRADIENT

controls the display of observations on contour plots. The keyword `OUTLINE` displays the observations as circles, `GRADIENT` displays gradient-colored dots, `OUTLINEGRADIENT` displays gradient-filled-circles, and `NONE` suppresses the display of the observations. The default is `CDISPLAY=OUTLINEGRADIENT`.

CGRADIENT=RESIDUAL | DEPENDENT

specifies what the gradient-shading of the observed values on the `CONTOUR` *plot-type* represents. The `RESIDUAL` keyword shades the observations by the raw residual value and displays the fitted surface as a line contour plot. The `DEPENDENT` keyword shades the observations by the response variable value and displays the fitted surface as a contour shaded on the same scale. The default is `CGRADIENT=DEPENDENT`.

DEPTH=depth

specifies the number of overlapping observations that can be distinguished by adjusting their transparency; you can specify $1 \leq \text{depth} \leq 100$. By default, `DEPTH=1`. The `DEPTH=` option is available with `FIT`, `SLICEFIT`, and `INTERACTION` *plot-types*.

DISTANCE

displays observations on `FIT` *plot-types* with a color-gradient that indicates how far the observation is from the `AT` and `PLOTBY=` level. This option is ignored unless an `AT` or `PLOTBY=` option is specified.

The distance is computed as the square root of the following number: for each continuous `AT` and `PLOTBY=` variable, add the square of the difference from the observed value divided by the range of the variable; for each `CLASS AT` and `PLOTBY=` variable, add 1 if the `CLASS` levels are different. Thus the largest possible distance is the square root of the number of `AT` and `PLOTBY=` variables. Observations at zero distance are displayed with the darkest color, and the color fades as the distance increases.

Note that the `UNPACKED` panels compute the maximum distance within each panel and hence do not use the same gradient across all panels. Also, the `PANELS` *panel-type* computes the maximum distance within each `PLOTBY=` level, so a different gradient is used for each `PLOTBY=` level. All other *panel-types* compute the maximum distance across all observations and therefore use the same gradient on every plot.

FITATCLASS

computes fitted values only for class levels that are observed in the data set. This option is ignored when the GLM parameterization is used.

FRINGE

displays observations in a fringe (rug) plot at the bottom of the plot. This option is available only with `FIT` and `SLICEFIT` *plot-types*.

JITTER< (jitter-options) >

shifts (*jitters*) the observations. By default, the jittering in the X direction is achieved by adding a random number that is generated according to a normal distribution with `mean=0` and standard deviation = `jitter/2` and truncating at $\pm \text{jitter}$, where `jitter=0.01` times the range of the X axis;

the jittering in the Y direction is performed independently but in the same fashion. The JITTER option is not available with the **BOX** *plot-type*. The following *jitter-options* are available:

FACTOR=*factor* sets the jitter to *factor* times the range of the axis, and jitters in both the X and Y directions. You can specify $0 \leq \textit{factor} \leq 1$.

SEED=*seed* specifies an integer to use as the initial seed for the random number generator. If you do not specify a seed, or if you specify a value less than or equal to zero, then the time of day from the computer clock is used to generate an initial seed.

X=*x-jitter* sets the jitter to *x-jitter* for the X direction; the jitter in the Y direction is assumed to be 0 unless the Y= option is also specified. You can specify $\textit{x-jitter} \geq 0$. The X= option is not available for the **INTERACTION** *plot-type*. This option is ignored if the **FACTOR=** option is also specified.

Y=*y-jitter* sets the jitter to *y-jitter* for the Y direction; the jitter in the X direction is assumed to be 0 unless the X= option is also specified. You can specify $\textit{y-jitter} \geq 0$. This option is ignored if the **FACTOR=** option is also specified.

LABEL<=OBS>

labels markers with their observation number.

LOCATION=*location*

specifies where the observed values for polytomous response models are displayed when the **SLICEBY=** variable is the response. This option is available only with the **SLICEFIT** and **INTERACTION** *plot-types*. The observations are always displayed at their appropriate X-axis value, but their Y-axis location can depend on the specification of the **YRANGE=** option or on the minimum and maximum computed predicted values in addition to the specified *location*. The following *locations* are available:

BOTTOM<=*factor***>** displays the first response level at the minimum predicted value, and displays succeeding response levels above the first level at $\textit{factor} \times \textit{range}$ intervals, where *range* is the range of the predicted values. You can specify $0 \leq \textit{factor} \leq 1$, but the largest usable value, which corresponds to **LOCATION=SPREAD**, is $\textit{factor} = \frac{1}{k}$, where $k + 1$ is the number of response levels that are displayed. By default, $\textit{factor} = 0.03$.

CURVE displays the observations for polytomous response models at their predicted values. For displays on the LINK scale, the reference level is displayed at the maximum value. This method is the default.

FIRST displays the observations for a response level at the first displayed predicted value for that response level.

MAX displays the observations for a response level at the maximum displayed predicted value for that response level.

MIDDLE displays the observations for a response level at the middle of the displayed predicted values for that response level.

MIN displays the observations for a response level at the minimum displayed predicted value for that response level.

SPREAD displays the observations with the response levels evenly spread across the Y axis.

TOP<=*factor*> displays the last response level at the maximum predicted value, and displays preceding response levels below the last level at $factor \times range$ intervals, where *range* is the range of the predicted values. You can specify $0 \leq factor \leq 1$, but the largest usable value, which corresponds to LOCATION=SPREAD, is $factor = \frac{1}{k}$, where $k+1$ is the number of response levels that are displayed. By default, $factor = 0.03$.

PLOTBY< (*panel-type*)>=*effect*<=*numeric-list*>

specifies a variable or CLASS effect at whose levels the predicted values are computed and the plots are displayed. You can specify the response variable as the *effect* for polytomous response models. The *panel-type* argument specifies the method in which the plots are grouped for the display. The following *panel-types* are available.

COLUMNS

specifies that the columns within each panel correspond to different levels of the PLOTBY=*effect* and hence the rows correspond to different AT levels.

PACK

specifies that plots be displayed in the panels as they are produced with no control over the placement of the PLOTBY= and AT levels.

PANELS | LEVELS

specifies that each level of the PLOTBY=*effect* begin a new panel of plots and the AT levels define the plots within the panels.

ROWS

specifies that the rows within each panel correspond to different levels of the PLOTBY=*effect* and hence the columns correspond to different AT levels.

This option is ignored with the BOX *plot-type*; box plots are always displayed in an unpacked fashion, grouped by the PLOTBY= and AT levels. If you specify a continuous variable as the *effect*, then you can either specify a *numeric-list* of values at which to display that variable or, by default, five equally spaced values from the minimum variable value to its maximum are displayed.

The default *panel-type* is based on the number of PLOTBY= and AT levels as shown in the following table.

Number of PLOTBY Levels	Number of AT Levels	Resulting <i>panel-type</i>
1	1	(UNPACK)
>1	1	PACK
1	>1	PACK
2	>1	ROWS
3	>1	COLUMNS
>3	>1	PANELS

The default dimensions of the panels are also based on the number of PLOTBY= and AT levels; see the NCOLS= option for details.

Specification of the *panel-type* is honored except in the following cases. If you specify a *panel-type* but produce only one plot, specify the NROWS=1 and NCOLS=1 options, or specify the UNPACK

option, then the plots are produced as if you specified only the **UNPACK** option. If you specify the **PANELS** *panel-type* with only one **AT** level, then the plots are produced with the **UNPACK** option. However, if you specify the **PANELS** *panel-type* but the **PLOTBY=** effect has only one level, then the *panel-type* is changed to **PACK**.

PLOTBYLEN=*n*

specifies the maximum length ($1 \leq n \leq 256$) of the levels of the **PLOTBY=** variables, which are displayed in footnotes and headers. By default, up to 256 characters of the **CLASS** levels are displayed. **CAUTION:** If the levels of your **PLOTBY=** variables are not unique when the first *n* characters are displayed, then the levels are combined in the plots but not in the underlying computations.

POLYBAR

displays polytomous response data as a stacked histogram with bar heights defined by the individual predicted value. Your response variable must be the *effect* specified in the **SLICEBY=** option. If you specify the **INDIVIDUAL** option, then the histogram bars are displayed in a side-by-side fashion. If you specify the **CLM** option, then error bars are displayed on the side-by-side histogram bars.

PREDLABEL='label'

specifies a label to be displayed on the Y axis. The default Y axis label is determined by your model. For the **CONTOUR** *plot-type*, this option changes the title to “*label* for Y.”

SHOWCLEGEND

displays the gradient-legend for the **CONTOUR** *plot-type*. This option has no effect when the **OBS(CGRADIENT=RESIDUAL)** option is also specified.

SLICEBY=NONE | *effect*< =*numeric-list*>

displays the fitted values at the different levels of the specified variable or **CLASS** effect. You can specify the response variable as the *effect* for polytomous response models. Use this option to modify **SLICEFIT**, **INTERACTION**, and **BOX** *plot-types*. If you specify a continuous variable as the *effect*, then you can either specify a *numeric-list* of values at which to display that variable or, by default, five equally spaced values from the minimum variable value to its maximum are displayed. The **NONE** keyword is available for preventing the **INTERACTION** *plot-type* from slicing by a second class covariate. Note that the **SLICEBY=NONE** option is not available for the **SLICEFIT** *plot-type*, since that is the same as the **FIT** *plot-type*. The **BOX** *plot-type* accepts only classification effects.

SMOOTH

overlays a loess smooth on the **FIT** *plot-type* for models that have only one continuous predictor. This option is not available for binary or polytomous response models.

UNPACK

suppresses paneling. By default, multiple plots can appear in some output *panels*. Specify **UNPACK** to display each plot separately.

X=*effect*

specifies values to display on the X axis. For **BOX** and **INTERACTION** *plot-types*, *effect* can be a **CLASS** effect in the **MODEL** statement. For **FIT**, **SLICEFIT**, and **CONTOUR** *plot-types*, *effect* can be any continuous variable in the model.

Y=args

specifies values to display on the Y axis for the **CONTOUR** *plot-type*. The Y= argument can be any continuous variable in the model.

YRANGE=CLIP | (< min > < , max >)

displays the predicted values on the Y axis in the range [*min*,*max*]. The YRANGE=CLIP option has the same effect as specifying the minimum predicted value as *min* and the maximum predicted value as *max*. The axis might extend beyond your specified values. By default, when the Y axis displays predicted probabilities, the entire Y axis, [0,1], is displayed. This option is useful if your predicted probabilities are all contained in some subset of this range. This option is not available with the **CONTOUR** *plot-type*.

ODS Graphics: EFFECTPLOT Statement

To produce the EFFECTPLOT displays, ODS Graphics must be enabled. For more information about ODS Graphics, see Chapter 21, “Statistical Graphics Using ODS.” The available graph names are provided in Table 19.17.

Table 19.17 Graphs Produced by the EFFECTPLOT Statement

ODS Graph Name	Plot Description
BoxFitPlot	A box plot of the responses at each level of one classification effect, overlaid with a plot of the predicted values
ContourFitPlot	A contour plot of the fitted surface against two continuous covariates
ContourFitPanel	A panel of ContourFitPlots
FitPlot	A curve of the predicted values plotted against one continuous covariate
FitPanel	A panel of FitPlots
InteractionPlot	A plot of the predicted values (connected by a line) against one classification effect, possibly for each level of a second classification effect
InteractionPanel	A panel of InteractionPlots
SliceFitPlot	A curve of the predicted values against one continuous covariate for each level of a second classification covariate
SliceFitPanel	A panel of SliceFitPlots

Examples: EFFECTPLOT Statement

Example 19.1: A Saddle Surface

Myers (1976) analyzes an experiment reported by Frankel (1961) which is aimed at maximizing the yield of mercaptobenzothiazole (MBT) by varying processing time and temperature. Myers uses a two-factor model in which the estimated surface does not have a unique optimum. The objective is to find the settings of time and temperature in the processing of a chemical that maximize the yield. The following statements create the data set d:

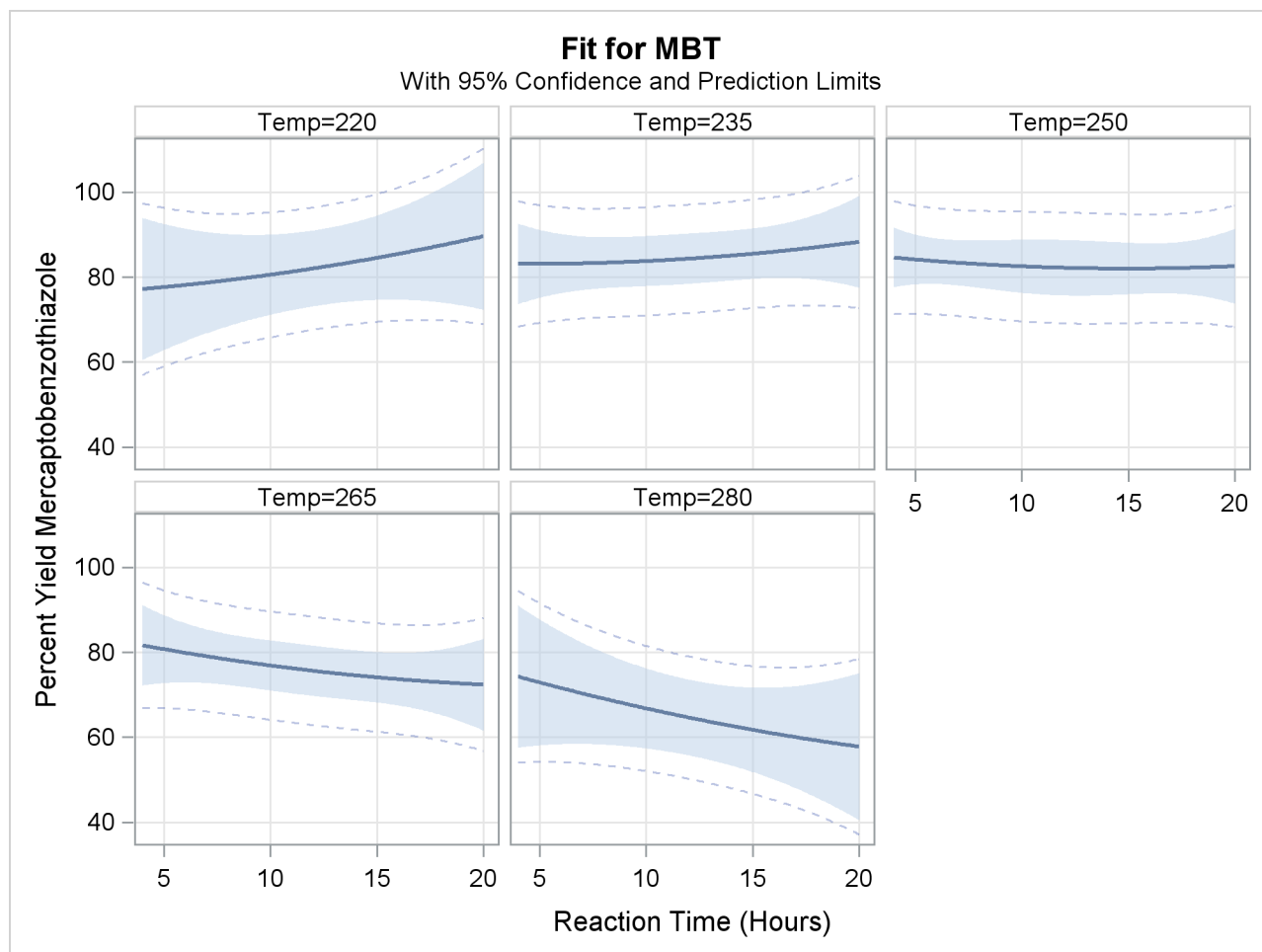
```
data d;
  input Time Temp MBT @@;
  label Time = "Reaction Time (Hours)"
         Temp = "Temperature (Degrees Centigrade)"
         MBT = "Percent Yield Mercaptobenzothiazole";
  datalines;
  4.0 250 83.8    20.0 250 81.7    12.0 250 82.4
  12.0 250 82.9    12.0 220 84.7    12.0 280 57.9
  12.0 250 81.2     6.3 229 81.3     6.3 271 83.1
  17.7 229 85.3    17.7 271 72.7     4.0 250 82.0
  ;
```

In the following statements, the ORTHOREG procedure fits a response surface regression model to the data and uses the EFFECTPLOT statement to create a slice of the response surface. The *FIT plot-type* requests plots of the predicted yield against the Time variable, and the PLOTBY= option specifies that the Temp variable is fixed at five equally spaced values so that five fitted regression curves are displayed in Output 19.1.1.

```
ods graphics on;
proc orthoreg data=d;
  model MBT=Time|Time|Temp|Temp@2;
  effectplot fit(x=time plotby=temp);
run;
ods graphics off;
```

The displays in Output 19.1.1 show that the slope of the surface changes as the temperature increases.

Output 19.1.1 Panel of Fit Plots

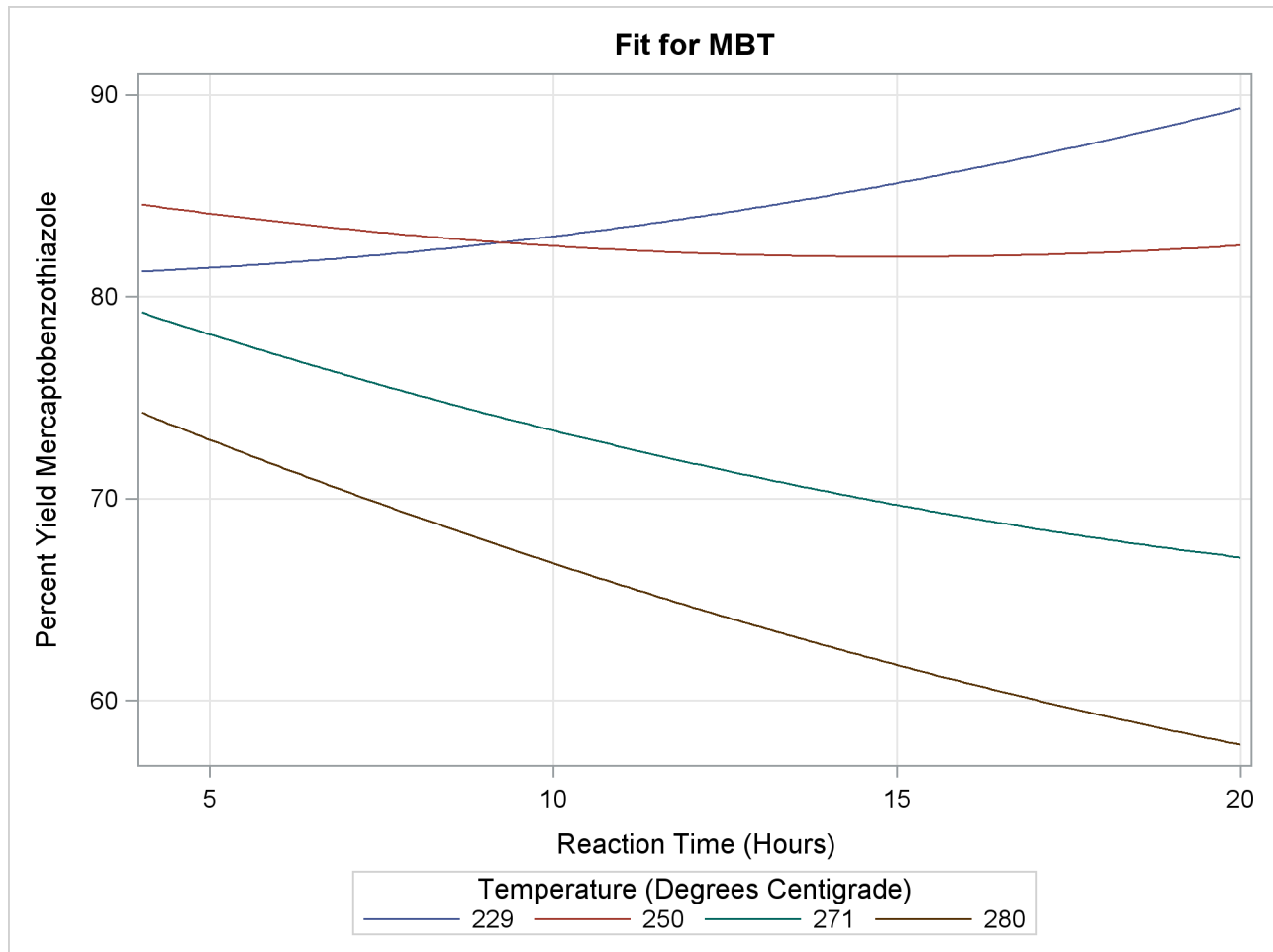


It might be more informative to see these results in one graphic, so the following statements specify the `SLICEFIT plot-type` to overlay plots of the predicted yield versus time, fixed at several values of temperature. In this case, the `SLICEBY=` option is specified to explicitly use the same four temperatures as used in the experiment.

```
ods graphics on;
proc orthoreg data=d;
  model MBT=Time|Time|Temp|Temp@2;
  effectplot slicefit(x=time sliceby=temp=229 250 271 280);
run;
ods graphics off;
```

Output 19.1.2 shows that you should choose either low temperatures and long times to optimize the yield, or maybe high temperatures and short times.

Output 19.1.2 Fit Plot Grouped (Sliced) by Temp

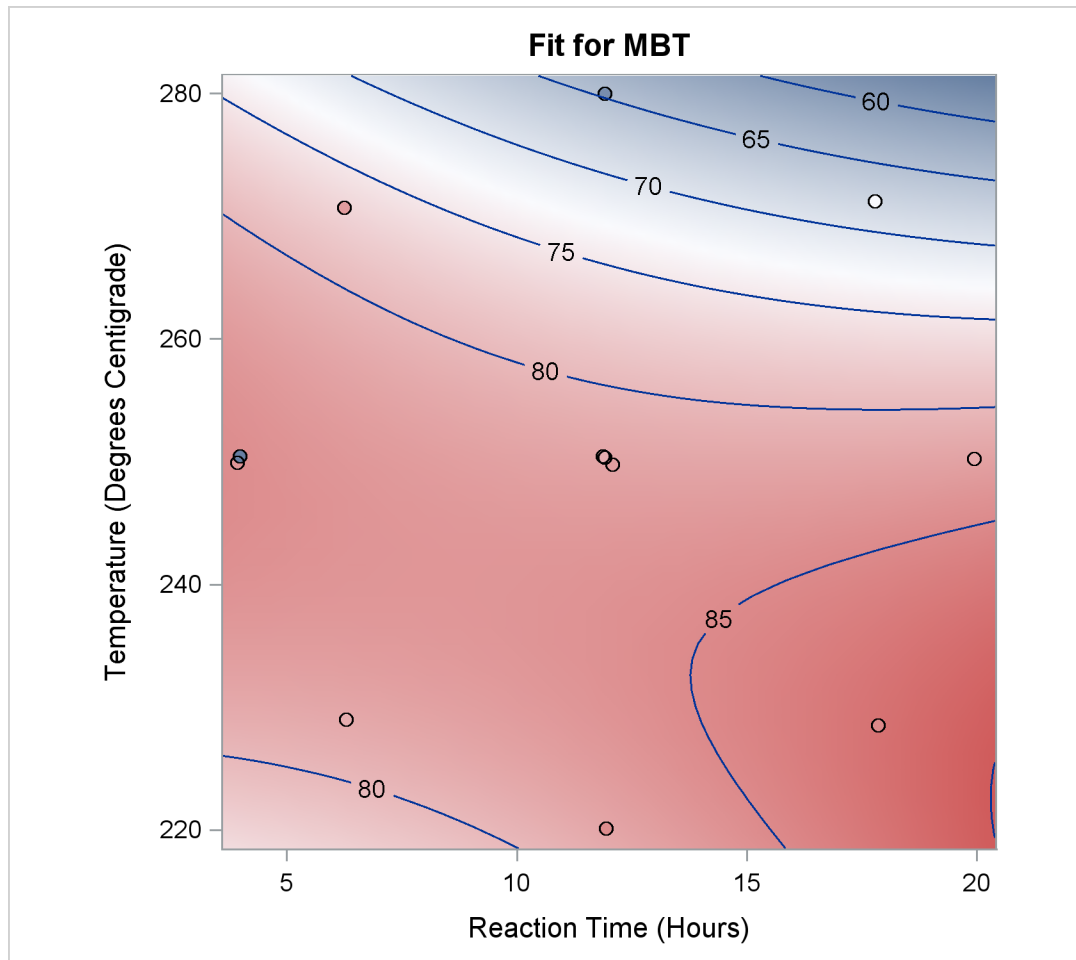


Another plot might explain the reason for this more clearly. The following statements produces the default EFFECTPLOT statement display, enhanced by the **OBS(JITTER)** option to jitter the observations so that you can see the replicated points.

```
ods graphics on;
proc orthoreg data=d;
  model MBT=Time|Time|Temp|Temp@2;
  effectplot / obs(jitter(seed=39393));
run;
ods graphics off;
```

Output 19.1.3 shows the reason for the changing slopes is that the surface is at a saddle point. This surface does not have an optimum point.

Output 19.1.3 Contour Fit Plot with Jittered Observations



Example 19.2: Unbalanced Two-Way ANOVA

This example uses data from Kutner (1974, p. 98) to illustrate a two-way analysis of variance. The original data source is Afifi and Azen (1972, p. 166). The following statements create the data set *a*:

```

data a;
  input drug disease @;
  do i=1 to 6;
    input y @;
    output;
  end;
  datalines;
1 1 42 44 36 13 19 22
1 2 33 . 26 . 33 21
1 3 31 -3 . 25 25 24
2 1 28 . 23 34 42 13
2 2 . 34 33 31 . 36
2 3 3 26 28 32 4 16
3 1 . . 1 29 . 19
3 2 . 11 9 7 1 -6
3 3 21 1 . 9 3 .
4 1 24 . 9 22 -2 15
4 2 27 12 12 -5 16 15
4 3 22 7 25 5 12 .
;

```

In the following statements, PROC GENMOD fits two classification variables and their interaction to Y. The first EFFECTPLOT statement displays the default graphic, which plots the predicted values against Disease for each of the three Drug levels. The **OBS** option also displays the observations on the plot. The second EFFECTPLOT statement modifies the default to plot the predicted values against Drug for each of the three Disease levels. The **CLM** option is specified to produce 95% confidence bars for the means.

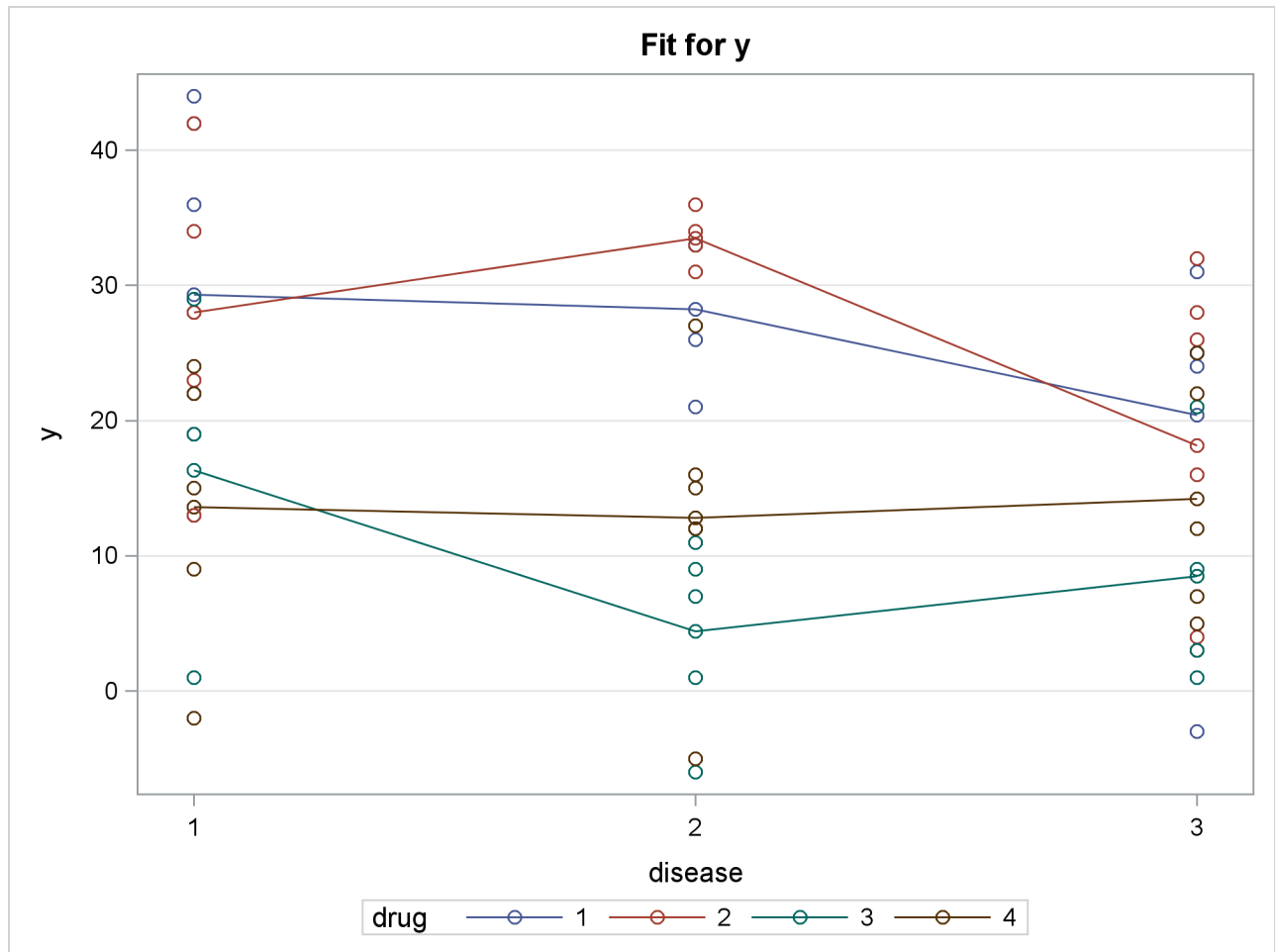
```

ods graphics on;
proc genmod data=a;
  class drug disease;
  model y=disease drug disease*drug / d=n;
  effectplot / obs;
  effectplot interaction(sliceby=disease) / clm;
run;
ods graphics off;

```

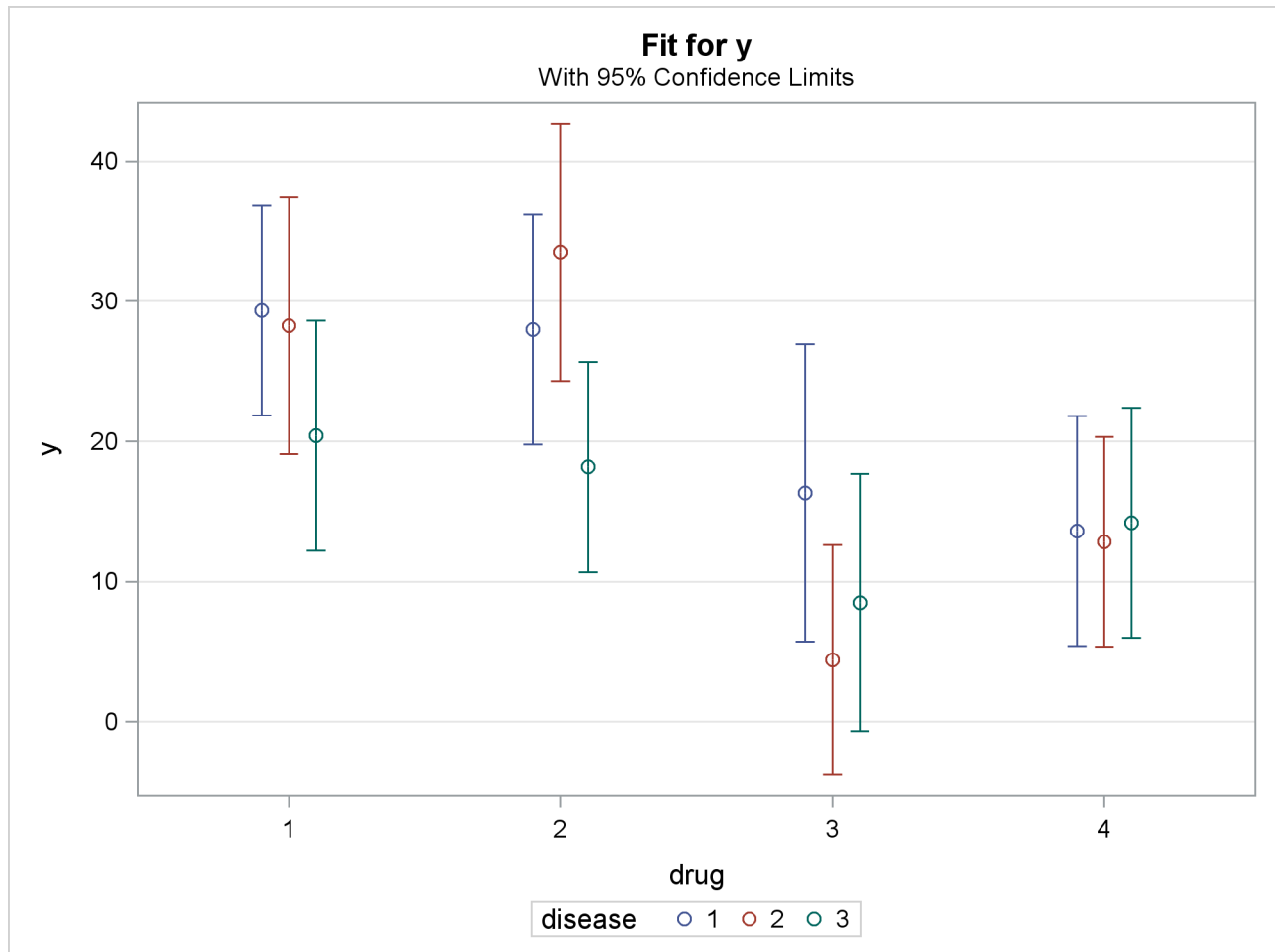
In [Output 19.2.1](#), the default interaction plot is produced, and the observations are also displayed. From this plot, you can compare the performance of the drugs for a given disease. The predicted values are connected with a line to provide something for your eye to follow—obviously a line has no intrinsic meaning in this graphic. Drugs 3 and 4 are consistently outperformed by the first two drugs.

Output 19.2.1 Interaction Plot: Default with Observations



By default, the first classification variable is displayed on the X axis and the second classification variable is used for grouping. Specifying the `SLICEBY=DISEASE` option in the second `EFFECTPLOT` statement reverses this, displays the classification variable with the most levels on the X axis, and slices by fewer levels, resulting in a more readable display. **Output 19.2.2** shows how well a given drug performs on each disease.

Output 19.2.2 Interaction Plot with Specified SLICEBY= Effect

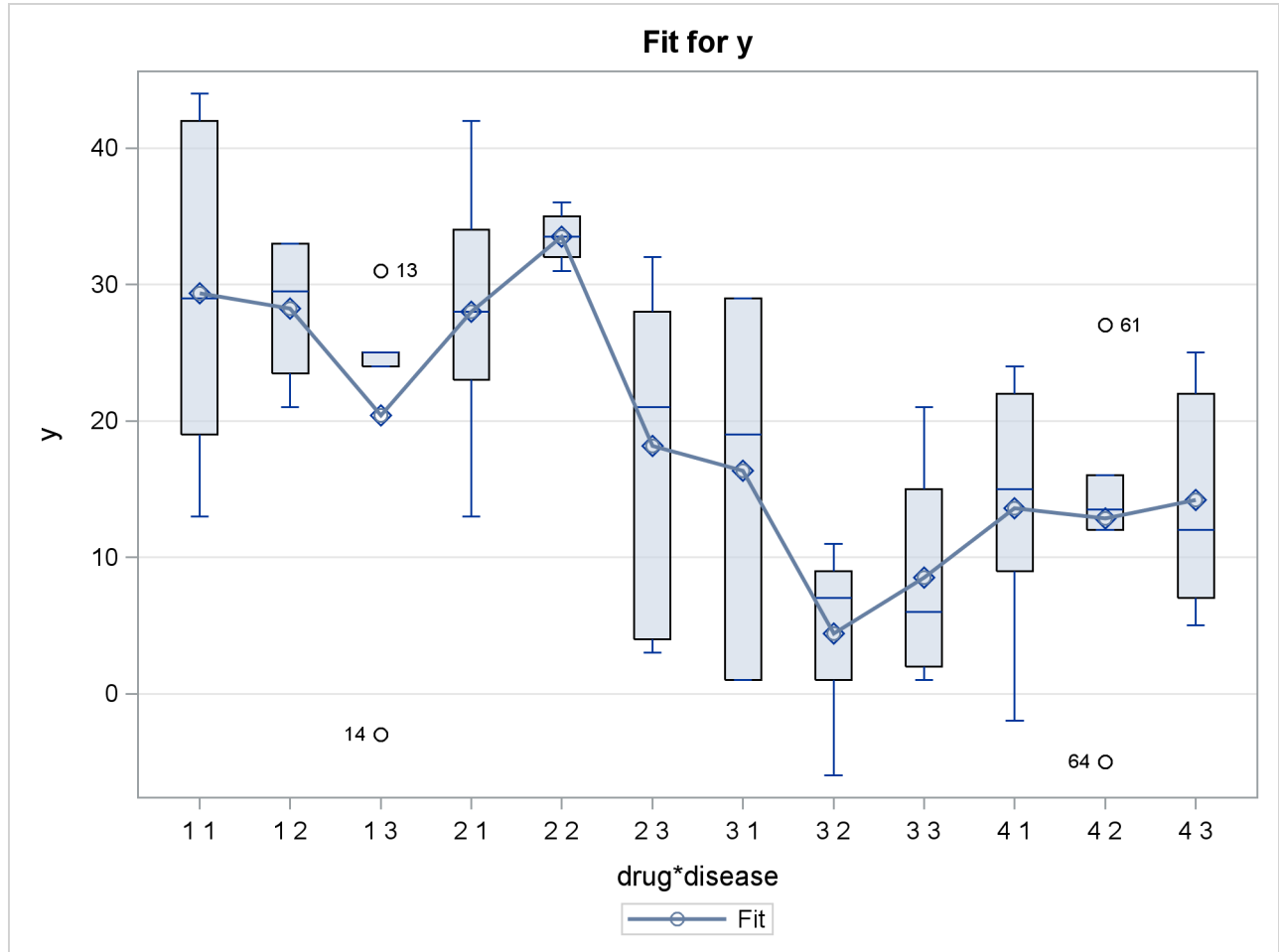


In the following statements, the **BOX** *plot-type* is requested to display box plots of the predictions by each drug and disease combination. The second **EFFECTPLOT** statement displays the same information by using an **INTERACTION** *plot-type* and specifies the **OBS** option to display the individual observations. The third **EFFECTPLOT** statement creates an interaction plot of predictions versus drug for each of the Disease levels, and displays them in a panel.

```
ods graphics on;
proc genmod data=a;
  class drug disease;
  model y=drug disease drug*disease / d=n;
  effectplot box;
  effectplot interaction(x=drug*disease) / obs;
  effectplot interaction(plotby=disease);
run;
ods graphics off;
```

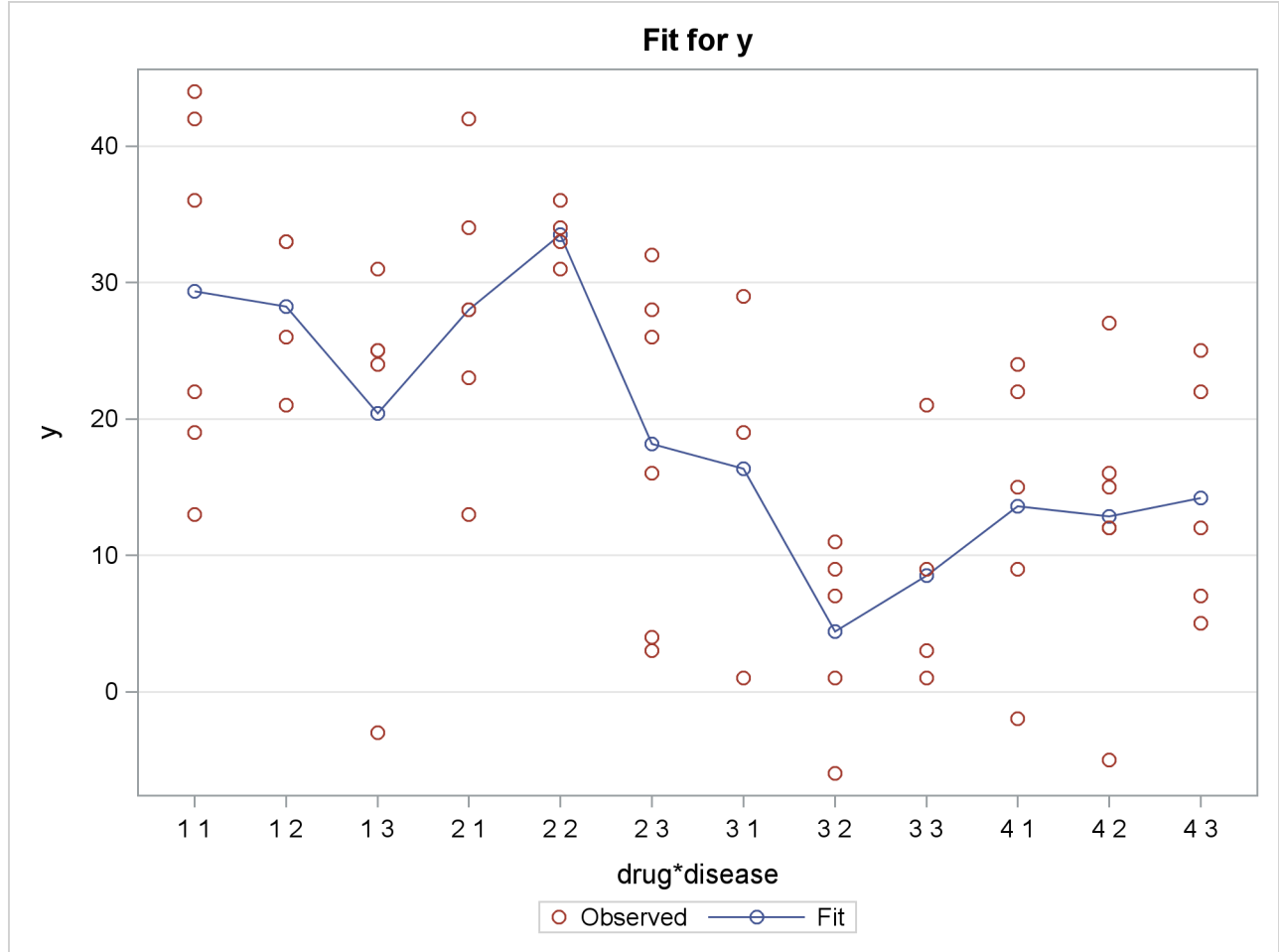

In the box plot in [Output 19.2.3](#), the predicted values are displayed as circles; they coincide with the mean of the data at each level which are displayed as diamonds. The predicted values are again connected by lines. It is difficult to make any conclusions from this graphic.

Output 19.2.3 Box Fit Plot



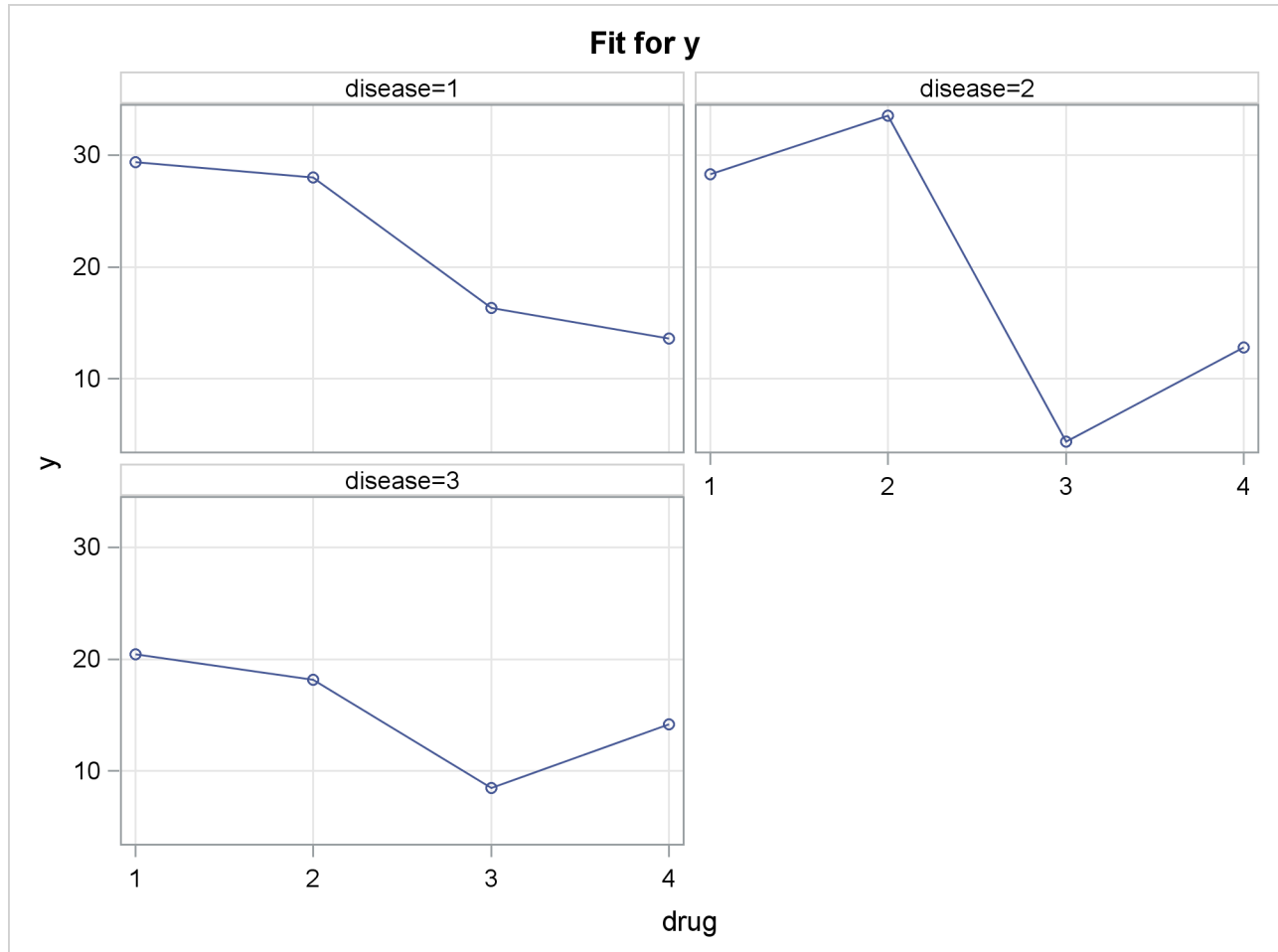
Output 19.2.4 shows the interaction plot at every combination of Drug and Disease. This plot is identical to the preceding box plot, except the boxes are replaced by the actual observations. Again, it is difficult to see any pattern in the plot.

Output 19.2.4 Interaction Plot with Specified X= Effect



Output 19.2.5 groups the observations by Disease, and for each disease displays the effectiveness of the four drugs in a panel of plots.

Output 19.2.5 Interaction Plot with Specified PLOTBY= Effect



Example 19.3: Logistic Regression

Consider a study of the analgesic effects of treatments on elderly patients with neuralgia. Two test treatments and a placebo are compared. The response variable is whether the patient reported pain or not. Researchers recorded the age and gender of 60 patients and the duration of complaint before the treatment began. The following DATA step creates the data set Neuralgia:

```
data Neuralgia;
  input Treatment $ Sex $ Age Duration Pain $ @@;
  datalines;
P F 68 1 No B M 74 16 No P F 67 30 No
P M 66 26 Yes B F 67 28 No B F 77 16 No
A F 71 12 No B F 72 50 No B F 76 9 Yes
A M 71 17 Yes A F 63 27 No A F 69 18 Yes
B F 66 12 No A M 62 42 No P F 64 1 Yes
A F 64 17 No P M 74 4 No A F 72 25 No
P M 70 1 Yes B M 66 19 No B M 59 29 No
A F 64 30 No A M 70 28 No A M 69 1 No
B F 78 1 No P M 83 1 Yes B F 69 42 No
B M 75 30 Yes P M 77 29 Yes P F 79 20 Yes
A M 70 12 No A F 69 12 No B F 65 14 No
B M 70 1 No B M 67 23 No A M 76 25 Yes
P M 78 12 Yes B M 77 1 Yes B F 69 24 No
P M 66 4 Yes P F 65 29 No P M 60 26 Yes
A M 78 15 Yes B M 75 21 Yes A F 67 11 No
P F 72 27 No P F 70 13 Yes A M 75 6 Yes
B F 65 7 No P F 68 27 Yes P M 68 11 Yes
P M 67 17 Yes B M 70 22 No A M 65 15 No
P F 67 1 Yes A M 67 10 No P F 72 11 Yes
A F 74 1 No B M 80 21 Yes A F 69 3 No
;
```

The Neuralgia data set contains five variables. The Pain variable is the response. A specification of Pain=Yes indicates that the patient felt pain, and Pain=No indicates that the patient did not feel pain. The variable Treatment is a categorical variable with three levels: A and B represent the two test treatments, and P represents the placebo treatment. The gender of the patients is given by the categorical variable Sex. The variable Age is the age of the patients, in years, when treatment began. The duration of complaint, in months, before the treatment began is given by the variable Duration.

In the following statements, a complex model that includes classification and continuous covariates and an interaction term is fit to the Neuralgia data. When you try to create a default effect plot from this model, computations stop because the best type of plot cannot easily be determined.

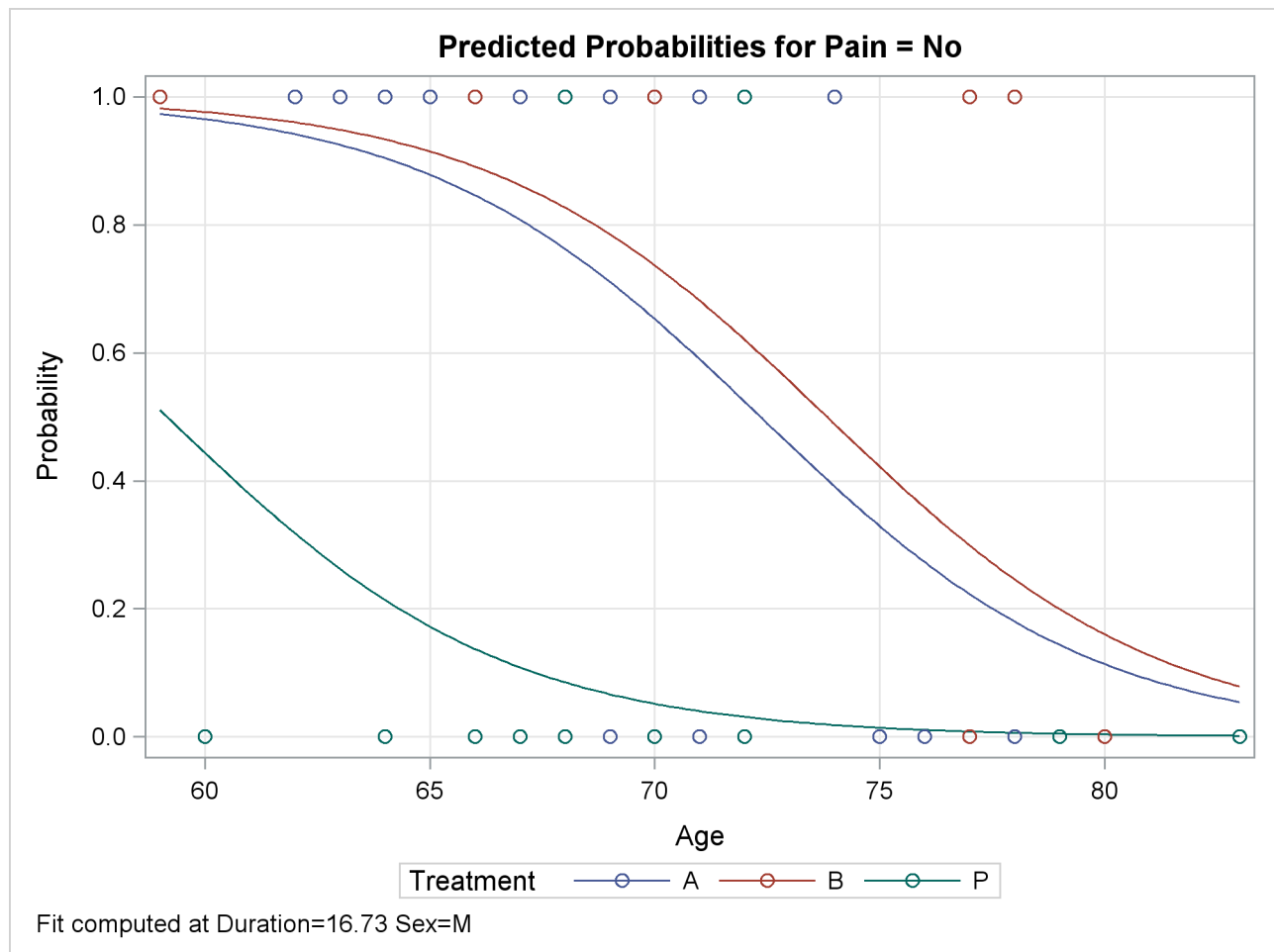
```
ods graphics on;
proc logistic data=Neuralgia;
  class Treatment Sex / param=ref;
  model Pain= Treatment|Sex Age Duration;
  effectplot;
run;
ods graphics off;
```

To produce an effect plot for this model, you need to first choose the type of plot to be created. In this case, since there are both classification and continuous covariates on the model, a `SLICEFIT` *plot-type* displays the first continuous covariate (Age) on the X axis and displays fit curves that correspond to each level of the first classification covariate (Treatment). The following statements produce [Output 19.3.1](#).

```
ods graphics on;
proc logistic data=Neuralgia;
  class Treatment Sex / param=ref;
  model Pain= Treatment|Sex Age Duration;
  effectplot slicefit;
run;
ods graphics off;
```

By default, effect plots from PROC LOGISTIC are displayed on the probability scale. The predicted values are computed at the mean of the Duration variable, 16.73, and at the reference level of the Sex variable, M. Observations are also displayed on the sliced-fit plot in [Output 19.3.1](#). While the display of binary responses can give you a feel for the spread of the data, it does not enable you to evaluate the fit of the model.

Output 19.3.1 Default Fit Plot Sliced by Treatment

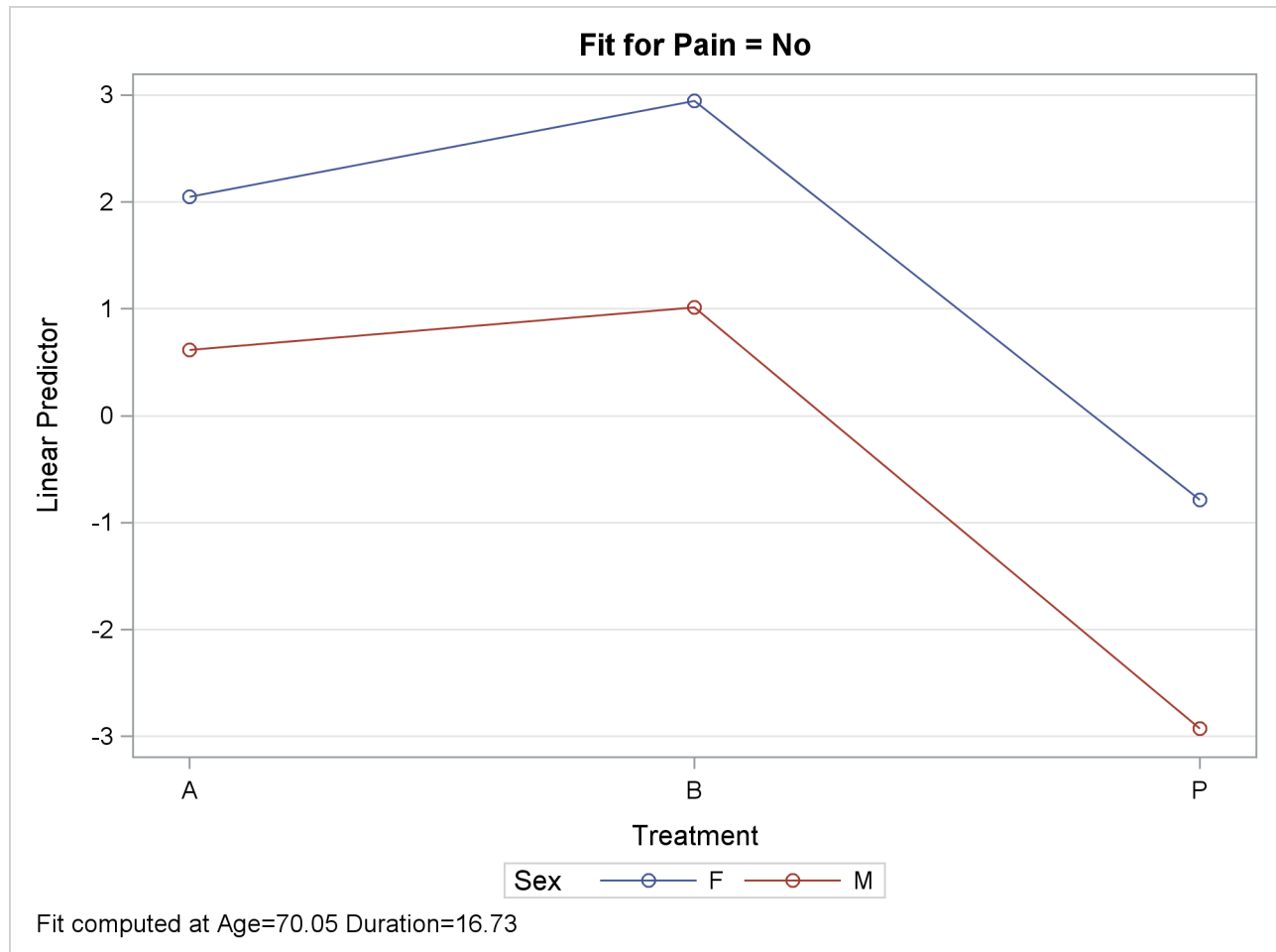


In the following statements, an **INTERACTION** *plot-type* is specified for the Treatment variable, with the Sex effect chosen for grouping the fits. The Age and Duration variables are set to their mean values for computing the predicted values. The **NOOBS** option suppresses the display of the binary observations on this plot. The **LINK** option is specified to display the fit on the LOGIT scale; if there is no interaction between Treatment and Sex, then the resulting curves shown in [Output 19.3.2](#) will have similar slopes across the treatments.

```
ods graphics on;
proc logistic data=Neuralgia;
  class Treatment Sex / param=ref;
  model Pain= Treatment|Sex Age Duration;
  effectplot interaction(x=Treatment sliceby=Sex) / noobs link;
run;
ods graphics off;
```

In [Output 19.3.2](#), the slopes of the lines seem “parallel” across the treatments, corroborating the nonsignificance of the interaction terms.

Output 19.3.2 Interaction Plot of an Interaction Effect

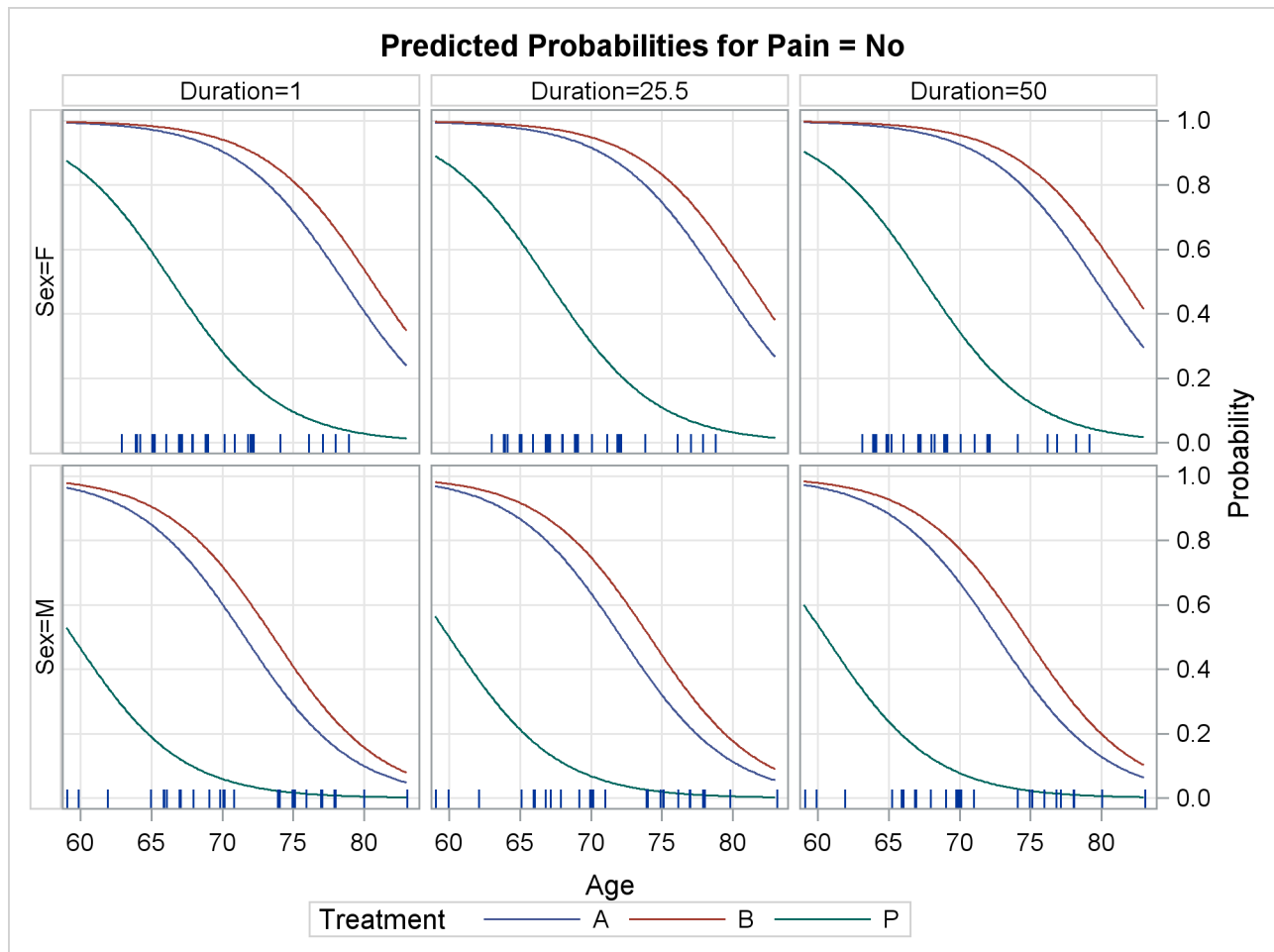


In the following statements, the interaction effect is removed, and the Duration variable is investigated further. The `PLOTBY(ROWS)=` option displays the Sex levels in the rows of a panel of plots, and the `AT` option computes the fits for several values of the Duration main effect in the columns of the panel. The `OBS(FRINGER)` option moves the observations to a fringe (rug) plot at the bottom of the plot, the observations are subsetting and displayed according to the value of the `PLOTBY=` variable, and the `JITTER` option makes overlaid fringes more visible. A `STORE` statement is also specified to save the model information for a later display. These statements produce [Output 19.3.3](#).

```
ods graphics on;
proc logistic data=Neuralgia;
  class Treatment Sex / param=ref;
  model Pain= Treatment Sex Age Duration;
  effectplot slicefit(sliceby=Treatment plotby(rows)=Sex)
    / at(Duration=min midrange max) obs(fringe jitter(seed=39393));
  store logimodel;
run;
ods graphics off;
```

The predicted probability curves in [Output 19.3.3](#) look very similar across the different values of the Duration variable, which agrees with the nonsignificance of Duration in this model. The fringe plot displays only female patients in the `SEX=F` row of the panel and displays only male patients in the `SEX=M` row, because the `PLOTBY=SEX` option subsets the observations.

Output 19.3.3 Sliced-Fit Plot with AT Option

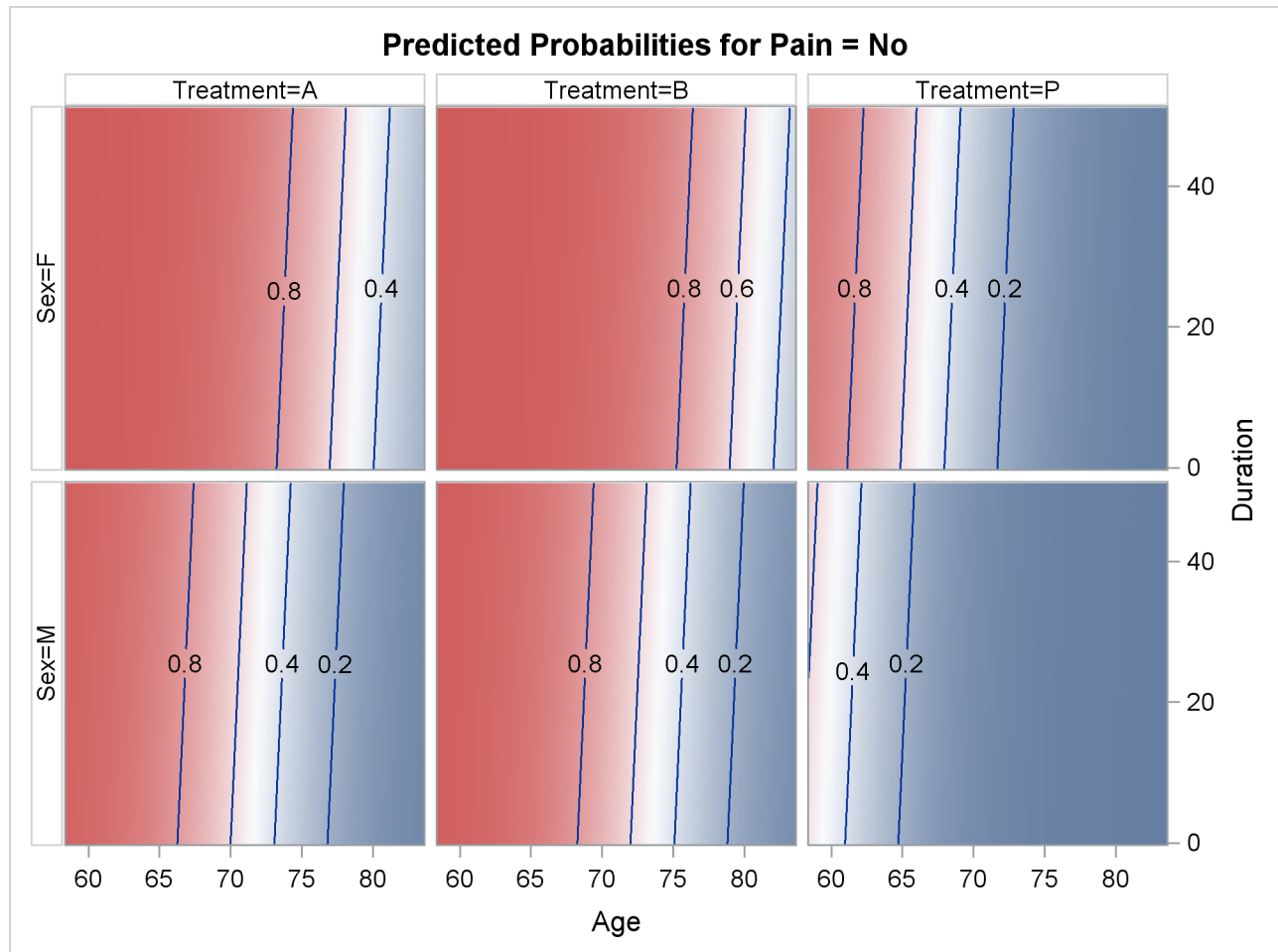


The following statements use the stored model and the PLM procedure to display a panel of contour plots:

```
ods graphics on;
proc plm restore=logimodel;
  effectplot contour(plotby=Treatment) / at(Sex=all);
run;
ods graphics off;
```

Output 19.3.4 again confirms that Duration is not significant.

Output 19.3.4 Contour Fit Panel



ESTIMATE Statement

This statement documentation applies to the following SAS/STAT procedures: LIFEREG, LOGISTIC, ORTHOREG, PHREG, PLM, PROBIT, QUANTREG, SURVEYLOGISTIC, SURVEYPHREG, and SURVEYREG. It also applies to the RELIABILITY procedure in SAS/QC software.

The ESTIMATE statement in the GENMOD, GLIMMIX, GLM, and MIXED procedures are documented in the respective procedure chapters.

The ESTIMATE statement provides a mechanism for obtaining custom hypothesis tests. Estimates are formed as linear estimable functions of the form $L\beta$. You can perform hypothesis tests for the estimable functions, construct confidence limits, and obtain specific nonlinear transformations.

Syntax: ESTIMATE Statement

```
ESTIMATE <'label'> estimate-specification <(divisor=n)>
      < , <'label'> estimate-specification <(divisor=n)> > < , ... >
      </options>;
```

The basic element of the ESTIMATE statement is the *estimate-specification*, which consists of model effects and their coefficients. A *estimate-specification* takes the general form

effect name < effect values ... >

The following variables can appear in the ESTIMATE statement:

<i>label</i>	is an optional label that identifies the particular row of the estimate in the output.
<i>effect</i>	identifies an effect that appears in the MODEL statement. The keyword INTERCEPT can be used as an effect when an intercept is fitted in the model. You do not need to include all effects that are in the MODEL statement.
<i>values</i>	are constants that are elements of the L matrix and are associated with the fixed and random effects. There are two basic methods of specifying the entries of the L matrix. The traditional representation—also known as the positional syntax—relies on entering coefficients in the position they assume in the L matrix. For example, in the following statements the elements of L that are associated with the b main effect receive a 1 in the first position and a –1 in the second position:

```
class a b;
model y = a b a*b;
estimate 'B at A2' b 1 -1 a*b 0 0 1 -1;
```

The elements that are associated with the interaction receive a 1 in the third position and a –1 in the fourth position. In order to specify coefficients correctly for the interaction term, you need to know how the levels of a and b vary in the interaction, which is governed by the order of the variables in the CLASS statement. The nonpositional syntax is designed to make it easier to enter coefficients for interactions and is necessary to enter coefficients for effects that are constructed with the EFFECT statement. In square brackets you enter the coefficient followed by the associated levels of the CLASS variables. If B has two levels and A has three levels, the previous ESTIMATE statement, by using nonpositional syntax for the interaction term, becomes the following statement:

```
estimate 'B at A2' b 1 -1 a*b [1, 2 1] [-1, 2 2];
```

The previous statement assigns value 1 to the interaction where A is at level 2 and B is at level 1, and it assigns -1 to the interaction where both classification variables are at level 2. The comma that separates the entry for the **L** matrix from the level indicators is optional. Further details about the nonpositional contrast syntax and its use with constructed effects can be found in the section “Positional and Nonpositional Syntax for Coefficients in Linear Functions” on page 448.

Based on the *estimate-specifications* in your ESTIMATE statement, the procedure constructs the matrix **L** to test the hypothesis $H: \mathbf{L}\boldsymbol{\beta} = \mathbf{0}$. The procedure supports nonpositional syntax for the coefficients of model effects in the ESTIMATE statement. For details see the section “Positional and Nonpositional Syntax for Coefficients in Linear Functions” on page 448.

The procedure then produces for each row *l* of **L** an approximate *t* test of the hypothesis $H: \mathbf{l}\boldsymbol{\beta} = 0$. You can also obtain multiplicity-adjusted *p*-values and confidence limits for multirow estimates with the **ADJUST=** option.

Note that multirow estimates are permitted. Unlike releases prior to SAS 9.22, you do not need to specify a ‘*label*’ for every row of the estimate; the procedure constructs a default label if a label is not specified.

If the procedure finds the estimate to be nonestimable, then it displays “Non-est” for the estimate entry.

Table 19.18 summarizes important options in the ESTIMATE statement. All ESTIMATE options are subsequently discussed in alphabetical order.

Table 19.18 ESTIMATE Statement Options

Option	Description
Construction and Computation of Estimable Functions	
DIVISOR=	Specifies a list of values to divide the coefficients
NOFILL	Suppresses the automatic fill-in of coefficients for higher-order effects
SINGULAR=	Tunes the estimability checking difference
Degrees of Freedom and <i>p</i>-values	
ADJUST=	Determines the method for multiple comparison adjustment of estimates
ALPHA=α	Determines the confidence level ($1 - \alpha$)
LOWER	Performs one-sided, lower-tailed inference
STEPDOWN	Adjusts multiplicity-corrected <i>p</i> -values further in a step-down fashion
TESTVALUE=	Specifies values under the null hypothesis for tests
UPPER	Performs one-sided, upper-tailed inference

Table 19.18 *continued*

Option	Description
Statistical Output	
CL	Constructs confidence limits
CORR	Displays the correlation matrix of estimates
COV	Displays the covariance matrix of estimates
E	Prints the L matrix
JOINT	Produces a joint <i>F</i> or chi-square test for the estimable functions
PLOTS=	Requests ODS statistical graphics if the analysis is sampling-based
SEED=	Specifies the seed for computations that depend on random numbers
Generalized Linear Modeling	
CATEGORY=	Specifies how to construct estimable functions with multinomial data
EXP	Exponentiates and displays estimates
ILINK	Computes and displays estimates and standard errors on the inverse linked scale

You can specify the following options in the ESTIMATE statement after a slash (/).

ADJDFE=SOURCE**ADJDFE=ROW**

specifies how denominator degrees of freedom are determined when *p*-values and confidence limits are adjusted for multiple comparisons with the **ADJUST=** option. When you do not specify the **ADJDFE=** option, or when you specify **ADJDFE=SOURCE**, the denominator degrees of freedom for multiplicity-adjusted results are the denominator degrees of freedom for the final effect that is listed in the ESTIMATE statement from the “Type III” table.

The **ADJDFE=ROW** setting is useful if you want multiplicity adjustments to take into account that denominator degrees of freedom are not constant across estimates. For example, this can be the case when the denominator degrees of freedom are computed by the Satterthwaite method or according to Kenward and Roger (1997).

The **ADJDFE=** option has an effect only in mixed models that use these degree-of-freedom methods. It is not supported by the procedures that perform chi-square-based inference (**LOGISTIC**, **PHREG**, and **SURVEYLOGISTIC**).

ADJUST=BON**ADJUST=SCHEFFE****ADJUST=SIDAK****ADJUST=SIMULATE**< (*simoptions*) >**ADJUST=T**

requests a multiple comparison adjustment for the *p*-values and confidence limits for the estimates. The adjusted quantities are produced in addition to the unadjusted quantities. Adjusted confidence limits are produced if the **CL** or **ALPHA=** option is in effect. For a description of the adjustments,

see Chapter 42, “The GLM Procedure,” and Chapter 61, “The MULTTEST Procedure,” and the documentation for the `ADJUST=` option in the `LSMEANS` statement.

If the `STEPDOWN` option is in effect, the p -values are further adjusted in a step-down fashion.

ALPHA=*number*

requests that a t type confidence interval be constructed with confidence level $1 - \textit{number}$. The value of *number* must be between 0 and 1; the default is 0.05. If the “Estimates” table shows infinite degrees of freedom, then the confidence interval is a z type interval.

CATEGORY=*category-options*

specifies how to construct estimates and multiplicity corrections for models with multinomial data (ordinal or nominal). This option is also important for constructing sets of estimable functions for F or chi-square tests with the `JOINT` option.

The *category-options* are used to indicate how response variable levels are treated in constructing the estimable functions. Possible values for the *category-options* are the following:

JOINT

computes the estimable functions for every nonredundant category and treats them as a set. For example, a three-row ESTIMATE statement in a model with three response categories leads to six estimable functions.

SEPARATE

computes the estimable functions for every nonredundant category in turn. For example, a three-row ESTIMATE statement in a model with three response categories leads to two sets of three estimable functions.

quoted-value-list

computes the estimable functions only for the list of values given. The list must consist of formatted values of the response categories.

Consider the following ESTIMATE statements in the LOGISTIC procedure for an ordinal model with response categories ‘vg’, ‘g’, ‘m’, ‘b’, and ‘vb’. Because there are five response categories, there are four nonredundant categories for the cumulative link model.

```
proc logistic data=icecream;
  class brand / param=glm;
  model taste(order=data) = brand / link=logit;
  freq count;

  estimate brand 1 -1,
           intercept 1 brand 0 1 / category='m', 'vg';

  estimate intercept 1 brand 1      / category=joint
           adjust=simulate(seed=1);

  estimate brand 1 -1,
           brand 1 1 -2              / category=separate
           adjust=bon;

run;
```

The first ESTIMATE statement requests a two-row estimable function. The result is produced for two of the four nonredundant response categories. The second ESTIMATE statement produces four t tests, one for each nonredundant category. The multiplicity adjustment with p -value computation by simulation treats the four estimable functions as a unit for family-wise Type I error protection. The third ESTIMATE statement computes a two-row estimable function and reports its results separately for all nonredundant categories. The Bonferroni adjustment in this statement applies to a family of two tests that correspond to the two-row estimable function. Four Bonferroni adjustments for sets of size two are performed.

The CATEGORY= option is supported only by the procedures that support generalized linear modeling (LOGISTIC and SURVEYLOGISTIC) and by PROC PLM when it is used to perform statistical analyses on item stores created by these procedures.

CHISQ

requests that chi-square tests be performed in addition to F tests, when you request an F test with the JOINT option. This option has no effect in procedures that produce chi-square statistics by default.

CL

requests that t type confidence limits be constructed. If the procedure shows the degrees of freedom in the “Estimates” table as infinite, then the confidence limits are z intervals. The confidence level is 0.95 by default, and you can change the confidence level with the ALPHA= option. The confidence intervals are adjusted for multiplicity when you specify the ADJUST= option. However, if a step-down p -value adjustment is requested with the STEPDOWN option, only the p -values are adjusted for multiplicity.

CORR

displays the estimated correlation matrix of the linear combination of the parameter estimates.

COV

displays the estimated covariance matrix of the linear combination of the parameter estimates.

DF=*number*

specifies the degrees of freedom for the t test and confidence limits. This option is not supported by the procedures that perform chi-square-based inference (LOGISTIC, PHREG, and SUVEYLOGISTIC).

DIVISOR=*value-list*

specifies a list of values by which to divide the coefficients so that fractional coefficients can be entered as integer numerators. If you do not specify *value-list*, a default value of 1.0 is assumed. Missing values in the *value-list* are converted to 1.0.

If the number of elements in *value-list* exceeds the number of rows of the estimate, the extra values are ignored. If the number of elements in *value-list* is less than the number of rows of the estimate, the last value in *value-list* is copied forward.

If you specify a row-specific divisor as part of the specification of the estimate row, this value multiplies the corresponding divisor that is implied by the *value-list*. For example, the following statement divides the coefficients in the first row by 8, and the coefficients in the third and fourth row by 3:

```
estimate 'One vs. two'   A 2 -2 (divisor=2),
         'One vs. three' A 1  0 -1      ,
         'One vs. four'  A 3  0  0 -3    ,
         'One vs. five'  A 1  0  0  0 -1 / divisor=4,.,3;
```

Coefficients in the second row are not altered.

E

requests that the **L** matrix coefficients be displayed.

EXP

requests exponentiation of the estimate. When you model data with the logit, cumulative logit, or generalized logit link functions, and the estimate represents a log odds ratio or log cumulative odds ratio, the EXP option produces an odds ratio. In proportional hazards model, this option produces estimates of hazard ratios. If you specify the **CL** or **ALPHA=** option, the (adjusted) confidence bounds are also exponentiated.

The EXP option is supported only by PROC PHREG, PROC SURVEYPHREG, the procedures that support generalized linear modeling (LOGISTIC and SURVEYLOGISTIC), and by PROC PLM when it is used to perform statistical analyses on item stores created by these procedures.

ILINK

requests that the estimate and its standard error also be reported on the scale of the mean (the inverse linked scale). The computation of the inverse linked estimate depends on the estimation mode. For example, if the analysis is based on a posterior sample when a BAYES statement is present, the inversely linked estimate is the average of the inversely linked values across the sample of posterior parameter estimates. If the analysis is not based on a sample of parameter estimates, the procedure computes the value on the mean scale by applying the inverse link to the estimate. The interpretation of this quantity depends on the *effect values* specified in your ESTIMATE statement and on the link function. For example, in a model for binary data with logit link the following statements compute

$$\frac{1}{1 + \exp\{-(\alpha_1 - \alpha_2)\}}$$

where α_1 and α_2 are the fixed-effects solutions that are associated with the first two levels of the classification effect A:

```
class A;
model y = A / dist=binary link=logit;
estimate 'A one vs. two' A 1 -1 / ilink;
```

This quantity is not the difference of the probabilities that are associated with the two levels,

$$\pi_1 - \pi_2 = \frac{1}{1 + \exp\{-\beta_0 - \alpha_1\}} - \frac{1}{1 + \exp\{-\beta_0 - \alpha_2\}}$$

The standard error of the inversely linked estimate is based on the delta method. If you also specify the **CL** option, the procedure computes confidence limits for the estimate on the mean scale. In multinomial models for nominal data, the limits are obtained by the delta method. In other models they are obtained from the inverse link transformation of the confidence limits for the estimate. The ILINK option is specific to an ESTIMATE statement.

The ILINK option is supported only by the procedures that support generalized linear modeling (LOGISTIC and SURVEYLOGISTIC) and by PROC PLM when it is used to perform statistical analyses on item stores created by these procedures.

JOINT< *joint-test-options* >

requests that a joint F or chi-square test be produced for the rows of the estimate. The JOINT option in the ESTIMATE statement essentially replaces the CONTRAST statement.

When the **LOWERTAILED** or the **UPPERTAILED** options are in effect, or if the **BOUNDS** option described below is in effect, the JOINT option produces the chi-bar-square statistic according to Silvapulle and Sen (2004). This statistic uses a simulation-based approach to compute p -values in situations where the alternative hypotheses of the estimable functions are not simple two-sided hypotheses. See the section “**Joint Hypothesis Tests with Complex Alternatives, the Chi-Bar-Square Statistic**” on page 451 for more information about this test statistic.

You can specify the following *joint-test-options* in parentheses:

ACC= γ

specifies the accuracy radius for determining the necessary sample size in the simulation-based approach of Silvapulle and Sen (2004) for tests with order restrictions. The value of γ must be strictly between 0 and 1; the default value is 0.005.

EPS= ϵ

specifies the accuracy confidence level for determining the necessary sample size in the simulation-based approach of Silvapulle and Sen (2004) for tests with order restrictions. The value of ϵ must be strictly between 0 and 1; the default value is 0.01.

LABEL='label'

assigns an identifying label to the joint test. If you do not specify a label, the first non-default label for the ESTIMATE rows is used to label the joint test.

NOEST**ONLY**

performs only the F or chi-square test and suppresses other results from the ESTIMATE statement. This option is useful for emulating the CONTRAST statement that is available in other procedures.

NSAMP= n

specifies the number of samples for the simulation-based method of Silvapulle and Sen (2004). If n is not specified, it is constructed from the values of the **ALPHA**= α , the **ACC**= γ , and the **EPS**= ϵ options. With the default values for γ , ϵ , and α (0.005, 0.01, and 0.05, respectively), **NSAMP**=12,604 by default.

CHISQ

adds a chi-square test if the procedure produces an F test by default.

BOUNDS=*value-list*

specifies boundary values for the estimable linear function. The null value of the hypothesis is always zero. If you specify a positive boundary value z , the hypotheses are $H: \theta = 0$, $H_a: \theta > 0$ with the added constraint that $\theta < z$. The same is true for negative boundary values. The alternative hypothesis is then $H_a: \theta < 0$ subject to the constraint $\theta > -|z|$. If you specify a missing value, the hypothesis is assumed to be two-sided. The **BOUNDS** option enables you to specify sets of one- and two-sided joint hypotheses. If all values in *value-list* are set to missing, the procedure performs a simulation-based p -value calculation for a two-sided test.

LOWER**LOWERTAILED**

requests that the p -value for the t test be based only on values that are less than the test statistic. A two-tailed test is the default. A lower-tailed confidence limit is also produced if you specify the **CL** or **ALPHA=** option.

Note that for **ADJUST=SCHEFFE** the one-sided adjusted confidence intervals and one-sided adjusted p -values are the same as the corresponding two-sided statistics, because this adjustment is based on only the right tail of the F distribution.

If you request a joint test with the **JOINT** option, then a one-sided left-tailed order restriction is applied to all estimable functions, and the corresponding chi-bar-square statistic of Silvapulle and Sen (2004) is computed in addition to the two-sided, standard, F or chi-square statistic. See the **JOINT** option for how to control the computation of the simulation-based chi-bar-square statistic.

NOFILL

suppresses the automatic fill-in of coefficients of higher-order effects.

PLOTS=*plot-options*

produces ODS statistical graphics of the distribution of estimable functions if the procedure performs the analysis in a sampling-based mode. For example, this is the case when procedures support a **BAYES** statement and perform a Bayesian analysis. The estimable functions are then computed for each of the posterior parameter estimates, and the “Estimates” table reports simple descriptive statistics for the evaluated functions. The **PLOTS=** option enables you in this situation to visualize the distribution of the estimable function. The following *plot-options* are available:

ALL

produces all possible plots with their default settings.

BOXPLOT< (*boxplot-options*) >

produces box plots of the distribution of the estimable function across the posterior sample. A separate box is generated for each estimable function, and all boxes appear on a single graph by default. You can affect the appearance of the box plot graph with the following options:

ORIENTATION=VERTICAL | HORIZONTAL**ORIENT=VERT | HORIZ**

specifies the orientation of the boxes. The default is vertical orientation of the box plots.

NPANELPOS=*number*

specifies how to break the series of box plots across multiple panels. If the **NPANELPOS** option is not specified, or if *number* equals zero, then all box plots are displayed in a single graph; this is the default. If a negative number is specified, then exactly up to $|number|$ of box plots are displayed per panel. If *number* is positive, then the number of boxes per panel is balanced to achieve small variation in the number of box plots per graph.

DISTPLOT< (*distplot-options*) >**DIST**< (*distplot-options*) >

generates panels of histograms with a kernel density overlaid. A separate plot in each panel contains the results for each estimable function. You can specify the following *distplot-options* in parentheses:

BOX | NOBOX

controls the display of a horizontal box plot of the estimable function's distribution across the posterior sample below the graph. The BOX option is enabled by default.

HIST | NOHIST

controls the display of the histogram of the estimable function's distribution across the posterior sample. The HIST option is enabled by default.

NORMAL | NONORMAL

controls the display of a normal density estimate on the graph. The NONORMAL option is enabled by default.

KERNEL | NOKERNEL

controls the display of a kernel density estimate on the graph. The KERNEL option is enabled by default.

NROWS=*number*

specifies the highest number of rows in a panel. The default is 3.

NCOLS=*number*

specifies the highest number of columns in a panel. The default is 3.

UNPACK

unpacks the panel into separate graphics.

NONE

does not produce any plots.

SEED=*number*

specifies the seed for the sampling-based components of the computations for the ESTIMATE statement (for example, chi-bar-square statistics and simulated p -values). The value of *number* must be an integer. The seed is used to start the pseudo-random number generator for the simulation. If you do not specify a seed, or if you specify a value less than or equal to zero, the seed is generated from reading the time of day from the computer clock. There could be multiple ESTIMATE statements with SEED= specifications and there could be other statements that can supply a random number seed. Since the procedure has only one random number stream, the initial seed is shown in the SAS log.

SINGULAR=*number*

tunes the estimability checking. If \mathbf{v} is a vector, define $\text{ABS}(\mathbf{v})$ to be the largest absolute value of the elements of \mathbf{v} . If $\text{ABS}(\mathbf{L} - \mathbf{L}\mathbf{T})$ is greater than $c * \text{number}$ for any row of \mathbf{L} in the contrast, then $\mathbf{L}\boldsymbol{\beta}$ is declared nonestimable. Here, \mathbf{T} is the Hermite form matrix $(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{X}$, and c is $\text{ABS}(\mathbf{L})$, except when it equals 0, and then c is 1. The value for *number* must be between 0 and 1; the default is $1\text{E}-4$.

STEPDOWN< (*step-down-options*) >

requests that multiplicity adjustments for the p -values of estimates be further adjusted in a step-down fashion. Step-down methods increase the power of multiple testing procedures by taking advantage of the fact that a p -value is never declared significant unless all smaller p -values are also declared significant. The STEPDOWN adjustment combined with ADJUST=BON corresponds to the methods of Holm (1979) and "Method 2" of Shaffer (1986); this is the default. Using step-down-adjusted p -values combined with ADJUST=SIMULATE corresponds to the method of Westfall (1997).

If the ESTIMATE statement is applied with a STEPDOWN option in a mixed model where the degrees-of-freedom method is that of Kenward and Roger (1997) or of Satterthwaite, then step-down-adjusted p -values are produced only if the ADJDFE=ROW option is in effect.

Also, the STEPDOWN option affects only p -values, not confidence limits. For ADJUST=SIMULATE, the generalized least squares hybrid approach of Westfall (1997) is used to increase Monte Carlo accuracy. You can specify the following *step-down-options* in parentheses after the STEPDOWN option:

MAXTIME= n

specifies the time (in seconds) to be spent computing the maximal logically consistent sequential subsets of equality hypotheses for TYPE=LOGICAL. The default is MAXTIME=60. If the MAXTIME value is exceeded, the adjusted tests are not computed. When this occurs, you can try increasing the MAXTIME value. However, note that there are common multiple comparisons problems for which this computation requires a huge amount of time—for example, all pairwise comparisons between more than 10 groups. In such cases, try to use TYPE=FREE (the default) or TYPE=LOGICAL(n) for small n .

ORDER=PVALUE

ORDER=ROWS

specifies the order in which the step-down tests to be performed. ORDER=PVALUE is the default, with estimates being declared significant only if all estimates with smaller (unadjusted) p -values are significant. If you specify ORDER=ROWS, then significances are evaluated in the order in which they are specified in the syntax.

REPORT

specifies that a report on the step-down adjustment be displayed, including a listing of the sequential subsets (Westfall 1997) and, for ADJUST=SIMULATE, the step-down simulation results.

TYPE=LOGICAL< (n) >

TYPE=FREE

specifies how step-down adjustment are made. If you specify TYPE=LOGICAL, the step-down adjustments are computed by using maximal logically consistent sequential subsets of equality hypotheses (Shaffer 1986; Westfall 1997). Alternatively, for TYPE=FREE, sequential subsets are computed ignoring logical constraints. The TYPE=FREE results are more conservative than those for TYPE=LOGICAL, but they can be much more efficient to produce for many estimates. For example, it is not feasible to take logical constraints between all pairwise comparisons of more than about 10 groups. For this reason, TYPE=FREE is the default.

However, you can reduce the computational complexity of taking logical constraints into account by limiting the depth of the search tree used to compute them, specifying the optional depth parameter as a number n in parentheses after TYPE=LOGICAL. As with TYPE=FREE, results for TYPE=LOGICAL(n) are conservative relative to the true TYPE=LOGICAL results. But even for TYPE=LOGICAL(0) they can be appreciably less conservative than TYPE=FREE, and they are computationally feasible for much larger numbers of estimates. If you do not specify n or if $n = -1$, the full search tree is used.

TESTVALUE=*value-list*

TESTMEAN=*value-list*

specifies the value under the null hypothesis for testing the estimable functions in the ESTIMATE statement. The rules for specifying the *value-list* are very similar to those for specifying the divisor list in the DIVISOR= option. If no TESTVALUE= is specified, all tests are performed as $H: \mathbf{L}\boldsymbol{\beta} = 0$. Missing values in the *value-list* also are translated to zeros. If you specify fewer values than rows in the ESTIMATE statement, the last value in *value-list* is carried forward.

The TESTVALUE= option affects only p -values from individual, joint, and multiplicity-adjusted tests. It does not affect confidence intervals.

The TESTVALUE option is not available for the multinomial distribution, and the values are ignored when you perform a sampling-based (Bayesian) analysis.

UPPER

UPPERTAILED

requests that the p -value for the t test be based only on values that are greater than the test statistic. A two-tailed test is the default. An upper-tailed confidence limit is also produced if you specify the CL or ALPHA= option.

Note that for ADJUST=SCHEFFE the one-sided adjusted confidence intervals and one-sided adjusted p -values are the same as the corresponding two-sided statistics, because this adjustment is based on only the right tail of the F distribution.

If you request a joint test with the JOINT option, then a one-sided right-tailed order restriction is applied to all estimable functions, and the corresponding chi-bar-square statistic of Silvapulle and Sen (2004) is computed in addition to the two-sided, standard, F or chi-square statistic. See the JOINT option for how to control the computation of the simulation-based chi-bar-square statistic.

Positional and Nonpositional Syntax for Coefficients in Linear Functions

When you define custom linear hypotheses with the ESTIMATE statement, the procedure sets up an \mathbf{L} vector or matrix that conforms to the model effect solutions. (Note that the following remarks also apply to the LSMESTIMATE statement, where you specify coefficients of the matrix \mathbf{K} which is then converted into a coefficient matrix that conforms to the model effects solutions.)

There are two methods for specifying the entries in a coefficient matrix (hereafter simply referred to as the \mathbf{L} matrix); they are called the positional and nonpositional methods. In the positional form, which is the traditional method, you provide a list of values that occupy the elements of the \mathbf{L} matrix that is associated with the effect in question in the order in which the values are listed. For traditional model effects that consist of continuous and classification variables, the positional syntax is simpler in some cases (main effects) and more cumbersome in others (interactions). When you work with effects that are constructed through the EFFECT statement, the nonpositional syntax is essential.

For example, consider the following two-way model with interactions where factors A and B have three and two levels, respectively:

```
proc logistic;
  class a b;
  model y = a b a*b;
run;
```

To test the difference of the B levels at the second level of A with an **ESTIMATE** statement (a slice), you need to assign coefficients 1 and -1 to the levels of B and to the levels of the interaction where A is at the second level. Two examples of equivalent **ESTIMATE** statements that use positional and nonpositional syntax are as follows:

```
estimate 'B at A2' b 1 -1 a*b 0 0 1 -1 ;
estimate 'B at A2' b 1 -1 a*b [1 2 1] [-1 2 2];
```

Because A precedes B in the **CLASS** statement, the levels of the interaction are formed as $\alpha_1\beta_1, \alpha_1\beta_2, \alpha_2\beta_1, \alpha_2\beta_2, \dots$. If B precedes A in the **CLASS** statement, you need to modify the coefficients accordingly:

```
proc logistic;
  class b a;
  model y = a b a*b;
  estimate 'B at A2' b 1 -1 a*b 0 1 0 0 -1 ;
  estimate 'B at A2' b 1 -1 a*b [1 1 2] [-1 2 2];
  estimate 'B at A2' b 1 -1 a*b [1, 1 2] [-1, 2 2];
run;
```

You can optionally separate the **L** value entry from the level indicators with a comma, as in the last **ESTIMATE** statement.

The general syntax for defining coefficients with the nonpositional syntax is as follows:

effect-name [*multiplier* <, > *level-values*] ... <[*multiplier* <, > *level-values*] >

The first entry in square brackets is the multiplier that is applied to the elements of **L** for the effect after the *level-values* have been resolved and any necessary action that forms **L** has been taken.

The *level-values* are organized in a specific form:

- The number of entries should equal the number of terms that are needed to construct the effect. For effects that do not contain any constructed effects, this number is simply the number of terms in the name of the effect.
- Values of continuous variables that are needed for the construction of the **L** matrix precede the level indicators of **CLASS** variables.
- If the effect involves constructed effects, then you need to provide as many continuous and classification variables as are needed for the effect formation. For example, if a collection effect is defined as

```
class c;
effect v = collection(x1 x2 c);
```

then a proper nonpositional syntax would be

```
v [0.5, 0.2 0.3 3]
```

- If an effect contains both regular terms (old-style effects) and constructed effects, then the order of the coefficients is as follows: continuous values for old-style effects, class levels for classification variables in old-style effects, continuous values for constructed effects, and finally class levels that are needed for constructed effects. Assume that C has four levels so that effect v contributes six elements to the L matrix. When the procedure resolves this syntax, the values 0.2 and 0.3 are assigned to the positions for x1 and x2 and a 1 is associated with the third level of C. The resulting vector is then multiplied by 0.5 to produce

```
[0.1 0.15 0 0 0.5 0]
```

Note that you enter the **levels** of the classification variables in the square brackets, not their formatted values. The ordering of the levels of classification variables can be gleaned from the “Class Level Information” table.

To specify values for continuous variables, simply give their value as one of the terms in the effect. The nonpositional syntax in the following **ESTIMATE** statement is read as “1 times the value 0.4 in the column that is associated with level 2 of A”

```
proc phreg;
  class a / param=glm;
  model y = a a*x / s;
  lsmeans a / e at x=0.4;
  estimate 'A2 at x=0.4' intercept 1 a 0 1 a*x [1,0.4 2] / e;
run;
```

Because the value before the comma serves as a multiplier, the same estimable function could also be constructed with the following statements:

```
estimate 'A2 at x=0.4' intercept 1 a 0 1 a*x [ 4, 0.1 2];
estimate 'A2 at x=0.4' intercept 1 a 0 1 a*x [ 2, 0.2 2];
estimate 'A2 at x=0.4' intercept 1 a 0 1 a*x [-1, -0.4 2];
```

Note that continuous variables that are needed to construct an effect are always listed before any CLASS variables.

When you work with constructed effects, the nonpositional syntax works in the same way. For example, the following model contains a classification effect and a B-spline. The first two **ESTIMATE** statements produce predicted values for level 1 of C when the continuous variable x takes on the values 20 and 10, respectively.

```
proc orthoreg;
  class c;
  effect spl = spline(x / knotmethod=equal(5));
  model y = c spl;
  estimate 'C = 1 @ x=20' intercept 1 c 1 spl [1,20],
          'C = 1 @ x=10' intercept 1 c 1 spl [1,10];
  estimate 'Difference' spl [1,20] [-1,10];
run;
```

In this example, the ORTHOREG procedure computes the spline coefficients for the first `ESTIMATE` statement based on $x = 20$, and similarly in the second statement for $x = 10$. The third `ESTIMATE` statement computes the difference of the predicted values. Because the spline effect does not interact with the classification variable, this difference does not depend on the level of C . If such an interaction is present, you can estimate the difference in predicted values for a given level of C by using the nonpositional syntax. Because the effect `C*spl` contains both old-style terms (`C`) and a constructed effect, you specify the values for the old-style terms before assigning values to constructed effects.

```
proc orthoreg;
  class c;
  effect spl = spline(x / knotmethod=equal(5));
  model y = spl*c;
  estimate 'C2 = 1, x=20' intercept 1 c*spl [1,1 20];
  estimate 'C2 = 2, x=20' intercept 1 c*spl [1,2 20];
  estimate 'C diff at x=20' c*spl [1,1 20] [-1,2 20];
run;
```

It is recommended that you add the `E` option to the `ESTIMATE` or `LSMESTIMATE` statement to verify that the `L` matrix is formed according to your expectations.

In any row of an `ESTIMATE` statement you can choose positional and nonpositional syntax separately for each effect. However, you cannot mix the two forms of syntax for coefficients of a single effect. For example, the following statement is not proper because both forms of syntax are used for the interaction effect:

```
estimate 'A1B1 - A1B2' b 1 -1 a*b 0 1 [-1, 1 2];
```

Joint Hypothesis Tests with Complex Alternatives, the Chi-Bar-Square Statistic

Silvapulle and Sen (2004) propose a test statistic for testing hypotheses where the null or the alternative hypothesis or both involve inequalities. You can test special cases of these hypotheses with the `JOINT` option in the `ESTIMATE` and the `LSMESTIMATE` statement. Consider the k estimable functions $\mathbf{L}\boldsymbol{\beta}$ and the hypotheses $H_0: \mathbf{L}\boldsymbol{\beta} = \mathbf{0}$ and $H_a: \mathbf{L}\boldsymbol{\beta} \geq \mathbf{0}$. The alternative hypothesis defines a convex cone \mathcal{C} at the origin. Suppose that under the null hypothesis $\mathbf{L}\hat{\boldsymbol{\beta}}$ follows a multivariate normal distribution with mean $\mathbf{0}$ and variance \mathbf{V} . The restricted alternative prevents you from using the usual F or chi-square test machinery, since the distribution of the test statistic under the alternative might not follow the usual rules. Silvapulle and Sen (2004) coined a statistic that takes into account the projection of the observed estimate onto the convex cone formed by the alternative parameter space. This test statistic is called the chi-bar-square statistic, and p -values are obtained by simulation; see, in particular, Chapter 3.4 in Silvapulle and Sen (2004).

Briefly, let \mathbf{U} be a multivariate normal random variable with mean $\mathbf{0}$ and variance matrix \mathbf{V} . The chi-bar-square statistic is the random variable

$$\begin{aligned}\bar{\chi}^2 &= \mathbf{U}'\mathbf{V}^{-1}\mathbf{U} - Q \\ Q &= \min_{\boldsymbol{\theta} \in \mathcal{C}} (\mathbf{U} - \boldsymbol{\theta})'\mathbf{V}^{-1}(\mathbf{U} - \boldsymbol{\theta})\end{aligned}$$

and it can be motivated by a geometric argument. The quadratic form in Q is the \mathbf{V} -projection of \mathbf{U} onto the cone \mathcal{C} . Suppose that this projected point is $\tilde{\mathbf{U}}$. If $\mathbf{U} \in \mathcal{C}$, then $Q = 0$ and $\tilde{\mathbf{U}} = \mathbf{U}$. If \mathbf{U} is completely

outside of the cone \mathcal{C} , then $\tilde{\mathbf{U}}$ is a point on the surface of the cone. Similarly, $\mathbf{U}'\mathbf{V}^{-1}\mathbf{U}$ is the length of the segment from the origin to \mathbf{U} in the \mathbf{V} -space with norm $\|x\| = (\mathbf{x}'\mathbf{V}^{-1}\mathbf{x})^{1/2}$. If you apply the Pythagorean theorem, you can see that the chi-bar-square statistic measures the length of the segment from the origin to the projected point $\tilde{\mathbf{U}}$ in \mathcal{C} .

To calculate p -values for chi-bar-square statistics, a simulation-based approach is taken. Consider again the set of k estimable functions $\mathbf{L}\boldsymbol{\beta}$ with estimate $\mathbf{L}\hat{\boldsymbol{\beta}} = \mathbf{U}$ and variance $\mathbf{L}\text{Var}[\hat{\boldsymbol{\beta}}]\mathbf{L}' = \mathbf{V}$.

First, the observed value of the statistic is computed as

$$\bar{\chi}_{obs}^2 = \mathbf{U}'\mathbf{V}^{-1}\mathbf{U} - Q$$

Then, n independent random samples $\mathbf{Z}_1, \dots, \mathbf{Z}_n$ are drawn from an $N(\mathbf{0}, \mathbf{V})$ distribution and the following chi-bar-statistics are computed for the sample:

$$\begin{aligned} \bar{\chi}_1^2 &= \mathbf{Z}_1'\mathbf{V}^{-1}\mathbf{Z}_1 - \min_{\boldsymbol{\theta} \in \mathcal{C}} (\mathbf{Z}_1 - \boldsymbol{\theta})'\mathbf{V}^{-1}(\mathbf{Z}_1 - \boldsymbol{\theta}) \\ &\vdots \\ \bar{\chi}_n^2 &= \mathbf{Z}_n'\mathbf{V}^{-1}\mathbf{Z}_n - \min_{\boldsymbol{\theta} \in \mathcal{C}} (\mathbf{Z}_n - \boldsymbol{\theta})'\mathbf{V}^{-1}(\mathbf{Z}_n - \boldsymbol{\theta}) \end{aligned}$$

The p -value is estimated by the fraction of simulated statistics that are greater than or equal to the observed value $\bar{\chi}_{obs}^2$.

Notice that unless \mathbf{U} is interior to the cone \mathcal{C} , finding the value of Q requires the solution to a quadratic optimization problem. When k is large, or when many simulations are requested, the computation of p -values for chi-bar-square statistics might require considerable computing time.

ODS Table Names: ESTIMATE Statement

Each table created by the `ESTIMATE` statement has a name associated with it, and you can use this name to refer to the table when you use the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in Table 19.19. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

Table 19.19 ODS Tables Produced by the `ESTIMATE` statement

Table Name	Description	Required Option
Coef	\mathbf{L} matrix coefficients	E
Estimates	<code>ESTIMATE</code> statement results	Default
Contrasts	Joint test results	JOINT

ODS Graphics: ESTIMATE Statement

This section describes the use of ODS Graphics for creating statistical graphs of the distribution of estimable functions with the `ESTIMATE` statement. The plots can be produced only in association with the `LIFEREG`

and PHREG procedures, which can perform Bayesian analysis. The plots are available via these procedures directly, and also via PROC PLM when it is run using an item store that was created by these procedures.

To request these graphs you must do the following:

- ensure that ODS Graphics is enabled
- use a BAYES statement with PROC LIFEREG or PROC PHREG, or use PROC PLM to perform statistical analysis on an item store that was saved from a Bayesian analysis
- request plots with the PLOTS= option in the ESTIMATE statement

For more information about ODS Graphics, see Chapter 21, “Statistical Graphics Using ODS.” The available graphs are summarized in Table 19.20.

Table 19.20 Graphs Produced by the ESTIMATE statement

ODS Graph Name	Plot Description	Required Option
BoxPlot	Displays box plots of estimable functions across a posterior sample.	PLOTS=BOXPLOT
DistPanel	Displays panels of histograms with kernel density curves overlaid. Each plot contains the results for the posterior sample of each estimable function.	PLOTS=DISTPLOT
DistPlot	Displays a histogram with a kernel density curve overlaid. The plot contains the results for the posterior sample of the estimable function.	PLOTS=DISTPLOT(UNPACK)

For details about the *plot-options* of the ESTIMATE statement, see the PLOTS= option in the section “ESTIMATE Statement” on page 437.

LSMEANS Statement

This statement documentation applies to the following procedures: GENMOD, LIFEREG, LOGISTIC, ORTHOREG, PHREG, PLM, PROBIT, SURVEYLOGISTIC, SURVEYPHREG, and SURVEYREG. It also applies to the RELIABILITY procedure in SAS/QC software. The GLIMMIX, GLM, and MIXED procedures also support LSMEANS statements. The relevant statement documentation for these procedures can be found in the specific procedure chapter.

The LSMEANS statement computes least squares means (LS-means) of fixed effects. In the GLM, MIXED, and GLIMMIX procedures, LS-means are *predicted population margins*—that is, they estimate the marginal

means over a balanced population. In a sense, LS-means are to unbalanced designs as class and subclass arithmetic means are to balanced designs.

Thus it is important not to interpret the name with a strict association with least squares estimation. Least squares is the predominant estimation technique for the type of models in which LS-means were first applied. Their interpretation and importance reaches beyond the least squares principle, however. A more appropriate approach to LS-means views them as linear combinations of the parameter estimates that are constructed in such a way that they correspond to average predicted values in a population where the levels of classification variables are balanced.

This contemporary—and historically correct—interpretation of the concept of least squares means underlines their importance in all classes of models where predicted values are reasonably formed as linear combinations of the parameter estimates. LS-means distinguish themselves from general estimable functions in that they take the structure for the model and data into account through the structure of the \mathbf{X} and $\mathbf{X}'\mathbf{X}$ matrix in your model. For example, in a generalized linear model the structure of the \mathbf{X} matrix informs the analysis about the possible levels of classification variables and predictions on the linear (the linked) scale are computed as $\mathbf{x}'\boldsymbol{\beta}$. LS-means are thus meaningful quantities in such models when the linear estimable function that corresponds to an averaged prediction is constructed on the linked scale. For example, in a binomial model with logit link, the least squares means are predicted population margins of the logits. You can then transform the least squares means to the data scale with the `ILINK` option, and you can display differences of least squares means in terms of odds ratios with the `ODDSRATIO` option. The underlying principle—unless you perform a Bayesian analysis—is to construct the estimates or their differences on the linked scale and to apply appropriate transformations in a second step.

Least squares means computations are also supported for multinomial models.

LS-means are computed as $\mathbf{L}\boldsymbol{\beta}$ where the \mathbf{L} matrix that is constructed to compute the predicted values is the same as the \mathbf{L} matrix that is formed in `PROC GLM`.

Each LS-mean is computed as $\mathbf{L}\hat{\boldsymbol{\beta}}$, where \mathbf{L} is the coefficient matrix that is associated with the least squares mean and $\hat{\boldsymbol{\beta}}$ is the estimate of the fixed-effects parameter vector. The approximate standard error for the LS-mean is computed as the square root of $\mathbf{L}\widehat{\text{Var}}[\hat{\boldsymbol{\beta}}]\mathbf{L}'$. The approximate variance matrix of the fixed-effects estimates depends on the estimation method.

Syntax: LSMEANS Statement

```
LSMEANS < model-effects > < / options > ;
```

LS-means can be computed for any effect in the statistical model that involves only `CLASS` variables. You can specify multiple effects in one `LSMEANS` statement or in multiple `LSMEANS` statements, and all `LSMEANS` statements must appear after the `MODEL` statement. If you do not specify *model-effects*, the options in the `LSMEANS` statement are applied to all suitable model effects.

As in the `ESTIMATE` statement, the \mathbf{L} matrix is tested for estimability; if this test fails, the procedure displays “Non-est” for the LS-means entries. Note that linear functions of LS-means, such as differences, can be estimable, even if the means themselves are not estimable. Estimability checks for differences are thus applied separately from checks for the means.

Assuming the LS-mean is estimable, the procedure constructs an approximate t test to test the null hypothesis that the associated population quantity equals zero.

Table 19.21 summarizes important options in the LSMEANS statement. All LSMEANS options are subsequently discussed in alphabetical order.

Table 19.21 LSMEANS Statement Options

Option	Description
Construction and Computation of LS-Means	
AT	Modifies the covariate value in computing LS-means
BYLEVEL	Computes separate margins
DIFF	Requests differences of LS-means
OM=	Specifies the weighting scheme for LS-means computation as determined by the input data set
SINGULAR=	Tunes estimability checking
Degrees of Freedom and p-values	
ADJUST=	Determines the method for multiple-comparison adjustment of LS-means differences
ALPHA= α	Determines the confidence level ($1 - \alpha$)
STEPDOWN	Adjusts multiple-comparison p -values further in a step-down fashion
Statistical Output	
CL	Constructs confidence limits for means and mean differences
CORR	Displays the correlation matrix of LS-means
COV	Displays the covariance matrix of LS-means
E	Prints the L matrix
LINES	Produces a “Lines” display for pairwise LS-means differences
MEANS	Prints the LS-means
PLOTS=	Requests graphs of means and mean comparisons
SEED=	Specifies the seed for computations that depend on random numbers
Generalized Linear Modeling	
EXP	Exponentiates and displays estimates of LS-means or LS-means differences
ILINK	Computes and displays estimates and standard errors of LS-means (but not differences) on the inverse linked scale
ODDSRATIO	Reports (simple) differences of least squares means in terms of odds ratios if permitted by the link function

You can specify the following options in the LSMEANS statement after a slash (/):

ADJDFE=ROW

ADJDFE=SOURCE

specifies how denominator degrees of freedom are determined when p -values and confidence limits are adjusted for multiple comparisons with the ADJUST= option. When you do not specify the ADJDFE= option or when you specify ADJDFE=SOURCE, the denominator degrees of freedom for

multiplicity-adjusted results are the denominator degrees of freedom for the LS-mean effect in the “Type III Tests of Fixed Effects” table. When you specify `ADJDFE=ROW`, the denominator degrees of freedom for multiplicity-adjusted results correspond to the degrees of freedom that are displayed in the DF column of the “Differences of Least Squares Means” table.

The `ADJDFE=ROW` setting is particularly useful if you want multiplicity adjustments to take into account that denominator degrees of freedom are not constant across LS-mean differences.

In one-way models with heterogeneous variance, combining certain `ADJUST=` options with the `ADJDFE=ROW` option corresponds to particular methods of performing multiplicity adjustments in the presence of heteroscedasticity. For example, the following statements fit a heteroscedastic one-way model and perform Dunnett’s T3 method (Dunnett 1980), which is based on the studentized maximum modulus (`ADJUST=SMM`):

```
proc glimmix;
  class A;
  model y = A / ddfm=satterth;
  random _residual_ / group=A;
  lsmeans A / adjust=smm adjdfe=row;
run;
```

If you combine the `ADJDFE=ROW` option with `ADJUST=SIDAK`, the multiplicity adjustment corresponds to the T2 method of Tamhane (1979), and `ADJUST=TUKEY` corresponds to the method of Games-Howell (Games and Howell 1976). Note that `ADJUST=TUKEY` gives the exact results for the case of fractional degrees of freedom in the one-way model, but it does not take into account that the degrees of freedom are subject to variability. A more conservative method, such as `ADJUST=SMM`, might protect the overall error rate better.

Unless the `ADJUST=` option is specified in the `LSMEANS` statement, the `ADJDFE=` option has no effect. The option is not supported by the procedures that perform chi-square-based inference (`GENMOD`, `LOGISTIC`, `PHREG`, and `SURVEYLOGISTIC`).

ADJUST=BON

ADJUST=DUNNETT

ADJUST=NELSON

ADJUST=SCHEFFE

ADJUST=SIDAK

ADJUST=SIMULATE< (*simoptions*) >

ADJUST=SMM | GT2

ADJUST=TUKEY

requests a multiple comparison adjustment for the p -values and confidence limits for the differences of LS-means. The adjusted quantities are produced in addition to the unadjusted quantities. By default, the procedure performs all pairwise differences. If you specify `ADJUST=DUNNETT`, the procedure analyzes all differences with a control level. If you specify `ADJUST=NELSON`, ANOM differences are taken. The `ADJUST=` option implies the `DIFF` option.

The BON (Bonferroni) and SIDAK adjustments involve correction factors described in Chapter 42, “The GLM Procedure,” and Chapter 61, “The MULTTEST Procedure”; also see Westfall and Young

(1993) and Westfall et al. (1999). When you specify ADJUST=TUKEY and your data are unbalanced, the procedure uses the approximation described in Kramer (1956) and identifies the adjustment as “Tukey-Kramer” in the results. Similarly, when you specify ADJUST=DUNNETT or ADJUST=NELSON and the LS-means are correlated, the procedure uses the factor-analytic covariance approximation described in Hsu (1992) and identifies the adjustment in the results as “Dunnnett-Hsu” or “Nelson-Hsu,” respectively. The approximation derives an approximate “effective sample sizes” for which exact critical values are computed. Computing the exact adjusted p -values and critical values for unbalanced designs can be computationally intensive, in particular for ADJUST=NELSON. A simulation-based approach, as specified by the ADJUST=SIM option, while nondeterministic, can provide inferences that are sufficiently accurate in much less time. The preceding references also describe the SCHEFFE and SMM adjustments.

Nelson’s adjustment applies only to the analysis of means (Ott 1967; Nelson 1982, 1991, 1993), where LS-means are compared against an average LS-mean. It does not apply to all pairwise differences of least squares means. See the DIFF=ANOM option for more details regarding the analysis of means with the procedure.

The SIMULATE adjustment computes adjusted p -values and confidence limits from the simulated distribution of the maximum or maximum absolute value of a multivariate t random vector. All covariance parameters, except the residual scale parameter, are fixed at their estimated values throughout the simulation, potentially resulting in some underdispersion. The simulation estimates q , the true $(1 - \alpha)$ quantile, where $1 - \alpha$ is the confidence coefficient. The default α is 0.05, and you can change this value with the ALPHA= option in the LSMEANS statement.

The number of samples is set so that the tail area for the simulated q is within γ of $1 - \alpha$ with $100(1 - \epsilon)\%$ confidence. In equation form,

$$\Pr(|F(\hat{q}) - (1 - \alpha)| \leq \gamma) = 1 - \epsilon$$

where \hat{q} is the simulated q and F is the true distribution function of the maximum; see Edwards and Berry (1987) for details. By default, $\gamma = 0.005$ and $\epsilon = 0.01$, placing the tail area of \hat{q} within 0.005 of 0.95 with 99% confidence. You can specify the following *simoptions* in parentheses after the ADJUST=SIMULATE option:

ACC=value

specifies the target accuracy radius γ of a $100(1 - \epsilon)\%$ confidence interval for the true probability content of the estimated $(1 - \alpha)$ quantile. The default value is ACC=0.005.

EPS=value

specifies the value ϵ for a $100 \times (1 - \epsilon)\%$ confidence interval for the true probability content of the estimated $(1 - \alpha)$ quantile. The default value for the accuracy confidence is 99%, which corresponds to EPS=0.01.

NSAMP=n

specifies the sample size for the simulation. By default, n is set based on the values of the target accuracy radius γ and accuracy confidence $100 \times (1 - \epsilon)\%$ for an interval for the true probability content of the estimated $(1 - \alpha)$ quantile. With the default values for γ , ϵ , and α (0.005, 0.01, and 0.05, respectively), NSAMP=12,604 by default.

SEED=number

specifies an integer that is used to start the pseudo-random number generator for the simulation. If you do not specify a seed, or specify a value less than or equal to zero, the seed is by default generated from reading the time of day from the computer's clock.

THREADS

specifies that the computational work for the simulation be divided into parallel threads, where the number of threads is the value of the SAS system option CPUCOUNT=. For large simulations (as specified directly using the NSAMP= *simoption* or indirectly using the ACC= or EPS= *simoptions*), parallel processing can markedly speed up the computation of adjusted *p*-values and confidence intervals. However, because the parallel processing has different pseudo-random number streams, the precise results are different from the default ones, which are computed in sequence rather than in parallel. This option overrides the SAS system option THREADS | NOTTHREADS.

NOTTHREADS

specifies that the computational work for the simulation be performed in sequence rather than in parallel. NOTTHREADS is the default. This option overrides the SAS system option THREADS | NOTTHREADS.

If the **STEPDOWN** option is in effect, the *p*-values are further adjusted in a step-down fashion. For certain options and data, this adjustment is exact under an iid $N(0, \sigma^2)$ model for the dependent variable, in particular for the following:

- for ADJUST=DUNNETT when the means are uncorrelated
- for ADJUST=TUKEY with STEPDOWN(TYPE=LOGICAL) when the means are balanced and uncorrelated.

The first case is a consequence of the nature of the successive step-down hypotheses for comparisons with a control; the second uses an extension of the maximum studentized range distribution appropriate for partition hypotheses (Royen 1989). Finally, for **STEPDOWN(TYPE=FREE)**, ADJUST=TUKEY employs the Royen (1989) extension in such a way that the resulting *p*-values are conservative.

ALPHA=number

requests that a *t* type confidence interval be constructed for each of the LS-means with confidence level $1 - \text{number}$. The value of *number* must be between 0 and 1; the default is 0.05.

AT variable=value**AT (variable-list)=(value-list)****AT MEANS**

modifies the values of the covariates that are used in computing LS-means. By default, all covariate effects are set equal to their mean values for computation of standard LS-means. The AT option enables you to assign arbitrary values to the covariates. Additional columns in the output table indicate the values of the covariates.

If there is an effect that contains two or more covariates, the AT option sets the effect equal to the product of the individual means rather than the mean of the product (as with standard LS-means calculations). The AT MEANS option sets covariates equal to their mean values (as with standard LS-means) and incorporates this adjustment to crossproducts of covariates.

As an example, consider the following statements:

```
class A;
model Y = A x1 x2 x1*x2;
lsmeans A;
lsmeans A / at means;
lsmeans A / at x1=1.2;
lsmeans A / at (x1 x2)=(1.2 0.3);
```

For the first two LSMEANS statements, the LS-means coefficient for x_1 is \bar{x}_1 (the mean of x_1) and for x_2 is \bar{x}_2 (the mean of x_2). However, for the first LSMEANS statement, the coefficient for x_1*x_2 is $\bar{x}_1\bar{x}_2$, but for the second LSMEANS statement, the coefficient is $\bar{x}_1 \times \bar{x}_2$. The third LSMEANS statement sets the coefficient for x_1 equal to 1.2 and leaves it at \bar{x}_2 for x_2 , and the final LSMEANS statement sets these values to 1.2 and 0.3, respectively.

Even if you specify a WEIGHT variable, the unweighted covariate means are used for the covariate coefficients if there is no AT specification. If you specify the AT option, WEIGHT or FREQ variables are taken into account as follows. The weighted covariate means are then used for the covariate coefficients for which no explicit AT values are given, or if you specify AT MEANS. Observations that do not contribute to the analysis because of a missing dependent variable are included in computing the covariate means. Use the E option in conjunction with the AT option to check that the modified LS-means coefficients are the ones you want.

The AT option is disabled if you specify the BYLEVEL option.

BYLEVEL

requests that separate margins be computed for each level of the LSMEANS effect.

The standard LS-means have equal coefficients across classification effects. The BYLEVEL option changes these coefficients to be proportional to the observed margins. This adjustment is reasonable when you want your inferences to apply to a population that is not necessarily balanced but has the margins observed in the input data set. In this case, the resulting LS-means are actually equal to raw means for fixed-effects models and certain balanced random-effects models, but their estimated standard errors account for the covariance structure that you have specified. If a WEIGHT statement is specified, the procedure uses weighted margins to construct the LS-means coefficients.

If the AT option is specified, the BYLEVEL option disables it.

CL

requests that t type confidence limits be constructed for each of the LS-means. The confidence level is 0.95 by default; this can be changed with the ALPHA= option. If you specify an ADJUST= option, then the confidence limits are adjusted for multiplicity. But if you also specify STEPDOWN, then only p -values are step-down adjusted, not the confidence limits.

CORR

displays the estimated correlation matrix of the least squares means as part of the “Least Squares Means” table.

COV

displays the estimated covariance matrix of the least squares means as part of the “Least Squares Means” table.

DF=number

specifies the degrees of freedom for the t test and confidence limits. The default is the denominator degrees of freedom taken from the “Type III Tests” table that corresponds to the LS-means effect. The option is not supported by the procedures that perform chi-square-based inference (GENMOD, LOGISTIC, PHREG and SURVEYLOGISTIC).

DIFF<=difftype>**PDIF<=difftype>**

requests that differences of the LS-means be displayed. You can use one of the following optional *difftype* values to specify which differences to produce:

ALL

requests all pairwise differences; this is the default.

ANOM

requests differences between each LS-mean and the average LS-mean, as in the *analysis of means* (Ott 1967). The average is computed as a weighted mean of the LS-means, the weights being inversely proportional to the diagonal entries of the $\mathbf{L}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{L}'$ matrix. If LS-means are nonestimable, this design-based weighted mean is replaced with an equally weighted mean. Note that the ANOM procedure in SAS/QC software implements both tables and graphics for the analysis of means with a variety of response types. For one-way designs and normal data with identity link, the DIFF=ANOM computations are equivalent to the results of PROC ANOM. If the LS-means being compared are uncorrelated, exact adjusted p -values and critical values for confidence limits can be computed in the analysis of means; see Nelson (1982, 1991, 1993) and Guirguis and Tobias (2004) in addition to the documentation for the ADJUST=NELSON option.

CONTROL

requests differences with a control, which, by default, is the first valid level of each of the specified LSMEANS effects. For example, suppose the effects A and B are classification variables, both of them have two levels 1 and 2, and the A=1, B=1 cell is missing. Unless the procedure supports a MISSING option in the CLASS statement and the option is in effect, the following LSMEANS statement uses the level (1,2) of A*B as the control:

```
lsmeans A*B / diff=control;
```

Nevertheless, you can still specify a valid level as the control—for example, (2,1) of A*B. To specify which levels of the effects are the controls, list the quoted formatted values in parentheses after the CONTROL keyword. For example, if the effects A, B, and C are classification variables, each having two levels, 1 and 2, the following LSMEANS statement specifies the (1,2) level of A*B and the (2,1) level of B*C as controls:

```
lsmeans A*B B*C / diff=control('1' '2' '2' '1');
```

For multiple effects, the results depend upon the order of the list, and so you should check the output to make sure that the controls are correct.

Two-tailed tests and confidence limits are associated with the CONTROL *difftype*. For one-tailed results, use either the CONTROLL or CONTROLU *difftype*.

CONTROLL

tests whether the noncontrol levels are significantly smaller than the control; the upper confidence limits for the control minus the noncontrol levels are considered to be infinity and are displayed as missing.

CONTROLU

tests whether the noncontrol levels are significantly larger than the control; the upper confidence limits for the noncontrol levels minus the control are considered to be infinity and are displayed as missing.

If you want to perform multiple comparison adjustments on the differences of LS-means, you must specify the **ADJUST=** option.

The differences of the LS-means are displayed in a table titled “Differences of Least Squares Means.”

E

requests that the **L** matrix coefficients for the LSMEANS effects be displayed.

EXP

requests exponentiation of the LS-means or LS-mean differences. When you model data with the logit, cumulative logit, or generalized logit link functions, and the estimate represents a log odds ratio or log cumulative odds ratio, the **EXP** option produces an odds ratio. In proportional hazards model, the exponentiation of the LS-mean differences produces estimates of hazard ratios. If you specify the **CL** or **ALPHA=** option, the (adjusted) confidence bounds are also exponentiated.

The **EXP** option is supported only by PROC PHREG, PROC SURVEYPHREG, the procedures that support generalized linear modeling (GENMOD, LOGISTIC, and SURVEYLOGISTIC), and PROC PLM when it is used to perform statistical analyses on item stores that are created by these procedures.

ILINK

requests that estimates and their standard errors in the “Least Squares Means” table also be reported on the scale of the mean (the inverse linked scale). This enables you to obtain estimates of predicted probabilities and their standard errors in logistic models, for example. The option is specific to an LSMEANS statement. If you also specify the **CL** option, the procedure computes confidence intervals for the predicted means by applying the inverse link transform to the confidence limits on the linked (linear) scale. Standard errors on the inverse linked scale are computed by the delta method.

The **ILINK** option is supported only by the procedures that support generalized linear modeling (GENMOD, LOGISTIC and SURVEYLOGISTIC) and by PROC PLM when it is used to perform statistical analyses on item stores that are created by these procedures.

LINES

presents results of comparisons between all pairs of least squares means by listing the means in descending order and indicating nonsignificant subsets by line segments beside the corresponding LS-means. When all differences have the same variance, these comparison lines are guaranteed to accurately reflect the inferences that are based on the corresponding tests, which are made by comparing the respective *p*-values to the value of the **ALPHA=** option (0.05 by default). However, equal variances might not be the case for differences between LS-means. If the variances are not all the same, then the comparison lines might be conservative, in the sense that if you base your inferences on the lines alone, you will detect fewer significant differences than the tests indicate. If there are any such differences, the procedure lists the pairs of means that are inferred to be significantly different

by the tests but not by the comparison lines. However, even though the variances in many cases are unequal, they are similar enough that the comparison lines accurately reflect the test inferences.

MEANS | NOMEANS

determines whether to print the least squares means themselves. For most procedure, MEANS is the default behavior. For example, the NOMEANS option is the default for the PHREG procedure. You can then use the MEANS option to produce the table of least squares means, if desired.

ODDSRATIO

OR

requests that LS-mean differences (**DIFF**, **ADJUST=** options) are also reported in terms of odds ratios. The ODDSRATIO option is ignored unless you use either the logit, cumulative logit, or generalized logit link function. If you specify the **CL** or **ALPHA=** option, confidence intervals for the odds ratios are also computed. These intervals are adjusted for multiplicity when you specify the **ADJUST=** option.

The ODDSRATIO option is supported only by the procedures that support generalized linear modeling (GENMOD, LOGISTIC and SURVEYLOGISTIC) and by PROC PLM when it is used to perform statistical analyses on item stores created by these procedures.

OBSMARGINS< =OM-data-set >

OM< =OM-data-set >

specifies a potentially different weighting scheme for the computation of LS-means coefficients. The standard LS-means have equal coefficients across classification effects; however, the OM option changes these coefficients to be proportional to those found in the *OM-data-set*. This adjustment is reasonable when you want your inferences to apply to a population that is not necessarily balanced but has the margins that are observed in *OM-data-set*.

By default, *OM-data-set* is the same as the analysis data set. You can optionally specify another data set that describes the population for which you want to make inferences. This data set must contain all model variables except for the dependent variable (which is ignored if it is present). In addition, the levels of all CLASS variables must be the same as those that occur in the analysis data set. If a level of a classification effect in the original data set is not present in the *OM-data-set*, the LS-means for that level are undefined. The corresponding rows of the LSMeans table are displayed as missing. Specifying an *OM-data-set* enables you to construct arbitrarily weighted LS-means.

In computing the observed margins, the procedure uses all observations for which there are no missing or invalid independent variables, including those for which there are missing dependent variables. Also, if you use a WEIGHT statement, the procedure computes weighted margins to construct the LS-means coefficients. If your data are balanced, the LS-means are unchanged by the OM option.

The **BYLEVEL** option modifies the observed-margins LS-means. Instead of computing the margins across all of the *OM-data-set*, the procedure computes separate margins for each level of the LSMEANS effect in question. In this case the resulting LS-means are actually equal to raw means for fixed-effects models and certain balanced random-effects models, but their estimated standard errors account for the covariance structure that you have specified.

You can use the **E** option in conjunction with either the OM or **BYLEVEL** option to verify that the modified LS-means coefficients are the ones you want. It is possible that the modified LS-means are not estimable when the standard ones are estimable, or vice versa.

PDIFF

is the same as the **DIFF** option.

PLOT | PLOTS<=*plot-request*< (*options*) >>**PLOT | PLOTS**<=*(plot-request*< (*options*)> <...*plot-request*< (*options*)> >)>

requests that graphics related to least squares means be produced via ODS Graphics, provided that ODS Graphics is enabled and the *plot-request* does not conflict with other options in the LSMEANS statement. For general information about ODS Graphics, see Chapter 21, “Statistical Graphics Using ODS.”

The available options and suboptions are as follows:

ALL

requests that the default plots that correspond to this LSMEANS statement be produced. The default plot depends on the options in the statement.

ANOMPLOT**ANOM**

requests an analysis-of-means display in which least squares means are compared to an average least squares mean. Least squares mean ANOM plots are produced only for those model effects that are listed in LSMEANS statements and have options that do not contradict with the display. For example, the following statements produce analysis-of-mean plots for effects A and C:

```
lsmeans A / diff=anom plot=anom;
lsmeans B / diff      plot=anom;
lsmeans C /          plot=anom;
```

The **DIFF** option in the second LSMEANS statement implies all pairwise differences.

BOXPLOT< *boxplot-options* >

produces box plots of the distribution of the least squares mean or least squares mean differences across a posterior sample. For example, this plot is available in procedures that support a Bayesian analysis through the BAYES statement.

A separate box is generated for each estimable function, and all boxes appear on a single graph by default. You can affect the appearance of the box plot graph with the following options:

ORIENTATION=VERTICAL | HORIZONTAL**ORIENT=VERT | HORIZ**

specifies the orientation of the boxes. The default is vertical orientation of the box plots.

NPANELPOS=*number*

specifies how to break the series of box plots across multiple panels. If the NPANELPOS option is not specified, or if *number* equals zero, then all box plots are displayed in a single graph; this is the default. If a negative number is specified, then exactly up to $|number|$ of box plots are displayed per panel. If *number* is positive, then the number of boxes per panel is balanced to achieve small variation in the number of box plots per graph.

CONTROLPLOT**CONTROL**

requests a display in which least squares means are visually compared against a reference level. These plots are produced only for statements with options that are compatible with control differences. For example, the following statements produce control plots for effects A and C:

```
lsmeans A / diff=control('1') plot=control;
lsmeans B / diff                plot=control;
lsmeans C                      plot=control;
```

The **DIFF** option in the second LSMEANS statement implies all pairwise differences.

DIFFPLOT<(diffplot-options)>

DIFFOGRAM<(diffplot-options)>

DIFF<(diffplot-options)>

requests a display of all pairwise least squares mean differences and their significance. The display is also known as a “mean-mean scatter plot” when it is based on arithmetic means (Hsu 1996; Hsu and Peruggia 1994). For each comparison a line segment, centered at the LS-means in the pair, is drawn. The length of the segment corresponds to the projected width of a confidence interval for the least squares mean difference. Segments that fail to cross the 45-degree reference line correspond to significant least squares mean differences.

LS-mean difference plots are produced only for statements with options that are compatible with the display. For example, the following statements request differences against a control level for the A effect, all pairwise differences for the B effect, and the least squares means for the C effect:

```
lsmeans A / diff=control('1') plot=diff;
lsmeans B / diff                plot=diff;
lsmeans C                      plot=diff;
```

The **DIFF=** type in the first statement is incompatible with a display of all pairwise differences.

You can specify the following *diffplot-options*:

ABS

determines the positioning of the line segments in the plot. This is the default *diffplot-options*. When the ABS option is in effect, all line segments are shown on the same side of the reference line.

NOABS

determines the positioning of the line segments in the plot. The NOABS option separates comparisons according to the sign of the difference.

CENTER

marks the center point for each comparison. This point corresponds to the intersection of two least squares means.

NOLINES

suppresses the display of the line segments that represent the confidence bounds for the differences of the least squares means. The NOLINES option implies the CENTER option. The default is to draw line segments in the upper portion of the plot area without marking the center point.

DISTPLOT< *distplot-options* >**DIST**< *distplot-options* >

generates panels of histograms with a kernel density overlaid if the analysis has access to a set of posterior parameter estimates. For example, this plot is available in procedures that support a Bayesian analysis through the BAYES statement. A separate plot in each panel contains the results for each least squares mean or least squares mean differences. You can specify the following *distplot-options* in parentheses:

BOX | NOBOX

controls the display of a horizontal box plot of the estimable function's distribution across the posterior sample below the graph. The BOX option is enabled by default.

HIST | NOHIST

controls the display of the histogram of the estimable function's distribution across the posterior sample. The HIST option is enabled by default.

NORMAL | NONORMAL

controls the display of a normal density estimate on the graph. The NONORMAL option is enabled by default.

KERNEL | NOKERNEL

controls the display of a kernel density estimate on the graph. The KERNEL option is enabled by default.

NROWS=*number*

specifies the highest number of rows in a panel. The default is 3.

NCOLS=*number*

specifies the highest number of columns in a panel. The default is 3.

UNPACK

unpacks the panel into separate graphics.

MEANPLOT< (*meanplot-options*) >

requests displays of the least squares means.

The following *meanplot-options* control the display of the least squares means.

ASCENDING

displays the least squares means in ascending order. This option has no effect if means are displayed in separate plots.

CL

displays upper and lower confidence limits for the least squares means. By default, 95% limits are drawn. You can change the confidence level with the ALPHA= option. Confidence limits are drawn by default if the CL option is specified in the LSMEANS statement.

CLBAND

displays confidence limits as bands. This option implies the JOIN option.

DESCENDING

displays the least squares means in descending order. This option has no effect if means are displayed in separate plots.

ILINK

requests that means (and confidence limits) be displayed on the inverse linked scale.

JOIN**CONNECT**

connects the least squares means with lines. This option is implied by the CLBAND option. If the effect contains nested variables and a SLICEBY= effect contains classification variables that appear as crossed effects, this option is ignored.

SLICEBY=*fixed-effect*

specifies an effect by which to group the means in a single plot. For example, the following statement requests a plot in which the levels of A are placed on the horizontal axis and the means that belong to the same level of B are joined by lines:

```
lsmeans A*B / plot=meanplot(sliceby=b join);
```

Unless the LS-mean effect contains at least two classification variables, the SLICEBY= option has no effect. The *fixed-effect* does not have to be an effect in your MODEL statement, but it must consist entirely of classification variables and it must be contained in the LS-mean effect.

PLOTBY=*fixed-effect*

specifies an effect by which to break interaction plots into separate displays. For example, the following statement requests for each level of C one plot of the A*B cell means that are associated with that level of C:

```
lsmeans A*B*C / plot=meanplot(sliceby=b plotby=c clband);
```

In each plot, levels of A are displayed on the horizontal axis, and confidence bands are drawn around the means that share the same level of B.

The PLOTBY= option has no effect unless the LS-mean effect contains at least three classification variables. The *fixed-effect* does not have to be an effect in the MODEL statement, but it must consist entirely of classification variables and it must be contained in the LS-mean effect.

NONE

requests that no plots be produced.

When LS-mean calculations are adjusted for multiplicity by using the ADJUST= option, the plots are adjusted accordingly.

SEED=*number*

specifies the seed for the sampling-based components of the computations for the LSMEANS statement (for example, chi-bar-square statistics and simulated *p*-values). The value of *number* must be an integer. The seed is used to start the pseudo-random-number generator for the simulation. If you do not specify a seed, or if you specify a value less than or equal to zero, the seed is generated

from reading the time of day from the computer clock. Note that there could be multiple LSMEANS statements with SEED= specifications and there could be other statements that can supply a random number seed. Since the procedure has only one random number stream, the initial seed is shown in the SAS log.

SINGULAR=number

tunes the estimability checking. If \mathbf{v} is a vector, define $\text{ABS}(\mathbf{v})$ to be the largest absolute value of the elements of \mathbf{v} . If $\text{ABS}(\mathbf{K}' - \mathbf{K}'\mathbf{T})$ is greater than $c*\text{number}$ for any row of \mathbf{K}' in the contrast, then $\mathbf{K}'\boldsymbol{\beta}$ is declared nonestimable. Here, \mathbf{T} is the Hermite form matrix $(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{X}$, and c is $\text{ABS}(\mathbf{K}')$, except when it equals 0, and then c is 1. The value for *number* must be between 0 and 1; the default is 1E-4.

STEPDOWN<(step-down-options)>

requests that multiple comparison adjustments for the p -values of LS-mean differences be further adjusted in a step-down fashion. Step-down methods increase the power of multiple comparisons by taking advantage of the fact that a p -value is never declared significant unless all smaller p -values are also declared significant. The STEPDOWN adjustment combined with ADJUST=BON corresponds to the methods of Holm (1979) “Method 2” of Shaffer (1986); this is the default. Using step-down-adjusted p -values combined with ADJUST=SIMULATE corresponds to the method of Westfall (1997).

If the denominator degrees of freedom are computed by the Kenward-Roger (Kenward and Roger 1997) or Satterthwaite method in a mixed model, then step-down-adjusted p -values are produced only if the ADJDFE=ROW option is in effect.

Also, STEPDOWN affects only p -values, not confidence limits. For ADJUST=SIMULATE, the generalized least squares hybrid approach of Westfall (1997) is used to increase Monte Carlo accuracy.

You can specify the following *step-down-options* in parentheses:

MAXTIME=n

specifies the time (in seconds) to be spent computing the maximal logically consistent sequential subsets of equality hypotheses for TYPE=LOGICAL. The default is MAXTIME=60. If the MAXTIME value is exceeded, the adjusted tests are not computed. When this occurs, you can try increasing the MAXTIME value. However, note that there are common multiple comparisons problems for which this computation requires a huge amount of time—for example, all pairwise comparisons between more than 10 groups. In such cases, try to use TYPE=FREE (the default) or TYPE=LOGICAL(n) for small n .

REPORT

specifies that a report on the step-down adjustment be displayed, including a listing of the sequential subsets (Westfall 1997) and, for ADJUST=SIMULATE, the step-down simulation results.

TYPE=LOGICAL<(n)>

TYPE=FREE

specifies how step-down adjustment are made. If you specify TYPE=LOGICAL, the step-down adjustments are computed by using maximal logically consistent sequential subsets of equality hypotheses (Shaffer 1986; Westfall 1997). Alternatively, for TYPE=FREE, sequential subsets are computed ignoring logical constraints. The TYPE=FREE results are more conservative than those for TYPE=LOGICAL, but they can be much more efficient to produce for many

comparisons. For example, it is not feasible to take logical constraints between all pairwise comparisons of more than 10 groups. For this reason, `TYPE=FREE` is the default.

However, you can reduce the computational complexity of taking logical constraints into account by limiting the depth of the search tree used to compute them, specifying the optional depth parameter as a number n in parentheses after `TYPE=LOGICAL`. As with `TYPE=FREE`, results for `TYPE=LOGICAL(n)` are conservative relative to the true `TYPE=LOGICAL` results. But even for `TYPE=LOGICAL(0)` they can be appreciably less conservative than `TYPE=FREE`, and they are computationally feasible for much larger numbers of comparisons. If you do not specify n or if $n = -1$, the full search tree is used.

ODS Table Names: LSMEANS Statement

Each table created by the `LSMEANS` statement has a name associated with it, and you can use this name to refer to the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in Table 19.22. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

Table 19.22 ODS Tables Produced by the `LSMEANS` statement

Table Name	Description	Required Option
Coef	L matrix coefficients	E
Diffs	Differences of LS-means	DIFF or ADJUST= or STEPDOWN
LSMeans	LS-means	Default
LSMLines	Lines display for LS-means	LINES

ODS Graphics: LSMEANS Statement

This section describes the use of ODS Graphics for creating graphics that are related to LS-means in procedures that support the common `LSMEANS` or `SLICE` statement. There are two groups of available plots: those that can be produced by all procedures that support these two statements, and those that can be produced only in association with the three procedures that can perform Bayesian analysis (`PROC GENMOD`, `PROC LIFEREG`, and `PROC PHREG`). Plots that are associated with the Bayesian analysis are available via these procedures directly, and also by using `PROC PLM` with an item store that was created by these procedures.

Plots in the first group depict the LS-means and their differences; when LS-mean comparisons are adjusted for multiplicity by using the `ADJUST=` option, the plots are adjusted accordingly. To request plots in this group, ODS Graphics must be enabled and you must request plots with the appropriate `PLOTS=` option in the `LSMEANS` or `SLICE` statement. Plots in the second group depict the posterior sample distribution of LS-means and their differences. To request plots in this group, you must also use a `BAYES` statement with `PROC GENMOD`, `PROC PHREG`, or `PROC LIFEREG`, or you must use `PROC PLM` to perform statistical analysis on an item store that was saved from a Bayesian analysis.

For more information about ODS Graphics, see Chapter 21, “Statistical Graphics Using ODS.” The available graphs are summarized in [Table 19.23](#) and [Table 19.24](#).

Table 19.23 Graphs Produced by All Procedures That Support the Common LSMEANS or SLICE Statement

ODS Graph Name	Plot Description	Required Option
AnomPlot	Requests an analysis of means display in which least squares means are compared to an average least squares mean.	PLOTS=ANOM
ControlPlot	Requests a display in which least squares means are compared to a reference level.	PLOTS=CONTROL
DiffPlot	Displays all pairwise least squares mean differences and their significance. This plot is also known as a “mean-mean scatter plot” when based on arithmetic means.	PLOTS=DIFF
MeanPlot	Displays least squares means.	PLOTS=MEANPLOT

Table 19.24 Graphs Produced by Procedures That Support the LSMEANS or SLICE Statement and Bayesian Analysis

ODS Graph Name	Plot Description	Required Option
BoxPlot	Displays box plots of LS-means or LS-mean differences across a posterior sample.	PLOTS=BOXPLOT
DistPanel	Displays panels of histograms with kernel density curves overlaid. Each plot contains the results for the posterior sample of each LS-mean or LS-mean difference.	PLOTS=DISTPLOT
DistPlot	Displays a histogram with a kernel density curve overlaid. The plot contains the results for the posterior sample of the LS-mean or LS-mean difference.	PLOTS=DISTPLOT(UNPACK)

You can supply the same *plot-options* to the SLICE statement to produce these graphs. For details about the *plot-options* of the LSMEANS or SLICE statement, see the PLOTS= option in the section “LSMEANS Statement” on page 453. For more details about the DIFFPLOT in particular, see the section “Graphics for LS-Mean Comparisons” on page 3122 in Chapter 41, “The GLIMMIX Procedure.”

LSMESTIMATE Statement

This statement documentation applies to the following SAS/STAT procedures: GENMOD, LIFEREG, LOGISTIC, MIXED, ORTHOREG, PHREG, PLM, PROBIT, SURVEYLOGISTIC, SURVEYPHREG, and SURVEYREG. It also applies to the RELIABILITY procedure in SAS/QC software. The LSMESTIMATE statement in the GLIMMIX procedure is documented in Chapter 41, “The GLIMMIX Procedure.”

The LSMESTIMATE statement provides a mechanism for obtaining custom hypothesis tests among least squares means. In contrast to the LSMEANS statement, the LSMESTIMATE statement does not produce the least squares means or their differences; instead, you can estimate any linear function of the least squares means (including the means themselves or their differences). In contrast to the linear functions that are constructed with the ESTIMATE statement, you do not specify coefficients for the individual parameter estimates. Instead, with the LSMESTIMATE statement you specify coefficients for the least squares means; these are then converted for you into estimable functions for the parameter estimates.

The LSMESTIMATE statement thus combines important and convenient features of the LSMEANS and the ESTIMATE statement. As with the LSMEANS statement, the following conditions are true:

- You need to specify only a single effect; the mapping into linear estimable functions in terms of the parameter estimates is performed by the procedure.
- You can use the AT=, BYLEVEL, and OBSMARGINS options to affect the computation of the underlying least squares means.

As with the ESTIMATE statement you can do the following:

- specify multiple-row linear combinations.
- perform multiplicity corrections to control the familywise Type I error probability with the ADJUST= option.
- construct general linear functions of the least squares means.
- perform joint F or chi-square tests with or without order restrictions through the JOINT option.
- rely on positional or nonpositional syntax to specify coefficients for linear functions. For details about using nonpositional syntax, see the section “Positional and Nonpositional Syntax for Coefficients in Linear Functions” on page 448.

The computation of an LSMESTIMATE involves two coefficient matrices. Suppose that there are n_l levels for a valid least squares means effect (an effect that is part of your model and consists of classification variables only). Then the LS-means are formed as $\mathbf{L}_1 \hat{\boldsymbol{\beta}}$, where \mathbf{L}_1 is a $(n_l \times p)$ coefficient matrix. The $(k \times n_l)$ coefficient matrix \mathbf{K} is formed from the *values* that you supply in the k rows of the LSMESTIMATE statement. The least squares means estimates then represent the $(k \times 1)$ vector

$$\mathbf{KL}_1\boldsymbol{\beta} = \mathbf{L}\boldsymbol{\beta}$$

Because the analytic features and capabilities of the LSMESTIMATE statement are an amalgam of the LSMEANS and the ESTIMATE statement, the syntax of the statement follows the same pattern.

Syntax: LSMESTIMATE Statement

```
LSMESTIMATE model-effect <'label'> values <divisor=n>
            <,<'label'> values <divisor=n>> <,&hellip;>
            </options>;
```

In contrast to a multirow estimate in the ESTIMATE statement, you specify only a single effect in the LSMESTIMATE statement. The row labels are optional and follow the *model-effect* specification. For example, the following statements fit a split-split-plot design and compare the average of the third and fourth LS-mean of the whole-plot factor A to the first LS-mean of the factor:

```
proc glimmix;
  class a b block;
  model y = a b a*b / s;
  random int a / sub=block;
  lsmestimate A 'a1 vs avg(a3,a4)' 2 0 -1 -1 divisor=2;
run;
```

The order in which coefficients are assigned to the least squares means corresponds to the order in which they are displayed in the “Least Squares Means” table. You can use the ELSM option to see how coefficients are matched to levels of the fixed effect.

The optional *divisor=n* specification enables you to assign a separate divisor to each row of the LSMESTIMATE. You can also assign divisor values through the DIVISOR= option. See the description of the DIVISOR= option that follows for the interaction between the two ways of specifying divisors.

Table 19.25 summarizes important options in the LSMESTIMATE statement. All LSMESTIMATE options are subsequently discussed in alphabetical order.

Table 19.25 LSMESTIMATE Statement Options

Option	Description
Construction and Computation of LS-Means	
AT	Modifies covariate values in computing LS-means
BYLEVEL	Computes separate margins
DIVISOR=	Specifies a list of values to divide the coefficients
OM=	Specifies the weighting scheme for LS-means computation as determined by a data set
SINGULAR=	Tunes estimability checking

Table 19.25 *continued*

Option	Description
Degrees of Freedom and p-values	
ADJUST=	Determines the method for multiple-comparison adjustment of LS-means differences
ALPHA= α	Determines the confidence level ($1 - \alpha$)
LOWER	Performs one-sided, lower-tailed inference
STEPDOWN	Adjusts multiple-comparison p -values further in a step-down fashion
TESTVALUE=	Specifies values under the null hypothesis for tests
UPPER	Performs one-sided, upper-tailed inference
Statistical Output	
CL	Constructs confidence limits for means and mean differences
CORR	Displays the correlation matrix of LS-means
COV	Displays the covariance matrix of LS-means
E	Prints the L matrix
ELSM	Prints the K matrix
JOINT	Produces a joint F or chi-square test for the LS-means and LS-means differences
PLOTS=	Requests graphs of means and mean comparisons
SEED=	Specifies the seed for computations that depend on random numbers
Generalized Linear Modeling	
CATEGORY=	Specifies how to construct estimable functions with multinomial data
EXP	Exponentiates and displays LS-means estimates
ILINK	Computes and displays estimates and standard errors of LS-means (but not differences) on the inverse linked scale

You can specify the following options in the LSMESTIMATE statement after a slash (/):

ADJDFE=SOURCE**ADJDFE=ROW**

specifies how denominator degrees of freedom are determined when p -values and confidence limits are adjusted for multiple comparisons with the **ADJUST=** option. When you do not specify the **ADJDFE=** option or when you specify **ADJDFE=SOURCE**, the denominator degrees of freedom for multiplicity-adjusted results are the denominator degrees of freedom for the LS-mean effect in the “Type III Tests of Fixed Effects” table.

The **ADJDFE=ROW** setting is useful if you want multiplicity adjustments to take into account that denominator degrees of freedom are not constant across estimates. For example, this can be the case when the denominator degrees of freedom are computed by the Satterthwaite or Kenward-Roger method (Kenward and Roger 1997) in a mixed model.

The ADJDFE= option is not supported by the procedures that perform chi-square-based inference (GENMOD, LOGISTIC, PHREG and SURVEYLOGISTIC).

ADJUST=BON**ADJUST=SCHEFFE****ADJUST=SIDAK****ADJUST=SIMULATE**< (*simoptions*) >**ADJUST=T**

requests a multiple comparison adjustment for the p -values and confidence limits for the LS-mean estimates. The adjusted quantities are produced in addition to the unadjusted p -values and confidence limits. Adjusted confidence limits are produced if the CL or ALPHA= option is in effect. For a description of the adjustments, see Chapter 42, “The GLM Procedure,” and Chapter 61, “The MULTTEST Procedure,” in addition to the documentation for the ADJUST= option in the LSMEANS statement.

Not all adjustment methods of the LSMEANS statement are available for the LSMESTIMATE statement. Multiplicity adjustments in the LSMEANS statement are designed specifically for differences of least squares means.

If you specify the STEPDOWN option, the p -values are further adjusted in a step-down fashion.

ALPHA=number

requests that a t type confidence interval be constructed for each of the LS-means with confidence level $1 - \text{number}$. The value of *number* must be between 0 and 1; the default is 0.05.

AT variable=value**AT (variable-list)=(value-list)****AT MEANS**

modifies the values of the covariates used in computing LS-means. See the AT option in the LSMEANS statement for details.

BYLEVEL

requests that the procedure compute separate margins for each level of the LSMEANS effect.

The standard LS-means have equal coefficients across classification effects. The BYLEVEL option changes these coefficients to be proportional to the observed margins. This adjustment is reasonable when you want your inferences to apply to a population that is not necessarily balanced but has the margins observed in the input data set. In this case, the resulting LS-means are actually equal to raw means for fixed-effects models and certain balanced random-effects models, but their estimated standard errors account for the covariance structure that you have specified. If a WEIGHT statement is specified, the procedure uses weighted margins to construct the LS-means coefficients.

If the AT option is specified, the BYLEVEL option disables it.

CATEGORY=category-options

specifies how to construct estimates and multiplicity corrections for models with multinomial data (ordinal or nominal). This option is also important for constructing sets of estimable functions for F tests with the JOINT option.

The *category-options* indicate how response variable levels are treated in constructing the estimable functions. Possible value for the *category-options* are the following:

JOINT

computes the estimable functions for every nonredundant category and treats them as a set. For example, a three-row LSMESTIMATE statement in a model with three response categories leads to six estimable functions.

SEPARATE

computes the estimable functions for every nonredundant category in turn. For example, a three-row LSMESTIMATE statement in a model with three response categories leads to two sets of three estimable functions.

quoted-value-list

computes the estimable functions only for the list of values given. The list must consist of formatted values of the response categories.

For further details about using the `CATEGORY=` option in models for multinomial data, see the documentation for the `CATEGORY=` option in the `ESTIMATE` statement.

The `CATEGORY=` option is supported only by the procedures that support generalized linear modeling (`GENMOD`, `LOGISTIC`, and `SURVEYLOGISTIC`) and by `PROC PLM` when it is used to perform statistical analyses on item stores that were created by these procedures.

CHISQ

requests that chi-square tests be performed in addition to F tests, when you request an F test with the `JOINT` option. This option has no effect in procedures that produce chi-square statistics by default.

CL

requests that t type confidence limits be constructed for each of the LS-means. The confidence level is 0.95 by default; this can be changed with the `ALPHA=` option. If you specify an `ADJUST=` option, then the confidence limits are adjusted for multiplicity. But if you also specify `STEPDOWN`, then only p -values are step-down adjusted, not the confidence limits.

CORR

displays the estimated correlation matrix of the linear combination of the least squares means.

COV

displays the estimated covariance matrix of the linear combination of the least squares means.

DF=number

specifies the degrees of freedom for the tests and confidence limits. The option is not supported by the procedures that perform chi-square-based inference (`GENMOD`, `LOGISTIC`, `PHREG`, and `SURVEYLOGISTIC`).

DIVISOR=value-list

specifies a list of values by which to divide the coefficients so that fractional coefficients can be entered as integer numerators. If you do not specify *value-list*, a default value of 1.0 is assumed. Missing values in the *value-list* are converted to 1.0.

If the number of elements in *value-list* exceeds the number of rows of the estimate, the extra values are ignored. If the number of elements in *value-list* is less than the number of rows of the estimate, the last value in *value-list* is carried forward.

If you specify a row-specific divisor as part of the specification of the estimate row, this value multiplies the corresponding value in the *value-list*. For example, the following statement divides the coefficients in the first row by 8, and the coefficients in the third and fourth row by 3:

```

lsmestimate A 'One vs. two' 8 -8 divisor=2,
              'One vs. three' 1 0 -1
              'One vs. four' 3 0 0 -3
              'One vs. five' 3 0 0 0 -3 / divisor=4,.,3;

```

Coefficients in the second row are not altered.

E

requests that the **L** coefficients of the estimable function be displayed. These are the coefficients that apply to the fixed-effect parameter estimates. The E option displays the coefficients that you would need to enter in an equivalent **ESTIMATE** statement.

ELSM

requests that the **K** matrix coefficients be displayed. These are the coefficients that apply to the LS-means. This option is useful to ensure that you assigned the coefficients correctly to the LS-means.

EXP

requests exponentiation of the least squares means estimate. When you model data with the logit link function and the estimate represents a log odds ratio, the EXP option produces an odds ratio. If you specify the **CL** or **ALPHA=** option, the (adjusted) confidence limits for the estimate are also exponentiated.

The EXP option is supported only by PROC PHREG, PROC SURVEYPHREG, the procedures that support generalized linear modeling (GENMOD, LOGISTIC, and SURVEYLOGISTIC), and by PROC PLM when it is used to perform statistical analyses on item stores that were created by these procedures.

ILINK

requests that the estimate and its standard error also be reported on the scale of the mean (the inverse linked scale). The computation of the inverse linked estimate depends on the estimation mode. For example, if the analysis is based on a posterior sample when a BAYES statement is present, the inversely linked estimate is the average of the inversely linked values across the sample of posterior parameter estimates. If the analysis is not based on a sample of parameter estimates, the procedure computes the value on the mean scale by applying the inverse link to the estimate.

The interpretation of the inversely linked quantity depends on the coefficients that are specified in your LSMESTIMATE statement and the link function. For example, in a model for binary data with logit link the following LSMESTIMATE statement computes

$$q = \frac{1}{1 + \exp\{-(\tau_1 - \tau_2)\}}$$

where τ_1 and τ_2 are the least squares means that are associated with the first two levels of the classification effect A:

```

proc logistic;
  class A / param=glm;
  model y = A / dist=binary link=logit;
  lsmestimate A 1 -1 / ilink;
run;

```

The quantity q is not the difference of the probabilities associated with the two levels,

$$\pi_1 - \pi_2 = \frac{1}{1 + \exp\{-\tau_1\}} - \frac{1}{1 + \exp\{-\tau_2\}}$$

The standard error of the inversely linked estimate is based on the delta method. If you also specify the **CL** or **ALPHA=** option, the procedure computes confidence intervals for the inversely linked estimate. These intervals are obtained by applying the inverse link to the confidence intervals on the linked scale.

The **ILINK** option is supported only by the procedures that support generalized linear modeling (**GENMOD**, **LOGISTIC**, and **SURVEYLOGISTIC**) and by **PROC PLM** when it is used to perform statistical analyses on item stores that were created by these procedures.

JOINT<(joint-test-options)>

requests that a joint F or chi-square test be produced for the rows of the estimate. For more information about the simulation-based p -value calculation, see the section “[Joint Hypothesis Tests with Complex Alternatives, the Chi-Bar-Square Statistic](#)” on page 451. You can specify the following *joint-test-options* in parentheses:

ACC= γ

specifies the accuracy radius for determining the necessary sample size in the simulation-based approach of Silvapulle and Sen (2004) for tests with order restrictions. The value of γ must be strictly between 0 and 1; the default value is 0.005.

EPS= ϵ

specifies the accuracy confidence level for determining the necessary sample size in the simulation-based approach of Silvapulle and Sen (2004) for F tests with order restrictions. The value of ϵ must be strictly between 0 and 1; the default value is 0.01.

LABEL=‘label’

assigns an identifying label to the joint test. If you do not specify a label, the first non-default label for the **ESTIMATE** rows is used to label the joint test.

NOEST

ONLY

performs only the joint test and suppresses other results from the **ESTIMATE** statement. This option is useful for emulating the **CONTRAST** statement that is available in other procedures.

NSAMP= n

specifies the number of samples for the simulation-based method of Silvapulle and Sen (2004). If n is not specified, it is constructed from the values of the **ALPHA**= α , the **ACC**= γ , and the **EPS**= ϵ options. With the default values for γ , ϵ , and α (0.005, 0.01, and 0.05, respectively), **NSAMP**=12,604 by default.

CHISQ

adds a chi-square test if the procedure produces an F test by default.

BOUNDS=value-list

specifies boundary values for the estimable linear function. The null value of the hypothesis is always zero. If you specify a positive boundary value z , the hypotheses are $H: \theta = 0$,

$H_a: \theta > 0$ with the added constraint that $\theta < z$. The same is true for negative boundary values. The alternative hypothesis is then $H_a: \theta < 0$ subject to the constraint $\theta > -|z|$. If you specify a missing value, the hypothesis is assumed to be two-sided. The BOUNDS option enables you to specify sets of one- and two-sided joint hypotheses. If all values in *value-list* are set to missing, the procedure performs a simulation-based *p*-value calculation for a two-sided test.

LOWER

LOWERTAILED

requests that the *p*-value for the *t* test be based only on values that are less than the test statistic. A two-tailed test is the default. A lower-tailed confidence limit is also produced if you specify the CL or ALPHA= option.

Note that for ADJUST=SCHEFFE the one-sided adjusted confidence intervals and one-sided adjusted *p*-values are the same as the corresponding two-sided statistics, because this adjustment is based on only the right tail of the *F* distribution.

If you request an *F* test with the JOINT option, then a one-sided left-tailed order restriction is applied to all estimable functions, and the corresponding chi-bar-square statistic of Silvapulle and Sen (2004) is computed in addition to the two-sided, standard, *F* or chi-square statistic. See the JOINT option for how to control the computation of the simulation-based chi-bar-square statistic.

OBSMARGINS< =OM-data-set >

OM< =OM-data-set >

specifies a potentially different weighting scheme for the computation of LS-means coefficients. The standard LS-means have equal coefficients across classification effects; however, the OM option changes these coefficients to be proportional to those found in the *OM-data-set*. This adjustment is reasonable when you want your inferences to apply to a population that is not necessarily balanced but has the margins observed in *OM-data-set*. See the OBSMARGINS option in the LSMEANS statement for further details.

PLOTS=*plot-options*

produces ODS statistical graphics of the distribution of estimable functions if the procedure performs the analysis in a sampling-based mode. For example, this is the case when procedures support a BAYES statement and perform a Bayesian analysis. The estimable functions are then computed for each of the posterior parameter estimates, and the “Least Squares Means Estimates” table reports simple descriptive statistics for the evaluated functions. In this situation, the PLOTS= option enables you to visualize the distribution of the estimable function. The following *plot-options* are available:

ALL

produces all possible plots with their default settings.

BOXPLOT< (*boxplot-options*) >

produces box plots of the distribution of the estimable function across the posterior sample. A separate box plot is generated for each estimable function and all box plots appear on a single graph by default. You can affect the appearance of the box plot graph with the following options:

ORIENTATION=VERTICAL | HORIZONTAL**ORIENT=VERT | HORIZ**

specifies the orientation of the boxes. The default is vertical orientation of the box plots.

NPANELPOS=*number*

specifies how to break the series of box plots across multiple panels. If the NPANELPOS option is not specified, or if *number* equals zero, then all box plots are displayed in a single graph; this is the default. If a negative number is specified, then exactly up to $|number|$ of box plots are displayed per panel. If *number* is positive, then the number of boxes per panel is balanced to achieve small variation in the number of box plots per graph.

DISTPLOT<(distplot-options)>**DIST<(distplot-options)>**

generates panels of histograms with a kernel density overlaid. A separate plot in each panel contains the results for each estimable function. You can specify the following *distplot-options* in parentheses:

BOX | NOBOX

controls the display of a horizontal box plot below the histogram. The BOX option is enabled by default.

HIST | NOHIST

controls the display of the histogram of the estimable function's distribution across the posterior sample. The HIST option is enabled by default.

NORMAL | NONORMAL

controls the display of a normal density estimate on the graph. The NONORMAL option is enabled by default.

KERNEL | NOKERNEL

controls the display of a kernel density estimate on the graph. The KERNEL option is enabled by default.

NROWS=*number*

specifies the highest number of rows in a panel. The default is 3.

NCOLS=*number*

specifies the highest number of columns in a panel. The default is 3.

UNPACK

unpacks the panel into separate graphics.

NONE

does not produce any plots.

SEED=*number*

specifies the seed for the sampling-based components of the computations for the LSMESTIMATE statement (for example, chi-bar-square statistics and simulated *p*-values). The value of *number* must be an integer. The seed is used to start the pseudo-random-number generator for the simulation. If you do not specify a seed, or if you specify a value less than or equal to zero, the seed is generated from

reading the time of day from the computer clock. Note that there could be multiple LSMESTIMATE statements with SEED= specifications and there could be other statements that can supply a random number seed. Since the procedure has only one random number stream, the initial seed is shown in the SAS log.

SINGULAR=number

tunes the estimability checking as documented for the SINGULAR= option in the ESTIMATE statement.

STEPDOWN<(step-down-options)>

requests that multiplicity adjustments for the p -values of estimable functions be further adjusted in a step-down fashion. Step-down methods increase the power of multiple testing procedures by taking advantage of the fact that a p -value is never declared significant unless all smaller p -values are also declared significant. The STEPDOWN adjustment combined with ADJUST=BON corresponds to the methods of Holm (1979) and “Method 2” of Shaffer (1986); this is the default. Using step-down-adjusted p -values combined with ADJUST=SIMULATE corresponds to the method of Westfall (1997).

If the ESTIMATE statement is applied with a STEPDOWN option in a mixed model where the degrees-of-freedom method is that of Kenward and Roger (1997) or of Satterthwaite, then step-down-adjusted p -values are produced only if the ADJDFE=ROW option is in effect.

Also, the STEPDOWN option affects only p -values, not confidence limits. For ADJUST=SIMULATE, the generalized least squares hybrid approach of Westfall (1997) is used to increase Monte Carlo accuracy.

You can specify the following *step-down-options* in parentheses:

MAXTIME= n

specifies the time (in seconds) to be spent computing the maximal logically consistent sequential subsets of equality hypotheses for TYPE=LOGICAL. The default is MAXTIME=60. If the MAXTIME value is exceeded, the adjusted tests are not computed. When this occurs, you can try increasing the MAXTIME value. However, note that there are common multiple comparisons problems for which this computation requires a huge amount of time—for example, all pairwise comparisons between more than 10 groups. In such cases, try to use TYPE=FREE (the default) or TYPE=LOGICAL(n) for small n .

ORDER=PVALUE

ORDER=ROWS

specifies the order in which the step-down tests are performed. ORDER=PVALUE is the default, with LS-mean estimates being declared significant only if all LS-mean estimates with smaller (unadjusted) p -values are significant. If you specify ORDER=ROWS, then significances are evaluated in the order in which they are specified.

REPORT

specifies that a report on the step-down adjustment be displayed, including a listing of the sequential subsets (Westfall 1997) and, for ADJUST=SIMULATE, the step-down simulation results.

TYPE=LOGICAL< (*n*) >**TYPE=FREE**

specifies how step-down adjustment are made. If you specify TYPE=LOGICAL, the step-down adjustments are computed by using maximal logically consistent sequential subsets of equality hypotheses (Shaffer 1986; Westfall 1997). Alternatively, for TYPE=FREE, sequential subsets are computed ignoring logical constraints. The TYPE=FREE results are more conservative than those for TYPE=LOGICAL, but they can be much more efficient to produce for many estimates. For example, it is not feasible to take logical constraints between all pairwise comparisons of more than about 10 groups. For this reason, TYPE=FREE is the default.

However, you can reduce the computational complexity of taking logical constraints into account by limiting the depth of the search tree used to compute them, specifying the optional depth parameter as a number *n* in parentheses after TYPE=LOGICAL. As with TYPE=FREE, results for TYPE=LOGICAL(*n*) are conservative relative to the true TYPE=LOGICAL results. But even for TYPE=LOGICAL(0), they can be appreciably less conservative than TYPE=FREE, and they are computationally feasible for much larger numbers of estimates. If you do not specify *n* or if *n* = -1, the full search tree is used.

TESTVALUE=*value-list***TESTMEAN=***value-list*

specifies the value under the null hypothesis for testing the estimable functions in the LSMESTIMATE statement. The rules for specifying the *value-list* are very similar to those for specifying the divisor list in the **DIVISOR=** option. If no TESTVALUE= is specified, all tests are performed as $H: \mathbf{L}\boldsymbol{\beta} = 0$. Missing values in the *value-list* also are translated to zeros. If you specify fewer values than rows in the LSMESTIMATE statement, the last value in *value-list* is carried forward.

The TESTVALUE= option affects only *p*-values from individual, joint, and multiplicity-adjusted tests. It does not affect confidence intervals.

The TESTVALUE option is not available for the multinomial distribution, and the values are ignored when you perform a sampling-based (Bayesian) analysis.

UPPER**UPPERTAILED**

requests that the *p*-value for the *t* test be based only on values that are greater than the test statistic. A two-tailed test is the default. An upper-tailed confidence limit is also produced if you specify the **CL** or **ALPHA=** option.

Note that for **ADJUST=SCHEFFE** the one-sided adjusted confidence intervals and one-sided adjusted *p*-values are the same as the corresponding two-sided statistics, because this adjustment is based on only the right tail of the *F* distribution.

If you request a joint test with the **JOINT** option, then a one-sided right-tailed order restriction is applied to all estimable functions, and the corresponding chi-bar-square statistic of Silvapulle and Sen (2004) is computed in addition to the two-sided, standard, *F* or chi-square statistic. See the **JOINT** option for how to control the computation of the simulation-based chi-bar-square statistic.

ODS Table Names: LSMESTIMATE Statement

Each table created by the `LSMESTIMATE` statement has a name associated with it, and you can use this name to refer to the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in [Table 19.26](#). For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

Table 19.26 ODS Tables Produced by the `LSMESTIMATE` statement

Table Name	Description	Required Option
Coef	L matrix coefficients or K matrix coefficients	E or ELSM
LSMEstimates	Estimates among LS-means	Default
Contrasts	Joint test results for LS-means estimates	JOINT

ODS Graphics: LSMESTIMATE Statement

This section describes the use of ODS for creating statistical graphs of the distribution of LS-means and LS-mean differences with the `LSMESTIMATE` statement. The plots can be produced only in association with the three procedures that can perform Bayesian analysis (`PROC GENMOD`, `PROC LIFEREG`, and `PROC PHREG`). The plots are available via these procedures directly, and also via `PROC PLM` when run using an item store that was created by these procedures. To request these graphs, you must do the following:

- ensure that ODS Graphics is enabled
- use a `BAYES` statement with `PROC GENMOD`, `PROC LIFEREG`, or `PROC PHREG`, or use `PROC PLM` to perform statistical analysis on an item store that was saved from a Bayesian analysis
- request plots with the `PLOTS=` option in the `LSMESTIMATE` statement

For more information about ODS Graphics, see Chapter 21, “Statistical Graphics Using ODS.” The available graphs are summarized in [Table 19.27](#).

Table 19.27 Graphs Produced by the `LSMESTIMATE` statement

ODS Graph Name	Plot Description	Required Option
BoxPlot	Displays box plots of LS-means or LS-mean differences across a posterior sample.	<code>PLOTS=BOXPLOT</code>
DistPanel	Displays panels of histograms with kernel density curves overlaid. Each plot contains the results for the posterior sample of each LS-mean or LS-mean difference.	<code>PLOTS=DISTPLOT</code>

Table 19.27 continued

ODS Graph Name	Plot Description	Required Option
DistPlot	Displays a histogram with a kernel density curve overlaid. The plot contains the results for the posterior sample of the LS-mean or LS-mean difference.	PLOTS=DISTPLOT(UNPACK)

For details about the *plot-options* of the `LSMESTIMATE` statement, see the `PLOTS=` option in the section “`LSMESTIMATE` Statement” on page 470.

NLOPTIONS Statement

This section applies to the following procedures:

CALIS, GLIMMIX, HPMIXED, PHREG, SURVEYPHREG, and VARIOGRAM. See the individual procedure chapters for deviations from the common syntax and defaults shown here.

Syntax: NLOPTIONS Statement

The `NLOPTIONS` statement provides you with syntax to control aspects of the nonlinear optimizations in the `CALIS`, `GLIMMIX`, `HPMIXED`, `PHREG`, `SURVEYPHREG`, and `VARIOGRAM` procedures.

NLOPTIONS < options > ;

The nonlinear optimization options are described in alphabetical order after Table 19.28, which summarizes the options by category. The notation used in describing the options is generic in the sense that $\boldsymbol{\psi}$ denotes the $p \times 1$ vector of parameters for the optimization and ψ_i is its i th element. The objective function being minimized, its $p \times 1$ gradient vector, and its $p \times p$ Hessian matrix are denoted as $f(\boldsymbol{\psi})$, $\mathbf{g}(\boldsymbol{\psi})$, and $\mathbf{H}(\boldsymbol{\psi})$, respectively. The gradient with respect to the i th parameter is denoted as $g_i(\boldsymbol{\psi})$. Superscripts in parentheses denote the iteration count; for example, $f(\boldsymbol{\psi})^{(k)}$ is the value of the objective function at iteration k . In the mixed model procedures, the parameter vector $\boldsymbol{\psi}$ might consist of fixed effects only, covariance parameters only, or fixed effects and covariance parameters. In the `CALIS` procedure, $\boldsymbol{\psi}$ consists of all independent parameters that are defined in the models and in the `PARAMETERS` statement.

Table 19.28 Options to Control Aspects of the Optimization

Option	Description
Optimization	
HESCAL=	Determines the type of Hessian scaling
INHESIAN=	Specifies the start for approximated Hessian
LINESEARCH=	Specifies the line-search method
LSPRECISION=	Specifies the line-search precision
RESTART=	Specifies the iteration number for update restart
TECHNIQUE=	Determines the minimization technique

Table 19.28 *continued*

Option	Description
UPDATE=	Determines the update technique
Termination Criteria	
ABSCONV=	Tunes an absolute function convergence criterion
ABSFCONV=	Tunes an absolute function difference convergence criterion
ABSGCONV=	Tunes the absolute gradient convergence criterion
ABSXCONV=	Tunes the absolute parameter convergence criterion
FCONV=	Tunes the relative function convergence criterion
FCONV2=	Tunes another relative function convergence criterion
FSIZE=	Specifies the value used in the FCONV and GCONV criteria
GCONV=	Tunes the relative gradient convergence criterion
GCONV2=	Tunes another relative gradient convergence criterion
MAXFUNC=	Specifies the maximum number of function calls
MAXITER=	Specifies the maximum number of iterations
MAXTIME=	Specifies the upper limit for seconds of CPU time
MINITER=	Specifies the minimum number of iterations
XCONV=	Specifies the relative parameter convergence criterion
XSIZE=	Specifies the value used in the XCONV criterion
Step Length	
DAMPSTEP=	Dampens steps in a line search
INSTEP=	Specifies the initial trust region radius
MAXSTEP=	Specifies the maximum trust region radius
Printed Output	
PALL	Displays (almost) all printed output
PHISTORY	Displays optimization history
NOPRINT	Suppresses all printed output
Covariance Matrix Tolerances	
ASINGULAR=	Specifies the absolute singularity for inertia
MSINGULAR=	Specifies the relative M singularity for inertia
VSINGULAR=	Specifies the relative V singularity for inertia
Constraint Specifications	
LCEPSILON=	Specifies the range for active constraints
LCDEACT=	Specifies the LM tolerance for deactivating
LCSINGULAR=	Specifies the tolerance for dependent constraints
Remote Monitoring	
SOCKET=	Specifies the fileref for remote monitoring

ABSCONV=*r***ABSTOL=*r***

specifies an absolute function convergence criterion: for minimization, termination requires $f(\boldsymbol{\psi}^{(k)}) \leq r$. The default value of r is the negative square root of the largest double-precision value, which serves only as a protection against overflows.

ABSFCNV=*r* < *n* >**ABSFTOL=*r* < *n* >**

specifies an absolute function difference convergence criterion:

- For all techniques except NMSIMP (specified by the **TECHNIQUE=** option), termination requires a small change of the function value in successive iterations,

$$|f(\boldsymbol{\psi}^{(k-1)}) - f(\boldsymbol{\psi}^{(k)})| \leq r$$

- The same formula is used for the NMSIMP technique, but $\boldsymbol{\psi}^{(k)}$ is defined as the vertex with the lowest function value, and $\boldsymbol{\psi}^{(k-1)}$ is defined as the vertex with the highest function value in the simplex.

The default value is $r = 0$. The optional integer value n specifies the number of successive iterations for which the criterion must be satisfied before the process can be terminated.

ABSGCONV=*r* < *n* >**ABSGTOL=*r* < *n* >**

specifies an absolute gradient convergence criterion:

- For all techniques except NMSIMP (specified by the **TECHNIQUE=** option), termination requires the maximum absolute gradient element to be small:

$$\max_j |g_j(\boldsymbol{\psi}^{(k)})| \leq r$$

- This criterion is not used by the NMSIMP technique.

The default value is $r = 1\text{E-}5$. The optional integer value n specifies the number of successive iterations for which the criterion must be satisfied before the process can be terminated.

ABSXCONV=*r* < *n* >**ABSXTOL=*r* < *n* >**

specifies an absolute parameter convergence criterion:

- For all techniques except NMSIMP, termination requires a small Euclidean distance between successive parameter vectors,

$$\|\boldsymbol{\psi}^{(k)} - \boldsymbol{\psi}^{(k-1)}\|_2 \leq r$$

- For the NMSIMP technique, termination requires either a small length $\alpha^{(k)}$ of the vertices of a restart simplex,

$$\alpha^{(k)} \leq r$$

or a small simplex size,

$$\delta^{(k)} \leq r$$

where the simplex size $\delta^{(k)}$ is defined as the L1 distance from the simplex vertex $\xi^{(k)}$ with the smallest function value to the other p simplex points $\psi_l^{(k)} \neq \xi^{(k)}$:

$$\delta^{(k)} = \sum_{\psi_l \neq y} \|\psi_l^{(k)} - \xi^{(k)}\|_1$$

The default is $r = 1\text{E-}8$ for the NMSIMP technique and $r = 0$ otherwise. The optional integer value n specifies the number of successive iterations for which the criterion must be satisfied before the process can terminate.

ASINGULAR= r

ASING= r

specifies an absolute singularity criterion for the computation of the inertia (number of positive, negative, and zero eigenvalues) of the Hessian and its projected forms. The default value is the square root of the smallest positive double-precision value.

DAMPSTEP<= r >

specifies that the initial step length value $\alpha^{(0)}$ for each line search (used by the QUANEW, CONGRA, or NEWRAP technique) cannot be larger than r times the step length value used in the former iteration. If the DAMPSTEP option is specified but r is not specified, the default is $r = 2$. The DAMPSTEP= option can prevent the line-search algorithm from repeatedly stepping into regions where some objective functions are difficult to compute or where they could lead to floating-point overflows during the computation of objective functions and their derivatives. The DAMPSTEP= option can save time-consuming function calls during the line searches of objective functions that result in very small steps.

FCONV= r < n >

FTOL= r < n >

specifies a relative function convergence criterion:

- For all techniques except NMSIMP, termination requires a small relative change of the function value in successive iterations,

$$\frac{|f(\psi^{(k)}) - f(\psi^{(k-1)})|}{\max(|f(\psi^{(k-1)})|, \text{FSIZE})} \leq r$$

where FSIZE is defined by the **FSIZE=** option.

- The same formula is used for the NMSIMP technique, but $\psi^{(k)}$ is defined as the vertex with the lowest function value and $\psi^{(k-1)}$ is defined as the vertex with the highest function value in the simplex.

The default is $r = 10^{-\text{FDIGITS}}$, where FDIGITS is by default $-\log_{10}\{\epsilon\}$ and ϵ is the machine precision. Some procedures, such as the GLIMMIX procedure, enable you to change the value with the FDIGITS= option in the PROC statement. The optional integer value n specifies the number of successive iterations for which the criterion must be satisfied before the process can terminate.

FCONV2=r<n>**FTOL2=r<n>**

specifies a second function convergence criterion:

- For all techniques except NMSIMP, termination requires a small predicted reduction,

$$df^{(k)} \approx f(\boldsymbol{\psi}^{(k)}) - f(\boldsymbol{\psi}^{(k)} + \mathbf{s}^{(k)})$$

of the objective function. The predicted reduction

$$\begin{aligned} df^{(k)} &= -\mathbf{g}^{(k)'} \mathbf{s}^{(k)} - \frac{1}{2} \mathbf{s}^{(k)'} \mathbf{H}^{(k)} \mathbf{s}^{(k)} \\ &= -\frac{1}{2} \mathbf{s}^{(k)'} \mathbf{g}^{(k)} \leq r \end{aligned}$$

is computed by approximating the objective function f by the first two terms of the Taylor series and substituting the Newton step,

$$\mathbf{s}^{(k)} = -[\mathbf{H}^{(k)}]^{-1} \mathbf{g}^{(k)}$$

- For the NMSIMP technique, termination requires a small standard deviation of the function values of the $p + 1$ simplex vertices $\boldsymbol{\psi}_l^{(k)}$, $l = 0, \dots, p$,

$$\sqrt{\frac{1}{n+1} \sum_l \left[f(\boldsymbol{\psi}_l^{(k)}) - \bar{f}(\boldsymbol{\psi}^{(k)}) \right]^2} \leq r$$

where $\bar{f}(\boldsymbol{\psi}^{(k)}) = \frac{1}{p+1} \sum_l f(\boldsymbol{\psi}_l^{(k)})$. If there are p_{act} boundary constraints active at $\boldsymbol{\psi}^{(k)}$, the mean and standard deviation are computed only for the $n + 1 - p_{act}$ unconstrained vertices.

The default value is $r = 1\text{E-}6$ for the NMSIMP technique and $r = 0$ otherwise. The optional integer value n specifies the number of successive iterations for which the criterion must be satisfied before the process can terminate.

FSIZE=rspecifies the FSIZE parameter of the relative function and relative gradient termination criteria. The default value is $r = 0$. For more details, see the **FCONV=** and **GCONV=** options.**GCONV=r<n>****GTOL=r<n>**

specifies a relative gradient convergence criterion:

- For all techniques except CONGRA and NMSIMP, termination requires that the normalized predicted function reduction be small,

$$\frac{\mathbf{g}(\boldsymbol{\psi}^{(k)})' [\mathbf{H}^{(k)}]^{-1} \mathbf{g}(\boldsymbol{\psi}^{(k)})}{\max(|f(\boldsymbol{\psi}^{(k)})|, \text{FSIZE})} \leq r$$

where FSIZE is defined by the **FSIZE=** option. For the CONGRA technique (where a reliable Hessian estimate \mathbf{H} is not available), the following criterion is used:

$$\frac{\| \mathbf{g}(\boldsymbol{\psi}^{(k)}) \|_2^2 \quad \| \mathbf{s}(\boldsymbol{\psi}^{(k)}) \|_2}{\| \mathbf{g}(\boldsymbol{\psi}^{(k)}) - \mathbf{g}(\boldsymbol{\psi}^{(k-1)}) \|_2 \max(|f(\boldsymbol{\psi}^{(k)})|, \text{FSIZE})} \leq r$$

- This criterion is not used by the NMSIMP technique.

The default value is $r = 1\text{E-}8$. The optional integer value n specifies the number of successive iterations for which the criterion must be satisfied before the process can terminate.

GCONV2=r<n>**GTOL2=r<n>**

specifies another relative gradient convergence criterion:

- For least squares problems and the TRUREG, LEVMAR, NRRIDG, and NEWRAP techniques, the following criterion of Browne (1982) is used:

$$\max_j \frac{|g_j(\boldsymbol{\psi}^{(k)})|}{\sqrt{f(\boldsymbol{\psi}^{(k)})\mathbf{H}_{j,j}^{(k)}}} \leq r$$

- This criterion is not used by the other techniques.

The default value is $r = 0$. The optional integer value n specifies the number of successive iterations for which the criterion must be satisfied before the process can terminate.

HESCAL=0 | 1 | 2 | 3**HS=0 | 1 | 2 | 3**

specifies the scaling version of the Hessian (or crossproduct Jacobian) matrix used in NRRIDG, TRUREG, LEVMAR, NEWRAP, or DBLDOG optimization.

If HS is not equal to 0, the first iteration and each restart iteration set the diagonal scaling matrix $D^{(0)} = \text{diag}(d_i^{(0)})$:

$$d_i^{(0)} = \sqrt{\max(|H_{i,i}^{(0)}|, \epsilon)}$$

where $H_{i,i}^{(0)}$ are the diagonal elements of the Hessian (or crossproduct Jacobian). In every other iteration, the diagonal scaling matrix $D^{(0)} = \text{diag}(d_i^{(0)})$ is updated depending on the HS option:

HS=0 specifies that no scaling be done.

HS=1 specifies the Moré (1978) scaling update:

$$d_i^{(k+1)} = \max \left[d_i^{(k)}, \sqrt{\max(|H_{i,i}^{(k)}|, \epsilon)} \right]$$

HS=2 specifies the Dennis, Gay, and Welsch (1981) scaling update:

$$d_i^{(k+1)} = \max \left[0.6 * d_i^{(k)}, \sqrt{\max(|H_{i,i}^{(k)}|, \epsilon)} \right]$$

HS=3 specifies that d_i be reset in each iteration:

$$d_i^{(k+1)} = \sqrt{\max(|H_{i,i}^{(k)}|, \epsilon)}$$

In each scaling update, ϵ is the relative machine precision. The default value is HS=0. Scaling of the Hessian can be time-consuming in the case where general linear constraints are active.

INHESIAN=<math>r>**INHES=<math>r>**

specifies how the initial estimate of the approximate Hessian is defined for the quasi-Newton techniques QUANEW and DBLDOG. There are two alternatives:

- If you do not use the r specification, the initial estimate of the approximate Hessian is set to the Hessian at $\psi^{(0)}$.
- If you do use the r specification, the initial estimate of the approximate Hessian is set to the multiple of the identity matrix $r\mathbf{I}$.

By default (if you do not specify the option INHESIAN= r), the initial estimate of the approximate Hessian is set to the multiple of the identity matrix $r\mathbf{I}$, where the scalar r is computed from the magnitude of the initial gradient.

INSTEP=<math>r>**SALPHA=<math>r>****RADIUS=<math>r>**

reduces the length of the first trial step during the line search of the first iterations. For highly nonlinear objective functions, such as the EXP function, the default initial radius of the trust-region algorithm TRUREG or DBLDOG or the default step length of the line-search algorithms can result in arithmetic overflows. If this occurs, you should specify decreasing values of $0 < r < 1$ such as INSTEP=1E-1, INSTEP=1E-2, INSTEP=1E-4, and so on, until the iteration starts successfully.

- For trust-region algorithms (TRUREG or DBLDOG), the INSTEP= option specifies a factor $r > 0$ for the initial radius $\Delta^{(0)}$ of the trust region. The default initial trust-region radius is the length of the scaled gradient. This step corresponds to the default radius factor of $r = 1$.
- For line-search algorithms (NEWRAP, CONGRA, or QUANEW), the INSTEP= option specifies an upper bound for the initial step length for the line search during the first five iterations. The default initial step length is $r = 1$.
- For the Nelder-Mead simplex algorithm, by using TECH=NMSIMP, the INSTEP= r option defines the size of the start simplex.

LCDEACT=<math>r>**LCD=<math>r>**

specifies a threshold r for the Lagrange multiplier that determines whether an active inequality constraint remains active or can be deactivated. For maximization, r must be greater than zero; for minimization, r must be smaller than zero. An active inequality constraint can be deactivated only if its Lagrange multiplier is less than the threshold value. The default value is

$$r = \pm \min(0.01, \max(0.1 \times \text{ABSGCONV}, 0.001 \times g_{\max}^{(k)}))$$

where “+” is for maximization, “-” is for minimization, ABSGCONV is the value of the absolute gradient criterion, and $g_{\max}^{(k)}$ is the maximum absolute element of the gradient or the projected gradient.

LCEPSILON=*r***LCEPS=*r*****LCE=*r***

specifies the range r for active and violated boundary constraints, where $r \geq 0$. If the point $\psi^{(k)}$ satisfies the following condition, the constraint i is recognized as an active constraint:

$$\left| \sum_{j=1}^k a_{ij} \psi_j^{(k)} - b_i \right| \leq r \times (|b_i| + 1)$$

Otherwise, the constraint i is either an inactive inequality or a violated inequality or equality constraint. The default value is $r = 1\text{E}-8$. During the optimization process, the introduction of rounding errors can force the optimization to increase the value of r by a factor of 10^k for some $k > 0$. If this happens, it is indicated by a message displayed in the log.

LCSINGULAR=*r***LCSING=*r*****LCS=*r***

specifies a criterion r , where $r \geq 0$, that is used in the update of the QR decomposition and that determines whether an active constraint is linearly dependent on a set of other active constraints. The default value is $r = 1\text{E}-8$. The larger r becomes, the more the active constraints are recognized as being linearly dependent. If the value of r is larger than 0.1, it is reset to 0.1.

LINESEARCH=*i***LIS=*i***

specifies the line-search method for the CONGRA, QUANEW, and NEWRAP optimization techniques. See Fletcher (1987) for an introduction to line-search techniques. The value of i can be 1, . . . , 8 as follows. The default is LIS=2.

- | | |
|-------|---|
| LIS=1 | specifies a line-search method that needs the same number of function and gradient calls for cubic interpolation and cubic extrapolation; this method is similar to one used by the Harwell subroutine library. |
| LIS=2 | specifies a line-search method that needs more function than gradient calls for quadratic and cubic interpolation and cubic extrapolation; this method is implemented as shown in Fletcher (1987) and can be modified to an exact line search by using the LSPRECISION= option. This is the default. |
| LIS=3 | specifies a line-search method that needs the same number of function and gradient calls for cubic interpolation and cubic extrapolation; this method is implemented as shown in Fletcher (1987) and can be modified to an exact line search by using the LSPRECISION= option. |
| LIS=4 | specifies a line-search method that needs the same number of function and gradient calls for stepwise extrapolation and cubic interpolation. |
| LIS=5 | specifies a line-search method that is a modified version of LIS=4. |
| LIS=6 | specifies a golden-section line search (Polak 1971), which uses only function values for linear approximation. |
| LIS=7 | specifies a bisection line search (Polak 1971), which uses only function values for linear approximation. |

LIS=8 specifies the Armijo line-search technique (Polak 1971), which uses only function values for linear approximation.

LSPRECISION=*r*

LSP=*r*

specifies the degree of accuracy that should be obtained by the line-search algorithms **LIS=2** and **LIS=3**. Usually an imprecise line search is inexpensive and successful. For more difficult optimization problems, a more precise and expensive line search might be necessary (Fletcher 1987). The **LIS=2** line-search method (which is the default for the **NEWRAP**, **QUANEW**, and **CONGRA** techniques) and the **LIS=3** line-search method approach exact line search for small **LSPRECISION=** values. If you have numerical problems, try to decrease the **LSPRECISION=** value to obtain a more precise line search. The default values are shown in [Table 19.29](#).

Table 19.29 Default Values for Line-Search Precision

TECH=	UPDATE=	LSP Default
QUANEW	DBFGS, BFGS	$r = 0.4$
QUANEW	DDFP, DFP	$r = 0.06$
CONGRA	All	$r = 0.1$
NEWRAP	No update	$r = 0.9$

For more details, see Fletcher (1987).

MAXFUNC=*i*

MAXFU=*i*

specifies the maximum number *i* of function calls in the optimization process. The default values are as follows:

- 125 for the **TRUREG**, **NRRIDG**, **NEWRAP**, and **LEVMAR** techniques
- 500 for the **QUANEW** and **DBLDOG** techniques
- 1000 for the **CONGRA** technique
- 3000 for the **NMSIMP** technique

Optimization can terminate only after completing a full iteration. Therefore, the number of function calls that are actually performed can exceed the number that is specified by the **MAXFUNC=** option.

MAXITER=*i*

MAXIT=*i*

specifies the maximum number *i* of iterations in the optimization process. The default values are as follows:

- 50 for the **TRUREG**, **NRRIDG**, **NEWRAP**, and **LEVMAR** techniques
- 200 for the **QUANEW** and **DBLDOG** techniques
- 400 for the **CONGRA** technique
- 1000 for the **NMSIMP** technique

These default values are also valid when *i* is specified as a missing value.

MAXSTEP= $r < n$ >

specifies an upper bound for the step length of the line-search algorithms during the first n iterations. By default, r is the largest double-precision value and n is the largest integer available. Setting this option can improve the speed of convergence for the CONGRA, QUANEW, and NEWRAP techniques.

MAXTIME= r

specifies an upper limit of r seconds of CPU time for the optimization process. The default value is the largest floating-point double representation of your computer. The time specified by the MAXTIME= option is checked only once at the end of each iteration. Therefore, the actual running time can be much longer than that specified by the MAXTIME= option. The actual running time includes the rest of the time needed to finish the iteration and the time needed to generate the output of the results.

MINITER= i **MINIT= i**

specifies the minimum number of iterations. The default value is 0. If you request more iterations than are actually needed for convergence to a stationary point, the optimization algorithms can behave strangely. For example, the effect of rounding errors can prevent the algorithm from continuing for the required number of iterations.

MSINGULAR= r **MSING= r**

specifies a relative singularity criterion r , where $r > 0$, for the computation of the inertia (number of positive, negative, and zero eigenvalues) of the Hessian and its projected forms. The default value is $1E-12$.

NOPRINT

suppresses output that is related to optimization, such as the iteration history. This option, along with all NLOPTIONS statement options for displayed output, are ignored by the GLIMMIX and HPMIXED procedures.

PALL

displays all optional output for optimization. This option is supported only by the CALIS and SURVEYPHREG procedures.

PHISTORY**PHIST**

displays the optimization history. The PHISTORY option is implied if the PALL option is specified. The PHISTORY option is supported only by the CALIS and SURVEYPHREG procedures.

RESTART= i **REST= i**

specifies that the QUANEW or CONGRA technique is restarted with a steepest search direction after at most i iterations, where $i > 0$. Default values are as follows:

- When TECHNIQUE=CONGRA and UPDATE=PB, restart is performed automatically; so i is not used.
- When TECHNIQUE=CONGRA and UPDATE \neq PB, $i = \min(10p, 80)$, where p is the number of parameters.
- When TECHNIQUE=QUANEW, i is the largest integer available.

SINGULAR=*r***SING=*r***

specifies the singularity criterion r , $0r \leq 1$, that is used for the inversion of the Hessian matrix. The default value is 1E-8.

SOCKET=*fileref*

specifies the fileref that contains the information needed for remote monitoring.

TECHNIQUE=*value***TECH=*value*****OMETHOD=*value*****OM=*value***

specifies the optimization technique. You can find additional information about choosing an optimization technique in the section “[Choosing an Optimization Algorithm](#)” on page 494. Valid values for the TECHNIQUE= option are as follows:

- CONGRA
 - performs a conjugate-gradient optimization, which can be more precisely specified with the **UPDATE=** option and modified with the **LINESEARCH=** option. When you specify this option, **UPDATE=PB** by default.
- DBLDOG
 - performs a version of double-dogleg optimization, which can be more precisely specified with the **UPDATE=** option. When you specify this option, **UPDATE=DBFGS** by default.
- LEVMAR
 - performs a highly stable, but for large problems memory- and time-consuming, Levenberg-Marquardt optimization technique, a slightly improved variant of the Moré (1978) implementation. You can also specify this technique with the alias LM or MARQUARDT. In the CALIS procedure, this is the default optimization technique if there are fewer than 40 parameters to estimate. The GLIMMIX and HPMIXED procedures do not support this optimization technique.
- NMSIMP
 - performs a Nelder-Mead simplex optimization. The CALIS procedure does not support this optimization technique.
- NONE
 - does not perform any optimization. This option can be used for the following:
 - to perform a grid search without optimization
 - to compute estimates and predictions that cannot be obtained efficiently with any of the optimization techniques
 - to obtain inferences for known values of the covariance parameters
- NEWRAP
 - performs a Newton-Raphson optimization that combines a line-search algorithm with ridging. The line-search algorithm **LIS=2** is the default method.
- NRRIDG
 - performs a Newton-Raphson optimization with ridging. This is the default optimization technique in the SURVEYPHREG procedure.

- QUANEW
performs a quasi-Newton optimization, which can be defined more precisely with the **UPDATE=** option and modified with the **LINESEARCH=** option.
- TRUREG
performs a trust-region optimization.

UPDATE=method**UPD=method**

specifies the update method for the quasi-Newton, double-dogleg, or conjugate-gradient optimization technique. Not every update method can be used with each optimizer.

The following are the valid methods for the **UPDATE=** option:

- BFGS
performs the original Broyden, Fletcher, Goldfarb, and Shanno (BFGS) update of the inverse Hessian matrix.
- DBFGS
performs the dual BFGS update of the Cholesky factor of the Hessian matrix. This is the default update method.
- DDFP
performs the dual Davidon, Fletcher, and Powell (DFP) update of the Cholesky factor of the Hessian matrix.
- DFP
performs the original DFP update of the inverse Hessian matrix.
- PB
performs the automatic restart update method of Powell (1977) and Beale (1972).
- FR
performs the Fletcher-Reeves update (Fletcher 1987).
- PR
performs the Polak-Ribiere update (Fletcher 1987).
- CD
performs a conjugate-descent update of Fletcher (1987).

VERSION=1 | 2**VS=1 | 2**

specifies the version of the quasi-Newton optimization technique with nonlinear constraints.

VS=1 specifies the update of the μ vector as in Powell (1978b, a) (update like VF02AD).

VS=2 specifies the update of the μ vector as in Powell (1982b, a) (update like VMCWD).

The default is **VERSION=2**.

VSINGULAR=*r***VSING=*r***

specifies a relative singularity criterion r , where $r > 0$, for the computation of the inertia (number of positive, negative, and zero eigenvalues) of the Hessian and its projected forms. The default value is $r = 1\text{E-}8$.

XCONV=*r*<*n*>**XTOL=*r*<*n*>**

specifies the relative parameter convergence criterion:

- For all techniques except NMSIMP, termination requires a small relative parameter change in subsequent iterations:

$$\frac{\max_j |\psi_j^{(k)} - \psi_j^{(k-1)}|}{\max(|\psi_j^{(k)}|, |\psi_j^{(k-1)}|, \text{XSIZE})} \leq r$$

- For the NMSIMP technique, the same formula is used, but $\psi_j^{(k)}$ is defined as the vertex with the lowest function value and $\psi_j^{(k-1)}$ is defined as the vertex with the highest function value in the simplex.

The default value is $r = 1\text{E-}8$ for the NMSIMP technique and $r = 0$ otherwise. The optional integer value n specifies the number of successive iterations for which the criterion must be satisfied before the process can be terminated.

XSIZE=*r*

specifies the XSIZE parameter r of the relative parameter termination criterion, where $r \geq 0$. The default value is $r = 0$. For more details, see the **XCONV=** option.

Choosing an Optimization Algorithm

First- or Second-Order Algorithms

The factors that go into choosing a particular optimization technique for a particular problem are complex. Trial and error can be involved.

For many optimization problems, computing the gradient takes more computer time than computing the function value. Computing the Hessian sometimes takes *much* more computer time and memory than computing the gradient, especially when there are many decision variables. Unfortunately, optimization techniques that do not use some kind of Hessian approximation usually require many more iterations than techniques that do use a Hessian matrix, and, as a result, the total run time of these techniques is often longer. Techniques that do not use the Hessian also tend to be less reliable. For example, they can terminate more easily at stationary points than at global optima.

Table 19.30 shows which derivatives are required for each optimization technique.

Table 19.30 Derivatives Required

Algorithm	First-Order	Second-Order
LEVMAR	x	x
TRUREG	x	x
NEWRAP	x	x
NRRIDG	x	x
QUANEW	x	-
DBLDOG	x	-
CONGRA	x	-
NMSIMP	-	-

The second-derivative methods TRUREG, NEWRAP, and NRRIDG are best for small problems where the Hessian matrix is not expensive to compute. Sometimes the NRRIDG algorithm can be faster than the TRUREG algorithm, but TRUREG can be more stable. The NRRIDG algorithm requires only one matrix with $p(p + 1)/2$ double words; TRUREG and NEWRAP require two such matrices. Here, p denotes the number of parameters in the optimization.

The first-derivative methods QUANEW and DBLDOG are best for medium-sized problems where the objective function and the gradient are much faster to evaluate than the Hessian. In general, the QUANEW and DBLDOG algorithms require more iterations than TRUREG, NRRIDG, and NEWRAP, but each iteration can be much faster. The QUANEW and DBLDOG algorithms require only the gradient to update an approximate Hessian, and they require slightly less memory than TRUREG or NEWRAP (essentially one matrix with $p(p + 1)/2$ double words).

The first-derivative method CONGRA is best for large problems where the objective function and the gradient can be computed much faster than the Hessian and where too much memory is required to store the (approximate) Hessian. In general, the CONGRA algorithm requires more iterations than QUANEW or DBLDOG, but each iteration can be much faster. Because CONGRA requires only a factor of p double-word memory, many large applications can be solved only by CONGRA.

The no-derivative method NMSIMP is best for small problems where derivatives are not continuous or are very difficult to compute.

Each optimization method uses one or more convergence criteria that determine when it has converged. An algorithm is considered to have converged when any one of the convergence criteria is satisfied. For example, under the default settings, the QUANEW algorithm will converge if $\text{ABSGCONV} < 1\text{E-}5$, $\text{FCONV} < 10^{-\text{FDIGITS}}$, or $\text{GCONV} < 1\text{E-}8$.

Algorithm Descriptions

Trust Region Optimization (TRUREG)

The trust region method uses the gradient $\mathbf{g}(\boldsymbol{\psi}^{(k)})$ and the Hessian matrix $\mathbf{H}(\boldsymbol{\psi}^{(k)})$; thus, it requires that the objective function $f(\boldsymbol{\psi})$ have continuous first- and second-order derivatives inside the feasible region.

The trust region method iteratively optimizes a quadratic approximation to the nonlinear objective function within a hyperelliptic trust region with radius Δ that constrains the step size that corresponds to the quality of the quadratic approximation. The trust region method is implemented based on Dennis, Gay, and Welsch (1981); Gay (1983) and Moré and Sorensen (1983).

The trust region method performs well for small- to medium-sized problems, and it does not need many function, gradient, and Hessian calls. However, if the computation of the Hessian matrix is computationally expensive, one of the (dual) quasi-Newton or conjugate gradient algorithms might be more efficient.

Newton-Raphson Optimization with Line Search (NEWRAP)

The NEWRAP technique uses the gradient $\mathbf{g}(\boldsymbol{\psi}^{(k)})$ and the Hessian matrix $\mathbf{H}(\boldsymbol{\psi}^{(k)})$; thus, it requires that the objective function have continuous first- and second-order derivatives inside the feasible region. If second-order derivatives are computed efficiently and precisely, the NEWRAP method can perform well for medium-sized to large problems, and it does not need many function, gradient, and Hessian calls.

This algorithm uses a pure Newton step when the Hessian is positive definite and when the Newton step reduces the value of the objective function successfully. Otherwise, a combination of ridging and line search is performed to compute successful steps. If the Hessian is not positive definite, a multiple of the identity matrix is added to the Hessian matrix to make it positive definite (Eskow and Schnabel 1991).

In each iteration, a line search is performed along the search direction to find an approximate optimum of the objective function. The default line-search method uses quadratic interpolation and cubic extrapolation (LIS=2).

Newton-Raphson Ridge Optimization (NRRIDG)

The NRRIDG technique uses the gradient $\mathbf{g}(\boldsymbol{\psi}^{(k)})$ and the Hessian matrix $\mathbf{H}(\boldsymbol{\psi}^{(k)})$; thus, it requires that the objective function have continuous first- and second-order derivatives inside the feasible region.

This algorithm uses a pure Newton step when the Hessian is positive definite and when the Newton step reduces the value of the objective function successfully. If at least one of these two conditions is not satisfied, a multiple of the identity matrix is added to the Hessian matrix.

The NRRIDG method performs well for small- to medium-sized problems, and it does not require many function, gradient, and Hessian calls. However, if the computation of the Hessian matrix is computationally expensive, one of the (dual) quasi-Newton or conjugate gradient algorithms might be more efficient.

Because the NRRIDG technique uses an orthogonal decomposition of the approximate Hessian, each iteration of NRRIDG can be slower than that of the NEWRAP technique, which works with a Cholesky decomposition. Usually, however, NRRIDG requires fewer iterations than NEWRAP.

Quasi-Newton Optimization (QUANEW)

The (dual) quasi-Newton method uses the gradient $\mathbf{g}(\boldsymbol{\psi}^{(k)})$, and it does not need to compute second-order derivatives because they are approximated. It works well for medium-sized to moderately large optimization problems, where the objective function and the gradient are much faster to compute than the Hessian. However, in general, it requires more iterations than the TRUREG, NEWRAP, and NRRIDG techniques, which compute second-order derivatives. QUANEW is the default optimization algorithm because it provides an appropriate balance between the speed and stability required for most nonlinear mixed model applications.

The QUANEW technique is one of the following, depending upon the value of the `UPDATE=` option:

- the original quasi-Newton algorithm, which updates an approximation of the inverse Hessian
- the dual quasi-Newton algorithm, which updates the Cholesky factor of an approximate Hessian (this is the default)

You can specify four update formulas with the `UPDATE=` option:

- DBFGS performs the dual Broyden, Fletcher, Goldfarb, and Shanno (BFGS) update of the Cholesky factor of the Hessian matrix. This is the default.
- DDFP performs the dual Davidon, Fletcher, and Powell (DFP) update of the Cholesky factor of the Hessian matrix.
- BFGS performs the original BFGS update of the inverse Hessian matrix.
- DFP performs the original DFP update of the inverse Hessian matrix.

In each iteration, a line search is performed along the search direction to find an approximate optimum. The default line-search method uses quadratic interpolation and cubic extrapolation to obtain a step size α that satisfies the Goldstein conditions. One of the Goldstein conditions can be violated if the feasible region defines an upper limit of the step size. Violating the left-side Goldstein condition can affect the positive definiteness of the quasi-Newton update. In that case, either the update is skipped or the iterations are restarted with an identity matrix, resulting in the steepest descent or ascent search direction. You can specify line-search algorithms other than the default with the LIS= option.

The QUANEW algorithm uses its own line-search technique. Of the options and parameters that control the line search for other algorithms, only the INSTEP= option applies here. In several applications, large steps in the first iterations are troublesome. You can use the INSTEP= option to impose an upper bound for the step size α during the first five iterations. You can also use the INHESSIAN= option to specify a different starting approximation for the Hessian. If you specify only the INHESSIAN option, the Cholesky factor of a (possibly ridged) finite-difference approximation of the Hessian is used to initialize the quasi-Newton update process.

Double-Dogleg Optimization (DBLDOG)

The double-dogleg optimization method combines the ideas of the quasi-Newton and trust region methods. In each iteration, the double-dogleg algorithm computes the step $s^{(k)}$ as the linear combination of the steepest descent or ascent search direction $s_1^{(k)}$ and a quasi-Newton search direction $s_2^{(k)}$,

$$s^{(k)} = \alpha_1 s_1^{(k)} + \alpha_2 s_2^{(k)}$$

The step is requested to remain within a prespecified trust region radius; see Fletcher (1987, p, 107). Thus, the DBLDOG subroutine uses the dual quasi-Newton update but does not perform a line search. You can specify two update formulas with the UPDATE= option:

- DBFGS performs the dual Broyden, Fletcher, Goldfarb, and Shanno update of the Cholesky factor of the Hessian matrix. This is the default.
- DDFP performs the dual Davidon, Fletcher, and Powell update of the Cholesky factor of the Hessian matrix.

The double-dogleg optimization technique works well for medium-sized to moderately large optimization problems, where the objective function and the gradient are much faster to compute than the Hessian. The implementation is based on Dennis and Mei (1979); Gay (1983), but it is extended for dealing with boundary and linear constraints. The DBLDOG technique generally requires more iterations than the TRUREG, NEWRAP, and NRRIDG techniques, which require second-order derivatives; however, each of the DBLDOG iterations is computationally cheap. Furthermore, the DBLDOG technique requires only gradient calls for the update of the Cholesky factor of an approximate Hessian.

Conjugate Gradient Optimization (CONGRA)

Second-order derivatives are not required by the CONGRA algorithm and are not even approximated. The CONGRA algorithm can be expensive in function and gradient calls, but it requires only $O(p)$ memory for unconstrained optimization. In general, many iterations are required to obtain a precise solution, but each of the CONGRA iterations is computationally cheap. You can specify four different update formulas for generating the conjugate directions by using the `UPDATE=` option:

- PB performs the automatic restart update method of Powell (1977) and Beale (1972). This is the default.
- FR performs the Fletcher-Reeves update (Fletcher 1987).
- PR performs the Polak-Ribiere update (Fletcher 1987).
- CD performs a conjugate-descent update of Fletcher (1987).

The default often behaves best for typical examples, whereas `UPDATE=CD` can perform poorly.

The CONGRA subroutine should be used for optimization problems with large p . For the unconstrained or boundary-constrained case, CONGRA requires only $O(p)$ bytes of working memory, whereas all other optimization methods require order $O(p^2)$ bytes of working memory. During p successive iterations, uninterrupted by restarts or changes in the working set, the conjugate gradient algorithm computes a cycle of p conjugate search directions. In each iteration, a line search is performed along the search direction to find an approximate optimum of the objective function. The default line-search method uses quadratic interpolation and cubic extrapolation to obtain a step size α that satisfies the Goldstein conditions. One of the Goldstein conditions can be violated if the feasible region defines an upper limit for the step size. Other line-search algorithms can be specified with the `LIS=` option.

Nelder-Mead Simplex Optimization (NMSIMP)

The Nelder-Mead simplex method does not use any derivatives and does not assume that the objective function has continuous derivatives. The objective function itself needs to be continuous. This technique is quite expensive in the number of function calls, and it might be unable to generate precise results for $p \gg 40$.

The original Nelder-Mead simplex algorithm is implemented and extended to boundary constraints. This algorithm does not compute the objective for infeasible points, but it changes the shape of the simplex adapting to the nonlinearities of the objective function, which contributes to an increased speed of convergence. It uses a special termination criterion.

SLICE Statement

This statement applies to the following SAS/STAT procedures:

GENMOD, GLIMMIX, LIFEREG, LOGISTIC, MIXED, ORTHOREG, PHREG, PLM, PROBIT, SURVEYLOGISTIC, SURVEYPHREG, and SURVEYREG. It also applies to the RELIABILITY procedure in SAS/QC software.

The SLICE statement is similar to the LSMEANS statement. You use it to perform inferences on model effects that consist entirely of classification variables. With the SLICE statement, these effects must be higher-order effects of at least two classification variables. The effect is then partitioned into subsets that correspond to variables used in forming the effect. You can use the same options as you use for the LSMEANS statement to perform an analysis for the partitions. This analysis is also known as an analysis of simple effects (Winer 1971).

By default, the interaction effect is partitioned by all main effects. For example, the following statements produce simple-effect differences among the A levels for each level of B and simple-effect differences among the B levels for each level of A:

```
class a b;
model y = a b a*b;
slice a*b / diff nof;
```

For example, if the *model-effect* is a three-way interaction effect, the default output includes comparisons of the two-way interaction means.

Suppose, for example, that the interaction effect A*B is significant in your analysis and that you want to test the effect of A for each level of B. The appropriate statement is

```
slice A*B / sliceBy = B;
```

This produces an *F* test for each level of B that compares the equality of the levels of A.

For example, assume that in a balanced design factors A and B have $a = 4$ and $b = 3$ levels, respectively. Consider the following statements:

```
class a b;
model y = a b a*b;
slice a*b / sliceby=a diff;
```

The SLICE statement produces four *F* tests, one per level of A. The first of these tests is constructed by extracting the three rows that correspond to the first level of A from the coefficient matrix for the A*B interaction. Call this matrix \mathbf{L}_{a1} and its rows $\mathbf{l}_{a1}^{(1)}$, $\mathbf{l}_{a1}^{(2)}$, and $\mathbf{l}_{a1}^{(3)}$. The slice tests the two-degrees-of-freedom hypothesis

$$H: \begin{cases} \left(\mathbf{l}_{a1}^{(1)} - \mathbf{l}_{a1}^{(2)} \right) \boldsymbol{\beta} = 0 \\ \left(\mathbf{l}_{a1}^{(1)} - \mathbf{l}_{a1}^{(3)} \right) \boldsymbol{\beta} = 0 \end{cases}$$

In a balanced design, where μ_{ij} denotes the mean response if A is at level i and B is at level j , this hypothesis is equivalent to $H: \mu_{11} = \mu_{12} = \mu_{13}$. The DIFF option considers the three rows of \mathbf{L}_{a1} in turn and performs tests of the difference between pairs of rows. By default, all pairwise differences within the subset of \mathbf{L} are considered; in the example this corresponds to tests of the form

$$H: \left(\mathbf{l}_{a1}^{(1)} - \mathbf{l}_{a1}^{(2)} \right) \boldsymbol{\beta} = 0$$

$$H: \left(\mathbf{l}_{a1}^{(1)} - \mathbf{l}_{a1}^{(3)} \right) \boldsymbol{\beta} = 0$$

$$H: \left(\mathbf{l}_{a1}^{(2)} - \mathbf{l}_{a1}^{(3)} \right) \boldsymbol{\beta} = 0$$

In the example, with $a = 4$ and $b = 3$, this produces four sets of least squares means differences. Within each set, factor A is held fixed at a particular level and each set consists of three comparisons.

Syntax: SLICE Statement

SLICE *model-effect* </ options> ;

You can specify all options of the **LSMEANS** statement in the **SLICE** statement. The philosophy of the **SLICE** statement is to apply the analysis according to the options to the subsets of the **L** matrix that correspond to chosen partitions.

The following behavior differences between the **SLICE** and the **LSMEANS** statement are noteworthy:

- The specification of the *model-effect* is optional in the **LSMEANS** statement and required in the **SLICE** statement.
- Only a single **SLICE model-effect** can be specified before the option slash (/). However, you can specify multiple partitioning rules with the **SLICEBY** option.
- The **MEANS** option is the default for most procedures in the **LSMEANS** statement. For the **SLICE** statement, the default is the **NOMEANS** option.

Also, the three generalized linear modeling options: **EXP**, **ILINK**, and **ODDSRATIO** in the **SLICE** statement are additionally supported by **PROC GLIMMIX** and by **PROC PLM** when it is used to perform statistical analyses on item stores that were created by **PROC GLIMMIX**.

In addition to the options in the **LSMEANS** statement, you can specify the following options in the **SLICE** statement after the slash (/):

SLICEBY <=> *slice-specification*

SIMPLE <=> *slice-specification*

SLICEBY(*slice-specification* <, *slice-specification* <, ...>)

SIMPLE(*slice-specification* <, *slice-specification* <, ...>)

determines how to construct the partition of the least squares means for the *model-effect*. A *slice-specification* consists of an effect name followed by an optional list of formatted values. For example, the following statements creates partitions of the A*B interaction effect for all levels of variable A:

```
class a b;
model y = a b a*b;
slice a*b / sliceby=a;
```

The following statements produces two partitions of the interaction:

```
class a b;
model y = a b a*b;
slice a*b / sliceby(b='2' a='1') diff;
```

In the first partition the variable B takes on formatted value '2'. In the second partition the variable A takes on the formatted value '1'.

NOF

suppresses the F test for testing the mutual equality of the estimable functions in the partition.

ODS Table Names: SLICE Statement

Each table created by the `SLICE` statement has a name associated with it, and you can use this name to refer to the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in Table 19.31. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

Table 19.31 ODS Tables Produced by the `SLICE` statement

Table Name	Description	Required Option
Coef	L matrix coefficients	E
Slices	LS-means slices	MEANS
SliceDiffs	Simple differences of LS-means slices	DIFF or ADJUST= or STEPDOWN or NOF
SliceLines	Lines display for LS-means slices	LINES
SliceTests	Tests for LS-means slices	Default

STORE Statement

This statement applies to the following SAS/STAT procedures:

GENMOD, GLIMMIX, GLM, GLMSELECT, LOGISTIC, MIXED, ORTHOREG, PHREG, PROBIT, SURVEYLOGISTIC, SURVEYPHREG, and SURVEYREG. It also applies to the RELIABILITY procedure in SAS/QC software.

The `STORE` statement requests that the procedure save the context and results of the statistical analysis into an item store. An item store is a binary file format that cannot be modified by the user. The contents of the item store can be processed with the `PLM` procedure. One example of item store technology is to perform a time-consuming analysis and to store its results by using the `STORE` statement. At a later time you can then perform specific statistical analysis tasks based on the saved results of the previous analysis, without having to fit the model again. The following statements show an example in which a mixed model is fit with the `MIXED` procedure and the postprocessing analysis is performed with the `PLM` procedure:

```
proc mixed data=MyBigDataSet;
  class Env A B sub;
  model y = A B x / ddfm=KenwardRoger;
  random int A*B / sub=Env;
  repeated / subject=Env*A*B type=AR(1);
  store sasuser.mixed;
run;
```



```
proc plm restore=sasuser.mixed;
  show cov ParmS;
  lsmeans A B / diff;
  score data=NewData out=ScoreResults;
run;
```

The STORE statement in the PROC MIXED step requests that the MIXED procedure save those results that are needed to perform statistical tasks with the PLM procedure. For example, the MIXED procedure saves the necessary pieces of information that relate to the Kenward-Roger degree-of-freedom method. The results from the LSMEANS statement in the PROC PLM step thus apply this technique for calculating denominator degrees of freedom. The SHOW statement in the PLM procedure reveals the contents of the item store in terms of ODS tables, and the SCORE statement computes predicted values in a new data set. For more information about postprocessing tasks based on item stores, see the documentation for the PLM procedure.

Syntax: STORE Statement

```
STORE <OUT=>item-store-name </ LABEL='label'> ;
```

The *item-store-name* is a usual one- or two-level SAS name, like the names that are used for SAS data sets. If you specify a one-level name, then the item store resides in the WORK library and is deleted at the end of the SAS session. Since item stores usually are used to perform postprocessing tasks, typical usage specifies a two-level name of the form libname.membername.

If an item store by the same name as specified in the STORE statement already exists, the existing store is replaced.

You can add a custom label with the LABEL= option in the STORE statement after the slash (/). When the PLM procedure processes an item store, the label appears in the PROC PLM output along with other identifying information.

TEST Statement

This statement documentation applies to the following procedures: LIFEREG, ORTHOREG, PLM, PROBIT, SURVEYPHREG, and SURVEYREG. It also applies to the RELIABILITY procedure in SAS/QC software.

The TEST statement enables you to perform F tests for model effects that test Type I, II, or Type III hypotheses. See Chapter 15, “The Four Types of Estimable Functions,” for details about the construction of Type I, II, and III estimable functions.

Syntax: TEST Statement

TEST < *model-effects* > < / *options* > ;

Table 19.32 summarizes options in the TEST statement.

Table 19.32 TEST Statement Options

Option	Description
CHISQ	Requests chi-square tests
DDF=	Specifies denominator degrees of freedom for fixed effects
E	Requests Type I, Type II, and Type III coefficients
E1	Requests Type I coefficients
E2	Requests Type II coefficients
E3	Requests Type III coefficients
HTYPE=	Indicates the type of hypothesis test to perform
INTERCEPT	Adds a row that corresponds to the overall intercept

You can specify the following options in the TEST statement after the slash (/):

CHISQ

requests that chi-square tests be performed for the relevant effects in addition to the *F* tests. Type III tests are the default; you can produce the Type I and Type II tests by using the HTYPE= option. This option has no effect when the procedure produces chi-square statistics by default.

DDF=*value-list*

DF=*value-list*

specifies the denominator degrees of freedom for the fixed effects. The *value-list* specification is a list of numbers or missing values (.) separated by commas. The order of degrees of freedom should match the order of the fixed effects that are specified in the TEST statement; otherwise it should match the order in which the effects appear in the “Type III Tests of Fixed Effects” table. If you want to retain the default degrees of freedom for a particular effect, use a missing value for its location in the list. In the following example, the first TEST statement assigns 3 denominator degrees of freedom to A and 4.7 to A*B, while those for B remain the same, and the second TEST statement assigns 5 denominator degrees of freedom to A and uses the default degrees of freedom for B.

```
model Y = A B A*B;
test / ddf=3, ., 4.7;
test B A / ddf=., 5;
```

E

requests that Type I, Type II, and Type III L matrix coefficients be displayed for all relevant effects.

E1 | EI

requests that Type I L matrix coefficients be displayed for all relevant effects.

E2 | EII

requests that Type II **L** matrix coefficients be displayed for all relevant effects.

E3 | EIII

requests that Type III **L** matrix coefficients be displayed for all relevant effects.

HTYPE=*value-list*

indicates the type of hypothesis test to perform on the fixed effects. Valid entries for values in the *value-list* are 1, 2, and 3, which correspond to Type I, Type II, and Type III tests, respectively. The default value is 3.

INTERCEPT**INT**

adds a row to the tables for Type I, II, and III tests that correspond to the overall intercept.

ODS Table Names: TEST Statement

Each table created by the **TEST** statement has a name associated with it, and you can use this name to refer to the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in Table 19.33. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

Table 19.33 ODS Tables Produced by the **TEST** statement

Table Name	Description	Required Option
Coef	L matrix coefficients	E
Tests1	Type I tests of fixed effects	HTYPE=1
Tests2	Type II tests of fixed effects	HTYPE=2
Tests3	Type III tests of fixed effects	Default

Programming Statements

This section applies to the following procedures:

CALIS, GLIMMIX, MCMC, NLIN, NLMIXED, PHREG, and SURVEYPHREG.

The majority of the SAS/STAT modeling procedures can take advantage of the fact that the statistical model can easily be translated into programming syntax (statements and options). However, several procedures require additional flexibility in specifying models—for example, when the model contains general nonlinear functions, when it is necessary to specify complicated restrictions, or when user-supplied expressions need to be evaluated. Procedures that are listed at the beginning of the section support—in addition to the usual procedure statements and options—programming statements that can be used in the SAS DATA step.

The following are valid statements:

```

ABORT;
ARRAY arrayname < [ dimensions ] > < $ > < variables-and-constants >;
CALL name < (expression < , expression ... >) >;
DELETE;
DO < variable = expression < TO expression > < BY expression > >
    < , expression < TO expression > < BY expression > > ...
    < WHILE expression > < UNTIL expression >;
END;
GOTO statement-label;
IF expression;
IF expression THEN program-statement;
    ELSE program-statement;
variable = expression;
variable + expression;
LINK statement-label;
PUT < variable > < = > ...;
RETURN;
SELECT < (expression) >;
STOP;
SUBSTR(variable, index, length)= expression;
WHEN (expression)program-statement;
    OTHERWISE program-statement;

```

For the most part, these programming statements work the same as they do in the SAS DATA step, as documented in *SAS Language Reference: Concepts*. However, there are several differences:

- The ABORT statement does not allow any arguments.
- The DO statement does not allow a character index variable. Thus

```
do i = 1,2,3;
```

is supported, whereas the following statement is not supported:

```
do i = 'A', 'B', 'C';
```

- Not all procedures support LAG functionality. For example, the GLIMMIX procedure does not support lags.
- The PUT statement, used mostly for program debugging, supports only some of the features of the DATA step PUT statement, and it has some features that are not available with the DATA step PUT statement:
 - The PUT statement does not support line pointers, factored lists, iteration factors, overprinting, `_INFILE_`, the colon (:) format modifier, or “\$”.
 - The PUT statement does support expressions, but the expression must be enclosed in parentheses. For example, the following statement displays the square root of x:

```
put (sqrt(x));
```

- The PUT statement supports the item `_PDV_` to display a formatted listing of all variables in the program. For example:

```
put _pdv_;
```

- The WHEN and OTHERWISE statements enable you to specify more than one target statement. That is, DO/END groups are not necessary for multiple-statement WHENs. For example, the following syntax is valid:

```
select;
  when (exp1) stmt1;
           stmt2;
  when (exp2) stmt3;
           stmt4;
end;
```

- The LINK statement is used in a program to jump immediately to the label *statement_label* and to continue program execution at that point. It is not used to specify a link function in a generalized linear model.

Please consult the individual chapters for other, procedure-specific differences between programming statements and the SAS DATA step and for procedure-specific details, limitations, and rules.

When coding your programming statements, avoid defining variables that begin with an underscore (`_`), because they might conflict with internal variables that are created by procedures that support programming statements.

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Chapter 20

Using the Output Delivery System

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Overview: Using the Output Delivery System

Most SAS procedures use the Output Delivery System (ODS) to manage their output. ODS enables you to do the following:

- display your output in hypertext markup language (HTML), rich text format (RTF), portable document format (PDF), PostScript, SAS listing, or other formats
- create SAS data sets directly from tables or graphs
- select or exclude individual pieces of output
- customize the layout, format, headers, and style of your output
- produce graphs with ODS Graphics (see Chapter 21, “[Statistical Graphics Using ODS](#)”)

This chapter discusses some typical applications of ODS with SAS software. For complete documentation about the Output Delivery System, see the *SAS Output Delivery System: User’s Guide*. For more information about ODS Graphics, see Chapter 21, “[Statistical Graphics Using ODS](#),” and Chapter 22, “[ODS Graphics Template Modification](#).”

Output Defaults

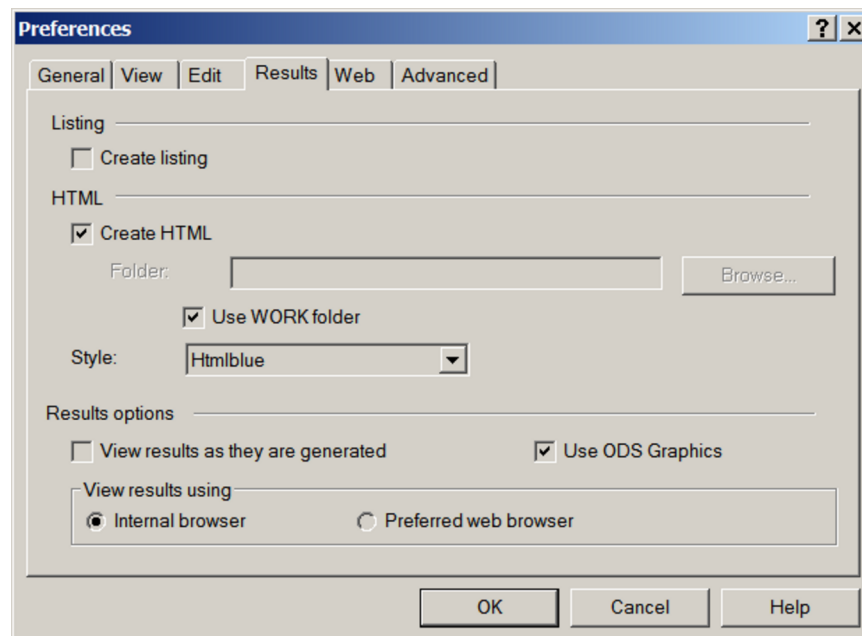
HTML output with ODS Graphics enabled is the default in the SAS windowing environment for Microsoft Windows and UNIX. LISTING output with ODS Graphics disabled is the default when you run SAS in batch mode or on the mainframe. Your actual defaults might be different due to your registry, system option, or configuration file settings. The following sections explain these defaults and how to change them.

HTML Output in the SAS Windowing Environment

The default destination in the SAS windowing environment is HTML and ODS Graphics is enabled by default.¹ These defaults have several advantages. Graphs are integrated with tables, and all output is displayed in the same HTML file. The HTML destination uses the HTMLBLUE style, which is an all-color style, that is designed to integrate tables and modern statistical graphics.

You can view and modify the default settings by selecting **Tools ► Options ► Preferences** from the menu at the top of the main SAS window. Then click the **Results** tab. You can remember this sequence using the mnemonic TOPR (pronounced “topper”). See [Figure 20.1](#).

¹HTML output with ODS Graphics enabled is the default in the SAS windowing environment for Microsoft Windows and UNIX, but not on the mainframe.

Figure 20.1 SAS Results Tab with the Default Settings

The default settings are as follows:

- HTML output is created when **Create HTML** is selected, and all output is viewed in the Results Viewer window.
- ODS Graphics is enabled when **Use ODS Graphics** is selected.
- The default style, HTMLBLUE, is selected from the **Style** list.
- Results are viewed in an internal SAS browser when **Internal browser** is selected.
- Graph image files are saved in the Work folder (not in your current folder) when **Use WORK folder** is selected.
- LISTING output is not created when the **Create listing** box is cleared.

In many cases, graphs are an integral part of a data analysis. However, when you run large computational programs (such as when you use procedures with many BY groups), you might not want to create graphs. In those cases, you should disable ODS Graphics, which will improve the performance of your program. You can disable and re-enable ODS Graphics in your SAS programs with the ODS GRAPHICS OFF and ODS GRAPHICS ON statements. You can also change the ODS Graphics default in the **Results** tab.

In the SAS windowing environment, the current folder is displayed in the status line at the bottom of the main SAS window. When **Use WORK folder** is cleared, graph image files are saved in the current folder and are available after your SAS session ends. They can accumulate with time and take up a great deal of space. When **Use WORK folder** is selected, graph image files are stored in the Work folder and are not available after your SAS session ends.

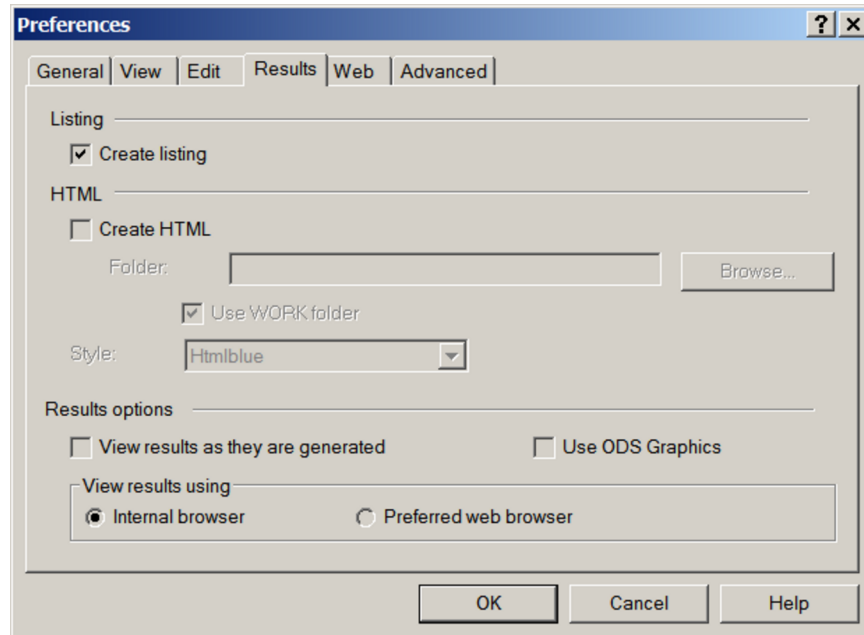
LISTING Output in the SAS Windowing Environment

In the LISTING destination, tables are displayed in monospace, and graphs are not integrated with tables. You can create LISTING output by selecting **Tools ► Options ► Preferences** from the menu at the top of the main SAS window. Then click the **Results** tab. Select **Create listing**, and clear **Create HTML**. See

Figure 20.2. Tabular results are viewed in the Output window. Graphical results are viewed by selecting graphs in the Results window.

You can enable or disable ODS Graphics by default by using the **Use ODS Graphics** check box, and you can use the ODS GRAPHICS ON and ODS GRAPHICS OFF statements to enable and disable ODS Graphics in your SAS programs.

Figure 20.2 SAS Results Tab for LISTING Output



Assumptions about ODS Defaults in this Chapter

Default settings such as destinations and whether ODS Graphics is enabled vary depending on your operating system, registry settings, configuration file settings, system options, and whether you are using the SAS windowing environment or batch mode. For this reason, this chapter makes no assumptions about these defaults. Instead, all destinations are explicitly closed before some steps without assuming which destination (usually LISTING or HTML) is open, destinations are explicitly opened when needed, and ODS Graphics is explicitly enabled and disabled as needed. In some examples, when all destinations are closed, the LISTING destination is opened at the end of the step so that some destination is available for subsequent output. If you know the defaults for your environment, you do not need to use many of the ODS statements that are used in this chapter.

The HTMLBLUE Style

In the SAS windowing environment, the default ODS style for HTML output is the HTMLBLUE style. However, if you use the ODS HTML statement in batch mode, the default style is DEFAULT. You can see examples of the HTMLBLUE style in this chapter in [Output 20.1.1](#), [Output 20.8.2](#), and [Output 20.8.3](#). The HTMLBLUE style inherits most of its attributes from the STATISTICAL style, but it has a brighter appearance and color coordination between the tables and graphs. In the HTMLBLUE style, the dominant color is blue; in the DEFAULT style, the dominant color is gray. See Chapter 21, “Statistical Graphics Using ODS,” for a comparison of the HTMLBLUE style and other styles.

Default Open Destination

By default, either the LISTING or the HTML destination is open. You can change the default destination three ways, which are described in the next three subsections. The fourth subsection of this section explains how to use ODS statements to open and close destinations.

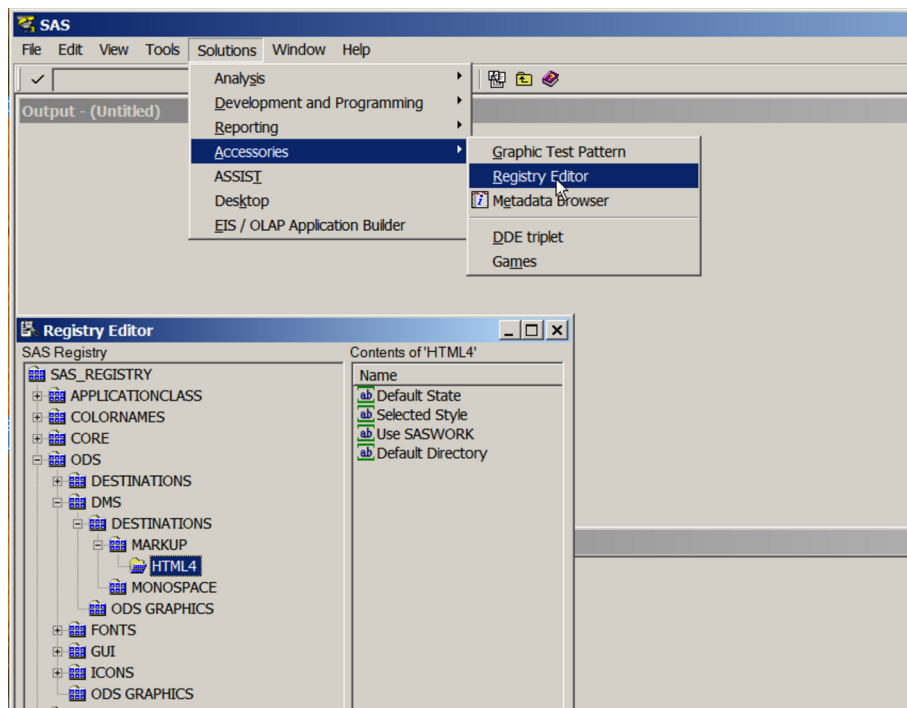
Setting the Default Destination in the Results Tab

You can change the default destination in the SAS windowing environment by selecting **Tools ► Options ► Preferences** from the menu at the top of the main SAS window. Then select the **Results** tab. See sections “HTML Output in the SAS Windowing Environment” on page 512 and “LISTING Output in the SAS Windowing Environment” on page 513. Changing defaults in the SAS windowing environment affects only the SAS windowing environment; it does not affect batch jobs.

Setting the Default Destination in the SAS Registry

You can change the default destination by editing the SAS registry (see Figure 20.3) or by changing system options in your SAS configuration file.

Figure 20.3 SAS Registry Window



Registry customization is generally performed by more advanced users who have experience and knowledge about the SAS System and their operating environment. Incorrect registry entries can corrupt your SAS registry. For more information about SAS configuration files and the SAS registry, see the *SAS Companion* for your operating system.

Setting the Default Destination in SAS System Options

The ODSDEST system option controls the default destination. This option is specified only at SAS start-up time. Other relevant system options that correspond to entries in the **Results** tab in Figure 20.1 include ODSGRAPHICS (which specifies whether ODS Graphics is enabled by default) and ODSSTYLE (which specifies the default style for the HTML destination in the SAS windowing environment). See the *SAS System Options: Reference* for more information.

Setting the Destination in ODS Statements

You can use ODS destination statements to explicitly set destinations. These statements are described in this chapter and in detail in the *SAS Output Delivery System: User's Guide*. When you open a new destination, you should close all other open destinations unless you really need multiple destinations to be open. When multiple destinations are open, each piece of output is created multiple times, once per destination. Closing unneeded destinations increases efficiency.

You can create HTML output in any environment by using the ODS HTML statement as in the following example:

```
ods _all_ close;
ods html file='MyFile.html';

proc reg data=sashelp.class;
  model height=weight;
run; quit;

ods html close;
ods listing;
```

The first statement closes all open destinations. The second statement opens the HTML destination and specifies the HTML output file *MyFile.html*. The last two statements close the HTML destination and open the LISTING destination for subsequent output.

You can create LISTING output in any environment by using the ODS LISTING statement as in the following example:

```
ods _all_ close;
ods listing;

proc reg data=sashelp.class;
  model height=weight;
run; quit;
```

The first statement closes all open destinations. The second statement opens the LISTING destination which sends output to the SAS listing. In this example, the LISTING destination is not closed so that subsequent steps can append more information to the listing.

If the LISTING destination is open, then you can simultaneously create LISTING and HTML output as follows:

```
* The ODS LISTING destination is not closed,
  which is not recommended for efficiency reasons;

ods html file='Reg.htm';
```

```
proc reg data=sashelp.class;
    model height=weight;
run; quit;

ods html close;
```

Sometimes you see ODS Graphics notes or warnings multiple times when multiple destinations are open. The messages appear once for each affected graph for each destination.

Output Objects and ODS Destinations

All SAS procedures produce *output objects* that ODS delivers to various *ODS destinations*, according to the default specifications for the procedure or according to your own specifications. Typically, you see the output objects displayed as tables, data sets, or graphs. Underlying all output (for example, a table of parameter estimates) are two component parts:

- the data component, which consists of the results computed by a SAS procedure
- the template, which contains the instructions for formatting and displaying the results

Each output object has an associated template, provided by the SAS System, that defines its presentation format. You can use the `TEMPLATE` procedure to view or alter these templates or to create new templates by changing the headers, formats, column order, and so on. For more information, see the chapter titled “The Template Procedure” in the *SAS Output Delivery System: User’s Guide*.

You define the form that the output should take by specifying an ODS destination. Some supported destinations are as follows:

- LISTING, the standard SAS monospace listing
- HTML, for viewing in a browser
- RTF, for inclusion in Microsoft Word
- PDF, PostScript, and PCL, for high-fidelity printers
- OUTPUT, for saving results to SAS data sets
- DOCUMENT, for saving, modifying, and replaying your output

You can open multiple ODS destinations at the same time so that a single procedure step can produce output for multiple destinations. If you do not supply any ODS statements, ODS delivers all output to the default destination (which is usually LISTING or HTML). See the section “[Output Defaults](#)” on page 512 for more information about default destinations. You can specify an output style for each ODS destination. The style controls the foreground, background, colors, lines, fonts, and so on.

The following statements provide an example of temporarily closing all open destinations for PROC REG and then opening the LISTING destination for PROC PRINT. PROC REG with the ODS OUTPUT statement makes an output data set, `Parms`, from the parameter estimates table. Closing unneeded open destinations is not required, but it is done in many examples in this chapter for efficiency. Closing the superfluous destinations suppresses the generation of output that is not needed or used. This is particularly beneficial with graphics. This example uses the `Sashelp.Class` data set, one of the sample data sets in the Sashelp library that are automatically available for your use. The following statements produce [Figure 20.4](#):


```

title 'Getting Started with ODS';

ods _all_ close;

proc reg data=sashelp.class;
  model height=weight;
  ods output ParameterEstimates=parms;
run; quit;

ods listing;

proc print noobs data=parms;
run;

```

The ODS OUTPUT statement contains an object name, an equal sign, and the name of the output SAS data set to create. You can use the ODS TRACE statement to find the object names. The ODS TRACE statement is described in the section “[Paths and Selection](#)” on page 519. Also see [Example 20.4](#) for more information.

Figure 20.4 PROC REG Parameter Estimates Table

Getting Started with ODS							
Model	Dependent	Variable	DF	Estimate	StdErr	tValue	Probt
MODEL1	Height	Intercept	1	42.57014	2.67989	15.89	<.0001
MODEL1	Height	Weight	1	0.19761	0.02616	7.55	<.0001

You could accomplish the same thing using ODS SELECT statements as follows:

```

ods select none;

proc reg data=sashelp.class;
  model height=weight;
  ods output ParameterEstimates=parms;
run; quit;

ods select all;

proc print noobs data=parms;
run;

```

You can specify ODS EXCLUDE ALL instead of ODS SELECT NONE and ODS EXCLUDE NONE instead of ODS SELECT ALL. These statements remain in effect until a new ODS SELECT or ODS EXCLUDE statement changes the selection list.

The ODS Statement

You use the ODS statement to provide instructions to ODS. You can use the ODS statement to specify options for different destinations, specify the output style, and select and exclude output. Here are some examples:

```
/* open the HTML destination with the HTMLBlue style */
ods html style=HTMLBlue;

/* select only the parameter estimates table */
ods select ParameterEstimates;

/* output the parameter estimates table to a SAS data set*/
ods output ParameterEstimates=Parms;

/* exclude the number of observations, ANOVA, and fit statistics tables */
ods exclude NObs ANOVA FitStatistics;
```

Paths and Selection

Each output output (tables, graphs, notes, and so on) produced by a SAS procedure has a name and a label. Each name is part of a name path. For example, PROC GLM has a table called ErrorSSCP, and the name path (fully qualified name) is **GLM.Repeated.MANOVA.Model.Error.ErrorSSCP**. Each level in the name path corresponds to a part of the PROC GLM hierarchy of output. Each piece of output also has a label and a label path. For example, the PROC GLM ErrorSSCP table is labeled '**SSCP Matrix**', and the label path is '**The GLM Procedure**'.'**Repeated Measures Analysis**'.'**MANOVA**'.'**Model**'.'**Error**'.'**SSCP Matrix**'.

You need to know the name or label to select, exclude, or modify a table or graph. You can obtain this information in several ways:

- You can obtain names from the individual procedure documentation chapter or from the individual procedure section of the SAS online Help system. See the sections “ODS Table Names” and “ODS Graphics” from within the “Details” section of the procedure documentation chapter.
- You can use the SAS Results window to view the name of each piece of output that is created in your SAS session (see the section “[The SAS Results Window](#)” on page 523 for more information).
- You can use the ODS TRACE statement to find the name and label of each piece of output that is created in your SAS session. The ODS TRACE statement writes identifying information to the SAS log or listing for each generated output object.

If you are working interactively with reasonably small data sets, then the ODS TRACE statement is usually the most convenient way to find the names. Specify the ODS TRACE ON statement prior to the procedure statements that create the output for which you want information. For example, the following statements write the trace record for the output created in the REG procedure step:

```
ods trace on;
ods graphics on;
proc reg data=sashelp.class;
  model weight=height;
  model age=height;
run; quit;
ods trace off;
```

By default, the trace output is written to the SAS log. Some of the trace output from the previous step is as follows:

Output Added:

```
-----
Name:          NObs
Label:         Number of Observations
Template:      Stat.Reg.NObs
Path:         Reg.MODEL1.Fit.Weight.NObs
-----
```

Output Added:

```
-----
Name:          ANOVA
Label:         Analysis of Variance
Template:      Stat.REG.ANOVA
Path:         Reg.MODEL1.Fit.Weight.ANOVA
-----
```

Output Added:

```
-----
Name:          FitStatistics
Label:         Fit Statistics
Template:      Stat.REG.FitStatistics
Path:         Reg.MODEL1.Fit.Weight.FitStatistics
-----
```

Output Added:

```
-----
Name:          ParameterEstimates
Label:         Parameter Estimates
Template:      Stat.REG.ParameterEstimates
Path:         Reg.MODEL1.Fit.Weight.ParameterEstimates
-----
```

Output Added:

```
-----
Name:          DiagnosticsPanel
Label:         Fit Diagnostics
Template:      Stat.REG.Graphics.DiagnosticsPanel
Path:         Reg.MODEL1.ObswiseStats.Weight.DiagnosticPlots.DiagnosticsPanel
-----
```

Output Added:

```
-----
Name:      ResidualPlot
Label:     Height
Template:  Stat.REG.Graphics.ResidualPlot
Path:     Reg.MODEL1.ObswiseStats.Weight.ResidualPlots.ResidualPlot
-----
```

Output Added:

```
-----
Name:      FitPlot
Label:     Fit Plot
Template:  Stat.REG.Graphics.Fit
Path:     Reg.MODEL1.ObswiseStats.Weight.FitPlot
-----
```

Output Added:

```
-----
Name:      NObs
Label:     Number of Observations
Template:  Stat.Reg.NObs
Path:     Reg.MODEL2.Fit.Age.NObs
-----
```

.
.
.

Output Added:

```
-----
Name:      FitPlot
Label:     Fit Plot
Template:  Stat.REG.Graphics.Fit
Path:     Reg.MODEL2.ObswiseStats.Age.FitPlot
-----
```

Alternatively, you can specify the LISTING option (`ods trace on / listing;`), which writes the trace record, interleaved with the procedure output, to the LISTING destination (if it is open).

The trace record contains the name of each output object created and its associated label, template, and fully qualified name path. The label provides a description of the table or graph. The fully qualified name path shows the output hierarchy. (An example of the hierarchy is shown in [Figure 20.5](#). The SAS Results window displays the labels, rather than the names of objects, but the hierarchy is the same for both names and labels.) The hierarchy has a level for the REG procedure, a level for the model (MODEL1 or MODEL2), a level for the fit results, a level for the dependent variable (Weight or Age), and a level for the name (for example, NObs, ANOVA, FitStatistics, ParameterEstimates).

When you specify ODS objects in an ODS statement, you can often omit the first few levels and instead use a partially qualified name path. A partially qualified name path consists of any part of the fully qualified name path that begins immediately after a period and continues to the end of the fully qualified name path. For example, the table `Reg.Model1.Fit.Weight.ParameterEstimates` can be referenced in any of the following ways:

<code>ParameterEstimates</code>	name
<code>Weight.ParameterEstimates</code>	partially qualified name path
<code>Fit.Weight.ParameterEstimates</code>	partially qualified name path
<code>Model1.Fit.Weight.ParameterEstimates</code>	partially qualified name path
<code>Reg.Model1.Fit.Weight.ParameterEstimates</code>	fully qualified name path

When a procedure creates multiple output objects that have the same name, as shown in the preceding trace output, you have several selection options for referring to the object. You can specify the name, a fully qualified name path, or a partially qualified name path in ODS statements such as ODS SELECT, ODS EXCLUDE, or ODS OUTPUT. You can also specify a WHERE clause. For example, you can specify any of the following statements (in addition to other possibilities) to display both tables of parameter estimates:

```
ods select ParameterEstimates;

ods select Weight.ParameterEstimates Age.ParameterEstimates;

ods select Reg.Model1.Fit.Weight.ParameterEstimates
           Reg.Model2.Fit.Age.ParameterEstimates;

ods select where = (_path_ ? 'Parameter');
```

The first ODS SELECT statement specifies the object name, which is shared by both tables. The second statement specifies a partially qualified name path for both tables. The third statement specifies the fully qualified name path for each table. The fourth statement selects every object that contains the string 'Parameter' anywhere in its path.

In the first three statements, selection is case insensitive. Any combination of uppercase and lowercase letters works. This is not true in the fourth statement, which uses an ordinary SAS comparison of character strings. For case insensitivity in WHERE clause selection, use the LOWCASE function as in the following example:

```
ods select where = (lowcase(_path_) ? 'parameter');
```

You can also select objects based on a WHERE clause and the label path. The following statements turn on the trace record, display a label path in addition to the name path, and select all objects that have the string 'var' in the label:

```
ods trace on / label;
ods select where = (lowcase(_label_) ? 'var');
```

A subset of the trace record for PROC REG with this ODS SELECT list, showing just the name path and label path, is as follows:

```
Path:          Reg.MODEL1.Fit.Weight.ANOVA
Label Path:    'The Reg Procedure'. 'MODEL1'. 'Fit'.Weight. 'Analysis of Variance'
Path:          Reg.MODEL2.Fit.Age.ANOVA
Label Path:    'The Reg Procedure'. 'MODEL2'. 'Fit'.Age. 'Analysis of Variance'
```

The ODS SELECT statement selects the ANOVA tables, because they have the string '**Analysis of Variance**' (which when lowercased contains '**var**') in their labels. WHERE clause selection is also useful for selecting all of the objects within a group or level of the path hierarchy (the group '**MODEL2**' or '**Fit**'). You can specify any part of the name path or label path—for example, '**.Age.**' matches the variable **Age** and ignores any '**Age**' that might be in the middle of a word, '**2.F**' matches Model 2 fit tables and any other object that has the string '**2.F**' in its path, and so on.

ODS records the specified object names in its internal selection or exclusion list, and then it processes the output it receives. ODS maintains an overall selection or exclusion list that pertains to all ODS destinations, and it maintains a separate selection or exclusion list for each ODS destination. The list for a specific destination provides the primary filtering step. The restrictions that you specify in the overall list are added to the destination-specific lists.

Suppose, for example, that your LISTING exclusion list (that is, the list of objects you want to exclude from the LISTING destination) contains the **FitStatistics** table, which you specify with the following statement:

```
ods listing exclude FitStatistics;
```

Suppose also that your overall selection list (that is, the list of objects you want to select for all destinations) contains the tables **ParameterEstimates** and **FitStatistics**, which you specify with the following statement:

```
ods select ParameterEstimates FitStatistics;
```

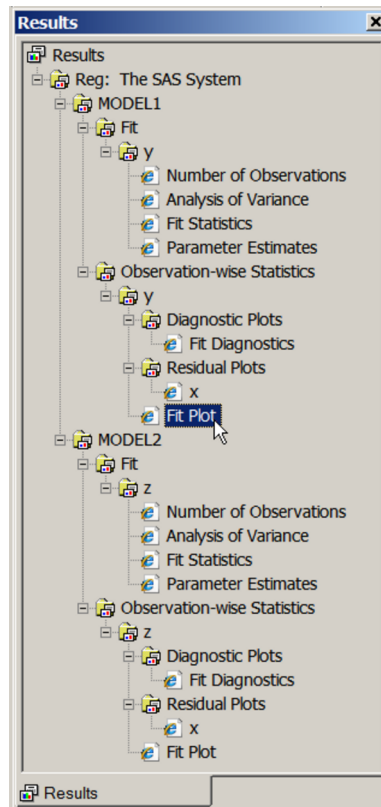
ODS then sends only the **ParameterEstimates** and **FitStatistics** tables to all open destinations except the LISTING destination. It sends only the **ParameterEstimates** table to the LISTING destination because the table **FitStatistics** is excluded from that destination.

RUN-Group Processing

Some SAS procedures, such as PROC REG and PROC GLM, support RUN-group processing, which means that a RUN statement does not end the procedure. A QUIT statement explicitly ends such procedures. If you omit the QUIT statement, a PROC or a DATA statement implicitly ends such procedures. When you use ODS with procedures that support RUN-group processing, it is good programming practice to specify a QUIT statement at the end of the procedure. This causes ODS to clear the selection or exclusion list, and you are less likely to encounter unexpected results.

The SAS Results Window

The SAS Results window contains a running record of the output from your SAS session. In the SAS windowing environment, select **View ► Results** to open the Results window. [Figure 20.5](#) displays the Results window from the PROC REG step shown previously.

Figure 20.5 The Results Window from the SAS Explorer

When you click the output names in the Results window, you link directly to the output in the Output Results window (for the HTML destination) or the Output window or graph viewer window (for the LISTING destination). The Results window contains an entry for each level of the label path and for each object. You can also use the Results window to determine the names of the templates associated with each object. Right-click the name, and then select **Properties**. You can see all of the templates from the Results window by selecting **View ► Templates ► Sashelp.Tmplmst**. Then click a product such as **Stat**, a procedure such as **REG**, and a template such as **ParameterEstimates**.

The ODS PATH Statement

The ODS PATH statement controls where ODS stores new templates that you create and where ODS finds the templates that your programs use.² Compiled templates are stored in a template store, which is a type of item store. (An item store is a special type of SAS file.)

By default, the templates that you write are stored in `Sasuser.Templat`, and the templates that the SAS System provides are stored in `Sashelp.Tmplmst`. Templates are found in `Sashelp.Tmplmst` unless you compile and store them in `Sasuser.Templat`.

You can see the list of active template stores by submitting the following statement:

²Other types of paths include the name path and label path, which are discussed in the section “Paths and Selection” on page 519.

```
ods path show;
```

By default, the results are as follows:

```
Current ODS PATH list is:
```

1. SASUSER.TEMPLAT (UPDATE)
2. SASHELP.TMPLMST (READ)

You can see a list of all of the templates in a template store as follows:

```
proc template;
  list / store=sasuser.templat;
run;
```

See the sections “The Master Template Store” on page 525 and “Controlling Output Appearance with Templates” on page 526 for more information about the template search path and template stores.

The Master Template Store

By default, the ODS path includes the name of the template store that provides the templates that are shipped with the SAS system. You can use the ODS PATH SHOW statement to see the list of active template stores:

```
ods path show;
```

By default, the results are as follows:

```
Current ODS PATH list is:
```

1. SASUSER.TEMPLAT (UPDATE)
2. SASHELP.TMPLMST (READ)

The ODS PATH statement template search path name Sashelp.Tmplmst refers to the template stores that are shipped with the SAS System. More precisely, the ODS PATH name Sashelp.Tmplmst refers to multiple template store files including Sashelp.Tmplmst, Sashelp.Tmplstat, Sashelp.Tmplets, Sashelp.Tmplqc, Sashelp.Tmpliml, and others. The name Sashelp.Tmplmst refers to both the entire template store that is shipped with the SAS System and one particular file in that template store. In earlier releases of the SAS System, there was just one template store file, namely Sashelp.Tmplmst, and there was a one-to-one correspondence between the ODS PATH statement name and the template store file name. Now there are multiple files (because certain products have their own template store files), but the ODS PATH statement syntax for selecting all of them is unchanged. You do not need to be concerned about this, and you should not specify any of these template stores individually. You simply specify Sashelp.Tmplmst to get the item stores that are shipped with the SAS System. However, you will see these other names sometimes in the SAS log and output when you are working with templates, so you need to know what that means.

If you see a template store name of the form Sashelp followed by a period and a name, it refers to part of the overall template store that you can reference with the name Sashelp.Tmplmst. For example, submit the following step:


```
proc template;
  source Stat.REG.ANOVA;
run;
```

The following is displayed in the SAS log file:

```
NOTE: Path 'Stat.Reg.ANOVA' is in: SASHELP.TMPLSTAT.
```

Submit the following step:

```
proc template;
  list Stat.REG;
  list ETS.ARIMA;
  list QC.Shewhart;
run;
```

The names Sashelp.Tmplstat, Sashelp.Tmpltets, and Sashelp.Tmplqc are displayed in the headers of the tables that list the procedure templates.

Controlling Output Appearance with Templates

A template is a description of how output should appear when it is formatted. Templates describe several characteristics of the output, including headers, column ordering, style information, justification, and formats. Each object in the output has a template, and all SAS templates are stored in the Sashelp library. You can find the template associated with a particular output object or table column by using the ODS TRACE statement or the SAS Results window. You can create or modify a template with the `TEMPLATE` procedure. For example, you can specify different column headings or different orders of columns in a table.

There are a number of different types of templates including column and table templates, graphical templates, and style templates. A column or table template applies to the specific columns or tables that refer to the template. Graphical templates are discussed in more detail in Chapter 21, “[Statistical Graphics Using ODS](#).” A style template applies to an entire SAS program, including all tables and graphs, and can be specified with the `STYLE=` option in a valid ODS destination, such as HTML, RTF, or PDF. You can specify a style as follows:

```
ods html style=HTMLBlue;
```

A style template controls stylistic elements such as colors, fonts, and presentation attributes. You can change the style to give your output different looks and color schemes. You can also refer to style information in table templates for individual headers and data cells. You can modify all types of templates with `PROC TEMPLATE`. For information about creating your own styles, see the *SAS Output Delivery System: User's Guide*.

You can display the contents of a template by running `PROC TEMPLATE` with a `SOURCE` statement and a template name, as in the following example:

```
proc template;
  source Stat.REG.ANOVA;
  source Stat.GLM.OverallANOVA;
run;
```

In many cases, a template definition is based at least in part on another template. When you see the `PAR-ENT=template` option in a template definition, you need to look at the specified template to learn more about the rest of the template definition. To illustrate, consider the following PROC GLM step:

```
proc glm data=sashelp.class;
  model height=weight;
run; quit;
```

The ANOVA table from this step is displayed in [Figure 20.6](#).

Figure 20.6 PROC GLM ANOVA Table with the Default Template

Getting Started with ODS					
The GLM Procedure					
Dependent Variable: Height					
Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	1	364.5762619	364.5762619	57.08	<.0001
Error	17	108.5879486	6.3875264		
Corrected Total	18	473.1642105			

The sums of squares and mean squares are presented with eight decimal places. You can change the templates to change the formats of those columns to use fewer decimal places. First, you can use the ODS TRACE statement when you run PROC GLM to determine the name of the template:

```
ods trace output;
proc glm data=sashelp.class;
  model height=weight;
run; quit;
ods trace off;
```

The trace output results include the following:

```
Output Added:
-----
Name:      OverallANOVA
Label:     Overall ANOVA
Template:  stat.GLM.OverallANOVA
Path:     GLM.ANOVA.Height.OverallANOVA
-----
```

From this, you can see that the template for the overall ANOVA table is `stat.GLM.OverallANOVA`. You can submit the following statements to see the overall ANOVA table template:

```
proc template;
  source stat.glm.overallanova;
run;
```

The results are as follows:

```
define table Stat.GLM.Overallanova;
  notes "Over-all ANOVA";
  top_space = 1;
  parent = Stat.GLM.ANOVA;
  double_space;
end;
```

The results show that this template inherits its definition from a parent template named `Stat.GLM.ANOVA`. Submit the following statements to see the parent template:

```
proc template;
  source stat.glm.anova;
run;
```

Some of the results are as follows:

```
define SS;
  parent = Stat.GLM.SS;
end;

define MS;
  parent = Stat.GLM.MS;
end;
```

These columns inherit their definitions from the parent columns named `Stat.GLM.SS` and `Stat.GLM.MS`. This is all of the information that you need to redefine these columns, but you can run PROC TEMPLATE again as follows to see more information about how these templates are defined:

```
proc template;
  source Stat.GLM.SS;
  source Stat.GLM.MS;
run;
```

The results are as follows:

```
define column Stat.GLM.Ss;
  notes "Parent for GLM ANOVA Sums of Squares columns";
  parent = Common.ANOVA.SS;
end;
define column Stat.GLM.Ms;
  notes "Parent for GLM ANOVA Mean Squares columns";
  parent = Common.ANOVA.MS;
end;
```

These columns inherit their definitions from the columns named `Common.ANOVA.SS` and `Common.ANOVA.MS`. You can run PROC TEMPLATE as follows to see their definitions:

```
proc template;
  source Common.ANOVA.SS;
  source Common.ANOVA.MS;
run;
```

The results are as follows:

```
define column Common.ANOVA.Ss;
  notes "Default ANOVA Sum of squares column";
  header = "Sum of Squares";
  translate _val_=_ into "";
end;
define column Common.ANOVA.Ms;
  notes "Default ANOVA Mean square column";
  header = "Mean Square";
  translate _val_=_ into "";
end;
```

You can redefine `Common.ANOVA.SS` and `Common.ANOVA.MS` to change all **SS** and **MS** columns in ANOVA tables. This would be the most general redefinition. More specifically, you can redefine `Stat.GLM.SS` and `Stat.GLM.MS` to change **SS** and **MS** columns in ANOVA tables produced by PROC GLM. Finally, and most specifically, you can change the **SS** and **MS** columns in just the overall ANOVA table template.

In this example, the `Stat.GLM.SS` and `Stat.GLM.MS` columns are redefined as follows, so that results are displayed with fewer decimal places:

```
proc template;
  edit Stat.GLM.SS;
    choose_format=max format_width=8;
  end;
  edit Stat.GLM.MS;
    choose_format=max format_width=8;
  end;
run;
```

The `CHOOSE_FORMAT=MAX` option along with the `FORMAT_WIDTH=8` option chooses the format for each column based on the maximum value in that column and an overall width of eight. You are editing and not replacing the definition, so the column header and other information in the definition is not lost. The following step uses the new templates:

```
proc glm data=sashelp.class;
  model height=weight;
run; quit;
```

The new ANOVA results, using the edited templates, are shown in [Figure 20.7](#). You can see that the original results in [Figure 20.6](#) have eight decimal places, whereas the new results in [Figure 20.7](#) have only five decimal places and an overall format width of eight.

Figure 20.7 PROC GLM ANOVA Table after Template Customization

Getting Started with ODS					
The GLM Procedure					
Dependent Variable: Height					
Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	1	364.5763	364.5763	57.08	<.0001
Error	17	108.5879	6.3875		
Corrected Total	18	473.1642			

The preceding PROC TEMPLATE step produces the following notes:

```
NOTE: Overwriting existing template/link: Stat.GLM.Ss
NOTE: COLUMN 'Stat.GLM.Ss' has been saved to: SASUSER.TEMPLAT
NOTE: Overwriting existing template/link: Stat.GLM.Ms
NOTE: COLUMN 'Stat.GLM.Ms' has been saved to: SASUSER.TEMPLAT
```

When you run PROC TEMPLATE to modify or edit a template, the template is stored by default in your Sasuser library. You can delete your custom template and restore the default template as follows:

```
proc template;
  delete Stat.GLM.SS / store=sasuser.templat;
  delete Stat.GLM.MS / store=sasuser.templat;
run;
```

The preceding PROC TEMPLATE step produces the following notes:

```
NOTE: 'Stat.GLM.SS' has been deleted from: SASUSER.TEMPLAT
NOTE: 'Stat.GLM.MS' has been deleted from: SASUSER.TEMPLAT
```

It is good practice to delete any template redefinitions that you do not want to be permanent, because otherwise they persist beyond the duration of your SAS session. The option STORE=SASUSER.TEMPLAT is not required. However, if you have administrator privileges on your computer, this option helps you ensure that you do not accidentally delete templates from Sashelp.Tmplmst.

You can modify the template search path with the ODS PATH statement—for example, so you can access these new templates in a later SAS session. This enables you to create a new default set of templates to modify the display format for all of your SAS output. You can specify the SHOW option in the ODS PATH statement to determine the current template search path. The following statements illustrate the template search path:

```
ods path show;
libname mytpls '.';
ods path (prepend) mytpls.template(update);
ods path show;
```

```
proc template;
  edit Stat.GLM.SS;
    choose_format=max format_width=8;
  end;
  edit Stat.GLM.MS;
    choose_format=max format_width=8;
  end;
run;
```

The results of the first statement are as follows:

Current ODS PATH list is:

1. SASUSER.TEMPLAT (UPDATE)
2. SASHELP.TMPLMST (READ)

This shows that the Sasuser.Templat template store is open for storing new templates and retrieving templates for use. After that, the Sashelp.Tmplmst template store is used, but it is open only for read access.³ The LIBNAME and second ODS PATH statements add a template store to the front of this list in the current directory. The final ODS PATH SHOW statement shows the new template search path, which is as follows:

Current ODS PATH list is:

1. MYTPLS.TEMPLATE (UPDATE)
2. SASUSER.TEMPLAT (UPDATE)
3. SASHELP.TMPLMST (READ)

The PROC TEMPLATE step produces the following notes, which show that the templates are now stored in MYTPLS.TEMPLATE:

```
NOTE: Overwriting existing template/link: Stat.GLM.Ss
NOTE: COLUMN 'Stat.GLM.Ss' has been saved to: MYTPLS.TEMPLATE
NOTE: Overwriting existing template/link: Stat.GLM.Ms
NOTE: COLUMN 'Stat.GLM.Ms' has been saved to: MYTPLS.TEMPLATE
```

In all cases, the original template definitions in Sashelp.Tmplmst are not changed. You can delete your custom template and restore the default template as follows:

```
proc template;
  delete Stat.GLM.SS / store=mytpls.template;
  delete Stat.GLM.MS / store=mytpls.template;
run;
```

If you would like all template modifications to be automatically deleted at the end of your SAS session, you can modify the template search path so that an updatable template store is placed in the Work directory in the front of the current path in either of the two equivalent ways:

³Most SAS users cannot modify templates in Sashelp. However, if you have computer administrator privileges, you might be able to modify templates in Sashelp, so you should be careful to not do so.

```
ods path (prepend) work.templat(update);
ods path work.templat(update) sasuser.templat(update) sashelp.tmplmst(read);
```

Alternatively, you can replace Sasuser.Templat with Sashelp.Templat as follows:

```
ods path work.templat(update) sashelp.tmplmst(read);
```

When you are done, you can reset the default template search path as follows:

```
ods path reset;
```

ODS and the NOPRINT Option

Many SAS procedures support a NOPRINT option that you can use when you want to create an output data set without displaying any output. You use an option (such as the OUTEST= option or an OUTPUT statement with an OUT= option) in addition to the procedure's NOPRINT option to create a data set and suppress displayed output.

You can also use the ODS OUTPUT statement to create output data sets. However, if you specify the NOPRINT option, the procedure might not send any output to ODS. In most procedures that support a NOPRINT option, NOPRINT means no ODS. (However, there are a few procedures that for historical reasons still might produce some output even when NOPRINT is specified.) When you want to create output data sets through the ODS OUTPUT statement and you want to suppress the display of all output, specify the following statement instead of using the NOPRINT option:

```
ods select none;
```

Alternatively, you can close the active ODS destinations like this:

```
ods _all_ close;
```

ODS statements do not instruct a procedure to generate output. Instead, they specify how ODS should manage output after it is created. You must ensure that the proper procedure options are in effect, or the output is not generated. For example, the following statements do not create the requested data set ParmS because the SOLUTION option is not specified in the MODEL statement:

```
proc glm data=sashelp.class;
  ods output ParameterEstimates=ParmS;
  class sex;
  model height=sex;
run; quit;
```

Since PROC GLM did not create the table, ODS cannot make the output data set. When you execute these statements, the following message is displayed in the log:

```
WARNING: Output 'ParameterEstimates' was not created.
```

The following step creates the output data set:

```
proc glm data=sashelp.class;
  ods output ParameterEstimates=Parms;
  class sex;
  model height=sex / solution;
run; quit;
```

Examples: Using the Output Delivery System

This section provides examples of creating HTML output, selecting and excluding output, tracing ODS output, using the Results window, creating ODS output data sets, modifying templates, creating hyperlinks, and using ODS Graphics.

Example 20.1: Creating HTML Output with ODS

This example demonstrates how you can use the ODS HTML statement to display your output in HTML. The following statements create the data set `Scores`, which contains the golf scores of boys and girls in a physical education class:

```
title 'Comparing Group Means';

data Scores;
  input Gender $ Score @@;
  datalines;
f 75  f 76  f 80  f 77  f 80  f 77  f 73
m 82  m 80  m 85  m 85  m 78  m 87  m 82
;
```

The `TTEST` procedure is used to compare the scores. The ODS HTML statement specifies the name of the file to contain the HTML output. The following statements create the HTML file `ttest.htm`:

```
ods html body='ttest.htm' style=HTMLBlue;

proc ttest;
  class Gender;
  var Score;
run;

ods html close;
```

In many cases, the LISTING destination is open by default. See the section “Output Defaults” on page 512 for more information about default destinations. When the LISTING destination is open, the LISTING destination receives all output generated during your SAS session. In this example, the ODS HTML statement also opens the HTML destination, and both destinations receive the generated output. If you are in the SAS windowing environment and are using the internal browser, you do not need to close the HTML destination

before viewing your output. However, when you write to an HTML file, you must specify the following statement before you can view your output in an external browser:

```
ods html close;
```

If you do not close the HTML destination, your HTML file might contain no output or incomplete output, or you might experience other unexpected results.

The following statements use ODS to display the output in HTML with a table of contents:

```
ods _all_ close;
ods html body='ttest.htm' contents='ttestc.htm' frame='ttestf.htm'
      style=HTMLBlue;
ods graphics on;

proc ttest;
  class Gender;
  var Score;
run;

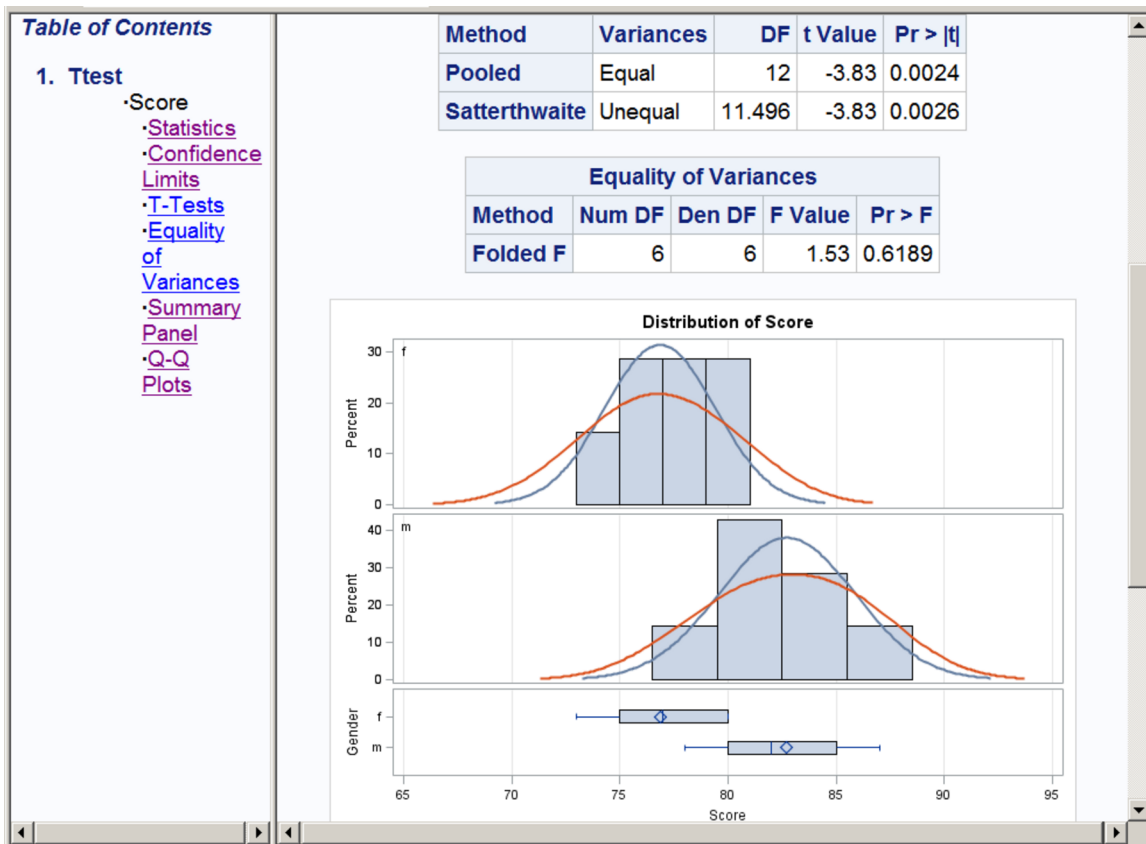
ods html close;
ods listing;
```

The ODS `_ALL_ CLOSE` statement closes all open destinations. The ODS HTML statement specifies three files and the HTMLBLUE style of output. The `BODY=` option specifies the file that contains the SAS output. The `CONTENTS=` option specifies the file that contains the table of contents. The `FRAME=` option specifies the file that displays both the table of contents and the output. You can open the `FRAME=` file (*ttestf.htm*) in your browser to view the table of contents together with the generated output (see [Output 20.1.1](#)). By default, the HTML files are generated in your current working directory. You can instead specify a path, such as `frame='html/ttestf.htm'`, to store a file in a subdirectory.

If you specify the ODS HTML statement with only the `BODY=` argument, no table of contents is created. The table of contents contains the descriptive label for each output object produced in the PROC TTEST step. You can select any label in the table of contents, and the corresponding output is displayed on the right side of the browser window.

The ODS GRAPHICS ON statement enables ODS Graphics, which creates the graph displayed in [Output 20.1.1](#). For general information about ODS Graphics, see Chapter 21, “Statistical Graphics Using ODS.”

Output 20.1.1 HTML Output with a Table of Contents and a Frame



Example 20.2: Selecting ODS Tables for Display

You can use the ODS SELECT statement to deliver only a subset of the tables or graphs to ODS destinations. The following statements create an input SAS data set and use PROC GLM to perform an analysis of an unbalanced two-way experimental design:

```

title 'Unbalanced Two-way Design';
data twoway;
  input Treatment Block y @@;
  datalines;
1 1 17  1 1 28  1 1 19  1 1 21  1 1 19  1 2 43
1 2 30  1 2 39  1 2 44  1 2 44  1 3 16
2 1 21  2 1 21  2 1 24  2 1 25  2 2 39  2 2 45
2 2 42  2 2 47  2 3 19  2 3 22  2 3 16
3 1 22  3 1 30  3 1 33  3 1 31  3 2 46  3 3 26
3 3 31  3 3 26  3 3 33  3 3 29  3 3 25
;

proc glm data=twoway;
  class Treatment Block;
  model y = Treatment | Block;
  means Treatment;
  lsmeans Treatment;

```

```

ods select ModelANOVA Means;
ods trace on;
ods show;
run;

```

The ODS SELECT statement selects only two tables (ModelANOVA and Means) for display in the ODS destinations. In this example, no ODS destinations are explicitly opened. Therefore, only the default destination (usually LISTING or HTML) receives the procedure output. See the section “[Output Defaults](#)” on page 512 for more information about default destinations. The ODS SHOW statement displays the current overall selection list in the SAS log. The ODS SHOW statement is not required; it is used here simply to show the effects of the ODS SELECT statement. The results of the ODS SHOW statement are as follows:

```

Current OVERALL select list is:
1. ModelANOVA
2. Means

```

The ODS TRACE statement writes the trace record of the ODS output objects to the SAS log. The trace record is as follows:

```

Output Added:
-----
Name:      ModelANOVA
Label:     Type I Model ANOVA
Template:  stat.GLM.Tests
Path:      GLM.ANOVA.y.ModelANOVA
-----

Output Added:
-----
Name:      ModelANOVA
Label:     Type III Model ANOVA
Template:  stat.GLM.Tests
Path:      GLM.ANOVA.y.ModelANOVA
-----

Output Added:
-----
Name:      Means
Label:     Means
Template:  stat.GLM.Means
Path:      GLM.Means.Treatment.Means
-----

```

There are two tables with the name ModelANOVA. One contains the “Type I Model ANOVA” table, and the other contains the “Type III Model ANOVA” table. If you want to select only one of them, you can specify either of the labels in the ODS SELECT statement instead of the name. You specify one of the following:

```

ods select 'Type I Model ANOVA' Means;
ods select 'Type III Model ANOVA' Means;

```

In the following statements, the ODS SHOW statement writes the current overall selection list to the SAS log, the QUIT statement ends the PROC GLM step, and the second ODS SHOW statement writes the selection list to the log after PROC GLM terminates:

```
ods show;
quit;
ods show;
```

The results of these statements are as follows:

```
ods show;
```

```
Current OVERALL select list is:
1. ModelANOVA
2. Means
```

```
quit;
ods show;
```

```
Current OVERALL select list is: ALL
```

PROC GLM supports interactive RUN-group processing. Before the QUIT statement is executed, PROC GLM is active and the ODS selection list remains at its previous setting. The list includes only the two tables, ModelANOVA and Means. After the QUIT statement, when PROC GLM is no longer active, the selection list is reset to ALL. The displayed output, shown in [Output 20.2.1](#), consists of the three selected tables (two ModelANOVA tables and the Means table). The LS-means results are not displayed even though an LSMEANS statement was specified. This is because the LS-means table, named LSMeans, is not specified in the ODS SELECT statement. Other tables are suppressed as well.

Output 20.2.1 Selected Tables from PROC GLM

Unbalanced Two-way Design					
The GLM Procedure					
Dependent Variable: y					
Source	DF	Type I SS	Mean Square	F Value	Pr > F
Treatment	2	8.060606	4.030303	0.24	0.7888
Block	2	2621.864124	1310.932062	77.95	<.0001
Treatment*Block	4	32.684361	8.171090	0.49	0.7460
Source	DF	Type III SS	Mean Square	F Value	Pr > F
Treatment	2	266.130682	133.065341	7.91	0.0023
Block	2	1883.729465	941.864732	56.00	<.0001
Treatment*Block	4	32.684361	8.171090	0.49	0.7460

Output 20.2.1 *continued*

Unbalanced Two-way Design			
The GLM Procedure			
Level of Treatment	N	-----y----- Mean	Std Dev
1	11	29.0909091	11.5104695
2	11	29.1818182	11.5569735
3	11	30.1818182	6.3058414

For more information about ODS exclusion and selection lists, see the section “The ODS Statement” on page 519.

Example 20.3: Excluding ODS Tables from Display

The following example demonstrates how you can use the ODS EXCLUDE statement to exclude particular objects from ODS destinations. This example also creates a SAS data set from the excluded table and uses it to create a specialized plot.

The data are from Hemmerle and Hartley (1973). The response variable consists of measurements from an oven experiment, and the model contains a fixed effect a and random effects b and $a*b$. The following statements create the input SAS data set:

```

title 'Oven Measurements';

data hh;
  input a b y @@;
  datalines;
1 1 237  1 1 254  1 1 246
1 2 178  1 2 179
2 1 208  2 1 178  2 1 187
2 2 146  2 2 145  2 2 141
3 1 186  3 1 183
3 2 142  3 2 125  3 2 136
;

```

The following ODS statements are submitted before the analysis, which will be done with the MIXED procedure:

```

ods _all_ close;
ods html body='mixed.htm' contents='mixedc.htm' frame='mixedf.htm'
  style=HTMLBlue;

ods exclude ParmSearch(persist);
ods show;

```

The ODS HTML statement specifies the filenames to contain the output generated from the statements that follow. The ODS EXCLUDE statement excludes the table ParmSearch from display. Although the table

is excluded from the displayed output, the information contained in the ParmSearch table is graphically summarized in a later step.

The PERSIST option in the ODS EXCLUDE statement excludes the object for the entire SAS session or until you execute an ODS SELECT statement or an ODS EXCLUDE NONE statement. If you omit the PERSIST option, the exclusion list is cleared when the procedure terminates. The resulting exclusion list is displayed next:

```
Current OVERALL exclude list is:
1. ParmSearch(PERSIST)
```

The MIXED procedure is run to fit the model:

```
proc mixed data=hh;
  class a b;
  model y = a;
  random b a*b;
  parms (17 to 20 by 0.1) (.3 to .4 by .005) (1.0);
  ods output ParmSearch=parms;
run;

ods show;
```

All output from PROC MIXED, except the ParmSearch table, is delivered to the HTML destination. The ODS OUTPUT statement outputs the table ParmSearch to a SAS data set called Parms.

The ODS SHOW statement again displays the overall current exclusion list after PROC MIXED has terminated. The results of the ODS SHOW statement are displayed next:

```
Current OVERALL exclude list is:
1. ParmSearch(PERSIST)
```

The ParmSearch table is saved in the Parms data set (as specified in the ODS OUTPUT statement). The following steps plot the surface of the residual log likelihood as a function of the covariance parameters and produce [Output 20.3.1](#):

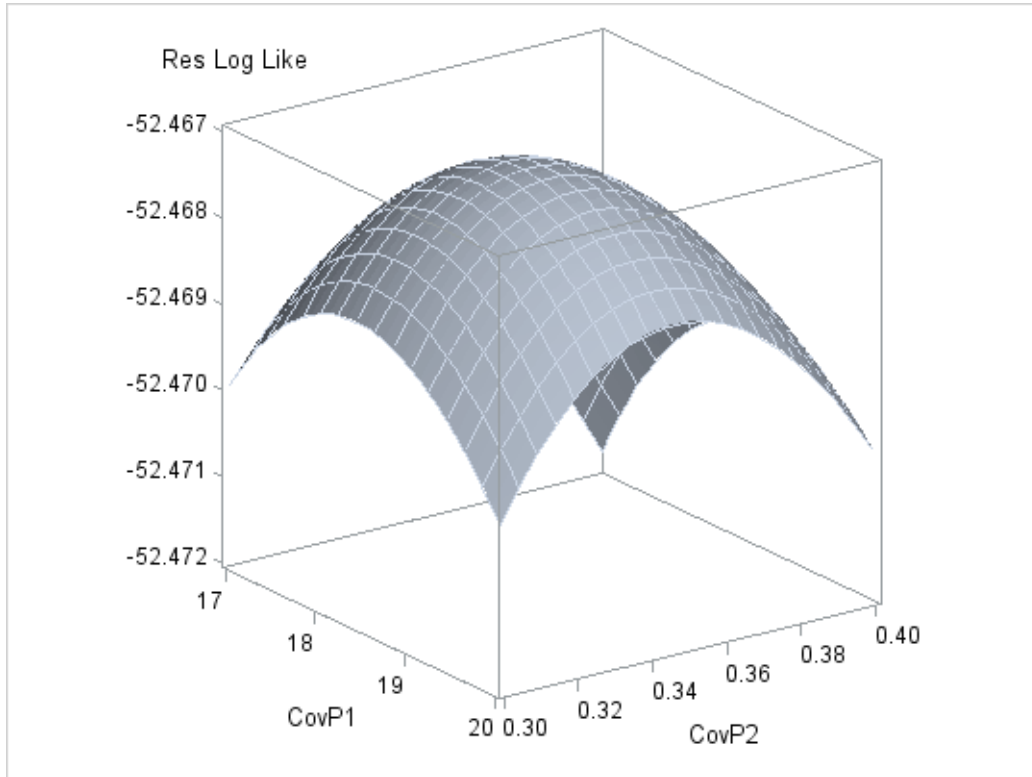
```
proc template;
  define statgraph surface;
    begingraph;
      layout overlay3d;
        surfaceplotparm x=CovP1 y=CovP2 z=ResLogLike;
      endlayout;
    endgraph;
  end;
run;

proc sgrender data=parms template=surface;
run;

ods html close;
```

PROC TEMPLATE is used to create a template for displaying the data as a three-dimensional surface plot. The plot is displayed with the ODS Graphics procedure SGRENDER. For more information about ODS Graphics, see Chapter 21, “Statistical Graphics Using ODS.”

Output 20.3.1 HTML Output from PROC MIXED



Example 20.4: Creating an Output Data Set from an ODS Table

In this example, the GENMOD procedure is used to perform Poisson regression, and part of the resulting procedure output is written to a SAS data set with the ODS OUTPUT statement. Insurance claims data are classified by two factors: age group (with two levels) and car type (with three levels). The following statements create the data set Insure:

```

title 'Insurance Claims';

data Insure;
  input n c Car $ Age;
  ln = log(n);
  datalines;
  500  42  Small  1
 1200  37  Medium 1
  100   1  Large  1
  400 101  Small  2
  500  73  Medium 2
  300  14  Large  2
;

```

The variable *n* represents the number of insurance policyholders, and the variable *c* represents the number of insurance claims. The variable *Car* represents the type of car involved (classified into three groups), and the variable *Age* is the age of a policyholder (classified into two groups).

You can use PROC GENMOD to perform a Poisson regression analysis of these data with a log link function. Assume that the number-of-claims variable, *c*, has a Poisson probability distribution and the log of its mean, μ_i , is related to the factors *Car* and *Age*.

The following statements obtain the names of the objects produced by this PROC GENMOD run. The ODS TRACE statement lists the trace record. If you already know the names, such as by looking them up in the procedure documentation, you do not have to run this step. The following step displays the trace information:

```
ods trace on;

proc genmod data=insure;
  class car age;
  model c = car age / dist=poisson link=log offset=ln obstats;
run;

ods trace off;
```

The trace record from the SAS log is displayed next:

Output Added:

```
Name:      ModelInfo
Label:     Model Information
Template:  Stat.Genmod.ModelInfo
Path:     Genmod.ModelInfo
-----
```

Output Added:

```
Name:      NObs
Label:     Number of observations summary
Template:  Stat.Genmod.NObs
Path:     Genmod.NObs
-----
```

Output Added:

```
Name:      ClassLevels
Label:     Class Level Information
Template:  Stat.Genmod.Classlevels
Path:     Genmod.ClassLevels
-----
```


The KEEP= data set option in the ODS OUTPUT statement specifies that only the variables Car, Age, and Pred are written to the data set. The RENAME= data set option changes the name of variable Pred to PredictedValue. The following statements sort the output data set myObStats, select all output, and produce Output 20.4.1:

```
proc sort data=myObStats;
  by descending PredictedValue;
run;

ods select all;
proc print data=myObStats noobs;
  title2 'Values of Car, Age, and the Predicted Values';
run;
```

The ODS SELECT NONE statement remains in effect until it is explicitly canceled (for example, with the ODS SELECT ALL statement).

Output 20.4.1 The ObStats Table Created as a SAS Data Set

Insurance Claims		
Values of Car, Age, and the Predicted Values		
Car	Age	Predicted Value
Small	2	107.2011
Medium	2	67.025444
Medium	1	42.974556
Small	1	35.798902
Large	2	13.773459
Large	1	1.2265414

Example 20.5: Creating an Output Data Set: Subsetting the Data

This example demonstrates how you can create an output data set with the ODS OUTPUT statement and also use data set selection keywords to limit the output that ODS writes to a SAS data set. The data set, called Color, contains the eye color and hair color of children from two different regions of Europe. The data are recorded as cell counts, where the variable Count contains the number of children who exhibit each of the 15 combinations of eye and hair color. The following statements create the SAS data set:

```
title 'Hair Color of European Children';

data Color;
  input Region Eyes $ Hair $ Count @@;
  label Eyes ='Eye Color'
        Hair ='Hair Color'
        Region='Geographic Region';
  datalines;
1 blue fair 23 1 blue red 7 1 blue medium 24
```

```

1 blue dark 11 1 green fair 19 1 green red 7
1 green medium 18 1 green dark 14 1 brown fair 34
1 brown red 5 1 brown medium 41 1 brown dark 40
1 brown black 3 2 blue fair 46 2 blue red 21
2 blue medium 44 2 blue dark 40 2 blue black 6
2 green fair 50 2 green red 31 2 green medium 37
2 green dark 23 2 brown fair 56 2 brown red 42
2 brown medium 53 2 brown dark 54 2 brown black 13
;

```

The following statements exclude all output and sort the observations in the Color data set by the Region variable:

```

ods select none;

proc sort data=Color;
  by Region;
run;

```

The following ODS OUTPUT statement creates the ChiSq table as a SAS data set named myStats:

```

ods output ChiSq=myStats(drop=Table
                        where=(Statistic =: 'Chi' or
                               Statistic =: 'Like'));

```

You specify the table name in the ODS OUTPUT statement.⁴ The DROP= data set option excludes variables from the new data set. The WHERE= data set option selects observations for output to the new data set myStats—specifically, those that begin with 'Chi' or 'Like'.

The following statements create [Output 20.5.1](#):

```

proc freq data=Color order=data;
  weight Count;
  tables Eyes*Hair / testp=(30 12 30 25 3);
  by Region;
run;

ods select all;
proc print data=myStats noobs;
run;

```

The FREQ procedure is used to create and analyze a crosstabulation table from the two categorical variables Eyes and Hair, for each value of the variable Region.

⁴You can obtain the names of the objects created by any procedure in the individual procedure documentation chapter or from the individual procedure section of the SAS online Help system. (See the “ODS Table Names” section in the “Details” section of the documentation.) You can also determine the names of objects with the ODS TRACE statement (see [Example 20.4](#) and [Example 20.2](#)).

Output 20.5.1 Output Data Set from PROC FREQ and ODS

Hair Color of European Children				
Region	Statistic	DF	Value	Prob
1	Chi-Square	8	12.6331	0.1251
1	Likelihood Ratio Chi-Square	8	14.1503	0.0779
2	Chi-Square	8	18.2839	0.0192
2	Likelihood Ratio Chi-Square	8	23.3021	0.0030

Example 20.6: RUN-Group Processing

Some SAS procedures, such as PROC REG and PROC GLM, permit you to submit statements, followed by a RUN statement, followed by more statements and more RUN statements. Each group of statements, followed by a RUN statement, is called a RUN group. These procedures can produce several blocks of output for each of several RUN groups. The procedure stays active until a QUIT statement, a DATA statement, another PROC statement, or the end of the SAS session is encountered. However, ODS settings are cleared by default at RUN-group boundaries. In the following analysis, PROC REG is used to compute the covariance matrix of the estimates for two different models, and the covariance matrices are saved in a single SAS data set. The PERSIST= option in the ODS OUTPUT statement is required to make this happen. The PERSIST= option maintains ODS settings across RUN statements for procedures that support RUN-group processing.

Consider the following population growth trends. The population of the United States from 1790 to 1970 is fit to linear and quadratic functions of time. The quadratic term, YearSq, is created in the DATA step; this is necessary since polynomial effects such as Year*Year cannot be specified in the MODEL statement in PROC REG. The data are as follows:

```

title1 'US Population Study';
title2 'Concatenating Two Tables into One Data Set';

data USPopulation;
  input Population @@;
  retain Year 1780;
  Year=Year+10;
  YearSq=Year*Year;
  Population=Population/1000;
  datalines;
3929 5308 7239 9638 12866 17069 23191 31443 39818 50155
62947 75994 91972 105710 122775 131669 151325 179323 203211
;

```

In the following statements, PROC REG is used, and the ODS OUTPUT statement with the PERSIST= option creates a data set with the CovB table (the covariance matrix of the estimates):

```

proc reg data=USPopulation;
  ods output covb(persist=run)=Bmatrix;
  var YearSq;
  model Population = Year / covb;
run;

```

The MODEL statement defines the regression model, and the COVB matrix is requested. The RUN statement executes PROC REG and the model is fit, producing a covariance matrix of the estimates with two rows and two columns. The results are displayed in [Output 20.6.1](#) and [Output 20.6.2](#).

Output 20.6.1 Regression Results for the Model Population

US Population Study					
Concatenating Two Tables into One Data Set					
The REG Procedure					
Model: MODEL1					
Dependent Variable: Population					
Number of Observations Read		19			
Number of Observations Used		19			
Analysis of Variance					
Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	1	66336	66336	201.87	<.0001
Error	17	5586.29253	328.60544		
Corrected Total	18	71923			
Root MSE		18.12748	R-Square	0.9223	
Dependent Mean		69.76747	Adj R-Sq	0.9178	
Coeff Var		25.98271			
Parameter Estimates					
Variable	DF	Parameter Estimate	Standard Error	t Value	Pr > t
Intercept	1	-1958.36630	142.80455	-13.71	<.0001
Year	1	1.07879	0.07593	14.21	<.0001

Output 20.6.2 CovB Matrix for the Model Population

Covariance of Estimates		
Variable	Intercept	Year
Intercept	20393.138485	-10.83821461
Year	-10.83821461	0.0057650078

In the next step, the YearSq variable is added to the model and the model is fit again, producing a covariance matrix of the estimates with three rows and three columns:

```
add YearSq;
print;
run; quit;
```

The new COVB matrix is displayed in [Output 20.6.3](#).

Output 20.6.3 CovB Matrix for the Model Population

US Population Study Concatenating Two Tables into One Data Set			
The REG Procedure Model: MODEL1.1 Dependent Variable: Population			
Covariance of Estimates			
Variable	Intercept	Year	YearSq
Intercept	711450.62602	-757.2493826	0.2013282694
Year	-757.2493826	0.8061328943	-0.000214361
YearSq	0.2013282694	-0.000214361	5.7010894E-8

The PERSIST=RUN option maintains the ODS selection list across RUN statements for procedures that support RUN-group processing. If the PERSIST=RUN option is omitted, the selection list is cleared when the RUN statement is encountered and only the first COVB matrix is selected. Because the PERSIST=RUN option is specified, the selection list remains in effect throughout the PROC REG step. This ensures that each of the COVB matrices is selected and output. The following statements display the ODS OUTPUT SAS data set and create [Output 20.6.4](#):

```
proc print;
run;
```

Output 20.6.4 Results of the ODS OUTPUT Statement: Specifying the PERSIST Option

US Population Study Concatenating Two Tables into One Data Set						
Obs	_Run_	Model	Dependent Variable	Intercept	Year	YearSq
1	1	MODEL1	Population Intercept	20393.138485	-10.83821461	.
2	1	MODEL1	Population Year	-10.83821461	0.0057650078	.
3	2	MODEL1.1	Population Intercept	711450.62602	-757.2493826	0.2013282694
4	2	MODEL1.1	Population Year	-757.2493826	0.8061328943	-0.000214361
5	2	MODEL1.1	Population YearSq	0.2013282694	-0.000214361	5.7010894E-8

Even though the two COVB matrices do not have the same rows or columns, ODS automatically combines the two tables into one data set.

Example 20.7: ODS Output Data Sets and Using PROC TEMPLATE to Customize Output

You can use ODS statements, the DATA step, and PROC TEMPLATE to modify the appearance of your displayed tables or to display results in forms that are not directly produced by any procedure. The following example, similar to that given in Olinger and Tobias (1998), runs an analysis with PROC GLM. This example has several parts. It creates output data sets with the ODS OUTPUT statement, combines and manipulates those data sets, displays the results by using a standard SAS template, modifies a template by using PROC TEMPLATE, and displays the output data sets by using the modified template. Each step works toward the final goal of taking multiple tables and creating a custom display of those tables in a way that cannot be done directly by PROC GLM.

The following statements create a SAS data set named Histamine that contains the experimental data:

```

title1 'Histamine Study';

data Histamine;
  input Drug $12. Depleted $ hist0 hist1 hist3 hist5;
  logHist0 = log(hist0); logHist1 = log(Hist1);
  logHist3 = log(hist3); logHist5 = log(Hist5);
  datalines;
Morphine      N   .04   .20   .10   .08
Morphine      N   .02   .06   .02   .02
Morphine      N   .07  1.40   .48   .24
Morphine      N   .17   .57   .35   .24
Morphine      Y   .10   .09   .13   .14
Morphine      Y   .07   .07   .06   .07
Morphine      Y   .05   .07   .06   .07
Trimethaphan  N   .03   .62   .31   .22
Trimethaphan  N   .03  1.05   .73   .60
Trimethaphan  N   .07   .83  1.07   .80
Trimethaphan  N   .09  3.13  2.06  1.23
Trimethaphan  Y   .10   .09   .09   .08
Trimethaphan  Y   .08   .09   .09   .10
Trimethaphan  Y   .13   .10   .12   .12
Trimethaphan  Y   .06   .05   .05   .05
;

```

The data set comes from a preclinical drug experiment (Cole and Grizzle 1966). In order to study the effect of two different drugs on histamine levels in the blood, researchers administer the drugs to 13 animals and measure the levels of histamine in the animals' blood after 0, 1, 3, and 5 minutes. The response variable is the logarithm of the histamine level.

In the analysis that follows, PROC GLM is used to perform a repeated measures analysis, naming the drug and depletion status as between-subject factors in the MODEL statement and naming post-administration measurement time as the within-subject factor. For more information about this study and its analysis, see [Example 42.7](#) in Chapter 42, “The GLM Procedure.”

The following PROC GLM statements begin the analysis:

```
ods graphics off;
ods trace output;

proc glm data=Histamine;
  class Drug Depleted;
  model LogHist0--LogHist5 = Drug Depleted Drug*Depleted / nouni;
  repeated Time 4 (0 1 3 5) polynomial / summary printe;
run; quit;
```

The portion of the trace output that contains the fully qualified name paths is shown next:

```
Path:      GLM.Data.ClassLevels
Path:      GLM.Data.NObs
Path:      GLM.Repeated.RepeatedLevelInfo
Path:      GLM.Repeated.PartialCorr
Path:      GLM.Repeated.MANOVA.Model.Error.ErrorSSCP
Path:      GLM.Repeated.MANOVA.Model.Error.PartialCorr
Path:      GLM.Repeated.MANOVA.Model.Error.Sphericity
Path:      GLM.Repeated.MANOVA.Model.Time.MultStat
Path:      GLM.Repeated.MANOVA.Model.Time_Drug.MultStat
Path:      GLM.Repeated.MANOVA.Model.Time_Depleted.MultStat
Path:      GLM.Repeated.MANOVA.Model.Time_Drug_Depleted.MultStat
Path:      GLM.Repeated.BetweenSubjects.ModelANOVA
Path:      GLM.Repeated.WithinSubject.ModelANOVA
Path:      GLM.Repeated.WithinSubject.Epsilons
Path:      GLM.Repeated.Summary.Time_1.ModelANOVA
Path:      GLM.Repeated.Summary.Time_2.ModelANOVA
Path:      GLM.Repeated.Summary.Time_3.ModelANOVA
```

The goal here is to output the within-subjects multivariate statistics and the between-subjects ANOVA table to SAS data sets for use in subsequent steps. The following statements run the analysis and save the desired results to output data sets:

```
ods select none;

proc glm data=Histamine;
  class Drug Depleted;
  model LogHist0--LogHist5 = Drug Depleted Drug*Depleted / nouni;
  repeated Time 4 (0 1 3 5) polynomial / summary printe;
  ods output MultStat          = HistWithin
             BetweenSubjects.ModelANOVA = HistBetween;
run; quit;

ods select all;
```

No output is displayed due to the ODS SELECT statements. The ODS OUTPUT statement creates two SAS data sets, named HistWithin and HistBetween, from the two ODS tables. This analysis creates the following tables:

```
Path:      GLM.Repeated.MANOVA.Model.Time.MultStat
Path:      GLM.Repeated.MANOVA.Model.Time_Drug.MultStat
Path:      GLM.Repeated.MANOVA.Model.Time_Depleted.MultStat
Path:      GLM.Repeated.MANOVA.Model.Time_Drug_Depleted.MultStat
Path:      GLM.Repeated.BetweenSubjects.ModelANOVA
```


Here is the full trace output for the model ANOVA table:

```

Output Added:
-----
Name:          ModelANOVA
Label:         Type III Model ANOVA
Template:      stat.GLM.Tests
Path:          GLM.Repeated.BetweenSubjects.ModelANOVA
-----

```

All of the multivariate test results are routed to the HistWithin data set because all multivariate test tables are named MultStat, even though they occur in different directories in the output directory hierarchy. Only the between-subject ANOVA table appears in the HistBetween data set, even though there are also other tables named ModelANOVA. ODS selects just the one specific table for the HistBetween data set because of the partial name path (**BetweenSubjects.ModelANOVA**) in the second specification. For more information about names and qualified path names, see the discussion in the section “[The ODS Statement](#)” on page 519.

The following statements show the names and the variable labels for the two data sets and produce [Output 20.7.1](#):

```

proc contents data=HistBetween varnum;
  ods select position;
run;

proc contents data=HistWithin varnum;
  ods select position;
run;

```

Output 20.7.1 Variable Names and Labels for the Two Data Sets

Histamine Study					
The CONTENTS Procedure					
Variables in Creation Order					
#	Variable	Type	Len	Format	Label
1	Dependent	Char	15		
2	HypothesisType	Num	8	BEST8.	
3	Source	Char	20		
4	DF	Num	8	BEST6.	
5	SS	Num	8	12.8	Type III SS
6	MS	Num	8	12.8	Mean Square
7	FValue	Num	8	7.2	F Value
8	ProbF	Num	8	PVALUE6.4	Pr > F

Output 20.7.1 *continued*

Histamine Study					
The CONTENTS Procedure					
Variables in Creation Order					
#	Variable	Type	Len	Format	Label
1	Hypothesis	Char	32		
2	Error	Char	55		
3	Statistic	Char	22		
4	Value	Num	8	12.8	
5	FValue	Num	8	7.2	F Value
6	NumDF	Num	8	BEST6.	Num DF
7	DenDF	Num	8	BEST6.	Den DF
8	ProbF	Num	8	PVALUE6.4	Pr > F
9	PValue	Num	8	PVALUE6.4	P-Value

The following statements create a new data set that contains the two data sets created in the preceding PROC GLM step and display the results in [Output 20.7.2](#):

```

title2 'The Combined Data Set';

data temp1;
  set HistBetween HistWithin;
run;

proc print label;
run;

```

Output 20.7.2 Listing of the Combined Data Set: Histamine Study

Histamine Study				
The Combined Data Set				
Obs	Dependent	Hypothesis Type	Source	DF
1	BetweenSubjects	3	Drug	1
2	BetweenSubjects	3	Depleted	1
3	BetweenSubjects	3	Drug*Depleted	1
4	BetweenSubjects	3	Error	11
5		.		.
6		.		.
7		.		.
8		.		.
9		.		.
10		.		.
11		.		.
12		.		.
13		.		.
14		.		.
15		.		.
16		.		.
17		.		.
18		.		.
19		.		.
20		.		.

Output 20.7.2 *continued*

Histamine Study				
The Combined Data Set				
Obs	Type III SS	Mean Square	F Value	Pr > F
1	5.99336243	5.99336243	2.71	0.1281
2	15.44840703	15.44840703	6.98	0.0229
3	4.69087508	4.69087508	2.12	0.1734
4	24.34683348	2.21334850	—	—
5	.	.	24.03	0.0001
6	.	.	24.03	0.0001
7	.	.	24.03	0.0001
8	.	.	24.03	0.0001
9	.	.	5.78	0.0175
10	.	.	5.78	0.0175
11	.	.	5.78	0.0175
12	.	.	5.78	0.0175
13	.	.	21.31	0.0002
14	.	.	21.31	0.0002
15	.	.	21.31	0.0002
16	.	.	21.31	0.0002
17	.	.	12.48	0.0015
18	.	.	12.48	0.0015
19	.	.	12.48	0.0015
20	.	.	12.48	0.0015

Obs	Hypothesis	Error
1		
2		
3		
4		
5	Time	Error SSCP Matrix
6	Time	Error SSCP Matrix
7	Time	Error SSCP Matrix
8	Time	Error SSCP Matrix
9	Time_Drug	Error SSCP Matrix
10	Time_Drug	Error SSCP Matrix
11	Time_Drug	Error SSCP Matrix
12	Time_Drug	Error SSCP Matrix
13	Time_Depleted	Error SSCP Matrix
14	Time_Depleted	Error SSCP Matrix
15	Time_Depleted	Error SSCP Matrix
16	Time_Depleted	Error SSCP Matrix
17	Time_Drug_Depleted	Error SSCP Matrix
18	Time_Drug_Depleted	Error SSCP Matrix
19	Time_Drug_Depleted	Error SSCP Matrix
20	Time_Drug_Depleted	Error SSCP Matrix

Output 20.7.2 continued

Histamine Study The Combined Data Set					
Obs	Statistic	Value	Num DF	Den DF	P-Value
1	
2	
3	
4	
5	Wilks' Lambda	0.11097706	3	9	.
6	Pillai's Trace	0.88902294	3	9	.
7	Hotelling-Lawley Trace	8.01087137	3	9	.
8	Roy's Greatest Root	8.01087137	3	9	.
9	Wilks' Lambda	0.34155984	3	9	.
10	Pillai's Trace	0.65844016	3	9	.
11	Hotelling-Lawley Trace	1.92774470	3	9	.
12	Roy's Greatest Root	1.92774470	3	9	.
13	Wilks' Lambda	0.12339988	3	9	.
14	Pillai's Trace	0.87660012	3	9	.
15	Hotelling-Lawley Trace	7.10373567	3	9	.
16	Roy's Greatest Root	7.10373567	3	9	.
17	Wilks' Lambda	0.19383010	3	9	.
18	Pillai's Trace	0.80616990	3	9	.
19	Hotelling-Lawley Trace	4.15915732	3	9	.
20	Roy's Greatest Root	4.15915732	3	9	.

The next steps are designed to produce a more parsimonious display of the most important information in [Output 20.7.2](#). The next step creates a data set named HistTests. Only the observations from the input data sets that are needed for interpretation are included. The variable Hypothesis in the HistWithin data set is renamed Source, and the NumDF variable is renamed DF. The renamed variables correspond to the variable names found in the HistBetween data set. These names are chosen since the template for the ModelANOVA table is used in subsequent steps. An explicit length for the new variable Source is provided since the input variables, Hypothesis and Source, have different lengths. The following statements produce [Output 20.7.3](#):

```
data HistTests;
  length Source $ 20;
  set HistBetween(where =(Source ^= 'Error'))
    HistWithin (rename=(Hypothesis = Source NumDF=DF)
                where =(Statistic = 'Hotelling-Lawley Trace'));
run;

proc print label;
  title2 'Listing of the Combined Data Set';
run;
```

Output 20.7.3 Listing of the HistTests Data Set: Histamine Study

Histamine Study						
Listing of the Combined Data Set						
Obs	Source	Dependent	Hypothesis Type	Num DF	Type III SS	
1	Drug	BetweenSubjects	3	1	5.99336243	
2	Depleted	BetweenSubjects	3	1	15.44840703	
3	Drug*Depleted	BetweenSubjects	3	1	4.69087508	
4	Time		.	3	.	
5	Time_Drug		.	3	.	
6	Time_Depleted		.	3	.	
7	Time_Drug_Depleted		.	3	.	

Obs	Mean Square	F Value	Pr > F	Error	Statistic
1	5.99336243	2.71	0.1281		
2	15.44840703	6.98	0.0229		
3	4.69087508	2.12	0.1734		
4	.	24.03	0.0001	Error SSCP Matrix	Hotelling-Lawley Trace
5	.	5.78	0.0175	Error SSCP Matrix	Hotelling-Lawley Trace
6	.	21.31	0.0002	Error SSCP Matrix	Hotelling-Lawley Trace
7	.	12.48	0.0015	Error SSCP Matrix	Hotelling-Lawley Trace

Obs	Value	Den DF	P-Value
1	.	.	.
2	.	.	.
3	.	.	.
4	8.01087137	9	.
5	1.92774470	9	.
6	7.10373567	9	.
7	4.15915732	9	.

The amount of information contained in the HistTests data set is appropriate for interpreting the analysis; however, there is still extra information, and the information of interest is not being displayed in a compact or useful form. This data set consists of multiple tables, an ANOVA table with between-subjects information, and multivariate statistics tables with the variables renamed to match the names in the ANOVA table. This form was chosen so that the data set could be displayed using PROC GLM's ANOVA template. A template specifies how the data set should be displayed and which columns should be displayed. The output from the ODS TRACE statements shows that the template associated with PROC GLM's ANOVA table is named **Stat.GLM.Tests**. You can use the **Stat.GLM.Tests** template to display the SAS data set HistTests, as follows:

```

title2 'Listing of the Selections, Using a Standard Template';
proc sgrender data=histtests template=Stat.GLM.Tests;
run;

```

The SGRENDER procedure displays the DATA= data set with the specified TEMPLATE= template. (You can use PROC SGRENDER to display both graphs and tables.) The results are displayed in **Output 20.7.4**.

Output 20.7.4 Listing of the Data Set Using a Standard PROC GLM ANOVA Template

Histamine Study					
Listing of the Selections, Using a Standard Template					
Source	DF	SS	Mean Square	F Value	Pr > F
Drug	1	5.99336243	5.99336243	2.71	0.1281
Depleted	1	15.44840703	15.44840703	6.98	0.0229
Drug*Depleted	1	4.69087508	4.69087508	2.12	0.1734
Time	3	.	.	24.03	0.0001
Time_Drug	3	.	.	5.78	0.0175
Time_Depleted	3	.	.	21.31	0.0002
Time_Drug_Depleted	3	.	.	12.48	0.0015

Alternatively, you could display the results by using a DATA step as follows:

```

title2 'Listing of the Selections, Using a Standard Template';

data _null_;
  set histtests;
  file print ods=(template='Stat.GLM.Tests');
  put _ods_;
run;

```

The next steps create a final display of these results, this time by using a custom template. This example shows you how to use PROC TEMPLATE to do the following:

- redefine the format for the SS and Mean Square columns
- include the table title and footnote in the body of the table
- translate the missing values for SS and Mean Square in the rows that correspond to multivariate tests to asterisks
- add a footnote to a table
- add a column that depicts the level of significance of each effect

The following statements create a custom template:

```

proc template;
  define table CombinedTests;
    parent=Stat.GLM.Tests;

    header '#Histamine Study##';
    footer '## - Test computed using Hotelling-Lawley trace';

    column Source DF SS MS FValue ProbF Star;

    define Source; width=20; end;
    define DF; format=bestd3.; end;
    define SS;
      parent=Stat.GLM.SS
      choose_format=max format_width=7;
      translate _val_ = . into ' *';
    end;

```

```

define MS;
  parent=Stat.GLM.MS
  choose_format=max format_width=7;
  translate _val_ = . into ' *';
end;
define Star;
  compute as ProbF;
  translate _val_ <= 0.001 into 'xxx',
           _val_ <= 0.01  into 'xx',
           _val_ <= 0.05  into 'x',
           _val_ > 0.05  into '';
  pre_space=1 width=3 just=l;
end;
end;
run;

```

The CHOOSE_FORMAT=MAX option along with FORMAT_WIDTH=7 chooses the format for each column based on the maximum value and an overall width of 7. Alternatively, you could have specified a format directly by specifying, for example, FORMAT=7.2 or FORMAT=D8.3. The TRANSLATE statements provide values to display in place of the original values. The first two TRANSLATE statements display missing values as an asterisk with leading blanks added to ensure alignment with the decimal place. The third TRANSLATE statement displays *p*-values greater than 0.05 as a blank, values greater than 0.01 but less than or equal to 0.05 as a single 'x', and so on. The ProbF column is printed twice—once in the usual way as a numeric column with a PVALUE format and once with a column of blanks or x's. For detailed information about PROC TEMPLATE, see the section “The Template Procedure” in the *SAS Output Delivery System: User's Guide*. The following statements use the customized template to display the HistTests data set:

```

title2 'Listing of the Selections, Using a Customized Template';

proc sgrender data=HistTests template=CombinedTests;
run;

```

The results are displayed in [Output 20.7.5](#).

Output 20.7.5 Display of the Data Sets Using a Customized Template: Histamine Study

Histamine Study					
Listing of the Selections, Using a Customized Template					
Histamine Study					
Source	Num DF	Sum of Squares	Mean Square	F Value	Pr > F
Drug	1	5.9934	5.9934	2.71	0.1281
Depleted	1	15.4484	15.4484	6.98	0.0229 x
Drug*Depleted	1	4.6909	4.6909	2.12	0.1734
Time	3	*	*	24.03	0.0001 xxx
Time_Drug	3	*	*	5.78	0.0175 x
Time_Depleted	3	*	*	21.31	0.0002 xxx
Time_Drug_Depleted	3	*	*	12.48	0.0015 xx

* - Test computed using Hotelling-Lawley trace

These next steps display the same table, but this time changing the background color for the entire row to highlight effects with p -values less than 0.001 and also those with p -values less than 0.01. The table is displayed three times. [Output 20.7.6](#) displays the results by using bold green and yellow backgrounds and a bold font. [Output 20.7.7](#) displays the results by using subtler cyan and yellow backgrounds and a bold font. [Output 20.7.8](#) displays the results by using very subtle cyan and gray backgrounds and a normal font. This control is provided by the CELLSTYLE statement in PROC TEMPLATE. You can do many things with the CELLSTYLE statement to enhance your output. Several more are shown in other examples in this chapter. These next steps create the custom template with varying colors and fonts and display the results by using PROC SGRENDER:

```
%macro highlight(c1,c2);
  proc template;
    define table CombinedTests;
      parent=Stat.GLM.Tests;

      header '#Histamine Study##';
      footer '* - Test computed using Hotelling-Lawley trace';

      column Source DF SS MS FValue ProbF;

      cellstyle probf <= 0.001 as {background=&c1},
                probf <= 0.01  as {background=&c2};

      define DF; format=bestd3.; end;
      define SS;
        parent=Stat.GLM.SS
        choose_format=max format_width=7;
        translate _val_ = . into ' *';
      end;
      define MS;
        parent=Stat.GLM.MS
        choose_format=max format_width=7;
        translate _val_ = . into ' *';
      end;
    end;
  run;

  proc sgrender data=HistTests template=CombinedTests;
  run;
%mend;

title2;
ods _all_ close;
ods html style=HTMLBlue;

%highlight(CX22FF22 fontweight=bold, CXFFFF22 fontweight=bold)
%highlight(CXAAFFFF fontweight=bold, CXFFFFDD fontweight=bold)
%highlight(CXEFAFA, CXEEEEEE)

ods html close;
ods listing;
```

Output 20.7.6 Rows Boldly Highlighted: Histamine Study

Histamine Study					
Histamine Study					
Source	Num DF	Sum of Squares	Mean Square	F Value	Pr > F
Drug	1	5.9934	5.9934	2.71	0.1281
Depleted	1	15.4484	15.4484	6.98	0.0229
Drug*Depleted	1	4.6909	4.6909	2.12	0.1734
Time	3	*	*	24.03	0.0001
Time_Drug	3	*	*	5.78	0.0175
Time_Depleted	3	*	*	21.31	0.0002
Time_Drug_Depleted	3	*	*	12.48	0.0015
* - Test computed using Hotelling-Lawley trace					

Output 20.7.7 Rows Subtly Highlighted: Histamine Study

Histamine Study					
Histamine Study					
Source	Num DF	Sum of Squares	Mean Square	F Value	Pr > F
Drug	1	5.9934	5.9934	2.71	0.1281
Depleted	1	15.4484	15.4484	6.98	0.0229
Drug*Depleted	1	4.6909	4.6909	2.12	0.1734
Time	3	*	*	24.03	0.0001
Time_Drug	3	*	*	5.78	0.0175
Time_Depleted	3	*	*	21.31	0.0002
Time_Drug_Depleted	3	*	*	12.48	0.0015
* - Test computed using Hotelling-Lawley trace					

Output 20.7.8 Rows Very Subtly Highlighted: Histamine Study

Histamine Study					
Histamine Study					
Source	Num DF	Sum of Squares	Mean Square	F Value	Pr > F
Drug	1	5.9934	5.9934	2.71	0.1281
Depleted	1	15.4484	15.4484	6.98	0.0229
Drug*Depleted	1	4.6909	4.6909	2.12	0.1734
Time	3	*	*	24.03	0.0001
Time_Drug	3	*	*	5.78	0.0175
Time_Depleted	3	*	*	21.31	0.0002
Time_Drug_Depleted	3	*	*	12.48	0.0015
* - Test computed using Hotelling-Lawley trace					

All colors are specified in values of the form *CXrrggbb*, where the last six characters specify RGB (red, green, blue) values on the hexadecimal scale of 00 to FF (or 0 to 255 base 10). You can run the following step to see the correspondence between the integer and HEX formatting of values in the range 0 to 255:

```

data _null_;
  do color = 0 to 255;
    put color 3. +1 color hex2.;
  end;
run;

```

The results of this step are not shown. Hexadecimal values 0 through F represent the numbers 0 to 15. A hex value xy can be converted to an integer as follows: $16x + y$. For example, BC is $16 \times 11 + 12 = 188$. Common colors are CXFF0000 (red), CX00FF00 (green), CX0000FF (blue), CXFFFF00 (yellow, a mix of red and green), CXFF00FF (magenta, a mix of red and blue), CX00FFFF (cyan, a mix of green and blue), CXFFFFFF (white, a mix of red, green, and blue), CX000000 (black, no color), CXDDDDDD (very light gray), CX222222 (very dark gray), and so on. Colors become lighter as the RGB values increase and darker as they decrease. For example, cyan (CX00FFFF) can be lightened by increasing the red component from 00 to FF until eventually it becomes indistinguishable from white. It can be darkened by jointly decreasing the green and blue values until it becomes indistinguishable from black.

The three CELLSTYLE statements that set the colors after the macro variables are substituted are as follows:

```

cellstyle probf <= 0.001 as {background=CX22FF22 fontweight=bold},
  probf <= 0.01 as {background=CXFFFF22 fontweight=bold};
cellstyle probf <= 0.001 as {background=CXAAFFFF fontweight=bold},
  probf <= 0.01 as {background=CXFFFFDD fontweight=bold};
cellstyle probf <= 0.001 as {background=CXEFAFA},
  probf <= 0.01 as {background=CXEFFFFFF};

```

The first color, CX22FF22, for the smallest p -values in the first table is a bold green color. The first table uses almost pure green and pure yellow, but a little red and blue are added to slightly lighten the colors. The second table uses a cyan and yellow that are very light due to the addition of AA (170) red and DD (221) blue, respectively. The third table uses a cyan that is not much different from light gray, and a light gray that is not much different from white.

Example 20.8: HTML Output with Hyperlinks between Tables

This example demonstrates how you can use ODS to provide links between different parts of your HTML procedure output. This example creates a table where each row contains a link to another table with more information about that row.

Suppose that you are analyzing a 4×4 factorial experiment for an industrial process, testing for differences in the number of defective products that are manufactured by different machines and use different sources of raw material. The data set Experiment is created as follows:

```

title 'Product Defects Experiment';

data Experiment;
  do Supplier = 'A', 'B', 'C', 'D';
    do Machine = 1 to 4;
      do rep = 1 to 5;
        input Defects @@;
        output;
      end;
    end;
  end;

```

```

    end;
  end;
  datalines;
  2  6  3  3  6  8  6  6  4  4  4  2  4  0  4  5  5  7  8  5
13 12 12 11 12 16 15 14 14 13 11 10 12 12 10 13 13 14 15 12
  2  6  3  6  6  6  4  4  6  6  0  3  2  0  2  4  6  7  6  4
20 19 18 21 22 22 24 23 20 20 17 19 18 16 17 23 20 20 22 21
;

```

Suppose that you are interested in fitting a model to determine the effect that the supplier of raw material and machine type have on the number of defects in the products. If the F test for a factor is significant, you might want to follow up with a multiple-comparison test for the levels of that factor. The tables of interest are the model ANOVA and the multiple-comparison output. Since this is a balanced experiment, the ANOVA procedure computes the appropriate analysis. The following statements produce these tables and Figure 20.8.1:

```

ods _all_ close;
ods html body='anovab.htm' style=HTMLBlue anchor='anova1';
ods trace output;

proc anova data=Experiment;
  ods select ModelANOVA MCLines;
  class Supplier Machine;
  model Defects = Supplier Machine;
  means Supplier Machine / tukey;
run; quit;

ods html close;
ods listing;

```

All destinations are first closed to avoid generating the output multiple times. ODS writes the HTML output to the file *anovab.htm*. The ANCHOR= option specifies *anova1* as the root name for the HTML anchor tags. This means that within the HTML document, the URL for the first table will be *anova1*, the URL for the second table will be *anova2*, and so on.

Output 20.8.1 ANOVA and Multiple-Comparison Results: Histamine Study

Product Defects Experiment					
The ANOVA Procedure					
Dependent Variable: Defects					
Source	DF	Anova SS	Mean Square	F Value	Pr > F
Supplier	3	3441.637500	1147.212500	580.72	<.0001
Machine	3	163.137500	54.379167	27.53	<.0001

Output 20.8.1 *continued***Product Defects Experiment****The ANOVA Procedure****Tukey's Studentized Range (HSD) Test for Defects**

Means with the same letter are not significantly different.

Tukey Grouping	Mean	N	Supplier
A	20.1000	20	D
B	12.7000	20	B
C	4.6000	20	A
C			
C	4.1500	20	C

Product Defects Experiment**The ANOVA Procedure****Tukey's Studentized Range (HSD) Test for Defects**

Means with the same letter are not significantly different.

Tukey Grouping	Mean	N	Machine
A	11.7500	20	2
A			
A	11.5000	20	4
B	10.1500	20	1
C	8.1500	20	3

The ODS trace output (not shown) shows that PROC ANOVA uses the `Stat.GLM.Tests` template to format the ANOVA table. The following statements demonstrate how you can link a row of the ANOVA table to the corresponding multiple-comparison table by modifying the table template, using the original values and the URLs for the second and third tables (*anova2* and *anova3*):

```
proc template;
  edit Stat.GLM.Tests;
  edit Source;
    cellstyle _val_ = 'Supplier' as {url="#ANOVA2"},
              _val_ = 'Machine' as {url="#ANOVA3"};
  end;
end;
run;
```

This template uses the CELLSTYLE statement to alter the values in the `Source` column ('Supplier' and 'Machine') of the ANOVA tests table. The values of 'Supplier' and 'Machine' are displayed as hyperlinks in the HTML, and clicking them takes you to the links *anova2* and *anova3*, which are the multiple-comparison tables.

You can find the value to use in the URL by viewing the HTML source file, *anovab.htm*. You can either open the HTML file in a text editor or view it in a browser window and select **View ► Source**. Search for '`<a name=`' to find the URL names. The first table is *anova1*, the second is *anova2*, the third is *anova3*, and so on. If the ANCHOR= option had not been used in the ODS HTML statement, the names would have been *IDX*, *IDX1*, *IDX2*, and so on. If you do not use the ODS SELECT statement or if you do anything to change the tables that are produced, the names will be different. The statements create the *Supplier* label as a link that enables you to open the table of means from the “Tukey’s Studentized Range Test for Defects” associated with the Supplier variable. Similarly, *Machine* provides a link to the table of means from the “Tukey’s Studentized Range Test for Defects” associated with the Machine variable.

Next, the analysis is run again, this time using the modified template. The following statements produce the results:

```
ods _all_ close;
ods html body='anovab.htm' style=HTMLBlue anchor='anova1';

proc anova data=Experiment;
  ods select ModelANOVA MCLines;
  class Supplier Machine;
  model Defects = Supplier Machine;
  means Supplier Machine / tukey;
run; quit;

ods html close;
ods listing;
```

The ANOVA table is displayed in [Output 20.8.2](#).

Output 20.8.2 HTML Output from PROC ANOVA: Linked Output

Product Defects Experiment
The ANOVA Procedure

Dependent Variable: Defects

Source	DF	Anova SS	Mean Square	F Value	Pr > F
<u>Supplier</u>	3	3441.637500	1147.212500	580.72	<.0001
<u>Machine</u>	3	163.137500	54.379167	27.53	<.0001

Product Defects Experiment
The ANOVA Procedure
Tukey's Studentized Range (HSD) Test for Defects

The underlined text displayed in Output 20.8.2 shows the links, *Supplier* and *Machine*, that you created with the modified template. When you click a link, the appropriate multiple-comparison table opens in your browser. Output 20.8.3 shows the table from the *Supplier* link.

Output 20.8.3 Linked Output: Multiple-Comparison Table from PROC ANOVA

Product Defects Experiment
The ANOVA Procedure
Tukey's Studentized Range (HSD) Test for Defects

Means with the same letter are not significantly different.			
Tukey Grouping	Mean	N	Supplier
A	20.1000	20	D
B	12.7000	20	B
C	4.6000	20	A
C			
C	4.1500	20	C

When you run the PROC TEMPLATE step shown previously, the following note is printed in the SAS log:

NOTE: TABLE 'Stat.GLM.Tests' has been saved to: SASUSER.TEMPLAT

You can see that there is a version of the template in Sasuser by running the following statements:

```
proc template;
  list Stat.GLM.Tests;
run;
```

These statements produce [Output 20.8.4](#).

Output 20.8.4 Templates

Product Defects Experiment		
Listing of: SASUSER.TEMPLAT		
Path Filter is: Stat.GLM.Tests		
Sort by: PATH/ASCENDING		
Obs	Path	Type
1	Stat.GLM.Tests	Table
Listing of: SASHELP.TMPLSTAT		
Path Filter is: Stat.GLM.Tests		
Sort by: PATH/ASCENDING		
Obs	Path	Type
1	Stat.GLM.Tests	Table
Listing of: SASHELP.TMPLMST		
Path Filter is: Stat.GLM.Tests		
Sort by: PATH/ASCENDING		
Obs	Path	Type
1	Stat.GLM.Tests	Table

You can delete your custom template and restore the default template as follows:

```
proc template;
  delete Stat.GLM.Tests / store=sasuser.templat;
run;
```

The following note is printed in the SAS log:

NOTE: 'Stat.GLM.Tests' has been deleted from: SASUSER.TEMPLAT

Example 20.9: HTML Output with Graphics and Hyperlinks

This example demonstrates how you can use ODS to create links between each bar in a bar chart ([Output 20.9.1](#)) and other parts of the analysis ([Output 20.9.2](#)). The data in this example are selected from a

larger experiment on the use of drugs in the treatment of leprosy (Snedecor and Cochran 1967, p. 422). Variables in the study are as follows:

Drug two antibiotics ('a' and 'd') and a control ('f')
 PreTreatment a pretreatment score of leprosy bacilli
 PostTreatment a posttreatment score of leprosy bacilli

The data set is created as follows:

```
title 'Treatment of Leprosy';

data drugtest;
  input Drug $ PreTreatment PostTreatment @@;
  datalines;
a 11 6 a 8 0 a 5 2 a 14 8 a 19 11
a 6 4 a 10 13 a 6 1 a 11 8 a 3 0
d 6 0 d 6 2 d 7 3 d 8 1 d 18 18
d 8 4 d 19 14 d 8 9 d 5 1 d 15 9
f 16 13 f 13 10 f 11 18 f 9 5 f 21 23
f 16 12 f 12 5 f 12 16 f 7 1 f 12 20
;
```

The following statement opens the HTML destination:

```
ods _all_ close;
ods html body='glmb.htm' contents='glmc.htm' frame='glmf.htm' style=HTMLBlue;
```

The ODS HTML statement specifies the body filename, generates a table of contents for the output, and generates a frame to contain the body and table of contents. The following statements perform the analysis:

```
proc glm data=drugtest;
  class drug;
  model PostTreatment = drug | PreTreatment / solution;
  lsmeans drug / stderr pdiff;
  ods output LSMeans=lsmeans;
run; quit;
```

The ODS OUTPUT statement writes the table of LS-means to the data set named lsmeans. PROC GLM performs an analysis of covariance and computes LS-means for the variable Drug.

The following steps demonstrate how you can create links to connect the results of different analyses. In this example, the table of LS-means is graphically summarized in a horizontal bar chart. Each bar is linked to a plot that displays the relationship between the PostTreatment response variable and the PreTreatment variable for the drug that corresponds to the bar.

NOTE: PROC GLM can use ODS Graphics to create LS-means graphs that are different from the one constructed here. You do not have to run the following steps to get PROC GLM's standard LS-means plots.

The following DATA step creates a new variable named DrugClick that matches each drug value with an HTML file:

```
data lsmeans;
  set lsmeans;
  if drug='a' then DrugClick='drug1.htm';
  if drug='d' then DrugClick='drug2.htm';
```

```

    if drug='f' then DrugClick='drug3.htm';
run;

```

The variable DrugClick is used in the chart. The variable provides the connection information for linking the two parts of the analysis together. The files referred to in these statements are created in a later step. The following statements create the chart:

```

ods graphics / imagemap=yes height=2in width=6.4in;

proc sgplot data=lsmeans;
  title 'Chart of LS-Means for Drug Type';
  hbar drug / response=lsmean stat=mean
           url=drugclick;
  footnote j=1 'Click on the bar to see a plot of PostTreatment '
             'versus PreTreatment for the corresponding drug.';
  format lsmean 6.3;
run;

ods graphics off;
footnote;
ods html close;

```

The chart is created with the ODS Graphics procedure SGPLOT. For more information about ODS Graphics, see Chapter 21, “[Statistical Graphics Using ODS](#).” The ODS GRAPHICS statement is not required before you run SG procedures. However, in this case, it is necessary to specify IMAGEMAP=YES so that the URL= option works properly. The size of the graph is also specified with the HEIGHT= and WIDTH= options. PROC SGPLOT is used, and the HBAR statement requests a horizontal bar chart for the variable Drug. The lengths of the bars represent the values of the LSMEAN variable. The URL= option specifies the variable DrugClick as the HTML linking variable. The FOOTNOTE statement provides text that indicates how to use the links in the graph.

The following statements provide the second analysis. The three files referred to by the DrugClick variable are created as follows:

```

ods html body='drug1.htm' newfile=page style=HTMLBlue;

proc sgplot data=drugtest;
  title 'Plot of PostTreatment versus PreTreatment';
  scatter y=PostTreatment x=PreTreatment;
  by drug notsorted;
run;
ods html close;

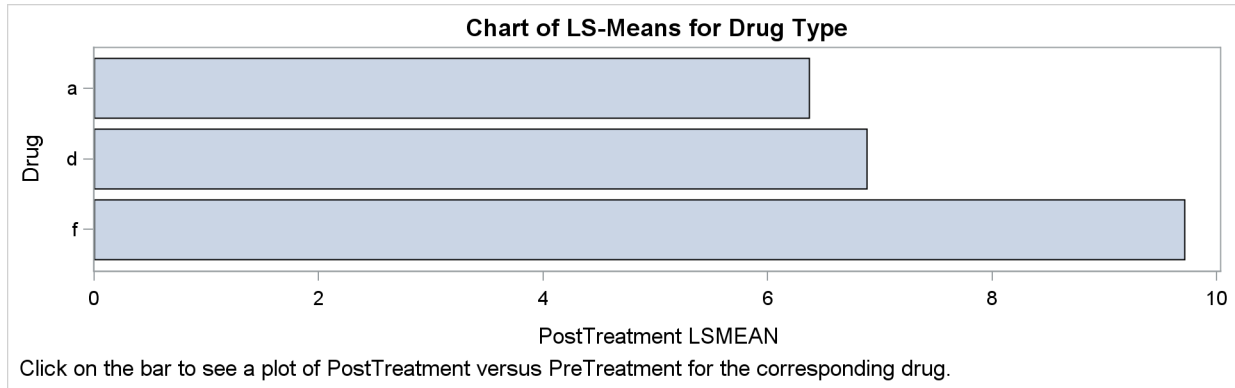
```

The NEWFILE= option in the ODS HTML statement creates a new HTML file for each page of output. (Page breaks occur only when a procedure explicitly starts a new page.) The NEWFILE= option also increments the filename numeric suffix for each new HTML file created, with the first filename corresponding to that given in the BODY= option, *drug1.htm*.

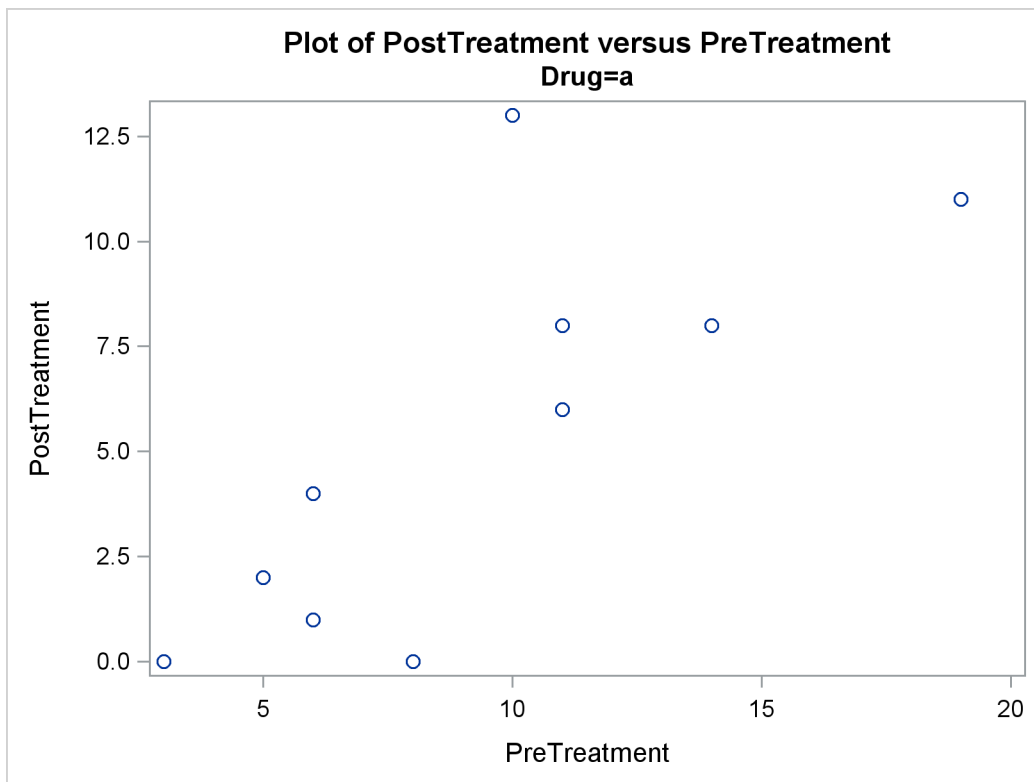
PROC SGPLOT is used, producing a plot of the variable PostTreatment versus the variable PreTreatment for each value of the Drug variable. Three plots are created, and each plot is contained in a separate HTML file. The files are named *drug1.htm*, *drug2.htm*, and *drug3.htm*. The filenames match those filenames specified as values of the DrugClick variable. By default, the HTML files are generated in your current working directory. You can instead specify a path, such as `frame='html/drug2.htm'`, to put a file in a subdirectory. The

chart in [Output 20.9.1](#) displays the difference in LS-means for each drug type. When you click on a bar that represents a value of the variable Drug, the browser opens the plot of PostTreatment versus PostTreatment variables that corresponds to that value of the variable Drug. [Output 20.9.2](#) displays the plots for each drug type.

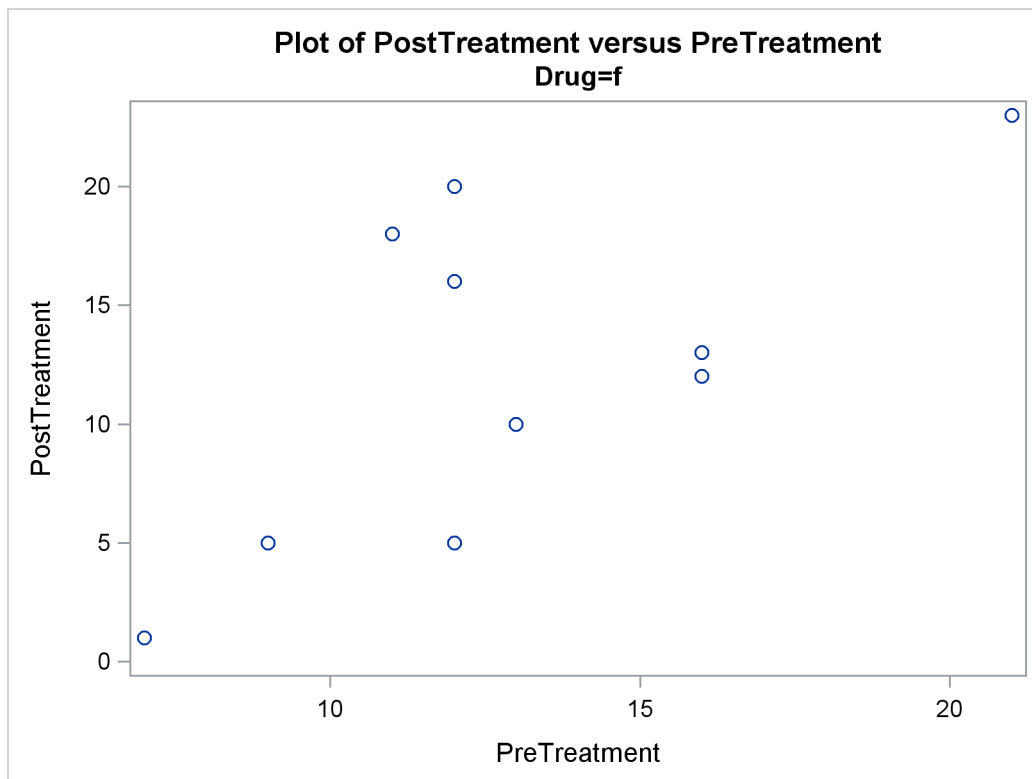
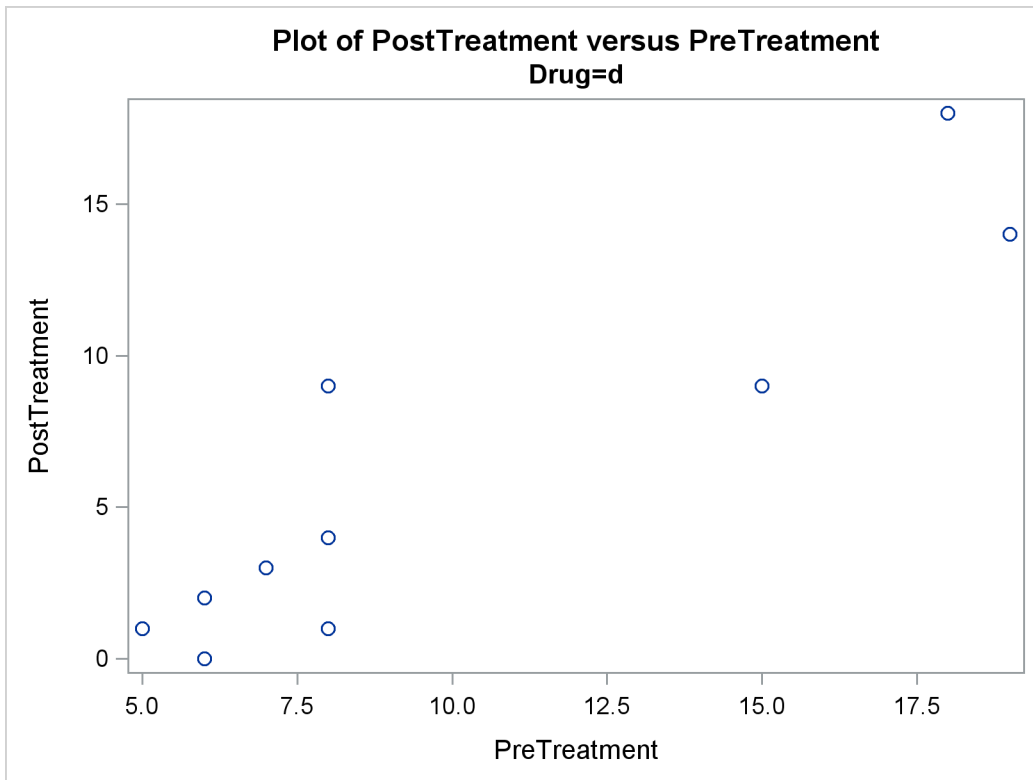
Output 20.9.1 Bar Chart of LS-Means by Drug Type with Links to Plots



Output 20.9.2 Plots by Drug Type



Output 20.9.2 continued



Example 20.10: Correlation and Covariance Matrices

This example demonstrates how you can use ODS to set the background color of individual cells in a table. The color is set to reflect the magnitude of the value in the cell. You can use color to call attention to larger values and to see the pattern in the data in a way that is hard to visualize just by looking at the numbers. This is illustrated with correlation and covariance matrices. The data for this first part of this example are ratings of automobiles. The following statements create the data set:

```

title 'Rating of Automobiles';

data cars;
  input Origin $ 1-8 Make $ 10-19 Model $ 21-36
        (MPG Reliability Acceleration Braking Handling Ride
         Visibility Comfort Quiet Cargo) (1.);
  datalines;
GMC      Buick      Century      3334444544
GMC      Buick      Electra      2434453555
GMC      Buick      Lesabre     2354353545

... more lines ...

GMC      Pontiac   Sunbird     3134533234
;

```

The following steps edit the template that PROC CORR uses to display the correlation matrix. The CELLSTYLE statement sets the background color to light gray for correlations equal to 1 or -1 . Values less than -0.75 or greater than 0.75 are set to red. Values less than -0.50 or greater than 0.50 are set to blue. Values less than -0.25 or greater than 0.25 are set to cyan. Values in the range -0.25 to 0.25 are set to white. PROC CORR is then run using the custom template. Finally, the default template is restored. The following statements produce [Output 20.10.1](#):

```

proc template;
  edit Base.Corr.StackedMatrix;
    column (RowName RowLabel) (Matrix) * (Matrix2);
    edit matrix;
      cellstyle _val_ = -1.00 as {backgroundcolor=CXEFFFFFFE},
                _val_ <= -0.75 as {backgroundcolor=red},
                _val_ <= -0.50 as {backgroundcolor=blue},
                _val_ <= -0.25 as {backgroundcolor=cyan},
                _val_ <= 0.25 as {backgroundcolor=white},
                _val_ <= 0.50 as {backgroundcolor=cyan},
                _val_ <= 0.75 as {backgroundcolor=blue},
                _val_ < 1.00 as {backgroundcolor=red},
                _val_ = 1.00 as {backgroundcolor=CXEFFFFFFE};
    end;
  end;
run;

ods _all_ close;
ods html body='corr.html' style=HTMLBlue;

```

```

proc corr data=cars noprob;
  ods select PearsonCorr;
run;

ods html close;
ods listing;

proc template;
  delete Base.Corr.StackedMatrix / store=sasuser.templat;
run;

```

Output 20.10.1 Correlation Matrix from PROC CORR

Rating of Automobiles										
The CORR Procedure										
Pearson Correlation Coefficients, N = 50										
	MPG	Reliability	Acceleration	Braking	Handling	Ride	Visibility	Comfort	Quiet	Cargo
MPG	1.00000	0.22003	-0.19454	0.41475	0.25594	-0.23705	0.67924	-0.06567	-0.49128	-0.03075
Reliability	0.22003	1.00000	-0.08512	0.25881	-0.09443	0.27406	0.33356	0.36607	0.45302	0.35261
Acceleration	-0.19454	-0.08512	1.00000	0.06688	0.07119	0.33888	-0.13280	0.06369	0.00934	-0.12112
Braking	0.41475	0.25881	0.06688	1.00000	0.22335	0.30309	0.44938	0.26165	0.00164	0.20880
Handling	0.25594	-0.09443	0.07119	0.22335	1.00000	0.12435	0.12599	-0.07516	-0.02418	-0.14274
Ride	-0.23705	0.27406	0.33888	0.30309	0.12435	1.00000	0.16114	0.75173	0.48498	0.39108
Visibility	0.67924	0.33356	-0.13280	0.44938	0.12599	0.16114	1.00000	0.29830	-0.18347	0.35585
Comfort	-0.06567	0.36607	0.06369	0.26165	-0.07516	0.75173	0.29830	1.00000	0.44917	0.53836
Quiet	-0.49128	0.45302	0.00934	0.00164	-0.02418	0.48498	-0.18347	0.44917	1.00000	0.33846
Cargo	-0.03075	0.35261	-0.12112	0.20880	-0.14274	0.39108	0.35585	0.53836	0.33846	1.00000

The preceding statements used a small number of discrete colors to show the range of values. In contrast, the following statements use a color gradient. The SAS autocall macro **Paint** is available for generating the CELLSTYLE colors list with a list of interpolated colors. If your site has installed the autocall libraries supplied by the SAS System and uses the standard configuration of software supplied by the SAS System, you need to ensure that the SAS System option MAUTOSOURCE is in effect before you begin using autocall macros. The macros do not have to be included (for example, with a %INCLUDE statement). They can be called directly once they are properly installed. For more information about autocall libraries, see *SAS Macro Language: Reference*.

Usually, you can use the **Paint** macro by specifying a list of values and a list of colors. Here is an example for values that range from 0 to 10:

```

%paint(values=0 to 10 by 0.5,
       colors=white cyan blue magenta red)

proc print data=colors;
run;

```

The **Paint** macro prints the following information to the SAS log:

Legend:

0 = White
 2.5 = Cyan
 5 = Blue
 7.5 = Magenta
 10 = Red

A value of 0 maps to white, a value of 2.5 maps to cyan, values in the range 0 to 2.5 map to colors in the range from white to cyan, and so on. The **Paint** macro for this step creates an output data set, **Colors**, which is shown in [Output 20.10.2](#).

Output 20.10.2 Color Interpolation

Rating of Automobiles		
Obs	Start	_RGB_
1	0.0	CXFFFFFF
2	0.5	CXCFFFFFF
3	1.0	CX97FFFF
4	1.5	CX63FFFF
5	2.0	CX2FFFFF
6	2.5	CX05FFFF
7	3.0	CX00D1FF
8	3.5	CX009CFF
9	4.0	CX0068FF
10	4.5	CX0034FF
11	5.0	CX0000FF
12	5.5	CX3400FF
13	6.0	CX6800FF
14	6.5	CX9C00FF
15	7.0	CXD100FF
16	7.5	CXFA00FF
17	8.0	CXFF00D1
18	8.5	CXFF009C
19	9.0	CXFF0068
20	9.5	CXFF0034
21	10.0	CXFF0000

This shows the color interpolation for a series of points. You could use a smaller **BY** value in the **Paint** macro to get more points along the color gradient. However, a few dozen colors are usually sufficient for most purposes.

The following steps use the **Paint** macro to create a color gradient for a correlation matrix, edit the template, display the results, and restore the default template:

```
%paint(values=-1 to 1 by 0.05, macro=setstyle,
        colors=CXEFFFFFFE red magenta blue cyan white
              cyan blue magenta red CXEFFFFFFE
              -1 -0.99 -0.75 -0.5 -0.25 0 0.25 0.5 0.75 0.99 1)
```

```

proc template;
  edit Base.Corr.StackedMatrix;
    column (RowName RowLabel) (Matrix) * (Matrix2);
    edit matrix;
      %setstyle(backgroundcolor)
    end;
  end;
run;

ods _all_ close;
ods html body='corr.html' style=HTMLBlue;
proc corr data=cars noprob;
  ods select PearsonCorr;
run;
ods html close;
ods listing;

proc template;
  delete Base.Corr.StackedMatrix / store=sasuser.templat;
run;

```

The `VALUES=` option creates a range of values from -1 to 1 with an increment of 0.05 . The `Paint` macro generates a `CELLSTYLE _val_ <= value as {backgroundcolor= color}`, line for each value in the list. Specifically, it generates a macro named `SETSTYLE` (from the `MACRO=` option) that contains the entire `CELLSTYLE` statement for use in `PROC TEMPLATE`. The argument to the macro is the option that you want to set. In this case, it is the background color. You could specify `foreground` instead to set the color of the numbers themselves. The first part of the generated statement is as follows:

```

cellstyle _val_<=-1 as {backgroundcolor=CXEFEEEE},
  _val_<=-0.95 as {backgroundcolor=CXFF0020},
  _val_<=-0.9 as {backgroundcolor=CXFF0062},
  _val_<=-0.85 as {backgroundcolor=CXFF008D},
  _val_<=-0.8 as {backgroundcolor=CXFF00CF},

```

The color mapping for a correlation matrix can be a bit more involved than it is for most tables. This is because you might want the maximum correlations, 1 and -1 , to be displayed using colors outside the gradient that is used for other values. Usually, you specify the color list, and the `Paint` macro maps the first color to the minimum value, the last color to the maximum value, and colors in between using equal increments and values based on the minimum and maximum. Alternatively, you can provide these values, as shown in this example. The legend, displayed in the SAS log, is as follows for the `Paint` macro step:

```

Legend:
  -1 = CXEEEEEE
 -0.99 = Red
 -0.75 = Magenta
 -0.5 = Blue
 -0.25 = Cyan
  0 = White
  0.25 = Cyan
  0.5 = Blue
  0.75 = Magenta
  0.99 = Red
  1 = CXEEEEEE

```


Values in the range -0.99 to 0.99 follow the interpolation red to magenta to blue to cyan to white to cyan to blue to magenta to red. Of course, the actual correlations for these data do not span this entire range, so a pure red background does not appear in the matrix. Correlations of 1 and -1 are displayed as light gray. The resulting correlation matrix is displayed in [Output 20.10.3](#). Notice that there are now a number of shades of colors, particularly shades of blues, not just a few discrete colors. The largest values are displayed in shades of purple and magenta.

Output 20.10.3 Correlation Matrix from PROC CORR with a Color Gradient

Rating of Automobiles										
The CORR Procedure										
Pearson Correlation Coefficients, N = 50										
	MPG	Reliability	Acceleration	Braking	Handling	Ride	Visibility	Comfort	Quiet	Cargo
MPG	1.00000	0.22003	-0.19454	0.41475	0.25594	-0.23705	0.67924	-0.06567	-0.49128	-0.03075
Reliability	0.22003	1.00000	-0.08512	0.25881	-0.09443	0.27406	0.33356	0.36607	0.45302	0.35261
Acceleration	-0.19454	-0.08512	1.00000	0.06688	0.07119	0.33888	-0.13280	0.06369	0.00934	-0.12112
Braking	0.41475	0.25881	0.06688	1.00000	0.22335	0.30309	0.44938	0.26165	0.00164	0.20880
Handling	0.25594	-0.09443	0.07119	0.22335	1.00000	0.12435	0.12599	-0.07516	-0.02418	-0.14274
Ride	-0.23705	0.27406	0.33888	0.30309	0.12435	1.00000	0.16114	0.75173	0.48498	0.39108
Visibility	0.67924	0.33356	-0.13280	0.44938	0.12599	0.16114	1.00000	0.29830	-0.18347	0.35585
Comfort	-0.06567	0.36607	0.06369	0.26165	-0.07516	0.75173	0.29830	1.00000	0.44917	0.53836
Quiet	-0.49128	0.45302	0.00934	0.00164	-0.02418	0.48498	-0.18347	0.44917	1.00000	0.33846
Cargo	-0.03075	0.35261	-0.12112	0.20880	-0.14274	0.39108	0.35585	0.53836	0.33846	1.00000

Next, the same technique is used to display the covariance and correlation matrices of a heteroscedastic autoregressive model. The data are based on the famous growth measurement data of Pothoff and Roy (1964), but are modified here to illustrate the technique of painting the entries of a matrix. The data consist of four repeated growth measurements of 11 girls and 16 boys. The measurements from two adjacent children in the original data were combined and rearranged here to emulate a repeated measures sequence with eight observations. The following statements create the data set:

```

title 'Analysis of Repeated Growth Measures';

data pr;
  input Person Gender $ y1 y2 y3 y4 y5 y6 y7 y8;
  array y{8};
  do time=5,7,8,4,3,2,1;
    Response = y{time};
    Age      = time+7;
    output;
  end;
  datalines;
1  F  21.0  20.0  21.5  23.0  21.0  21.5  24.0  25.5
2  F  20.5  24.0  24.5  26.0  23.5  24.5  25.0  26.5
3  F  21.5  23.0  22.5  23.5  20.0  21.0  21.0  22.5
4  F  21.5  22.5  23.0  25.0  23.0  23.0  23.5  24.0
5  F  20.0  21.0  22.0  21.5  16.5  19.0  19.0  19.5
6  F  24.5  25.0  28.0  28.0  26.0  25.0  29.0  31.0
7  M  21.5  22.5  23.0  26.5  23.0  22.5  24.0  27.5

```

```

8 M 25.5 27.5 26.5 27.0 20.0 23.5 22.5 26.0
9 M 24.5 25.5 27.0 28.5 22.0 22.0 24.5 26.5
10 M 24.0 21.5 24.5 25.5 23.0 20.5 31.0 26.0
11 M 27.5 28.0 31.0 31.5 23.0 23.0 23.5 25.0
12 M 21.5 23.5 24.0 28.0 17.0 24.5 26.0 29.5
13 M 22.5 25.5 25.5 26.0 23.0 24.5 26.0 30.0
;

```

The following statements create a macro that sets colors for the covariance matrix (SETSTYLE1), create a macro that sets colors for the correlation matrix (SETSTYLE2), edit the templates, run the analysis with PROC GLIMMIX, and restore the default templates:

```

* You need to run the analysis once to know that 20 is a good maximum;
%paint(values=0 to 20 by 0.25,
       colors=cyan blue magenta red, macro=setstyle1)

%paint(values=0 to 1 by 0.05,
       colors=cyan blue magenta red, macro=setstyle2)

proc template;
  edit Stat.Glimmix.V;
    column Subject Index Row Col;
  edit Col;
    %setstyle1(backgroundcolor)
  end;
end;
edit Stat.Glimmix.VCorr;
  column Subject Index Row Col;
  edit Col;
    %setstyle2(backgroundcolor)
  end;
end;
run;

ods _all_ close;
ods html body='ar1.html' style=HTMLBlue;
proc glimmix data=pr;
  class person gender time;
  model response = gender age gender*age;
  random _residual_ / sub=person type=arh(1) v residual vcorr;
  ods select v vcorr;
run;
ods html close;
ods listing;

proc template;
  delete Stat.Glimmix.V / store=sasuser.templat;
  delete Stat.Glimmix.VCorr / store=sasuser.templat;
run;

```

The results are displayed in [Output 20.10.4](#) and [Output 20.10.5](#). Both the covariance and correlation matrices have a structure that is more obvious when colors are added to the display. In particular, the colors clearly show the banded structure of the correlation matrix.

Output 20.10.4 Heteroscedastic AR(1) Covariance Matrix

Analysis of Repeated Growth Measures
The GLIMMIX Procedure

Estimated V Matrix for Person 1

Row	Col1	Col2	Col3	Col4	Col5	Col6	Col7
1	19.1973	10.5505	7.3707	4.5756	2.4983	1.4814	0.9697
2	10.5505	11.8104	8.2508	5.1220	2.7966	1.6582	1.0855
3	7.3707	8.2508	11.7407	7.2885	3.9795	2.3596	1.5446
4	4.5756	5.1220	7.2885	9.2159	5.0318	2.9836	1.9530
5	2.4983	2.7966	3.9795	5.0318	5.5959	3.3181	2.1720
6	1.4814	1.6582	2.3596	2.9836	3.3181	4.0075	2.6232
7	0.9697	1.0855	1.5446	1.9530	2.1720	2.6232	3.4976

Output 20.10.5 Heteroscedastic AR(1) Correlation Matrix

Estimated V Correlation Matrix for Person 1

Row	Col1	Col2	Col3	Col4	Col5	Col6	Col7
1	1.0000	0.7007	0.4910	0.3440	0.2410	0.1689	0.1183
2	0.7007	1.0000	0.7007	0.4910	0.3440	0.2410	0.1689
3	0.4910	0.7007	1.0000	0.7007	0.4910	0.3440	0.2410
4	0.3440	0.4910	0.7007	1.0000	0.7007	0.4910	0.3440
5	0.2410	0.3440	0.4910	0.7007	1.0000	0.7007	0.4910
6	0.1689	0.2410	0.3440	0.4910	0.7007	1.0000	0.7007
7	0.1183	0.1689	0.2410	0.3440	0.4910	0.7007	1.0000

Alternatively, you could just use the **Paint** macro to do the color interpolation and use its output data set to create other types of style effects. The following statements show one way to set the font to bold and set the foreground color based on the values of the covariances:

```

%let inc = 0.25;

%paint(values=0 to 20 by &inc, colors=blue magenta red)

data cntlin;
  set colors;
  fmtname = 'paintfmt';
  label = _rgb_;
  end = start + &inc;
  keep start end label fmtname;
run;

proc format cntlin=cntlin;
run;

proc template;
  edit Stat.Glimmix.V;
  column Subject Index Row Col;
  edit Col;
  style = {foreground=paintfmt8. font_weight=bold};
  end;
end;
run;

ods _all_ close;
ods html body='ar1.html' style=HTMLBlue;
proc glimmix data=pr;
  class person gender time;
  model response = gender age gender*age;
  random _residual_ / sub=person type=arh(1) v residual;
  ods select v;
run;
ods html close;
ods listing;

proc template;
  delete Stat.Glimmix.V / store=sasuser.templat;
run;

```

The **Paint** macro creates the SAS data set **Colors** with the result of the interpolation. This data set can be processed to create a format. The **DATA** step creates a range of values from **Start** to **End** and assigns a color to **Label** based on the color computed by the **Paint** macro. This data set is input to **PROC FORMAT** to create the format **PAINTFMT**. **PROC TEMPLATE** uses this format to set the color of the values in the table. The cell value is evaluated using the specified **FOREGROUND=** format for every cell in the table, and the appropriate color is assigned. **PROC GLIMMIX** does the analysis, and the results are displayed in [Output 20.10.6](#).

Output 20.10.6 Heteroscedastic AR(1) Covariance Matrix

Analysis of Repeated Growth Measures

The GLIMMIX Procedure

Estimated V Matrix for Person 1							
Row	Col1	Col2	Col3	Col4	Col5	Col6	Col7
1	19.1973	10.5505	7.3707	4.5756	2.4983	1.4814	0.9697
2	10.5505	11.8104	8.2508	5.1220	2.7966	1.6582	1.0855
3	7.3707	8.2508	11.7407	7.2885	3.9795	2.3596	1.5446
4	4.5756	5.1220	7.2885	9.2159	5.0318	2.9836	1.9530
5	2.4983	2.7966	3.9795	5.0318	5.5959	3.3181	2.1720
6	1.4814	1.6582	2.3596	2.9836	3.3181	4.0075	2.6232
7	0.9697	1.0855	1.5446	1.9530	2.1720	2.6232	3.4976

Many other effects could be achieved by using this approach and different options in the STYLE= specification.

References

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- Hemmerle, W. J. and Hartley, H. O. (1973), "Computing Maximum Likelihood Estimates for the Mixed AOV Model Using the W-Transformation," *Technometrics*, 15, 819–831.
- Olinger, C. R. and Tobias, R. D. (1998), "It Chops, It Dices, It Makes Julienne Slices! ODS for Data Analysis Output As-You-Like-It in Version 7," in *Proceedings of the Twenty-third Annual SAS Users Group International Conference*, Cary, NC: SAS Institute Inc.
- Pothoff, R. F. and Roy, S. N. (1964), "A Generalized Multivariate Analysis of Variance Model Useful Especially for Growth Curve Problems," *Biometrika*, 51, 313–326.
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Chapter 21

Statistical Graphics Using ODS

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Introduction

Effective graphics are indispensable for modern statistical analysis. They reveal patterns, differences, and uncertainty that are not readily apparent in tabular output. Graphics provoke questions that stimulate deeper investigation, and they add visual clarity and rich content to reports and presentations.

In earlier SAS releases, creating graphs with statistical procedures typically required additional programming steps such as creating output data sets with the values to plot, modifying these data sets with a DATA step program, and using traditional SAS/GRAPH procedures to produce the plots.

ODS Graphics eliminates the need for additional programming. ODS Graphics is an extension of ODS (the Output Delivery System). ODS manages procedure output and lets you display it in a variety of destinations,

such as HTML and RTF. With ODS Graphics, statistical procedures produce graphs as automatically as they produce tables, and graphs are integrated with tables in the ODS output. ODS Graphics is available in procedures in SAS/STAT, Base SAS, SAS/ETS, SAS/QC, and other products (see the section “[Procedures That Support ODS Graphics](#)” on page 609). Note that ODS Graphics is automatically provided with Base SAS software.

ODS Graphics might or might not be enabled by default depending on your operating system, whether you are in the SAS windowing environment, your registry, system options, and configuration file settings. For more information about default settings and enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600.

You can enable ODS Graphics with the following statement:

```
ods graphics on;
```

When ODS Graphics is enabled, procedures that support ODS Graphics create appropriate graphs, either by default or when you specify procedure options for requesting specific graphs. These options are documented in the “Syntax” section of each procedure chapter, and the “Details” section of each chapter provides an “ODS Graphics” subsection that lists the graphs that are available. Once ODS Graphics is enabled, it stays enabled for the duration of your SAS session unless you disable it.

You can disable ODS Graphics with the following statement:

```
ods graphics off;
```

You might consider disabling ODS Graphics if your goal is solely to produce computational results. Often though, you can enable ODS Graphics and then leave it enabled. Throughout this chapter, ODS Graphics is enabled only once per section.

Chapter Reading Guide

This chapter provides a basic introduction to ODS Graphics along with more detailed information. The following list provides a guide to reading this chapter:

- If you want to see a few of the many graphs that are produced by statistical procedures by using ODS Graphics, see the section “[Getting Started with ODS Statistical Graphics](#)” on page 582.
- If you are using ODS Graphics for the first time, read the section “[A Primer on ODS Statistical Graphics](#)” on page 599, which provides the minimum information that you need to get started.
- If you need to create plots of raw data or your own customized plots of statistical results, see the section “[Statistical Graphics Procedures](#)” on page 682, which describes SAS procedures that use ODS Graphics.
- If you need information about specialized topics such as accessing your graphs, making changes to your graphs, and working with ODS styles, see the detailed discussions starting with the section “[Syntax](#)” on page 610 and including the section “[Examples of ODS Statistical Graphics](#)” on page 692.

If you are unfamiliar with ODS, see Chapter 20, “[Using the Output Delivery System](#).” For complete documentation about the Output Delivery System, see the *SAS Output Delivery System: User’s Guide*. For an introduction to graph template modification, see Chapter 22, “[ODS Graphics Template Modification](#).” For

an introduction to ODS Graphics, ODS styles, the graph template language, the style template language, the statistical graphics procedures, and graph template modification, see Kuhfeld (2010). For complete documentation about ODS graph templates, see the *SAS/GRAPH: Graph Template Language User's Guide* and the *SAS/GRAPH: Graph Template Language Reference*. For complete documentation about the ODS Graphics Editor, see the *SAS/GRAPH: ODS Graphics Editor User's Guide*. Also see the *SAS/GRAPH: Statistical Graphics Procedures Guide* for information about the statistical graphics procedures.

Assumptions about ODS Defaults in This Chapter

Default settings such as destinations and whether or not ODS Graphics is enabled vary depending on your operating system, registry settings, configuration file settings, system options, and whether you are using the SAS windowing environment or batch mode. For this reason, this chapter makes no assumptions about these defaults. Instead, destinations are often explicitly closed without assuming which destination (usually LISTING or HTML) is open, destinations are explicitly opened when needed, and ODS Graphics is explicitly enabled and disabled as needed. In some examples, when all destinations are closed, the LISTING destination is opened at the end of the step so that some destination is available for subsequent output. If you know the defaults for your environment, you do not need to use many of the ODS statements that are used in this chapter.

Getting Started with ODS Statistical Graphics

This section provides examples that illustrate the most basic uses of ODS Graphics with a few of the many plots that are produced by statistical procedures.

Default Plots for Simple Linear Regression with PROC REG

This example is based on the section “Getting Started: REG Procedure” on page 6616 of Chapter 79, “The REG Procedure.” The Class data set used in this example is available in the Sashelp library. The following statements use PROC REG to fit a simple linear regression model in which Weight is the response variable and Height is the independent variable:

```
ods graphics on;

proc reg data=sashelp.class;
    model Weight = Height;
run; quit;
```

The ODS GRAPHICS ON statement requests ODS Graphics in addition to the usual tabular output. The statement ODS GRAPHICS OFF is not used here, but it can be specified to disable ODS Graphics.

The graphical output consists of a fit diagnostics panel, a residual plot, and a fit plot. These plots are integrated with the tabular output and are shown in [Figure 21.1](#), [Figure 21.2](#), and [Figure 21.3](#), respectively. The results are displayed in the HTMLBLUE style.

Figure 21.1 Fit Diagnostics Panel

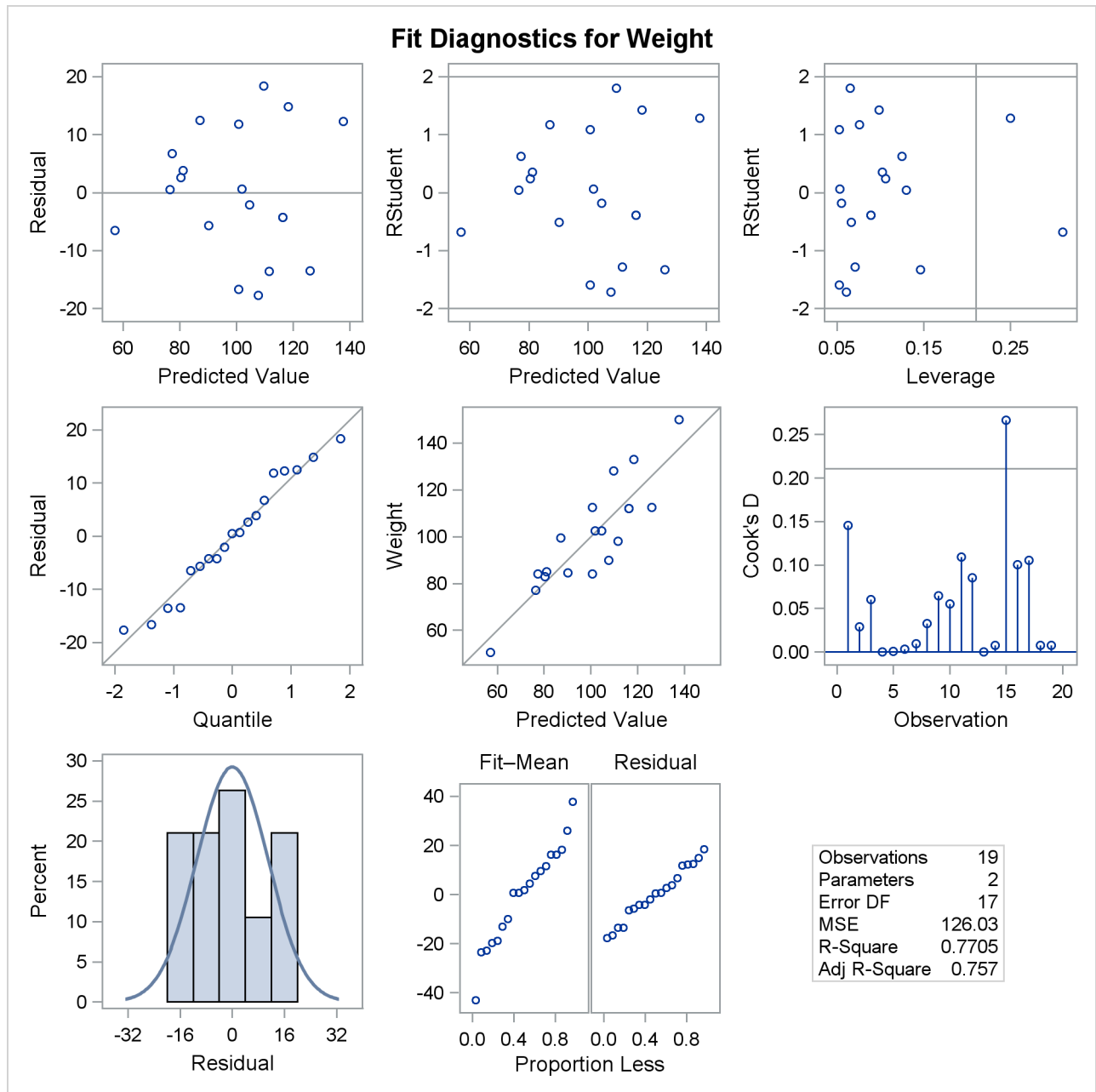


Figure 21.2 Residual Plot

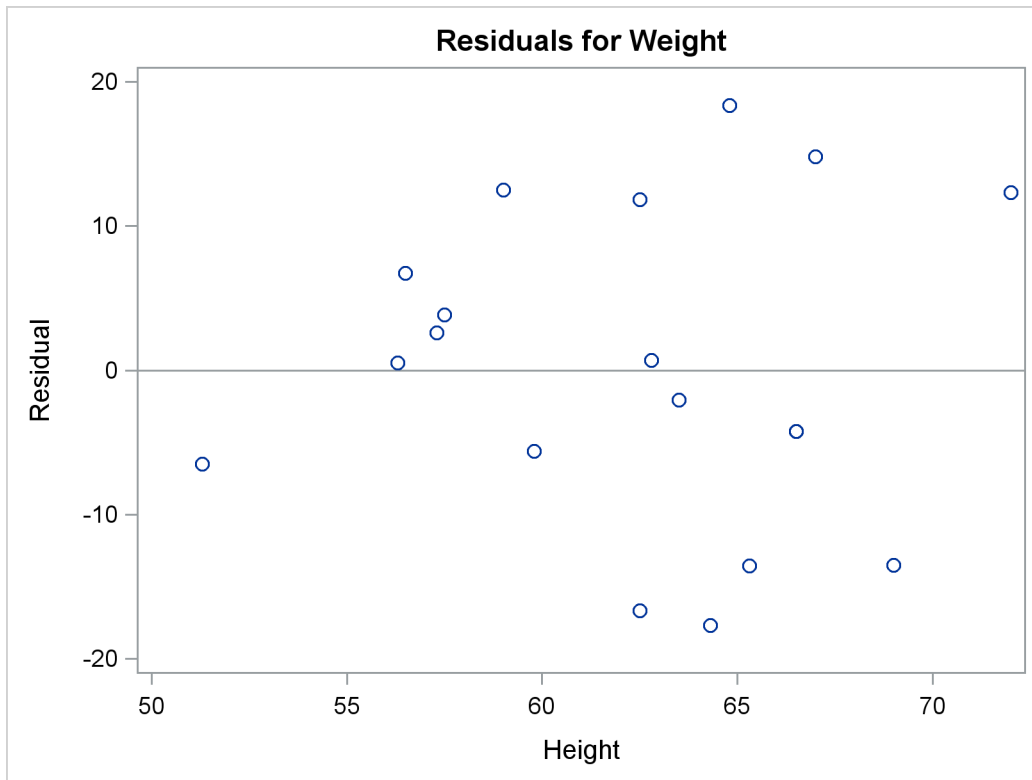
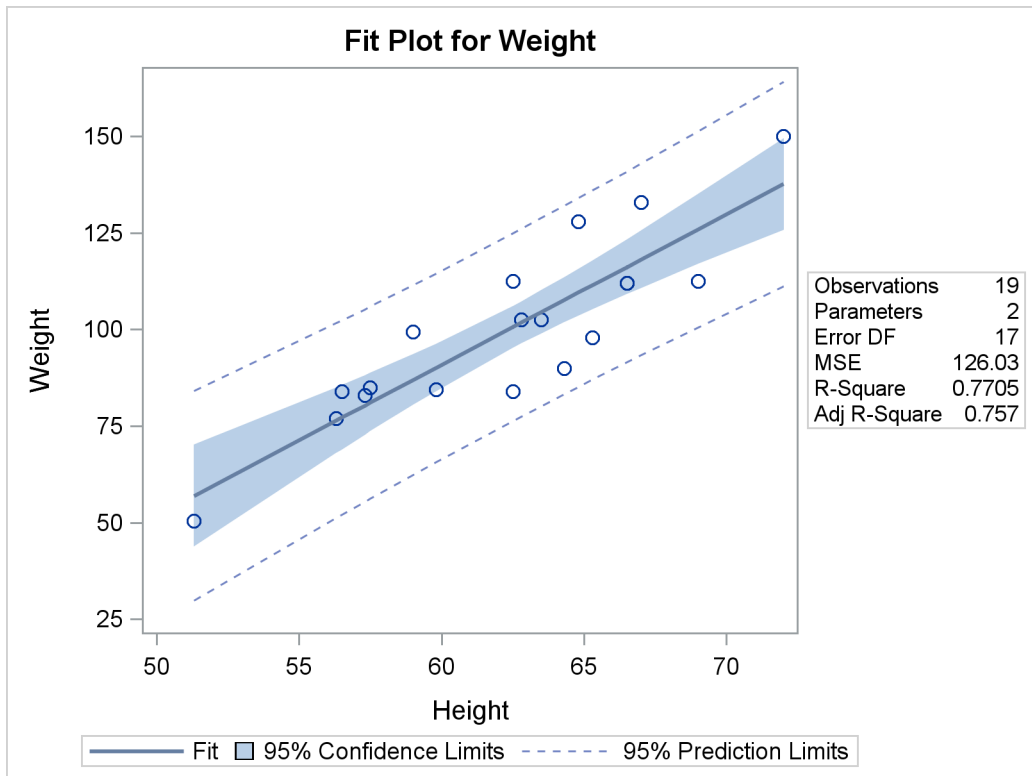


Figure 21.3 Fit Plot



ODS styles control the colors and general appearance of all graphs and tables, and the SAS System provides several styles that are recommended for use with statistical graphics. The default style that you see when you run SAS depends on the ODS destination, system options, and SAS registry settings. For more information about styles, see the section “Graph Styles” on page 601 and the section “Styles” on page 635.

Survival Estimate Plot with PROC LIFETEST

This example is taken from [Example 52.2](#) of Chapter 52, “The LIFETEST Procedure.” It shows how to construct a product-limit survival estimate plot. Both the ODS GRAPHICS statement and procedure options are used to request the plot. This example uses the bone marrow transplant data set, which is available from the Sashelp library. The data set contains disease-free times for three risk categories.

The following statements use PROC LIFETEST to compute the product-limit estimate of the survivor function for each risk category:

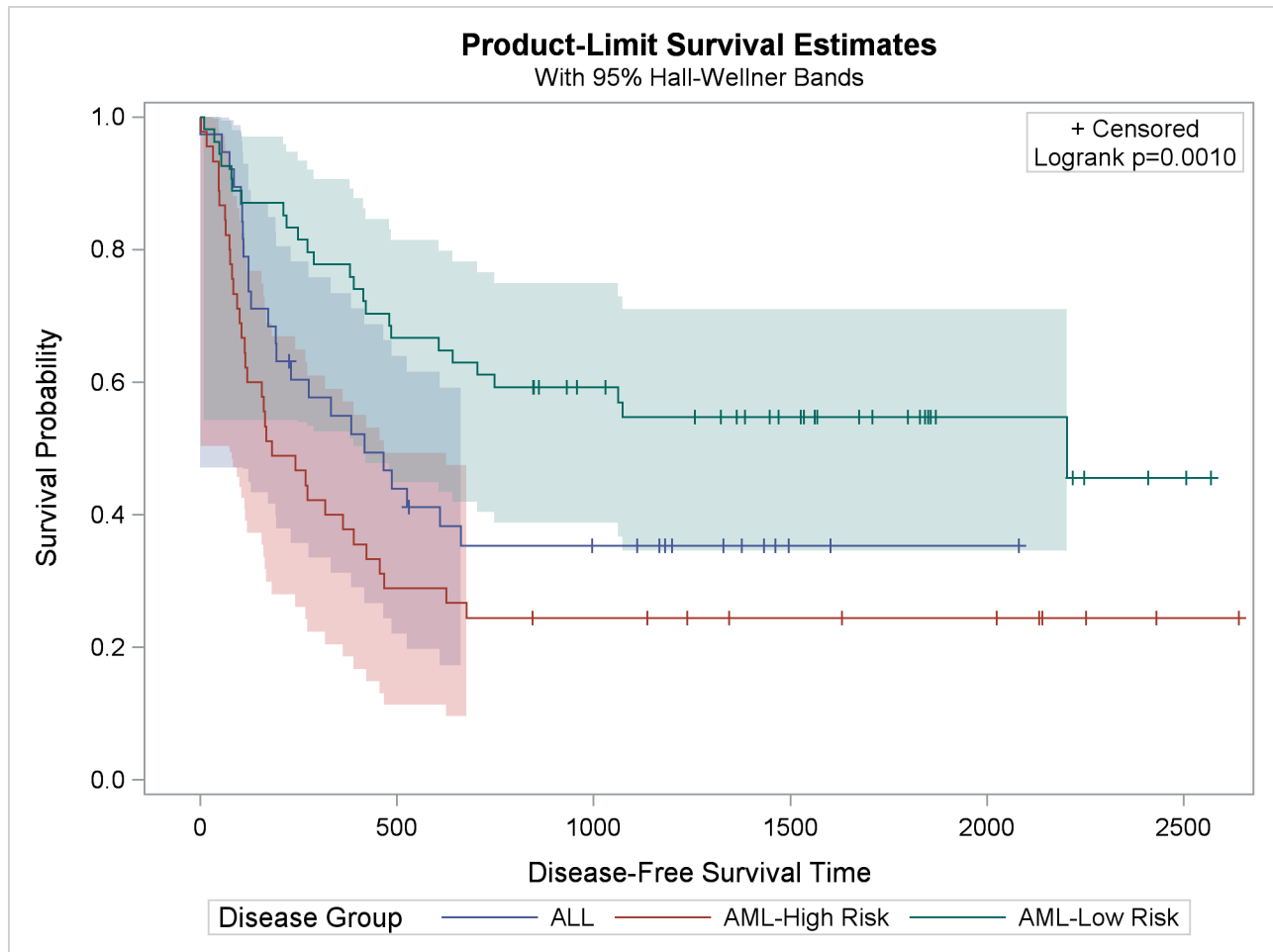
```
ods graphics on;

proc lifetest data=sashelp.BMT plots=survival(cb=hw test);
  time T * Status(0);
  strata Group / test=logrank;
run;
```

The ODS GRAPHICS ON statement enables ODS Graphics, and the PLOTS=SURVIVAL option requests a plot of the estimated survival curves. The CB=HW suboption requests Hall-Wellner confidence bands, and the TEST suboption displays the p -value for the log-rank test in a plot inset.

[Figure 21.4](#) displays the plot; note that tabular output is not shown. Patients in the AML-Low Risk group are disease-free longer than those in the ALL group, who in turn fare better than those in the AML-High Risk group.

Figure 21.4 Survival Plot



Contour and Surface Plots with PROC KDE

This example is taken from the section “Getting Started: KDE Procedure” on page 3748 in Chapter 48, “The KDE Procedure.” Here, in addition to the ODS GRAPHICS statement, procedure options are used to request plots. The following statements simulate 1,000 observations from a bivariate normal density with means (0,0), variances (10,10), and covariance 9:

```
data bivnormal;
  do i = 1 to 1000;
    z1 = rannor(104);
    z2 = rannor(104);
    z3 = rannor(104);
    x = 3*z1+z2;
    y = 3*z1+z3;
    output;
  end;
run;
```

The following statements request a bivariate kernel density estimate for the variables x and y :

```
ods graphics on;  
  
proc kde data=bivnormal;  
  bivar x y / plots=contour surface;  
run;
```

The PLOTS= option requests a contour plot and a surface plot of the estimate (displayed in [Figure 21.5](#) and [Figure 21.6](#), respectively). For more information about the graphs available in PROC KDE, see the section “ODS Graphics” on page 3767 of Chapter 48, “The KDE Procedure.”

Figure 21.5 Contour Plot of Estimated Density

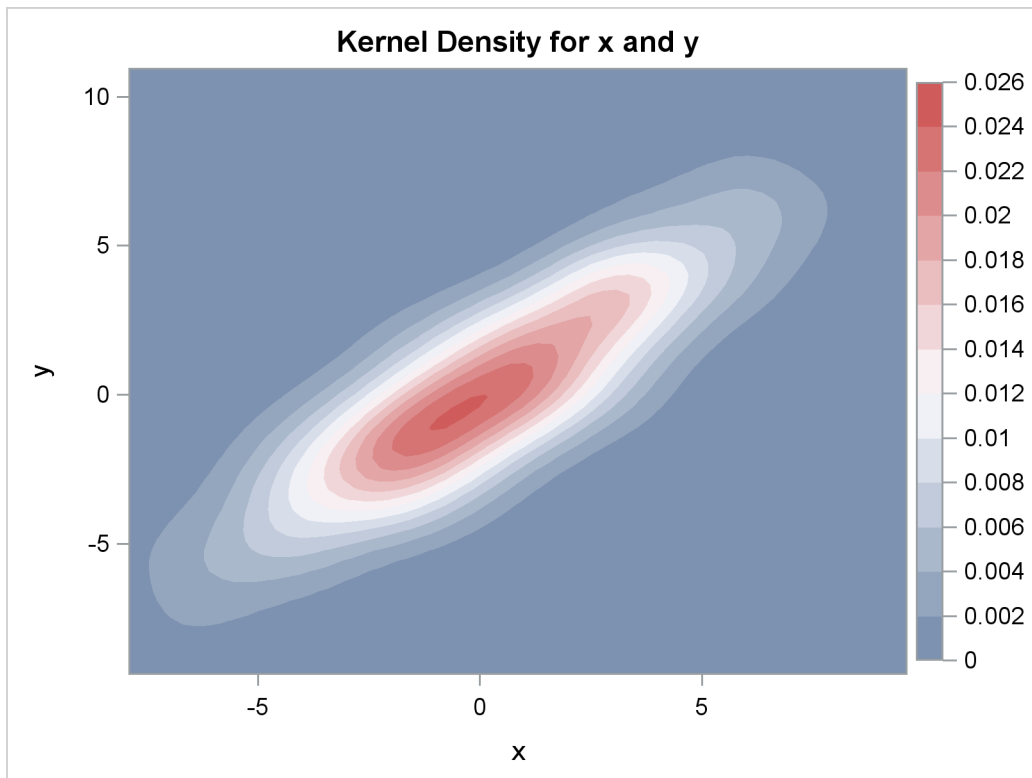
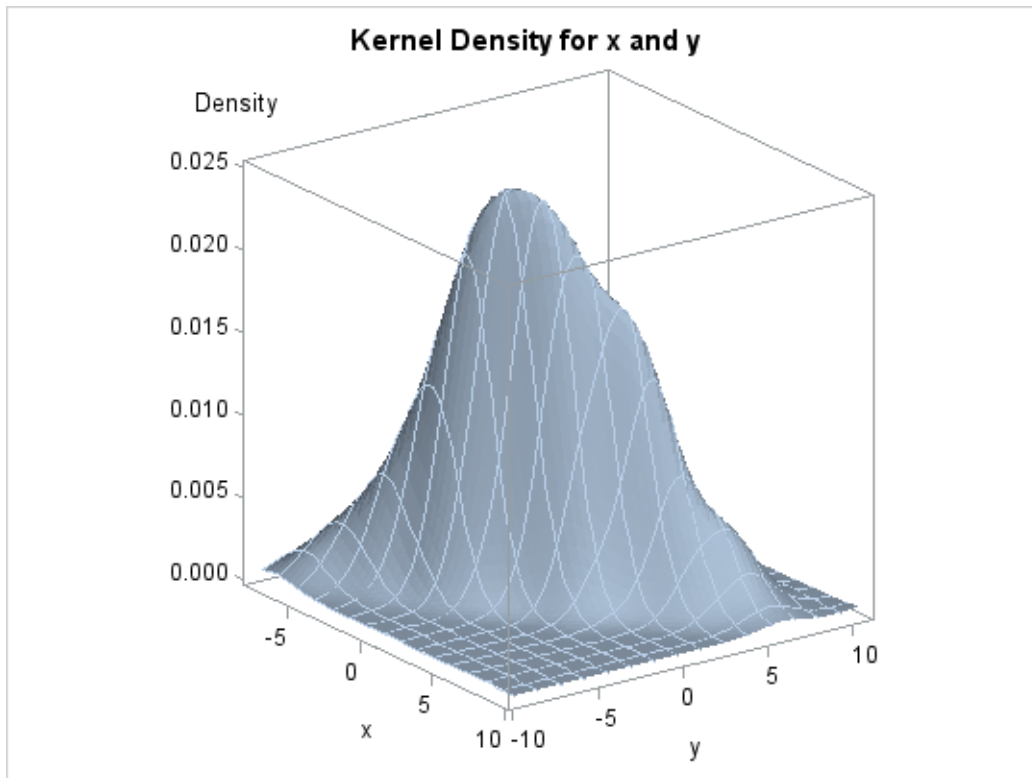


Figure 21.6 Surface Plot of Estimated Density

Contour Plots with PROC KRIGE2D

This example is taken from [Example 49.2](#) of Chapter 49, “The KRIGE2D Procedure.” The coal seam thickness data set is available from the Sashelp library. The following statements create a SAS data set that contains a copy of these data along with some artificially added missing data:

```
data thick;
  set sashelp.thick;
  if _n_ in (41, 42, 73) then thick = .;
run;
```

The following statements run PROC KRIGE2D:

```
ods graphics on;

proc krige2d data=thick outest=predictions
  plots=(observ(showmissing)
         pred(fill=pred line=pred obs=linegrad)
         pred(fill=se line=se obs=linegrad));
  coordinates xc=East yc=North;
  predict var=Thick r=60;
  model scale=7.2881 range=30.6239 form=gauss;
  grid x=0 to 100 by 2.5 y=0 to 100 by 2.5;
run;
```

The PLOTS=OBSERV(SHOWMISSING) option produces a scatter plot of the data along with the locations of any missing data. The PLOTS=PRED option produces maps of the kriging predictions and standard errors. Two instances of the PLOTS=PRED option are specified with suboptions that customize the plots. The results are shown in Figure 21.7.

Figure 21.7 Spatial Distribution

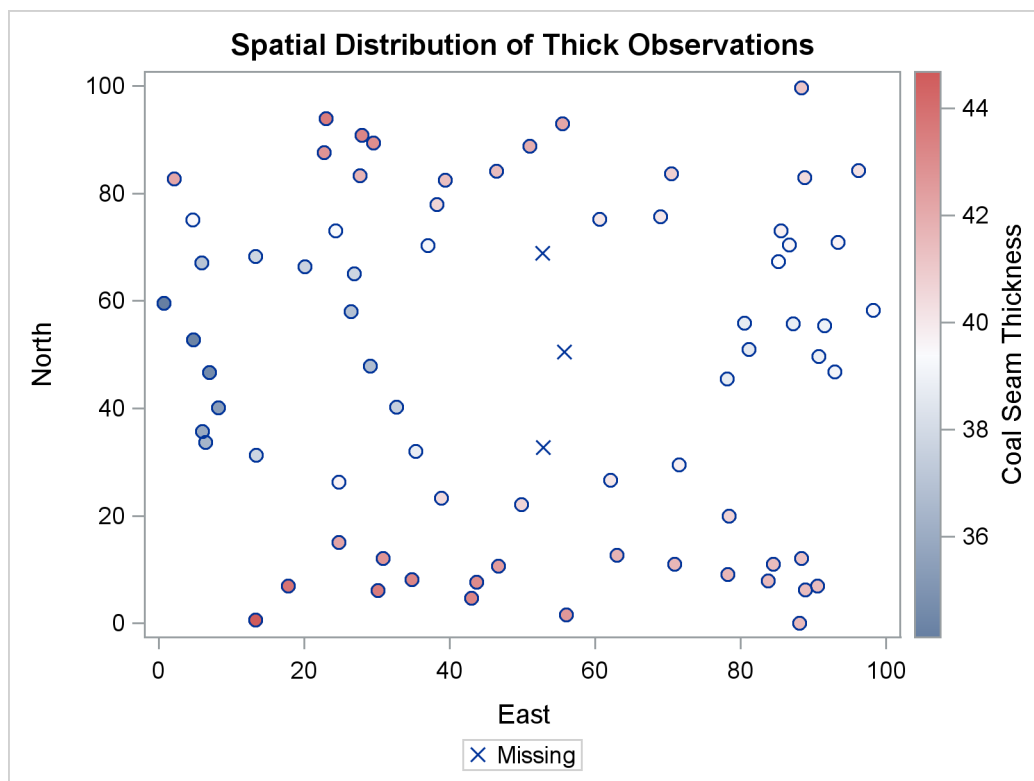
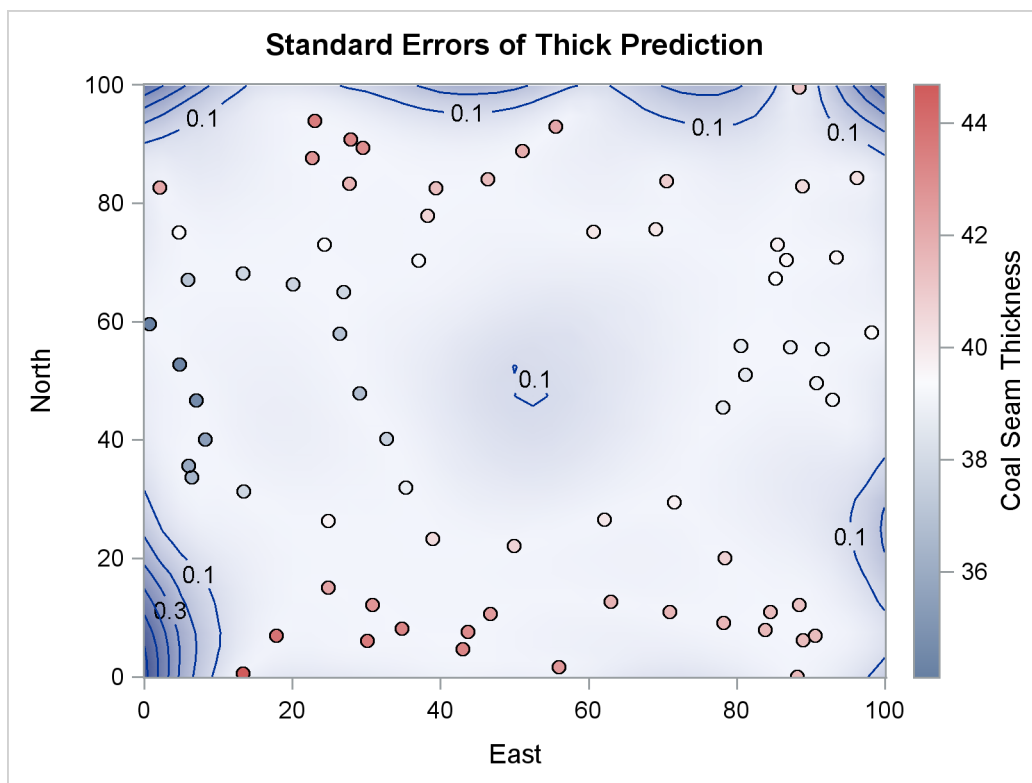
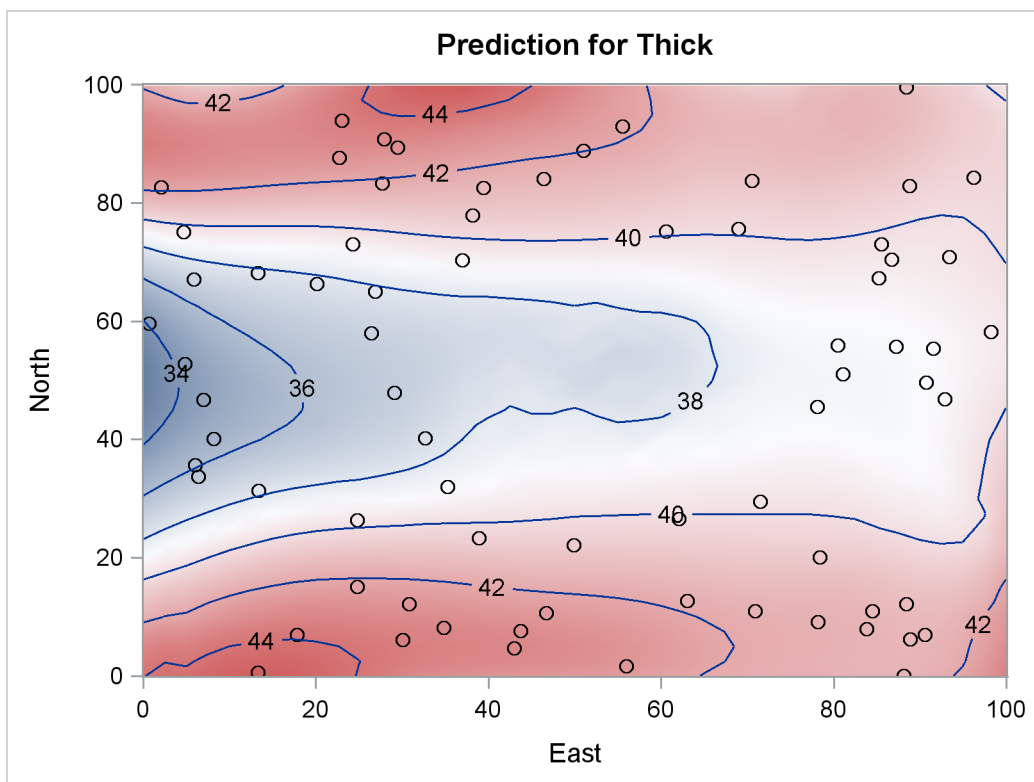


Figure 21.7 continued



Partial Least Squares Plots with PROC PLS

This example is taken from the section “Getting Started: PLS Procedure” on page 5865 of Chapter 70, “The PLS Procedure.” The following statements create a SAS data set that contains measurements of biological activity in the Baltic Sea:

```
data Sample;
  input obsnam $ v1-v27 ls ha dt @@;
  datalines;
EM1  2766 2610 3306 3630 3600 3438 3213 3051 2907 2844 2796
      2787 2760 2754 2670 2520 2310 2100 1917 1755 1602 1467
      1353 1260 1167 1101 1017          3.0110 0.0000 0.00
EM2  1492 1419 1369 1158  958  887  905  929  920  887  800

      ... more lines ...

;
```

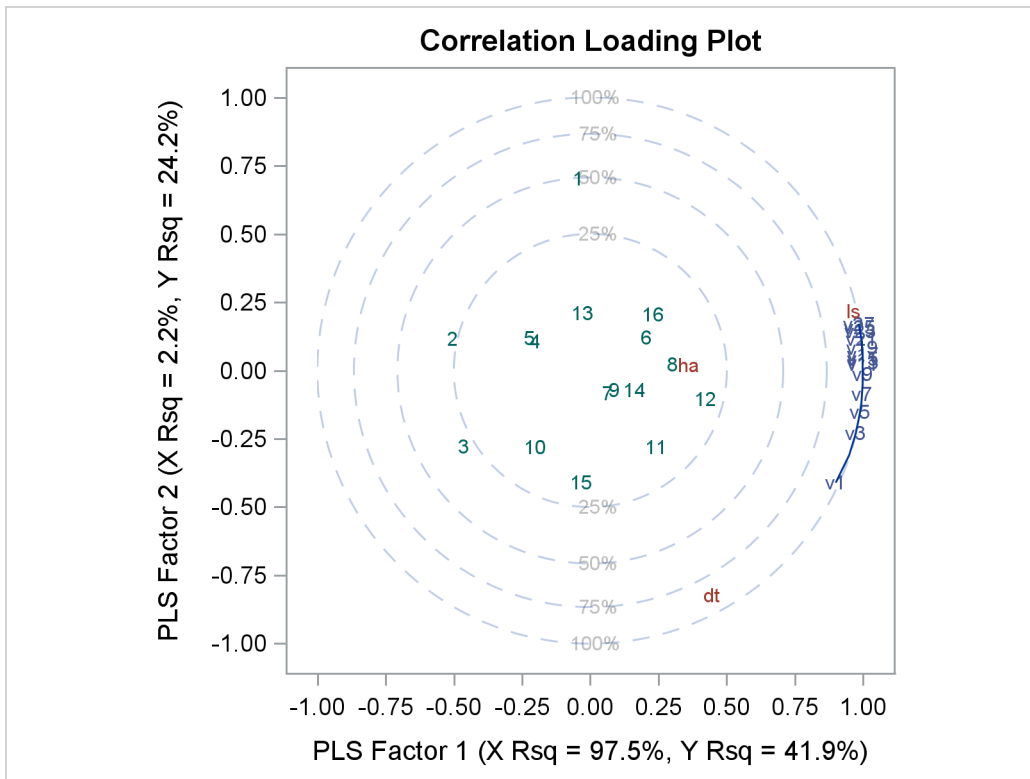
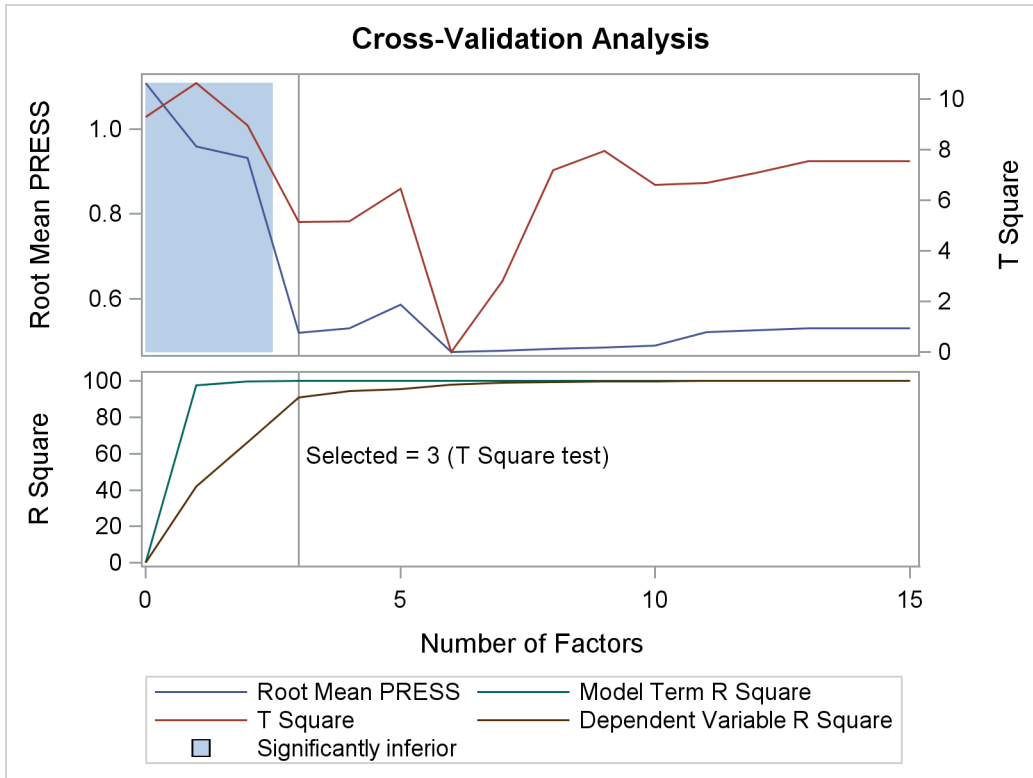
The following statements run PROC PLS:

```
ods graphics on;

proc pls data=sample cv=split cvtest(seed=104);
  model ls ha dt = v1-v27;
run;
```

By default, the procedure produces a plot for the cross validation analysis and a correlation loading plot (see Figure 21.8).

Figure 21.8 Partial Least Squares



Box-Cox Transformation Plot with PROC TRANSREG

This example is taken from [Example 97.2](#) of Chapter 97, “The TRANSREG Procedure.” The following statements create a SAS data set that contains failure times for yarn:

```
proc format;
  value a -1 = 8 0 = 9 1 = 10;
  value l -1 = 250 0 = 300 1 = 350;
  value o -1 = 40 0 = 45 1 = 50;
run;

data yarn;
  input Fail Amplitude Length Load @@;
  format amplitude a. length l. load o.;
  label fail = 'Time in Cycles until Failure';
  datalines;
674 -1 -1 -1    370 -1 -1 0    292 -1 -1 1    338 0 -1 -1
266 0 -1 0    210 0 -1 1    170 1 -1 -1    118 1 -1 0

... more lines ...

;
```

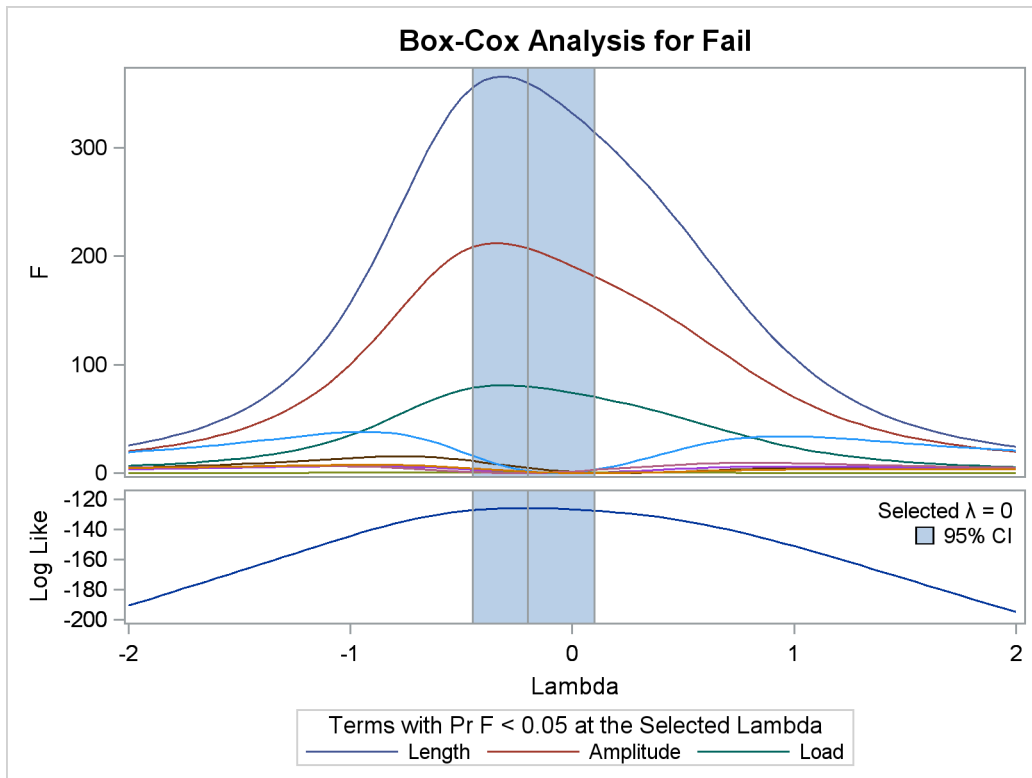
The following statements run PROC TRANSREG:

```
ods graphics on;

proc transreg data=yarn;
  model BoxCox(fail / convenient lambda=-2 to 2 by 0.05) =
    qqpoint(length amplitude load);
run;
```

The log-likelihood plot in [Figure 21.9](#) suggests a Box-Cox transformation with $\lambda = 0$.

Figure 21.9 Box-Cox “Significant Effects”



LS-Means Diffogram with PROC GLIMMIX

This example is taken from the section “Graphics for LS-Mean Comparisons” on page 3122 of Chapter 41, “The GLIMMIX Procedure.” The following statements create a SAS data set that contains measurements from an experiment that investigates how snapdragons grow in various soils:

```
data plants;
  input Type $ @;
  do Block = 1 to 3;
    input StemLength @;
    output;
  end;
  datalines;
Clarion  32.7 32.3 31.5
Clinton  32.1 29.7 29.1

... more lines ...

;
```

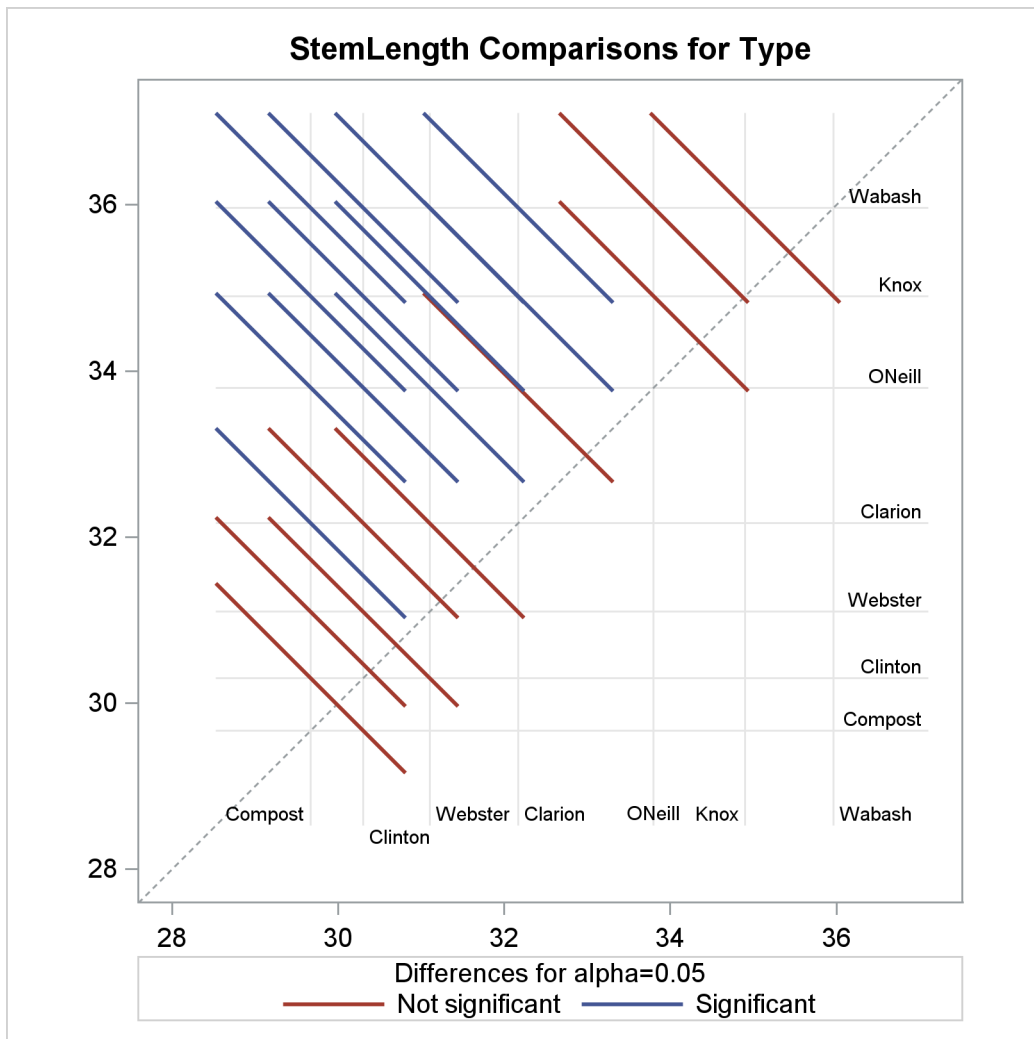
The following statements run PROC GLIMMIX:

```
ods graphics on;

proc glimmix data=plants order=data plots=diffogram;
  class Block Type;
  model StemLength = Block Type;
  lsmeans Type;
run;
```

The PLOTS=DIFFOGRAM option produces a diffogram, shown in Figure 21.10, that displays all of the pairwise least squares mean differences and indicates which are significant.

Figure 21.10 LS-Means Diffogram



Principal Component Analysis Plots with PROC PRINCOMP

This example is taken from [Example 73.3](#) of Chapter 73, “The PRINCOMP Procedure.” The following statements create a SAS data set that contains ratings of job performance of police officers:

```
options validvarname=any;

data Jobratings;
  input ('Communication Skills'n
        'Problem Solving'n
        'Learning Ability'n
        'Judgment Under Pressure'n
        'Observational Skills'n
        'Willingness to Confront Problems'n
        'Interest in People'n
        'Interpersonal Sensitivity'n
        'Desire for Self-Improvement'n
        'Appearance'n
        'Dependability'n
        'Physical Ability'n
        'Integrity'n
        'Overall Rating'n) (1.);
  datalines;
26838853879867
74758876857667

... more lines ...

;
```

The following statements run PROC PRINCOMP:

```
ods graphics on;

proc princomp data=Jobratings(drop='Overall Rating'n) n=2
  plots=(Matrix PatternProfile);
run;
```

The plots are requested by the PLOTS=(MATRIX PATTERNPROFILE) option. The results, shown in [Figure 21.11](#), contain the default scree and variance-explained plots, along with a scatter plot matrix of component scores and a pattern profile plot.

Figure 21.11 Principal Component Analysis

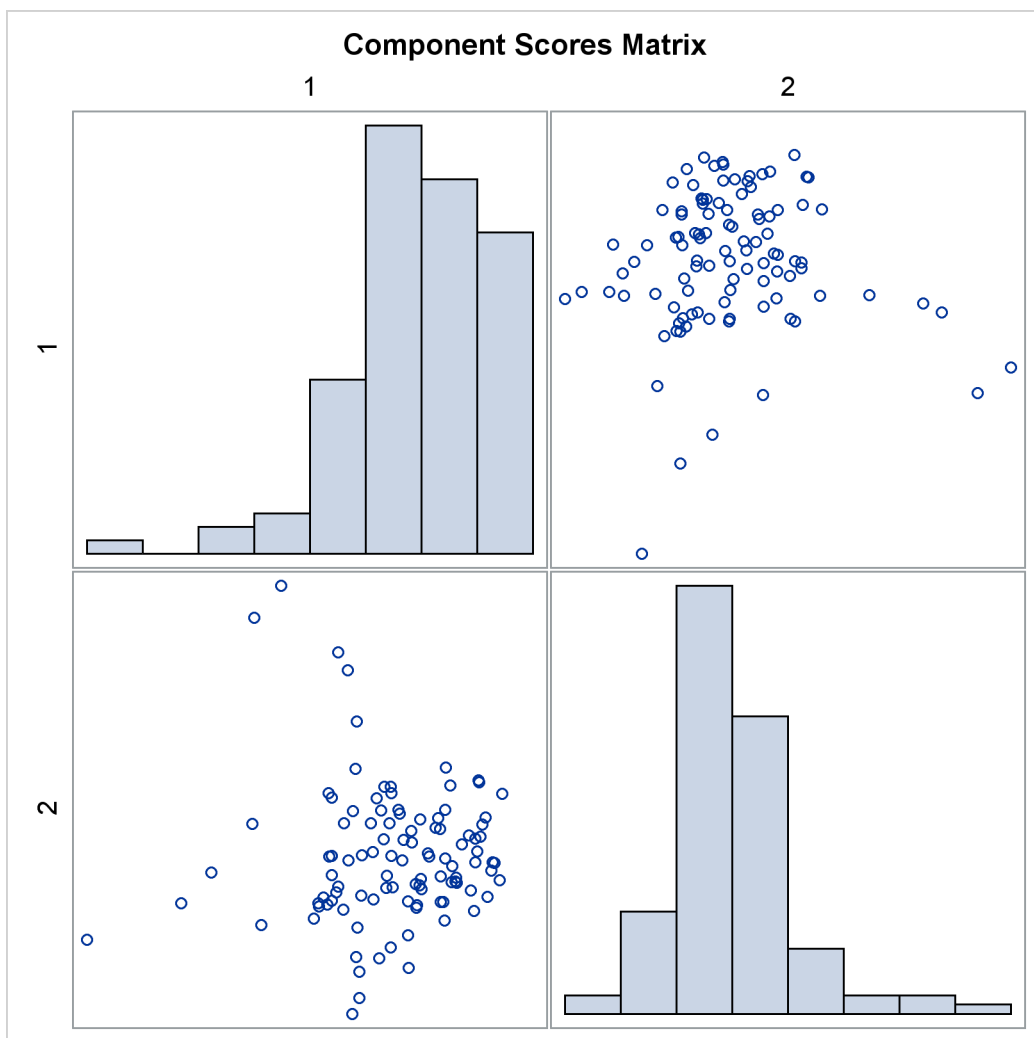
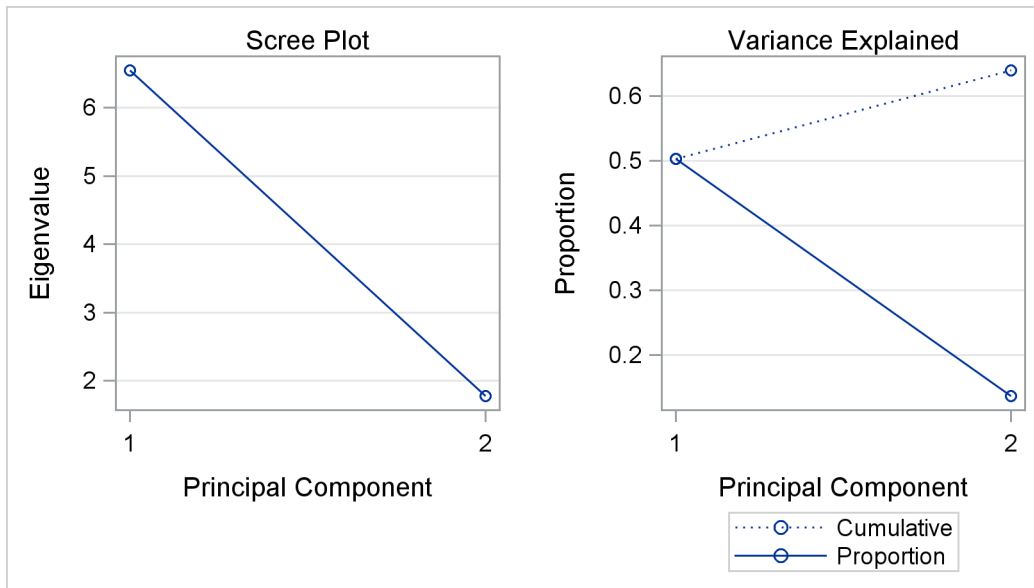
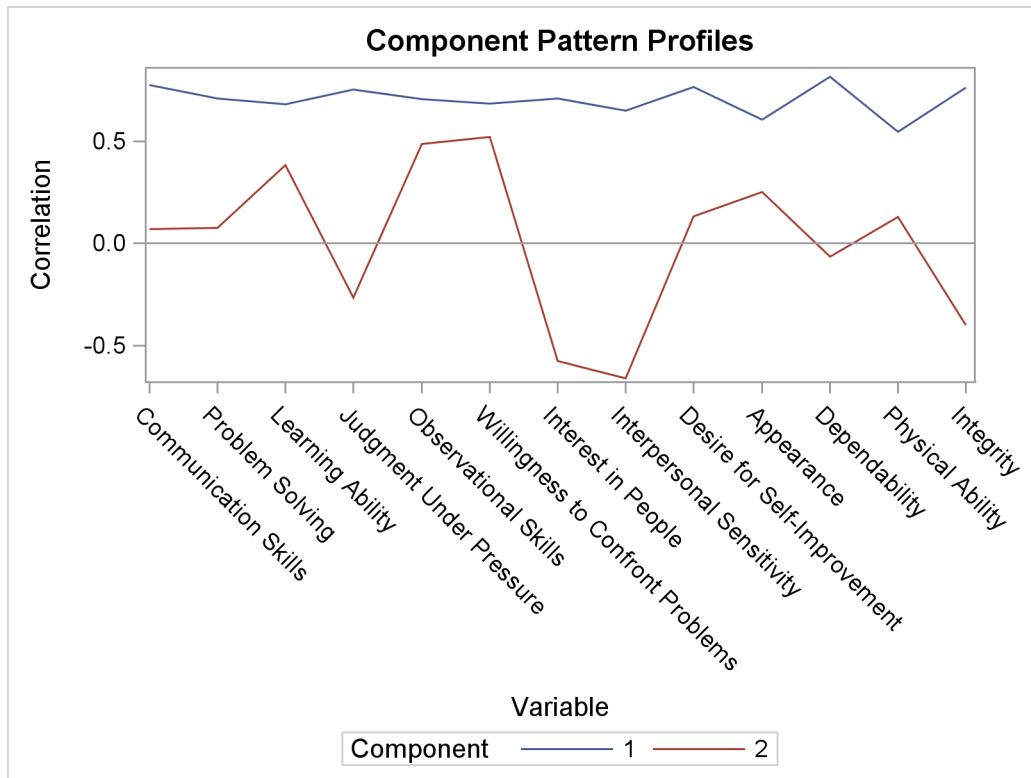


Figure 21.11 continued



Grouped Scatter Plot with PROC SGPLOT

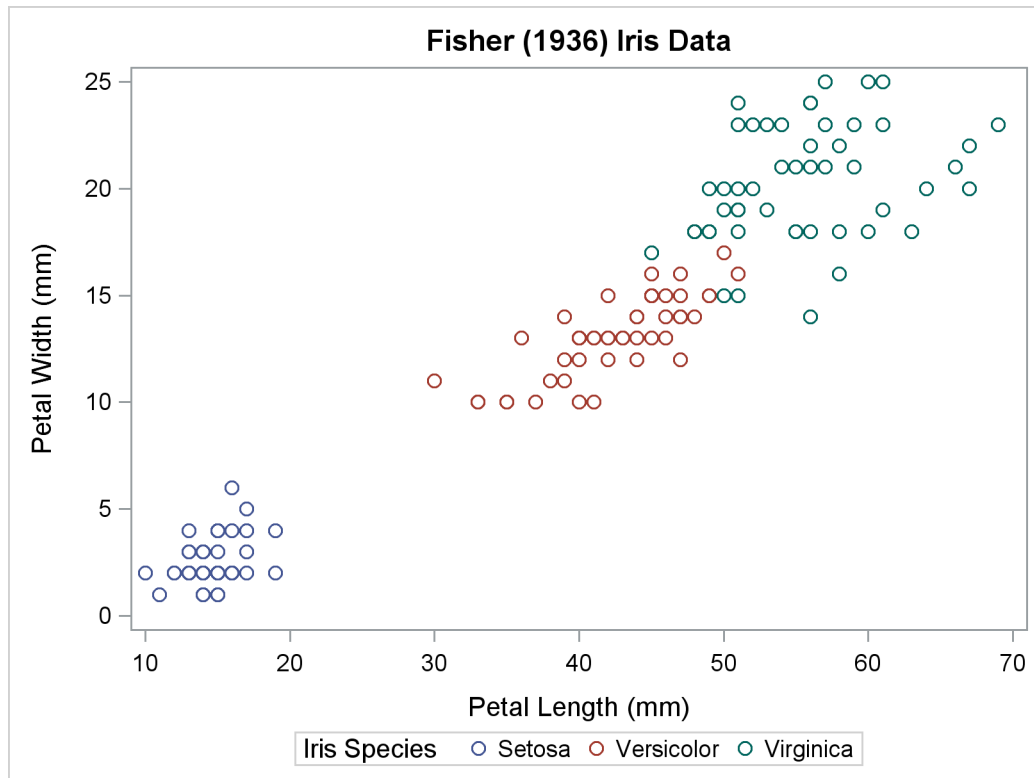
This example is taken from Example 33.1 of Chapter 33, “The DISCRIM Procedure.” It uses the Fisher iris data set, which is available from the Sashelp library.

The following statements run PROC SGPLOT to make a scatter plot, grouped by iris species:

```
proc sgplot data=sashelp.iris;
  title 'Fisher (1936) Iris Data';
  scatter x=petallength y=petalwidth / group=species;
run;
```

The results are shown in Figure 21.12.

Figure 21.12 Iris Data



See the section “[Statistical Graphics Procedures](#)” on page 682 and the *SAS/GRAPH: Statistical Graphics Procedures Guide* for more information about PROC SGPLOT (statistical graphics plot) and other SG procedures. You do not need to enable ODS Graphics in order to use SG procedures (because making plots with ODS Graphics is their sole function).

A Primer on ODS Statistical Graphics

You can enable ODS Graphics by specifying the following statement:

```
ods graphics on;
```

ODS Graphics remains enabled for all procedure steps until you disable it with the following statement:

```
ods graphics off;
```

Once ODS Graphics is enabled, creating graphical output with procedures is as simple as creating tabular output. For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600. See the section “[Syntax](#)” on page 610 for details about the more commonly used ODS GRAPHICS statement options.

You can control your output in the following ways:

- ODS destination statements (such as ODS HTML or ODS RTF) specify where you want your graphs displayed. See [Figure 21.20](#) for an example of HTML output. See the section “[ODS Destination Statements](#)” on page 613 for a list of the supported destinations. See the section “[Syntax](#)” on page 610 for details about the more commonly used ODS destination statement options.
- ODS SELECT and ODS EXCLUDE statements select and exclude graphs from your output. See the section “[Selecting and Excluding Graphs](#)” on page 620 for an example of how to select graphs.
- ODS OUTPUT statements create SAS data sets from the data object used to make the plot. See the section “[Specifying an ODS Destination for Graphics](#)” on page 616 for an example.
- Procedure options specify which graphs to create. For each procedure, these options are described in the “[Syntax](#)” section of the procedure chapter. Typically, you use the PLOTS= option to control all graphs. The available graphs are listed in the “[ODS Graphics](#)” section, which is found in the “[Details](#)” section of each procedure chapter. Many graphs are produced by default.
- ODS styles control the general appearance and consistency of all graphs and tables. See the sections “[Graph Styles](#)” on page 601 and “[Styles](#)” on page 635 for more information about styles.
- ODS templates modify the layout and details of each graph. See the section “[Graph Templates](#)” on page 706 in Chapter 22, “[ODS Graphics Template Modification](#),” for more information about templates.

NOTE: A default template is provided by SAS for each graph, so you do not need to know anything about templates to create statistical graphics.

You can also access individual graphs, control the resolution and size of graphs, and modify your graphs (as explained in the sections beginning with “[Selecting and Viewing Graphs](#)” on page 616). Alternatively, you can use special statistical graphics procedures to create custom graphs directly (see the section “[Statistical Graphics Procedures](#)” on page 682).

Enabling and Disabling ODS Graphics

You can enable ODS Graphics by specifying the following statement:

```
ods graphics on;
```

ODS Graphics remains enabled for all procedure steps until you disable it with the following statement:

```
ods graphics off;
```

ODS Graphics might or might not be enabled by default. This depends on a number of factors. ODS Graphics is typically enabled by default in the SAS windowing environment; ODS Graphics is typically disabled by default when you invoke SAS in other ways. However, these defaults can be changed in a number of ways. You can enable or disable ODS Graphics by default in an *autoexec.sas* file, a configuration file such as *SASV9.CFG*, or in the SAS registry. You can change the default in the SAS windowing environment by selecting **Tools ► Options ► Preferences** from the menu at the top of the main SAS window. Then on the **Results** tab, select the **Use ODS Graphics** check box to enable ODS Graphics by default or clear the

check box to disable ODS Graphics by default. You can also change the default output destination (HTML or LISTING) on the **Results** tab. See the section “[HTML Output in the SAS Windowing Environment](#)” on page 512 for more information about default ODS Graphics settings and default destinations.

When ODS Graphics is enabled, procedures that support ODS Graphics create graphs, either by default or when you specify procedure options for requesting specific graphs. Often, you can leave ODS Graphics enabled for the duration of your SAS session. However, you might consider disabling ODS Graphics if your goal is solely to produce computational results, particularly for large data sets or with many BY groups.

Graph Styles

ODS styles control the overall appearance of graphs and tables. They specify colors, fonts, line styles, symbol markers, and other attributes of graph elements. There are many more ODS styles than are listed here. Most styles are not designed for statistical work. The following styles are used most often for statistical work:

- The HTMLBLUE style is a modern color style that is recommended for use in Web pages or color print media. See [Figure 21.20](#) for an example. The HTMLBLUE style inherits most of its attributes from the STATISTICAL style, which inherits from the DEFAULT style. The HTMLBLUE style has a brighter appearance than its parents, and it has color coordination between the tables and graphs. The dominant color is blue.

The HTMLBLUE style is one of the default styles for the HTML destination (depending on SAS option and registry settings). It is also the default style in SAS/STAT documentation. It is an all-color style; groups of observations are distinguished by color instead of by line style or symbol changes.¹ Most other styles simultaneously vary colors, line styles, and marker symbols to show group membership. Output that is created with the HTMLBLUE style does not print well on black-and-white devices. If you need an alternative to the HTMLBLUE style that varies colors, lines, and markers, use the HTMLBLUECML style or some other style. If you need an alternative to the HTMLBLUE style that is designed for printer destinations such as PRINTER, PDF, PS, and RTF, see the PEARL and SAPPHIRE styles.

- The HTMLBLUECML style is a modern color style that is recommended for use in Web pages or color print media. See [Figure 21.21](#) for an example. It inherits most of its attributes from the HTMLBLUE style. The dominant color is blue. Groups of observations are distinguished by simultaneous color, line style, and symbol changes. If you need an alternative to the HTMLBLUECML style that is all-color, use the HTMLBLUE style instead.
- The SAPPHIRE style is a modern color style that is recommended for use in documents that are created with printer destinations such as PRINTER, PDF, PS, and RTF. See [Figure 21.28](#) for an example. The SAPPHIRE style shares most of its attributes with the PEARL style. Both styles inherit most of their attributes from the HTMLBLUE style; hence the dominant color is blue. However, unlike HTMLBLUE (which has a very light blue background), SAPPHIRE has a white background. The SAPPHIRE style has a light blue background for row and column table headers, whereas the PEARL style has a white background. The SAPPHIRE and PEARL styles use fonts that are appropriate for

¹More precisely, the HTMLBLUE style is an all-color style for the first 12 groups of observations, which are more than are shown in most analyses. Markers and lines change for groups 13–24 and then again for groups 25–36. [Figure 21.40](#) shows how colors, markers, and line styles change in the HTMLBLUE style, and [Figure 21.39](#) shows how these change in most other styles.

printer destinations. Groups of observations are distinguished by color. Output that is created with the SAPPHIRE style might not print well on black-and-white devices.

- The PEARL style is a modern color style that is recommended for use in documents that are created with printer destinations such as PRINTER, PDF, PS, and RTF. See [Figure 21.27](#) for an example. The PEARL style shares most of its attributes with the SAPPHIRE style. Both styles inherit most of their attributes from the HTMLBLUE style; hence the dominant color is blue. However, unlike HTMLBLUE (which has a very light blue background), PEARL has a white background. The PEARL style also has a white background for row and column table headers, whereas the SAPPHIRE style has a light blue background. The PEARL and SAPPHIRE styles use fonts that are appropriate for printer destinations. Groups of observations are distinguished by color. Output that is created with the PEARL style might not print well on black-and-white devices.
- The JOURNAL family of styles (JOURNAL, JOURNAL2, and JOURNAL3) consists of black-and-white or gray-scale styles that are recommended for graphs that appear in journals and in other black-and-white publications. See [Figure 21.24](#) for an example of the JOURNAL style, see [Figure 21.9](#) for an example of the JOURNAL2 style, and see [Example 21.3](#) for a comparison of the three styles. See the PEARL and SAPPHIRE styles for color alternatives to the JOURNAL family of styles.
- The DEFAULT style is a legacy color style. See [Figure 21.19](#) for an example. Most other styles inherit some of their elements from this style. The DEFAULT style is one of the default styles for the HTML destination (depending on SAS registry and option settings). The dominant color is gray. Groups of observations are distinguished by simultaneous color, line style, and symbol changes. Output that is created with the DEFAULT style might not print well on black-and-white devices.
- The STATISTICAL style is a legacy color style. See [Figure 21.22](#) for an example. The STATISTICAL style inherits elements from the DEFAULT style, and it is similar in some ways (other than color) to the ANALYSIS style. The dominant colors are blue and gray. Groups of observations are distinguished by simultaneous color, line style, and symbol changes. Output that is created with the STATISTICAL style might not print well on black-and-white devices.
- The ANALYSIS style is a legacy color style. See [Figure 21.23](#) for an example. The ANALYSIS style inherits elements from the DEFAULT style, and it is similar in some ways (other than color) to the STATISTICAL style. The dominant colors are green and yellow. Groups of observations are distinguished by simultaneous color, line style, and symbol changes. Output that is created with the ANALYSIS style might not print well on black-and-white devices.
- The RTF style is a legacy color style designed for graphs that will be inserted into a Microsoft Word document or a Microsoft PowerPoint slide. See [Figure 21.26](#) for an example of the RTF style, which is the default style for the RTF destination. The RTF style inherits elements from the DEFAULT style. The dominant color is gray. Groups of observations are distinguished by simultaneous color, line style, and symbol changes. Output that is created with the RTF style might not print well on black-and-white devices. See the PEARL and SAPPHIRE styles for alternatives to the RTF style that are brighter and less gray.
- The LISTING style is a legacy color style that is similar to the DEFAULT style, but with a lighter background. See [Figure 21.25](#) for an example. It is the default style for the LISTING destination. The LISTING style inherits elements from the DEFAULT style. The dominant colors are black and white. Groups of observations are distinguished by simultaneous color, line style, and symbol changes. Output that is created with the LISTING style might not print well on black-and-white devices.

You specify a style with the `STYLE=` option in the ODS destination statement. For example, the following statement creates RTF output with the `JOURNAL` style:

```
ods rtf style=Journal;
```

The following statement sets the style for the `LISTING` destination:

```
ods listing style=HTMLBlue;
```

The style specified with the `STYLE=` option in the `ODS LISTING` statement applies only to graphs. SAS monospace format is used for tables.

Most color styles (except the `HTMLBLUE`, `PEARL`, and `SAPPHIRE` styles) are compromise styles in the sense that some graph elements are intentionally overdistinguished to facilitate black-and-white printing. For example, fit lines that correspond to different classification levels are distinguished by both colors and line patterns. You can use the `HTMLBLUE`, `PEARL`, and `SAPPHIRE` styles when you want groups to be distinguished only by color. You can easily modify any style to be an all-color style. For example:

```
proc template;
  define style styles.Default2;
    parent = default;
    style Graph from Graph / attrpriority = "Color";
  end;
run;
```

The `AttrPriority = "Color"` option makes a style an all-color style.

To modify some other style so that it relies only on color for distinguishability, you can use the `%MODSTYLE` SAS autocall macro instead (see the sections “[Creating an All-Color Style](#)” on page 669 and “[Style Template Modification Macro](#)” on page 667). More generally, you can modify the colors, fonts, and other attributes of graph elements in a style by editing the style template. More information is provided in the section “[Styles](#)” on page 635, and detailed information is in the *SAS Output Delivery System: User’s Guide*.

ODS Destinations

ODS can send your graphs and tables to a number of different destinations including RTF (rich text format), HTML (hypertext markup language), `LISTING` (the SAS `LISTING` destination), `DOCUMENT` (the ODS document), and PDF (portable document format). You use an ODS statement to open a destination, as in the following examples:

```
ods html body='b.htm';
ods rtf;
ods listing;
ods document name=MyDoc(write);
ods pdf file="contour.pdf";
```

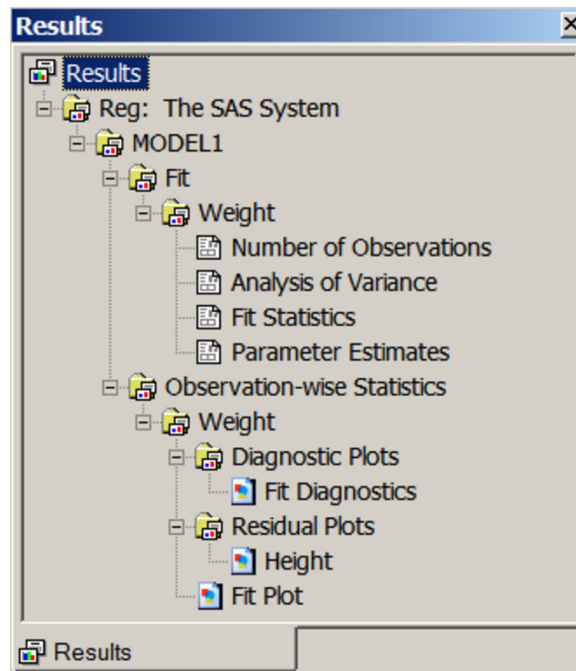
You can close destinations individually or all at once, as in the following examples:

```
ods html close;
ods rtf close;
ods listing close;
ods document close;
```

```
ods pdf close;
ods _all_ close;
```

For most ODS destinations (for example, HTML, RTF, and PDF), graphs and tables are integrated in the output, and you view your output with an appropriate viewer, such as a web browser for HTML. However, the LISTING destination is different. If you are using the LISTING destination in the SAS windowing environment, you view your graphs individually by clicking the graph icons in the Results window, shown in Figure 21.13. This action invokes a host-dependent graph viewer (for example, Microsoft Photo Editor on Windows). The graphs produced with ODS Graphics are *not* displayed with traditional graphs in the Graph window.

Figure 21.13 SAS Results Window



If you are using the SAS windowing environment and you prefer to view integrated output, you should use a destination such as HTML or RTF. In many cases, HTML is the default destination in the SAS windowing environment (see the section “HTML Output in the SAS Windowing Environment” on page 512). You can change destinations in the SAS windowing environment by selecting **Tools ► Options ► Preferences** from the menu at the top of the main SAS window and then selecting the **Results** tab.

Instead, you can prevent the Output window from appearing by using ODS statements to close the LISTING destination, as follows:

```
ods listing close;
ods html;
```

A graph is created for every open destination. When you open a new destination, you should close all destinations that you do not need. Closing destinations makes your jobs run faster and with fewer resources, because fewer tables and graphs are produced.

Accessing Individual Graphs

If you are writing a paper or creating a presentation, you need to access your graphs individually. There are various ways to do this, depending on the ODS destination. Three particularly useful methods are as follows:

- If you are viewing RTF output, you can simply copy and paste your graphs from the viewer into a Microsoft Word document or a Microsoft PowerPoint slide.
- If you are viewing HTML output, you can copy and paste your graphs from the viewer, or you can right-click the graph and save it to a file. Copying and pasting from RTF is preferable because the default resolution is higher than with HTML. See the section “[Specifying the Size and Resolution of Graphs](#)” on page 605 for details.
- You can save your graphs in image files and then include them into a paper or presentation. For example, you can save your graphs as PNG files and include them into a paper that you are writing with \LaTeX or into an HTML document.

You can specify the graphics image format and the filename in the ODS GRAPHICS statement. For example, the following statements, when submitted before a procedure step that produces multiple graphs, save the graphs in PostScript files named *myname.ps*, *myname1.ps*, and so on:

```
ods _all_ close;
ods latex;
ods graphics on / outputfmt=ps imagename='myname';
```

See the section “[Image File Types](#)” on page 622 for details about the file types available with various destinations, how they are named, and how they are saved.

If you are using the LISTING destination and the SAS windowing environment, you can also copy from the viewer into a Microsoft Word document or a Microsoft PowerPoint slide.

Specifying the Size and Resolution of Graphs

Two factors to consider when you are creating graphs for a paper or presentation are the size of the graph and its resolution. You can specify the size of a graph in the ODS GRAPHICS statement. The following examples show typical ways to change the size of your graphs:

```
ods graphics on / width=6in;
ods graphics on / height=4in;
ods graphics on / width=4.5in height=3.5in;
```

You can change the resolution with the `IMAGE_DPI=` option in any ODS destination statement, as in the following example:

```
ods html image_dpi=300;
```


The default resolution of graphs created with the HTML and LISTING destinations is 96 DPI (dots per inch), whereas the default with the RTF destination is 200 DPI. An increase in resolution often improves the quality of the graphs, but it also increases the size of the image file. See the section “[Graph Size and Resolution](#)” on page 628 for more information about graph size and resolution.

Modifying Your Graphs

Although ODS Graphics is designed to automate the creation of high-quality statistical graphics, on occasion you might need to modify your graphs. There are two ways you can make modifications, depending on whether the changes you want to make are data-dependent and immediate (for a specific graph you are preparing for a paper or presentation), or whether they are persistent (applied to a graph each time you run the procedure). You can make immediate, ad hoc changes by using the ODS Graphics Editor, which provides a point-and-click interface. You can make persistent changes by modifying the ODS graph template for a particular plot. For an introduction to graph template modification, see Chapter 22, “[ODS Graphics Template Modification](#).” A graph template is a program, written in the Graph Template Language (GTL), that specifies the layout and details of a graph.

NOTE: The SAS system provides a template for each graph it creates, so you do not need to know anything about templates to create statistical graphics.

You can use the ODS Graphics Editor to customize titles and labels, annotate data points, add text, and change the properties of graph elements. After you have modified your graph, you can save it as a PNG image file or as an SGE file, which preserves the editing context. You can open SGE files with the ODS Graphics Editor and resume editing.

You can invoke the ODS Graphics Editor in the SAS windowing environment, provided that you have enabled ODS Graphics to create editable graphs. The steps for doing this are described in the section “[ODS Graphics Editor](#)” on page 630. Also see *SAS/GRAPH: ODS Graphics Editor User’s Guide*.

Figure 21.14 shows the ODS Graphics Editor window for a fit plot created by PROC REG. Figure 21.15 shows modifications made with tools in the ODS Graphics Editor. The title has been changed, and the legend has been repositioned.

Figure 21.14 ODS Graphics Editor Invoked with a Fit Plot

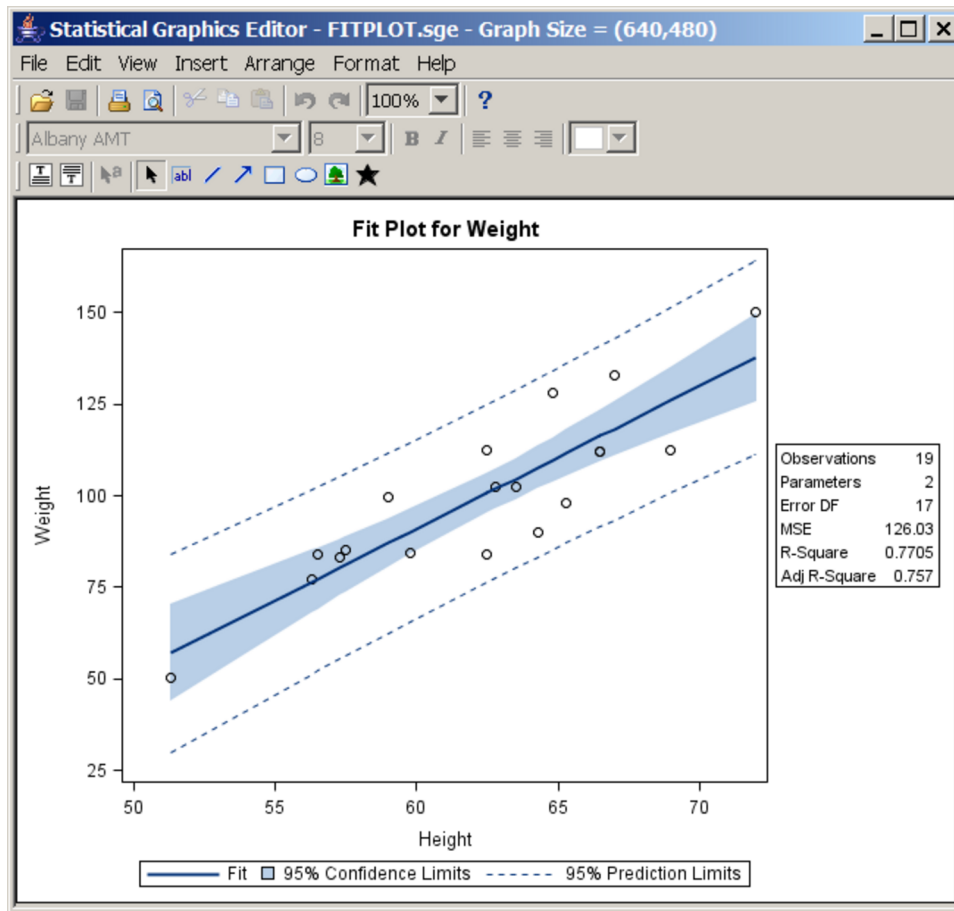
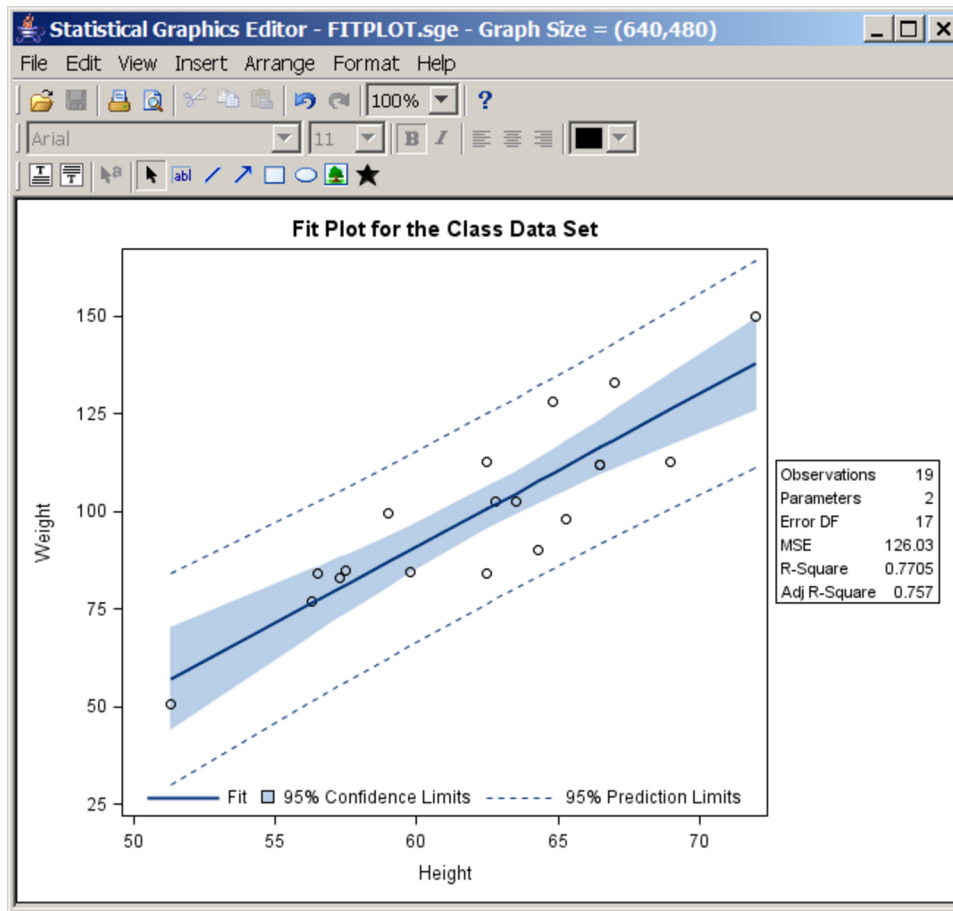


Figure 21.15 Point-and-Click Modifications Made with the ODS Graphics Editor

Procedures That Support ODS Graphics

SAS procedures that support ODS Graphics include the following:

SAS/STAT		SAS/QC	SAS/ETS
ADAPTIVEREG	NPAR1WAY	ANOM	ARIMA
ANOVA	ORTHOREG	CAPABILITY	AUTOREG
BOXPLOT	PHREG	CUSUM	COPULA
CALIS	PLM	MACONTROL	COUNTREG
CLUSTER	PLS	MVPDIAGNOSE	ENTROPY
CORRESP	POWER	MVPMONITOR	ESM
FACTOR	PRINCOMP	MVPMODEL	EXPAND
FMM	PRINQUAL	PARETO	MODEL
FREQ	PROBIT	RELIABILITY	PANEL
GAM	QUANTLIFE	SHEWHART	QLIM
GENMOD	QUANTREG		SEVERITY
GLIMMIX	QUANTSELECT	Base SAS	SIMILARITY
GLM	REG	CORR	SSM
GLMPower	ROBUSTREG	FREQ	SYSLIN
GLMSELECT	RSREG	UNIVARIATE	TIMEDATA
KDE	SEQDESIGN		TIMEID
KRIGE2D	SEQTEST		TIMESERIES
LIFEREG	SIM2D	Other	UCM
LIFETEST	STDRATE	HPF	VARMAX
LOESS	SURVEYFREQ	HPFENGINE	X12
LOGISTIC	SURVEYLOGISTIC		
MCMC	SURVEYPHREG	SAS Risk	
MDS	SURVEYREG	Dimensions	
MI	TPSPLINE		
MIXED	TRANSREG		
MULTTEST	TTEST		
NLIN	VARCLUS		
	VARIOGRAM		

For details about the specific graphs available with a particular procedure, see the PLOTS= option syntax and the “ODS Graphics” section in the corresponding procedure chapter. For the SAS/STAT procedures, the procedure names in the preceding table are links to the “ODS Graphics” section.

Procedures That Support ODS Graphics and Traditional Graphics

A number of procedures that support ODS Graphics produced traditional graphics in previous releases of SAS. These include the UNIVARIATE procedure in Base SAS software; the LIFEREG, LIFETEST, and REG procedures in SAS/STAT software; and the ANOM, CAPABILITY, CUSUM, MACONTROL, PARETO, RELIABILITY, and SHEWHART procedures in SAS/QC software. All of these procedures continue to produce traditional graphics, but in some cases, they do so only when ODS Graphics is not enabled. For more information about the interaction between traditional graphics and ODS graphics in other procedures, see the documentation for that procedure.

Traditional graphs are saved in SAS graphics catalogs and are controlled by the GOPTIONS statement. In contrast, ODS Graphics produces graphs in standard image file formats (not graphics catalogs), and their appearance and layout are controlled by ODS styles and templates.

Syntax

The following sections document some of the most commonly used options in the ODS GRAPHICS statement (section “[ODS GRAPHICS Statement](#)” on page 610) and other statements used with ODS Graphics (section “[ODS Destination Statements](#)” on page 613). You can find the complete syntax in the *SAS Output Delivery System: User’s Guide*. In addition, information about the PLOTS= option is provided in the section “[PLOTS= Option](#)” on page 614. Statistical procedures that produce ODS Graphics all have a PLOTS= option that is used to select graphs and control some aspects of the graphs.

ODS GRAPHICS Statement

ODS GRAPHICS < OFF | ON > < / options > ;

The ODS GRAPHICS statement enables ODS to create graphs. You can enable ODS Graphics by using either of the following equivalent statements:

```
ods graphics on;
ods graphics;
```

You specify one of these statements prior to your procedure invocation, as illustrated in the examples beginning with “[Default Plots for Simple Linear Regression with PROC REG](#)” on page 582. Any procedure that supports ODS Graphics then produces graphs, either by default or when you specify procedure options for requesting particular graphs.

To disable ODS Graphics, specify the following statement:

```
ods graphics off;
```

ODS Graphics might or might not be enabled by default depending on your operating system, whether you are in the SAS windowing environment, your registry, system options, and configuration file settings. For more information about default settings and enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600.

The following is a subset of the options, syntax, and capabilities available in the ODS GRAPHICS statement. See the *SAS Output Delivery System: User’s Guide* for more information.

ANTIALIAS=ON | OFF

controls the use of antialiasing to smooth the components of a graph. Without antialiasing, pixels are simply set or not set. With antialiasing, pixels at the edge of a line or other object are set to an intermediate color, which makes smoother and more professional looking graphics. Text displayed in a graph is always antialiased. Antialiasing is very time-consuming for larger graphical displays, and its benefits decrease as the number of points increases, so it is disabled by default for plots with many points. If the number of observations in the ODS output object exceeds the ANTIALIASMAX= threshold (10,000 by default), then antialiasing is not used, even if you specify the option ANTIALIAS=ON. The default is ANTIALIAS=ON.

ANTIALIASMAX=*n*

specifies the maximum number of markers or lines to be antialiased before antialiasing is disabled. For example, if there are more than 10,000 point markers and ANTIALIASMAX=10,000 (the default), then no markers are antialiased.

BORDER=ON | OFF

specifies whether to draw the graph with a border. BORDER=ON is the default.

BYLINE=FOOTNOTE | TITLE | NOBYLINE

specifies how the BY group line is displayed in graphs when the analysis is run with a BY statement. By default, a BY line is not displayed. Specify BYLINE=FOOTNOTE (recommended) to display the BY line as a left-justified graph footnote or BYLINE=TITLE (not recommended) to display the BY line as a centered graph title. The placement of the BY line is controlled in each graph template as follows:

```

if (_BYTITLE_)
  entrytitle _BYLINE_ / textattrs=GraphValueText;
else
  if (_BYFOOTNOTE_)
    entryfootnote halign=left _BYLINE_;
  endif;
endif;

```

You can modify the graph template if you want the BY line to be displayed in some other way. Since most graphs have titles and few graphs have footnotes, the BY line looks better when it is displayed as a footnote.

HEIGHT=*dimension*

specifies the height of the graph. The default is HEIGHT=480PX (480 pixels). You can also specify height in inches (for example, HEIGHT=5IN) or centimeters (for example, HEIGHT=12CM).

IMAGEMAP=ON | OFF

controls tooltip generation in the HTML destination. The default is IMAGEMAP=OFF, which means that no tooltips are generated. Tooltips are text boxes that appear in HTML output when you rest your mouse pointer over a part of the plot (see [Example 21.1](#)).

IMAGENAME=*< base-file-name >*

specifies the base image filename. The default is the name of the output object. You can determine the name of the output object by using the ODS TRACE statement (see the section “[Determining Graph Names and Labels](#)” on page 618). The base image name should not include an extension. ODS automatically adds the increment value and the appropriate extension (which is specific to the output destination). See the section “[Specifying Base Filenames](#)” on page 625 for an example.

LABELMAX=*n*

specifies the maximum number of labeled areas before labeling is disabled. For example, if LABELMAX=50, and there are more than 50 points with labels, then no points are labeled. The default is LABELMAX=200.

MAXLEGENDAREA=*n*

specifies the maximum percentage of the overall graph area that a legend can occupy. The default is MAXLEGENDAREA=20. Larger legends are dropped from the display.

OUTPUTFMT=< *image-file-type* | STATIC >

specifies the image format for graphs. The OUTPUTFMT= option was previously named the IMAGEFMT= option. By default, OUTPUTFMT=STATIC and ODS dynamically uses the best quality static image format for the active output destination. The available image formats include: BMP (Microsoft Windows device-independent bitmap), DIB (Microsoft Windows device-independent bitmap), EMF (Microsoft NT enhanced metafile), EPSI (Adobe encapsulated PostScript interchange), GIF (graphic interchange format), JFIF (JPEG file interchange format), JPEG (Joint Photographic Experts Group), PBM (portable bitmap), PCD (Photo CD), PCL (Printer Command Language), PDF (portable document format), PICT (the QuickDraw picture format), PNG (Portable Network Graphics), PS (PostScript image file format), SVG (Scalable Vector Graphics), TIFF (Tagged Image File Format), WMF (Microsoft Windows Metafile format), XBM (X Bitmap), and XPM (X-Windows Pixelmap). If the specified image format is not valid for the active output destination, the device is automatically remapped to the default image format.

RESET< =*option* >

resets one or more ODS GRAPHICS options to their default settings. The RESET and RESET=ALL options are equivalent. If you want to reset more than one option, but not all of the options, then you must specify RESET= separately for each option you reset (for example, `ods graphics on / reset=antialias reset=index;`). The RESET= options include the following:

ALL

resets all of the resettable options to their defaults.

ANTIALIAS

resets the ANTIALIAS= option to its default.

ANTIALIASMAX

resets the ANTIALIASMAX= option to its default.

BORDER

resets the BORDER= option to its default.

INDEX

resets the index counter that is appended to static image files.

HEIGHT

resets the HEIGHT= option to its default.

IMAGEMAP

resets the IMAGEMAP= option to its default.

LABELMAX

resets the LABELMAX= option to its default.

SCALE

resets the SCALE= option to its default.

TIPMAX

resets the TIPMAX= option to its default.

WIDTH

resets the WIDTH= option to its default.

SCALE=ON | OFF

specifies whether the fonts and symbol markers are scaled proportionally with the size of the graph. The default is SCALE=ON. For examples, see [Figure 21.58](#) and [Figure 21.59](#).

SCALEMARKERS=ON | OFF

specifies whether markers are scaled in nested layouts. The default is SCALE=ON.

TIPMAX=*n*

specifies the maximum number of distinct tooltips permitted before tooltips are disabled. Tooltips are text boxes that appear when you rest your mouse pointer over a part of the plot. For example, if TIPMAX=400, and there are more than 400 points in a scatter plot, then no tooltips appear. The default is TIPMAX=500.

WIDTH=*dimension*

specifies the width of the graph. The default is WIDTH=640PX (640 pixels). You can also specify widths in inches (for example, WIDTH=5in) or centimeters (for example, WIDTH=12cm).

ODS Destination Statements

ODS has a number of statements that control the destination of ODS output. The ODS destination statements that are most commonly used with ODS Graphics are: ODS DOCUMENT, ODS HTML, ODS LISTING, ODS PCL, ODS PDF, ODS PS, and ODS RTF. Specifying a statement opens a destination, unless the CLOSE option is specified. Each of the following statements opens an ODS destination:

```
ods html;
ods rtf;
ods html image_dpi=300;
ods listing style=HTMLBlue;
```

Each of the following statements closes an ODS destination:

```
ods html close;
ods rtf close;
ods listing close;
```

The following statement closes all open destinations:

```
ods _all_ close;
```

The following two options are commonly used in ODS destination statements to control aspects of ODS Graphics:

IMAGE_DPI=*dpi*

specifies the dots per inch (DPI), which is the image resolution for graphical output. The default varies depending on the destination. For example, the default is 96 for HTML and 200 for RTF.

STYLE=*style-name*

specifies the output style. Commonly used styles include HTMLBLUE, HTMLBLUECML, PEARL, SAPPHIRE, DEFAULT, LISTING, STATISTICAL, JOURNAL, JOURNAL2, JOURNAL3, RTF, and ANALYSIS.

Other options provide you with ways to control the files that are created. For example, the following statement opens the HTML destination:

```
ods html body='b.html' contents='c.html' frame='a.html';
```

This statement also writes the body of the output to the file *b.html*, the table of contents to the file *c.html*, and an overall frame that contains both the contents and the output to the file *a.html*. Alternatively, you can specify FILE= instead of BODY=.

If you are using a destination for which individual graphs are created (for example, LISTING or HTML), you can use the GPATH= option to specify the directory where your graphics files are saved, as in the following example:

```
ods html gpath="C:\figures";
```

See the sections “Image File Types” on page 622, “Saving Graphics Image Files” on page 626, “LISTING Destination” on page 626, and “HTML Destination” on page 627 for more information about individual image files and options specified in the ODS Destination statements. For complete details about the ODS destination statements, see the *SAS Output Delivery System: User’s Guide*.

PLOTS= Option

Each statistical procedure that supports ODS Graphics has a PLOTS= option that is used to select graphs and specify some options. The syntax of the PLOTS= option is as follows:

```
PLOTS <(global-plot-options)> <= plot-request <(options)>>
```

```
PLOTS <(global-plot-options)> <= (plot-request <(options)> <... plot-request <(options)>>>
```

The PLOTS= option has a common overall syntax for all statistical procedures, but the specific global plot options, plot requests, and plot options vary across procedures. This section discusses only a few of the options available in the PLOTS= option. For more information about the PLOTS= option, see the “Syntax” section for each procedure that produces ODS Graphics. There are only a limited number of things that you can control with the PLOTS= option. Most graphical details are controlled either by graph templates (see the section “Graph Templates” on page 706 in Chapter 22, “ODS Graphics Template Modification,”) or by styles (see the section “Styles” on page 635).

The PLOTS= option is usually specified in the PROC statement. However, for some procedures, certain analyses and hence certain plots can appear only if an additional statement is specified. These procedures might have a PLOTS= option in that other statement. For example, the PHREG procedure has a PLOTS= option in the BAYES statement, which is used to perform a Bayesian analysis. See the “Syntax” section of each procedure chapter for more information. The following examples illustrate the syntax of the PLOTS= option:

```

plots=all
plots=none
plots=residuals
plots=residuals(smooth)
plots=(trace autocorr)
plots(unpack)
plots(unpack)=diagnostics
plots=diagnostics(unpack)
plots(only)=freqplot
plots=(scree(unpack) loadings(plotref) preloadings(flip))
plots(unpack maxparmlabel=0 stepaxis=number)=coefficients
plots(sigonly)=(rawprob adjusted(unpack))

```

Also see the “Getting Started” sections “Survival Estimate Plot with PROC LIFETEST” on page 585, “Contour and Surface Plots with PROC KDE” on page 586, “Contour Plots with PROC KRIGE2D” on page 588, “LS-Means Diffogram with PROC GLIMMIX” on page 594, and “Principal Component Analysis Plots with PROC PRINCOMP” on page 596 for examples of the PLOTS= option.

The simplest PLOTS= specifications are of the form PLOTS=*plot-request* or PLOTS=(*plot-requests*). When there is more than one plot request, the plot-request list must appear in parentheses. Each plot request either requests a plot (for example, RESIDUALS) or provides you with a place to specify plot-specific options (for example, DIAGNOSTICS(UNPACK)). Some simple and typical plot requests are explained next:

- PLOTS=ALL requests all plots that are relevant to the analysis. This does not mean that all plots that the procedure can produce are produced. Plots that are produced for one set of options might not appear with PLOTS=ALL and a different set of options. In some cases, certain plots are not produced unless certain options or statements outside the PLOTS= option are specified.
- PLOTS=NONE disables ODS Graphics for just that step. You can use this option instead of specifying ODS GRAPHICS OFF before a procedure step and ODS GRAPHICS ON after the step when you want to suppress graphics for only that step.
- PLOTS=RESIDUALS requests a plot of residuals in a modeling procedure such as PROC REG.
- PLOTS=RESIDUALS(SMOOTH) requests the residuals plot along with a smooth fit function.
- PLOTS=(TRACE AUTOCORR) requests trace and autocorrelation plots in procedures with Bayesian analysis options.

Global plot options appear in parentheses after the option name and before the equal sign. These options affect many or all of the plots. The UNPACK option is a commonly used global plot option. It specifies that plots that are normally produced with multiple plots per panel (or “packed”) should be unpacked and appear in multiple panels with one plot in each panel. The specification PLOTS(UNPACK)=(*plot-requests*) unpacks all paneled plots. The UNPACK option is also used as an option in a plot request when you want to unpack only certain panels. For example, the option PLOTS=(DIAGNOSTICS(UNPACK) PARTIAL PREDICTIONS) unpacks only the diagnostics panel. In some cases, unpacked plots contain additional information that is not found in the smaller packed versions. The UNPACK option is not available for all plot requests; it is available only with plots that have multiple panels by default.

Another commonly used global plot option is the ONLY option. Many procedures produce default plots, and additional plots can be requested in the PLOTS= option. Specifying PLOTS=(*plot-requests*) while

omitting the default plots does not prevent the default plots from being produced. The ONLY option is used when you want to see only the plots specifically listed in the plot-request list. Procedures that produce no default plots typically do not provide an ONLY option. You can use ODS SELECT and ODS EXCLUDE (see the section “[Selecting and Excluding Graphs](#)” on page 620) to select and exclude graphs, but in some situations the ONLY option is more convenient. It is typically more efficient to select plots by using the PLOTS(ONLY)= option, because the procedure does not do extra work to generate a plot that is excluded by the PLOTS(ONLY)= option. In contrast, ODS SELECT and ODS EXCLUDE have their effect after the procedure has done the work to generate the plot.

Selecting and Viewing Graphs

This section describes techniques for selecting and viewing your graphs. Topics include:

- specifying an ODS destination for graphics
- viewing your graphs in the SAS windowing environment
- referring to graphs by name when using ODS
- selecting and excluding graphs from your output

Specifying an ODS Destination for Graphics

If you do not specify an ODS destination, then either the LISTING or the HTML destination is used by default. Here is an example of how you can explicitly specify the HTML destination:

```
ods graphics on;
ods html;

proc reg data=sashelp.class;
  model Weight = Height;
run; quit;

ods html close;
```

This ODS HTML statement creates an HTML file with a default name. See the section “[Specifying a File for ODS Output](#)” on page 617 to see how to specify a filename. Other destinations are specified in a similar way. For example, you can specify an RTF destination with the following statements:

```
ods graphics on;
ods rtf;

. . .

ods rtf close;
```

The destinations that ODS supports for graphics are as follows:

Destination	Destination Family
DOCUMENT	
HTML	MARKUP
LATEX*	MARKUP
LISTING	
PCL	PRINTER
PDF	PRINTER
PS	PRINTER
RTF	

* The LATEX destination is experimental.

You can close all open destinations if you are interested only in displaying your output in a nondefault destination. For example, if you want to see your output only in the RTF destination, you can specify the following statements:

```
ods graphics on;
ods _all_ close;
ods rtf;

. . .

ods rtf close;
ods listing;
```

Closing unneeded destinations makes your jobs run faster and creates fewer files. More generally, it makes your jobs consume fewer resources, because a graph is created for every open destination. The last statement opens the LISTING destination after you are finished using the RTF destination.

You can also use the ODS OUTPUT destination to create an output data set from the data object used to make a plot. Here is an example:

```
ods graphics on;

proc reg data=sashelp.class;
  ods output fitplot=myfitplot;
  model Weight = Height;
run; quit;
```

Specifying a File for ODS Output

You can specify a filename for your output with the FILE= option in the ODS destination statement, as in the following example:

```
ods html file="test.htm";
```

The output is written to the file *test.htm*, which is saved in the SAS current folder. At start-up, the SAS current folder is the same directory in which you started your SAS session. If you are using the SAS windowing environment, then the current folder is displayed in the status line at the bottom of the main SAS window. If you do not specify a filename for your output, then the SAS System provides a default filename, which depends on the ODS destination. This file is saved in the SAS current folder. You can always check

the SAS log to verify the name of the file in which your output is saved. For example, suppose you specify the following statement:

```
ods html;
```

Then the following message is displayed in the SAS log:

```
NOTE: Writing HTML Body file: sashtml.htm
```

The default filenames for each destination are specified in the SAS Registry. For example, Figure 21.60 shows that the default filename in the SAS Registry for the RTF destination is *sasrtf.rtf*. For more information, see the *SAS Companion* for your operating system.

Viewing Your Graphs in the SAS Windowing Environment

The mechanism for viewing graphs created with ODS can vary depending on your operating system, which viewers are installed on your computer, and the ODS destination you have selected. If you do not specify an ODS destination, then the default destination is either HTML or LISTING.

If you are using the SAS windowing environment and the HTML destination, then the results are displayed by default in the SAS Results Viewer unless you chose to use an external browser. To use an external viewer, select **Tools ► Options ► Preferences** from the menu at the top of the main SAS window. Then select the **Results** and **Web** tabs to make your selection.

If you are using the PS destination, you must use a PostScript viewer, such as GSview. For information about the windowing environment in a different operating system, see the *SAS Companion* for that operating system.

If you do not want to view the results as they are being generated, then select **Tools ► Options ► Preferences** from the menu at the top of the main SAS window. Then on the **Results** tab, clear the **View results as they are generated** checkbox.

If you are using the SAS windowing environment and the LISTING destination, go to the Results window and find the icon for the corresponding graph. You can double-click the graph icon to display the graph in the default viewer that is configured on your computer for the corresponding image file type (see Figure 21.13).

Determining Graph Names and Labels

Procedures assign a name to each graph they create with ODS Graphics. This enables you to refer to ODS graphs in the same way that you refer to ODS tables (see the section “The ODS Statement” on page 519 in Chapter 20, “Using the Output Delivery System,”). You can determine the names of graphs in several ways:

- You can look up graph names in the “ODS Graphics” section of chapters for procedures that use ODS Graphics. For example, see the section “ODS Graphics” on page 6745 in Chapter 79, “The REG Procedure.”
- You can use the Results window to view the names of ODS graphs created in your SAS session. See the section “The SAS Results Window” on page 523 in Chapter 20, “Using the Output Delivery System,” for more information.

- You can use the ODS TRACE ON statement to list the names of graphs created by your SAS session. This statement adds identifying information in the SAS log (or optionally in the SAS LISTING) for each graph that is produced. See the section “The ODS Statement” on page 519 in Chapter 20, “Using the Output Delivery System,” for more information.

The graph name is not the same as the name of the image file that contains the graph (see the section “Naming Graphics Image Files” on page 624).

This example revisits the analysis described in the section “Contour and Surface Plots with PROC KDE” on page 586. To determine which output objects are created by ODS, you specify the ODS TRACE ON statement prior to the procedure statements as follows:

```
ods graphics on;
ods trace on;

proc kde data=bivnormal;
  bivar x y / plots=contour surface;
run;

ods trace off;
```

The trace record from the SAS log is as follows:

Output Added:

```
Name:      Inputs
Template:  Stat.KDE.Inputs
Path:      KDE.Bivar1.x_y.Inputs
-----
```

Output Added:

```
Name:      Controls
Template:  Stat.KDE.Controls
Path:      KDE.Bivar1.x_y.Controls
-----
```

Output Added:

```
Name:      ContourPlot
Label:     Contour Plot
Template:  Stat.KDE.Graphics.Contour
Path:      KDE.Bivar1.x_y.ContourPlot
-----
```

Output Added:

```
Name:      SurfacePlot
Label:     Density Surface
Template:  Stat.KDE.Graphics.Surface
Path:      KDE.Bivar1.x_y.SurfacePlot
-----
```

By default, PROC KDE creates table objects named Inputs and Controls, and it creates graph objects named ContourPlot and SurfacePlot. In addition to the name, the trace record provides the label, template, and path for each output object. Graph templates are distinguished from table templates by a naming convention that uses the procedure name in the second level and **Graphics** in the third level. For example, the fully qualified template name for the surface plot created by PROC KDE is **Stat.KDE.Graphics.SurfacePlot**.

You can specify the LISTING option in the ODS TRACE ON statement to write the trace record to the LISTING destination as follows:

```
ods trace on / listing;
```

Each table and graph has a path (or name path), which was previously shown in the trace output. The path consists of the plot name preceded by the names of one or more output groups. Each table and graph also has a label path, which can be seen by adding the LABEL option to the ODS TRACE ON statement, after a slash, as follows:

```
ods trace on / label;

proc kde data=bivnormal;
  bivar x y / plots=contour surface;
run;

ods trace off;
```

A portion of the trace output is shown next:

```
Path:          KDE.Bivar1.x_y.Inputs
Label Path:    'The KDE Procedure'. 'Bivariate Analysis'. 'x and y'. 'KDE.Bivar1.x_y'

Path:          KDE.Bivar1.x_y.Controls
Label Path:    'The KDE Procedure'. 'Bivariate Analysis'. 'x and y'. 'KDE.Bivar1.x_y'

Path:          KDE.Bivar1.x_y.ContourPlot
Label Path:    'The KDE Procedure'. 'Bivariate Analysis'. 'x and y'. 'Contour Plot'

Path:          KDE.Bivar1.x_y.SurfacePlot
Label Path:    'The KDE Procedure'. 'Bivariate Analysis'. 'x and y'. 'Density Surface'
```

The label path contains the information that you see in the HTML table of contents. Names are fixed, they do not vary, and they are not data- or context-dependent. In contrast, labels often reflect data- or context-dependent information.

Selecting and Excluding Graphs

You can use the ODS SELECT and ODS EXCLUDE statements along with graph and table names to specify which ODS outputs are displayed. See the section “The ODS Statement” on page 519 in Chapter 20, “Using the Output Delivery System,” for more information about how to use these statements.

This section shows several examples of selecting and excluding graphs by using the data set and trace output that are created in the section “[Determining Graph Names and Labels](#)” on page 618. The following statements use the ODS SELECT statement to select only two graphs, ContourPlot and SurfacePlot, for display in the output:

```
proc kde data=bivnormal;
  ods select ContourPlot SurfacePlot;
  bivar x y / plots=contour surface;
run;
```

Equivalently, the following statements use the ODS EXCLUDE statement to exclude the two tables:

```
proc kde data=bivnormal;
  ods exclude Inputs Controls;
  bivar x y / plots=contour surface;
run;
```

You can select or exclude graphs by using either the name or the label. Labels must be specified in quotes. In the context of this example, the following two statements are equivalent:

```
ods select contourplot;
ods select 'Contour Plot';
```

You can also specify multiple levels of the path, as in the following example:

```
ods select x_y.contourplot;
ods select 'x and y'. 'Contour Plot';
ods select 'x and y'.contourplot;
ods select x_y.'Contour Plot';
```

Name and label paths can be mixed, as in the last two statements. All four of the preceding statements select the same plot. Furthermore, selection based directly on the names and labels is case-insensitive. The following statements all select the same plot:

```
ods select x_y.contourplot;
ods select 'x and y'. 'Contour Plot';
ods select X_Y.CONTOURPLOT;
ods select 'X AND Y'. 'CONTOUR PLOT';
```

It is sometimes useful to specify a WHERE clause in an ODS SELECT or ODS EXCLUDE statement. This enables you to specify expressions based on either the name path or the label path. You can base your selection on two automatic variables `_path_` and `_label_`. The following two statements select every object whose path contains the string ‘plot’ and every object whose label path contains the string ‘plot’, respectively, ignoring the case in the name and label:

```
ods select where = (lowercase(_path_) ? 'plot');
ods select where = (lowercase(_label_) ? 'plot');
```

The question mark operator means that the second expression (the string ‘plot’) is contained in the first expression (the lowercase version of the name or label). For example, all of the following names match ‘plot’ in the WHERE clause: plot, SurfacePlot, SURFACEPLOT, FitPlot, pLoTtInG, Splotch, and so on. Since WHERE clause selection is based on SAS string comparisons, selection is case-sensitive. The LOWCASE function is used to ensure a match even when the specified string does not match the case of the actual name or label.

WHERE clauses are particularly useful when you want to select all of the objects in a group. A group is a level of the name path or label path hierarchy before the last level. In the following step, all of the objects whose name path contains 'DiagnosticPlots' are selected:

```
proc reg data=sashelp.class plots(unpack);  
  ods select where = (_path_ ? 'DiagnosticPlots');  
  model Weight = Height;  
run; quit;
```

These are the plots that come from unpacking the PROC REG diagnostics panel of plots. All are in a group named 'DiagnosticPlots'.

Graphics Image Files

Accessing your graphs as individual image files is useful when you want to include them in various types of documents. The default image file type depends on the ODS destination, but there are other supported image file types that you can specify. You can also specify the names for your graphics image files and the directory in which you want to save them. This section describes the image file types supported by ODS Graphics, and it explains how to name and save graphics image files.

Image File Types

If you are using the LISTING or HTML destinations, your graphs are individually produced in a specific image file type, such as PNG (Portable Network Graphics). If you are using a destination in the PRINTER family or the RTF destination, the graphs are contained in the ODS output file and cannot be accessed as individual image files. However, you can open an RTF output file in Microsoft Word and then copy and paste the graphs into another document, such as a Microsoft PowerPoint presentation. This is illustrated in [Example 21.2](#).

[Table 21.1](#) shows the various ODS destinations supported by ODS Graphics, the viewer that is appropriate for displaying graphs in each destination, and the image file types supported for each destination.

Table 21.1 Destinations and Image File Types Supported by ODS Graphics

Destination	Destination Family	Recommended Viewer	Image File Types
DOCUMENT		Not applicable	Not applicable
HTML	MARKUP	Web browser	PNG (default), GIF, JPEG,
LATEX	MARKUP	PostScript or PDF viewer after compiling the \LaTeX file	PostScript (default), EPSI, GIF, JPEG, PDF, PNG
LISTING		Default viewer in your system for the specified file type	PNG (default), GIF, BMP, DIB, EMF, EPSI, GIF, JFIF, JPEG, PBM, PS, TIFF, WMF
PCL	PRINTER	Not applicable	Contained in PRN file
PDF	PRINTER	PDF viewer, such as Adobe Reader	Contained in PDF file
PS	PRINTER	PostScript viewer, such as GSview	Contained in PostScript file
RTF		Word processor, such as Microsoft Word	Contained in RTF file

For destinations such as PDF and RTF, you can control the types of the images that are contained in the file even though individual files are not made for each image. The default image file type is PNG, and other image types are available. See the *SAS Output Delivery System: User's Guide* for more information.

Scalable Vector Graphics

Scalable vector graphics output is now supported in ODS Graphics. The output type support varies based on the ODS destination that you use. You can specify the `OUTPUTFMT=` option in the ODS GRAPHICS statement to specify the output type for any destination. For destinations that generate vector graphics by default, you can get image output by specifying the option `OUTPUTFMT=STATIC`.

Vector graphics are not supported for all graph types. When vector graphics are requested but not supported, the graph automatically changes to image output. Vector graphics are not supported for the following graph types:

- three-dimensional graph
- contour plots with smooth gradient fills
- graphs with continuous legends
- graphs with data skins
- graphs with rotated annotation images
- graphs with transparency (EMF and PS only)

The LISTING destination can generate all of the supported forms of vector-based output: PDF, PS, EMF, SVG, and PCL. Each graph is generated in a separate file that can be included into a larger report. The default output format is a PNG image.

Like the LISTING destination, the ODS PRINTER destination can generate all of the supported vector output types. The output format depends on the type of printer you select. If you select the PDF, SVG, or PCL5C printers, vector-based output is automatically produced. However, if you select PS or EMF printers, you need to set the OUTPUTFMT= option in the ODS GRAPHICS statement to PS or EMF, respectively, to create vector-based output. By default, the output from this destination is in one file instead of individual files for each graph.

The PDF destination renders PDF vector output by default, except for the exceptions noted. You can specify the OUTPUTFMT=STATIC option in the ODS GRAPHICS statement to produce an embedded image in the PDF file.

The experimental LATEX destination renders PS vector output by default, except for the exceptions noted. You can specify the OUTPUTFMT=STATIC option in the ODS GRAPHICS statement to produce an embedded image in the postscript file.

The RTF destination renders PNG image output by default. Vector-based EMF output is also supported for this destination. You can specify the OUTPUTFMT=EMF option in the ODS GRAPHICS statement to select this output type. If one of the noted exceptions occurs, the output type for that graph changes to a PNG image.

The HTML destination renders PNG image output by default. Vector-based SVG output is also supported for this destination. You can specify the OUTPUTFMT=SVG option in the ODS GRAPHICS statement to select this output type. If one of the noted exceptions occurs, the output type for that graph changes to a PNG image.

In most cases, the file size with vector graphics is much smaller than a comparable static image file. However, in some cases, the vector graphics file size is larger than the image version. This is likely for scatter plots of data sets with a large number of observations.

Naming Graphics Image Files

The following discussion applies to the destinations where ODS graphs are created as individual image files (for example, HTML, and LISTING). The names of graphics image files are determined by a base filename, an index counter, and an extension. By default, the base filename is the ODS graph name (see the section “Determining Graph Names and Labels” on page 618). There is an index counter for each base filename. The extension indicates the image file type. The first time a graph object with a given base filename is created, the filename consists only of the base filename and the extension. If a graph with the same base filename is created multiple times, then an index counter is appended to the base filename to avoid overwriting previously created images.

To illustrate, consider the following statements:

```
proc kde data=bivnormal;
  ods select ContourPlot SurfacePlot;
  bivar x y / plots=contour surface;
run;
```

If you run this step at the beginning of a SAS session, the two graphics image files created are *ContourPlot.png* and *SurfacePlot.png*. If you immediately rerun these statements, then ODS creates the same graphs in different image files named *ContourPlot1.png* and *SurfacePlot1.png*. The next time, the image files are named *ContourPlot2.png* and *SurfacePlot2.png*. The index starts at zero, and one is added each time the same name is used. Note, however, that when the index is at zero, 0 is not added to the filename.

Resetting the Index Counter

You can specify the RESET=INDEX option in the ODS GRAPHICS statement to reset the index counter. This is useful when you need to have predictable names. It is particularly useful when you are running a SAS program multiple times in the same session. The following statement resets the index:

```
ods graphics on / reset=index;
```

The index counter is reinitialized at the beginning of your SAS session or if you specify the RESET=INDEX option in the ODS GRAPHICS statement. Graphics image files with the same name are overwritten.

Specifying Base Filenames

You can specify a base filename for all your graphics image files with the IMAGENAME= option in the ODS GRAPHICS statement as follows:

```
ods graphics on / imagename="MyName";
```

You can also specify the RESET=INDEX option as follows:

```
ods graphics on / reset=index imagename="MyName";
```

The IMAGENAME= option overrides the default base filename. With the preceding statement, the graphics image files are named *MyName*, *MyName1*, *MyName2*, and so on.

Specifying Image File Types

You can specify the image file type for the LISTING, HTML, or LATEX destinations with the OUTPUTFMT= option in the ODS GRAPHICS statement as follows:

```
ods graphics on / outputfmts=gif;
```

For more information, see the section “ODS GRAPHICS Statement” on page 610.

Naming Graphics Image Files with Multiple Destinations

Since the index counter depends only on the base filename, if you specify multiple ODS destinations for your output, then the index counter is increased independently of the destination. For example, the following statements create image files named *ContourPlot.png* and *SurfacePlot.png* that correspond to the LISTING destination, and *ContourPlot1.png* and *SurfacePlot1.png* that correspond to the HTML destination:

```
ods listing;
ods html;
ods graphics on / reset;

proc kde data=bivnormal;
  ods select ContourPlot SurfacePlot;
  bivar x y / plots=contour surface;
run;

ods _all_ close;
ods listing;
```

When you specify one of the destinations in the PRINTER family or the RTF destination, your ODS graphs are embedded in the document, so the index counter is not affected. For example, the following statements create image files *ContourPlot.png* and *SurfacePlot.png* for the LISTING destinations, but no image files for the RTF destination:

```
ods listing;
ods rtf;
ods graphics on / reset;

proc kde data=bivnormal;
  ods select ContourPlot SurfacePlot;
  bivar x y / plots=contour surface;
run;

ods _all_ close;
```

Saving Graphics Image Files

Knowing where your graphics image files are saved and how they are named is particularly important if you are running in batch mode, if you have disabled the SAS Results window (see the section “[Viewing Your Graphs in the SAS Windowing Environment](#)” on page 618), or if you plan to access the files for inclusion in a paper or presentation. The following discussion assumes you are running SAS under the Windows operating system. If you are running on a different operating system, see the *SAS Companion* for your operating system.

In the SAS windowing environment, the current folder is displayed in the status line at the bottom of the main SAS window. When **Use WORK folder** is cleared in the **Tools ► Options ► Preferences ► Results** tab, graph image files are saved in the current folder and are available after your SAS session ends. They can accumulate with time and take up a great deal of space. When **Use WORK folder** is selected, graph image files are stored in the Work folder and are not available after your SAS session ends.

If you are running your SAS programs in batch mode, the graphs are saved by default in the same directory where you started your SAS session. For example, suppose the SAS current folder is *C:\myfiles*. If ODS Graphics is enabled, then your graphics image files are saved in the directory *C:\myfiles*. Traditional graphics are always saved in a catalog in your Work directory.

With the LISTING, HTML, and LATEX destinations, you can specify a directory for saving your graphics image files. With a destination in the PRINTER family and with the RTF destination, you can specify a directory only for your output file. The remainder of this discussion provides details for each destination type.

LISTING Destination

If you are using the LISTING destination, the individual graphs are created as PNG files by default. You can use the GPATH= option in the ODS LISTING statement to specify the directory where your graphics files are saved. For example, if you want to save your graphics image files in *C:\figures*, then you can specify the following:

```
ods listing gpath="C:\figures";
```

It is important to note that the GPATH= option applies only to ODS Graphics. It does not affect the behavior of graphs created with traditional SAS/GRAPH procedures.

HTML Destination

If you are using the HTML destination, the individual graphs are created as PNG files by default. You can use the PATH= and GPATH= options in the ODS HTML statement to specify the directory where your HTML and graphics files are saved, respectively. This also gives you more control over your graphs. For example, if you want to save your HTML file named *test.htm* in the *C:\myfiles* directory, but you want to save your graphics image files in *C:\myfiles\png*, then you can specify the following:

```
ods html path = "C:\myfiles"
      gpath = "C:\myfiles\png"
      file = "test.htm";
```

When you specify the URL= suboption with the GPATH= option, SAS creates relative paths for the links and references to the graphics image files in the HTML file. This is useful for building output files that are easily moved from one location to another. For example, the following statements create a relative path to the *png* directory in all the links and references contained in *test.htm*:

```
ods html path = "C:\myfiles"
      gpath = "C:\myfiles\png" (url="png/")
      file = "test.htm";
```

If you do not specify the URL= suboption, SAS creates absolute paths that are hard-coded in the HTML file. These can cause broken links if you move the files. For more information, see the ODS HTML statement in the *SAS Output Delivery System: User's Guide*.

LATEX Destination

L^AT_EX is a document preparation system for high-quality typesetting. The ODS LATEX statement produces output in the form of a L^AT_EX source file that is ready to compile in L^AT_EX. When you request ODS Graphics for a LATEX destination², ODS creates the requested graphs as PostScript files by default, and the L^AT_EX source file includes references to these image graphics files. You can compile the L^AT_EX file, or you can ignore this file and simply access the individual PostScript files to include your graphs in a different L^AT_EX document, such as a paper that you are writing. You can specify the PATH= and GPATH= options in the ODS LATEX statement, as explained previously for the ODS HTML statement. See [Example 21.3](#) for an illustration. The ODS LATEX statement is an alias for the ODS MARKUP statement with the TAGSET=LATEX option. For more information, see the *SAS Output Delivery System: User's Guide*.

The default image file type for the LATEX destination is PostScript. When you use L^AT_EX to compile your document, the graphics format for included images is Postscript. However, if you prefer to use pdfL^AT_EX, you can specify a different format such as JPEG, PDF, or PNG, any of which can be directly included into your pdfL^AT_EX document. To specify one of these formats, you use the OUTPUTFMT= option in the ODS GRAPHICS statement. For more information, see the L^AT_EX documentation for the `graphicx` package.

²The LATEX destination is experimental.

Creating Graphs in Multiple Destinations

This section illustrates how to send your output to more than one destination with a single execution of your SAS statements. For example, to create LISTING, HTML, and RTF output, you can specify the ODS LISTING, ODS HTML, and the ODS RTF statements before your procedure statements. The ODS `_ALL_CLOSE` statement closes all open destinations before and after the other statements are run.

```
ods _all_ close;
ods listing;
ods html;
ods rtf;

. . .

ods _all_ close;
```

You can also specify multiple instances of the same destination. For example, using the data in the section “Contour and Surface Plots with PROC KDE” on page 586, the following statements save the contour plot to the file *contour.pdf* and the surface plot to the file *surface.pdf*:

```
ods _all_ close;
ods pdf file="contour.pdf";
ods pdf select ContourPlot;
ods pdf(id=srf) file="surface.pdf";
ods pdf(id=srf) select SurfacePlot;
ods graphics on;

proc kde data=bivnormal;
  ods select ContourPlot SurfacePlot;
  bivar x y / plots=contour surface;
run;

ods _all_ close;
```

The `ID=` option assigns the name `srf` to the second instance of the PDF destination. Without the `ID=` option, the second ODS PDF statement closes the destination that was opened by the previous ODS PDF statement, and it opens a new instance of the PDF destination. In that case, the file *contour.pdf* is not created. For more information, see the ODS PDF statement in the *SAS Output Delivery System: User's Guide*.

Graph Size and Resolution

ODS provides options for specifying the size and resolution of graphs. You can specify the size of a graph in the ODS GRAPHICS statement and the resolution in an ODS destination statement. There are two other ways to change the size of a graph, but they are rarely needed. The three methods are as follows:

- Usually, you specify the `WIDTH=` or `HEIGHT=` option (or both) in the ODS GRAPHICS statement to change the size of a graph.

- To modify the size of a particular graph, specify the dimensions with the DESIGNHEIGHT= and DESIGNWIDTH= options in the BEGINGRAPH statement in the template. Some templates contain the specification DESIGNWIDTH=DEFAULTDESIGNHEIGHT, which sets the width of the graph to the default height, or DESIGNHEIGHT=DEFAULTDESIGNWIDTH, which sets the height of the graph to the default width.
- To modify the size of all of your ODS graphs, specify the dimensions with the OUTPUTHEIGHT= and OUTPUTWIDTH= options in the style template.

The following examples show typical ways to change the size of your graphs:

```
ods graphics on / width=6in;
ods graphics on / height=4in;
ods graphics on / width=4.5in height=3.5in;
```

The dimensions of the graph can be specified in pixels (for example, 200PX), inches (for example, 3IN), or centimeters (for example, 8CM). The default dimensions of ODS Graphics are 640 pixels wide and 480 pixels high, and these values determine the default aspect ratio. The actual size of the graph in inches depends on your printer or display device. For example, if the resolution of your printer is 100 dots per inch and you want a graph that is 4 inches wide, you should set the width to 400 pixels.

If you specify only one dimension, the other is determined by the default aspect ratio—that is, height=0.75 × width. For best results, you should create your graphs by using the exact size that is used to display the graphs in your paper or presentation. In other words, avoid generating them at one size and then expanding or shrinking them for inclusion into the your document.

By default, fonts and symbol markers are automatically scaled with the size of the graph. You can suppress this scaling with the SCALE= option, as in the following example:

```
ods graphics on / scale=off;
```

The default resolution of graphs created with HTML and LISTING is 96 DPI (dots per inch), whereas the default with RTF is 200 DPI. The 200 DPI value is recommended if you are copying and pasting graphs into a Microsoft PowerPoint presentation or a Microsoft Word document. Graphs shown in SAS/STAT documentation are typically generated at 300 DPI for display in PDF and 96 DPI for display in HTML.

You can change the resolution with the IMAGE_DPI= option in any ODS destination statement, as in the following example:

```
ods html image_dpi=300;
```

An increase in resolution often improves the quality of the graphs, but it also greatly increases the size of the image file. Going from 96 DPI to 300 DPI increases the size of the image file by roughly a factor of $(300/96)^2 = 9.77$. Even when you are using a higher DPI for most of your graphs, you should consider using a lower DPI for some, such as contour plots, that create large files even at a lower DPI.

If you increase the resolution, you might need to compensate by reducing the size of the graph, as in the following example:

```
ods graphics on / width=4.5in height=3.5in;
```


Increasing DPI also increases the amount of memory needed for your program to complete. You can increase the amount of memory available to ODS Graphics with an option when you invoke SAS, as in the following example:

```
-jreoptions '(-Xmx256m)'
```

You can modify the default amount of memory available to ODS Graphics by changing JREOPTIONS in your SAS configuration file to the settings `-Xmxnnm -Xmsnnm`, where *nnn* is the amount of memory in megabytes. An example is `-Xmx256m -Xms256m`. In either case, the exact syntax varies depending on your operating system and the amount of memory that you can allocate varies from system to system. For more information, see the *SAS Companion* for your operating system.

ODS Graphics Editor

The ODS Graphics Editor is a point-and-click interface that you can use to modify a specific graph created by ODS Graphics. For example, if you need to enhance a graph for a paper or presentation, you can use the ODS Graphics Editor to customize the title, modify the axis labels, annotate particular data points, and change graph element properties such as fonts, colors, and line styles.

This section explains how to enable ODS Graphics to create editable graphs and how to invoke the ODS Graphics Editor. You can use the ODS Graphics Editor in the SAS windowing environment, provided that the LISTING destination is open and that you have first enabled ODS Graphics to create editable graphs. **NOTE:** The LISTING destination is typically open by default. There are three steps you must take to edit a graph:

1 You must first enable the creation of editable graphs in one of three ways:

- use an ODS statement to temporarily enable this feature
- use a SAS command to temporarily enable this feature
- use the SAS Registry Editor to permanently enable this feature

Creating editable graphs takes additional resources, so you might not want to permanently enable this feature.

2 You submit your SAS code and create editable graphs.

3 You invoke the ODS Graphics Editor and edit the plot.

Step 2 involves submitting SAS code in the usual way, and no special instructions are needed for creating graphs that can be edited. Steps 1 and 3 are explained in more detail in the following sections.

Enabling the Creation of Editable Graphs

Temporarily Enable Creation of Editable Graphs by Using an ODS Statement

You can enable the creation of editable graphs within a SAS session by submitting one of the following statements:

```
ods listing sge=on;
ods html sge=on;
```

You can disable the creation of editable graphs by submitting one of the following statements:

```
ods listing sge=off;
ods html sge=off;
```

Permanently Enable Creation of Editable Graphs across SAS Sessions

You can create a default setting that enables or disables the creation of editable graphs across SAS sessions via the ‘ODS Graphics Editor’ setting in the SAS Registry. You can change this setting in the SAS windowing environment as follows:

- 1 Open the Registry Editor by entering **regedit** on the command line.
- 2 Select **SAS_REGISTRY ► ODS ► GUI ► RESULTS**.
- 3 In the **Value Data** field, click **ODS Graphics Editor** to open the Edit String Value window, and type **On** to enable the creation of editable graphs or type **Off** to disable it.
- 4 Click **OK**.

Editing a Graph with the ODS Graphics Editor

The ODS Graphics Editor is illustrated using the following example:

```
data sasuser.growth;
  input country $ GDP LFG EQP NEQ GAP;
  datalines;
Argentin  0.0089 0.0118 0.0214 0.2286 0.6079
Austria   0.0332 0.0014 0.0991 0.1349 0.5809
Belgium   0.0256 0.0061 0.0684 0.1653 0.4109

  ... more lines ...

Zambia   -0.0110 0.0275 0.0702 0.2012 0.8695
Zimbabwe  0.0110 0.0309 0.0843 0.1257 0.8875
;

ods graphics on;
ods html style=Statistical sge=on;

proc robustreg data=sasuser.growth plots=(ddplot histogram);
  model GDP = LFG GAP EQP NEQ / diagnostics leverage;
  output out=robout r=resid sr=stdres;
run;

ods _all_ close;
ods listing;
```

The DATA and the PROC ROBUSTREG steps are submitted to the SAS System, in this case from the SAS windowing environment, as shown in Figure 21.16. Two versions of the graph are created: one in an uneditable PNG file (for example, *DDPlot.png*) and one in an editable SGE file (for example, *DDPlot.sge*). Both are saved in the SAS current folder. You can edit the graph in one of three ways:

- In the Results window, double-click the second graph icon for the graph you want to edit (see Figure 21.16). The second icon corresponds to the SGE file, and the first icon corresponds to the PNG file. Clicking the first graph icon invokes a host-dependent graph viewer (for example, Microsoft Photo Editor on Windows), not the ODS Graphics Editor. **NOTE:** The Editor window might be hidden behind other windows in the SAS windowing environment.
- You can edit the graph by selecting it in the SAS Explorer window. You must first navigate to the SAS current folder and to the SGE files.
- You can open the graph from outside of the SAS System. For example, if you are running the SAS System under the Windows operating system, you can click on the graph's SGE file to open it with the ODS Graphics Editor.

Figure 21.16 Results Window with Icons for Editable Plots

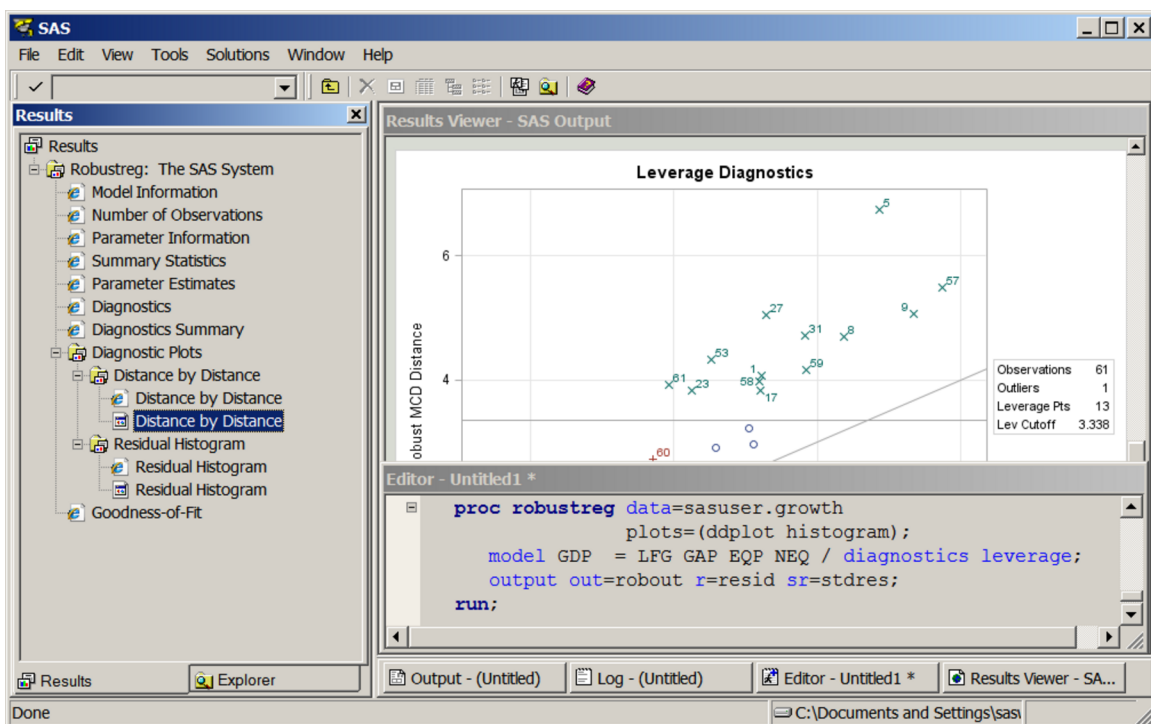


Figure 21.17 shows the ODS Graphics Editor window for the editable diagnostic plot created by PROC ROBUSTREG. In Figure 21.18, various tools in the ODS Graphics Editor are used to modify the title and annotate a particular point. The edited plot can be saved as a PNG file or as an SGE file by selecting **File ► Save As**. After saving the plot, you can edit it again through the SAS Explorer window or by selecting **File ► Open** from the ODS Graphics Editor window. Alternatively, you can reopen the saved plot for editing without first invoking the SAS System. For example, if you are running the SAS System under the Windows operating system, you can click on the plot to open it with the ODS Graphics Editor.

The ODS Graphics Editor does not permit you to make structural changes to a graph (such as moving the positions of data points). The ODS Graphics Editor provides you with a point-and-click way to make one-time changes to a specific graph, whereas the template language (see the section “[Graph Templates](#)” on page 706 in Chapter 22, “[ODS Graphics Template Modification](#),”) provides you with a programmatic way to make template changes that persist every time you run the procedure. For complete details about the tools available in the ODS Graphics Editor, see *SAS/GRAPH: ODS Graphics Editor User’s Guide*.

Figure 21.17 Diagnostic Plot before Editing

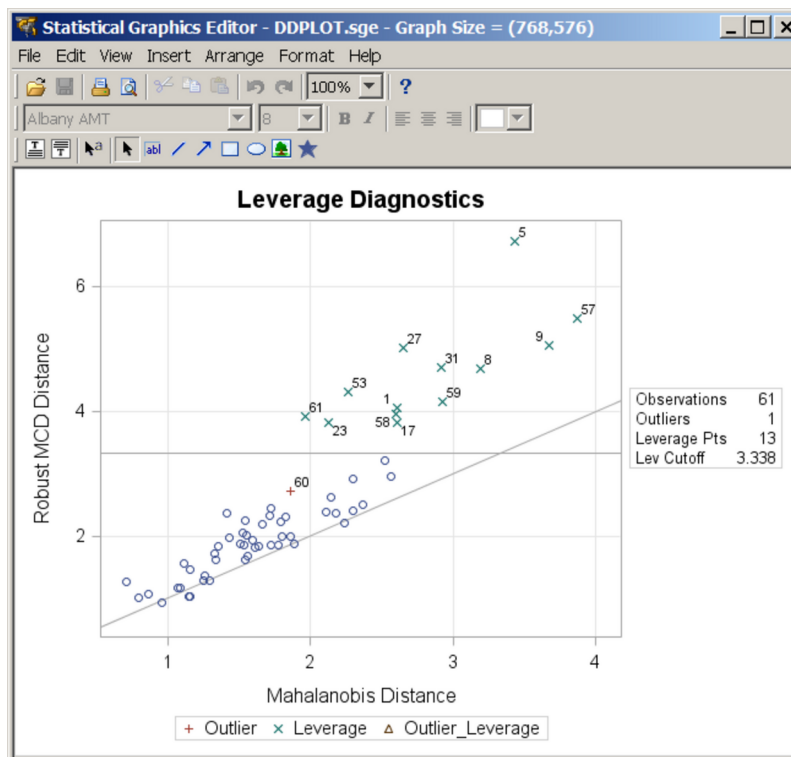
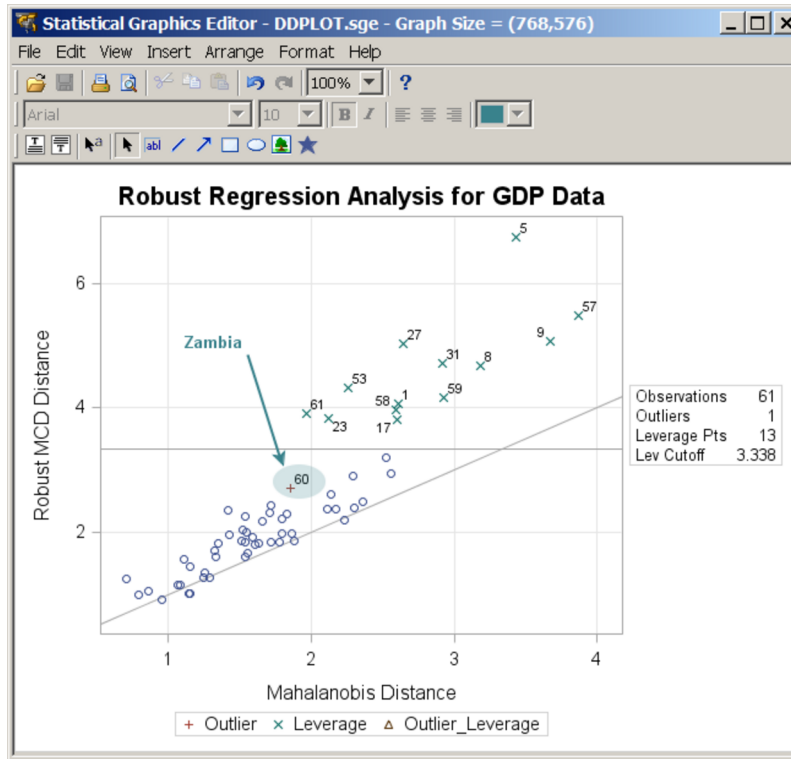


Figure 21.18 Diagnostic Plot after Editing



The Default Template Stores and the Template Search Path

Compiled templates are stored in a template store, which is a type of item store. (An item store is a special type of SAS file.) You can see the list of template stores by submitting the following statement:

```
ods path show;
```

The results are as follows:

```
Current ODS PATH list is:
```

1. SASUSER.TEMPLAT (UPDATE)
2. SASHELP.TMPLMST (READ)

These results show that the default template search path consists of Sasuser.Templat followed by Sashelp.Tmplmst. You can add template stores that you create or change the order in which the template stores are searched. This is discussed in detail in the sections “Saving Customized Templates” on page 715, “Using Customized Templates” on page 716, and “Reverting to the Default Templates” on page 717 in Chapter 22, “ODS Graphics Template Modification,” and in the sections “The ODS PATH Statement” on page 524 and “Controlling Output Appearance with Templates” on page 526 in Chapter 20, “Using the Output Delivery System.”

This section discusses the default template stores that you use when you have not modified the template search path with the ODS PATH statement. By default, templates that you write are stored in Sasuser.Templat. If you stored a modified template in Sasuser.Templat, ODS finds and uses your modified template. Otherwise, ODS finds the templates it provides in Sashelp.Tmplmst. You can see a list of all of the templates that you have modified as follows:

```
proc template;
  list / store=sasuser.templat;
run;
```

You can delete any template that you modified (so that ODS finds the default SAS template) by specifying it in a DELETE statement, as in the following statement:

```
proc template;
  delete Stat.REG.Graphics.ResidualPlot / store=sasuser.templat;
run;
```

The option STORE=SASUSER.TEMPLAT is not required. However, if you have administrator privileges on your computer, this option helps you ensure that you do not accidentally delete templates from Sashelp.Tmplmst. Unless you have administrator privileges, ODS never deletes a template in Sashelp.Tmplmst, so you can safely run the preceding step without the STORE= option, even if the template you specify does not exist in Sasuser.Templat. You can run the following step to delete the entire Sasuser.Templat template store of customized templates so that ODS uses only the templates supplied by the SAS System:

```
ods path sashelp.tmplmst(read);
proc datasets library=sasuser nolist;
  delete templat(memtype=itemstor);
run;
ods path sasuser.templat(update) sashelp.tmplmst(read);
```

It is good practice to delete templates that you have customized when you are done with them, so that they are not unexpectedly used later. See the section “Reverting to the Default Templates” on page 717 in Chapter 22, “ODS Graphics Template Modification,” for more information.

Styles

ODS styles control the overall appearance of your output. Usually, the only thing you need to do with styles is specify them in an ODS destination statement, as in the following example:

```
ods html body='b.html' style=HTMLBlue;
```

However, you can also modify existing styles and even write your own styles. You can also specify style elements in custom templates that you write, or you can modify which style elements are used in templates supplied by SAS. This section provides an overview of styles and style elements, which are the components of a style. It also describes how to customize a style template and how to specify a default style for your output. Only the most commonly used styles, style elements, and style changes are discussed here. For complete details about styles, see the *SAS Output Delivery System: User's Guide*.

An Overview of Styles

An ODS style template provides formatting information for specific visual aspects of your SAS output (see the section “[Style Elements and Attributes](#)” on page 638). The appearance of tables and graphs is coordinated within a particular style. For tables, this information includes a list of fonts and a list of colors. Each font definition specifies a family, size, weight, and style. Colors are associated with common areas of output, including titles, footnotes, BY groups, table headers, and table cells. For graphs, styles also control the appearance of graph elements including lines, markers, fonts and colors. ODS styles also include elements specific to statistical graphics, such as the style of fitted lines, confidence bands, and prediction limits. For more information about styles, see Kuhfeld (2010) and the *SAS Output Delivery System: User’s Guide*.

You can specify a style by using the `STYLE=` option in an ODS destination statement such as HTML, PDF, RTF, or PRINTER. You can also specify a style in the LISTING destination; however, it affects graphs but not tables. Output produced with different styles has the same content, but a different visual appearance. For example, the following statement requests output produced with the JOURNAL style:

```
ods rtf style=Journal;
```

You can use any SAS style or any style that you define yourself. The following statements list the names of all of the styles and then display five of them:

```
proc template;  
  list styles;  
  source Styles.Default;  
  source Styles.Statistical;  
  source Styles.Journal;  
  source Styles.RTF;  
  source Styles.HTMLBlue;  
run;
```

The results of this step (not shown) are a list of over fifty styles in the SAS listing and five style templates in the SAS log. Style templates are often hundreds of lines long. See the section “[Style Templates and Colors](#)” on page 639 for more information about style templates. Although you can use any style, only a few styles are typically used with ODS Graphics. They are described in [Table 21.2](#).

Table 21.2 Styles

Style	Default in	Description
HTMLBLUE	HTML and SAS/STAT documentation	An all-color style whose dominant colors are shades of blue with sans-serif fonts. See Figure 21.20 .
HTMLBLUECML		A color style whose dominant colors are shades of blue with sans-serif fonts. See Figure 21.21 .
PEARL		A color style with a white background whose dominant colors are shades of blue with sans-serif fonts. See Figure 21.27 .
SAPPHIRE		A color style with a white background and light blue table header background whose dominant colors are shades of blue with sans-serif fonts. See Figure 21.28 .
DEFAULT	HTML	A color style whose dominant colors are gray, blue, and white, with bold sans-serif fonts. See Figure 21.19 .
STATISTICAL		A color style whose dominant colors are blue, creamy gray, and white, with sans-serif fonts. See Figure 21.22 .
LISTING	LISTING	A color style, similar to DEFAULT but with a white background. See Figure 21.25 .
JOURNAL		A black-and-white style with filled areas, with sans-serif fonts. See Figure 21.24 .
JOURNAL2		A black-and-white style, similar to JOURNAL but with empty areas. Grouped bar charts use crosshatching to show groups. See Output 21.3.2 .
JOURNAL3		A black-and-white style, similar to JOURNAL2 but with a mix of filled areas and crosshatching in grouped bar charts. See Output 21.3.3 .
RTF	RTF	A color style whose dominant colors are blue, white, and black, with Times Roman fonts. See Figure 21.26 .
ANALYSIS		A color style, similar to STATISTICAL, whose dominant color is tan. See Figure 21.23 .

Each ODS destination has its own default style, as shown in Table 21.2. Most output in SAS/STAT documentation uses the HTMLBLUE style. However, throughout this chapter, you can see examples of other styles. For more information about styles, see the *SAS Output Delivery System: User's Guide*.

Style Elements and Attributes

An ODS style template is composed of a set of *style elements*. A style element is a collection of *style attributes* that applies to a particular feature or aspect of the output. A value is specified for each attribute in a style template. For example, **GraphFit** is the style element used for fit lines, and its attributes include: **LineThickness**, **LineStyle**, **MarkerSize**, **MarkerSymbol**, **ContrastColor**, and **Color**.

In general, style templates control the overall appearance of ODS tables and graphs. For tables, style templates specify features such as background color, table borders, and color scheme, and they specify the fonts, sizes, and color for the text and values in a table and its headers. For graphs, style templates specify the following features:

- background color
- graph dimensions (height and width)
- borders
- line styles for axes and grid lines
- fonts, sizes, and colors for titles, footnotes, axis labels, axis values, and data labels (see the section “[Modifying Graph Fonts in Styles](#)” on page 675 for an illustration)
- marker symbols, colors, and sizes for data points and outliers
- line styles for needles
- line and curve styles for fitted models and predicted values (see the section “[Modifying Other Graph Elements in Styles](#)” on page 678 for an illustration)
- line and curve styles for confidence and prediction limits
- fill colors for histogram bars, confidence bands, and confidence ellipses
- colors for box plot features
- colors for surfaces
- color ramps for contour plots

The SAS System supplies a graph template for each graph that is created by statistical procedures. A graph template is a program that specifies the layout and details of a graph. See the section “[Graph Templates](#)” on page 706 in Chapter 22, “[ODS Graphics Template Modification](#),” for more information about templates. Some template options are specified with a style reference of the form **style-element**, or occasionally **style-element:attribute**. For example, the symbol, color, and size of markers for basic scatter plots are specified in a template SCATTERPLOT statement as follows:

```
scatterplot x=x y=y / markerattrs=GraphDataDefault;
```

The preceding statement specifies that the appearance for markers is controlled by the **GraphDataDefault** element. Consistent use of this element guarantees a common appearance of markers across all scatter plots, based on the style template that you are using.

In general, ODS Graphics features are determined by style element attributes unless they are overridden by a statement or option in the graph template. For example, suppose that a classification variable is specified with the **GROUP=** option in a **SCATTERPLOT** template statement as follows:

```
scatterplot x=X y=Y / group=GroupVar;
```

Then the colors for markers that correspond to the classification levels are assigned by using the style element attributes **GraphData1:ContrastColor** through **GraphData12:ContrastColor**.

Style templates are created and modified with **PROC TEMPLATE**. For more information, see the *SAS Output Delivery System: User's Guide*. You need to understand the relationships between style elements and graph features if you want to create your own style template or modify a style template. These relationships are explained in the following sections.

Style Templates and Colors

The default style templates that the SAS System provides are stored in the *Styles* directory of *Sashelp.Tmplmst*. You can display, edit, and save style templates by using the same methods available for modifying graph and table templates, as explained in the section “[The Default Template Stores and the Template Search Path](#)” on page 634 and the series of sections beginning with the section “[Displaying Templates](#)” on page 712 in Chapter 22, “[ODS Graphics Template Modification](#).” In particular, you can display a style template by using one of these methods:

- From the Templates window in the SAS windowing environment, expand the *Sashelp.Tmplmst* node under **Templates**, and then select **Styles** to display the contents of this folder. To open the Templates window, type **odst** on the command line.
- Use the **SOURCE** statement in **PROC TEMPLATE**.

For example, the following statements display the **DEFAULT** style template in the SAS log:

```
proc template;
  source Styles.Default;
run;
```

Some of the results are as follows:

```
define style Styles.Default;
. . .
class GraphColors
  "Abstract colors used in graph styles" /
. . .
'gconramp3cend' = cxFF0000
'gconramp3cneutral' = cxFF00FF
'gconramp3cstart' = cx0000FF
. . .
'gdata12' = cxDDD17E
'gdata11' = cxB7AEF1
'gdata10' = cx87C873
'gdata9' = cxCF974B
'gdata8' = cxCD7BA1
'gdata6' = cxBABC5C
'gdata7' = cx94BDE1
'gdata4' = cxA9865B
'gdata5' = cxB689CD
'gdata3' = cx66A5A0
'gdata2' = cxDE7E6F
'gdata1' = cx7C95CA;
. . .
```

The first part of this list shows that the shading for certain filled plots, such as some contour plots goes from blue ('gconramp3cstart' = cx0000FF) to magenta ('gconramp3cneutral' = cxFF00FF) to red ('gconramp3cend' = cxFF0000). All colors are specified in values of the form CXrrggbb, where the last six characters specify RGB (red, green, blue) values on the hexadecimal scale of 00 to FF (or 0 to 255 base 10). The second part of the list ('gdata1' = cx7C95CA) shows that the dominant component of the **GraphData1** color is blue because the blue component of the color (CA, which corresponds to 202 base 10) is greater than both the green component (95, which corresponds to 149 base 10) and the red component (7C, which corresponds to 124 base 10).

You can change any part of the style and then submit the style back into the SAS System, after first submitting a PROC TEMPLATE statement. See the sections “Saving Customized Templates” on page 715, “Using Customized Templates” on page 716, and “Reverting to the Default Templates” on page 717 in Chapter 22, “ODS Graphics Template Modification,” for more information about modifying, using, and restoring templates. The principles discussed in those sections apply to all templates—table, style, and graph.

Some Common Style Elements

This section explains some common style elements and produces most of the graphs displayed in the section “Style Comparisons” on page 646.

The DEFAULT style is the parent for the styles used for statistical graphics work. You can see all of the elements of the DEFAULT style by running the following step:

```
proc template;
  source styles.default;
run;
```

The source listing of the definition of the DEFAULT style is hundreds of lines long. If you run PROC TEMPLATE with the SOURCE statement for most other styles, you see `parent = styles.default` (or in the case of the HTMLBLUE style, you see `parent = styles.statistical`, which inherits from the DEFAULT style), and you do not see all of the elements in the style unless you also run the preceding step with a SOURCE statement for all parent styles.

Only a few of the style elements are referenced in the templates that the SAS System provides for statistical procedures. The most commonly used style elements, along with the defaults for the noncolor attributes of the DEFAULT style, are shown next (`Color` applies to filled areas, and `ContrastColor` applies to markers and lines):

Graph	graph size, outer border appearance, and background color Padding = 0 BackgroundColor
GraphConfidence	primary fit confidence interval LineThickness = 1px LineStyle = 1 MarkerSize = 7px MarkerSymbol = "triangle" ContrastColor Color
GraphData1	attributes related to first grouped data items MarkerSymbol = "circle" LineStyle = 1 ContrastColor Color
GraphData2	attributes related to second grouped data items MarkerSymbol = "plus" LineStyle = 4 ContrastColor Color
GraphData3	attributes related to third grouped data items MarkerSymbol = "X" LineStyle = 8 ContrastColor Color
GraphData4	attributes related to fourth grouped data items MarkerSymbol = "triangle" LineStyle = 5 ContrastColor Color
GraphData<i>n</i>	attributes related to <i>n</i> th grouped data items MarkerSymbol LineStyle ContrastColor Color

GraphDataDefault	attributes related to data items that are not grouped EndColor NeutralColor StartColor MarkerSize = 7px MarkerSymbol = "circle" LineThickness = 1px LineStyle = 1 ContrastColor Color
GraphFit	primary fit line, such as a normal density curve LineThickness = 2px LineStyle = 1 MarkerSize = 7px MarkerSymbol = "circle" ContrastColor Color
GraphFit2	secondary fit line, such as a kernel density curve LineThickness = 2px LineStyle = 4 MarkerSize = 7px MarkerSymbol = "X" ContrastColor Color
GraphGridLines	horizontal and vertical grid lines drawn at major tick marks Displayopts = "auto" LineThickness = 1px LineStyle = 1 ContrastColor Color
GraphOutlier	outlier data for the graph LineThickness = 2px LineStyle = 42 MarkerSize = 7px MarkerSymbol = "circle" ContrastColor Color
GraphPredictionLimits	fills for prediction limits LineThickness = 1px LineStyle = 2 MarkerSize = 7px MarkerSymbol = "chain" ContrastColor Color

GraphReference	horizontal and vertical reference lines and drop lines LineThickness = 1px LineStyle = 1 ContrastColor
GraphDataText	text font and color for point and line labels Font = GraphFonts('GraphDataFont') (where 'GraphDataFont' = (" <sans-serif>, <MTsans-serif> ", 7pt)) Color
GraphValueText	text font and color for axis tick values and legend values Font = GraphFonts('GraphValueFont') (where 'GraphValueFont' = (" <sans-serif>, <MTsans-serif> ", 9pt)) Color
GraphLabelText	text font and color for axis labels and legend title Font = GraphFonts('GraphLabelFont') (where 'GraphLabelFont' = (" <sans-serif>, <MTsans-serif> ", 10pt, bold)) Color
GraphFootnoteText	text font and color for footnotes Font = GraphFonts('GraphFootnoteFont') (where 'GraphFootnoteFont' = (" <sans-serif>, <MTsans-serif> ", 10pt)) Color
GraphTitleText	text font and color for titles Font = GraphFonts('GraphTitleFont') (where 'GraphTitleFont' = (" <sans-serif>, <MTsans-serif> ", 11pt, bold)) Color
GraphWalls	vertical walls bounded by axes LineThickness = 1px LineStyle = 1 FrameBorder = on ContrastColor BackgroundColor Color

You refer to these elements in graph templates as `style-element` or as `style-element:attribute` (for example `GraphDataDefault:ContrastColor`). The default values are not shown for the color attributes since they are typically defined indirectly. For example, `Graph:BackgroundColor` (the color that fills the box outside the graph) is defined elsewhere in the style as `colors('docbg')`. The style also defines `'docbg' = color_list('bgA')` and `'bgA' = cxE0E0E0`. This shows that the background is a shade of gray that is much closer to white (CXFFFFFF) than to black (CX000000). You can see the background color in Figure 21.29. This shade of gray might seem darker (closer to CX000000) than you might expect based on just the RGB values. Your perception of a color change is not a linear function of the change in RGB values.

You can use the following program to see the color and other attributes for a number of style elements:

```
proc format;
  value vf 5 = 'GraphValueText';
run;

data x1;
  array y[20] y0 - y19;
  do x = 1 to 20; y[x] = x - 0.5; end;
  do x = 0 to 10 by 5; output; end;
  label y0 = 'GraphLabelText' x = 'GraphLabelText';
  format x y0 vf.;
run;

%macro d;
  %do i = 1 %to 12;
    reg y=y%eval(19-&i) x=x / lineattrs=GraphData&i markerattrs=GraphData&i
      curvelabel=" GraphData&i" curvelabelpos=max;
  %end;
%mend;

%macro l(i, l);
  reg y=y&i x=x / lineattrs=&l markerattrs=&l curvelabel=" &l"
    curvelabelpos=max;
%mend;

ods listing style=default;

proc sgplot noautolegend data=x1;
  title 'GraphTitleText';
  %d
  %l(19, GraphDataDefault)
  %l( 6, GraphFit)
  %l( 5, GraphFit2)
  %l( 4, GraphPredictionLimits)
  %l( 3, GraphConfidence)
  %l( 2, GraphGridLines)
  %l( 1, GraphOutlier)
  %l( 0, GraphReference)
  xaxis values=(0 5 10);
run;
```

The results in [Figure 21.29](#) display the attributes for a number of the elements of the DEFAULT style.

When there is a group or classification variable, the colors, markers, and lines that distinguish the groups are derived from the **GraphData***n* elements that are defined with the style. In the DEFAULT style, these are elements **GraphData1** through **GraphData12**. There can be any number of groups even though only 12 **GraphData***n* style elements are defined in the DEFAULT style. The following steps create a data set with 40 groups, display one line per group, and produce [Figure 21.39](#):

```
data x2;
  do y = 40 to 1 by -1;
    group = 'Group' || put(41 - y, 2. -L);
    do x = 0 to 10 by 5;
      if x = 10 then do; z = 11; l = group; end;
      else do; z = .; l = ' '; end;
      output;
    end;
  end;
run;

proc sgplot data=x2;
  title 'Colors, Markers, Lines Patterns for Groups';
  series y=y x=x / group=group markers;
  scatter y=y x=z / group=group markerchar=l;
run;
```

The colors, markers, and line patterns in [Figure 21.39](#) repeat in cycles. The **GraphData1** – **GraphData8** lines in [Figure 21.29](#) exactly match the **Group1** – **Group8** lines in [Figure 21.39](#). After that, there are differences due to the cyclic construction of the grouped style. This is explained next.

The DEFAULT style defines a marker symbol only in **GraphData1** through **GraphData7**. The seven markers are: circle, plus, X, triangle, square, asterisk, and diamond. With the explicit style reference in [Figure 21.29](#), the actual symbol, when no symbol is specified, is the circle. This is what you see for **GraphData8** through **GraphData12**. With the group variable in [Figure 21.39](#), the symbols repeat in cycles. Hence, **Group1**, **Group8**, **Group15**, and so on, are all circles. Similarly, **Group2**, **Group9**, **Group16**, and so on, are all pluses. The DEFAULT style defines 11 different line styles for **GraphData1** through **GraphData11**. You specify line styles by specifying an integer. The default lines styles are: 1, 4, 8, 5, 14, 26, 15, 20, 41, 42, and 2. Hence, **Group1**, **Group12**, **Group23**, and so on, all have the same line style, which is a solid line (line style 1). Similarly, **Group2**, **Group13**, **Group24**, and so on, all have line style 4. There are twelve different colors, so **Group1**, **Group13**, **Group25**, and so on, all have the same colors. Overall, there are $12 \times 11 \times 7 = 924$ color/line/marker combinations that appear before any combination repeats. You can use the %MODSTYLE SAS autocall macro (see the sections “[Creating an All-Color Style](#)” on page 669 and “[Style Template Modification Macro](#)” on page 667) to conveniently change these style attributes.

The HTMLBLUE style is an all-color style for the first 12 groups of observations. Most analyses have fewer than 12 groups. Markers and lines change for groups 13–24 and then again for groups 25–36. [Figure 21.40](#) shows how colors, markers, and line styles change in the HTMLBLUE style. [Figure 21.39](#) and [Figure 21.40](#) through [Figure 21.48](#) show how these elements change in other styles.

Style Comparisons

In this section, some of the most commonly used styles are compared with a series of figures, most of which were generated in the preceding section. Figure 21.19 through Figure 21.28 show tables and graphs in each of eight styles, for the following analysis:

```
proc reg data=sashelp.class;  
    model Weight = Height;  
run; quit;
```

Figure 21.29 through Figure 21.38 show some of the more common style elements. Figure 21.39 through Figure 21.46 show how groups of observations are displayed in the graph.

The style comparisons are as follows:

- Figure 21.19, Figure 21.29, and Figure 21.39 show the DEFAULT style.
- Figure 21.20, Figure 21.30, and Figure 21.40 show the HTMLBLUE style.
- Figure 21.21, Figure 21.31, and Figure 21.41 show the HTMLBLUECML style.
- Figure 21.22, Figure 21.32, and Figure 21.42 show the STATISTICAL style.
- Figure 21.23, Figure 21.33, and Figure 21.43 show the ANALYSIS style.
- Figure 21.24, Figure 21.34, and Figure 21.44 show the JOURNAL style.
- Figure 21.25, Figure 21.35, and Figure 21.45 show the LISTING style.
- Figure 21.26, Figure 21.36, and Figure 21.46 show the RTF style.
- Figure 21.27, Figure 21.37, and Figure 21.47 show the SAPPHIRE style.
- Figure 21.28, Figure 21.38, and Figure 21.48 show the SAPPHIRE style.

Figure 21.19 Statistical Output with the DEFAULT Style

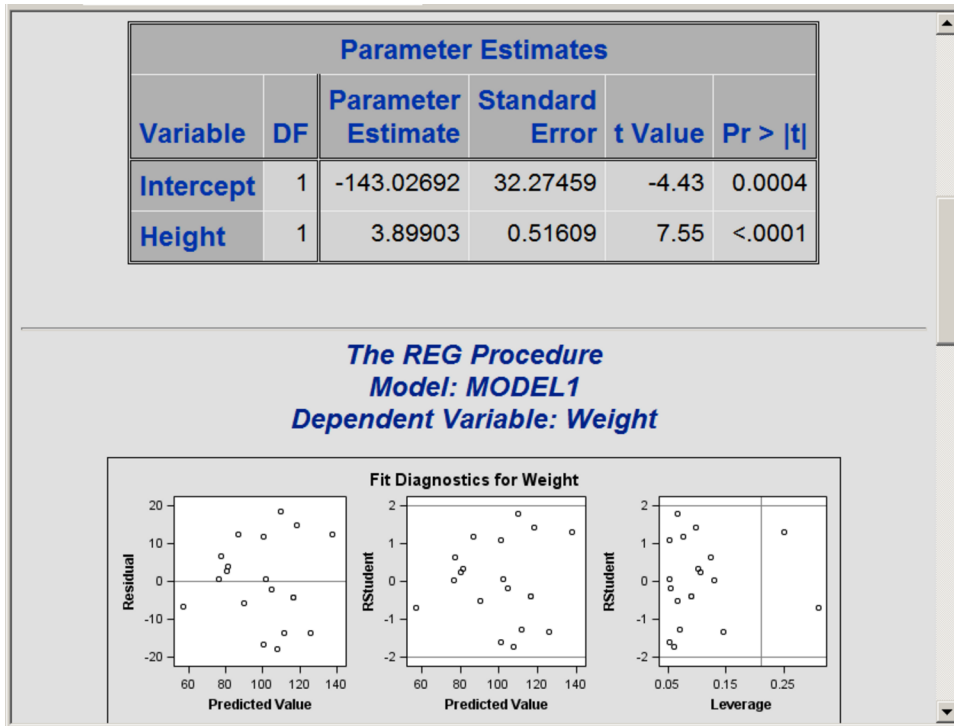


Figure 21.20 Statistical Output with the HTMLBLUE Style

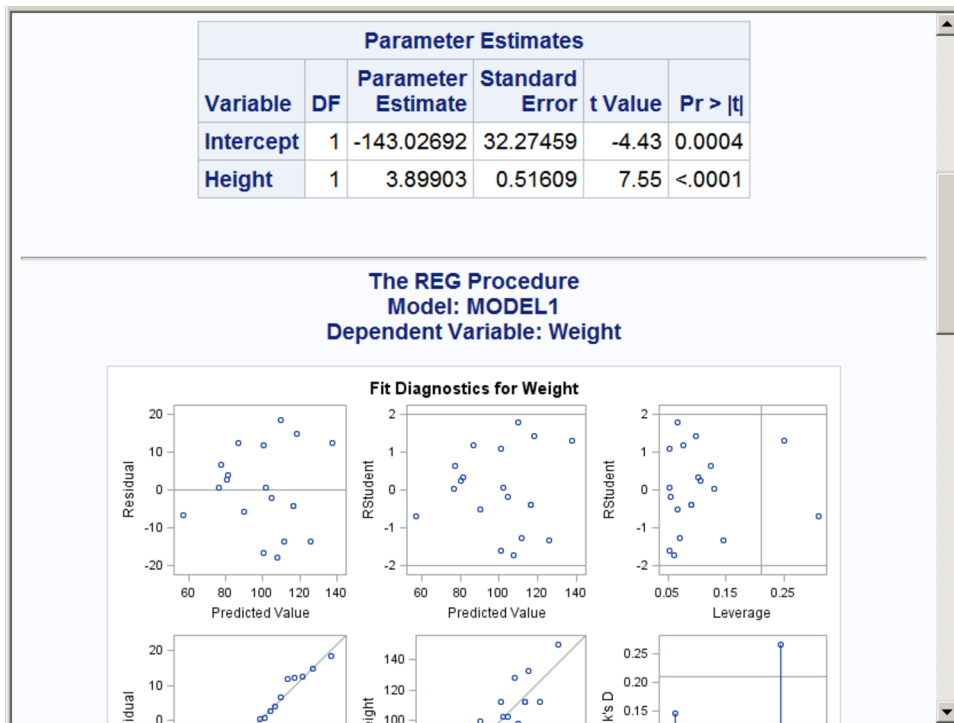


Figure 21.21 Statistical Output with the HTMLBLUECML Style

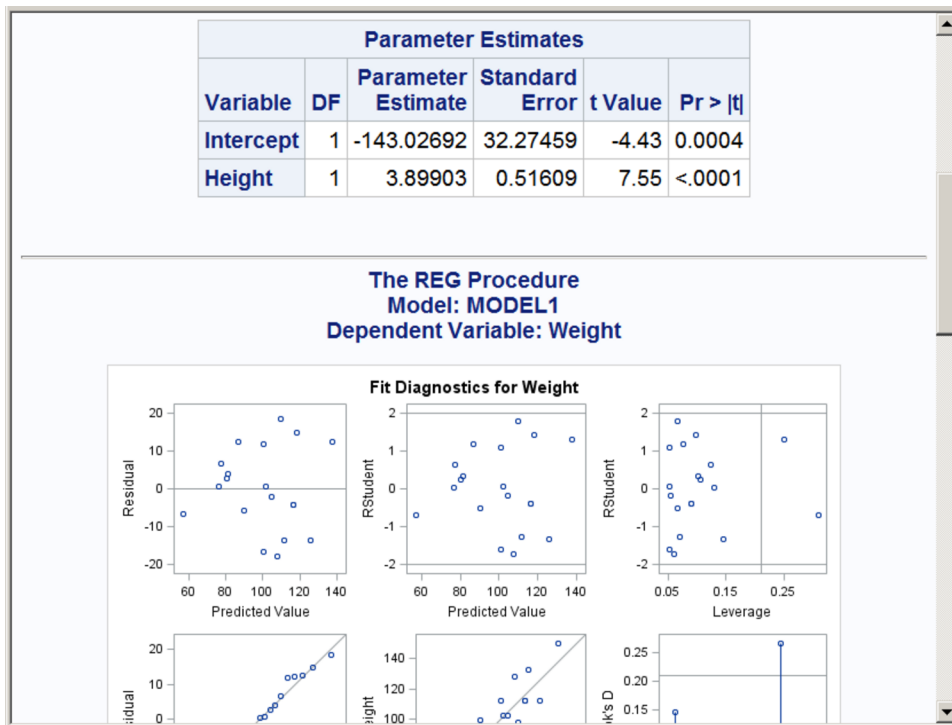


Figure 21.22 Statistical Output with the STATISTICAL Style

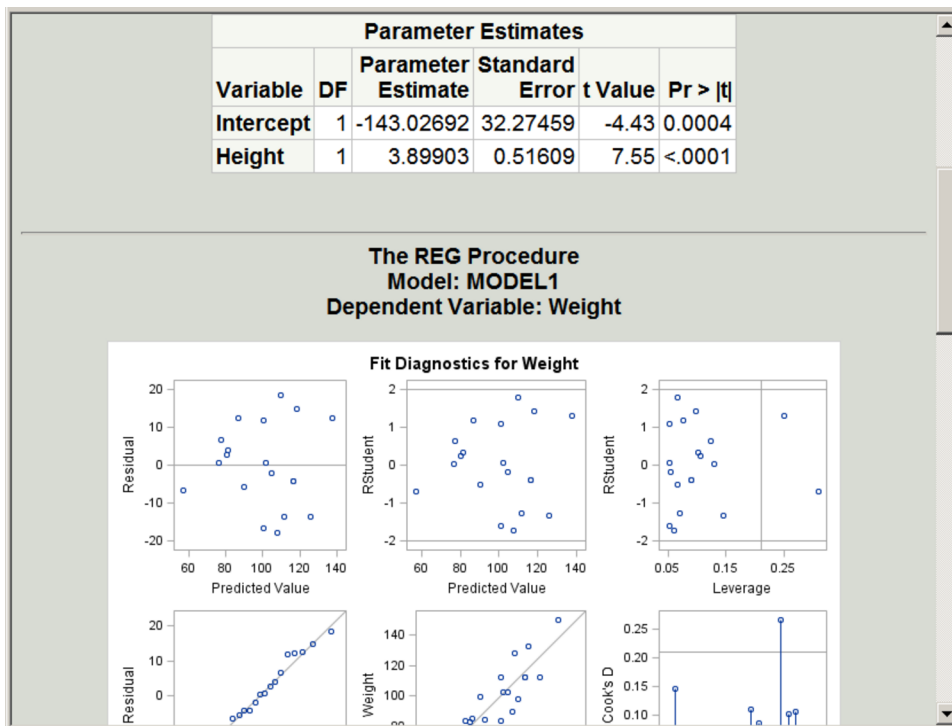


Figure 21.23 Statistical Output with the ANALYSIS Style

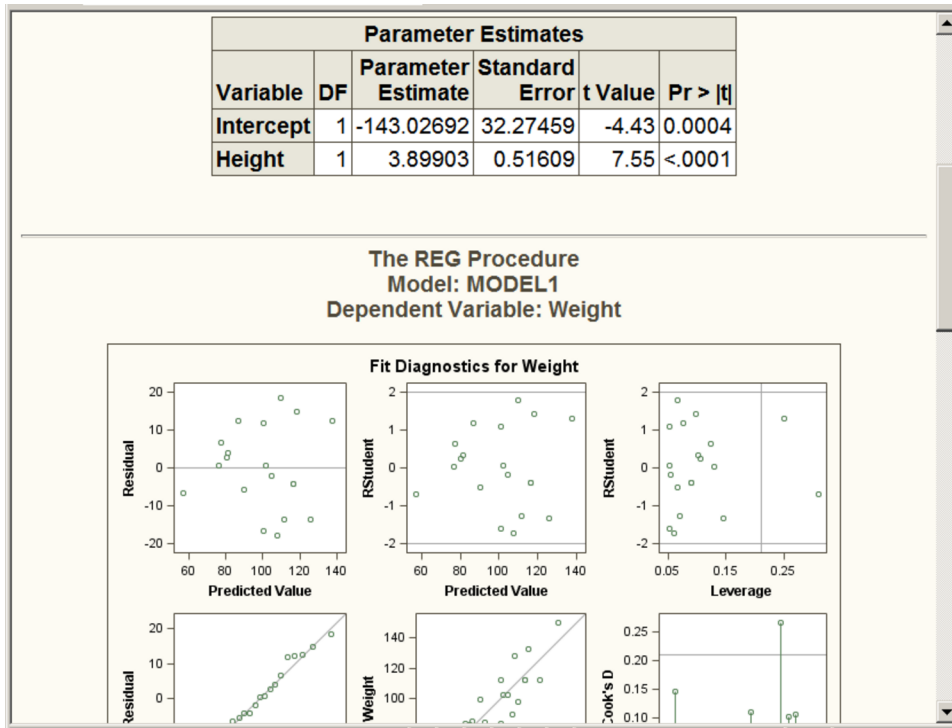


Figure 21.24 Statistical Output with the JOURNAL Style

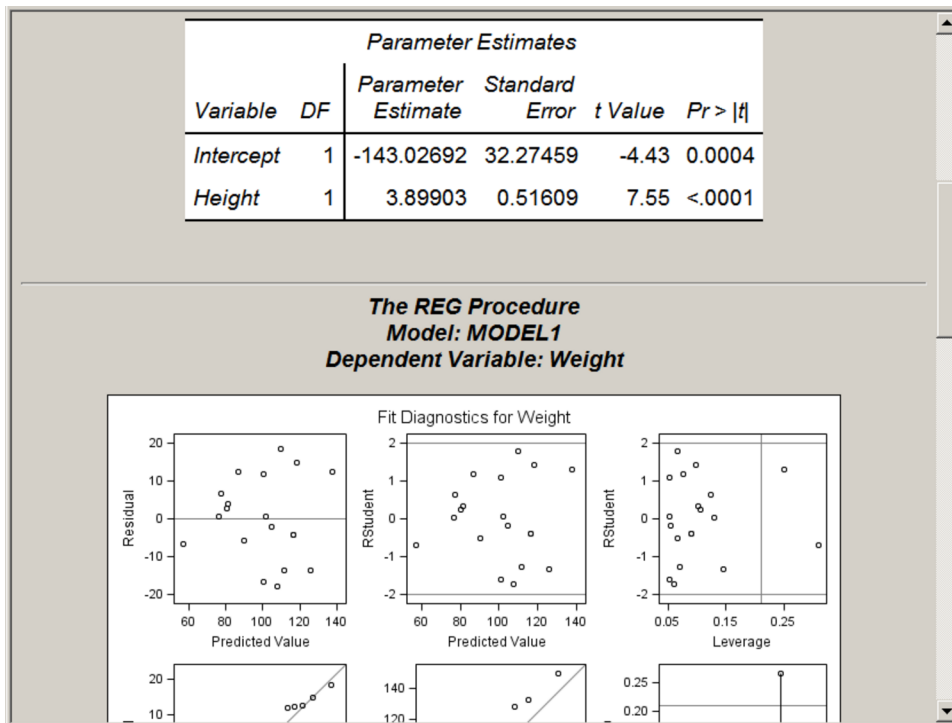


Figure 21.25 Statistical Output with the LISTING Style

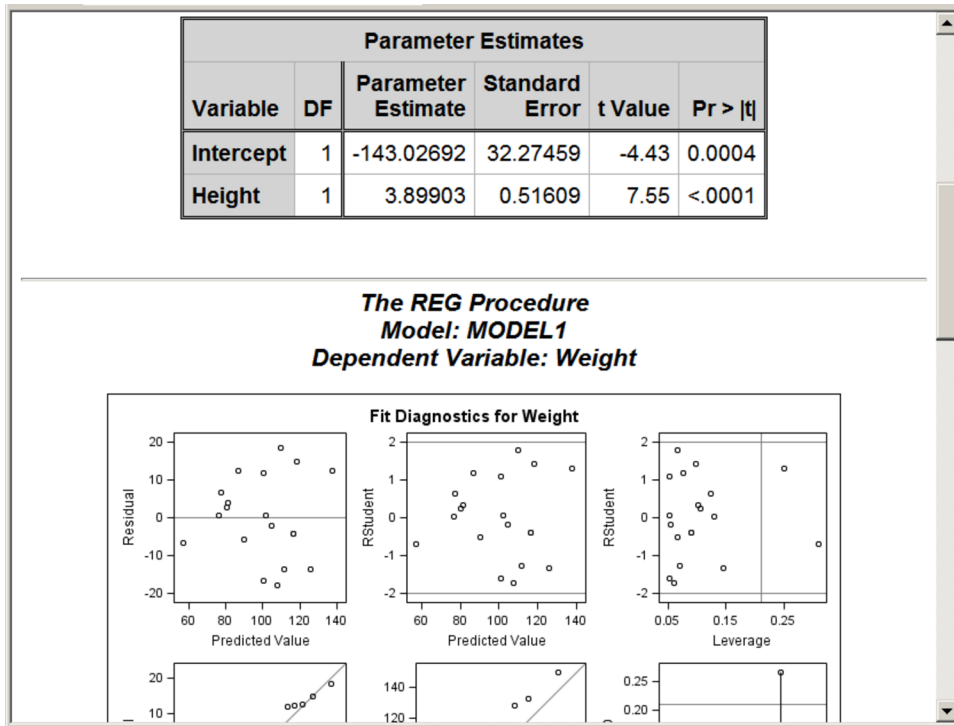


Figure 21.26 Statistical Output with the RTF Style

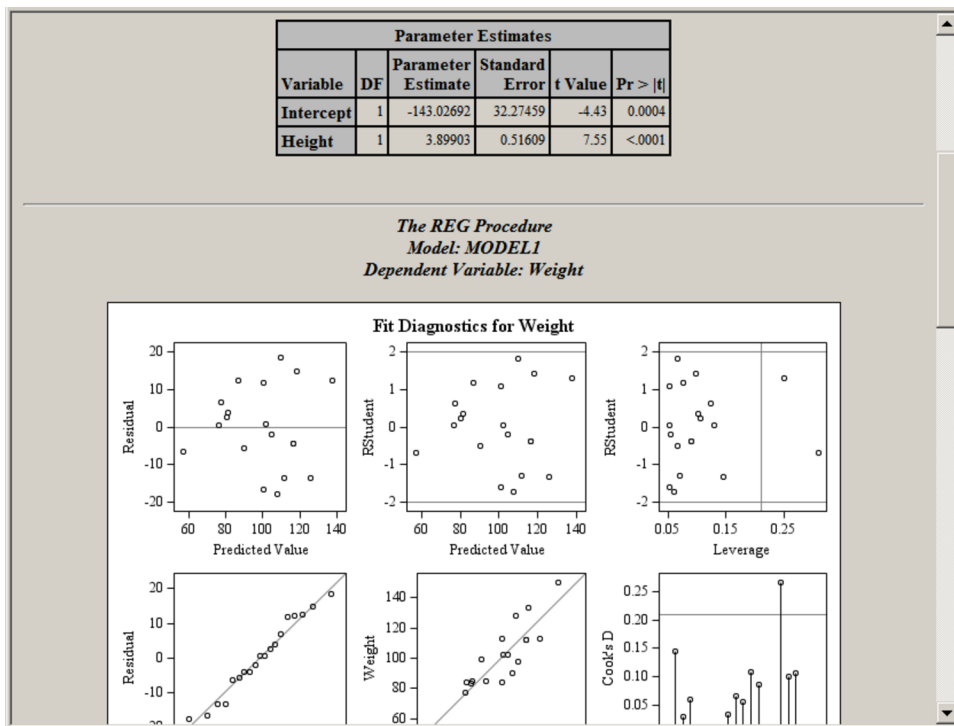


Figure 21.27 Statistical Output with the PEARL Style

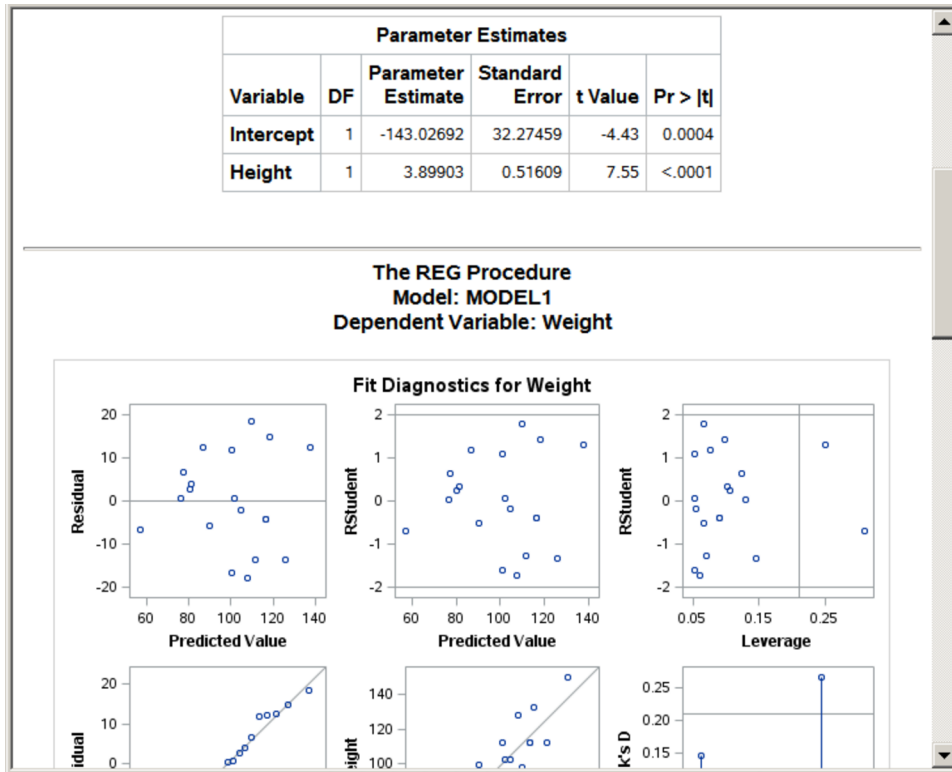


Figure 21.28 Statistical Output with the SAPPHERE Style

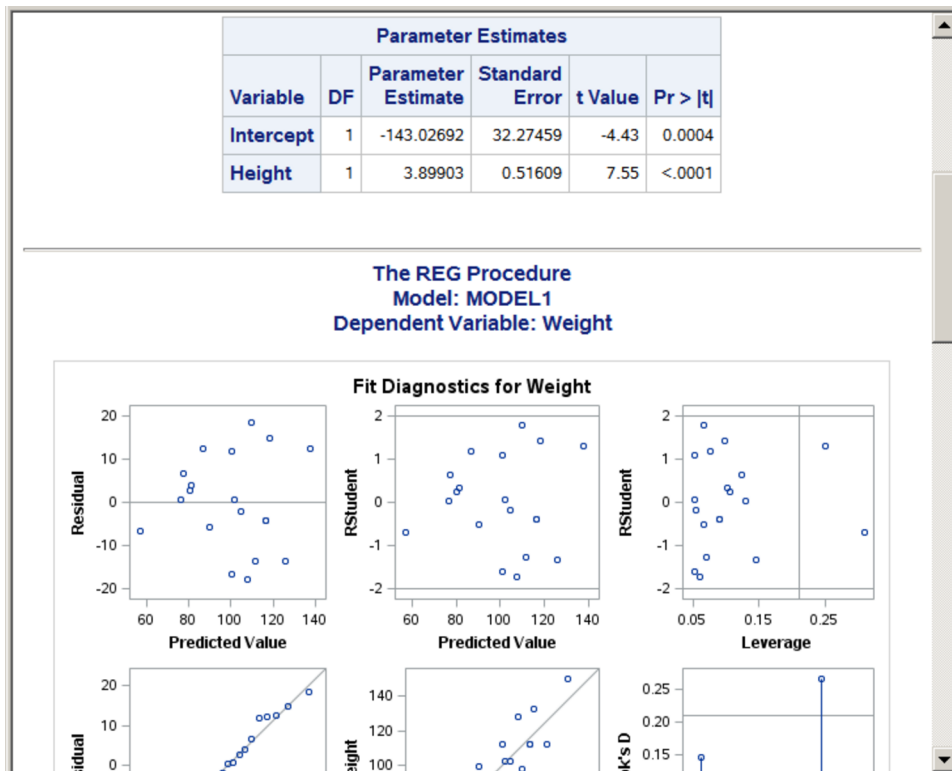


Figure 21.29 Attributes of Style Elements in the DEFAULT Style

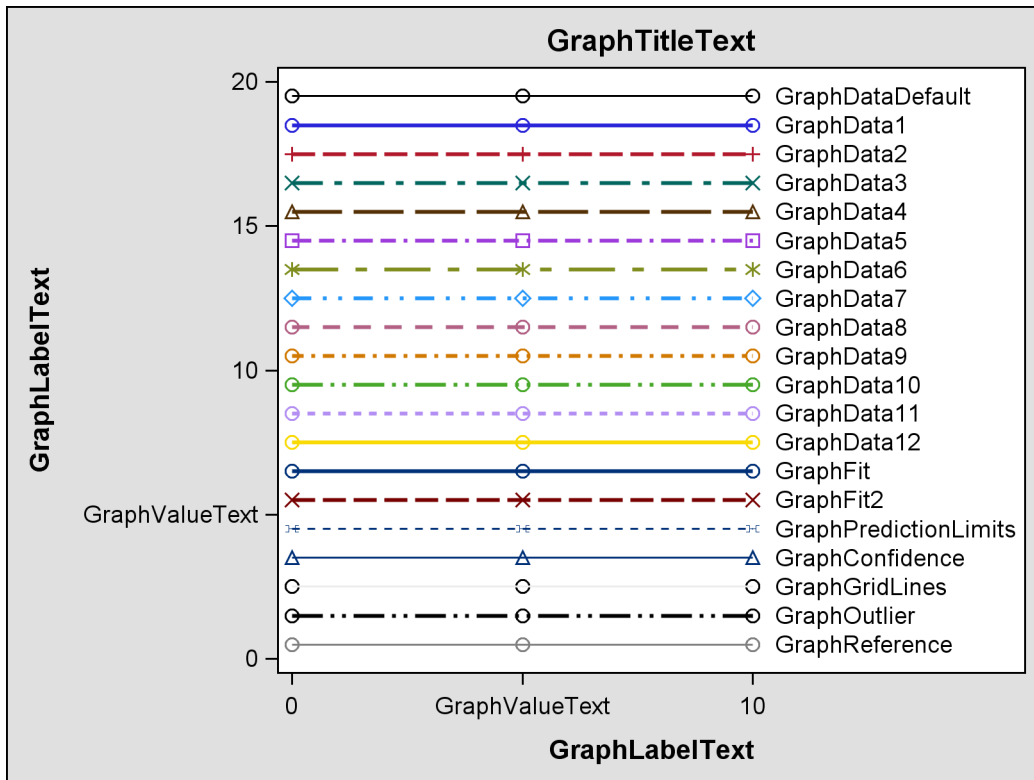


Figure 21.30 Attributes of Style Elements in the HTMLBLUE Style

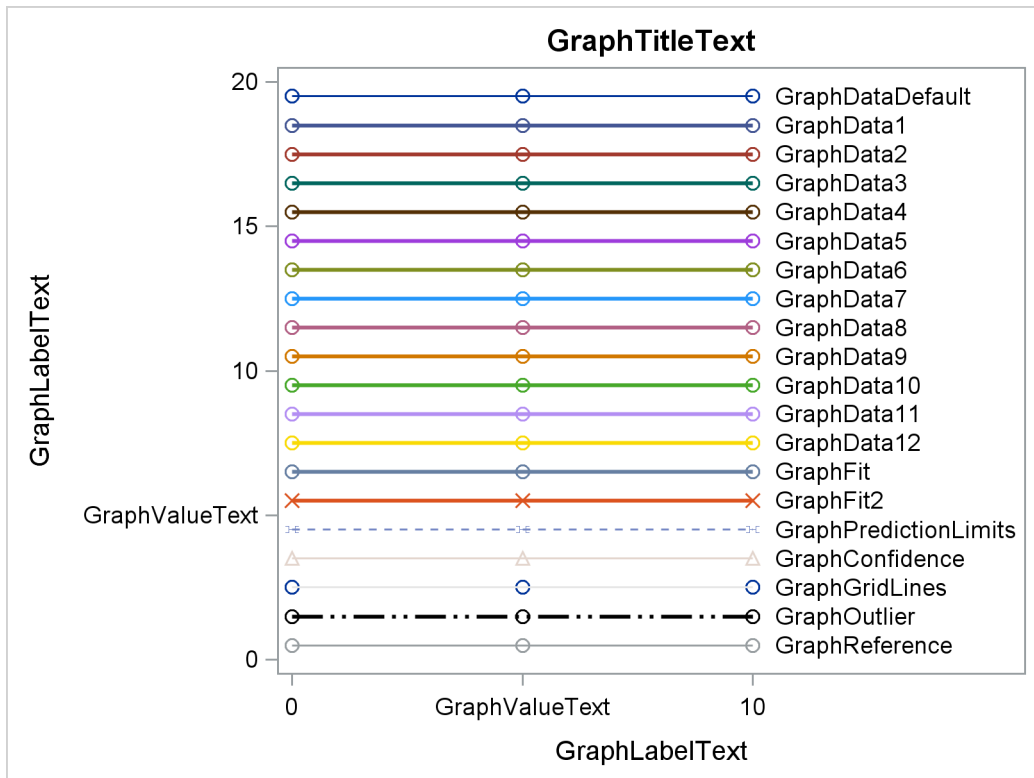


Figure 21.31 Attributes of Style Elements in the HTMLBLUECML Style

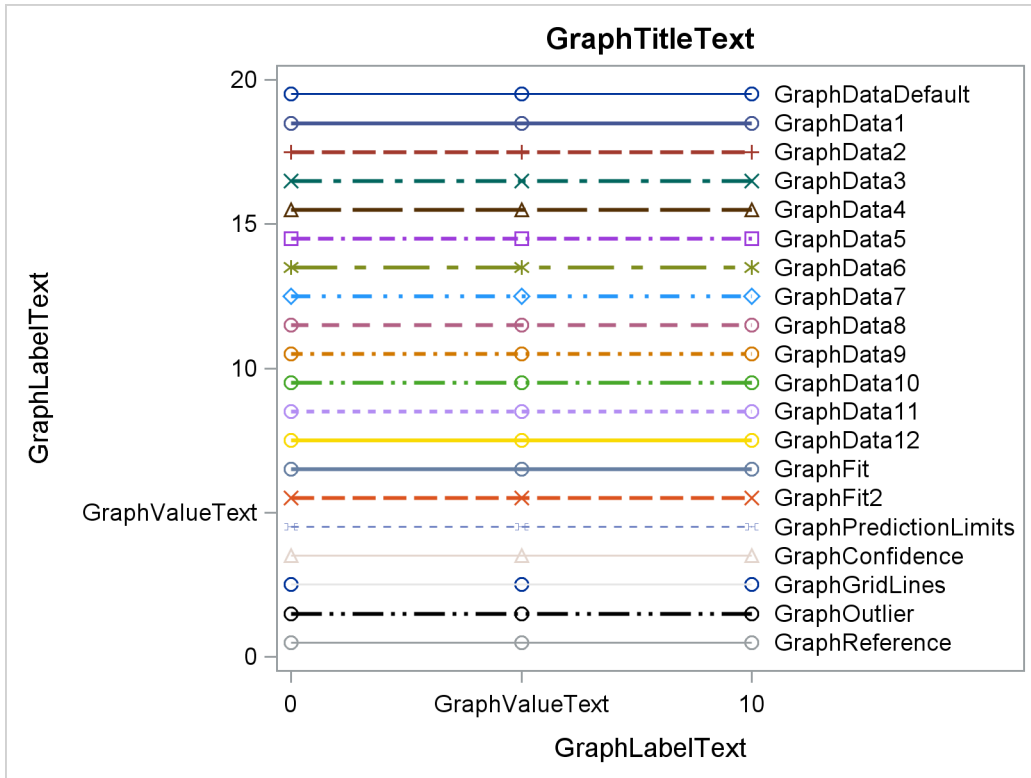


Figure 21.32 Attributes of Style Elements in the STATISTICAL Style

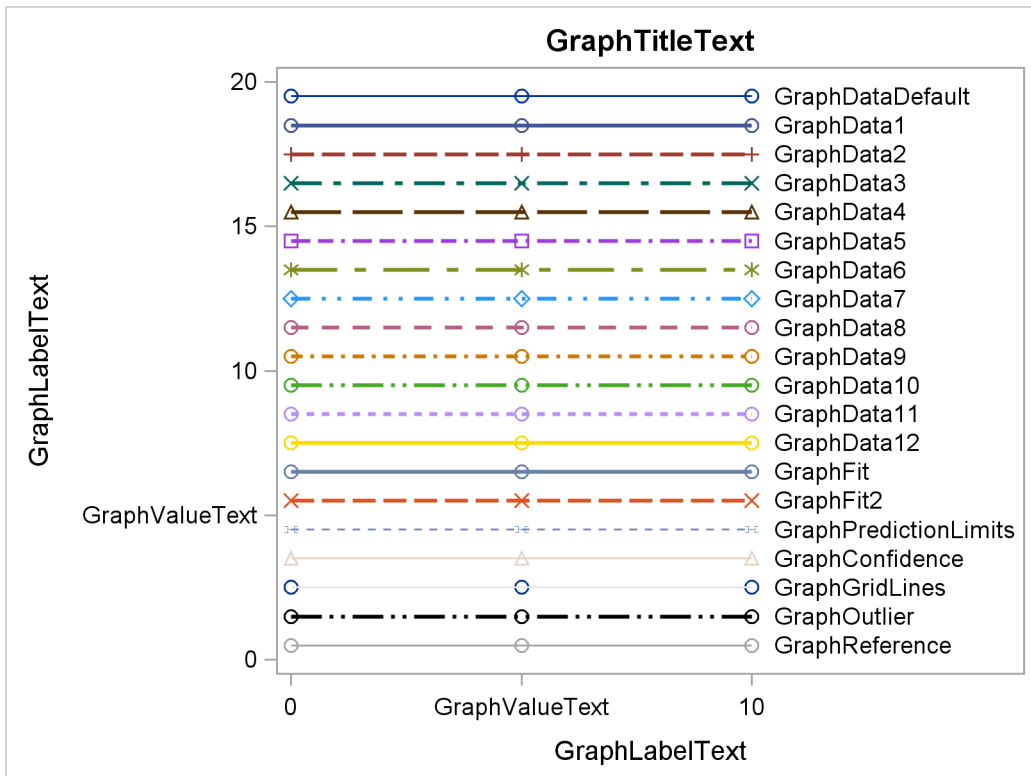


Figure 21.33 Attributes of Style Elements in the ANALYSIS Style

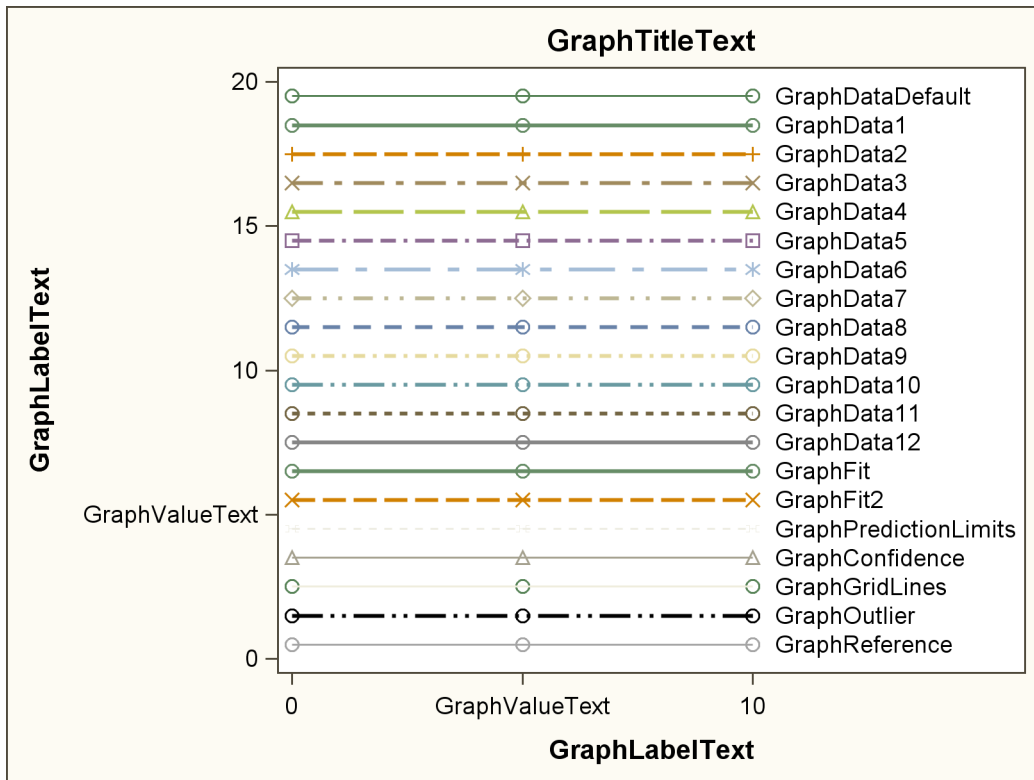


Figure 21.34 Attributes of Style Elements in the JOURNAL Style

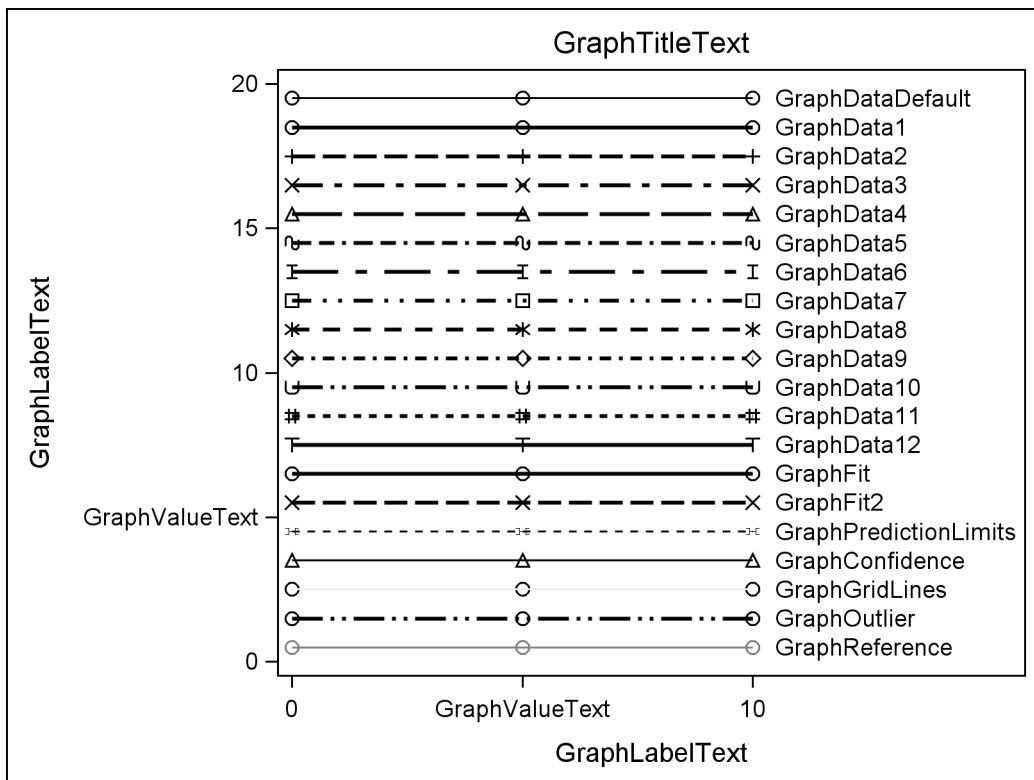


Figure 21.35 Attributes of Style Elements in the LISTING Style

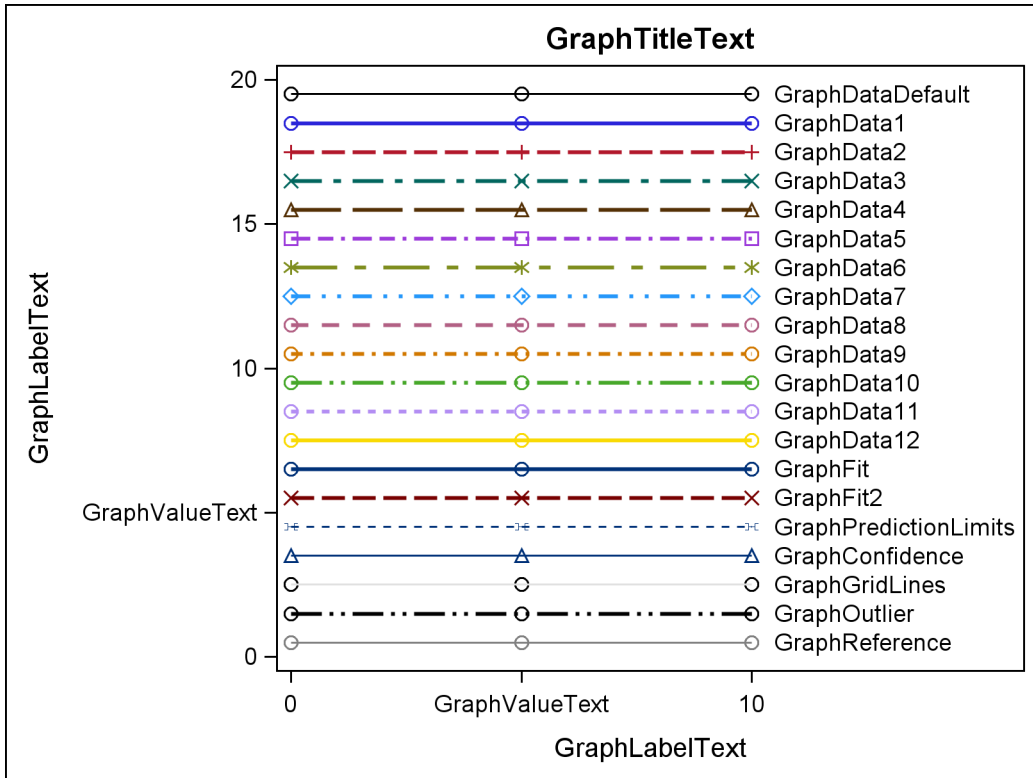


Figure 21.36 Attributes of Style Elements in the RTF Style

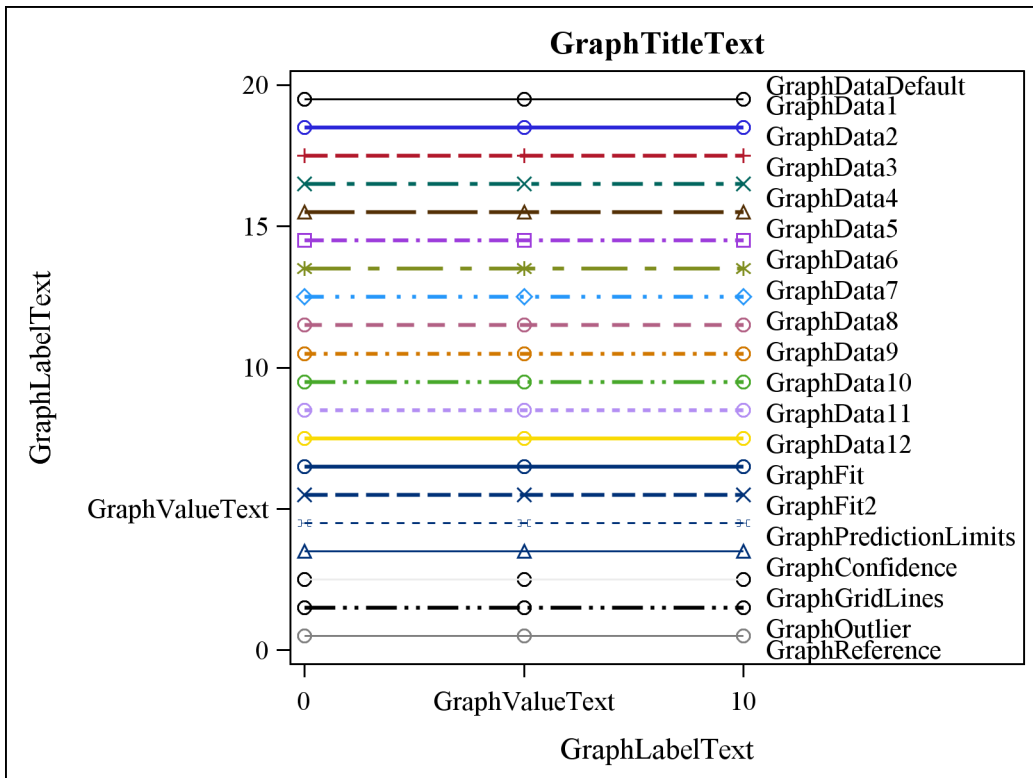


Figure 21.37 Attributes of Style Elements in the PEARL Style

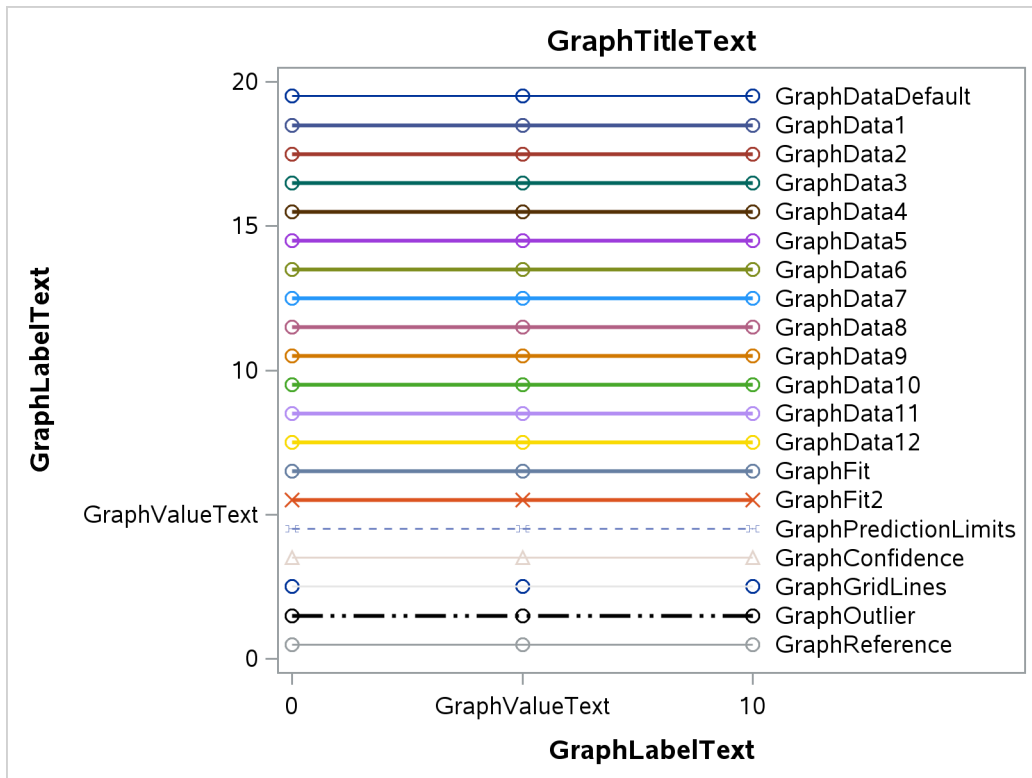


Figure 21.38 Attributes of Style Elements in the SAPPHIRE Style

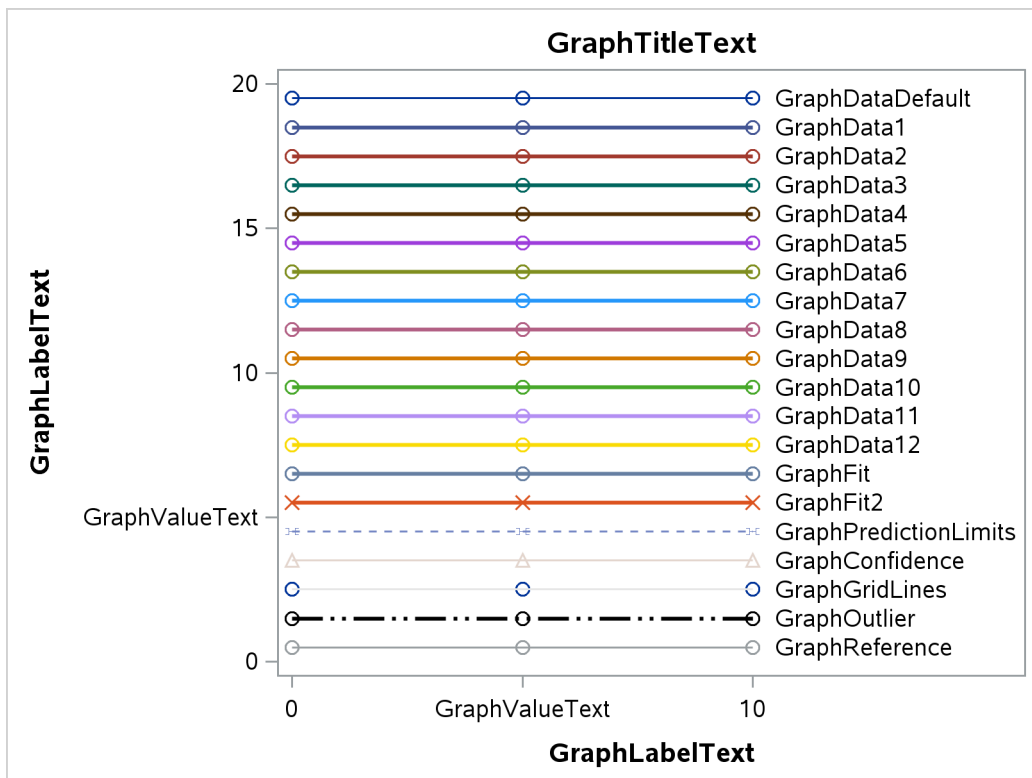


Figure 21.39 Markers, Lines, and Colors with Groups in the DEFAULT Style

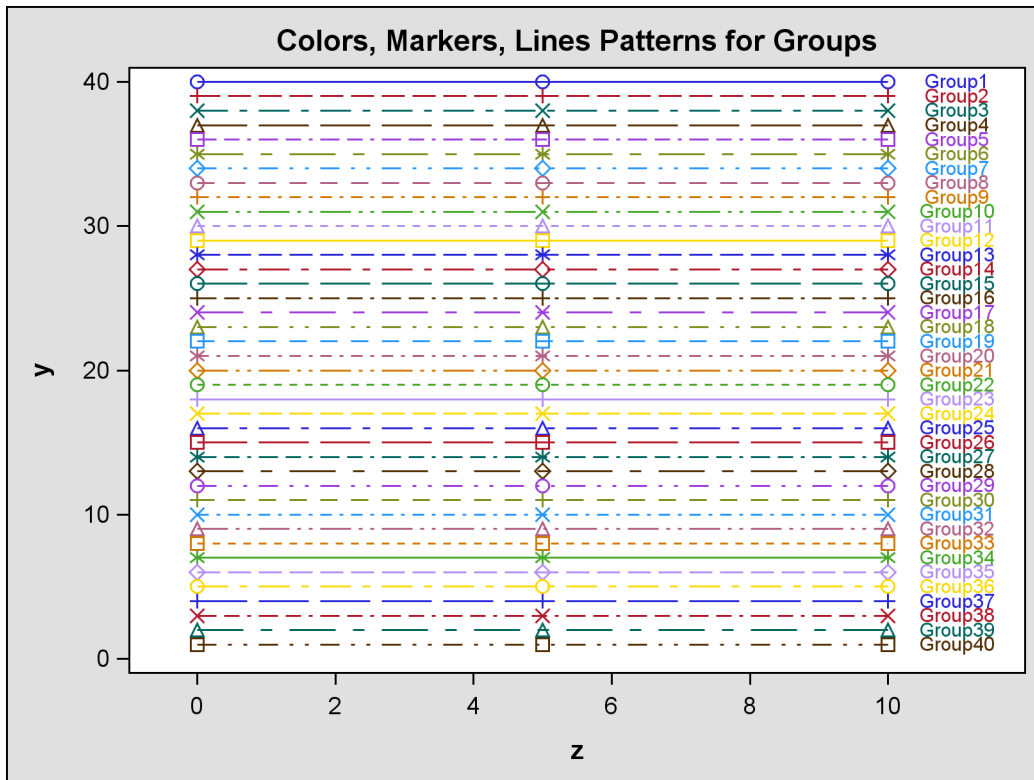


Figure 21.40 Markers, Lines, and Colors with Groups in the HTMLBLUE Style

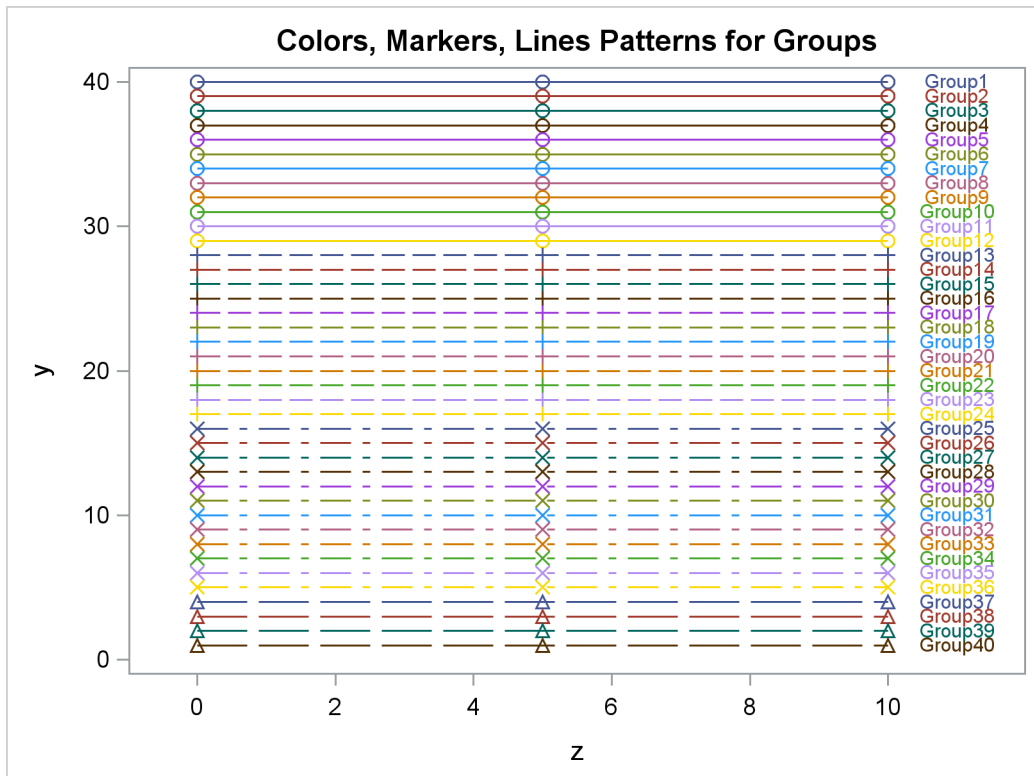


Figure 21.41 Markers, Lines, and Colors with Groups in the HTMLBLUECML Style

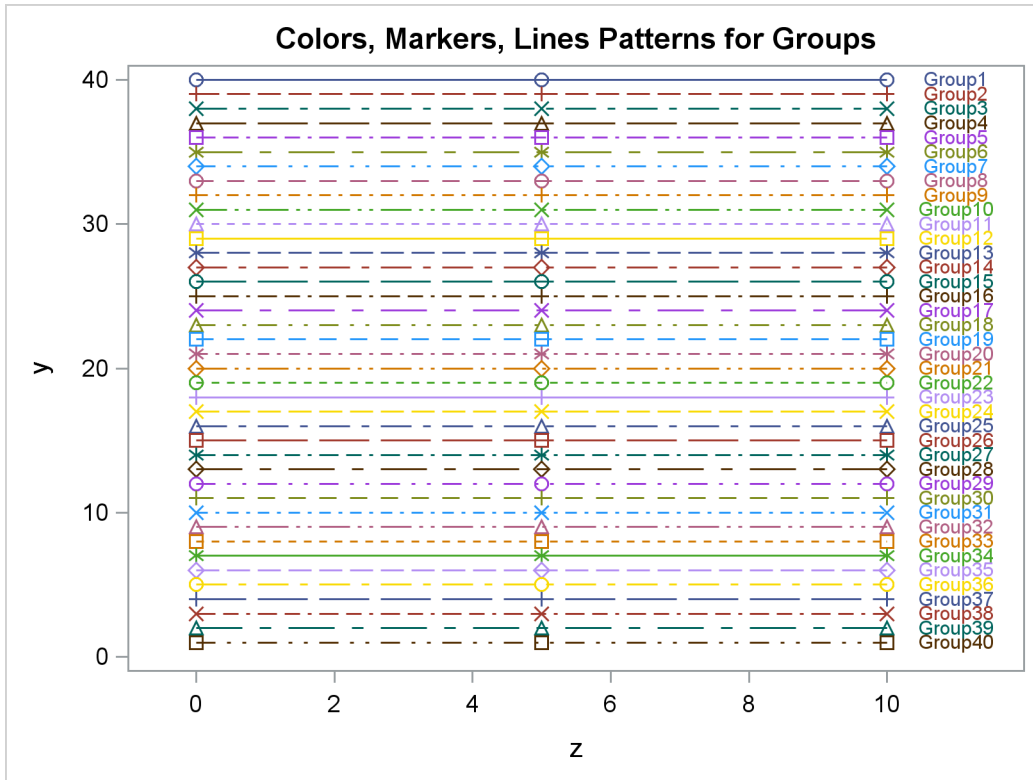


Figure 21.42 Markers, Lines, and Colors with Groups in the STATISTICAL Style

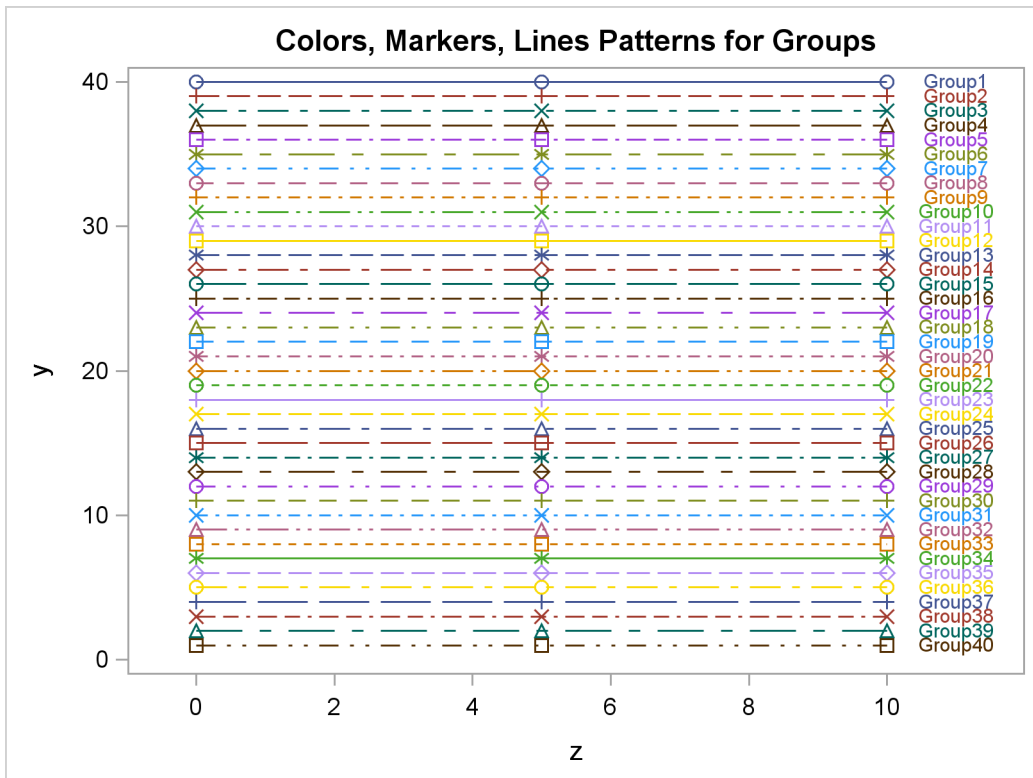


Figure 21.43 Markers, Lines, and Colors with Groups in the ANALYSIS Style

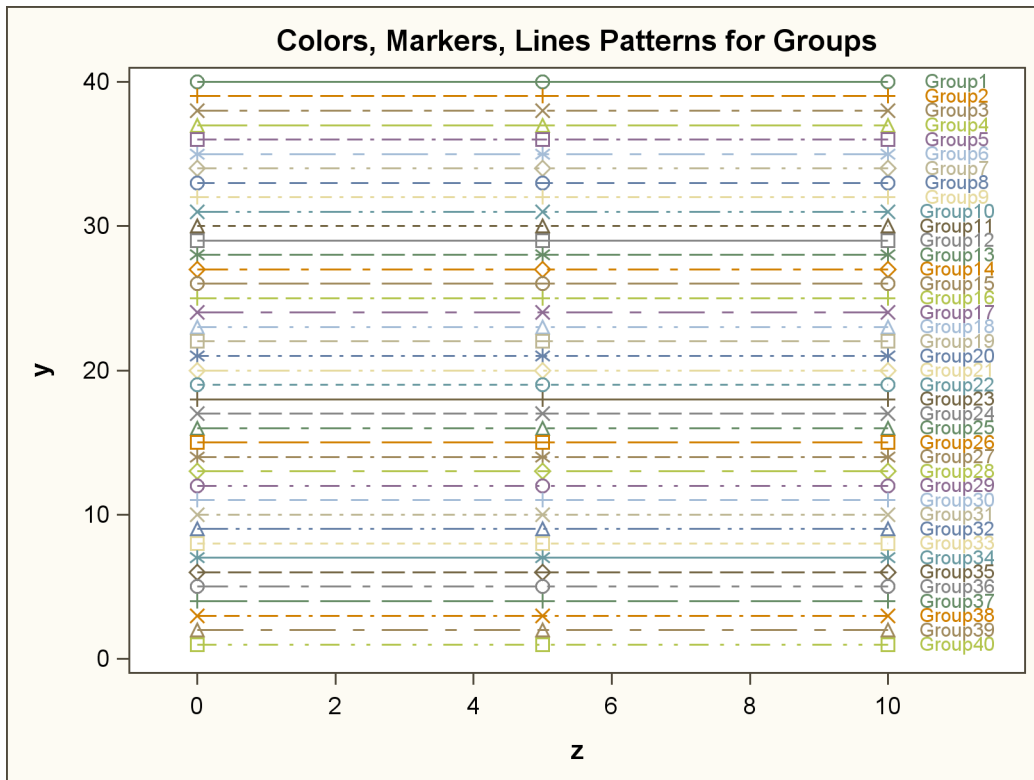


Figure 21.44 Markers, Lines, and Colors with Groups in the JOURNAL Style

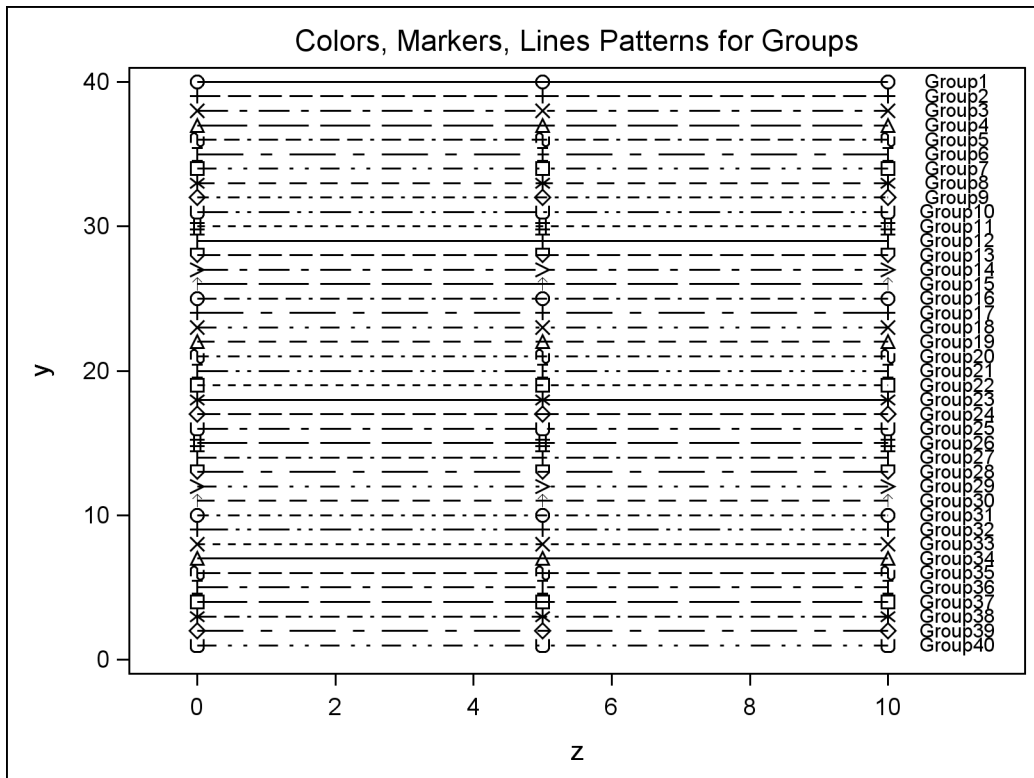


Figure 21.45 Markers, Lines, and Colors with Groups in the LISTING Style

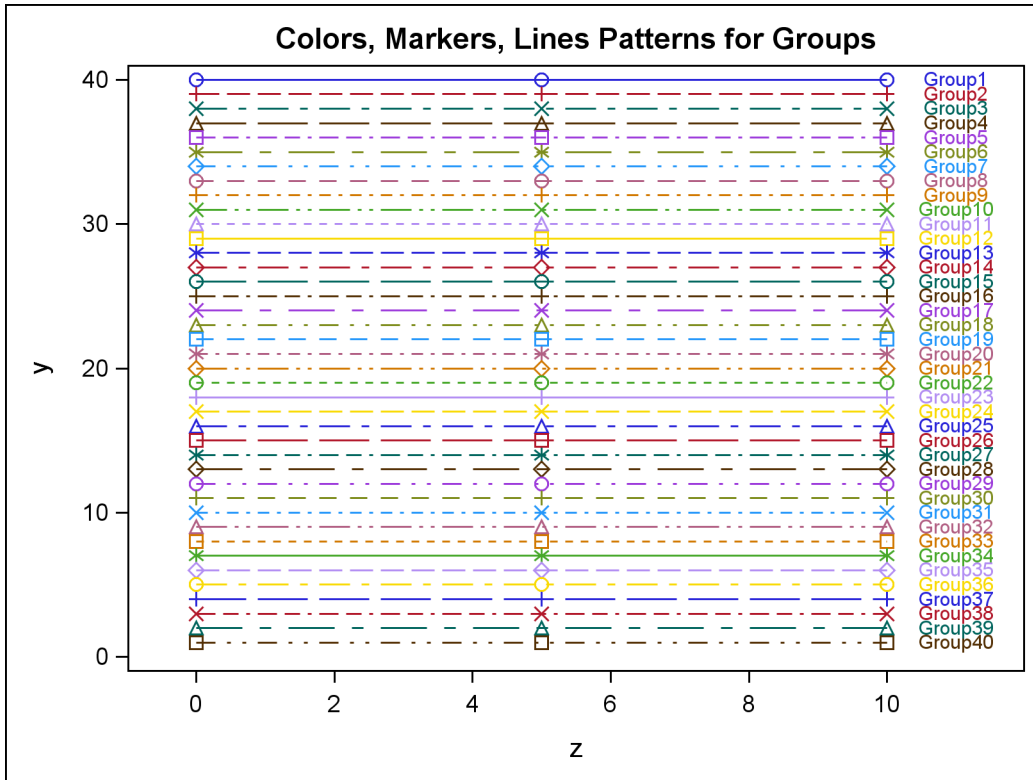


Figure 21.46 Markers, Lines, and Colors with Groups in the RTF Style

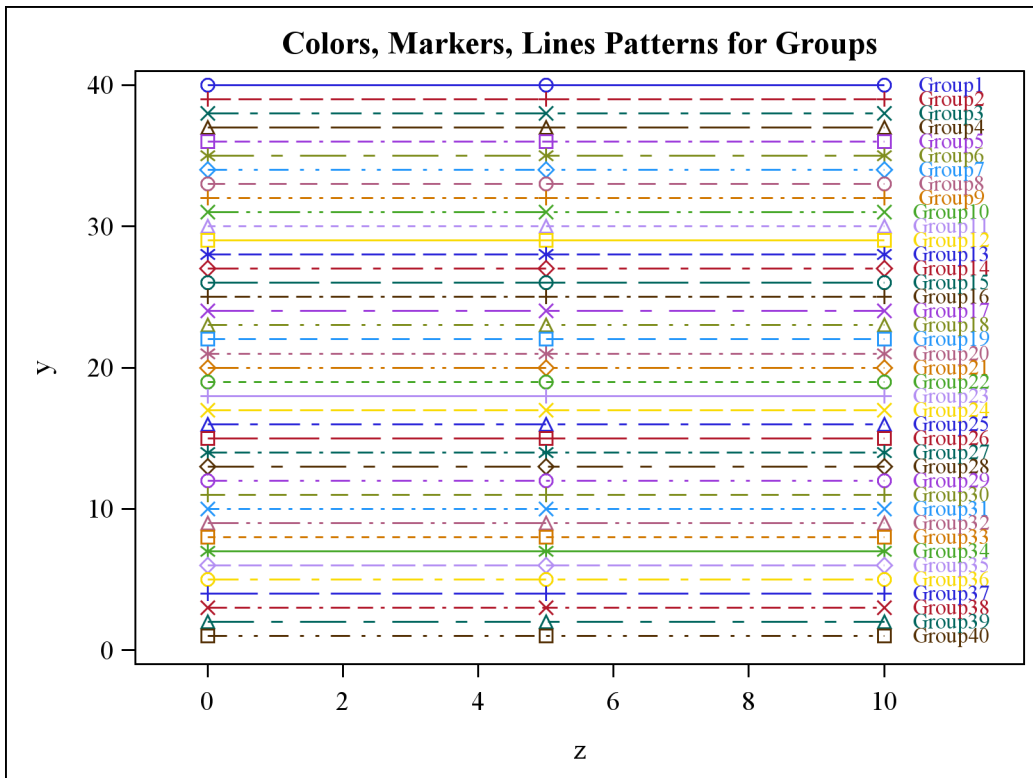


Figure 21.47 Markers, Lines, and Colors with Groups in the PEARL Style

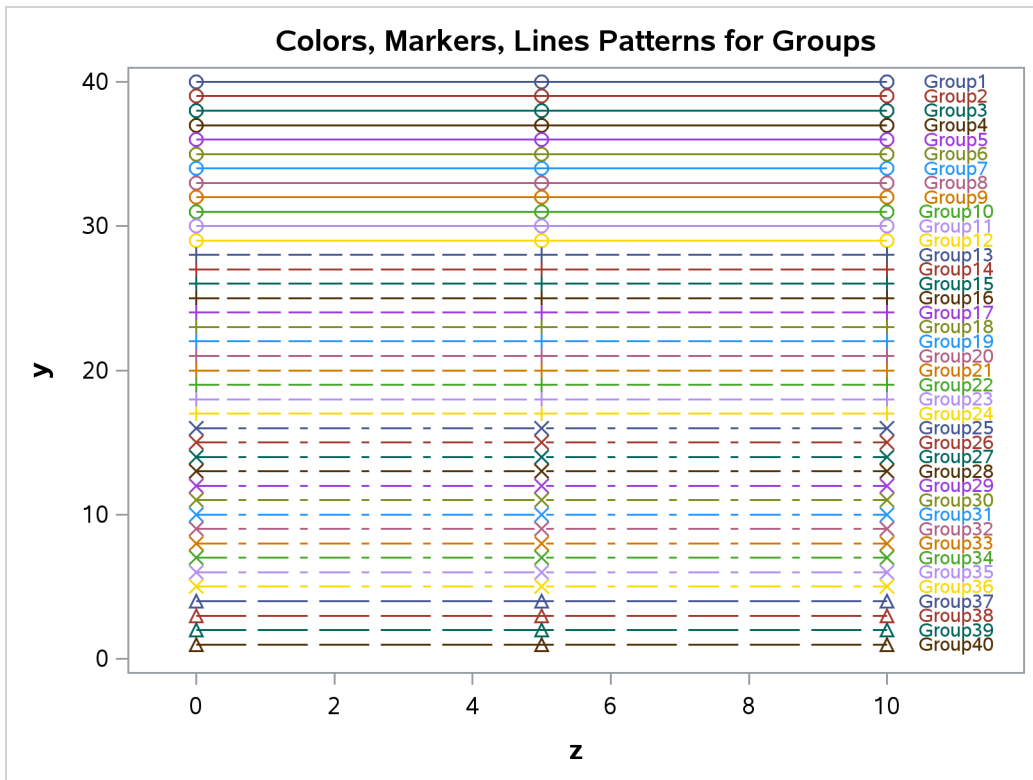
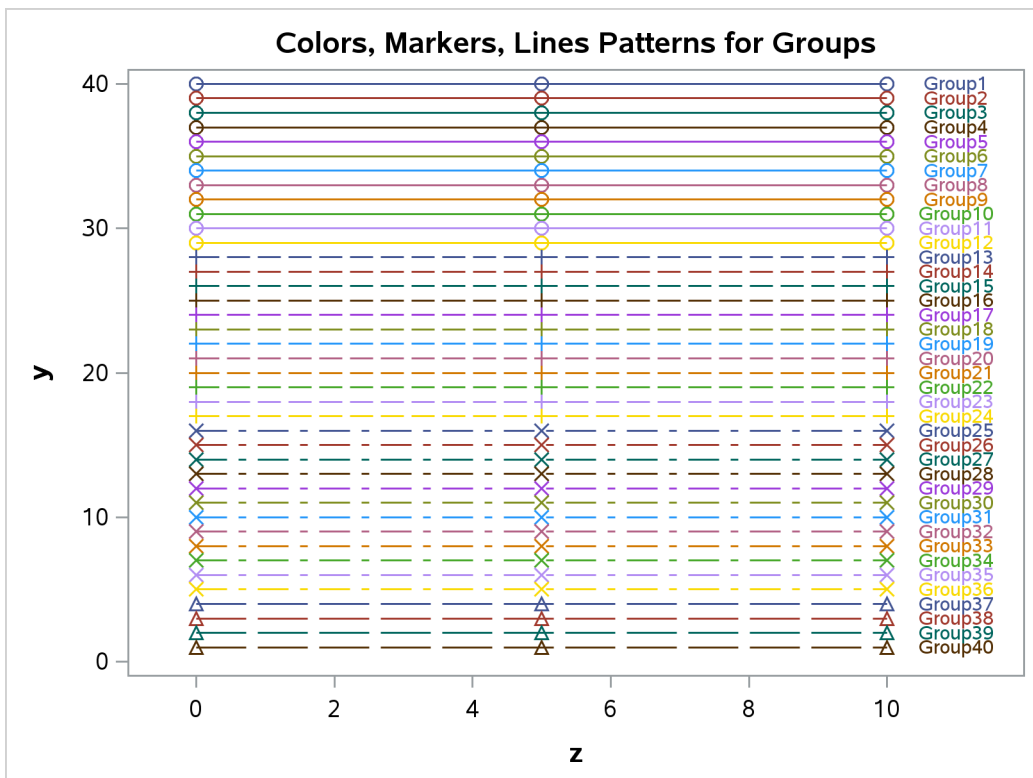


Figure 21.48 Markers, Lines, and Colors with Groups in the SAPPHIRE Style



Modifying the HTMLBLUE Style

The HTMLBLUE style is an all-color style for the first 12 groups of observations. After each set of 12 groups, the line style and marker change for the next 12 groups. See Figure 21.40. The HTMLBLUECML style is a color style in which groups of observations are distinguished by simultaneous color, line style, and symbol changes. See Figure 21.41. For some graphs, you might want more differentiation than you get in an all-color style like HTMLBLUE but without the overkill differentiation of the HTMLBLUECML style and other styles. This section defines four new styles for this purpose:

HTMLBLUEL – line styles and colors vary together with fixed markers for each set of 11 groups

HTMLBLUEM – markers and colors vary together with fixed line styles for each set of 11 groups

HTMLBLUEFL – line styles and colors vary together with fixed filled markers for each set of 11 groups

HTMLBLUEFM – filled markers and colors vary together with fixed line styles for each set of 5 groups

The following statements show part of the style definition for each of these styles:

```
define style Styles.HTMLBlueL;    parent = styles.htmlbluecml;
  style GraphFit2    from GraphFit2    /                               linestyle = 1;
  style GraphData1   from GraphData1   / markersymbol = "circle" linestyle = 1;
  style GraphData2   from GraphData2   / markersymbol = "circle" linestyle = 4;
  style GraphData3   from GraphData3   / markersymbol = "circle" linestyle = 8;
  style GraphData4   from GraphData4   / markersymbol = "circle" linestyle = 5;
  style GraphData5   from GraphData5   / markersymbol = "circle" linestyle = 14;
  style GraphData6   from GraphData6   / markersymbol = "circle" linestyle = 26;
  style GraphData7   from GraphData7   / markersymbol = "circle" linestyle = 15;
  style GraphData8   from GraphData8   / markersymbol = "circle" linestyle = 20;
  style GraphData9   from GraphData9   / markersymbol = "circle" linestyle = 41;
  style GraphData10  from GraphData10  / markersymbol = "circle" linestyle = 42;
  style GraphData11  from GraphData11  / markersymbol = "circle" linestyle = 2;
  style GraphData12  from GraphData12  / markersymbol = "square" linestyle = 1;
  style GraphData13  from GraphData1   / markersymbol = "square" linestyle = 4;
  style GraphData14  from GraphData2   / markersymbol = "square" linestyle = 8;
  style GraphData15  from GraphData3   / markersymbol = "square" linestyle = 5;
  . . .
end;
define style Styles.HTMLBlueM;    parent = styles.htmlbluecml;
  style GraphFit2    from GraphFit2    /                               linestyle = 1;
  style GraphData1   from GraphData1   / markersymbol = "circle"   linestyle = 1;
  style GraphData2   from GraphData2   / markersymbol = "square"  linestyle = 1;
  style GraphData3   from GraphData3   / markersymbol = "diamond" linestyle = 1;
  style GraphData4   from GraphData4   / markersymbol = "asterisk" linestyle = 1;
  style GraphData5   from GraphData5   / markersymbol = "plus"    linestyle = 1;
  style GraphData6   from GraphData6   / markersymbol = "triangle" linestyle = 1;
  style GraphData7   from GraphData7   / markersymbol = "circlefilled" linestyle = 1;
  style GraphData8   from GraphData8   / markersymbol = "starfilled" linestyle = 1;
  style GraphData9   from GraphData9   / markersymbol = "squarefilled" linestyle = 1;
  style GraphData10  from GraphData10  / markersymbol = "diamondfilled" linestyle = 1;
  style GraphData11  from GraphData11  / markersymbol = "trianglefilled" linestyle = 1;
  style GraphData12  from GraphData12  / markersymbol = "circle"   linestyle = 4;
  style GraphData13  from GraphData1   / markersymbol = "square"   linestyle = 4;
  style GraphData14  from GraphData2   / markersymbol = "diamond"  linestyle = 4;
  style GraphData15  from GraphData3   / markersymbol = "asterisk"  linestyle = 4;
  . . .
end;
```

```

define style Styles.HTMLBlueFL;    parent = styles.htmlbluecml;
  style GraphFit2    from GraphFit2    /                               linestyle = 1;
  style GraphData1  from GraphData1  / markersymbol = "circlefilled" linestyle = 1;
  style GraphData2  from GraphData2  / markersymbol = "circlefilled" linestyle = 4;
  style GraphData3  from GraphData3  / markersymbol = "circlefilled" linestyle = 8;
  style GraphData4  from GraphData4  / markersymbol = "circlefilled" linestyle = 5;
  style GraphData5  from GraphData5  / markersymbol = "circlefilled" linestyle = 14;
  style GraphData6  from GraphData6  / markersymbol = "circlefilled" linestyle = 26;
  style GraphData7  from GraphData7  / markersymbol = "circlefilled" linestyle = 15;
  style GraphData8  from GraphData8  / markersymbol = "circlefilled" linestyle = 20;
  style GraphData9  from GraphData9  / markersymbol = "circlefilled" linestyle = 41;
  style GraphData10 from GraphData10 / markersymbol = "circlefilled" linestyle = 42;
  style GraphData11 from GraphData11 / markersymbol = "circlefilled" linestyle = 2;
  style GraphData12 from GraphData12 / markersymbol = "starfilled"   linestyle = 1;
  style GraphData13 from GraphData1  / markersymbol = "starfilled"   linestyle = 4;
  style GraphData14 from GraphData2  / markersymbol = "starfilled"   linestyle = 8;
  style GraphData15 from GraphData3  / markersymbol = "starfilled"   linestyle = 5;
  . . .
end;
define style Styles.HTMLBlueFM;    parent = styles.htmlbluecml;
  style GraphFit2    from GraphFit2    /                               linestyle = 1;
  style GraphData1  from GraphData1  / markersymbol = "circlefilled" linestyle = 1;
  style GraphData2  from GraphData2  / markersymbol = "starfilled"   linestyle = 1;
  style GraphData3  from GraphData3  / markersymbol = "squarefilled"  linestyle = 1;
  style GraphData4  from GraphData4  / markersymbol = "diamondfilled"  linestyle = 1;
  style GraphData5  from GraphData5  / markersymbol = "trianglefilled"  linestyle = 1;
  style GraphData6  from GraphData6  / markersymbol = "circlefilled"  linestyle = 4;
  style GraphData7  from GraphData7  / markersymbol = "starfilled"   linestyle = 4;
  style GraphData8  from GraphData8  / markersymbol = "squarefilled"  linestyle = 4;
  style GraphData9  from GraphData9  / markersymbol = "diamondfilled"  linestyle = 4;
  style GraphData10 from GraphData10 / markersymbol = "trianglefilled"  linestyle = 4;
  style GraphData11 from GraphData11 / markersymbol = "circlefilled"  linestyle = 8;
  style GraphData12 from GraphData12 / markersymbol = "starfilled"   linestyle = 8;
  style GraphData13 from GraphData1  / markersymbol = "squarefilled"  linestyle = 8;
  style GraphData14 from GraphData2  / markersymbol = "diamondfilled"  linestyle = 8;
  style GraphData15 from GraphData3  / markersymbol = "trianglefilled"  linestyle = 8;
  . . .
end;

```

New `GraphData n` style elements are created that inherit colors from the `GraphData1` through `GraphData12` style elements. The line styles and markers are explicitly set in the new style definitions. The `style GraphFit2 from GraphFit2 / linestyle = 1` statement creates a solid second fit line. You can remove that statement if you prefer a dashed second fit line.

The following statements use SAS macros to generate these four new styles:

```

proc template;
  %let m = circle square diamond asterisk plus triangle circlefilled
          starfilled squarefilled diamondfilled trianglefilled;
  %let ls = 1 4 8 5 14 26 15 20 41 42 2;
  %macro makestyle;
    %let l = %eval(%sysfunc(mod(&k,12))+1);
    %let k = %eval(&k+1);
    style GraphData&k from GraphData&l /
      linestyle=%scan(&ls, &j) markersymbol="%scan(&m, &i)";
  %mend;

```

```

define style styles.HTMLBlueL;
  parent=styles.htmlbluecml;
  style GraphFit2 from GraphFit2 / linestyle = 1;
  %macro htmlblue1;
    %let k = 0;
    %do i = 1 %to 11; %do j = 1 %to 11; %makestyle %end; %end;
  %mend;
  %htmlblue1
end;
define style styles.HTMLBlueM;
  parent=styles.htmlbluecml;
  style GraphFit2 from GraphFit2 / linestyle = 1;
  %macro htmlbluem;
    %let k = 0;
    %do j = 1 %to 11; %do i = 1 %to 11; %makestyle %end; %end;
  %mend;
  %htmlbluem
end;
%let m = circlefilled starfilled squarefilled diamondfilled trianglefilled;
define style styles.HTMLBlueFL;
  parent=styles.htmlbluecml;
  style GraphFit2 from GraphFit2 / linestyle = 1;
  %macro htmlblue1;
    %let k = 0;
    %do i = 1 %to 5; %do j = 1 %to 11; %makestyle %end; %end;
  %mend;
  %htmlblue1
end;
define style styles.HTMLBlueFM;
  parent=styles.htmlbluecml;
  style GraphFit2 from GraphFit2 / linestyle = 1;
  %macro htmlbluem;
    %let k = 0;
    %do j = 1 %to 11; %do i = 1 %to 5; %makestyle %end; %end;
  %mend;
  %htmlbluem
end;
run;

```

The %LET *m* statement provides the list of markers. The %LET *ls* statement provides the list of line styles. The MAKESTYLE macro makes the *k*th style element from the **GraphData***n* style element for $n = \text{mod}(k - 1, 12) + 1$. The remaining macros vary markers and line styles in the appropriate order over the elements in each list.

The following step that was used in the section “Style Comparisons” on page 646 is used with the different styles to produce Figure 21.49 through Figure 21.52:

```

proc sgplot data=x2;
  title 'Colors, Markers, Lines Patterns for Groups';
  series y=y x=x / group=group markers;
  scatter y=y x=z / group=group markerchar=1;
run;

```

Figure 21.49 Markers, Lines, and Colors with Groups in the HTMLBLUEL Style

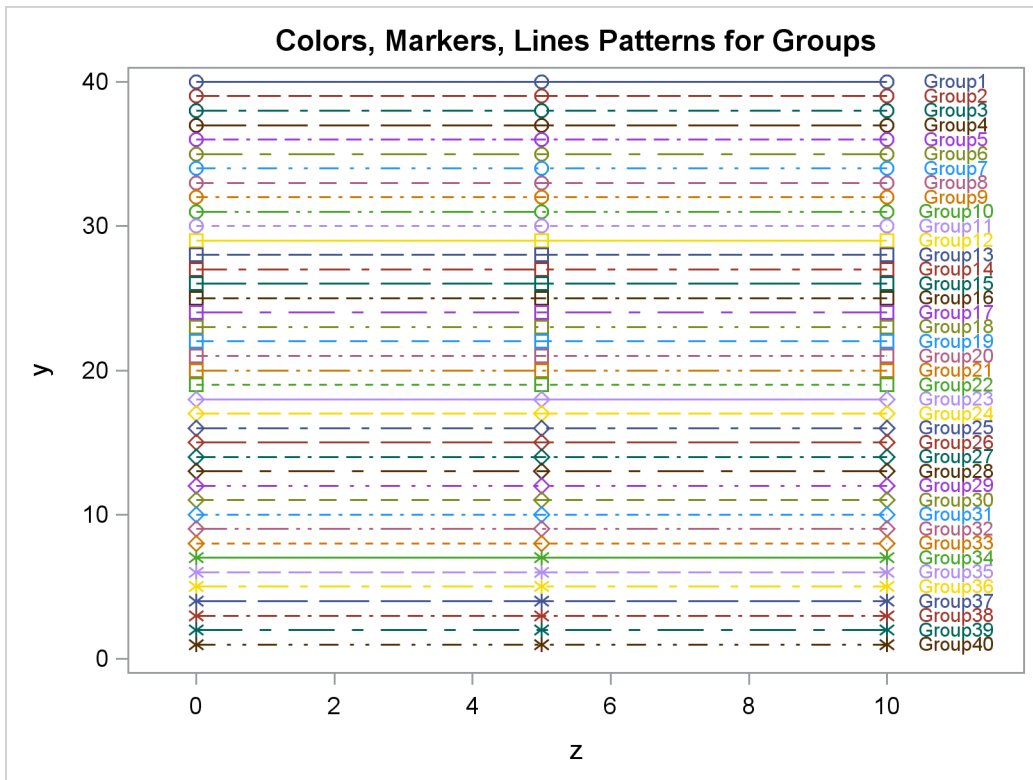


Figure 21.50 Markers, Lines, and Colors with Groups in the HTMLBLUEM Style

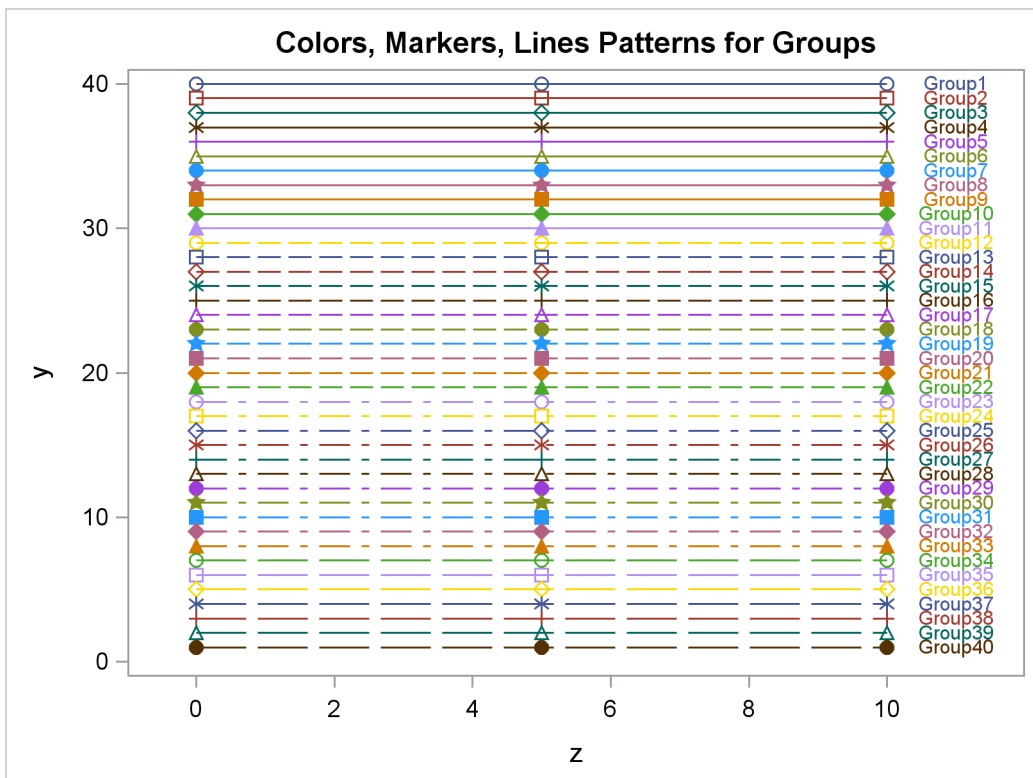


Figure 21.51 Markers, Lines, and Colors with Groups in the HTMLBLUEFL Style

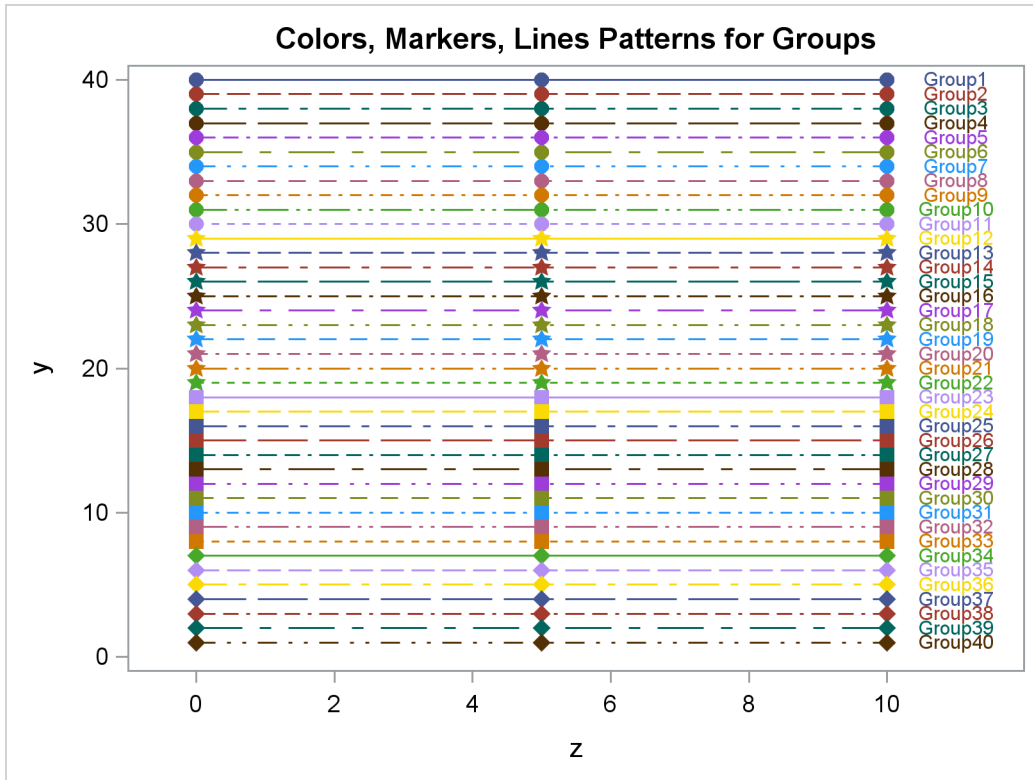
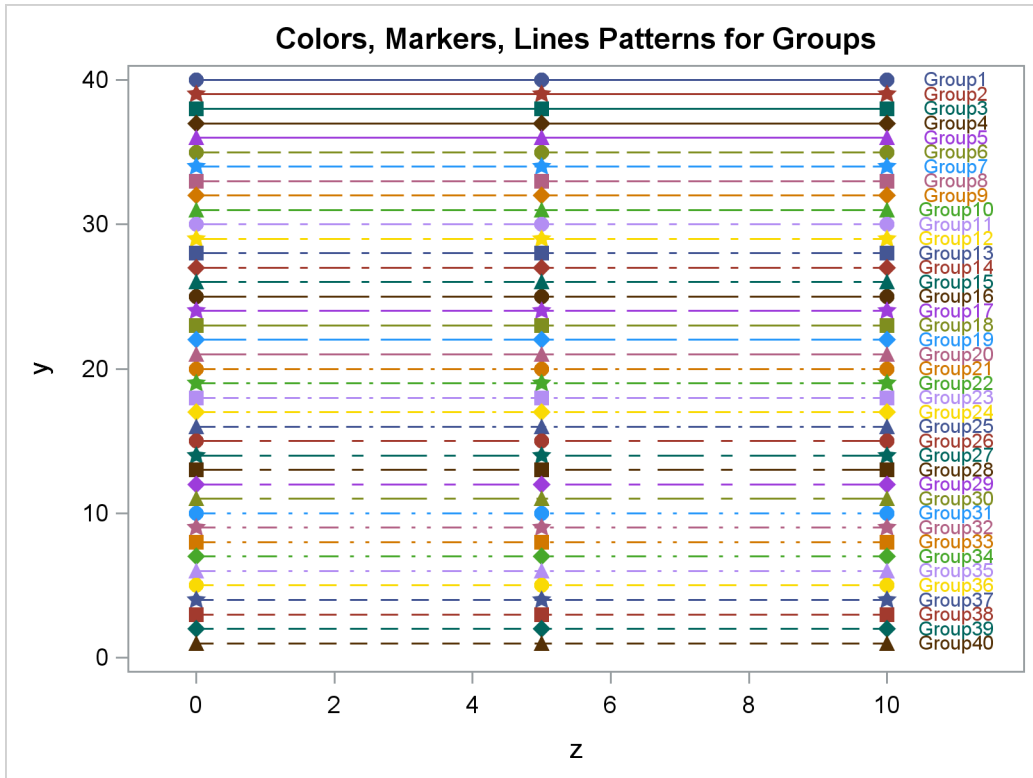


Figure 21.52 Markers, Lines, and Colors with Groups in the HTMLBLUEFM Style



Style Template Modification Macro

The `%ModStyle` macro provides easy ways to customize the style elements (`GraphData1–GraphDatan`) that control how groups of observations are distinguished. Examples of using the `%ModStyle` macro can be found in the sections “Creating an All-Color Style” on page 669 and “Changing the Default Markers and Lines” on page 671. Also see Kuhfeld (2009) for more information about this macro.

You do not need to include autocall macros (for example, with a `%include` statement). You can call them directly once they are properly installed. If your site has installed the autocall libraries supplied by the SAS System and uses the standard configuration of SAS software, you need to ensure that the SAS system option MAUTOSOURCE is in effect to begin using the autocall macros. For more information about autocall libraries, see the *SAS Macro Language: Reference*. For details about installing autocall macros, consult your host documentation.

The `%ModStyle` macro has the following options:

COLORS=*color-list*

specifies a space-delimited list of colors for markers and lines. If you do not specify this option, then the colors from the parent style are used. You can specify the colors using any SAS color notation such as `CXrrggbb`.

`COLORS=GRAYS` generates seven distinguishable grayscale colors from blackest to whitest. The colors should be mixed up to be more easily distinguished when you need fewer colors, but you can do that with your own `COLORS=` list. The HLS (hue/light/saturation) coding generates colors by setting hue and saturation to 0 and incrementing the lightness for each gray. You can also use the keywords `BLUES`, `PURPLES`, `MAGENTAS`, `REDS`, `ORANGES`, `YELLOWS`, `GREENS`, and `CYANS` to generate seven colors with a fixed hue and a saturation of AA (hex).

`COLORS=SHADES INT` generates seven colors as described previously, except that you specify an integer $0 \leq \text{INT} < 360$. See *SAS/GRAPH: Reference*. The available hues include: `GRAY`, `GREY`, `BLUE=0`, `PURPLE=30`, `MAGENTA=60`, `RED=120`, `ORANGE=150`, `YELLOW=180`, `GREEN=240`, and `CYAN=300`.

DISPLAY=*n*

specifies whether to display the generated template. By default, the template is not displayed. Specify `DISPLAY=1` to display the generated template.

FILLCOLORS=*color-list*

specifies a space-delimited list of colors for bands and fills. If you do not specify this option, then the colors from the parent style are used.

Fill colors from the parent style are designed to work well with the colors from the parent style. If you specify a `COLORS=` list, then you might want to redefine the `FILLCOLORS=` list as well. You need to have at least as many fill colors as you have colors (any extra fill colors are ignored). Two shortcuts are available: `FILLCOLORS=COLORS` uses the `COLORS=` colors for the fills (your confidence bands should have transparency for this to be useful) and `FILLCOLORS=LIGHTCOLORS` modifies the lightness associated with each color generated by `COLORS=SHADES` (this is allowed only with `COLORS=SHADES`).

LINESTYLES=*line-style-list*

specifies a space-delimited list of line styles. The default is:

```
LineStyle=Solid MediumDash MediumDashShortDash LongDash
DashDashDot LongDashShortDash DashDotDot Dash
ShortDashDot MediumDashDotDot ShortDash
```

Line style numbers can range from 1 to 46. Some line styles have names associated with them. You can specify either the name or the number for the following number/name pairs: 1 Solid, 2 ShortDash, 4 MediumDash, 5 LongDash, 8 MediumDashShortDash, 14 DashDashDot, 15 DashDotDot, 20 Dash, 26 LongDashShortDash, 34 Dot, 35 ThinDot, 41 ShortDashDot, and 42 MediumDashDotDot.

MARKERS=*marker-list*

specifies a space-delimited list of marker symbols. By default, **Markers=Circle Plus X Triangle Square Asterisk Diamond**. The available marker symbols are listed in *SAS/GRAPH: Graph Template Language Reference*. Two shortcuts are available: **MARKERS=FILLED** is an alias for the specification **Markers=CircleFilled TriangleFilled SquareFilled DiamondFilled StarFilled HomeDownFilled**, and **MARKERS=EMPTY** is an alias for the specification **Markers=Circle Triangle Square Diamond Star HomeDown**.

NAME=*style-name*

specifies the name of the new style that you are creating. This name is used when you specify the style in an ODS destination statement (for example, ODS HTML STYLE=*style-name*). The default is **NAME=NEWSTYLE**.

NUMBEROFGROUPS=*n*

specifies *n*, the number of **GraphData n** style elements to create. The **GraphData1–GraphData n** style elements contain *n* combinations of colors, markers, and line styles. By default, 32 combinations are created.

PARENT=*style-name*

specifies the parent style. The new style inherits most of its attributes from the parent style. The default is **PARENT=DEFAULT** (which is one of the default styles for HTML and the parent style for all of the styles that are recommended for statistical graphics). If your goals are to change colors or create an all-color style, you can use any style as the parent style. However, if your goal is to change markers or line styles without creating an all-color style, do not use the **HTMLBLUE** style as a parent. The **HTMLBLUE** style is an all-color style that is different from most other styles due to its use of the **ATTRPRIORITY=** style option.

TYPE=*type-specification*

specifies how your new style cycles through colors, markers, and line styles. The default is **TYPE=LMbyC**.

These first three methods work well with all plots, because cycling line styles and markers together ensures that both scatterplot markers and series plot lines are distinguishable:

CLM

cycles through colors, line styles, and markers simultaneously. The first group uses the first color, line style, and marker; the second group uses the second color, line style, and marker; and so on. This is the method used by the ODS Graphics styles.

LMbyC

fixes line style and marker, cycles through colors, and then moves to the next line style and marker. This is the default and creates a style where the first groups are distinguished entirely by color.

CbyLM

fixes color, cycles through line style and marker, and then moves to the next color. This option uses the smaller of the number of line styles or the number of markers when cycling within a color.

The following two methods might not work well with all plots:

CbyLbyM

fixes color and line style, then cycles through markers, increments line style, and then cycles through markers. After all line styles have been used, then this option moves to the next color and continues.

LbyMbyC

fixes line style and marker, then cycles through colors, increments marker, and then cycles through colors. After all markers have been used, then this option moves to the next line style and continues. This is closest to the legacy SAS/GRAPH method.

Creating an All-Color Style

Many styles are designed to make color plots where lines, functions, and groups of observations can be distinguished even when the plot is sent to a black-and-white printer. Hence, lines differ not only in color but also in pattern. Similarly, markers differ in both color and symbol. This is not true with the HTMLBLUE, PEARL, and SAPPHIRE styles, which are all-color styles.

You can easily modify any style to be an all-color style by using the ATTRPRIORITY= option. For example:

```
proc template;
  define style styles.StatColor;
    parent = statistical;
    style Graph from Graph / attrpriority = "Color";
  end;
run;
```

Alternatively, you can make an all-color style with the %MODSTYLE autocall macro. It creates a new style by modifying a parent style and reordering the colors, line patterns, and marker symbols in the **GraphData** style elements (see the section “[Some Common Style Elements](#)” on page 640). By default, the macro creates a new style that distinguishes lines and groups only by color. The macro is documented in the section “[Style Template Modification Macro](#)” on page 667.

The following example illustrates the default use of the macro and is taken from the section “[Fitting a Curve through a Scatter Plot](#)” on page 8154 of Chapter 97, “[The TRANSREG Procedure](#).” The data come from an experiment in which nitrogen oxide emissions from a single cylinder engine are measured for various combinations of fuel and equivalence ratio. This gas data set is available from the Sashelp library.

The following statements fit separate curves for each group and produce [Figure 21.53](#) and [Figure 21.54](#):


```
ods graphics on;
ods listing style=statistical;

proc transreg data=sashelp.Gas ss2 plots=transformation lprefix=0;
  model identity(nox) = class(Fuel / zero=none) * pbspline(EqRatio);
run;

%modstyle(parent=statistical, name=StatColor)
ods listing style=StatColor;

proc transreg data=sashelp.Gas ss2 plots=transformation lprefix=0;
  model identity(nox) = class(Fuel / zero=none) * pbspline(EqRatio);
run;
```

The first PROC TRANSREG step uses the STATISTICAL style to create the fit plot in Figure 21.53, which uses different colors, line patterns, and markers for each group. Then the macro creates a new style, called STATCOLOR, that inherits its characteristics from the STATISTICAL style. Only the attributes of the lines and markers are changed. In Figure 21.54, which is created with the modified style, the groups are differentiated only by color. This is the easiest and most common way for you to use this macro. However, you can use it to perform other style modifications as illustrated in the section “Changing the Default Markers and Lines” on page 671. The macro is documented in the section “Style Template Modification Macro” on page 667.

Figure 21.53 Fit Plot with the STATISTICAL Style

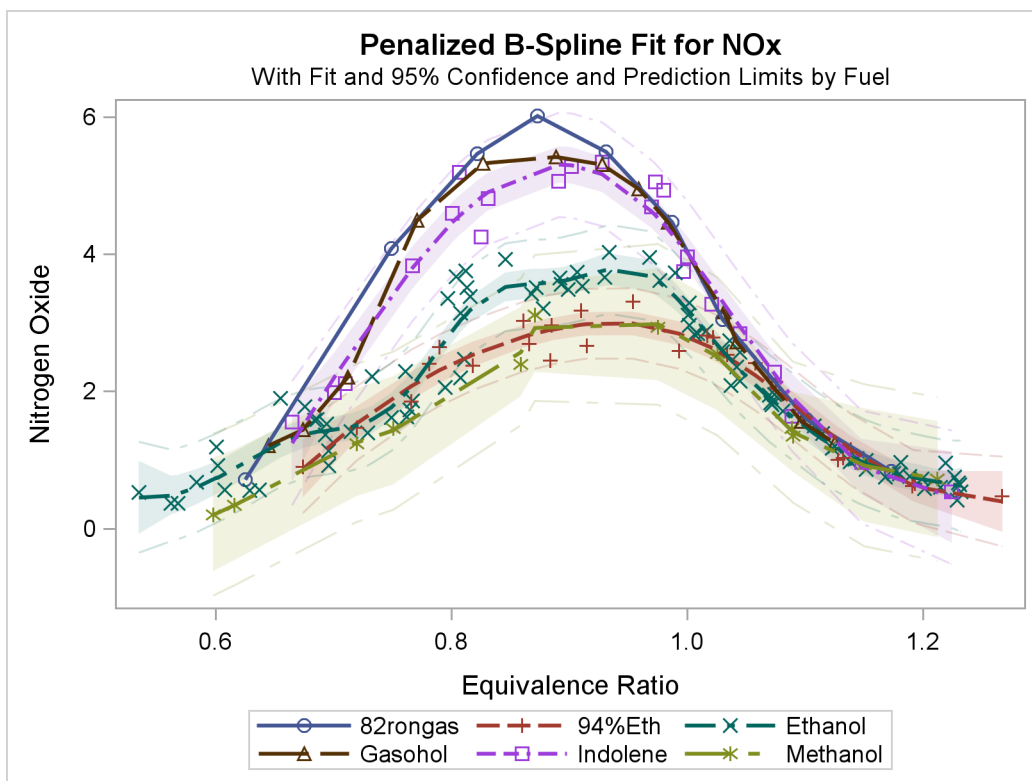
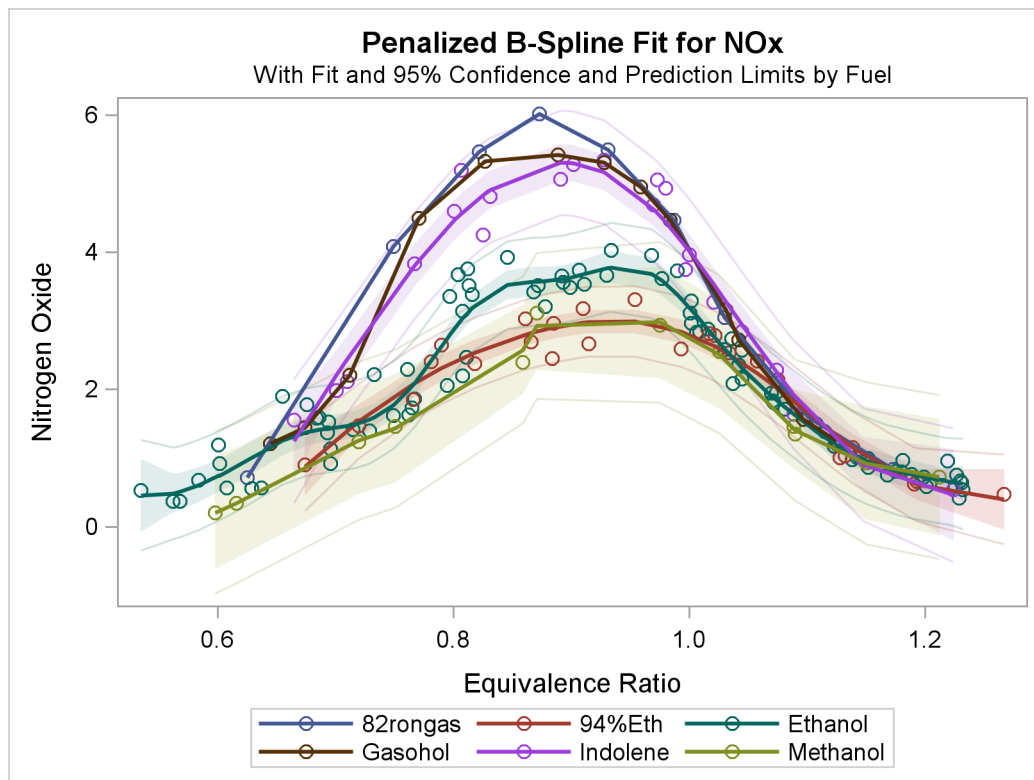


Figure 21.54 Fit Plot with the Modified Style

Changing the Default Markers and Lines

The preceding section shows how to use the `%MODSTYLE` autocall macro to create an all-color style. You can also use the `%MODSTYLE` macro to change markers and line styles. This example creates a new style called `MARKSTYLE` that inherits from the `STATISTICAL` style but uses a different set of markers. The following statements create artificial data, change the marker list, and display the results:

```
data x;
  do g = 1 to 12;
    do x = 1 to 10;
      y = 13 - g + sin(x * 0.1 * g);
      output;
    end;
  end;
run;

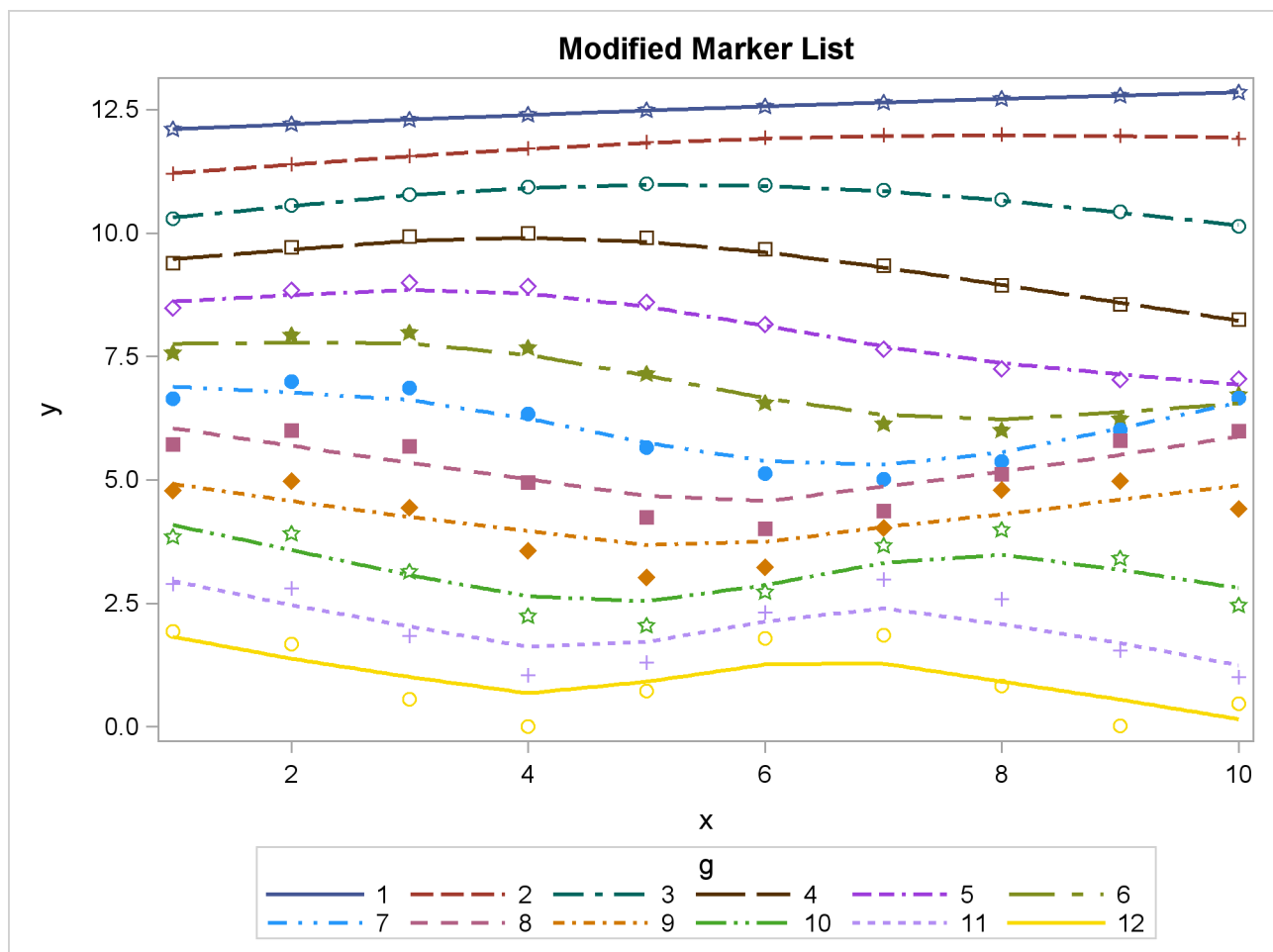
%modstyle(name=markstyle, parent=statistical, type=CLM,
          markers=star plus circle square diamond starfilled
              circlefilled squarefilled diamondfilled)

ods listing style=markstyle;
```

```
proc sgplot;
  title 'Modified Marker List';
  loess y=y x=x / group=g;
run;
```

The NAME= option specifies the new style name, and the PARENT= option specifies the parent style. The TYPE= option controls the method of cycling through colors, lines, and markers. The default, TYPE=LMbyC, fixes (holds constant) the line styles and markers, while cycling through the color list. This is illustrated in the section “Creating an All-Color Style” on page 669. This example uses TYPE=CLM to cycle through colors, line styles, and markers (holding none of them fixed). Other TYPE= values are described in the section “Style Template Modification Macro” on page 667. The values specified with the TYPE= option are case-sensitive (‘by’ is lower case and the ‘L’, ‘C’, and ‘M’ are upper case). The new marker list is specified with the MARKERS= option. The results are displayed in Figure 21.55. The marker list is reused in the tenth and subsequent groups since only nine markers are defined.

Figure 21.55 A Modified Style with a New List of Markers



The following statements create a new style called `LINESTYLE` that inherits from the `STATISTICAL` style and changes the line list:

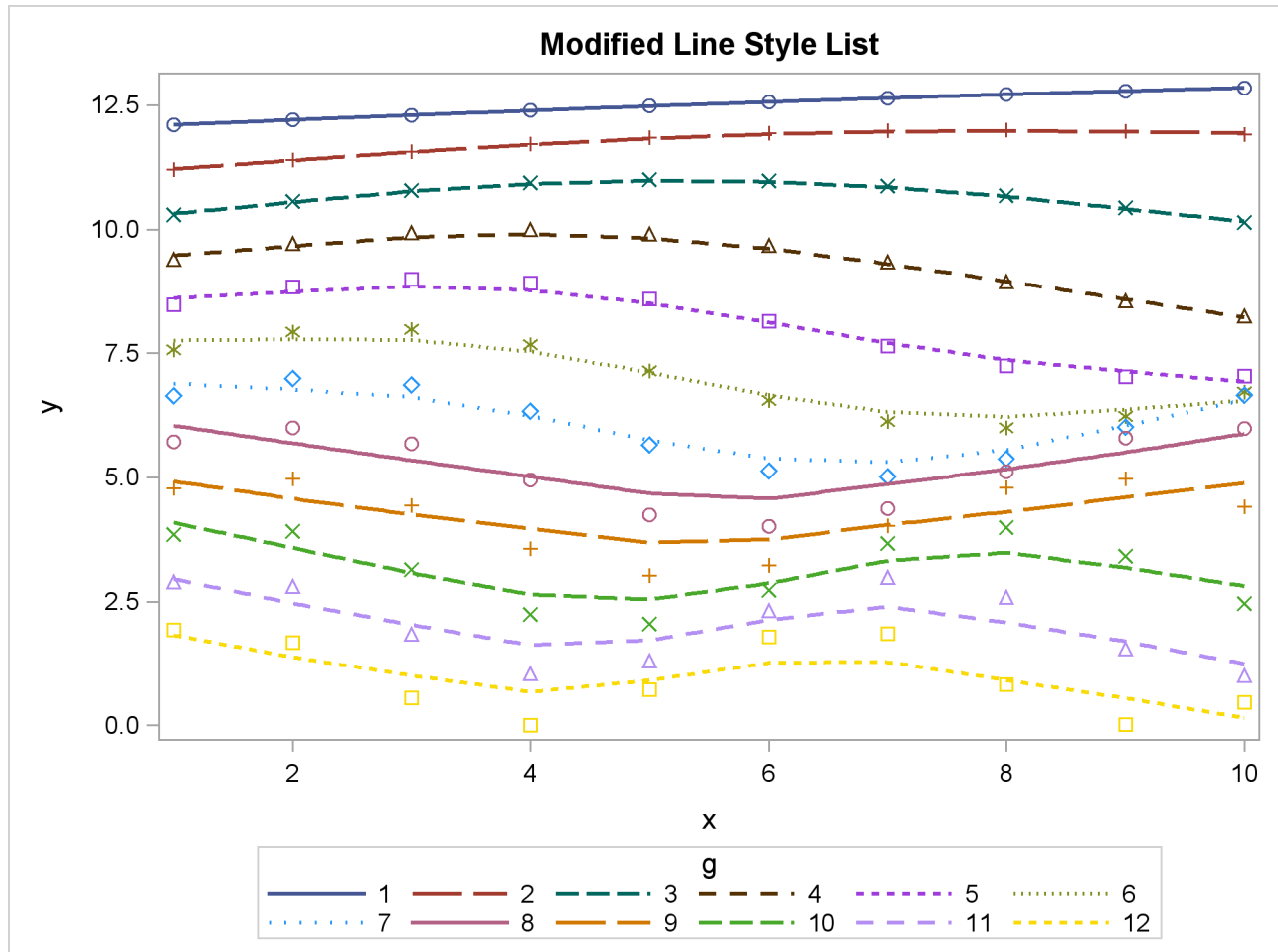
```
%modstyle(name=linestyle, parent=statistical, type=CLM,
          linestyle=Solid LongDash MediumDash Dash ShortDash Dot ThinDot)

ods listing style=linestyle;

proc sgplot;
  title 'Modified Line Style List';
  loess y=y x=x / group=g;
run;
```

The new line list is specified with the `LINESTYLES=` option. The results are displayed in [Figure 21.56](#). In this example, each of the first seven groups uses a dash pattern that is shorter than the previous group. The line list is reused in the eighth and subsequent groups since only seven line patterns are defined.

Figure 21.56 Modified Style with a New List of Line Styles



You can learn more about style modification by examining the new styles, as in the following example:

```
proc template;
  source styles.markstyle;
  source styles.linestyle;
run;
```

The results show the definitions of **GraphData1** through **GraphData32** that the macro created. An abridged listing of the results follows:

```
define style Styles.Markstyle;
  parent = Styles.statistical;
  . . .
  style GraphData1 /
    markersymbol = "star"
    linestyle = 1
    contrastcolor = ColorStyles('c1')
    color = FillStyles('f1');
  . . .
  style GraphData32 /
    markersymbol = "diamond"
    linestyle = 42
    contrastcolor = ColorStyles('c8')
    color = FillStyles('f8');
end;

define style Styles.Linestyle;
  parent = Styles.statistical;
  . . .
  style GraphData1 /
    markersymbol = "circle"
    linestyle = 1
    contrastcolor = ColorStyles('c1')
    color = FillStyles('f1');
  . . .
  style GraphData32 /
    markersymbol = "triangle"
    linestyle = 20
    contrastcolor = ColorStyles('c8')
    color = FillStyles('f8');
end;
```

You can use the **NUMBEROFGROUPS=** option in the **%MODSTYLE** macro to control the number of **GraphData*n*** style elements created in the new style.

Modifying Graph Fonts in Styles

You can modify an ODS style to customize the general appearance of plots produced with ODS Graphics, just as you can modify a style to customize the general appearance of ODS tables. This section shows you how to customize fonts used in graphs. The following step displays the HTMLBLUE style and its parent styles, STATISTICAL and DEFAULT:

```
proc template;
  source Styles.HTMLBlue;
  source Styles.Statistical;
  source Styles.Default;
run;
```

If you search for ‘font’, you find the style elements that control graph fonts:

```
style GraphFonts /
  'GraphDataFont' = ("<sans-serif>, <MTsans-serif>", 7pt)
  'GraphUnicodeFont' = ("<MTsans-serif-unicode>", 9pt)
  'GraphValueFont' = ("<sans-serif>, <MTsans-serif>", 9pt)
  'GraphLabel2Font' = ("<sans-serif>, <MTsans-serif>", 10pt)
  'GraphLabelFont' = ("<sans-serif>, <MTsans-serif>", 10pt)
  'GraphFootnoteFont' = ("<sans-serif>, <MTsans-serif>", 10pt)
  'GraphTitleFont' = ("<sans-serif>, <MTsans-serif>", 11pt, bold)
  'GraphTitle1Font' = ("<sans-serif>, <MTsans-serif>", 14pt, bold)
  'GraphAnnoFont' = ("<sans-serif>, <MTsans-serif>", 10pt);
```

The fonts **GraphTitle1Font** and **GraphLabel2Font** are not used with ODS Graphics. The following fonts are the ones typically used for the text in most graphs:

- **GraphDataFont** is the smallest font. It is used for text that needs to be small (labels for points in scatter plots, labels for contours, and so on)
- **GraphValueFont** is the next largest font. It is used for axis value (tick marks) labels and legend entry labels.
- **GraphLabelFont** is the next largest font. It is used for axis labels and legend titles.
- **GraphFootnoteFont** is the next largest font. It is used for all footnotes.
- **GraphTitleFont** is the largest font. It is used for all titles.
- **GraphUnicodeFont** is used for special characters. See the section “Unicode and Special Characters” on page 742.

The following statements define a style named NEWSTYLE that replaces the graph fonts in the DEFAULT style with italic Times New Roman fonts, which are available with the Windows operating system:

```
proc template;
  define style Styles.NewStyle;
    parent=Styles.Statistical;
    replace GraphFonts /
      'GraphDataFont'      = ("<MTserif>, Times New Roman", 7pt)
      'GraphUnicodeFont'  = ("<MTserif>, Times New Roman", 9pt)
      'GraphValueFont'    = ("<MTserif>, Times New Roman", 9pt)
      'GraphLabel2Font'   = ("<MTserif>, Times New Roman", 10pt)
      'GraphLabelFont'    = ("<MTserif>, Times New Roman", 10pt)
      'GraphFootnoteFont' = ("<MTserif>, Times New Roman", 10pt)
      'GraphTitleFont'    = ("<MTserif>, Times New Roman", 11pt)
      'GraphTitle1Font'   = ("<MTserif>, Times New Roman", 14pt)
      'GraphAnnoFont'     = ("<MTserif>, Times New Roman", 10pt);
  end;
run;
```

For more information about the DEFINE, PARENT, and REPLACE statements, see the *SAS/GRAPH: Graph Template Language Reference*.

The “Getting Started” section of Chapter 80, “The ROBUSTREG Procedure,” creates the following data set to illustrate the use of the PROC ROBUSTREG for robust regression:

```
data stack;
  input x1 x2 x3 y @@;
  datalines;
80 27 89 42   80 27 88 37   75 25 90 37   62 24 87 28   62 22 87 18
62 23 87 18   62 24 93 19   62 24 93 20   58 23 87 15   58 18 80 14
58 18 89 14   58 17 88 13   58 18 82 11   58 19 93 12   50 18 89 8
50 18 86 7    50 19 72 8    50 19 79 8    50 20 80 9    56 20 82 15
70 20 91 15
;
```

The following statements create a Q-Q plot that uses the HTMLBLUE style (see Figure 21.57) and the NEWSTYLE style (see Figure 21.58):

```
ods listing style=HTMLBlue;
ods graphics on;

proc robustreg data=stack plots=qqplot;
  ods select QQPlot;
  model y = x1 x2 x3;
run;

ods listing close;
ods listing style=NewStyle;

proc robustreg data=stack plots=qqplot;
  ods select QQPlot;
  model y = x1 x2 x3;
run;
```

Figure 21.57 Q-Q Plot That Uses the HTMLBLUE Style

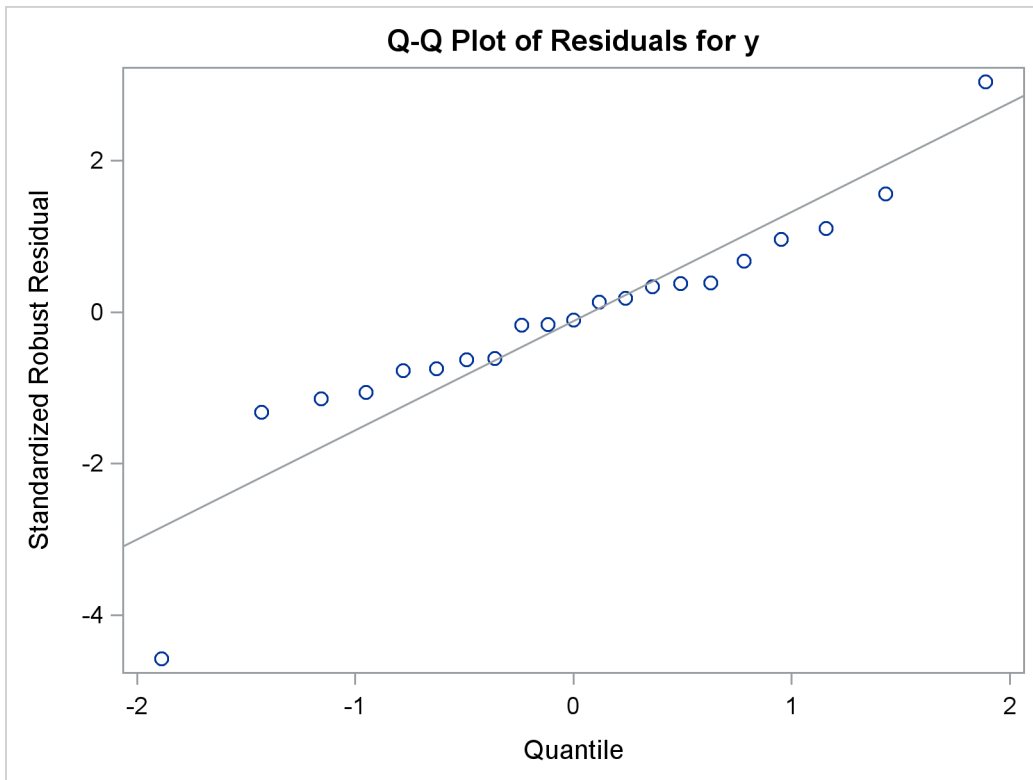
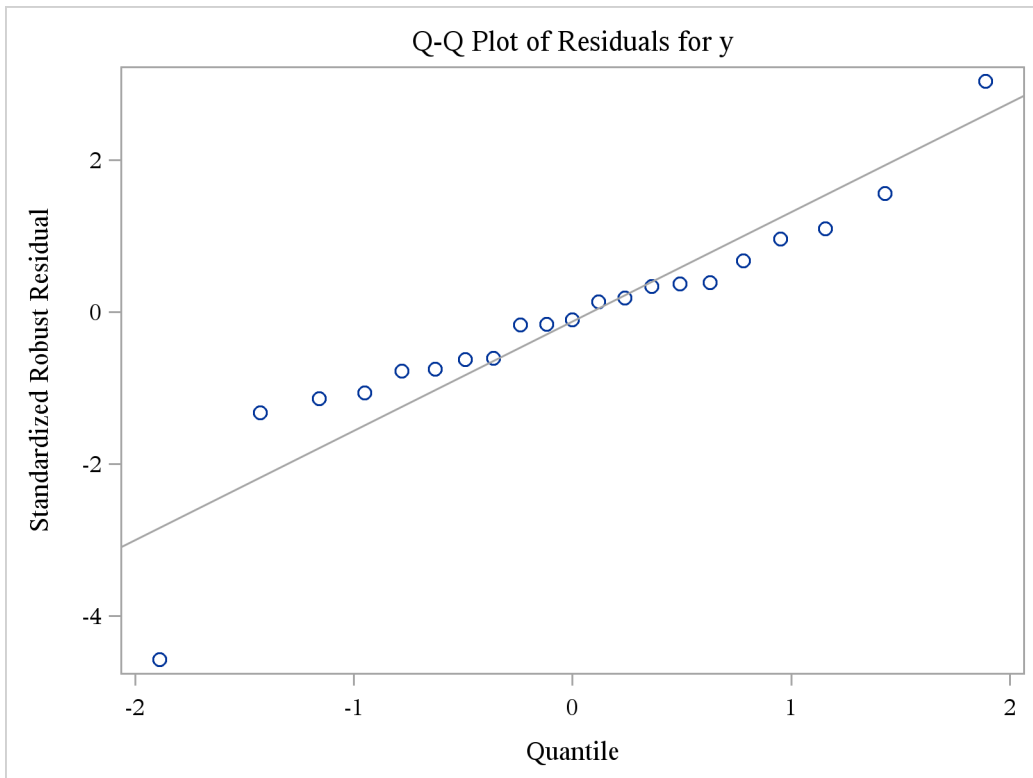


Figure 21.58 Q-Q Plot That Uses the NEWSTYLE Style



Although this example illustrates the use of a style with graphical output from a particular procedure, a style is applied to *all* of your output (graphs and tables) in the destination for which you specify the style. See the section “[Changing the Default Style](#)” on page 680 for information about specifying a default style for all your output.

Modifying Other Graph Elements in Styles

This section illustrates how to modify other style elements for graphics, specifically the style element **GraphReference**, which controls the attributes of reference lines. You can run the following statements to learn more about the **GraphReference** style element:

```
proc template;
  source styles.HTMLBlue;
run;
```

The following are the first two lines of the source listing:

```
define style Styles.HTMLBlue;
  parent = styles.statistical;
```

There is no mention of **GraphReference** in the complete listing of the source because **GraphReference** is inherited from a parent style. Most styles inherit many of their attributes from other styles. To find out more, you must list the parent style, as in the following example:

```
proc template;
  source styles.statistical;
run;
```

Most styles that you typically use with ODS Graphics inherit most of their attributes from only one style, the **DEFAULT** style. The **HTMLBLUE** style inherits from the **STATISTICAL** style, which inherits from the **DEFAULT** style. A few of the other styles inherit from several parents. You might have to repeat this process multiple times to find the first parent. The following step displays the **HTMLBLUE** style and its parent styles, **STATISTICAL** and **DEFAULT**:

```
proc template;
  source Styles.HTMLBlue;
  source Styles.Statistical;
  source Styles.Default;
run;
```

Styles are listed in the order: style of interest, then its parent, and then its grandparent. If you search the results from the top, you will find the most recent specification of a style element first. The `GraphReference` style element is defined as follows:

```
class GraphReference /
  linethickness = 1px
  linestyle = 1
  contrastcolor = GraphColors('referencelines');
```

To specify a line thickness of 4 pixels for all reference lines, add the following statement to the definition of the `NEWSTYLE` style in the section “[Modifying Graph Fonts in Styles](#)” on page 675:

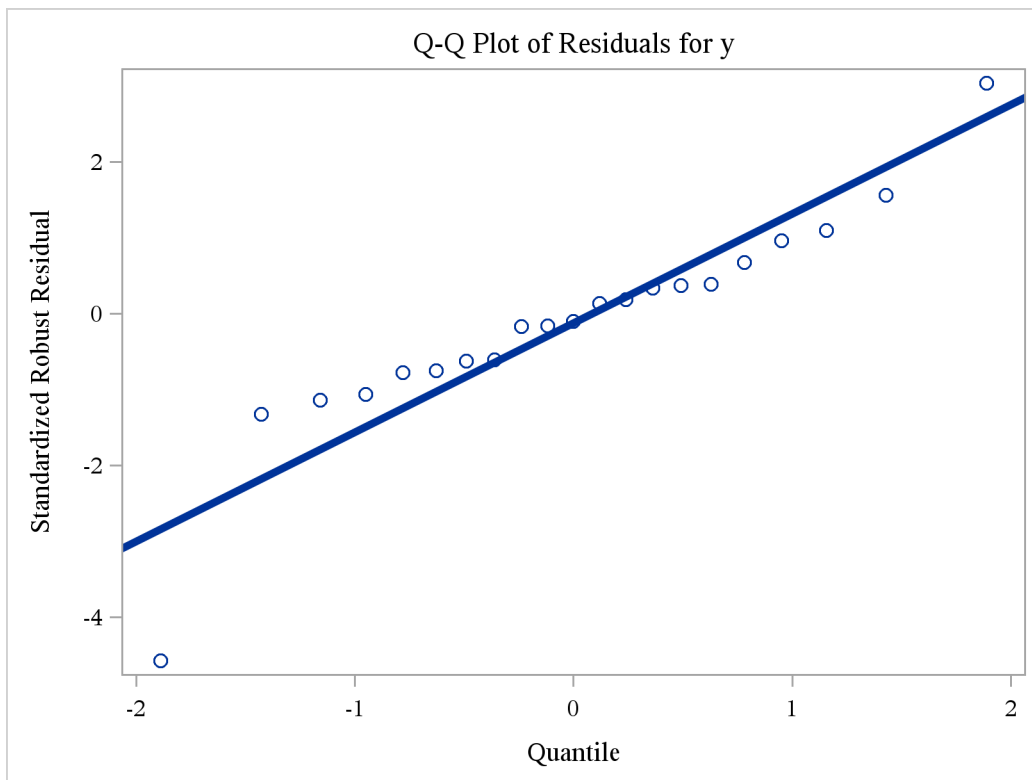
```
replace GraphReference / linethickness=4px;
```

The following statements modify the style and produce the Q-Q plot shown in [Figure 21.59](#):

```
proc template;
  define style Styles.NewStyle;
    parent=Styles.Statistical;
    replace GraphFonts /
      'GraphDataFont' = ("<MTserif>, Times New Roman", 7pt)
      'GraphUnicodeFont' = ("<MTserif>, Times New Roman", 9pt)
      'GraphValueFont' = ("<MTserif>, Times New Roman", 9pt)
      'GraphLabel2Font' = ("<MTserif>, Times New Roman", 10pt)
      'GraphLabelFont' = ("<MTserif>, Times New Roman", 10pt)
      'GraphFootnoteFont' = ("<MTserif>, Times New Roman", 10pt)
      'GraphTitleFont' = ("<MTserif>, Times New Roman", 11pt)
      'GraphTitle1Font' = ("<MTserif>, Times New Roman", 14pt)
      'GraphAnnoFont' = ("<MTserif>, Times New Roman", 10pt);
    replace GraphReference / linethickness=4px;
  end;
run;

ods listing style=NewStyle;
ods graphics on;

proc robustreg data=stack plots=qqplot;
  ods select QQPlot;
  model y = x1 x2 x3;
run;
```

Figure 21.59 Q-Q Plot That Uses the NEWSTYLE Style with a Thicker Line

You can use this approach to modify other attributes of the line, such as **LineStyle** and **ContrastColor**. These style modifications apply to all graphs that display reference lines, and not just to Q-Q plots produced by PROC ROBUSTREG. You can control the attributes of specific graphs by modifying the graph template, as discussed in the section “[Graph Templates](#)” on page 706 in Chapter 22, “[ODS Graphics Template Modification](#).” Values specified directly in a graph template override style attributes.

When you are done with the NEWSTYLE style, you do not need to restore the HTMLBLUE style template since you did not modify it. Rather, you inherited from the HTMLBLUE style.

Changing the Default Style

The default style for each ODS destination is specified in the SAS Registry. For example, the default style for the HTML destination is DEFAULT (or HTMLBLUE in the SAS windowing environment) and the default style for the RTF destination is RTF. You can specify a default style for all of your output in a particular ODS destination. This is useful if you want to use a different SAS style, if you have modified one of the styles supplied by the SAS System (see the section “[Style Templates and Colors](#)” on page 639), or if you have defined your own style. For example, you can specify the JOURNAL style as the default style for RTF output.

The recommended approach for specifying a default style is as follows. Open the SAS Registry Editor by typing **regedit** on the command line. Expand the node **ODS ► DESTINATIONS** and select a destination (for example, select **RTF**). Double-click the **Selected Style** item, shown in [Figure 21.60](#), and specify a style. This can be any style supplied by the SAS System or a user-defined style, as long as it can be found with the

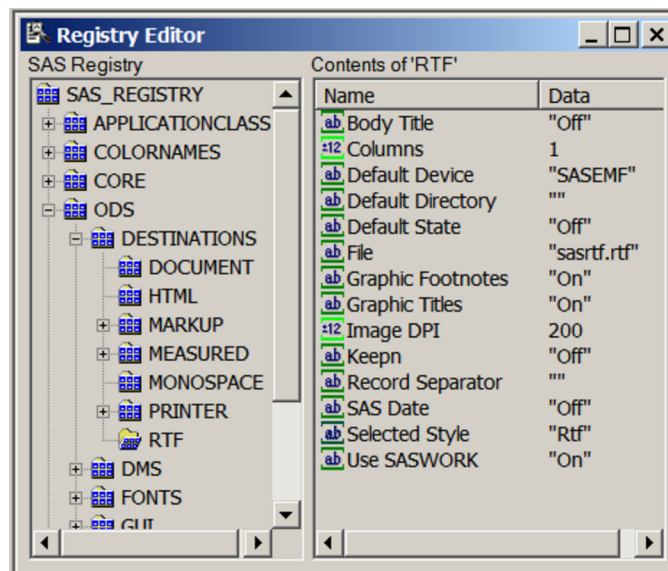
current template search path (for example, specify **Journal**). You can specify a default style for the other destinations in a similar way.

In a few cases the default style is specified in more than one place. Assume that you are using the SAS windowing environment and Microsoft Windows or UNIX in the following;

- If you expand the node **ODS ► DESTINATIONS ► HTML**, you see that the **Selected Style** is DEFAULT.
- If you expand the node **ODS ► MARKUP ► HTML4**, you see that the **Selected Style** is DEFAULT.
- If you expand the node **ODS ► DMS ► DESTINATIONS ► MARKUP ► HTML4**, you see that the **Selected Style** is HTMLBLUE.

The HTMLBLUE style is the default style for HTML output in the SAS windowing environment, yet the DEFAULT style is the default style for HTML output in other contexts.

Figure 21.60 SAS Registry Editor



ODS searches sequentially through each element of the template search path for the first style template that matches the name of the style specified in the SAS Registry. The first style template found is used. (See the sections “Saving Customized Templates” on page 715, “Using Customized Templates” on page 716, and “Reverting to the Default Templates” on page 717 in Chapter 22, “ODS Graphics Template Modification,” for more information about the template search path.) If you are specifying a customized style as your default style, the following are useful suggestions:

- If you save your style in Sasuser.Templat, verify that the name of your default style matches the name of the style specified in the SAS Registry. For example, suppose the RTF style is specified for the RTF destination in the SAS Registry. You can name your style RTF and save it in Sasuser.Templat. This blocks the RTF style in Sashelp.Tmplmst (provided that you did not alter the default template search path).

- If you save your style in a user-defined template store, verify that this template store is the first in the current template search path. Include the ODS PATH statement in your SAS autoexec file so that it is executed at start-up.

For the HTML destination, an alternative approach for specifying a default style is as follows. From the menu at the top of the main SAS window, select **Tools ► Options ► Preferences**. On the **Results** tab, select the **Create HTML** check box and select a style from the **Style** list.

Statistical Graphics Procedures

Three Base SAS statistical graphics procedures use ODS Graphics and provide a convenient syntax for creating a variety of graphs from raw data or from procedure output.

SGSCATTER	creates single-cell and multi-cell scatter plots and scatter plot matrices with optional fits and ellipses.
SGPLOT	creates single-cell plots with a variety of plot and chart types.
SGPANEL	creates single-page or multi-page panels of plots and charts conditional on classification variables.

You do not need to enable ODS Graphics in order to use these procedures, which are called SG (statistical graphics) procedures. In addition, the Base SAS SGRENDER procedure provides a way to create plots from graph templates that you have modified or written yourself. See the *SAS/GRAPH: Statistical Graphics Procedures Guide* and Kuhfeld (2010) for more information about the SG procedures and PROC SGRENDER.

These procedures do much more than make scatter plots. They can produce density plots, dot plots, needle plots, series plots, horizontal and vertical bar charts, histograms, and box plots. They can also compute and display loess fits, polynomial fits, penalized B-spline fits, reference lines, bands, and ellipses. PROC SGRENDER is the most flexible because it uses the Graph Template Language. The syntax for the other SG procedures is much simpler than that of the GTL, and so these procedures are recommended for creating most plots commonly required in statistical work.

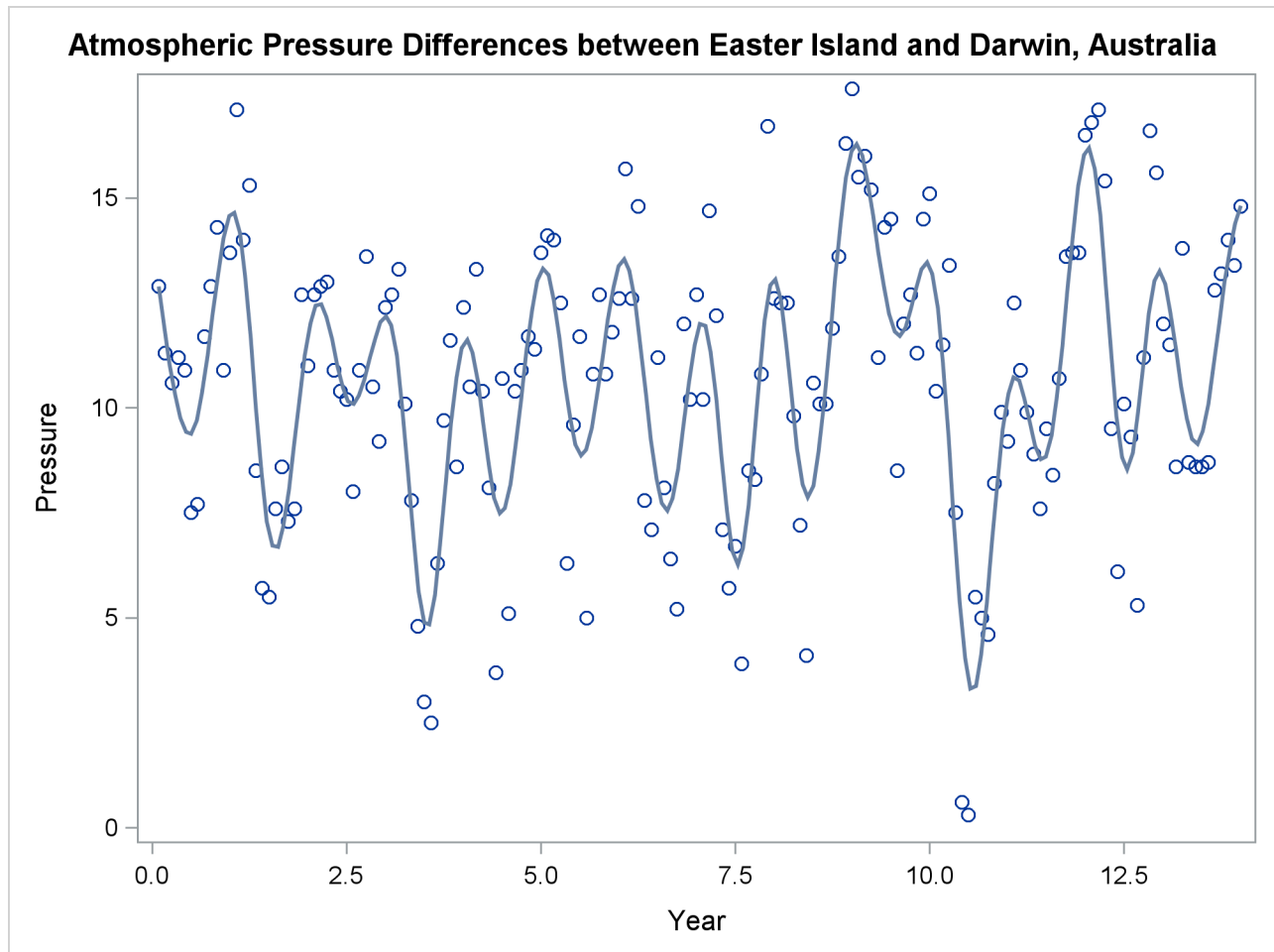
The SGPLOT Procedure

PROC SGPLOT provides a simple way to make a variety of scatter plots. This example is taken from Example 53.4 of Chapter 53, “The LOESS Procedure.” The ENSO data set, which contains information about differences in ocean pressure over time, is available from the Sashelp library.

The following statements create a scatter plot of points along with a penalized B-spline fit to the data and produce Figure 21.61:

```
proc sgplot data=sashelp.enso noautolegend;
  title 'Atmospheric Pressure Differences between '
        'Easter Island and Darwin, Australia';
  pbspline y=pressure x=year;
run;
```

Figure 21.61 Penalized B-Spline Fit with PROC SGPLOT



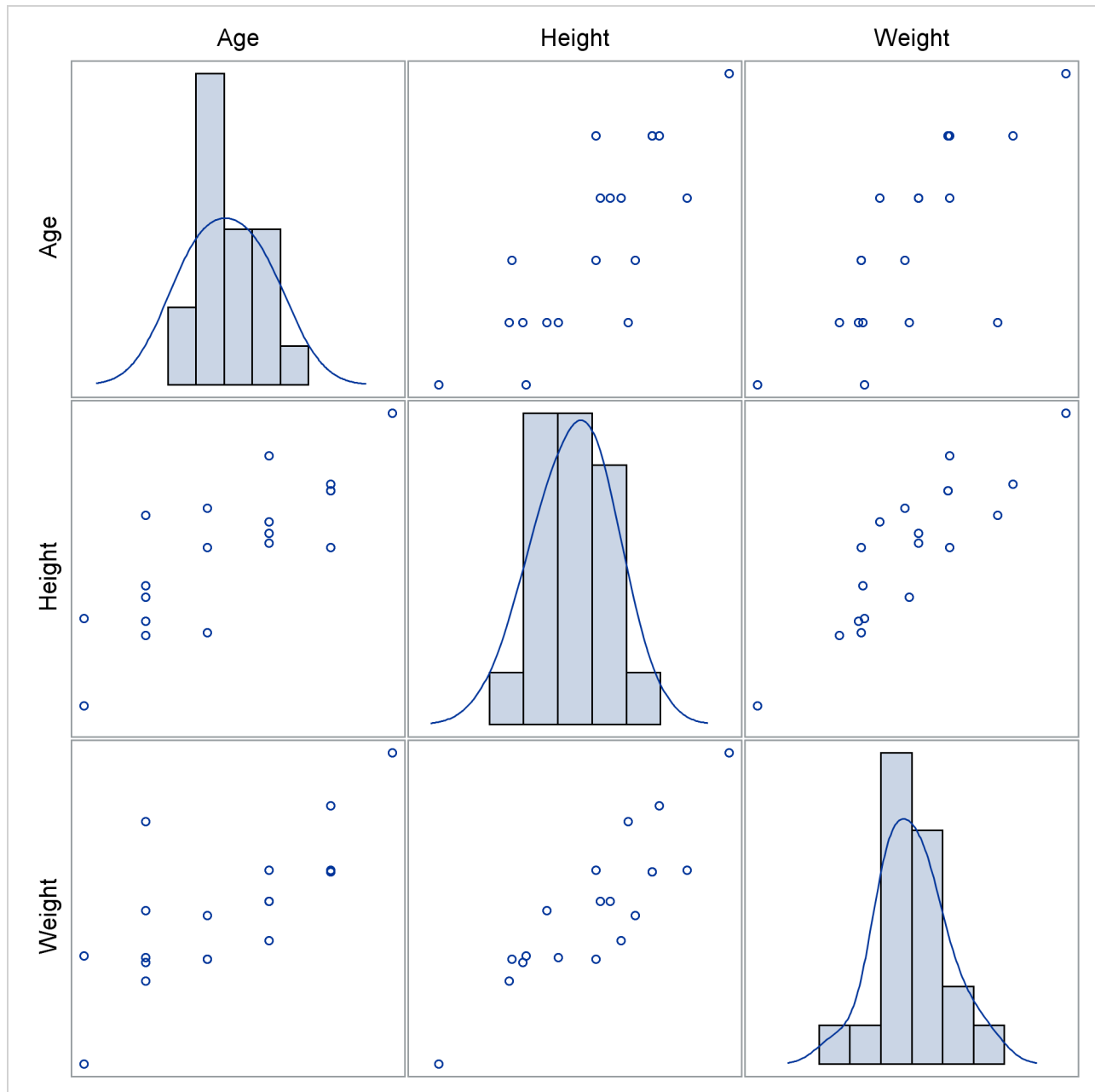
See Chapter 97, “The TRANSREG Procedure,” for more information about penalized B-splines. Also see the section “Grouped Scatter Plot with PROC SGPLOT” on page 598 and Figure 21.12 for an example of a scatter plot with groups of observations.

The SGSCATTER Procedure

You can use the SGSCATTER procedure to produce scatter plot matrices. The following step creates a scatter plot matrix from all of the numeric variables in the `Class` data set (available in the `Sashelp` library) and produces Figure 21.62:

```
proc sgscatter data=sashelp.class;
  matrix _numeric_ / diagonal=(kernel histogram);
run;
```

The diagonal cells of Figure 21.62 contain a histogram and a kernel density fit. The off-diagonal cells contain all pairs of scatter plots.

Figure 21.62 Scatter Plot Matrix with PROC SGSCATTER

The MATRIX statement creates a symmetric $n \times n$ scatter plot matrix. Other statements are also available. The PLOT statement creates a panel that contains one or more individual scatter plots. The COMPARE statement creates a rectangular $m \times n$ scatter plot matrix. Linear and nonlinear fits can be added, and many graphical features can be requested with options.

The SGPANEL Procedure

The SGPANEL procedure creates paneled plots and charts with one or more classification variables. Classification variables can be designated as row or column variables, or there can be multiple classifications.

Graphs are drawn for each combination of the levels of classification variables, showing a subset of the data in each cell.

This example is taken from [Example 41.6](#) of Chapter 41, “The GLIMMIX Procedure.” The following statements create the input SAS data sets:

```

data times;
  input time1-time23;
  datalines;
122 150 166 179 219 247 276 296 324 354 380 445
478 508 536 569 599 627 655 668 723 751 781
;

data cows;
  if _n_ = 1 then merge times;
  array t{23} time1 - time23;
  array w{23} weight1 - weight23;
  input cow iron infection weight1-weight23 @@;
  do i=1 to 23;
    weight = w{i};
    tpoint = (t{i}-t{1})/10;
    output;
  end;
  keep cow iron infection tpoint weight;
  datalines;
1 0 0 4.7 4.905 5.011 5.075 5.136 5.165 5.298 5.323
5.416 5.438 5.541 5.652 5.687 5.737 5.814 5.799
5.784 5.844 5.886 5.914 5.979 5.927 5.94
2 0 0 4.868 5.075 5.193 5.22 5.298 5.416 5.481 5.521
... more lines ...
;

```

First, PROC GLIMMIX is run to fit the model, and then the results are prepared for plotting:

```

proc glimmix data=cows;
  t2 = tpoint / 100;
  class cow iron infection;
  model weight = iron infection iron*infection tpoint;
  random t2 / type=rsmooth subject=cow
           knotmethod=kdtree(bucket=100 knotinfo);
  output out=gmxout pred(blup)=pred;
  nloptions tech=newrap;
run;

data plot;
  set gmxout;
  length Group $ 26;
  if (iron=0) and (infection=0) then group='Control Group (n=4)';
  else if (iron=1) and (infection=0) then group='Iron - No Infection (n=3)';
  else if (iron=0) and (infection=1) then group='No Iron - Infection (n=9)';
  else group = 'Iron - Infection (n=10)';
run;

```



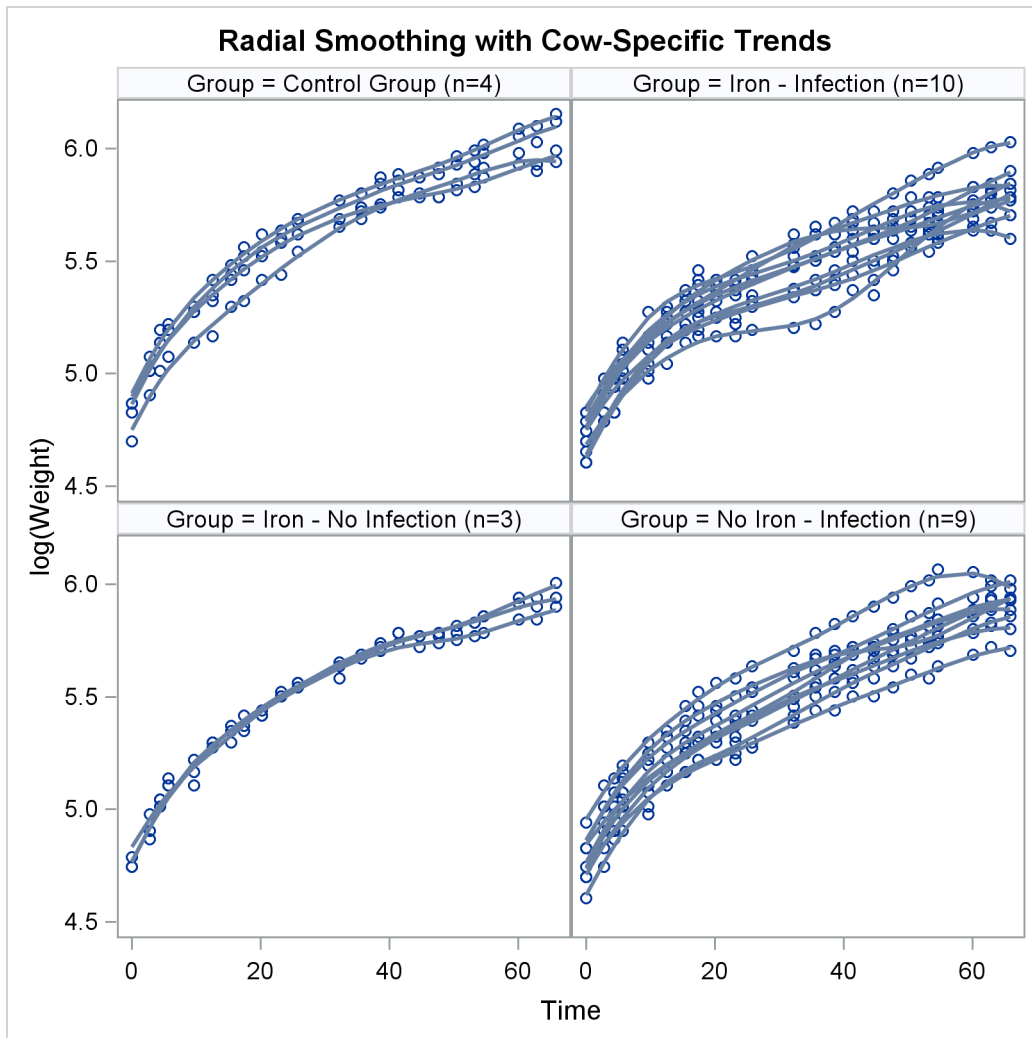
```
proc sort data=plot; by group cow;
run;
```

The following statements produce graphs of the observed data and fitted profiles in the four groups:

```
proc sgpanel data=plot noautolegend;
  title 'Radial Smoothing with Cow-Specific Trends';
  label tpoint='Time' weight='log(Weight)';
  panelby group / columns=2 rows=2;
  scatter x=tpoint y=weight;
  series x=tpoint y=pred / group=cow lineattrs=GraphFit;
run;
```

The results are shown in Figure 21.63.

Figure 21.63 Fit Using PROC SGPANEL



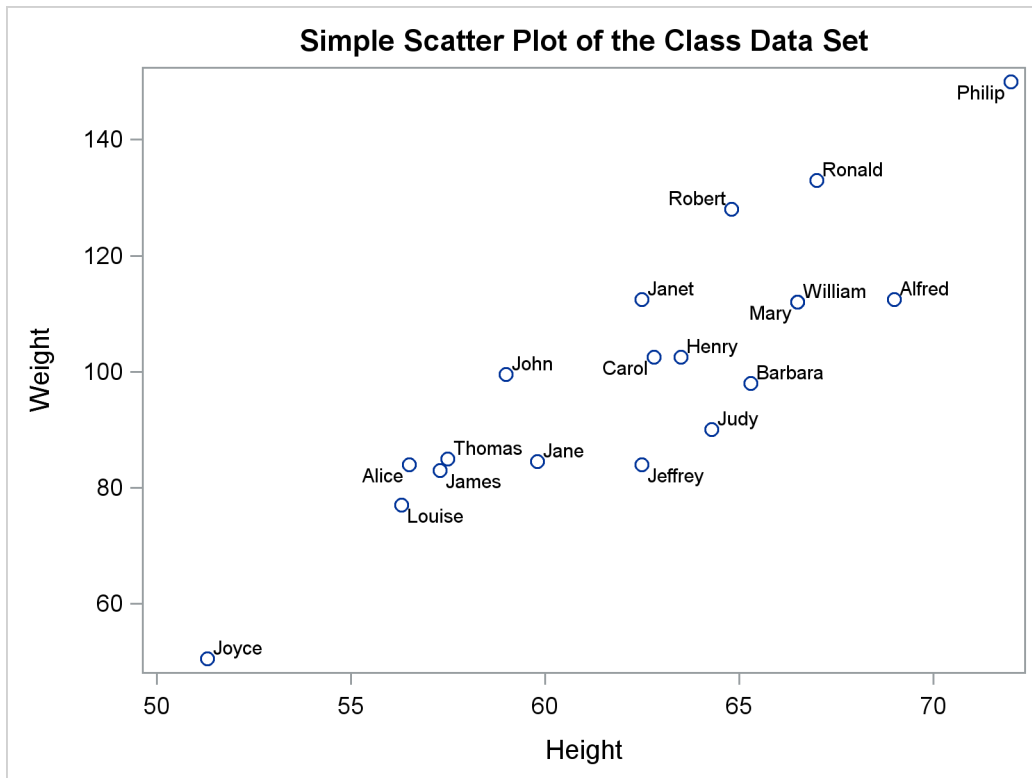
The SGRENDER Procedure

The SGRENDER procedure produces a graph from an input SAS data set and an ODS graph template. With PROC SGRENDER and the Graph Template Language (GTL), you can create highly customized graphs. The following steps create a simple scatter plot of the Class data set (available in the Sashelp library) and produce Figure 21.64:

```
proc template;
  define statgraph Scatter;
    begingraph;
      entrytitle "Simple Scatter Plot of the Class Data Set";
      layout overlay;
        scatterplot y=weight x=height / datalabel=name;
      endlayout;
    endgraph;
  end;
run;

proc sgrender data=sashelp.class template=scatter;
run;
```

The template definition consists of an outer block that begins with a DEFINE statement and ends with an END statement. Inside of that is a BEGINGRAPH/ENDGRAPH block. Inside that block, the ENTRYTITLE statement provides the plot title, and the LAYOUT OVERLAY block contains the statement or statements that define the graph. In this case, there is just a single SCATTERPLOT statement that names the Y-axis (vertical) variable, the X-axis (horizontal) variable, and an optional variable that contains labels for the points. The PROC SGRENDER statement simply specifies the input data set and the template. The real work in using PROC SGRENDER is writing the template.

Figure 21.64 Scatter Plot of Labeled Points with PROC SGRENDER

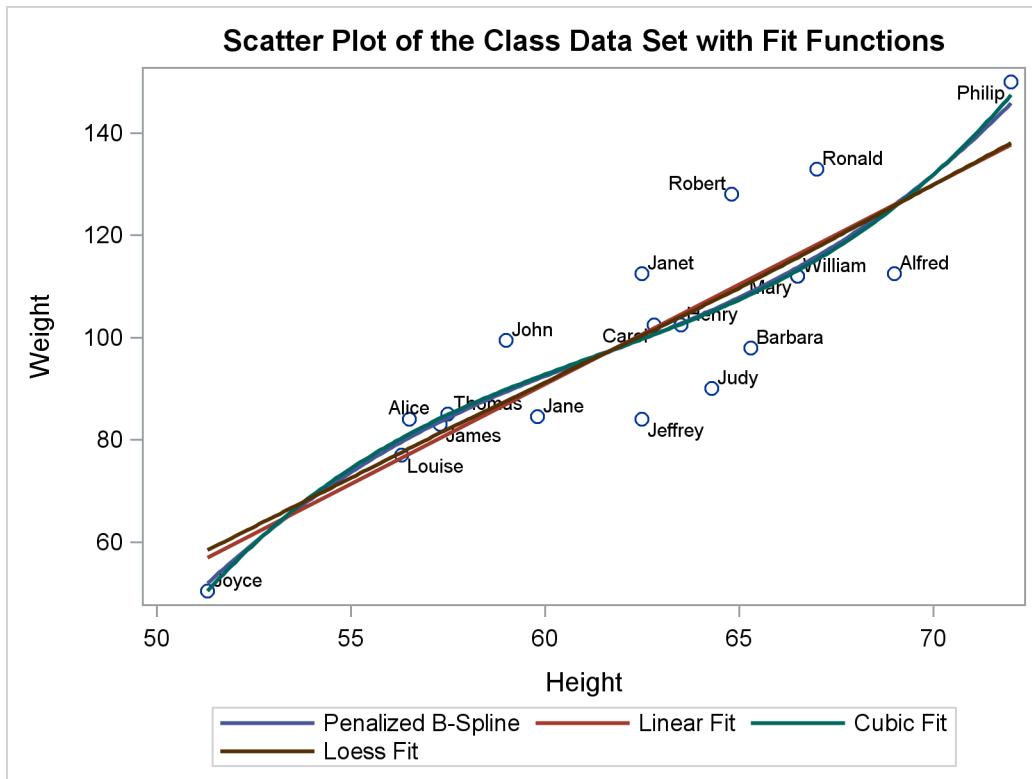
The following steps add a series of fit functions to the scatter plot and create a legend by adding statements to the **Scatter** template:

```
proc template;
  define statgraph Scatter;
    begingraph;
      entrytitle "Scatter Plot of the Class Data Set with Fit Functions";
      layout overlay;
        scatterplot y=weight x=height / datalabel=name;
        pbsplineplot y=weight x=height / name='pbs'
          legendlabel='Penalized B-Spline'
          lineattrs=GraphData1;
        regressionplot y=weight x=height / degree=1 name='line'
          legendlabel='Linear Fit'
          lineattrs=GraphData2;
        regressionplot y=weight x=height / degree=3 name='cubic'
          legendlabel='Cubic Fit'
          lineattrs=GraphData3;
        loessplot y=weight x=height / name='loess'
          legendlabel='Loess Fit'
          lineattrs=GraphData4;
        discretelegend 'pbs' 'line' 'cubic' 'loess';
      endlayout;
    endgraph;
  end;
run;
```

```
proc sgrender data=sashelp.class template=scatter;
run;
```

The line attributes for each function are specified with different style elements, **GraphData1** through **GraphData4**, so that the functions are adequately identified in the legend. The preceding statements create Figure 21.65.

Figure 21.65 Scatter Plot and Fit Functions with PROC SGRENDER



The following statements create a four-panel display of the Class data set and produce [Figure 21.66](#):

```
proc template;
  define statgraph Panel;
    beginngraph;
      entrytitle "Paneled Display of the Class Data Set";

      layout lattice / rows=2 columns=2 rowgutter=10 columngutter=10;

        layout overlay;
          scatterplot y=weight x=height;
          pbsplineplot y=weight x=height;
        endlayout;

        layout overlay / xaxisopts=(label='Weight');
          histogram weight;
        endlayout;

        layout overlay / yaxisopts=(label='Height');
          boxplot y=height;
        endlayout;

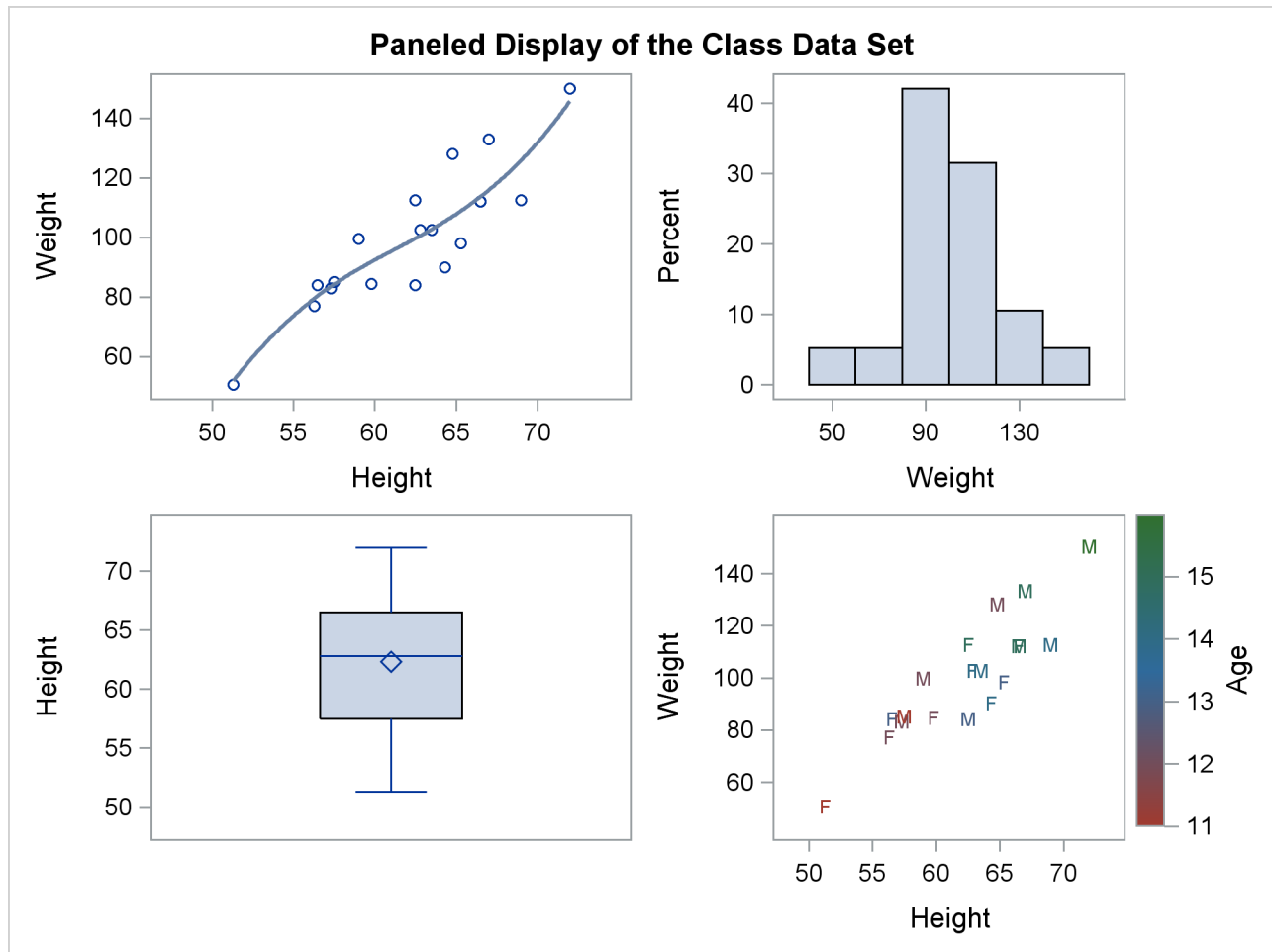
        layout overlay / xaxisopts=(offsetmin=0.1 offsetmax=0.1)
          yaxisopts=(offsetmin=0.1 offsetmax=0.1);
          scatterplot y=weight x=height / markercharacter=sex
            name='color' markercolorgradient=age;
          continuouslegend 'color' / title='Age';
        endlayout;

      endlayout;
    endngraph;
  end;
run;

proc sgrender data=sashelp.class template=panel;
run;
```

In this template, the outermost layout is a `LAYOUT LATTICE`. It creates a 2×2 panel of plots with a 10-pixel separation (or gutter) between each plot. Inside the lattice are four `LAYOUT OVERLAY` blocks—each defining one of the graphs. The first is a simple scatter plot with a nonlinear penalized B-spline fit. The second is a histogram of the dependent variable `Weight`. The third is a box plot of the independent variable `Height`. The fourth simultaneously shows height, weight, age, and sex for the students in the class. Each axis has an offset added at both the maximum and minimum. This provides padding between the axes and the data.

Figure 21.66 Multiple Panels Using PROC SGRENDER



Many other types of graphs are available with the SG procedures. However, even the few examples provided here show the power and flexibility available for making professional-quality statistical graphics. See the *SAS/GRAPH: Graph Template Language User's Guide* and the *SAS/GRAPH: Statistical Graphics Procedures Guide* for more information.

Examples of ODS Statistical Graphics

Example 21.1: Creating Graphs with Tool Tips in HTML

This example demonstrates how to request graphs in HTML that are enhanced with tooltip displays, which appear when you move a mouse over certain features of the graph. When you specify the HTML destination and the `IMAGEMAP=ON` option in the ODS GRAPHICS statement, an image map of coordinates for tooltips is generated along with the HTML output file. Individual graphs are saved as PNG files.

Example 59.2 and Example 59.8 of Chapter 59, “The MIXED Procedure,” analyze a data set with repeated growth measurements for 27 children. The following step creates the data set:

```
data pr;
  input Person Gender $ y1 y2 y3 y4 @@;
  y=y1; Age=8; output;
  y=y2; Age=10; output;
  y=y3; Age=12; output;
  y=y4; Age=14; output;
  drop y1-y4;
  datalines;
1  F  21.0  20.0  21.5  23.0      2  F  21.0  21.5  24.0  25.5
3  F  20.5  24.0  24.5  26.0      4  F  23.5  24.5  25.0  26.5

... more lines ...

;
```

The following statements fit a mixed model with random intercepts and slopes for each child:

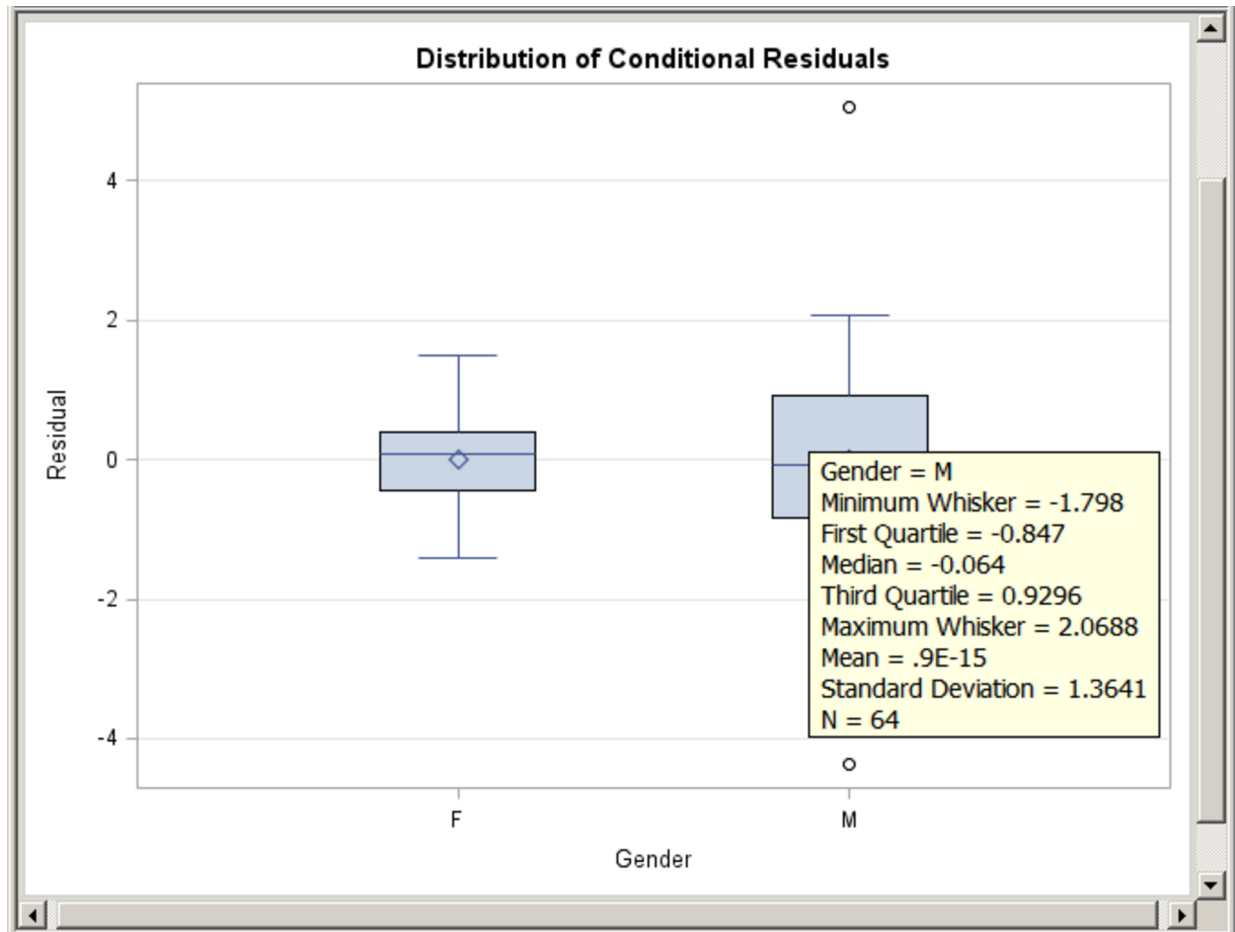
```
ods _all_ close;
ods html body='b.html' style=HTMLBlue;
ods graphics on / imagemap=on;

proc mixed data=pr method=ml plots=boxplot;
  ods select 'Conditional Residuals by Gender';
  class Person Gender;
  model y = Gender Age Gender*Age;
  random intercept Age / type=un subject=Person;
run;

ods html close;
```

The `PLOTS=BOXPLOT` option in the PROC MIXED statement requests box plots of observed values and residuals for each classification main effect in the model (Gender and Person). Only the by-gender box plots are actually created due to the ODS SELECT statement, which uses the plot label to select the plot. Output 21.1.1 displays the results. Moving the mouse over a box plot displays a tooltip with summary statistics for the class level. Graphics with tooltips are supported for only the HTML destination.

Output 21.1.1 Box Plot with Tool Tips



Example 21.2: Creating Graphs for a Presentation

The RTF destination provides an easy way to create graphs for inclusion into a paper or presentation. You can specify the ODS RTF statement to create a file that is easily imported into a document (such as Microsoft Word or WordPerfect) or a presentation (such as Microsoft PowerPoint).

The following statements request a loess fit and save the output in the file *loess.rtf*:

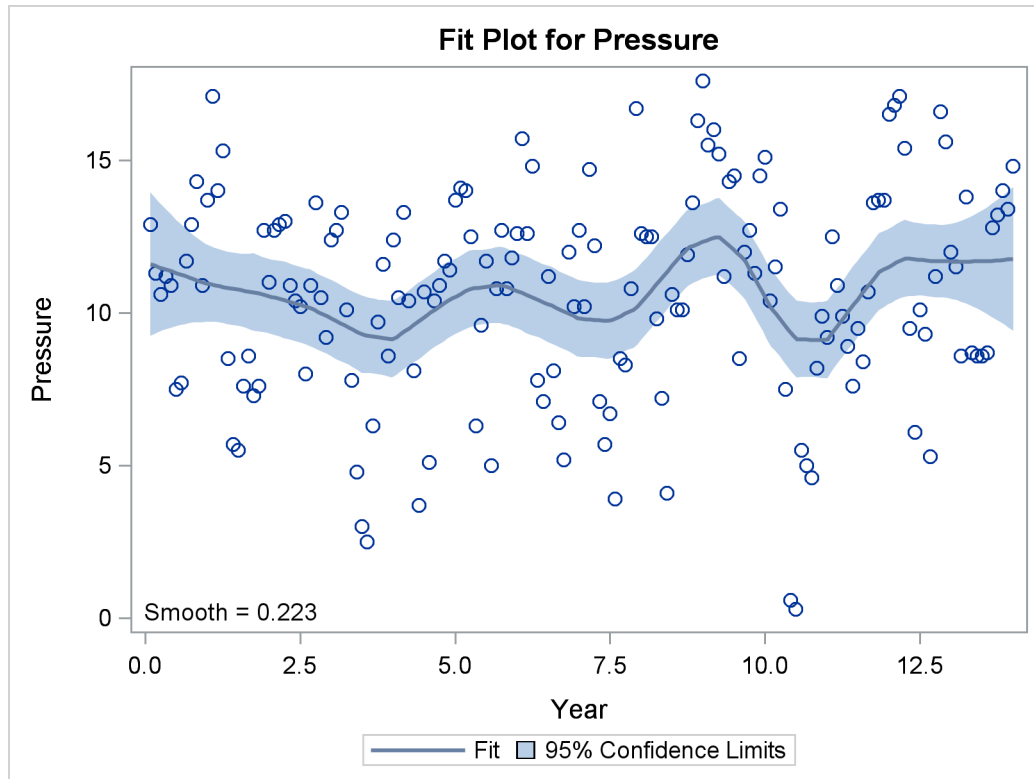
```
ods _all_ close;
ods rtf file="loess.rtf" style=HTMLBlue;
ods graphics on;

proc loess data=sashelp.enso;
  model pressure = year / clm residual;
run;

ods rtf close;
ods listing;
```


The output file includes various tables and the following plots: a plot of the selection criterion versus smoothing parameter, a fit plot with 95% confidence bands, a plot of residual by regressors, and a diagnostics panel. The fit plot is produced with the HTMLBLUE style and is shown in [Output 21.2.1](#).

Output 21.2.1 Loess Fit Plot with the HTMLBLUE Style



If you are running the SAS System in the Microsoft Windows operating system, you can open the RTF file in Microsoft Word and simply copy and paste the graphs into Microsoft PowerPoint. In general, RTF output is convenient for exchange of graphical results between Microsoft Windows applications through the clipboard.

Alternatively, if you use the LISTING or HTML destinations, then your individual graphs are created as PNG files by default. You can insert these files into a Microsoft PowerPoint presentation. See the sections “[Naming Graphics Image Files](#)” on page 624 and “[Saving Graphics Image Files](#)” on page 626 for information about how the image files are named and saved.

Example 21.3: Creating Graphs in PostScript Files

This example illustrates how to create individual graphs in PostScript files. This is particularly useful when you want to include them in a \LaTeX document.

The following statements close all open destinations, open the \LaTeX ³ destination with the JOURNAL style, and request a grouped bar chart for the Sashelp.Class data set:

³The \LaTeX destination is experimental.

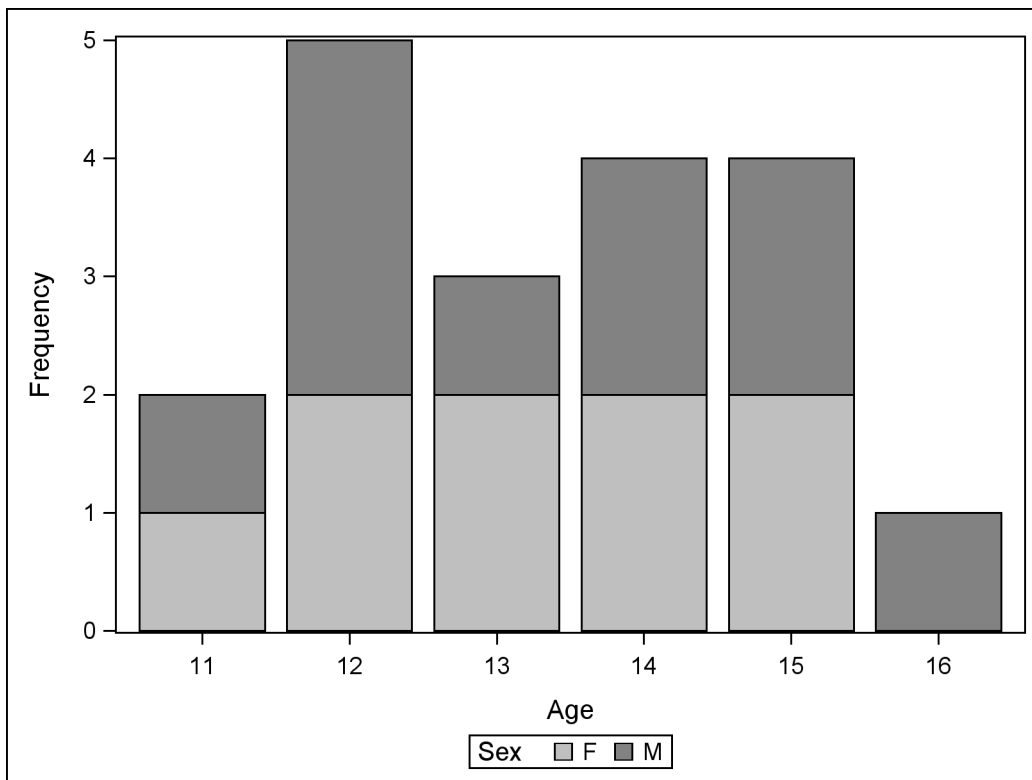
```
ods graphics on / reset=index;
ods _all_ close;
ods latex style=Journal;

proc sgplot data=sashelp.class;
  vbar age / group=sex;
run;

ods latex close;
ods listing;
```

The JOURNAL style displays gray-scale graphs that are suitable for a journal. When you specify the ODS LATEX destination, ODS creates a PostScript file for each individual graph in addition to a L^AT_EX source file that includes the tabular output and references to the PostScript files. By default, these files are saved in the SAS current folder. The bar chart shown in [Output 21.3.1](#) is saved by default in a file named *SGPlot.ps*. See the section “[Naming Graphics Image Files](#)” on page 624 for details about how graphics image files are named. If both the default destination (LISTING or HTML) and the LATEX destination are open, then two files are created: *SGPlot.png* and *SGPlot1.ps*. If the RESET=INDEX option is not specified in the ODS GRAPHICS statement and you run the step again, the next names are based on an incremented index (*SGPlot2.png* and *SGPlot3.ps*).

Output 21.3.1 Bar Chart Using the JOURNAL Style



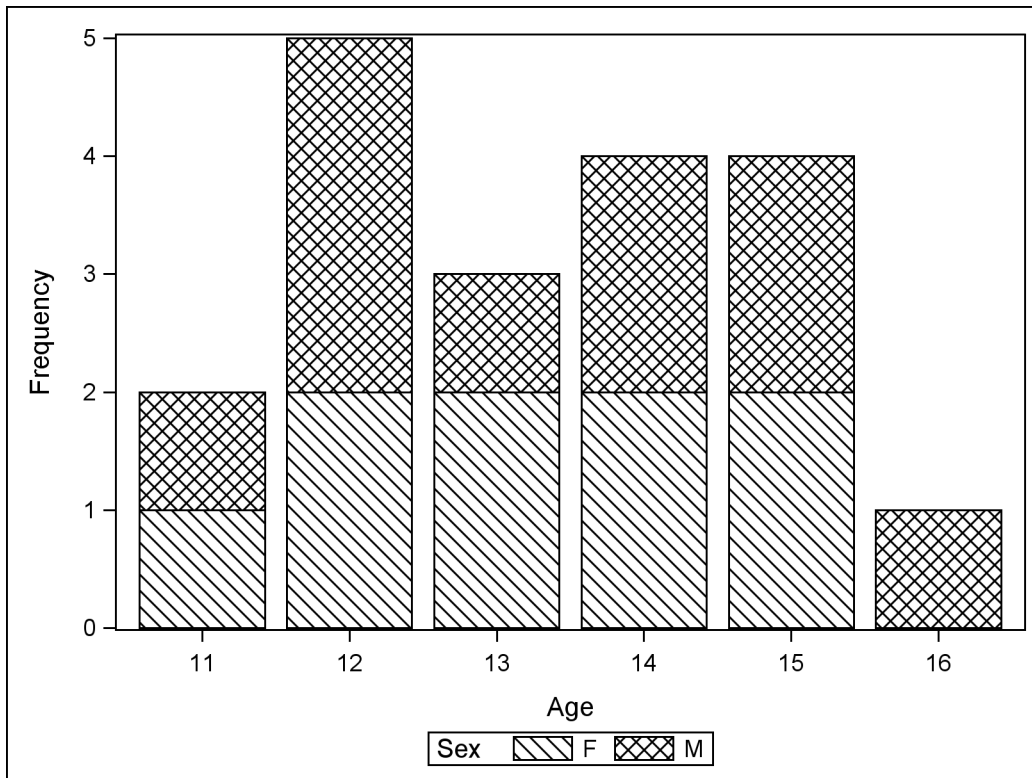
You can use the JOURNAL2 style for a different appearance—the bars are not shaded. Crosshatching is used to indicate group membership. The following step produces [Output 21.3.2](#):

```
ods graphics on / reset=index;
ods _all_ close;
ods latex style=Journal2;

proc sgplot data=sashelp.class;
  vbar age / group=sex;
run;

ods latex close;
ods listing;
```

Output 21.3.2 Bar Chart Using the JOURNAL2 Style

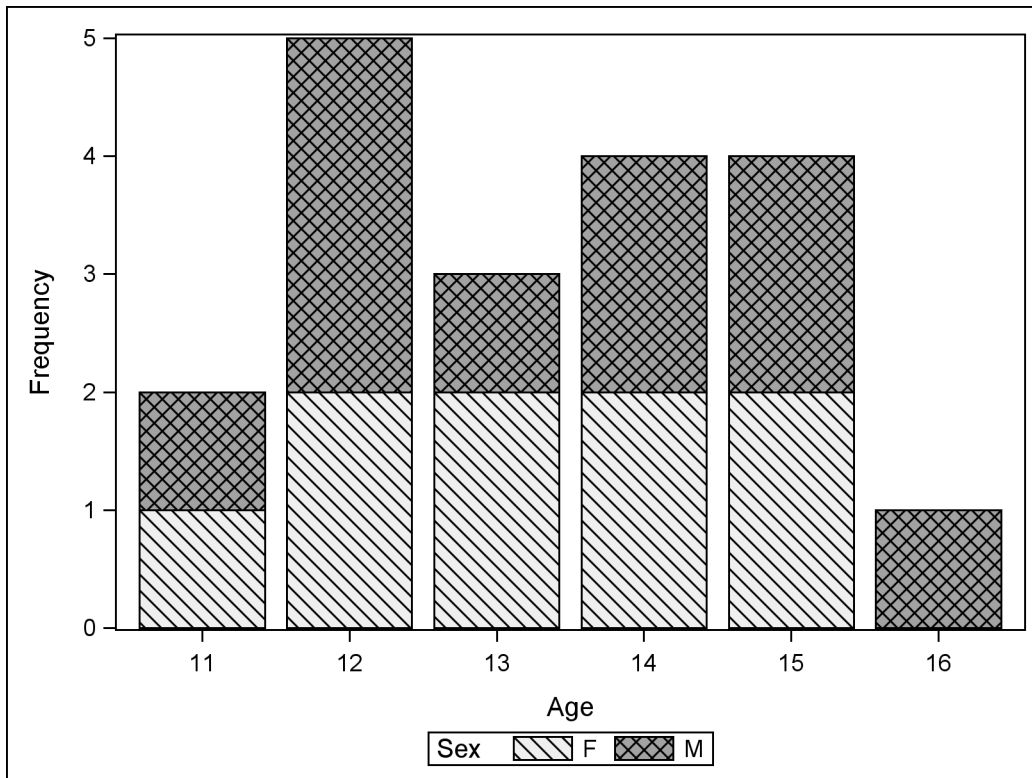


You can use the JOURNAL3 style for a different kind of appearance from the JOURNAL style. A mix of filled areas and crosshatching is used in grouped bar charts. The following step produces [Output 21.3.3](#):

```
ods graphics on / reset=index;
ods _all_ close;
ods latex style=Journal3;

proc sgplot data=sashelp.class;
  vbar age / group=sex;
run;

ods latex close;
ods listing;
```

Output 21.3.3 Bar Chart Using the JOURNAL3 Style

If you are writing a paper, you can include the graphs in your own \LaTeX source file by referencing the names of the individual PostScript graphics files. In this situation, you might not find it necessary to use the \LaTeX source file created by the SAS System. Alternatively, you can include PNG files into a \LaTeX document, after using some other ODS destination (such as HTML) to create the PNG files.

Example 21.4: Displaying Graphs Using the DOCUMENT Procedure

This example illustrates the use of the ODS DOCUMENT destination and the DOCUMENT procedure to display your ODS graphs. You can use this approach whenever you want to generate and save your output (both tables and graphs) and then display or replay it later, potentially in subsets or more than once. This approach is particularly useful when you want to display your output in multiple ODS destinations, or when you want to use different styles without rerunning your SAS program. This approach is also useful when you want to break your output into separate parts for inclusion into different parts of a document such as a \LaTeX file.

Consider again the data set Stack created by the following statements:

```
data stack;
  input x1 x2 x3 y @@;
  datalines;
80 27 89 42   80 27 88 37   75 25 90 37   62 24 87 28   62 22 87 18
62 23 87 18   62 24 93 19   62 24 93 20   58 23 87 15   58 18 80 14
58 18 89 14   58 17 88 13   58 18 82 11   58 19 93 12   50 18 89 8
50 18 86 7    50 19 72 8    50 19 79 8    50 20 80 9    56 20 82 15
70 20 91 15
;
```

The following statements request a Q-Q plot from PROC ROBUSTREG with the Stack data:

```
ods graphics on;
ods _all_ close;
ods document name=QQDoc(write);

proc robustreg data=stack plots=qqplot;
  model y = x1 x2 x3;
run; quit;

ods document close;
ods listing;
```

The ODS DOCUMENT statement opens an ODS document named `QQDoc`. All of the results—tables, graphs, titles, notes, footnotes, headers—are stored in the ODS document. None of them are displayed since no other destination is open. In order to display the Q-Q plot with PROC DOCUMENT, you first need to determine its name. You can do this by specifying the ODS TRACE ON statement prior to the procedure statements (see the section “[Determining Graph Names and Labels](#)” on page 618 for more information). Alternatively, you can type `odsdocuments` (or `odsd` for short) on the command line to open the Documents window, which you can then use to manage your ODS documents.

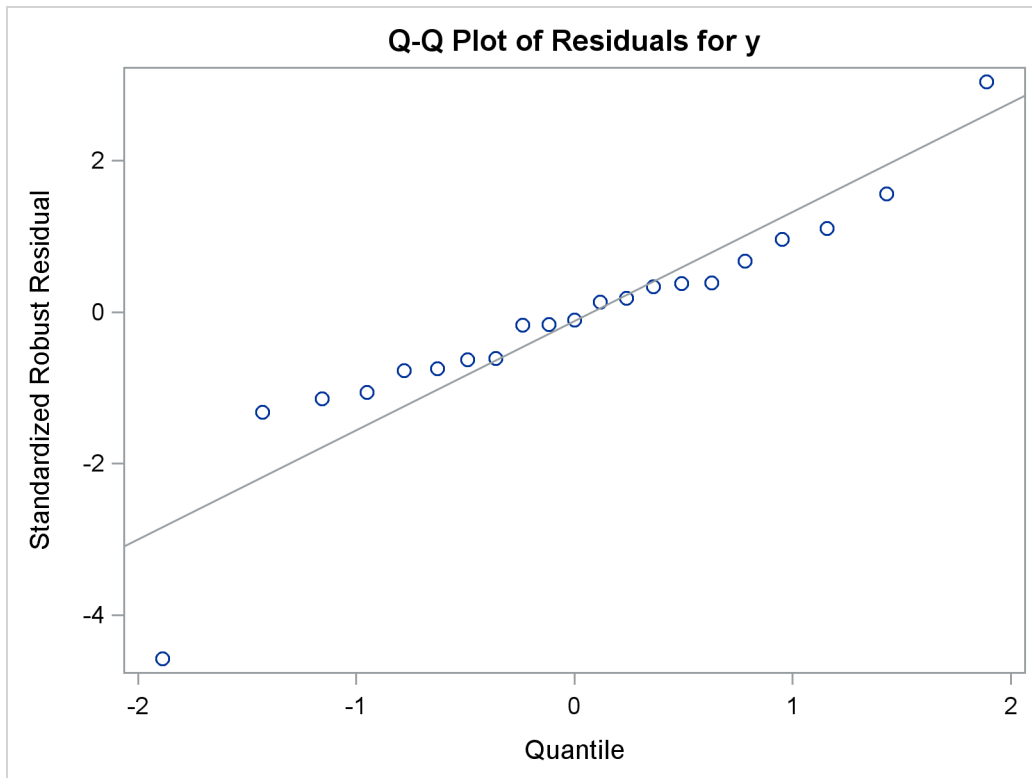
The following statements specify an HTML destination and display the residual Q-Q plot by using the REPLAY statement in PROC DOCUMENT:

```
ods html body='b.htm';

proc document name=QQDoc;
  ods select QQPlot;
  replay;
run; quit;

ods html close;
```

Subsequent steps can replay one or more objects from the same ODS document. By default, the REPLAY statement attempts to display every output object stored in the ODS document, but here only the Q-Q plot is displayed because it is specified by the ODS SELECT statement. The plot is displayed in [Output 21.4.1](#).

Output 21.4.1 Q-Q Plot Displayed by PROC DOCUMENT

As an alternative to running PROC DOCUMENT with an ODS SELECT statement, you can run PROC DOCUMENT with a *document path* for the Q-Q plot in the REPLAY statement. This approach is preferable when the ODS document contains a large volume of output, so that PROC DOCUMENT does not attempt to process every piece of output stored in the ODS document.

You can determine the ODS document path for the Q-Q plot by specifying the LIST statement with the LEVELS=ALL option in PROC DOCUMENT as follows:

```
proc document name=QQDoc;
  list / levels=all;
run; quit;
```

The contents of the ODS document `QQDoc` are shown in [Output 21.4.2](#).

Output 21.4.2 Contents of the ODS Document `QQDoc`

```
Listing of: \Work.Qqdoc\
Order by: Insertion
Number of levels: All
```

Obs	Path	Type
1	\Robustreg#1	Dir
2	\Robustreg#1\ModelInfo#1	Table
3	\Robustreg#1\NObs#1	Table
4	\Robustreg#1\ParmInfo#1	Table
5	\Robustreg#1\SummaryStatistics#1	Table
6	\Robustreg#1\ParameterEstimates#1	Table
7	\Robustreg#1\DiagSummary#1	Table
8	\Robustreg#1\DiagnosticPlots#1	Dir
9	\Robustreg#1\DiagnosticPlots#1\QQPlot#1	Graph
10	\Robustreg#1\GoodFit#1	Table

The ODS document path of the `QQPlot` entry in the `QQDoc` ODS document, as shown in [Output 21.4.2](#), is `\Robustreg#1\DiagnosticPlots#1\QQPlot#1`.

You can use this path to display the residual Q-Q plot with PROC DOCUMENT as follows:

```
proc document name=QQDoc;
  replay \Robustreg#1\DiagnosticPlots#1\QQPlot#1;
run; quit;
```

You can also determine the ODS document path from the Results window or the Documents window. Right-click the object icon and select **Properties**.

The SAS/STAT documentation preparation process uses the ODS document. SAS output is saved into an ODS document that is then replayed into sections of the documentation, which is prepared using L^AT_EX. In general, when you send your output to the DOCUMENT destination, you can use PROC DOCUMENT to rearrange, duplicate, or remove output from the results of a procedure or a database query. For more information, see the ODS DOCUMENT statement in the section “Dictionary of ODS Language Statements” and the chapter “The DOCUMENT Procedure” in the *SAS Output Delivery System: User’s Guide*.

Example 21.5: Customizing the Style for Box Plots

This example demonstrates how to modify the style for box plots. This example is taken from [Example 21.1](#). The following step creates the data set:

```
data pr;
  input Person Gender $ y1 y2 y3 y4 @@;
  y=y1; Age=8; output;
  y=y2; Age=10; output;
  y=y3; Age=12; output;
  y=y4; Age=14; output;
  drop y1-y4;
  datalines;
1 F 21.0 20.0 21.5 23.0      2 F 21.0 21.5 24.0 25.5
3 F 20.5 24.0 24.5 26.0      4 F 23.5 24.5 25.0 26.5
... more lines ...
;
```

The following step displays the HTMLBLUE style and its parent styles, STATISTICAL and DEFAULT:

```
proc template;
  source Styles.HTMLBlue;
  source Styles.Statistical;
  source Styles.Default;
run;
```

If you search for ‘box’, you find the style element that controls some aspects of the box plot:

```
class GraphBox /
  capstyle = "serif"
  connect = "mean"
  displayopts = "fill caps median mean outliers";
```

You can learn more about the **GraphBox** style element and its attributes in the section on the BOXPLOT statement in the *SAS/GRAPH: Graph Template Language Reference* and in the section on “ODS Style Elements” in the *SAS Output Delivery System: User’s Guide*.

The following statements create two new styles by modifying attributes of the **GraphBox** style element. The first style is a sparse style; the box is outlined (not filled), and the median is shown but not the mean. In contrast, the second style produces a filled box, with caps on the whiskers that shows the mean, median, and outliers. In addition, the box is notched.

The following statements create the two styles:

```
proc template;
  define style BoxStyleSparse;
    parent=styles.HTMLBlue;
    style GraphBox / capstyle = "line" displayopts = "median";
  end;
  define style BoxStyleRich;
    parent=styles.HTMLBlue;
    style GraphBox / capstyle = "bracket"
      displayopts = "fill caps median mean outliers notches";
  end;
run;
```

The following steps run PROC MIXED and create box plots that use the two styles:

```
ods graphics on;
ods listing style=boxstylesparse;

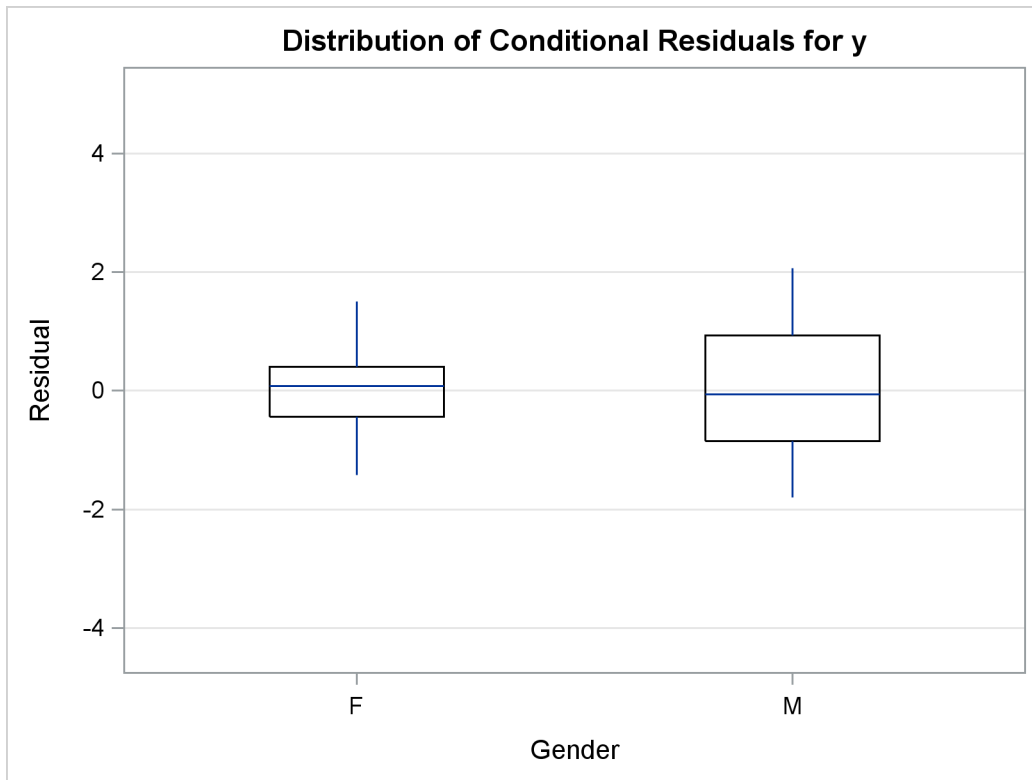
proc mixed data=pr method=ml plots=boxplot;
  ods select 'Conditional Residuals by Gender';
  class Person Gender;
  model y = Gender Age Gender*Age;
  random intercept Age / type=un subject=Person;
run;

ods listing style=boxstylerich;

proc mixed data=pr method=ml plots=boxplot;
  ods select 'Conditional Residuals by Gender';
  class Person Gender;
  model y = Gender Age Gender*Age;
  random intercept Age / type=un subject=Person;
run;
```

The results with the sparse style are displayed in [Output 21.5.1](#), and the results with the richer style are displayed in [Output 21.5.2](#). See [Output 21.1.1](#) in [Example 21.1](#) to see the results of using the HTMLBLUE style.

Output 21.5.1 Box Plot with the Sparse Style



Output 21.5.2 Box Plot with the Richer Style



References

Kuhfeld, W. F. (2009), “Modifying ODS Statistical Graphics Templates in SAS 9.2,” <http://support.sas.com/rnd/app/papers/ods/modtmplt.pdf>.

Kuhfeld, W. F. (2010), *Statistical Graphics in SAS: An Introduction to the Graph Template Language and the Statistical Graphics Procedures*, Cary, NC: SAS Press.

Chapter 22

ODS Graphics Template Modification

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Graph Templates

This chapter discusses the graph template language and graph template modification in ODS Graphics. Be sure that you are familiar with Chapter 21, “Statistical Graphics Using ODS,” before reading this chapter.

Graph templates control the layout and details of graphs produced with ODS Graphics. The SAS System provides a template for every graph produced by statistical procedures. Graph template definitions are written in the Graph Template Language (GTL). This powerful language includes statements for specifying plot layouts (such as lattices or overlays), plot types (such as scatter plots and histograms), and text elements (such as titles, footnotes, and insets). It also provides support for built-in computations (such as histogram binning) and the evaluation of expressions. Options are available for specifying colors, marker symbols, and other attributes of plot features.

Graphs, like all SAS output, are constructed from two underlying components, a data component (or data object) and a template. Procedures supply a table of data values and statistical results to plot. Together, the data object and the template form an output object that ODS displays in one or more output destinations. You can control this display in two ways. You can use the ODS Graphics Editor (discussed in the section “ODS Graphics Editor” on page 630 in Chapter 21, “Statistical Graphics Using ODS,”) to modify the output object (but not the underlying data object or template), and you can use the GTL to modify the template. With just a little knowledge of the GTL, you can modify or edit templates, even when you do not understand most of the syntax used in the template definition. See examples starting with [Example 22.1](#).

NOTE: You do not need to know anything about the GTL to create statistical graphics.

This section provides an overview of the Graph Template Language. It also describes how to locate, display, edit, and save templates. A *template definition* is a set of SAS statements that is used together with PROC TEMPLATE to create a compiled template. In addition to graph templates, two other common types of templates are table templates and style templates. A table template describes how to display the output for an output object that is rendered as a table. A style template provides formatting information for visual aspects of your SAS output, including both tables and graphs. In most applications, you do not have to modify the templates that are supplied by SAS. However, when customization is necessary, you can modify the default template with the template language and PROC TEMPLATE.

Compiled templates are stored in a template store, which is a type of item store. (An item store is a special type of SAS file.) The default templates supplied by SAS are stored in the Sashelp.Tmplmst template store. If you are using the SAS windowing environment, an easy way to display, edit, and save your templates is by using the Templates window. For an introduction to the graph template language, see Kuhfeld (2010).

For detailed information about managing templates, see the *SAS Output Delivery System: User’s Guide* and the *SAS/GRAPH: Graph Template Language User’s Guide*. For details about the syntax of the graph template language, see the *SAS/GRAPH: Graph Template Language Reference*.

The Graph Template Language

Graph template definitions begin with a `DEFINE STATGRAPH` statement in `PROC TEMPLATE`, and they end with an `END` statement. Embedded in every graph template is a `BEGINGRAPH/ENDGRAPH` block, and embedded in that block are one or more `LAYOUT` blocks. You can specify the `DYNAMIC` statement to define dynamic variables (which the procedure uses to pass values to the template definition), the `MVAR` and `NMVAR` statements to define macro variables (which you can use to pass values to the template definition), and the `NOTES` statement to provide descriptive information about the graph. The default templates supplied by SAS for statistical procedures are often lengthy and complex, because they provide ODS Graphics with comprehensive and detailed information about graph construction. Here is one of the simpler graph templates for a statistical procedure:

```
define statgraph Stat.MDS.Graphics.Fit;
  notes "MDS Fit Plot";
  dynamic head;
  beginnograph / designwidth=defaultdesignheight;
    entrytitle HEAD;
    layout overlayequated / equatetype=square;
      scatterplot y=FITDATA x=FITDIST / markerattrs=(size=5px);
      lineparm slope=1 x=0 y=0 / extend=true lineattrs=GRAPHREFERENCE;
    endlayout;
  endnograph;
end;
```

This template, supplied for the MDS procedure, creates a scatter plot of two variables, `FitData` and `FitDist`, along with a diagonal reference line that passes through the origin. The plot is square and the axes are equated so that a centimeter on one axis represents the same data range as a centimeter on the other axis. The plot title is provided by the evaluation of the dynamic variable `Head`, which is set by the procedure. It is not unusual for this plot to contain hundreds or even thousands of points, so a five-pixel marker is specified, which is smaller than the seven-pixel marker used by default in most styles.

The statements available in the graph template language can be classified as follows:

- Control statements specify the conditional or iterative flow of control. By default, flow of control is sequential. In other words, each statement is used in the order in which it appears.
- Layout statements specify the arrangement of the components of the graph. Layout statements are arranged in blocks that begin with a `LAYOUT` statement and end with an `ENDLAYOUT` statement. The blocks can be nested. Within a layout block, there can be plot, text, and other statements that define one or more graph components. Options provide control for attributes of layouts and components.
- Plot statements specify a number of commonly used displays, including scatter plots, histograms, contour plots, surface plots, and box plots. Plot statements are always provided within a layout block. The plot statements include options to specify the data columns from the data object that is used in the graph. For example, in the `SCATTERPLOT` statement, there are mandatory `X=` and `Y=` arguments that specify which data columns are used for the X (horizontal) and Y (vertical) axes in the plot. (In the preceding example, `FitData` and `FitDist` are the names of columns in the data object that `PROC MDS` creates for this graph.) There is also a `GROUP=` option that specifies a data column as an optional classification variable.

- Text statements specify the descriptions that accompany graphs. An entry is any textual description, including titles, footnotes, and legends; it can include symbols to identify graph elements.

The following statements display another of the simpler template definitions—the definition of the scatter plot available in PROC KDE (see Figure 48.6.1 in Chapter 48, “The KDE Procedure,”):

```
proc template;
  define statgraph Stat.KDE.Graphics.ScatterPlot;
    dynamic _TITLE _DEPLABEL _DEPLABEL2;
    BeginGraph;
      EntryTitle _TITLE;
      layout Overlay;
        scatterplot x=X y=Y / markerattrs=GRAPHDATADEFAULT;
      EndLayout;
    EndGraph;
  end;
run;
```

Here, the PROC TEMPLATE and RUN statements have been added to show how you would compile the template if you wanted to modify it. The DEFINE STATGRAPH statement in PROC TEMPLATE begins the graph template definition, and the END statement ends the definition. The DYNAMIC statement defines three dynamic variables that PROC KDE sets at run time. The variable `_Title` provides the title of the graph. The variables `_DepLabel` and `_DepLabel2` contain the names of the X- and Y-variables, respectively. If you were to modify this template, you could use these dynamic text variables in any text element of the graph definition.

The overall display is specified with the LAYOUT OVERLAY statement inside the BEGIN-GRAPH/ENDGRAPH block. The title of the graph is specified with the ENTRYTITLE statement. The main plot is a scatter plot specified with the SCATTERPLOT statement. The options in the SCATTERPLOT statement are given after the slash and specify display options such as marker attributes (symbol, color, and size). These attributes can be specified directly, as in the PROC MDS template, or more typically by using indirect references to style attributes, as in the PROC KDE template. The values of these attributes are specified in the definition of the style you are using and are automatically set to different values if you specify a different style. For more information about style references, see the section “Styles” on page 635 in Chapter 21, “Statistical Graphics Using ODS.” The ENDLAYOUT statement ends the main layout block. For details about the syntax of the graph template language, see the *SAS/GRAPH: Graph Template Language Reference*.

You can write your own templates and use them to display raw data or output from procedures. For example, consider the iris data from [Example 33.1](#) of Chapter 33, “The DISCRIM Procedure.” The iris data set is available from the Sashelp library.

The following statements create a template for a scatter plot of the variables PetalLength and PetalWidth with a legend:

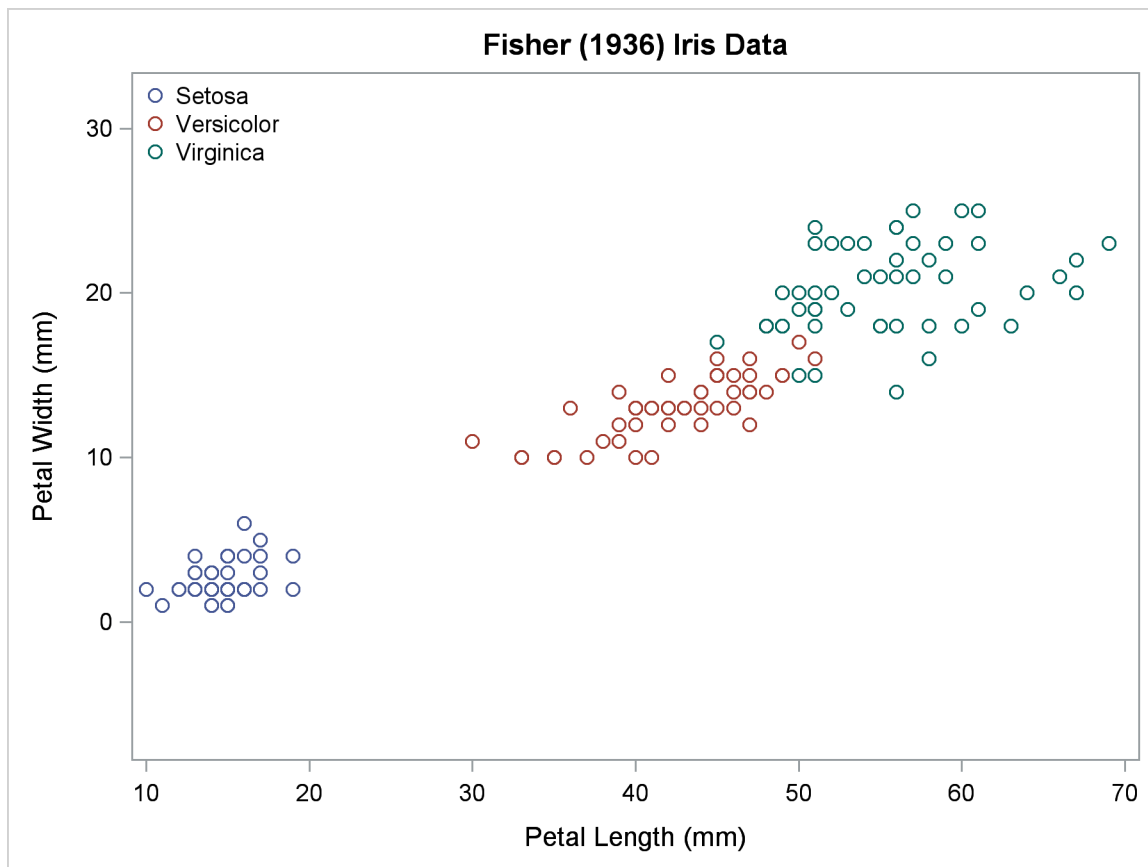
```
proc template;
  define statgraph scatter;
    beginnograph;
      entrytitle 'Fisher (1936) Iris Data';
      layout overlayequated / equatetype=fit;
        scatterplot x=petalength y=petalwidth /
          group=species name='iris';
      layout gridded / autoalign=(topleft);
        discretelegend 'iris' / border=false opaque=false;
      endlayout;
    endlayout;
  endnograph;
end;
run;
```

The layout is OVERLAYEQUATED, which equates the axes in the plot. However, unlike the PROC MDS template, which used EQUATETYPE=SQUARE to make a square plot, the EQUATETYPE=FIT option specifies that the lengths of the axes in this plot should fill the entire plotting area. A legend is placed internally in the top-left portion of the plot. There are three groups of observations, indicated by the three species, and each group is plotted with a separate color and symbol that depends on the ODS style. The legend identifies each group. The NAME= option provides the link between the SCATTERPLOT statement and the DISCRETELEGEND statement. An explicit link is needed since some graphical displays are based on multiple plotting statements.

The following step creates the plot by using the SGRENDER procedure, the Sashelp.Iris data set, and the custom template `scatter`:

```
proc sgrender data=sashelp.iris template=scatter;
run;
```

The syntax of PROC SGRENDER is very simple, because all of the graphical options appear in the template. The scatter plot in [Figure 22.1](#) shows the results.

Figure 22.1 Petal Width and Petal Length in Three Iris Species

The intent of this example is to illustrate how you can write a template to create a scatterplot. PROC TEMPLATE and PROC SGRENDER provide you with the power to create highly customized displays. However, usually you can use the SGPLOT, SGSCATTER or SGPANEL procedures instead, which are much simpler to use. These procedures are discussed in the section “Statistical Graphics Procedures” on page 682 in Chapter 21, “Statistical Graphics Using ODS.” See the section “Grouped Scatter Plot with PROC SGPLOT” on page 598 and Figure 21.12 in Chapter 21, “Statistical Graphics Using ODS,” for an example that plots these data with PROC SGPLOT.

Locating Templates

Before you can customize a graph, you must determine which template is used to create the original graph. You can do this by submitting the ODS TRACE ON statement before the procedure statements that create the graph. The fully qualified template name is displayed in the SAS log. Here is an example:

```
ods trace on;
ods graphics on;

proc reg data=sashelp.class;
  model Weight = Height;
run; quit;
```

The preceding statements create the following trace output, which provides information about both the graphs and tables produced by PROC REG:

Output Added:

Name: NObs
 Label: Number of Observations
 Template: Stat.Reg.NObs
 Path: Reg.MODEL1.Fit.Weight.NObs

Output Added:

Name: ANOVA
 Label: Analysis of Variance
 Template: Stat.REG.ANOVA
 Path: Reg.MODEL1.Fit.Weight.ANOVA

Output Added:

Name: FitStatistics
 Label: Fit Statistics
 Template: Stat.REG.FitStatistics
 Path: Reg.MODEL1.Fit.Weight.FitStatistics

Output Added:

Name: ParameterEstimates
 Label: Parameter Estimates
 Template: Stat.REG.ParameterEstimates
 Path: Reg.MODEL1.Fit.Weight.ParameterEstimates

Output Added:

Name: DiagnosticsPanel
 Label: Fit Diagnostics
 Template: Stat.REG.Graphics.DiagnosticsPanel
 Path: Reg.MODEL1.ObwiseStats.Weight.DiagnosticPlots.DiagnosticsPanel

Output Added:

Name: ResidualPlot
 Label: Height
 Template: Stat.REG.Graphics.ResidualPlot
 Path: Reg.MODEL1.ObwiseStats.Weight.ResidualPlots.ResidualPlot

Output Added:

```

-----
Name:          FitPlot
Label:         Fit Plot
Template:      Stat.REG.Graphics.Fit
Path:          Reg.MODEL1.ObwiseStats.Weight.FitPlot
-----

```

This is also illustrated in [Example 22.1](#) and the section “The ODS Statement” on page 519 in Chapter 20, “Using the Output Delivery System.”

Displaying Templates

Once you have found the fully qualified name of a template, you can display its definition (source program) by using one of these methods:

- Open the Templates window by issuing the command **odstemplates** (**odst** for short) in the command line of the SAS windowing environment. The template window is shown in [Figure 22.2](#). If you expand the Sashelp.Tmplmst node, you can view all the available templates and double-click any template icon to display its definition. This is illustrated in [Example 22.1](#).
- Use the SOURCE statement in PROC TEMPLATE to display a template definition in the SAS log or write the definition to a file.

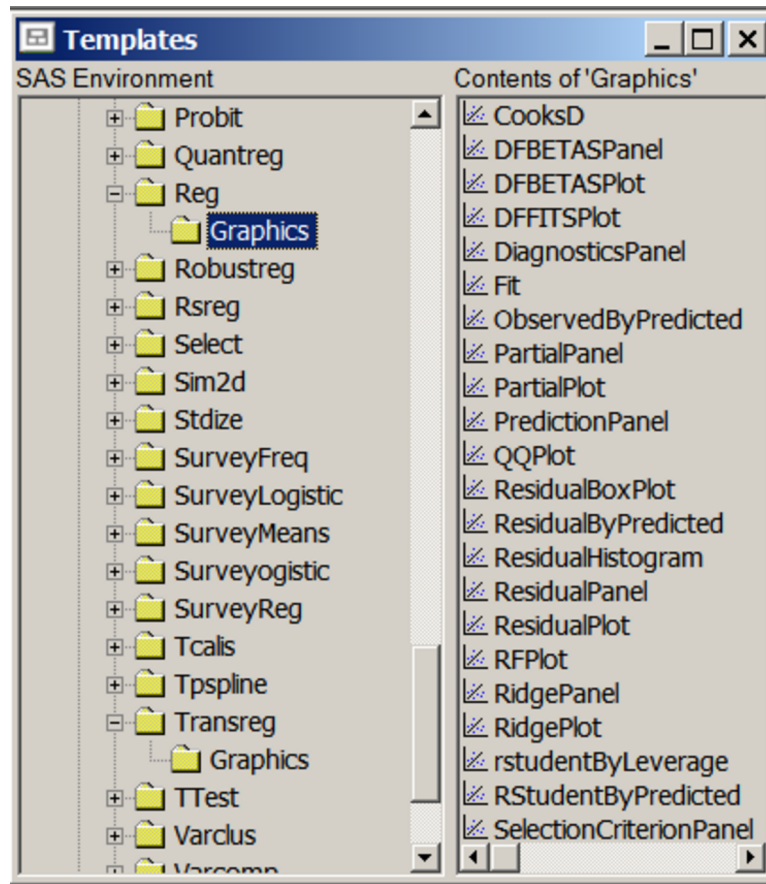
For example, the following statements display the template for the PROC REG residual plot:

```

proc template;
  source Stat.REG.Graphics.ResidualPlot;
run;

```

Figure 22.2 Requesting the Templates Window in the Command Line



The template is displayed as follows:

```

define statgraph Stat.Reg.Graphics.ResidualPlot;
  notes "Residual Plot";
  dynamic _XVAR _SHORTXLABEL _TITLE _LOESSLABEL _DEPNAME
    _MODELLABEL _SMOOTH;
  BeginGraph;
    entrytitle halign=left textattrs=GRAPHVALUETEXT
      _MODELLABEL halign=center
      textattrs=GRAPHTITLETEXT _TITLE " for " _DEPNAME;
    entrytitle textattrs=GRAPHVALUETEXT _LOESSLABEL;
    layout overlay / xaxisopts=(shortlabel=_SHORTXLABEL);
    referenceline y=0;
    scatterplot y=RESIDUAL x=_XVAR / primary=true
      rolename=(tip1=OBSERVATION _id1=ID1 _id2=ID2
        _id3=ID3 _id4=ID4 _id5=ID5) tip=(y x
        _tip1 _id1 _id2 _id3 _id4 _id5);
    if (EXISTS(_SMOOTH))
      loessplot y=_SMOOTH x=_XVAR /
        tiplabel=(y="Smoothed Residual");
    endif;
  endlayout;
EndGraph;
end;

```

PROC TEMPLATE also tells you where the template is located. In this case, it prints the following note:

```
NOTE: Path 'Stat.Reg.Graphics.ResidualPlot' is in: SASHELP.TMPLMST.
```

The word “Path” in ODS has several meanings. In this context, it refers to any name or label hierarchy. In the note, the levels of the template name form a path. In the trace output, the levels of the plot name form a different path.

Editing Templates

You can modify the format and appearance of a particular graph by doing the following:

- Modify its template definition (source program).
- Submit the revised template to create a new compiled template, which is stored in a template store.
- Ensure that the ODS template search path includes the template store that contains your new template.

Template stores are designated read-only (such as Sashelp.Tmplmst) or updatable (such as Sasuser.Templat).

If you view the templates in an updatable template store from the Templates window, you can select **Open** or **Edit** from the pop-up menu. Either the Template Browser or Template Editor window opens. In the Template Editor window, you can make changes and submit the code directly. For read-only templates or when you select **Open**, the Template Browser window opens and you must copy the definition to an editor window to make changes. Since templates supplied by SAS are in the read-only Sashelp library, an easy way to obtain an editable program file is to use the SOURCE statement with the FILE= option in PROC TEMPLATE to write the template definition to a file as follows:

```
proc template;
  source Stat.REG.Graphics.ResidualPlot / file="residtpl.sas";
run;
```

By default, the file is saved in the SAS current folder. Alternatively, you can omit the slash and the FILE= option and copy and paste the source from the SAS log into an editor. Either way, you must add a PROC TEMPLATE statement before the generated source statements and optionally a RUN statement after the END statement before you submit your modified definition.

Graph definitions are self-contained and do not support inheritance (via the PARENT= option) as do table definitions. Consequently, the EDIT statement in PROC TEMPLATE is not supported for graph definitions.

Here are some important points about what you can and cannot change in a template supplied by SAS while preserving its overall functionality:

- Do not change the template name. A statistical procedure can access only a predefined list of templates. If you change the name, the procedure cannot find your template. You must keep the original name and make sure that it is in a template store that is searched before Sashelp.Tmplmst. You control this with the ODS PATH statement (see the section “[The Default Template Stores and the Template](#)”).

[Search Path](#)” on page 634 in Chapter 21, “[Statistical Graphics Using ODS](#),” the section “[Saving Customized Templates](#)” on page 715, and subsequent sections for more information about the template search path and the ODS PATH statement).

- Do not change the names of columns. The underlying data object contains predefined column names that you must use. Be very careful if you change how a column is used in a template. Usually, columns are not interchangeable.
- Do not change the names of DYNAMIC variables. Procedures set values only for a predefined list of dynamic variables. Changing dynamic variable names can lead to runtime errors. Do not add dynamic variables, because the procedure cannot set their values. A few procedures document additional dynamic variables that can be defined in the template if you want to add more information to the output, such additional statistics in an inset table. See the sections “[Modifying the Layout and Adding a New Inset Table](#)” on page 766 and “[Displaying Survival Summary Statistics](#)” on page 784 for examples.
- Do not change the names of statements (for example, from a SCATTERPLOT to a NEEDLEPLOT or other type of plot).

You can change any of the following:

- You can add macro variables that behave like dynamic variables. They are resolved at the time that the statistical procedure is run, and not at the time that the template is compiled. They are defined with an MVAR or NMVAR statement at the beginning the template. You can set the value of each macro variable with a %LET statement before the statistical procedure is run. See [Example 22.6](#). You can also move a variable from a DYNAMIC statement to an MVAR or NMVAR statement if you want to set it yourself rather than letting the procedure set it.
- You can change the graph size.
- You can change graph titles, footnotes, axis labels, and any other text that appears in the graph.
- You can change which plot features are displayed.
- You can change axis features, such as grid lines, offsets, view ports, tick value formatting, and so on.
- You can change the content and arrangement of insets (small tables of statistics embedded in some graphs).
- You can change the legend location, contents, border, background, title, and so on.

See the *SAS/GRAPH: Graph Template Language Reference* for information about the syntax of the statements in the Graph Template Language.

Saving Customized Templates

After you edit the template definition, you can submit your PROC TEMPLATE statements as you would any other SAS program. If you are using the Template Editor window, select **Submit** from the **Run** menu. See [Example 22.1](#). Alternatively, submit your PROC TEMPLATE statements from the Program Editor. ODS automatically saves the compiled template in the first template store that it can update, according to the

currently defined template search path. If you have not changed the template search path, then the modified template is saved in the Sasuser.Templat template store. You can display the current template search path with the following statement:

```
ods path show;
```

The log messages for the default template search path are as follows:

```
Current ODS PATH list is:
```

1. SASUSER.TEMPLAT (UPDATE)
2. SASHELP.TMPLMST (READ)

If you want to store modified templates in another template store, you can use the ODS PATH statement to add that template store to the front of the list. To use these templates, you must make sure the template search path is set correctly before you attempt to access them in the other SAS sessions. See the section “Using Customized Templates” on page 716.

Using Customized Templates

When you create ODS output (either graphs or tables), ODS searches sequentially through each template store in the template search path for a template that matches the one requested. If you have not changed the default template search path, then ODS searches the Sasuser.Templat store first, then Sashelp.Tmplmst. ODS uses the first template that it finds with the requested name. **NOTE:** Templates with the same name can exist in more than one template store.

The ODS PATH statement specifies the template stores to search, as well as the order in which to search them. You can change the default template search path by using the ODS PATH statement. For example, the following statement sets the template search path so that the template store Work.Mystore is searched first, followed by Sashelp.Tmplmst:

```
ods path work.mystore(update) sashelp.tmplmst(read);
```

The UPDATE option provides update access as well as read access to Work.Mystore. The READ option provides read-only access to Sashelp.Tmplmst. With this path, the template store Sasuser.Templat is no longer searched. You can verify this with the following statement:

```
ods path show;
```

The log messages generated by the preceding statement are as follows:

```
Current ODS PATH list is:
```

1. WORK.MYSTORE (UPDATE)
2. SASHELP.TMPLMST (READ)

For more information, see the *SAS Output Delivery System: User’s Guide* and the *SAS/GRAPH: Graph Template Language User’s Guide*. [Example 22.1](#) illustrates all the steps of displaying, editing, saving, and using customized templates.

Reverting to the Default Templates

Customized templates are stored in `Sasuser.Templat` or in some other template store that you create. The templates supplied by SAS are in the read-only template store `Sashelp.Tmplmst`. If you have modified any of the supplied templates and you want to use the original default templates, you can change your template search path as follows:

```
ods path sashelp.tmplmst(read) sasuser.templat(update);
```

This way the default templates are found first. Alternatively, you can save all of your customized templates in a user-defined template store (for example `Mylib.Mystore`). To access these templates, you submit the following statement before running your analysis:

```
libname mylib '.';
ods path mylib.mystore(update) sashelp.tmplmst(read);
```

When you are done, you can reset the default template search path as follows:

```
ods path reset;
```

This restores the template search path to its original state (`sasuser.templat(update) sashelp.tmplmst(read)`). You can also save your customized template as part of your SAS program. You can delete your customized template from the `Sasuser.Templat` template store when you are done, as in the following statements:

```
proc template;
  delete Stat.REG.Graphics.ResidualPlot / store=sasuser.templat;
run;
```

The option `STORE=SASUSER.TEMPLAT` is not required. However, if you have administrator privileges on your computer, this option helps you ensure that you do not accidentally delete templates from `Sashelp.Tmplmst`.

The following note is printed in the SAS log:

```
NOTE: 'Stat.REG.Graphics.ResidualPlot' has been deleted from: SASUSER.TEMPLAT
```

You can run the following step to delete the entire `Sasuser.Templat` store of customized templates:

```
ods path sashelp.tmplmst(read);
proc datasets library=sasuser nolist;
  delete templat(memtype=itemstor);
run;
ods path sasuser.templat(update) sashelp.tmplmst(read);
```

Graph Template Modification Macro

You can use the `%ModTmpl` autocall macro to insert BY line information, titles, and footnotes in ODS Graphics. You can also use it to remove titles and perform other template modifications. See Kuhfeld (2009) for more information about this macro.

You do not have to include autocall macros (for example, with a `%include` statement). You can call them directly once they are properly installed. If your site has installed the autocall libraries supplied by SAS and uses the standard configuration of SAS supplied software, you need to ensure that the SAS system option MAUTOSOURCE is in effect to begin using the autocall macros. For more information about autocall libraries, see the *SAS Macro Language: Reference*. For details about installing autocall macros, consult your host documentation.

The `%ModTmpl1t` macro has the following options:

BY=*by-variable-list*

specifies the list of BY variables. Also see BYLIST=. When graphs are produced (by default or when the STEPS= value contains 'G'), you must specify the BY= option. Otherwise, when you are only modifying the template, you do not need to specify the BY= option. **NOTE:** This option has been rendered obsolete by the BYLINE= option in the ODS GRAPHICS statement.

BYLIST=*by-statement-list*

specifies the full syntax of the BY statement. You can specify a full BY statement syntax including the DESCENDING or NOTSORTED options. If only BY variables are needed, specify only BY=. If you also need options, then specify the BY variables in the BY= option and the full syntax in the BYLIST= option (for example, specify BY=A B and BYLIST=A DESCENDING B). **NOTE:** This option has been rendered obsolete by the BYLINE= option in the ODS GRAPHICS statement.

DATA=*SAS-data-set*

specifies the input SAS data set. If you do not specify the DATA= option, the macro uses the most recently created SAS data set.

FILE=*filename*

specifies the file in which to store the original templates. This is a temporary file. You can specify either a quoted file name or the name from a FILENAME statement that you provide before you call the macro. The default is *"template.txt"*.

OPTIONS=*options*

specifies one or more of the following options (case is ignored):

LOG

displays a note in the SAS log when each BY group has finished.

FIRST

adds the ENTRYTITLE or ENTRYFOOTNOTE statements as the first titles or footnotes. By default, the statements are added after the last titles or footnotes. Most graph templates provided by SAS do not use footnotes; so this option usually affects only entry titles.

NOQUOTES

specifies that the values of the system titles and footnotes are to be moved to the ENTRYTITLE or ENTRYFOOTNOTE statements without the outer quotation marks. With OPTIONS=NOQUOTES, you can specify options in the titles or footnotes in addition to the text. However, you must ensure that you quote the text that provides the actual title or footnote.

The following is an example of an ordinary footnote:

```
footnote "My Footer";
```

With this FOOTNOTE statement and without OPTIONS=NOQUOTES, the macro creates the following ENTRYFOOTNOTE statement:

```
entryfootnote "My Footer";
```

The following footnotes are used with OPTIONS=NOQUOTES:

```
footnote 'halign=left "My Footer"';
footnote2 '"My Second Footer"';
```

With these FOOTNOTE statements and OPTIONS=NOQUOTES, the macro creates the following ENTRYFOOTNOTE statements:

```
entryfootnote halign=left "My Footer";
entryfootnote "My Second Footer";
```

REPLACE

replaces the unconditionally added entry titles and entry footnotes in the templates (those that are not part of IF or ELSE statements) with the system titles and footnotes. The system titles and footnotes are those that are specified in the TITLE or FOOTNOTE statements. You can instead use the TITLES=*SAS-data-set* option to specify titles and footnotes with a data set. If OPTIONS=REPLACE is specified, then OPTIONS=TITLES is ignored.

SOURCE

displays the generated source code. By default, the template source code is not displayed.

TITLES

displays the system titles and footnotes with the graphs. The system titles and footnotes are those that are specified in the TITLE or FOOTNOTE statements. You can instead use the TITLES=*SAS-data-set* option to specify titles and footnotes with a data set. If you also specify OPTIONS=FIRST, the system titles and footnotes are inserted before the previously existing entry titles and entry footnotes in the templates. Otherwise, they are inserted at the end.

You can specify OPTIONS=TITLES or OPTIONS=REPLACE, or insert BY lines, or do both. If you do both, and you do not like where the BY line is inserted relative to your titles and footnotes, just specify OPTIONS=NOQUOTES and `_ByLine0` to place the BY line wherever you choose. The following TITLE statements illustrate:

```
title1 '"My First Title"';
title2 '_byline0';
title3 '"My Last Title"';
```

Also, you can embed BY information in a title or a footnote, again with OPTIONS=NOQUOTES. For example:

```
title '"Spline Fit By Sex, " _byline0';
```

When `_ByLine0` is specified in any of the titles or footnotes, then the usual BY line is not added.

The following example removes all titles and footnotes:

```

footnote;
title;
%modtmpl (options=replace, template=Stat.Transreg.Graphics, steps=t)

```

STATEMENT=*entry-statement-fragment*

specifies the statement that contains the BY line that gets added to the template along with any statement options. The default is **Statement=EntryFootNote halign=left TextAttrs=GraphValueText**. Other examples include:

```

Statement=EntryTitle
Statement=EntryFootNote halign=left TextAttrs=GraphLabelText

```

STEPS=*steps*

specifies the macro steps to run. Case and white space are ignored. the macro modifies the templates (when 'T' is specified), produces the graphs for each BY group (when 'G' is specified), and deletes the modified templates (when 'D' is specified). The default is STEPS=TGD. You can instead have it perform a subset of these three tasks by specifying a subset of terms in the STEPS= option.

When you use the %ModTmpl macro to add BY lines, you usually do not need to delete the templates before you run your procedure again in the normal way. The template modification inserts the BY line through a macro variable and an MVAR statement. When the macro variable _ByLine0 is undefined, the ENTRYTITLE or ENTRYFOOTNOTE statement drops out as if it were not there at all.

```

STMTOPTS1= n ADD | REPLACE | DELETE | BEFORE | AFTER statement-name < options >
STMTOPTS2= n ADD | REPLACE | DELETE | BEFORE | AFTER statement-name < options >
STMTOPTS3= n ADD | REPLACE | DELETE | BEFORE | AFTER statement-name < options >
STMTOPTS4= n ADD | REPLACE | DELETE | BEFORE | AFTER statement-name < options >
STMTOPTS5= n ADD | REPLACE | DELETE | BEFORE | AFTER statement-name < options >
STMTOPTS6= n ADD | REPLACE | DELETE | BEFORE | AFTER statement-name < options >
STMTOPTS7= n ADD | REPLACE | DELETE | BEFORE | AFTER statement-name < options >
STMTOPTS8= n ADD | REPLACE | DELETE | BEFORE | AFTER statement-name < options >
STMTOPTS9= n ADD | REPLACE | DELETE | BEFORE | AFTER statement-name < options >
STMTOPTS10= n ADD | REPLACE | DELETE | BEFORE | AFTER statement-name < options >

```

These ten options add or replace options in up to 10 selected statements. The following example illustrates:

```

%modtmpl (template=Stat.glm.graphics.residualhistogram, steps=t,
          stmtopts1=. add discretelegend autoalign=(topleft),
          stmtopts2=1 add densityplot legendlabel='Normal Density',
          stmtopts3=2 add densityplot legendlabel='Kernel Density',
          stmtopts4=1 add overlay yaxisopts=(griddisplay=on)
          yaxisopts=(label='Normal and Kernel Density'))

proc glm plots=diagnostics(unpack) data=sashelp.class;
  model weight = height;
run;

```

```
%modtmpl (template=Stat.glm.graphics.residualhistogram, steps=d)
```

These options require you to specify a series of values. The first value is the statement number (or missing to modify options on all statements that match the statement name). The second value is: ADD, REPLACE, DELETE, BEFORE, or AFTER. When the second value is ADD or REPLACE, it controls whether you add new options or replace existing options. Alternatively, the second value can be BEFORE or AFTER to add a new statement before or after the named statement. When the value is DELETE, the corresponding statement is deleted. The third value is a statement name. All remaining options are options for the statement named by the third value (with ADD and REPLACE) or for a new statement (with BEFORE and AFTER). In the STMTOPTS1= example, an option is added to all DISCRETELEGEND statements. In the STMTOPTS2= example, an option is added to the first DensityPlot statement. In the STMTOPTS4= example, an option is added to the LAYOUT OVERLAY statement. In most cases, the statement name is the first name that begins the statement. The LAYOUT statement is an exception. In the case of layouts, specify the second name (OVERLAY, GRIDDED, LATTICE, and so on) for the third value. Note that a statement such as **if (expression) EntryTitle...**; is an IF statement not an ENTRYTITLE statement.

If an option is specified multiple times on a GTL statement, the last specification overrides previous specifications. Hence, you do not need to know and respecify all of the options. You can just add an option to the end, and it overrides the previous value. You can use these options only to modify statements that contain a slash, and only to modify the options that come after the slash. Note that in STMTOPTS4=, the YAXISOPTS= option is specified twice. It could have been equivalently specified once as follows:

```
yaxisopts=(griddisplay=on label='Normal and Kernel Density'))
```

The actual specification adds the GRIDDISPLAY=ON to the Y axis options (which by default has only a label specification). The old label is unchanged until the LABEL= option in the second YAXISOPTS= specification overrides it. In other words, YAXISOPTS=(GRIDDISPLAY=ON) augments the old YAXISOPTS= option; it does not replace it.

The following steps delete the legend and instead provide a footnote:

```
%modtmpl (template=Stat.glm.graphics.residualhistogram, steps=t,
          stmtopts1=. delete discretelegend,
          stmtopts2=1 after begingraph entryfootnote
              textattrs=GraphLabelText (color=cx445694) 'Normal '
              textattrs=GraphLabelText (color=cxA23A2E) 'Kernel')

proc glm plots=diagnostics(unpack) data=sashelp.class;
  model weight = height;
run;

%modtmpl (template=Stat.glm.graphics.residualhistogram, steps=d)
```

TEMPLATE=SAS-template

specifies the name of the template to modify. You can specify just the first few levels to modify a series of templates. For example, to modify all of PROC REG's graph templates, specify TEMPLATE=Stat.Reg.Graphics. This option is required.

TITLES=SAS-data-set

specifies a data set that contains titles or footnotes or both. By default, when the system titles or footnotes are used (when `OPTIONS=TITLES` or `OPTIONS=REPLACE` is specified), PROC SQL is used to determine the titles and footnotes. You can instead create this data set yourself so that you can set the graph titles independently from the system titles and footnotes. The data set must contain two variables: `Type` (`Type='T'` for titles and `Type='F'` for footnotes), and `Text`, which contains the titles and footnotes. Other variables are ignored. Specify the titles and footnotes in the order in which you want them to appear.

TITLEOPTS=entry-statement-options

specifies the options for system titles and footnotes. For example, you can specify the `HALIGN=` and `TEXTATTRS=` options as in the `STATEMENT=` option. By default, no title options are used. With `OPTIONS=NOQUOTES`, you can specify options individually.

Examples of ODS Graphics Template Modification

Example 22.1: Customizing Graphs Through Template Changes

This example shows how to use PROC TEMPLATE to customize the appearance and content of an ODS graph. It is divided into several parts; each part illustrates a different aspect of the template that you can easily change. You are never required to change a template, but you can if you want to change aspects of the plot.

Modifying Graph Titles and Axis Labels

This section illustrates the discussion in the section “Graph Templates” on page 706 in the context of changing the default title and Y-axis label for a Q-Q plot created with PROC ROBUSTREG. The data set `Stack` is created by the following statements:

```
data stack;
  input  x1 x2 x3 y @@;
  datalines;
80 27 89 42    80 27 88 37    75 25 90 37
62 24 87 28    62 22 87 18    62 23 87 18
... more lines ...
;
```

The following statements request a Q-Q plot for robust residuals created by PROC ROBUSTREG:

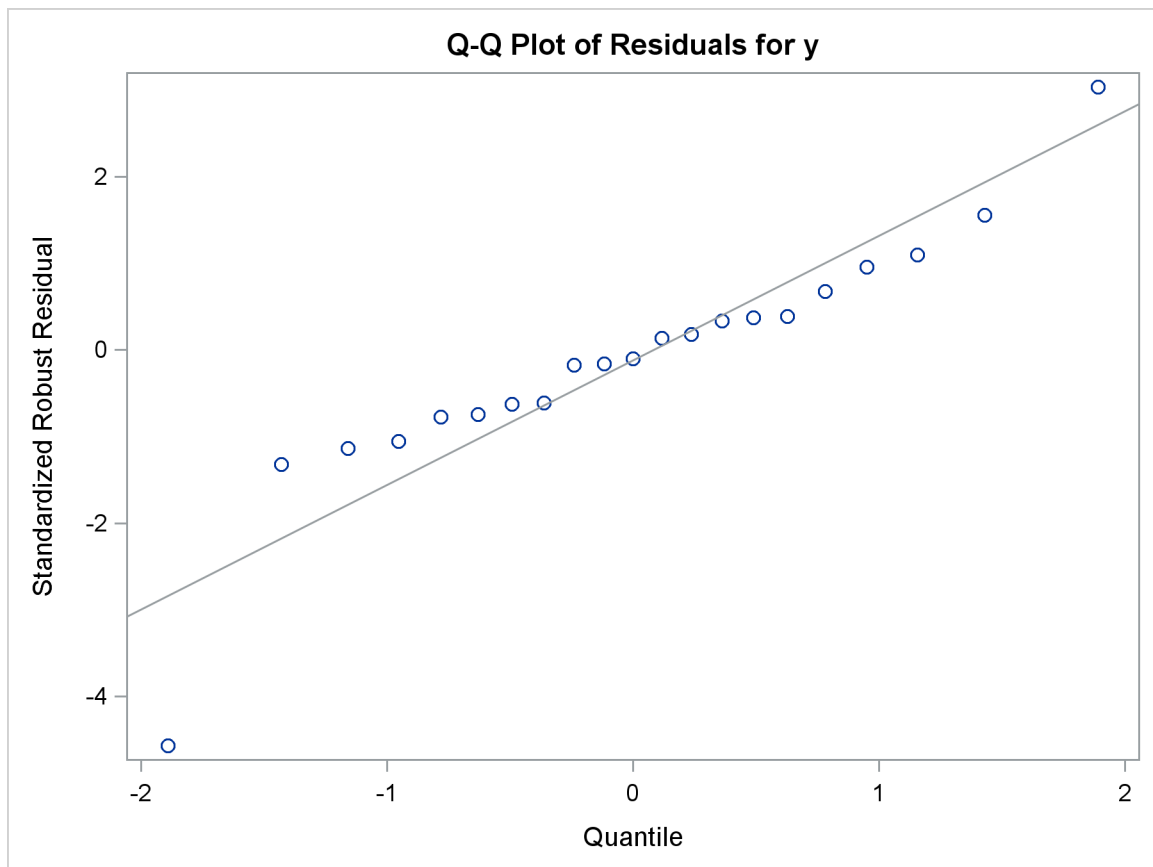
```
ods trace on;
ods graphics on;

proc robustreg data=stack plots=qqplot;
  ods select QQPlot;
  model y = x1 x2 x3;
run;

ods trace off;
```

The Q-Q plot is shown in [Output 22.1.1](#).

Output 22.1.1 Default Q-Q Plot from PROC ROBUSTREG



The ODS TRACE ON statement requests a record of all the ODS output objects created by PROC ROBUSTREG. The trace output is as follows:

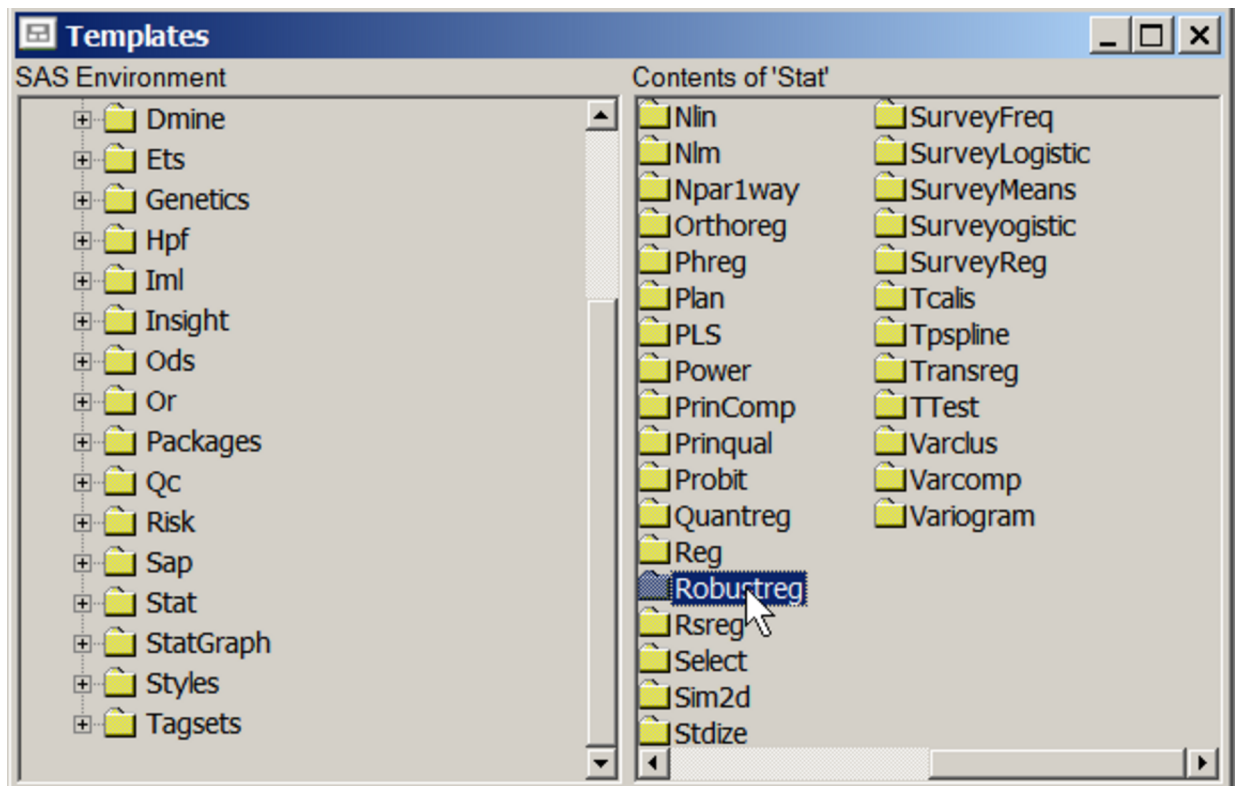
Output Added:

```
-----
Name:      QQPlot
Label:     Residual Q-Q Plot
Template:  Stat.Robustreg.Graphics.QQPlot
Path:     Robustreg.DiagnosticPlots.QQPlot
-----
```

ODS Graphics creates the Q-Q plot from an ODS data object named QQPlot and a graph template named `Stat.Robustreg.Graphics.QQPlot`, which is the default template provided by SAS. Default templates supplied by SAS are saved in the Sashelp.Tmplmst template store (see the section “Graph Templates” on page 706).

To display the default template definition, open the Templates window by typing `odstemplates` (or `odst` for short) in the command line. Expand Sashelp.Tmplmst and click the **Stat** folder. [Output 22.1.2](#) shows the contents of the **Stat** folder.

Output 22.1.2 The Template Window



Next, open the **Robustreg** folder and then open the **Graphics** folder. Then right-click the **QQPlot** template icon and select **Open**. This opens the Template Browser window shown in Output 22.1.3. You can copy this template to an editor to edit it.

Output 22.1.3 Default Template Definition for Q-Q Plot

```

roc template;
  define statgraph Stat.Robustreg.Graphics.QQPlot;
    notes "Q-Q Plot for Standardized Robust Residuals";
    dynamic _DEPLABEL Residual;
    BeginGraph;
      ENTRYTITLE "Q-Q Plot of Residuals for " _DEPLABEL;
      layout Overlay / yaxisopts=(label="Standardized Robust Residual")
        xaxisopts=(label="Quantile");
        SCATTERPLOT y=eval (SORT(DROPMISSING(RESIDUAL))) x=eval (
          PROBIT((NUMERATE(SORT(DROPMISSING(RESIDUAL))) -0.375)/(0.25 + N
(RESIDUAL)))) / primary=true markerattrs=GRAPHDATADEFAULT rolename=(q=eval (
          PROBIT((NUMERATE(SORT(DROPMISSING(RESIDUAL))) -0.375)/(0.25 + N
(RESIDUAL)))) s=eval (SORT(DROPMISSING(RESIDUAL))) tip=(q s) tiplabel=(q=
          "Quantile" s="Residual");
        lineparm slope=eval (STDDEV(RESIDUAL)) Y=eval (MEAN(RESIDUAL)) X=0
          / lineattrs=GRAPHREFERENCE extend=true;
      EndLayout;
    EndGraph;
  end;
run;

```

Alternatively, you can submit the following statements to display the `QQPlot` template definition in the SAS log:

```
proc template;
  source Stat.Robustreg.Graphics.QQPlot;
run;
```

The `SOURCE` statement specifies the fully qualified template name. You can copy and paste the template source into the Program Editor and modify it. The template, with a `PROC TEMPLATE` and `RUN` statement added, is shown next:

```
proc template;
  define statgraph Stat.Robustreg.Graphics.QQPlot;
    notes "Q-Q Plot for Standardized Robust Residuals";
    dynamic _DEPLABEL Residual;
    BeginGraph;
      ENTRYTITLE "Q-Q Plot of Residuals for " _DEPLABEL;
      layout Overlay / yaxisopts=(label="Standardized Robust Residual")
        xaxisopts=(label="Quantile");
      SCATTERPLOT y=eval (SORT(DROPMISSING(RESIDUAL))) x=eval (
        PROBIT((NUMERATE(SORT(DROPMISSING(RESIDUAL))) -0.375)/(0.25
        + N(RESIDUAL)))) / primary=true markerattrs=GRAPHDATADEFAULT
        rolename=(q=eval (
        PROBIT((NUMERATE(SORT(DROPMISSING(RESIDUAL))) -0.375)/(0.25
        + N(RESIDUAL)))) s=eval (SORT(DROPMISSING(RESIDUAL))))
        tip=(q s) tiplabel=(q="Quantile" s="Residual");
      lineparm slope=eval (STDDEV(RESIDUAL)) Y=eval (MEAN(RESIDUAL))
        X=0 / lineattrs=GRAPHREFERENCE extend=true;
    EndLayout;
  EndGraph;
end;
run;
```

In the template, the default title of the Q-Q plot is specified by the `ENTRYTITLE` statement. The variable `_DepLabel` is a dynamic variable that provides the name of the dependent variable in the regression analysis. In this case, the name is `y`. In this template, the label for the axes are specified by the `LABEL=` suboption of the `YAXISOPTS=` option for the `LAYOUT OVERLAY` statement. In other templates, the axis labels come from the column labels of the X-axis and Y-axis columns of the data object. You can see these labels by specifying `ODS OUTPUT` with the plot data object and running `PROC CONTENTS` with the resulting SAS data set.

Suppose you want to change the default title to “Analysis of Residuals”, and you want the Y-axis label to display the name of the dependent variable. First, replace the `ENTRYTITLE` statement with the following statement:

```
entrytitle "Analysis of Residuals";
```

Next, replace the `LABEL=` suboption with the following:

```
label=("Standardized Robust Residual for " _DEPLABEL)
```

You can use dynamic text variables such as `_DepLabel` in any text element.

You can then submit the modified template definition as you would any SAS program, for example, by selecting **Submit** from the **Run** menu. After submitting the PROC TEMPLATE statements, you should see the following message in the SAS log:

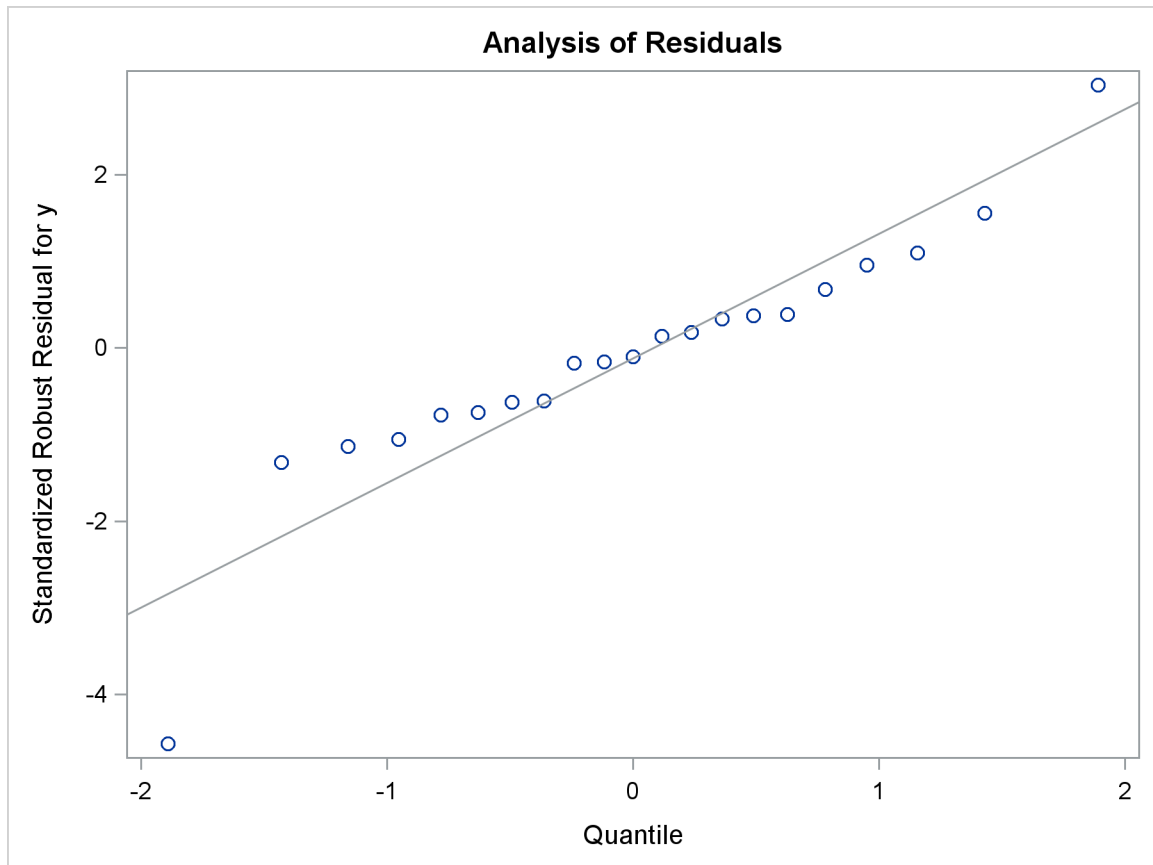
```
NOTE: STATGRAPH 'Stat.Robustreg.Graphics.QQPlot' has been
      saved to: SASUSER.TEMPLAT
```

For more information about graph definitions and the graph template language, see the section “Graph Templates” on page 706.

Finally, resubmit the PROC ROBUSTREG statements to display the Q-Q plot created with your modified template. The following statements create [Output 22.1.4](#):

```
proc template;
  define statgraph Stat.Robustreg.Graphics.QQPlot;
    notes "Q-Q Plot for Standardized Robust Residuals";
    dynamic _DEPLABEL Residual;
    BeginGraph;
      entrytitle "Analysis of Residuals";
      layout Overlay /
        yaxisopts=(label=("Standardized Robust Residual for " _DEPLABEL))
        xaxisopts=(label="Quantile");
        SCATTERPLOT y=eval (SORT(DROPMISSING(RESIDUAL))) x=eval (
          PROBIT((NUMERATE(SORT(DROPMISSING(RESIDUAL))) -0.375)/(0.25
            + N(RESIDUAL)))) / primary=true markerattrs=GRAPHDATADEFAULT
          rolename=(q=eval (
            PROBIT((NUMERATE(SORT(DROPMISSING(RESIDUAL))) -0.375)/(0.25
              + N(RESIDUAL)))) s=eval (SORT(DROPMISSING(RESIDUAL))))
            tip=(q s) tiplabel=(q="Quantile" s="Residual");
          lineparm slope=eval (STDDEV(RESIDUAL)) Y=eval (MEAN(RESIDUAL))
            X=0 / lineattrs=GRAPHREFERENCE extend=true;
      EndLayout;
    EndGraph;
  end;
run;

proc robustreg data=stack plots=qqplot;
  ods select QQPlot;
  model y = x1 x2 x3;
run;
```

Output 22.1.4 Q-Q Plot with Modified Title and Y-Axis Label

If you have not changed the default template search path, the modified template `QQPlot` is used automatically because `Sasuser.Templat` occurs before `Sashelp.Tmplmst` in the ODS search path. See the sections “Saving Customized Templates” on page 715, “Using Customized Templates” on page 716, and “Reverting to the Default Templates” on page 717 for more information about the template search path and the ODS PATH statement.

You do not need to rerun the PROC ROBUSTREG analysis after you modify a graph template if you have stored the plot in an ODS document. After you modify your template, you can submit the PROC DOCUMENT statements in Example 21.4 in Chapter 21, “Statistical Graphics Using ODS,” to replay the Q-Q plot with the modified template. You can run the following statements to revert to the default template:

```
proc template;
  delete Stat.Robustreg.Graphics.QQPlot / store=sasuser.templat;
run;
```

Modifying Colors, Line Styles, and Markers

This section shows you how to customize colors, line attributes, and marker symbol attributes by modifying a graph template. In the `QQPlot` template definition shown in Output 22.1.3, the SCATTERPLOT statement specifies a scatter plot of normal quantiles versus ordered standardized residuals. The attributes of the marker symbol in the scatter plot are specified by: `MarkerAttrs=GraphDataDefault`. This is a reference

to the style element `GraphDataDefault`. See the section “Style Elements and Attributes” on page 638 in Chapter 21, “Statistical Graphics Using ODS,” for more information.

The actual value of the marker symbol depends on the style that you are using. In this case, since the `HTMLBLUE` style is used, the marker symbol is a circle. You can specify a filled circle as the marker symbol by overriding the symbol portion of the style specification as follows: `MarkerAttrs=GraphDataDefault(symbol=CircleFilled)`.

The value of the `SYMBOL=` option can be any valid marker symbol or a reference to a style attribute of the form `style-element:attribute`. It is recommended that you use style attributes because they are chosen to provide consistency and appropriate emphasis based on display principles for statistical graphics. If you specify values directly in a template, you are overriding the style and you run the risk of creating a graph that is inconsistent with the style definition. For more information about the syntax of the Graph Template Language and style elements for graphics, see the *SAS/GRAPH: Graph Template Language Reference* and the *SAS Output Delivery System: User's Guide*.

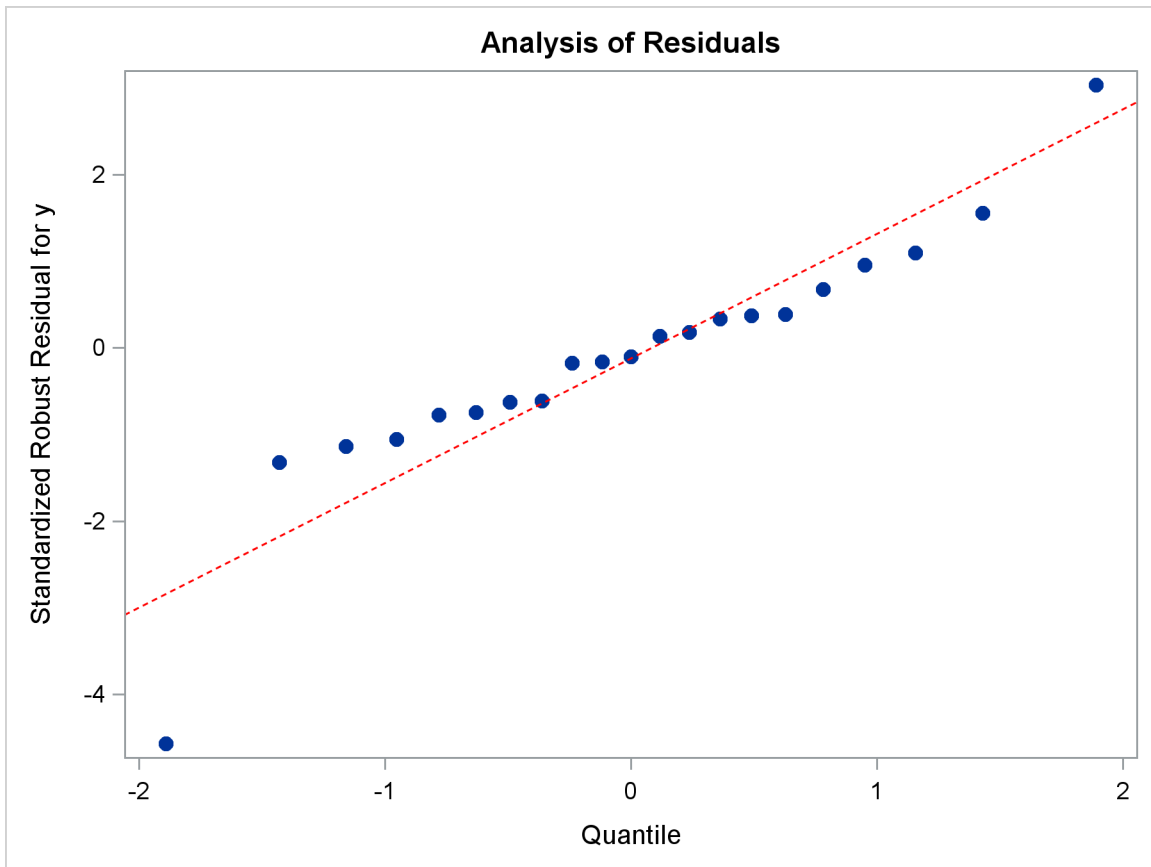
Similarly, you can change the line color and pattern with the `LINEATTRS=` option in the `LINEPARM` statement. The `LINEPARM` statement displays a straight line specified by slope and intercept parameters. The following option changes the color of the line to red and the line pattern to dashed, by overriding those aspects of the style specification: `LineAttrs=GraphReference(color=red pattern=dash)`. To see the results, submit the modified template definition and the `PROC ROBUSTREG` statements as follows to create [Output 22.1.5](#):

```
proc template;
  define statgraph Stat.Robustreg.Graphics.QQPlot;
    notes "Q-Q Plot for Standardized Robust Residuals";
    dynamic _DEPLABEL Residual;
    BeginGraph;
      entrytitle "Analysis of Residuals";
      layout Overlay /
        yaxisopts=(label=("Standardized Robust Residual for " _DEPLABEL))
        xaxisopts=(label="Quantile");
        SCATTERPLOT y=eval (SORT(DROPMISSING(RESIDUAL))) x=eval (
          PROBIT( (NUMERATE(SORT(DROPMISSING(RESIDUAL))) -0.375)/(0.25
            + N(RESIDUAL)))) / primary=true
          markerattrs=GraphDataDefault(symbol=CircleFilled)
          rolename=(q=eval (
            PROBIT( (NUMERATE(SORT(DROPMISSING(RESIDUAL))) -0.375)/(0.25
              + N(RESIDUAL)))) s=eval (SORT(DROPMISSING(RESIDUAL))))
            tip=(q s) tiplabel=(q="Quantile" s="Residual");
        lineparm slope=eval (STDDEV(RESIDUAL)) Y=eval (MEAN(RESIDUAL))
          X=0 / lineattrs=GraphReference(color=red pattern=dash)
          extend=true;
      EndLayout;
    EndGraph;
  end;
run;

ods graphics on;

proc robustreg data=stack plots=qqplot;
  ods select QQPlot;
  model y = x1 x2 x3;
run;
```

Output 22.1.5 Q-Q Plot with Modified Marker Symbols and Line



Alternatively, you can replay the plot with PROC DOCUMENT, as in [Example 21.4](#) in Chapter 21, “Statistical Graphics Using ODS.”

Modifying Tick Marks and Grid Lines

This section illustrates how to modify axis tick marks and control grid lines. For example, you can specify the following statement to request tick marks ranging from -4 to 2 in the Y-axis:

```
layout Overlay / yaxisopts=(linearopts=(tickvaluelist=(-4 -3 -2 -1 0 1 2)));
```

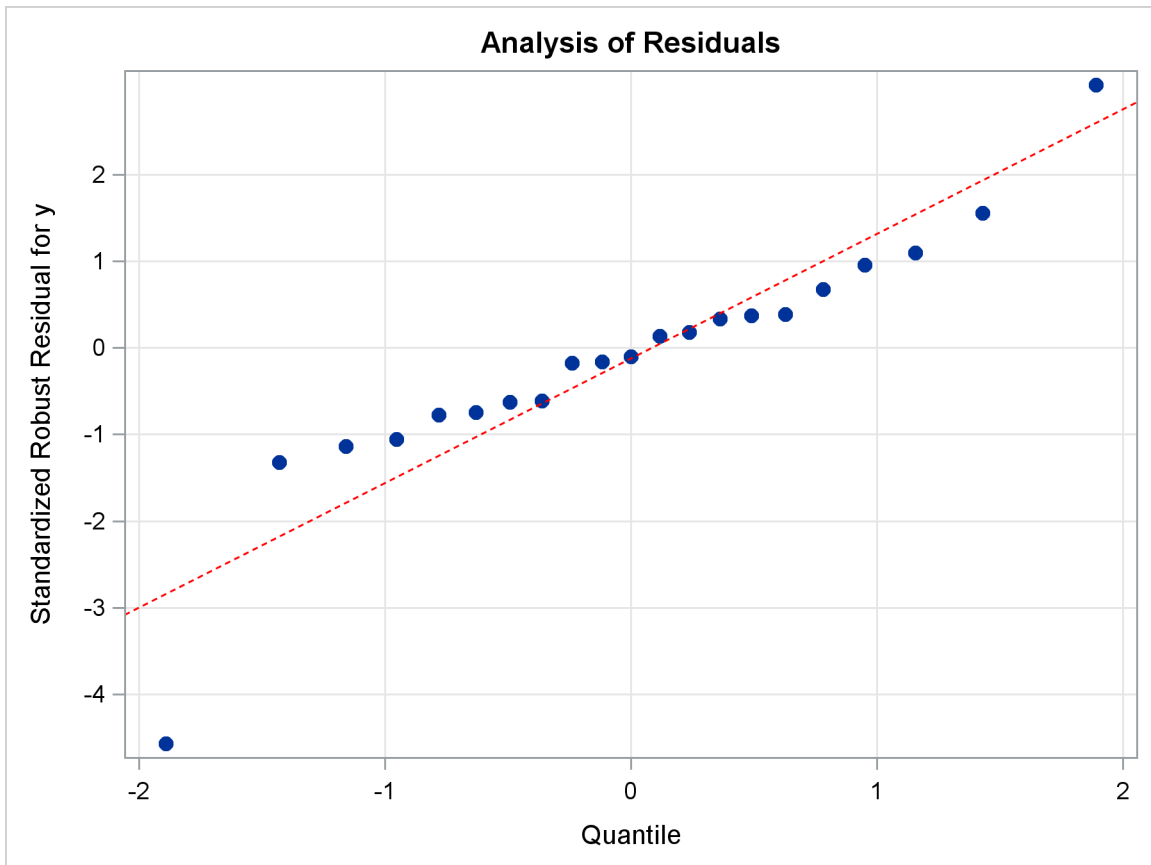
The LINEAROPTS= option is used for standard linearly scaled axes (as opposed to log-scaled axes). You use the TICKVALUELIST= to specify the tick marks.

You can control the grid lines by using the GRIDDISPLAY= suboption in the YAXISOPTS= option. Typically, you specify either GRIDDISPLAY=AUTO_OFF (grid lines are not displayed unless the `GraphGridLines` element in the current style contains `DisplayOpts="ON"`) or GRIDDISPLAY=AUTO_ON (grid lines are displayed unless the `GraphGridLines` element in the current style contains `DisplayOpts="OFF"`). Here, the template is modified by specifying GRIDDISPLAY=AUTO_ON for both axes. The following statements produce [Output 22.1.6](#):

```
proc template;
  define statgraph Stat.Robustreg.Graphics.QQPlot;
    notes "Q-Q Plot for Standardized Robust Residuals";
    dynamic _DEPLABEL Residual;
    BeginGraph;
      entrytitle "Analysis of Residuals";
      layout Overlay / yaxisopts=(gridDisplay=Auto_On
        linearopts=(tickvaluelist=(-4 -3 -2 -1 0 1 2))
        label=("Standardized Robust Residual for " _DEPLABEL))
        xaxisopts=(gridDisplay=Auto_On label="Quantile");
      SCATTERPLOT y=eval (SORT(DROPMISSING(RESIDUAL))) x=eval(
        PROBIT((NUMERATE(SORT(DROPMISSING(RESIDUAL))) -0.375)/(0.25
          + N(RESIDUAL)))) / primary=true
        markerattrs=GraphDataDefault(symbol=CircleFilled)
        rolename=(q=eval (
          PROBIT((NUMERATE(SORT(DROPMISSING(RESIDUAL))) -0.375)/(0.25
            + N(RESIDUAL)))) s=eval (SORT(DROPMISSING(RESIDUAL))))
        tip=(q s) tiplabel=(q="Quantile" s="Residual");
      lineparm slope=eval (STDDEV(RESIDUAL)) Y=eval (MEAN(RESIDUAL))
        X=0 / lineattrs=GraphReference(color=red pattern=dash)
        extend=true;
    EndLayout;
  EndGraph;
end;
run;

ods graphics on;

proc robustreg data=stack plots=qqplot;
  ods select QQPlot;
  model y = x1 x2 x3;
run;
```

Output 22.1.6 Q-Q Plot with Modified Y-Axis Tick Marks and Grids

You can restore the default template by running the following step:

```
proc template;
  delete Stat.Robustreg.Graphics.QQPlot / store=sasuser.templat;
run;
```

See the section “[Modifying the Style to Show Grid Lines](#)” on page 731 for more information about grid lines.

Modifying the Style to Show Grid Lines

The section “[Modifying Tick Marks and Grid Lines](#)” on page 730 explains that grid lines in graphs are controlled both by template options and by the style. Some graphs never display grid lines because they would interfere with the display. Some graphs always display grid lines because they are a critical part of the display. In both cases, grid control is so important that the template writer is not willing to give control to the style. If you want to change the grid display setting for these graphs, you must edit their templates. Most templates, however, let the style control the grid lines. They either do not display grid lines unless the style forces them on, or they display grid lines unless the style forces them off. The HTMLBLUE, STATISTICAL, DEFAULT, and most other styles use the setting `DisplayOpts = "Auto"`. Then templates that specify `GRIDDISPLAY=AUTO_OFF` (the default) do not display grid lines, and templates that specify `GRIDDISPLAY=AUTO_ON` do display grid lines. You can easily make a new style with `DisplayOpts`

= "On" or `DisplayOpts = "Off"` if you would prefer to see grid lines more or less often. This example shows how to set `DisplayOpts = "On"`.

First, you need to find the style source for setting grid lines. The following step displays the HTMLBLUE style and its parent styles, STATISTICAL and DEFAULT:

```
proc template;
  source Styles.HTMLBlue;
  source Styles.Statistical;
  source Styles.Default;
run;
```

The advantage of displaying all three styles together is that you can do one search of the results. If grids are defined in the HTMLBLUE style, you will find that first. Otherwise, you will first find the definition in one of the parent styles. An abridged version of the results follows:

```
. . .
class GraphGridLines /
  displayopts = "auto"
  linethickness = 1px
  linestyle = 1
  contrastcolor = GraphColors('ggrid')
  color = GraphColors('ggrid');
. . .
```

You can use this to create a new style that inherits from the HTMLBLUE style, but sets the display options for grids to ON, as in the following example:

```
proc template;
  define style Styles.MyGrids;
    parent=styles.HTMLBlue;
    class GraphGridLines /
      displayopts = "on"
      linethickness = 1px
      linestyle = 1
      contrastcolor = GraphColors('ggrid')
      color = GraphColors('ggrid');
    end;
  run;
```

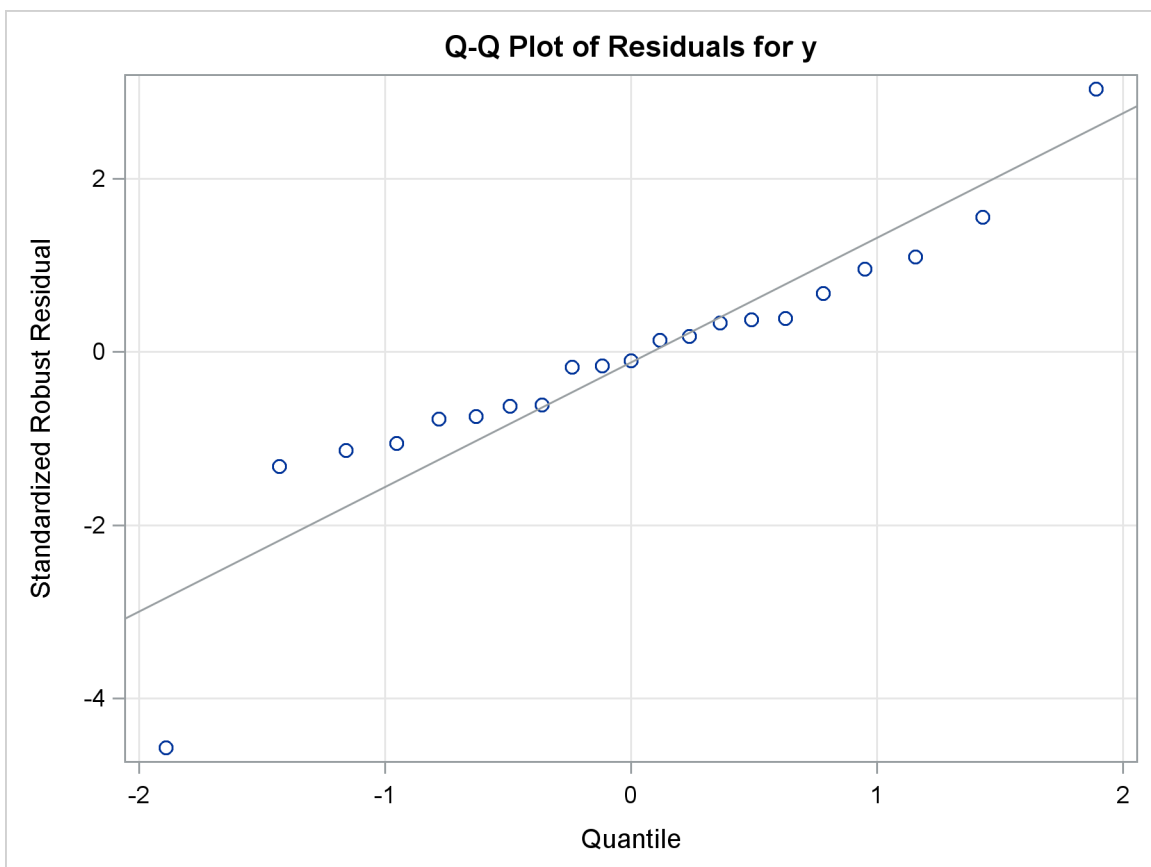
You can use this new style as in the following example:

```
ods graphics on;
ods listing style=mygrids;

proc robustreg data=stack plots=qqplot;
  ods select QQPlot;
  model y = x1 x2 x3;
run;
```

The preceding statements produce [Output 22.1.7](#), which shows the Q-Q plot with grid lines displayed. The default graph template, supplied by SAS, is used because the custom template created in the section “[Modifying Tick Marks and Grid Lines](#)” on page 730 is deleted at the end of that section.

Output 22.1.7 A Style that Makes Grid Lines the Typical Default



Example 22.2: Adding Equations and Special Characters to Fit Plots

This example shows how to run the REG and TRANSREG procedures to get fit plots. The R square, mean, and equation for the regression model are output to data sets, and the results are processed and then displayed in subsequent fit plots. This example also illustrates Unicode and how to add special characters to graphs (for example, $\hat{\mu}$ and R^2). The Unicode Consortium <http://unicode.org/> provides a list of character codes at <http://www.unicode.org/charts/charindex.html>.

Simple Linear Regression

The following step runs PROC REG to fit a simple regression model and creates [Output 22.2.2](#) and [Output 22.2.1](#):

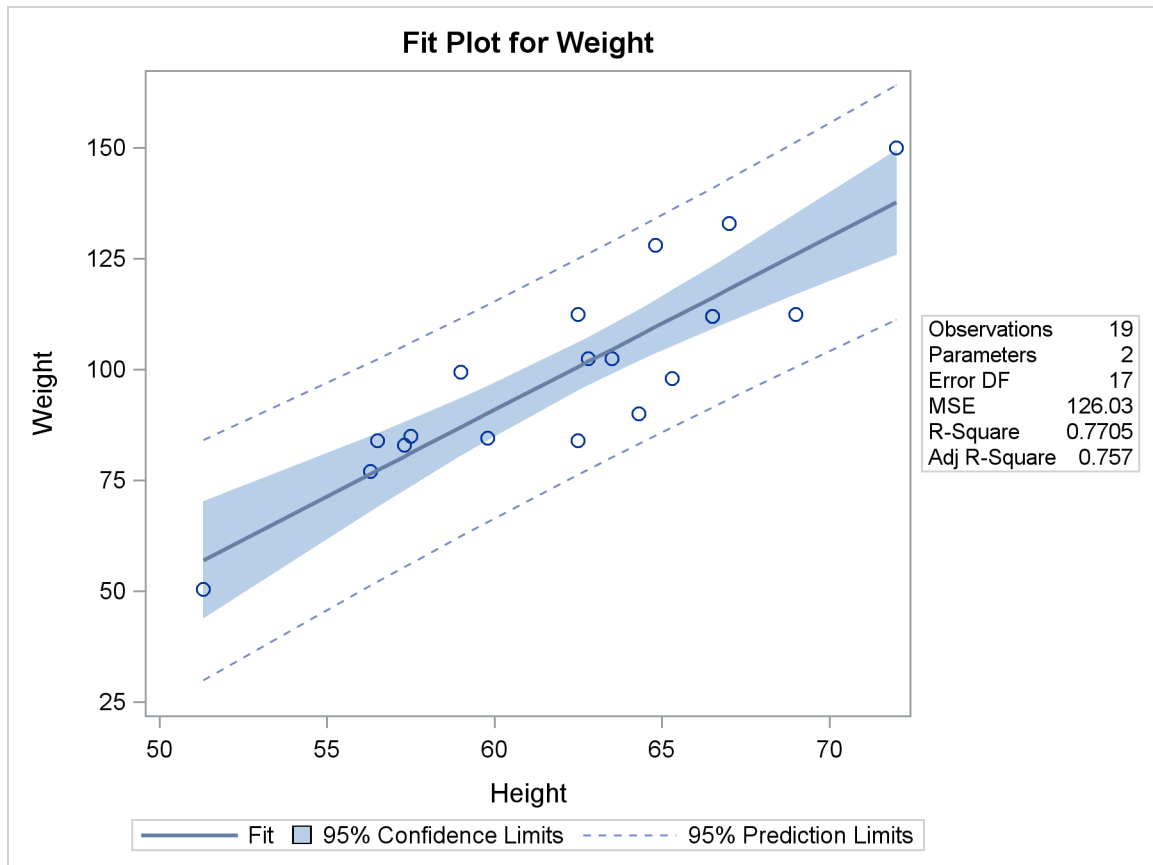
```
ods graphics on;
ods trace on;

proc reg data=sashelp.class;
  model weight = height;
run;
```

Output 22.2.1 PROC REG Output

The REG Procedure					
Model: MODEL1					
Dependent Variable: Weight					
Number of Observations Read		19			
Number of Observations Used		19			
Analysis of Variance					
Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	1	7193.24912	7193.24912	57.08	<.0001
Error	17	2142.48772	126.02869		
Corrected Total	18	9335.73684			
Root MSE		11.22625	R-Square	0.7705	
Dependent Mean		100.02632	Adj R-Sq	0.7570	
Coeff Var		11.22330			
Parameter Estimates					
Variable	DF	Parameter Estimate	Standard Error	t Value	Pr > t
Intercept	1	-143.02692	32.27459	-4.43	0.0004
Height	1	3.89903	0.51609	7.55	<.0001

Output 22.2.2 PROC REG Fit Plot



The fit statistics table following the “Analysis of Variance” table displays the R square and the mean. The last table displays the parameter estimates. This information is produced and processed for inclusion in the fit plot as follows:

```
proc reg data=sashelp.class;
  ods output fitstatistics=fs ParameterEstimates=c;
  model weight = height;
run;

data _null_;
  set fs;
  if _n_ = 1 then call symputx('R2' , put (nvalue2, 4.2) , 'G');
  if _n_ = 2 then call symputx('mean', put (nvalue1, best6.), 'G');
run;
```

```

data _null_;
  set c;
  length s $ 200;
  retain s ' ';
  if _n_ = 1 then
    s = trim(dependent) || ' = ' ||                /* dependent =          */
      put(estimate, best5. -L);                    /* intercept            */
  else if abs(estimate) > 1e-8 then do;           /* skip zero coefficients */
    s = trim(s) || ' ' ||                          /* string so far        */
      scan('+ -', 1 + (estimate < 0), ' ')        /* + (add) or - (subtract) */
      || ' ' ||
      trim(put(abs(estimate), best5. -L))          /* abs(coefficient)     */
      || ' ' || variable;                          /* variable name        */
  end;
  call symputx('formula', trim(s) || ' + e', 'G'); /* e for error added next */
run;

```

Two SAS data sets are made from the tabular output, and the R square, mean, and equation for the regression model are stored in macro variables. The following step uses PROC SGPLOT with an INSET statement to display the linear fit plot along with the R square, mean, and equation for the regression model:

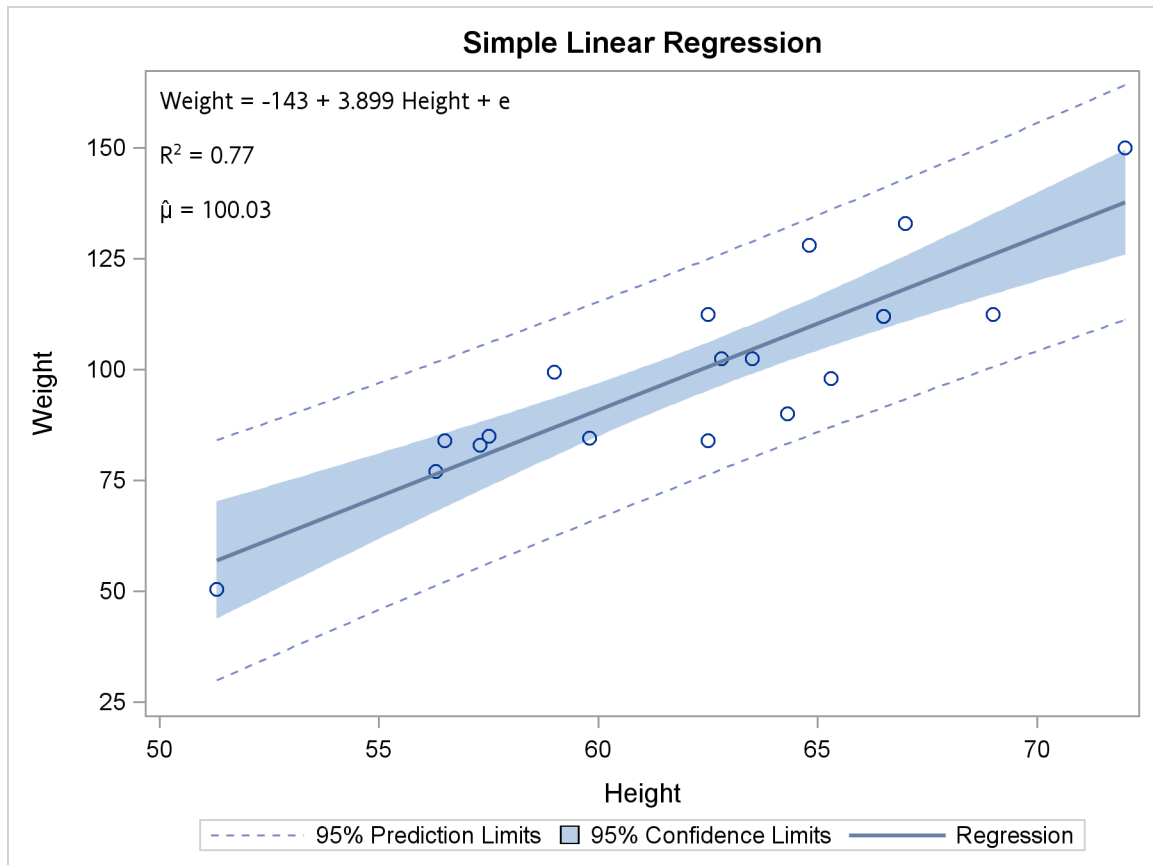
```

proc sgplot data=sashelp.class;
  title 'Simple Linear Regression';
  inset "&formula"
        "R(*ESC*){sup '2'} = &r2"
        "(*ESC*){unicode mu}(*ESC*){unicode hat} = &mean" / position=topleft;
  reg y=weight x=height / clm cli;
run;

```

The results are displayed in [Output 22.2.3](#).

Each separate string in the INSET statement is displayed in a separate line. The first string is the formula, which is generated in the second DATA step. The next string is the R square, and it consists of an 'R', an escaped superscript 2, and the value of R square (which is stored in a macro variable). The string for the mean consists of two Unicode specifications, one for the Greek letter μ , and one to put a hat over it. These special character specifications appear in quotes and are escaped with `(*ESC*)` so that they are processed as special characters rather than as literal text. Typically, you must escape special characters in quotes, and not escape them when they are not in quotes. See the section “Unicode and Special Characters” on page 742 for a list of a few of the more commonly used Unicode characters.

Output 22.2.3 Fit Plot from PROC SGPLOT with Equation

The same information can be added to the graph that PROC REG produces by adding the following statements to the PROC REG template for a fit plot:

```
mvar formula;

layout gridded / autoalign=(topleft topright bottomleft
                           bottomright);
  entry halign=left formula;
  entry halign=left "R"2 " = " eval(put(_rsquare, 4.2));
  entry halign=left "(*ESC*){unicode mu}{(*ESC*){unicode hat} = "
    eval(put(_depmean, best6.))
  / textattrs=GraphValueText
    (family=GraphUnicodeText:FontFamily);

endlayout;
```

The MVAR statement names macro variables whose values are added to the graph. The MVAR statement is added to the PROC REG fit plot template near the top. The LAYOUT GRIDDED block creates a table that consists of the equation, R square, and mean. The LAYOUT GRIDDED block is added to the PROC REG fit plot template inside the LAYOUT OVERLAY. The option `autoalign=(topleft topright bottomleft bottomright)` is used to position the table in a part of the graph that is open, first trying the top left corner.

In this example, in the LAYOUT GRIDDED block, two dynamic variables for R square, and the mean are used instead of the macro variables that were made in previous steps. The origin of the names of

the two dynamic variables that are used in this example are revealed in the next step when the source code for the PROC REG fit plot is displayed. The first ENTRY statement creates a text line for the formula and left-justifies it. The second ENTRY statement creates the R square line. It consists of a literal 'R', a specification for a superscript of 2 (`{sup 2}`), an equal sign surrounded by spaces, and the formatted value of the dynamic variable with the R square. The third ENTRY statement creates the mean line. It consists of two Unicode specifications, one for the Greek letter μ , and one to put a hat over it. These special character specifications appear in quotes (unlike the `{sup 2}`) and are escaped with `(*ESC*)` so that they are processed as special characters rather than as literal text. Typically, you must escape special characters in quotes, and not escape them when they are not in quotes. Note that `sup` along with `sub` (subscript) must not appear in quotes in the GTL, but they can appear in quotes in PROC SGPLOT (as was previously shown). The option `textattrs=GraphValueText (family=GraphUnicodeText:FontFamily)` is specified to ensure that a font that recognizes Unicode characters is used. See the section “Unicode and Special Characters” on page 742 for a list of a few of the more commonly used Unicode characters.

You can use the trace information from the PROC REG step (not shown) and the following step to display the template for the fit plot:

```
proc template;
  source Stat.Reg.Graphics.Fit;
run;
```

Some of the results are as follows:

```
define statgraph Stat.Reg.Graphics.Fit;
  notes "Fit Plot";
  dynamic _DEPLABEL _DEPNAME _MODELLABEL _SHOWSTATS _NSTATSCOLS _SHOWNObs
    _SHOWTOTFREQ _SHOWNParm _SHOWEDF _SHOWMSE _SHOWRSquare _SHOWAdjRSq
    _SHOWSSE _SHOWDepMean _SHOWCV _SHOWAIC _SHOWBIC _SHOWCP _SHOWGMSEP
    _SHOWJP _SHOWPC _SHOWSBC _SHOWSP _NObs _NParm _EDF _MSE _RSquare
    _AdjRSq _SSE _DepMean _CV _AIC _BIC _CP _GMSEP _JP _PC _SBC _SP
    _PREDLIMITS _CONFLIMITS _XVAR _SHOWCLM _SHOWCLI _WEIGHT _SHORTXLABEL
    _SHORTYLABEL _TITLE _TOTFreq;
  BeginGraph;
  entrytitle halign=left textattrs=GRAPHVALUETEXT _MODELLABEL
    halign=center textattrs=GRAPHTITLETEXT _TITLE " for " _DEPNAME;
  layout Overlay / yaxisopts=(label=_DEPLABEL shortlabel=_SHORTYLABEL)
    xaxisopts=(shortlabel=_SHORTXLABEL);
    .
    .
    .
  if (_SHOWRSQUARE^=0)
    entry halign=left "R-Square" / valign=top;
    entry halign=right eval (PUT(_RSQUARE,BEST6.)) / valign=top;
  endif;
    .
    .
    .
  if (_SHOWDEPMEAN^=0)
    entry halign=left "Dependent Mean" / valign=top;
    entry halign=right eval (PUT(_DEPMEAN,BEST6.)) / valign=top;
  endif;
    .
    .
    .
  endif;
```

```

    endlayout;
  EndGraph;
end;

```

The preceding results show that the dynamic variables `_RSquare` and `_DepMean` contain the R square and the mean of the dependent variable. The `MVAR` statement and the `LAYOUT GRIDDED` block can be added to the template, and in the interest of maximizing graph size, the table of statistics can be removed, creating the following template:

```

proc template;
  define statgraph Stat.Reg.Graphics.Fit;
    notes "Fit Plot";
    mvar formula;
    dynamic _DEPLABEL _DEPNAME _MODELLABEL _SHOWSTATS _NSTATSCOLS _SHOWNObs
      _SHOWTOTFREQ _SHOWNParm _SHOWEDF _SHOWMSE _SHOWRSquare _SHOWAdjRSq
      _SHOWSSE _SHOWDepMean _SHOWCV _SHOWAIC _SHOWBIC _SHOWCP _SHOWGMSEP
      _SHOWJP _SHOWPC _SHOWSBC _SHOWSP _NObs _NParm _EDF _MSE _RSquare
      _AdjRSq _SSE _DepMean _CV _AIC _BIC _CP _GMSEP _JP _PC _SBC _SP
      _PREDLIMITS _CONFLIMITS _XVAR _SHOWCLM _SHOWCLI _WEIGHT _SHORTXLABEL
      _SHORTYLABEL _TITLE _TOTFREQ;
    BeginGraph;
    entrytitle halign=left textattrs=GRAPHVALUETEXT _MODELLABEL
      halign=center textattrs=GRAPHTITLETEXT _TITLE " for " _DEPNAME;
    layout Overlay / yaxisopts=(label=_DEPLABEL shortlabel=_SHORTYLABEL)
      xaxisopts=(shortlabel=_SHORTXLABEL);
    if (_SHOWCLM=1)
      BANDPLOT limitupper=UPPERCLMEAN limitlower=LOWERCLMEAN x=_XVAR /
        fillattrs=GRAPHCONFIDENCE connectorder=axis name="Confidence"
        LegendLabel=_CONFLIMITS;
    endif;
    layout gridded / autoalign=(topleft topright bottomleft
      bottomright);
    entry halign=left formula;
    entry halign=left "R"2 " = " eval(put(_rsquare, 4.2));
    entry halign=left "(*ESC*){unicode mu}(*ESC*){unicode hat} = "
      eval(put(_depmean, best6.))
      / textattrs=GraphValueText
      (family=GraphUnicodeText:FontFamily);
    endlayout;
    if (_SHOWCLI=1)
      if (_WEIGHT=1)
        SCATTERPLOT y=PREDICTEDVALUE x=_XVAR / markerattrs=(size=0)
          datatransparency=.6 yerrorupper=UPPERCL yerrorlower=LOWERCL
          name="Prediction" LegendLabel=_PREDLIMITS;
      else
        BANDPLOT limitupper=UPPERCL limitlower=LOWERCL x=_XVAR /
          display=(outline) outlineattrs=GRAPHPREDICTIONLIMITS
          connectorder=axis name="Prediction"
          LegendLabel=_PREDLIMITS;
      endif;
    endif;
    SCATTERPLOT y=DEPVAR x=_XVAR / markerattrs=GRAPHDATADEFAULT primary=
      true rolename=( _tip1=OBSERVATION _id1=ID1 _id2=ID2 _id3=ID3 _id4=
      ID4 _id5=ID5) tip=(y x _tip1 _id1 _id2 _id3 _id4 _id5);
    SERIESPLOT y=PREDICTEDVALUE x=_XVAR / lineattrs=GRAPHFIT
      connectorder=xaxis name="Fit" LegendLabel="Fit";
    if (_SHOWCLI=1 OR _SHOWCLM=1)

```

```

DISCRETELEGEND "Fit" "Confidence" "Prediction" / across=3 HALIGN=
CENTER VALIGN=BOTTOM;
endif;
endlayout;
EndGraph;
end;
run;

```

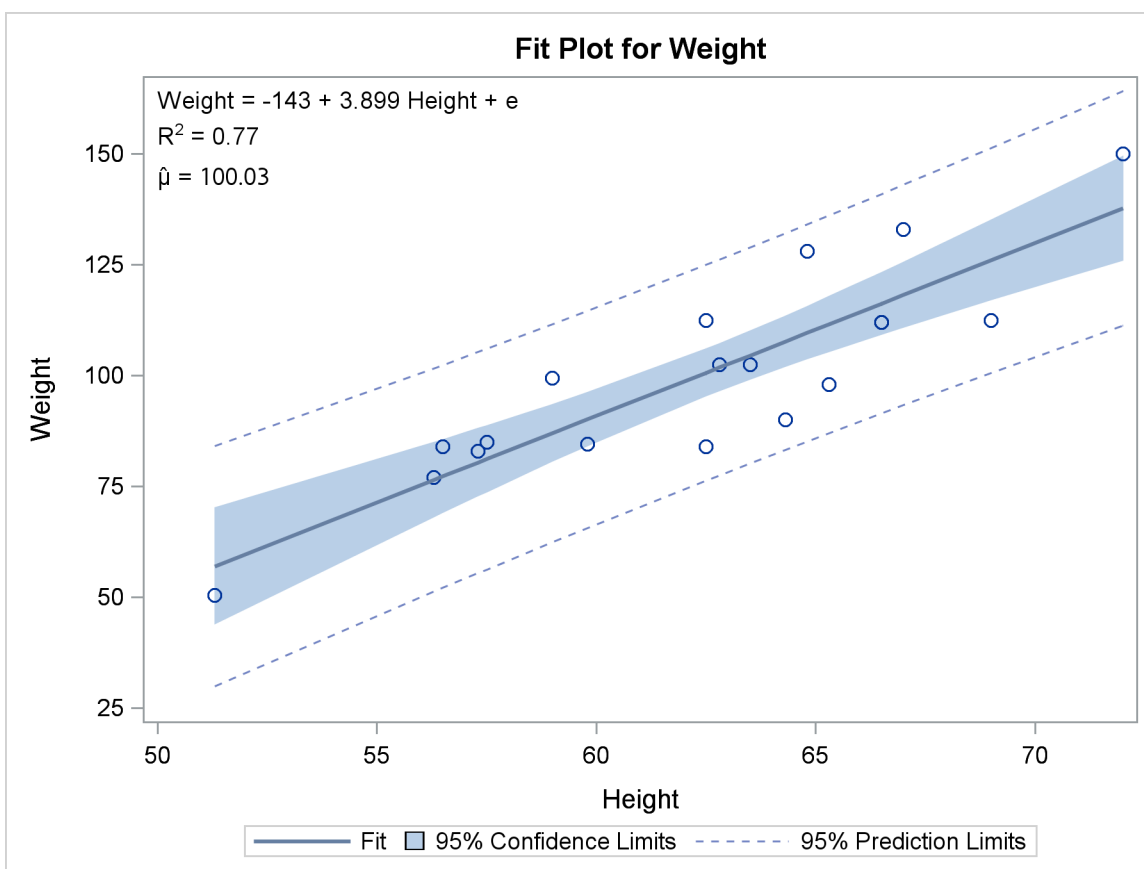
The following step uses the modified template to create [Output 22.2.4](#):

```

proc reg data=sashelp.class;
  model weight = height;
run;

```

Output 22.2.4 PROC REG Fit Plot with the Equation



You can restore the default template by running the following step:

```

proc template;
  delete Stat.Reg.Graphics.Fit / store=sasuser.templat;
run;

```

Cubic Fit Function

The following steps run PROC TRANSREG to find a cubic fit function and display the equation in a plot generated by PROC SGPLOT:

```
proc transreg data=sashelp.class ss2;
  ods output fitstatistics=fs coef=c;
  model identity(weight) = pspline(height);
run;

data _null_;
  set fs;
  if _n_ = 1 then call symputx('R2' , put(value2, 4.2) , 'G');
  if _n_ = 2 then call symputx('mean', put(value1, best6.), 'G');
run;

data _null_;
  set c end=eof;
  length s $ 200 c $ 1;
  retain s ' ';
  if _n_ = 1 then
    s = scan(dependent, 2, '()') || ' = ' || /* dependent = */
      put(coefficient, best5. -L); /* intercept */
  else if abs(coefficient) > 1e-8 then do; /* skip zero coefficients */
    s = trim(s) || ' ' || /* string so far */
      scan('+ -', 1 + (coefficient < 0), ' ') /* + (add) or - (subtract) */
      || ' ' ||
      trim(put(abs(coefficient), best5. -L )) /* abs(coefficient) */
      || ' ' || scan(variable, 2, '._'); /* variable name */
    c = scan(variable, 2, '._'); /* grab power */
    if c ne '1' then /* skip power for linear */
      s = trim(s) || /* string so far */
        "(*ESC*){sup '" || c || "'}"; /* add superscript */
  end; /* e for error added next */
  if eof then call symputx('formula', trim(s) || ' + e', 'G');
run;

proc sgplot data=sashelp.class;
  title 'Cubic Fit Function';
  inset "&formula"
    "R(*ESC*){sup '2'} = &r2"
    "(*ESC*){unicode mu}(*ESC*){unicode hat} = &mean" / position=topleft;
  reg y=weight x=height / degree=3 cli clm;
run;
```

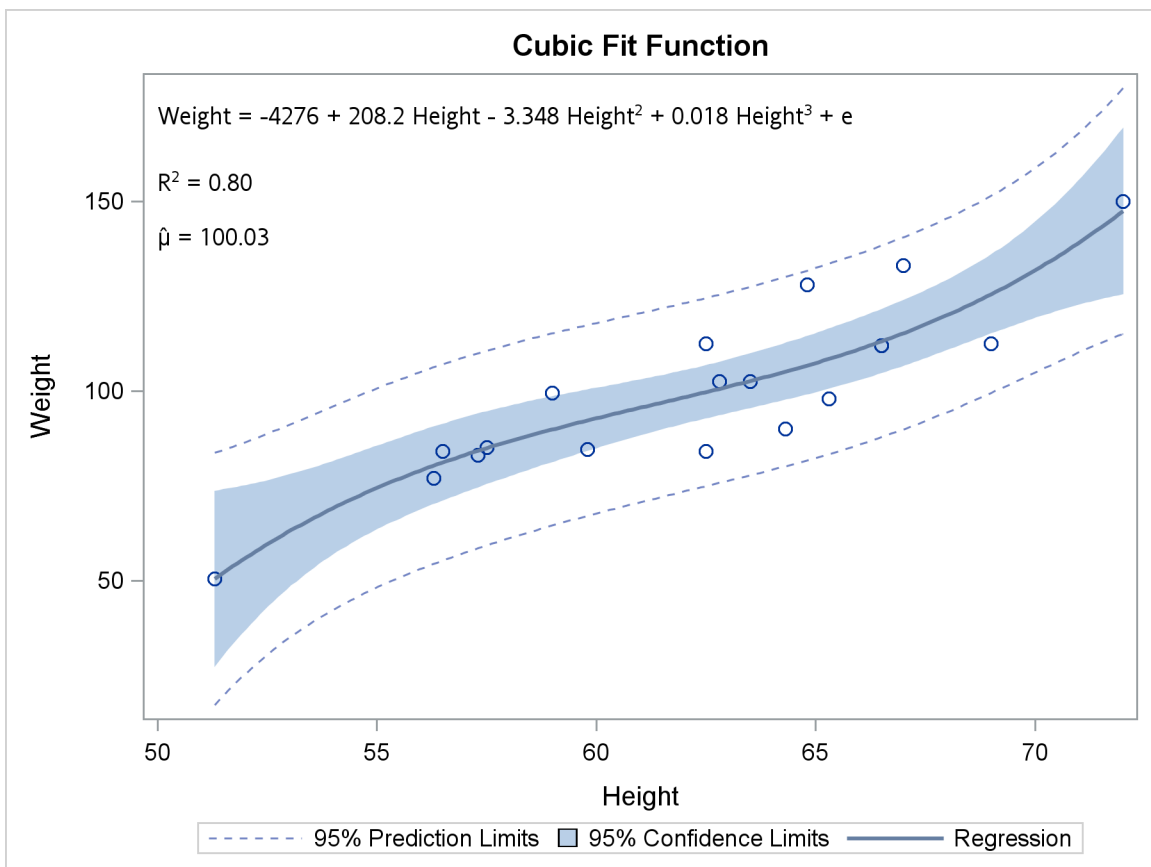
These steps create [Output 22.2.5](#).

The PROC TRANSREG MODEL statement fits a model with an untransformed dependent variable and a cubic polynomial function of the independent variable. By default, PSPLINE fits a cubic polynomial spline with no knots, which is simply a cubic polynomial. The fit statistics and parameter estimates are output to data sets, and their values are stored in macro variables. There are three independent variables plus the intercept. Variable names and exponents are extracted from the TRANSREG parameter names of Pspline.Height_1, Pspline.Height_2, and Pspline.Height_3 by using the SCAN function. Exponents are added by using the specifications "(*ESC*){sup '2'}" and "(*ESC*){sup '3'}", which are explained in

more detail with the INSET statement.

PROC SGPLOT with an INSET statement makes the plot. Each separate string is displayed in a separate line. The first string is the formula, which is generated in the second DATA step. The next string is the R square: it consists of an ‘R’, an escaped superscript 2, and the value of R square (which is stored in a macro variable). The string for the mean consists of two Unicode specifications, one for the Greek letter μ , and one to put a hat over it. These special character specifications appear in quotes and are escaped with `(*ESC*)` so that they are processed as special characters rather than as literal text. Typically, you must escape special characters in quotes, and not escape them when they are not in quotes. See section “Simple Linear Regression” on page 734 for more information about Unicode characters. See the section “Unicode and Special Characters” on page 742 for a list of a few of the more commonly used Unicode characters.

Output 22.2.5 Cubic Fit Function with the Equation



Unicode and Special Characters

The following steps illustrate Unicode specifications for a number of commonly used characters and create Output 22.2.6 and Output 22.2.7, which are charts of Unicode characters:

```
%let l = halign=left;
proc template;
  define statgraph class;
    begingraph / designheight=550px designwidth=520px;
```

```

layout overlay / xaxisopts=(display=none) yaxisopts=(display=none);
  layout gridded / columns=3 autoalign=(topleft);
    entry &l textattrs=(weight=bold) 'Description';
    entry &l textattrs=(weight=bold) 'Displayed';
    entry &l textattrs=(weight=bold) "Unicode";
    entry &l 'R Square';
    entry &l 'R' {sup '2'};
    entry &l "'R' {sup '2'}";
    entry &l 'y hat sub i';
    entry &l 'y' {unicode hat}{sub 'i'};
    entry &l "'y' {unicode hat}{sub 'i'}";
    entry &l 'less than or equal';
    entry &l 'a ' {unicode '2264'x} ' b';
    entry &l "'a ' {unicode '2264'x} ' b'";
    entry &l 'greater than or equal';
    entry &l 'b ' {unicode '2265'x} ' a';
    entry &l "'b ' {unicode '2265'x} ' a'";
    entry &l 'infinity';
    entry &l {unicode '221e'x};
    entry &l "{unicode '221e'x}";
    entry &l 'almost equal';
    entry &l 'a ' {unicode '2248'x} ' b';
    entry &l "'a ' {unicode '2248'x} ' b'";
    entry &l 'combining tilde';
    entry &l 'El nin' {unicode tilde} 'o';
    entry &l "'El nin' {unicode tilde} 'o'";
    entry &l 'grave accent';
    entry &l 'cre' {unicode '0300'x} 'me';
    entry &l "'cre' {unicode '0300'x} 'me'";
    entry &l 'circumflex, acute accent';
    entry &l 'bru' {unicode '0302'x} 'le' {unicode '0301'x} 'e';
    entry &l "'bru' {unicode '0302'x} 'le' {unicode '0301'x} 'e'";
    entry &l 'alpha';
    entry &l {unicode alpha} ' ' {unicode alpha_u};
    entry &l "{unicode alpha} ' ' {unicode alpha_u}";
    entry &l 'beta';
    entry &l {unicode beta} ' ' {unicode beta_u};
    entry &l "{unicode beta} ' ' {unicode beta_u}";
    entry &l 'gamma';
    entry &l {unicode gamma} ' ' {unicode gamma_u};
    entry &l "{unicode gamma} ' ' {unicode gamma_u}";
    entry &l 'delta';
    entry &l {unicode delta} ' ' {unicode delta_u};
    entry &l "{unicode delta} ' ' {unicode delta_u}";
    entry &l 'epsilon';
    entry &l {unicode epsilon} ' ' {unicode epsilon_u};
    entry &l "{unicode epsilon} ' ' {unicode epsilon_u}";
    entry &l 'zeta';
    entry &l {unicode zeta} ' ' {unicode zeta_u};
    entry &l "{unicode zeta} ' ' {unicode zeta_u}";
    entry &l 'eta';
    entry &l {unicode eta} ' ' {unicode eta_u};
    entry &l "{unicode eta} ' ' {unicode eta_u}";
    entry &l 'theta';

```

```

entry &l {unicode theta} ' ' {unicode theta_u};
entry &l "{unicode theta} ' ' {unicode theta_u}";
entry &l 'iota';
entry &l {unicode iota} ' ' {unicode iota_u};
entry &l "{unicode iota} ' ' {unicode iota_u}";
entry &l 'kappa';
entry &l {unicode kappa} ' ' {unicode kappa_u};
entry &l "{unicode kappa} ' ' {unicode kappa_u}";
entry &l 'lambda';
entry &l {unicode lambda} ' ' {unicode lambda_u};
entry &l "{unicode lambda} ' ' {unicode lambda_u}";
entry &l 'mu';
entry &l {unicode mu} ' ' {unicode mu_u};
entry &l "{unicode mu} ' ' {unicode mu_u}";
entry &l 'nu';
entry &l {unicode nu} ' ' {unicode nu_u};
entry &l "{unicode nu} ' ' {unicode nu_u}";
entry &l 'xi';
entry &l {unicode xi} ' ' {unicode xi_u};
entry &l "{unicode xi} ' ' {unicode xi_u}";
entry &l 'omicron';
entry &l {unicode omicron} ' ' {unicode omicron_u};
entry &l "{unicode omicron} ' ' {unicode omicron_u}";
entry &l 'pi';
entry &l {unicode pi} ' ' {unicode pi_u};
entry &l "{unicode pi} ' ' {unicode pi_u}";
entry &l 'rho';
entry &l {unicode rho} ' ' {unicode rho_u};
entry &l "{unicode rho} ' ' {unicode rho_u}";
entry &l 'sigma';
entry &l {unicode sigma} ' ' {unicode sigma_u};
entry &l "{unicode sigma} ' ' {unicode sigma_u}";
entry &l 'tau';
entry &l {unicode tau} ' ' {unicode tau_u};
entry &l "{unicode tau} ' ' {unicode tau_u}";
entry &l 'upsilon';
entry &l {unicode upsilon} ' ' {unicode upsilon_u};
entry &l "{unicode upsilon} ' ' {unicode upsilon_u}";
entry &l 'phi';
entry &l {unicode phi} ' ' {unicode phi_u};
entry &l "{unicode phi} ' ' {unicode phi_u}";
entry &l 'chi';
entry &l {unicode chi} ' ' {unicode chi_u};
entry &l "{unicode chi} ' ' {unicode chi_u}";
entry &l 'psi';
entry &l {unicode psi} ' ' {unicode psi_u};
entry &l "{unicode psi} ' ' {unicode eta_u}";
entry &l 'omega';
entry &l {unicode omega} ' ' {unicode omega_u};
entry &l "{unicode omega} ' ' {unicode omega_u}";
endlayout;
scatterplot y=weight x=height / markerattrs=(size=0);
endlayout;
endgraph;

```

```

end;
run;

proc sgrender data=sashelp.class template=class;
run;

%macro m(u);
  entry halign=left "(*ESC*){unicode &u.x} {unicode &u.x}" /
    textattrs=GraphValueText (family=GraphUnicodeText:FontFamily);
%mend;

proc template;
  define statgraph markers;
    begingraph / designheight=510px designwidth=350px;
    layout overlay / xaxisopts=(display=none) yaxisopts=(display=none);
    layout gridded / columns=1 autoalign=(topright);
      entry " ";
      %m('2193')    %m('002A')    %m('25cb')    %m('25cf')
      %m('25c7')    %m('2666')    %m('003e')    %m('0023')
      %m('2336')    %m('002b')    %m('25a1')    %m('25a0')
      %m('2606')    %m('2605')    %m('22a4')    %m('223c')
      %m('25b3')    %m('25b2')    %m('222a')    %m('0058')
      %m('0059')    %m('005a')
    endlayout;
    scatterplot x=x1 y=y / group=m;
    scatterplot x=x2 y=y / markercharacter=m;
    scatterplot x=x3 y=y / markerattrs=(size=0);
    endlayout;
  endgraph;
end;
run;

%modstyle(name=mark, parent=statistical, markers=
  ArrowDown Asterisk Circle CircleFilled Diamond DiamondFilled GreaterThan
  Hash IBeam Plus Square SquareFilled Star StarFilled Tack Tilde Triangle
  TriangleFilled Union X Y Z, linestyle=1, colors=black)

data x;
  retain x1 1 x2 2 x3 3;
  length m $ 20;
  input m @@;
  y = -_n_;
  datalines;
ArrowDown Asterisk Circle CircleFilled Diamond DiamondFilled GreaterThan
Hash IBeam Plus Square SquareFilled Star StarFilled Tack Tilde Triangle
TriangleFilled Union X Y Z
;

ods listing style=mark;
proc sgrender data=x template=markers;
run;
ods listing;

```

Output 22.2.6 Commonly Used Unicode and Special Characters

Description	Displayed Unicode	
R Square	R^2	'R' {sup '2'}
y hat sub i	\hat{y}_i	'y' {unicode hat}{sub 'i'}
less than or equal	$a \leq b$	'a' {unicode '2264'x} ' b'
greater than or equal	$b \geq a$	'b' {unicode '2265'x} ' a'
infinity	∞	{unicode '221e'x}
almost equal	$a \approx b$	'a' {unicode '2248'x} ' b'
combining tilde	El niño	'El nin' {unicode tilde} 'o'
grave accent	crème	'cre' {unicode '0300'x} 'me'
circumflex, acute accent	brûlée	'bru' {unicode '0302'x} 'le' {unicode '0301'x} 'e'
alpha	α A	{unicode alpha} ' ' {unicode alpha_u}
beta	β B	{unicode beta} ' ' {unicode beta_u}
gamma	γ Γ	{unicode gamma} ' ' {unicode gamma_u}
delta	δ Δ	{unicode delta} ' ' {unicode delta_u}
epsilon	ϵ E	{unicode epsilon} ' ' {unicode epsilon_u}
zeta	ζ Z	{unicode zeta} ' ' {unicode zeta_u}
eta	η H	{unicode eta} ' ' {unicode eta_u}
theta	θ Θ	{unicode theta} ' ' {unicode theta_u}
iota	ι I	{unicode iota} ' ' {unicode iota_u}
kappa	κ K	{unicode kappa} ' ' {unicode kappa_u}
lambda	λ Λ	{unicode lambda} ' ' {unicode lambda_u}
mu	μ M	{unicode mu} ' ' {unicode mu_u}
nu	ν N	{unicode nu} ' ' {unicode nu_u}
xi	ξ Ξ	{unicode xi} ' ' {unicode xi_u}
omicron	o O	{unicode omicron} ' ' {unicode omicron_u}
pi	π Π	{unicode pi} ' ' {unicode pi_u}
rho	ρ P	{unicode rho} ' ' {unicode rho_u}
sigma	σ Σ	{unicode sigma} ' ' {unicode sigma_u}
tau	τ T	{unicode tau} ' ' {unicode tau_u}
upsilon	u Y	{unicode upsilon} ' ' {unicode upsilon_u}
phi	ϕ Φ	{unicode phi} ' ' {unicode phi_u}
chi	χ X	{unicode chi} ' ' {unicode chi_u}
psi	ψ Ψ	{unicode psi} ' ' {unicode eta_u}
omega	ω Ω	{unicode omega} ' ' {unicode omega_u}

Output 22.2.7 Markers, Marker Names, Unicode Characters, Unicode Specifications

↓	ArrowDown	↓ {unicode '2193'x}
*	Asterisk	* {unicode '002A'x}
○	Circle	○ {unicode '25cb'x}
●	CircleFilled	● {unicode '25cf'x}
◇	Diamond	◇ {unicode '25c7'x}
◆	DiamondFilled	◆ {unicode '2666'x}
>	GreaterThan	> {unicode '003e'x}
#	Hash	# {unicode '0023'x}
⊥	IBeam	⊥ {unicode '2336'x}
+	Plus	+ {unicode '002b'x}
□	Square	□ {unicode '25a1'x}
■	SquareFilled	■ {unicode '25a0'x}
☆	Star	☆ {unicode '2606'x}
★	StarFilled	★ {unicode '2605'x}
⊥	Tack	⊥ {unicode '22a4'x}
~	Tilde	~ {unicode '223c'x}
△	Triangle	△ {unicode '25b3'x}
▲	TriangleFilled	▲ {unicode '25b2'x}
∪	Union	∪ {unicode '222a'x}
X	X	X {unicode '0058'x}
Y	Y	Y {unicode '0059'x}
Z	Z	Z {unicode '005a'x}

The Unicode Consortium <http://unicode.org/> provides a list of character codes at <http://www.unicode.org/charts/charindex.html>.

The following rules apply to Unicode and special character specifications in ODS graphics:

- Each character can be specified by looking up its code and specifying it as a hexadecimal constant. Example: `{unicode '221e' x}`.
- Lower case Greek letters can be specified by using names instead of hexadecimal constants. Example: `{unicode alpha}`.
- Upper case Greek letters can be specified by using names followed by `_u` instead of a hexadecimal constants. Example: `{unicode alpha_u}`.
- Superscript and subscript have special abbreviations. Examples: `{sup 2}` and `{sub 2}`.
- The `sup` and `sub` specifications must not appear escaped and in quotes in the GTL. They must appear outside of quotes.
- Some characters overprint the character that comes before. Example: `'El nin' {tilde} 'o'`, which is equivalent to `'El nin' {unicode '0303' x} 'o'` creates 'El niño'.
- Specifications inside quotes are escaped. Example: `"(*ESC*){unicode beta}"`.
- Specifications outside quotes are not escaped. Example: `{unicode beta}`.

Example 22.3: Customizing Survival Plots

The LIFETEST procedure, like other statistical procedures, provides a PLOTS= option and other options for modifying its output without requiring template changes. See Chapter 52, “The LIFETEST Procedure,” for more information. Those options are sufficient for many purposes. This example shows ways that you can change the graph by changing the graph template when those options are not sufficient. The first part of this example shows how to find the name of the template, display the template by using PROC TEMPLATE and the SOURCE statement, and change the title. This approach is sufficient for simple changes.

As this example progresses, a more aggressive approach to template modification is introduced. The survival plot template in PROC LIFETEST is long, and it has distinct components for different scenarios (single stratum versus multiple strata). The same options are often repeated in multiple statements. The next part of the example rewrites the template using macros and macro variables so that it is more modular and easier to modify. The subsequent parts of this example modify the template in other ways by using the rewritten template as the starting point. If you need to change the survival plot template, you too might find it easier to use this rewritten template as a starting point instead of the template as it is displayed by using PROC TEMPLATE and the SOURCE statement.

This example consists of the following parts:

- **Modifying the plot title:** This part identifies the template, displays it, explains its overall structure, and modifies the titles. See the section “Modifying the Plot Title” on page 749.
- **Modifying the axes:** This part explains the options that control the X and Y axes, and shows how to modify the ticks and axis labels. See the section “Modifying the Axes” on page 753.

- **Creating a template that is easy to modify:** This part shows how you can reorganize and modularize the entire template to make it easy to customize it in various ways. See the section “[Creating a Template That Is Easy to Modify](#)” on page 756.
- **Modifying the plot title in the revised template:** This part shows how to change the title by using the revised template. See the section “[Modifying the Plot Title in the Revised Template](#)” on page 762.
- **Modifying the legend and inset table:** This part removes the small inset table and moves the legend inside the graph. The censoring information above the X axis is moved outside the graph. See the section “[Modifying the Legend and Inset Table](#)” on page 763.
- **Modifying the layout and adding a new inset table:** This part moves the event and total information out of the graph and the legend in. It also moves the small inset table. See the section “[Modifying the Layout and Adding a New Inset Table](#)” on page 766.
- **Changing line styles:** This part shows how to modify a style template to change line colors and styles. See the section “[Changing Line Styles](#)” on page 773.
- **Changing fonts:** This part shows how to change the graph template and the style template to change some of the fonts that are used in the graph. See the section “[Changing Fonts](#)” on page 776.
- **Changing how censored data are displayed:** This part shows how to change or remove the plus marks that are used to display censored observations. See the section “[Changing How Censored Data Are Displayed](#)” on page 781.
- **Displaying survival summary statistics:** This part adds to the graph a table with event, censoring and survival information. See the section “[Displaying Survival Summary Statistics](#)” on page 784.

This example uses the bone marrow transplant data set `Sashelp.BMT`, which is also used in Chapter 52, “[The LIFETEST Procedure](#).”

Modifying the Plot Title

This first part of this example changes the default title of the survival plot in PROC LIFETEST from “Product-Limit Survival Estimates” to “Kaplan-Meier Plot” through a template change.

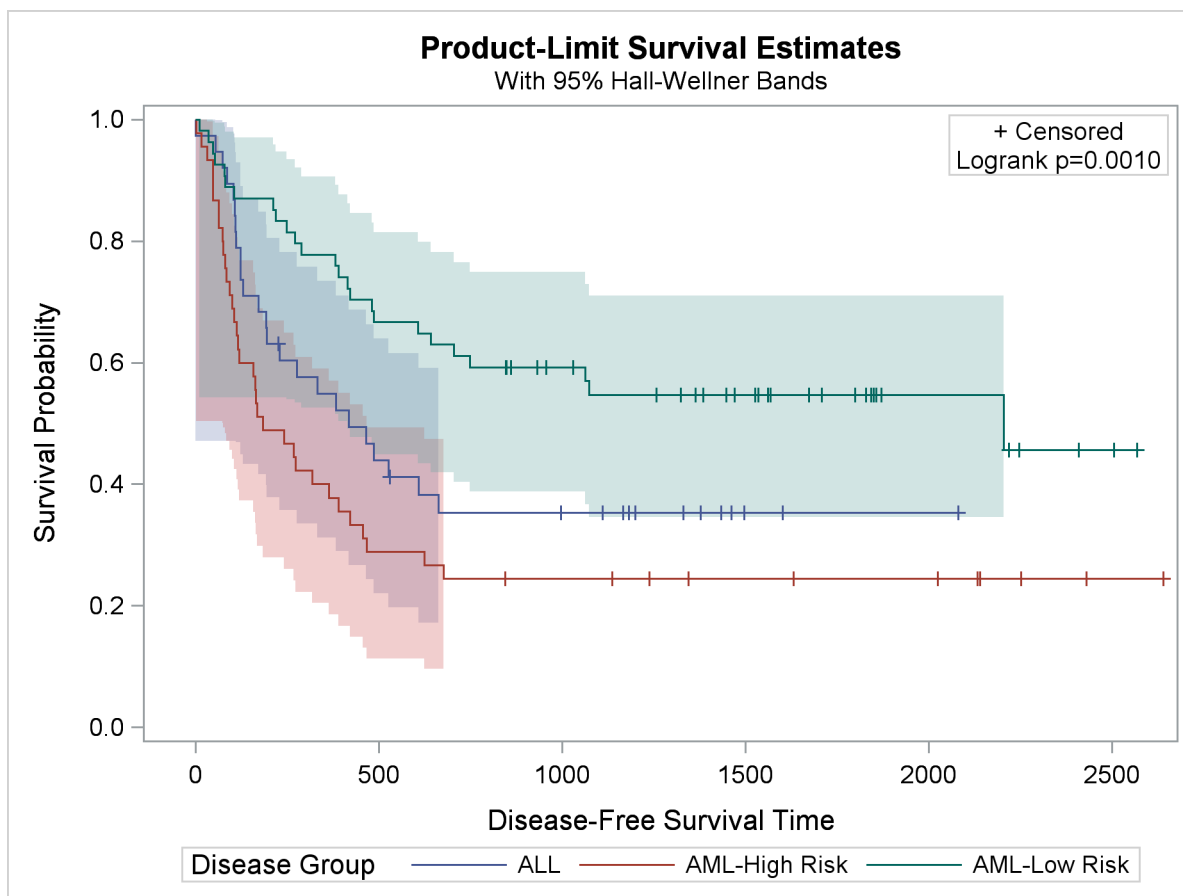
The following statements run PROC LIFETEST to display the survival plot and to determine the template name:

```
ods graphics on;
ods trace on;

proc lifetest data=sashelp.BMT plots=survival(cb=hw test);
  time T * Status(0);
  strata Group;
run;

ods trace off;
```

The survival plot is displayed in [Output 22.3.1](#). Notice that the Hall-Welner bands by design stop at the last event.

Output 22.3.1 Product Limit Survival Plot

The relevant part of the trace output from the SAS log is as follows:

Output Added:

```
-----
Name:      SurvivalPlot
Label:     Survival Curves
Template:  Stat.Lifetest.Graphics.ProductLimitSurvival
Path:     Lifetest.SurvivalPlot
-----
```

The trace output shows that the template name for the survival plot is:

```
Stat.Lifetest.Graphics.ProductLimitSurvival.
```

The following statements display the template:

```
proc template;
  source Stat.Lifetest.Graphics.ProductLimitSurvival;
run;
```

The results, at 158 lines, are lengthy. A partial display of the results is as follows:

```
define statgraph Stat.Lifetest.Graphics.ProductLimitSurvival;
  dynamic NStrata xName plotAtRisk plotCensored plotCL plotHW plotEP labelCL
  labelHW labelEP maxTime xtickVals xtickValFitPol method StratumID
  classAtRisk plotBand plotTest GroupName yMin Transparency SecondTitle
  TestName pValue;
  BeginGraph;
  if (NSTRATA=1)
    if (EXISTS(STRATUMID))
      entrytitle METHOD " " "Survival Estimate" " for " STRATUMID;
    else
      entrytitle METHOD " " "Survival Estimate";
    endif;
  if (PLOTATRISK=1)
    entrytitle "with Number of Subjects at Risk" / textattrs=
      GRAPHVALUETEXT;
  endif;
  layout overlay / xaxisopts=(shortlabel=XNAME offsetmin=.05 linearopts=
    (viewmax=MAXTIME tickvaluelist=XTICKVALS tickvaluefitpolicy=
    XTICKVALFITPOL)) yaxisopts=(label="Survival Probability" shortlabel=
    "Survival" linearopts=(viewmin=0 viewmax=1 tickvaluelist=(0 .2 .4
    .6 .8 1.0)));
  .
  .
  .
  endlayout;
else
  entrytitle METHOD " " "Survival Estimates";
  if (EXISTS(SECONDTITLE))
    entrytitle SECONDTITLE / textattrs=GRAPHVALUETEXT;
  endif;
  layout overlay / xaxisopts=(shortlabel=XNAME offsetmin=.05 linearopts=
    (viewmax=MAXTIME tickvaluelist=XTICKVALS tickvaluefitpolicy=
    XTICKVALFITPOL)) yaxisopts=(label="Survival Probability" shortlabel=
    "Survival" linearopts=(viewmin=0 viewmax=1 tickvaluelist=(0 .2 .4
    .6 .8 1.0)));
  .
  .
  .
  endlayout;
endif;
EndGraph;
end;
```

This template has a two-part structure. The graph is created one way for a single stratum (in the statements that follow `if (NSTRATA=1)`); otherwise it is created a different way (in the statements that follow the `ELSE` near the middle of the template). You can change the title by locating and changing `ENTRYTITLE` statements, which are the GTL statements that provide graph titles. Change just the entry titles that provide the first title lines. In most templates, all `ENTRYTITLE` statements are near the top of the template. They are not near the top of this template due to the two-part structure. The following step shows the changes that you could make to change the title (as displayed in [Output 22.3.2](#)):

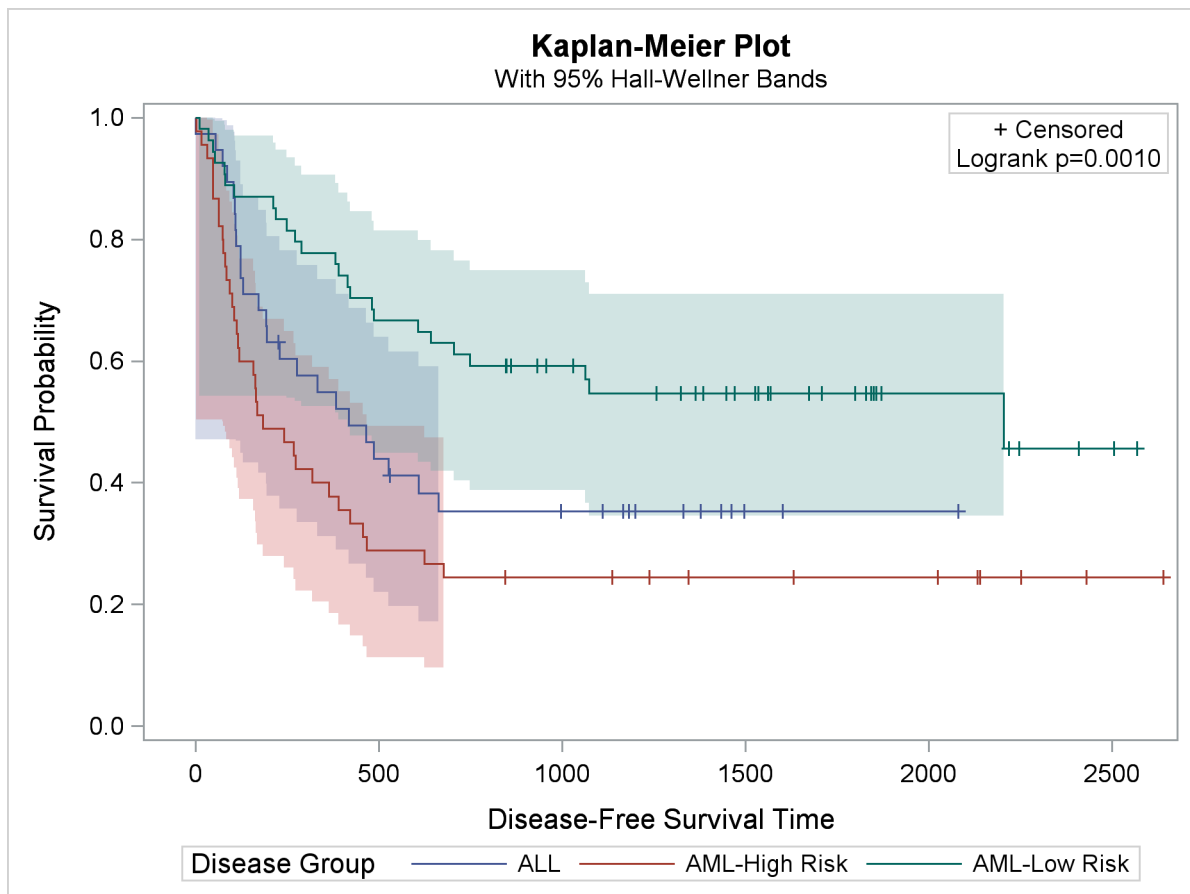
```
proc template;
  define statgraph Stat.Lifetest.Graphics.ProductLimitSurvival;
    dynamic NStrata xName plotAtRisk plotCensored plotCL plotHW plotEP labelCL
      labelHW labelEP maxTime xtickVals xtickValFitPol method StratumID
      classAtRisk plotBand plotTest GroupName yMin Transparency SecondTitle
      TestName pValue;
    BeginGraph;
      if (NSTRATA=1)
        if (EXISTS(STRATUMID))
          entrytitle "Kaplan-Meier Plot for " STRATUMID;
        else
          entrytitle "Kaplan-Meier Plot";
        endif;
      if (PLOTATRISK=1)
        entrytitle "with Number of Subjects at Risk" / textattrs=
          GRAPHVALUETEXT;
      endif;
      layout overlay / xaxisopts=(shortlabel=XNAME offsetmin=.05 linearopts=
        (viewmax=MAXTIME tickvaluelist=XTICKVALS tickvaluefitpolicy=
          XTICKVALFITPOL)) yaxisopts=(label="Survival Probability" shortlabel=
          "Survival" linearopts=(viewmin=0 viewmax=1 tickvaluelist=(0 .2 .4
            .6 .8 1.0)));
      .
      .
      .
      endlayout;
    else
      entrytitle "Kaplan-Meier Plot";
      if (EXISTS(SECONDTITLE))
        entrytitle SECONDTITLE / textattrs=GRAPHVALUETEXT;
      endif;
      layout overlay / xaxisopts=(shortlabel=XNAME offsetmin=.05 linearopts=
        (viewmax=MAXTIME tickvaluelist=XTICKVALS tickvaluefitpolicy=
          XTICKVALFITPOL)) yaxisopts=(label="Survival Probability" shortlabel=
          "Survival" linearopts=(viewmin=0 viewmax=1 tickvaluelist=(0 .2 .4
            .6 .8 1.0)));
      .
      .
      .
      endlayout;
    endif;
  EndGraph;
end;
run;
```

Three ENTRYTITLE statements are changed. Notice that you must provide a PROC TEMPLATE statement and optionally a RUN statement in addition to making the title changes. Submit the PROC TEMPLATE step to SAS along with the following PROC LIFETEST step to create the modified graph:

```
proc lifetest data=sashelp.BMT plots=survival(cb=hw test);
  time T * Status(0);
  strata Group;
run;
```

The results are displayed in [Output 22.3.2](#).

Output 22.3.2 Kaplan-Meier Plot



Modifying the Axes

The template option `linearopts=(viewmin=0 viewmax=1 tickvaluelist=(0 .2 .4 .6 .8 1.0))` controls the minimum value displayed, the maximum value displayed, and the ticks on the vertical axis. You can change the range of the vertical axis or the ticks in either version of the template by changing this option everywhere that it occurs. The following specification changes the ticks but not the range of values: `linearopts=(viewmin=0 viewmax=1 tickvaluelist=(0 .25 .5 .75 1.0))`.

When there is a single stratum, the LAYOUT OVERLAY statement (which controls the axes) is as follows:

```
layout overlay / xaxisopts=(shortlabel=XNAME offsetmin=.05
  linearopts=(viewmax=MAXTIME tickvaluelist=XTICKVALS
  tickvaluefitpolicy=XTICKVALFITPOL)) yaxisopts=(label=
  "Survival Probability" shortlabel="Survival" linearopts=(viewmin=
  0 viewmax=1 tickvaluelist=(0 .2 .4 .6 .8 1.0)));
```

The LAYOUT OVERLAY statement with more than one stratum is identical. With added comments, the statement is as follows:

```
layout overlay /                               /*-----*/
  xaxisopts=(                                  /* X axis options      */
                                                    /* label= is not specified, so */
                                                    /* it comes from data object  */
                                                    /* column label             */
  shortlabel=XNAME                             /* alternative shorter label */
                                                    /* comes from dynamic         */
  offsetmin=.05                               /* add 5% padding on minimum */
                                                    /* side of the x axis        */
  linearopts=(                                 /* linear axis (not log axis) */
  viewmax=MAXTIME                             /* largest value to display,  */
                                                    /* comes from dynamic         */
  tickvaluelist=XTICKVALS                     /* tick value list comes from */
                                                    /* a dynamic                  */
  tickvaluefitpolicy=                          /* fit policy comes from a    */
  XTICKVALFITPOL))                            /* dynamic - controls tick    */
                                                    /* value collision avoidance   */
                                                    /* strategies including       */
                                                    /* rotation                   */
                                                    /*-----*/
  yaxisopts=(                                  /* Y axis options      */
  label="Survival Probability"                 /* axis label           */
  shortlabel="Survival"                       /* shorter label for short axes*/
  linearopts=(                                 /* linear axis (not log axis) */
  viewmin=0                                   /* smallest value to display  */
  viewmax=1                                   /* largest value to display   */
  tickvaluelist=                              /* list of tick values to    */
  (0 .2 .4 .6 .8 1.0)));                      /* display                 */
                                                    /*-----*/
```

You can change any of these values in several ways:

- You can specify literal values or macro variables when previously a dynamic variable was used. Example: change VIEWMAX=MAXTIME to VIEWMAX=2000.
- You can change literal specifications. Example: change VIEWMAX=1 TICKVALUELIST=(0 .2 .4 .6 .8 1.0) to VIEWMAX=0.75 TICKVALUELIST=(0 .25 .5 .75) to restrict the range on the Y axis.
- You can add options. Example: specify LABEL="Time" in the XAXISOPTS= option. Example: specify LABELATTRS=(SIZE=12PX) in the XAXISOPTS= and YAXISOPTS= options to change the font size for the labels. Example: specify TICKVALUEATTRS=(SIZE=10PX) in the XAXISOPTS= and YAXISOPTS= options to change the font size for the ticks.
- You can delete options. Example: delete VIEWMIN=0 VIEWMAX=1 from the YAXISOPTS= option.

If you frequently find yourself changing the title or the axes, you can make it easier by creating a template where those options are controlled by macro variables. For example, this template is easier to modify than the default template:

```
%let TitleText0 = METHOD " Survival Estimate";
%let TitleText1 = &titletext0 " for " STRATUMID;
%let TitleText2 = &titletext0 "s";
%let yOptions   = label="Survival Probability"
                  shortlabel="Survival"
                  linearopts=(viewmin=0 viewmax=1
                              tickvaluelist=(0 .2 .4 .6 .8 1.0));
%let xOptions   = shortlabel=XNAME
                  offsetmin=.05
                  linearopts=(viewmax=MAXTIME tickvaluelist=XTICKVALS
                              tickvaluefitpolicy=XTICKVALFITPOL);

proc template;
  define statgraph Stat.Lifetest.Graphics.ProductLimitSurvival;
    dynamic NStrata xName plotAtRisk plotCensored plotCL plotHW plotEP labelCL
      labelHW labelEP maxTime xtickVals xtickValFitPol method StratumID
      classAtRisk plotBand plotTest GroupName yMin Transparency SecondTitle
      TestName pValue;
    BeginGraph;
      if (NSTRATA=1)
        if (EXISTS(STRATUMID))
          entrytitle &titletext1;
        else
          entrytitle &titletext0;
        endif;
      if (PLOTATRISK=1)
        entrytitle "with Number of Subjects at Risk" / textattrs=
          GRAPHVALUETEXT;
      endif;
      layout overlay / xaxisopts=(&xoptions) yaxisopts=(&yoptions);
      .
      .
      .
      endlayout;
    else
      entrytitle &titletext2;
      if (EXISTS(SECONDTITLE))
        entrytitle SECONDTITLE / textattrs=GRAPHVALUETEXT;
      endif;
      layout overlay / xaxisopts=(&xoptions) yaxisopts=(&yoptions);
      .
      .
      .
      endlayout;
    endif;
  EndGraph;
end;
run;
```

Creating a Template That Is Easy to Modify

This example shows how you can modularize the entire template. The goal is to modularize the template and use macros such that simple changes, such as title changes, are no more complicated than the following:

```
%SurvivalTemplateRestore

%let TitleText0 = "Kaplan-Meier Plot";
%let TitleText1 = &titletext0 " for " STRATUMID;
%let TitleText2 = &titletext0;

%SurvivalTemplate
```

You can modularize the entire template as follows:

```
%macro SurvivalTemplateRestore;

  %global TitleText0 TitleText1 TitleText2 yOptions xOptions tips
         tipl groups bandopts gridopts blockopts censored censorstr;

  %let TitleText0 = METHOD " Survival Estimate";
  %let TitleText1 = &titletext0 " for " STRATUMID;
  %let TitleText2 = &titletext0 "s";          /* plural: Survival Estimates */

  %let yOptions   = label="Survival Probability"
                   shortlabel="Survival"
                   linearopts=(viewmin=0 viewmax=1
                               tickvaluelist=(0 .2 .4 .6 .8 1.0));

  %let xOptions   = shortlabel=XNAME
                   offsetmin=.05
                   linearopts=(viewmax=MAXTIME tickvaluelist=XTICKVALS
                               tickvaluefitpolicy=XTICKVALFITPOL);

  %let tips       = rolename=( _tip1= ATRISK _tip2=EVENT)
                   tiplabel=( _tip1="Number at Risk" _tip2="Observed Events")
                   tip=(x y _tip1 _tip2);

  %let tipl       = tiplabel=(y="Survival Probability");

  %let groups     = group=STRATUM index=STRATUMNUM;

  %let bandopts   = &groups modelname="Survival";

  %let gridopts   = autoalign=(TOPRIGHT BOTTOMLEFT TOP BOTTOM)
                   border=true BackgroundColor=GraphWalls:Color Opaque=true;

  %let blockopts  = repeatedvalues=true valuealign=start
                   valuefitpolicy=truncate labelposition=left
                   labelattrs=GRAPHVALUETEXT includemissingclass=false
                   valueattrs=GRAPHDATATEXT(size=7pt);

  %let censored   = markerattrs=(symbol=plus);
  %let censorstr  = "+ Censored";

%mend
```

```

%macro SurvivalTemplate;
  proc template;
    define statgraph Stat.Lifetest.Graphics.ProductLimitSurvival;
      dynamic NStrata xName plotAtRisk plotCL plotHW plotEP labelCL
        %if %nrbquote(&censored) ne %then plotCensored;
        labelHW labelEP maxTime xtickVals xtickValFitPol method StratumID
        classAtRisk plotBand plotTest GroupName yMin Transparency
        SecondTitle TestName pValue;
      BeginGraph;

        if (NSTRATA=1)
          if (EXISTS(STRATUMID))
            entrytitle &titletext1;
          else
            entrytitle &titletext0;
          endif;
          if (PLOTATRISK=1)
            entrytitle "with Number of Subjects at Risk" / textattrs=
              GRAPHVALUETEXT;
          endif;

          layout overlay / xaxisopts=(&xoptions) yaxisopts=(&yoptions);
            %singlestratum
          endlayout;

        else
          entrytitle &titletext2;
          if (EXISTS(SECONDTITLE))
            entrytitle SECONDTITLE / textattrs=GRAPHVALUETEXT;
          endif;

          layout overlay / xaxisopts=(&xoptions) yaxisopts=(&yoptions);
            %multiplestrata
          endlayout;

        endif;

      EndGraph;
    end;
  run;
%mend;

%macro entry_p;
  if (PVALUE < .0001)
    entry TESTNAME " p " eval (PUT(PVALUE, PVALUE6.4));
  else
    entry TESTNAME " p=" eval (PUT(PVALUE, PVALUE6.4));
  endif;
%mend;

```



```

%macro SingleStratum;
  if (PLOTBW=1 AND PLOTEP=0)
    bandplot LimitUpper=HW_UCL LimitLower=HW_LCL x=TIME /
      modelname="Survival" fillattrs=GRAPHCONFIDENCE
      name="HW" legendlabel=LABELHW;
  endif;
  if (PLOTBW=0 AND PLOTEP=1)
    bandplot LimitUpper=EP_UCL LimitLower=EP_LCL x=TIME /
      modelname="Survival" fillattrs=GRAPHCONFIDENCE
      name="EP" legendlabel=LABELEP;
  endif;
  if (PLOTBW=1 AND PLOTEP=1)
    bandplot LimitUpper=HW_UCL LimitLower=HW_LCL x=TIME /
      modelname="Survival" fillattrs=GRAPHDATA1 datatransparency=.55
      name="HW" legendlabel=LABELHW;
    bandplot LimitUpper=EP_UCL LimitLower=EP_LCL x=TIME /
      modelname="Survival" fillattrs=GRAPHDATA2
      datatransparency=.55 name="EP" legendlabel=LABELEP;
  endif;
  if (PLOTCL=1)
    if (PLOTBW=1 OR PLOTEP=1)
      bandplot LimitUpper=SDF_UCL LimitLower=SDF_LCL x=TIME /
        modelname="Survival" display=(outline)
        outlineattrs=GRAPHPREDICTIONLIMITS name="CL" legendlabel=LABELCL;
    else
      bandplot LimitUpper=SDF_UCL LimitLower=SDF_LCL x=TIME /
        modelname="Survival" fillattrs=GRAPHCONFIDENCE name="CL"
        legendlabel=LABELCL;
    endif;
  endif;

  stepplot y=SURVIVAL x=TIME / name="Survival" &tips legendlabel="Survival";

  if (PLOTCEM=1)
    scatterplot y=CENSORED x=TIME / &censored &tipl
      name="Censored" legendlabel="Censored";
  endif;

  if (PLOTCL=1 OR PLOTBW=1 OR PLOTEP=1)
    discretelegend "Censored" "CL" "HW" "EP" / location=outside
      halign=center;
  else
    if (PLOTCEM=1)
      discretelegend "Censored" / location=inside
        autoalign=(topright bottomleft);
    endif;
  endif;
  if (PLOTATRISK=1)
    innermargin / align=bottom;
    blockplot x=TATRISK block=ATRISK / display=(label values)
      &blockopts;
    endinnermargin;
  endif;
%mend;

```

```

%macro MultipleStrata;
  if (PLOTBW)
    bandplot LimitUpper=HW_UCL LimitLower=HW_LCL x=TIME / &bandopts
             datatransparency=Transparency;
  endif;
  if (PLOTTEP)
    bandplot LimitUpper=EP_UCL LimitLower=EP_LCL x=TIME / &bandopts
             datatransparency=Transparency;
  endif;
  if (PLOTCL)
    if (PLOTBAND)
      bandplot LimitUpper=SDF_UCL LimitLower=SDF_LCL x=TIME / &bandopts
               display=(outline);
    else
      bandplot LimitUpper=SDF_UCL LimitLower=SDF_LCL x=TIME / &bandopts
               datatransparency=Transparency;
    endif;
  endif;

  stepplot y=SURVIVAL x=TIME / &groups name="Survival" &tips;

  if (PLOTCECENSORED)
    scatterplot y=CENSORED x=TIME / &groups &censored &tipl;
  endif;

  if (PLOTATRISK=1)
    innermargin / align=bottom;
    blockplot x=TATRISK block=ATRISK / class=CLASSATRISK
              display=(label values) &blockopts;
    endinnermargin;
  endif;

  DiscreteLegend "Survival" / title=GROUPNAME location=outside;

  if (PLOTCECENSORED)
    if (PLOTTEST)
      layout gridded / rows=2 &gridopts;
      entry &cursorstr;
      %entry_p
      endlayout;
    else
      layout gridded / rows=1 &gridopts;
      entry &cursorstr;
      endlayout;
    endif;
  else
    if (PLOTTEST)
      layout gridded / rows=1 &gridopts;
      %entry_p
      endlayout;
    endif;
  endif;
%mend;

%SurvivalTemplate
%mend;

```

This modularized template is available in the SAS sample library. If you are using the SAS windowing environment, select **Help ► Getting Started with SAS Software**. Select the **Contents** tab. Expand **Learning to Use SAS**, expand **SAS Sample Programs**, and expand **SAS/STAT**. Select **Samples**. Search for and select **PROC LIFETEST Template**.

The following changes were made to the template:

- The outer macro, **%SurvivalTemplateRestore**, defines a set of macros and a set of global macro variables. This macro makes it easier to restore the default macros and macro variables. You should not use this outer macro to modify the templates. You should use it only to provide and restore all of the defaults.
- Many options, including most of the options that are specified in multiple places in the template, are extracted to macro variables.
- The main body of the template is in a macro, **%SurvivalTemplate**, so that it is easier to recompile the template after making changes.
- The table for p -values is stored in the macro, **%Entry_P**.
- The revised template for the single-stratum case is stored in the macro **%SingleStratum**.
- The revised template for the multiple-stratum case is stored in the macro **%MultipleStrata**.
- The template has been re-indented.

These changes make it easier to identify the relevant parts of the template, modify them, and recompile the template. All subsequent parts of this example modify this rewritten and more modular template.

Do not edit the template inside the **%SurvivalTemplateRestore** macro. Rather, copy the **%LET** statements and macro definitions and modify them outside the context of the **%SurvivalTemplateRestore** macro. If you work this way, then you can restore the defaults with a two step process:

- 1 You can restore the default macros and macro variables by running the following step:

```
%SurvivalTemplateRestore
```

- 2 You can restore the default template by running the following step:

```
proc template;  
  delete Stat.Lifetest.Graphics.ProductLimitSurvival / store=sasuser.templat;  
run;
```

A simple, complete program, with set up, template modification, and clean up works as follows:

```

                                /* Make the macros and macro      */
%SurvivalTemplateRestore          /* variables available        */

%let TitleText0 = "Kaplan-Meier Plot"; /* Change the title.      */
%let TitleText1 = &titletext0 " for " STRATUMID;
%let TitleText2 = &titletext0;

%SurvivalTemplate                 /* Compile the template with */
                                /* the new title.           */

proc lifetest data=sashelp.BMT      /* Perform the analysis and make */
      plots=survival(cb=hw test); /* the graph.                 */
  time T * Status(0);
  strata Group;
run;

%SurvivalTemplateRestore          /* Restore the default macros  */
                                /* and macro variables.       */

proc template;                    /* Restore the default template. */
  delete Stat.Lifetest.Graphics.ProductLimitSurvival / store=sasuser.templat;
run;

```

The results of this step are not shown, but this same template modification is discussed in the next section. The `%SurvivalTemplateRestore` macro creates the macros and macro variables that you can modify to change the template. The `%SurvivalTemplate` macro compiles the template with the macro variable changes and macro changes (if any were performed). By default, the compiled template is stored in the `Sasuser.Templat` item store. PROC LIFETEST makes the graph. The `%SurvivalTemplateRestore` macro restores the default macros and macro variables. The `%SurvivalTemplateRestore` macro ends by calling the `%SurvivalTemplate` macro, so it also compiles and stores the default template in the `Sasuser.Templat` item store. The PROC TEMPLATE step deletes the compiled template from the `Sasuser.Templat` item store so that the original template from the `Sashelp.Tmplmst` item store is used in subsequent runs.

Deleting the compiled template from the `Sasuser.Templat` item store does not change the macros or macro variables. Hence, if you do not restore the macros and macro variables, but you delete the compiled template, change a different macro variable, and recompile the template in the same SAS session, you will see the effects of both changes. In practice, you do not need to restore the default macros and macro variables when you are done unless (as is the case in this example) you go on in the same SAS session to make other template changes and you do not want your previous template changes to affect subsequent graphs.

If you modify and manipulate this template frequently, you might find it more convenient to modify the `%SurvivalTemplateRestore` macro along the following lines:

```
%macro SurvivalTemplateRestore(action);
.
.
.
  %if      &action = compile %then %SurvivalTemplate;
  %else %if &action = delete  %then %do;
    proc template;
      delete Stat.Lifetest.Graphics.ProductLimitSurvival / store=sasuser.templat;
    run;
  %end;
%mend;
```

This modification enables you to clean up with a single step.

Modifying the Plot Title in the Revised Template

This example changes the title of the survival plot in PROC LIFETEST from “Product-Limit Survival Estimates” to “Kaplan-Meier Plot” as follows, using the modularized template with macros:

```
%SurvivalTemplateRestore

%let TitleText0 = "Kaplan-Meier Plot";
%let TitleText1 = &titletext0 " for " STRATUMID;
%let TitleText2 = &titletext0;

%SurvivalTemplate
```

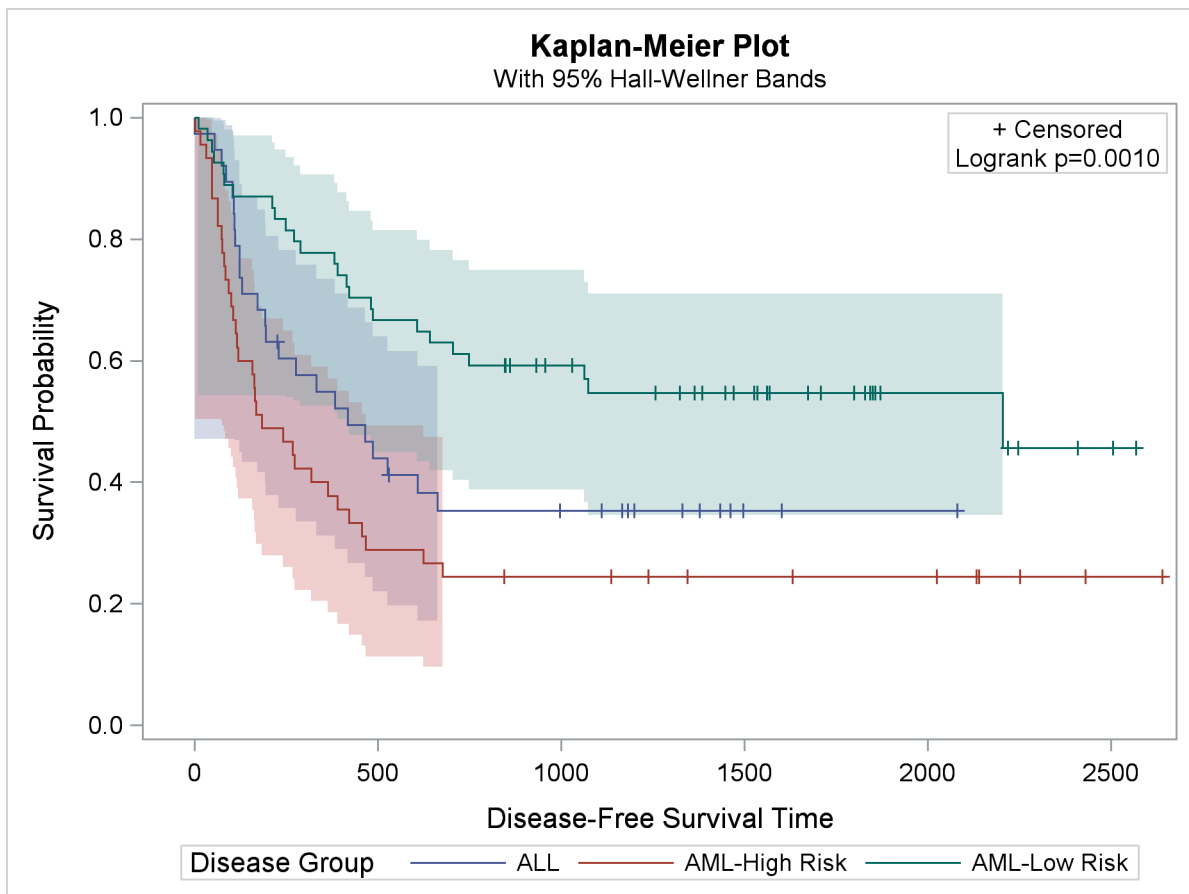
The `%SurvivalTemplateRestore` macro from the preceding section, “[Creating a Template That Is Easy to Modify](#)” on page 756, provides the modularized template code. The three `%LET` statements modify the titles, and the `%SurvivalTemplate` macro compiles the modified template. The following step, along with the modified template, creates [Output 22.3.3](#):

```
proc lifetest data=sashelp.BMT plots=survival(cb=hw test);
  time T * Status(0);
  strata Group;
run;
```

You can restore the default macros, macro variables, and template by running the following steps:

```
%SurvivalTemplateRestore

proc template;
  delete Stat.Lifetest.Graphics.ProductLimitSurvival / store=sasuser.templat;
run;
```

Output 22.3.3 Kaplan-Meier Plot Created with the Revised Template

Modifying the Legend and Inset Table

You can easily modify many other features of this template. For example, you can change the locations of the inset table and the legend, which are controlled by the following statements:

```
%let gridopts = autoalign=(TOPRIGHT BOTTOMLEFT TOP BOTTOM)
                    border=true BackgroundColor=GraphWalls:Color Opaque=true;
layout gridded / rows=2 &gridopts;
```

```
DiscreteLegend "Survival" / title=GROUPNAME location=outside;
```

The LAYOUT GRIDDED statement produces the two-row inset table displayed in the top right corner. The AUTOALIGN= option provides the preferred locations inside the plot for this table, ordered from most preferred to least preferred. You can add new locations or rearrange the existing locations. The DISCRETELEGEND statement places the legend outside of the plot. You can move it inside and print only one legend entry across each row instead of three. This has the effect of changing the orientation of the legend from a row to a column. The modified statements are as follows:

```
%let gridopts = autoalign=(BottomRight TOPRIGHT BOTTOMLEFT TOP BOTTOM)
                    border=true BackgroundColor=GraphWalls:Color Opaque=true;
layout gridded / rows=2 &gridopts;
```

```
DiscreteLegend "Survival" / title=GROUPNAME across=1 location=inside
                    autoalign=(TopRight BottomLeft Top Bottom);
```

These changes are incorporated into the template as follows:

```

%SurvivalTemplateRestore

%let TitleText0 = "Kaplan-Meier Plot";
%let TitleText1 = &titletext0 " for " STRATUMID;
%let TitleText2 = &titletext0;

%let gridopts = autoalign=(BottomRight TOPRIGHT BOTTOMLEFT TOP BOTTOM)
                border=true BackgroundColor=GraphWalls:Color Opaque=true;

%macro multiplestrata;
  if (PLOTBW)
    bandplot LimitUpper=HW_UCL LimitLower=HW_LCL x=TIME / &bandopts
             datatransparency=Transparency;
  endif;
  if (PLOTTEP)
    bandplot LimitUpper=EP_UCL LimitLower=EP_LCL x=TIME / &bandopts
             datatransparency=Transparency;
  endif;
  if (PLOTCL)
    if (PLOTBAND)
      bandplot LimitUpper=SDF_UCL LimitLower=SDF_LCL x=TIME / &bandopts
               display=(outline);
    else
      bandplot LimitUpper=SDF_UCL LimitLower=SDF_LCL x=TIME / &bandopts
               datatransparency=Transparency;
    endif;
  endif;

  stepplot y=SURVIVAL x=TIME / &groups name="Survival" &tips;

  if (PLOTCECENSORED)
    scatterplot y=CENSORED x=TIME / &groups &censored &tipl;
  endif;

  if (PLOTATRISK=1)
    innermargin / align=bottom;
    blockplot x=TATRISK block=ATRISK / class=CLASSATRISK
              display=(label values) &blockopts;
    endinnermargin;
  endif;

  DiscreteLegend "Survival" / title=GROUPNAME across=1 location=inside
                 autoalign=(TopRight BottomLeft Top Bottom);

  if (PLOTCECENSORED)
    if (PLOTTEST)
      layout gridded / rows=2 &gridopts;
      entry &cursorstr;
      %entry_p
    endlayout;
  else

```

```

        layout gridded / rows=1 &gridopts;
            entry &cursorstr;
        endlayout;
    endif;
else
    if (PLOTTEST)
        layout gridded / rows=1 &gridopts;
            %entry_p
        endlayout;
    endif;
endif;
%mend;

%SurvivalTemplate

```

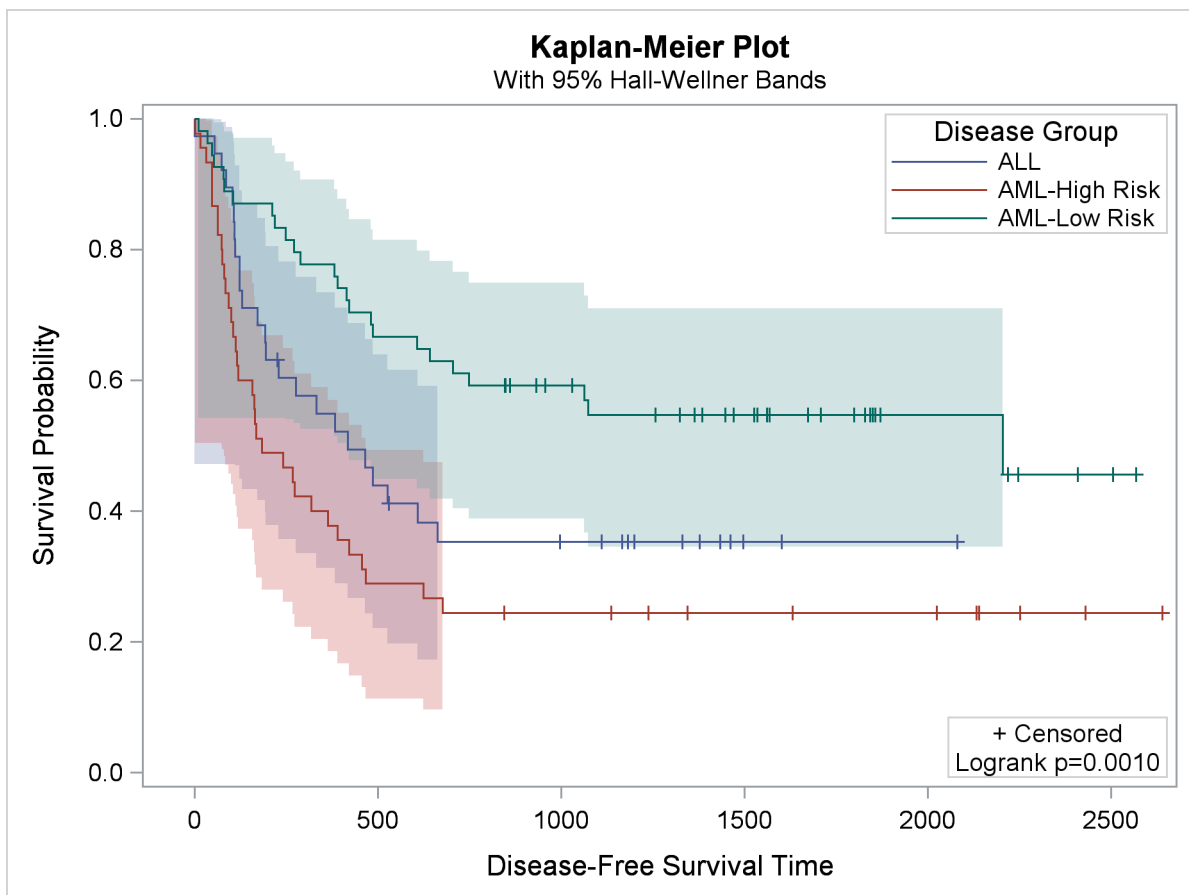
The new template along with the following statements produce [Output 22.3.4](#):

```

proc lifetest data=sashelp.BMT plots=survival(cb=hw test);
    time T * Status(0);
    strata Group;
run;

```

Output 22.3.4 Kaplan-Meier Plot with Legend Modifications



You can restore the default macros, macro variables, and template by running the following steps:

```
%SurvivalTemplateRestore

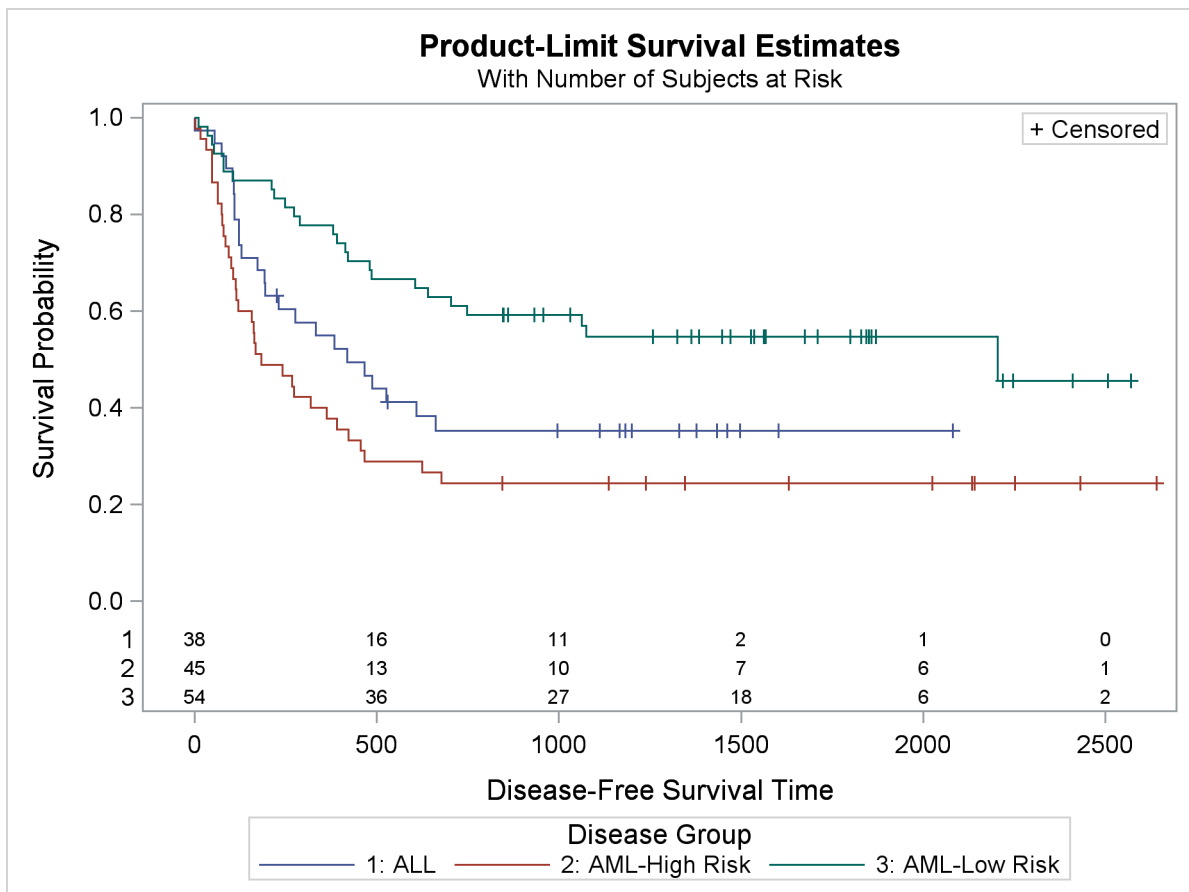
proc template;
  delete Stat.Lifetest.Graphics.ProductLimitSurvival / store=sasuser.template;
run;
```

Modifying the Layout and Adding a New Inset Table

You can use the following statements to make the plot shown in [Output 22.3.5](#) with the default at-risk table:

```
proc lifetest data=sashelp.BMT plots=survival(atrisk=0 to 2500 by 500);
  ods select SurvivalPlot;
  time T * Status(0);
  strata Group;
run;
```

Output 22.3.5 Survival Plot with Number of Subjects At Risk

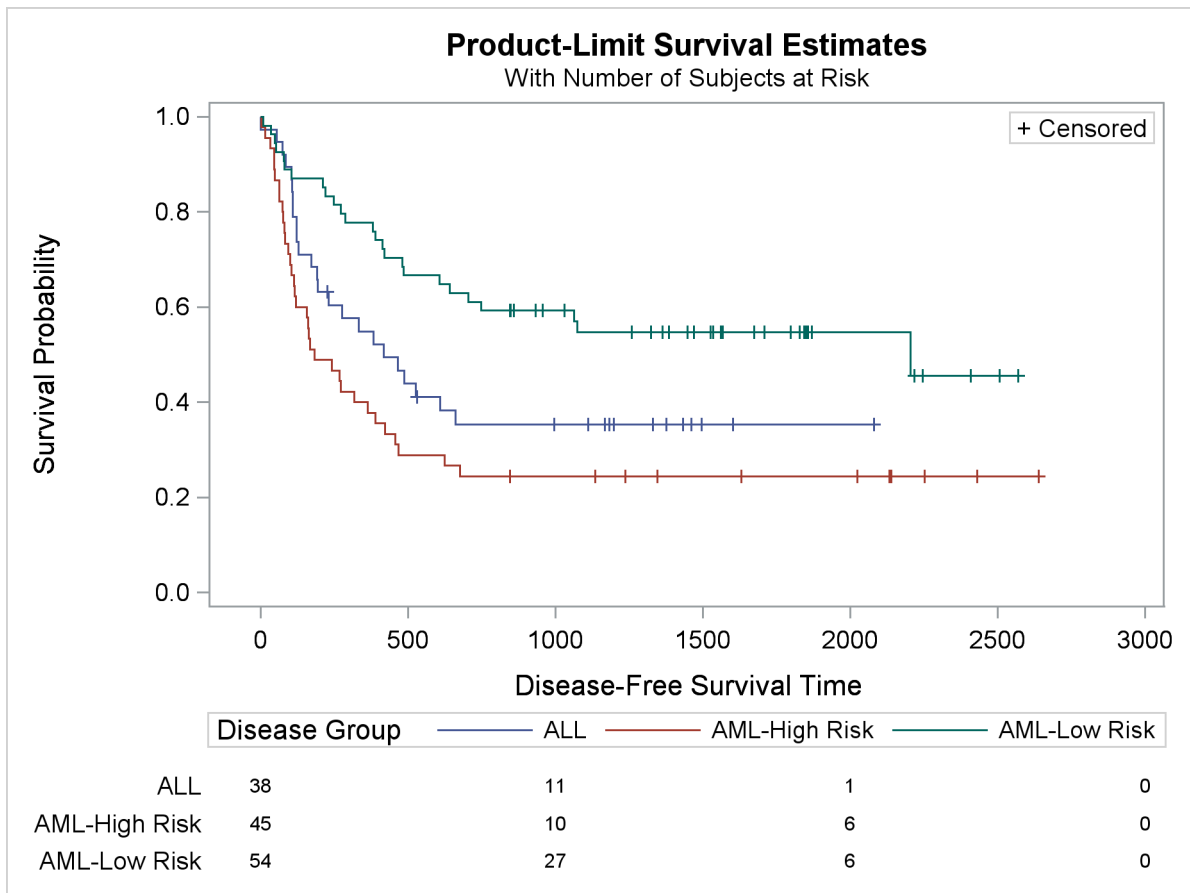


Output 22.3.5 displays the estimated disease-free survival functions for the three leukemia groups with the number of subjects at risk at 0, 500, 1,000, 1,500, 2,000, and 2,500 days.

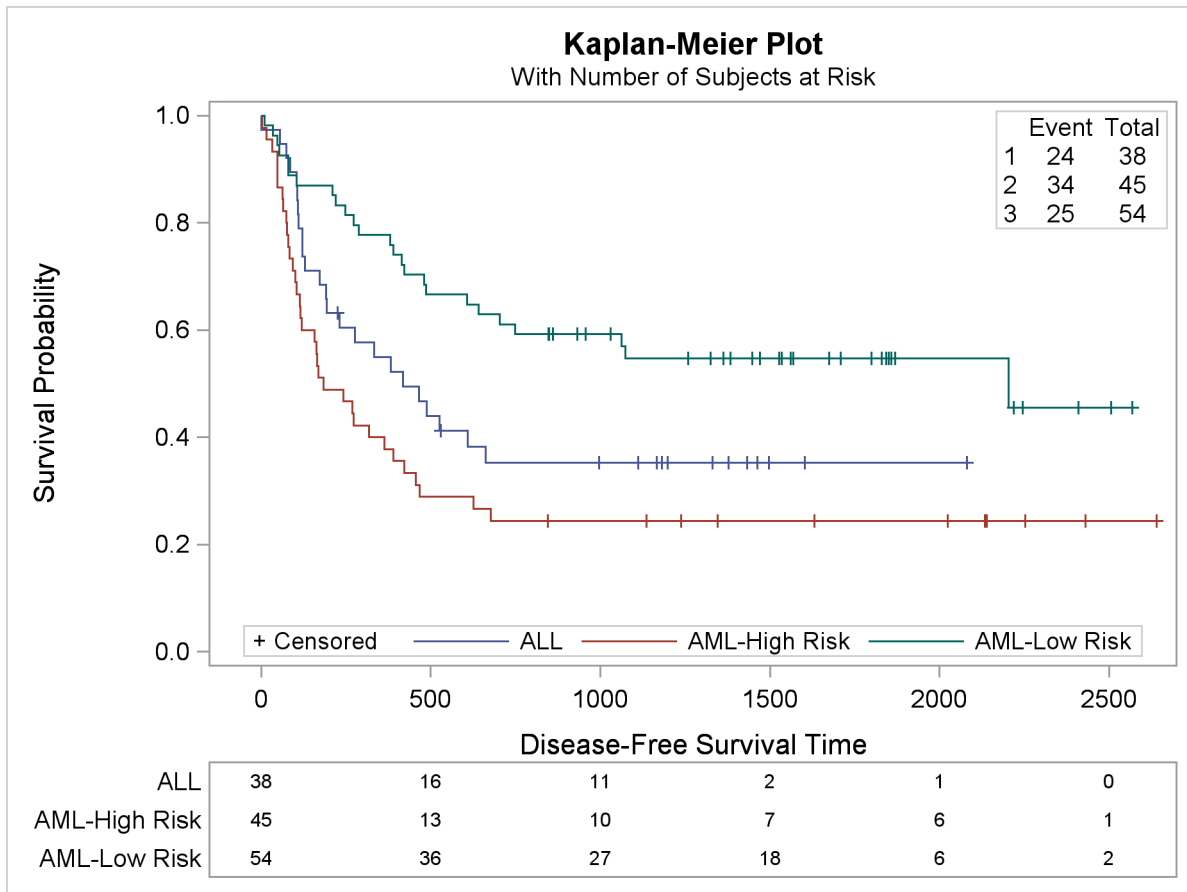
You can display this table outside the graph, display the table in 15% of the available space, and display row labels up to 13 characters long as follows:

```
proc lifetest data=sashelp.BMT
  plots=survival(atrisk(maxlen=13 outside(0.15)));
  ods select SurvivalPlot;
  time T * Status(0);
  strata Group;
run;
```

Output 22.3.6 Survival Plot with an External At-Risk Table



The rest of this example shows you how to modify the template to produce the plot displayed in Output 22.3.7. This new plot differs from the old plot in several ways. It has a new inset table in the top right corner with the number of observations and the number of events in the each stratum. The legend has been moved inside the plot and combined with the old inset table that showed the marker for censored observations. The information about the subjects at risk has been moved into a table below the plot. Also, the title change from the first part of the example is retained. These changes are easy, if they are broken down and performed one step at a time.

Output 22.3.7 Kaplan-Meier Plot with a Different Layout

You can begin this step by submitting the original macro definitions from the section “[Creating a Template That Is Easy to Modify](#)” on page 756:

```
%SurvivalTemplateRestore
```

Notice that the survival plot template has two major parts: a layout that is used when there is only one stratum and a layout that is used with more than one stratum. You can see the two major parts in the definition of the `%SurvivalTemplate` macro. Every section of this example has more than one stratum, so it is the changes to the second layout and the `%MultipleStrata` macro (or more precisely the ELSE portion of the template) that are affecting the results.

PROC LIFETEST makes available a series of dynamic variables that it does not display by default. See the section “[Additional Dynamic Variables for Survival Plots Using ODS Graphics](#)” on page 4060 in Chapter 52, “[The LIFETEST Procedure](#),” for information about these dynamic variables. You can use these dynamic variables to add the new inset table to the plot. The following statements show how to add a gridded layout to the graph:

```
dynamic NObs1 NObs2 NObs3 NEvent1 NEvent2 NEvent3;
layout gridded / columns=3 border=TRUE autoalign=(TopRight);
  entry "";      entry "Event";  entry "Total";
  entry "1";     entry NEvent1;  entry NObs1;
  entry "2";     entry NEvent2;  entry NObs2;
  entry "3";     entry NEvent3;  entry Nobs3;
endlayout;
```

These statements are added to the end of the `%MultipleStrata` macro.

The at-risk information in [Output 22.3.5](#) is produced by the following `BLOCKPLOT` statement, which is displayed in the context of the `IF` and `INNERMARGIN` statements that go with it:

```
if (PLOTATRISK=1)
  innermargin / align=bottom;
  blockplot x=TATRISK block=ATRISK / class=CLASSATRISK
    display=(label values) &blockopts;
  endinnermargin;
endif;
```

In the next step, the at-risk block plot is moved out of the plot and into a table below the plot. The template has a new overall layout—a `LAYOUT LATTICE` that has two panels stacked vertically, one for the plot and one for the at-risk information. Using `ROWWEIGHTS=(.85 .15)`, the plot on top occupies 85% of the display and the at-risk information in the second panel occupies 15%. The option `COLUMN-DATARANGE=UNIONALL` creates a common axis across the two panels. In these next steps, you also move the legend inside (similar to a previous part of this example) and rearrange the three inset boxes.

The new template structure is as follows:

```
%let TitleText2 = "Kaplan-Meier Plot";

%macro SurvivalTemplate;
  proc template;
    define statgraph Stat.Lifetest.Graphics.ProductLimitSurvival;
      dynamic NStrata xName plotAtRisk plotCL plotHW plotEP labelCL
        %if %nrquote(&censored) ne %then plotCensored;
      labelHW labelEP maxTime xtickVals xtickValFitPol method StratumID
      classAtRisk plotBand plotTest GroupName yMin Transparency
      SecondTitle TestName pValue;
      BeginGraph;

      entrytitle &titletext2;
      if (EXISTS(SECONDTITLE))
        entrytitle SECONDTITLE / textattrs=GRAPHVALUETEXT;
      endif;

      layout lattice / rows=2 columns=1 columndatarange=unionall
        rowweights=(.85 .15);
      layout overlay / xaxisopts=(&xoptions) yaxisopts=(&yoptions);
      %multiplestrata
      endlayout;

      layout overlay / xaxisopts=(display=none);
      blockplot x=TATRISK block=ATRISK / class=CLASSATRISK
        display=(label values) &blockopts;
      endlayout;
    endlayout;

      EndGraph;
    end;
  run;
%mend;
```

```

%macro multiplestrata;
  if (PLOTBW)
    bandplot LimitUpper=HW_UCL LimitLower=HW_LCL x=TIME / &bandopts
             datatransparency=Transparency;
  endif;
  if (PLOTTEP)
    bandplot LimitUpper=EP_UCL LimitLower=EP_LCL x=TIME / &bandopts
             datatransparency=Transparency;
  endif;
  if (PLOTCL)
    if (PLOTBAND)
      bandplot LimitUpper=SDF_UCL LimitLower=SDF_LCL x=TIME / &bandopts
               display=(outline);
    else
      bandplot LimitUpper=SDF_UCL LimitLower=SDF_LCL x=TIME / &bandopts
               datatransparency=Transparency;
    endif;
  endif;

  stepplot y=SURVIVAL x=TIME / &groups name="Survival" &tips;

  if (PLOTCECENSORED)
    scatterplot y=CENSORED x=TIME / &groups &censored &tipl;
  endif;

  DiscreteLegend "Survival" / title=GROUPNAME location=outside;

  if (PLOTCECENSORED)
    if (PLOTTEST)
      layout gridded / rows=2 &gridopts;
      entry &sensorstr;
      %entry_p
    endlayout;
    else
      layout gridded / rows=1 &gridopts;
      entry &sensorstr;
    endlayout;
  endif;
  else
    if (PLOTTEST)
      layout gridded / rows=1 &gridopts;
      %entry_p
    endlayout;
  endif;
endif;

dynamic NObs1 NObs2 NObs3 NEvent1 NEvent2 NEvent3;
layout gridded / columns=3 border=TRUE autoalign=(TopRight);
  entry "";      entry "Event";  entry "Total";
  entry "1";     entry NEvent1;  entry NObs1;
  entry "2";     entry NEvent2;  entry NObs2;
  entry "3";     entry NEvent3;  entry Nobs3;
endlayout;
%mend;

%SurvivalTemplate

```

You can further simplify the plot by moving the legend inside, removing the title from the legend (which is currently the variable name Group), and instead adding “+ Censored” (the contents of the inset table) to the legend in place of the title, as in the following statement:

```
DiscreteLegend "Survival" / title="+ Censored"
  titleattrs=GraphValueText location=inside autoalign=(Bottom);
```

The option TITLEATTRS=GRAPHVALUETEXT is specified so that the “+ Censored” appears in the same font as the other entries in the legend and appears to be just another part of the legend. All of the statements for making the old inset table can now be removed from the template. The full template also plots bands, which are not used in this example, so they can also be removed. The resulting template is as follows:

```
%let TitleText2 = "Kaplan-Meier Plot";

%macro SurvivalTemplate;
  proc template;
    define statgraph Stat.Lifetest.Graphics.ProductLimitSurvival;
      dynamic NStrata xName plotAtRisk plotCL plotHW plotEP labelCL
        %if %nrbracequote(&censored) ne %then plotCensored;
        labelHW labelEP maxTime xtickVals xtickValFitPol method StratumID
        classAtRisk plotBand plotTest GroupName yMin Transparency
        SecondTitle TestName pValue;
      BeginGraph;

        entrytitle &titletext2;
        if (EXISTS(SECONDTITLE))
          entrytitle SECONDTITLE / textattrs=GRAPHVALUETEXT;
        endif;

        layout lattice / rows=2 columns=1 columndatarange=unionall
          rowweights=(.85 .15);
          layout overlay / xaxisopts=(&xoptions) yaxisopts=(&yoptions);
            %multiplestrata
          endlayout;

          layout overlay / xaxisopts=(display=none);
            blockplot x=TATRISK block=ATRISK / class=CLASSATRISK
              display=(label values) &blockopts;
            endlayout;
          endlayout;

      EndGraph;
    end;
  run;
%mend;
```

```

%macro MultipleStrata;

    stepplot y=SURVIVAL x=TIME / &groups name="Survival" &tips;

    if (PLOTCEASURED)
        scatterplot y=CENSORED x=TIME / &groups &censored &tipl;
    endif;

    DiscreteLegend "Survival" / title="+ Censored"
        titleattrs=GraphValueText location=inside autoalign=(Bottom);

    dynamic NObs1 NObs2 NObs3 NEvent1 NEvent2 NEvent3;
    layout gridded / columns=3 border=TRUE autoalign=(TopRight);
        entry "";          entry "Event";    entry "Total";
        entry "1";         entry NEvent1;  entry NObs1;
        entry "2";         entry NEvent2;  entry NObs2;
        entry "3";         entry NEvent3;  entry Nobs3;
    endlayout;
%mend;

%SurvivalTemplate

```

The following step uses the new template to create the desired plot:

```

proc lifetest data=sashelp.BMT
    plots=survival(maxlen=13 atrisk=0 to 2500 by 500);
    ods select SurvivalPlot;
    time T * Status(0);
    strata Group;
run;

```

The plot is displayed in [Output 22.3.7](#) at the beginning of this section.

This example removed a great deal of functionality from the default template so that the final, modified template would be relatively simple and understandable, but this is not necessary. The template could have been modified without deleting the first LAYOUT OVERLAY and other statements. The strategy for template modification illustrated in this example can be applied to any complicated template: identify the overall structure, isolate the relevant pieces, and then make changes in stages. Since the modified template no longer works for all analyses, it is important that you delete it when you are done, as in the following example:

```

%SurvivalTemplateRestore

proc template;
    delete Stat.Lifetest.Graphics.ProductLimitSurvival / store=sasuser.templat;
run;

```

Changing Line Styles

The survival plot for multiple strata has a separate step function for each stratum. The information that goes into making each stratum appears as a separate group of observations in the data object that is displayed in the graph. The template options `GROUP=STRATUM` and `INDEX=STRATUMNUM` specify the data object columns that provide the information for identifying each stratum. The `GROUP=` column provides the stratum name, and the `INDEX=` column provides a numeric index that identifies each group. There are no options that explicitly control the colors or other aspects of the appearance of information about each stratum. The number of groups can be large, and it is not known at the time the template is written how many groups must be accommodated. Therefore, group information is controlled by ODS styles. The style elements `GraphData1`, `GraphData2`, `GraphData3`, and so on control the appearance of groups. See the section “[Some Common Style Elements](#)” on page 640 for more information.

You can use the `HTMLBLUE` style when you want groups to be distinguished only by color. Alternatively, you can easily modify any other style to be an all-color style like `HTMLBLUE`. For example:

```
proc template;
  define style styles.Statistical2;
    parent = Statistical;
    style Graph from Graph / attrpriority = "Color";
  end;
run;
```

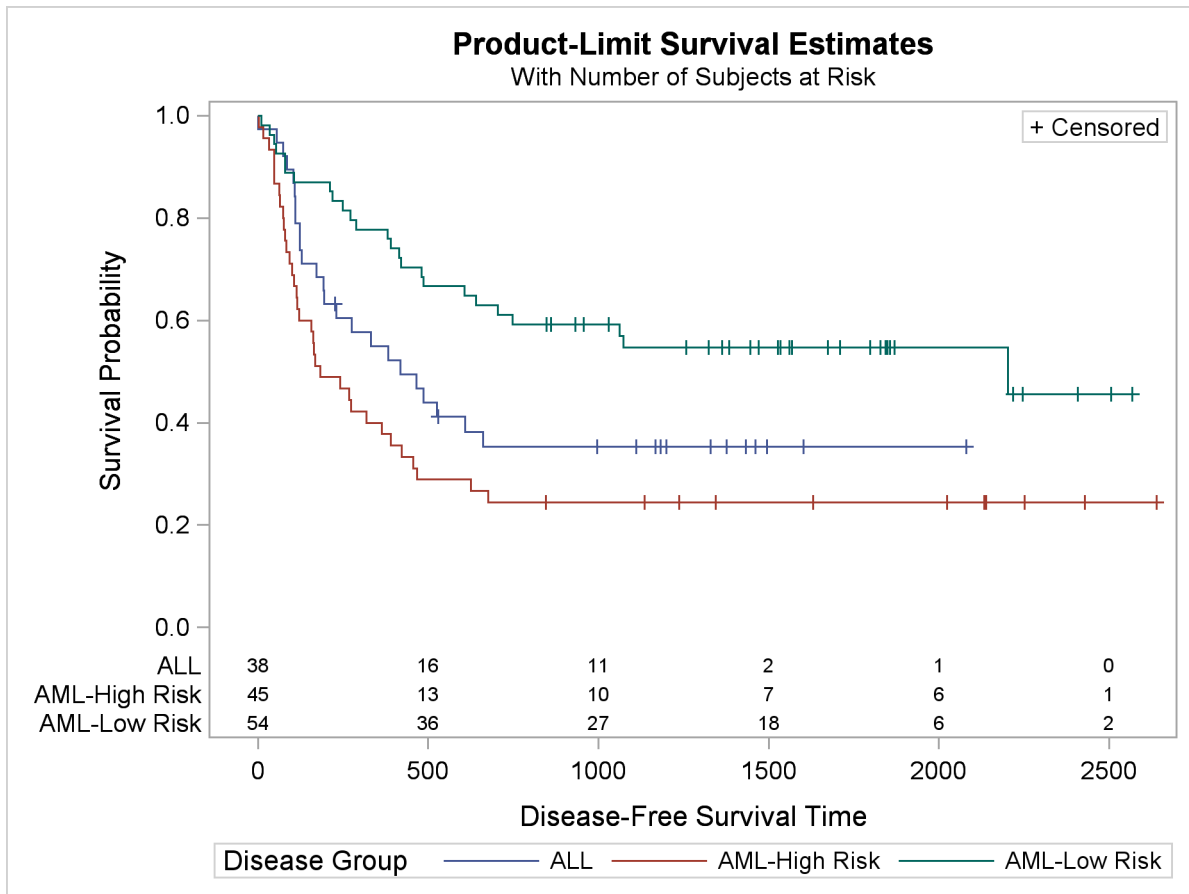
You can instead use the SAS autocall macro `%ModStyle`. See the section “[Creating an All-Color Style](#)” on page 669 in Chapter 21, “[Statistical Graphics Using ODS](#),” for more information. The easiest way to use the `%ModStyle` macro is as follows:

```
%modstyle(name=StatColor, parent=statistical)

ods listing style=StatColor;

proc lifetest data=sashelp.BMT
  plots=survival(maxlen=13 atrisk=0 to 2500 by 500);
  ods select SurvivalPlot;
  time T * Status(0);
  strata Group;
run;
```

A new style called `STATCOLOR` is created that inherits from the `STATISTICAL` style. The result (since no other options were specified) is an all-color style. All lines have the same solid line style instead of the default, which uses different line styles. The results are displayed in [Output 22.3.8](#).

Output 22.3.8 Survival Plot with an All-Color Style

There are many other changes you can make to styles, and many other ways to use the `%ModStyle` macro. The following steps illustrate three ways to change the colors. The first uses the `%ModStyle` macro and an explicit color list to create an all-color style for the first three groups. The second creates an all-color style by redefining `GraphData1` through `GraphData3`. The third creates a new style by redefining `GraphData1` through `GraphData3`, inheriting from the old style elements, but overriding the colors. Only the last style change is actually used in this example to make a graph. The following steps create the graph displayed in [Output 22.3.9](#):

```
%modstyle(name=StatColor, parent=HTMLBlue, colors=purple orange silver)
```

```
proc template;
  define style Styles.StatColor;
    parent = Styles.HTMLBlue;
    style GraphData1 / contrastcolor = purple;
    style GraphData2 / contrastcolor = orange;
    style GraphData3 / contrastcolor = silver;
  end;
run;
```

```
proc template;
  define style Styles.StatColor;
    parent = Styles.HTMLBlue;
```

```

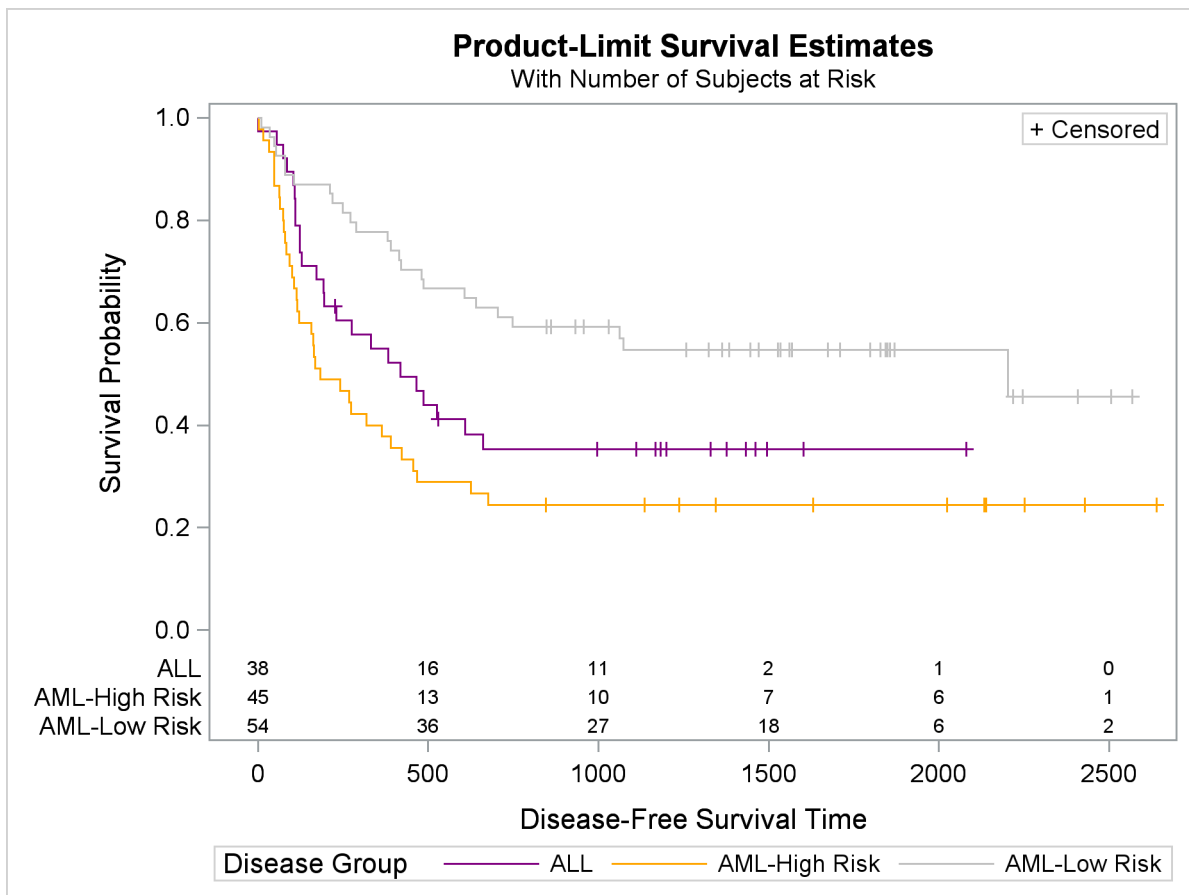
style GraphData1 from GraphData1 / contrastcolor = purple;
style GraphData2 from GraphData2 / contrastcolor = orange;
style GraphData3 from GraphData3 / contrastcolor = silver;
end;
run;

ods listing style=StatColor;

proc lifetest data=sashelp.BMT
  plots=survival(maxlen=13 atrisk=0 to 2500 by 500);
  ods select SurvivalPlot;
  time T * Status(0);
  strata Group;
run;

```

Output 22.3.9 Survival Plot with a Modified Style



Most other examples in this section change the graph template. This example creates a new style template. Since a new template is created instead of modifying an existing template, there is nothing that must be cleaned up in this example. However, you can delete the new style template as follows:

```

proc template;
  delete Styles.StatColor / store=sasuser.templat;
run;

```

Alternatively, there is no harm in leaving it around since it has no effect unless you explicitly specify it on a destination statement.

Changing Fonts

You can change the fonts for the axis labels by using the LABELATTRS= option for both the X and Y axes. You can change the fonts for the tick values by using the TICKVALUEATTRS= option for both the X and Y axes. The following steps illustrate:

```
%SurvivalTemplateRestore

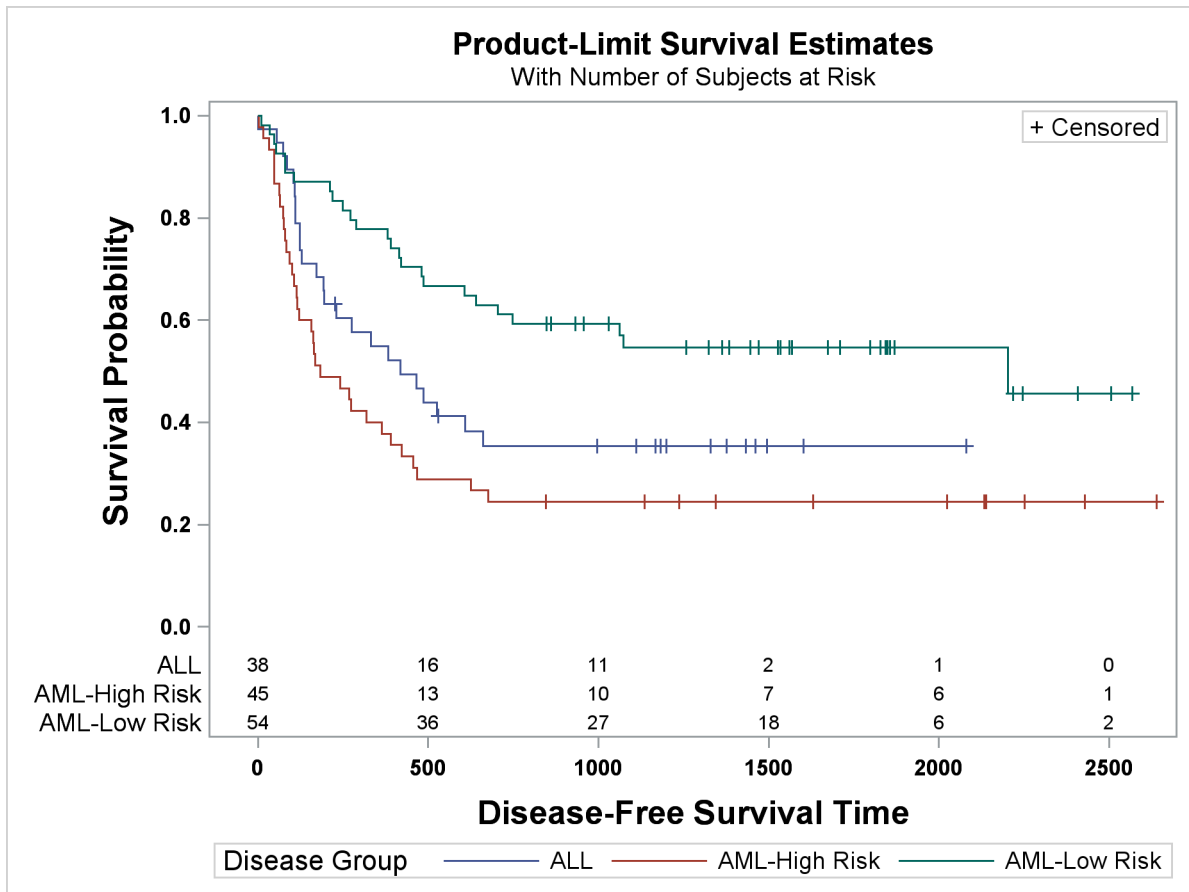
%let yOptions    = label="Survival Probability"
                  shortlabel="Survival"
                  labelattrs=(size=12pt weight=bold)
                  tickvalueattrs=(size=8pt weight=bold)
                  linearopts=(viewmin=0 viewmax=1
                              tickvaluelist=(0 .2 .4 .6 .8 1.0));

%let xOptions    = shortlabel=XNAME
                  offsetmin=.05
                  labelattrs=(size=12pt weight=bold)
                  tickvalueattrs=(size=8pt weight=bold)
                  linearopts=(viewmax=MAXTIME tickvaluelist=XTICKVALS
                              tickvaluefitpolicy=XTICKVALFITPOL);

%SurvivalTemplate

proc lifetest data=sashelp.BMT
  plots=survival(maxlen=13 atrisk=0 to 2500 by 500);
  ods select SurvivalPlot;
  time T * Status(0);
  strata Group;
run;
```

These steps create axis label fonts that are greater than the default (12-point rather than 10-point) and are bold. The tick value fonts are smaller than the default (8-point rather than 9-point) and again are bold. The results are displayed in [Output 22.3.10](#).

Output 22.3.10 Survival Plot with a Modified Axis Label Font

You can restore the default macros, macro variables, and template by running the following steps:

```
%SurvivalTemplateRestore
```

```
proc template;
  delete Stat.Lifetest.Graphics.ProductLimitSurvival / store=sasuser.templat;
run;
```

Instead of changing a graph template to change fonts, you can change the fonts by modifying the ODS style. The following steps write the HTMLBLUE style and its parent style STATISTICAL to a file and display only those lines that pertain to fonts:

```
filename temp1 'temp1.tpl' lrecl=100;
filename temp2 'temp2.tpl' lrecl=100;
filename temp ('temp1.tpl' 'temp2.tpl') lrecl=100;

proc template;
  source styles.htmlblue / file=temp1;
  source styles.statistical / file=temp2;
run;
```

```

data _null_;
  infile temp pad;
  input line $ 1-100;
  file print;
  if index(lowercase(line), 'font') then put line;
run;

```

The results are displayed in [Output 22.3.11](#).

Output 22.3.11 The Part of the HTMLBLUE Style That Pertains to Fonts

```

style fonts /
'TitleFont2' = ("<sans-serif>, <MTsans-serif>, Helvetica, Helv",2,bold)
'TitleFont' = ("<sans-serif>, <MTsans-serif>, Helvetica, Helv",3,bold)
'StrongFont' = ("<sans-serif>, <MTsans-serif>, Helvetica, Helv",2,bold)
'EmphasisFont' = ("<sans-serif>, <MTsans-serif>, Helvetica, Helv",2,italic)
'FixedFont' = ("<monospace>, Courier",2)
'BatchFixedFont' = ("SAS Monospace, <monospace>, Courier, monospace",2)
'FixedHeadingFont' = ("<monospace>, Courier, monospace",2)
'FixedStrongFont' = ("<monospace>, Courier, monospace",2,bold)
'FixedEmphasisFont' = ("<monospace>, Courier, monospace",2,italic)
'headingEmphasisFont' = ("<sans-serif>, <MTsans-serif>, Helvetica, Helv",2,bold italic)
'headingFont' = ("<sans-serif>, <MTsans-serif>, Helvetica, Helv",2,bold)
'docFont' = ("<sans-serif>, <MTsans-serif>, Helvetica, Helv",2);
style GraphFonts /
'GraphDataFont' = ("<sans-serif>, <MTsans-serif>",7pt)
'GraphUnicodeFont' = ("<MTsans-serif-unicode>",9pt)
'GraphValueFont' = ("<sans-serif>, <MTsans-serif>",9pt)
'GraphLabel12Font' = ("<sans-serif>, <MTsans-serif>",10pt)
'GraphLabelFont' = ("<sans-serif>, <MTsans-serif>",10pt)
'GraphFootnoteFont' = ("<sans-serif>, <MTsans-serif>",10pt)
'GraphTitleFont' = ("<sans-serif>, <MTsans-serif>",11pt,bold)
'GraphTitle1Font' = ("<sans-serif>, <MTsans-serif>",14pt,bold)
'GraphAnnoFont' = ("<sans-serif>, <MTsans-serif>",10pt);
font = fonts('HeadingFont')
font = fonts('HeadingFont')
font = fonts('HeadingFont')
font = fonts('HeadingFont')
font = fonts('DocFont')
font = fonts('DocFont')
font = Fonts('headingEmphasisFont');
font = Fonts('TitleFont2');
font = Fonts('docFont');

```

If neither of these styles contains the right information, you can also display the DEFAULT style, which is the parent of the STATISTICAL style, as follows:

```

filename temp1 'temp1.tpl' lrecl=100;
filename temp2 'temp2.tpl' lrecl=100;
filename temp3 'temp3.tpl' lrecl=100;
filename temp ('temp1.tpl' 'temp2.tpl' 'temp3.tpl') lrecl=100;

proc template;
  source styles.htmlblue / file=temp1;
  source styles.statistical / file=temp2;
  source styles.default / file=temp3;
run;

data _null_;
  infile temp pad;
  input line $ 1-100;
  file print;
  if index(lowercase(line), 'font') then put line;
run;

```

The results of this step are not shown.

The following step creates a new style, `STATBIGFONT`, that redefines the `GraphLabelFont` style element from an ordinary 10-point font to a bold 12-point font and the `GraphValueFont` style element from an ordinary 9-point font to a bold 8-point font:

```

proc template;
  define style Styles.StatBigFont;
    parent = Styles.HTMLBlue;
    style graphfonts from graphfonts /
      'GraphLabelFont' = ("<sans-serif>, <MTsans-serif>", 12pt, bold)
      'GraphValueFont' = ("<sans-serif>, <MThsans-serif>", 8pt, bold);
  end;
run;

```

The following step creates the graph that is displayed in [Output 22.3.12](#):

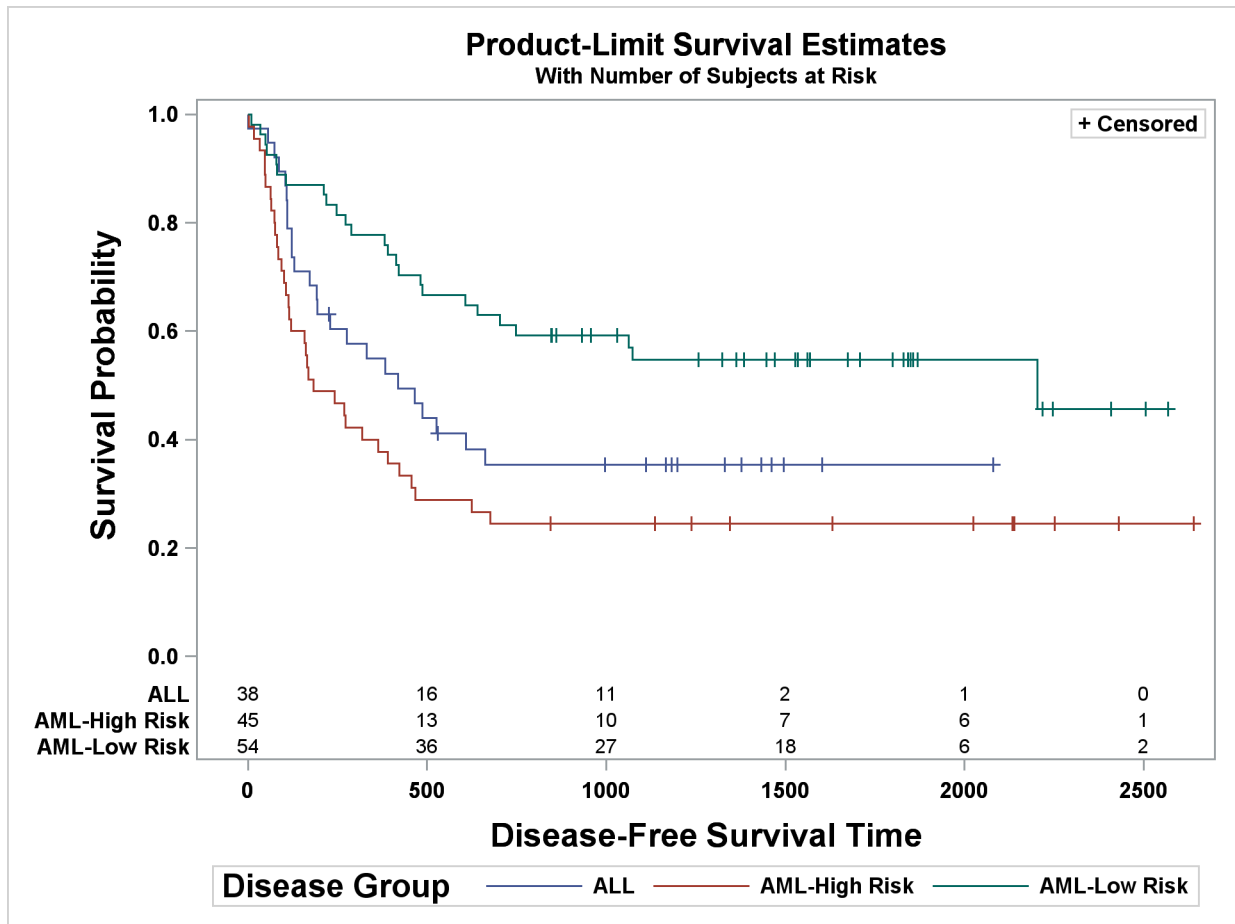
```

ods listing style=StatBigFont;

proc lifetest data=sashelp.BMT
  plots=survival(maxlen=13 atrisk=0 to 2500 by 500);
  ods select SurvivalPlot;
  time T * Status(0);
  strata Group;
run;

```

The graph displayed in [Output 22.3.12](#) is almost identical to the one displayed in [Output 22.3.10](#). They differ since the `GraphLabelFont` style element also controls the title for the legend, and the `GraphValueFont` style element also controls the labels for the at-risk information table.

Output 22.3.12 Survival Plot with a Modified `GraphLabelFont` Style Element

You can delete the new style template as follows:

```
proc template;
  delete Styles.StatBigFont / store=sasuser.templat;
run;
```

Changing How Censored Data Are Displayed

By default, PROC LIFETEST displays a plus to indicate censoring. This example illustrates how to change that symbol to a small filled circle both on the step plots and in the inset box. The following steps change the template and create **Output 22.3.13**:

```
%SurvivalTemplateRestore

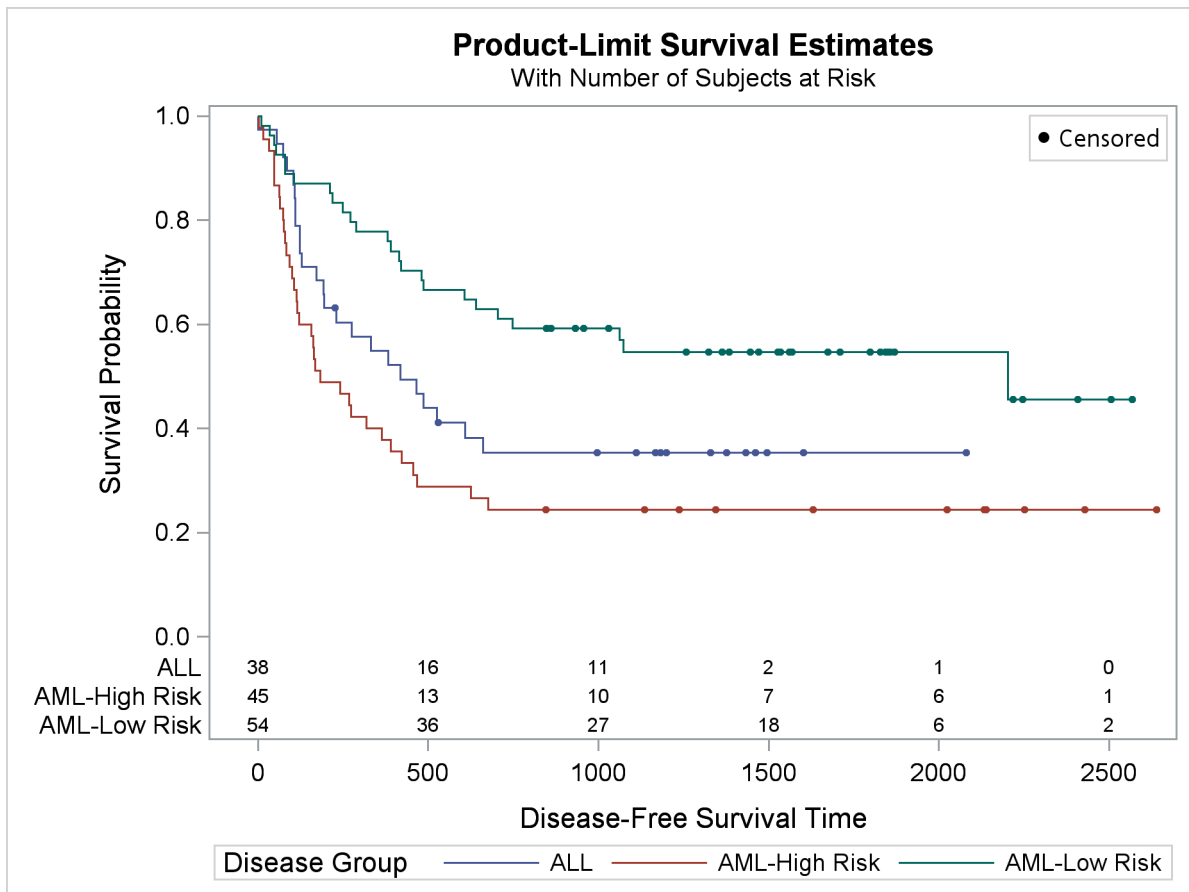
%let censored = markerattrs=(symbol=circlefilled size=3px);
%let censorstr = "(*ESC*){Unicode '25cf'x} Censored"
                / textattrs=GraphValueText (family=GraphUnicodeText:FontFamily);

%SurvivalTemplate

proc lifetest data=sashelp.BMT
  plots=survival(maxlen=13 atrisk=0 to 2500 by 500);
  ods select SurvivalPlot;
  time T * Status(0);
  strata Group;
run;
```

The Unicode Consortium <http://unicode.org/> provides a list of character codes at <http://www.unicode.org/charts/charindex.html>.

Output 22.3.13 Survival Plot with a Modified Display of Censoring



The following step suppresses the censoring information by using the NOCENSOR option in the survival plot request:

```
proc lifetest data=sashelp.BMT
  plots=survival(nocensor maxlen=13 atrisk=0 to 2500 by 500);
  ods select SurvivalPlot;
  time T * Status(0);
  strata Group;
run;
```

Alternatively, you could make a template change to have the same effect and create [Output 22.3.14](#) as follows:

```
%let censored = ;

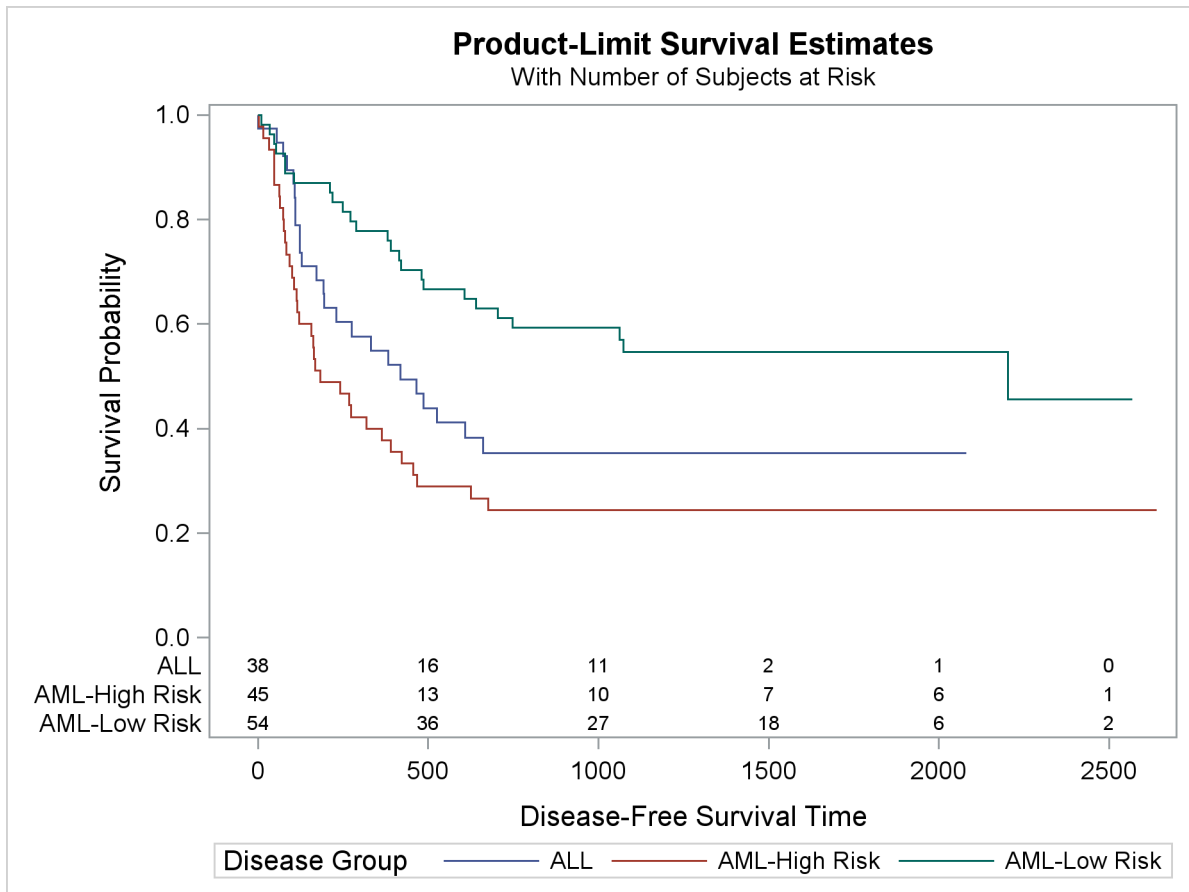
%SurvivalTemplate;

proc lifetest data=sashelp.BMT
  plots=survival(maxlen=13 atrisk=0 to 2500 by 500);
  ods select SurvivalPlot;
  time T * Status(0);
  strata Group;
run;
```

This step works because the modularized template was written to include the following DYNAMIC statement:

```
dynamic NStrata xName plotAtRisk plotCL plotHW plotEP labelCL
  %if %nrbquote(&censored) ne %then plotCensored;
  labelHW labelEP maxTime xtickVals xtickValFitPol method StratumID
  classAtRisk plotBand plotTest GroupName yMin Transparency
  SecondTitle TestName pValue;
```

The DYNAMIC statement names the variables that are set by the procedure and control aspects of the graph. The plotCensored dynamic variable controls whether the censoring information is plotted. It is omitted from the list of dynamic variables when the macro variable Censored is null, so all aspects of the graph that are conditionally displayed based on the value of the dynamic variable plotCensored are suppressed.

Output 22.3.14 Survival Plot with No Display of Censoring

You can restore the default macros, macro variables, and template by running the following steps:

```
%SurvivalTemplateRestore
```

```
proc template;
```

```
  delete Stat.Lifetest.Graphics.ProductLimitSurvival / store=sasuser.templat;
```

```
run;
```

Displaying Survival Summary Statistics

PROC LIFETEST passes a number of summary statistics as dynamic variables to the survival plot template. See the section “Additional Dynamic Variables for Survival Plots Using ODS Graphics” on page 4060 in Chapter 52, “The LIFETEST Procedure,” for information about these dynamic variables. In this example, the graph template is modified to display survival summary statistics.

The following steps create [Output 22.3.15](#):

```

%SurvivalTemplateRestore

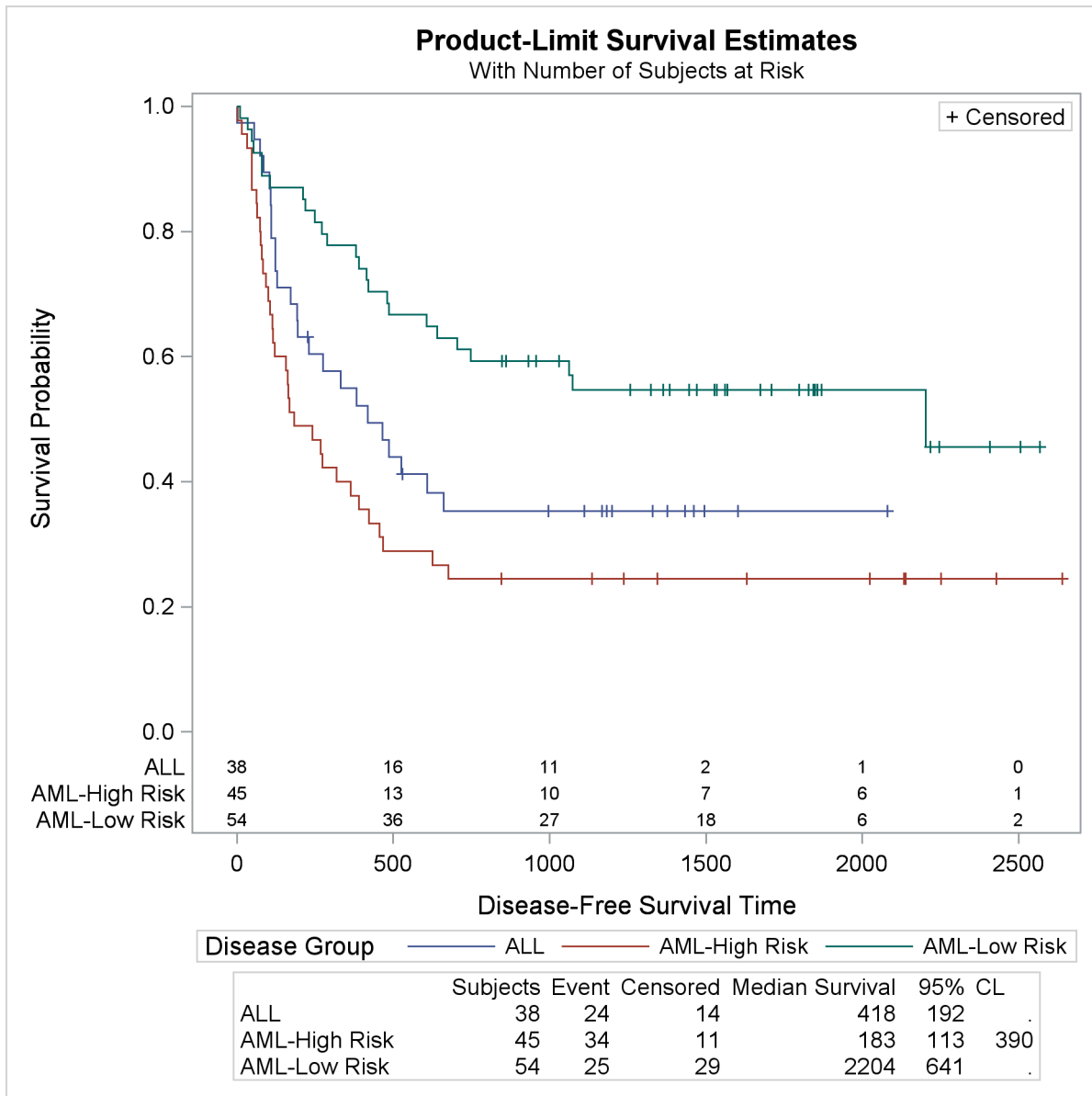
%let fmt = bestd6.;

%macro header;
  entry halign=right "Subjects";
  entry halign=right "Event";
  entry halign=right "Censored";
  entry halign=right "Median Survival";
  entry halign=right PctMedianConfid;
  entry halign=left  "CL";
%mend;

%macro table1;
  columnheaders;
  layout overlay / pad=(top=5);
  layout gridded / columns=6 border=TRUE;
  dynamic PctMedianConfid NObs NEvent Median
          MedianLower MedianUpper;
  %header
  entry halign=right NObs;
  entry halign=right NEvent;
  entry halign=right eval(NObs-NEvent);
  entry halign=right eval(put(Median, &fmt));
  entry halign=right eval(put(MedianLower, &fmt));
  entry halign=right eval(put(MedianUpper, &fmt));
  endlayout;
  endlayout;
  endcolumnheaders;
%mend;

```

Output 22.3.15 Survival Plot with Survival Summary Statistics



```

%macro table2;
  columnheaders;
  layout overlay / pad=(top=5);
  layout gridded / columns=7 border=TRUE;
  dynamic PctMedianConfid;
  entry " ";
  %header
  %do i = 1 %to 6;
    dynamic StrVal&i NObs&i NEvent&i Median&i
      LowerMedian&i UpperMedian&i;
    if (&i <= nstrata)
      entry halign=left StrVal&i;
      entry halign=right NObs&i;
  %enddo;
%macro table2;

```

```

        entry halign=right NEvent&i;
        entry halign=right eval (NObs&i-NEvent&i);
        entry halign=right eval (put (Median&i, &fmt));
        entry halign=right eval (put (LowerMedian&i, &fmt));
        entry halign=right eval (put (UpperMedian&i, &fmt));
    endif;
%end;
endlayout;
endlayout;
endcolumnheaders;
%mend;

%macro SurvivalTemplate;
proc template;
define statgraph Stat.Lifetest.Graphics.ProductLimitSurvival;
dynamic NStrata xName plotAtRisk plotCL plotHW plotEP labelCL
%if %nrbracequote(&censored) ne %then plotCensored;
labelHW labelEP maxTime xtickVals xtickValFitPol method StratumID
classAtRisk plotBand plotTest GroupName yMin Transparency
SecondTitle TestName pValue;
BeginGraph / designheight=defaultdesignwidth;

if (NSTRATA=1)
if (EXISTS(STRATUMID))
entrytitle &titletext1;
else
entrytitle &titletext0;
endif;
if (PLOTATRISK=1)
entrytitle "with Number of Subjects at Risk" / textattrs=
GRAPHVALUETEXT;
endif;

layout lattice / rows=1 columns=1;
layout overlay / xaxisopts=(&xoptions) yaxisopts=(&yoptions);
%singlestratum
endlayout;
%table1
endlayout;

else
entrytitle &titletext2;
if (EXISTS(SECONDTITLE))
entrytitle SECONDTITLE / textattrs=GRAPHVALUETEXT;
endif;

layout lattice / rows=1 columns=1;
layout overlay / xaxisopts=(&xoptions) yaxisopts=(&yoptions);
%multiplestrata
endlayout;
%table2
endlayout;
endif;
EndGraph;

```

```

        end;
    run;
%mend;

%SurvivalTemplate

proc lifetest data=sashelp.BMT
    plots=survival(maxlen=13 atrisk=0 to 2500 by 500);
    ods select SurvivalPlot;
    time T * Status(0);
    strata Group;
run;

```

This example adds new macros that provide the portions of the template that produce the survival summary statistics table. This template allows for the display of tables with up to six strata. The template could be modified to handle more strata, particularly if the height of the graphical display area is increased, but the graph starts getting busy with too many strata.

The **%Header** macro provides a header for the table of summary statistics. In the single-stratum case, it provides all of the column headers. In the multiple-strata case, a blank header for the first column must be provided in addition to the column headers in the **%Header** macro.

The **%Table1** macro provides the summary statistics table for the single-stratum case. A **LAYOUT OVERLAY** statement adds padding to the top of the table so that it is separated from the legend. A **LAYOUT GRIDDED** statement creates a table with six columns. The six **ENTRY** statements in the **%Header** macro provide the column headers, and the six **ENTRY** statements in the **%Table1** macro provide the one-line body of the table.

The **%Table2** macro provides the summary statistics table for the multiple-strata case. A **LAYOUT OVERLAY** statement adds padding to the top of the table so that it is separated from the legend. A **LAYOUT GRIDDED** statement creates a table with seven columns. The blank **ENTRY** statement along with the eight **ENTRY** statements in the **%Header** macro provide the column headers, and the seven **ENTRY** statements in the **%Table2** macro provide the multi-line body of the table. These **ENTRY** statements are in a macro **DO** loop and are repeated six times for up to six strata. This macro also has a **DYNAMIC** statement that declares the dynamic variables whose values appear in the table.

The **%SurvivalTemplate** macro is modified to accommodate the table. For both the single-stratum and multiple-strata cases, a **LAYOUT LATTICE** statement is added so that a **COLUMNHEADERS** block can be added with the survival summary statistics table. The **%Table1** and **%Table2** macros are then added. The new statements could have been directly added to the **%SurvivalTemplate** macro instead of creating two additional macros. The additional macros were created solely to provide a more modular and readable template.

You can restore the default macros, macro variables, and template by running the following steps:

```

%SurvivalTemplateRestore

proc template;
    delete Stat.Lifetest.Graphics.ProductLimitSurvival / store=sasuser.templat;
run;

```

Example 22.4: Customizing Panels

This example illustrates how to modify the regression fit diagnostics panel shown in Figure 21.1 in Chapter 21, “Statistical Graphics Using ODS,” so that it displays a subset of the component plots. The original panel consists of eight plots and a summary statistics box. The ODS trace output from PROC REG shown previously shows that the template for the diagnostics panel is `Stat.REG.Graphics.DiagnosticsPanel`. The following statements display the template:

```
proc template;
  source Stat.REG.Graphics.DiagnosticsPanel;
run;
```

An abridged version of the results is shown next:

```
define statgraph Stat.Reg.Graphics.DiagnosticsPanel;
  notes "Diagnostics Panel";
  dynamic . . .;
  BeginGraph / designheight=defaultDesignWidth;
  entrytitle halign=left textattrs=GRAPHVALUETEXT _MODELLABEL
    halign=center textattrs=GRAPHTITLETEXT "Fit Diagnostics"
    " for " _DEPNAME;
  layout lattice / columns=3 rowgutter=10 columngutter=10
    shrinkfonts=true rows=3;
  layout overlay / xaxisopts=(shortlabel='Predicted');
  . . .
  endlayout;
  layout overlay / xaxisopts=(shortlabel='Predicted');
  . . .
  endlayout;
  layout overlay / xaxisopts=(label='Leverage' offsetmax=0.05)
  . . .
  endlayout;
  layout overlay / yaxisopts=(label="Residual" shortlabel=
    "Resid") xaxisopts=(label="Quantile");
  . . .
  endlayout;
  layout overlayequated / xaxisopts=(shortlabel='Predicted')
  . . .
  endlayout;
  layout overlay / xaxisopts=(linearopts=(integer=true) label=
    "Observation" shortlabel="Obs" offsetmax=0.05) yaxisopts=(
    offsetmin=0.05 offsetmax=0.05);
  . . .
  endlayout;
  layout overlay / xaxisopts=(label="Residual") yaxisopts=(label
    ="Percent");
  . . .
  endlayout;
  layout lattice / columns=2 rows=1 rowdatarange=unionall
    columngutter=0;
  . . .
  endlayout;
```

```

    if (_SHOWSTATS =1)
        layout overlay;
        . . .
    endLayout;
    endif;
    if (_SHOWSTATS = 2)
        layout overlay / yaxisopts=(gridDisplay=auto_off label=
            "Residual");
        . . .
    endlayout;
    endif;
endlayout;
EndGraph;
end;

```

The outermost components of the template are a BEGINGRAPH/ENDGRAPH block with a lattice layout with ROWS=3 and COLUMNS=3 that defines the 3×3 panel of plots. Inside that are nine layouts, one for each cell, the last of which is conditionally defined. The LAYOUT statements define the components of the panel from left to right and top to bottom. You can eliminate some of the panels and produce a 2×2 panel as follows:

```

proc template;
  define statgraph Stat.Reg.Graphics.DiagnosticsPanel;
    notes "Diagnostics Panel";
    dynamic _DEPLABEL _DEPNAME _MODELLABEL _OUTLEVLABEL _TOTFREQ _NPARM
      _NOBS _OUTCOOKSDLABEL _SHOWSTATS _NSTATSCOLS _DATALABEL _SHOWNObs
      _SHOWTOTFREQ _SHOWNParm _SHOWEDF _SHOWMSE _SHOWRSquare
      _SHOWAdjRSq _SHOWSSE _SHOWDepMean _SHOWCV _SHOWAIC _SHOWBIC
      _SHOWCP _SHOWGMSEP _SHOWJP _SHOWPC _SHOWSBC _SHOWSP _EDF _MSE
      _RSquare _AdjRSq _SSE _DepMean _CV _AIC _BIC _CP _GMSEP _JP _PC
      _SBC _SP;
    BeginGraph / designheight=defaultDesignWidth;
    entrytitle halign=left textattrs=GRAPHVALUETEXT _MODELLABEL
      halign=center textattrs=GRAPHTITLETEXT "Fit Diagnostics"
      " for " _DEPNAME;
    layout lattice / columns=2 rowgutter=10 columngutter=10
      shrinkfonts=true rows=2;
    layout overlay / xaxisopts=(shortlabel='Predicted');
      referenceline y=-2;
      referenceline y=2;
      scatterplot y=RSTUDENT x=PREDICTEDVALUE / primary=true
        datalabel=_OUTLEVLABEL rolename=( _tip1=OBSERVATION _id1=
          ID1 _id2=ID2 _id3=ID3 _id4=ID4 _id5=ID5) tip=(y x _tip1
            _id1 _id2 _id3 _id4 _id5);
    endlayout;
    layout overlay / yaxisopts=(label="Residual" shortlabel=
      "Resid") xaxisopts=(label="Quantile");
      lineparm slope=eval (STDDEV(RESIDUAL)) y=eval (
        MEAN(RESIDUAL)) x=0 / extend=true lineattrs=
        GRAPHREFERENCE;
      scatterplot y=eval (SORT(DROPMISSING(RESIDUAL))) x=eval (
        PROBIT((NUMERATE(SORT(DROPMISSING(RESIDUAL))) -0.375)/
          (0.25 + N(RESIDUAL)))) / markerattrs=GRAPHDATADEFAULT
        primary=true

```



```

        rolename=(s=eval (SORT(DROPMISSING(RESIDUAL))) nq=eval (
        PROBIT((NUMERATE(SORT(DROPMISSING(RESIDUAL))) -0.375)
        /(0.25 + N(RESIDUAL)))) tiplabel=(nq="Quantile"
        s="Residual")
        tip=(nq s);
    endlayout;
    layout overlayequated / xaxisopts=(shortlabel='Predicted')
        yaxisopts=(label=_DEPLABEL shortlabel="Observed")
        equatetype=square;
    lineparm slope=1 x=0 y=0 / extend=true lineattrs=
        GRAPHREFERENCE;
    scatterplot y=DEPVAR x=PREDICTEDVALUE / primary=true
        datalabel=_OUTLEVLABEL rolename=( _tip1=OBSERVATION _id1=
        ID1 _id2=ID2 _id3=ID3 _id4=ID4 _id5=ID5) tip=(y x _tip1
        _id1 _id2 _id3 _id4 _id5);
    endlayout;
    layout overlay / xaxisopts=(label="Residual") yaxisopts=(label
        ="Percent");
    histogram RESIDUAL / primary=true;
    densityplot RESIDUAL / name="Normal" legendlabel="Normal"
        lineattrs=GRAPHFIT;
    endlayout;
    endlayout;
    EndGraph;
end;
run;

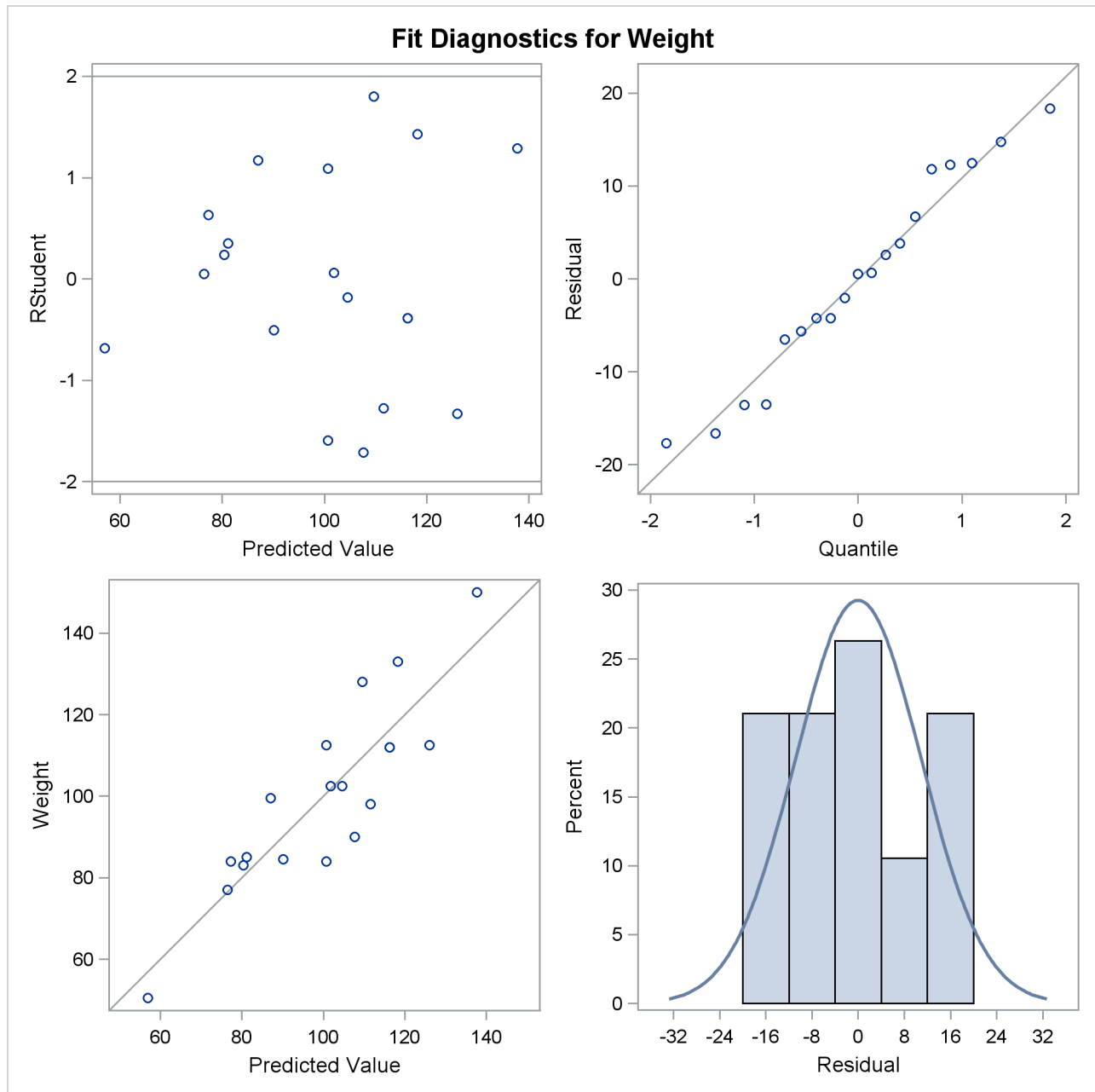
ods graphics on;

proc reg data=sashelp.class;
    model Weight = Height;
run; quit;

```

This template plots the residuals by predicted values, the Q-Q plot, the actual by predicted plot, and the residual histogram. The results are shown in [Output 22.4.1](#).

Output 22.4.1 Diagnostics Panel with Four Plots



This new template is a straightforward modification of the original template. The COLUMNS=2 and ROWS=2 options in the LAYOUT LATTICE statement request a 2×2 lattice. The LAYOUT statement blocks for components 1, 3, 6, 8, and 9 are deleted. **NOTE:** You do not need to understand every aspect of a template to modify it if you can recognize the overall structure and a few key options.

You can restore the original template as follows:

```
proc template;
  delete Stat.REG.Graphics.DiagnosticsPanel / store=sasuser.templat;
run;
```

Example 22.5: Customizing Axes and Reference Lines

This example illustrates several ways that you can change the plot axes in a scatter plot. The example uses PROC CORRESP to perform a correspondence analysis. It is taken from the section “Getting Started: CORRESP Procedure” on page 1996 in Chapter 32, “The CORRESP Procedure.” It uses the following data:

```

title "Number of Ph.D.'s Awarded from 1973 to 1978";

data PhD;
  input Science $ 1-19 y1973-y1978;
  label y1973 = '1973'
        y1974 = '1974'
        y1975 = '1975'
        y1976 = '1976'
        y1977 = '1977'
        y1978 = '1978';
  datalines;
Life Sciences      4489 4303 4402 4350 4266 4361
Physical Sciences  4101 3800 3749 3572 3410 3234
Social Sciences    3354 3286 3344 3278 3137 3008
Behavioral Sciences 2444 2587 2749 2878 2960 3049
Engineering        3338 3144 2959 2791 2641 2432
Mathematics        1222 1196 1149 1003  959  959
;

```

The following steps perform the correspondence analysis and create [Output 22.5.1](#):

```

ods graphics on;
ods trace on;

proc corresp data=PhD short;
  ods select configplot;
  var y1973-y1978;
  id Science;
run;

```

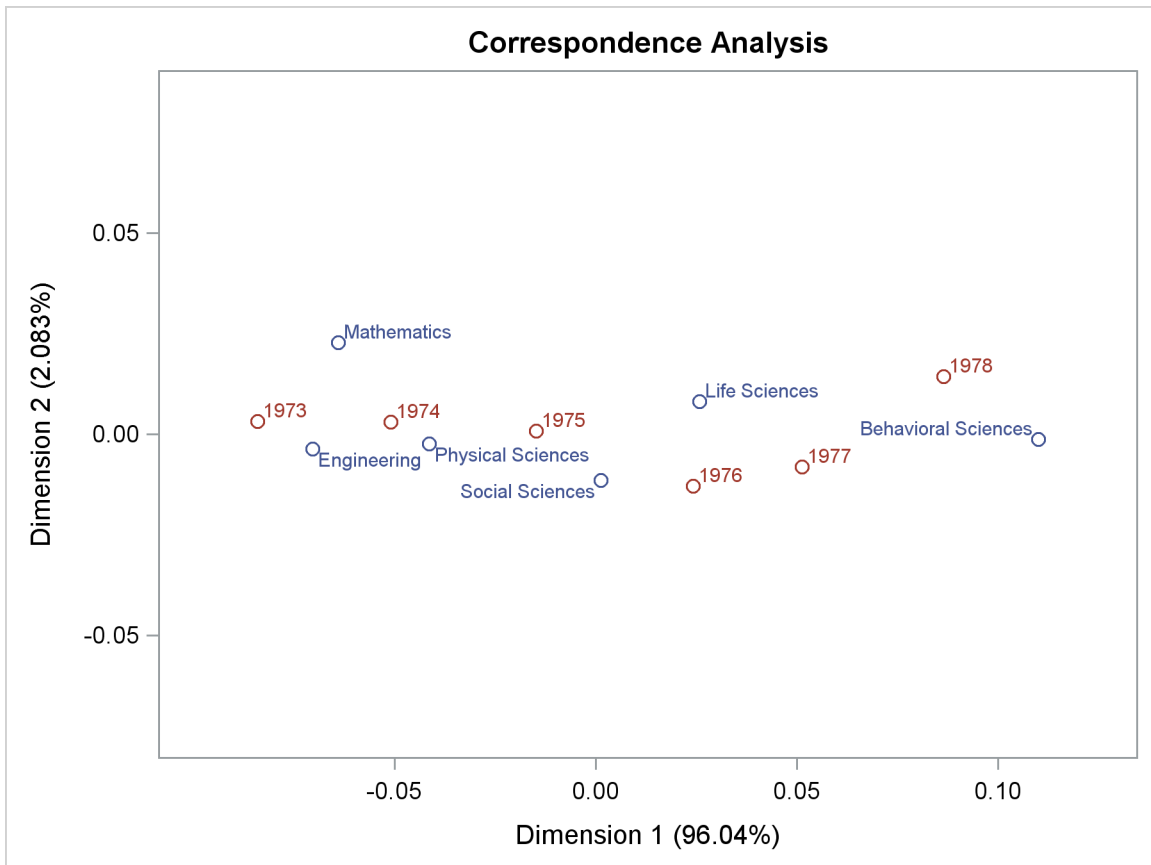
The trace output for this step (not shown) shows that the template for this plot is `Stat.Corresp.Graphics.Configuration`. The following step displays this template:

```

proc template;
  source Stat.Corresp.Graphics.Configuration;
run;

```

Output 22.5.1 Default Scatter Plot



The results are as follows:

```

define statgraph Stat.Corresp.Graphics.Configuration;
  dynamic xVar yVar head legend;
  begingraph;
  entrytitle HEAD;
  layout overlayequated / equatetype=fit xaxisopts=(offsetmin=0.1
    offsetmax=0.1) yaxisopts=(offsetmin=0.1 offsetmax=0.1);
  scatterplot y=YVAR x=XVAR / group=GROUP index=INDEX
    datalabel=LABEL datalabelattrs=GRAPHVALUETEXT
    name="Type" tip=(y x datalabel group)
    tiplabel=(group="Point");
  if (LEGEND)
    discretelegend "Type";
  endif;
  endlayout;
endgraph;
end;

```

You can add reference lines to the scatter plot at specified X and Y values by using the REFERENCELINE statement, as in the following example:

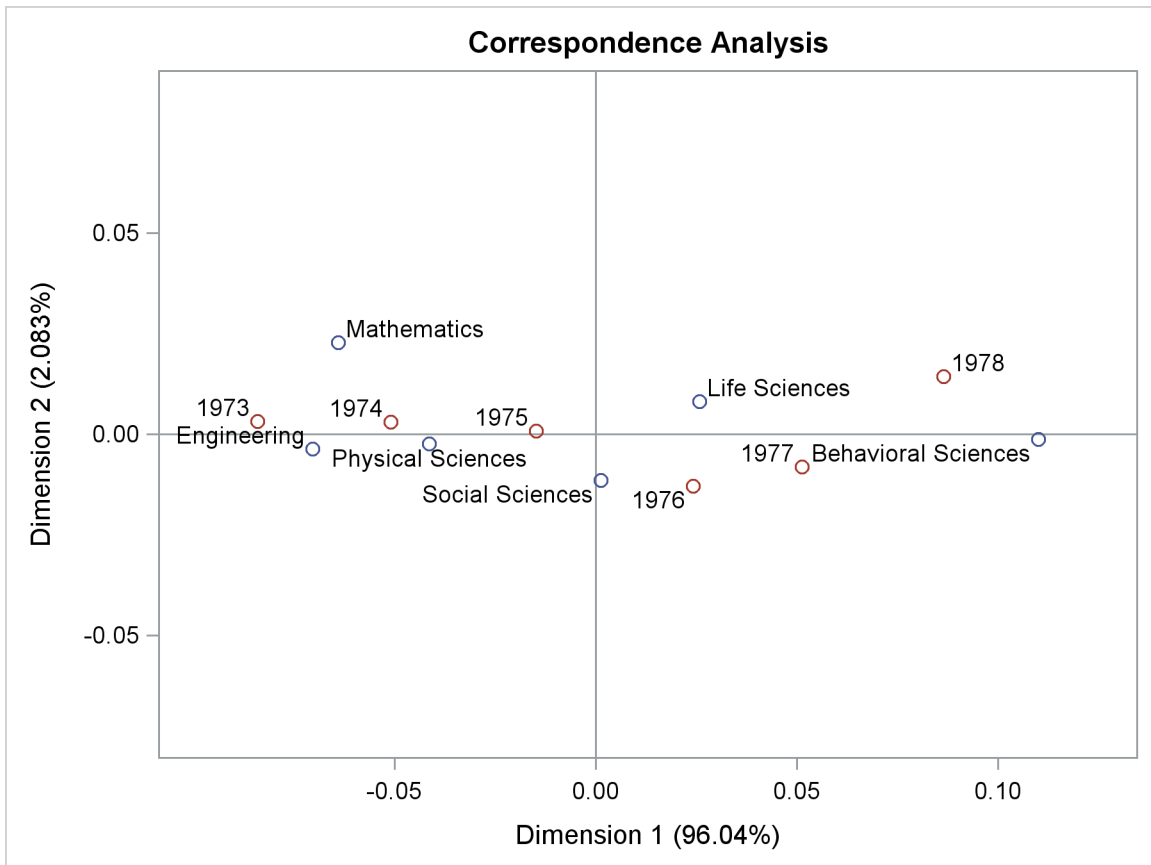
```
proc template;
  define statgraph Stat.Corresp.Graphics.Configuration;
    dynamic xVar yVar head legend;
    begingraph;
      entrytitle HEAD;
      layout overlayequated / equatetype=fit xaxisopts=(offsetmin=0.1
        offsetmax=0.1) yaxisopts=(offsetmin=0.1 offsetmax=0.1);

      referenceline x=0;
      referenceline y=0;

      scatterplot y=YVAR x=XVAR / group=GROUP index=INDEX
        datalabel=LABEL datalabelattrs=GRAPHVALUETEXT
        name="Type" tip=(y x datalabel group)
        tiplabel=(group="Point");
      if (LEGEND)
        discretelegend "Type";
      endif;
    endlayout;
  endgraph;
end;
run;

proc corresp data=PhD short;
  ods select configplot;
  var y1973-y1978;
  id Science;
run;
```

When you modify templates, it is important to note that the order of the statements within the LAYOUT OVERLAYEQUATED (or more typically, the LAYOUT OVERLAY) is significant. Here, the reference lines are added before the scatter plot so that the reference lines are drawn before the scatter plot. Consequently, labels and markers that coincide with the reference lines are drawn over the reference lines. The results, with reference lines, are displayed in [Output 22.5.2](#).

Output 22.5.2 Scatter Plot with Reference Lines Added

You can restore the default graph template as follows:

```
proc template;
  delete Stat.Corresp.Graphics.Configuration / store=sasuser.templat;
run;
```

The next steps show how you can change the style so that a frame is not shown:

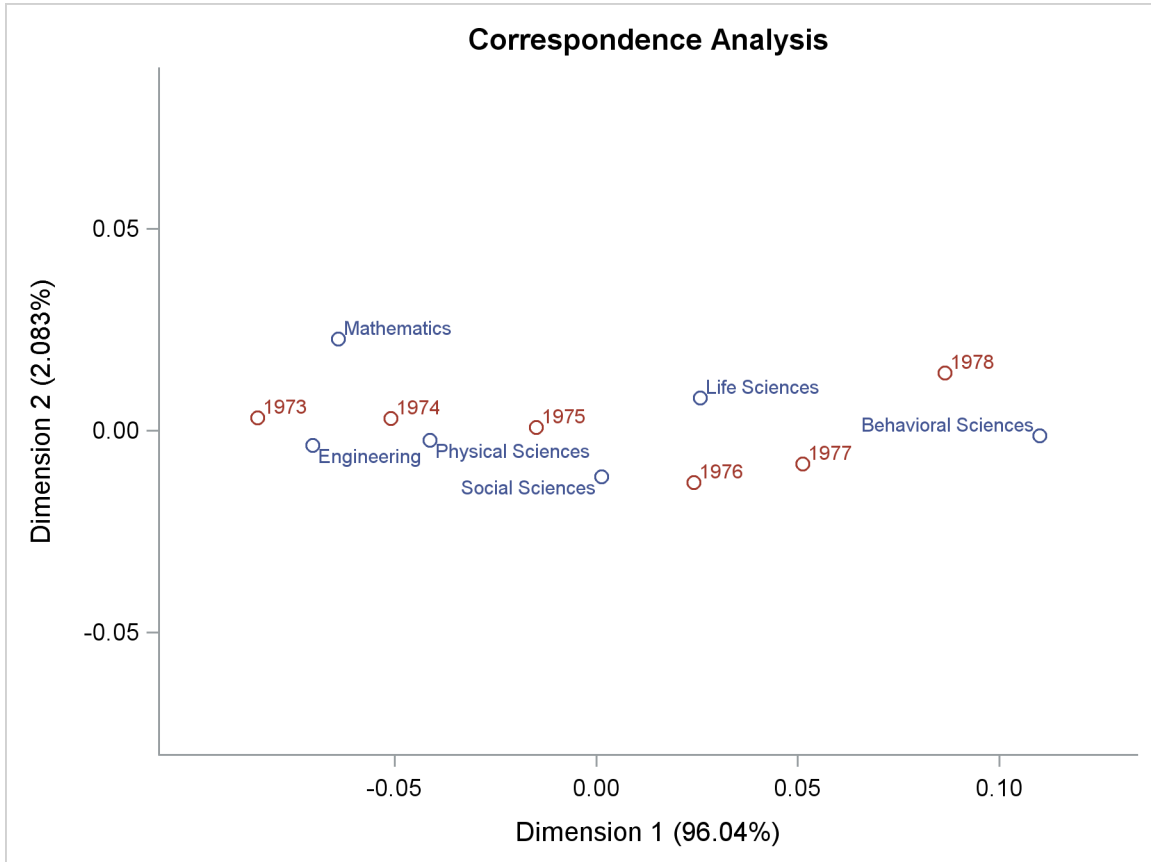
```
proc template;
  define style noframe;
    parent=styles.htmlblue;
    style graphwalls from graphwalls / frameborder=off;
  end;
run;

ods listing style=noframe;

proc corresp data=PhD short;
  ods select configplot;
  var y1973-y1978;
  id Science;
run;
```

The results, shown in [Output 22.5.3](#), display an X-axis and a Y-axis without a frame. Unlike the previous change, which affects only the ConfigPlot display, this change affects all plots created with the NOFRAME style.

Output 22.5.3 Scatter Plot with No Axis Frame



Alternatively, you can also add reference lines and delete the entire axis frame using the WALLDISPLAY=NONE and the DISPLAY= option in the graph template, as in the following example:

```
proc template;
  define statgraph Stat.Corresp.Graphics.Configuration;
    dynamic xVar yVar head legend;
    begingraph;
    entrytitle HEAD;

    layout overlayequated / equatetype=fit walldisplay=none
      xaxisopts=(display=(tickvalues) offsetmin=0.1 offsetmax=0.1)
      yaxisopts=(display=(tickvalues) offsetmin=0.1 offsetmax=0.1);

    referenceline x=0;
    referenceline y=0;

    scatterplot y=YVAR x=XVAR / group=GROUP index=INDEX
      datalabel=LABEL datalabelattrs=GRAPHVALUETEXT
      name="Type" tip=(y x datalabel group)
  end;
end;
```

```

        tiplabel=(group="Point");
    if (LEGEND)
        discretelegend "Type";
    endif;
endlayout;
endgraph;
end;
run;

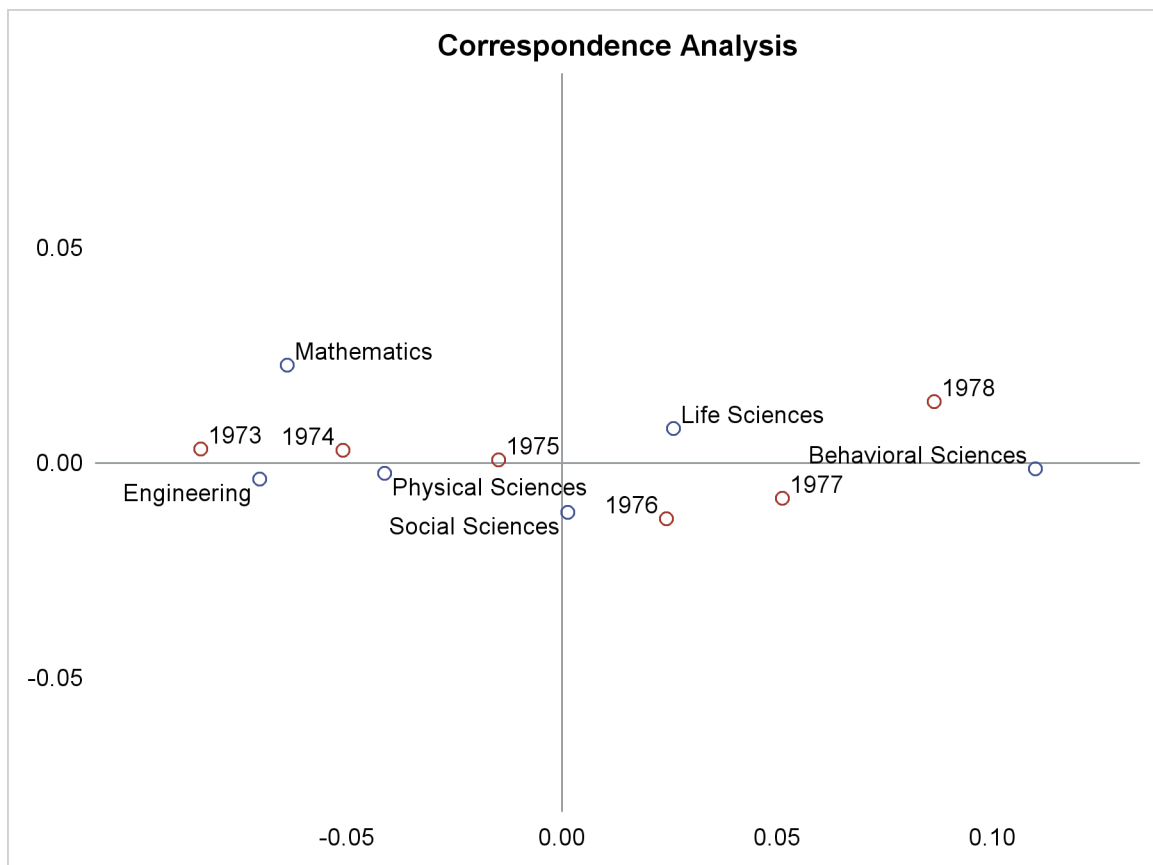
ods listing style=htmlblue;

proc corresp data=PhD short;
    ods select configplot;
    var y1973-y1978;
    id Science;
run;

```

The results are shown in [Output 22.5.4](#).

Output 22.5.4 Scatter Plot with Internal Axes



Instead of `DISPLAY=(TICKVALUES)`, you can use `DISPLAY=NONE` (not shown) to remove the tick values from the display as well. You can change the tick values, as in the following example:

```
proc template;
  define statgraph Stat.Corresp.Graphics.Configuration;
    dynamic xVar yVar head legend;
    begingraph;
      entrytitle HEAD;

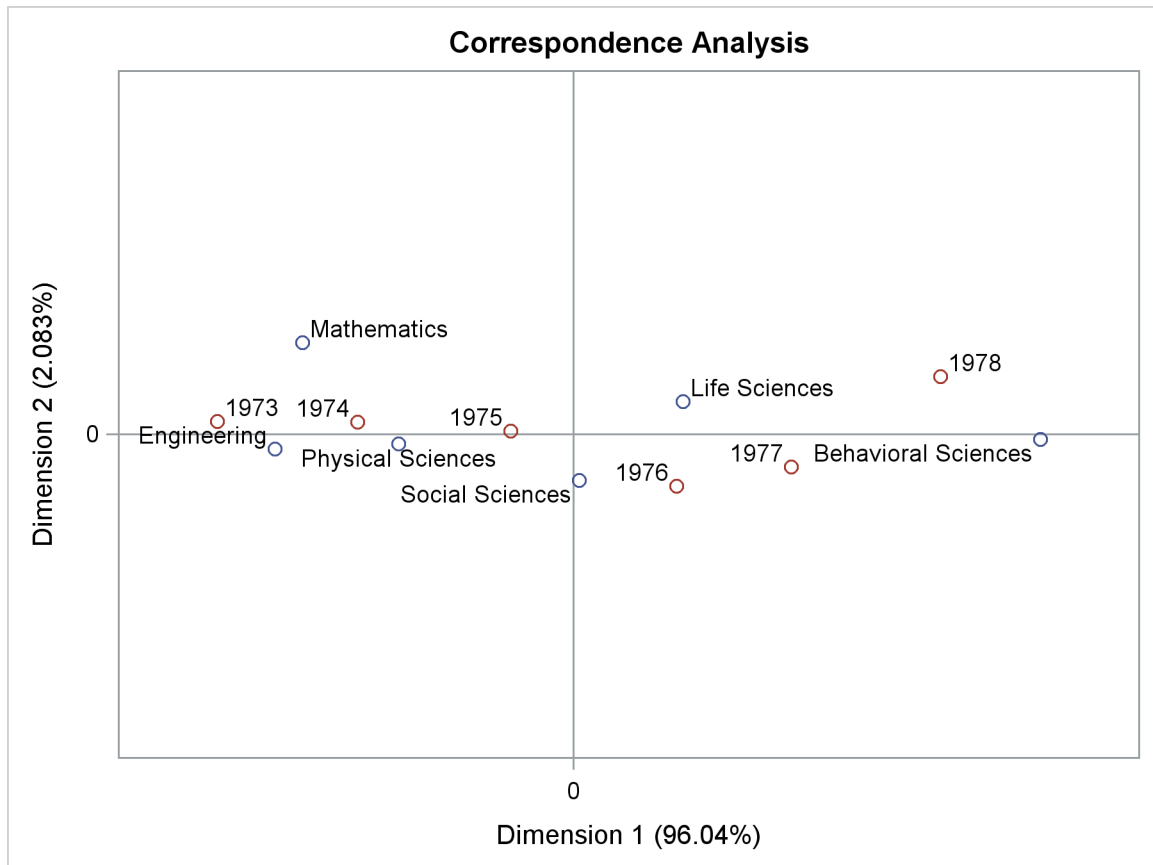
      layout overlayequated / equatetype=fit
        commonaxisopts=(tickvaluelist=(0))
        xaxisopts=(offsetmin=0.1 offsetmax=0.1)
        yaxisopts=(offsetmin=0.1 offsetmax=0.1);

        referenceline x=0;
        referenceline y=0;

        scatterplot y=YVAR x=XVAR / group=GROUP index=INDEX
          datalabel=LABEL datalabelattrs=GRAPHVALUETEXT
          name="Type" tip=(y x datalabel group)
          tiplabel=(group="Point");
        if (LEGEND)
          discretelegend "Type";
        endif;
      endlayout;
    endgraph;
  end;
run;

proc corresp data=PhD short;
  ods select configplot;
  var y1973-y1978;
  id Science;
run;
```

Since the axes in this plot are equated, the ticks are specified using the option `commonaxisopts = (tickvaluelist = (tick-value-list))`. This example only shows ticks at zero, but you can specify lists of values instead. The results are shown in [Output 22.5.5](#).

Output 22.5.5 Scatter Plot with Tick Marks Specified

If the axes are not equated, then the tick value list is specified with the `LINEAROPTS=` option, as in the following statement:

```
layout overlay / xaxisopts=(linearopts=(viewmin=-0.1 viewmax=0.1
                                     tickvaluelist=(-0.1 0 0.1))
                   offsetmin=0.1 offsetmax=0.1)
                 yaxisopts=(linearopts=(viewmin=-0.1 viewmax=0.1
                                     tickvaluelist=(-0.1 0 0.1))
                   offsetmin=0.1 offsetmax=0.1);
```

The preceding statement uses the `VIEWMIN=` and `VIEWMAX=` options to specify the beginning and end of the data range that is shown. Specifying a tick value list does not extend or restrict the range of data shown in the plot. When axes share common options, it might be more convenient to use a macro to specify the options. The following two statements are equivalent to the preceding statement:

```
%let opts = linearopts=(viewmin=-0.1 viewmax=0.1
                       tickvaluelist=(-0.1 0 0.1)) offsetmin=0.1 offsetmax=0.1;
layout overlay / xaxisopts=(&opts) yaxisopts=(&opts);
```

You can restore the default graph template as follows:

```
proc template;
  delete Stat.Corresp.Graphics.Configuration / store=sasuser.templat;
run;
```

Example 22.6: Adding Text to Every Graph

This example shows how to add text to one or more graphs. For example, you can create a macro variable, with project and date information, as follows:

```
%let date = Project 17.104, &sysdate;
```

In order to add this information to a set of graphs, you need to first know the names of their templates. You can list the names of every graph template for SAS/STAT procedures or for a particular procedure as follows:

```
proc template;
  list stat      / where=(type='Statgraph');
  list stat.reg / where=(type='Statgraph');
run;
```

The results for PROC REG are shown in [Output 22.6.1](#).

Output 22.6.1 PROC REG Templates

Obs	Path	Type
1	Stat.Reg.Graphics.CooksD	Statgraph
2	Stat.Reg.Graphics.DFBETASPanel	Statgraph
3	Stat.Reg.Graphics.DFBETASPlot	Statgraph
4	Stat.Reg.Graphics.DFFITSPLOT	Statgraph
5	Stat.Reg.Graphics.DiagnosticsPanel	Statgraph
6	Stat.Reg.Graphics.Fit	Statgraph
7	Stat.Reg.Graphics.FitHeatMap	Statgraph
8	Stat.Reg.Graphics.ObservedByPredicted	Statgraph
9	Stat.Reg.Graphics.PartialPanel	Statgraph
10	Stat.Reg.Graphics.PartialPlot	Statgraph
11	Stat.Reg.Graphics.PredictionPanel	Statgraph
12	Stat.Reg.Graphics.QQPlot	Statgraph
13	Stat.Reg.Graphics.RFPlot	Statgraph
14	Stat.Reg.Graphics.RStudentByPredicted	Statgraph
15	Stat.Reg.Graphics.ResidualBoxPlot	Statgraph
16	Stat.Reg.Graphics.ResidualByPredicted	Statgraph
17	Stat.Reg.Graphics.ResidualHeatMap	Statgraph
18	Stat.Reg.Graphics.ResidualHeatPanel	Statgraph
19	Stat.Reg.Graphics.ResidualHistogram	Statgraph
20	Stat.Reg.Graphics.ResidualPanel	Statgraph
21	Stat.Reg.Graphics.ResidualPlot	Statgraph
22	Stat.Reg.Graphics.RidgePanel	Statgraph
23	Stat.Reg.Graphics.RidgePlot	Statgraph
24	Stat.Reg.Graphics.SelectionCriterionPanel	Statgraph
25	Stat.Reg.Graphics.SelectionCriterionPlot	Statgraph
26	Stat.Reg.Graphics.StepSelectionCriterionPanel	Statgraph
27	Stat.Reg.Graphics.StepSelectionCriterionPlot	Statgraph
28	Stat.Reg.Graphics.VIFPlot	Statgraph
29	Stat.Reg.Graphics.rstudentByLeverage	Statgraph

Output 22.6.1 *continued*

```
Listing of: SASHELP.TMPLMST
Path Filter is: Stat.Reg
Sort by: PATH/ASCENDING
```

Obs	Path	Type
1	Stat.Reg.Graphics.CooksD	Statgraph
2	Stat.Reg.Graphics.DFBETASPanel	Statgraph
3	Stat.Reg.Graphics.DFBETASPlot	Statgraph
4	Stat.Reg.Graphics.DFFITSPlot	Statgraph
5	Stat.Reg.Graphics.DiagnosticsPanel	Statgraph
6	Stat.Reg.Graphics.Fit	Statgraph
7	Stat.Reg.Graphics.ObservedByPredicted	Statgraph
8	Stat.Reg.Graphics.PartialPanel	Statgraph
9	Stat.Reg.Graphics.PartialPlot	Statgraph
10	Stat.Reg.Graphics.PredictionPanel	Statgraph
11	Stat.Reg.Graphics.QQPlot	Statgraph
12	Stat.Reg.Graphics.RFPlot	Statgraph
13	Stat.Reg.Graphics.RStudentByPredicted	Statgraph
14	Stat.Reg.Graphics.ResidualBoxPlot	Statgraph
15	Stat.Reg.Graphics.ResidualByPredicted	Statgraph
16	Stat.Reg.Graphics.ResidualHistogram	Statgraph
17	Stat.Reg.Graphics.ResidualPanel	Statgraph
18	Stat.Reg.Graphics.ResidualPlot	Statgraph
19	Stat.Reg.Graphics.RidgePanel	Statgraph
20	Stat.Reg.Graphics.RidgePlot	Statgraph
21	Stat.Reg.Graphics.SelectionCriterionPanel	Statgraph
22	Stat.Reg.Graphics.SelectionCriterionPlot	Statgraph
23	Stat.Reg.Graphics.StepSelectionCriterionPanel	Statgraph
24	Stat.Reg.Graphics.StepSelectionCriterionPlot	Statgraph
25	Stat.Reg.Graphics.VIFPlot	Statgraph
26	Stat.Reg.Graphics.rstudentByLeverage	Statgraph

You can show the source for the graph templates for SAS/STAT procedures or for a particular procedure as follows:

```
options ls=96;
proc template;
  source stat      / where=(type='Statgraph');
  source stat.reg / where=(type='Statgraph');
options ls=80;
```

The results of this step are not shown. However, [Example 22.4](#) shows a portion of the template for the PROC REG diagnostics panel. Here, the OPTIONS statement is used to set a line size of 96, which sometimes works better than the smaller default line size when showing the source for large and complicated templates.

An abridged version of the first few lines of the diagnostics panel template is displayed next:

```
define statgraph Stat.Reg.Graphics.DiagnosticsPanel;
  notes "Diagnostics Panel";
  dynamic . . .;
  BeginGraph / designheight=defaultDesignWidth;
  entrytitle halign=left textattrs=GRAPHVALUETEXT _MODELLABEL
    halign=center textattrs=GRAPHTITLETEXT "Fit Diagnostics"
    " for " _DEPNAME;
  . . .
```

Adding a Date and Project Stamp to a Few Graphs

You can add the project and date to the bottom of all graphs produced with PROC REG by putting a PROC TEMPLATE statement in front of the template source code, and adding an MVAR and ENTRYFOOTNOTE statement after every BEGINGRAPH statement, as in the following example:

```
proc template;
  define statgraph Stat.Reg.Graphics.DiagnosticsPanel;
    notes "Diagnostics Panel";
    dynamic . . .;
    BeginGraph / designheight=defaultDesignWidth;

    mvar date;
    entryfootnote halign=left textattrs=GraphValueText date;

    entrytitle halign=left textattrs=GRAPHVALUETEXT _MODELLABEL
      halign=center textattrs=GRAPHTITLETEXT "Fit Diagnostics"
      " for " _DEPNAME;
    . . .
```

The MVAR statement enables you to dynamically customize the template and graph at procedure run time, just as the DYNAMIC statement enables the procedure to dynamically customize the template and graph. With the MVAR statement, you can modify the template once and reuse that modification as the macro changes over time: Alternatively, you can modify the templates as follows:

```
entryfootnote halign=left textattrs=GRAPHVALUETEXT "&date";
```

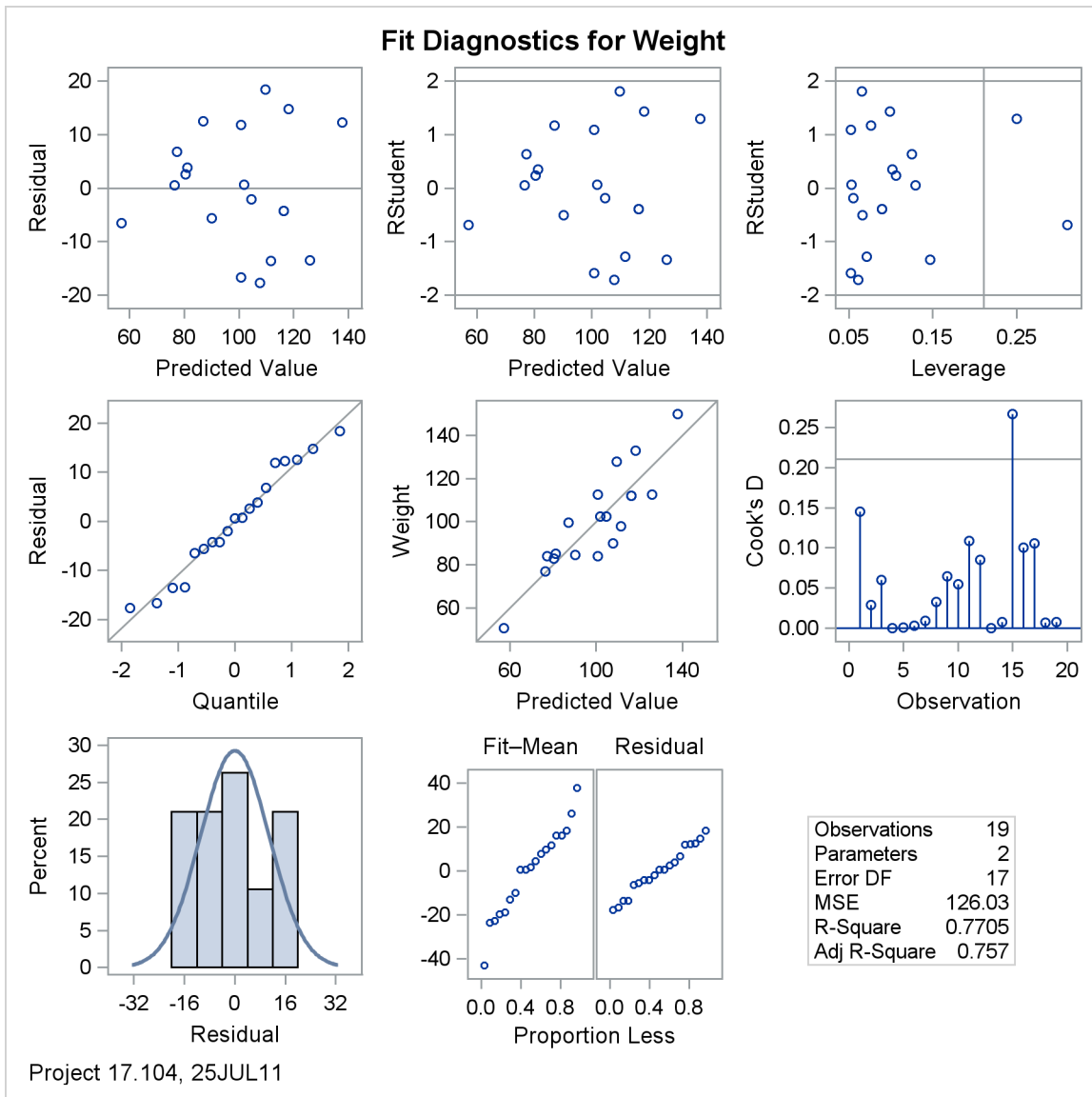
However, you would then have to resubmit your templates every time the macro variable changed. The substitution for the macro variable `date` occurs at different times in the two preceding cases. In the former case, ODS looks for the value of the macro variable `date` at the time the template is used, and then the current date variable is used to set the text in the ENTRYFOOTNOTE statement, every time the template is used. In the latter case, SAS substitutes the value of the macro variable once, at the time that the PROC TEMPLATE step is executed.

The following steps use the Class data set and produce [Output 22.6.2](#):

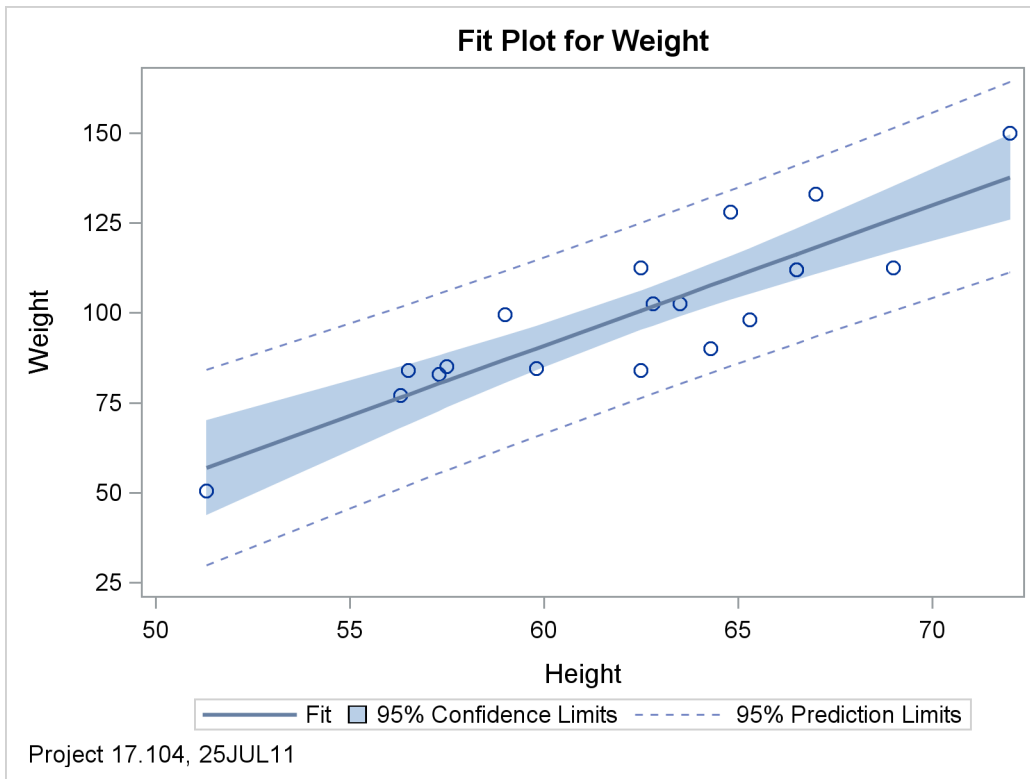
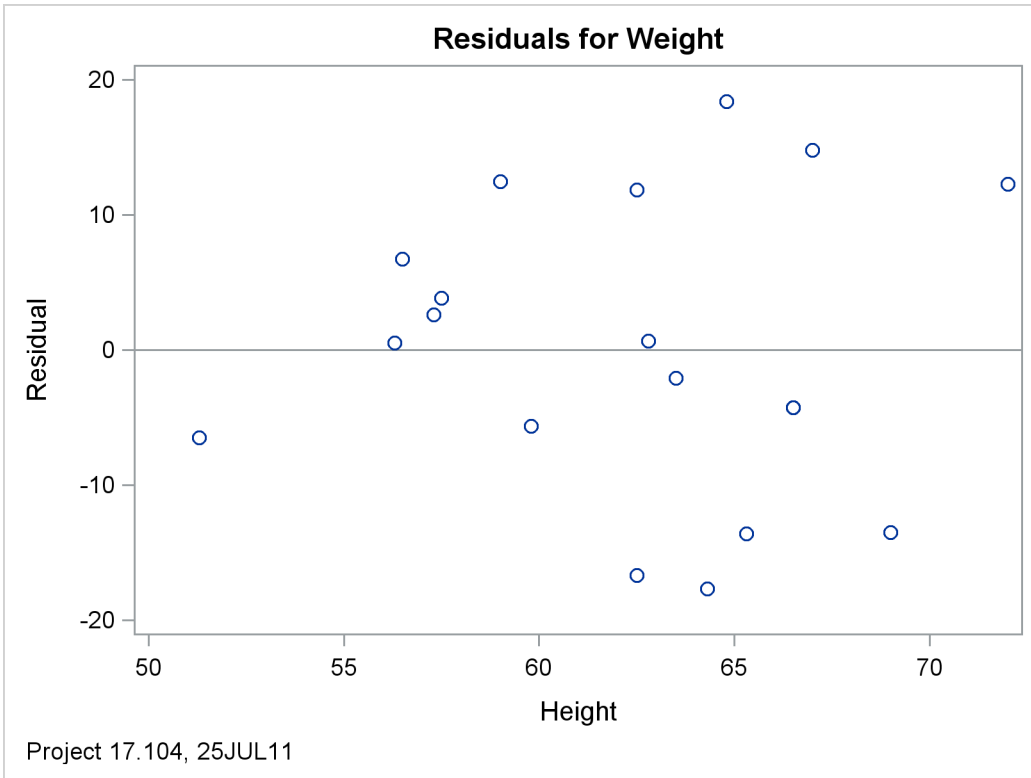
```
ods graphics on;

proc reg data=sashelp.class plots=fit(stats=none);
  model weight = height;
run; quit;
```

Output 22.6.2 PROC REG Plots with Project and Date Stamp



Output 22.6.2 continued



You can restore all of the default templates for PROC REG by running the following step:

```
proc template;
  delete stat.reg / store=sasuser.templat;
run;
```

Alternatively, you can specify **delete stat** to restore all SAS/STAT templates to their default definitions.

You can add text to the top or the bottom of a graph by using the ENTRYTITLE or the ENTRYFOOTNOTE statement, respectively. With both statements, you can put the text in the HALIGN=RIGHT, HALIGN=LEFT, or HALIGN=CENTER positions. You can add text to titles even if they already have a centered title. For example, the ENTRYTITLE statement in the diagnostic panel has text on the left (which is conditionally displayed) and a centered title:

```
entrytitle halign=left textattrs=GraphValueText _MODELLABEL
  halign=center textattrs=GraphTitleText "Fit Diagnostics"
  " for " _DEPNAME;
```

The current title can be followed by HALIGN=RIGHT and more text.

Adding Data Set Information to a Graph

You might, for example, want to add text to a set of graphs that indicates the most recently created data set. The following example shows you how you can do this with the syslast macro variable:

```
%let data = &syslast;
. . .
mvar data;
entrytitle halign=left textattrs=GraphValueText "Data: " data
  halign=center textattrs=GraphTitleText "Fit Diagnostics"
  " for " _DEPNAME;
. . .
```

Of course, this only makes sense when you are analyzing the last data set created. Alternatively, you can incorporate the name of the data set in the title, as in the following example:

```
%let data = &syslast;
. . .
mvar data;
entrytitle halign=center textattrs=GraphTitleText
  "Fit Diagnostics for Data Set " data;
. . .
```


Adding a Date and Project Stamp to All Graphs

Sometimes, you can automate the process of template modification. For example, you can automatically add an MVAR and ENTRYFOOTNOTE statement to every graph template, as in the following example:

```
ods path sashelp.tmplmst(read);
proc datasets library=sasuser nolist;
  delete templat(memtype=itemstor);
run;
ods path sasuser.templat(update) sashelp.tmplmst(read);

options ls=256;

proc template;
  source / where=(type='Statgraph') file="tpls.sas";
run;

options ls=80;

data _null_;
  infile 'tpls.sas' lrecl=256 pad;
  input line $ 1-256;
  file 'newtpls.sas';
  put line;
  line = left(lowercase(line));
  if line =: 'begingraph' then
    put 'mvar __date;' /
      'entryfootnote halign=left textattrs=GraphValueText __date;';

  file log;
  if index(line, '__date') then
    put 'ERROR: Name __date already used.' / line;
  if index(line, 'entryfootnote') then put line;
run;

proc template;
  %include 'newtpls.sas' / nosource;
run;
```

These statements write all ODS graph templates to a file, read that file, and write out a new file with an MVAR and ENTRYFOOTNOTE statement added after every BEGINGRAPH statement. Then these new templates are compiled with PROC TEMPLATE. These steps assume that no BEGINGRAPH statement is longer than 256 characters. Most graphs do not have footnotes. Those that do will now have multiple footnotes. You might want to manually combine them or write a more complicated program to handle them. These steps also assume that the name `__date` is not used anywhere. However, the program does check this and also lists all ENTRYFOOTNOTE statements. Be careful to check the SAS log to ensure that all templates compile without error. Also, before using templates that are automatically modified, make sure your modifications are reasonable.

You can delete Sasuser.Templat and hence all modified templates (assuming the default template search path) as follows:

```
ods path sashelp.tmplmst(read);
proc datasets library=sasuser nolist;
  delete templat(memtype=itemstor);
run;
ods path sasuser.templat(update) sashelp.tmplmst(read);
```

Example 22.7: PROC TEMPLATE Statement Order and Primary Plots

This example uses artificial data to illustrate two basic principles of template writing: that statement order matters and that one of the plotting statements is the primary statement. The data are a sample from a bivariate normal distribution. A custom graph template and PROC SGRENDER are used to plot the data along with vectors and ellipses. The plot consists of four components: a scatterplot of the data; vectors whose end points come from other variables in the data set; ellipses whose parameters are specified in the template; and reference lines whose locations are specified in the template. Initially, thick lines are used to show what happens at the places where the lines and points intersect.

The following steps create the input SAS data set:

```
data x;
  input x y;
  label x = 'Normal(0, 4)' y = 'Normal(0, 1)';
  datalines;
-4 0
 4 0
 0 -2
 0 2
;

data y(drop=i);
  do i = 1 to 2500;
    r1 = normal( 104 );
    r2 = normal( 104 ) * 2;
    output;
  end;
run;

data all;
  merge x y;
run;
```

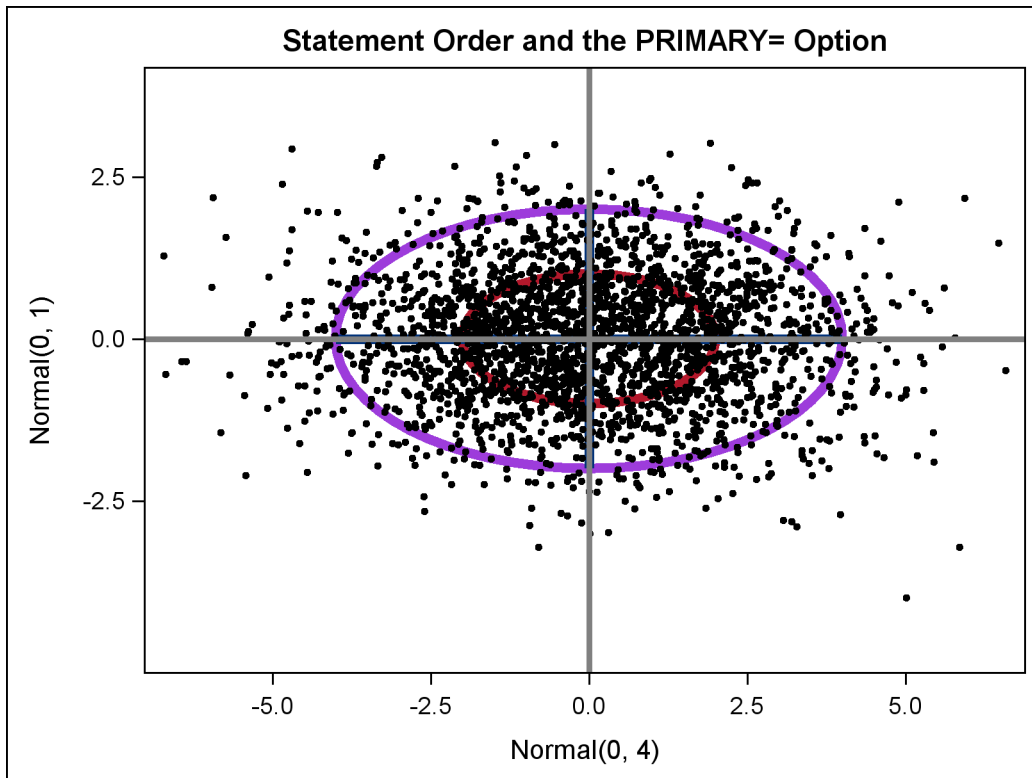
The data set All contains four variables. The variables r1 and r2 contain the random data. These variables contain 2500 nonmissing observations. The data set also contains the variables x and y, which contain the end points for the vectors. These variables contain four nonmissing observations and 2496 observations that are all missing. A data set like this is not unusual when creating overlaid plots. Different overlays often require input data with very different sizes. First, the data are plotted by using a template that is deliberately constructed to demonstrate a number of problems that can occur with statement order.

The following steps create [Output 22.7.1](#):

```
proc template;
  define statgraph Plot;
    begingraph;
      entrytitle 'Statement Order and the PRIMARY= Option';
      layout overlayequated / equatetype=fit;
        ellipseparm semimajor=eval(sqrt(4)) semiminor=1
          slope=0 xorigin=0 yorigin=0 /
          outlineattrs=GraphData2(pattern=solid thickness=5);
        ellipseparm semimajor=eval(2 * sqrt(4)) semiminor=2
          slope=0 xorigin=0 yorigin=0 /
          outlineattrs=GraphData5(pattern=solid thickness=5);
        vectorplot y=y x=x xorigin=0 yorigin=0 /
          arrowheads=false lineattrs=GraphFit(thickness=5);
        scatterplot y=r1 x=r2 /
          markerattrs=(symbol=circlefilled size=3);
        referenceline x=0 / lineattrs=(thickness=3);
        referenceline y=0 / lineattrs=(thickness=3);
      endlayout;
    endgraph;
  end;
run;

ods listing style=listing;

proc sgrender data=all template=plot;
run;
```

Output 22.7.1 Statements Specified in a Nonoptimal Order

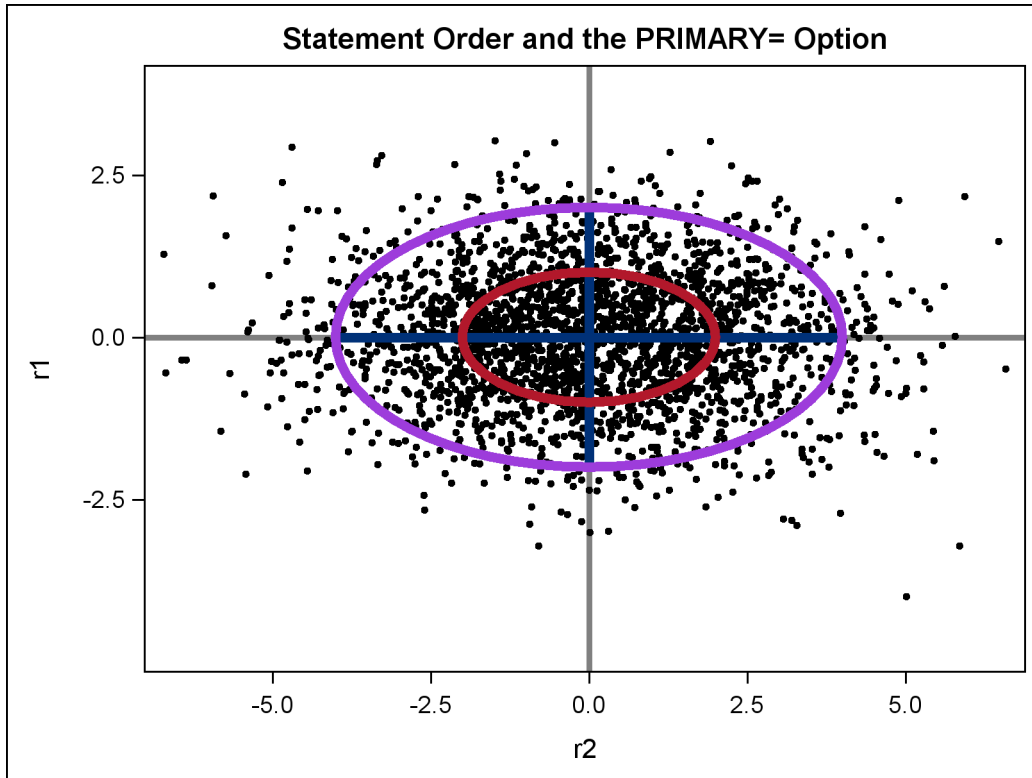
There are a number of problems with the plot in [Output 22.7.1](#). The reference lines obliterate the vectors, and the data are on top of everything but the reference lines. It might be more reasonable to plot the reference lines first, the data next, the vectors next, and the ellipses last. The following steps do this and produce [Output 22.7.2](#):

```
proc template;
  define statgraph Plot;
    begingraph;
      entrytitle 'Statement Order and the PRIMARY= Option';
      layout overlayequated / equatetype=fit;
        referenceline x=0 / lineattrs=(thickness=3);
        referenceline y=0 / lineattrs=(thickness=3);
        scatterplot y=r1 x=r2 /
          markerattrs=(symbol=circlefilled size=3);
        vectorplot y=y x=x xorigin=0 yorigin=0 /
          arrowheads=false lineattrs=GraphFit(thickness=5);
        ellipseparm semimajor=eval(sqrt(4)) semiminor=1
          slope=0 xorigin=0 yorigin=0 /
          outlineattrs=GraphData2(pattern=solid thickness=5);
        ellipseparm semimajor=eval(2 * sqrt(4)) semiminor=2
          slope=0 xorigin=0 yorigin=0 /
          outlineattrs=GraphData5(pattern=solid thickness=5);
      endlayout;
    endgraph;
  end;
run;
```

```
ods listing style=listing;

proc sgrender data=all template=plot;
run;
```

Output 22.7.2 Statement Order Fixed



Output 22.7.2 looks better than Output 22.7.1, but the labels for the axes have changed. Output 22.7.1 has the labels of the variables x and y as axis labels, whereas Output 22.7.2 uses the names of the variables $r1$ and $r2$. This is because in the Output 22.7.1, the first plot is the vector plot of x and y (which have labels), and in Output 22.7.2, the first plot is the scatter plot of $r1$ and $r2$ (which do not have labels). By default, the first plot is the *primary plot*, and the primary plot is used to determine the axis type and labels. You can designate the vector plot as the primary plot with the PRIMARY=TRUE option.

The following statements make the final plot, this time with default line thicknesses, and produce [Output 22.7.3](#):

```
proc template;
  define statgraph Plot;
    begingraph;
      entrytitle 'Statement Order and the PRIMARY= Option';
      layout overlayequated / equatetype=fit;
      referenceline x=0;
      referenceline y=0;
      scatterplot y=r1 x=r2 / markerattrs=(symbol=circlefilled size=3);

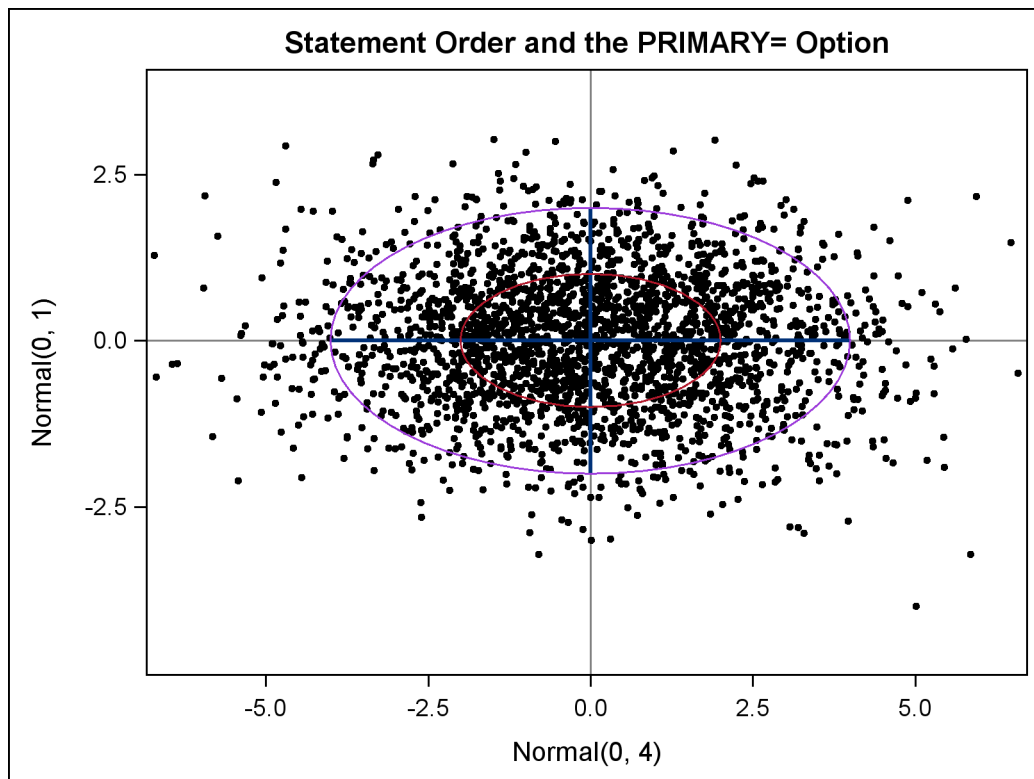
      vectorplot y=y x=x xorigin=0 yorigin=0 / primary=true
        arrowheads=false lineattrs=GraphFit;

      ellipseparm semimajor=eval(sqrt(4)) semiminor=1
        slope=0 xorigin=0 yorigin=0 /
        outlineattrs=GraphData2(pattern=solid);
      ellipseparm semimajor=eval(2 * sqrt(4)) semiminor=2
        slope=0 xorigin=0 yorigin=0 /
        outlineattrs=GraphData5(pattern=solid);
    endlayout;
  endgraph;
end;
run;

ods listing style=listing;

proc sgrender data=all template=plot;
run;
```

Output 22.7.3 Statement Order Fixed and Primary Plot Specified



The axis labels in [Output 22.7.3](#) and the overprinting of plot elements look better than in the previous plots. You can further adjust the line thicknesses if you want to emphasize or deemphasize components of this plot. The following list discusses the syntax of the GTL statements used in this example.

- The template has an `ENTRYTITLE` statement that specifies the title.
- The template has an equated overlay. This means that a centimeter on one axis represents the same data range as a centimeter on the other axis. This is done instead of the more common `LAYOUT OVERLAY` since with these data, the shape and geometry of the data have meaning even though the ranges of the two axis variables are different. The option `EQUATETYPE=SQUARE` is used to make a square plot, but since the X-axis variable has a larger range than the Y-axis variable, and since the default plot size is wider than high, `EQUATETYPE=FIT` is specified. The axes are equated but use the available space.
- A vertical reference line is drawn at $X=0$, and a horizontal reference line is drawn at $Y=0$.
- The scatter plot is based on the Y-axis variable `r2` and the X-axis variable `r1`. The markers are filled circles with a size of three pixels. This is smaller than the default size and works well with a plot that displays many points.
- The vector plot is based on the Y-axis variable `y` and the X-axis variable `x`. The vectors are solid lines with no heads emanating from the origin ($X=0$ and $Y=0$). The color and other line attributes such as thickness come from the attributes of the `GraphFit` style element. This is the primary plot, so the default axis labels are the variable labels for the X= and Y= variables if they exist or the variable names if the variables do not have labels.
- The plot also displays two ellipses with $X=0$ and $Y=0$ at their center. Their widths are expressions, and their heights are constant. The expressions are not needed in this example; they are used to illustrate the syntax. The `SEMIMAJOR=` option specifies half the length of the major axis for the ellipse, and the `SEMIMINOR=` option specifies half the length of the minor axis for the ellipse. The `SLOPE=` option specifies the slope of the major axis for the ellipse. The colors of the ellipses and other line properties are based on the `GraphData2` and `GraphData5` style elements, but the line pattern attribute from the style is overridden.

References

- Kuhfeld, W. F. (2009), "Modifying ODS Statistical Graphics Templates in SAS 9.2," <http://support.sas.com/rnd/app/papers/ods/modtplt.pdf>.
- Kuhfeld, W. F. (2010), *Statistical Graphics in SAS: An Introduction to the Graph Template Language and the Statistical Graphics Procedures*, Cary, NC: SAS Press.

Chapter 23

The ACECLUS Procedure

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Overview: ACECLUS Procedure

The ACECLUS (approximate covariance estimation for clustering) procedure obtains approximate estimates of the pooled within-cluster covariance matrix when the clusters are assumed to be multivariate normal with equal covariance matrices. Neither cluster membership nor the number of clusters needs to be known. PROC ACECLUS is useful for preprocessing data to be subsequently clustered by the CLUSTER or FASTCLUS procedure.

Many clustering methods perform well with spherical clusters but poorly with elongated elliptical clusters (Everitt 1980, pp. 77–97). If the elliptical clusters have roughly the same orientation and eccentricity, you can apply a linear transformation to the data to yield a spherical within-cluster covariance matrix—that is, a covariance matrix proportional to the identity. Equivalently, the distance between observations can be measured in the metric of the inverse of the pooled within-cluster covariance matrix. The remedy is difficult to apply, however, because you need to know what the clusters are in order to compute the sample within-cluster covariance matrix. One approach is to estimate iteratively both cluster membership and within-cluster covariance (Wolfe 1970; Hartigan 1975). Another approach is provided by Art, Gnanadesikan, and

Kettenring (1982). They have devised an ingenious method for estimating the within-cluster covariance matrix without knowledge of the clusters. The method can be applied before any of the usual clustering techniques, including hierarchical clustering methods.

First, Art, Gnanadesikan, and Kettenring (1982) obtain a decomposition of the total-sample sum-of-squares-and-crossproducts (SSCP) matrix into within-cluster and between-cluster SSCP matrices computed from pairwise differences between observations, rather than differences between observations and means. Then, they show how the within-cluster SSCP matrix based on pairwise differences can be approximated without knowing the number or the membership of the clusters. The approximate within-cluster SSCP matrix can be used to compute distances for cluster analysis, or it can be used in a canonical analysis similar to canonical discriminant analysis. For more information, see Chapter 29, “The CANDISC Procedure.”

Art, Gnanadesikan, and Kettenring demonstrate by Monte Carlo calculations that their method can produce better clusters than the Euclidean metric even when the approximation to the within-cluster SSCP matrix is poor or the within-cluster covariances are moderately heterogeneous. The algorithm used by the ACECLUS procedure differs slightly from the algorithm used by Art, Gnanadesikan, and Kettenring. In the following sections, the PROC ACECLUS algorithm is described first; then, differences between PROC ACECLUS and the method used by Art, Gnanadesikan, and Kettenring are summarized.

Background

It is well known from the literature on nonparametric statistics that variances and, hence, covariances can be computed from pairwise differences instead of deviations from means. (For example, Puri and Sen (1971, pp. 51–52) show that the variance is a U statistic of degree 2.) Let $\mathbf{X} = (x_{ij})$ be the data matrix with n observations (rows) and v variables (columns), and let \bar{x}_j be the mean of the j th variable. The sample covariance matrix $\mathbf{S} = (s_{jk})$ is usually defined as

$$s_{jk} = \frac{1}{n-1} \sum_{i=1}^n (x_{ij} - \bar{x}_j)(x_{ik} - \bar{x}_k)$$

The matrix \mathbf{S} can also be computed as

$$s_{jk} = \frac{1}{n(n-1)} \sum_{i=2}^n \sum_{h=1}^{i-1} (x_{ij} - x_{hj})(x_{ik} - x_{hk})$$

Let $\mathbf{W} = (w_{jk})$ be the pooled within-cluster covariance matrix, q be the number of clusters, n_c be the number of observations in the c th cluster, and

$$d''_{ic} = \begin{cases} 1 & \text{if observation } i \text{ is in cluster } c \\ 0 & \text{otherwise} \end{cases}$$

The matrix \mathbf{W} is normally defined as

$$w_{jk} = \frac{1}{n-q} \sum_{c=1}^q \sum_{i=1}^{n_c} d''_{ic} (x_{ij} - \bar{x}_{cj})(x_{ik} - \bar{x}_{ck})$$

where \bar{x}_{cj} is the mean of the j th variable in cluster c . Let

$$d'_{ih} = \begin{cases} \frac{1}{n_c} & \text{if observations } i \text{ and } h \text{ are in cluster } c \\ 0 & \text{otherwise} \end{cases}$$

The matrix \mathbf{W} can also be computed as

$$w_{jk} = \frac{1}{n-q} \sum_{i=2}^n \sum_{h=1}^{i-1} d'_{ih} (x_{ij} - x_{hj})(x_{ik} - x_{hk})$$

If the clusters are not known, d'_{ih} cannot be determined. However, an approximation to \mathbf{W} can be obtained by using instead

$$d_{ih} = \begin{cases} 1 & \text{if } \sum_{j=1}^v \sum_{k=1}^v m_{jk} (x_{ij} - x_{hj})(x_{ik} - x_{hk}) \leq u^2 \\ 0 & \text{otherwise} \end{cases}$$

where u is an appropriately chosen value and $\mathbf{M} = (m_{jk})$ is an appropriate metric. Let $\mathbf{A} = (a_{jk})$ be defined as

$$a_{jk} = \frac{\sum_{i=2}^n \sum_{h=1}^{i-1} d_{ih} (x_{ij} - x_{hj})(x_{ik} - x_{hk})}{2 \sum_{i=2}^n \sum_{h=1}^{i-1} d_{ih}}$$

If all of the following conditions hold, \mathbf{A} equals \mathbf{W} :

- All within-cluster distances in the metric \mathbf{M} are less than or equal to u .
- All between-cluster distances in the metric \mathbf{M} are greater than u .
- All clusters have the same number of members n_c .

If the clusters are of unequal size, \mathbf{A} gives more weight to large clusters than \mathbf{W} does, but this discrepancy should be of little importance if the population within-cluster covariance matrices are equal. There might be large differences between \mathbf{A} and \mathbf{W} if the cutoff u does not discriminate between pairs in the same cluster and pairs in different clusters. Lack of discrimination might occur for one of the following reasons:

- The clusters are not well separated.
- The metric \mathbf{M} or the cutoff u is not chosen appropriately.

In the former case, little can be done to remedy the problem. The remaining question concerns how to choose \mathbf{M} and u . Consider \mathbf{M} first. The best choice for \mathbf{M} is \mathbf{W}^{-1} , but \mathbf{W} is not known. The solution is to use an iterative algorithm:

1. Obtain an initial estimate of \mathbf{A} , such as the identity or the total-sample covariance matrix. See the `INITIAL=` option in the PROC ACECLUS statement for more information.
2. Let \mathbf{M} equal \mathbf{A}^{-1} .
3. Recompute \mathbf{A} by using the preceding formula.
4. Repeat steps 2 and 3 until the estimate stabilizes.

Convergence is assessed by comparing values of \mathbf{A} on successive iterations. Let \mathbf{A}_i be the value of \mathbf{A} on the i th iteration and \mathbf{A}_0 be the initial estimate of \mathbf{A} . Let \mathbf{Z} be a user-specified $v \times v$ matrix. See the `METRIC=` option in the PROC ACECLUS statement for more information. The convergence measure is

$$e_i = \frac{1}{v} \|\mathbf{Z}'(\mathbf{A}_i - \mathbf{A}_{i-1})\mathbf{Z}\|$$

where $\|\dots\|$ indicates the Euclidean norm—that is, the square root of the sum of the squares of the elements of the matrix. In PROC ACECLUS, \mathbf{Z} can be the identity or an inverse factor of \mathbf{S} or `diag(S)`. Iteration stops when e_i falls below a user-specified value. See the `CONVERGE=` option or the `MAXITER=` option in the PROC ACECLUS statement for more information.

The remaining question of how to choose u has no simple answer. In practice, you must try several different values. PROC ACECLUS provides four different ways of specifying u :

- You can specify a constant value for u . This method is useful if the initial estimate of \mathbf{A} is quite good. See the `ABSOLUTE` option and the `THRESHOLD=` option in the PROC ACECLUS statement for more information.
- You can specify a threshold value $t > 0$ that is multiplied by the root mean square distance between observations in the current metric on each iteration to give u . Thus, the value of u changes from iteration to iteration. This method is appropriate if the initial estimate of \mathbf{A} is poor. See the `THRESHOLD=` option in the PROC ACECLUS statement for more information.
- You can specify a value p , $0 < p < 1$, to be transformed into a distance u such that approximately a proportion p of the pairwise Mahalanobis distances between observations in a random sample from a multivariate normal distribution will be less than u in repeated sampling. The transformation can be computed only if the number of observations exceeds the number of variables, preferably by at least 10 percent. This method also requires a good initial estimate of \mathbf{A} . See the `PROPORTION=` option and the `ABSOLUTE` option in the PROC ACECLUS statement for more information.
- You can specify a value p , $0 < p < 1$, to be transformed into a value t that is then multiplied by $1/\sqrt{2v}$ times the root mean square distance between observations in the current metric on each iteration to yield u . The value of u changes from iteration to iteration. This method can be used with a poor initial estimate of \mathbf{A} . See the `PROPORTION=` option in the PROC ACECLUS statement for more information.

In most cases, the analysis should begin with the last method, using values of p between 0.5 and 0.01 and using the full covariance matrix as the initial estimate of \mathbf{A} .

Proportions p are transformed to distances t by using the formula

$$t^2 = 2v \left\{ \left[F_{v, n-v}^{-1}(p) \right]^{\frac{n-v}{n-1}} \right\}$$

where $F_{v, n-v}^{-1}$ is the quantile (inverse cumulative distribution) function of an F random variable with v and $n - v$ degrees of freedom. The squared Mahalanobis distance between a single pair of observations sampled from a multivariate normal distribution is distributed as $2v$ times an F random variable with v and $n - v$ degrees of freedom. The distances between two pairs of observations are correlated if the pairs have an observation in common. The quantile function is raised to the power given in the preceding formula to compensate approximately for the correlations among distances between pairs of observations that share a

member. Monte Carlo studies indicate that the approximation is acceptable if the number of observations exceeds the number of variables by at least 10 percent.

If \mathbf{A} becomes singular, step 2 in the iterative algorithm cannot be performed because \mathbf{A} cannot be inverted. In this case, let \mathbf{Z} be the matrix as defined in discussing the convergence measure, and let $\mathbf{Z}'\mathbf{A}\mathbf{Z} = \mathbf{R}'\mathbf{\Lambda}\mathbf{R}$, where $\mathbf{R}'\mathbf{R} = \mathbf{R}\mathbf{R}' = \mathbf{I}$ and $\mathbf{\Lambda} = (\lambda_{jk})$ is diagonal. Let $\mathbf{\Lambda}^* = (\lambda_{jk}^*)$ be a diagonal matrix, where $\lambda_{jj}^* = \max(\lambda_{jj}, g \text{ trace}(\mathbf{\Lambda}))$, and $0 < g < 1$ is a user-specified singularity criterion (see the `SINGULAR=` option in the PROC ACECLUS statement for more information). Then \mathbf{M} is computed as $\mathbf{Z}\mathbf{R}'(\mathbf{\Lambda}^*)^{-1}\mathbf{R}\mathbf{Z}'$.

The ACECLUS procedure differs from the method used by Art, Gnanadesikan, and Kettenring (1982) in several respects:

- The Art, Gnanadesikan, and Kettenring method uses the identity matrix as the initial estimate, whereas the ACECLUS procedure enables you to specify any symmetric matrix as the initial estimate and defaults to the total-sample covariance matrix. The default initial estimate in PROC ACECLUS is chosen to yield invariance under nonsingular linear transformations of the data but might sometimes obscure clusters that become apparent if the identity matrix is used.
- The Art, Gnanadesikan, and Kettenring method carries out all computations with SSCP matrices, whereas the ACECLUS procedure uses estimated covariance matrices because covariances are easier to interpret than crossproducts.
- The Art, Gnanadesikan, and Kettenring method uses the m pairs with the smallest distances to form the new estimate at each iteration, where m is specified by the user, whereas the ACECLUS procedure uses all pairs closer than a given cutoff value. Kettenring (1984) says that the m -closest-pairs method seems to give the user more direct control. PROC ACECLUS uses a distance cutoff because it yields a slight decrease in computer time and because in some cases, such as widely separated spherical clusters, the results are less sensitive to the choice of distance cutoff than to the choice of m . Much research remains to be done on this issue.
- The Art, Gnanadesikan, and Kettenring method uses a different convergence measure. Let \mathbf{A}_i be computed on each iteration by using the m -closest-pairs method, and let $\mathbf{B}_i = \mathbf{A}_{i-1}^{-1}\mathbf{A}_i - \mathbf{I}$, where \mathbf{I} is the identity matrix. The convergence measure is equivalent to $\text{trace}(\mathbf{B}_i^2)$.

Analyses of the Fisher (1936) iris data, consisting of measurements of petal and sepal length and width for 50 specimens from each of three iris species, are summarized in Table 23.1. The number of misclassified observations out of 150 is given for four clustering methods:

- k -means as implemented in PROC FASTCLUS with MAXC=3, MAXITER=99, and CONV=0
- Ward's minimum variance method as implemented in PROC CLUSTER
- average linkage on Euclidean distances as implemented in PROC CLUSTER
- the centroid method as implemented in PROC CLUSTER

Each hierarchical analysis is followed by the TREE procedure with NCL=3 to determine cluster assignments at the three-cluster level. Clusters with 20 or fewer observations are discarded by using the DOCK=20 option. The observations in a discarded cluster are considered unclassified.

Each method is applied to the following data:

- the raw data
- the data standardized to unit variance by the STANDARD procedure
- two standardized principal components accounting for 95 percent of the standardized variance and having an identity total-sample covariance matrix, computed by the PRINCOMP procedure with the STD option
- four standardized principal components having an identity total-sample covariance matrix, computed by PROC PRINCOMP with the STD option
- the data transformed by PROC ACECLUS, using seven different settings of the PROPORTION= (P=) option
- four canonical variables having an identity pooled within-species covariance matrix, computed using the CANDISC procedure

Theoretically, the best results should be obtained by using the canonical variables from PROC CANDISC. PROC ACECLUS yields results comparable to those from PROC CANDISC for values of the PROPORTION= option ranging from 0.005 to 0.02. At PROPORTION=0.04, average linkage and the centroid method show some deterioration, but *k*-means and Ward's method continue to produce excellent classifications. At larger values of the PROPORTION= option, all methods perform poorly, although no worse than with four standardized principal components.

Table 23.1 Number of Misclassified and Unclassified Observations Using the Fisher (1936) Iris Data

Data	Clustering Method			
	<i>k</i> -means	Ward's	Average Linkage	Centroid
Raw Data	16	16	25+12	14
Standardized Data	25	26	33+4	33+4
Two Standardized Principal Components	29	31	30+9	27+32
Four Standardized Principal Components	39	27	32+7	45+11
Transformed by ACECLUS, P=0.32	39	10+9	7+25	
Transformed by ACECLUS, P=0.16	39	18+9	7+19	7+26
Transformed by ACECLUS, P=0.08	19	9	3+13	5+16
Transformed by ACECLUS, P=0.04	4	5	1+19	3+12
Transformed by ACECLUS, P=0.02	4	3	3	3
Transformed by ACECLUS, P=0.01	4	4	3	4
Transformed by ACECLUS, P=0.005	4	4	4	4
Canonical Variables	3	5	4	4+1

— A single number represents misclassified observations with no unclassified observations.

— Where two numbers are separated by a plus sign, the first is the number of observations; the second is the number of unclassified observations.

This example demonstrates the following:

- PROC ACECLUS can produce results as good as those from the optimal transformation.
- PROC ACECLUS can be useful even when the within-cluster covariance matrices are moderately heterogeneous.
- The choice of the distance cutoff as specified by the PROPORTION= or the THRESHOLD= option is important, and several values should be tried.
- Commonly used transformations such as standardization and principal components can produce poor classifications.

Although experience with the Art, Gnanadesikan, and Kettenring and PROC ACECLUS methods is limited, the results so far suggest that these methods help considerably more often than they hinder the subsequent cluster analysis, especially with normal-mixture techniques such as *k*-means and Ward's minimum variance method.

Getting Started: ACECLUS Procedure

The following example demonstrates how you can use the ACECLUS procedure to obtain approximate estimates of the pooled within-cluster covariance matrix and to compute canonical variables for subsequent analysis. You use PROC ACECLUS to preprocess data before you cluster it by using the FASTCLUS or CLUSTER procedure.

Suppose you want to determine whether national figures for birth rates, death rates, and infant death rates can be used to determine certain types or categories of countries. You want to perform a cluster analysis to determine whether the observations can be formed into groups suggested by the data. Previous studies indicate that the clusters computed from this type of data can be elongated and elliptical. Thus, you need to perform a linear transformation on the raw data before the cluster analysis.

The following data¹ from Rouncefield (1995) are the birth rates, death rates, and infant death rates for 97 countries. The following statements create the SAS data set Poverty:

```
data poverty;
  input Birth Death InfantDeath Country &$20. @@;
  datalines;
24.7  5.7  30.8 Albania           12.5 11.9  14.4 Bulgaria
13.4 11.7  11.3 Czechoslovakia    12 12.4   7.6 Former E. Germany
... more lines ...

41.7 10.3   66 Zimbabwe
;
```

The data set Poverty contains the character variable Country and the numeric variables Birth, Death, and InfantDeath, which represent the birth rate per thousand, death rate per thousand, and infant death rate per thousand, respectively. The \$20. format in the INPUT statement specifies that the variable Country is a

¹ These data have been compiled from the United Nations *Demographic Yearbook* 1990 (United Nations publications, Sales No. E/F.91.XII.1, copyright 1991, United Nations, New York) and are reproduced with the permission of the United Nations.

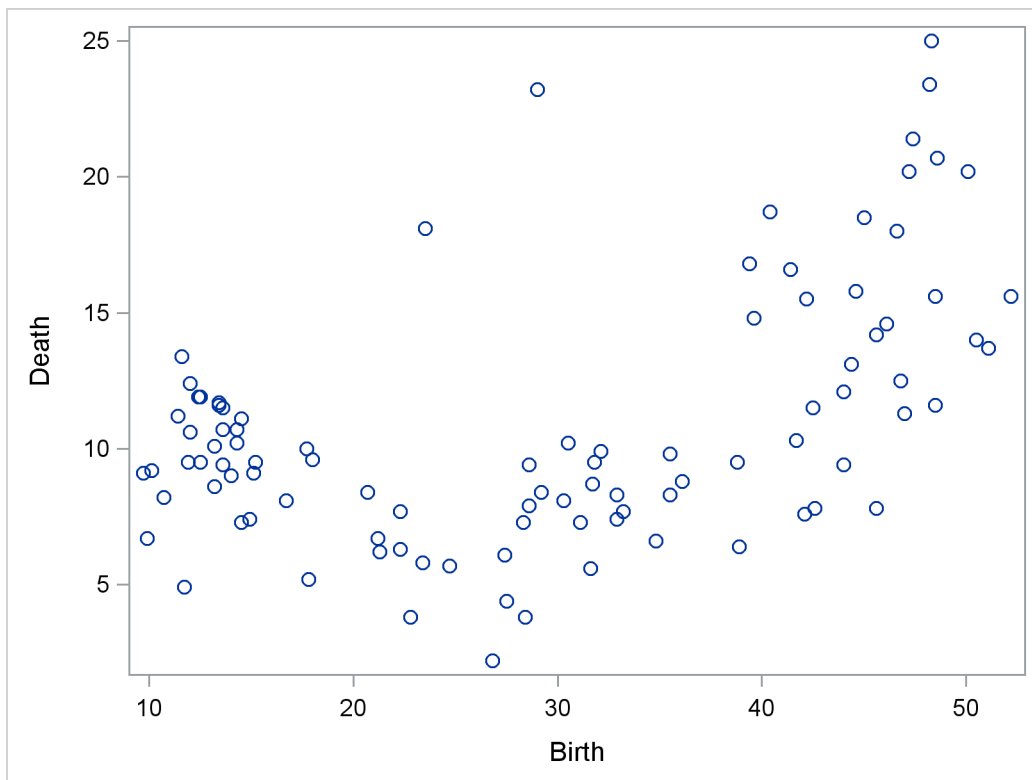
character variable with a length of 20. The preceding & enables the reading of blanks in the middle of the country names. The double trailing at sign (@@) in the INPUT statement specifies that observations are input from each line until all values have been read.

It is often useful when beginning a cluster analysis to look at the data graphically. The following statements use the SGLOT procedure to make a scatter plot of the variables Birth and Death.

```
proc sgplot data=poverty;
  scatter y=Death x=Birth;
run;
```

The plot, displayed in Figure 23.1, indicates the difficulty of dividing the points into clusters. Plots of the other variable pairs (not shown) display similar characteristics. The clusters that comprise these data might be poorly separated and elongated. Data with poorly separated or elongated clusters must be transformed.

Figure 23.1 Scatter Plot of Original Poverty Data: Birth Rate versus Death Rate



If you know the within-cluster covariances, you can transform the data to make the clusters spherical. However, since you do not know what the clusters are, you cannot calculate exactly the within-cluster covariance matrix. The ACECLUS procedure estimates the within-cluster covariance matrix to transform the data, even when you have no knowledge of cluster membership or the number of clusters.

The following statements perform the ACECLUS procedure transformation by using the SAS data set Poverty:

```
proc aceclus data=poverty out=ace proportion=.03;
  var Birth Death InfantDeath;
run;
```

The OUT= option creates an output data set called Ace to contain the canonical variable scores. The PROPORTION= option specifies that approximately 3 percent of the pairs are included in the estimation of the within-cluster covariance matrix. The VAR statement specifies that the variables Birth, Death, and InfantDeath are used in computing the canonical variables.

The results of this analysis are displayed in [Figure 23.2](#) through [Figure 23.5](#).

[Figure 23.2](#) displays the number of observations, the number of variables, and the settings for the PROPORTION and CONVERGE options. The PROPORTION option is set at 0.03, as specified in the previous statements. The CONVERGE parameter is set at its default value of 0.001. [Figure 23.2](#) next displays the means, standard deviations, and sample covariance matrix of the analytical variables.

Figure 23.2 Means, Standard Deviations, and Covariance Matrix from the ACECLUS Procedure

The ACECLUS Procedure			
Approximate Covariance Estimation for Cluster Analysis			
Observations	97	Proportion	0.0300
Variables	3	Converge	0.00100
Means and Standard Deviations			
Variable	Mean	Standard Deviation	
Birth	29.2299	13.5467	
Death	10.8361	4.6475	
InfantDeath	54.9010	45.9926	
COV: Total Sample Covariances			
	Birth	Death	InfantDeath
Birth	183.512951	30.610056	534.794969
Death	30.610056	21.599205	139.925900
InfantDeath	534.794969	139.925900	2115.317811

The type of matrix used for the initial within-cluster covariance estimate is displayed in [Figure 23.3](#). In this example, that initial estimate is the full covariance matrix. The threshold value that corresponds to the PROPORTION=0.03 setting is given as 0.292815.

Figure 23.3 Table of Iteration History from the ACECLUS Procedure

```

Initial Within-Cluster Covariance Estimate = Full Covariance Matrix

Threshold = 0.292815

Iteration History

Iteration      RMS      Distance      Pairs      Convergence
Distance      Cutoff      Within      Measure
Cutoff

-----
1             2.449      0.717      385.0      0.552025
2            12.534      3.670      446.0      0.008406
3            12.851      3.763      521.0      0.009655
4            12.882      3.772      591.0      0.011193
5            12.716      3.723      628.0      0.008784
6            12.821      3.754      658.0      0.005553
7            12.774      3.740      680.0      0.003010
8            12.631      3.699      683.0      0.000676

Algorithm converged.
    
```

Figure 23.3 displays the iteration history. For each iteration, PROC ACECLUS displays the following measures:

- root mean square distance between all pairs of observations
- distance cutoff for including pairs of observations in the estimate of within-cluster covariances (equal to RMS*Threshold)
- number of pairs within the cutoff
- convergence measure

Figure 23.4 displays the approximate within-cluster covariance matrix and the table of eigenvalues from the canonical analysis. The first column of the eigenvalues table contains numbers for the eigenvectors. The next column of the table lists the eigenvalues of $Inv(ACE)*(COV-ACE)$.

Figure 23.4 Approximate Within-Cluster Covariance Estimates

```

ACE: Approximate Covariance Estimate Within Clusters

Birth      Death      InfantDeath
Birth      5.94644949  -0.63235725  6.28151537
Death     -0.63235725  2.33464129  1.59005857
InfantDeath 6.28151537  1.59005857  35.10327233
    
```

Figure 23.4 continued

Eigenvalues of $\text{Inv}(\text{ACE}) * (\text{COV} - \text{ACE})$				
	Eigenvalue	Difference	Proportion	Cumulative
1	63.5500	54.7313	0.8277	0.8277
2	8.8187	4.4038	0.1149	0.9425
3	4.4149		0.0575	1.0000

The next three columns of the eigenvalue table (Figure 23.4) display measures of the relative size and importance of the eigenvalues. The first column lists the difference between each eigenvalue and its successor. The last two columns display the individual and cumulative proportions that each eigenvalue contributes to the total sum of eigenvalues.

The raw and standardized canonical coefficients are displayed in Figure 23.5. The coefficients are standardized by multiplying the raw coefficients with the standard deviation of the associated variable. The ACECLUS procedure uses these standardized canonical coefficients to create the transformed canonical variables, which are the linear transformations of the original input variables, Birth, Death, and InfantDeath.

Figure 23.5 Raw and Standardized Canonical Coefficients from the ACECLUS Procedure

Eigenvectors (Raw Canonical Coefficients)			
	Can1	Can2	Can3
Birth	0.125610	0.457037	0.003875
Death	0.108402	0.163792	0.663538
InfantDeath	0.134704	-.133620	-.046266
Standardized Canonical Coefficients			
	Can1	Can2	Can3
Birth	1.70160	6.19134	0.05249
Death	0.50380	0.76122	3.08379
InfantDeath	6.19540	-6.14553	-2.12790

The following statements invoke the CLUSTER procedure, using the SAS data set Ace created in the previous ACECLUS procedure:

```
proc cluster data=ace outtree=tree noprint method=ward;
  var can1 can2 can3 ;
  copy Birth--Country;
run;
```

The OUTTREE= option creates the output SAS data set Tree that is used in a subsequent step to display cluster membership. The NOPRINT option suppresses the display of the output. The METHOD= option specifies Ward's minimum-variance clustering method.

The VAR statement specifies that the canonical variables computed in the ACECLUS procedure are used in the cluster analysis. The COPY statement specifies that all the variables from the SAS data set Poverty (Birth—Country) are added to the output data set Tree.

The following statements use PROC TREE to create an output SAS data set called New. The NCLUSTERS= option specifies the number of clusters desired in the SAS data set New. The NOPRINT option suppresses the display of the output.

```
proc tree data=tree out=new nclusters=3 noprint;
  copy Birth Death InfantDeath can1 can2 ;
  id Country;
run;
```

The COPY statement copies the canonical variables Can1 and Can2 (computed in the preceding ACECLUS procedure) and the original analytical variables Birth, Death, and InfantDeath into the output SAS data set New.

The following statements invoke the SGPLOT procedure, using the SAS data set created by PROC TREE:

```
proc sgplot data=new;
  scatter y=Death x=Birth / group=cluster;
  keylegend / title="Cluster Membership";
run;

proc sgplot data=new;
  scatter y=can2 x=can1 / group=cluster;
  keylegend / title="Cluster Membership";
run;
```

The first PROC SGPLOT statement requests a scatter plot of the two variables Birth and Death, using the variable CLUSTER as the identification variable.

The second PROC SGPLOT statement requests a plot of the two canonical variables, using the value of the variable CLUSTER as the identification variable.

Figure 23.6 and Figure 23.7 display the separation of the clusters when three clusters are calculated.

Figure 23.6 Scatter Plot of Poverty Data, Identified by Cluster

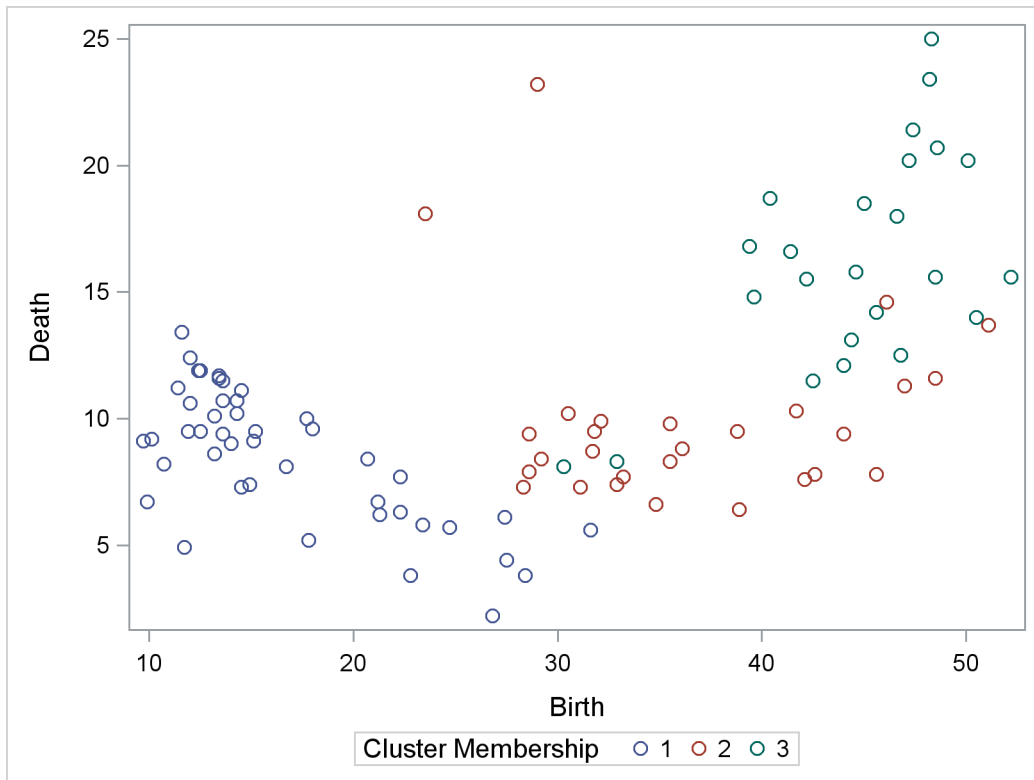
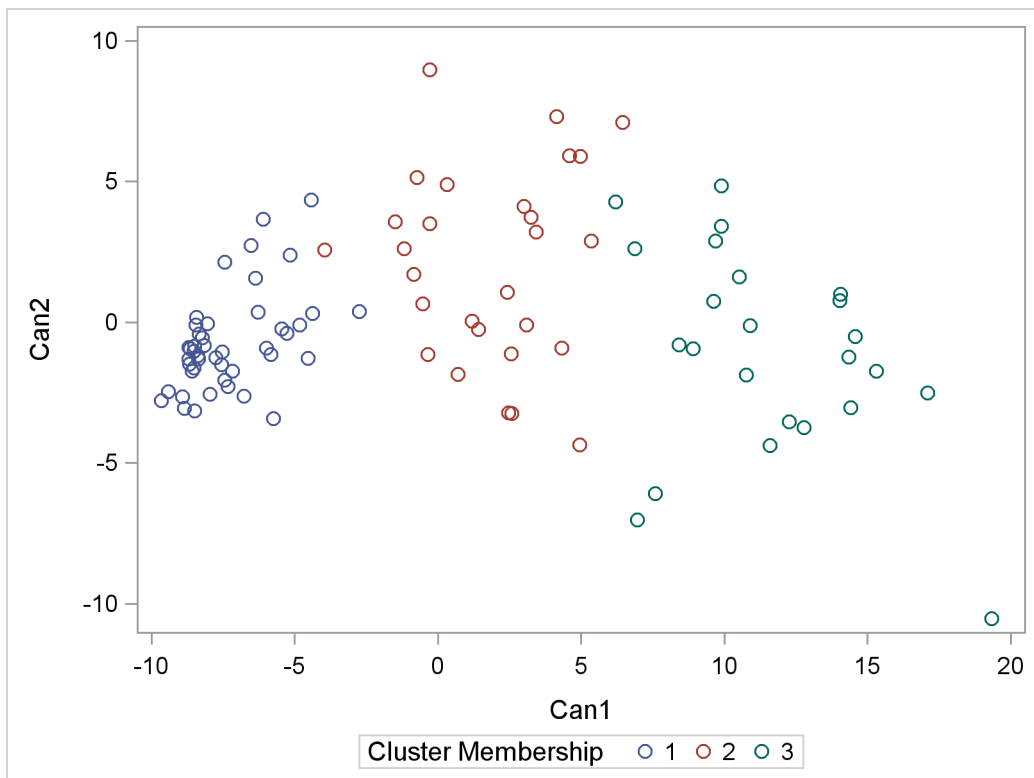


Figure 23.7 Scatter Plot of Canonical Variables



Syntax: ACECLUS Procedure

The following statements are available in the ACECLUS procedure:

```
PROC ACECLUS PROPORTION=p | THRESHOLD=t < options > ;
  BY variables ;
  FREQ variable ;
  VAR variables ;
  WEIGHT variable ;
```

Usually you need only the VAR statement in addition to the required PROC ACECLUS statement. The optional BY, FREQ, VAR, and WEIGHT statements are described in alphabetical order after the PROC ACECLUS statement.

PROC ACECLUS Statement

```
PROC ACECLUS PROPORTION=p | THRESHOLD=t < options > ;
```

The PROC ACECLUS statement invokes the ACECLUS procedure. Table 23.2 summarizes the options available in the PROC ACECLUS statement. These options are also discussed in the following sections. Note that, if you specify the METHOD=COUNT option, you must specify either the PROPORTION= or the MPAIRS= option. Otherwise, you must specify either the PROPORTION= or THRESHOLD= option.

Table 23.2 Summary of PROC ACECLUS Statement Options

Options	Description
Specify clustering options	
METHOD=	Specifies the clustering method
MPAIRS=	Specifies number of pairs for estimating within-cluster covariance (when you specify the option METHOD=COUNT)
PROPORTION=	Specifies proportion of pairs for estimating within-cluster covariance
THRESHOLD=	Specifies the threshold for including pairs in the estimation of the within-cluster covariance
Specify input and output data sets	
DATA=	Specifies input data set name
OUT=	Specifies output data set name
OUTSTAT=	Specifies output data set name containing various statistics
Specify iteration options	
ABSOLUTE	Uses absolute instead of relative threshold
CONVERGE=	Specifies convergence criterion
INITIAL=	Specifies initial estimate of within-cluster covariance matrix
MAXITER=	Specifies maximum number of iterations
METRIC=	Specifies metric in which computations are performed
SINGULAR=	Specifies singularity criterion
Specify canonical analysis options	
N=	Specifies number of canonical variables
PREFIX=	Specifies prefix for naming canonical variables

Table 23.2 continued

Options	Description
Control displayed output	
NOPRINT	Suppresses the display of the output
PP	Produces PP-plot of distances between pairs from last iteration
QQ	Produces QQ-plot of power transformation of distances between pairs from last iteration
SHORT	Omits all output except for iteration history and eigenvalue table

The following list provides details about the options.

ABSOLUTE

causes the THRESHOLD= value or the threshold computed from the PROPORTION= option to be treated absolutely rather than relative to the root mean square distance between observations. Use the ABSOLUTE option only when you are confident that the initial estimate of the within-cluster covariance matrix is close to the final estimate, such as when the INITIAL= option specifies a data set created by a previous execution of PROC ACECLUS by using the OUTSTAT= option.

CONVERGE=*c*

specifies the convergence criterion. By default, CONVERGE= 0.001. Iteration stops when the convergence measure falls below the value specified by the CONVERGE= option or when the iteration limit as specified by the MAXITER= option is exceeded, whichever happens first.

DATA=*SAS-data-set*

specifies the SAS data set to be analyzed. By default, PROC ACECLUS uses the most recently created SAS data set.

INITIAL=*name*

specifies the matrix for the initial estimate of the within-cluster covariance matrix. Valid values for *name* are as follows:

DIAGONAL D	uses the diagonal matrix of sample variances as the initial estimate of the within-cluster covariance matrix.
FULL F	uses the total-sample covariance matrix as the initial estimate of the within-cluster covariance matrix.
IDENTITY I	uses the identity matrix as the initial estimate of the within-cluster covariance matrix.
INPUT=<i>SAS-data-set</i>	specifies a SAS data set from which to obtain the initial estimate of the within-cluster covariance matrix. The data set can be TYPE=CORR, COV, UCORR, UCOV, SSCP, or ACE, or it can be an ordinary SAS data set. See Appendix A, “Special SAS Data Sets,” for descriptions of CORR, COV, UCORR, UCOV, and SSCP data sets. See the section “Output Data Sets” on page 831 for a description of ACE data sets.

If you do not specify the INITIAL= option, the default is the matrix specified by the METRIC= option. If neither the INITIAL= nor the METRIC= option is specified, INITIAL=FULL is used if there are enough observations to obtain a nonsingular total-sample covariance matrix; otherwise, INITIAL=DIAGONAL is used.

MAXITER=*n*

specifies the maximum number of iterations. By default, MAXITER=10.

METHOD=COUNT | C | THRESHOLD | T

specifies the clustering method. The METHOD=THRESHOLD option requests a method (also the default) that uses all pairs closer than a given cutoff value to form the estimate at each iteration. The METHOD=COUNT option requests a method that uses a number of pairs, *m*, with the smallest distances to form the estimate at each iteration.

METRIC=*name*

specifies the metric in which the computations are performed, implies the default value for the INITIAL= option, and specifies the matrix **Z** used in the formula for the convergence measure e_i and for checking singularity of the **A** matrix. Valid values for *name* are as follows:

DIAGONAL | D uses the diagonal matrix of sample variances $\text{diag}(\mathbf{S})$ and sets $\mathbf{Z} = \text{diag}(\mathbf{S})^{-\frac{1}{2}}$, where the superscript $-\frac{1}{2}$ indicates an inverse factor.

FULL | F uses the total-sample covariance matrix **S** and sets $\mathbf{Z} = \mathbf{S}^{-\frac{1}{2}}$.

IDENTITY | I uses the identity matrix **I** and sets $\mathbf{Z} = \mathbf{I}$.

If you do not specify the METRIC= option, METRIC=FULL is used if there are enough observations to obtain a nonsingular total-sample covariance matrix; otherwise, METRIC=DIAGONAL is used.

The option METRIC= is rather technical. It affects the computations in a variety of ways, but for well-conditioned data the effects are subtle. For most data sets, the METRIC= option is not needed.

MPAIRS=*m*

specifies the number of pairs to be included in the estimation of the within-cluster covariance matrix when METHOD=COUNT is requested. The values of *m* must be greater than 0 but less than or equal to $(\text{totfq} \times (\text{totfq} - 1)) / 2$, where *totfq* is the sum of nonmissing frequencies specified in the FREQ statement. If there is no FREQ statement, *totfq* equals the number of total nonmissing observations.

N=*n*

specifies the number of canonical variables to be computed. The default is the number of variables analyzed. N=0 suppresses the canonical analysis.

NOPRINT

suppresses the display of all output. Note that this option temporarily disables the Output Delivery System (ODS). For more information, see Chapter 20, “Using the Output Delivery System.”

OUT=*SAS-data-set*

creates an output SAS data set that contains all the original data as well as the canonical variables having an estimated within-cluster covariance matrix equal to the identity matrix. If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*.

OUTSTAT=*SAS-data-set*

specifies a TYPE=ACE output SAS data set that contains means, standard deviations, number of observations, covariances, estimated within-cluster covariances, eigenvalues, and canonical coefficients. If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*.

PROPORTION=*p***PERCENT=*p*****P=*p***

specifies the percentage of pairs to be included in the estimation of the within-cluster covariance matrix. The value of *p* must be greater than 0. If *p* is greater than or equal to 1, it is interpreted as a percentage and divided by 100; PROPORTION=0.02 and PROPORTION=2 are equivalent. When you specify METHOD=THRESHOLD, a threshold value is computed from the PROPORTION= option under the assumption that the observations are sampled from a multivariate normal distribution.

When you specify METHOD=COUNT, the number of pairs, *m*, is computed from PROPORTION=*p* as

$$m = \text{floor} \left(\frac{p}{2} \times \text{totfq} \times (\text{totfq} - 1) \right)$$

where *totfq* is the number of total nonmissing observations.

PP

produces a PP probability plot of distances between pairs of observations computed in the last iteration.

PREFIX=*name*

specifies a prefix for naming the canonical variables. By default the names are Can1, Can2, ..., CANN. If you specify PREFIX=ABC, the variables are named ABC1, ABC2, ABC3, and so on. The number of characters in the prefix plus the number of digits required to designate the variables should not exceed the name length defined by the VALIDVARNAME= system option. For more information about the VALIDVARNAME= system option, see *SAS System Options: Reference*.

QQ

produces a QQ probability plot of a power transformation of the distances between pairs of observations computed in the last iteration. **CAUTION:** The QQ plot can require an enormous amount of computer time.

SHORT

omits all items from the standard output except for the iteration history and the eigenvalue table.

SINGULAR=*g***SING=*g***

specifies a singularity criterion $0 < g < 1$ for the total-sample covariance matrix **S** and the approximate within-cluster covariance estimate **A**. The default is SINGULAR=1E-4.

THRESHOLD=*t***T=*t***

specifies the threshold for including pairs of observations in the estimation of the within-cluster covariance matrix. A pair of observations is included if the Euclidean distance between them is less than or equal to *t* times the root mean square distance computed over all pairs of observations.

BY Statement

BY variables ;

You can specify a BY statement with PROC ACECLUS to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the ACECLUS procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

If you specify the INITIAL=INPUT= option and the INITIAL=INPUT= data set does not contain any of the BY variables, the entire INITIAL=INPUT= data set provides the initial value for the matrix **A** for each BY group in the DATA= data set.

If the INITIAL=INPUT= data set contains some but not all of the BY variables, or if some BY variables do not have the same type or length in the INITIAL=INPUT= data set as in the DATA= data set, then PROC ACECLUS displays an error message and stops.

If all the BY variables appear in the INITIAL=INPUT= data set with the same type and length as in the DATA= data set, then each BY group in the INITIAL=INPUT= data set provides the initial value for **A** for the corresponding BY group in the DATA= data set. All BY groups in the DATA= data set must also appear in the INITIAL= INPUT= data set. The BY groups in the INITIAL=INPUT= data set must be in the same order as in the DATA= data set. If you specify NOTSORTED in the BY statement, identical BY groups must occur in the same order in both data sets. If you do not specify NOTSORTED, some BY groups can appear in the INITIAL= INPUT= data set, but not in the DATA= data set; such BY groups are not used in the analysis.

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

FREQ Statement

FREQ variable ;

If a variable in your data set represents the frequency of occurrence for the observation, include the name of that variable in the FREQ statement. The procedure then treats the data set as if each observation appears n times, where n is the value of the FREQ variable for the observation. If a value of the FREQ variable is not integral, it is truncated to the largest integer not exceeding the given value. Observations with FREQ values

less than one are not included in the analysis. The total number of observations is considered equal to the sum of the FREQ variable.

VAR Statement

VAR *variables* ;

The VAR statement specifies the numeric variables to be analyzed. If the VAR statement is omitted, all numeric variables not specified in other statements are analyzed.

WEIGHT Statement

WEIGHT *variable* ;

If you want to specify relative weights for each observation in the input data set, place the weights in a variable in the data set and specify that variable name in a WEIGHT statement. This is often done when the variance associated with each observation is different and the values of the weight variable are proportional to the reciprocals of the variances. The values of the WEIGHT variable can be nonintegral and are not truncated. An observation is used in the analysis only if the value of the WEIGHT variable is greater than zero.

The WEIGHT and FREQ statements have a similar effect, except in calculating the divisor of the **A** matrix.

Details: ACECLUS Procedure

Missing Values

Observations with missing values are omitted from the analysis and are given missing values for canonical variable scores in the OUT= data set.

Output Data Sets

OUT= Data Set

The OUT= data set contains all the variables in the original data set plus new variables containing the canonical variable scores. The N= option determines the number of new variables. The OUT= data set is not created if N=0. The names of the new variables are formed by concatenating the value given by the PREFIX= option (or the prefix CAN if the PREFIX= option is not specified) and the numbers 1, 2, 3, and so on. The OUT= data set can be used as input to PROC CLUSTER or PROC FASTCLUS. The cluster analysis should be performed on the canonical variables, not on the original variables.

OUTSTAT= Data Set

The OUTSTAT= data set is a TYPE=ACE data set containing the following variables:

- the BY variables, if any
- the two new character variables, `_TYPE_` and `_NAME_`
- the variables analyzed—that is, those in the VAR statement, or, if there is no VAR statement, all numeric variables not listed in any other statement

Each observation in the new data set contains some type of statistic as indicated by the `_TYPE_` variable. The values of the `_TYPE_` variable are as follows:

MEAN	mean of each variable
STD	standard deviation of each variable
N	number of observations on which the analysis is based. This value is the same for each variable.
SUMWGT	sum of the weights if a WEIGHT statement is used. This value is the same for each variable.
COV	covariances between each variable and the variable named by the <code>_NAME_</code> variable. The number of observations with <code>_TYPE_=COV</code> is equal to the number of variables being analyzed.
ACE	estimated within-cluster covariances between each variable and the variable named by the <code>_NAME_</code> variable. The number of observations with <code>_TYPE_=ACE</code> is equal to the number of variables being analyzed.
EIGENVAL	eigenvalues of $INV(ACE)*(COV-ACE)$. If the N= option requests fewer than the maximum number of canonical variables, only the specified number of eigenvalues are produced, with missing values filling out the observation.
RAWSCORE	raw canonical coefficients. To obtain the canonical variable scores, these coefficients should be multiplied by the raw data centered by means obtained from the observation with <code>_TYPE_='MEAN'</code> .
SCORE	standardized canonical coefficients. The <code>_NAME_</code> variable contains the name of the corresponding canonical variable as constructed from the PREFIX= option. The number of observations with <code>_TYPE_=SCORE</code> equals the number of canonical variables computed. To obtain the canonical variable scores, these coefficients should be multiplied by the standardized data, using means obtained from the observation with <code>_TYPE_='MEAN'</code> and standard deviations obtained from the observation with <code>_TYPE_='STD'</code> .

The OUTSTAT= data set can be used in the following conditions:

- to initialize another execution of PROC ACECLUS
- to compute canonical variable scores with the SCORE procedure
- as input to the FACTOR procedure, specifying METHOD=SCORE, to rotate the canonical variables

Computational Resources

Let

n = number of observations

v = number of variables

i = number of iterations

Memory

The memory in bytes required by PROC ACECLUS is approximately

$$8(2n(v + 1) + 21v + 5v^2)$$

bytes. If you request the PP or QQ option, an additional $4n(n - 1)$ bytes are needed.

Time

The time required by PROC ACECLUS is roughly proportional to

$$2nv^2 + 10v^3 + i \left(\frac{n^2v}{2} + nv^2 + 5v^3 \right)$$

Displayed Output

Unless the SHORT option is specified, the ACECLUS procedure displays the following items:

- Means and Standard Deviations of the input variables
- the S matrix, labeled COV: Total Sample Covariances
- the name or value of the matrix used for the Initial Within-Cluster Covariance Estimate
- the Threshold value if the PROPORTION= option is specified

For each iteration, PROC ACECLUS displays the following items:

- the Iteration number
- RMS Distance, the root mean square distance between all pairs of observations
- the Distance Cutoff (u) for including pairs of observations in the estimate of the within-cluster covariances, which equals the RMS distance times the threshold

- the number of Pairs Within Cutoff
- the Convergence Measure (e_i) as specified by the METRIC= option

If the SHORT option is not specified, PROC ACECLUS also displays the **A** matrix, labeled ACE: Approximate Covariance Estimate Within Clusters.

The ACECLUS procedure displays a table of eigenvalues from the canonical analysis containing the following items:

- Eigenvalues of $\text{Inv}(\text{ACE}) * (\text{COV} - \text{ACE})$
- the Difference between successive eigenvalues
- the Proportion of variance explained by each eigenvalue
- the Cumulative proportion of variance explained

If the SHORT option is not specified, PROC ACECLUS displays the following items:

- the Eigenvectors or raw canonical coefficients
- the standardized eigenvectors or standard canonical coefficients

ODS Table Names

PROC ACECLUS assigns a name to each table it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in the following table. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

Table 23.3 ODS Tables Produced by PROC ACECLUS

ODS Table Name	Description	Statement	Option
ConvergenceStatus	Convergence status	PROC	default
DataOptionInfo	Data and option information	PROC	default
Eigenvalues	Eigenvalues of $\text{Inv}(\text{ACE}) * (\text{COV} - \text{ACE})$	PROC	default
Eigenvectors	Eigenvectors (raw canonical coefficients)	PROC	default
InitWithin	Initial within-cluster covariance estimate	PROC	INITIAL=INPUT
IterHistory	Iteration history	PROC	default
SimpleStatistics	Simple statistics	PROC	default
StdCanCoef	Standardized canonical coefficients	PROC	default
Threshold	Threshold value	PROC	PROPORTION=

Table 23.3 continued

ODS Table Name	Description	Statement	Option
TotSampleCov	Total sample covariances	PROC	default
Within	Approximate covariance estimate within clusters	PROC	default

Example: ACECLUS Procedure

Example 23.1: Transformation and Cluster Analysis of Fisher Iris Data

The iris data published by Fisher (1936) have been widely used for examples in discriminant analysis and cluster analysis. The sepal length, sepal width, petal length, and petal width are measured in millimeters on 50 iris specimens from each of three species, *Iris setosa*, *I. versicolor*, and *I. virginica*. Mezzich and Solomon (1980) discuss a variety of cluster analyses of the iris data.

In this example PROC ACECLUS is used to transform the iris data, which is available from the Sashelp library, and the clustering is performed by PROC FASTCLUS. Compare this with the example in Chapter 36, “The FASTCLUS Procedure.” The results from the FREQ procedure display fewer misclassifications when PROC ACECLUS is used.

The following statements produce [Output 23.1.1](#) through [Output 23.1.5](#):

```

title 'Fisher (1936) Iris Data';

proc aceclus data=sashelp.iris out=ace p=.02 outstat=score;
  var SepalLength SepalWidth PetalLength PetalWidth ;
run;

proc sgplot data=ace;
  scatter y=can2 x=can1 / group=Species;
  keylegend / title="Species";
run;

proc fastclus data=ace maxc=3 maxiter=10 conv=0 out=clus;
  var can:;
run;

proc freq;
  tables cluster*Species;
run;

```

Output 23.1.1 Using PROC ACECLUS to Transform Fisher's Iris Data

```

Fisher (1936) Iris Data

The ACECLUS Procedure

Approximate Covariance Estimation for Cluster Analysis

Observations      150   Proportion      0.0200
Variables          4    Converge       0.00100

Means and Standard Deviations
Standard
Variable          Mean   Deviation   Label
SepalLength      58.4333    8.2807   Sepal Length (mm)
SepalWidth       30.5733    4.3587   Sepal Width (mm)
PetalLength      37.5800   17.6530   Petal Length (mm)
PetalWidth       11.9933    7.6224   Petal Width (mm)

COV: Total Sample Covariances

SepalLength      SepalWidth      PetalLength      PetalWidth
SepalLength      68.5693512     -4.2434004      127.4315436     51.6270694
SepalWidth       -4.2434004     18.9979418     -32.9656376     -12.1639374
PetalLength      127.4315436   -32.9656376     311.6277852     129.5609396
PetalWidth       51.6270694    -12.1639374     129.5609396     58.1006264

Initial Within-Cluster Covariance Estimate = Full Covariance Matrix

Threshold = 0.334211

Iteration History

RMS      Distance      Pairs      Convergence
Iteration Distance   Cutoff     Within     Measure
-----
1         2.828         0.945     408.0     0.465775
2         11.905        3.979     559.0     0.013487
3         13.152        4.396     940.0     0.029499
4         13.439        4.491    1506.0     0.046846
5         13.271        4.435    2036.0     0.046859
6         12.591        4.208    2285.0     0.025027
7         12.199        4.077    2366.0     0.009559
8         12.121        4.051    2402.0     0.003895
9         12.064        4.032    2417.0     0.002051
10        12.047        4.026    2429.0     0.000971

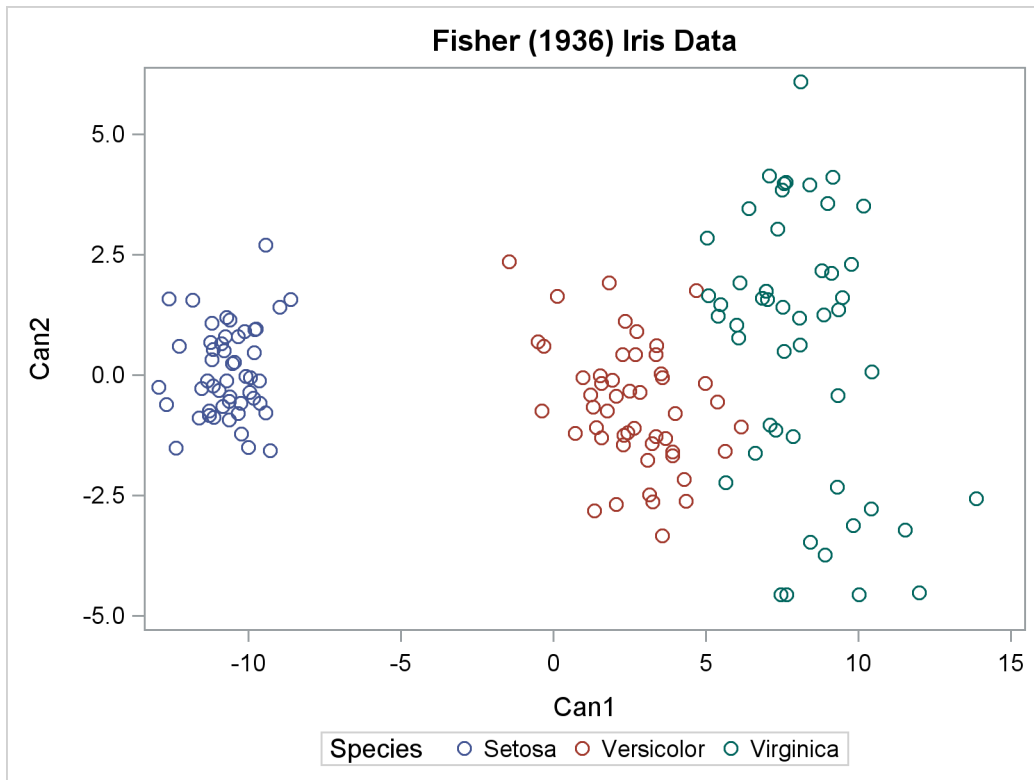
Algorithm converged.

```

Output 23.1.2 Eigenvalues, Raw Canonical Coefficients, and Standardized Canonical Coefficients

ACE: Approximate Covariance Estimate Within Clusters					
	SepalLength	SepalWidth	PetalLength	PetalWidth	
SepalLength	11.73342939	5.47550432	4.95389049	2.02902429	
SepalWidth	5.47550432	6.91992590	2.42177851	1.74125154	
PetalLength	4.95389049	2.42177851	6.53746398	2.35302594	
PetalWidth	2.02902429	1.74125154	2.35302594	2.05166735	
Eigenvalues of Inv(ACE)*(COV-ACE)					
	Eigenvalue	Difference	Proportion	Cumulative	
1	63.7716	61.1593	0.9367	0.9367	
2	2.6123	1.5561	0.0384	0.9751	
3	1.0562	0.4167	0.0155	0.9906	
4	0.6395		0.00939	1.0000	
Eigenvectors (Raw Canonical Coefficients)					
		Can1	Can2	Can3	Can4
SepalLength	Sepal Length (mm)	-0.012009	-0.098074	-0.059852	0.402352
SepalWidth	Sepal Width (mm)	-0.211068	-0.000072	0.402391	-0.225993
PetalLength	Petal Length (mm)	0.324705	-0.328583	0.110383	-0.321069
PetalWidth	Petal Width (mm)	0.266239	0.870434	-0.085215	0.320286
Standardized Canonical Coefficients					
		Can1	Can2	Can3	Can4
SepalLength	Sepal Length (mm)	-0.09944	-0.81211	-0.49562	3.33174
SepalWidth	Sepal Width (mm)	-0.91998	-0.00031	1.75389	-0.98503
PetalLength	Petal Length (mm)	5.73200	-5.80047	1.94859	-5.66782
PetalWidth	Petal Width (mm)	2.02937	6.63478	-0.64954	2.44134

Output 23.1.3 Plot of Transformed Iris Data: PROC SGPLOT



Output 23.1.4 Clustering of Transformed Iris Data: Partial Output from PROC FASTCLUS

```

Fisher (1936) Iris Data

The FASTCLUS Procedure
Replace=FULL Radius=0 Maxclusters=3 Maxiter=10 Converge=0

Cluster Summary

```

Cluster	Frequency	RMS Std Deviation	Maximum Distance from Seed to Observation	Radius Exceeded	Nearest Cluster
1	50	1.4138	5.3152		2
2	50	1.8880	6.8298		1
3	50	1.1016	5.2768		1

```

Cluster Summary

Distance Between  
Cluster Centroids

```

Cluster	Distance Between Cluster Centroids
1	5.8580
2	5.8580
3	13.2845

Output 23.1.4 *continued*

Statistics for Variables				
Variable	Total STD	Within STD	R-Square	RSQ/(1-RSQ)
Can1	8.04808	1.48537	0.966394	28.756658
Can2	1.90061	1.85646	0.058725	0.062389
Can3	1.43395	1.32518	0.157417	0.186826
Can4	1.28044	1.27550	0.021025	0.021477
OVER-ALL	4.24499	1.50298	0.876324	7.085666

Pseudo F Statistic = 520.80

Approximate Expected Over-All R-Squared = 0.80391

Cubic Clustering Criterion = 5.179

WARNING: The two values above are invalid for correlated variables.

Cluster Means				
Cluster	Can1	Can2	Can3	Can4
1	2.54528754	-0.59273569	-0.78905317	-0.26079612
2	8.12988211	0.52566663	0.51836499	0.14915404
3	-10.67516964	0.06706906	0.27068819	0.11164209

Cluster Standard Deviations				
Cluster	Can1	Can2	Can3	Can4
1	1.572366584	1.393565864	1.303411851	1.372050319
2	1.799159552	2.743869556	1.270344142	1.370523175
3	0.953761025	0.931943571	1.398456061	1.058217627

Output 23.1.5 Crosstabulation of Cluster by Species for Fisher's Iris Data: PROC FREQ

Fisher (1936) Iris Data				
The FREQ Procedure				
Table of CLUSTER by Species				
CLUSTER(Cluster)	Species(Iris Species)			
	Setosa	Versicol or	Virginic a	Total
Frequency				
Percent				
Row Pct				
Col Pct				
1	0	48	2	50
	0.00	32.00	1.33	33.33
	0.00	96.00	4.00	
	0.00	96.00	4.00	
2	0	2	48	50
	0.00	1.33	32.00	33.33
	0.00	4.00	96.00	
	0.00	4.00	96.00	
3	50	0	0	50
	33.33	0.00	0.00	33.33
	100.00	0.00	0.00	
	100.00	0.00	0.00	
Total	50	50	50	150
	33.33	33.33	33.33	100.00

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Chapter 24

The ADAPTIVEREG Procedure

(Experimental)

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Overview: ADAPTIVEREG Procedure

The ADAPTIVEREG procedure fits multivariate adaptive regression splines as defined by Friedman (1991b). The method is a nonparametric regression technique that combines both regression splines and model selection methods. It does not assume parametric model forms and does not require specification

of knot values for constructing regression spline terms. Instead, it constructs spline basis functions in an adaptive way by automatically selecting appropriate knot values for different variables and obtains reduced models by applying model selection techniques.

PROC ADAPTIVEREG supports models with classification variables (Friedman 1991a) and offers options for improving modeling speed (Friedman 1993). PROC ADAPTIVEREG also extends the method to data with response variables that are distributed in the exponential family as suggested in Buja et al. (1991). The procedure can take advantage of multicore processors to distribute the computation to multiple threads.

SAS/STAT software offers various tools for nonparametric regression, including the GAM, LOESS, and TPSPLINE procedures. Typical nonparametric regression methods involve a large number of parameters in order to capture nonlinear trends in data; thus the model space is much larger than it is in more restricted parametric models. The fitting algorithms for nonparametric regression models are usually more complicated than for parametric regression models. Also, the sparsity of data in high dimensions often causes slow convergence or failure in many nonparametric regression methods. As the number of predictors increases, the model variance increases rapidly because of the sparsity. This phenomenon is referred as the “curse of dimensionality” (Bellman 1961). Hence, the LOESS and TPSPLINE procedures are limited to problems in low dimensions. PROC GAM fits generalized additive models with the additivity assumption. By using the local scoring algorithm (Hastie and Tibshirani 1990), PROC GAM can handle larger data sets than the other two procedures. However, the computation time for the local scoring algorithm to converge increases rapidly as data size grows, and the convergence for nonnormal distributions is not guaranteed. PROC ADAPTIVEREG uses the multivariate adaptive regression splines method, which is similar to the method used for the recursive partitioning models (Breiman et al. 1984). It creates an overfitted model first with the fast-update algorithm (Friedman 1991b); then prunes it back with the backward selection technique.

The main features of the ADAPTIVEREG procedure are as follows:

- supports classification variables with ordering options
- enables you to force effects in the final model or restrict variables in linear forms
- supports options for fast forward selection
- supports data with response variables that are distributed in the exponential family
- supports partitioning of data into training, validation, and testing roles
- provides leave-one-out and k -fold cross validation
- produces a graphical representation of the selection process, model fit, functional components, and fit diagnostics
- produces an output data set that contains predicted values and residuals
- produces an output data set that contains the design matrix of formed basis functions
- supports multiple SCORE statements

Getting Started: ADAPTIVEREG Procedure

This example concerns city-cycle fuel efficiency and automobile characteristics for 361 vehicle models made from year 1970 to 1982. The data can be downloaded from the UCI Machine Learning Repository (Asuncion and Newman 2007). The following DATA step creates the data set autmpg:

```

title 'Automobile MPG Study';
data Autmpg;
  input MPG Cylinders Displacement Horsepower Weight
        Acceleration Year Origin Name $35.;
  datalines;
18.0 8 307.0 130.0 3504 12.0 70 1 Chevrolet Chevelle Malibu
15.0 8 350.0 165.0 3693 11.5 70 1 Buick Skylark 320
18.0 8 318.0 150.0 3436 11.0 70 1 Plymouth Satellite
16.0 8 304.0 150.0 3433 12.0 70 1 AMC Rebel SST

... more lines ...

44.0 4 97.00 52.00 2130 24.6 82 2 VW Pickup
32.0 4 135.0 84.00 2295 11.6 82 1 Dodge Rampage
28.0 4 120.0 79.00 2625 18.6 82 1 Ford Ranger
31.0 4 119.0 82.00 2720 19.4 82 1 Chevy S-10
;

```

There are nine variables in the data set. The response variable MPG is city-cycle mileage per gallon (MPG). Seven predictor variables (Cylinders, Displacement, HorsePower, Weight, Acceleration, Year, and Origin) provide vehicle attributes. Among them, Cylinders, Year, and Origin are categorical variables. The last variable, Name, contains the specific name of each vehicle model.

The dependency of vehicle fuel efficiency on various factors might be nonlinear. There might also be redundant predictor variables as a result of dependency structures within predictors. For example, a vehicle model with more cylinders is likely to have more horsepower. The objective of this example is to explore the nonlinear dependency structure and also to produce a parsimonious model that does not overfit and thus has good predictive power. The following invocation of the ADAPTIVEREG procedure fits an additive model with linear spline terms of continuous predictors. By default, PROC ADAPTIVEREG fits a nonparametric regression model that includes two-way interaction between spline basis functions. You can try models with even higher interaction orders by specifying the `MAXORDER=` option in the `MODEL` statement. For this particular data set, the sample size is relatively small. Restricting model complexity by specifying an additive model can both improve model interpretability and reduce model variance without sacrificing much predictive power. The additive model consists of terms of nonparametric transformations of variables. The transformation of each variable and the selection of transformed terms are performed in an adaptive and automatic way.

```

ods graphics on;

proc adaptivereg data=autmpg plots=all;
  class cylinders year origin;
  model mpg = cylinders displacement horsepower
            weight acceleration year origin / additive;
run;

```


PROC ADAPTIVEREG summarizes important information about the model that you are fitting in Figure 24.1.

Figure 24.1 Model Information and Fit Controls

Automobile MPG Study	
The ADAPTIVEREG Procedure	
Model Information	
Data Set	WORK.AUTOMPG
Response Variable	MPG
Class Variables	Cylinders Year Origin
Distribution	Normal
Link Function	Identity
Fit Controls	
Maximum Number of Bases	21
Maximum Order of Interaction	1
Degrees of Freedom per Knot	2
Knot Separation Parameter	0.05
Penalty for Variable Reentry	0
Missing Value Handling	Include

In addition to listing classification variables in the “Model Information” table, PROC ADAPTIVEREG displays level information about the classification variables that are specified in the CLASS statement. The table in Figure 24.2 lists the levels of the classification variables Cylinders, Year, and Origin. Although the values of Cylinders and Year are naturally ordered, they are treated as ordinary classification variables.

Figure 24.2 Class Level Information

Class Level Information		
Class	Levels	Values
Cylinders	5	3 4 5 6 8
Year	13	70 71 72 73 74 75 76 77 78 79 80 81 82
Origin	3	1 2 3

The “Fit Statistics” table (Figure 24.3) lists summary statistics of the fitted regression spline model. Because the final model is essentially a linear model, several fit statistics are reported as if the model were fitted with basis functions as predetermined effects. However, because the model selection process and the determination of basis functions are highly nonlinear, additional statistics that incorporate the extra source of degrees of freedom are also displayed. The statistics include effective degrees of freedom, the generalized cross validation (GCV) criterion, and the GCV R-square value.

Figure 24.3 Fit Statistics

Fit Statistics	
GCV	11.55804
GCV R-Square	0.81128
Effective Degrees of Freedom	23
R-Square	0.83161
Adjusted R-Square	0.82682
Mean Square Error	10.57977
Average Square Error	10.26079

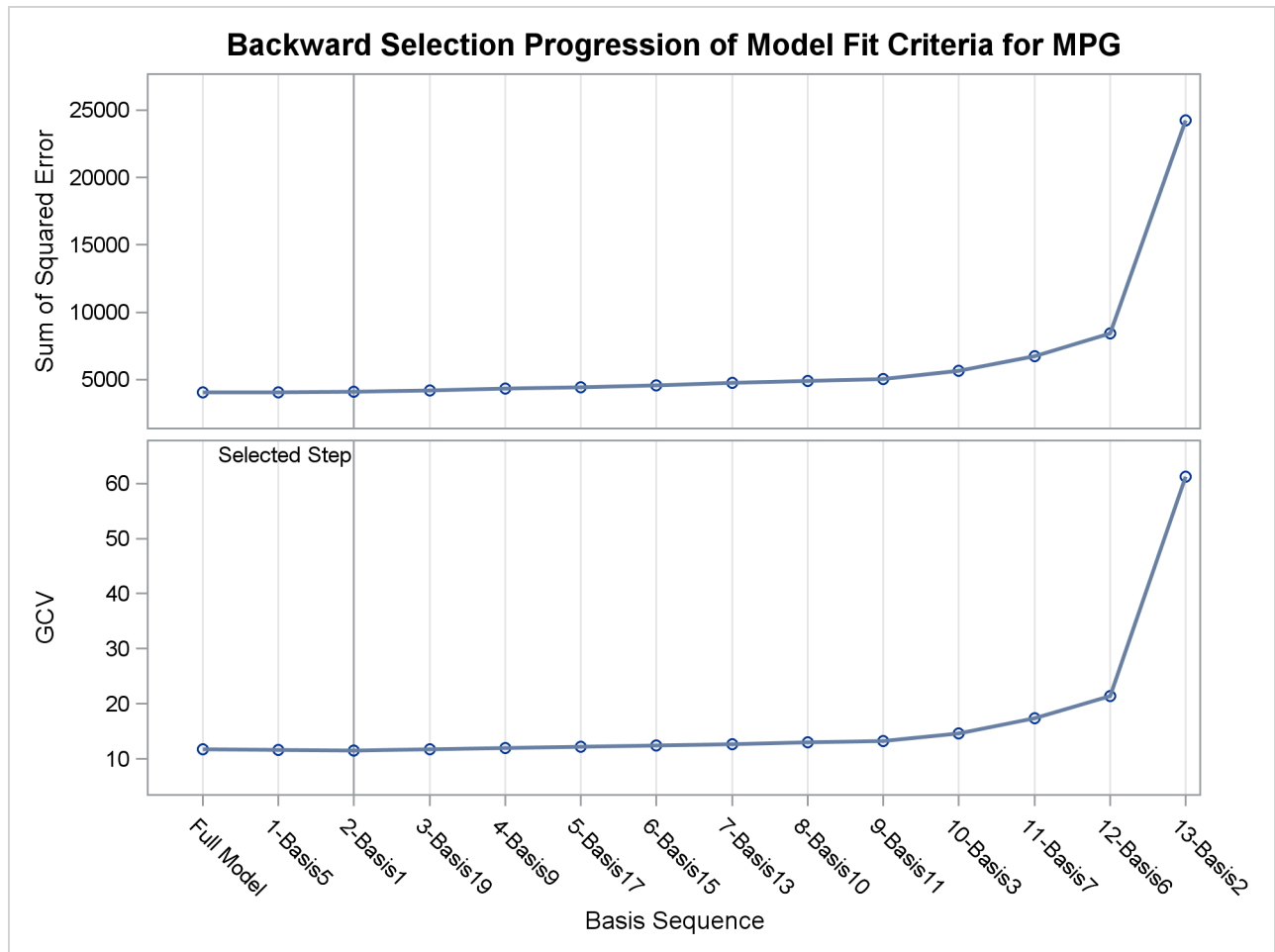
The “Parameter Estimates” table (Figure 24.4) displays both parameter estimates for constructed basis functions and each function’s construction components. The basis functions are constructed as two-way interaction terms from parent basis functions and transformations of variables. For continuous variables, the transformations are linear spline functions with knot values specified in the Knot column. For classification variables, the transformations are formed by dichotomizing the variables based on levels specified in the Levels column.

Figure 24.4 Parameter Estimates

Regression Spline Model after Backward Selection					
Name	Coefficient	Parent	Variable	Knot	Levels
Basis0	29.4394		Intercept		
Basis2	0.004412	Basis0	Weight	3139.00	
Basis3	-21.2899	Basis0	Horsepower	.	
Basis6	0.1534	Basis3	Horsepower	158.00	
Basis7	2.3920	Basis3	Year		10 12 11 9 8 7 3
Basis9	1.6658	Basis0	Acceleration	21.0000	
Basis10	0.4672	Basis0	Acceleration	21.0000	
Basis11	-8.1766	Basis0	Cylinders		0 3
Basis13	-10.0976	Basis4	Origin		0
Basis15	2.1354	Basis0	Origin		2
Basis17	6.7675	Basis0	Cylinders		3
Basis19	1.4987	Basis0	Year		3 10 12 11 9

During the model construction and selection process, some basis function terms are removed. You can view the backward elimination process in the selection plot (Figure 24.5). The plot displays how the model sum of squared error and the corresponding GCV criterion change along with the backward elimination process. The sum of squared error increases as more basis functions are removed from the full model. The GCV criterion decreases at first when two basis functions are dropped and increases afterward. The vertical line indicates the selected model that has the minimum GCV value.

Figure 24.5 Selection Plot



The formed model is an additive model. Basis functions of same variables can be grouped together to form functional components. The “ANOVA Decomposition” table (Figure 24.6) shows functional components and their contribution to the final model.

Figure 24.6 ANOVA Decomposition

ANOVA Decomposition				
Functional Component	Number of Bases	DF	---Change If Omitted--- Lack of Fit	GCV
Weight	1	2	299.55	0.7165
Horsepower	1	2	1324.81	3.5875
Year	2	4	1183.22	3.0358
Acceleration	2	4	287.76	0.5546
Cylinders	2	4	321.11	0.6470
Origin	2	4	316.04	0.6330

Another criterion that focuses on the contribution of each individual variable is variable importance. It is defined to be the square root of the GCV value of a submodel from which all basis functions that involve a variable have been removed, minus the square root of the GCV value of the selected model, then scaled to have the largest importance value, 100. The table in [Figure 24.7](#) lists importance values, sorted in descending order, for the variables that compose the selected model.

Figure 24.7 Variable Importance

Variable Importance		
Variable	Number of Bases	Importance
Horsepower	1	100.00
Year	2	85.46
Weight	1	21.10
Cylinders	2	19.08
Origin	2	18.67
Acceleration	2	16.38

The component panel (Figure 24.8) displays the fitted functional components against their forming variables.

Figure 24.8 Component Panel

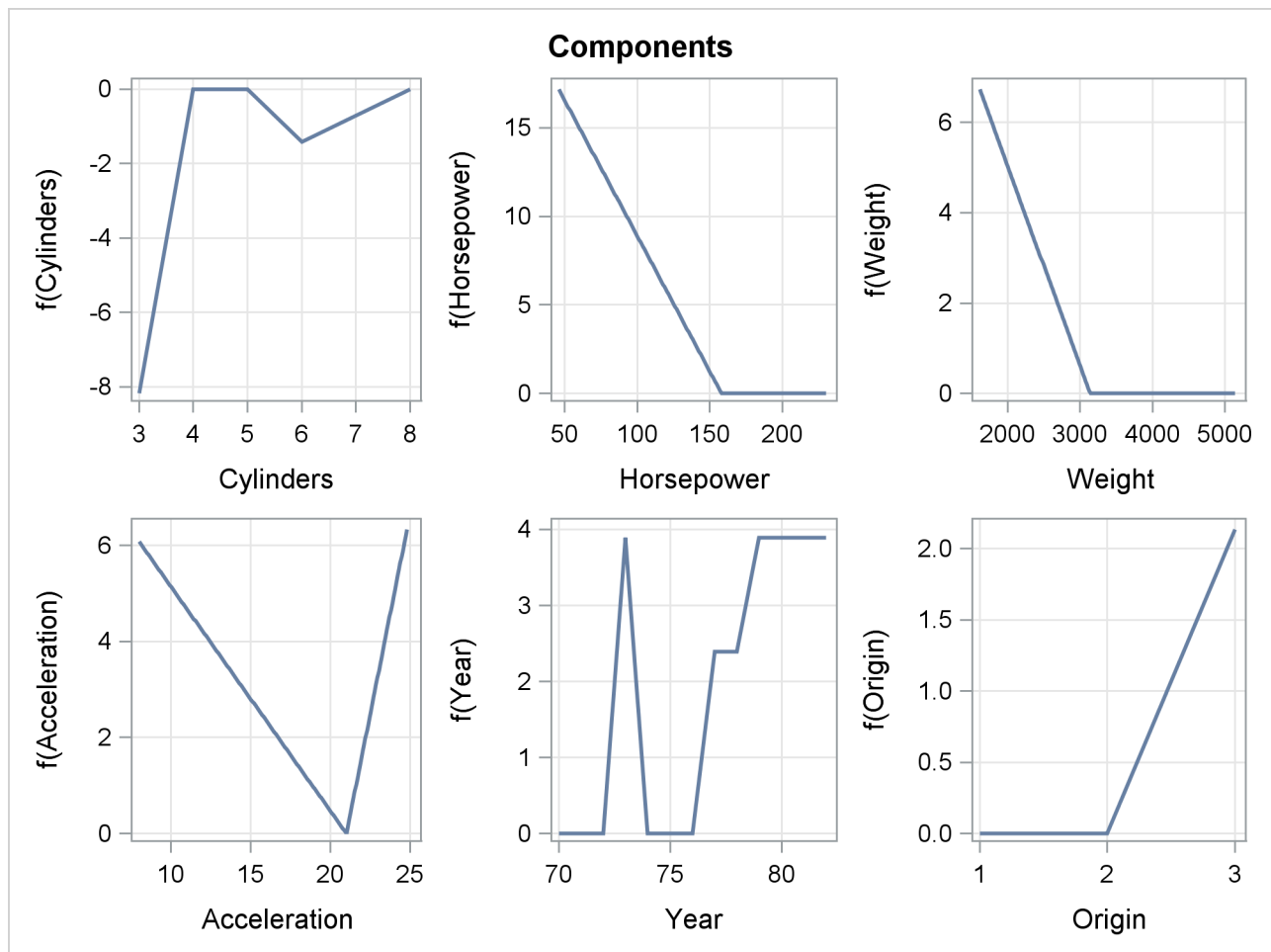
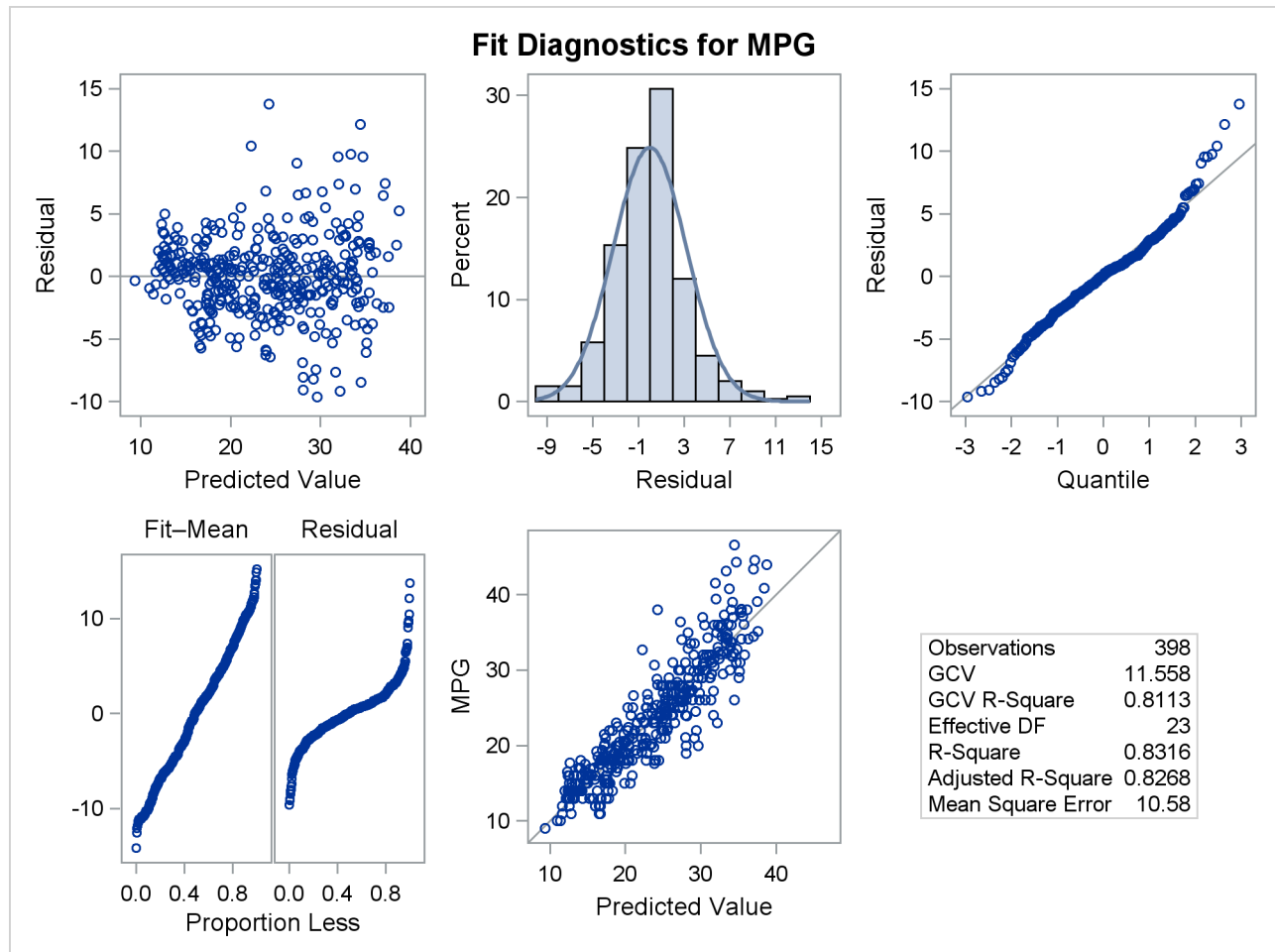


Figure 24.9 shows a panel of fit diagnostics for the selected model that indicate a reasonable fit.

PROC ADAPTIVEREG provides an adaptive way to fit parsimonious regression spline models. The non-parametric transformation of variables is automatically determined, and model selection methods are used to reduce model complexity. The final model based on piecewise linear splines is easy to interpret and highly portable. It can also be used to suggest parametric forms based on the nonlinear trend.

Figure 24.9 Diagnostics Panel



Syntax: ADAPTIVEREG Procedure

The following statements are available in the ADAPTIVEREG procedure:

```

PROC ADAPTIVEREG < options > ;
  BY variables ;
  CLASS variables < / options > ;
  FREQ variable ;
  MODEL dependent < (options) > = < effects > < / options > ;
  OUTPUT < OUT=SAS-data-set > < keyword < (keyword-options) > < =name > > ...
    < keyword < (keyword-options) > < =name > > ;
  PARTITION < options > ;
  SCORE < DATA=SAS-data-set > < OUT=SAS-data-set >
    < keyword < =name > > ... < keyword < =name > > ;
  WEIGHT variable ;

```

The syntax of the ADAPTIVEREG procedure is similar to that of other regression procedures in the SAS System. The PROC ADAPTIVEREG and MODEL statements are required, and the MODEL statement must appear after the CLASS statement if a CLASS statement is included. The SCORE statement can appear multiple times; all other statements can appear only once.

The following sections describe the PROC ADAPTIVEREG statement and then describe the other statements in alphabetical order.

PROC ADAPTIVEREG Statement

PROC ADAPTIVEREG < options > ;

The PROC ADAPTIVEREG statement invokes the procedure.

Table 24.1 summarizes the options available in the PROC ADAPTIVEREG statement.

Table 24.1 PROC ADAPTIVEREG Statement Options

Option	Description
Data Set Options	
DATA=	Specifies the input SAS data set
TESTDATA=	Names a data set that contains test data
VALDATA=	Names a data set that contains validation data
Computational Options	
NLOPTIONS	Sets optimization parameters for fitting generalized linear models
SINGULAR=	Sets the singularity tolerance
Display Options	
NAMELEN=	Sets the length of effect names in tables and output data sets
PLOTS=	Controls plots produced through ODS Graphics
DETAILS=	Displays detailed modeling information
Other Options	
NOTHREADS	Requests the computation in single-threaded mode
OUTDESIGN=	Requests a data set that contains the design matrix
SEED=	Sets the seed used for pseudo-random number generation
THREADS=	Specifies the number of threads for the computation

You can specify the following *options*.

DATA=*SAS-data-set*

specifies the SAS data set to be read by PROC ADAPTIVEREG. If you do not specify the DATA= option, PROC ADAPTIVEREG uses the most recently created SAS data set.

DETAILS< =(detail-options) >

requests detailed model fitting information. You can specify the following *detail-options*:

BASES

displays the “Bases Information” table.

BWDSUMMARY

displays the “Backward Selection Summary” table.

FWDSUMMARY

displays the “Forward Selection Summary” table.

FWDPARAMS

displays the “Forward Selection Parameter Estimates” table.

If you do not specify a *detail-option*, PROC ADAPTIVEREG produces all the preceding tables by default.

NAMELEN=number

specifies the length to which long effect names are shortened. The default and minimum value is 20.

NLOPTIONS(options)

specifies options for the nonlinear optimization methods if you are applying the multivariate adaptive regression splines algorithm to generalized linear models. You can specify the following *options*:

ABSCONV=r**ABSTOL=r**

specifies an absolute function convergence criterion by which minimization stops when $f(\boldsymbol{\psi}^{(k)}) \leq r$, where $\boldsymbol{\psi}$ is the vector of parameters in the optimization and $f(\cdot)$ is the objective function. The default value of r is the negative square root of the largest double-precision value, which serves only as a protection against overflows.

ABSFCONV=r**ABSFTOL=r**

specifies an absolute function difference convergence criterion. For all techniques except NMSIMP, termination requires a small change of the function value in successive iterations,

$$|f(\boldsymbol{\psi}^{(k-1)}) - f(\boldsymbol{\psi}^{(k)})| \leq r$$

where $\boldsymbol{\psi}$ denotes the vector of parameters that participate in the optimization and $f(\cdot)$ is the objective function. The same formula is used for the NMSIMP technique, but $\boldsymbol{\psi}^{(k)}$ is defined as the vertex with the lowest function value, and $\boldsymbol{\psi}^{(k-1)}$ is defined as the vertex with the highest function value in the simplex. The default value is $r=0$.

ABSGCONV=r**ABSGTOL=r**

specifies an absolute gradient convergence criterion. Termination requires the maximum absolute gradient element to be small,

$$\max_j |g_j(\boldsymbol{\psi}^{(k)})| \leq r$$

where $\boldsymbol{\psi}$ denotes the vector of parameters that participate in the optimization and $g_j(\cdot)$ is the gradient of the objective function with respect to the j th parameter. This criterion is not used by the NMSIMP technique. The default value is $r = 1\text{E-}5$.

FCONV=r**FTOL=r**

specifies a relative function convergence criterion. For all techniques except NMSIMP, termination requires a small relative change of the function value in successive iterations,

$$\frac{|f(\boldsymbol{\psi}^{(k)}) - f(\boldsymbol{\psi}^{(k-1)})|}{|f(\boldsymbol{\psi}^{(k-1)})|} \leq r$$

where $\boldsymbol{\psi}$ denotes the vector of parameters that participate in the optimization and $f(\cdot)$ is the objective function. The same formula is used for the NMSIMP technique, but $\boldsymbol{\psi}^{(k)}$ is defined as the vertex with the lowest function value, and $\boldsymbol{\psi}^{(k-1)}$ is defined as the vertex with the highest function value in the simplex. The default is $r = 10^{-\text{FDIGITS}}$, where FDIGITS is by default $-\log_{10}\{\epsilon\}$ and ϵ is the machine precision.

GCONV=r**GTOL=r**

specifies a relative gradient convergence criterion. For all techniques except CONGRA and NMSIMP, termination requires the normalized predicted function reduction to be small,

$$\frac{\mathbf{g}(\boldsymbol{\psi}^{(k)})' [\mathbf{H}^{(k)}]^{-1} \mathbf{g}(\boldsymbol{\psi}^{(k)})}{|f(\boldsymbol{\psi}^{(k)})|} \leq r$$

where $\boldsymbol{\psi}$ denotes the vector of parameters that participate in the optimization, $f(\cdot)$ is the objective function, and $\mathbf{g}(\cdot)$ is the gradient. For the CONGRA technique (where a reliable Hessian estimate \mathbf{H} is not available), the following criterion is used:

$$\frac{\|\mathbf{g}(\boldsymbol{\psi}^{(k)})\|_2 \|\mathbf{s}(\boldsymbol{\psi}^{(k)})\|_2}{\|\mathbf{g}(\boldsymbol{\psi}^{(k)}) - \mathbf{g}(\boldsymbol{\psi}^{(k-1)})\|_2 |f(\boldsymbol{\psi}^{(k)})|} \leq r$$

This criterion is not used by the NMSIMP technique. The default value is $r = 1\text{E-}8$.

HESSIAN=hessian-options

specifies the Hessian matrix type used in the optimization of likelihood functions, if the Newton-Raphson technique is used. You can specify the following *hessian-options*:

EXPECTED

requests that the Hessian matrix in optimization be computed as the negative of the expected information matrix.

OBSERVED

requests that the Hessian matrix in optimization be computed as the negative of the observed information matrix. For many specified distribution families and link functions, the observed information matrix is equal to the expected information matrix.

The default is HESSIAN=EXPECTED.

MAXFUNC=*n***MAXFU=*n***

specifies the maximum number of function calls in the optimization process. The default values are as follows, depending on the optimization technique:

- TRUREG, NRRIDG, and NEWRAP: 125
- QUANEW and DBLDOG: 500
- CONGRA: 1000
- NMSIMP: 3000

The optimization can terminate only after completing a full iteration. Therefore, the number of function calls that are actually performed can exceed the number that is specified by this option. You can select the optimization technique by specifying the **TECHNIQUE=** option.

MAXITER=*n***MAXIT=*n***

specifies the maximum number of iterations in the optimization process. The default values are as follows, depending on the optimization technique:

- TRUREG, NRRIDG, and NEWRAP: 50
- QUANEW and DBLDOG: 200
- CONGRA: 400
- NMSIMP: 1000

These default values also apply when *n* is specified as a missing value. You can select the optimization technique by specifying the **TECHNIQUE=** option.

MAXTIME=*r*

specifies an upper limit of *r* seconds of CPU time for the optimization process. The default value is the largest floating-point double representation of your computer. The time that is specified by the **MAXTIME=** option is checked only once at the end of each iteration. Therefore, the actual running time can be longer than the time specified by this option.

MINITER=*n***MINIT=*n***

specifies the minimum number of iterations. The default value is 0. If you request more iterations than are actually needed for convergence to a stationary point, the optimization algorithms can behave strangely. For example, the effect of rounding errors can prevent the algorithm from continuing for the required number of iterations.

TECHNIQUE=*keyword*

specifies the optimization technique to obtain maximum likelihood estimates for nonnormal distributions. You can choose from the following techniques by specifying the appropriate *keyword*:

CONGRA	performs a conjugate-gradient optimization.
DBLDOG	performs a version of double-dogleg optimization.
NEWRAP	performs a Newton-Raphson optimization that combines a line-search algorithm with ridging.

NMSIMP	performs a Nelder-Mead simplex optimization.
NONE	performs no optimization.
NR RIDG	performs a Newton-Raphson optimization with ridging.
QUANEW	performs a dual quasi-Newton optimization.
TRUREG	performs a trust-region optimization.

The default is `TECHNIQUE=NEWRAP`.

For more information about these optimization methods, see the section “Choosing an Optimization Algorithm” on page 494 in Chapter 19, “Shared Concepts and Topics.”

NOTHEADS

forces single-threaded execution of the analytic computations. This overrides the SAS system option `THREADS | NOTHEADS`. Specifying this option is equivalent to specifying the `THREADS=1` option.

OUTDESIGN<(options)>=*SAS-data-set*

creates a data set that contains the design matrix of constructed basis functions. The design matrix column names consist of a prefix followed by an index. The default naming prefix is `_X`. The default output is the design matrix of basis functions after backward selection.

You can specify the following *options* in parentheses to control the content of the `OUTDESIGN=` data set:

BACKWARDMODEL | BACKWARD

produces the design matrix for the selected model after the backward selection.

FORWARDMODEL | FORWARD

produces the design matrix for the selected model after the forward selection.

PREFIX=*prefix*

requests that the design matrix column names consist of a prefix followed by an index.

STARTMODEL

produces the design matrix for the initial model specified in the `MODEL` statement.

PLOTS <(global-plot-options)> <=*plot-request* <(options)>>

PLOTS <(global-plot-options)> <=*(plot-request* <(options)> <... *plot-request* <(options)>>>

controls the plots produced through ODS Graphics. When you specify only one *plot-request*, you can omit the parentheses around the *plot-request*. For example:

```
plots=all
plots=components(unpack)
plots(unpack)=(components diagnostics)
```

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;

proc adaptivereg plots=all;
  model y=x1 x2;
run;

ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS](#).”

You can specify the following *global-plot-option*, which applies to all plots that the ADAPTIVEREG procedure generates:

UNPACK | UNPACKPANEL

suppresses paneling. By default, multiple plots can appear in some output panels. Specify UNPACK to get each plot individually. You can also specify UNPACK as a suboption with COMPONENTS and DIAGNOSTICS.

You can specify the following *plot-requests* and their options:

ALL

requests that all default plots be produced.

COMPONENTS <(component-options)>

plots a panel of functional components of the fitted model. You can specify the following *component-options*:

COMMONAXES

specifies that the functional component plots use a common vertical axis except for contour plots. This enables you to visually judge relative effect size.

UNPACK | UNPACKPANEL

displays the component plots individually.

DIAGNOSTICS <(UNPACK | UNPACKPANEL)>

produces a summary panel of fit diagnostics that consists of the following:

- residuals versus the predicted values
- a histogram of the residuals
- a normal quantile plot of the residuals
- a residual-fit (RF) plot that consists of side-by-side quantile plots of the centered fit and the residuals
- response values versus the predicted values

You can request the five plots in this panel as individual plots by specifying the UNPACK suboption. The fit diagnostics panel is not produced for dependent variable with nonnormal distributions.

FIT <(NODATA | NOOBS)>

produces a plot of the predicted values against the variables that form the selected model. By default, a scatter plot of the input data is overlaid. You can suppress the scatter plot by specifying the NODATA | NOOBS option.

The plot is not produced if the number of variables in the selected model exceeds two. The plot is not produced for dependent variables with nonnormal distributions.

NONE

suppresses all plots.

SELECTION<(selection-panel-options)>

plots a panel of model fit criteria. The panel consists of two plots. The upper plot shows the progression of the model lack-of-fit criterion as the selection process proceeds. The lower plot shows the progression of the model validation criterion as the selection process proceeds. By default, the selection panel shows the progression for the backward selection process. You can specify the following *selection-panel-options*:

BACKWARDMODEL | BACKWARD

displays the progression of model fit criteria for the backward selection process.

FORWARDMODEL | FORWARD

displays the progression of model fit criteria for the forward selection process.

SEED=number

specifies an integer used to start the pseudorandom number generator for random cross validation and random partitioning of data for training, testing, and validation. If you do not specify a seed, or if you specify a value less than or equal to 0, the seed is generated from the time of day, which is read from the computer's clock.

SINGULAR=number**EPSILON=number**

sets the tolerance for testing singularity of the $X'WX$ matrix that is formed from the design matrix X . Roughly, the test requires that a pivot be at least this number times the original diagonal value. By default, *number* is 10^7 times the machine epsilon. The default *number* is approximately 10^{-9} on most machines.

TESTDATA=SAS-data-set

names a SAS data set that contains test data. This data set must contain all the variables specified in the MODEL statement. Furthermore, when a BY statement is used and the TESTDATA=data set contains any of the BY variables, then the TESTDATA= data set must also contain all the BY variables sorted in the order of the BY variables. In this case, only the test data for a specific BY group are used with the corresponding BY group in the analysis data. If the TESTDATA= data set contains none of the BY variables, then the entire TESTDATA = data set is used with each BY group of the analysis data.

If you specify a TESTDATA= data set, then you cannot also specify a PARTITION statement to reserve observations for testing.

THREADS=*n*

specifies the number of threads for analytic computations and overrides the SAS system option `THREADS` | `NOTHREADS`. If you do not specify the `THREADS=` option or if you specify `THREADS=0`, the number of threads is determined based on the data size and the number of CPUs on the host on which the analytic computations execute. If the specified number of threads is more than the number of actual CPUs, PROC ADAPTIVEREG by default sets the value to the number of actual CPUs.

VALDATA=*SAS-data-set*

names a SAS data set that contains validation data. This data set must contain all the variables specified in the `MODEL` statement. Furthermore, when a `BY` statement is used and the `VALDATA=` data set contains any of the `BY` variables, then the `VALDATA=` data set must also contain all the `BY` variables sorted in the order of the `BY` variables. In this case, only the validation data for a specific `BY` group are used with the corresponding `BY` group in the analysis data. If the `VALDATA=` data set contains none of the `BY` variables, then the entire `VALDATA =` data set is used with each `BY` group of the analysis data.

If you specify a `VALDATA=` data set, then you cannot also specify a `PARTITION` statement to reserve observations for validation.

BY Statement

BY variables ;

You can specify a `BY` statement with PROC ADAPTIVEREG to obtain separate analyses of observations in groups that are defined by the `BY` variables. When a `BY` statement appears, the procedure expects the input data set to be sorted in order of the `BY` variables. If you specify more than one `BY` statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the `SORT` procedure with a similar `BY` statement.
- Specify the `NOTSORTED` or `DESCENDING` option in the `BY` statement for the ADAPTIVEREG procedure. The `NOTSORTED` option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the `BY` variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the `BY` variables by using the `DATASETS` procedure (in Base SAS software).

For more information about `BY`-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the `DATASETS` procedure, see the discussion in the *Base SAS Procedures Guide*.

CLASS Statement

CLASS *variables* </ options > ;

The CLASS statement names the classification *variables* to be used in the analysis. Typical class variables are Treatment, Sex, Race, Group, and Replication. If the CLASS statement is used, it must appear before the MODEL statement.

Classification variables can be either character or numeric. Class levels are determined from the formatted values of the *variables*. Thus, you can use formats to group values into levels. See the discussion of the FORMAT procedure in the *Base SAS Procedures Guide* and the discussions of the FORMAT statement and SAS formats in *SAS Formats and Informats: Reference*.

You can specify the following *options* for classification *variables*:

DESCENDING

DESC

reverses the sort order of the classification variable. If you specify both the DESCENDING and ORDER= options, PROC ADAPTIVEREG orders the categories according to the ORDER= option and then reverses that order.

ORDER=*order-type*

specifies the sort order for the categories of categorical variables. This ordering determines which parameters in the model correspond to each level in the data. When the default ORDER=FORMATTED is in effect for numeric variables for which you have supplied no explicit format, the levels are ordered by their internal values. Table 24.2 shows how PROC ADAPTIVEREG interprets values of the ORDER= option.

Table 24.2 Sort Order for Categorical Variables

<i>order-type</i>	Levels Sorted By
DATA	Order of appearance in the input data set
FORMATTED	External formatted value, except for numeric variables with no explicit format, which are sorted by their unformatted (internal) value
FREQ	Descending frequency count; levels with the most observations come first in the order
FREQDATA	Order of descending frequency count, and within counts by order of appearance in the input data set when counts are tied
FREQFORMATTED	Order of descending frequency count, and within counts by formatted value (as above) when counts are tied
FREQINTERNAL	Order of descending frequency count, and within counts by unformatted value when counts are tied
INTERNAL	Unformatted value

For the FORMATTED and INTERNAL values, the sort order is machine-dependent. If you specify the ORDER= option in the MODEL statement and the ORDER= option in the CLASS statement, the former takes precedence.

For more information about sort order, see the chapter on the SORT procedure in the *Base SAS Procedures Guide* and the discussion of BY-group processing in *SAS Language Reference: Concepts*.

FREQ Statement

FREQ *variable* ;

The FREQ statement names a variable that provides frequencies for each observation in the DATA= data set. Specifically, if n is the value of the FREQ variable for a given observation, then that observation is used n times.

The analysis produced using a FREQ statement reflects the expanded number of observations. You can produce the same analysis without the FREQ statement by first creating a new data set that contains the expanded number of observations. For example, if the value of the FREQ variable is 5 for the first observation, the first five observations in the new data set are identical. Each observation in the old data set is replicated n_i times in the new data set, where n_i is the value of the FREQ variable for that observation.

If the value of the FREQ variable is missing or is less than 1, the observation is not used in the analysis. If the value is not an integer, only the integer portion is used.

MODEL Statement

MODEL *dependent* < *options* > = < *effects* > < / *options* > ;

MODEL *events/trials* = < *effects* > < / *options* > ;

The MODEL statement names the response variable and the explanatory effects, including covariates, main effects, interactions, and nested effects; see the section “[Specification of Effects](#)” on page 3324 for more information. If you omit the explanatory effects, the procedure fits an intercept-only model. You must specify exactly one MODEL statement.

You can specify two forms of the MODEL statement. The first form, referred to as *single-trial* syntax, is applicable to binary, ordinal, and nominal response data. The second form, referred to as *events/trials* syntax, is restricted to binary response data. You use the *single-trial* syntax when each observation in the DATA= data set contains information about only a single trial, such as a single subject in an experiment. When each observation contains information about multiple binary response trials, such as the counts of the number of observed subjects and the number of subjects who respond, then you can use the *events/trials* syntax.

In the *events/trials* syntax, you specify two variables that contain count data for a binomial experiment. These two variables are separated by a slash. The value of the first variable, *events*, is the number of positive responses (or events). The value of the second variable, *trials*, is the number of trials. The values of both *events* and (*trials*–*events*) must be nonnegative and the value of *trials* must be positive for the response to be valid.

In the single-trial syntax, you specify one variable (on the left side of the equal sign) as the response variable. This variable can be character or numeric. You can specify variable options specific to the response variable immediately after the response variable with parentheses around them.

For both forms of the MODEL statement, explanatory *effects* follow the equal sign. Variables can be either continuous or classification variables. Classification variables can be character or numeric, and they must be declared in the CLASS statement. When an *effect* is a classification variable, the procedure inserts a set of coded columns into the design matrix instead of directly entering a single column that contains the values of the variable.

Table 24.3 summarizes the *options* available in the MODEL statement.

Table 24.3 MODEL Statement Options

Option	Description
Response Variable Options	
DESCENDING	Reverses the order of the response categories
EVENT=	Specifies the event category for the binary response
ORDER=	Specifies the sort order for the categorical response
REFERENCE=	Specifies the reference category for the categorical response
Statistical Modeling Options	
ADDITIVE	Requests an additive model
ALPHA	Controls the knot selection
CVMETHOD=	Specifies how subsets for cross validation are formed
DFPERBASIS	Specifies degrees of freedom per basis function
DIST=	Specifies the distribution family
FAST	Controls the fast-forward selection algorithm
FORWARDONLY	Requests that the backward selection process be skipped
KEEP=	Specifies effects to be included in the final model
LINEAR=	Specifies linear effects to be examined in model selection
LINK=	Specifies the link function
MAXBASIS=	Specifies the maximum number of basis functions allowed
MAXORDER=	Specifies the maximum order of interactions allowed
NOMISS	Requests removal of missing values from modeling
OFFSET=	Specifies an offset for the linear predictor
VARPENALTY=	Specifies the penalty for variable reentry

You can specify the following *options* in the MODEL statement.

Response Variable Options

Response variable options determine how the ADAPTIVEREG procedure models probabilities for binary data. You can specify the following response variable options by enclosing them in parentheses after the response variable.

DESCENDING

DESC

reverses the order of the response categories. If both the DESCENDING and ORDER= options are specified, PROC ADAPTIVEREG orders the response categories according to the ORDER= option and then reverses that order.

EVENT='category' | FIRST | LAST

specifies the event category for the binary response model. PROC ADAPTIVEREG models the probability of the event category. You can specify one of the following values for this option:

'category' specifies the formatted value of the reference category.

FIRST designates the first ordered category as the event.

LAST designates the last ordered category as the event.

The default is `EVENT=FIRST`.

One of the most common sets of response levels is $\{0, 1\}$, with 1 representing the event for which the probability is to be modeled. Consider the example where Y takes the value 1 for event and 0 for nonevent, and X is the explanatory variable. To specify the value 1 as the event category, use the following MODEL statement:

```
model Y (event='1') = X;
```

ORDER=order-type

specifies the sort order for the categories of categorical variables. This ordering determines which parameters in the model correspond to each level in the data. When the default `ORDER=FORMATTED` is in effect for numeric variables for which you have supplied no explicit format, the levels are ordered by their internal values. Table 24.4 shows how PROC ADAPTIVEREG interprets values of the `ORDER=` option.

Table 24.4 Sort Order for Categorical Variables

<i>order-type</i>	Levels Sorted By
DATA	Order of appearance in the input data set
FORMATTED	External formatted value, except for numeric variables with no explicit format, which are sorted by their unformatted (internal) value
FREQ	Descending frequency count; levels with the most observations come first in the order
FREQDATA	Order of descending frequency count, and within counts by order of appearance in the input data set when counts are tied
FREQFORMATTED	Order of descending frequency count, and within counts by formatted value (as above) when counts are tied
FREQINTERNAL	Order of descending frequency count, and within counts by unformatted value when counts are tied
INTERNAL	Unformatted value

For the `FORMATTED` and `INTERNAL` values, the sort order is machine-dependent. If you specify the `ORDER=` option in the MODEL statement and the `ORDER=` option in the CLASS statement, the former takes precedence.

For more information about sort order, see the chapter on the SORT procedure in the *Base SAS Procedures Guide* and the discussion of BY-group processing in *SAS Language Reference: Concepts*.

REFERENCE='category' | FIRST | LAST

REF='category' | FIRST | LAST

specifies the reference category for the binary or multinomial response model. For the binary response model, specifying one response category as the reference is the same as specifying the other response category as the event category. You can specify one of the following values for this option:

- ‘*category*’ specifies the formatted value of the reference category.
- FIRST** designates the first ordered category as the reference.
- LAST** designates the last ordered category as the reference.

The default is REFERENCE=LAST.

Model Options

You can specify the following model *options*.

ADDITIVE

requests an additive model for which only main effects are included in the fitted model. If you do not specify the ADDITIVE option, PROC ADAPTIVEREG fits a model that has both main effects and two-way interaction terms.

ALPHA=*number*

specifies the parameter that controls the number of knots considered for each variable. Friedman (1991b) uses the following as the number of observations between interior knots:

$$-\frac{2}{5} \log_2 \left[-\frac{\log(1 - \alpha)}{pn_m} \right]$$

Friedman also uses the following as the number of observations between extreme knots and the corresponding variable boundary values,

$$3 - \log_2 \frac{\alpha}{p}$$

where p is the number of variables and n_m is the number of observations for which a parent basis $B_m > 0$. The value of α should be greater than 0 and less than 1. The default is ALPHA=0.05.

CVMETHOD=RANDOM <(*n*)>

CVMETHOD=INDEX (*variable*)

specifies the method for subdividing the training data into n parts when you request n -fold cross validation when you do backward selection. CVMETHOD=RANDOM assigns each training observation randomly to one of the n parts. CVMETHOD=INDEX(*variable*) assigns observations to parts based on the formatted value of the named *variable*. This input data set variable is treated as a classification variable, and the number of parts n is the number of distinct levels of this variable. By optionally naming this variable in a CLASS statement, you can use the ORDER= option in the CLASS statement to control how this variable is leveled.

The value of n defaults to 5 with CVMETHOD=RANDOM.

DFPERBASIS=*d*

DF=*d*

specifies the degrees of freedom (d) that are “charged” for each basis function that is used in the lack-of-fit function for backward selection. Larger values of d lead to fewer spline knots and thus smoother function estimates. The default is DFPERBASIS=2.

DIST=*distribution-id*

specifies the distribution family used in the model.

If you do not specify a *distribution-id*, the ADAPTIVEREG procedure defaults to the normal distribution for continuous response variables and to the binary distribution for classification or character variables, unless the *events/trial* syntax is used in the MODEL statement. If you choose the *events/trial* syntax, the ADAPTIVEREG procedure defaults to the binomial distribution.

Table 24.5 lists the values of the DIST= option and the corresponding default link functions. For generalized linear models with these distributions, you can find expressions for the log-likelihood functions in the section “Log-Likelihood Functions” on page 2802.

Table 24.5 Values of the DIST= Option

<i>distribution-id</i>	Aliases	Distribution	Default Link Function
BINOMIAL		Binomial	Logit
GAMMA	GAM, G	Gamma	Reciprocal
GAUSSIAN	NORMAL, N, NOR	Normal	Identity
IGAUSSIAN	IG	Inverse Gaussian	Inverse squared (power(-2))
NEGBIN	NB	Negative binomial	Log
POISSON	POI	Poisson	Log

FAST< (*fast-options*) >

improves the speed of the modeling. Because of the computation complexity in the original multivariate adaptive regression splines algorithm, Friedman (1993) proposes modifications to improve the speed by tuning several parameters. See the section “Fast Algorithm” on page 874 for more information about the improvement of the multivariate adaptive regression splines algorithm. You can specify the following *fast-options*:

BETA=*beta*

specifies the “aging” factor in the priority queue of candidate parent bases. Larger values of *beta* result in low-improvement parents rising fast into top list of candidates. The default value is BETA=1.

H=*h*

specifies the parameter that controls how often the improvement is recomputed for a parent basis B_m over all candidate variables. Larger values of *h* cause fewer computations of improvement. The default value is H=1.

K=*k*

specifies the number of top candidates in the priority queue of parent bases for selecting new bases. Larger values of *k* cause more parent bases to be considered. The default is to use all eligible parent bases at every iteration.

FORWARDONLY

skips the backward selection step after forward selection is finished.

KEEP=effects

specifies a list of variables to be included in the final model.

LINEAR=effects

specifies a list of variables to be considered without nonparametric transformation. They should appear in the linear form if they are selected.

LINK=keyword

specifies the link function in the model. Not all link functions are available for all distribution families. The *keywords* and expressions for the associated link functions are shown in Table 24.6.

Table 24.6 Link Functions in MODEL Statement of the ADAPTIVEREG Procedure

<i>keyword</i>	Alias	Link Function	$g(\mu) = \eta =$
CLOGLOG	CLL	Complementary log-log	$\log(-\log(1 - \mu))$
IDENTITY	ID	Identity	μ
LOG		Log	$\log(\mu)$
LOGIT		Logit	$\log(\mu/(1 - \mu))$
POWERMINUS2		Power with exponent -2	$1/\mu^2$
PROBIT	NORMIT	Probit	$\Phi^{-1}(\mu)$
RECIPROCAL	INVERSE	Reciprocal	$1/\mu$

MAXBASIS=number

specifies the maximum number of basis functions (M_{\max}) that can be used in the final model. The default value is the larger value between 21 and one plus two times the number of nonintercept effects specified in the MODEL statement.

MAXORDER=number

specifies the maximum interaction levels for effects that could potentially enter the model. The default value is MAXORDER=2.

NOMISS

excludes all observations with missing values from the model fitting. By default, the ADAPTIVEREG procedure takes the missingness into account when an explanatory variable has missing values. For more information about how PROC ADAPTIVEREG handles missing values, see the section “Missing Values” on page 875.

OFFSET=variable

specifies an offset for the linear predictor. An offset plays the role of a predictor whose coefficient is known to be 1. For example, you can use an offset in a Poisson model when counts have been obtained in time intervals of different lengths. With a log link function, you can model the counts as Poisson variables with the logarithm of the time interval as the offset variable. The offset variable cannot appear in the CLASS statement or elsewhere in the MODEL statement.

VARPENALTY= γ

specifies the incremental penalty γ for increasing the number of variables in the adaptive regression model. To discourage a model with too many variables, at each iteration of the forward selection the model improvement is reduced by a factor of $(1 - \gamma)$ for any new variable that is introduced.

For highly collinear designs, the `VARPENALTY=` option helps PROC ADAPTIVEREG produce models that are nearly equivalent in terms of residual sum of squares but have fewer independent variables. Friedman (1991b) suggests the following values for γ :

0.0	no penalty (default value)
0.05	moderate penalty
0.1	heavy penalty

The best value depends on the specific situation. Some experimenting with different values is usually required. You should use this option with care.

OUTPUT Statement

```
OUTPUT <OUT=SAS-data-set> <keyword <(keyword-options)> <=name>> ...
      <keyword <(keyword-options)> <=name>> ;
```

The OUTPUT statement creates a new SAS data set to contain diagnostic measures that are calculated for the selected model. If you do not specify a *keyword*, then the only diagnostic included is the predicted response.

All the variables in the original data set are included by the new data set, along with variables created in the OUTPUT statement. These new variables contain the values of a variety of statistics and diagnostic measures that are calculated for each observation in the data set. If you specify a BY statement, then a variable `_BY_` that indexes the BY groups is included. For each observation, the value of `_BY_` is the index of the BY group to which this observation belongs.

If you have requested n -fold cross validation, then a variable `_CVINDEX_` is included in the output data set. For each observation that is used for model training, the value of `_CVINDEX_` is i if that observation is omitted in forming the i th subset of the training data. See the `CVMETHOD=` for additional details. The value of `_CVINDEX_` is 0 for all observations in the input data set that are not used for model training.

If you have partitioned the input data by using a `PARTITION` statement, then a character variable `_ROLE_` is included in the output data set. For each observation the value of `_ROLE_` is as follows:

<u><code>_ROLE_</code></u>	<u>Observation Role</u>
TEST	Testing
TRAIN	Training
VALIDATE	Validation

If you want to create a permanent SAS data set, you must specify a two-level name. For more information about permanent SAS data sets, see *SAS Language Reference: Concepts*.

Details about the specifications in the OUTPUT statement follow.

keyword <(keyword-options)> <=name>

specifies the statistics to include in the output data set and optionally names the new variables that contain the statistics. You can use the *keyword-options* to control which type of a particular statistic to compute for generalized linear models. You can specify the following *keyword-options* for associated statistics:

ILINK	computes the prediction on the scale of the data $\hat{\mu} = g^{-1}(\hat{\eta})$.
RAW	requests the raw residual value $r = y - \hat{\eta}$.
PEARSON	requests the Pearson residual value $r = (y - \hat{\eta}) / \sqrt{V(\hat{\mu})}$.
DEVIANCE	requests the deviance residual value $r = \text{sign}(y - \hat{\mu}) \sqrt{\hat{d}^2}$.

You can specify a *keyword* for each desired statistic (see the following list of keywords), followed optionally by an equal sign, and a variable to contain the statistic.

If you specify *keyword=name*, the new variable that contains the requested statistic has the specified name. If you omit the optional *=name* after a *keyword*, then the new variable name is formed by default names.

You can specify the following *keywords* for the corresponding statistics:

PREDICTED | PRED | P requests predicted values. The default name is Pred.

RESIDUAL | RESID | R requests residuals, calculated as ACTUAL – PREDICTED. The default name is Resid.

OUT=SAS-data-set

specifies the name of the new data set to contain the diagnostic measures. If the OUT= option is omitted, the procedure uses the DATA*n* convention to name the output data set.

PARTITION Statement

PARTITION < options > ;

The PARTITION statement specifies how observations in the input data set are logically partitioned into disjoint subsets for model training, validation, and testing. Either you can designate a variable in the input data set and a set of formatted values of that variable to determine the role of each observation, or you can specify proportions to use for random assignment of observations for each role.

An alternative to using a PARTITION statement is to provide a variable named `_ROLE_` in the input data set to define roles of observations in the input data. If you specify a PARTITION statement, then the `_ROLE_` variable is ignored if it is present in the input data set. If you do not specify a PARTITION statement and the input data do not contain a variable named `_ROLE_`, then all observations in the input data set are assigned to model training.

You can specify the following mutually exclusive *options*:

ROLEVAR=*variable* (< **TEST=**'value' > < **TRAIN=**'value' > < **VALIDATE=**'value' >)

ROLE=*variable* (< **TEST=**'value' > < **TRAIN=**'value' > < **VALIDATE=**'value' >)

names the *variable* in the input data set whose values are used to assign roles to each observation. The formatted values of this variable that are used to assign observations roles are specified in the TEST=, TRAIN=, and VALIDATE= suboptions. If you do not specify the TRAIN= suboption, then all observations whose role is not determined by the TEST= or VALIDATE= suboptions are assigned to training. If you specify a TESTDATA= data set in the PROC ADAPTIVEREG statement, then you cannot also specify the TEST= suboption in the PARTITION statement. If you specify a VALDATA= data set in the PROC ADAPTIVEREG statement, then you cannot also specify the VALIDATE= suboption in the PARTITION statement.

FRACTION(**< TEST=fraction >** **< VALIDATE=fraction >**)

randomly assigns training and validation roles to the observations in the input data according to the proportions that are specified by the fraction values in the TEST= and VALIDATE= suboptions. If you specify both the TEST= and VALIDATE= suboptions, then the sum of the specified fractions must be less than 1 and the remaining fraction of the observations are assigned to the training role. If you specify a TESTDATA= data set in the PROC ADAPTIVEREG statement, then you cannot also specify the TEST= suboption in the PARTITION statement. If you specify a VALDATA= data set in the PROC ADAPTIVEREG statement, then you cannot also specify the VALIDATE= suboption in the PARTITION statement.

SCORE Statement

SCORE **< DATA=SAS-data-set >** **< OUT=SAS-data-set >**
< keyword < =name > > . . . < keyword < =name > > ;

The SCORE statement creates a new SAS data set to contain predicted values and optionally residuals for data in a new data set that you name. If you do not specify a DATA= data set, then the input data are scored. If you want to predict multiple data sets, you can specify multiple SCORE statements. If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*.

When you specify a BY statement, the DATA= data set must either contain all the BY variables sorted in the order of the BY variables or contain none of the BY variables. If the DATA= data set contains all the BY variables, then the model that is selected for a given BY group is used to score just the matching observations in that data set. If the DATA= set contains none of the BY variables, then the entire data set is scored for each BY group.

All observations in the DATA= data set are retained in the output data set. All the variables in the input data set are included in the output data set, along with variables that contain predicted values and optionally residuals.

You can specify the following arguments in the SCORE statement:

DATA=SAS data set

names the data set to be scored. If you omit this option, then the input data set that is named in the DATA= option in the PROC ADAPTIVEREG statement is scored.

keyword < =name >

specifies the statistics to include in the output data set and optionally names the new variables that contain the statistics. Specify one of the following *keyword* for each desired statistic, followed optionally by an equal sign, and a variable to contain the statistic.

If you specify *keyword=name*, the new variable that contains the requested statistic has the specified name. If you omit the optional *=name* after a *keyword*, then the new variable name is formed by using a prefix of one or more characters that identify the statistic, followed by an underscore (_), followed by the dependent variable name.

You can specify the following keywords, which represent the statistics shown:

PREDICTED PRED P	includes predicted values in the output data set. The prefix for the default name is Pred.
RESIDUAL RESID R	includes residuals (which are calculated as ACTUAL – PREDICTED), in the output data set. The prefix for the default name is Resid.

OUT=SAS data set

specifies the name of the new output data set. By default, PROC ADAPTIVEREG uses the DATA n convention to name the new data set.

WEIGHT Statement

WEIGHT *variable* ;

When you specify a WEIGHT statement, each observation in the input data set is weighted by the value of *variable*. The value of *variable* can be nonintegral. Observations that have a negative, zero, or missing value for the WEIGHT variable are not used in model fitting.

Details: ADAPTIVEREG Procedure

Fitting Algorithms

The multivariate adaptive regression splines algorithm (Friedman 1991b) is a predictive modeling algorithm that combines nonparametric variable transformations with a recursive partitioning scheme.

The algorithm originates with Smith (1982), who proposes a nonparametric method that applies the model selection method (stepwise regression) to a large number of truncated power spline functions, which are evaluated at different knot values. This method constructs spline functions and selects relevant knot values automatically with the model selection method. However, the method is applicable only to problems in low dimensions. For multiple variables, the number of tensor products between spline basis functions is too large to fit even a single model. The multivariate adaptive regression splines algorithm avoids this situation by using forward selection to build the model gradually instead of using the full set of tensor products of spline basis functions.

Like the recursive partitioning algorithm, which has “growing” and “pruning” steps, the multivariate adaptive regression splines algorithm contains two stages: forward selection and backward selection. During the forward selection process, bases are created from interactions between existing parent bases and nonparametric transformations of continuous or classification variables as candidate effects. After the model grows to a certain size, the backward selection process begins by deleting selected bases. The deletion continues until the null model is reached, and then an overall the best model is chosen based on some goodness-of-fit criterion. The next three subsections give details about the selection process and methods of nonparametric transformation of variables. The fourth subsection describes how the multivariate adaptive regression splines algorithm is applied to fit generalized linear models. The fifth subsection describes the fast algorithm (Friedman 1993) for speeding up the fitting process.

Forward Selection

The forward selection process in the multivariate adaptive regression splines algorithm is as follows:

1. Initialize by setting $\mathbf{B}_0 = \mathbf{1}$ and $M = 1$.
2. Repeat the following steps until the maximum number of bases M_{\max} has been reached or the model cannot be improved by any combination of \mathbf{B}_m , \mathbf{v} , and t .
 - a) Set the lack-of-fit criterion $\text{LOF}^* = \infty$.
 - b) For each selected basis: $\mathbf{B}_m, m \in \{0, \dots, M - 1\}$ do the following for each variable \mathbf{v} that \mathbf{B}_m does not consist of $\mathbf{v} \notin \{\mathbf{v}(k, m) | 1 \leq k \leq K_m\}$
 - i. For each knot value (or a subset of categories) t of $\mathbf{v} : t \in \{\mathbf{v} | \mathbf{B}_m > 0\}$, form a model with all currently selected bases $\sum_{i=0}^{M-1} \mathbf{B}_i$ and two new bases: $\mathbf{B}_m \mathbf{T}_1(\mathbf{v}, t)$ and $\mathbf{B}_m \mathbf{T}_2(\mathbf{v}, t)$.
 - ii. Compute the lack-of-fit criterion for the new model LOF.
 - iii. If $\text{LOF} < \text{LOF}^*$, then update $\text{LOF}^* = \text{LOF}$, $m^* = m$, $\mathbf{v}^* = \mathbf{v}$, and $t^* = t$.
 - c) Update the model by adding two bases that improve the most $\mathbf{B}_{m^*} \mathbf{T}_1(\mathbf{v}^*, t^*)$ and $\mathbf{B}_{m^*} \mathbf{T}_2(\mathbf{v}^*, t^*)$.
 - d) Set $M = M + 2$.

The essential part of each iteration is to search a combination of \mathbf{B}_m , \mathbf{v} , and t such that adding two corresponding bases most improve the model. The objective of the forward selection step is to build a model that overfits the data. The lack-of-fit criterion for linear models is usually the residual sum of squares (RSS).

Backward Selection

The backward selection process in the multivariate adaptive regression splines algorithm is as follows:

1. Initialize by setting the overall lack-of-fit criterion: $\text{LOF}^* = \infty$.
2. Repeat the following steps until the null model is reached. The final model is the best one that is found during the backward deletion process.
 - a) For a selected basis $\mathbf{B}_m, m \in \{1, \dots, M\}$:
 - i. Compute the lack-of-fit criterion, LOF, for a model that excludes \mathbf{B}_m .
 - ii. If $\text{LOF} < \text{LOF}^*$, save the model as the best one. Let $m^* = m$.
 - iii. Delete \mathbf{B}_{m^*} from the current model.
 - b) Set $M = M - 1$.

The objective of the backward selection is to “prune” back the overfitted model to find the best model that has good predictive performance. So the lack-of-fit criteria that characterize model loyalty to original data are not appropriate. Instead, the multivariate adaptive regression splines algorithm uses a quantity similar to the generalized cross validation criterion. See the section “[Goodness-of-Fit Criteria](#)” on page 873 for more information.

Variable Transformations

The type of transformation depends on the variable type:

- For a continuous variable, the transformation is a linear truncated power spline,

$$\mathbf{T}_1(\mathbf{v}, t) = (v - t)_+ = \begin{cases} v - t, & \text{if } v > t \\ 0, & \text{otherwise} \end{cases}$$

$$\mathbf{T}_2(\mathbf{v}, t) = [-(v - t)]_+ = \begin{cases} 0, & \text{if } v > t \\ t - v, & \text{otherwise} \end{cases}$$

where t is a knot value for variable \mathbf{v} and v is an observed value for \mathbf{v} . Instead of examining every unique value of \mathbf{v} , a series of knot values with a minimum span are used by assuming the smoothness of the underlying function. Friedman (1991b) uses the following formula to determine a reasonable number of counts between knots (span size). For interior knots, the span size is determined by

$$-\frac{2}{5} \log_2 \left[-\frac{\log(1 - \alpha)}{pn_m} \right]$$

For boundary knots, the span size is determined by

$$3 - \log_2 \frac{\alpha}{p}$$

where α is the parameter that controls the knot density, p is the number of variables, and n_m is the number of observations that a parent basis $\mathbf{B}_m > 0$.

- For a classification variable, the transformation is an indicator function,

$$\mathbf{T}_1(\mathbf{v}, t) = \begin{cases} 1, & \text{if } v \in \{c_1, \dots, c_t\} \\ 0, & \text{otherwise} \end{cases}$$

$$\mathbf{T}_2(\mathbf{v}, t) = \begin{cases} 0, & \text{if } v \in \{c_1, \dots, c_t\} \\ 1, & \text{otherwise} \end{cases}$$

where $\{c_1, \dots, c_t\}$ is a subset of all categories of variable \mathbf{v} . The smoothing is applied to categorical variables by assuming that subsets of categories tend to have similar properties, analogous to the assumption that a local neighborhood has close predictions for continuous variables.

If a categorical variable has k distinct categories, then there are a total of $2^{k-1} - 1$ possible subsets to consider. The computation cost is equal to all-subsets selection in regression, which is expensive for large k values. The multivariate adaptive regression splines algorithm use the stepwise selection method to select categories to form the subset $\{c_1, \dots, c_t\}$. The method is still greedy, but it reduces computation and still yields reasonable final models.

Goodness-of-Fit Criteria

Like other nonparametric regression procedures, the multivariate adaptive regression splines algorithm can yield complicated models that involve high-order interactions in which many knot values or subsets are considered. Besides the basis functions, both the forward selection and backward selection processes are also highly nonlinear. Because of the trade-off between bias and variance, the complicated models that contain many parameters tend to have low bias but high variance. To select models that achieve good prediction performance, Craven and Wahba (1979) propose the widely used generalized cross validation criterion (GCV),

$$\text{GCV} = \frac{1}{n} \sum_{i=1}^n \left(\frac{y_i - \hat{f}_i}{1 - \text{trace}(\mathbf{S})/n} \right)^2 = \frac{\text{RSS}}{n(1 - \text{trace}(\mathbf{S})/n)^2}$$

where y is the response, \hat{f} is an estimate of the underlying smooth function, and \mathbf{S} is the smoothing matrix such that $\hat{\mathbf{y}} = \mathbf{S}\mathbf{y}$. The effective degrees of freedom for the smoothing spline can be defined as $\text{trace}(\mathbf{S})$. In the multivariate adaptive regression splines algorithm, Friedman (1991b) uses a similar quantity as the lack-of-fit criterion,

$$\text{LOF} = \frac{\text{RSS}}{n(1 - (M + d(M - 1)/2)/n)^2}$$

where d is the degrees-of-freedom cost for each nonlinear basis function and M is total number of linearly independent bases in the model. Because any candidate model that is evaluated at each step of the multivariate adaptive regression splines algorithm is a linear model, M is actually the trace of the hat matrix. The only difference between the GCV criterion and the LOF criterion is the extra term $d(M - 1)$. The corresponding effective degrees of freedom is defined as $M + d(M - 1)/2$. The quantity d takes into account the extra nonlinearity in forming new bases, and it operates as a smoothing parameter. Larger values of d tend to result in smoother function estimates. Based on many practical experiments and some theoretic work (Owen 1991), Friedman suggests that the value of d is typically in the range of $[2, 4]$. For data that have complicated structures, the value of d could be much larger.

Alternatively, you can use the cross validation as the goodness-of-fit criterion or use a separate validation data set to select models and a separate testing data set to evaluate selected models.

Generalized Linear Models

Friedman (1991b) applies the multivariate adaptive regression splines algorithm to a logistic model by using the squared error loss between the response and inversely linked values in the goodness-of-fit criterion:

$$\sum_{i=1}^n \left(y_i - \frac{1}{1 + \exp(\mathbf{x}'\boldsymbol{\beta})} \right)^2$$

When a final model is obtained, the ordinary logistic model is fitted on selected bases. Some realizations of the multivariate adaptive regression splines algorithm ignore the distributional properties and derive model bases that are based on the least squares criterion. The reason to ignore the distributional properties or use least squares approximations is that examining the lack-of-fit criterion for each combination of \mathbf{B}_m , \mathbf{v} , and t is computationally formidable, because one generalized linear model fit involves multiple steps of weighted least squares. The ADAPTIVEREG procedure extends the multivariate adaptive regression splines algorithm to generalized linear models as suggested by Buja et al. (1991).

In the forward selection process, the ADAPTIVEREG procedure extends the algorithm in the following way. Suppose there are $(2k + 1)$ bases after the k th iteration. Then a generalized linear model is fitted against the data by using the selected bases. Then the weighted least squares method uses the working weights and working response in the last step of the iterative reweighted least squares algorithm as the weight and response for selecting new bases in the $(k + 1)$ th iteration. Then the residual chi-square statistic is used to select two new bases. This is similar to the forward selection scheme that the LOGISTIC procedure uses. For more information about the score chi-square statistic, see the section “Testing Individual Effects Not in the Model” on page 4247 in Chapter 54, “The LOGISTIC Procedure.”

In the backward selection process, the ADAPTIVEREG procedure extends the algorithm in the following way. Suppose there are M bases in the selected model. The Wald chi-square statistic is used to determine which basis to delete. After one basis is selected for deletion, a generalized linear model is refitted with the remaining bases. This is similar to the backward deletion scheme that the LOGISTIC procedure uses. For more information about the Wald chi-square statistic, see the section “Testing Linear Hypotheses about the Regression Coefficients” on page 4262 in Chapter 54, “The LOGISTIC Procedure.”

Accordingly, the lack-of-fit criterion in the forward selection for generalized linear models is the score chi-square statistic. For the lack-of-fit criterion in the backward selection process for generalized linear models, the residual sum of squares term is replaced by the model deviance.

Fast Algorithm

The original multivariate adaptive regression splines algorithm is computationally expensive. To improve the computation speed, Friedman (1993) proposes the fast algorithm. The essential idea of the fast algorithm is to reduce the number of combinations of \mathbf{B} , \mathbf{v} , and t that are examined at each step of forward selection.

Suppose there are $(2k + 1)$ bases that are formed after the k th iteration, where a parent basis \mathbf{B}_m is selected to construct two new bases. Consider a queue with bases as its elements. At the top of the queue are the two newly constructed bases, \mathbf{B}_{2k} and \mathbf{B}_{2k+1} . The rest of the queue is sorted based on the minimum lack-of-fit criterion for each basis:

$$J(\mathbf{B}_i) = \min_{\substack{\text{for all eligible } \mathbf{v} \\ \text{for all knot } t}} \text{LOF}(\mathbf{v}, t | \mathbf{B}_i), \quad i = 1, \dots, 2k - 1$$

When k is not small, there are a relatively large number of bases in the model, and adding more bases is unlikely to dramatically improve the fit. Thus the ranking of the bases in the priority queue is not likely to change much during adjacent iterations. So the candidate parent bases can be restricted to the top K ones in the queue for $(k + 1)$ th iteration. After the k th iteration, the top bases have new $J(\mathbf{B}_i)$ values, whereas the values of the bottom bases are unchanged. The queue is reordered based on $J(\mathbf{B}_i)$ values. This corresponds to the $\mathbf{K} =$ option value for the FAST option in the MODEL statement.

To avoid losing the candidate bases that are ranked at the bottom of the queue and to allow them to rise back to the top, a natural “aging” factor is introduced into each basis. This is accomplished by defining the priority for each basis function to be

$$P(\mathbf{B}_i) = R(\mathbf{B}_i) + \beta(k_c - k_r)$$

where $R(\mathbf{B}_i)$ is the rank of i th basis in the queue, k_c is the current iteration number, and k_r is the number of the iteration where the $J(\mathbf{B}_i)$ value was last computed. The top K candidate bases are then sorted again based on this priority. Large β values cause bases that have low improvement during previous iterations to rise faster to the top of the list. This corresponds to the $\mathbf{BETA} =$ value for the FAST option in the MODEL statement.

For a candidate basis in the top of the priority queue, the minimum lack-of-fit criterion $J(\mathbf{B}_i)$ is recomputed for all eligible variables \mathbf{v} for the $(k + 1)$ iteration. An optimal variable is likely to be the same as the one that was found during the previous iteration. So the fast multivariate adaptive regression splines algorithm introduces another factor H to save the computation cost. The factor specifies how often $J(\mathbf{B}_i)$ should be recomputed for all eligible variables. If $H = 1$, then optimization over all variables is done at each iteration when a parent basis is considered. If $H = 5$, the complete optimization is done after five iterations. For an iteration count less than the specified H , the optimization is done only for the optimal variable found in the last complete optimization. The only exceptions are the top three candidates, \mathbf{B}_{2k-1} (which is the parent basis \mathbf{B}_m used to construct two new bases) and two new ones, \mathbf{B}_{2k} and \mathbf{B}_{2k+1} . The complete optimization for them is performed at each iteration. This corresponds to the `H=` option value for the `FAST` option in the `MODEL` statement.

Missing Values

When fitting a model, the `ADAPTIVEREG` procedure excludes observations that have missing values for the response variable, weight variable, or frequency variable. It also excludes observations with invalid response, weight, or frequency values. For observations that have valid response, weight, and frequency values but missing predictor values, the `ADAPTIVEREG` procedure can either include them in model fitting or exclude them.

By default, observations with missing values in the predictor variables are included in the model fitting. Suppose a variable \mathbf{v} contains missing values. The `ADAPTIVEREG` procedure automatically forms two candidate bases, \mathbf{B}_m and \mathbf{B}_{m+1} , in the forward selection step when variable \mathbf{v} is considered. When \mathbf{v} is missing, $\mathbf{B}_{m+1} = I(\mathbf{v} \text{ is missing})$. When \mathbf{v} is not missing, $\mathbf{B}_m = I(\mathbf{v} \text{ is not missing})$. $I(\cdot)$ is a scalar-valued indicator function that returns a 1 when the argument is true and a 0 when the argument is false.

If the transformation of \mathbf{v} with a parent basis \mathbf{B}_i and a knot (or a subset) t turns out to be the best one during this iteration, then two more bases are added to the model:

$$\mathbf{B}_{m+2} = \mathbf{B}_i \mathbf{B}_m \mathbf{T}_1(\mathbf{v} - t)$$

$$\mathbf{B}_{m+3} = \mathbf{B}_i \mathbf{B}_{m+1} \mathbf{T}_2(\mathbf{v} - t)$$

The indicator function does not contribute to the interaction order of the constructed bases. This approach assumes that the missingness in the training data is representative of missingness in future data to be predicted.

Alternatively, you can specify the `NOMISS` option in the `MODEL` statement to exclude from the model fitting all observations that have missing values in the predictor variables.

ANOVA Decomposition

The model that is produced by the multivariate adaptive regression splines algorithm can be formed as

$$\begin{aligned} \hat{f}(\mathbf{x}) &= \beta_0 + \sum_{m=1}^M \beta_m \mathbf{B}_m \\ &= \beta_0 + \sum_{m=1}^M \beta_m \prod_{k=1}^{K_m} \mathbf{T}_m(\mathbf{x}_{k,m}, t_{k,m}) \end{aligned}$$

Here \hat{f} is the nonparametric estimate of the response variable in linear models and of the linked response variable in generalized linear models. M is the number of nonconstant bases. For each formed basis, K_m is the order of interaction, \mathbf{T}_m is the variable transformation function that depends on the variable type, $\mathbf{x}_{k,m}$ is variable for the k th component of the basis, and $t_{k,m}$ is the corresponding knot value or subset categories for the variable.

The function estimate can be recast into the form

$$\hat{f}(\mathbf{x}) = \beta_0 + \sum_{i:K_m=1} f_i(\mathbf{x}_i) + \sum_{i,j:K_m=2} f_{ij}(\mathbf{x}_i, \mathbf{x}_j) + \sum_{i,j,k:K_m=3} f_{ijk}(\mathbf{x}_i, \mathbf{x}_j, \mathbf{x}_k) + \dots$$

where f_i represents the sum of bases that involve a single variable \mathbf{x}_i , f_{ij} represents the sum of bases that involve two-way interactions between transformations of two variables, and so on. The univariate function f_i is a linear regression spline for variable \mathbf{x}_i , which represent the univariate contribution of \mathbf{x}_i to the model. Let

$$f_{ij}^* = f_i(\mathbf{x}_i) + f_j(\mathbf{x}_j) + f_{ij}(\mathbf{x}_i, \mathbf{x}_j)$$

Then this bivariate function is a tensor product regression spline that represents the joint contribution by both \mathbf{x}_i and \mathbf{x}_j . Multivariate functions can be formed similarly if higher-order interaction terms are present in the model. Because of its similarity to the analysis of variance for contingency tables, this is referred as the ANOVA decomposition of the multivariate adaptive regression splines model.

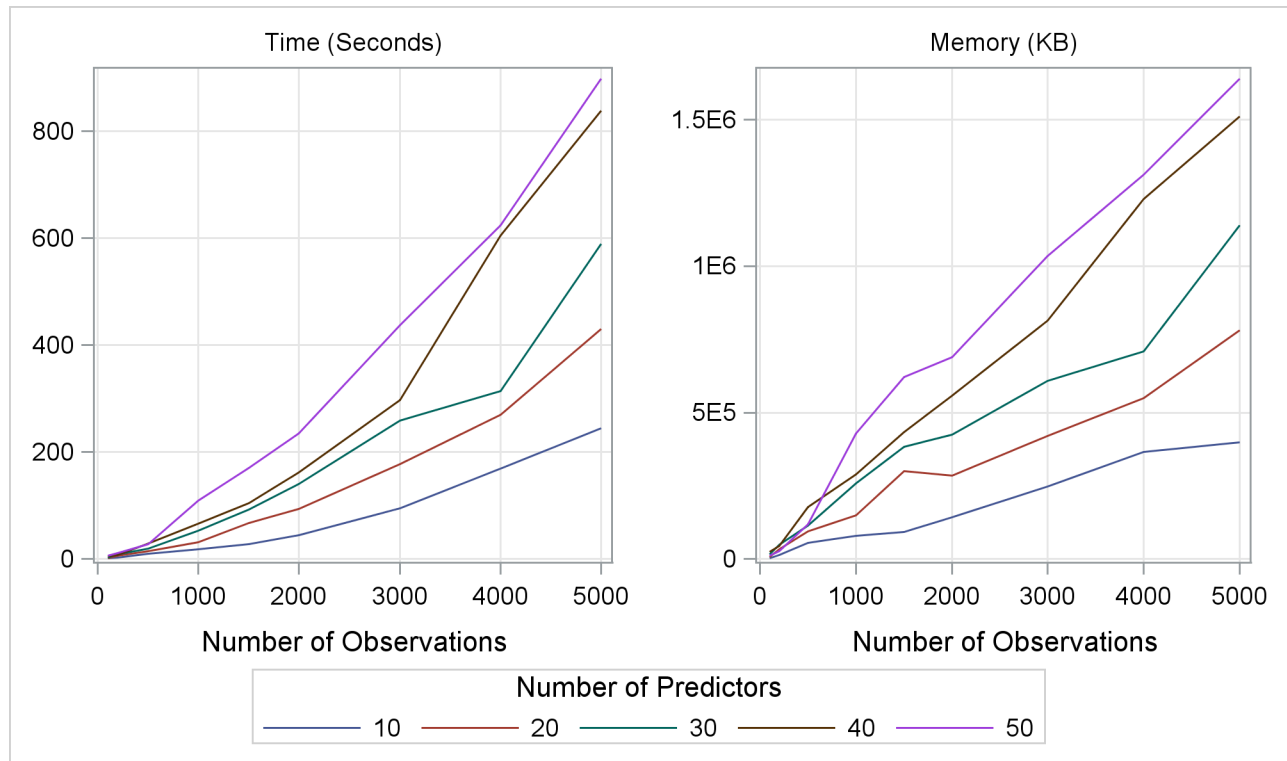
Computational Resources

The multivariate adaptive regression splines algorithm is computationally intensive and requires a significant amount of memory for large data sets. However, the core algorithm is fairly scalable, so you might expect performance improvement if you use multicore machines. You can even further improve the fitting speed by carefully tuning the parameters of the **FAST** option in the **MODEL** statement.

A general formula does not exist for predicting amount of memory that is required for PROC ADAPTIVEREG. The procedure uses logical utility files to store values that are associated with observations. If sufficient random access memory (RAM) is available, the utility files reside in RAM to allow fast access. Otherwise, the utility files are stored on hard drives, which have slower read/write speed.

Because of the model selection nature, the multivariate adaptive regression splines algorithm essentially fits a large number of candidate models with different sets of basis functions. The original prototype requires computation that is proportional to pNM_{\max}^4 . The implemented algorithm that takes advantage of the special structure of linear truncated power functions to reduce the computation to be proportional to pNM_{\max}^3 . With the fast algorithm, the computational can be reduced even further.

To provide a feel for how the number of variables and the number of observations affect the fitting performance, a series of simulations are carried out on a server with a 12-way 2.6GHz AMD Opteron processor and 32GB of RAM. Data sets are created in different sizes with the number of variables ranging from 10 to 50 and the number of observations ranging from 100 to 5,000. For each data set, the true model is the same as the one used in [Example 24.1](#). At each data size, the experiment is repeated three times to measure minimum running times and corresponding memory consumption. PROC ADAPTIVEREG sets the maximum number of basis function to 50 and uses all other default options. [Figure 24.10](#) displays the results of the simulations.

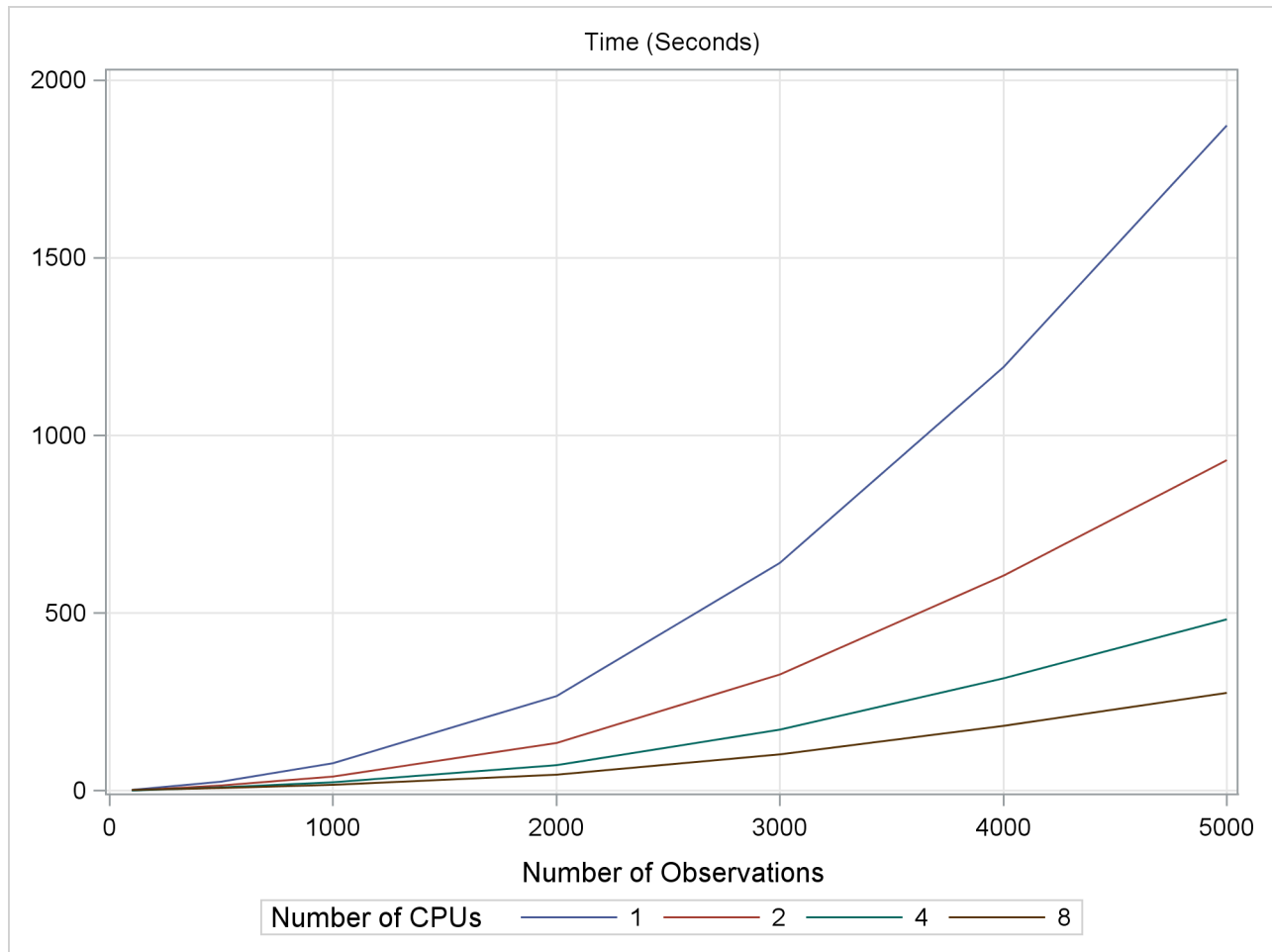
Figure 24.10 Time and Memory Used

The graphs in Figure 24.10 show that computational times grow with respect to the number of observations at a speed that is slightly faster than linear. The growth of the memory consumption is close to linear. Also, the increment with respect to number of variables is approximately in fixed ratios.

To show how PROC ADAPTIVEREG scales as the number of CPUs grows, another series of experiments is performed with the following settings. SAS DATA steps use the same mechanism as in previous simulations to generate data sets. The number of observations range from 100 to 5,000, and the number of variables is 10. PROC ADAPTIVEREG fits models to these data sets with the maximum number of basis functions set to 50. Each fitting uses four threading settings with 1, 2, 4, and 8 CPUs.

Figure 24.11 displays the simulation results. The computation times scale well with the number of CPUs. The more CPUs you have, the less time you need to fit a model by using PROC ADAPTIVEREG.

Figure 24.11 Time Used with Different Number of Threads



ODS Table Names

PROC ADAPTIVEREG assigns a name to each table that it creates. You can use these names to refer to the table when you use the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in Table 24.7. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

Table 24.7 ODS Tables Produced by PROC ADAPTIVEREG

ODS Table Name	Description	Statement	Option
ANOVA	ANOVA functional decomposition	PROC	Default
Bases	Bases transformation information	PROC	<code>DETAILS=BASES</code>
BWDParams	Parameter estimates after backward selection	PROC	Default
ClassInfo	Classification variable levels information	CLASS	Default
FitControls	Fit control parameters	PROC	Default

Table 24.7 *continued*

ODS Table Name	Description	Statement	Option
FitStatistics	Model fit statistics	PROC	Default
FWDPParams	Parameter estimates after forward selection	PROC	DETAILS=FWDPARAMS
FWDSummary	Forward selection summary	PROC	DETAILS=FWDSUMMARY
ModelInfo	Model information	PROC	Default
NObs	Number of observations	PROC	Default
SelectionSummary	Backward selection summary	PROC	DETAILS=BWDSUMMARY
VarImp	Variable importance information	PROC	Default

ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “[Statistical Graphics Using ODS](#).”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS](#).”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “[A Primer on ODS Statistical Graphics](#)” on page 599 in Chapter 21, “[Statistical Graphics Using ODS](#).”

You must also specify the PLOTS= option in the PROC ADAPTIVEREG statement.

PROC ADAPTIVEREG assigns a name to each graph that it creates using ODS. You can use these names to refer to the graphs when using ODS. The names are listed in [Table 24.8](#).

Table 24.8 Graphs Produced by PROC ADAPTIVEREG

ODS Graph Name	Plot Description	PLOTS Option
BoxPlot	Box plot of the response at each level of one categorical predictor, overlaid with a plot of predicted values	FIT
ComponentPanel	Panel of partial prediction curves for components that contain up to two predictors	COMPONENTS
ContourPlot	Contour plot of the fitted surface by two continuous predictors overlaid on scatter plot of data	FIT
DiagnosticPanel	Panel of fit diagnostics	DIAGNOSTICS
FitPlot	Plot of fitted values by single continuous predictor (or with one categorical variable) overlaid on scatter plot of data	FIT
IntPlot	Plot of fitted values by two categorical predictors overlaid on scatter plot of data	FIT
ObservedByPredicted	Dependent variable versus fitted values	DIAGNOSTICS(UNPACK)

Table 24.8 continued

ODS Graph Name	Plot Description	PLOTS Option
QQPlot	Normal quantile plot of residuals	DIAGNOSTICS(UNPACK)
ResidualByPredicted	Residuals versus fitted values	DIAGNOSTICS(UNPACK)
ResidualHistogram	Histogram of fit residuals	DIAGNOSTICS(UNPACK)
RFPlot	Side-by-side plots of quantiles of centered fit and residuals	DIAGNOSTICS(UNPACK)
SelectionPlot	Model fit criteria by step	SELECTION

Examples: ADAPTIVEREG Procedure

Example 24.1: Surface Fitting with Many Noisy Variables

This example shows how you can use PROC ADAPTIVEREG to fit a surface model from a data set that contains many nuisance variables.

Consider a simulated data set that contains a response variable and 10 continuous predictors. Each continuous predictor is sampled independently from the uniform distribution $U(0, 1)$. The true model is formed by x_1 and x_2 :

$$y = \frac{40 \exp(8((x_1 - 0.5)^2 + (x_2 - 0.5)^2))}{\exp(8((x_1 - 0.2)^2 + (x_2 - 0.7)^2)) + \exp(8((x_1 - 0.7)^2 + (x_2 - 0.2)^2))}$$

The values of the response variable are generated by adding errors from the standard normal distribution $N(0, 1)$ to the true model. The generating mechanism is adapted from Gu et al. (1990). There are 400 generated observations in all. The following statements create an artificial data set:

```
data artificial;
  drop i;
  array X{10};
  do i=1 to 400;
    do j=1 to 10;
      X{j} = ranuni(1);
    end;
    Y = 40*exp(8*((X1-0.5)**2+(X2-0.5)**2)) /
      (exp(8*((X1-0.2)**2+(X2-0.7)**2)) +
       exp(8*((X1-0.7)**2+(X2-0.2)**2)))+rannor(1);
  output;
end;
run;
```

The standard deviation for the response without noise is 3, whereas the standard deviation for the error term is 1. So the response variable Y has a signal-to-noise ratio of 3. When eight more variables are introduced, it is harder to search for the true model because of the extra variability that the nuisance variables create. The objective is to fit a nonparametric surface model that can well approximate the true model without experiencing much interference from the nuisance variables.

The following statements invoke the ADAPTIVEREG procedure to fit the model:

```
ods graphics on;

proc adaptivereg data=artificial plots=fit;
  model y=x1-x10;
run;
```

The `PLOTS=FIT` option in the PROC ADAPTIVEREG statement requests a fit plot. PROC ADAPTIVEREG might not produce the fit plot because the number of predictors in the final model is unknown. If the final model has no more than two variables, then the fit can be graphically presented.

PROC ADAPTIVEREG selects the two variables that form the true model (X_1 , X_2) and does not include other nuisance variables. The “Fit Statistics” table (Output 24.1.1) lists summary statistics of the fitted surface model. The model has 27 effective degrees of freedom and 14 basis functions formed by X_1 or X_2 or both. The fit statistics suggest that this is a reasonable fit.

Output 24.1.1 Fit Statistics

The ADAPTIVEREG Procedure	
Fit Statistics	
GCV	1.55656
GCV R-Square	0.86166
Effective Degrees of Freedom	27
R-Square	0.87910
Adjusted R-Square	0.87503
Mean Square Error	1.40260
Average Square Error	1.35351

Output 24.1.2 lists both parameter estimates and construction components (parent basis function, new variable, and optimal knot for the new variable) for the basis functions.

Output 24.1.2 Parameter Estimates

Regression Spline Model after Backward Selection				
Name	Coefficient	Parent	Variable	Knot
Basis0	12.3031		Intercept	
Basis1	13.1804	Basis0	X1	0.05982
Basis3	-23.4892	Basis0	X2	0.1387
Basis4	-171.03	Basis0	X2	0.1387
Basis5	-86.1867	Basis3	X1	0.6333
Basis7	-436.86	Basis4	X1	0.5488
Basis8	397.18	Basis4	X1	0.5488
Basis9	11.4682	Basis1	X2	0.6755
Basis10	-19.1796	Basis1	X2	0.6755
Basis13	126.84	Basis11	X1	0.6018
Basis14	40.8134	Basis11	X1	0.6018
Basis15	22.2884	Basis0	X1	0.7170
Basis17	-53.8746	Basis12	X1	0.2269
Basis19	598.89	Basis4	X1	0.2558

Output 24.1.3 shows all the ANOVA functional components that form the final model. The function estimate consists of two basis functions for each of X1 and X2 and nine bivariate functions of both variables. Because the true model contains the interaction between X1 and X2, PROC ADAPTIVEREG automatically selects many interaction terms.

Output 24.1.3 ANOVA Decomposition

ANOVA Decomposition				
Functional Component	Number of Bases	DF	---Change If Omitted---	Lack of Fit GCV
X1	2	4	405.18	1.1075
X2	2	4	947.87	2.6348
X2 X1	9	18	2583.21	6.6187

To compute predictions for the contour plot of the fitted model, you can use the `SCORE` statement. The following statements produce the graph that shows both the true model and the fitted model:

```

data score;
  do X1=0 to 1 by 0.01;
    do X2=0 to 1 by 0.01;
      Y=40*exp(8*((X1-0.5)**2+(X2-0.5)**2))/
        (exp(8*((X1-0.2)**2+(X2-0.7)**2))+
         exp(8*((X1-0.7)**2+(X2-0.2)**2)));
      output;
    end;
  end;
run;

proc adaptivereg data=artificial;
  model y=x1-x10;
  score data=score out=scoreout;
run;

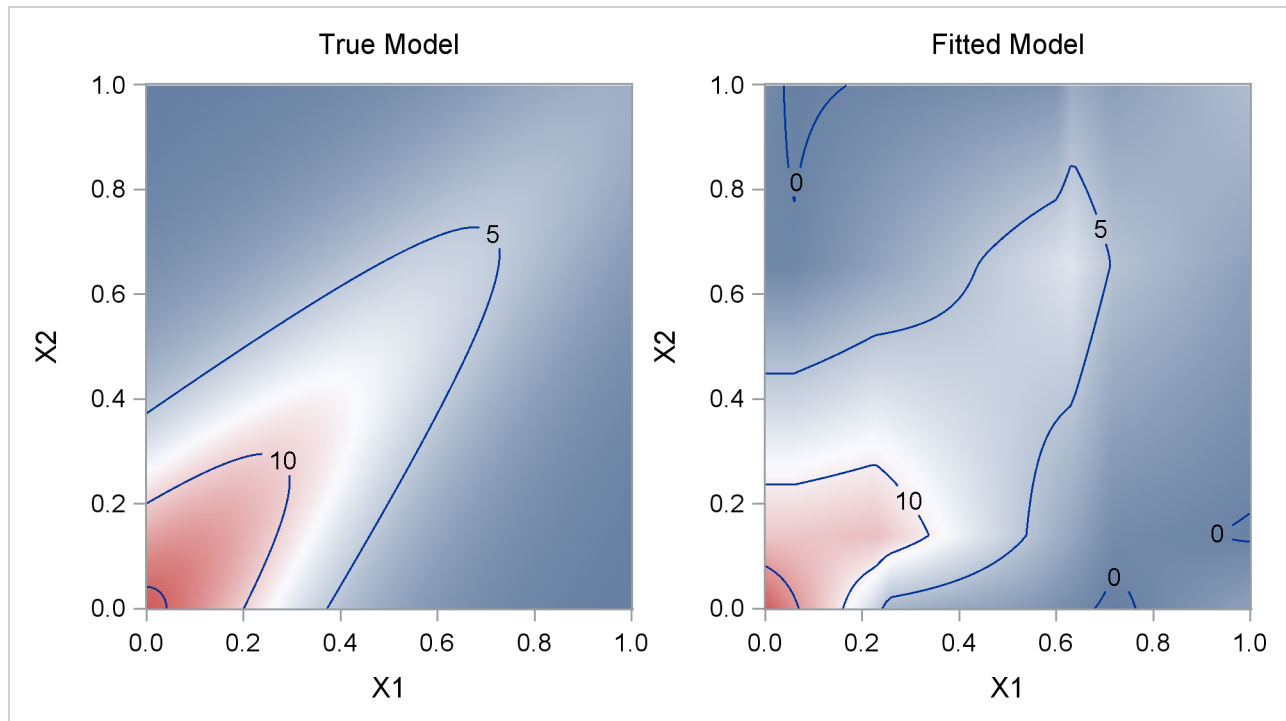
proc template;
  define statgraph surfaces;
    begingraph / designheight=360px;
    layout lattice/columns=2;
      layout overlay/xaxisopts=(offsetmin=0 offsetmax=0)
        yaxisopts=(offsetmin=0 offsetmax=0);
        entry "True Model" / location=outside valign=top
          textattrs=graphlabeltext;
        contourplotparm z=y y=x2 x=x1;
      endlayout;
      layout overlay/xaxisopts=(offsetmin=0 offsetmax=0)
        yaxisopts=(offsetmin=0 offsetmax=0);
        entry "Fitted Model" / location=outside valign=top
          textattrs=graphlabeltext;
        contourplotparm z=pred y=x2 x=x1;
      endlayout;
    endlayout;
  endgraph;
end;

proc sgrender data=scoreout template=surfaces;
run;

```

Output 24.1.4 displays surfaces for both the true model and the fitted model. The fitted model approximates the underlying true model well.

Output 24.1.4 True Model and Fitted Model



For high-dimensional data sets with complex underlying data-generating mechanisms, many different models can almost equally approximate the true mechanisms. Because of the sequential nature of the selection mechanism, any change in intermediate steps due to perturbations from local structures might yield completely different models. Therefore, PROC ADAPTIVEREG might find models that contain noisy variables. For example, if you change the random number seed in generating the data (as in the following statements), PROC ADAPTIVEREG might return different models with more variables. You can use the information from the variable importance table (Output 24.1.5) to aid further analysis.

```

data artificial;
  drop i;
  array x{10};
  do i=1 to 400;
    do j=1 to 10;
      x{j} = ranuni(12345);
    end;
    y = 40*exp(8*((x1-0.5)**2+(x2-0.5)**2)) /
      (exp(8*((x1-0.2)**2+(x2-0.7)**2)) +
       exp(8*((x1-0.7)**2+(x2-0.2)**2)))+rannor(1);
    output;
  end;
run;

proc adaptivereg data=artificial;
  model y=x1-x10;
run;

```

Output 24.1.5 shows that the variables X1 and X2 are two dominating factors for predicting the response, whereas the relative importance of the variable X8 compared to the other two is negligible. You might want to remove the variable if you fit a new model.

Output 24.1.5 Variable Importance

The ADAPTIVEREG Procedure		
Variable Importance		
Variable	Number of Bases	Importance
x1	13	100.00
x2	12	98.58
x8	2	0.22

Example 24.2: Fitting Data with Mixture Structures

This example shows how you can use PROC ADAPTIVEREG to fit a model from a data set that contains mixture structures. It also demonstrates how to use the CLASS statement.

Consider a simulated data set that contains a response variable and two predictors, one continuous and the other categorical. The continuous predictor is sampled from the uniform distribution $U(0, 1)$, and the classification variable is sampled from $U(0, 3)$ and then rounded to integers. The response variable is constructed from three different models that depend on the CLASS variable levels, with error sampled from the standard normal distribution.

$$y = \begin{cases} \exp(5(x - 0.3)^2), & \text{if } c = 0 \\ \log(x - x^2), & \text{if } c = 1 \\ 7x, & \text{if } c = 2 \end{cases}$$

The following statements create the artificial data set Mixture:

```
data Mixture;
  drop i;
  do i=1 to 1000;
    X1 = ranuni(1);
    C1 = int(3*ranuni(1));
    if C1=0 then Y=exp(5*(X1-0.3)**2)+rannor(1);
    else if C1=1 then Y=log(X1*(1-X1))+rannor(1);
    else Y=7*X1+rannor(1);
    output;
  end;
run;
```


The standard deviation for the response without noise is 3.14. So the response variable Y in the data set Mixture has a signal-to-noise ratio of 3.14. With a classification variable and a continuous variable in the data set, the objective is to fit a nonparametric model that can reveal the underlying three different data-generating processes. The following statements use the ADAPTIVEREG procedure to fit the data:

```
ods graphics on;
proc adaptivereg data=Mixture plots=fit;
  class c1;
  model y=c1 x1;
run;
```

Because the data contain two explanatory variables, graphical presentation of the fitted model is possible. The `PLOTS=FIT` option in the PROC ADAPTIVEREG statement requests the fit plot. The `CLASS` statement specifies that C1 is a classification variable.

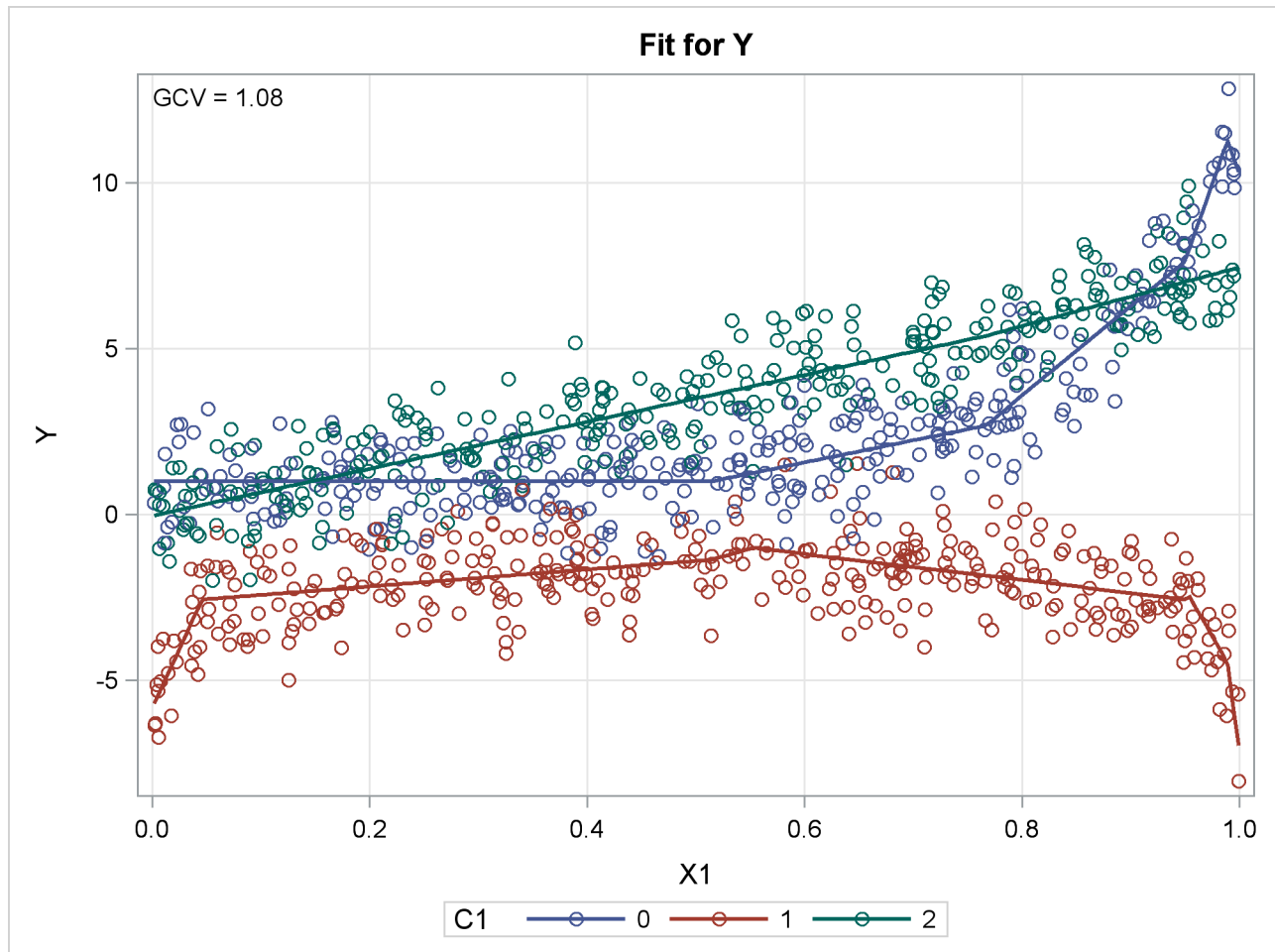
Output 24.2.1 displays the parameter estimates for the 13 selected basis functions after backward selection. For Basis1, the coefficient estimate is -4.3871. It is constructed from the intercept and the classification variable C1 at levels 0 and 1.

Output 24.2.1 Parameter Estimates

The ADAPTIVEREG Procedure					
Regression Spline Model after Backward Selection					
Name	Coefficient	Parent	Variable	Knot	Levels
Basis0	5.3829		Intercept		
Basis1	-4.3871	Basis0	C1		1 0
Basis3	32.7761	Basis0	C1		1
Basis5	20.2859	Basis4	X1	0.7665	
Basis7	-11.4183	Basis2	X1	0.7665	
Basis8	-7.0758	Basis2	X1	0.7665	
Basis9	58.4911	Basis3	X1	0.5531	
Basis10	-71.6388	Basis3	X1	0.5531	
Basis11	-69.0764	Basis3	X1	0.04580	
Basis13	-119.71	Basis3	X1	0.9526	
Basis15	66.5733	Basis1	X1	0.9499	
Basis17	6.6681	Basis1	X1	0.5143	
Basis19	-185.21	Basis1	X1	0.9890	

Output 24.2.2 displays the fitted linear splines overlaid with the original data. PROC ADAPTIVEREG captures the three underlying data-generating processes. For observations with C1 at level 0, the shape of the fitted splines is quite similar to the exponential function. For observations with C1 at level 1, the shape of the fitted spline suggests a symmetric function along X1 with a symmetry point approximately equal to 0.5. The function at each side of the symmetry point is analogous to the logarithmic transformation. For the rest of the observations with C1 at level 2, PROC ADAPTIVEREG suggests a strict linear model. The fitted model is very close to the true model. PROC ADAPTIVEREG fits the model in an automatic and adaptive way, except that it needs the `CLASS` statement to name the classification variable.

Output 24.2.2 Raw Data and Fitted Model



You might notice that some basis functions have their parent basis functions not listed in the parameter estimates table (Output 24.2.1). This is because their parent basis functions are dropped during the model selection process. You can view the complete set of basis functions used in the model selection by specifying the `DETAILS=BASES` option in the PROC ADAPTIVEREG statement, as in the following statements:

```
proc adaptivereg data=Mixture details=bases;
  class c1;
  model y=c1 x1;
run;
```

Output 24.2.3 Basis Function Information

The ADAPTIVEREG Procedure	
Basis Information	
Name	Transformation
Basis0	None
Basis1	Basis0*(C1 = 1 OR C1 = 0)
Basis2	Basis0*NOT(C1 = 1 OR C1 = 0)
Basis3	Basis0*(C1 = 1)
Basis4	Basis0*NOT(C1 = 1)
Basis5	Basis4*MAX(X1 - 0.7665019053, 0)
Basis6	Basis4*MAX(0.7665019053 - X1, 0)
Basis7	Basis2*MAX(X1 - 0.7665019053, 0)
Basis8	Basis2*MAX(0.7665019053 - X1, 0)
Basis9	Basis3*MAX(X1 - 0.5530566455, 0)
Basis10	Basis3*MAX(0.5530566455 - X1, 0)
Basis11	Basis3*MAX(X1 - 0.045800759, 0)
Basis12	Basis3*MAX(0.045800759 - X1, 0)
Basis13	Basis3*MAX(X1 - 0.9526330293, 0)
Basis14	Basis3*MAX(0.9526330293 - X1, 0)
Basis15	Basis1*MAX(X1 - 0.9499325226, 0)
Basis16	Basis1*MAX(0.9499325226 - X1, 0)
Basis17	Basis1*MAX(X1 - 0.5142821095, 0)
Basis18	Basis1*MAX(0.5142821095 - X1, 0)
Basis19	Basis1*MAX(X1 - 0.9889635476, 0)
Basis20	Basis1*MAX(0.9889635476 - X1, 0)

You can produce a SAS DATA step for scoring new observations by using the information provided in the parameter estimate table and the basis information table, as shown in the following statements:

```

data New;
  basis1 = (c1=1 OR c1=0);
  basis3 = (c1=1);
  basis5 = NOT(c1=1) *MAX(x1-0.7665019053, 0);
  basis7 = NOT(c1=1 OR c1=0) *MAX(x1-0.7665019053, 0);
  basis8 = NOT(c1=1 OR c1=0) *MAX(0.7665019053-x1, 0);
  basis9 = (c1=1) *MAX(x1-0.5530566455, 0);
  basis10 = (c1=1) *MAX(0.5530566455-x1, 0);
  basis11 = (c1=1) *MAX(x1-0.045800759, 0);
  basis13 = (c1=1) *MAX(x1-0.9526330293, 0);
  basis15 = (c1=1 OR c1=0) *MAX(x1-0.9499325226, 0);
  basis17 = (c1=1 OR c1=0) *MAX(x1-0.5142821095, 0);
  basis19 = (c1=1 OR c1=0) *MAX(x1-0.9889635476, 0);
  pred    = 5.3829 - 4.3871*basis1 + 32.7761*basis3 +
            20.2859*basis5 - 11.4183*basis7 - 7.0758*basis8 +
            58.4911*basis9 - 71.6388*basis10 - 69.0764*basis11 -
            119.71*basis13 + 66.5733*basis15 + 6.6681*basis17 -
            185.21*basis19;
run;

```

Example 24.3: Predicting E-Mail Spam

This example shows how you can use PROC ADAPTIVEREG to fit a classification model for a data set with a binary response. It illustrates how you can use the PARTITION statement to create subsets of data for training and testing purposes. It also demonstrates how to use the OUTPUT statement. Finally, it shows how you can improve the modeling speed by changing some default settings.

This example concerns a study on classifying whether an e-mail is junk e-mail (coded as 1) or not (coded as 0). The data were collected in Hewlett-Packard labs and donated by George Forman. The data set contains 4,601 observations with 58 variables. The response variable is a binary indicator of whether an e-mail is considered spam or not. The 57 variables are continuous variables that record frequencies of some common words and characters in e-mails and lengths of uninterrupted sequences of capital letters. The data set is publicly available at the UCI Machine Learning repository (Asuncion and Newman 2007).

The following DATA step downloads the data from the UCI Machine Learning repository and creates a SAS data set called spambase:

```
%let base = http://archive.ics.uci.edu/ml/machine-learning-databases;
data spambase;
  infile "&base/spambase/spambase.data" device=url dsd dlm=' ';
  input Make Address All _3d Our Over Remove Internet Order Mail Receive
        Will People Report Addresses Free Business Email You Credit Your Font
        _000 Money Hp Hpl George _650 Lab Labs Telnet _857 Data _415 _85
        Technology _1999 Parts Pm Direct Cs Meeting Original Project Re Edu
        Table Conference Semicol Paren Bracket Bang Dollar Pound Cap_Avg
        Cap_Long Cap_Total Class;
run;
```

This example shows how you can use PROC ADAPTIVEREG to build a model with good predictive power and then use it to classify observations in independent data sets. PROC ADAPTIVEREG enables you to partition your data into subsets for training, validation, and testing. The training set is used to build models, the validation set is used to estimate prediction errors and select models, and the testing set is used independently to evaluate the final model. When the sample size is not large enough, sample reusing approaches are used instead, such as bootstrap and cross validation. For this data set, the sample size is sufficient to support a random partitioning. Because the GCV model selection criterion itself serves as an estimate of prediction error, this data set is split into two separate subsets. The training set is used to build the classification model, and the test set is used to evaluate the model. The PARTITION statement performs the random partitioning for you, as shown in the following statements:

```

proc adaptivereg data=spambase seed=10359;
  class Class;
  model class = _000      _85      _415      _650      _857
                _1999    _3d      address  addresses all
                bang     bracket  business cap_avg  cap_long
                cap_total conference credit   cs       data
                direct    dollar   edu      email   font
                free      george   hp       hpl     internet
                lab       labs     mail    make   meeting
                money     order   original our     over
                paren     parts   people  pm     pound
                project   re     receive remove report
                semicol   table  technology telnet will
                you       your   / additive dist=binomial;
  partition fraction(test=0.333);
  output out=spamout p(ilink);
run;

```

The **FRACTION** option in the **PARTITION** statement specifies that 33.3% of observations in the spambase data set are randomly selected to form the testing set while the rest of the data form the training set. If you want to use the same partitioning for further analysis, you can specify the seed for the random number generator so that the exact same random number stream can be duplicated. For the preceding statements, the seed is 10359, which is specified in the **PROC ADAPTIVEREG** statement. The response variable is a two-level variable, which is specified in the **CLASS** statement. The **ADDITIVE** option specifies that this is an additive model without interactions between spline basis functions; this option makes the predictive model more interpretable. The **DIST=BINOMIAL** option specifies the distribution of the response variable. The **ILINK** option in the **OUTPUT** statement requests predicted probabilities for each observation.

The “Model Information” table in [Output 24.3.1](#) includes the distribution, link function, and the random number seed.

Output 24.3.1 Model Information

The ADAPTIVEREG Procedure	
Model Information	
Data Set	WORK.SPAMBASE
Response Variable	Class
Distribution	Binomial
Link Function	Logit
Random Number Seed	10359

The “Number of Observations” table in [Output 24.3.2](#) lists the total number of observations used. It also lists number of observations for the training set and the test set.

Output 24.3.2 Number of Observations

Number of Observations Read	4601
Number of Observations Used	4601
Number of Observations Used for Training	3028
Number of Observations Used for Testing	1573

The response variable is a binary classification variable. PROC ADAPTIVEREG produces the “Response Profile” table in [Output 24.3.3](#). The table shows the response level frequencies for the training set and the probability that PROC ADAPTIVEREG models.

Output 24.3.3 Response Profile

Response Profile		
Ordered Value	Class	Total Frequency
1	0	2788
2	1	1813

Probability modeled is Class='0'.

The “Fit Statistics” table in [Output 24.3.3](#) shows that the final model for the training set contains large effective degrees freedom.

Output 24.3.4 Fit Statistics

Fit Statistics	
GCV	0.23427
GCV R-Square	0.82508
Effective Degrees of Freedom	173
Log Likelihood	-315.30998
Deviance (Train)	630.61996
Deviance (Test)	806.74112

To classify e-mails from the test set, the following rule is used. For each observation, the e-mail is classified as spam if the predicted probability of Class = ‘0’ is greater than the predicted probability of Class = ‘1’, and ham (a good e-mail) otherwise. Because the response is binary, you can classify an e-mail as spam if the predicted probability of Class = ‘0’ is less than 0.5. The following statements evaluate classification errors:

```

data test;
  set spamout(where=(_ROLE_='TEST'));
  if ((pred>0.5 & class=0) | (pred<0.5 & class=1))
  then Error=0;
  else error=1;
run;

proc freq data=test;
  tables class*error/nocol;
run;

```

Output 24.3.5 shows the misclassification errors for all observations and observations of each response category. Compared to the results from other statistical learning algorithms that use different training subsets (Hastie, Tibshirani, and Friedman 2001), these results from PROC ADAPTIVEREG are competitive.

Output 24.3.5 Crosstabulation Table for Test Set Prediction

The FREQ Procedure				
Table of Class by Error				
Class	Error			
Frequency				
Percent				
Row Pct	0	1	Total	
0	885	59	944	
	56.26	3.75	60.01	
	93.75	6.25		
1	592	37	629	
	37.64	2.35	39.99	
	94.12	5.88		
Total	1477	96	1573	
	93.90	6.10	100.00	

It takes approximately 3GB of memory and about five and a half minutes to fit the model on a workstation with a 12-way 2.6GHz AMD Opteron processor. The following analyses illustrate how you can change some default settings to improve the modeling speed without sacrificing much predictive capability. As discussed in the section “Computational Resources” on page 876, the computation cost for PROC ADAPTIVEREG is proportional to pNM_{\max}^3 . For the same data set, you can significantly increase the modeling speed by reducing the maximum number of basis functions that are allowed for the forward selection.

PROC ADAPTIVEREG uses 115 as the maximum number of basis functions. Suppose you want to set the maximum number to 61, which is approximately half the default value. The following program fits a multivariate adaptive regression splines model with `MAXBASIS=` set to 61. The same random number seed is used to get the exact same data partitioning.

```
proc adaptivereg data=spambase seed=10359;
  class Class;
  model class = _000      _85      _415      _650      _857
                _1999    _3d      address  addresses all
                bang     bracket  business cap_avg  cap_long
                cap_total conference credit    cs      data
                direct    dollar    edu      email   font
                free      george    hp       hpl     internet
                lab       labs     mail    make   meeting
                money     order    original our     over
                paren     parts    people  pm     pound
                project    re      receive remove report
                semicol    table   technology telnet  will
                you       your    / maxbasis=61 additive dist=binomial;
  partition fraction(test=0.333);
  output out=spamout2 p(ilink);
run;
```

The “Fit Statistics” table in [Output 24.3.6](#) displays summary statistics for the second model. The log likelihood of the second model is smaller than that of the first model, which is expected because the effective degrees of freedom is 95, much smaller than the effective degrees of freedom of the first model. This means that the fitted model is much simpler than the first model. Both the GCV and GCV R-square values show that the estimated prediction capability of the second model is slightly less than the first model.

Output 24.3.6 Fit Statistics

The ADAPTIVEREG Procedure	
Fit Statistics	
GCV	0.27971
GCV R-Square	0.79115
Effective Degrees of Freedom	95
Log Likelihood	-397.32916
Deviance (Train)	794.65833
Deviance (Test)	682.79427

By predicting observations in the test set, the second model has an overall misclassification error of 5.28%, which is slightly lower than that of the first model. This shows that the predictive power of the second model is actually greater than of the first model due to reduced model complexity. The computation takes around 80 seconds on the same workstation and consumes approximately 170MB of memory. This is a significant improvement in both computation speed and memory cost.

You can further improve the modeling speed by using the **FAST** option in the **MODEL** statement. The **FAST** option avoids evaluating certain combinations of parent basis functions and variables. For example, you can specify the **FAST(K=20)** option so that in each forward selection iteration, PROC ADAPTIVEREG uses only the top 20 parent basis functions (based on their maximum improvement from the previous iteration) to construct and evaluate new basis functions. The underlying assumption, as discussed in the section “Fast Algorithm” on page 874, is that parent basis functions that offer low improvement at previous steps are less likely to yield new basis functions that offer large improvement at the current step. The following statements illustrate the **FAST** option:

```
proc adaptivereg data=spambase seed=10359;
  class Class;
  model class = _000      _85      _415      _650      _857
                _1999    _3d      address  addresses all
                bang     bracket  business cap_avg  cap_long
                cap_total conference credit   cs       data
                direct    dollar   edu      email   font
                free      george   hp       hpl     internet
                lab       labs     mail    make    meeting
                money     order   original our     over
                paren     parts   people  pm      pound
                project   re     receive remove report
                semicol   table  technology telnet  will
                you       your   / maxbasis=61 fast(k=20) additive dist=binomial;
  partition fraction(test=0.333);
  output out=spamout3 p(ilink);
run;
```

The fitted model is the same as the second model. The computation time reduces further to 70 seconds. You should tune the parameters for the **FAST** option with care because the underlying assumption does not always hold.

With this investigation, the second model can serve as a good classifier. It contains 26 variables. The “Variable Importance” table (Output 24.3.7) lists all variables and their importance values in descending order. Two variables in the model, **George** and **Hp**, are important factors in classifying e-mails as not spam. George Forman, the donor of the original data set, collected e-mails from filed work and personal e-mails at Hewlett-Packard labs. Thus these two variables are strong indicators of e-mails that are not spam. This confirms the results from the fitted multivariate adaptive regression splines model by PROC ADAPTIVEREG.

Output 24.3.7 Variable Importance

Variable Importance		
Variable	Number of Bases	Importance
George	1	100.00
Hp	1	78.35
Edu	3	61.25
Remove	2	49.21
Bang	3	44.14
Free	2	34.18
Meeting	3	32.57
_1999	2	29.71
Dollar	2	28.30
Money	3	26.39
Cap_Long	3	24.41
Our	2	19.46
Semicol	2	14.98
Re	2	13.52
Business	3	13.48
Over	3	12.63
Cap_Total	3	12.50
Will	1	10.81
Pound	2	9.73
Internet	1	5.88
_000	1	4.57
You	2	3.17

Example 24.4: Nonparametric Poisson Model for Mackerel Egg Density

This example demonstrates how you can use PROC ADAPTIVEREG to fit a nonparametric Poisson regression model.

The example concerns a study of mackerel egg density. The data are a subset of the 1992 mackerel egg survey conducted over the Porcupine Bank west of Ireland. The survey took place in the peak spawning area. Scientists took samples by hauling a net up from deep sea to the sea surface. Then they counted the number of spawned mackerel eggs and used other geographic information to estimate the sizes and distributions of spawning stocks. The data set is used as an example in Bowman and Azzalini (1997).

The following SAS DATA step creates the data set Mackerel. This data set contains 634 observations and five variables. The response variable Egg_Count is the number of mackerel eggs collected from each sampling net. Longitude and Latitude are the location values in degrees east and north, respectively, of each sample station. Net_Area is the area of the sampling net in square meters. Depth records the sea bed depth in meters at the sampling location. And Distance is the distance in geographic degrees from the sample location to the continental shelf edge.

```

title 'Mackerel Egg Density Study';
data Mackerel;
  input Egg_Count Longitude Latitude Net_Area Depth Distance;
  datalines;
0      -4.65      44.57      0.242      4342      0.8395141177
0      -4.48      44.57      0.242      4334      0.8591926336
0      -4.3       44.57      0.242      4286      0.8930152895
1      -2.87      44.02      0.242      1438      0.3956408691
4      -2.07      44.02      0.242      166       0.0400088237
3      -2.13      44.02      0.242      460       0.0974234463
0      -2.27      44.02      0.242      810       0.2362566569

  ... more lines ...

22     -4.22      46.25      0.19       205       0.1181120828
21     -4.28      46.25      0.19       237       0.129990854
0      -4.73      46.25      0.19      2500      0.3346500536
5      -4.25      47.23      0.19       114       0.718192582
3      -3.72      47.25      0.19       100      0.9944669778
0      -3.25      47.25      0.19        64      1.2639918431
;

```

The response values are counts, so the Poisson distribution might be a reasonable model. The study of interest is the mackerel egg density, which can be formed as

$$\text{density} = E(\text{count})/\text{net_area}$$

This is equivalent to a Poisson regression with the response variable `Egg_Count` and an offset variable $\log(\text{net_area})$ and other covariates.

The following statements produce the plot of the mackerel egg density with respect to the sampling station location:

```

data temp;
  set mackerel;
  density = egg_count/net_area;
run;

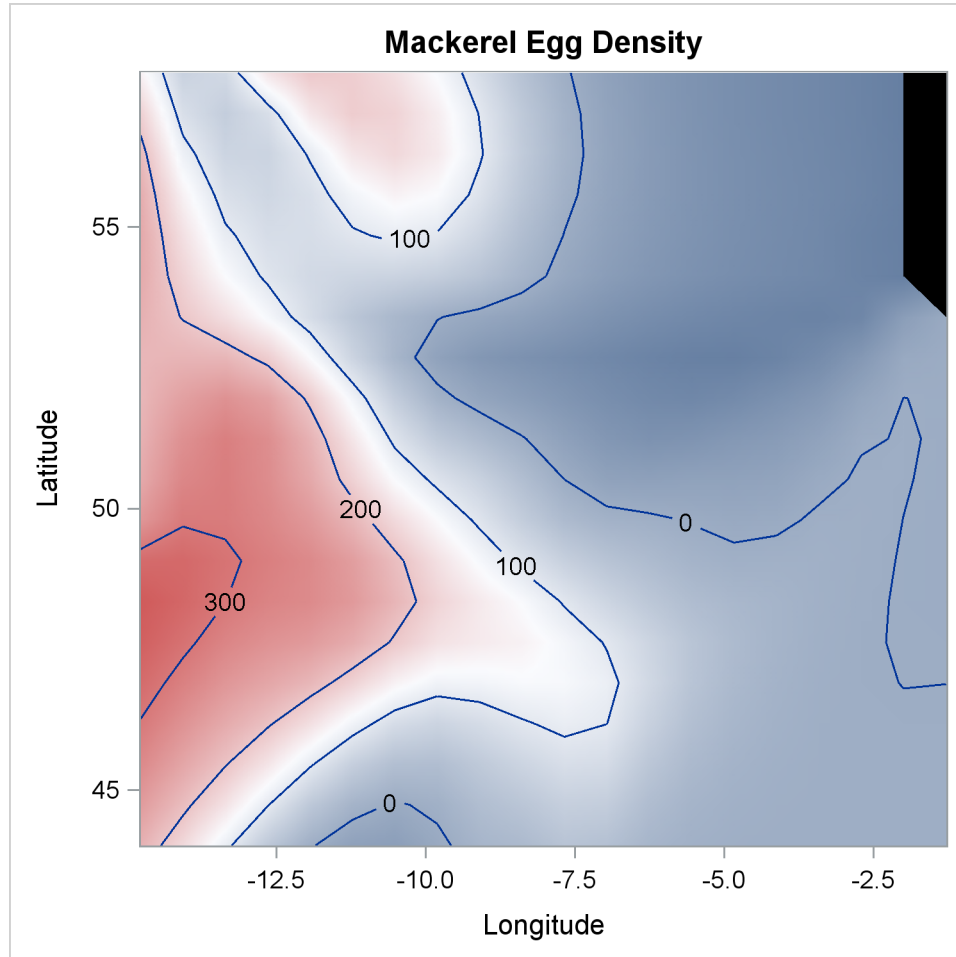
proc template;
  define statgraph surface;
    dynamic _title _z;
    begingraph / designwidth=defaultDesignHeight;
    entrytitle _title;
    layout overlay / xaxisopts=(offsetmin=0 offsetmax=0
                               linearopts=(thresholdmin=0 thresholdmax=0))
                   yaxisopts=(offsetmin=0 offsetmax=0
                               linearopts=(thresholdmin=0 thresholdmax=0));
    contourplotparm z=_z y=latitude x=longitude / gridded=FALSE;
    endlayout;
  endgraph;
end;
run;

```

```
ods graphics on;
proc sgrender data=temp template=surface;
  dynamic _title='Mackerel Egg Density'
    _z='density';
run;
```

Output 24.4.1 displays the mackerel egg density in the sampling area. The black hole in the upper right corner is due to missing values in that area.

Output 24.4.1 Mackerel Egg Density



In this example, the dependent variable is the mackerel egg counts, the independent variables are the geographical information about each of the sampling stations, and the logarithm of the sampling area is the offset variable. The following statements fit the nonparametric Poisson regression model:

```
data mackerel;
  set mackerel;
  log_net_area = log(net_area);
run;
```

```

proc adaptivereg data=mackerel;
  model egg_count = longitude latitude depth distance
    / offset=log_net_area dist=poisson;
  output out=mackerelout p(ilink);
run;

```

Output 24.4.2 lists basic model information such as the offset variable, distribution, and link function.

Output 24.4.2 Model Information

Mackerel Egg Density Study	
The ADAPTIVEREG Procedure	
Model Information	
Data Set	WORK.MACKEREL
Response Variable	Egg_Count
Offset Variable	log_net_area
Distribution	Poisson
Link Function	Log

Output 24.4.3 lists fit statistics for the final model.

Output 24.4.3 Fit Statistics

Fit Statistics	
GCV	6.94340
GCV R-Square	0.79204
Effective Degrees of Freedom	29
Log Likelihood	-2777.21279
Deviance	4008.60601

The final model consists of basis functions and interactions between basis functions of three geographic variables. Output 24.4.4 lists seven functional components of the final model, including three one-way spline transformations and four two-way spline interactions.

Output 24.4.4 ANOVA Decomposition

ANOVA Decomposition				
Functional Component	Number of Bases	DF	---Change If Omitted---	
			Lack of Fit	GCV
Longitude	3	6	2035.77	3.3216
Depth	1	2	420.59	0.6780
Latitude	1	2	265.05	0.4104
Longitude Latitude	2	4	199.17	0.2496
Depth Distance	3	6	552.75	0.8030
Depth Latitude	2	4	680.45	1.0723
Depth Longitude	2	4	415.77	0.6198

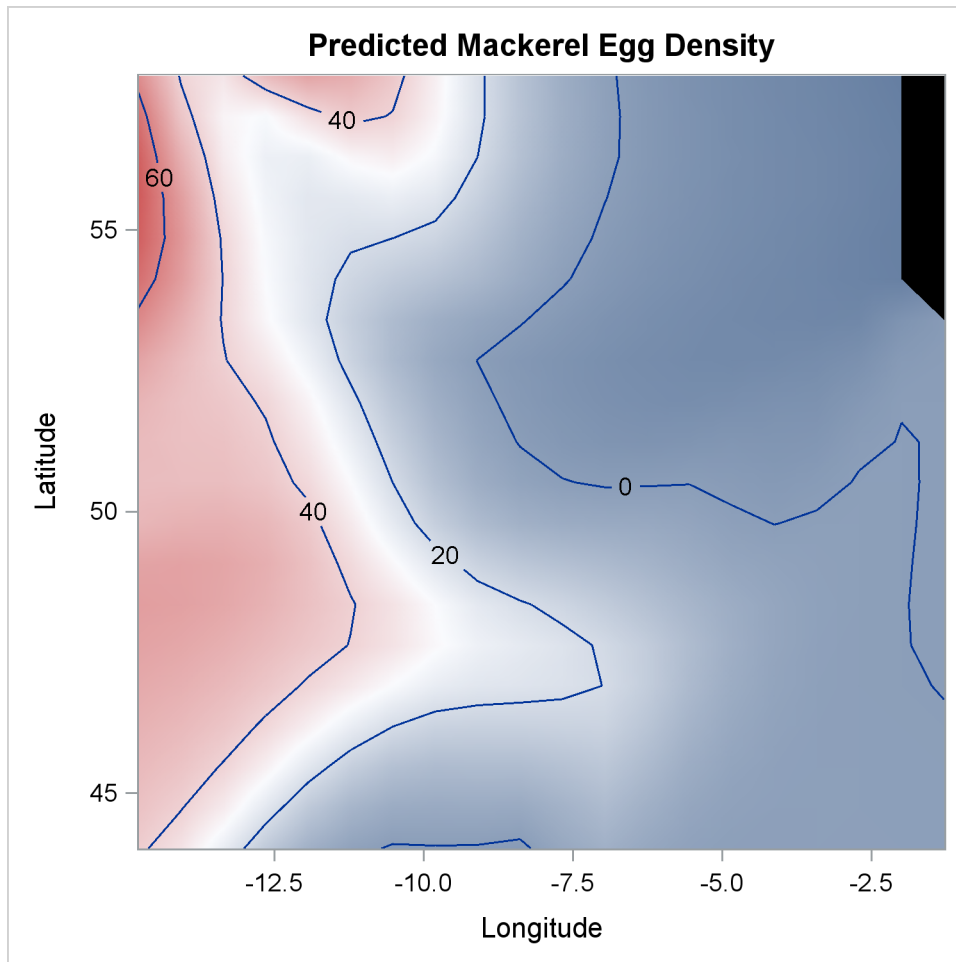
The “Variable Importance” table in [Output 24.4.5](#) displays the relative variable importance among the four variables. Longitude is the most important one.

Output 24.4.5 Variable Importance

Variable Importance		
Variable	Number of Bases	Importance
Longitude	7	100.00
Depth	8	30.26
Latitude	5	18.93
Distance	3	8.56

[Output 24.4.6](#) displays the predicted mackerel egg density over the spawning area.

Output 24.4.6 Predicted Mackerel Egg Density



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Chapter 25

The ANOVA Procedure

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Overview: ANOVA Procedure

The ANOVA procedure performs *analysis of variance* (ANOVA) for balanced data from a wide variety of experimental designs. In analysis of variance, a continuous response variable, known as a *dependent variable*, is measured under experimental conditions identified by classification variables, known as *independent variables*. The variation in the response is assumed to be due to effects in the classification, with random error accounting for the remaining variation.

The ANOVA procedure is one of several procedures available in SAS/STAT software for analysis of variance. The ANOVA procedure is designed to handle balanced data (that is, data with equal numbers of observations for every combination of the classification factors), whereas the GLM procedure can analyze both balanced and unbalanced data. Because PROC ANOVA takes into account the special structure of a balanced design, it is faster and uses less storage than PROC GLM for balanced data.

Use PROC ANOVA for the analysis of balanced data only, with the following exceptions: one-way analysis of variance, Latin square designs, certain partially balanced incomplete block designs, completely nested (hierarchical) designs, and designs with cell frequencies that are proportional to each other and are also proportional to the background population. These exceptions have designs in which the factors are all orthogonal to each other.

For further discussion, see Searle (1971, p. 138). PROC ANOVA works for designs with block diagonal $X'X$ matrices where the elements of each block all have the same value. The procedure partially tests this requirement by checking for equal cell means. However, this test is imperfect: some designs that cannot be analyzed correctly might pass the test, and designs that can be analyzed correctly might not pass. If your design does not pass the test, PROC ANOVA produces a warning message to tell you that the design is unbalanced and that the ANOVA analyses might not be valid; if your design is not one of the special cases described here, then you should use PROC GLM instead. Complete validation of designs is not performed in PROC ANOVA since this would require the whole $X'X$ matrix; if you are unsure about the validity of PROC ANOVA for your design, you should use PROC GLM.

CAUTION: If you use PROC ANOVA for analysis of unbalanced data, you must assume responsibility for the validity of the results.

The ANOVA procedure automatically produces graphics as part of its ODS output. For general information about ODS graphics, see the section “ODS Graphics” on page 941 and Chapter 21, “Statistical Graphics Using ODS.”

Getting Started: ANOVA Procedure

The following examples demonstrate how you can use the ANOVA procedure to perform analyses of variance for a one-way layout and a randomized complete block design.

One-Way Layout with Means Comparisons

A one-way analysis of variance considers one treatment factor with two or more treatment levels. The goal of the analysis is to test for differences among the means of the levels and to quantify these differences. If there are two treatment levels, this analysis is equivalent to a t test comparing two group means.

The assumptions of analysis of variance (Steel and Torrie 1980) are that treatment effects are additive and experimental errors are independently random with a normal distribution that has mean zero and constant variance.

The following example studies the effect of bacteria on the nitrogen content of red clover plants. The treatment factor is bacteria strain, and it has six levels. Five of the six levels consist of five different *Rhizobium trifolii* bacteria cultures combined with a composite of five *Rhizobium meliloti* strains. The sixth level is a composite of the five *Rhizobium trifolii* strains with the composite of the *Rhizobium meliloti*. Red clover plants are inoculated with the treatments, and nitrogen content is later measured in milligrams. The data are derived from an experiment by Erdman (1946) and are analyzed in Chapters 7 and 8 of Steel and Torrie (1980). The following DATA step creates the SAS data set Clover:

```

title1 'Nitrogen Content of Red Clover Plants';
data Clover;
  input Strain $ Nitrogen @@;
  datalines;
3DOK1  19.4 3DOK1  32.6 3DOK1  27.0 3DOK1  32.1 3DOK1  33.0
3DOK5  17.7 3DOK5  24.8 3DOK5  27.9 3DOK5  25.2 3DOK5  24.3
3DOK4  17.0 3DOK4  19.4 3DOK4   9.1 3DOK4  11.9 3DOK4  15.8
3DOK7  20.7 3DOK7  21.0 3DOK7  20.5 3DOK7  18.8 3DOK7  18.6
3DOK13 14.3 3DOK13 14.4 3DOK13 11.8 3DOK13 11.6 3DOK13 14.2
COMPOS 17.3 COMPOS 19.4 COMPOS 19.1 COMPOS 16.9 COMPOS 20.8
;

```

The variable Strain contains the treatment levels, and the variable Nitrogen contains the response. The following statements produce the analysis.

```

proc anova data = Clover;
  class strain;
  model Nitrogen = Strain;
run;

```

The classification variable is specified in the **CLASS** statement. Note that, unlike the GLM procedure, PROC ANOVA does not allow continuous variables on the right-hand side of the model. Figure 25.1 and Figure 25.2 display the output produced by these statements.

Figure 25.1 Class Level Information

Nitrogen Content of Red Clover Plants							
The ANOVA Procedure							
Class Level Information							
Class	Levels	Values					
Strain	6	3DOK1	3DOK13	3DOK4	3DOK5	3DOK7	COMPOS
Number of Observations Read						30	
Number of Observations Used						30	

The “Class Level Information” table shown in Figure 25.1 lists the variables that appear in the CLASS statement, their levels, and the number of observations in the data set.

Figure 25.2 displays the ANOVA table, followed by some simple statistics and tests of effects.

Figure 25.2 ANOVA Table

Nitrogen Content of Red Clover Plants					
The ANOVA Procedure					
Dependent Variable: Nitrogen					
Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	5	847.046667	169.409333	14.37	<.0001
Error	24	282.928000	11.788667		
Corrected Total	29	1129.974667			
	R-Square	Coeff Var	Root MSE	Nitrogen Mean	
	0.749616	17.26515	3.433463	19.88667	
Source	DF	Anova SS	Mean Square	F Value	Pr > F
Strain	5	847.046667	169.409333	14.37	<.0001

The degrees of freedom (DF) column should be used to check the analysis results. The model degrees of freedom for a one-way analysis of variance are the number of levels minus 1; in this case, $6 - 1 = 5$. The Corrected Total degrees of freedom are always the total number of observations minus one; in this case $30 - 1 = 29$. The sum of Model and Error degrees of freedom equals the Corrected Total.

The overall F test is significant ($F = 14.37$, $p < 0.0001$), indicating that the model as a whole accounts for a significant portion of the variability in the dependent variable. The F test for Strain is significant, indicating that some contrast between the means for the different strains is different from zero. Notice that the Model and Strain F tests are identical, since Strain is the only term in the model.

The F test for Strain ($F = 14.37$, $p < 0.0001$) suggests that there are differences among the bacterial strains, but it does not reveal any information about the nature of the differences. Mean comparison methods can be used to gather further information. The interactivity of PROC ANOVA enables you to do this without re-running the entire analysis. After you specify a model with a MODEL statement and execute the ANOVA procedure with a RUN statement, you can execute a variety of statements (such as MEANS, MANOVA, TEST, and REPEATED) without PROC ANOVA recalculating the model sum of squares.

The following additional statements request means of the Strain levels with Tukey’s studentized range procedure.

```
means strain / tukey;
run;
```

Results of Tukey's procedure are shown in [Figure 25.3](#).

Figure 25.3 Tukey's Multiple Comparisons Procedure

Nitrogen Content of Red Clover Plants				
The ANOVA Procedure				
Tukey's Studentized Range (HSD) Test for Nitrogen				
Alpha				0.05
Error Degrees of Freedom				24
Error Mean Square				11.78867
Critical Value of Studentized Range				4.37265
Minimum Significant Difference				6.7142
Means with the same letter are not significantly different.				
Tukey Grouping		Mean	N	Strain
	A	28.820	5	3DOK1
	A			
B	A	23.980	5	3DOK5
B				
B	C	19.920	5	3DOK7
B	C			
B	C	18.700	5	COMPOS
	C			
	C	14.640	5	3DOK4
	C			
	C	13.260	5	3DOK13

Examples of implications of the multiple comparisons results are as follows:

- Strain 3DOK1 fixes significantly more nitrogen than all but 3DOK5.
- While 3DOK5 is not significantly different from 3DOK1, it is also not significantly better than all the rest, though it is better than the bottom two groups.

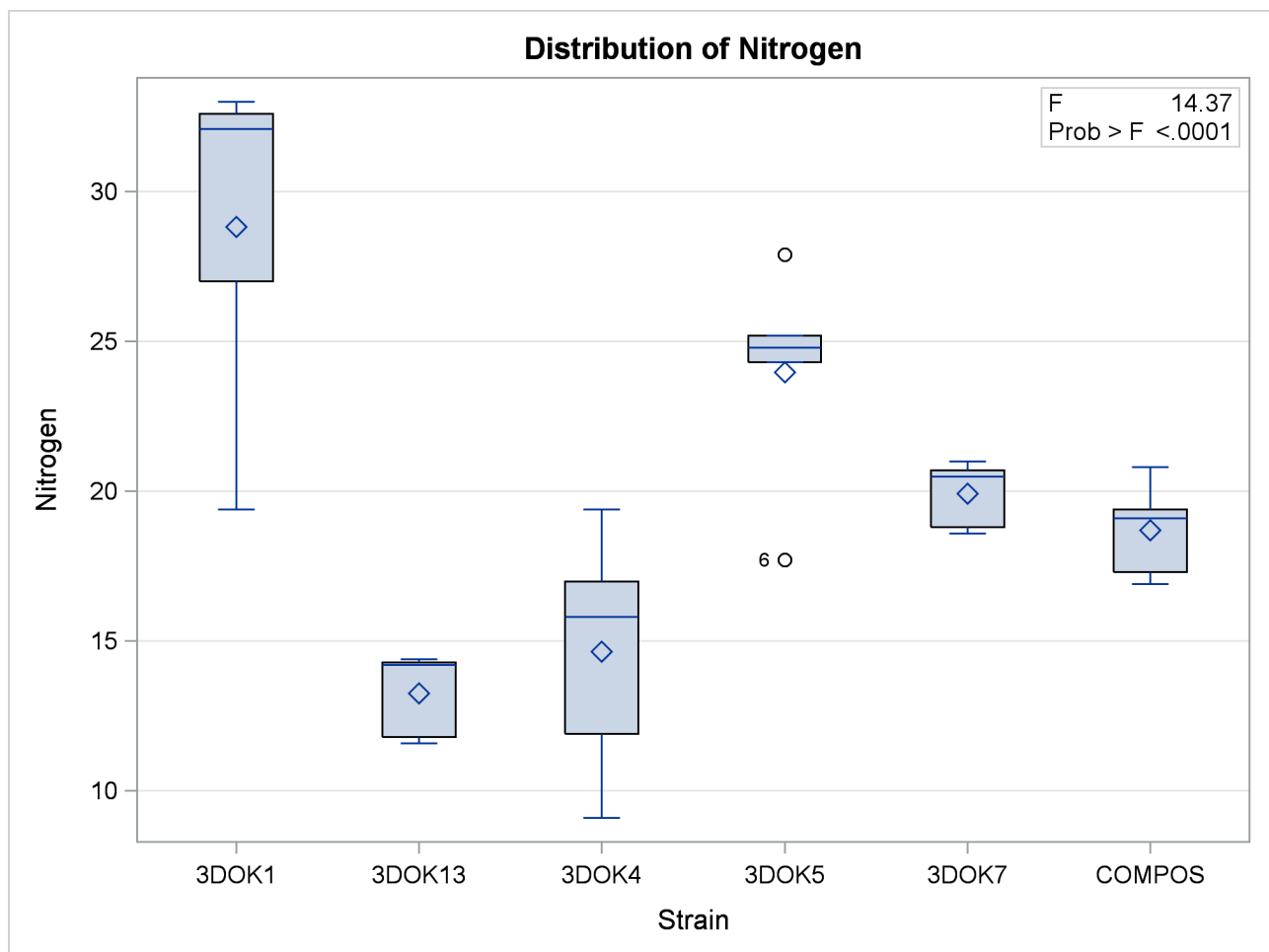
Although the experiment has succeeded in separating the best strains from the worst, more experimentation is required in order to clearly distinguish the very best strain.

If ODS Graphics is enabled, ANOVA also displays by default a plot that enables you to visualize the distribution of nitrogen content for each treatment. The following statements, which are the same as the previous analysis but with ODS graphics enabled, additionally produce [Figure 25.4](#).

```
ods graphics on;
proc anova data = Clover;
  class strain;
  model Nitrogen = Strain;
run;
ods graphics off;
```

When ODS Graphics is enabled and you fit a one-way analysis of variance model, the ANOVA procedure output includes a box plot of the dependent variable values within each classification level of the independent variable. For general information about ODS Graphics, see Chapter 21, “Statistical Graphics Using ODS.” For specific information about the graphics available in the ANOVA procedure, see the section “ODS Graphics” on page 941.

Figure 25.4 Box Plot of Nitrogen Content for each Treatment



Randomized Complete Block with One Factor

This example illustrates the use of PROC ANOVA in analyzing a randomized complete block design. Researchers are interested in whether three treatments have different effects on the yield and worth of a particu-

lar crop. They believe that the experimental units are not homogeneous. So, a blocking factor is introduced that allows the experimental units to be homogeneous within each block. The three treatments are then randomly assigned within each block.

The data from this study are input into the SAS data set RCB:

```

title1 'Randomized Complete Block';
data RCB;
  input Block Treatment $ Yield Worth @@;
  datalines;
1 A 32.6 112    1 B 36.4 130    1 C 29.5 106
2 A 42.7 139    2 B 47.1 143    2 C 32.9 112
3 A 35.3 124    3 B 40.1 134    3 C 33.6 116
;

```

The variables Yield and Worth are continuous response variables, and the variables Block and Treatment are the classification variables. Because the data for the analysis are balanced, you can use PROC ANOVA to run the analysis.

The statements for the analysis are

```

proc anova data=RCB;
  class Block Treatment;
  model Yield Worth=Block Treatment;
run;

```

The Block and Treatment effects appear in the **CLASS** statement. The **MODEL** statement requests an analysis for each of the two dependent variables, Yield and Worth.

Figure 25.5 shows the “Class Level Information” table.

Figure 25.5 Class Level Information

Randomized Complete Block		
The ANOVA Procedure		
Class Level Information		
Class	Levels	Values
Block	3	1 2 3
Treatment	3	A B C
Number of Observations Read		9
Number of Observations Used		9

The “Class Level Information” table lists the number of levels and their values for all effects specified in the **CLASS** statement. The number of observations in the data set are also displayed. Use this information to make sure that the data have been read correctly.

The overall ANOVA table for Yield in Figure 25.6 appears first in the output because it is the first response variable listed on the left side in the MODEL statement.

Figure 25.6 Overall ANOVA Table for Yield

Randomized Complete Block					
The ANOVA Procedure					
Dependent Variable: Yield					
Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	4	225.2777778	56.3194444	8.94	0.0283
Error	4	25.1911111	6.2977778		
Corrected Total	8	250.4688889			
	R-Square	Coeff Var	Root MSE	Yield Mean	
	0.899424	6.840047	2.509537	36.68889	

The overall F statistic is significant ($F = 8.94, p = 0.0283$), indicating that the model as a whole accounts for a significant portion of the variation in Yield and that you can proceed to evaluate the tests of effects.

The degrees of freedom (DF) are used to ensure correctness of the data and model. The Corrected Total degrees of freedom are one less than the total number of observations in the data set; in this case, $9 - 1 = 8$. The Model degrees of freedom for a randomized complete block are $(b - 1) + (t - 1)$, where $b =$ number of block levels and $t =$ number of treatment levels. In this case, this formula leads to $(3 - 1) + (3 - 1) = 4$ model degrees of freedom.

Several simple statistics follow the ANOVA table. The R-Square indicates that the model accounts for nearly 90% of the variation in the variable Yield. The coefficient of variation (C.V.) is listed along with the Root MSE and the mean of the dependent variable. The Root MSE is an estimate of the standard deviation of the dependent variable. The C.V. is a unitless measure of variability.

The tests of the effects shown in Figure 25.7 are displayed after the simple statistics.

Figure 25.7 Tests of Effects for Yield

Source	DF	Anova SS	Mean Square	F Value	Pr > F
Block	2	98.1755556	49.0877778	7.79	0.0417
Treatment	2	127.1022222	63.5511111	10.09	0.0274

For Yield, both the Block and Treatment effects are significant ($F = 7.79, p = 0.0417$ and $F = 10.09, p = 0.0274$, respectively) at the 95% level. From this you can conclude that blocking is useful for this variable and that some contrast between the treatment means is significantly different from zero.

Figure 25.8 shows the ANOVA table, simple statistics, and tests of effects for the variable Worth.

Figure 25.8 ANOVA Table for Worth

Randomized Complete Block					
The ANOVA Procedure					
Dependent Variable: Worth					
Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	4	1247.333333	311.833333	8.28	0.0323
Error	4	150.666667	37.666667		
Corrected Total	8	1398.000000			
	R-Square	Coeff Var	Root MSE	Worth Mean	
	0.892227	4.949450	6.137318	124.0000	
Source	DF	Anova SS	Mean Square	F Value	Pr > F
Block	2	354.6666667	177.3333333	4.71	0.0889
Treatment	2	892.6666667	446.3333333	11.85	0.0209

The overall F test is significant ($F = 8.28, p = 0.0323$) at the 95% level for the variable Worth. The Block effect is not significant at the 0.05 level but is significant at the 0.10 confidence level ($F = 4.71, p = 0.0889$). Generally, the usefulness of blocking should be determined before the analysis. However, since there are two dependent variables of interest, and Block is significant for one of them (Yield), blocking appears to be generally useful. For Worth, as with Yield, the effect of Treatment is significant ($F = 11.85, p = 0.0209$).

Issuing the following command produces the Treatment means.

```
means Treatment;
run;
```

Figure 25.9 displays the treatment means and their standard deviations for both dependent variables.

Figure 25.9 Means of Yield and Worth

Randomized Complete Block					
The ANOVA Procedure					
Level of Treatment	N	Yield		Worth	
		Mean	Std Dev	Mean	Std Dev
A	3	36.8666667	5.22908532	125.000000	13.5277493
B	3	41.2000000	5.43415127	135.666667	6.6583281
C	3	32.0000000	2.19317122	111.333333	5.0332230

Syntax: ANOVA Procedure

The following statements are available in the ANOVA procedure:

```

PROC ANOVA < options > ;
CLASS variables < / option > ;
MODEL dependents = effects < / options > ;
ABSORB variables ;
BY variables ;
FREQ variable ;
MANOVA < test-options > < / detail-options > ;
MEANS effects < / options > ;
REPEATED factor-specification < / options > ;
TEST < H=effects > E=effect ;
    
```

The **PROC ANOVA**, **CLASS**, and **MODEL** statements are required, and they must precede the first **RUN** statement. The **CLASS** statement must precede the **MODEL** statement. If you use the **ABSORB**, **FREQ**, or **BY** statement, it must precede the first **RUN** statement. The **MANOVA**, **MEANS**, **REPEATED**, and **TEST** statements must follow the **MODEL** statement, and they can be specified in any order. These four statements can also appear after the first **RUN** statement.

Table 25.1 summarizes the function of each statement (other than the **PROC** statement) in the ANOVA procedure:

Table 25.1 Statements in the ANOVA Procedure

Statement	Description
ABSORB	Absorbs classification effects in a model
BY	Specifies variables to define subgroups for the analysis
CLASS	Declares classification variables
FREQ	Specifies a frequency variable
MANOVA	Performs a multivariate analysis of variance
MEANS	Computes and compares means
MODEL	Defines the model to be fit

Table 25.1 *continued*

Statement	Description
REPEATED	Performs multivariate and univariate repeated measures analysis of variance
TEST	Constructs tests that use the sums of squares for effects and the error term you specify

PROC ANOVA Statement

PROC ANOVA < options > ;

The PROC ANOVA statement invokes the ANOVA procedure. Table 25.2 summarizes the options available in the PROC ANOVA statement.

Table 25.2 PROC ANOVA Statement Options

Option	Description
Specify input and output data sets	
DATA=	Specifies input SAS data set
MANOVA	Requests the multivariate mode of eliminating observations with missing values
MULTIPASS	Requests that the input data set be reread when necessary, instead of using a utility file
NAMELEN=	Specifies the length of effect names
NOPRINT	Suppresses the normal display of results
ORDER=	Specifies the sort order for the levels of the classification variables
OUTSTAT=	Names an output data set for information and statistics on each model effect
PLOTS	Controls the plots produced through ODS Graphics.

You can specify the following options in the PROC ANOVA statement:

DATA=SAS-data-set

names the SAS data set used by the ANOVA procedure. By default, PROC ANOVA uses the most recently created SAS data set.

MANOVA

requests the multivariate mode of eliminating observations with missing values. If any of the dependent variables have missing values, the procedure eliminates that observation from the analysis. The MANOVA option is useful if you use PROC ANOVA in interactive mode and plan to perform a multivariate analysis.

MULTIPASS

requests that PROC ANOVA reread the input data set, when necessary, instead of writing the values of dependent variables to a utility file. This option decreases disk space usage at the expense of increased execution times and is useful only in rare situations where disk space is at an absolute premium.

NAMELEN=*n*

specifies the length of effect names to be *n* characters long, where *n* is a value between 20 and 200 characters. The default length is 20 characters.

NOPRINT

suppresses the normal display of results. The NOPRINT option is useful when you want to create only the output data set with the procedure. Note that this option temporarily disables the Output Delivery System (ODS); see Chapter 20, “Using the Output Delivery System,” for more information.

ORDER=DATA | FORMATTED | FREQ | INTERNAL

specifies the sort order for the levels of the classification variables (which are specified in the **CLASS** statement). This option applies to the levels for all classification variables, except when you use the (default) ORDER=FORMATTED option with numeric classification variables that have no explicit format. With this option, the levels of such variables are ordered by their internal value.

The ORDER= option can take the following values:

Value of ORDER=	Levels Sorted By
DATA	Order of appearance in the input data set
FORMATTED	External formatted value, except for numeric variables with no explicit format, which are sorted by their unformatted (internal) value
FREQ	Descending frequency count; levels with the most observations come first in the order
INTERNAL	Unformatted value

By default, ORDER=FORMATTED. For ORDER=FORMATTED and ORDER=INTERNAL, the sort order is machine-dependent.

OUTSTAT=SAS-data-set

names an output data set that contains sums of squares, degrees of freedom, *F* statistics, and probability levels for each effect in the model. If you use the CANONICAL option in the **MANOVA** statement and do not use an M= specification in the **MANOVA** statement, the data set also contains results of the canonical analysis. See the section “Output Data Set” on page 936 for more information.

PLOTS <(MAXPOINTS=NONE | number)> <=NONE >**PLOTS=NONE**

controls the plots produced through ODS Graphics. When ODS Graphics is enabled, the ANOVA procedure can display a grouped box plot of the input data with groups defined by an effect in the model. Such a plot is produced by default if you have a one-way model, with only a single classification variable, or if you use a **MEANS** statement. Specify the PLOTS=NONE option to prevent these plots from being produced when ODS Graphics is enabled.

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;
proc anova data = Clover;
  class strain;
  model Nitrogen = Strain;
run;
ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The following option can be specified in parentheses after PLOTS.

MAXPOINTS=NONE | *number*

specifies that plots with elements that require processing of more than *number* points be suppressed. The default is MAXPOINTS=5000. This limit is ignored if you specify MAXPOINTS=NONE.

ABSORB Statement

ABSORB *variables* ;

Absorption is a computational technique that provides a large reduction in time and memory requirements for certain types of models. The *variables* are one or more variables in the input data set.

For a main effect variable that does not participate in interactions, you can absorb the effect by naming it in an ABSORB statement. This means that the effect can be adjusted out before the construction and solution of the rest of the model. This is particularly useful when the effect has a large number of levels.

Several variables can be specified, in which case each one is assumed to be nested in the preceding variable in the ABSORB statement.

NOTE: When you use the ABSORB statement, the data set (or each BY group, if a BY statement appears) must be sorted by the variables in the ABSORB statement. Including an absorbed variable in the CLASS list or in the MODEL statement might produce erroneous sums of squares. If the ABSORB statement is used, it must appear before the first RUN statement or it is ignored.

When you use an ABSORB statement and also use the INT option in the MODEL statement, the procedure ignores the option but produces the uncorrected total sum of squares (SS) instead of the corrected total SS.

See the section “Absorption” on page 3343 in Chapter 42, “The GLM Procedure,” for more information.

BY Statement

BY *variables* ;

You can specify a BY statement with PROC ANOVA to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the ANOVA procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

Since sorting the data changes the order in which PROC ANOVA reads observations, the sort order for the levels of the classification variables might be affected if you have also specified the **ORDER=DATA** option in the **PROC ANOVA** statement.

If the BY statement is used, it must appear before the first RUN statement, or it is ignored. When you use a BY statement, the interactive features of PROC ANOVA are disabled.

When both a **BY** and an **ABSORB** statement are used, observations must be sorted first by the variables in the **BY** statement, and then by the variables in the **ABSORB** statement.

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

CLASS Statement

```
CLASS variable <(REF= option)> ... <variable <(REF= option)>> </global-options> ;
```

The CLASS statement names the classification variables to be used in the model. Typical classification variables are Treatment, Sex, Race, Group, and Replication. If you use the CLASS statement, it must appear before the MODEL statement.

Classification variables can be either character or numeric. By default, class levels are determined from the entire set of formatted values of the CLASS variables.

NOTE: Prior to SAS 9, class levels were determined by using no more than the first 16 characters of the formatted values. To revert to this previous behavior, you can use the TRUNCATE option in the CLASS statement.

In any case, you can use formats to group values into levels. See the discussion of the FORMAT procedure in the *Base SAS Procedures Guide* and the discussions of the FORMAT statement and SAS formats in *SAS Formats and Informats: Reference*. You can adjust the order of CLASS variable levels with the **ORDER=** option in the **PROC ANOVA** statement. You can specify the following REF= option to indicate how the levels of an individual classification variable are to be ordered by enclosing it in parentheses after the variable name:

REF= 'level' | FIRST | LAST

specifies a level of the classification variable to be put at the end of the list of levels. This level thus corresponds to the reference level in the usual interpretation of the estimates with PROC ANOVA's singular parameterization. You can specify the *level* of the variable to use as the reference level; specify a value that corresponds to the formatted value of the variable if a format is assigned. Alternatively, you can specify REF=FIRST to designate that the first ordered level serve as the reference, or

REF=LAST to designate that the last ordered level serve as the reference. To specify that REF=FIRST or REF=LAST be used for all classification variables, use the **REF=** *global-option* after the slash (/) in the CLASS statement.

You can specify the following *global-options* in the CLASS statement after a slash (/):

REF=FIRST | LAST

specifies a level of all classification variables to be put at the end of the list of levels. This level thus corresponds to the reference level in the usual interpretation of the estimates with PROC ANOVA's singular parameterization. Specify REF=FIRST to designate that the first ordered level for each classification variable serve as the reference. Specify REF=LAST to designate that the last ordered level serve as the reference. This option applies to all the variables specified in the CLASS statement. To specify different reference levels for different classification variables, use **REF=** options for individual variables.

TRUNCATE

specifies that class levels be determined by using only up to the first 16 characters of the formatted values of CLASS variables. When formatted values are longer than 16 characters, you can use this option to revert to the levels as determined in releases prior to SAS 9.

FREQ Statement

FREQ *variable* ;

The FREQ statement names a variable that provides frequencies for each observation in the **DATA=** data set. Specifically, if n is the value of the FREQ variable for a given observation, then that observation is used n times.

The analysis produced by using a FREQ statement reflects the expanded number of observations. For example, means and total degrees of freedom reflect the expanded number of observations. You can produce the same analysis (without the FREQ statement) by first creating a new data set that contains the expanded number of observations. For example, if the value of the FREQ variable is 5 for the first observation, the first 5 observations in the new data set would be identical. Each observation in the old data set would be replicated n_i times in the new data set, where n_i is the value of the FREQ variable for that observation.

If the value of the FREQ variable is missing or is less than 1, the observation is not used in the analysis. If the value is not an integer, only the integer portion is used.

If the FREQ statement is used, it must appear before the first RUN statement or it is ignored.

MANOVA Statement

MANOVA < *test-options* > < *detail-options* > ;

If the MODEL statement includes more than one dependent variable, you can perform multivariate analysis of variance with the MANOVA statement. The *test-options* define which effects to test, while the *detail-options* specify how to execute the tests and what results to display.

When a MANOVA statement appears before the first RUN statement, PROC ANOVA enters a multivariate mode with respect to the handling of missing values; in addition to observations with missing independent

variables, observations with *any* missing dependent variables are excluded from the analysis. If you want to use this mode of handling missing values but do not need any multivariate analyses, specify the MANOVA option in the `PROC ANOVA` statement.

Table 25.3 summarizes the options available in the MANOVA statement.

Table 25.3 MANOVA Statement Options

Option	Description
Test Options	
<code>H=</code>	Specifies hypothesis effects
<code>E=</code>	Specifies the error effect
<code>M=</code>	Specifies a transformation matrix for the dependent variables
<code>MNAMES=</code>	Provides names for the transformed variables
<code>PREFIX=</code>	Alternatively identifies the transformed variables
Detail Options	
<code>CANONICAL</code>	Displays a canonical analysis of the H and E matrices
<code>MSTAT=</code>	Specifies the method of evaluating the multivariate test statistics
<code>ORTH</code>	Orthogonalizes the rows of the transformation matrix
<code>PRINTE</code>	Displays the error SSCP matrix E
<code>PRINTH</code>	Displays the hypothesis SSCP matrix H
<code>SUMMARY</code>	Produces analysis-of-variance tables for each dependent variable

Test Options

You can specify the following options in the MANOVA statement as *test-options* in order to define which multivariate tests to perform.

`H=effects` | `INTERCEPT` | `_ALL_`

specifies effects in the preceding model to use as hypothesis matrices. For each SSCP matrix **H** associated with an effect, the `H=` specification computes an analysis based on the characteristic roots of $\mathbf{E}^{-1}\mathbf{H}$, where **E** is the matrix associated with the error effect. The characteristic roots and vectors are displayed, along with the Hotelling-Lawley trace, Pillai's trace, Wilks' lambda, and Roy's greatest root. By default, these statistics are tested with approximations based on the *F* distribution. To test them with exact (but computationally intensive) calculations, use the `MSTAT=EXACT` option.

Use the keyword `INTERCEPT` to produce tests for the intercept. To produce tests for all effects listed in the `MODEL` statement, use the keyword `_ALL_` in place of a list of effects.

For background and further details, see the section “[Multivariate Analysis of Variance](#)” on page 3366 in Chapter 42, “[The GLM Procedure](#).”

`E=effect`

specifies the error effect. If you omit the `E=` specification, the ANOVA procedure uses the error SSCP (residual) matrix from the analysis.

M=*equation, . . . , equation* | (*row-of-matrix, . . . , row-of-matrix*)

specifies a transformation matrix for the dependent variables listed in the **MODEL** statement. The equations in the **M=** specification are of the form

$$c_1 \times \text{dependent-variable} \pm c_2 \times \text{dependent-variable} \\ \dots \pm c_n \times \text{dependent-variable}$$

where the c_i values are coefficients for the various *dependent-variables*. If the value of a given c_i is 1, it can be omitted; in other words $1 \times Y$ is the same as Y . Equations should involve two or more dependent variables. For sample syntax, see the section “**Examples**” on page 921.

Alternatively, you can input the transformation matrix directly by entering the elements of the matrix with commas separating the rows, and parentheses surrounding the matrix. When this alternate form of input is used, the number of elements in each row must equal the number of dependent variables. Although these combinations actually represent the columns of the **M** matrix, they are displayed by rows.

When you include an **M=** specification, the analysis requested in the MANOVA statement is carried out for the variables defined by the equations in the specification, not the original dependent variables. If you omit the **M=** option, the analysis is performed for the original dependent variables in the **MODEL** statement.

If an **M=** specification is included without either the **MNAMES=** or the **PREFIX=** option, the variables are labeled MVAR1, MVAR2, and so forth by default.

For further information, see the section “**Multivariate Analysis of Variance**” on page 3366 in Chapter 42, “**The GLM Procedure**.”

MNAMES=*names*

provides names for the variables defined by the equations in the **M=** specification. Names in the list correspond to the **M=** equations or the rows of the **M** matrix (as it is entered).

PREFIX=*name*

is an alternative means of identifying the transformed variables defined by the **M=** specification. For example, if you specify **PREFIX=DIFF**, the transformed variables are labeled DIFF1, DIFF2, and so forth.

Detail Options

You can specify the following options in the MANOVA statement after a slash as *detail-options*:

CANONICAL

produces a canonical analysis of the **H** and **E** matrices (transformed by the **M** matrix, if specified) instead of the default display of characteristic roots and vectors.

MSTAT=FAPPROX**MSTAT=EXACT**

specifies the method of evaluating the multivariate test statistics. The default is **MSTAT=FAPPROX**, which specifies that the multivariate tests are evaluated by using the usual approximations based on the F distribution, as discussed in the “Multivariate Tests” section in Chapter 4, “[Introduction to Regression Procedures](#).” Alternatively, you can specify **MSTAT=EXACT** to compute exact p -values for three of the four tests (Wilks’ lambda, the Hotelling-Lawley trace, and Roy’s greatest root) and an improved F -approximation for the fourth (Pillai’s trace). While **MSTAT=EXACT** provides better control of the significance probability for the tests, especially for Roy’s Greatest Root, computations for the exact p -values can be appreciably more demanding, and are in fact infeasible for large problems (many dependent variables). Thus, although **MSTAT=EXACT** is more accurate for most data, it is not the default method. For more information about the results of **MSTAT=EXACT**, see the section “[Multivariate Analysis of Variance](#)” on page 3366 in Chapter 42, “[The GLM Procedure](#).”

ORTH

requests that the transformation matrix in the **M=** specification of the MANOVA statement be orthonormalized by rows before the analysis.

PRINTE

displays the error SSCP matrix **E**. If the **E** matrix is the error SSCP (residual) matrix from the analysis, the partial correlations of the dependent variables given the independent variables are also produced.

For example, the statement

```
manova / printe;
```

displays the error SSCP matrix and the partial correlation matrix computed from the error SSCP matrix.

PRINTH

displays the hypothesis SSCP matrix **H** associated with each effect specified by the **H=** specification.

SUMMARY

produces analysis-of-variance tables for each dependent variable. When no **M** matrix is specified, a table is produced for each original dependent variable from the **MODEL** statement; with an **M** matrix other than the identity, a table is produced for each transformed variable defined by the **M** matrix.

Examples

The following statements give several examples of using a MANOVA statement.

```
proc anova;
  class A B;
  model Y1-Y5=A B(A);
  manova h=A e=B(A) / printh printe;
  manova h=B(A) / printe;
  manova h=A e=B(A) m=Y1-Y2, Y2-Y3, Y3-Y4, Y4-Y5
    prefix=diff;

  manova h=A e=B(A) m=(1 -1 0 0 0,
                      0 1 -1 0 0,
                      0 0 1 -1 0,
                      0 0 0 1 -1) prefix=diff;

run;
```

The first MANOVA statement specifies A as the hypothesis effect and B(A) as the error effect. As a result of the **PRINTH** option, the procedure displays the hypothesis SSCP matrix associated with the A effect; and, as a result of the **PRINTE** option, the procedure displays the error SSCP matrix associated with the B(A) effect.

The second MANOVA statement specifies B(A) as the hypothesis effect. Since no error effect is specified, PROC ANOVA uses the error SSCP matrix from the analysis as the **E** matrix. The **PRINTE** option displays this **E** matrix. Since the **E** matrix is the error SSCP matrix from the analysis, the partial correlation matrix computed from this matrix is also produced.

The third MANOVA statement requests the same analysis as the first MANOVA statement, but the analysis is carried out for variables transformed to be successive differences between the original dependent variables. The **PREFIX=DIFF** specification labels the transformed variables as DIFF1, DIFF2, DIFF3, and DIFF4.

Finally, the fourth MANOVA statement has the identical effect as the third, but it uses an alternative form of the **M=** specification. Instead of specifying a set of equations, the fourth MANOVA statement specifies rows of a matrix of coefficients for the five dependent variables.

As a second example of the use of the **M=** specification, consider the following:

```
proc anova;
  class group;
  model dose1-dose4=group / nouni;
  manova h = group
    m = -3*dose1 - dose2 + dose3 + 3*dose4,
        dose1 - dose2 - dose3 + dose4,
        -dose1 + 3*dose2 - 3*dose3 + dose4
    mnames = Linear Quadratic Cubic
    / printe;

run;
```

The **M=** specification gives a transformation of the dependent variables dose1 through dose4 into orthogonal polynomial components, and the **MNAMES=** option labels the transformed variables as **LINEAR**, **QUADRATIC**, and **CUBIC**, respectively. Since the **PRINTE** option is specified and the default residual matrix is used as an error term, the partial correlation matrix of the orthogonal polynomial components is also produced.

For further information, see the section “Multivariate Analysis of Variance” on page 3366 in Chapter 42, “The GLM Procedure.”

MEANS Statement

MEANS *effects* </ options > ;

PROC ANOVA can compute means of the dependent variables for any effect that appears on the right-hand side in the **MODEL** statement.

You can use any number of MEANS statements, provided that they appear after the **MODEL** statement. For example, suppose A and B each have two levels. Then, if you use the following statements

```
proc anova;
  class A B;
  model Y=A B A*B;
  means A B / tukey;
  means A*B;
run;
```

means, standard deviations, and Tukey’s multiple comparison tests are produced for each level of the main effects A and B, and just the means and standard deviations for each of the four combinations of levels for A*B. Since multiple comparisons options apply only to main effects, the single MEANS statement

```
means A B A*B / tukey;
```

produces the same results.

Options are provided to perform multiple comparison tests for only main effects in the model. PROC ANOVA does not perform multiple comparison tests for interaction terms in the model; for multiple comparisons of interaction terms, see the LSMEANS statement in Chapter 42, “The GLM Procedure.”

Table 25.4 summarizes the options available in the MEANS statement.

Table 25.4 Options Available in the MEANS Statement

Option	Description
Perform multiple comparison tests	
BON	Performs Bonferroni t tests of differences between means for all main effect means
DUNCAN	Performs Duncan’s multiple range test on all main effect means
DUNNETT	Performs Dunnett’s two-tailed t test
DUNNETTL	Performs Dunnett’s one-tailed t test, testing if any treatment is significantly less than the control
DUNNETTU	Performs Dunnett’s one-tailed t test, testing if any treatment is significantly greater than the control
GABRIEL	Performs Gabriel’s multiple-comparison procedure on all main effect means
REGWQ	Performs the Ryan-Einot-Gabriel-Welsch multiple range test
SCHEFFE	Performs Scheffé’s multiple-comparison procedure
SIDAK	Performs pairwise t tests on differences between means with levels adjusted according to Sidak’s inequality

Table 25.4 *continued*

Option	Description
SMM or GT2	Performs pairwise comparisons based on the studentized maximum modulus and Sidak's uncorrelated-t inequality
SNK	Performs the Student-Newman-Keuls multiple range test
T or LSD	Performs pairwise t tests
TUKEY	Performs Tukey's studentized range test (HSD)
WALLER	Performs the Waller-Duncan k-ratio t test
Specify additional details for multiple comparison tests	
ALPHA=	Specifies the level of significance for comparisons among the means.
CLDIFF	Presents results from options as confidence intervals
CLM	Options as intervals for the mean of each level of the variables specified
E=	Specifies the error mean square used in the multiple comparisons
KRATIO=	Specifies the Type 1/Type 2 error seriousness ratio for the Waller-Duncan test
LINES	Presents results of options by listing the means in descending order and indicating nonsignificant subsets by line segments
NOSORT	Prevents the means from being sorted into descending order
Test for homogeneity of variances	
HOVTEST	Requests a homogeneity of variance test
Compensate for heterogeneous variances	
WELCH	Requests the Welch (1951) variance-weighted one-way ANOVA

Descriptions of these options follow. For a further discussion of these options, see the section “Multiple Comparisons” on page 3349 in Chapter 42, “The GLM Procedure.”

ALPHA= p

specifies the level of significance for comparisons among the means. By default, ALPHA=0.05. You can specify any value greater than 0 and less than 1.

BON

performs Bonferroni t tests of differences between means for all main effect means in the MEANS statement. See the CLDIFF and LINES options, which follow, for a discussion of how the procedure displays results.

CLDIFF

presents results of the BON, GABRIEL, SCHEFFE, SIDAK, SMM, GT2, T, LSD, and TUKEY options as confidence intervals for all pairwise differences between means, and the results of the DUNNETT, DUNNETTU, and DUNNETTL options as confidence intervals for differences with the control. The CLDIFF option is the default for unequal cell sizes unless the DUNCAN, REGWQ, SNK, or WALLER option is specified.

CLM

presents results of the BON, GABRIEL, SCHEFFE, SIDAK, SMM, T, and LSD options as intervals for the mean of each level of the variables specified in the MEANS statement. For all options except GABRIEL, the intervals are confidence intervals for the true means. For the GABRIEL option, they

are *comparison intervals* for comparing means pairwise: in this case, if the intervals corresponding to two means overlap, the difference between them is insignificant according to Gabriel's method.

DUNCAN

performs Duncan's multiple range test on all main effect means given in the MEANS statement. See the [LINES](#) option for a discussion of how the procedure displays results.

DUNNETT <(formatted-control-values)>

performs Dunnett's two-tailed *t* test, testing if any treatments are significantly different from a single control for all main effects means in the MEANS statement.

To specify which level of the effect is the control, enclose the formatted value in quotes in parentheses after the keyword. If more than one effect is specified in the MEANS statement, you can use a list of control values within the parentheses. By default, the first level of the effect is used as the control. For example,

```
means a / dunnett('CONTROL');
```

where CONTROL is the formatted control value of A. As another example,

```
means a b c / dunnett('CNTLA' 'CNTLB' 'CNTLC');
```

where CNTLA, CNTLB, and CNTLC are the formatted control values for A, B, and C, respectively.

DUNNETTL <(formatted-control-value)>

performs Dunnett's one-tailed *t* test, testing if any treatment is significantly less than the control. Control level information is specified as described previously for the [DUNNETT](#) option.

DUNNETTU <(formatted-control-value)>

performs Dunnett's one-tailed *t* test, testing if any treatment is significantly greater than the control. Control level information is specified as described previously for the [DUNNETT](#) option.

E=effect

specifies the error mean square used in the multiple comparisons. By default, PROC ANOVA uses the residual Mean Square (MS). The effect specified with the E= option must be a term in the model; otherwise, the procedure uses the residual MS.

GABRIEL

performs Gabriel's multiple-comparison procedure on all main effect means in the MEANS statement. See the [CLDIFF](#) and [LINES](#) options for discussions of how the procedure displays results.

GT2

see the [SMM](#) option.

HOVTEST**HOVTEST=BARTLETT****HOVTEST=BF****HOVTEST=LEVENE <(TYPE=ABS | SQUARE)>****HOVTEST=OBRIEN <(W=*number*)>**

requests a homogeneity of variance test for the groups defined by the MEANS effect. You can optionally specify a particular test; if you do not specify a test, Levene's test (Levene 1960) with TYPE=SQUARE is computed. Note that this option is ignored unless your MODEL statement specifies a simple one-way model.

The HOVTEST=BARTLETT option specifies Bartlett's test (Bartlett 1937), a modification of the normal-theory likelihood ratio test.

The HOVTEST=BF option specifies Brown and Forsythe's variation of Levene's test (Brown and Forsythe 1974).

The HOVTEST=LEVENE option specifies Levene's test (Levene 1960), which is widely considered to be the standard homogeneity of variance test. You can use the TYPE= option in parentheses to specify whether to use the absolute residuals (TYPE=ABS) or the squared residuals (TYPE=SQUARE) in Levene's test. The default is TYPE=SQUARE.

The HOVTEST=OBRIEN option specifies O'Brien's test (O'Brien 1979), which is basically a modification of HOVTEST=LEVENE(TYPE=SQUARE). You can use the W= option in parentheses to tune the variable to match the suspected kurtosis of the underlying distribution. By default, W=0.5, as suggested by O'Brien (1979, 1981).

See the section "Homogeneity of Variance in One-Way Models" on page 3362 in Chapter 42, "The GLM Procedure," for more details on these methods. Example 42.10 in the same chapter illustrates the use of the HOVTEST and WELCH options in the MEANS statement in testing for equal group variances.

KRATIO=*value*

specifies the Type 1/Type 2 error seriousness ratio for the Waller-Duncan test. Reasonable values for KRATIO are 50, 100, and 500, which roughly correspond for the two-level case to ALPHA levels of 0.1, 0.05, and 0.01. By default, the procedure uses the default value of 100.

LINES

presents results of the BON, DUNCAN, GABRIEL, REGWQ, SCHEFFE, SIDAK, SMM, GT2, SNK, T, LSD TUKEY, and WALLER options by listing the means in descending order and indicating non-significant subsets by line segments beside the corresponding means. The LINES option is appropriate for equal cell sizes, for which it is the default. The LINES option is also the default if the DUNCAN, REGWQ, SNK, or WALLER option is specified, or if there are only two cells of unequal size. If the cell sizes are unequal, the harmonic mean of the cell sizes is used, which might lead to somewhat liberal tests if the cell sizes are highly disparate. The LINES option cannot be used in combination with the DUNNETT, DUNNETTL, or DUNNETTU option. In addition, the procedure has a restriction that no more than 24 overlapping groups of means can exist. If a mean belongs to more than 24 groups, the procedure issues an error message. You can either reduce the number of levels of the variable or use a multiple comparison test that allows the CLDIFF option rather than the LINES option.

LSD

see the **T** option.

NOSORT

prevents the means from being sorted into descending order when the **CLDIFF** or **CLM** option is specified.

REGWQ

performs the Ryan-Einot-Gabriel-Welsch multiple range test on all main effect means in the **MEANS** statement. See the **LINES** option for a discussion of how the procedure displays results.

SCHEFFE

performs Scheffé's multiple-comparison procedure on all main effect means in the **MEANS** statement. See the **CLDIFF** and **LINES** options for discussions of how the procedure displays results.

SIDAK

performs pairwise t tests on differences between means with levels adjusted according to Sidak's inequality for all main effect means in the **MEANS** statement. See the **CLDIFF** and **LINES** options for discussions of how the procedure displays results.

SMM**GT2**

performs pairwise comparisons based on the studentized maximum modulus and Sidak's uncorrelated- t inequality, yielding Hochberg's GT2 method when sample sizes are unequal, for all main effect means in the **MEANS** statement. See the **CLDIFF** and **LINES** options for discussions of how the procedure displays results.

SNK

performs the Student-Newman-Keuls multiple range test on all main effect means in the **MEANS** statement. See the **LINES** option for a discussion of how the procedure displays results.

T**LSD**

performs pairwise t tests, equivalent to Fisher's least-significant-difference test in the case of equal cell sizes, for all main effect means in the **MEANS** statement. See the **CLDIFF** and **LINES** options for discussions of how the procedure displays results.

TUKEY

performs Tukey's studentized range test (HSD) on all main effect means in the **MEANS** statement. (When the group sizes are different, this is the Tukey-Kramer test.) See the **CLDIFF** and **LINES** options for discussions of how the procedure displays results.

WALLER

performs the Waller-Duncan k -ratio t test on all main effect means in the **MEANS** statement. See the **KRATIO=** option for information about controlling details of the test, and see the **LINES** option for a discussion of how the procedure displays results.

WELCH

requests Welch's (1951) variance-weighted one-way ANOVA. This alternative to the usual analysis of variance for a one-way model is robust to the assumption of equal within-group variances. This option is ignored unless your **MODEL** statement specifies a simple one-way model.

Note that using the WELCH option merely produces one additional table consisting of Welch's ANOVA. It does not affect all of the other tests displayed by the ANOVA procedure, which still require the assumption of equal variance for exact validity.

See the section “Homogeneity of Variance in One-Way Models” on page 3362 in Chapter 42, “The GLM Procedure,” for more details on Welch's ANOVA. Example 42.10 in the same chapter illustrates the use of the HOVTEST and WELCH options in the MEANS statement in testing for equal group variances.

MODEL Statement

MODEL *dependents = effects* </ options > ;

The MODEL statement names the dependent variables and independent effects. The syntax of effects is described in the section “Specification of Effects” on page 932. For any model effect involving classification variables (interactions as well as main effects), the number of levels cannot exceed 32,767. If no independent effects are specified, only an intercept term is fit. This tests the hypothesis that the mean of the dependent variable is zero. All variables in effects that you specify in the MODEL statement must appear in the CLASS statement because PROC ANOVA does not allow for continuous effects.

You can specify the following options in the MODEL statement; they must be separated from the list of independent effects by a slash.

INTERCEPT

INT

displays the hypothesis tests associated with the intercept as an effect in the model. By default, the procedure includes the intercept in the model but does not display associated tests of hypotheses. Except for producing the uncorrected total SS instead of the corrected total SS, the INT option is ignored when you use an ABSORB statement.

NOUNI

suppresses the display of univariate statistics. You typically use the NOUNI option with a multivariate or repeated measures analysis of variance when you do not need the standard univariate output. The NOUNI option in a MODEL statement does not affect the univariate output produced by the REPEATED statement.

REPEATED Statement

REPEATED *factor-specification* </ options > ;

When values of the dependent variables in the MODEL statement represent repeated measurements on the same experimental unit, the REPEATED statement enables you to test hypotheses about the measurement factors (often called *within-subject factors*), as well as the interactions of within-subject factors with independent variables in the MODEL statement (often called *between-subject factors*). The REPEATED statement provides multivariate and univariate tests as well as hypothesis tests for a variety of single-degree-of-freedom contrasts. There is no limit to the number of within-subject factors that can be specified. For more details, see the section “Repeated Measures Analysis of Variance” on page 3367 in Chapter 42, “The GLM Procedure.”

The REPEATED statement is typically used for handling repeated measures designs with one repeated response variable. Usually, the variables on the left-hand side of the equation in the MODEL statement represent one repeated response variable.

This does not mean that only one factor can be listed in the REPEATED statement. For example, one repeated response variable (hemoglobin count) might be measured 12 times (implying variables Y1 to Y12 on the left-hand side of the equal sign in the MODEL statement), with the associated within-subject factors treatment and time (implying two factors listed in the REPEATED statement). See the section “Examples” on page 931 for an example of how PROC ANOVA handles this case.

Designs with two or more repeated response variables can, however, be handled with the IDENTITY transformation; see Example 42.9 in Chapter 42, “The GLM Procedure,” for an example of analyzing a doubly-multivariate repeated measures design.

When a REPEATED statement appears, the ANOVA procedure enters a multivariate mode of handling missing values. If any values for variables corresponding to each combination of the within-subject factors are missing, the observation is excluded from the analysis.

The simplest form of the REPEATED statement requires only a *factor-name*. With two repeated factors, you must specify the *factor-name* and number of levels (*levels*) for each factor. Optionally, you can specify the actual values for the levels (*level-values*), a *transformation* that defines single-degree-of freedom contrasts, and *options* for additional analyses and output. When more than one within-subject factor is specified, *factor-names* (and associated level and transformation information) must be separated by a comma in the REPEATED statement. These terms are described in the following section, “Syntax Details.”

Syntax Details

Table 25.5 summarizes the options available in the REPEATED statement.

Table 25.5 PROC REPEATED Statement Options

Option	Description
CANONICAL	Performs a canonical analysis of the H and E matrices
MSTAT=FAPPROX	Specifies the method of evaluating the multivariate test statistics
NOM	Displays only the results of the univariate analyses
NOU	Displays only the results of the multivariate analyses
PRINTE	Displays the E matrix
PRINTH	Displays the H (SSCP) matrix
PRINTM	Displays the transformation matrices that define the contrasts
PRINTRV	Produces the characteristic roots and vectors
SUMMARY	Produces analysis-of-variance tables for each contrast
UEPSDEF=	Specifies the univariate <i>F</i> test adjustment

You can specify the following terms in the REPEATED statement.

factor-specification

The *factor-specification* for the REPEATED statement can include any number of individual factor specifications, separated by commas, of the following form:

factor-name levels <(level-values)> <transformation>

where

factor-name names a factor to be associated with the dependent variables. The name should not be the same as any variable name that already exists in the data set being analyzed and should conform to the usual conventions of SAS variable names.

When specifying more than one factor, list the dependent variables in the **MODEL** statement so that the within-subject factors defined in the **REPEATED** statement are nested; that is, the first factor defined in the **REPEATED** statement should be the one with values that change least frequently.

levels specifies the number of levels associated with the factor being defined. When there is only one within-subject factor, the number of levels is equal to the number of dependent variables. In this case, *levels* is optional. When more than one within-subject factor is defined, however, *levels* is required, and the product of the number of levels of all the factors must equal the number of dependent variables in the **MODEL** statement.

(level-values) specifies values that correspond to levels of a repeated-measures factor. These values are used to label output; they are also used as spacings for constructing orthogonal polynomial contrasts if you specify a **POLYNOMIAL** transformation. The number of level values specified must correspond to the number of levels for that factor in the **REPEATED** statement. Enclose the *level-values* in parentheses.

The following *transformation* keywords define single-degree-of-freedom contrasts for factors specified in the **REPEATED** statement. Since the number of contrasts generated is always one less than the number of levels of the factor, you have some control over which contrast is omitted from the analysis by which transformation you select. The only exception is the **IDENTITY** transformation; this transformation is not composed of contrasts, and it has the same degrees of freedom as the factor has levels. By default, the procedure uses the **CONTRAST** transformation.

CONTRAST< (*ordinal-reference-level*) >

generates contrasts between levels of the factor and a reference level. By default, the procedure uses the last level; you can optionally specify a reference level in parentheses after the keyword **CONTRAST**. The reference level corresponds to the ordinal value of the level rather than the level value specified. For example, to generate contrasts between the first level of a factor and the other levels, use

```
contrast (1)
```

HELMERT

generates contrasts between each level of the factor and the mean of subsequent levels.

IDENTITY

generates an identity transformation corresponding to the associated factor. This transformation is *not* composed of contrasts; it has n degrees of freedom for an n -level factor, instead of $n - 1$. This can be used for doubly-multivariate repeated measures.

MEAN< (ordinal-reference-level) >

generates contrasts between levels of the factor and the mean of all other levels of the factor. Specifying a reference level eliminates the contrast between that level and the mean. Without a reference level, the contrast involving the last level is omitted. See the **CONTRAST** transformation for an example.

POLYNOMIAL

generates orthogonal polynomial contrasts. Level values, if provided, are used as spacings in the construction of the polynomials; otherwise, equal spacing is assumed.

PROFILE

generates contrasts between adjacent levels of the factor.

For examples of the transformation matrices generated by these contrast transformations, see the section “Repeated Measures Analysis of Variance” on page 3367 in Chapter 42, “The GLM Procedure.”

You can specify the following options in the REPEATED statement after a slash:

CANONICAL

performs a canonical analysis of the **H** and **E** matrices corresponding to the transformed variables specified in the REPEATED statement.

MSTAT=FAPPROX**MSTAT=EXACT**

specifies the method of evaluating the multivariate test statistics. The default is **MSTAT=FAPPROX**, which specifies that the multivariate tests are evaluated by using the usual approximations based on the *F* distribution, as discussed in the “Multivariate Tests” section in Chapter 4, “Introduction to Regression Procedures.” Alternatively, you can specify **MSTAT=EXACT** to compute exact *p*-values for three of the four tests (Wilks’ lambda, the Hotelling-Lawley trace, and Roy’s greatest root) and an improved *F*-approximation for the fourth (Pillai’s trace). While **MSTAT=EXACT** provides better control of the significance probability for the tests, especially for Roy’s Greatest Root, computations for the exact *p*-values can be appreciably more demanding, and are in fact infeasible for large problems (many dependent variables). Thus, although **MSTAT=EXACT** is more accurate for most data, it is not the default method. For more information about the results of **MSTAT=EXACT**, see the section “Multivariate Analysis of Variance” on page 3366 in Chapter 42, “The GLM Procedure.”

NOM

displays only the results of the univariate analyses.

NOU

displays only the results of the multivariate analyses.

PRINTE

displays the **E** matrix for each combination of within-subject factors, as well as partial correlation matrices for both the original dependent variables and the variables defined by the transformations specified in the REPEATED statement. In addition, the **PRINTE** option provides sphericity tests for each set of transformed variables. If the requested transformations are not orthogonal, the **PRINTE** option also provides a sphericity test for a set of orthogonal contrasts.

PRINTH

displays the **H** (SSCP) matrix associated with each multivariate test.

PRINTM

displays the transformation matrices that define the contrasts in the analysis. PROC ANOVA always displays the **M** matrix so that the transformed variables are defined by the rows, not the columns, of the displayed **M** matrix. In other words, PROC ANOVA actually displays **M'**.

PRINTRV

produces the characteristic roots and vectors for each multivariate test.

SUMMARY

produces analysis-of-variance tables for each contrast defined by the within-subjects factors. Along with tests for the effects of the independent variables specified in the **MODEL** statement, a term labeled **MEAN** tests the hypothesis that the overall mean of the contrast is zero.

UEPSDEF=unbiased-epsilon-definition

specifies the type of adjustment for the univariate *F* test that is displayed in addition to the Greenhouse-Geisser adjustment. The default is **UEPSDEF=HFL**, corresponding to the corrected form of the Huynh-Feldt adjustment (Huynh and Feldt 1976; Lecoutre 1991). Other alternatives are **UEPSDEF=HF**, the uncorrected Huynh-Feldt adjustment (the only available method in previous releases of SAS/STAT software), and **UEPSDEF=CM**, the adjustment of Chi et al. (2012). See the section “[Hypothesis Testing in Repeated Measures Analysis](#)” on page 3370 in Chapter 42, “[The GLM Procedure](#),” for details about these adjustments.

Examples

When specifying more than one factor, list the dependent variables in the **MODEL** statement so that the within-subject factors defined in the **REPEATED** statement are nested; that is, the first factor defined in the **REPEATED** statement should be the one with values that change least frequently. For example, assume that three treatments are administered at each of four times, for a total of twelve dependent variables on each experimental unit. If the variables are listed in the **MODEL** statement as Y1 through Y12, then the following **REPEATED** statement

```
repeated trt 3, time 4;
```

implies the following structure:

	Dependent Variables											
	Y1	Y2	Y3	Y4	Y5	Y6	Y7	Y8	Y9	Y10	Y11	Y12
Value of trt	1	1	1	1	2	2	2	2	3	3	3	3
Value of time	1	2	3	4	1	2	3	4	1	2	3	4

The **REPEATED** statement always produces a table like the preceding one.

For more information about repeated measures analysis and about using the **REPEATED** statement, see the section “[Repeated Measures Analysis of Variance](#)” on page 3367 in Chapter 42, “[The GLM Procedure](#).”

TEST Statement

TEST < **H= effects** > **E= effect** ;

Although an F value is computed for all SS in the analysis by using the residual MS as an error term, you can request additional F tests that use other effects as error terms. You need a TEST statement when a nonstandard error structure (as in a split plot) exists.

CAUTION: The ANOVA procedure does not check any of the assumptions underlying the F statistic. When you specify a TEST statement, you assume sole responsibility for the validity of the F statistic produced. To help validate a test, you might want to use the GLM procedure with the RANDOM statement and inspect the expected mean squares. In the GLM procedure, you can also use the TEST option in the RANDOM statement.

You can use as many TEST statements as you want, provided that they appear after the MODEL statement.

You can specify the following terms in the TEST statement.

H=effects

specifies which effects in the preceding model are to be used as hypothesis (numerator) effects.

E=effect

specifies one, and only one, effect to use as the error (denominator) term. The **E=** specification is required.

The following example uses two TEST statements and is appropriate for analyzing a split-plot design.

```
proc anova;
  class a b c;
  model y=a|b(a)|c;
  test h=a e=b(a);
  test h=c a*c e=b*c(a);
run;
```

Details: ANOVA Procedure

Specification of Effects

In SAS analysis-of-variance procedures, the variables that identify levels of the classifications are called *classification variables*, and they are declared in the CLASS statement. Classification variables are also called *categorical*, *qualitative*, *discrete*, or *nominal variables*. The values of a classification variable are called *levels*. Classification variables can be either numeric or character. This is in contrast to the *response* (or *dependent*) variables, which are continuous. Response variables must be numeric.

The analysis-of-variance model specifies *effects*, which are combinations of classification variables used to explain the variability of the dependent variables in the following manner:

- Main effects are specified by writing the variables by themselves in the **CLASS** statement: A B C. Main effects used as independent variables test the hypothesis that the mean of the dependent variable is the same for each level of the factor in question, ignoring the other independent variables in the model.
- Crossed effects (interactions) are specified by joining the **CLASS** variables with asterisks in the **MODEL** statement: A*B A*C A*B*C. Interaction terms in a model test the hypothesis that the effect of a factor does not depend on the levels of the other factors in the interaction.
- Nested effects are specified by following a main effect or crossed effect with a **CLASS** variable or list of **CLASS** variables enclosed in parentheses in the **MODEL** statement. The main effect or crossed effect is nested within the effects listed in parentheses: B(A) C*D(A B). Nested effects test hypotheses similar to interactions, but the levels of the nested variables are not the same for every combination within which they are nested.

The general form of an effect can be illustrated by using the **CLASS** variables A, B, C, D, E, and F:

A * B * C(D E F)

The crossed list should come first, followed by the nested list in parentheses. Note that no asterisks appear within the nested list or immediately before the left parenthesis.

Main Effects Models

For a three-factor main effects model with A, B, and C as the factors and Y as the dependent variable, the necessary statements are

```
proc anova;
  class A B C;
  model Y=A B C;
run;
```

Models with Crossed Factors

To specify interactions in a factorial model, join effects with asterisks as described previously. For example, these statements specify a complete factorial model, which includes all the interactions:

```
proc anova;
  class A B C;
  model Y=A B C A*B A*C B*C A*B*C;
run;
```

Bar Notation

You can shorten the specifications of a full factorial model by using bar notation. For example, the preceding statements can also be written


```
proc anova;
  class A B C;
  model Y=A|B|C;
run;
```

When the bar (|) is used, the expression on the right side of the equal sign is expanded from left to right by using the equivalents of rules 2–4 given in Searle (1971, p. 390). The variables on the right- and left-hand sides of the bar become effects, and the cross of them becomes an effect. Multiple bars are permitted. For instance, $A|B|C$ is evaluated as follows:

$$\begin{aligned} A|B|C &\rightarrow \{A|B\}|C \\ &\rightarrow \{A\ B\ A*B\}|C \\ &\rightarrow A\ B\ A*B\ C\ A*C\ B*C\ A*B*C \end{aligned}$$

You can also specify the maximum number of variables involved in any effect that results from bar evaluation by specifying that maximum number, preceded by an @ sign, at the end of the bar effect. For example, the specification $A|B|C@2$ results in only those effects that contain two or fewer variables; in this case, $A\ B\ A*B\ C\ A*C$ and $B*C$.

The following table gives more examples of using the bar and at operators.

$A C(B)$	is equivalent to	$A\ C(B)\ A*C(B)$
$A(B) C(B)$	is equivalent to	$A(B)\ C(B)\ A*C(B)$
$A(B) B(D\ E)$	is equivalent to	$A(B)\ B(D\ E)$
$A B(A) C$	is equivalent to	$A\ B(A)\ C\ A*C\ B*C(A)$
$A B(A) C@2$	is equivalent to	$A\ B(A)\ C\ A*C$
$A B C D@2$	is equivalent to	$A\ B\ A*B\ C\ A*C\ B*C\ D\ A*D\ B*D\ C*D$

Consult the section “Specification of Effects” on page 3324 in Chapter 42, “The GLM Procedure,” for further details on bar notation.

Nested Models

Write the effect that is nested within another effect first, followed by the other effect in parentheses. For example, if A and B are main effects and C is nested within A and B (that is, the levels of C that are observed are not the same for each combination of A and B), the statements for PROC ANOVA are

```
proc anova;
  class A B C;
  model y=A B C(A B);
run;
```

The identity of a level is viewed within the context of the level of the containing effects. For example, if City is nested within State, then the identity of City is viewed within the context of State.

The distinguishing feature of a nested specification is that nested effects never appear as main effects. Another way of viewing nested effects is that they are effects that pool the main effect with the interaction of the nesting variable.

See the “Automatic Pooling” section, which follows.

Models Involving Nested, Crossed, and Main Effects

Asterisks and parentheses can be combined in the `MODEL` statement for models involving nested and crossed effects:

```
proc anova;
  class A B C;
  model Y=A B(A) C(A) B*C(A);
run;
```

Automatic Pooling

In line with the general philosophy of the GLM procedure, there is no difference between the statements

```
model Y=A B(A);
```

and

```
model Y=A A*B;
```

The effect `B` becomes a nested effect by virtue of the fact that it does not occur as a main effect. If `B` is not written as a main effect in addition to participating in `A*B`, then the sum of squares that is associated with `B` is pooled into `A*B`.

This feature allows the automatic pooling of sums of squares. If an effect is omitted from the model, it is automatically pooled with all the higher-level effects containing the `CLASS` variables in the omitted effect (or within-error). This feature is most useful in split-plot designs.

Using PROC ANOVA Interactively

PROC ANOVA can be used interactively. After you specify a model in a `MODEL` statement and run PROC ANOVA with a `RUN` statement, a variety of statements (such as `MEANS`, `MANOVA`, `TEST`, and `REPEATED`) can be executed without PROC ANOVA recalculating the model sum of squares.

The section “Syntax: ANOVA Procedure” on page 912 describes which statements can be used interactively. You can execute these interactive statements individually or in groups by following the single statement or group of statements with a `RUN` statement. Note that the `MODEL` statement cannot be repeated; the ANOVA procedure allows only one `MODEL` statement.

If you use PROC ANOVA interactively, you can end the procedure with a `DATA` step, another PROC step, an `ENDSAS` statement, or a `QUIT` statement. The syntax of the `QUIT` statement is

```
quit;
```

When you use PROC ANOVA interactively, additional `RUN` statements do not end the procedure but tell PROC ANOVA to execute additional statements.

When a `WHERE` statement is used with PROC ANOVA, it should appear before the first `RUN` statement. The `WHERE` statement enables you to select only certain observations for analysis without using a subsetting `DATA` step. For example, the statement `where group ne 5` omits observations with `GROUP=5` from the analysis. See *SAS Statements: Reference* for details about this statement.

When a **BY** statement is used with PROC ANOVA, interactive processing is not possible; that is, once the first RUN statement is encountered, processing proceeds for each BY group in the data set, and no further statements are accepted by the procedure.

Interactivity is also disabled when there are different patterns of missing values among the dependent variables. For details, see the section “Missing Values,” which follows.

Missing Values

For an analysis involving one dependent variable, PROC ANOVA uses an observation if values are nonmissing for that dependent variable and for all the variables used in independent effects.

For an analysis involving multiple dependent variables without the **MANOVA** or **REPEATED** statement, or without the **MANOVA** option in the PROC ANOVA statement, a missing value in one dependent variable does not eliminate the observation from the analysis of other nonmissing dependent variables. For an analysis with the **MANOVA** or **REPEATED** statement, or with the **MANOVA** option in the PROC ANOVA statement, the ANOVA procedure requires values for all dependent variables to be nonmissing for an observation before the observation can be used in the analysis.

During processing, PROC ANOVA groups the dependent variables by their pattern of missing values across observations so that sums and cross products can be collected in the most efficient manner.

If your data have different patterns of missing values among the dependent variables, interactivity is disabled. This could occur when some of the variables in your data set have missing values and either of the following conditions obtain:

- You do not use the **MANOVA** option in the PROC ANOVA statement.
- You do not use a **MANOVA** or **REPEATED** statement before the first RUN statement.

Output Data Set

The **OUTSTAT=** option in the PROC ANOVA statement produces an output data set that contains the following:

- the BY variables, if any
- **_TYPE_**, a new character variable. This variable has the value ‘ANOVA’ for observations corresponding to sums of squares; it has the value ‘CANCORR’, ‘STRUCTUR’, or ‘SCORE’ if a canonical analysis is performed through the **MANOVA** statement and no **M=** matrix is specified.
- **_SOURCE_**, a new character variable. For each observation in the data set, **_SOURCE_** contains the name of the model effect from which the corresponding statistics are generated.
- **_NAME_**, a new character variable. The variable **_NAME_** contains the name of one of the dependent variables in the model or, in the case of canonical statistics, the name of one of the canonical variables (CAN1, CAN2, and so on).

- four new numeric variables, SS, DF, F, and PROB, containing sums of squares, degrees of freedom, F values, and probabilities, respectively, for each model or contrast sum of squares generated in the analysis. For observations resulting from canonical analyses, these variables have missing values.
- if there is more than one dependent variable, then variables with the same names as the dependent variables represent
 - for `_TYPE_='ANOVA'`, the crossproducts of the hypothesis matrices
 - for `_TYPE_='CANCORR'`, canonical correlations for each variable
 - for `_TYPE_='STRUCTUR'`, coefficients of the total structure matrix
 - for `_TYPE_='SCORE'`, raw canonical score coefficients

The output data set can be used to perform special hypothesis tests (for example, with the IML procedure in SAS/IML software), to reformat output, to produce canonical variates (through the SCORE procedure), or to rotate structure matrices (through the FACTOR procedure).

Computational Method

Let \mathbf{X} represent the $n \times p$ design matrix. The columns of \mathbf{X} contain only 0s and 1s. Let \mathbf{Y} represent the $n \times 1$ vector of dependent variables.

In the GLM procedure, $\mathbf{X}'\mathbf{X}$, $\mathbf{X}'\mathbf{Y}$, and $\mathbf{Y}'\mathbf{Y}$ are formed in main storage. However, in the ANOVA procedure, only the diagonals of $\mathbf{X}'\mathbf{X}$ are computed, along with $\mathbf{X}'\mathbf{Y}$ and $\mathbf{Y}'\mathbf{Y}$. Thus, PROC ANOVA saves a considerable amount of storage as well as time. The memory requirements for PROC ANOVA are asymptotically linear functions of n^2 and nr , where n is the number of dependent variables and r the number of independent parameters.

The elements of $\mathbf{X}'\mathbf{Y}$ are cell totals, and the diagonal elements of $\mathbf{X}'\mathbf{X}$ are cell frequencies. Since PROC ANOVA automatically pools omitted effects into the next higher-level effect containing the names of the omitted effect (or within-error), a slight modification to the rules given by Searle (1971, p. 389) is used.

1. PROC ANOVA computes the sum of squares for each effect as if it is a main effect. In other words, for each effect, PROC ANOVA squares each cell total and divides by its cell frequency. The procedure then adds these quantities together and subtracts the correction factor for the mean (total squared over N).
2. For each effect involving two **CLASS** variable names, PROC ANOVA subtracts the SS for any main effect with a name that is contained in the two-factor effect.
3. For each effect involving three **CLASS** variable names, PROC ANOVA subtracts the SS for all main effects and two-factor effects with names that are contained in the three-factor effect. If effects involving four or more **CLASS** variable names are present, the procedure continues this process.

Displayed Output

PROC ANOVA first displays a table that includes the following:

- the name of each variable in the **CLASS** statement
- the number of different values or Levels of the **CLASS** variables
- the Values of the **CLASS** variables
- the Number of observations in the data set and the number of observations excluded from the analysis because of missing values, if any

PROC ANOVA then displays an analysis-of-variance table for each dependent variable in the **MODEL** statement. This table breaks down the Total Sum of Squares for the dependent variable into the portion attributed to the Model and the portion attributed to Error. It also breaks down the Mean Square term, which is the Sum of Squares divided by the degrees of freedom (DF). The analysis-of-variance table also lists the following:

- the Mean Square for Error (MSE), which is an estimate of σ^2 , the variance of the true errors
- the F Value, which is the ratio produced by dividing the Mean Square for the Model by the Mean Square for Error. It tests how well the model as a whole (adjusted for the mean) accounts for the dependent variable's behavior. This *F* test is a test of the null hypothesis that all parameters except the intercept are zero.
- the significance probability associated with the *F* statistic, labeled "Pr > F"
- R-Square, R^2 , which measures how much variation in the dependent variable can be accounted for by the model. The R square statistic, which can range from 0 to 1, is the ratio of the sum of squares for the model divided by the sum of squares for the corrected total. In general, the larger the R square value, the better the model fits the data.
- C.V., the coefficient of variation, which is often used to describe the amount of variation in the population. The C.V. is 100 times the standard deviation of the dependent variable divided by the Mean. The coefficient of variation is often a preferred measure because it is unitless.
- Root MSE, which estimates the standard deviation of the dependent variable. Root MSE is computed as the square root of Mean Square for Error, the mean square of the error term.
- the Mean of the dependent variable

For each effect (or source of variation) in the model, PROC ANOVA then displays the following:

- DF, degrees of freedom
- Anova SS, the sum of squares, and the associated Mean Square
- the F Value for testing the hypothesis that the group means for that effect are equal

- $Pr > F$, the significance probability value associated with the F Value

When you specify a **TEST** statement, PROC ANOVA displays the results of the requested tests. When you specify a **MANOVA** statement and the model includes more than one dependent variable, PROC ANOVA produces these additional statistics:

- the characteristic roots and vectors of $E^{-1}H$ for each **H** matrix
- the Hotelling-Lawley trace
- Pillai's trace
- Wilks' lambda
- Roy's greatest root

See [Example 42.6](#) in Chapter 42, “The GLM Procedure,” for an example of the MANOVA results. These MANOVA tests are discussed in Chapter 4, “Introduction to Regression Procedures.”

ODS Table Names

PROC ANOVA assigns a name to each table it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in [Table 25.6](#). For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

Table 25.6 ODS Tables Produced by PROC ANOVA

ODS Table Name	Description	Statement / Option
AltErrTests	Anova tests with error other than MSE	TEST E=
Bartlett	Bartlett's homogeneity of variance test	MEANS / HOVTEST=BARTLETT
CLDiffs	Multiple comparisons of pairwise differences	MEANS / CLDIFF or DUNNETT or (Unequal cells and not LINES)
CLDiffsInfo	Information for multiple comparisons of pairwise differences	MEANS / CLDIFF or DUNNETT or (Unequal cells and not LINES)
CLMeans	Multiple comparisons of means with confidence/comparison interval	MEANS / CLM with (BON or GABRIEL or SCHEFFE or SIDAK or SMM or T or LSD)
CLMeansInfo	Information for multiple comparisons of means with confidence/comparison interval	MEANS / CLM
CanAnalysis	Canonical analysis	(MANOVA or REPEATED) / CANONICAL
CanCoef	Canonical coefficients	(MANOVA or REPEATED) / CANONICAL

Table 25.6 continued

ODS Table Name	Description	Statement / Option
CanStructure	Canonical structure	(MANOVA or REPEATED) / CANONICAL
CharStruct	Characteristic roots and vectors	(MANOVA / not CANONICAL) or (REPEATED / PRINTRV)
ClassLevels	Classification variable levels	CLASS statement
DependentInfo	Simultaneously analyzed dependent variables	default when there are multiple dependent variables with different patterns of missing values
Epsilons	Greenhouse-Geisser and Huynh-Feldt epsilons	REPEATED statement
ErrorSSCP	Error SSCP matrix	(MANOVA or REPEATED) / PRINTE
FitStatistics	R-Square, C.V., Root MSE, and dependent mean	default
HOVFTest	Homogeneity of variance ANOVA	MEANS / HOVTEST
HypothesisSSCP	Hypothesis SSCP matrix	(MANOVA or REPEATED) / PRINTE
MANOVATransform	Multivariate transformation matrix	MANOVA / M=
MCLines	Multiple comparisons output	MEANS / LINES or ((DUNCAN or WALLER or SNK or REGWQ) and not (CLDIFF or CLM)) or (Equal cells and not CLDIFF)
MCLinesInfo	Information for multiple comparison output	MEANS / LINES or ((DUNCAN or WALLER or SNK or REGWQ) and not (CLDIFF or CLM)) or (Equal cells and not CLDIFF)
MCLinesRange	Ranges for multiple range MC tests	MEANS / LINES or ((DUNCAN or WALLER or SNK or REGWQ) and not (CLDIFF or CLM)) or (Equal cells and not CLDIFF)
Means	Group means	MEANS statement
ModelANOVA	ANOVA for model terms	default
MultStat	Multivariate tests	MANOVA statement
NObs	Number of observations	default
OverallANOVA	Over-all ANOVA	default
PartialCorr	Partial correlation matrix	(MANOVA or REPEATED) / PRINTE
RepeatedTransform	Repeated transformation matrix	REPEATED (CONTRAST or HELMERT or MEAN or POLYNOMIAL or PROFILE)

Table 25.6 *continued*

ODS Table Name	Description	Statement / Option
RepeatedLevelInfo	Correspondence between dependents and repeated measures levels	REPEATED statement
Sphericity Tests	Sphericity tests Summary ANOVA for specified MANOVA H= effects	REPEATED / PRINTE MANOVA / H= SUMMARY
Welch	Welch's ANOVA	MEANS / WELCH

ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “Statistical Graphics Using ODS.”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “A Primer on ODS Statistical Graphics” on page 599 in Chapter 21, “Statistical Graphics Using ODS.”

When ODS Graphics is enabled, if you specify a one-way analysis of variance model, with just one independent classification variable, or if you use a MEANS statement, then the ANOVA procedure will produce a grouped box plot of the response values versus the classification levels. For an example of the box plot, see the section “One-Way Layout with Means Comparisons” on page 904.

ODS Graph Names

PROC ANOVA produces a single graph, the name of which you can use for referencing it in ODS. The name is listed in Table 25.7.

Table 25.7 ODS Graphic Produced by PROC ANOVA

ODS Graph Name	Plot Description
BoxPlot	Box plot of observed response values by classification levels

Examples: ANOVA Procedure

Example 25.1: Randomized Complete Block With Factorial Treatment Structure

This example uses statements for the analysis of a randomized block with two treatment factors occurring in a factorial structure. The data, from Neter, Wasserman, and Kutner (1990, p. 941), are from an experiment examining the effects of codeine and acupuncture on post-operative dental pain in male subjects. Both treatment factors have two levels. The codeine levels are a codeine capsule or a sugar capsule. The acupuncture levels are two inactive acupuncture points or two active acupuncture points. There are four distinct treatment combinations due to the factorial treatment structure. The 32 subjects are assigned to eight blocks of four subjects each based on an assessment of pain tolerance.

The data for the analysis are balanced, so PROC ANOVA is used. The data are as follows:

```

title1 'Randomized Complete Block With Two Factors';
data PainRelief;
  input PainLevel Codeine Acupuncture Relief @@;
  datalines;
1 1 1 0.0 1 2 1 0.5 1 1 2 0.6 1 2 2 1.2
2 1 1 0.3 2 2 1 0.6 2 1 2 0.7 2 2 2 1.3
3 1 1 0.4 3 2 1 0.8 3 1 2 0.8 3 2 2 1.6
4 1 1 0.4 4 2 1 0.7 4 1 2 0.9 4 2 2 1.5
5 1 1 0.6 5 2 1 1.0 5 1 2 1.5 5 2 2 1.9
6 1 1 0.9 6 2 1 1.4 6 1 2 1.6 6 2 2 2.3
7 1 1 1.0 7 2 1 1.8 7 1 2 1.7 7 2 2 2.1
8 1 1 1.2 8 2 1 1.7 8 1 2 1.6 8 2 2 2.4
;

```

The variable PainLevel is the blocking variable, and Codeine and Acupuncture represent the levels of the two treatment factors. The variable Relief is the pain relief score (the higher the score, the more relief the patient has).

The following statements invokes PROC ANOVA. The blocking variable and treatment factors appear in the CLASS statement. The bar between the treatment factors Codeine and Acupuncture adds their main effects as well as their interaction Codeine*Acupuncture to the model.

```

proc anova data=PainRelief;
  class PainLevel Codeine Acupuncture;
  model Relief = PainLevel Codeine|Acupuncture;
run;

```

The results from the analysis are shown in [Output 25.1.1](#), [Output 25.1.2](#), and [Output 25.1.3](#).

Output 25.1.1 Class Level Information

```

Randomized Complete Block With Two Factors

The ANOVA Procedure

Class Level Information

Class          Levels  Values
PainLevel      8      1 2 3 4 5 6 7 8
Codeine        2      1 2
Acupuncture    2      1 2

Number of Observations Read      32
Number of Observations Used      32
    
```

Output 25.1.2 ANOVA Table

```

Randomized Complete Block With Two Factors

The ANOVA Procedure

Dependent Variable: Relief

Source          DF          Sum of Squares    Mean Square    F Value    Pr > F
Model           10          11.33500000        1.13350000     78.37     <.0001
Error           21           0.30375000        0.01446429
Corrected Total 31          11.63875000

R-Square      Coeff Var      Root MSE      Relief Mean
0.973902      10.40152       0.120268      1.156250
    
```

The Class Level Information and ANOVA table are shown in [Output 25.1.1](#) and [Output 25.1.2](#). The classification level information summarizes the structure of the design. It is good to check these consistently in search of errors in the DATA step. The overall *F* test is significant, indicating that the model accounts for a significant amount of variation in the dependent variable.

Output 25.1.3 Tests of Effects

Source	DF	Anova SS	Mean Square	F Value	Pr > F
PainLevel	7	5.59875000	0.79982143	55.30	<.0001
Codeine	1	2.31125000	2.31125000	159.79	<.0001
Acupuncture	1	3.38000000	3.38000000	233.68	<.0001
Codeine*Acupuncture	1	0.04500000	0.04500000	3.11	0.0923

Output 25.1.3 shows tests of the effects. The blocking effect is significant; hence, it is useful. The interaction between codeine and acupuncture is significant at the 90% level but not at the 95% level. The significance level of this test should be determined before the analysis. The main effects of both treatment factors are highly significant.

Example 25.2: Alternative Multiple Comparison Procedures

The following is a continuation of the first example in the section “One-Way Layout with Means Comparisons” on page 904. You are studying the effect of bacteria on the nitrogen content of red clover plants, and the analysis of variance shows a highly significant effect. The following statements create the data set and compute the analysis of variance as well as Tukey’s multiple comparisons test for pairwise differences between bacteria strains; the results are shown in Figure 25.1, Figure 25.2, and Figure 25.3

```

title1 'Nitrogen Content of Red Clover Plants';
data Clover;
  input Strain $ Nitrogen @@;
  datalines;
3DOK1 19.4 3DOK1 32.6 3DOK1 27.0 3DOK1 32.1 3DOK1 33.0
3DOK5 17.7 3DOK5 24.8 3DOK5 27.9 3DOK5 25.2 3DOK5 24.3
3DOK4 17.0 3DOK4 19.4 3DOK4 9.1 3DOK4 11.9 3DOK4 15.8
3DOK7 20.7 3DOK7 21.0 3DOK7 20.5 3DOK7 18.8 3DOK7 18.6
3DOK13 14.3 3DOK13 14.4 3DOK13 11.8 3DOK13 11.6 3DOK13 14.2
COMPOS 17.3 COMPOS 19.4 COMPOS 19.1 COMPOS 16.9 COMPOS 20.8
;

proc anova data=Clover;
  class Strain;
  model Nitrogen = Strain;
  means Strain / tukey;
run;

```

The interactivity of PROC ANOVA enables you to submit further MEANS statements without re-running the entire analysis. For example, the following command requests means of the Strain levels with Duncan’s multiple range test and the Waller-Duncan k -ratio t test.

```

  means Strain / duncan waller;
run;

```

Results of the Waller-Duncan k -ratio t test are shown in Output 25.2.1.

Output 25.2.1 Waller-Duncan K -ratio t Test

Nitrogen Content of Red Clover Plants			
The ANOVA Procedure			
Waller-Duncan K -ratio t Test for Nitrogen			
Kratio			100
Error Degrees of Freedom			24
Error Mean Square		11.78867	
F Value		14.37	
Critical Value of t		1.91873	
Minimum Significant Difference		4.1665	
Means with the same letter are not significantly different.			
Waller Grouping	Mean	N	Strain
A	28.820	5	3DOK1
B	23.980	5	3DOK5
B			
C B	19.920	5	3DOK7
C			
C D	18.700	5	COMPOS
D			
E D	14.640	5	3DOK4
E			
E	13.260	5	3DOK13

The Waller-Duncan k -ratio t test is a multiple range test. Unlike Tukey's test, this test does not operate on the principle of controlling Type I error. Instead, it compares the Type I and Type II error rates based on Bayesian principles (Steel and Torrie 1980).

The Waller Grouping column in [Output 25.2.1](#) shows which means are significantly different. From this test, you can conclude the following:

- The mean nitrogen content for strain 3DOK1 is higher than the means for all other strains.
- The mean nitrogen content for strain 3DOK5 is higher than the means for COMPOS, 3DOK4, and 3DOK13.
- The mean nitrogen content for strain 3DOK7 is higher than the means for 3DOK4 and 3DOK13.
- The mean nitrogen content for strain COMPOS is higher than the mean for 3DOK13.
- Differences between all other means are not significant based on this sample size.

[Output 25.2.2](#) shows the results of Duncan's multiple range test. Duncan's test is a result-guided test that compares the treatment means while controlling the comparison-wise error rate. You should use this test for planned comparisons only (Steel and Torrie 1980). The results and conclusions for this example are the same as for the Waller-Duncan k -ratio t test. This is not always the case.

Output 25.2.2 Duncan's Multiple Range Test

	Alpha				0.05
	Error Degrees of Freedom				24
	Error Mean Square				11.78867
Number of Means	2	3	4	5	6
Critical Range	4.482	4.707	4.852	4.954	5.031
Means with the same letter are not significantly different.					
	Duncan Grouping	Mean	N	Strain	
	A	28.820	5	3DOK1	
	B	23.980	5	3DOK5	
	B				
C	B	19.920	5	3DOK7	
C					
C	D	18.700	5	COMPOS	
	D				
E	D	14.640	5	3DOK4	
E					
E		13.260	5	3DOK13	

Tukey and Least Significant Difference (LSD) tests are requested with the following **MEANS** statement. The **CLDIFF** option requests confidence intervals for both tests.

```
means Strain/ lsd tukey cldiff ;
run;
```

The **LSD** tests for this example are shown in **Output 25.2.3**, and they give the same results as the previous two multiple comparison tests. Again, this is not always the case.

Output 25.2.3 T Tests (LSD)

Nitrogen Content of Red Clover Plants	
The ANOVA Procedure	
t Tests (LSD) for Nitrogen	
Alpha	0.05
Error Degrees of Freedom	24
Error Mean Square	11.78867
Critical Value of t	2.06390
Least Significant Difference	4.4818

Output 25.2.3 continued

Comparisons significant at the 0.05 level are indicated by ***.

Strain Comparison	Difference Between Means	95% Confidence Limits		
3DOK1 - 3DOK5	4.840	0.358	9.322	***
3DOK1 - 3DOK7	8.900	4.418	13.382	***
3DOK1 - COMPOS	10.120	5.638	14.602	***
3DOK1 - 3DOK4	14.180	9.698	18.662	***
3DOK1 - 3DOK13	15.560	11.078	20.042	***
3DOK5 - 3DOK1	-4.840	-9.322	-0.358	***
3DOK5 - 3DOK7	4.060	-0.422	8.542	
3DOK5 - COMPOS	5.280	0.798	9.762	***
3DOK5 - 3DOK4	9.340	4.858	13.822	***
3DOK5 - 3DOK13	10.720	6.238	15.202	***
3DOK7 - 3DOK1	-8.900	-13.382	-4.418	***
3DOK7 - 3DOK5	-4.060	-8.542	0.422	
3DOK7 - COMPOS	1.220	-3.262	5.702	
3DOK7 - 3DOK4	5.280	0.798	9.762	***
3DOK7 - 3DOK13	6.660	2.178	11.142	***
COMPOS - 3DOK1	-10.120	-14.602	-5.638	***
COMPOS - 3DOK5	-5.280	-9.762	-0.798	***
COMPOS - 3DOK7	-1.220	-5.702	3.262	
COMPOS - 3DOK4	4.060	-0.422	8.542	
COMPOS - 3DOK13	5.440	0.958	9.922	***
3DOK4 - 3DOK1	-14.180	-18.662	-9.698	***
3DOK4 - 3DOK5	-9.340	-13.822	-4.858	***
3DOK4 - 3DOK7	-5.280	-9.762	-0.798	***
3DOK4 - COMPOS	-4.060	-8.542	0.422	
3DOK4 - 3DOK13	1.380	-3.102	5.862	
3DOK13 - 3DOK1	-15.560	-20.042	-11.078	***
3DOK13 - 3DOK5	-10.720	-15.202	-6.238	***
3DOK13 - 3DOK7	-6.660	-11.142	-2.178	***
3DOK13 - COMPOS	-5.440	-9.922	-0.958	***
3DOK13 - 3DOK4	-1.380	-5.862	3.102	

If you only perform the **LSD** tests when the overall model F test is significant, then this is called Fisher's protected **LSD** test. Note that the **LSD** tests should be used for planned comparisons.

The **TUKEY** tests shown in Output 25.2.4 find fewer significant differences than the other three tests. This is not unexpected, as the **TUKEY** test controls the Type I experimentwise error rate. For a complete discussion of multiple comparison methods, see the section "Multiple Comparisons" on page 3349 in Chapter 42, "The GLM Procedure."

Output 25.2.4 Tukey's Studentized Range Test

Alpha	0.05	
Error Degrees of Freedom	24	
Error Mean Square	11.78867	
Critical Value of Studentized Range	4.37265	
Minimum Significant Difference	6.7142	
Comparisons significant at the 0.05 level are indicated by ***.		
Strain Comparison	Difference Between Means	Simultaneous 95% Confidence Limits
3DOK1 - 3DOK5	4.840	-1.874 11.554
3DOK1 - 3DOK7	8.900	2.186 15.614 ***
3DOK1 - COMPOS	10.120	3.406 16.834 ***
3DOK1 - 3DOK4	14.180	7.466 20.894 ***
3DOK1 - 3DOK13	15.560	8.846 22.274 ***
3DOK5 - 3DOK1	-4.840	-11.554 1.874
3DOK5 - 3DOK7	4.060	-2.654 10.774
3DOK5 - COMPOS	5.280	-1.434 11.994
3DOK5 - 3DOK4	9.340	2.626 16.054 ***
3DOK5 - 3DOK13	10.720	4.006 17.434 ***
3DOK7 - 3DOK1	-8.900	-15.614 -2.186 ***
3DOK7 - 3DOK5	-4.060	-10.774 2.654
3DOK7 - COMPOS	1.220	-5.494 7.934
3DOK7 - 3DOK4	5.280	-1.434 11.994
3DOK7 - 3DOK13	6.660	-0.054 13.374
COMPOS - 3DOK1	-10.120	-16.834 -3.406 ***
COMPOS - 3DOK5	-5.280	-11.994 1.434
COMPOS - 3DOK7	-1.220	-7.934 5.494
COMPOS - 3DOK4	4.060	-2.654 10.774
COMPOS - 3DOK13	5.440	-1.274 12.154
3DOK4 - 3DOK1	-14.180	-20.894 -7.466 ***
3DOK4 - 3DOK5	-9.340	-16.054 -2.626 ***
3DOK4 - 3DOK7	-5.280	-11.994 1.434
3DOK4 - COMPOS	-4.060	-10.774 2.654
3DOK4 - 3DOK13	1.380	-5.334 8.094
3DOK13 - 3DOK1	-15.560	-22.274 -8.846 ***
3DOK13 - 3DOK5	-10.720	-17.434 -4.006 ***
3DOK13 - 3DOK7	-6.660	-13.374 0.054
3DOK13 - COMPOS	-5.440	-12.154 1.274
3DOK13 - 3DOK4	-1.380	-8.094 5.334

Example 25.3: Split Plot

In some experiments, treatments can be applied only to groups of experimental observations rather than separately to each observation. When there are two nested groupings of the observations on the basis of treatment application, this is known as a *split plot design*. For example, in integrated circuit fabrication it is of interest to see how different manufacturing methods affect the characteristics of individual chips.

However, much of the manufacturing process is applied to a relatively large wafer of material, from which many chips are made. Additionally, a chip's position within a wafer might also affect chip performance. These two groupings of chips—by wafer and by position-within-wafer—might form the *whole plots* and the *subplots*, respectively, of a split plot design for integrated circuits.

The following statements produce an analysis for a split-plot design. The **CLASS** statement includes the variables Block, A, and B, where B defines subplots within BLOCK*A whole plots. The **MODEL** statement includes the independent effects Block, A, Block*A, B, and A*B. The **TEST** statement asks for an *F* test of the A effect that uses the Block*A effect as the error term. The following statements produce [Output 25.3.1](#) and [Output 25.3.2](#):

```

title1 'Split Plot Design';
data Split;
  input Block 1 A 2 B 3 Response;
  datalines;
142 40.0
141 39.5
112 37.9
111 35.4
121 36.7
122 38.2
132 36.4
131 34.8
221 42.7
222 41.6
212 40.3
211 41.6
241 44.5
242 47.6
231 43.6
232 42.8
;

proc anova data=Split;
  class Block A B;
  model Response = Block A Block*A B A*B;
  test h=A e=Block*A;
run;

```

Output 25.3.1 Class Level Information and ANOVA Table

Split Plot Design		
The ANOVA Procedure		
Class Level Information		
Class	Levels	Values
Block	2	1 2
A	4	1 2 3 4
B	2	1 2

Output 25.3.1 continued

Number of Observations Read		16			
Number of Observations Used		16			
Split Plot Design					
The ANOVA Procedure					
Dependent Variable: Response					
Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	11	182.0200000	16.5472727	7.85	0.0306
Error	4	8.4300000	2.1075000		
Corrected Total	15	190.4500000			
R-Square	Coeff Var	Root MSE	Response Mean		
0.955736	3.609007	1.451723	40.22500		

First, notice that the overall F test for the model is significant.

Output 25.3.2 Tests of Effects

Source	DF	Anova SS	Mean Square	F Value	Pr > F
Block	1	131.1025000	131.1025000	62.21	0.0014
A	3	40.1900000	13.3966667	6.36	0.0530
Block*A	3	6.9275000	2.3091667	1.10	0.4476
B	1	2.2500000	2.2500000	1.07	0.3599
A*B	3	1.5500000	0.5166667	0.25	0.8612
Tests of Hypotheses Using the Anova MS for Block*A as an Error Term					
Source	DF	Anova SS	Mean Square	F Value	Pr > F
A	3	40.19000000	13.39666667	5.80	0.0914

The effect of Block is significant. The effect of A is not significant: look at the F test produced by the **TEST** statement, not at the F test produced by default. Neither the B nor A*B effects are significant. The test for Block*A is irrelevant, as this is simply the main-plot error.

Example 25.4: Latin Square Split Plot

The data for this example is taken from Smith (1951). A Latin square design is used to evaluate six different sugar beet varieties arranged in a six-row (Rep) by six-column (Column) square. The data are collected over two harvests. The variable Harvest then becomes a split plot on the original Latin square design for whole plots. The following statements produce [Output 25.4.1](#), [Output 25.4.2](#), and [Output 25.4.3](#):

```

title1 'Sugar Beet Varieties';
title3 'Latin Square Split-Plot Design';
data Beets;
  do Harvest=1 to 2;
    do Rep=1 to 6;
      do Column=1 to 6;
        input Variety Y @;
        output;
      end;
    end;
  end;
  datalines;
3 19.1 6 18.3 5 19.6 1 18.6 2 18.2 4 18.5
6 18.1 2 19.5 4 17.6 3 18.7 1 18.7 5 19.9
1 18.1 5 20.2 6 18.5 4 20.1 3 18.6 2 19.2
2 19.1 3 18.8 1 18.7 5 20.2 4 18.6 6 18.5
4 17.5 1 18.1 2 18.7 6 18.2 5 20.4 3 18.5
5 17.7 4 17.8 3 17.4 2 17.0 6 17.6 1 17.6
3 16.2 6 17.0 5 18.1 1 16.6 2 17.7 4 16.3
6 16.0 2 15.3 4 16.0 3 17.1 1 16.5 5 17.6
1 16.5 5 18.1 6 16.7 4 16.2 3 16.7 2 17.3
2 17.5 3 16.0 1 16.4 5 18.0 4 16.6 6 16.1
4 15.7 1 16.1 2 16.7 6 16.3 5 17.8 3 16.2
5 18.3 4 16.6 3 16.4 2 17.6 6 17.1 1 16.5
;

proc anova data=Beets;
  class Column Rep Variety Harvest;
  model Y=Rep Column Variety Rep*Column*Variety
        Harvest Harvest*Rep
        Harvest*Variety;
  test h=Rep Column Variety e=Rep*Column*Variety;
  test h=Harvest          e=Harvest*Rep;
run;

```

Output 25.4.1 Class Level Information

```

                Sugar Beet Varieties

                Latin Square Split-Plot Design

                The ANOVA Procedure

                Class Level Information

Class          Levels   Values

Column         6       1 2 3 4 5 6

Rep            6       1 2 3 4 5 6

Variety        6       1 2 3 4 5 6

Harvest        2       1 2

Number of Observations Read      72
Number of Observations Used      72
    
```

Output 25.4.2 ANOVA Table

```

                Sugar Beet Varieties

                Latin Square Split-Plot Design

                The ANOVA Procedure

Dependent Variable: Y

Source          DF          Sum of
                Squares    Mean Square    F Value    Pr > F

Model          46          98.9147222    2.1503200    7.22    <.0001

Error          25          7.4484722    0.2979389

Corrected Total  71          106.3631944

R-Square      Coeff Var    Root MSE    Y Mean

0.929971      3.085524    0.545838    17.69028
    
```

Output 25.4.2 *continued*

Source	DF	Anova SS	Mean Square	F Value	Pr > F
Rep	5	4.32069444	0.86413889	2.90	0.0337
Column	5	1.57402778	0.31480556	1.06	0.4075
Variety	5	20.61902778	4.12380556	13.84	<.0001
Column*Rep*Variety	20	3.25444444	0.16272222	0.55	0.9144
Harvest	1	60.68347222	60.68347222	203.68	<.0001
Rep*Harvest	5	7.71736111	1.54347222	5.18	0.0021
Variety*Harvest	5	0.74569444	0.14913889	0.50	0.7729

First, note from [Output 25.4.2](#) that the overall model is significant.

Output 25.4.3 Tests of Effects

Tests of Hypotheses Using the Anova MS for Column*Rep*Variety as an Error Term					
Source	DF	Anova SS	Mean Square	F Value	Pr > F
Rep	5	4.32069444	0.86413889	5.31	0.0029
Column	5	1.57402778	0.31480556	1.93	0.1333
Variety	5	20.61902778	4.12380556	25.34	<.0001
Tests of Hypotheses Using the Anova MS for Rep*Harvest as an Error Term					
Source	DF	Anova SS	Mean Square	F Value	Pr > F
Harvest	1	60.68347222	60.68347222	39.32	0.0015

[Output 25.4.3](#) shows that the effects for Rep and Harvest are significant, while the Column effect is not. The average Y s for the six different Varieties are significantly different. For these four tests, look at the output produced by the two **TEST** statements, not at the usual ANOVA procedure output. The Variety*Harvest interaction is not significant. All other effects in the default output should either be tested by using the results from the **TEST** statements or are irrelevant as they are only error terms for portions of the model.

Example 25.5: Strip-Split Plot

In this example, four different fertilizer treatments are laid out in vertical strips, which are then split into subplots with different levels of calcium. Soil type is stripped across the split-plot experiment, and the entire experiment is then replicated three times. The dependent variable is the yield of winter barley. The data come from the notes of G. Cox and A. Rotti.

The input data are the 96 values of Y , arranged so that the calcium value (Calcium) changes most rapidly, then the fertilizer value (Fertilizer), then the Soil value, and, finally, the Rep value. Values are shown for Calcium (0 and 1); Fertilizer (0, 1, 2, 3); Soil (1, 2, 3); and Rep (1, 2, 3, 4). The following example produces [Output 25.5.1](#), [Output 25.5.2](#), [Output 25.5.3](#), and [Output 25.5.4](#).

```

title1 'Strip-split Plot';
data Barley;
  do Rep=1 to 4;
    do Soil=1 to 3; /* 1=d 2=h 3=p */
      do Fertilizer=0 to 3;
        do Calcium=0,1;
          input Yield @;
          output;
        end;
      end;
    end;
  end;
  datalines;
4.91 4.63 4.76 5.04 5.38 6.21 5.60 5.08
4.94 3.98 4.64 5.26 5.28 5.01 5.45 5.62
5.20 4.45 5.05 5.03 5.01 4.63 5.80 5.90
6.00 5.39 4.95 5.39 6.18 5.94 6.58 6.25
5.86 5.41 5.54 5.41 5.28 6.67 6.65 5.94
5.45 5.12 4.73 4.62 5.06 5.75 6.39 5.62
4.96 5.63 5.47 5.31 6.18 6.31 5.95 6.14
5.71 5.37 6.21 5.83 6.28 6.55 6.39 5.57
4.60 4.90 4.88 4.73 5.89 6.20 5.68 5.72
5.79 5.33 5.13 5.18 5.86 5.98 5.55 4.32
5.61 5.15 4.82 5.06 5.67 5.54 5.19 4.46
5.13 4.90 4.88 5.18 5.45 5.80 5.12 4.42
;

proc anova data=Barley;
  class Rep Soil Calcium Fertilizer;
  model Yield =
    Rep
    Fertilizer Fertilizer*Rep
    Calcium Calcium*Fertilizer Calcium*Rep(Fertilizer)
    Soil Soil*Rep
    Soil*Fertilizer Soil*Rep*Fertilizer
    Soil*Calcium Soil*Fertilizer*Calcium
    Soil*Calcium*Rep(Fertilizer);
  test h=Fertilizer          e=Fertilizer*Rep;
  test h=Calcium calcium*fertilizer e=Calcium*Rep(Fertilizer);
  test h=Soil                e=Soil*Rep;
  test h=Soil*Fertilizer     e=Soil*Rep*Fertilizer;
  test h=Soil*Calcium
    Soil*Fertilizer*Calcium e=Soil*Calcium*Rep(Fertilizer);
  means Fertilizer Calcium Soil Calcium*Fertilizer;
run;

```

Output 25.5.1 Class Level Information

```

Strip-split Plot
The ANOVA Procedure
Class Level Information

Class          Levels  Values
Rep            4      1 2 3 4
Soil           3      1 2 3
Calcium        2      0 1
Fertilizer     4      0 1 2 3

Number of Observations Read      96
Number of Observations Used      96
    
```

Output 25.5.2 ANOVA Table

```

Strip-split Plot
The ANOVA Procedure
Dependent Variable: Yield

Source          DF      Sum of
                Sums of    Mean Square    F Value    Pr > F
                Squares

Model           95      31.89149583    0.33569996    .          .
Error           0          0.00000000    .
Corrected Total 95      31.89149583

R-Square      Coeff Var    Root MSE    Yield Mean
1.000000      .            .            5.427292
    
```

Output 25.5.2 continued

Source	DF	Anova SS	Mean Square	F Value	Pr > F
Rep	3	6.27974583	2.09324861	.	.
Fertilizer	3	7.22127083	2.40709028	.	.
Rep*Fertilizer	9	6.08211250	0.67579028	.	.
Calcium	1	0.27735000	0.27735000	.	.
Calcium*Fertilizer	3	1.96395833	0.65465278	.	.
Rep*Calcium(Fertili)	12	1.76705833	0.14725486	.	.
Soil	2	1.92658958	0.96329479	.	.
Rep*Soil	6	1.66761042	0.27793507	.	.
Soil*Fertilizer	6	0.68828542	0.11471424	.	.
Rep*Soil*Fertilizer	18	1.58698125	0.08816563	.	.
Soil*Calcium	2	0.04493125	0.02246562	.	.
Soil*Calcium*Fertili	6	0.18936042	0.03156007	.	.
Rep*Soil*Calc(Ferti)	24	2.19624167	0.09151007	.	.

Notice in [Output 25.5.2](#) that the default tests against the residual error rate are all unavailable. This is because the `Soil*Calcium*Rep(Fertilizer)` term in the model takes up all the degrees of freedom, leaving none for estimating the residual error rate. This is appropriate in this case since the `TEST` statements give the specific error terms appropriate for testing each effect. [Output 25.5.3](#) displays the output produced by the various `TEST` statements. The only significant effect is the `Calcium*Fertilizer` interaction.

Output 25.5.3 Tests of Effects

Tests of Hypotheses Using the Anova MS for Rep*Fertilizer as an Error Term					
Source	DF	Anova SS	Mean Square	F Value	Pr > F
Fertilizer	3	7.22127083	2.40709028	3.56	0.0604
Tests of Hypotheses Using the Anova MS for Rep*Calcium(Fertili) as an Error Term					
Source	DF	Anova SS	Mean Square	F Value	Pr > F
Calcium	1	0.27735000	0.27735000	1.88	0.1950
Calcium*Fertilizer	3	1.96395833	0.65465278	4.45	0.0255
Tests of Hypotheses Using the Anova MS for Rep*Soil as an Error Term					
Source	DF	Anova SS	Mean Square	F Value	Pr > F
Soil	2	1.92658958	0.96329479	3.47	0.0999
Tests of Hypotheses Using the Anova MS for Rep*Soil*Fertilizer as an Error Term					
Source	DF	Anova SS	Mean Square	F Value	Pr > F
Soil*Fertilizer	6	0.68828542	0.11471424	1.30	0.3063

Output 25.5.3 *continued*

Tests of Hypotheses Using the Anova MS for Rep*Soil*Calc(Ferti) as an Error Term					
Source	DF	Anova SS	Mean Square	F Value	Pr > F
Soil*Calcium	2	0.04493125	0.02246562	0.25	0.7843
Soil*Calcium*Fertili	6	0.18936042	0.03156007	0.34	0.9059

Output 25.5.4 Results of MEANS statement

Level of Fertilizer		N	-----Yield-----	
			Mean	Std Dev
0		24	5.18416667	0.48266395
1		24	5.12916667	0.38337082
2		24	5.75458333	0.53293265
3		24	5.64125000	0.63926801

Level of Calcium		N	-----Yield-----	
			Mean	Std Dev
0		48	5.48104167	0.54186141
1		48	5.37354167	0.61565219

Level of Soil		N	-----Yield-----	
			Mean	Std Dev
1		32	5.54312500	0.55806369
2		32	5.51093750	0.62176315
3		32	5.22781250	0.51825224

Level of Calcium	Level of Fertilizer	N	-----Yield-----	
			Mean	Std Dev
0	0	12	5.34666667	0.45029956
0	1	12	5.08833333	0.44986530
0	2	12	5.62666667	0.44707806
0	3	12	5.86250000	0.52886027
1	0	12	5.02166667	0.47615569
1	1	12	5.17000000	0.31826233
1	2	12	5.88250000	0.59856077
1	3	12	5.42000000	0.68409197

Output 25.5.4 shows the results of the **MEANS** statement, displaying for various effects and combinations of effects, as requested. You can examine the Calcium*Fertilizer means to understand the interaction better.

In this example, you could reduce memory requirements by omitting the Soil*Calcium*Rep(Fertilizer) effect from the model in the **MODEL** statement. This effect then becomes the

ERROR effect, and you can omit the last **TEST** statement in the statements shown earlier. The test for the Soil*Calcium effect is then given in the Analysis of Variance table in the top portion of output. However, for all other tests, you should look at the results from the **TEST** statement. In large models, this method might lead to significant reductions in memory requirements.

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Chapter 26

The BOXPLOT Procedure

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Overview: BOXPLOT Procedure

The BOXPLOT procedure creates side-by-side box-and-whiskers plots of measurements organized in groups. A box-and-whiskers plot displays the mean, quartiles, and minimum and maximum observations for a group. Throughout this chapter, this type of plot, which can contain one or more box-and-whiskers plots, is referred to as a *box plot*.

The PLOT statement of the BOXPLOT procedure produces a box plot. You can specify more than one PLOT statement to produce multiple box plots. You can use options in the PLOT statement to do the following:

- control the style of the box-and-whiskers plots
- specify one of several methods for calculating quantile statistics (percentiles)
- add block legends and symbol markers to reveal stratification in data
- display vertical and horizontal reference lines
- control axis values and labels
- overlay the box plot with plots of additional variables
- control the layout and appearance of the plot

The INSET and INSETGROUP statements produce boxes or tables (referred to as *insets*) of summary statistics or other data on a box plot. An INSET statement produces an inset of statistics pertaining to the entire box plot. An INSETGROUP statement produces an inset containing statistics calculated separately for each group. An INSET or INSETGROUP statement by itself does not produce a display; it must be used with a PLOT statement.

You can use options in an INSET or INSETGROUP statement to control insets in these ways:

- specify the position of the inset
- specify a header for the inset
- specify graphical enhancements, such as background colors, text colors, text height, text font, and drop shadows

Traditional Graphics and ODS Graphics

The BOXPLOT procedure can produce two kinds of graphical output:

- traditional graphics
- ODS Statistical Graphics output

Traditional graphics are saved in graphics catalogs with entry type GRSEG. Their appearance is controlled by global statements such as the GOPTIONS, AXIS, and SYMBOL statements (as described in *SAS/GRAPH: Reference*) and numerous specialized PLOT statement options. You must have a SAS/GRAPH® license to produce traditional graphics.

ODS Statistical Graphics (or ODS Graphics for short) is an extension to the Output Delivery System (ODS). Graphs are produced in standard image file formats (such as PNG) instead of graphics catalogs, and the details of their appearance and layout are controlled by ODS styles and templates. When ODS Graphics is enabled (for example, with the ODS GRAPHICS ON statement) PROC BOXPLOT produces ODS Graphics output. Otherwise, it produces traditional graphics. See Chapter 21, “Statistical Graphics Using ODS,” for a thorough discussion of ODS Graphics.

Global graphics statements (GOPTIONS, AXIS, and SYMBOL, for example) and PLOT statement options that specify details of graph appearance (such as CBOXFILL= and FONT=) are ignored when ODS Graphics is enabled. Some PLOT statement options do affect ODS Graphics output, as indicated in the section “PLOT Statement Options” on page 979.

See the section “Getting Started: BOXPLOT Procedure” on page 963 for examples producing box plots via the traditional graphics system and ODS Graphics.

NOTE: Prior to SAS 9.2, traditional graphics produced by PROC BOXPLOT were extremely basic by default. Producing attractive graphical output required the careful selection of colors, fonts, and other elements, which were specified via SAS/GRAPH statements and PLOT statement options. Beginning with SAS 9.2, the default appearance of traditional box plots is governed by the prevailing ODS style, which automatically produces attractive, consistent output. You can specify the NOGSTYLE system option to prevent the ODS style from affecting the appearance of traditional graphs.

Getting Started: BOXPLOT Procedure

This section introduces the BOXPLOT procedure with simple examples demonstrating commonly used options. Complete syntax for the BOXPLOT procedure is presented in the section “Syntax: BOXPLOT Procedure” on page 971, and advanced examples are presented in the section “Examples: BOXPLOT Procedure” on page 1022.

Creating Box Plots from Raw Data

A petroleum company uses a turbine to heat water into steam that is pumped into the ground to make oil less viscous and easier to extract. This process occurs 20 times daily, and the amount of power (in kilowatts) used to heat the water to the desired temperature is recorded. The following statements create a SAS data set called Turbine that contains the power output measurements for 10 nonconsecutive days:

```
data Turbine;
  informat Day date7.;
  format Day date5.;
  label KWatts='Average Power Output';
  input Day @;
```

```

do i=1 to 10;
  input KWatts @;
  output;
end;
drop i;
datalines;
05JUL94 3196 3507 4050 3215 3583 3617 3789 3180 3505 3454
05JUL94 3417 3199 3613 3384 3475 3316 3556 3607 3364 3721
06JUL94 3390 3562 3413 3193 3635 3179 3348 3199 3413 3562
06JUL94 3428 3320 3745 3426 3849 3256 3841 3575 3752 3347
07JUL94 3478 3465 3445 3383 3684 3304 3398 3578 3348 3369
07JUL94 3670 3614 3307 3595 3448 3304 3385 3499 3781 3711
08JUL94 3448 3045 3446 3620 3466 3533 3590 3070 3499 3457
08JUL94 3411 3350 3417 3629 3400 3381 3309 3608 3438 3567
11JUL94 3568 2968 3514 3465 3175 3358 3460 3851 3845 2983
11JUL94 3410 3274 3590 3527 3509 3284 3457 3729 3916 3633
12JUL94 3153 3408 3741 3203 3047 3580 3571 3579 3602 3335
12JUL94 3494 3662 3586 3628 3881 3443 3456 3593 3827 3573
13JUL94 3594 3711 3369 3341 3611 3496 3554 3400 3295 3002
13JUL94 3495 3368 3726 3738 3250 3632 3415 3591 3787 3478
14JUL94 3482 3546 3196 3379 3559 3235 3549 3445 3413 3859
14JUL94 3330 3465 3994 3362 3309 3781 3211 3550 3637 3626
15JUL94 3152 3269 3431 3438 3575 3476 3115 3146 3731 3171
15JUL94 3206 3140 3562 3592 3722 3421 3471 3621 3361 3370
18JUL94 3421 3381 4040 3467 3475 3285 3619 3325 3317 3472
18JUL94 3296 3501 3366 3492 3367 3619 3550 3263 3355 3510
;

```

In the data set *Turbine*, each observation contains the date and the power output for a single heating. The first 20 observations contain the outputs for the first day, the second 20 observations contain the outputs for the second day, and so on. Because the variable *Day* classifies the observations into groups, it is referred to as the *group variable*. The variable *KWatts* contains the output measurements and is referred to as the *analysis variable*.

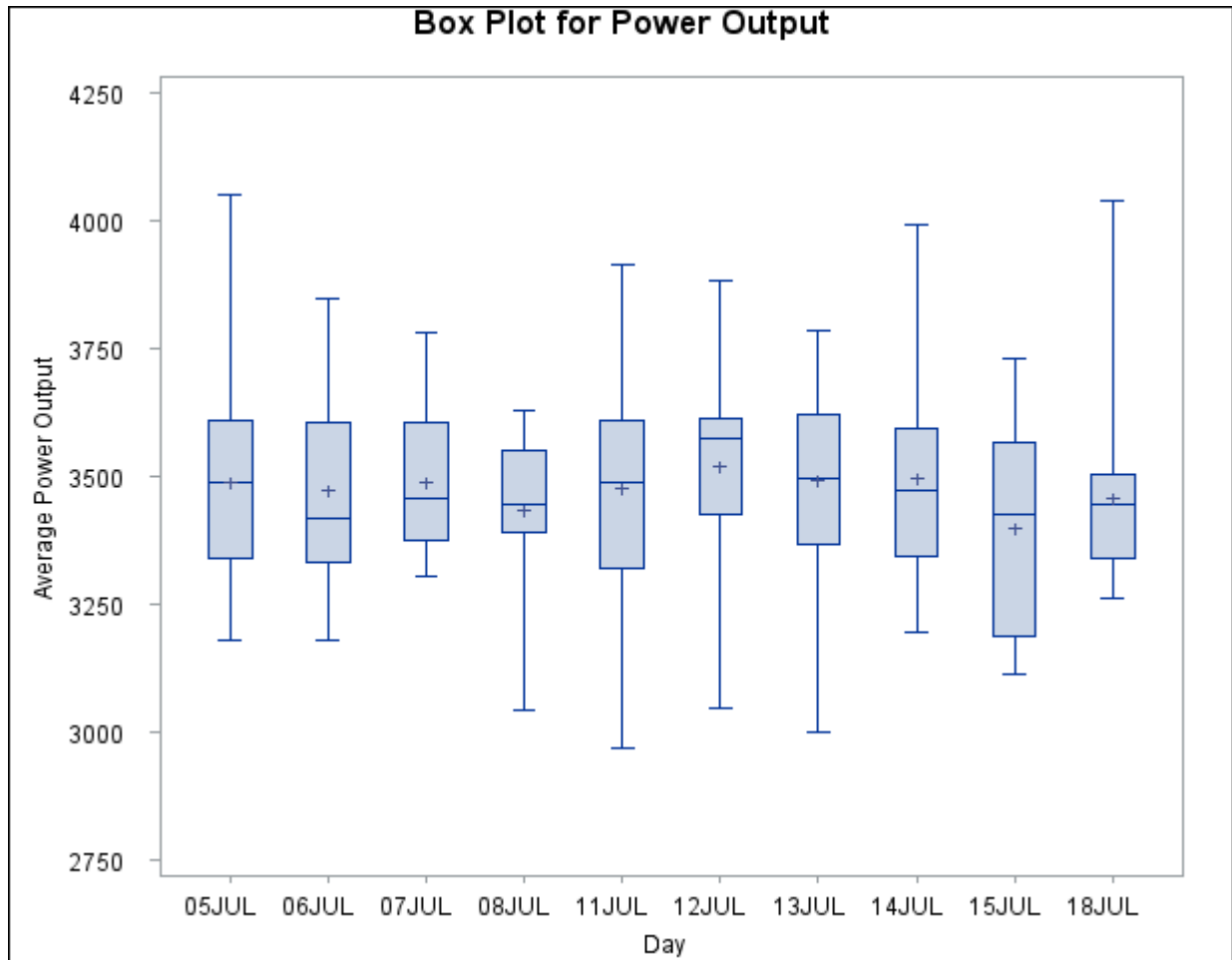
The following statements create a box plot showing the distribution of power output for each day:

```

ods graphics off;
title 'Box Plot for Power Output';
proc boxplot data=Turbine;
  plot KWatts*Day;
run;

```

The input data set *Turbine* is specified with the `DATA=` option in the PROC BOXPLOT statement. The PLOT statement requests a box-and-whiskers plot for each group of data. After the keyword PLOT, you specify the analysis variable (in this case, *KWatts*), followed by an asterisk and the group variable (*Day*). The ODS GRAPHICS OFF statement specified before the PROC BOXPLOT statement disables ODS Graphics, so the box plot is produced using traditional graphics. The box plot is shown in [Figure 26.1](#).

Figure 26.1 Box Plot for Power Output Data

The box plot displayed in Figure 26.1 represents summary statistics for the analysis variable KWatts. Each of the 10 box-and-whiskers plots describes the variable KWatts for a particular day. The plot elements and the statistics they represent are as follows:

- The length of the box represents the interquartile range (the distance between the 25th and 75th percentiles).
- The symbol in the box interior represents the group mean.
- The horizontal line in the box interior represents the group median.
- The vertical lines (called *whiskers*) issuing from the box extend to the group minimum and maximum values.

Creating Box Plots from Summary Data

The previous example illustrates how you can create box plots from raw data. However, in some applications the data are provided as summary statistics. This example illustrates how you can use the BOXPLOT procedure with data of this type.

The following statements create the data set Oilsum, which provides the data from the preceding example in summarized form:

```
data Oilsum;
  input Day KWattsL KWatts1 KWattsX KWattsM
        KWatts3 KWattsH KWattsS KWattsN;
  informat Day date7. ;
  format Day date5. ;
  label Day      ='Date of Measurement'
        KWattsL='Minimum Power Output'
        KWatts1='25th Percentile'
        KWattsX='Average Power Output'
        KWattsM='Median Power Output'
        KWatts3='75th Percentile'
        KWattsH='Maximum Power Output'
        KWattsS='Standard Deviation of Power Output'
        KWattsN='Group Sample Size';
  datalines;
05JUL94 3180 3340.0 3487.40 3490.0 3610.0 4050 220.3 20
06JUL94 3179 3333.5 3471.65 3419.5 3605.0 3849 210.4 20
07JUL94 3304 3376.0 3488.30 3456.5 3604.5 3781 147.0 20
08JUL94 3045 3390.5 3434.20 3447.0 3550.0 3629 157.6 20
11JUL94 2968 3321.0 3475.80 3487.0 3611.5 3916 258.9 20
12JUL94 3047 3425.5 3518.10 3576.0 3615.0 3881 211.6 20
13JUL94 3002 3368.5 3492.65 3495.5 3621.5 3787 193.8 20
14JUL94 3196 3346.0 3496.40 3473.5 3592.5 3994 212.0 20
15JUL94 3115 3188.5 3398.50 3426.0 3568.5 3731 199.2 20
18JUL94 3263 3340.0 3456.05 3444.0 3505.5 4040 173.5 20
;
```

Oilsum contains exactly one observation for each group. Note that, as in the previous example, the groups are indexed by the variable Day. A listing of Oilsum is shown in [Figure 26.2](#).

Figure 26.2 The Summary Data Set Oilsum

Box Plot for Power Output								
Day	KWatts L	KWatts1	KWattsX	KWatts M	KWatts3	KWatts H	KWatts S	KWatts N
05JUL	3180	3340.0	3487.40	3490.0	3610.0	4050	220.3	20
06JUL	3179	3333.5	3471.65	3419.5	3605.0	3849	210.4	20
07JUL	3304	3376.0	3488.30	3456.5	3604.5	3781	147.0	20
08JUL	3045	3390.5	3434.20	3447.0	3550.0	3629	157.6	20
11JUL	2968	3321.0	3475.80	3487.0	3611.5	3916	258.9	20
12JUL	3047	3425.5	3518.10	3576.0	3615.0	3881	211.6	20
13JUL	3002	3368.5	3492.65	3495.5	3621.5	3787	193.8	20
14JUL	3196	3346.0	3496.40	3473.5	3592.5	3994	212.0	20
15JUL	3115	3188.5	3398.50	3426.0	3568.5	3731	199.2	20
18JUL	3263	3340.0	3456.05	3444.0	3505.5	4040	173.5	20

There are eight summary variables in Oilsum:

- KWattsL contains the group minima (low values).
- KWatts1 contains the 25th percentile (first quartile) for each group.
- KWattsX contains the group means.
- KWattsM contains the group medians.
- KWatts3 contains the 75th percentile (third quartile) for each group.
- KWattsH contains the group maxima (high values).
- KWattsS contains the group standard deviations.
- KWattsN contains the group sizes.

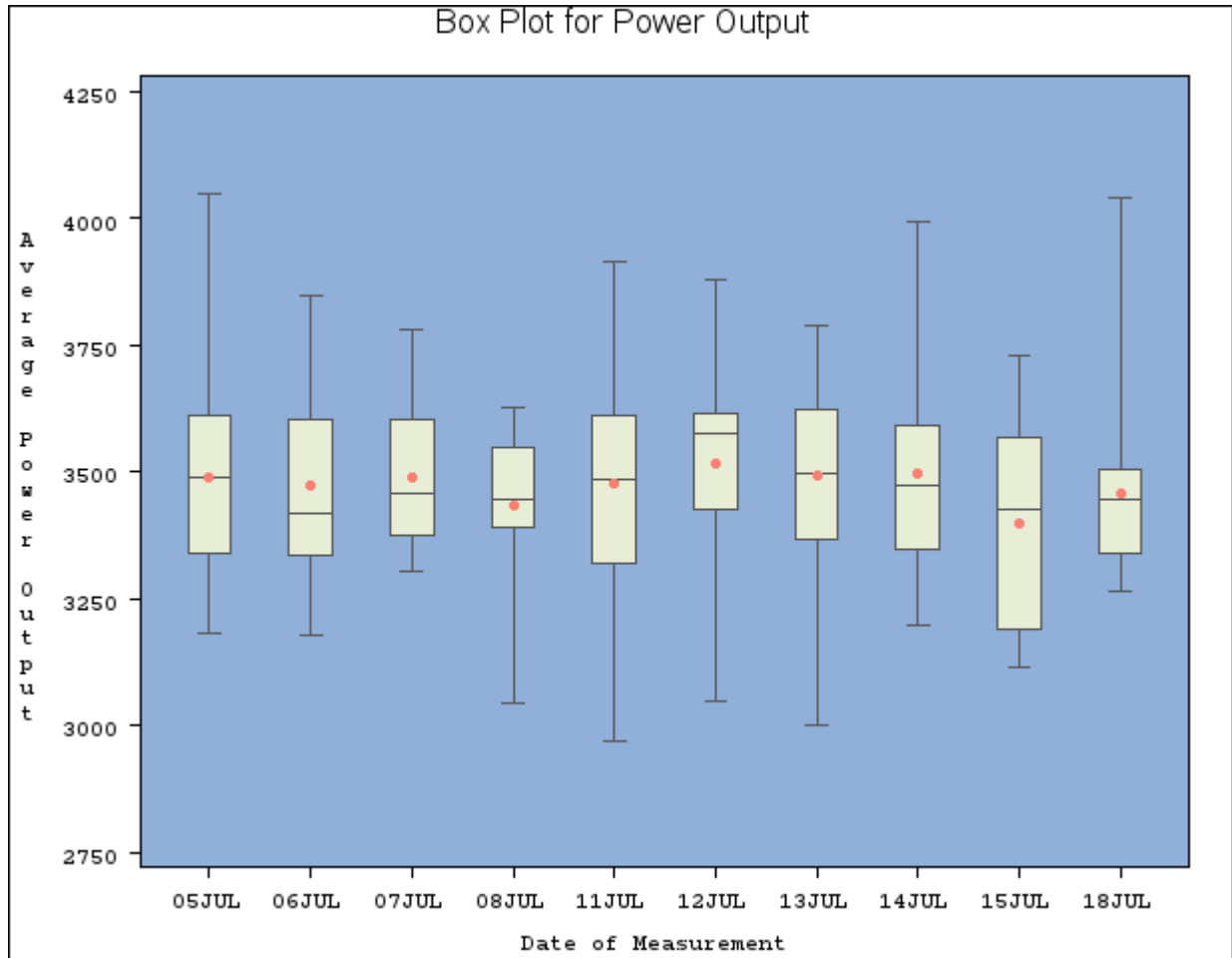
You can use this data set as input to the BOXPLOT procedure by specifying it with the `HISTORY=` option in the PROC BOXPLOT statement. Detailed requirements for `HISTORY=` data sets are presented in the section “`HISTORY= Data Set`” on page 1006.

The following statements produce a box plot of the summary data from the Oilsum data set:

```
options nogstyle;
title 'Box Plot for Power Output';
symbol value=dot color=salmon;
proc boxplot history=Oilsum;
  plot KWatts*Day / cframe = vligb
                    cboxes = dagr
                    cboxfill = ywh;
run;
options gstyle;
options reset=symbol;
```

The NOGSTYLE system option causes PROC BOXPLOT to ignore ODS styles when producing the box plot. Instead, the SYMBOL statement and options specified after the slash (/) in the PLOT statement control its appearance. The GSTYLE system option restores the use of ODS styles for subsequent high-resolution graphics output. For more information about SYMBOL statements, see *SAS/GRAPH: Reference*. The resulting box plot is shown in Figure 26.3.

Figure 26.3 High-Resolution Box Plot with NOGSTYLE



Saving Summary Data with Outliers

In a *schematic* box plot, outlier values within a group are plotted as separate points beyond the whiskers of the box-and-whiskers plot. See the section “[Styles of Box Plots](#)” on page 1007 and the description of the `BOXSTYLE=` option for a complete description of schematic box plots.

The following statements use the `BOXSTYLE=` option to produce a schematic box plot of the data from the Turbine data set. The `OUTBOX=` option creates a summary data set named `OilSchematic`. The `ODS GRAPHICS ON` statement specified before the `PROC BOXPLOT` statement enables ODS Graphics, so the box plot is created using ODS Graphics instead of traditional graphics.

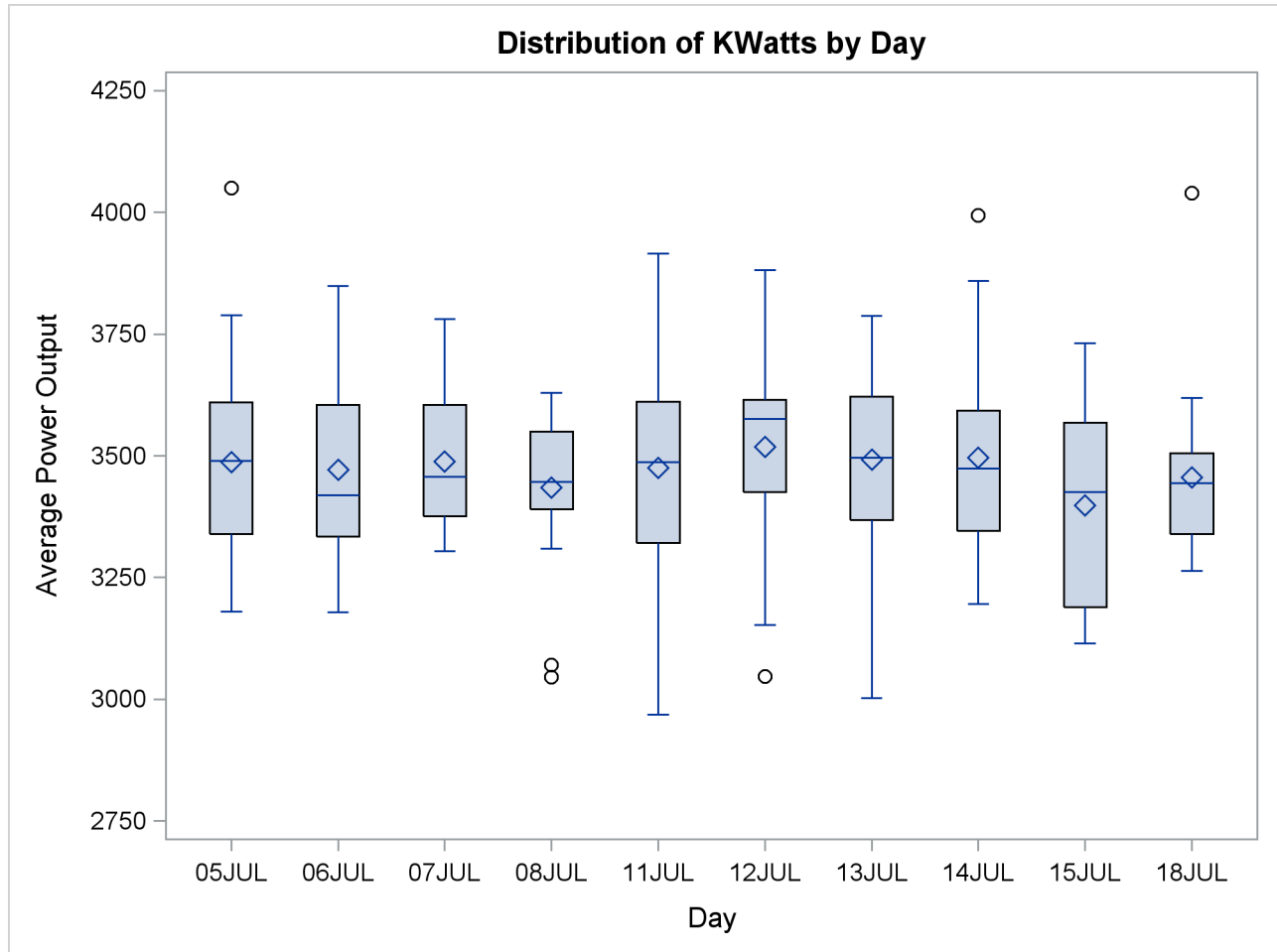
```

title 'Schematic Box Plot for Power Output';
ods graphics on;
proc boxplot data=Turbine;
  plot KWatts*Day / boxstyle = schematic
        outbox    = OilSchematic;
run;

```

The schematic box plot is shown in Figure 26.4. Note the outliers plotted for several of the groups.

Figure 26.4 Schematic Box Plot of Power Output



Whereas the Oilsum data set from the section “Creating Box Plots from Summary Data” on page 966 contains a *variable* for each summary statistic and one observation per group, the OUTBOX= data set OilSchematic contains one *observation* for each summary statistic in each group. The _TYPE_ variable identifies the statistic and the _VALUE_ variable contains its value. In addition, the OilSchematic data set contains an observation recording each outlier value for each group. Figure 26.5 shows a partial listing of the OilSchematic data set.

Figure 26.5 The Summary Data Set OilSchematic

Schematic Box Plot for Power Output			
Day	_VAR_	_TYPE_	_VALUE_
05JUL	KWatts	N	20.00
05JUL	KWatts	MIN	3180.00
05JUL	KWatts	Q1	3340.00
05JUL	KWatts	MEAN	3487.40
05JUL	KWatts	MEDIAN	3490.00
05JUL	KWatts	Q3	3610.00
05JUL	KWatts	MAX	4050.00
05JUL	KWatts	STDDEV	220.26
05JUL	KWatts	HIWHISKR	3789.00
05JUL	KWatts	HIGH	4050.00
06JUL	KWatts	N	20.00
06JUL	KWatts	MIN	3179.00
06JUL	KWatts	Q1	3333.50
06JUL	KWatts	MEAN	3471.65
06JUL	KWatts	MEDIAN	3419.50
06JUL	KWatts	Q3	3605.00
06JUL	KWatts	MAX	3849.00
06JUL	KWatts	STDDEV	210.43
07JUL	KWatts	N	20.00
07JUL	KWatts	MIN	3304.00
07JUL	KWatts	Q1	3376.00
07JUL	KWatts	MEAN	3488.30
07JUL	KWatts	MEDIAN	3456.50
07JUL	KWatts	Q3	3604.50
07JUL	KWatts	MAX	3781.00
07JUL	KWatts	STDDEV	147.02
08JUL	KWatts	N	20.00
08JUL	KWatts	MIN	3045.00
08JUL	KWatts	Q1	3390.50
08JUL	KWatts	MEAN	3434.20
08JUL	KWatts	MEDIAN	3447.00
08JUL	KWatts	Q3	3550.00
08JUL	KWatts	MAX	3629.00
08JUL	KWatts	STDDEV	157.64
08JUL	KWatts	LOWHISKR	3309.00
08JUL	KWatts	LOW	3070.00
08JUL	KWatts	LOW	3045.00
11JUL	KWatts	N	20.00
11JUL	KWatts	MIN	2968.00
11JUL	KWatts	Q1	3321.00

Observations with the `_TYPE_` variable values “HIGH” and “LOW” contain outlier values. If you want to use a summary data set to re-create a schematic box plot, you *must* create an `OUTBOX=` data set in order to save the outlier data.

Syntax: BOXPLOT Procedure

The following statements are available in the BOXPLOT procedure:

```

PROC BOXPLOT options ;
  BY variables ;
  ID variables ;
  INSET keywords </ options> ;
  INSETGROUP keywords </ options> ;
  PLOT analysis-variable * group-variable <( block-variables)> <=symbol-variable> </ options > ;

```

Both the PROC BOXPLOT and PLOT statements are required. You can specify any number of PLOT statements within a single PROC BOXPLOT invocation.

PROC BOXPLOT Statement

```

PROC BOXPLOT options ;

```

The PROC BOXPLOT statement invokes the BOXPLOT procedure. Table 26.1 summarizes the options available in the PROC BOXPLOT statement.

Table 26.1 PROC BOXPLOT Statement Options

Statement	Description
ANNOTATE=	Enhances traditional graphics box plots
BOX=	Names an input data set containing group summary statistics and outlier values
DATA=	Names an input data set containing raw data to be analyzed
GOUT=	Specifies the SAS catalog in which to save traditional graphics output
HISTORY=	Names an input data set containing group summary statistics

The following options can appear in the PROC BOXPLOT statement.

ANNOTATE=*SAS-data-set*

ANNO=*SAS-data-set*

specifies an ANNOTATE= type data set, as described in *SAS/GRAPH: Reference*, which enhances traditional graphics box plots requested in subsequent PLOT statements. **NOTE:** The ANNOTATE= option is ignored when ODS Graphics is enabled.

BOX=*SAS-data-set*

names an input data set containing group summary statistics and outlier values. Typically, this data set is created as an **OUTBOX=** data set in a previous run of PROC BOXPLOT. Each group summary statistic or outlier value is recorded in a separate observation in a BOX= data set, so there are multiple observations per group. You cannot use a BOX= data set together with a DATA= or HISTORY= data set. If you do not specify one of these input data sets, the procedure uses the most recently created SAS data set as a DATA= data set.

DATA=SAS-data-set

names an input data set containing raw data to be analyzed. You cannot use a DATA= data set together with a BOX= or HISTORY= data set. If you do not specify one of these input data sets, the procedure uses the most recently created SAS data set as a DATA= data set.

GOUT=< libref.>output catalog

specifies the SAS catalog in which to save traditional graphics output that is produced by the BOXPLOT procedure. If you omit the libref, PROC BOXPLOT looks for the catalog in the temporary library called WORK and creates the catalog if it does not exist. **NOTE:** The GOUT= option is ignored when ODS Graphics is enabled.

HISTORY=SAS-data-set**HIST=SAS-data-set**

names an input data set containing group summary statistics. Typically, this data set is created as an OUTHISTORY= data set in a previous run of PROC BOXPLOT, but it can also be created using a SAS summarization procedure such as the MEANS procedure. The HISTORY= data set can contain only one observation for each value of the group variable. You cannot use a HISTORY= data set with a DATA= or BOX= data set. If you do not specify one of these three input data sets, PROC BOXPLOT uses the most recently created data set as a DATA= data set.

BY Statement

BY variables ;

You can specify a BY statement with PROC BOXPLOT to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the BOXPLOT procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

ID Statement

ID *variables* ;

The ID statement specifies variables used to identify observations. The ID variables must be variables in the input data set.

If you specify the keyword SCHEMATICID or SCHEMATICIDFAR with the **BOXSTYLE=** option, the value of an ID variable is used to label each extreme observation. When you specify a **BOX=** data set, the label values come from the variable `_ID_`, if it is present in the data set. When you specify a **DATA=** or **HISTORY=** input data set, or a **BOX=** data set that does not contain the variable `_ID_`, the labels come from the first variable listed in the ID statement. If ID statement is specified, the outliers are not labeled.

INSET Statement

INSET *keywords* *</ options>* ;

A PLOT statement in the BOXPLOT procedure can be followed by a series of INSET and INSETGROUP statements. Each INSET statement in that series produces one inset in the box plot produced by the preceding PLOT statement. If the box plot occupies multiple panels, the inset appears on each panel.

The data requested using the *keywords* are displayed in the order in which they are specified. Summary statistics requested with an INSET statement are calculated using the observations in all groups.

keywords identify summary statistics or other data to be displayed in the inset. By default, inset statistics are identified with appropriate labels, and numeric values are printed using appropriate formats. However, you can provide customized labels and formats. You provide the customized label by specifying the *keyword* for that statistic followed by an equal sign (=) and the label in quotes. Labels can have up to 24 characters. You provide the numeric format in parentheses after the *keyword*. Note that if you specify both a label and a format for a statistic, the label must appear before the format.

The available keywords are listed in [Table 26.2](#).

options control the appearance of the inset. Most of these options apply only to traditional graphics and are ignored when ODS Graphics is enabled. [Table 26.3](#) summarizes the options available in the INSET statement. It also lists options and identifies those that are valid when ODS Graphics is enabled. Complete descriptions for each option follow.

Table 26.2 INSET Statement Keywords

Keyword	Description
DATA=	(label, value) pairs from <i>SAS-data-set</i>
MEAN	mean of all observations
MIN	minimum observed value
MAX	maximum observed value
NMIN	minimum group size
NMAX	maximum group size
NOBS	number of observations in box plot
STDDEV	pooled standard deviation

The DATA= keyword specifies a SAS data set containing (label, value) pairs to be displayed in an inset. The data set must contain the variables `_LABEL_` and `_VALUE_`. `_LABEL_` is a character variable of up to 24 characters whose values provide labels for inset entries. `_VALUE_` can be character or numeric, and provides values displayed in the inset. The label and value from each observation in the DATA= data set occupy one line in the inset.

The *pooled standard deviation* requested with the STDDEV keyword is defined as

$$s_p = \sqrt{\frac{\sum_{i=1}^N s_i^2 (n_i - 1)}{\sum_{i=1}^N (n_i - 1)}}$$

where N is the number of groups, n_i is the size of the i th group, and s_i^2 is the variance of the i th group.

Table 26.3 INSET Statement Options

Option	Description	ODS Graphics
CFILL=	Specifies color of inset background	
CFILLH=	Specifies color of inset header background	
CFRAME=	Specifies color of inset frame	
CHEADER=	Specifies color of inset header text	
CSHADOW=	Specifies color of inset drop shadow	
CTEXT=	Specifies color of inset text	
DATA	Specifies data units for POSITION=(x, y) coordinates	
FONT=	Specifies font of inset text	
FORMAT=	Specifies format of values in inset	✓
HEADER=	Specifies inset header text	✓
HEIGHT=	Specifies height of inset and header text	
NOFRAME	Suppresses frame around inset	✓
POSITION=	Specifies position of inset	✓
REFPOINT=	Specifies reference point of inset positioned with POSITION=(x, y) coordinates	

Following are descriptions of the options that you can specify in the INSET statement after a slash (/). Only those options marked with † are applicable when ODS Graphics is enabled.

CFILL=*color* | BLANK

specifies the color of the inset background (including the header background if you do not specify the **CFILLH=** option).

If you do not specify the **CFILL=** option, then by default the background is empty. This means that items that overlap the inset (such as box-and-whiskers plots or reference lines) show through the inset. If you specify any value for the **CFILL=** option, then overlapping items no longer show through the inset. Specify **CFILL=BLANK** to leave the background uncolored and also to prevent items from showing through the inset.

CFILLH=*color*

specifies the color of the header background. By default, if you do not specify a **CFILLH=** color, the **CFILL=** color is used.

CFRAME=*color*

specifies the color of the frame around the inset. By default, the frame is the same color as the axis of the plot.

CHEADER=*color*

specifies the color of the header text. By default, if you do not specify a **CHEADER=** color, the INSET statement **CTEXT=** color is used.

CSHADOW=*color*

CS=*color*

specifies the color of the drop shadow. If you do not specify the **CSHADOW=** option, a drop shadow is not displayed.

CTEXT=*color*

CT=*color*

specifies the color of the text in the inset. By default, the inset text color is the same as the other text in the box plot.

DATA

specifies that data coordinates be used in positioning the inset with the **POSITION=** option. The **DATA** option is available only when you specify **POSITION= (x, y)**, and it must be placed immediately after the coordinates (x, y) . See the entry for the **POSITION=** option.

FONT=*font*

specifies the font of the text.

† **FORMAT=*format***

specifies a format for all the values displayed in an inset. If you specify a format for a particular statistic, then this format overrides the format you specified with the **FORMAT=** option.

† **HEADER=*'string'***

specifies the header text. The *string* can be up to 40 characters. If you do not specify the **HEADER=** option, no header line appears in the inset.

HEIGHT=*value*

specifies the height of the inset and header text.

† **NOFRAME**

suppresses the frame drawn around the inset.

† **POSITION=***position*† **POS=***position*

determines the position of the inset. The *position* can be a compass point keyword, a margin keyword, or (for traditional graphics) a pair of coordinates (x, y) . You can specify coordinates in axis percent units or axis data units. For more information, see the section “Positioning Insets” on page 1011. By default, POSITION=NW, which positions the inset in the upper-left (northwest) corner of the plot.

REFPOINT=BR | BL | TR | TL**RP=**BR | BL | TR | TL

specifies the reference point for an inset that is positioned by a pair of coordinates with the POSITION= option. Use the REFPOINT= option with POSITION= coordinates. The REFPOINT= option specifies which corner of the inset frame you want positioned at coordinates (x, y) . The keywords BL, BR, TL, and TR represent bottom left, bottom right, top left, and top right, respectively. The default is REFPOINT=BL.

If you specify the position of the inset as a compass point or margin keyword, the REFPOINT= option is ignored.

INSETGROUP Statement

INSETGROUP *keywords* </ *options* > ;

A PLOT statement in the BOXPLOT procedure can be followed by a series of INSET and INSETGROUP statements. Each INSETGROUP statement in that series displays statistics associated with individual groups in the box plot produced by the preceding PLOT statement. No more than two INSETGROUP statements can be associated with a given PLOT statement: one that displays group statistics above the box plot and one that displays group statistics below it. The data requested using the *keywords* are displayed in the order in which they are specified.

keywords identify summary statistics to be displayed in the insets. By default, inset statistics are identified with appropriate labels, and numeric values are printed using appropriate formats. However, you can provide customized labels and formats. You provide the customized label by specifying the *keyword* for that statistic followed by an equal sign (=) and the label in quotes. Labels can have up to 24 characters. You provide the numeric format in parentheses after the *keyword*. Note that if you specify both a label and a format for a statistic, the label must appear before the format. The keywords are listed in Table 26.4.

options control the appearance of the insets. Table 26.5 lists all the options in the INSETGROUP statement. Complete descriptions for each option follow.

Table 26.4 INSETGROUP Statement Keywords

Keyword	Description
MEAN	group mean
MIN	group minimum value or low whisker value
MAX	group maximum value or high whisker value
N	number of observations in group
NHIGH	number of outliers above upper fence
NLOW	number of outliers below lower fence
NOUT	total number of outliers in group
Q1	first quartile of group values
Q2	second quartile of group values
Q3	third quartile of group values
RANGE	range of group values
STDDEV	group standard deviation

NOTE: When ODS Graphics is enabled, the MIN and MAX keywords display the low whisker and high whisker values, respectively. Otherwise, the group minimum and maximum data values are displayed.

Table 26.5 summarizes the options available in the INSETGROUP statement. All of these options apply to traditional graphics only. They are ignored when ODS Graphics is enabled.

Table 26.5 INSETGROUP Statement Options

Option	Description
CFILL=	Specifies color of inset background
CFILLH=	Specifies color of inset header background
CFRAME=	Specifies color of inset frame
CHEADER=	Specifies color of inset header text
CTEXT=	Specifies color of inset text
FONT=	Specifies font of inset text
FORMAT=	Specifies format of values in inset
HEADER=	Specifies inset header text
HEIGHT=	Specifies height of inset and header text
NOFRAME	Suppresses frame around inset
POSITION=	Specifies position of inset

Following are descriptions of the options that you can specify in the INSETGROUP statement after a slash (/).

CFILL=*color*

specifies the color of the inset background (including the header background if you do not specify the CFILLH= option). If you do not specify the CFILL= option, then by default the background is empty.

CFILLH=*color*

specifies the color of the header background. By default, if you do not specify a CFILLH= color, the CFILL= color is used.

CFRAME=*color*

specifies the color of the frame around the inset. By default, the frame is the same color as the axis of the plot.

CHEADER=*color*

specifies the color of the header text. By default, if you do not specify a CHEADER= color, the CTEXT= color is used.

CTEXT=*color***CT=***color*

specifies the color of the inset text. By default, the inset text color is the same as the other text in the plot.

FONT=*font*

specifies the font of the inset text. By default, the font is SIMPLEX.

FORMAT=*format*

specifies a format for all the values displayed in an inset. If you specify a format for a particular statistic, then this format overrides the format you specified with the FORMAT= option.

HEADER='*string*'

specifies the header text. The *string* can be up to 40 characters. If you do not specify the HEADER= option, no header line appears in the inset.

HEIGHT=*value*

specifies the height of the inset and header text.

NOFRAME

suppresses the frame drawn around the inset.

POSITION=*position***POS=***position*

determines the position of the inset. Valid positions are TOP, TOPOFF, AXIS, and BOTTOM. By default, POSITION=TOP.

Position Keyword	Description
TOP	top of plot, immediately above axis frame
TOPOFF	top of plot, offset from axis frame
AXIS	bottom of plot, immediately above horizontal axis
BOTTOM	bottom of plot, below horizontal axis label

PLOT Statement

```
PLOT (analysis-variables)* group-variable <(block-variables)> <=symbol-variable>
  </ options > ;
```

You can specify multiple PLOT statements after the PROC BOXPLOT statement. The components of the PLOT statement are as follows:

analysis-variables identify one or more variables to be analyzed. An analysis variable is required. If you specify more than one analysis variable, enclose the list in parentheses. For example, the following statements request distinct box plots for the variables Weight, Length, and Width:

```
proc boxplot data=Summary;
  plot (Weight Length Width)*Day;
run;
```

group-variable specifies the variable that identifies groups in the data. The group variable is required. In the preceding PLOT statement, Day is the group variable.

block-variables specify optional variables that group the data into blocks of consecutive groups. These blocks are labeled in a legend, and each block variable provides one level of labels in the legend.

symbol-variable specifies an optional variable whose levels (unique values) determine the symbol marker used to plot the means. Distinct symbol markers are displayed for points corresponding to the various levels of the symbol variable. You can specify the symbol markers with SYMBOL*n* statements (see *SAS/GRAPH: Reference* for complete details).

options enhance the appearance of the box plot, request additional analyses, save results in data sets, and so on. Complete descriptions of each option follow.

PLOT Statement Options

Many PLOT statement options apply only to traditional graphics and are ignored when ODS Graphics is enabled. Table 26.6 summarizes the options available in the PLOT statement. It also lists options by function and indicates which are applicable with ODS Graphics.

Table 26.6 PLOT Statement Options

Option	Description	ODS Graphics
Options for Controlling Box Appearance		
BOXCONNECT=	Connects features of adjacent box-and-whiskers plots with line segments	✓
BOXSTYLE=	Specifies style of box-and-whiskers plots	✓
BOXWIDTH=	Specifies width of box-and-whiskers plots	
BOXWIDTHSCALE=	Specifies that widths of box-and-whiskers plots vary proportionately to group size	✓
CBOXES=	Specifies color for outlines of box-and-whiskers plots	
CBOXFILL=	Specifies fill color for interior of box-and-whiskers plots	

Table 26.6 continued

Option	Description	ODS Graphics
IDCOLOR=	Specifies outlier symbol color in schematic box-and-whiskers plots	
IDCTEXT=	Specifies outlier label color in schematic box-and-whiskers plots	
IDFONT=	Specifies outlier label font in schematic box-and-whiskers plots	
IDHEIGHT=	Specifies outlier label height in schematic box-and-whiskers plots	
IDSYMBOL=	Specifies outlier symbol in schematic box-and-whiskers plots	
LBOXES=	Specifies line types for outlines of box-and-whiskers plots	
NOSERIFS	Eliminates serifs from whiskers of box-and-whiskers plots	✓
NOTCHES	Specifies that box-and-whiskers plots be notched	✓
PCTLDEF=	Specifies percentile definition used for box-and-whiskers plots	✓
Options for Plotting and Labeling Points		
ALLLABEL=	Labels means of box-and-whiskers plots	
CLABEL=	Specifies color for labels requested with ALLLABEL= option	
CCONNECT=	Specifies color for line segments requested with BOXCONNECT= option	
LABELANGLE=	Specifies angle for labels requested with ALLLABEL= option	
SYMBOLLEGEND=	Specifies LEGEND statement for levels of symbol variable	
SYMBOLORDER=	Specifies order in which symbols are assigned for levels of symbol variable	
Reference Line Options		
CHREF=	Specifies color for lines requested by HREF= option	
CVREF=	Specifies color for lines requested by VREF= option	
FRONTREF	Draws reference lines in front of boxes	
HREF=	Requests reference lines perpendicular to horizontal axis	✓
HREFLABELS=	Specifies labels for HREF= lines	✓
HREFLABPOS=	Specifies position of HREFLABELS= labels	
LHREF=	Specifies line type for HREF= lines	
LVREF=	Specifies line type for VREF= lines	
NOBYREF	Specifies that reference line information in a data set be applied uniformly to plots created for all BY groups	✓
VREF=	Requests reference lines perpendicular to vertical axis	✓
VREFLABELS=	Specifies labels for VREF= lines	✓
VREFLABPOS=	Specifies position of VREFLABELS= labels	
Block Variable Legend Options		
BLOCKLABELPOS=	Specifies position of label for block variable legend	
BLOCKLABTYPE=	Specifies text size of block variable legend	
BLOCKPOS=	Specifies vertical position of block variable legend	✓

Table 26.6 continued

Option	Description	ODS Graphics
BLOCKREP	Repeats identical consecutive labels in block variable legend	✓
CBLOCKLAB=	Specifies colors for filling frames enclosing block variable labels	
CBLOCKVAR=	Specifies colors for filling background of block variable legend	
Axis and Axis Label Options		
CAXIS=	Specifies color for axis lines and tick marks	
CFRAME=	Specifies fill color for frame for plot area	
CONTINUOUS	Produces horizontal axis for continuous group variable values (traditional graphics only)	
CTEXT=	Specifies color for tick mark values and axis labels	
HAXIS=	Specifies major tick mark values for horizontal axis	
HEIGHT=	Specifies height of axis label and axis legend text	
HMINOR=	Specifies number of minor tick marks between major tick marks on horizontal axis	
HOFFSET=	Specifies length of offset at both ends of horizontal axis	
NOHLABEL	Suppresses horizontal axis label	✓
NOTICKREP	Specifies that only first occurrence of repeated, adjacent character group values be labeled on horizontal axis	
NOVANGLE	Requests vertical axis labels that are strung out vertically	
SKIPLABELS=	Specifies thinning factor for tick mark labels on horizontal axis	
TURNHLABELS	Requests horizontal tick labels that are strung out vertically	
VAXIS=	Specifies major tick mark values for vertical axis	✓
VFORMAT=	Specifies format for vertical axis tick marks	✓
VMINOR=	Specifies number of minor tick marks between major tick marks on vertical axis	
VOFFSET=	Specifies length of offset at both ends of vertical axis	
VZERO	Forces origin to be included in vertical axis	
WAXIS=	Specifies width of axis lines	
Input Data Set Options		
MISSBREAK	Specifies that a missing value between identical character group values signify the start of a new group	✓
Output Data Set Options		
OUTBOX=	Produces an output data set containing group summary statistics and outlier values	✓
OUTHISTORY=	Produces an output data set containing group summary statistics	✓
Graphical Enhancement Options		
ANNOTATE=	Specifies annotate data set that adds features to box plot	
BWSLEGEND	Displays a legend identifying the function of group size specified with BOXWIDTHSCALE= option	

Table 26.6 continued

Option	Description	ODS Graphics
DESCRIPTION=	Specifies string that appears in description field of PROC GREPLAY master menu for high-resolution graphics box plot	
FONT=	Specifies font for labels and legends on plots	
HORIZONTAL	Requests a horizontal box plot with ODS Graphics	✓
HTML=	Specifies URLs to be associated with box-and-whiskers plots	
NAME=	Specifies name that appears in name field of PROC GREPLAY master menu for high-resolution graphics box plot	
NLEGEND	Requests legend displaying group sizes	
OUTHIGHHTML=	Specifies URLs to be associated with high outliers on box-and-whiskers plots	
OUTLOWHTML=	Specifies URLs to be associated with low outliers on box-and-whiskers plots	
PAGENUM=	Specifies form of label used in pagination	
PAGENUMPOS=	Specifies position of page number requested with PAGENUM= option	
Grid Options		
CGRID=	Specifies color for grid requested with ENDGRID or GRID option	
ENDGRID	Adds grid after last box-and-whiskers plot	
GRID	Adds grid to box plot	✓
LENDGRID=	Specifies line type for grid requested with ENDGRID option	
LGRID=	Specifies line type for grid requested with GRID option	
WGRID=	Specifies width of grid lines	

Table 26.6 *continued*

Option	Description	ODS Graphics
Plot Layout Options		
INTERVAL=	Specifies natural time interval between consecutive group positions when time, date, or datetime format is associated with numeric group variable	
INTSTART=	Specifies first major tick mark value on horizontal axis when date, time, or datetime format is associated with numeric group variable	
MAXPANELS=	Specifies maximum number of panels used for box plot	✓
NOCHART	Suppresses creation of box plot	✓
NOFRAME	Suppresses frame for plot area	
NPANELPOS=	Specifies number of group positions per panel	✓
REPEAT	Repeats last group position on panel as first group position of next panel	✓
TOTPANELS=	Specifies number of panels to be used to display box plot	✓
Overlay Options		
CCOVERLAY=	Specifies colors for line segments connecting points on overlays	
COVERLAY=	Specifies colors for points on overlays	
LOVERLAY=	Specifies line types for line segments connecting points on overlays	
NOOVERLAYLEGEND	Suppresses overlay legend	✓
OVERLAY=	Specifies variables to be plotted on overlays	✓
OVERLAYHTML=	Specifies URLs to be associated with overlay plot points	
OVERLAYID=	Specifies labels for overlay plot points	
OVERLAYLEGLAB=	Specifies label for overlay legend	✓
OVERLAYSYM=	Specifies symbols used for overlays	
OVERLAYSYMHT=	Specifies heights for overlay symbols	
WOVERLAY=	Specifies widths for line segments connecting points on overlays	
Clipping Options		
CCLIP=	Specifies color for plot symbol for clipped points	
CLIPFACTOR=	Determines extent to which extreme values are clipped	
CLIPLEGEND=	Specifies text for clipping legend	
CLIPLEGPOS=	Specifies position of clipping legend	
CLIPSUBCHAR=	Specifies substitution character for CLIPLEGEND= text	
CLIPSYMBOL=	Specifies plot symbol for clipped points	
CLIPSYMBOLHT=	Specifies symbol marker height for clipped points	
COVERLAYCLIP=	Specifies color for clipped points on overlays	
OVERLAYCLIPSYM=	Specifies symbol for clipped points on overlays	
OVERLAYCLIPSYMHT=	Specifies symbol height for clipped points on overlays	

Table 26.6 continued

Option	Description	ODS Graphics
Options for Box Plots Produced Using Styles		
BLOCKVAR=	Groups block legends whose backgrounds are filled with colors from style	✓
BOXES=	Groups boxes whose outlines are drawn with colors from style	
BOXFILL=	Groups boxes that are filled with colors from style	

Following are explanations of the options you can specify in the PLOT statement after a slash (/). Only those options marked with † are applicable when ODS Graphics is enabled.

ALLLABEL=VALUE | (*variable*)

labels the point plotted for the mean of each box-and-whiskers plot with the mean (when ALLLABEL=VALUE) or with the value of the ALLLABEL=*variable* from the input data set.

ANNOTATE=SAS-data-set

specifies an ANNOTATE= type data set, as described in *SAS/GRAPH: Reference*.

BLOCKLABELPOS=ABOVE | **LEFT**

specifies the position of a block variable label in the block legend. The keyword ABOVE places the label immediately above the legend, and LEFT places the label to the left of the legend. Use the keyword LEFT with labels that are short enough to fit in the margin of the plot; otherwise, they are truncated. The default keyword is ABOVE.

BLOCKLABTYPE=SCALED | **TRUNCATED****BLOCKLABTYPE=height**

specifies how lengthy block variable values are treated when there is insufficient space to display them in the block legend. If you specify BLOCKLABTYPE=SCALED, the values are uniformly reduced in height so that they fit. If you specify BLOCKLABTYPE=TRUNCATED, lengthy values are truncated on the right until they fit. You can also specify a text height in vertical percent screen units for the values. By default, lengthy values are not displayed. For more information, see the section “Displaying Blocks of Data” on page 1016.

† **BLOCKPOS=*n***

specifies the vertical position of the legend for the values of the block variables. Values of *n* and the corresponding positions are as follows. By default, BLOCKPOS=1.

n	Legend Position
1	top of plot, offset from axis frame
2	top of plot, immediately above axis frame
3	bottom of plot, immediately above horizontal axis
4	bottom of plot, below horizontal axis label

† BLOCKREP

specifies that block variable values for all groups be displayed. By default, only the first block variable value in any block is displayed, and repeated block variable values are not displayed.

† BLOCKVAR=*variable* | (*variable-list*)

specifies variables whose values are used to assign colors for filling the background of the legend associated with block variables. A list of BLOCKVAR= variables must be enclosed in parentheses. BLOCKVAR= variables are matched with block variables by their order in the respective variable lists. While the values of a CBLOCKVAR= variable are color names, values of a BLOCKVAR= variable are used to group block legends for assigning fill colors from the ODS style. Block legends with the same BLOCKVAR= variable value are filled with the same color.

† BOXCONNECT=MEAN | MEDIAN | MAX | MIN | Q1 | Q3**† BOXCONNECT**

specifies that the points in adjacent box-and-whiskers plots representing group means, medians, maximum values, minimum values, first quartiles, or third quartiles be connected with line segments. If the BOXCONNECT option is specified without a keyword identifying the points to be connected, group means are connected. By default, no points are connected.

BOXES=(*variable*)

specifies a variable whose values are used to assign colors for the outlines of box-and-whiskers plots. While the values of a CBOXES= variable are color names, values of the BOXES= variable are used to group box-and-whiskers plots for assigning outline colors from the ODS style. The outlines of box-and-whiskers plots of groups with the same BOXES= variable value are drawn using the same color.

BOXFILL=(*variable*)

specifies a variable whose values are used to assign fill colors for box-and-whiskers plots. While the values of a CBOXFILL= variable are color names, values of the BOXFILL= variable are used to group box-and-whiskers plots for assigning fill colors from the ODS style. Box-and-whiskers plots of groups with the same BOXFILL= variable value are filled with the same color.

† BOXSTYLE=*keyword*

specifies the style of the box-and-whiskers plots displayed. If you specify BOXSTYLE=SKELETAL, the whiskers are drawn from the edges of the box to the extreme values of the group. This plot is sometimes referred to as a skeletal box-and-whiskers plot. By default, the whiskers are drawn with serifs. You can specify the NOSERIFS option to draw the whiskers without serifs.

In the following descriptions, the terms *fence* and *far fence* refer to the distance from the first and third quartiles (25th and 75th percentiles, respectively), expressed in terms of the interquartile range (IQR). For example, the lower fence is located at $1.5 \times \text{IQR}$ below the 25th percentile; the upper fence is located at $1.5 \times \text{IQR}$ above the 75th percentile. Similarly, the lower far fence is located at $3 \times \text{IQR}$ below the 25th percentile; the upper far fence is located at $3 \times \text{IQR}$ above the 75th percentile.

If you specify BOXSTYLE=SCHEMATIC, a whisker is drawn from the upper edge of the box to the largest observed value within the upper fence, and another is drawn from the lower edge of the box to the smallest observed value within the lower fence. Serifs are added to the whiskers by default. Observations outside the fences are identified with a special symbol. For traditional graphics you can specify the shape and color for this symbol with the **IDSYMBOL=** and **IDCOLOR=** options. The default symbol is a square. This type of plot corresponds to the schematic box-and-whiskers plot

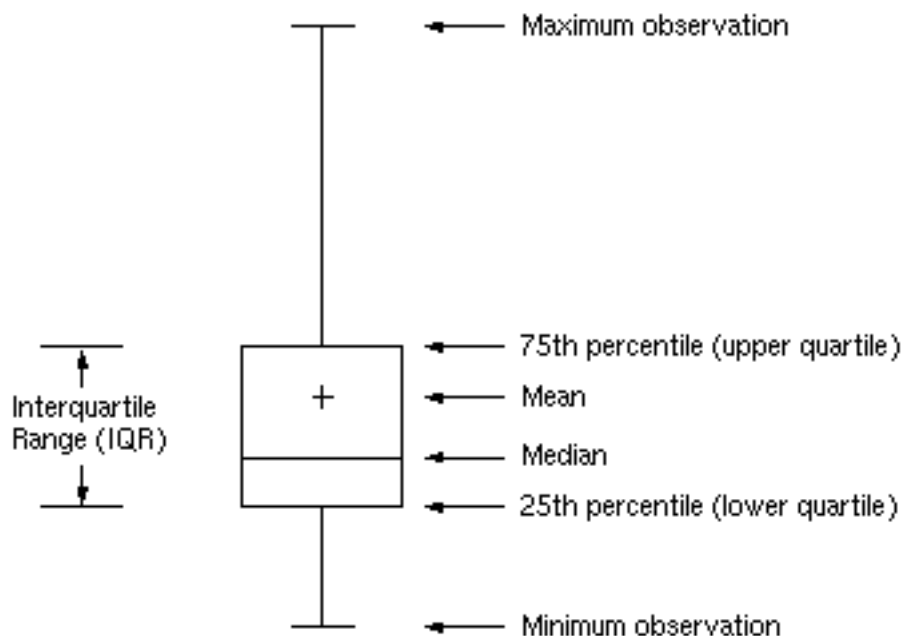
described in Chapter 2 of Tukey (1977). See Figure 26.8 and the discussion in the section “Styles of Box Plots” on page 1007 for more information.

If you specify `BOXSTYLE=SCHEMATICID`, a schematic box-and-whiskers plot is displayed in which an ID variable value is used to label the symbol marking each observation outside the upper and lower fences. A `BOX=` data set can contain a variable named `_ID_` that is used as the ID variable. Otherwise, the first variable listed in the ID statement provides the labels.

If you specify `BOXSTYLE=SCHEMATICIDFAR`, a schematic box-and-whiskers plot is displayed in which the value of the ID variable is used to label the symbol marking each observation outside the lower and upper far fences. Observations between the fences and the far fences are identified with a symbol but are not labeled with the ID variable.

Figure 26.6 illustrates the elements of a skeletal box-and-whiskers plot.

Figure 26.6 Skeletal Box-and-Whiskers Plot



The skeletal style of the box-and-whiskers plot shown in Figure 26.6 is the default.

BOXWIDTH=value

specifies the width (in horizontal percent screen units) of the box-and-whiskers plots.

† **BOXWIDTHSCALE=value**

specifies that the box-and-whiskers plot width is to vary proportionately to a particular function of the group size n . The function is determined by the *value*.

If you specify a positive value, the widths are proportional to n^{value} . In particular, if you specify `BOXWIDTHSCALE=1`, the widths are proportional to the group size. If you specify `BOXWIDTHSCALE=0.5`, the widths are proportional to \sqrt{n} , as described by McGill, Tukey, and Larsen (1978). If you specify `BOXWIDTHSCALE=0`, the widths are proportional to $\log(n)$. See Example 26.4 for an illustration of the `BOXWIDTHSCALE=` option.

You can specify the **BWSLEGEND** option to display a legend identifying the function of n used to determine the box-and-whiskers plot widths.

By default, the box widths are constant.

BWSLEGEND

displays a legend identifying the function of group size n specified with the **BOXWIDTHSCALE=** option. No legend is displayed if all group sizes are equal. The **BWSLEGEND** option is not applicable unless you also specify the **BOXWIDTHSCALE=** option.

CAXIS=*color*

CAXES=*color*

CA=*color*

specifies the color for the axes and tick marks. This option overrides any **COLOR=** specifications in an **AXIS** statement.

CBLOCKLAB=*color* | (*color-list*)

specifies fill colors for the frames that enclose the block variable labels in a block legend. By default, these areas are not filled. Colors in the **CBLOCKLAB=** list are matched with block variables in the order in which they appear in the **PLOT** statement.

CBLOCKVAR=*variable* | (*variable-list*)

specifies variables whose values are colors for filling the background of the legend associated with block variables. **CBLOCKVAR=** variables are matched with block variables by their order in the respective variable lists. Each **CBLOCKVAR=** variable must be a character variable of no more than eight characters in the input data set, and its values must be valid SAS/GRAPH color names (see *SAS/GRAPH: Reference* for complete details). A list of **CBLOCKVAR=** variables must be enclosed in parentheses.

The procedure matches the **CBLOCKVAR=** variables with block variables in the order specified. That is, each block legend is filled with the color value of the **CBLOCKVAR=** variable of the first observation in each block. In general, values of the i th **CBLOCKVAR=** variable are used to fill the block of the legend corresponding to the i th block variable.

By default, fill colors are not used for the block variable legend. The **CBLOCKVAR=** option is available only when block variables are used in the **PLOT** statement.

CBOXES=*color* | (*variable*)

specifies the colors for the outlines of the box-and-whiskers plots created with the **PLOT** statement. You can use one of the following approaches:

- You can specify **CBOXES=***color* to provide a single outline color for all the box-and-whiskers plots.
- You can specify **CBOXES=**(*variable*) to provide a distinct outline color for each box-and-whiskers plot as the value of the variable. The variable must be a character variable of up to eight characters in the input data set, and its values must be valid SAS/GRAPH color names (see *SAS/GRAPH: Reference* for complete details). The outline color of the plot displayed for a particular group is the value of the variable in the observations corresponding to this group. Note that if there are multiple observations per group in the input data set, the values of the variable should be identical for all the observations in a given group.

CBOXFILL=*color* | (*variable*)

specifies the interior fill colors for the box-and-whiskers plots. You can use one of the following approaches:

- You can specify **CBOXFILL=***color* to provide a single color for all of the box-and-whiskers plots.
- You can specify **CBOXFILL=**(*variable*) to provide a distinct color for each box-and-whiskers plot as the value of the variable. The variable must be a character variable of up to eight characters in the input data set, and its values must be valid SAS/GRAPH color names (or the value **EMPTY**, which you can use to suppress color filling). See *SAS/GRAPH: Reference* for complete details. The interior color of the box displayed for a particular group is the value of the variable in the observations corresponding to this group. Note that if there are multiple observations per group in the input data set, the values of the variable should be identical for all the observations in a given group.

By default, the interiors are not filled.

CCLIP=*color*

specifies a color for the plotting symbol that is specified with the **CLIPSYMBOL=** option to mark clipped values. The default color is the color specified in the **COLOR=** option in the **SYMBOL1** statement.

CCONNECT=*color*

specifies the color for line segments connecting points on the plot. The default color is the color specified in the **COLOR=** option in the **SYMBOL1** statement. This option is not applicable unless you also specify the **BOXCONNECT=** option.

CCOVERLAY=(*color-list*)

specifies the colors for line segments connecting points on overlay plots. Colors in the **CCOVERLAY=** list are matched with variables in the corresponding positions in the **OVERLAY=** list. By default, points are connected by line segments of the same color as the plotted points. You can specify the value **NONE** to suppress the line segments connecting points of an overlay plot.

CFRAME=*color*

specifies the color for filling the rectangle enclosed by the axes and the frame. By default, this area is not filled. The **CFRAME=** option cannot be used in conjunction with the **NOFRAME** option.

CGRID=*color*

specifies the color for the grid requested by the **ENDGRID** or **GRID** option. By default, the grid is the same color as the axes.

CHREF=*color*

specifies the color for the lines requested by the **HREF=** option.

CLABEL=*color*

specifies the color for labels produced by the **ALLLABEL=** option. The default color is the **CTEXT=** color.

CLIPFACTOR=*factor*

requests clipping of extreme values on the box plot. The *factor* that you specify determines the extent to which these values are clipped, and it must be greater than 1.

For examples of the CLIPFACTOR= option, see [Figure 26.17](#) and [Figure 26.18](#). Related clipping options are CCLIP=, CLIPLEGEND=, CLIPLEGPOS=, CLIPSUBCHAR=, and CLIPSYMBOL=.

CLIPLEGEND=*'label'*

specifies the *label* for the legend that indicates the number of clipped boxes when the CLIPFACTOR= option is used. The *label* must be no more than 16 characters and must be enclosed in quotes. For an example, see [Figure 26.18](#).

CLIPLEGPOS= TOP | BOTTOM

specifies the position for the legend that indicates the number of clipped boxes when the CLIPFACTOR= option is used. The keyword TOP or BOTTOM positions the legend at the top or bottom of the chart, respectively. Do not specify CLIPLEGPOS=TOP together with the BLOCKPOS=1 or BLOCKPOS=2 option. By default, CLIPLEGPOS=BOTTOM.

CLIPSUBCHAR=*'character'*

specifies a substitution character (such as '#') for the label provided with the CLIPLEGEND= option. The substitution character is replaced with the number of boxes that are clipped. For example, suppose that the following statements produce a chart in which three boxes are clipped:

```
proc boxplot data=Pistons;
  plot Diameter*Hour /
    clipfactor = 1.5
    cliplegend = 'Boxes clipped=#'
    clipsubchar = '#' ;
run;
```

Then the clipping legend displayed on the chart will be “Boxes clipped=3”.

CLIPSYMBOL=*symbol*

specifies a plot symbol used to identify clipped points on the chart and in the legend when the CLIPFACTOR= option is used. You should use this option in conjunction with the CLIPFACTOR= option. The default *symbol* is CLIPSYMBOL=SQUARE.

CLIPSYMBOLHT=*value*

specifies the height for the symbol marker used to identify clipped points on the chart when the CLIPFACTOR= option is used. The default is the height specified with the H= option in the SYMBOL statement.

For general information about clipping options, see the section “[Clipping Extreme Values](#)” on page 1018.

CONTINUOUS

specifies that numeric group variable values be treated as continuous values. By default, the values of a numeric group variable are considered discrete values unless the HAXIS= option is specified.

NOTE: The CONTINUOUS option is not supported for ODS Graphics output. For more information, see the discussion in the section “[Continuous Group Variables](#)” on page 1009.

COVERLAY=(color-list)

specifies the colors used to plot overlay variables. Colors in the COVERLAY= list are matched with variables in the corresponding positions in the OVERLAY= list.

COVERLAYCLIP=color

specifies the color used to plot clipped values on overlay plots when the CLIPFACTOR= option is used.

CTEXT=color

specifies the color for tick mark values and axis labels. The default color is the color specified in the CTEXT= option in the most recent GOPTIONS statement.

CVREF=color

specifies the color for the lines requested by the VREF= option.

DESCRIPTION='string'**DES='string'**

specifies a description of a box plot produced with high-resolution graphics. The description appears in the PROC GREPLAY master menu and can be no longer than 256 characters. The default description is the analysis variable name.

ENDGRID

adds a grid to the rightmost portion of the plot, beginning with the first labeled major tick mark position that follows the last box-and-whiskers plot. You can use the HAXIS= option to force space to be added to the horizontal axis.

FONT=font

specifies a font for labels and legends. You can also specify fonts for axis labels in an AXIS statement. The FONT= font takes precedence over the FTEXT= font specified in the GOPTIONS statement. See *SAS/GRAPH: Reference* for more information about the GOPTIONS statement.

FRONTREF

draws reference lines specified with the HREF= and VREF= options in front of box-and-whiskers plots. By default, reference lines are drawn behind the box-and-whiskers plots and can be obscured by filled boxes.

† GRID

adds a grid to the box plot. Grid lines are horizontal lines positioned at labeled major tick marks, and they cover the length and height of the plotting area.

HAXIS=value-list**HAXIS=AXIS n**

specifies tick mark values for the horizontal (group) axis. If the group variable is numeric, the values must be numeric and equally spaced. If the group variable is character, values must be quoted strings of up to 16 characters. Optionally, you can specify an axis name defined in a previous AXIS statement. See *SAS/GRAPH: Reference* for more information about the AXIS statement.

If you are producing traditional graphics, specifying the HAXIS= option with a numeric group variable causes the group variable values to be treated as continuous values. For more information, see the description of the CONTINUOUS option and the discussion in the section “Continuous Group Variables” on page 1009. Numeric values can be given in an explicit or implicit list. If a date, time,

or datetime format is associated with a numeric group variable, SAS datetime literals can be used. Examples of HAXIS= lists follow:

- haxis=0 2 4 6 8 10
- haxis=0 to 10 by 2
- haxis='LT12A' 'LT12B' 'LT12C' 'LT15A' 'LT15B' 'LT15C'
- haxis='20MAY88'D to '20AUG88'D by 7
- haxis='01JAN88'D to '31DEC88'D by 30

If the group variable is numeric, the HAXIS= list must span the group variable values. If the group variable is character, the HAXIS= list must include all of the group variable values. You can add group positions to the box plot by specifying HAXIS= values that are not group variable values.

If you specify a large number of HAXIS= values, some of these can be thinned to avoid collisions between tick mark labels. To avoid thinning, use one of the following methods.

- Shorten values of the group variable by eliminating redundant characters. For example, if your group variable has values LOT1, LOT2, LOT3, and so on, you can use the SUBSTR function in a DATA step to eliminate LOT from each value, and you can modify the horizontal axis label to indicate that the values refer to lots.
- Use the [TURNHLABELS](#) option to turn the labels vertically.
- Use the [NPANELPOS=](#) option to force fewer group positions per panel.

HEIGHT=*value*

specifies the height (in vertical screen percent units) of the text for axis labels and legends. This value takes precedence over the HTEXT= value specified in the GOPTIONS statement. This option is recommended for use with fonts specified with the [FONT=](#) option or with the FTEXT= option in the GOPTIONS statement. See *SAS/GRAPH: Reference* for complete information about the GOPTIONS statement.

HMINOR=*n*

HM=*n*

specifies the number of minor tick marks between major tick marks on the horizontal axis. Minor tick marks are not labeled. The default is HMINOR=0.

HOFFSET=*value*

specifies the length (in percent screen units) of the offset at both ends of the horizontal axis. You can eliminate the offset by specifying HOFFSET=0.

† HORIZONTAL

produces a horizontal box plot, with group variable values on the vertical axis and analysis variable values on the horizontal axis. The HORIZONTAL option is supported only with ODS Graphics.

† HREF=*value-list*

HREF=*SAS-data-set*

draws reference lines perpendicular to the horizontal (group) axis on the box plot. You can use this option in the following ways:

- You can specify the values for the lines with an HREF= list. If the group variable is numeric, the values must be numeric. If the group variable is character, the values must be quoted strings of up to 16 characters. If the group variable is formatted, the values must be given as internal values. Examples of HREF= values follow:

```
href=5
href=5 10 15 20 25 30
href='Shift 1' 'Shift 2' 'Shift 3'
```

- You can specify reference line values as the values of a variable named `_REF_` in an HREF= data set. The type and length of `_REF_` must match those of the group variable specified in the PLOT statement. Optionally, you can provide labels for the lines as values of a variable named `_REFLAB_`, which must be a character variable of up to 16 characters. If you want distinct reference lines to be displayed in plots for different analysis variables specified in the PLOT statement, you must include a character variable named `_VAR_`, whose values are the analysis variable names. If you do not include the variable `_VAR_`, all of the lines are displayed in all of the plots. Each observation in an HREF= data set corresponds to a reference line. If BY variables are used in the input data set, the same BY variable structure must be used in the reference line data set unless you specify the `NOBYREF` option.

Unless the `CONTINUOUS` or `HAXIS=` option is specified, numeric group variable values are treated as discrete values, and only HREF= values matching these discrete values are valid. Other values are ignored.

† **HREFLABELS=**'label1' ... 'labeln'

† **HREFLABEL=**'label1' ... 'labeln'

† **HREFLAB=**'label1' ... 'labeln'

specifies labels for the reference lines requested by the `HREF=` option. The number of labels must equal the number of lines. Enclose each label in quotes. Labels can be up to 16 characters.

HREFLABPOS=*n*

specifies the vertical position of the `HREFLABELS=` label, as described in the following table. By default, *n*=2.

HREFLABPOS=	Label Position
1	along top of plot area
2	staggered from top to bottom of plot area
3	along bottom of plot area
4	staggered from bottom to top of plot area

HTML=*variable*

specifies uniform resource locators (URLs) as values of the specified character variable (or formatted values of a numeric variable). These URLs are associated with box-and-whiskers plots when graphics output is directed into HTML. The value of the HTML= variable should be the same for each observation with a given value of the group variable.

IDCOLOR=*color*

specifies the color of the symbol marker used to identify outliers in schematic box-and-whiskers plots (that is, when you specify the keyword SCHEMATIC, SCHEMATICID, or SCHEMATICIDFAR with the **BOXSTYLE=** option). The default color is the color specified with the **CBOXES=** option.

IDTEXT=*color*

specifies the color for the text used to label outliers when you specify the keyword SCHEMATICID or SCHEMATICIDFAR with the **BOXSTYLE=** option. The default value is the color specified with the **CTEXT=** option.

IDFONT=*font*

specifies the font for the text used to label outliers when you specify the keyword SCHEMATICID or SCHEMATICIDFAR with the **BOXSTYLE=** option. The default font is SIMPLEX.

IDHEIGHT=*value*

specifies the height for the text used to label outliers when you specify the keyword SCHEMATICID or SCHEMATICIDFAR with the **BOXSTYLE=** option. The default value is the height specified with the **HTEXT=** option in the **GOPTIONS** statement. See *SAS/GRAPH: Reference* for complete information about the **GOPTIONS** statement.

IDSYMBOL=*symbol*

specifies the symbol marker used to identify outliers in schematic box plots. The default symbol is SQUARE.

INTERVAL=DAY | DTDAY | HOUR | MINUTE | MONTH | QTR | SECOND

specifies the natural time interval between consecutive group positions when a time, date, or datetime format is associated with a numeric group variable. By default, the **INTERVAL=** option uses the number of group positions per panel (screen or page) that you specify with the **NPANELPOS=** option. The default time interval keywords for various time formats are shown in the following table.

Format	Default Keyword	Format	Default Keyword
DATE	DAY	MONYY	MONTH
DATETIME	DTDAY	TIME	SECOND
DDMMYY	DAY	TOD	SECOND
HHMM	HOUR	WEEKDATE	DAY
HOUR	HOUR	WORDDATE	DAY
MMDDYY	DAY	YYMMDD	DAY
MMSS	MINUTE	YYQ	QTR

You can use the **INTERVAL=** option to modify the effect of the **NPANELPOS=** option, which specifies the number of group positions per panel. The **INTERVAL=** option enables you to match the scale of the horizontal axis to the scale of the group variable without having to associate a different format with the group variable.

For example, suppose that your formatted group values span an overall time interval of 100 days and a **DATETIME** format is associated with the group variable. Since the default interval for the **DATETIME** format is **DTDAY** and since **NPANELPOS=25** by default, the plot is displayed with four panels.

Now, suppose that your data span an overall time interval of 100 hours and a DATETIME format is associated with the group variable. The plot for these data is created in a single panel, but the data occupy only a small fraction of the plot since the scale of the data (hours) does not match that of the horizontal axis (days). If you specify INTERVAL=HOUR, the horizontal axis is scaled for 25 hours, matching the scale of the data, and the plot is displayed with four panels.

You should use the INTERVAL= option only in conjunction with the CONTINUOUS or HAXIS= option, which produces a horizontal axis of continuous group variable values. For more information, see the descriptions of the CONTINUOUS and HAXIS= options, and the discussion in the section “Continuous Group Variables” on page 1009.

INTSTART=*value*

specifies the starting value for a numeric horizontal axis when a date, time, or datetime format is associated with the group variable. If the value specified is greater than the first group variable value, this option has no effect.

LABELANGLE=*angle*

specifies the angle at which labels requested with the ALLLABEL= option are drawn. A positive angle rotates the labels counterclockwise; a negative angle rotates them clockwise. By default, labels are oriented horizontally.

LBOXES=*linetype*

LBOXES=*(variable)*

specifies the line types for the outlines of the box-and-whiskers plots. You can use one of the following approaches:

- You can specify LBOXES=*linetype* to provide a single linetype for all of the box-and-whiskers plots.
- You can specify LBOXES=*(variable)* to provide a distinct line type for each box-and-whiskers plot. The variable must be a numeric variable in the input data set, and its values must be valid SAS/GRAPH linetype values (numbers ranging from 1 to 46). The line type for the plot displayed for a particular group is the value of the variable in the observations corresponding to this group. Note that if there are multiple observations per group in the input data set, the values of the variable should be identical for all of the observations in a given group.

The default value is 1, which produces solid lines. See the description of the SYMBOL statement in *SAS/GRAPH: Reference* for more information about valid linytypes.

LENDGRID=*linetype*

specifies the line type for the grid requested with the ENDGRID option. The default value is 1, which produces a solid line. If you use the LENDGRID= option, you do not need to specify the ENDGRID option. See the description of the SYMBOL statement in *SAS/GRAPH: Reference* for more information about valid linytypes.

LGRID=*linetype*

specifies the line type for the grid requested with the GRID option. The default value is 1, which produces a solid line. If you use the LGRID= option, you do not need to specify the GRID option. See the description of the SYMBOL statement in *SAS/GRAPH: Reference* for more information about valid linytypes.

LHREF=*linetype*

LH=*linetype*

specifies the line type for reference lines requested with the **HREF=** option. The default value is 2, which produces a dashed line. See the description of the **SYMBOL** statement in *SAS/GRAPH: Reference* for more information about valid linetypes.

LOVERLAY=(*linetypes*)

specifies line types for the line segments connecting points on overlay plots. Line types in the **LOVERLAY=** list are matched with variables in the corresponding positions in the **OVERLAY=** list.

LVREF=*linetype*

LV=*linetype*

specifies the line type for reference lines requested by the **VREF=** option. The default value is 2, which produces a dashed line. See the description of the **SYMBOL** statement in *SAS/GRAPH: Reference* for more information about valid linetypes.

† **MAXPANELS=***n*

specifies the maximum number of panels used to display a box plot. By default, *n* = 20.

† **MISSBREAK**

determines how groups are formed when observations are read from a **DATA=** data set and a character group variable is provided. When you specify the **MISSBREAK** option, observations with missing values of the group variable are not processed. Furthermore, the next observation with a nonmissing value of the group variable is treated as the beginning observation of a new group even if this value is identical to the most recent nonmissing group value. In other words, by specifying the option **MISSBREAK** and by inserting an observation with a missing group variable value into a group of consecutive observations with the same group variable value, you can split the group into two distinct groups of observations.

By default (that is, when you omit the **MISSBREAK** option), observations with missing values of the group variable are not processed, and all remaining observations with the same consecutive value of the group variable are treated as a single group.

NAME='*string*'

specifies a name for the box plot, not more than eight characters, that appears in the **PROC GREPLAY** master menu.

NLEGEND

requests a legend displaying group sizes. If the size is the same for each group, that number is displayed. Otherwise, the minimum and maximum group sizes are displayed.

† **NOBYREF**

specifies that the reference line information in an **HREF=** or **VREF=** data set be applied uniformly to box plots created for all the **BY** groups in the input data set. If you specify the **NOBYREF** option, you do not need to provide **BY** variables in the reference line data set. By default, you must provide **BY** variables.

† **NOCHART**

suppresses the creation of the box plot. You typically specify the **NOCHART** option when you are using the procedure to compute group summary statistics and save them in an output data set.

NOFRAME

suppresses the default frame drawn around the plot.

† NOHLABEL

suppresses the label for the horizontal (group) axis. Use the NOHLABEL option when the meaning of the axis is evident from the tick mark labels, such as when a date format is associated with the group variable.

† NOOVERLAYLEGEND

suppresses the legend for overlay plots that is displayed by default when the OVERLAY= option is specified.

† NOSERIFS

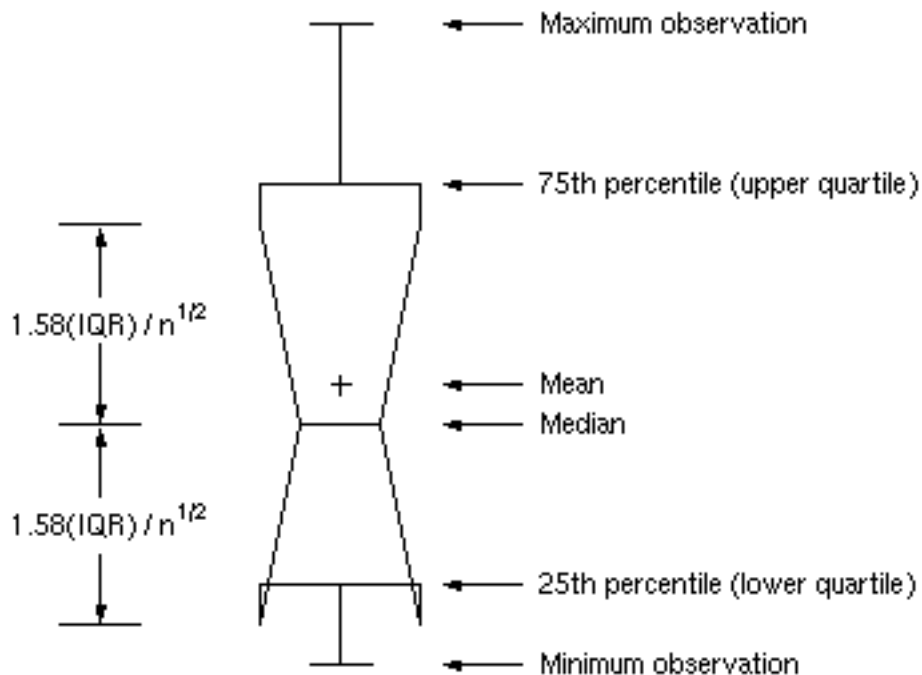
eliminates serifs from the whiskers of box-and-whiskers plots.

† NOTCHES

specifies that box-and-whiskers plots be notched. The endpoints of the notches are located at the median plus and minus $1.58(\text{IQR}/\sqrt{n})$, where IQR is the interquartile range and n is the group size. The medians (central lines) of two box-and-whiskers plots are significantly different at approximately the 0.95 confidence level if the corresponding notches do not overlap.

See McGill, Tukey, and Larsen (1978) for more information. Figure 26.7 illustrates the NOTCHES option. Notice the folding effect at the bottom, which happens when the endpoint of a notch is beyond its corresponding quartile. This situation typically occurs when the group size is small.

Figure 26.7 Box Plot: The NOTCHES Option



NOTICKREP

applies to character-valued group variables and specifies that only the first occurrence of repeated, adjacent group values be labeled on the horizontal axis.

NOVANGLE

requests that the vertical axis label be strung out vertically.

† NPANELPOS=*n***NPANEL=*n***

specifies the number of group positions per panel. You typically specify the NPANELPOS= option to display more box-and-whiskers plots on a panel than the default number, which is $n = 25$.

You can specify a positive or negative number for n . The absolute value of n must be at least 5. If n is positive, the number of positions is adjusted so that it is approximately equal to n and so that all panels display approximately the same number of group positions. If n is negative, no balancing is done, and each panel (except possibly the last) displays approximately $|n|$ positions. In this case, the approximation is due only to axis scaling.

You can use the **INTERVAL=** option to change the effect of the NPANELPOS= option when a date or time format is associated with the group variable. The INTERVAL= option enables you to match the scale of the horizontal axis to the scale of the group variable without having to associate a different format with the group variable.

† OUTBOX=*SAS-data-set*

creates an output data set that contains group summary statistics and outlier values for a box plot. You can use an OUTBOX= data set as a **BOX=** input data set in a subsequent run of the procedure. See the section “**OUTBOX= Data Set**” on page 1002 for details.

OUTHIGHTHTML=*variable*

specifies a variable whose values are URLs to be associated with outlier points above the upper fence on a schematic box plot when graphics output is directed into HTML.

† OUTHISTORY=*SAS-data-set*

creates an output data set that contains the group summary statistics. You can use an OUTHISTORY= data set as a **HISTORY=** input data set in a subsequent run of the procedure. See the section “**OUTHISTORY= Data Set**” on page 1003 for details.

OUTLOWHTML=*variable*

specifies a variable whose values are URLs to be associated with outlier points below the lower fence on a schematic box plot when graphics output is directed into HTML.

† OVERLAY=(*variable-list*)

specifies variables to be plotted as overlays on the box plot. One value for each overlay variable is plotted at each group position. If there are multiple observations with the same group variable value in the input data set, the overlay variable values from the first observation in each group are plotted. By default, the points in an overlay plot are connected with line segments.

OVERLAYCLIPSYM=*symbol*

specifies the symbol used to plot clipped values on overlay plots when the **CLIPFACTOR=** option is used.

OVERLAYCLIPSYMHT=*value*

specifies the height for the symbol used to plot clipped values on overlay plots when the **CLIPFACTOR=** option is used.

OVERLAYHTML=(*variable-list*)

specifies variables whose values are URLs to be associated with points on overlay plots when graphics output is directed into HTML. Variables in the **OVERLAYHTML=** list are matched with variables in the corresponding positions in the **OVERLAY=** list.

OVERLAYID=(*variable-list*)

specifies variables whose formatted values are used to label points on overlays. Variables in the **OVERLAYID=** list are matched with variables in the corresponding positions in the **OVERLAY=** list. The value of the **OVERLAYID=** variable should be the same for each observation with a given value of the group variable.

† OVERLAYLEGLAB='label'

specifies the label displayed to the left of the overlay legend produced by the **OVERLAY=** option. The label can be up to 16 characters and must be enclosed in quotes. The default label is "Overlays:".

OVERLAYSYM=(*symbol-list*)

specifies symbols used to plot overlay variables. Symbols in the **OVERLAYSYM=** list are matched with variables in the corresponding positions in the **OVERLAY=** list.

OVERLAYSYMHT=(*value-list*)

specifies the heights of symbols used to plot overlay variables. Symbol heights in the **OVERLAYSYMHT=** list are matched with variables in the corresponding positions in the **OVERLAY=** list.

PAGENUM='string'

specifies the form of the label used for pagination. The string can be up to 16 characters, and it must include one or two occurrences of the substitution character '#'. The first '#' is replaced with the page number, and the optional second '#' is replaced with the total number of pages.

The **PAGENUM=** option is useful when you are working with a large number of groups, resulting in multiple pages of output. For example, suppose that each of the following **PLOT** statements produces multiple pages:

```
proc boxplot data=Pistons;
  plot Diameter*Hour / pagenum='Page #';
  plot Diameter*Hour / pagenum='Page # of #';
  plot Diameter*Hour / pagenum='#/#';
run;
```

The third page produced by the first statement would be labeled "Page 3". The third page produced by the second statement would be labeled "Page 3 of 5". The third page produced by the third statement would be labeled "3/5".

By default, no page number is displayed.

PAGENUMPOS=TL | TR | BL | BR | TL100 | TR100 | BL0 | BR0

specifies where to position the page number requested with the **PAGENUM=** option. The keywords TL, TR, BL, and BR correspond to the positions top left, top right, bottom left, and bottom right, respectively. You can use the TL100 and TR100 keywords to ensure that the page number appears at the very top of a page when a title is displayed. The BL0 and BR0 keywords ensure that the page number appears at the very bottom of a page when footnotes are displayed.

The default value is BR.

† PCTLDEF=*index*

specifies one of five definitions used to calculate percentiles in the construction of box-and-whiskers plots. The index can be 1, 2, 3, 4, or 5. The five corresponding percentile definitions are discussed in the section “[Percentile Definitions](#)” on page 1008. The default index is 5.

† REPEAT**† REP**

specifies that the horizontal axis of a plot that spans multiple panels be arranged so that the last group position on a panel is repeated as the first group position on the next panel. The REPEAT option facilitates cutting and pasting panels together. When a SAS DATETIME format is associated with the group variable, the REPEAT option is the default.

SKIPHLABELS=*n***SKIPHLABEL=*n***

specifies the number *n* of consecutive tick mark labels, beginning with the second tick mark label, that are thinned (not displayed) on the horizontal (group) axis. For example, specifying SKIPHLABEL=1 causes every other label to be skipped. Specifying SKIPHLABEL=2 causes the second and third labels to be skipped, the fifth and sixth labels to be skipped, and so forth.

The default value of the SKIPHLABELS= option is the smallest value *n* for which tick mark labels do not collide. A specified *n* will be overridden to avoid collision. To reduce thinning, you can use the [TURNHLABELS](#) option.

SYMBOLLEGEND=LEGEND*n***SYMBOLLEGEND=NONE**

controls the legend for the levels of a symbol variable (see [Example 26.1](#)). You can specify SYMBOLLEGEND=LEGEND*n*, where *n* is the number of a LEGEND statement defined previously. You can specify SYMBOLLEGEND=NONE to suppress the default legend. See *SAS/GRAPH: Reference* for more information about the LEGEND statement.

SYMBOLORDER=DATA | INTERNAL | FORMATTED**SYMORD=DATA | INTERNAL | FORMATTED**

specifies the order in which symbols are assigned for levels of the symbol variable. The DATA keyword assigns symbols to values in the order in which values appear in the input data set. The INTERNAL keyword assigns symbols based on sorted order of internal values of the symbol variable, and the FORMATTED keyword assigns them based on sorted formatted values. The default value is FORMATTED.

† **TOTPANELS**=*n*

specifies the total number of panels to be used to display the plot. This option overrides the **NPAN-ELPOS**= option.

TURNHLABELS**TURNHLABEL**

turns the major tick mark labels for the horizontal (group) axis so that they are arranged vertically. By default, labels are arranged horizontally.

Note that arranging the labels vertically might leave insufficient vertical space on the panel for a plot.

† **VAXIS**=*value-list***VAXIS**=**AXIS***n*

specifies major tick mark values for the vertical axis of a box plot. The values must be listed in increasing order, must be evenly spaced, and must span the range of values displayed in the plot. You can specify the values with an explicit list or with an implicit list, as shown in the following example:

```
proc boxplot;
  plot Width*Hour / vaxis=0 2 4 6 8;
  plot Width*Hour / vaxis=0 to 8 by 2;
run;
```

You can also specify a previously defined **AXIS** statement with the **VAXIS**= option.

† **VFORMAT**=*format*

specifies a format to be used for displaying tick mark labels on the vertical axis of the box plot.

VMINOR=*n***VM**=*n*

specifies the number of minor tick marks between major tick marks on the vertical axis. Minor tick marks are not labeled. By default, **VMINOR**=0.

VOFFSET=*value*

specifies the length in percent screen units of the offset at the ends of the vertical axis.

† **VREF**=*value-list*† **VREF**=*SAS-data-set*

draws reference lines perpendicular to the vertical axis. You can use this option in the following ways:

- Specify the values for the lines with a **VREF**= list:

```
vref=20
vref=20 40 80
```

- Specify the values for the lines as the values of a numeric variable named **_REF_** in a **VREF**= data set. Optionally, you can provide labels for the lines as values of a variable named **_REFLAB_**, which must be a character variable of up to 16 characters. If you want distinct reference lines to be displayed in plots for different analysis variables specified in the **PLOT** statement, you must include a character variable named **_VAR_**, whose values are the names of the analysis variables. If you do not include the variable **_VAR_**, all of the lines are displayed in all of the

plots. Each observation in the VREF= data set corresponds to a reference line. If BY variables are used in the input data set, the same BY-variable structure must be used in the VREF= data set unless you specify the NOBYREF option.

† VREFLABELS='label1' ... 'labeln'

† VREFLABEL='label1' ... 'labeln'

† VREFLAB='label1' ... 'labeln'

specifies labels for the reference lines requested by the VREF= option. The number of labels must equal the number of lines. Enclose each label in quotes. Labels can be up to 16 characters.

VREFLABPOS=*n*

specifies the horizontal position of the VREFLABELS= label, as described in the following table. By default, *n* = 1.

n	Label Position
1	left-justified in plot area
2	right-justified in plot area
3	left-justified in right margin

VZERO

forces the origin to be included in the vertical axis for a box plot.

WAXIS=*n*

specifies the width in pixels for the axis and frame lines. By default, *n* = 1.

WGRID=*n*

specifies the width in pixels for grid lines requested with the ENDGRID and GRID options. By default, *n* = 1.

WOVERLAY=(*value-list*)

specifies the widths in pixels for the line segments connecting points on overlay plots. Widths in the WOVERLAY= list are matched with variables in the corresponding positions in the OVERLAY= list. By default, all overlay widths are 1.

Details: BOXPLOT Procedure

Summary Statistics Represented by Box Plots

Table 26.7 lists the summary statistics represented in each box-and-whiskers plot.

Table 26.7 Summary Statistics Represented by Box Plots

Group Summary Statistic	Feature of Box-and-Whiskers Plot
maximum	endpoint of upper whisker
third quartile (75th percentile)	upper edge of box
median (50th percentile)	line inside box
mean	symbol marker
first quartile (25th percentile)	lower edge of box
minimum	endpoint of lower whisker

Note that you can request different box plot styles, as discussed in the section “Styles of Box Plots” on page 1007, and as illustrated in [Example 26.2](#).

Output Data Sets

OUTBOX= Data Set

The OUTBOX= data set saves group summary statistics and outlier values. The following variables can be saved:

- the group variable
- the variable `_VAR_`, containing the analysis variable name
- the variable `_TYPE_`, identifying features of box-and-whiskers plots
- the variable `_VALUE_`, containing values of box-and-whiskers plot features
- the variable `_ID_`, containing labels for outliers
- the variable `_HTML_`, containing URLs associated with plot features

`_ID_` is included in the OUTBOX= data set only if the keyword SCHEMATICID or SCHEMATICIDFAR is specified with the `BOXSTYLE=` option. `_HTML_` is present only if one or more of the `HTML=`, `OUT-HIGHHTML=`, and `OUTLOWHTML=` options are specified.

Each observation in an OUTBOX= data set records the value of a single feature of one group’s box-and-whiskers plot, such as its mean. The `_TYPE_` variable identifies the feature whose value is recorded in `_VALUE_`. [Table 26.8](#) lists valid `_TYPE_` variable values.

Table 26.8 Valid `_TYPE_` Values in an `OUTBOX=` Data Set

<code>_TYPE_</code>	Description
N	group size
MIN	minimum group value
Q1	group first quartile
MEDIAN	group median
MEAN	group mean
Q3	group third quartile
MAX	group maximum value
STDDEV	group standard deviation
LOW	low outlier value
HIGH	high outlier value
LOWHISKR	low whisker value, if different from MIN
HIWHISKR	high whisker value, if different from MAX
FARLOW	low far outlier value
FARHIGH	high far outlier value

Additionally, the following variables, if specified, are included:

- block variables
- symbol variable
- BY variables
- ID variables

OUTHISTORY= Data Set

The `OUTHISTORY=` data set saves group summary statistics. The following variables are saved:

- the group variable
- group minimum variables named by *analysis-variable* suffixed with *L*
- group first-quartile variables named by *analysis-variable* suffixed with *1*
- group mean variables named by *analysis-variable* suffixed with *X*
- group median variables named by *analysis-variable* suffixed with *M*
- group third-quartile variables named by *analysis-variable* suffixed with *3*
- group maximum variables named by *analysis-variable* suffixed with *H*
- group standard deviation variables named by *analysis-variable* suffixed with *S*
- group size variables named by *analysis-variable* suffixed with *N*

If an analysis variable name has the maximum length of 32 characters, PROC BOXPLOT forms summary statistic names from its first 16 characters, its last 15 characters, and the appropriate suffix.

Subgroup summary variables are created for each analysis variable specified in the PLOT statement. For example, consider the following statements:

```
proc boxplot data=Steel;
  plot (Width Diameter)*Lot / outhistory=Summary;
run;
```

The data set Summary contains variables named Lot, WidthL, Width1, WidthM, WidthX, Width3, WidthH, WidthS, WidthN, DiameterL, Diameter1, DiameterM, DiameterX, Diameter3, DiameterH, DiameterS, and DiameterN.

Additionally, the following variables, if specified, are included:

- BY variables
- block variables
- symbol variable
- ID variables

Note that an OUTHISTORY= data set does not contain outlier values, and therefore cannot be used, in general, to save a schematic box plot. You can use an OUTBOX= data set to save a schematic box plot summary.

Input Data Sets

DATA= Data Set

You can read analysis variable measurements from a data set specified with the DATA= option in the PROC BOXPLOT statement. Each analysis variable specified in the PLOT statement must be a SAS variable in the data set. This variable provides measurements that are organized into groups indexed by the group variable. The group variable, specified in the PLOT statement, must also be a SAS variable in the DATA= data set. Each observation in a DATA= data set must contain a value for each analysis variable and a value for the group variable. If the i th group contains n_i measurements, there should be n_i consecutive observations for which the value of the group variable is the index of the i th group. For example, if each group contains 20 items and there are 30 groups, the DATA= data set should contain 600 observations. Other variables that can be read from a DATA= data set include the following:

- block variables
- symbol variable
- BY variables
- ID variables

BOX= Data Set

You can read group summary statistics and outlier information from a BOX= data set specified in the PROC BOXPLOT statement. This enables you to reuse OUTBOX= data sets that have been created in previous runs of the BOXPLOT procedure to reproduce schematic box plots.

A BOX= data set must contain the following variables:

- the group variable
- `_VAR_`, containing the analysis variable name
- `_TYPE_`, identifying features of box-and-whiskers plots
- `_VALUE_`, containing values of those features

Each observation in a BOX= data set records the value of a single feature of one group's box-and-whiskers plot, such as its mean. Consequently, a BOX= data set contains multiple observations per group. These must appear consecutively in the BOX= data set.

The `_TYPE_` variable identifies the feature whose value is recorded in a given observation. The following table lists valid `_TYPE_` variable values.

Table 26.9 Valid `_TYPE_` Values in a BOX= Data Set

<code>_TYPE_</code>	Description
N	group size
MIN	group minimum value
Q1	group first quartile
MEDIAN	group median
MEAN	group mean
Q3	group third quartile
MAX	group maximum value
STDDEV	group standard deviation
LOW	low outlier value
HIGH	high outlier value
LOWHISKR	low whisker value, if different from MIN
HIWHISKR	high whisker value, if different from MAX
FARLOW	low far outlier value
FARHIGH	high far outlier value

The features identified by `_TYPE_` values N, MIN, Q1, MEDIAN, MEAN, Q3, and MAX are required for each group.

Other variables that can be read from a BOX= data set include the following:

- the variable `_ID_`, containing labels for outliers
- the variable `_HTML_`, containing URLs to be associated with features on box plots

- block variables
- symbol variable
- BY variables
- ID variables

When you specify the keyword SCHEMATICID or SCHEMATICIDFAR with the `BOXSTYLE=` option, values of `_ID_` are used as outlier labels. If `_ID_` does not exist in the `BOX=` data set, the values of the first variable listed in the ID statement are used.

HISTORY= Data Set

You can read group summary statistics from a `HISTORY=` data set specified in the `PROC BOXPLOT` statement. This enables you to reuse `OUTHISTORY=` data sets that have been created in previous runs of the `BOXPLOT` procedure or to read output data sets created with SAS summarization procedures, such as `PROC UNIVARIATE`.

Note that a `HISTORY=` data set does *not* contain outlier information. Therefore, in general you cannot reproduce a schematic box plot from summary statistics saved in an `OUTHISTORY=` data set. To save and reproduce schematic box plots, use `OUTBOX=` and `BOX=` data sets.

A `HISTORY=` data set must contain the following:

- the group variable
- a group minimum variable for each analysis variable
- a group first-quartile variable for each analysis variable
- a group median variable for each analysis variable
- a group mean variable for each analysis variable
- a group third-quartile variable for each analysis variable
- a group maximum variable for each analysis variable
- a group standard deviation variable for each analysis variable
- a group size variable for each analysis variable

The names of the group summary statistics variables must be the analysis variable name concatenated with the following special suffix characters.

Group Summary Statistic	Suffix Character
group minimum	L
group first quartile	1
group median	M
group mean	X
group third quartile	3
group maximum	H
group standard deviation	S
group size	N

For example, consider the following statements:

```
proc boxplot history=Summary;
  plot (Weight Yieldstrength) * Batch;
run;
```

The data set Summary must include the variables Batch, WeightL, Weight1, WeightM, WeightX, Weight3, WeightH, WeightS, WeightN, YieldstrengthL, Yieldstrength1, YieldstrengthM, YieldstrengthX, Yieldstrength3, YieldstrengthH, YieldstrengthS, and YieldstrengthN.

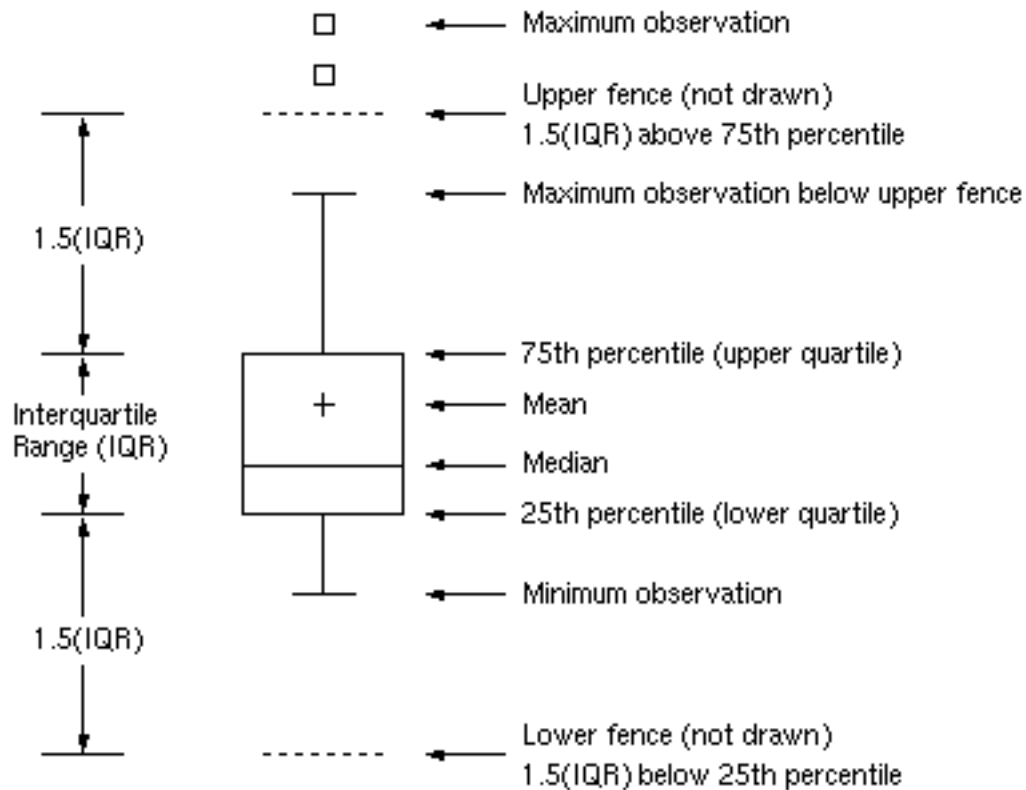
Note that if you specify an analysis variable whose name contains the maximum of 32 characters, the summary variable names must be formed from the first 16 characters and the last 15 characters of the analysis variable name, suffixed with the appropriate character.

These other variables can be read from a HISTORY= data set:

- block variables
- symbol variable
- BY variables
- ID variables

Styles of Box Plots

A box-and-whiskers plot is displayed for the measurements in each group on the box plot. The *skeletal* style of the box-and-whiskers plot shown in Figure 26.6 is the default. You can produce a *schematic* box plot by specifying the `BOXSTYLE=SCHEMATIC` option in the PLOT statement. Figure 26.8 illustrates a typical schematic box plot and the locations of the fences (which are not displayed in actual output). See the description of the `BOXSTYLE=` option for complete details.

Figure 26.8 Schematic Box-and-Whiskers Plot

You can draw connecting lines between adjacent box-and-whiskers plots by using the `BOXCONNECT=keyword` option. For example, `BOXCONNECT=MEAN` connects the points representing the means of adjacent groups. Other available keywords are `MIN`, `Q1`, `MEDIAN`, `Q3`, and `MAX`. Specifying `BOXCONNECT` without a keyword is equivalent to specifying `BOXCONNECT=MEAN`. You can specify the color for the connecting lines with the `CCONNECT=` option.

Percentile Definitions

You can use the `PCTLDEF=` option to specify one of five definitions for computing quantile statistics (percentiles). Suppose that n is the number of nonmissing values for a variable and that x_1, x_2, \dots, x_n represent the ordered values of the analysis variable. For the t th percentile, set $p = t/100$.

For the following definitions numbered 1, 2, 3, and 5, express np as

$$np = j + g$$

where j is the integer part of np , and g is the fractional part of np . For definition 4, let

$$(n + 1)p = j + g$$

The t th percentile (call it y) can be defined as follows:

PCTLDEF=1	weighted average at x_{np} $y = (1 - g)x_j + gx_{j+1}$ where x_0 is taken to be x_1 .
PCTLDEF=2	observation numbered closest to np $y = x_i$ where i is the integer part of $np + 1/2$ if $g \neq 1/2$. If $g = 1/2$, then $y = x_j$ if j is even, or $y = x_{j+1}$ if j is odd.
PCTLDEF=3	empirical distribution function $y = x_j \text{ if } g = 0$ $y = x_{j+1} \text{ if } g > 0$
PCTLDEF=4	weighted average aimed at $x_{p(n+1)}$ $y = (1 - g)x_j + gx_{j+1}$ where x_{n+1} is taken to be x_n .
PCTLDEF=5	empirical distribution function with averaging $y = (x_j + x_{j+1})/2 \text{ if } g = 0$ $y = x_{j+1} \text{ if } g > 0$

Missing Values

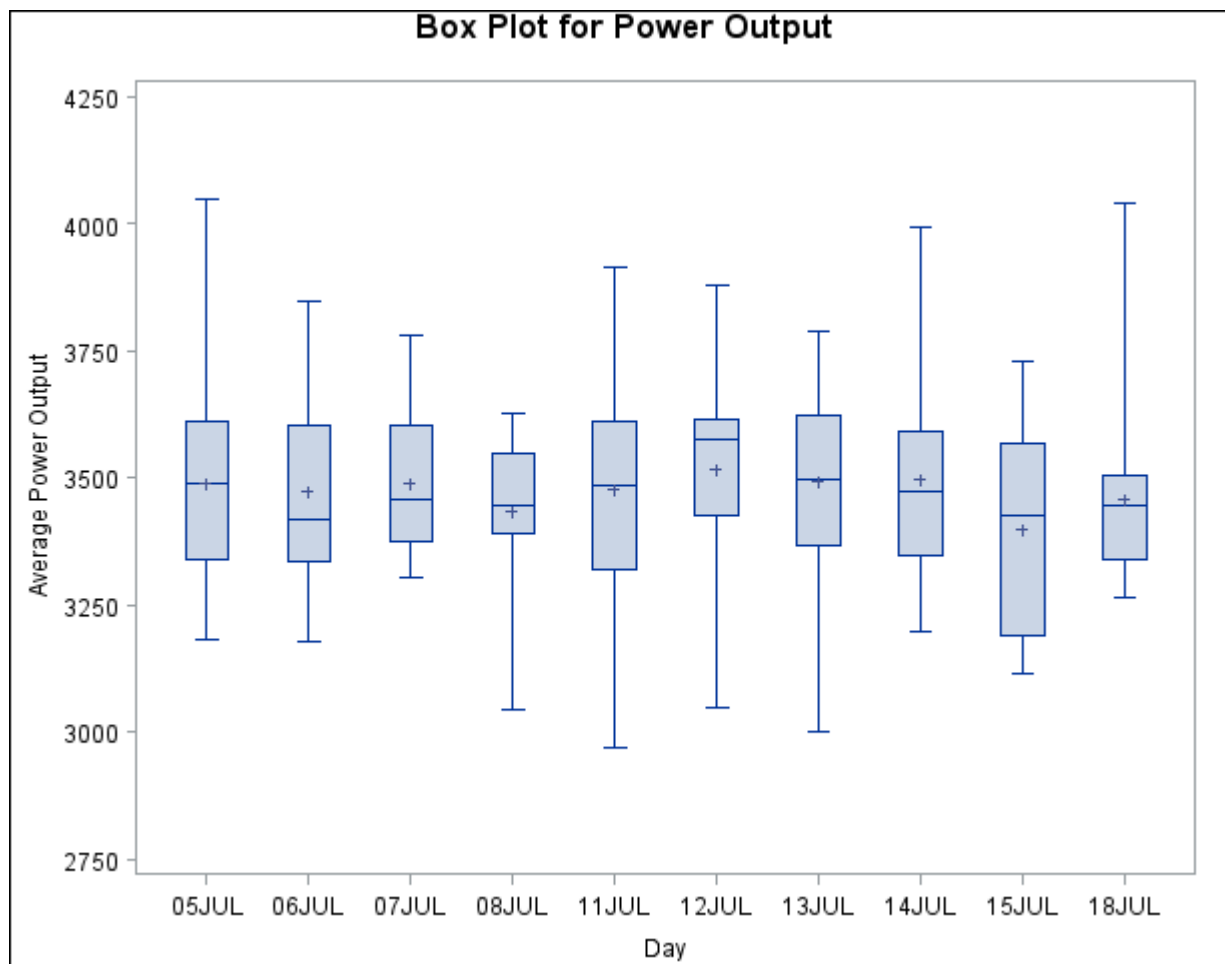
An observation read from an input data set is not analyzed if the value of the group variable is missing. For a particular analysis variable, an observation read from a `DATA=` data set is not analyzed if the value of the analysis variable is missing.

Continuous Group Variables

By default, the `PLOT` statement treats numerical group variable values as *discrete* values and spaces the boxes evenly on the plot. The following statements produce the box plot in [Figure 26.9](#):

```
ods graphics off;
title 'Box Plot for Power Output';
proc boxplot data=Turbine;
  plot KWatts*Day;
run;
```

Figure 26.9 Box Plot with Discrete Group Variable



The labels on the horizontal axis in Figure 26.9 do not represent 10 consecutive days, but the box-and-whiskers plots are evenly spaced.

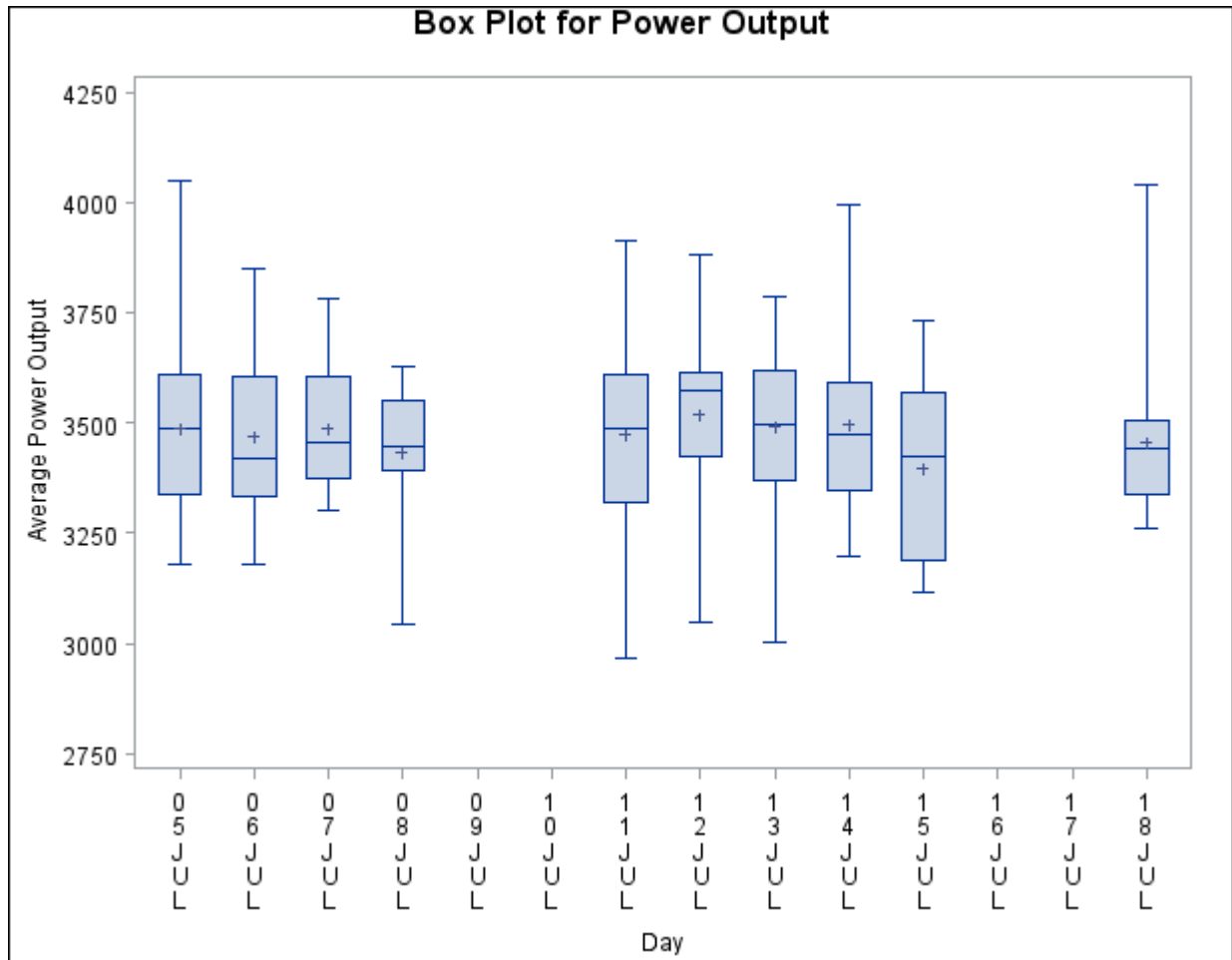
In order to treat the group variable as *continuous*, you can specify the `CONTINUOUS` or `HAXIS=` option when producing traditional graphics. Either option produces a box plot with a horizontal axis scaled for continuous group variable values. (ODS Graphics does not support a continuous group axis.)

The following statements produce the plot shown in Figure 26.10. The `TURNHLABELS` option orients the horizontal axis labels vertically so there is room to display them all.

```

title 'Box Plot for Power Output';
proc boxplot data=Turbine;
  plot KWatts*Day / turnhlabels
          continuous;
run;

```

Figure 26.10 Box Plot with Continuous Group Variable

Note that the tick values on the horizontal axis represent consecutive days and that no box-and-whiskers plots are displayed for days when no turbine data were collected.

Positioning Insets

This section provides details on three different methods of positioning INSET boxes by using the POSITION= option. With the POSITION= option, you can specify the following:

- compass points
- keywords for margin positions
- coordinates in data units or percent axis units

Positioning the Inset Using Compass Points

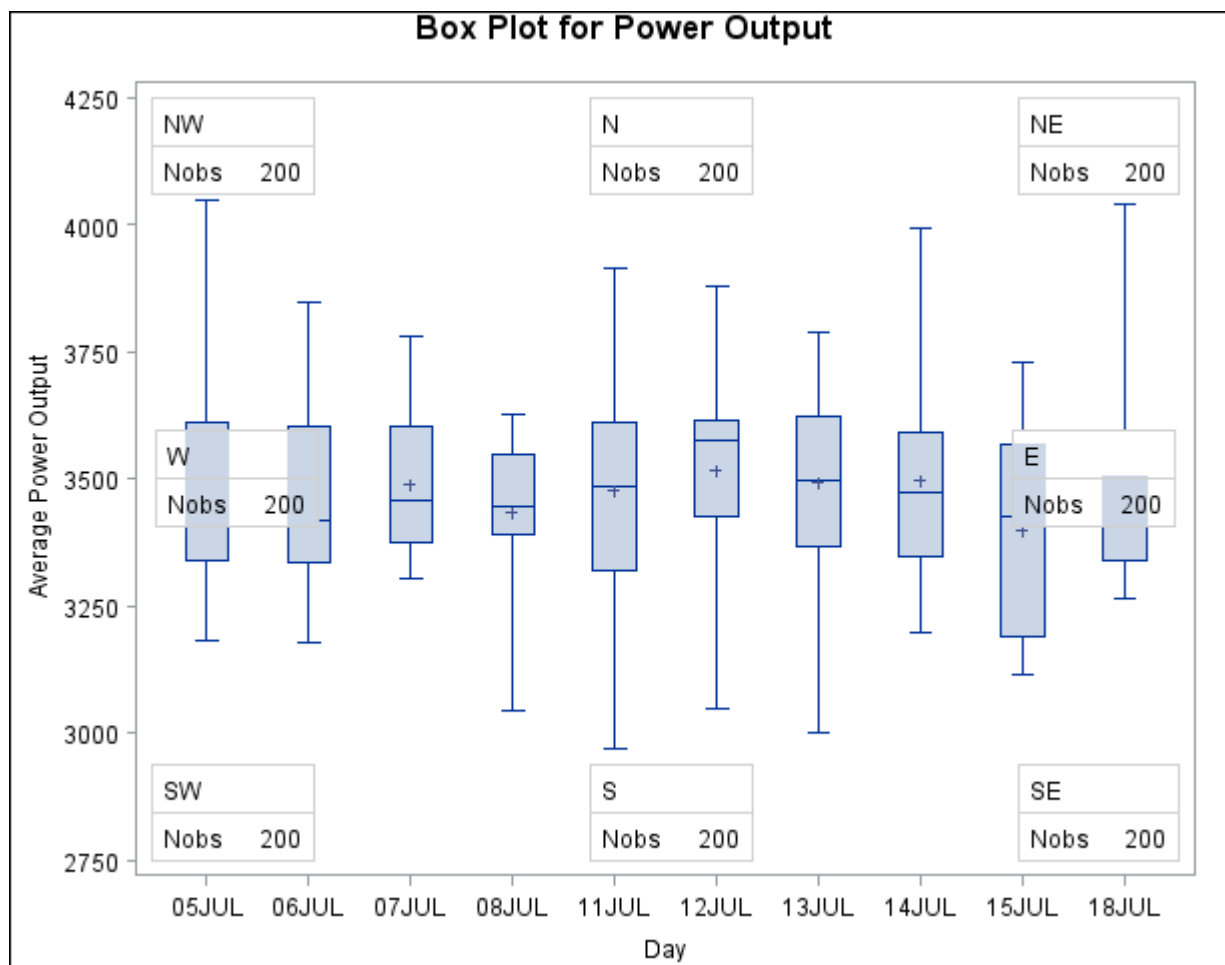
You can specify the eight compass points (N, NE, E, SE, S, SW, W, and NW) as keywords for the POSITION= option. The default inset position is NW. The following statements create the display in Figure 26.11, which illustrates all eight compass positions:

```

title 'Box Plot for Power Output';
proc boxplot data=Turbine;
  plot KWatts*Day;
  inset nobs / height=2.5 cfill=blank header='NW' pos=nw;
  inset nobs / height=2.5 cfill=blank header='N ' pos=n ;
  inset nobs / height=2.5 cfill=blank header='NE' pos=ne;
  inset nobs / height=2.5 cfill=blank header='E ' pos=e ;
  inset nobs / height=2.5 cfill=blank header='SE' pos=se;
  inset nobs / height=2.5 cfill=blank header='S ' pos=s ;
  inset nobs / height=2.5 cfill=blank header='SW' pos=sw;
  inset nobs / height=2.5 cfill=blank header='W ' pos=w ;
run;

```

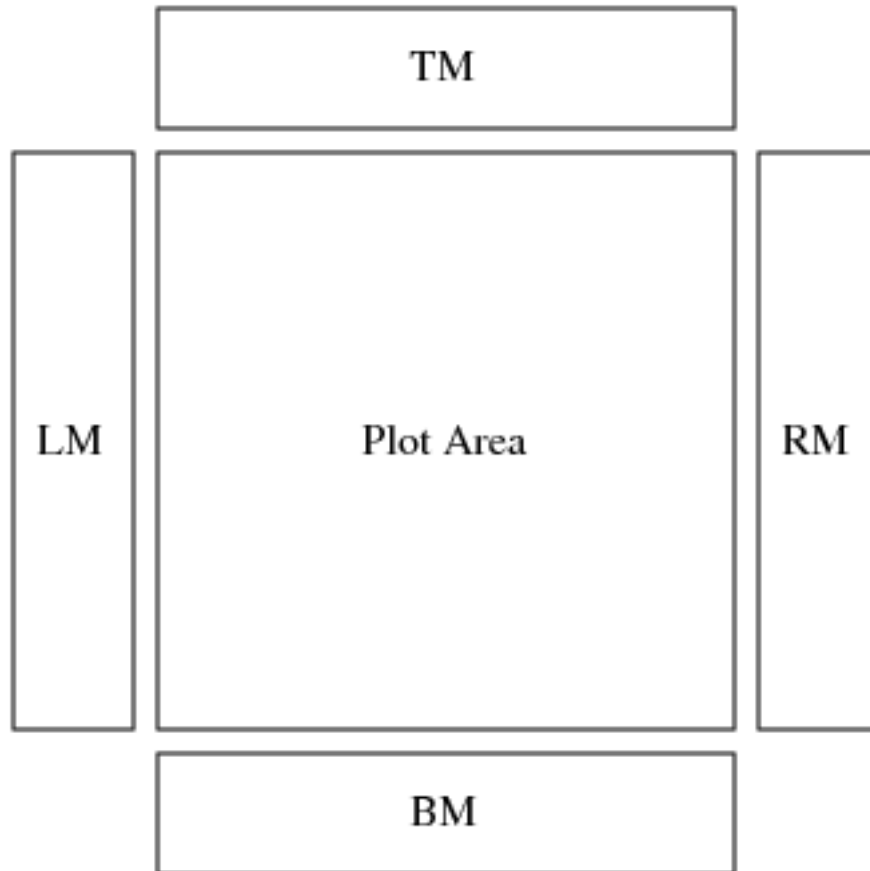
Figure 26.11 Insets Positioned Using Compass Points



Positioning the Inset in the Margins

You can also use the INSET statement to position an inset in one of the four margins surrounding the plot area by using the margin keyword LM, RM, TM, or BM, as illustrated in Figure 26.12.

Figure 26.12 Positioning Insets in the Margins



For an example of an inset placed in the top margin, see [Output 26.1.1](#). Margin positions are recommended for insets containing a large number of statistics. If you attempt to display a lengthy inset in the interior of the plot, it is likely that the inset will collide with the data display.

Positioning the Inset Using Coordinates

You can also specify the position of an inset with coordinates by using the POSITION= (*x*, *y*) option. You can specify coordinates in axis percent units (the default) or in axis data units.

Data Unit Coordinates

If you specify the DATA option immediately following the coordinates, the inset is positioned using axis data units. For example, the following statements place the bottom-left corner of the inset at 07JUL on the horizontal axis and 3950 on the vertical axis:

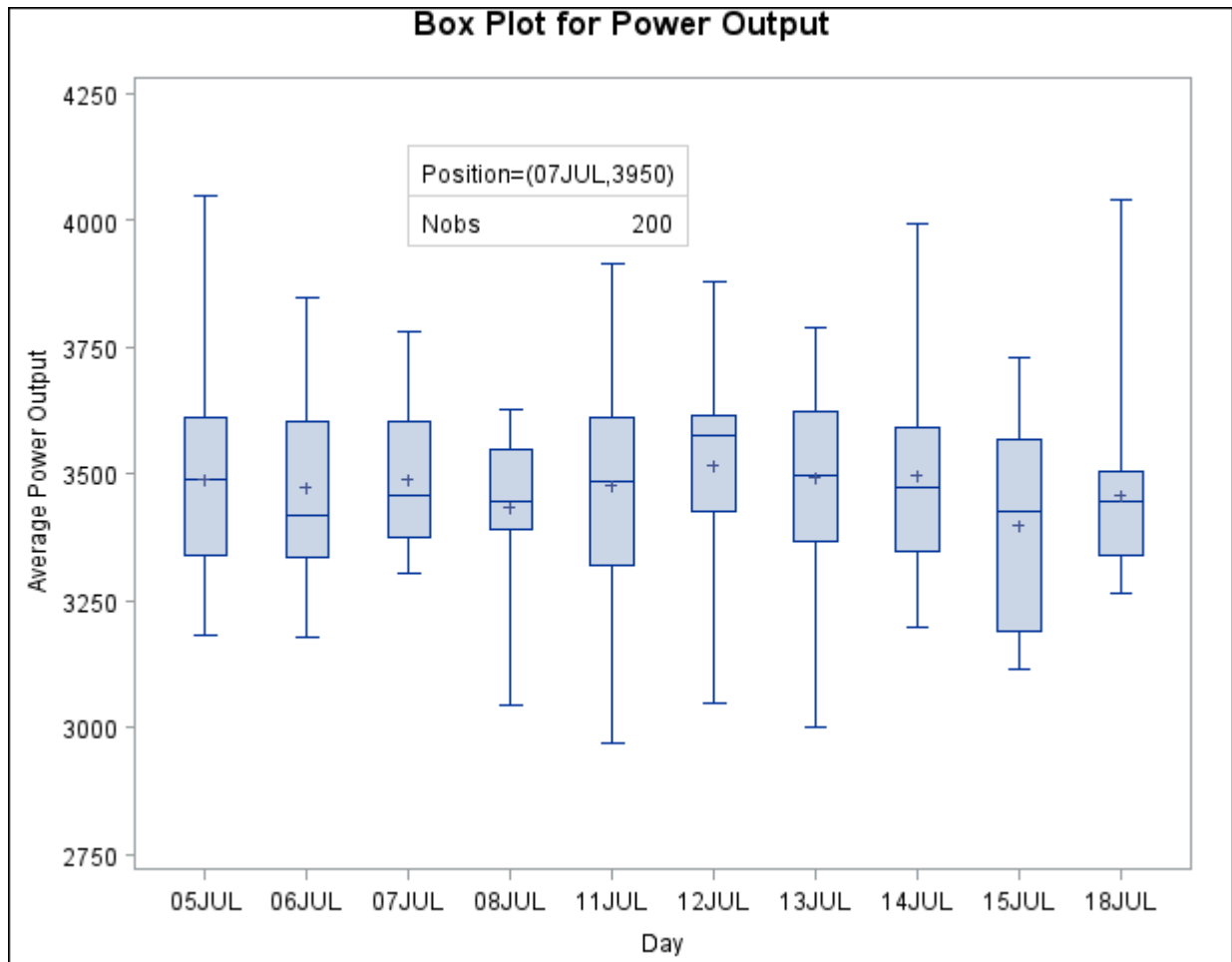

```

title 'Box Plot for Power Output';
proc boxplot data=Turbine;
plot KWatts*Day;
inset nobis /
  header   = 'Position=(07JUL,3950)'
  position = ('07JUL94'd, 3950) data;
run;

```

The box plot is displayed in Figure 26.13. By default, the specified coordinates determine the position of the bottom-left corner of the inset. You can change this reference point with the `REFPOINT=` option, as in the next example.

Figure 26.13 Inset Positioned Using Data Unit Coordinates



Axis Percent Unit Coordinates

If you do not use the `DATA` option, the inset is positioned using axis percent units. The coordinates of the bottom-left corner of the display are (0, 0), while the coordinates of the top-right corner are (100, 100). For example, the following statements create a box plot with two insets, both positioned using coordinates in axis percent units:

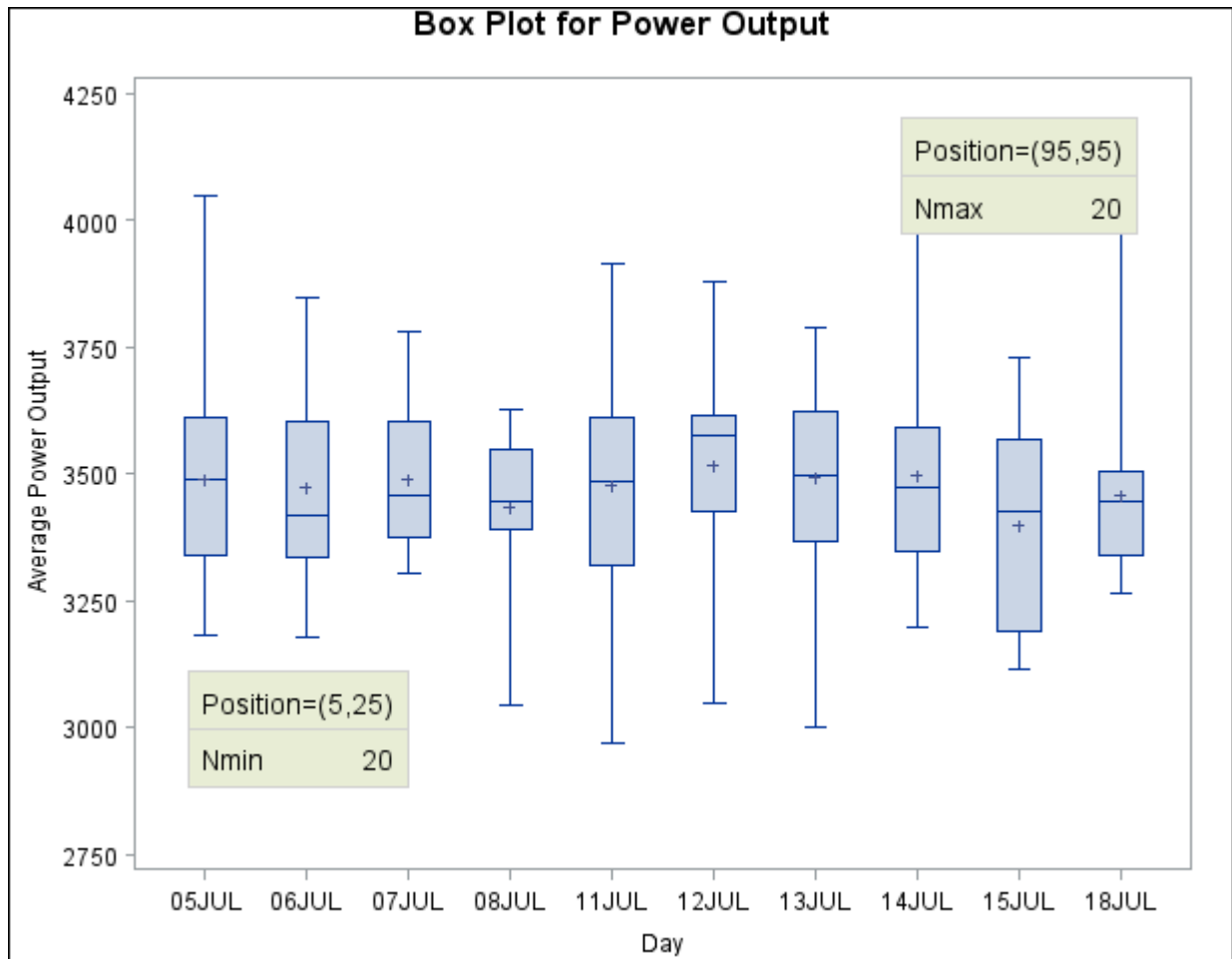
```

title 'Box Plot for Power Output';
proc boxplot data=Turbine;
plot KWatts*Day;
inset nmin / position = (5,25)
           header = 'Position=(5,25) '
           height = 3
           cfill = ywh
           refpoint = tl;
inset nmax / position = (95,95)
           header = 'Position=(95,95) '
           height = 3
           cfill = ywh
           refpoint = tr;
run;

```

The display is shown in Figure 26.14. Notice that the REFPOINT= option is used to determine which corner of the inset is placed at the coordinates specified with the POSITION= option. The first inset has REFPOINT=TL, so the top-left corner of the inset is positioned 5% of the way across the horizontal axis and 25% of the way up the vertical axis. The second inset has REFPOINT=TR, so the top-right corner of the inset is positioned 95% of the way across the horizontal axis and 95% of the way up the vertical axis. Note also that coordinates in axis percent units must be *between* 0 and 100.

Figure 26.14 Inset Positioned Using Axis Percent Unit Coordinates



Displaying Blocks of Data

To display data organized in blocks of consecutive observations, specify one or more *block variables* in parentheses after the group variable in the PLOT statement. The block variables must be variables in the input data set. The BOXPLOT procedure displays a legend identifying blocks of consecutive observations with identical values of the block variables. The legend displays one track of values for each block variable containing formatted values of the block variable.

The values of a block variable must be the same for all observations with the same value of the group variable. In other words, groups must be nested within blocks determined by block variables.

The following statements create a SAS data set containing diameter measurements for a part produced on three different machines:

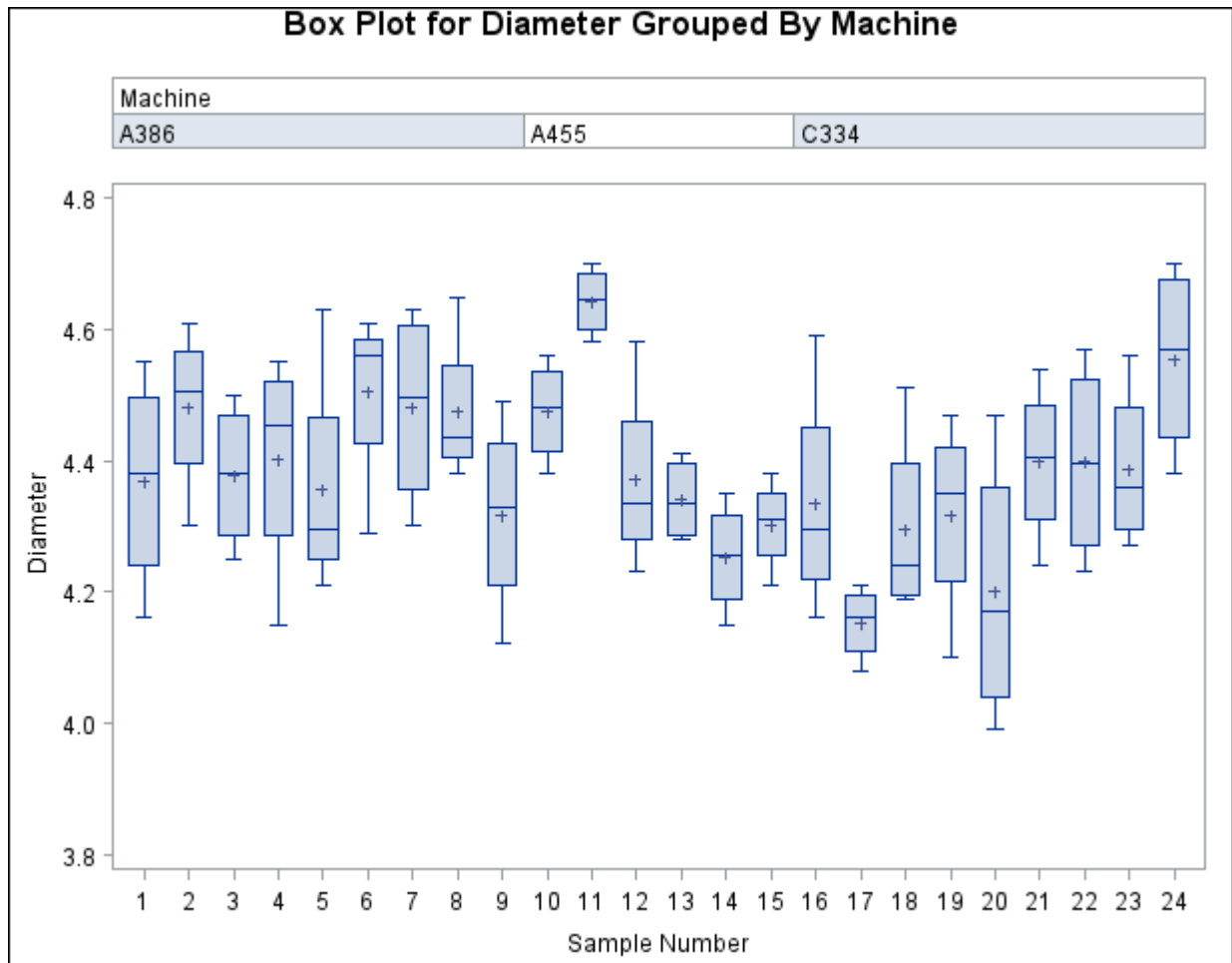
```
data Parts;
  length Machine $ 4;
  input Sample Machine $ @;
  do i= 1 to 4;
    input Diam @;
    output;
  end;
  drop i;
  datalines;
1  A386  4.32 4.55 4.16 4.44
2  A386  4.49 4.30 4.52 4.61
3  A386  4.44 4.32 4.25 4.50
4  A386  4.55 4.15 4.42 4.49
5  A386  4.21 4.30 4.29 4.63
6  A386  4.56 4.61 4.29 4.56
7  A386  4.63 4.30 4.41 4.58
8  A386  4.38 4.65 4.43 4.44
9  A386  4.12 4.49 4.30 4.36
10 A455  4.45 4.56 4.38 4.51
11 A455  4.62 4.67 4.70 4.58
12 A455  4.33 4.23 4.34 4.58
13 A455  4.29 4.38 4.28 4.41
14 A455  4.15 4.35 4.28 4.23
15 A455  4.21 4.30 4.32 4.38
16 C334  4.16 4.28 4.31 4.59
17 C334  4.14 4.18 4.08 4.21
18 C334  4.51 4.20 4.28 4.19
19 C334  4.10 4.33 4.37 4.47
20 C334  3.99 4.09 4.47 4.25
21 C334  4.24 4.54 4.43 4.38
22 C334  4.23 4.48 4.31 4.57
23 C334  4.27 4.40 4.32 4.56
24 C334  4.70 4.65 4.49 4.38
;
```

The following statements create a box plot for the measurements in the Parts data set grouped into blocks by the block variable Machine:

```
ods graphics off;
title 'Box Plot for Diameter Grouped By Machine';
proc boxplot data=Parts;
  plot Diam*Sample (Machine);
  label Sample = 'Sample Number'
        Machine = 'Machine'
        Diam = 'Diameter';
run;
```

Note the LABEL statement used to provide labels for the axes and for the block legend. The plot is shown in Figure 26.15.

Figure 26.15 Box Plot Using a Block Variable



The unique consecutive values of Machine (A386, A455, and C334) are displayed in a legend above the plot. That is the default location of the block legend. You can control the position of the block legend with the BLOCKPOS= option. See the BLOCKPOS= option for details.

By default, block variable values that are too long to fit into the available space in a block legend are not displayed. You can specify the BLOCKLABTYPE= option to display lengthy labels. Specify BLOCKLABTYPE=SCALED to scale down the text size of the values so they all fit. Use BLOCKLAB-

TYPE=TRUNCATED to truncate lengthy values. You can also use BLOCKLABTYPE=*height* to specify a text height in vertical percent screen units for the values.

You can control the position of legend labels with the BLOCKLABELPOS= option. Valid BLOCKLABELPOS= values are ABOVE (the default, as shown in Figure 26.15) and LEFT.

Clipping Extreme Values

By default a box plot's vertical axis is scaled to accommodate all the values in all groups. If the variation between groups is large with respect to the variation within groups, or if some groups contain extreme outlier values, the vertical axis scale can become so large that the box-and-whiskers plots are compressed. In such cases, you can clip the extreme values to produce a more readable plot, as illustrated in the following example.

A company produces copper tubing. The diameter measurements (in millimeters) for 15 batches of five tubes each are provided in the data set Newtubes:

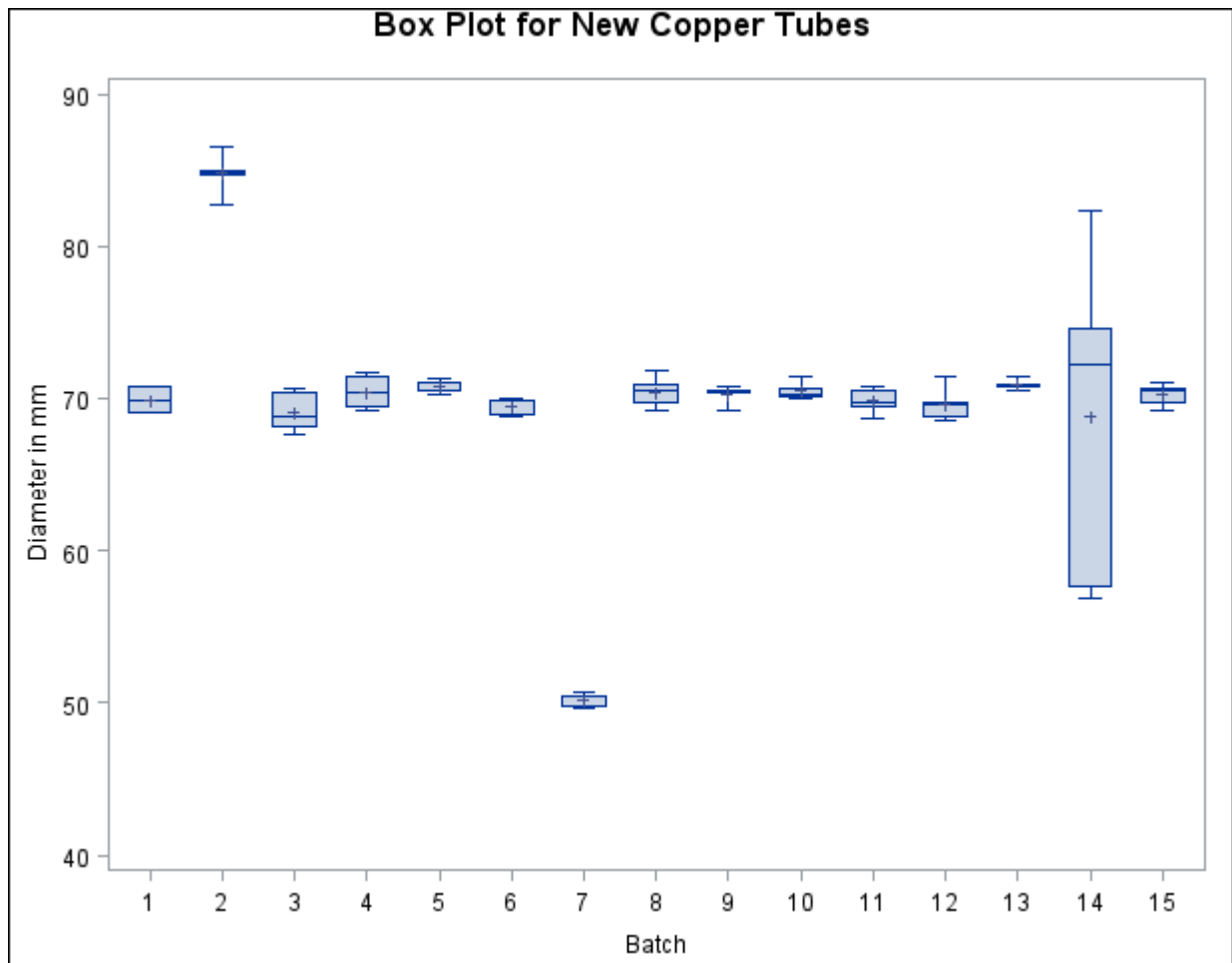
```
data Newtubes;
  label Diameter='Diameter in mm';
  do Batch = 1 to 15;
    do i = 1 to 5;
      input Diameter @@;
      output;
    end;
  end;
  datalines;
69.13 69.83 70.76 69.13 70.81
85.06 82.82 84.79 84.89 86.53
67.67 70.37 68.80 70.65 68.20
71.71 70.46 71.43 69.53 69.28
71.04 71.04 70.29 70.51 71.29
69.01 68.87 69.87 70.05 69.85
50.72 50.49 49.78 50.49 49.69
69.28 71.80 69.80 70.99 70.50
70.76 69.19 70.51 70.59 70.40
70.16 70.07 71.52 70.72 70.31
68.67 70.54 69.50 69.79 70.76
68.78 68.55 69.72 69.62 71.53
70.61 70.75 70.90 71.01 71.53
74.62 56.95 72.29 82.41 57.64
70.54 69.82 70.71 71.05 69.24
;
```

The following statements create a box plot of the tube diameters:

```
ods graphics off;
title 'Box Plot for New Copper Tubes' ;
proc boxplot data=Newtubes;
  plot Diameter*Batch;
run;
```

The box plot is shown in Figure 26.16.

Figure 26.16 Compressed Box Plots



Note that the diameters in batch 2 are significantly larger, and those in batch 7 significantly smaller, than those in most of the other batches. The default vertical axis scaling causes the box-and-whiskers plots to be compressed.

You can produce a more useful box plot by specifying the `CLIPFACTOR=factor` option, where *factor* is a value greater than one. Clipping is applied as follows:

1. The mean of the first quartile values ($\overline{Q1}$) and the mean of the third quartile values ($\overline{Q3}$) are computed across all groups.
2. The following values define the clipping range:

$$y_{\max} = \overline{Q1} + (\overline{Q3} - \overline{Q1}) \times factor$$

and

$$y_{\min} = \overline{Q3} - (\overline{Q3} - \overline{Q1}) \times factor$$

Any statistic greater than y_{\max} or less than y_{\min} is ignored during vertical axis scaling.

NOTE:

- Clipping is applied only to the plotted statistics and not to the statistics saved in an output data set.
- A special symbol is used for clipped points (the default symbol is a square), and a legend is added to the chart indicating the number of boxes that were clipped.

The following statements use a clipping factor of 1.5 to create a box plot of the same data plotted in Figure 26.16:

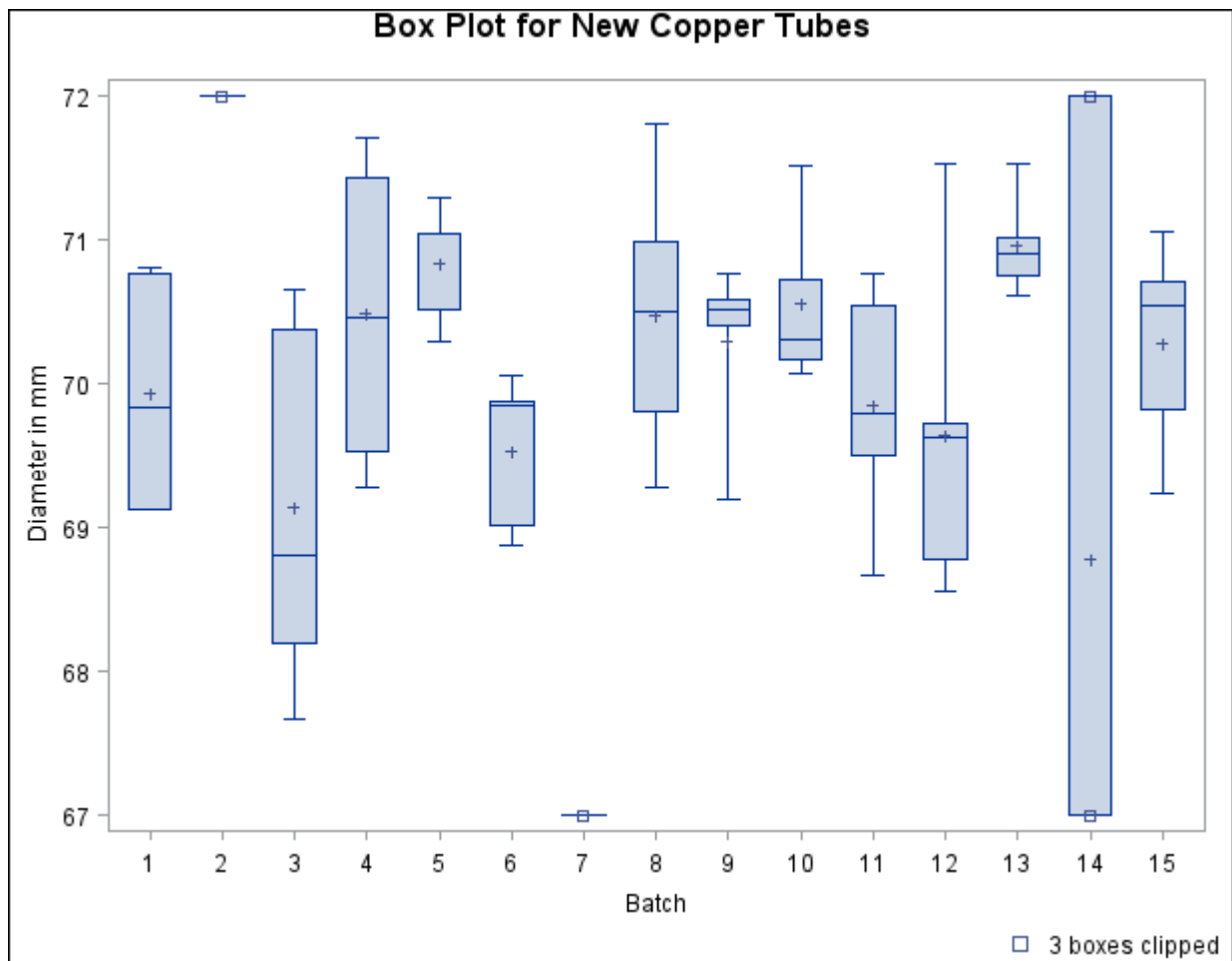
```

title 'Box Plot for New Copper Tubes' ;
proc boxplot data=Newtubes;
  plot Diameter*Batch /
    clipfactor = 1.5;
run;

```

The clipped box plot is shown in Figure 26.17.

Figure 26.17 Box Plot with Clip Factor of 1.5



In Figure 26.17 the extreme values are clipped, making the box plot more readable. The box-and-whiskers plots for batches 2 and 7 are clipped completely, while the plot for batch 14 is clipped at both the top and bottom. Clipped points are marked with a square, and a clipping legend is added at the lower right of the display.

Other clipping options are available, as illustrated by the following statements:

```

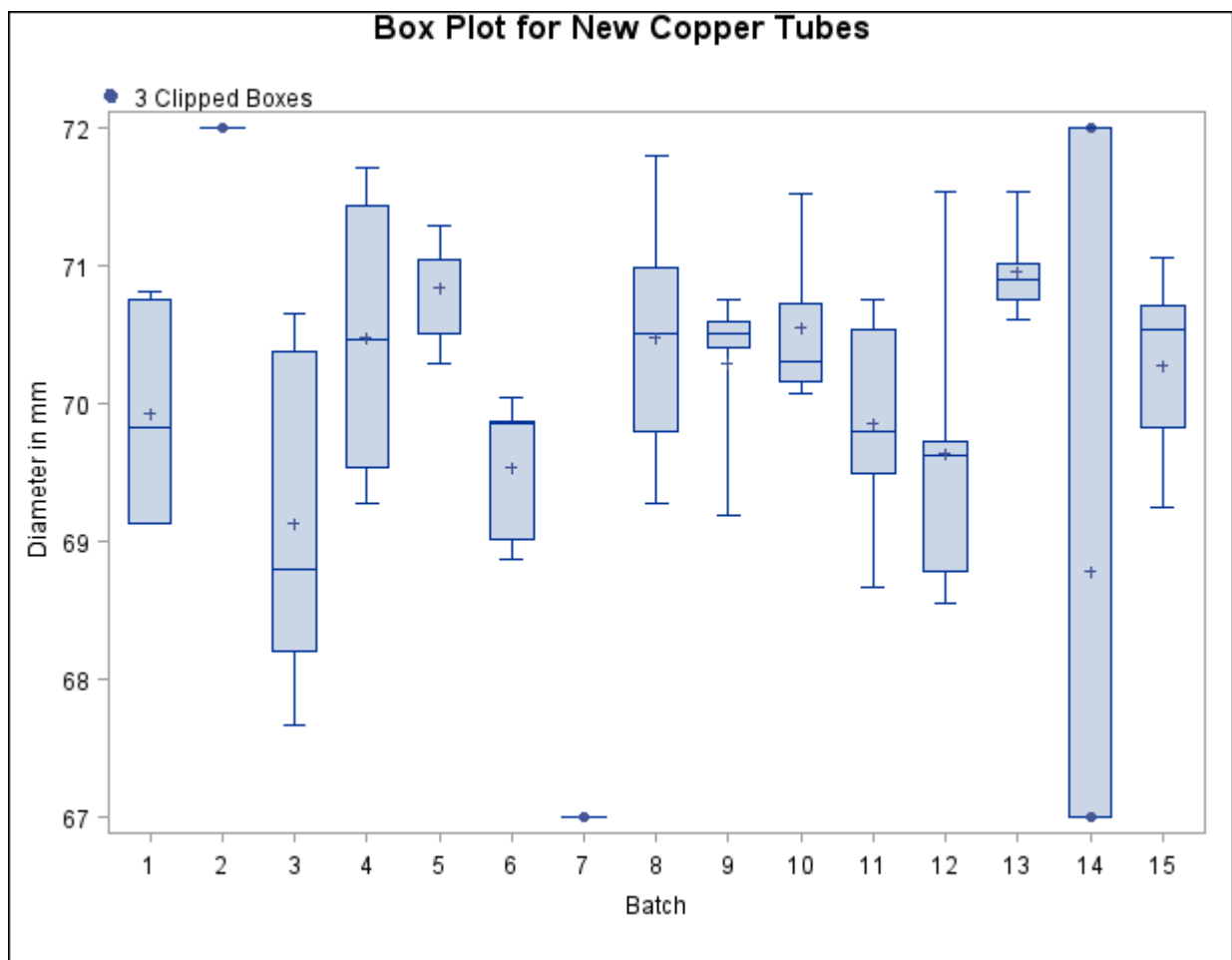
title 'Box Plot for New Copper Tubes' ;
proc boxplot data=Newtubes;
  plot Diameter*Batch /
    clipfactor = 1.5
    clipsymbol = dot
    cliplegpos = top
    cliplegend = '# Clipped Boxes'
    clipsubchar = '#';
run;

```

Specifying `CLIPSYMBOL=DOT` marks the clipped points with a dot instead of the default square. Specifying `CLIPLEGPOS=TOP` positions the clipping legend at the top of the chart. The options `CLIPLEGEND='# Clipped Boxes'` and `CLIPSUBCHAR='#'` request the clipping legend “3 Clipped Boxes”.

Figure 26.18 shows the modified box plot.

Figure 26.18 Box Plot Using Clipping Options



For more information about clipping options, see the appropriate entries in the section “PLOT Statement Options” on page 979.

ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “Statistical Graphics Using ODS.”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “A Primer on ODS Statistical Graphics” on page 599 in Chapter 21, “Statistical Graphics Using ODS.”

The appearance of a box plot produced using ODS Graphics is determined by the style associated with the ODS destination where the graph is produced. PLOT statement options used to control the appearance of traditional high-resolution graphs are ignored for ODS Graphics output.

When producing ODS graphical displays, the PLOT statement assigns a name to each graph it creates. You can use this name to reference the graph when using ODS. The name is listed in Table 26.10.

Table 26.10 Graphs Produced by PROC BOXPLOT

ODS Graph Name	Plot Description
Boxplot	box-and-whiskers plots for groups

Examples: BOXPLOT Procedure

This section provides advanced examples of the PLOT statement.

Example 26.1: Displaying Summary Statistics in a Box Plot

This example demonstrates how you can use the INSET and INSETGROUP statements to include tables of summary statistics in your box plots. The following statements produce a box plot of the Turbine data set from the section “Getting Started: BOXPLOT Procedure” on page 963, augmented with insets containing summary statistics:

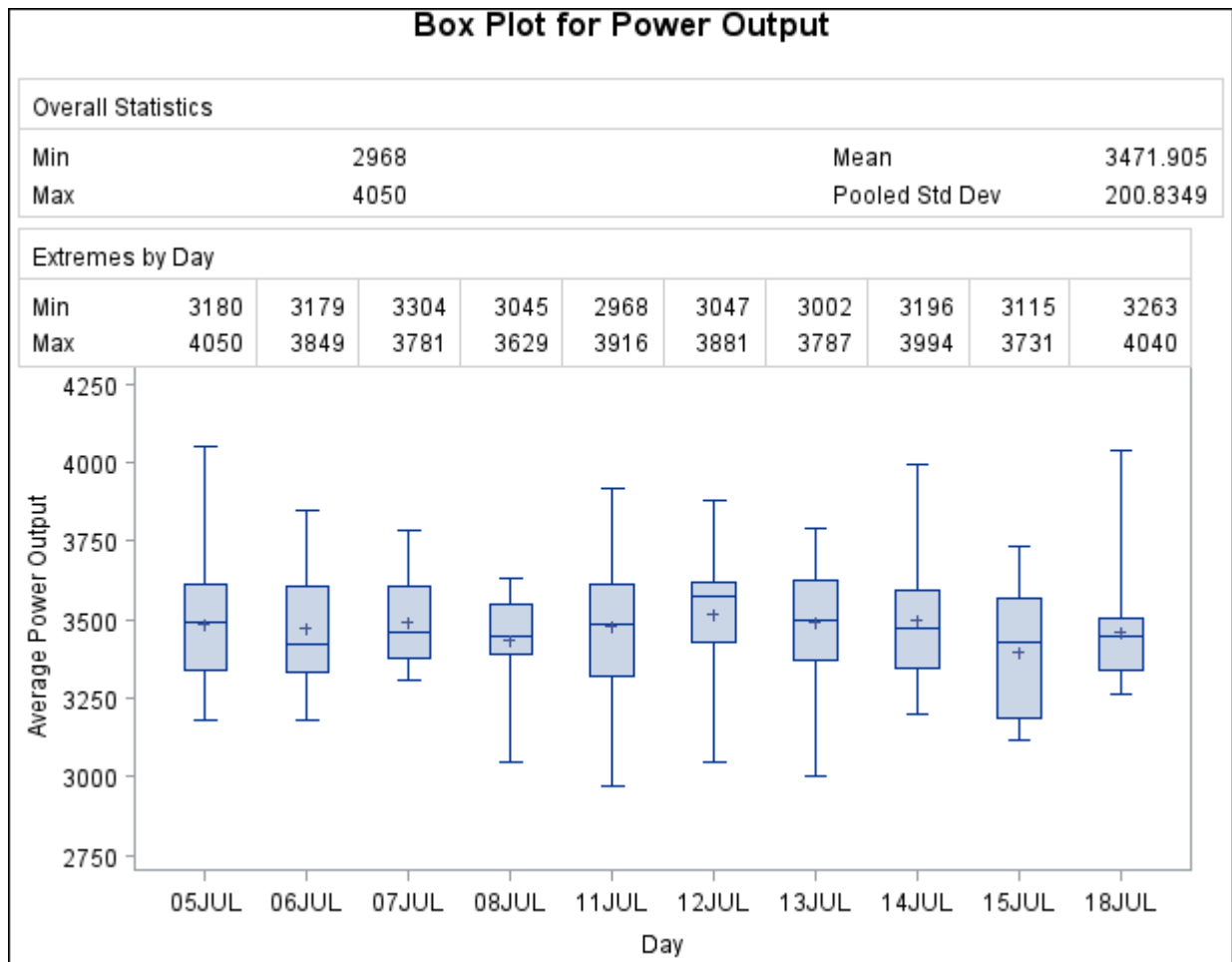
```
ods graphics off;
title 'Box Plot for Power Output';
proc boxplot data=Turbine;
plot KWatts*Day;
inset min mean max stddev /
  header = 'Overall Statistics'
  pos    = tm;
insetgroup min max /
  header = 'Extremes by Day';
run;
```

The INSET statement produces an inset of overall summary statistics. The keywords listed before the slash (/) request the minimum, mean, maximum, and standard deviation computed over all days. The POS=TM option places the inset in the top margin of the plot.

The INSETGROUP statement produces an inset containing statistics calculated for each group separately. The MIN and MAX keywords request the minimum and maximum observations from each day, respectively.

The resulting plot is shown in [Output 26.1.1](#).

Output 26.1.1 Box Plot with Insets



Example 26.2: Using Box Plots to Compare Groups

In this example a box plot is used to compare the delay times of airline flights during the Christmas holidays with the delay times prior to the holiday period. The following statements create a data set named Times with the delay times in minutes for 25 flights each day. When a flight is canceled, the delay is recorded as a missing value.

```

data Times;
  informat Day date7. ;
  format Day date7. ;
  input Day @ ;
  do Flight=1 to 25;
    input Delay @ ;
    output;
  end;
datalines;
16DEC88  4 12  2  2 18  5  6 21  0  0
          0 14  3  .  2  3  5  0  6 19
          7  4  9  5 10
17DEC88  1 10  3  3  0  1  5  0  .  .
          1  5  7  1  7  2  2 16  2  1
          3  1 31  5  0
18DEC88  7  8  4  2  3  2  7  6 11  3
          2  7  0  1 10  2  3 12  8  6
          2  7  2  4  5
19DEC88 15  6  9  0 15  7  1  1  0  2
          5  6  5 14  7 20  8  1 14  3
         10  0  1 11  7
20DEC88  2  1  0  4  4  6  2  2  1  4
          1 11  .  1  0  6  5  5  4  2
          2  6  6  4  0
21DEC88  2  6  6  2  7  7  5  2  5  0
          9  2  4  2  5  1  4  7  5  6
          5  0  4 36 28
22DEC88  3  7 22  1 11 11 39 46  7 33
         19 21  1  3 43 23  9  0 17 35
         50  0  2  1  0
23DEC88  6 11  8 35 36 19 21  .  .  4
          6 63 35  3 12 34  9  0 46  0
          0 36  3  0 14
24DEC88 13  2 10  4  5 22 21 44 66 13
          8  3  4 27  2 12 17 22 19 36
          9 72  2  4  4
25DEC88  4 33 35  0 11 11 10 28 34  3
         24  6 17  0  8  5  7 19  9  7
         21 17 17  2  6
26DEC88  3  8  8  2  7  7  8  2  5  9
          2  8  2 10 16  9  5 14 15  1
         12  2  2 14 18
;

```

In the following statements, the MEANS procedure is used to count the number of canceled flights for each day. This information is then added to the data set Times.

```
proc means data=Times noprint;
  var Delay;
  by Day;
  output out=Cancel nmiss=ncancel;
run;

data Times;
  merge Times Cancel;
  by Day;
run;
```

The following statements create a data set named Weather containing information about possible causes for delays, and then merge this data set with the data set Times:

```
data Weather;
  informat Day date7. ;
  format Day date7. ;
  length Reason $ 16 ;
  input Day Flight Reason & ;
  datalines;
16DEC88 8 Fog
17DEC88 18 Snow Storm
17DEC88 23 Sleet
21DEC88 24 Rain
21DEC88 25 Rain
22DEC88 7 Mechanical
22DEC88 15 Late Arrival
24DEC88 9 Late Arrival
24DEC88 22 Late Arrival
;

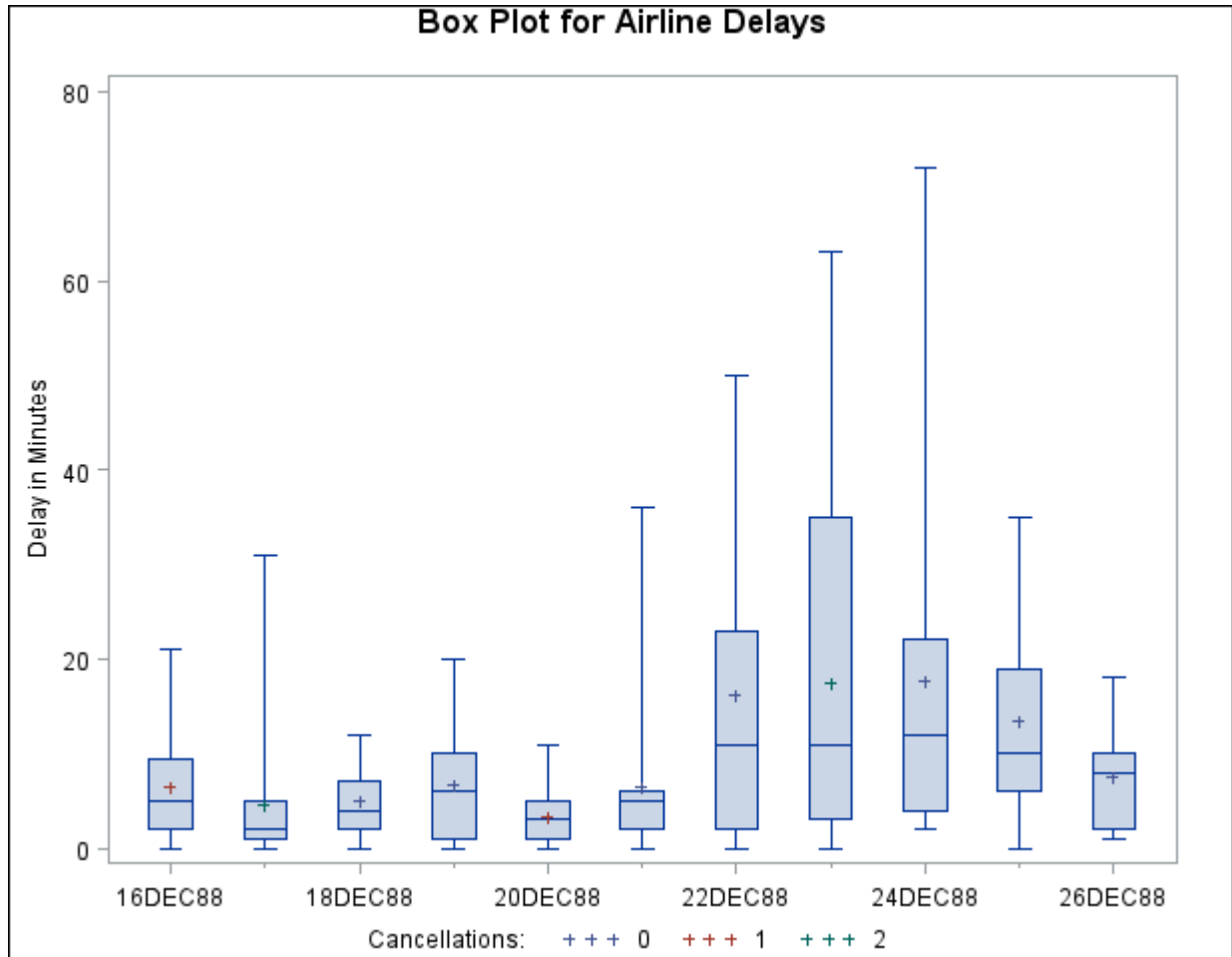
data Times;
  merge Times Weather;
  by Day Flight;
run;
```

The following statements create a box plot for the complete set of data:

```
ods graphics off;
symbol1 v=plus;
symbol2 v=square;
symbol3 v=triangle;
title 'Box Plot for Airline Delays';
proc boxplot data=Times;
  plot Delay*Day = ncancel /
    nohlabel
    symbollegend = legend1;
  legend1 label = ('Cancellations:');
  label Delay = 'Delay in Minutes';
run;
goptions reset=symbol;
```

The level of the *symbol variable* `ncancel` determines the symbol marker for each group mean, and the `SYMBOLLEGEND=` option controls the appearance of the legend for the symbols. The `NOHLABEL` option suppresses the horizontal axis label. The resulting box plot is shown in [Output 26.2.1](#).

Output 26.2.1 Box Plot for Airline Data



The delay distributions from December 22 through December 25 are drastically different from the delay distributions during the preholiday period. Both the mean delay and the variability of the delays are much greater during the holiday period.

Example 26.3: Creating Various Styles of Box-and-Whiskers Plots

This example uses the flight delay data of the preceding example to illustrate how you can create box plots with various styles of box-and-whiskers plots. The following statements create a plot that displays skeletal box-and-whiskers plots:

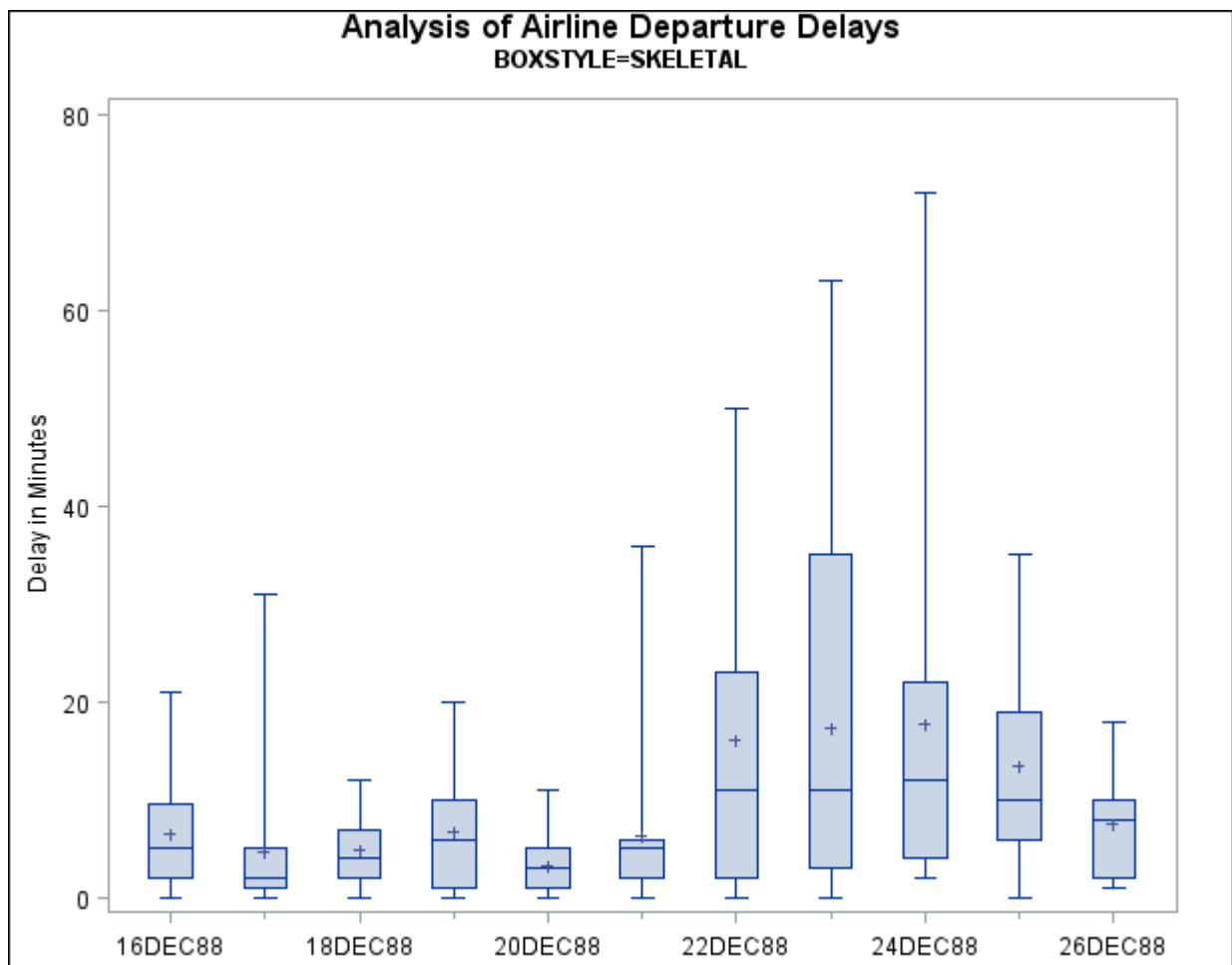
```

title 'Analysis of Airline Departure Delays';
title2 'BOXSTYLE=SKELETAL';
proc boxplot data=Times;
  plot Delay*Day /
    boxstyle = skeletal
    nohlabel;
  label Delay = 'Delay in Minutes';
run;

```

In a skeletal box-and-whiskers plot, the whiskers are drawn from the quartiles to the extreme values of the group. The skeletal box plot is the default style, so you can also produce a skeletal box plot by omitting the `BOXSTYLE=` option. [Output 26.3.1](#) shows the skeletal box plot.

Output 26.3.1 BOXSTYLE=SKELETAL



The following statements request a schematic box:

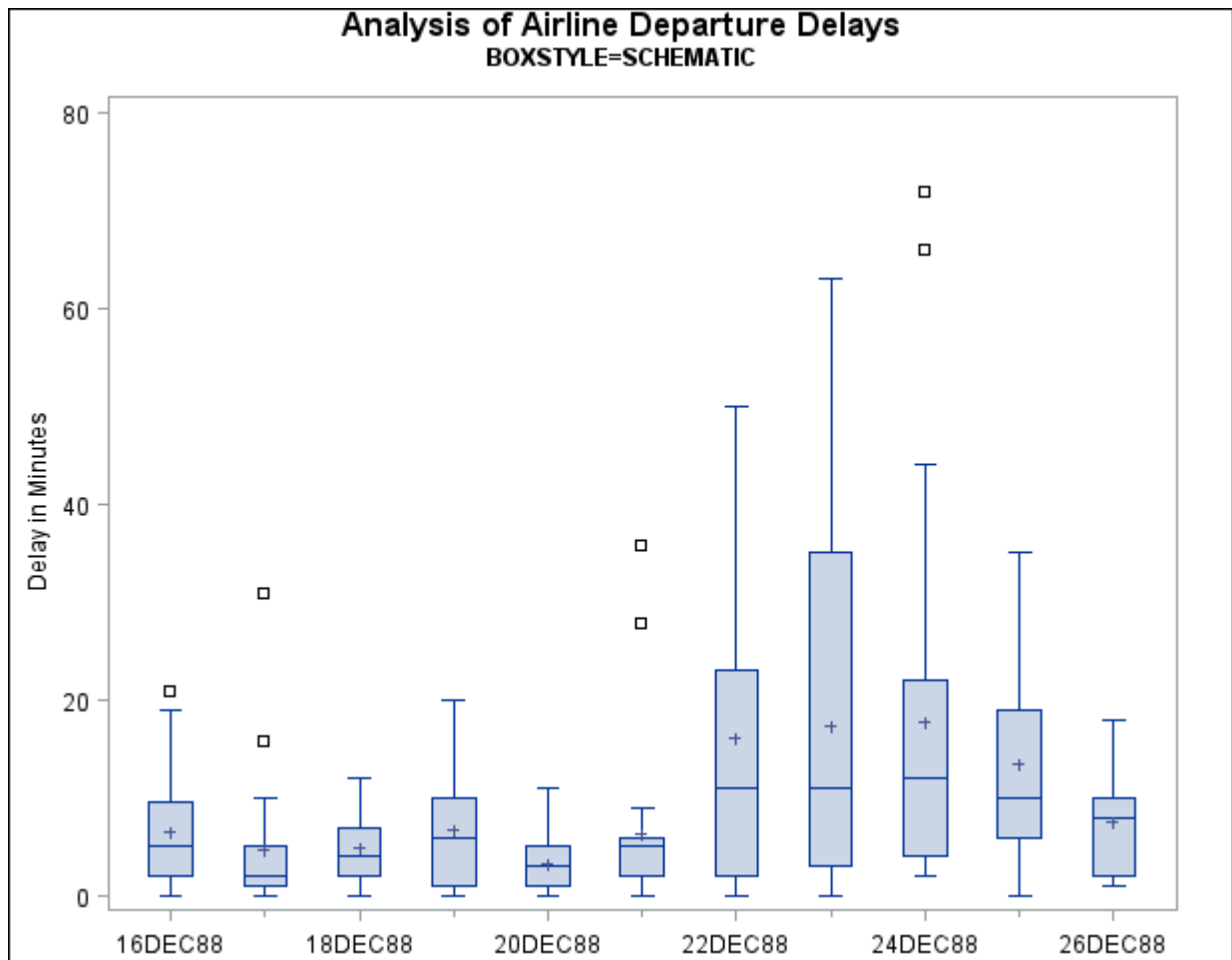
```

title 'Analysis of Airline Departure Delays';
title2 'BOXSTYLE=SCHEMATIC';
proc boxplot data=Times;
  plot Delay*Day /
    boxstyle = schematic
    nohlabel;
  label Delay = 'Delay in Minutes';
run;

```

When you specify `BOXSTYLE=SCHEMATIC`, the whiskers are drawn to the most extreme points in the group that lie within the *fences*. The *upper fence* is defined as the third quartile (represented by the upper edge of the box) plus 1.5 times the interquartile range (IQR). The *lower fence* is defined as the first quartile (represented by the lower edge of the box) minus 1.5 times the interquartile range. Observations outside the fences are identified with a special symbol. The default symbol is a square, and you can specify the shape and color for this symbol with the `IDSYMBOL=` and `IDCOLOR=` options. Serifs are added to the whiskers by default. For further details, see the entry for the `BOXSTYLE=` option. The plot is shown in [Output 26.3.2](#).

Output 26.3.2 BOXSTYLE=SCHEMATIC



The following statements create a schematic box plot in which the observations outside the fences are labeled:

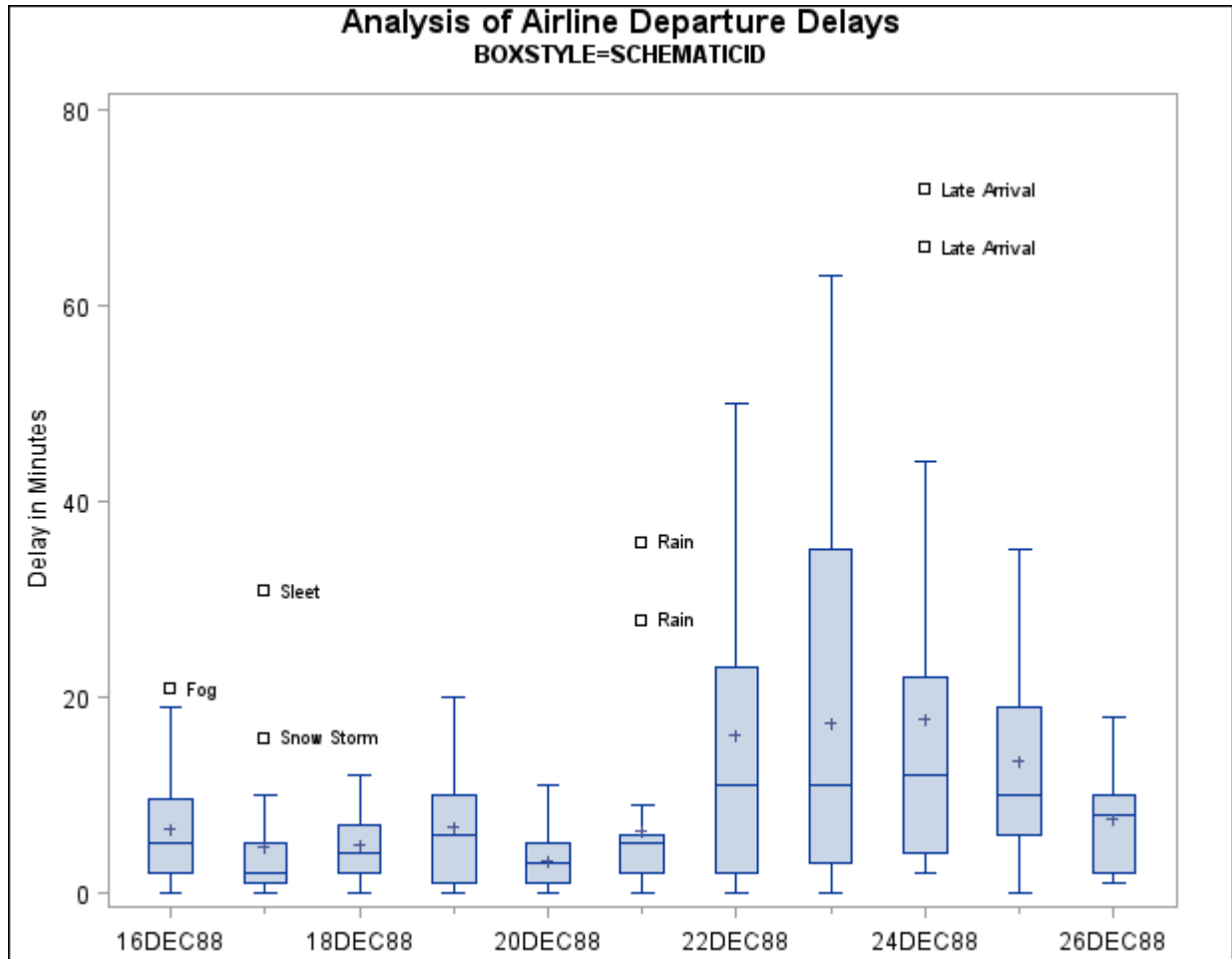
```

title 'Analysis of Airline Departure Delays';
title2 'BOXSTYLE=SCHEMATICID';
proc boxplot data=Times;
  plot Delay*Day /
    boxstyle = schematicid
    nohlabel;
  id Reason;
  label Delay = 'Delay in Minutes';
run;

```

If you specify BOXSTYLE=SCHEMATICID, schematic box-and-whiskers plots are created and the value of the first ID variable (in this case, Reason) is used to label each observation outside the fences. The box plot is shown in Output 26.3.3.

Output 26.3.3 BOXSTYLE=SCHEMATICID



The following statements create a box plot with schematic box-and-whiskers plots in which only the extreme observations outside the fences are labeled:

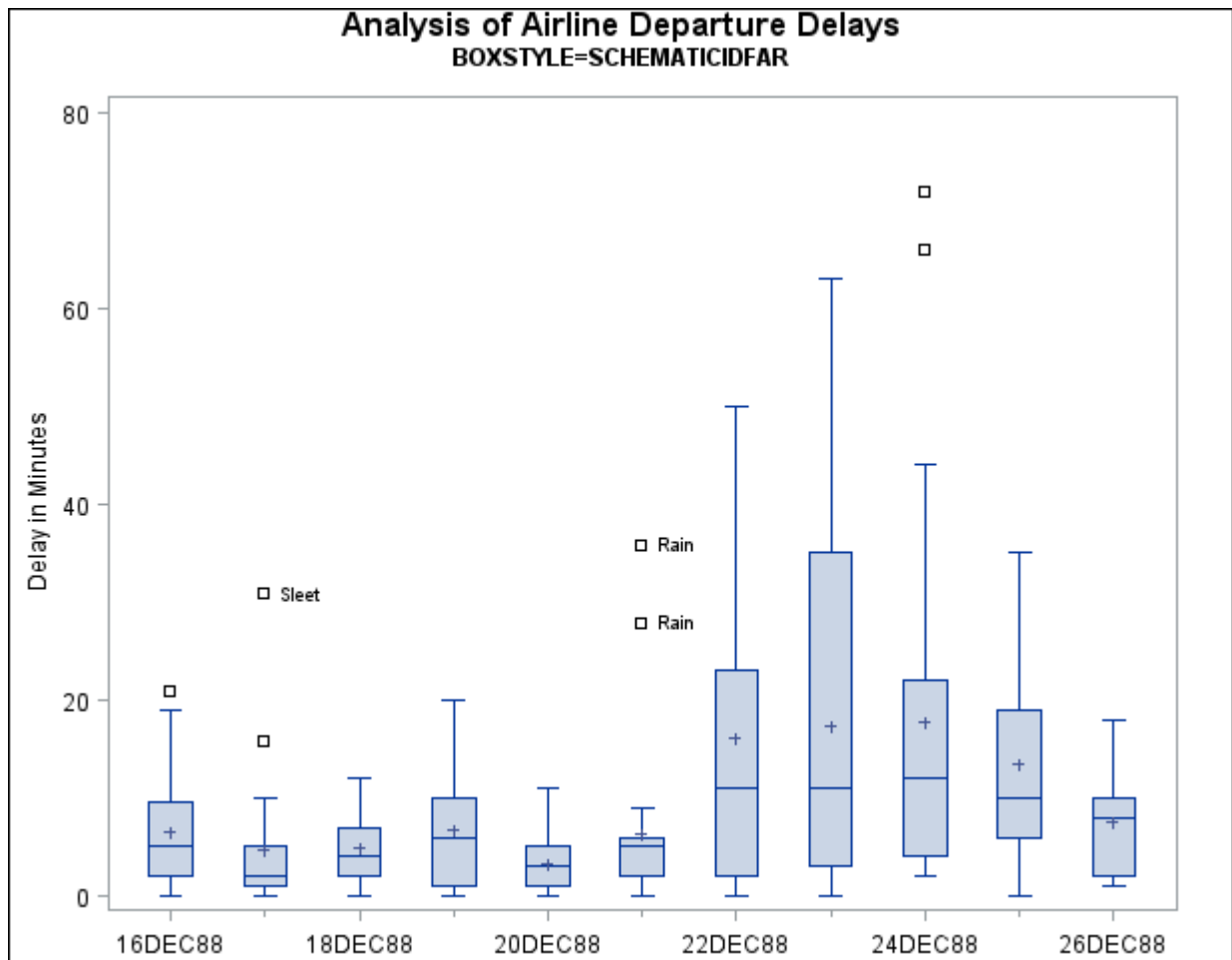
```

title 'Analysis of Airline Departure Delays';
title2 'BOXSTYLE=SCHEMATICIDFAR';
proc boxplot data=Times;
  plot Delay*Day /
    boxstyle = schematicidfar
    nohlabel;
  id Reason;
  label Delay = 'Delay in Minutes';
run;

```

If you specify `BOXSTYLE=SCHEMATICIDFAR`, the value of the first ID variable is used to label each observation outside the lower and upper *far fences*. The lower and upper far fences are located $3 \times \text{IQR}$ below the 25th percentile and $3 \times \text{IQR}$ above the 75th percentile, respectively. Observations between the fences and the far fences are identified with a symbol but are not labeled. The box plot is shown in [Output 26.3.4](#).

Output 26.3.4 BOXSTYLE=SCHEMATICIDFAR



Other options for controlling the display of high-resolution graphics box plots include the `BOXWIDTH=`, `BOXWIDTHSCALE=`, `CBOXES=`, `CBOXFILL=`, and `LBOXES=` options.

Example 26.4: Creating Notched Box-and-Whiskers Plots

The following statements use the flight delay data of Example 26.1 to create box-and-whiskers plots with notches:

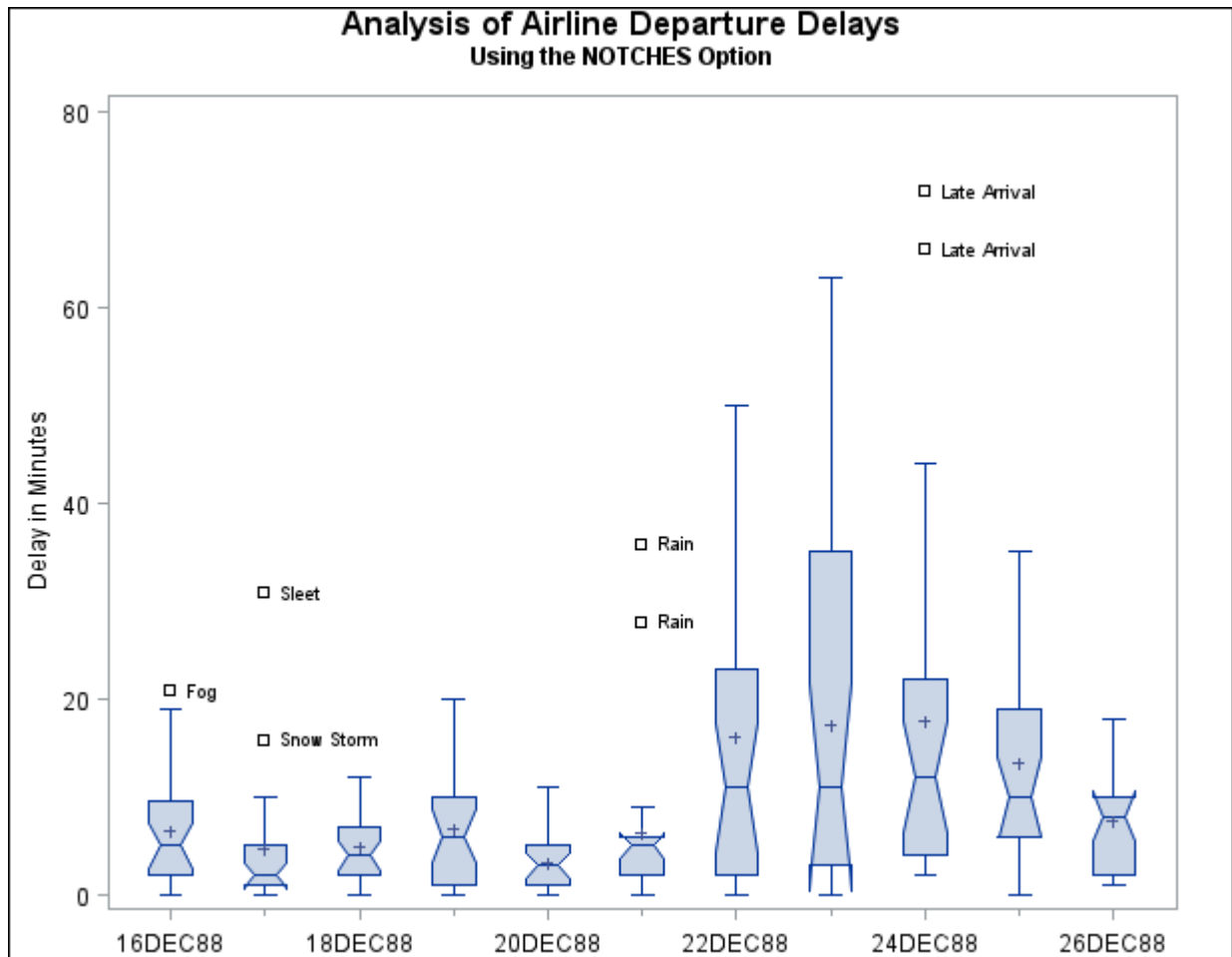
```

title 'Analysis of Airline Departure Delays';
title2 'Using the NOTCHES Option';
proc boxplot data=Times;
  plot Delay*Day /
    boxstyle = schematicid
    nohlabel
    notches;
  id Reason;
  label Delay = 'Delay in Minutes';
run;

```

The notches, requested with the `NOTCHES` option, measure the significance of the difference between two medians. The medians of two box plots are significantly different at approximately the 0.95 confidence level if the corresponding notches do not overlap. For example, in [Output 26.4.1](#), the median for December 20 is significantly different from the median for December 24.

Output 26.4.1 Notched Side-by-Side Box-and-Whiskers Plots



Example 26.5: Creating Box-and-Whiskers Plots with Varying Widths

This example shows how to create a box plot with box-and-whiskers plots whose widths vary proportionately with the group size. The following statements create a SAS data set named Times2 that contains flight departure delays (in minutes) recorded daily for eight consecutive days:

```
data Times2;
  label Delay = 'Delay in Minutes';
  informat Day date7. ;
  format Day date7. ;
  input Day @ ;
  do Flight=1 to 25;
    input Delay @ ;
    output;
  end;
  datalines;
01MAR90 12 4 2 2 15 8 0 11 0 0
          0 12 3 . 2 3 5 0 6 25
          7 4 9 5 10
02MAR90 1 . 3 . 0 1 5 0 . .
          1 5 7 . 7 2 2 16 2 1
          3 1 31 . 0
03MAR90 6 8 4 2 3 2 7 6 11 3
          2 7 0 1 10 2 5 12 8 6
          2 7 2 4 5
04MAR90 12 6 9 0 15 7 1 1 0 2
          5 6 5 14 7 21 8 1 14 3
          11 0 1 11 7
05MAR90 2 1 0 4 . 6 2 2 1 4
          1 11 . 1 0 . 5 5 . 2
          3 6 6 4 0
06MAR90 8 6 5 2 9 7 4 2 5 1
          2 2 4 2 5 1 3 9 7 8
          1 0 4 26 27
07MAR90 9 6 6 2 7 8 . . 10 8
          0 2 4 3 . . . 7 . 6
          4 0 . . .
08MAR90 1 6 6 2 8 8 5 3 5 0
          8 2 4 2 5 1 6 4 5 10
          2 0 4 1 1
;
```

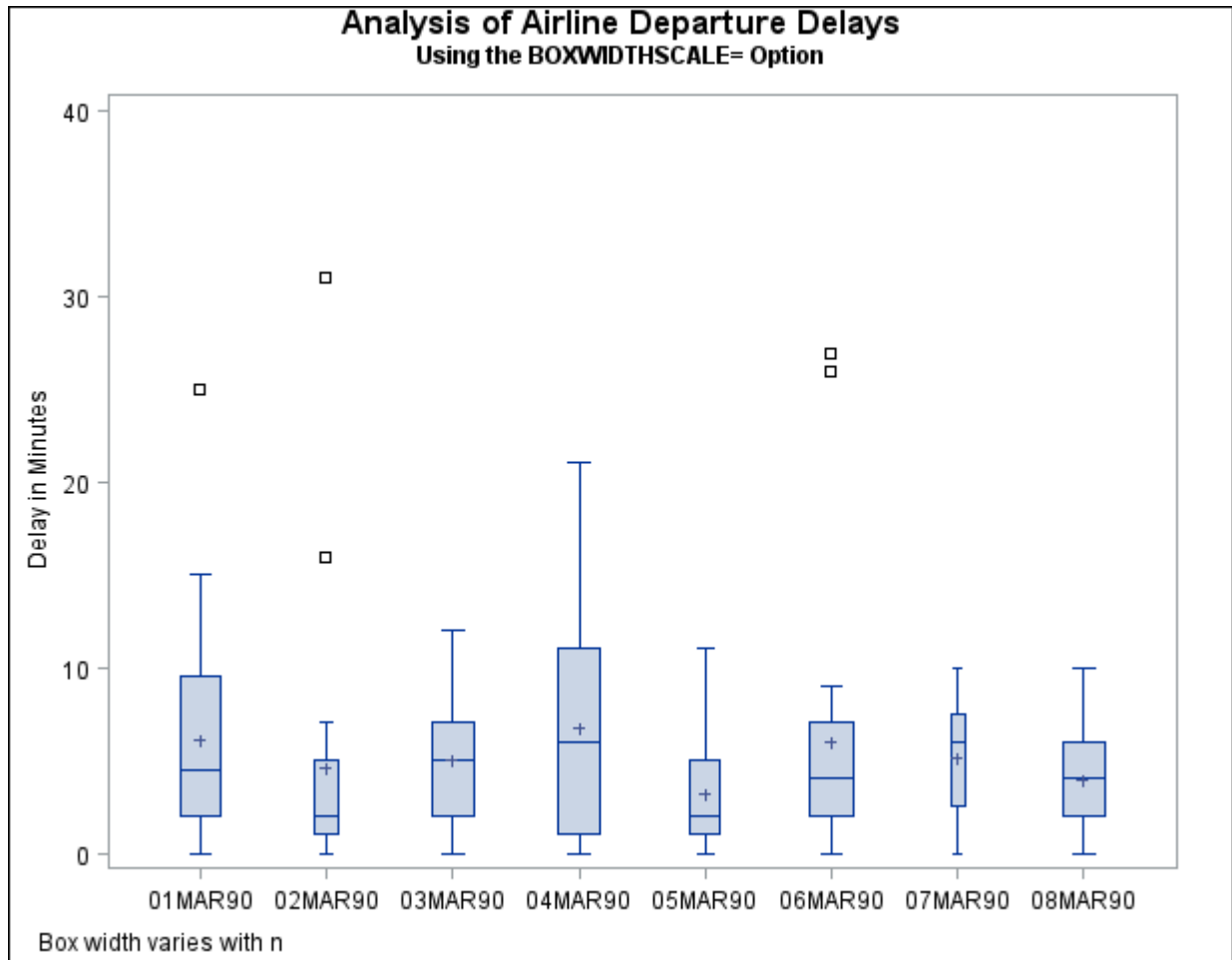
The following statements create a box plot with varying box widths:

```
title 'Analysis of Airline Departure Delays';
title2 'Using the BOXWIDTHSCALE= Option';
proc boxplot data=Times2;
  plot Delay*Day /
    nohlabel
    boxstyle      = schematic
    boxwidthscale = 1
    bwslegend;
run;
```

The `BOXWIDTHSCALE=value` option specifies that the widths of the box-and-whiskers plots vary in proportion to a particular function of the group size n . The function is determined by *value* and is identified on the box plot with a legend if the `BWSLEGEND` option is specified. The `BOXWIDTHSCALE=` option is useful in situations where the group sizes vary widely.

Output 26.5.1 shows the resulting box plot.

Output 26.5.1 Box Plot with Box-and-Whiskers Plots of Varying Widths

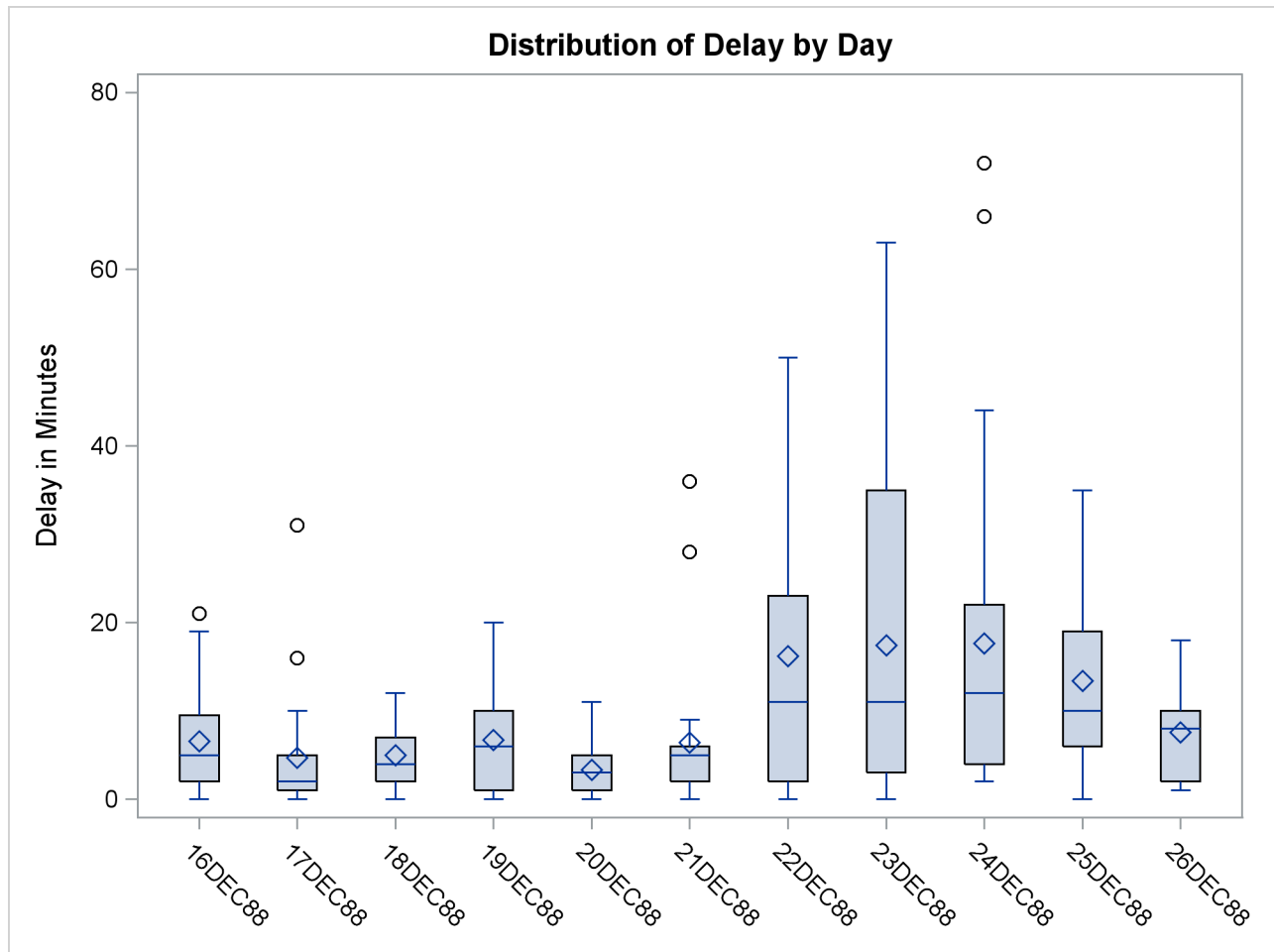


Example 26.6: Creating Box-and-Whiskers Plots Using ODS Graphics

The following statements use ODS Graphics to produce a box plot of the flight delay data from Example 26.2.

```
ods graphics on;
proc boxplot data=Times;
  plot Delay*Day /
    boxstyle = schematic
    nohlabel;
  label Delay = 'Delay in Minutes';
run;
```

The resulting box plot is shown in Output 26.6.1.

Output 26.6.1 Box Plot Produced Using ODS Graphics

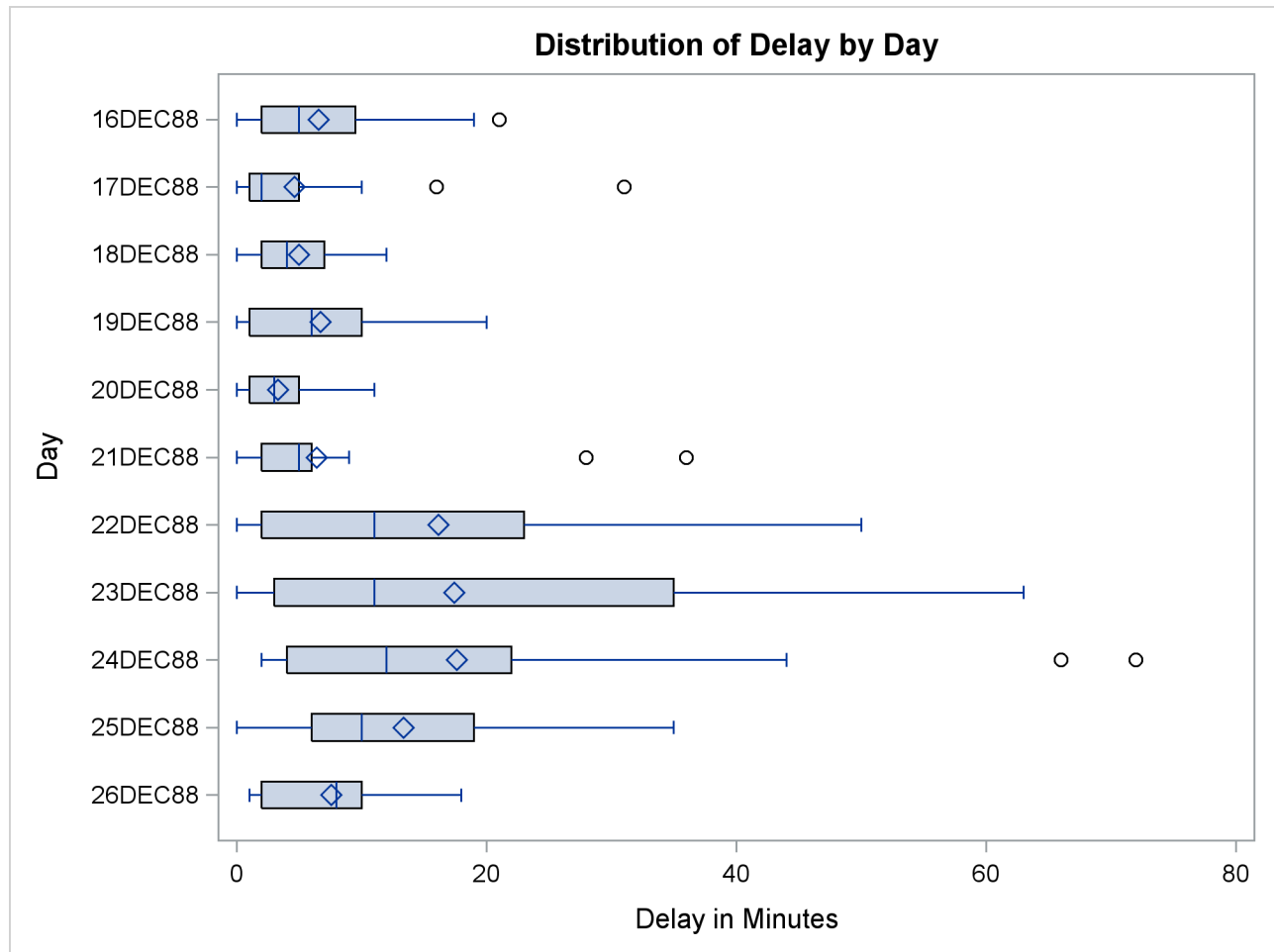
ODS graphical displays, like traditional high-resolution graphs in SAS 9.2, are controlled by the ODS style currently in effect for the output destination where the box plots are produced. However, unlike high-resolution graphs, ODS graphs are unaffected by GOPTIONS and SYMBOL statements, and by PLOT statement options used to specify colors, fonts, and other features affecting box plot appearance. Options such as **BOXSTYLE=** and **NOHLABEL** are honored by the PLOT statement when producing ODS graphical output.

The following statements use the **HORIZONTAL** option, which is supported only by ODS Graphics, to produce a horizontal box plot:

```
proc boxplot data=Times;
  plot Delay*Day /
    boxstyle = schematic
    horizontal;
  label Delay = 'Delay in Minutes';
run;
```

The horizontal box plot is shown in [Output 26.6.2](#).

Output 26.6.2 Horizontal Box Plot



References

McGill, R., Tukey, J. W., and Larsen, W. A. (1978), "Variations of Box Plots," *The American Statistician*, 32, 12–16.

Tukey, J. W. (1977), *Exploratory Data Analysis*, Reading, MA: Addison-Wesley.

Chapter 27

The CALIS Procedure

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Overview: CALIS Procedure

Structural equation modeling is an important statistical tool in social and behavioral sciences. Structural equations express relationships among a system of variables that can be either observed variables (manifest variables) or unobserved hypothetical variables (latent variables). For an introduction to latent variable models, see Loehlin (2004); Bollen (1989b); Everitt (1984), or Long (1983); and for manifest variables with measurement errors, see Fuller (1987).

In structural models, as opposed to functional models, all variables are taken to be random rather than having fixed levels. For maximum likelihood (default) and generalized least squares estimation in PROC CALIS, the random variables are assumed to have an approximately multivariate normal distribution. Nonnormality, especially high kurtosis, can produce poor estimates and grossly incorrect standard errors and hypothesis tests, even in large samples. Consequently, the assumption of normality is much more important than in models with nonstochastic exogenous variables. You should remove outliers and consider transformations of nonnormal variables before using PROC CALIS with maximum likelihood (default) or generalized least squares estimation. Alternatively, model outliers can be downweighted during model estimation with robust methods. If the number of observations is sufficiently large, Browne's asymptotically distribution-free (ADF) estimation method can be used. If your data sets contain random missing data, the full information maximum likelihood (FIML) method can be used.

You can use the CALIS procedure to estimate parameters and test hypotheses for constrained and unconstrained problems in various situations, including but not limited to the following:

- exploratory and confirmatory factor analysis of any order
- linear measurement-error models or regression with errors in variables
- multiple and multivariate linear regression
- multiple-group structural equation modeling with mean and covariance structures
- path analysis and causal modeling
- simultaneous equation models with reciprocal causation
- structured covariance and mean matrices in various forms

To specify models in PROC CALIS, you can use a variety of modeling languages:

- **COSAN**—a generalized version of the COSAN program (McDonald 1978, 1980), uses general mean and covariance structures to define models
- **FACTOR**—supports the input of latent factor and observed variable relations
- **LINEQS**—like the EQS program (Bentler 1995), uses equations to describe variable relationships
- **LISMOD**—utilizes LISREL (Jöreskog and Sörbom 1985) model matrices to define models
- **MSTRUCT**—supports direct parameterizations in the mean and covariance matrices

- **PATH**—provides an intuitive causal path specification interface
- **RAM**—utilizes the formulation of the reticular action model (McArdle and McDonald 1984) to define models
- **REFMODEL**—provides a quick way for model referencing and respecification

Various modeling languages are provided to suit a wide range of researchers' background and modeling philosophy. However, statistical situations might arise where one modeling language is more convenient than the others. This will be discussed in the section “Which Modeling Language?” on page 1077.

In addition to basic model specification, you can set various parameter constraints in PROC CALIS. Equality constraints on parameters can be achieved by simply giving the same parameter names in different parts of the model. **Boundary**, **linear**, and **nonlinear** constraints are supported as well. If parameters in the model are dependent on additional parameters, you can define the dependence by using the **PARAMETERS** and the **SAS programming statements**.

Before the data are analyzed, researchers might be interested in studying some statistical properties of the data. PROC CALIS can provide the following statistical summary of the data:

- covariance and mean matrices and their properties
- descriptive statistics like means, standard deviations, univariate skewness, and kurtosis measures
- multivariate measures of kurtosis
- coverage of covariances and means, missing patterns summary, and means of the missing patterns when the FIML estimation is used
- weight matrix and its descriptive properties
- robust covariance and mean matrices with the robust methods

After a model is fitted and accepted by the researcher, PROC CALIS can provide the following supplementary statistical analysis:

- computing squared multiple correlations and determination coefficients
- direct and indirect effects partitioning with standard error estimates
- model modification tests such as Lagrange multiplier and Wald tests
- computing fit summary indices
- computing predicted moments of the model
- residual analysis on the covariances and means
- case-level residual diagnostics with graphical plots
- factor rotations
- standardized solutions with standard errors

- testing parametric functions, individually or simultaneously

When fitting a model, you need to choose an estimation method. The following estimation methods are supported in the CALIS procedure:

- diagonally weighted least squares (DWLS, with optional weight matrix input)
- full information maximum likelihood (FIML, which can treat observations with random missing values)
- generalized least squares (GLS, with optional weight matrix input)
- maximum likelihood (ML, for multivariate normal data); this is the default method
- robust estimation with maximum likelihood model evaluation (ROBUST option)
- unweighted least squares (ULS)
- weighted least squares or asymptotically distribution-free method (WLS or ADF, with optional weight matrix input)

Estimation methods implemented in PROC CALIS do not exhaust all alternatives in the field. For example, the partial least squares (PLS) method is not implemented. See the section “[Estimation Criteria](#)” on page 1309 for details about estimation criteria used in PROC CALIS. Note that there is a SAS/STAT procedure called PROC PLS, which employs the partial least squares technique but for a different class of models than those of PROC CALIS. For general path analysis with latent variables, consider using PROC CALIS.

All estimation methods need some starting values for the parameter estimates. You can provide starting values for any parameters. If there is any estimate without a starting value provided, PROC CALIS determines the starting value by using one or any combination of the following methods:

- approximate factor analysis
- default initial values
- instrumental variable method
- matching observed moments of exogenous variables
- McDonald’s method (McDonald and Hartmann 1992) method
- ordinary least squares estimation
- random number generation, if a seed is provided
- two-stage least squares estimation

Although no methods for initial estimates are completely foolproof, the initial estimation methods provided by PROC CALIS behave reasonably well in most common applications.

With initial estimates, PROC CALIS will iterate the solutions so as to achieve the optimum solution as defined by the estimation criterion. This is a process known as optimization. Because numerical problems

can occur in any optimization process, the CALIS procedure offers several optimization algorithms so that you can choose alternative algorithms when the one being used fails. The following optimization algorithms are supported in PROC CALIS:

- Levenberg-Marquardt algorithm (Moré 1978)
- trust-region algorithm (Gay 1983)
- Newton-Raphson algorithm with line search
- ridge-stabilized Newton-Raphson algorithm
- various quasi-Newton and dual quasi-Newton algorithms: Broyden-Fletcher-Goldfarb-Shanno and Davidon-Fletcher-Powell, including a sequential quadratic programming algorithm for processing nonlinear equality and inequality constraints
- various conjugate gradient algorithms: automatic restart algorithm of Powell (1977), Fletcher-Reeves, Polak-Ribiere, and conjugate descent algorithm of Fletcher (1980)
- iteratively reweighted least squares for robust estimation

In addition to the ability to save output tables as data sets by using the ODS OUTPUT statement, PROC CALIS supports the following types of output data sets so that you can save your analysis results for later use:

- **OUTEST=** data sets for storing parameter estimates and their covariance estimates
- **OUTFIT=** data sets for storing fit indices and some pertinent modeling information
- **OUTMODEL=** data sets for storing model specifications and final estimates
- **OUTSTAT=** data sets for storing descriptive statistics, robust covariances and means, residuals, predicted moments, and latent variable scores regression coefficients
- **OUTWGT=** data sets for storing the weight matrices used in the modeling

The **OUTEST=**, **OUTMODEL=**, and **OUTWGT=** data sets can be used as input data sets for subsequent analyses. That is, in addition to the input data provided by the **DATA=** option, PROC CALIS supports the following input data sets for various purposes in the analysis:

- **INEST=** data sets for providing initial parameter estimates. An **INEST=** data set could be an **OUTEST=** data set created from a previous analysis.
- **INMODEL=** data sets for providing model specifications and initial estimates. An **INMODEL=** data set could be an **OUTMODEL=** data set created from a previous analysis.
- **INWGT=** data sets for providing the weight matrices. An **INWGT=** data set could be an **OUTWGT=** data set created from a previous analysis.

The CALIS procedure uses ODS Graphics to create graphs as part of its output. High-quality residual histograms are available in PROC CALIS. See Chapter 21, “Statistical Graphics Using ODS,” for general information about ODS Graphics. See the section “ODS Graphics” on page 1384 and the **PLOTS=** option on page 1112 for specific information about the statistical graphics available with the CALIS procedure.

Structural Equation Modeling Application

The Structural Equation Modeling Application is a graphical user interface to structural equation modeling techniques. You can specify models in graphical form to represent the hypothesized relationships among the variables. It is accessed from JMP software and uses the CALIS procedure for its computations.

The application enables you to define model variables in a path diagram by dragging data set variables to the diagram and to define the relationship between the model variables by using an arrow tool. You can move the variables to arrange the path diagram exactly the way you want. You can easily make a copy of a model, modify it, and analyze the new model, and you can compare several models with appropriate fit statistics. Finally, you can save the model specifications and the results for later use.

The Structural Equation Modeling Application provides access to a subset of the capabilities in the CALIS procedure. It supports mainly the PATH model specification through the path diagram interface. It does not support many other advanced features in PROC CALIS. For details, see *SAS Structural Equation Modeling for JMP*.

Changes and Enhancements

The following sections describe the new features of this version of PROC CALIS.

Case-Level Residual Diagnostics

Residual analysis at the case level or observation level is available when you provide raw data input. The main features include graphical and nongraphical residual diagnostic tools for identifying outliers and leverage observations, for detecting departures from the theoretical residual distribution, and for studying the distribution of residuals over the range of predicted values of the dependent observed variables. Use the **RESIDUAL** option to request nongraphical output for residual diagnostics. Use the **PLOTS=** option to request graphical plots for residual diagnostics. See the section “Case-Level Residuals, Outliers, Leverage Observations, and Residual Diagnostics” on page 1339 for details about these new features. See [Example 27.14](#) for an example that illustrates the use of the residual diagnostic tools provided by PROC CALIS.

Robust Estimation

Robust estimation is available with the **ROBUST** option. Robust estimation methods downweight the model outliers during the estimation process so that estimates are not contaminated by outliers. Two robust methods are implemented in PROC CALIS. The direct robust method applies individual (casewise) weights to observations during the model estimation. This is the default robust method that you get when you specify the **ROBUST** option. The two-stage robust method estimates robust covariance and mean matrices in the first stage, and then it does an ML estimation of the model by inputting the robust covariance and mean matrices in the second stage. You can specify this method with the **ROBUST=SAT** option. See the **ROBUST** option for details about variants of the robust methods. See the section “Robust Estimation” on page 1315 for technical details of the robust estimation implemented in PROC CALIS.

Inputting Customized Baseline Model Fit

A class of fit indices, called incremental fit indices (see the section “[Incremental Indices](#)” on page 1335 for details), measures model fit by comparing the relative fit of the target model to that of a baseline model. Traditionally, this baseline model is the uncorrelatedness model, where the covariances of observed variables are all zero. PROC CALIS follows this tradition and uses the uncorrelatedness model as the baseline model when computing the incremental fit indices. However, if you have a situation where the uncorrelatedness model is not desirable, you can now define and fit your own baseline model in a separate analysis. PROC CALIS provides tools for you to input the fit information of your customized baseline model. If you use PROC CALIS to fit your customized baseline model, you can save the fit information in an `OUTFIT=` data set and then specify the data set as a `BASEFIT=` data set when fitting your target model. PROC CALIS can extract the fit information of the customized baseline model for the computations of incremental fit indices (and a few other indices that assume the degrees of freedom of a baseline model). Alternatively, you can directly input the fit function value and the degrees of freedom of your customized baseline model by using the `BASEFUNC=` option. See the `BASEFIT=` and the `BASEFUNC=` options for details.

Compatibility with the CALIS Procedure in SAS/STAT 9.2 or Earlier

In addition to the many important feature enhancements of the CALIS procedure since SAS/STAT 9.22, there have also been some rudimentary changes in the procedure. To help users make a smoother transition from earlier versions (SAS/STAT 9.2 or earlier), this section describes some of the major changes of the CALIS procedure since SAS/STAT 9.22.

Changes in Default Analysis Type and Parameterization

Table 27.1 lists some important changes in the default analysis type and parameterization since SAS/STAT 9.22. Some items that did not change are also included to make the scope of the changes clear. Notice that the part of this table about default parameterization applies only to models that have functional relations between variables. This class of functional models includes the following types of models: FACTOR, LINEQS, LISMOD, PATH, and RAM, although LISMOD and PATH models did not exist prior to SAS/STAT 9.22. This table does not apply to the default parameterization of the COSAN and MSTRUCT models. For these models, see the descriptions in the `COSAN` and `MSTRUCT` statements, or see the sections “[The MSTRUCT Model](#)” on page 1285 and “[The COSAN Model](#)” on page 1259.

Table 27.1 Default Analysis Type and Parameterization

Default Setting	SAS/STAT 9.22 or Later	Prior to SAS/STAT 9.22
Analysis type	Covariance analysis	Correlation analysis
Variances of independent factors and errors	Free parameters	Zero variances
Variances of independent observed variables	Free parameters	Free parameters
Covariances between independent factors	Free parameters ¹	Fixed zeros
Covariances between error variables	Fixed zeros	Fixed zeros
Covariances between independent observed variables	Free parameters	Free parameters

1. The exploratory FACTOR model is an exception. Covariances between unrotated factors are set to zeros by default.

- Covariance structure analysis is the default analysis type in SAS/STAT 9.22 or later.

Covariance structure analysis has been the default since SAS/STAT 9.22. The statistical theory for structural equation modeling has been developed largely for covariance structures rather than correlation structures. Also, most practical structural equation models nowadays are concerned with covariance structures. Therefore, the default analysis type with covariance structure analysis is more reasonable. You must now use the **CORR** option for correlation structure analysis.

- Variances of any types of variables are free parameters by default in SAS/STAT 9.22 or later.

Variances of any types of variables are assumed to be free parameters in almost all applications for functional models. Prior to SAS/STAT 9.22, default variances of independent factors and errors were set to fixed zeros. This default has changed since SAS/STAT 9.22. Variances of any types of variables in functional models are now free parameters by default. This eliminates the need to specify these commonly assumed variance parameters.

- Covariances between all exogenous variables (factors or observed variables), except for error variables, are free parameters by default in functional models in SAS/STAT 9.22 or later.

Since SAS/STAT 9.22, covariances between all exogenous variables, except for error variables, are free parameters by default in functional models such as LINEQS, LISMOD, PATH, RAM, and confirmatory FACTOR models. In exploratory FACTOR models, covariances between unrotated factors are set to zeros by default. This change of default setting reflects the structural equation modeling practice much better. The default covariances between error variables, or between errors and other exogenous variables, are fixed at zero in all versions. Also, the default covariances between independent observed variables are free parameters in all versions.

Certainly, you can override all default parameters by specifying various statements in SAS/STAT 9.22 or later. You can use the **PVAR**, **RAM**, **VARIANCE**, or specific **MATRIX** statement to override default fixed or free variance parameters. You can use the **COV**, **PCOV**, **RAM**, or specific **MATRIX** statement to override default fixed or free covariance parameters.

Changes in the Role of the VAR Statement in Model Specification

Like many other SAS procedures, PROC CALIS enables you to use the **VAR** statement to define the set of observed variables in the data set for analysis. Unlike many other SAS procedures, PROC CALIS has other statements for more flexible model specifications. Because you can specify observed variables in these model specification statements and in the **VAR** statement with PROC CALIS, a question might arise when the set of observed variables specified in the **VAR** statement is not exactly the same as the set of observed variables specified in the model specification statements. Which set of observed variables does PROC CALIS use for analysis? The answer might depend on which version of PROC CALIS you use.

For observed variables that are specified in both the **VAR** statement and at least one of the model specification statements (such as the **LINEQS**, **PATH**, **RAM**, **COV**, **PCOV**, **PVAR**, **STD**, and **VARIANCE** statements), PROC CALIS recognizes the observed variables without any difficulty (that is, if they actually exist in the data set) no matter which SAS version you are using.

For observed variables that are specified only in the model specification statements and not in the VAR statement specifications (if the VAR statement is used at all), PROC CALIS does not recognize the observed variables as they are because the VAR statement has been used to preselect the legitimate set of observed variables to analyze. In most models, these observed variables are instead treated as latent variables. Again, this behavior is the same for all versions of PROC CALIS. If mistreating observed variables as latent variables is a major concern, a simple solution is not to use the VAR statement at all. This ensures that PROC CALIS uses all the observed variable as they are if they are specified in the model specification statements.

Finally, for observed variables that are specified only in the VAR statement and not in any of the model specification statements, the behavior depends on which SAS version you are using. Prior to SAS/STAT 9.22, PROC CALIS simply ignored these observed variables. For SAS/STAT 9.22 or later, PROC CALIS still includes these observed variables for analysis. In this case, PROC CALIS treats these “extra” variables as exogenous variables in the model so that some default parameterization applies. See the section “[Default Analysis Type and Default Parameterization](#)” on page 1257 for explanations of why this could be useful.

Changes in the LINEQS Model Specifications

Prior to SAS/STAT 9.22, LINEQS was the most popular modeling language supported by PROC CALIS. Since then, PROC CALIS has implemented a new syntax system that does not require the use of parameter names. Together with the change in default parameterization and some basic modeling methods, the specification of LINEQS models becomes much simpler and intuitive in SAS/STAT 9.22 or later. [Table 27.2](#) lists the major syntax changes in LINEQS model specifications, followed by some notes.

Table 27.2 Changes in the LINEQS Model Syntax

Syntax	SAS/STAT 9.22 or Later	Prior to SAS/STAT 9.22
Free parameter specifications	Parameter names optional	Parameter names required
Error terms in equations	Required	Not required
Mean structure analysis	With the MEANSTR option	With the UCOV and AUG options
Intercept parameter specifications	With the Intercept or Intercep variable	With the INTERCEP variable
Mean parameter specifications	With the MEAN statement specifications	As covariances between variables and the INTERCEP variable
Treatment of short parameter lists	Free parameters after the last parameter specification	Replicating the last parameter specification
Parameter-prefix notation	With two trailing underscores (__) as suffix	With the suffix ‘:’

The explanations of these changes are as follows:

- The use of parameter names for free parameters is optional in SAS/STAT 9.22 or later.

Prior to SAS/STAT 9.22, you must use parameter names to specify free parameters. In SAS/STAT 9.22 or later, the use of parameter names is optional. For example, prior to SAS/STAT 9.22, you might use the following LINEQS model specifications:

```

lineqs
  A = x1 * B + x2(.5) * C + E1;
std
  B = var_b, C = var_c(1.2);
cov
  B C = cov_b_c;

```

In SAS/STAT 9.22 or later, you can simply use the following:

```

lineqs
  A = * B + (.5) * C + E1;
variance
  B, C = (1.2);
cov
  B C;

```

This example shows that the parameter names `x1`, `x2`, `var_b`, `var_c`, and `cov_b_c` for free parameters are not necessary in SAS/STAT 9.22 or later. PROC CALIS generates names for these unnamed free parameters automatically. Also, you can specify initial estimates in parentheses without using parameter names. Certainly, you can still use parameter names wherever you want to, especially when you need to constrain parameters by referring to their names. Notice that the STD statement prior to SAS/STAT 9.22 has a more meaningful alias, VARIANCE, in SAS/STAT 9.22 or later.

- An error term is required in each equation in the LINEQS statement in SAS/STAT 9.22 or later.

Prior to SAS/STAT 9.22, you can set an equation in the LINEQS statement without providing an error term such as the following:

```

lineqs
  A = x1 * F1;

```

This means that A is perfectly predicted from F1 without an error. In SAS/STAT 9.22 or later, you need to provide an error term in each equation, and the preceding specification is not syntactically valid. If a perfect relationship is indeed desirable, you can equivalently set the corresponding error variance to zero. For example, the following specification in SAS/STAT 9.22 or later achieves the purpose of specifying a perfect relationship between A and F1:

```

lineqs
  A = x1 * F1 + E1;
variance
  E1 = 0.;

```

In the VARIANCE statement, the error variance of E1 is fixed at zero, resulting in a perfect relationship between A and F1.

- Mean structure analysis is invoked by the `MEANSTR` option in SAS/STAT 9.22 or later.

Prior to SAS/STAT 9.22, you use the AUG and UCOV options together in the PROC CALIS statement to invoke the analysis of mean structures. These two options became obsolete in SAS/STAT 9.22.

This change actually reflects more than a name change. Prior to SAS/STAT 9.22, mean structures are analyzed as augmented covariance structures in the uncorrected covariance matrix (hence the AUG and UCOV options). There are many problems with this “augmented” matrix approach. In SAS/STAT 9.22 or later, the augmented matrix was abandoned in favor of the direct parameterization approach for the mean structures. Now you must use the **MEANSTR** option in the PROC CALIS statement to invoke the analysis of mean structures. Alternatively, you can specify the intercepts directly in the **LINEQS** statement or specify the means directly in the **MEAN** statement. See the next two items for more information.

- Intercept parameters are set as the coefficient effects of the Intercept variable in SAS/STAT 9.22 or later.

Prior to SAS/STAT 9.22, you specify the intercept variable in the equations of the **LINEQS** statement by using the special “variable” named ‘INTERCEP’. For example, in the following specification, *a1* is the intercept parameter for the equation with dependent variable *A*:

```
proc calis ucov aug;
lineqs
  A = a1 * INTERCEP + b1 * B + E1;
```

In SAS/STAT 9.22 or later, although ‘INTERCEP’ is still accepted by PROC CALIS, a more meaningful alias ‘Intercept’ is also supported, as shown in the following:

```
proc calis;
lineqs
  A = a1 * Intercept + b1 * B + E1;
```

Intercept or INTERCEP can be typed in uppercase, lowercase, or mixed case in all versions. In addition, with the use of the Intercept variable in the **LINEQS** statement specification, mean structure analysis is automatically invoked for all parts of the model without the need to use the **MEANSTR** option in the PROC CALIS statement in SAS/STAT 9.22 or later.

- Mean parameters are specified directly in the **MEAN** statement in SAS/STAT 9.22 or later.

Prior to SAS/STAT 9.22, you need to specify mean parameters as covariances between the corresponding variables and the INTERCEP variable. For example, the following statements specify the mean parameters, *mean_b* and *mean_c*, of variables *B* and *C*, respectively:

```
proc calis ucov aug;
lineqs
  A = a1 * INTERCEP + b1 * B + b2 * C + E1;
cov
  B INTERCEP = mean_b (3),
  C INTERCEP = mean_c;
```

In SAS/STAT 9.22 or later, you can specify these mean parameters directly in the **MEAN** statement, as in the following example:

```

proc calis;
lineqs
  A = a1 * Intercept + b1 * B + b2 * C + E1;
mean
  B = mean_b (3),
  C = mean_c;

```

This way, the types of parameters that are being specified are clearer.

- Short parameter lists do not generate constrained parameters in SAS/STAT 9.22 or later.

Prior to SAS/STAT 9.22, if you provide a shorter parameter list than expected, the last parameter specified is replicated automatically. For example, the following specification results in replicating `varx` as the variance parameters for variables `x2–x10`:

```

std
  x1-x10 = var0 varx;

```

This means that all variances for the last nine variables in the list are constrained to be the same. In SAS/STAT 9.22 or later, this is not the case. That is, `var0` and `varx` are the variance parameters for `x1` and `x2`, respectively, while the variances for `x3–x10` are treated as unconstrained free parameters.

If you want to constrain the remaining parameters to be the same in the current version of PROC CALIS, you can use the following continuation syntax `[...]` at the end of the parameter list:

```

std
  x1-x10 = var0 varx [...];

```

The continuation syntax `[...]` repeats the specification of `varx` for all the remaining variance parameters for `x3–x10`.

- The parameter-prefix uses a new notation in SAS/STAT 9.22 or later.

Prior to SAS/STAT 9.22, you can use the parameter-prefix to generate parameter names as in the following example:

```

lineqs
  A = x: * B + x: * C + E1;
std
  B = var:, C = var: ;

```

In SAS/STAT 9.22 or later, you must replace the `:` notation with two trailing underscores, `__`, as in the following:

```

lineqs
  A = x__ * B + x__ * C + E1;
variance
  B = var__, C = var__;

```

Both versions generate parameter names by appending unique integers to the prefix, as if the following has been specified:

```

lineqs
  A = x1 * B + x2 * C + E1;
variance
  B = var1, C = var2;

```

In SAS/STAT 9.22 or later, you can even omit the parameter-prefix altogether. For example, you can specify the following with a null parameter-prefix:

```

lineqs
  A = __ * B + __ * C + E1;
variance
  B = __, C = __;

```

In this case, PROC CALIS uses the internal prefix ‘_Parm’ to generate names, as if the following has been specified:

```

lineqs
  A = _Parm1 * B + _Parm2 * C + E1;
variance
  B = _Parm3, C = _Parm4;

```

Compatibility with the TCALIS Procedure in SAS/STAT 9.2

Prior to the extensive changes and feature enhancements of the CALIS procedure in SAS/STAT 9.22, an experimental version of the CALIS procedure, called PROC TCALIS, was made available in SAS/STAT 9.2. In fact, the CALIS procedure in SAS/STAT 9.22 or later builds on the foundations of the TCALIS procedure. Although the experimental TCALIS procedure and the current CALIS procedure have some similar features, they also have some major differences. This section describes these major differences so that users who have experience in using the TCALIS procedure can adapt better to the current version of the CALIS procedure. In this section, whenever the CALIS procedure is mentioned without version reference, it is assumed to be the PROC CALIS version in SAS/STAT 9.22 or later.

Naming Parameters Is Optional in PROC CALIS

In essence, the CALIS procedure does not require the use of parameter names in specifications, whereas the TCALIS procedure (like the PROC CALIS versions prior to SAS/STAT 9.22) does require the use of parameter names. For example, in the TCALIS procedure you might specify the following LINEQS model:

```

proc tcalis;
  lineqs
    X1 = 1.      * F1 + E1,
    X2 = 12     * F1 + E2,
    X3 = 13 (.2) * F1 + E3;
  cov
    E1 E2 = cv12;
run;

```

Two parameters for factor loadings are used in the specification: l_1 and l_2 . The initial value of l_2 is set to 0.2. The covariance between the error terms E_1 and E_2 is named $cv12$. These parameters are not constrained, and therefore names for these parameters are not required in PROC CALIS, as shown in the following specifications:

```
proc calis;
  lineqs
    X1 = 1.      * F1 + E1,
    X2 =        * F1 + E2,
    X3 = (0.2) * F1 + E3;
  cov
    E1 E2;
run;
```

Parameter names for the two loadings in the second and the third equations are automatically generated by PROC CALIS. So is the error covariance parameter between E_1 and E_2 . Except for the names of these parameters, the preceding PROC TCALIS and PROC CALIS specifications generate the same model.

Names for parameters are only optional in PROC CALIS, but they are not prohibited. PROC CALIS enables you to specify models efficiently without the burden of having to create parameter names unnecessarily. But you can still use parameter names and the corresponding syntax in PROC CALIS wherever you want to, much as you do in PROC TCALIS.

Another example is the following PATH model specification in PROC TCALIS:

```
proc tcalis;
  path
    X1 <--- F1    1. ,
    X2 <--- F1    l2 ,
    X3 <--- F1    l3 (0.2);
  pcov
    X1 X2 = cv12;
run;
```

Again, naming the unconstrained parameters l_1 , l_2 , and $cv12$ is not required with the CALIS procedure, as shown in the following specification:

```
proc calis;
  path
    X1 <--- F1    = 1. ,      /* path entry 1 */
    X2 <--- F1    ,          /* path entry 2 */
    X3 <--- F1    = (0.2);   /* path entry 3 */
  pcov
    X1 X2;
run;
```

Without any parameter specification (that is, neither a name nor a value), the second path entry specifies a free parameter for the path effect (or coefficient) of F_1 on X_2 . The corresponding parameter name for the effect is generated by PROC CALIS internally. In the third path entry, only an initial value is specified. Again, a parameter name is not necessary there. Similarly, PROC CALIS treats this as a free path effect parameter with a generated parameter name. Lastly, the error covariance between X_1 and X_2 is also a free parameter with a generated parameter name.

Although in PROC CALIS naming unconstrained free parameters in the PATH model is optional, PROC CALIS requires the use of equal signs before the specifications of parameters, fixed values, or initial values. The TCALIS procedure does not enforce this rule. Essentially, this stricter syntax rule in PROC CALIS makes the parameter specifications distinguishable from path specifications in path entries and therefore is necessary for the development of the multiple-path syntax, which is explained in the next section.

Changes in the PATH Statement Syntax

The PATH statement syntax was first available in the TCALIS procedure and was also a major addition to the CALIS procedure in SAS/STAT 9.22. This statement is essential to the PATH modeling language for specifying general structural equation models. Table 27.3 summarizes the major differences between the two versions.

Table 27.3 Changes in the PATH Statement Syntax

Syntax	PROC CALIS	PROC TCALIS
Naming unconstrained free parameters	Optional	Required
Equal signs before parameter specifications	Required	Not used
Treatment of unspecified path parameters	Free parameters	Fixed constants at 1
Multiple-path syntax	Supported	Not supported
Extended path syntax	Supported	Not supported

The following example shows how to specify a PATH model in PROC TCALIS:

```
proc tcalis;
  path
    F1 ---> X1      ,
    F1 ---> X2      a2 (.3) ,
    F1 ---> X3      a3      ,
    F2 ---> X4      1.      ,
    F2 ---> X5      a5      ,
    F2 ---> X6      a6      ;
  pvar
    F1 F2 = fvar1 fvar2,
    X1-X6 = evar1-evar6;
  pcov
    F1 F2 = covF1F2;

run;
```

The following statements show to specify the preceding PATH model in PROC CALIS equivalently:

```
proc calis;
  path
    F1 ---> X1      = 1.      ,      /* path entry 1 */
    F1 ---> X2      = (.3)    ,      /* path entry 2 */
    F1 ---> X3      ,      /* path entry 3 */
    F2 ---> X4-X6 = 1. a5 a6 ,      /* path entry 4 */
    F1 <--> F1      ,      /* path entry 5 */
    F2 <--> F2      ,      /* path entry 6 */
    F1 <--> F2      = covF1F2 ,      /* path entry 7 */
    <--> X1-X6      = evar1-evar6; /* path entry 8 */

run;
```


The differences in specifications between the two versions are as follows:

- In PROC CALIS, naming unconstrained free parameters in the PATH statement is optional.

For example, in the PROC TCALIS specification, the parameter names `a2` and `a3` have been used for path entries 2 and 3, respectively. They can be omitted with the PROC CALIS specification.

- In PROC CALIS, you must use equal signs before parameter specifications in all path entries.

For example, equal signs are necessary in path entries 1, 2, 4, 7, and 8 to separate the parameter specifications from the path specifications. However, because equal signs are not part of the syntax in PROC TCALIS, the TCALIS procedure cannot distinguish parameter specifications from path specifications in path entries. Consequently, PROC TCALIS is incapable of handling multiple-path syntax such as path entry 4 and extended path syntax such as path entry 8.

- In PROC CALIS, unspecified parameters are treated as free parameters.

For example, path entries 3, 5, and 6 are free parameters for the path effect of F1 on X3, the variance of F1, and the variance of F2, respectively. In contrast, these unspecified parameters are treated as fixed constants 1 in PROC TCALIS. That is also why path entry 1 must specify a fixed value of 1 explicitly with the PROC CALIS specification. Otherwise, PROC CALIS treats it as a free parameter for the path effect.

- In PROC CALIS, you can use the multiple-path syntax.

For example, path entry 4 specifies three different paths from F2 in a single entry. The parameter specifications after the equal sign are distributed to the multiple paths specified in order (that is, to X4, X5, and X6, respectively). However, in PROC TCALIS you must specify these paths separately in three path entries.

- In PROC CALIS, you can use the extended path syntax to specify all kinds of parameters in the PATH statement.

For example, path entries 5 and 6 specify the variance parameters for F1 and F2, respectively. Because these variances are unconstrained free parameters, you do not need to use parameter names (but you can use them if you want). In PROC TCALIS, however, you must specify these variance parameters in the PVAR statement. Path entries 7 and 8 in the PROC CALIS specification provide other examples of the extended path syntax available only in PROC CALIS. Path entry 7 specifies the covariance parameter between F1 and F2 as `CovF1F2` (although the name for this free parameter could have been omitted). You must specify this covariance parameter in the PCOV statement if you use PROC TCALIS. Path entry 8 specifies the error variances for X1–X6 as `evar1–evar6`, respectively. You must specify these error variance parameters in the PVAR statement if you use PROC TCALIS. Essentially, in PROC CALIS you can specify all types of parameters in the PATH model as path entries in the PATH statement. See the [PATH](#) statement for details about the extended path syntax.

Changes in the Automatic Free Parameters in Functional Models

The CALIS and the TCALIS procedures differ in their treatment of automatic free parameters in functional models. Functional models refer to those models that can (but do not necessarily have to) analyze predictor-outcome or exogenous-endogenous relationships. In general, models that use the following statements are functional models: FACTOR, LINEQS, LISMOD, PATH, and RAM. Automatic free parameters in these functional models are those parameters that are free to estimate by default even if you do not specify them explicitly in the syntax. Table 27.4 indicates which types of parameters are automatic free parameters in PROC CALIS and PROC TCALIS.

Table 27.4 Automatic Free Parameters in PROC CALIS and PROC TCALIS

Automatic Free Parameters	PROC CALIS	PROC TCALIS
Variances		
Exogenous observed variables	Yes	Yes
Exogenous latent factors	Yes	Yes
Error variables	Yes	Yes
Covariances		
Between exogenous observed variables	Yes	Yes
Between exogenous latent factors	Yes ¹	No
Between exogenous observed variables and exogenous latent factors	Yes	No
Between error variables	No	No
Means		
Exogenous observed variables	Yes	Yes
Exogenous latent factors	No	No
Intercepts		
Endogenous observed variables	Yes	No
Endogenous latent factors	No	No

1. This does not apply to exploratory FACTOR models, where covariances between latent factors in the unrotated factor solution are fixed zeros.

Regarding the treatment of automatic free parameters, this table shows that unlike the CALIS procedure, PROC TCALIS does not set default free parameters in (1) the covariances between exogenous latent factors themselves and between any pairs of exogenous latent factors and observed variables, and (2) the intercepts for the endogenous observed variables.

You can compare these two schemes of setting automatic free parameters in the following three scenarios.

First, when no functional relationships are specified in the model (and hence no latent factors and no intercept parameters), the treatment of automatic free parameters by either PROC CALIS or PROC TCALIS leads to just-identified or saturated covariance and mean structures, which is certainly a reasonable “baseline” parameterization that saturates the relationships among observed variables.

Second, when there are functional relationships between observed variables in the model and no latent factors are involved, the treatment by PROC CALIS is more reasonable because it leads to a parameterization similar to that of linear regression models. That is, PROC CALIS sets the intercepts to free parameters. However, the treatment by PROC TCALIS would lead to restrictive linear regression models with zero intercepts.

Finally, when latent factors are involved, the treatment by PROC CALIS is more “natural” in the sense that the covariances among all exogenous variables are saturated in the model, rather than being restricted to zeros for the parts pertaining to latent factors, as in PROC TCALIS. Saturating the covariances between latent factors is seen to be more natural because all variables in empirical research are usually believed to be correlated, no matter how small the correlation.

Therefore, in general the PROC CALIS treatment of automatic free parameters is recommended. The treatment by PROC TCALIS might be more compatible to models that assume independent or uncorrelated latent factors such as the unrotated exploratory factor model. In this situation, to use PROC CALIS you must use the `PATH`, `PVAR`, `RAM`, `VARIANCE`, or specific `MATRIX` statements to set the covariances between factors to fixed zeros.

A Guide to the PROC CALIS Documentation

The CALIS procedure uses a variety of modeling languages to fit structural equation models. This chapter provides documentation for all of them. Additionally, some sections provide introductions to the model specification, the theory behind the software, and other technical details. While some introductory material and examples are provided, this chapter is not a textbook for structural equation modeling and related topics. For didactic treatment of structural equation models with latent variables, see Bollen (1989b) and Loehlin (2004).

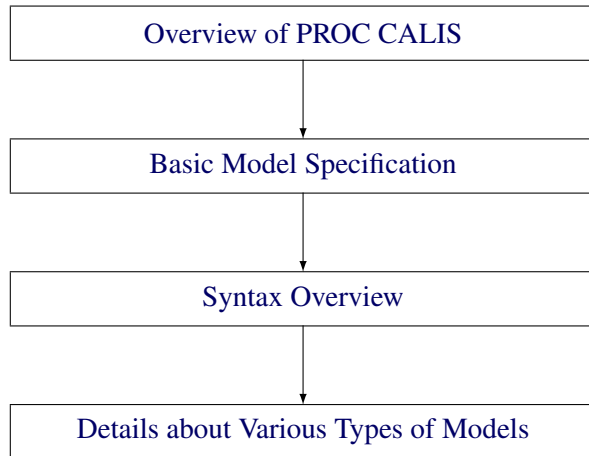
Reading this chapter sequentially is not a good strategy for learning about PROC CALIS. This section provides a guide or “road map” to the rest of the PROC CALIS chapter, starting with the basics and continuing through more advanced topics. Many sections assume that you already have a basic understanding of structural equation modeling.

The following table shows three different skill levels of using the CALIS procedure ([basic](#), [intermediate](#), and [advanced](#)) and their milestones.

Level	Milestone	Starting Section
Basic	You are able to specify simple models, but might make mistakes.	“ Guide to the Basic Skill Level ” on page 1057
Intermediate	You are able to specify more sophisticated models with few syntactic and semantic mistakes.	“ Guide to the Intermediate Skill Level ” on page 1062
Advanced	You are able to use the advanced options provided by PROC CALIS.	“ Guide to the Advanced Skill Level ” on page 1063

In the next three sections, each skill level is discussed, followed by an introductory section of the reference topics that are not covered in any of the skill levels.

Guide to the Basic Skill Level



Overview of PROC CALIS

The section “[Overview: CALIS Procedure](#)” on page 1040 gives you an overall picture of the CALIS procedure but without the details.

Basic Model Specification

The structural equation example in the section “[Getting Started: CALIS Procedure](#)” on page 1067 provides the starting point to learn the basic model specification. You learn how to represent your theory by using a path diagram and then translate the diagram into the [PATH model](#) for PROC CALIS to analyze. Because the PATH modeling language is new, this example is useful whether or not you have previous experience with PROC CALIS. The PATH model is specified in the section “[PATH Model](#)” on page 1068. The corresponding results are shown and discussed in [Example 27.17](#).

After you learn about the PATH modeling language and an example of its application, you can do either of the following:

- You can continue to learn more modeling languages in the section “[Getting Started: CALIS Procedure](#)” on page 1067.
- You can skip to the section “[Syntax Overview](#)” on page 1061 for an overview of the PROC CALIS syntax and learn other modeling languages at a later time.

You do not need to learn all of the modeling languages in PROC CALIS. Any one of the modeling languages (LINEQS, LISMOD, PATH, or RAM) is sufficient for specifying a very wide class of structural equation models. PROC CALIS provides different kinds of modeling languages because different researchers might have previously learned different modeling languages or approaches. To get a general idea about different kinds of modeling languages, the following subsections in the “[Getting Started: CALIS Procedure](#)” section are useful:

- LINEQS: Section “[LINEQS Model](#)” on page 1071
- RAM: Section “[RAM Model](#)” on page 1070

- LISMOD: Section “LISMOD Model” on page 1072
- FACTOR: Section “A Factor Model Example” on page 1073
- MSTRUCT: Section “Direct Covariance Structures Analysis” on page 1075

After studying the examples in the “Getting Started: CALIS Procedure” section, you can strengthen your understanding of the various modeling languages by studying more examples such as those in section “Examples: CALIS Procedure” on page 1385. Unlike the examples in the “Getting Started: CALIS Procedure” section, the examples in the “Examples: CALIS Procedure” section include the analysis results in addition to the explanations of the model specifications.

You can start with the following two sets of basic examples:

- MSTRUCT model examples
The basic MSTRUCT model examples demonstrate the testing of covariance structures directly on the covariance matrices. Although the MSTRUCT model is not the most common structural equation models in applications, these MSTRUCT examples can help you understand the basic form of covariance structures and the corresponding specifications in PROC CALIS.
- PATH model examples
The basic PATH model examples demonstrate how you can represent your model by path diagrams and by the PATH modeling language. These examples show the most common applications of structural equation modeling.

The following is a summary of the basic MSTRUCT model examples:

- “Example 27.1: Estimating Covariances and Correlations” on page 1385 shows how you can estimate the covariances and correlations with standard error estimates for the variables in your model. The model you fit is a saturated covariance structure model.
- “Example 27.2: Estimating Covariances and Means Simultaneously” on page 1390 extends Example 27.1 to include the mean structures in the model. The model you fit is a saturated mean and covariance structure model.
- “Example 27.3: Testing Uncorrelatedness of Variables” on page 1392 shows a very basic covariance structure model, in which the covariance structures can be specified directly. The variables in this model are uncorrelated. You learn how to specify the covariance pattern directly.
- “Example 27.4: Testing Covariance Patterns” on page 1395 extends Example 27.3 to include other covariance structures that you can specify directly.
- “Example 27.5: Testing Some Standard Covariance Pattern Hypotheses” on page 1397 illustrates the use of built-in covariance patterns supported by PROC CALIS.

The following is a summary of the basic PATH model examples:

- “Example 27.6: Linear Regression Model” on page 1401 shows how you can fit a linear regression model with the PATH modeling language of PROC CALIS. This example also introduces the path diagram representation of “causal” models. You compare results obtained from PROC CALIS and from the REG procedure, which is designed specifically for regression analysis.

- “[Example 27.7: Multivariate Regression Models](#)” on page 1406 extends [Example 27.6](#) in several different ways. You fit covariance structure models with more than one predictor, with direct and indirect effects. This example also discusses how you can choose the “best” model for your data.
- “[Example 27.8: Measurement Error Models](#)” on page 1424 explores the case where the predictor in simple linear regression is measured with error. The concept of latent true score variable is introduced. You use PROC CALIS to fit a simple measurement error model.
- “[Example 27.9: Testing Specific Measurement Error Models](#)” on page 1430 extends [Example 27.8](#) to test special measurement error models with constraints. By using PROC CALIS, you can constrain your measurement error models in many different ways. For example, you can constrain the error variances or the intercepts to test specific hypotheses.
- “[Example 27.10: Measurement Error Models with Multiple Predictors](#)” on page 1437 extends [Example 27.8](#) to include more predictors in the measurement error models. The measurement errors in the predictors can be correlated in the model.

More elaborate examples about the MSTRUCT and PATH models are listed as follows:

- “[Example 27.17: Path Analysis: Stability of Alienation](#)” on page 1499 shows you how to specify a simple PATH model and interpret the basic estimation results. The results are shown in considerable detail. The output and analyses include: a model summary, an initial model specification, an initial estimation method, an optimization history and results, residual analyses, residual graphics, estimation results, squared multiple correlations, and standardized results.
- “[Example 27.19: Fitting Direct Covariance Structures](#)” on page 1521 shows you how to fit your covariance structures directly on the covariance matrix by using the MSTRUCT modeling language. You also learn how to use the FITINDEX statement to create a customized model fit summary and how to save the fit summary statistics into an external file.
- “[Example 27.21: Testing Equality of Two Covariance Matrices Using a Multiple-Group Analysis](#)” on page 1537 uses the MSTRUCT modeling language to illustrate a simple multiple-group analysis. You also learn how to use the ODS SELECT statement to customize your printed output.
- “[Example 27.22: Testing Equality of Covariance and Mean Matrices between Independent Groups](#)” on page 1542 uses the COVPATTERN= and MEANPATTERN= options to show some tests of equality of covariance and mean matrices between independent groups. It also illustrates how you can improve your model fit by the exploratory use of the Lagrange multiplier statistics for releasing equality constraints.
- “[Example 27.24: Testing Competing Path Models for the Career Aspiration Data](#)” on page 1576 illustrates how you can fit competing models by using the OUTMODEL= and INMODEL= data sets for transferring and modifying model information from one analysis to another. This example also demonstrates how you can choose the best model among several competing models for the same data.

After studying the PATH and MSTRUCT modeling languages, you are able to specify most commonly used structural equation models by using PROC CALIS. To broaden your scope of structural equation modeling, you can study some basic examples that use the FACTOR and LINEQS modeling languages. These basic examples are listed as follows:

- “[Example 27.11: Measurement Error Models Specified As Linear Equations](#)” on page 1442 explores another way to specify measurement error models in PROC CALIS. The LINEQS modeling language is introduced. You learn how to specify linear equations of the measurement error model by using the LINEQS statement. Unlike the PATH modeling language, in the LINEQS modeling language, you need to specify the error terms explicitly in the model specification.
- “[Example 27.12: Confirmatory Factor Models](#)” on page 1448 introduces a basic confirmatory factor model for test items. You use the FACTOR modeling language to specify the factor-variable relationships.
- “[Example 27.13: Confirmatory Factor Models: Some Variations](#)” on page 1459 extends [Example 27.12](#) to include some variants of the confirmatory factor model. With the flexibility of the FACTOR modeling language, this example shows how you fit models with parallel items, tau-equivalent items, or partially parallel items.

More advanced examples that use the PATH, LINEQS, and FACTOR modeling languages are listed as follows:

- “[Example 27.14: Residual Diagnostics and Robust Estimation](#)” on page 1469 illustrates the use of several graphical residual plots to detect model outliers and leverage observations, to study the departures from the theoretical case-level residual distribution, and to examine the linearity and homoscedasticity of variance. In addition, this example illustrates the use of robust estimation technique to downweight the outliers and to estimate the model parameters.
- “[Example 27.15: The Full Information Maximum Likelihood Method](#)” on page 1483 shows how you can use the full information maximum likelihood (FIML) method to estimate your model when your data contain missing values. It illustrates the analysis of the data coverage of the sample variances, covariances, and means and the analysis of missing patterns and the mean profile. It also shows that the full information maximum likelihood method makes the maximum use of the available information from the data, as compared with the default ML (maximum likelihood) methods.
- “[Example 27.16: Comparing the ML and FIML Estimation](#)” on page 1493 discusses the similarities and differences between the ML and FIML estimation methods as implemented in PROC CALIS. It uses an empirical example to show how ML and FIML obtain the same estimation results when the data do not contain missing values.
- “[Example 27.18: Simultaneous Equations with Mean Structures and Reciprocal Paths](#)” on page 1514 is an econometric example that shows you how to specify models using the LINEQS modeling language. This example also illustrates the specification of reciprocal effects, the simultaneous analysis of the mean and covariance structures, the setting of bounds for parameters, and the definitions of metaparameters by using the [PARAMETERS](#) statement and [SAS programming statements](#). You also learn how to shorten your output results by using some [global display options](#) such as the [PSHORT](#) and [NOSTAND](#) options in the PROC CALIS statement.
- “[Example 27.20: Confirmatory Factor Analysis: Cognitive Abilities](#)” on page 1524 uses the FACTOR modeling language to illustrate confirmatory factor analysis. In addition, you use the [MODIFICATION](#) option in the PROC CALIS statement to compute LM test indices for model modifications.
- “[Example 27.25: Fitting a Latent Growth Curve Model](#)” on page 1591 is an advanced example that illustrates the use of structural equation modeling techniques for fitting latent growth curve models.

You learn how to specify random intercepts and random slopes by using the LINEQS modeling language. In addition to the modeling of the covariance structures, you also learn how to specify the mean structure parameters.

If you are familiar with the traditional Keesling-Wiley-Jöreskog measurement and structural models (Keesling 1972; Wiley 1973; Jöreskog 1973) or the RAM model (McArdle 1980), you can use the LISMOD or RAM modeling languages to specify structural equation models. The following example shows how to specify these types of models:

- “[Example 27.23: Illustrating Various General Modeling Languages](#)” on page 1567 extends [Example 27.17](#), which uses the PATH modeling language, and shows how to use the other general modeling languages: RAM, LINEQS, and LISMOD. These modeling languages enable you to specify the same path model as in [Example 27.17](#) and get equivalent results. This example shows the connections between the general modeling languages supported in PROC CALIS. A good understanding of [Example 27.17](#) is a prerequisite for this example.

Once you are familiar with various modeling languages, you might wonder which modeling language should be used in a given situation. The section “[Which Modeling Language?](#)” on page 1077 provides some guidelines and suggestions.

Syntax Overview

The section “[Syntax: CALIS Procedure](#)” on page 1078 shows the syntactic structure of PROC CALIS. However, reading the “[Syntax: CALIS Procedure](#)” section sequentially might not be a good strategy. The statements used in PROC CALIS are classified in the section “[Classes of Statements in PROC CALIS](#)” on page 1079. Understanding this section is a prerequisite for understanding single-group and multiple-group analyses in PROC CALIS. Syntax for single-group analyses is described in the section “[Single-Group Analysis Syntax](#)” on page 1082, and syntax for multiple-group analyses is described in the section “[Multiple-Group Multiple-Model Analysis Syntax](#)” on page 1082.

You might also want to get an overview of the options in the `PROC CALIS` statement. However, you can skip the [detailed listing](#) of the available options in the PROC CALIS statement. Most of these details serve as references, so you can consult them only when you need to. You can just read the summary tables for the available options in the PROC CALIS statement in the following subsections:

- “[Data Set Options](#)” on page 1083
- “[Model and Estimation Options](#)” on page 1084
- “[Options for Fit Statistics](#)” on page 1084
- “[Options for Statistical Analysis](#)” on page 1085
- “[Global Display Options](#)” on page 1085
- “[Optimization Options](#)” on page 1087

Details about Various Types of Models

Several subsections in the section “[Details: CALIS Procedure](#)” on page 1236 can help you gain a deeper understanding of the various types of modeling languages, as shown in the following table:

Language	Section
COSAN	“ The COSAN Model ” on page 1259
FACTOR	“ The FACTOR Model ” on page 1263
LINEQS	“ The LINEQS Model ” on page 1270
LISMOD	“ The LISMOD Model and Submodels ” on page 1277
MSTRUCT	“ The MSTRUCT Model ” on page 1285
PATH	“ The PATH Model ” on page 1288
RAM	“ The RAM Model ” on page 1294

The specification techniques you learn from the examples cover only parts of the modeling language. A more complete treatment of the modeling languages is covered in these subsections. In addition, you can also learn the mathematical models, model restrictions, and default parameterization of all supported modeling languages in these subsections. To get an overall idea about the default parameterization rules used in PROC CALIS, the section “[Default Analysis Type and Default Parameterization](#)” on page 1257 would be very useful. Understanding how PROC CALIS set default parameters would help you specify your models more efficiently and accurately.

Guide to the Intermediate Skill Level

At the intermediate level, you learn to minimize your mistakes in model specification and to establish more sophisticated modeling techniques. The following topics in the “[Details: CALIS Procedure](#)” section or elsewhere can help:

- The section “[Naming Variables and Parameters](#)” on page 1302 summarizes the naming rules and conventions for variable and parameter names in specifying models.
- The section “[Setting Constraints on Parameters](#)” on page 1303 covers various techniques of constraining parameters in model specifications.
- The section “[Automatic Variable Selection](#)” on page 1308 discusses how PROC CALIS treats variables in the models and variables in the data sets. It also discusses situations where the `VAR` statement specification is deemed necessary.
- The section “[Computational Problems](#)” on page 1360 discusses computational problems that occur quite commonly in structural equation modeling. It also discusses some possible remedies of the computational problem.
- The section “[Missing Values and the Analysis of Missing Patterns](#)” on page 1348 describes the default treatment of missing values.
- The statements `REFMODEL` on page 1223 and `RENAMEPARM` on page 1225 are useful when you need to make references to well-defined models when specifying a “new” model. See [Example 27.28](#) for an application.

Revisit topics and examples covered at the [basic](#) level, as needed, to help you better understand the topics at the intermediate level.

You can also study the following more advanced examples:

- “[Example 27.26: Higher-Order and Hierarchical Factor Models](#)” on page 1597 is an advanced example for confirmatory factor analysis. It involves the specifications of higher-order and hierarchical factor models. Because higher-order factor models cannot be specified by the FACTOR modeling language, you need to use the LINEQS model specification instead. A second-order factor model and a bifactor model are fit. Linear constraints on parameters are illustrated by using the PARAMETERS statement and SAS programming statements. Relationships between the second-order factor model and the bifactor model are numerically illustrated.
- “[Example 27.27: Linear Relations among Factor Loadings](#)” on page 1613 is an advanced example of a first-order confirmatory factor analysis that uses the FACTOR modeling language. In this example, you learn how to use the PARAMETERS statement and SAS programming statements to set up dependent parameters in your model. You also learn how to specify the correlation structures for a specific confirmatory factor model.
- “[Example 27.28: Multiple-Group Model for Purchasing Behavior](#)” on page 1622 is a sophisticated example of analyzing a path model. The PATH modeling language is used. In this example, a two-group analysis of mean and covariance structures is conducted. You learn how to use the REFMODEL statement to reference properly defined models and the SIMTESTS statement to test a priori simultaneous hypotheses.
- “[Example 27.29: Fitting the RAM and EQS Models by the COSAN Modeling Language](#)” on page 1648 introduces the COSAN modeling language by connecting it with general RAM and EQS models. The model matrices of the RAM or EQS model are described. You specify these model matrices and the associated parameters in the COSAN modeling language.
- “[Example 27.30: Second-Order Confirmatory Factor Analysis](#)” on page 1681 constructs the covariance structure model of the second-order confirmatory factor model. You define the model matrices by using the COSAN modeling language.
- “[Example 27.31: Linear Relations among Factor Loadings: COSAN Model Specification](#)” on page 1689 shows how you can set linear constraints among model parameters under the COSAN model.
- “[Example 27.32: Ordinal Relations among Factor Loadings](#)” on page 1695 shows how you can set ordinal constraints among model parameters under the COSAN model.
- “[Example 27.33: Longitudinal Factor Analysis](#)” on page 1699 defines the covariance structures of a longitudinal factor model and shows how you can specify the covariance structure model with the COSAN modeling language.

Guide to the Advanced Skill Level

At the advanced level, you learn to use the advanced data analysis and output control tools supported by PROC CALIS.

Advanced Data Analysis Tools

The following advanced data analysis topics are discussed:

- Assessment of fit

The section “[Assessment of Fit](#)” on page 1326 presents the fit indices used in PROC CALIS. However, the more important topics covered in this section are about how model fit indices are organized and used, how residuals can be used to gauge the fitting of individual parts of the model, and how the coefficients of determination are defined for equations.

To customize your fit summary table, you can use the options on the [FITINDEX](#) statement.

- Case-level residual diagnostics

The section “[Case-Level Residuals, Outliers, Leverage Observations, and Residual Diagnostics](#)” on page 1339 describes details about how the residual diagnostics at the individual data level are accomplished in general structural equation modeling, and how they lead to the graphical techniques for detecting outliers and leverage observations, studying residual distributions, and examining linear relationships and heteroscedasticity of error variances.

- Effect partitioning

The section “[Total, Direct, and Indirect Effects](#)” on page 1343 discusses the total, direct, and indirect effects and their computations. The stability coefficient of reciprocal causation is also defined.

To customize the effect analysis, you can use the [EFFPART](#) statement.

- Counting and adjusting degrees of freedom

The section “[Counting the Degrees of Freedom](#)” on page 1323 describes how PROC CALIS computes model fit degrees of freedom and how you can use some options on the PROC CALIS statement to make degrees-of-freedom adjustments.

To adjust the model fit degrees of freedom, you can use the [DFREDUCE=](#) and [NOADJDF](#) options in the PROC CALIS statement.

- Standardized solutions

Standardization schemes used in PROC CALIS are described and discussed in the section “[Standardized Solutions](#)” on page 1345.

Standardized solutions are displayed by default. You can turn them off by using the [NOSTAND](#) option of the PROC CALIS statement.

- Model modifications

In the section “[Modification Indices](#)” on page 1346, modification indices such as Lagrange multiplier test indices and Wald statistics are defined and discussed. These indices can be used either to enhance your model fit or to make your model more precise.

To limit the modification process only to those parameters of interest, you can use the [LMTESTS](#) statement to customize the sets of LM tests conducted on potential parameters.

- A Priori Parametric Function Testing

You can use the [TESTFUNC](#) statement to test a priori hypotheses individually. You can use the [SIMTESTS](#) statement to test a priori hypotheses simultaneously.

Advanced Output Control Tools

To be more effective in presenting your analysis results, you need to be more sophisticated in controlling your output. Some customization tools have been discussed in the previous section “Advanced Data Analysis Tools” on page 1064 and might have been mentioned in the examples included in the *basic* and the *intermediate* levels. In the following topics, these output control tools are presented in a more organized way so that you can have a systematic study scheme of these tools.

- Global output control tools in PROC CALIS

You can control output displays in PROC CALIS either by the *global display options* or by the individual output printing options. Each global display option typically controls more than one output display, while each individual output display controls only one output display. The global display options can both enable and suppress output displays, and they can also alter the format of the output.

See the *ALL*, *PRINT*, *PSHORT*, *PSUMMARY*, and *NOPRINT* options for ways to control the appearances of the output. See the section “Global Display Options” on page 1085 for details about the global display options and their relationships with the individual output display options. Also see the *ORDERALL*, *ORDERGROUPS*, *ORDERMODELS*, *ORDERSPEC*, *PARMNAME*, *PRIMAT*, *NOORDERSPEC*, *NOPARMNAME*, *NOSTAND*, and *NOSE* options which control the output formats.

- Customized analysis tools in PROC CALIS

Many individual output displays in PROC CALIS can be customized via specific options or statements. If you do not use these customization tools, the default output will usually contain a large number of displays or displays with very large dimensions. These customized analysis tools are as follows:

- The *ON=*, *OFF=*, *ON(ONLY)=* options in the *FITINDEX* statement enable you to select individual or groups of model fit indices or modeling information to display. You can still save the information of *all* fit indices in an external file by using the *OUTFIT=* option.
- The *EFFPART* statement enables you to customize the effect analysis. You display only those effects of substantive interest.
- The *LMTESTS* statement enables you to customize the sets of LM tests of interest. You test only those potential parameters that are theoretically and substantively possible.

- Output selection and destinations by the ODS system

This kind of output control is used not only for PROC CALIS, but is used for all procedures that support the ODS system. The most common uses include output selection and output destinations assignment. You use the *ODS SELECT* statement together with the ODS table names or graph names to select particular output displays. See the section “ODS Table Names” on page 1368 for these names in PROC CALIS.

The default output destination of PROC CALIS is the listing destination. You can add or change the destinations by using statements such as *ods html* (for html output), *ods rtf* (for rich text output), and so on. For details, see Chapter 20, “Using the Output Delivery System.”

Reference Topics

Some topics in the “[Details: CALIS Procedure](#)” section are intended primarily for references—you consult them only when you encounter specific problems in the PROC CALIS modeling or when you need to know the very fine technical details in certain special situations. Many of these reference topics in the “[Details: CALIS Procedure](#)” section are not required for practical applications of structural equation modeling. The following technical topics are discussed:

- Measures of multivariate kurtosis and skewness

This is covered in the section “[Measures of Multivariate Kurtosis](#)” on page 1349.

- Estimation criteria and the mathematical functions for estimation

The section “[Estimation Criteria](#)” on page 1309 presents formulas for various estimation criteria. The relationships among these criteria are shown in the section “[Relationships among Estimation Criteria](#)” on page 1318. To optimize an estimation criterion, you usually need its gradient and Hessian functions. These functions are detailed in the section “[Gradient, Hessian, Information Matrix, and Approximate Standard Errors](#)” on page 1321, where you can also find information about the computation of the standard error estimates in PROC CALIS. Unlike other estimation methods, the robust estimation methods do not optimize a discrepancy function themselves. The robust estimation methods that are implemented in PROC CALIS use the iteratively reweighted least squares (IRLS) method to obtain parameter convergence. The robust estimation technique is detailed in the section “[Robust Estimation](#)” on page 1315.

- Initial estimation

Initial estimates are necessary for all kinds of iterative optimization techniques. They are described in section “[Initial Estimates](#)” on page 1351.

- Use of optimization techniques

Optimization techniques are covered in section “[Use of Optimization Techniques](#)” on page 1352. See this section if you need to fine-tune the optimization.

- Output displays and control

The output displays in PROC CALIS are listed in the section “[Displayed Output](#)” on page 1363. General requirements for the displays are also shown.

With the ODS system, each table and graph has a name, which can be used on the ODS OUTPUT or ODS SELECT statement. See the section “[ODS Table Names](#)” on page 1368 for the ODS table and graph names.

- Input and output files

PROC CALIS supports several input and output data files for data, model information, weight matrices, estimates, fit indices, and estimation and descriptive statistics. The uses and the structures of these input and output data files are described in the sections “[Input Data Sets](#)” on page 1236 and “[Output Data Sets](#)” on page 1240.

Getting Started: CALIS Procedure

A Structural Equation Example

This example from Wheaton et al. (1977) illustrates the basic uses of the CALIS procedure and the relationships among the LINEQS, LISMOD, PATH, and RAM modeling languages. Different structural models for these data are analyzed in Jöreskog and Sörbom (1985) and in (Bentler 1995, p. 28). The data contain the following six (manifest) variables collected from 932 people in rural regions of Illinois:

Anomie67:	Anomie 1967
Powerless67:	Powerlessness 1967
Anomie71:	Anomie 1971
Powerless71:	Powerlessness 1971
Education:	Education level (years of schooling)
SEI:	Duncan’s socioeconomic index (SEI)

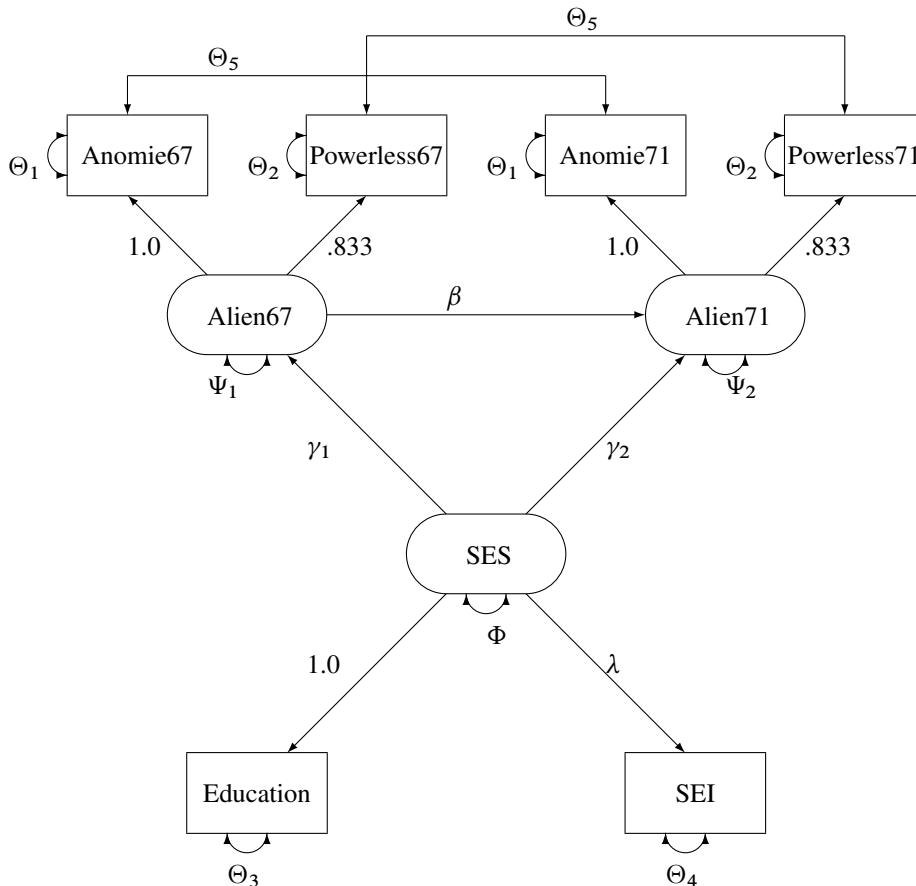
The covariance matrix of these six variables is stored in the data set named *Wheaton*.

It is assumed that anomie and powerlessness are indicators of an alienation factor and that education and SEI are indicators for a socioeconomic status (SES) factor. Hence, the analysis contains three latent variables (factors):

Alien67:	Alienation 1967
Alien71:	Alienation 1971
SES:	Socioeconomic status (SES)

The following path diagram shows the structural model used in Bentler (1985, p. 29) and slightly modified in Jöreskog and Sörbom (1985, p. 56):

Figure 27.1 Path Diagram of Stability and Alienation Example



In the path diagram shown in Figure 27.1, regressions of variables are represented by one-headed arrows. Regression coefficients are indicated along these one-headed arrows. Variances and covariances among the variables are represented by two-headed arrows. Error variances and covariances are also represented by two-headed arrows. This scheme of representing paths, variances and covariances, and error variances and covariances (McArdle 1988; McDonald 1985) is helpful in translating the path diagram to the PATH or RAM model input in the CALIS procedure.

PATH Model

Specification by using the PATH modeling language is direct and intuitive in PROC CALIS once a path diagram is drawn. The following statements specify the path diagram almost intuitively:

```
proc calis nob=932 data=Wheaton;
  path
    Anomie67 <=== Alien67 = 1.0,
    Powerless67 <=== Alien67 = 0.833,
```

```

    Anomie71      <=== Alien71      = 1.0,
    Powerless71  <=== Alien71      = 0.833,
    Education    <=== SES           = 1.0,
    SEI          <=== SES           = lambda,
    Alien67      <=== SES           = gamma1,
    Alien71      <=== SES           = gamma2,
    Alien71      <=== Alien67      = beta;
pvar
    Anomie67     = theta1,
    Powerless67  = theta2,
    Anomie71     = theta1,
    Powerless71  = theta2,
    Education    = theta3,
    SEI          = theta4,
    Alien67      = psi1,
    Alien71      = psi2,
    SES          = phi;
pcov
    Anomie67     Anomie71      = theta5,
    Powerless67  Powerless71   = theta5;
run;

```

In the PROC CALIS statement, you specify *Wheaton* as the input data set, which contains the covariance matrix of the variables.

In the PATH model specification, all the one-headed arrows in the path diagram are represented as path entries in the **PATH** statement, with entries separated by commas. In each path entry, you specify a pair of variables and the direction of the path (either **<===** or **===>**), followed by a path coefficient, which is either a fixed constant or a parameter with a name in the specification.

All the two-headed arrows each with the same source and destination are represented as entries in the **PVAR** statement, with entries separated by commas. In the **PVAR** statement, you specify the variance or error (or partial) variance parameters. In each entry, you specify a variable and then a parameter name or a fixed parameter value. If the variable involved is exogenous in the model (serves only as a predictor; never being pointed at by one-headed arrows), you are specifying a variance parameter for an exogenous variable in the **PVAR** statement. Otherwise, you are specifying an error variance (or a partial variance) parameter for an endogenous variable.

All other two-headed arrows are represented as entries in the **PCOV** statement, with entries separated by commas. In the **PCOV** statement, you specify the covariance or error (or partial) covariance parameters. In each entry, you specify a pair of variables and then a parameter name or a fixed parameter value. If both variables involved in an entry are exogenous, you are specifying a covariance parameter. If both variables involved in an entry are endogenous, you are specifying an error (or partial) covariance parameter. When one variable is exogenous and the other is endogenous in an entry, you are specifying a partial covariance parameter that can be interpreted as the covariance between the exogenous variable and the error of the endogenous variable.

See [Example 27.17](#) for the results of the current PATH model analysis. For more information about the PATH modeling language, see the section “[The PATH Model](#)” on page 1288 and the [PATH statement](#) on page 1202.

RAM Model

The PATH modeling language is not the only specification method that you can use to represent the path diagram. You can also use the RAM, LINEQS or LISMOD modeling language to represent the diagram equivalently.

The RAM model specification in PROC CALIS resembles that of the PATH model, as shown in the following statements:

```
proc calis nobs=932 data=Wheaton;
  ram
    var = Anomie67      /* 1 */
          Powerless67 /* 2 */
          Anomie71     /* 3 */
          Powerless71 /* 4 */
          Education    /* 5 */
          SEI          /* 6 */
          Alien67     /* 7 */
          Alien71     /* 8 */
          SES,        /* 9 */
    A 1 7 1.0,
    A 2 7 0.833,
    A 3 8 1.0,
    A 4 8 0.833,
    A 5 9 1.0,
    A 6 9 lambda,
    A 7 9 gamma1,
    A 8 9 gamma2,
    A 8 7 beta,
    P 1 1 theta1,
    P 2 2 theta2,
    P 3 3 theta1,
    P 4 4 theta2,
    P 5 5 theta3,
    P 6 6 theta4,
    P 7 7 psi1,
    P 8 8 psi2,
    P 9 9 phi,
    P 1 3 theta5,
    P 2 4 theta5;
run;
```

In the **RAM** statement, you specify a list of entries for parameters, with entries separated by commas. In each entry, you specify the type of parameter (PATH, PVAR, or PCOV in the code), the associated variable or pair of variables and the path direction if applicable, and then a parameter name or a fixed parameter value. The types of parameters you specify in this RAM model are for path coefficients, variances or partial variances, and covariances or partial covariances. They bear the same meanings as those in the PATH model specified previously. The RAM model specification is therefore quite similar to the PATH model specification—except that in the RAM model you put all parameter specification in the same list under the RAM statement, whereas you specify different types of parameters separately under different statements in the PATH model.

See [Example 27.23](#) for partial results of the current RAM model analysis. For more information about the RAM modeling language, see the section “[The RAM Model](#)” on page 1294 and the [RAM statement](#) on page 1216.

LINEQS Model

The LINEQS modeling language uses equations to specify functional relationships among variables, as shown in the following statements:

```
proc calis nobs=932 data=Wheaton;
  lineqs
    Anomie67      = 1.0      * f_Alien67 + E1,
    Powerless67   = 0.833    * f_Alien67 + E2,
    Anomie71      = 1.0      * f_Alien71 + E3,
    Powerless71   = 0.833    * f_Alien71 + E4,
    Education     = 1.0      * f_SES      + E5,
    SEI           = lambda   * f_SES      + E6,
    f_Alien67     = gamma1   * f_SES      + D1,
    f_Alien71     = gamma2   * f_SES      + beta * Alien67 + D2;
  std
    E1            = theta1,
    E2            = theta2,
    E3            = theta1,
    E4            = theta2,
    E5            = theta3,
    E6            = theta4,
    D1            = psi1,
    D2            = psi2,
    f_SES         = phi;
  cov
    E1 E3         = theta5,
    E2 E4         = theta5;
run;
```

In the **LINEQS** statement, equations are separated by commas. In each equation, you specify an endogenous variable on the left-hand side, and then predictors and path coefficients on the right-hand side of the equal side. The set of equations specified in this **LINEQS** model is equivalent to the system of paths specified in the preceding **PATH** (or **RAM**) model. However, there are some notable differences between the **LINEQS** and the **PATH** specifications.

First, in the **LINEQS** modeling language you must specify the error terms explicitly as exogenous variables. For example, E1, E2, and D1 are error terms in the specification. In the **PATH** (or **RAM**) modeling language, you do not need to specify error terms explicitly.

Second, equations specified in the **LINEQS** modeling language are oriented by the endogenous variables. Each endogenous variable can appear on the left-hand side of an equation only *once* in the **LINEQS** statement. All the corresponding predictor variables must then be specified on the right-hand side of the equation. For example, f_Alien71 is predicted from f_Alien67 and f_SES in the last equation of the **LINEQS** statement. In the **PATH** or **RAM** modeling language, however, you would specify the same functional relationships in two separate paths.

Third, you must follow some naming conventions for latent variables when using the **LINEQS** modeling language. The names of latent variables that are not errors or disturbances must start with an ‘f’ or ‘F’. Also, the names of the error variables must start with ‘e’ or ‘E’ and the names of the disturbance variables must start with ‘d’ or ‘D’. For example, variables Alien67, Alien71, and SES serve as latent factors in the previous **PATH** or **RAM** model specification. To comply with the naming conventions, these variables are named with an extra prefix ‘f_’ in the **LINEQS** model specification—that is, f_Alien67, f_Alien71, and

f_SES, respectively. In addition, because of the naming conventions of the LINEQS modeling language, E1–E6 serve as error terms and D1–D1 serve as disturbances in the specification.

A consequence of explicit specification of error terms in the LINEQS statement is that the partial variance and partial covariance concepts used in the PATH and RAM modeling languages are no longer needed. They are replaced by the variances or covariances of the error terms or disturbances. Errors and disturbances are exogenous variables by nature. Hence, in terms of variance and covariance specification, they are treated exactly the same way as other non-error exogenous variables in the LINEQS modeling language. That is, variance parameters for all exogenous variables, including errors and disturbances, are specified in the VARIANCE statement, and covariance parameters among exogenous variables, including errors and disturbances, are specified in COV statement.

See Example 27.23 for partial results of the current LINEQS model analysis. For more information about the LINEQS modeling language, see the section “The LINEQS Model” on page 1270 and the LINEQS statement on page 1156.

LISMOD Model

The LISMOD language is quite different from the LINEQS, PATH, and RAM modeling languages. In the LISMOD specification, you define parameters as entries in model matrices, as shown in the following statements:

```
proc calis nobs=932 data=Wheaton;
  lismod
    yvar = Anomie67 Powerless67 Anomie71 Powerless71,
    xvar = Education SEI,
    etav = Alien67 Alien71,
    xiv = SES;
  matrix _LAMBDAY_ [1,1] = 1.0,
                    [2,1] = 0.833,
                    [3,2] = 1.0,
                    [4,2] = 0.833;
  matrix _LAMBDA_ [1,1] = 1.0,
                  [2,1] = lambda;
  matrix _GAMMA_ [1,1] = gamma1,
                [2,1] = gamma2;
  matrix _BETA_ [2,1] = beta;
  matrix _THETAY_ [1,1] = theta1,
                  [2,2] = theta2,
                  [3,3] = theta1,
                  [4,4] = theta2,
                  [3,1] = theta5,
                  [4,2] = theta5;
  matrix _THETAX_ [1,1] = theta3,
                  [2,2] = theta4;
  matrix _PSI_ [1,1] = psi1,
               [2,2] = psi2;
  matrix _PHI_ [1,1] = phi;
run;
```

In the LISMOD statement, you specify the lists of variables in the model. In the MATRIX statements, you specify the parameters in the LISMOD model matrices. Each MATRIX statement contains the matrix name of interest and then locations of the parameters, followed by the parameter names or fixed parameter

values. It would be difficult to explain the LISMOD specification here without better knowledge about the formulation of the mathematical model. For this purpose, see the section “[The LISMOD Model and Submodels](#)” on page 1277 and the [LISMOD statement](#) on page 1162. See also [Example 27.23](#) for partial results of the current LISMOD model analysis.

COSAN Model

The COSAN model specification is even more abstract than all of the modeling languages considered. Like the LISMOD model specification, to specify a COSAN model you need to define parameters as entries in model matrices. In addition, you must also provide the definitions of the model matrices and the matrix formula for the covariance structures in the COSAN model specification. Therefore, the COSAN model specification requires sophisticated knowledge about the formulation of the mathematical model. For this reason, the COSAN model specification of the preceding path model is not discussed here (but see [Example 27.29](#)). For more details about the COSAN model specification, see the section “[The COSAN Model](#)” on page 1259 and the [COSAN statement](#) on page 1122.

A Factor Model Example

In addition to the general modeling languages such as PATH, RAM, LINEQS, and LISMOD, the CALIS procedure provides a specialized language for factor analysis. In the FACTOR modeling language, you can specify either exploratory or confirmatory factor models. For exploratory factor models, you can specify the number of factors, factor extraction method, and rotation algorithm, among many other options. For confirmatory factor models, you can specify the variable-factor relationships, factor variances and covariances, and the error variances.

For example, the following is an exploratory factor model fitted to the Wheaton et al. (1977) data by using PROC CALIS:

```
proc calis nobs=932 data=Wheaton;
  factor n=2 rotate=varimax;
run;
```

In this model, you want to get the varimax-rotated solution with two factors. By default, the factor extraction method is maximum likelihood (`METHOD=ML`). Maximum likelihood exploratory factor analysis by PROC CALIS can also be done equivalently by the FACTOR procedure, as shown in the following statements for the Wheaton et al. (1977) data:

```
proc factor nobs=932 data=Wheaton n=2 rotate=varimax method=ml;
run;
```

Note that `METHOD=ML` is necessary because maximum likelihood is not the default method in PROC FACTOR.

Whereas you can use either the CALIS or FACTOR procedure to fit certain exploratory factor models, you can only use the CALIS procedure to fit confirmatory factor models. In a confirmatory factor model, you are assumed to have some prior knowledge about the variable-factor relations. For example, in your substantive theory, some observed variables are not related to certain factors in the model. The following statements illustrate the specification of a confirmatory factor model for Wheaton et al. (1977) data:

```

proc calis nobs=932 data=Wheaton;
  factor
    Alien67 ==> Anomie67 Powerless67    = 1.0 load1,
    Alien71 ==> Anomie71 Powerless71    = 1.0 load2,
    SES      ==> Education SEI          = 1.0 load3;
  pvar
    Alien67      = phi11,
    Alien71      = phi22,
    SES          = phi33,
    Anomie67     = theta1,
    Powerless67  = theta2,
    Anomie71     = theta3,
    Powerless71  = theta4,
    Education    = theta5,
    SEI          = theta6;
  cov
    Alien71 Alien67 = phi21,
    SES     Alien67 = phi31,
    SES     Alien71 = phi32;
run;

```

Unlike the model fitted by the PATH, RAM, LINEQS, or LISMOD modeling language in previous sections, the confirmatory factor model considered here is purely a measurement model—that is, there are no functional relationships among factors in the model (beyond the covariances among factors) and hence it is a different model. In the **FACTOR** statement, you specify factors on the left-hand side of the entries, followed by arrows and the manifest variables that are related to the factors. On the right-hand side of the entries, you specify either parameter names or fixed parameter values for the corresponding factor loadings. In this example, there are three factors with three loadings to estimate. In the **PVAR** statement, you specify the parameters for factor variances and error variances of manifest variables. In the **COV** statement, you specify the factor covariances. As compared with the PATH, RAM, LINEQS, or LISMOD, the factor modeling language has more restrictions on parameters. These restrictions are listed as follows:

- factor-factor paths and variable-to-factor paths are not allowed
- error covariances and factor-error covariances are not allowed

For more information about exploratory and confirmatory factor models and the **FACTOR** modeling language, see the section “[The FACTOR Model](#)” on page 1263 or the **FACTOR** statement on page 1138.

Direct Covariance Structures Analysis

Previous examples are concerned with the implied covariance structures from the functional relationships among manifest and latent variables. In some cases, direct modeling of the covariance structures is not only possible, but indeed more convenient. The MSTRUCT modeling language in PROC CALIS is designed for this purpose. Consider the following four variables from the Wheaton et al. (1977) data:

Anomie67: Anomie 1967
 Powerless67: Powerlessness 1967
 Anomie71: Anomie 1971
 Powerless71: Powerlessness 1971

The covariance structures are hypothesized as follows:

$$\Sigma = \begin{pmatrix} \phi_1 & \theta_1 & \theta_2 & \theta_1 \\ \theta_1 & \phi_2 & \theta_1 & \theta_3 \\ \theta_2 & \theta_1 & \phi_1 & \theta_1 \\ \theta_1 & \theta_3 & \theta_1 & \phi_2 \end{pmatrix}$$

where:

ϕ_1 : Variance of Anomie
 ϕ_2 : Variance of Powerlessness
 θ_1 : Covariance between Anomie and Powerlessness
 θ_2 : Covariance between Anomie measures
 θ_3 : Covariance between Powerlessness measures

In the hypothesized covariance structures, the variances of Anomie and Powerlessness measures are assumed to stay constant over the two time points. Their covariances are also independent of the time of measurements. To test the tenability of this covariance structure model, you can use the following statements of the MSTRUCT modeling language:

```

proc calis nobs=932 data=Wheaton;
  mstruct
    var = Anomie67 Powerless67 Anomie71 Powerless71;
  matrix _COV_ [1,1] = phi1,
               [2,2] = phi2,
               [3,3] = phi1,
               [4,4] = phi2,
               [2,1] = theta1,
               [3,1] = theta2,
               [3,2] = theta1,
               [4,1] = theta1,
               [4,2] = theta3,
               [4,3] = theta1;
run;

```

In the **MSTRUCT** statement, you specify the list of variables of interest with the **VAR=** option. The order of the variables in the list will be the order in the hypothesized covariance matrix. Next, you use the **MATRIX _COV_** statement to specify the parameters in the covariance matrix. The specification is a direct translation from the hypothesized covariance matrix. For example, the [1, 1] element of the covariance matrix is fitted by the free parameter **phi1**. Depending on the hypothesized model, you can also specify fixed constants for the elements in the covariance matrix. If an element in the covariance matrix is not specified by either a parameter name or a constant, it is assumed to be a fixed zero.

The analysis of this model is carried out in [Example 27.19](#).

The **MSTRUCT** modeling language appears to be more restrictive than any of the other modeling languages discussed, in regard to the following limitations:

- It does not explicitly support latent variables in modeling.
- It does not explicitly support modeling of linear functional relations among variables (for example, paths).

However, these limitations are more apparent than real. In **PROC CALIS**, the parameters defined in models can be dependent. These dependent parameters can be defined further as functions of other parameters in the **PARAMETERS** and the **SAS programming statements**. With these capabilities, it is possible to fit structural models with latent variables and with linear functional relations by using the **MSTRUCT** modeling language. However, this requires a certain level of sophistication in statistical knowledge and in programming. Therefore, it is recommended that the **MSTRUCT** modeling language be used only when the covariance and mean structures are modeled directly.

For more information about the MSTRUCT modeling language, see the section “The MSTRUCT Model” on page 1285 and the [MSTRUCT statement](#) on page 1194.

Which Modeling Language?

Various modeling languages are supported in PROC CALIS because researchers are trained in or adhere to different schools of modeling. Different modeling languages reflect different modeling terminology and philosophies. The statistical and mathematical consequences by using these various modeling languages, however, might indeed be the same. In other words, you can use more than one modeling languages for certain types of models without affecting the statistical analysis. Given the choices, which modeling language is preferred? There are two guidelines for this:

- Use the modeling language that you are most familiar with.
- Use the most specialized modeling language whenever it is possible.

The first guideline calls for researchers’ knowledge about a particular modeling language. Use the language you know the best. For example, some researchers might find equation input language like LINEQS the most suitable, while others might feel more comfortable using matrix input language like LISMOD.

The second guideline depends on the nature of the model at hand. For example, to specify a factor analysis model in the CALIS procedure, the specialized FACTOR language, instead of the LISMOD language, is recommended. Using a more specialized the modeling language is less error-prone. In addition, using a specialized language like FACTOR in this case amounts to giving the CALIS procedure additional information about the specific mathematical properties of the model. This additional information is used to enhance computational efficiency and to provide more specialized results. Another example is fitting an equi-covariance model. You can simply use the MSTRUCT model specification, in which you specify the same parameter for all off-diagonal elements of the covariance elements. This is direct and intuitive. Alternatively, you could tweak a LINEQS model that would predict the same covariance for all variables. However, this is indirect and error-prone, especially for novice modelers.

In PROC CALIS, the FACTOR and MSTRUCT modeling languages are considered more specialized, while other languages are more general in applications. Whenever possible, you should use the more specialized languages. However, if your model involves some novel covariance or mean structures that are not covered by the more specialized modeling languages, you can consider the more generalized modeling languages. See [Example 27.33](#) for an application of the generalized COSAN model.

Syntax: CALIS Procedure

The following statements are available in the CALIS procedure:

```
PROC CALIS < options > ;  
  BOUNDS boundary-constraints ;  
  BY variables ;  
  COSAN model-specifications ;  
  COV covariance-parameters ;  
  DETERM variables ;  
  EFFPART effects ;  
  FACTOR model-specifications ;  
  FITINDEX fit-options ;  
  FREQ variable ;  
  GROUP group-number < / options > ;  
  LINCON linear-constraints ;  
  LINEQS equations ;  
  LISMOD variable-lists ;  
  LMTESTS test-options ;  
  MATRIX parameter-specifications ;  
  MEAN mean-parameters ;  
  MODEL model-number < / options > ;  
  MSTRUCT variable-list ;  
  NLINCON nonlinear-constraints ;  
  NLOPTIONS optimization-options ;  
  OUTFILES file-options ;  
  PARAMETERS parameter-specifications ;  
  PARTIAL variables ;  
  PATH paths ;  
  PCOV covariance-parameters ;  
  PVAR variance-parameters ;  
  RAM model-specifications ;  
  REFMODEL model-number < / options > ;  
  RENAMEPARM parameter-assignments ;  
  SIMTESTS simultaneous-tests ;  
  STD variance-parameters ;  
  STRUCTEQ variables < label > ;  
  TESTFUNC parametric-functions ;  
  VAR variables ;  
  VARIANCE variance-parameters ;  
  VARNAMES name-assignments ;  
  WEIGHT variable ;  
  Programming statements ;
```

Classes of Statements in PROC CALIS

To better understand the syntax of PROC CALIS, it is useful to classify the statements into classes. These classes of statements are described in the following sections.

PROC CALIS Statement

is the main statement that invokes the CALIS procedure. You can specify options for input and output data sets, printing, statistical analysis, and computations in this statement. The options specified in the PROC CALIS statement will propagate to all groups and models, but are superseded by the options specified in the individual **GROUP** or **MODEL** statements.

GROUP Statement

signifies the beginning of a group specification. A group in the CALIS procedure is an independent sample of observations. You can specify options for input and output data sets, printing, and statistical computations in this statement. Some of these group options in the **GROUP** statement can also be specified in the **MODEL** or PROC CALIS statement, but the options specified in the **GROUP** statement supersede those specified in the **MODEL** or PROC CALIS statement for the group designated in the **GROUP** statement. For group options that are available in both of the **GROUP** and PROC CALIS statements, see the section “Options Available in the **GROUP** and PROC CALIS Statements” on page 1153. For group options that are available in the **GROUP**, **MODEL**, and PROC CALIS statements, see the section “Options Available in **GROUP**, **MODEL**, and PROC CALIS Statements” on page 1154. If no **GROUP** statement is used, a single-group analysis is assumed. The group options for a single-group analysis are specified in the PROC CALIS statement.

The **GROUP** statement can be followed by **subsidiary group specification statements**, which specify further data processing procedures for the group designated in the **GROUP** statement.

Subsidiary Group Specification Statements

are for specifying additional data processing attributes for the input data. These statements are summarized in the following table:

Statement	Description
FREQ on page 1152	Specifies the frequency variable for the input observations
PARTIAL on page 1202	Specifies the partial variables
VAR on page 1228	Specifies the set of variables in analysis
WEIGHT on page 1235	Specifies the weight variable for the input observations

These statements can be used after the PROC CALIS statement or each **GROUP** statement. Again, the specifications within the scope of the **GROUP** statement supersede those specified after the PROC CALIS statement for the group designated in the **GROUP** statement.

MODEL Statement

signifies the beginning of a model specification. In the **MODEL** statement, you can specify the fitted groups, input and output data sets for model specification or estimates, printing options, statistical analysis, and computational options. Some of the options in the **MODEL** statement can also be specified in the PROC CALIS

statement. These options are called model options. Model options specified in the **MODEL** statement supersede those specified in the **PROC CALIS** statement. For model options that are available in both of the **MODEL** and **PROC CALIS** statements, see the section “Options Available in the **MODEL** and **PROC CALIS** Statements” on page 1193. If no **MODEL** statement is used, a single model is assumed and the model options are specified in the **PROC CALIS** statement.

Some of the options in the **MODEL** statement can also be specified in the **GROUP** statement. These options are called group options. The group options in the **MODEL** statement are transferred to the groups being fitted, but they are superseded by the group options specified in the associated **GROUP** statement. For group options that are available in the **GROUP** and the **MODEL** statements, see the section “Options Available in **GROUP**, **MODEL**, and **PROC CALIS** Statements” on page 1154.

The **MODEL** statement itself does not define the model being fitted to the data; the main and subsidiary model specification statements that follow immediately after the **MODEL** statement do. These statements are described in the next two sections.

Main Model Specification Statements

are for specifying the type of the modeling language and the main features of the model. These statements are summarized in the following table:

Statement	Description
COSAN on page 1122	Specifies general mean and covariance structures in matrix terms
FACTOR on page 1138	Specifies confirmatory or exploratory factor models
LINEQS on page 1156	Specifies models by using linear equations
LISMOD on page 1162	Specifies models in terms of LISREL-like model matrices
MSTRUCT on page 1194	Specifies parameters directly in the mean and covariance matrices
PATH on page 1202	Specifies models by using the causal paths of variables
RAM on page 1216	Specifies models by using RAM-like lists of parameters
REFMODEL on page 1223	Specifies a base model from which the target model is modified

You can use one of these statements for specifying one model. Each statement in the list represents a particular type of modeling language. After the main model specification statement, you might need to add subsidiary model specification statements, as described in the following section, to complete the model specification.

Subsidiary Model Specification Statements

are used to supplement the model specification. They are specific to the types of the modeling languages invoked by the main model specification statements, as shown in the following table:

Statement	Specification	Modeling Languages
COV on page 1132	Covariance parameters	FACTOR, LINEQS
MATRIX on page 1175	Parameters in matrices	COSAN, LISMOD, MSTRUCT
MEAN on page 1189	Mean or intercept parameters	FACTOR, LINEQS, PATH
PCOV on page 1212	(Partial) covariance parameters	PATH
PVAR on page 1214	(Partial) variance parameters	FACTOR, PATH
RENAMEPARM on page 1225	New parameters by renaming	REFMODEL
VARIANCE on page 1231	Variance parameters	LINEQS

Notice that the RAM modeling language does not have any subsidiary model specification statements, because all model specification can be done in the [RAM](#) statement.

Model Analysis Statements

are used to request specific statistical analysis, as shown in the following table:

Statement	Analysis
DETERM on page 1136	Sets variable groups for computing the determination coefficients; same as the STRUCTEQ statement
EFFPART on page 1097	Displays and partitions the effects in the model
FITINDEX on page 1148	Controls the fit summary output
LMTTESTS on page 1166	Defines the Lagrange multiplier test regions
SIMTESTS on page 1226	Defines simultaneous parametric function tests
STRUCTEQ on page 1136	Sets variable groups for computing the determination coefficients; same as the DETERM statement
TESTFUNC on page 1227	Tests individual parametric functions

Notice that the [DETERM](#) and the [STRUCTEQ](#) statements function exactly the same way.

Optimization Statements

are used to define additional parameters and parameter constraints, to fine-tune the optimization techniques, or to set the printing options in optimization, as shown in the following table:

Statement	Description
BOUNDS on page 1120	Defines the bounds of parameters
LINCON on page 1155	Defines the linear constraints of parameters
NLINCON on page 1196	Defines the nonlinear constraints of parameters
NLOPTIONS on page 1197	Sets the optimization techniques and printing options

Other Statements

that are not listed in preceding sections are summarized in the following table:

Statement	Description
BY on page 1121	Fits a model to different groups separately
OUTFILES on page 1197	Controls multiple output data sets
PARAMETERS on page 1199	Defines additional parameters or superparameters
SAS programming statements on page 1226	Define parameters or functions

Note that [SAS programming statements](#) include the [ARRAY](#) statement and the mathematical statements for defining parameter interdependence.

Single-Group Analysis Syntax

```

PROC CALIS < options > ;
  subsidiary group specification statements ;
  main model specification statement ;
  subsidiary model specification statements ;
  model analysis statements ;
  optimization statements ;
  other statements ;

```

In a single-group analysis, there is only one group and one model. Because all model or group specifications are unambiguous, the **MODEL** and **GROUP** statements are not necessary. The order of the statements is not important for parsing purposes, although you might still like to order them in a particular way to aid understanding. Notice that the **OUTFILES** statement is not necessary in single-group analyses, as it is designed for multiple-group situations. Output file options in a single-group analysis can be specified in the **PROC CALIS** statement.

Multiple-Group Multiple-Model Analysis Syntax

```

PROC CALIS < options > ;
  subsidiary group specification statements ;
  model analysis statements ;
  GROUP 1 < / group options > ;
    subsidiary group specification statements ;
  GROUP 2 < / group options > ;
    subsidiary group specification statements ;
  MODEL 1 < / model options > ;
    main model specification statement ;
    subsidiary model specification statements ;
    model analysis statements ;
  MODEL 2 < / model options > ;
    main model specification statement ;
    subsidiary model specification statements ;
    model analysis statements ;
  optimization statements ;
  other statements ;

```

The multiple uses of the **GROUP** and the **MODEL** statements characterize the multiple-group multiple-model analysis. Unlike the single-group analysis, the order of some statements in a multiple-group multiple-model syntax is important for parsing purposes.

A **GROUP** statement signifies the beginning of a group specification block and designates a group number for the group. The scope of a **GROUP** statement extends to the subsequent subsidiary group specification statements until another **MODEL** or **GROUP** statement is encountered. In the preceding syntax, **GROUP 1** and **GROUP 2** have separate blocks of subsidiary group specification statements. By using additional **GROUP** statements, you can add as many groups as your situation calls for. Subsidiary group specification statements declared before the first **GROUP** statement are in the scope of the **PROC CALIS** statement. This

means that these subsidiary group specification statements are applied globally to all groups unless they are respecified locally within the scopes of individual **GROUP** statements.

A **MODEL** statement signifies the beginning of a model specification block and designates a model number for the model. The scope of a **MODEL** statement extends to the subsequent main and subsidiary model specification statements until another **MODEL** or **GROUP** statement is encountered. In the preceding syntax, MODEL 1 and MODEL 2 have separate blocks of main and subsidiary model specification statements. By using additional **MODEL** statements, you can add as many models as your situation calls for. If you use at least one **MODEL** statement, any main and subsidiary model specification statements declared before the first **MODEL** statement are ignored.

Some model analysis statements are also bounded by the scope of the **MODEL** statements. These statements are: **DETERM**, **EFFPART**, **LMTESTS**, and **STRUCTEQ**. These statements are applied only locally to the model in which they belong. To apply these statements globally to all models, put these statements before the first **MODEL** statement.

Other model analysis statements are not bounded by the scope of the **MODEL** statements. These statements are: **FITINDEX**, **SIMTESTS**, and **TESTFUNC**. Because these statements are not model-specific, you can put these statements anywhere in a PROC CALIS run.

Optimization and other statements are not bounded by the scope of either the **GROUP** or **MODEL** statements. You can specify them anywhere between the PROC CALIS and the run statements without affecting the parsing of the models and the groups. For clarity of presentation, they are shown as last statement block in the syntax. Notice that the **BY** statement is not supported in a multiple-group setting.

PROC CALIS Statement

PROC CALIS < options > ;

The PROC CALIS statement invokes the CALIS procedure. There are many options in the PROC CALIS statement. These options, together with brief descriptions, are classified into different categories in the next few sections. An alphabetical listing of these options with more details then follows.

Data Set Options

You can use the following options to specify input and output data sets:

Option	Description
BASEFIT=	Inputs the fit information of the customized baseline model
DATA=	Inputs the data
INEST=	Inputs the initial values and constraints
INMODEL=	Inputs the model specifications
INWGT=	Inputs the weight matrix
OUTEST=	Outputs the estimates and their covariance matrix
OUTFIT=	Outputs the fit indices
OUTMODEL=	Outputs the model specifications
OUTSTAT=	Outputs the statistical results
OUTWGT=	Outputs the weight matrix
READADDPARM	Inputs the generated default parameters in the INMODEL= data set

Model and Estimation Options

You can use these options to specify details about estimation, models, and computations:

Option	Description
CORRELATION	Analyzes correlation matrix
COVARIANCE	Analyzes covariance matrix
COVPATTERN=	Specifies one of the built-in covariance structures
DEMPHAS=	Emphasizes the diagonal entries
EDF=	Defines number of observations by the number of error degrees of freedom
INWGTINV	Specifies that the INWGT= data set contains the inverse of the weight matrix
MEANPATTERN=	Specifies one of the built-in mean patterns
MEANSTR	Analyzes the mean structures
METHOD=	Specifies the estimation method
NOBS=	Defines the number of observations
NOMEANSTR	Deactivates the inherited MEANSTR option
RANDOM=	Specifies the seed for randomly generated initial values
RDF=	Defines nob _s by the number of regression <i>df</i>
RIDGE=	Specifies the ridge factor for the covariance matrix
ROBPHI=	Specifies the tuning parameter for robust methods
ROBUST=	Specifies the type of robust method
START=	Specifies a constant for initial values
VARDEF=	Specifies the variance divisor
WPENALTY=	Specifies the penalty weight to fit correlations
WRIDGE=	Specifies the ridge factor for the weight matrix

Options for Fit Statistics

You can use these options to modify the default behavior of fit index computations, to control the display of fit indices, and specify output file for fit indices:

Option	Description
ALPHAECV=	Specifies the α level for computing the confidence interval of ECV (Browne and Cudeck 1993)
ALPHARMS=	Specifies the α level for computing the confidence interval of RMSEA (Steiger and Lind 1980)
BASEFUNC=	Specifies the function value and the degrees of freedom of the customized baseline model
CHICORRECT=	Specifies the chi-square correction factor
CLOSEFIT=	Defines the close fit value
DFREDUCE=	Reduces the degrees of freedom for model fit chi-square test
NOADJDF	Requests no degrees-of-freedom adjustment be made for active constraints
NOINDEXTYPE	Suppresses the printing of fit index types
OUTFIT=	Specifies the output data set for storing fit indices

These options can also be specified in the **FITINDEX** statement. However, to control the display of individual fit indices, you must use the **ON=** and **OFF=** options of the **FITINDEX** statement.

Options for Statistical Analysis

You can use these options to request specific statistical analysis and display and to set the parameters for statistical analysis:

Option	Description
ALPHALEV=	Specifies the α -level criterion for detecting leverage points
ALPHAOUT=	Specifies the α -level criterion for detecting outliers
ASYCOV=	Specifies the formula for computing asymptotic covariances
BIASKUR	Computes the skewness and kurtosis without bias corrections
EFFPART TOTEFF	Displays total, direct, and indirect effects
EXTENDPATH	Displays the extended path estimates
G4=	Specifies the algorithm for computing standard errors
KURTOSIS	Computes and displays kurtosis
MAXMISSPAT=	Specifies the maximum number of missing patterns to display
MODIFICATION	Computes modification indices
NOMISSPAT	Suppresses the display of missing pattern analysis
NOMOD	Suppresses modification indices
NOSTAND	Suppresses the standardized output
NOSTDERR	Suppresses standard error computations
PCORR	Displays analyzed and estimated moment matrix
PCOVES	Displays the covariance matrix of estimates
PDETERM	Computes the determination coefficients
PESTIM	Prints parameter estimates
PINITIAL	Prints initial pattern and values
PLATCOV	Computes the latent variable covariances and score coefficients
PLOTS=	Specifies ODS Graphics selection
PWEIGHT	Displays the weight matrix
RESIDUAL=	Specifies the type of residuals being computed
SIMPLE	Prints univariate statistics
SLMW=	Specifies the probability limit for Wald tests
STDERR	Computes the standard errors
TMISSPAT=	Specifies the data proportion threshold for displaying the missing patterns

Global Display Options

There are two different kinds of global display options: one is for selecting output; the other is for controlling the format or order of output.

You can use the following options to select printed output:

Option	Description
NOPRINT	Suppresses the displayed output
PALL	Displays all displayed output (ALL)
PRINT	Adds default displayed output
PSHORT	Reduces default output (SHORT)
PSUMMARY	Displays fit summary only (SUMMARY)

In contrast to individual output printing options described in the section “Options for Statistical Analysis” on page 1085, the global display options typically control more than one output or analysis. The relations between these two types of options are summarized in the following table:

Options	PALL	PRINT	default	PSHORT	PSUMMARY
fit indices	*	*	*	*	*
linear dependencies	*	*	*	*	*
PESTIM	*	*	*	*	
iteration history	*	*	*	*	
PINITIAL	*	*	*		
SIMPLE	*	*	*		
STDERR	*	*	*		
RESIDUAL	*	*			
KURTOSIS	*	*			
PLATCOV	*	*			
TOTEFF	*	*			
PCORR	*				
MODIFICATION	*				
PWEIGHT	*				
PCOVES					
PDETERM					
PRIMAT					

Each column in the table represents a global display option. An “*” in the column means that the individual output or analysis option listed in the corresponding row turns on when the global display option in the corresponding column is specified.

Note that the column labeled with “default” is for default printing. If the **NOPRINT** option is not specified, a default set of output is displayed. The **PRINT** and **PALL** options add to the default output, while the **PSHORT** and **PSUMMARY** options reduce from the default output.

Note also that the **PCOVES**, **PDETERM**, and **PRIMAT** options cannot be turned on by any global display options. They must be specified individually.

The following global display options are for controlling formats and order of the output:

Option	Description
NOORDERSPEC	Displays model specifications and results according to the input order
NOPARMNAME	Suppresses the printing of parameter names in results
ORDERALL	Orders all output displays according to the model numbers, group numbers, and parameter types
ORDERGROUPS	Orders the group output displays according to the group numbers
ORDERMODELS	Orders the model output displays according to the model numbers
ORDERSPEC	Orders the model output displays according to the parameter types within each model
PARMNAME	Displays parameter names in model specifications and results
PRIMAT	Displays estimation results in matrix form

Optimization Options

You can use the following options to control the behavior of the optimization. Most of these options are also available in the `NLOPTIONS` statement.

Option	Description
<code>ASINGULAR=</code>	Specifies the absolute singularity criterion for inverting the information matrix
<code>COVSING=</code>	Specifies the singularity tolerance of the information matrix
<code>FCONV=</code>	Specifies the relative function convergence criterion
<code>GCONV=</code>	Specifies the gradient convergence criterion
<code>INSTEP=</code>	Specifies the initial step length (<code>RADIUS=</code> , <code>SALPHA=</code>)
<code>LINESEARCH=</code>	Specifies the line-search method
<code>LSPRECISION=</code>	Specifies the line-search precision (<code>SPRECISION=</code>)
<code>MAXFUNC=</code>	Specifies the maximum number of function calls
<code>MAXITER=</code>	Specifies the maximum number of iterations
<code>MSINGULAR=</code>	Specifies the relative M singularity of the information matrix
<code>OMETHOD TECHNIQUE=</code>	Specifies the minimization method
<code>ROBITER=</code>	Specifies the maximum number of iterations for estimating robust covariance and mean matrices
<code>SINGULAR=</code>	Specifies the singularity criterion for matrix inversion
<code>UPDATE=</code>	Specifies the update method for some optimization techniques
<code>VSINGULAR=</code>	Specifies the relative V singularity of information matrix
<code>XCONV=</code>	Specifies the relative parameter convergence criterion

PROC CALIS Statement Options

ALPHAECV= α

specifies a $(1 - \alpha)100\%$ confidence interval ($0 \leq \alpha \leq 1$) for the Browne and Cudeck (1993) expected cross-validation index (ECVI). The default value is $\alpha = 0.1$, which corresponds to a 90% confidence interval for the ECVI.

ALPHALEV | ALPHALEVERAGE= α

specifies the α -level criterion for detecting leverage observations (or leverage points) in case-level (observation-level) residual diagnostics. The default `ALPHALEV=` value is 0.01. An observation is a leverage observation if the p -value of its squared Mahalanobis distance (M-distance) for its predictor variables (including observed and latent variables) is smaller than the specified α -level, where the p -value is computed according to an appropriate theoretical chi-square distribution. The larger the `ALPHALEV=` value, the more liberal the criterion for detecting leverage observations.

In addition to displaying the leverage observations as defined by the `ALPHALEV=` criterion, PROC CALIS also displays the next 5 observations with the largest leverage M-distances for reference. However, the total number of observations in the displayed output cannot exceed 30 or the number of original observations, whichever is smaller.

This option is relevant only when residual analysis is requested with the `RESIDUAL` option and with raw data input.

ALPHAOUT | ALPHAOUTLIER= α

specifies the α -level criterion for detecting outliers in case-level (observation-level) residual diagnostics. The default ALPHAOUT= value is 0.01. An observation is an outlier if the p -value of its squared residual M-distance is smaller than the specified α -level, where the p -value is computed according to an appropriate theoretical chi-square distribution. The larger the ALPHAOUT= value, the more liberal the criterion for detecting outliers.

In addition to displaying the outliers as defined by the ALPHAOUT= criterion, PROC CALIS also displays the next 5 observations with the largest residual M-distances for reference. However, the total number of observations in the displayed output in the displayed output cannot exceed 30 or the number of original observations, whichever is smaller.

This option is relevant only when residual analysis is requested with the **RESIDUAL** option and with raw data input.

ALPHARMS | ALPHARMSEA= α

specifies a $(1 - \alpha)100\%$ confidence interval ($0 \leq \alpha \leq 1$) for the Steiger and Lind (1980) root mean square error of approximation (RMSEA) coefficient (see Browne and Du Toit 1992). The default value is $\alpha = 0.1$, which corresponds to a 90% confidence interval for the RMSEA.

ASINGULAR | ASING= r

specifies an absolute singularity criterion r ($r > 0$), for the inversion of the information matrix, which is needed to compute the covariance matrix. The default value for r or ASING= is the square root of the smallest positive double precision value.

When inverting the information matrix, the following singularity criterion is used for the diagonal pivot $d_{j,j}$ of the matrix:

$$|d_{j,j}| \leq \max(\text{ASING}, \text{VSING} * |H_{j,j}|, \text{MSING} * \max(|H_{1,1}|, \dots, |H_{n,n}|))$$

where *VSING* and *MSING* are the specified values in the **VSINGULAR=** and **MSINGULAR=** options, respectively, and $H_{j,j}$ is the j th diagonal element of the information matrix. Note that in many cases a normalized matrix $\mathbf{D}^{-1}\mathbf{H}\mathbf{D}^{-1}$ is decomposed (where $\mathbf{D}^2 = \text{diag}(\mathbf{H})$), and the singularity criteria are modified correspondingly.

ASYCOV | ASC=*name*

specifies the formula for asymptotic covariances used in the weight matrix **W** for WLS and DWLS estimation. The ASYCOV option is effective only if **METHOD=** WLS or **METHOD=** DWLS and no **INWGT=** input data set is specified. The following formulas are implemented:

- BIASED:** Browne (1984) formula (3.4)
biased asymptotic covariance estimates; the resulting weight matrix is at least positive semidefinite. This is the default for analyzing a covariance matrix.
- UNBIASED:** Browne (1984) formula (3.8)
asymptotic covariance estimates corrected for bias; the resulting weight matrix can be indefinite (that is, can have negative eigenvalues), especially for small N .
- CORR:** Browne and Shapiro (1986) formula (3.2)
(identical to DeLeeuw (1983) formulas (2,3,4)) the asymptotic variances of the diagonal elements are set to the reciprocal of the value r specified by the **WPENALTY=** option (default: $r=100$). This formula is the default for analyzing a correlation matrix.

By default, `AYSCOV=BIASED` is used for covariance analyses and `ASYCOV=CORR` is used for correlation analyses. Therefore, in almost all cases you do not need to set the `ASYCOV=` option once you specify the covariance or correlation analysis by the `COV` or `CORR` option.

BASEFIT | INBASEFIT=SAS-data-set

inputs the *SAS-data-set* that contains the fit information of the baseline model of your choice. This customized baseline model replaces the default uncorrelatedness model for computing several fit indices of your target model. Typically, you create the `BASEFIT=` data set by using the `OUTFIT=` option in a previous PROC CALIS fitting of your customized baseline model. Using the `BASEFIT=` option assumes that you fit your customized baseline model and your target model with the same data, number of groups (for multiple-group analysis), and estimation method. Typically, your baseline model should be more restrictive (or have fewer parameters) than your target model.

For example, the following statements use the compound symmetry model (`COVPATTERN=COMPSYM`) as the customized baseline model for the subsequent factor model with two factors:

```
proc calis data=abc outfit=outf method=glis covpattern=compsym;
    var=x1-x10;
run;

proc calis data=abc method=glis basefit=outf;
    factor n=2;
    var=x1-x10;
run;
```

The fit information of the customized baseline model is saved as an `OUTFIT=` data set called `outf`, which is then read as a `BASEFIT=` data set in the next PROC CALIS run for fitting the target factor model. Notice that in this example the baseline model and the target factor model use the same data set, `abc`, and the same GLS estimation method.

Alternatively, you can use the `BASEFUNC=` option to input the function value and the degrees of freedom of your customized baseline model. See the `BASEFUNC=` option for details. The `BASEFIT=` option is ignored if you also specify the `BASEFUNC=` option.

Notice that the fit information in the `BASEFIT=` data set does not affect the computation of all fit indices. Mainly, it affects the incremental fit indices, because these indices are defined as the incremental fit of a target model over a baseline model. Among all absolute and parsimonious fit indices, only the parsimonious goodness-of-fit (PGFI) index (Mulaik et al. 1989) is affected by the input fit information provided in the `BASEFIT=` data set.

If you specify `METHOD=LSDWLS`, `LSFIML`, `LSGLS`, or `LSML` for your target model, the fit information in the `BASEFIT=` data set is assumed to have been obtained from the DWLS, FIML, GLS, or ML estimation of your customized baseline model. Hence, the fit information in the `BASEFIT=` data set applies only to the second estimation of your target model. The unweighted least squares (ULS) estimation of the target model still uses the uncorrelatedness model as the baseline model for computing fit indices.

If you use a `BASEFIT=` data set to input the fit information of your customized baseline model in a multiple-group analysis, then the baseline model function values, chi-squares, and degrees of freedom for individual groups are not known and hence not displayed in the multiple-group fit summary table. The Bentler-Bonett normed fit index (NFI) is also not displayed in the multiple-group fit summary

table, because the baseline model function values for individual groups are not saved in the BASEFIT= data set.

BASEFUNC= r ($< DF = > i$)

BASEFUNC($< DF = > i$)= r

inputs the fit function value r and the degrees of freedom i of the baseline model of your choice. This customized baseline model replaces the default uncorrelatedness model for computing several fit indices of your target model. To use this option, you must first fit your customized baseline model and then use this option to input the baseline model fit information when you fit your target model.

Using the BASEFUNC= option assumes that you fit your customized baseline model and your target model with the same data, number of groups (for multiple-group analysis), and estimation method. Typically, your baseline model should be more restrictive (or have fewer parameters) than your target model.

For example, assume that after fitting a customized baseline model you find that the function value of the baseline model is 20.54 and the model degrees of freedom are 15. The following code inputs the function value and the degrees of freedom of the customized baseline model by using the BASEFUNC= option:

```
proc calis data=abc basefunc(df=15)=20.54;
  path
    f1 ==> x1-x5 = 1.,
    f2 ==> x6-x10 = 1.,
    f1 ==> f2;
run;
```

You can use the following equivalent syntax to provide the same baseline model fit information:

```
basefunc(df=15)=20.54
basefunc(15)=20.54
basefunc=20.54(df=15)
basefunc=20.54(15)
```

It is emphasized here that you should input the fit function value, but not the model fit chi-square value, of the baseline model in the BASEFUNC= option. For all estimation methods except the full information maximum likelihood (FIML) method in PROC CALIS, the model fit chi-square values are some multiples of the fit function values. See the section “[Estimation Criteria](#)” on page 1309 for the definitions of the various fit functions that are assumed by the BASEFUNC= option.

Alternatively, it might be easier to use the BASEFIT= option to specify the SAS data set that contains the baseline model fit information. Such a SAS data set is typically created by using the [OUTFIT=](#) option in the PROC CALIS fitting of your customized baseline model. See the [BASEFIT=](#) option for details. However, the BASEFIT= option is ignored if you also specify the BASEFUNC= option.

Notice that the specified values in the BASEFUNC= option do not affect the computation of all fit indices. Mainly, they affect the incremental fit indices, because these indices are defined as the incremental fit of a target model over a baseline model. Among all absolute and parsimonious fit indices, only the parsimonious goodness-of-fit (PGFI) index (Mulaik et al. 1989) is affected by the values provided in the BASEFUNC= option.

If you specify **METHOD=LSDWLS**, **LSFIML**, **LSGLS**, or **LSML** for your target model, the fit information provided by the **BASEFUNC=** option is assumed to have been obtained from the **DWLS**, **FIML**, **GLS**, or **ML** estimation of your customized baseline model. Hence, the fit information provided by the **BASEFUNC=** option applies only to the second estimation of your target model. The unweighted least squares (**ULS**) estimation of the target model still uses the uncorrelatedness model as the baseline model for computing fit indices.

If you use the **BASEFUNC=** option to input the fit information of your customized baseline model in a multiple-group analysis, then the baseline model function values, chi-squares, and degrees of freedom for individual groups are not known and hence not displayed in the multiple-group fit summary table. The Bentler-Bonett **NFI** is also not displayed in the multiple-group fit summary table, because the baseline model function values for individual groups are not provided with the **BASEFUNC=** option.

BIASKUR

computes univariate skewness and kurtosis by formulas uncorrected for bias.

See the section “[Measures of Multivariate Kurtosis](#)” on page 1349 for more information.

CHICORRECT | **CHICORR=** *name* | *c*

specifies a correction factor *c* for the chi-square statistics for model fit. You can specify a *name* for a built-in correction factor or a value between 0 and 1 as the **CHICORRECT=** value. The model fit chi-square statistic is computed as:

$$\chi^2 = (1 - c)(N - k)F$$

where *N* is the total number of observations, *k* is the number of independent groups, and *F* is the optimized function value. Application of these correction factors requires appropriate specification of the covariance structural model suitable for the chi-square correction. For example, using **CHICORRECT=UNCORR** assumes that you are fitting a covariance structure with free parameters on the diagonal elements and fixed zeros off-diagonal elements of the covariance matrix. Because all the built-in correction factors assume multivariate normality in their derivations, the appropriateness of applying these built-in chi-square corrections to estimation methods other than **METHOD=ML** is not known.

Valid *names* for the **CHICORRECT=** value are as follows:

COMPSYM | **EQVARCOV** specifies the correction factor due to Box (1949) for testing equal variances and equal covariances in a covariance matrix. The correction factor is:

$$c = \frac{p(p + 1)^2(2p - 3)}{6n(p - 1)(p^2 + p - 4)}$$

where *p* (*p* > 1) represents the number of variables and *n* = (*N* - 1), with *N* denoting the number of observations in a single group analysis. This option is not applied when you also analyze the mean structures or when you fit multiple-group models.

EQCOVMAT specifies the correction factor due to Box (1949) for testing equality of covariance matrices. The correction factor is:

$$c = \frac{2p^2 + 3p - 1}{6(p + 1)(k - 1)} \left(\sum_{i=1}^k \frac{1}{n_i} - \frac{1}{\sum_{i=1}^k n_i} \right)$$

where p represents the number of variables, k ($k > 1$) represents the number of groups, and $n_i = (N_i - 1)$, with N_i denoting the number of observations in the i th group. This option is not applied when you also analyze the mean structures or when you fit single-group models.

FIXCOV specifies the correction factor due to Bartlett (1954) for testing a covariance matrix against a hypothetical fixed covariance matrix. The correction factor is:

$$c = \frac{1}{6n} \left(2p + 1 - \frac{2}{p + 1} \right)$$

where p represents the number of variables and $n = (N - 1)$, with N denoting the number of observations in a single group analysis. This option is not applied when you also analyze the mean structures or when you fit multiple-group models.

SPHERICITY specifies the correction factor due to Box (1949) for testing a spherical covariance matrix (Mauchly 1940). The correction factor is:

$$c = \frac{2p^2 + p + 2}{6np}$$

where p represents the number of variables and $n = (N - 1)$, with N denoting the number of observations in a single group analysis. This option is not applied when you also analyze the mean structures or when you fit multiple-group models.

TYPEH specifies the correction factor for testing the H pattern (Huynh and Feldt 1970) directly. The correction factor is:

$$c = \frac{2p^2 - 3p + 3}{6n(p - 1)}$$

where p ($p > 1$) represents the number of variables and $n = (N - 1)$, with N denoting the number of observations in a single group analysis. This option is not applied when you also analyze the mean structures or when you fit multiple-group models.

This correction factor is derived by substituting p with $p - 1$ in the correction formula applied to Mauchly's sphericity test. The reason is that testing the H pattern of p variables is equivalent to testing the sphericity of the $(p - 1)$ orthogonal contrasts of the same set of variables (Huynh and Feldt 1970). See pp. 295–296 of Morrison (1990) for more details.

UNCORR specifies the correction factor due to Bartlett (1950) and Box (1949) for testing a diagonal pattern of a covariance matrix, while the diagonal elements (variances) are unconstrained. This test is sometimes called Bartlett's test of sphericity—not to be confused with the sphericity test due to Mauchly (1940), which requires all variances in the covariance matrix to be equal. The correction factor is:

$$c = \frac{2p + 5}{6n}$$

where p represents the number of variables and $n = (N - 1)$, with N denoting the number of observations in a single group analysis. This option is not applied when you also analyze the mean structures or when you fit multiple-group models.

CLOSEFIT=*p*

defines the criterion value p for indicating a close fit. The smaller the better fit. The default value for close fit is .05.

CORRELATION | CORR

analyzes the correlation matrix, instead of the default covariance matrix. See the [COVARIANCE](#) option for more details.

COVARIANCE | COV

analyzes the covariance matrix. Because this is also the default analysis in PROC CALIS, you can simply omit this option when you analyze covariance rather than correlation matrices. If the [DATA=](#) input data set is a [TYPE=CORR](#) data set (containing a correlation matrix and standard deviations), the default COV option means that the covariance matrix is computed and analyzed.

Unlike many other SAS/STAT procedures (for example, the FACTOR procedure) that analyze correlation matrices by default, PROC CALIS uses a different default because statistical theories of structural equation modeling or covariance structure analysis are mostly developed for covariance matrices. You must use the [CORR](#) option if correlation matrices are analyzed.

COVPATTERN | COVPAT=*name*

specifies one of the built-in covariance structures for the data. The purpose of this option is to fit some commonly-used direct covariance structures efficiently without the explicit use of the MSTRUCT model specifications. With this option, the covariance structures are defined internally in PROC CALIS. The following *names* for the built-in covariance structures are supported:

COMPSYM | EQVARCOV specifies the compound symmetry pattern for the covariance matrix. That is, a covariance matrix with equal variances for all variables and equal covariance between any pairs of variables (EQVARCOV). PROC CALIS names the common variance parameter `_varparm` and the common covariance parameter `_covparm`. For example, if there are four variables in the analysis, the covariance pattern generated by PROC CALIS is:

$$\Sigma = \begin{pmatrix} _varparm & _covparm & _covparm & _covparm \\ _covparm & _varparm & _covparm & _covparm \\ _covparm & _covparm & _varparm & _covparm \\ _covparm & _covparm & _covparm & _varparm \end{pmatrix}$$

If you request a single-group maximum likelihood (METHOD=ML) covariance structure analysis by specifying the COVPATTERN=COMPSYM or COVPATTERN=EQVARCOV option and the mean structures are not modeled, the chi-square correction due to Box (1949) is applied automatically when the number of variables is greater than or equal to 2. See the [CHICORRECT=COMPSYM](#) option for the definition of the correction factor.

EQCOVMAT

specifies the equality of covariance matrices between multiple groups. That is, this option tests the null hypothesis that

$$H_0 : \Sigma_1 = \Sigma_2 = \dots = \Sigma_k = \Sigma$$

where Σ is a common covariance matrix for the k Σ_j 's ($j = 1, \dots, k; k > 1$). The elements of Σ are named `_cov_xx_yy` automatically by PROC CALIS, where

xx represents the row number and yy represents the column number. For example, if there are four variables in the analysis, the common Σ is defined as

$$\Sigma = \begin{pmatrix} _cov_1_1 & _cov_1_2 & _cov_1_3 & _cov_1_4 \\ _cov_2_1 & _cov_2_2 & _cov_2_3 & _cov_2_4 \\ _cov_3_1 & _cov_3_2 & _cov_3_3 & _cov_3_4 \\ _cov_4_1 & _cov_4_2 & _cov_4_3 & _cov_4_4 \end{pmatrix}$$

If you request a multiple-group maximum likelihood (METHOD=ML) covariance structure analysis by specifying the COVPATTERN=EQCOVMAT and the mean structures are not modeled, the chi-square correction due to Box (1949) is applied automatically. See the CHICORRECT=EQCOVMAT option for the definition of the correction factor.

SATURATED

specifies a saturated covariance structure model. This is the default option when you specify the MEANPATTERN= option without using the COVPATTERN= option. The elements of Σ are named $_cov_xx_yy$ automatically by PROC CALIS, where xx represents the row number and yy represents the column number. For example, if there are three variables in the analysis, Σ is defined as

$$\Sigma = \begin{pmatrix} _cov_1_1 & _cov_1_2 & _cov_1_3 \\ _cov_2_1 & _cov_2_2 & _cov_2_3 \\ _cov_3_1 & _cov_3_2 & _cov_3_3 \end{pmatrix}$$

SPHERICITY | SIGSQI specifies the spheric pattern of the covariance matrix (Mauchly 1940). That is, this option tests the null hypothesis that

$$H_0 : \Sigma = \sigma^2 \mathbf{I}$$

where σ^2 is a common variance parameter and \mathbf{I} is an identity matrix. PROC CALIS names the common variance parameter $_varparm$. For example, if there are three variables in the analysis, the covariance pattern generated by PROC CALIS is:

$$\Sigma = \begin{pmatrix} _varparm & 0 & 0 \\ 0 & _varparm & 0 \\ 0 & 0 & _varparm \end{pmatrix}$$

If you request a single-group maximum likelihood (METHOD=ML) covariance structure analysis by specifying the COVPATTERN=SPHERICITY or COVPATTERN=SIGSQI option and the mean structures are not modeled, the chi-square correction due to Box (1949) is applied automatically. See the CHICORRECT=SPHERICITY option for the definition of the correction factor.

UNCORR | DIAG

specifies the diagonal pattern of the covariance matrix. That is, this option tests the null hypothesis of uncorrelatedness—all correlations (or covariances) between variables are zero and the variances are unconstrained. PROC CALIS names the variance parameters $_varparm_xx$, where xx represents the row or column number. For example, if there are three variables in the analysis, the covariance pattern generated by PROC CALIS is:

$$\Sigma = \begin{pmatrix} _varparm_1 & 0 & 0 \\ 0 & _varparm_2 & 0 \\ 0 & 0 & _varparm_3 \end{pmatrix}$$

If you request a single-group maximum likelihood (METHOD=ML) covariance structure analysis by specifying the COVPATTERN=UNCORR or COVPATTERN=DIAG option and the mean structures are not modeled, the chi-square correction due to Bartlett (1950) is applied automatically. See the [CHICORRECT=UNCORR](#) option for the definition of the correction factor. Under the multivariate normal assumption, COVPATTERN=UNCORR is also a test of independence of the variables in the analysis.

When you specify the covariance structure model by means of the COVPATTERN= option, you can define the set of variables in the analysis by the [VAR](#) statement (either within the scope of the PROC CALIS statement or the [GROUP](#) statements). If the VAR statement is not used, PROC CALIS uses all numerical variables in the data sets.

Except for the EQCOVMAT pattern, all other built-in covariance patterns are primarily designed for single-group analysis. However, you can still use these covariance pattern options for multiple-group situations. For example, consider the following three-group analysis:

```
proc calis covpattern=compsym;
  group 1 / data=set1;
  group 2 / data=set2;
  group 3 / data=set3;
run;
```

In this specification, all three groups are fitted by the compound symmetry pattern. However, there would be no constraints across these groups. PROC CALIS generates two distinct parameters for each group: `_varparm_md1` and `_covparm_md1` for Group 1, `_varparm_md2` and `_covparm_md2` for Group 2, and `_varparm_md3` and `_covparm_md3` for Group 3. Similarly, the `_mdlxx` suffix, where `xx` represents the model number, is applied to the parameters defined by the SATURATED, SPHERICITY (or SIGSQI), and UNCORR (or DIAG) covariance patterns in multiple-group situations. However, chi-square correction, whenever it is applicable to single-group analysis, is not applied to such multiple-group analyses.

You can also apply the COVPATTERN= option partially to the groups in the analysis. For example, the following statements apply the spheric pattern to Group 1 and Group 2 only:

```
proc calis covpattern=sphericity;
  group 1 / data=set1;
  group 2 / data=set2;
  group 3 / data=set3;
  model 3 / group=3;
  path    x1 ==> y3;
run;
```

Group 3 is fitted by Model 3, which is specified explicitly by a PATH model with distinct covariance structures.

If the EQCOVMAT pattern is specified instead, as shown in the following statements, the equality of covariance matrices still holds for Groups 1 and 2:

```

proc calis covpattern=eqcovmat;
  group 1 / data=set1;
  group 2 / data=set2;
  group 3 / data=set3;
  model 3 / group=3;
  path   x1 ==> y3;
run;

```

However, Group 3 has its own covariance structures as specified in Model 3. In this case, the chi-square correction due to Box (1949) is not applied because the null hypothesis is no longer testing the equality of covariance matrices among the groups in the analysis.

Use the **MEANPATTERN=** option if you also want to analyze some built-in mean structures along with the covariance structures.

COVSING=*r*

specifies a nonnegative threshold r , which determines whether the eigenvalues of the information matrix are considered to be zero. If the inverse of the information matrix is found to be singular (depending on the **VSINGULAR=**, **MSINGULAR=**, **ASINGULAR=**, or **SINGULAR=** option), a generalized inverse is computed using the eigenvalue decomposition of the singular matrix. Those eigenvalues smaller than r are considered to be zero. If a generalized inverse is computed and you do not specify the **NOPRINT** option, the distribution of eigenvalues is displayed.

DATA=SAS-data-set

specifies an input data set that can be an ordinary SAS data set or a specially structured **TYPE=**CORR, **TYPE=**COV, **TYPE=**UCORR, **TYPE=**UCOV, **TYPE=**SSCP, or **TYPE=**FACTOR SAS data set, as described in the section “Input Data Sets” on page 1236. If the **DATA=** option is omitted, the most recently created SAS data set is used.

DEMPHAS | DE=*r*

changes the initial values of all variance parameters by the relationship:

$$s_{new} = r(|s_{old}| + 1)$$

where s_{new} is the new initial value and s_{old} is the original initial value. The initial values of all variance parameters should always be nonnegative to generate positive definite predicted model matrices in the first iteration. By using values of $r > 1$, for example, $r = 2$, $r = 10$, and so on, you can increase these initial values to produce predicted model matrices with high positive eigenvalues in the first iteration. The **DEMPHAS=** option is effective independent of the way the initial values are set; that is, it changes the initial values set in the model specification as well as those set by an **INMODEL=** data set and those automatically generated for the **FACTOR**, **LINEQS**, **LISMOD**, **PATH**, or **RAM** models. It also affects the initial values set by the **START=** option, which uses, by default, **DEMPHAS=100** if a covariance matrix is analyzed and **DEMPHAS=10** for a correlation matrix.

DFREDUCE | DFRED=*i*

reduces the degrees of freedom of the model fit χ^2 test by i . In general, the number of degrees of freedom is the total number of nonredundant elements in all moment matrices minus the number of parameters, t . Because negative values of i are allowed, you can also increase the number of degrees of freedom by using this option.

EDF | DFE=*n*

makes the effective number of observations $n + 1$. You can also use the **NOBS=** option to specify the number of observations.

EFFPART | PARTEFF | TOTEFF | TE

computes and displays total, direct, and indirect effects for the unstandardized and standardized estimation results. Standard errors for the effects are also computed. Note that this displayed output is not automatically included in the output generated by the **PALL** option.

Note also that in some situations computations of total effects and their partitioning are not appropriate. While total and indirect effects must converge in recursive models (models with no cyclic paths among variables), they do not always converge in nonrecursive models. When total or indirect effects do not converge, it is not appropriate to partition the effects. Therefore, before partitioning the total effects, the convergence criterion must be met. To check the convergence of the effects, PROC CALIS computes and displays the “stability coefficient of reciprocal causation”—that is, the largest modulus of the eigenvalues of the β matrix, which is the square matrix that contains the path coefficients of all endogenous variables in the model. Stability coefficients less than one provide a necessary and sufficient condition for the convergence of the total and the indirect effects. Otherwise, PROC CALIS does not show results for total effects and their partitioning. See the section “[Stability Coefficient of Reciprocal Causation](#)” on page 1345 for more information about the computation of the stability coefficient.

EXTENDPATH | GENPATH

displays the extended path estimates such as the variances, covariances, means, and intercepts in the table that contains the ordinary path effect (coefficient) estimates. This option applies to the PATH model only.

FCONV | FTOL=*r*

specifies the relative function convergence criterion. The optimization process is terminated when the relative difference of the function values of two consecutive iterations is smaller than the specified value of r ; that is,

$$\frac{|f(x^{(k)}) - f(x^{(k-1)})|}{\max(|f(x^{(k-1)})|, FSIZE)} \leq r$$

where $FSIZE$ can be defined by the **FSIZE=** option in the **NLOPTIONS** statement. The default value is $r = 10^{-FDIGITS}$, where $FDIGITS$ either can be specified in the **NLOPTIONS** statement or is set by default to $-\log_{10}(\epsilon)$, where ϵ is the machine precision.

G4=*i*

instructs that the algorithm to compute the approximate covariance matrix of parameter estimates used for computing the approximate standard errors and modification indices when the information matrix is singular. If the number of parameters t used in the model you analyze is smaller than the value of i , the time-expensive Moore-Penrose (G4) inverse of the singular information matrix is computed by eigenvalue decomposition. Otherwise, an inexpensive pseudo (G1) inverse is computed by sweeping. By default, $i = 60$.

See the section “[Estimation Criteria](#)” on page 1309 for more details.

GCONV | GTOL=*r*

specifies the relative gradient convergence criterion.

Termination of all techniques (except the CONGRA technique) requires the following normalized predicted function reduction to be smaller than *r*. That is,

$$\frac{[g(x^{(k)})]'[\mathbf{G}^{(k)}]^{-1}g(x^{(k)})}{\max(|f(x^{(k)})|, FSIZE)} \leq r$$

where *FSIZE* can be defined by the *FSIZE=* option in the **NLOPTIONS** statement. For the CONGRA technique (where a reliable Hessian estimate **G** is not available),

$$\frac{\|g(x^{(k)})\|_2^2 \|s(x^{(k)})\|_2}{\|g(x^{(k)}) - g(x^{(k-1)})\|_2 \max(|f(x^{(k)})|, FSIZE)} \leq r$$

is used. The default value is $r = 10^{-8}$.

INEST | INVAR | ESTDATA=*SAS-data-set*

specifies an input data set that contains initial estimates for the parameters used in the optimization process and can also contain boundary and general linear constraints on the parameters. Typical applications of this option are to specify an **OUTEST=** data set from a previous PROC CALIS analysis. The initial estimates are taken from the values of the **PARMS** observation in the **INEST=** data set.

INMODEL | INRAM=*SAS-data-set*

specifies an input data set that contains information about the analysis model. A typical use of the **INMODEL=** option is when you run an analysis with its model specifications saved as an **OUTMODEL=** data set from a previous PROC CALIS run. Instead of specifying the **main** or **subsidiary** model specification statements in the new run, you use the **INMODEL=** option to input the model specification saved from the previous run.

Sometimes, you might create an **INMODEL=** data set from modifying an existing **OUTMODEL=** data set. However, editing and modifying **OUTMODEL=** data sets requires good understanding of the formats and contents of the **OUTMODEL=** data sets. This process could be error-prone for novice users. For details about the format of **INMODEL=** or **OUTMODEL=** data sets, see the section “**Input Data Sets**” on page 1236.

It is important to realize that **INMODEL=** or **OUTMODEL=** data sets contain only the information about the specification of the model. These data sets do not store any information about the bounds on parameters, linear and nonlinear parametric constraints, and programming statements for computing dependent parameters. If required, these types of information must be provided in the corresponding statement specifications (for example, **BOUNDS**, **LINCON**, and so on) in addition to the **INMODEL=** data set.

An **OUTMODEL=** data set might also contain default parameters added automatically by PROC CALIS from a previous run (for example, observations with **_TYPE_=ADDP**COV, **ADDMEAN**, or **ADDP**VAR). When reading the **OUTMODEL=** model specification as an **INMODEL=** data set in a new run, PROC CALIS ignores these added parameters so that the model being read is exactly like the previous PROC CALIS specification (that is, before default parameters were added automatically). After interpreting the specification in the **INMODEL=** data set, PROC CALIS will then add default parameters appropriate to the new run. The purpose of doing this is to avoid inadvertent parameter constraints in the new run, where another set of automatic default parameters might have the same generated names as those of the generated parameter names in the **INMODEL=** data set.

If you want the default parameters in the INMODEL= data set to be read as a part of model specification, you must also specify the [READADDPARM](#) option. However, using the [READADDPARM](#) option should be rare.

INSTEP=*r*

For highly nonlinear objective functions, such as the EXP function, the default initial radius of the trust-region algorithms (TRUREG, DBLDOG, and LEVMAR) or the default step length of the line-search algorithms can produce arithmetic overflows. If an arithmetic overflow occurs, specify decreasing values of $0 < r < 1$ such as INSTEP=1E-1, INSTEP=1E-2, INSTEP=1E-4, and so on, until the iteration starts successfully.

- For trust-region algorithms (TRUREG, DBLDOG, and LEVMAR), the INSTEP option specifies a positive factor for the initial radius of the trust region. The default initial trust-region radius is the length of the scaled gradient, and it corresponds to the default radius factor of $r = 1$.
- For line-search algorithms (NEWRAP, CONGRA, and QUANEW), INSTEP specifies an upper bound for the initial step length for the line search during the first five iterations. The default initial step length is $r = 1$.

For more details, see the section “[Computational Problems](#)” on page 1360.

INWGT | INWEIGHT<(INV)>=*SAS-data-set*

specifies an input data set that contains the weight matrix **W** used in generalized least squares (GLS), weighted least squares (WLS, ADF), or diagonally weighted least squares (DWLS) estimation, if you do not specify the INV option at the same time. The weight matrix must be positive definite because its inverse must be defined in the computation of the objective function. If the weight matrix **W** defined by an INWGT= data set is not positive definite, it can be ridged using the [WRIDGE=](#) option. See the section “[Estimation Criteria](#)” on page 1309 for more information. If you specify the INWGT(INV)= option, the INWGT= data set contains the inverse of the weight matrix, rather than the weight matrix itself. Specifying the INWGT(INV)= option is equivalent to specifying the INWGT= and [INWGTINV](#) options simultaneously. With the INWGT(INV)= specification, the input matrix is not required to be positive definite. See the [INWGTINV](#) option for more details. If no INWGT= data set is specified, default settings for the weight matrices are used in the estimation process. The INWGT= data set is described in the section “[Input Data Sets](#)” on page 1236. Typically, this input data set is an [OUTWGT=](#) data set from a previous PROC CALIS analysis.

INWGTINV

specifies that the INWGT= data set contains the inverse of the weight matrix, rather than the weight matrix itself. This option is effective only with an input weight matrix specified in the [INWGT=](#) data set and with the generalized least squares (GLS), weighted least squares (WLS or ADF), or diagonally weighted least squares (DWLS) estimation. With this option, the input matrix provided in the INWGT= data set is not required to be positive definite. Also, the ridging requested by the [WRIDGE=](#) option is ignored when you specify the INWGTINV option.

KURTOSIS | KU

computes and displays univariate kurtosis and skewness, various coefficients of multivariate kurtosis, and the numbers of observations that contribute most to the normalized multivariate kurtosis. See the section “[Measures of Multivariate Kurtosis](#)” on page 1349 for more information. Using the KURTOSIS option implies the [SIMPLE](#) display option. This information is computed only if the [DATA=](#) data set is a raw data set, and it is displayed by default if the [PRINT](#) option is specified. The

multivariate least squares kappa and the multivariate mean kappa are displayed only if you specify **METHOD=WLS** and the weight matrix is computed from an input raw data set. All measures of skewness and kurtosis are corrected for the mean. Using the **BIASKUR** option displays the biased values of univariate skewness and kurtosis.

LINESEARCH | LIS | SMETHOD | SM=*i*

specifies the line-search method for the CONGRA, QUANEW, and NEWRAP optimization techniques. See Fletcher (1980) for an introduction to line-search techniques. The value of *i* can be any integer between 1 and 8, inclusively; the default is *i*=2.

LIS=1 specifies a line-search method that needs the same number of function and gradient calls for cubic interpolation and cubic extrapolation; this method is similar to one used by the Harwell subroutine library.

LIS=2 specifies a line-search method that needs more function calls than gradient calls for quadratic and cubic interpolation and cubic extrapolation; this method is implemented as shown in Fletcher (1987) and can be modified to an exact line search by using the **LSPRECISION=** option.

LIS=3 specifies a line-search method that needs the same number of function and gradient calls for cubic interpolation and cubic extrapolation; this method is implemented as shown in Fletcher (1987) and can be modified to an exact line search by using the **LSPRECISION=** option.

LIS=4 specifies a line-search method that needs the same number of function and gradient calls for stepwise extrapolation and cubic interpolation.

LIS=5 specifies a line-search method that is a modified version of LIS=4.

LSPRECISION | LSP=*r*

SPRECISION | SP=*r*

specifies the degree of accuracy that should be obtained by the line-search algorithms **LIS=2** and **LIS=3**. Usually an imprecise line search is inexpensive and successful. For more difficult optimization problems, a more precise and more expensive line search might be necessary (Fletcher 1980, p. 22). The second (default for NEWRAP, QUANEW, and CONGRA) and third line-search methods approach exact line search for small **LSPRECISION=** values. If you have numerical problems, you should decrease the **LSPRECISION=** value to obtain a more precise line search. The default **LSPRECISION=** values are displayed in the following table.

OMETHOD=	UPDATE=	LSP default
QUANEW	DBFGS, BFGS	<i>r</i> = 0.4
QUANEW	DDFP, DFP	<i>r</i> = 0.06
CONGRA	all	<i>r</i> = 0.1
NEWRAP	no update	<i>r</i> = 0.9

For more details, see Fletcher (1980, pp. 25–29).

MAXFUNC | MAXFU=*i*

specifies the maximum number *i* of function calls in the optimization process. The default values are displayed in the following table.

OMETHOD=	MAXFUNC default
LEVMAR, NEWRAP, NRRIDG, TRUREG	$i = 125$
DBLDOG, QUANEW	$i = 500$
CONGRA	$i = 1000$

The default is used if you specify `MAXFUNC=0`. The optimization can be terminated only after completing a full iteration. Therefore, the number of function calls that is actually performed can exceed the number that is specified by the `MAXFUNC=` option.

MAXITER | MAXIT= $i < n$ >

specifies the maximum number i of iterations in the optimization process. Except for the iteratively reweighted least squares (IRLS) algorithm for the robust estimation of model parameters, the default values are displayed in the following table.

OMETHOD=	MAXITER default
LEVMAR, NEWRAP, NRRIDG, TRUREG	$i = 50$
DBLDOG, QUANEW	$i = 200$
CONGRA	$i = 400$

The default maximum number of iterations for IRLS is 5000. The default value is used if you specify `MAXITER=0` or if you omit the `MAXITER` option.

The optional second value n is valid only for `OMETHOD=QUANEW` with nonlinear constraints. It specifies an upper bound n for the number of iterations of an algorithm and reduces the violation of nonlinear constraints at a starting point. The default is $n = 20$. For example, specifying

```
maxiter= . 0
```

means that you do not want to exceed the default number of iterations during the main optimization process and that you want to suppress the feasible point algorithm for nonlinear constraints.

MAXMISSPAT= n

specifies the maximum number of missing patterns to display in the output, where n is between 1 and 9,999. The default `MAXMISSPAT=` value is 10 or the number of missing patterns in the data, whichever is smaller. The number of missing patterns to display cannot exceed this `MAXMISSPAT=` value. This option is relevant only when there are incomplete observations (with some missing values in the analysis variables) in the input raw data set and when you use `METHOD=FIML` or `METHOD=LSFIML` for estimation.

Because the number of missing patterns could be quite large, PROC CALIS displays a limited number of the most frequent missing patterns in the output. The `MAXMISSPAT=` and the `TMISSPAT=` options are used in determining the number of missing patterns to display. The missing patterns are ordered according to the data proportions they account for, from the largest to the smallest. PROC CALIS displays a minimum number of the highest-frequency missing patterns. This minimum number is the smallest among five, the actual number of missing patterns, and the `MAXMISSPAT=` value. Then, PROC CALIS displays the subsequent high-frequency missing patterns if the data proportion accounted for by each of these patterns is at least as large as the proportion threshold set by the `TMISSPAT=` value (default at 0.05) until the total number of missing patterns displayed reaches the maximum set by the `MAXMISSPAT=` option.

MEANPATTERN | MEANPAT=*name*

specifies one of the built-in mean structures for the data. The purpose of this option is to fit some commonly-used direct mean structures efficiently without the explicit use of the MSTRUCT model specifications. With this option, the mean structures are defined internally in PROC CALIS. The following *names* for the built-in mean structures are supported:

EQMEANVEC specifies the equality of mean vectors between multiple groups. That is, this option tests the null hypothesis that

$$H_0 : \mu_1 = \mu_2 = \dots = \mu_k = \mu$$

where μ is a common mean vector for the k μ_j 's ($j = 1, \dots, k$). The elements of μ are named `_mean_xx` automatically by PROC CALIS, where `xx` represents the row number. For example, if there are four variables in the analysis, the common μ is defined as

$$\mu = \begin{pmatrix} \text{_mean_1} \\ \text{_mean_2} \\ \text{_mean_3} \\ \text{_mean_4} \end{pmatrix}$$

If you use the `COVPATTERN=EQCOVMAT` and `MEANPATTERN=EQMEANVEC` together in a maximum likelihood (METHOD=ML) analysis, you are testing a null hypothesis of the same multivariate normal distribution for the groups.

If you use the `MEANPATTERN=EQMEANVEC` option for a single-group analysis, the parameters for the single group are still created accordingly. However, the mean model for the single group contains only unconstrained parameters that would result in saturated mean structures for the model.

SATURATED specifies a saturated mean structure model. This is the default mean structure pattern when the covariance structures are specified by the `COVPATTERN=` pattern and the mean structure analysis is invoked by `MEANSTR` option. The elements of μ are named `_mean_xx` automatically by PROC CALIS, where `xx` represents the row number. For example, if there are three variables in the analysis, μ is defined as

$$\mu = \begin{pmatrix} \text{_mean_1} \\ \text{_mean_2} \\ \text{_mean_3} \end{pmatrix}$$

UNIFORM specifies a mean vector with a uniform mean parameter `_meanparm`. For example, if there are three variables in the analysis, the mean pattern generated by PROC CALIS is

$$\mu = \begin{pmatrix} \text{_meanparm} \\ \text{_meanparm} \\ \text{_meanparm} \end{pmatrix}$$

ZERO specifies a zero vector for the mean structures. For example, if there are four variables in the analysis, the mean pattern generated by PROC CALIS is:

$$\mu = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

When you specify the mean structure model by means of the MEANPATTERN= option, you can define the set of variables in the analysis by the VAR statement (either within the scope of the PROC CALIS statement or the GROUP statements). If the VAR statement is not used, PROC CALIS uses all numerical variables in the data sets.

Except for the EQMEANVEC pattern, all other built-in mean patterns are primarily designed for single-group analysis. However, you can still use these mean pattern options for multiple-group situations. For example, consider the following three-group analysis:

```
proc calis meanpattern=uniform;
  group 1 / data=set1;
  group 2 / data=set2;
  group 3 / data=set3;
run;
```

In this specification, all three groups are fitted by the uniform mean pattern. However, there would be no constraints across these groups. PROC CALIS generates a distinct mean parameter for each group: `_meanparm_md1` for Group 1, `_meanparm_md2` for Group 2, and `_meanparm_md3` for Group 3. Similarly, the `_mdlxx` suffix, where `xx` represents the model number, is applied to the parameters defined by the SATURATED mean pattern in multiple-group situations.

You can also apply the MEANPATTERN= option partially to the groups in the analysis. For example, the following statements apply the ZERO mean pattern to Group 1 and Group 2 only:

```
proc calis meanpattern=zero;
  group 1 / data=set1;
  group 2 / data=set2;
  group 3 / data=set3;
  model 3 / group=3;
  path    x1 ==> y3;
  means  x1 = mean_x1;
run;
```

Group 3 is fitted by Model 3, which is specified explicitly by a PATH model with a distinct mean parameter `mean_x1`.

If the EQMEANVEC pattern is specified instead, as shown in the following statements, the equality of mean vectors still holds for Groups 1 and 2:

```
proc calis meanpattern=eqmeanvec;
  group 1 / data=set1;
  group 2 / data=set2;
  group 3 / data=set3;
  model 3 / group=3;
    path    x1 ==> y3;
    means x1 = mean_x1;
run;
```

However, Group 3 has its own mean structures as specified in Model 3.

Use the `COVPATTERN=` option if you also want to analyze some built-in covariance structures along with the mean structures. If you use the `MEANPATTERN=` option but do not specify the `COVPATTERN=` option, a saturated covariance structure model (that is, `COVPATTERN=SATURATED`) is assumed by default.

MEANSTR

invokes the analysis of mean structures. By default, no mean structures are analyzed. You can specify the `MEANSTR` option in both the `PROC CALIS` and the `MODEL` statements. When this option is specified in the `PROC CALIS` statement, it propagates to all models. When this option is specified in the `MODEL` statement, it applies only to the local model. Except for the `COSAN` model, the `MEANSTR` option adds default mean parameters to the model. For the `COSAN` model, the `MEANSTR` option adds null mean vectors to the model. Instead of using the `MEANSTR` option to analyze the mean structures, you can specify the mean and the intercept parameters explicitly in the model by some model specification statements. That is, you can specify the intercepts in the `LINEQS` statement, the intercepts and means in the `PATH` or the `MEAN` statement, the `_MEAN_` matrix in the `MATRIX` statement, or the mean structure formula in the `COSAN` statement. The explicit mean structure parameter specifications are useful when you need to constrain the mean parameters or to create your own references of the parameters.

METHOD | MET | M=name

specifies the method of parameter estimation. The default is `METHOD=ML`. Valid values for *name* are as follows:

FIML

performs full information maximum-likelihood (FIML) or direct maximum likelihood parameter estimation for data with missing values. This method assumes raw input data sets. When there are no missing values in the analysis, the FIML method yields the same estimates as those by using the regular maximum likelihood (`METHOD=ML`) method with `VARDEF=N`.

Because the FIML method recomputes the mean estimates iteratively during estimation, it must intrinsically analyze the mean structures of models. If you do not specify the `MEANSTR` option or any mean parameters for your models (which is not required for using the FIML method), `PROC CALIS` assumes saturated mean structures for models. However, when computing fit statistics, these saturated mean structures would be ignored as if they were never modeled. If you do specify the `MEANSTR` option

	or any mean parameters for your models, these mean structures would be taken into account when computing fit statistics.
ML M MAX	performs normal-theory maximum-likelihood parameter estimation. The ML method requires a nonsingular covariance or correlation matrix.
GLS G	performs generalized least squares parameter estimation. If no INWGT= data set is specified, the GLS method uses the inverse sample covariance or correlation matrix as the weight matrix W . Therefore, METHOD=GLS requires a nonsingular covariance or correlation matrix.
WLS W ADF	performs weighted least squares parameter estimation. If no INWGT= data set is specified, the WLS method uses the inverse matrix of estimated asymptotic covariances of the sample covariance or correlation matrix as the weight matrix W . In this case, the WLS estimation method is equivalent to Browne's asymptotically distribution-free estimation (Browne 1982, 1984). The WLS method requires a nonsingular weight matrix.
DWLS D	performs diagonally weighted least squares parameter estimation. If no INWGT= data set is specified, the DWLS method uses the inverse diagonal matrix of asymptotic variances of the input sample covariance or correlation matrix as the weight matrix W . The DWLS method requires a nonsingular diagonal weight matrix.
ULS LS U	performs unweighted least squares parameter estimation.
LSFIML	performs unweighted least squares followed by full information maximum-likelihood parameter estimation.
LSML LSM LSMAX	performs unweighted least squares followed by normal-theory maximum-likelihood parameter estimation.
LSGLS LSG	performs unweighted least squares followed by generalized least squares parameter estimation.
LSWLS LSW LSADF	performs unweighted least squares followed by weighted least squares parameter estimation.
LSDWLS LSD	performs unweighted least squares followed by diagonally weighted least squares parameter estimation.
NONE NO	uses no estimation method. This option is suitable for checking the validity of the input information and for displaying the model matrices and initial values.

MODIFICATION | MOD

computes and displays Lagrange multiplier (LM) test indices for constant parameter constraints, equality parameter constraints, and active boundary constraints, as well as univariate and multivariate Wald test indices. The modification indices are not computed in the case of unweighted or diagonally weighted least squares estimation.

The Lagrange multiplier test (Bentler 1986; Lee 1985; Buse 1982) provides an estimate of the χ^2 reduction that results from dropping the constraint. For constant parameter constraints and active boundary constraints, the approximate change of the parameter value is displayed also. You can use this value to obtain an initial value if the parameter is allowed to vary in a modified model. See the section “[Modification Indices](#)” on page 1346 for more information.

Relying solely on the LM tests to modify your model can lead to unreliable models that capitalize purely on sampling errors. See MacCallum, Roznowski, and Necowitz (1992) for the use of LM tests.

MSINGULAR | MSING=*r*

specifies a relative singularity criterion r ($r > 0$) for the inversion of the information matrix, which is needed to compute the covariance matrix. If you do not specify the **SINGULAR=** option, the default value for r or **MSING=** is $1E-12$; otherwise, the default value is $1E-4 \times SING$, where $SING$ is the specified **SINGULAR=** value.

When inverting the information matrix, the following singularity criterion is used for the diagonal pivot $d_{j,j}$ of the matrix:

$$|d_{j,j}| \leq \max(ASING, VSING * |H_{j,j}|, MSING * \max(|H_{1,1}|, \dots, |H_{n,n}|))$$

where $ASING$ and $VSING$ are the specified values of the **ASINGULAR=** and **VSINGULAR=** options, respectively, and $H_{j,j}$ is the j th diagonal element of the information matrix. Note that in many cases a normalized matrix $\mathbf{D}^{-1}\mathbf{H}\mathbf{D}^{-1}$ is decomposed (where $\mathbf{D}^2 = \text{diag}(\mathbf{H})$), and the singularity criteria are modified correspondingly.

NOADJDF

turns off the automatic adjustment of degrees of freedom when there are active constraints in the analysis. When the adjustment is in effect, most fit statistics and the associated probability levels will be affected. This option should be used when you believe that the active constraints observed in the current sample will have little chance to occur in repeated sampling. See the section “Adjustment of Degrees of Freedom” on page 1325 for more discussion on the issue.

NOBS=*nobs*

specifies the number of observations. If the **DATA=** input data set is a raw data set, $nobs$ is defined by default to be the number of observations in the raw data set. The **NOBS=** and **EDF=** options override this default definition. You can use the **RDF=** option to modify the $nobs$ specification. If the **DATA=** input data set contains a covariance, correlation, or scalar product matrix, you can specify the number of observations either by using the **NOBS=**, **EDF=**, and **RDF=** options in the PROC CALIS statement or by including a **_TYPE_='N'** observation in the **DATA=** input data set.

NOINDEXTYPE

disables the display of index types in the fit summary table.

NOMEANSTR

deactivates the inherited **MEANSTR** option for the analysis of mean structures. You can specify the **NOMEANSTR** option in both the PROC CALIS and the **MODEL** statements. When this option is specified in the PROC CALIS statement, it does not have any apparent effect because by default the mean structures are not analyzed. When this option is specified in the MODEL statement, it deactivates the inherited **MEANSTR** option from the PROC CALIS statement. In other words, this option is mainly used for resetting the default behavior in the local model that is specified within the scope of a particular MODEL statement. If you specify both the **MEANSTR** and **NOMEANSTR** options in the same statement, the **NOMEANSTR** option is ignored.

CAUTION: This option does not remove the mean structure specifications from the model. It only deactivates the **MEANSTR** option inherited from the PROC CALIS statement. The mean structures

of the model are analyzed as long as there are mean structure specifications in the model (for example, when you specify the means or intercepts in any of the **main** or **subsidiary** model specification statements).

NOMISSPAT

suppresses the display of the analytic results of the missing patterns. This option is relevant only when there are incomplete observations (with some missing values in the analysis variables) in the input raw data set and when you use **METHOD=FIML** or **METHOD=LSFIML** for estimation.

NOMOD

suppresses the computation of modification indices. The **NOMOD** option is useful in connection with the **PALL** option because it saves computing time.

NOORDERSPEC

prints the model results in the order they appear in the input specifications. This is the default printing behavior. In contrast, the **ORDERSPEC** option arranges the model results by the types of parameters. You can specify the **NOORDERSPEC** option in both the **PROC CALIS** and the **MODEL** statements. When this option is specified in the **PROC CALIS** statement, it does not have any apparent effect because by default the model results display in the same order as that in the input specifications. When this option is specified in the **MODEL** statement, it deactivates the inherited **ORDERSPEC** option from the **PROC CALIS** statement. In other words, this option is mainly used for resetting the default behavior in the local model that is specified within the scope of a particular **MODEL** statement. If you specify both the **ORDERSPEC** and **NOORDERSPEC** options in the same statement, the **NOORDERSPEC** option is ignored.

NOPARMNAME

suppresses the printing of parameter names in the model results. The default is to print the parameter names. You can specify the **NOPARMNAME** option in both the **PROC CALIS** and the **MODEL** statements. When this option is specified in the **PROC CALIS** statement, it propagates to all models. When this option is specified in the **MODEL** statement, it applies only to the local model.

NOPRINT | NOP

suppresses the displayed output. Note that this option temporarily disables the Output Delivery System (ODS). See Chapter 20, “Using the Output Delivery System,” for more information.

NOSTAND

suppresses the printing of standardized results. The default is to print the standardized results.

NOSTDERR | NOSE

suppresses the printing of the standard error estimates. Standard errors are not computed for unweighted least squares (ULS) or diagonally weighted least squares (DWLS) estimation. In general, standard errors are computed even if the **STDERR** display option is not used (for file output). You can specify the **NOSTDERR** option in both the **PROC CALIS** and the **MODEL** statements. When this option is specified in the **PROC CALIS** statement, it propagates to all models. When this option is specified in the **MODEL** statement, it applies only to the local model.

OMETHOD | OM=name

TECHNIQUE | TECH=name

specifies the optimization method or technique. Because there is no single nonlinear optimization algorithm available that is clearly superior (in terms of stability, speed, and memory) for all applications,

different types of optimization methods or techniques are provided in the CALIS procedure. The optimization method or technique is specified by using one of the following *names* in the `OMETHOD=` option:

- CONGRA | CG** chooses one of four different conjugate-gradient optimization algorithms, which can be more precisely defined with the `UPDATE=` option and modified with the `LINESEARCH=` option. The conjugate-gradient techniques need only $O(t)$ memory compared to the $O(t^2)$ memory for the other three techniques, where t is the number of parameters. On the other hand, the conjugate-gradient techniques are significantly slower than other optimization techniques and should be used only when memory is insufficient for more efficient techniques. When you choose this option, `UPDATE=PB` by default. This is the default optimization technique if there are more than 999 parameters to estimate.
- DBLDOG | DD** performs a version of double dogleg optimization, which uses the gradient to update an approximation of the Cholesky factor of the Hessian. This technique is, in many aspects, very similar to the dual quasi-Newton method, but it does not use line search. The implementation is based on Dennis and Mei (1979) and (Gay 1983).
- LEVMAP | LM | MARQUARDT** performs a highly stable (but for large problems, memory- and time-consuming) Levenberg-Marquardt optimization technique, a slightly improved variant of the (Moré 1978) implementation. This is the default optimization technique for estimation methods other than the FIML if there are fewer than 500 parameters to estimate.
- NEWRAP | NRA** performs a usually stable (but for large problems, memory- and time-consuming) Newton-Raphson optimization technique. The algorithm combines a line-search algorithm with ridging, and it can be modified with the `LINESEARCH=` option.
- NRRIDG | NRR | NR | NEWTON** performs a usually stable (but for large problems, memory- and time-consuming) Newton-Raphson optimization technique. This algorithm does not perform a line search. Since `OMETHOD=NRRIDG` uses an orthogonal decomposition of the approximate Hessian, each iteration of `OMETHOD=NRRIDG` can be slower than that of `OMETHOD=NEWRAP`, which works with Cholesky decomposition. However, usually `OMETHOD=NRRIDG` needs fewer iterations than `OMETHOD=NEWRAP`. The `NRRIDG` technique is the default optimization for the FIML estimation if there are fewer than 500 parameters to estimate.
- QUANEW | QN** chooses one of four different quasi-Newton optimization algorithms that can be more precisely defined with the `UPDATE=` option and modified with the `LINESEARCH=` option. If boundary constraints are used, these techniques sometimes converge slowly. When you choose this option, `UPDATE=DBFGS` by default. If nonlinear constraints are specified in the `NLINCON` statement, a modification of Powell's VMCWD algorithm (Powell 1982a, b) is used, which is a sequential quadratic programming (SQP) method. This algorithm can be modified by specifying `VERSION=1`, which replaces the update of the Lagrange multiplier estimate vector μ to the original update of Powell (1978b, a)

that is used in the VF02AD algorithm. This can be helpful for applications with linearly dependent active constraints. The QUANEW technique is the default optimization technique if there are nonlinear constraints specified or if there are more than 499 and fewer than 1,000 parameters to estimate. The QUANEW algorithm uses only first-order derivatives of the objective function and, if available, of the nonlinear constraint functions.

TRUREG TR	performs a usually very stable (but for large problems, memory- and time-consuming) trust-region optimization technique. The algorithm is implemented similar to Gay (1983) and Moré and Sorensen (1983).
NONE NO	does not perform any optimization. This option is similar to METHOD=NONE , but OMETHOD=NONE also computes and displays residuals and goodness-of-fit statistics. If you specify METHOD=ML , METHOD=LSML , METHOD=GLS , METHOD=LSGLS , METHOD=WLS , or METHOD=LSWLS , this option enables computing and displaying (if the display options are specified) of the standard error estimates and modification indices corresponding to the input parameter estimates.

For fewer than 500 parameters ($t < 500$), **OMETHOD=NRRIDG** (Newton-Raphson Ridge) is the default optimization technique for the FIML estimation, and **OMETHOD=LEVVAR** (Levenberg-Marquardt) is the default optimization technique for the all other estimation methods. For $500 \leq t < 1,000$, **OMETHOD=QUANEW** (quasi-Newton) is the default method, and for $t \geq 1,000$, **OMETHOD=CONGRA** (conjugate gradient) is the default method. Each optimization method or technique can be modified in various ways. See the section “Use of Optimization Techniques” on page 1352 for more details.

ORDERALL

prints the model and group results in the order of the model or group numbers, starting from the smallest number. It also arrange some model results by the parameter types. In effect, this option turns on the **ORDERGROUPS**, **ORDERMODELS**, and **ORDERSPEC** options. The **ORDERALL** is not a default option. By default, the printing of the results follow the order of the input specifications.

ORDERGROUPS | ORDERG

prints the group results in the order of the group numbers, starting from the smallest number. The default behavior, however, is to print the group results in the order they appear in the input specifications.

ORDERMODELS | ORDERMO

prints the model results in the order of the model numbers, starting from the smallest number. The default behavior, however, is to print the model results in the order they appear in the input specifications.

ORDERSPEC

arranges some model results by the types of parameters. The default behavior, however, is to print the results in the order they appear in the input specifications. You can specify the **ORDERSPEC** option in both the PROC CALIS and the **MODEL** statements. When this option is specified in the PROC CALIS statement, it propagates to all models. When this option is specified in the MODEL statement, it applies only to the local model.

OUTEST=SAS-data-set

creates an output data set that contains the parameter estimates, their gradient, Hessian matrix, and boundary and linear constraints. For **METHOD=ML**, **METHOD=GLS**, and **METHOD=WLS**, the **OUTEST=** data set also contains the information matrix, the approximate covariance matrix of the parameter estimates ((generalized) inverse of information matrix), and approximate standard errors. If linear or nonlinear equality or active inequality constraints are present, the Lagrange multiplier estimates of the active constraints, the projected Hessian, and the Hessian of the Lagrange function are written to the data set.

See the section “**OUTEST= Data Set**” on page 1240 for a description of the **OUTEST=** data set. If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*.

OUTFIT=SAS-data-set

creates an output data set that contains the values of the fit indices. See the section “**OUTFIT= Data Set**” on page 1254 for details.

OUTMODEL | OUTRAM=SAS-data-set

creates an output data set that contains the model information for the analysis, the parameter estimates, and their standard errors. An **OUTMODEL=** data set can be used as an input **INMODEL=** data set in a subsequent analysis by PROC CALIS. If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*.

OUTSTAT=SAS-data-set

creates an output data set that contains the BY group variables, the analyzed covariance or correlation matrices, and the predicted and residual covariance or correlation matrices of the analysis. You can specify the correlation or covariance matrix in an **OUTSTAT=** data set as an input **DATA=** data set in a subsequent analysis by PROC CALIS. See the section “**OUTSTAT= Data Set**” on page 1250 for a description of the **OUTSTAT=** data set. If the model contains latent variables, this data set also contains the predicted covariances between latent and manifest variables and the latent variable score regression coefficients (see the **PLATCOV** option on page 1112). If the **FACTOR** statement is used, the **OUTSTAT=** data set also contains the rotated and unrotated factor loadings, the unique variances, the matrix of factor correlations, the transformation matrix of the rotation, and the matrix of standardized factor loadings.

You can use the latent variable score regression coefficients with PROC SCORE to compute factor scores.

If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*.

OUTWGT | OUTWEIGHT=SAS-data-set

creates an output data set that contains the elements of the weight matrix **W** or the its inverse **W⁻¹** used in the estimation process. The inverse of the weight matrix is output only when you specify an **INWGT=** data set with the **INWGT=** and **INWGTINV** options (or the **INWGT(INV)=** option alone) in the same analysis. As a result, the entries in the **INWGT=** and **OUTWGT=** data sets are consistent. In other situations where the weight matrix is computed by the procedure or obtained from the **OUTWGT=** data set without the **INWGTINV** option, the weight matrix is output in the **OUTWGT=** data set. Furthermore, if the weight matrix is computed by the procedure, the **OUTWGT=**

data set contains the elements of the weight matrix on which the **WRIDGE=** and the **WPENALTY=** options are applied.

You cannot create an **OUTWGT=** data set with an unweighted least squares or maximum likelihood estimation. The weight matrix is defined only in the GLS, WLS (ADF), or DWLS fit function. An **OUTWGT=** data set can be used as an input **INWGT=** data set in a subsequent analysis by PROC CALIS. See the section “**OUTWGT= Data Set**” on page 1254 for the description of the **OUTWGT=** data set. If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*.

PALL | ALL

displays all optional output except the output generated by the **PCOVES** and **PDETERM** options.

CAUTION: The **PALL** option includes the very expensive computation of the modification indices. If you do not really need modification indices, you can save computing time by specifying the **NOMOD** option in addition to the **PALL** option.

PARMNAME

prints the parameter names in the model results. This is the default printing behavior. In contrast, the **NOPARMNAME** option suppresses the printing of the parameter names in the model results. You can specify the **PARMNAME** option in both the PROC CALIS and the **MODEL** statements. When this option is specified in the PROC CALIS statement, it does not have any apparent effect because by default model results show the parameter names. When this option is specified in the **MODEL** statement, it deactivates the inherited **NOPARMNAME** option from the PROC CALIS statement. In other words, this option is mainly used for resetting the default behavior in the local model that is specified within the scope of a particular **MODEL** statement. If you specify both the **PARMNAME** and **NOPARMNAME** options in the same statement, the **PARMNAME** option is ignored.

PCORR | CORR

displays the covariance or correlation matrix that is analyzed and the predicted model covariance or correlation matrix.

PCOVES | PCE

displays the following:

- the information matrix
- the approximate covariance matrix of the parameter estimates (generalized inverse of the information matrix)
- the approximate correlation matrix of the parameter estimates

The covariance matrix of the parameter estimates is not computed for estimation methods ULS and DWLS. This displayed output is not included in the output generated by the **PALL** option.

PDETERM | PDE

displays three coefficients of determination: the determination of all equations (DETAE), the determination of the structural equations (DETSE), and the determination of the manifest variable equations (DETMV). These determination coefficients are intended to be global means of the squared multiple correlations for different subsets of model equations and variables. The coefficients are displayed only when you specify a **FACTOR**, **LINEQS**, **LISMOD**, **PATH**, or **RAM** model, but they are displayed for all five estimation methods: ULS, GLS, ML, WLS, and DWLS.

You can use the **STRUCTEQ** statement to define which equations are structural equations. If you do not use the **STRUCTEQ** statement, PROC CALIS uses its own default definition to identify structural equations.

The term “structural equation” is not defined in a unique way. The LISREL program defines the structural equations by the user-defined BETA matrix. In PROC CALIS, the default definition of a structural equation is an equation that has a dependent left-side variable that appears at least once on the right side of another equation, or an equation that has at least one right-side variable that appears at the left side of another equation. Therefore, PROC CALIS sometimes identifies more equations as structural equations than the LISREL program does.

PESTIM | PES

displays the parameter estimates. In some cases, this includes displaying the standard errors and *t* values.

PINITIAL | PIN

displays the model specification with initial estimates and the vector of initial values.

PLATCOV | PLATMOM | PLC

displays the following:

- the estimates of the covariances among the latent variables
- the estimates of the covariances between latent and manifest variables
- the estimates of the latent variable means for mean structure analysis
- the latent variable score regression coefficients

The estimated covariances between latent and manifest variables and the latent variable score regression coefficients are written to the **OUTSTAT=** data set. You can use the score coefficients with PROC SCORE to compute factor scores.

PLOTS | PLOT < = *plot-request* >

PLOTS | PLOT < = (*plot-request* < ... *plot-request* >) >

specifies the ODS Graphics plots. When you specify only one *plot-request*, you can omit the parentheses around the *plot-request*. For example:

```
PLOTS=ALL
PLOTS=RESIDUALS
PLOTS=(PP RESBYPRED QQ)
```

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;
proc calis plots;
  path y <=== x,
        y <=== z;
run;
ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS](#).”

You can specify the following *plot-requests*:

- ALL** displays all plots.
- CASERESID | CASERESIDUAL | CASERESIDUALS** displays all the case-level ODS Graphics plots enabled by the following *plot-requests*: CRESHIST, PP, QQ, RESBYLEV, and RESBYPRED. This option requires raw data input.
- CRESHIST | CRESIDUALHISTOGRAM** produces the ODS Graphics plot CaseResidualHistogram, which displays the distribution of the case-level (observation-level) residuals in the form of a histogram, where residuals are measured in terms of M-distances. This option requires raw data input.
- NONE** suppresses ODS Graphics plots.
- PP | PFPLOT** produces the ODS Graphics plot ResPercentileByExpPercentile, which plots the observed percentiles of the residual M-distances against the theoretical percentiles. This plot is useful for showing departures from the theoretical distribution in terms of percentiles, and it is especially sensitive to departures in the middle region of the distribution. This option requires raw data input.
- QQ | QQPLOT** produces the ODS Graphics plot ResidualByQuantile, which plots the residual M-distances (observed quantiles) against the theoretical quantiles. This plot is useful for showing departures from the theoretical distribution in terms of quantiles, and it is especially sensitive to departures at the upper tail of the distribution. This option requires raw data input.
- RESBYLEV | RESIDUALBYLEVERAGE** produces the ODS Graphics plot ResidualByLeverage, which plots the residual M-distances against the leverage M-distances. This plot is useful for showing outliers and leverage observations graphically. See the [ALPHAOUT=](#) and [ALPHALEV=](#) options for detection criteria of outliers and leverage observations. This option requires raw data input.
- RESBYPRED | RESONFIT | RESIDUALBYPREDICTED | RESIDUALONFIT<(VAR= var-list)>** produces the ODS Graphics plot ResidualByPredicted, which plots the residuals against the predicted values of the dependent observed variables in the model. You can restrict the set of dependent variables to display by specifying *var-list* in the VAR= option. If *var-list* is not specified in the VAR= option, plots for all dependent observed variables are displayed. The residual on fit plots are useful for detecting nonlinear relationships in the model. If the relationships are linear and the residual variance is homoscedastic, the residuals should not show systematic pattern with the predicted values. This option requires raw data input.
- RESIDUAL | RESIDUALS** produces the ODS Graphics plot for the histogram of residuals in covariances and means rather than the case-level residuals. With this ODS Graphics plot, the nongraphical (legacy) output for the bar chart of residual tallies is redundant and therefore is suppressed. To display this bar chart together with the ODS Graphics for residual histogram, you must use the [RESIDUAL\(TALLY\)](#) option in the PROC CALIS statement. This option does not require raw data input.

PRIMAT | PMAT

displays parameter estimates, approximate standard errors, and *t* values in matrix form if you specify the analysis model using the [RAM](#) or [LINEQS](#) statement.

PRINT | PRI

adds the options **KURTOSIS**, **RESIDUAL**, **PLATCOV**, and **TOTEFF** to the default output.

PSHORT | SHORT | PSH

excludes the output produced by the **PINITIAL**, **SIMPLE**, and **STDERR** options from the default output.

PSUMMARY | SUMMARY | PSUM

displays the fit assessment table only.

PWEIGHT | PW

displays the weight matrix **W** used in the estimation. The weight matrix is displayed after the **WRIDGE=** and the **WPENALTY=** options are applied to it. However, if you specify an **INWGT=** data set by the **INWGT=** and **INWGTINV** options (or the **INWGT(INV)=** option alone) in the same analysis, this option displays the elements of the inverse of the weight matrix.

RADIUS=*r*

is an alias for the **INSTEP=** option for Levenberg-Marquardt minimization.

RANDOM=*i*

specifies a positive integer as a seed value for the pseudo-random number generator to generate initial values for the parameter estimates for which no other initial value assignments in the model definitions are made. Except for the parameters in the diagonal locations of the central matrices in the model, the initial values are set to random numbers in the range $0 \leq r \leq 1$. The values for parameters in the diagonals of the central matrices are random numbers multiplied by 10 or 100. See the section “Initial Estimates” on page 1351 for more information.

RDF | DFR=*n*

makes the effective number of observations the actual number of observations minus the **RDF=** value. The degree of freedom for the intercept should not be included in the **RDF=** option. If you use PROC CALIS to compute a regression model, you can specify **RDF= *number-of-regressor-variables*** to get approximate standard errors equal to those computed by PROC REG.

READADDPARM | READADD

inputs the generated default parameters (for example, observations with **_TYPE_=ADDP**COV, **AD-DMEAN**, or **ADDP**VAR) in the **INMODEL=** data set as if they were part of the original model specification. Typically, these default parameters in the **INMODEL=** data set were generated automatically by PROC CALIS in a previous analysis and stored in an **OUTMODEL=** data set, which is then used as the **INMODEL=** data set in a new run of PROC CALIS. By default, PROC CALIS does not input the observations for default parameters in the **INMODEL=** data set. In most applications, you do not need to specify this option because PROC CALIS is able to generate a new set of default parameters that are appropriate to the new situation after it reads in the **INMODEL=** data set. Undistinguished uses of the **READADDPARM** option might lead to unintended constraints on the default parameters.

RESIDUAL | RES <(TALLY | TALLIES)> < = NORM | VARSTAND | ASYSTAND >

displays the raw and normalized residual covariance matrix, the rank order of the largest residuals, and a bar chart of the residual tallies. If mean structures are modeled, mean residuals are also displayed and ranked.

For raw data input, this option also displays tables for case-level (observation-level) residual analysis, including outlier and leverage detections and departures of residuals from the theoretical residual

distributions. To set the criterion for detecting outliers, use the `ALPHAOUT=` option. To set the criterion for leverage observations, use the `ALPHALEV=` option. Case-level residual analysis is not available when you specify `METHOD=FIML`.

For the covariance and mean residuals, three types of normalized or standardized residual matrices can be chosen with the `RESIDUAL=` specification.

RESIDUAL= NORM	normalized residuals
RESIDUAL= VARSTAND	variance standardized residuals
RESIDUAL= ASYSTAND	asymptotically standardized residuals

When `ODS Graphics plots` of covariance and mean residuals are also requested, the bar charts of residual tallies are suppressed. They are replaced with high quality graphical histograms showing residual distributions. If you still want to display the bar charts in this situation, use the `RESIDUAL(TALLY)` or `RESIDUAL(TALLY)=` option.

The `RESIDUAL` option is also enabled by the `PRINT` option. See the section “Assessment of Fit” on page 1326 for more details about the definitions of residuals.

RIDGE< =*r* >

defines a ridge factor r for the diagonal of the covariance or correlation matrix \mathbf{S} that is analyzed. The matrix \mathbf{S} is transformed to:

$$\mathbf{S} \longrightarrow \tilde{\mathbf{S}} = \mathbf{S} + r(\text{diag}(\mathbf{S}))$$

If you do not specify r in the `RIDGE` option, PROC CALIS tries to ridge the covariance or correlation matrix \mathbf{S} so that the smallest eigenvalue is about 10^{-3} . Because the weight matrix in the GLS method is the same as the observed covariance or correlation matrix, the `RIDGE=` option also applies to the weight matrix for the GLS estimation, unless you input the weight matrix by the `INWGT=` option.

CAUTION: The covariance or correlation matrix in the `OUTSTAT=` output data set does not contain the ridged diagonal.

ROBITER | ROBUSTITER =*i*

specifies the maximum number i of iterations for the iteratively reweighted least squares (IRLS) method to compute the robust mean and covariance matrices with the two-stage robust estimation. This option is relevant only with the use of the `ROBUST=` option and with raw data input. The default value is 5,000.

You can also specify this option in the `GROUP` statement so that different groups can use different `ROBITER=` values. Notice that the `ROBITER=` option does not specify the maximum number of iterations for the IRLS algorithm used in the direct robust estimation or in the second stage of the two-stage robust estimation. You can specify the `MAXITER=` option for this purpose.

ROBPHI | ROBUSTPHI =*r*

sets the tuning parameter r ($0 < r < 1$) for the robust estimation method that you specify using the `ROBUST=` option. The `ROBPHI=` value controls the criterion for downweighting observations. This value indicates approximately the proportion of observations that would receive weights less than 1 (that is, would be downweighted) according to certain theoretical distributions. The larger the `ROBPHI=` value, the more observations are downweighted (that is, with weights less than 1). The default value is 0.05.

You can also specify this option in the **GROUP** statement so that different groups can use different **ROBPHI=** values for the tuning parameters.

ROBUST | ROB < =name>

invokes the robust estimation method that downweights the outliers in estimation. You can use the **ROBUST** option only in conjunction with the **ML** method (**METHOD=ML**). More accurately, the robust estimation is done by using the iteratively reweighted least squares (IRLS) method under the normal distribution assumption. The model fit of robust estimation is evaluated with the **ML** discrepancy function.

You must provide raw data input for the robust estimation method to work. With the robust method, the Huber weights are applied to the observations so that outliers are downweighted during estimation. See the section “[Robust Estimation](#)” on page 1315 for details.

You can request the three different types of robust methods by using one of the following *names*:

RESIDUAL | DIRECT | RESID | RES <(E)> specifies a direct robust method that downweights observations with large residuals during the iterative estimation of the model. This method treats the disturbances (the error terms of endogenous latent factors) as errors or residuals (hence the keyword **E**) in the associated factor model when computing residual **M**-distances and factor scores during the robust estimation. The **(E)**specification is irrelevant if there are no endogenous latent factors in the model. This is the default robust method.

RESIDUAL | DIRECT | RESID | RES (F) specifies a direct robust method that downweights observations with large estimated residuals during the iterative estimation of the model. Unlike the **(E)**method, this method treats the disturbances (the error terms of endogenous latent factors) as factors (hence the keyword **F**) in the associated factor model when computing residual **M**-distances and factor scores during the robust estimation. The **(F)**specification is irrelevant if there are no endogenous latent factors in the model.

SAT | TWOSTAGE | UNSTRUCT | UNS specifies a two-stage robust method that downweights the observations with large **M**-distances in all observed variable dimensions when computing the covariance matrix and mean vector from the input raw data. As a result, this option produces a robust covariance matrix and a mean vector for a subsequent model estimation where no reweighting would be applied at the observational level. Hence, this is a two-stage method that applies weights only in the first stage for computing the robust covariance and mean matrices. This is in contrast with the **RES(E)** or **RES(F)** option, where weighting and reweighting of observations are applied directly during model estimation.

For details about these robust methods, see the section “[Robust Estimation](#)” on page 1315.

To control the proportion of the observations that are downweighted during the robust estimation, you can specify the value of the tuning parameter φ , which is between 0 and 1, by using the **ROBPHI=** option. Approximately, $\varphi \times 100\%$ of observations would receive weights less than 1 according to certain theoretical distributions. By default, the value of the tuning parameter φ is set to 0.05 for all robust methods in PROC CALIS.

By default, the robust method uses a maximum of 5,000 iterations to obtain parameter convergence through the IRLS algorithm. You can override this default maximum number of iterations by spec-

ifying the **ROBITER=** option. The default relative parameter convergence criterion for the robust method is $1E-8$. See the **XCONV=** option for the mathematical definition of this criterion and for information about overriding the default convergence criterion.

Because all robust methods reweight the observations iteratively, the observed variable means are always implicitly updated with the robust weights. Therefore, in a sense all robust methods intrinsically analyze the mean structures of models. If you do not specify the **MEANSTR** option or any mean parameters for your models, PROC CALIS assumes appropriate saturated mean structures for the models. However, when you are computing fit statistics, these saturated mean structures are ignored as if they were never modeled. If you do specify the **MEANSTR** option or any mean parameters for your models, these mean structures are taken into account in computing fit statistics.

In this release, robust estimation with the IRLS method is not supported when you specify the **BOUNDS**, **LINCON**, or **NLINCON** statement. However, you can still set parameter constraints by using the same parameter names or by specifying the **PARAMETERS** statement and the **SAS programming statements**. See the section “**Setting Constraints on Parameters**” on page 1303 for techniques to set up implicit parameter constraints by using the **PARAMETERS** statement and SAS programming statements.

SALPHA=*r*

is an alias for the **INSTEP=** option for line-search algorithms.

SIMPLE | S

displays means, standard deviations, skewness, and univariate kurtosis if available. This information is displayed when you specify the **PRINT** option. If the **KURTOSIS** option is specified, the **SIMPLE** option is set by default.

SINGULAR | SING =*r*

specifies the singularity criterion r ($0 < r < 1$) used, for example, for matrix inversion. The default value is the square root of the relative machine precision or, equivalently, the square root of the largest double precision value that, when added to 1, results in 1.

SLMW=*r*

specifies the probability limit used for computing the stepwise multivariate Wald test. The process stops when the univariate probability is smaller than r . The default value is $r=0.05$.

SPRECISION | SP=*r*

is an alias for the **LSPRECISION=** option.

START=*r*

specifies initial estimates for parameters as multiples of the r value. In all CALIS models, you can supply initial estimates individually as parenthesized values after each parameter name. Unspecified initial estimates are usually computed by various reasonable initial estimation methods in PROC CALIS. If none of the initialization methods is able to compute all the unspecified initial estimates, then the remaining unspecified initial estimates are set to r , $10|r|$, or $100|r|$. For variance parameters, $100|r|$ is used for covariance structure analyses and $10|r|$ is used for correlation structure analyses. For other types of parameters, r is used. The default value is $r = 0.5$. If the **DEMPHAS=** option is used, the initial values of the variance parameters are multiplied by the value specified in the **DEMPHAS=** option. See the section “**Initial Estimates**” on page 1351 for more information.

STDERR | SE

displays approximate standard errors if estimation methods other than unweighted least squares (ULS) or diagonally weighted least squares (DWLS) are used (and the **NOSTDERR** option is not specified). In contrast, the **NOSTDERR** option suppresses the printing of the standard error estimates. If you specify neither the **STDERR** nor the **NOSTDERR** option, the standard errors are computed for the **OUTMODEL=** data set. This information is displayed by default when you specify the **PRINT** option.

You can specify the **STDERR** option in both the **PROC CALIS** and the **MODEL** statements. When this option is specified in the **PROC CALIS** statement, it does not have any apparent effect because by default the model results display the standard error estimates (for estimation methods other than ULS and DWLS). When this option is specified in the **MODEL** statement, it deactivates the inherited **NOSTDERR** or **NOSE** option from the **PROC CALIS** statement. In other words, this option is mainly used for resetting the default behavior in the local model that is specified within the scope of a particular **MODEL** statement. If you specify both the **STDERR** and **NOSTDERR** options in the same statement, the **STDERR** option is ignored.

TMISSPAT | THRESHOLDMISSPAT | THRESMISSPAT=*n*

specifies the proportion threshold for the missing patterns to display in the output, where *n* is between 0 and 1. The default **TMISSPAT=** value is 0.05. This option is relevant only when there are incomplete observations (with some missing values in the analysis variables) in the input raw data set and when you use **METHOD=FIML** or **METHOD=LSFIML** for estimation.

Because the number of missing patterns could be quite large, **PROC CALIS** displays a limited number of the most frequent missing patterns in the output. Together with the **MAXMISSPAT=** option, this option controls the number of missing patterns to display in the output. See the **MAXMISSPAT=** option for a detailed description about how the number of missing patterns to display is determined.

UPDATE | UPD=*name*

specifies the update method for the quasi-Newton or conjugate-gradient optimization technique.

For **OMETHOD=CONGRA**, the following updates can be used:

- PB** performs the automatic restart update method of Powell (1977) and Beale (1972). This is the default.
- FR** performs the Fletcher-Reeves update (Fletcher 1980, p. 63).
- PR** performs the Polak-Ribiere update (Fletcher 1980, p. 66).
- CD** performs a conjugate-descent update of Fletcher (1987).

For **OMETHOD=DBLDOG**, the following updates (Fletcher 1987) can be used:

- DBFGS** performs the dual Broyden, Fletcher, Goldfarb, and Shanno (BFGS) update of the Cholesky factor of the Hessian matrix. This is the default.
- DDFP** performs the dual Davidon, Fletcher, and Powell (DFP) update of the Cholesky factor of the Hessian matrix.

For **OMETHOD=QUANEW**, the following updates (Fletcher 1987) can be used:

- BFGS** performs original BFGS update of the inverse Hessian matrix. This is the default for earlier releases.
- DFP** performs the original DFP update of the inverse Hessian matrix.
- DBFGS** performs the dual BFGS update of the Cholesky factor of the Hessian matrix. This is the default.
- DDFP** performs the dual DFP update of the Cholesky factor of the Hessian matrix.

VARDEF= DF | N | WDF | WEIGHT | WGT

specifies the divisor used in the calculation of covariances and standard deviations. The default value is VARDEF=N for the METHOD=FIML, and VARDEF=DF for other estimation methods. The values and associated divisors are displayed in the following table, where k is the number of partial variables specified in the PARTIAL statement. When a WEIGHT statement is used, w_j is the value of the WEIGHT variable in the j th observation, and the summation is performed only over observations with positive weight.

Value	Description	Divisor
DF	Degrees of freedom	$N - k - 1$
N	Number of observations	N
WDF	Sum of weights DF	$\sum_j^N w_j - k - 1$
WEIGHT WGT	Sum of weights	$\sum_j^N w_j$

VSINGULAR | VSING= r

specifies a relative singularity criterion r ($r > 0$) for the inversion of the information matrix, which is needed to compute the covariance matrix. If you do not specify the SINGULAR= option, the default value for r or VSING= is 1E-8; otherwise, the default value is SING, which is the specified SINGULAR= value.

When inverting the information matrix, the following singularity criterion is used for the diagonal pivot $d_{j,j}$ of the matrix:

$$|d_{j,j}| \leq \max(ASING, VSING * |H_{j,j}|, MSING * \max(|H_{1,1}|, \dots, |H_{n,n}|))$$

where ASING and MSING are the specified values of the ASINGULAR= and MSINGULAR= options, respectively, and $H_{j,j}$ is the j th diagonal element of the information matrix. Note that in many cases a normalized matrix $\mathbf{D}^{-1}\mathbf{H}\mathbf{D}^{-1}$ is decomposed (where $\mathbf{D}^2 = \text{diag}(\mathbf{H})$), and the singularity criteria are modified correspondingly.

WPENALTY | WPEN= r

specifies the penalty weight $r \geq 0$ for the WLS and DWLS fit of the diagonal elements of a correlation matrix (constant 1s). The criterion for weighted least squares estimation of a correlation structure is

$$\mathbf{F}_{WLS} = \sum_{i=2}^n \sum_{j=1}^{i-1} \sum_{k=2}^n \sum_{l=1}^{k-1} w^{ij,kl} (s_{ij} - c_{ij})(s_{kl} - c_{kl}) + r \sum_i^n (s_{ii} - c_{ii})^2$$

where r is the penalty weight specified by the WPENALTY= r option and the $w^{ij,kl}$ are the elements of the inverse of the reduced $(n(n - 1)/2) \times (n(n - 1)/2)$ weight matrix that contains only the nonzero rows and columns of the full weight matrix \mathbf{W} . The second term is a penalty term to fit the

diagonal elements of the correlation matrix. The default value is 100. The reciprocal of this value replaces the asymptotic variance corresponding to the diagonal elements of a correlation matrix in the weight matrix \mathbf{W} , and it is effective only with the `ASYCOV=``CORR` option, which is the default for correlation analyses. The often used value $r = 1$ seems to be too small in many cases to fit the diagonal elements of a correlation matrix properly. The default `WPENALTY=` value emphasizes the importance of the fit of the diagonal elements in the correlation matrix. You can decrease or increase the value of r if you want to decrease or increase the importance of the diagonal elements fit. This option is effective only with the WLS or DWLS estimation method and the analysis of a correlation matrix.

See the section “[Estimation Criteria](#)” on page 1309 for more details.

CAUTION: If you input the weight matrix by the `INWGT=` option, the `WPENALTY=` option is ignored.

WRIDGE= r

defines a ridge factor r for the diagonal of the weight matrix \mathbf{W} used in GLS, WLS, or DWLS estimation. The weight matrix \mathbf{W} is transformed to

$$\mathbf{W} \longrightarrow \tilde{\mathbf{W}} = \mathbf{W} + r(\text{diag}(\mathbf{W}))$$

The `WRIDGE=` option is applied on the weight matrix before the following actions occur:

- the `WPENALTY=` option is applied on it
- the weight matrix is written to the `OUTWGT=` data set
- the weight matrix is displayed

CAUTION: If you input the weight matrix by the `INWGT=` option, the `OUTWGT=` data set will contain the same weight matrix without the ridging requested by the `WRIDGE=` option. This ensures that the entries in the `INWGT=` and `OUTWGT=` data sets are consistent. The `WRIDGE=` option is ignored if you input the inverse of the weight matrix by the `INWGT=` and `INWGTINV` options (or the `INWGT(INV)=` option alone).

XCONV | XTOL= r

specifies the relative parameter convergence criterion. Termination requires a small relative parameter (x) change in subsequent iterations, that is,

$$\frac{\max_j |x_j^{(k)} - x_j^{(k-1)}|}{\max(|x_j^{(k)}|, |x_j^{(k-1)}|, XSIZE)} \leq r$$

The default value for r is 1E–8 for robust estimation (see the `ROBUST` option) with the iteratively reweighted least squares method, and it is 0 for other estimation methods. The default value for `XSIZE` is 0. You can change this default value by specifying the `XSIZE=` option in the `NLOPTIONS` statement.

BOUNDS Statement

BOUNDS *constraint* <, *constraint* ... >;

where *constraint* represents

< number operator > parameter-list < operator number >

You can use the BOUNDS statement to define boundary constraints for any independent parameter that has its name specified in the main or subsidiary model specification statements, the **PARAMETERS** statement, or the **INMODEL=** data set. You cannot define boundary constraints for dependent parameters created in **SAS programming statements** or elsewhere.

Valid operators are <=, <, >=, >, and = (or, equivalently, LE, LT, GE, GT, and EQ). The following is an example of the BOUNDS statement:

```
bounds      0.    <= a1-a9 x    <= 1.  ,
           -1.    <= c2-c5
                b1-b10 y    >= 0.  ;
```

You must separate boundary constraints with a comma, and you can specify more than one BOUNDS statement. The feasible region for a parameter is the intersection of all boundary constraints specified for that parameter; if a parameter has a maximum lower boundary constraint greater than its minimum upper bound, the parameter is set equal to the minimum of the upper bounds.

The active set strategies made available in PROC CALIS treat strict inequality constraints < or > as if they were just inequality constraints <= or >=. For example, if you require x be strictly greater than zero so as to prevent an undefined value for $y = \log(x)$, specifying the following statement is insufficient:

```
BOUNDS x > 0;
```

Specify the following statement instead:

```
BOUNDS x > 1E-8;
```

If the CALIS procedure encounters negative variance estimates during the minimization process, serious convergence problems can occur. You can use the BOUNDS statement to constrain these parameters to nonnegative values. Although allowing negative values for variances might lead to a better model fit with smaller χ^2 value, it adds difficulties in interpretation.

BY Statement

BY variables ;

You can specify a BY statement with PROC CALIS to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the CALIS procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.

- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

The BY statement is not supported if you define more than one group by using the **GROUP** statements.

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

COSAN Statement

COSAN < **VAR**=*variable-list*, > *term* < + *term* . . . > ;

where *variable-list* is a list of observed variables and *term* represents either one of the following forms:

matrix-definition < * *matrix-definition* . . . > < *mean-definition* >

or

mean-definition

where *matrix-definition* is of the following form:

matrix-name < (*number-of-columns* < , *matrix-type* < , *transformation* > >) >

and *mean-definition* is one of the following forms:

[/ *mean-vector*]

or

[**MEAN**=*mean-vector*]

where *mean-vector* is a vector name.

COSAN stands for covariance structure analysis (McDonald 1978, 1980). The COSAN model in PROC CALIS is a generalized version of the original COSAN model. See the section “The COSAN Model” on page 1259 for details of the generalized COSAN model. You can analyze a very wide class of mean and covariance structures with the COSAN modeling language, which consists of the COSAN statement as the **main model specification statement** and the **MATRIX** statement as the **subsidiary model specification statement**. Use the following syntax to specify a COSAN model:

```
COSAN < VAR=variable-list, > term < + term . . . > ;
MATRIX matrix-name parameters-in-matrix ;
/* Repeat the MATRIX statement as needed */ ;
VARNAMES name-assignments ;
```

The PROC CALIS statement invokes the COSAN modeling language. You can specify at most one COSAN statement in a model within the scope of either the PROC CALIS statement or a **MODEL** statement. To complete the COSAN model specification, you might need to add as many **MATRIX** statements as needed. Optionally, you can provide the variable names for the COSAN model matrices in the **VARNAMES** statement.

In the COSAN statement, you specify the list of observed variables for analysis in the **VAR=** option and the formulas for covariance and mean structures in the *terms*. If specified at all, the **VAR=** option must be

specified at the very beginning of the COSAN statement. The order of the variables in the VAR= option is important. It is the same order assumed for the row and column variables in the mean and covariance structures defined in the *terms*. If you do not specify the VAR= option, PROC CALIS selects all the numerical variables in the associated groups for analysis. To avoid confusion about the variables being analyzed in the model, it is recommended that you set the VAR= list explicitly in the COSAN statement.

To define the matrix formulas for the covariance and mean structures, you specify the *terms*, *matrix-definitions*, and *mean-vector* in the COSAN statement. The forms of the covariance and mean structures that are supported in PROC CALIS are mentioned in the section “The COSAN Model” on page 1259. In each *term*, you specify the covariance structures by listing the matrices in the *matrix-definitions*. These matrices must be in the proper order such that their matrix product produces the intended covariance structures. If you want to analyze the corresponding mean structures, specify the trailing *mean-vectors* in the *terms* whenever needed.

To illustrate the COSAN statement syntax, consider a factor-analytic model with six variables (var1–var6) and two factors. The covariance structures of the six variables are described by the matrix formula

$$\Sigma = \mathbf{F}\mathbf{P}\mathbf{F}' + \mathbf{U}$$

where Σ is a 6×6 symmetric matrix for the covariance matrix, \mathbf{F} is a 6×2 factor loading matrix, \mathbf{P} is a 2×2 (symmetric) factor covariance matrix, and \mathbf{U} is a 6×6 diagonal matrix of unique variances. You can use the following COSAN statement to specify the covariance structures of this factor model:

```
cosan var = var1-var6,
      F(2,GEN) * P(2,SYM) + U(6,DIA);
```

In the VAR= option of the COSAN statement, you define a list of six observed variables in the covariance structures. The order of the variables in the VAR= list determines the order of the row variables in the first matrix of each term in the model. That is, both matrices \mathbf{F} and \mathbf{U} have these six observed variables as their row variables, which are ordered the same way as in the VAR= list.

Next, you define the formula for the covariance structures by listing the matrices in the desired order *up to the central covariance matrix in each term*. In the first *term* of this example, you need to specify only $\mathbf{F}\mathbf{P}$ instead of the complete covariance structure formula $\mathbf{F}\mathbf{P}\mathbf{F}'$. The reason is that the latter part of the term (that is, after the central covariance matrix) contains only the transpose of the matrices that have already been defined. Hence, PROC CALIS can easily generate the complete term with the nonredundant information given.

In each of the *matrix-definitions*, you can provide the number of columns in the first argument (that is, the *number-of-columns* field) inside a pair of parentheses. You do not need to provide the number of rows because this information can be deduced from the given covariance structure formula. By using some keywords, you can optionally provide the matrix type in the second argument (that is, the *matrix-type* field) and the matrix transformation in the third argument (that is, the *transformation* field).

In the current example, $\mathbf{F}(2, \mathbf{GEN})$ represents a general rectangular (GEN) matrix \mathbf{F} with two columns. Implicitly, it has six rows because it is the first matrix of the first term in the covariance structure formula. $\mathbf{P}(2, \mathbf{SYM})$ represents a symmetric (SYM) matrix \mathbf{P} with two columns. Implicitly, it has two rows because it is premultiplied with \mathbf{F} , which has two columns. In the second term, $\mathbf{U}(6, \mathbf{DIA})$ represents a diagonal (DIA) matrix \mathbf{U} with six rows and six columns. Because you do not specify the third argument in these *matrix-definitions*, no transformation is applied to any of the matrices in the covariance structure formula.

PROC CALIS supports the following keywords for *matrix-type*:

IDE	specifies an identity matrix. If the matrix is not square, this specification describes an identity submatrix followed by a rectangular zero submatrix.
ZID	specifies an identity matrix. If the matrix is not square, this specification describes a rectangular zero submatrix followed by an identity submatrix.
DIA	specifies a diagonal matrix. If the matrix is not square, this specification describes a diagonal submatrix followed by a rectangular zero submatrix.
ZDI	specifies a diagonal matrix. If the matrix is not square, this specification describes a rectangular zero submatrix followed by a diagonal submatrix.
LOW	specifies a lower triangular matrix. The matrix can be rectangular.
UPP	specifies an upper triangular matrix. The matrix can be rectangular.
SYM	specifies a symmetric matrix. The matrix cannot be rectangular.
GEN	specifies a general rectangular matrix (default).

If you omit the *matrix-type* argument, PROC CALIS sets the type of matrix by default. For central covariance matrices, the default for *matrix-type* is SYM. For all other matrices, the default for *matrix-type* is GEN. For example, if **A** is not a central covariance matrix in the covariance structure formula, the following specifications are equivalent for a general matrix **A** with three columns:

```
A (3, GEN)
A (3)
A (3, )
A (3, , )
```

PROC CALIS supports the following two keywords for *transformation*:

INV	uses the inverse of the matrix.
IMI	uses the inverse of the difference between the identity and the matrix. For example, A (3, GEN , IMI) represents $(\mathbf{I} - \mathbf{A})^{-1}$.

Both INV or IMI require square (but not necessarily symmetric) matrices to transform. If you omit the *transformation* argument, no transformation is applied.

CAUTION: You can specify the same matrix by using the same *matrix-name* in different locations of the matrix formula in the COSAN statement. The *number-of-columns* and the *matrix-type* fields for matrices with identical *matrix-names* must be consistent. This consistency can be maintained easily by specifying each of these two fields only once in any of the locations of the same matrix. However, there is no restriction on the transformation for the same matrix in different locations. For example, while **R** must be the same 3×3 symmetric matrix throughout the formula in the following specification, the INV transformation of **R** applies only to the **R** matrix in the second term, but not to the same **R** matrix in the first term:

```
cosan var = var1-var6,  
      B (3, GEN) * R (3, SYM) + H (3, DIA) * R (3, SYM, INV) ;
```

Mean and Covariance Structures

Suppose now you want to analyze the mean structures in addition to the covariance structures of the preceding factor model. The mean structure formula for μ of the observed variables is

$$\mu = Fv + a$$

where μ is a 6×1 vector for the observed variable means, v is a 2×1 vector for the factor means, and a is a 6×1 vector for the intercepts of the observed variables. To include the mean structures in the COSAN model, you need to specify the mean vector at the end of the *terms*, as shown in the following statement:

```
cosan var = var1-var6,
          F(2,GEN) * P(2,SYM) [/ v] + U(6,DIA) [/ a];
```

If you take the mean vectors within the brackets away from each of the *terms*, the formula for the covariance structures is generated as

$$\Sigma = FPF' + U$$

which is exactly the same covariance structure as described in a preceding example. Now, with the mean vectors specified at the end of each *term*, you analyze the corresponding mean structures simultaneously with the covariance structures.

To generate the mean structure formula, PROC CALIS replaces the central covariance matrices with the mean vectors in the *terms*. In the current example the mean structure formula is formed by replacing P and U with v and a , respectively. Hence, the first term of the mean structure formula is $F * v$, and the second term of the mean structure formula is simply a . Adding these two terms yields the desired mean structure formula for the model.

To make the mean vector specification more explicit, you can use the following equivalent syntax with the MEAN= option:

```
cosan var = var1-var6,
          F(2,GEN) * P(2,SYM) [mean=v] + U(6,DIA) [mean=a];
```

If a *term* in the specification does not have a mean vector (covariance matrix) specification, a zero mean vector (null covariance matrix) is assumed. For example, the following specification generates the same mean and covariance structures as the preceding example:

```
cosan var = var1-var6,
          F(2,GEN) * P(2,SYM) [/ v] + U(6,DIA) + [/ a];
```

The covariance structure formula for this specification is

$$\Sigma = FPF' + U + \mathbf{0}$$

where $\mathbf{0}$ in the last term represents a null matrix. The corresponding mean structure formula is

$$\mu = Fv + \mathbf{0} + a$$

where $\mathbf{0}$ in the second term represents a zero vector.

Specifying Models with No Explicit Central Covariance Matrices

In some situations, the central covariance matrices in the covariance structure formula are not defined explicitly. For example, the covariance structure formula for an orthogonal factor model is:

$$\Sigma = \mathbf{F}\mathbf{F}' + \mathbf{U}$$

Again, assuming that \mathbf{F} is a 6×2 factor loading matrix and \mathbf{U} is a 6×6 diagonal matrix for unique variances, you can specify the covariance structure formula as in the following COSAN statement:

```
cosan var = var1-var6,
          F(2,GEN) + U(6,DIA);
```

In determining the proper formula for the covariance structures, PROC CALIS detects whether the last matrix specified in each *term* is symmetric. If you specify this last matrix explicitly with the SYM, IDE (with the same number of rows and columns), or DIA type, it is certainly a symmetric matrix. If you specify this last matrix without an explicit *matrix-type* and it has the same number of rows and columns, it is also treated as a symmetric matrix for the central covariance matrix of the *term*. Otherwise, this last matrix is not symmetric and PROC CALIS treats the *term* as if an identity matrix has been inserted for the central covariance matrix. For example, for the orthogonal factor model specified in the preceding statement, PROC CALIS correctly generates the first term as $\mathbf{F}\mathbf{F}' = \mathbf{F}\mathbf{I}\mathbf{F}'$ and the second term as \mathbf{U} .

Certainly, you might also specify your own central covariance matrix explicitly for the orthogonal factor model. That is, you add an identity matrix into the COSAN model specification as shown in the following statement:

```
cosan var = var1-var6,
          F(2,GEN) * I(2,IDE) + U(6,DIA);
```

Specifying Mean Structures for Models with No Central Covariance Matrices

When you specify covariance structures with central covariance matrices explicitly defined in the *terms*, the corresponding mean structure formula is formed by replacing the central covariance matrices with the *mean-vectors* that are specified in the brackets. However, when there is no central covariance matrix explicitly specified in a *term*, the last matrix of the *term* in the covariance structure formula is replaced with the *mean-vector* to generate the mean structure formula. Consider the following specification where there is no central covariance matrix defined explicitly in the first *term* of the COSAN model:

```
cosan var = var1-var6,
          A(6,GEN) [ / v];
```

The generated formulas for the covariance and mean structures are

$$\begin{aligned}\Sigma &= \mathbf{A}\mathbf{A}' \\ \mu &= \mathbf{v}\end{aligned}$$

If, instead, you intend to fit the following covariance and mean structures

$$\begin{aligned}\Sigma &= \mathbf{A}\mathbf{A}' \\ \mu &= \mathbf{A}\mathbf{v}\end{aligned}$$

you must put an explicit identity matrix for the central covariance matrix in the first *term*. That is, you can use the following specification:

```

cosan var = var1-var6,
          A(6,GEN) * I(6,IDE) [ / v];

```

Specifying Parameters in Matrices

By specifying the COSAN statement, you define the covariance and mean structures in matrix formulas for the observed variables. To specify the parameters in the model matrices, you need to use the **MATRIX** statements.

For example, for an orthogonal factor model with six variables (var1–var6) and two factors, the 6×2 factor loading matrix **F** might take the following form:

$$\mathbf{F} = \begin{pmatrix} x & 0 \\ x & 0 \\ x & 0 \\ 0 & x \\ 0 & x \\ 0 & x \end{pmatrix}$$

The 6×6 unique variance matrix **U** might take the following form:

$$\mathbf{U} = \begin{pmatrix} x & 0 & 0 & 0 & 0 & 0 \\ 0 & x & 0 & 0 & 0 & 0 \\ 0 & 0 & x & 0 & 0 & 0 \\ 0 & 0 & 0 & x & 0 & 0 \\ 0 & 0 & 0 & 0 & x & 0 \\ 0 & 0 & 0 & 0 & 0 & x \end{pmatrix}$$

where each x in the matrices represents a free parameter to estimate and 0 represents a fixed zero value. The covariance structures for the observed variables are described by the following formula:

$$\Sigma = \mathbf{F}\mathbf{F}' + \mathbf{U}$$

To specify the entire model, you use the following statements to define the covariance structure formula and the free parameters in the model matrices:

```

cosan var = var1-var6,
          F(2,GEN) + U(6,DIA);
matrix F [1 to 3,@1],[4 to 6,@2];
matrix U [1,1],[2,2],[3,3],[4,4],[5,5],[6,6];

```

In the **MATRIX** statements, you specify the free parameters in the matrices. For the factor loading matrix **F**, you specify that rows 1, 2, and 3 in column 1 and rows 4, 5, and 6 in column 2 are free parameters. For the unique variance matrix **U**, you specify that all diagonal elements are free parameters. All other unspecified entries in the matrices are fixed zeros by default. Certainly, you can also specify fixed zeros explicitly. For the current example, you can specify matrix **F** equivalently as:

```

matrix F [1 to 3,@1],[4 to 6,@2],
          [4 to 6,@1] = 0. 0. 0.,
          [1 to 3,@2] = 0. 0. 0.;

```

See the **MATRIX** statement on page 1175 for various ways to specify the parameters in matrices.

Matrix Names versus Parameter Names

Although parameter names and matrix names in PROC CALIS are both arbitrary SAS names for denoting mathematical entities in the model, their usages are very different in one aspect. That is, parameter names are globally defined in the procedure, while matrix names are only locally defined in models.

Consider the following two-group analysis example:

```
proc calis;
  group 1 / data=g1;
  group 2 / data=g2;
  model 1 / group=1;
    cosan var = var1-var6,
      F(2,GEN) * I(2,IDE) + U(6,DIA);
  matrix F [1 to 3,@1],[4 to 6,@2];
  matrix U [1,1] = u1-u6;
  model 2 / group=2;
    cosan var = var1-var6,
      F(1,GEN) * I(1,IDE) + D(6,DIA);
  matrix F [1 to 6,@1];
  matrix D [1,1] = u1-u6;
run;
```

In this example, you fit Model 1 to Group 1 and Model 2 to Group 2. You specify a matrix called **F** in each of the models. However, the two models are not constrained by this “same” matrix **F**. In fact, matrix **F** in Model 1 is a 6×2 matrix but matrix **F** in Model 2 is a 6×1 matrix. In addition, none of the parameters in the **F** matrices are constrained by the parameter names (simply because no parameter names are used). This illustrates that matrix names in PROC CALIS are defined only locally within models.

In contrast, in this example you use different matrix names for the second terms of the two models. In Model 1, you define a 6×6 diagonal matrix **U** for the second term; and in Model 2, you define a 6×6 diagonal matrix **D** for the second term. Are these two matrices necessarily different? The answer depends on how you define the parameters in these matrices. In the **MATRIX** statement for **U**, all diagonal elements of **U** are specified as free parameters u_1 – u_6 . Similarly, in the **MATRIX** statement for **D**, all diagonal elements of **D** are also specified as free parameters u_1 – u_6 . Because you use the same sets of parameter names in both of these **MATRIX** statements, matrices **U** and **D** are essentially constrained to be the same even though their names are different. This illustrates that parameter names are defined globally in PROC CALIS.

The following points summarize how PROC CALIS treats matrix and parameter names differently:

- Matrices with the same name in the same model are treated as identical.
- Matrices with the same name in different models are not treated as identical.
- Parameters with the same name are identical throughout the entire PROC CALIS specification.
- Cross-model constraints on matrix elements are set by using the same parameter names, but not the same matrix names.

Row and Column Variable Names for Matrices

You can use the `VARNAMES` statement to define the column variable names for the model matrices of a COSAN model. However, you do not specify the row variable names for the model matrices directly because they are determined by the column variable names of the related matrices in the covariance and mean structure formulas. For example, the following specification names the column variables of matrices **F** and **I**:

```

cosan var = var1-var6,
          F(2,GEN) * I(2,IDE) + U(6,DIA) ;
varnames
          F = [Factor1 Factor2],
          I = F;

```

The column names for matrix **F** are Factor1 and Factor2. The row names of matrix **F** are var1–var6 because it is the first matrix in the first term. Matrix **I** has the same column variable names as those for matrix **F**, as specified in the last specification of the `VARNAMES` statement. Because matrix **I** is a central covariance matrix, its row variable names are the same as its column variable names: Factor1 and Factor2. You do not specify the column variable names for matrix **U** in the `VARNAMES` statement. However, because it is the first matrix in the second term, its row variable names are the same as that of the `VAR=` list in the COSAN statement. Because matrix **U** is also the central covariance matrix in the second term, its column variable names are the same as its row variable names, which has been determined to be var1–var6. See the `VARNAMES` statement for more details.

Default Parameters

Unlike other modeling languages in PROC CALIS, the COSAN modeling language does not set any default free parameters for the model matrices. There is only one type of default parameters in the COSAN model: fixed values for matrix elements. These fixed values can be 0 or 1. For matrices with the IDE or ZID type, all elements are predetermined with either 0 or 1. They are fixed matrices in the sense that you cannot override these default fixed values. For all other matrix types, PROC CALIS sets their elements to fixed zeros by default. You can override these default zeros by specifying them explicitly in the `MATRIX` statements.

Modifying a COSAN Model from a Reference Model

In this section, it is assumed that you use a `REFMODEL` statement within the scope of a `MODEL` statement and the reference model (or base model) is also a COSAN model. The reference model is referred to as the old model, while the model that makes reference to this old model is referred to as the new model. If the new model is not intended to be an exact copy of the old model, you can use the following extended COSAN modeling language to make modifications within the scope of the `MODEL` statement for the new model. The syntax is similar to, but not exactly the same as, the ordinary COSAN modeling language. (See the section “COSAN Statement” on page 1122.) The respecification syntax for a COSAN model is as follows:

```

COSAN ;
          MATRIX matrix-name parameters-in-matrix ;
          /* Repeat the MATRIX statement as needed */ ;
          VARNAMES name-assignments ;

```

In the respecification, the COSAN statement is optional. In fact, the purpose of using the COSAN statement at all is to remind yourself that a COSAN model is used in the model definition. If you use the COSAN statement, you cannot specify the `VAR=` option or the covariance and mean structure formula. This means

that the model form and the observed variable references of the new model must be the same as the old (reference) model. The reason for enforcing these model structures is to ensure that the MATRIX statement respecifications are consistently interpreted.

You can optionally use the VARNAMES statement in the respecification. If the variable names for a COSAN matrix are defined in the old model but not redefined in the new model, all variable names for that matrix are duplicated in the new model. However, specification of variable names for a COSAN matrix in the new model overrides the corresponding specification in the old model.

You can respecify or modify the elements of the COSAN model matrices by using the **MATRIX** *matrix-name* statements. The syntax of the MATRIX statements for respecifications is the same as that in the ordinary COSAN modeling language, but with one more feature. In the respecification syntax, you can use the missing value '.' to drop a parameter specification from the old model.

The new model is formed by integrating with the old model in the following ways:

- Duplication: If you do not specify in the new model a parameter location that exists in the old model, the old parameter specification is duplicated in the new model.
- Addition: If you specify in the new model a parameter location that does not exist in the old model, the new parameter specification is used in the new model.
- Deletion: If you specify in the new model a parameter location that also exists in the old model and the new parameter is denoted by the missing value '.', the old parameter specification is not copied into the new model.
- Replacement: If you specify in the new model a parameter location that also exists in the old model and the new parameter is not denoted by the missing value '.', the new parameter specification replaces the old one in the new model.

For example, the following two-group analysis specifies Model 2 by referring to Model 1 in the **REF-MODEL** statement:

```
proc calis;
  group 1 / data=d1;
  group 2 / data=d2;
  model 1 / group=1;
  cosan
    var = x1-x6,
    F(2,GEN) * PHI(2,SYM) + PSI(6,SYM);
  matrix F
    [1,1] = 1.,
    [2,1] = load2,
    [3,1] = load3,
    [4,2] = 1.,
    [5,2] = load5,
    [6,2] = load6;
  matrix PHI
    [1,1] = phi1,
    [2,2] = phi2,
    [2,1] = phi21;
  matrix PSI
    [1,1] = psi1,
    [2,2] = psi2,
    [3,3] = psi3,
    [4,4] = psi4,
    [5,5] = psi5;
```

```

                                [6,6] = psi6;
varnames F    = [Factor1 Factor2],
        PHI = F;
model 2 / group=2;
  refmodel 1;
  matrix F          [3,1] = load2;    /* replacement */
  matrix PHI        [2,1] = .;        /* deletion */
  matrix PSI        [3,1] = psi31;    /* addition */
  varnames F    = [FF1 FF2],
run;

```

In this example, Model 2 is the new model which refers to the old model, Model 1. It illustrates the four types of model integration by using the MATRIX statements:

- Duplication: Except for the $F[3, 1]$ and $PHI[2, 1]$ elements, all parameter specifications in the old model are duplicated in the new model.
- Addition: The $PSI[3, 1]$ element is added with a new parameter $psi31$ in the new model. This indicates the presence of a correlated error in Model 2, but not in Model 1.
- Deletion: The $PHI[2, 1]$ element is no longer a free parameter in the new model. This means that the two latent factors are correlated in Model 1, but not in Model 2.
- Replacement: The $F[3, 1]$ element defined in Model 2 replaces the definition in the old model. This element is now a free parameter named $load2$. Because the $F[2, 1]$ element (via duplication from the old model) is also a free parameter with this same name, $F[3, 1]$ and $F[2, 1]$ are constrained to be the same in Model 2, but not in Model 1.

With the VARNAMES statement specification in Model 1, the two columns of matrix F are labeled with Factor1 and Factor2, respectively. In addition, because $PHI=F$ is specified in the VARNAMES statement of Model 1, the row and column of matrix PHI in Model 1 also contain Factor1 and Factor2 as the variable names. In Model 2, with the explicit VARNAMES specifications the two columns of matrix F are labeled with FF1 and FF2, respectively. These names are not the same as those for matrix F in the old (reference) model. However, because $PHI=F$ is *not* specified in the VARNAMES statement of Model 2, the row and column of matrix PHI in Model 2 contain Factor1 and Factor2 as the variable names, which are duplicated from the old (reference) model.

COSAN Models and Other Models

Because the COSAN model is a more general model than any other model considered in PROC CALIS, you can virtually fit any other type of model in PROC CALIS by using the COSAN modeling language. See the section “[Special Cases of the Generalized COSAN Model](#)” on page 1261, [Example 27.29](#), and [Example 27.30](#) for illustrations and discussions.

In general, it is recommended that you use the more specific modeling languages such as FACTOR, LINEQS, LISMOD, MSTRUCT, PATH, and RAM. Because the COSAN model is very general in its formulation, PROC CALIS cannot exploit the specific model structures to generate reasonable initial estimates the way it does with other specific models such as FACTOR and PATH. If you do not provide initial estimates for a COSAN model, PROC CALIS uses some default starting values such as 0.5. See the **START=** option for controlling the starting value. See the **RANDOM=** option for setting random starting values. There are

other reasons for preferring specific modeling languages whenever possible. The section “Which Modeling Language?” on page 1077 discusses these various reasons. However, when the covariance structures are complicated and are difficult to specify otherwise, the COSAN modeling language is a very useful tool. See Example 27.31 and Example 27.33 for illustrations.

COV Statement

COV *assignment* <, *assignment* ... >;

where *assignment* represents

var-list < * *var-list2* > < = *parameter-spec* >

The COV statement is a subsidiary model specification statement for the confirmatory **FACTOR** and **LINEQS** models. In the LINEQS model, the COV statement defines the covariances among the exogenous variables, including errors and disturbances. In the confirmatory FACTOR model, the COV statement defines the factor covariances. In each *assignment* of the COV statement, you specify variables in the *var-list* and the *var-list2* lists, followed by the covariance parameter specification in the *parameter-spec* list. The latter two specifications are optional.

You can specify the following five types of the parameters for the covariances:

- an unnamed free parameter
- an initial value
- a fixed value
- a free parameter with a name provided
- a free parameter with a name and initial value provided

Consider a LINEQS model with exogenous variables V1, V2, V3, and V4. The following COV statement shows the five types of specifications in five *assignments*:

```

cov v2 v1 ,
    v3 v1 = (0.3) ,
    v3 v2 = 1.0 ,
    v4 v1 = phi1 ,
    v4 v2 = phi2 (0.2) ;

```

In this statement, **cov(v2,v1)** is specified as an unnamed free parameter. For this covariance, PROC CALIS generates a parameter name with the `_Parm` prefix and appended with a unique integer (for example, `_Parm1`). **cov(v3,v1)** is an unnamed free parameter but with an initial value of 0.3. PROC CALIS also generates a parameter name for this covariance. **cov(v3,v2)** is a fixed value of 1.0. This value stays the same in the estimation. **cov(v4,v1)** is a free parameter named `phi1`. **cov(v4,v2)** is a free parameter named `phi2` with an initial value of 0.2.

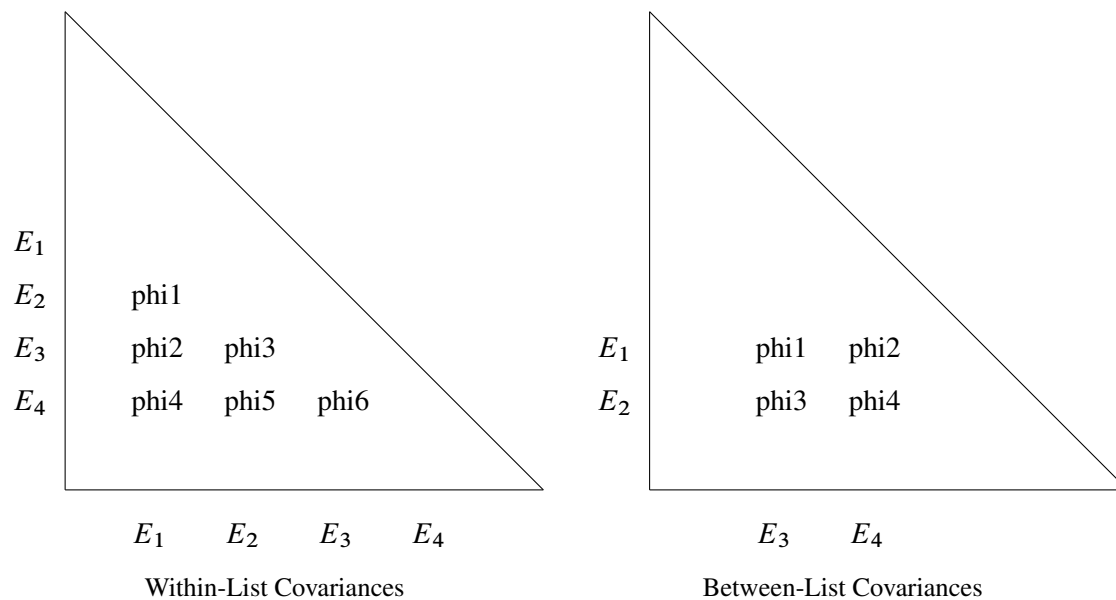
Note that the *var-list* and *var-list2* lists on the left-hand side of the equal sign of the COV statement should contain only names of *exogenous* variables. Hence, the COV statement is different from the **PCOV** statement

in which you can list both exogenous and endogenous variables, although the COV and PCOV statements share the same syntax.

You can use the COV statement for specifying covariance parameters in the **FACTOR** and **LINEQS** models. In the **FACTOR** model, the COV statement specifies the covariances among latent factors. In the **LINEQS** model, the COV statement specifies the covariances among all observed or latent exogenous variables, including error and disturbance terms.

If you specify only the *var-list* list, then you are specifying the so-called within-list covariances. If you specify both of the *var-list* and *var-list2* lists, then you are specifying the so-called between-list covariances. An asterisk is used to separate the two variable lists. You can use one of these two alternatives to specify the covariance parameters. **Figure 27.2** illustrates the within-list and between-list covariance specifications.

Figure 27.2 Within-List and Between-List Covariances



Within-List Covariances

The left panel of the figure shows that the same set of four variables are used in both the rows and columns. This yields six nonredundant covariances to specify. In general, with a *var-list* list with k variables in the COV statement, there are $k(k - 1)/2$ distinct covariance parameters you can specify. The variable order of the *var-list* list is important. For example, the left panel of **Figure 27.2** corresponds to the following COV statement specification:

```
cov E1-E4 = phi1-phi6;
```

This specification is equivalent to the following specification:

```
cov E2 E1 = phi1,
    E3 E1 = phi2, E3 E2 = phi3,
    E4 E1 = phi4, E4 E2 = phi5, E4 E3 = phi6;
```

Another way to assign distinct parameter names with the same prefix is to use the so-called prefix-name. For example, the following COV statement specification is exactly the same as the preceding specification:


```
cov E1-E4 = 6*phi__; /* phi with two trailing underscores */
```

In the COV statement, `phi__` is a prefix-name with the root `phi`. The notation `6*` means this prefix-name is applied six times, resulting in a generation of the six parameter names `phi1`, `phi2`, ..., `phi6` for the six covariance parameters.

The root of the prefix-name should have few characters so that the generated parameter name is not longer than 32 characters. To avoid unintentional equality constraints, the prefix-names should not coincide with other parameter names.

You can also specify the within-list covariances as unnamed free parameters, as shown in the following statement:

```
cov E1-E4;
```

This specification is equivalent to the following specification:

```
cov E2 E1,
    E3 E1, E3 E2,
    E4 E1, E4 E2, E4 E3;
```

Between-List Covariances

The right panel of [Figure 27.2](#) illustrates the application of the between-list covariance specification. The set of row variables is different from the set of column variables. You intend to specify the cross covariances of the two sets of variables. There are four of these covariances in the figure. In general, with k_1 and k_2 variable names in the two variable lists (separated by an asterisk) in a COV statement, there are $k_1 \times k_2$ distinct covariances to specify. Again, variable order is very important. For example, the right panel of [Figure 27.2](#) corresponds to the following between-list covariance specification:

```
cov E1 E2 * E3 E4 = phi1-phi4;
```

This is equivalent to the following specification:

```
cov E1 E3 = phi1, E1 E4 = phi2,
    E2 E3 = phi3, E2 E4 = phi4;
```

You can also use the prefix-name specification for the same specification, as shown in the following statement:

```
cov E1 E2 * E3 E4 = 4*phi__ ; /* phi with two trailing underscores */
```

Mixed Parameter Lists

You can specify different types of parameters for the list of covariances. For example, you use a list of parameters with mixed types in the following statement:

```
cov E1-E4 = phi1(0.1) 0.2 phi3 phi4(0.4) (0.5) phi6;
```

This specification is equivalent to the following specification:

```

cov E2 E1 = phi1(0.1) ,
    E3 E1 = 0.2          , E3 E2 = phi3,
    E4 E1 = phi4(0.4) , E4 E2 = (0.5), E4 E3 = phi6;

```

Notice that an initial value that follows a parameter name is associated with the free parameter. Therefore, in the original mixed list specification, 0.1 is interpreted as the initial value for the parameter `phi1`, but not as the initial estimate for the covariance between E3 and E1. Similarly, 0.4 is the initial value for the parameter `phi4`, but not the initial estimate for the covariance between E4 and E2.

However, if you indeed want to specify that `phi1` is a free parameter *without* an initial value and 0.1 is an initial estimate for the covariance between E3 and E1 (while keeping all other things the same), you can use a null initial value specification for the parameter `phi1`, as shown in the following statement:

```

cov E1-E4 = phi1() (0.1) phi3 phi4(0.4) (0.5) phi6;

```

This way 0.1 becomes the initial estimate for the covariance between E3 and E1. Because a parameter list with mixed types might be confusing, you can break down the specifications into separate *assignments* to remove ambiguities. For example, you can use the following equivalent specification:

```

cov E2 E1 = phi1 ,
    E3 E1 = (0.1)          , E3 E2 = phi3,
    E4 E1 = phi4(0.4) , E4 E2 = (0.5), E4 E3 = phi6;

```

Shorter and Longer Parameter Lists

If you provide fewer parameters than the number of covariances in the variable lists, all the remaining parameters are treated as unnamed free parameters. For example, the following specification assigns a fixed value to `cov(E1, E3)` while treating all the other three covariances as unnamed free parameters:

```

cov E1 E2 * E3 E4 = 1.0;

```

This specification is equivalent to the following specification:

```

cov E1 E3 = 1.0, E1 E4, E2 E3, E2 E4;

```

If you intend to fill up all values by the last parameter specification in the list, you can use the continuation syntax `[...]`, `[. . .]`, or `[.]`, as shown in the following example:

```

cov E1 E2 * E3 E4 = 1.0 phi [...];

```

This means that `cov(E1, E3)` is a fixed value of 1 and all the remaining three covariances are free parameter named `phi`. The last three covariances are thus constrained to be equal by using the same parameter name.

However, you must be careful not to provide too many parameters. For example, the following specification results in an error:

```

cov E1 E2 * E3 E4 = 1.0 phi2(2.0) phi3 phi4 phi5 phi6;

```

The parameters after `phi4` are excessive.

Default Covariance Parameters

In the confirmatory FACTOR model, by default all factor covariances are free parameters. In the LINEQS model, by default all covariances among exogenous manifest and latent variables (excluding error or disturbance variables) are also free parameters. For these default free parameters, PROC CALIS generate the parameter names with the `_Add` prefix and appended with unique integer suffixes. You can also use the COV statement specification to override these default covariance parameters in situations where you want to set parameter constraints, provide initial or fixed values, or make parameter references.

Another type of default covariances are fixed zeros. In the LINEQS model, covariances among errors or disturbances are all fixed zeros by default. Again, you can override the default fixed values by providing explicit specification of these covariances in the COV statement.

Modifying a Covariance Parameter Specification from a Reference Model

If you define a new model by using a reference (old) model in the `REFMODEL` statement, you might want to modify some parameter specifications from the COV statement of the reference model before transferring the specifications to the new model. To change a particular covariance specification from the reference model, you can simply respecify the same covariance with the desired parameter specification in the COV statement of the new model. To delete a particular covariance parameter from the reference model, you can specify the desired covariance with a missing value specification in the COV statement of the new model.

For example, suppose that the covariance between variables V1 and V2 is specified in the reference model but you do not want this covariance specification be transferred to the new model. You can use the following COV statement specification in the new model:

```
cov v1 v2 = . ;
```

Note that the missing value syntax is valid only when you use it with the `REFMODEL` statement. See the section “[Modifying a LINEQS Model from a Reference Model](#)” on page 1160 for a more detailed example of the LINEQS model respecification with the `REFMODEL` statement. See the section “[Modifying a FACTOR Model from a Reference Model](#)” on page 1146 for a more detailed example of the FACTOR model respecification with the `REFMODEL` statement.

As discussed in a preceding section, PROC CALIS generates some default free covariance parameters for the LINEQS and FACTOR models if you do not specify them explicitly in the COV statement. When you use the `REFMODEL` statement for defining a reference model, these default free covariance parameters in the old (reference) model are not transferred to the new model. Instead, the new model generates its own set of default free covariance parameters *after* it is resolved from the reference model, the `REFMODEL` statement options, the `RENAMEPARM` statement, and the COV statement specifications in the new model. This also implies that if you want any of the covariance parameters to be constrained across the models by means of the `REFMODEL` specification, you must specify them explicitly in the COV statement of the reference model so that the same covariance specification is transferred to the new model.

DETERM Statement

```
DETERM | STRUCTEQ variables </ option > ;
```

where *option* represents:

LABEL | NAME= *name*

The DETERM statement is used to compute the determination coefficient of the listed dependent *variables* in the model. The precursor of the DETERM statement is the STRUCTEQ statement, which enables you to define the list of the dependent variables of the structural equations. Because the term *structural equation* is not defined in a unique way, a more generic concept of determination coefficients is revealed by the DETERM statement.

You can specify the DETERM statement as many times as you want for computing determination coefficients for the sets of dependent *variables* of interest. You can label each set of dependent variables by using the LABEL= option. Note that you cannot use the DETERM statement in an MSTRUCT model because there are no dependent variables in this type of model.

EFFPART Statement

EFFPART *effect* <, *effect*> ;

where *effect* represents:

var-list < *direction var-list2*>

and *direction* is the direction of the effect, as indicated by one of the following: ==>, --->, ==>, -->, =>, ->, >, <==, <---, <==, <--, <=, <-, or <.

In the EFFPART statement, you select those effects you want to analyze by partitioning the total effects into direct and indirect effects, with estimated standard errors. The EFFPART or TOTEFF option of the PROC CALIS statement also enables you to analyze effects. The difference is that the EFFPART or TOTEFF option displays effects on *all* endogenous variables, while the EFFPART statement shows only the effects of interest. In addition, the EFFPART statement enables you to arrange the effects in any way you like. Hence, the EFFPART statement offers a more precise and organized way to present various results of effects.

The EFFPART statement supports the following three types of effect specifications:

- >, =>, ->, ==>, -->, ===>, or ----> direction

Example:

```
effpart x1 x3-x5 ==> y1 y2;
```

This will display *four* separate tables, respectively for the effects of X1, X3, X4, and X5 on Y1 and Y2. Each table contains the total, direct, and indirect effects of an X-variable on the two Y-variables.

- <, <=, <-, <==, <--, <===, or <---- direction

Example:

```
effpart Y1 Y2 <=== X1 X3-X5;
```

This will display *two* separate tables, respectively for the effects on Y1 and Y2, by X1, X3, X4, and X5. Each table contains the total, direct, and indirect effects of the four X-variables on a Y-variable. Certainly, the results produced from this statement are essentially the same as the previous statement. The difference is about the organization of the effects in the tables.

- no direction

Example:

```
effpart Y1 Y2 X1-X3;
```

In this case, variables on the list are analyzed one by one to determine the nature of the effects. If a variable has nonzero effects on any other variables in the model, a table of the total, direct, and indirect effects of the variable on those variables is displayed. If a variable is endogenous, a table of total, direct, and indirect effects of those variables that have nonzero effects on the variable is displayed. Note that an endogenous variable in a model might also have effects on other endogenous variables. Therefore, the two cases mentioned are not mutually exclusive—a variable listed in the EFFPART statement might yield two tables for effect analysis.

FACTOR Statement

```
FACTOR < EFA-options | CFA-spec > ;
```

where *EFA-options* are options for the exploratory factor analysis that are described in the section “[Exploratory Factor Analysis](#)” on page 1138 and *CFA-spec* is a specification of confirmatory factor analysis that is described in the section “[Confirmatory Factor Analysis](#)” on page 1142.

In the FACTOR statement, you can specify either *EFA-options*, *CFA-spec*, or neither of these. However, you cannot specify both *EFA-options* and *CFA-spec* at the same time. If no option is specified or there is at least one *EFA-option* (exploratory factor analysis option) specified in the FACTOR statement, an [exploratory factor model](#) is analyzed. Otherwise, a [confirmatory factor model](#) is analyzed with the *CFA-spec*. These two types of models are discussed in the next two sections.

Exploratory Factor Analysis

```
FACTOR < EFA-options > ;
```

For the exploratory factor model with orthogonal factors, PROC CALIS assumes the following model structures for the population covariance or correlation matrix Σ :

$$\Sigma = \mathbf{F}\mathbf{F}' + \mathbf{U}$$

where \mathbf{F} is the factor loading matrix and \mathbf{U} is a diagonal matrix of error variances. In this section, p denotes the number of manifest variables corresponding to the rows and columns of matrix Σ , and n denotes the number of factors (or components, if the [COMPONENT](#) option is specified in the FACTOR statement)

corresponding to the columns of the factor loading matrix \mathbf{F} . While the number of manifest variables is set automatically by the number of variables in the **VAR** statement or in the input data set, the number of factors can be set by the **N=** option in the **FACTOR** statement.

The unrestricted exploratory factor model is not identified because any orthogonal rotated factor loading matrix $\tilde{\mathbf{F}} = \mathbf{F}\mathbf{\Theta}$ satisfies the same model structures as \mathbf{F} does, where $\mathbf{\Theta}$ is any orthogonal matrix so that $\mathbf{\Theta}'\mathbf{\Theta} = \mathbf{\Theta}\mathbf{\Theta}' = \mathbf{I}$. Mathematically, the covariance or correlation structures can be expressed as:

$$\Sigma = \tilde{\mathbf{F}}\tilde{\mathbf{F}}' + \mathbf{U} = \mathbf{F}\mathbf{\Theta}\mathbf{\Theta}'\mathbf{F}' + \mathbf{U} = \mathbf{F}\mathbf{F}' + \mathbf{U}$$

To obtain an identified orthogonal factor solution as a starting point, the $n(n - 1)/2$ elements in the upper triangle of \mathbf{F} are constrained to zeros in **PROC CALIS**. Initial estimates for factor loadings and unique variances are computed by an algebraic method of approximate factor analysis. Given the initial estimates, final estimates are obtained through the iterative optimization of an objective function, which depends on the estimation method specified in the **METHOD=** option (default with **ML**—maximum likelihood) of the **PROC CALIS** statement.

To make the factor solution more interpretable, you can use the **ROTATE=** option in the **FACTOR** statement to obtain a rotated factor loading matrix with a “simple” pattern. Rotation can be orthogonal or oblique. The rotated factors remain uncorrelated after an orthogonal rotation but would be correlated after an oblique rotation. The model structures of an oblique solution are expressed in the following equation:

$$\Sigma = \tilde{\mathbf{F}}\tilde{\mathbf{P}}\tilde{\mathbf{F}}' + \mathbf{U}$$

where $\tilde{\mathbf{F}}$ is the rotated factor loading matrix and $\tilde{\mathbf{P}}$ is a symmetric matrix for factor correlations. See the sections “[The FACTOR Model](#)” on page 1263 and “[Exploratory Factor Analysis Models](#)” on page 1265 for more details about exploratory factor models.

You can also do exploratory factor analysis by the more dedicated **FACTOR** procedure. Even though extensive comparisons of the factor analysis capabilities between the **FACTOR** and **CALIS** procedures are not attempted here, some general points can be made here. In general, the **FACTOR** procedure provides more factor analysis options than the **CALIS** procedure does, although both procedures have some unique factor analysis features that are not shared by the other. **PROC CALIS** requires more computing time and memory than **PROC FACTOR** because it is designed for more general structural estimation problems and is not able to exploit all the special properties of the unconstrained factor analysis model. For maximum likelihood analysis, you can use either **PROC FACTOR** (with **METHOD=ML**, which is not the default method in **PROC FACTOR**) or **PROC CALIS**. Because the initial unrotated factor solution obtained by **PROC FACTOR** uses a different set of identification constraints than that of **PROC CALIS**, you would observe different initial **ML** factor solutions for the procedures. Nonetheless, the initial solutions by both procedures are statistically equivalent.

The following *EFA-options* are available in the **FACTOR** statement:

COMPONENT | COMP

computes a component analysis instead of a factor analysis (the diagonal matrix \mathbf{U} in the model is set to 0). Note that the rank of $\mathbf{F}\mathbf{F}'$ is equal to the number n of components in \mathbf{F} . If n is smaller than the number of variables in the moment matrix Σ , the matrix of predicted model values is singular and maximum likelihood estimates for \mathbf{F} cannot be computed. You should compute **ULS** estimates in this case.

HEYWOOD | HEY

constrains the diagonal elements of **U** to be nonnegative. Equivalently, you can constrain these elements to positive values by the **BOUNDS** statement.

GAMMA=*p*

specifies the orthomax weight used with the option **ROTATE=ORTHOMAX**. Alternatively, you can use **ROTATE=ORTHOMAX(*p*)** with *p* representing the orthomax weight. There is no restriction on valid values for the orthomax weight, although the most common values are between 0 and the number of variables. The default **GAMMA=** value is one, resulting in the varimax rotation.

N=*n*

specifies the number of first-order factors or components. The number of factors (*n*) should not exceed the number of manifest variables (*p*) in the analysis. For the saturated model with $n = p$, the **COMP** option should generally be specified for **U** = 0; otherwise, $df < 0$. For $n = 0$ no factor loadings are estimated, and the model is $\Sigma = U$, with a diagonal **U** matrix. By default, $n = 1$.

NORM< = KAISER | NONE >

Kaiser-normalizes the rows of the factor pattern for rotation. **NORM=KAISER**, which is the default, has exactly the same effect as **NORM**. You can turn off the normalization by **NORM=NONE**.

RCONVERGE=*p***RCONV=*p***

specifies the convergence criterion for rotation cycles. Rotation stops when the scaled change of the simplicity function value is less than the **RCONVERGE=** value. The default convergence criterion is:

$$|f_{new} - f_{old}|/K < \epsilon$$

where f_{new} and f_{old} are simplicity function values of the current cycle and the previous cycle, respectively, $K = \max(1, |f_{old}|)$ is a scaling factor, and ϵ is 1E-9 by default and is modified by the **RCONVERGE=** value.

RITER=*i*

specifies the maximum number of cycles *i* for factor rotation. The default *i* is the greater of 10 times the number of variables and 100.

ROTATE | R=*name*

specifies an orthogonal or oblique rotation of the initial factor solution. Although **ROTATE=PRINCIPAL** is actually not a rotation method, it is put here for convenience. By default, **ROTATE=NONE**.

Valid *names* for orthogonal rotations are as follows:

BIQUARTIMAX | BIQMAX specifies orthogonal biquartimax rotation. This corresponds to the specification **ROTATE=ORTHOMAX(0.5)**.

EQUAMAX | E specifies orthogonal equamax rotation. This corresponds to the specification **ROTATE=ORTHOMAX** with **GAMMA=*n*/2**.

FACTORPARSIMAX | FPA specifies orthogonal factor parsimax rotation. This corresponds to the specification **ROTATE=ORTHOMAX** with **GAMMA=*n***.

NONE | N specifies that no rotation be performed, leaving the original orthogonal solution.

ORTHCF($p1,p2$) | **ORCF**($p1,p2$) specifies the orthogonal Crawford-Ferguson rotation (Crawford and Ferguson 1970) with the weights $p1$ and $p2$ for variable parsimony and factor parsimony, respectively. See the definitions of weights in Chapter 35, “The FACTOR Procedure.”

ORTHGENCF($p1,p2,p3,p4$) | **ORGENCF**($p1,p2,p3,p4$) specifies the orthogonal generalized Crawford-Ferguson rotation (Jennrich 1973), with the four weights $p1$, $p2$, $p3$, and $p4$. For the definitions of these weights, see the section “Simplicity Functions for Rotations” on page 2244 in Chapter 35, “The FACTOR Procedure.”

ORTHOMAX<($p1$)> | **ORMAX**<($p1$)> specifies the orthomax rotation (see Harman 1976) with orthomax weight $p1$. If ROTATE=ORTHOMAX is used, the default $p1$ value is 1 unless specified otherwise in the GAMMA= option. Alternatively, ROTATE=ORTHOMAX($p1$) specifies $p1$ as the orthomax weight or the GAMMA= value. For the definitions of the orthomax weight, see the section “Simplicity Functions for Rotations” on page 2244 in Chapter 35, “The FACTOR Procedure.”

PARSIMAX | **PA** specifies orthogonal parsimax rotation. This corresponds to the specification ROTATE=ORTHOMAX with

$$\text{GAMMA} = \frac{p \times (n - 1)}{p + n - 2}$$

PRINCIPAL | **PC** specifies a principal axis rotation. If ROTATE=PRINCIPAL is used with a factor rather than a component model, the following rotation is performed:

$$\mathbf{F}_{new} = \mathbf{F}_{old} \mathbf{T}, \quad \text{with} \quad \mathbf{F}'_{old} \mathbf{F}_{old} = \mathbf{T} \mathbf{\Lambda} \mathbf{T}'$$

where the columns of matrix \mathbf{T} contain the eigenvectors of $\mathbf{F}'_{old} \mathbf{F}_{old}$.

QUARTIMAX | **QMAX** | **Q** specifies orthogonal quartimax rotation. This corresponds to the specification ROTATE=ORTHOMAX(0).

VARIMAX | **V** specifies orthogonal varimax rotation. This corresponds to the specification ROTATE=ORTHOMAX with GAMMA=1.

Valid *names* for oblique rotations are as follows:

BIQUARTIMIN | **BIQMIN** specifies biquartimin rotation. It corresponds to the specification ROTATE=OBLIMIN(.5) or ROTATE=OBLIMIN with TAU=.5.

COVARIMIN | **CVMIN** specifies covarimin rotation. It corresponds to the specification ROTATE=OBLIMIN(1) or ROTATE=OBLIMIN with TAU=1.

OBBIQUARTIMAX | **OBIQMAX** specifies oblique biquartimax rotation.

OBEQUAMAX | **OE** specifies oblique equamax rotation.

OBFACTORPARSIMAX | **OFPA** specifies oblique factor parsimax rotation.

OBLICF($p1,p2$) | **OBCF**($p1,p2$) specifies the oblique Crawford-Ferguson rotation (Crawford and Ferguson 1970) with the weights $p1$ and $p2$ for variable parsimony and factor parsimony, respectively. For the definitions of these weights, see the section “Simplicity Functions for Rotations” on page 2244 in Chapter 35, “The FACTOR Procedure.”

OBLIGENCF($p1, p2, p3, p4$) | **OBGENCF**($p1, p2, p3, p4$) specifies the oblique generalized Crawford-Ferguson rotation (Jennrich 1973) with the four weights $p1$, $p2$, $p3$, and $p4$. For the definitions of these weights, see the section “Simplicity Functions for Rotations” on page 2244 in Chapter 35, “The FACTOR Procedure.”

OBLIMIN<($p1$)> | **OBMIN**<($p1$)> specifies the oblimin rotation with oblimin weight $p1$. If **ROTATE=OBLIMIN** is used, the default $p1$ value is zero unless specified otherwise in the **TAU=** option. Alternatively, **ROTATE=OBLIMIN**($p1$) specifies $p1$ as the oblimin weight or the **TAU=** value. For the definitions of the oblimin weight, see the section “Simplicity Functions for Rotations” on page 2244 in Chapter 35, “The FACTOR Procedure.”

OBPARSIMAX | **OPA** specifies oblique parsimax rotation.

OBQUARTIMAX | **OQMAX** specifies oblique quartimax rotation. This is the same as the **QUARTIMIN** method.

OBVARIMAX | **OV** specifies oblique varimax rotation.

QUARTIMIN | **QMIN** specifies quartimin rotation. It is the same as the oblique quartimax method. It also corresponds to the specification **ROTATE=OBLIMIN**(0) or **ROTATE=OBLIMIN** with **TAU=0**.

TAU= p

specifies the oblimin weight used with the option **ROTATE=OBLIMIN**. Alternatively, you can use **ROTATE=OBLIMIN**(p) with p representing the oblimin weight. There is no restriction on valid values for the oblimin weight, although for practical purposes a negative or zero value is recommended. The default **TAU=** value is 0, resulting in the quartimin rotation.

Confirmatory Factor Analysis

FACTOR *factor-variables-relation* <, *factor-variables-relation* . . . > ;

where each *factor-variables-relation* is defined as

factor *right-arrow* *var-list* < = *parameter-spec* >

where *right-arrow* is one of the following: **===>**, **---->**, **==>**, **--->**, **=>**, **->**, or **>**.

To complete the specification of a confirmatory factor model, you might need to use the **PVAR**, **COV**, and **MEAN** statements to specify the variance, partial variance, covariance, and mean parameters in the model, as shown in the following syntax:

```
FACTOR factor-variable-relation <, factor-variables-relation . . . > ;
PVAR partial-variance-parameters ;
COV covariance-parameters ;
MEAN mean-parameters ;
```

The model structures for the covariance matrix Σ of the confirmatory factor model are described in the equation

$$\Sigma = \mathbf{FPF}' + \mathbf{U}$$

where \mathbf{F} is the factor loading matrix, \mathbf{P} is a symmetric matrix for factor correlations, and \mathbf{U} is a diagonal matrix of error variances.

If the mean structures are also analyzed, the model structures for the mean vector $\boldsymbol{\mu}$ of the confirmatory factor model are described in the equation

$$\boldsymbol{\mu} = \boldsymbol{\alpha} + \mathbf{F}\boldsymbol{\nu}$$

where $\boldsymbol{\alpha}$ is the intercept vector for the observed variables and $\boldsymbol{\nu}$ is the vector for factor means. See the sections “The FACTOR Model” on page 1263 and “Confirmatory Factor Analysis Models” on page 1266 for more details about confirmatory factor models.

The FACTOR statement is the main model specification statement for the confirmatory factor model. The specifications in the FACTOR statement concern the factor loading pattern in the \mathbf{F} matrix. More details follow after a brief description of the subsidiary model specification statements: PVAR, COV, and MEAN.

By default, the factor variance parameters in the diagonal of matrix \mathbf{P} and the error variances in the diagonal of matrix \mathbf{U} are free parameters in the confirmatory factor model. However, you can override these default parameters by specifying them explicitly in the PVAR statement. For example, in some confirmatory factor models, you might want to set some of these variances to fixed constants, or you might want to set equality constraints by using the same parameter name at different parameter locations in your model.

By default, factor covariances, which are the off-diagonal elements of matrix \mathbf{P} , are free parameters in the confirmatory factor model. However, you can override these default covariance parameters by specifying them explicitly in the COV statement. Note that you cannot use the COV statement to specify the error covariances—they are always fixed zeros in the confirmatory factor analysis model.

By default, all factor means are fixed zeros and all intercepts are free parameters if the mean structures are analyzed. You can override these defaults by explicitly specifying the means of the factors in vector $\boldsymbol{\nu}$ and the intercepts of the manifest variables in vector $\boldsymbol{\alpha}$ in the MEAN statement.

Because the default parameterization of the confirmatory FACTOR model already covers most commonly used parameters in matrices \mathbf{P} , \mathbf{U} , $\boldsymbol{\alpha}$, and $\boldsymbol{\nu}$, the specifications in the PVAR, COV, and MEAN statements are secondary to the specifications in the FACTOR statement, which specifies the factor pattern of the \mathbf{F} matrix. The following example statement introduces the syntax of the confirmatory FACTOR statement. Suppose that there are nine manifest variables V1–V9 in your sample and you want to fit a model with four factors, as shown in the following FACTOR statement:

```
factor
  g_factor    ===>  V1-V9 ,
  factor_a    ===>  V1-V3 ,
  factor_b    ===>  V4-V6 ,
  factor_c    ===>  V7-V9 ;
```

In this factor model, you assume a general factor `g_factor` and three group-factors: `factor_a`, `factor_b`, and `factor_c`. The general factor `g_factor` is related to all manifest variables in the sample, while each group-factor is related only to three manifest variables. This example fits the following pattern of factor pattern of \mathbf{F} :

	g_factor	factor_a	factor_b	factor_c
V1	x	x		
V2	x	x		
V3	x	x		
V4	x		x	
V5	x		x	
V6	x		x	
V7	x			x
V8	x			x
V9	x			x

where an x represents an unnamed free parameter and all other cells that are blank are fixed zeros. For each of these unnamed parameters, PROC CALIS generates a parameter name with the `_Parm` prefix and appended with a unique integer (for example, `_Parm1`, `_Parm2` and so on).

An unnamed free parameter is only one of the following five types of parameters (*parameter-spec*) you can specify at the end of each *factor-variables-relation*:

- an unnamed free parameter
- an initial value
- a fixed value
- a free parameter with a name provided
- a free parameter with a name and initial value provided

To illustrate these different types of parameter specifications, consider the following factor pattern for **F**:

	g_factor	factor_a	factor_b	factor_c
V1	<code>g_load1</code>	1.		
V2	<code>g_load2</code>	x		
V3	<code>g_load3</code>	x		
V4	<code>g_load4</code>		1.	
V5	<code>g_load5</code>		<code>load_a</code>	
V6	<code>g_load6</code>		<code>load_b</code>	
V7	<code>g_load7</code>			1.
V8	<code>g_load8</code>			<code>load_c</code>
V9	<code>g_load9</code>			<code>load_c</code>

where an x represents an unnamed free parameter, a constant 1 represents a fixed value, and each name in a cell represents a name for a free parameter. You can specify this factor pattern by using the following FACTOR statement:

```
factor
  g_factor  ==>  V1-V9    = g_load1-g_load9 (9*0.6),
  factor_a  ==>  V1-V3    = 1. (.7 .8),
  factor_b  ==>  V4-V6    = 1. load_a (.9) load_b,
  factor_c  ==>  V7-V9    = 1. 2*load_c ;
```

In the first entry of the FACTOR statement, you specify that the loadings of V1–V9 on g_factor are free parameters g_load1–g_load9 with all given an initial estimate of 0.6. The syntax 9*0.6 means that 0.6 is repeated nine times. Because they are enclosed in a pair parentheses, all these values are treated as initial estimates, but not fixed values.

The second entry of the FACTOR statement can be split into the following specification:

```
factor_a    ===>  V1    = 1.  ,
factor_a    ===>  V2    = (.7) ,
factor_a    ===>  V3    = (.8) ,
```

This means that the first loading is a fixed value of 1, while the other loadings are unnamed free parameters with initial estimates 0.7 and 0.8, respectively. For each of these unnamed parameters with initial values, PROC CALIS also generates a parameter name with the _Parm prefix and appended with a unique integer.

The third entry of the FACTOR statement can be split into the following specification:

```
factor_b    ===>  V4    = 1.  ,
factor_b    ===>  V5    = load_a (.9) ,
factor_b    ===>  V6    = load_b ,
```

This means that the first loading is a fixed value of 1, the second loading is a free parameter named load_a with an initial estimate of 0.9, and the third loading is a free parameter named load_b without an initial estimate. PROC CALIS generates the initial value for this free parameter.

The fourth entry of the FACTOR statement states that the first loading is a fixed 1 and the remaining two loadings are free parameters named load_c. No initial estimate is given. But because the two loadings have the same parameter name, they are constrained to be equal in the estimation.

Notice that an initial value that follows after a parameter name is associated with the free parameter. For example, in the third entry of the FACTOR statement, the specification (.9) after load_a is interpreted as the initial value for the parameter load_a, but not as the initial estimate for the next loading for V6.

However, if you indeed want to specify that load_a is a free parameter *without* an initial value and (0.9) is an initial estimate for the loading for V6, you can use a null initial value specification for the parameter load_a, as shown in the following specification:

```
factor_b    ===>  V4-V6  = 1. load_a() (.9) ,
```

This way 0.9 becomes the initial estimate of the loading for V6. Because a parameter list with mixed parameter types might be confusing, you can split the specification into separate entries to remove ambiguities. For example, you can use the following equivalent specification:

```
factor_b    ===>  V4    = 1. ,
factor_b    ===>  V5    = load_a ,
factor_b    ===>  V6    = (.9) ,
```

Shorter and Longer Parameter Lists

If you provide fewer parameters than the number of loadings that are specified in the corresponding *factor-variable-relation*, all the remaining parameters are treated as unnamed free parameters. For example, the following specification assigns a fixed value of 1.0 to the first loading, while treating the remaining two loadings as unnamed free parameters:

```
factor
  factor_a   ==>  V1-V3   = 1.;
```

This specification is equivalent to the following specification:

```
factor
  factor_a   ==>  V1      = 1.,
  factor_a   ==>  V2 V3   ;
```

If you intend to fill up all values with the last parameter specification in the list, you can use the continuation syntax [...], [...], or [...], as shown in the following example:

```
factor
  g_factor   ==>  V1-V30   = 1. (.5) [...];
```

This means that the loading of V1 on g_factor is a fixed value of 1.0, while the remaining 29 loadings are unnamed free parameters with all given an initial estimate of 0.5.

However, you must be careful not to provide too many parameters. For example, the following specification results in an error:

```
factor
  g_factor   ==>  V1-V3   = load1-load6;
```

The parameter list has six parameters for three loadings. Parameters after load3 are excessive.

Default Parameters

It is important to understand the default parameters in the FACTOR model. First, if you know which parameters are default free parameters, you can make your specification more efficient by omitting the specifications of those parameters that can be set by default. For example, because all error variances in the confirmatory FACTOR model are free parameters by default, you do not need to specify them with the PVAR statement if these error variances are not constrained. Second, if you know which parameters are default free parameters, you can specify your model accurately. For example, because all factor variance and covariances in the confirmatory FACTOR model are free parameters by default, you must use the COV statement to restrict the covariances among the factors if you want to fit an orthogonal factor model. See the section “Default Parameters in the FACTOR Model” on page 1270 for details about the default parameters of the FACTOR model.

Modifying a FACTOR Model from a Reference Model

This section assumes that you use a REFMODEL statement within the scope of a MODEL statement and that the reference model (or base model) is a factor model, either exploratory or confirmatory. The reference model is called the old model, and the model that refers to the old model is called the new model. If the new model is not intended to be an exact copy of the old FACTOR model, you can use the extended FACTOR modeling language described in this section to make modifications from the old model before transferring the specifications to the new model.

Using the **REFMODEL** statement for defining new factor models is not recommended in the following cases:

- If your old model is an exploratory factor analysis model, then specification by using the **FACTOR** modeling language in the new model replaces the old model completely. In this case, the use of the **REFMODEL** statement is superfluous and should be avoided.
- If your old model is a confirmatory factor analysis model, then specification of an exploratory factor model by using the **FACTOR** statement in the new model also replaces the old model completely. Again, the use of the **REFMODEL** statement is superfluous and should be avoided.

The nontrivial case where you might find the **REFMODEL** statement useful is when you modify an old confirmatory factor model to form a new confirmatory factor model. This nontrivial case is the focus of discussion in the remaining of the section.

The extended **FACTOR** modeling language for modifying model specification bears the same syntax as that of the ordinary **FACTOR** modeling language (see the section “**Confirmatory Factor Analysis**” on page 1142). The syntax is:

```
FACTOR factor-variable-relation ;
PVAR partial-variance-parameters ;
COV covariance-parameters ;
MEAN mean-parameters ;
```

The new model is formed by integrating with the old model in the following ways:

- Duplication: If you do not specify in the new model a parameter location that exists in the old model, the old parameter specification is duplicated in the new model.
- Addition: If you specify in the new model a parameter location that does not exist in the old model, the new parameter specification is added in the new model.
- Deletion: If you specify in the new model a parameter location that also exists in the old model and the new parameter is denoted by the missing value ‘.’, the old parameter specification is not copied into the new model.
- Replacement: If you specify in the new model a parameter location that also exists in the old model and the new parameter is not denoted by the missing value ‘.’, the new parameter specification replaces the old one in the new model.

For example, consider the following two-group analysis:

```

proc calis;
  group 1 / data=d1;
  group 2 / data=d2;
  model 1 / group=1;
    factor
      F1 ==> V1-V3    = 1. load1 load2,
      F2 ==> V4-V6    = 1. load3 load4,
      F3 ==> V7-V9    = 1. load5 load6;
    cov
      F1 F2 = c12,
      F2 F3 = c23;
    pvar
      F1-F3 = c1-c3,
      V1-V9 = ev1-ev9;
  model 2 / group=2;
    refmodel 1;
    factor
      F1 ==> V1      = loada,
      F2 ==> V4      = loadb,
      F3 ==> V7      = loadc;
    cov
      F1 F2 = .,
      F1 F3 = c13;
run;

```

In this specification, you specify Model 2 by referring to Model 1 in the **REFMODEL** statement; Model 2 is the new model which refers to the old model, Model 1. Because the **PVAR** statement is not used in new model, all variance and partial variance parameter specifications in the **PVAR** statement of the old model are duplicated in the new model. The covariance parameter **c23** for covariance between F2 and F3 in the **COV** statement of the old model is also duplicated in the new model. Similarly, loading parameters **load1**–**load6** for some specific factor matrix locations are duplicated from the old model to the new model.

The new model has an additional parameter specification that the old model does not have. In the **COV** statement of the new model, covariance parameter **c13** for the covariance between F1 and F3 is added.

In the same statement, the covariance between F1 and F2 is denoted by the missing value ‘.’. The missing value indicates that this parameter location in the old model should not be included in the new model. The consequence of this deletion from the old model is that the covariance between F1 and F2 is a fixed zero in the new model.

Finally, the three new loading specifications in the **FACTOR** statement of the new model replace the fixed ones in the old model. They are now free parameters **loada**, **loadb**, and **loadc** in the new model.

FITINDEX Statement

FITINDEX *option* < *option* ... > ;

You can use the **FITINDEX** statement to set the options for computing and displaying the fit indices, or to output the fit indices. All but the **OFF=** and **ON=** options of the **FITINDEX** statement are also available in the **PROC CALIS** statement. The options set in the **FITINDEX** statement will overwrite those set in the **PROC CALIS** statement.

For the listing of fit indices and their definitions, see the section “Overall Model Fit Indices” on page 1329. Note that not all fit indices are available with all estimation methods, which is specified by the **METHOD=** option of the PROC CALIS statement. See the section “Fit Indices and Estimation Methods” on page 1336 for more details.

The options of the FITINDEX statement are as follows:

ALPHAECV= α

specifies a $(1 - \alpha)100\%$ confidence interval ($0 \leq \alpha \leq 1$) for the Browne and Cudeck (1993) expected cross validation index (ECVI). See the **ALPHAECV=** option of the PROC CALIS statement on page 1087.

ALPHARMS= α

specifies a $(1 - \alpha)100\%$ confidence interval ($0 \leq \alpha \leq 1$) for the Steiger and Lind (1980) root mean square error of approximation (RMSEA) coefficient. See the **ALPHARMS=** option of the PROC CALIS statement on page 1088.

BASEFIT | INBASEFIT=*SAS-data-set*

inputs the *SAS-data-set* that contains the fit information of the baseline model of your choice. See the **BASEFIT=** option of the PROC CALIS statement on page 1089.

BASEFUNC= $r(< DF=>i)$

BASEFUNC($< DF=>i$)= r

inputs the fit function value r and the degrees of freedom i of the baseline model of your choice. See the **BASEFUNC=** option of the PROC CALIS statement on page 1090.

CHICORRECT | CHICORR = *name* | *c*

specifies a correction factor c for the chi-square statistics for model fit. See the **CHICORRECT=** option of the PROC CALIS statement on page 1091.

CLOSEFIT= ρ

defines the criterion value ρ for indicating a close fit. See the **CLOSEFIT=** option of the PROC CALIS statement on page 1093.

DFREDUCE= i

reduces the degrees of freedom of the χ^2 test by i . See the **DFREDUCE=** option of the PROC CALIS statement on page 1096.

NOADJDF

turns off the automatic adjustment of degrees of freedom when there are active constraints in the analysis. See the **NOADJDF** option of the PROC CALIS statement on page 1106.

NOINDEXTYPE

disables the display of index types in the fit summary table. See the **NOINDEXTYPE** option of the PROC CALIS statement on page 1106.

OFF | OFFLIST= [*names*] | {*names*}

turns off the printing of one or more fit indices or modeling information as indicated by *names*, where a *name* represents a fit index, a group of fit indices, or modeling information. *Names* must be specified inside a pair of parentheses and separated by spaces. By default, all fit indices are printed. See the **ON=** option for the value of *names*.

ON | ONLIST < (ONLY) > = [names] | {names}

turns on the printing of one or more fit indices or modeling information as indicated by *names*, where a *name* represents a fit index, a group of fit indices, or modeling information. *Names* must be specified inside a pair of parentheses and separated by spaces. Because all fit indices and modeling information are printed by default, using an ON= list alone is redundant. When both ON= and OFF= lists are specified, the ON= list will override the OFF= list for those fit indices or modeling information that appear on both lists. If an ON(ONLY)= list is used, only those fit indices or modeling information specified in the list will be printed. Effectively, an ON(ONLY)= list is the same as the specification with an ON= list with the same selections and an OFF=ALL list in the FITINDEX statement.

Output Control of Fit Index Groups and Modeling Information Group

You can use the following *names* to refer to the groups of fit indices or modeling information available in PROC CALIS:

ABSOLUTE	Absolute or stand-alone fit indices that measures the model fit without using a baseline model.
ALL	All fit indices available in PROC CALIS.
INCREMENTAL	Incremental fit indices that measure model fit by comparing with a baseline model.
MODELINFO	General modeling information including sample size, number of variables, number of variables, and so on.
PARSIMONY	Fit indices that take model parsimony into account.

Output Control of Modeling Information

You can use the following *names* to refer to the individual modeling information available in PROC CALIS:

BASECHISQ	Chi-square statistic for the baseline model.
BASEDF	Degrees of freedom of the chi-square statistic for the baseline model.
BASEFUNC	Baseline model function value.
BASELOGLIKE	Baseline model -2 log-likelihood function value for METHOD=FIML.
BASEPROBCHI	p -value of the chi-square statistic for the baseline model fit.
BASESTATUS	Status of the baseline model fitting for METHOD=FIML.
NACTCON	Number of active constraints.
NIOBS	Number of incomplete observations for METHOD=FIML.
NMOMENTS	Number of elements in the moment matrices being modeled.
NOBS	Number of observations assumed in the analysis.
NPARAM NPARMS	Number of independent parameters.
NVAR	Number of variables.
SATFUNC	Saturated model function value for METHOD=FIML.
SATLOGLIKE	Saturated model -2 log-likelihood function value for METHOD=FIML.
SATSTATUS	Status of the saturated model fitting for METHOD=FIML.

Output Control of Absolute Fit Indices

You can use the following *names* to refer to the individual absolute fit indices available in PROC CALIS:

CHISQ	Chi-square statistic for model fit.
CN CRITICAL_N	Hoelter's critical N.
CONTLIKE	Percentage contribution to the Log-likelihood function value of each group in multiple-group analyses with METHOD=FIML.
CONTRIBUTION CONTCHI	Percentage contribution to the chi-square value for multiple-group analyses.
DF	Degrees of freedom for the chi-square test for model fit.
ELLIPTIC	Elliptical chi-square statistic for ML and GLS methods in single-group analyses without mean structures. This index is computed only when you input the raw data with the KURTOSIS option specified.
FUNCVL	Optimized function value.
GFI	Goodness-of-fit index by Jöreskog and Sörbom.
LOGLIKE	Fitted model -2 log-likelihood function value for METHOD=FIML.
PROBCHI	<i>P</i> -value of the chi-square statistic for model fit.
PROBELLIPTIC	<i>P</i> -value of the elliptical chi-square statistic.
RMR	Root mean square residual.
SRMR	Standardized root mean square residual.
ZTEST	Z-test of Wilson and Hilferty.

Output Control of Parsimonious Fit Indices

You can use the following *names* to refer to the individual parsimonious fit indices available in PROC CALIS:

AGFI	Adjusted GFI.
AIC	Akaike information criterion.
CAIC	Bozdogan corrected AIC.
CENTRALITY	McDonald centrality measure.
ECVI	Expected cross-validation index.
ECVI_LL LL_ECVI	Lower confidence limit for ECVI.
ECVI_UL UL_ECVI	Upper confidence limit for ECVI.
PGFI	Parsimonious GFI.
PROBCLFIT	Probability of close fit.
RMSEA	Root mean squares of error approximation.
RMSEA_LL LL_RMSEA	Lower confidence limit for RMSEA.
RMSEA_UL UL_RMSEA	Upper confidence limit for RMSEA.

SBC Schwarz Bayesian criterion.

Output Control of Incremental Fit Indices

You can use the following *names* to refer to the individual incremental fit indices available in PROC CALIS:

BENTLRCFI | **CFI** Bentler comparative fit index.

BENTLERNFI Bentler-Bonett normed fit index.

BENTLERNNFI Bentler-Bonett nonnormed fit index.

BOLLENNFI Bollen normed fit index (Rho1).

BOLLENNNFI Bollen nonnormed fit index (Delta2).

PNFI James et al. parsimonious normed fit index.

OUTFIT=SAS-data-set

creates an output data set containing the values of the fit indices. This is the same as the **OUTFIT=** option of the PROC CALIS statement on page 1110. See the section “**OUTFIT= Data Set**” on page 1254 for details.

FREQ Statement

FREQ *variable* ;

If one variable in your data set represents the frequency of occurrence for the other values in the observation, specify the variable’s name in a FREQ statement. PROC CALIS then treats the data set as if each observation appears n_i times, where n_i is the value of the FREQ variable for observation i . Only the integer portion of the value is used. If the value of the FREQ variable is less than 1 or is missing, that observation is not included in the analysis. The total number of observations is considered to be the sum of the FREQ values. You can use only one FREQ statement within the scope of each **GROUP** or the PROC CALIS statement.

GROUP Statement

GROUP i *</ options >* ;

where i is an assigned group number between 1 and 9999, inclusively.

The GROUP statement signifies the beginning of a group specification block and designates a group number for the group. All [subsidiary group specification statements](#) after a GROUP statement belong in that group until another **MODEL** or **GROUP** statement is used. The subsidiary group specification statements refer to one of the following four statements:

- [FREQ](#) statement on page 1152
- [PARTIAL](#) statement on page 1202
- [VAR](#) statement on page 1228
- [WEIGHT](#) statement on page 1235

For example, consider the following statements:

```
proc calis;
  var X1-X4;
  group 1 / label='Women' data=women_data;
    freq Z;
  group 2 / label='Men' data=men_data;
    partial P;
  model 1 / group = 1-2;
    factor N=1; /* One factor exploratory factor analysis */
run;
```

In the GROUP statements, two groups are defined. Group 1, labeled as ‘Women’, refers to the data set `women_data`. Group 2, labeled as ‘Men’, refers to the data set `men_data`. Both groups are fitted by an exploratory factor model defined in Model 1, as indicated in the GROUP= option of the MODEL statement. While the frequency variable Z defined in the FREQ statement is applicable only to Group 1, the partial variable P defined in the PARTIAL statement is applicable only to Group 2. However, the VAR statement, which appears before the definitions of both groups, applies globally to both Group 1 and Group 2. Therefore, variables X1–X4 are the analysis variables in the two groups.

You can set group-specific *options* in each GROUP statement. All but one (that is, the LABEL= option) of these *options* are also available in the MODEL and PROC CALIS statements. If you set these group-specific *options* in the PROC CALIS statement, they will apply to all groups unless you respecify them in the GROUP statement. If you set these group-specific *options* in the MODEL statement, they will apply to all groups that are fitted by the associated model. In general, the group-specific options are transferred from the PROC CALIS statement to the MODEL statements (if present) and then to the fitted groups. In the transferring process, options are overwritten by the newer ones. If you want to apply some group-specific options to a particular group only, you should set those options in the GROUP statement corresponding to that group.

Option Available in the GROUP Statement Only

LABEL | NAME=*name*

specifies a label for the current group. You can use any valid SAS names up to 256 characters for labels. You can also use quote strings for the labels. This option can be specified only in the GROUP statement, not the PROC CALIS statement.

Options Available in the GROUP and PROC CALIS Statements

These options are available in the GROUP and PROC CALIS statements:

Option	Description
DATA= on page 1096	Specifies the input data set
INWGT= on page 1099	Specifies the data set that contains the weight matrix
OUTSTAT= on page 1110	Specifies the data set for storing the statistical results
OUTWGT= on page 1110	Specifies the data set for storing the weight matrix
ROBITER= on page 1115	Specifies the maximum number of iterations for estimating robust covariance and mean matrices
ROBPHI= on page 1115	Specifies the tuning parameter for robust methods

See the section “PROC CALIS Statement Options” on page 1087 for more details about these options. If you specify these options in the PROC CALIS statement, they are transferred to *all* GROUP statements. They might be overwritten by the respecifications in the individual GROUP statements.

Options Available in GROUP, MODEL, and PROC CALIS Statements

These options are available in the GROUP, MODEL, and PROC CALIS statements:

Option	Description
ALPHALEV= on page 1087	Specifies the α -level criterion for detecting leverage points
ALPHAOUT= on page 1088	Specifies the α -level criterion for detecting outliers
BIASKUR on page 1091	Computes the skewness and kurtosis without bias corrections
EDF= on page 1097	Defines nob _s by the number of error <i>df</i>
INWGTINV on page 1099	Specifies that the INWGT= data set contains the inverse of the weight matrix
KURTOSIS on page 1099	Computes and displays kurtosis
MAXMISSPAT= on page 1101	Specifies the maximum number of missing patterns to display
NOBS= on page 1106	Defines the number of observations (nob _s)
NOMISSPAT on page 1107	Suppresses the display of missing pattern analysis
PCORR on page 1111	Displays analyzed and estimated moment matrix
PLOTS= on page 1112	Specifies ODS Graphics selection
PWEIGHT on page 1235	Displays the weight matrix
RDF DFR= on page 1114	Defines nob _s by the number of regression <i>df</i>
RESIDUAL RES on page 1114	Computes the default residuals
RESIDUAL RES= on page 1114	Specifies the type of residuals
RIDGE on page 1115	Specifies the ridge factor for covariance matrix
SIMPLE on page 1117	Prints univariate statistics
TMISSPAT= on page 1118	Specifies the data proportion threshold for displaying the missing patterns
VARDEF= on page 1119	Specifies variance divisor
WPENALTY= on page 1119	Specifies the penalty weight to fit correlations
WRIDGE= on page 1120	Specifies the ridge factor for the weight matrix

If you specify these options in the PROC CALIS statement, they are transferred to all MODEL statements. These options are overwritten by the respecifications in the individual MODEL statements. After these options are resolved in a given MODEL statement, they are transferred further to the GROUP statements

of which the associated groups are fitted by the model. Again, these options might be overwritten by the respecifications in the individual GROUP statements.

LINCON Statement

LINCON *constraint* <, *constraint* ... > ;

where *constraint* represents one of the following:

- *number operator linear-term*
- *linear-term operator number*

and *linear-term* is

< +|- > < *coefficient* * > *parameter* < +|- > < *coefficient* * > *parameter* ... >

The LINCON statement specifies a set of linear equality or inequality constraints of the following form:

$$\sum_{j=1}^n a_{ij} x_j \leq b_i, \quad i = 1, \dots, m$$

The constraints must be separated by commas. Each linear constraint i in the statement consists of a linear combination $\sum_j a_{ij} x_j$ of a subset of the n parameters x_j , $j = 1, \dots, n$, and a constant value b_i separated by a comparison operator. Valid operators are <=, <, >=, >, and = or, equivalently, LE, LT, GE, GT, and EQ. PROC CALIS cannot enforce the strict inequalities < or >. Note that the coefficients a_{ij} in the linear combination must be constant numbers and must be followed by an asterisk and the name of a parameter (that is, listed in the PARMS, **main**, or **subsidiary** model specification statements). The following is an example of the LINCON statement that sets a linear constraint on parameters x_1 and x_2 :

```
lincon      x1 + 3 * x2 <= 1;
```

Although you can express boundary constraints of individual parameters in LINCON statements, it is much more convenient to specify these boundary constraints with the **BOUNDS** statement. For example, the following LINCON statement essentially specifies boundary constraints on four parameters:

```
lincon      x1 <= 1,
            x2 <= 1,
            v1 > 0,
            v2 > 0;
```

Instead of using the LINCON statement, you can specify the following **BOUNDS** statement:

```
bounds      x1 x2 <= 1,
            v1 v2 > 0;
```

Another advantage of using the **BOUNDS** statement for setting bounds for individual parameters is that when a boundary constraint becomes active in the solution (that is, when the final estimate is on the boundary), a Lagrange multiplier test on releasing the boundary constraint would be conducted when you also specify the **MOD** option. However, no Lagrange multiplier test would be conducted if you specified the boundary constraint with the LINCON statement.

LINEQS Statement

LINEQS < equation <, equation ... >> ;

where *equation* represents:

dependent = *term* < + *term* ... >

and each *term* represents one of the following:

- *coefficient-name* < (*number*) > < * > *variable-name*
- *prefix-name* < (*number*) > < * > *variable-name*
- < *number* > < * > *variable-name*

The LINEQS statement is a **main model specification statement** that invokes the LINEQS modeling language. You can specify at most one LINEQS statement in a model, within the scope of either the PROC CALIS statement or a MODEL statement. To completely specify a LINEQS model, you might need to add some **subsidiary model specification statements** such as the VARIANCE, COV, and MEAN statements. The syntax for the LINEQS modeling language is as follows:

```
LINEQS < equation <, equation ... >> ;
VARIANCE partial-variance-parameters ;
COV covariance-parameters ;
MEAN mean-parameters ;
```

In the LINEQS statement, you use equations to specify the linear functional relations among manifest and latent variables. Equations in the LINEQS statement are separated by commas.

In the **VARIANCE** statement, you specify the variance parameters. In the **COV** statement, you specify the covariance parameters. In the **MEAN** statement, you specify the mean parameters. For details of these subsidiary model specification statements, see the syntax of these statements.

In the LINEQS statement, in addition to the functional relations among variables, you specify the coefficient parameters of interest in the equations. There are five types of parameters you can specify in equations, as shown in the following example:

```
lineqs
  V1 =           * F1 + E1,
  V2 = (.5)      * F1 + E2,
  V3 = 1.        * F1 + E3,
  V4 = b4       * F1 + E4;
  V5 = b5 (.4) * F1 + E5;
```

In this example, you have manifest variables V1–V5, which are related to a latent factor, denoted by F1, as specified in the equations. In each equation, you have one outcome variable (V-variable), one predictor variable (F1, which is assumed to be a latent factor, the so-called F-variable), and one error variable (E-variable). The following four types of parameters have been specified:

- an unnamed free parameter

The effect of F1 on V1 in the first equation is an unnamed free parameter. Although you specify nothing before the asterisk sign, the effect parameter is effectively specified. For an unnamed free

parameter, PROC CALIS generates a parameter name with the `_Parm` prefix and appended with a unique integer (for example, `_Parm1`, `_Parm2`, and so on).

- an initial value

The effect of F1 on V2 in the second equation is an unnamed free parameter with an initial estimate of 0.5. PROC CALIS also generates a parameter name for this specification. Notice that you must use a pair of parentheses for the initial value specification because it is interpreted as a fixed value otherwise, as described in the next case.

- a fixed value

The effect of F1 on V3 in the third equation is an unnamed free parameter with a fixed value of 0.5. A fixed value remains the same in the estimation. There is no parameter name for a fixed constant in the model.

- a free parameter with a name

The effect of F1 on V4 in the fourth equation is a free parameter named `b4`. You do not provide an initial estimate for this free parameter.

- a free parameter with a name and an initial estimate

The effect of F1 on V5 in the fifth equation is a free parameter named `b5` with an initial estimate of 0.4. Parameters with no starting values are initialized by various heuristic and effective methods in PROC CALIS. See the section “[Initial Estimates](#)” on page 1351 for details.

Notice that there must be an error term in each equation. The error terms in equation must start with the prefix ‘E’, ‘e’, ‘D’, or ‘d’. See the section “[Representing Latent Variables in the LINEQS Model](#)” on page 1158 for details about naming the factors and error terms. The effect or the path coefficient attached to an error term must be 1.0. This is implicitly specified as in the preceding example. For example, there is no parameter specification nor an asterisk sign before the error term `E1` in the first equation, as shown in the following:

$$V1 = \quad * F1 + E1,$$

This specification is the same as the following explicit specification with a fixed constant 1.0 for the effect of the error term `E1`:

$$V1 = \quad * F1 + 1. * E1,$$

The equivalence shown here implies that you can also specify the third equation in the following equivalent way:

$$V3 = F1 + E3,$$

This implicitly specifies a constant 1.0 for the effect of F1 on V3. You must be very careful about the distinction between this specification and the following one with an asterisk before F1:

$$V3 = * F1 + E3,$$

With an asterisk sign, the effect of F1 on V3 becomes an unnamed free parameter in the current specification. This interpretation is very different from the preceding one without an asterisk sign before F1, which assumes a fixed constant of 1.0.

Except for the unnamed free parameter specification, you can omit the asterisk signs in all other types of parameter specifications. That is, you can use the following equivalent statement for the preceding LINEQS specification:

```

lineqs
  V1 =          * F1 + E1,
  V2 = (.5)      F1 + E2,
  V3 = 1.        F1 + E3,
  V4 = b4        F1 + E4;
  V5 = b5 (.4)   F1 + E5;

```

Again, you cannot omit the asterisk in the first equation because it is intended to denote an unnamed free parameter.

If your model contains many unconstrained parameters and it is too cumbersome to find different parameter names, you can specify all those parameters by the same prefix-name. A prefix name is a short name called “root” followed by two underscores __. Whenever a prefix-name is encountered, the CALIS procedure generates a parameter name by appending a unique integer to the root. Hence, the prefix-name should have few characters so that the generated parameter name is not longer than thirty-two characters. To avoid unintentional equality constraints, the prefix names should not coincide with explicitly defined parameter names. The following statement illustrates the uses prefix-names:

```

lineqs
  V1 = 1.    * F1 + E1,
  V2 = b__  * F1 + E2,
  V3 = b__  * F1 + E3,
  V4 = b__  * F1 + E4;
  V5 = b__  * F1 + E5;

```

In the five equations, only the first equation has a fixed constant 1.0 for the effect of F1 on V1. For all the remaining equations, the effects of F1 on the variables are all free parameters with the prefix b. The generated parameter names for these effects have unique integers appended to this prefix. For example, b1, b2, b3, and b4 are the parameter names for these effects.

Representing Latent Variables in the LINEQS Model

Because latent variables are widely used in structural equation modeling, PROC CALIS needs a way to identify different types of latent variables that are specified in the LINEQS model. This is accomplished by following some naming conventions for the latent variables. See the section “[Naming Variables in the LINEQS Model](#)” on page 1272 for details about these naming rules. Essentially, latent factors (systematic sources) must start with the letter ‘F’ or ‘f’. Error terms must start with the letter ‘E’, ‘e’, ‘D’, or ‘d’. Prefix ‘E’ or ‘e’ represents the error term of an endogenous *manifest* variable. Prefix ‘D’ or ‘d’ represents the disturbance (or error) term of an endogenous *latent* variable. Although D- and E- variables are conceptually different, for modeling purposes ‘D’ and ‘E’ prefixes are interchangeable in the LINEQS modeling language. Essentially, only the distinction between latent factors (systematic sources) and errors or disturbances (unsystematic sources) is critical in specifying a proper LINEQS model. Manifest variables in the LINEQS model do not need to follow additional naming rules beyond those required by the general SAS System—they are recognized by PROC CALIS by referring to the variables in the input data sets.

Types of Variables and Semantic Rules of Equations

Depending on their roles in the system of equations, variables in a LINEQS model can be classified into endogenous or exogenous. An endogenous variable is a variable that serves as an outcome variable (left-hand side of an equation) in one of the equations. All other variables are exogenous variables, including those manifest variables that do not appear in any equations but are included in the model because they are specified in the `VAR` statement for the analysis.

Merely following the syntactic rules described so far is not sufficient to define a proper system of equations that PROC CALIS can analyze. You also need to observe the following semantic rules:

- Only manifest or latent variables can be endogenous. This means that you cannot specify any error or disturbances variables on the left-hand side of the equations. This also means that error and disturbance variables are always exogenous in the LINEQS model.
- An endogenous variable that appears on the left-hand side of an equation cannot appear on the left-hand side of another equation. In other words, you have to specify all the predictors for an endogenous variable in a single equation.
- An endogenous variable that appears on the left-hand side of an equation cannot appear on the right-hand side of the same equation. This prevents a variable to have a direct effect on itself (but indirect effect on itself is possible).
- Each equation must contain one and only one *unique* error term, be it an E-variable for a manifest outcome variable or a D-variable for a latent outcome variable. If, indeed, you want to specify an equation without an error term, you can equivalently set the variance of the error term to a fixed zero in the `VARIANCE` statement.

Mean Structures in Equations

To fit a LINEQS model with mean structures, you can specify the `MEANSTR` option in the PROC CALIS or the associated `MODEL` statement. This generates the default mean and intercept parameters for the model (see the section “Default Parameters” on page 1160). Alternatively, you can specify the intercept parameters with the `Intercept` variable in the equations or the mean parameters in the `MEAN` statement. The `Intercept` variable in the LINEQS model is a special “variable” that contains the value 1 for each observation. You do not need to have this variable in your input data set, nor do you need to generate it in the DATA step. It serves as a notational convenience in the LINEQS modeling language. The actual intercept parameter is expressed as a coefficient parameter with the intercept variable. For example, consider the following LINEQS model specification:

```

lineqs
  V1 = a1 (10) * Intercept + 1.0      * F1 + E1,
  V2 =          * Intercept +          * F1 + E2,
  V3 =          + b2          * F1 + E3,
  V4 = a2      * Intercept + b2      * F1 + E4,
  V5 = a2      * Intercept + b4 (.4) * F1 + E5;

```

In the first equation, `a1`, with a starting value at 10, is the intercept parameter of `V1`. In the second equation, the intercept parameter of `V2` is an unnamed free parameter. In the third equation, although you do not specify the `Intercept` variable, the intercept parameter of manifest variable `V3` is assumed to be a free parameter

by default. See the section “Default Parameters” on page 1160 for more details about default parameters. In the fourth and the fifth equations, the intercept parameters are both named `a2`. This means that these intercepts are constrained to be the same in the estimation.

In some cases, you might need to set the intercepts to fixed constants such as zeros. You can use the following syntax:

```
lineqs
  V1 = 0 * Intercept + F_intercept + a2 * F_slope + E1;
```

This sets the intercept parameter of `V1` to a fixed zero. An example of this application is the analysis of latent growth curve model in which you define the intercept as a random variable represented by a latent factor (for example, `F_intercept` in the specification). See [Example 27.25](#) for a detailed example.

To complete the specification of the mean structures in the LINEQS model, you might want to use the `MEAN` statement to specify the mean parameters. For example, the following statements specify the means of `F_intercept` and `F_slope` as unnamed free parameters in the LINEQS model:

```
lineqs
  V1 = 0 * Intercept + F_intercept + 1 * F_slope + E1;
mean
  F_intercept F_slope;
```

See the [MEAN](#) statement for details.

Default Parameters

It is important to understand the default parameters in the LINEQS model. First, if you know which parameters are default free parameters, you can make your specification more efficient by omitting the specifications of those parameters that can be set by default. For example, because all variances and covariances among exogenous variables (excluding error terms) are free parameters by default, you do not need to specify them with the `COV` and `VARIANCE` statements if these variances and covariances are not constrained. Second, if you know which parameters are default fixed zero parameters, you can specify your model accurately. For example, because all error covariances in the LINEQS model are fixed zeros by default, you must use the `COV` statement to specify the covariances among the errors if you want to fit a model with correlated errors. See the section “Default Parameters in the LINEQS Model” on page 1276 for details about the default parameters of the LINEQS model.

Modifying a LINEQS Model from a Reference Model

This section assumes that you use a `REFMODEL` statement within the scope of a `MODEL` statement and that the reference model (or base model) is a LINEQS model. The reference model is called the old model, and the model being defined is called the new model. If the new model is not intended to be an exact copy of the old model, you can use the extended LINEQS modeling language described in this section to make modifications within the scope of the `MODEL` statement for the new model.

The syntax of the extended LINEQS modeling language is the same as that of the ordinary LINEQS modeling language (see the section “LINEQS Statement” on page 1156):

```
LINEQS < equation <, equation ... >>;
  VARIANCE partial-variance-parameters;
  COV covariance-parameters;
  MEAN mean-parameters;
```

The new model is formed by integrating with the old model in the following ways:

- Duplication:** If you do not specify in the new model an equation with an outcome variable (that is, a variable on the left side of the equal sign) that exists in the old model, the equation with that outcome variable in the old model is duplicated in the new model. For specifications other than the LINEQS statement, if you do not specify in the new model a parameter location that exists in the old model, the old parameter specification is duplicated in the new model.
- Addition:** If you specify in the new model an equation with an outcome variable that does not exist as an outcome variable in the equations of the old model, the equation is added in the new model. For specifications other than the LINEQS statement, if you specify in the new model a parameter location that does not exist in the old model, the new parameter specification is added in the new model.
- Deletion:** If you specify in the new model an equation with an outcome variable that also exists as an outcome variable in an equation of the old model and you specify the missing value '.' as the only term on the right-hand side of the equation in the new model, the equation with the same outcome variable in the old model is not copied into the new model. For specifications other than the LINEQS statement, if you specify in the new model a parameter location that also exists in the old model and the new parameter is denoted by the missing value '.', the old parameter specification is not copied into the new model.
- Replacement:** If you specify in the new model an equation with an outcome variable that also exists as an outcome variable in an equation of the model and the right-hand side of the equation in the new model is not denoted by the missing value '.', the new equation replaces the old equation with the same outcome variable in the new model. For specifications other than the LINEQS statement, if you specify in the new model a parameter location that also exists in the old model and the new parameter is not denoted by the missing value '.', the new parameter specification replaces the old one in the new model.

For example, the following two-group analysis specifies Model 2 by referring to Model 1 in the **REFMODEL** statement:

```
proc calis;
  group 1 / data=d1;
  group 2 / data=d2;
  model 1 / group=1;
    lineqs
      V1 = 1 * F1 + E1,
      V2 = load1 * F1 + E2,
      V3 = load2 * F1 + E3,
      F1 = b1 * V4 + b2 * V5 + b3 * V6 + D1;
    variance
      E1-E3 = ve1-ve3,
      D1 = vd1,
      V4-V6 = phi4-phi6;
    cov
      E1 E2 = cve12;
  model 2 / group=2;
  refmodel 1;
```

```

lineqs
  V3   = load1 * F1 + E3;
cov
  E1 E2 = .,
  E2 E3 = cve23;
run;

```

Model 2 is the new model which refers to the old model, Model 1. This example illustrates the four types of model integration:

- Duplication: All equations, except the one with outcome variable V3, in the old model are duplicated in the new model. All specifications in the VARIANCE and COV statements, except the covariance between E1 and E2, in the old model are also duplicated in the new model.
- Addition: The parameter `cve23` for the covariance between E2 and E3 is added in the new model.
- Deletion: The specification of covariance between E1 and E2 in the old model is not copied into the new model, as indicated by the missing value '.' specified in the new model.
- Replacement: The equation with V3 as the outcome variable in the old model is replaced with a new equation in the model. The new equation uses parameter `load1` so that it is now constrained to be the same as the regression coefficient in the equation with V2 as the outcome variable.

LISMOD Statement

LISMOD < *var-lists* > ;

where *var-lists* represent one or more of the following:

- **YVAR** | **YV** | **Y** = *var-list*
- **XVAR** | **XV** | **X** = *var-list*
- **ETAVAR** | **ETAV** | **ETA** = *var-list*
- **XIVAR** | **XIV** | **XI** | **KSIVAR** | **KSIV** | **KSI** = *var-list*

LISMOD stands for LISREL modeling, where LISREL is the program developed by Jöreskog and Sörbom (1988). Like the original implementation of LISREL, LISMOD uses a matrix specification interface. To complete the LISMOD specification, you might need to add as many **MATRIX** statements as needed, as shown in the following statement structure for the LISMOD model:

```

LISMOD var-lists ;
MATRIX matrix-name parameters-in-matrix ;
Repeat the MATRIX statement as needed ;

```

The *matrix-name* in the **MATRIX** statement should be one of the twelve model matrices in LISMOD, as listed in the following:

- Matrices in the structural model: `_ALPHA_`, `_KAPPA_`, `_BETA_`, `_GAMMA_`, `_PHI_`, or `_PSI_`
- Matrices in the measurement model for y-variables: `_NUY_`, `_LAMBDAY_`, or `_THETAY_`
- Matrices in the measurement model for x-variables: `_NUX_`, `_LAMBDA_`, or `_THETAX_`

See the section “[Model Matrices in the LISMOD Model](#)” on page 1279 for definitions of these matrices and their roles in the LISMOD modeling language. See the [MATRIX statement](#) on page 1175 for the details of parameter specification.

In the LISMOD statement, you can specify the following four lists of variables:

- `YVAR=` list is for manifest variables y that are directly related to the endogenous latent variables η (eta). Variables in the list are called y-variables.
- `XVAR=` list is for manifest variables x that are directly related to the exogenous latent variables ξ (xi or ksi). Variables in the list are called x-variables.
- `ETAVAR=` list is for endogenous latent variables η . Variables in the list are called η -variables.
- `XIVAR=` list is for exogenous latent variables ξ . Variables in the list are called ξ -variables.

The order of variables in the lists of the LISMOD statement is used to define the variable order in rows and columns of the LISMOD model matrices.

Depending on the model of interest, you might not need to specify all the lists of variables. When some variable lists are not specified, the full model reduces to specialized submodels. However, to be a proper submodel in the LISMOD modeling language, it is necessary (but not sufficient) that at least one of the `YVAR=` or `XVAR=` lists is defined. See the section “[LISMOD Submodels](#)” on page 1282 for the details about LISMOD submodels that PROC CALIS can handle.

An example of a LISMOD model specification is shown as follows:

```
proc calis;
  lismod xvar=x1-x3 yvar=y1-y6 xivar=xi etavar=eta1-eta2;
  matrix _LAMBDAY_  [,1] = 1. load3 load4,
                  [,2] = 0. 0. 0. 1. load5 load6;
  matrix _THETAY_  [1,1] = ey1-ey3,
                  [2,1] = cey;
  matrix _LAMBDA_  [,] = 1. load1 load2;
  matrix _THETAX_  [1,1] = 3*ex;
  matrix _GAMMA_   [,1] = beta1 beta2;
  matrix _PHI_     [1,1] = phi;
  matrix _PSI_     [1,1] = psi1-psi2;
run;
```

In this example, you have three x-variables x_1 – x_3 , six y-variables y_1 – y_6 , one ξ -variable ξ , and two η -variables η_1 – η_2 . The numbers of variables in these lists define the dimensions of the LISMOD model matrices. For example, matrix `_LAMBDAY_` is 6×2 , with y_1 – y_6 as the row variables and η_1 – η_2 as the column variables. Matrix `_THETAX_` is 3×3 , with x_1 – x_3 as the row and column variables. In the MATRIX statements, you specify parameters in the elements of the matrices. After the matrix name, you specify in square brackets ‘[’ and ‘]’ the starting row and column numbers of the first element to be parameterized. After the equal sign, you specify fixed or free parameters for the matrix elements.

Depending on how you specify the starting row and column numbers, the parameter specification might proceed differently. See the **MATRIX statement** on page 1175 for a detailed description. In this example, the first specification of the parameters in the `_LAMBDAY_` matrix starts from [1,1]—meaning that it starts from the first column and proceeds downwards. As a result, the [1,1] element is a fixed constant 1.0, the [2,1] element is a free parameter called `load3`, and the [3,1] element is a free parameter called `load4`. Similarly, in the second specification in the `_LAMBDAY_` matrix, the [1,2], [2,2], [3,2], and [4,2] elements take constant values 0, 0, 0, and 1, respectively, and the [5,2] and [6,2] elements are free parameters `load5` and `load6`, respectively.

You can also use similar notation to specify the parameters of a row. For example, with the notation [2,] for the starting row and column numbers, specification proceeds to the left with the same second row in the matrix.

If you have specified both starting row and column numbers, such as those in the first specification in matrix `_THETAY_`, the parameter specification starts from [1,1] and proceeds to the next row and column numbers—that is [2,2], [3,3], and so on. This results in specifying the diagonal elements of matrix `_THETAY_` as free parameters `ey1`, `ey2`, and `ey3`.

With the notation [,], no starting row and column numbers are specified. Specification starts from the first valid element in the matrix and proceeds row-wise for all valid elements in the matrix. For example, in the matrix `_LAMBDA_X_` statement, the [1,1] element of matrix `_LAMBDA_X_` is a fixed constant 1, and the [1,2] and [1,3] elements are free parameters `load1` and `load2`, respectively.

Default Parameters

It is important to understand the default parameters in the LISMOD model. First, if you know which parameters are default free parameters, you can make your specification more efficient by omitting some specifications. For example, because all variances and covariances among the exogenous ξ -variables (excluding error terms) are free parameters by default, you do not need to specify them with **MATRIX** statement if these variances and covariances are not constrained. Second, if you know which parameters are default fixed zero parameters, you can specify your model accurately. For example, because all measurement errors in the LISMOD model are fixed zeros by default, you must use the **MATRIX** statement to specify the covariances among the errors in the Θ_x (`_THETA_X_`) or Θ_y (`_THETA_Y_`) matrices if you want to fit a model with some correlated measurement errors. See the section “[Default Parameters in the LISMOD Model](#)” on page 1285 for details about the default parameters of the LISMOD model.

Modifying a LISMOD Model from a Reference Model

This section assumes that you use a **REFMODEL** statement within the scope of a **MODEL** statement and that the reference model (or base model) is also a LISMOD model. The reference model is called the old model, and the model that refers to this old model is called the new model. If the new model is not intended to be an exact copy of the old model, you can use the extended LISMOD modeling language described in this section to make modifications within the scope of the **MODEL** statement for the new model. The syntax is similar to, but not exactly the same as, the ordinary LISMOD modeling language (see the section “[LISMOD Statement](#)” on page 1162). The respecification syntax for a LISMOD model is shown as follows:

```
LISMOD ;
MATRIX matrix-name parameters-in-matrix ;
Repeat the MATRIX statement as needed ;
```


First, in the respecification you should not put any variable lists in the LISMOD statement. The reason is that the parameter respecifications in the new model refer to the variable lists of the old model. Therefore, the variable lists in the new model are implicitly assumed to be exactly the same as those in the old model. Because of this, the LISMOD statement is entirely optional for the respecification in the new model.

Second, you can use **MATRIX** *matrix-name* statements to modify the old model by using the same syntax as in the LISMOD modeling language. The *matrix-name* can be one of the twelve possible LISMOD matrices. In addition, in the respecification syntax you can use the missing value '.' to drop a parameter specification from the old model.

The new model is formed by integrating with the old model in the following ways:

- Duplication: If you do not specify in the new model a parameter location that exists in the old model, the old parameter specification is duplicated in the new model.
- Addition: If you specify in the new model a parameter location that does not exist in the old model, the new parameter specification is used in the new model.
- Deletion: If you specify in the new model a parameter location that also exists in the old model and the new parameter is denoted by the missing value '.', the old parameter specification is not copied into the new model.
- Replacement: If you specify in the new model a parameter location that also exists in the old model and the new parameter is not denoted by the missing value '.', the new parameter specification replaces the old one in the new model.

For example, the following two-group analysis specifies Model 2 by referring to Model 1 in the **REF-MODEL** statement:

```
proc calis;
  group 1 / data=d1;
  group 2 / data=d2;
  model 1 / group=1;
    lismod xvar=X1-X3 yvar=Y1-Y6 xivar=xi etavar=eta1-eta2;
    matrix _LAMBDAY_  [,1] = 1. load3 load4,
                      [,2] = 0. 0. 0. 1. load5 load6;
    matrix _THETAY_   [1,1] = ey1-ey3,
                      [2,1] = cey;
    matrix _LAMBDA_X_ [,] = 1. load1 load2;
    matrix _THETA_X_  [1,1] = 3*ex;
    matrix _GAMMA_    [,1] = beta1 beta2;
    matrix _PHI_      [1,1] = phi;
    matrix _PSI_      [1,1] = psi1-psi2;
  model 2 / group=2;
    refmodel 1;
    matrix _THETAY_   [2,1] = .;
    matrix _THETA_X_  [1,1] = ex1-ex3;
    matrix _BETA_     [2,1] = beta;
run;
```

In this example, Model 2 is the new model which refers to the old model, Model 1. It illustrates the four types of model integration:

- **Duplication:** All parameter locations and specifications in the old model are duplicated in the new model, except for the [2,1] element in matrix `_THETAY_` and the diagonal of matrix `_THETAX_`, which are modified in the new model.
- **Addition:** The `_BETA_[2,1]` parameter location is added with a new parameter `beta` in the new model. This indicates that *eta1* is a predictor variable of *eta2* in the new model, but not in the old model.
- **Deletion:** Because the missing value ‘.’ is used for the parameter value, the `_THETAY_[2,1]` parameter location is no longer defined as a free parameter in the new model. In the old model, the same location is defined by the free parameter `cey`.
- **Replacement:** The diagonal elements of the `_THETAX_` matrix in the new model are now defined by three distinct parameters `ex1–ex3`. This replaces the old specification where a single constrained parameter `ex` is applied to all the diagonal elements in the `_THETAX_` matrix.

LMTESTS Statement

LMTESTS | **LMTEST** *option* < *option* ... > ;

where *option* represents one of the following:

- *display-option*
- *test-set*

and *test-set* represents one of the following:

- *set-name* = [*regions*]
- *set-name* = { *regions* }

where *set-name* is the name of the set of Lagrange multiplier (LM) tests defined by the *regions* that follow after the equal sign and *regions* are keywords denoting specific sets of parameters in the model.

You can use the LMTESTS statement to set *display-options* or to customize the *test-sets* for the LM tests. The LMTESTS statement is one of the [model analysis statements](#). It can be used within the scope of the CALIS statement so that the options will apply to all models. It can also be used within the scope of each MODEL statement so that the options will apply only locally. Therefore, different models within a CALIS run can have very different LMTESTS *options*.

The LM Tests Display Options

The following are the *display-options* for the LM tests:

DEFAULT

conducts the default sets of LM tests for freeing fixed parameters in the model. This option is used when you need to reset the default sets of LM tests in the local model. For example, you might have turned off the default LM tests by using the NODEFAULT option in the LMTESTS statement within the scope of PROC CALIS statement. However, for the model under the scope of a particular MODEL statement, you can use this DEFAULT option in the local LMTESTS statement to turn on the default LM tests again.

MAXRANK

sets the maximum number of rankings within a set of LM tests. The actual number of test rankings might be smaller because the number of possible LM tests within a set might be smaller than the maximum number requested.

NODEFAULT

turns off the default sets of LM tests for freeing fixed parameters in the model. As a result, only the customized LM tests defined in the *test-sets* of the LMTESTS statement are conducted and displayed. Note that the LM tests for equality and active boundary constraints are not turned off by this option. If you specify this option in the LMTESTS statement within the scope of the PROC CALIS statement, it will propagate to all models.

NORANK

turns off the ranking of the LM tests. Ranking of the LM tests is done automatically when the model modification indices are requested. The NORANK option is ignored if you also set the MAXRANK option.

LMMAT

prints the sets of LM tests in matrix form, in addition to the normal LM test results.

The Customized Sets of LM Tests: Syntax of the Test-sets

In addition to the *display-options*, you can define customized sets of LM tests as *test-sets* in the LMTESTS statement. You can define as many *test-sets* as you like. Ranking of the LM tests will be done individually for each *test-set*. For example, the following LMTESTS statement requests that the default sets of LM tests not be conducted by the NODEFAULT option. Instead, two customized *test-sets* are defined.

```
lmtests nodefault MyFirstSet=[ALL] MySecondSet=[COVEXOG COVERR];
```

The first customized set MyFirstSet pulls all possible parameter locations together for the LM test ranking (ALL keyword). The second customized set MySecondSet pulls only the covariances among exogenous variables (COVEXOG keyword) and among errors (COVERR keyword) together for the LM test ranking.

Two different kinds of *regions* for LM tests are supported in PROC CALIS: matrix-based or non-matrix-based.

The matrix-based *regions* can be used if you are familiar with the matrix representations of various types of models. Note that defining *test-sets* by using matrix-based *regions* does not mean that LM tests are printed in matrix format. It means only that the parameter locations within the specified matrices are included into the specific *test-sets* for LM test ranking. For matrix output of LM tests, use the LMMAT option in the LMTESTS statement.

Non-matrix-based *regions* do not assume the knowledge of the model matrices. They are easier to use in most situations. In addition, non-matrix-based *regions* can cover special subsets of parameter locations that cannot be defined by model matrices and submatrices. For example, because of the compartmentalization according to independent and dependent variables in the LINEQS model matrices, the sets of LM tests defined by the LINEQS matrix-based *regions* are limited. For example, you cannot use any matrix-based *regions* to request LM tests for new paths to existing independent variables in the LINEQS model. Such a matrix does not exist in the original specification. However, you can use the non-matrix based *region* NEWENDO to refer to these new paths.

The *regions* for parameter locations are specified by keywords in the LMTESTS statement. Because the *regions* are specific to the types of models, they are described separately for each model type in the following.

The LM Test Regions for COSAN Models

ALLMAT

specifies all parameter locations in all matrices.

CENTRAL

specifies all parameter locations in the central covariance matrices in all terms.

MATRIX | MAT | MATSET = [*set-of-matrices*] | {*set-of-matrices*}

specifies the parameter locations in the matrices specified in *set-of-matrices*.

MEANVEC

specifies all parameter locations in the central mean vectors in all terms.

OUTER

specifies all parameter locations in all matrices except for the central covariance matrices and central mean vectors in all terms.

The LM Test Regions for FACTOR Models

The keywords for the matrix-based regions are associated with the FACTOR model matrices. See the section “[Summary of Matrices in the FACTOR Model](#)” on page 1268 for the definitions and properties of these matrices.

Keywords for Matrix-Based Regions

FACTERRV | FACTERRV

specifies the error variances.

FACTFCOV | FACTFCOV

specifies the covariances among factors.

FACTINTE | FACTINTE

specifies the intercepts.

FACTLOAD | FACTLOAD

specifies the factor loadings.

FACTMEAN | FACTMEAN

specifies the factor means.

Keywords for Non-Matrix-Based Regions

ALL

specifies all parameter locations.

COV

specifies the covariances among factors.

COVERR

specifies the covariances among errors.

COVFACT | COVLV

specifies the covariances among factors.

FIRSTMOMENTS

specifies the means of factors and the intercepts.

INTERCEPTS

specifies the intercepts.

LOADINGS

specifies the factor loadings.

MEANS | MEAN

specifies the means of factors.

The LM Test Regions for LINEQS Models

Keywords for Matrix-Based Regions

The keywords for the matrix-based regions are associated with the LINEQS model matrices. See the section “[Matrix Representation of the LINEQS Model](#)” on page 1272 for definitions of these model matrices and see the section “[Summary of Matrices and Submatrices in the LINEQS Model](#)” on page 1274 for the names and properties and the model matrices and submatrices.

EQSALPHA | EQSALPHA

specifies the intercepts of dependent variables.

EQSBETA | EQSBETA

specifies effects of dependent variables on dependent variables.

EQSGAMMA | _EQSGAMMA_SUB_ | EQSGAMMA | EQSGAMMASUB

specifies the effects of independent variables (excluding errors) on dependent variables. Because effects of errors on dependent variables are restricted to ones in the LINEQS model, LM tests on **_EQSGAMMA_** and **_EQSGAMMA_SUB_** (submatrix of **_EQSGAMMA_**) are the same.

EQSNU | _EQSNU_SUB_ | EQSNU | EQSNUSUB

specifies the means of independent variables (excluding errors). Because means of errors are restricted to zero in the LINEQS model, LM tests on **_EQSNU_** and **_EQSNU_SUB_** (submatrix of **_EQSNU_**) are the same.

EQSPHI | EQSPHI

specifies variances and covariances among all independent variables, including errors.

EQSPHI11 | EQSPHI11

specifies variances and covariances among independent variables, excluding errors.

EQSPHI21 | EQSPHI21

specifies covariances between errors and disturbances with other independent variables.

EQSPHI22 | EQSPHI22

specifies variances and covariances among errors and disturbances.

Keywords for Non-Matrix-Based Regions

ALL

specifies all possible parameter locations.

COV

specifies all covariances among independent variables, including errors and disturbances.

COVERR

specifies covariances among errors or disturbances.

COVEXOG

specifies covariances among independent variables, excluding errors and disturbances.

COVEXOGERR

specifies covariances of errors and disturbances with other independent variables.

COVLV | COVFACT

specifies covariances among latent variables (excluding errors and disturbances).

COVMV | COVOV

specifies covariance among independent manifest variables.

EQUATION | EQUATIONS

specifies all possible linear relationships among variables.

FIRSTMOMENTS

specifies means and intercepts.

INTERCEPTS | INTERCEPT

specifies intercepts of dependent variables.

LV==>LV | LV->LV

specifies all possible effects of latent factors on latent factors.

LV==>MV | LV->MV | MV<==LV | MV<-LV

specifies all possible effects of latent factors on manifest variables.

LV<==MV | LV<-MV | MV==>LV | MV->LV

specifies all possible effects of manifest variables on latent factors.

MEANS | MEAN

specifies the means of independent factors.

MV==>MV | MV->MV

specifies all possible effects of manifest variables on manifest variables.

NEWDEP | NEWENDO

specifies effects of other variables on the independent variables in the original model.

PATHS | PATH

specifies all possible linear relationships among variables.

The LM Test Regions for LISMOD Models

The keywords for the matrix-based regions are associated with the LISMOD model matrices. See the section “Model Matrices in the LISMOD Model” on page 1279 for the definitions and properties of these matrices.

Keywords for Matrix-Based Regions**_ALPHA_ | ALPHA**

specifies the _ALPHA_ matrix.

BETA | BETA

specifies the _BETA_ matrix.

GAMMA | GAMMA

specifies the _GAMMA_ matrix.

KAPPA | KAPPA

specifies the _KAPPA_ matrix.

LAMBDA | LAMBDA

specifies the _LAMBDA_X_ and _LAMBDA_Y_ matrices.

_LAMBDA_X_ | LAMBDA_X

specifies the _LAMBDA_X_ matrix.

_LAMBDA_Y_ | LAMBDA_Y

specifies the _LAMBDA_Y_ matrix.

NU | NU

specifies the _NU_X_ and _NU_Y_ matrices.

_NU_X_ | NU_X

specifies the _NU_X_ matrix.

_NU_Y_ | NU_Y

specifies the _NU_Y_ matrix.

PHI | PHI

specifies the _PHI_ matrix.

PSI | PSI

specifies the _PSI_ matrix.

THETA | THETA

specifies the _THETA_X_ and _THETA_Y_ matrices.

THETAX | THETAX

specifies the `_THETAX_` matrix.

THETAY | THETAY

specifies the `_THETAY_` matrix.

Keywords for Non-Matrix-Based Regions**ALL**

specifies all model matrices.

COV

specifies all covariance parameters in `_THETAY_`, `_THETAX_`, `_PHI_`, and `_PSI_`.

COVERR

specifies all covariances for errors or disturbances in `_THETAY_`, `_THETAX_`, and `_PSI_`.

COVFACT | COVLV

specifies all covariances among latent factors in `_PHI_` when the ξ -variables exist, and in `_PSI_` when the η -variables exist without the presence of the ξ -variables.

FIRSTMOMENTS

specifies all intercepts and means in `_NUY_`, `_NUX_`, `_ALPHA_`, and `_KAPPA_`.

INTERCEPTS | INTERCEPT

specifies all intercepts in `_NUY_`, `_NUX_`, and `_ALPHA_`.

LOADING | LOADINGS

specifies the coefficients in `_LAMBDAY_` and `_LAMBDA_X_`.

LV==>LV | LV->LV

specifies the effects of latent variables on latent variables. Depending on the type of LISMOD model, the `_BETA_` and `_GAMMA_` might be involved.

LV==>MV | LV->MV | MV<==LV | MV<-LV

specifies the effects of latent variables on manifest variables. Depending on the type of LISMOD model, the `_LAMBDAY_`, `_LAMBDA_X_`, and `_GAMMA_` matrices might be involved.

MEANS | MEAN

specifies the mean parameters. Depending on the type of LISMOD model, the `_ALPHA_` and `_KAPPA_` matrices might be involved.

MV==>MV | MV->MV

specifies effects of manifest variables on manifest variables. Depending on the type of LISMOD model, the `_BETA_` and `_GAMMA_` matrices might be involved.

PATHS | PATH

specifies all path coefficients. Depending on the type of LISMOD model, the `_LAMBDAY_`, `_LAMBDA_X_`, `_BETA_`, and `_GAMMA_` matrices might be involved.

The LM Test Regions for MSTRUCT Models

The keywords for the matrix-based regions are associated with the MSTRUCT model matrices. See the section “[Model Matrices in the MSTRUCT Model](#)” on page 1286 for the definitions and properties of these matrices.

Keywords for Matrix-Based Regions

MSTRUCTCOV | _COV_ | MSTRUCTCOV
specifies the `_MSTRUCTCOV_` or `_COV_` matrix.

MSTRUCTMEAN | _MEAN_ | MSTRUCTMEAN
specifies the `_MSTRUCTMEAN_` or `_MEAN_` vector.

Keywords for Non-Matrix-Based Regions

ALL
specifies the `_MSTRUCTCOV_` (or `_COV_`) and `_MSTRUCTMEAN_` (or `_MEAN_`) matrices.

COV
specifies the `_MSTRUCTCOV_` or `_COV_` matrix.

MEANS | MEAN
specifies the `_MSTRUCTMEAN_` or `_MEAN_` matrix.

The LM Test Regions for PATH and RAM Models

The keywords for the matrix-based regions are associated with the submatrices of the RAM model matrices. See the section “[Partitions of the RAM Model Matrices and Some Restrictions](#)” on page 1296 for the definitions of these submatrices and the section “[Summary of Matrices and Submatrices in the RAM Model](#)” on page 1298 for the summary of the names and properties of these submatrices.

Keywords for Matrix-Based Regions

RAMA | _A_ | RAMA
specifies the `_RAMA_` matrix.

_RAMA_LEFT_ | _A_LEFT_ | RAMALEFT
specifies the left portion of the `_RAMA_` matrix.

_RAMA_LL_ | _A_LL_ | RAMALL
specifies the lower left portion of the `_RAMA_` matrix.

_RAMA_LR_ | _A_LR_ | RAMALR
specifies the lower right portion of the `_RAMA_` matrix.

_RAMA_LOWER_ | _A_LOWER_ | RAMALOWER
specifies the lower portion of the `_RAMA_` matrix. This is equivalent to the region specified by the `NEWENDO` keyword.

_RAMA_RIGHT_ | _A_RIGHT_ | RAMARIGHT
specifies the right portion of the `_RAMA_` matrix.

_RAMA_UPPER_ | _A_UPPER_ | RAMAUPPER
specifies the upper portion of the `_RAMA_` matrix.

RAMALPHA | RAMALPHA
specifies the `_RAMALPHA_` matrix.

RAMBETA | RAMBETA
specifies the `_RAMBETA_` matrix.

RAMGAMMA | RAMGAMMA
specifies the `_RAMGAMMA_` matrix.

RAMNU | RAMNU
specifies the `_RAMNU_` matrix.

RAMP | _P_ | RAMP
specifies the `_RAMP_` matrix.

RAMP11 | RAMP11
specifies the `_RAMP11_` matrix.

RAMP21 | RAMP21
specifies the `_RAMP21_` matrix.

RAMP22 | RAMP22
specifies the `_RAMP22_` matrix.

RAMW | _W_ | RAMW
specifies the `_RAMW_` vector.

Keywords for Non-Matrix-Based Regions

ALL
specifies all possible parameter locations.

ARROWS | ARROW
specifies all possible paths (that is, the entries in the `_RAMA_` matrix).

COV
specifies all covariances and partial covariances (that is, the entries in the `_RAMP_` matrix).

COVERR
specifies partial covariances among endogenous variables (that is, the entries in the `_RAMP11_` matrix).

COVEXOG
specifies covariances among exogenous variables (that is, the entries in the `_RAMP22_` matrix).

COVEXOGERR
specifies partial covariances of endogenous variables with exogenous variables (that is, the entries in the `_RAM21_` matrix).

COVLV | COVFACT

specifies covariance among latent factors (that is, entries in `_RAMP11_` pertaining to latent variables).

COVMV | COVOV

specifies covariance among manifest variables (that is, entries in `_RAMP11_` pertaining to manifest variables).

FIRSTMOMENTS

specifies means or intercepts (that is, entries in `_RAMW_` vector).

INTERCEPTS | INTERCEPT

specifies intercepts for endogenous variables (that is, entries in `_RAMALPHA_` vector).

LV==>LV | LV->LV

specifies effects of latent variables on latent variables.

LV==>MV | LV->MV | MV<==LV | MV<-LV

specifies effects of latent variables on manifest variables.

LV<==MV | LV<-MV | MV==>LV | MV->LV

specifies effects of manifest variables on latent variables.

MEANS | MEAN

specifies the means of exogenous variables (that is, entries in the `_RAMNU_` vector).

MV==>MV | MV->MV

specifies effects of manifest variables on manifest variables.

NEWENDO

specifies new paths to the exogenous variables in the original model.

PATHS | PATH

specifies all possible paths (that is, the entries in the `_RAMA_` matrix).

MATRIX Statement

MATRIX *matrix-name* < *location* <= *parameter-spec* > < , *location* <= *parameter-spec* ... >>> ;

MATRIX statement specifies the matrix elements (locations) and their parameters. Parameters can be fixed or free, with or without initial estimates. The *matrix-name* indicates the matrix to specify in the MATRIX statement. The *location* indicates the starting row and column numbers of the matrix being specified and the *parameter-spec* is a list of free or fixed parameters for the elements that are indicated by the *location*.

The MATRIX statement is a [subsidiary model specification statement](#) of the COSAN, LISMOD, and MSTRUCT modeling languages. You might need to use the MATRIX statements as many times as needed for specifying your model. However, you can use the MATRIX statement at most once for each distinct model matrix.

Valid Matrix Names for the COSAN Model

The valid *matrix-names* depend on the your specification in the COSAN statement in which you define the COSAN model matrices and their properties. Except for those fixed matrices with the IDE or ZID type, you can use the MATRIX statement to specify any COSAN model matrices you define in the COSAN statement.

Valid Matrix Names for the LISMOD Model

There are 12 model matrices in the LISMOD model, and they correspond to the following valid *matrix-names* :

- matrices and their types in the measurement model for the y-variables

LAMBDAY the matrix of regression coefficients of the y-variables on the η -variables (general, GEN)

NUY the vector of intercept terms of the y-variables (general, GEN)

THETAY the error covariance matrix for the y-variables (symmetric, SYM)

- matrices and their types in the measurement model for the x-variables

_LAMBDA_X_ the matrix of regression coefficients of the x-variables on the ξ -variables (general, GEN)

NUX the vector of intercept terms of the x-variables (general, GEN)

_THETA_X_ the error covariance matrix for the x-variables (symmetric, SYM)

- matrices and their types in the structural model

ALPHA the vector of intercept terms of the η -variables (general, GEN)

BETA the matrix of regression coefficients of the η -variables on the η -variables (general, GEN)

GAMMA the matrix of regression coefficients of the η -variables on the ξ -variables (general, GEN)

KAPPA the mean vector for the ξ -variables (general, GEN)

PHI the covariance matrix for the ξ -variables (symmetric, SYM)

PSI the error covariance matrix for the η -variables (symmetric, SYM)

Valid Matrix Names for the MSTRUCT Modeling Language

The following *matrix-names* are valid for the MSTRUCT modeling language:

COV the covariance matrix (symmetric, SYM)

MEAN the mean vector (general, GEN)

Specifying Locations in Model Matrices

The five main types of matrix *locations* (elements) specification in the MATRIX statement are briefly described in the following:

- **Unspecified *location*:** Blank or [,]
Use this notation to specify the [1,1] element of the matrix, and to specify the remaining *valid* elements of the matrix in a prescribed order until all the parameters in the *parameter-spec* list are assigned.
- **Row-and-column *location*:** [i, j], [@i, j], [i, @j], or [@i, @j]
Use this notation to specify the [i, j] element of a matrix, and to specify the remaining elements of the matrix in the order indicated by the *location* notation until all the parameters in the *parameter-spec* list are assigned.
- **Row *location* only:** [i,], [@i,], or [iset,]
Use this notation to specify the first *valid* matrix element in the [i]-th row (for the first two notations) or the [i1]-th row (for the [iset,] notation, where *iset*=(i1, i2, ...) is a set of row numbers), and to specify the remaining elements of the matrix in the order indicated by the *location* notation until all the parameters in the *parameter-spec* list are assigned.
- **Column *location* only:** [, j], [, @j], or [, jset]
Use this notation to specify the first *valid* matrix element in the [j]-th column (for the first two notations) or the [j1]-th column (for the [, jset] notation, where *jset*=(j1, j2, ...) is a set of columns), and to specify the remaining elements of the matrix in the order indicated by the *location* notation until all the parameters in the *parameter-spec* list are assigned.
- **Row-and-column-sets *location*:** [iset, jset], [iset, j], or [i, jset]
Use this notation to specify the [i1, j1] element of the matrix, where *i1* is either the same as *i* or the first row number specified in *iset*, and *j1* is either the same as *j* or the first column number specified in *jset*, and to specify the remaining elements of the matrix in the order indicated by the *location* notation until all the parameters in the *parameter-spec* list are assigned.

Consider the following points about the *location* specifications:

- In the description of the various *location* specifications, the starting matrix element for parameter assignment is relatively well-defined. However, if the *parameter-spec* list has more than one parameter, there are more matrix elements to assign with the parameters in the *parameter-spec* list. If there is no *parameter-spec* list, a set of matrix elements are specified as unnamed free parameters. Hence, the actual number of elements specified by these *location* specifications depends on the length of the *parameter-spec* list.
- Because more than one matrix element could be specified in any of these *location* specifications, it is important to understand the order that PROC CALIS uses to assign the matrix elements.
- In some of the *location* specifications, either the row or column is unspecified and the assignment of the matrix element starts with the first *valid* element given the column or the row number. This first *valid* element depends on the type of the matrix in question.

The next few sections describe the parameter assignments in more detail for each of these *location* specifications in the MATRIX statement.

Unspecified Location: Blank or [,]

This notation means that all valid elements started with the [1,1] element of the matrix specified in the model. If no *parameter-spec* list is specified, all valid elements in the matrix are unnamed free parameters. For these elements, PROC CALIS generates parameter names with the `_Parm` prefix followed by a unique integer (for example, `_Parm1`, `_Parm2`, and so on). If a *parameter-spec* list is specified, the assignment of parameters starts with the [1,1] element and proceeds to the next *valid* elements in the same row. If the entire row of valid elements is assigned with parameters, it proceeds to the next row and so on, until all the parameters in the *parameter-spec* list are assigned. The valid element given the row or column number depends on the type of matrix in question. The following examples illustrate the usage of the unspecified *location* notation.

Suppose that `_GAMMA_` is a general 3×3 matrix. The following statement specifies four elements of this matrix:

```
matrix _GAMMA_ [,] = gg1-gg4;
```

Equivalently, you can use the following blank *location* specification:

```
matrix _GAMMA_ = gg1-gg4;
```

Both specifications are equivalent to the following elementwise specification:

```
matrix _GAMMA_ [1,1] = gg1,
                [1,2] = gg2,
                [1,3] = gg3,
                [2,1] = gg4;
```

With the unspecified *location* for the matrix `_GAMMA_`, the first row is filled up with the parameters first. Then it proceeds to the next row and so on until all parameters in the *parameter-spec* list are assigned. Because there are four parameters and `_GAMMA_` has three columns, the parameter `gg4` is assigned to the `_GAMMA_[2, 1]` element.

However, if the preceding specification is for a 3×3 matrix symmetric matrix `_PHI_`, the parameters are assigned differently. That is, the following specification has different matrix elements assigned with the parameters:

```
matrix _PHI_ = gg1-gg4;
```

Because symmetric matrices contain redundant elements, parameters are assigned only to the lower triangular elements (including the diagonal elements). As a result, the following elementwise specification reflects the preceding specification of matrix `_PHI_`:

```
matrix _PHI_ [1,1] = gg1,
              [2,1] = gg2,
              [2,2] = gg3,
              [3,1] = gg4;
```

The case for lower triangular matrices is the same as the case for symmetric matrices. That is, only the lower triangular elements are valid elements for the parameter assignments.

For upper triangular matrices, only the upper triangular elements (including the diagonal elements) are valid for the parameter assignments. For example, consider the following specification of a 3×3 upper triangular matrix `UPP`:

```
matrix UPP = gg1-gg4;
```

The matrix elements assigned with the parameters are the same as the following elementwise specification:

```
matrix UPP [1,1] = gg1,
           [1,2] = gg2,
           [1,3] = gg3,
           [2,2] = gg4;
```

If a 4×4 diagonal matrix is specified by the preceding MATRIX statement, the parameters are assigned to the following elements: [1, 1], [2, 2], [3, 3], and [4, 4].

Lastly, if there is no *parameter-spec* list for the unspecified *location* notation, all valid parameters in the matrix being specified are unnamed free parameters. For example, if **A** is a 4×4 general rectangular matrix, the following specification assigns 16 unnamed free parameters to all of the elements in **A**:

```
matrix A [ , ];
```

PROC CALIS generates parameters `_Parm1`, `_Parm2`, ..., `_Parm16` to the elements [1, 1], [1, 2], [1, 3], ..., [4, 3], [4, 4], respectively.

However, if **S** is a 4×4 *symmetric* matrix, the following specification assigns only 10 unnamed free parameters to the lower triangular elements of **S**:

```
matrix S;
```

PROC CALIS generates parameters `_Parm1`, `_Parm2`, ..., `_Parm10` to the elements [1, 1], [2, 1], [2, 2], ..., [4, 3], [4, 4], respectively.

Row-and-Column Location: [*i*, *j*], [*@i*, *j*], [*i*, *@j*], or [*@i*, *@j*]

All these notations provide the starting row (*i*) and column (*j*) numbers for the assignment of the parameters in the *parameter-spec* list. The notations are different in the way they proceed to the next element in the matrix. If no *parameter-spec* list is specified, only the single element [*i*, *j*] is an unnamed free parameter. For this [*i*, *j*] element, PROC CALIS generates a parameter name with the `_Parm` prefix followed by a unique integer (for example, `_Parm1`). If a *parameter-spec* list is specified, the assignment of parameters starts with the [*i*, *j*] element and proceeds to next element until all the parameters in the *parameter-spec* list are assigned. The following summarizes how the assignment of parameter proceeds, depending on the uses of the @ sign before the starting row or column number:

- [*i*, *j*] specifies the [*i*, *j*] element, and proceeds to [*i*+1, *j*+1], [*i*+2, *j*+2], and so on.
- [*@i*, *j*] specifies the [*i*, *j*] element, and proceeds to [*i*, *j*+1], [*i*, *j*+2], [*i*, *j*+3], and so on.
- [*i*, *@j*] specifies the [*i*, *j*] element, and proceeds to [*i*+1, *j*], [*i*+2, *j*], [*i*+3, *j*], and so on.
- [*@i*, *@j*] specifies the [*i*, *j*] element only.

The following examples illustrates the usage of the row-and-column *location* notation.

The simplest case is the specification of a single element as an unnamed free parameter. For example, the following statement specifies that [1, 4] in matrix **A** is an unnamed free parameter:

```
matrix A [1,4];
```

PROC CALIS generates a parameter name with the `_Parm` prefix for this element. In this case, using the `@` sign before the row or column number is optional. That is, the following statements are all the same specification:

```
matrix A [1,4];
matrix A [@1,4];
matrix A [1,@4];
matrix A [@1,@4];
```

You can specify more than one unnamed free parameter by using multiple *location* specifications, as shown in the following example:

```
matrix A [1,4], [3,5];
```

Elements `[1,4]` and `[3,5]` of matrix `A` are both unnamed free parameters. However, when a *parameter-spec* list is specified after the *location*, more than one parameters might be specified. The use of the `@` determines how the elements in the matrix are assigned with the parameters in the *parameter-spec* list. The following examples illustrate this under various situations.

For example, consider the following specification of a 4×4 matrix general matrix `A`:

```
matrix A
  [1,1] = a b c;
```

The three parameters `a`, `b`, and `c`, are assigned to the matrix elements `[1,1]`, `[2,2]`, and `[3,3]`, respectively. That is, this specification is equivalent to the following elementwise specification:

```
matrix A
  [1,1] = a ,
  [2,2] = b ,
  [3,3] = c ;
```

However, with the `@` sign, the assignment is different. For example, consider the `@` sign attached to the row number in the following specification:

```
matrix A
  [@1,1] = a b c;
```

The `@` sign fixes the row number to 1. As a result, this specification is equivalent to the following elementwise specification:

```
matrix A
  [1,1] = a ,
  [1,2] = b ,
  [1,3] = c ;
```

Using the `@` sign before the column number fixes the column number. For example, consider the following specification of matrix `A`:

```
matrix A
  [2,@2] = a b c;
```

The @ sign fixes the column number to 2. As a result, this specification is equivalent to the following elementwise specification:

```
matrix A
  [2,2] = a ,
  [3,2] = b ,
  [4,2] = c ;
```

If you put the @ sign in both of the row and column numbers, only one element is intended to be assigned. For example, the following specification means that only $A[2, 3]$ is assigned with the parameter a:

```
matrix A
  [@2,@3] = a;
```

But you could specify this simply as the statement without the @ sign:

```
matrix A
  [2,3] = a;
```

Notice that the matrix type does not play a role in determining the elements for the parameter assignments in the row-and-column *location* specification. You have to make sure that the parameters are assigned in the valid elements of the matrix. For example, suppose that S is a 4×4 symmetric matrix and you specify the following statement for its elements:

```
matrix A
  [@3,2] = a b c;
```

The elements to be assigned with the parameters a, b, and c, are $[3, 2]$, $[3, 3]$, and $[3, 4]$, respectively. However, because S is symmetric, you can specify only the nonredundant elements in the lower triangular of S . Hence, the specification of the $[3, 4]$ element is not valid and it generates an error.

Row Location Only: $[i,]$, $[@i,]$, or $[iset,]$

All these notations provide the starting row $[i1,]$ for the assignment of the parameters in *parameter-spec*, where $i1$ is i for the first two *location* notations or $i1$ is the first row specified in *iset*, where $iset = (i1, i2, \dots)$ is a set of row numbers. Because no column location is specified, the starting element is the first valid element in the $i1$ -th row of the matrix.

If no *parameter-spec* list is specified, all the valid elements in the entire $i1$ -th row of the matrix are unnamed free parameters. If a set of row numbers is specified in *iset*, all the valid elements in the all the rows specified in *iset* are unnamed free parameters.

If a *parameter-spec* list is specified, the assignment of parameters starts with the first valid elements of the $i1$ -th row. The assignment proceeds to next valid elements in the same row. The $[i,]$ specification proceeds row by row for parameter assignment while the $[@i,]$ specification stays at the same i -th row. The $[iset,]$ specification indicates and limits the sequence of rows to be assigned with the parameter in the *parameter-spec* list. The assignment stops when all the parameters in the *parameter-spec* list are assigned. The following summarizes how the assignment of parameters proceeds in more precise terms:

- $[i,]$ specifies the first valid element in row i and proceeds to the valid elements in rows $i, i+1, i+2, \dots$, until all parameters in the *parameter-spec* list are assigned.

- `[@i,]` specifies the first valid elements in row `i` and proceeds to the valid elements in the *same* row until all parameters in the *parameter-spec* list are assigned.
- `[iset,]` specifies the first valid elements in row `i1`, where `i1, i2, ...` are the rows specified in *iset*. It proceeds to the valid elements in rows `i1, i2, ...`, until all parameters in the *parameter-spec* list are assigned.

The following examples illustrates the usage of the row *locations*.

The simplest case is the specification of all valid elements of a single row as unnamed free parameters. For example, the following specification of a 3×3 rectangular matrix `A` assigns unnamed free parameters to all the elements in the second row of matrix `A`:

```
matrix A [2,];
```

PROC CALIS generates parameter names with the `_Parm` prefix for these elements. For example, the `[2, 1]`, `[2, 2]`, and `[2, 3]` elements are named with `_Parm1`, `_Parm2`, and `_Parm3`, respectively.

Using the `@` sign before the row number in this case is optional. That is, the following statement is the same specification:

```
matrix A [@2,];
```

If you specify a set of row numbers without the *parameter-spec* list, all valid elements of the specified rows are unnamed free parameters. For example, consider the following specification of a 6×6 symmetric matrix `S`:

```
matrix S [1 3 5,];
```

This specification specifies unnamed free parameters for the lower triangular elements in the first, third, and fifth rows of matrix `S`. It is equivalent to the following specification:

```
matrix S [1,],
          [3,],
          [5,];
```

As a result, this means that the following elements in matrix `S` are free parameters: `[1, 1]`, `[3, 1]`, `[3, 2]`, `[3, 3]`, `[5, 1]`, `[5, 2]`, `[5, 3]`, `[5, 4]`, and `[5, 5]`. Notice that only the elements in the lower triangular of those specified rows in `S` are free parameters. This shows that parameter assignment with the row *location* notation depends on the matrix type.

With the use of the *parameter-spec* list, the parameter assignment with the row *location* notation stops when all the parameters are assigned. For example, consider the following specification of a 4×4 *general* (rectangular) matrix `A`:

```
matrix A
  [2,] = a b c;
```

The three parameters `a`, `b`, and `c`, are assigned to the matrix elements `[2, 1]`, `[2, 2]`, and `[2, 3]`, respectively. However, a different assignment of the parameters applies if you use the same specification for a 4×4 *symmetric* matrix `S`, as shown in the following statement:

```
matrix S
  [2, ] = a b c;
```

Because there are redundant elements in a symmetric matrix, you can specify only the lower triangular elements. Therefore, the row *location* specification is equivalent to the following elementwise specification:

```
matrix S
  [2, 1] = a ,
  [2, 2] = b ,
  [3, 1] = c ;
```

When all the valid row elements are assigned with the parameters, the assignment proceeds to the next row. This is why the last parameter assignment is for $S[3, 1]$. The same assignment sequence applies to matrices with the lower triangular type (LOW).

For matrices with the upper triangular matrix type (UPP), only the elements in the upper triangular are assigned. For example, consider a 4×4 upper triangular matrix U with the following row *location* specification:

```
matrix U
  [2, ] = a b c d;
```

The assignment of parameters is the same as the following elementwise specification:

```
matrix U
  [2, 2] = a ,
  [2, 3] = b ,
  [2, 4] = c ,
  [3, 3] = d;
```

The first valid element in the second row of the U matrix is $U[2, 2]$. Because all the valid elements in the second row are assigned with parameters, the last element has to go to the valid element in the next row. Hence, the parameter d is assigned to $U[3, 3]$.

For matrices with the diagonal matrix type (DIA), only the diagonal elements are assigned. For example, consider a 4×4 upper diagonal matrix D with the following row *location* specification:

```
matrix D
  [2, ] = a b c;
```

The assignment of parameters is the same as the following elementwise specification:

```
matrix D
  [2, 2] = a ,
  [3, 3] = b ,
  [4, 4] = c ;
```

If you use an $@$ sign before the row number in the row *location* specification, the row number cannot move—it cannot proceed to the next row even if the valid elements in that row are already filled with the parameters in *parameter-spec*. All other behavior of the $[@i,]$ specification is the same as that of the $[i,]$ specification. For example, consider the following specification of a 4×4 *general* (rectangular) matrix A :

```
matrix A
  [@2,] = a b c d;
```

The four parameters a, b, c, and d, are assigned to the matrix elements [2, 1], [2, 2], [2, 3], and [2, 4], respectively. This is exactly the same result as the following specification without the @ sign:

```
matrix A
  [2,] = a b c d;
```

Here, all the elements of the second row of matrix A are assigned with elements. However, if one more parameter is specified in the *parameter-spec* list, the behavior for the two types of row *location* specifications are different. The following specification without the @ sign proceeds to the next row for the last parameter:

```
matrix A
  [2,] = a b c d e;
```

That is, the parameter e is assigned to the A[3, 1] element. However, the following specification *with* the @ sign results in an out-of-bound error:

```
matrix A
  [@2,] = a b c d e;
```

The out-of-bound error is due to the fact that the row number must be fixed so that the parameter e is forced to be assigned to A[2, 5], which does not exist.

However, the distinction between the row *location* specifications with and without the @ sign is not very important in common practice because in most cases you do not want the parameter assignment to proceed row after row automatically with a long list of parameters. For example, consider the following specification of a 4×4 *symmetric* matrix S:

```
matrix S
  [2,] = s21 s22 s31 s32 s33 s41 s42 s43;
```

This specification is equivalent to the following specification:

```
matrix S
  [2,] = s21 s22,
  [3,] = s31 s32 s33,
  [4,] = s41 s42 s43;
```

Although this specification is not as concise as the preceding one, it specifies more clearly about how parameters are assigned to each of the three rows of the S matrix. In this specification, you make sure that each of the three row *location* specifications has just enough parameters for the given row without proceeding to the next row for additional parameter assignments. With this kind of “careful” row *location* specifications, you do not need to use the @ sign before the row numbers at all.

The last type of row *location* specification is the [*iset*,] notation, where *iset* means a set of row numbers. This specification type provides the set of row numbers for the assignment of the parameters in the *parameter-spec* list. For example, consider the following specification of a 4×4 *general* matrix A:

```
matrix A
  [2 4,] = a21 a22 a23 a24 a41 a42 a43 a44;
```

This specification is equivalent to the following statement with two row *location* specifications:

```
matrix A
  [2,] = a21 a22 a23 a24,
  [4,] = a41 a42 a43 a44;
```

In other words, the assignment of parameters follows the order of rows provided in the *iset*. Notice that the *iset* notation merely provides the order of rows to be assigned with the parameters in the *parameter-spec* list; it is not an error if you provide a shorter parameter list than that of the total number of elements in the rows. For example, the following specification of a 4×4 *general* matrix **A** is valid:

```
matrix A
  [2 4,] = a21 a22 a23 a24;
```

This specification has the same results as the following statement with one row *location*:

```
matrix A
  [2,] = a21 a22 a23 a24;
```

However, a valid specification does not mean it is a good representation of the problem. Providing more rows in the *iset* specification than intended is simply not a good practice.

Although a shorter *parameter-spec* list is acceptable, a longer list results in an error. For example, the following specification of a 4×4 *symmetric* matrix **S** results in an error:

```
matrix S
  [2 to 3,] = s21 s22 s31 s32 s33 extra1 extra2;
```

The `[2 to 3,]` not only gives the sequence of the rows for the parameter assignment, it also limits the set of rows to assign. Because matrix **S** is symmetric and because only the second and the third rows are supposed to be assigned with the *iset* specification, the parameters `extra1` and `extra2` are excessive.

Column Location Only: `[, j]`, `[, @j]`, or `[, jset]`

These notations mirror that of the row *location* notations. Instead of the rows being specified, the columns are specified by these notations. Therefore, you can understand the column *location* notations the same way as the row *location* notations.

All these column *location* notations provide the starting column `[, j1]` for the assignment of the parameters in *parameter-spec*, where `j1` is `j` for the first two *location* notations or `j1` is the first column specified in *jset*, where *jset* = (`j1`, `j2`, ...) is a set of column numbers. Because no row location is specified, the starting element is the first valid element in the `j1`-th column of the matrix.

If no *parameter-spec* list is specified, all the valid elements in the entire `j1`-th column of the matrix are unnamed free parameters. If a set of column numbers is specified in *jset*, all the valid elements in the all the columns specified in *jset* are unnamed free parameters.

If a *parameter-spec* list is specified, the assignment of parameters starts with the first valid elements of the `j1`-th column. The assignment proceeds to next valid elements in the same column. The `[, j]` specification proceeds column by column for parameter assignment while the `[, @j]` specification stays at the same `j`-th column. The `[, jset]` specification indicates and limits the sequence of columns to be assigned with the parameter in the *parameter-spec* list. The assignment stops when all the parameters in the *parameter-spec* list are assigned. The following list summarizes how the assignment of parameters proceeds:

- `[, j]` specifies the first valid element in column `j` and proceeds to the valid elements in columns `j`, `j+1`, `j+2`, ..., until all parameters in the *parameter-spec* list are assigned.

- `[, @j]` specifies the first valid elements in column `j` and proceeds to the valid elements in the *same* column until all parameters in the *parameter-spec* list are assigned.
- `[, jset]` specifies the first valid elements in column `j1`, where `j1, j2, ...` are the columns specified in *jset*. It proceeds to the valid elements in columns `j1, j2, ...`, until all parameters in the *parameter-spec* list are assigned.

See the section “Row Location Only: `[i,]`, `[@i,]`, or `[iset,]`” on page 1181 for examples, which are applicable to the usage of the column *locations*.

Row-and-Column-Sets Location: `[iset, jset]`, `[iset, j]`, or `[i, jset]`

These notations specify the sets of row and column elements for the assignment of the parameters in the *parameter-spec* list. In the first notation, you specify the set of row numbers in *iset* = (`i1, i2, ...`), and the set of column numbers in *jset* = (`j1, j2, ...`). The last two notations are special cases of the first notation. The `[iset, j]` notation specifies only one column with *jset* = `j1 = j`. The `[i, jset]` notation specifies only one row with *iset* = `i1 = i`. For the last two notations, adding the `@` sign before `j` or `i` is optional. In general, the row-and-column-sets *locations* specify the matrix elements in the following order:

```
[i1, j1], [i1, j2], ...,
[i2, j1], [i2, j2], ...,
[i3, j1], [i3, j2], ...,
..., ..., ...,
[ir, j1], [ir, j2], ..., [ir, js]
```

where `r` represents the number of rows in the *iset* and `s` represents the number of columns in the *jset*. Note that this ordering of elements does not necessarily mean that all these elements are specified. The number of elements specified depends on the length of the *parameter-spec* list.

If no *parameter-spec* list is specified after the *location* notation, all the `r × s` elements specified in the *iset* and *jset* are unnamed free parameters. PROC CALIS generates parameter names with the `_Parm` prefix for these elements.

If a *parameter-spec* list is specified after the *location* notation, the total number of matrix elements that are assigned with the parameters is the same as the number of parameter specifications in the *parameter-spec* list.

The following examples illustrates the usage of the row-and-column-sets *locations*.

The simplest case is the specification of all elements in the *iset* and *jset* as free parameters, as shown in the following statement:

```
matrix _Gamma_ [2 3, 4 1];
```

This means that `_Gamma_[2, 4]`, `_Gamma_[2, 1]`, `_Gamma_[3, 4]`, and `_Gamma_[3, 1]` are all free parameters in the matrix. For these elements, PROC CALIS generates parameter names with the `_Parm` prefix followed by a unique integer (for example, `_Parm1`, `_Parm2`, ...). This row-and-column-sets *location* specification is the same as the following specification:

```
matrix _Gamma_ [2, 4 1], [3, 4 1];
```

It is also equivalent to the following elementwise specification:

```
matrix _Gamma_ [2,4], [2,1], [3,4], [3,1];
```

If you provide a *parameter-spec* list after the row-and-column-sets *location*, the parameters in the list are assigned to the matrix elements. For example, consider the following specification:

```
matrix _Gamma_ [2 3,4 1] = gamma1-gamma4;
```

This specification is equivalent to the following elementwise specification:

```
matrix _Gamma_ [2,4] = gamma1,
                [2,1] = gamma2,
                [3,4] = gamma3,
                [3,1] = gamma4;
```

It is not necessary for all the elements specified in the row-and-column-sets *location* to be assigned with the parameters in the *parameter-spec* list. For example, the following *iset* and *jset* specify a maximum of six elements, but only five parameters are assigned as a result of a shorter *parameter-spec* list:

```
matrix _Gamma_ [2 to 4,1 5] = gamma1-gamma4;
```

This specification is equivalent to the following elementwise specification:

```
matrix _Gamma_ [2,1] = gamma1,
                [2,5] = gamma2,
                [3,1] = gamma3,
                [3,5] = gamma4,
                [4,1] = gamma5;
```

In this case, `_Gamma_[4,5]` is not specified and is fixed at zero by default.

With the row-and-column-sets *location* specifications, you need to be aware of the matrix type being specified. For example, the following specification of the symmetric matrix **S** results in an out-of-bounds error:

```
matrix S [1 2,1 2] = s1-s4;
```

This specification is equivalent to the following elementwise specification:

```
matrix S [1,1] = s1,
          [1,2] = s2,
          [2,1] = s3,
          [2,2] = s4;
```

The specification of the `S[1,2]` element is not valid because you can specify only the lower triangular elements of a symmetric matrix in PROC CALIS. The upper triangular elements are redundant and are taken into account by PROC CALIS during computations.

Specifying Fixed and Free Parameters in Model Matrices

For clarity in describing various *location* notations, the *parameter-spec* list contains only free parameters in the examples. In general, you can specify fixed values, free parameters, and initial values in the *parameter-spec* list. The syntax for the *parameter-spec* list is the same as the *parameter-spec* list for the **VARIANCE** statement. You can specify the following five types of the parameters in the **MATRIX** statement:

- an unnamed free parameter
- an initial value
- a fixed value
- a free parameter with a name provided
- a free parameter with a name and initial value provided

The following example demonstrates these five types of specifications:

```
matrix A [1,2],
         [1,3] = (.2),
         [1,4] = .3,
         [2,3] = a1,
         [2,4] = a2(.5);
```

In this statement, $A[1, 2]$ is an unnamed free parameter. For this element, PROC CALIS generates a parameter name with the `_Parm` prefix and appended with a unique integer (for example, `_Parm1`). $A[1, 3]$ is an unnamed free parameter with an initial value of 0.2. PROC CALIS also generates a parameter name for this element. $A[1, 4]$ is fixed at 0.3. This value does not change in estimation. $A[2, 3]$ is a free parameter named `a1`. No initial value is given for this element. $A[2, 4]$ is a free parameter named `a2` with an initial value of 0.5.

You can also specify different types of parameters in the *parameter-spec* list. The preceding specification is equivalent to the following specification:

```
matrix A [1,2],
         [1 2,3 4] = (.2) .3 a1-a2 (.5);
```

Notice that 0.5 is the initial value for `a2` but not for `a1` because this specification is the same as:

```
matrix A [1,2],
         [1 2,3 4] = (.2) .3 a1 a2(.5);
```

When you use *parameter-spec* lists with mixed parameters, you must be careful about how the initial value syntax is interpreted with and without a parameter name before it. With a parameter before the initial value, the initial value is for the parameter, as shown in the following statement:

```
matrix S [1,1] = s1 s2 (.2);
```

This specification is the same as the following elementwise specification:

```
matrix S [1,1] = s1,
         [2,2] = s2(.2);
```

This means that 0.2 is the initial value of parameter `s2`, but not interpreted as an unnamed free parameter for $S[3, 3]$. If you do intend to set the free parameter `s2` for $S[2, 2]$ without an initial value and set the initial value 0.2 for $S[3, 3]$, you can use a null initial value for the `s2` parameter, as shown in the following:

```
matrix S [1,1] = s1 s2() (.2);
```

This specification is the same as the following elementwise specification:

```
matrix S [1,1] = s1,
          [2,2] = s2,
          [3,3] = (.2);
```

Modifying a Parameter Specification from a Reference Model

If you define a new COSAN, LISMOD, or MSTRUCT model by using a reference (old) model in the [REFMODEL](#) statement, you might want to modify some parameter specifications from the [MATRIX](#) statement of the reference model before transferring the specifications to the new model. To change a particular matrix element specification from the reference model, you can simply respecify the same matrix element with the desired parameter specification in the [MATRIX](#) statement of the new model. To delete a particular matrix parameter from the reference model, you can specify the desired matrix element with a missing value specification in the [MATRIX](#) statement of the new model.

For example, suppose that `_PHI_[1,2]` is a free parameter in the reference model but you do not want this matrix element be a free parameter in the new model, you can use the following specification in the new model:

```
matrix _PHI_ [1,2] = .;
```

Notice that the missing value syntax is valid only when you use the [REFMODEL](#) statement. See the section “[Modifying a COSAN Model from a Reference Model](#)” on page 1129 for a more detailed example of COSAN model respecification. See the section “[Modifying a LISMOD Model from a Reference Model](#)” on page 1164 for a more detailed example of LISMOD model respecification. See the section “[Modifying an MSTRUCT Model from a Reference Model](#)” on page 1195 for a more detailed example of MSTRUCT model respecification.

MEAN Statement

```
MEAN assignment <, assignment ... >;
```

where *assignment* represents:

```
var-list < = parameter-spec >
```

The [MEAN](#) statement specifies the mean or intercept parameters in connection with the [FACTOR](#), [LINEQS](#), and [PATH](#) modeling languages. With the [MEAN](#) statement specification, [PROC CALIS](#) analyzes the mean structures in addition to the covariance structures.

In each *assignment* of the [MEAN](#) statement, you list the *var-list* that you want to specify for their means or intercepts. Optionally, you can provide a list of parameter specifications in a *parameter-spec* after an equal sign for each *var-list*. The syntax of the [MEAN](#) statement is exactly the same as that of the [VARIANCE](#) statement. See the [VARIANCE statement](#) on page 1231 for details about the syntax.

For the confirmatory [FACTOR](#) or [PATH](#) model, the variables in a *var-list* can be exogenous or endogenous. You specify the mean of a variable if the variable is exogenous. You specify the intercept of a variable if

the variable is endogenous. However, for the LINEQS model, you can specify only the means of exogenous variables whose type is not error (that is, not the E- or D- variables) in the MEAN statement. You cannot specify the intercept parameters in the MEAN statement for the LINEQS model. Instead, you must specify the intercepts in the equations of the LINEQS statement. For the exploratory FACTOR model, the MEAN statement is used merely to include the mean structures into analysis. In this case, the parameter specification by the *assignment* syntax is not interpreted. Instead, the intercept parameters for the exploratory factor model are automatically generated by PROC CALIS.

You can specify the following five types of the parameters for the means or intercepts in the MEAN statement:

- an unnamed free parameter
- an initial value
- a fixed value
- a free parameter with a name provided
- a free parameter with a name and initial value provided

For example, consider a PATH model with exogenous variables x1, x2, and x3 and endogenous variables y4 and y5. The following MEAN statement illustrates the five types of specifications in five *assignments*:

```
mean x1 ,
      x2 = (3.0) ,
      x3 = 1.5 ,
      y4 = intercept1 ,
      y5 = intercept2 (0.6) ;
```

In this statement, the mean of x1 is specified as an unnamed free parameter. For this mean, PROC CALIS generates a parameter name with the `_Parm` prefix and appended with a unique integer (for example, `_Parm1`). The mean of x2 is an unnamed free parameter with an initial value of 3.0. PROC CALIS also generates a parameter name for this mean. The mean of x3 is a fixed value of 1.5. This value stays the same during the estimation. The intercept of endogenous variable y4 is a free parameter named `intercept1`. The intercept of endogenous variable y5 is a free parameter named `intercept2` with an initial value of 0.6.

The syntax of the MEAN statement is the same as the syntax of the VARIANCE statement. See the [VARIANCE](#) statement for more illustrations about the usage.

Default Mean and Intercept Parameters

If the mean structures are analyzed, either the means or intercepts of the *manifest* variables in the FACTOR, LINEQS, or PATH model are free parameters by default. If a manifest variable is exogenous, then its mean is a free parameter by default. If a manifest variable is endogenous, then its intercept is a free parameter by default. Except for the exploratory FACTOR model, PROC CALIS generates parameter names for these default free mean or intercept parameters that include the `_Add` prefix and are appended with unique integer suffixes. The default intercepts of the exploratory FACTOR model use the `_a` prefix instead. For the confirmatory FACTOR model and the PATH model, you can use the MEAN statement to override these default mean or intercept parameters in situations where you want to set parameter constraints, provide initial or fixed values, or make parameter references. However, you cannot override any default intercept

parameters for the exploratory FACTOR model. For the LINEQS model, you can use the MEAN statement specification to override only the default mean parameters. The intercept parameters of the LINEQS model must be specified in the equations of the LINEQS statement.

Fixed zero is another type of default mean or intercept parameters for the FACTOR, LINEQS, or PATH model. All the intercepts and means of the *latent* variables in these models are fixed zeros by default. For the confirmatory FACTOR and PATH models, you can override these default fixed zeros by using the MEAN statement specifications. However, you cannot override the fixed zero factor means for the exploratory FACTOR model. For the LINEQS model, you can override only the default fixed zeros of latent variables whose type is not error. That is, you can use the MEAN statement to override the default zero mean for the exogenous latent factors (excluding the error or disturbance variables) or use the LINEQS statement to override the default zero intercept for the endogenous latent factors. The fixed zero means for the error or disturbance variables in the LINEQS model reflects model restrictions—there is no way you can override these default zero means.

Modifying a Mean or Intercept Parameter Specification from a Reference Model

If you define a new FACTOR (confirmatory factor model only), LINEQS, or PATH model by using a reference (old) model in the REFMODEL statement, you might want to modify some parameter specifications from the MEAN statement of the reference model before transferring the specifications to the new model. To change a particular mean or intercept specification from the reference model, you can simply respecify the same mean or intercept with the desired parameter specification in the MEAN statement of the new model. To delete a particular mean or intercept parameter from the reference model, you can specify the desired mean or intercept with a missing value specification in the MEAN statement of the new model.

For example, suppose that the mean of F1 is specified in the reference model, but you do not want this mean specification be transferred to the new model. You can use the following MEAN statement specification in the new model:

```
mean F1 = . ;
```

Note that the missing value syntax is valid only when you use with the REFMODEL statement. See the section “[Modifying a FACTOR Model from a Reference Model](#)” on page 1146 for a more detailed example of FACTOR model respecification. See the section “[Modifying a LINEQS Model from a Reference Model](#)” on page 1160 for a more detailed example of LINEQS model respecification. See the section “[Modifying a PATH Model from a Reference Model](#)” on page 1211 for a more detailed example of PATH model respecification.

As discussed in a preceding section, PROC CALIS generates default free mean or intercept parameters for manifest variables in the FACTOR, LINEQS, or PATH model if you do not specify them explicitly in the MEAN statement (and the LINEQS statement for the LINEQS model). When you use the REFMODEL statement for defining a reference model, these default free mean or intercept parameters in the old (reference) model are not transferred to the new model. Instead, the new model generates its own set of default free mean or intercept parameters *after* the new model is resolved from the reference model, the REFMODEL statement options, the RENAMEPARM statement, and the MEAN statement (and the LINEQS statement for the LINEQS model) specifications in the new model. This also implies that if you want any of the mean or intercept parameters to be constrained across the models by means of the REFMODEL specification, you must specify them explicitly in the MEAN statement (or the LINEQS statement for the LINEQS model) of the reference model so that the same mean or intercept specification is transferred to the new model.

MODEL Statement

MODEL *i* </options>;

where *i* is an assigned model number between 1 and 9999, inclusively.

A MODEL statement signifies the beginning of a model specification block and designates a model number for the model. All **main** and **subsidiary** model specification statements after a MODEL statement belong in that model until another MODEL or **GROUP** statement is encountered.

The MODEL statement itself does not serve the purpose of model specification, which is actually done by the **main** and **subsidiary** model specification statements that follow it. The MODEL statement serves as a “place-holder” of specification of a single model. It also makes the reference to a model easier with an assigned model number. For example, consider the following statements:

```
proc calis;
  group 1 / data=women_data;
  group 2 / data=men_data;
  model 1 / group=1 label='Women Model';
    {model 1 specification here}
  model 2 / group=2 label='Men Model';
    {model 2 specification here}
run;
```

This example illustrates a two-group analysis with two models. One is **model 1** labeled as ‘Women Model’ in a MODEL statement. Another is **model 2** labeled as ‘Men Model’ in another MODEL statement. The two groups, **group 1** and **group 2**, as defined in two separate **GROUP** statements, are fitted by **model 1** and **model 2**, respectively, as indicated by the GROUP= option of the MODEL statements. Within the scope of **model 1**, you provide model specification statements by using the **main** and **subsidiary** model specification statements. Usually, one of the following main model specification statements is used: **FACTOR**, **LINEQS**, **LISMOD**, **MSTRUCT**, **PATH**, **RAM**, or **REFMODEL**. Similarly, you provide another set of model specification statements within the scope of **model 2**.

Hence, for an analysis with a single group, the use of the MODEL statement is not necessary because the model that fits the group is unambiguous.

You can set model-specific *options* in each MODEL statement. All but two of these *options* are also available in the **PROC CALIS** statement. If you set these *options* in the PROC CALIS statement, they apply to all models, unless you respecify them in the local MODEL statements. If you want to apply some *options* only to a particular model, specify these *options* in the MODEL statement that corresponds to that model.

You can also set group-specific *options* in the MODEL statement. These group *options* apply to the groups that are specified in GROUP= option of the MODEL statement. See the section “Options Available in the **GROUP** and **PROC CALIS** Statements” on page 1153 for a detailed descriptions of these group *options*.

Options Available Only in the MODEL Statement

LABEL | **NAME**=*name*

specifies a label for the model. You can use any valid SAS names up to 256 characters for labels. You can also use quoted strings for labels.

GROUP | GROUPS=*int-list*

specifies a list of integers which represent the groups to be fitted by the model.

Options Available in the MODEL and PROC CALIS Statements

The following options are available in the MODEL and PROC CALIS statements. If you specify these options in the PROC CALIS statement, they are transferred to all MODEL statements. These options might be overwritten by the respecifications in the local MODEL statements.

Option	Description
DEMPHAS= on page 1096	Emphasizes the diagonal entries
EFFPART TOTEFF on page 1097	Displays total, direct, and indirect effects
EXTENDPATH GENPATH on page 1097	Displays the extended path estimates that include variances and covariances
INEST= on page 1098	Specifies the data set that contains the initial values and constraints
INMODEL INRAM= on page 1098	Specifies the data set that contains the model specifications
MEANSTR on page 1104	Analyzes the mean structures
MODIFICATION on page 1105	Computes modification indices
NOMEANSTR on page 1106	Deactivates the inherited MEANSTR option
NOMOD on page 1107	Suppresses modification indices
NOORDERSPEC on page 1107	Displays model specifications and results according to the input order
NOPARMNAME on page 1107	Suppresses the printing of parameter names in results
NOSTAND on page 1107	Suppresses the standardized output
NOSTDERR on page 1107	Suppresses standard error computations
ORDERSPEC on page 1109	Orders the model output displays according to the parameter types within each model
OUTEST= on page 1110	Specifies the data set that outputs the estimates and their covariance matrix
OUTMODEL OUTRAM= on page 1110	Specifies the output data set for storing the model specification and results
PARMNAME on page 1111	Displays parameter names in model specifications and results
PDETERM on page 1111	Computes the determination coefficients
PESTIM on page 1112	Prints parameter estimates
PINITIAL on page 1112	Prints initial pattern and values
PLATCOV on page 1112	Computes the latent variable covariances and scoring coefficients
PRIMAT on page 1113	Displays results in matrix forms
READADDPARM on page 1114	Instructs generated default parameters be read in the INMODEL= data set
STDERR on page 1118	Computes the standard errors

Options Available in MODEL, GROUP, and PROC CALIS Statements

Some options in the **GROUP** statement can also be specified in the **MODEL** statements. Group options that are specified the **MODEL** statements are transferred to the **GROUP** statements that define the groups that are fitted by the associated models in the **MODEL** statements. This is a little more convenient than setting the common group options individually in the **GROUP** statements for all fitted groups by a model. See the section “Options Available in **GROUP**, **MODEL**, and **PROC CALIS** Statements” on page 1154 for a reference of these options.

MSTRUCT Statement

MSTRUCT <VAR=*var-list*> ;

MSTRUCT stands for matrix structures. As opposed to other modeling languages, in which the mean and covariance structures are implied from paths, equations, or complicated model matrix computations, the **MSTRUCT** language is for direct structured mean and covariance models.

In the **MSTRUCT** statement, you define the list of variables. You can use **MATRIX** statements to specify the parameters in the mean and covariance structures:

```
MSTRUCT <VAR=var-list> ;
MATRIX _COV_ parameters-in-matrix ;
MATRIX _MEAN_ parameters-in-matrix ;
```

You use the **MATRIX _COV_** statement to specify the covariance and variance parameters in the structured covariance matrix. When applicable, you use the **MATRIX _MEAN_** statement to specify the parameters in the structured mean vector. Each of these matrices can be specified no more than once within a model. See the **MATRIX statement** on page 1175 for details. If you do not use any **MATRIX** statement for specifying parameters, a saturated model is assumed. This means that all elements in the covariance and mean (if modeled) matrices are free parameters in the model.

The order of variables in the *var-list* of the **MSTRUCT** statement is important; it is used to refer to the row and column variables of the **_COV_** and the **_MEAN_** matrices. The variables specified in the list should be present in the input data set that is intended for the **MSTRUCT** model. With direct mean and covariance structures on the observed variables, no latent variables are explicitly involved in the **MSTRUCT** modeling language. However, this does not mean that the **MSTRUCT** modeling language cannot handle latent variable models. With additional specifications in the **PARAMETERS** and the **SAS programming statements**, it is possible to fit certain latent variable models by using the **MSTRUCT** modeling language. Despite this, the code might get too complicated and error-prone. Hence, using the **MSTRUCT** modeling language for latent variable modeling is not recommended for novice users. The **LINEQS**, **LISMOD**, **PATH**, or **RAM** modeling language should be considered first for latent variable modeling.

Default Parameters

It is important to understand the default parameters in the **MSTRUCT** model. If you know which parameters are default free parameters, you can make your specification more efficient by omitting the specifications of those parameters that can be set by default. For example, you do not need to specify any elements of the **_COV_** matrix if all elements are supposed to free parameters. See the section “Default Parameters in the **MSTRUCT Model**” on page 1287 for details about the default parameters of the **FACTOR** model.

Modifying an MSTRUCT Model from a Reference Model

This section assumes that you use a `REFMODEL` statement within the scope of a `MODEL` statement and that the reference model (or base model) is also an MSTRUCT model. The reference model is called the old model, and the model that refers to the old model is called the new model. If the new model is not intended to be an exact copy of the old model, you can use the following extended MSTRUCT modeling language to make modifications within the scope of the `MODEL` statement for the new model. The syntax is similar to, but not exactly the same as, the ordinary MSTRUCT modeling language, as described in the section “MSTRUCT Statement” on page 1194. The syntax for respecifying or modifying an MSTRUCT model takes the following form:

```
MSTRUCT ;
MATRIX _COV_ parameters-in-matrix ;
MATRIX _MEAN_ parameters-in-matrix ;
```

In the respecification, you should not put any `VAR=` list in the MSTRUCT statement, as you would do for specifying the original base model. The reason is that parameter respecifications in the new model refer to the variables in the `VAR=` list of the old model. Therefore, the `VAR=` list in the new model is implicitly assumed to be exactly the same as that in the old model. This renders the specification of a `VAR=` list of the MSTRUCT statement of the new model unnecessary. Because the `VAR=` option is the only possible option in the MSTRUCT statement, it also implies that the entire MSTRUCT statement is optional for the new model.

You can use the `MATRIX _COV_` and `MATRIX _MEAN_` statements to modify from the old model by using the same syntax as in ordinary MSTRUCT modeling language. In addition, in the respecification syntax, you can use the missing value `'.'` to drop a parameter location from the old model.

The new model is formed by integrating with the old model in the following ways:

- Duplication: If you do not specify in the new model a parameter location that exists in the old model, the old parameter specification is duplicated in the new model.
- Addition: If you specify in the new model a parameter location that does not exist in the old model, the new parameter specification is used in the new model.
- Deletion: If you specify in the new model a parameter location that also exists in the old model and the new parameter is denoted by the missing value `'.'`, the old parameter specification is not copied into the new model.
- Replacement: If you specify in the new model a parameter location that also exists in the old model and the new parameter is not denoted by the missing value `'.'`, the new parameter specification replaces the old one in the new model.

For example, consider the following statements for a two-group analysis:

```
proc calis;
  group 1 / data=d1;
  group 2 / data=d2;
  model 1 / group=1;
    mstruct var=V1-V6;
    matrix _COV_ [1,1] = 6*vparm (8.),
                  [2,] = cv21,
                  [3,] = cv31,
                  [4,] = cv41 cv42 cv43,
```



```

[5,] = cv51 cv52 cv53 cv54,
[6,] = cv61 cv62 cv63 cv64 cv65;
model 2 / group=2;
  refmodel 1;
  matrix _COV_ [2,] = 3.,
                [3,2] = cv32,
                [4,] = . . . ,
                [5,] = . . . ,
                [6,] = . . . ;
run;

```

In these statements, you specify Model 2 by referring to Model 1 in the **REFMODEL** statement. Hence, Model 2 is called the new model that refers to the old model, Model 1. Because they are not respecified in the new model, all parameters on the diagonal of the covariance matrix are duplicated from the old model for the new model. Similarly, parameter locations associated with the **cv54**, **cv64**, and **cv65** parameters are also duplicated in the new model.

An added parameter in the new model is **cv32** for the covariance between **V3** and **V2**. This parameter location is not specified in the old model.

In the new model, parameters for the covariances between the variable sets {**V1 V2 V3**} and {**V4 V5 V6**} are all deleted from the old model. The corresponding parameter locations for these covariances are given missing values ‘.’ in the new model, indicating that they are no longer free parameters as in the old model. Deleting these parameters amounts to setting the corresponding covariances to fixed zeros in the new model.

Finally, covariance between **V2** and **V1** is changed from a free parameter **cv21** in the old model to a fixed constant 3 in the new model. This illustrates the replacement rule of the respecification syntax.

NLINCON Statement

NLINCON | **NLC** *constraint* <, *constraint* ... >;

where *constraint* represents one of the following:

- *number operator variable-list number operator*
- *variable-list number operator*
- *number operator variable-list*

You can specify nonlinear equality and inequality constraints with the **NLINCON** or **NLC** statement. The **QUANEW** optimization subroutine is used when you specify nonlinear constraints by using the **NLINCON** statement.

The syntax of the **NLINCON** statement is similar to that of the **BOUNDS** statement, except that the **NLINCON** statement must contain the names of variables that are defined in the program statements and are defined as continuous functions of parameters in the model. They must not be confused with the variables in the data set.

As with the **BOUNDS** statement, one- or two-sided constraints are allowed in the **NLINCON** statement; equality constraints must be one sided. Valid operators are **<=**, **<**, **>=**, **>**, and **=** (or, equivalently, **LE**, **LT**, **GE**, **GT**, and **EQ**).

PROC CALIS cannot enforce the strict inequalities **<** or **>** but instead treats them as **<=** and **>=**, respectively. The listed nonlinear constraints must be separated by commas. The following is an example of the **NLINCON** statement that constrains the nonlinear parametric function $x_1 * x_1 + u_1$ to a fixed value of 1:

```
nlincon    xx = 1;
xx = x1 * x1 + u1;
```

Note that x_1 and u_1 are parameters defined in the model. The following three NLINCON statements, which require xx_1 , xx_2 , and xx_3 to be between zero and ten, are equivalent:

```
nlincon 0. <= xx1-xx3,
          xx1-xx3 <= 10;
nlincon 0. <= xx1-xx3 <= 10.;
nlincon 10. >= xx1-xx3 >= 0.;
```

NLOPTIONS Statement

NLOPTIONS *options* ;

Many options that are available in SAS/OR PROC NLP can be specified for the optimization subroutines in PROC CALIS by using the NLOPTIONS statement. The NLOPTIONS statement provides more displayed and file output control on the results of the optimization process, and it permits the same set of termination criteria as in PROC NLP. These are more technical options that you might not need to specify in most cases.

Several statistical procedures support the use of NLOPTIONS statement. The syntax of NLOPTIONS statement is common to all these procedures and can be found in the section “NLOPTIONS Statement” on page 482 in Chapter 19, “Shared Concepts and Topics.”

See the section “Use of Optimization Techniques” on page 1352 for more information about the use of optimization techniques in PROC CALIS.

OUTFILES Statement

OUTFILES | **OUTFILE** *file-option* < *file-option* ... > ;

where *file-option* represents one of the following:

- **OUTMODEL** | **OUTRAM**= *file-name* [**MODEL**= *int-list* < , *int-list* >]
- **OUTSTAT**= *file-name* [**GROUP**= *int-list* < , *int-list* >]
- **OUTWGT**= *file-name* [**GROUP**= *int-list* < , *int-list* >]

with *file-name* representing an output file name and *int-list* representing list of model or group numbers

Use the OUTFILES statement when you need to output multiple-group or multiple-model information to output files in a complex way. In each OUTFILES statement, each possible *file-option* should appear no more than once. However, as needed, you can use the OUTFILES statement more than once. For example, suppose you want to create two **OUTWGT**= files for different sets of groups. You can specify the OUTFILES statement twice, as shown in the following specification:

```
outfiles outwgt=file1 [group=1,2];
outfiles outwgt=file2 [group=3,4];
```


In the first OUTFILES statement, the weights for groups 1 and 2 are output to the file file1. In the second OUTFILES statement, the weights for groups 3 and 4 are output to the file file2.

When the **OUTMODEL=**, **OUTSTAT=**, or **OUTWGT=** option is intended for *all* groups or models, you can simply specify the option in the PROC CALIS statement. Only when you need to output the group (model) information from *more than one* group (model), *but not all* groups (models), to a single output file does the use the OUTFILES statement become necessary. For example, consider the following specification:

```
proc calis method=glis;
  outfiles outmodel=outmodel [model=1,3]
           outwgt=outwgt [group=1,2]
           outstat=outstat [group=2,3];
  group 1 / data=g1;
  group 2 / data=g2;
  group 3 / data=g3 outwgt=outwgt3;
  model 1 / group=1;
           factor N=3;
  model 2 / group=2;
           factor N=2;
  model 3 / group=3;
           factor N=3;
run;
```

You fit three different factor models to three groups: Model 1 for Group 1, Model 2 for Group 2, and Model 3 for group 3. In the OUTFILES statement, you output model information from models 1 and 3 to an output file named outmodel, weight matrices from groups 1 and 2 to outwgt, and statistics from groups 2 and 3 to outstat. In each of these output files, you have information from more than one (but not all) groups or models. In the **GROUP** statement for group 3, you have another **OUTWGT=** file named outwgt3 for group 3 alone.

Note that you cannot specify the preceding output file organization by using the following statements:

```
proc calis method=glis;
  group 1 / data=g1 outwgt=outwgt;
  group 2 / data=g2 outwgt=outwgt outstat=outstat;
  group 3 / data=g3 outwgt=outwgt3 outstat=outstat;
  model 1 / group=1 outmodel=outmodel;
           factor N=3;
  model 2 / group=2;
           factor N=2;
  model 3 / group=3 outmodel=outmodel;
           factor N=3;
run;
```

This specification will not work because SAS forbids the repeated specification of the same output file in the same PROC CALIS run. That is, you cannot specify **OUTWGT=outwgt**, **OUTSTAT=outstat**, or **OUTMODEL=outmodel** more than once in the PROC CALIS run without causing file invocation problems (however, multiple specification of the same input file is not a problem).

If you specify any of the output files for a group (or a model) in both of the OUTFILES and the **GROUP** (or **MODEL**) statements, the destination specified in the more specific **GROUP** (or **MODEL**) statement will be used. For example, for the following specification PROC CALIS will save the Model 2 information in the **OUTMODEL=outmodel2** data set, but not in the **OUTMODEL=outfile1** data set:

```

proc calis method=glis;
  outfiles outmodel=outfile1 [model=1,2];
  group 1 / data=g1;
  group 2 / data=g2;
  model 1 / group=1;
    factor N=3;
  model 2 / group=2 outmodel=outmodel2;
    factor N=2;
run;

```

The OUTFILES statement is intended for arranging output files in a complex way. The use of the OUTFILES statement is unnecessary in the following situations:

- If you have a single-sample analysis, you do not need to use the **GROUP** statement. As a result, you can simply use the **OUTSTAT=** or **OUTWGT=** options in the **PROC CALIS** statement for specifying the output destinations. Therefore, the OUTFILES statement is not needed.
- If you have a single model in your analysis, you do not need to use the **MODEL** statement. As a result, you can simply use the **OUTMODEL=** options in the **PROC CALIS** statement for specifying the output destination. Therefore, the OUTFILES statement is not needed.
- If you have multiple groups or multiple models in your analysis and information for all groups or models is output to the same file, you do not need to use the OUTFILES statement. You can simply use the **OUTSTAT=**, **OUTWGT=**, or **OUTMODEL=** options in the **PROC CALIS** statement because the output file information is automatically propagated from the PROC CALIS statement to the groups or models.
- If you have multiple groups or multiple models in your analysis and each group or model has a unique output data file destination (including cases where some groups or models might not have any output files), you do not need to use the OUTFILES statement. You can simply specify the **OUTSTAT=**, **OUTWGT=**, or **OUTMODEL=** options in the **GROUP** or **MODEL** statements.

PARAMETERS Statement

```

PARAMETERS | PARMS parameters <<=> numbers | (numbers)>
  <<,> parameters <<=> numbers | (numbers)> ... >;

```

The PARAMETERS statement defines parameters that are useful in the modeling. You can specify more than one PARAMETERS statement.

The three main uses of the PARAMETERS statement are as follows:

- Define independent parameters that are not specified in your model. In some modeling situations, it is more convenient (practically or conceptually) to define the model parameters as functions of these independent parameters. PROC CALIS computes the estimates and their standard errors for these independent parameters.

- Define dependent parameters of interest. These dependent parameters are then defined as functions of the model parameters in the SAS programming statements. PROC CALIS computes the estimates and their standard errors for these dependent parameters.
- Provide initial values for the free parameters in the model if they have not been specified in the model specification statements.

For example, the following statements illustrate the three main uses of the PARAMETERS statement:

```
proc calis;
  path
    v1 <=== v2 = b1,
    v1 <=== v3 = b2,
    v2 <=== v4 = b3 (0.9) ,
    v3 <=== v5 = b4;
  parameters a1 (0.1) a2 (0.2) b3 (0.3) b4 (0.4) b5;
  b1 = -a1 / a2;
  b2 = 1 / a2;
  b5 = b3 - b4;
run;
```

In the PARAMETERS statement, you specify five parameters that take different roles in the modeling. Parameters *a1* and *a2* are independent parameters that are not specified in the PATH statement, which specifies four paths with four parameters for the path coefficients *b1*, *b2*, *b3*, and *b4*. The two SAS programming statements immediately after the PARAMETERS statement define parameters *b1* and *b2* as functions of parameters *a1* and *a2*. Because *a1* and *a2* appear only on the right side of the programming statements, they are independent parameters of the model. In addition, *b1* and *b2* are dependent parameters because they appear on the left side of the first two programming statements. Independent parameters *a1* and *a2* are provided with initial values 0.1 and 0.2, respectively, in the PARAMETERS statement. Because the initial values these two independent parameters are used, dependent parameters *b1* and *b2* are also initialized with values -0.5 and 5 , respectively.

Parameters *b3* and *b4* appear in both the PATH and PARAMETERS statements. Because these two parameters are already specified in the PATH statement, their initial values might have been defined in the model. For example, parameter *b3* in the PATH statement has an initial value of 0.9. This initial value is *not* replaced by the initial value of 0.3 specified in the PARAMETERS statement. However, because you do not specify an initial value for parameter *b4* in the PATH statement, the initial value of 0.4 specified in the PARAMETERS statement is used. In general, the initial values that are specified in the PARAMETERS statement do not replace the initial values that have already been specified for the same parameters in the model.

Parameter *b5* in the PARAMETERS statement is a dependent parameter, which is defined as the difference between the model parameters *b3* and *b4* in the last SAS programming statement. No initial value for this dependent parameter is provided (nor is it needed). By definition, dependent parameters are functions of other parameters, so their initial values are computed. In this example, parameter *b5* takes an initial value of 0.5, the difference between the initial values of *b3* and *b4*.

It is not necessary to provide initial values for the parameters in the PARAMETERS statement. For the independent parameters without initial values specified, PROC CALIS generates the initial values from the `START=` value in the PROC CALIS statement. The default `START=` value is 0.5. If you specify the `RANDOM=` option in the PROC CALIS statement, random numbers are generated for the initial values of

the independent parameters. For the dependent parameters, PROC CALIS computes the initial values by using the SAS programming statements.

In general, the number of parameters and the number of initial values do not have to match. When you specify fewer initial values than parameter names, PROC CALIS either generates or computes the initial values. When you specify more values than parameter names, the extra values are ignored.

For example, consider the following statements:

```
parameters c1 c2 c3 c4 (0.2 0.3 0.4);
parameters d1 d2 d3 d4 (0.1 0.2 0.3 0.4 0.5);
run;
```

The first PARAMETERS statement has a shorter initial value list than the parameter list. The initial values 0.2, 0.3, and 0.4 are assigned to c2, c3, and c4, respectively. PROC CALIS generates the initial value for c1. The second PARAMETERS statement has a longer initial value list than the parameter list. The initial values 0.1, 0.2, 0.3, and 0.4 are assigned to d1, d2, d3, and d4, respectively. The extra initial value 0.5 is ignored.

When the lengths of the parameter list and the initial value list match, you can use an equal sign between the lists freely without affecting the assignments of the initial values. For example, each of the following PARAMETERS statements assigns the initial values alpha=0.5 and beta=-0.5:

```
parameters alfa 0.5 beta -0.5;
parameters alfa = 0.5 beta = -0.5;
parameters alfa (0.5) beta (-0.5);
parameters alfa = (0.5) beta = (-0.5);
parameters alfa beta 0.5 -0.5;
parameters alfa beta = 0.5 -0.5;
parameters alfa beta (0.5 -0.5);
parameters alfa beta = (0.5 -0.5);
```

However, when the parameter list is longer than the initial value list, the equal sign affects the assignments of the initial values. For example, the following statement assigns the initial values to the last three parameters, c2, c3, and c4:

```
parameters c1 c2 c3 c4 (0.2 0.3 0.4);
```

But with an equal sign between the lists, the following statement assigns the initial values to the first three parameters, c1, c2, and c3:

```
parameters c1 c2 c3 c4 = (0.2 0.3 0.4);
```

To make initial value assignments less ambiguous, you can use commas to separate parameter lists. For example, the following statement clearly assigns the initial values to c2, c3, and c4:

```
parameters c1, c2 c3 c4 (0.2 0.3 0.4);
```

This specification is equivalent to the same specification without the comma. But the specification is certainly less ambiguous with the comma.

Proper grouping of the parameter and initial value lists with the use of commas helps make the specification in the PARAMETERS statement clear. For example, consider the following specification:

```
parameters c1 c2 c3 c4 = (0.1 0.2 0.3) c5 c6 (0.6);
```

Initial values 0.1, 0.2, 0.3, and 0.6 are assigned to parameters c1, c2, c3, and c6, respectively. Initial values for other parameters are either generated or computed by PROC CALIS. A much better practice is to use the following equivalent specification:

```
parameters c1 c2 c3 (0.1 0.2 0.3), c4 c5, c6 (0.6);
```

Matching the number of parameters and the number of initial values (if provided) in entries separated by commas in the PARAMETERS statement is highly recommended. It reduces ambiguities and makes your code more interpretable.

It is important to notice that PROC CALIS does not have better alternatives to generate initial values (such as those for setting the initial values of the model parameters) for the independent parameters specified in the PARAMETERS statement other than using either the `START=` value or random values generated by using the `RANDOM=` option. These ad hoc initial values are arbitrary and might not always lead to converged solutions. Therefore, you should try to provide good initial values for those independent parameters that are defined only in the PARAMETERS statement.

Do not confuse the PARAMETERS statement with the `VAR` statement. While you specify the parameters of the model in the PARAMETERS statement, you specify analysis variables in the `VAR` statement. See the [VAR statement](#) on page 1228 for more details.

CAUTION: The `OUTMODEL=` and `OUTRAM=` data sets do not contain any information about the PARAMETERS statement or the SAS programming statements.

PARTIAL Statement

PARTIAL *variables* ;

If you want the analysis to be based on a partial correlation or covariance matrix, use the PARTIAL statement to list the variables used to partial out the variables in the analysis. You can specify only one PARTIAL statement within the scope of each `GROUP` or PROC CALIS statement.

PATH Statement

PATH *path* <, *path* ... > ;

where *path* represents any of the following specifications:

- single-headed path for defining functional relationship
- double-headed path for specifying variances or covariances
- 1-path for specifying means or intercepts

For example, the following PATH statement contains only the single-headed paths:

```

path
v1    <==== v2,
v2    <==== v4 v5,    /* same as: v2 <==== v4 and v2 <==== v5 */
v3    <==== v5,      /* same as: v5 <==== v3 */
v4 v5 <==== v6 v7;   /* same as: v4 <==== v6, v4 <==== v7,
                    v5 <==== v6, and v5 <==== v7 */

```

Although the most common definition of paths refer to these single-headed paths, PROC CALIS extends the definition of paths to include the so-called “variance-paths,” “covariance-paths,” and “1-paths” that refer to the variance, covariance, and the mean or intercept parameters, respectively. Corresponding to these extended path definitions, PROC CALIS provides the double-headed path and 1-path syntax. For example, the following PATH statement contains single-headed paths for specifying functional relationships and double-headed paths for specifying variances and covariances:

```

path
v1    <==== v3-v5,    /* same as: v1 <==== v3, v1 <==== v4, and v1 <==== v5 */
v2    <==== v4 v5,
v3    <==== v5,
v1    <====> v1,      /* error variance of v1 */
<====> v2 v3,        /* error variances of v2 and v3 */
v2    <====> v3,      /* error covariance between v2 and v3 */
<====> [v4 v5];     /* variances and covariance for v4 and v5 */

```

The following PATH statement contains single-headed paths for specifying functional relationships and 1-paths for specifying means and intercepts:

```

path
v1    <==== v3-v5,
v2    <==== v4 v5,
v3    <==== v5,
1     <====> v1,      /* intercepts for v1 */
1     <====> v2-v3,   /* intercepts for v2 and v3 */
1     <====> v4 v5;   /* means of v4 and v5 */

```

Details about the syntax of these three different types of *paths* are described later. Instead of using double-headed paths and 1-paths, you can also specify these parameters by the [subsidiary model specification statements](#) such as the PVAR, PCOV, and the MEAN statements, as shown in the following syntactic structure of the PATH modeling language:

```

PATH path <, path ... > ;
PVAR partial-variance-parameters ;
PCOV partial-covariance-parameters ;
MEAN mean-parameters ;

```

Typically, in this syntactic structure the *paths* contains only single-headed paths for representing the functional relationships among variables, which could be observed or latent. The *paths* are separated by commas. You can specify at most one PATH statement in a model within the scope of either the PROC CALIS statement or a MODEL statement.

Next, the PVAR statement specifies the parameters for the variances or error (partial) variances. The PCOV statement specifies the parameters for the covariances or error (partial) covariances. The MEAN statement specifies the parameters for the means or intercepts. For details about these subsidiary model specification statements, see the syntax of the individual statements.

A natural question now arises. For the specification of variances, covariances, intercepts, and means, should you use the extended path syntax that includes double-headed paths and 1-paths or the subsidiary model specification statements such as the PVAR, PCOV, and MEAN statements? If you want to specify all parameters in a single statement and hence output and view all the parameter estimates in a single output table, then the extended path syntax would be your choice. If you want to use more common language for specifying and viewing the parameters or the estimates of variances, covariances, means, and intercepts, then the subsidiary model specification statements serve the purpose better.

You are not restricted to using extended path syntax or the subsidiary model statements exclusively in a PATH model specification. For example, you might specify the variance of *v1* by using the double-headed path syntax and the variance of *v2* by using the PVAR statement. The only restriction is that you cannot specify the same parameter twice. In addition, even if you specify your PATH model without using double-headed paths or 1-paths, you can include the estimation results associated with these extended paths in the same output table for the single-headed paths by using the **EXTENDPATH** or **GENPATH** option. This way all the estimates of the PATH model can be shown in a single output table.

The Single-Headed Path Syntax for Specifying Functional Relationships

var-list *arrow* *var-list2* < = *parameter-spec* >

where *var-list* and *var-list2* are lists of variables, *parameter-spec* is an optional specification of parameters, and *arrow* represents either a *left-arrow* is one of the following forms:

<===, <---, <==, <--, <=, <-, or <

or a *right-arrow* is one of the following forms:

===>, --->, ==>, -->, =>, ->, or >

In each single-headed path, you specify two lists of variables: *var-list* and *var-list2*. Depending on the direction of the *arrow* specification, one group of variables contains the outcome variables and the other group contains the predictor variables. Optionally, you can specify the *parameter-spec* at the end of each path entry. You can specify the following five types of the parameters for the path entries:

- unnamed free parameters
- initial values
- fixed values
- free parameters with names provided
- free parameters with names and initial values provided

For example, in the following statement you specify a model with five paths:

```
path
  v1 <=== f1 ,
  v2 <=== f1 = (0.5) ,
  v3 <=== f1 = 1. ,
  v4 <=== f1 = b1 ,
  v5 <=== f1 = b2 (.4) ;
```

The first path entry specifies a path from *f1* to *v1*. The effect of *f1* (or the path coefficient) on *v1* is an unnamed free parameter. For this path effect parameter, PROC CALIS generates a parameter name with the `_Parm` prefix and appended with a unique integer (for example, `_Parm1`). The second path entry specifies a path from *f1* to *v2*. The effect of *f1* is also an unnamed free parameter with an initial estimate of 0.5. PROC CALIS also generates a parameter name for effect parameter. The third path entry specifies a path from *f1* to *v3*. The effect of *f1* is also a fixed value of 1.0. This value stays the same in the model estimation. The fourth path entry specifies a path from *f1* to *v4*. The effect of *f1* is a free parameter named *b1*. The fifth path entry specifies a path from *f1* to *v5*. The effect of *f1* is a free parameter named *b2*, with an initial value of 0.4.

You can specify multiple variables in the *var-list* and *var-list2* lists. For example, the following statement specifies five paths from *f1* to *v1-v5*:

```
path
  f1 ==> v1-v5;
```

All the five effects of *f1* on the five variables are unnamed free parameters. If both *var-list* and *var-list2* lists contain multiple variables, you must be careful about the order of the variables when you also specify parameters at the end of the path entry. For example, the following statement specifies the paths from the predictor variables *x1-x2* to the outcome variables *y1-y3*:

```
path
  y1-y3 <=== x1-x2 = a1-a6;
```

The PATH statement specifies six paths in the path entry. These six paths have effect parameters *a1-a6*. This specification is equivalent to the following specification:

```
path
  y1 <=== x1 = a1;
  y1 <=== x2 = a2;
  y2 <=== x1 = a3;
  y2 <=== x2 = a4;
  y3 <=== x1 = a5;
  y3 <=== x2 = a6;
```

The following statement shows another example of multiple-path specification:

```
path
  x1-x2 ==> y1-y3 = b1-b6;
```

This specification is equivalent to the following specification with separate path specifications:

```
path
  x1 ==> y1 = b1;
  x1 ==> y2 = b2;
  x2 ==> y3 = b3;
  x2 ==> y1 = b4;
  x2 ==> y2 = b5;
  x2 ==> y3 = b6;
```

You can also specify parameter with mixed types in any path entry, as shown in the following specification:


```

path
  f1 ==> y1-y3    = 1.  b1(.5) (.3),
  f2 ==> y4-y6    = 1.  b2  b3(.7);

```

This specification is equivalent to the following expanded version:

```

path
  f1 ==> y1      = 1.,
  f1 ==> y2      = b1(.5),
  f1 ==> y3      = (.3),
  f2 ==> y4      = 1.,
  f2 ==> y5      = b2,
  f2 ==> y6      = b3(.7);

```

Notice that in the original specification with multiple-path entries, 0.5 is interpreted as the initial value for the parameter `b1`, but not as the initial estimate for the path from `f1` to `y3`. In general, an initial value that follows a parameter name is associated with the free parameter.

If you indeed want to specify that `b1` is a free parameter *without* an initial estimate and 0.5 is the initial estimate for the path from `f1` to `y3` (while keeping all other specification the same), you can use a null initial value specification, as shown in the following statement:

```

path
  f1 ==> y1-y3    = 1.  b1() (.5) ,
  f2 ==> y4-y6    = 1.  b2  b3(.7);

```

This way 0.5 becomes the initial value for the path from `f1` to `y3`. Because a parameter list with mixed types might be confusing, you can break down the specifications into separate path entries to remove ambiguities. For example, you can use the following specification equivalently:

```

path
  f1 ==> y1      = 1.,
  f1 ==> y2      = b1,
  f1 ==> y3      = (.5) ,
  f2 ==> y4-y6   = 1.  b2  b3(.7);

```

The equal signs in the path entries are optional when the parameter lists do not start with a parameter name. For example, the preceding specification is the same as the following specification:

```

path
  f1 ==> y1      1.,
  f1 ==> y2      = b1,
  f1 ==> y3      (.5) ,
  f2 ==> y4-y6   1.  b2  b3(.7);

```

Notice that in the second path entry, you must retain the equal sign because `b1` is a parameter name. Omitting the equal sign makes the specification erroneous because `b1` is treated as a variable. This might cause serious estimation problems. Omitting the equal signs might be cosmetically appealing in specifying fixed values or initial values (for example, the first and the third path entries). However, the gain of doing that is not much as compared to the clarity of specification that results from using the equal signs consistently.

NOTE: You do not need to specify single-headed paths from the errors or disturbances (that is, error terms) in the PATH model specification, even though the functional relationships between variables are not assumed to be perfect. Essentially, the roles of error terms in the PATH model are in effect represented by the

associated default error variances of the endogenous variables, making it unnecessary to specify any single-headed paths from error or disturbance variables.

The Double-Headed Path Syntax That Uses Two Variable Lists for Specifying Variances and Covariances

```
var-list two-headed-arrow var-list2 < = parameter-spec >
```

where a *two-headed-arrow* is one of the following forms:

```
<==>, <-->, <=>, <->, or <>
```

This syntax enables you to specify covariances between the variables in *var-list* and the variables in *var-list2*. Consider the following example:

```
path
  v1      <==>  v2,
  v3 v4   <==>  v5 v6 v7 = cv1-cv6;
```

The first double-headed path specifies the covariance between v1 and v2 as an unnamed free parameter. PROC CALIS generates a name for this unnamed free parameter. The second double-headed path specifies six covariances with parameters named cv1–cv6. This multiple-covariance specification is equivalent to the following elementwise covariance specification:

```
path
  v3 <==> v5   = cv1,
  v3 <==> v6   = cv2,
  v3 <==> v7   = cv3,
  v4 <==> v5   = cv4,
  v4 <==> v6   = cv5,
  v4 <==> v7   = cv6;
```

Note that the order of variables in the list is important for determining the assignment of the parameters in the *parameter-spec* list.

If the same variable appears in both of the *var-list* and *var-list2* lists, the “covariance” specification becomes a variance specification for that variable. For example, the following statement specifies two variances:

```
path
  v1      <==>  v1      = 1.0,
  v2      <==>  v2 v3 = sigma2 cv23;
```

The first double-headed path entry specifies the variance of v1 as a fixed value of 1.0. The second double-headed path entry specifies the variance of v2 as a free parameter named sigma2, and then the covariance between v2 and v3 as a free parameter named cv23.

It results in an error if you attempt to use this syntax to specify the variance and covariances among a set of variables. For example, suppose you intend to specify the variances and covariances among v1–v3 as unnamed free parameters by the following statement:

```
path
  v1-v3 <==> v1-v3 ;
```

This specification expands to the following elementwise specification:

```

path
  v1 <==> v1 ,
  v1 <==> v2 ,
  v1 <==> v3 ,
  v2 <==> v1 ,
  v2 <==> v2 ,
  v2 <==> v3 ,
  v3 <==> v1 ,
  v3 <==> v2 ,
  v3 <==> v3 ;

```

There are nine variance or covariance specifications, but all of the covariances are specified twice. This is treated as a duplication error. The correct way is to specify only the nonredundant covariances, as shown in the following elementwise specification:

```

path
  v1 <==> v1 ,
  v2 <==> v1 ,
  v2 <==> v2 ,
  v3 <==> v1 ,
  v3 <==> v2 ,
  v3 <==> v3 ;

```

However, the elementwise specification is quite tedious when the number of variables is large. Fortunately, there is another syntax for double-headed paths to deal with this situation. This syntax is discussed next.

The Double-Headed Path Syntax That Uses a Single Variable List for Specifying Variances

two-headed-arrow var-list < = parameter-spec >

This syntax enables you to specify variances among the variables in *var-list*. Consider the following example:

```

path
  <==> v1 = (0.8) ,
  <==> v2-v4 ;

```

The first double-headed path entry specifies the variance of v1 as an unnamed free parameter with an initial estimate of 0.8. The second double-headed path entry specifies the variances of v2–v4 as unnamed free parameters. No initial values are given for these three variances. PROC CALIS generates names for all these variance parameters. You can specify these variances equivalently by the elementwise covariance specification syntax, as shown in the following, but former syntax is much more efficient.

```

path
  v1 <==> v1 = (0.8) ,
  v2 <==> v2 ,
  v3 <==> v3 ,
  v4 <==> v4 ;

```

The Double-Headed Path Syntax That Uses a Single Variable List for Specifying Variances and Covariances

two-headed-arrow [*var-list*] < = *parameter-spec* >

This syntax enables you to specify all the variances and covariances among the variables in *var-list*. For example, the following statement specifies all the variances and covariances among v2–v4:

```
path
  <==> [v2-v4] = 1.0 cv32 cv33(0.5) cv42 .7 cv44;
```

This specification is more efficient as compared with the following equivalent specification with element-wise variance or covariance definitions:

```
path
  v2 <==> v2 = 1.0,
  v3 <==> v2 = cv32,
  v3 <==> v3 = cv33(0.5),
  v4 <==> v2 = cv42,
  v4 <==> v3 = .7,
  v4 <==> v4 = cv44;
```

The double-headed path Syntax for Specifying Nonredundant Covariances

two-headed-arrow (*var-list*)< = *parameter-spec* >

This syntax enables you to specify all the nonredundant covariances among the variables in *var-list*. For example, the following statement specifies all the nonredundant covariances between v2–v4:

```
path
  <==> (v2-v5) = cv1-cv6;
```

This specification is equivalent to the following elementwise specification:

```
path
  v3 <==> v2 = cv1,
  v4 <==> v2 = cv2,
  v4 <==> v3 = cv3,
  v5 <==> v2 = cv4,
  v5 <==> v3 = cv5,
  v5 <==> v4 = cv6;
```

The 1-path Syntax for Specifying Means and Intercepts

1 *right-arrow* *var-list* < = *parameter-spec* >

where a *right-arrow* is one of the following forms:

====>, ---->, ==>, -->, =>, ->, or >

This syntax enables you to specify the means or intercepts of the variables in *var-list* as paths from the constant **1**. Consider the following example:

```

path
  v1 <=== v2-v4,
  1 ==> v1 = alpha,
  1 ==> v2-v4 = 3*kappa;

```

The first single-headed path specifies that v_1 is predicted by variables v_2 , v_3 , and v_4 . Next, the first 1-path entry specifies either the intercept of v_1 as a free parameter named α . It is the intercept, rather than the mean, of v_1 because endogenous in the PATH model. The second 1-path entry specifies the means of v_2 – v_4 as constrained parameters. All these means or intercepts are named κ so that they have the same estimate.

Therefore, whether the parameter is a mean or an intercept specified with the 1-path syntax depends on whether the associated variable is endogenous or exogenous in the model. The intercept is specified if the variable is endogenous. Otherwise, the mean of the variable is specified. Fortunately, any variable in the model can have either a mean or intercept (but not both) to specify. Therefore, the 1-path syntax is applicable to either the mean or intercept specification without causing conflicts.

Shorter and Longer Parameter Lists

If you provide fewer parameters in *parameter-spec* than the number of paths in a *path* entry, all the remaining parameters are treated as unnamed free parameters. For example, the following specification specifies the free parameter β to the first path and assigns unnamed free parameters to the remaining four paths:

```

path
  f1 ==> y1 z1 z2 z3 z4 = beta;

```

This specification is equivalent to the following specification:

```

path
  f1 ==> y1 = beta,
  f1 ==> z1 z2 z3 z4;

```

If you intend to fill up all values with the last parameter specification in the list, you can use the continuation syntax [...], [...], or [...], as shown in the following example:

```

path
  f1 ==> y1 z1 z2 z3 z4 = beta gamma [...];

```

This specification is equivalent to the following specification:

```

path
  f1 ==> y1 z1 z2 z3 z4 = beta 4*gamma;

```

The repetition factor $4*$ means that γ repeats 4 times.

However, you must be careful not to provide too many parameters. For example, the following specification results in an error:

```

path
  SES_Factor ==> y1 z1 z2 z3 z4 = beta gamma1-gamma6;

```

Because there are only five paths in the specification, parameters γ_5 and γ_6 are excessive.

Default Parameters

It is important to understand the default parameters in the PATH model. First, knowing which parameters are default free parameters makes your specification more efficient by omitting the specifications of those parameters that can be set by default. For example, because all variances and covariances among exogenous variables (excluding error terms) are free parameters by default, you do not need to specify them in the PATH model if these variances and covariances are not constrained. Second, knowing which parameters are default fixed zero parameters enables you to specify your model accurately. For example, because all error covariances in the PATH model are fixed zeros by default, you must use the PCOV statement or the double-headed path syntax to specify the partial (error) covariances among the endogenous variables if you want to fit a model with correlated errors. See the section “[Default Parameters in the PATH Model](#)” on page 1293 for details about the default parameters of the PATH model.

Modifying a PATH Model from a Reference Model

If you define a new model by using a reference (old) model in the **REFMODEL** statement, you might want to modify some path specifications from the PATH statement of the reference model before transferring the specifications to the new model. To change a particular path specification from the reference model, you can simply respecify the same path with the desired parameter specification in the PATH statement of the new model. To delete a particular path and its associated parameter from the reference model, you can specify the desired path with a missing value specification in the PATH statement of the new model.

```
PATH path <, path ... >;
PVAR partial-variance-parameters;
PCOV partial-covariance-parameters;
MEAN mean-parameters;
```

The new model is formed by integrating with the old model in the following ways:

- Duplication: If you do not specify in the new model a parameter location that exists in the old model, the old parameter specification is duplicated in the new model.
- Addition: If you specify in the new model a parameter location that does not exist in the old model, the new parameter specification is used in the new model.
- Deletion: If you specify in the new model a parameter location that also exists in the old model and the new parameter is denoted by the missing value ‘.’, the old parameter specification is not copied into the new model.
- Replacement: If you specify in the new model a parameter location that also exists in the old model and the new parameter is not denoted by the missing value ‘.’, the new parameter specification replaces the old one in the new model.

For example, consider the following specification of a two-group analysis:

```
proc calis;
  group 1 / data=d1;
  group 2 / data=d2;
  model 1 / group=1;
  path
    v1 <=== f1 = 1.,
    v2 <=== f1 = load1,
    v3 <=== f1 = load2,
```

```

        f1 <=== v4   = b1,
        f1 <=== v5   = b2,
        f1 <=== v6   = b3;
    pvar
        E1-E3      = ve1-ve3,
        f1         = vd1,
        v5-v6      = phi4-phi6;
    pcov
        v1 v2      = cve12;
model 2 / group=2;
    refmodel 1;
    path
        v3 <=== f1  = load1,
    pcov
        v1 v2      = .,
        v2 v3      = cve23;
run;

```

You specify Model 2 by referring to Model 1 in the **REFMODEL** statement. Model 2 is the new model that refers to the old model, Model 1. This example illustrates the four types of model integration rules for the new model:

- **Duplication:** All parameter specifications, except for the partial covariance between $v1$ and $v2$ and the $v3 <=== f1$ path in the old model, are duplicated in the new model.
- **Addition:** The parameter $cve23$ for the partial covariance between $v2$ and $v3$ is added in the new model because there is no corresponding specification in the old model.
- **Deletion:** The specification of partial covariance between $v1$ and $v2$ in the old model is not copied into the new model, as indicated by the missing value '.' specified in the new model.
- **Replacement:** The new path $v3 <=== f1$ replaces the same path in the old model with parameter $load1$ for the path coefficient. Thus, in the new model paths $v3 <=== f1$ and $v2 <=== f1$ are now constrained to have the same path coefficient parameter $load1$.

PCOV Statement

PCOV *assignment* <, *assignment* ... >;

where *assignment* represents:

var-list < * *var-list2* > < = *parameter-spec* >

The PCOV statement is a subsidiary model specification statement for the **PATH** model. You can use the PCOV statement only with the PATH modeling language. The PCOV statement specifies the covariances of exogenous variables, or the error covariances of endogenous variables in the PATH model. It can also specify the covariance between an exogenous variable and the error term of an endogenous variables, although this usage is rare in practice.

In each *assignment* of the COV statement, you specify variables in the *var-list* and the *var-list2* lists, followed by the covariance parameter specification in the *parameter-spec* list. The latter two specifications

are optional. The syntax of the PCOV statement is the same as that of the COV statement. See the COV statement on page 1132 for details about specifying within- and between-list (partial) covariances.

The concept behind the PCOV statement is broader than that of the COV statement. The PCOV statement supports the partial covariance parameter specification in addition to the covariance parameter specification, which is the only type of parameter that the COV statement supports. This difference is also reflected from the sets of *var-list* and *var-list2* that you can use in the PCOV statement. In the COV statement, variables on the left-hand side of an *assignment* must be exogenous. However, in the PCOV statement, you can specify both exogenous and endogenous variables. If a pair of variables are both exogenous in a specification, you are defining a covariance parameter between the variables. If a pair of variables are both endogenous in a specification, you are defining a partial covariance parameter between of the variables. This partial covariance is usually interpreted as the error covariance between the two endogenous variables. If one variable is exogenous while the other is endogenous, you are defining a covariance parameter between the exogenous variable and the error term for the endogenous variable.

You can specify the following five types of the parameters for the partial covariances in the PCOV statement:

- an unnamed free parameter
- an initial value
- a fixed value
- a free parameter with a name provided
- a free parameter with a name and initial value provided

For example, consider a PATH model with exogenous variables *x1*, *x2*, and *x3* and endogenous variables *y4*, *y5* and *y6*. The following PCOV statement shows the five types of specifications in five *assignments*:

```
pcov x1 x2 ,
     x1 x3 = (0.5) ,
     x2 x3 = 2.0 ,
     y4 y5 = psi1 ,
     y5 y6 = psi2(0.4) ;
```

In this statement, the covariance between *x1* and *x2* is specified as an unnamed free parameter. For this covariance, PROC CALIS generates a parameter name with the `_Parm` prefix and appended with a unique integer (for example, `_Parm1`). The covariance between *x1* and *x3* is an unnamed free parameter with an initial value of 0.5. PROC CALIS also generates a parameter name for this covariance. The covariance between *x2* and *x3* is a fixed value of 2.0. This value stays the same during the estimation. The error covariance between endogenous variables *y4* and *y5* is a free parameter named `psi1`. The error covariance between endogenous variables *y5* and *y6* is a free parameter named `psi2` with an initial value of 0.4.

The syntax of the PCOV statement is the same as the syntax of the COV statement. See the COV statement for more illustrations about the usage.

Default Covariance Parameters

Although the PCOV statement specification is conceptually broader than the COV statement specification, their related default set of covariance parameters is the same—that is, all covariances among *exogenous* manifest and latent variables (excluding error or disturbance variables) are free parameters. Because the

PCOV statement applies only to the PATH model, it is easy to understand why the covariances do not apply to the error or disturbance terms. The PATH model, as implemented in PROC CALIS, simply does not use any explicit error or disturbance terms. For the default free covariance parameters, PROC CALIS generate the parameter names with the `_Add` prefix and appended with unique integer suffixes. You can also use the PCOV statement specification to override these default covariance parameters in situations where you want to set parameter constraints, provide initial or fixed values, or make parameter references.

Another type of default partial covariances are fixed zeros. This default applies to the partial (error) covariances among all *endogenous* variables, and to the partial covariances between all *exogenous* variables and all *endogenous* variables in the path model. Again, you can override the default fixed values by providing explicit specification of these partial or error covariances in the PCOV statement.

Modifying a Covariance or Partial Covariance Parameter Specification from a Reference Model

If you define a new PATH model by using a reference (old) model in the `REFMODEL` statement, you might want to modify some parameter specifications from the PCOV statement of the reference model before transferring the specifications to the new model. To change a particular partial covariance specification from the reference model, you can simply respecify the same covariance with the desired parameter specification in the PCOV statement of the new model. To delete a particular partial covariance parameter from the reference model, you can specify the desired partial covariance with a missing value specification in the PCOV statement of the new model.

For example, suppose that you are defining a new PATH model by using the `REFMODEL` statement and that the covariance between variables `f1` and `v2` is defined as a fixed or free parameter in the reference model. If you do not want this fixed parameter specification to be copied into your new model, you can use the following specification in the new model:

```
pcov f1 v2 = . ;
```

Note that the missing value syntax is valid only when you use it with the `REFMODEL` statement. See the section “[Modifying a PATH Model from a Reference Model](#)” on page 1211 for a more detailed example of the PATH model respecification.

As discussed in the section “[Default Covariance Parameters](#)” on page 1213, PROC CALIS generates some default free covariance parameters for the PATH model if you do not specify them explicitly in the PCOV statement. When you use the `REFMODEL` statement for defining a reference model, these default free covariance parameters in the old (reference) model are not transferred to the new model. Instead, the new model generates its own set of default free covariance parameters *after* the new model is resolved from the reference model, the `REFMODEL` statement options, the `RENAMEPARM` statement, and the PCOV statement specifications in the new model. This also implies that if you want any of the (partial) covariance parameters to be constrained across the models by means of the `REFMODEL` specification, you must specify them explicitly in the PCOV statement of the reference model so that the same (partial) covariance specification is transferred to the new model.

PVAR Statement

```
PVAR assignment <, assignment ... > ;
```

where *assignment* represents:

var-list <= *parameter-spec* >

The PVAR statement specifies the variance or error (partial) variance parameters in connection with the confirmatory FACTOR and PATH models.

In each *assignment* of the PVAR statement, you list the *var-list* that you want to specify for their variances or error (partial) variances. Optionally, you can provide a list of parameter specifications (*parameter-spec*) after an equal sign for each *var-list* list. The syntax of the PVAR statement is exactly the same as that of the VARIANCE statement. See the VARIANCE statement on page 1231 for details about the syntax.

The concept behind the PVAR statement is broader than that of the VARIANCE statement. The PVAR statement supports the partial variance parameter specification in addition to the variance parameter specification, which is the only type of parameters that the VARIANCE statement supports. This difference is reflected from the set of *var-list* you can use in the PVAR statement. You can specify both exogenous variables and endogenous variables in the *var-list* list of the PVAR statement, but you can specify only exogenous variables in the *var-list* list of the VARIANCE statement. This conceptualization of the PVAR statement is needed in the FACTOR and PATH modeling languages because error variables are not explicitly defined in these models. You specify the variance of a variable if the variable in the *var-list* list of the PVAR statement is an exogenous (independent) variable in the FACTOR or PATH model. You specify the error (partial) variance of a variable if the variable in the *var-list* list of the PVAR statement is an endogenous (dependent) variable in the FACTOR or PATH model.

You can specify the following five types of the parameters for the partial variances in the PVAR statement:

- an unnamed free parameter
- an initial value
- a fixed value
- a free parameter with a name provided
- a free parameter with a name and initial value provided

For example, consider a PATH model with exogenous variables x1, x2, and x3 and endogenous variables y4 and y5. The following PVAR statement illustrates the five types of specifications in five *assignments*:

```
pvar x1 ,
      x2 = (2.0) ,
      x3 = 1.0 ,
      y4 = psi1 ,
      y5 = psi2(0.6) ;
```

In this statement, the variance of x1 is specified as an unnamed free parameter. For this variance, PROC CALIS generates a parameter name with the `_Parm` prefix and appended with a unique integer (for example, `_Parm1`). The variance of x2 is an unnamed free parameter with an initial value of 2.0. PROC CALIS also generates a parameter name for this variance. The variance of x3 is a fixed value of 1.0. This value stays the same during the estimation. The error variance of endogenous variable y4 is a free parameter named `psi1`. The error variance of endogenous variable y5 is a free parameter named `psi2` with an initial value of 0.6.

The syntax of the PVAR statement is the same as the syntax of the VARIANCE statement. See the VARIANCE statement for more illustrations about the usage.

Default Partial Variance Parameters

By default, all variances of the *exogenous* manifest and latent variables and all error (partial) variances of the *endogenous* manifest and latent variables are free parameters in the FACTOR or PATH model. For these default free variance parameters, PROC CALIS generates the parameter names with the `_Add` prefix and appended with unique integer suffixes. You can also use the PVAR statement specification to override these default variance parameters in situations where you want to specify parameter constraints, provide initial or fixed values, or make parameter references.

In the FACTOR or PATH model, a variable can either be exogenous or endogenous. Therefore, the default free parameters covers all the possible variance or partial variance parameters in the model. There are no default fixed zeros for any variances or partial variances in the model.

Modifying a Variance or Partial Variance Parameter Specification from a Reference Model

If you define a new FACTOR or PATH model by using a reference (old) model in the `REFMODEL` statement, you might want to modify some parameter specifications from the PVAR statement of the reference model before transferring the specifications to the new model. To change a particular variance or partial variance specification from the reference model, you can simply respecify the same variance or partial variance with the desired parameter specification in the PVAR statement of the new model. To delete a particular variance parameter from the reference model, you can specify the desired variance or partial variance with a missing value specification in the PVAR statement of the new model.

For example, suppose that the variance of V1 is specified in the reference PATH model but you do not want this variance specification to be transferred to the new model. You can use the following PVAR statement specification in the new model:

```
pvar
  v2 = .;
```

Note that the missing value syntax is valid only when you use the `REFMODEL` statement. See the section “[Modifying a FACTOR Model from a Reference Model](#)” on page 1146 for a more detailed example of FACTOR model respecification. See the section “[Modifying a PATH Model from a Reference Model](#)” on page 1211 for a more detailed example of PATH model respecification.

As discussed the section “[Default Partial Variance Parameters](#)” on page 1216, PROC CALIS generates default free variance parameters for the exogenous variables and default free error variance parameters for the endogenous variables in the confirmatory FACTOR or PATH model. When you use the `REFMODEL` statement for defining a reference model, these default free variance parameters in the old (reference) model are not transferred to the new model. Instead, the new model generates its own set of default free variance parameters *after* the new model is resolved from the reference model, the `REFMODEL` statement options, the `RENAMEPARAM` statement, and the PVAR statement specifications in the new model. If you want any of the variance or error (partial) variance parameters to be constrained across the models by means of the `REFMODEL` specification, you must specify them explicitly in the PVAR statement of the reference model so that the same variance or error (partial) variance specification is transferred to the new model.

RAM Statement

```
RAM < VAR=variable-list | [ variable-list=number-list <, variable-list=number-list ... > ], > < ram-entry
  <, ram-entry ... >>;
```

where *variable-list* is a list of variables for the rows and columns of the `_A_` and `_P_` matrices and the rows of the `_W_` vector of the RAM model, *number-list* is a list of positive integers that denote the order of the specified variables, and *ram-entry* is a parameter specification for an element in one of the three RAM model matrices. You can specify latent variables in addition to observed variables in the VAR= option.

RAM stands for the reticular action model developed by McArdle (1980). The RAM model implemented in PROC CALIS extends the original RAM model with the specification of the mean vector in the `_W_` vector. See the section “The RAM Model” on page 1294 for details about the model.

The RAM statement specification consists of the list of the variables in the model and the parameters and their locations the RAM model matrices. For example, consider the following simple RAM model specification:

```
ram var= x1-x2 y3,
      _A_ 3 1,
      _A_ 3 2;
```

In this statement, variables `x1`, `x2`, and `y3` are specified in the VAR= option. The variable order in the VAR= option is important. The same variable order applies to the rows and columns of the `_A_` matrix. Next, there are two *ram-entries*. The first *ram-entry* specifies that the third variable (`y3`) has a path from the first variable (`x1`). Similarly, the second *ram-entry* specifies that `y3` has a path from `x2`.

Specifying the VAR= Option

In the VAR= option, you specify the list of observed and latent variables in the RAM model. There are two ways to specify the VAR= list. The first way is a simple listing of variables. For example, you specify a total of 18 variables in the RAM model in the following statement:

```
ram var= a b c x1-x5 y1-y10;
```

The order of the variables in this VAR= list is important. The same variable order applies to the rows and columns of the `_A_` and `_P_` matrices and the rows of the `_W_` matrices. Although it is not required to arrange the variables according to whether they are observed or latent in the VAR= list, you can do so for your own convenience. PROC CALIS checks each variable in the VAR= list against the associated data sets to determine whether the variable is observed or latent.

When you specify the parameters in the *ram-entries*, you represent variables by the variable numbers that refer to the VAR= list. Therefore, it is important to make correct association of the variables and their order on the VAR= list. To this end, you can add some comments in your VAR= list to make the variable numbers explicit. For example,

```
ram var= a      /* 1 */
        b      /* 2 */
        c      /* 3 */
        x1-x5  /* 4-8 */
        y1-y10 /* 9-18 */;
```

Another way to specify VAR= list is to provide the *variable-lists* together with explicit ordering indicated in the *number-lists*. For example, in the following statement you specify exactly the same variable list as that in the preceding example:

```
ram var= [x1-x5 = 4 to 8, c = 3, y1-y10 = 9 to 18, a = 1, b = 2];
```

Apart from showing how you can construct the VAR= list in a very general way with the *number-lists*, there is no particular reason why the *variable-lists* in the preceding specification are not in either an ascending or a descending order. Perhaps a more natural and useful way to use this type of explicit ordering specification is to place variables in exactly the same order as intended. For example, the following VAR= specification serves as a “key” of the variable numbers in the subsequent *ram-entries*:

```
ram var= [x1 = 1, x2 = 2, y1 = 3, y2 = 4, y3 = 5],
  _A_ 1 2 ,
  _P_ 2 2 ;
```

With reference to the explicit variable numbers in the VAR= list, you can interpret the `_A_[1, 2]` specification immediately as the effect from x2 to x1, and the `_P_[2, 2]` specification as the variance of x2.

If the VAR= option is not specified in the RAM statement, the *n* observed variables in the VAR statement are used as the first *n* variables in the VAR= list. If you specify neither the VAR= option in the RAM statement nor the VAR statement, all *n* numerical variables in the associated data sets serve as the first *n* variables in the RAM model matrices. If there are more than *n* variables used in the *ram-entries*, the extra variables are all treated as latent variables in the RAM model.

Latent variables generated by PROC CALIS for the RAM model are named in two different ways, depending on whether your RAM model is specified under a MODEL statement. If you do not use the MODEL statement (for example, in situations with single-group analyses), latent variables are named `_Factor1`, `_Factor2`, and so on. If your RAM model is defined within the scope of a MODEL statement, latent variables are named `_Mdlk_F1`, `_Mdlk_F2`, and so on, where *k* is substituted with the model number that is specified in the MODEL statement. For example, `_Mdl2_F1` is a latent factor that is specified under a RAM model within the scope of the MODEL statement with 2 as its model number.

Because data sets might contain nonnumerical variables, implicit variable ordering deduced from the data sets is sometimes obscured. Therefore, it is highly recommended that you use the VAR= option to list all the variables in the RAM model.

Specifying a *ram-entry*

```
matrix-name | matrix-number row-number column-number <parameter-spec>
```

A *ram-entry* is a parameter specification of a matrix element of the RAM model. In each *ram-entry*, you first specify the matrix by using either the *matrix-name* or the *matrix-number*. Then you specify the *row-number* and the *column-number* of the element of the matrix. At the end of the *ram-entry*, you can optionally specify various kinds of parameters in *parameter-spec*. You can specify as many *ram-entries* as needed in your RAM model. *Ram-entries* are separated by commas. For example, consider the following specification:

```
ram var= x1-x2 y3,
  _A_ 3 1 1.,
  _A_ 3 2;
```

You specify three variables in the VAR= option of the RAM statement. In the first *ram-entry*, variable y3 has a path from variable x1 with a fixed path coefficient 1. In the second *ram-entry*, variable y3 has a path from variable x2. Because the *parameter-spec* is blank, the corresponding path coefficient (or the effect from x2 on y3) is a free parameter by default.

Specifying the matrix-name or matrix-number

The three model matrices in the RAM model are: `_A_`, `_P_`, and `_W_`. See the section “The RAM Model” on page 1294 for the mathematical formulation of the RAM model. The *matrix-name* or *matrix-number* specifications in the *ram-entries* refer to these model matrices. You can use the following keywords for *matrix-name* or *matrix-number*:

`_A_`, `_RAMA_`, or 1 for the elements in the **A** matrix, which is for path coefficients or effects
`_P_`, `_RAMP_`, or 2 for the elements in the **P** matrix, which is for variances and covariances
`_W_`, `_RAMW_`, or 3 for the elements in the **W** vector, which is for intercepts and means

Specifying the row-number and column-number

After you specify the *matrix-name* or *matrix-number* in a *ram-entry*, you need to specify the *row-number* and *column-number* that correspond to the intended element of the matrix being specified.

Specifying the parameter-spec

You can specify three types of parameters in *parameter-spec*:

- A free parameter without an initial estimate: blank or *parameter-name*

You can specify a free parameter for the matrix element in a *ram-entry* by either omitting the *parameter-spec* (that is, leaving it blank) or specifying a *parameter-name*. For example, both of the following *ram-entries* specify that `_A_[3,1]` is a free parameter in the RAM model:

```
_A_ 3 1
```

and

```
_A_ 3 1 beta
```

The difference is that in the latter you name the effect (path coefficient) for the `_A_[3,1]` element as `beta`, while in the former PROC CALIS generates a free parameter name (prefixed with `_Parm` and followed by a unique parameter number) for the specified element. Leaving the *parameter-spec* blank is handy if you do not need to refer to this parameter in your code. But when you need to specify parameter constraints by referring to parameter names, the *parameter-name* syntax becomes necessary. For example, the following specification constrains the `_A_[3,1]` and `_A_[3,2]` paths to have equal effects (path coefficients) because they have the same *parameter-name* `beta`:

```
ram var= x1-x2 y3,
      _A_ 3 1 beta,
      _A_ 3 2 beta;
```

- A free parameter with an initial estimate: (*number*) or *parameter-name* (*number*)

You can specify a free parameter with an initial estimate in a *ram-entry* by either specifying the initial estimate within parentheses or specifying a *parameter-name* followed by the parenthesized initial estimate. For example, both of the following *ram-entries* specify that `_A_[3,1]` is a free parameter with an initial estimate of 0.3 in the RAM model:

```
_A_ 3 1 (0.3)
```

and

```
_A_ 3 1 beta (0.3)
```

In the latter you name the effect (path coefficient) for the `_A_[3,1]` element as `beta`, while in the former PROC CALIS generates a free parameter name (prefixed with `_Parm` and followed by a unique parameter number). The latter syntax is necessary when you need to specify parameter constraints by referring to the parameter name `beta`. The former syntax is more convenient when you do not need to refer to this parameter in other specifications.

For the latter syntax with a *parameter-name* specified, you can omit the pair of parentheses or exchange the position of *parameter-name* and *number* (or both) without changing the nature of the parameter. That is, you can use the following equivalent specifications for a named free parameter with initial values:

```
_A_ 3 1 beta 0.3
```

and

```
_A_ 3 1 .3 beta
```

- A fixed parameter value: *number*

You can specify a fixed value by simply providing it as the *parameter-spec* in a *ram-entry*. For example, in the following syntax you specify that `_A_[3,1]` is a fixed value of 0.3:

```
_A_ 3 1 0.3
```

The fixed value for `_A_[3,1]` does not change during the estimation. To distinguish this syntax from the initial value specification, notice that you do not put `0.3` inside parentheses, nor do you put a *parameter-name* before or after the provided value.

Notes and Cautions about Specifying *ram-entries*

- Older versions of PROC CALIS treat a blank *parameter-spec* in the *ram-entry* as a fixed constant 1. This is no longer the case in this version of PROC CALIS. Fixed values such as 1.0 must be specified explicitly.
- The *row-number* and *column-number* in the *ram-entries* refer to the VAR= variable list of the RAM statement. An exception is for the `_W_` vector, of which the *column-number* should always be 1 and does not refer to any particular variable.
- When a *row-number* or *column-number* in a *ram-entry* (except for the *column-number* of `_W_`) does not have any reference in the VAR= variable list (or is greater than the number of default observed variables when the VAR= option is not specified), PROC CALIS treats the corresponding row or column variable as a latent variable and generates variable names for it.

- The largest row or column number used in any *ram-entry* should not exceed the sum of observed and latent variables intended in the RAM model. Otherwise, some extraneous latent variables might be created.

Default Parameters

It is important to understand the default parameters in the RAM model. First, if you know which parameters are default free parameters, you can make your specification more efficient by omitting the specifications of those parameters that can be set by default. For example, because all exogenous variances and error variances in the RAM model are free parameters by default, you do not need to specify the diagonal elements of the *_P_* matrix if they are not constrained in the model. Second, if you know which parameters are default free parameters, you can specify your model accurately. For example, because all the error covariances in the RAM model are fixed zeros by default, you must specify the corresponding off-diagonal elements of the *_P_* matrix in the *ram-entries*. See the section “Default Parameters in the RAM Model” on page 1301 for details about the default parameters of the RAM model.

Modifying a RAM Model from a Reference Model

This section assumes that you use a **REFMODEL** statement within the scope of a **MODEL** statement and that the reference model (or base model) is also a RAM model. The reference model is called the old model, and the model that refers to this old model is called the new model. If the new model is not intended to be an exact copy of the old model, you can use the following extended RAM modeling language to make modifications on the model specification. The syntax for modifications is very much the same as the ordinary RAM modeling language (see the section “RAM Statement” on page 1216), except that you cannot specify the **VAR=** option in the RAM statement. The reason is that the **VAR=** variable list in the new RAM model should be exactly the same as the old model; otherwise, the *row-number* and *column-number* in the *ram-entries* would not have the same references and thus would make model referencing meaningless. Hence, the syntax for respecifying (modifying) the RAM model contains only the *ram-entries*:

```
RAM ram-entry <, ram-entry ... > ;
```

The syntax of the *ram-entry* is the same as that of the original RAM statement, with an addition of the missing value specification for the *parameter-spec*, which denotes the deletion of a parameter location.

The new model is formed by integrating with the old model in the following ways:

- | | |
|--------------|--|
| Duplication: | If you do not specify in the new model a parameter location (matrix element) that exists in the old model, the old parameter specification is duplicated in the new model. |
| Addition: | If you specify in the new model a parameter location (matrix element) that does not exist in the old model, the new parameter specification is added to the new model. |
| Deletion: | If you specify in the new model a parameter location (matrix element) that also exists in the old model and the new <i>parameter-spec</i> is denoted by the missing value ‘.’, the old parameter specification is not copied into the new model. |
| Replacement: | If you specify in the new model a parameter location (matrix element) that also exists in the old model and the new parameter is not denoted by the missing value ‘.’, the new parameter specification replaces the old one in the new model. |

For example, consider the following two-group analysis:


```

proc calis;
  group 1 / data=d1;
  group 2 / data=d2;
  model 1 / group=1;
    ram
      var = [V1-V6 = 1 to 6, F1 = 7],
      _A_ 1 7 1.,
      _A_ 2 7 load1,
      _A_ 3 7 load2,
      _A_ 7 4 ,
      _A_ 7 5 ,
      _A_ 7 6 ,
      _P_ 1 1 ,
      _P_ 2 2 ,
      _P_ 3 3 ,
      _P_ 7 7 ,
      _P_ 4 4 ,
      _P_ 5 5 ,
      _P_ 6 6 ,
      _P_ 1 2 cve12;
  model 2 / group=2;
    refmodel 1;
    ram
      _A_ 3 7 load1,
      _P_ 1 2 .,
      _P_ 2 3 cve23;
run;

```

In this example, you specify Model 2 by referring to Model 1 in the **REFMODEL** statement. Model 2 is the new model which refers to the old model, Model 1. This example illustrates the four types of model integration process by PROC CALIS:

- Duplication: All parameter specifications, except for **_A_[3, 7]** and **_P_[1, 2]**, in the old model are duplicated in the new model.
- Addition: The new parameter **cve23** is added for the matrix element **_P_[2, 3]** in the new model.
- Deletion: The parameter location **_P_[1, 2]** and associated parameter **cve12** are not copied into the new model, as indicated by the missing value **'.'** in the new model specification.
- Replacement: The **_A_[3, 7]** path in the new model replaces the same path in the old model with another parameter for the path coefficient. As a result, in the new model paths specified by **_A_[3, 7]** and **_A_[2, 7]** are constrained to have the same path coefficient parameter **load1**.

PROC CALIS might have generated some default parameters (named with the **'_Add'** prefix) for the old (reference) model. These default parameters in the old (reference) model do *not* transfer to the new model. Only after the new model is resolved from the reference model, the **REFMODEL** statement options, the **RENAMEPARAM** statement, and the model respecification are the default parameters of the new RAM model generated. In this way, the generated parameters in the new model are not constrained to be the same as the corresponding parameters in the old (reference) model. If you want any of these default parameters to be constrained across the models, you must specify them explicitly in the *ram-entries* of the RAM statement

of the reference model so that these specifications are duplicated to the new model via the [REFMODEL](#) statement.

REFMODEL Statement

```
REFMODEL model-number </ options > ;
```

The REFMODEL statement is not a modeling language itself. It is a tool for referencing and modifying models. It is classified into one of the modeling languages because its role is similar to other modeling languages.

```
REFMODEL model-number </ options > ;
RENAMEPARM parameter renaming ;
main model specification statement ;
subsidiary model specification statements ;
```

In the REFMODEL statement, you specify the *model-number* (between 1 and 9,999, inclusive) of the model you are making reference to. The reference model must be well-defined in the same PROC CALIS run. In the *options*, you can rename all the parameters in the reference model by adding a prefix or suffix so that the current model has a new set of parameters. The [RENAMEPARM](#) statement renames individual parameters in the reference model to new names. In the [main model specification statement](#) and the [subsidiary model specification statements](#), you can respecify or modify the specific parts of the reference model. The specification of these statements must be compatible with the model type of the reference model.

NOTE: The REFMODEL statement does *not* simply copy model specifications from a reference model. If you do not change any of the parameter names of the reference model by any of the REFMODEL statement options, the REFMODEL statement copies only the *explicit* specifications from the reference model to the new model. However, the REFMODEL statement does not copy the default parameters from the reference model to the new model. For example, consider the following statements:

```
proc calis;
  group 1 / data=a1;
  group 2 / data=a2;
  model 1 / group=1;
    path x1 ==> x2;
  model 2 / group=2;
    refmodel 1;
run;
```

In this example, Model 2 makes reference to Model 1. This means that the path relationship between x1 and x2 as specified in Model 1 is exactly the same path relationship you want Model 2 to have. The path coefficients in these two models are constrained to be the same. However, the variance parameter of x1 and the error variance parameter for x2 are not constrained in these models. Rather, these two parameters are set by default in these models separately. If you intend to constrain all parameters in the two models, you can specify all the parameters in Model 1 explicitly and use the REFMODEL statement for Model 2, as shown in the following statements:

```
proc calis;
  group 1 / data=a1;
  group 2 / data=a2;
  model 1 / group=1;
```

```

    path x1 ==> x2;
    pvar x1 x2;
    model 2 / group=2;
    refmodel 1;
run;

```

This way Model 2 makes reference to all the explicitly specified parameters in Model 1. Hence the two models are completely constrained. However, a simpler way to fit exactly the same model to two groups is to use a single model definition, as shown in the following statements:

```

proc calis;
  group 1 / data=a1;
  group 2 / data=a2;
  model 1 / group=1,2;
  path x1 ==> x2;
run;

```

This specification has the same estimation results as those for the preceding specification.

When you also use one of the REFMODEL statement options, the REFMODEL statement is no longer a simple copy of explicit parameter specifications from the reference model. All parameters are renamed in the new model in the model referencing process. The following options are available in the REFMODEL statement:

ALLNEWPARMS

appends to the parameter names in the reference model with `_mdl` and then an integer suffix denoting the model number of the current model. For example, if `qq` is a parameter in the reference model for a current model with model number 3, then this option creates `qq_mdl3` as a new parameter name.

PARAM_PREFIX=prefix

inserts to all parameter names in the reference model with the *prefix* provided. For example, if `qq` is a parameter in the reference model for a current model, then **PARAM_PREFIX=pre_** creates `pre_qq` as a new parameter name.

PARAM_SUFFIX=suffix

appends to all parameter names in the reference model with the *suffix* provided. For example, if `qq` is a parameter in the reference model for a current model, then **PARAM_SUFFIX=_suf** creates `qq_suf` as a new parameter name.

Instead of renaming all parameters, you can also rename parameters individually by using the **RENAMEPARAM** statement within the scope of the REFMODEL statement.

You can also add the main and subsidiary model specification statements to modify a particular part from the reference model. For example, you might like to add or delete some equations or paths, or to change a fixed parameter to a free parameter or vice versa in the new model. All can be done in the respecification in the main and subsidiary model specification statements within the scope of the **MODEL** statement to which the REFMODEL statement belongs. Naturally, the modeling language used in respecification must be the same as that of the reference model. See the individual statements for modeling languages for the syntax of respecification. Note that when you respecify models by using the main and subsidiary model specification statements together with the **RENAMEPARAM** statement or the REFMODEL options for changing parameter names, the parameter name changes occur after respecifications.

RENAMEPARM Statement

RENAMEPARM *assignment* <, *assignment* ... > ;

where *assignment* represents:

old_parameters = *parameter-spec*

You can use the RENAMEPARM statement to rename parameters or to change the types of parameters of a reference model so that new parameters are transferred to the new model in question. The RENAMEPARM statement is a subsidiary model specification statement that should be used together with the REFMODEL statement. The syntax of the RENAMEPARM statement is similar to that of the VARIANCE statement—except that in the RENAMEPARM statement, you put parameter names on the left-hand side of equal signs, whereas you put variable names on the left-hand side in the VARIANCE statement. You can use no more than one RENAMEPARM statement within the scope of each REFMODEL statement.

In the REFMODEL statement, you transfer all the model specification information from a base model to the new model being specified. The RENAMEPARM statement enables you to modify the parameter names or types in the base model before transferring them to the new model. For example, in the following example, you define Model 2, which is a new model, by referring it to Model 1, the base model, in the REFMODEL statement.

```

model 1;
  lineqs
    V1 =    F1 + E1,
    V2 = b2 F1 + E2,
    V3 = b3 F1 + E3,
    V4 = b4 F1 + E4;
  variance F1 = vF1,
    E1-E4 = ve1-ve4;
model 2;
  refmodel 1;
  renameparm ve1-ve4=new1-new4, b2=newb2(.2), b4=.3;

```

Basically, the LINEQS model specification in Model 1 is transferred to Model 2. In addition, you redefine some parameters in the base model by using the RENAMEPARM statement. This example illustrates two kinds of modifications that the RENAMEPARM statement can do:

- creating new parameters in the new model

The error variances for E1–E4 in Model 2 are different from those defined in Model 1 because new parameters new1–new4 are now used. Parameter b2 is renamed as newb2 with a starting value at 0.2 in Model 2. So the two models have distinct path coefficients for the F1-to-V2 path.

- changing free parameters into fixed constants

By using the specification **b4=.3** in the RENAMEPARM statement, b4 is no longer a free parameter in Model 2. The path coefficient for the F1-to-V4 path in Model 2 is now fixed at 0.3.

The RENAMEPARM statement is handy when you have just few parameters to change in the reference model defined by the REFMODEL statement. However, when there are a lot of parameters to modify, the

RENAMEPARAM statement might not be very efficient. For example, to make all parameters unique to the current model, you might consider using the `ALLNEWPARAMS`, `PARAM_PREFIX=`, or `PARAM_SUFFIX=` option in the `REFMODEL` statement.

SAS Programming Statements

You can use SAS programming statements to define dependent parameters, parametric functions, and equality constraints among parameters.

Several statistical procedures support the use of SAS programming statements. The syntax of SAS programming statements are common to all these procedures and can be found in the section “Programming Statements” on page 504 in Chapter 19, “Shared Concepts and Topics.”

SIMTESTS Statement

SIMTESTS | **SIMTEST** *sim-test* < *sim-test* ... > ;

where *sim-test* represents one of the following:

- *test-name* = [*functions*]
- *test-name* = { *functions* }

and *functions* are either parameters in the model or parametric functions computed in the [SAS programming statements](#).

When the estimates in a model are asymptotically multivariate-normal, continuous and differentiable functions of the estimates are also multivariate-normally distributed. In the `SIMTESTS` statement, you can test these parametric functions simultaneously. The null hypothesis for the simultaneous tests is assumed to have the following form:

$$H_0 : h_1(\theta) = 0, h_2(\theta) = 0, \dots$$

where θ is the set of model parameters (independent or dependent) in the analysis and each $h_i()$ is a continuous and differentiable function of the model parameters.

To test parametric functions simultaneously in the `SIMTESTS` statement, you first assign a name for the simultaneously test in *test-name*. Then you put the parametric functions for the simultaneous test inside a pair of parentheses: either the ‘{’ and ‘}’ pair, or the ‘[’ and ‘]’ pair. For example, if θ_1 , θ_2 , θ_3 , and θ_4 are parameters in the model and you want to test the equality of θ_1 and θ_2 and the equality of θ_3 and θ_4 simultaneously, you can use the following statements:

```
simtests
  Equality_test = [t1_t2_diff t3_t4_diff];
t1_t2_diff     = theta1 - theta2;
t3_t4_diff     = theta3 - theta4;
```

In the `SIMTESTS` statement, you test two functions `t1_t2_diff` and `t3_t4_diff` simultaneously in the test named `Equality_test`. The two parametric functions `t1_t2_diff` and `t3_t4_diff` are computed in the [SAS programming statements](#) as differences of some parameters in the model.

See also the [TESTFUNC](#) statement on page 1227 for testing parametric functions individually.

STD Statement

STD *assignment* <, *assignment* ... > ;

where *assignment* represents:

var-list = *parameter-spec*

The STD statement functions exactly the same as the [VARIANCE](#) statement. The STD statement is obsolete and might not be supported in future versions of PROC CALIS. Use the [VARIANCE](#) statement instead.

STRUCTEQ Statement

STRUCTEQ *variables* </ *label*> ;

where *label* represents:

LABEL | NAME = *name*

The STRUCTEQ statement functions exactly the same as the [DETERM](#) statement.

TESTFUNC Statement

TESTFUNC *functions* ;

where *functions* are either parameters in the model or parametric functions computed in the [SAS programming statements](#).

When the estimates in a model are asymptotically multivariate-normal, any continuous and differentiable function of the estimates is also normally distributed. In the TESTFUNC statement, you can test these parametric functions using z-tests. The form of the null hypothesis is as follows:

$$H_0 : h(\theta) = 0$$

where θ is the set of model parameters (independent or dependent) in the analysis and $h()$ is a continuous and differentiable function of the model parameters.

For example, if θ_1 , θ_2 , and θ_3 are parameters in the model, and you want to test whether θ_1 and θ_2 are the same and whether θ_3 is the same as the average of θ_1 and θ_2 , you can use the following statements:

```
testfunc    t1_t2_diff t3_t1t2_diff;
t1_t2_diff  = theta1 - theta2;
t3_t1t2_diff = theta3 - (theta1 + theta2)/2;
```

In the TESTFUNC statement, you test two functions: `t1_t2_diff` and `t3_t1t2_diff`. These two functions are defined in the [SAS programming statements](#) that follow after the TESTFUNC statement. Thus, `t1_t2_diff` represents the difference between θ_1 and θ_2 , and `t3_t1t2_diff` represents the difference between θ_3 and the average of θ_1 and θ_2 .

See the [SIMTESTS](#) statement if you want to test several null hypotheses simultaneously.

VAR Statement

VAR *variables* ;

The VAR statement defines and limits the set of observed variables that are available for the corresponding model analysis. It is one of the [subsidiary group specification statements](#). You can use the VAR statement no more than once within the scope of each [GROUP](#) or the PROC CALIS statement. The set of variables in the VAR statement must be present in the data set specified in the associated [GROUP](#) or the PROC CALIS statement.

The following example shows the specification of 16 variables (x1, x2, . . . , x9, x10, y, z1, z2, . . . , z5) in the VAR statement:

```
var x1-x10 y z1-z5;
```

The VAR statement in PROC CALIS does not support the specification of variable lists with syntax that refers to consecutive variables in the data set. For example, if QQ, RR, SS, and TT are consecutive variables in a data set, the following specification of these four variables in the VAR statement is not supported by PROC CALIS:

```
var QQ-TT;
```

The VAR statement should not be confused with the [PARAMETERS](#) statement. In the [PARAMETERS](#) statement, you specify additional *parameters* in the model. Parameters are population quantities that characterize the functional relationships, variations, or covariation among variables. Unfortunately, parameters are sometimes referred to as *var-list* in the optimization context. You have to make sure that all variables specified in the VAR statement refer to the variables in the input data set, while the parameters specified in the [PARAMETERS](#) statement are population quantities that characterize distributions of the variables and their relationships.

In some modeling languages of PROC CALIS, you can also specify the observed variables either directly (for example, through the VAR= or similar option in some [main model specification statements](#)) or indirectly (for example, through the specification of functional relationships between observed variables). How does the VAR statement specifications interplay with the observed variables specified in the model? This depends on the types of models specified. Four different cases are considered in the following.

Case 1. Exploratory Factor Models With No VAR= option in the FACTOR statement. For exploratory factor models specified using the [FACTOR](#) statement, it is important for you to use the VAR statement to select and limit the set of the observed variables for analysis. The reason is simply that there is no other options in the [FACTOR](#) statement that will serve the same purpose. For example, you analyze only v1–v3 in the following exploratory factor model even though there might be more observed variables available in the data set:

```
proc calis;
  var v1-v3;
  factor n=1;
```

If you do not specify the VAR statement, PROC CALIS simply selects all numerical variables for analysis. However, to avoid confusions it is a good practice to specify the observed variables explicitly in the VAR statement.

Case 2. Models With a VAR= or Similar Option for Defining the Set of Observed Variables for Analysis. The classes of models considered here are: **COSAN**, **LISMOD**, **MSTRUCT**, and **RAM**. Except for the LISMOD models, in all other three classes of models you can specify the observed variables in the model by using the a VAR= option in the respective **main model specification statement**. For the LISMOD models, you can specify all observed variables that should be included in the model in the XVAR= and YVAR= options of the LISMOD statement. Therefore, the use of the VAR statement for these models might become unnecessary. For example, the following MSTRUCT statement specifies the observed variables v1–v6 in the VAR= option:

```
proc calis;
  mstruct var=v1-v6;
```

It would have been redundant to use a VAR statement to specify v1–v6 additionally. The same conclusion applies to the **COSAN** and the **RAM** models.

Another example is when you specify a LISMOD model. In the following LISMOD specification, variables v1–v8 would be the set of observed variables for analysis:

```
proc calis;
  var v1-v8;
  lismod xvar = v1-v4,
         yvar = v5-v8,
         eta = factor1,
         xi  = factor2;
```

Again, there is no need to add a VAR statement merely repeating the specification of variables v1–v8.

If you do specify the VAR statement in addition to the specification of variable lists in these models, PROC CALIS will check the consistency between the lists. Conflicts arise if the two lists do not match.

For example, the following statements will generate an error in model specification because v6 specified in the MSTRUCT model is not defined as an observed variable available for analysis in the VAR statement (even if v6 might indeed be present in the data set):

```
proc calis;
  var v1-v5;
  mstruct var=v1-v6;
```

So it is an error when you specify fewer observed variables in the VAR statement than in the VAR= option in the model. How about if you specify more variables in the VAR statement? PROC CALIS will also general an error because the extra variables in VAR statement will not be well-undefined in the model. For example, v7–v10 specified in the VAR statement are supposed to be included into the model, but they not listed on either the XVAR= or YVAR= list in the following LISMOD statement:

```
proc calis;
  var v1-v10;
  lismod xvar = v1-v3,
         yvar = v4-v6,
         eta = factor1,
         xi  = factor2;
```

Therefore, if you must specify the VAR statement for these models, the specifications of the observed variables must be consistent in the VAR statement and in the relevant model options. However, to avoid

potential conflicts in these situations, you are recommended to specify the observed variables in the VAR=, XVAR=, or YVAR= lists only.

When the VAR= option is not specified in the COSAN, MSTRUCT, or RAM statement, the VAR statement specification will be used as the list of observed variables in the model. If both of the VAR= option and VAR statement specification are lacking, then all numerical variables in the associated data set will be used in the model. However, to avoid confusions the preferred method is to specify the list of observed variables explicitly on the VAR=, XVAR=, or YVAR= option of the [main model specification statements](#).

Case 3. Models With Indirect Ways to Include the Set of Observed Variables for Analysis. Two types of models are considered here: LINEQS and PATH. For these models, the main use of the VAR statement is to include those observed variables that are not mentioned in model specifications.

For example, in the following statements for a LINEQS model variable v3 is not mentioned in the LINEQS statement:

```
proc calis;
  var v1-v3;
  lineqs v1 = a1 * v2 + e1;
```

With the specification in the VAR statement, however, variable v3 is included into the model as an exogenous manifest variable. Similarly, the same applies to the following PATH model specification:

```
proc calis;
  var v1-v3;
  path v1 <=== v2;
```

Again, variable v3 is included into the PATH model because it is specified in the VAR statement.

The two preceding examples also suggest that you do not need to use the VAR statement when your already mentions all observed variables in the model specification. For example, if your target set of observed variables are v1–v3, the use of the VAR statement in the following specification is *unnecessary*:

```
proc calis;
  var v1-v3;
  path v1 <=== v2;
  pvar v3;
```

For the two types of models considered here, you can also use the VAR statement to define and limit the set of observed variables for analysis. For example, you might have v1, v2, v3 in your data set as observed variables for analysis; but somehow in your model v2 should be treated as a latent variable. You might use the following code to exclude v2 as an observed variable in the model:

```
proc calis;
  var v1 v3;
  path v1 <=== v2;
  pvar v3;
```

The role of the VAR statement here is to define and limit the set of observed variables available for the model. Hence, only variables v1 and v3 are supposed to be observed variables in the model while variable v2 in the PATH model is treated as latent.

In sum, in the current situation the use of the VAR statement should depend on whether a variable should or should not be included as an observed variable in your theoretical model.

Case 4. Confirmatory Factor Model With the FACTOR statement. In this case, the VAR statement still limits the set of observed variables being analyzed in the confirmatory factor model. However, because all observed variables in a [confirmatory factor analysis](#) must be loaded on (or related to) some factors through the specification of *factor-variable-relations* in the [FACTOR](#) statement, all observed variables in the model should have been specified (or mentioned) in the [FACTOR](#) statement already, making it redundant to use the VAR statement for the same purpose.

VARIANCE Statement

VARIANCE *assignment* <, *assignment* ... > ;

where *assignment* represents:

var-list < =*parameter-spec* >

The VARIANCE statement specifies the variance parameters in connection with the [LINEQS](#) model. Notice that the VARIANCE statement is different from the [VAR](#) statement, which specifies variables for analysis. In previous versions of PROC CALIS, the STD statement name was used instead of the VARIANCE statement name. Although these two names result in the same functionalities, the VARIANCE statement name reflects the intended usages better.

In the [LINEQS](#) model, variance parameters are defined only for *exogenous* manifest and latent variables (including error and disturbance variables) in the model. Therefore, you cannot list any *endogenous* variables in the *var-list* list of the VARIANCE statement. You can specify no more than one VARIANCE statement for each [LINEQS](#) model.

In each *assignment* of the VARIANCE statement, you list the *var-list* whose variances you want to specify. Optionally, you can provide a list of parameter specifications (*parameter-spec*) after an equal sign for each *var-list* list.

You can specify the following five types of the parameters for the variances of the exogenous variables in the VARIANCE statement:

- an unnamed free parameter
- an initial value
- a fixed value
- a free parameter with a name provided
- a free parameter with a name and initial value provided

Consider a [LINEQS](#) model with exogenous variables V1, V2, F1, D2, and E3. The following VARIANCE statement illustrates the five types of parameter specifications in five *assignments*:

```
variance
  V1 ,
  V2 = (.5),
  F1 = 1.0,
```

```
D2 = dvar,
E3 = evar(0.7);
```

In this statement, the variance of V1 is specified as an unnamed free parameter. For this variance, PROC CALIS generates a parameter name with the `_Parm` prefix and appended with a unique integer (for example, `_Parm1`). The variance of V2 is an unnamed free parameter with an initial value of 0.5. PROC CALIS also generates a parameter name for this variance. The variance of F1 is a fixed value of 1.0. This value stays the same during the estimation. The variance of D2 is a free parameter named `dvar`. The variance of E3 is a free parameter named `evar` with an initial value of 0.7.

When you need to specify a long parameter name list, you can consider using the prefix-name specification for the parameter list. For example, the following statement specifies 100 unique parameter names for the variances of E1–E100:

```
variance
  E1-E100 = 100 * evar__ ; /* evar with two trailing underscores */
```

In the VARIANCE statement, `evar__` is a prefix-name with the root `evar`. The notation `100*` means this prefix-name is applied 100 times, resulting in a generation of the 100 unique parameter names `evar001`, `evar002`, ..., `evar100`.

The root of the prefix-name should have few characters so that the generated parameter name is not longer than 32 characters. To avoid unintentional equality constraints, the prefix-names should not coincide with other parameter names.

Mixed Parameter Lists

You can specify different types of parameters for the list of variances. For example, the following statement uses a list of parameters with mixed types:

```
variance
  E1-E6 = vp1 vp2(2.0) vp3 4. (.3) vp6(.4);
```

This is equivalent to the following specification:

```
variance
  E1 = vp1
  E2 = vp2(2.0) ,
  E3 = vp3 ,
  E4 = 4. ,
  E5 = (.3) ,
  E6 = vp6(.4);
```

Notice that an initial value followed after a parameter name is associated with the free parameter. For example, in the original mixed list specification, the specification `(2.0)` after `vp2` is interpreted as the initial value for the parameter `vp2`, but not as the initial estimate for the variance of E3.

However, if you indeed want to specify that `vp2` is a free parameter *without* an initial value and 2.0 is an initial estimate for the variance of E3 (while keeping all other things the same), you can use a null initial value specification for the parameter `vp2`, as shown in the following statement:

```

variance
  E1-E6 = vp1 vp2 () (2.0) 4. (.3) vp6(.4);

```

This way 2.0 becomes the initial estimate for the variance of E3. Because a parameter list with mixed types might be confusing, you can break down the specifications into separate *assignments* to remove ambiguities. For example, you can use the following equivalent specification:

```

variance
  E1 = vp1
  E2 = vp2,
  E3 = (2.),
  E4 = 4. ,
  E5 = (.3),
  E6 = vp6(.4);

```

Shorter and Longer Parameter Lists

If you provide fewer parameters than the number of variances in the *var-list* list, all the remaining parameters are treated as unnamed free parameters. For example, the following specification assigns a fixed value of 1.0 to the variance of F1 while treating the other three variances as unnamed free parameters:

```

variance
  F1-F4 = 1.0;

```

This specification is equivalent to the following specification:

```

variance
  F1 = 1.0, F2-F4;

```

If you intend to fill up all values with the last parameter specification in the list, you can use the continuation syntax [...], [...], or [...], as shown in the following example:

```

variance
  E1-E100 = 1.0 psi [...];

```

This means that the variance of E1 is fixed at 1.0, while the variances of E1–E100 are all free parameter named psi. All variances except that for E1 are thus constrained to be equal by using the same parameter name.

However, you must be careful not to provide too many parameters. For example, the following specification results in an error:

```

variance
  E1-E6 = 1.0 psi2-psi6 extra;

```

The parameters after psi6 are excessive.

Default Variance Parameters

In the LINEQS model, by default all variances of exogenous manifest and latent variables (including error and disturbance variables) are free parameters. For these default free parameters, PROC CALIS generates the parameter names with the *_Add* prefix and appended with unique integer suffixes. You can also use the

VARIANCE statement specification to override these default variance parameters in situations where you want to specify parameter constraints, provide initial or fixed values, or make parameter references.

Because only exogenous variables can have variance parameters in the LINEQS model and all these exogenous variances are free parameters by default, there are no default fixed zeros for any variances in the LINEQS model.

Modifying a Variance Parameter Specification from a Reference Model

If you define a new LINEQS model by using a reference (old) model in the `REFMODEL` statement, you might want to modify some parameter specifications from the `VARIANCE` statement of the reference model before transferring the specifications to the new model. To change a particular variance specification from the reference model, you can simply respecify the same variance with the desired parameter specification in the `VARIANCE` statement of the new model. To delete a particular variance parameter from the reference model, you can specify the desired variance with a missing value specification in the `VARIANCE` statement of the new model.

For example, suppose that the variance of `V1` is specified in the reference model but you do not want this variance specification to be transferred to the new model, you can use the following `VARIANCE` statement specification in the new model:

```
variance V1 = .;
```

Note that the missing value syntax is valid only when you use the `REFMODEL` statement. See the section “Modifying a LINEQS Model from a Reference Model” on page 1160 for a more detailed example of the LINEQS model respecification.

As discussed in a preceding section, PROC CALIS generates default free variance parameters for the LINEQS model if you do not specify them explicitly in the `VARIANCE` statement. When you use the `REFMODEL` statement for defining a reference model, these default free variance parameters in the old (reference) model are not transferred to the new model. Instead, the new model generates its own set of default free variance parameters *after* the new model is resolved from the reference model, the `REFMODEL` statement options, the `RENAMEPARM` statement, and the `VARIANCE` statement specifications in the new model. This also implies that if you want any of the variance parameters to be constrained across the models by means of the `REFMODEL` specification, you must specify them explicitly in the `VARIANCE` statement of the reference model so that the same variance specification is transferred to the new model.

VARNAMES Statement

```
VARNAMES name-assignment <, name-assignment ... > ;
```

```
VARNAME name-assignment <, name-assignment ... > ;
```

```
VNAMES name-assignment <, name-assignment ... > ;
```

where *name-assignment* represents one of the following forms:

```
matrix-name variable-names
```

```
matrix-name = [variable-names]
```

```
matrix-name = matrix-name
```

You can use the VARNAMES statement in connection with the COSAN modeling language to assign variable names for matrices. The *matrix-name* refers to any matrix you define in the COSAN statement. The *variable-names* that follow the *matrix-name* are assigned to the column variables of the matrix of interest. This applies to the first two types of VARNAMES specifications. For example,

```
varnames F f1-f3;
```

is exactly the same as

```
varnames F = [ f1-f3 ];
```

Both of these assign f1, f2, and f3 as the names for the first three column variables of matrix F.

You can also use another kind of *name-assignment* in connection with a COSAN statement. Two matrix names equated by an equal sign assign the column names of the matrix on the right-hand side to the column names of the matrix on the left-hand side. This assignment assumes that the column names of at least one of the two matrices are already defined. For example, assuming that J and A are model matrices defined in a COSAN statement, the following VARNAMES statement specification specifies that both J and A have the same set of column variable names V1–V6 and F1–F3:

```
varnames J = [ V1-V6 F1-F3 ] ,
        A = J ;
```

This is the same as the following specification:

```
varnames J = [ V1-V6 F1-F3 ] ,
        A = [ V1-V6 F1-F3 ] ;
```

The VARNAMES statement appears to enable you to specify only the column variable names for matrices. However, PROC CALIS also uses these column variable names to assign row variable names of the related matrices in the covariance and mean structure formulas for the COSAN model. PROC CALIS uses the following rules to determine the row variable names of a matrix in the model:

- If a matrix is the first matrix of any term in the covariance or mean structure formula, the row variable names are the names of the manifest variables.
- If a matrix is the central covariance matrix of any term in the covariance structure formula, the row variable names are the same as the column variable names.
- For any other matrices, the row variable names are the same as the column variable names of the preceding matrix in the multiplicative formula for the covariance or mean structures.

WEIGHT Statement

WEIGHT *variable* ;

The WEIGHT statement specifies the weight variable for the observations. It is one of the [subsidiary group specification statements](#). You can use the WEIGHT statement no more than once within the scope of each GROUP statement or the PROC CALIS statement.

Weighting is often done when the error variance associated with each observation is different and the values of the weight variable are proportional to the reciprocals of the variances. The **WEIGHT** and **FREQ** statements have a similar effect, except the **WEIGHT** statement does not alter the number of observations unless **VARDEF=WGT** or **VARDEF=WDF**. An observation is used in the analysis only if the **WEIGHT** variable is greater than 0 and is not missing.

Details: CALIS Procedure

Input Data Sets

You can use four different kinds of input data sets in the CALIS procedure, and you can use them simultaneously. The **DATA=** data set contains the data to be analyzed, and it can be an ordinary SAS data set containing raw data or a special **TYPE=COV**, **TYPE=UCOV**, **TYPE=CORR**, **TYPE=UCORR**, **TYPE=SSCP**, or **TYPE=FACTOR** data set containing previously computed statistics. The **INEST=** data set specifies an input data set that contains initial estimates for the parameters used in the optimization process, and it can also contain boundary and general linear constraints on the parameters. If the model does not change too much, you can use an **OUTEST=** data set from a previous PROC CALIS analysis; the initial estimates are taken from the values of the **_TYPE_=PARMS** observation. The **INMODEL=** or **INRAM=** data set contains information of the analysis models (except for user-written programming statements). Often the **INMODEL=** data set is created as the **OUTMODEL=** data set from a previous PROC CALIS analysis. See the section “**OUTMODEL=** or **OUTRAM=** Data Set” on page 1243 for the structure of both **OUTMODEL=** and **INMODEL=** data sets. Using the **INWGT=** data set enables you to read in the weight matrix **W** that can be used in generalized least squares, weighted least squares, or diagonally weighted least squares estimation.

BASEFIT= or INBASEFIT= Data Set

The **BASEFIT=** or **INBASEFIT=** data set saves the fit function value and the degrees of freedom of a baseline model for computing various fit indices, especially the incremental fit indices. Typically, the **BASEFIT=** data set is created as an **OUTFIT=** data set from a previous PROC CALIS fitting of a customized baseline model. See the section “**OUTFIT=** Data Set” on page 1254 for details about the format of the **OUTFIT=** and **BASEFIT=** data sets.

DATA= Data Set

A **TYPE=COV**, **TYPE=UCOV**, **TYPE=CORR**, or **TYPE=UCORR** data set can be created by the **CORR** procedure or various other procedures. It contains means, standard deviations, the sample size, the covariance or correlation matrix, and possibly other statistics depending on which procedure is used.

If your data set has many observations and you plan to run PROC CALIS several times, you can save computer time by first creating a **TYPE=COV**, **TYPE=UCOV**, **TYPE=CORR**, or **TYPE=UCORR** data set and using it as input to PROC CALIS.

For example, assuming that PROC CALIS is first run with an **OUTMODEL=MODEL** option, you can run the following statements in subsequent analyses with the same model in the first run:

```

/* create TYPE=COV data set */
proc corr cov nocorr data=raw outp=cov(type=cov);
run;
/* analysis using correlations */
proc calis corr data=cov inmodel=model;
run;
/* analysis using covariances */
proc calis data=cov inmodel=model;
run;

```

Most procedures automatically set the TYPE= option of an output data set appropriately. However, the CORR procedure sets TYPE=CORR unless an explicit TYPE= option is used. Thus, (TYPE=COV) is needed in the preceding PROC CORR request, since the output data set is a covariance matrix. If you use a DATA step with a SET statement to modify this data set, you must declare the TYPE=COV, TYPE=UCOV, TYPE=CORR, or TYPE=UCORR attribute in the new data set.

You can use a VAR statement with PROC CALIS when reading a TYPE=COV, TYPE=UCOV, TYPE=CORR, TYPE=UCORR, or TYPE=SSCP data set to select a subset of the variables or change the order of the variables.

CAUTION: Problems can arise from using the CORR procedure when there are missing data. By default, PROC CORR computes each covariance or correlation from all observations that have values present for the pair of variables involved (“pairwise deletion”). The resulting covariance or correlation matrix can have negative eigenvalues. A correlation or covariance matrix with negative eigenvalues is recognized as a singular matrix in PROC CALIS, and you cannot compute (default) generalized least squares or maximum likelihood estimates. You can specify the RIDGE option to ridge the diagonal of such a matrix to obtain a positive definite data matrix. If the NOMISS option is used with the CORR procedure, observations with any missing values are completely omitted from the calculations (“listwise deletion”), and there is no possibility of negative eigenvalues (but there is still a chance for a singular matrix).

PROC CALIS can also create a TYPE=COV, TYPE=UCOV, TYPE=CORR, or TYPE=UCORR data set that includes all the information needed for repeated analyses.

If the data set DATA=RAW does not contain missing values, the following statements should give the same PROC CALIS results as the previous example:

```

/* using correlations */
proc calis corr data=raw outstat=cov inmodel=model;
run;
/* using covariances */
proc calis data=cov inmodel=model;
run;

```

You can create a TYPE=COV, TYPE=UCOV, TYPE=CORR, TYPE=UCORR, or TYPE=SSCP data set in a DATA step. Be sure to specify the TYPE= option in parentheses after the data set name in the DATA statement and include the _TYPE_ and _NAME_ variables. If you want to analyze the covariance matrix but your DATA= data set is a TYPE=CORR or TYPE=UCORR data set, you should include an observation with _TYPE_=STD giving the standard deviation of each variable. By default, PROC CALIS analyzes the recomputed covariance matrix even when a TYPE=CORR data set is provided, as shown in the following statements:


```

data correl(type=corr);
  input _type_ $ _name_ $ X1-X3;
  datalines;
std    .    4.  2.  8.
corr  X1  1.0  .   .
corr  X2   .7  1.0  .
corr  X3   .5  .4  1.0
;
proc calis inmodel=model;
run;

```

INEST= Data Set

You can use the `INEST=` (or `INVAR=`) input data set to specify the initial values of the parameters used in the optimization and to specify boundary constraints and the more general linear constraints that can be imposed on these parameters.

The variables of the `INEST=` data set must correspond to the following:

- a character variable `_TYPE_` that indicates the type of the observation
- n numeric variables with the parameter names used in the specified PROC CALIS model
- the BY variables that are used in a `DATA=` input data set
- a numeric variable `_RHS_` (right-hand side); needed only if linear constraints are used
- additional variables with names corresponding to constants used in the programming statements

The content of the `_TYPE_` variable defines the meaning of the observation of the `INEST=` data set. PROC CALIS recognizes observations with the following `_TYPE_` specifications.

PARMS	specifies initial values for parameters that are defined in the model statements of PROC CALIS. The <code>_RHS_</code> variable is not used. Additional variables can contain the values of constants that are referred to in programming statements. At the beginning of each run of PROC CALIS, the values of the constants are read from the PARMS observation for initializing the constants in the SAS programming statements.
UPPERBD UB	specifies upper bounds with nonmissing values. The use of a missing value indicates that no upper bound is specified for the parameter. The <code>_RHS_</code> variable is not used.
LOWERBD LB	specifies lower bounds with nonmissing values. The use of a missing value indicates that no lower bound is specified for the parameter. The <code>_RHS_</code> variable is not used.
LE <= <	specifies the linear constraint $\sum_j a_{ij}x_j \leq b_i$. The n parameter values contain the coefficients a_{ij} , and the <code>_RHS_</code> variable contains the right-hand-side b_i . The use of a missing value indicates a zero coefficient a_{ij} .

- GE |>=|> specifies the linear constraint $\sum_j a_{ij}x_j \geq b_i$. The n parameter values contain the coefficients a_{ij} , and the `_RHS_` variable contains the right-hand-side b_i . The use of a missing value indicates a zero coefficient a_{ij} .
- EQ |= specifies the linear constraint $\sum_j a_{ij}x_j = b_i$. The n parameter values contain the coefficients a_{ij} , and the `_RHS_` variable contains the right-hand-side b_i . The use of a missing value indicates a zero coefficient a_{ij} .

The constraints specified in the `INEST=`, `INVAR=`, or `ESTDATA=` data set are added to the constraints specified in `BOUNDS` and `LINCON` statements.

You can use an `OUTEST=` data set from a PROC CALIS run as an `INEST=` data set in a new run. However, be aware that the `OUTEST=` data set also contains the boundary and general linear constraints specified in the previous run of PROC CALIS. When you are using this `OUTEST=` data set without changes as an `INEST=` data set, PROC CALIS adds the constraints from the data set to the constraints specified by a `BOUNDS` and `LINCON` statement. Although PROC CALIS automatically eliminates multiple identical constraints, you should avoid specifying the same constraint a second time.

INMODEL= or INRAM= Data Set

This data set is usually created in a previous run of PROC CALIS. It is useful if you want to reanalyze a problem in a different way such as using a different estimation method. You can alter an existing `OUTMODEL=` data set in the DATA step to create the `INMODEL=` data set that describes a modified model. See the section “`OUTMODEL=` or `OUTRAM=` Data Set” on page 1243 for more details about the `INMODEL=` data set.

INWGT= Data Set

This data set enables you to specify a weight matrix other than the default matrix for the generalized, weighted, and diagonally weighted least squares estimation methods. If you also specify the `INWGT-INV` option (or use the `INWGT(INV)=option`), the `INWGT=` data set is assumed to contain the inverse of the weight matrix, rather than the weight matrix itself. The specification of any `INWGT=` data set for unweighted least squares or maximum likelihood estimation is ignored. For generalized and diagonally weighted least squares estimation, the `INWGT=` data set must contain a `_TYPE_` and a `_NAME_` variable as well as the manifest variables used in the analysis. The value of the `_NAME_` variable indicates the row index i of the weight w_{ij} . For weighted least squares, the `INWGT=` data set must contain `_TYPE_`, `_NAME_`, `_NAM2_`, and `_NAM3_` variables as well as the manifest variables used in the analysis. The values of the `_NAME_`, `_NAM2_`, and `_NAM3_` variables indicate the three indices i, j, k of the weight $w_{ij,kl}$. You can store information other than the weight matrix in the `INWGT=` data set, but only observations with `_TYPE_=WEIGHT` are used to specify the weight matrix \mathbf{W} . This property enables you to store more than one weight matrix in the `INWGT=` data set. You can then run PROC CALIS with each of the weight matrices by changing only the `_TYPE_` observation in the `INWGT=` data set with an intermediate DATA step.

See the section “`OUTWGT=` Data Set” on page 1254 for more details about the `INWGT=` data set.

Output Data Sets

OUTEST= Data Set

The `OUTEST=` (or `OUTVAR=`) data set is of `TYPE=EST` and contains the final parameter estimates, the gradient, the Hessian, and boundary and linear constraints. For `METHOD=ML`, `METHOD=GLS`, and `METHOD=WLS`, the `OUTEST=` data set also contains the approximate standard errors, the information matrix (crossproduct Jacobian), and the approximate covariance matrix of the parameter estimates ((generalized) inverse of the information matrix). If there are linear or nonlinear equality or active inequality constraints at the solution, the `OUTEST=` data set also contains Lagrange multipliers, the projected Hessian matrix, and the Hessian matrix of the Lagrange function.

The `OUTEST=` data set can be used to save the results of an optimization by PROC CALIS for another analysis with either PROC CALIS or another SAS procedure. Saving results to an `OUTEST=` data set is advised for expensive applications that cannot be repeated without considerable effort.

The `OUTEST=` data set contains the BY variables, two character variables `_TYPE_` and `_NAME_`, t numeric variables corresponding to the parameters used in the model, a numeric variable `_RHS_` (right-hand side) that is used for the right-hand-side value b_i of a linear constraint or for the value $f = f(x)$ of the objective function at the final point x^* of the parameter space, and a numeric variable `_ITER_` that is set to zero for initial values, set to the iteration number for the `OUTITER` output, and set to missing for the result output.

The `_TYPE_` observations in Table 27.5 are available in the `OUTEST=` data set, depending on the request.

Table 27.5 `_TYPE_` Observations in the `OUTEST=` Data Set

<code>_TYPE_</code>	Description								
ACTBC	If there are active boundary constraints at the solution x^* , three observations indicate which of the parameters are actively constrained, as follows: <table border="1" data-bbox="537 1255 1102 1432"> <thead> <tr> <th><code>_NAME_</code></th> <th>Description</th> </tr> </thead> <tbody> <tr> <td>GE</td> <td>indicates the active lower bounds</td> </tr> <tr> <td>LE</td> <td>indicates the active upper bounds</td> </tr> <tr> <td>EQ</td> <td>indicates the active masks</td> </tr> </tbody> </table>	<code>_NAME_</code>	Description	GE	indicates the active lower bounds	LE	indicates the active upper bounds	EQ	indicates the active masks
<code>_NAME_</code>	Description								
GE	indicates the active lower bounds								
LE	indicates the active upper bounds								
EQ	indicates the active masks								
COV	Contains the approximate covariance matrix of the parameter estimates; used in computing the approximate standard errors.								
COVRANK	contains the rank of the covariance matrix of the parameter estimates.								
CRPJ_LF	Contains the Hessian matrix of the Lagrange function (based on <code>CRPJAC</code>).								
CRPJAC	Contains the approximate Hessian matrix used in the optimization process. This is the inverse of the information matrix.								

Table 27.5 continued

TYPE	Description										
EQ	If linear constraints are used, this observation contains the i th linear constraint $\sum_j a_{ij}x_j = b_i$. The parameter variables contain the coefficients a_{ij} , $j = 1, \dots, n$, the _RHS_ variable contains b_i , and _NAME_=ACTLC or _NAME_=LDACTLC .										
GE	If linear constraints are used, this observation contains the i th linear constraint $\sum_j a_{ij}x_j \geq b_i$. The parameter variables contain the coefficients a_{ij} , $j = 1, \dots, n$, and the _RHS_ variable contains b_i . If the constraint i is active at the solution x^* , then _NAME_=ACTLC or _NAME_=LDACTLC .										
GRAD	Contains the gradient of the estimates.										
GRAD_LF	Contains the gradient of the Lagrange function. The _RHS_ variable contains the value of the Lagrange function.										
HESSIAN	Contains the Hessian matrix.										
HESS_LF	Contains the Hessian matrix of the Lagrange function (based on HESSIAN).										
INFORMAT	Contains the information matrix of the parameter estimates (only for METHOD=ML , METHOD=GLS , or METHOD=WLS).										
INITGRAD	Contains the gradient of the starting estimates.										
INITIAL	Contains the starting values of the parameter estimates.										
JACNLC	Contains the Jacobian of the nonlinear constraints evaluated at the final estimates.										
LAGM BC	Contains Lagrange multipliers for masks and active boundary constraints.										
<table border="1"> <thead> <tr> <th>_NAME_</th> <th>Description</th> </tr> </thead> <tbody> <tr> <td>GE</td> <td>Indicates the active lower bounds</td> </tr> <tr> <td>LE</td> <td>Indicates the active upper bounds</td> </tr> <tr> <td>EQ</td> <td>Indicates the active masks</td> </tr> </tbody> </table>		_NAME_	Description	GE	Indicates the active lower bounds	LE	Indicates the active upper bounds	EQ	Indicates the active masks		
NAME	Description										
GE	Indicates the active lower bounds										
LE	Indicates the active upper bounds										
EQ	Indicates the active masks										
LAGM LC	Contains Lagrange multipliers for linear equality and active inequality constraints in pairs of observations containing the constraint number and the value of the Lagrange multiplier.										
<table border="1"> <thead> <tr> <th>_NAME_</th> <th>Description</th> </tr> </thead> <tbody> <tr> <td>LEC_NUM</td> <td>Number of the linear equality constraint</td> </tr> <tr> <td>LEC_VAL</td> <td>Corresponding Lagrange multiplier value</td> </tr> <tr> <td>LIC_NUM</td> <td>Number of the linear inequality constraint</td> </tr> <tr> <td>LIC_VAL</td> <td>Corresponding Lagrange multiplier value</td> </tr> </tbody> </table>		_NAME_	Description	LEC_NUM	Number of the linear equality constraint	LEC_VAL	Corresponding Lagrange multiplier value	LIC_NUM	Number of the linear inequality constraint	LIC_VAL	Corresponding Lagrange multiplier value
NAME	Description										
LEC_NUM	Number of the linear equality constraint										
LEC_VAL	Corresponding Lagrange multiplier value										
LIC_NUM	Number of the linear inequality constraint										
LIC_VAL	Corresponding Lagrange multiplier value										

Table 27.5 continued

TYPE	Description										
LAGM NLC	contains Lagrange multipliers for nonlinear equality and active inequality constraints in pairs of observations that contain the constraint number and the value of the Lagrange multiplier.										
	<table border="1"> <thead> <tr> <th>_NAME_</th> <th>Description</th> </tr> </thead> <tbody> <tr> <td>NLEC_NUM</td> <td>Number of the nonlinear equality constraint</td> </tr> <tr> <td>NLEC_VAL</td> <td>Corresponding Lagrange multiplier value</td> </tr> <tr> <td>NLIC_NUM</td> <td>Number of the linear inequality constraint</td> </tr> <tr> <td>NLIC_VAL</td> <td>Corresponding Lagrange multiplier value</td> </tr> </tbody> </table>	_NAME_	Description	NLEC_NUM	Number of the nonlinear equality constraint	NLEC_VAL	Corresponding Lagrange multiplier value	NLIC_NUM	Number of the linear inequality constraint	NLIC_VAL	Corresponding Lagrange multiplier value
NAME	Description										
NLEC_NUM	Number of the nonlinear equality constraint										
NLEC_VAL	Corresponding Lagrange multiplier value										
NLIC_NUM	Number of the linear inequality constraint										
NLIC_VAL	Corresponding Lagrange multiplier value										
LE	If linear constraints are used, this observation contains the i th linear constraint $\sum_j a_{ij}x_j \leq b_i$. The parameter variables contain the coefficients a_{ij} , $j = 1, \dots, n$, and the _RHS_ variable contains b_i . If the constraint i is active at the solution x^* , then _NAME_ =ACTLC or _NAME_ =LDACTLC.										
LOWERBD LB	If boundary constraints are used, this observation contains the lower bounds. Those parameters not subjected to lower bounds contain missing values. The _RHS_ variable contains a missing value, and the _NAME_ variable is blank.										
NACTBC	All parameter variables contain the number n_{abc} of active boundary constraints at the solution x^* . The _RHS_ variable contains a missing value, and the _NAME_ variable is blank.										
NACTLC	All parameter variables contain the number n_{alc} of active linear constraints at the solution x^* that are recognized as linearly independent. The _RHS_ variable contains a missing value, and the _NAME_ variable is blank.										
NLC_EQ NLC_GE NLC_LE	Contains values and residuals of nonlinear constraints. The _NAME_ variable is described as follows: <table border="1"> <thead> <tr> <th>_NAME_</th> <th>Description</th> </tr> </thead> <tbody> <tr> <td>NLC</td> <td>Inactive nonlinear constraint</td> </tr> <tr> <td>NLCACT</td> <td>Linear independent active nonlinear constraint</td> </tr> <tr> <td>NLCACTLD</td> <td>Linear dependent active nonlinear constraint</td> </tr> </tbody> </table>	_NAME_	Description	NLC	Inactive nonlinear constraint	NLCACT	Linear independent active nonlinear constraint	NLCACTLD	Linear dependent active nonlinear constraint		
NAME	Description										
NLC	Inactive nonlinear constraint										
NLCACT	Linear independent active nonlinear constraint										
NLCACTLD	Linear dependent active nonlinear constraint										
NLDACTBC	Contains the number of active boundary constraints at the solution x^* that are recognized as linearly dependent. The _RHS_ variable contains a missing value, and the _NAME_ variable is blank.										

Table 27.5 continued

TYPE	Description
NLDACTLC	Contains the number of active linear constraints at the solution x^* that are recognized as linearly dependent. The _RHS_ variable contains a missing value, and the _NAME_ variable is blank.
NOBS	Contains the number of observations.
PARMS	Contains the final parameter estimates. The _RHS_ variable contains the value of the objective function.
PCRPJ_LF	Contains the projected Hessian matrix of the Lagrange function (based on CRPJAC).
PHESS_LF	Contains the projected Hessian matrix of the Lagrange function (based on HESSIAN).
PROJCRPJ	Contains the projected Hessian matrix (based on CRPJAC).
PROJGRAD	If linear constraints are used in the estimation, this observation contains the $n - n_{act}$ values of the projected gradient $\mathbf{g}_z = \mathbf{Z}'\mathbf{g}$ in the variables corresponding to the first $n - n_{act}$ parameters. The _RHS_ variable contains a missing value, and the _NAME_ variable is blank.
PROJHESS	Contains the projected Hessian matrix (based on HESSIAN).
STDERR	Contains approximate standard errors (only for METHOD=ML , METHOD=GLS , or METHOD=WLS).
TERMINAT	The _NAME_ variable contains the name of the termination criterion.
UPPERBD UB	If boundary constraints are used, this observation contains the upper bounds. Those parameters not subjected to upper bounds contain missing values. The _RHS_ variable contains a missing value, and the _NAME_ variable is blank.

If the technique specified by the **OMETHOD=** option cannot be performed (for example, no feasible initial values can be computed or the function value or derivatives cannot be evaluated at the starting point), the **OUTEST=** data set can contain only some of the observations (usually only the **PARMS** and **GRAD** observations).

OUTMODEL= or OUTRAM= Data Set

The **OUTMODEL=** (or **OUTRAM=**) data set is of **TYPE=CALISMDL** and contains the model specification, the computed parameter estimates, and the standard error estimates. This data set is intended to be reused as an **INMODEL=** data set to specify good initial values in a subsequent analysis by **PROC CALIS**.

The **OUTMODEL=** data set contains the following variables:

- the **BY** variables, if any

- an `_MDLNUM_` variable for model numbers, if used
- a character variable `_TYPE_`, which takes various values that indicate the type of model specification
- a character variable `_NAME_`, which indicates the model type, parameter name, or variable name
- a character variable `_MATNR_`, which indicates the matrix number (COSAN models only)
- a character variable `_VAR1_`, which is the name or number of the first variable in the specification
- a character variable `_VAR2_`, which is the name or number of the second variable in the specification
- a numerical variable `_ESTIM_` for the final estimate of the parameter location
- a numerical variable `_STDERR_` for the standard error estimate of the parameter location
- a numerical variable `_SDEST_` for the final standardized estimate of the parameter location
- a numerical variable `_SDSE_` for the standard error of the standardized estimate of the parameter location

Although the `_SDEST_` and `_SDSE_` variables are created for COSAN models, the values for these two variables are always missing because there are no rules to carry out the standardization of COSAN models.

Each observation (record) of the `OUTMODEL=` data set contains a piece of information regarding the model specification. Depending on the type of the specification indicated by the value of the `_TYPE_` variable, the meanings of `_NAME_`, `_VAR1_`, and `_VAR2_` differ. The following tables summarize the meanings of the `_NAME_`, `_MATNR_` (COSAN models only), `_VAR1_`, and `_VAR2_` variables for each value of the `_TYPE_` variable, given the type of the model.

COSAN Models

<code>_TYPE_</code>	Description	<code>_NAME_</code>	<code>_MATNR_</code>	<code>_VAR1_</code>	<code>_VAR2_</code>
MDLTYPE	Model type	COSAN			
VAR	Variable	Variable name	Matrix number	Column location	
MATRIX	Matrix	Matrix name	Matrix number	Number of rows	Number of columns
MODEL	Model formula	COV or MEAN	Matrix number	Term number	Location in term
ESTIM	Parameters	Parameter name	Matrix number	Row number	Column number

The value of the `_NAME_` variable is COSAN for the `_TYPE_=MDLTYPE` observation.

The `_TYPE_=VAR` observations store the information about the column variables in matrices. The `_NAME_` variable stores the variable names. The value of `_VAR1_` indicates the column location of the variable in the matrix with the matrix number stored in `_MATNR_`.

The `_TYPE_=MATRIX` observations store the information about the model matrices. The `_NAME_` variable stores the matrix names. The value of `_MATNR_` indicates the corresponding matrix number. The values of `_VAR1_` and `_VAR2_` indicates the numbers of rows and columns, respectively, of the matrix.

The `_TYPE_=MODEL` observations store the covariance and mean structure formulas. The `_NAME_` variable indicates whether the mean (MEAN) or covariance (COV) structure information is stored. The value of `_MATNR_` indicates the matrix number in the mean or covariance structure formula. The `_VAR1_` variable indicates the term number, and the `_VAR2_` variable indicates the location of the matrix in the term.

The `_TYPE_=ESTIM` observations store the information about the parameters and their estimates. The `_NAME_` variable stores the parameter names. The value of `_MATNR_` indicates the matrix number. The values of `_VAR1_` and `_VAR2_` indicate the associated row and column numbers, respectively, of the parameter.

FACTOR Models

<code>_TYPE_</code>	Description	<code>_NAME_</code>	<code>_VAR1_</code>	<code>_VAR2_</code>
MDLTYPE	Model type	Model type		
FACTVAR	Variable	Variable name	Variable number	Variable type
LOADING	Factor loading	Parameter name	Manifest variable	Factor variable
COV	Covariance	Parameter name	First variable	Second variable
PVAR	(Partial) variance	Parameter name	Variable	
MEAN	Mean or intercept	Parameter name	Variable	
ADDCOV	Added covariance	Parameter name	First variable	Second variable
ADDPVAR	Added (partial) variance	Parameter name	Variable	
ADDMEAN	Added mean or intercept	Parameter name	Variable	

For factor models, the value of the `_NAME_` variable is either EFACOR (exploratory factor model) or CFACOR (confirmatory factor model) for the `_TYPE_=MDLTYPE` observation.

The `_TYPE_=FACTVAR` observations store the information about the variables in the model. The `_NAME_` variable stores the variable names. The value of `_VAR1_` indicates the variable number. The value of `_VAR2_` indicates the type of the variable: either DEPV for dependent observed variables or INDF for latent factors.

Other observations specify the parameters and their estimates in the model. The `_NAME_` values for these observations are the parameter names. Observation with `_TYPE_=LOADING`, `_TYPE_=COV`, or `_TYPE_=ADDCOV` are for parameters that are associated with two variables. The `_VAR1_` and `_VAR2_` values of these two types of observations indicate the variables involved.

Observations with `_TYPE_=PVAR`, `_TYPE_=MEAN`, `_TYPE_=ADDPVAR`, or `_TYPE_=ADDMEAN` are for parameters that are associated with a single variable. The value of `_VAR1_` indicates the variable involved.

LINEQS Models

<code>_TYPE_</code>	Description	<code>_NAME_</code>	<code>_VAR1_</code>	<code>_VAR2_</code>
MDLTYPE	Model type	LINEQS		
EQSVAR	Variable	Variable name	Variable number	Variable type
EQUATION	Path coefficient	Parameter	Outcome variable	Predictor variable
COV	Covariance	Parameter	First variable	Second variable
VARIANCE	Variance	Parameter	Variable	
MEAN	Mean	Parameter	Variable	
ADDCOV	Added covariance	Parameter	First variable	Second variable
ADDVARIA	Added variance	Parameter	Variable	
ADDINTE	Added intercept	Parameter	Variable	
ADDMEAN	Added mean	Parameter	Variable	

The value of the `_NAME_` variable is `LINEQS` for the `_TYPE_=MDLTYPE` observation.

The `_TYPE_=EQSVAR` observations store the information about the variables in the model. The `_NAME_` variable stores the variable names. The value of `_VAR1_` indicates the variable number. The value of `_VAR2_` indicates the type of the variable. There are six types of variables in the `LINEQS` model:

- `DEPV` for dependent observed variables
- `INDV` for independent observed variables
- `DEPF` for dependent latent factors
- `INDF` for independent latent factors
- `INDD` for independent error terms
- `INDE` for independent disturbance terms

Other observations specify the parameters and their estimates in the model. The `_NAME_` values for these observations are the parameter names. Observation with `_TYPE_=EQUATION`, `_TYPE_=COV`, or `_TYPE_=ADDCOV` are for parameters that are associated with two variables. The `_VAR1_` and `_VAR2_` values of these two types of observations indicate the variables involved.

Observations with `_TYPE_=VARIANCE`, `_TYPE_=MEAN`, `_TYPE_=ADDVARIA`, `_TYPE_=ADDINTE`, or `_TYPE_=ADDMEAN` are for parameters associated with a single variable. The value of `_VAR1_` indicates the variable involved.

LISMOD Models

TYPE	Description	_NAME_	_VAR1_	_VAR2_
MDLTYPE	model type	LISMOD		
XVAR	x-variable	Variable	Variable number	
YVAR	y-variable	Variable	Variable number	
ETAVAR	η -variable	Variable	Variable number	
XIVAR	ξ -variable	Variable	Variable number	
ALPHA	_ALPHA_ entry	Parameter	Row number	
BETA	_BETA_ entry	Parameter	Row number	Column number
GAMMA	_BETA_ entry	Parameter	Row number	Column number
KAPPA	_KAPPA_ entry	Parameter	Row number	
LAMBDAX	_LAMBDAX_ entry	Parameter	Row number	Column number
LAMBDAY	_LAMBDAY_ entry	Parameter	Row number	Column number
NUX	_NUX_ entry	Parameter	Row number	
NUY	_NUY_ entry	Parameter	Row number	
PHI	_PHI_ entry	Parameter	Row number	Column number
PSI	_PSI_ entry	Parameter	Row number	Column number
THETAX	_THETAX_ entry	Parameter	Row number	Column number
THETAY	_THETAY_ entry	Parameter	Row number	Column number
ADDALPHA	Added _ALPHA_ entry	Parameter	Row number	
ADDKAPPA	Added _KAPPA_ entry	Parameter	Row number	
ADDNUX	Added _NUX_ entry	Parameter	Row number	
ADDNUY	Added _NUY_ entry	Parameter	Row number	
ADDPHI	Added _PHI_ entry	Parameter	Row number	Column number
ADDPSI	Added _PSI_ entry	Parameter	Row number	Column number
ADTHETAX	Added _THETAX_ entry	Parameter	Row number	Column number
ADTHETAY	Added _THETAY_ entry	Parameter	Row number	Column number

The value of the `_NAME_` variable is LISMOD for the `_TYPE_=MDLTYPE` observation. Other observations specify either the variables or the parameters in the model.

Observations with `_TYPE_` values equal to XVAR, YVAR, ETAVAR, and XIVAR indicate the variables in the respective lists in the model. The `_NAME_` variable of these observations stores the names of the variables, and the `_VAR1_` variable stores the variable numbers in the respective list. The variable numbers in this data set are not arbitrary—that is, they define the variable orders in the rows and columns of the LISMOD model matrices. The `_VAR2_` variable of these observations is not used.

All other observations in this data set specify the parameters in the model. The `_NAME_` values of these observations are the parameter names. The corresponding `_VAR1_` and `_VAR2_` values of these observations indicate the row and column locations of the parameters in the LISMOD model matrices that are specified in the `_TYPE_` variable. For example, when the value of `_TYPE_` is ADDPHI or PHI, the parameter specified is located in the `_PHI_` matrix, with its row and column numbers indicated by the `_VAR1_` and `_VAR2_` values, respectively. Some observations for specifying parameters do not have values in the `_VAR2_` variable. This means that the associated LISMOD matrices are vectors so that the column numbers are always 1 for these observations.

MSTRUCT Models

TYPE	Description	_NAME_	_VAR1_	_VAR2_
MDLTYPE	Model type	MSTRUCT		
VAR	Variable	Variable	Variable number	
COVMAT	Covariance	Parameter	Row number	Column number
MEANVEC	Mean	Parameter	Row number	
ADCOVMAT	Added covariance	Parameter	Row number	Column number
AMEANVEC	Added mean	Parameter	Row number	

The value of the `_NAME_` variable is MSTRUCT for the `_TYPE_=MDLTYPE` observation. Other observations specify either the variables or the parameters in the model.

Observations with `_TYPE_` values equal to VAR indicate the variables in the model. The `_NAME_` variable of these observations stores the names of the variables, and the `_VAR1_` variable stores the variable numbers in the variable list. The variable numbers in this data set are not arbitrary—that is, they define the variable orders in the rows and columns of the mean and covariance matrices. The `_VAR2_` variable of these observations is not used.

All other observations in this data set specify the parameters in the model. The `_NAME_` values of these observations are the parameter names. The corresponding `_VAR1_` and `_VAR2_` values of these observations indicate the row and column locations of the parameters in the mean or covariance matrix, as specified in the `_TYPE_` model. For example, when `_TYPE_=COVMAT`, the parameter specified is located in the covariance matrix, with its row and column numbers indicated by the `_VAR1_` and `_VAR2_` values, respectively. For observations with `_TYPE_=MEANVEC`, the `_VAR2_` variable is not used because the column numbers are always 1 for parameters in the mean vector.

PATH Models

TYPE	Description	_NAME_	_VAR1_	_VAR2_
MDLTYPE	Model type	PATH		
PATHVAR	Variable	Variable name	Variable number	Variable type
LEFT	Path coefficient	Parameter	Outcome variable	Predictor variable
RIGHT	Path coefficient	Parameter	Predictor variable	Outcome variable
PCOV	(Partial) covariance	Parameter	First variable	Second variable
PCOVPATH	(Partial) covariance path	Parameter	First variable	Second variable
PVAR	(Partial) variance	Parameter	Variable	
PVARPATH	(Partial) variance path	Parameter	Variable	Variable
MEAN	Mean or intercept	Parameter	Variable	
ONEPATH	Mean or intercept path	Parameter	<code>_ONE_</code>	Variable
ADDPcov	Added (partial) covariance	Parameter	First variable	Second variable
ADDPVAR	Added (partial) variance	Parameter	Variable	
ADDMEAN	Added mean	Parameter	Variable	

The value of the `_NAME_` variable is PATH for the `_TYPE_=MDLTYPE` observation.

The `_TYPE_=PATHVAR` observations store the information about the variables in the model. The `_NAME_` variable stores the variable names. The value of `_VAR1_` indicates the variable number. The value of `_VAR2_` indicates the type of the variable. There are four types of variables in the PATH model:

- DEPV for dependent observed variables

- INDV for independent observed variables
- DEPF for dependent latent factors
- INDF for independent latent factors

Other observations specify the parameters in the model. The `_NAME_` values for these observations are the parameter names. Observation with `_TYPE_=LEFT`, `_TYPE_=RIGHT`, `_TYPE_=PCOV`, or `_TYPE_=ADDP` are for parameters that are associated with two variables. The `_VAR1_` and `_VAR2_` values of these two types of observations indicate the variables involved.

Observations with `_TYPE_=PVAR`, `_TYPE_=MEAN`, `_TYPE_=ADDPVAR`, or `_TYPE_=ADDMEAN` are for parameters that are associated with a single variable. The value of `_VAR1_` indicates the variable involved.

RAM Models

<code>_TYPE_</code>	Description	<code>_NAME_</code>	<code>_VAR1_</code>	<code>_VAR2_</code>
MDLTYPE	Model type	RAM		
RAMVAR	Variable name	Variable	Variable number	Variable type
<code>_A_</code>	<code>_A_</code> entry	Parameter	Row number	Column number
<code>_P_</code>	<code>_P_</code> entry	Parameter	Row number	Column number
<code>_W_</code>	<code>_W_</code> entry	Parameter	Row number	Column number
ADD_P_	Added <code>_P_</code> entry	Parameter	Row number	Column number
ADD_W_	Added <code>_W_</code> entry	Parameter	Row number	Column number

The value of the `_NAME_` variable is RAM for the `_TYPE_=MDLTYPE` observation.

For the `_TYPE_=RAMVAR` observations, the `_NAME_` variable stores the variable names, the `_VAR1_` variable stores the variable number, and the `_VAR2_` variable stores the variable type. There are four types of variables in the PATH model:

- DEPV for dependent observed variables
- INDV for independent observed variables
- DEPF for dependent latent factors
- INDF for independent latent factors

Other observations specify the parameters in the model. The `_NAME_` variable stores the parameter name. The `_TYPE_` variable indicates the associated matrix with the row number indicated in `_VAR1_` and column number indicated in `_VAR2_`.

Reading an OUTMODEL= Data Set As an INMODEL= Data Set in Subsequent Analyses

When the `OUTMODEL=` data set is treated as an `INMODEL=` data set in subsequent analyses, you need to pay attention to observations with `_TYPE_` values prefixed by “ADD”, “AD”, or “A” (for example, `ADDCOV`, `ADTHETAY`, or `AMEANVEC`). These observations represent default parameter locations that are generated by PROC CALIS in a previous run. Because the context of the new analyses might be different, these observations for added parameter locations might no longer be suitable in the new runs. Hence, these observations are *not* read as input model information. Fortunately, after reading the `INMODEL=` specification in the new

analyses, CALIS analyzes the new model specification again. It then adds an appropriate set of parameters in the new context when necessary. If you are certain that the added parameter locations in the INMODEL= data set are applicable, you can force the input of these observations by using the `READADDPARM` option in the PROC CALIS statement. However, you must be very careful about using the `READADDPARM` option. The added parameters from the INMODEL= data set might have the same parameter names as those for the generated parameters in the new run. This might lead to unnecessary constraints in the model.

OUTSTAT= Data Set

The `OUTSTAT=` data set is similar to the `TYPE=COV`, `TYPE=UCOV`, `TYPE=CORR`, or `TYPE=UCORR` data set produced by the CORR procedure. The `OUTSTAT=` data set contains the following variables:

- the BY variables, if any
- the `_GPNUM_` variable for groups numbers, if used in the analysis
- two character variables, `_TYPE_` and `_NAME_`
- the manifest and the latent variables analyzed

The `OUTSTAT=` data set contains the following information (when available) in the observations:

- the mean and standard deviation
- the skewness and kurtosis (if the `DATA=` data set is a raw data set and the `KURTOSIS` option is specified)
- the number of observations
- if the `WEIGHT` statement is used, sum of the weights
- the correlation or covariance matrix to be analyzed
- the robust covariances, standard deviations, and means for robust estimation
- the predicted correlation or covariance matrix
- the standardized or normalized residual correlation or covariance matrix
- if the model contains latent variables, the predicted covariances between latent and manifest variables and the latent variable (or factor) score regression coefficients (see the `PLATCOV` option on page 1112)

In addition, for FACTOR models the `OUTSTAT=` data set contains:

- the unrotated factor loadings, the error variances, and the matrix of factor correlations
- the standardized factor loadings and factor correlations
- the rotation matrix, rotated factor loadings, and factor correlations

- standardized rotated factor loadings and factor correlations

If effects are analyzed, the `OUTSTAT=` data set also contains:

- direct, indirect, and total effects and their standard error estimates
- standardized direct, indirect, and total effects and their standard error estimates

Each observation in the `OUTSTAT=` data set contains some type of statistic as indicated by the `_TYPE_` variable. The values of the `_TYPE_` variable are shown in the following tables:

Basic Descriptive Statistics

Value of <code>_TYPE_</code>	Contents
ADJCOV	Adjusted covariances
ADJSTD	Adjusted standard deviations
CORR	Correlations
COV	Covariances
KURTOSIS	Univariate kurtosis
MEAN	Means
N	Sample size
NPARTIAL	Number of partial variables
PARTCOV	Covariances after partialling
PARTCORR	Correlations after partialling
PARTMEAN	Means after partialling
PARTSTD	Standard deviations after partialling
ROBCOV	Robust covariances
ROBMEAN	Robust means
ROBSTD	Robust standard deviations
SKEWNESS	Univariate skewness
STD	Standard deviations
SUMWGT	Sum of weights (if the <code>WEIGHT</code> statement is used)
VARDIV	Variance divisor
VARDIVAJ	Variance divisor adjustment

For the `_TYPE_=CORR` or `COV` observations, the `_NAME_` variable contains the name of the manifest variable that corresponds to each row for the covariance or correlation. For other observations, `_NAME_` is blank.

Predicted Moments and Residuals

value of <code>_TYPE_</code>	Contents
METHOD=DWLS	
DWLSPRED	DWLS predicted moments
DWLSRES	DWLS raw residuals
DWLSRES	DWLS variance standardized residuals
METHOD=GLS	
GLSASRES	GLS asymptotically standardized residuals
GLSNRES	GLS normalized residuals
GLSPRED	GLS predicted moments
GLSRES	GLS raw residuals
GLSSRES	GLS variance standardized residuals
METHOD=ML or FIML	
MAXASRES	ML asymptotically standardized residuals
MAXNRES	ML normalized residuals
MAXPRED	ML predicted moments
MAXRES	ML raw residuals
MAXSRES	ML variance standardized residuals
METHOD=ULS	
ULSPRED	ULS predicted moments
ULSRES	ULS raw residuals
ULSSRES	ULS variance standardized residuals
METHOD=WLS	
WLSASRES	WLS asymptotically standardized residuals
WLSNRES	WLS normalized residuals
WLSPRED	WLS predicted moments
WLSRES	WLS raw residuals
WLSRES	WLS variance standardized residuals

For residuals or predicted moments of means, the `_NAME_` variable is a fixed value denoted by `_Mean_`. For residuals or predicted moments for covariances or correlations, the `_NAME_` variable is used for names of variables.

Effects and Latent Variable Scores Regression Coefficients

Value of _TYPE_	Contents
Unstandardized Effects	
DEFFECT	Direct effects
DEFF_SE	Standard error estimates for direct effects
IEFFECT	Indirect effects
IEFF_SE	Standard error estimates for indirect effects
TEFFECT	Total effects
TEFF_SE	Standard error estimates for total effects
Standardized Effects	
SDEFF	Standardized direct effects
SDEFF_SE	Standard error estimates for standardized direct effects
SIEFF	Standardized indirect effects
SIEFF_SE	Standard error estimates for standardized indirect effects
STEFF	Standardized total effects
STEFF_SE	Standard error estimates for standardized total effects
Latent Variable Scores Coefficients	
LSSCORE	Latent variable (or factor) scores regression coefficients for ULS method
SCORE	Latent variable (or factor) scores regression coefficients other than ULS method

For latent variable or factor scores coefficients, the **_NAME_** variable contains factor or latent variables in the observations. For other observations, the **_NAME_** variable contains manifest or latent variable names.

You can use the latent variable score regression coefficients with PROC SCORE to compute factor scores. If the analyzed matrix is a covariance rather than a correlation matrix, the **_TYPE_=STD** observation is not included in the **OUTSTAT=** data set. In this case, the standard deviations can be obtained from the diagonal elements of the covariance matrix. Dropping the **_TYPE_=STD** observation prevents PROC SCORE from standardizing the observations before computing the factor scores.

Factor Analysis Results

Value of _TYPE_	Contents
ERRVAR	Error variances
FCOV	Factor correlations or covariances
LOADINGS	Unrotated factor loadings
RFCOV	Rotated factor correlations or covariances
RLOADING	Rotated factor loadings
ROTMAT	Rotation matrix
STDFCOV	Standardized factor correlations
STDLOAD	Standardized factor loadings
STDRFCOV	Standardized rotated factor correlations or covariances
STDRLOAD	Standardized rotated factor loadings

For the **_TYPE_=ERRVAR** observation, the **_NAME_** variable is blank. For all other observations, the **_NAME_** variable contains factor names.

OUTWGT= Data Set

You can create an **OUTWGT=** data set that is of **TYPE=WEIGHT** and contains the weight matrix used in generalized, weighted, or diagonally weighted least squares estimation. The **OUTWGT=** data set contains the weight matrix on which the **WRIDGE=** and the **WPENALTY=** options are applied. However, if you input the inverse of the weight matrix with the **INWGT=** and **INWGTINV** options (or the **INWGT(INV)=** option alone) in the same analysis, the **OUTWGT=** data set contains the same elements of the inverse of the weight matrix. For unweighted least squares or maximum likelihood estimation, no **OUTWGT=** data set can be written. The weight matrix used in maximum likelihood estimation is dynamically updated during optimization. When the ML solution converges, the final weight matrix is the same as the predicted covariance or correlation matrix, which is included in the **OUTSTAT=** data set (observations with **_TYPE_=MAXPRED**).

For generalized and diagonally weighted least squares estimation, the weight matrices **W** of the **OUTWGT=** data set contain all elements w_{ij} , where the indices i and j correspond to all manifest variables used in the analysis. Let $varnam_i$ be the name of the i th variable in the analysis. In this case, the **OUTWGT=** data set contains n observations with the variables shown in the following table:

Variable	Contents
TYPE	WEIGHT (character)
NAME	Name of variable $varnam_i$ (character)
$varnam_1$	Weight w_{i1} for variable $varnam_1$ (numeric)
⋮	⋮
$varnam_n$	Weight w_{in} for variable $varnam_n$ (numeric)

For weighted least squares estimation, the weight matrix **W** of the **OUTWGT=** data set contains only the nonredundant elements $w_{ij,kl}$. In this case, the **OUTWGT=** data set contains $n(n+1)(2n+1)/6$ observations with the variables shown in the following table:

Variable	Contents
TYPE	WEIGHT (character)
NAME	Name of variable $varnam_i$ (character)
NAM2	Name of variable $varnam_j$ (character)
NAM3	Name of variable $varnam_k$ (character)
$varnam_1$	Weight $w_{ij,k1}$ for variable $varnam_1$ (numeric)
⋮	⋮
$varnam_n$	Weight $w_{ij,kn}$ for variable $varnam_n$ (numeric)

Symmetric redundant elements are set to missing values.

OUTFIT= Data Set

You can create an **OUTFIT=** data set that is of **TYPE=CALISFIT** and that contains the values of the fit indices of your analysis. If you use two estimation methods such as LSML or LSWLS, the fit indices are for the second analysis. An **OUTFIT=** data set contains the following variables:

- a character variable **_TYPE_** for the types of fit indices
- a numerical variable **IndexCode** for the codes of the fit indices

- a character variable `FitIndex` for the names of the fit indices
- a numerical variable `FitValue` for the numerical values of the fit indices
- a character variable `PrintChar` for the character-formatted fit index values.

The possible values of `_TYPE_` are:

ModelInfo: basic modeling statistics and information
 Absolute: stand-alone fit indices
 Parsimony: fit indices that take model parsimony into account
 Incremental: fit indices that are based on comparison with a baseline model

Possible Values of FitIndex When _TYPE_=ModelInfo

Value of FitIndex	Description
Number of Observations	Number of observations used in the analysis
Number of Complete Observations	Number of complete observations (METHOD=FIML)
Number of Incomplete Observations	Number of incomplete observations (METHOD=FIML)
Number of Variables	Number of variables
Number of Moments	Number of mean or covariance elements
Number of Parameters	Number of parameters
Number of Active Constraints	Number of active constraints in the solution
Saturated Model Estimation	Estimation status of the saturated model (METHOD=FIML)
Saturated Model Function Value	Saturated model function value (METHOD=FIML)
Saturated Model -2 Log-Likelihood	Saturated model -2 log-likelihood function value (METHOD=FIML)
Baseline Model Estimation	Estimation status of the baseline model (METHOD=FIML)
Baseline Model Function Value	Baseline model function value
Baseline Model -2 Log-Likelihood	Baseline model -2 log-likelihood function value (METHOD=FIML)
Baseline Model Chi-Square	Baseline model chi-square value
Baseline Model Chi-Square DF	Baseline model chi-square degrees of freedom
Baseline Model DF	Baseline model degrees of freedom (METHOD=ULS or METHOD=DWLS)
Pr > Baseline Model Chi-Square	<i>p</i> value of the baseline model chi-square

Possible Values of FitIndex When *_TYPE_*=Absolute

Value of FitIndex	Description
Fit Function	Fit function value
-2 Log-Likelihood	-2 log-likelihood function value for the model (METHOD=FIML)
Chi-Square	Model chi-square value
Chi-Square DF	Degrees of freedom for the model chi-square test
Model DF	Degrees of freedom for model (METHOD=ULS or METHOD=DWLS)
Pr > Chi-Square	Probability of obtaining a larger chi-square than the observed value
Percent Contribution to Chi-Square	Percentage contribution to the chi-square value
Percent Contribution to Likelihood	Percentage contribution to the -2 log-likelihood function value (METHOD=FIML)
Elliptic Corrected Chi-Square	Elliptic-corrected chi-square value
Pr > Elliptic Corr. Chi-Square	Probability of obtaining a larger elliptic-corrected chi-square value
Z-test of Wilson and Hilferty	Z-test of Wilson and Hilferty
Hoelter Critical N	N value that makes a significant chi-square when multiplied to the fit function value
Root Mean Square Residual (RMR)	Root mean square residual
Standardized RMR (SRMR)	Standardized root mean square residual
Goodness of Fit Index (GFI)	Jöreskog and Sörbom goodness-of-fit index

Possible Values of FitIndex When *_TYPE_*=Parsimony

Value of FitIndex	Description
Adjusted GFI (AGFI)	Goodness-of-fit index adjusted for the degrees of freedom of the model
Parsimonious GFI	Mulaik et al. (1989) modification of the GFI
RMSEA Estimate	Steiger and Lind (1980) root mean square error approximation
RMSEA Lower <i>r</i> % Confidence Limit	Lower <i>r</i> % ¹ confidence limit for RMSEA
RMSEA Upper <i>r</i> % Confidence Limit	Upper <i>r</i> % ¹ confidence limit for RMSEA
Probability of Close Fit	Browne and Cudeck (1993) test of close fit
ECVI Estimate	Expected cross-validation index
ECVI Lower <i>r</i> % Confidence Limit	Lower <i>r</i> % ² confidence limit for ECVI
ECVI Upper <i>r</i> % Confidence Limit	Upper <i>r</i> % ² confidence limit for ECVI
Akaike Information Criterion	Akaike information criterion
Bozdogan CAIC	Bozdogan (1987) consistent AIC
Schwarz Bayesian Criterion	Schwarz (1978) Bayesian criterion
McDonald Centrality	McDonald and Marsh (1988) measure of centrality

1. The value of *r* is one minus the ALPHARMS= value. By default, *r*=90.

2. The value of *r* is one minus the ALPHAECV= value. By default, *r*=90.

Possible Values of FitIndex When `_TYPE_=Incremental`

Value of FitIndex	Description
Bentler Comparative Fit Index	Bentler (1985) comparative fit index
Bentler-Bonett NFI	Bentler and Bonett (1980) normed fit index
Bentler-Bonett Non-normed Index	Bentler and Bonett (1980) nonnormed fit index
Bollen Normed Index Rho1	Bollen normed ρ_1
Bollen Non-normed Index Delta2	Bollen nonnormed δ_2
James et al. Parsimonious NFI	James, Mulaik, and Brett (1982) parsimonious normed fit index

Default Analysis Type and Default Parameterization

This section describes the default analysis type and default parameterization of PROC CALIS. Because various types of models supported by PROC CALIS have their own specific features, the following table outlines only those major default settings of PROC CALIS in SAS/STAT 9.22 or later:

Moment Structures Analyzed

Covariance structures	Covariance structures are analyzed by default (COVARIANCE option).
Mean structures	Not analyzed by default. Use the MEANSTR option, the 'Intercept' variable in the LINEQS statement, the MEAN statement, or specific MATRIX statements to specify mean or intercept parameters.

Default Parameterization

Variance parameters	Free variance parameters for independent latent factors, observed variables, and errors.
Covariance parameters	Free covariance parameters for all pairs of independent latent factors and observed variables (except for the latent factors in exploratory factor models). Fixed zero covariances for all pairs of error variables, all pairs between errors and other exogenous variables, and all pairs of latent factors in exploratory factor models.
Mean parameters	Free mean parameters for all exogenous observed variables. Fixed zero means for all exogenous latent factors and error terms.
Intercept parameters	Free intercept parameters for all endogenous observed variables; Fixed zero intercepts for all endogenous latent factors.

Role of the VAR Statement in Model Specification

Inclusion of Variables	If the VAR statement is used, observed variables that are listed in the VAR statement but not mentioned in corresponding model specification are included as exogenous variables in the model. Default variance, covariance, and mean parameterization apply to these exogenous variables.
------------------------	--

Exclusion of Variables	If the VAR statement is used, observed variables that are not listed in the VAR statement are not recognized as observed variables in model specification. They might be treated as latent variables instead.
------------------------	---

In general, the default settings of PROC CALIS in SAS/STAT 9.22 and later are more consistent with conventional practice of structural equation modeling. For example, because statistical theory of structural equation modeling is based mainly on the analysis of covariance structures, the default analysis type of PROC CALIS in SAS/STAT 9.22 or later is for covariance structures. This means that the **CORR** option must be specified if you want to analyze correlation matrices. Mean structures in PROC CALIS have also been parameterized more naturally since SAS/STAT 9.22 so that users can make statistical inferences directly on the mean and intercept estimates. Default variance and covariance parameters for all independent factors and observed variables have been implemented since SAS/STAT 9.22 to reflect the common belief that no exogenous variables are absolutely uncorrelated (except for the unrotated factors in the initial solution of exploratory FACTOR models).

For comparisons of these and other default settings before and after SAS/STAT 9.22, see the section “[Compatibility with the CALIS Procedure in SAS/STAT 9.2 or Earlier](#)” on page 1045.

For details about the default parameters in specific types of model, see the **FACTOR**, **LINEQS**, **LISMOD**, **PATH**, and **RAM** statements. Because there are no explicit latent variables and the exogenous/endogenous variable distinction is not used in the COSAN and MSTRUCT modeling languages, the default parameterization outlined in the preceding table does not apply to these two types of models. See the **COSAN** and the **MSTRUCT** statements for details. See the following sections for details about model parameterization in various types of models:

- “[The COSAN Model](#)” on page 1259
- “[The FACTOR Model](#)” on page 1263
- “[The LINEQS Model](#)” on page 1270
- “[The LISMOD Model and Submodels](#)” on page 1277
- “[The PATH Model](#)” on page 1288
- “[The RAM Model](#)” on page 1294
- “[The MSTRUCT Model](#)” on page 1285

By default, PROC CALIS in SAS/STAT 9.22 or later treats observed variables specified in the **VAR** statement as exogenous variables in the **FACTOR**, **PATH**, **LINEQS**, and **RAM** models. This minimizes the routine specifications in the **COVARIANCE**, **MEAN**, **PCOV**, **PVAR**, or **VARIANCE** for those “standalone” exogenous observed variables—observed variables that are not functionally related to any other variables in the model. Including these standalone exogenous observed variables into the model is useful during the model modification process (by the **MODIFICATION** option) where you can do Lagrange multiplier tests to see whether relating these variables to other variables can improve the model fit.

Notice that the use of the VAR statement specification is optional in PROC CALIS. If you have specified all the observed variables that you want in the model specification statements, it is not necessary to use the VAR statement specifications for the purpose of specifying the set of observed variable for analysis.

The COSAN Model

The original COSAN (covariance structure analysis) model is proposed by McDonald (1978, 1980) for analyzing general covariance structure models. PROC CALIS enables you to analyze a generalized form of the original COSAN model. The generalized COSAN model extends the original COSAN model with the inclusion of addition terms in the covariance structure formula and the associated mean structure formula.

The covariance structure formula of the generalized COSAN model is

$$\Sigma = \mathbf{F}_1 \mathbf{P}_1 \mathbf{F}'_1 + \cdots + \mathbf{F}_m \mathbf{P}_m \mathbf{F}'_m$$

and the corresponding mean structure formula of the generalized COSAN model is

$$\boldsymbol{\mu} = \mathbf{F}_1 \mathbf{v}_1 + \cdots + \mathbf{F}_m \mathbf{v}_m$$

where Σ is a symmetric correlation or covariance matrix for the observed variables, $\boldsymbol{\mu}$ is a vector for the observed variable means, each \mathbf{P}_k is a symmetric matrix, each \mathbf{v}_k is a mean vector, and each \mathbf{F}_k ($k = 1, \dots, m$) is the product of $n(k)$ matrices $\mathbf{F}_{k_1}, \dots, \mathbf{F}_{k_{n(k)}}$; that is,

$$\mathbf{F}_k = \mathbf{F}_{k_1} \cdots \mathbf{F}_{k_{n(k)}}, \quad k = 1, \dots, m$$

The matrices \mathbf{F}_{k_j} and \mathbf{P}_k in the model can be one of the forms

$$\mathbf{F}_{k_j} = \begin{cases} \mathbf{G}_{k_j} \\ \mathbf{G}_{k_j}^{-1} \\ (\mathbf{I} - \mathbf{G}_{k_j})^{-1} \end{cases} \quad j = 1, \dots, n(k) \quad \text{and} \quad \mathbf{P}_k = \begin{cases} \mathbf{Q}_k \\ \mathbf{Q}_k^{-1} \end{cases}$$

where \mathbf{G}_{k_j} and \mathbf{Q}_k are basic model matrices that are not expressed as functions of other matrices.

The COSAN model matrices and vectors are \mathbf{G}_{k_j} , \mathbf{Q}_k , and \mathbf{v}_k (when the mean structures are analyzed). The elements of these model matrices and vectors are either parameters (free or constrained) or fixed values. Matrix \mathbf{P}_k is referred to as the central covariance matrix for the k th term in the covariance structure formula.

Essentially, the COSAN modeling language enables you to define the covariance and mean structure formulas of the generalized COSAN model, the basic COSAN model matrices \mathbf{G}_{k_j} , \mathbf{Q}_k , and \mathbf{v}_k , and the parameters and fixed values in the model matrices.

You can also specify a generalized COSAN model without using an explicit central covariance matrix in any term. For example, you can define the k th term in the covariance structure formula as

$$\mathbf{F}_k \mathbf{F}'_k = \mathbf{F}_{k_1} \cdots \mathbf{F}_{k_{n-1}} \mathbf{F}_{k_n} \mathbf{F}'_{k_n} \mathbf{F}'_{k_{n-1}} \cdots \mathbf{F}'_{k_1}$$

The corresponding term for the mean structure becomes

$$\mathbf{F}_{k_1} \cdots \mathbf{F}_{k_{n-1}} \mathbf{v}_m$$

In the covariance structure formula, $\mathbf{F}_{k_n} \mathbf{F}'_{k_n}$ serves as an implicit central covariance matrix in this term of the covariance structure formula. Because of this, \mathbf{F}_{k_n} does not appear in the corresponding mean structure formula.

To take advantage of the modeling flexibility of the COSAN model specifications, you are required to provide the correct covariance and mean structure formulas for the analysis problem. If you are not familiar with the mathematical formulations of structural equation models, you can consider using simpler modeling languages such as PATH or LINEQS.

An Example: Specifying a Second-Order Factor Model

This example illustrates how to specify the covariance structures in the COSAN statement. Consider a second-order factor analysis model with the following formula for the covariance structures of observed variables v_1 – v_9

$$\Sigma = \mathbf{F}_1(\mathbf{F}_2\mathbf{P}_2\mathbf{F}_2' + \mathbf{U}_2)\mathbf{F}_1' + \mathbf{U}_1$$

where \mathbf{F}_1 is a 9×3 first-order factor matrix, \mathbf{F}_2 is a 3×2 second-order factor matrix, \mathbf{P}_2 is a 2×2 covariance matrix for the second-order factors, \mathbf{U}_2 is a 3×3 diagonal matrix for the unique variances of the first-order factors, and \mathbf{U}_1 is a 9×9 diagonal matrix for the unique variances of the observed variables.

To fit this covariance structure model, you first rewrite the covariance structure formula in the form of the generalized COSAN model as

$$\Sigma = \mathbf{F}_1\mathbf{F}_2\mathbf{P}_2\mathbf{F}_2'\mathbf{F}_1' + \mathbf{F}_1\mathbf{U}_2\mathbf{F}_1' + \mathbf{U}_1$$

You can specify the list of observed variables and the three terms for the covariance structure formula in the following COSAN statement:

```
cosan var= v1-v9,
      F1(3) * F2(2) * P2(2, SYM) + F1(3) * U2(3, DIA) + U1(9, DIA);
```

The VAR= option specifies the nine observed variables in the model. Next, the three terms of the covariance structure formula are specified. Because each term in the covariance structure formula is a symmetric product, you only need to specify each term up to the central covariance matrix. For example, although the first term in the covariance structure formula is $\mathbf{F}_1\mathbf{F}_2\mathbf{P}_2\mathbf{F}_2'\mathbf{F}_1'$, you only need to specify **F1(3) * F2(2) * P2(2, SYM)**. PROC CALIS generates the redundant information for the term. Similarly, you specify the other two terms of the covariance structure formula.

In each matrix specification of the COSAN statement, you can specify the following three matrix properties as the arguments in the trailing parentheses: the number of columns, the matrix type, and the transformation of the matrix. For example, **F1(3)** means that the number of columns of \mathbf{F}_1 is 3 (while the number of rows is 9 because this number has to match the number of observed variables specified in the VAR= option), **F2(2)** means that the number of columns of \mathbf{F}_2 is 2 (while the number of rows is 3 because the number has to match the number of columns of the preceding matrix, \mathbf{F}_1). You can specify the type of the matrix in the second argument. For example, **P2(2, SYM)** means that \mathbf{P}_2 is a symmetric (SYM) matrix and **U2(2, DIA)** means that \mathbf{U}_2 is a diagonal (DIA) matrix. You can also specify the transformation of the matrix in the third argument. Because there is no transformation needed in the current second-order factor model, this argument is omitted in the specification. See the COSAN statement for details about the matrix types and transformation that are supported by the COSAN modeling language.

Suppose now you also want to analyze the mean structures of the second-order factor model. The corresponding mean structure formula is

$$\mu = \mathbf{F}_1\mathbf{F}_2\mathbf{v} + \mathbf{u}$$

where \mathbf{v} is a 2×1 mean vector for the second-order factors and \mathbf{u} is a 6×1 vector for the intercepts of the observed variables. To analyze the mean and covariance structures simultaneously, you can use the following COSAN statement:

```
cosan var= v1-v9,
          F1(3) * F2(2) * P2(2,SYM) [mean = v] + F1(3) * U2(3,DIA)
          + U1(9,DIA) [mean = u];
```

In addition to the covariance structure specified, you now add the trailing MEAN= options in the first and the third terms. PROC CALIS then generates the mean structure formula by the following steps:

- Remove the last matrix (that is, the central covariance matrix) in each term of the covariance structure formula.
- Append to each term the vector that is specified in the MEAN= option of the term, or if no MEAN= option is specified in a term, that term becomes a zero vector in the mean structure formula.

Following these steps, the mean structure formula generated for the second-order factor model is

$$\boldsymbol{\mu} = \mathbf{F}_1 \mathbf{F}_2 \mathbf{v} + \mathbf{0} + \mathbf{u}$$

which is what you expect for the mean structures of the second-order factor model. To complete the COSAN model specification, you can use **MATRIX** statements to specify the parameters and fixed values in the COSAN model matrices. See [Example 27.29](#) for a complete example.

Special Cases of the Generalized COSAN Model

It is illustrative to see how you can view different types of models as a special case of the generalized COSAN model. This section describes two such special cases.

The Original COSAN Model

The original COSAN (covariance structure analysis) model (McDonald 1978, 1980) specifies the following covariance structures:

$$\boldsymbol{\Sigma} = \mathbf{F}_1 \cdots \mathbf{F}_n \mathbf{P} \mathbf{F}_n' \cdots \mathbf{F}_1'$$

This is the generalized COSAN with only one term for the covariance structure model formula. Hence, using the COSAN statement to specify the original COSAN model is straightforward.

Reticular Action Model

The RAM (McArdle 1980; McArdle and McDonald 1984) model fits the covariance structures

$$\boldsymbol{\Sigma}_a = (\mathbf{I} - \mathbf{A})^{-1} \mathbf{P} (\mathbf{I} - \mathbf{A})^{-1'}$$

where $\boldsymbol{\Sigma}_a$ is the symmetric covariance for all latent and observed variables in the RAM model, \mathbf{A} is a square matrix for path coefficients, \mathbf{I} is an identity matrix with the same dimensions as \mathbf{A} , and \mathbf{P} is a symmetric covariance matrix. For details about the RAM model, see the section “[The RAM Model](#)” on page 1294.

Correspondingly, the RAM model fits the mean structure formula

$$\boldsymbol{\mu}_a = (\mathbf{I} - \mathbf{A})^{-1} \mathbf{w}$$

where μ_a is the mean vector for all latent and observed variables in the RAM model and w is a vector for mean or intercepts of the variables.

To extract the covariance and mean structures for the observed variables, a selection matrix G is used. The selection matrix G contains zeros and ones as its elements. Each row of G has exactly one nonzero element at the position that corresponds to the location of a manifest row variable in Σ_a or μ_a . The covariance structure formula for the observed variables in the RAM model becomes

$$\Sigma = G(I - A)^{-1}P(I - A)^{-1'}G'$$

The mean structure formula for the observed variables in the RAM model becomes

$$\mu = G(I - A)^{-1}w$$

These formulas suggest that the RAM model is special case of the generalized COSAN model with one term. For example, suppose that there are 10 observed variables (var1–var10) and 3 latent variables in a RAM model. The following COSAN statement represents the RAM model:

```
cosan var= v1-v10,
      G(13,GEN) * A(13,GEN,IMI) * P(13,SYM) [Mean = w];
```

In the COSAN statement, you define the 10 variables in the VAR= option. Next, you provide the formulas for the mean and covariance structures. G is 10×13 general matrix (GEN), A is a 13×13 general matrix with the IMI transformation (that is, $(I - A)^{-1}$), P is a 13×13 symmetric matrix (SYM), and w is a 13×1 vector. With these COSAN statement specifications, your mean and covariance structure formulas represent exactly those of the RAM model. To complete the entire model specification, your next step is to use the **MATRIX** statements to specify the parameters and fixed values in the model matrices G , A , P , and w .

Similarly, it is possible to use the COSAN modeling language to represent any other model types such as models defined by the FACTOR, LINEQS, LISMOD, MSTRUCT, PATH, and RAM statements. But this is not an automatic recommendation of using the COSAN modeling languages in all situations. When an analysis can be specified by either the COSAN or a more specific modeling language (for example, PATH), you should consider using the specific modeling language because the specific modeling language can exploit specific model features so that it does the following:

- enables more supplemental analysis (effect analysis, standardized solutions, and so on), which COSAN has no general way to display
- supports better initial estimation methods (the COSAN model can only set initial estimates to certain default or random values)
- leads to more efficient computations due to the availability of more specific formulas and algorithms

Certainly, the COSAN modeling language is still very useful when you fit some nonstandard model structures that cannot be handled otherwise by the more specific modeling languages.

Naming Variables in the COSAN Model

Although you can define the list of observed (manifest) variables in the VAR= option of the COSAN statement, the COSAN modeling language does not support a direct specification of the latent or error variables in the model. In the COSAN statement, you can define the model matrices and how they multiply together

to form the covariance and mean structures. However, except for the row variables of the first matrix in each term, you do not need to *identify* the row and column variables in all other matrices. However, you can use the `VARNAMES` statement to *label* the column variables of the matrices. The names in the `VARNAMES` statement follow the general naming rules required by the general SAS system. They should not contain special characters and cannot be longer than 32 characters. Also, they do not need to use certain prefixes like what the `LINEQS` modeling language requires. It is important to realize that the `VARNAME` statement only *labels*, but does not *identify*, the column variables (and the row variables, by propagation). This means that while keeping all other things equal, changing the names in the `VARNAMES` statements does not change the mathematical model or the estimation of the model. For example, you can label all columns of a `COSAN` matrix with the same name but it does not mean that these columns refer to the same variable in the model. See the section “[Naming Variables and Parameters](#)” on page 1302 for the general rules about naming variables and parameters.

Default Parameters in the COSAN Model

The default parameters of the `COSAN` model matrices depend on the types of the matrices. Each element of the `IDE` or `ZID` matrix (identity matrix with or without an additional zero matrix) is either a fixed one or a fixed zero. You cannot override the default parameter values of these fixed matrices. For `COSAN` model matrices with types other than `IDE` or `ZID`, all elements are fixed zeros by default. You can override these default zeros by specifying them explicitly in the `MATRIX` statements.

The FACTOR Model

The `FACTOR` modeling language is used for specifying exploratory and confirmatory factor analysis models. You can use other general modeling languages such as `LINEQS`, `LISMOD`, `PATH`, and `RAM` to specify a factor model. But the `FACTOR` modeling language is more convenient for specifying factor models and is more specialized in displaying factor-analytic results. For convenience, models specified by the `FACTOR` modeling language are called `FACTOR` models.

Types of Variables in the FACTOR Model

Each variable in the `FACTOR` model is either manifest or latent. Manifest variables are those variables that are measured in the research. They must be present in the input data set. Latent variables are not directly observed. Each latent variable in the `FACTOR` model can be either a factor or an error term.

Factors are unmeasured hypothetical constructs for explaining the covariances among manifest variables, while errors are the unique parts of the manifest variables that are not explained by the (common) factors.

In the `FACTOR` model, all manifest variables are endogenous, which means that they are predicted from the latent variables. In contrast, all latent variables in the `FACTOR` model are exogenous, which means that they serve as predictors only.

Naming Variables in the FACTOR Model

Manifest variables in the `FACTOR` model are referenced in the input data set. In the `FACTOR` model specification, you use their names as they appear in the input data set. Manifest variable names must not be longer than 32 characters. There are no further restrictions on these names beyond those required by the SAS System.

Error variables in the FACTOR model are not named explicitly, although they are assumed in the model. You can name latent factors only in confirmatory FACTOR models. Factor names must not be longer than 32 characters and must be distinguishable from the manifest variable names in the same analysis. You do not need to name factors in exploratory FACTOR models, however. Latent factors named Factor1, Factor2, and so on are generated automatically in exploratory FACTOR models.

Model Matrices in the FACTOR Model

Suppose in the FACTOR model that there are p manifest variables and n factors. The FACTOR model matrices are described in the following subsections.

Matrix \mathbf{F} ($p \times n$) : Factor Loading Matrix

The rows of \mathbf{F} represent the p manifest variables, while the columns represent the n factors. Each row of \mathbf{F} contains the factor loadings of a variable on all factors in the model.

Matrix \mathbf{P} ($n \times n$) : Factor Covariance Matrix

The \mathbf{P} matrix is a symmetric matrix for the variances of and covariances among the n factors.

Matrix \mathbf{U} ($p \times p$) : Error Covariance Matrix

The \mathbf{U} matrix represents a $p \times p$ diagonal matrix for the error variances for the manifest variables. Elements in this matrix are the parts of variances of the manifest variables that are not explained by the common factors. Note that all off-diagonal elements of \mathbf{U} are fixed zeros in the FACTOR model.

Vector \mathbf{a} ($p \times 1$) : Intercepts

If the mean structures are analyzed, vector \mathbf{a} represents the intercepts of the manifest variables.

Vector \mathbf{v} ($n \times 1$) : Factor Means

If the mean structures are analyzed, vector \mathbf{v} represents the means of the factors.

Matrix Representation of the FACTOR Model

Let \mathbf{y} be a $p \times 1$ vector of manifest variables, $\boldsymbol{\xi}$ be an $n \times 1$ vector of latent factors, and \mathbf{e} be a $p \times 1$ vector of errors. The factor model is written as

$$\mathbf{y} = \mathbf{a} + \mathbf{F}\boldsymbol{\xi} + \mathbf{e}$$

With the model matrix definitions in the previous section, the covariance matrix $\boldsymbol{\Sigma}$ ($p \times p$) of manifest variables is structured as

$$\boldsymbol{\Sigma} = \mathbf{F}\mathbf{P}\mathbf{F}' + \mathbf{U}$$

The mean vector $\boldsymbol{\mu}$ ($p \times p$) of manifest variables is structured as

$$\boldsymbol{\mu} = \mathbf{a} + \mathbf{F}\mathbf{v}$$

$$\mathbf{P} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

and

$$\mathbf{U} = \begin{pmatrix} * & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & * & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & * & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & * & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & * & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & * & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & * & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & * & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & * \end{pmatrix}$$

If METHOD=FIML or METHOD=LSFIML, the elements of the intercept vector \mathbf{a} are all free parameters, as shown in the following:

$$\mathbf{a} = \begin{pmatrix} * \\ * \\ * \\ * \\ * \\ * \\ * \\ * \\ * \\ * \end{pmatrix}$$

The factor mean vector \mathbf{v} is a fixed zero vector.

If an initial factor solution is rotated afterward, some of these matrix patterns are changed. In general, rotating a factor solution eliminates the fixed zero pattern in the upper triangle of the factor loading matrix \mathbf{F} . If you apply an orthogonal rotation, the factor covariance matrix \mathbf{P} does not change. It is an identity matrix before and after rotation. However, if you apply an oblique rotation, in general the rotated factor covariance matrix \mathbf{P} is not an identity matrix and the off-diagonal elements are not zeros.

The error covariance matrix \mathbf{U} remains unchanged after rotation. That is, it would still be a diagonal matrix. For the FIML estimation, the rotation does not affect the estimation of the intercept vector \mathbf{a} and the fixed factor mean vector \mathbf{v} .

Confirmatory Factor Analysis Models

In confirmatory FACTOR models, there are no imposed patterns on the \mathbf{F} , \mathbf{P} , \mathbf{a} , and \mathbf{v} model matrices. All elements in these model matrices can be specified. However, for model identification, you might need to specify some factor loadings or factor variances as constants.

The only model restriction in confirmatory FACTOR models is placed on \mathbf{U} , which must be a diagonal matrix, as in exploratory FACTOR models too.

For example, for a confirmatory factor analysis with nine variables and three factors, you might specify the following patterns for the model matrices, where * denotes free parameters in the model matrices:

$$\mathbf{F} = \begin{pmatrix} 1 & 0 & 0 \\ * & 0 & 0 \\ * & 0 & 0 \\ 0 & 1 & 0 \\ 0 & * & 0 \\ 0 & * & 0 \\ 0 & 0 & 1 \\ 0 & 0 & * \\ 0 & 0 & * \end{pmatrix}$$

$$\mathbf{P} = \begin{pmatrix} * & * & * \\ * & * & * \\ * & * & * \end{pmatrix}$$

and

$$\mathbf{U} = \begin{pmatrix} * & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & * & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & * & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & * & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & * & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & * & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & * & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & * & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & * \end{pmatrix}$$

In this confirmatory factor model, mean structures are not modeled. In addition, there are some distinctive features that underscore the differences between confirmatory and exploratory models:

- Factor loading matrix \mathbf{F} contains mostly zero elements and few nonzero free parameters, a pattern which is seen in most confirmatory factor models. In contrast, in exploratory factor models most elements in the \mathbf{F} matrix are nonzero parameters.
- Factor loading matrix \mathbf{F} contains fixed values of ones. These fixed values are used for model identification purposes (that is, identifying the scales of the latent variables). In general, you always have to make sure that your confirmatory factor models are identified by putting fixed values in appropriate parameter locations in the model matrices. However, this is not a concern in exploratory FACTOR models because identification has been ensured by imposing certain patterns on the model matrices.
- The nonzero off-diagonal parameters in the factor covariance matrix \mathbf{P} indicate that correlated factors are hypothesized in the confirmatory factor model. This cannot be the case with the initial model of exploratory FACTOR models, where the \mathbf{P} matrix must be an identity matrix before rotation.

Summary of Matrices in the FACTOR Model

Let p be the number of manifest variables and n be the number of factors in the FACTOR model. The names, roles, and dimensions of the FACTOR model matrices are shown in the following table.

Matrix	Name	Description	Dimensions
F	<code>_FACTLOAD_</code>	Factor loading matrix	$p \times n$
P	<code>_FACTFCOV_</code>	Factor covariance matrix	$n \times n$
U	<code>_FACTERRV_</code>	Error covariance matrix	$p \times p$
a	<code>_FACTINTE_</code>	Intercepts	$p \times 1$
v	<code>_FACTMEAN_</code>	Factor means	$n \times 1$

Specification of the Exploratory Factor Model

Because all initial model matrices of exploratory FACTOR models are predefined in PROC CALIS, you do not need to specify any other parameters in the model matrices. To obtain desired factor solutions, you can use various options for exploratory factor analysis in the **FACTOR** statement. These options are the *EFA-options* in the **FACTOR** statement. Two main types of *EFA-options* are shown as follows:

- options for factor extraction: `COMPONENT`, `HEYWOOD`, and `N=`.
- options for factor rotation: `GAMMA=`, `NORM=`, `RCONVERGE=`, `RITER=`, `ROTATE=`, and `TAU=`.

For example, the following statement requests that three factors be extracted, followed by a varimax rotation of the initial factor solution:

```
factor n=3 rotate=varimax;
```

See the **FACTOR** statement on page 1138 for details about the *EFA-options*.

Specification of the Confirmatory Factor Model

To specify a confirmatory FACTOR model, you specify the factor-variable relationships in the **FACTOR** statement, the factor variances and error variances in the **PVAR** statement, the factor covariances in the **COV** statement, and the means and intercepts in the **MEAN** statement.

Specification of Factor-Variable Relationships

The *CFA-spec* in the **FACTOR** statement is for specifying the factor-variables relationships. For example, in the following statement you specify three factors F1, F2, and F3 that are related to different clusters of observed variables V1–V9:

```
factor
  F1 ==> V1-V3 = 1. parm1 (.4) parm2 (.4),
  F2 ==> V4-V6 = 1. parm3 parm4,
  F3 ==> V7-V9 = 1. parm5 parm6 (.3);
```

In the specification, variable V1 has a fixed loading of 1.0 on F1. Variables V2 and V3 have loadings on F1 also. These two loadings are free parameters named `parm1` and `parm2`, respectively. Initial estimates can be set in parentheses after the free parameters. For example, both `parm1` and `parm2` have initial values at 0.4. Similarly, relationships of factor F2 with V4–V6 and of factor F3 with V7–V9 are defined in the same

FACTOR statement. Providing initial estimates for parameters is optional. In this example, `parm3`, `parm4`, and `parm5` are all free parameters without initial values provided. PROC CALIS can determine appropriate initial estimates for these parameters. See the descriptions of *CFA-spec* in the **FACTOR statement** on page 1138 for more details about the syntax.

Specification of Factor Variances and Error Variances

You can specify the factor variances and error variances in the **PVAR** statement. For example, consider the following statement:

```
pvar F1-F3 = fvar1-fvar3,
      V1-V9 = evar1-evar9 (9*10.);
```

In the **PVAR** statement, you specify the variances of factors F1, F2, and F3 as free parameters `fvar1`, `fvar2`, and `fvar3`, respectively, and the error variances for manifest variables V1–V9 as free parameters `evar1`–`evar9`, respectively. Each of the error variance parameters is given a starting value at 10. See the **PVAR statement** on page 1214 for more details about the syntax.

Specification of Factor Covariances

You can specify the factor covariances in the **COV** statement. For example, you specify the covariances among factors F1, F2, and F3 in the following statement:

```
cov F1 F2 = cov12,
     F1 F3 = cov13,
     F2 F3 = cov23;
```

The covariance parameters are named `cov12`, `cov13`, and `cov23`, respectively. They represent the lower triangular elements of the factor covariance matrix **P**. See the **COV statement** on page 1132 for more details about the syntax.

Specification of Means and Intercepts

If mean structures are of interest, you can also specify the factor means and the intercepts for the manifest variables in the **MEAN** statement. For example, consider the following statement:

```
mean F1-F3 = fmean1-fmean3,
      V1-V9 = 9*12.;
```

In this statement, you specify the factor means of F1, F2, and F3 as free parameters `fmean1`, `fmean2`, and `fmean3`, respectively, and the intercepts for variables V1–V9 as fixed parameters at 12. See the **MEAN statement** on page 1189 for more details about the syntax.

Naming the Factors

For the exploratory FACTOR model, PROC CALIS generates the names for the factors automatically. For the confirmatory FACTOR model, you can specify the names for the factors. Unlike the LINEQS model, in the confirmatory FACTOR model you do not need to use the ‘F’ or ‘f’ prefix to denote factors in the model. You can use any valid SAS variable names for the factors, especially those names that reflect the nature of the factors. To avoid confusions with other names in the model, some general rules are recommended. See the section “Naming Variables and Parameters” on page 1302 for these general rules about naming variables and parameters.

Default Parameters in the FACTOR Model

Default parameters in the FACTOR model are different for exploratory and confirmatory factor models.

For the exploratory FACTOR model, all fixed and free parameters of the model are prescribed. These prescribed parameters include a fixed pattern for the factor loading matrix \mathbf{F} , a diagonal pattern for the error variance matrix \mathbf{U} , and an identity matrix for factor covariance matrix \mathbf{P} . This means that factors are uncorrelated in the estimation. However, if you specify an oblique rotation after the estimation of the factor solution, the factors could become correlated. See the section “[Exploratory Factor Analysis Models](#)” on page 1265 for more details about the patterns of the exploratory FACTOR model. Because all these patterns are prescribed, you cannot override any of these parameters for the exploratory FACTOR model.

For the confirmatory FACTOR model, the set of default free parameters of the confirmatory FACTOR model includes the following:

- the error variances of the observed variables; these correspond to the diagonal elements of the uniqueness matrix \mathbf{U}
- the variances and covariances among the factors; these correspond to all elements of the factor covariance matrix \mathbf{P}
- the intercepts of the observed variables if the mean structures are modeled; these correspond to all elements of the intercept vector \mathbf{a}

PROC CALIS names the default free parameters with the `_Add` prefix (or the `_a` prefix for the case of default intercept parameters in `a` for exploratory factor models), followed by a unique integers for each parameter. Except for the exploratory factor model, you can override the default free parameters by explicitly specifying them as free, constrained, or fixed parameters in the `COV`, `MEAN`, or `PVAR` statement.

In addition to default free parameters, another type of default parameter is the fixed zeros applied to the unspecified parameters in the loading matrix \mathbf{F} and the factor means in the \mathbf{v} vector. Certainly, you use the `FACTOR` and `MEAN` specifications to override those default zero loadings or factor means and set them to free, constrained, or fixed parameters. Notice that the uniqueness matrix \mathbf{U} in the confirmatory factor model is a diagonal element. You cannot specify any of its off-diagonal elements—they are always fixed zeros by the model restriction.

The LINEQS Model

The LINEQS modeling language is adapted from the EQS (equations) program by Bentler (1995). The statistical models that LINEQS or EQS analyzes are essentially the same as other general modeling languages such as LISMOD, RAM, and PATH. However, the terminology and approach of the LINEQS or EQS modeling language are different from other languages. They are based on the theoretical model developed by Bentler and Weeks (1980). For convenience, models that are analyzed using the LINEQS modeling language are called LINEQS models. Note that these so-called LINEQS models can also be analyzed by other general modeling languages in PROC CALIS.

In the LINEQS (or the original EQS) model, relationships among variables are represented by a system of equations. For example:

$$Y_1 = a_0 + a_1X_1 + a_2X_2 + E_1$$

$$Y_2 = b_0 + b_1X_1 + b_2Y_1 + E_2$$

On the left-hand side of each equation, an outcome variable is hypothesized to be a linear function of one or more predictor variables and an error, which are all specified on the right-hand side of the equation. The parameters specified in an equation are the effects (or regression coefficients) of the predictor variables. For example, in the preceding equations, Y_1 and Y_2 are outcome variables; E_1 and E_2 are error variables; a_1 , a_2 , b_1 , and b_2 are effect parameters (or regression coefficients); and a_0 and b_0 are intercept parameters. Variables X_1 and X_2 serve as predictors in the first equation, while variables X_1 and Y_1 serve as predictors in the second equation.

This is almost the same representation as in multiple regression models. However, the LINEQS model entails more. It supports a system of equations that can also include latent variables, measurement errors, and correlated errors.

Types of Variables in the LINEQS Model

The distinction between dependent and independent variables is important in the LINEQS model.

A variable is dependent if it appears on the left-hand side of an equation in the model. A dependent variable might be observed (manifest) or latent. It might or might not appear on the right-hand side of other equations, but it cannot appear on the left-hand sides of two or more equations. Error variables cannot be dependent in the LINEQS model.

A variable in the LINEQS model is independent if it is not dependent. Independent variables can be observed (manifest) or latent. All error variables must be independent in the LINEQS model.

Dependent variables are also referred to as endogenous variables; these names are interchangeable. Similarly, independent variables are interchangeable with exogenous variables.

Whereas an outcome variable in any equation must be a dependent variable, a predictor variable in an equation is not necessarily an independent variable in the entire LINEQS model. For example, Y_1 is a predictor variable in the second equation of the preceding example, but it is a dependent variable in the LINEQS model. In summary, the predictor-outcome nature of a variable is determined within a single equation, while the exogenous-endogenous (independent-dependent) nature of variable is determined within the entire system of equations.

In addition to the dependent-independent variable distinction, variables in the LINEQS model are distinguished according to whether they are observed in the data. Variables that are observed in research are called observed or manifest variables. Hypothetical variables that are not observed in the LINEQS model are latent variables.

Two types of latent variables should be distinguished: one is error variables; the other is non-error variables. An error variable is unique to an equation. It serves as the unsystematic source of effect for the outcome variable in an equation. If the outcome variable in the equation is latent, the corresponding error variable is also called disturbance. In contrast, non-error or systematic latent variables are called factors. Factors are unmeasured hypothetical constructs in your model. They are systematic sources that explain or describe functional relationships in your model.

Both manifest variables and latent factors can be dependent or independent. However, error or disturbance terms must be independent (or exogenous) variables in your model.

Naming Variables in the LINEQS Model

Whether a variable in each equation is an outcome or a predictor variable is prescribed by the modeler. Whether a variable is independent or dependent can be determined by analyzing the entire system of equations in the model. Whether a variable is observed or latent can be determined if it is referenced in your data set. However, whether a latent variable serves as a factor or an error can be determined only if you provide the specific information.

To distinguish latent factors from errors and both from manifest variables, the following rules for naming variables in the LINEQS model are followed:

- Manifest variables are referenced in the input data set. You use their names in the LINEQS model specification directly. There is no additional naming rule for the manifest variables in the LINEQS model beyond those required by the SAS System.
- Latent factor variables must start with letter F or f (for factor).
- Error variables must start with letter E or e (for error), or D or d (for disturbance). Although you might enforce the use of D- (or d-) variables for disturbances, it is not required. For flexibility, disturbance variables can also start with letter E or e in the LINEQS model.
- The names of latent variables, errors, and disturbances (F-, E-, and D-variables) should not coincide with the names of manifest variables.
- You should not use Intercept as a name for any variable. This name is reserved for the intercept specification in LINEQS model equations.

See the section “Naming Variables and Parameters” on page 1302 for the general rules about naming variables and parameters.

Matrix Representation of the LINEQS Model

As a programming language, the LINEQS model uses equations to describes relationships among variables. But as a mathematical model, the LINEQS model is more conveniently described by matrix terms. In this section, the LINEQS matrix model is described.

Suppose in a LINEQS model that there are n_i independent variables and n_d dependent variables. The vector of the independent variables is denoted by ξ , in the order of manifest variables, latent factors, and error variables. The vector of dependent variables is denoted by η , in the order of manifest variables and latent factors. The LINEQS model matrices are defined as follows:

- α ($n_d \times 1$): intercepts of dependent variables
- β ($n_d \times n_d$): effects of dependent variables (in columns) on dependent variables (in rows)
- γ ($n_d \times n_i$): effects of independent variables (in columns) on dependent variables (in rows)
- Φ ($n_i \times n_i$): covariance matrix of independent variables
- ν ($n_i \times 1$): means of independent variables

The model equation of the LINEQS model is

$$\eta = \alpha + \beta\eta + \gamma\xi$$

Assuming that $(\mathbf{I} - \beta)$ is invertible, under the model the covariance matrix of all variables $(\eta', \xi)'$ is structured as

$$\Sigma_a = \begin{pmatrix} (\mathbf{I} - \beta)^{-1} \gamma \Phi \gamma' (\mathbf{I} - \beta)^{-1'} & (\mathbf{I} - \beta)^{-1} \gamma \Phi \\ \Phi \gamma' (\mathbf{I} - \beta)^{-1'} & \Phi \end{pmatrix}$$

The mean vector of all variables $(\eta', \xi)'$ is structured as

$$\mu_a = \begin{pmatrix} (\mathbf{I} - \beta)^{-1} (\alpha + \gamma \nu) \\ \nu \end{pmatrix}$$

As is shown in the structured covariance and mean matrices, the means \mathbf{G} and covariances of independent variables are direct model parameters in ν and Φ ; whereas the means and covariances of dependent variables are functions of various model matrices and hence functions of model parameters.

The covariance and mean structures of all observed variables are obtained by selecting the elements in Σ_a and μ_a . Mathematically, define a selection matrix \mathbf{G} of dimensions $n \times (n_d + n_i)$, where n is the number of observed variables in the model. The selection matrix \mathbf{G} contains zeros and ones as its elements. Each row of \mathbf{G} has exactly one nonzero element at the position that corresponds to the location of an observed row variable in Σ_a or μ_a . With each row of \mathbf{G} selecting a distinct observed variable, the structured covariance matrix of all observed variables is represented by

$$\Sigma = \mathbf{G} \Sigma_a \mathbf{G}'$$

The structured mean vector of all observed variables is represented by

$$\mu = \mathbf{G} \mu_a$$

Partitions of Some LINEQS Model Matrices and Their Restrictions

There are some restrictions in some of the LINEQS model matrices. Although these restrictions do not affect the derivation of the covariance and mean structures, they are enforced in the LINEQS model specification.

Model Restrictions on the β Matrix

The diagonal of the β matrix must be zeros. This prevents the direct regression of dependent variables on themselves. Hence, in the LINEQS statement you cannot specify the same variable on both the left-hand and the right-hand sides of the same equation.

Partitions of the γ Matrix and the Associated Model Restrictions

The columns of the γ matrix refer to the variables in ξ , in the order of manifest variables, latent factors, and error variables. In the LINEQS model, the following partition of the γ matrix is assumed:

$$\gamma = (\gamma_0 \quad \mathbf{E})$$

where γ_0 is an $n_d \times (n_i - n_d)$ matrix for the effects of independent manifest variables and latent factors on the dependent variables and \mathbf{E} is an $n_d \times n_d$ permutation matrix for the effects of errors on the dependent variables.

The dimension of submatrix \mathbf{E} is $n_d \times n_d$ because in the LINEQS model each dependent variable signifies an equation with an error term. In addition, because \mathbf{E} is a permutation matrix (which is formed by exchanging rows of an identity matrix of the same order), the partition of the $\boldsymbol{\gamma}$ matrix ensures that each dependent variable is associated with a *unique* error term and that the effect of each error term on its associated dependent variable is 1.

As a result of the error term restriction, in the LINEQS statement you must specify a unique error term in each equation. The coefficient associated with the error term can only be a fixed value at one, either explicitly (with 1.0 inserted immediately before the error term) or implicitly (with no coefficient specified).

Partitions of the $\boldsymbol{\nu}$ Vector and the Associated Model Restrictions

The $\boldsymbol{\nu}$ vector contains the means of independent variables, in the order of the manifest, latent factor, and error variables. In the LINEQS model, the following partition of the $\boldsymbol{\nu}$ vector is assumed:

$$\boldsymbol{\nu} = \begin{pmatrix} \boldsymbol{\nu}_0 \\ 0 \end{pmatrix}$$

where $\boldsymbol{\nu}_0$ is an $(n_i - n_d) \times 1$ vector for the means of independent manifest variables and latent factors and 0 is a null vector of dimension n_d for the means of errors or disturbances. Again, the dimension of the null vector is n_d because each dependent variable is associated uniquely with an error term. This partition restricts the means of errors or disturbances to zeros.

Hence, when specifying a LINEQS model, you cannot specify the means of errors (or disturbances) as free parameter or fixed values other than zero in the MEAN statement.

Partitions of the Φ matrix

The Φ matrix is for the covariances of the independent variables, in the order of the manifest, latent factor, and error variables. The following partition of the Φ matrix is assumed:

$$\Phi = \begin{pmatrix} \Phi_{11} & \Phi'_{21} \\ \Phi_{21} & \Phi_{22} \end{pmatrix}$$

where Φ_{11} is an $(n_i - n_d) \times (n_i - n_d)$ covariance matrix for the independent manifest variables and latent factors, Φ_{22} is an $n_d \times n_d$ covariance matrix for the errors, and Φ_{21} is an $n_d \times (n_i - n_d)$ covariance matrix for the errors with other independent variables in the LINEQS model. Because Φ is symmetric, Φ_{11} and Φ_{22} are also symmetric.

There are actually no model restrictions placed on the submatrices of the partition. However, in most statistical applications, errors represent unsystematic sources of effects and therefore they are not to be correlated with other systematic sources. This implies that submatrix Φ_{21} is a null matrix. However, Φ_{21} being null is not enforced in the LINEQS model specification. If you ever specify a covariance between an error variable and a non-error independent variable in the COV statement, as a workaround trick or otherwise, you should provide your own theoretical justifications.

Summary of Matrices and Submatrices in the LINEQS Model

Let n_d be the number of dependent variables and n_i be the number of independent variables. The names, roles, and dimensions of the LINEQS model matrices and submatrices are summarized in the following table.

Matrix	Name	Description	Dimensions
Model Matrices			
α	_EQSALPHA_	Intercepts of dependent variables	$n_d \times 1$
β	_EQSBETA_	Effects of dependent (column) variables on dependent (row) variables	$n_d \times n_d$
γ	_EQSGAMMA_	Effects of independent (column) variables on dependent (row) variables	$n_d \times n_i$
ν	_EQSNU_	Means of independent variables	$n_i \times 1$
Φ	_EQSPHI_	Covariance matrix of independent variables	$n_i \times n_i$
Submatrices			
γ_0	_EQSGAMMA_SUB_	Effects of independent variables, excluding errors, on dependent variables	$n_d \times (n_i - n_d)$
ν_0	_EQSNU_SUB_	Means of independent variables, excluding errors	$(n_i - n_d) \times 1$
Φ_{11}	_EQSPHI11_	Covariance matrix of independent variables, excluding errors	$(n_i - n_d) \times (n_i - n_d)$
Φ_{21}	_EQSPHI21_	Covariances of errors with other independent variables	$n_d \times (n_i - n_d)$
Φ_{22}	_EQSPHI22_	Covariance matrix of errors	$n_d \times n_d$

Specification of the LINEQS Model

Specification in Equations

In the **LINEQS** statement, you specify intercepts and effect parameters (or regression coefficients) along with the variable relationships in equations. In terms of model matrices, you specify the α vector and the β and γ matrices in the **LINEQS** statement without using any matrix language.

For example:

$$Y = b_0 + b_1 * X_1 + b_2 * F_2 + E_1$$

In this equation, you specify Y as an outcome variable, X_1 and F_2 as predictor variables, and E_1 as an error variable. The parameters in the equation are the intercept b_0 and the path coefficients (or effects) b_1 and b_2 .

This kind of model equation is specified in the **LINEQS** statement. For example, the previous equation translates into the following **LINEQS** statement specification:

```
lineqs Y = b0 * Intercept + b1 * X1 + b2 * F2 + E1;
```

If the mean structures of the model are not of interest, the intercept term can be omitted. The specification becomes:

```
lineqs Y = b1 * X1 + b2 * F2 + E1;
```

See the [LINEQS statement](#) on page 1156 for the details about the syntax.

Because of the LINEQS model restrictions (see the section “[Partitions of Some LINEQS Model Matrices and Their Restrictions](#)” on page 1273), you must also follow these rules when specifying LINEQS model equations:

- A dependent variable can appear only on the left-hand side of an equation once. In other words, you must put all predictor variables for a dependent variable in one equation. This is different from some econometric models where a dependent variable can appear on the left-hand sides of two equations to represent an equilibrium point. However, this limitation can be resolved by reparameterization in some cases. See [Example 27.18](#).
- A dependent variable that appears on the left-hand side of an equation cannot appear on the right-hand side of the same equation. If you measure the same characteristic at different time points and the previous measurement serves as a predictor of the next measurement, you should use different variable names for the measurements so as to comply with this rule.
- An error term must be specified in each equation and must be unique. The same error name cannot appear in two or more equations. When an equation is truly intended to have no error term, it should be represented equivalently in the LINEQS equation by introducing an error term with zero variance (specified in the [VARIANCE](#) statement).
- The regression coefficient (effect) that is associated with an error term must be fixed at one (1.0). This is done automatically by omitting any fixed constants or parameters that are associated with the error terms. Inserting a parameter or a fixed value other than 1 immediately before an error term is not allowed.

Mean, Variance, and Covariance Parameter Specification

In addition to the intercept and effect parameters that are specified in equations, the means, variances, and covariances among all independent variables are parameters in the LINEQS model. An exception is that the means of all error variables are restricted to fixed zeros in the LINEQS model. To specify the mean, variance, and covariance parameters, you use the [MEAN](#), [VARIANCE](#), and the [COV](#) statements, respectively.

The means, variances, and covariances among dependent variables are not parameters themselves in the model. Rather, they are complex functions of the model parameters. See the section “[Matrix Representation of the LINEQS Model](#)” on page 1272 for mathematical details.

Default Parameters in the LINEQS Model

There are two types of default parameters of the LINEQS model, as implemented in PROC CALIS. One is the free parameters; the other is the fixed constants.

The following sets of parameters are free parameters by default:

- the variances of all exogenous (independent) observed or latent variables (*including* error and disturbance variables)

- the covariances among all exogenous (independent) manifest or latent variables (*excluding* error and disturbance variances)
- the means of all exogenous (independent) observed variables if the mean structures are modeled
- the intercepts of all endogenous (dependent) manifest variables if the mean structures are modeled

PROC CALIS names the default free parameters with the `_Add` prefix and a unique integer suffix. You can override the default free parameters by explicitly specifying them as free, constrained, or fixed parameters in the COV, LINEQS, MEAN, or VARIANCE statement.

Parameters that are not default free parameters in the LINEQS model are fixed constants by default. You can override almost all of the default fixed constants of the LINEQS model by using the COV, LINEQS, MEAN, or VARIANCE statement. You cannot override the following two sets of fixed constants:

- fixed zero parameters for the direct effects (path coefficients) of variables on their own. You cannot have an equation in the LINEQS statement that has the same variable specified on the left-hand and the right-hand sides.
- fixed one effects from the error or disturbance variables. You cannot set the path coefficient (effect) of the error or disturbance term to any value other than 1 in the LINEQS statement.

These two sets of fixed parameters reflect the LINEQS model restrictions so that they cannot be modified. Other than these two sets of default fixed parameters, all other default fixed parameters are zeros. You can override these default zeros by explicitly specifying them as free, constrained, or fixed parameters in the COV, LINEQS, MEAN, or VARIANCE statement.

The LISMOD Model and Submodels

As a statistical model, the LISMOD modeling language is derived from the LISREL model proposed by Jöreskog and others (see Keesling 1972; Wiley 1973; Jöreskog 1973). But as a computer language, the LISMOD modeling language is quite different from the LISREL program. To maintain the consistence of specification syntax within the CALIS procedure, the LISMOD modeling language departs from the original LISREL programming language. In addition, to make the programming a little easier, some terminological changes from LISREL are made in LISMOD.

For brevity, models specified by the LISMOD modeling language are called LISMOD models, although you can also specify these LISMOD models by other general modeling languages that are supported in PROC CALIS.

The following descriptions of LISMOD models are basically the same as those of the original LISREL models. The main modifications are the names for the model matrices.

The LISMOD model is described by three component models. The first one is the structural equation model that describes the relationships among latent constructs or factors. The other two are measurement models that relate latent factors to manifest variables.

Structural Equation Model

The structural equation model for latent factors is

$$\eta = \alpha + \beta\eta + \Gamma\xi + \zeta$$

where:

η is a random vector of n_η endogenous latent factors

ξ is a random vector of n_ξ exogenous latent factors

ζ is a random vector of errors

α is a vector of intercepts

β is a matrix of regression coefficients of η variables on other η variables

Γ is a matrix of regression coefficients of η on ξ

There are some assumptions in the structural equation model. To prevent a random variable in η from regressing directly on itself, the diagonal elements of β are assumed to be zeros. Also, $(I - \beta)^{-1}$ is assumed to be nonsingular, and ζ is uncorrelated with ξ .

The covariance matrix of ζ is denoted by Ψ and its expected value is a null vector. The covariance matrix of ξ is denoted by Φ and its expected value is denoted by κ .

Because variables in the structural equation model are not observed, to analyze the model these latent variables must somehow relate to the manifest variables. The measurement models, which are discussed in the subsequent sections, provide such relations.

Measurement Model for y

$$y = \nu_y + \Lambda_y\eta + \epsilon$$

where:

y is a random vector of n_y manifest variables

ϵ is a random vector of errors for y

ν_y is a vector of intercepts for y

Λ_y is a matrix of regression coefficients of y on η

It is assumed that ϵ is uncorrelated with either η or ξ . The covariance matrix of ϵ is denoted by Θ_y and its expected value is the null vector.

Measurement Model for x

$$x = \nu_x + \Lambda_x\xi + \delta$$

where:

x is a random vector of n_x manifest variables

δ is a random vector of errors for x

ν_x is a vector of intercepts for x

Λ_x is a matrix of regression coefficients of x on ξ

It is assumed that δ is uncorrelated with ξ , ϵ , or ζ . The covariance matrix of δ is denoted by Θ_x and its expected value is a null vector.

Covariance and Mean Structures

Under the structural and measurement equations and the model assumptions, the covariance structures of the manifest variables (y', x')' are expressed as

$$\Sigma = \begin{pmatrix} \Lambda_y(I - \beta)^{-1}(\Gamma\Phi\Gamma' + \Psi)(I - \beta')^{-1}\Lambda'_y + \Theta_y & \Lambda_y(I - \beta)^{-1}\Gamma\Phi\Lambda'_x \\ \Lambda_x\Phi\Gamma'(I - \beta')^{-1}\Lambda'_y & \Lambda_x\Phi\Lambda'_x + \Theta_x \end{pmatrix}$$

The mean structures of the manifest variables (y', x')' are expressed as

$$\mu = \begin{pmatrix} \nu_y + \Lambda_y(I - \beta)^{-1}(\alpha + \Gamma\kappa) \\ \nu_x + \Lambda_x\kappa \end{pmatrix}$$

Model Matrices in the LISMOD Model

The parameters of the LISMOD model are elements in the model matrices, which are summarized as follows.

Matrix	Name	Description	Dimensions	Row Variables	Column Variables
α	_ALPHA_	Intercepts for η	$n_\eta \times 1$	η (ETAVAR=)	N/A
β	_BETA_	Effects of η on η	$n_\eta \times n_\eta$	η (ETAVAR=)	η (ETAVAR=)
Γ	_GAMMA_	Effects of ξ on η	$n_\eta \times n_\xi$	η (ETAVAR=)	ξ (XIVAR=)
Ψ	_PSI_	Error covariance matrix for η	$n_\eta \times n_\eta$	η (ETAVAR=)	η (ETAVAR=)
Φ	_PHI_	Covariance matrix for ξ	$n_\xi \times n_\xi$	ξ (XIVAR=)	ξ (XIVAR=)
κ	_KAPPA_	Mean vector for ξ	$n_\xi \times 1$	ξ (XIVAR=)	N/A
ν_y	_NUY_	Intercepts for y	$n_y \times 1$	y (YVAR=)	N/A
Λ_y	_LAMBDAY_	Effects of η on y	$n_y \times n_\eta$	y (YVAR=)	η (ETAVAR=)
Θ_y	_THETAY_	Error covariance matrix for y	$n_y \times n_y$	y (YVAR=)	y (YVAR=)
ν_x	_NUX_	Intercepts for x	$n_x \times 1$	x (XVAR=)	N/A
Λ_x	_LAMBDA_X_	Effects of ξ on x	$n_x \times n_\xi$	x (XVAR=)	ξ (XIVAR=)
Θ_x	_THETAX_	Error covariance matrix for x	$n_x \times n_x$	x (XVAR=)	x (XVAR=)

There are twelve model matrices in the LISMOD model. Not all of them are used in all situations. See the section “LISMOD Submodels” on page 1282 for details. In the preceding table, each model matrix is given a name in the column Name, followed by a brief description of the parameters in the matrix, the dimensions, and the row and column variables being referred to. In the second column of the table, the LISMOD matrix

names are used in the **MATRIX** statements when specifying the LISMOD model. In the last two columns of the table, following the row or column variables is the variable list (for example, ETAVAR=, YVAR=, and so on) in parentheses. These lists are used in the LISMOD statement for defining variables.

Specification of the LISMOD Model

The LISMOD specification consists of two tasks. The first task is to define the variables in the model. The second task is to specify the parameters in the LISMOD model matrices.

Specifying Variables

The first task is accomplished in the **LISMOD** statement. In the **LISMOD** statement, you define the lists of variables of interest: **YVAR=**, **XVAR=**, **ETAVAR=**, and **XIVAR=** lists, respectively for the **y**-variables, **x**-variables, η -variables, and the ξ -variables. While you provide the names of variables in these lists, you also define implicitly the numbers of four types of variables: n_y , n_x , n_η , and n_ξ . The variables in the **YVAR=** and **XVAR=** lists are manifest variables and therefore must be present in the analyzed data set. The variables in the **ETAVAR=** and **XIVAR=** lists are latent factors, the names of which are assigned by the researcher to represent their roles in the substantive theory. After these lists are defined, the dimensions of the model matrices are also defined by the number of variables on various lists. In addition, the variable orders in the lists are referred to by the row and column variables of the model matrices.

Unlike the **LINEQS** model, in the **LISMOD** model you do not need to use the ‘F’ or ‘f’ prefix to denote factors in the **ETAVAR=** or **XIVAR=** list. You can use any valid SAS variable names for the factors, especially those names that reflect the nature of the factors. To avoid confusion with other names in the model, some general rules are recommended. See the section “**Naming Variables and Parameters**” on page 1302 for these general rules about naming variables and parameters.

Specifying Parameters in Model Matrices

The second task is accomplished by the **MATRIX** statements. In each **MATRIX** statement, you specify the model matrix by using the matrix names described in the previous table. Then you specify the parameters (free or fixed) in the locations of the model matrix. You can use as many **MATRIX** statements as needed for defining your model. But each model matrix can be specified only in one **MATRIX** statement, and each **MATRIX** statement is used for specifying only one model matrix.

An Example

In the section “**LISMOD Model**” on page 1072, the **LISMOD** modeling language is used to specify the model described in the section “**A Structural Equation Example**” on page 1067. In the **LISMOD** statement, you define four lists of variables, as shown in the following statement:

```
lismod
  yvar = Anomie67 Powerless67 Anomie71 Powerless71,
  xvar = Education SEI,
  etav = Alien67 Alien71,
  xivar = SES;
```

Endogenous latent factors are specified in the ETAVAR= list. Exogenous latent factors are specified in the XIVAR= list. In this case, Alien67 and Alien71 are the η -variables, and SES is the only ξ -variable in the model. Manifest variables that are indicators of endogenous latent factors in η are specified in the YVAR= list. In this case, they are the Anomie and Powerless variables, measured at two different time points. Manifest variables that are indicators of exogenous latent factors in ξ are specified in the XVAR= list. In this case, they are the Education and the SEI variables. Implicitly, the dimensions of the model matrices are defined by these lists already; that is, $n_y = 4$, $n_x = 2$, $n_\eta = 2$, and $n_\xi = 1$.

The **MATRIX** statements are used to specify parameters in the model matrices. For example, in the following statement you define the **_LAMBDA_** (Λ_x) matrix with two nonzero entries:

```
matrix _LAMBDA_ [1,1] = 1.0,
                [2,1] = lambda;
```

The first parameter location is for [1, 1], which is the effect of SES (the first variable in the XIVAR= list) on Education (the first element in the XVAR= list). A fixed value of 1.0 is specified there. The second parameter location is for [2, 1], which is the effect of SES (the first variable in the XIVAR= list) on SEI (the second variable in the XVAR= list). A parameter named lambda without an initial value is specified there.

Another example is shown as follows:

```
matrix _THETAY_ [1,1] = theta1,
                [2,2] = theta2,
                [3,3] = theta1,
                [4,4] = theta2,
                [3,1] = theta5,
                [4,2] = theta5;
```

In this **MATRIX** statement, the error variances and covariances (that is, the Θ_y matrix) for the y-variables are specified. The diagonal elements of the **_THETAY_** matrix are specified by parameters theta1, theta2, theta1, and theta2, respectively, for the four y-variables Anomie67, Powerless67, Anomie71, and Powerless71. By using the same parameter name theta1, the error variances for Anomie67 and Anomie71 are implicitly constrained. Similarly, the error variances for Powerless67 and Powerless71 are also implicitly constrained. Two more parameter locations are specified. The error covariance between Anomie67 and Anomie71 and the error covariance between Powerless67 and Powerless71 are both represented by the parameter theta5. Again, this is an implicit constraint on the covariances. All other unspecified elements in the **_THETAY_** matrix are treated as fixed zeros.

In this example, no parameters are specified for matrices **_ALPHA_**, **_KAPPA_**, **_NUY_**, or **_NUX_**. Therefore, mean structures are not modeled.

LISMOD Submodels

It is not necessary to specify all four lists of variables in the LISMOD statement. When some lists are unspecified in the LISMOD statement, PROC CALIS analyzes submodels derived logically from the specified lists of variables. For example, if only y- and x-variable lists are specified, the submodel being analyzed would be a multivariate regression model with manifest variables only. Not all combinations of lists lead to meaningful submodels, however. To determine whether and how a submodel (which is formed by a certain combination of variable lists) can be analyzed, the following three principles in the LISMOD modeling language are applied:

- Submodels with at least one of the YVAR= and XVAR= lists are required.
- Submodels that have an ETAVAR= list but no YVAR= list cannot be analyzed.
- When a submodel has a YVAR= (or an XVAR=) list but without an ETAVAR= (or a XIVAR=) list, it is assumed that the set of y-variables (x-variables) is equivalent to the η -variables (ξ -variables). Hereafter, this principle is referred to as an equivalence interpretation.

Apparently, the third principle is the same as the situation where the latent factors η (or ξ) are perfectly measured by the manifest variables y (or x). That is, in such a perfect measurement model, Λ_y (Λ_x) is an identity matrix and Θ_y (Θ_x) and ν_y (ν_x) are both null. This can be referred to as a perfect measurement interpretation. However, the equivalence interpretation stated in the last principle presumes that there are actually no measurement equations at all. This is important because under the equivalence interpretation, matrices Λ_y (Λ_x), Θ_y (Θ_x) and ν_y (ν_x) are nonexistent rather than fixed quantities, which is assumed under the perfect measurement interpretation. Hence, the x-variables are treated as *exogenous* variables with the equivalence interpretation, but they are still treated as *endogenous* with the perfect measurement interpretation. Ultimately, whether x-variables are treated as exogenous or endogenous affects the default or automatic parameterization. See the section “Default Parameters” on page 1164 for more details.

By using these three principles, the models and submodels that PROC CALIS analyzes are summarized in the following table, followed by detailed descriptions of these models and submodels.

Presence of Lists	Description	Model Equations	Nonfixed Model Matrices
Presence of Both x- and y-variables			
1 YVAR=, ETAVAR=, XVAR=, XIVAR=	Full model	$y = \nu_y + \Lambda_y \eta + \epsilon$ $x = \nu_x + \Lambda_x \xi + \delta$ $\eta = \alpha + \beta \eta + \Gamma \xi + \zeta$	$\nu_y, \Lambda_y, \Theta_y$ $\nu_x, \Lambda_x, \Theta_x, \kappa, \Phi$ $\alpha, \beta, \Gamma, \Psi$
2 YVAR=, XVAR=, XIVAR=	Full model with $y \equiv \eta$	$x = \nu_x + \Lambda_x \xi + \delta$ $y = \alpha + \beta y + \Gamma \xi + \zeta$	$\nu_x, \Lambda_x, \Theta_x, \kappa, \Phi$ $\alpha, \beta, \Gamma, \Psi$
3 YVAR=, ETAVAR=, XVAR=	Full model with $x \equiv \xi$	$y = \nu_y + \Lambda_y \eta + \epsilon$ $\eta = \alpha + \beta \eta + \Gamma x + \zeta$	$\nu_y, \Lambda_y, \Theta_y$ $\alpha, \beta, \Gamma, \Psi, \kappa, \Phi$
4 YVAR=, XVAR=	Regression ($y \equiv \eta$) ($x \equiv \xi$)	$y = \alpha + \beta y + \Gamma x + \zeta$, or $(I - \beta)^{-1} y = \alpha + \Gamma x + \zeta$	$\alpha, \beta, \Gamma, \Psi, \kappa, \Phi$
Presence of x-variables and Absence of y-variables			
5 XVAR=, XIVAR=	Factor model for x	$x = \nu_x + \Lambda_x \xi + \delta$	$\nu_x, \Lambda_x, \Theta_x, \kappa, \Phi$
6 XVAR=	x-structures ($x \equiv \xi$)		κ, Φ
Presence of y-variables and Absence of x-variables			
7 YVAR=, ETAVAR=	Factor model for y	$y = \nu_y + \Lambda_y \eta + \epsilon$ $\eta = \alpha + \beta \eta + \zeta$	$\nu_y, \Lambda_y, \Theta_y$ α, β, Ψ
8 YVAR=	y-structures ($y \equiv \eta$)	$y = \alpha + \beta y + \zeta$, or $(I - \beta)^{-1} y = \alpha + \zeta$	α, β, Ψ
9 YVAR=, ETAVAR=, XIVAR=	Second-order factor model	$y = \nu_y + \Lambda_y \eta + \epsilon$ $\eta = \alpha + \beta \eta + \Gamma \xi + \zeta$	$\nu_y, \Lambda_y, \Theta_y$ $\alpha, \beta, \Gamma, \Psi, \kappa, \Phi$
10 YVAR=, XIVAR=	Factor model ($y \equiv \eta$)	$y = \alpha + \beta y + \Gamma \xi + \zeta$, or $(I - \beta)^{-1} y = \alpha + \Gamma \xi + \zeta$	$\alpha, \beta, \Gamma, \Psi, \kappa, \Phi$

Models 1, 2, 3, and 4—Presence of Both x- and y-Variables

Submodels 1, 2, 3, and 4 are characterized by the presence of both x- and y-variables in the model. In fact, Model 1 is the full model with the presence of all four types of variables. All twelve model matrices are parameter matrices in this model.

Depending on the absence of the latent factor lists, manifest variables can replace the role of the latent factors in Models 2–4. For example, the absence of the ETAVAR= list in Model 2 means y is equivalent to η ($y \equiv \eta$). Consequently, you cannot, nor do you need to, use the **MATRIX** statement to specify parameters in the **_LAMBDAY_**, **_THETAY_**, or **_NUY_** matrices under this model. Similarly, because x is equivalent to ξ ($x \equiv \xi$) in Model 3, you cannot, nor do you need to, use the **MATRIX** statement to specify the parameters in the **_LAMBDA_X_**, **_THETA_X_**, or **_NUX_** matrices. In Model 4, y is equivalent to η ($y \equiv \eta$) and x is equivalent to ξ ($x \equiv \xi$). None of the six model matrices in the measurement equations are defined in the

model. Matrices in which you can specify parameters by using the **MATRIX** statement are listed in the last column of the table.

Describing Model 4 as a regression model is a simplification. Because y can regress on itself in the model equation, the regression description is not totally accurate for Model 4. Nonetheless, if β is a null matrix, the equation describes a multivariate regression model with outcome variables y and predictor variables x . This model is the TYPE 2A model in LISREL VI (Jöreskog and Sörbom 1985).

You should also be aware of the changes in meaning of the model matrices when there is an equivalence between latent factors and manifest variables. For example, in Model 4 the Φ and κ are now the covariance matrix and mean vector, respectively, of manifest variables x , while in Model 1 (the complete model) these matrices are of the latent factors ξ .

Models 5 and 6 — Presence of x -Variables and Absence of y -Variables

Models 5 and 6 are characterized by the presence of the x -variables and the absence of y -variables.

Model 5 is simply a factor model for measured variables x , with Λ_x representing the factor loading matrix, Θ_x the error covariance matrix, and Φ the factor covariance matrix. If mean structures are modeled, κ represents the factor means and ν_x is the intercept vector. This is the TYPE 1 submodel in LISREL VI (Jöreskog and Sörbom 1985).

Model 6 is a special case where there is no model equation. You specify the mean and covariance structures (in κ and Φ , respectively) for the manifest variables x directly. The x -variables are treated as exogenous variables in this case. Because this submodel uses direct mean and covariance structures for measured variables, it can also be handled more easily by the MSTRUCT modeling language. See the **MSTRUCT** statement and the section “The **MSTRUCT** Model” on page 1285 for more details.

Note that because η -variables cannot exist in the absence of y -variables (see one of the three aforementioned principles for deriving submodels), adding the ETAVAR= list alone to these two submodels does not generate new submodels that can be analyzed by PROC CALIS.

Models 7, 8, 9 and 10—Presence of y -Variables and Absence of x -Variables

Models 7–10 are characterized by the presence of the y -variables and the absence of x -variables.

Model 7 is a factor model for y -variables (TYPE 3B submodel in LISREL VI). It is similar to Model 5, but with regressions among latent factors allowed. When β is null, Model 7 functions the same as Model 5. It becomes a factor model for y -variables, with Λ_y representing the factor loading matrix, Θ_y the error covariance matrix, Ψ the factor covariance matrix, α the factor means, and ν_y the intercept vector.

Model 8 (TYPE 2B submodel in LISREL VI) is a model for studying the mean and covariance structures of y -variables, with regression among y -variables allowed. When β is null, the mean structures of y are specified in α and the covariance structures are specified in Ψ . This is similar to Model 6. However, there is an important distinction. In Model 6, the x -variables are treated as exogenous (no model equation at all). But the y -variables are treated as endogenous in Model 8 (with or without $\beta = 0$). Consequently, the default parameterization would be different for these two submodels. See the section “Default Parameters” on page 1164 for details about the default parameterization.

Model 9 represents a modified version of the second-order factor model for y . It would be a standard second-order factor model when β is null. This is the TYPE 3A submodel in LISREL VI. With β being null, η represents the first-order factors and ξ represents the second-order factors. The first- and second-order factor loading matrices are Λ_y and Γ , respectively.

Model 10 is another form of factor model when β is null, with factors represented by ξ and manifest variables represented by y . However, if β is indeed a null matrix in applications, you might want to use Model 5, in which the factor model specification is more direct and intuitive.

Default Parameters in the LISMOD Model

When a model matrix is defined in a LISMOD model, you can specify fixed values or free parameters for the elements of the matrix by the **MATRIX** statement. All other unspecified elements in the matrix are set by default. There are two types of default parameters for the LISMOD model matrices: one is free parameters; the other is fixed zeros.

The following sets of parameters are free parameters by default:

- the diagonal elements of the **_THETAX_**, **_THETAY_**, and **_PSI_** matrices; these elements represent the error variances in the model
- all elements of the **_PHI_** matrix; these elements represent the variances and covariance among exogenous variables in the model
- all elements in the **_NUX_** and **_NUY_** vectors if the mean structures are modeled; these elements represent the intercepts of the observed variables
- all elements in the **_ALPHA_** vector if a **YVAR=** list is specified but an **ETAVAR=** list is not specified and the mean structures are modeled; these elements represent the intercepts of the y -variables
- all elements in the **_KAPPA_** vector if an **XVAR=** list is specified but an **XIVAR=** list is not specified and the mean structures are modeled; these elements represent the means of the x -variables

PROC CALIS names the default free parameters with the **_Add** prefix and a unique integer suffix. You can override the default free parameters by explicitly specifying them as free, constrained, or fixed parameter in the **MATRIX** statements for the matrices.

Parameters that are not default free parameters in the LISMOD model are fixed zeros by default. You can override almost all of these default fixed zeros of the LISMOD model by using the **MATRIX** statements for the matrices. The only set of default fixed zeros that you cannot override is the set of the diagonal elements of the **_BETA_** matrix. These fixed zeros reflect a model restriction that precludes variables from having direct effects on themselves.

The MSTRUCT Model

In contrast to other modeling languages where the mean and covariance structures are implied from the specification of equations, paths, variable-factor relations, mean parameters, variance parameters, or covariance parameters, the MSTRUCT modeling language is supported in PROC CALIS for modeling mean and covariance structures directly.

A simple example for using the MSTRUCT modeling language is the testing of a covariance model with equal variances and covariances. Suppose that a variable was measured five times in an experiment. The covariance matrix of these five measurements is hypothesized to have the structure

$$\Sigma = \Sigma(\theta)$$

where

$$\theta = (\phi, \tau)$$

and

$$\Sigma(\theta) = \begin{pmatrix} \phi & \tau & \tau & \tau & \tau \\ \tau & \phi & \tau & \tau & \tau \\ \tau & \tau & \phi & \tau & \tau \\ \tau & \tau & \tau & \phi & \tau \\ \tau & \tau & \tau & \tau & \phi \end{pmatrix}$$

For model structures that are hypothesized directly in the covariance matrix, the MSTRUCT modeling language is the most convenient to use. You can also use other general modeling languages such as LINEQS, PATH, or RAM to fit the same model structures, but the specification is less straightforward and more error-prone. For convenience, models that are specified using the MSTRUCT modeling language are called MSTRUCT models.

Model Matrices in the MSTRUCT Model

Suppose that there are p observed variables. The two model matrices, their names, their roles, and their dimensions are summarized in the following table.

Matrix	Name	Description	Dimensions
Σ	<code>_COV_</code> or <code>_MSTRUCTCOV_</code>	Structured covariance matrix	$p \times p$
μ	<code>_MEAN_</code> or <code>_MSTRUCTMEAN_</code>	Structured mean vector	$p \times 1$

Specification of the MSTRUCT Model

Specifying Variables

In the MSTRUCT statement, you specify the list of p manifest variables of interest in the VAR= list. For example, you specify v1–v5 as the variables to be analyzed in your MSTRUCT model by this statement:

```
mstruct VAR= v1 v2 v3 v4 v5;
```

See the MSTRUCT statement on page 1194 for details about the syntax.

The manifest variables in the VAR= list must be referenced in the input set. The number of variables in the VAR= list determines the dimensions of the `_COV_` and the `_MEAN_` matrices in the model. In addition, the order of variables determines the order of row and column variables in the model matrices.

Specifying Parameters in Model Matrices

Denote the parameter vector in the MSTRUCT model as θ . The dimension of θ depends on your hypothesized model. In the preceding example, θ contains two parameters in ϕ and τ . You can use the MATRIX statement to specify these parameters in the `_COV_` matrix:

```
matrix _COV_ [1,1] = 5*phi, /* phi for all diagonal elements */
              [2, ] = tau, /* tau for all off-diagonal elements */
              [3, ] = 2*tau,
              [4, ] = 3*tau,
              [5, ] = 4*tau;
```

In this **MATRIX** statement, the five diagonal elements, starting from the [1, 1] element of the covariance matrix, are fitted by the phi parameter. The specification **5*phi** is a shorthand for specifying phi five times, once for each of the five diagonal elements in the covariance matrix. All other lower triangular elements are fitted by the tau parameter, as shown in the **MATRIX** statement. For example, with [3, 1] the elements starting from the first element of the third row of the **_COV_** matrix are parameterized by the tau parameter. The specification **2*tau** repeats the specification two times, meaning that the [3, 1] and [3, 2] elements are both fitted by the same parameter tau. Similarly, all lower triangular elements (not including the diagonal elements) of the **_COV_** matrix are fitted by the tau parameter. The specification of the upper triangular elements (diagonal excluded) of the **_COV_** matrix is not needed because the **_COV_** matrix is symmetric. The specification in the lower triangular elements is transferred automatically to the upper triangular elements. See the **MATRIX statement** on page 1175 for details about the syntax.

Default Parameters in the MSTRUCT Model

By using the **MATRIX** statements, you can specify either fixed values or free parameters (with or without initial values) for the elements in the **_COV_** and **_MEAN_** model matrices. If some or all elements are not specified, default parameters are applied to the **MSTRUCT**. There are two types of default parameters: one is free parameters; the other is fixed zeros. They are applied in different situations.

If you do not specify *any* elements of the **_COV_** matrix with the **MATRIX** statement, all elements of the **_COV_** matrix are free parameters by default. **PROC CALIS** names the default free parameters with the **_Add** prefix and a unique integer suffix. However, if you specify *at least one* fixed or free parameter of the **_COV_** matrix with the **MATRIX** statement, then all other unspecified elements of the **_COV_** matrix are fixed zeros by default.

If the mean structures are modeled, the same treatment applies to the **_MEAN_** vector. That is, if you do not specify any elements of the **_MEAN_** vector with the **MATRIX** statement, all elements of the **_MEAN_** vector are free parameters by default. However, if you specify *at least one* fixed or free parameter of the **_MEAN_** vector with the **MATRIX** statement, then all other unspecified elements of the **_MEAN_** vector are fixed zeros by default.

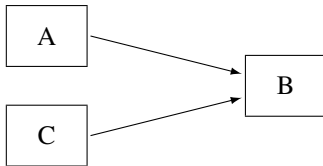
How and Why the Default Parameters Are Treated Differently in the MSTRUCT Model

Notice that the default parameter treatment of the **MSTRUCT** model is quite different from other types of models such as **FACTOR**, **LINEQS**, **LISMOD**, **RAM**, or **PATH**. For these models, unspecified variances and covariances among exogenous variables are all free parameters by default. However, for the **MSTRUCT** model, either default free parameters or fixed zeros are generated depending on whether at least one element of the covariance matrix is specified. The reason for this different treatment is that you fit the covariance structure directly by using the **MSTRUCT** modeling language. Hence, in an **MSTRUCT** model there is no information regarding the functional relationships among the variables that indicates whether the variables are exogenous or endogenous in the model. Hence, **PROC CALIS** cannot assume default free parameters based on the exogenous or endogenous variable types.

Because of this special default parameter treatment, when fitting an **MSTRUCT** model you must make sure that each diagonal element in your **_COV_** matrix is set as a free, constrained, or fixed parameter, in accordance with your theoretical model. If you specify some elements in the model matrix but omit the specification of other diagonal elements, the default fixed zero variances would lead to a nonpositive definite **_COV_** model matrix, making the model fitting problematic.

The PATH Model

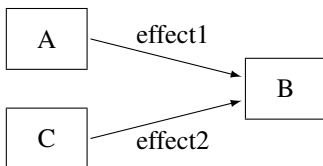
The PATH modeling language is supported in PROC CALIS as a more intuitive modeling tool. It is designed so that specification by using the PATH modeling language translates effortlessly from the path diagram. For example, consider the following simple path diagram:



You can use the following PATH statement to specify the paths easily:

```
path    A ==> B ,
        C ==> B ;
```

There are two path entries in the PATH statement: one is for the path **A ==> B**, and the other is for the path **C ==> B**. Sometimes you might want to name the effect parameters in the path diagram, as shown in the following:



You can specify the paths and the parameters together in the following statement:

```
path    A ==> B   = effect1,
        C ==> B   = effect2;
```

In the first entry of the PATH statement, the path **A ==> B** is specified together with the path coefficient (effect) **effect1**. Similarly, in the second entry, the **C ==> B** path is specified together with the effect parameter **effect2**. In addition to the path coefficients (effects) in the path diagram, you can also specify other types of parameters by using the **PVAR** and **PCOV** statements. See the section “A Structural Equation Example” on page 1067 for a more detailed example of the PATH model specification.

Despite its simple representation of the path diagram, the PATH modeling language is general enough to handle a wide class of structural models that can also be handled by other general modeling languages such as LINEQS, LISMOD, or RAM. For brevity, models specified by the PATH modeling language are called PATH models.

Types of Variables in the PATH Model

When you specify the paths in the PATH model, you typically use arrows (such as **<==** or **==>**) to denote “causal” paths. For example, in the preceding path diagram or the PATH statement, you specify that **B** is an outcome variable with predictors **A** and **C**, respectively, in two paths. An outcome variable is the variable being pointed to in a path specification, while the predictor variable is the one where the arrow starts from.

Whereas the outcome–predictor relationship describes the roles of variables in each single path, the endogenous–exogenous relationship describes the roles of variables in the entire system of paths. In a

system of path specification, a variable is endogenous if it is pointed to by at least one single-headed arrow or it serves as an outcome variable in at least one path. Otherwise, it is exogenous. In the preceding path diagram, for example, variable B is endogenous and both variables A and C are exogenous. Note that although any variable that serves as an outcome variable at least in one path must be endogenous, it does not mean that all endogenous variables must serve only as outcome variables in all paths. An endogenous variable in a model might also serve as a predictor variable in a path. For example, variable B in the following PATH statement is an endogenous variable, and it serves as an outcome variable in the first path but as a predictor variable in the second path.

```
path    A ==> B    = effect1,
        B ==> C    = effect2;
```

A variable is a manifest or observed variable in the PATH model if it is measured and exists in the input data set. Otherwise, it is a latent variable. Because error variables are not explicitly defined in the PATH modeling language, all latent variables that are named in the PATH model are *factors*, which are considered to be the systematic source of effects in the model. Each manifest variable in the PATH model can be endogenous or exogenous. The same is true for any latent factor in the PATH model.

Because you do not name error variables in the PATH model, you do not need to specify paths from errors to any endogenous variables. Error terms are implicitly assumed for all endogenous variables in the PATH model. Although error variables are not named in the PATH model, the error variances are expressed equivalently as partial variances of the associated endogenous variables. These partial variances are set by default in the PATH modeling language. Therefore, you do not need to specify error variance parameters explicitly unless constraints on these parameters are desirable in the model. You can use the **PVAR** statement to specify the error variance or partial variance parameters explicitly.

Naming Variables in the PATH Model

Manifest variables in the PATH model are referenced in the input data set. Their names must not be longer than 32 characters. There are no further restrictions beyond those required by the SAS System. You use the names of manifest variables directly in the PATH model specification.

Because you do not name error variables in the PATH model, all latent variables named in the PATH model specification are factors (non-errors). Factor names in the PATH model must not be longer than 32 characters, and they should be different from the manifest variables. Unlike the LINEQS model, you do not need to use ‘F’ or ‘f’ prefix to denote latent factors in the PATH model. As a general naming convention, you should not use Intercept as either a manifest or latent variable name. See the section “[Naming Variables and Parameters](#)” on page 1302 for these general rules about naming variables and parameters.

Specification of the PATH Model

(1) Specification of Effects or Paths

You specify the “causal” paths or linear functional relationships among variables in the PATH statement. For example, if there is a path from v2 to v1 in your model and the effect parameter is named parm1 with a starting value at 0.5, you can use either of these specifications:

```
path    v1 <=== v2    = parm1 (0.5);
```

```
path    v2 ==> v1    = parm1(0.5);
```

If you have more than one path in your model, path specifications should be separated by commas, as shown in the following **PATH** statement:

```
path
  v1 <=== v2    = parm1(0.5),
  v2 <=== v3    = parm2(0.3);
```

Because the **PATH** statement can be used only once in each model specification, all paths in the model must be specified together in a single **PATH** statement. See the **PATH** statement on page 1202 for more details about the syntax.

(2) Specification of Variances and Partial (Error) Variances

If *v2* is an exogenous variable in the **PATH** model and you want to specify its variance as a parameter named *parm2* with a starting value at 10, you can use the following **PVAR** statement specification:

```
pvar    v2    = parm2(10.);
```

If *v1* is an endogenous variable in the **PATH** model and you want to specify its partial variance or error variance as a parameter named *parm3* with a starting value at 5.0, you can also use the following **PVAR** statement specification:

```
pvar    v1 = parm3(5.0);
```

Therefore, the **PVAR** statement can be used for both exogenous and endogenous variables. When a variable in the statement is exogenous (which can be automatically determined by PROC CALIS), you are specifying the variance parameter of the variable. Otherwise, you are specifying the partial or error variance for an endogenous variable.

You do not need to supply the parameter names for the variances or partial variances if these parameters are not constrained. For example, the following statement specifies the unnamed free parameters for variances or partial variances of *v1* and *v2*:

```
pvar    v1 v2;
```

If you have more than one variance or partial variance parameter to specify in your model, you can put a variable list on the left-hand side of the equal sign, and a parameter list on the right-hand side, as shown in the following **PVAR** statement specification:

```
pvar
  v1 v2 v3 = parm1(0.5) parm2 parm3;
```

In the specification, variance or partial variance parameters for variables *v1*–*v3* are *parm1*, *parm2*, and *parm3*, respectively. Only *parm1* is given an initial value at 0.5. The initial values for other parameters are generated by PROC CALIS.

You can also separate the specifications into several entries in the **PVAR** statement. Entries should be separated by commas. For example, the preceding specification is equivalent to the following specification:

```

pvar
  v1 = parm1 (0.5) ,
  v2 = parm2 ,
  v3 = parm3 ;

```

Because the **PVAR** statement can be used only once in each model specification, all variance and partial variance parameters in the model must be specified together in a single **PVAR** statement. See the **PVAR statement** on page 1214 for more details about the syntax.

(3) Specification of Covariances and Partial Covariances

If you want to specify the (partial) covariance between two variables *v3* and *v4* as a parameter named *parm4* with a starting value at 3, you can use the following **PCOV** statement specification:

```

pcov v3 v4 = parm4 (5.) ;

```

Whether *parm4* is a covariance or partial covariance parameter depends on the variable types of *v3* and *v4*. If both *v3* and *v4* are exogenous variables (manifest or latent), *parm4* is a covariance parameter between *v3* and *v4*. If both *v3* and *v4* are endogenous variables (manifest or latent), *parm4* is a parameter for the covariance between the errors for *v3* and *v4*. In other words, it is a partial covariance or error covariance parameter for *v3* and *v4*.

A less common case is when one of the variables is exogenous and the other is endogenous. In this case, *parm4* is a parameter for the partial covariance between the endogenous variable and the exogenous variable, or the covariance between the error for the endogenous variable and the exogenous variable. Fortunately, such covariances are relatively uncommon in statistical modeling. Their uses confuse the roles of systematic and unsystematic sources in the model and lead to difficulties in interpretations. Therefore, you should almost always avoid this kind of partial covariance.

Like the syntax of the **PVAR** statement, you can specify a list of (partial) covariance parameters in the **PCOV** statement. For example, consider the following statement:

```

pcov
  v1 v2 = parm4 ,
  v1 v3 = parm5 ,
  v2 v3 = parm6 ;

```

In the specification, three (partial) covariance parameters *parm4*, *parm5*, and *parm6* are specified, respectively, for the variable pairs (*v1,v2*), (*v1,v3*), and (*v2,v3*). Entries for (partial) covariance specification are separated by commas.

Again, if all these covariances are not constrained, you can omit the names for the parameters. For example, the preceding specification can be specified as the following statement when the three covariances are free parameters in the model:

```

pcov
  v1 v2 ,
  v1 v3 ,
  v2 v3 ;

```

Or, you can simply use the following within-list covariance specification:

```
pcov
  v1 v2 v3;
```

Three covariance parameters are generated by this specification.

Because the **PCOV** statement can be used only once in each model specification, all covariance and partial covariance parameters in the model must be specified together in a single **PCOV** statement. See the **PCOV statement** on page 1212 for more details about the syntax.

(4) Specification of Means and Intercepts

Means and intercepts are specified when the mean structures of the model are of interest. You can specify mean and intercept parameters in the **MEAN** statement. For example, consider the following statement:

```
mean      v5 = parm5(11.);
```

If **V5** is an exogenous variable (which is determined by PROC CALIS automatically), you are specifying **parm5** as the mean parameter of **V5**. If **V5** is an endogenous variable, you are specifying **parm5** as the intercept parameter for **V5**.

Because each named variable in the PATH model is either exogenous or endogenous (exclusively), each variable in the PATH model would have either a mean or an intercept parameter (but not both) to specify in the **MEAN** statement. Like the syntax of the **PVAR** statement, you can specify a list of mean or intercept parameters in the **MEAN** statement. For example, in the following statement you specify a list of mean or intercept parameters for variables **v1–v4**:

```
mean
  v1-v4 = parm6-parm9;
```

This specification is equivalent to the following specification with four entries of parameter specifications:

```
mean
  v1 = parm6,
  v2 = parm7,
  v3 = parm8,
  v4 = parm9;
```

Again, entries in the **MEAN** statement must be separated by commas, as shown in the preceding statement.

Because the **MEAN** statement can be used only once in each model specification, all mean and intercept parameters in the model must be specified together in a single **MEAN** statement. See the **MEAN statement** on page 1189 for more details about the syntax.

Specifying Parameters without Initial Values

If you do not have any knowledge about the initial value for a parameter, you can omit the initial value specification and let PROC CALIS compute it. For example, you can provide just the parameter locations and parameter names as in the following specification:

```
path      v1 <=== v2      = parm1;
  pvar    v2 = parm2,
          v1 = parm3;
```

Specifying Fixed Parameter Values

If you want to specify a fixed parameter value, you do not need to provide a parameter name. Instead, you provide the fixed value (without parentheses) in the specification.

For example, in the following statement the path coefficient for the path is fixed at 1.0 and the (partial) variance of F1 is also fixed at 1.0:

```
path    v1 <=== F1 = 1.;
      pvar
        F1 = 1.;
```

A Complete PATH Model Specification Example

The following specification shows a more complete PATH model specification:

```
path    v1 <=== v2 ,
        v1 <=== v3 ;
      pvar v1,
          v2 = parm3,
          v3 = parm3;
      pcov v3 v2 = parm5(5.);
```

The two paths specified in the PATH statement have unnamed free effect parameters. These parameters are named by PROC CALIS with the `_Parm` prefix and unique integer suffixes. The error variance of v1 is an unnamed parameter, while the variances of v2 and v3 are constrained by using the same parameter parm3. The covariance between v2 and v3 is a free parameter named parm5, with a starting value of 5.0.

Default Parameters in the PATH Model

There are two types of default parameters of the PATH model. One is the free parameters; the other is the fixed constants.

The following sets of parameters are free parameters by default:

- the variances or partial (or error) variances of all variables, manifest or latent
- the covariances among all exogenous (independent) manifest or latent variables
- the means of all exogenous (independent) manifest variables if the mean structures are modeled
- the intercepts of all endogenous (dependent) manifest variables if the mean structures are modeled

For each of the default free parameters, PROC CALIS generates a parameter name with the `_Add` prefix and a unique integer suffix. Parameters that are not default free parameters in the PATH model are fixed zeros by default. You can override almost all of the default zeros of the PATH model by using the MEAN, PATH, PCOV, and MEAN statements. The only exception is the single-headed path that has the same variable on both sides. That is, the following specification is not accepted by PROC CALIS:

```
path    v1 <=== v1 = parm;
```

This path should always has a zero coefficient, which is treated as a model restriction that prevents a variable from having a direct effect on itself.

Relating the PATH Model to the RAM Model

Mathematically, the PATH model is essentially the RAM model. You can consider the PATH model to share exactly the same set of model matrices as in the RAM model. See the section “[Model Matrices in the RAM Model](#)” on page 1295 and the section “[Summary of Matrices and Submatrices in the RAM Model](#)” on page 1298 for details about the RAM model matrices. In the RAM model, the **A** matrix contains effects or path coefficients for describing relationships among variables. In the PATH model, you specify these effect or coefficient parameters in the **PATH** statement. The **P** matrix in the RAM model contains (partial) variance and (partial) covariance parameters. In the PATH model, you use the **PVAR** and **PCOV** statements to specify these parameters. The **W** vector in the RAM model contains the mean and intercept parameters, while in the PATH model you use the **MEAN** statement to specify these parameters. By using these model matrices in the PATH model, the covariance and mean structures are derived in the same way as they are derived in the RAM model. See the section “[The RAM Model](#)” on page 1294 for derivations of the model structures.

The RAM Model

The RAM modeling language is adapted from the basic RAM model developed by McArdle (1980). For brevity, models specified by the RAM modeling language are called RAM models. You can also specify these so-called RAM models by other general modeling languages that are supported in PROC CALIS.

Types of Variables in the RAM Model

A variable in the RAM model is manifest if it is observed and is defined in the input data set. A variable in the RAM model is latent if it is not manifest. Because error variables are not explicitly named in the RAM model, all latent variables in the RAM model are considered as factors (non-error-type latent variables).

A variable in the RAM model is endogenous if it ever serves as an outcome variable in the RAM model. That is, an endogenous variable has at least one path (or an effect) from another variable in the model. A variable is exogenous if it is not endogenous. Endogenous variables are also referred to as dependent variables, while exogenous variables are also referred to as independent variables.

In the RAM model, distinctions between exogenous and endogenous and between latent and manifest for variables are not essential to the definitions of model matrices, although they are useful for conceptual understanding when the model matrices are partitioned.

Naming Variables in the RAM Model

Manifest variables in the RAM model are referenced in the input data set. Their names must not be longer than 32 characters. There are no further restrictions beyond those required by the SAS System.

Latent variables in the RAM model are those not being referenced in the input data set. Their names must not be longer than 32 characters. Unlike the LINEQS model, you do not need to use any specific prefix (for example, ‘F’ or ‘f’) for the latent factor names. The reason is that error or disturbance variables in the RAM model are not named explicitly in the RAM model. Thus, any variable names that are not referenced in the input data set are for latent factors.

As a general naming convention, you should not use Intercept as either a manifest or latent variable name.

Model Matrices in the RAM Model

In terms of the number of model matrices involved, the RAM model is the simplest among all the general structural equations models that are supported by PROC CALIS. Essentially, there are only three model matrices in the RAM model: one for the interrelationships among variables, one for the variances and covariances, and one for the means and intercepts. These matrices are discussed in the following subsections.

Matrix \mathbf{A} ($n_a \times n_a$): Effects of Column Variables on Row Variables

The row and column variables of matrix \mathbf{A} are the set of manifest and latent variables in the RAM model. Unlike the LINEQS model, the set of latent variables in the RAM model matrix does not include the error or disturbance variables. Each entry or element in the \mathbf{A} matrix represents an effect of the associated column variable on the associated row variable or a path coefficient from the associated column variable to the associated row variable. A zero entry means an absence of a path or an effect.

The pattern of matrix \mathbf{A} determines whether a variable is endogenous or exogenous. A variable in the RAM model is endogenous if its associated row in the \mathbf{A} matrix has at least one nonzero entry. Any other variable in the RAM model is exogenous.

Mathematically, you do not need to arrange the set of variables for matrix \mathbf{A} in a particular order, as long as the order of variables is the same for the rows and the columns. However, arranging the variables according to whether they are endogenous or exogenous is useful for showing the partitions of the model matrices and certain mathematical properties. See the section “Partitions of the RAM Model Matrices and Some Restrictions” on page 1296 for details.

Matrix \mathbf{P} ($n_a \times n_a$): Variances, Covariances, Partial Variances, and Partial Covariances

The row and column variables of matrix \mathbf{P} refer to the same set of manifest and latent variables that are defined in the RAM model matrix \mathbf{A} . The diagonal entries of \mathbf{P} contain variances or partial variances of variables. If a variable is exogenous, then the corresponding diagonal element in the \mathbf{P} matrix represents its variance. Otherwise, the corresponding diagonal element in the \mathbf{P} matrix represents its partial variance. This partial variance is an unsystematic source of variance that is not explained by the interrelationships of variables in the model. In most cases, you can interpret a partial variance as the error variance for an endogenous variable.

The off-diagonal elements of \mathbf{P} contain covariances or partial covariances among variables. An off-diagonal element in \mathbf{P} that is associated with exogenous row and column variables represents covariance between the two exogenous variables. An off-diagonal element in \mathbf{P} that is associated with endogenous row and column variables represents *partial* covariance between the two variables. This partial covariance is unsystematic, in the sense that it is not explained by the interrelationships of variables in the model. In most cases, you can interpret a partial covariance as the error covariance between the two endogenous variables involved. An off-diagonal element in \mathbf{P} that is associated with one exogenous variable and one endogenous variable in the row and column represents the covariance between the exogenous variable and the error of the endogenous variable. While this interpretation sounds a little awkward and inelegant, this kind of covariance, fortunately, is rare in most applications.

Vector \mathbf{W} ($n_a \times 1$): Intercepts and Means

The row variables of vector \mathbf{W} refer to the same set of manifest and latent variables that are defined in the RAM model matrix \mathbf{A} . Elements in \mathbf{W} represent either intercepts or means. An element in \mathbf{W} that is associated with an exogenous row variable represents the mean of the variable. An element in \mathbf{W} that is associated with an endogenous row variable represents the intercept term for the variable.

Covariance and Mean Structures

Assuming that $(\mathbf{I} - \mathbf{A})$ is invertible, where \mathbf{I} is an identity matrix of the same dimension as \mathbf{A} , the structured covariance matrix of all variables (including latent variables) in the RAM model is shown as follows:

$$\Sigma_a = (\mathbf{I} - \mathbf{A})^{-1} \mathbf{P} (\mathbf{I} - \mathbf{A})^{-1'}$$

The structured mean vector of all variables is shown as follows:

$$\mu_a = (\mathbf{I} - \mathbf{A})^{-1} \mathbf{W}$$

The covariance and mean structures of all manifest variables are obtained by selecting the elements in Σ_a and μ_a . This can be achieved by defining a selection matrix \mathbf{G} of dimensions $n \times n_a$, where n is the number of manifest variables in the model. The selection matrix \mathbf{G} contains zeros and ones as its elements. Each row of \mathbf{G} has exactly one nonzero element at the position that corresponds to the location of a manifest row variable in Σ_a or μ_a . With each row of \mathbf{G} selecting a distinct manifest variable, the structured covariance matrix of all manifest variables is expressed as the following:

$$\Sigma = \mathbf{G} \Sigma_a \mathbf{G}'$$

The structured mean vector of all observed variables is expressed as the following:

$$\mu = \mathbf{G} \mu_a$$

Partitions of the RAM Model Matrices and Some Restrictions

There are some model restrictions in the RAM model matrices. Although these restrictions do not affect the derivation of the covariance and mean structures, they are enforced in the RAM model specification.

For convenience, it is useful to assume that n_a variables are arranged in the order of n_d endogenous (or dependent) variables and the n_i exogenous (independent) variables in the rows and columns of the model matrices.

Model Restrictions on the A Matrix

The \mathbf{A} matrix is partitioned as

$$\mathbf{A} = \begin{pmatrix} \boldsymbol{\beta} & \boldsymbol{\gamma} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}$$

where $\boldsymbol{\beta}$ is an $n_d \times n_d$ matrix for paths or effects from (column) endogenous variables to (row) endogenous variables and $\boldsymbol{\gamma}$ is an $n_d \times n_i$ matrix for paths (effects) from (column) exogenous variables to (row) endogenous variables.

As shown in the matrix partitions, there are four submatrices. The two submatrices at the lower parts are seemingly structured to zeros. However, this should not be interpreted as restrictions imposed by the model. The zero submatrices are artifacts created by the exogenous-endogenous arrangement of the row and column variables. The only restriction on the \mathbf{A} matrix is that the diagonal elements must all be zeros. This implies that the diagonal elements of the submatrix $\boldsymbol{\beta}$ are also zeros. This restriction prevents a direct path from any endogenous variable to itself. There are no restrictions on the pattern of $\boldsymbol{\gamma}$.

It is useful to denote the lower partitions of the \mathbf{A} matrix by \mathbf{A}_{LL} (lower left) and \mathbf{A}_{LR} (lower right) so that

$$\mathbf{A} = \begin{pmatrix} \boldsymbol{\beta} & \boldsymbol{\gamma} \\ \mathbf{A}_{LL} & \mathbf{A}_{LR} \end{pmatrix}$$

Although they are zero matrices in the initial model specification, their entries could become non-zero (paths) in an improved model when you modify your model by using the Lagrange multiplier statistics (see the section “Modification Indices” on page 1346 or the **MODIFICATION** option). Hence, you might need to reference these two submatrices when you apply the customized LM tests on them during the model modification process (see the **LMTESTS** statement).

For the purposes of defining specific parameter regions in customized LM tests, you might also partition the **A** matrix in other ways. First, you can partition **A** into the left and right portions,

$$\mathbf{A} = (\mathbf{A}_{Left} \quad \mathbf{A}_{Right})$$

where \mathbf{A}_{Left} is top-down concatenation of the $\boldsymbol{\beta}$ and \mathbf{A}_{LL} matrices and \mathbf{A}_{Right} is the top-down concatenation of the $\boldsymbol{\gamma}$ and \mathbf{A}_{LR} matrices. Second, you can partition **A** into the upper and lower portions,

$$\mathbf{A} = \begin{pmatrix} \mathbf{A}_{Upper} \\ \mathbf{A}_{Lower} \end{pmatrix}$$

where \mathbf{A}_{Upper} is the side-by-side concatenation of the $\boldsymbol{\beta}$ and $\boldsymbol{\gamma}$ matrices and \mathbf{A}_{Lower} is the side-by-side concatenation of the \mathbf{A}_{LL} and \mathbf{A}_{LR} matrices.

In your initial model, because of the arrangement of the endogenous and exogenous variables \mathbf{A}_{Lower} is a null matrix. But if you improve your model by applying the LM tests on the entries in \mathbf{A}_{Lower} , some of these entries might become free paths in your improved model. Hence, some exogenous variables in your initial model now become endogenous variables in your improved model. For this reason, \mathbf{A}_{Lower} is also designated as a parameter region for *new* endogenous variables, which is exactly what the **NEWENDO** region means in the **LMTESTS** statement.

Partition of the P Matrix

The **P** matrix is partitioned as

$$\mathbf{P} = \begin{pmatrix} \mathbf{P}_{11} & \mathbf{P}'_{21} \\ \mathbf{P}_{21} & \mathbf{P}_{22} \end{pmatrix}$$

where \mathbf{P}_{11} is an $n_d \times n_d$ partial covariance matrix for the endogenous variables, \mathbf{P}_{22} is an $n_i \times n_i$ covariance matrix for the exogenous variables, and \mathbf{P}_{21} is an $n_i \times n_d$ covariance matrix between the exogenous variables and the error terms for the endogenous variables. Because **P** is symmetric, \mathbf{P}_{11} and \mathbf{P}_{22} are also symmetric.

There are virtually no model restrictions placed on these submatrices. However, in most statistical applications, errors for endogenous variables represent unsystematic sources of effects and therefore they are not to be correlated with other systematic sources such as the exogenous variables in the RAM model. This means that in most practical applications \mathbf{P}_{21} would be a null matrix, although this is not enforced in **PROC CALIS**.

Partition of the W Vector

The **W** vector is partitioned as

$$\mathbf{W} = \begin{pmatrix} \boldsymbol{\alpha} \\ \boldsymbol{\nu} \end{pmatrix}$$

where $\boldsymbol{\alpha}$ is an $n_d \times 1$ vector for intercepts of the endogenous variables and $\boldsymbol{\nu}$ is an $n_i \times 1$ vector for the means of the exogenous variables. There is no model restriction on these subvectors.

Summary of Matrices and Submatrices in the RAM Model

Let n_a be the total number of manifest and latent variables in the RAM model. Of these n_a variables, n_d are endogenous and n_i are exogenous. Suppose that the rows and columns of the RAM model matrices **A** and **P** and the rows of **W** are arranged in the order of n_d endogenous variables and then n_i exogenous variables. The names, roles, and dimensions of the RAM model matrices and submatrices are summarized in the following table.

Matrix	Name	Description	Dimensions
Model Matrices			
A	<code>_A_</code> or <code>_RAMA_</code>	Effects of column variables on row variables, or paths from the column variables to the row variables	$n_a \times n_a$
P	<code>_P_</code> or <code>_RAMP_</code>	(Partial) variances and covariances	$n_a \times n_a$
W	<code>_W_</code> or <code>_RAMW_</code>	Intercepts and means	$n_a \times 1$
Submatrices			
β	<code>_RAMBETA_</code>	Effects of endogenous variables on endogenous variables	$n_d \times n_d$
γ	<code>_RAMGAMMA_</code>	Effects of exogenous variables on endogenous variables	$n_d \times n_i$
\mathbf{A}_{LL}	<code>_RAMA_LL_</code>	The null submatrix at the lower left portion of <code>_A_</code>	$n_i \times n_d$
\mathbf{A}_{LR}	<code>_RAMA_LR_</code>	The null submatrix at the lower right portion of <code>_A_</code>	$n_i \times n_i$
\mathbf{A}_{Left}	<code>_RAMA_LEFT_</code>	The left portion of <code>_A_</code> , including β and \mathbf{A}_{LL}	$n_a \times n_d$
\mathbf{A}_{Right}	<code>_RAMA_RIGHT_</code>	The right portion of <code>_A_</code> , including γ and \mathbf{A}_{LR}	$n_a \times n_i$
\mathbf{A}_{Upper}	<code>_RAMA_UPPER_</code>	The upper portion of <code>_A_</code> , including β and γ	$n_d \times n_a$
\mathbf{A}_{Lower}	<code>_RAMA_LOWER_</code>	The lower portion of <code>_A_</code> , including \mathbf{A}_{LL} and \mathbf{A}_{LR}	$n_i \times n_a$
\mathbf{P}_{11}	<code>_RAMP11_</code>	Error variances and covariances for endogenous variables	$n_d \times n_d$
\mathbf{P}_{21}	<code>_RAMP21_</code>	Covariances between exogenous variables and error terms for endogenous variables	$n_d \times n_i$
\mathbf{P}_{22}	<code>_RAMP22_</code>	Variances and covariances for exogenous variables	$n_i \times n_i$
α	<code>_RAMALPHA_</code>	Intercepts for endogenous variables	$n_d \times 1$
ν	<code>_RAMNU_</code>	Means for exogenous variables	$n_i \times 1$

Specification of the RAM Model

In PROC CALIS, the RAM model specification is a matrix-oriented modeling language. That is, you have to define the row and column variables for the model matrices and specify the parameters in terms of matrix entries. The VAR= option specifies the variables (including manifest and latent) in the model. For example, the following statement specifies five variables in the model:

RAM

```
var= v1 v2 v3;
```

The order of variables in the VAR= option is important. The same order is used for the row and column variables in the model matrices. After you specify the variables in the model, you can specify three types of parameters, which correspond to the elements in the three model matrices. The three types of RAM entries are described in the following.

(1) Specification of Effects or Paths in Model Matrix A

If there is a path from V2 to V1 in your model and the associated effect parameter is named parm1 with 0.5 as the starting value, you can use the following RAM statement:

RAM

```
var= v1 v2 v3,
_A_ 1 2 parm1(0.5);
```

The *ram-entry* that starts with `_A_` means that an element of the ram matrix A is being specified. The row number and the column number of this element are 1 and 2, respectively. With reference to the VAR= list, the row number 1 refers to variable v1, and the column number 2 refers to variable v2. Therefore, the effect of V2 on V1 is a parameter named parm1, with an initial value of 0.5.

You can specify fixed values in the *ram-entries* too. Suppose the effect of v3 on v1 is fixed at 1.0. You can use the following specification:

RAM

```
var= v1 v2 v3,
_A_ 1 2 parm1(0.5),
_A_ 1 3 1.0;
```

(2) Specification of the Latent Factors in the Model

In the RAM model, you specify the list of variables in VAR= list of the RAM statement. The list of variables can include the latent variables in the model. Because observed variables have references in the input data sets, those variables that do not have references in the data sets are treated as latent factors automatically. Unlike the LINEQS model, you do not need to use 'F' or 'f' prefix to denote latent factors in the RAM model. It is recommended that you use meaningful names for the latent factors. See the section “[Naming Variables and Parameters](#)” on page 1302 for the general rules about naming variables and parameters.

For example, suppose that SES_Factor and Education_Factor are names that are not used as variable names in the input data set. These two names represent two latent factors in the model, as shown in the following specification:

RAM

```
var= v1 v2 v3 SES_FACTOR Education_Factor,
_A_ 1 4 b1,
_A_ 2 5 b2,
_A_ 3 5 1.0;
```

This specification shows that the effect of SES_Factor on v1 is a free parameter named b1, and the effects of Education_Factor on v2 and v3 are a free parameter named b2 and a fixed value of 1.0, respectively.

However, naming latent factors is not compulsory. The preceding specification is equivalent to the following specification:

```
RAM
var= v1 v2 v3,
_A_  1   4  b1,
_A_  2   5  b2,
_A_  3   5  1.0;
```

Although you do not name the fourth and the fifth variables in the VAR= list, PROC CALIS generates the names for these two latent variables. In this case, the fourth variable is named `_Factor1` and the fifth variable is named `_Factor2`.

(3) Specification of (Partial) Variances and (Partial) Covariances in Model Matrix P

Suppose now you want to specify the variance of `v2` as a free parameter named `parm2`. You can add a new *ram-entry* for this variance parameter, as shown in the following statement:

```
RAM
var= v1 v2 v3,
_A_  1   2  parm1(0.5),
_A_  1   3  1.0,
_P_  2   2  parm2;
```

The *ram-entry* that starts with `_P_` means that an element of the RAM matrix **P** is being specified. The (2,2) element of **P**, which is the variance of `v2`, is a parameter named `parm2`. You do not specify an initial value for this parameter.

You can also specify the error variance of `v1` similarly, as shown in the following statement:

```
RAM
var= v1 v2 v3,
_A_  1   2  parm1(0.5),
_A_  1   3  1.0,
_P_  2   2  parm2,
_P_  1   1;
```

In the last *ram-entry*, the (1,1) element of **P**, which is the error variance of `v1`, is an unnamed free parameter.

Covariance parameters are specified in the same manner. For example, the following specification adds a *ram-entry* for the covariance parameter between `v2` and `v3`:

```
RAM
var= v1 v2 v3,
_A_  1   2  parm1(0.5),
_A_  1   3  1.0,
_P_  2   2  parm2,
_P_  1   1,
_P_  2   3  (.5);
```

The covariance between `v2` and `v3` is an unnamed parameter with an initial value of 0.5.

(4) Specification of Means and Intercepts in Model Matrix W

To specifying means or intercepts, you need to start the *ram-entries* with the `_W_` keyword. For example, the last two entries of following statement specify the intercept of `v1` and the mean of `v2`, respectively:

RAM

```

var= v1 v2 v3,
_A_  1  2  parm1 (0.5),
_A_  1  3  1.0,
_P_  2  2  parm2,
_P_  1  1  ,
_P_  2  3  (.5),
_W_  1  1  int_v1,
_W_  2  2  mean_v2;

```

The intercept of v1 is a free parameter named `int_v1`, and the mean of v2 is a free parameter named `mean_v2`.

Default Parameters in the RAM Model

There are two types of default of parameters of the RAM model in PROC CALIS. One is the free parameters; the other is the fixed zeros.

By default, certain sets of model matrix elements in the RAM model are free parameters. These parameters are set automatically by PROC CALIS, although you can also specify them explicitly in the *ram-entries*. In general, default free parameters enable you to specify only what are absolutely necessary for defining your model. PROC CALIS automatically sets those commonly assumed free parameters so that you do not need to specify them routinely. The sets of default free parameters of the RAM model are as follows:

- Diagonal elements of the `_P_` matrix—this includes the variance of exogenous variables (latent or observed) and error variances of all endogenous variables (latent or observed)
- The off-diagonal elements that pertain to the exogenous variables of the `_P_` matrix—this includes all the covariances among exogenous variables, latent or observed
- If the mean structures are modeled, the elements that pertain to the observed variables (but not the latent variables) in the `_W_` vector— this includes all the means of exogenous observed variables and the intercepts of all endogenous observed variables

For example, suppose you are fitting a RAM model with three observed variables `x1`, `x2`, and `y3`, you specify a simple multiple-regression model with `x1` and `x2` predicting `y3` by the following statements:

```

proc calis meanstr;
  ram var= x1-x2 y3,
      _A_ 3 1 ,
      _A_ 3 2 ;

```

In the RAM statement, you specify that path coefficients represented by `_A_[3,1]` and `_A_[3,2]` are free parameters in the model. In addition to these free parameters, PROC CALIS sets several other free parameters by default. `_P_[1,1]`, `_P_[2,2]`, and `_P_[3,3]` are set as free parameters for the variance of `x1`, the variance of `x2`, and the error variance of `x3`, respectively. `_P_[2,1]` (and hence `_P_[1,2]`) is set as a free parameter for the covariance between the exogenous variables `x1` and `x2`. Because the mean structures are also analyzed by the `MEANSTR` option in the PROC CALIS statement, `_W_[1,1]`, `_W_[2,1]`, and `_W_[3,1]` are also set as free parameters for the mean of `x1`, the mean of `x2`, and the intercept of `x3`, respectively. In the current situation, this default parameterization is consistent with using PROC REG for multiple regression analysis, where you only need to specify the functional relationships among variables.

If a matrix element is not a default free parameter in the RAM model, then it is a fixed zero by default. You can override almost all default fixed zeros in the RAM model matrices by specifying the *ram-entries*. The diagonal elements of the *_A_* matrix are exceptions. These elements are always fixed zeros. You cannot set these elements to free parameters or other fixed values—this reflects a model restriction that prevents a variable from having a direct effect on itself.

Naming Variables and Parameters

Follow these rules when you name your variables:

- Use the usual naming conventions of the SAS System.
- Variable names are not more than 32 characters.
- When you create latent variable names, make sure that they are not used in the input data set that is being analyzed.
- For the LINEQS model, error or disturbance variables must start with ‘E’, ‘e’, ‘D’, or ‘d’.
- For the LINEQS model, non-error-type latent variables (that is, factors) must start with ‘F’ or ‘f’.
- For modeling languages other than LINEQS, names for errors or disturbances are not needed. As a result, you do not need to distinguish latent factors from errors or disturbances by using particular prefixes. Variable names that are not referenced in the analyzed data set are supposed to be latent factors.
- You should not use Intercept (case-insensitive) as a variable name in your data set or as a latent variable name in your model.

Follow these rules when you name your parameters:

- Use the usual naming conventions of the SAS System.
- Parameter names are not more than 32 characters.
- Use a prefix-name when you want to generate new parameter names automatically. A prefix-name contains a short string of characters called a “root,” followed by double underscores ‘__’. Each occurrence of such a prefix-name generates a new parameter name by replacing the two trailing underscores with a unique integer. For example, occurrences of Gen__ generate Gen1, Gen2, and so on.
- A special prefix-name is the one without a root—that is, it contains only double underscores ‘__’. Occurrences of ‘__’ generate _Parm1, _Parm2, and so on.
- PROC CALIS generates parameter names for default parameters to safeguard ill-defined models. These generated parameter names start with the *_Add* prefix and unique integer suffixes. For example, *_Add1*, *_Add2*, and so on.
- Avoid using parameter names that start with either *_*, *_Add*, or *_Parm*. These names might get confused with the names generated by PROC CALIS. The confusion might lead to unintended constraints to your model if the parameter names that you use match those generated by PROC CALIS.

- Avoid using parameter names that are roots of prefix-names. For example, you should not use `Gen` as a parameter name if `Gen__` is also used in the same model specification. Although violation of this rule might not distort the model specification, it might cause ambiguities and confusion.

Finally, parameter names and variable names in PROC CALIS are not distinguished by explicit declarations. That is, a valid SAS name can be used as a parameter name or a variable name in any model that is supported by PROC CALIS. Whether a name in a model specification is for a parameter or a variable is determined by the syntactic structure. For example, consider the following path specification:

```
proc calis;
  path
    a ==> b    = c;
run;
```

PROC CALIS parses the path specification according to the syntactic structure of the PATH statement and determines that `a` and `b` are variable names and `c` is a parameter name. Consider another specification as follows:

```
proc calis;
  path
    a ==> b    = b;
run;
```

This is a syntactically correct specification. Variables `a` and `b` are defined in a path relationship with a path coefficient parameter also named `b`. While such a name conflict between parameter and variable names would not confuse PROC CALIS in terms of model specification and fitting, it would create unnecessary confusion in programming and result interpretations. Hence, using parameter names that match variable names exactly is a bad practice and should be avoided.

Setting Constraints on Parameters

The CALIS procedure offers a very flexible way to constrain parameters. There are two main methods for specifying constraints. One is explicit specification by using specially designed statements for constraints. The other is implicit specification by using the [SAS programming statements](#).

Explicit Specification of Constraints

Explicit constraints can be set in the following ways:

- specifying boundary constraints on independent parameters in the [BOUNDS](#) statement
- specifying general linear equality and inequality constraints on independent parameters in the [LIN-CON](#) statement
- specifying general nonlinear equality and inequality constraints on parametric functions in the [NLIN-CON](#) statement

BOUNDS Statement

You can specify one-sided or two-sided boundaries on independent parameters in the **BOUNDS** statement. For example, in the following statement you constrain parameter `var1` to be nonnegative and parameter `effect` to be between 0 and 5.

```
bounds    var1 >= 0,
          0. <= effect <= 5.;
```

Note that if your upper and lower bounds are the same for a parameter, it effectively sets a fixed value for that parameter. As a result, PROC CALIS will reduce the number of independent parameters by one automatically. Note also that only independent parameters are allowed to be bounded in the **BOUNDS** statement.

LINCON Statement

You can specify equality or inequality linear constraints on independent parameters in the **LINCON** statement. For example, in the following statement you specify a linear inequality constraint on parameters `beta1`, `beta2`, and `beta3` and an equality constraint on parameters `gamma1` and `gamma2`.

```
lincon   beta1 - .5 * beta2 - .5 * beta3 >= 0.,
          gamma1 - gamma2 = 0.;
```

In the inequality constraint, `beta1` is set to be at least as large as the average of `beta2` and `beta3`. In the equality constraint, `gamma1` and `gamma2` are set to be equal. Note that in PROC CALIS a nonredundant linear equality constraint on independent parameters effectively reduces the number of parameters by one.

NLINCON Statement

You can specify equality or inequality nonlinear constraints for parameters in the **NLINCON** statement. While you can only constrain the independent parameters in the **BOUNDS** and the **LINCON** statements, you can constrain any of the following in the **NLINCON** statement:

- independent parameters
- dependent parameters
- parametric functions computed by the SAS programming statements

For example, consider the following statements:

```
nlincon
  IndParm >= 0,           /* constraint 1 */
  0 <= DepParm <= 10,    /* constraint 2 */
  ParmFunc1 >= 3,        /* constraint 3 */
  0 <= ParmFunc2 <= 8;   /* constraint 4 */

/* SAS Programming statements in the following */
DepParm   = Indparm1 + IndParm5;
ParmFunc1 = IndParm1 - .5 * IndParm2 - .5 * IndParm3;
ParmFunc2 = (IndParm1 - 7.)**2 + SQRT(DepParm * IndParm4) * ParmFunc1;
```

You specify four nonlinear constraints by using the `NLINCON` statement. Labeled in a comment as “constraint 1” is a one-sided boundary constraint for independent parameter `IndParm`. Labeled in a comment as “constraint 2” is a two-sided boundary constraint for dependent parameter `DepParm`. Labeled in a comment as “constraint 3” is a one-sided inequality constraint on parametric function named `ParmFunc1`. Finally, labeled in a comment as “constraint 4” is a two-sided inequality constraint on parametric function named `ParmFunc2`. Parametric functions `ParmFunc1` and `ParmFunc2` are defined and computed in the [SAS programming statements](#) after the `NLINCON` statement specification.

Constraint 1 could have been set in the `BOUNDS` statement because it is just a simple boundary constraint on an independent parameter. Constraint 3 could have been set in the `LINCON` statement because the definition of `ParmFunc1` in a SAS programming statement shows that it is a linear function of independent parameters. The purpose of including these special cases of “nonlinear constraints” in this example is to show the flexibility of the `NLINCON` statement. However, whenever possible, the `BOUNDS` or the `LINCON` statement specification should be considered first because computationally they are more efficient than the equivalent specification in the `NLINCON` statement.

Specification in the `NLINCON` statement becomes necessary when you want to constrain dependent parameters or nonlinear parametric functions. For example, constraint 2 is a two-sided boundary constraint on the dependent parameter `DepParm`, which is defined as a linear function of independent parameters in a SAS programming statement. Constraints on dependent parameters are not allowed in the `BOUNDS` statement. Constraint 4 is a two-sided inequality constraint on the nonlinear parametric function `ParmFunc2`, which is defined as a nonlinear function of other parametric functions and parameters in the [SAS programming statements](#). Again, you cannot use the `LINCON` statement to specify nonlinear constraints.

Implicit Constraint Specification

An implicit way to specify constraints is to use your own [SAS programming statements](#) together with the `PARAMETERS` statement to express special properties of the parameter estimates. This kind of reparameterization tool is also present in McDonald’s COSAN implementation (McDonald 1978) but is considerably easier to use in the CALIS procedure. PROC CALIS is able to compute analytic first- and second-order derivatives that you would have to specify using the COSAN program.

Some traditional ways to enforce parameter constraints by using reparameterization or parameter transformation (McDonald 1980) are considered in the following:

- **one-sided boundary constraints of the form:**

$$q \geq a \quad \text{or} \quad q \leq b$$

where the parameter of interest is q , which should be at least as large as (or at most as small as) a given constant value a (or b). This inequality constraint can be expressed as an equality constraint:

$$q = a + x^2 \quad \text{or} \quad q = b - x^2$$

in which the new parameter x is unconstrained.

For example, inequality constraint $q \geq 7$ can be accomplished by the following statements:

```
parameters x (0.);
q = 7 + x * x;
```

In this specification, you essentially redefine q as a parametric function of x , which is not constrained and has a starting value at 0.

- **two-sided boundary constraints of the form:**

$$a \leq q \leq b$$

where the parameter of interest is q , which should be located between two given constant values a and b , with $a < b$. This inequality constraint can be expressed as the following equality constraint:

$$q = a + (b - a) \frac{\exp(x)}{1 + \exp(x)}$$

where the new parameter x is unconstrained.

For example, to implement $1 \leq q \leq 5$ in PROC CALIS, you can use the following statements:

```
parameters x (0.);
u = exp(x);
q = 1 + 4 * u / (1 + u);
```

In this specification, q becomes a dependent parameter which is nonlinearly related to independent parameter x , which is an independent parameter defined in the **PARAMETERS** statement with a starting value of 0.

- **one-sided order constraints of the form:**

$$q_1 \leq q_2, \quad q_1 \leq q_3, \quad \dots, \quad q_1 \leq q_k$$

where q_1, \dots, q_k are the parameters of interest. These inequality constraints can be expressed as the following set of equality constraints:

$$q_1 = x_1, \quad q_2 = x_1 + x_2^2, \quad \dots, \quad q_k = x_1 + x_k^2$$

where the new parameters x_1, \dots, x_k are unconstrained.

For example, to implement $q_1 \leq q_2$, $q_1 \leq q_3$, and $q_1 \leq q_4$ simultaneously, you can use the following statements:

```
parameters x1-x4 (4*0.);
q1 = x1;
q2 = x1 + x2 * x2;
q3 = x1 + x3 * x3;
q4 = x1 + x4 * x4;
```

In this specification, you essentially redefine $q_1 - q_4$ as dependent parameters that are functions of $x_1 - x_4$, which are defined as independent parameters in the **PARAMETERS** statement with starting values of zeros. No constraints on x_i 's are needed. The way that q_i 's are computed in the SAS programming statements guarantees the required order constraints on q_i 's are satisfied.

- **two-sided order constraints of the form:**

$$q_1 \leq q_2 \leq q_3 \leq \dots \leq q_k$$

These inequality constraints can be expressed as the following set of equality constraints:

$$q_1 = x_1, \quad q_2 = q_1 + x_2^2, \quad \dots \quad q_k = q_{k-1} + x_k^2$$

where the new parameters x_1, \dots, x_k are unconstrained.

For example, to implement $q_1 \leq q_2 \leq q_3 \leq q_4$ simultaneously, you can use the following statements:

```
parameters x1-x4 (4*0.);
q1 = x1;
q2 = q1 + x2 * x2;
q3 = q2 + x3 * x3;
q4 = q3 + x4 * x4;
```

In this specification, you redefine $q_1 - q_4$ as dependent parameters that are functions of $x_1 - x_4$, which are defined as independent parameters in the **PARAMETERS** statement. Each x_i has a starting value of zero without being constrained in estimation. The order relation of q_i 's are satisfied by the way they are computed in the **SAS programming statements**.

- **linear equation constraints of the form:**

$$\sum_i^k b_i q_i = a$$

where q_i 's are the parameters of interest, b_i 's are constant coefficients, a is a constant, and k is an integer greater than one. This linear equation can be expressed as the following system of equations with unconstrained new parameters x_1, x_2, \dots, x_k :

$$q_i = x_i / b_i \quad (i < k)$$

$$q_k = (a - \sum_j^{k-1} x_j) / b_k$$

For example, consider the following linear constraint on independent parameters $q_1 - q_3$:

$$3q_1 + 2q_2 - 5q_3 = 8$$

You can use the following statements to implement the linear constraint:

```
parameters x1-x2 (2*0.);
q1 = x1 / 3;
q2 = x2 / 2;
q3 = -(8 - x1 - x2) / 5;
```

In this specification, $q_1 - q_3$ become dependent parameters that are functions of x_1 and x_2 . The linear constraint on q_1 and q_3 are satisfied by the way they are computed. In addition, after reparameterization the number of independent parameters drops to two.

See McDonald (1980) and Browne (1982) for further notes on reparameterization techniques.

Explicit or Implicit Specification of Constraints?

Explicit and implicit constraint techniques differ in their specifications and lead to different computational steps in optimizing a solution. The explicit constraint specification that uses the supported statements incurs additional computational routines within the optimization steps. In contrast, the implicit reparameterization method does not incur additional routines for evaluating constraints during the optimization. Rather, it changes the constrained problem to a non-constrained one. This costs more in computing function derivatives and in storing parameters.

If the optimization problem is small enough to apply the Levenberg-Marquardt or Newton-Raphson algorithm, use the `BOUNDS` and the `LINCON` statements to set explicit boundary and linear constraints. If the problem is so large that you must use a quasi-Newton or conjugate gradient algorithm, reparameterization techniques might be more efficient than the `BOUNDS` and `LINCON` statements.

Automatic Variable Selection

When you specify your model, you use the `main` and `subsidiary` model statements to define variable relationships and parameters. PROC CALIS checks the variables mentioned in these statements against the variable list of the input data set. If a variable in your model is also found in your data set, PROC CALIS knows that it is a manifest variable. Otherwise, it is either a latent variable or an invalid variable.

To save computational resources, only manifest variables defined in your model are automatically selected for analysis. For example, even if you have 100 variables in your input data set, only a covariance matrix of 10 manifest variables is computed for the analysis of the model if only 10 variables are selected for analysis.

In some special circumstances, the automatic variable selection performed for the analysis might be a drawback. For example, if you are interested in modification indices connected to some of the variables that are not used in the model, automatic variable selection in the specification stage will exclude those variables from consideration in computing modification indices. Fortunately, a little trick can be done. You can use the `VAR` statement to include as many exogenous manifest variables as needed. Any variables in the `VAR` statement that are defined in the input data set but are not used in the `main` and `subsidiary` model specification statements are included in the model as exogenous manifest variables.

For example, the first three steps in a stepwise regression analysis of the Werner Blood Chemistry data (Jöreskog and Sörbom 1988, p. 111) can be performed as follows:

```
proc calis data=dixon method=glS nobs=180 print mod;
  var    x1-x7;
  lineqs y = e;
  variance    e = var;
run;
proc calis data=dixon method=glS nobs=180 print mod;
  var    x1-x7;
  lineqs y = g1 x1 + e;
  variance    e = var;
run;
proc calis data=dixon method=glS nobs=180 print mod;
  var    x1-x7;
  lineqs y = g1 x1 + g6 x6 + e;
  variance    e = var;
run;
```

In the first analysis, no independent manifest variables are included in the regression equation for dependent variable y . However, x_1 – x_7 are specified in the **VAR** statement so that in computing the Lagrange multiplier tests these variables would be treated as potential predictors in the regression equation for dependent variable y . Similarly, in the next analysis, x_1 is already a predictor in the regression equation, while x_2 – x_7 are treated as potential predictors in the LM tests. In the last analysis, x_1 and x_6 are predictors in the regression equation, while other x -variables are treated as potential predictors in the LM tests.

Estimation Criteria

The following seven estimation methods are available in PROC CALIS:

- unweighted least squares (ULS)
- full information maximum likelihood (FIML)
- generalized least squares (GLS)
- normal-theory maximum likelihood (ML)
- weighted least squares (WLS, ADF)
- diagonally weighted least squares (DWLS)
- robust estimation (ROBUST) under the normal theory (ML)

Default weight matrices \mathbf{W} are computed for GLS, WLS, and DWLS estimation. You can also provide your own weight matrices by using an **INWGT=** data set. The weight matrices in these estimation methods provide weights for the moment matrices. In contrast, weights that are applied to individual observations are computed in robust estimation. These observation weights are updated during iteration steps of robust estimation. The ULS, GLS, ML, WLS, ADF, and DWLS methods can analyze sample moment matrices as well as raw data, while the FIML and robust methods must analyze raw data.

PROC CALIS does not implement all estimation methods in the field. As mentioned in the section “**Overview: CALIS Procedure**” on page 1040, partial least squares (PLS) is not implemented. The PLS method is developed under less restrictive statistical assumptions. It circumvents some computational and theoretical problems encountered by the existing estimation methods in PROC CALIS; however, PLS estimates are less efficient in general. When the statistical assumptions of PROC CALIS are tenable (for example, large sample size, correct distributional assumptions, and so on), ML, GLS, or WLS methods yield better estimates than the PLS method. Note that there is a SAS/STAT procedure called PROC PLS that employs the partial least squares technique, but for a different class of models than those of PROC CALIS. For example, in a PROC CALIS model each latent variable is typically associated with only a subset of manifest variables (predictor or outcome variables). However, in PROC PLS latent variables are not prescribed with subsets of manifest variables. Rather, they are extracted from linear combinations of all manifest predictor variables. Therefore, for general path analysis with latent variables you should use PROC CALIS.

ULS, GLS, and ML Discrepancy Functions

In each estimation method, the parameter vector is estimated iteratively by a nonlinear optimization algorithm that minimizes a discrepancy function F , which is also known as the fit function in the literature. With p denoting the number of manifest variables, \mathbf{S} the sample $p \times p$ covariance matrix for a sample with size N , $\bar{\mathbf{x}}$ the $p \times 1$ vector of sample means, $\boldsymbol{\Sigma}$ the fitted covariance matrix, and $\boldsymbol{\mu}$ the vector of fitted means, the discrepancy function for unweighted least squares (ULS) estimation is:

$$F_{ULS} = 0.5\text{Tr}[(\mathbf{S} - \boldsymbol{\Sigma})^2] + (\bar{\mathbf{x}} - \boldsymbol{\mu})'(\bar{\mathbf{x}} - \boldsymbol{\mu})$$

The discrepancy function for generalized least squares estimation (GLS) is:

$$F_{GLS} = 0.5\text{Tr}[(\mathbf{W}^{-1}(\mathbf{S} - \boldsymbol{\Sigma}))^2] + (\bar{\mathbf{x}} - \boldsymbol{\mu})'\mathbf{W}^{-1}(\bar{\mathbf{x}} - \boldsymbol{\mu})$$

By default, $\mathbf{W} = \mathbf{S}$ is assumed so that F_{GLS} is the normal theory generalized least squares discrepancy function.

The discrepancy function for normal-theory maximum likelihood estimation (ML) is:

$$F_{ML} = \text{Tr}(\mathbf{S}\boldsymbol{\Sigma}^{-1}) - p + \ln(|\boldsymbol{\Sigma}|) - \ln(|\mathbf{S}|) + (\bar{\mathbf{x}} - \boldsymbol{\mu})'\boldsymbol{\Sigma}^{-1}(\bar{\mathbf{x}} - \boldsymbol{\mu})$$

In each of the discrepancy functions, \mathbf{S} and $\bar{\mathbf{x}}$ are considered to be given and $\boldsymbol{\Sigma}$ and $\boldsymbol{\mu}$ are functions of model parameter vector $\boldsymbol{\Theta}$. That is:

$$F = F(\boldsymbol{\Sigma}(\boldsymbol{\Theta}), \boldsymbol{\mu}(\boldsymbol{\Theta}); \mathbf{S}, \bar{\mathbf{x}})$$

Estimating $\boldsymbol{\Theta}$ by using a particular estimation method amounts to choosing a vector $\boldsymbol{\theta}$ that minimizes the corresponding discrepancy function F .

When the mean structures are not modeled or when the mean model is saturated by parameters, the last term of each fit function vanishes. That is, they become:

$$F_{ULS} = 0.5\text{Tr}[(\mathbf{S} - \boldsymbol{\Sigma})^2]$$

$$F_{GLS} = 0.5\text{Tr}[(\mathbf{W}^{-1}(\mathbf{S} - \boldsymbol{\Sigma}))^2]$$

$$F_{ML} = \text{Tr}(\mathbf{S}\boldsymbol{\Sigma}^{-1}) - p + \ln(|\boldsymbol{\Sigma}|) - \ln(|\mathbf{S}|)$$

If, instead of being a covariance matrix, \mathbf{S} is a correlation matrix in the discrepancy functions, $\boldsymbol{\Sigma}$ would naturally be interpreted as the fitted correlation matrix. Although whether \mathbf{S} is a covariance or correlation matrix makes no difference in minimizing the discrepancy functions, correlational analyses that use these functions are problematic because of the following issues:

- The diagonal of the fitted correlation matrix $\boldsymbol{\Sigma}$ might contain values other than ones, which violates the requirement of being a correlation matrix.
- Whenever available, standard errors computed for correlation analysis in PROC CALIS are straightforward generalizations of those of covariance analysis. In very limited cases these standard errors are good approximations. However, in general they are not even asymptotically correct.
- The model fit chi-square statistic for correlation analysis might not follow the theoretical distribution, thus making model fit testing difficult.

Despite these issues in correlation analysis, if your primary interest is to obtain the estimates in the correlation models, you might still find PROC CALIS results for correlation analysis useful.

The statistical techniques used in PROC CALIS are primarily developed for the analysis of covariance structures, and hence **COVARIANCE** is the default option. Depending on the nature of your research, you can add the mean structures in the analysis by specifying mean and intercept parameters in your models. However, you cannot analyze mean structures simultaneously with correlation structures (see the **CORRELATION** option) in PROC CALIS.

FIML Discrepancy Function

The full information maximum likelihood method (FIML) assumes multivariate normality of the data. Suppose that you analyze a model that contains p observed variables. The discrepancy function for FIML is

$$F_{FIML} = \frac{1}{N} \sum_{j=1}^N (\ln(|\Sigma_j|) + (\mathbf{x}_j - \boldsymbol{\mu}_j)' \Sigma_j^{-1} (\mathbf{x}_j - \boldsymbol{\mu}_j) + K_j)$$

where \mathbf{x}_j is a data vector for observation j , and K_j is a constant term (to be defined explicitly later) independent of the model parameters Θ . In the current formulation, \mathbf{x}_j 's are not required to have the same dimensions. For example, \mathbf{x}_1 could be a complete vector with all p variables present while \mathbf{x}_2 is a $(p-1) \times 1$ vector with one missing value that has been excluded from the original $p \times 1$ data vector. As a consequence, subscript j is also used in $\boldsymbol{\mu}_j$ and Σ_j to denote the submatrices that are extracted from the entire $p \times 1$ structured mean vector $\boldsymbol{\mu}$ ($\boldsymbol{\mu} = \boldsymbol{\mu}(\Theta)$) and $p \times p$ covariance matrix Σ ($\Sigma = \Sigma(\Theta)$). In other words, in the current formulation $\boldsymbol{\mu}_j$ and Σ_j do not mean that each observation is fitted by distinct mean and covariance structures (although theoretically it is possible to formulate FIML in such a way). The notation simply signifies that the dimensions of \mathbf{x}_j and of the associated mean and covariance structures could vary from observation to observation.

Let p_j be the number of variables without missing values for observation j . Then \mathbf{x}_j denotes a $p_j \times 1$ data vector, $\boldsymbol{\mu}_j$ denotes a $p_j \times 1$ vector of means (structured with model parameters), Σ_j is a $p_j \times p_j$ matrix for variances and covariances (also structured with model parameters), and K_j is defined by the following formula, which is a constant term independent of model parameters:

$$K_j = \ln(2\pi) * p_j$$

As a general estimation method, the FIML method is based on the same statistical principle as the ordinary maximum likelihood (ML) method for multivariate normal data—that is, both methods maximize the normal theory likelihood function given the data. In fact, F_{FIML} used in PROC CALIS is related to the log-likelihood function L by the following formula:

$$F_{FIML} = \frac{-2L}{N}$$

Because the FIML method can deal with observations with various levels of information available, it is primarily developed as an estimation method that could deal with data with random missing values. See the section “[Relationships among Estimation Criteria](#)” on page 1318 for more details about the relationship between FIML and ML methods.

Whenever you use the FIML method, the mean structures are automatically assumed in the analysis. This is due to fact that there is no closed-form formula to obtain the saturated mean vector in the FIML discrepancy function if missing values are present in the data. You can certainly provide explicit specification of the

mean parameters in the model by specifying intercepts in the **LINEQS** statement or means and intercepts in the **MEAN** or **MATRIX** statement. However, usually you do not need to do the explicit specification if all you need to achieve is to saturate the mean structures with p parameters (that is, the same number as the number of observed variables in the model). With **METHOD=FIML**, PROC CALIS uses certain default parameterizations for the mean structures automatically. For example, all intercepts of endogenous observed variables and all means of exogenous observed variables are default parameters in the model, making the explicit specification of these mean structure parameters unnecessary.

WLS and ADF Discrepancy Functions

Another important discrepancy function to consider is the weighted least squares (WLS) function. Let $\mathbf{u} = (\mathbf{s}, \bar{\mathbf{x}})$ be a $p(p+3)/2$ vector containing all nonredundant elements in the sample covariance matrix \mathbf{S} and sample mean vector $\bar{\mathbf{x}}$, with $\mathbf{s} = \text{vecs}(\mathbf{S})$ representing the vector of the $p(p+1)/2$ lower triangle elements of the symmetric matrix \mathbf{S} , stacking row by row. Similarly, let $\boldsymbol{\eta} = (\boldsymbol{\sigma}, \boldsymbol{\mu})$ be a $p(p+3)/2$ vector containing all nonredundant elements in the fitted covariance matrix $\boldsymbol{\Sigma}$ and the fitted mean vector $\boldsymbol{\mu}$, with $\boldsymbol{\sigma} = \text{vecs}(\boldsymbol{\Sigma})$ representing the vector of the $p(p+1)/2$ lower triangle elements of the symmetric matrix $\boldsymbol{\Sigma}$.

The WLS discrepancy function is:

$$F_{WLS} = (\mathbf{u} - \boldsymbol{\eta})' \mathbf{W}^{-1} (\mathbf{u} - \boldsymbol{\eta})$$

where \mathbf{W} is a positive definite symmetric weight matrix with $(p(p+3)/2)$ rows and columns. Because $\boldsymbol{\eta}$ is a function of model parameter vector $\boldsymbol{\Theta}$ under the structural model, you can write the WLS function as:

$$F_{WLS} = (\mathbf{u} - \boldsymbol{\eta}(\boldsymbol{\Theta}))' \mathbf{W}^{-1} (\mathbf{u} - \boldsymbol{\eta}(\boldsymbol{\Theta}))$$

Suppose that \mathbf{u} converges to $\boldsymbol{\eta}_o = (\boldsymbol{\sigma}_o, \boldsymbol{\mu}_o)$ with increasing sample size, where $\boldsymbol{\sigma}_o$ and $\boldsymbol{\mu}_o$ denote the population covariance matrix and mean vector, respectively. By default, the WLS weight matrix \mathbf{W} in PROC CALIS is computed from the raw data as a consistent estimate of the asymptotic covariance matrix $\boldsymbol{\Gamma}$ of $\sqrt{N}(\mathbf{u} - \boldsymbol{\eta}_o)$, with $\boldsymbol{\Gamma}$ partitioned as

$$\boldsymbol{\Gamma} = \begin{pmatrix} \boldsymbol{\Gamma}_{ss} & \boldsymbol{\Gamma}'_{\bar{x}s} \\ \boldsymbol{\Gamma}_{\bar{x}s} & \boldsymbol{\Gamma}_{\bar{x}\bar{x}} \end{pmatrix}$$

where $\boldsymbol{\Gamma}_{ss}$ denotes the $(p(p+1)/2) \times (p(p+1)/2)$ asymptotic covariance matrix for $\sqrt{N}(\mathbf{s} - \boldsymbol{\sigma}_o)$, $\boldsymbol{\Gamma}_{\bar{x}\bar{x}}$ denotes the $p \times p$ asymptotic covariance matrix for $\sqrt{N}(\bar{\mathbf{x}} - \boldsymbol{\mu}_o)$, and $\boldsymbol{\Gamma}_{\bar{x}s}$ denotes the $p \times (p(p+1)/2)$ asymptotic covariance matrix between $\sqrt{N}(\bar{\mathbf{x}} - \boldsymbol{\mu}_o)$ and $\sqrt{N}(\mathbf{s} - \boldsymbol{\sigma}_o)$.

To compute the default weight matrix \mathbf{W} as a consistent estimate of $\boldsymbol{\Gamma}$, define a similar partition of the weight matrix \mathbf{W} as:

$$\mathbf{W} = \begin{pmatrix} \mathbf{W}_{ss} & \mathbf{W}'_{\bar{x}s} \\ \mathbf{W}_{\bar{x}s} & \mathbf{W}_{\bar{x}\bar{x}} \end{pmatrix}$$

Each of the submatrices in the partition can now be computed from the raw data. First, define the biased sample covariance for variables i and j as:

$$t_{ij} = \frac{1}{N} \sum_{r=1}^N (x_{ri} - \bar{x}_i)(x_{rj} - \bar{x}_j)$$

and the sample fourth-order central moment for variables i, j, k , and l as:

$$t_{ij,kl} = \frac{1}{N} \sum_{r=1}^N (x_{ri} - \bar{x}_i)(x_{rj} - \bar{x}_j)(x_{rk} - \bar{x}_k)(x_{rl} - \bar{x}_l)$$

The submatrices in \mathbf{W} are computed by:

$$[\mathbf{W}_{ss}]_{ij,kl} = t_{ij,kl} - t_{ij}t_{kl}$$

$$[\mathbf{W}_{\bar{x}s}]_{i,kl} = \frac{1}{N} \sum_{r=1}^N (x_{ri} - \bar{x}_i)(x_{rk} - \bar{x}_k)(x_{rl} - \bar{x}_l)$$

$$[\mathbf{W}_{\bar{x}\bar{x}}]_{ij} = t_{ij}$$

Assuming the existence of finite eighth-order moments, this default weight matrix \mathbf{W} is a consistent but biased estimator of the asymptotic covariance matrix $\mathbf{\Gamma}$.

By using the `ASYCOV=` option, you can use Browne's unbiased estimator (Browne 1984, formula (3.8)) of $\mathbf{\Gamma}_{ss}$ as:

$$[\mathbf{W}_{ss}]_{ij,kl} = \frac{N(N-1)}{(N-2)(N-3)}(t_{ij,kl} - t_{ij}t_{kl}) - \frac{N}{(N-2)(N-3)}(t_{ik}t_{jl} + t_{il}t_{jk} - \frac{2}{N-1}t_{ij}t_{kl})$$

There is no guarantee that \mathbf{W}_{ss} computed this way is positive semidefinite. However, the second part is of order $O(N^{-1})$ and does not destroy the positive semidefinite first part for sufficiently large N . For a large number of independent observations, default settings of the weight matrix \mathbf{W} result in asymptotically distribution-free parameter estimates with unbiased standard errors and a correct χ^2 test statistic (Browne 1982, 1984).

With the default weight matrix \mathbf{W} computed by PROC CALIS, the WLS estimation is also called as the asymptotically distribution-free (ADF) method. In fact, as options in PROC CALIS, `METHOD=WLS` and `METHOD=ADF` are totally equivalent, even though WLS in general might include cases with special weight matrices other than the default weight matrix.

When the mean structures are not modeled, the WLS discrepancy function is still the same quadratic form statistic. However, with only the elements in covariance matrix being modeled, the dimensions of \mathbf{u} and $\boldsymbol{\eta}$ are both reduced to $p(p+1)/2 \times 1$, and the dimension of the weight matrix is now $(p(p+1)/2) \times (p(p+1)/2)$. That is, the WLS discrepancy function for covariance structure models is:

$$F_{WLS} = (\mathbf{s} - \boldsymbol{\sigma})' \mathbf{W}_{ss}^{-1} (\mathbf{s} - \boldsymbol{\sigma})$$

If \mathbf{S} is a correlation rather than a covariance matrix, the default setting of the \mathbf{W}_{ss} is a consistent estimator of the asymptotic covariance matrix $\mathbf{\Gamma}_{ss}$ of $\sqrt{N}(\mathbf{s} - \boldsymbol{\sigma}_o)$ (Browne and Shapiro 1986; DeLeeuw 1983), with \mathbf{s} and $\boldsymbol{\sigma}_o$ representing vectors of sample and population correlations, respectively. Elementwise, \mathbf{W}_{ss} is expressed as:

$$[\mathbf{W}_{ss}]_{ij,kl} = r_{ij,kl} - \frac{1}{2}r_{ij}(r_{ii,kl} + r_{jj,kl}) - \frac{1}{2}r_{kl}(r_{kk,ij} + r_{ll,ij}) + \frac{1}{4}r_{ij}r_{kl}(r_{ii,kk} + r_{ii,ll} + r_{jj,kk} + r_{jj,ll})$$

where

$$r_{ij} = \frac{t_{ij}}{\sqrt{t_{ii}t_{jj}}}$$

and

$$r_{ij,kl} = \frac{t_{ij,kl}}{\sqrt{t_{ii}t_{jj}t_{kk}t_{ll}}}$$

The asymptotic variances of the diagonal elements of a correlation matrix are 0. That is,

$$[\mathbf{W}_{ss}]_{ii,ii} = 0$$

for all i . Therefore, the weight matrix computed this way is always singular. In this case, the discrepancy function for weighted least squares estimation is modified to:

$$F_{WLS} = \sum_{i=2}^p \sum_{j=1}^{i-1} \sum_{k=2}^p \sum_{l=1}^{k-1} [\mathbf{W}_{ss}]^{ij,kl} ([\mathbf{S}]_{ij} - [\boldsymbol{\Sigma}]_{ij})([\mathbf{S}]_{kl} - [\boldsymbol{\Sigma}]_{kl}) \\ + r \sum_i^p ([\mathbf{S}]_{ii} - [\boldsymbol{\Sigma}]_{ii})^2$$

where r is the penalty weight specified by the `WPENALTY=r` option and the $[\mathbf{W}_{ss}]^{ij,kl}$ are the elements of the inverse of the reduced $(p(p-1)/2) \times (p(p-1)/2)$ weight matrix that contains only the nonzero rows and columns of the full weight matrix \mathbf{W}_{ss} .

The second term is a penalty term to fit the diagonal elements of the correlation matrix \mathbf{S} . The default value of $r = 100$ can be decreased or increased by the `WPENALTY=` option. The often used value of $r = 1$ seems to be too small in many cases to fit the diagonal elements of a correlation matrix properly.

Note that when you model correlation structures, no mean structures can be modeled simultaneously in the same model.

DWLS Discrepancy Functions

Storing and inverting the huge weight matrix \mathbf{W} in WLS estimation requires considerable computer resources. A compromise is found by implementing the diagonally weighted least squares (DWLS) method that uses only the diagonal of the weight matrix \mathbf{W} from the WLS estimation in the following discrepancy function:

$$F_{DWLS} = (\mathbf{u} - \boldsymbol{\eta})' [\text{diag}(\mathbf{W})]^{-1} (\mathbf{u} - \boldsymbol{\eta}) \\ = \sum_{i=1}^p \sum_{j=1}^i [\mathbf{W}_{ss}]_{ij,ij}^{-1} ([\mathbf{S}]_{ij} - [\boldsymbol{\Sigma}]_{ij})^2 + \sum_{i=1}^p [\mathbf{W}_{\bar{x}\bar{x}}]_{ii}^{-1} (\bar{x}_i - \boldsymbol{\mu}_i)^2$$

When only the covariance structures are modeled, the discrepancy function becomes:

$$F_{DWLS} = \sum_{i=1}^p \sum_{j=1}^i [\mathbf{W}_{ss}]_{ij,ij}^{-1} ([\mathbf{S}]_{ij} - [\boldsymbol{\Sigma}]_{ij})^2$$

For correlation models, the discrepancy function is:

$$F_{DWLS} = \sum_{i=2}^p \sum_{j=1}^{i-1} [\mathbf{W}_{ss}]_{ij,ij}^{-1} ([\mathbf{S}]_{ij} - [\boldsymbol{\Sigma}]_{ij})^2 + r \sum_{i=1}^p ([\mathbf{S}]_{ii} - [\boldsymbol{\Sigma}]_{ii})^2$$

where r is the penalty weight specified by the `WPENALTY=r` option. Note that no mean structures can be modeled simultaneously with correlation structures when using the DWLS method.

As the statistical properties of DWLS estimates are still not known, standard errors for estimates are not computed for the DWLS method.

Input Weight Matrices

In GLS, WLS, or DWLS estimation you can change from the default settings of weight matrices \mathbf{W} by using an `INWGT=` data set. The CALIS procedure requires a positive definite weight matrix that has positive diagonal elements.

Multiple-Group Discrepancy Function

Suppose that there are k independent groups in the analysis and N_1, N_2, \dots, N_k are the sample sizes for the groups. The overall discrepancy function $F(\boldsymbol{\Theta})$ is expressed as a weighted sum of individual discrepancy functions F_i 's for the groups:

$$F(\boldsymbol{\Theta}) = \sum_{i=1}^k t_i F_i(\boldsymbol{\Theta})$$

where

$$t_i = \frac{N_i - 1}{N - k}$$

is the weight of the discrepancy function for group i , and

$$N = \sum_{i=1}^k N_i$$

is the total number of observations in all groups. In PROC CALIS, all discrepancy function F_i 's in the overall discrepancy function must belong to the same estimation method. You cannot specify different estimation methods for the groups in a multiple-group analysis. In addition, the same analysis type must be applied to all groups—that is, you can analyze either covariance structures, covariance and mean structures, and correlation structures for all groups.

Robust Estimation

Two robust estimation methods that are proposed by Yuan and Zhong (2008) and Yuan and Hayashi (2010) are implemented in PROC CALIS. The first method is the two-stage robust method, which estimates robust covariance and mean matrices in the first stage and then feeds the robust covariance and mean matrices (in place of the ordinary sample covariance and mean matrices) for ML estimation in the second stage. Weighting of the observations is done only in the first stage. The `ROBUST=SAT` option invokes the two-stage robust estimation. The second method is the direct robust method, which iteratively estimates

model parameters with simultaneous weightings of the observations. The **ROBUST**, **ROBUST=RES(E)**, or **ROBUST=RES(F)** option invokes the direct robust estimation method.

The procedural difference between the two robust methods results in differential treatments of model outliers and leverage observations (or leverage points). In producing the robust covariance and mean matrices in the first stage, the two-stage robust method downweights outlying observations in all variable dimensions without regard to the model structure. This method downweights potential model outliers and leverage observations (which are not necessarily model outliers) in essentially the same way before the ML estimation in the second stage.

However, the direct robust method downweights the model outliers only. “Good” leverage observations (those that are not outliers at the same time) are not downweighted for model estimation. Therefore, it could be argued that the direct robust method is more desirable if you can be sure that the model is a reasonable one. The reason is that the direct robust method can retain the information from the “good” leverage observations for estimation, while the two-stage robust method downweights all leverage observations indiscriminately during its first stage. However, if the model is itself uncertain, the two-stage robust estimation method might be more foolproof.

Both robust methods employ weights on the observations. Weights are functions of the Mahalanobis distances (M-distances) of the observations and are computed differently for the two robust methods. The following two sections describe the weighting scheme and the estimation procedure of the two robust methods in more detail.

Two-Stage Robust Method

For the two-stage robust method, the following conventional M-distance d_s for an observed random vector \mathbf{x} is computed as

$$d_s = \sqrt{(\mathbf{x} - \boldsymbol{\mu})' \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu})}$$

where $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ are the unstructured mean and covariance matrices, respectively.

Two sets of weights are computed as functions of the M-distances of the observations. The weighting functions are essentially the same form as that of Huber (see, for example, Huber 1981). Let d_i be the M-distance of observation i , computed from the d_s formula. The first set of weights $w_1(d_i)$ applies to the first moments of the data and is defined as

$$\begin{aligned} w_1(d_i) &= 1 && \text{(if } d_i \leq \rho) \\ &= \rho/d_i && \text{(if } d_i > \rho) \end{aligned}$$

where ρ is the critical value corresponding to the $(1 - \varphi) \times 100$ quantile of the $\chi_r = \sqrt{\chi_r^2}$ distribution, with r being the degrees of freedom. For the two-stage robust method, r is simply the number of observed variables in the analysis. The tuning parameter φ controls the approximate proportion of observations to be downweighted (that is, with $w_1(d_i)$ less than 1). The default φ value is set to 0.05. You can override this value by using the **ROBPHI=** option.

The second set of weights $w_2(d_i)$ applies to the second moments of the data and is defined as

$$w_2(d_i) = (w_1(d_i))^2 / \kappa$$

where κ is a constant that adjusts the sum $\sum_{i=1}^N w_2(d_i)$ to 1 approximately. After the tuning parameter φ is determined, the critical value ρ and the adjustment κ are computed automatically by PROC CALIS.

With these two sets of weights, the two-stage robust method (ROBUST=SAT) estimates the mean and covariance by the so-called iteratively reweighted least squares (IRLS) algorithm. Specifically, the updating formulas at the $j+1$ iteration are

$$\begin{aligned}\boldsymbol{\mu}^{(j+1)} &= \frac{\sum_{i=1}^N w_1(d_i^{(j)})\mathbf{x}_i}{\sum_{i=1}^N w_1(d_i^{(j)})} \\ \boldsymbol{\Sigma}^{(j+1)} &= \frac{1}{N} \sum_{i=1}^N w_2(d_i^{(j)})(\mathbf{x}_i - \boldsymbol{\mu}^{(j)})(\mathbf{x}_i - \boldsymbol{\mu}^{(j)})'\end{aligned}$$

where $d_i^{(j)}$ is the M-distance evaluated at $\boldsymbol{\mu}^{(j)}$ and $\boldsymbol{\Sigma}^{(j)}$ obtained in the j th iteration. Carry out the iterations until $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ converge. The final iteration yields the robust estimates of mean and covariance matrices. PROC CALIS uses the relative parameter convergence criterion for the IRLS algorithm. The default criterion is $1E-8$. See the XCONV= option for the definition of the relative parameter convergence criterion. After the IRLS algorithm converges in the first stage, the two-stage robust method proceeds to treat the robust mean and covariance estimates as if they were sample mean and covariance matrices for a maximum likelihood estimation (METHOD=ML) of the model.

Direct Robust Method

The direct robust method computes the following residual M-distance d_r for an observation with residual random vector $\hat{\mathbf{e}}$ (say, of dimension $h \times 1$, where h is the number of dependent observed variables \mathbf{y}):

$$d_r = \sqrt{(\mathbf{L}\hat{\mathbf{e}})'(\mathbf{L}\boldsymbol{\Omega}_{\hat{\mathbf{e}}}\mathbf{L}')^{-1}(\mathbf{L}\hat{\mathbf{e}})}$$

where \mathbf{L} ($(h - q) \times h$) is a loading matrix that reduces $\hat{\mathbf{e}}$ to $(h - q)$ independent components and q is the number of independent factors to be estimated from the dependent observed variables \mathbf{y} . The reduction of the residual vector into independent components is necessary when the number of factors q is not zero in the model. For $q > 0$, the residual covariance matrix $\boldsymbol{\Omega}_{\hat{\mathbf{e}}}$ is not invertible and cannot be used in computing the residual M-distances. Hence, the covariance matrix $\mathbf{L}\boldsymbol{\Omega}_{\hat{\mathbf{e}}}\mathbf{L}'$ of independent components $\mathbf{L}\hat{\mathbf{e}}$ is used instead. See Yuan and Hayashi (2010) for details about the computation of the residuals in the context of structural equation modeling.

The direct robust method also computes two sets of weights as functions of the residual M-distances. Let d_i be the M-distance of observation i , computed from the d_r formula. The first set of weights $w_1(d_i)$ applies to parameters in the first moments and is defined as

$$\begin{aligned}w_1(d_i) &= 1 \quad (\text{if } d_i \leq \rho) \\ &= \rho/d_i \quad (\text{if } d_i > \rho)\end{aligned}$$

The second set of weights $w_2(d_i)$ applies to the parameters in the second moments and is defined as

$$w_2(d_i) = (w_1(d_i))^2/\kappa$$

These are essentially the same Huber-type weighting functions as those for the two-stage robust method. The only difference is that the d_r , instead of the d_s , formula is used in the weighting functions for the direct robust method. The definition of ρ is also the same as that in the two-stage robust method, but it is now based on a different theoretical chi-square distribution. That is, in the direct robust method, ρ is the critical value that corresponds to the $(1 - \varphi) \times 100$ quantile of the $\chi_r = \sqrt{\chi_r^2}$ distribution, with $r = (h - q)$ being

the degrees of freedom. Again, φ is a tuning parameter and is set to 0.05 by default. You can override this value by using the **ROBPHI=** option. The calculation of the number of “independent factors” q depends on the variants of the direct robust estimation that you choose. With the **ROBUST=RES(E)** option, q is the same as the number of exogenous factors specified in the model. With the **ROBUST=RES(F)** option, the disturbances of the endogenous factors in the model are also treated as “independent factors,” so q is the total number of latent factors specified in the model.

The direct robust method (**ROBUST=RES(E)** or **ROBUST=RES(F)**) employs the IRLS algorithm in model estimation. Let the following expression be a vector of nonredundant first and second moments structured in terms of model parameters θ :

$$\mathbf{m}(\theta) = \begin{pmatrix} \boldsymbol{\mu}(\theta) \\ \text{vech}(\boldsymbol{\Sigma}(\theta)) \end{pmatrix}$$

where $\text{vech}()$ extracts the lower-triangular nonredundant elements in $\boldsymbol{\Sigma}(\theta)$. The updating formulas for θ at the $j+1$ iteration is

$$\theta^{(j+1)} = \theta^{(j)} + \Delta\theta^{(j)}$$

where $\theta^{(j)}$ is the parameter values at the j th iteration and $\Delta\theta^{(j)}$ is defined by the following formula:

$$\Delta\theta^{(j)} = (\dot{\mathbf{m}}'(\theta^{(j)})\mathbf{W}(\theta^{(j)})\dot{\mathbf{m}}(\theta^{(j)}))^{-1}\dot{\mathbf{m}}'(\theta^{(j)})\mathbf{W}(\theta^{(j)})\mathbf{g}_j$$

where $\dot{\mathbf{m}}(\theta) = \frac{\partial \mathbf{m}(\theta)}{\partial \theta}$ is the model Jacobian, $\mathbf{W}(\theta)$ is the (normal theory) weight matrix for the moments (see Yuan and Zhong 2008 for the formula of the weight matrix), and \mathbf{g}_j is defined as

$$\mathbf{g}_j = \begin{pmatrix} \frac{1}{\sum_{i=1}^N w_1(d_i)} \sum_{i=1}^N w_1(d_i) \mathbf{x}_i - \boldsymbol{\mu}(\theta^{(j)}) \\ \frac{1}{N} \sum_{i=1}^N w_2(d_i) \text{vech}[(\mathbf{x}_i - \boldsymbol{\mu}(\theta^{(j)}))(\mathbf{x}_i - \boldsymbol{\mu}(\theta^{(j)}))'] - \boldsymbol{\Sigma}(\theta^{(j)}) \end{pmatrix}$$

Starting with some reasonable initial estimates for θ , PROC CALIS iterates the updating formulas until the relative parameter convergence criterion of the IRLS algorithm is satisfied. The default criterion value is $1\text{E}-8$. This essentially means that the IRLS algorithm converges when $\Delta\theta$ is sufficiently small. See the **XCONV=** option for the definition of the relative parameter convergence criterion.

Although the iterative formulas and the IRLS steps for robust estimation have been presented for single-group analysis, they are easily generalizable to multiple-group analysis. For the two-stage robust method, you only need to repeat the robust estimation of the means and covariances for the groups and then apply the obtained robust moments as if they were sample moments for regular maximum likelihood estimation (**METHOD=ML**). For the direct robust method, you need to expand the dimensions of the model Jacobian matrix $\dot{\mathbf{m}}(\theta)$, the weight matrix $\mathbf{W}(\theta)$, and the vector \mathbf{g} to include moments from several groups/models. Therefore, the multiple-group formulas are conceptually quite simple but tedious to present. For this reason, they are omitted here.

Relationships among Estimation Criteria

There is always some arbitrariness to classify the estimation methods according to certain mathematical or numerical properties. The discussion in this section is not meant to be a thorough classification of the estimation methods available in PROC CALIS. Rather, classification is done here with the purpose of clarifying the uses of different estimation methods and the theoretical relationships of estimation criteria.

Assumption of Multivariate Normality

GLS, ML, and FIML assume multivariate normality of the data, while ULS, WLS, and DWLS do not. Although the ML method with covariance structure analysis alone can also be based on the Wishart distribution of the sample covariance matrix, for convenience GLS, ML, and FIML are usually classified as normal-theory based methods, while ULS, WLS, and DWLS are usually classified as distribution-free methods.

An intuitive or even naive notion is usually that methods without distributional assumptions such as WLS and DWLS are preferred to normal theory methods such as ML and GLS in practical situations where multivariate normality is doubtful. This notion might need some qualifications because there are simply more factors to consider in judging the quality of estimation methods in practice. For example, the WLS method might need a very large sample size to enjoy its purported asymptotic properties, while the ML might be robust against the violation of multi-normality assumption under certain circumstances. No recommendations regarding which estimation criterion should be used are attempted here, but you should make your choice based more than the assumption of multivariate normality.

Contribution of the Off-Diagonal Elements to the Estimation of Covariance or Correlation Structures

If only the covariance or correlation structures are considered, the six estimation functions, F_{ULS} , F_{GLS} , F_{ML} , F_{FIML} , F_{WLS} , and F_{DWLS} , belong to the following two groups:

- The functions F_{ULS} , F_{GLS} , F_{ML} , and F_{FIML} take into account all n^2 elements of the symmetric residual matrix $\mathbf{S} - \mathbf{\Sigma}$. This means that the off-diagonal residuals contribute twice to the discrepancy function F , as lower and as upper triangle elements.
- The functions F_{WLS} and F_{DWLS} take into account only the $n(n + 1)/2$ lower triangular elements of the symmetric residual matrix $\mathbf{S} - \mathbf{\Sigma}$. This means that the off-diagonal residuals contribute to the discrepancy function F only once.

The F_{DWLS} function used in PROC CALIS differs from that used by the LISREL 7 program. Formula (1.25) of the LISREL 7 manual (Jöreskog and Sörbom 1985, p. 23) shows that LISREL groups the F_{DWLS} function in the first group by taking into account all n^2 elements of the symmetric residual matrix $\mathbf{S} - \mathbf{\Sigma}$.

- Relationship between DWLS and WLS:
PROC CALIS: The F_{DWLS} and F_{WLS} discrepancy functions deliver the same results for the special case that the weight matrix $\mathbf{W} = \mathbf{W}_{ss}$ used by WLS estimation is a diagonal matrix.
LISREL 7: This is not the case.
- Relationship between DWLS and ULS:
LISREL 7: The F_{DWLS} and F_{ULS} estimation functions deliver the same results for the special case that the diagonal weight matrix $\mathbf{W} = \mathbf{W}_{ss}$ used by DWLS estimation is an identity matrix.
PROC CALIS: To obtain the same results with F_{DWLS} and F_{ULS} estimation, set the diagonal weight matrix $\mathbf{W} = \mathbf{W}_{ss}$ used in DWLS estimation to:

$$[\mathbf{W}_{ss}]_{ik,ik} = \begin{cases} 1. & \text{if } i = k \\ 0.5 & \text{otherwise} \end{cases} \quad (k \leq i)$$

Because the reciprocal elements of the weight matrix are used in the discrepancy function, the off-diagonal residuals are weighted by a factor of 2.

ML and FIML Methods

Both the ML and FIML methods can be derived from the log-likelihood function for multivariate normal data. The preceding section “[Estimation Criteria](#)” on page 1309 mentions that F_{FIML} is essentially the same as $\frac{-2L}{N}$, where L is the log-likelihood function for multivariate normal data. For the ML estimation, you can also consider $\frac{-2L}{N}$ as a part of the F_{ML} discrepancy function that contains the information regarding the model parameters (while the rest the F_{ML} function contains some constant terms given the data). That is, with some algebraic manipulations and assuming that there is no missing value in the analysis (so that all μ_j and Σ_j are the same as μ and Σ , respectively), it can be shown that

$$\begin{aligned} F_{FIML} &= \frac{-2L}{N} \\ &= \frac{1}{N} \sum_{j=1}^n (\ln(|\Sigma|) + (\mathbf{x}_j - \boldsymbol{\mu})' \Sigma^{-1} (\mathbf{x}_j - \boldsymbol{\mu}) + K) \\ &= \ln(|\Sigma|) + \text{Tr}(\mathbf{S}_N \Sigma^{-1}) + (\bar{\mathbf{x}} - \boldsymbol{\mu})' \Sigma^{-1} (\bar{\mathbf{x}} - \boldsymbol{\mu}) + K \end{aligned}$$

where $\bar{\mathbf{x}}$ is the sample mean and \mathbf{S}_N is the biased sample covariance matrix. Compare this FIML function with the ML function shown in the following expression, which shows that both functions are very similar:

$$F_{ML} = \ln(|\Sigma|) + \text{Tr}(\mathbf{S} \Sigma^{-1}) + (\bar{\mathbf{x}} - \boldsymbol{\mu})' \Sigma^{-1} (\bar{\mathbf{x}} - \boldsymbol{\mu}) - p - \ln(|\mathbf{S}|)$$

The two expressions differ only in the constant terms, which are independent of the model parameters, and in the formulas for computing the sample covariance matrix. While the FIML method assumes the biased formula (with N as the divisor, by default) for the sample covariance matrix, the ML method (as implemented in PROC CALIS) uses the unbiased formula (with $N - 1$ as the divisor, by default).

The similarity (or dissimilarity) of the ML and FIML discrepancy functions leads to some useful conclusions here:

- Because the constant terms in the discrepancy functions play no part in parameter estimation (except for shifting the function values), overriding the default ML method with `VARDEF=N` (that is, using N as the divisor in the covariance matrix formula) leads to the same estimation results as that of the FIML method, given that there are no missing values in the analysis.
- Because the FIML function is evaluated at the level of individual observations, it is much more expensive to compute than the ML function. As compared with ML estimation, FIML estimation takes longer and uses more computing resources. Hence, for data without missing values, the ML method should always be chosen over the FIML method.
- The advantage of the FIML method lies solely in its ability to handle data with random missing values. While the FIML method uses the information maximally from each observation, the ML method (as implemented in PROC CALIS) simply throws away any observations with at least one missing value. If it is important to use the information from observations with random missing values, the FIML method should be given consideration over the ML method.

See [Example 27.15](#) for an application of the FIML method and [Example 27.16](#) for an empirical comparison of the ML and FIML methods.

Gradient, Hessian, Information Matrix, and Approximate Standard Errors

For a single-sample setting with a discrepancy function $F = F(\boldsymbol{\Sigma}(\boldsymbol{\Theta}), \boldsymbol{\mu}(\boldsymbol{\Theta}); \mathbf{S}, \bar{\mathbf{x}})$, the gradient is defined as the first partial derivatives of the discrepancy function with respect to the model parameters $\boldsymbol{\Theta}$:

$$g(\boldsymbol{\Theta}) = \frac{\partial}{\partial \boldsymbol{\Theta}} F(\boldsymbol{\Theta})$$

The Hessian is defined as the second partial derivatives of the discrepancy function with respect to the model parameters $\boldsymbol{\Theta}$:

$$H(\boldsymbol{\Theta}) = \frac{\partial^2}{\partial \boldsymbol{\Theta} \partial \boldsymbol{\Theta}'} F(\boldsymbol{\Theta})$$

Suppose that the mean and covariance structures fit perfectly with $\boldsymbol{\Theta} = \boldsymbol{\Theta}_o$ in the population. The information matrix is defined as

$$I(\boldsymbol{\Theta}_o) = \frac{1}{2} \mathcal{E}(H(\boldsymbol{\Theta}_o))$$

where the expectation $\mathcal{E}(\cdot)$ is taken over the sampling space of $\mathbf{S}, \bar{\mathbf{x}}$.

The information matrix plays a significant role in statistical theory. Under certain regularity conditions, the inverse of the information matrix $I^{-1}(\boldsymbol{\Theta}_o)$ is the asymptotic covariance matrix for $\sqrt{N}(\hat{\boldsymbol{\Theta}} - \boldsymbol{\Theta}_o)$, where N denotes the sample size and $\hat{\boldsymbol{\Theta}}$ is an estimator.

In practice, $\boldsymbol{\Theta}_o$ is never known and can only be estimated. The information matrix is therefore estimated by the so-called empirical information matrix:

$$I(\hat{\boldsymbol{\Theta}}) = \frac{1}{2} H(\hat{\boldsymbol{\Theta}})$$

which is evaluated at the values of the sample estimates $\hat{\boldsymbol{\Theta}}$. Notice that this empirical information matrix, rather than the unknown $I(\boldsymbol{\Theta}_o)$, is the “information matrix” displayed in PROC CALIS output.

Taking the inverse of the empirical information matrix with sample size adjustment, PROC CALIS approximates the estimated covariance matrix of $\hat{\boldsymbol{\Theta}}$ by:

$$((N - 1)I(\hat{\boldsymbol{\Theta}}))^{-1} = ((N - 1)\frac{1}{2}H(\hat{\boldsymbol{\Theta}}))^{-1} = \frac{2}{N - 1} H^{-1}(\hat{\boldsymbol{\Theta}})$$

Approximate standard errors for $\hat{\boldsymbol{\Theta}}$ can then be computed as the square roots of the diagonal elements of the estimated covariance matrix. The theory about the empirical information matrix, the approximate covariance matrix of the parameter estimates, and the approximate standard errors applies to all but the ULS and DWLS estimation methods. Standard errors are therefore not computed with the ULS and DWLS estimation methods.

If a given Hessian or information matrix is singular, PROC CALIS offers two ways to compute a generalized inverse of the matrix and, therefore, two ways to compute approximate standard errors of implicitly constrained parameter estimates, t values, and modification indices. Depending on the G4= specification, either a Moore-Penrose inverse or a G2 inverse is computed. The expensive Moore-Penrose inverse computes an estimate of the null space by using an eigenvalue decomposition. The cheaper G2 inverse is produced by sweeping the linearly independent rows and columns and zeroing out the dependent ones.

Multiple-Group Extensions

In the section “Multiple-Group Discrepancy Function” on page 1315, the overall discrepancy function for multiple-group analysis is defined. The same notation is applied here. To begin with, the overall discrepancy function $F(\Theta)$ is expressed as a weighted sum of individual discrepancy functions F_i 's for the groups as follows:

$$F(\Theta) = \sum_{i=1}^k t_i F_i(\Theta)$$

where

$$t_i = \frac{N_i - 1}{N - k}$$

is the weight for group i ,

$$N = \sum_{i=1}^k N_i$$

is the total sample size, and N_i is the sample size for group i .

The gradient $g(\Theta)$ and the Hessian $H(\Theta)$ are now defined as weighted sum of individual functions. That is,

$$g(\Theta) = \sum_{i=1}^k t_i g_i(\Theta) = \sum_{i=1}^k t_i \frac{\partial}{\partial \Theta} F_i(\Theta)$$

and

$$H(\Theta) = \sum_{i=1}^k t_i H_i(\Theta) = \sum_{i=1}^k t_i \frac{\partial^2}{\partial \Theta \partial \Theta'} F_i(\Theta)$$

Suppose that the mean and covariance structures fit perfectly with $\Theta = \Theta_o$ in the population. If each t_i converges to a fixed constant τ_i ($\tau_i > 0$) with increasing total sample size, the information matrix can be written as:

$$I(\Theta_o) = \frac{1}{2} \sum_{i=1}^k \tau_i \mathcal{E}(H_i(\Theta_o))$$

To approximate this information matrix, an empirical counterpart is used:

$$I(\hat{\Theta}) = \frac{1}{2} \sum_{i=1}^k t_i H_i(\hat{\Theta})$$

which is evaluated at the values of the sample estimates $\hat{\Theta}$. Again, this empirical information matrix, rather than the unknown $I(\Theta_o)$, is the “information matrix” output in PROC CALIS results.

Taking the inverse of the empirical information matrix with sample size adjustment, PROC CALIS approximates the estimated covariance matrix of $\hat{\Theta}$ in multiple-group analysis by:

$$((N - k)I(\hat{\Theta}))^{-1} = ((N - k)\frac{1}{2}H(\hat{\Theta}))^{-1} = \frac{2}{N - k} \sum_{i=1}^k t_i H_i^{-1}(\hat{\Theta})$$

Approximate standard errors for $\hat{\Theta}$ can then be computed as the square roots of the diagonal elements of the estimated covariance matrix. Again, for ULS and DWLS estimation, the theory does not apply and so there are no standard errors computed in these cases.

Testing Rank Deficiency in the Approximate Covariance Matrix for Parameter Estimates

When computing the approximate covariance matrix and hence the standard errors for the parameter estimates, inversion of the scaled information matrix or Hessian matrix is involved. The numerical condition of the information matrix can be very poor in many practical applications, especially for the analysis of unscaled covariance data. The following four-step strategy is used for the inversion of the information matrix.

1. The inversion (usually of a normalized matrix $\mathbf{D}^{-1}\mathbf{H}\mathbf{D}^{-1}$) is tried using a modified form of the Bunch and Kaufman (1977) algorithm, which allows the specification of a different singularity criterion for each pivot. The following three criteria for the detection of rank loss in the information matrix are used to specify thresholds:
 - *ASING* specifies absolute singularity.
 - *MSING* specifies relative singularity depending on the whole matrix norm.
 - *VSING* specifies relative singularity depending on the column matrix norm.

If no rank loss is detected, the inverse of the information matrix is used for the covariance matrix of parameter estimates, and the next two steps are skipped.

2. The linear dependencies among the parameter subsets are displayed based on the singularity criteria.
3. If the number of parameters t is smaller than the value specified by the **G4=** option (the default value is 60), the Moore-Penrose inverse is computed based on the eigenvalue decomposition of the information matrix. If you do not specify the **NOPRINT** option, the distribution of eigenvalues is displayed, and those eigenvalues that are set to zero in the Moore-Penrose inverse are indicated. You should inspect this eigenvalue distribution carefully.
4. If PROC CALIS did not set the right subset of eigenvalues to zero, you can specify the **COVSING=** option to set a larger or smaller subset of eigenvalues to zero in a further run of PROC CALIS.

Counting the Degrees of Freedom

When fitting covariance and mean structure models, the population moments are hypothesized to be functions of model parameters Θ . The population moments refer to the first-order moments (means) and the second-order central moments (variances of and covariances among the variables). Usually, the number of nonredundant population moments is greater than the number of model parameters for a structural model. The difference between the two is the degrees of freedom (*df*) of your model.

Formally, define a multiple-group situation where you have k independent groups in your model. The set of variables in each group might be different so that you have p_1, p_2, \dots, p_k manifest or observed variables for the k groups. It is assumed that the primary interest is to study the covariance structures. The inclusion of mean structures is optional for each of these groups. Define $\delta_1, \delta_2, \dots, \delta_k$ as zero-one indicators of the

mean structures for the groups. If δ_i takes the value of one, it means that the mean structures of group i is modeled. The total number of nonredundant elements in the moment matrices is thus computed by:

$$q = \sum_{i=1}^k (p_i(p_i + 1)/2 + \delta_i p_i)$$

The first term in the summation represents the number of lower triangular elements in the covariance or correlation matrix, while the second term represents the number of elements in the mean matrix. Let t be the total number of independent parameters *in the model*. The degrees of freedom is:

$$df = q - (t - c)$$

where c represents the number of linear equality constraints imposed on the independent parameters in the model. In effect, the $(t - c)$ expression means that each nonredundant linear equality constraint reduces one independent parameter.

Counting the Number of Independent Parameters

To count the number of independent parameters in the model, first you have to distinguish them from the dependent parameters. Dependent parameters are expressed as functions of other parameters in the [SAS programming statements](#). That is, a parameter is dependent if it appears at the left-hand side of the equal sign in a SAS programming statement.

A parameter is independent if it is not dependent. An independent parameter can be specified in the [main](#) or [subsidiary](#) model specification statements or the [PARAMETERS](#) statement, or it is generated automatically by PROC CALIS as additional parameters. Quite intuitively, all independent parameter specified in the main or subsidiary model specification statements are independent parameters *in the model*. All automatic parameters added by PROC CALIS are also independent parameters *in the model*.

Intentionally or not, some independent parameters specified in the [PARMS](#) statement might not be counted as independent parameters in the model. Independent parameters in the [PARMS](#) statement belong in the model only when they are used to define at least one dependent parameter specified in the main or subsidiary model specification statements. This restriction eliminates the counting of superfluous independent parameters which have no bearing of model specification.

Note that when counting the number of independent parameters, you are counting the number of distinct independent parameter names but not the number of distinct parameter locations for independent parameters. For example, consider the following statement for defining the error variances in a [LINEQS](#) model:

```
variance    E1-E3 = vare1 vare2 vare3;
```

You define three variance parameter locations with three independent parameters `vare1`, `vare2`, and `vare3`. However, in the following specification:

```
variance    E1-E3 = vare vare vare;
```

you still have three variance parameter locations to define, but the number of independent parameter is only one, which is the parameter named `vare`.

Counting the Number of Linear Equality Constraints

The linear equality constraints refer to those specified in the **BOUNDS** or **LINCON** statement. For example, consider the following specification:

```
bounds 3 <= parm01 <= 3;
lincon 3 * parm02 + 2 * parm03 = 12;
```

In the **BOUNDS** statement, `parm01` is constrained to a fixed number 3, and in the **LINCON** statement, `parm02` and `parm03` are constrained linearly. In effect, these two statements reduce two independent parameters from the model. In the degrees of freedom formula, the value of c is 2 for this example.

Adjustment of Degrees of Freedom

In some cases, computing degrees of freedom for model fit is not so straightforward. Two important cases are considered in the following.

The first case is when you set linear inequality or boundary constraints in your model, and these inequality or boundary constraints become “active” in your final solution. For example, you might have set inequality boundary and linear constraints as:

```
bounds 0 <= var01;
lincon 3 * beta1 + 2 * beta2 >= 7;
```

The optimal solution occurs at the boundary point so that you observe in the final solution the following two equalities:

```
var01 = 0,
3 * beta1 + 2 * beta2 = 7
```

These two active constraints reduce the number of independent parameters of your original model. As a result, PROC CALIS will automatically increase the degrees of freedom by the number of active linear constraints. Adjusting degrees of freedom not only affects the significance of the model fit chi-square statistic, but it also affects the computation of many fit statistics and indices. See Dijkstra (1992) for a discussion of the validity of statistical inferences with active boundary constraints.

Automatically adjusting df in such a situation might not be totally justified in all cases. Statistical estimation is subject to sampling fluctuation. Active constraints might not occur when fitting the same model in new samples. If the researcher believes that those linear inequality and boundary constraints have a small chance of becoming active in repeated sampling, it might be more suitable to turn off the automatic adjustment by using the **NOADJDF** option in the PROC CALIS statement.

Another case where you need to pay attention to the computation of degrees of freedom is when you fit correlation models. The degrees-of-freedom calculation in PROC CALIS applies mainly to models with covariance structures with or without mean structures. When you model correlation structures, the degrees of freedom calculation in PROC CALIS is a straightforward generalization of the covariance structures. It does not take the fixed ones at the diagonal elements of the sample correlation matrix into account. Some might argue that with correlation structures, the degrees of freedom should be reduced by the total number of diagonal elements in the correlation matrices in the model. While PROC CALIS does not do this automatically, you can use the **DFREDUCE= i** option to specify the adjustment, where i can be any positive or negative integer. The df value is reduced by the **DFREDUCE=** value.

A Different Type of Degrees of Freedom

The degrees of freedom for model fitting has to be distinguished from another type of degrees of freedom. In a regression problem, the number of degrees of freedom for the error variance estimate is the number of observations in the data set minus the number of parameters. The `NOBS=`, `DFR=` (`RDF=`), and `DFE=` (`EDF=`) options refer to degrees of freedom in this sense. However, these values are not related to the degrees of freedom for the model fit statistic. The `NOBS=`, `DFR=`, and `DFE=` options should be used in PROC CALIS to specify the effective number of observations in the input data set only.

Assessment of Fit

In PROC CALIS, there are three main tools for assessing model fit:

- residuals for the fitted means or covariances
- overall model fit indices
- squared multiple correlations and determination coefficients

This section contains a collection of formulas for these assessment tools. The following notation is used:

- N for the total sample size
- k for the total number of independent groups in analysis
- p for the number of manifest variables
- t for the number of parameters to estimate
- Θ for the t -vector of parameters, $\hat{\Theta}$ for the estimated parameters
- $S = (s_{ij})$ for the $p \times p$ input covariance or correlation matrix
- $\bar{x} = (\bar{x}_i)$ for the p -vector of sample means
- $\hat{\Sigma} = \Sigma(\hat{\Theta}) = (\hat{\sigma}_{ij})$ for the predicted covariance or correlation matrix
- $\hat{\mu} = (\hat{\mu}_i)$ for the predicted mean vector
- δ for indicating the modeling of the mean structures
- W for the weight matrix
- f_{min} for the minimized function value of the fitted model
- d_{min} for the degrees of freedom of the fitted model

In multiple-group analyses, subscripts are used to distinguish independent groups or samples. For example, $N_1, N_2, \dots, N_r, \dots, N_k$ denote the sample sizes for k groups. Similarly, notation such as $p_r, S_r, \bar{x}_r, \hat{\Sigma}_r, \hat{\mu}_r, \delta_r,$ and W_r is used for multiple-group situations.

Residuals in the Moment Matrices

Residuals indicate how well each entry or element in the mean or covariance matrix is fitted. Large residuals indicate bad fit.

PROC CALIS computes four types of residuals and writes them to the `OUTSTAT=` data set when requested.

- **raw residuals**

$$s_{ij} - \hat{\sigma}_{ij}, \quad \bar{x}_i - \hat{\mu}_i$$

for the covariance and mean residuals, respectively. The raw residuals are displayed whenever the `PALL`, `PRINT`, or `RESIDUAL` option is specified.

- **variance standardized residuals**

$$\frac{s_{ij} - \hat{\sigma}_{ij}}{\sqrt{s_{ii}s_{jj}}}, \quad \frac{\bar{x}_i - \hat{\mu}_i}{\sqrt{s_{ii}}}$$

for the covariance and mean residuals, respectively. The variance standardized residuals are displayed when you specify one of the following:

- the `PALL`, `PRINT`, or `RESIDUAL` option and `METHOD=NONE`, `METHOD=ULS`, or `METHOD=DWLS`
- `RESIDUAL=VARSTAND`

The variance standardized residuals are equal to those computed by the EQS 3 program (Bentler 1995).

- **asymptotically standardized residuals**

$$\frac{s_{ij} - \hat{\sigma}_{ij}}{\sqrt{v_{ij,ij}}}, \quad \frac{\bar{x}_i - \hat{\mu}_i}{\sqrt{u_{ii}}}$$

for the covariance and mean residuals, respectively; with

$$v_{ij,ij} = (\hat{\Gamma}_1 - \mathbf{J}_1 \widehat{\text{Cov}}(\hat{\Theta}) \mathbf{J}'_1)_{ij,ij}$$

$$u_{ii} = (\hat{\Gamma}_2 - \mathbf{J}_2 \widehat{\text{Cov}}(\hat{\Theta}) \mathbf{J}'_2)_{ii}$$

where $\hat{\Gamma}_1$ is the $p^2 \times p^2$ estimated asymptotic covariance matrix of sample covariances, $\hat{\Gamma}_2$ is the $p \times p$ estimated asymptotic covariance matrix of sample means, \mathbf{J}_1 is the $p^2 \times t$ Jacobian matrix $d\boldsymbol{\Sigma}/d\boldsymbol{\Theta}$, \mathbf{J}_2 is the $p \times t$ Jacobian matrix $d\boldsymbol{\mu}/d\boldsymbol{\Theta}$, and $\widehat{\text{Cov}}(\hat{\Theta})$ is the $t \times t$ estimated covariance matrix of parameter estimates, all evaluated at the sample moments and estimated parameter values. See the next section for the definitions of $\hat{\Gamma}_1$ and $\hat{\Gamma}_2$. Asymptotically standardized residuals are displayed when one of the following conditions is met:

- The `PALL`, the `PRINT`, or the `RESIDUAL` option is specified, and `METHOD=ML`, `METHOD=GLS`, or `METHOD=WLS`, and the expensive information and Jacobian matrices are computed for some other reason.
- `RESIDUAL=ASYSTAND` is specified.

The asymptotically standardized residuals are equal to those computed by the LISREL 7 program (Jöreskog and Sörbom 1988) except for the denominator in the definition of matrix $\hat{\Gamma}_1$.

• **normalized residuals**

$$\frac{s_{ij} - \hat{\sigma}_{ij}}{\sqrt{(\hat{\Gamma}_1)_{ij,ij}}}, \quad \frac{\bar{x}_i - \hat{\mu}_i}{\sqrt{(\hat{\Gamma}_2)_{ii}}}$$

for the covariance and mean residuals, respectively; with $\hat{\Gamma}_1$ as the $p^2 \times p^2$ estimated asymptotic covariance matrix of sample covariances; and $\hat{\Gamma}_2$ as the $p \times p$ estimated asymptotic covariance matrix of sample means.

Diagonal elements of $\hat{\Gamma}_1$ and $\hat{\Gamma}_2$ are defined for the following methods:

- **GLS:** $(\hat{\Gamma}_1)_{ij,ij} = \frac{1}{(N-1)}(s_{ii}s_{jj} + s_{ij}^2)$ and $(\hat{\Gamma}_2)_{ii} = \frac{1}{(N-1)}s_{ii}$
- **ML:** $(\hat{\Gamma}_1)_{ij,ij} = \frac{1}{(N-1)}(\hat{\sigma}_{ii}\hat{\sigma}_{jj} + \hat{\sigma}_{ij}^2)$ and $(\hat{\Gamma}_2)_{ii} = \frac{1}{(N-1)}\hat{\sigma}_{ii}$
- **WLS:** $(\hat{\Gamma}_1)_{ij,ij} = \frac{1}{(N-1)}W_{ij,ij}$ and $(\hat{\Gamma}_2)_{ii} = \frac{1}{(N-1)}s_{ii}$

where **W** in the **WLS** method is the weight matrix for the second-order moments.

Normalized residuals are displayed when one of the following conditions is met:

- The **PALL**, **PRINT**, or **RESIDUAL** option is specified, and **METHOD=ML**, **METHOD=GLS**, or **METHOD=WLS**, and the expensive information and Jacobian matrices are **not** computed for some other reasons.
- **RESIDUAL=NORM** is specified.

The normalized residuals are equal to those computed by the LISREL VI program (Jöreskog and Sörbom 1985) except for the definition of the denominator in computing matrix $\hat{\Gamma}_1$.

For estimation methods that are not “best” generalized least squares estimators (Browne 1982, 1984), such as **METHOD=NONE**, **METHOD=ULS**, or **METHOD=DWLS**, the assumption of an asymptotic covariance matrix Γ_1 of sample covariances does not seem to be appropriate. In this case, the normalized residuals should be replaced by the more relaxed variance standardized residuals. Computation of asymptotically standardized residuals requires computing the Jacobian and information matrices. This is computationally very expensive and is done only if the Jacobian matrix has to be computed for some other reasons—that is, if at least one of the following items is true:

- The default, **PRINT**, or **PALL** displayed output is requested, and neither the **NOMOD** nor **NOSTDERR** option is specified.
- Either the **MODIFICATION** (included in **PALL**), **PCOVES**, or **STDERR** (included in default, **PRINT**, and **PALL** output) option is requested or **RESIDUAL=ASYSTAND** is specified.
- The **LEVMAR** or **NEWRAP** optimization technique is used.
- An **OUTMODEL=** data set is specified without using the **NOSTDERR** option.
- An **OUTEST=** data set is specified without using the **NOSTDERR** option.

Since normalized residuals use an overestimate of the asymptotic covariance matrix of residuals (the diagonals of Γ_1 and Γ_2), the normalized residuals cannot be greater than the asymptotically standardized residuals (which use the diagonal of the form $\Gamma - \mathbf{J}\widehat{\text{Cov}}(\hat{\Theta})\mathbf{J}'$).

Together with the residual matrices, the values of the average residual, the average off-diagonal residual, and the rank order of the largest values are displayed. The distributions of the normalized and standardized residuals are displayed also.

Overall Model Fit Indices

Instead of assessing the model fit by looking at a number of residuals of the fitted moments, an overall model fit index measures model fit by a single number. Although an overall model fit index is precise and easy to use, there are indeed many choices of overall fit indices. Unfortunately, researchers do not always have a consensus on the best set of indices to use in all occasions.

PROC CALIS produces a large number of overall model fit indices in the fit summary table. If you prefer to display only a subset of these fit indices, you can use the ONLIST(ONLY)= option of the FITINDEX statement to customize the fit summary table.

Fit indices are classified into three classes in the fit summary table of PROC CALIS:

- absolute or standalone Indices
- parsimony indices
- incremental indices

Absolute or Standalone Indices

These indices are constructed so that they measure model fit without comparing with a baseline model and without taking the model complexity into account. They measure the absolute fit of the model.

- **fit function or discrepancy function**

The fit function or discrepancy function F is minimized during the optimization. See the section “[Estimation Criteria](#)” on page 1309 for definitions of various discrepancy functions available in PROC CALIS. For a multiple-group analysis, the fit function can be written as a weighted average of discrepancy functions for k independent groups as:

$$F = \sum_{r=1}^k a_r F_r$$

where $a_r = \frac{(N_j - 1)}{(N - k)}$ and F_r are the group weight and the discrepancy function for the r th group, respectively. Notice that although the groups are assumed to be independent in the model, in general F_r 's are not independent when F is being minimized. The reason is that F_r 's might have shared parameters in Θ during estimation.

The minimized function value of F will be denoted as f_{min} , which is always positive, with small values indicating good fit.

- **χ^2 test statistic**

For the ML, GLS, and the WLS estimation, the overall χ^2 measure for testing model fit is:

$$\chi^2 = (N - k) * f_{min}$$

where f_{min} is the function value at the minimum, N is the total sample size, and k is the number of independent groups. The associated degrees of freedom is denoted by d_{min} .

For the ML estimation, this gives the likelihood ratio test statistic of the specified structural model in the null hypothesis against an unconstrained saturated model in the alternative hypothesis. The χ^2 test is valid only if the observations are independent and identically distributed, the analysis is based on the unstandardized sample covariance matrix S , and the sample size N is sufficiently large (Browne 1982; Bollen 1989b; Jöreskog and Sörbom 1985). For ML and GLS estimates, the variables must also have an approximately multivariate normal distribution.

In the output fit summary table of PROC CALIS, the notation “Prob > Chi-Square” means “the probability of obtaining a greater χ^2 value than the observed value under the null hypothesis.” This probability is also known as the p -value of the chi-square test statistic.

- **adjusted χ^2 value (Browne 1982)**

If the variables are p -variate elliptic rather than normal and have significant amounts of multivariate kurtosis (leptokurtic or platykurtic), the χ^2 value can be adjusted to:

$$\chi_{ell}^2 = \frac{\chi^2}{\eta_2}$$

where η_2 is the multivariate relative kurtosis coefficient.

- **Z-test (Wilson and Hilferty 1931)**

The Z-test of Wilson and Hilferty assumes a p -variate normal distribution:

$$Z = \frac{\sqrt[3]{\frac{\chi^2}{d}} - (1 - \frac{2}{9d})}{\sqrt{\frac{2}{9d}}}$$

where d is the degrees of freedom of the model. See McArdle (1988) and Bishop, Fienberg, and Holland (1975, p. 527) for an application of the Z-test.

- **critical N index (Hoelter 1983)**

The critical N (Hoelter 1983) is defined as

$$CN = \text{int}\left(\frac{\chi_{crit}^2}{f_{min}}\right)$$

where χ_{crit}^2 is the critical chi-square value for the given d degrees of freedom and probability $\alpha = 0.05$, and $\text{int}()$ takes the integer part of the expression. See Bollen (1989b, p. 277). Conceptually, the CN value is the largest number of observations that could still make the chi-square model fit statistic insignificant if it were to apply to the actual sample fit function value f_{min} . Hoelter (1983) suggests that CN should be at least 200; however, Bollen (1989b) notes that the CN value might lead to an overly pessimistic assessment of fit for small samples.

Note that when you have a perfect model fit for your data (that is, $f_{min} = 0$) or a zero degree of freedom for your model (that is, $d = 0$), CN is not computable.

- **root mean square residual (RMR)**

For a single-group analysis, the RMR is the root of the mean squared residuals:

$$\text{RMR} = \sqrt{\frac{1}{b} \left[\sum_i^p \sum_j^i (s_{ij} - \hat{\sigma}_{ij})^2 + \delta \sum_i^p (\bar{x}_i - \hat{\mu}_i)^2 \right]}$$

where

$$b = \frac{p(p + 1 + 2\delta)}{2}$$

is the number of distinct elements in the covariance matrix and in the mean vector (if modeled).

For multiple-group analysis, PROC CALIS uses the following formula for the overall RMR:

$$\text{overall RMR} = \sqrt{\sum_{r=1}^k \frac{w_r}{\sum_{r=1}^k w_r} \left[\sum_i^p \sum_j^i (s_{ij} - \hat{\sigma}_{ij})^2 + \delta \sum_i^p (\bar{x}_i - \hat{\mu}_i)^2 \right]}$$

where

$$w_r = \frac{N_r - 1}{N - k} b_r$$

is the weight for the squared residuals of the r th group. Hence, the weight w_r is the product of group size weight $\frac{N_r - 1}{N - k}$ and the number of distinct moments b_r in the r th group.

- **standardized root mean square residual (SRMR)**

For a single-group analysis, the SRMR is the root of the mean of the standardized squared residuals:

$$\text{SRMR} = \sqrt{\frac{1}{b} \left[\sum_i^p \sum_j^i \frac{(s_{ij} - \hat{\sigma}_{ij})^2}{s_{ii} s_{jj}} + \delta \sum_i^p \frac{(\bar{x}_i - \hat{\mu}_i)^2}{s_{ii}} \right]}$$

where b is the number of distinct elements in the covariance matrix and in the mean vector (if modeled). The formula for b is defined exactly the same way as it appears in the formula for RMR.

Similar to the calculation of the overall RMR, an overall measure of SRMR in a multiple-group analysis is a weighted average of the standardized squared residuals of the groups. That is,

$$\text{overall SRMR} = \sqrt{\sum_{r=1}^k \frac{w_r}{\sum_{r=1}^k w_r} \left[\sum_i^p \sum_j^i \frac{(s_{ij} - \hat{\sigma}_{ij})^2}{s_{ii} s_{jj}} + \delta \sum_i^p \frac{(\bar{x}_i - \hat{\mu}_i)^2}{s_{ii}} \right]}$$

where w_r is the weight for the squared residuals of the r th group. The formula for w_r is defined exactly the same way as it appears in the formula for SRMR.

- **goodness-of-fit index (GFI)**

For a single-group analysis, the goodness-of-fit index for the ULS, GLS, and ML estimation methods is:

$$\text{GFI} = 1 - \frac{\text{Tr}((\mathbf{W}^{-1}(\mathbf{S} - \hat{\Sigma}))^2) + \delta(\bar{\mathbf{x}} - \hat{\boldsymbol{\mu}})' \mathbf{W}^{-1}(\bar{\mathbf{x}} - \hat{\boldsymbol{\mu}})}{\text{Tr}((\mathbf{W}^{-1}\mathbf{S})^2) + \delta\bar{\mathbf{x}}' \mathbf{W}^{-1}\bar{\mathbf{x}}}$$

with $\mathbf{W} = \mathbf{I}$ for ULS, $\mathbf{W} = \mathbf{S}$ for GLS, and $\mathbf{W} = \hat{\Sigma}$. For WLS and DWLS estimation,

$$\text{GFI} = 1 - \frac{(\mathbf{u} - \hat{\boldsymbol{\eta}})' \mathbf{W}^{-1} (\mathbf{u} - \hat{\boldsymbol{\eta}})}{\mathbf{u}' \mathbf{W}^{-1} \mathbf{u}}$$

where \mathbf{u} is the vector of observed moments and $\hat{\boldsymbol{\eta}}$ is the vector of fitted moments. When the mean structures are modeled, vectors \mathbf{u} and $\hat{\boldsymbol{\eta}}$ contains all the nonredundant elements $\text{vecs}(\mathbf{S})$ in the covariance matrix and all the means. That is,

$$\mathbf{u} = (\text{vecs}'(\mathbf{S}), \bar{\mathbf{x}}')', \quad \hat{\boldsymbol{\eta}} = (\text{vecs}'(\hat{\Sigma}), \hat{\boldsymbol{\mu}})'$$

and the symmetric weight matrix \mathbf{W} is of dimension $p \times (p + 3)/2$. When the mean structures are not modeled, vectors \mathbf{u} and $\hat{\boldsymbol{\eta}}$ contains all the nonredundant elements $\text{vecs}(\mathbf{S})$ in the covariance matrix only. That is,

$$\mathbf{u} = \text{vecs}(\mathbf{S}), \quad \hat{\boldsymbol{\eta}} = \text{vecs}(\hat{\Sigma})$$

and the symmetric weight matrix \mathbf{W} is of dimension $p \times (p + 1)/2$. In addition, for the DWLS estimation, \mathbf{W} is a diagonal matrix.

For a constant weight matrix \mathbf{W} , the goodness-of-fit index is 1 minus the ratio of the minimum function value and the function value before any model has been fitted. The GFI should be between 0 and 1. The data probably do not fit the model if the GFI is negative or much greater than 1.

For a multiple-group analysis, individual GFI_r 's are computed for groups. The overall measure is a weighted average of individual GFI_r 's, using weight $a_r = \frac{N_r - 1}{N - k}$. That is,

$$\text{overall GFI} = \sum_{r=1}^k a_r \text{GFI}_r$$

Parsimony Indices

These indices are constructed so that the model complexity is taken into account when assessing model fit. In general, models with more parameters (fewer degrees of freedom) are penalized.

- **adjusted goodness-of-fit index (AGFI)**

The AGFI is the GFI adjusted for the degrees of freedom d of the model,

$$\text{AGFI} = 1 - \frac{c}{d} (1 - \text{GFI})$$

where

$$c = \sum_{r=1}^k \frac{p_k(p_k + 1 + 2\delta_k)}{2}$$

computes the total number of elements in the covariance matrices and mean vectors for modeling. For single-group analyses, the AGFI corresponds to the GFI in replacing the total sum of squares by the mean sum of squares.

CAUTION:

- Large p and small d can result in a negative AGFI. For example, $GFI=0.90$, $p=19$, and $d=2$ result in an AGFI of -8.5 .
- AGFI is not defined for a saturated model, due to division by $d = 0$.
- AGFI is not sensitive to losses in d .

The AGFI should be between 0 and 1. The data probably do not fit the model if the AGFI is negative or much greater than 1. For more information, see Mulaik et al. (1989).

- **parsimonious goodness-of-fit index (PGFI)**

The PGFI (Mulaik et al. 1989) is a modification of the GFI that takes the parsimony of the model into account:

$$\text{PGFI} = \frac{d_{\min}}{d_0} \text{GFI}$$

where d_{\min} is the model degrees of freedom and d_0 is the degrees of freedom for the independence model. See the section “Incremental Indices” on page 1335 for the definition of independence model. The PGFI uses the same parsimonious factor as the parsimonious normed Bentler-Bonett index (James, Mulaik, and Brett 1982).

- **RMSEA index (Steiger and Lind 1980; Steiger 1998)**

The root mean square error approximation (RMSEA) coefficient is:

$$\epsilon = \sqrt{k} \sqrt{\max\left(\frac{f_{\min}}{d_{\min}} - \frac{1}{(N-k)}, 0\right)}$$

The lower and upper limits of the $(1 - \alpha)\%$ -confidence interval are computed using the cumulative distribution function of the noncentral chi-square distribution $\Phi(x|\lambda, d)$. With $x = (N - k)f_{\min}$, λ_L satisfying $\Phi(x|\lambda_L, d_{\min}) = 1 - \frac{\alpha}{2}$, and λ_U satisfying $\Phi(x|\lambda_U, d_{\min}) = \frac{\alpha}{2}$:

$$(\epsilon_{\alpha_L}; \epsilon_{\alpha_U}) = \left(\sqrt{k} \sqrt{\frac{\lambda_L}{(N-k)d_{\min}}}; \sqrt{k} \sqrt{\frac{\lambda_U}{(N-k)d_{\min}}} \right)$$

See Browne and Du Toit (1992) for more details. The size of the confidence interval can be set by the option `ALPHARMS= α` , $0 \leq \alpha \leq 1$. The default is $\alpha = 0.1$, which corresponds to the 90% confidence interval for the RMSEA.

- **probability for test of close fit (Browne and Cudeck 1993)**

The traditional exact χ^2 test hypothesis $H_0: \epsilon = 0$ is replaced by the null hypothesis of close fit $H_0: \epsilon \leq 0.05$ and the exceedance probability P is computed as:

$$P = 1 - \Phi(x|\lambda^*, d_{\min})$$

where $x = (N - k)f_{\min}$ and $\lambda^* = 0.05^2(N - k)d_{\min}/k$. The null hypothesis of close fit is rejected if P is smaller than a prespecified level (for example, $P < 0.05$).

- **ECVI: expected cross validation index (Browne and Cudeck 1993)**

The following formulas for ECVI are limited to the case of single-sample analysis without mean structures and with either the GLS, ML, or WLS estimation method. For other cases, ECVI is not defined in PROC CALIS. For GLS and WLS, the estimator c of the ECVI is linearly related to AIC, Akaike's Information Criterion (Akaike 1974, 1987):

$$c = f_{min} + \frac{2t}{N - 1}$$

For ML estimation, c_{ML} is used:

$$c_{ML} = f_{min} + \frac{2t}{N - p - 2}$$

For GLS and WLS, the confidence interval ($c_L; c_U$) for ECVI is computed using the cumulative distribution function $\Phi(x|\lambda, d_{min})$ of the noncentral chi-square distribution,

$$(c_L; c_U) = \left(\frac{\lambda_L + p(p+1)/2 + t}{(N-1)}; \frac{\lambda_U + p(p+1)/2 + t}{(N-1)} \right)$$

with $x = (N-1)f_{min}$, $\Phi(x|\lambda_U, d_{min}) = \frac{\alpha}{2}$, and $\Phi(x|\lambda_L, d_{min}) = 1 - \frac{\alpha}{2}$.

For ML, the confidence interval ($c_L^*; c_U^*$) for ECVI is:

$$(c_L^*; c_U^*) = \left(\frac{\lambda_L^* + p(p+1)/2 + t}{N - p - 2}; \frac{\lambda_U^* + p(p+1)/2 + t}{N - p - 2} \right)$$

where $x = (N - p - 2)f_{min}$, $\Phi(x|\lambda_U^*, d_{min}) = \frac{\alpha}{2}$ and $\Phi(x|\lambda_L^*, d_{min}) = 1 - \frac{\alpha}{2}$. See Browne and Cudeck (1993). The size of the confidence interval can be set by the option `ALPHAECV= α` , $0 \leq \alpha \leq 1$. The default is $\alpha = 0.1$, which corresponds to the 90% confidence interval for the ECVI.

- **Akaike's information criterion (AIC) (Akaike 1974, 1987)**

This is a criterion for selecting the best model among a number of candidate models. The model that yields the smallest value of AIC is considered the best.

$$AIC = h + 2t$$

where h is the -2 times the likelihood function value for the FIML method or the χ^2 value for other estimation methods.

- **consistent Akaike's information criterion (CAIC) (Bozdogan 1987)**

This is another criterion, similar to AIC, for selecting the best model among alternatives. The model that yields the smallest value of CAIC is considered the best. CAIC is preferred by some people to AIC or the χ^2 test.

$$CAIC = h + (\ln(N) + 1)t$$

where h is the -2 times the likelihood function value for the FIML method or the χ^2 value for other estimation methods. Notice that N includes the number of incomplete observations for the FIML method while it includes only the complete observations for other estimation methods.

- **Schwarz's Bayesian criterion (SBC) (Schwarz 1978; Sclove 1987)**

This is another criterion, similar to AIC, for selecting the best model. The model that yields the smallest value of SBC is considered the best. SBC is preferred by some people to AIC or the χ^2 test.

$$\text{SBC} = h + \ln(N)t$$

where h is the -2 times the likelihood function value for the FIML method or the χ^2 value for other estimation methods. Notice that N includes the number of incomplete observations for the FIML method while it includes only the complete observations for other estimation methods.

- **McDonald's measure of centrality (McDonald and Marsh 1988)**

$$\text{CENT} = \exp\left(-\frac{(\chi^2 - d_{\min})}{2N}\right)$$

Incremental Indices

These indices are constructed so that the model fit is assessed through the comparison with a baseline model. The baseline model is usually the independence model where all covariances among manifest variables are assumed to be zeros. The only parameters in the independence model are the diagonals of covariance matrix. If modeled, the mean structures are saturated in the independence model. For multiple-group analysis, the overall independence model consists of component independence models for each group.

In the following, let f_0 and d_0 denote the minimized discrepancy function value and the associated degrees of freedom, respectively, for the independence model; and f_{\min} and d_{\min} denote the minimized discrepancy function value and the associated degrees of freedom, respectively, for the model being fitted in the null hypothesis.

- **Bentler comparative fit index (Bentler 1995)**

$$\text{CFI} = 1 - \frac{\max((N - k)f_{\min} - d_{\min}, 0)}{\max((N - k)f_0 - d_0, 0)}$$

- **Bentler-Bonett normed fit index (NFI) (Bentler and Bonett 1980)**

$$\Delta = \frac{f_0 - f_{\min}}{f_0}$$

Mulaik et al. (1989) recommend the parsimonious weighted form called parsimonious normed fit index (PNFI) (James, Mulaik, and Brett 1982).

- **Bentler-Bonett nonnormed coefficient (Bentler and Bonett 1980)**

$$\rho = \frac{f_0/d_0 - f_{\min}/d_{\min}}{f_0/d_0 - 1/(N - k)}$$

See Tucker and Lewis (1973).

- **normed index ρ_1 (Bollen 1986)**

$$\rho_1 = \frac{f_0/d_0 - f_{\min}/d_{\min}}{f_0/d_0}$$

ρ_1 is always less than or equal to 1; $\rho_1 < 0$ is unlikely in practice. See the discussion in Bollen (1989a).

- **nonnormed index Δ_2 (Bollen 1989a)**

$$\Delta_2 = \frac{f_0 - f_{min}}{f_0 - \frac{d_{min}}{(N-k)}}$$

is a modification of Bentler and Bonett's Δ that uses d and "lessens the dependence" on N . See the discussion in (Bollen 1989b). Δ_2 is identical to the IFI2 index of Mulaik et al. (1989).

- **parsimonious normed fit index (James, Mulaik, and Brett 1982)**

The PNFI is a modification of Bentler-Bonett's normed fit index that takes parsimony of the model into account,

$$\text{PNFI} = \frac{d_{min}}{d_0} \frac{(f_0 - f_{min})}{f_0}$$

The PNFI uses the same parsimonious factor as the parsimonious GFI of Mulaik et al. (1989).

Fit Indices and Estimation Methods

Note that not all fit indices are reasonable or appropriate for all estimation methods set by the **METHOD=** option of the PROC CALIS statement. The availability of fit indices is summarized as follows:

- Adjusted (elliptic) chi-square and its probability are available only for **METHOD=ML** or **GLS** and with the presence of raw data input.
- For **METHOD=ULS** or **DWLS**, probability of the chi-square value, RMSEA and its confidence intervals, probability of close fit, ECVI and its confidence intervals, critical N index, Z-test, AIC, CAIC, SBC, and measure of centrality are not appropriate and therefore not displayed.

Individual Fit Indices for Multiple Groups

When you compare the fits of individual groups in a multiple-group analysis, you can examine the residuals of the groups to gauge which group is fitted better than the others. While examining residuals is good for knowing specific locations with inadequate fit, summary measures like fit indices for individual groups would be more convenient for overall comparisons among groups.

Although the overall fit function is a weighted sum of individual fit functions for groups, these individual functions are not statistically independent. Therefore, in general you cannot partition the degrees of freedom or χ^2 value according to the groups. This eliminates the possibility of breaking down those fit indices that are functions of degrees of freedom or χ^2 for group comparison purposes. Bearing this fact in mind, PROC CALIS computes only a limited number of descriptive fit indices for individual groups.

- **fit function**

The overall fit function is:

$$F = \sum_{r=1}^k a_r F_r$$

where $a_r = \frac{(N_j - 1)}{(N - k)}$ and F_r are the group weight and the discrepancy function for group r , respectively. The value of unweighted fit function F_r for the r th group is denoted by:

$$f_r$$

This f_r value provides a measure of fit in the r th group without taking the sample size into account. The larger the f_r , the worse the fit for the group.

- **percentage contribution to the chi-square**

The percentage contribution of group r to the chi-square is:

$$\text{percentage contribution} = a_r f_r / f_{min} \times 100\%$$

where f_r is the value of F_r with F minimized at the value f_{min} . This percentage value provides a descriptive measure of fit of the moments in group r , weighted by its sample size. The group with the largest percentage contribution accounts for the most lack of fit in the overall model.

- **root mean square residual (RMR)**

For the r th group, the total number of moments being modeled is:

$$g = \frac{p_r(p_r + 1 + 2\delta_r)}{2}$$

where p_r is the number of variables and δ_r is the indicator variable of the mean structures in the r th group. The root mean square residual for the r th group is:

$$\text{RMR}_r = \sqrt{\frac{1}{g} \left[\sum_i^{p_r} \sum_j^i ([S_r]_{ij} - [\hat{\Sigma}_r]_{ij})^2 + \delta_r \sum_i^{p_r} ([\bar{x}_r]_i - [\hat{\mu}_r]_i)^2 \right]}$$

- **standardized root mean square residual (SRMR)**

For the r th group, the standardized root mean square residual is:

$$\text{SRMR} = \sqrt{\frac{1}{g} \left[\sum_i^{p_r} \sum_j^i \frac{([S_r]_{ij} - [\hat{\Sigma}_r]_{ij})^2}{[S_r]_{ii}[S_r]_{jj}} + \delta_r \sum_i^{p_r} \frac{([\bar{x}_r]_i - [\hat{\mu}_r]_i)^2}{[S_r]_{ii}} \right]}$$

- **goodness-of-fit index (GFI)**

For the ULS, GLS, and ML estimation, the goodness-of-fit index (GFI) for the r th group is:

$$\text{GFI} = 1 - \frac{\text{Tr}((\mathbf{W}_r^{-1}(\mathbf{S}_r - \hat{\Sigma}_r))^2) + \delta_r (\bar{\mathbf{x}}_r - \hat{\mathbf{u}}_r)' \mathbf{W}_r^{-1} (\bar{\mathbf{x}}_r - \hat{\mathbf{u}}_r)}{\text{Tr}((\mathbf{W}_r^{-1} \mathbf{S}_r)^2) + \delta_r \bar{\mathbf{x}}_r' \mathbf{W}_r^{-1} \bar{\mathbf{x}}_r}$$

with $\mathbf{W}_r = \mathbf{I}$ for ULS, $\mathbf{W}_r = \mathbf{S}_r$ for GLS, and $\mathbf{W}_r = \hat{\Sigma}_r$. For the WLS and DWLS estimation,

$$\text{GFI} = 1 - \frac{(\mathbf{u}_r - \hat{\boldsymbol{\eta}}_r)' \mathbf{W}_r^{-1} (\mathbf{u}_r - \hat{\boldsymbol{\eta}}_r)}{\mathbf{u}_r' \mathbf{W}_r^{-1} \mathbf{u}_r}$$

where \mathbf{u}_r is the vector of observed moments and $\hat{\boldsymbol{\eta}}_r$ is the vector of fitted moments for the r th group ($r = 1, \dots, k$).

When the mean structures are modeled, vectors \mathbf{u}_r and $\hat{\boldsymbol{\eta}}_r$ contain all the nonredundant elements $\text{vecs}(\mathbf{S}_r)$ in the covariance matrix and all the means, and \mathbf{W}_r is the weight matrix for covariances and means. When the mean structures are not modeled, \mathbf{u}_r , $\hat{\boldsymbol{\eta}}_r$, and \mathbf{W}_r contain elements pertaining to the covariance elements only. Basically, formulas presented here are the same as the case for a single-group GFI. The only thing added here is the subscript r to denote individual group measures.

- **Bentler-Bonett normed fit index (NFI)**

For the r th group, the Bentler-Bonett NFI is:

$$\Delta_r = \frac{f_{0r} - f_r}{f_{0r}}$$

where f_{0r} is the function value for fitting the independence model to the r th group. The larger the value of Δ_r , the better is the fit for the group. Basically, the formula here is the same as the overall Bentler-Bonett NFI. The only difference is that the subscript r is added to denote individual group measures.

Squared Multiple Correlations and Determination Coefficients

In the section, squared multiple correlations for endogenous variables are defined. Squared multiple correlation is computed for all of these five estimation methods: ULS, GLS, ML, WLS, and DWLS. These coefficients are also computed as in the LISREL VI program of Jöreskog and Sörbom (1985). The DETAE, DETSE, and DETMV determination coefficients are intended to be multivariate generalizations of the squared multiple correlations for different subsets of variables. These coefficients are displayed only when you specify the **PDETERM** option.

- **R² values corresponding to endogenous variables**

$$R^2 = 1 - \frac{\widehat{\text{Evar}}(y)}{\widehat{\text{Var}}(y)}$$

where y denotes an endogenous variable, $\widehat{\text{Var}}(y)$ denotes its variance, and $\widehat{\text{Evar}}(y)$ denotes its error (or unsystematic) variance. The variance and error variance are estimated under the model.

- **total determination of all equations**

$$\text{DETAE} = 1 - \frac{|\widehat{\text{Ecov}}(\mathbf{y}, \boldsymbol{\eta})|}{|\widehat{\text{Cov}}(\mathbf{y}, \boldsymbol{\eta})|}$$

where the \mathbf{y} vector denotes all manifest dependent variables, the $\boldsymbol{\eta}$ vector denotes all latent dependent variables, $\widehat{\text{Cov}}(\mathbf{y}, \boldsymbol{\eta})$ denotes the covariance matrix of \mathbf{y} and $\boldsymbol{\eta}$, and $\widehat{\text{Ecov}}(\mathbf{y}, \boldsymbol{\eta})$ denotes the error covariance matrix of \mathbf{y} and $\boldsymbol{\eta}$. The covariance matrices are estimated under the model.

- **total determination of latent equations**

$$\text{DETSE} = 1 - \frac{|\widehat{\text{Ecov}}(\boldsymbol{\eta})|}{|\widehat{\text{Cov}}(\boldsymbol{\eta})|}$$

where the $\boldsymbol{\eta}$ vector denotes all latent dependent variables, $\widehat{\text{Cov}}(\boldsymbol{\eta})$ denotes the covariance matrix of $\boldsymbol{\eta}$, and $\widehat{\text{Ecov}}(\boldsymbol{\eta})$ denotes the error covariance matrix of $\boldsymbol{\eta}$. The covariance matrices are estimated under the model.

- **total determination of the manifest equations**

$$\text{DETMV} = 1 - \frac{|\widehat{\text{Ecov}}(\mathbf{y})|}{|\widehat{\text{Cov}}(\mathbf{y})|}$$

where the \mathbf{y} vector denotes all manifest dependent variables, $\widehat{\text{Cov}}(\mathbf{y})$ denotes the covariance matrix of \mathbf{y} , $\widehat{\text{Ecov}}(\mathbf{y})$ denotes the error covariance matrix of \mathbf{y} , and $|\mathbf{A}|$ denotes the determinant of matrix \mathbf{A} . All the covariance matrices in the formula are estimated under the model.

You can also use the **DETERM** statement to request the computations of determination coefficients for any subsets of dependent variables.

Case-Level Residuals, Outliers, Leverage Observations, and Residual Diagnostics

Residual M-Distances and Outlier Detection

In structural equation modeling, residual analysis has been developed traditionally for the elements in the moment matrices such as mean vector and covariance matrix. See the section “Residuals in the Moment Matrices” on page 1327 for a detailed description of this type of residual. In fact, almost all fit indices in the field were developed more or less based on measuring the overall magnitude of the residuals in the moment matrices. See the section “Assessment of Fit” on page 1326 for examples of fit indices such as standardized root mean square residual (SRMR), adjusted goodness-of-fit index (AGFI), and so on.

However, recent research advances make it possible to study case-level or observational-level residuals. Although case-level residuals have not yet been used to assess overall model fit, they are quite useful as model diagnostic tools. This section describes how case-level residuals are computed and applied to the detection of outliers, the identification of leverage observations, and various residual diagnostics.

The main difficulty of case-level residual analysis in general structural equation modeling is the presence of latent variables in the model. Another difficulty is the involvement of multivariate responses. Both are nonissues in multiple regression analysis because there is no latent variable and there is only a single response variable. Hence, a good starting point for this section is to explain how PROC CALIS handles these two issues in general structural equation modeling. The residual diagnostic techniques described in the following draw heavily from Yuan and Hayashi (2010).

Latent variables in models are not observed, and their values must be predicted from the data. Although the indeterminacy of factor scores is a well-known issue, it does not mean that factor scores cannot be reasonably derived or predicted from the observed data. One of the factor score estimation methods is Bartlett’s method. Suppose for a factor model that Λ represents a $p \times m$ factor matrix and Ψ represents a $p \times p$ error covariance matrix, where p is the number of manifest variables and m is the number of factors. Bartlett’s factor scores are defined by the formula

$$\mathbf{f} = (\Lambda' \Psi^{-1} \Lambda)^{-1} \Lambda' \Psi^{-1} \mathbf{y}$$

where \mathbf{f} represents an $m \times 1$ random vector of factors and \mathbf{y} represents a $p \times 1$ random vector of manifest variables. Yuan and Hayashi (2010) generalize Bartlett’s formulas to a certain class of structural equation models. Essentially, they provide formulas that the quantities Λ and Ψ are computable functions from the parameter estimates of the structural equation models. PROC CALIS adopts their formulas. With the estimation of factor scores, residuals in structural equation models can be computed as if all values of factors are present. Hence, case-level residual analysis becomes possible.

With the possibility of a multivariate residual vector in structural equation models, a summary measure for the overall magnitude of the residuals in observations is needed. Yuan and Hayashi (2010) consider

the Mahalanobis distance (M-distance) of case-level residuals. For observation i with residual vector \hat{e}_i of dimension $h \times 1$, the residual M-distance of observation i is defined as

$$d_{r_i} = \sqrt{(\mathbf{L}\hat{e}_i)'(\mathbf{L}\Omega_{\hat{e}}\mathbf{L}')^{-1}(\mathbf{L}\hat{e}_i)}$$

where \mathbf{L} ($(h - q) \times h$) is a matrix that reduces \hat{e} to $(h - q)$ independent components, q is the number of independent factors to be estimated in the structural equation model, and $\Omega_{\hat{e}}$ is the covariance matrix of \hat{e} . The reduction of the residual vector into independent components is necessary when the number of factors q is not zero in the model. For $q > 0$, $\Omega_{\hat{e}}$ is not invertible and cannot be used in computing the M-distances for residuals. Hence, the covariance matrix $\mathbf{L}\Omega_{\hat{e}}\mathbf{L}'$ of independent components $\mathbf{L}\hat{e}$ is used instead. In practice, \hat{e}_i and $\Omega_{\hat{e}}$ are evaluated at the estimated parameter values. \mathbf{L} can be computed after $\Omega_{\hat{e}}$ is estimated.

Because the residual M-distance d_{r_i} is nonnegative and is a distance measure, the interpretation of d_{r_i} is straightforward—the larger it is, the farther away observation i is from the origin of the residuals. Therefore, the residual M-distance d_{r_i} can be used to detect outliers. The criterion for defining outliers is based on a selection of an α -level for the residual M-distance distribution. Under the multivariate normality distribution of the residuals, Yuan and Hayashi (2010) find that d_{r_i} is distributed as a χ_r variate (that is, the square root of the corresponding χ_r^2 variate), where $r = h - q$ is the degrees of freedom of the distribution. Therefore, a probability-based criterion for outlier detection can be used. An observation is an outlier according to the α -level criterion if its residual M-distance d_{r_i} is located within the upper $\alpha \times 100\%$ region of the χ_r distribution. Mathematically, an observation with d_{r_i} satisfying the following criterion is an outlier if

$$\text{prob}(\chi_r \geq d_{r_i}) < \alpha$$

The larger the α , the more liberal the criterion for detecting outliers. By default, PROC CALIS sets α to 0.01. You can override this value by using the `ALPHAOUT=` option.

Leverage Observations

Leverage observations are those with large M-distances in the exogenous variables of the model. For example, in the context of a confirmatory factor model, Yuan and Hayashi (2010) define the M-distance of exogenous latent factors d_{f_i} by the formula

$$d_{f_i} = \sqrt{\mathbf{f}_i'(\Omega_f)^{-1}\mathbf{f}_i}$$

where \mathbf{f}_i is the Bartlett's factor scores for observation i and Ω_f is the covariance matrix of the factor scores. See Yuan and Hayashi (2010) for the formulas for \mathbf{f}_i and Ω_f . PROC CALIS uses a more general formula to compute the M-distance of exogenous observed variables \mathbf{x}_i and latent variables \mathbf{f}_i in structural equation models. That is, with exogenous variables $\mathbf{v}_i = (\mathbf{x}_i \mathbf{f}_i)'$, the leverage M-distance d_{v_i} is computed as

$$d_{v_i} = \sqrt{\mathbf{v}_i'(\Omega_v)^{-1}\mathbf{v}_i}$$

where Ω_v is the covariance matrix of the exogenous variables. Leverage observations are those judged to have large leverage M-distances.

As with outlier detection, you need to set a criterion for declaring leverage observations. Specifically, an observation with d_{v_i} satisfying the following criterion is a leverage observation (or leverage point):

$$\text{prob}(\chi_c \geq d_{v_i}) < \alpha$$

where χ_c is the square root of the χ_c^2 variate, with c being the dimension of \mathbf{v}_i . The larger the α , the more liberal the criterion for declaring leverage observations. The default α value is 0.01. You can override this value by using the `ALPHALEV=` option.

Unlike the outliers that are usually judged as undesirable in models, leverage observations might or might not be bad for model estimation. Simply stated, a leverage observation is bad if it is also an outlier according to its residual M-distance value d_{ri} . Otherwise, it is a “good” leverage observation and should not be removed in model estimation.

Residual Diagnostics

Case-level residuals analysis can be very useful in detecting outliers, anomalies in residual distributions, and nonlinear functional relationships. All these techniques are graphical in nature and can be found in most textbooks in regression analysis (see, for example, Belsley, Kuh, and Welsch 1980). PROC CALIS provides these graphical analyses in the context of structural equation modeling. However, because PROC CALIS deals with multivariate responses and predictors in general, in some residual analysis the residuals are measured in terms of M-distances, which are always positive. PROC CALIS can produce the following graphical plots (with their ODS graph names in parentheses) for residual diagnostics:

- Residual histogram (CaseResidualHistogram): the distribution of residual M-distances is shown as a histogram. The residual M-distances are theoretically distributed as a χ -variate. Use the `PLOTS=CRESHIST` option to request this plot.
- Residual by leverage plot (ResidualByLeverage): the observations are plotted in a two-dimensional space according to their M-distances for residuals and leverages. Criteria for classifying outliers and leverage observations are shown in the plot so that outliers and leverage observations are located in well-defined regions of the two-dimensional space. Use the `PLOTS=RESBYLEV` option to request this plot.
- Residual by predicted values (ResidualByPredicted): the residuals (not the M-distances) of a dependent observed variable are plotted against the predicted values. This is also called the residual on fit plot. If the relationship of the dependent variable to the predictors is truly linear in the model, the residuals should be randomly dispersed in the plot. If the residuals show some systematic pattern with the predicted values, unexplained nonlinear relationships of the dependent observed variable with other variables or heteroscedasticity of error variance might exist. Use the `PLOTS=RESBYPRED` option to request this plot.
- Residual by quantile plot or Q-Q plot (ResidualByQuantile): the residual M-distances are plotted against their theoretical quantiles. Observations that depart significantly from the theoretical line (with slope=1) are problematic observations. Use the `PLOTS=QQPLOT` option to request this plot.
- Residual percentile by theoretical percentile plot or P-P plot (ResPercentileByExpPercentile): the observed residual M-distance percentiles are plotted against the theoretical percentiles. Observations that depart significantly from the theoretical line (with slope=1) are problematic observations. Use the `PLOTS=PPPLOT` option to request this plot.

Residual Diagnostics with Robust Estimation

With the presence of multiple outliers in a data set, estimation might suffer from the so-called masking effect. This problem refers to the fact that some prominent outliers in the data might have biased the estimation so that usual residual diagnostic tools might fail to detect some less prominent outliers. As a result, subsequent analyses that are based on the data set with outliers removed might actually not be free from the effects of the outliers.

Robust estimation deals with the outliers differently. Instead of relying on diagnostic tools for detection and removal of outliers, robust methods downweight the outliers during the estimation so that the undesirable outlier effect on estimation is minimized effectively. No outliers need to be removed during or after the robust estimation. Hence, the masking effect is not an issue. In addition, with the use of robust estimation, residual diagnostics for the purpose of outlier removal become a redundant concept. In such a scenario, outlier diagnostics are more important for the purpose of identification than for removal. You can use the ROBUST=RES option (or the default ROBUST option) to downweight the outliers during model estimation.

Similarly, detecting leverage observations might also suffer from the masking effect. That is, some leverage observations might not be detected if the diagnostic results are based on model estimation that includes the leverage observations themselves. Unfortunately, the ROBUST=RES option downweights only the residual outliers and does not downweight the leverage observations during estimation. However, the ROBUST=SAT option does downweight outlying observations in all variable dimensions, and hence it could be used if the masking effect of leverage observations is a concern.

Following the recommendation by Yuan and Hayashi (2010), PROC CALIS uses an eclectic approach to compute the residual and leverage M-distances. That is, when a robust estimation is requested (using either the ROBUST=SAT or ROBUST=RES option) with case-level residual analysis (using the RESIDUAL option), the residual M-distances are computed from the robust estimation results that downweight the model outliers only (that is, the procedure invoked by the ROBUST=RES(E) or RES(F) option); but the leverage M-distances are computed from the robust estimation results that downweight the outlying observations in all variable dimensions (that is, the procedure invoked by the ROBUST=SAT option). Consequently, both the residual M-distances and the leverage M-distances calculated from this eclectic approach are free from the respective masking effects—and this is true for any robust estimation methods implemented in PROC CALIS.

It is important to note that this eclectic approach applies only to the computations of the residual and leverage M-distances. The parameter estimates, fit statistics, and the case-level residuals that are displayed in the residual on fit plots are still obtained from the specific robust method requested. Table 27.7 summarizes the robust methods that PROC CALIS uses to compute the parameter estimates, fit statistics, case-level residuals, and residual and leverage M-distances with different robust options.

Table 27.7 Robust Methods for the Computations of Various Results

	Robust Option Specified		
	ROBUST=SAT	ROBUST=RES(E)	ROBUST=RES(F)
Estimates	ROBUST=SAT	ROBUST=RES(E)	ROBUST=RES(F)
Model fit	ROBUST=SAT	ROBUST=RES(E)	ROBUST=RES(F)
Case-level residuals	ROBUST=SAT	ROBUST=RES(E)	ROBUST=RES(F)
Residual M-distances	ROBUST=RES(E)	ROBUST=RES(E)	ROBUST=RES(F)
Leverage M-distances	ROBUST=SAT	ROBUST=SAT	ROBUST=SAT

One important implication from this table is that ROBUST=SAT and ROBUST=RES(E) lead to the same residual and leverage diagnostic results, which are all free from masking effects.

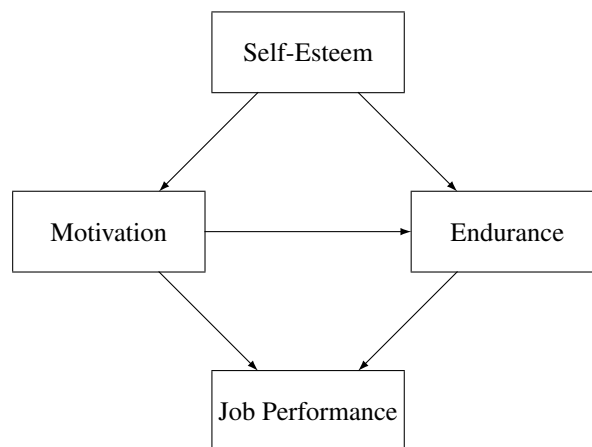
In conclusion, even though outlier removal is unnecessary with robust estimation, case-level residual diagnostics are still useful for identifying outliers and leverage observations. Needless to say, other residual diagnostics such as residual M-distance distribution, Q-Q plots, P-P plots, and residual on fit plots are useful whether you use robust estimation or not.

Total, Direct, and Indirect Effects

Most structural equation models involve the specification of the effects of variables on each other. Whenever you specify equations in the LINEQS model, paths in the PATH model, path coefficient parameters in the RAM model, variable-factor relations in the FACTOR model, or regression coefficients in model matrices of the LISMOD model, you are specifying direct effects of predictor variables on outcome variables. All direct effects are represented by the associated regression coefficients, either fixed or free, in the specifications. You can examine the direct effect estimates easily in the output for model estimation.

However, direct effects are not the only effects that are important. In some cases, the indirect effects or total effects are of interest too. For example, suppose Self-Esteem is an important factor of Job Performance in your theory. Although it does not have a direct effect on Job Performance, it affects Job Performance through its influences on Motivation and Endurance. Also, Motivation has a direct effect on Endurance in your theory. The following path diagram summarizes such a theory:

Figure 27.3 Direct and Indirect Effects of Self-Esteem on Job Performance



Clearly, each path in the diagram represents a direct effect of a predictor variable on an outcome variable. Less apparent are the total and indirect effects implied by the same path diagram. Despite this, interesting theoretical questions regarding the total and indirect effects can be raised in such a model. For example, even though there is no direct effect of Self-Esteem on Job Performance, what is its indirect effect on Job Performance? In addition to its direct effect on Job Performance, Motivation also has an indirect effect on Job Performance via its effect on Endurance. So, what is the total effect of Motivation on Job Performance and what portion of this total effect is indirect? The **TOTEFF** option of the CALIS statement and the **EFFPART** statement are designed to address these questions. By using the **TOTEFF** option or the **EFFPART** statement, PROC CALIS can compute the total, direct, and indirect effects of any sets of predictor variables on any sets of outcome variables. In this section, formulas for computing these effects are presented.

Formulas for Computing Total, Direct and Indirect Effects

No matter which modeling language is used, variables in a model can be classified into three groups. The first group is the so-called dependent variables, which serve as outcome variables at least once in the model. The other two groups consist of the remaining independent variables, which never serve as outcome variables in the model. The second group consists of independent variables that are unsystematic sources such as error and disturbance variables. The third group consists of independent variables that are systematic sources only.

Any variable, no matter which group it falls into, can have effects on the first group of variables. By definition, however, effects of variables in the first group on the other two groups do not exist. Because the effects of unsystematic sources in the second group are treated as residual effects on the first group of dependent variables, these effects are trivial in the sense that they always serve as direct effects only. That is, the effects from the second group of unsystematic sources partition trivially—total effects are always the same as the direct effects for this group. Therefore, for the purpose of effect analysis or partitioning, only the first group (dependent variables) and the third group (systematic independent variables) are considered.

Define \mathbf{u} to be the set of n_u dependent variables in the first group and w to be the set of n_w systematic independent variables in the third group. Variables in both groups can be manifest or latent. All variables in the effect analysis is thus represented by the vector $(\mathbf{u}', \mathbf{w}')'$.

The $(n_u + n_w) \times (n_u + n_w)$ matrix \mathbf{D} of *direct* effects refers to the path coefficients from all column variables to the row variables. This matrix is represented by:

$$\mathbf{D} = \begin{pmatrix} \boldsymbol{\beta} & \boldsymbol{\gamma} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}$$

where $\boldsymbol{\beta}$ is an $(n_u \times n_u)$ matrix for direct effects of dependent variables on dependent variables and $\boldsymbol{\gamma}$ is an $(n_u \times n_w)$ matrix for direct effects of systematic independent variables on dependent variables. By definition, there should not be any direct effects on independent variables, and therefore the lower submatrices of \mathbf{D} are null. In addition, by model restrictions the diagonal elements of matrix $\boldsymbol{\beta}$ must be zeros.

Correspondingly, the $(n_u + n_w) \times (n_u + n_w)$ matrix \mathbf{T} of *total* effects of column variables on the row variables is computed by:

$$\mathbf{T} = \begin{pmatrix} (\mathbf{I} - \boldsymbol{\beta})^{-1} - \mathbf{I} & (\mathbf{I} - \boldsymbol{\beta})^{-1} \boldsymbol{\gamma} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}$$

Finally, the $(n_u + n_w) \times (n_u + n_w)$ matrix $\boldsymbol{\mu}$ of *indirect* effects of column variables on the row variables is computed by the difference between \mathbf{T} and \mathbf{D} as:

$$\boldsymbol{\mu} = \begin{pmatrix} (\mathbf{I} - \boldsymbol{\beta})^{-1} - \mathbf{I} - \boldsymbol{\beta} & (\mathbf{I} - \boldsymbol{\beta})^{-1} \boldsymbol{\gamma} - \boldsymbol{\gamma} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}$$

In PROC CALIS, any subsets of \mathbf{D} , \mathbf{T} , and $\boldsymbol{\mu}$ can be requested via the specification in the `EFFPART` statement. All you need to do is to specify the sets of column variables (variables that have effects on others) and row variables (variables that receive the effects, direct or indirect). Specifications of the column and row variables are done conveniently by specifying variable names—no matrix terminology is needed. This feature is very handy if you have some focused subsets of effects that you want to analyze a priori. See the `EFFPART` statement on page 1137 for details about specifications.

Stability Coefficient of Reciprocal Causation

For recursive models (that is, models without cyclical paths of effects), using the preceding formulas for computing the total effect and the indirect effect is appropriate without further restrictions. However, for non-recursive models (that is, models with reciprocal effects or cyclical effects) the appropriateness of the preceding formulas for effect computations is restricted to situations with the convergence of the total effects.

A necessary and sufficient condition for the convergence of total effects (with or without cyclical paths) is when all eigenvalues, complex or real, of the β matrix fall into a unit circle (see Bentler and Freeman 1983). Equivalently, define the stability coefficient of reciprocal causation as the largest length (modulus) of the eigenvalues of the β matrix. A stability coefficient less than one would ensure that all eigenvalues, complex or real, of the β matrix fall into a unit circle. Hence, stability coefficient that is less than one is a necessary and sufficient condition for the convergence of the total effects, which in turn substantiates the appropriateness of total and indirect effect computations. Whenever effect analysis or partitioning is requested, PROC CALIS will check the appropriateness of effect computations by evaluating the stability coefficient of reciprocal causation. If the stability coefficient is greater than one, computations of the total and indirect effects will not be done.

Standardized Solutions

Standardized solutions are useful when you want to compare parameter values that are measured on quite different scales. PROC CALIS provides standardized solutions routinely. In standardizing a solution, parameters are classified into five groups:

- **path coefficients, regression coefficients, or direct effects**

With each parameter α in this group, there is an associated outcome variable and a predictor variable. Denote the predicted variance of the outcome variable by σ_o^2 and the variance of the predictor variable by σ_p^2 , the standardized parameter α^* is:

$$\alpha^* = \alpha \frac{\sigma_p}{\sigma_o}$$

- **fixed ones for the path coefficients attached to error or disturbance terms**

These fixed values are unchanged in standardization.

- **variances and covariances among exogenous variables, excluding errors and disturbances**

Let σ_{ij} be the covariance between variables i and j . In this notation, σ_{ii} is the variance of variable i . The standardized covariance σ_{ij}^* is:

$$\sigma_{ij}^* = \frac{\sigma_{ij}}{\sqrt{\sigma_{ii}\sigma_{jj}}}$$

When $i = j$, σ_{ii}^* takes the value of 1 for all i . Also, σ_{ij}^* is the correlation between the i th and j th variables.

- **variances and covariances among errors or disturbances**

Denote the error covariance parameter as θ_{ij} so that θ_{ii} represents the variance parameter of error variable i . Associated with each error or disturbance variable i is a unique outcome variable. Let the

variance of such an outcome variable be σ_{ii} . In the standardized solution, the error covariance θ_{ij} is rescaled as:

$$\theta_{ij}^* = \frac{\theta_{ij}}{\sqrt{\sigma_{ii}\sigma_{jj}}}$$

Notice that when $i = j$, θ_{ii}^* is not standardized to 1 in general. In fact, the error (disturbance) variance is simply rescaled by the reciprocal of the variance of the associated dependent variable. As a result, the rescaled error (disturbance) variance represents the proportion of variation of the dependent variable due to the unsystematic source. By the same token, θ_{ij}^* does not represent the correlation between errors i and j . It is a rescaled covariance of the errors involved.

- **intercepts and means of variables**

These parameters are fixed zeros in the standardized solution.

While formulas for the standardized solution are useful in computing the parameter values in the standardized solution, it is conceptually more useful to explain how variables are being transformed in the standardization process. The following provides a summary of the transformation process:

- Observed and latent variables, excluding errors or disturbances, are centered and then divided by their corresponding standard deviations. Therefore, in the standardized solution, all these variables will have variance equal to 1. In other words, these variables are truly standardized.
- Errors or disturbances are divided by the standard deviations of the corresponding outcome variables. In the standardized solution, these variables will not have variance equal to 1 in general. However, the rescaled error variances represent the proportion of unexplained or unsystematic variance of the corresponding outcome variables. Therefore, errors or disturbances in the standardized solution are simply rescaled but not standardized.

Standardized total, direct, and indirect effects are computed using formulas presented in the section “[Total, Direct, and Indirect Effects](#)” on page 1343, but with the standardized parameter values substituted into the formulas.

Although parameter values associated with different scales are made more comparable in the standardized solution, a precaution should be mentioned. In the standardized solution, the original constraints on parameters in the unstandardized solution are usually lost. These constraints, however, might underscore some important theoretical position that needs to be maintained in the model. Destroying these constraints in the standardized solution means that interpretations or comparisons of parameter values in the standardized solution are made without maintaining the original theoretical position. You must judge whether such a departure from the original constraints poses conceptual difficulties for interpreting the standardized solution.

Modification Indices

While fitting structural equation models is mostly a confirmatory analytic procedure, it does not prevent you from exploring what might have been a better model given the data. After fitting your theoretical structural equation model, you might want to modify the original model in order to do one of the following:

- add free parameters to improve the model fit significantly
- reduce the number of parameters without affecting the model fit too much

The first kind of model modification can be achieved by using the Lagrange multiplier (LM) test indices. Parameters that have the largest LM indices would increase the model fit the most. In general, adding more parameters to your model improves the overall model fit, as measured by those absolute or standalone fit indices (see the section “Overall Model Fit Indices” on page 1329 for more details). However, adding parameters liberally makes your model more prone to sampling errors. It also makes your model more complex and less interpretable in most cases. A disciplined use of LM test indices is highly recommended. In addition to the model fit improvement indicated by the LM test indices, you should also consider the theoretical significance when adding particular parameters. See [Example 27.28](#) for an illustration of the use of LM test indices for improving model fit.

The second kind of model modification can be achieved by using the Wald statistics. Parameters that are not significant in your model may be removed from the model without affecting the model fit too much. In general, removing parameters from your model decreases the model fit, as measured by those absolute or standalone fit indices (see the section “Overall Model Fit Indices” on page 1329 for more details). However, for just a little sacrifice in model fit, removing non-significant parameters increases the simplicity and precision of your model, which is the virtue that any modeler should look for.

Whether adding parameters by using the LM test indices or removing unnecessary parameters by the Wald statistics, you should not treat your modified model as if it were your original hypothesized model. That is, you should not publish your modified model as if it were hypothesized a priori. It is perfectly fine to use modification indices to gain additional insights for future research. But if you want to publish your modified model together with your original model, you should report the modification process that leads to your modified model. Theoretical justifications of the modified model should be supplemented if you want to make strong statements to support your modified model. Whenever possible, the best practice is to show reasonable model fit of the modified model with new data.

To modify your model either by LM test indices or Wald statistics, you can use the **MODIFICATION** or **MOD** option in the PROC CALIS statement. To customize the LM tests by setting specific regions of parameters, you can use the **LMTESTS** statements. PROC CALIS computes and displays the following default set of modification indices:

- **univariate Lagrange multiplier (LM) test indices for parameters in the model**

These are second-order approximations of the decrease in the χ^2 value that would result from allowing the *fixed parameter values* in the model to be freed to estimate. LM test indices are ranked within their own parameter regions in the model. The ones that suggest greatest model improvements (that is, greatest χ^2 drop) are ranked first. Depending on the type of your model, the set of possible parameter regions varies. For example, in a RAM model, modification indices are ranked in three different parameter regions for the covariance structures: path coefficients, variances of and covariances among exogenous variables, and the error variances and covariances. In addition to the value of the Lagrange multiplier, the corresponding *p*-value (*df* = 1) and the approximate change of the parameter value are displayed.

If you use the LMMAT option in the **LMTESTS** statement, LM test indices are shown as elements in model matrices. Not all elements in a particular model matrix will have LM test indices. Elements that are already free parameters in the model do not have LM test indices. Instead, the parameter names are shown. Elements that are model restricted values (for example, direct path from a variable

to itself must be zero) are labeled Excluded in the matrix output. When you customize your own regions of LM tests, some elements might also be excluded from a custom set of LM tests. These elements are also labeled as Excluded in the matrix output. If an LM test for freeing a parameter would result in a singular information matrix, the corresponding element in the matrix is labeled as Singular.

- **univariate Lagrange multiplier test indices for releasing equality constraints**

These are second-order approximations of the decrease in the χ^2 value that would result from the release of *equality constraints*. Multiple equality constraints containing $n > 2$ parameters are tested successively in n steps, each assuming the release of one of the equality-constrained parameters. The expected change of the parameter values of the separated parameter and the remaining parameter cluster are displayed, too.

- **univariate Lagrange multiplier test indices for releasing active boundary constraints**

These are second-order approximations of the decrease in the χ^2 value that would result from the release of the *active boundary constraints* specified in the `BOUNDS` statement.

- **stepwise multivariate Wald statistics for constraining free parameters to 0**

These are second-order approximations of the increases in χ^2 value that would result from constraining free parameters to zero in a stepwise fashion. In each step, the parameter that would lead to the smallest increase in the multivariate χ^2 value is set to 0. Besides the multivariate χ^2 value and its p -value, the univariate increments are also displayed. The process stops when the univariate p -value is smaller than the specified value in the `SLMW=` option, of which the default value is 0.05.

All of the preceding tests are approximations. You can often obtain more accurate tests by actually fitting different models and computing likelihood ratio tests. For more details about the Wald and the Lagrange multiplier test, see MacCallum (1986), Buse (1982), Bentler (1986), or Lee (1985). Note that relying solely on the LM tests to modify your model can lead to unreliable models that capitalize purely on sampling errors. See MacCallum, Roznowski, and Necowitz (1992) for the use of LM tests.

For large model matrices, the computation time for the default modification indices can considerably exceed the time needed for the minimization process.

The modification indices are not computed for unweighted least squares or diagonally weighted least squares estimation.

Missing Values and the Analysis of Missing Patterns

If the `DATA=` data set contains raw data (rather than a covariance or correlation matrix), in general observations with missing values for any variables in the analysis are omitted from the computations. The only exception is with `METHOD=FIML`. Incomplete observations with at least one nonmissing variables in the analysis are also used for the estimation.

If a covariance or correlation matrix is read, missing values are allowed as long as every pair of variables has at least one nonmissing value. Unlike the raw data input, `METHOD=FIML` does not allow missing values in the covariance or correlation matrix.

When you use `METHOD=FIML`, PROC CALIS provide several analyses on the missing patterns of the raw input data sets. First, PROC CALIS shows the coverage results for the means and covariances. The

coverage results refer to the proportions of data present for computing the means and the covariances. Because distinct missing patterns in the data sets are possible, the coverage proportions for the individual means and covariances could vary. Average coverage proportions of the means and covariances give you an overall idea about the missingness (or the lack of). In order to help locate the problematic means and covariances that have the low coverage, PROC CALIS shows the rank orders of the smallest coverages of mean and covariance elements. The number of smallest coverages shown for the means is equal to half of the total number of variables. The number of smallest coverages shown for the covariances is equal to half of the total number of the distinct elements in the lower triangular of the covariance matrix. However, in both cases at most 10 smallest coverages would be shown.

Second, PROC CALIS ranks the most frequent missing patterns in the data set (the nonmissing pattern is excluded in the ranking). Because the number of missing patterns could be quite large, PROC CALIS displays only a limited number of most frequent missing patterns in the output. You can use the `MAXMISSPAT=` and the `TMISSPAT=` options to control the number of missing patterns to display. See these options for details.

Third, PROC CALIS shows the means of the most frequent missing patterns, along with the means for the nonmissing pattern for comparison.

See [Example 27.15](#) for an illustration of the use of the full information maximum likelihood method and the analysis of missing patterns.

Measures of Multivariate Kurtosis

In many applications, the manifest variables are not even approximately multivariate normal. If this happens to be the case with your data set, the default generalized least squares and maximum likelihood estimation methods are not appropriate, and you should compute the parameter estimates and their standard errors by an asymptotically distribution-free method, such as the WLS estimation method. If your manifest variables are multivariate normal, then they have a zero relative multivariate kurtosis, and all marginal distributions have zero kurtosis (Browne 1982). If your `DATA=` data set contains raw data, PROC CALIS computes univariate skewness and kurtosis and a set of multivariate kurtosis values. By default, the values of univariate skewness and kurtosis are corrected for bias (as in PROC UNIVARIATE), but using the `BIASKUR` option enables you to compute the uncorrected values also. The values are displayed when you specify the PROC CALIS statement option `KURTOSIS`.

In the following formulas, N denotes the sample size and p denotes the number of variables.

- **corrected variance for variable z_j**

$$\sigma_j^2 = \frac{1}{N-1} \sum_i^N (z_{ij} - \bar{z}_j)^2$$

- **uncorrected univariate skewness for variable z_j**

$$\gamma_{1(j)} = \frac{N \sum_i^N (z_{ij} - \bar{z}_j)^3}{\sqrt{N [\sum_i^N (z_{ij} - \bar{z}_j)^2]^3}}$$

- **corrected univariate skewness for variable z_j**

$$\gamma_{1(j)} = \frac{N}{(N-1)(N-2)} \frac{\sum_i^N (z_{ij} - \bar{z}_j)^3}{\sigma_j^3}$$

- **uncorrected univariate kurtosis for variable z_j**

$$\gamma_{2(j)} = \frac{N \sum_i^N (z_{ij} - \bar{z}_j)^4}{[\sum_i^N (z_{ij} - \bar{z}_j)^2]^2} - 3$$

- **corrected univariate kurtosis for variable z_j**

$$\gamma_{2(j)} = \frac{N(N+1)}{(N-1)(N-2)(N-3)} \frac{\sum_i^N (z_{ij} - \bar{z}_j)^4}{\sigma_j^4} - \frac{3(N-1)^2}{(N-2)(N-3)}$$

- **Mardia's multivariate kurtosis**

$$\gamma_2 = \frac{1}{N} \sum_i^N [(z_i - \bar{z})' S^{-1} (z_i - \bar{z})]^2 - p(p+2)$$

where S is the biased sample covariance matrix with N as the divisor.

- **relative multivariate kurtosis**

$$\eta_2 = \frac{\gamma_2 + p(p+2)}{p(p+2)}$$

- **normalized multivariate kurtosis**

$$\kappa_0 = \frac{\gamma_2}{\sqrt{8p(p+2)/N}}$$

- **Mardia based kappa**

$$\kappa_1 = \frac{\gamma_2}{p(p+2)}$$

- **mean scaled univariate kurtosis**

$$\kappa_2 = \frac{1}{3p} \sum_j^p \gamma_{2(j)}$$

- **adjusted mean scaled univariate kurtosis**

$$\kappa_3 = \frac{1}{3p} \sum_j^p \gamma_{2(j)}^*$$

with

$$\gamma_{2(j)}^* = \begin{cases} \gamma_{2(j)} & , \quad \text{if } \gamma_{2(j)} > \frac{-6}{p+2} \\ \frac{-6}{p+2} & , \quad \text{otherwise} \end{cases}$$

If variable Z_j is normally distributed, the uncorrected univariate kurtosis $\gamma_{2(j)}$ is equal to 0. If Z has an p -variate normal distribution, Mardia's multivariate kurtosis γ_2 is equal to 0. A variable Z_j is called *leptokurtic* if it has a positive value of $\gamma_{2(j)}$ and is called *platykurtic* if it has a negative value of $\gamma_{2(j)}$. The values of κ_1 , κ_2 , and κ_3 should not be smaller than the following lower bound (Bentler 1985):

$$\hat{\kappa} \geq \frac{-2}{p+2}$$

PROC CALIS displays a message if κ_1 , κ_2 , or κ_3 falls below the lower bound.

If weighted least squares estimates (METHOD=WLS or METHOD=ADF) are specified and the weight matrix is computed from an input raw data set, the CALIS procedure computes two more measures of multivariate kurtosis.

- **multivariate mean kappa**

$$\kappa_4 = \frac{1}{m} \sum_i^p \sum_j^i \sum_k^j \sum_l^k \hat{\kappa}_{ij,kl} - 1$$

where

$$\hat{\kappa}_{ij,kl} = \frac{s_{ij,kl}}{s_{ij}s_{kl} + s_{ik}s_{jl} + s_{il}s_{jk}}$$

and $m = p(p+1)(p+2)(p+3)/24$ is the number of elements in the vector $s_{ij,kl}$ (Bentler 1985).

- **multivariate least squares kappa**

$$\kappa_5 = \frac{s_4' s_2}{s_2' s_2} - 1$$

where s_2 is the vector of the elements in the denominator of $\hat{\kappa}$ (Bentler 1985) and s_4 is the vector of the $s_{ij,kl}$, which is defined as

$$s_{ij,kl} = \frac{1}{N} \sum_{r=1}^N (z_{ri} - \bar{z}_i)(z_{rj} - \bar{z}_j)(z_{rk} - \bar{z}_k)(z_{rl} - \bar{z}_l)$$

The occurrence of significant nonzero values of Mardia's multivariate kurtosis γ_2 and significant amounts of some of the univariate kurtosis values $\gamma_{2(j)}$ indicate that your variables are not multivariate normal distributed. Violating the multivariate normality assumption in (default) generalized least squares and maximum likelihood estimation usually leads to the wrong approximate standard errors and incorrect fit statistics based on the χ^2 value. In general, the parameter estimates are more stable against violation of the normal distribution assumption. For more details, see Browne (1974, 1982, 1984).

Initial Estimates

Each optimization technique requires a set of initial values for the parameters. To avoid local optima, the initial values should be as close as possible to the globally optimal solution. You can check for local optima

by running the analysis with several different sets of initial values; the `RANDOM=` option in the PROC CALIS statement is useful in this regard.

Except for the case of exploratory FACTOR model, you can specify initial estimates manually for all different types of models. If you do not specify some of the initial estimates and the `RANDOM=` option is not used, PROC CALIS will use a combination of good strategic methods to compute initial estimates for your model.

These initial estimation methods are used in PROC CALIS:

- two-stage least squares estimation
- instrumental variable method (Hägglund 1982; Jennrich 1987)
- approximate factor analysis method
- ordinary least squares estimation
- estimation method of McDonald (McDonald and Hartmann 1992)
- observed moments of manifest exogenous variables

The choice of initial estimation methods is dependent on the data and on the model. In general, it is difficult to tell in advance which initial estimation methods will be used for a given analysis. However, PROC CALIS displays the methods used to obtain initial estimates in the output. Notice that none of these initial estimation methods can be applied to the COSAN model because of the general formulation of the COSAN model. If you do not provide initial parameter estimates for the COSAN model, the default values or random values are used (see the `START=` and the `RANDOM=` options).

Poor initial values can cause convergence problems, especially with maximum likelihood estimation. Sufficiently large positive initial values for variance estimates (as compared with the covariance estimates) might help prevent a nonnegative definite initial predicted covariance model matrix from happening. If maximum likelihood estimation fails to converge, it might help to use `METHOD=LSML`, which uses the final estimates from an unweighted least squares analysis as initial estimates for maximum likelihood. Or you can fit a slightly different but better-behaved model and produce an `OUTMODEL=` data set, which can then be modified in accordance with the original model and used as an `INMODEL=` data set to provide initial values for another analysis.

If you are analyzing a covariance or scalar product matrix, be sure to take into account the scales of the variables. The default initial values might be inappropriate when some variables have extremely large or small variances.

Use of Optimization Techniques

No algorithm for optimizing general nonlinear functions exists that can always find the global optimum for a general nonlinear minimization problem in a reasonable amount of time. Since no single optimization technique is invariably superior to others, PROC CALIS provides a variety of optimization techniques that work well in various circumstances. However, you can devise problems for which none of the techniques in PROC CALIS can find the correct solution. All optimization techniques in PROC CALIS use $O(n^2)$

memory except the conjugate gradient methods, which use only $O(n)$ of memory and are designed to optimize problems with many parameters.

The PROC CALIS statement NLOPTIONS can be especially helpful for tuning applications with nonlinear equality and inequality constraints on the parameter estimates. Some of the options available in NLOPTIONS can also be invoked as PROC CALIS options. The NLOPTIONS statement can specify almost the same options as the SAS/OR NLP procedure.

Nonlinear optimization requires the repeated computation of the following:

- the function value (optimization criterion)
- the gradient vector (first-order partial derivatives)
- for some techniques, the (approximate) Hessian matrix (second-order partial derivatives)
- values of linear and nonlinear constraints
- the first-order partial derivatives (Jacobian) of nonlinear constraints

For the criteria used by PROC CALIS, computing the gradient takes more computer time than computing the function value, and computing the Hessian takes *much* more computer time and memory than computing the gradient, especially when there are many parameters to estimate. Unfortunately, optimization techniques that do not use the Hessian usually require many more iterations than techniques that do use the (approximate) Hessian, and so they are often slower. Techniques that do not use the Hessian also tend to be less reliable (for example, they might terminate at local rather than global optima).

The available optimization techniques are displayed in the following table and can be chosen by the OMETHOD=*name* option.

OMETHOD=	Optimization Technique
LEVVAR	Levenberg-Marquardt method
TRUREG	Trust-region method
NEWRAP	Newton-Raphson method with line search
NRRIDG	Newton-Raphson method with ridging
QUANEW	Quasi-Newton methods (DBFGS, DDFP, BFGS, DFP)
DBLDOG	Double-dogleg method (DBFGS, DDFP)
CONGRA	Conjugate gradient methods (PB, FR, PR, CD)

The following table shows, for each optimization technique, which derivatives are needed (first-order or second-order) and what kind of constraints (boundary, linear, or nonlinear) can be imposed on the parameters.

OMETHOD=	Derivatives		Constraints		
	First Order	Second Order	Boundary	Linear	Nonlinear
LEVVAR	X	X	X	X	-
TRUREG	X	X	X	X	-
NEWRAP	X	X	X	X	-
NRRIDG	X	X	X	X	-
QUANEW	X	-	X	X	X
DBLDOG	X	-	X	X	-
CONGRA	X	-	X	X	-

The Levenberg-Marquardt, trust-region, and Newton-Raphson techniques are usually the most reliable, work well with boundary and general linear constraints, and generally converge after a few iterations to a precise solution. However, these techniques need to compute a Hessian matrix in each iteration. Computing the approximate Hessian in each iteration can be very time- and memory-consuming, especially for large problems (more than 200 parameters, depending on the computer used). For large problems, a quasi-Newton technique, especially with the BFGS update, can be far more efficient.

For a poor choice of initial values, the Levenberg-Marquardt method seems to be more reliable.

If memory problems occur, you can use one of the conjugate gradient techniques, but they are generally slower and less reliable than the methods that use second-order information.

There are several options to control the optimization process. You can specify various termination criteria. You can specify the `GCONV=` option to specify a relative gradient termination criterion. If there are active boundary constraints, only those gradient components that correspond to inactive constraints contribute to the criterion. When you want very precise parameter estimates, the `GCONV=` option is useful. Other criteria that use relative changes in function values or parameter estimates in consecutive iterations can lead to early termination when active constraints cause small steps to occur. The small default value for the `FCONV=` option helps prevent early termination. Using the `MAXITER=` and `MAXFUNC=` options enables you to specify the maximum number of iterations and function calls in the optimization process. These limits are especially useful in combination with the `INMODEL=` and `OUTMODEL=` options; you can run a few iterations at a time, inspect the results, and decide whether to continue iterating.

Nonlinearly Constrained QN Optimization

The algorithm used for nonlinearly constrained quasi-Newton optimization is an efficient modification of Powell's Variable Metric Constrained WatchDog (VMCWD) algorithm (Powell 1978a, b, 1982a, b). A similar but older algorithm (VF02AD) is part of the Harwell library. Both VMCWD and VF02AD use Fletcher's VE02AD algorithm (also part of the Harwell library) for positive definite quadratic programming. The PROC CALIS QUANEW implementation uses a quadratic programming subroutine that updates and down-dates the approximation of the Cholesky factor when the active set changes. The nonlinear QUANEW algorithm is not a feasible point algorithm, and the value of the objective function might not necessarily decrease (minimization) or increase (maximization) monotonically. Instead, the algorithm tries to reduce a linear combination of the objective function and constraint violations, called the *merit function*.

The following are similarities and differences between this algorithm and VMCWD:

- A modification of this algorithm can be performed by specifying `VERSION=1`, which replaces the update of the Lagrange vector μ with the original update of Powell (1978a, b), which is used in VF02AD. This can be helpful for some applications with linearly dependent active constraints.
- If the `VERSION=` option is not specified or `VERSION=2` is specified, the evaluation of the Lagrange vector μ is performed in the same way as Powell (1982a, b) describes.
- Instead of updating an approximate Hessian matrix, this algorithm uses the dual BFGS (or DFP) update that updates the Cholesky factor of an approximate Hessian. If the condition of the updated matrix gets too bad, a restart is done with a positive diagonal matrix. At the end of the first iteration after each restart, the Cholesky factor is scaled.
- The Cholesky factor is loaded into the quadratic programming subroutine, automatically ensuring positive definiteness of the problem. During the quadratic programming step, the Cholesky factor of

the projected Hessian matrix $Z'_k G Z_k$ and the QT decomposition are updated simultaneously when the active set changes. See Gill et al. (1984) for more information.

- The line-search strategy is very similar to that of Powell (1982a, b). However, this algorithm does not call for derivatives during the line search; hence, it generally needs fewer derivative calls than function calls. The VMCWD algorithm always requires the same number of derivative and function calls. It was also found in several applications of VMCWD that Powell's line-search method sometimes uses steps that are too long during the first iterations. In those cases, you can use the `INSTEP=` option specification to restrict the step length α of the first iterations.
- The watchdog strategy is similar to that of Powell (1982a, b). However, this algorithm does not return automatically after a fixed number of iterations to a former better point. A return here is further delayed if the observed function reduction is close to the expected function reduction of the quadratic model.
- Although Powell's termination criterion still is used (as `FCONV2`), the `QUANEW` implementation uses two additional termination criteria (`GCONV` and `ABSGCONV`).

This algorithm is automatically invoked when you specify the `NLINCON` statement. The nonlinear `QUANEW` algorithm needs the Jacobian matrix of the first-order derivatives (constraints normals) of the constraints:

$$(\nabla c_i) = \left(\frac{\partial c_i}{\partial x_j} \right), \quad i = 1, \dots, nc, j = 1, \dots, n$$

where nc is the number of nonlinear constraints for a given point x .

You can specify two update formulas with the `UPDATE=` option:

- `UPDATE=DBFGS` performs the dual BFGS update of the Cholesky factor of the Hessian matrix. This is the default.
- `UPDATE=DDFP` performs the dual DFP update of the Cholesky factor of the Hessian matrix.

This algorithm uses its own line-search technique. All options and parameters (except the `INSTEP=` option) controlling the line search in the other algorithms do not apply here. In several applications, large steps in the first iterations are troublesome. You can specify the `INSTEP=` option to impose an upper bound for the step size α during the first five iterations. The values of the `LCSINGULAR=`, `LCEPSILON=`, and `LCDEACT=` options (which control the processing of linear and boundary constraints) are valid only for the quadratic programming subroutine used in each iteration of the nonlinear constraints `QUANEW` algorithm.

Optimization and Iteration History

The optimization and iteration histories are displayed by default because it is important to check for possible convergence problems. The optimization history includes the following summary of information about the initial state of the optimization:

- the number of constraints that are active at the starting point, or more precisely, the number of constraints that are currently members of the working set. If this number is followed by a plus sign, there are more active constraints, of which at least one is temporarily released from the working set due to negative Lagrange multipliers.

- the value of the objective function at the starting point
- if the (projected) gradient is available, the value of the largest absolute (projected) gradient element
- for the TRUREG and LEVMAR subroutines, the initial radius of the trust region around the starting point

The optimization history ends with some information concerning the optimization result:

- the number of constraints that are active at the final point, or more precisely, the number of constraints that are currently members of the working set. If this number is followed by a plus sign, there are more active constraints, of which at least one is temporarily released from the working set due to negative Lagrange multipliers.
- the value of the objective function at the final point
- if the (projected) gradient is available, the value of the largest absolute (projected) gradient element
- other information specific to the optimization technique

The iteration history generally consists of one line of displayed output containing the most important information for each iteration.

The iteration history always includes the following:

- the iteration number
- the number of iteration restarts
- the number of function calls
- the number of active constraints
- the value of the optimization criterion
- the difference between adjacent function values
- the maximum of the absolute gradient components that correspond to inactive boundary constraints

An apostrophe trailing the number of active constraints indicates that at least one of the active constraints is released from the active set due to a significant Lagrange multiplier.

For the Levenberg-Marquardt technique (LEVMAR), the iteration history also includes the following information:

- an asterisk trailing the iteration number when the computed Hessian approximation is singular and consequently ridged with a positive lambda value. If all or the last several iterations show a singular Hessian approximation, the problem is not sufficiently identified. Thus, there are other locally optimal solutions that lead to the same optimum function value for different parameter values. This implies that standard errors for the parameter estimates are not computable without the addition of further constraints.

- the value of the Lagrange multiplier (λ). This value is 0 when the optimum of the quadratic function approximation is inside the trust region (a trust-region-scaled Newton step can be performed) and is greater than 0 when the optimum of the quadratic function approximation is located at the boundary of the trust region (the scaled Newton step is too long to fit in the trust region and a quadratic constraint optimization is performed). Large values indicate optimization difficulties. For a nonsingular Hessian matrix, the value of λ should go to 0 during the last iterations, indicating that the objective function can be well approximated by a quadratic function in a small neighborhood of the optimum point. An increasing λ value often indicates problems in the optimization process.
- the value of the ratio ρ (rho) between the actually achieved difference in function values and the predicted difference in the function values on the basis of the quadratic function approximation. Values much less than 1 indicate optimization difficulties. The value of the ratio ρ indicates the goodness of the quadratic function approximation. In other words, $\rho \ll 1$ means that the radius of the trust region has to be reduced; a fairly large value of ρ means that the radius of the trust region does not need to be changed. And a value close to or greater than 1 means that the radius can be increased, indicating a good quadratic function approximation.

For the Newton-Raphson technique (NRRIDG), the iteration history also includes the following information:

- the value of the ridge parameter. This value is 0 when a Newton step can be performed, and it is greater than 0 when either the Hessian approximation is singular or a Newton step fails to reduce the optimization criterion. Large values indicate optimization difficulties.
- the value of the ratio ρ (rho) between the actually achieved difference in function values and the predicted difference in the function values on the basis of the quadratic function approximation. Values much less than 1.0 indicate optimization difficulties.

For the Newton-Raphson with line-search technique (NEWRAP), the iteration history also includes the following information:

- the step size α (alpha) computed with one of the line-search algorithms
- the slope of the search direction at the current parameter iterate. For minimization, this value should be significantly negative. Otherwise, the line-search algorithm has difficulty reducing the function value sufficiently.

For the trust-region technique (TRUREG), the iteration history also includes the following information:

- an asterisk after the iteration number when the computed Hessian approximation is singular and consequently ridged with a positive λ value.
- the value of the Lagrange multiplier (λ). This value is zero when the optimum of the quadratic function approximation is inside the trust region (a trust-region-scaled Newton step can be performed) and is greater than zero when the optimum of the quadratic function approximation is located at the boundary of the trust region (the scaled Newton step is too long to fit in the trust region and a quadratically constrained optimization is performed). Large values indicate optimization difficulties. As in Gay (1983), a negative λ value indicates the special case of an indefinite Hessian matrix (the smallest eigenvalue is negative in minimization).

- the value of the radius Δ of the trust region. Small trust-region radius values combined with large lambda values in subsequent iterations indicate optimization problems.

For the quasi-Newton (QUANEW) and conjugate gradient (CONGRA) techniques, the iteration history also includes the following information:

- the step size (alpha) computed with one of the line-search algorithms
- the descent of the search direction at the current parameter iterate. This value should be significantly smaller than 0. Otherwise, the line-search algorithm has difficulty reducing the function value sufficiently.

Frequent update restarts (rest) of a quasi-Newton algorithm often indicate numerical problems related to required properties of the approximate Hessian update, and they decrease the speed of convergence. This can happen particularly if the ABSGCONV= termination criterion is too small—that is, when the requested precision cannot be obtained by quasi-Newton optimization. Generally, the number of automatic restarts used by conjugate gradient methods are much higher.

For the nonlinearly constrained quasi-Newton technique, the iteration history also includes the following information:

- the maximum value of all constraint violations,

$$\text{conmax} = \max(|c_i(x)| : c_i(x) < 0)$$

- the value of the predicted function reduction used with the GCONV and FCONV2 termination criteria,

$$\text{pred} = |g(x^{(k)})_S(x^{(k)})| + \sum_{i=1}^m |\lambda_i c_i(x^{(k)})|$$

- the step size α of the quasi-Newton step. Note that this algorithm works with a special line-search algorithm.
- the maximum element of the gradient of the Lagrange function,

$$\begin{aligned} \text{lfgmax} &= \nabla_x L(x^{(k)}, \lambda^{(k)}) \\ &= \nabla_x f(x^{(k)}) - \sum_{i=1}^m \lambda_i^{(k)} \nabla_x c_i(x^{(k)}) \end{aligned}$$

For the double dogleg technique, the iteration history also includes the following information:

- the parameter λ of the double-dogleg step. A value $\lambda = 0$ corresponds to the full (quasi) Newton step.
- the slope of the search direction at the current parameter iterate. For minimization, this value should be significantly negative.

Line-Search Methods

In each iteration k , the (dual) quasi-Newton, hybrid quasi-Newton, conjugate gradient, and Newton-Raphson minimization techniques use iterative line-search algorithms that try to optimize a linear, quadratic, or cubic approximation of the nonlinear objective function f of n parameters x along a feasible descent search direction $s^{(k)}$ as follows:

$$f(x^{(k+1)}) = f(x^{(k)} + \alpha^{(k)}s^{(k)})$$

by computing an approximately optimal scalar $\alpha^{(k)} > 0$. Since the outside iteration process is based only on the approximation of the objective function, the inside iteration of the line-search algorithm does not have to be perfect. Usually, it is satisfactory that the choice of α significantly reduces (in a minimization) the objective function. Criteria often used for termination of line-search algorithms are the Goldstein conditions (Fletcher 1987).

Various line-search algorithms can be selected by using the **LIS= option** on page 1100. The line-search methods **LIS=1**, **LIS=2**, and **LIS=3** satisfy the left-hand-side and right-hand-side Goldstein conditions (Fletcher 1987).

The line-search method **LIS=2** seems to be superior when function evaluation consumes significantly less computation time than gradient evaluation. Therefore, **LIS=2** is the default value for Newton-Raphson, (dual) quasi-Newton, and conjugate gradient optimizations.

Restricting the Step Length

Almost all line-search algorithms use iterative extrapolation techniques that can easily lead to feasible points where the objective function f is no longer defined (resulting in indefinite matrices for ML estimation) or is difficult to compute (resulting in floating point overflows). Therefore, PROC CALIS provides options that restrict the step length or trust region radius, especially during the first main iterations.

The inner product $\mathbf{g}'\mathbf{s}$ of the gradient \mathbf{g} and the search direction \mathbf{s} is the slope of $f(\alpha) = f(\mathbf{x} + \alpha\mathbf{s})$ along the search direction \mathbf{s} with step length α . The default starting value $\alpha^{(0)} = \alpha^{(k,0)}$ in each line-search algorithm ($\min_{\alpha>0} f(\mathbf{x} + \alpha\mathbf{s})$) during the main iteration k is computed in three steps:

1. Use either the difference $df = |f^{(k)} - f^{(k-1)}|$ of the function values during the last two consecutive iterations or the final stepsize value α^- of the previous iteration $k - 1$ to compute a first value $\alpha_1^{(0)}$.

- Using the **DAMPSTEP<r>** option:

$$\alpha_1^{(0)} = \min(1, r\alpha^-)$$

The initial value for the new step length can be no greater than r times the final step length α^- of the previous iteration. The default is $r = 2$.

- Not using the **DAMPSTEP** option:

$$\alpha_1^{(0)} = \begin{cases} step & \text{if } 0.1 \leq step \leq 10 \\ 10 & \text{if } step > 10 \\ 0.1 & \text{if } step < 0.1 \end{cases}$$

with

$$step = \begin{cases} df/|\mathbf{g}'\mathbf{s}| & \text{if } |\mathbf{g}'\mathbf{s}| \geq \epsilon \max(100df, 1) \\ 1 & \text{otherwise} \end{cases}$$

This value of $\alpha_1^{(0)}$ can be too large and can lead to a difficult or impossible function evaluation, especially for highly nonlinear functions such as the EXP function.

2. During the first five iterations, the second step enables you to reduce $\alpha_1^{(0)}$ to a smaller starting value $\alpha_2^{(0)}$ using the `INSTEP=r` option:

$$\alpha_2^{(0)} = \min(\alpha_1^{(0)}, r)$$

After more than five iterations, $\alpha_2^{(0)}$ is set to $\alpha_1^{(0)}$.

3. The third step can further reduce the step length by

$$\alpha_3^{(0)} = \min(\alpha_2^{(0)}, \min(10, u))$$

where u is the maximum length of a step inside the feasible region.

The `INSTEP=r` option lets you specify a smaller or larger radius of the trust region used in the first iteration by the trust-region, double-dogleg, and Levenberg-Marquardt algorithms. The default initial trust region radius is the length of the scaled gradient (Moré 1978). This default length for the initial trust region radius corresponds to the default radius factor of $r = 1$. This choice is successful in most practical applications of the TRUREG, DBLDOG, and LEVMAR algorithms. However, for bad initial values used in the analysis of a covariance matrix with high variances or for highly nonlinear constraints (such as using the EXP function) in your SAS programming statements, the default start radius can result in arithmetic overflows. If this happens, you can try decreasing values of `INSTEP=r` ($0 < r < 1$), until the iteration starts successfully. A small factor r also affects the trust region radius of the next steps because the radius is changed in each iteration by a factor $0 < c \leq 4$ depending on the ρ ratio. Reducing the radius corresponds to increasing the ridge parameter λ that produces smaller steps directed closer toward the gradient direction.

Computational Problems

First Iteration Overflows

Analyzing a covariance matrix that includes high variances in the diagonal and using bad initial estimates for the parameters can easily lead to arithmetic overflows in the first iterations of the minimization algorithm. The line-search algorithms that work with cubic extrapolation are especially sensitive to arithmetic overflows. If this occurs with quasi-Newton or conjugate gradient minimization, you can specify the `INSTEP=` option to reduce the length of the first step. If an arithmetic overflow occurs in the first iteration of the Levenberg-Marquardt algorithm, you can specify the `INSTEP=` option to reduce the trust region radius of the first iteration. You also can change the minimization technique or the line-search method. If none of these help, you can consider doing the following:

- scaling the covariance matrix
- providing better initial values
- changing the model

No Convergence of Minimization Process

If convergence does not occur during the minimization process, perform the following tasks:

- If there are *negative variance estimates*, you can do either of the following:
 - Specify the **BOUNDS** statement to obtain nonnegative variance estimates.
 - Specify the **HEYWOOD** option, if the **FACTOR** statement is specified.
- Change the estimation method to obtain a better set of initial estimates. For example, if you use **METHOD=ML**, you can do either of the following:
 - Change to **METHOD=LSML**.
 - Run some iterations with **METHOD=DWLS** or **METHOD=GLS**, write the results in an **OUTMODEL=** data set, and use the results as initial values specified by an **INMODEL=** data set in a second run with **METHOD=ML**.
- Change the optimization technique. For example, if you use the default **OMETHOD=LEVMAR**, you can do either of the following:
 - Change to **OMETHOD=QUANEW** or to **OMETHOD=NEWRAP**.
 - Run some iterations with **OMETHOD=CONGRA**, write the results in an **OUTMODEL=** data set, and use the results as initial values specified by an **INMODEL=** data set in a second run with a different **OMETHOD=** technique.
- Change or modify the update technique or the line-search algorithm or both when using **OMETHOD=QUANEW** or **OMETHOD=CONGRA**. For example, if you use the default update formula and the default line-search algorithm, you can do any or all of the following:
 - Change the update formula with the **UPDATE=** option.
 - Change the line-search algorithm with the **LIS=** option.
 - Specify a more precise line search with the **LSPRECISION=** option, if you use **LIS=2** or **LIS=3**.
- Add more iterations and function calls by using the **MAXIT=** and **MAXFU=** options.
- Change the initial values. For many categories of model specifications, PROC CALIS computes an appropriate set of initial values automatically. However, for some of the model specifications (for example, structural equations with latent variables on the left-hand side and manifest variables on the right-hand side), PROC CALIS might generate very obscure initial values. In these cases, you have to set the initial values yourself.
 - Increase the initial values of the variance parameters by one of the following ways:
 - * Set the variance parameter values in the model specification manually.
 - * Use the **DEMPHAS=** option to increase all initial variance parameter values.
 - Use a slightly different, but more stable, model to obtain preliminary estimates.
 - Use additional information to specify initial values, for example, by using other SAS software like the **FACTOR**, **REG**, **SYSLIN**, and **MODEL (SYSNLIN)** procedures for the modified, unrestricted model case.

Unidentified Model

The parameter vector Θ in the structural model

$$\Sigma = \Sigma(\Theta)$$

is said to be identified in a parameter space G , if

$$\Sigma(\Theta) = \Sigma(\tilde{\Theta}), \quad \tilde{\Theta} \in G$$

implies $\Theta = \tilde{\Theta}$. The parameter estimates that result from an unidentified model can be very far from the parameter estimates of a very similar but identified model. They are usually machine dependent. Do not use parameter estimates of an unidentified model as initial values for another run of PROC CALIS.

Singular Predicted Covariance Model Matrix

Sometimes you might inadvertently specify models with singular predicted covariance model matrices (for example, by fixing diagonal elements to zero). In such cases, you cannot compute maximum likelihood estimates (the ML function value F is not defined). Since singular predicted covariance model matrices can also occur temporarily in the minimization process, PROC CALIS tries in such cases to change the parameter estimates so that the predicted covariance model matrix becomes positive definite. This process does not always work well, especially if there are fixed instead of free diagonal elements in the predicted covariance model matrices. A famous example where you cannot compute ML estimates is a component analysis with fewer components than given manifest variables. See the section “**FACTOR Statement**” on page 1138 for more details. If you continue to obtain a singular predicted covariance model matrix after changing initial values and optimization techniques, then your model might be specified so that ML estimates cannot be computed.

Saving Computing Time

For large models, the most computing time is needed to compute the modification indices. If you do not really need the Lagrange multipliers or multiple Wald test indices (the univariate Wald test indices are the same as the t values), using the **NOMOD** option can save a considerable amount of computing time.

Predicted Covariance Matrices with Negative Eigenvalues

A covariance matrix cannot have negative eigenvalues, since a negative eigenvalue means that some linear combination of the variables has negative variance. PROC CALIS displays a warning if the predicted covariance matrix has negative eigenvalues but does not actually compute the eigenvalues. Sometimes this warning can be triggered by 0 or very small positive eigenvalues that appear negative because of numerical error. If you want to be sure that the predicted covariance matrix you are fitting can be considered to be a variance-covariance matrix, you can use the SAS/IML command `VAL=EIGVAL(U)` to compute the vector `VAL` of eigenvalues of matrix `U`.

Negative R^2 Values

The estimated squared multiple correlations R^2 of the endogenous variables are computed using the estimated error variances:

$$R_i^2 = 1 - \frac{\widehat{var}(\xi_i)}{\widehat{var}(\eta_i)}$$

When $\widehat{var}(\zeta_i) > \widehat{var}(\eta_i)$, R_i^2 is negative. This might indicate poor model fit or R square is an inappropriate measure for the model. For the latter case, for example, negative R square might be due to cyclical (nonrecursive) paths in the model so that the R square interpretation is not appropriate.

Displayed Output

The output of PROC CALIS includes the following:

- a list of basic modeling information such as: the data set, the number of records read and used in the raw data set, the number of observations assumed by the statistical analysis, and the model type. When a multiple-group analysis is specified, the groups and their corresponding models are listed. This output assumes at least the **PSHORT** option.
- a list of all variables in the models. This output is displayed by default or by the **PINITIAL** option. It will not be displayed when you use the **PSHORT** or the **PSUMMARY** option.

Depending on the modeling language, the variable lists vary, as shown in the following:

- **FACTOR**: a list of the variables and the factors
- **LINEQS**, **PATH**, and **RAM**: a list of the endogenous and exogenous variables specified in the model
- **LISMOD**: a list of x -, y -, ξ -, and η - variables specified in the model
- **MSTRUCT**: a list of the manifest variables specified in the model
- initial model specification. This output is displayed by default or by the **PINITIAL** option. It will not be displayed when you use the **PSHORT** or the **PSUMMARY** option.

Depending on the modeling language, the sets of output vary, as shown in the following:

- **FACTOR**: factor loading matrix, factor covariance matrix, intercepts, factor means, and error variances as specified initially in the model. The initial values for free parameters, the fixed values, and the parameter names are also displayed.
- **LINEQS**: linear equations, variance and covariance parameters, and mean parameters as specified initially in the model. The initial values for free parameters, the fixed values, and the parameter names are also displayed.
- **LISMOD**: all model matrices as specified initially in the model. The initial values for free parameters, the fixed values, and the parameter names are also displayed.
- **MSTRUCT**: initial covariance matrix and mean vectors, with parameter names and initial values displayed.
- **PATH**: the path list, variance and covariance parameters, intercept and mean parameters as specified initially in the model. The initial values for free parameters, the fixed values, and the parameter names are also displayed.
- **RAM**: a list of parameters, their types, names, and initial values.

- mean and standard deviation of each manifest variable if you specify the **SIMPLE** option, as well as skewness and kurtosis if the **DATA=** data set is a raw data set and you specify the **KURTOSIS** option.
- various coefficients of multivariate kurtosis and the numbers of observations that contribute most to the normalized multivariate kurtosis if the **DATA=** data set is a raw data set and the **KURTOSIS** option is used or you specify at least the **PRINT** option. See the section “Measures of Multivariate Kurtosis” on page 1349 for more information.
- covariance coverage, variable coverage, average coverage of covariances and means, rank orders of the variable (mean) and covariance coverage, most frequent missing patterns in the input data set, and the means of the missing patterns when there are incomplete observations (with some missing values in the analysis variables) in the input raw data set and when you use **METHOD=FIML** or **METHOD=LSFIML** for estimation.
- covariance or correlation matrix to be analyzed and the value of its determinant if you specify the output option **PCORR** or **PALL**. A zero determinant indicates a singular data matrix. In this case, the generalized least squares estimates with default weight matrix **S** and maximum likelihood estimates cannot be computed.
- robust covariance matrix and its determinant and robust mean vector if you specify the output option **PCORR** or **PALL** for robust estimation with the **ROBUST** option. Raw data input is required.
- the weight matrix **W** or its inverse is displayed if GLS, WLS, or DWLS estimation is used and you specify the **PWEIGHT** or **PALL** option.
- initial estimation methods for generating initial estimates. This output is displayed by default. It will not be displayed when you use the **PSHORT** or the **PSUMMARY** option.
- vector of parameter names and initial values and gradients. This output is displayed by default, unless you specify the **PSUMMARY** or **NOPRINT** option.
- special features of the optimization technique chosen if you specify at least the **PSHORT** option.
- optimization history if at least the **PSHORT** option is specified. For more details, see the section “Use of Optimization Techniques” on page 1352.
- specific output requested by options in the **NLOPTIONS** statement; for example, parameter estimates, gradient, constraints, projected gradient, Hessian, projected Hessian, Jacobian of nonlinear constraints, estimated covariance matrix of parameter estimates, and information matrix. Note that the estimated covariance of parameter estimates and the information matrix are not printed for the ULS and DWLS estimation methods.
- fit summary table with various model fit test statistics or fit indices, and some basic modeling information. For the listing of fit indices and their definitions, see the section “Overall Model Fit Indices” on page 1329. Note that for ULS and DWLS estimation methods, many of those fit indices that are based on model fit χ^2 are not displayed. See the section “Overall Model Fit Indices” on page 1329 for details. This output can be suppressed by the **NOPRINT** option.
- fit comparison for multiple-group analysis. See the section “Individual Fit Indices for Multiple Groups” on page 1336 for the fit indices for group comparison. This output can be suppressed by the **NOPRINT** option.

- the predicted covariance matrix and its determinant and mean vector, if you specify the output option **PCORR** or **PALL**.
- outlier, leverage, and case-level residual analysis if you specify the **RESIDUAL** option (or at least the **PRINT** option) with raw data input.
- leverage and outlier plot, quantile and percentile plots of residual M-distances, distribution of residual M-distances, and residual on fit plots if you request ODS Graphics by using the relevant **PLOTS=** option.
- residual and normalized residual matrix if you specify the **RESIDUAL** option or at least the **PRINT** option. The variance standardized or asymptotically standardized residual matrix can be displayed also. The average residual and the average off-diagonal residual are also displayed. Note that normalized or asymptotically standardized residuals are not applicable for the ULS and DWLS estimation methods.

See the section “Residuals in the Moment Matrices” on page 1327 for more details.

- rank order of the largest normalized residuals if you specify the **RESIDUAL** option or at least the **PRINT** option.
- bar chart of the normalized residuals if you specify the **RESIDUAL** option or at least the **PRINT** option.
- plotting of smoothed density functions of residuals if you request ODS Graphics by the relevant **PLOTS=** option.
- equations of linear dependencies among the parameters used in the model specification if the information matrix is recognized as singular at the final solution.
- the estimation results and the standardized results. Except for ULS or DWLS estimates, the approximate standard errors and *t* values are also displayed. This output is displayed by default or if you specify the **PESTIM** option or at least the **PSHORT** option.

Depending on the modeling language, the sets of output vary, as shown in the following:

- **FACTOR**: factor loading matrix, rotation matrix, rotated factor loading matrix (if rotation requested), factor covariance matrix, intercepts, factor means, and error variances in the model. Factor rotation matrix is printed for the unstandardized solution.
 - **LINEQS**: linear equations, variance and covariance parameters, and mean parameters in the model.
 - **LISMOD**: all model matrices in the model.
 - **MSTRUCT**: covariance matrix and mean vectors.
 - **PATH**: the path list, variance and covariance parameters, intercept and mean parameters.
 - **RAM**: a list of parameters, their types, names, and initial values.
- squared multiple correlations table which displays the error variance, total variance, and the squared multiple correlation of each endogenous variable in the model. The total variances are the diagonal elements of the predicted covariance matrix. This output is displayed if you specify the **PESTIM** option or at least the **PSHORT** option.

- the total determination of all equations, the total determination of the latent equations, and the total determination of the manifest equations if you specify the **PDETERM** or the **PALL** option. See the section “Assessment of Fit” on page 1326 for more details. If you specify subsets of variables in the **DETERM** statements, the corresponding determination coefficients will also be shown. If one of the determinants in the formula for computing the determination coefficient is zero, the corresponding coefficient is displayed as the missing value ‘.’.
- the matrix of estimated covariances among the latent variables in the model if you specify the **PLATCOV** option or at least the **PRINT** option.
- the matrix of estimated covariances between latent and manifest variables in the model if you specify the **PLATCOV** option or at least the **PRINT** option.
- the vector of estimated means for the latent and manifest variables in the model if you specify the **PLATCOV** option or at least the **PRINT** option.
- the matrix **FSR** of latent variable scores regression coefficients if you specify the **PLATCOV** option or at least the **PRINT** option. The **FSR** matrix is a generalization of Lawley and Maxwell (1971, p. 109) factor scores regression matrix,

$$\mathbf{FSR} = \hat{\Sigma}_{yx} \hat{\Sigma}_{xx}^{-1}$$

where $\hat{\Sigma}_{xx}$ is the $p \times p$ predicted covariance matrix among manifest variables and $\hat{\Sigma}_{yx}$ is the $m \times p$ matrix of the predicted covariances between latent and manifest variables, with p being the number of manifest variables, and m being the number of latent variables. You can multiply the observed values by this matrix to estimate the scores of the latent variables used in your model.

- stability coefficient of reciprocal causation if you request the effect analysis by using the **EFFPART** or **TOTEFF** option, and you must not use the **NOPRINT** option.
- the matrices for the total, direct, and indirect effects if you specify the **EFFPART** or **TOTEFF** option or at least the **PRINT** option, and you must not use the **NOPRINT** option. Unstandardized and standardized effects are printed in separate tables. Standard errors for the all estimated effects are also included in the output. Additional tables for effects are available if you request specialized effect analysis in the **EFFPART** statements.
- the matrix of rotated factor loadings and the orthogonal transformation matrix if you specify the **ROTATE=** and **PESTIM** options or at least the **PSHORT** options. This output is available for the **FACTOR** models.

- factor scores regression matrix, if you specify the **PESTIM** option or at least the **PSHORT** option. The determination of manifest variables is displayed only if you specify the **PDETERM** option.
- univariate Lagrange multiplier indices if you specify the **MODIFICATION** (or **MOD**) or the **PALL** option. The value of a Lagrange multiplier (LM) index indicates the approximate drop in χ^2 when the corresponding fixed parameter in the original model is freely estimated. The corresponding probability (with $df = 1$) and the estimated change of the parameter value are printed. Ranking of the LM indices is automatically done for prescribed parameter subsets of the original model. The LM indices with greatest improvement of χ^2 model fit appear in the beginning of the ranking list. Note that LM indices are not applicable to the ULS and the DWLS estimation methods. See the section “**Modification Indices**” on page 1346 for more detail.
- matrices of univariate Lagrange multiplier (LM) indices if you specify the **MODIFICATION** (or **MOD**) or the **PALL** option, and the **LMMAT** option in the **LMTESTS** statement. These matrices are predefined in **PROC CALIS**, or you can specify them in the **LMTESTS** statements. If releasing a fixed parameter in the matrix would result in a singular information matrix, the string ‘Singular’ is displayed instead of the Lagrange multiplier index. If a fixed entry in the matrix is restricted by the model (for example, fixed ones for coefficients associated with error terms) or being excluded in the specified subsets in the **LMTESTS** statement, the string ‘Excluded’ is displayed. Note that matrices for LM indices are not printed for the ULS and the DWLS estimation methods. See the section “**Modification Indices**” on page 1346 for more detail.
- univariate Lagrange multiplier test indices for releasing equality constraints if you specify the **MODIFICATION** (or **MOD**) or the **PALL** option. Note that this output is not applicable to the ULS and the DWLS estimation methods. See the section “**Modification Indices**” on page 1346 for more detail.
- univariate Lagrange multiplier test indices for releasing active boundary constraints specified by the **BOUNDS** statement if you specify the **MODIFICATION** (or **MOD**) or the **PALL** option. Note that this output is not applicable to the ULS and the DWLS estimation methods. See the section “**Modification Indices**” on page 1346 for more detail.
- the stepwise multivariate Wald test for constraining estimated parameters to zero constants if the **MODIFICATION** (or **MOD**) or the **PALL** option is specified and the univariate probability is greater than the value specified in the **PMW=** option (default **PMW=0.05**). Note that this output is not applicable to the ULS and the DWLS estimation methods. See the section “**Modification Indices**” on page 1346 for more details.

ODS Table Names

PROC CALIS assigns a name to each table it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

There are numerous ODS tables in the CALIS procedure. The conditions for these ODS tables to display vary a lot. For convenience in presentation, the ODS tables for the PROC CALIS procedure are organized in the following categories:

- ODS tables for descriptive statistics, missing patterns, and residual analysis
- ODS tables for model specification and results
- ODS tables for supplementary model analysis
- ODS tables for modification indices
- ODS tables for optimization control and results

Many ODS tables are displayed when you set either a specialized option in a certain statement or a **global display option** in the PROC CALIS statement. Rather than requesting displays by setting specialized options separately, you can request a group of displays by using a global display option.

There are five global display levels, represented by five options: **PALL** (highest), **PRINT**, *default*, **PSHORT**, and **PSUMMARY**. The higher the level, the more output requested. The *default* printing level is in effect when you do not specify any other global printing options in the PROC CALIS statement. See the section “Global Display Options” on page 1085 for details.

In the following description of ODS tables whenever applicable, the lowest level of global printing options for an ODS table to print is listed. It is understood that global printing options at higher levels can also be used. For example, if **PSHORT** is the global display option to print an ODS table, you can also use **PALL**, **PRINT**, or *default*.

ODS Tables for Descriptive Statistics, Missing Patterns, and Residual Analysis

These ODS tables are group-oriented, meaning that each group has its own set of tables in the output. To display these tables in your output, you can set a specialized option in either the PROC CALIS or **GROUP** statement. If the specialized option is set in the PROC CALIS statement, it will apply to all groups. If the option is set in the **GROUP** statement, it will apply to the associated group only. Alternatively, you can set a global printing option in the PROC CALIS statement to print these tables. Either a specialized or a global printing option is sufficient to print the tables.

Table Names for Descriptive Statistics

ODS Table Name	Description	Specialized Option	Global Display Option
ContKurtosis	Contributions to kurtosis from observations	KURTOSIS	PRINT
CovRobust	Robust covariance matrix, with raw data input	PCORR ¹	PRINT
CovDetRobust	Determinant of the robust covariance matrix, with raw data input	PCORR ¹	PRINT
InCorr	Input correlation matrix	PCORR	PALL
InCorrDet	Determinant of the input correlation matrix	PCORR	PALL
InCov	Input covariance matrix	PCORR	PALL
InCovDet	Determinant of the input covariance matrix	PCORR	PALL
InMean	Input mean vector	PCORR	PALL
Kurtosis	Kurtosis, with raw data input	KURTOSIS	PRINT
MeanRobust	Robust mean vector, with raw data input	PCORR ¹	PRINT
PredCorr	Predicted correlation matrix	PCORR	PALL
PredCorrDet	Determinant of the predicted correlation matrix	PCORR	PALL
PredCov	Predicted covariance matrix	PCORR	PALL
PredCovDet	Determinant of the predicted covariance matrix	PCORR	PALL
PredMean	Predicted mean vector	PCORR	PALL
RidgedCovRobust	Ridged robust covariance matrix, with raw data input	PCORR ¹	PRINT
RidgedCovDetRobust	Determinant of the ridged robust covariance matrix, with raw data input	PCORR ¹	PRINT
RidgedInCorr	Ridged input correlation matrix	PCORR	PALL
RidgedInCorrDet	Determinant of the ridged input correlation matrix	PCORR	PALL
RidgedInCov	Ridged input covariance matrix	PCORR	PALL
RidgedInCovDet	Determinant of the ridged input covariance matrix	PCORR	PALL
SimpleStatistics	Simple statistics, with raw data input	SIMPLE	Default
Weights	Weight matrix	PWEIGHT	PALL
WeightsDet	Determinant of the weight matrix	PWEIGHT	PALL

1. Robust estimation with the **ROBUST** option is required.

Table Names for Missing Pattern Analysis

ODS Table Name	Description	Specialized Option	Global Display Option
AveCoverage	Average proportion coverages of means (variances) and covariances	SIMPLE or PCORR ¹	Default ²
MeanCovCoverage	Proportions of data present for means (variances) and covariances	SIMPLE or PCORR ¹	Default ²
MissPatternsMeans	Means of the nonmissing and the most frequent missing patterns	SIMPLE or PCORR ¹	Default ²
RankCovCoverage	Rank order of the covariance coverages	SIMPLE or PCORR ¹	Default ²
RankMissPatterns	Rank order of the most frequent missing patterns	SIMPLE or PCORR ¹	Default ²
RankVariableCoverage	Rank order of the proportion coverages of the variables	SIMPLE or PCORR ¹	Default ²

1. You can use the **NOMISSPAT** option in the **PROC CALIS** statement to suppress the analytic output of the missing patterns. If you use the **NOMISSPAT** option in the **GROUP** statements, only the output of the missing pattern analysis for the corresponding groups are suppressed.

2. **PROC CALIS** outputs these tables by default only when there are incomplete observations in the data sets and you use **METHOD=FIML** or **METHOD=LSFIML** for estimation.

Table Names for Residual Displays

ODS Table Name	Description	Specialized Option	Global Display Option
Residuals in the Moment Matrices			
AsymStdRes	Asymptotically standardized residual matrix	RESIDUAL=ASYSTAND ¹	PALL
AveAsymStdRes	Average of absolute asymptotically standardized residual values	RESIDUAL=ASYSTAND ¹	PALL
AveNormRes	Average of absolute normalized residual values	RESIDUAL=NORM ¹	PALL
AveRawRes	Average of absolute raw residual values	RESIDUAL	PALL
AveVarStdRes	Average of absolute variance standardized residual values	RESIDUAL=VARSTAND ¹	PALL
DistAsymStdRes	Distribution of asymptotically standardized residuals	RESIDUAL=ASYSTAND ¹	PALL
DistNormRes	Distribution of normalized residuals	RESIDUAL=NORM ¹	PALL
DistRawRes	Distribution of raw residuals	RESIDUAL	PALL
DistVarStdRes	Distribution of variance standardized residuals	RESIDUAL=VARSTAND ¹	PALL
NormRes	Normalized residual matrix	RESIDUAL=NORM ¹	PALL
RawRes	Raw residual matrix	RESIDUAL ²	PALL
RankAsymStdRes	Rank order of asymptotically standardized residuals	RESIDUAL=ASYSTAND ¹	PALL
RankNormRes	Rank order of normalized residuals	RESIDUAL=NORM ¹	PALL
RankRawRes	Rank order of raw residuals	RESIDUAL	PALL
RankVarStdRes	Rank order of variance standardized residuals	RESIDUAL=VARSTAND ¹	PALL
VarStdRes	Variance standardized residual matrix	RESIDUAL=VARSTAND ¹	PALL
Case-Level Residuals³			
DepartResidualDist	Departures from the theoretical distribution for the residual M-distances	RESIDUAL	PALL
Leverage	Observations with largest leverage M-distances	RESIDUAL	PALL
Outlier	Observations with largest residual M-distances	RESIDUAL	PALL

1. The **RESIDUAL=** option specifies the **RESIDUAL** option and the type of residuals. For example, RESIDUAL=ASYSTAND requests asymptotically standardized residuals, in addition to the tables enabled by the **RESIDUAL** option. In some cases, the requested types of residuals are not available due to the specific estimation method or the data type used. When this occurs, PROC

CALIS will determine the appropriate types of normalized or standardized residuals to display.

2. Raw residuals are also printed for correlation analysis even if `RESIDUAL` or `PALL` is not specified.
3. Raw data input is required.

ODS Tables for Model Specification and Results

Some ODS tables of this group are model-oriented. Others are not. Model-oriented ODS tables are printed for each model, while others are printed no more than once no matter how many models you have.

Non-Model-Oriented ODS Tables

The ODS tables that are not model-oriented are listed in the following table:

ODS Table Name	Description	Global Display Option	Additional Specification Required
AddParms	Estimates for additional parameters	PSHORT	PARAMETERS statement
AddParmsInit	Initial values for additional parameters	PSHORT	PARAMETERS statement
Fit	Fit summary	PSUMMARY	
GroupFit	Fit comparison among groups	PSUMMARY	Multiple groups
ModelingInfo	General modeling information	PSHORT	
ModelSummary	Summary of models and their labels and types	PSHORT	Multiple models ¹
ParmFunc	Parametric function testing	PSHORT	TESTFUNC statement
Simtests	Simultaneous tests of parametric functions	PSHORT	SIMTESTS statement

1. This table is displayed when you have multiple models that have labels specified by the `LABEL=` option, or when you define a model with more than a single level of reference by using the `REFMODEL` option. Otherwise, the `ModelingInfo` table contains all pertinent information regarding the models in the analysis.

Model-Oriented ODS Tables

These ODS tables are model-oriented, meaning that each model has its own set of ODS tables in the output. There are three types of model specification and results printing in PROC CALIS: initial specification, (unstandardized) estimated model results, and standardized model results. To distinguish these three types of ODS tables, different suffixes for the ODS table names are used. An “Init” suffix indicates initial specification, while a “Std” suffix indicates standardized solutions. All other tables are for unstandardized solutions.

These ODS tables require some specialized options to print. If you set the specialized option in the PROC CALIS statement, it applies to all models. If you set the specialized option in the `MODEL` statement, it applies to the associated model only. Alternatively, to print *all* these ODS tables, you can use the `PSHORT` or any higher level `global printing` option in the PROC CALIS statement. Either a specialized or a global printing option is sufficient to print these ODS tables. The following is a summary of the specialized and global printing options for these three types of ODS tables:

Type of ODS Tables	Table Name Suffix	Specialized Option	Global Display Option
Initial specification	Init	PINITIAL	PSHORT
Unstandardized solutions	(none)	PESTIM	PSHORT
Standardized solutions	Std	PESTIM, and NOSTAND not used	PSHORT

In the following list of ODS tables, the prefixes of the ODS table names indicate the modeling language required for the ODS tables to print. The last column of the list indicates whether the **PRIMAT** option is needed to print the corresponding ODS tables in matrix formats. You can use the **PRIMAT** option either in the PROC CALIS or **MODEL** statement. If you want matrix output for all models, set this option in the PROC CALIS statement. If you want matrix output for a specific model, set this option in the associated **MODEL** statement only.

ODS Table Name	Description	Additional Option
COSANVariables	Variables in the COSAN model	
COSANModel	Mean and covariance structure formulas	
COSANMatrixSummary	Summary of COSAN model matrices	
COSANMatrix	Estimated model matrix	
COSANMatrixInit	Initial model matrix	
FACTORCov	Estimated factor covariances	
FACTORCovInit	Initial factor covariances	
FACTORCovStd	Factor correlations	
FACTORErrVar	Estimated error variances	
FACTORErrVarInit	Initial error variances	
FACTORErrVarStd	Standardized results for error variances	
FACTORIntercepts	Estimated intercepts	
FACTORInterceptsInit	Initial intercepts	
FACTORLoadings	Estimated factor loadings	
FACTORLoadingsInit	Initial factor loadings	
FACTORLoadingsStd	Standardized factor loadings	
FACTORMeans	Estimated factor means	
FACTORMeansInit	Initial factor means	
FACTORRotCov	Estimated rotated factor covariances	
FACTORRotCovStd	Rotated factor correlations	
FACTORRotErrVar	Error variances in rotated solution	
FACTORRotErrVarStd	Standardized results for error variances in rotated solution	
FACTORRotLoadings	Rotated factor loadings	
FACTORRotLoadingsStd	Standardized rotated factor loadings	
FACTORRotMat	Rotation matrix	
FACTORScoresRegCoef	Factor scores regression coefficients	
FACTORVariables	Variables in the analysis	
LINEQSAalpha	Estimated intercept vector	PRIMAT
LINEQSAalphaInit	Initial intercept vector	PRIMAT

ODS Table Name	Description	Additional Option
LINEQSBeta	Estimated _EQSBETA_ matrix	PRIMAT
LINEQSBetaInit	Initial _EQSBETA_ matrix	PRIMAT
LINEQSBetaStd	Standardized results for _EQSBETA_ matrix	PRIMAT
LINEQSCovExog	Estimated covariances among exogenous variables	
LINEQSCovExogInit	Initial covariances among exogenous variables	
LINEQSCovExogStd	Standardized results for covariances among exogenous variables	
LINEQSEq	Estimated equations	
LINEQSEqInit	Initial equations	
LINEQSEqStd	Standardized equations	
LINEQSGamma	Estimated _EQSGAMMA_ matrix	PRIMAT
LINEQSGammaInit	Initial _EQSGAMMA_ matrix	PRIMAT
LINEQSGammaStd	Standardized results for _EQSGAMMA_ matrix	PRIMAT
LINEQSMean	Estimated means for exogenous variables	
LINEQSMeanInit	Initial means for exogenous variables	
LINEQSNu	Estimated mean vector	PRIMAT
LINEQSNuInit	Initial mean vector	PRIMAT
LINEQSPhi	Estimated _EQSPHI_ matrix	PRIMAT
LINEQSPhiInit	Initial _EQSPHI_ matrix	PRIMAT
LINEQSPhiStd	Standardized results for _EQSPHI_ matrix	PRIMAT
LINEQSVarExog	Estimated variances of exogenous variables	
LINEQSVarExogInit	Initial variances of exogenous variables	
LINEQSVarExogStd	Standardized results for variances of exogenous variables	
LINEQSVariables	Exogenous and endogenous variables	
LISMODAlpha	Estimated _ALPHA_ vector	
LISMODAlphaInit	Initial _ALPHA_ vector	
LISMODBeta	Estimated _BETA_ matrix	
LISMODBetaInit	Initial _BETA_ matrix	
LISMODBetaStd	Standardized _BETA_ matrix	
LISMODGamma	Estimated _GAMMA_ matrix	
LISMODGammaInit	Initial _GAMMA_ matrix	
LISMODGammaStd	Standardized _GAMMA_ matrix	
LISMODKappa	Estimated _KAPPA_ vector	
LISMODKappaInit	Initial _KAPPA_ vector	
LISMODLambdaX	Estimated _LAMBDA_X_ matrix	
LISMODLambdaXInit	Initial _LAMBDA_X_ matrix	
LISMODLambdaXStd	Standardized _LAMBDA_X_ matrix	
LISMODLambdaY	Estimated _LAMBDA_Y_ matrix	
LISMODLambdaYInit	Initial _LAMBDA_Y_ matrix	
LISMODLambdaYStd	Standardized _LAMBDA_Y_ matrix	
LISMODNuX	Estimated _NUX_ vector	
LISMODNuXInit	Initial _NUX_ vector	
LISMODNuY	Estimated _NUY_ vector	

ODS Table Name	Description	Additional Option
LISMODNuYInit	Initial _NUY_ vector	
LISMODPhi	Estimated _PHI_ matrix	
LISMODPhiInit	Initial _PHI_ matrix	
LISMODPhiStd	Standardized _PHI_ matrix	
LISMODPsi	Estimated _PSI_ matrix	
LISMODPsiInit	Initial _PSI_ matrix	
LISMODPsiStd	Standardized _PSI_ matrix	
LISMODThetaX	Estimated _THETAX_ matrix	
LISMODThetaXInit	Initial _THETAX_ matrix	
LISMODThetaXStd	Standardized _THETAX_ matrix	
LISMODThetaY	Estimated _THETAY_ matrix	
LISMODThetaYInit	Initial _THETAY_ matrix	
LISMODThetaYStd	Standardized _THETAY_ matrix	
LISMODVariables	Variables in the model	
MSTRUCTCov	Estimated _COV_ matrix	
MSTRUCTCovInit	Initial _COV_ matrix	
MSTRUCTCovStd	Standardized _COV_ matrix	
MSTRUCTMean	Estimated _MEAN_ vector	
MSTRUCTMeanInit	Initial _MEAN_ vector	
MSTRUCTVariables	Variables in the model	
PATHCovErrors	Estimated error covariances	
PATHCovErrorsInit	Initial error covariances	
PATHCovErrorsStd	Standardized error covariances	
PATHCovVarErr	Estimated covariances between exogenous variables and errors	
PATHCovVarErrInit	Initial covariances between exogenous variables and errors	
PATHCovVarErrStd	Standardized results for covariances between exogenous variables and errors	
PATHCovVars	Estimated covariances among exogenous variables	
PATHCovVarsInit	Initial covariances among exogenous variables	
PATHCovVarsStd	Standardized results for covariances among exogenous variables	
PATHList	Estimated path list	
PATHListInit	Initial path list	
PATHListStd	Standardized path list	
PATHMeansIntercepts	Estimated intercepts	
PATHMeansInterceptsInit	Initial intercepts	
PATHVariables	Exogenous and endogenous variables	
PATHVarParms	Estimated variances or error variances	
PATHVarParmsInit	Initial variances or error variances	
PATHVarParmsStd	Standardized results for variances or error variances	
RAMAMat	Estimated _A_ matrix	PRIMAT

ODS Table Name	Description	Additional Option
RAMAMatInit	Initial <i>_A_</i> matrix	PRIMAT
RAMAMatStd	Standardized results of <i>_A_</i> matrix	PRIMAT
RAMList	List of RAM estimates	
RAMListInit	List of initial RAM estimates	
RAMListStd	Standardized results for RAM estimates	
RAMPMat	Estimated <i>_P_</i> matrix	PRIMAT
RAMPMatInit	Initial <i>_P_</i> matrix	PRIMAT
RAMPMatStd	Standardized results of <i>_P_</i> matrix	PRIMAT
RAMVariables	Exogenous and endogenous variables	
RAMWVec	Estimated mean and intercept vector	PRIMAT
RAMWVecInit	Initial mean and intercept vector	PRIMAT

ODS Tables for Supplementary Model Analysis

These ODS tables are model-oriented. They are printed for each model in your analysis. To display these ODS tables, you can set some specialized *options* in either the PROC CALIS or MODEL statement. If the specialized options are used in the PROC CALIS statement, they apply to all models. If the specialized options are used in the MODEL statement, they apply to the associated model only. For some of these ODS tables, certain specialized *statements* for the model might also enable the printing. Alternatively, you can use the global printing options in the PROC CALIS statement to print these ODS tables. Either a specialized option (or statement) or a global printing option is sufficient to print a particular ODS table.

ODS Table Name	Description	Specialized Option or Statement	Global Display Option
Determination	Coefficients of determination	PDETERM DETERM ⁴	Default
DirectEffects	Direct effects	TOTEFF ¹	PRINT
DirectEffectsStd	Standardized direct effects	TOTEFF ^{1,3}	PRINT
EffectsOf	Effects of the listed variables	EFFPART ²	PRINT
EffectsOn	Effects on the listed variables	EFFPART ²	PRINT
IndirectEffects	Indirect effects	TOTEFF ¹	PRINT
IndirectEffectsStd	Standardized indirect effects	TOTEFF ^{1,3}	PRINT
LatentScoresRegCoef	Latent variable scores regression coefficients	PLATCOV	PRINT
PredCovLatent	Predicted covariances among latent variables	PLATCOV	PRINT
PredCovLatMan	Predicted covariances between latent and manifest variables	PLATCOV	PRINT
PredMeanLatent	Predicted means of latent variables	PLATCOV	PRINT
SqMultCorr	Squared multiple correlations	PESTIM	PSHORT
Stability	Stability coefficient of reciprocal causation	PDETERM, DETERM ⁴	Default
StdEffectsOf	Standardized effects of the listed variables	EFFPART ^{2,3}	PSHORT
StdEffectsOn	Standardized effects on the listed variables	EFFPART ^{2,3}	PSHORT
TotalEffects	Total effects	TOTEFF ¹	PRINT
TotalEffectsStd	Standardized total effects	TOTEFF ^{1,3}	PRINT

1. This refers to the **TOTEFF** or **EFFPART** option in the PROC CALIS or **MODEL** statement.

2. This refers to the **EFFPART** statement specifications.

3. **NOSTAND** option must not be specified in the **MODEL** or PROC CALIS statement.

4. **PDETERM** is an option specified in the PROC CALIS or **MODEL** statement, while **DETERM** is a statement name.

ODS Tables for Model Modification Indices

To print the ODS tables for model modification indices, you can use the **MODIFICATION** option in either the PROC CALIS or **MODEL** statement. When this option is set in the PROC CALIS statement, it applies to all models. When this option is set in the **MODEL** statement, it applies to the associated model only. Alternatively, you can also use the **PALL** option in the PROC CALIS statement to print these ODS tables.

If the **NOMOD** option is set in the PROC CALIS statement, these ODS tables are not printed for all models, unless the **MODIFICATION** is respecified in the individual **MODEL** statements. If the **NOMOD** option is set in the **MODEL** statement, then the ODS tables for modification do not print for the associated model.

For convenience in presentation, three different classes of ODS tables for model modifications are described in the following. First, ODS tables for ranking of LM indices are the default printing when the **MODIFICATION** option is specified. Second, ODS tables for LM indices in matrix forms require an additional option to print. Last, ODS tables for other modification indices, including the Wald test indices, require specific

data-analytic conditions to print. While the first two classes of ODS tables are model-oriented (that is, each model has its own sets of output), the third one is not.

ODS Table Names for Ranking of LM indices

Rankings of the LM statistics in different regions of parameter space are the default printing format when you specify the **MODIFICATION** option in the PROC CALIS or MODEL statement. You can also turn off these default printing by the **NODEFAULT** option in the LMTESTS statement for models. If you want to print matrices of LM test statistics rather than the rankings of LM test statistics, you can use the **NORANK** or **MAXRANK=0** option in the **LMTESTS** statement.

These ODS tables for ranking LM statistics are specific to the types of modeling languages used. This is noted in the last column of the following table.

ODS Table Name	Description	Model
LMRankCosanMatrix	Any COSAN model matrix	COSAN
LMRankCov	Covariances among variables	MSTRUCT
LMRankCovErr	Covariances among errors	LINEQS
LMRankCovErrorfVar	Covariances among errors of variables	PATH
LMRankCovExog	Covariances among existing exogenous variables	LINEQS or PATH
LMRankCovFactors	Covariance among factors	FACTOR
LMRankCustomSet	Customized sets of parameters defined in LMTESTS statements	any model
LMRankErrorVar	Error variances	FACTOR
LMRankFactMeans	Factor means	FACTOR
LMRankIntercepts	Intercepts	FACTOR, LINEQS, or PATH
LMRankLisAlpha	LISMOD _ALPHA_	LISMOD
LMRankLisBeta	LISMOD _BETA_	LISMOD
LMRankLisGamma	LISMOD _GAMMA_	LISMOD
LMRankLisKappa	LISMOD _KAPPA_	LISMOD
LMRankLisLambdaX	LISMOD _LAMBDA_X_	LISMOD
LMRankLisLambdaY	LISMOD _LAMBDA_Y_	LISMOD
LMRankLisNuX	LISMOD _NUX_	LISMOD
LMRankLisNuY	LISMOD _NUY_	LISMOD
LMRankLisPhi	LISMOD _PHI_	LISMOD
LMRankLisPsi	LISMOD _PSI_	LISMOD
LMRankLisThetaX	LISMOD _THETA_X_	LISMOD
LMRankLisThetaY	LISMOD _THETA_Y_	LISMOD
LMRankLoadings	Factor loadings	FACTOR
LMRankMeans	Means of existing variables	LINEQS, MSTRUCT, or PATH
LMRankPaths	All possible paths in the model	PATH
LMRankPathsFromEndo	Paths from existing endogenous variables	LINEQS
LMRankPathsFromExog	Paths from existing exogenous variables	LINEQS
LMRankPathsNewEndo	Paths to existing exogenous variables	LINEQS

ODS Table Name	Description	Model
LMRankRamA	_RAMA_ matrix	RAM
LMRankRamAlpha	_RAMALPHA_ matrix	RAM
LMRankRamNu	_RAMNU_ matrix	RAM
LMRankRamP11	_RAMP11_ matrix	RAM
LMRankRamP22	_RAMP22_ matrix	RAM

ODS Table Names for Lagrange Multiplier Tests in Matrix Form

To print matrices of LM test indices for a model, you must also use the LMMAT option in the LMTESTS statement for the model. Some of these matrices are printed by default, while others are printed only when certain regions of parameter are specified in the LM test sets. In the following tables, the ODS table names for LM test statistics in matrix form are listed for each model type.

The COSAN Model

ODS Table Name	Description	Selected Region in Test Sets
LMCosanMatrix	Any COSAN model matrix	(default)

The FACTOR Model

ODS Table Name	Description	Selected Region in Test Sets
LMFactErrv	Vector of error variances	FACTERRV (default)
LMFactFcov	Factor covariance matrix	FACTFCOV (default)
LMFactInte	Intercept vector	FACTINTE (default)
LMFactLoad	Factor loading matrix	FACTLOAD (default)
LMFactMean	Factor mean vector	FACTMEAN (default)

The LINEQS Model

ODS Table Name	Description	Selected Regions in Test Sets
LMEqsAlpha	_EQSALPHA_ vector	_EQSALPHA_ (default)
LMEqsBeta	_EQSBETA_ matrix	_EQSBETA_ (default)
LMEqsGammaSub	_EQSGAMMA_ matrix, excluding entries with error variables in columns	_EQSGAMMA_ (default)
LMEqsNewDep	New rows for expanding _EQSBETA_ and _EQSGAMMA_ matrices	NEWDEP
LMEqsNuSub	_EQSNU_ vector, excluding fixed zero means for error variables	_EQSNU_ (default)
LMEqsPhi	_EQSPHI_ matrix	_EQSPHI_ alone or _EQSPHI11_, _EQSPHI21_ and _EQSPHI22_ together
LMEqsPhi11	Upper left portion (exogenous variances and covariances) of the _EQSPHI_ matrix	_EQSPHI11_ (default)

ODS Table Name	Description	Selected Regions in Test Sets
LMEqsPhi21	Lower left portion (error variances and covariances) of the <code>_EQSPHI_</code> matrix	<code>_EQSPHI21_</code>
LMEqsPhi22	Lower right portion (error variances and covariances) of the <code>_EQSPHI_</code> matrix	<code>_EQSPHI22_</code> (default)

The LISMOD Model

ODS Table Name	Description	Selected Regions in Test Sets
LMLisAlpha	LISMOD <code>_ALPHA_</code> vector	<code>_ALPHA_</code> (default)
LMLisBeta	LISMOD <code>_BETA_</code> matrix	<code>_BETA_</code> (default)
LMLisGamma	LISMOD <code>_GAMMA_</code> matrix	<code>_GAMMA_</code> (default)
LMLisKappa	LISMOD <code>_KAPPA_</code> vector	<code>_KAPPA_</code> (default)
LMLisLambdaX	LISMOD <code>_LAMBDA_X_</code> matrix	<code>_LAMBDA_X_</code> (default) or <code>_LAMBDA_</code>
LMLisLambdaY	LISMOD <code>_LAMBDA_Y_</code> matrix	<code>_LAMBDA_Y_</code> (default) or <code>_LAMBDA_</code>
LMLisNuX	LISMOD <code>_NUX_</code> vector	<code>_NUX_</code> (default) or <code>_NU_</code>
LMLisNuY	LISMOD <code>_NUY_</code> vector	<code>_NUY_</code> (default) or <code>_NU_</code>
LMLisPhi	LISMOD <code>_PHI_</code> matrix	<code>_PHI_</code> (default)
LMLisPsi	LISMOD <code>_PSI_</code> matrix	<code>_PSI_</code> (default)
LMLisThetaX	LISMOD <code>_THETA_X_</code> matrix	<code>_THETA_X_</code> (default) or <code>_THETA_</code>
LMLisThetaY	LISMOD <code>_THETA_Y_</code> matrix	<code>_THETA_Y_</code> (default) or <code>_THETA_</code>

The MSTRUCT Model

ODS Table Name	Description	Selected Regions in Test Sets
LMMstructCov	Covariance matrix	<code>MSTRUCTCOV</code> (default) or <code>_COV_</code>
LMMstructMean	Mean vector	<code>MSTRUCTMEAN</code> (default) or <code>_MEAN_</code>

The PATH Model

ODS Table Name	Description	Selected Regions in Test Sets
LMRamA	<code>_RAMA_</code> matrix	<code>ARROWS</code> or <code>_RAMA_</code> (default)
LMRamALeft	Left portion of the <code>_RAMA_</code> matrix	<code>_RAMA_LEFT_</code> alone or <code>_RAMBETA_</code> and <code>_RAMA_LL_</code> together
LMRamALL	Lower left portion of the <code>_RAMA_</code> matrix	<code>_RAMA_LL_</code>

ODS Table Name	Description	Selected Regions in Test Sets
LMRamALower	Lower portion of the <code>_RAMA_</code> matrix	NEWENDO or <code>_RAMA_LOWER_</code> or <code>_RAMA_LL_</code> and <code>_RAMA_LR_</code> together
LMRamALR	Lower right portion of the <code>_RAMA_</code> matrix	<code>_RAMA_LR_</code>
LMRamARight	Right portion of the <code>_RAMA_</code> matrix	<code>_RAMA_RIGHT_</code>
LMRamAUpper	Upper portion of the <code>_RAMA_</code> matrix	<code>_RAMA_UPPER_</code> alone or <code>_RAMBETA_</code> and <code>_RAMGAMMA_</code> together
LMRamAlpha	<code>_RAMALPHA_</code> matrix	INTERCEPTS (default)
LMRamBeta	Upper left portion of the <code>_RAMA_</code> matrix	<code>_RAMBETA_</code>
LMRamGamma	Upper right portion of the <code>_RAMA_</code> matrix	<code>_RAMGAMMA_</code>
LMRamNu	<code>_RAMNU_</code> matrix	MEANS (default)
LMRamP	<code>_RAMP_</code> matrix	<code>_RAMP_</code> alone or <code>_RAMP11_</code> , <code>_RAMP21_</code> , and <code>_RAMP22_</code> together
LMRamP11	Upper left portion of the <code>_RAMP_</code> matrix	COVERR (default)
LMRamP21	Lower left portion of the <code>_RAMP_</code> matrix	COVEXOGERR
LMRamP22	Lower right portion of the <code>_RAMP_</code> matrix	COVEXOG (default)
LMRamW	<code>_RAMW_</code> matrix	FIRSTMOMENTS alone or MEANS and INTERCEPTS together

The RAM Model

ODS Table Name	Description	Selected Regions in Test Sets
LMRamA	<code>_RAMA_</code> matrix	<code>_RAMA_</code> (default)
LMRamALeft	Left portion of the <code>_RAMA_</code> matrix	<code>_RAMA_LEFT_</code> alone or <code>_RAMBETA_</code> and <code>_RAMA_LL_</code> together
LMRamALL	Lower left portion of the <code>_RAMA_</code> matrix	<code>_RAMA_LL_</code>
LMRamALower	Lower portion of the <code>_RAMA_</code> matrix	NEWENDO or <code>_RAMA_LOWER_</code> or <code>_RAMA_LL_</code> and <code>_RAMA_LR_</code> together
LMRamALR	Lower right portion of the <code>_RAMA_</code> matrix	<code>_RAMA_LR_</code>
LMRamARight	Right portion of the <code>_RAMA_</code> matrix	<code>_RAMA_RIGHT_</code>
LMRamAUpper	Upper portion of the <code>_RAMA_</code> matrix	<code>_RAMBETA_</code> and <code>_RAMGAMMA_</code>
LMRamAlpha	<code>_RAMALPHA_</code> matrix	<code>_RAMALPHA_</code> (default)
LMRamBeta	Upper left portion of the <code>_RAMA_</code> matrix	<code>_RAMBETA_</code>
LMRamGamma	Upper right portion of the <code>_RAMA_</code> matrix	<code>_RAMGAMMA_</code>
LMRamNu	<code>_RAMNU_</code> matrix	<code>_RAMNU_</code> (default)
LMRamP	<code>_RAMP_</code> matrix	<code>_RAMP_</code> alone or <code>_RAMP11_</code> , <code>_RAMP21_</code> , and <code>_RAMP22_</code> together

ODS Table Name	Description	Selected Regions in Test Sets
LMRamP11	Upper left portion of the <code>_RAMP_</code> matrix	<code>_RAMP11_</code> (default)
LMRamP21	Lower left portion of the <code>_RAMP_</code> matrix	<code>_RAMP21_</code>
LMRamP22	Lower right portion of the <code>_RAMP_</code> matrix	<code>_RAMP22_</code> (default)
LMRamW	<code>_RAMW_</code> matrix	<code>_RAMW_</code>

ODS Table Names for Other Modification Indices

The following table shows the ODS tables for the remaining modification indices.

ODS Table Name	Description	Additional Requirement
LagrangeBoundary	LM tests for active boundary constraints	Presence of active boundary constraints
LagrangeDepParmEquality	LM tests for equality constraints in dependent parameters	Presence of equality constraints in dependent parameters
LagrangeEquality	LM tests for equality constraints	Presence of equality constraints in independent parameters
WaldTest	Wald tests for testing existing parameters equaling zeros	At least one insignificant parameter value

ODS Table for Optimization Control and Results

To display the ODS tables for optimization control and results, you must specify any of the following global display options in the PROC CALIS statement: `PRINT`, `PALL`, or default (that is, `NOPRINT` is not specified). Also, you must not use the `NOPRINT` option in the `NLOPTIONS` statement. For some of these tables, you must also specify additional options, either in the PROC CALIS or the `NLOPTIONS` statement. Some restrictions might apply. Additional options and restrictions are noted in the last column.

ODS Table Name	Description	Additional Option Required or Restriction
CovParm	Covariances of parameters	PCOVES ¹ or PALL ² , restriction ³
ConvergenceStatus	Convergence status	
DependParmsResults	Final dependent parameter estimates	Restriction ⁴
DependParmsStart	Initial dependent parameter estimates	Restriction ⁴
Information	Information matrix	PCOVES ¹ or PALL ² , restriction ³
InitEstMethods	Initial estimation methods	
InputOptions	Optimization options	PALL ²
IterHist	Iteration history	
IterStart	Iteration start	
IterStop	Iteration stop	
Lagrange	First and second order Lagrange multipliers	PALL ²
LinCon	Linear constraints	PALL ² , restriction ⁵
LinConDel	Deleted constraints	PALL ² , restriction ⁵
LinConSol	Linear constraints evaluated at solution	PALL ² , restriction ⁵
LinDep	Linear dependencies of parameter estimates	Restriction ⁶
ParameterEstimatesResults	Final estimates	
ParameterEstimatesStart	Initial estimates	
ProblemDescription	Problem description	
ProjGrad	Projected gradient	PALL ²

1. PCOVES option is specified in the PROC CALIS statement.

2. PALL option is specified in the NLOPTIONS statement.

3. Estimation method must not be ULS or DWLS.

4. Existence of dependent parameters.

5. Linear equality or boundary constraints are imposed.

6. Existence of parameter dependencies during optimization, but not due to model specification.

ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “Statistical Graphics Using ODS.”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “A Primer on ODS Statistical Graphics” on page 599 in Chapter 21, “Statistical Graphics Using ODS.”

In the following table, ODS graph names and the options to display the graphs are listed.

Table 27.17 Graphs Produced by PROC CALIS

ODS Graph Name	Plot Description	Option
Distribution of Residuals in the Moment Matrices		
AsymStdResidualHistogram	Asymptotically standardized residuals	PLOTS=RESIDUALS and RESIDUAL=ASYMSTD, METHOD= is not ULS or DWLS
NormResidualHistogram	Normalized residuals	PLOTS=RESIDUALS and RESIDUAL=NORM
RawResidualHistogram	Raw residuals	PLOTS=RESIDUALS
VarStdResidualHistogram	Variance standardized residuals	PLOTS=RESIDUALS and RESIDUAL=VARSTD
Case-Level Residual Diagnostics		
CaseResidualHistogram	Distribution of the residual M-distances	PLOTS=CRESHIST or CASERESIDUAL
ResidualByLeverage	Residual M-distances against the leverage M-distances	PLOTS=RESBYLEV or CASERESIDUAL
ResidualByPredicted	Residuals against the predicted values of dependent variables	PLOTS=RESBYPRED or CASERESIDUAL
ResidualByQuantile	Residual M-distances against the theoretical quantiles	PLOTS=QQ or CASERESIDUAL
ResPercentileByExpPercentile	Percentiles of residual M-distances against the theoretical percentiles	PLOTS=PP or CASERESIDUAL

Examples: CALIS Procedure

Example 27.1: Estimating Covariances and Correlations

This example shows how you can use PROC CALIS to estimate the covariances and correlations of the variables in your data set. Estimating the covariances introduces you to the most basic form of covariance structures—a saturated model with all variances and covariances as parameters in the model. To fit such a saturated model when there is no need to specify the functional relationships among the variables, you can use the **MSTRUCT** modeling language of PROC CALIS.

The following data set contains four variables **q1–q4** for the quarterly sales (in millions) of a company. The 14 observations represent 14 retail locations in the country. The input data set is shown in the following DATA step:

```
data sales;
  input q1 q2 q3 q4;
  datalines;
1.03  1.54  1.11  2.22
1.23  1.43  1.65  2.12
3.24  2.21  2.31  5.15
1.23  2.35  2.21  7.17
.98   2.13  1.76  2.38
1.02  2.05  3.15  4.28
1.54  1.99  1.77  2.00
1.76  1.79  2.28  3.18
1.11  3.41  2.20  3.21
1.32  2.32  4.32  4.78
1.22  1.81  1.51  3.15
1.11  2.15  2.45  6.17
1.01  2.12  1.96  2.08
1.34  1.74  2.16  3.28
;
```

Use the following PROC CALIS specification to estimate a saturated covariance structure model with all variances and covariances as parameters:

```
proc calis data=sales pcorr;
  mstruct var=q1-q4;
run;
```

In the PROC CALIS statement, specify the data set with the **DATA=** option. Use the **PCORR** option to display the observed and predicted covariance matrix. Next, use the **MSTRUCT** statement to fit a covariance matrix of the variables that are provided in the **VAR=** option. Without further specifications such as the **MATRIX** statement, PROC CALIS assumes all elements in the covariance matrix are model parameters. Hence, this is a saturated model.

Output 27.1.1 shows the modeling information. Information about the model is displayed: the name and location of the data set, the number of data records read and used, and the number of observations in the analysis. The number of data records read is the actual number of records (or observations) that PROC CALIS processes from the data set. The number of data records used might or might not be the same as the

actual number of records read from the data set. For example, records with missing values are read but not used in the analysis for the default maximum likelihood (ML) method. The number of observations refers to the N used for testing statistical significance and model fit. This number might or might not be the same as the number of records used for at least two reasons. First, if you use a frequency variable in the **FREQ** statement, the number of observations used is a weighted sum of the number of records, with the frequency variable being the weight. Second, if you use the **NOBS=** option in the **PROC CALIS** statement, you can override the number of observations that are used in the analysis. Because the current data set does not have any missing data and there are no frequency variables or an **NOBS=** option specified, these three numbers are all 14.

The model type is **MSTRUCT** because you use the **MSTRUCT** statement to define your model. The analysis type is covariances, which is the default. **Output 27.1.1** then shows the four variables in the covariance structure model.

Output 27.1.1 Modeling Information of the Saturated Covariance Structure Model for the Sales Data

```

Estimating the Covariance Matrix by the MSTRUCT Modeling Language

                The CALIS Procedure
Covariance Structure Analysis: Model and Initial Values

                Modeling Information
                Maximum Likelihood Estimation

Data Set           WORK.SALES
N Records Read     14
N Records Used     14
N Obs              14
Model Type         MSTRUCT
Analysis           Covariances

                Variables in the Model

                q1  q2  q3  q4

                Number of Variables = 4

```

Output 27.1.2 shows the initial covariance structure model for these four variables. All lower triangular elements (including the diagonal elements) of the covariance matrix are parameters in the model. **PROC CALIS** generates the names for these parameters: **_Add01–_Add10**. Because the covariance matrix is symmetric, all upper triangular elements of the matrix are redundant. The initial estimates for covariance are denoted by missing values no initial values were specified.

Output 27.1.2 Initial Saturated Covariance Structure Model for the Sales Data

Initial MSTRUCT _COV_ Matrix				
	q1	q2	q3	q4
q1
	[_Add01]	[_Add02]	[_Add04]	[_Add07]
q2
	[_Add02]	[_Add03]	[_Add05]	[_Add08]
q3
	[_Add04]	[_Add05]	[_Add06]	[_Add09]
q4
	[_Add07]	[_Add08]	[_Add09]	[_Add10]

The PCORR option in the PROC CALIS statement displays the sample covariance matrix in [Output 27.1.3](#). By default, PROC CALIS computes the unbiased sample covariance matrix (with variance divisor equal to $N - 1$) and uses it for the covariance structure analysis.

Output 27.1.3 Sample Covariance Matrix for the Sales Data

Covariance Matrix (DF = 13)				
	q1	q2	q3	q4
q1	0.33830	0.00020	0.03610	0.22137
q2	0.00020	0.22466	0.12653	0.24425
q3	0.03610	0.12653	0.60633	0.63012
q4	0.22137	0.24425	0.63012	2.66552

The fit summary and the fitted covariance matrix are shown in [Output 27.1.4](#) and [Output 27.1.5](#), respectively.

Output 27.1.4 Fit Summary of the Saturated Covariance Structure Model for the Sales Data

Fit Summary	
Chi-Square	0.0000
Chi-Square DF	0
Pr > Chi-Square	.

Output 27.1.5 Fitted Covariance Matrix for the Sales Data

MSTRUCT _COV_ Matrix: Estimate/StdErr/t-value				
	q1	q2	q3	q4
q1	0.3383	0.000198	0.0361	0.2214
	0.1327	0.0765	0.1260	0.2704
	2.5495	0.002587	0.2865	0.8186
q2	0.000198	0.2247	0.1265	0.2443
	0.0765	0.0881	0.1082	0.2251
	0.002587	2.5495	1.1693	1.0853
q3	0.0361	0.1265	0.6063	0.6301
	0.1260	0.1082	0.2378	0.3935
	0.2865	1.1693	2.5495	1.6012
q4	0.2214	0.2443	0.6301	2.6655
	0.2704	0.2251	0.3935	1.0455
	0.8186	1.0853	1.6012	2.5495

In [Output 27.1.4](#), the model fit chi-square is 0 ($df = 0$). The p -value cannot be computed because the degrees of freedom is zero. This fit is perfect because the model is saturated.

[Output 27.1.5](#) shows the fitted covariance matrix, along with standard error estimates and t values in each cell. The variance and covariance estimates match exactly those of the sample covariance matrix shown in [Output 27.1.3](#).

A common practice for determining statistical significance for estimates in structural equation modeling is to require the absolute value of t to be greater than 1.96, which is the critical value of a standard normal variate at $\alpha=0.05$. While all diagonal elements in [Output 27.1.5](#) show statistical significance, all off-diagonal elements are not significantly different from zero. The t values for these elements range from 0.002 to 1.601.

[Output 27.1.6](#) shows the standardized estimates of the variance and covariance elements. This is also the correlation matrix under the MSTRUCT model. Standard error estimates and t values are computed with the correlation estimates. Note that because the diagonal element values are fixed at 1, no standard errors or t values are shown.

Output 27.1.6 Standardized Covariance Matrix for the Sales Data

Standardized MSTRUCT _COV_ Matrix: Estimate/StdErr/t-value				
	q1	q2	q3	q4
q1	1.0000	0.000717 0.2773 0.002587	0.0797 0.2756 0.2892	0.2331 0.2623 0.8888
q2	0.000717 0.2773 0.002587	1.0000	0.3428 0.2448 1.4008	0.3156 0.2497 1.2640
q3	0.0797 0.2756 0.2892	0.3428 0.2448 1.4008	1.0000	0.4957 0.2092 2.3692
q4	0.2331 0.2623 0.8888	0.3156 0.2497 1.2640	0.4957 0.2092 2.3692	1.0000

Sometimes researchers do not need to estimate the standard errors that are in their models. You can suppress the standard error and *t* value computations by using the **NOSE** option in the PROC CALIS statement:

```
proc calis data=sales nose;
  mstruct var=q1-q4;
run;
```

Output 27.1.7 shows the fitted covariance matrix with the NOSE option. These values are exactly the same as in the sample covariance matrix shown in Output 27.1.3.

Output 27.1.7 Fitted Covariance Matrix without Standard Error Estimates for the Sales Data

MSTRUCT _COV_ Matrix				
	q1	q2	q3	q4
q1	0.3383	0.000198	0.0361	0.2214
q2	0.000198	0.2247	0.1265	0.2443
q3	0.0361	0.1265	0.6063	0.6301
q4	0.2214	0.2443	0.6301	2.6655

This example shows a very simple application of PROC CALIS: estimating the covariance matrix with standard error estimates. The covariance structure model is saturated. Several extensions of this very simple model are possible. To estimate the means and covariances simultaneously, see Example 27.2. To fit nonsaturated covariance structure models with certain hypothesized patterns, see Example 27.3 and Example 27.4. To fit structural models with implied covariance structures that are based on specified functional relationships among variables, see Example 27.6.

Example 27.2: Estimating Covariances and Means Simultaneously

This example uses the same data set that is used in [Example 27.1](#) and estimates the means and covariances. Use the **MSTRUCT** model specification as shown in the following statements:

```
proc calis data=sales meanstr nostand;
  mstruct var=q1-q4;
run;
```

In the PROC CALIS statement, specify the **MEANSTR** option to request the mean structure analysis in addition to the default covariance structure analysis. If you are not interested in the standardized solution, specify the **NOSTAND** option in the PROC CALIS statement to suppress computation of the standardized estimates. Without further model specification (such as the **MATRIX** statement), PROC CALIS assumes a saturated structural model with all means, variances, and covariances as model parameters.

[Output 27.2.1](#) shows the modeling information. With the **MEANSTR** option specified in the PROC CALIS statement, the current analysis type is Means and Covariances, instead of the default Covariances in [Example 27.1](#).

Output 27.2.1 Modeling Information of the Saturated Mean and Covariance Structure Model for the Sales Data

```

Saturated Means and Covariance Structures Using MSTRUCT

                The CALIS Procedure
Mean and Covariance Structures: Model and Initial Values

                Modeling Information
                Maximum Likelihood Estimation

Data Set              WORK.SALES
N Records Read        14
N Records Used        14
N Obs                 14
Model Type            MSTRUCT
Analysis              Means and Covariances

                Variables in the Model

                q1  q2  q3  q4

                Number of Variables = 4

```

[Output 27.2.2](#) shows the fit summary of the current model. Again, this is a perfect model fit with 0 chi-square value and 0 degrees of freedom.

Output 27.2.2 Fit Summary of the Saturated Mean and Covariance Structure Model for the Sales Data

Fit Summary	
Chi-Square	0.0000
Chi-Square DF	0
Pr > Chi-Square	.

Output 27.2.3 shows the estimates of the means, together with the standard error estimates and the *t* values. These estimated means are exactly the same as the sample means, which are not shown here.

Output 27.2.3 Mean Estimates for the Sales Data

MSTRUCT _Mean_ Vector			
Variable	Estimate	Standard Error	t Value
q1	1.36714	0.16132	8.47491
q2	2.07429	0.13146	15.77902
q3	2.20286	0.21596	10.20008
q4	3.65500	0.45281	8.07176

Output 27.2.4 shows the variance and covariance estimates. These estimates are exactly the same as the elements in the sample covariance matrix. In addition, these estimates match the estimates in Output 27.1.5 of Example 27.1, where only the covariance structures are analyzed.

Output 27.2.4 Variance and Covariance Estimates for the Sales Data

MSTRUCT _COV_ Matrix: Estimate/StdErr/t-value				
	q1	q2	q3	q4
q1	0.3383 0.1327 2.5495	0.000198 0.0765 0.002587	0.0361 0.1260 0.2865	0.2214 0.2704 0.8186
q2	0.000198 0.0765 0.002587	0.2247 0.0881 2.5495	0.1265 0.1082 1.1693	0.2443 0.2251 1.0853
q3	0.0361 0.1260 0.2865	0.1265 0.1082 1.1693	0.6063 0.2378 2.5495	0.6301 0.3935 1.6012
q4	0.2214 0.2704 0.8186	0.2443 0.2251 1.0853	0.6301 0.3935 1.6012	2.6655 1.0455 2.5495

These estimates are essentially the same as the sample means, variances, and covariances. This kind of analysis is much easier using PROC CORR with the NOMISS option. However, the main purpose of [Example 27.1](#) and [Example 27.2](#) is to introduce the MSTRUCT modeling language and some basic but important options in PROC CALIS. You can apply the MSTRUCT modeling language to more sophisticated situations that are beyond the saturated mean and covariance structure models. [Example 27.3](#) and [Example 27.4](#) fit some patterned covariance models that are nonsaturated. Also, options such as NOSE, NOSTAND, and MEANSTR are useful for all modeling languages in PROC CALIS.

Example 27.3: Testing Uncorrelatedness of Variables

This example uses the sales data in [Example 27.1](#) and tests the uncorrelatedness of the variables in the model by using the MSTRUCT model specification. With the multivariate normality assumption, this is also the test of independence of the variables. The MATRIX statement defines the parameters in the model.

The uncorrelatedness model assumes that the correlations or covariances among the four variables are zero. Therefore, only the four diagonal elements of the covariance matrix, which represent the variances of the variables, are free parameters in the covariance structure model. To specify these parameters, use the MATRIX statement with the MSTRUCT model specification:

```
proc calis data=sales;
  mstruct var=q1-q4;
  matrix _cov_ [1,1], [2,2], [3,3], [4,4];
run;
```

[Example 27.1](#) specifies exactly the same MSTRUCT statement for the four variables. The difference here is the addition of the MATRIX statement. Without a MATRIX statement, the MSTRUCT model assumes that all nonredundant elements in the covariance matrix are model parameters. This assumption is not the case in the current specification. The MATRIX statement specification for the covariance matrix (denoted by the `_cov_` keyword) specifies four free parameters on the diagonal of the covariance matrix: `[1, 1]`, `[2, 2]`, `[3, 3]`, and `[4, 4]`. All other unspecified elements in the covariance matrix are fixed zeros by default.

The uncorrelatedness model is displayed in the output for the initial model specification. [Output 27.3.1](#) shows that all off-diagonal elements of the covariance matrix are fixed zeros while the diagonal elements are missing and labeled with `_Parm1–_Parm4`. PROC CALIS generates these parameter names automatically and estimates these four parameters in the analysis.

Output 27.3.1 Initial Uncorrelatedness Model for the Sales Data

Initial MSTRUCT _COV_ Matrix				
	q1	q2	q3	q4
q1	.	0	0	0
	[_Parm1]			
q2	0	.	0	0
		[_Parm2]		
q3	0	0	.	0
			[_Parm3]	
q4	0	0	0	.
				[_Parm4]

Output 27.3.2 shows the model fit chi-square test of the uncorrelatedness model. The chi-square is 6.528 ($df = 6, p = 0.3667$), which is not significant. This means that you fail to reject the uncorrelatedness model. In other words, the data is consistent with the uncorrelatedness model (zero covariances or correlations among the quarterly sales).

Output 27.3.2 Fit Summary of the Uncorrelatedness Model for the Sales Data

Fit Summary	
Chi-Square	6.5280
Chi-Square DF	6
Pr > Chi-Square	0.3667

Output 27.3.3 shows the estimates of the covariance matrix under the uncorrelatedness model, together with standard error estimates and t values. All off-diagonal elements are fixed zeros in the estimation results.

Output 27.3.3 Estimates of Variance under the Uncorrelatedness Model for the Sales Data

MSTRUCT _COV_ Matrix: Estimate/StdErr/t-value				
	q1	q2	q3	q4
q1	0.3383 0.1327 2.5495 [_Parm1]	0	0	0
q2	0	0.2247 0.0881 2.5495 [_Parm2]	0	0
q3	0	0	0.6063 0.2378 2.5495 [_Parm3]	0
q4	0	0	0	2.6655 1.0455 2.5495 [_Parm4]

This example shows how to specify free parameters in the MSTRUCT model by using the **MATRIX** statement. To specify the covariance matrix, use the **_COV_** keyword in the **MATRIX** statement. To specify the parameters in the mean structures, you need use an additional **MATRIX** statement with the **_MEAN_** keyword.

Two important notes regarding the MSTRUCT model specification are now in order:

- When you use the **MSTRUCT** statement without any **MATRIX** statements, *all* elements in the covariance matrix are *free parameters* in the model (for example, see [Example 27.1](#)). However, if the **MATRIX** statement includes at least one free or fixed parameter in the covariance matrix, PROC CALIS assumes that all other unspecified elements in the covariance matrix are *fixed zeros* (such as the current example).
- Using parameter names in the **MATRIX** statement specification is optional. In the context of the current example, naming the parameters is optional because there is no need to refer to them anywhere in the specification. PROC CALIS automatically generates unique names for these parameters. Alternatively, you can specify your own parameter names in the **MATRIX** statement. Naming parameters is not only useful for references, but is also indispensable when you need to constrain model parameters by referring to their names. See [Example 27.4](#) to use parameter names to define a covariance pattern.

Example 27.4: Testing Covariance Patterns

In the test for sphericity, a covariance matrix is hypothesized to be a constant multiple of an identity matrix. That is, the null hypothesis for the population covariance matrix is

$$\Sigma = \sigma^2 \mathbf{I}$$

where σ^2 is an unknown positive constant and \mathbf{I} is an identity matrix. When this covariance pattern is applied to the sales data in [Example 27.1](#), this hypothesis states that all four variables have the same variance σ^2 and are uncorrelated with each other. This model is more restricted than the uncorrelatedness model in [Example 27.3](#), which requires uncorrelatedness but does not require equal variances. Use the following specification to conduct a sphericity test for the sales data:

```
proc calis data=sales;
  mstruct var=q1-q4;
  matrix _cov_ [1,1] = 4*sigma_sq;
run;
```

This specification is similar to that of [Example 27.3](#). The major difference is the **MATRIX** statement specification. The current example uses a parameter name `sigma_sq` to represent the unknown variance parameter σ^2 , whereas [Example 27.3](#) specifies only the locations of the four free variance parameters.

The current **MATRIX** statement specification uses a shorthand notation. On the left-hand side of the equal sign, `[1,1]` indicates the starting location of the covariance matrix. The matrix entries automatically proceed to `[2,2]`, `[3,3]` and so on, depending on the length of the parameter list specified on the right-hand side of the equal sign. For example, if there is just one parameter on the right-hand side, the matrix specification contains only `[1,1]`. In the current example, the specification `4*sigma_sq` means that `sigma_sq` appears four times in the specification. As a result, the preceding **MATRIX** statement specification is equivalent to the following statement:

```
matrix _cov_ [1,1] = sigma_sq,
             [2,2] = sigma_sq,
             [3,3] = sigma_sq,
             [4,4] = sigma_sq;
```

This matrix is what is required by the sphericity test. Use either the expanded notation or the shorthand notation for specifying the covariance pattern. For details about various types of shorthand notation for parameter specifications, see the **MATRIX** statement.

Output 27.4.1 shows the initial model specification under the test of sphericity. All the diagonal elements are labeled with the same name `sigma_sq`, indicating that they are the same parameter.

Output 27.4.1 Covariance Model under Sphericity for the Sales Data

Initial MSTRUCT _COV_ Matrix				
	q1	q2	q3	q4
q1	.	0	0	0
	[sigma_sq]			
q2	0	.	0	0
		[sigma_sq]		
q3	0	0	.	0
			[sigma_sq]	
q4	0	0	0	.
				[sigma_sq]

Output 27.4.2 shows that the model fit chi-square is 31.5951 ($df = 9$, $p = 0.0002$). This means that the covariance pattern under the sphericity hypothesis is not supported.

Output 27.4.2 Fit Summary of the Sphericity Test for the Sales Data

Fit Summary	
Chi-Square	31.5951
Chi-Square DF	9
Pr > Chi-Square	0.0002

Output 27.4.3 shows the estimated covariance matrix under the sphericity hypothesis. The variance estimate for all four diagonal elements is 0.9587 (standard error=0.1880).

Output 27.4.3 Fitted Covariance Matrix under the Sphericity Hypothesis for the Sales Data

MSTRUCT _COV_ Matrix: Estimate/StdErr/t-value				
	q1	q2	q3	q4
q1	0.9587 0.1880 5.0990 [sigma_sq]	0	0	0
q2	0	0.9587 0.1880 5.0990 [sigma_sq]	0	0
q3	0	0	0.9587 0.1880 5.0990 [sigma_sq]	0
q4	0	0	0	0.9587 0.1880 5.0990 [sigma_sq]

This example shows how you can specify a simple covariance pattern by using the MATRIX statement. Use the same parameter names to constrain variance parameters that are supposed to be the same under the model. Constraining parameters by using the same parameter names is applicable not only to the MSTRUCT models, but also to more complicated covariance structure models, such as multiple-group modeling (see Example 27.19 and Example 27.21).

The MSTRUCT modeling language is handy when you can directly specify the covariance pattern or structures in your model. However, in most applications of structural equation modeling, it is difficult to specify such direct covariance structures. Instead, the covariance structures are usually implied from the functional relationships among the variables in the model. Using the MSTRUCT modeling language in such a situation is not easy. Fortunately, PROC CALIS supports other modeling languages that enable you to specify the functional relationships among variables. The functional relationships can be in the form of a set of path-like descriptions, a system of linear equations, or parameter specifications in matrices. See Example 27.6 for an introduction to using the PATH modeling language for specifying path models.

Example 27.5: Testing Some Standard Covariance Pattern Hypotheses

In Example 27.3, you test the uncorrelatedness of variables by using the MSTRUCT model specification. In Example 27.4, you test the sphericity of the covariance matrix by using the same model specification technique. In both examples, you need to specify the parameters in the covariance structure model explicitly by using the MATRIX statements.

Some covariance patterns are well-known in multivariate statistics, including the two tests in Example 27.3 and Example 27.4. To facilitate the tests of these “standard” covariance patterns, PROC CALIS provides the

COVPATTERN= option to specify those standard covariance patterns more efficiently. With the COVPATTERN=option, you do not need to use the MSTRUCT and MATRIX statements to specify the covariance patterns explicitly. See the COVPATTERN= option for the supported covariance patterns. This example illustrates the use of the COVPATTERN= option.

In Example 27.3, you conduct a test of uncorrelatedness for the four variables in the sales data (see Example 27.1 for the data set). That is, the variables are hypothesized to be uncorrelated and only the four variances on the diagonal of the covariance matrix are population parameters of interest. The null hypothesis for the population covariance matrix is

$$\Sigma = \begin{pmatrix} x & 0 & 0 & 0 \\ 0 & x & 0 & 0 \\ 0 & 0 & x & 0 \\ 0 & 0 & 0 & x \end{pmatrix}$$

where each x represents a distinct parameter (that is, the diagonal elements are not constrained with each other). You can test the diagonal covariance pattern easily by the following specification:

```
proc calis data=sales covpattern=diag;
run;
```

The COVPATTERN=DIAG option specifies the required diagonal covariance pattern for the test. PROC CALIS then sets up the covariance structures automatically. Output 27.5.1 shows the initial specification of the covariance pattern. As required, only the diagonal elements are parameters in the test and the other elements are fixed to zero. PROC CALIS names the variance parameters automatically—that is, `_varparm_1–_varparm_4` are the four parameters for the variances. This is the same pattern as shown in Output 27.3.1 of Example 27.3, although the parameter names are different.

Output 27.5.1 Initial Diagonal Pattern for the Covariance Matrix of the Sales Data

Initial MSTRUCT _COV_ Matrix				
	q1	q2	q3	q4
q1	.	0	0	0
	[_varparm_1]			
q2	0	.	0	0
		[_varparm_2]		
q3	0	0	.	0
			[_varparm_3]	
q4	0	0	0	.
				[_varparm_4]

Output 27.5.2 shows the results of the chi-square test of the diagonal covariance pattern. The chi-square is 5.44 ($df = 6$, $p = 0.4887$), which is not significant. You fail to reject the null hypothesis of the diagonal covariance pattern in the population.

Output 27.5.2 Fit Summary of the Diagonal Covariance Pattern Test for the Sales Data

Fit Summary	
Chi-Square	5.4400
Chi-Square DF	6
Pr > Chi-Square	0.4887

The numerical results shown in [Output 27.5.2](#) are different from those of the same test by using the MSTRUCT model specification, which is shown in [Output 27.3.2](#) of [Example 27.3](#), although you do not reject the null hypothesis in both cases. The reason is that with the use of COVPATTERN= option, PROC CALIS applies the appropriate chi-square correction to the test statistic automatically. In the current example, the chi-square correction due to Bartlett (1950) has been applied. Test results with chi-square corrections are theoretically more accurate.

To obtain the same numerical results as those in [Output 27.3.2](#), you can turn off the chi-square correction by using the CHICORRECT=0 option, as shown in the following specification:

```
proc calis data=sales covpattern=diag chicorrect=0;
run;
```

[Output 27.5.3](#) shows the fit summary results without any chi-square correction. The numerical results match exactly to those shown in [Output 27.3.2](#) of [Example 27.3](#).

Output 27.5.3 Fit Summary of the Diagonal Covariance Pattern Test for the Sales Data: No Chi-Square Correction

Fit Summary	
Chi-Square	6.5280
Chi-Square DF	6
Pr > Chi-Square	0.3667

[Example 27.4](#) tests the sphericity of the covariance matrix of the same data set. The null hypothesis for the population covariance matrix is

$$\Sigma = \sigma^2 \mathbf{I}$$

where σ^2 is an unknown positive constant and \mathbf{I} is an identity matrix. You can use the following specification to test this hypothesis easily:

```
proc calis data=sales covpattern=sigsqi;
run;
```

[Output 27.5.4](#) shows the initial specification of the covariance pattern. As required, the diagonal elements are all the same parameter named `_varparm`, and all the off-diagonal elements are fixed to zero. This is the same pattern as shown in [Output 27.4.1](#) of [Example 27.4](#).

Output 27.5.4 Initial Covariance Pattern for the Sphericity Test on the Sales Data

Initial MSTRUCT _COV_ Matrix				
	q1	q2	q3	q4
q1	.	0	0	0
	[_varparm]			
q2	0	.	0	0
		[_varparm]		
q3	0	0	.	0
			[_varparm]	
q4	0	0	0	.
				[_varparm]

Output 27.5.5 shows the fit summary of the sphericity test. The chi-square is 27.747 ($df = 9$, $p = 0.0011$), which is statistically significant. You reject the sphericity hypothesis for the population covariance matrix.

Output 27.5.5 Fit Summary of the Sphericity Test on the Sales Data

Fit Summary	
Chi-Square	27.7470
Chi-Square DF	9
Pr > Chi-Square	0.0011

Again, the numerical results in Output 27.5.5 are different from those shown in Output 27.4.2 of Example 27.4. This is because with the COVPATTERN=SIGSQI option, the chi-square correction due to Box (1949) has been applied in the current example. To turn off the automatic chi-square correction, you can use the following specification:

```
proc calis data=sales covpattern=sigsqi chicorrect=0;
run;
```

As expected, the numerical results in Output 27.5.6 match exactly to those of in Output 27.4.2 of Example 27.4.

Output 27.5.6 Fit Summary of the Sphericity Test on the Sales Data: No Chi-Square Correction

Fit Summary	
Chi-Square	31.5951
Chi-Square DF	9
Pr > Chi-Square	0.0002

This example shows that for the tests of some standard covariance patterns, you can use the `COVPATTERN=` option directly. As compared with the use of the explicit `MSTRUCT` model specifications, which are shown in [Example 27.3](#) and [Example 27.4](#), the use of `COVPATTERN=` option is more efficient and less error-prone in coding. In addition, it can apply chi-square corrections in appropriate situations.

`PROC CALIS` also provides the test of some “standard” mean patterns by the `MEANPATTERN=` option. You can use the `COVPATTERN=` and `MEANPATTERN=` options together to define the desired combinations of covariance and mean patterns. See these two options for details. See [Example 27.22](#) for a multiple-group analysis with the simultaneous use of the `COVPATTERN=` and `MEANPATTERN=` options. Certainly, the `COVPATTERN=` and `MEANPATTERN=` options are limited to the standard covariance and mean patterns provided by `PROC CALIS`. When you need to fit some specific (nonstandard) covariance or mean patterns, the `MSTRUCT` model specification would be indispensable. See [Example 27.19](#) and [Example 27.22](#) for applications.

Example 27.6: Linear Regression Model

This example shows how you can use `PROC CALIS` to fit the basic regression models. Unlike the preceding examples ([Example 27.1](#), [Example 27.2](#), [Example 27.3](#), and [Example 27.4](#)) where you specify the covariance structures directly, in this example the covariance structures being analyzed are implied by the functional relationships specified in the model. The `PATH` modeling language introduced in the current example requires you to specify only the functional or path relationships among variables. `PROC CALIS` analyzes the implied covariance structures that are derived from the specified functional or path relationships.

Consider the same sales data as in [Example 27.1](#). This example demonstrates a simple linear regression that uses `q1` (the sales in the first quarter) to predict `q4` (the sales in the fourth quarter).

In covariance structural analysis, or in general structural equation modeling, relationships among variables are usually represented by the so-called path diagram. For example, you can represent the linear regression of `q4` on `q1` by the following simple path diagram:



In the path diagram, `q1` is an exogenous (or independent) variable and `q4` is an endogenous (or dependent) variable. Formally, a variable in a path diagram is endogenous if there is at least one single-headed arrow pointing to it. Otherwise, the variable is exogenous. In some situations, researchers apply “causal” interpretations among variables in the path diagram, with the single-headed arrows indicating the causal directions. However, causal interpretations are not a requirement for using covariance structure analysis or structural equation modeling.

It is easy to transcribe the preceding path diagram into the `PATH` model specification in `PROC CALIS`, as shown in the following statements:

```

proc calis data=sales;
  path   q1 ==> q4;
run;

```

Output 27.6.1 shows the modeling information of the linear regression model. It shows that all 14 observations are used and the model type is PATH. PROC CALIS analyzes the (implied) covariance structure model for the data. In the next table of Output 27.6.1, PROC CALIS shows the nature of the variables in the model: q4 is an endogenous manifest variable and q1 is an exogenous manifest variable. There is no latent variable in this simple path model.

Output 27.6.1 Modeling Information of the Linear Regression Model for the Sales Data

```

Simple Linear Regression Model by the PATH Modeling Language

                The CALIS Procedure
Covariance Structure Analysis: Model and Initial Values

                Modeling Information
                Maximum Likelihood Estimation

Data Set           WORK.SALES
N Records Read     14
N Records Used     14
N Obs             14
Model Type        PATH
Analysis          Covariances

                Variables in the Model

Endogenous   Manifest   q4
              Latent
Exogenous    Manifest   q1
              Latent

Number of Endogenous Variables = 1
Number of Exogenous Variables = 1

```

Output 27.6.2 shows the initial model specification. The path is in the first table. A parameter name is attached to the path. The name `_Parm1`, which is generated automatically by PROC CALIS, denotes the effect parameter of q1 on q4. In the context of linear regression, `_Parm1` also denotes the regression coefficient.

Output 27.6.2 Initial Specification of the Linear Regression Model for the Sales Data

```

                Initial Estimates for PATH List

-----Path-----   Parameter   Estimate
q1    ==>    q4    _Parm1           .

```

Output 27.6.2 *continued*

Initial Estimates for Variance Parameters			
Variance Type	Variable	Parameter	Estimate
Exogenous	q1	_Add1	.
Error	q4	_Add2	.

NOTE: Parameters with prefix '_Add' are added by PROC CALIS.

Next, [Output 27.6.2](#) shows the variance parameters in the model. You do not need to specify any of these parameters in the preceding PATH model specification—because PROC CALIS adds these parameters by default. `_Add1` denotes the variance parameter for the exogenous variable `q1`. `_Add2` denotes the error variance parameter for the endogenous variable `q4`.

In the PATH model of PROC CALIS, all variances of exogenous variables and all error variances of endogenous variables are free parameters by default. In most practical applications, these parameters are usually free parameters in models and it would be laborious to specify them each time when you fit a covariance structure model. Therefore, to make the PATH model specification more efficient and easier, PROC CALIS sets these free parameters by default. In fact, with these default parameters in the PATH model, PROC CALIS produces essentially the same regression analysis results as those produced by common linear regression procedures such as PROC REG. This consistency is shown in the subsequent estimation results for the current example.

You can also explicitly specify those otherwise default parameters of the PATH model in PROC CALIS. Depending on the modeling situation, you can set any parameter in the PATH model as a free, fixed, or constrained parameter. You can also provide names for the parameters. Naming parameters is very useful for parameter referencing and for setting up parameter constraints. See [Example 27.4](#). For details, see the `PATH` statement and the section “[The PATH Model](#)” on page 1288.

[Output 27.6.3](#) shows some fit statistics from the linear regression model. The model fit chi-square is 0 with 0 degrees of freedom. This is a perfect model fit. The fit is perfect because the covariance model contains three distinct elements (variance of `q1`, variance of `q4`, and covariance between `q1` and `q4`) that are fitted perfectly by three parameters: `_Parm1` for the effect of `q1` on `q4`, `_Add1` for the variance of variable `q1`, and `_Add2` for the error variance of variable `q4`. Thus, the unconstrained linear regression model estimates are simply a transformation of the covariance elements. Hence, the model is saturated with a perfect fit and zero degrees of freedom.

Output 27.6.3 Model Fit of the Linear Regression Model for the Sales Data

Fit Summary	
Chi-Square	0.0000
Chi-Square DF	0
Pr > Chi-Square	.
Standardized RMR (SRMR)	0.0000
RMSEA Estimate	.

Output 27.6.4 shows the estimates of the model. The effect of q1 on q4 is 0.6544 (standard error=0.7571). The associated t value is 0.86433, which is not significantly different from zero. The estimated variance of q1 is 0.3383 and the estimated error variance for q4 is 2.5207. Both estimates are significant.

Output 27.6.4 Parameter Estimates of the Linear Regression Model for the Sales Data

PATH List					
-----Path-----	Parameter	Estimate	Standard Error	t Value	
q1 ==> q4	_Parm1	0.65436	0.75707	0.86433	
Variance Parameters					
Variance Type	Variable	Parameter	Estimate	Standard Error	t Value
Exogenous	q1	_Add1	0.33830	0.13269	2.54951
Error	q4	_Add2	2.52066	0.98869	2.54951

For a simple linear regression such as this one, you could have used PROC REG. You get essentially the same estimates by specifying the following statements:

```
proc reg data=sales;
  model q4 = q1;
run;
```

Output 27.6.5 shows the parameter estimates from PROC REG. The intercept estimate is 2.7604 (standard error=1.1643) and the regression coefficient is 0.6544 (standard error=0.7880). The regression coefficient estimate matches PROC CALIS. However, the corresponding standard error estimate in PROC CALIS is 0.7571, which is slightly different from PROC REG. This difference is due to the different variance divisors that are used in calculating the standard error estimates. PROC CALIS uses $(N - 1)$ as the divisor (by default) while PROC REG uses $(N - q - 1)$, where N is the number of observations and q is the number of regression coefficients. In the current example, q is 1 so that the variance divisor in PROC REG is 1 less than the divisor in PROC CALIS. If you have at least a moderate sample size and the number of regression parameters is relatively small compared to the sample size, the discrepancy due to using different variance divisors is of little consequence.

Output 27.6.5 Parameter Estimates from PROC REG for the Sales Data

Parameter Estimates					
Variable	DF	Parameter Estimate	Standard Error	t Value	Pr > t
Intercept	1	2.76040	1.16430	2.37	0.0353
q1	1	0.65436	0.78798	0.83	0.4225

By default, PROC CALIS analyzes only the covariance structures, which are properties of the second-order moments of the data. PROC CALIS does not automatically produce intercept estimates, which are properties of the first-order moments of the data.

In order to produce the intercept estimate in the linear regression context, you can add the **MEANSTR** (mean structures) option in the PROC CALIS statement, as shown in the following statements:

```
proc calis data=sales meanstr;
  path  q1 ==> q4;
run;
```

Output 27.6.6 shows the parameter estimates of the model with the MEANSTR option added. Compared with Output 27.6.4, Output 27.6.6 produces one more table: estimates of the mean and intercept. The intercept estimate for q4 is 2.7604, which matches the intercept estimate from PROC REG. The estimated mean of q1 is 1.3671. All other estimates are the same for the analyses with and without the MEANSTR option.

Output 27.6.6 Parameter Estimates of the Linear Regression Model with the MEANSTR option for the Sales Data

PATH List					
-----Path-----	Parameter	Estimate	Standard Error	t Value	
q1 ==> q4	_Parm1	0.65436	0.75707	0.86433	
Variance Parameters					
Variance Type	Variable	Parameter	Estimate	Standard Error	t Value
Exogenous	q1	_Add1	0.33830	0.13269	2.54951
Error	q4	_Add2	2.52066	0.98869	2.54951
Means and Intercepts					
Type	Variable	Parameter	Estimate	Standard Error	t Value
Intercept	q4	_Add3	2.76040	1.12480	2.45413
Mean	q1	_Add4	1.36714	0.16132	8.47491

Linear regression estimates from PROC CALIS are comparable to those obtained from PROC REG, although the two procedures have different default treatments of the variance divisor in calculating the standard error estimates. With the **MEANSTR** option in the PROC CALIS statement, you can analyze the mean and covariance structures simultaneously. PROC CALIS prints the estimates of the intercepts and means when you model the mean structures.

This example shows how you can fit the linear regression model as a PATH model in PROC CALIS. You need to specify only path relationships among the variables in the PATH statement, because the implied

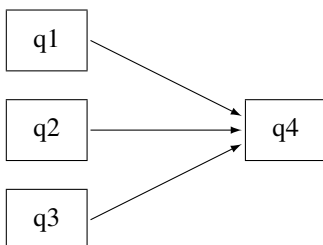
covariance structures are generated and analyzed by PROC CALIS. To make model specification more efficient, PROC CALIS sets default variance parameters for exogenous variables and default error variance parameters for endogenous variables. You can also overwrite these default parameters by explicit specifications. See [Example 27.7](#) for some sophisticated regression models that you can specify with PROC CALIS. See [Example 27.17](#) for a more elaborate path model specification.

Example 27.7: Multivariate Regression Models

This example shows how to analyze different types of multivariate regression models with PROC CALIS. [Example 27.6](#) fits a simple linear regression model to the sales data that are described in [Example 27.1](#). The simple linear regression model predicts the fourth quarter sales (q4) from the first quarter sales (q1). There is only one dependent (outcome) variable (q4) and one independent (predictor) variable (q1) in the analysis. Also, there are no constraints on the parameters. This example fits more sophisticated regression models. The models include more than one predictor. Some variables can serve as outcome variables and predictor variables at the same time. This example also illustrates the use of parameter constraints in model specifications and the use of the model fit statistics to search for a “best” model for the sales data.

Multiple Regression Model for the Sales Data

Consider a multiple regression model for q4. Instead of using just q1 as the predictor in the model as in [Example 27.6](#), use all previous sales q1–q3 to predict the fourth-quarter sale (q4). The path model representation is shown in the following path diagram:



You can transcribe this path diagram into the following PATH model specification:

```

proc calis data=sales;
  path  q1 q2 q3 ==> q4;
run;
  
```

In the path statement, the shorthand path specification

```

path  q1 q2 q3 ==> q4;
  
```

is equivalent to the following specification:

```

path  q1 ==> q4,
      q2 ==> q4,
      q3 ==> q4;
  
```

The shorthand notation provides a more convenient way to specify the path model. Some of the model fit statistics are shown in [Output 27.7.1](#). This is a saturated model with perfect fit and zero degrees of freedom.

Because the chi-square statistic is always smallest in a saturated model (with a zero chi-square value), it does not make much sense to judge the model quality solely by looking at the chi-square value. However, a saturated model is useful for serving as a baseline model with which other nonsaturated competing models are compared.

Output 27.7.1 Model Fit of the Multiple Regression Model for the Sales Data

Fit Summary	
Chi-Square	0.0000
Chi-Square DF	0
Pr > Chi-Square	.
Standardized RMR (SRMR)	0.0000
RMSEA Estimate	.
Akaike Information Criterion	20.0000
Bozdogan CAIC	36.3906
Schwarz Bayesian Criterion	26.3906

In addition to the model fit chi-square statistic, [Output 27.7.1](#) also shows Akaike’s information criterion (AIC), Bozdogan’s CAIC, and Schwarz’s Bayesian criterion (SBC) of the saturated model. The AIC, CAIC, and SBC are derived from information theory and henceforth they are referred to as the information-theoretic fit indices. These information-theoretic fit indices measure the model quality by taking the model parsimony into account. The root mean square error of approximation (RMSEA) also takes the model parsimony into account, but it is not an information-theoretic fit index. The values of these information-theoretic fit indices themselves do not indicate the quality of the model. However, when you fit several different models to the same data, you can order the models by these fit indices. The better the model, the smaller the fit index values. Unlike the chi-square statistic, these fit indices do not always favor a saturated model because a saturated model lacks model parsimony (the saturated model uses the most parameters to explain the data). The subsequent discussion uses these fit indices to select the “best” model for the sales data.

[Output 27.7.2](#) shows the parameter estimates of the multiple regression model. In the first table, all path effect estimates are not statistically significant—that is, all *t* values are less than 1.96. The next table in [Output 27.7.2](#) shows the variance estimates of q1–q3 and the error variance estimate for q4. All of these estimates are significant. The last table in [Output 27.7.2](#) shows the covariances among the exogenous variables q1–q3. These covariance estimates are small and are not statistically significant.

Output 27.7.2 Parameter Estimates of the Multiple Regression Model for the Sales Data

PATH List						
-----Path-----	Parameter	Estimate	Standard Error	t Value		
q1 ==> q4	_Parm1	0.55980	0.64938	0.86205		
q2 ==> q4	_Parm2	0.58946	0.84558	0.69711		
q3 ==> q4	_Parm3	0.88290	0.51635	1.70988		

Output 27.7.2 continued

Variance Parameters					
Variance Type	Variable	Parameter	Estimate	Standard Error	t Value
Exogenous	q1	_Add1	0.33830	0.13269	2.54951
	q2	_Add2	0.22466	0.08812	2.54951
	q3	_Add3	0.60633	0.23782	2.54951
Error	q4	_Add4	1.84128	0.72221	2.54951

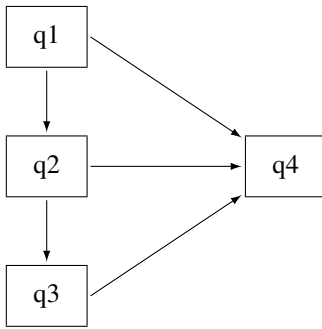
Covariances Among Exogenous Variables					
Var1	Var2	Parameter	Estimate	Standard Error	t Value
q2	q1	_Add5	0.0001978	0.07646	0.00259
q3	q1	_Add6	0.03610	0.12601	0.28649
q3	q2	_Add7	0.12653	0.10821	1.16931

In Output 27.7.2, the total number of parameter estimates is 10 (_Parm1–_Parm3 and _Add1–_Add7). Under the covariance structure model, these 10 parameters explain the 10 nonredundant elements in the covariance matrix for the sales data. That is why the model has a perfect fit with zero degrees of freedom.

In Output 27.7.2, notice that some parameters have the prefix ‘_Parm’, while others have the prefix ‘_Add’. Both types of parameter names are generated by PROC CALIS. The parameters named with the ‘_Parm’ prefix are those that were specified in the model, but were not named. In the current example, the parameters specified but not named are the path coefficients (effects) for the three paths in the PATH statement. The parameters named with the ‘_Add’ prefix are default parameters added by PROC CALIS. In the current multiple regression example, the variances and covariances among the predictors (q1–q3) and the error variance for the outcome variable (q4) are default parameters in the model. In general, variances and covariances among exogenous variables and error variances of endogenous variables are default parameters in the PATH model. Avoid using parameter names with the ‘_Parm’ and ‘_Add’ prefixes to avoid confusion with parameters that are generated by PROC CALIS.

Direct and Indirect Effects Model for the Sales Data

In the multiple regression model, q1–q3 are all predictors that have direct effects on q4. This example considers the possibility of adding indirect effects into the multiple regression model. Because of the time ordering, it is reasonable to assume that there is a causal sequence $q1 \implies q2 \implies q3$. To implement this idea into the model, put two more paths into the preceding path diagram to form the following new path diagram:



With the $q1 \implies q2$ and $q2 \implies q3$ paths, $q2$ and $q3$ are no longer exogenous in the model. They become endogenous. The only exogenous variable in the model is $q1$, which has a direct effect in addition to indirect effects on $q4$. The direct effect is indicated by the $q1 \implies q4$ path. The indirect effects are indicated by the following two causal chains: $q1 \implies q2 \implies q4$ and $q1 \implies q2 \implies q3 \implies q4$. Similarly, $q2$ has a direct and an indirect effect on $q4$. However, $q3$ has only a direct effect on $q4$. You can use the following statements to specify this *direct and indirect effects* model:

```

proc calis data=sales;
  path   q1      ==>  q2,
         q2      ==>  q3,
         q1 q2 q3 ==>  q4;
run;

```

Although the *direct and indirect effects* model has two more paths in the PATH statement than does the preceding multiple regression model, the current model is more precise because it has one fewer parameter. By introducing the causal paths $q1 \implies q2$ and $q2 \implies q3$, the six variances and covariances among $q1$ – $q3$ are explained by: the two causal effects, the exogenous variance of $q1$, and the error variances for $q2$ and $q3$ (that is, five parameters in the model). Hence, the current *direct and indirect effects* model has one fewer parameter than the preceding multiple regression model.

Output 27.7.3 shows some model fit indices of the direct and indirect effects model. The model fit chi-square is 0.0934 with one degree of freedom. It is not significant. Therefore, you cannot reject the model on statistical grounds. The standardized root mean squares of residuals (SRMR) is 0.028 and the root mean square error of approximation (RMSEA) is close to zero. Both indices point to a very good model fit. The AIC, CAIC, and SBC are all smaller than those of the saturated model, as shown in **Output 27.7.1**. This suggests that the *direct and indirect effects* model is better than the saturated model.

Output 27.7.3 Model Fit of the Direct and Indirect Effects Model for the Sales Data

Fit Summary	
Chi-Square	0.0934
Chi-Square DF	1
Pr > Chi-Square	0.7600
Standardized RMR (SRMR)	0.0280
RMSEA Estimate	0.0000
Akaike Information Criterion	18.0934
Bozdogan CAIC	32.8449
Schwarz Bayesian Criterion	23.8449

Output 27.7.4 shows the parameter estimates of the *direct and indirect effects* model. All the path effects are not significant, while all the variance or error variance estimates are significant. Unlike the saturated model where you have covariance estimates among several exogenous variables (as shown in Output 27.7.2), in the *direct and indirect effects* model there is only one exogenous variable (q1) and hence there is no covariance estimate in the results.

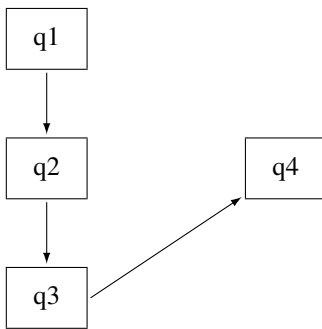
Output 27.7.4 Parameter Estimates of the Direct and Indirect Effects Model for the Sales Data

PATH List						
-----Path-----		Parameter	Estimate	Standard Error	t Value	
q1	====>	q2	_Parm1	0.0005847	0.22602	0.00259
q2	====>	q3	_Parm2	0.56323	0.42803	1.31587
q1	====>	q4	_Parm3	0.55980	0.64705	0.86515
q2	====>	q4	_Parm4	0.58946	0.84524	0.69739
q3	====>	q4	_Parm5	0.88290	0.51450	1.71603
Variance Parameters						
Variance Type	Variable	Parameter	Estimate	Standard Error	t Value	
Exogenous	q1	_Add1	0.33830	0.13269	2.54951	
Error	q2	_Add2	0.22466	0.08812	2.54951	
	q3	_Add3	0.53506	0.20987	2.54951	
	q4	_Add4	1.84128	0.72221	2.54951	

Although the current *direct and indirect effects* model is better than the saturated model and both the SRMR and RMSEA indicate a good model fit, the nonsignificant path effect estimates are unsettling. You continue to explore alternative models for the data.

Indirect Effects Model for the Sales Data

The saturated model includes only the direct effects of q1–q3 on q4, while the *direct and indirect effects* model includes both the direct and indirect effects of q1 and q2 on q4. An alternative model with only the indirect effects of q1 and q2 on q4, but without their direct effects, is possible. Such an *indirect effects* model is represented by the following path diagram:



You can easily transcribe this path diagram into the following PATH model specification:

```

proc calis data=sales;
  path  q1  ==> q2,
        q2  ==> q3,
        q3  ==> q4;
run;

```

Output 27.7.5 shows some model fit indices for the *indirect effects* model. The chi-square model fit statistic is not statistically significant, so the model is not rejected. The standardized RMR is 0.0905, which is a bit higher than the conventional value of 0.05 for an acceptable good model fit. However, the RMSEA is close to zero, which shows a very good model fit. The AIC, CAIC and SBC are all smaller than the *direct and indirect effects* model. These information-theoretic fit indices suggest that the *indirect effects* model is better.

Output 27.7.5 Model Fit of the Indirect Effects Model for the Sales Data

Fit Summary	
Chi-Square	1.2374
Chi-Square DF	3
Pr > Chi-Square	0.7440
Standardized RMR (SRMR)	0.0905
RMSEA Estimate	0.0000
Akaike Information Criterion	15.2374
Bozdogan CAIC	26.7108
Schwarz Bayesian Criterion	19.7108

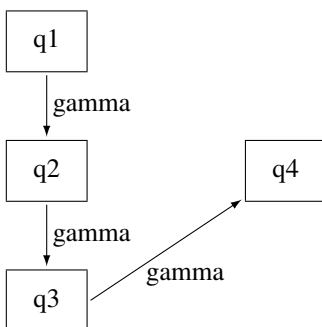
Output 27.7.6 shows the parameter estimates of the *indirect effects* model. All the variance and error variance estimates are statistically significant. However, only the path effect of q3 on q4 is statistically significant, and all other path effects are not. Having significant variances with nonsignificant paths raises some concerns about accepting the current model even though the AIC, CAIC, and SBC values suggest that it is the best model so far.

Output 27.7.6 Parameter Estimates of the Indirect Effects Model for the Sales Data

PATH List						
-----Path-----	Parameter	Estimate	Standard Error	t Value		
q1 ==> q2	_Parm1	0.0005847	0.22602	0.00259		
q2 ==> q3	_Parm2	0.56323	0.42803	1.31587		
q3 ==> q4	_Parm3	1.03924	0.50506	2.05765		
Variance Parameters						
Variance Type	Variable	Parameter	Estimate	Standard Error	t Value	
Exogenous Error	q1	_Add1	0.33830	0.13269	2.54951	
	q2	_Add2	0.22466	0.08812	2.54951	
	q3	_Add3	0.53506	0.20987	2.54951	
	q4	_Add4	2.01067	0.78865	2.54951	

Constrained Indirect Effects Model for the Sales Data

In the preceding *indirect effects* model, some path effects are not significant. In the current model, all the path effects are constrained to be equal. The following path diagram represents the *constrained indirect effects* model:



Except for one notable difference, this path diagram is the same as the path diagram for the preceding *indirect effects* model. The current path diagram labels all the paths with the same name (gamma) to signify that they are the same parameter. You can specify this *constrained indirect effects* model with this chosen constraint on the path effects by the using following statements:

```

proc calis data=sales;
  path   q1  ==> q2    = gamma,
        q2  ==> q3    = gamma,
        q3  ==> q4    = gamma;
run;

```

In the PATH statement, append an equal sign and a parameter name gamma in each of the path entries. This specification means that all the associated path effects are the same parameter named gamma.

Output 27.7.7 shows some fit indices for the *constrained indirect effects* model. Again, the model fit chi-square statistic is not significant. However, the SRMR is 0.2115, which is too large to accept as a good model. The RMSEA is 0.0499, which still indicates a good model fit. The AIC, CAIC, and SBC values are a bit smaller than those of the preceding unconstrained *indirect effects* model. Therefore, it seems that constraining the path effects leads to a slightly better model.

Output 27.7.7 Model Fit of the Constrained Indirect Effects Model for the Sales Data

Fit Summary	
Chi-Square	5.1619
Chi-Square DF	5
Pr > Chi-Square	0.3964
Standardized RMR (SRMR)	0.2115
RMSEA Estimate	0.0499
Akaike Information Criterion	15.1619
Bozdogan CAIC	23.3572
Schwarz Bayesian Criterion	18.3572

Output 27.7.8 shows the parameter estimates of the *constrained indirect effects* model. Again, all variance and error variance estimates are significant, and all path effects are not significant. The effect estimate is 0.24 (standard error=0.19, $t = 1.25$).

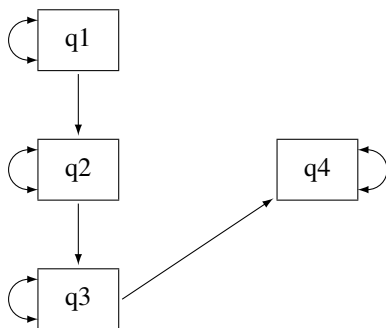
Output 27.7.8 Parameter Estimates of the Constrained Indirect Effects Model for the Sales Data

PATH List					
-----Path-----	Parameter	Estimate	Standard Error	t Value	
q1 ==> q2	gamma	0.24014	0.19152	1.25390	
q2 ==> q3	gamma	0.24014	0.19152	1.25390	
q3 ==> q4	gamma	0.24014	0.19152	1.25390	
Variance Parameters					
Variance Type	Variable	Parameter	Estimate	Standard Error	t Value
Exogenous	q1	_Add1	0.33830	0.13269	2.54951
Error	q2	_Add2	0.24407	0.09573	2.54951
	q3	_Add3	0.55851	0.21907	2.54951
	q4	_Add4	2.39783	0.94051	2.54951

Constrained Indirect Effects and Error Variances Model for the Sales Data

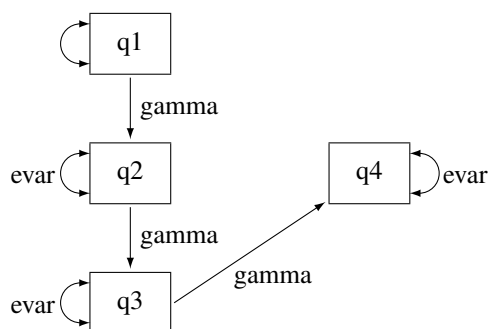
In addition to constraining all the path effects in the preceding model, the current model constrains all the error variances. Before using a path diagram to represent the current constrained indirect effects and constrained error variances, it is important to realize that you have not manually defined variances and covariances in the path diagrams for all of the preceding models. The default parameterization in PROC CALIS defined those parameters.

Represent the variances and covariances in a path diagram with double-headed arrows. When a double-headed arrow points to a single variable, it represents the variance parameter. When a double-headed arrow points to two distinct variables, it represents the covariance between the two variables. Consider the unconstrained *indirect effects* model for the sales data as an example. A more complete path diagram representation is as follows:



In this path diagram, a double-headed arrow on each variable represents variance or error variance. For q1, the double-headed arrow represents the variance parameter of q1. For other variables, the double-headed arrows represent error variances because those variables are endogenous (that is, they are predicted from other variables) in the model.

In order to represent the equality-constrained parameters in the model, you can put parameter names in the respective parameter locations in the path diagram. For the current *constrained indirect effects and error variances* model, you can represent the model by the following path diagram:



In the path diagram, label all the path effects by the parameter gamma and all error variances by the parameter evar. The double-headed arrow attached to q1 is not labeled by any name. This means that it is an unnamed free parameter in the model.

You can transcribe the path diagram into the following statements:

```
proc calis data=sales;
  path   q1   ==> q2       = gamma,
         q2   ==> q3       = gamma,
         q3   ==> q4       = gamma;
  pvar   q2 q3 q4 = 3 * evar;
run;
```

The specification in the PATH statement is the same as the preceding PATH model specification for the *constrained indirect effects* model. The new specification here is the PVAR statement. You use the PVAR statement to specify partial variances, which include the (total) variances of exogenous variables and the error variances of the endogenous variables. In the PVAR statement, you specify the variables for which you intend to define variances. If you do not specify anything after the list of variables, the variances of these variables are unnamed free parameters. If you put an equal sign after the variable lists, you can specify parameter names, initial values, or fixed parameters for the variances of the variables. See the PVAR statement for details. In the current model, `3*evar` means that you want to specify `evar` three times (for the error variance parameters of `q2`, `q3`, and `q4`).

Note that you did not specify the variance of `q1` in the PVAR statement. This variance is a default parameter in the model, and therefore you do not need to specify it in the PVAR statement. Alternatively, you can specify it explicitly in the PVAR statement by giving it a parameter name. For example, you can specify the following:

```
pvar   q2 q3 q4 = 3 * evar,
       q1       = MyOwnName;
```

Or, you can specify it explicitly without giving it a parameter name, as shown in following statement:

```
pvar   q2 q3 q4 = 3 * evar,
       q1 ;
```

All these specifications lead to the same estimation results. The difference between the two specifications is the explicit parameter name for the variance of `q1`. Without putting `q1` in the PVAR statement, the variance parameter is named with the prefix `_Add`, which is generated as a default parameter by PROC CALIS. With the explicit specification of `q1`, the variance parameter is named `MyOwnName`. With the explicit specification of `q1`, but without giving it a parameter name in the PVAR statement, the variance parameter is named with the prefix `_Parm`, which PROC CALIS generates for unnamed free parameters.

Output 27.7.9 shows some fit indices for the *constrained indirect effects and error variances* model. The model fit chi-square is 19.7843, which is significant at the 0.05 α -level. In practice, the model fit chi-square statistic is not the only criterion for judging model fit. In fact, it might not even be the most commonly used criterion for measuring model fit. Other criteria such as the SRMR and RMSEA are more popular or important. Unfortunately, the values of these two fit indices do not support the current constrained model either. The SRMR is 1.5037 and the RMSEA is 0.3748. Both are much greater than the commonly accepted 0.05 criterion.

Output 27.7.9 Model Fit of the Constrained Indirect Effects and Error Variances Model for the Sales Data

Fit Summary	
Chi-Square	19.7843
Chi-Square DF	7
Pr > Chi-Square	0.0061
Standardized RMR (SRMR)	1.5037
RMSEA Estimate	0.3748
Akaike Information Criterion	25.7843
Bozdogan CAIC	30.7015
Schwarz Bayesian Criterion	27.7015

The AIC, CAIC, and SBC values are all much greater than those of the preceding *constrained indirect effects* model. Therefore, constraining the error variances in addition to the constrained indirect effects does not lead to a better model.

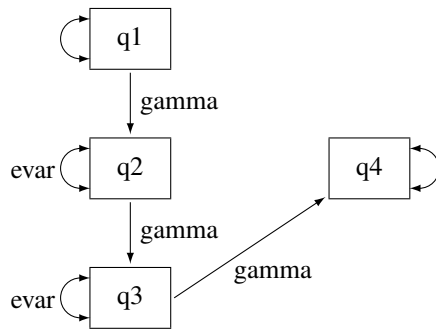
Output 27.7.10 shows the parameter estimates of the *constrained indirect effects and error variances* model. All estimates are significant in the model, which is often desirable. However, because of the bad model fit, this model is not acceptable.

Output 27.7.10 Parameter Estimates of the Constrained Indirect Effects and Error Variances Model for the Sales Data

PATH List						
-----Path-----	Parameter	Estimate	Standard Error	t Value		
q1 ==> q2	gamma	0.64733	0.16128	4.01368		
q2 ==> q3	gamma	0.64733	0.16128	4.01368		
q3 ==> q4	gamma	0.64733	0.16128	4.01368		
Variance Parameters						
Variance Type	Variable	Parameter	Estimate	Standard Error	t Value	
Error	q2	evar	1.00220	0.22695	4.41588	
	q3	evar	1.00220	0.22695	4.41588	
	q4	evar	1.00220	0.22695	4.41588	
Exogenous	q1	_Add1	0.33830	0.13269	2.54951	

Partially Constrained Model for the Sales Data

In the preceding model, constraining all error variances to be same shows that the model fit is unacceptable, even though all parameter estimates are significant. Relaxing those constraints a little might improve the model. The following path diagram represents such a *partially constrained* model:



The only difference between the current *partially constrained* model and the preceding *constrained indirect effects and error variances* model is that the error variance for q4 is no longer constrained to be equal to the error variances of q2 and q3. In the path diagram, `evar` is no longer attached to the double-headed arrow that is associated with the error variance of q4. You can transcribe this path diagram representation into the following PATH model specification:

```

proc calis data=sales;
  path   q1  ==> q2      = gamma,
         q2  ==> q3      = gamma,
         q3  ==> q4      = gamma;
  pvar   q2 q3 = 2 * evar,
         q4 q1;
run;

```

Now, the PVAR statement has only the error variances of q2 and q3 constrained to be equal. The error variance of q4 and the variance of q1 are free parameters without constraints.

Output 27.7.11 shows some fit indices for the *partially constrained* model. The chi-square model fit test statistic is not significant. The SRMR is 0.3877 and the RMSEA is 0.1164. These are far from the conventional acceptance level of 0.05. However, the AIC, CAIC, and SBC values are all slightly smaller than the *constrained indirect effects* model, as shown in Output 27.7.7. In fact, these information-theoretic fit indices suggest that the *partially constrained* model is the best model among all models that have been considered.

Output 27.7.11 Model Fit of the Partially Constrained Model for the Sales Data

Fit Summary	
Chi-Square	7.0575
Chi-Square DF	6
Pr > Chi-Square	0.3156
Standardized RMR (SRMR)	0.3877
RMSEA Estimate	0.1164
Akaike Information Criterion	15.0575
Bozdogan CAIC	21.6138
Schwarz Bayesian Criterion	17.6138

Output 27.7.12 shows the parameter estimates of the *partially constrained* model. Again, all variance and error variance parameters are statistically significant. However, the path effects are only marginally significant.

Output 27.7.12 Parameter Estimates of the Partially Constrained Model for the Sales Data

PATH List						
-----Path-----		Parameter	Estimate	Standard Error	t Value	
q1	====>	q2	gamma	0.35546	0.18958	1.87497
q2	====>	q3	gamma	0.35546	0.18958	1.87497
q3	====>	q4	gamma	0.35546	0.18958	1.87497
Variance Parameters						
Variance Type	Variable	Parameter	Estimate	Standard Error	t Value	
Error	q2	evar	0.40601	0.11261	3.60555	
	q3	evar	0.40601	0.11261	3.60555	
	q4	_Parm1	2.29415	0.89984	2.54951	
Exogenous	q1	_Parm2	0.33830	0.13269	2.54951	

Which Model Should You Choose?

You fit various models in this example for the sales data. The fit summary of the models is shown in the following table:

	1	2	3	4	5	6
	Saturated	Direct and Indirect Effects	Indirect Effects	Constrained Indirect Effects	Constrained Indirect Effects and Error Variances	Partially Constrained
<i>df</i>	0	1	3	5	7	6
<i>p</i> -value	.	0.76	0.74	0.40	0.01	0.32
SRMR	0	0.03	0.09	0.21	1.50	0.39
RMSEA	.	0.00	0.00	0.05	0.37	0.12
AIC	20.00	18.09	15.24	15.16	25.78	15.06
CAIC	36.39	32.84	26.71	23.36	30.70	21.61
SBC	26.39	23.84	19.71	18.36	27.70	17.61

As discussed previously, the model fit chi-square test statistic always favors models with a lot of parameters. It does not take model parsimony into account. In particular, a saturated model (Model 1) always has a perfect fit. However, it does not explain the data in a concise way. Therefore, the model fit chi-square statistic is not used here for comparing the competing models.

The standardized root mean square residual (SRMR) also does not take the model parsimony into account. It tells you how the fitted covariance matrix is different from the observed covariance matrix in a certain

standardized way. Again, it always favors models with a lot of parameters. As shown in the preceding table, the more parameters (the fewer degrees of freedom) the model has, the smaller the SRMR is. A conventional criterion is to accept a model with SRMR less than 0.05. Applying this criterion, only the saturated model (Model 1) and the *direct and indirect effects* (Model 2) models are acceptable. The *indirect effects* model (Model 3) is marginally acceptable.

The root mean square error of approximation (RMSEA) fit index does take model parsimony into account. With the ‘RMSEA less than 0.05 criterion’, the *constrained indirect effects and error variances* model (Model 5) and the *partially constrained* model (Model 6) are not acceptable.

The information-theoretic fit indices such as the AIC, CAIC, and SBC also take model parsimony into account. All of these indices point to the *partially constrained* model (Model 6) as the best model among the competing models. However, because this model has a relatively bad absolute fit, as indicated by the large SRMR value (0.39), accepting this model is questionable. In addition, the information-theoretic fit indices of the *indirect effects* model (Model 3) and of the *constrained indirect effects* model (Model 4) are not too different from those of the *partially constrained* model (Model 6). The indirect effects model is especially promising because it has relatively small SRMR and RMSEA values. The drawback is that some path effect estimates in the indirect effects model are not significant. Perhaps collecting and analyzing more data might confirm these promising models with significant path effects.

You might not be able to draw a unanimous conclusion about the best model for the sales data of this example. Different fit indices in structural equation modeling do not always point to the same conclusions. The analyses in the current example show some of the complexity of structural equation modeling. Some interesting questions about model selections are:

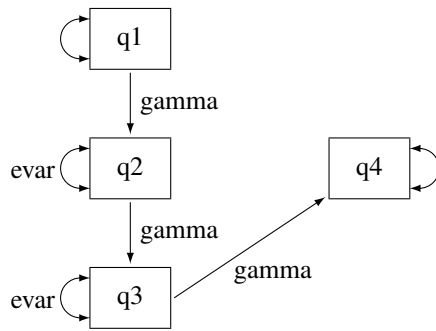
- Do you choose a model based on a single fit criterion? Or, do you consider a set of model fit criteria to weigh competing models?
- Which fit index criterion is the most important for judging model fit?
- In selecting your “best” model, how do you take “chance” into account?
- How would you use your substantive theory to guide your model search?

The answers to these interesting research questions might depend on the context. Nonetheless, PROC CALIS can help you in the model selection process by computing various kinds of fit indices. (Only a few of these fit indices are shown in the output of this example. See the [FITINDEX](#) statement for a wide variety of fit indices that you can obtain from PROC CALIS.)

Alternative PATH Model Specifications for Variances and Covariances

The PATH modeling language of PROC CALIS is designed to map the path diagram representation into the PATH statement syntax efficiently. For any path that is denoted by a single-headed arrow in the path diagram, you can specify a path entry in the PATH statement. You can also specify double-headed arrows in the PATH statement.

Consider the preceding path diagram for the *partially constrained* model for the sales data. You use double-headed arrows to denote variances or error variances of the variables. The path diagram is shown in the following:



As discussed previously, you can use the PVAR statement to specify these variances or error variances as in following syntax:

```
pvar  q2 q3 = 2 * evar,
      q4 q1;
```

Alternatively, you can specify these double-headed arrows directly as paths in the PATH statement, as shown in the following statements:

```
proc calis data=sales;
  path  q1  ==> q2      = gamma,
        q2  ==> q3      = gamma,
        q3  ==> q4      = gamma,
        <==> q2 q3      = 2 * evar,
        <==> q4 q1;
run;
```

To specify the double-headed paths pointing to individual variables, you begin with the double-headed arrow notation `<==>`, followed by the list of variables. For example, in the preceding specification, the error variance of q4 and the variance of q1 are specified in the last path entry of the PATH statement. If you want to define the parameter names for the variances, you can add a parameter list after an equal sign in the path entries. For example, the error variances of q2 and q3 are denoted by the free parameter `evar` in a path entry in the PATH statement.

Alternatively, you can specify the double-headed arrow paths literally in a PATH statement, as shown in the following equivalent specification:

```
proc calis data=sales;
  path  q1  ==> q2      = gamma,
        q2  ==> q3      = gamma,
        q3  ==> q4      = gamma,
        q2  <==> q2      = evar,
        q3  <==> q3      = evar,
        q4  <==> q4,
        q1  <==> q1;
run;
```

For example, the path entry `q1 <==> q1` specifies the variance of q1. It is an unnamed free parameter in the model.

Output 27.7.13 show the parameter estimates for this alternative specification method. All these estimates match exactly those with the PVAR statement specification, as shown in Output 27.7.12. The only difference is that all estimation results are now presented under one PATH List, as shown in Output 27.7.13, instead of as two tables as shown in Output 27.7.12.

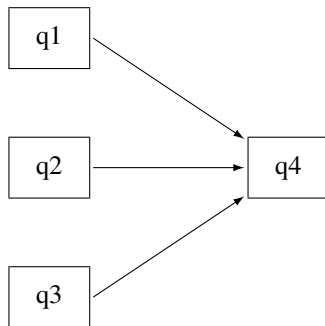
Output 27.7.13 Path Estimates of the Partially Constrained Model for the Sales Data

PATH List						
-----Path-----	Parameter	Estimate	Standard Error	t Value		
q1 ==> q2	gamma	0.35546	0.18958	1.87497		
q2 ==> q3	gamma	0.35546	0.18958	1.87497		
q3 ==> q4	gamma	0.35546	0.18958	1.87497		
q2 <==> q2	evar	0.40601	0.11261	3.60555		
q3 <==> q3	evar	0.40601	0.11261	3.60555		
q4 <==> q4	_Parm1	2.29415	0.89984	2.54951		
q1 <==> q1	_Parm2	0.33830	0.13269	2.54951		

The double-headed arrow path syntax applies to covariance specification as well. For example, the following PATH statement specifies the covariances among variables x1–x3:

```
path    x2 <==> x1,
        x3 <==> x1,
        x3 <==> x2;
```

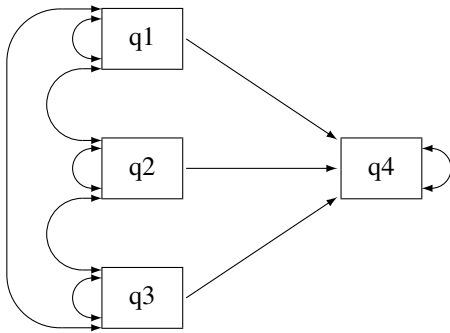
In the beginning of the current example, you use the following path diagram to represent the multiple regression model for the sales data:



The following statements specify the multiple regression model:

```
proc calis data=sales;
  path    q1 q2 q3 ==> q4;
run;
```

You do not represent the covariances and variances among the exogenous variables explicitly in the path diagram, nor in the PATH statement specification. However, PROC CALIS generates them as free parameters by default. Some researchers might prefer to represent the exogenous variances and covariances explicitly in the path diagram, as shown in the following path diagram:



In the path diagram, there are three single-head arrows and seven double-headed arrows. These 10 paths represent the 10 parameters in the covariance structure model. To represent all these parameters in the PATH model specification, you can use the following statements:

```

proc calis data=sales;
  path   q1   ==>  q4   ,
         q2   ==>  q4   ,
         q3   ==>  q4   ,
         q1   <==> q1   ,
         q2   <==> q2   ,
         q3   <==> q3   ,
         q1   <==> q2   ,
         q2   <==> q3   ,
         q1   <==> q3   ,
         q4   <==> q4   ;
run;
  
```

The first three path entries in the PATH statement reflect the single-headed paths in the path diagram. The next six path entries in the PATH statement reflect the double-headed paths among the exogenous variables q1–q3 in the path diagram. The last path entry in the PATH statement reflects the double-headed path attached to the endogenous variable q4 in the path diagram. With this specification, the parameter estimates for the multiple regression model are all shown in [Output 27.7.14](#).

Output 27.7.14 Path Estimates of the Multiple Regression Model for the Sales Data

PATH List						
-----Path-----	Parameter	Estimate	Standard Error	t Value		
q1 ==> q4	_Parm01	0.55980	0.64938	0.86205		
q2 ==> q4	_Parm02	0.58946	0.84558	0.69711		
q3 ==> q4	_Parm03	0.88290	0.51635	1.70988		
q1 <==> q1	_Parm04	0.33830	0.13269	2.54951		
q2 <==> q2	_Parm05	0.22466	0.08812	2.54951		
q3 <==> q3	_Parm06	0.60633	0.23782	2.54951		
q1 <==> q2	_Parm07	0.0001978	0.07646	0.00259		
q2 <==> q3	_Parm08	0.12653	0.10821	1.16931		
q1 <==> q3	_Parm09	0.03610	0.12601	0.28649		
q4 <==> q4	_Parm10	1.84128	0.72221	2.54951		

These estimates are the same as those in [Output 27.7.2](#), where the estimates are shown in three different tables, instead of in one table for all paths as in [Output 27.7.14](#).

Sometimes, specification of some single-headed and double-headed paths can become very laborious. Fortunately, PROC CALIS provides shorthand notation for the PATH statement to make the specification more efficient. For example, a more concise way to specify the preceding multiple regression model is shown in the following statements:

```
proc calis data=sales;
  path   q1 q2 q3 ==> q4 ,
        <==> [q1-q3] ,
        <==> q4 ;
run;
```

The first path entry `q1 q2 q3 ==> q4` in the PATH statement represents the three single-headed arrows in the path diagram. The second path entry `<==> [q1-q3]` generates the variances and covariances for the set of variables specified in the rectangular brackets. The last path entry represents the error variance of `q4`. Consequently, expanding the preceding shorthand specification generates the following specification:

```
proc calis data=sales;
  path   q1   ==> q4 ,
        q2   ==> q4 ,
        q3   ==> q4 ,
        q1 <==> q1 ,
        q2 <==> q1 ,
        q2 <==> q2 ,
        q3 <==> q1 ,
        q3 <==> q2 ,
        q3 <==> q3 ,
        q4 <==> q4 ;
run;
```

Notice that the third through ninth path entries correspond to the lower triangular elements of the covariance matrix for `q1-q3`.

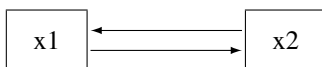
CAUTION: The double-headed path specification does *not* represent a reciprocal relationship. That is, the following statement specifies the covariance between `x2` and `x1`:

```
path   x2 <==> x1,
```

But the following statement specifies that `x2` and `x1` have reciprocal causal effects:

```
path   x2 <==> x1,
        x1 ==> x2;
```

The reciprocal causal effects specification reflects the following path diagram:



Example 27.8: Measurement Error Models

In this example, you use PROC CALIS to fit some measurement error models. You use latent variables to define “true” scores variables that are measured without errors. You constrain parameters by using parameter names or fixed values in the PATH model specification.

Consider a simple linear regression model with dependent variable y and predictor variable x . The path diagram for this simple linear regression model is depicted as follows:



Suppose you have the following SAS data set for the regression analysis of y on x :

```

data measures;
  input x y @@;
  datalines;
  7.91736 13.8673 6.10807 11.7966 6.94139 12.2174
  7.61290 12.9761 6.77190 11.6356 6.33328 11.7732
  7.60608 12.8040 6.65642 12.8866 6.26643 11.9382
  7.32266 13.2590 5.76977 10.7654 5.62881 11.5041
  7.57418 13.2502 7.17305 13.3416 8.23123 13.9876
  7.17199 13.1750 8.04604 14.5968 5.77692 11.5077
  5.72741 11.3299 6.66033 12.5159 7.14944 12.4988
  7.51832 12.3588 5.48877 11.2211 7.50323 13.3735
  7.15814 13.1556 7.35485 13.8457 8.91648 14.4929
  5.37445 9.6366 6.00419 11.7654 6.89546 13.1493
  ;
  
```

This data set contains 30 observations for the x and y variables. You can fit the simple linear regression model to the measures data by the PATH model specification of PROC CALIS, as shown in the following statements:

```

proc calis data=measures;
  path
    x ==> y;
run;
  
```

Output 27.8.1 shows that the regression coefficient estimate (denoted as `_Parm1` in the PATH List) is 1.1511 (standard error = 0.1002).

Output 27.8.1 Estimates of the Linear Regression Model for the Measures Data

PATH List					
-----Path-----	Parameter	Estimate	Standard Error	t Value	
x ==> y	_Parm1	1.15112	0.10016	11.49241	

Output 27.8.1 continued

Variance Parameters					
Variance Type	Variable	Parameter	Estimate	Standard Error	t Value
Exogenous	x	_Add1	0.79962	0.20999	3.80789
Error	y	_Add2	0.23265	0.06110	3.80789

You can also do the simple linear regression by PROC REG by the following statement:

```
proc reg data=measures;
  model y = x;
run;
```

Output 27.8.2 shows that PROC REG essentially gives the same regression coefficient estimate with a similar standard error estimate. The discrepancy in the standard error estimates produced by the two procedures is due to the different variance divisors in computing standard errors in the two procedures. But the discrepancy is negligible when the sample size becomes large.

Output 27.8.2 PROC REG Estimates of the Linear Regression Model for the Measures Data

Parameter Estimates					
Variable	DF	Parameter Estimate	Standard Error	t Value	Pr > t
Intercept	1	4.62455	0.70790	6.53	<.0001
x	1	1.15112	0.10194	11.29	<.0001

There are two main differences between PROC CALIS and PROC REG regarding the parameter estimation results. First, PROC CALIS does not give the estimate of the intercept because by default PROC CALIS analyzes only the covariance structures. Therefore, it does not estimate the intercept. To obtain the intercept estimate, you can add the MEANSTR option in the PROC CALIS statement, as is shown in Example 27.9. Second, in Output 27.8.1 of PROC CALIS, the variance estimate of x and the error variance estimate of y are shown. The corresponding results are not shown as parameter estimates in the PROC REG results. In PROC CALIS, these two variances are model parameters in covariance structure analysis. PROC CALIS adds these variances as default parameters. You can also represent these two variance parameters by double-headed arrows in the path diagram, as shown in the following:



The two double-headed arrows attached to x and y represent the variances. Although it is not necessary to specify these default parameters, you can use the PVAR statement to specify them explicitly, as shown in the following statements:

```

proc calis data=measures meanstr;
  path
    x ==> y;
  pvar
    x y;
run;

```

In the PROC CALIS statement, you specify the MEANSTR option to request the analysis of mean structures together with covariance structures. [Output 27.8.3](#) shows the estimation results.

Output 27.8.3 Estimates of the Measurement Error Model with Error in x

PATH List					
-----Path-----	Parameter	Estimate	Standard Error	t Value	
x ==> y	_Parm1	1.15112	0.10016	11.49241	
Variance Parameters					
Variance Type	Variable	Parameter	Estimate	Standard Error	t Value
Exogenous	x	_Parm2	0.79962	0.20999	3.80789
Error	y	_Parm3	0.23265	0.06110	3.80789
Means and Intercepts					
Type	Variable	Parameter	Estimate	Standard Error	t Value
Intercept	y	_Add1	4.62455	0.69578	6.64658
Mean	x	_Add2	6.88865	0.16605	41.48504

The regression coefficient estimate and the variance estimates are the same as those in [Output 27.8.1](#). However, in [Output 27.8.3](#), there is an additional table for the mean and intercept estimates. The intercept estimate for y is 4.6246 (standard error=0.6958), which match closely to the results obtained from PROC REG, as shown in [Output 27.8.2](#).

Measurement Error in x

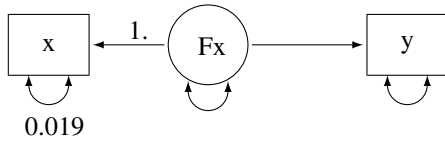
PROC CALIS can also handle more complicated regression situations where the variables are measured with errors. This is beyond the application of PROC REG.

Suppose that the predictor variable x is measured with error and from prior studies you know that the size of the measurement error variance is about 0.019. You can use PROC CALIS to incorporate this information into the model. First, think of the measured variable x as composed of two components: one component is the “true” score measure F_x and the other is the measurement error e_1 . Both of these components are not

observed (that is, latent) but they sum up to yield x . That is,

$$x = Fx + e1$$

Because x is contaminated with measurement error, what you are interested in knowing is the regression effect of the true score Fx on x . The following path diagram represents this regression scenario:



In path diagrams, latent variables are usually represented by circles or ovals, while observed variables are represented by rectangles. In the current path diagram, Fx is a latent variable and is represented by a circle. The other two variables are observed variables and are represented by rectangles. There are five arrows in the path diagram. Two of them are single-headed arrows that represent functional relationships, while the other three are double-headed arrows that represent variances or error variances. Two paths are labeled with fixed values. The path effect from Fx to x is fixed at 1, as assumed in the measurement error model. The error variance for measuring x is fixed at 0.019 due to the prior knowledge about the measurement error variance. The remaining three arrows represent free parameters in the model: the regression coefficient of y on Fx , the variance of Fx , and the error variance of y . The following statements specify the model for this path diagram:

```
proc calis data=measures;
  path
    x <=== Fx = 1.,
    Fx ==> y;
  pvar
    x = 0.019,
    Fx, y;
run;
```

You specify all the single-headed paths in the PATH statement and all the double-headed arrows in the PVAR statement. For paths with fixed values, you put the equality at the back of the specifications to tell PROC CALIS about the fixed values. For example, the path coefficient in the path $x <=== Fx$ is fixed at 1 and the error variance for x is fixed at 0.019. All other specifications represent unnamed free parameters in the model.

Output 27.8.4 shows the estimation results. The effect of Fx on y is 1.1791 (standard error=0.1029). This effect is slightly greater than the corresponding effect (1.1511) of x on y in the preceding model where the measurement error of x has not been taken into account, as shown in Output 27.8.3.

Output 27.8.4 Estimates of the Measurement Error Model with Error in x

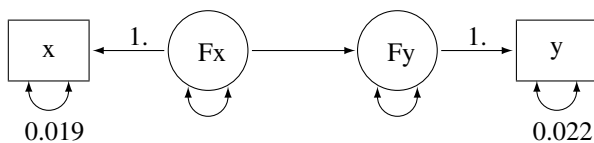
PATH List					
-----Path-----	Parameter	Estimate	Standard Error	t Value	
x <=== Fx		1.00000			
Fx ==> y	_Parm1	1.17914	0.10288	11.46153	

Output 27.8.4 continued

Variance Parameters					
Variance Type	Variable	Parameter	Estimate	Standard Error	t Value
Error	x		0.01900		
Exogenous	Fx	_Parm2	0.78062	0.20999	3.71741
Error	y	_Parm3	0.20686	0.06126	3.37667

Measurement Errors in x and y

Measurement error can occur in the y variable too. Suppose that both x and y are measured with errors. From prior studies, the measurement error variance of x is known to be 0.019 (as in the preceding modeling scenario) and the measurement error variance of y is known to be 0.022. The following path diagram represents the current modeling scenario:



In the current path diagram the true score variable Fy and its measurement indicator y have the same kind of relationship as the relationship between the true score variable Fx and its measurement indicator x in the previous description. The error variance for measuring y is treated as a known constant 0.022. You can transcribe this path diagram easily to the following PROC CALIS specification:

```

proc calis data=measures;
  path
    x <=== Fx = 1.,
    Fx ===> Fy ,
    Fy ===> y = 1.;
  pvar
    x = 0.019,
    y = 0.022,
    Fx Fy;
run;

```

Again, you specify all the single-headed paths in the PATH statement and the double-headed paths in the PVAR statement. You provide the fixed parameter values by appending the required equalities after the individual specifications.

Output 27.8.5 shows the estimation results of the model with measurement errors in both x and y. The effect of Fx on Fy is 1.1791 (standard error=0.1029). This is essentially the same effect of Fx on y as in the preceding measurement model in which no measurement error in y is assumed.

Output 27.8.5 Estimates of the Measurement Error Model with Errors in x and y

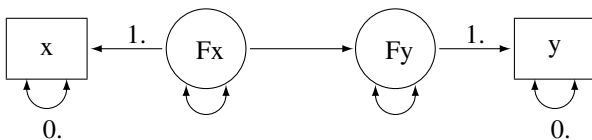
PATH List					
-----Path-----	Parameter	Estimate	Standard Error	t Value	
x <=== Fx		1.00000			
Fx ==> Fy	_Parm1	1.17914	0.10288	11.46153	
Fy ==> y		1.00000			

Variance Parameters					
Variance Type	Variable	Parameter	Estimate	Standard Error	t Value
Error	x		0.01900		
	y		0.02200		
Exogenous Error	Fx	_Parm2	0.78062	0.20999	3.71741
	Fy	_Parm3	0.18486	0.06126	3.01755

The estimated error variance for Fy in the current model is 0.1849 and the measurement error variance of y is fixed at 0.022, as shown in the last table of [Output 27.8.5](#). The sum is 0.2069, which is the same amount of error variance for y in the preceding model with measurement error assumed only in x. Hence, the assumption of the measurement error in y does not change the structural effect of Fx on y (same amount of effect Fx on Fy, which is 1.1791). It only changes the variance components of y. In the preceding model with measurement error assumed only in x, the total error variance in y is 0.2069. In the current model, this total error variance is partitioned into the measurement error variance (which is fixed at 0.022) and the error variance in the regression on Fx (which is estimated at 0.1849).

Linear Regression Model as a Special Case of Structural Equation Model

By using the current measurement error model as an illustration, it is easy to see that the structural equation model is a more general model that includes the linear regression model as a special case. If you restrict the measurement error variances in x and y to zero, the measurement error model (which represents the structural equation model in this example) reduces to the linear regression model. That is, the path diagram becomes:



You can then specify the PATH model by the following statements:

```

proc calis data=measures;
  path
    x <=== Fx = 1.,
    Fx ==> Fy ,
    Fy ==> y = 1.;
  pvar

```



```

x = 0.,
y = 0.,
Fx Fy;
run;

```

Output 27.8.6 shows the estimation results of this measurement error model with zero measurement errors. The estimate of the regression coefficient is 1.1511, which is essentially the same result as in Output 27.8.2 by using PROC REG.

Output 27.8.6 Estimates of the Measurement Error Model with Zero Measurement Errors

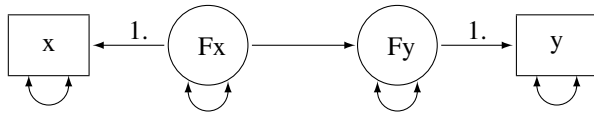
PATH List					
-----Path-----	Parameter	Estimate	Standard Error	t Value	
x <==== F _x		1.00000			
F _x ==> F _y	_Parm1	1.15112	0.10016	11.49241	
F _y ==> y		1.00000			
Variance Parameters					
Variance Type	Variable	Parameter	Estimate	Standard Error	t Value
Error	x		0		
	y		0		
Exogenous Error	F _x	_Parm2	0.79962	0.20999	3.80789
	F _y	_Parm3	0.23265	0.06110	3.80789

This example shows that you can apply PROC CALIS to fit measurement error models. You treat true scores variables as latent variables in the structural equation model. The linear regression model is a special case of the structural equation model (or measurement error model) where measurement error variances are assumed to be zero. Structural equation modeling by PROC CALIS is not limited to this simple modeling scenario. PROC CALIS can treat more complicated measurement error models. In Example 27.9 and Example 27.10, you fit measurement error models with parameter constraints and with more than one predictor. You can also fit measurement error models with correlated errors.

Example 27.9: Testing Specific Measurement Error Models

In Example 27.8, you used the PATH modeling language of PROC CALIS to fit some basic measurement error models. In this example, you continue to fit the same kind of measurement error models but you restrict some model parameters to test some specific hypotheses.

This example uses the same data set as is used in [Example 27.8](#). This data set contains 30 observations for the x and y variables. The general measurement error model with measurement errors in both x and y is shown in the following path diagram:

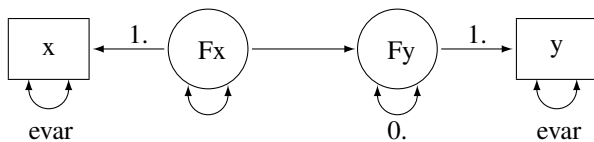


In the path diagram, two paths are fixed with a path coefficient of 1. They are required in the model for representing the relationships between true scores (latent) and measured indicators (observed). In [Example 27.8](#), you consider several different modeling scenarios, all of which require you to make some parameter restrictions to estimate the models. You fix the measurement error variances to certain values that are based on prior knowledge or studies. Without those fixed error variances, those models would have been overparameterized and the parameters would not have been estimable.

For example, in the current path diagram, five of the single- or double-headed paths are not labeled with fixed numbers. Each of these paths represents a free parameter in the model. However, in the covariance structure model analysis, you fit these free parameters to the three nonredundant elements of the sample covariance matrix, which is a 2×2 symmetric matrix. Hence, to have an identified model, you can at most have three free parameters in your covariance structure model. However, the path diagram shows that you have five free parameters in the model. You must introduce additional parameter constraints to make the model identified.

If you do not have prior knowledge about the measurement error variances (as those described in [Example 27.8](#)), then you might need to make some educated guesses about how to restrict the overparameterized model. For example, if x and y are of the same kind of measurements, perhaps you can assume that they have an equal amount of measurement error variance. Furthermore, if the measurement errors have been taken into account, in some physical science studies you might be able to assume that the relationship between the true scores F_x and F_y is almost deterministic, resulting in a near zero error variance of F_y .

The assumptions here are not comparable to prior knowledge or studies about the measurement error variances. If you suppose they are reasonable enough in a particular field, you can use these assumptions to give you an identified model to work with (at least as an exploratory study) when the required prior knowledge is lacking. The following path diagram incorporates these two assumptions in the measurement error model:



In the path diagram, you use *evar* to denote the error variances of x and y . This implicitly constrains the two error variances to be equal. The error variance of F_y is labeled zero, indicating a fixed parameter value and a deterministic relationship between x and y . You can transcribe this path diagram into the following PATH modeling specification:

```

proc calis data=measures;
  path
    x <=== Fx = 1.,
    Fx ===> Fy ,
    Fy ===> y = 1.;
  pvar
    x = evar,
    y = evar,
    Fy = 0.,
    Fx;
run;

```

In the PVAR statement, you specify the same parameter name `evar` for the error variances of `x` and `y`. This way their estimates are constrained to be the same in the estimation. In addition, the error variance for `Fy` is fixed at zero, which reflects the “near-deterministic” assumption about the relationship between `Fx` and `Fy`. These two assumptions effectively reduce the overparameterized model by two parameters so that the new model is just-identified and estimable.

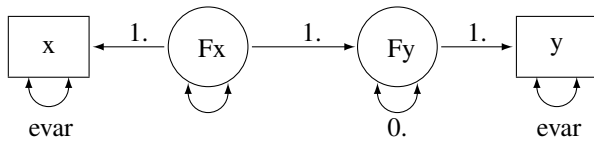
Output 27.9.1 shows the estimation results. The estimated effect of `Fx` on `Fy` is 1.3028 (standard error = 0.1134). The measurement error variances for `x` and `y` are both estimated at 0.0931 (standard error = 0.0244).

Output 27.9.1 Estimates of the Measurement Error Model with Equal Measurement Error Variances

PATH List					
-----Path-----	Parameter	Estimate	Standard Error	t Value	
x <=== Fx		1.00000			
Fx ===> Fy	_Parm1	1.30275	0.11336	11.49241	
Fy ===> y		1.00000			
Variance Parameters					
Variance Type	Variable	Parameter	Estimate	Standard Error	t Value
Error	x	evar	0.09307	0.02444	3.80789
	y	evar	0.09307	0.02444	3.80789
	Fy		0		
Exogenous	Fx	_Parm2	0.70655	0.20962	3.37057

Testing the Effect of `Fx` on `Fy`

Suppose you are interested in testing the hypothesis that the effect of `Fx` on `Fy` (that is, the regression slope) is 1. The following path diagram represents the model under the hypothesis:



Now you label the path from Fx to Fy with a fixed constant 1, which reflects the hypothesis you want to test. You can transcribe the current path diagram easily into the following PROC CALIS specification:

```
proc calis data=measures;
  path
    x <=== Fx = 1.,
    Fx ===> Fy = 1., /* Testing a fixed constant effect */
    Fy ===> y = 1.;
  pvar
    x = evar,
    y = evar,
    Fy = 0.,
    Fx;
run;
```

Output 27.9.2 shows the model fit chi-square statistic. The model fit chi-square test here essentially is a test of the null hypothesis of the constant effect at 1 because the alternative hypothesis is a saturated model. The chi-square value is 8.1844 ($df = 1, p = .0042$), which is statistically significant. This means that the hypothesis of constant effect at 1 is rejected.

Output 27.9.2 Fit Summary for Testing Constant Effect

Fit Summary	
Chi-Square	8.1844
Chi-Square DF	1
Pr > Chi-Square	0.0042

Output 27.9.3 shows the estimates under this restricted model. In the first table of Output 27.9.3, all path effects or coefficients are fixed at 1. In the second table of Output 27.9.3, estimates of the error variances are 0.1255 (standard error = 0.0330) for both x and y. The error variance of Fy is a fixed zero, as required in the hypothesis. The variance estimate of Fx is 0.9205 (standard error = 0.2587).

Output 27.9.3 Estimates of Constant Effect Measurement Error Model

PATH List				
-----Path-----		Estimate	Standard Error	t Value
x	<=== Fx	1.00000		
Fx	===> Fy	1.00000		
Fy	===> y	1.00000		

Output 27.9.3 continued

Variance Parameters					
Variance Type	Variable	Parameter	Estimate	Standard Error	t Value
Error	x	evar	0.12545	0.03295	3.80789
	y	evar	0.12545	0.03295	3.80789
	Fy		0		
Exogenous	Fx	_Parm1	0.92046	0.25872	3.55771

Testing a Zero Intercept

Suppose you are interested in testing the hypothesis that the intercept for the regression of Fy on Fx is zero, while the regression effect is freely estimated. Because the intercept parameter belongs to the mean structures, you need to specify this parameter in PROC CALIS to test the hypothesis.

There are two ways to include the mean structure analysis. First, you can include the MEANSTR option in the PROC CALIS statement. Alternatively, you can use the MEAN statement to specify the means and intercepts in the model. The following statements specify the model under the zero intercept hypothesis:

```
proc calis data=measures;
  path
    x <=== Fx = 1.,
    Fx ==> Fy , /* regression effect is freely estimated */
    Fy ==> y = 1.;
  pvar
    x = evar,
    y = evar,
    Fy = 0.,
    Fx;
  mean
    x y = 0. 0., /* Intercepts are zero in the measurement error model */
    Fy = 0., /* Fixed to zero under the hypothesis */
    Fx; /* Mean of Fx is freely estimated */
run;
```

In the PATH statement, the regression effect of Fx on Fy is freely estimated. In the MEAN statement, you specify the means or intercepts of the variables. Each variable in your measurement error model has either a mean or an intercept (but not both) to specify. If a variable is exogenous (independent), you can specify its mean in the MEAN statement. Otherwise, you can specify its intercept in the MEAN statement. Variables x and y in the measurement error model are both endogenous. They are measured indicators of their corresponding true scores Fx and Fy. Under the measurement error model, their intercepts are fixed zeros. The intercept for Fy is zero under the current hypothesized model. The mean of Fx is freely estimated under the model. This parameter is specified in the MEAN statement but is not named.

Output 27.9.4 shows the model fit chi-square statistic. The chi-square value is 10.5397 ($df = 1, p = .0012$), which is statistically significant. This means that the zero intercept hypothesis for the regression of Fy on Fx is rejected.

Output 27.9.4 Fit Summary for Testing Zero Intercept

Fit Summary	
Chi-Square	10.5397
Chi-Square DF	1
Pr > Chi-Square	0.0012

Output 27.9.5 shows the estimates under the hypothesized model. The effect of Fx on Fy is 1.8169 (standard error = 0.0206). In the last table of Output 27.9.5, the estimate of the mean of Fx is 6.9048 (standard error = 0.1388). The intercepts for all other variables are fixed at zero under the hypothesized model.

Output 27.9.5 Estimates of the Zero Intercept Measurement Error Model

PATH List					
-----Path-----	Parameter	Estimate	Standard Error	t Value	
x <=== Fx		1.00000			
Fx ==> Fy	_Parm1	1.81689	0.02055	88.42473	
Fy ==> y		1.00000			
Variance Parameters					
Variance Type	Variable	Parameter	Estimate	Standard Error	t Value
Error	x	evar	0.13684	0.03594	3.80789
	y	evar	0.13684	0.03594	3.80789
	Fy		0		
Exogenous	Fx	_Parm2	0.42280	0.11990	3.52614
Means and Intercepts					
Type	Variable	Parameter	Estimate	Standard Error	t Value
Intercept	x		0		
	y		0		
	Fy		0		
Mean	Fx	_Parm3	6.90483	0.13881	49.74314

Measurement Model with Means and Intercepts Freely Estimated

In the preceding model, you fit a restricted regression model with a zero intercept. You reject the null hypothesis and conclude that this intercept is significantly different from zero. The alternative hypothesis is a saturated model with the intercept freely estimated. The model under the alternative hypothesis is specified in the following statements:

```

proc calis data=measures;
  path
    x <=== Fx = 1.,
    Fx ===> Fy ,
    Fy ===> y = 1.;
  pvar
    x = evar,
    y = evar,
    Fy = 0.,
    Fx;
  mean
    x y = 0. 0.,
    Fy Fx;
run;

```

Output 27.9.6 shows that model fit chi-square statistic is zero. This is expected because you are fitting a measurement error model with saturated mean and covariance structures.

Output 27.9.6 Fit Summary of the Saturated Measurement Model with Mean Structures

Fit Summary	
Chi-Square	0.0000
Chi-Square DF	0
Pr > Chi-Square	.

Output 27.9.7 shows the estimates under the measurement model with saturated mean and covariance structures. The effect of Fx on Fy is 1.3028 (standard error=0.1134), which is considerably smaller than the corresponding estimate in the restricted model with zero intercept, as shown in Output 27.9.5. The intercept estimate of Fy is 3.5800 (standard error = 0.7864), with a significant *t* value of 4.55.

Output 27.9.7 Estimates of the Saturated Measurement Model with Mean Structures

PATH List					
-----Path-----	Parameter	Estimate	Standard Error	t Value	
x <=== Fx		1.00000			
Fx ===> Fy	_Parm1	1.30275	0.11336	11.49241	
Fy ===> y		1.00000			
Variance Parameters					
Variance Type	Variable	Parameter	Estimate	Standard Error	t Value
Error	x	evar	0.09307	0.02444	3.80789
	y	evar	0.09307	0.02444	3.80789
	Fy		0		
Exogenous	Fx	_Parm2	0.70655	0.20962	3.37057

Output 27.9.7 *continued*

Means and Intercepts					
Type	Variable	Parameter	Estimate	Standard Error	t Value
Intercept	x		0		
	y		0		
Mean	Fy	_Parm3	3.57998	0.78641	4.55234
	Fx	_Parm4	6.88865	0.16605	41.48504

In this example, you fit some measurement error models with some parameter constraints that reflect the hypothesized models of interest. You can set equality constraints by simply providing the same parameter names in the PATH model specification of PROC CALIS. You can also fix parameters to constants. In the MEAN statement, you can specify the intercepts and means of the variables in the measurement error models. You can apply all these techniques to more complicated measurement error models with multiple predictors, as shown in [Example 27.10](#), where you also fit measurement error models with correlated errors.

Example 27.10: Measurement Error Models with Multiple Predictors

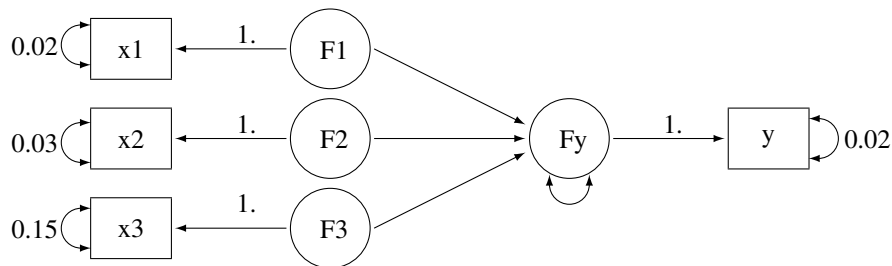
In [Example 27.8](#) and [Example 27.9](#), you fit various measurement error models with only one predictor. This example illustrates the case in which you have more than one predictor, all measured with errors. The measurement errors might also be correlated.

The data from 37 observations are summarized in a covariance matrix as shown in the following SAS DATA step:

```
data multiple(type=cov);
  input _type_ $ 1-4  _name_ $ 6-8 @10 y x1 x2 x3;
  datalines;
mean      0.93  1.33  1.34  4.11
cov y      1.31  .      .      .
cov x1     1.24  1.42  .      .
cov x2     0.21  0.18  1.15  .
cov x3     3.91  4.21  0.58  14.11
;
```

In this data set, four variables are measured. Variables x1–x3 are predictors of y. Instead of the raw data, you can input the sample covariance matrix in the form of a SAS data set for PROC CALIS to analyze.

You assume all of these variables in the data set are measured with errors. From prior studies, you establish the knowledge about the measurement errors of these variables. You create the true score counterparts for each of these variables in the same manner as you do in [Example 27.8](#) and [Example 27.9](#). The following path diagram represents your measurement error model for the data:



In the path diagram, variables F1–F3 and Fy are latent variables that represent the true score for the measured indicators x1–x3 and y, respectively. All paths from the true scores to the corresponding measured indicators are labeled with the fixed constant 1, as required by the measurement model. Each measured indicator is attached with a double-headed arrow that indicates the error variance. Because you have knowledge about these measurement error variances, you put fixed constant values adjacent to these double-headed arrows. For example, the measurement error variance of y is 0.02 and the measurement error variance of x3 is 0.15. The path diagram also indicates that the paths from F1–F3 to Fy and the error variance for Fy are free parameters to estimate in the model.

Notice that for brevity the variances and covariances among the three exogenous true score variables F1–F3 are not represented in the path diagram. These six variance and covariance parameters could have been represented by double-headed arrows in the path diagram. However, because PROC CALIS always assumes the exogenous variances and covariances as default model parameters, this information is not represented to reduce clutter in the path diagram.

You can transcribe the path diagram easily to the following PATH model specification:

```
proc calis data=multiple nobs=37;
  path
    Fy <=== F1 F2 F3,
    F1 ===> x1 = 1.,
    F2 ===> x2 = 1.,
    F3 ===> x3 = 1.,
    Fy ===> y = 1.;
  pvar
    x1 x2 x3 y = .02 .03 .15 .02,
    Fy;
run;
```

In the first entry of the PATH statement, you specify that F1–F3 predicts Fy. In the next four path entries you specify the measurement model for the true scores and how they are related to the observed variables. In the PVAR statement, you specify all the known measurement error variances for the observed variables. They are all fixed constants in the model. In the last entry in the PVAR statement, you specify the error variance of Fy as a free (unnamed) parameter. You could have omitted this entry because error variances for all endogenous variables in the PATH model are free parameters by default. Setting these default parameters explicitly as free parameters would not affect model fitting.

Output 27.10.1 shows the parameter estimates of the model. The path coefficient or effect from F2 to Fy is not significant, while the other two path coefficients are at least marginally significant.

Output 27.10.1 Parameter Estimates of the Measurement Model with Multiple Predictors

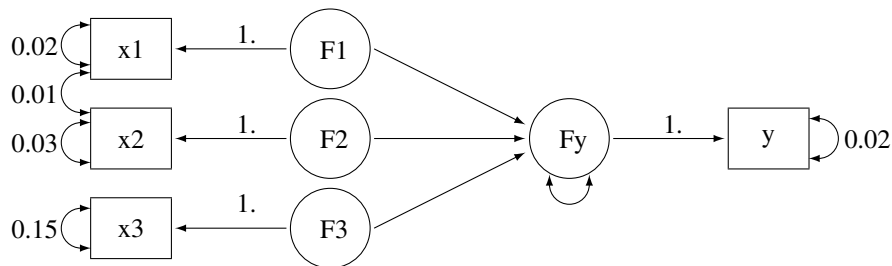
PATH List						
-----Path-----	Parameter	Estimate	Standard Error	t Value		
Fy <=== F1	_Parm1	0.46507	0.22682	2.05035		
Fy <=== F2	_Parm2	0.04123	0.07069	0.58323		
Fy <=== F3	_Parm3	0.13812	0.07175	1.92490		
F1 ===> x1		1.00000				
F2 ===> x2		1.00000				
F3 ===> x3		1.00000				
Fy ===> y		1.00000				

Variance Parameters						
Variance Type	Variable	Parameter	Estimate	Standard Error	t Value	
Error	x1		0.02000			
	x2		0.03000			
	x3		0.15000			
	y		0.02000			
	Fy	_Parm4	0.16461	0.04522	3.64028	
Exogenous	F1	_Add1	1.40000	0.33470	4.18289	
	F2	_Add2	1.12000	0.27106	4.13196	
	F3	_Add3	13.96000	3.32576	4.19754	

Covariances Among Exogenous Variables						
Var1	Var2	Parameter	Estimate	Standard Error	t Value	
F2	F1	_Add4	0.18000	0.21508	0.83688	
F3	F1	_Add5	4.21000	1.02416	4.11070	
F3	F2	_Add6	0.58000	0.67829	0.85509	

The second table of [Output 27.10.1](#) shows the variance estimates. As specified in the model, all measurement error variances for the observed variables are fixed constants. The error variance of Fy is 0.1646 (standard error = 0.0452). Although you do not specify them in the PATH model specification, variances of F1–F3 are free parameters in the model. The second table of [Output 27.10.1](#) shows their estimates. The last table of [Output 27.10.2](#) shows the covariances among the latent true scores. Only the covariance between F3 and F1 is significant.

PROC CALIS not only can handle measurement error variance with multiple true score predictors, but it also can handle correlated errors. Suppose that the measurement errors for variables x1 and x2 are correlated. From prior studies, you determine that their covariance is 0.01. The path diagram with this new piece of information added is shown in the following:



In the path diagram, the double-headed arrow that connects x_1 and x_2 represents the covariance between the error terms for the two variables. The value attached to this double-headed arrow is 0.01, which represents a fixed constant in the model. The PATH model specification is similar to the preceding specification, with one more entry added in the PCOV statement, as shown in the following statements:

```
proc calis data=multiple nobs=37;
  path
    Fy <=== F1 F2 F3,
    F1 <=== x1 = 1.,
    F2 <=== x2 = 1.,
    F3 <=== x3 = 1.,
    Fy <=== y = 1.;
  pvar
    x1 x2 x3 y = .02 .03 .15 .02,
    Fy;
  pcov
    x1 x2 = 0.01;
run;
```

Except for the PCOV statement specification, everything else is the same as in the preceding specification. In the PCOV statement, you can specify covariance or error covariances between exogenous or endogenous variables. In the current model, because both x_1 and x_2 are endogenous in the model, the specification is for their error covariance, which is fixed at 0.01 as required.

Output 27.10.2 shows the parameter estimates of the measurement model with correlated errors. The estimates do not change much from the preceding analysis in which correlated errors is not assumed. Perhaps the correlation between the errors in the current model is so small that it is ignorable. The last table in Output 27.10.2 shows the covariance estimates among errors. This table is unique to the current model. It shows that the measurement errors for x_1 and x_2 have a covariance of 0.01, which is treated as a fixed constant in the current model.

Output 27.10.2 Parameter Estimates of the Measurement Model with Multiple Predictors: Correlated Errors

PATH List						
-----Path-----	Parameter	Estimate	Standard Error	t Value		
Fy <=== F1	_Parm1	0.46839	0.22695	2.06386		
Fy <=== F2	_Parm2	0.04549	0.07074	0.64306		
Fy <=== F3	_Parm3	0.13694	0.07194	1.90351		
F1 ==> x1		1.00000				
F2 ==> x2		1.00000				
F3 ==> x3		1.00000				
Fy ==> y		1.00000				

Variance Parameters						
Variance Type	Variable	Parameter	Estimate	Standard Error	t Value	
Error	x1		0.02000			
	x2		0.03000			
	x3		0.15000			
	y		0.02000			
Exogenous	Fy	_Parm4	0.16421	0.04523	3.63046	
	F1	_Add1	1.40000	0.33470	4.18289	
	F2	_Add2	1.12000	0.27106	4.13196	
	F3	_Add3	13.96000	3.32576	4.19754	

Covariances Among Exogenous Variables						
Var1	Var2	Parameter	Estimate	Standard Error	t Value	
F2	F1	_Add4	0.17000	0.21508	0.79039	
F3	F1	_Add5	4.21000	1.02416	4.11070	
F3	F2	_Add6	0.58000	0.67829	0.85509	

Covariances Among Errors						
Error of	Error of	Estimate	Standard Error	t Value		
x1	x2	0.01000				

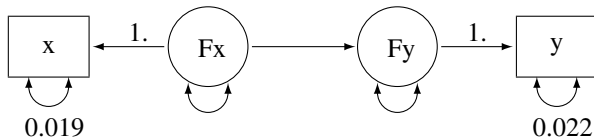
This example shows how you can use PROC CALIS to fit measurement error models with multiple true score predictors. You can also fit models with correlated errors. The model specification tool is the PATH modeling language, which ties closely to the path diagram representations.

However, some researchers might prefer to use linear equations to represent the measurement error models. PROC CALIS provides the LINEQS modeling language for specifying the measurement error models, or

mean and covariance structure models in general. Example 27.11 illustrates the LINEQS model specification of the measurement error models.

Example 27.11: Measurement Error Models Specified As Linear Equations

In Example 27.8, you fit a simple measurement error model with errors in both of the predictor variable x and the outcome variable y . From prior studies, the measurement error variance of x is 0.019 and the measurement error variance of y is 0.022. You use the following path diagram to represent the model:

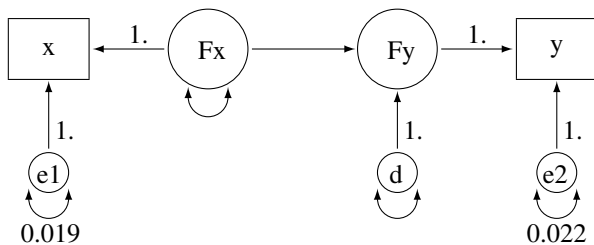


With this path diagram, you use the PATH modeling language of PROC CALIS to specify the model, as shown in the following:

```
proc calis data=measures;
  path
    x <=== Fx = 1.,
    Fx ==> Fy ,
    Fy ==> y = 1.;
  pvar
    x = 0.019,
    y = 0.022,
    Fx Fy;
run;
```

In the path diagram and in the PATH model specification, there are no explicit representations of the error terms in the model. You express the error variances of x , y , and Fy as partial variances of the endogenous variables. In the path diagram, you represent these partial variances by the double-headed arrows. Correspondingly, in the PATH statement of PROC CALIS, you specify these partial variances in the PVAR statement.

In practice, some researchers might prefer to express the error terms in the model explicitly. For example, with the error terms added to the preceding measurement error model, the new path diagram becomes:



In the path diagram, you add paths from error variables $e1$, $e2$, and d to the endogenous variables x , y , and Fy , respectively. All these paths from the error terms have a fixed path coefficient of 1. The error variances are represented by double-headed arrows directly attached to them. For example, the variance of $e1$ is fixed at 0.019, and the variance of $e2$ is fixed at 0.022. The variance of d , which is sometime called

the disturbance, is a free unnamed parameter in the path diagram. Similarly, the variance of F_x is a free unnamed parameter in the model.

Corresponding to this new path diagram, you can use the LINEQS modeling language for specifying your model in PROC CALIS, as shown in the following statements:

```
proc calis data=measures;
  lineqs
    x  = 1. * Fx + e1,
    y  = 1. * Fy + e2,
    Fy =      * Fx + d;
  variance
    e1 = 0.019,
    e2 = 0.022,
    Fx d;
run;
```

The LINEQS model specification in PROC CALIS emphasizes the linear equation input. In each of the linear equations in the LINEQS statement, you specify an endogenous variable and how it is related to other variables. An endogenous variable in the path diagram is a variable that has at least one single-headed arrow pointing to it. You need to list all endogenous variables on the left-hand side of the linear equations of the LINEQS statement. In the current model, variables x , y , and F_y are endogenous, and therefore you specify three linear equations in the LINEQS statement. The first two equations represent the measurement model for the observed variables, while the third equation represents the structural equation of the model. Notice that in the third equation, you do not specify the path coefficient that is attached to F_x . PROC CALIS treats unspecified path coefficients as free parameters. The effect of F_x on F_y is freely estimated, as required in the path diagram representation.

In the VARIANCE statement, you specify the variances of the exogenous variables in the model. The specifications in the VARIANCE statement of the LINEQS model are very similar to those in the PVAR statement of the PATH model. The main difference is the use of error variable names in the VARIANCE statement. With the LINEQS model specification, you can only specify exogenous variables in the VARIANCE statement. Hence, you must specify the error variables e_1 , e_2 , and d in the VARIANCE statement of the LINEQS model, instead of the corresponding endogenous variables x , y , and F_y in the PVAR statement of the PATH model.

Output 27.11.1 shows the parameter estimates of the LINEQS model.

Output 27.11.1 LINEQS Parameter Estimates of the Measurement Model for the Measures Data

		Linear Equations	
x	=	1.0000 Fx	+ 1.0000 e1
y	=	1.0000 Fy	+ 1.0000 e2
Fy	=	1.1791*Fx	+ 1.0000 d
Std Err		0.1029	_Parm1
t Value		11.4615	

Output 27.11.1 *continued*

Estimates for Variances of Exogenous Variables					
Variable Type	Variable	Parameter	Estimate	Standard Error	t Value
Error	e1		0.01900		
	e2		0.02200		
Latent	Fx	_Parm2	0.78062	0.20999	3.71741
Disturbance	d	_Parm3	0.18486	0.06126	3.01755

All these estimates are essentially the same as those obtained from the PATH model specification, as shown in Output 27.11.2.

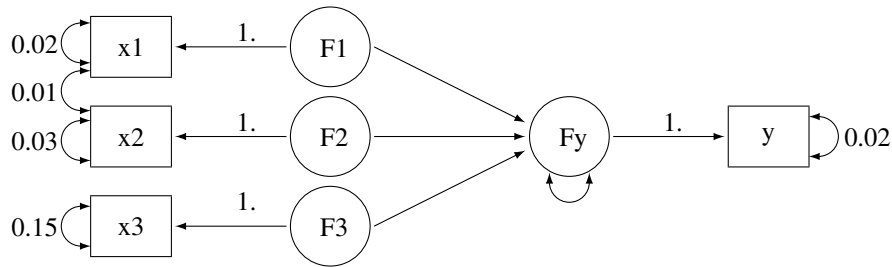
Output 27.11.2 PATH Parameter Estimates of the Measurement Model for the Measures Data

PATH List					
-----Path-----	Parameter	Estimate	Standard Error	t Value	
x <=== Fx		1.00000			
Fx ==> Fy	_Parm1	1.17914	0.10288	11.46153	
Fy ==> y		1.00000			
Variance Parameters					
Variance Type	Variable	Parameter	Estimate	Standard Error	t Value
Error	x		0.01900		
	y		0.02200		
Exogenous	Fx	_Parm2	0.78062	0.20999	3.71741
Error	Fy	_Parm3	0.18486	0.06126	3.01755

You can use either the LINEQS or PATH model specification in PROC CALIS for your analysis problems. They give you the same estimation results.

So far the measurement error model is concerned with one predictor. With more predictors in the model, you might also want to model the correlated measurement errors in the x variables. You can analyze this kind of model by using the PATH model specification, as shown in Example 27.10. With measurement error terms explicitly assumed, you can also use the LINEQS model specification. This example illustrates how you can do that by using the same data set and the measurement error model with correlated errors in Example 27.10.

In the data set, you have four observed variables: x1–x3 and y. All are measured with errors, as represented by the following path diagram:

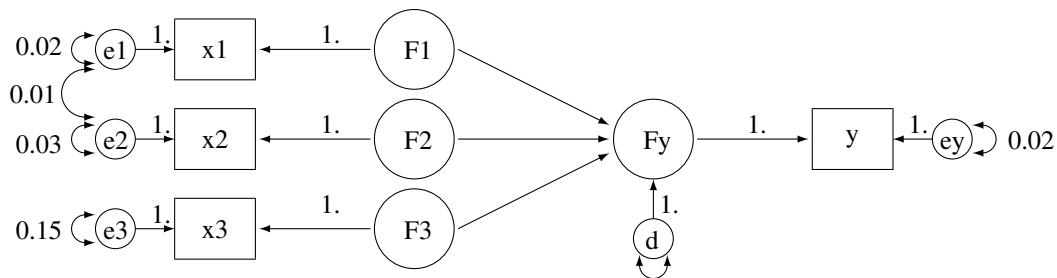


In the path diagram, F1–F3 and Fy represent true scores for the measurement indicators x1–x3 and y, respectively. You predict Fy by F1–F3, which represents the structural relationships in the model. Measurement error variances of the observed variables are treated as known and are represented by the double-headed arrows attached to the observed variables. For example, the error variance of x3 is 0.15. In addition, the error covariance between x1 and x2 is treated as known. The double-headed arrow that connects x1 and x2 represents the error covariance, and this covariance is fixed at 0.01 in the model.

You transcribe this path diagram representation into the following PATH model specification:

```
proc calis data=multiple nobs=37;
  path
    Fy <=== F1 F2 F3,
    F1 ==> x1 = 1.,
    F2 ==> x2 = 1.,
    F3 ==> x3 = 1.,
    Fy ==> y = 1.;
  pvar
    x1 x2 x3 y = .02 .03 .15 .02,
    Fy;
  pcov
    x1 x2 = 0.01;
run;
```

To represent the error terms explicitly, you can add the error terms to the path diagram with some modifications, as shown in the following:



In the path diagram, you attach error variables e1–e3, ey, and d to the associated endogenous variables in the model. The error variances and covariances, which are attached to the endogenous variables directly, are now attached to the corresponding error variables. With this new path diagram, you can use the following LINEQS model specification for the model:


```

proc calis data=multiple nobs=37;
  lineqs
    Fy =      * F1 + * F2 + * F3 + d,
    x1 = 1. * F1 + e1,
    x2 = 1. * F2 + e2,
    x3 = 1. * F3 + e3,
    y = 1. * Fy + ey;
  variance
    e1-e3 ey = .02 .03 .15 .02,
    d;
  cov
    e1 e2 = 0.01;
run;

```

Again, in each linear equation of the LINEQS statement, you specify the functional relationship of an endogenous variable with other variables, including the error variable. The first equation is the structural equation in the model. You want to estimate the effects of F1, F2, and F3 on Fy. The error or disturbance variable is d. In the next four equations, you relate the observed variables with their true scores counterparts.

In the VARIANCE statement, you specify the error variances with reference to the error variables in the path diagram. Four of the error variances are fixed constants, as required in the model. The last specification represents a free parameter for the variance of d. The specifications in the VARIANCE statement of the LINEQS model are similar to those in the PVAR statement of the PATH model specification. The difference is that in the PATH model specification the reference variables are the endogenous variables in the PATH model, while in the LINEQS model specification the reference variables are the associated error variables.

In the COV statement, you specify the covariance between the error variables e1 and e2. Again, this is similar to the corresponding specification of the PATH model, where the same error covariance is specified as the partial covariance between x1 and x2 in the PCOV statement.

Output 27.11.3 shows the parameter estimates that result from using the LINEQS model specification. Estimates in the equations, variances, and covariances are shown respectively.

Output 27.11.3 Parameter Estimates of the Measurement Model with Multiple Predictors: LINEQS Model

		Linear Equations			
Fy	=	0.4684*F1	+ 0.0455*F2	+ 0.1369*F3	+ 1.0000 d
Std Err		0.2269 _Parm1	0.0707 _Parm2	0.0719 _Parm3	
t Value		2.0639	0.6431	1.9035	
x1	=	1.0000 F1	+ 1.0000 e1		
x2	=	1.0000 F2	+ 1.0000 e2		
x3	=	1.0000 F3	+ 1.0000 e3		
y	=	1.0000 Fy	+ 1.0000 ey		

Output 27.11.3 *continued*

Estimates for Variances of Exogenous Variables					
Variable Type	Variable	Parameter	Estimate	Standard Error	t Value
Error	e1		0.02000		
	e2		0.03000		
	e3		0.15000		
	ey		0.02000		
Disturbance	d	_Parm4	0.16421	0.04523	3.63046
Latent	F1	_Add1	1.40000	0.33470	4.18289
	F2	_Add2	1.12000	0.27106	4.13196
	F3	_Add3	13.96000	3.32576	4.19754

Covariances Among Exogenous Variables					
Var1	Var2	Parameter	Estimate	Standard Error	t Value
e1	e2		0.01000		
F2	F1	_Add4	0.17000	0.21508	0.79039
F3	F1	_Add5	4.21000	1.02416	4.11070
F3	F2	_Add6	0.58000	0.67829	0.85509

Output 27.11.4 shows the parameter estimates that result from using the PATH model specification. The estimates in the path list shown in Output 27.11.4 correspond to those of the equation output in Output 27.11.3. The variance estimates in Output 27.11.4 correspond to those variance estimates of the exogenous variables of the LINEQS model, as shown in Output 27.11.3. Finally, the last two tables in Output 27.11.4 correspond to the covariance estimates among the exogenous variables of the LINEQS model, as shown in Output 27.11.3. Again, the LINEQS and PATH model specification give you exactly the same estimation results, but in different output formats.

Output 27.11.4 Parameter Estimates of the Measurement Model with Multiple Predictors: PATH Model

PATH List					
-----Path-----	Parameter	Estimate	Standard Error	t Value	
Fy <=== F1	_Parm1	0.46839	0.22695	2.06386	
Fy <=== F2	_Parm2	0.04549	0.07074	0.64306	
Fy <=== F3	_Parm3	0.13694	0.07194	1.90351	
F1 <===> x1		1.00000			
F2 <===> x2		1.00000			
F3 <===> x3		1.00000			
Fy <===> y		1.00000			

Output 27.11.4 continued

Variance Parameters					
Variance Type	Variable	Parameter	Estimate	Standard Error	t Value
Error	x1		0.02000		
	x2		0.03000		
	x3		0.15000		
	y		0.02000		
Exogenous	Fy	_Parm4	0.16421	0.04523	3.63046
	F1	_Add1	1.40000	0.33470	4.18289
	F2	_Add2	1.12000	0.27106	4.13196
	F3	_Add3	13.96000	3.32576	4.19754

Covariances Among Exogenous Variables					
Var1	Var2	Parameter	Estimate	Standard Error	t Value
F2	F1	_Add4	0.17000	0.21508	0.79039
F3	F1	_Add5	4.21000	1.02416	4.11070
F3	F2	_Add6	0.58000	0.67829	0.85509

Covariances Among Errors					
Error of	Error of	Parameter	Estimate	Standard Error	t Value
x1	x2		0.01000		

In this example, you fit measurement error models by using the LINEQS and PATH model specifications of PROC CALIS. The two different model specification languages give you essentially the same estimation results. The measurement models can have multiple true scores predictors and correlated errors. The measurement error models considered so far have only one measured indicator for each true score latent variable. This is usually not the case in many psychometric or sociological applications where latent factors usually have several observed indicators. The confirmatory factor model is a typical example of this kind of applications. See [Example 27.12](#) for an application of PROC CALIS to fit confirmatory factor models. See [Example 27.17](#) for an application of PROC CALIS to fit a general structural equation model where latent variables have more than one measured indicators.

Example 27.12: Confirmatory Factor Models

This example shows how you can fit a confirmatory factor analysis model by the FACTOR modeling language. Thirty-two students take tests of their verbal and math abilities. Six tests are administered separately. Tests x1–x3 test their verbal skills and tests y1–y3 test their math skills.

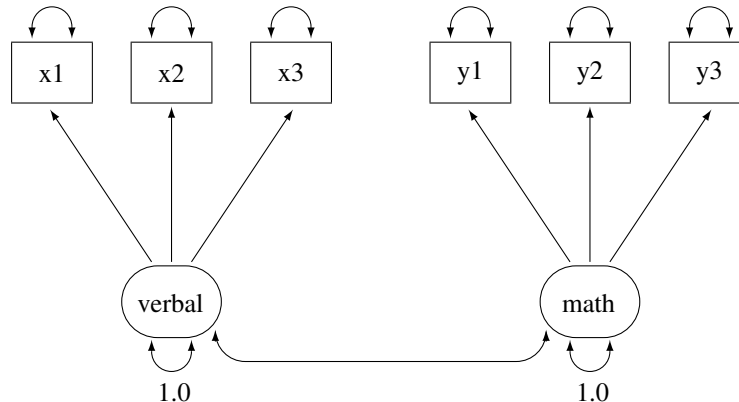
The data are shown in the following DATA step:

```

data scores;
  input x1 x2 x3 y1 y2 y3;
  datalines;
23 17 16 15 14 16
29 26 23 22 18 19
14 21 17 15 16 18
20 18 17 18 21 19
25 26 22 26 21 26
26 19 15 16 17 17
14 17 19 4 6 7
12 17 18 14 16 13
25 19 22 22 20 20
7 12 15 10 11 8
29 24 30 14 13 16
28 24 29 19 19 21
12 9 10 18 19 18
11 8 12 15 16 16
20 14 15 24 23 16
26 25 21 24 23 24
20 16 19 22 21 20
14 19 15 17 19 23
14 20 13 24 26 25
29 24 24 21 20 18
26 28 26 28 26 23
20 23 24 22 23 22
23 24 20 23 22 18
14 18 17 13 16 14
28 34 27 25 21 21
17 12 10 14 12 16
8 1 13 14 15 14
22 19 19 13 11 14
18 21 18 15 18 19
12 12 10 13 13 16
22 14 20 20 18 19
29 21 22 13 17 12
;

```

Because of the unambiguous nature of the tests, you hypothesize that this is a confirmatory factor model with two factors: one is the verbal ability factor and the other is the math ability factor. You can represent such a confirmatory factor model by the following path diagram:



In the path diagram, there are two clusters of variables. One cluster is for the verbal factor and the other is for the math factor. The single-headed arrows in the path diagram represent functional relationships between factors and the observed variables. The double-headed arrows that point to single variables represent variances of the factors or error variances of the observed variables. The double-headed arrow that connects the two factors represents their covariance. All but two of these arrows are not labeled with numbers. Each of the unlabeled arrows represents a free parameter in the confirmatory factor model. You label the double-headed arrows that attach to the two factors with the constant 1. This means that the variances of the factors are fixed at 1.0 in the model.

You can specify the confirmatory factor model by the FACTOR model language of PROC CALIS, as shown in the following statements:

```
proc calis data=scores;
  factor
    verbal ==> x1-x3,
    math   ==> y1-y3;
  pvar
    verbal = 1.,
    math   = 1.;
run;
```

In each of the entry of the FACTOR statement, you specify a latent factor, followed by a list of observed variables that are functionally related to the latent factor. For example, in the first entry, the verbal factor is related to variables x1–x3, as shown by the single-headed arrows in the path diagram. In fact, all single-headed arrows in the path diagram are specified in the FACTOR statement. Notice that each entry of the FACTOR statement must take the format of

```
factor_name ==> variable_list
```

You cannot reverse the arrow specification as in the following:

```
variable_list <=== factor_name
```

Nor you can have a specification such as the following:

```
variable_list ==> factor_name
```

However, you can specify the functional relationships between factors and variables in different entries. For example, you can specify the same confirmatory factor model by the following statements:

```
title "Basic Confirmatory Factor Model: Separate Path Entries";
title2 "FACTOR Model Specification";
proc calis data=scores;
  factor
    verbal ==> x1,
    verbal ==> x2,
    verbal ==> x3,
    math   ==> y1,
    math   ==> y2,
    math   ==> y3;
  pvar
    verbal = 1.,
    math   = 1.;
  fitindex noindextype on(only)=[chisq df probchi rmsea srmr bentlercfi];
run;
```

In the PVAR statement, which is for the specification of variances or error variances, you fix the variances of the latent factors to 1. This completes the model specification of the confirmatory factor model, although you do not specify other arrows in the path diagram as free parameters in these statements. The reason is that in the FACTOR modeling language, the variances and covariances among factors and the error variances of the observed variables are default parameters in the confirmatory factor model. It is not necessary to specify these parameters (or the corresponding arrows in the path diagram) explicitly if they are free parameters in the model. You can also specify these free parameters explicitly without affecting the estimation. However, if these parameters (or the corresponding double-headed arrows in the path diagram) are intended to be constrained parameters or fixed values, you must specify them explicitly. For example, in the current confirmatory factor model, you must provide explicit specifications for the variances of the verbal and the math factors because these parameters are fixed at 1.

Output 27.12.1 shows the modeling information and the variables in the confirmatory factor model.

Output 27.12.1 Modeling Information and Variables of the CFA Model: Scores Data

Simple Confirmatory Factor Model	
FACTOR Model Specification	
The CALIS Procedure	
Covariance Structure Analysis: Model and Initial Values	
Modeling Information	
Maximum Likelihood Estimation	
Data Set	WORK.SCORES
N Records Read	32
N Records Used	32
N Obs	32
Model Type	FACTOR
Analysis	Covariances

Output 27.12.1 *continued*

```

Variables in the Model

Variables   x1  x2  x3  y1  y2  y3
Factors    verbal  math

Number of Variables = 6
Number of Factors   = 2

```

In the beginning of the output, PROC CALIS shows the data set, the number of observations, the model type, and the analysis type. The default analysis type in PROC CALIS is covariances (that is, covariance structures). If you want to analyze the correlation structures instead, you can use the **CORR** option in the PROC CALIS statement. Next, PROC CALIS shows the list of variables and factors in the model. As expected, the number of variables is 6 and the number of factors is 2.

Output 27.12.2 shows the initial model specifications of the confirmatory factor model.

Output 27.12.2 Initial Specification of the CFA Model: Scores Data

```

Initial Factor Loading Matrix

           verbal           math
x1         .                0
   [_Parm1]
x2         .                0
   [_Parm2]
x3         .                0
   [_Parm3]
y1         0                .
           [_Parm4]
y2         0                .
           [_Parm5]
y3         0                .
           [_Parm6]

Initial Factor Covariance Matrix

           verbal           math
verbal    1.0000           .
           [_Add1]
math      .                1.0000
           [_Add1]

```

Output 27.12.2 *continued*

Initial Error Variances		
Variable	Parameter	Estimate
x1	_Add2	.
x2	_Add3	.
x3	_Add4	.
y1	_Add5	.
y2	_Add6	.
y3	_Add7	.

NOTE: Parameters with prefix '_Add' are added by PROC CALIS.

The first table of [Output 27.12.2](#) shows the pattern of factor loadings of the variables on the two latent factors. As expected, x1–x3 have nonzero loadings only on the verbal factor, while y1–y3 have nonzero loadings on the math factor. PROC CALIS names these free parameters automatically with the “_Parm” prefix and unique numerical suffixes. There are six parameters in the factor loading matrix with six different parameter names.

The next table of [Output 27.12.2](#) shows the covariance matrix of the factors. The variances of the factors are fixed at one, as shown on the diagonal of the covariance matrix. The covariance between the two factors is a free parameter named _Add1. You did not specify this covariance parameter explicitly in the factor model specification. By default, PROC CALIS assumes that latent factors are correlated. Default free parameters added by PROC CALIS have the _Add prefix for their names. If you do not want to assume the covariances among the factors, you must specify zero covariances in the COV statement. For example, the following statement specifies that the math and verbal factors have zero covariance:

```
COV
  math verbal = 0.;
```

The last table of [Output 27.12.2](#) shows the error variance parameters of the observed variables. By default PROC CALIS assumes these error variances are free parameters in the confirmatory factor model. These added parameters are named with the _Add prefix. However, as all other default parameters that are assumed by PROC CALIS, you can overwrite the default by using explicit specifications. You can specify the error variances of a confirmatory factor model explicitly in the PVAR statement. See specifications in [Example 27.13](#).

[Output 27.12.3](#) shows the fit summary of the confirmatory factor model for the scores data.

Output 27.12.3 Fit Summary of the CFA Model: Scores Data

Fit Summary	
Chi-Square	9.8052
Chi-Square DF	8
Pr > Chi-Square	0.2790
Standardized RMR (SRMR)	0.0571
RMSEA Estimate	0.0853
Bentler Comparative Fit Index	0.9887

The model fit chi-square is 9.805 ($df = 8, p = 0.279$). This shows that statistically you cannot reject the confirmatory factor model for the test scores. However, the root mean square error of approximation (RMSEA) estimate is 0.0853, which is greater than the conventional 0.05 value for a good model fit. The standardized root mean square residual (SRMR) is 0.0571, which is close to the conventional 0.05 value for a good model fit. Bentler's comparative fit index is 0.9887, which indicates a very good model fit. Overall, the model seems to be quite reasonable for the data.

Output 27.12.4 shows the loading and factor covariance estimates of the confirmatory factor model for the scores data. The first table shows the loading estimates, together with the standard error estimates and the t values. In structural equation modeling, the significance of the parameter estimates is usually inferred by comparing the t values with the critical value of a standardized normal variate (that is, the z -table). Therefore, estimates with associated (absolute) t values greater than 1.96 are significant at $\alpha = .05$. In Output 27.12.4, all the t values for the loading estimates are greater than 2. This indicates that the prescribed relationships between the variables and the factors are significant.

Output 27.12.4 Loading and Factor Covariance Estimates of the CFA Model: Scores Data

Factor Loading Matrix: Estimate/StdErr/t-value		
	verbal	math
x1	5.8406 0.9962 5.8629	0
	[_Parm1]	
x2	5.8182 0.9537 6.1004	0
	[_Parm2]	
x3	4.6619 0.7814 5.9662	0
	[_Parm3]	
y1	0	5.2804 0.6998 7.5455
		[_Parm4]
y2	0	4.2003 0.6220 6.7532
		[_Parm5]
y3	0	3.7596 0.6341 5.9289
		[_Parm6]

Output 27.12.4 *continued*

Factor Covariance Matrix: Estimate/StdErr/t-value		
	verbal	math
verbal	1.0000	0.5175 0.1429 3.6221 [_Add1]
math	0.5175 0.1429 3.6221 [_Add1]	1.0000

The second table of [Output 27.12.4](#) shows the covariance matrix of the verbal and the math factors. Because the factor variances are fixed at one, the covariance estimate is also the correlation between the two factors. [Output 27.12.4](#) shows that the two factors are moderately correlated with a correlation estimate of 0.5175, which is statistically significant.

[Output 27.12.5](#) shows the estimates of the error variances. All but the error variance of y1 are significant. This suggests that y1 might have an almost perfect relationship with the math factor.

Output 27.12.5 Error Variance Estimates of the CFA Model: Scores Data

Error Variances				
Variable	Parameter	Estimate	Standard Error	t Value
x1	_Add2	11.52376	4.26398	2.70259
x2	_Add3	9.14503	3.83219	2.38637
x3	_Add4	6.68169	2.59770	2.57216
y1	_Add5	0.78580	1.29440	0.60708
y2	_Add6	2.88069	1.09395	2.63329
y3	_Add7	5.15573	1.46854	3.51080

[Output 27.12.6](#) echoes this same fact. The R-squares in this table shows the percentages of variance of the variables that are overlapped with the factors. While all these percentages (0.74 – 0.97) are quite high for all variables, the percentage is especially high for y1. It shares 97% of the variance with the math factor. So, it appears that the observed variable y1 is almost a perfect indicator of the math factor.

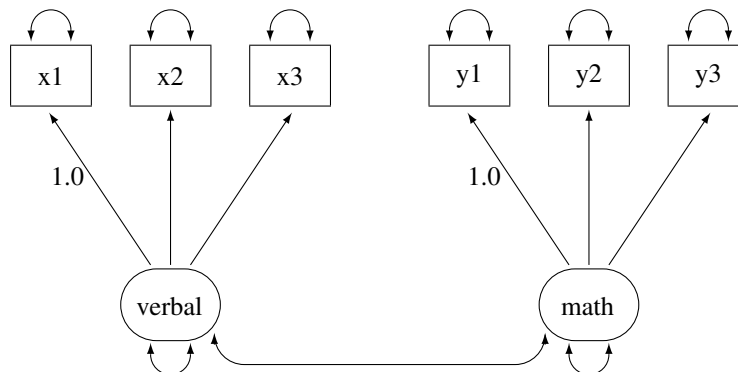
Output 27.12.6 Squared Multiple Correlations of the CFA Model: Scores Data

Squared Multiple Correlations			
Variable	Error Variance	Total Variance	R-Square
x1	11.52376	45.63609	0.7475
x2	9.14503	42.99597	0.7873
x3	6.68169	28.41532	0.7649
y1	0.78580	28.66835	0.9726
y2	2.88069	20.52319	0.8596
y3	5.15573	19.29032	0.7327

Alternative Identification Constraints

Setting the variances of the latent factors to 1 in the preceding FACTOR model specification makes the model identified. This is necessary because the scales of the latent factors are arbitrary and the constraints imposed on the factor variances fix the scales of the factors.

In practice, there is another way to fix the scales of the factors. For each factor, you can fix the loading of one of its measured indicators to a constant. This fixed loading value is usually set at 1. For example, you can represent the confirmatory factor model for the scores data by the following alternative path diagram:



This path diagram is essentially the same as the preceding one. However, the fixed constants adjacent to the double-headed arrows that attach to the two factors in the preceding path diagram are now moved to two of the single-headed paths in the current path diagram.

You can specify this path diagram by the following FACTOR model specification of PROC CALIS:

```
proc calis data=scores;
  factor
    verbal ==> x1-x3 = 1. ,
    math   ==> y1-y3 = 1. ;
run;
```

In the FACTOR statement, you assign a fixed constant to each of the path entries. In the first entry, the constant 1 is assigned to the loading of x_1 on the verbal factor, while all other loadings in this entry are (unnamed) free parameters. Similarly, in the second entry, the fixed constant 1 is assigned to the loading of y_1 on the math factor, while all other loadings in this entry are (unnamed) free parameters. This completes the specification of the confirmatory factor model because all the double-headed arrows in the path diagram correspond to default free parameters in the FACTOR modeling language of PROC CALIS.

Output 27.12.7 shows some fit indices for the current confirmatory factor model for the scores data.

Output 27.12.7 Fit Summary of the CFA Model with Alternative Identification Constraints: Scores Data

Fit Summary	
Chi-Square	9.8052
Chi-Square DF	8
Pr > Chi-Square	0.2790
Standardized RMR (SRMR)	0.0571
RMSEA Estimate	0.0853
Bentler Comparative Fit Index	0.9887

The model fit chi-square is 9.805 ($df = 8$, $p = 0.279$). This is the same model fit chi-square as that for the preceding CFA model specification with factor variances constrained to 1. In fact, all fit information in Output 27.12.7 are identical to Output 27.12.3.

Output 27.12.8 shows the parameter estimates under the current model specification. The loading of x_1 on the verbal factor is a fixed at 1, as required for the identification of the scale of the verbal factor. Similarly, the loading of y_1 on the math factor is a fixed at 1 for the identification of the scale of the math factor. All other loading estimates in Output 27.12.8 are not the same as those in the preceding model specification, as shown in Output 27.12.4. The reason is that the scales of the factors (as measured by the estimated standard deviations of the factors) in the two specifications are not the same. In the current model specification, the verbal factor has an estimated variance of 34.1123 and the math factor has an estimated variance of 27.8825, as shown in the second table of Output 27.12.8. Hence, the estimated standard deviations of these two factors are 5.8406 and 5.2804, respectively. But the standard deviations of the factors in the preceding confirmatory factor model specification are fixed at 1.

Output 27.12.8 Loading and Factor Covariance Estimates of the CFA Model with Alternative Identification Constraints: Scores Data

Factor Loading Matrix: Estimate/StdErr/t-value		
	verbal	math
x1	1.0000	0
x2	0.9962 0.1576 6.3194 [_Parm1]	0
x3	0.7982 0.1286 6.2083 [_Parm2]	0
y1	0	1.0000
y2	0	0.7955 0.0718 11.0820 [_Parm3]
y3	0	0.7120 0.0858 8.3027 [_Parm4]
Factor Covariance Matrix: Estimate/StdErr/t-value		
	verbal	math
verbal	34.1123 11.6366 2.9315 [_Add1]	15.9585 6.7270 2.3723 [_Add3]
math	15.9585 6.7270 2.3723 [_Add3]	27.8825 7.3905 3.7727 [_Add2]

However, if you multiply the loading estimates in [Output 27.12.8](#) by the corresponding estimated factor standard deviation, you get the same set of loading estimates as in [Output 27.12.4](#). For example, the loading of x1 on the verbal factor is 1.0 in [Output 27.12.8](#). Multiplying this loading by the estimated standard deviation 5.8406 of the verbal factor gives you the same corresponding loading as in [Output 27.12.4](#). Another

example is the loading of y3 on the math factor. This loading is 0.7120 in [Output 27.12.8](#). Multiplying this estimate by the estimated standard deviation 5.2804 of the verbal factor gives an estimate of 3.7596, which matches the corresponding loading estimate in [Output 27.12.4](#). Therefore, the discrepancies in the loading estimates are due to different factor scales in the two specifications. The loading estimates in [Output 27.12.8](#) are simply rescaled version of the loading estimates in [Output 27.12.4](#).

However, the scales of the factors do not affect the estimates of the error variances, as shown in [Output 27.12.9](#). These estimates are the same as those for the preceding model specification, as shown in the [Output 27.12.5](#).

Output 27.12.9 Error Variance Estimates of the CFA Model with Alternative Identification Constraints:
Scores Data

Error Variances				
Variable	Parameter	Estimate	Standard Error	t Value
x1	_Add4	11.52376	4.26398	2.70259
x2	_Add5	9.14503	3.83219	2.38637
x3	_Add6	6.68169	2.59770	2.57216
y1	_Add7	0.78580	1.29440	0.60708
y2	_Add8	2.88069	1.09395	2.63329
y3	_Add9	5.15573	1.46854	3.51080

This example shows how you can fit a basic confirmatory factor model by the FACTOR modeling language of PROC CALIS. You can set the identification constraints and get statistically equivalent estimation results in two different ways. By setting up additional parameter constraints, you can also fit some variations of the basic confirmatory factor model. See [Example 27.13](#) for illustrations of some restricted confirmatory factor models for the scores data.

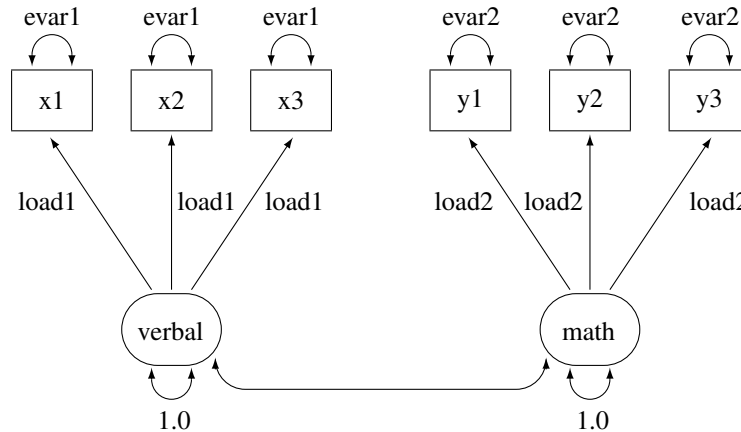
When your data have missing values, with the default ML estimation method PROC CALIS deletes all observations with missing values for the analysis. This might result in a serious loss of information. [Example 27.15](#) considers a hypothetical situation where some observations in the scores data have missing values in the observed variables. Only 16 observations have complete data. By using the full information maximum likelihood (FIML) method for treating the missing data, [Example 27.15](#) shows how you can fully use the information from the scores data set with missing values.

Example 27.13: Confirmatory Factor Models: Some Variations

This example shows how you can fit some variations of the basic confirmatory factor analysis model by the FACTOR modeling language. You apply these models to the scores data set that is described in [Example 27.12](#). The data set contains six test scores of verbal and math abilities. Thirty-two students take the tests. Tests x1–x3 test their verbal skills and tests y1–y3 test their math skills.

The Parallel Tests Model

In classical measurement theory, test items for a latent factor are parallel if they have the same loadings on the factor and the same error variances (or reliability). Suppose for the scores data, the items within each of the verbal and the math factors are parallel. You can use the following path diagram to represent such a parallel tests model:



In the path diagram, the variances of the verbal and the math are both fixed at 1, as indicated by the constants 1.0 adjacent to the double-headed arrows that are attached to factors. You label all the single-headed paths in the path diagram by parameter names. For the three paths (loadings) from the verbal factor, you use the same parameter name `load1`. This means that these loadings are the same parameter. You also label the double-headed arrows that are attached to `x1–x3` by the parameter name `evar1`. This means that the corresponding error variances for these three observed variables are exactly the same. Hence, `x1–x3` are parallel tests for the verbal factor, as required by the current confirmatory factor model.

Similarly, you define parallel tests `y1–y3` for the math factor by using `load2` as the common factor loading parameter and `evar2` as the common error variances for the observed variables.

Corresponding to this path diagram, you can specify the model by the following FACTOR model specification of PROC CALIS:

```
proc calis data=scores;
  factor
    verbal ==> x1-x3 = load1 load1 load1,
    math   ==> y1-y3 = load2 load2 load2;
  pvar
    verbal = 1.,
    math   = 1.,
    x1-x3  = 3*evar1,
    y1-y3  = 3*evar2;
run;
```

In each entry of the **FACTOR** statement, you specify the factor-variables relationships, followed by a list of parameters. For example, the three loading parameters of x_1 – x_3 on the verbal factor are all named **load1**. This effectively constrains the corresponding loading estimates to be the same. Similarly, in the next entry you set equality constraints on the loading estimates y_1 – y_3 on the math factor by using the same parameter name **load2**.

To make the tests parallel, you also need to constrain the error variances for each variable cluster. In the **PVAR** statement, in addition to setting the factor variances to 1 for identification, you set all the error variances of x_1 – x_3 to be the same by using the same parameter name **evar1**. The notation **3*evar1** means that you want to specify **evar1** three times, one time each for the error variances for the three observed variables in the variable list of the entry. Similarly, you set the equality of the error variances of y_1 – y_3 by using the same parameter name **evar2**.

Output 27.13.1 shows some fit indices of the parallel tests model for the scores data. The model fit chi-square is 26.128 ($df = 16$, $p = 0.0522$). The SRMR value is 0.1537 and the RMSEA value is 0.1429. All these indices show that the model does not fit very well. However, Bentler's CFI is 0.9366, which shows a good model fit.

Output 27.13.1 Model Fit of the Parallel Tests Model: Scores Data

Fit Summary	
Chi-Square	26.1283
Chi-Square DF	16
Pr > Chi-Square	0.0522
Standardized RMR (SRMR)	0.1537
RMSEA Estimate	0.1429
Bentler Comparative Fit Index	0.9366

Output 27.13.2 shows the parameter estimates of the parallel tests model. The first table of **Output 27.13.2** shows the required factor pattern for parallel tests. Variables x_1 – x_3 all have the same loading estimates on the verbal factor, and variables y_1 – y_3 all have the same loading estimates on the math factor. All loading estimates are statistically significant.

Output 27.13.2 Parameter Estimates of the Parallel Tests Model: Scores Data

Factor Loading Matrix: Estimate/StdErr/t-value		
	verbal	math
x1	5.4226 0.7655 7.0833 [load1]	0
x2	5.4226 0.7655 7.0833 [load1]	0
x3	5.4226 0.7655 7.0833 [load1]	0
y1	0	4.4001 0.5926 7.4246 [load2]
y2	0	4.4001 0.5926 7.4246 [load2]
y3	0	4.4001 0.5926 7.4246 [load2]
Factor Covariance Matrix: Estimate/StdErr/t-value		
	verbal	math
verbal	1.0000	0.5024 0.1497 3.3569 [_Add1]
math	0.5024 0.1497 3.3569 [_Add1]	1.0000

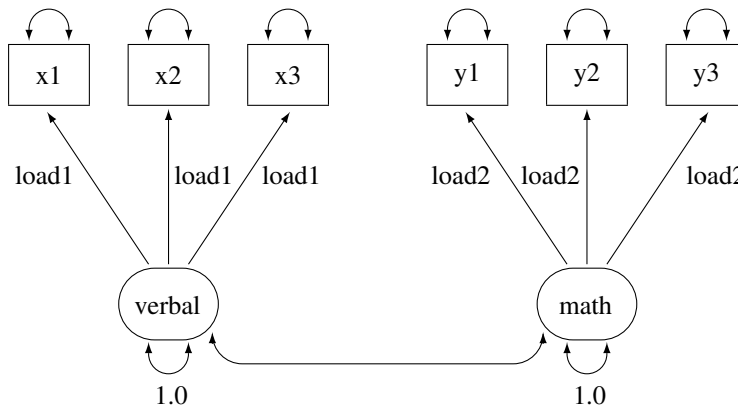
Output 27.13.2 *continued*

Error Variances				
Variable	Parameter	Estimate	Standard Error	t Value
x1	evar1	9.61122	1.72623	5.56776
x2	evar1	9.61122	1.72623	5.56776
x3	evar1	9.61122	1.72623	5.56776
y1	evar2	3.46673	0.62264	5.56776
y2	evar2	3.46673	0.62264	5.56776
y3	evar2	3.46673	0.62264	5.56776

In the second table of [Output 27.13.2](#), the factor covariance (or correlation) estimate is 0.5024, showing moderate relationship between the verbal and the math factors. The last table of [Output 27.13.2](#) shows the error variances of the variables. As required by the parallel tests model, the error variance estimates of x1–x3 are all 9.6112, and the error variance estimates of y1–y3 are all 3.4667.

The Tau-Equivalent Tests Model

Because the parallel tests model does not fit well, you are looking for a less constrained model for the scores data. The tau-equivalent tests model is such a model. It requires only the equality of factor loadings but not the equality of error variances within each factor. The following path diagram represents the tau-equivalent tests model for the scores data:



This path diagram is much the same as that for the parallel tests model except that now you do not use parameter names to label the double-headed arrows that are attached to the observed variables. This means that you allow the corresponding error variances to be free parameters in the tau-equivalent tests model. You can use the following FACTOR model specification of PROC CALIS to specify the tau-equivalent tests model for the scores data:

```

proc calis data=scores;
  factor
    verbal ==> x1-x3 = load1 load1 load1,
    math   ==> y1-y3 = load2 load2 load2;
  pvar
    verbal = 1.,
    math   = 1.;
run;

```

This specification is the same as that for the parallel tests model except that you remove the specifications about the error variances in the PVAR statement in the current tau-equivalent model. This effectively allows the error variances of the observed variables to be (default) free parameters in the model.

Output 27.13.3 shows some model fit indices of the tau-equivalent tests model for the scores data. The chi-square is 22.0468 ($df = 12$, $p = 0.037$). The SRMR is 0.1398 and the RMSEA is 0.1643. The comparative fit index (CFI) is 0.9371. Except for the CFI value, all other values do not support a good model fit. This model has a degrees of freedom of 12, which is less restrictive (has more parameters) than the parallel tests model, which has a degrees of freedom of 16, as shown in Output 27.13.1. However, it seems that the tau-equivalent tests model is still too restrictive for the data.

Output 27.13.3 Model Fit of the Tau-Equivalent Tests Model: Scores Data

Fit Summary	
Chi-Square	22.0468
Chi-Square DF	12
Pr > Chi-Square	0.0370
Standardized RMR (SRMR)	0.1398
RMSEA Estimate	0.1643
Bentler Comparative Fit Index	0.9371

Output 27.13.4 shows the parameter estimates. The first table of Output 27.13.4 shows the required pattern of factor loadings under the tau-equivalent tests model. The third table of Output 27.13.4 shows the error variance estimates. The error variance parameters are no longer constrained under the tau-equivalent tests model. Each has a unique estimate.

Output 27.13.4 Parameter Estimates of the Tau-Equivalent Tests Model: Scores Data

Factor Loading Matrix: Estimate/StdErr/t-value		
	verbal	math
x1	5.2418 0.7374 7.1085 [load1]	0
x2	5.2418 0.7374 7.1085 [load1]	0
x3	5.2418 0.7374 7.1085 [load1]	0
y1	0	4.4462 0.5932 7.4953 [load2]
y2	0	4.4462 0.5932 7.4953 [load2]
y3	0	4.4462 0.5932 7.4953 [load2]
Factor Covariance Matrix: Estimate/StdErr/t-value		
	verbal	math
verbal	1.0000	0.4514 0.1569 2.8772 [_Add1]
math	0.4514 0.1569 2.8772 [_Add1]	1.0000

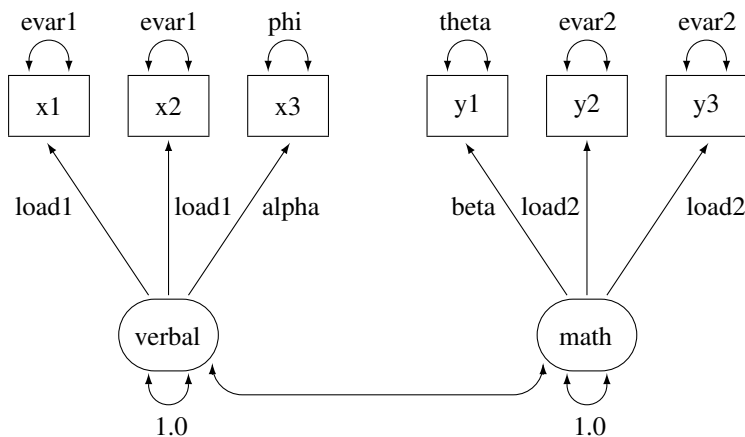
Output 27.13.4 continued

Error Variances				
Variable	Parameter	Estimate	Standard Error	t Value
x1	_Add2	13.05681	4.19549	3.11210
x2	_Add3	10.80421	3.70322	2.91752
x3	_Add4	5.43527	2.72147	1.99719
y1	_Add5	3.29858	1.24673	2.64578
y2	_Add6	1.90435	1.02393	1.85984
y3	_Add7	5.09724	1.61477	3.15663

The Partially Constrained Parallel Tests Model

Because both the parallel tests and tau-equivalent tests models do not fit the data well, you can explore an alternative model for the scores data. Suppose that for each factor only two (but not all) of their measured variables (tests) are parallel. For example, suppose you know that tests x1 and x2 are very similar to each other (for example, both are speeded tests with forced-choice answers), while x3 is a little different in the way it is administered (for example, open-ended questions). Although all tests are designed for measuring the verbal factor, only x1 and x2 are parallel tests while x3 is congeneric to the verbal factor. Similarly, suppose you can argue that y2 and y3 are parallel tests while y1 is only congeneric to the math factor.

The current modeling idea is represented by the following path diagram:



In the path diagram, x1 and x2 have the same parameter load1 for the paths from the verbal factor. Their error variances are also the same, as labeled with the evar1 parameter adjacent to the double-headed arrows that are attached to the variables. The test x3 has distinct parameter names for its associated path and the attached double-headed arrow. The corresponding loading and error variance parameters are alpha and phi, respectively. Similarly, with the use of specific parameter names, you define y2 and y3 as parallel tests for the math factor, while y1 is congeneric to the same factor but with distinct loading and error variance parameters. Lastly, you fix the variances of the factors to 1.0 for identification of the factor scales.

You can specify such a partially constrained parallel tests model by the following FACTOR model specification of PROC CALIS:

```
proc calis data=scores;
  factor
    verbal ==> x1-x3 = load1 load1 alpha,
    math   ==> y1-y3 = beta  load2 load2;
  pvar
    verbal = 1.,
    math   = 1.,
    x1-x3  = evar1 evar1 phi,
    y1-y3  = theta evar2 evar2;
run;
```

First, in the FACTOR statement, you name the loading parameters that reflect the parallel tests constraints. For example, the loading parameters of x1 and x2 on the verbal factor are both named load1. This means that they are the same. However, the loading parameter of x3 on the verbal factor is named alpha, which means that it is a separate parameter. Similarly, you apply the load2 parameter name to the loading parameters of y2 and y3 on the math factor, but the loading parameter of y1 on the math factor is a distinct parameter named beta.

In the PVAR statement, the two factor variances are set to a constant 1 for the identification of latent factor scales. Next, you use the same naming techniques as in the FACTOR statement to constrain some parts of the error variances. As a result, together with the specifications in the FACTOR statement, x1 and x2 are parallel tests for the verbal factor and y2 and y3 are parallel tests for the math factor, while x3 and y1 are only congeneric tests for their respective factors.

Output 27.13.5 shows some fit indices of the partially constrained parallel tests model. The model fit chi-square is 12.6784 ($df = 12$, $p = 0.3928$). The SRMR is 0.0585 and the RMSEA is close to 0.0427. The comparative fit index (CFI) is 0.9958. All these fit indices point to a quite reasonable model fit for the scores data.

Output 27.13.5 Model Fit of the Partially Constrained Parallel Tests Model: Scores Data

Fit Summary	
Chi-Square	12.6784
Chi-Square DF	12
Pr > Chi-Square	0.3928
Standardized RMR (SRMR)	0.0585
RMSEA Estimate	0.0427
Bentler Comparative Fit Index	0.9958

Notice that the current model actually has the same degrees of freedom as that of the tau-equivalent tests model, as shown in Output 27.13.3. Both models have nine parameters. But the current partially constrained parallel tests model is definitely a better model for the data. This shows that sometimes you do not have to add more parameters to improve the model fit. Structurally different models might explain the data quite differently, even though they might use the same number of parameters.

Output 27.13.6 show the parameter estimates of the partially constrained parallel tests model for the scores data. The estimates in the factor loading matrix and error variances table confirm the prescribed nature of

the tests—that is, x1 and x2 are parallel tests for the verbal factor and y2 and y3 are parallel tests for the math factor.

Output 27.13.6 Parameter Estimates of the Partially Constrained Parallel Tests Model: Scores Data

Factor Loading Matrix: Estimate/StdErr/t-value		
	verbal	math
x1	5.8306 0.8593 6.7853 [load1]	0
x2	5.8306 0.8593 6.7853 [load1]	0
x3	4.6623 0.7814 5.9664 [alpha]	0
y1	0	5.2784 0.7010 7.5294 [beta]
y2	0	3.9789 0.5732 6.9419 [load2]
y3	0	3.9789 0.5732 6.9419 [load2]
Factor Covariance Matrix: Estimate/StdErr/t-value		
	verbal	math
verbal	1.0000	0.5203 0.1425 3.6497 [_Add1]
math	0.5203 0.1425 3.6497 [_Add1]	1.0000

Output 27.13.6 *continued*

Error Variances				
Variable	Parameter	Estimate	Standard Error	t Value
x1	evar1	10.31998	2.57827	4.00268
x2	evar1	10.31998	2.57827	4.00268
x3	phi	6.67832	2.59902	2.56956
y1	theta	0.80714	1.35247	0.59679
y2	evar2	4.07534	1.00371	4.06028
y3	evar2	4.07534	1.00371	4.06028

Example 27.14: Residual Diagnostics and Robust Estimation

This example illustrates case-level residual diagnostics and robust estimation with PROC CALIS. The data set is available in Mardia, Kent, and Bibby (1979). It contains 88 responses on five subjects: mechanics, vector, algebra, analysis, and statistics. Yuan and Hayashi (2010) use the same data set to illustrate the uses of residual diagnostics in the context of robust estimation. Inspired by their illustrations, this example mirrors their one-factor model, with some modifications.

Case-Level Residual Diagnostics

The following DATA step specifies and inputs five observed variables for the data set mardia:

```
data mardia;
  input mechanics vector algebra analysis statistics;
  datalines;
77.000    82.000    67.000    67.000    81.000
63.000    78.000    80.000    70.000    81.000
75.000    73.000    71.000    66.000    81.000
.         .         .         .         .
.         .         .         .         .
  { More Data }
.         .         .         .         .
.         .         .         .         .
.         .         .         .         .
.         .         .         .         .
;
```

You specify a one-factor model for the five variables by using the following statements:

```
ods graphics on;

proc calis data=mardia residual plots=caseresid;
  path
    fact1 ==> mechanics vector algebra analysis statistics = 1. ;
run;

ods graphics off;
```


In the PATH statement, all observed variables are indicators of the latent factor fact1. The first factor loading for mechanics is fixed at 1 for identification of the latent variable scale, while the remaining four loadings are free parameters in the model. The RESIDUAL option that is specified in the PROC CALIS statement requests residual analysis. Because raw data are input, case-level residual analysis is done. To request all the available ODS Graphics output for case-level residual diagnostics, you specify the PLOTS=CASERESID option. To enable ODS Graphics, you specify the ODS GRAPHICS ON statement before running the CALIS procedure.

Output 27.14.1 shows some of the fit statistics of the one-factor model. The model fit chi-square is 8.9782 ($df = 5, p = 0.1099$). Therefore, you fail to reject the one-factor model for the data. The SRMR is 0.0411, which shows a good fit. But the RMSEA is 0.0956, which does not show that the one-factor model is a very good approximating model for the data. Output 27.14.2 shows the loading estimates. All are statistically significant.

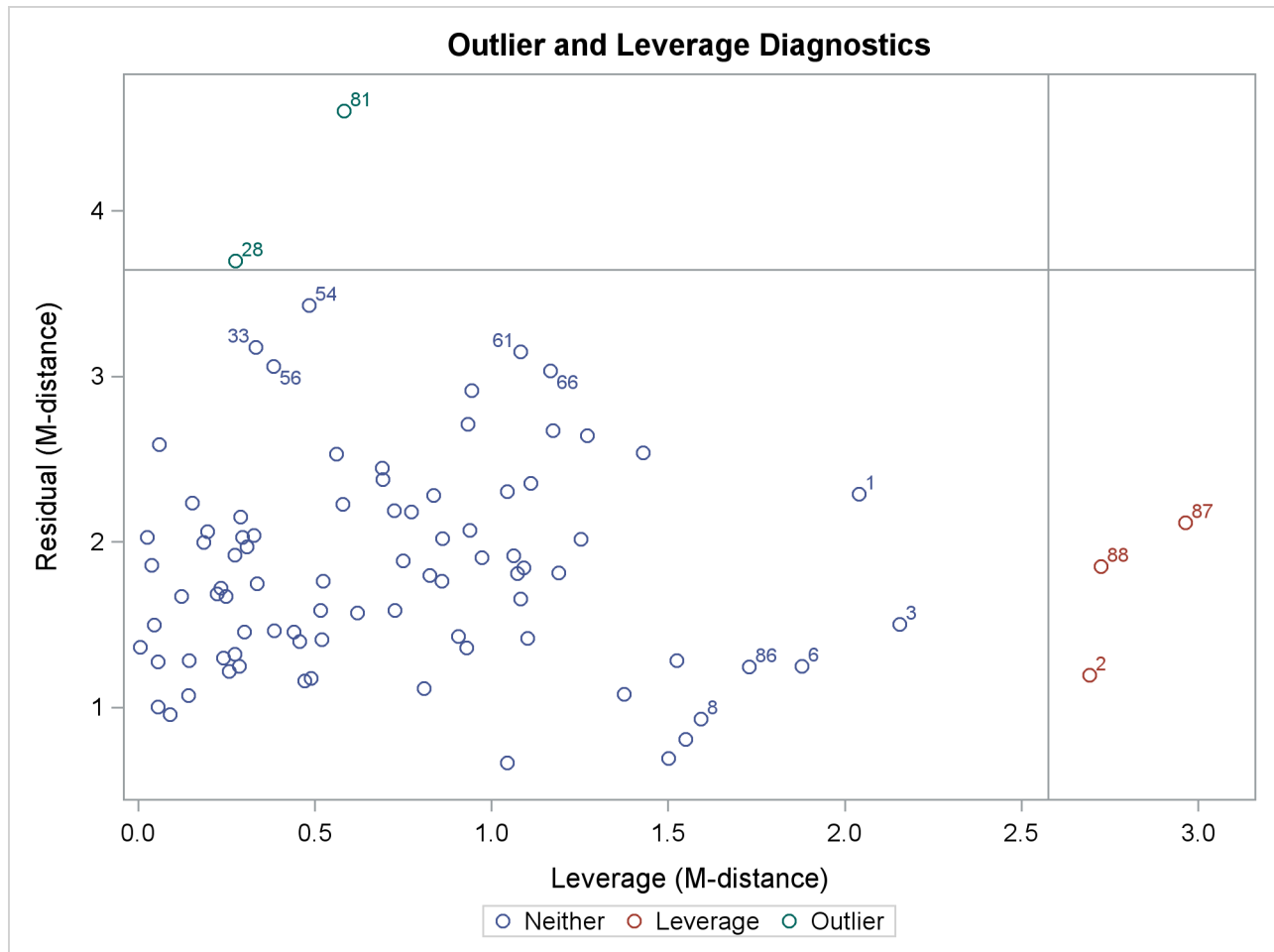
Output 27.14.1 Model Fit of Mardia Data

Fit Summary	
Chi-Square	8.9782
Chi-Square DF	5
Pr > Chi-Square	0.1099
Standardized RMR (SRMR)	0.0475
RMSEA Estimate	0.0956

Output 27.14.2 Estimates of Loadings

PATH List					
-----Path-----	Parameter	Estimate	Standard Error	t Value	
fact1 ==> mechanics		1.00000			
fact1 ==> vector	_Parm1	0.83770	0.16598	5.04687	
fact1 ==> algebra	_Parm2	0.93064	0.15369	6.05521	
fact1 ==> analysis	_Parm3	1.09480	0.19611	5.58262	
fact1 ==> statistics	_Parm4	1.19229	0.22309	5.34440	

Output 27.14.3 shows the classifications of outlier and leverage observations in a two-dimensional space. Four regions are clearly shown.

Output 27.14.3 Outliers and Leverage Observations

The upper and the lower regions are separated by a horizontal line that represents the criterion for outlier detection. This criterion is set by a certain α -level that has a probability meaning. Loosely speaking, if the model is true and the distribution of the residuals is multivariate normal, you would expect that about $\alpha \times 100\%$ of observations will have their residual M-distances above the criterion. The larger the α value, the more liberal the outlier detection criterion. This α -level is set to 0.01 by default. You can change this default by using the `ALPHAOUT=` option.

Notice that all residuals and the criterion are measured in terms of M-distances. Hence, these measures are always positive. [Output 27.14.3](#) classifies observations 81 and 28 as outliers (in the residual dimension). In addition to these two outlying observations, PROC CALIS also labels the next five observations with the largest residual M-distances. [Output 27.14.3](#) shows that observations 33, 54, 56, 61, and 66 are the closest to being labeled as outliers.

The right and left regions are separated by a vertical line that represents the criterion for leverage observations. Again, this criterion is set by a certain α -level that has a probability meaning. If the model is true and the distribution of the predictor variables (in this case, the factor variable fact1) is multivariate normal, you would expect that about $\alpha \times 100\%$ of observations will have their leverage M-distances above the criterion. The larger the α value, the more liberal the leverage observation detection criterion. This α -level is also set to 0.01 by default. You can change this default by using the `ALPHALEV=` option.

Output 27.14.3 classifies observations 2, 87, and 88 as leverage points or observations. In addition to these three observations, PROC CALIS also labels the next five observations with the largest leverage M-distances. Output 27.14.3 shows that observations 1, 3, 6, 8, and 86 are the closest to being labeled as leverage observations.

The lower left region in Output 27.14.3 contains observations that are neither outliers nor leverage observations. This region contains the majority of the observations. The upper right region in Output 27.14.3 contains observations that are classified as both outliers and leverage observations. For the current model, no observations are classified as such.

To supplement the graphical depiction of outliers and leverage observations, PROC CALIS shows two tables that contain more numerical information. Output 27.14.4 shows the seven observations that have the largest residual M-distances. The table reflects the outlier classification in Output 27.14.3 numerically. Two outliers are flagged in the table. However, none of the seven observations are leverage observations. Output 27.14.5 shows the eight observations that have the largest leverage M-distances. Again, this table reflects the classification of leverage observations in Output 27.14.3 numerically. Three leverage observations are flagged, but none of these observations are residual outliers at the same time.

Output 27.14.4 Largest Residual Outliers

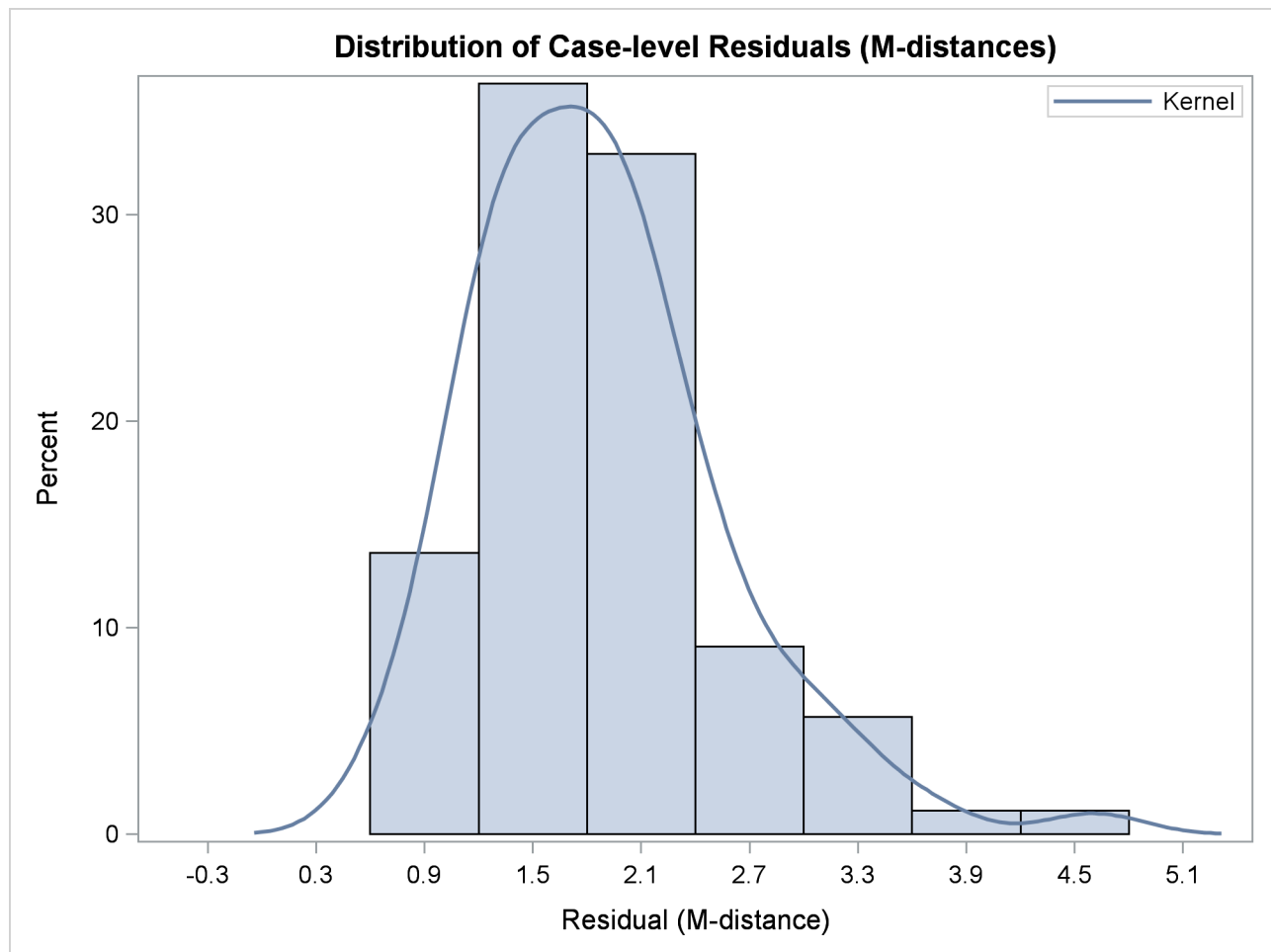
Diagnostics of the 7 Largest Case-Level Residuals (alpha=0.01)				
Case Number	Residual (M-Distance)	----Diagnostics-----		
		Outlier	Leverage	
81	4.60511	*		
28	3.69953	*		
54	3.43068			
33	3.17659			
61	3.15104			
56	3.06094			
66	3.03262			

Output 27.14.5 Largest Leverage Observations

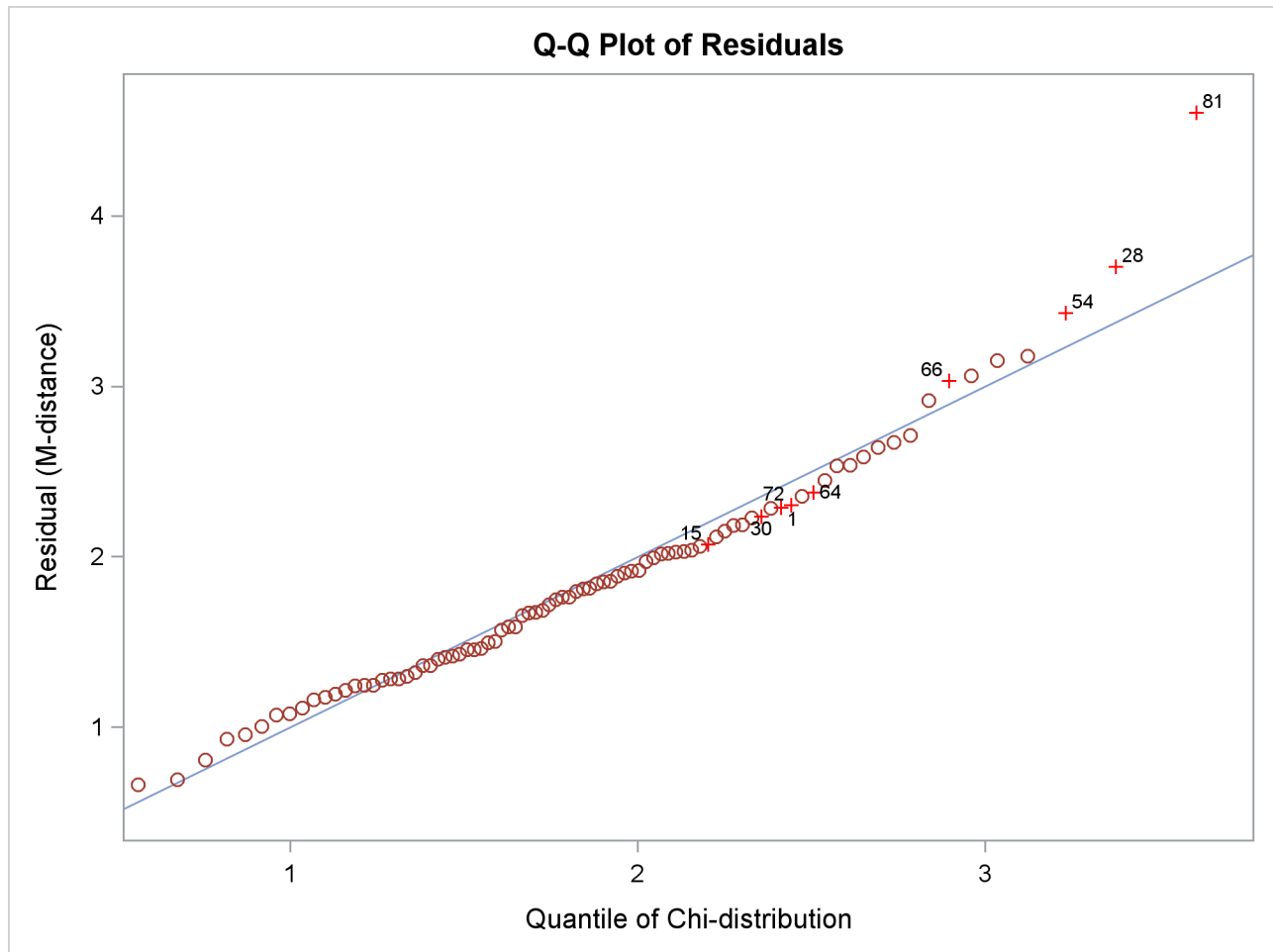
Diagnostics of the 8 Largest Case-Level Leverages (alpha=0.01)				
Case Number	Leverage (M-Distance)	----Diagnostics-----		
		Leverage	Outlier	
87	2.96438	*		
88	2.72441	*		
2	2.69293	*		
3	2.15519			
1	2.04014			
6	1.87894			
86	1.72950			
8	1.59242			

Output 27.14.6 shows the histogram and its kernel density function of the residual M-distances. Theoretically, the density should look like a χ^2 -distribution (that is, the distribution of the square root of the corresponding χ^2 variate). While this histogram provides an overall impression of the empirical distribution of the residual M-distances, it is not very useful in diagnosing the observations that do not conform to the theoretical distribution of the residual M-distances. To this end, Output 27.14.7 and Output 27.14.8 are more useful.

Output 27.14.6 Distribution of Case-Level Residuals

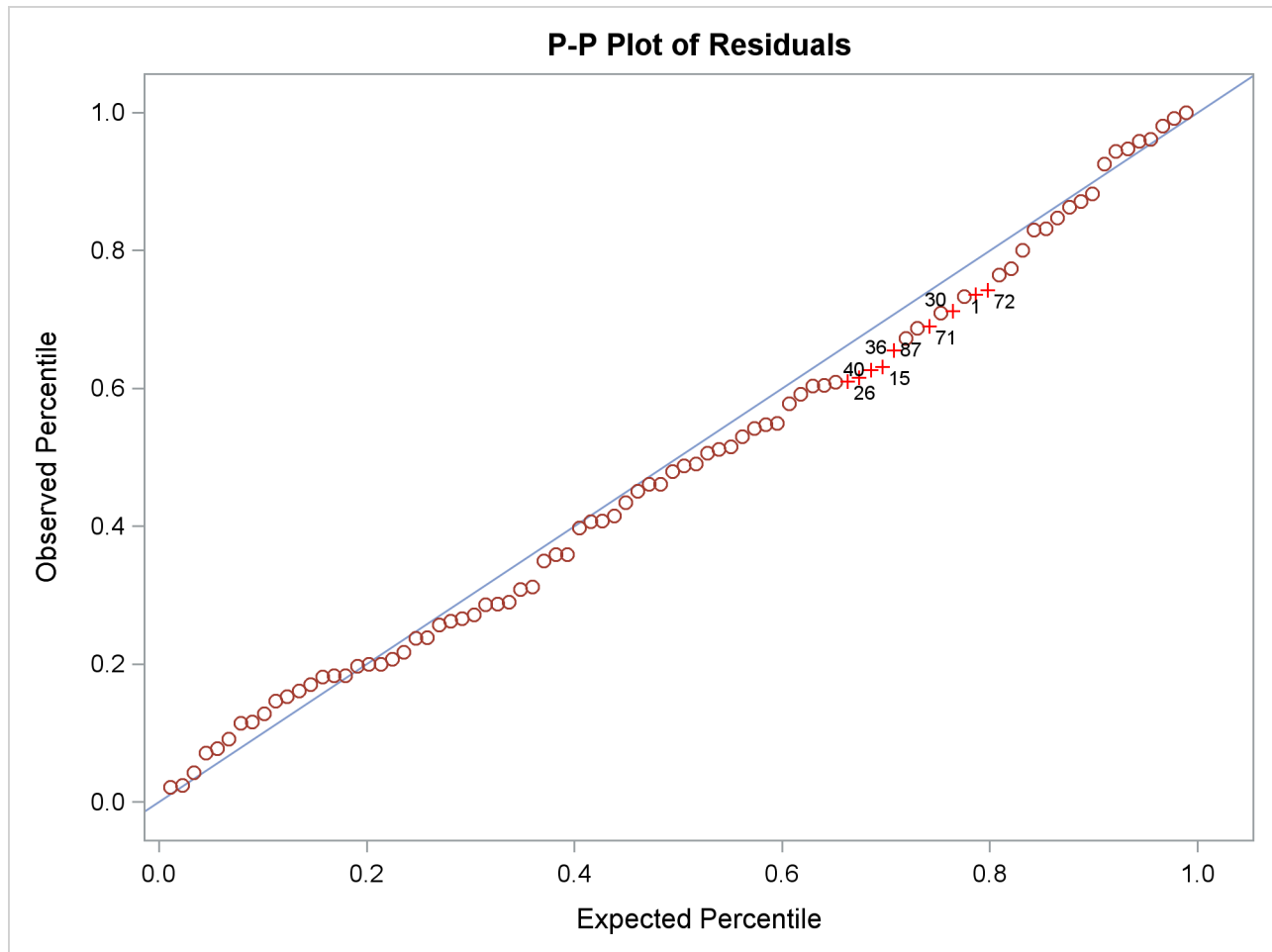


Output 27.14.7 shows the so-called Q-Q plot for the residual M-distances. The Y coordinates represent the observed quantiles, and the X coordinates represent the theoretical quantiles. Output 27.14.8 shows the so-called P-P plots for the residual M-distances. The Y coordinates represent the observed percentiles, and the X coordinates represent the theoretical percentiles. If the observed residual M-distances distribute exactly like the theoretical χ^2 -distribution, all observations should lie on the straight lines with a slope of 1 in both plots. In Output 27.14.7 and Output 27.14.8, observations with the largest departures from the straight lines are labeled.

Output 27.14.7 Q-Q Plot of Residual M-Distances

In terms of quantiles, the Q-Q plot in [Output 27.14.7](#) shows that observations 81, 28, and 54 have the largest departures from the theoretical distribution for the residual M-distances. Notice that observations 81 and 28 were also identified as outliers previously.

Output 27.14.8 P-P Plot of Residual M-Distances



In terms of percentiles, the P-P plot in [Output 27.14.8](#) shows that several observations in the middle of the distribution have the largest departures from the theoretical distribution. However, it is not clear from the plot which observations have the largest departures.

To supplement the Q-Q and the P-P plots with numerical information, PROC CALIS outputs the table in [Output 27.14.9](#), which shows the observations with the largest departures from the theoretical residual M-distance distribution in terms of quantiles and percentiles. The observations in the table are arranged by their percentile regions. Approximately 10% of the observations with the largest departures in terms of quantile and in terms of percentile, respectively, are shown in this table. However, the final percentage of observations shown in the table might not add up to 20%, because some observations could have large departures in terms of both quantile and percentile. [Output 27.14.9](#) shows that observations 1, 15, 30, and 72 are this kind of observation. However, none of these are residual outliers.

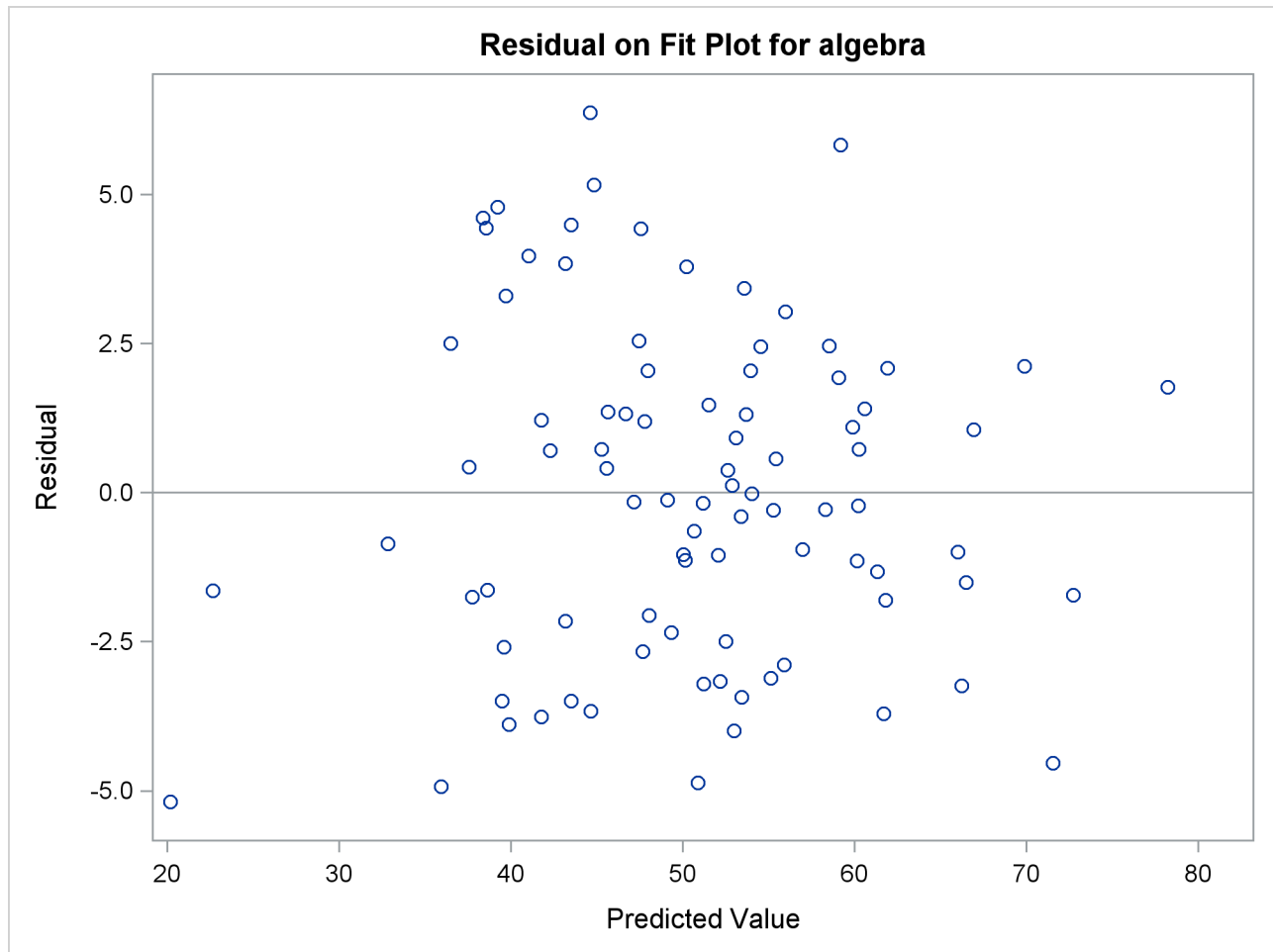
Output 27.14.9 Largest Departures from the Theoretical Residual Distribution

Largest Departures From the Theoretical Residual Distribution			
Percentile Region	Case Number	Quantile Deviation	Percentile Deviation
(.65, .90)	26		-0.05302
	36		-0.05836
	40		-0.05863
	15	-0.13087	-0.06509
	87		-0.05257
	71		-0.05145
	30	-0.11973	-0.05198
	1	-0.12344	-0.05065
	72	-0.13739	-0.05498
	64	-0.12550	
(.90, .95)	66	0.13803	
	54	0.20039	
	28	0.32398	
	81	0.99843	
> .95			

Output 27.14.10 shows the residual on fit plot for the variable algebra. Notice that unlike the preceding residual diagnostic plots where the M-distances (nonnegative) for residuals are plotted, the residuals (which can be positive or negative) themselves are plotted against the predicted values for algebra in the current residual on fit (or residual on predicted) plot. If the linear relationship as described by the one-factor model is reasonable, then the residuals should show no systematic trend with the predicted values. That is, the residuals should be randomly scattered around the plot in the range of the predicted values. The pattern of residuals in Output 27.14.10 looks sufficiently “random,” and therefore it gives support to the prescribed linear relationship between the variable algebra and the factor fact1. PROC CALIS also outputs the residual on fit plots for other dependent observed variables. To conserve space, they are not shown here. You can also control the amount of graphical output by specifying the desirable set of dependent observed variables for the residual on fit plots. For example, the following requests the residual on fit plots for the variables mechanics and analysis only, even though there are five dependent observed variables in the model:

```
PLOTS=RESBYPRED (VAR=mechanics analysis)
```

See the PLOTS= option for details.

Output 27.14.10 Residual on Fit Plot for the Variable Algebra

Direct Robust Estimation

Usually, the outlier detection process in residual diagnostics implies some treatments after their detections. For example, in the preceding analysis, observations 28 and 81 were detected as outliers. You would naturally think that the next step is to do an additional model fitting with these two outlying observations removed. While this thinking is intuitively appealing, the outlier issues are usually more complicated than can be resolved by such a “pick-and-remove” strategy. One issue is the so-called masking effect of outliers. In the preceding analysis, outliers are detected based on a criterion that is a function of the chosen criterion level (for example, the $\text{ALPHAOUT} =$ value set by the researcher) and the parameter estimates. However, because the outliers have contributed to the estimation of the parameters, you might wonder whether the outlier detection process has been contaminated by the outliers themselves. If such a masking effect is present and an additional analysis is done after employing the pick-and-remove strategy for the outliers, you would be likely to discover more outliers. As a result, you might wonder whether the outlier removal process should be carried out indefinitely.

Robust estimation provides an alternative way to resolve the issue of masking effect. In robust estimation, outlying observations are downweighted simultaneously with the estimation. Iterative steps are used to reweight the observations according to the updated parameter estimates. Hence, with robust estimation you

do not need to make a decision about removing outliers because they are already downweighted during the estimation. The issue of masking effect is avoided.

PROC CALIS provides two major methods of robust estimation—direct and two-stage. This section illustrates the direct robust estimation method, in which the model is estimated simultaneously with the (re)weighting of the observations. The next section illustrates the two-stage estimation method, in which the robust mean and covariance matrices obtained in the first stage are analyzed by the maximum likelihood (ML) estimation in the second stage. Both methods are based on the methodology proposed by Yuan and Zhong (2008) and Yuan and Hayashi (2010).

The following statements request direct robust estimation of the model for the mardia data set:

```
ods graphics on;

proc calis data=mardia residual robust plots=caseresid pcorr;
  path
    fact1 ==> mechanics vector algebra analysis statistics = 1. ;
run;

ods graphics off;
```

The ROBUST option invokes the direct robust estimation method. The direct robust method reweights the observations according to the magnitudes of the residuals during iterative steps. For this reason, you can also specify ROBUST=RES to signify direct robust estimation with residual (M-distance) weighting. Following Yuan and Hayashi (2010), there are two variants of the direct robust estimation. One treats the disturbances (that is, error terms for endogenous latent factors) as factors to estimate (see the ROBUST=RES(F) option), and the other treats the disturbances as true error terms (see the ROBUST=RES(E) option). See the ROBUST= option and the section “Robust Estimation” on page 1315 for details. These variants would not make any difference for the current one-factor model estimation, and the ROBUST option that is used in the specification is the same as ROBUST=RES(E).

You also request case-level residual analysis by using the RESIDUAL option, even though the intention now is to identify rather than to remove the outliers.

Output 27.14.11 shows the fit summary of the direct robust estimation. The model fit chi-square is 6.0031 ($df = 5$, $p = 0.3059$). Again, you fail to reject the one-factor model for the data. Unlike the regular ML estimation in the preceding analysis, both SRMR (0.0321) and RMSEA (0.0480) show good model fit. This result can be attributed to the downweighting of the outlying observations in the direct robust estimation. Output 27.14.12 shows that all loading estimates are statistically significant.

Output 27.14.11 Model Fit of Mardia Data with Direct Robust Estimation

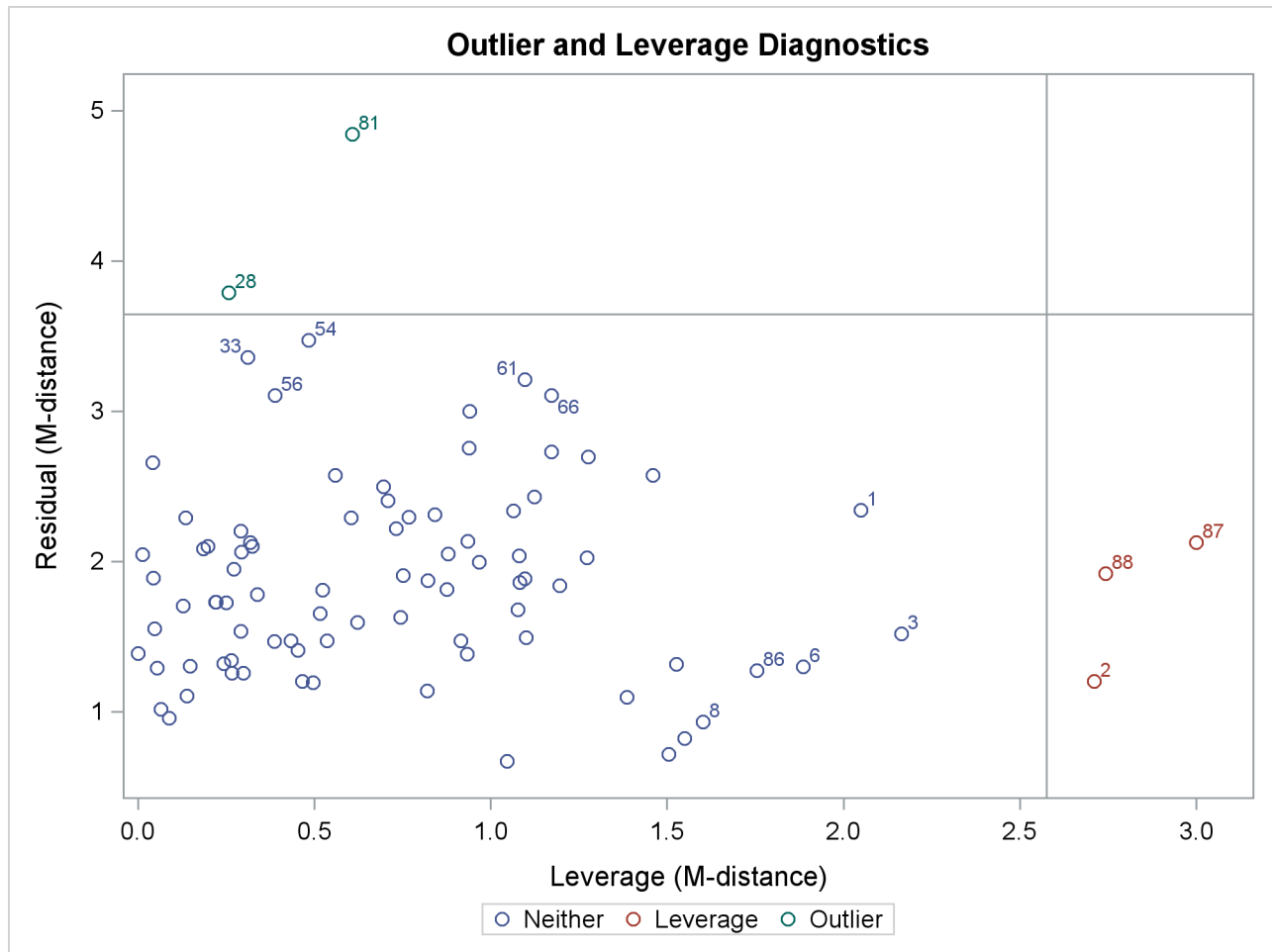
Fit Summary	
Chi-Square	6.0031
Chi-Square DF	5
Pr > Chi-Square	0.3059
Standardized RMR (SRMR)	0.0370
RMSEA Estimate	0.0480
NOTE: Saturated mean structure parameters are excluded from the computations of fit indices.	

Output 27.14.12 Estimates of Loadings with Direct Robust Estimation

PATH List						
-----Path-----	Parameter	Estimate	Standard Error	t Value		
fact1 ==> mechanics		1.00000				
fact1 ==> vector	_Parm1	0.83279	0.15680	5.31106		
fact1 ==> algebra	_Parm2	0.92854	0.14763	6.28950		
fact1 ==> analysis	_Parm3	1.08665	0.18855	5.76317		
fact1 ==> statistics	_Parm4	1.18799	0.21487	5.52890		

Output 27.14.13 shows the outlier and leverage classifications by the direct robust estimation. This plot has a similar pattern to the one obtained from the preceding regular ML estimation (see Output 27.14.3). Both plots show that observations 28 and 81 are the only outliers. Thus, the results from the direct robust estimation eliminate the concern of the masking effect.

Output 27.14.13 Outliers and Leverage Observations with Direct Robust Estimation



As a by-product of the direct robust estimation, robust (unstructured) covariance and mean matrices are computed with the **PCORR** option. **Output 27.14.14** shows the robust covariance and mean matrices obtained for the current direct robust estimation for the *mardia* data set. These matrices are essentially computed by the usual formulas for covariance and mean matrices, but with weights obtained from the final estimates of the direct robust estimation of the model. For the current analysis, outlying observations (28 and 81) receive weights of less than 1 whereas all other observations receive weights of 1 in the computation.

Output 27.14.14 Robust Covariance and Mean Matrices with Direct Robust Estimation

Robust Covariance Matrix					
	mechanics	vector	algebra	analysis	statistics
mechanics	299.05121	118.73107	104.04139	111.35028	122.12239
vector	118.73107	162.60829	86.88667	97.18075	102.10393
algebra	104.04139	86.88667	114.69031	113.43289	124.09414
analysis	111.35028	97.18075	113.43289	220.34769	156.62425
statistics	122.12239	102.10393	124.09414	156.62425	296.42019

Output 27.14.14 *continued*

	Determinant	33723890038	Ln	24.241472	
	Robust Means				
mechanics	vector	algebra	analysis	statistics	
39.11015	50.80549	50.61153	46.70196	42.21135	

Two-Stage Robust Estimation

In addition to the direct robust estimation method, PROC CALIS implements another robust estimation method for structural equation models. The two-stage robust estimation method estimates the robust means and covariance matrices in the first stage. It then fits the model to the robust mean and covariance matrix by using the ML method in the second stage. During the first stage, the robust method downweights the outlying observations in all variable dimensions. The robust properties are then propagated to the second stage of estimation.

In PROC CALIS, you can use the ROBUST=SAT option to invoke the two-stage robust estimation method, as shown in the following statements for fitting the one-factor model to the mardia data set:

```
proc calis data=mardia robust=sat pcorr;
  path
    fact1 ==> mechanics vector algebra analysis statistics = 1. ;
run;
```

With the PCORR option, the (unstructured) robust mean and covariance matrices are displayed in [Output 27.14.15](#). Although the robust covariance and mean matrices obtained here are numerically similar to those obtained from the direct robust estimation (see [Output 27.14.14](#)), they are obtained with totally different methods. The robust mean and covariance matrices in the direct robust estimation are the by-products of the model estimation, while the robust mean and covariance matrices in the two-stage robust estimation are the initial inputs for model estimation.

Output 27.14.15 Robust Covariance and Mean Matrices with Two-Stage Robust Estimation

	Robust Covariance Matrix				
	mechanics	vector	algebra	analysis	statistics
mechanics	298.83513	119.28292	99.65134	105.47098	116.68242
vector	119.28292	165.11323	84.25310	94.28855	98.70260
algebra	99.65134	84.25310	110.93012	110.46759	121.18480
analysis	105.47098	94.28855	110.46759	219.56424	155.24377
statistics	116.68242	98.70260	121.18480	155.24377	298.80146
	Determinant	36001000868	Ln	24.306813	

Output 27.14.15 *continued*

Robust Means				
mechanics	vector	algebra	analysis	statistics
39.10571	50.74232	50.65677	46.73882	42.33179

Output 27.14.16 shows the fit summary of the two-stage robust estimation. The model fit chi-square is 7.2941 ($df = 5$, $p = 0.1997$). As in direct robust estimation, you fail to reject the one-factor model for the data. Unlike the case with direct robust estimation, only SRMR (0.0366) shows a good model fit. RMSEA is 0.0726 and is not very close to a good model fit.

Output 27.14.16 Model Fit of Mardia Data with Two-Stage Robust Estimation

Fit Summary	
Chi-Square	7.2941
Chi-Square DF	5
Pr > Chi-Square	0.1997
Standardized RMR (SRMR)	0.0422
RMSEA Estimate	0.0726
NOTE: Saturated mean structure parameters are excluded from the computations of fit indices.	

Output 27.14.16 shows the estimates of loadings with the two-stage robust estimation. All the estimates are statistically significant. All the numerical results are similar to that of the direct robust estimation in Output 27.14.12.

Output 27.14.17 Estimates of Loadings with Two-Stage Robust Estimation

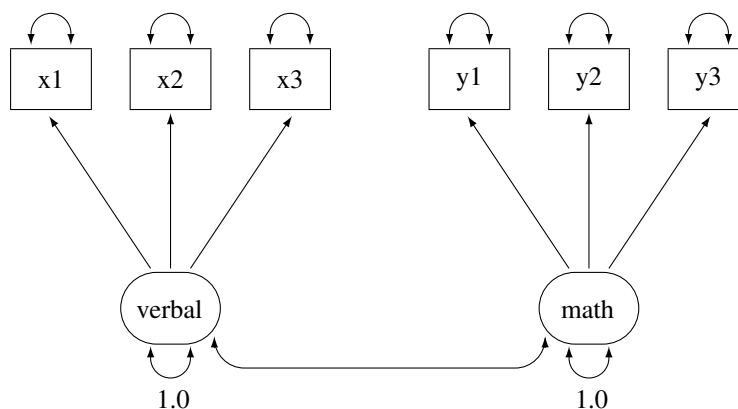
PATH List					
-----Path-----	Parameter	Estimate	Standard Error	t Value	
fact1 ==> mechanics		1.00000			
fact1 ==> vector	_Parm1	0.84322	0.16538	5.09856	
fact1 ==> algebra	_Parm2	0.93683	0.15485	6.04996	
fact1 ==> analysis	_Parm3	1.10397	0.19849	5.56172	
fact1 ==> statistics	_Parm4	1.21080	0.22686	5.33712	

The outlier and leverage observation detection in two-stage robust estimation is essentially the same method as that in direct robust estimation. Therefore, the corresponding results for the two-stage robust estimation are not shown here. See the section “Residual Diagnostics with Robust Estimation” on page 1342 for details about case-level residual analysis with robust estimation.

Example 27.15: The Full Information Maximum Likelihood Method

This example shows how you can fully utilize all available information from the data when there is a high proportion of observations with random missing value. You use the full information maximum likelihood method for model estimation.

In Example 27.12, 32 students take six tests. These six tests are indicator measures of two ability factors: verbal and math. You conduct a confirmatory factor analysis in Example 27.12 based on a data set without any missing values. The path diagram for the confirmatory factor model is shown the following:



Suppose now due to sickness or unexpected events, some students cannot take part in one of these tests. Now, the data test contains missing values at various locations, as indicated by the following DATA step:

```
data missing;
  input x1 x2 x3 y1 y2 y3;
  datalines;
23 . 16 15 14 16
29 26 23 22 18 19
14 21 . 15 16 18
20 18 17 18 21 19
25 26 22 . 21 26
26 19 15 16 17 17
. 17 19 4 6 7
12 17 18 14 16 .
25 19 22 22 20 20
7 12 15 10 11 8
29 24 . 14 13 16
28 24 29 19 19 21
12 9 10 18 19 .
11 . 12 15 16 16
20 14 15 24 23 16
26 25 . 24 23 24
20 16 19 22 21 20
14 . 15 17 19 23
14 20 13 24 . .
29 24 24 21 20 18
26 . 26 28 26 23
20 23 24 22 23 22
23 24 20 23 22 18
14 . 17 . 16 14
28 34 27 25 21 21
17 12 10 14 12 16
. 1 13 14 15 14
22 19 19 13 11 14
18 21 . 15 18 19
12 12 10 13 13 16
22 14 20 20 18 19
29 21 22 13 17 .
;
```

This data set is similar to the scores data set used in [Example 27.12](#), except that some values are replaced at random with missing values. You can still fit the same confirmatory factor analysis model described in [Example 27.12](#) to this data set by the default maximum likelihood (ML) method, as shown in the following statement:

```

proc calis data=missing;
  factor
    verbal ==> x1-x3,
    math   ==> y1-y3;
  pvar
    verbal = 1.,
    math   = 1.;
run;

```

The data set, the number of observations, the model type, and analysis type are shown in the first table of [Output 27.15.1](#). Although PROC CALIS reads all 32 records in the data set, only 16 of these records are used. The remaining 16 records contain at least one missing value in the tests. They are discarded from the analysis. Therefore, the maximum likelihood method only uses those 16 observations without missing values.

Output 27.15.1 Modeling Information of the CFA Model: Missing Data

Confirmatory Factor Model With \Dataset{Missing} Data: ML	
FACTOR Model Specification	
The CALIS Procedure	
Covariance Structure Analysis: Model and Initial Values	
Modeling Information	
Maximum Likelihood Estimation	
Data Set	WORK.MISSING
N Records Read	32
N Records Used	16
N Obs	16
Model Type	FACTOR
Analysis	Covariances

Output 27.15.2 shows the parameter estimates.

Output 27.15.2 Parameter Estimates of the CFA Model: Missing Data

Factor Loading Matrix: Estimate/StdErr/t-value		
	verbal	math
x1	5.1110 1.3110 3.8984 [_Parm1]	0
x2	5.6261 1.2561 4.4790 [_Parm2]	0
x3	4.8739 1.1410 4.2717 [_Parm3]	0
y1	0	4.4529 0.8530 5.2205 [_Parm4]
y2	0	3.8562 0.8303 4.6444 [_Parm5]
y3	0	2.6338 0.7416 3.5513 [_Parm6]
Factor Covariance Matrix: Estimate/StdErr/t-value		
	verbal	math
verbal	1.0000	0.7050 0.1464 4.8165 [_Add1]
math	0.7050 0.1464 4.8165 [_Add1]	1.0000

Output 27.15.2 *continued*

Error Variances				
Variable	Parameter	Estimate	Standard Error	t Value
x1	_Add2	11.27773	5.19739	2.16988
x2	_Add3	6.33003	4.25356	1.48817
x3	_Add4	6.47402	3.61040	1.79316
y1	_Add5	0.57143	1.51781	0.37648
y2	_Add6	2.57992	1.47618	1.74770
y3	_Add7	4.59651	1.77777	2.58555

Most of the factor loading estimates shown in [Output 27.15.2](#) are similar to those estimated from the data set without missing values, as shown in [Output 27.12.4](#). The loading estimate of y3 on the math factor shows the largest discrepancy. With only half of the data used in the current estimation, this loading estimate is 2.6338 in the current analysis, while it is 3.7596 if no data were missing, as shown in [Output 27.12.4](#). Another obvious difference between the two sets of results is that the standard error estimates for the loadings are consistently larger in the current analysis than in the analysis in [Example 27.12](#) where there are no missing data. This is expected because you have only half of the data set available in the current analysis.

Similarly, the estimates for the factor covariance and error variances are mostly similar to those in the analysis with complete data, but the standard error estimates in the current analysis are consistently higher.

The maximum likelihood method, as implemented in PROC CALIS, deletes all observations with at least one missing value in the estimation. In a sense, the partially available information of these deleted observations is wasted. This greatly reduces the efficiency of the estimation, which results in higher standard error estimates.

To fully utilize all available information from the data set with the presence of missing values, you can use the full information maximum likelihood (FIML) method in PROC CALIS, as shown in the following statements:

```
proc calis method=fiml data=missing;
  factor
    verbal ==> x1-x3,
    math   ==> y1-y3;
  pvar
    verbal = 1.,
    math   = 1.;
run;
```

In the PROC CALIS statement, you use METHOD=FIML to request the full information maximum likelihood method. Instead of deleting observations with missing values, the full information maximum likelihood method uses all available information in all observations. [Output 27.15.3](#) shows some modeling information of the FIML estimation of the confirmatory factor model on the missing data.

Output 27.15.3 Modeling Information of the CFA Model with FIML: Missing Data

Confirmatory Factor Model With Missing Data: FIML	
FACTOR Model Specification	
The CALIS Procedure	
Mean and Covariance Structures: Model and Initial Values	
Modeling Information	
Full Information Maximum Likelihood Estimation	
Data Set	WORK.MISSING
N Records Read	32
N Complete Records	16
N Incomplete Records	16
N Complete Obs	16
N Incomplete Obs	16
Model Type	FACTOR
Analysis	Means and Covariances

PROC CALIS shows you that the number of complete observations is 16 and the number of incomplete observations is 16 in the data set. All these observations are included in the estimation. The analysis type is ‘Means and Covariances’ because with full information maximum likelihood, the sample means have to be analyzed during the estimation.

For the full information maximum likelihood estimation, PROC CALIS outputs several tables to summarize the missing data patterns and statistics. [Output 27.15.4](#) shows the proportions of data that are present for the variables, individually or jointly by pairs.

Output 27.15.4 Proportions of Data Present for the Variables: Missing Data

Proportions of Data Present for Means (Diagonal) and Covariances (Off-Diagonal)						
	x1	x2	x3	y1	y2	y3
x1	0.9375					
x2	0.7813	0.8438				
x3	0.8125	0.7188	0.8750			
y1	0.8750	0.8125	0.8125	0.9375		
y2	0.9063	0.8125	0.8438	0.9063	0.9688	
y3	0.8125	0.7188	0.7500	0.8125	0.8750	0.8750
Average Proportion Coverage of Means					0.906250	
Average Proportion Coverage of Covariances					0.816667	

The diagonal elements of the table in [Output 27.15.4](#) show the proportions of data coverage by each of the variables. The off-diagonal elements shows the proportions of joint data coverage by all possible pairs of variables. For example, the first diagonal element of the table shows that about 94% of the observations have x1 values that are not missing. This percentage value is referred to as the proportion coverage for x1 or the proportion coverage for computing the means of x1. The off-diagonal element for x1 and x2 shows

that about 78% of the observations have nonmissing values for both their x1 and x2 values. This percentage value is referred to as the joint proportion coverage of x1 and x2 or the proportion coverage for computing the covariance between x1 and x2. The larger the coverage proportions this table shows, the more relative information the data contain for estimating the corresponding moments.

To summarize the proportion coverage, **Output 27.15.4** shows that on average about 91% of the data are nonmissing for computing the means, and about 82% of the data are nonmissing for computing the covariances.

Output 27.15.5 shows the lowest coverage proportions of the means and the covariances.

Output 27.15.5 Ranking the Lowest Coverage Proportions: Missing Data

Rank Order of the 3 Smallest Variable (Mean) Coverages		
Variable	Coverage	
x2	0.8438	
x3	0.8750	
y3	0.8750	

Rank Order of the 7 Smallest Covariance Coverages		
Var1	Var2	Coverage
x3	x2	0.7188
y3	x2	0.7188
y3	x3	0.7500
x2	x1	0.7813
x3	x1	0.8125
y1	x2	0.8125
y1	x3	0.8125

The first table of **Output 27.15.5** shows that x2 has the lowest proportion coverage at about 84%, and x3 and y3 are the next at about 88%. The second table of **Output 27.15.5** shows that the joint proportion coverage by the x3–x2 pair and the y3–x2 pair are the lowest at about 72%, followed by the y3–x3 pair at 75%. These two tables are useful to diagnose which variables most lack the information for estimation. For this data set, these tables show that estimation related to the moments of x2, x3, and y3 suffers the missing data problem the most. However, because the worst proportion coverage is still higher than 70%, the missingness problem does not seem to be very serious based on percentage.

In **Output 27.15.6**, PROC CALIS outputs two tables that show an overall picture of the missing patterns in the data set.

Output 27.15.6 The Most Frequent Missing Patterns and Their Mean Profiles: Missing Data

Rank Order of the 5 Most Frequent Missing Patterns					
Total Number of Distinct Patterns with Missing Values = 7					
	Pattern	NVar Miss	Freq	Proportion	Cumulative
1	x.xxxx	1	4	0.1250	0.1250
2	xx.xxx	1	4	0.1250	0.2500
3	xxxxx.	1	3	0.0938	0.3438
4	.xxxxx	1	2	0.0625	0.4063
5	xxxx..	2	1	0.0313	0.4375

NOTE: Nonmissing Pattern Proportion = 0.5000 (N=16)

Means of the Nonmissing and the Most Frequent Missing Patterns						
Variable	Nonmissing (N=16)	-----Missing Pattern-----				
		1 (N=4)	2 (N=4)	3 (N=3)	4 (N=2)	5 (N=1)
x1	21.75000	18.50000	21.75000	17.66667	.	14.00000
x2	19.37500	.	22.75000	15.66667	9.00000	20.00000
x3	19.31250	17.25000	.	16.66667	16.00000	13.00000
y1	19.00000	18.75000	17.00000	15.00000	9.00000	24.00000
y2	18.12500	18.75000	17.50000	17.33333	10.50000	.
y3	17.75000	19.50000	19.25000	.	10.50000	.

The first table of [Output 27.15.6](#) shows that “x.xxxx” and “xx.xxx” are the two most frequent missing patterns in the data set. Each has a frequency of 4. An “x” in the missing pattern denotes a nonmissing value, while a “.” denotes a missing value. Hence, the first pattern has all missing values for the second variable, and the second pattern has all missing values for the third variable. Each of these two missing patterns accounts for 12.5% of the total observations. Together, the five missing patterns shown in [Output 27.15.6](#) account for about 43.8% of the total observations. The note after this table shows that 50% of the total observations do not have any missing values.

To determine exactly which variables are missing in the missing patterns, it is useful to consult the second table in [Output 27.15.6](#). In this table, the variable means of the most frequent missing patterns are shown, together with the variable means of the nonmissing pattern for comparisons. Missing means in this table show that the corresponding variables are not present in the missing patterns. For example, the column labeled “Nonmissing” is for the group of 16 observations that do not have any missing values. Each of the variable means is computed based on 16 observations. The next column labeled “1” is the first missing pattern that has four observations. The variable mean for x2 is missing for this missing pattern group, while each of the other variable means is computed based on four observations. Comparing these means with those in the nonmissing group, it shows that the means for x1, x3, and y1 in the first missing pattern are smaller than those in the nonmissing group, while the means for y2 and y3 are greater. This comparison does not seem to suggest any systematic bias in the means of the first missing pattern group.

However, the nonmissing means in the third missing pattern (the column labeled “3” do show a consistent downward bias, as compared with the means in the nonmissing group. This might mean that respondents

with low scores in x1–x3, y1, and y2 tend not to respond to y3 for some reason. Similarly, the fourth missing pattern shows a consistent downward bias in x2, x3, and y1–y3. Whether these patterns suggest a systematic (or nonrandom) pattern of missingness must be judged in the substantive context. Nonetheless, the numerical results in [Output 27.15.6](#) provide some insight on this matter.

The tables shown in [Output 27.15.6](#) do not show all the missing patterns. In general, PROC CALIS shows only the most frequent or dominant missing patterns so that the output results are more focused. By default, if the total number of missing patterns in a data set is below six, then PROC CALIS shows all the missing patterns. If the total number of missing patterns is at least six, PROC CALIS shows up to 10 missing patterns provided that each of these missing patterns accounts for at least 5% of the total observations. The 10 missing patterns is the default maximum number of missing patterns to show, and the 5% is the default proportion threshold for a missing pattern to display. You can override the default maximum number of missing patterns by the `MAXMISSPAT=` option and the proportion threshold by the `TMISSPAT=` option.

[Output 27.15.7](#) shows the parameter estimates by the FIML estimation.

Output 27.15.7 Parameter Estimates of the CFA Model with FIML: Missing Data

Factor Loading Matrix: Estimate/StdErr/t-value		
	verbal	math
x1	5.5003	0
	1.0025	
	5.4867	
	[_Parm1]	
x2	5.7134	0
	0.9956	
	5.7385	
	[_Parm2]	
x3	4.4417	0
	0.7669	
	5.7918	
	[_Parm3]	
y1	0	4.9277
		0.6798
		7.2491
		[_Parm4]
y2	0	4.1215
		0.5716
		7.2100
		[_Parm5]
y3	0	3.3834
		0.6145
		5.5058
		[_Parm6]

Output 27.15.7 *continued*

Factor Covariance Matrix: Estimate/StdErr/t-value				
		verbal	math	
verbal		1.0000	0.5014	
			0.1473	
			3.4029	
			[_Add01]	
math		0.5014	1.0000	
		0.1473		
		3.4029		
		[_Add01]		
Error Variances				
Variable	Parameter	Estimate	Standard Error	t Value
x1	_Add08	12.72770	4.77627	2.66478
x2	_Add09	9.35994	4.48806	2.08552
x3	_Add10	5.67393	2.69872	2.10246
y1	_Add11	1.86768	1.36676	1.36650
y2	_Add12	1.49942	0.97322	1.54067
y3	_Add13	5.24973	1.54121	3.40623

First, you can compare the current FIML results with the results in [Example 27.12](#), where maximum likelihood method is used with the complete data set. Overall, the estimates of loadings, factor covariance, and error variances are similar in the two analyses. Next, you compare the current FIML results with the results in [Output 27.15.2](#), where the default ML method is applied to the same data set with missing values. Except for the standard error estimate of the factor covariance, which are very similar with ML and FIML, the standard error estimates with FIML are consistently smaller than those with ML in [Output 27.15.2](#). This means that with FIML, you improve the estimation efficiency by including the partial information in those observations with missing values.

When you have a data set with no missing values, the ML and FIML methods, as implemented in PROC CALIS, are theoretically the same. Both are equally efficient and produce similar estimates (see [Example 27.16](#)). FIML and ML are the same estimation technique that maximizes the likelihood function under the multivariate normal distribution. However, in PROC CALIS, the distinction between of ML and FIML concerns different treatments of the missing values. With METHOD=ML, all observations with one or more missing values are discarded from the analysis. With METHOD=FIML, all observations with at least one nonmissing value are included in the analysis.

Example 27.16: Comparing the ML and FIML Estimation

This example uses the complete data set from [Example 27.12](#) to illustrate how the maximum likelihood (ML) and full information maximum likelihood (FIML) methods are theoretically equivalent when you apply them to data set without missing values. In [Example 27.15](#), you apply a confirmatory factor model to a data set with missing values. You find that with METHOD=FIML, you can get more stable estimates than with METHOD=ML (which is the default estimation method). Near the end of [Example 27.15](#), you learn that ML and FIML are theoretically equivalent estimation methods when you apply them to data sets *without* missing values.

However, the ML and FIML methods have two major computational differences in their implementations in PROC CALIS. First, with METHOD=FIML the first-order properties (that is, the means of the variables) of the data are automatically included in the analysis. However, by default you analyze only the second-order properties (that is, the covariances of the variables) with METHOD=ML. Second, the biased sample covariance formula (with N as the variance divisor) is used with METHOD=FIML, while the unbiased sample covariance formula (with $DF=N - 1$ as the variance divisor) is used with METHOD=ML. See the section “[Relationships among Estimation Criteria](#)” on page 1318 for more details about the similarities and differences between the ML and FIML methods.

If you take care of these two differences between ML and FIML in PROC CALIS, you can obtain exactly the same results with these two methods when you apply them to data sets without missing values.

For example, with the complete data set scores from [Example 27.12](#), you specify the FIML estimation in the following statements:

```
proc calis method=fiml data=scores;
  factor
    verbal ===> x1-x3,
    math   ===> y1-y3;
  pvar
    verbal = 1.,
    math   = 1.;
run;
```

An equivalent specification with the ML method is shown in the following statements:

```
proc calis method=ml meanstr vardef=n data=scores;
  factor
    verbal ===> x1-x3,
    math   ===> y1-y3;
  pvar
    verbal = 1.,
    math   = 1.;
run;
```


In the PROC CALIS statement, you specify two options to make the ML estimation exactly equivalent to the FIML estimation in PROC CALIS. First, the MEANSTR option requests the first-order properties (the mean structures) to be analyzed with the covariance structures. Second, the VARDEF=N option defines the variance divisor to N, instead of the default DF, which is the same as N-1. These two options make the ML estimation equivalent to the FIML estimation.

Output 27.16.1 and Output 27.16.2 show some fit summary statistics under the FIML and ML methods, respectively.

Output 27.16.1 Model Fitting by the FIML Method: Scores Data

Fit Summary	
Fit Function	31.7837
Chi-Square	10.1215
Chi-Square DF	8
Pr > Chi-Square	0.2566
Standardized RMR (SRMR)	0.0571
RMSEA Estimate	0.0910
Bentler Comparative Fit Index	0.9872
NOTE: Saturated mean structure parameters are excluded from the computations of fit indices.	

Output 27.16.2 Model Fitting by the ML Method: Scores Data

Fit Summary	
Fit Function	0.3163
Chi-Square	10.1215
Chi-Square DF	8
Pr > Chi-Square	0.2566
Standardized RMR (SRMR)	0.0504
RMSEA Estimate	0.0910
Bentler Comparative Fit Index	0.9872

Except for the fit function values, both FIML and ML methods produce the same set of fit statistics. The difference in the fit function values is expected because the FIML function has a constant term which is derived from the likelihood function. This constant term does not depend on the model parameters. Hence, the FIML and ML discrepancy functions that are used in PROC CALIS are equivalent when VARDEF=N is used in the ML method for analyzing mean and covariance structures.

The parameter estimates are shown in Output 27.16.3 and Output 27.16.4 for the FIML and ML methods, respectively. Except for very tiny numerical differences in some estimates, the FIML and ML estimates match.

Output 27.16.3 Parameter Estimates by the FIML Method: Scores Data

Factor Loading Matrix: Estimate/StdErr/t-value		
	verbal	math
x1	5.7486 0.9651 5.9567 [_Parm1]	0
x2	5.7265 0.9239 6.1980 [_Parm2]	0
x3	4.5886 0.7570 6.0618 [_Parm3]	0
y1	0	5.1972 0.6779 7.6662 [_Parm4]
y2	0	4.1342 0.6025 6.8612 [_Parm5]
y3	0	3.7004 0.6143 6.0237 [_Parm6]
Factor Covariance Matrix: Estimate/StdErr/t-value		
	verbal	math
verbal	1.0000	0.5175 0.1406 3.6804 [_Add01]
math	0.5175 0.1406 3.6804 [_Add01]	1.0000

Output 27.16.3 *continued*

Intercepts				
Variable	Parameter	Estimate	Standard Error	t Value
x1	_Add02	19.90625	1.17540	16.93575
x2	_Add03	18.81250	1.14089	16.48928
x3	_Add04	18.68750	0.92749	20.14856
y1	_Add05	17.90625	0.93161	19.22084
y2	_Add06	17.84375	0.78823	22.63773
y3	_Add07	17.75000	0.76419	23.22725
Error Variances				
Variable	Parameter	Estimate	Standard Error	t Value
x1	_Add08	11.16406	4.06574	2.74589
x2	_Add09	8.85978	3.65403	2.42466
x3	_Add10	6.47248	2.47685	2.61319
y1	_Add11	0.76135	1.23420	0.61687
y2	_Add12	2.79060	1.04306	2.67539
y3	_Add13	4.99466	1.40025	3.56698

Output 27.16.4 Parameter Estimates by the ML Method: Scores Data

Factor Loading Matrix: Estimate/StdErr/t-value		
	verbal	math
x1	5.7486 0.9651 5.9567 [_Parm1]	0
x2	5.7265 0.9239 6.1981 [_Parm2]	0
x3	4.5885 0.7570 6.0617 [_Parm3]	0
y1	0	5.1972 0.6779 7.6662 [_Parm4]
y2	0	4.1341 0.6025 6.8612 [_Parm5]
y3	0	3.7004 0.6143 6.0238 [_Parm6]
Factor Covariance Matrix: Estimate/StdErr/t-value		
	verbal	math
verbal	1.0000	0.5175 0.1406 3.6800 [_Add01]
math	0.5175 0.1406 3.6800 [_Add01]	1.0000

Output 27.16.4 *continued*

Intercepts				
Variable	Parameter	Estimate	Standard Error	t Value
x1	_Add02	19.90625	1.17540	16.93575
x2	_Add03	18.81250	1.14089	16.48928
x3	_Add04	18.68750	0.92749	20.14856
y1	_Add05	17.90625	0.93161	19.22084
y2	_Add06	17.84375	0.78823	22.63773
y3	_Add07	17.75000	0.76419	23.22725

Error Variances				
Variable	Parameter	Estimate	Standard Error	t Value
x1	_Add08	11.16365	4.06567	2.74583
x2	_Add09	8.85925	3.65397	2.42456
x3	_Add10	6.47288	2.47689	2.61331
y1	_Add11	0.76124	1.23420	0.61679
y2	_Add12	2.79066	1.04307	2.67543
y3	_Add13	4.99461	1.40024	3.56697

The equivalence between METHOD=ML and METHOD=FIML implies that if you do not have any missing data in your data, you can just use METHOD=ML because it is computationally more efficient than the FIML method.

While the equivalence between ML and FIML is established here with the use of the VARDEF= and MEANSTR options (for data without missing values), it is not necessary in practice to use these options with METHOD=ML. The VARDEF= option is used in this example only to demonstrate the theoretical equivalence between METHOD=ML and METHOD=FIML. The VARDEF= option has very little effect if you have at least a moderate sample size (for example, 30 or more observations).

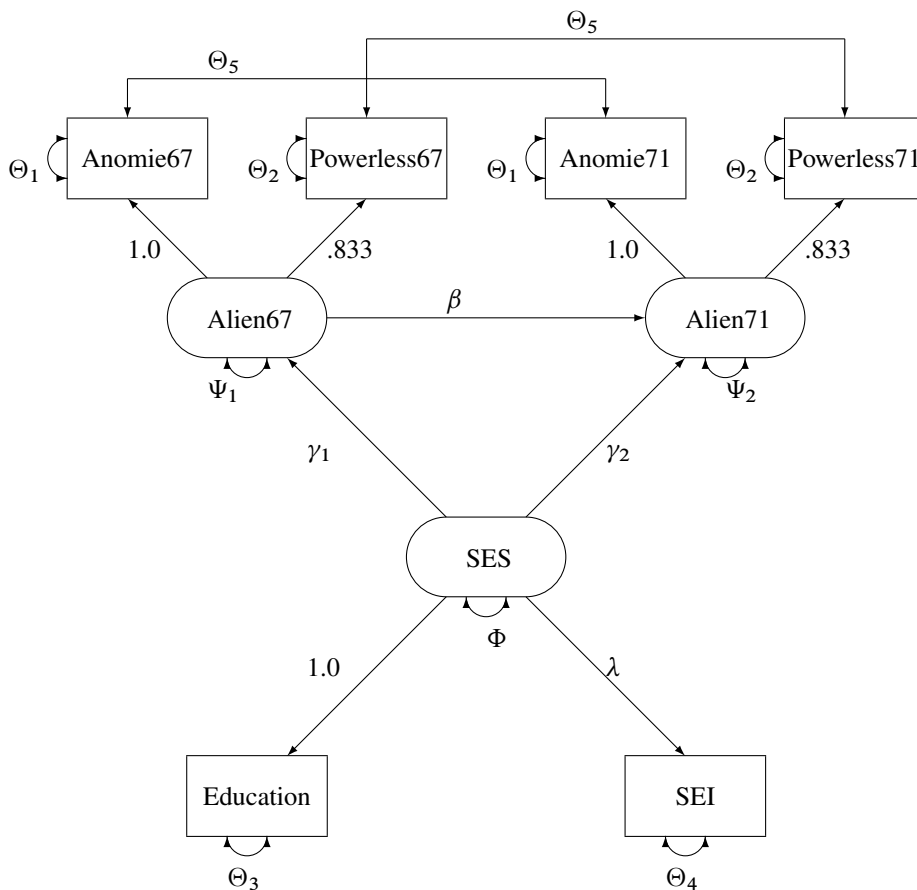
Merely adding the MEANSTR option to an analysis for data without missing values amounts to adding a saturated mean structure to a covariance structure analysis. In this case, the MEANSTR option only gives you more estimates that pertain to the mean structures, but the parameter estimates that pertain to the covariance structures do not change. Therefore, use the MEANSTR option only when you need to estimate certain mean structure parameters or when you fit models with nonsaturated mean structures.

However, use METHOD=FIML when there are missing values in your data and you need to use every bit of information from the incomplete observations with random missing values.

Example 27.17: Path Analysis: Stability of Alienation

The following covariance matrix from Wheaton et al. (1977) has served to illustrate the performance of several implementations for the analysis of structural equation models. Two different models have been analyzed by an early implementation of LISREL and are mentioned in Jöreskog (1978). You can also find a more detailed discussion of these models in the LISREL VI manual (Jöreskog and Sörbom 1985). A slightly modified model for this covariance matrix is included in the EQS 2.0 manual (Bentler 1985, p. 28). However, for the analysis with the EQS implementation, the SEI variable is rescaled by a factor of 0.1 to make the matrix less ill-conditioned. Since the Levenberg-Marquardt or Newton-Raphson optimization techniques are used with PROC CALIS, rescaling the data matrix is not necessary and, therefore, is not done here. The results reported here reflect the estimates based on the original covariance matrix.

The path diagram of this model is displayed in Figure 27.1 and is reproduced in the following:



You use the PATH modeling language of PROC CALIS to specify this path model, as shown in the following statements:

```

title "Stability of Alienation";
title2 "Data Matrix of WHEATON, MUTHEN, ALWIN & SUMMERS (1977)";
data Wheaton(TYPE=COV);
  _type_ = 'cov';
  input _name_ $ 1-11 Anomie67 Powerless67 Anomie71 Powerless71
          Education SEI;
  label Anomie67='Anomie (1967)' Powerless67='Powerlessness (1967)'
        Anomie71='Anomie (1971)' Powerless71='Powerlessness (1971)'
        Education='Education' SEI='Occupational Status Index';
  datalines;
Anomie67      11.834      .      .      .      .      .
Powerless67   6.947      9.364      .      .      .      .
Anomie71      6.819      5.091     12.532      .      .      .
Powerless71   4.783      5.028      7.495      9.986      .      .
Education     -3.839     -3.889     -3.841     -3.625      9.610      .
SEI           -21.899    -18.831    -21.748    -18.775     35.522     450.288
;

ods graphics on;

proc calis nob=932 data=Wheaton plots=residuals;
  path
    Anomie67   Powerless67 <=== Alien67   = 1.0 0.833,
    Anomie71   Powerless71 <=== Alien71   = 1.0 0.833,
    Education  SEI          <=== SES       = 1.0 lambda,
    Alien67    Alien71      <=== SES       = gamma1 gamma2,
    Alien71    <=== Alien67   = beta;
  pvar
    Anomie67   = theta1,
    Powerless67 = theta2,
    Anomie71   = theta1,
    Powerless71 = theta2,
    Education  = theta3,
    SEI        = theta4,
    Alien67    = psi1,
    Alien71    = psi2,
    SES        = phi;
  pcov
    Anomie67   Anomie71   = theta5,
    Powerless67 Powerless71 = theta5;
run;

ods graphics off;

```

Since no `METHOD=` option is used in the PROC CALIS statement, maximum likelihood estimates are computed by default.

In the PATH statement, you specify the functional relationships of the variables in the model. These functional relationships are represented as single-headed paths in the path diagram. There are five entries in the PATH statement. You specify the relationships between the latent constructs and the observed variables in the first three path entries. For example, the first entry states that Anomie and Powerless67 are measured indicators of the latent variable Alien67. The path effects or coefficients from the latent factor to these measured indicators are fixed at 1.0 and 0.833, respectively. Similarly, in the next two path entries, you

define the relationships between the latent factors Alien71 and SES and their measured indicators. The last two path entries in the PATH statement represent the functional relationships among the latent variables in the model. SES has effects on Alien67 and Alien71. These effect parameters are labeled or named with gamma1 and gamma2, respectively. Alien67 also has an effect on Alien71, with the effect parameter named beta.

In the PVAR statement, you specify the variance or error variance parameters in the model. These parameters correspond to the double-headed arrows pointing to the individual variables in the path diagram. In the first six entries of the PVAR statement, you specify the error variance parameters of the observed variables. You also give names to these parameters that correspond to the notation in the path diagram. Although you can choose any names for the parameters, it is important to remember that parameters with the same name are identical and will have the same estimates. For example, the error variances of Anomie67 and Anomie71 are the same parameter named theta1. Similarly, you constrain the error variances of Powerless67 and Powerless71. However, the error variance parameters of Education and SEI are unique. They are not constrained with other parameters in the model because they have unique parameter names. Next, you specify the error variance parameters of Alien67 and Alien71. They also have unique parameter names and therefore they are not constrained with any other parameters in the model. Lastly, you specify the variance parameter phi of SES.

In the PCOV statement, you specify the covariances or error covariances among variables in the model. These parameters correspond to the double-headed arrows pointing to distinct pairs of variables in the path diagram. Observed variables Anomie67 and Anomie71 have correlated errors and you specify this error covariance parameter as theta5. Similarly, observed variables Powerless67 and Powerless71 have correlated errors and you also specify this error covariance parameter as theta5. This way, the two error covariances are constrained to be equal.

PROC CALIS can produce a high-quality residual histogram that is useful for showing the distribution of residuals. Before you request the residual histogram, ODS Graphics must be enabled. For example, you can specify the ODS GRAPHICS ON statement, as shown in the preceding statements before the PROC CALIS statement. Then, the residual histogram is requested by the `plots=residuals` option in the PROC CALIS statement.

Output 27.17.1 displays the modeling information and variables in the analysis.

Output 27.17.1 Model Specification and Variables

PATH Model Specification	
The CALIS Procedure	
Covariance Structure Analysis: Model and Initial Values	
Modeling Information	
Maximum Likelihood Estimation	
Data Set	WORK.WHEATON
N Obs	932
Model Type	PATH
Analysis	Covariances

Output 27.17.1 *continued*

Variables in the Model					
Endogenous	Manifest	Anomie67	Anomie71	Education	Powerless67
		Powerless71	SEI		
Exogenous	Latent	Alien67	Alien71		
	Manifest				
	Latent	SES			
Number of Endogenous Variables = 8					
Number of Exogenous Variables = 1					

Output 27.17.1 shows that the data set Wheaton was used with 932 observations. The model is specified with the PATH modeling language. Variables in the model are classified into different categories according to their roles. All manifest variables are endogenous in the model. Also, three latent variables are hypothesized in the model: Alien67, Alien71, and SES. While Alien67 and Alien71 are endogenous, SES is exogenous in the model.

Output 27.17.2 echoes the initial specification of the PATH model.

Output 27.17.2 Initial Estimates

Initial Estimates for PATH List				
-----Path-----		Parameter	Estimate	
Anomie67	<===	Alien67	1.00000	
Powerless67	<===	Alien67	0.83300	
Anomie71	<===	Alien71	1.00000	
Powerless71	<===	Alien71	0.83300	
Education	<===	SES	1.00000	
SEI	<===	SES	lambda	.
Alien67	<===	SES	gamma1	.
Alien71	<===	SES	gamma2	.
Alien71	<===	Alien67	beta	.
Initial Estimates for Variance Parameters				
Variance Type	Variable	Parameter	Estimate	
Error	Anomie67	theta1	.	
	Powerless67	theta2	.	
	Anomie71	theta1	.	
	Powerless71	theta2	.	
	Education	theta3	.	
	SEI	theta4	.	
	Alien67	psi1	.	
Exogenous	Alien71	psi2	.	
	SES	phi	.	

Output 27.17.2 *continued*

Initial Estimates for Covariances Among Errors			
Error of	Error of	Parameter	Estimate
Anomie67	Anomie71	theta5	.
Powerless67	Powerless71	theta5	.

In [Output 27.17.2](#), numerical values for estimates are the initial values you input in the model specification. If the associated parameter name for a numerical estimate is blank, it means that the estimate is a fixed value, which would not be changed in the estimation. For example, the first five paths have fixed path coefficients with the fixed values given. For numerical estimates with parameter names given, the numerical values serve as initial values, which would be changed during the estimation. In [Output 27.17.2](#), you actually do not have this kind of specification. All free parameters specified in the model are with missing initial values, denoted by ‘.’. For example, lambda, gamma1, theta1, and psi1, among others, are free parameters without initial values given. PROC CALIS generates the initial values of these parameters automatically.

You can examine this output to ensure that the desired model is being analyzed. PROC CALIS outputs the initial specifications or the estimation results in the order you specify in the model, unless you use reordering options such as [ORDERSPEC](#) and [ORDERALL](#). Therefore, the input order of specifications is important—it determines how your output would look.

Simple descriptive statistics are displayed in [Output 27.17.3](#).

Output 27.17.3 Descriptive Statistics

Simple Statistics			
	Variable	Mean	Std Dev
Anomie67	Anomie (1967)	0	3.44006
Powerless67	Powerlessness (1967)	0	3.06007
Anomie71	Anomie (1971)	0	3.54006
Powerless71	Powerlessness (1971)	0	3.16006
Education	Education	0	3.10000
SEI	Occupational Status Index	0	21.21999

Because the input data set contains only the covariance matrix, the means of the manifest variables are assumed to be zero. Note that this has no impact on the estimation, unless a mean structure model is being analyzed.

Initial estimates are necessary in all kinds of optimization problems. You can provide these initial estimates or let PROC CALIS to generate them automatically. As shown in [Output 27.17.2](#), you did not provide any initial estimates for the parameters. PROC CALIS uses a combination of well-behaved mathematical methods to complete the initial estimation. The initial estimation methods for the current analysis are shown in [Output 27.17.4](#).

Output 27.17.4 Optimization Starting Point

Initial Estimation Methods			
1	Instrumental Variables Method		
2	McDonald Method		
3	Two-Stage Least Squares		
Optimization Start Parameter Estimates			
N	Parameter	Estimate	Gradient
1	lambda	4.99508	-0.00206
2	gamma1	-0.62322	-0.04069
3	gamma2	-0.20437	-0.03816
4	beta	0.66589	0.03789
5	theta1	3.51433	-0.00409
6	theta2	3.65991	0.01182
7	theta3	2.49860	-0.00578
8	theta4	272.85274	0.0000194
9	psi1	5.57764	-0.00217
10	psi2	3.79636	-0.00935
11	phi	7.11140	0.00108
12	theta5	0.45298	-0.06463
Value of Objective Function = 0.0365979443			

In this example, the instrumental variable Method, the McDonald and Hartmann method, and the two-stage least squares method have been used for initial estimation. In the same output, the vector of initial parameter estimates and their gradients are also shown. The initial objective function value is 0.0366.

Output 27.17.5 displays the optimization information, including technical details, iteration history and convergence status.

Output 27.17.5 Optimization

Optimization Start									
Active Constraints			0	Objective Function			0.0365979443		
Max Abs Gradient Element			0.0646338767	Radius			1		
Iter	Rest arts	Func Calls	Act Con	Objective Function	Obj Fun Change	Max Abs Gradient Element	Lambda	Actual Over Pred Change	
1	0	4	0	0.01453	0.0221	0.00142	0	1.013	
2	0	6	0	0.01448	0.000046	0.000249	0	1.001	
3	0	8	0	0.01448	1.007E-7	4.717E-6	0	1.006	
Optimization Results									
Iterations			3	Function Calls			11		
Jacobian Calls			5	Active Constraints			0		
Objective Function			0.0144844814	Max Abs Gradient Element			4.7172823E-6		
Lambda			0	Actual Over Pred Change			1.0060912391		
Radius			0.001390392						
Convergence criterion (ABSGCONV=0.00001) satisfied.									

The convergence status is important for the validity of your solution. In most cases, you should interpret your results only when the solution is converged. In this example, you obtain a converged solution, as shown in the message at the bottom of the table. The final objective function value is 0.01448, which is the minimized function value during the optimization. If problematic solutions such as nonconvergence are encountered, PROC CALIS issues an error message.

The fit summary statistics are displayed in [Output 27.17.6](#). By default, PROC CALIS displays all available fit indices and modeling information.

Output 27.17.6 Fit Summary

Fit Summary		
Modeling Info	Number of Observations	932
	Number of Variables	6
	Number of Moments	21
	Number of Parameters	12
	Number of Active Constraints	0
	Baseline Model Function Value	2.2894
	Baseline Model Chi-Square	2131.4327
	Baseline Model Chi-Square DF	15
	Pr > Baseline Model Chi-Square	<.0001
Absolute Index	Fit Function	0.0145
	Chi-Square	13.4851
	Chi-Square DF	9
	Pr > Chi-Square	0.1419
	Z-Test of Wilson & Hilferty	1.0754
	Hoelter Critical N	1169
	Root Mean Square Residual (RMR)	0.2281
	Standardized RMR (SRMR)	0.0150
	Goodness of Fit Index (GFI)	0.9953
Parsimony Index	Adjusted GFI (AGFI)	0.9890
	Parsimonious GFI	0.5972
	RMSEA Estimate	0.0231
	RMSEA Lower 90% Confidence Limit	0.0000
	RMSEA Upper 90% Confidence Limit	0.0470
	Probability of Close Fit	0.9705
	ECVI Estimate	0.0405
	ECVI Lower 90% Confidence Limit	0.0357
	ECVI Upper 90% Confidence Limit	0.0556
	Akaike Information Criterion	37.4851
	Bozdogan CAIC	107.5330
Schwarz Bayesian Criterion	95.5330	
McDonald Centrality	0.9976	
Incremental Index	Bentler Comparative Fit Index	0.9979
	Bentler-Bonett NFI	0.9937
	Bentler-Bonett Non-normed Index	0.9965
	Bollen Normed Index Rho1	0.9895
	Bollen Non-normed Index Delta2	0.9979
	James et al. Parsimonious NFI	0.5962

First, the fit summary table starts with some basic modeling information, as shown in [Output 27.17.6](#). You can check the number of observations, number of variables, number of moments being fitted, number of parameters, number of active constraints in the solution, and the independent model chi-square and its degrees of freedom in this modeling information category. Next, three types of fit indices are shown: absolute, parsimony, and incremental.

The absolute indices are fit measures that you interpret them without referring to any baseline model. These indices do not adjust for model parsimony. They always favor models with a large number of parameters. The chi-square test statistic is the best-known absolute index in this category. In this example, the p -value of the chi-square is 0.1419, which is greater than the conventional 0.05 value. From the statistical hypothesis testing point of view, you cannot reject this model. The Z-test of Wilson and Hilferty is also insignificant at $\alpha = .05$, which echoes the result of the chi-square test. You can consult other absolute indices as

well. Although it seems that there are no clear conventional levels for these absolute indices to indicate an acceptable model fit, you can always use these indices to compare the relative fit among competing models.

Next, the parsimony fit indices take the model parsimony into account. These indices adjust the model fit by the degrees of freedom (or the number of the parameters) of the model in certain ways. The advantage of these indices is that merely increasing the number of parameters in the model might not necessarily lead better model fit measures. These fit indices penalize models with large numbers of parameters. There is no universal way to interpret all these indices. However, for the relatively well-known RMSEA estimate, by convention values under 0.05 indicate good model fit. The RMSEA value for this example is 0.0231, and so this is a very good model fit. For interpretations of other parsimony indices, you can consult the original articles for these indices.

Last, the incremental fit indices are computed based on comparing the target model fit against the fit of a baseline model, which is usually the so-called uncorrelatedness model where all manifest variables are assumed to be uncorrelated. This is the baseline model that PROC CALIS uses. The baseline model fit statistic is shown under the 'Modeling Info' category of the same fit summary table. In this example, the model fit chi-square of the baseline model is 2131.43, with 15 degrees of freedom. The incremental indices show how well the hypothesized model improves over the baseline model for the data. Various incremental fit indices have been proposed. In the fit summary table, there are six of such fit indices. Large values for these indices are desired. It has been suggested that values greater than .9 for these indices indicate acceptable model fit. In this example, all incremental indices but James et al. parsimonious NFI show that the hypothesized model fits well.

There is no consensus as to which fit index is the best to judge model fit. Probably, with artificial data and model, all fit indices can be shown defective in some aspects of measuring model fit. Conventional wisdom is to look at all fit indices and determine whether the majority of them are close to the desirable ranges of values. In this example, almost all fit indices are good, and so it is safe to conclude that the model fits well.

Nowadays, most researchers pay less attention to the model fit chi-square statistic because it tends to reject all meaningful models with minimum departures from the truth. Although the model fit chi-square test statistic is an impeccable statistical inference tool when the underlying statistical assumptions are satisfied, for practical purposes it is just too powerful to accept any useful and reasonable models with only tiny imperfections. Some fit indices are more popular than others. Standardized RMR, RMSEA estimate, adjusted AGFI, and Bentler's comparative fit index are frequently reported in empirical research for judging model fit. In this example, all these measures show good model fit of the hypothesized model. While there are certainly legitimate reasons why these fit indices are more popular than others, they are out of the current scope of discussion.

PROC CALIS can perform a detailed residual analysis. Large residuals might indicate misspecification of the model. In [Output 27.17.7](#), raw residuals are reported and ranked.

Output 27.17.7 Raw Residuals and Ranking

Raw Residual Matrix				
		Anomie67	Powerless67	Anomie71
Anomie67	Anomie (1967)	-0.06997	0.03642	-0.01116
Powerless67	Powerlessness (1967)	0.03642	0.01261	0.15600
Anomie71	Anomie (1971)	-0.01116	0.15600	-0.08381
Powerless71	Powerlessness (1971)	-0.15200	0.01135	-0.00854
Education	Education	0.32892	-0.41712	0.22464
SEI	Occupational Status Index	0.47786	-0.19108	0.07976

Raw Residual Matrix				
		Powerless71	Education	SEI
Anomie67	Anomie (1967)	-0.15200	0.32892	0.47786
Powerless67	Powerlessness (1967)	0.01135	-0.41712	-0.19108
Anomie71	Anomie (1971)	-0.00854	0.22464	0.07976
Powerless71	Powerlessness (1971)	0.14067	-0.23832	-0.59248
Education	Education	-0.23832	0.00000	0.00000
SEI	Occupational Status Index	-0.59248	0.00000	0.00000

Average Absolute Residual	0.153940
Average Off-diagonal Absolute Residual	0.195044

Rank Order of the 10 Largest Raw Residuals		
Var1	Var2	Residual
SEI	Powerless71	-0.59248
SEI	Anomie67	0.47786
Education	Powerless67	-0.41712
Education	Anomie67	0.32892
Education	Powerless71	-0.23832
Education	Anomie71	0.22464
SEI	Powerless67	-0.19108
Anomie71	Powerless67	0.15600
Powerless71	Anomie67	-0.15200
Powerless71	Powerless71	0.14067

Because of the differential scaling of the variables, it is usually more useful to examine the standardized residuals instead. In [Output 27.17.8](#), for example, the table for the 10 largest asymptotically standardized residuals is displayed.

Output 27.17.8 Asymptotically Standardized Residuals and Ranking

Asymptotically Standardized Residual Matrix				
		Anomie67	Powerless67	Anomie71
Anomie67	Anomie (1967)	-0.30882	0.52686	-0.05619
Powerless67	Powerlessness (1967)	0.52686	0.05464	0.87613
Anomie71	Anomie (1971)	-0.05619	0.87613	-0.35460
Powerless71	Powerlessness (1971)	-0.86507	0.05735	-0.12169
Education	Education	2.55338	-2.76371	1.69781
SEI	Occupational Status Index	0.46484	-0.17015	0.07009

Asymptotically Standardized Residual Matrix				
		Powerless71	Education	SEI
Anomie67	Anomie (1967)	-0.86507	2.55338	0.46484
Powerless67	Powerlessness (1967)	0.05735	-2.76371	-0.17015
Anomie71	Anomie (1971)	-0.12169	1.69781	0.07009
Powerless71	Powerlessness (1971)	0.58521	-1.55750	-0.49608
Education	Education	-1.55750	0.00000	0.00000
SEI	Occupational Status Index	-0.49608	0.00000	0.00000

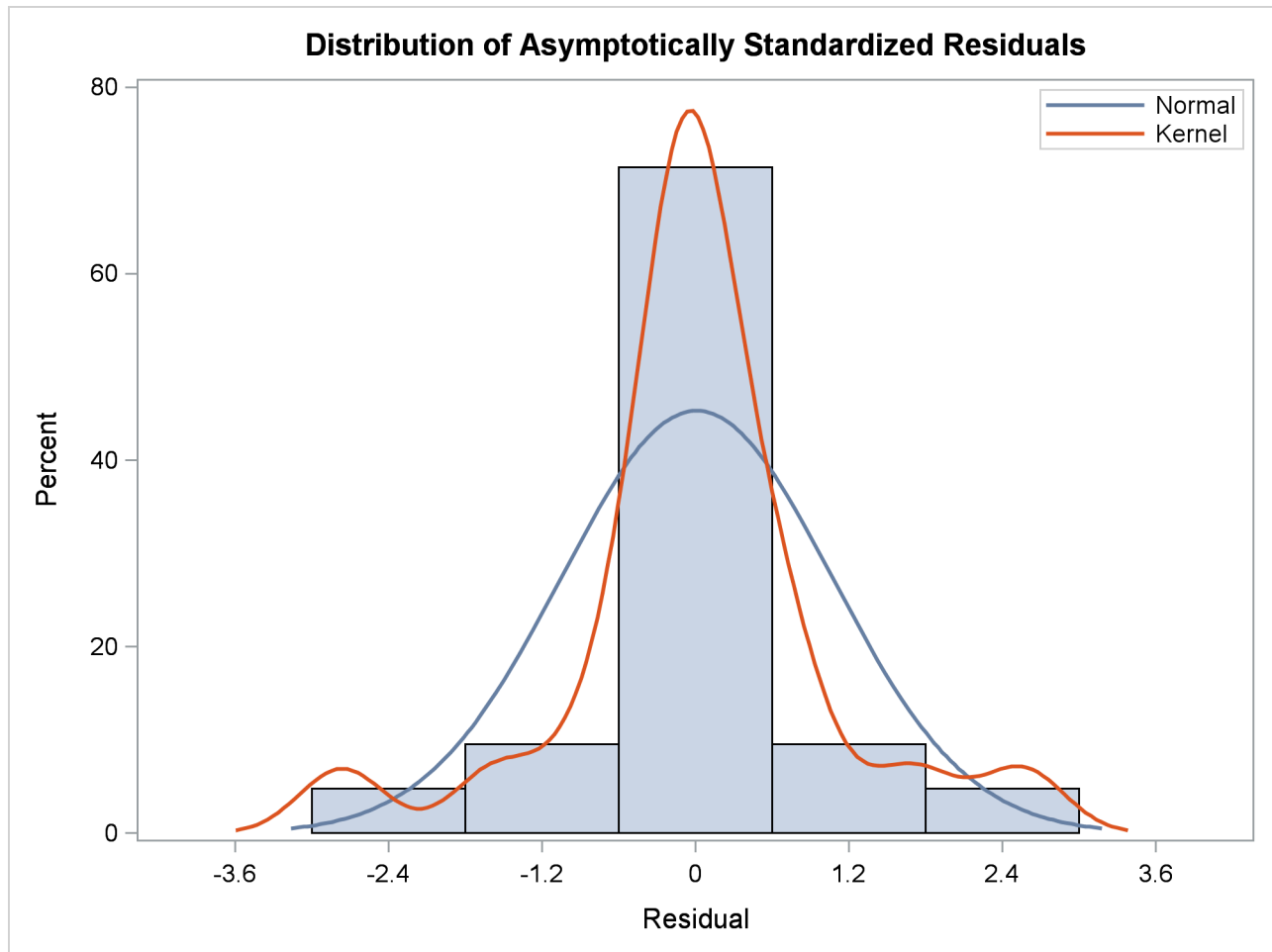
Average Standardized Residual	0.646672
Average Off-diagonal Standardized Residual	0.818456

Rank Order of the 10 Largest Asymptotically Standardized Residuals		
Var1	Var2	Residual
Education	Powerless67	-2.76371
Education	Anomie67	2.55338
Education	Anomie71	1.69781
Education	Powerless71	-1.55750
Anomie71	Powerless67	0.87613
Powerless71	Anomie67	-0.86507
Powerless71	Powerless71	0.58521
Powerless67	Anomie67	0.52686
SEI	Powerless71	-0.49608
SEI	Anomie67	0.46484

The model performs the poorest concerning the covariances of Education with all measures of Powerless and Anomie. This might suggest a misspecification of the functional relationships of Education with other variables in the model. However, because the model fit is quite good, such a possible misspecification should not be a serious concern in the analysis.

The histogram of the asymptotically standardized residuals is displayed in [Output 27.17.9](#), which also shows the normal and kernel approximations.

Output 27.17.9 Distribution of Asymptotically Standardized Residuals



The residual distribution looks quite symmetrical. It shows a small to medium departure from the normal distribution, as evidenced by the discrepancies between the kernel and the normal distribution curves.

Output 27.17.10 shows the estimation results.

Output 27.17.10 Estimation Results

PATH List						
-----Path-----	Parameter	Estimate	Standard Error	t Value		
Anomie67 <=== Alien67		1.00000				
Powerless67 <=== Alien67		0.83300				
Anomie71 <=== Alien71		1.00000				
Powerless71 <=== Alien71		0.83300				
Education <=== SES		1.00000				
SEI <=== SES	lambda	5.36883	0.43371	12.37880		
Alien67 <=== SES	gamma1	-0.62994	0.05634	-11.18092		
Alien71 <=== SES	gamma2	-0.24086	0.05489	-4.38836		
Alien71 <=== Alien67	beta	0.59312	0.04678	12.67884		

Output 27.17.10 *continued*

Variance Parameters					
Variance Type	Variable	Parameter	Estimate	Standard Error	t Value
Error	Anomie67	theta1	3.60796	0.20092	17.95717
	Powerless67	theta2	3.59488	0.16448	21.85563
	Anomie71	theta1	3.60796	0.20092	17.95717
	Powerless71	theta2	3.59488	0.16448	21.85563
	Education	theta3	2.99366	0.49861	6.00398
	SEI	theta4	259.57639	18.31151	14.17559
	Alien67	psi1	5.67046	0.42301	13.40500
	Alien71	psi2	4.51479	0.33532	13.46394
Exogenous	SES	phi	6.61634	0.63914	10.35190
Covariances Among Errors					
Error of	Error of	Parameter	Estimate	Standard Error	t Value
Anomie67	Anomie71	theta5	0.90580	0.12167	7.44472
Powerless67	Powerless71	theta5	0.90580	0.12167	7.44472

The paths, variances and partial (or error) variances, and covariances and partial covariances are shown. When you have fixed parameters such as the first five path coefficients in the output, the standard errors and *t* values are all blanks. For free or constrained estimates, standard errors and *t* values are computed. Researchers in structural equation modeling usually use the value 2 as an approximate critical value for the observed *t* values. The reason is that the estimates are asymptotically normal, and so the two-sided critical point with $\alpha = 0.05$ is 1.96, which is close to 2. Using this criterion, all estimates shown in **Output 27.17.10** are significantly different from zero, supporting the presence of these parameters in the model.

Squared multiple correlations are shown in **Output 27.17.11**.

Output 27.17.11 Squared Multiple Correlations

Squared Multiple Correlations			
Variable	Error Variance	Total Variance	R-Square
Anomie67	3.60796	11.90397	0.6969
Anomie71	3.60796	12.61581	0.7140
Education	2.99366	9.61000	0.6885
Powerless67	3.59488	9.35139	0.6156
Powerless71	3.59488	9.84533	0.6349
SEI	259.57639	450.28798	0.4235
Alien67	5.67046	8.29601	0.3165
Alien71	4.51479	9.00786	0.4988

For each endogenous variable in the model, the corresponding squared multiple correlation is computed by:

$$1 - \frac{\text{error variance}}{\text{total variance}}$$

In regression analysis, this is the percentage of explained variance of the endogenous variable by the predictors. However, this interpretation is complicated or even uninterpretable when your structural equation model has correlated errors or reciprocal casual relations. In these situations, it is not uncommon to see negative R-squares. Negative R-squares do not necessarily mean that your model is wrong or the model prediction is weak. Rather, the R-square interpretation is questionable in these situations.

When your variables are measured on different scales, comparison of path coefficients cannot be made directly. For example, in [Output 27.17.10](#), the path coefficient for path Education <=== SES is fixed at one, while the path coefficient for path SEI <=== SES is 5.369. It would be simple-minded to conclude that the effect of SES on SEI is greater than that SES on Education. Because SEI and Education are measured on different scales, direct comparison of the corresponding path coefficients is simply inappropriate.

In alleviating this problem, some might resort to the standardized solution for a better comparison. In a standardized solution, because the variances of manifest variables and systematic predictors are all standardized to ones, you hope the path coefficients are more comparable. In this example, PROC CALIS standardizes your results in [Output 27.17.12](#).

Output 27.17.12 Standardized Results

Standardized Results for PATH List					
-----Path-----	Parameter	Estimate	Standard Error	t Value	
Anomie67 <=== Alien67		0.83481	0.01093	76.35313	
Powerless67 <=== Alien67		0.78459	0.01163	67.47756	
Anomie71 <=== Alien71		0.84499	0.01031	81.97956	
Powerless71 <=== Alien71		0.79678	0.01107	71.96263	
Education <=== SES		0.82975	0.03172	26.15990	
SEI <=== SES	lambda	0.65079	0.03019	21.55331	
Alien67 <=== SES	gamma1	-0.56257	0.03456	-16.27961	
Alien71 <=== SES	gamma2	-0.20642	0.04483	-4.60430	
Alien71 <=== Alien67	beta	0.56920	0.04066	14.00001	
Standardized Results for Variance Parameters					
Variance Type	Variable	Parameter	Estimate	Standard Error	t Value
Error	Anomie67	theta1	0.30309	0.01825	16.60309
	Powerless67	theta2	0.38442	0.01825	21.06948
	Anomie71	theta1	0.28599	0.01742	16.41782
	Powerless71	theta2	0.36514	0.01764	20.69424
	Education	theta3	0.31152	0.05264	5.91822
	SEI	theta4	0.57647	0.03930	14.66804
	Alien67	psi1	0.68352	0.03888	17.57968
	Alien71	psi2	0.50121	0.03321	15.08974
Exogenous	SES	phi	1.00000		

Output 27.17.12 *continued*

Standardized Results for Covariances Among Errors					
Error of	Error of	Parameter	Estimate	Standard Error	t Value
Anomie67	Anomie71	theta5	0.07391	0.01013	7.29574
Powerless67	Powerless71	theta5	0.09440	0.01274	7.40922

Now, the standardized path coefficient for path Education \leftarrow SES is 0.830, while the standardized path coefficient for path SEI \leftarrow SES is 0.651. So the standardized effect of SES on SEI is actually smaller than that of SES on Education.

Furthermore, in PROC CALIS the standardized estimates are computed with standard error estimates and t values so that you can make statistical inferences on the standardized estimates as well.

PROC CALIS might differ from other software in its standardization scheme. Unlike other software that might standardize the path coefficients that attach to the error terms (unsystematic sources), PROC CALIS keeps these path coefficients at ones (not shown in the output). Unlike other software that might also standardize the corresponding error variances to ones, the error variances in the standardized solution of PROC CALIS are rescaled so as to keep the mathematical consistency of the model.

Essentially, in PROC CALIS only variances of manifest and non-error-type latent variables are standardized to ones. The error variances are rescaled, but not standardized. For example, in the standardized solution shown in [Output 27.17.12](#), the error variances for all endogenous variables are not ones (see the middle portion of the output). Only the variance for the latent variable SES is standardized to one. See the section “[Standardized Solutions](#)” on page 1345 for the logic of the standardization scheme adopted by PROC CALIS.

In appearance, the standardized solution is like a correlational analysis on the standardized manifest variables with standardized exogenous latent factors. Unfortunately, this statement is over-simplified, if not totally inappropriate. In standardizing a solution, the implicit equality constraints are likely destroyed. In this example, the unstandardized error variances for Anomie67 and Anomie71 are both 3.608, represented by a common parameter theta1. However, after standardization, these error variances have different values at 0.303 and 0.286, respectively. In addition, fixed parameter values are no longer fixed in a standardized solution (for example, the first five paths in the current example). The issue of standardization is common to all other SEM software and beyond the current discussion. PROC CALIS provides the standardized solution so that users can interpret the standardized estimates whenever they find them appropriate.

Example 27.18: Simultaneous Equations with Mean Structures and Reciprocal Paths

The supply-and-demand food example of Kmenta (1971, pp. 565, 582) is used to illustrate PROC CALIS for the estimation of intercepts and coefficients of simultaneous equations in econometrics. The model is specified by two simultaneous equations containing two endogenous variables Q and P , and three exogenous variables D , F , and Y :

$$Q_t(\text{demand}) = \alpha_1 + \beta_1 P_t + \gamma_1 D_t$$

$$Q_t(\text{supply}) = \alpha_2 + \beta_2 P_t + \gamma_2 F_t + \gamma_3 Y_t$$

for $t = 1, \dots, 20$.

To analyze this model in PROC CALIS, the second equation needs to be written in another form. For instance, in the LINEQS model each endogenous variable must appear on the left-hand side of exactly one equation. To satisfy this requirement, you can rewrite the second equation as an equation for P_t as:

$$P_t = -\frac{\alpha_2}{\beta_2} + \frac{1}{\beta_2} Q_t - \frac{\gamma_2}{\beta_2} F_t - \frac{\gamma_3}{\beta_2} Y_t$$

or, equivalently reparameterized as:

$$P_t = \theta_1 + \theta_2 Q_t + \theta_3 F_t + \theta_4 Y_t$$

where

$$\theta_1 = -\frac{\alpha_2}{\beta_2}, \quad \theta_2 = \frac{1}{\beta_2}, \quad \theta_3 = -\frac{\gamma_2}{\beta_2}, \quad \theta_4 = -\frac{\gamma_3}{\beta_2}$$

This new equation for P_t together with the first equation for Q_t suggest the following LINEQS model specification in PROC CALIS:

```

title 'Food example of KMENTA(1971, p.565 & 582)';
data food;
  input Q P D F Y;
  label Q='Food Consumption per Head'
        P='Ratio of Food Prices to General Price'
        D='Disposable Income in Constant Prices'
        F='Ratio of Preceding Years Prices'
        Y='Time in Years 1922-1941';
  datalines;
  98.485 100.323 87.4 98.0 1
  99.187 104.264 97.6 99.1 2
  102.163 103.435 96.7 99.1 3
  101.504 104.506 98.2 98.1 4
  104.240 98.001 99.8 110.8 5
  103.243 99.456 100.5 108.2 6
  103.993 101.066 103.2 105.6 7
  99.900 104.763 107.8 109.8 8
  100.350 96.446 96.6 108.7 9

```

```

102.820   91.228   88.9   100.6   10
 95.435   93.085   75.1    81.0   11
 92.424   98.801   76.9    68.6   12
 94.535  102.908   84.6    70.9   13
 98.757   98.756   90.6    81.4   14
105.797   95.119  103.1   102.3   15
100.225   98.451  105.1   105.0   16
103.522   86.498   96.4   110.5   17
 99.929  104.016  104.4    92.5   18
105.223  105.769  110.7    89.3   19
106.232  113.490  127.1    93.0   20
;

proc calis data=food pshort nostand;
  lineqs
    Q = alpha1 * Intercept + beta1 * P + gamma1 * D + E1,
    P = theta1 * Intercept + theta2 * Q + theta3 * F + theta4 * Y + E2;
  variance
    E1-E2 = eps1-eps2;
  cov
    E1-E2 = eps3;
  bounds
    eps1-eps2 >= 0. ;
run;

```

The LINEQS modeling language is used in this example because its specification is similar to the original equations. In the **LINEQS** statement, you essentially input the two model equations for Q and P. Parameters for intercepts and regression coefficients are also specified in the equations. Note that Intercept in the two equations is treated as a special variable that contains ones for all observations. Intercept is not a variable in the data set, nor do you need to create such a variable in your data set. Hence, the variable Intercept does not represent the intercept parameter itself. Instead, the intercept parameters for the two equations are the coefficients attached to Intercept. In this example, the intercept parameters are alpha1 and theta1, respectively, in the two equations. As required, error terms E1 and E2 are added to complete the equation specification.

In the **VARIANCE** statement, you specify eps1 and eps2, respectively, for the variance parameters of the error terms. In the **COV**, you specify eps3 for the covariance parameter between the error terms. In the **BOUNDS** statement, you set lower bounds for the error variances so that estimates of eps1 and eps2 would be nonnegative.

In this example, the **PSHORT** and the **NOSTAND** options are used in the PROC CALIS statement. The **PSHORT** option suppresses a large amount of the output. For example, initial estimates are not printed and simple descriptive statistics and standard errors are not computed. The **NOSTAND** option suppresses the printing of the standardized results. Because the default printing in PROC CALIS might produce a large amount of output, using these printing options make your output more concise and readable. Whenever appropriate, you may consider using these printing options.

The estimated equations are shown in [Output 27.18.1](#).

Output 27.18.1 Linear Equations

Linear Equations					
Q	=	93.6193*Intercept	+ -0.2295*P	+ 0.3100*D	
Std Err		7.5748 alpha1	0.0923 beta1	0.0448 gamma1	
t Value		12.3592	-2.4856	6.9186	
		+ 1.0000 E1			
Linear Equations					
P	=	-218.9*Intercept	+ 4.2140*Q	+ -0.9305*F	
Std Err		137.7 theta1	1.7540 theta2	0.3960 theta3	
t Value		-1.5897	2.4025	-2.3500	
		+ -1.5579*Y	+ 1.0000 E2		
		0.6650 theta4			
		-2.3429			

The estimates of intercepts and regression coefficients are shown directly in the equations. Any number in an equation followed by an asterisk is an estimate. For the estimates in equations, the parameter names are shown underneath the associated variables. Any number in an equation not followed by an asterisk is a fixed value. For example, the value 1.0000 attached to the error term in each of the output equation is fixed. Also, for fixed coefficients there are no parameter names underneath the associated variables.

All but the intercept estimates in the equation for predicting P are statistically significant at $\alpha = 0.05$ (when using an approximate critical value of 2). The t ratio for theta1 is -1.590 , which implies that this intercept might have been zero in the population. However, because you have reparameterized the original model to use the LINEQS model specification, transformed parameters like theta1 in this model might not be of primary interest. Therefore, you might not need to pay any attention to the significance of the theta1 estimate. There is a way to use the original econometric parameters to specify the LINEQS model. It is discussed in the later part of this example.

Estimates for variance, covariance, and mean parameters are shown in [Output 27.18.2](#).

Output 27.18.2 Variance, Covariance, and Mean Parameters

Estimates for Variances of Exogenous Variables					
Variable Type	Variable	Parameter	Estimate	Standard Error	t Value
Error	E1	eps1	3.51274	1.20204	2.92233
	E2	eps2	105.06749	83.89446	1.25238
Observed	D	_Add1	139.96029	45.40911	3.08221
	F	_Add2	161.51355	52.40192	3.08221
	Y	_Add3	35.00000	11.35550	3.08221

Output 27.18.2 *continued*

Covariances Among Exogenous Variables					
Var1	Var2	Parameter	Estimate	Standard Error	t Value
E1	E2	eps3	-18.87270	8.77951	-2.14963
F	D	_Add4	74.02539	38.44699	1.92539
Y	D	_Add5	22.99211	16.90102	1.36040
Y	F	_Add6	-21.58158	17.94544	-1.20262

Mean Parameters					
Variable Type	Variable	Parameter	Estimate	Standard Error	t Value
Observed	D	_Add7	97.53500	2.71410	35.93643
	F	_Add8	96.62500	2.91560	33.14071
	Y	_Add9	10.50000	1.35724	7.73628

Parameters with a name prefix `_Add` are added automatically by PROC CALIS. These parameters are added as free parameters to complete the model specification. In PROC CALIS, variances and covariances among the set of exogenous manifest variables must be parameters. You either specify them explicitly or let the CALIS procedure to add them. If you need to constrain or to fix these parameters, then you must specify them explicitly. When your model also fits the mean structures, the same principle applies to the means of the exogenous manifest variables. In this example, because variables D, F, and Y are all exogenous manifest variables, their associated means, variances and covariances must be parameters in the model.

The squared multiple correlations for the equations are shown in [Output 27.18.3](#).

Output 27.18.3 Squared Multiple Correlations

Squared Multiple Correlations			
Variable	Error Variance	Total Variance	R-Square
Q	3.51274	14.11128	0.7511
P	105.06749	35.11850	-1.9918

For endogenous variable P, the R-square is -1.9918 , which is obviously an invalid value. In fact, because there are correlated errors (between E1 and E2) and reciprocal paths (paths to and from Q and P), the model departs from the regular assumptions of multiple regression analysis. As a result, you should not interpret the R-squares for this example.

Specifying the LINEQS with the Original Econometric Parameters

If you are interested in estimating the parameters in the original econometric model (that is, α_2 , β_2 , γ_2 , and γ_3), the previous reparameterized LINEQS model does not serve your purpose well enough. However, using the relations between these original parameters with the θ parameters in the reparameterized LINEQS model, you can set up some “super-parameters” in the LINEQS model, as shown in the following statements:

```
proc calis data=Food pshort nostand;
  lineqs
    Q = alpha1 * Intercept + beta1 * P + gamma1 * D + E1,
    P = theta1 * Intercept + theta2 * Q + theta3 * F + theta4 * Y + E2;
  variance
    E1-E2 = eps1-eps2;
  cov
    E1-E2 = eps3;
  bounds
    eps1-eps2 >= 0. ;
  parameters alpha2 (50.) beta2 gamma2 gamma3 (3*.25);
    theta1 = -alpha2 / beta2;
    theta2 = 1 / beta2;
    theta3 = -gamma2 / beta2;
    theta4 = -gamma3 / beta2;
run;
```

In this new specification, only the **PARAMETERS** statement and the **SAS programming statements** following it are new. In the **PARAMETERS** statement, you define super-parameters alpha2, beta2, gamma2, and gamma3, and put initial values for them in parentheses. These parameters are the original econometric parameters of interest. The **SAS programming statements** that follow the **PARAMETERS** statement are used to define the functional relationships of the super-parameters with the parameters in the LINEQS model. Consequently, in this new specification, theta1, theta2, theta3, and theta4 are no longer independent parameters in the model, as they are in the previous reparameterized model. Instead, alpha2, beta2, gamma2, and gamma3 are independent parameters in this new specification. By fitting this new model, you get the same set of estimates as those in the previous LINEQS model. In addition, you get estimates of the super-parameters, as shown in [Output 27.18.4](#).

Output 27.18.4 Additional Parameters

Additional Parameters				
Type	Parameter	Estimate	Standard Error	t Value
Independent	alpha2	51.94452	11.70002	4.43969
	beta2	0.23731	0.09877	2.40262
	gamma2	0.22082	0.04161	5.30695
	gamma3	0.36971	0.07060	5.23649

You can now interpret the results in terms of the original econometric parameterization. As shown in [Output 27.18.4](#), all these estimates are significant, despite the fact that one of the transformed parameter estimates in the linear equations of the LINEQS model is not. You can obtain almost equivalent results by applying the SAS/ETS procedure SYSLIN on this problem.

Alternative Ways to Specify Your LINEQS Model

In specifying the linear equations in the LINEQS model, it might become cumbersome when you need to name a lot of parameters into the equations. If the parameters in your model are unconstrained, you need to be very careful to use unique parameter names to distinguish the free parameters because parameters with the same name are identical and will have the same estimate. To make model specification easier and to avoid accidental constraints, PROC CALIS provides an efficient way to specify these free parameters. That is, you can simply omit the parameter names in the specification. For example, in the first specification of the current example, except for the boundary constraints on the error variance parameters, all other parameters in the model are not constrained, as shown in the following statements:

```
proc calis data=food pshort nostand;
  lineqs
    Q = alpha1 * Intercept + beta1 * P + gamma1 * D + E1,
    P = theta1 * Intercept + theta2 * Q + theta3 * F + theta4 * Y + E2;
  variance
    E1-E2 = eps1-eps2;
  cov
    E1-E2 = eps3;
  bounds
    eps1-eps2 >= 0. ;
run;
```

Parameters such as alpha1, beta1, and so on are unique parameter names in the specific locations of the model. They are free parameters. Hence, you can use the following equivalent specification:

```
proc calis data=food pshort nostand;
  lineqs
    Q = * Intercept + * P + * D + E1,
    P = * Intercept + * Q + * F + * Y + E2;
  variance
    E1-E2 = eps1-eps2;
  cov
    E1 E2;
  bounds
    eps1-eps2 >= 0. ;
run;
```

Only the parameters eps1 and eps2 remain in this equivalent specification. You omit the specification of all other parameter names. But the estimation results are the same, as shown in [Output 27.18.5](#).

Output 27.18.5 Estimation Results With Generated Parameter Names

Linear Equations					
Q	=	93.6193*Intercept	+ -0.2295*P	+ 0.3100*D	
Std Err		7.5748 _Parm1	0.0923 _Parm2	0.0448 _Parm3	
t Value		12.3592	-2.4856	6.9186	
		+ 1.0000 E1			
Linear Equations					
P	=	-218.9*Intercept	+ 4.2140*Q	+ -0.9305*F	
Std Err		137.7 _Parm4	1.7540 _Parm5	0.3960 _Parm6	
t Value		-1.5897	2.4025	-2.3500	
		+ -1.5579*Y + 1.0000 E2			
		0.6650 _Parm7			
		-2.3429			
Estimates for Variances of Exogenous Variables					
Variable Type	Variable	Parameter	Estimate	Standard Error	t Value
Error	E1	eps1	3.51274	1.20204	2.92233
	E2	eps2	105.06749	83.89446	1.25238
Observed	D	_Add1	139.96029	45.40911	3.08221
	F	_Add2	161.51355	52.40192	3.08221
	Y	_Add3	35.00000	11.35550	3.08221
Covariances Among Exogenous Variables					
Var1	Var2	Parameter	Estimate	Standard Error	t Value
E1	E2	_Parm8	-18.87270	8.77951	-2.14963
F	D	_Add4	74.02539	38.44699	1.92539
Y	D	_Add5	22.99211	16.90102	1.36040
Y	F	_Add6	-21.58158	17.94544	-1.20262
Mean Parameters					
Variable Type	Variable	Parameter	Estimate	Standard Error	t Value
Observed	D	_Add7	97.53500	2.71410	35.93643
	F	_Add8	96.62500	2.91560	33.14071
	Y	_Add9	10.50000	1.35724	7.73628

The estimation results in [Output 27.18.5](#) are the same as those in [Output 27.18.2](#) and [Output 27.18.3](#) with the original LINEQS model specification, only now PROC CALIS generates the parameter names with the `_Parm` in the results, as shown in [Output 27.18.5](#). Note that you retain the parameter names `eps1` and `eps2` because you need to refer to them in the BOUNDS statement.

Example 27.19: Fitting Direct Covariance Structures

In the section “[Direct Covariance Structures Analysis](#)” on page 1075, the MSTRUCT modeling language is used to specify a model with direct covariance structures. In the model, four variables from the data set of Wheaton et al. (1977) are used. The analysis is carried out in this example to investigate the tenability of the hypothesized covariance structures.

The four variables used are: `Anomie67`, `Powerless67`, `Anomie71`, and `Powerless71`. The hypothesized covariance matrix is structured as:

$$\Sigma = \begin{pmatrix} \phi_1 & \theta_1 & \theta_2 & \theta_1 \\ \theta_1 & \phi_2 & \theta_1 & \theta_3 \\ \theta_2 & \theta_1 & \phi_1 & \theta_1 \\ \theta_1 & \theta_3 & \theta_1 & \phi_2 \end{pmatrix}$$

where:

- ϕ_1 : variance of anomie
- ϕ_2 : variance of powerlessness
- θ_1 : covariance between anomie and powerlessness
- θ_2 : covariance between anomie measures
- θ_3 : covariance between powerlessness measures

In this example, you hypothesize the covariance structures directly, as opposed to those models with implied covariance structures from path models (see [Example 27.17](#)), structural equations (see [Example 27.18](#)), or other types of models. The basic assumption of the direct covariance structures in this example is that `Anomie` and `Powerless` were invariant over the measurement periods employed. This implies that the time of measurement did not change the variances and covariances of the measures. Therefore, both `Anomie67` and `Anomie71` have the same variance parameter ϕ_1 , and both `Powerless67` and `Powerless71` have the same variance parameter ϕ_2 . These two parameters, ϕ_1 and ϕ_2 , are hypothesized on the diagonal of the covariance matrix Σ . In the same structured covariance matrix, θ_1 represents the covariance between `Anomie` and `Powerless`, without regard to the time of measurement. The θ_2 parameter represents the covariance between the `Anomie` measures, or the reliability of the `Anomie` measure. Similarly, the θ_3 parameter represents the covariance between the `Powerless` measures, or the reliability of the `Anomie` measure.

As explained in the section “[Direct Covariance Structures Analysis](#)” on page 1075, you can use the MSTRUCT modeling language to specify the hypothesized covariance structures directly, as shown in the following statements:

```

proc calis nobs=932 data=Wheaton psummary;
  fitindex on(only)=[chisq df probchi] outfit=savefit;
  mstruct
    var = Anomie67 Powerless67 Anomie71 Powerless71;
  matrix _COV_ [1,1] = phi1,
                [2,2] = phi2,
                [3,3] = phi1,
                [4,4] = phi2,
                [2,1] = theta1,
                [3,1] = theta2,
                [3,2] = theta1,
                [4,1] = theta1,
                [4,2] = theta3,
                [4,3] = theta1;
run;

```

In the **MSTRUCT** statement you specify the variables in the **VAR=** list. The order of variables in this **VAR=** list is assumed to be the same as that in the row and column of the hypothesized covariance matrix. Next, in the **MATRIX** statement you specify parameters as entries in the hypothesized covariance matrix **_COV_**. Only the lower diagonal elements need to be specified because covariance matrices, by nature, are symmetric. Redundant specification of the upper triangular elements are unnecessary as PROC CALIS has the information accounted for. You can also set initial estimates by putting parenthesized numbers after the parameter names. But in this example you let PROC CALIS determine all the initial estimates.

In the PROC CALIS statement, the **PSUMMARY** option is used. As a **global display option**, this option suppresses a lot of displayed output and requests only the fit summary table be printed. This way you can eliminate quite a lot of displayed output that is not of your primary interest. In this example, the specification of the covariance structures is straightforward, and you do not need any output regarding the initial estimation or standardized solution. Suppose that you are not even concerned with the estimates of the parameters because you are not yet sure if this model is good enough for the data. All you want to know at this stage is whether the hypothesized covariance structures fit the data well. Therefore, the **PSUMMARY** option would serve your purpose well in this example.

In fact, even the fit summary table can be trimmed down quite a bit if you only want to look at certain specific fit indices. In the **FITINDEX** statement of this example, the **ON(ONLY)=** option turns on the printing of the model fit chi-square, its *df*, and *p*-value only. This does not mean that you must lose the information of all other fit indices. In addition to the printed output, you can save all fit indices in an output data set. To this end, you can use the **OUTFIT=** option in the **FITINDEX** statement. In this example, you save the results of all fit indices in a SAS data set called **savefit**.

Output 27.19.1 shows the entire printed output.

Output 27.19.1 Testing Direct Covariance Structures

Fit Summary	
Chi-Square	221.5798
Chi-Square DF	5
Pr > Chi-Square	<.0001

The displayed output is very concise. It contains only a fit summary table with three statistics. The *p*-value for the model fit chi-square test indicates that the hypothesized structures should be rejected at $\alpha = 0.05$.

Therefore, this rather restrictive direct covariance structure model does not fit the data well. A less restrictive covariance structure model is needed to explain the variances and covariances.

All fit indices are saved in the savefit data set. To view it, you can use the following statement:

```
proc print data=savefit;
run;
```

Output 27.19.2 shows all indices, their types and values of all fit indices and information.

Output 27.19.2 Saved Fit Indices

Analysis of Direct Covariance Structures					
Testing Model by the MSTRUCT Language					
Obs	_TYPE_	Index Code	FitIndex	Fit Value	PrintChar
1	ModelInfo	101	Number of Observations	932.00	932
2	ModelInfo	103	Number of Variables	4.00	4
3	ModelInfo	104	Number of Moments	10.00	10
4	ModelInfo	105	Number of Parameters	5.00	5
5	ModelInfo	106	Number of Active Constraints	0.00	0
6	ModelInfo	111	Baseline Model Function Value	1.68	1.6799
7	ModelInfo	113	Baseline Model Chi-Square	1563.94	1563.9442
8	ModelInfo	114	Baseline Model Chi-Square DF	6.00	6
9	ModelInfo	115	Pr > Baseline Model Chi-Square	0.00	<.0001
10	Absolute	201	Fit Function	0.24	0.2380
11	Absolute	203	Chi-Square	221.58	221.5798
12	Absolute	204	Chi-Square DF	5.00	5
13	Absolute	205	Pr > Chi-Square	0.00	<.0001
14	Absolute	211	Z-Test of Wilson & Hilferty	12.25	12.2533
15	Absolute	212	Hoelter Critical N	47.00	47
16	Absolute	213	Root Mean Square Residual (RMR)	0.76	0.7649
17	Absolute	214	Standardized RMR (SRMR)	0.07	0.0701
18	Absolute	215	Goodness of Fit Index (GFI)	0.90	0.9036
19	Parsimony	301	Adjusted GFI (AGFI)	0.81	0.8071
20	Parsimony	302	Parsimonious GFI	0.75	0.7530
21	Parsimony	303	RMSEA Estimate	0.22	0.2157
22	Parsimony	304	RMSEA Lower 90% Confidence Limit	0.19	0.1920
23	Parsimony	305	RMSEA Upper 90% Confidence Limit	0.24	0.2404
24	Parsimony	306	Probability of Close Fit	0.00	<.0001
25	Parsimony	307	ECVI Estimate	0.25	0.2488
26	Parsimony	308	ECVI Lower 90% Confidence Limit	0.20	0.2003
27	Parsimony	309	ECVI Upper 90% Confidence Limit	0.31	0.3053
28	Parsimony	310	Akaike Information Criterion	231.58	231.5798
29	Parsimony	311	Bozdogan CAIC	260.77	260.7665
30	Parsimony	312	Schwarz Bayesian Criterion	255.77	255.7665
31	Parsimony	313	McDonald Centrality	0.89	0.8903
32	Incremental	401	Bentler Comparative Fit Index	0.86	0.8610
33	Incremental	402	Bentler-Bonett NFI	0.86	0.8583
34	Incremental	403	Bentler-Bonett Non-normed Index	0.83	0.8332
35	Incremental	404	Bollen Normed Index Rhol	0.83	0.8300
36	Incremental	405	Bollen Non-normed Index Delta2	0.86	0.8611
37	Incremental	406	James et al. Parsimonious NFI	0.72	0.7153

The results of various fit indices from this output data set confirm that the hypothesized model does not fit the data well.

As an aside, it is noted with some shorthand notation, the specification of the MSTRUCT model parameters that use the **MATRIX** statements can be made a little more precise for the current example. This is shown as follows:

```
proc calis nobs=932 data=Wheaton psummary;
  mstruct
    var = Anomie67 Powerless67 Anomie71 Powerless71;
  matrix _COV_ [1,1] = phi1 phi2 phi1 phi2,
              [2, ] = theta1,
              [3, ] = theta2 theta1,
              [4, ] = theta1 theta3 theta1;
  fitindex on(only)=[chisq df probchi] outfit=savefit;
run;
```

In the first entry of the **MATRIX** statement, the notation [1,1] represents that the parameter list specified after the equal sign starts with the [1,1] element of the **_COV_** matrix and proceeds down the diagonal. In the next three entries, the notations [2,], [3,], and [4,] represent that parameter lists start with the first elements of the second, third, and fourth rows, respectively, and proceed to the next (right) elements on the same rows. See the syntax of the **MATRIX** statement on page 1175 for more details about this kind of shorthand notation.

This example shows how you can use the MSTRUCT modeling language to test specific covariance patterns. You need to define the parameters of the covariance patterns explicitly by the **MATRIX** statements. See [Example 27.4](#) and [Example 27.21](#) for more applications.

However, some commonly-used covariance and mean patterns are built into PROC CALIS. For these covariance and mean patterns, you can simply use the **COVPATTERN=** and the **MEANPATTERN=** options without the need to specify the parameters in the **MATRIX** statements. See the **COVPATTERN=** and the **MEANPATTERN=** options for the supported covariance and mean patterns. See [Example 27.5](#) and [Example 27.22](#) for applications.

Example 27.20: Confirmatory Factor Analysis: Cognitive Abilities

In this example, cognitive abilities of 64 students from a middle school were measured. The fictitious data contain nine cognitive test scores. Three of the scores were for reading skills, three others were for math skills, and the remaining three were for writing skills. The covariance matrix for the nine variables was obtained. A confirmatory factor analysis with three factors was conducted. The following is the input data set:

```
title "Confirmatory Factor Analysis Using the FACTOR Modeling Language";
title2 "Cognitive Data";
data cognitivel(type=cov);
  _type_='cov';
  input _name_ $ reading1 reading2 reading3 math1 math2 math3
           writing1 writing2 writing3;
  datalines;
reading1 83.024      .      .      .      .      .      .      .      .
reading2 50.924 108.243  .      .      .      .      .      .      .
```

```

reading3 62.205 72.050 99.341 . . . . .
math1    22.522 22.474 25.731 82.214 . . . . .
math2    14.157 22.487 18.334 64.423 96.125 . . . . .
math3    22.252 20.645 23.214 49.287 58.177 88.625 . . . . .
writing1 33.433 42.474 41.731 25.318 14.254 27.370 90.734 . . . . .
writing2 24.147 20.487 18.034 22.106 26.105 22.346 53.891 96.543 . . . . .
writing3 13.340 20.645 23.314 19.387 28.177 38.635 55.347 52.999 98.445
;

```

Confirmatory Factor Model with Uncorrelated Factors

You first fit a confirmatory factor model with uncorrelated factors to the data, as shown in the following statements:

```

proc calis data=cognitivel nobs=64 modification;
  factor
    Read_Factor  ===> reading1-reading3 ,
    Math_Factor  ===> math1-math3      ,
    Write_Factor ===> writing1-writing3 ;
  pvar
    Read_Factor Math_Factor Write_Factor = 3 * 1.;
  cov
    Read_Factor Math_Factor Write_Factor = 3 * 0.;
run;

```

In the PROC CALIS statement, the number of observations is specified with the **NOBS=** option. With the **MODIFICATION** in the PROC CALIS statement, LM (Lagrange Multiplier) tests are conducted. The results of LM tests can suggest the inclusion of additional parameters for a better model fit.

The FACTOR modeling language is most handy when you specify confirmatory factor models. You use the **FACTOR** statement to invoke the FACTOR modeling language. Entries in the **FACTOR** statement are for specifying factor-variables relationships and are separated by commas. In each entry, you first specify a latent factor, followed by the right arrow sign **===>** (you can use **>**, **=>**, **==>**, or **===>**). Then you specify the observed variables that have nonzero loadings on the factor. For example, in the first entry of **FACTOR** statement, you specify that latent factor **Read_Factor** has nonzero loadings (free parameters) on variables **reading1-reading3**. Optionally, you can specify the parameter list after you specify the factor-variable relationships. For example, you can name the loading parameters as in the following specification:

```

factor
  Read_Factor  ===> reading1-reading3  = load1-load3;

```

This way, you name the factor loadings with parameter names **load1**, **load2**, and **load3**, respectively. However, in the current example, because the loading parameters are all unconstrained, you can just let PROC CALIS to generate the parameter names for you. In this example, there are three factors: **Read_Factor**, **Math_Factor**, and **Write_Factor**. These factors have simple cluster structures with the nine observed variables. Each observed variable has only one loading on exactly one factor.

In the **PVAR** statement, you can specify the variances of the factors and the error variances of the observed variables. The factor variances in this model are all fixed at 1.0 for identification purposes. You do not need to specify the error variances of the observed variables in the current model because PROC CALIS assumes these are free parameters by default.

Output 27.20.1 *continued*

Initial Factor Covariance Matrix			
	Read_Factor	Math_Factor	Write_Factor
Read_Factor	1.0000	0	0
Math_Factor	0	1.0000	0
Write_Factor	0	0	1.0000

Initial Error Variances		
Variable	Parameter	Estimate
reading1	_Add1	.
reading2	_Add2	.
reading3	_Add3	.
math1	_Add4	.
math2	_Add5	.
math3	_Add6	.
writing1	_Add7	.
writing2	_Add8	.
writing3	_Add9	.

NOTE: Parameters with prefix '_Add' are added by PROC CALIS.

In the table for initial factor loading matrix, the nine loading parameters are shown to have simple cluster relations with the factors. In the table for initial factor covariance matrix, the diagonal matrix shows that the factors are not correlated. The diagonal elements are fixed at ones so that this matrix is also a correlation matrix for the factors. In the table for initial error variances, the nine variance parameters are shown. As described previously, these error variances are generated by PROC CALIS as default parameters.

In [Output 27.20.2](#), initial estimates are generated by the instrumental variable method and the McDonald method.

Output 27.20.2 Optimization of the Uncorrelated Factor Model: Initial Estimates

Initial Estimation Methods	
1	Instrumental Variables Method
2	McDonald Method

Output 27.20.2 *continued*

Optimization Start Parameter Estimates			
N	Parameter	Estimate	Gradient
1	_Parm1	7.15372	0.00851
2	_Parm2	7.80225	-0.00170
3	_Parm3	8.70856	-0.00602
4	_Parm4	7.68637	0.00272
5	_Parm5	8.01765	-0.01096
6	_Parm6	7.05012	0.00932
7	_Parm7	8.76776	-0.0009955
8	_Parm8	5.96161	-0.01335
9	_Parm9	7.23168	0.01665
10	_Add1	31.84831	-0.00179
11	_Add2	47.36790	0.0003461
12	_Add3	23.50199	0.00257
13	_Add4	23.13374	-0.0008384
14	_Add5	31.84224	0.00280
15	_Add6	38.92075	-0.00167
16	_Add7	13.86035	-0.00579
17	_Add8	61.00217	0.00115
18	_Add9	46.14784	-0.00300

Value of Objective Function = 0.9103815918

These initial estimates turn out to be pretty good, in the sense that only three more iterations are needed to converge to the maximum likelihood estimates and the final function value 0.784 does not change much from the initial function value 0.910, as shown in [Output 27.20.3](#).

Output 27.20.3 Optimization of the Uncorrelated Factor Model: Iteration Summary

Iter	Rest arts	Func Calls	Act Con	Objective Function	Obj Fun Change	Max Abs Gradient Element	Lambda	Actual Over Pred Change
1	0	4	0	0.78792	0.1225	0.00175	0	0.932
2	0	6	0	0.78373	0.00419	0.000037	0	1.051
3	0	8	0	0.78373	5.087E-7	3.715E-9	0	1.001

Optimization Results

Iterations	3	Function Calls	11
Jacobian Calls	5	Active Constraints	0
Objective Function	0.783733415	Max Abs Gradient Element	3.7146571E-9
Lambda	0	Actual Over Pred Change	1.0006660673
Radius	0.0025042942		

Convergence criterion (ABSGCONV=0.00001) satisfied.

The fit summary is shown in [Output 27.20.4](#).

Output 27.20.4 Fit of the Uncorrelated Factor Model

Fit Summary		
Modeling Info	Number of Observations	64
	Number of Variables	9
	Number of Moments	45
	Number of Parameters	18
	Number of Active Constraints	0
	Baseline Model Function Value	4.3182
	Baseline Model Chi-Square	272.0467
	Baseline Model Chi-Square DF	36
	Pr > Baseline Model Chi-Square	<.0001
	Absolute Index	Fit Function
Chi-Square		49.3752
Chi-Square DF		27
Pr > Chi-Square		0.0054
Z-Test of Wilson & Hilferty		2.5474
Hoelter Critical N		52
Root Mean Square Residual (RMR)		19.5739
Standardized RMR (SRMR)		0.2098
Parsimony Index	Goodness of Fit Index (GFI)	0.8555
	Adjusted GFI (AGFI)	0.7592
	Parsimonious GFI	0.6416
	RMSEA Estimate	0.1147
	RMSEA Lower 90% Confidence Limit	0.0617
	RMSEA Upper 90% Confidence Limit	0.1646
	Probability of Close Fit	0.0271
	ECVI Estimate	1.4630
	ECVI Lower 90% Confidence Limit	1.2069
	ECVI Upper 90% Confidence Limit	1.8687
	Akaike Information Criterion	85.3752
	Bozdogan CAIC	142.2351
Schwarz Bayesian Criterion	124.2351	
Incremental Index	McDonald Centrality	0.8396
	Bentler Comparative Fit Index	0.9052
	Bentler-Bonett NFI	0.8185
	Bentler-Bonett Non-normed Index	0.8736
	Bollen Normed Index Rho1	0.7580
	Bollen Non-normed Index Delta2	0.9087
	James et al. Parsimonious NFI	0.6139

Using the chi-square model test criterion, the uncorrelated factor model should be rejected at $\alpha = 0.05$. The RMSEA estimate is 0.1147, which is not indicative of a good fit according to Browne and Cudeck (1993). Other indices might suggest only a marginal good fit. For example, Bentler's comparative fit index and Bollen nonnormed index delta2 are both above 0.90. However, many other do not attain this 0.90 level. For example, adjusted GFI is only 0.759. It is thus safe to conclude that there could be some improvements on the model fit.

The **MODIFICATION** option in the PROC CALIS statement has been used to request for computing the LM test indices for model modifications. The results are shown in [Output 27.20.5](#).

Output 27.20.5 Lagrange Multiplier Tests

Rank Order of the 10 Largest LM Stat for Factor Loadings				
Variable	Factor	LM Stat	Pr > ChiSq	Parm Change
writing1	Read_Factor	9.76596	0.0018	2.95010
math3	Write_Factor	3.58077	0.0585	1.89703
math1	Read_Factor	2.15312	0.1423	1.17976
writing3	Math_Factor	1.87637	0.1707	1.41298
math3	Read_Factor	1.02954	0.3103	0.95427
reading2	Write_Factor	0.91230	0.3395	0.99933
writing2	Math_Factor	0.86221	0.3531	0.95672
reading1	Write_Factor	0.63403	0.4259	0.73916
math1	Write_Factor	0.55602	0.4559	0.63906
reading2	Math_Factor	0.55362	0.4568	0.74628

Rank Order of the 3 Largest LM Stat for Covariances of Factors				
Var1	Var2	LM Stat	Pr > ChiSq	Parm Change
Write_Factor	Read_Factor	8.95268	0.0028	0.44165
Write_Factor	Math_Factor	7.07904	0.0078	0.40132
Math_Factor	Read_Factor	4.61896	0.0316	0.30411

Rank Order of the 10 Largest LM Stat for Error Variances and Covariances				
Error of	Error of	LM Stat	Pr > ChiSq	Parm Change
writing1	math2	5.45986	0.0195	-13.16822
writing1	math1	5.05573	0.0245	12.32431
writing3	math3	3.93014	0.0474	13.59149
writing3	math1	2.83209	0.0924	-9.86342
writing2	reading1	2.56677	0.1091	10.15901
writing2	math2	1.94879	0.1627	8.40273
writing2	reading3	1.75181	0.1856	-7.82777
writing3	reading1	1.57978	0.2088	-7.97915
writing1	reading2	1.34894	0.2455	7.77158
writing2	math3	1.11704	0.2906	-7.23762

Three different tables for ranking the LM test results are shown. In the first table, the new loading parameters that would improve the model fit the most are shown first. For example, in the first row a new factor loading of writing1 on the Read_Factor is suggested to improve the model fit the most. The ‘LM Stat’ value is 9.77. This is an approximation of the chi-square drop if this parameter was included in the model. The ‘Pr > ChiSq’ value of 0.0018 indicates a significant improvement of model fit at $\alpha = 0.05$. Nine more new loading parameters are suggested in the table, with less and less statistical significance in the change of model fit chi-square. Note that these approximate chi-squares are one-at-a-time chi-square changes. That means that the overall chi-square drop is not a simple sum of individual chi-square changes when you include two or more new parameters in the modified model.

The other two tables in [Output 27.20.5](#) shows the new parameters in factor covariances, error variances, or error covariances that would result in a better model fit. The table for the new parameters of the factor covariance matrix indicates that adding each of the covariances among factors might lead to a statistically significant improvement in model fit. The largest ‘LM Stat’ value in this table is 8.95, which is smaller than that of the largest ‘LM Stat’ for the factor loading parameters. Despite this, it is more reasonable to add the covariance parameters among factors first to determine whether that improves the model fit.

Confirmatory Factor Model with Correlated Factors

To fit the corresponding confirmatory factor model with correlated factors, you can remove the fixed zeros from the COV statement in the preceding specification, as shown in the following statements:

```
proc calis data=cognitive1 nobs=64 modification;
  factor
    Read_Factor   ==> reading1-reading3 ,
    Math_Factor   ==> math1-math3      ,
    Write_Factor  ==> writing1-writing3 ;
  pvar
    Read_Factor Math_Factor Write_Factor = 3 * 1.;
  cov
    Read_Factor Math_Factor Write_Factor /* = 3 * 0. */;
run;
```

In the COV statement, you comment out the fixed zeros so that the covariances among the latent factors are now free parameters. An alternative way is to delete the entire COV statement so that the covariances among factors are free parameters by the FACTOR model default.

The fit summary of the correlated factor model is shown in [Output 27.20.6](#).

Output 27.20.6 Fit of the Correlated Factor Model

Fit Summary		
Modeling Info	Number of Observations	64
	Number of Variables	9
	Number of Moments	45
	Number of Parameters	21
	Number of Active Constraints	0
	Baseline Model Function Value	4.3182
	Baseline Model Chi-Square	272.0467
	Baseline Model Chi-Square DF	36
	Pr > Baseline Model Chi-Square	<.0001
Absolute Index	Fit Function	0.4677
	Chi-Square	29.4667
	Chi-Square DF	24
	Pr > Chi-Square	0.2031
	Z-Test of Wilson & Hilferty	0.8320
	Hoelter Critical N	78
	Root Mean Square Residual (RMR)	5.7038
	Standardized RMR (SRMR)	0.0607
	Goodness of Fit Index (GFI)	0.9109
Parsimony Index	Adjusted GFI (AGFI)	0.8330
	Parsimonious GFI	0.6073
	RMSEA Estimate	0.0601
	RMSEA Lower 90% Confidence Limit	0.0000
	RMSEA Upper 90% Confidence Limit	0.1244
	Probability of Close Fit	0.3814
	ECVI Estimate	1.2602
	ECVI Lower 90% Confidence Limit	1.2453
	ECVI Upper 90% Confidence Limit	1.5637
	Akaike Information Criterion	71.4667
	Bozdogan CAIC	137.8032
Schwarz Bayesian Criterion	116.8032	
Incremental Index	McDonald Centrality	0.9582
	Bentler Comparative Fit Index	0.9768
	Bentler-Bonett NFI	0.8917
	Bentler-Bonett Non-normed Index	0.9653
	Bollen Normed Index Rho1	0.8375
	Bollen Non-normed Index Delta2	0.9780
	James et al. Parsimonious NFI	0.5945

The model fit chi-square value is 29.47, which is about 20 less than the model with uncorrelated factors. The p -value is 0.20, indicating a satisfactory model fit. The RMSEA value is 0.06, which is close to 0.05, a value recommended as an indication of good model fit by Browne and Cudeck (1993). More fit indices that do not attain the 0.9 level with the uncorrelated factor model now have values close to or above 0.9. These include the goodness-of-fit index (GFI), McDonald centrality, Bentler-Bonnet NFI, and Bentler-Bonnet nonnormed index. By all counts, the correlated factor model is a much better fit than the uncorrelated factor model.

In [Output 27.20.7](#), the estimation results for factor loadings are shown. All these loadings are statistically significant, indicating non-chance relationships with the factors.

Output 27.20.7 Estimation of the Factor Loading Matrix

Factor Loading Matrix: Estimate/StdErr/t-value			
	Read_Factor	Math_Factor	Write_Factor
reading1	6.7657 1.0459 6.4689 [_Parm01]	0	0
reading2	7.8579 1.1890 6.6090 [_Parm02]	0	0
reading3	9.1344 1.0712 8.5269 [_Parm03]	0	0
math1	0	7.5488 1.0128 7.4536 [_Parm04]	0
math2	0	8.4401 1.0838 7.7874 [_Parm05]	0
math3	0	6.8194 1.0910 6.2506 [_Parm06]	0
writing1	0	0	7.9677 1.1254 7.0797 [_Parm07]
writing2	0	0	6.8742 1.1986 5.7350 [_Parm08]
writing3	0	0	7.0949 1.2057 5.8844 [_Parm09]

In Output 27.20.8, the factor covariance matrix is shown. Because the diagonal elements are all ones, the off-diagonal elements are correlations among factors. The correlations range from 0.30–0.5. These factors are moderately correlated.

Output 27.20.8 Estimation of the Correlations of Factors

Factor Covariance Matrix: Estimate/StdErr/t-value			
	Read_Factor	Math_Factor	Write_Factor
Read_Factor	1.0000	0.3272 0.1311 2.4955 [_Parm10]	0.4810 0.1208 3.9813 [_Parm11]
Math_Factor	0.3272 0.1311 2.4955 [_Parm10]	1.0000	0.3992 0.1313 3.0417 [_Parm12]
Write_Factor	0.4810 0.1208 3.9813 [_Parm11]	0.3992 0.1313 3.0417 [_Parm12]	1.0000

In Output 27.20.9, the error variances for variables are shown.

Output 27.20.9 Estimation of the Error Variances

Error Variances				
Variable	Parameter	Estimate	Standard Error	t Value
reading1	_Add1	37.24939	8.33997	4.46637
reading2	_Add2	46.49695	10.69869	4.34604
reading3	_Add3	15.90447	9.26097	1.71737
math1	_Add4	25.22889	7.72269	3.26685
math2	_Add5	24.89032	8.98327	2.77074
math3	_Add6	42.12110	9.20362	4.57658
writing1	_Add7	27.24965	10.36489	2.62903
writing2	_Add8	49.28881	11.39812	4.32429
writing3	_Add9	48.10684	11.48868	4.18733

All t values except the one for reading3 are greater than 2, a value close to a critical t value at $\alpha = 0.05$. This means that the error variance for reading3 could have been zero in the population, or it could have been nonzero but the current sample just has this insignificant value by chance (that is, a Type 2 error). Further research is needed to confirm either way.

In addition to the parameter estimation results, PROC CALIS also outputs supplementary results that could be useful for interpretations. In Output 27.20.10, the squared multiple correlations and the factor scores regression coefficients are shown.

Output 27.20.10 Supplementary Estimation Results

Squared Multiple Correlations			
Variable	Error Variance	Total Variance	R-Square
reading1	37.24939	83.02400	0.5513
reading2	46.49695	108.24300	0.5704
reading3	15.90447	99.34100	0.8399
math1	25.22889	82.21400	0.6931
math2	24.89032	96.12500	0.7411
math3	42.12110	88.62500	0.5247
writing1	27.24965	90.73400	0.6997
writing2	49.28881	96.54300	0.4895
writing3	48.10684	98.44500	0.5113

Factor Scores Regression Coefficients			
	Read_Factor	Math_Factor	Write_Factor
reading1	0.0200	0.000681	0.001985
reading2	0.0186	0.000633	0.001847
reading3	0.0633	0.002152	0.006275
math1	0.001121	0.0403	0.002808
math2	0.001271	0.0457	0.003183
math3	0.000607	0.0218	0.001520
writing1	0.003195	0.002744	0.0513
writing2	0.001524	0.001309	0.0245
writing3	0.001611	0.001384	0.0259

The percentages of variance for the observed variables that can be explained by the factors are shown in the 'R-Square' column of the table for squared multiple correlations (R-squares). These R-squares can be interpreted meaningfully because there is no reciprocal relationships among variables or correlated errors in the model. All estimates of R-squares are bounded between 0 and 1.

In the table for factor scores regression coefficients, entries are coefficients for the variables you can use to create the factor scores. The larger the coefficient, the more influence of the corresponding variable for creating the factor scores. It makes intuitive sense to see the cluster pattern of these coefficients—the reading measures are more important to create the latent variable scores of Read_Factor and so on.

Example 27.21: Testing Equality of Two Covariance Matrices Using a Multiple-Group Analysis

You can use PROC CALIS to do multiple-group or multiple-sample analysis. The groups in the analysis must be independent. In this example, a relatively simple multiple-group analysis is carried out. The covariance matrices of two independent groups are tested for equality. Hence, individual covariance matrices are actually not structured. Rather, they are constrained to be the same under the null hypothesis. That is, you want to test the following null hypothesis:

$$H_0 : \Sigma_1 = \Sigma_2$$

where Σ_1 and Σ_2 represent the population covariance matrices of the two independent groups in question.

In PROC CALIS, you can use two different approaches to test the equality of covariance matrices. The first approach is to define an MSTRUCT model explicitly and to fit this model to the independent groups. The second approach is to use the `COVPATTERN=` option to invoke the required covariance structure model for the independent groups. Some standard covariance structures or patterns with the MSTRUCT modeling language are built into PROC CALIS internally. With appropriate keywords for the `COVPATTERN=` option, you can invoke the target built-in covariance patterns without defining the MSTRUCT model explicitly. This example considers these two approaches successively.

This example is concerned with a reaction time experiment that was conducted on two groups of individuals. One group ($N = 20$) was considered to be an expert group with prior training related to the tasks of the experiment. Another group ($N = 18$) was a control group without prior training. Three tasks of dexterity were administered to all individuals. These tasks differed by their required complexity levels of body skills. They were labeled as high, medium, and low complexities.

Apparently, the differential performance of the two groups under different task complexities was the primary research objective. In this example, however, you are interested in testing whether the groups have the same covariance matrix for the tasks. Equality of covariance matrices might be an essential assumption in some statistical tests for comparing group means. In this example, the sample covariance matrices for the two groups are stored in the data sets `Expert` and `Novice`, as shown in the following:

```
data expert(type=cov);
  input _type_ $ _name_ $ high medium low;
  datalines;
COV  high    5.88      .      .
COV  medium  2.88      7.16     .
COV  low     3.12      4.44     8.14
;

data novice(type=cov);
  input _type_ $ _name_ $ high medium low;
  datalines;
COV  high    6.42      .      .
COV  medium  1.24      8.25     .
COV  low     4.26      2.75     7.99
;
```

These data sets are read into the analysis through the `GROUP` statements in the following PROC CALIS specification:

```

proc calis;
  group 1 / data=expert nobs=20 label="Expert";
  group 2 / data=novice nobs=18 label="Novice";
  model 1 / groups=1,2;
    mstruct
      var=high medium low;
  fitindex NoIndexType On(only)=[chisq df probchi]
    chicorrect=eqcovmat;
  ods select ModelingInfo MSTRUCTVariables MSTRUCTCovInit Fit;
run;

```

The first **GROUP** statement defines **group 1** for the expert group. The second **GROUP** statement defines **group 2** for the novice group. You use the **NOBS=** option in both statements to provide the number of observations of these groups. You use the **LABEL=** option in these statements to provide meaningful group labels.

The **MODEL** statement defines **MODEL 1**. In the analysis, this model fits to both groups 1 and 2, as indicated by the **GROUPS=** option of the statement. This is done to test the null hypothesis of equality of covariance matrices in the two groups. An **MSTRUCT** model for **MODEL 1** is defined immediately afterward. Three variables, **high**, **medium**, and **low**, are specified in the **VAR=** option of the **MSTRUCT** statement.

Without further specification about the **MSTRUCT** model, **PROC CALIS** assumes all non redundant elements in the covariance matrix are free parameters. This is what is required under the null hypothesis of the equality of covariance matrices in the two groups—the groups have the same covariance matrix, but the covariance matrix itself is unconstrained. Your model under the null hypothesis is now well-defined and ready to run. In addition, you use **FITINDEX** and **ODS SELECT** statements to customize or fine tune the analysis.

By using the options in the **FITINDEX** statement, you can customize the fit summary table and control some analytic options. In the current example, you use the **NOINDEXTYPE** option to suppress the printing of the index types in the fit summary table. Then, you use the **ON(ONLY)=** option to specify the fit indices printed in the fit summary table. In this example, you request only the model fit chi-square statistic, degrees of freedom, and the probability value of the chi-square be printed. Finally, you use the **CHICORRECT=EQCOVMAT** option to request a chi-square correction for the test of equality of covariance matrices. This correction is due to Box (1949) and is implemented in **PROC CALIS** as a built-in chi-square correction option.

In addition, because you are not interested in all displayed output for the current hypothesized model, you use the **ODS SELECT** statement to display only those output (or ODS tables) of interest. In this example, you request only the modeling information, the variables involved, the initial covariance matrix specification, and the fit summary table be printed. All output in **PROC CALIS** are named as an ODS table. To locate a particular output in **PROC CALIS**, you must know the corresponding ODS table name. See the section “**ODS Table Names**” on page 1368 for a listing of ODS tables produced by **PROC CALIS**.

Output 27.21.1 displays some information regarding the basic model setup.

Output 27.21.1 Modeling Information and Initial Specification

Modeling Information						
Maximum Likelihood Estimation						
Group	Label	Data Set	N Obs	Model	Type	Analysis
1	Expert	WORK.EXPERT	20	Model 1	MSTRUCT	Covariances
2	Novice	WORK.NOVICE	18	Model 1	MSTRUCT	Covariances

Model 1. Variables in the Model			
high	medium	low	
Number of Variables = 3			

Model 1. Initial MSTRUCT _COV_ Matrix			
	high	medium	low
high	.	.	.
	[_Add1]	[_Add2]	[_Add4]
medium	.	.	.
	[_Add2]	[_Add3]	[_Add5]
low	.	.	.
	[_Add4]	[_Add5]	[_Add6]

The modeling information table summarizes some basic information about the two groups. Both of them are fitted by Model 1. The next table shows the variables involved: high, medium, and low. The order of variables in this table is the same as that of the row and column variables of the covariance model matrix, which is shown next in [Output 27.21.1](#). The parameters for the entries in the covariance matrix are shown. The names of parameters are displayed in parentheses. All these parameters are set by default and their names have the prefix `_Add`. No initial estimates are given as input, as indicated by the missing value ‘.’.

[Output 27.21.2](#) shows the customized fit summary table, which has been much simplified for the current example due to the uses of some options in the `FITINDEX` statement.

Output 27.21.2 Model Fit

Fit Summary	
Chi-Square	2.4924
Chi-Square DF	6
Pr > Chi-Square	0.8693

As shown in [Output 27.21.2](#), the chi-square test statistic is 2.4924. With six degrees of freedom, the test statistic is not significant at $\alpha = 0.01$. Therefore, the hypothesized model is supported, which means that the equality of the covariance matrices of the groups is supported.

Instead of using the MSTRUCT modeling language explicitly for defining the hypothesized covariance patterns (or structures), you can also invoke the same covariance patterns by using the **COVPATTERN=** option, as shown in the following statements:

```
proc calis covpattern=eqcovmat;
  var high medium low;
  group 1 / data=expert nobs=20 label="Expert";
  group 2 / data=novice nobs=18 label="Novice";
  fitindex NoIndexType On(only)=[chisq df probchi];
run;
```

The **COVPATTERN=EQCOVMAT** option in the PROC CALIS statement hypothesizes that the two population covariance matrices for the groups are the same. Next, you specify the set of variables in the covariance matrices in the VAR statement, followed by the specification of the data for the two groups. You use the FITINDEX statement to select a subset of fit indices to display in the output.

Output 27.21.3 shows the data sets and the corresponding MSTRUCT models that are generated by the **COVPATTERN=EQCOVMAT** option.

Output 27.21.3 Modeling Information with the **COVPATTERN=EQCOVMAT** Option

Modeling Information Maximum Likelihood Estimation						
Group	Label	Data Set	N Obs	Model	Type	Analysis
1	Expert	WORK.EXPERT	20	Model 1	MSTRUCT	Covariances
2	Novice	WORK.NOVICE	18	Model 2	MSTRUCT	Covariances

PROC CALIS generates Model 1 for the expert group and Model 2 for the novice group. Output 27.21.4 and Output 27.21.5 show the covariance matrices of these two models.

Output 27.21.4 Initial Specification of Model 1 for the Expert Group

Model 1. Variables in the Model			
	high	medium	low
	high	medium	low
	Number of Variables = 3		
Model 1. Initial MSTRUCT _COV_ Matrix			
	high	medium	low
high	.	.	.
	[_cov_1_1]	[_cov_2_1]	[_cov_3_1]
medium	.	.	.
	[_cov_2_1]	[_cov_2_2]	[_cov_3_2]
low	.	.	.
	[_cov_3_1]	[_cov_3_2]	[_cov_3_3]

Output 27.21.5 Initial Specification of Model 2 for the Novice Group

```

Model 2. Variables in the Model

      high  medium  low

Number of Variables = 3

Model 2. Initial MSTRUCT _COV_ Matrix

      high          medium          low

high      .          .          .
      [_cov_1_1]    [_cov_2_1]    [_cov_3_1]

medium    .          .          .
      [_cov_2_1]    [_cov_2_2]    [_cov_3_2]

low       .          .          .
      [_cov_3_1]    [_cov_3_2]    [_cov_3_3]

```

In [Output 27.21.4](#), the covariance matrix for the expert group has three variables: high, medium, and low. The second table of [Output 27.21.4](#) shows the parameters for the corresponding covariance matrix. PROC CALIS generates the parameter names for the elements in this covariance matrix: `_cov_1_1`, `_cov_2_1`, ..., `_cov_3_3`. In [Output 27.21.5](#), the covariance matrix for the novice group has exactly the same set of three variables: high, medium, and low. The second table of [Output 27.21.5](#) shows the parameters for the corresponding covariance matrix. These variance and covariance parameters are exactly the same as those in [Output 27.21.4](#), as required by the testing of equality of covariance matrices.

[Output 27.21.6](#) shows the fit summary of the test. The test results are exactly the same as those in [Output 27.21.2](#), as expected. The chi-square value is 2.4924. With six degrees of freedom, the test statistic is not significant at $\alpha = 0.01$. The hypothesis about the equality of the covariance matrices between the groups is supported.

Output 27.21.6 Model Fit with the COVPATTERN=EQCOVMAT Option

```

Fit Summary

Chi-Square          2.4924
Chi-Square DF       6
Pr > Chi-Square     0.8693

```

One advantage of using the built-in covariance patterns such as the current COVPATTERN=EQCOVMAT option is that it is more efficient and less error-prone than if you specify the covariance patterns manually by using the MSTRUCT and MATRIX statements. With the COVPATTERN= option, PROC CALIS generates the correct model specification internally. Another advantage is that when applicable, PROC CALIS applies the appropriate chi-square correction to the chi-square test statistic. For the current example, PROC CALIS displays the following message in the output:

NOTE: The chi-square correction due to Box for testing equality of covariance matrices was applied. Use the CHICORRECT=0 option if this correction is not desirable.

This shows that when you use the COVPATTERN=EQCOVMAT option, an appropriate chi-square correction is applied automatically to the chi-square test statistic. To turn off this automatic chi-square, you can use the CHICORRECT=0 in the PROC CALIS statement (although this should be a rare practice with the COVPATTERN= options).

To extend the test of the equality of covariance matrices to the test of the equality of mean vectors, see [Example 27.4](#). To extend the multiple-group analysis of covariance patterns to the multiple-group analysis of a general structural equation model, see [Example 27.28](#).

Example 27.22: Testing Equality of Covariance and Mean Matrices between Independent Groups

To make the specification of some standard MSTRUCT models for covariance and mean patterns more efficient, PROC CALIS defines these standard models internally. You can use two options to invoke these built-in covariance and mean patterns easily. For example, with the COVPATTERN= option, you can define the compound symmetry (COMPSYM) pattern for the covariance matrix or the equality of covariance matrices between groups (EQCOVMAT). With the MEANPATTERN= option, you can define uniform means (UNIFORM) for the mean vector or the equality of mean vectors between groups (EQMEANVEC). See the COVPATTERN= and the MEANPATTERN= options for details about the supported built-in covariance and mean patterns.

In [Example 27.21](#), you test of the equality of covariance matrices between two groups. This example extends the application to the test of equality of mean vectors between three independent groups by using the COVPATTERN= and MEANPATTERN= options together. The “best” fit model for the data is explored. The following DATA steps define the covariance and mean matrices for the three independent groups, respectively:

```
data g1(type=corr);
  Input _type_ $ 1-8 _name_ $ 9-11 x1-x9;
  datalines;
corr   x1  1.      .      .      .      .      .      .      .      .
corr   x2  .721    1.      .      .      .      .      .      .      .
corr   x3  .676    .379    1.      .      .      .      .      .      .
corr   x4  .149    .403    .450    1.      .      .      .      .      .
corr   x5  .422    .384    .445    .411    1.      .      .      .      .
corr   x6  .343    .456    .243    .308    .531    1.      .      .      .
corr   x7  .115    .225    .201    .481    .373    .198    1.      .      .
corr   x8  .213    .237    .434    .503    .267    .333    .355    1.      .
corr   x9  .236    .257    .159    .246    .126    .235    .601    .512    1.
mean   .  21.3    22.3    17.2    23.4    22.1    15.6    18.7    20.1    19.7
std    .  1.2     1.4     .87     1.33    2.2     1.4     2.3     2.1     1.8
n      .  21     21     21     21     21     21     21     21     21
;
```

```

data g2(type=corr);
  Input _type_ $ 1-8 _name_ $ 9-11 x1-x9;
  datalines;
corr   x1  1.      .      .      .      .      .      .      .      .
corr   x2  .733    1.      .      .      .      .      .      .      .
corr   x3  .576    .388    1.      .      .      .      .      .      .
corr   x4  .209    .414    .425    1.      .      .      .      .      .
corr   x5  .412    .286    .461    .398    1.      .      .      .      .
corr   x6  .323    .399    .212    .302    .522    1.      .      .      .
corr   x7  .215    .295    .188    .467    .334    .232    1.      .      .
corr   x8  .204    .257    .462    .522    .298    .355    .372    1.      .
corr   x9  .245    .272    .177    .301    .156    .246    .578    .422    1.
mean   .  22.1    19.8    16.9    23.3    21.9    17.3    17.9    19.1    19.8
std    .  1.3     1.3     .99    1.25    2.1     1.3     2.2     2.0     1.5
n      .  22     22     22     22     22     22     22     22     22
;

data g3(type=corr);
  Input _type_ $ 1-8 _name_ $ 9-11 x1-x9;
  datalines;
corr   x1  1.      .      .      .      .      .      .      .      .
corr   x2  .699    1.      .      .      .      .      .      .      .
corr   x3  .488    .328    1.      .      .      .      .      .      .
corr   x4  .235    .398    .413    1.      .      .      .      .      .
corr   x5  .377    .265    .471    .376    1.      .      .      .      .
corr   x6  .335    .412    .265    .314    .503    1.      .      .      .
corr   x7  .243    .216    .192    .423    .369    .212    1.      .      .
corr   x8  .217    .292    .423    .525    .219    .317    .376    1.      .
corr   x9  .211    .283    .152    .285    .147    .135    .633    .579    1.
mean   .  22.2    20.9    15.4    25.1    22.6    16.3    19.3    20.2    19.5
std    .  1.5     1.0     1.04   1.5     1.9     1.6     2.4     2.2     1.6
n      .  20     20     20     20     20     20     20     20     20
;

```

Each of these data sets contains the information about the correlations, means, standard deviations, and sample sizes. Even though these data sets contain correlations, by default PROC CALIS analyzes the covariances and means.

The first hypothesis to test is the equality of covariance matrices and mean vectors:

$$H_0 : \Sigma_1 = \Sigma_2 = \Sigma_3 \text{ and } \mu_1 = \mu_2 = \mu_3$$

where Σ_1 , Σ_2 , and Σ_3 are the population covariance matrices for the three independent groups, respectively, and μ_1 , μ_2 , and μ_3 are the population mean vectors for the three independent groups, respectively.

The following statements specify this test:

```

proc calis covpattern=eqcovmat meanpattern=eqmeanvec;
  var x1-x9;
  group 1 / data=g1;
  group 2 / data=g2;
  group 3 / data=g3;
  fitindex NoIndexType On(only)=[chisq df probchi rmsea aic caic sbc];
run;

```

In the PROC CALIS statement, the COVPATTERN=EQCOVMAT option specifies the same covariance matrix for the three groups and the MEANPATTERN=EQMEANVEC option specifies the same mean vector for the three groups. The VAR statement specifies that x1–9 are the variables in the hypothesis test. Next, the GROUP statements specify the data sets for the three independent groups. You use the FITINDEX statement to limit the amount of output fit statistics to the quantities specified: the chi-square test (CHISQ), the degrees of freedom (DF), the significance value of the test statistic (PROBCHI), the root mean square error approximation (RMSEA), Akaike’s information criterion (AIC), consistent Akaike’s information criterion (CAIC), and Schwarz’s Bayesian criterion (SBC). The first three quantities are useful for the chi-square model fit test, while the rest of the fit indices are useful for comparing competing models for the data. Because there are not many quantities in this customized fit summary table, the NOINDEXTYPE option is used to suppress the printing of the fit index types.

Output 27.22.1 shows the general modeling information, including the sample sizes, the models for the groups, the model types, and the analysis types.

Output 27.22.1 Modeling Information for Testing Equality of Covariance and Mean Matrices

Modeling Information					
Maximum Likelihood Estimation					
Group	Data Set	N Obs	Model	Type	Analysis
1	WORK.G1	21	Model 1	MSTRUCT	Means and Covariances
2	WORK.G2	22	Model 2	MSTRUCT	Means and Covariances
3	WORK.G3	20	Model 3	MSTRUCT	Means and Covariances

Output 27.22.2 shows the initial mean vector and the initial covariance matrix specifications for Model 1, which fits to Group 1. PROC CALIS generates the mean parameter names `_mean_1`, `_mean_2`, ..., and `_mean_9` for the nine elements in the mean vector. It also generates the covariance parameter names `_cov_1_1`, `_cov_2_1`, ..., and `_cov_9_9` for the 45 nonredundant elements in the covariance matrix.

Output 27.22.2 Initial Mean Vector and Covariance Matrix for Model 1

Model 1. Initial MSTRUCT _MEAN_ Vector		
Variable	Parameter	Estimate
x1	_mean_1	.
x2	_mean_2	.
x3	_mean_3	.
x4	_mean_4	.
x5	_mean_5	.
x6	_mean_6	.
x7	_mean_7	.
x8	_mean_8	.
x9	_mean_9	.

Output 27.22.2 *continued*

Model 1. Initial MSTRUCT _COV_ Matrix					
	x1	x2	x3	x4	x5
x1
	[_cov_1_1]	[_cov_2_1]	[_cov_3_1]	[_cov_4_1]	[_cov_5_1]
x2
	[_cov_2_1]	[_cov_2_2]	[_cov_3_2]	[_cov_4_2]	[_cov_5_2]
x3
	[_cov_3_1]	[_cov_3_2]	[_cov_3_3]	[_cov_4_3]	[_cov_5_3]
x4
	[_cov_4_1]	[_cov_4_2]	[_cov_4_3]	[_cov_4_4]	[_cov_5_4]
x5
	[_cov_5_1]	[_cov_5_2]	[_cov_5_3]	[_cov_5_4]	[_cov_5_5]
x6
	[_cov_6_1]	[_cov_6_2]	[_cov_6_3]	[_cov_6_4]	[_cov_6_5]
x7
	[_cov_7_1]	[_cov_7_2]	[_cov_7_3]	[_cov_7_4]	[_cov_7_5]
x8
	[_cov_8_1]	[_cov_8_2]	[_cov_8_3]	[_cov_8_4]	[_cov_8_5]
x9
	[_cov_9_1]	[_cov_9_2]	[_cov_9_3]	[_cov_9_4]	[_cov_9_5]

Model 1. Initial MSTRUCT _COV_ Matrix				
	x6	x7	x8	x9
x1
	[_cov_6_1]	[_cov_7_1]	[_cov_8_1]	[_cov_9_1]
x2
	[_cov_6_2]	[_cov_7_2]	[_cov_8_2]	[_cov_9_2]
x3
	[_cov_6_3]	[_cov_7_3]	[_cov_8_3]	[_cov_9_3]
x4
	[_cov_6_4]	[_cov_7_4]	[_cov_8_4]	[_cov_9_4]
x5
	[_cov_6_5]	[_cov_7_5]	[_cov_8_5]	[_cov_9_5]
x6
	[_cov_6_6]	[_cov_7_6]	[_cov_8_6]	[_cov_9_6]
x7
	[_cov_7_6]	[_cov_7_7]	[_cov_8_7]	[_cov_9_7]
x8
	[_cov_8_6]	[_cov_8_7]	[_cov_8_8]	[_cov_9_8]
x9
	[_cov_9_6]	[_cov_9_7]	[_cov_9_8]	[_cov_9_9]

Although not shown here, the initial mean vector and covariance matrices for Models 2 and 3 are exactly the same as those shown in [Output 27.22.2](#), as required by the equality of covariance and mean matrices in the null hypothesis H_0 .

[Output 27.22.3](#) shows the customized fit summary table. The chi-square test statistic is 203.2605. The degrees of freedom is 108 and the p -value is less than 0.0001. Therefore, the hypothesis H_0 of equality in covariance and mean matrices is rejected for the three independent groups. The RMSEA index is much greater than 0.05, which does not indicate a good model fit. Other fit indices such as AIC, CAIC, and SBC are not interpreted for the fit of the model itself, but are useful for comparing competing models in the later discussion.

Output 27.22.3 Fit Summary for Testing H_0 : Equality of Covariance and Mean Matrices

Fit Summary	
Chi-Square	203.2605
Chi-Square DF	108
Pr > Chi-Square	<.0001
RMSEA Estimate	0.2100
Akaike Information Criterion	311.2605
Bozdogan CAIC	480.9897
Schwarz Bayesian Criterion	426.9897

A less restrictive hypothesis is now considered. This hypothesis states the equality of covariance matrices only:

$$H_1 : \Sigma_1 = \Sigma_2 = \Sigma_3 (\mu_1, \mu_2, \text{ and } \mu_3 \text{ unconstrained})$$

H_1 differs from H_0 in that the population means in H_1 are not constrained. To test this hypothesis, you need to change the MEANPATTERN= option to use the SATURATED keyword, as shown in the following statements:

```
proc calis covpattern=eqcovmat meanpattern=saturated;
  var x1-x9;
  group 1 / data=g1;
  group 2 / data=g2;
  group 3 / data=g3;
  fitindex NoIndexType On(only)=[chisq df probchi rmsea aic caic sbc];
run;
```

[Output 27.22.4](#) shows the results of the testing H_1 .

Output 27.22.4 Fit Summary for Testing H_1 : Equality of Covariance Matrices but Unconstrained Means

Fit Summary	
Chi-Square	26.7897
Chi-Square DF	90
Pr > Chi-Square	1.0000
RMSEA Estimate	0.0000
Akaike Information Criterion	170.7897
Bozdogan CAIC	397.0954
Schwarz Bayesian Criterion	325.0954

The chi-square test statistic is 26.7897 ($df = 90$, $p = 1.000$). You cannot reject this null hypothesis about the equality of the population covariance matrices. The RMSEA value is virtually zero, which indicates a perfect fit. Comparing the models under H_0 and H_1 , it is clear that the three groups are significantly different with regard to their mean vectors. By relaxing all the equality constraints on the means in H_0 , H_1 is derived and is supported by the chi-square test. In addition, the RMSEA value for the model under H_1 is perfect. Because lower values of AIC, CAIC, and SBC values indicate better model fit (with the model complexity taken into account), these indices in [Output 27.22.3](#) and [Output 27.22.4](#) support that the model under H_1 is better than H_0 .

However, in getting a superior model fit, H_1 might have relaxed more constraints than absolutely necessary for an optimal fit. That is, it might be possible to impose equality constraints on only some (but not all, as in H_1) of the means to reach the same or even better model fit (by the RMSEA, AIC, CAIC, or SBC criterion) than the model under H_1 . But how can you determine this set of constrained means?

To answer this question, you conduct an exploratory analysis of the data by using some model modification techniques. Models established from exploratory analysis should be validated by external data in the future. However, this example demonstrates the exploratory part only.

Beginning with the model under H_0 , you can manually take away some particular constraints on the means and explore whether the revised model improves the fit. If the revised model fits better, you can repeat the process until you cannot improve more. Ultimately, you might be able to find the “best” model between the models specified under H_0 and H_1 . Such an exploratory analysis is laborious, considering the vast possibilities of constraints on the nine variable means in three independent groups that you could attempt to release. Fortunately, PROC CALIS provides some model modification statistics, called the LM (Lagrange multiplier) statistics, to assist this kind of exploratory analysis.

The following statements specify the model under H_0 , but now with the **MODIFICATION** option added to the PROC CALIS statement:

```
proc calis covpattern=eqcovmat meanpattern=eqmeanvec modification;
  var x1-x9;
  group 1 / data=g1;
  group 2 / data=g2;
  group 3 / data=g3;
  fitindex NoIndexType On(only)=[chisq df probchi rmsea aic caic sbc];
run;
```

The MODIFICATION option requests the so-called LM (Lagrange multiplier) statistics for releasing the parameter constraints. These constraints include the cross-group or within-group constraints and the fixed values in the model. For the model under H_0 , the covariances and the means are all constrained across groups.

These are the equality constraints that you would like to release to obtain a better model fit. [Output 27.22.5](#) shows the results of the LM statistics for releasing these equality constraints in variances, covariances, and means.

Output 27.22.5 Lagrange Multiplier Statistics for Releasing the Equality Constraints

Lagrange Multiplier Statistics for Releasing Equality Constraints								
Parm	---Released Parameter---				LM Stat	Pr > ChiSq	-----Changes-----	
	Model	Type	Var1	Var2			Original Parm	Released Parm
_cov_1_1	1	COV	x1	x1	0.01137	0.9151	0.0178	-0.0355
	2	COV	x1	x1	1.00150	0.3169	0.1729	-0.3212
	3	COV	x1	x1	1.28632	0.2567	-0.1818	0.3923
_cov_2_1	1	COV	x2	x1	2.19353	0.1386	0.2038	-0.4076
	2	COV	x2	x1	0.77014	0.3802	-0.1253	0.2327
	3	COV	x2	x1	0.36128	0.5478	-0.0796	0.1718
_cov_2_2	1	COV	x2	x2	3.12065	0.0773	-0.4344	0.8687
	2	COV	x2	x2	0.05704	0.8112	-0.0609	0.1132
	3	COV	x2	x2	4.14151	0.0418	0.4817	-1.0395
_cov_3_1	1	COV	x3	x1	0.00672	0.9347	0.00888	-0.0178
	2	COV	x3	x1	2.23758	0.1347	-0.1681	0.3122
	3	COV	x3	x1	2.10455	0.1469	0.1512	-0.3264
_cov_3_2	1	COV	x3	x2	2.18538	0.1393	-0.1940	0.3881
	2	COV	x3	x2	3.14532	0.0761	0.2416	-0.4487
	3	COV	x3	x2	0.10264	0.7487	-0.0405	0.0874
_cov_3_3	1	COV	x3	x3	1.56813	0.2105	0.1815	-0.3630
	2	COV	x3	x3	0.66118	0.4161	0.1223	-0.2272
	3	COV	x3	x3	4.42160	0.0355	-0.2934	0.6332
_cov_4_1	1	COV	x4	x1	0.31691	0.5735	-0.0667	0.1333
	2	COV	x4	x1	0.32615	0.5679	0.0702	-0.1304
	3	COV	x4	x1	0.0002277	0.9880	-0.00172	0.00371
_cov_4_2	1	COV	x4	x2	0.73377	0.3917	0.1242	-0.2484
	2	COV	x4	x2	0.53196	0.4658	-0.1097	0.2038
	3	COV	x4	x2	0.01445	0.9043	-0.0168	0.0362
_cov_4_3	1	COV	x4	x3	0.0000258	0.9959	0.000547	-0.00109
	2	COV	x4	x3	0.24892	0.6178	-0.0558	0.1036
	3	COV	x4	x3	0.25646	0.6126	0.0525	-0.1134
_cov_4_4	1	COV	x4	x4	0.04412	0.8336	0.0361	-0.0722
	2	COV	x4	x4	0.52198	0.4700	0.1288	-0.2392
	3	COV	x4	x4	0.90948	0.3403	-0.1577	0.3403
_cov_5_1	1	COV	x5	x1	0.0008607	0.9766	-0.00477	0.00953
	2	COV	x5	x1	0.01238	0.9114	0.0188	-0.0348
	3	COV	x5	x1	0.00712	0.9328	-0.0132	0.0285
_cov_5_2	1	COV	x5	x2	0.10637	0.7443	-0.0649	0.1297
	2	COV	x5	x2	0.00631	0.9367	-0.0164	0.0304
	3	COV	x5	x2	0.16971	0.6804	0.0789	-0.1702
_cov_5_3	1	COV	x5	x3	0.06645	0.7966	-0.0385	0.0771
	2	COV	x5	x3	0.0008275	0.9771	0.00446	-0.00829
	3	COV	x5	x3	0.05370	0.8167	0.0334	-0.0720
_cov_5_4	1	COV	x5	x4	0.24212	0.6227	0.0809	-0.1617
	2	COV	x5	x4	0.04459	0.8328	-0.0360	0.0669
	3	COV	x5	x4	0.07959	0.7779	-0.0446	0.0963
_cov_5_5	1	COV	x5	x5	0.01778	0.8939	-0.0431	0.0862
	2	COV	x5	x5	0.08223	0.7743	-0.0962	0.1787
	3	COV	x5	x5	0.18417	0.6678	0.1336	-0.2883

Output 27.22.5 continued

Lagrange Multiplier Statistics for Releasing Equality Constraints								
Parm	---Released Parameter---				LM Stat	Pr > ChiSq	-----Changes-----	
	Model	Type	Var1	Var2			Original Parm	Released Parm
_cov_6_1	1	COV	x6	x1	0.29558	0.5867	-0.0721	0.1442
	2	COV	x6	x1	0.26589	0.6061	-0.0710	0.1318
	3	COV	x6	x1	1.16570	0.2803	0.1378	-0.2974
_cov_6_2	1	COV	x6	x2	0.00228	0.9619	-0.00780	0.0156
	2	COV	x6	x2	1.00319	0.3165	0.1697	-0.3152
	3	COV	x6	x2	0.95767	0.3278	-0.1538	0.3320
_cov_6_3	1	COV	x6	x3	1.39116	0.2382	0.1513	-0.3027
	2	COV	x6	x3	0.08741	0.7675	-0.0394	0.0731
	3	COV	x6	x3	0.79586	0.3723	-0.1102	0.2378
_cov_6_4	1	COV	x6	x4	0.46031	0.4975	-0.0947	0.1894
	2	COV	x6	x4	0.04254	0.8366	0.0299	-0.0555
	3	COV	x6	x4	0.22665	0.6340	0.0640	-0.1381
_cov_6_5	1	COV	x6	x5	0.14991	0.6986	-0.0700	0.1399
	2	COV	x6	x5	0.04723	0.8280	0.0408	-0.0757
	3	COV	x6	x5	0.02874	0.8654	0.0295	-0.0636
_cov_6_6	1	COV	x6	x6	0.22550	0.6349	0.1079	-0.2158
	2	COV	x6	x6	0.04390	0.8340	0.0494	-0.0918
	3	COV	x6	x6	0.48451	0.4864	-0.1523	0.3286
_cov_7_1	1	COV	x7	x1	0.50774	0.4761	0.1203	-0.2406
	2	COV	x7	x1	0.01246	0.9111	-0.0196	0.0363
	3	COV	x7	x1	0.36926	0.5434	-0.0988	0.2131
_cov_7_2	1	COV	x7	x2	0.01235	0.9115	0.0228	-0.0455
	2	COV	x7	x2	0.16400	0.6855	-0.0861	0.1598
	3	COV	x7	x2	0.09159	0.7622	0.0597	-0.1288
_cov_7_3	1	COV	x7	x3	0.16844	0.6815	-0.0644	0.1288
	2	COV	x7	x3	0.15095	0.6976	0.0633	-0.1175
	3	COV	x7	x3	0.0003079	0.9860	0.00265	-0.00572
_cov_7_4	1	COV	x7	x4	0.22542	0.6349	-0.0776	0.1551
	2	COV	x7	x4	0.00754	0.9308	0.0147	-0.0273
	3	COV	x7	x4	0.15376	0.6950	0.0617	-0.1331
_cov_7_5	1	COV	x7	x5	0.07831	0.7796	-0.0631	0.1262
	2	COV	x7	x5	0.07552	0.7835	0.0643	-0.1195
	3	COV	x7	x5	3.293E-6	0.9986	0.000394	-0.00085
_cov_7_6	1	COV	x7	x6	0.13810	0.7102	0.0726	-0.1452
	2	COV	x7	x6	0.0001086	0.9917	0.00211	-0.00392
	3	COV	x7	x6	0.14999	0.6985	-0.0729	0.1572
_cov_7_7	1	COV	x7	x7	0.09334	0.7600	0.1051	-0.2101
	2	COV	x7	x7	0.00128	0.9714	0.0128	-0.0237
	3	COV	x7	x7	0.11994	0.7291	-0.1147	0.2474
_cov_8_1	1	COV	x8	x1	0.04800	0.8266	0.0353	-0.0706
	2	COV	x8	x1	0.19725	0.6569	0.0743	-0.1379
	3	COV	x8	x1	0.45888	0.4981	-0.1051	0.2268
_cov_8_2	1	COV	x8	x2	0.13689	0.7114	0.0727	-0.1453
	2	COV	x8	x2	0.31671	0.5736	-0.1147	0.2130
	3	COV	x8	x2	0.04084	0.8398	0.0382	-0.0825

Output 27.22.5 continued

Lagrange Multiplier Statistics for Releasing Equality Constraints								
Parm	---Released Parameter---				LM Stat	Pr > ChiSq	-----Changes-----	
	Model	Type	Var1	Var2			Original Parm	Released Parm
_cov_8_3	1	COV	x8	x3	0.37615	0.5397	-0.0904	0.1808
	2	COV	x8	x3	0.00452	0.9464	-0.0103	0.0191
	3	COV	x8	x3	0.47678	0.4899	0.0980	-0.2114
_cov_8_4	1	COV	x8	x4	0.00989	0.9208	0.0150	-0.0300
	2	COV	x8	x4	0.01001	0.9203	0.0157	-0.0291
	3	COV	x8	x4	0.04138	0.8388	-0.0296	0.0638
_cov_8_5	1	COV	x8	x5	0.01378	0.9066	-0.0267	0.0533
	2	COV	x8	x5	0.03154	0.8590	-0.0419	0.0778
	3	COV	x8	x5	0.09063	0.7634	0.0659	-0.1421
_cov_8_6	1	COV	x8	x6	0.0007193	0.9786	0.00510	-0.0102
	2	COV	x8	x6	0.01293	0.9095	0.0224	-0.0417
	3	COV	x8	x6	0.02067	0.8857	-0.0263	0.0568
_cov_8_7	1	COV	x8	x7	0.16543	0.6842	0.0952	-0.1904
	2	COV	x8	x7	0.29902	0.5845	-0.1328	0.2467
	3	COV	x8	x7	0.02206	0.8819	0.0335	-0.0722
_cov_8_8	1	COV	x8	x8	0.00581	0.9392	0.0244	-0.0487
	2	COV	x8	x8	0.00694	0.9336	-0.0276	0.0513
	3	COV	x8	x8	0.0000660	0.9935	0.00250	-0.00539
_cov_9_1	1	COV	x9	x1	0.19272	0.6607	-0.0532	0.1063
	2	COV	x9	x1	0.01910	0.8901	-0.0174	0.0323
	3	COV	x9	x1	0.34408	0.5575	0.0684	-0.1476
_cov_9_2	1	COV	x9	x2	0.09017	0.7640	-0.0446	0.0892
	2	COV	x9	x2	0.26496	0.6067	0.0794	-0.1474
	3	COV	x9	x2	0.04994	0.8232	-0.0320	0.0690
_cov_9_3	1	COV	x9	x3	0.44236	0.5060	0.0758	-0.1516
	2	COV	x9	x3	0.12761	0.7209	-0.0422	0.0784
	3	COV	x9	x3	0.09470	0.7583	-0.0338	0.0728
_cov_9_4	1	COV	x9	x4	0.04619	0.8298	0.0260	-0.0520
	2	COV	x9	x4	0.22996	0.6316	-0.0602	0.1117
	3	COV	x9	x4	0.07502	0.7842	0.0319	-0.0688
_cov_9_5	1	COV	x9	x5	0.02807	0.8669	0.0279	-0.0557
	2	COV	x9	x5	0.0006585	0.9795	-0.00443	0.00823
	3	COV	x9	x5	0.02058	0.8859	-0.0230	0.0496
_cov_9_6	1	COV	x9	x6	0.03989	0.8417	-0.0282	0.0563
	2	COV	x9	x6	0.15069	0.6979	-0.0568	0.1055
	3	COV	x9	x6	0.36051	0.5482	0.0815	-0.1759
_cov_9_7	1	COV	x9	x7	0.03398	0.8537	-0.0284	0.0567
	2	COV	x9	x7	0.05802	0.8097	0.0385	-0.0714
	3	COV	x9	x7	0.00362	0.9520	-0.00891	0.0192
_cov_9_8	1	COV	x9	x8	0.06050	0.8057	-0.0391	0.0781
	2	COV	x9	x8	0.56151	0.4537	0.1235	-0.2294
	3	COV	x9	x8	0.26945	0.6037	-0.0794	0.1713
_cov_9_9	1	COV	x9	x9	0.13296	0.7154	-0.0655	0.1310
	2	COV	x9	x9	0.00130	0.9712	-0.00673	0.0125
	3	COV	x9	x9	0.16526	0.6844	0.0703	-0.1517

Output 27.22.5 continued

Lagrange Multiplier Statistics for Releasing Equality Constraints								
Parm	---Released Parameter---				LM Stat	Pr > ChiSq	-----Changes-----	
	Model	Type	Var1	Var2			Original Parm	Released Parm
_mean_1	1	MEAN	x1		11.09173	0.0009	0.3453	-0.6906
	2	MEAN	x1		1.21196	0.2709	-0.1184	0.2200
	3	MEAN	x1		5.04550	0.0247	-0.2242	0.4838
_mean_2	1	MEAN	x2		21.46921	<.0001	-0.5837	1.1675
	2	MEAN	x2		15.27776	<.0001	0.5110	-0.9490
	3	MEAN	x2		0.47301	0.4916	0.0834	-0.1800
_mean_3	1	MEAN	x3		4.41967	0.0355	-0.2034	0.4067
	2	MEAN	x3		6.37770	0.0116	-0.2535	0.4708
	3	MEAN	x3		22.27732	<.0001	0.4395	-0.9485
_mean_4	1	MEAN	x4		3.26860	0.0706	0.1904	-0.3807
	2	MEAN	x4		0.03260	0.8567	0.0197	-0.0366
	3	MEAN	x4		4.06935	0.0437	-0.2045	0.4413
_mean_5	1	MEAN	x5		0.22210	0.6374	-0.0681	0.1362
	2	MEAN	x5		1.50172	0.2204	0.1837	-0.3412
	3	MEAN	x5		0.60673	0.4360	-0.1083	0.2338
_mean_6	1	MEAN	x6		1.61486	0.2038	0.1539	-0.3078
	2	MEAN	x6		6.72912	0.0095	-0.3260	0.6055
	3	MEAN	x6		1.88248	0.1701	0.1600	-0.3452
_mean_7	1	MEAN	x7		0.14035	0.7079	-0.0558	0.1116
	2	MEAN	x7		0.11034	0.7398	0.0514	-0.0954
	3	MEAN	x7		0.00153	0.9688	0.00560	-0.0121
_mean_8	1	MEAN	x8		0.12603	0.7226	-0.0510	0.1019
	2	MEAN	x8		1.96607	0.1609	0.2089	-0.3880
	3	MEAN	x8		1.16200	0.2811	-0.1490	0.3215
_mean_9	1	MEAN	x9		0.05301	0.8179	0.0248	-0.0496
	2	MEAN	x9		0.97965	0.3223	-0.1106	0.2054
	3	MEAN	x9		0.61083	0.4345	0.0810	-0.1748

To use the results of this table, you look for parameters that have large LM statistics (in the LM Stat column). Equivalently, you can look for parameters that have small *p*-values (in the Pr > ChiSq column). Loosely speaking, an LM statistic estimates the reduction of model fit chi-square statistic if you release the constraint on the corresponding parameter. The *p*-value indicates whether the improvement would be significant. Therefore, releasing those parameters with a high LM statistic and small *p*-value would be the key to model improvements. Bear in mind that the LM statistics are linear approximations and they might not be very accurate as estimates of the actual model improvement, which could only be accessed when you refit the model with the particular constraint released. Nonetheless, the LM statistics could still be very useful because they show which constraints could potentially improve the model the most.

Output 27.22.5 shows the results from releasing the constraints on the variances and covariances first. Each constrained element of the covariance matrix has three rows, respectively, for the three models (or groups). For example, the first parameter is `_cov_1_1`, which is the same variance parameter for x1 in the three models. The first row shows that if you release the variance of x1 in Model 1 from the constraint (while keeping the variances of x1 being constrained between Models 2 and 3), the LM statistic is 0.01127, and the corresponding *p*-value is 0.9155. This means that the model fit improvement would be very small and so you do not expect a significant model fit improvement by releasing this constraint. The columns entitled

“Changes” show the estimated parameter changes in the original parameters (that is, `_cov_1_1` for Models 2 and 3) and in the released parameter (that is, the new parameter for the variance of `x1` in Model 1) if you release the corresponding equality constraint. These two “Changes” columns are not very useful for the present purpose.

Looking through the results for the variance and covariance constraints, you can see that almost all the associated p -values are large (that is, as compared with the conventional 0.05 level for significance). Therefore, all these constraints on variances and covariances would not improve the model fit significantly. In contrast, the constraints on the means show that several of them could be released for a sizable model fit improvement. The largest LM statistic in the table is the one for `_mean_3` in Model 3. The LM statistic is 22.27678 and its corresponding p -value is less than 0.0001. This means that if the mean of `x3` in Model 3 were not constrained with the means of `x3` in Models 1 and 2, you would have expected a reduction in the model fit chi-square statistic that is estimated at 22.27678. Other notable LM statistics are those for `_mean_1` in Model 1, `_mean_2` in Model 1 or 2, and `_mean_6` in Model 2.

Two important points are noted about the use of the LM statistics. First, the LM statistics are not additive. You cannot expect that the total reduction in model fit chi-square for releasing a particular set of parameter constraints is the sum of the corresponding LM statistics. Second, once you release a particular constraint and refit the model, the LM statistics in the revised model might not follow the same pattern as those LM statistics in the original model. Basically, these are due to the nonlinearity of the fit function and the dependence of the parameter estimates. Therefore, in order to find the best model for the data, it would be more sensible to adopt a one-at-a-time approach to release the constraints. That is, you release one constraint at a time and refit the model to see if you can release more constraints to improve the model fit.

According to the results of LM statistics in [Output 27.22.5](#), you first release the constraint on the `_mean_3` parameter, which is for the mean of `x3` in Model 3. The following statements fit such a model:

```
proc calis modification;
  var x1-x9;
  group 1 / data=g1;
  group 2 / data=g2;
  group 3 / data=g3;
  model 1 / group = 1;
    mstruct;
    matrix _cov_ = cov01-cov45;
    matrix _mean_ = mean1-mean9;
  model 2 / group = 2;
    refmodel 1;
  model 3 / group = 3;
    refmodel 1;
    renameparm mean3=mean3_md13;
  fitindex NoIndexType On(only)=[chisq df probchi rmsea aic caic sbc];
run;
```

Because the revised model is no longer a supported built-in MSTRUCT model, you cannot use the `MEANPATTERN=` or the `COVPATTERN=` options any more. Instead, you now use the MSTRUCT modeling language to specify the covariance and mean patterns. Model 1, which fits to Group 1, is an MSTRUCT model with variance and covariance parameters `cov01-cov45` and mean parameters `mean1-mean9`. Model 2, which fits to Group 2, refers to the specifications of Model 1, as indicated in a `REFMODEL` statement. Hence, Model 1 and Model 2 are completely constrained in variances, covariances, and means. Model 3, which fits to Group 3, also refers to the specifications of Model 1, as indicated in another `REFMODEL` statement. However, the `RENAMEPARM` statement renames the parameter `mean3` in the reference model

(that is, Model 1) to a new name mean3_md13. As a result, all variance, covariance, and mean parameters except one in Model 3 are constrained to be the same as those in Model 1. The mean of x3 in Model 3 is the only parameter that is not constrained with any other parameters. This forms the first revised model from H_0 . The MODIFICATION option is specified again to determine whether a further model fit improvement is possible.

Output 27.22.6 shows the modeling information of the first revised model. It shows that Models 2 and 3 make references to Model 1. Therefore, parameters between models are constrained by referencing.

Output 27.22.6 Modeling Information for The First Revised Model

Modeling Information Maximum Likelihood Estimation						
Group	Data Set	N Obs	Model	Type	Base Model	Analysis
1	WORK.G1	21	Model 1	MSTRUCT		Means and Covariances
2	WORK.G2	22	Model 2	MSTRUCT	Model 1	Means and Covariances
3	WORK.G3	20	Model 3	MSTRUCT	Model 1	Means and Covariances

Output 27.22.7 shows the initial specifications of the means, variances, and covariances in Model 1.

Output 27.22.7 Initial Mean Vector and Covariance Matrix for Model 1 in the First Revised Model

Model 1. Initial MSTRUCT _MEAN_ Vector		
Variable	Parameter	Estimate
x1	mean1	.
x2	mean2	.
x3	mean3	.
x4	mean4	.
x5	mean5	.
x6	mean6	.
x7	mean7	.
x8	mean8	.
x9	mean9	.

Output 27.22.7 continued

Model 1. Initial MSTRUCT _COV_ Matrix					
	x1	x2	x3	x4	x5
x1
	[cov01]	[cov02]	[cov04]	[cov07]	[cov11]
x2
	[cov02]	[cov03]	[cov05]	[cov08]	[cov12]
x3
	[cov04]	[cov05]	[cov06]	[cov09]	[cov13]
x4
	[cov07]	[cov08]	[cov09]	[cov10]	[cov14]
x5
	[cov11]	[cov12]	[cov13]	[cov14]	[cov15]
x6
	[cov16]	[cov17]	[cov18]	[cov19]	[cov20]
x7
	[cov22]	[cov23]	[cov24]	[cov25]	[cov26]
x8
	[cov29]	[cov30]	[cov31]	[cov32]	[cov33]
x9
	[cov37]	[cov38]	[cov39]	[cov40]	[cov41]
Model 1. Initial MSTRUCT _COV_ Matrix					
	x6	x7	x8	x9	
x1	
	[cov16]	[cov22]	[cov29]	[cov37]	
x2	
	[cov17]	[cov23]	[cov30]	[cov38]	
x3	
	[cov18]	[cov24]	[cov31]	[cov39]	
x4	
	[cov19]	[cov25]	[cov32]	[cov40]	
x5	
	[cov20]	[cov26]	[cov33]	[cov41]	
x6	
	[cov21]	[cov27]	[cov34]	[cov42]	
x7	
	[cov27]	[cov28]	[cov35]	[cov43]	
x8	
	[cov34]	[cov35]	[cov36]	[cov44]	
x9	
	[cov42]	[cov43]	[cov44]	[cov45]	

Output 27.22.8 shows the initial specifications of the means in Model 2. The mean parameters in Model 2 are exactly the same as those in Model 1, as shown in Output 27.22.7. The variance and covariance parameters in Model 2 are also exactly the same as those in Model 1, but are not shown here to conserve space.

Output 27.22.8 Initial Mean Vector for Model 2 in the First Revised Model

Model 2. Initial MSTRUCT _MEAN_ Vector		
Variable	Parameter	Estimate
x1	mean1	.
x2	mean2	.
x3	mean3	.
x4	mean4	.
x5	mean5	.
x6	mean6	.
x7	mean7	.
x8	mean8	.
x9	mean9	.

Output 27.22.9 shows the initial specifications of the means in Model 3. All but one mean parameter in Model 3 are exactly the same as those in Models 1 and 2, as shown in Output 27.22.7 and Output 27.22.8, respectively. The mean for x3 in Model 3 is mean3_md13, which is now a distinct parameter, and therefore it is not constrained with any other parameters in the first or the second models for Groups 1 or 2. However, the variance and covariance parameters in Model 3 are exactly the same as those in Model 1. They are not shown here to conserve space.

Output 27.22.9 Initial Mean Vector for Model 3 in the First Revised Model

Model 3. Initial MSTRUCT _MEAN_ Vector		
Variable	Parameter	Estimate
x1	mean1	.
x2	mean2	.
x3	mean3_md13	.
x4	mean4	.
x5	mean5	.
x6	mean6	.
x7	mean7	.
x8	mean8	.
x9	mean9	.

Output 27.22.10 shows the fit summary of the first revised model. The model fit chi-square is 148.8865, which drops quite a bit from the original model under H_0 . The p -value of the model fit chi-square is 0.0046, which is statistically significant. The RMSEA value is 0.1399, which is also a sizable improvement. All the AIC, CAIC, and SBC values are reduced, indicating better model fit than the model under H_0 .

Output 27.22.10 Fit Summary for the First Revised Model

Fit Summary	
Chi-Square	148.8865
Chi-Square DF	107
Pr > Chi-Square	0.0046
RMSEA Estimate	0.1399
Akaike Information Criterion	258.8865
Bozdogan CAIC	431.7589
Schwarz Bayesian Criterion	376.7589

Output 27.22.11 shows the LM statistics for releasing the equality constraints in the first revised model. Almost all of the results for the variance and covariance constraints are omitted because their LM statistics are not significant. However, Output 27.22.11 shows all the LM statistics for releasing the constraints in means. The mean of x2 in Model 2 has the largest LM statistic at 26.25044.

Output 27.22.11 LM Statistics for Releasing the Equality Constraints in the First Revised Model

Lagrange Multiplier Statistics for Releasing Equality Constraints								
Parm	---Released Parameter---				LM Stat	Pr > ChiSq	-----Changes-----	
	Model	Type	Var1	Var2			Original Parm	Released Parm
cov01	1	COV	x1	x1	0.64999	0.4201	0.1050	-0.2100
	2	COV	x1	x1	0.41758	0.5181	0.0874	-0.1622
	3	COV	x1	x1	2.18923	0.1390	-0.1855	0.4004
					.			
					.			
mean1	1	MEAN	x1		9.26674	0.0023	0.2872	-0.5745
	2	MEAN	x1		3.00599	0.0830	-0.1702	0.3160
	3	MEAN	x1		2.13787	0.1437	-0.1481	0.3196
mean2	1	MEAN	x2		26.25115	<.0001	-0.6568	1.3135
	2	MEAN	x2		12.34638	0.0004	0.4674	-0.8680
	3	MEAN	x2		2.52683	0.1119	0.1962	-0.4234
mean3	1	MEAN	x3		0.58891	0.4428	-0.0787	0.0827
	2	MEAN	x3		0.58891	0.4428	0.0827	-0.0787
mean4	1	MEAN	x4		6.59009	0.0103	0.2746	-0.5493
	2	MEAN	x4		0.51343	0.4737	0.0796	-0.1478
	3	MEAN	x4		11.61610	0.0007	-0.3586	0.7739
mean5	1	MEAN	x5		0.52967	0.4667	-0.1042	0.2084
	2	MEAN	x5		0.22294	0.6368	0.0702	-0.1304
	3	MEAN	x5		0.06889	0.7930	0.0374	-0.0807
mean6	1	MEAN	x6		1.16656	0.2801	0.1270	-0.2540
	2	MEAN	x6		5.29599	0.0214	-0.2810	0.5218
	3	MEAN	x6		1.69412	0.1931	0.1518	-0.3275
mean7	1	MEAN	x7		0.03791	0.8456	-0.0291	0.0582
	2	MEAN	x7		0.44510	0.5047	0.1036	-0.1923
	3	MEAN	x7		0.23804	0.6256	-0.0704	0.1520
mean8	1	MEAN	x8		0.39420	0.5301	-0.0883	0.1765
	2	MEAN	x8		0.24231	0.6225	0.0719	-0.1335
	3	MEAN	x8		0.01951	0.8889	0.0200	-0.0431
mean9	1	MEAN	x9		0.00156	0.9685	0.00423	-0.00846
	2	MEAN	x9		1.06866	0.3012	-0.1150	0.2136
	3	MEAN	x9		1.05210	0.3050	0.1065	-0.2297

You now modify the preceding statements to specify the second revised model, as shown in the following statements:

```
proc calis modification;
  var x1-x9;
  group 1 / data=g1;
  group 2 / data=g2;
  group 3 / data=g3;
  model 1 / group = 1;
    mstruct;
    matrix _cov_ = cov01-cov45;
    matrix _mean_ = mean1-mean9;
  model 2 / group = 2;
    refmodel 1;
    renameparm mean2=mean2_new;    /* constraint a */
  model 3 / group = 3;
    refmodel 1;
    renameparm mean2=mean2_new,    /* constraint a */
              mean3=mean3_md13;
  fitindex NoIndexType On(only)=[chisq df probchi rmsea aic caic sbc];
run;
```

This second revised model must not constrain the mean of x_2 in Model 1 with any parameters. A straightforward way to do this is to rename the `mean2` parameter to a unique name in Model 1. However, for the current specification it is more convenient to rename the `mean2` parameter in Models 2 and 3 to another name. In the specification of the second revised model, Models 2 and 3 still make references to Model 1. However, in the respective `RENAMEPARM` statements, both Model 2 and 3 rename the `mean2` parameter that is referenced from Model 1 to the new name `mean2_new`. This way the mean for x_2 in Model 1 is not constrained with the means of x_2 in Models 2 and 3. But the means for x_2 in Models 2 and 3 are still constrained to be equal by the same parameter `mean2_new`. [Output 27.22.12](#) shows the fit summary of the second revised model.

Output 27.22.12 Fit Summary for the Second Revised Model

Fit Summary	
Chi-Square	86.3927
Chi-Square DF	106
Pr > Chi-Square	0.9183
RMSEA Estimate	0.0000
Akaike Information Criterion	198.3927
Bozdogan CAIC	374.4083
Schwarz Bayesian Criterion	318.4083

Again, a sizable improvement over the first revised model is shown in the second revised model. The model fit chi-square statistic is no longer significant ($p = 0.9183$), and the RMSEA value is perfect at 0. Large drops in the AIC, CAIC, and SBC values are also observed.

Output 27.22.13 suggests that the mean of x6 in Model 2 (which has the largest LM statistic at 11.41243) could be released from the equality constraints to achieve the largest model improvement over the current model.

Output 27.22.13 LM Statistics for Releasing the Equality Constraints in the Second Revised Model

Lagrange Multiplier Statistics for Releasing Equality Constraints								
Parm	---Released Parameter---				LM Stat	Pr > ChiSq	-----Changes-----	
	Model	Type	Var1	Var2			Original Parm	Released Parm
cov01	1	COV	x1	x1	2.77024	0.0960	0.1384	-0.2770
	2	COV	x1	x1	0.28728	0.5920	0.0462	-0.0860
	3	COV	x1	x1	5.00087	0.0253	-0.1791	0.3864
.								
.								
mean1	1	MEAN	x1		2.75437	0.0970	0.1646	-0.3292
	2	MEAN	x1		3.21093	0.0731	-0.1511	0.2806
	3	MEAN	x1		0.24923	0.6176	0.0424	-0.0915
mean3	1	MEAN	x3		0.74338	0.3886	-0.0877	0.0934
	2	MEAN	x3		0.74338	0.3886	0.0934	-0.0877
mean4	1	MEAN	x4		6.17449	0.0130	0.2672	-0.5343
	2	MEAN	x4		0.02087	0.8851	-0.0146	0.0272
	3	MEAN	x4		4.71344	0.0299	-0.2072	0.4470
mean5	1	MEAN	x5		1.65517	0.1983	-0.1853	0.3706
	2	MEAN	x5		1.16118	0.2812	0.1606	-0.2982
	3	MEAN	x5		0.04040	0.8407	0.0287	-0.0618
mean6	1	MEAN	x6		5.03834	0.0248	0.2712	-0.5423
	2	MEAN	x6		11.41247	0.0007	-0.4217	0.7831
	3	MEAN	x6		1.51175	0.2189	0.1460	-0.3150
mean7	1	MEAN	x7		0.32382	0.5693	-0.0853	0.1706
	2	MEAN	x7		0.82184	0.3646	0.1410	-0.2619
	3	MEAN	x7		0.12513	0.7235	-0.0512	0.1104
mean8	1	MEAN	x8		2.39207	0.1220	-0.2210	0.4420
	2	MEAN	x8		1.58292	0.2083	0.1867	-0.3467
	3	MEAN	x8		0.08641	0.7688	0.0427	-0.0922
mean9	1	MEAN	x9		0.00682	0.9342	0.00886	-0.0177
	2	MEAN	x9		1.20949	0.2714	-0.1225	0.2274
	3	MEAN	x9		1.10016	0.2942	0.1089	-0.2349
mean2_new	2	MEAN	x2		4.47814	0.0343	0.2983	-0.2661
	3	MEAN	x2		4.47814	0.0343	-0.2661	0.2983

The process of model refitting should now become familiar. You modify the previous model to release the constraint on the mean of x_6 in Model 2. As a result, the third revised model is specified by the following statements:

```
proc calis modification;
  var x1-x9;
  group 1 / data=g1;
  group 2 / data=g2;
  group 3 / data=g3;
  model 1 / group = 1;
    mstruct;
    matrix _cov_ = cov01-cov45;
    matrix _mean_ = mean1-mean9;
  model 2 / group = 2;
    refmodel 1;
    renameparm mean2=mean2_new,      /* constraint a */
              mean6=mean6_md12;
  model 3 / group = 3;
    refmodel 1;
    renameparm mean2=mean2_new,      /* constraint a */
              mean3=mean3_md13;
  fitindex NoIndexType On(only)=[chisq df probchi rmsea aic caic sbc];
run;
```

The only modification from the previous specification is to rename `mean6` to `mean6_md12` in the `RENAMEPARM` statement of Model 2. [Output 27.22.14](#) shows the model fit summary of the third revised model.

Output 27.22.14 Fit Summary for the Third Revised Model

Fit Summary	
Chi-Square	68.7869
Chi-Square DF	105
Pr > Chi-Square	0.9976
RMSEA Estimate	0.0000
Akaike Information Criterion	182.7869
Bozdogan CAIC	361.9456
Schwarz Bayesian Criterion	304.9456

The model improvement over the second revised model is still notable in the third revised model. The chi-square value drops about 20 points in the third revised model. The AIC, CAIC, and the SBC values are reduced notably, though not as impressively as with the previous improvements.

Output 27.22.15 suggests that the mean of x4 in Model 1 (which has the largest LM statistic at 7.01946) could be released from the equality constraint to improve model fit further.

Output 27.22.15 LM Statistics for Releasing the Equality Constraints in the Third Revised Model

Lagrange Multiplier Statistics for Releasing Equality Constraints								
Parm	---Released Parameter---				LM Stat	Pr > ChiSq	-----Changes-----	
	Model	Type	Var1	Var2			Original Parm	Released Parm
cov01	1	COV	x1	x1	2.43374	0.1187	0.1342	-0.2684
	2	COV	x1	x1	0.19037	0.6626	0.0390	-0.0723
	3	COV	x1	x1	4.11402	0.0425	-0.1679	0.3625
					.			
					.			
					.			
mean1	1	MEAN	x1		6.15722	0.0131	0.2550	-0.5101
	2	MEAN	x1		6.05791	0.0138	-0.2109	0.3917
	3	MEAN	x1		0.29302	0.5883	0.0463	-0.0999
mean3	1	MEAN	x3		2.89780	0.0887	-0.1796	0.1889
	2	MEAN	x3		2.89780	0.0887	0.1889	-0.1796
mean4	1	MEAN	x4		7.01915	0.0081	0.2850	-0.5701
	2	MEAN	x4		0.04916	0.8245	-0.0226	0.0419
	3	MEAN	x4		5.05102	0.0246	-0.2148	0.4635
mean5	1	MEAN	x5		0.21231	0.6450	-0.0672	0.1345
	2	MEAN	x5		0.07502	0.7842	-0.0443	0.0822
	3	MEAN	x5		0.55031	0.4582	0.1059	-0.2285
mean6	1	MEAN	x6		0.07013	0.7911	0.0503	-0.0486
	3	MEAN	x6		0.07013	0.7911	-0.0486	0.0503
mean7	1	MEAN	x7		0.98902	0.3200	-0.1513	0.3025
	2	MEAN	x7		2.42355	0.1195	0.2463	-0.4575
	3	MEAN	x7		0.34231	0.5585	-0.0858	0.1850
mean8	1	MEAN	x8		1.58481	0.2081	-0.1786	0.3572
	2	MEAN	x8		0.81634	0.3663	0.1347	-0.2502
	3	MEAN	x8		0.14503	0.7033	0.0549	-0.1184
mean9	1	MEAN	x9		0.13504	0.7133	0.0399	-0.0797
	2	MEAN	x9		2.54369	0.1107	-0.1796	0.3335
	3	MEAN	x9		1.61681	0.2035	0.1337	-0.2885
mean2_new	2	MEAN	x2		3.21203	0.0731	0.2484	-0.2280
	3	MEAN	x2		3.21203	0.0731	-0.2280	0.2484

To make the mean parameter for x4 in Model 1 unique, the mean parameters for x4 in Models 2 and 3 are renamed from mean4 to mean4_new, as shown in the following statements:

```
proc calis modification;
  var x1-x9;
  group 1 / data=g1;
  group 2 / data=g2;
  group 3 / data=g3;
  model 1 / group = 1;
    mstruct;
    matrix _cov_ = cov01-cov45;
    matrix _mean_ = mean1-mean9;
  model 2 / group = 2;
    refmodel 1;
    renameparm mean2=mean2_new,      /* constraint a */
               mean4=mean4_new,      /* constraint b */
               mean6=mean6_md12;
  model 3 / group = 3;
    refmodel 1;
    renameparm mean2=mean2_new,      /* constraint a */
               mean3=mean3_md13,
               mean4=mean4_new;      /* constraint b */
  fitindex NoIndexType On(only)=[chisq df probchi rmsea aic caic sbc];
run;
```

This forms the fourth revised model. [Output 27.22.16](#) shows the fit summary of this revised model. Again, the chi-square, AIC, CAIC, and SBC values all show improvements, as compared with the third revised model. However, the improvements do seem to slow down. For example, the CAIC value drops from 361.95 to the current value at 358.43—a mere 3 points reduction. The SBC value drops from 304.95 to the current value at 300.43—a mere 4 points reduction. These small reductions indicate that you might soon reach the point that no more model fit improvement would be possible with additional release of parameter constraints.

Output 27.22.16 Fit Summary for the Fourth Revised Model

Fit Summary	
Chi-Square	60.1265
Chi-Square DF	104
Pr > Chi-Square	0.9998
RMSEA Estimate	0.0000
Akaike Information Criterion	176.1265
Bozdogan CAIC	358.4283
Schwarz Bayesian Criterion	300.4283

Output 27.22.17 suggests that the mean of x1 in Model 1 (which has the largest LM statistic at 6.45785) could be released from the equality constraint to achieve the largest model improvement over the current model.

Output 27.22.17 LM Statistics for Releasing the Equality Constraints in the Fourth Revised Model

Lagrange Multiplier Statistics for Releasing Equality Constraints								
Parm	---Released Parameter---				LM Stat	Pr > ChiSq	-----Changes-----	
	Model	Type	Var1	Var2			Original Parm	Released Parm
cov01	1	COV	x1	x1	2.60531	0.1065	0.1376	-0.2751
	2	COV	x1	x1	0.28122	0.5959	0.0469	-0.0871
	3	COV	x1	x1	4.75001	0.0293	-0.1788	0.3859
					.			
					.			
					.			
mean1	1	MEAN	x1		6.45761	0.0110	0.2616	-0.5232
	2	MEAN	x1		5.00991	0.0252	-0.1921	0.3568
	3	MEAN	x1		0.05931	0.8076	0.0209	-0.0452
mean3	1	MEAN	x3		1.53300	0.2157	-0.1298	0.1406
	2	MEAN	x3		1.53300	0.2157	0.1406	-0.1298
mean5	1	MEAN	x5		0.09749	0.7549	-0.0457	0.0913
	2	MEAN	x5		0.19688	0.6572	-0.0716	0.1330
	3	MEAN	x5		0.56583	0.4519	0.1071	-0.2310
mean6	1	MEAN	x6		0.35800	0.5496	0.1141	-0.1113
	3	MEAN	x6		0.35800	0.5496	-0.1113	0.1141
mean7	1	MEAN	x7		4.53367E-6	0.9983	0.000350	-0.00070
	2	MEAN	x7		0.96363	0.3263	0.1572	-0.2920
	3	MEAN	x7		1.00890	0.3152	-0.1486	0.3208
mean8	1	MEAN	x8		0.20289	0.6524	-0.0676	0.1351
	2	MEAN	x8		0.12445	0.7243	0.0525	-0.0974
	3	MEAN	x8		0.00590	0.9388	0.0110	-0.0237
mean9	1	MEAN	x9		0.05893	0.8082	-0.0271	0.0542
	2	MEAN	x9		1.63723	0.2007	-0.1448	0.2689
	3	MEAN	x9		2.44241	0.1181	0.1652	-0.3565
mean2_new	2	MEAN	x2		3.05068	0.0807	0.2396	-0.2246
	3	MEAN	x2		3.05068	0.0807	-0.2246	0.2396
mean4_new	2	MEAN	x4		1.81983	0.1773	0.2306	-0.2003
	3	MEAN	x4		1.81983	0.1773	-0.2003	0.2306

To make the mean parameter for x1 in Model 1 unique, the mean parameters for x1 in Models 2 and 3 are renamed from mean1 to mean1_new, as shown in the following statements:

```
proc calis modification;
  var x1-x9;
  group 1 / data=g1;
  group 2 / data=g2;
  group 3 / data=g3;
  model 1 / group = 1;
    mstruct;
    matrix _cov_ = cov01-cov45;
    matrix _mean_ = mean1-mean9;
  model 2 / group = 2;
    refmodel 1;
    renameparm mean1=mean1_new,      /* constraint c */
               mean2=mean2_new,      /* constraint a */
               mean4=mean4_new,      /* constraint b */
               mean6=mean6_md12;
  model 3 / group = 3;
    refmodel 1;
    renameparm mean1=mean1_new,      /* constraint c */
               mean2=mean2_new,      /* constraint a */
               mean3=mean3_md13,
               mean4=mean4_new;      /* constraint b */
  fitindex NoIndexType On(only)=[chisq df probchi rmsea aic caic sbc];
run;
```

This forms the fifth revised model. [Output 27.22.18](#) shows the fit summary of the fifth revised model. Again, the chi-square, AIC, CAIC, and SBC values all show improvements, as compared with the fourth revised model. However, the improvements slow down even more. For example, the CAIC value drops from 358.43 to the current value at 356.32. The SBC value drops from 300.43 to the current value at 297.32. Because the model fit does not improve much, this is the point where you would cease to release more equality constraints for improving the model fit.

Output 27.22.18 Fit Summary for the Fifth Revised Model

Fit Summary	
Chi-Square	52.8821
Chi-Square DF	103
Pr > Chi-Square	1.0000
RMSEA Estimate	0.0000
Akaike Information Criterion	170.8821
Bozdogan CAIC	356.3270
Schwarz Bayesian Criterion	297.3270

Output 27.22.19 does not suggest the release of any equality constraints on the means, because all the p -values for the LM statistics are not significant (that is, all are greater than 0.05). Therefore, the same suggestion from examining the model fit improvements of the fifth revised model echoes here: this is the point that the “best” model for the data is found.

Output 27.22.19 LM Statistics for Releasing the Equality Constraints in the Fifth Revised Model

Lagrange Multiplier Statistics for Releasing Equality Constraints								
Parm	---Released Parameter---				LM Stat	Pr > ChiSq	-----Changes-----	
	Model	Type	Var1	Var2			Original Parm	Released Parm
cov01	1	COV	x1	x1	4.06279	0.0438	0.1590	-0.3180
	2	COV	x1	x1	0.48735	0.4851	0.0571	-0.1061
	3	COV	x1	x1	7.60892	0.0058	-0.2095	0.4520
				.				
				.				
mean3	1	MEAN	x3		0.08363	0.7724	-0.0312	0.0382
	2	MEAN	x3		0.08363	0.7724	0.0382	-0.0312
mean5	1	MEAN	x5		0.02394	0.8770	0.0229	-0.0458
	2	MEAN	x5		0.47076	0.4926	-0.1113	0.2067
	3	MEAN	x5		0.26015	0.6100	0.0728	-0.1571
mean6	1	MEAN	x6		0.97521	0.3234	0.1893	-0.1892
	3	MEAN	x6		0.97521	0.3234	-0.1892	0.1893
mean7	1	MEAN	x7		0.03746	0.8465	-0.0319	0.0638
	2	MEAN	x7		1.10428	0.2933	0.1683	-0.3126
	3	MEAN	x7		0.79474	0.3727	-0.1321	0.2851
mean8	1	MEAN	x8		0.86792	0.3515	-0.1426	0.2852
	2	MEAN	x8		0.47493	0.4907	0.1038	-0.1928
	3	MEAN	x8		0.03722	0.8470	0.0276	-0.0595
mean9	1	MEAN	x9		0.12190	0.7270	0.0401	-0.0801
	2	MEAN	x9		2.66768	0.1024	-0.1869	0.3472
	3	MEAN	x9		1.78114	0.1820	0.1417	-0.3058
mean1_new	2	MEAN	x1		1.28034	0.2578	-0.1794	0.1359
	3	MEAN	x1		1.28034	0.2578	0.1359	-0.1794
mean2_new	2	MEAN	x2		2.53131	0.1116	0.2117	-0.2112
	3	MEAN	x2		2.53131	0.1116	-0.2112	0.2117
mean4_new	2	MEAN	x4		2.25832	0.1329	0.2558	-0.2253
	3	MEAN	x4		2.25832	0.1329	-0.2253	0.2558

To see where the fifth revised model (equality in the covariance matrix and partial equality in the means) stands between the models under H_0 (equality in the covariance and mean matrices) and H_1 (equality in the covariance matrix only), the following table shows the fit statistics of these three models:

	H_0	“Fifth”	H_1
Chi-square	203.2605	52.8821	26.7897
Chi-square DF	108	103	90
Pr > chi-square	<0.0001	1.0000	1.0000
RMSEA estimate	0.2100	0.0000	0.0000
Akaike information criterion	311.2605	170.8821	170.7897
Bozdogan CAIC	480.9898	356.3270	397.0954
Schwarz Bayesian criterion	426.9898	297.3270	325.0954

The fifth revised model is labeled “Fifth” in the table. Compared with the model under H_0 , the fifth revised model is clearly superior. It uses only five more parameters (or five fewer degrees of freedom), but the improvement in the model fit chi-square and the RMSEA value are huge. The AIC, CAIC, and SBC are also much better.

Compared with the model under H_1 , the fifth revised model appears to be inferior in only the chi-square model fit statistic, although both models already have the highest possible p -value at 1.000 and smallest possible RMSEA value at 0. However, the model under H_1 uses 13 more parameters (or it has 13 fewer degrees of freedom), and hence it is more complex. In fact, because the model fit chi-square value does not take model complexity into account, it is often criticized as the basis for choosing competing models for the data. In contrast, the AIC, CAIC, and SBC measures take model complexity into account, and they are more reasonable as the basis for choosing competing models. Although the AIC values for the fifth revised model and the model under H_1 are very close, the CAIC and SBC values clearly favor the fifth revised model. Therefore, according to the CAIC and SBC criteria, the fifth revised model, which is a model with partial equality constraints on the means, is actually better than the model with all the means being unconstrained (that is, under H_1) for the current data with three independent groups.

Example 27.23: Illustrating Various General Modeling Languages

In PROC CALIS, you can use many different modeling languages to specify the same model. The choice of modeling language depends on personal preferences and the purposes of the analysis. See the section “Which Modeling Language?” on page 1077 for guidance. In this example, the data and the model in Example 27.17 are used to illustrate how a particular model can be specified by various general modeling languages.

RAM Model Specification

In Example 27.17, you use the PATH modeling language to specify the model because of its close resemblance to the path diagram. In this example, you consider another modeling language of PROC CALIS that is also closely related to the path diagram representation of structural equation models. The so-called RAM model language has syntax that represents the single- and double-headed paths (or arrows) in the path diagram. However, unlike the PATH modeling language, the RAM modeling language is matrix-based. The following statements show how you can specify the same path model with the RAM model specification for the data in Example 27.17:

```
proc calis nobs=932 data=Wheaton;
  ram
    var = Anomie67      /* 1 */
          Powerless67  /* 2 */
          Anomie71     /* 3 */
          Powerless71  /* 4 */
          Education    /* 5 */
          SEI          /* 6 */
          Alien67      /* 7 */
          Alien71      /* 8 */
          SES,         /* 9 */

    _A_ 1 7 1.0,
    _A_ 2 7 0.833,
    _A_ 3 8 1.0,
    _A_ 4 8 0.833,
    _A_ 5 9 1.0,
    _A_ 6 9 lambda,
    _A_ 7 9 gamma1,
    _A_ 8 9 gamma2,
    _A_ 8 7 beta,
    _P_ 1 1 theta1,
    _P_ 2 2 theta2,
    _P_ 3 3 theta1,
    _P_ 4 4 theta2,
    _P_ 5 5 theta3,
    _P_ 6 6 theta4,
    _P_ 7 7 psi1,
    _P_ 8 8 psi2,
    _P_ 9 9 phi,
    _P_ 1 3 theta5,
    _P_ 2 4 theta5;
run;
```

In the RAM model for covariance structure analysis, you have two important matrices to specify. The first one is the `_A_` matrix, which is for the specification of the single-headed paths (arrows) in the path diagram. The second one is the `_P_` matrix, which is for the specification of the double-headed paths (arrows) in the path diagram. Hence, to specify the RAM model is much like mapping the path diagram arrows into the parameter of the RAM model matrices.

In the RAM statement, you can specify the variables in the model in the `VAR=` option. The `VAR=` list contains all observed and latent variables in your path diagram (without the use of error terms). Although you can specify the variables in the `VAR=` list in any order you like, the variable order in the list is also the order of variables in the RAM model matrices. In `VAR=` list of the RAM statement, you put comments to note the order of the variables.

After you specify the variable list, you can specify the model parameter locations in the RAM statement entries. In the first nine entries, you specify the single-headed paths by mapping them into the elements of the `_A_` matrix of the RAM model. For example, the first entry represents the single-headed path of variable 1 (Anomie67) from variable 7 (Alien67). The corresponding path effect or coefficient is fixed at 1, which is also the value for `_A_[1,7]`. Another example is the ninth path entry. You specify a single-headed path of variable 8 (Alien71) from variable 7 (Alien67). The corresponding path effect or coefficient is a free parameter named `beta`, which is also the parameter for `_A_[8,7]`. Hence, you can specify all single-headed paths in the path diagram as elements in the `_A_` matrix of the RAM model.

To facilitate the comparisons between the RAN and PATH modeling languages, the PATH model specification in [Example 27.17](#) for the same data is reproduced in the following:

```
proc calis nob=932 data=Wheaton plots=residuals;
  path
    Anomie67    Powerless67 <==== Alien67    = 1.0  0.833,
    Anomie71    Powerless71 <==== Alien71    = 1.0  0.833,
    Education   SEI          <==== SES        = 1.0  lambda,
    Alien67     Alien71     <==== SES        = gamma1 gamma2,
    Alien71     <==== Alien67    = beta;
  pvar
    Anomie67    = theta1,
    Powerless67 = theta2,
    Anomie71    = theta1,
    Powerless71 = theta2,
    Education   = theta3,
    SEI         = theta4,
    Alien67     = psi1,
    Alien71     = psi2,
    SES         = phi;
  pcov
    Anomie67    Anomie71    = theta5,
    Powerless67 Powerless71 = theta5;
run;
```

It is clear that each of the path entries specified in the PATH statement corresponds to an matrix element entry of the `_A_` matrix in the RAM statement. How about the specifications of the double-headed arrows in the path diagram? Do the RAM and PATH model specifications correspond to each other?

The answer is yes. In the PATH modeling language, you specify all double-headed arrows in the path diagram as entries either in the PVAR or PCOV statement. In the RAM modeling language, you specify the corresponding entries as matrix element entries of the `_P_` matrix in the RAM statement. For example, the error variance of `Anomie67` is a parameter called `_Variabletheta1` in the PVAR statement of the PATH model. You specify the same parameter for the `_P_[1,1]` element in an entry of the RAM statement. Another example is the error covariance between `Powerless67` and `Powerless71`. You specify this a parameter called `theta5` in the last entry of the PCOV statement in the PATH model. You specify the same parameter for the `_P_[2,4]` element in the last entry of the RAM statement. Therefore, it is not difficult to find that the specifications in the PATH and the RAM model have some kind of one-to-one correspondence.

Output 27.23.1 shows the RAM model estimates for the Wheaton data. These RAM model estimates match the set of estimates using the PATH model specification, as shown in Output 27.17.10.

Output 27.23.1 RAM Model Estimates

RAM Pattern and Estimates						
Matrix	-----Row-----	---Column---	Parameter	Estimate	Standard Error	t Value
<code>_A_ (1)</code>	<code>Anomie67</code>	1 <code>Alien67</code>	7	1.00000		
	<code>Powerless67</code>	2 <code>Alien67</code>	7	0.83300		
	<code>Anomie71</code>	3 <code>Alien71</code>	8	1.00000		
	<code>Powerless71</code>	4 <code>Alien71</code>	8	0.83300		
	<code>Education</code>	5 <code>SES</code>	9	1.00000		
	<code>SEI</code>	6 <code>SES</code>	9 <code>lambda</code>	5.36883	0.43371	12.37880
	<code>Alien67</code>	7 <code>SES</code>	9 <code>gamma1</code>	-0.62994	0.05634	-11.18092
	<code>Alien71</code>	8 <code>SES</code>	9 <code>gamma2</code>	-0.24086	0.05489	-4.38836
	<code>Alien71</code>	8 <code>Alien67</code>	7 <code>beta</code>	0.59312	0.04678	12.67884
<code>_P_ (2)</code>	<code>Anomie67</code>	1 <code>Anomie67</code>	1 <code>theta1</code>	3.60796	0.20092	17.95717
	<code>Powerless67</code>	2 <code>Powerless67</code>	2 <code>theta2</code>	3.59488	0.16448	21.85563
	<code>Anomie71</code>	3 <code>Anomie71</code>	3 <code>theta1</code>	3.60796	0.20092	17.95717
	<code>Powerless71</code>	4 <code>Powerless71</code>	4 <code>theta2</code>	3.59488	0.16448	21.85563
	<code>Education</code>	5 <code>Education</code>	5 <code>theta3</code>	2.99366	0.49861	6.00398
	<code>SEI</code>	6 <code>SEI</code>	6 <code>theta4</code>	259.57639	18.31151	14.17559
	<code>Alien67</code>	7 <code>Alien67</code>	7 <code>psi1</code>	5.67046	0.42301	13.40500
	<code>Alien71</code>	8 <code>Alien71</code>	8 <code>psi2</code>	4.51479	0.33532	13.46394
	<code>SES</code>	9 <code>SES</code>	9 <code>phi</code>	6.61634	0.63914	10.35190
	<code>Anomie67</code>	1 <code>Anomie71</code>	3 <code>theta5</code>	0.90580	0.12167	7.44472
<code>Powerless67</code>	2 <code>Powerless71</code>	4 <code>theta5</code>	0.90580	0.12167	7.44472	

LINEQS Model Specification

Another way to specify the model in Example 27.17 is to use the LINEQS modeling language, which is shown in the following:

```

proc calis nobs=932 data=Wheaton;
  lineqs
    Anomie67      = 1.0      * f_Alien67 + e1,
    Powerless67   = 0.833    * f_Alien67 + e2,
    Anomie71      = 1.0      * f_Alien71 + e3,
    Powerless71   = 0.833    * f_Alien71 + e4,
    Education     = 1.0      * f_SES      + e5,
    SEI           = lambda   * f_SES      + e6,
    f_Alien67     = gamma1   * f_SES      + d1,
    f_Alien71     = gamma2   * f_SES      + beta * f_Alien67 + d2;
  variance
    E1            = theta1,
    E2            = theta2,
    E3            = theta1,
    E4            = theta2,
    E5            = theta3,
    E6            = theta4,
    D1            = psi1,
    D2            = psi2,
    f_SES         = phi;
  cov
    E1 E3        = theta5,
    E2 E4        = theta5;
run;

```

As compared with the PATH and RAM modeling languages, the most distinct feature of the LINEQS modeling language is the explicit use of error terms in equation specifications. In the LINEQS statement, you specify exactly one equation for each endogenous variable. In each equation, you list an endogenous variable on the left-hand-side of the equation and all its predictors on the right-hand-side of the equation. You must also include an error term in each equation. Because each endogenous variable in the LINEQS statement can only be specified in exactly one equation, the number of equations in the LINEQS model and the number of paths in the corresponding path diagram do not match necessarily. In this example, there are eight equations in the `LINEQS` statement, but there are nine paths in the corresponding path diagram.

In addition, in the LINEQS model, you need to follow a convention of naming latent variables. For latent variables that are neither errors nor disturbances, you must use either the ‘F’ or ‘f’ prefix. For error terms, you must use either the ‘E’ or ‘e’ prefix. For disturbances, you must use either the ‘D’ or ‘d’ prefix. However, in the PATH or RAM model specification, no such convention is imposed. For example, `f_Alien67`, `f_Alien71`, and `f_SES` are latent factors in the LINEQS model. They are not error terms, and so they must start with the ‘f’ prefix. However, this prefix is not needed in the PATH or RAM model. Furthermore, there are no explicit error terms that need to be specified in the PATH or RAM model, let alone specific prefixes for the error terms.

The `PVAR` statement in the PATH model is replaced with the `VARIANCE` statement in the LINEQS model, and the `PCOV` statement with the `COV` statement. The `PVAR` and `PCOV` statements in the PATH model are for the partial variance and partial covariance specifications. The partial variance or covariance concepts are used in the PATH or RAM model specification because error terms are not named explicitly. Specification of error variances in the PATH and RAM model is conceptualized as the specification of the partial variances of the corresponding variables. But in the LINEQS model, because errors or disturbances are named explicitly as *exogenous* variables, the partial variance or covariance concepts are no longer necessary. Instead, you specify the variances of the error terms directly, which reflects the conceptualization behind the `VARIANCE`

statement of the LINEQS modeling language. Similarly, you use the COV, but not PCOV, statement in the LINEQS modeling language because you can specify the covariances among variables or error terms without using the partial covariance conceptualization.

In this example, the variances of the errors (“E”-variables) and disturbances (“D”-variables) specified in the **VARIANCE** statement of the LINEQS model correspond to the partial variances of the endogenous variables specified in the **PVAR** statement of the PATH model. Similarly, covariances of errors specified in the **COV** statement of the LINEQS model correspond to the partial covariances of endogenous variables specified in the **PCOV** statement of the PATH model. The estimation results of the LINEQS model are shown in **Output 27.23.2**. Again, they are essentially the same estimates obtained from the PATH model specified in **Example 27.17**, as shown in **Output 27.17.10**.

Output 27.23.2 LINEQS Model Estimates

Linear Equations					
Anomie67	=	1.0000	f_Alien67	+	1.0000 e1
Powerless67	=	0.8330	f_Alien67	+	1.0000 e2
Anomie71	=	1.0000	f_Alien71	+	1.0000 e3
Powerless71	=	0.8330	f_Alien71	+	1.0000 e4
Education	=	1.0000	f_SES	+	1.0000 e5
SEI	=	5.3688	*f_SES	+	1.0000 e6
Std Err		0.4337	lambda		
t Value		12.3788			
f_Alien67	=	-0.6299	*f_SES	+	1.0000 d1
Std Err		0.0563	gamma1		
t Value		-11.1809			
f_Alien71	=	-0.2409	*f_SES	+	0.5931*f_Alien67 + 1.0000 d2
Std Err		0.0549	gamma2		0.0468 beta
t Value		-4.3884			12.6788

Estimates for Variances of Exogenous Variables					
Variable Type	Variable	Parameter	Estimate	Standard Error	t Value
Error	e1	theta1	3.60796	0.20092	17.95717
	e2	theta2	3.59488	0.16448	21.85563
	e3	theta1	3.60796	0.20092	17.95717
	e4	theta2	3.59488	0.16448	21.85563
	e5	theta3	2.99366	0.49861	6.00398
	e6	theta4	259.57639	18.31151	14.17559
Disturbance	d1	psi1	5.67046	0.42301	13.40500
	d2	psi2	4.51479	0.33532	13.46394
Latent	f_SES	phi	6.61634	0.63914	10.35190

Covariances Among Exogenous Variables					
Var1	Var2	Parameter	Estimate	Standard Error	t Value
e1	e3	theta5	0.90580	0.12167	7.44472
e2	e4	theta5	0.90580	0.12167	7.44472

LISMOD Specification

You can also specify general structural models by using the LISMOD modeling language. See the section “The LISMOD Model and Submodels” on page 1277 for details.

To use the LISMOD modeling language, you must recognize four types of variables in the model. The η -variables (eta-variables) are latent factors that are endogenous, or predicted by other latent factors. The ξ -variables (xi-variables) are exogenous latent variables that are not predicted by any other variables. The y-variables are manifest variables that are indicators of the η -variables, and the x-variables are manifest variables that are indicators of the ξ -variables. In this example, Alien67 and Alien71 are the η -variables, and SES is the ξ -variable in the model. Manifest indicators for Alien67 and Alien71 include Anomie67, Powerless67, Anomie71, and Powerless71, which are the y-variables. Manifest indicators for SES include Education and SEI, which are the x-variables.

After defining these four types of variables, the parameters of the model are defined as entries in the model matrices. The `_LAMBDAY_`, `_LAMBDA_X_`, `_GAMMA_`, and `_BETA_` are matrices for the path coefficients or effects. The `_THETAY_`, `_THETA_X_`, `_PSI_`, and `_PHI_` are matrices for the variances and covariances.

The following is the LISMOD specification for the model in [Example 27.17](#):

```
proc calis nobs=932 data=Wheaton;
  lismod
    yvar   = Anomie67 Powerless67 Anomie71 Powerless71,
    xvar   = Education SEI,
    etavar = Alien67 Alien71,
    xivar  = SES;
  matrix _LAMBDAY_
    [1,1] = 1,
    [2,1] = 0.833,
    [3,2] = 1,
    [4,2] = 0.833;
  matrix _LAMBDA_X_
    [1,1] = 1,
    [2,1] = lambda;
  matrix _GAMMA_
    [1,1] = gamma1,
    [2,1] = gamma2;
  matrix _BETA_
    [2,1] = beta;
  matrix _THETAY_
    [1,1] = theta1-theta2 theta1-theta2,
    [3,1] = theta5,
    [4,2] = theta5;
  matrix _THETA_X_
    [1,1] = theta3-theta4;
  matrix _PSI_
    [1,1] = psi1-psi2;
  matrix _PHI_
    [1,1] = phi;
run;
```

In the LISMOD statement, you specify the four lists of variables in the model. The orders of the variables in these lists define the order of the row and column variables in the model matrices, of which the parameter locations are specified in the MATRIX statements.

The estimated model is divided into three conceptual parts. The first part is the measurement model that relates the η -variables with the y-variables, as shown in Output 27.23.3:

Output 27.23.3 LISMOD Model Measurement Model for the η -Variables

LAMBDA Matrix: Estimate/StdErr/t-value				
	Alien67		Alien71	
Anomie67	1.0000		0	
Powerless67	0.8330		0	
Anomie71	0		1.0000	
Powerless71	0		0.8330	
THETA Matrix: Estimate/StdErr/t-value				
	Anomie67	Powerless67	Anomie71	Powerless71
Anomie67	3.6080 0.2009 17.9572 [theta1]	0	0.9058 0.1217 7.4447 [theta5]	0
Powerless67	0	3.5949 0.1645 21.8556 [theta2]	0	0.9058 0.1217 7.4447 [theta5]
Anomie71	0.9058 0.1217 7.4447 [theta5]	0	3.6080 0.2009 17.9572 [theta1]	0
Powerless71	0	0.9058 0.1217 7.4447 [theta5]	0	3.5949 0.1645 21.8556 [theta2]

The `_LAMBDAY_` matrix contains the coefficients or effects of the η -variables on the y -variables. All these estimates are fixed constants as specified. The `_THETAY_` matrix contains the error variances and covariances for the y -variables. Three free parameters are located in this matrix: `theta1`, `theta2`, and `theta5`.

The second part of the estimated model is the measurement model that relates the ξ -variable with the x -variables, as shown in [Output 27.23.4](#):

Output 27.23.4 LISMOD Model Measurement Model for the ξ -Variables

<code>_LAMBDAY_ Matrix: Estimate/StdErr/t-value</code>		
	<code>SES</code>	
<code>Education</code>	1.0000	
<code>SEI</code>	5.3688	
	0.4337	
	12.3788	
	[lambda]	
<code>_THETAX_ Matrix: Estimate/StdErr/t-value</code>		
	<code>Education</code>	<code>SEI</code>
<code>Education</code>	2.9937	0
	0.4986	
	6.0040	
	[theta3]	
<code>SEI</code>	0	259.5764
		18.3115
		14.1756
		[theta4]

The `_LAMBDAY_` matrix contains the coefficients or effects of the ξ -variable `SES` on the x -variables. The effect of `SES` on `Education` is fixed at one. The effect of `SES` on `SEI` is represented by the free parameter `lambda`, which is estimated at 5.3688. The `_THETAX_` matrix contains the error variances and covariances for the x -variables. Two free parameters are located in this matrix: `theta3` and `theta4`.

The last part of the estimated model is the structural model that relates the latent variables η and ξ , as shown in [Output 27.23.5](#):

Output 27.23.5 LISMOD Structural Model for the Latent Variables

<u>_BETA_ Matrix: Estimate/StdErr/t-value</u>		
	Alien67	Alien71
Alien67	0	0
Alien71	0.5931 0.0468 12.6788 [beta]	0
<u>_GAMMA_ Matrix: Estimate/StdErr/t-value</u>		
	SES	
Alien67	-0.6299 0.0563 -11.1809 [gamma1]	
Alien71	-0.2409 0.0549 -4.3884 [gamma2]	
<u>_PSI_ Matrix: Estimate/StdErr/t-value</u>		
	Alien67	Alien71
Alien67	5.6705 0.4230 13.4050 [psi1]	0
Alien71	0	4.5148 0.3353 13.4639 [psi2]

Output 27.23.5 *continued*

PHI Matrix: Estimate/StdErr/t-value	
	SES
SES	6.6163
	0.6391
	10.3519
	[phi]

The **_BETA_** matrix contains effects of η -variables on themselves. In the current example, there is only one such effect. The effect of Alien67 on Alien71 is represented by the free parameter beta. The **_GAMMA_** matrix contains effects of the ξ -variable, which is SES in this example, on the η -variables Alien67 on Alien71. These effects are represented by the free parameters gamma1 and gamma2. The **_PSI_** matrix contains the error variances and covariances in the structural model. In this example, psi1 and psi2 are two free parameters for the error variances. Finally, the **_PHI_** matrix is the covariance matrix for the ξ -variables. In this example, there is only one ξ -variable so that this matrix contains only the estimated variance of SES. This variance is represented by the parameter phi.

The estimates obtained from fitting the LISMOD model are the same as those from fitting the equivalent PATH, RAM, or LINEQS model. To some researchers the LISMOD modeling language might be more familiar, while for others modeling languages such as PATH, RAM, or LINEQS are more convenient to use.

Example 27.24: Testing Competing Path Models for the Career Aspiration Data

This example uses some well-known data from Haller and Butterworth (1960). The section “A Combined Measurement-Structural Model” on page 320 analyzes some models for these data. Inspired by the examples given in Loehlin (1987), this example shows additional applications to the same data set, but with a focus on testing nested models. By manipulating the **OUTMODEL=** data set, this example shows how you can specify new models in an efficient way. Various models and analyses of these data are also given by Duncan, Haller, and Portes (1968), Jöreskog and Sörbom (1988), and Loehlin (1987).

The study is concerned with the career aspirations of high school students and how these aspirations are affected by close friends. The data are collected from 442 seventeen-year-old boys in Michigan. There are 329 boys in the sample who named another boy in the sample as a best friend. The data from these 329 boys paired with the data from their best friends are analyzed.

Because of the dependency of the data, the effective sample size assumed in the example is 329, which you can specify in the **NOBS=** option in the PROC CALIS statements. See the section “A Combined Measurement-Structural Model” on page 320 for the justification of the use of this effective sample size.

The correlation matrix, taken from Jöreskog and Sörbom (1988), is shown in the following DATA step:

```

title 'Peer Influences on Aspiration: Haller & Butterworth (1960)';
data aspire(type=corr);
  _type_='corr';
  input _name_ $ riq rpa rses roa rea fiq fpa fses foa fea;
  label riq='Respondent: Intelligence'
        rpa='Respondent: Parental Aspiration'
        rses='Respondent: Family SES'
        roa='Respondent: Occupational Aspiration'
        rea='Respondent: Educational Aspiration'
        fiq='Friend: Intelligence'
        fpa='Friend: Parental Aspiration'
        fses='Friend: Family SES'
        foa='Friend: Occupational Aspiration'
        fea='Friend: Educational Aspiration';
  datalines;
riq  1.      .      .      .      .      .      .      .      .      .
rpa  .1839   1.      .      .      .      .      .      .      .      .
rses .2220   .0489   1.      .      .      .      .      .      .      .
roa  .4105   .2137   .3240   1.      .      .      .      .      .      .
rea  .4043   .2742   .4047   .6247   1.      .      .      .      .      .
fiq  .3355   .0782   .2302   .2995   .2863   1.      .      .      .      .
fpa  .1021   .1147   .0931   .0760   .0702   .2087   1.      .      .      .
fses .1861   .0186   .2707   .2930   .2407   .2950  -.0438   1.      .      .
foa  .2598   .0839   .2786   .4216   .3275   .5007   .1988   .3607   1.      .
fea  .2903   .1124   .3054   .3269   .3669   .5191   .2784   .4105   .6404   1.
;

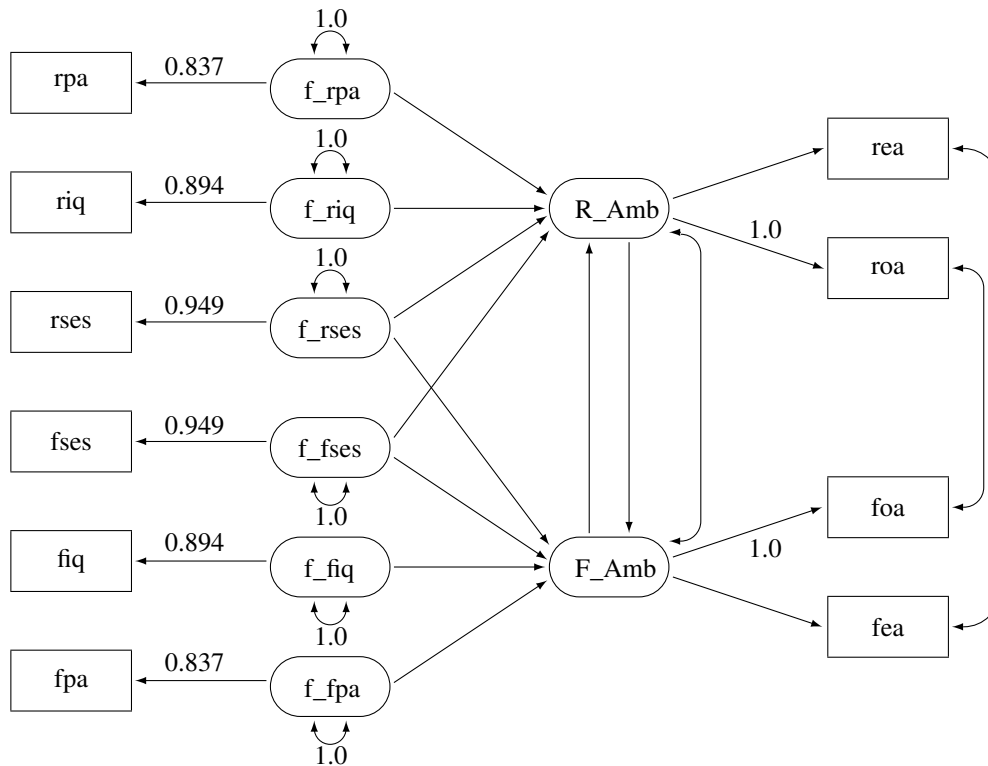
```

For illustration purposes, this correlation matrix is treated here as if it were a covariance matrix for PROC CALIS to analyze. The reason is that the chi-square tests shown in this example are valid only with covariance structure analysis. See [Example 27.27](#) for an illustration of covariance structure analysis on correlations.

Model 1: The Full Model

Loehlin (1987) analyzes the following path model for the data:

Figure 27.4 Path Diagram for Career Aspiration: Model 1



In Figure 27.4, the observed variables *rpa*, *riq*, *rses*, *fses*, *fiq*, and *fpa* are measured with errors. Their true scores counterparts *f_rpa*, *f_riq*, *f_rses*, *f_fses*, *f_fiq*, and *f_fpa* are latent variables in the model. Path coefficients from these latent variables to the observed variables are fixed coefficients, indicating the square roots of the theoretical reliabilities in the model. These latent variables, rather than the observed counterparts, serve as predictors of the ambition factors *R_Amb* and *F_Amb*. The error terms for these two latent factors are correlated, as indicated by a double-headed path (arrow) that connects the two factors. Correlated errors for the occupational aspiration variables (*roa* and *foa*) and the educational aspiration variables (*rea* and *fea*) are also shown in Figure 27.4. These correlated errors are also represented by two double-headed paths (arrows) in the path diagram.

Notice that the covariances among the six exogenous latent variables (*f_rpa*, *f_riq*, *f_rses*, *f_fses*, *f_fiq*, and *f_fpa*) are not represented in the path diagram for two reasons. First, there are 15 of these covariances and hence you need 15 double-headed arrows to represent them in the path diagram. Apparently, because of the space limitations, it would be difficult to put all these double-headed arrows in the path diagram without cluttering it. Second, covariances among exogenous latent variables are free parameters by default in PROC CALIS, and therefore omitting these double-headed arrows in the path diagram is compatible with the default model specification in PROC CALIS. Similarly, double-headed arrows for the error variances of the endogenous variables (*rpa*, *riq*, *rses*, *fses*, *fiq*, *fpa*, *R_Amb*, and *F_Amb*) in the path diagram are omitted because they are unconstrained free parameters and are set automatically by default in PROC CALIS .

The model represented by the path diagram in [Figure 27.4](#) is considered to be the full model for the data, in the sense that it has the largest number of parameters among the competing models considered this example. The same model is analyzed in the section “[A Combined Measurement-Structural Model](#)” on page 320 with the following specification:

```
proc calis data=aspire nobs=329;
  path
    /* measurement model for intelligence and environment */
    rpa    <=== f_rpa    = 0.837,
    riq    <=== f_riq    = 0.894,
    rses    <=== f_rses   = 0.949,
    fses    <=== f_fses   = 0.949,
    fiq     <=== f_fiq    = 0.894,
    fpa     <=== f_fpa    = 0.837,

    /* structural model of influences: 5 equality constraints */
    f_rpa   <===> R_Amb ,
    f_riq   <===> R_Amb ,
    f_rses  <===> R_Amb ,
    f_fses  <===> R_Amb ,
    f_rses  <===> F_Amb ,
    f_fses  <===> F_Amb ,
    f_fiq   <===> F_Amb ,
    f_fpa   <===> F_Amb ,
    F_Amb   <===> R_Amb ,
    R_Amb   <===> F_Amb ,

    /* measurement model for aspiration: 1 equality constraint */
    R_Amb   <===> rea ,
    R_Amb   <===> roa    = 1.,
    F_Amb   <===> foa    = 1.,
    F_Amb   <===> fea ;
  pvar
    f_rpa f_riq f_rses f_fpa f_fiq f_fses = 6 * 1.0;
  pcov
    R_Amb F_Amb      ,
    rea fea          ,
    roa foa          ;
run;
```

The PATH model specification represents each arrow (single-headed and double-headed) in the path diagram. You transcribe each arrow in [Figure 27.4](#) into an entry in the PATH model. The PATH statement specifies all the single-headed arrows in the path diagram. The PVAR statement specifies all the double-headed arrows that point to individual variables (that is, the fixed error variances of the exogenous latent variables) in the path diagram. The PCOV statement specifies all the double-headed arrows that connect paired variables (that is, the error covariances) in the path diagram.

Output 27.24.1 shows the fit summary of Model 1.

Output 27.24.1 Career Aspiration Data: Fit Summary of Model 1

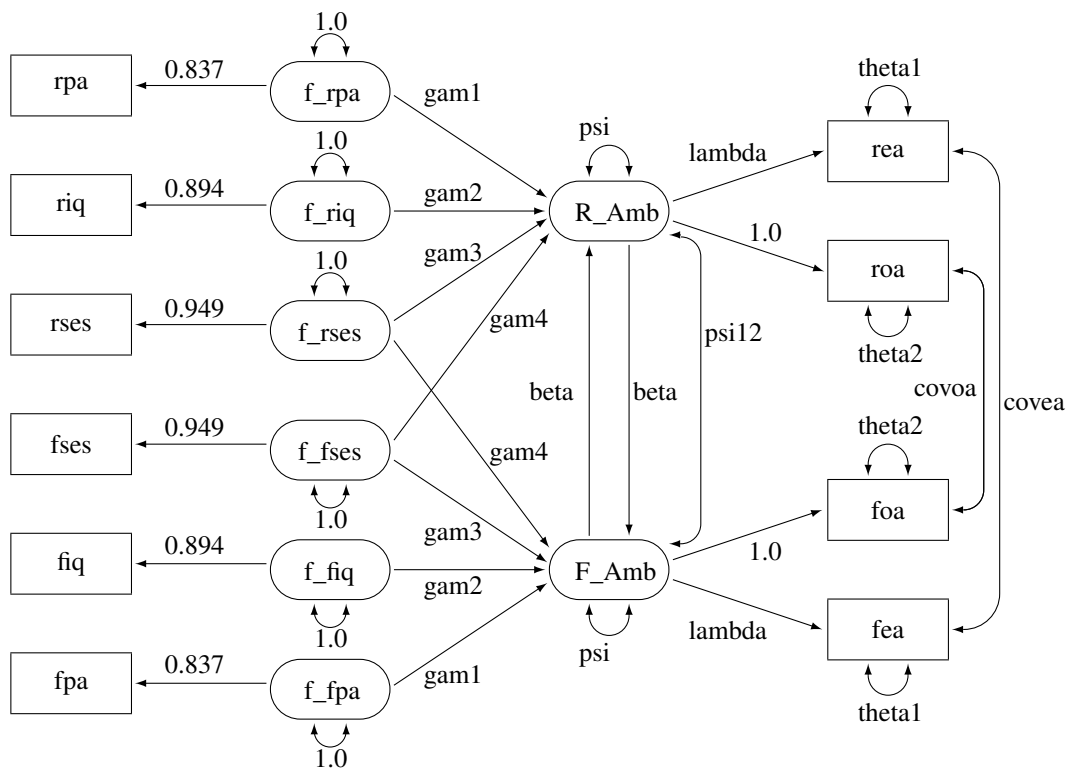
Fit Summary	
Chi-Square	12.0132
Chi-Square DF	13
Pr > Chi-Square	0.5266
Standardized RMR (SRMR)	0.0149
RMSEA Estimate	0.0000
Akaike Information Criterion	96.0132
Bozdogan CAIC	297.4476
Schwarz Bayesian Criterion	255.4476

Since the p -value for the chi-square test is 0.5266, this model clearly cannot be rejected. Both standardized RMR and RMSEA are very small. All these point to an excellent model fit. Three information-theoretic fit indices are also shown: Akaike's information criterion (AIC), Bozdogan's CAIC, and Schwarz's Bayesian Criterion (SBC). These indices are useful when you need to compare competing models for the data.

Model 2: The Model with Equality Constraints

You now consider a much more restrictive model with equality constraints in the model. The path diagram for this constrained model is shown in Figure 27.5.

Figure 27.5 Path Diagram for Career Aspiration: Model 2



The main idea about setting the equality constraints in this model is that there is some symmetry in the model components that correspond to the respondent and his friend. In particular, the corresponding coefficients or parameters should be equal. For example, the path $f_rpa \implies R_Amb$ for the respondent has the same effect as that of $f_fpa \implies F_Amb$. In the path diagram, they are both labeled by the same parameter γ_{am1} . Generalizing the same idea to other pairs of paths, [Output 27.5](#) shows nine pairs of these equality constraints, which are all represented by the same parameter names for distinct (single-headed or double-headed) paths.

However, because of the space limitation, there are six more equality constraints that are not shown in the path diagram. These six constraints concern the covariance structures of the exogenous latent factors f_rpa , f_riq , f_rses , f_fpa , f_fiq , and f_fses . The first three factors are for the respondent, and the last three are for his friend. Using the same symmetry argument, the covariance structures imposed on these exogenous latent factors are shown in the following:

	f_rpa	f_riq	f_rses	f_fpa	f_fiq	f_fses
f_rpa	1.					
f_riq	c1	1.				
f_rses	c2	c3	1.			
f_fpa	c4	c5	c6	1.		
f_fiq	c5	c7	c8	c1	1.	
f_fses	c6	c8	c9	c2	c3	1.

In this pattern of covariance structures, the covariance matrix (upper left portion) for the latent factors of the respondent is the same as that (lower right portion) for the latent factors of his friend. The cross-covariances among the factors between the friends (lower left portion) also display a symmetry pattern. There are six pairs of equality constraints in the covariance structures. Imposing these six pairs of equality constraints and the nine pairs of equality constraints in the path diagram lead to Model 2 of Loehlin (1987).

You can specify the current constrained model by the following PATH modeling language of PROC CALIS:

```
proc calis data=aspire nobs=329 outmodel=model2;
  path
    /* measurement model for intelligence and environment */
    rpa    <=== f_rpa    = 0.837,
    riq    <=== f_riq    = 0.894,
    rses    <=== f_rses   = 0.949,
    fses    <=== f_fses   = 0.949,
    fiq    <=== f_fiq    = 0.894,
    fpa    <=== f_fpa    = 0.837,

    /* structural model of influences: 5 equality constraints */
    f_rpa   ===> R_Amb   = gam1,
    f_riq   ===> R_Amb   = gam2,
    f_rses  ===> R_Amb   = gam3,
    f_fses  ===> R_Amb   = gam4,
    f_rses  ===> F_Amb   = gam4,
    f_fses  ===> F_Amb   = gam3,
    f_fiq   ===> F_Amb   = gam2,
    f_fpa   ===> F_Amb   = gam1,
    F_Amb   ===> R_Amb   = beta,
    R_Amb   ===> F_Amb   = beta,

    /* measurement model for aspiration: 1 equality constraint */
    R_Amb   ===> rea     = lambda,
    R_Amb   ===> roa     = 1.,
    F_Amb   ===> foa     = 1.,
    F_Amb   ===> fea     = lambda;
  pvar
    f_rpa f_riq f_rses f_fpa f_fiq f_fses = 6 * 1.0,
    R_Amb F_Amb           = 2 * psi,        /* 1 ec */
    rea fea              = 2 * theta1,     /* 1 ec */
    roa foa              = 2 * theta2;     /* 1 ec */
  pcov
    R_Amb F_Amb          = psi12,
    rea fea              = covea,
    roa foa              = covoa,
    f_rpa f_riq f_rses   = cov1-cov3,     /* 3 ec */
    f_fpa f_fiq f_fses   = cov1-cov3,
    f_rpa f_riq f_rses * f_fpa f_fiq f_fses = /* 3 ec */
    cov4 cov5 cov6 cov5 cov7 cov8 cov6 cov8 cov9;
run;
```

In the current PATH model specification, you specify the same set of paths as in Model 1. In addition, to set the required constraints in this path model, you use parameter names to label the related paths, variances, or covariances. Same parameter names mean equality constraints. The 15 equality constraints are labeled with comments in the specification. In the PROC CALIS statement, you use the OUTMODEL= option to output the model estimation results into the output data set model2, which is used for subsequent hypotheses tests.

Output 27.24.2 shows the fit summary of Model 2.

Output 27.24.2 Career Aspiration Data: Fit Summary of Model 2 in Loehlin (1987)

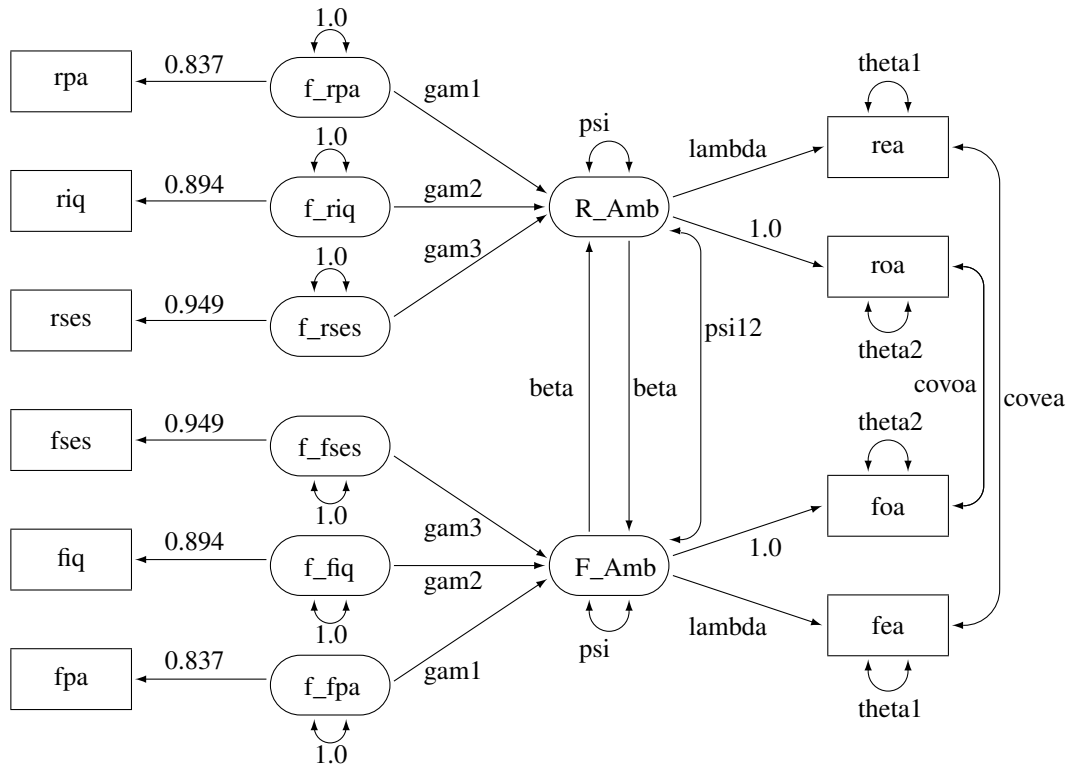
Fit Summary	
Chi-Square	19.0697
Chi-Square DF	28
Pr > Chi-Square	0.8960
Standardized RMR (SRMR)	0.0276
RMSEA Estimate	0.0000
Akaike Information Criterion	73.0697
Bozdogan CAIC	202.5632
Schwarz Bayesian Criterion	175.5632

The test of Model 2 against Model 1 (Loehlin 1987) yields a chi-square of $19.0697 - 12.0132 = 7.0565$ with 15 degrees of freedom, which is clearly not significant. This indicates that the restricted Model 2 fits at least as well as Model 1. Schwarz's Bayesian criterion (SBC) is also much lower for Model 2 (175.5623) than for Model 1 (255.4476). Hence, Model 2 seems preferable on both substantive and statistical grounds.

Model 3: No SES Paths

A question of substantive interest is whether the friend's socioeconomic status (SES) has a significant direct influence on a boy's ambition. This can be addressed by omitting the paths from `f_fses` to `R_Amb` and from `f_rses` to `F_Amb` designated by the parameter name `gam4`, yielding Model 3 of Loehlin (1987). The corresponding path diagram is shown in Figure 27.6.

Figure 27.6 Path Diagram for Career Aspiration: Model 3



In Figure 27.6, you drop the paths `f_rses====>F_Amb` and `f_fses====>R_Amb` from the previous model. Using the path diagram in Figure 27.6, you can specify the current model the same way you do for Model 2. However, because you have the estimation results from Model 2 in the SAS data set `model2`, you can modify this SAS data set to reflect the current model specification and then input the modified SAS data set as an `INMODEL=` file for PROC CALIS to analyze.

First, you create a new SAS data set model3 by the following DATA step:

```
data model3(type=calismdl);
  set model2;
  if _name_='gam4' then
    do;
      _name_=' ';
      _estim_=0;
    end;
run;
```

Essentially, by blanking out the parameter name for the target paths, you are stating that these paths are no longer associated with the free parameter gam4 in the new model. Instead, you put a fixed zero to these paths. This way you eliminate the paths $f_{rSES} \Rightarrow F_{Amb}$ and $f_{fSES} \Rightarrow R_{Amb}$ for Model 3, of which the model specification is now saved in the model3 data set.

Next, you input model3 as the INMODEL= data set for PROC CALIS to analyze, as shown in the following statements:

```
proc calis data=aspire nobs=329 inmodel=model3;
run;
```

PROC CALIS can now use the previous estimation results for fitting the required model. [Output 27.24.3](#) shows the fit summary of Model 3.

Output 27.24.3 Career Aspiration Data: Fit Summary of Model 3 in Loehlin (1987)

Fit Summary	
Chi-Square	23.0365
Chi-Square DF	29
Pr > Chi-Square	0.7749
Standardized RMR (SRMR)	0.0304
RMSEA Estimate	0.0000
Akaike Information Criterion	75.0365
Bozdogan CAIC	199.7340
Schwarz Bayesian Criterion	173.7340

The chi-square value for testing Model 3 versus Model 2 is $23.0365 - 19.0697 = 3.9668$ with one degree of freedom and a p -value of 0.0464. The chi-square test shows a marginal significance, which means that the paths might be needed in the model. However, the SBC (173.7340) indicates that Model 3 is slightly preferable to Model 2, which has an SBC value of 175.5632.

Model 4: No Reciprocal Influence between the Ambition Factors

Another important question is whether the reciprocal influences between the respondent's and friend's ambitions are needed in the model. To test whether these paths are zero, you can set the parameter beta for the paths linking R_Amb and F_Amb to zero to obtain Model 4 of Loehlin (1987).

Similar to Model 3, you can modify the model2 data set to form the new model data set model4 for PROC CALIS to analyze, as shown in the following statements:

```
data model4(type=calismdl);
  set model2;
  if _name_='beta' then
    do;
      _name_=' ';
      _estim_=0;
    end;
run;

proc calis data=aspire nobs=329 inmodel=model4;
run;
```

Output 27.24.4 shows the fit summary of Model 4.

Output 27.24.4 Career Aspiration Data: Fit Summary of Model 4 in Loehlin (1987)

Fit Summary	
Chi-Square	20.9981
Chi-Square DF	29
Pr > Chi-Square	0.8592
Standardized RMR (SRMR)	0.0304
RMSEA Estimate	0.0000
Akaike Information Criterion	72.9981
Bozdogan CAIC	197.6956
Schwarz Bayesian Criterion	171.6956

The chi-square value for testing Model 4 versus Model 2 is $20.9981 - 19.0697 = 1.9284$ with one degree of freedom and a p -value of 0.1649. Hence, there is little evidence of reciprocal influence.

Model 5: No Disturbance Correlation between the Ambition Factors

Model 2 of Loehlin (1987) has the direct paths connecting the latent ambition factors R_Amb and F_Amb and a covariance between the disturbance or error terms (that is, a double-headed arrow connecting the two factors in the path diagram shown in Figure 27.5). The presence of this disturbance correlation serves as a “wastebasket” that enables other omitted variables to have joint influences on the respondent’s and his friend’s ambition factors. To test the hypothesis that this disturbance correlation is zero, you use the following statements to set the parameter psi12 to zero in the model5 data set and fit the new model by PROC CALIS:

```
data model5(type=calismdl);
  set model2;
  if _name_='psi12' then
    do;
      _name_=' ';
      _estim_=0;
    end;
run;

proc calis data=aspire nobs=329 inmodel=model5;
run;
```

Output 27.24.5 displays the fit summary of Model 5.

Output 27.24.5 Career Aspiration Data: Fit Summary of Model 5 in Loehlin (1987)

Fit Summary	
Chi-Square	19.0745
Chi-Square DF	29
Pr > Chi-Square	0.9194
Standardized RMR (SRMR)	0.0276
RMSEA Estimate	0.0000
Akaike Information Criterion	71.0745
Bozdogan CAIC	195.7721
Schwarz Bayesian Criterion	169.7721

The chi-square value for testing Model 5 versus Model 2 is $19.0745 - 19.0697 = 0.0048$ with one degree of freedom. This test statistic is insignificant. Therefore, omitting the covariance between the disturbance terms causes hardly any deterioration in the fit of the model.

Model 7: No Reciprocal Influence and No Disturbance Correlation between the Ambition Factors

The test in Model 4 fails to provide evidence of a direct reciprocal influence between the respondent's and friend's ambitions, and the test in Model 5 fails to provide evidence of a covariance or correlation between the disturbance terms for the ambition factors. Because you consider these two tests separately, you cannot establish evidence to eliminate the reciprocal influence and the disturbance correlation jointly. Instead, to make such a joint inference, it is important to test both hypotheses together by setting both beta and psi12 to zero as in Model 7 of Loehlin (1987). The following statements show how you can do that by modifying the model2 data set to form a new INMODEL= data set model7 for PROC CALIS to analyze:

```
data model7(type=calismdl);
  set model2;
  if _name_='psi12'|_name_='beta' then
    do;
      _name_=' ';
      _estim_=0;
    end;
run;

proc calis data=aspire nobs=329 inmodel=model7;
run;
```

Output 27.24.6 shows the fit summary of Model 7.

Output 27.24.6 Career Aspiration Data: Fit Summary of Model 7 in Loehlin (1987)

Fit Summary	
Chi-Square	25.3466
Chi-Square DF	30
Pr > Chi-Square	0.7080
Standardized RMR (SRMR)	0.0363
RMSEA Estimate	0.0000
Akaike Information Criterion	75.3466
Bozdogan CAIC	195.2480
Schwarz Bayesian Criterion	170.2480

When Model 7 is tested against Models 2, 4, and 5, the p -values are respectively 0.0433, 0.0370, and 0.0123, indicating that the combined effect of the reciprocal influence and the covariance of the disturbance terms is statistically significant. Thus, the hypothesis tests indicate that it is acceptable to omit either the reciprocal influences or the covariance of the disturbances, but not both.

Model 6: No Error Correlations between the Friend's Educational and Occupational Aspiration

It is also of interest to test the covariances (covea and covoa) between the error terms for educational aspiration (that is, between re_a and fe_a) and occupational aspiration (that is, between ro_a and fo_a), because these terms are omitted from Jöreskog and Sörbom (1988) models. Constraining covea and covoa to zero produces Model 6 of Loehlin (1987). You can use the following statements to fit this model:

```
data model6(type=calismdl);
  set model2;
  if _name_='covea' | _name_='covoa' then
    do;
      _name_=' ';
      _estim_=0;
    end;
run;

proc calis data=aspire nobs=329 inmodel=model6;
run;
```

Output 27.24.7 shows the fit summary of Model 6.

Output 27.24.7 Career Aspiration Data: Model 6 of Loehlin (1987)

Fit Summary	
Chi-Square	33.4475
Chi-Square DF	30
Pr > Chi-Square	0.3035
Standardized RMR (SRMR)	0.0306
RMSEA Estimate	0.0187
Akaike Information Criterion	83.4475
Bozdogan CAIC	203.3489
Schwarz Bayesian Criterion	178.3489

The chi-square value for testing Model 6 versus Model 2 is $33.4476 - 19.0697 = 14.3779$ with two degrees of freedom and a p -value of 0.0008, indicating that there is considerable evidence of correlation between the error terms.

Summary of Competing Models

The following table summarizes the results from the seven models described in Loehlin (1987).

Model	χ^2	df	p-value	SBC
1. Full model	12.0132	13	0.5266	255.4476
2. Equality constraints	19.0697	28	0.8960	175.5632
3. No SES path	23.0365	29	0.7749	173.7340
4. No reciprocal influence	20.9981	29	0.8592	171.6956
5. No disturbance correlation	19.0745	29	0.9194	169.7721
6. No error correlation	33.4475	30	0.3035	178.3489
7. Constraints from both 4 and 5	25.3466	30	0.7080	170.2480

For comparing models, you can use a DATA step to compute the differences of the chi-square statistics and *p*-values, as shown in the following statements:

```
data _null_;
  array achisq[7] _temporary_
    (12.0132 19.0697 23.0365 20.9981 19.0745 33.4475 25.3466);
  array adf[7] _temporary_
    (13 28 29 29 29 30 30);
  retain indent 16;
  file print;
  input ho ha @@;
  chisq = achisq[ho] - achisq[ha];
  df = adf[ho] - adf[ha];
  p = 1 - probchi( chisq, df);
  if _n_ = 1 then put
    / +indent 'model comparison   chi**2   df p-value'
    / +indent '-----';
  put +indent +3 ho ' versus ' ha @18 +indent chisq 8.4 df 5. p 9.4;
  datalines;
2 1   3 2   4 2   5 2   7 2   7 4   7 5   6 2
;
```

The DATA step displays the table in [Output 27.24.8](#).

Output 27.24.8 Career Aspiration Data: Model Comparisons

Peer Influences on Aspiration: Haller & Butterworth (1960)				
model	comparison	chi**2	df	p-value

2	versus 1	7.0565	15	0.9561
3	versus 2	3.9668	1	0.0464
4	versus 2	1.9284	1	0.1649
5	versus 2	0.0048	1	0.9448
7	versus 2	6.2769	2	0.0433
7	versus 4	4.3485	1	0.0370
7	versus 5	6.2721	1	0.0123
6	versus 2	14.3778	2	0.0008

Although none of the seven models can be rejected when tested against the alternative of an unrestricted covariance matrix, the model comparisons make it clear that there are important differences among the models. Schwarz's Bayesian criterion indicates Model 5 as the model of choice. The constraints added to Model 5 in Model 7 can be rejected ($p = 0.0123$), while Model 5 cannot be rejected when tested against the less constrained Model 2 ($p = 0.9448$). Hence, among the small number of models considered, Model 5 has strong statistical support. However, as Loehlin (1987, p. 106) points out, many other models for these data could be constructed. Further analysis should consider, in addition to simple modifications of the models, the possibility that more than one friend could influence a boy's aspirations, and that a boy's ambition might have some effect on his choice of friends. Pursuing such theories would be statistically challenging.

Example 27.25: Fitting a Latent Growth Curve Model

Latent factors in structural equation modeling are constructed to represent important unobserved hypothetical constructs. However, with some manipulations latent factors can also represent random effects in models. In this example, a simple latent growth curve model is considered. You use latent factors to represent the random intercepts and slopes in the latent growth curve model.

Sixteen individuals were invited to a training program that was designed to boost self-confidence. During the training, the individuals' confidence levels were measured at five time points: initially and four more times separated by equal intervals. The data are stored in the following SAS data set:

```

data growth;
  input y1 y2 y3 y4 y5;
  datalines;
17.6 21.4 25.6 32.1 37.7
13.2 14.3 18.9 20.3 25.4
11.6 13.5 17.4 22.1 39.6
10.7 11.1 13.2 18.2 21.4
18.7 23.7 28.6 31.5 34.0
18.3 19.2 20.5 23.2 25.9
 9.2 13.5 17.8 19.2 21.1
18.3 23.5 27.9 30.2 34.6
11.2 15.6 20.8 22.7 30.4
17.0 22.9 26.9 31.9 35.6
10.4 13.6 18.0 25.6 29.3
17.7 19.0 22.5 28.5 30.7
14.5 19.4 21.1 28.8 31.5
20.0 21.4 28.9 30.2 35.6
14.6 19.3 21.7 28.5 32.0
11.7 15.2 19.1 23.7 28.7
;

```

First, consider a simple linear regression model for the confidence levels at time t due to training. That is,

$$y_t = \alpha + \beta T_t + e_t$$

where y_t represents the confidence level at time t ($t = 1, 2, \dots, 5$), α represents the intercept, β represents the slope or the effect of training, T_t represents the fixed time point at t ($T_1 = 0$ and $T_i = T_{i-1} + 1$), and e_t is the error term at time t .

This simple linear regression assumes that the effect of training (slope) and the intercept are constants for the individuals. However, individual differences are rules rather than exceptions. It is thus more reasonable to argue that an index i for individuals should be added to the intercept and slope in the model. As a result, the following individualized regression model is derived:

$$y_{it} = \alpha_i + \beta_i T_t + e_t$$

where $i = 1, 2, \dots, 16$. In this model, individuals are assumed to have different intercepts and slopes (regression coefficients). Note that theoretically e_t could also be “individualized” as e_{ti} in the model. But this is not done because such a model would be unnecessarily complicated without gaining additional insights in return.

Unfortunately, this individualized model with individual intercepts and slopes cannot be estimated directly. If you treat each α_i and β_i as fixed parameters, you are going to have too many parameters for the model to be identified or estimable. A workable solution is to treat α and β in the original linear regression model as random variables instead. That is, the latent growth curve model of interest is as follows:

$$y_t = \alpha + \beta T_t + e_t$$

where (α, β) is bivariate normal with unknown means, variances, and covariance. Therefore, instead of having 16 intercepts and 16 slopes to estimate in the individualized regression model, the final latent growth curve model has to estimate only two means, two variances and one covariance in the bivariate distribution of (α, β) .

To use PROC CALIS to fit this latent growth curve model, the random intercept and effect are treated as if they were covarying latent factors. To make them stand out more as latent variables, the random intercept and slope are renamed as f_α and f_β in the following structural equation:

$$y_t = f_\alpha + T_t f_\beta + e_t$$

where f_α and f_β are bivariate-normal latent variables. This model assumes that the error distribution is time dependent (with the index t). A simpler version is to make this error term invariant over time, which is then represented by the following model with constrained error variances:

$$y_t = f_\alpha + T_t f_\beta + e$$

This constrained model is considered first. The LINEQS modeling language is used to specify this constrained model, as shown in the following statements.

```
proc calis method=ml data=growth nostand noparmname;
  lineqs
    y1 = 0. * Intercept + f_alpha                + e1,
    y2 = 0. * Intercept + f_alpha + 1 * f_beta + e2,
    y3 = 0. * Intercept + f_alpha + 2 * f_beta + e3,
    y4 = 0. * Intercept + f_alpha + 3 * f_beta + e4,
    y5 = 0. * Intercept + f_alpha + 4 * f_beta + e5;
  variance
    f_alpha f_beta,
    e1-e5 = 5 * evar;
  mean
    f_alpha f_beta;
  cov
    f_alpha f_beta;
  fitindex on(only)=[chisq df probchi];
run;
```

In the LINEQS model specification, `f_alpha` and `f_beta` are treated as latent factors representing the random intercept and random slope, respectively. The `f_` prefix for latent factors is required as a convention in the LINEQS modeling language. See the sections “[Naming Variables in the LINEQS Model](#)” on page 1272 and “[Naming Variables and Parameters](#)” on page 1302 for details.

Notice that you need to set the ordinary (non-random) intercepts for endogenous variables to zero by the `0.*Intercept` specification because non-random intercepts for observed endogenous variables are default parameters in the LINEQS model. Because you have already used `f_alpha` as the random intercept, you must turn off the default non-random intercept term for the observed endogenous variables `y1–y5`. Otherwise, your latent growth curve model might be over-parameterized.

At $T_1 = 0$, y_1 represents the initial confidence measurement so that it is not subject to the random effect `f_beta`. The next four measurements y_2 , y_3 , y_4 , and y_5 are measured at time points T_2 , T_3 , T_4 , and T_5 , respectively. These are fixed time points with constant values 1, 2, 3, and 4, respectively, in the equations of the LINEQS statement.

The means, variances and covariances of `f_alpha` and `f_beta` are parameters in the model. The variances of these two latent variables are specified in the [VARIANCE](#) statement, while their covariance is specified in the [COV](#) statement. The means of `f_alpha` and `f_beta` are specified in the [MEAN](#) statement. Unlike the specification for the variances of `e1–e5`. All these parameters for the latent factors are unnamed because you do not need to constrain them by references.

The error variances for `e1–e5` are also specified in the [VARIANCE](#) statement. Using the shorthand notation `5 * evar`, the parameter name `evar` is repeated five times for the five error variances. This constrains the error variances for `e1–e5` to be equal.

You also use some special printing options in this example. In the PROC CALIS statement, the [NOSTAND](#) option is specified because standardized solution is not of interest. The reason is that `y1–y5` were already measured on comparable scales, making standardization unnecessary for interpretations. Another printing option specified is the [NOPARMNAME](#) option in the PROC CALIS statement. This option suppresses the printing of parameter names in the output for estimation. This makes the output look more concise when you do not need to make references to the parameter names. Still another printing option used is

the ON(ONLY)= option of the FITINDEX statement. This option trims down the display of fit indices to include only those listed in the option. See the FITINDEX statement on page 1148 for details.

Output 27.25.1 shows the fit summary table.

Output 27.25.1 Random Intercepts and Effects with Constrained Error Variances: Model Fit

Fit Summary	
Chi-Square	31.4310
Chi-Square DF	14
Pr > Chi-Square	0.0048

In Output 27.25.1, the chi-square value in the fit summary table is 31.431 ($df = 14$, $p < 0.01$), which is a statistically significant result that might indicate a poor model fit. Despite that, it is illustrative to continue to look at the main estimation results, which are shown in the following table.

Output 27.25.2 Estimation of Random Intercepts and Effects with Constrained Error Variances

Estimates for Variances of Exogenous Variables				
Variable Type	Variable	Estimate	Standard Error	t Value
Latent	f_alpha	13.89140	5.81540	2.38873
	f_beta	0.80742	0.42198	1.91342
Error	e1	3.32185	0.70031	4.74342
	e2	3.32185	0.70031	4.74342
	e3	3.32185	0.70031	4.74342
	e4	3.32185	0.70031	4.74342
	e5	3.32185	0.70031	4.74342
Covariances Among Exogenous Variables				
Var1	Var2	Estimate	Standard Error	t Value
f_alpha	f_beta	-0.35281	1.13815	-0.30998
Mean Parameters				
Variable Type	Variable	Estimate	Standard Error	t Value
Latent	f_alpha	14.15875	1.02906	13.75890
	f_beta	4.04813	0.27563	14.68665

In [Output 27.25.2](#), the estimated variance of the random intercept α , which is represented by the variance estimate of the latent factor `f_alpha`, is 13.891 ($t = 2.389$). In the next row of the same table, the variance estimate of the random effect β , which is represented by the variance estimate of the latent factor `f_beta`, is 0.807 ($t = 1.913$).

The covariance of the random intercept and the random effect is shown in the next table for “Covariances Among Exogenous Variables.” A negative estimate of -0.353 is shown. This means that the initial self-confidence level and the boosting effect of training are negatively correlated. The higher the initial self-confidence level, the smaller the training effect.

In the last table for the “Mean Parameters,” the estimated mean of the random intercept is 14.159, which is an estimate of the averaged initial self-confidence level. The estimated mean of random effect is 4.048, which is an estimate of the averaged training effect. They are both significantly different from zero.

Given that the model does not fit that well, perhaps you should not take the interpretations of these estimates so seriously. Knowing that the distribution of the errors might have been time-dependent, you now try to improve the fit of the model by relaxing the constraint about common error variances. You can use the following specifications:

```
proc calis method=ml data=growth nostand noparmname;
  lineqs
    y1 = 0. * Intercept + f_alpha          + e1,
    y2 = 0. * Intercept + f_alpha + 1 * f_beta + e2,
    y3 = 0. * Intercept + f_alpha + 2 * f_beta + e3,
    y4 = 0. * Intercept + f_alpha + 3 * f_beta + e4,
    y5 = 0. * Intercept + f_alpha + 4 * f_beta + e5;
  variance
    f_alpha f_beta,
    e1-e5;
  mean
    f_alpha f_beta;
  cov
    f_alpha f_beta;
  fitindex on(only)=[chisq df probchi];
run;
```

In this new specification, there is only one change in the **VARIANCE** statement from the previous specification. That is, you now specify only the error variables without putting parameter names for them. This makes the variances of `e1–e5` free (unconstrained) parameters in the model.

[Output 27.25.3](#) shows the model fit summary.

Output 27.25.3 Random Intercepts and Effects with Unconstrained Error Variances: Model Fit

Fit Summary	
Chi-Square	11.6250
Chi-Square DF	10
Pr > Chi-Square	0.3109

The chi-square for the unconstrained model is 11.625 ($df = 10$, $p > .10$). This indicates an acceptable model fit. The chi-square difference test can also be conducted for testing the previous constrained model

against this new model. The chi-square difference is $19.81 = 31.431 - 11.625$. With $df = 4$, this chi-square difference value is statistically significant at $\alpha=0.01$, indicating a significant improvement of model fit by using the unconstrained model.

Output 27.25.4 shows the estimation results.

Output 27.25.4 Estimation of Random Intercepts and Effects with Unconstrained Error Variances

Estimates for Variances of Exogenous Variables				
Variable Type	Variable	Estimate	Standard Error	t Value
Latent	f_alpha	14.70071	5.66943	2.59298
	f_beta	0.45059	0.29867	1.50867
Error	e1	2.81712	1.35332	2.08164
	e2	0.32213	0.46118	0.69848
	e3	1.94429	0.86824	2.23935
	e4	1.88569	1.21306	1.55448
	e5	14.65193	5.99354	2.44462
Covariances Among Exogenous Variables				
Var1	Var2	Estimate	Standard Error	t Value
f_alpha	f_beta	0.35291	0.90366	0.39054
Mean Parameters				
Variable Type	Variable	Estimate	Standard Error	t Value
Latent	f_alpha	14.03046	1.01534	13.81851
	f_beta	3.96793	0.22612	17.54781

The estimation results for the unconstrained model present a slightly different picture than the constrained model. While the estimates for the means and variances of the random intercept and the random training effect look similar in both models, estimates of the covariance between the random intercept and the random training effect are quite different in the two models. The covariance estimate is negative (-0.353) in the constrained model, but it is positive (0.353) in the unconstrained model. However, because the covariance estimates are not statistically significant in both models ($t = -0.310$ and 0.391 , respectively), you wonder whether the current data are showing strong evidence that supports one way or another. To get a clearer picture, perhaps you need to collect more data and fit the models again to examine the significance of the covariance between the random intercept and slope.

Example 27.26: Higher-Order and Hierarchical Factor Models

In this example, confirmatory higher-order and hierarchical factor models are fitted by PROC CALIS.

In higher-order factor models, factors are at different levels. The higher-order factors explain the relationships among factors at the next lower level, in the same way that the first-order factors explain the relationships among manifest variables. For example, in a two-level higher order factor model you have nine manifest variables V1–V9 with three first-order factors F1–F3. The first-order factor pattern of the model might appear like the following:

	F1	F2	F3
V1	x		
V2	x		
V3	x		
V4		x	
V5		x	
V6		x	
V7			x
V8			x
V9			x

where each “x” marks a nonzero factor loading and all other unmarked entries are fixed zeros in the model. To explain the correlations among the first-order factors, a second-order factor F4 is hypothesized with the following second-order factor pattern:

	F4
F1	x
F2	x
F3	x

If substantiated by your theory, you might have higher-order factor models with more than two levels.

In hierarchical factor models, all factors are at the same (first-order) level but are different in their clusters of manifest variables related. Using the terminology of Yung, Thissen, and McLeod (1999), factors in hierarchical factor models are classified into “layers.” The factors in the first layer partition the manifest variables into clusters so that each factor has a distinct cluster of related manifest variables. This part of the factor pattern of the hierarchical factor model is similar to that of the first-order factor model for manifest variables. The next layer of factors in the hierarchical factor model again partitions the manifest variables into clusters. However, this time each cluster contains at least two clusters of manifest variables that are formed in the previous layer. For example, the following is a factor pattern of a confirmatory hierarchical factor model with two layers:

	First Layer			Second Layer
	F1	F2	F3	F4
V1	x			x
V2	x			x
V3	x			x
V4		x		x
V5		x		x
V6		x		x
V7			x	x
V8			x	x
V9			x	x

F1–F3 are first-layer factors and F4 is the only second-layer factor. This special kind of two-layer hierarchical pattern is also known as the bifactor solution. In a bifactor solution, there are two classes of factors—group factors and a general factor. For example, in the preceding hierarchical factor pattern F1–F3 are group factors for different abilities and F4 is a general factor such as “intelligence” (see, for example, Holzinger and Swineford 1937). See Mulaik and Quartetti (1997) for more examples and distinctions among various types of hierarchical factor models. Certainly, if substantiated by your theory, hierarchical factor models with more than two layers are possible.

In this example, you use PROC CALIS to fit these two types of confirmatory factor models. First, you fit a second-order factor model to a real data set. Then you fit a bifactor model to the same data set. In the final section of this example, an informal account of the relationship between the higher-order and hierarchical factor models is attempted. Techniques for constraining parameters using PROC CALIS are also shown. This final section might be too technical in the first reading. Interested readers are referred to articles by Mulaik and Quartetti (1997), Schmid and Leiman (1957), and Yung, Thissen, and McLeod (1999) for more details.

A Second-Order Factor Analysis Model

In this section, a second-order confirmatory factor analysis model is applied to a correlation matrix of Thurstone reported by McDonald (1985). The correlation matrix is read into a SAS data set in the following statements:

```
data Thurst(type=corr);
title "Example of THURSTONE resp. McDONALD (1985, p.57, p.105)";
_type_ = 'corr'; input _name_ $ V1-V9;
label V1='Sentences' V2='Vocabulary' V3='Sentence Completion'
      V4='First Letters' V5='Four-letter Words' V6='Suffices'
      V7='Letter series' V8='Pedigrees' V9='Letter Grouping';
datalines;
V1 1. . . . . . . . .
V2 .828 1. . . . . . . .
V3 .776 .779 1. . . . . . .
V4 .439 .493 .460 1. . . . . .
V5 .432 .464 .425 .674 1. . . . .
V6 .447 .489 .443 .590 .541 1. . . . .
V7 .447 .432 .401 .381 .402 .288 1. . . .
V8 .541 .537 .534 .350 .367 .320 .555 1. .
V9 .380 .358 .359 .424 .446 .325 .598 .452 1.
;
```

Variables in this data set are measures of cognitive abilities. Three factors are assumed for these nine variable V1–V9. These three factors are the first-order factors in the analysis. A second-order factor is also assumed to explain the correlations among the three first-order factors.

The following statements define a second-order factor model by using the **LINEQS** modeling language.

```
proc calis corr data=Thurst method=max nobs=213 nose nostand;
  lineqs
    V1      = X11 * Factor1                                + E1,
    V2      = X21 * Factor1                                + E2,
    V3      = X31 * Factor1                                + E3,
    V4      =                X42 * Factor2                  + E4,
    V5      =                X52 * Factor2                  + E5,
    V6      =                X62 * Factor2                  + E6,
    V7      =                X73 * Factor3                  + E7,
    V8      =                X83 * Factor3                  + E8,
    V9      =                X93 * Factor3                  + E9,
    Factor1 =                L1g * FactorG + E10,
    Factor2 =                L2g * FactorG + E11,
    Factor3 =                L3g * FactorG + E12;
  variance
    FactorG = 1. ,
    E1-E12 = U1-U9 W1-W3;
  bounds
    0. <= U1-U9;
  fitindex ON(ONLY)=[chisq df probchi];
  /* SAS Programming Statements: Dependent parameter definitions */
    W1 = 1. - L1g * L1g;
    W2 = 1. - L2g * L2g;
    W3 = 1. - L3g * L3g;
run;
```

In the first nine equations of the **LINEQS** statement, variables V1–V3 are manifest indicators of latent factor Factor1, variables V4–V6 are manifest indicators of latent factor Factor2, and variables V7–V9 are manifest indicators of latent factor Factor3. In the last three equations of the **LINEQS** statement, the three first-order factors Factor1–Factor3 are explained by a common source: FactorG. Hence, Factor1–Factor3 are correlated due to the common source FactorG in the model.

An error term is added to each equation in the **LINEQS** statement. These error terms E1–E12 are needed because the factors are not assumed to be perfect predictors of the corresponding outcome variables.

In the **VARIANCE** statement, you specify variance parameters for all independent or exogenous variables in the model: FactorG, and E1–E12. The variance of FactorG is fixed at one for identification. Variances for E1–E9 are given parameter names U1–U9, respectively. Variances for E10–E12 are given parameter names W1–W3, respectively. Note that for model identification purposes, W1–W3 are defined as dependent parameters in the **SAS programming statements**. That is,

$$W_i = 1. - L_{ig}^2 \quad (i = 1, 2, 3)$$

These dependent parameter definitions ensure that the variances for Factor1–Factor3 are fixed at ones for identification.

In the **BOUNDS** statement, you specify that variance parameters U1–U9 must be positive in the solution.

In addition to the statements for model specification, you specify some output control options in the PROC CALIS statement. You use the **NOSE** and **NOSTAND** options suppress the display of standard errors and standardized results. In the **FITINDEX** statement, the **ON(ONLY)=** option requests only the model fit chi-square and its associated degrees of freedom and *p*-value be shown in the fit summary table. Using printing options in PROC CALIS to reduce the amount the of printout is a good practice. It makes your output more focused, as you output only what you need in a particular situation.

In **Output 27.26.1**, parameters and their initial values, gradients, and bounds are shown.

Output 27.26.1 Parameters in the Model

Optimization Start Parameter Estimates					
N	Parameter	Estimate	Gradient	Lower Bound	Upper Bound
1	X11	1.00000	0.13476	.	.
2	X21	1.01408	0.17327	.	.
3	X31	0.95518	0.12174	.	.
4	X42	1.00000	0.22548	.	.
5	X52	0.96603	0.21304	.	.
6	X62	0.88305	0.19782	.	.
7	X73	1.00000	0.21041	.	.
8	X83	1.03403	0.39324	.	.
9	X93	0.91752	0.19880	.	.
10	L1g	0.75060	-0.57492	.	.
11	L2g	0.64268	-0.50975	.	.
12	L3g	0.60919	-0.56538	.	.
13	U1	0.18879	0.14837	0	.
14	U2	0.16579	0.08989	0	.
15	U3	0.25988	-0.03231	0	.
16	U4	0.33068	0.20120	0	.
17	U5	0.37538	0.09124	0	.
18	U6	0.47808	-0.03595	0	.
19	U7	0.44813	0.20918	0	.
20	U8	0.40994	-0.12469	0	.
21	U9	0.53541	0.05959	0	.

Value of Objective Function = 0.5693888709

The Number of Dependent Parameters is 3

N	Parameter	Estimate
22	W1	0.43660
23	W2	0.58697
24	W3	0.62889

The first table contains all the independent parameters. There are twenty-one in total. Parameters W1–W3, which are defined in the [SAS programming statements](#), are shown in the next table for dependent parameters. Their initial values are computed as functions of the independent parameters.

Output 27.26.2 shows the information about optimization—iteration history and the convergence status.

Output 27.26.2 Optimization

Optimization Start									
Active Constraints			0	Objective Function			0.5693888709		
Max Abs Gradient Element			0.5749163348	Radius			1.8533033852		
Iter	Rest arts	Func Calls	Act Con	Objective Function	Obj Fun Change	Max Abs Gradient Element	Lambda	Actual Over Pred Change	
1	0	5	0	0.38684	0.1825	0.5158	3.214	1.174	
2	0	9	0	0.18706	0.1998	0.1003	0	1.181	
3	0	11	0	0.18039	0.00667	0.0273	0	0.987	
4	0	13	0	0.18020	0.000192	0.00581	0	0.881	
5	0	15	0	0.18017	0.000023	0.00295	0	0.967	
6	0	17	0	0.18017	3.08E-6	0.000686	0	1.083	
7	0	19	0	0.18017	4.606E-7	0.000379	0	1.195	
8	0	21	0	0.18017	7.365E-8	0.000096	0	1.283	
9	0	23	0	0.18017	1.228E-8	0.000054	0	1.342	
10	0	25	0	0.18017	2.098E-9	0.000018	0	1.377	
11	0	27	0	0.18017	3.63E-10	8.561E-6	0	1.397	

Optimization Results			
Iterations	11	Function Calls	30
Jacobian Calls	13	Active Constraints	0
Objective Function	0.1801712146	Max Abs Gradient Element	8.5605681E-6
Lambda	0	Actual Over Pred Change	1.3969225014
Radius	0.0000572561		

Convergence criterion (GCONV=1E-8) satisfied.

First, there are 21 independent parameters in the optimization by using 45 “Functions (Observations).” The so-called functions refer to the moments in the model that are structured with parameters. Nine lower bounds, which are specified for the error variance parameters, are specified in the optimization. The next table for iteration history shows that the optimization stops in 11 iterations. The notes at the bottom of table show that the solution converges without problems.

Output 27.26.3 shows the fit summary table. The chi-square model fit value is 38.196, with $df = 24$, and $p = 0.033$. This indicates a satisfactory model fit.

Output 27.26.3 Fit Summary

Fit Summary		
Chi-Square		38.1963
Chi-Square DF		24
Pr > Chi-Square		0.0331

Output 27.26.4 shows the fitted equations with final estimates. Interpretations of these loadings are not done here. The last table in this output shows various variance estimates. These estimates are classified by whether they are for the latent variables, error variables, or disturbance variables.

Output 27.26.4 Estimation Results

Linear Equations			
V1	=	0.9047*Factor1 + 1.0000 E1	
		X11	
V2	=	0.9138*Factor1 + 1.0000 E2	
		X21	
V3	=	0.8561*Factor1 + 1.0000 E3	
		X31	
V4	=	0.8358*Factor2 + 1.0000 E4	
		X42	
V5	=	0.7972*Factor2 + 1.0000 E5	
		X52	
V6	=	0.7026*Factor2 + 1.0000 E6	
		X62	
V7	=	0.7808*Factor3 + 1.0000 E7	
		X73	
V8	=	0.7202*Factor3 + 1.0000 E8	
		X83	
V9	=	0.7035*Factor3 + 1.0000 E9	
		X93	
Factor1	=	0.8221*FactorG + 1.0000 E10	
		L1g	
Factor2	=	0.7818*FactorG + 1.0000 E11	
		L2g	
Factor3	=	0.8150*FactorG + 1.0000 E12	
		L3g	

Output 27.26.4 *continued*

Estimates for Variances of Exogenous Variables			
Variable Type	Variable	Parameter	Estimate
Latent	FactorG		1.00000
Error	E1	U1	0.18150
	E2	U2	0.16493
	E3	U3	0.26713
	E4	U4	0.30150
	E5	U5	0.36450
	E6	U6	0.50642
	E7	U7	0.39033
	E8	U8	0.48137
Disturbance	E9	U9	0.50510
	E10	W1	0.32420
	E11	W2	0.38879
	E12	W3	0.33576

For illustration purposes, you might check whether the model constraints put on the variances of Factor1–Factor3 are honored (although this should have been taken care of in the optimization). For example, the variance of Factor1 should be:

$$1 = (\text{Loading on FactorG})^2 + \text{Variance of E10}$$

Extracting the estimates from the output, you indeed verify the required equality, as shown in the following:

$$1.0000 = (0.8221)^2 + 0.32420$$

A Bifactor Model

A bifactor model (or a hierarchical factor model with two layers) for the same data set is now considered. In this model, the same set of factors as in the preceding higher-order factor model are used. The most notable difference is that the second-order factor FactorG in the higher-order factor model is no longer a factor of the first-order factors Factor1–Factor3. Instead, FactorG, like Factor1–Factor3, now also serves as a factor of the observed variable V1–V9. Unlike Factor1–Factor3, FactorG is considered to be a *general* factor in the sense that *all* observed variables have direct functional relationships with it. In contrast, Factor1–Factor3 are *group* factors in the sense that each of them has a direct functional relationship with only one group of *observed* variables. Because of the coexistence of a general factor and group factors at the same factor level, such a hierarchical model is also called a bifactor model.

The bifactor model is specified in the following statements:

```

proc calis corr data=Thurst method=max nobs=213 nose nostand;
  lineqs
    V1 = X11 * Factor1                + X1g * FactorG + E1,
    V2 = X21 * Factor1                + X2g * FactorG + E2,
    V3 = X31 * Factor1                + X3g * FactorG + E3,
    V4 =           X42 * Factor2        + X4g * FactorG + E4,
    V5 =           X52 * Factor2        + X5g * FactorG + E5,
    V6 =           X62 * Factor2        + X6g * FactorG + E6,
    V7 =           X73 * Factor3 + X7g * FactorG + E7,
    V8 =           X83 * Factor3 + X8g * FactorG + E8,
    V9 =           X93 * Factor3 + X9g * FactorG + E9;
  variance
    Factor1-Factor3 = 3 * 1.,
    FactorG          = 1. ,
    E1-E9           = U1-U9;
  cov
    Factor1-Factor3 FactorG = 6 * 0.;
  bounds
    0. <= U1-U9;
  fitindex ON(ONLY)=[chisq df probchi];
run;

```

In the **LINEQS** statement, there are only nine equations for the manifest variables in the model. Unlike the second-order factor model fitted previously, Factor1–Factor3 are no longer functionally related to FactorG and therefore there are no equations with Factor1–Factor3 as outcome variables.

The factor variances are all fixed at 1 in the **VARIANCE** statement. The variance parameters for E1–E9 are named U1–U9, respectively. The **BOUNDS** statement, again, is specified so that only positive estimates are accepted for error variance estimates.

All factors in the bifactor model are uncorrelated. In the **COV** statement, you specify that the six covariances among Factor1–Factor3 and FactorG are all zero. This specification is necessary because by default exogenous variables (excluding error terms) in the **LINEQS** model are correlated.

Like the previous PROC CALIS run, options are specified in the PROC CALIS and the **FITINDEX** statements to reduce the amount of default output.

There are more parameters in this model than in the preceding higher-order factor model, as shown in [Output 27.26.5](#), which shows the optimization information.

Output 27.26.5 Optimization

Optimization Start			
Active Constraints	0	Objective Function	0.8380304146
Max Abs Gradient Element	2.4076251809	Radius	20.596787596

Output 27.26.5 *continued*

Iter	Rest arts	Func Calls	Act Con	Objective Function	Obj Fun Change	Max Abs Gradient Element	Lambda	Actual Over Pred Change
1	0	5	0	0.70566	0.1324	0.4851	0.00140	0.148
2	0	7	0	0.30090	0.4048	0.3269	0	1.292
3	0	9	0	0.17403	0.1269	0.2947	0	0.985
4	0	11	0	0.11759	0.0564	0.0677	0	1.190
5	0	13	0	0.11455	0.00304	0.0267	0	1.043
6	0	15	0	0.11426	0.000285	0.00242	0	1.153
7	0	17	0	0.11423	0.000027	0.00168	0	1.394
8	0	19	0	0.11423	5.552E-6	0.000478	0	1.413
9	0	21	0	0.11423	1.154E-6	0.000335	0	1.420
10	0	23	0	0.11423	2.405E-7	0.000105	0	1.427
11	0	25	0	0.11423	5.016E-8	0.000068	0	1.432
12	0	27	0	0.11423	1.047E-8	0.000023	0	1.436
13	0	29	0	0.11423	2.184E-9	0.000014	0	1.439
14	0	31	0	0.11423	4.56E-10	4.909E-6	0	1.442

Optimization Results

Iterations	14	Function Calls	34
Jacobian Calls	16	Active Constraints	0
Objective Function	0.1142278162	Max Abs Gradient Element	4.9090342E-6
Lambda	0	Actual Over Pred Change	1.4423534599
Radius	0.0002294218		

Convergence criterion (GCONV=1E-8) satisfied.

There are 27 parameters in the bifactor model: nine for the loadings on the group factors Factor1–Factor3, nine for the loadings on the general factor FactorG, and nine for the variances of errors E1–E9. The optimization converges in 14 iterations without problems.

A fit summary table is shown in [Output 27.26.6](#)

Output 27.26.6 Fit Summary

Fit Summary	
Chi-Square	24.2163
Chi-Square DF	18
Pr > Chi-Square	0.1481

The fit of this model is quite good. The chi-square value is 24.216, with $df = 18$ and $p = 0.148$. This is expected because the bifactor model has more parameters than the second-order factor model, which already has a good fit with fewer parameters.

Estimation results are shown in [Output 27.26.7](#). Estimates are left uninterpreted because they are not the main interest of this example.

Output 27.26.7 Estimation Results

Linear Equations			
V1 =	-0.4879*Factor1 +	0.7679*FactorG +	1.0000 E1
	X11	X1g	
V2 =	-0.4523*Factor1 +	0.7909*FactorG +	1.0000 E2
	X21	X2g	
V3 =	-0.4045*Factor1 +	0.7536*FactorG +	1.0000 E3
	X31	X3g	
V4 =	0.6140*Factor2 +	0.6084*FactorG +	1.0000 E4
	X42	X4g	
V5 =	0.5058*Factor2 +	0.5973*FactorG +	1.0000 E5
	X52	X5g	
V6 =	0.3943*Factor2 +	0.5718*FactorG +	1.0000 E6
	X62	X6g	
V7 =	-0.7273*Factor3 +	0.5669*FactorG +	1.0000 E7
	X73	X7g	
V8 =	-0.2468*Factor3 +	0.6623*FactorG +	1.0000 E8
	X83	X8g	
V9 =	-0.4091*Factor3 +	0.5300*FactorG +	1.0000 E9
	X93	X9g	
Estimates for Variances of Exogenous Variables			
Variable Type	Variable	Parameter	Estimate
Latent	Factor1		1.00000
	Factor2		1.00000
	Factor3		1.00000
	FactorG		1.00000
Error	E1	U1	0.17236
	E2	U2	0.16984
	E3	U3	0.26848
	E4	U4	0.25281
	E5	U5	0.38735
	E6	U6	0.51757
	E7	U7	0.14966
	E8	U8	0.50039
	E9	U9	0.55175

One might ask whether this bifactor (hierarchical) model provides a significantly better fit than the previous second-order model. Can one use a chi-square difference test for nested models to answer this question? The answer is yes.

Although it is not obvious that the previous second-order factor model is nested within the current bifactor model, a general nested relationship between the higher-order factor and the hierarchical factor model is formally proved by Yung, Thissen, and McLeod (1999). Therefore, a chi-square difference test can be conducted using the following DATA step:

```

data _null_;
  df0 = 24; chi0 = 38.1963;
  df1 = 18; chi1 = 24.2163;
  diff = chi0-chi1;
  p = 1.-probchi(chi0-chi1,df0-df1);
  put 'Chi-square difference = ' diff;
  put 'p-value = ' p;
run;

```

The results are shown in the following:

Output 27.26.8 Chi-square Difference Test

```

Chi-square difference = 13.98
p-value = 0.0298603746

```

The chi-square difference is 13.98, with $df = 6$ and $p = 0.02986$. If α -level is set at 0.05, the bifactor model indicates a significantly better fit. But if α -level is set at 0.01, statistically the two models fit equally well to the data.

In the next section, it is demonstrated that the second-order factor model is indeed nested within the bifactor model, and hence the chi-square test conducted in the previous section is justified. In addition, through the demonstration of the nested relationship between the two classes of models, you can see how some parameter constraints in structural equation model can be set up in PROC CALIS.

For some practical researchers, the technical details involved in the next section might not be of interest and therefore could be skipped.

A Constrained Bifactor Model and Its Equivalence to the Second-Order Factor Model

To demonstrate that the second-order factor model is indeed nested within the bifactor model, a constrained bifactor model is fitted in this section. This constrained bifactor model is essentially the same as the preceding bifactor model, but with additional constraints on the factor loadings. Hence, the constrained bifactor model is nested within the unconstrained bifactor model.

Furthermore, if it can be shown that the constrained bifactor model is equivalent to the previous second-order factor, then the second-order factor model must also be nested within the unconstrained bifactor model. As a result, it justifies the chi-square difference test conducted in the previous section.

The construction of such a constrained bifactor model is based on Yung, Thissen, and McLeod (1999). In the following statements, a constrained bifactor model is specified.

```

proc calis corr data=Thurst method=max nobs=213 nose nostand;
  lineqs
    V1 = X11 * Factor1                      + X1g * FactorG + E1,
    V2 = X21 * Factor1                      + X2g * FactorG + E2,
    V3 = X31 * Factor1                      + X3g * FactorG + E3,
    V4 =                X42 * Factor2        + X4g * FactorG + E4,
    V5 =                X52 * Factor2        + X5g * FactorG + E5,
    V6 =                X62 * Factor2        + X6g * FactorG + E6,
    V7 =                X73 * Factor3        + X7g * FactorG + E7,
    V8 =                X83 * Factor3        + X8g * FactorG + E8,
    V9 =                X93 * Factor3        + X9g * FactorG + E9;
  variance
    Factor1-Factor3 = 3 * 1.,
    FactorG          = 1. ,
    E1-E9           = U1-U9;
  cov
    Factor1-Factor3 FactorG = 6 * 0.;
  bounds
    0. <= U1-U9;
  fitindex ON(ONLY)=[chisq df probchi];
  parameters p1 (.5) p2 (.5) p3 (.5);
  /* Proportionality constraints */
  X1g = p1 * X11;
  X2g = p1 * X21;
  X3g = p1 * X31;
  X4g = p2 * X42;
  X5g = p2 * X52;
  X6g = p2 * X62;
  X7g = p3 * X73;
  X8g = p3 * X83;
  X9g = p3 * X93;
run;

```

In this constrained model, you add a **PARAMETERS** statement and nine **SAS programming statements** to the previous bifactor model. In the **PARAMETERS** statement, three new independent parameters are added: p_1 , p_2 , and p_3 . These parameters represent the proportions that constrain the factor loadings of the observed variables on the group factors Factor1–Factor3 and the general factor FactorG. They are all free parameters and have initial values at 0.5. The next nine **SAS programming statements** represent the proportionality constraints imposed. For example, X_{1g} – X_{3g} are now dependent parameters expressed as functions of p_1 , X_{11} , X_{21} , and X_{31} . Adding three new parameters (in the **PARAMETERS** statement) and redefining nine original parameters as dependent (in the **SAS programming statements**) is equivalent to adding six (=9–3) constraints to the original bifactor model. Mathematically, the additional statements in specifying the constrained bifactor model realizes the following six constraints:

$$\frac{X_{1g}}{X_{11}} = \frac{X_{2g}}{X_{21}} = \frac{X_{3g}}{X_{31}}$$

$$\frac{X_{4g}}{X_{42}} = \frac{X_{5g}}{X_{52}} = \frac{X_{6g}}{X_{62}}$$

$$\frac{X_{7g}}{X_{73}} = \frac{X_{8g}}{X_{83}} = \frac{X_{9g}}{X_{93}}$$

Obviously, with these six constraints the current constrained bifactor model is nested within the unconstrained version. What remains to be shown is that this constrained bifactor model is indeed equivalent to the previous second-order factor model. If so, the second-order factor model is also nested within the unconstrained bifactor model. One evidence for the equivalence of the current constrained bifactor model and the second-order factor model is from the fit summary table shown in [Output 27.26.10](#). But first, it is also useful to consider the optimization information of the constrained bifactor model, which is shown in [Output 27.26.9](#).

Output 27.26.9 Optimization

Optimization Start									
Active Constraints			0	Objective Function			6.8290849536		
Max Abs Gradient Element			8.9903038299	Radius			46.912034073		
Iter	Rest arts	Func Calls	Act Con	Objective Function	Obj Fun Change	Max Abs Gradient Element	Lambda	Actual Over Pred Change	
1*	0	4	0	4.42090	2.4082	1.5979	0.195	0.121	
2*	0	6	0	2.42951	1.9914	2.4449	0.195	1.700	
3*	0	8	0	1.52546	0.9040	2.1675	0.781	1.657	
4*	0	10	0	0.86547	0.6600	1.2570	0.781	1.552	
5*	0	12	0	0.50425	0.3612	0.4075	0.781	1.351	
6*	0	14	0	0.41864	0.0856	1.1698	0.195	0.216	
7*	0	16	0	0.28298	0.1357	0.2355	0.0488	0.983	
8	0	19	0	0.27010	0.0129	0.9602	0.00098	0.327	
9	0	21	0	0.21798	0.0521	0.2433	0	0.751	
10*	0	23	0	0.20781	0.0102	0.0373	0.0488	0.943	
11*	0	26	0	0.20251	0.00530	0.0273	0.0918	1.064	
12	0	28	0	0.19176	0.0108	0.0718	0.0515	1.008	
13	0	30	0	0.18575	0.00601	0.1407	0.00393	0.562	
14	0	32	0	0.18024	0.00551	0.0224	0	0.921	
15	0	34	0	0.18017	0.000064	0.00161	0	1.067	
16	0	36	0	0.18017	2.357E-6	0.000538	0	1.344	
17	0	38	0	0.18017	3.389E-7	0.000216	0	1.380	
18	0	40	0	0.18017	5.146E-8	0.000075	0	1.389	
19	0	42	0	0.18017	7.886E-9	0.000031	0	1.391	
20	0	44	0	0.18017	1.211E-9	0.000012	0	1.392	

Optimization Results									
Iterations	20			Function Calls	47				
Jacobian Calls	22			Active Constraints	0				
Objective Function	0.1801712147			Max Abs Gradient Element	0.0000117927				
Lambda	0			Actual Over Pred Change	1.3915929449				
Radius	0.0002502182								

Convergence criterion (GCONV=1E-8) satisfied.

As shown [Output 27.26.9](#), there are 21 independent parameters in the constrained bifactor model for the 45 “Functions (Observations).” These numbers match those of the second-order factor model exactly. The optimization shows some problems in initial iterations. The iteration numbers with asterisks indicate that the Hessian matrix is not positive definite in those iterations. But as long as the final converged iteration is not marked with an asterisk, the problems exhibited in early iterations do not raise any concern, as in the current case. Next, the fit summary is shown in [Output 27.26.10](#).

Output 27.26.10 Model Fit

Fit Summary	
Chi-Square	38.1963
Chi-Square DF	24
Pr > Chi-Square	0.0331

In [Output 27.26.10](#), the chi-square value in the fit summary table is 38.196, with $df = 24$, and $p = 0.033$. Again, these numbers match those of the second-order factor model exactly. These matches (same model fit with the same number of parameters) are necessary (but not sufficient) to show that the constrained bifactor model is equivalent to the second-order model. Stronger evidence is now presented.

In [Output 27.26.11](#), estimation results of the constrained bifactor model are shown.

Output 27.26.11 Estimation Results

Linear Equations			
V1 =	-0.5151*Factor1 +	0.7437*FactorG +	1.0000 E1
	X11	X1g	
V2 =	-0.5203*Factor1 +	0.7512*FactorG +	1.0000 E2
	X21	X2g	
V3 =	-0.4874*Factor1 +	0.7038*FactorG +	1.0000 E3
	X31	X3g	
V4 =	0.5211*Factor2 +	0.6534*FactorG +	1.0000 E4
	X42	X4g	
V5 =	0.4971*Factor2 +	0.6232*FactorG +	1.0000 E5
	X52	X5g	
V6 =	0.4381*Factor2 +	0.5493*FactorG +	1.0000 E6
	X62	X6g	
V7 =	0.4524*Factor3 +	0.6364*FactorG +	1.0000 E7
	X73	X7g	
V8 =	0.4173*Factor3 +	0.5869*FactorG +	1.0000 E8
	X83	X8g	
V9 =	0.4076*Factor3 +	0.5734*FactorG +	1.0000 E9
	X93	X9g	

Output 27.26.11 *continued*

Estimates for Variances of Exogenous Variables			
Variable Type	Variable	Parameter	Estimate
Latent	Factor1		1.00000
	Factor2		1.00000
	Factor3		1.00000
	FactorG		1.00000
Error	E1	U1	0.18150
	E2	U2	0.16493
	E3	U3	0.26713
	E4	U4	0.30150
	E5	U5	0.36450
	E6	U6	0.50641
	E7	U7	0.39034
	E8	U8	0.48136
	E9	U9	0.50511

According to Yung, Thissen, and McLeod (1999), two models are equivalent if there is a one-to-one correspondence of the parameters in the models. This fact is illustrated for the constrained bifactor model and the second-order factor model.

First, the error variances for E1–E9 in the second-order factor model are transformed directly (using an identity map) to that of the bifactor models. The nine error variances in [Output 27.26.4](#) for the second-order factor model match those of the constrained bifactor model exactly in [Output 27.26.11](#). In addition, the variances of factors are fixed at one in both models. The error variances and the factor loadings at both factor levels in [Output 27.26.4](#) for the second-order factor model are now transformed to yield the loading estimates in the constrained bifactor model.

Denote \mathbf{P}_1 as the first-order factor loading matrix, \mathbf{P}_2 as the second-order factor loading matrix, and \mathbf{U}_1^2 be the matrix of variances for disturbances. That is, for the second-order factor model,

$$\mathbf{P}_1 = \begin{pmatrix} 0.9047 & 0 & 0 \\ 0.9138 & 0 & 0 \\ 0.8561 & 0 & 0 \\ 0 & 0.8358 & 0 \\ 0 & 0.7972 & 0 \\ 0 & 0.7026 & 0 \\ 0 & 0 & 0.7808 \\ 0 & 0 & 0.7202 \\ 0 & 0 & 0.7035 \end{pmatrix}$$

$$\mathbf{P}_2 = \begin{pmatrix} 0.8221 \\ 0.7818 \\ 0.8150 \end{pmatrix}$$

$$\mathbf{U}_1^2 = \begin{pmatrix} 0.3242 & 0 & 0 \\ 0 & 0.3888 & 0 \\ 0 & 0 & 0.3358 \end{pmatrix}$$

According to Yung, Thissen, and McLeod (1999), the transformation to obtain the estimates in the equivalent constrained bifactor model is:

$$\begin{aligned} \mathbf{L}_1 &= \mathbf{P}_1 \mathbf{U}_1 \\ \mathbf{L}_2 &= \mathbf{P}_1 \mathbf{P}_2 \end{aligned}$$

where \mathbf{L}_1 is the matrix of the first-layer factor loadings (that is, loadings on group factors Factor1–Factor3), and \mathbf{L}_2 is the matrix of the second-layer factor loadings (that is, loadings on FactorG) in the constrained bifactor model. Carrying out the matrix calculations for \mathbf{L}_1 and \mathbf{L}_2 shows that:

$$\mathbf{L}_1 = \begin{pmatrix} 0.5151 & 0 & 0 \\ 0.5203 & 0 & 0 \\ 0.4875 & 0 & 0 \\ 0 & 0.5212 & 0 \\ 0 & 0.4971 & 0 \\ 0 & 0.4381 & 0 \\ 0 & 0 & 0.4525 \\ 0 & 0 & 0.4173 \\ 0 & 0 & 0.4077 \end{pmatrix}$$

$$\mathbf{L}_2 = \begin{pmatrix} 0.7438 \\ 0.7512 \\ 0.7038 \\ 0.6534 \\ 0.6232 \\ 0.5493 \\ 0.6364 \\ 0.5870 \\ 0.5734 \end{pmatrix}$$

With very minor numerical differences and ignorable sign changes, these transformation results match the estimated loadings observed in [Output 27.26.11](#) for the constrained bifactor model. Therefore, the second-order factor model is shown to be equivalent to the constrained bifactor model, and hence is nested within the unconstrained bifactor model.

Example 27.27: Linear Relations among Factor Loadings

In this example, you use the FACTOR modeling language of PROC CALIS to specify a confirmatory factor analysis model with linear constraints on loadings. You use [SAS programming statements](#) to set the constraints. This example also discusses the differences between fitting covariance structures and correlation structures in the current modeling context.

The correlation matrix of six variables from Kinzer and Kinzer (N=326) is used by Guttman (1957) as an example that yields an approximate simplex. McDonald (1980) uses this data set as an example of factor analysis where he assumes that the loadings on the second factor are linear functions of the loadings on the first factor. Let \mathbf{B} be the factor loading matrix containing the two factors and six variables so that:

$$\mathbf{B} = \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \\ b_{31} & b_{32} \\ b_{41} & b_{42} \\ b_{51} & b_{52} \\ b_{61} & b_{62} \end{pmatrix}$$

and

$$b_{j2} = \alpha + \beta b_{j1}, \quad j = 1, \dots, 6$$

The correlation structures are represented by:

$$\mathbf{P} = \mathbf{B}\mathbf{B}' + \mathbf{\Psi}$$

where $\mathbf{\Psi} = \text{diag}(\psi_{11}, \psi_{22}, \psi_{33}, \psi_{44}, \psi_{55}, \psi_{66})$ represents the diagonal matrix of unique variances for the variables.

With parameters α and β being unconstrained, McDonald (1980) has fitted an underidentified model with seven degrees of freedom. Browne (1982) imposes the following identification condition:

$$\beta = -1$$

In this example, Browne's identification condition is imposed. The following is the specification of the confirmatory factor model using the FACTOR modeling language.

```
data kinzer(type=corr);
title "Data Matrix of Kinzer & Kinzer, see GUTTMAN (1957)";
  _type_ = 'corr';
  input _name_ $ var1-var6;
  datalines;
var1  1.00  .    .    .    .    .
var2  .51  1.00  .    .    .    .
var3  .46  .51  1.00  .    .    .
var4  .46  .47  .54  1.00  .    .
var5  .40  .39  .49  .57  1.00  .
var6  .33  .39  .47  .45  .56  1.00
;
;
```



```

proc calis data=kinzer nobs=326 nose;
  factor
    factor1 ==> var1-var6   = b11 b21 b31 b41 b51 b61 (6 *.6),
    factor2 ==> var1-var6   = b12 b22 b32 b42 b52 b62;
  pvar
    factor1-factor2 = 2 * 1.,
    var1-var6       = psil-psi6 (6 *.3);
  cov
    factor1 factor2 = 0.;
  parameters alpha (1.);
  /* SAS Programming Statements to define dependent parameters */
  b12 = alpha - b11;
  b22 = alpha - b21;
  b32 = alpha - b31;
  b42 = alpha - b41;
  b52 = alpha - b51;
  b62 = alpha - b61;
  fitindex on(only)=[chisq df probchi];
run;

```

In the **FACTOR** statement, you specify two factors, named `factor1` and `factor2`, for the variables. In this model, all manifest variables have nonzero loadings on the two factors. These loading parameters are specified after the equal signs and are named with the prefix 'b.' You specify the initial estimates in the parentheses for the parameters in the first entry of the **FACTOR** statement. The loadings in the first entry are all free parameters with initial estimates of .6. In the second entry of the **FACTOR** statement, you specify the Loadings of `var1–var6` on `factor2`. However, these parameters are dependent, as shown in the [SAS programming statements](#). Initial values for these dependent parameters are thus unnecessary.

In the **PVAR** statement, the factor variances are fixed at ones, while the error variances of the variables are free parameters named `psi1–psi6`. Again, you provide initial estimates for these error variance parameters. All have the initial value of 0.3.

An additional parameter `alpha` is specified in the **PARAMETERS** statement with an initial value of 1. Then, you use six [SAS programming statements](#) to define the loadings on the second factor as functions of the loadings on the first factor. Lastly, the **FITINDEX** statement is used to trim the results in the fit summary table.

In the specification, there are twelve loadings in the **FACTOR** statement and six error variances in the **PVAR** statement. Adding the parameter `alpha` in the list, there are 19 parameters in total. However, the loading parameters are not all independent of each other. As defined in the [SAS programming statements](#), six loadings are dependent. This reduces the number of free parameters to 13. Hence the degrees of freedom for the model is $8 = 21 - 13$. Notice that the factor variances are fixed at 1, as specified in the **PVAR** statement, and covariance among the two factors is fixed at zero, as specified in the **COV** statement.

[Output 27.27.1](#) shows a concise fit summary table. The chi-square test statistic of model fit is 10.337 with $df = 8$ ($p = 0.242$). This indicates a good model fit.

Output 27.27.1 Fit of the Correlation Structures

Fit Summary		
Chi-Square		10.3374
Chi-Square DF		8
Pr > Chi-Square		0.2421

The estimated factor loading matrix is presented in [Output 27.27.2](#), and the estimated error variances and the estimate for alpha are presented in [Output 27.27.3](#).

Output 27.27.2 Loading Estimates

Factor Loading Matrix		
	factor1	factor2
var1	0.3609 [b11]	0.6174 [b12]
var2	0.3212 [b21]	0.6571 [b22]
var3	0.4859 [b31]	0.4923 [b32]
var4	0.5745 [b41]	0.4038 [b42]
var5	0.7985 [b51]	0.1797 [b52]
var6	0.6736 [b61]	0.3046 [b62]

Output 27.27.3 Unique Variances and the Additional Parameter

Error Variances		
Variable	Parameter	Estimate
var1	psi1	0.53036
var2	psi2	0.44986
var3	psi3	0.48756
var4	psi4	0.47278
var5	psi5	0.31125
var6	psi6	0.53815

Output 27.27.3 *continued*

Additional Parameters		
Type	Parameter	Estimate
Independent	alpha	0.97825

All these estimates are essentially the same as those reported in Browne (1982). Notice that there are no standard error estimates in the output, as requested by the **NOSE** option in the PROC CALIS statement. Standard error estimates are not of interest in this example.

In fitting the preceding factor model, wrong covariance structures rather than the intended correlation structures have been specified. As pointed out by Browne (1982), fitting such covariance structures directly is not entirely appropriate for analyzing correlations. For example, when fitting the correlation structures, the diagonal elements of **P** must always be fixed ones. This fact has never been enforced in the preceding specification. A simple check of the estimates will illustrate the problem. In **Output 27.27.2**, the loading estimates of VAR1 on the two factors are 0.3609 and 0.6174, respectively. In **Output 27.27.3**, the error variance estimate for VAR1 is 0.53036. The fitted variance of VAR1 can therefore be computed by the following equation:

$$\text{fitted variance} = 0.3609^2 + 0.6174^2 + 0.53036 = 1.0418$$

This fitted value is quite a bit off from 1.00, as required for the standardized variance of VAR1.

Fortunately, even though the wrong covariance structure model has been analyzed, the preceding analysis is not completely useless. For the current confirmatory factor model, according to Browne (1982) the estimates obtained from fitting the wrong covariance structure model are still consistent (as if they were estimating the population parameters in the correlation structures). However, the chi-square test statistic as reported previously is not correct.

Note that using the **CORR** option in the PROC CALIS statement will not solve the problem. By specifying the **CORR** option you merely request PROC CALIS to use the correlation matrix directly as a covariance matrix in the objective function for model fitting. It still would not constrain the fitting of the diagonal elements to 1 during estimation.

In the next section, a solution to the correlation analysis problem is suggested. It is not claimed that this is the only solution or the best solution. Alternative treatments of the problem are possible.

Fitting the Correct Correlation Structures

This main idea of this solution is to embed the intended correlation structures (with correct constraints on the diagonal elements of the correlation matrix) into a covariance structure model so that the estimation methods of PROC CALIS can be applied legitimately to the specially constructed covariance structures.

First, the issue of the fixed ones on the diagonal of the correlation structure model is addressed. That is, the diagonal elements of the correlation structures represented by $(\mathbf{B}\mathbf{B}' + \mathbf{\Psi})$ must be fitted by ones. This can be accomplished by constraining the error variances as dependent parameters of the loadings, as shown in the following:

$$\Psi_{jj} = 1. - b_{j1}^2 - b_{j2}^2, \quad j = 1, \dots, 6$$

Other constraints might also serve the purpose, but the proposed constraints here are the most convenient and intuitive.

Now, due to the fact that discrepancy functions used in PROC CALIS are derived for covariance matrices rather than correlation matrices, PROC CALIS is essentially set up for analyzing covariance structures (with or without mean structures), but not correlation structures. Hence, the statistical theory behind PROC CALIS applies to covariance structure analysis, but it might not generalize to correlation structure analysis in all situations. Despite that, with some manipulations PROC CALIS can fit the correct correlation structures to the current data without compromising the statistical theory. These manipulations are now discussed. Recall that the correlation structures are represented by:

$$\mathbf{P} = \mathbf{B}\mathbf{B}' + \mathbf{\Psi}$$

As before, in the \mathbf{B} matrix, there are six linear constraints on the factor loadings. In addition, the diagonal elements of $(\mathbf{B}\mathbf{B}' + \mathbf{\Psi})$ are constrained to ones, as done by defining the error variances as dependent parameters of the loadings in the preceding equation. To analyze the correlation structures by using PROC CALIS, a covariance structure model with such correlation structures embedded is now specified. That is, the covariance structure to be fitted by PROC CALIS is as follows:

$$\mathbf{\Sigma} = \mathbf{D}\mathbf{P}\mathbf{D}' = \mathbf{D}(\mathbf{B}\mathbf{B}' + \mathbf{\Psi})\mathbf{D}'$$

where \mathbf{D} is a 6 x 6 diagonal matrix containing the population standard deviations for the manifest variables. Theoretically, it is legitimate that you analyze this covariance structure model for studying the embedded correlation structures. In addition, it does not matter whether your input matrix is a correlation or covariance matrix, or any rescaled covariance matrix (by multiplying any variables by any positive constants). You would get correct results if you could somehow specify these covariance structures correctly in PROC CALIS. However, there seems to be nowhere in PROC CALIS that you can specify the diagonal matrix \mathbf{D} for the population standard deviations. So what can one do with this formulation? The answer is to rewrite the covariance structure model in a form similar to the usual confirmatory factor model, as presented in the following.

Let $\mathbf{T} = \mathbf{D}\mathbf{B}$ and $\mathbf{K} = \mathbf{D}\mathbf{\Psi}\mathbf{D}'$. The covariance structure model of interest can now be rewritten as:

$$\mathbf{\Sigma} = \mathbf{T}\mathbf{T}' + \mathbf{K}$$

This form of covariance structures implies a confirmatory factor model with factor loading matrix \mathbf{T} and error covariance matrix \mathbf{K} . This confirmatory factor model can certainly be specified using the FACTOR modeling language, in much the same way you specify a confirmatory factor model in the preceding section. However, because you are actually more interested in estimating the basic set of parameters in matrices \mathbf{B} and $\mathbf{\Psi}$ of the embedded correlation structures, you would define the model parameters as functions of this basic set of parameters of interest. This can be accomplished by using the [PARAMETERS](#) and the [SAS programming statements](#).

All in all, you can use the following statements to set up such a confirmatory factor model with the desired correlation structures embedded.

```

proc calis data=Kinzer nobs=326 nose;
  factor
    factor1 ==> var1-var6   = t11 t21 t31 t41 t51 t61,
    factor2 ==> var1-var6   = t12 t22 t32 t42 t52 t62;
  pvar
    factor1-factor2 = 2 * 1.,
    var1-var6       = k1-k6;
  cov
    factor1 factor2 = 0.;
  parameters alpha (1.) d1-d6 (6 * 1.)
    b11 b21 b31 b41 b51 b61 (6 *.6),
    b12 b22 b32 b42 b52 b62
    psi1-psi6;
  /* SAS Programming Statements */
  /* 12 Constraints on Correlation structures */
  b12 = alpha - b11;
  b22 = alpha - b21;
  b32 = alpha - b31;
  b42 = alpha - b41;
  b52 = alpha - b51;
  b62 = alpha - b61;
  psi1 = 1. - b11 * b11 - b12 * b12;
  psi2 = 1. - b21 * b21 - b22 * b22;
  psi3 = 1. - b31 * b31 - b32 * b32;
  psi4 = 1. - b41 * b41 - b42 * b42;
  psi5 = 1. - b51 * b51 - b52 * b52;
  psi6 = 1. - b61 * b61 - b62 * b62;
  /* Defining Covariance Structure Parameters */
  t11 = d1 * b11;
  t21 = d2 * b21;
  t31 = d3 * b31;
  t41 = d4 * b41;
  t51 = d5 * b51;
  t61 = d6 * b61;
  t12 = d1 * b12;
  t22 = d2 * b22;
  t32 = d3 * b32;
  t42 = d4 * b42;
  t52 = d5 * b52;
  t62 = d6 * b62;
  k1 = d1 * d1 * psi1;
  k2 = d2 * d2 * psi2;
  k3 = d3 * d3 * psi3;
  k4 = d4 * d4 * psi4;
  k5 = d5 * d5 * psi5;
  k6 = d6 * d6 * psi6;
  fitindex on(only)=[chisq df probchi];
run;

```

First, you notice that specifications in the **FACTOR** and the **PVAR** statements are essentially unchanged from the previous specification, except that the parameters are named differently here to reflect different model matrices. In the current specification, the factor loading parameters in matrix **T** are named with prefix 't,' and the error variance parameters in matrix **K** are named with prefix 'k.' Specification of these parameters reflects the covariance structures. As you see in the last block of the **SAS programming statements**, all these parameters are functions of the correlation structure parameters in **B**, Ψ , and **D**.

Next, in the **PARAMETERS** statement, all correlation structure parameters are defined with initial values provided. These are the parameters of interest: α is used to define dependencies among loadings, d 's are the population standard deviations, b 's are the loading parameters, and ψ 's are the error variance parameters. There are 25 parameters specified in this statement, but not all of them are free or independent.

In the first block of **SAS programming statements**, parameter dependencies or constraints on the correlation structures are specified. The first six statements realize the required linear relations among the factor loadings:

$$b_{j2} = \alpha - b_{j1}, \quad j = 1, \dots, 6$$

The next six statements constrain the error variances so as to ensure that an embedded correlation structure model is being fitted. That is, each error variance is dependent on the corresponding loadings, as prescribed by the following equation:

$$\Psi_{jj} = 1. - b_{j1}^2 - b_{j2}^2, \quad j = 1, \dots, 6$$

These twelve constraints reduce the number of independent parameters to 13, as expected.

The next block of **SAS programming statements** are essentially for relating the correlation structure parameters to the covariance structures that are specified in the **FACTOR** and the **PVAR** statements. These **SAS programming statements** realize the required relations: $\mathbf{T} = \mathbf{DB}$ and $\mathbf{K} = \mathbf{D}\Psi\mathbf{D}'$, but in non-matrix forms:

$$t_{ji} = d_j b_{ji} \quad (j = 1, \dots, 6; \quad i = 1, 2)$$

$$k_{jj} = d_j d_j \Psi_{jj} \quad (j = 1, \dots, 6)$$

where d_j denotes the j th diagonal element of **D**.

The fit summary is presented in **Output 27.27.4**. The chi-square test statistic is 14.63 with $df = 8$ ($p = 0.067$). This shows that the previous chi-square test based on fitting a wrong covariance structure model is indeed questionable.

Output 27.27.4 Model Fit of the Correlation Structures

Fit Summary	
Chi-Square	14.6269
Chi-Square DF	8
Pr > Chi-Square	0.0668

Estimates of the loadings and error variances are presented in [Output 27.27.5](#). These estimates are for the covariance structure model with loading matrix **T** and error covariance matrix **K**. They are rescaled versions of the correlation structure parameters and are not of primary interest themselves.

Output 27.27.5 Estimates of Loadings and Error Variances

Factor Loading Matrix		
	factor1	factor2
var1	0.3448 [t11]	0.6367 [t12]
var2	0.3200 [t21]	0.6512 [t22]
var3	0.4873 [t31]	0.4778 [t32]
var4	0.5703 [t41]	0.3948 [t42]
var5	0.7741 [t51]	0.1964 [t52]
var6	0.6778 [t61]	0.3126 [t62]
Factor Covariance Matrix		
	factor1	factor2
factor1	1.0000	0
factor2	0	1.0000
Error Variances		
Variable	Parameter	Estimate
var1	k1	0.49119
var2	k2	0.46780
var3	k3	0.51597
var4	k4	0.50070
var5	k5	0.35505
var6	k6	0.47685

The parameter estimates of the embedded correlation structures are shown in [Output 27.27.6](#) as “additional” parameters.

Output 27.27.6 Estimates of Correlation Structure Parameters

Additional Parameters		
Type	Parameter	Estimate
Independent	alpha	0.97400
	d1	1.00771
	d2	0.99712
	d3	0.99078
	d4	0.99085
	d5	0.99640
	d6	1.01687
	b11	0.34217
	b21	0.32095
	b31	0.49179
	b41	0.57553
	b51	0.77686
	b61	0.66659
	Dependent	b12
b22		0.65305
b32		0.48222
b42		0.39848
b52		0.19714
b62		0.30742
psi1		0.48371
psi2		0.47051
psi3		0.52561
psi4		0.50998
psi5		0.35762
psi6		0.46116

Except for the population standard deviation parameter d’s, all other parameters estimated in the current model can be compared with those from the previous fitting of an incorrect covariance structure model. Although estimates in the current model do not differ very much from those in the previous specification, it is at least reassuring that they are obtained from fitting a correctly specified covariance structure model with the intended correlation structures embedded.

Example 27.28: Multiple-Group Model for Purchasing Behavior

In this example, data were collected from customers who made purchases from a retail company during years 2002 and 2003. A two-group structural equation model is fitted to the data.

The variables are:

Spend02:	total purchase amount in 2002
Spend03:	total purchase amount in 2003
Courtesy:	rating of the courtesy of the customer service
Responsive:	rating of the responsiveness of the customer service
Helpful:	rating of the helpfulness of the customer service
Delivery:	rating of the timeliness of the delivery
Pricing:	rating of the product pricing
Availability:	rating of the product availability
Quality:	rating of the product quality

For the ratings scales, nine-point scales were used. Customers could respond 1 to 9 on these scales, with 1 representing “extremely unsatisfied” and 9 representing “extremely satisfied.” Data were collected from two different regions, which are labeled as Region 1 ($N = 378$) and Region 2 ($N = 423$), respectively. The ratings were collected at the end of year 2002 so that they represent customers’ purchasing experience in year 2002.

The central questions of the study are:

- How does the overall customer service affect the current purchases and predict future purchases?
- How does the overall product quality affect the current purchases and predict future purchases?
- Do current purchases predict future purchases?
- Do the two regions have different structural models for predicting the purchases?

In stating these research questions, you use several constructs that might or might not correspond to objective measurements. Current and future purchases are certainly measurable directly by the spending of the customers. That is, because customer service and product satisfaction and quality were surveyed between 2002 and 2003, Spend02 represents current purchases and Spend03 represents future purchases in the study. Both variables Spend02 and Spend03 are objective measurements without measurement errors. All you need to do is to extract the information from the transaction records. But how about hypothetical constructs such as customer service quality and product quality? How would you measure them in the model?

In measuring these hypothetical constructs, you might ask customers' perception about the service or product quality directly in a single question. A simple survey with two questions about the customer service and product qualities could then be what you need. These questions are called indicators (or indicator variables) of the underlying constructs. However, using just one indicator (question) for each of these hypothetical constructs would be quite unreliable—that is, measurement errors might dominate in the data collection process. Therefore, multiple indicators are usually recommended for measuring such hypothetical constructs.

There are two main advantages of using multiple indicators for hypothetical constructs. The first one is conceptual and the other is statistical and mathematical.

First, hypothetical constructs might conceptually be multifaceted themselves. Measuring a hypothetical construct by a single indicator does not capture the full meaning of the construct. For example, the product quality might refer to the durability of the product, the outlook of the product, the pricing of the product, and the availability of product, among others. The customer service quality might refer to the politeness of the customer service, the timeliness of the delivery, and the responsiveness of customer services, among others. Therefore, multiple indicators for a single hypothetical construct might be necessary if you want to cover the multifaceted aspects of a given hypothetical construct.

Second, from a statistical point of view, the reliability would be higher if you combine correlated indicators for a construct than if you use a single indicator only. Therefore, combining correlated indicators would lead to more accurate and reliable results.

One way to combine correlated indicators is to use a simple sum of them to represent the underlying hypothetical construct. However, a better way is to use the structural equation modeling technique that represents each indicator (variable) as a function of the underlying hypothetical construct plus an error term. In structural equation modeling, hypothetical constructs are constructed as latent factors, which are unobserved systematic (that is, non-error) variables. Theoretically, latent factors are free from measurement errors, and so the estimation through the structural equation modeling technique is more accurate than if you just use simple sums of indicators to represent hypothetical constructs. Therefore, a structural equation modeling approach is the method of the choice in the current analysis.

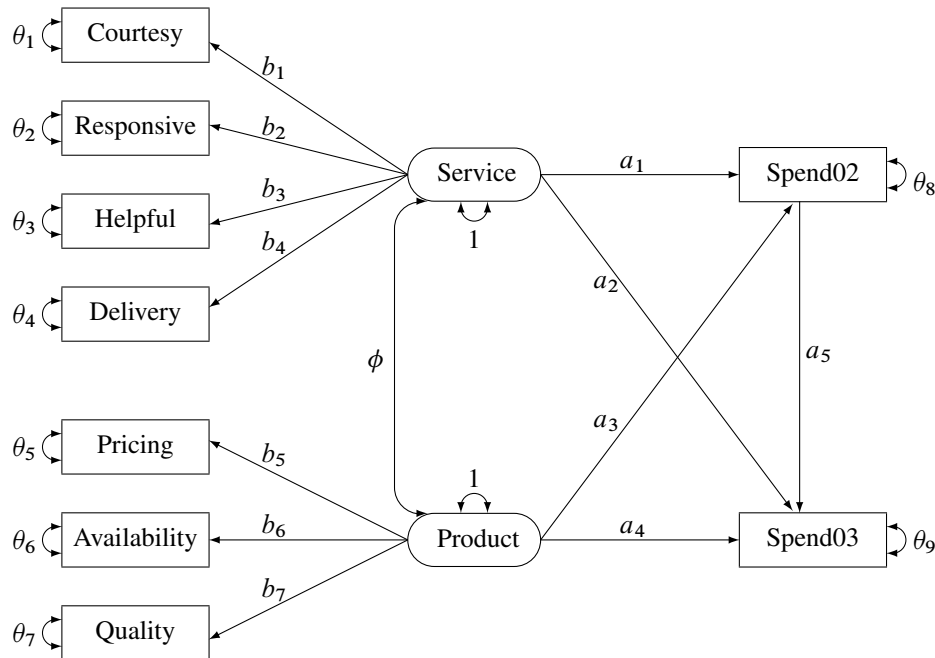
In practice, you must also make sure that there are enough indicators for the identification of the underlying latent factor, and hence the identification of the entire model. Necessary and sufficient rules for identification are very complicated to describe and are out of the scope of the current discussion (however, see Bollen 1989b for discussions of identification rules for various classes of structural equation models). Some simple rules of thumb might be useful as a guidance. For example, for unconstrained situations, you should at least have three indicators (variables) measured for a latent factor. Unfortunately, these rules of thumb do not guarantee identification in every case.

In this example, Service and Product are latent factors in the structural equation model which represent service and product qualities, respectively. In the model, these two latent factors are reflected by the ratings of the customers. Ratings on the Courtesy, Responsive, Helpful, and Delivery scales are indicators of Service. Ratings on the Pricing, Availability, and Quality scales are indicators of Product (that is, product quality).

A Path Diagram

A path diagram shown in Figure 27.7 represents the structural equation model for the purchase behavior. Observed or manifest variables are represented by rectangles, and latent variables are represented by ovals. As mentioned, two latent variables (factors), Service and Product, are created as overall measures of customer service and product qualities, respectively.

Figure 27.7 Path Diagram of Purchasing Behavior



The left part of the diagram represents the measurement model of the latent variables. The Service factor has four indicators: Courtesy, Responsive, Helpful, and Delivery. The path coefficients to these observed variables from the Service factor are b_1 , b_2 , b_3 , and b_4 , respectively. Similarly, the Product variable has three indicators: Pricing, Availability, and Quality, with path coefficients b_5 , b_6 , and b_7 , respectively.

The two latent factors are predictors of the purchase amounts Spend02 and Spend03. In addition, Spend02 also serves as a predictor of Spend03. Path coefficients (effects) for this part of functional relationships are represented by a_1 – a_5 in the diagram.

Each variable in the path diagram has a variance parameter. For endogenous or dependent variables, which serve as outcome variables in the model, the variance parameters are the error variances that are not accounted for by the predictors. For example, in the current model all observed variables are endogenous variables. The double-headed arrows that are attached to these variables represent error variances. In the diagram, θ_1 to θ_9 are the names of these error variance parameters. For exogenous or independent variables, which never serve as outcome variables in the model, the variance parameters are the (total) variances of these variables. For example, in the diagram the double-headed arrows that are attached to Service and Product represent the variances of these two latent variables. In the current model, both of these variances are fixed at one.

When the double-headed arrows point to two variables, they represent covariances in the path diagram. For example, in [Figure 27.7](#) the covariance between Service and Product is represented by the parameter ϕ .

The Basic Path Model Specification

For the moment, it is hypothesized that both ‘Region 1’ and ‘Region 2’ data are fitted by the same model as shown in [Figure 27.7](#). Once the path diagram is drawn, it is readily translated into the PATH modeling language. See the [PATH statement](#) on page 1202 for details about how to use the PATH modeling language to specify structural equation models.

To represent all the features in the path diagram in the PATH model language, you can use the following specification:

```

path
  Service ==> Spend02      = a1,
  Service ==> Spend03      = a1,
  Product ==> Spend02      = a3,
  Product ==> Spend03      = a4,
  Spend02 ==> Spend03      = a5,
  Service ==> Courtesy     = b1,
  Service ==> Responsive   = b2,
  Service ==> Helpful      = b3,
  Service ==> Delivery     = b4,
  Product ==> Pricing      = b5,
  Product ==> Availability = b6,
  Product ==> Quality      = b7;

pvar
  Courtesy Responsive Helpful
  Delivery Pricing
  Availability Quality = theta01-theta07,
  Spend02 = theta08,
  Spend03 = theta09,
  Service Product = 2 * 1.;

pcov
  Service Product = phi;

```

The [PATH](#) statement captures all the path coefficient specifications and the direction of the paths (single-headed arrows) in the path diagram. The first five paths define how Spend02 and Spend03 are predicted from the latent variables Service, Product, and Spend02. The next seven paths define the measurement model, which shows how the latent variables in the model relate to the observed indicator variables.

The [PVAR](#) statement captures the specification of the error variances and the variances of exogenous variables (that is, the double-headed arrows in the path diagram). The [PCOV](#) statement captures the specification of covariance between the two latent variables in the model (which is represented by the double-headed arrow that connects Service and Product in the path diagram).

You can also use the following simpler version of the PATH model specification for the path diagram:

```

path
  Service ==> Spend02 Spend03      ,
  Product ==> Spend02 Spend03      ,
  Spend02 ==> Spend03              ,
  Service ==> Courtesy Responsive
                Helpful Delivery   ,
  Product ==> Pricing Availability
                Quality            ;

pvar
  Courtesy Responsive Helpful Delivery Pricing
  Availability Quality Spend02 Spend03,
  Service Product = 2 * 1.;

pcov
  Service Product;

```

There are two simplifications in this PATH model specification. First, you do not need to specify the parameter names if they are unconstrained in the model. For example, parameter `a1` in the model is unique to the path effect from `Service` to `Spend02`. You do not need to name this effect because it is not constrained to be the same as any other parameter in the model. Similar, all the path coefficients (effects), error variances, and covariances in the path diagram are not constrained. Therefore, you can omit all the corresponding parameter name specifications in the PATH model specification. The only exceptions are the variances of `Service` and `Product`. Both are fixed constants 1 in the path diagram, and so you must specify them explicitly in the PVAR statement.

Second, you use a condensed way to specify the paths. In the first three path entries of the PATH statement, you specify how `Spend02` and `Spend03` are predicted from the latent variables `Service`, `Product`, and `Spend02`. Notice that in each path entry, you can define more than one path (single-headed arrow relationship). For example, in the first path entry, you specify two paths: one is `Service==>Spend02` and the other is `Service==>Spend03`. In the last two path entries of the PATH statement, you define the relationships between the two latent constructs `Spend` and `Service` and their measured indicators. Each of these path entries specifies multiple paths (single-headed arrow relationships).

You use this simplified PATH specifications in the subsequent analysis.

A Restrictive Model with Invariant Mean and Covariance Structures

In this section, you fit a mean and covariance structure model to the data from two regions, as shows in the following DATA steps:

```

data region1(type=cov);
  input _type_ $6. _name_ $12. Spend02 Spend03 Courtesy Responsive
        Helpful Delivery Pricing Availability Quality;
  datalines;
COV  Spend02      14.428  2.206  0.439  0.520  0.459  0.498  0.635  0.642  0.769
COV  Spend03      2.206 14.178  0.540  0.665  0.560  0.622  0.535  0.588  0.715
COV  Courtesy     0.439  0.540  1.642  0.541  0.473  0.506  0.109  0.120  0.126
COV  Responsive   0.520  0.665  0.541  2.977  0.582  0.629  0.119  0.253  0.184
COV  Helpful      0.459  0.560  0.473  0.582  2.801  0.546  0.113  0.121  0.139
COV  Delivery     0.498  0.622  0.506  0.629  0.546  3.830  0.120  0.132  0.145
COV  Pricing      0.635  0.535  0.109  0.119  0.113  0.120  2.152  0.491  0.538
COV  Availability 0.642  0.588  0.120  0.253  0.121  0.132  0.491  2.372  0.589
COV  Quality      0.769  0.715  0.126  0.184  0.139  0.145  0.538  0.589  2.753
MEAN  .           183.500 301.921 4.312 4.724 3.921 4.357 6.144 4.994 5.971
;

data region2(type=cov);
  input _type_ $6. _name_ $12. Spend02 Spend03 Courtesy Responsive
        Helpful Delivery Pricing Availability Quality;
  datalines;
COV  Spend02      14.489  2.193  0.442  0.541  0.469  0.508  0.637  0.675  0.769
COV  Spend03      2.193 14.168  0.542  0.663  0.574  0.623  0.607  0.642  0.732
COV  Courtesy     0.442  0.542  3.282  0.883  0.477  0.120  0.248  0.283  0.387
COV  Responsive   0.541  0.663  0.883  2.717  0.477  0.601  0.421  0.104  0.105
COV  Helpful      0.469  0.574  0.477  0.477  2.018  0.507  0.187  0.162  0.205
COV  Delivery     0.508  0.623  0.120  0.601  0.507  2.999  0.179  0.334  0.099
COV  Pricing      0.637  0.607  0.248  0.421  0.187  0.179  2.512  0.477  0.423
COV  Availability 0.675  0.642  0.283  0.104  0.162  0.334  0.477  2.085  0.675
COV  Quality      0.769  0.732  0.387  0.105  0.205  0.099  0.423  0.675  2.698
MEAN  .           156.250 313.670 2.412 2.727 5.224 6.376 7.147 3.233 5.119
;

```

To include the analysis of the mean structures, you need to introduce the mean and intercept parameters in the model. Although various researchers propose some representation schemes that include the mean parameters in the path diagram, the mean parameters are not depicted in [Figure 27.7](#). The reason is that representing the mean and intercept parameters in the path diagram would usually obscure the “causal” paths, which are of primary interest. In addition, it is a simple matter to specify the mean and intercept parameters in the [MEAN](#) statement without the help of a path diagram when you follow these principles:

- Each variable in the path diagram has a mean parameter that can be specified in the [MEAN](#) statement. For an exogenous variable, the mean parameter refers to the variable mean. For an endogenous variable, the mean parameter refers to the intercept of the variable.
- The means of exogenous observed variables are free parameters by default. The means of exogenous latent variables are fixed zeros by default.

- The intercepts of endogenous observed variables are free parameters by default. The intercepts of endogenous latent variables are fixed zeros by default.
- The total number of mean parameters should not exceed the number of observed variables.

Because all nine observed variables are endogenous (each has at least one single-headed arrow pointing to it) in the path diagram, you can specify these nine intercepts in the MEAN statement, as shown in the following specification:

```
mean
  Courtesy Responsive Helpful Delivery Pricing
  Availability Quality Spend02 Spend03;
```

However, the intercepts of endogenous observed variables are already free parameters by default and this MEAN statement specification is not necessary for the current situation. For the means of the latent variables Service and Product, you do not have any theoretical reasons to set them other than the default fixed zero. Hence, you do not need to set these mean parameters explicitly either. Consequently, to include the analysis of the mean structures with these default mean parameters, all you need to specify the MEANSTR option in the PROC CALIS statement, as shown in the following specification of the fitting of a constrained two-group model for the purchase data:

```
proc calis meanstr;
  group 1 / data=region1 label="Region 1" nobs=378;
  group 2 / data=region2 label="Region 2" nobs=423;
  model 1 / group=1,2;
  path
    Service ==> Spend02 Spend03      ,
    Product ==> Spend02 Spend03      ,
    Spend02 ==> Spend03                ,
    Service ==> Courtesy Responsive
                Helpful Delivery      ,
    Product ==> Pricing Availability
                Quality                ;
  pvar
    Courtesy Responsive Helpful Delivery Pricing
    Availability Quality Spend02 Spend03,
    Service Product = 2 * 1.;
  pcov
    Service Product;
run;
```

You use the **GROUP** statements to specify the data for the two regions. Using the **DATA=** options in the **GROUP** statements, you assign the ‘Region 1’ data to Group 1 and the ‘Region 2’ data to Group 2. You label the two groups by the **LABEL=** options. Because the number of observations is not defined in the data sets, you use the **NOBS=** options in the **GROUP** statements to provide this information.

In the **MODEL** statement, you specify in the **GROUP=** option that both Groups 1 and 2 are fitted by the same model—**model 1**. Next, the path model is specified. As discussed before, you do not need to specify the default mean parameters by using the **MEAN** statement because the **MEANSTR** option in the **PROC CALIS** statement already indicates the analysis of mean structures.

Output 27.28.1 presents a summary of modeling information. Each group is listed with its associated data set, number of observations, and its corresponding model and the model type. In the current analysis, the same model is fitted to both groups. Next, a table for the types of variables is presented. As intended, all nine observed (manifest) variables are endogenous, and all latent variables are exogenous in the model.

Output 27.28.1 Modeling Information and Variables

Modeling Information						
Maximum Likelihood Estimation						
Group	Label	Data Set	N Obs	Model	Type	Analysis
1	Region 1	WORK.REGION1	378	Model 1	PATH	Means and Covariances
2	Region 2	WORK.REGION2	423	Model 1	PATH	Means and Covariances
Model 1. Variables in the Model						
Endogenous	Manifest	Availability Courtesy Delivery Helpful Pricing Quality Responsive Spend02 Spend03				
	Latent					
Exogenous	Manifest					
	Latent	Product Service				
Number of Endogenous Variables = 9						
Number of Exogenous Variables = 2						

The optimization converges. The fit summary table is presented in [Output 27.28.2](#).

Output 27.28.2 Fit Summary

Fit Summary		
Modeling Info	Number of Observations	801
	Number of Variables	9
	Number of Moments	108
	Number of Parameters	31
	Number of Active Constraints	0
	Baseline Model Function Value	0.5003
	Baseline Model Chi-Square	399.7468
	Baseline Model Chi-Square DF	72
	Pr > Baseline Model Chi-Square	<.0001
	Absolute Index	Fit Function
Chi-Square		2820.2504
Chi-Square DF		77
Pr > Chi-Square		<.0001
Z-Test of Wilson & Hilferty		43.2575
Hoelter Critical N		29
Root Mean Square Residual (RMR)		28.2208
Standardized RMR (SRMR)		2.1367
Parsimony Index	Goodness of Fit Index (GFI)	0.9996
	Adjusted GFI (AGFI)	0.9995
	Parsimonious GFI	1.0690
	RMSEA Estimate	0.2986
	RMSEA Lower 90% Confidence Limit	0.2892
	RMSEA Upper 90% Confidence Limit	0.3081
	Probability of Close Fit	<.0001
	Akaike Information Criterion	2882.2504
	Bozdogan CAIC	3058.5121
	Schwarz Bayesian Criterion	3027.5121
Incremental Index	McDonald Centrality	0.1804
	Bentler Comparative Fit Index	0.0000
	Bentler-Bonett NFI	-6.0551
	Bentler-Bonett Non-normed Index	-6.8265
	Bollen Normed Index Rho1	-5.5970
	Bollen Non-normed Index Delta2	-7.4997
	James et al. Parsimonious NFI	-6.4756

The model chi-square statistic is 2820.25. With $df = 77$ and $p < .0001$, the null hypothesis for the mean and covariance structures is rejected. All incremental fit indices are negative. These negative indices indicate a bad model fit, as compared with the independence model. The same fact can be deduced by comparing the chi-square values of the baseline model and the fitted model. The baseline model has five degrees of freedom less (five parameters more) than the structural model but the chi-square value is only 399.747, much less than the model fit chi-square value of 2820.25. Because variables in social and behavioral sciences are almost always expected to correlate with each other, a structural model that explains relationships even worse than the baseline model is deemed inappropriate for the data. The RMSEA for the structural model is 0.2986, which also indicates a bad model fit. However, the GFI, AGFI, and parsimonious GFI indicate good model fit, which is a little surprising given the fact that all other indices indicate the opposite and the overall model is pretty restrictive in the first place.

There are some warnings in the output:

```
WARNING: Model 1. The estimated error variance for variable Spend02 is
negative.
WARNING: Model 1. Although all predicted variances for the observed and
latent variables are positive, the corresponding predicted
covariance matrix is not positive definite. It has one negative
eigenvalue.
```

PROC CALIS routinely checks the properties of the estimated variances and the predicted covariance matrix. It issues warnings when there are problems. In this case, the error variance estimate of Spend02 is negative, and the predicted covariance matrix for the observed and latent variables is not positive definite and has one negative eigenvalue. You can inspect [Output 27.28.3](#), which shows the variance parameter estimates of the variables.

Output 27.28.3 Variance Estimates

Model 1. Variance Parameters						
Variance Type	Variable	Parameter	Estimate	Standard Error	t Value	
Error	Courtesy	_Parm13	2.59181	0.13600	19.05743	
	Responsive	_Parm14	2.92423	0.15325	19.08205	
	Helpful	_Parm15	2.44625	0.12320	19.85656	
	Delivery	_Parm16	3.53408	0.18169	19.45095	
	Pricing	_Parm17	2.52948	0.12784	19.78694	
	Availability	_Parm18	1.57410	0.16884	9.32296	
	Quality	_Parm19	2.41658	0.13230	18.26611	
	Spend02	_Parm20	-14.40124	16.92863	-0.85070	
	Spend03	_Parm21	22.79309	5.75120	3.96319	
	Exogenous	Service		1.00000		
		Product		1.00000		

The error variance estimate for Spend02 is -14.40 , which is negative and might have led to the negative eigenvalue problem in the predicted covariance matrix for the observed and latent variables.

A Model with Unconstrained Parameters for the Two Regions

With all the bad model fit indications and the problematic predicted covariance matrix for the latent variables, you might conclude that an overly restricted model has been fit. Region 1 and Region 2 might not share exactly the same set of parameters. How about fitting a model at the other extreme with all parameters unconstrained for the two groups (regions)? Such a model can be easily specified, as shown in the following statements:

```
proc calis meanstr;
  group 1 / data=region1 label="Region 1" nobs=378;
  group 2 / data=region2 label="Region 2" nobs=423;
  model 1 / group=1;
    path
      Service ==> Spend02 Spend03      ,
      Product ==> Spend02 Spend03      ,
      Spend02 ==> Spend03              ,
      Service ==> Courtesy Responsive Helpful Delivery ,
      Product ==> Pricing Availability Quality ;
    pvar
      Courtesy Responsive Helpful Delivery Pricing
      Availability Quality Spend02 Spend03,
      Service Product = 2 * 1.;
    pcov
      Service Product;
  model 2 / group=2;
    refmodel 1/ allnewparms;
run;
```

Unlike the previous specification, in the current specification Group 2 is now fitted by a new model labeled as Model 2. This model is based on Model 1, as specified in `REFMODEL` statement. The `ALLNEWPARMS` option in the `REFMODEL` statement request that all parameters specified in Model 1 be renamed so that they become new parameters in Model 2. As a result, this specification gives different sets of estimates for Model 1 and Model 2, although both models have the same path structures and a comparable set of parameters.

The optimization converges without problems. The fit summary table is displayed in [Output 27.28.4](#). The chi-square statistic is 29.613 ($df = 46, p = .97$). The theoretical model is not rejected. Many other measures of fit also indicate very good model fit. For example, the GFI, AGFI, Bentler CFI, Bentler-Bonett NFI, and Bollen nonnormed index delta2 are all close to one, and the RMSEA is close to zero.

Output 27.28.4 Fit Summary

Fit Summary		
Modeling Info	Number of Observations	801
	Number of Variables	9
	Number of Moments	108
	Number of Parameters	62
	Number of Active Constraints	0
	Baseline Model Function Value	0.5003
	Baseline Model Chi-Square	399.7468
	Baseline Model Chi-Square DF	72
	Pr > Baseline Model Chi-Square	<.0001
	Absolute Index	Fit Function
Chi-Square		29.6131
Chi-Square DF		46
Pr > Chi-Square		0.9710
Z-Test of Wilson & Hilferty		-1.8950
Hoelter Critical N		1697
Root Mean Square Residual (RMR)		0.0670
Standardized RMR (SRMR)		0.0220
Goodness of Fit Index (GFI)		1.0000
Parsimony Index		Adjusted GFI (AGFI)
	Parsimonious GFI	0.6389
	RMSEA Estimate	0.0000
	RMSEA Lower 90% Confidence Limit	0.0000
	RMSEA Upper 90% Confidence Limit	0.0000
	Probability of Close Fit	1.0000
	Akaike Information Criterion	153.6131
	Bozdogan CAIC	506.1365
	Schwarz Bayesian Criterion	444.1365
	McDonald Centrality	1.0103
Incremental Index	Bentler Comparative Fit Index	1.0000
	Bentler-Bonett NFI	0.9259
	Bentler-Bonett Non-normed Index	1.0783
	Bollen Normed Index Rho1	0.8840
	Bollen Non-normed Index Delta2	1.0463
	James et al. Parsimonious NFI	0.5916

Notice that because there are no constraints between the two models for the groups, you might have fit the two sets of data by the respective models separately and gotten exactly the same results as in the current analysis. For example, you get two model fit chi-square values from separate analyses. Adding up these two chi-squares gives you the same overall chi-square as in [Output 27.28.4](#).

PROC CALIS also provides a table for comparing the relative model fit of the groups. In [Output 27.28.5](#), basic modeling information and some measures of fit for the two groups are shown along with the corresponding overall measures.

Output 27.28.5 Fit Comparison among Groups

Fit Comparison Among Groups			
		Overall	Region 1
Modeling Info	Number of Observations	801	378
	Number of Variables	9	9
	Number of Moments	108	54
	Number of Parameters	62	31
	Number of Active Constraints	0	0
	Baseline Model Function Value	0.5003	0.4601
	Baseline Model Chi-Square	399.7468	173.4482
	Baseline Model Chi-Square DF	72	36
	Fit Index	Fit Function	0.0371
Percent Contribution to Chi-Square		100	3
Root Mean Square Residual (RMR)		0.0670	0.0172
Standardized RMR (SRMR)		0.0220	0.0057
Goodness of Fit Index (GFI)		1.0000	1.0000
Bentler-Bonett NFI		0.9259	0.9950
Fit Comparison Among Groups			
		Region 2	
Modeling Info	Number of Observations	423	
	Number of Variables	9	
	Number of Moments	54	
	Number of Parameters	31	
	Number of Active Constraints	0	
	Baseline Model Function Value	0.5363	
	Baseline Model Chi-Square	226.2986	
	Baseline Model Chi-Square DF	36	
	Fit Index	Fit Function	0.0681
Percent Contribution to Chi-Square		97	
Root Mean Square Residual (RMR)		0.0907	
Standardized RMR (SRMR)		0.0298	
Goodness of Fit Index (GFI)		1.0000	
Bentler-Bonett NFI		0.8730	

When you examine the results of this table, the first thing you have to realize is that in general the group statistics are not independent. For example, although the overall chi-square statistic can be written as the weighted sum of fit functions of the groups, in general it does not imply that the individual terms are statistically independent. In the current two-group analysis, the overall chi-square is written as

$$T = (N_1 - 1)f_1 + (N_2 - 1)f_2$$

where N_1 and N_2 are sample sizes for the groups and f_1 and f_2 are the discrepancy functions for the groups. Even though T is chi-square distributed under the null hypothesis, in general the individual terms $(N_1 - 1)f_1$ and $(N_2 - 1)f_2$ are not chi-square distributed under the same null hypothesis. So when you compare the group fits by using the statistics in [Output 27.28.5](#), you should treat those as descriptive measures only.

The current model is a special case where f_1 and f_2 are actually independent of each other. The reason is that there are no constrained parameters for the models fitted to the two groups. This would imply that the individual terms $(N_1 - 1)f_1$ and $(N_2 - 1)f_2$ are chi-square distributed under the null hypothesis. Nonetheless, this fact is not important to the group comparison of the descriptive statistics in [Output 27.28.5](#). The values of f_1 and f_2 are shown in the row labeled “Fit Function.” Group 1 (Region 1) is fitted better by its model ($f_1 = 0.0023$) than is Group 2 (Region 2) by its model ($f_2 = 0.0681$). Next, the percentage contributions to the overall chi-square statistic for the two groups are shown. Group 1 contributes only 3% ($= (N_1 - 1)f_1/T \times 100\%$) while Group 2 contributes 97%. Other measures like RMR, SRMR, and Bentler-Bonett NFI show that Group 1 data are fitted better. The GFI’s show equal fits for the two groups, however.

Despite a very good fit, the current model is not intended to be the final model. It was fitted mainly for illustration purposes. The next section considers a partially constrained model for the two groups of data.

A Model with Partially Constrained Parameters for the Two Regions

For multiple-group analysis, cross-group constraints are of primary interest and should be explored whenever appropriate. The first fitting with all model parameters constrained for the groups has been shown to be too restrictive, while the current model with no cross-group constraints fits very well—so well that it might have overfit unnecessarily. A multiple-group model between these extremes is now explored. The following statements specify such a partially constrained model:

```

proc calis meanstr modification;
  group 1 / data=region1 label="Region 1" nobs=378;
  group 2 / data=region2 label="Region 2" nobs=423;
  model 3 / label="Model for References Only";
    path
      Service ==> Spend02 Spend03      ,
      Product ==> Spend02 Spend03      ,
      Spend02 ==> Spend03              ,
      Service ==> Courtesy Responsive
                        Helpful Delivery ,
      Product ==> Pricing Availability
                        Quality          ;
    pvar
      Courtesy Responsive Helpful Delivery Pricing
      Availability Quality Spend02 Spend03,
      Service Product = 2 * 1.;
    pcov
      Service Product;
  model 1 / groups=1;
    refmodel 3;
    mean
      Spend02 Spend03 = G1_InterSpend02 G1_InterSpend03,
      Courtesy Responsive Helpful
      Delivery Pricing Availability
      Quality = G1_intercept01-G1_intercept07;
  model 2 / groups=2;
    refmodel 3;
    mean
      Spend02 Spend03 = G2_InterSpend02 G2_InterSpend03,
      Courtesy Responsive Helpful
      Delivery Pricing Availability
      Quality = G2_intercept01-G2_intercept07;
  simtests
    SpendDiff          = (Spend02Diff Spend03Diff)
    MeasurementDiff    = (CourtesyDiff ResponsiveDiff
                          HelpfulDiff DeliveryDiff
                          PricingDiff AvailabilityDiff
                          QualityDiff);
    Spend02Diff        = G2_InterSpend02 - G1_InterSpend02;
    Spend03Diff        = G2_InterSpend03 - G1_InterSpend03;
    CourtesyDiff       = G2_intercept01 - G1_intercept01;
    ResponsiveDiff     = G2_intercept02 - G1_intercept02;
    HelpfulDiff        = G2_intercept03 - G1_intercept03;
    DeliveryDiff       = G2_intercept04 - G1_intercept04;
    PricingDiff        = G2_intercept05 - G1_intercept05;
    AvailabilityDiff   = G2_intercept06 - G1_intercept06;
    QualityDiff        = G2_intercept07 - G1_intercept07;
run;

```

In this specification, you use a special model definition. Model 3 serves as a reference model. You are not going to fit this model directly to any data set, but the specifications of other two models makes reference to it. Model 3 is no different from the basic path model specification used in preceding examples. The PATH model specification reflects the path diagram in [Figure 27.7](#).

Region 1 is fitted by Model 1, which makes reference to Model 3 by using the `REFMODEL` statement. In addition, you add the `MEAN` statement specification. You now specify the intercept parameters explicitly by using the parameter names `G1_intercept01–G1_intercept07`, `G1_InterSpend02`, and `G1_InterSpend03`. In previous examples, these intercept parameters are set by default by PROC CALIS. This explicit parameter naming serves the purpose of distinguishing these parameters from those for Model 2.

Region 2 is fitted by Model 2, which also refers to Model 3 by using the `REFMODEL` statement. You also specify a `MEAN` statement for this model with explicit specifications of the intercept parameters. You name these intercepts `G2_intercept01–G2_intercept07`, `G2_InterSpend02`, and `G2_InterSpend03`. The `G2` prefix distinguishes these parameters from the corresponding intercept parameters in the parent model. All in all, this means that both Models 1 and 2 refers to Model 3, except that Model 2 uses a different set of intercept parameters. In other words, in this multiple-group model the covariance structures for the two regions are constrained to be the same, while the means structures are allowed to be unconstrained.

You request additional statistics or tests in the current PROC CALIS analysis. The `MODIFICATION` option in the PROC CALIS statement requests that the Lagrange multiplier tests and Wald tests be conducted. The Lagrange multiplier tests provide information about which constrained or fixed parameters could be freed or added so as to improve the overall model fit. The Wald tests provide information about which existing parameters could be fixed at zeros (eliminated) without significantly affecting the overall model fit. These tests are discussed in more detail when the results are presented.

In the `SIMTESTS` statement, two simultaneous tests are requested. The first simultaneous test is named `SpendDiff`, which includes two parametric functions `Spend02Diff` and `Spend03Diff`. The second simultaneous test is named `MeasurementDiff`, which includes seven parametric functions: `CourtesyDiff`, `ResponsiveDiff`, `HelpfulDiff`, `DeliveryDiff`, `PricingDiff`, `AvailabilityDiff`, and `QualityDiff`. The null hypothesis of these simultaneous tests is of the form

$$H_0 : t_i = 0 \quad (i = 1 \dots k)$$

where k is the number of parametric functions within the simultaneous test. In the current analysis, the component parametric functions are defined in the [SAS programming statements](#), which are shown in the last block of the specification. Essentially, all these parametric functions represent the differences of the mean or intercept parameters between the two models for groups. The first simultaneous test is intended to test whether the mean or intercept parameters in the structural models are the same, while the second simultaneous test is intended to test whether the mean parameters in the measurement models are the same.

The fit summary table is shown in [Output 27.28.6](#).

Output 27.28.6 Fit Summary

Fit Summary		
Modeling Info	Number of Observations	801
	Number of Variables	9
	Number of Moments	108
	Number of Parameters	40
	Number of Active Constraints	0
	Baseline Model Function Value	0.5003
	Baseline Model Chi-Square	399.7468
	Baseline Model Chi-Square DF	72
	Pr > Baseline Model Chi-Square	<.0001
Absolute Index	Fit Function	0.1346
	Chi-Square	107.5461
	Chi-Square DF	68
	Pr > Chi-Square	0.0016
	Z-Test of Wilson & Hilferty	2.9452
	Hoelter Critical N	657
	Root Mean Square Residual (RMR)	0.1577
	Standardized RMR (SRMR)	0.0678
	Goodness of Fit Index (GFI)	1.0000
Parsimony Index	Adjusted GFI (AGFI)	0.9999
	Parsimonious GFI	0.9444
	RMSEA Estimate	0.0382
	RMSEA Lower 90% Confidence Limit	0.0237
	RMSEA Upper 90% Confidence Limit	0.0514
	Probability of Close Fit	0.9275
	Akaike Information Criterion	187.5461
	Bozdogan CAIC	414.9806
	Schwarz Bayesian Criterion	374.9806
McDonald Centrality	0.9756	
Incremental Index	Bentler Comparative Fit Index	0.8793
	Bentler-Bonett NFI	0.7310
	Bentler-Bonett Non-normed Index	0.8722
	Bollen Normed Index Rho1	0.7151
	Bollen Non-normed Index Delta2	0.8808
	James et al. Parsimonious NFI	0.6904

The chi-square value is 107.55 ($df = 68$, $p = 0.0016$), which is statistically significant. The null hypothesis of the mean and covariance structures is rejected if an α -level at 0.01 or larger is chosen. However, in practical structural equation modeling, the chi-square test is not the only criterion, or even an important criterion, for evaluating model fit. The RMSEA estimate for the current model is 0.0382, which indicates a good fit. The probability level of close fit is 0.9275, indicating that a good population fit hypothesis (that is, population RMSEA < 0.05) cannot be rejected. The GFI, AGFI, and parsimonious GFI all indicate good fit. However, the incremental indices show only a respectable model fit.

Comparison of the model fit to the groups is shown in [Output 27.28.7](#).

Output 27.28.7 Fit Comparison among Groups

Fit Comparison Among Groups			
		Overall	Region 1
Modeling Info	Number of Observations	801	378
	Number of Variables	9	9
	Number of Moments	108	54
	Number of Parameters	40	31
	Number of Active Constraints	0	0
	Baseline Model Function Value	0.5003	0.4601
	Baseline Model Chi-Square	399.7468	173.4482
	Baseline Model Chi-Square DF	72	36
Fit Index	Fit Function	0.1346	0.1261
	Percent Contribution to Chi-Square	100	44
	Root Mean Square Residual (RMR)	0.1577	0.1552
	Standardized RMR (SRMR)	0.0678	0.0792
	Goodness of Fit Index (GFI)	1.0000	1.0000
	Bentler-Bonett NFI	0.7310	0.7260
	Fit Comparison Among Groups		
		Region 2	
Modeling Info	Number of Observations	423	
	Number of Variables	9	
	Number of Moments	54	
	Number of Parameters	31	
	Number of Active Constraints	0	
	Baseline Model Function Value	0.5363	
	Baseline Model Chi-Square	226.2986	
Fit Index	Baseline Model Chi-Square DF	36	
	Fit Function	0.1422	
	Percent Contribution to Chi-Square	56	
	Root Mean Square Residual (RMR)	0.1599	
	Standardized RMR (SRMR)	0.0557	
	Goodness of Fit Index (GFI)	1.0000	
	Bentler-Bonett NFI	0.7348	

Looking at the percentage contribution to the chi-square, the Region 2 fitting shows a worse fit. However, this might be due to the larger sample size in Region 2. When comparing the fit of the two regions by using RMR, which does not take the sample size into account, the fitting of two groups are about the same. The standardized RMR even shows that Region 2 is fitted better. So, it seems to be safe to conclude that the models fit almost equally well (or badly) for the two regions.

The constrained parameter estimates for the two regions are shown in [Output 27.28.8](#).

Output 27.28.8 Estimates of Path Coefficients and Other Covariance Parameters

Model 1. PATH List						
-----Path-----	Parameter	Estimate	Standard Error	t Value		
Service ==> Spend02	_Parm01	0.37475	0.21318	1.75795		
Service ==> Spend03	_Parm02	0.53851	0.20840	2.58401		
Product ==> Spend02	_Parm03	0.80372	0.21939	3.66347		
Product ==> Spend03	_Parm04	0.59879	0.22144	2.70409		
Spend02 ==> Spend03	_Parm05	0.08952	0.03694	2.42326		
Service ==> Courtesy	_Parm06	0.72418	0.07989	9.06482		
Service ==> Responsive	_Parm07	0.90452	0.08886	10.17972		
Service ==> Helpful	_Parm08	0.64969	0.07683	8.45574		
Service ==> Delivery	_Parm09	0.64473	0.09021	7.14677		
Product ==> Pricing	_Parm10	0.63452	0.07916	8.01600		
Product ==> Availability	_Parm11	0.76737	0.08265	9.28516		
Product ==> Quality	_Parm12	0.79716	0.08922	8.93470		

Model 1. Variance Parameters					
Variance Type	Variable	Parameter	Estimate	Standard Error	t Value
Error	Courtesy	_Parm13	1.98374	0.13169	15.06379
	Responsive	_Parm14	2.02152	0.16159	12.51005
	Helpful	_Parm15	1.96535	0.12263	16.02727
	Delivery	_Parm16	2.97542	0.17049	17.45184
	Pricing	_Parm17	1.93952	0.12326	15.73583
	Availability	_Parm18	1.63156	0.13067	12.48646
	Quality	_Parm19	2.08849	0.15329	13.62464
	Spend02	_Parm20	13.47066	0.71842	18.75051
	Spend03	_Parm21	13.02883	0.68682	18.96966
Exogenous	Service		1.00000		
	Product		1.00000		

Model 1. Covariances Among Exogenous Variables					
Var1	Var2	Parameter	Estimate	Standard Error	t Value
Service	Product	_Parm22	0.33725	0.07061	4.77599

All parameter estimates but one are statistically significant at $\alpha = 0.05$. The parameter `_Parm01`, which represents the path coefficient from Service to Spend02, has a t value of 1.76. This is only marginally significant. Although all these results bear the title of Model 1, these estimates are the same for Model 2, of which the corresponding results are not shown here.

The mean and intercept parameters for the two models (regions) are shown in [Output 27.28.9](#).

Output 27.28.9 Estimates of Means and Intercepts

Model 1. Means and Intercepts					
Type	Variable	Parameter	Estimate	Standard Error	t Value
Intercept	Spend02	G1_InterSpend02	183.50000	0.19585	936.95628
	Spend03	G1_InterSpend03	285.49480	6.78127	42.10048
	Courtesy	G1_intercept01	4.31200	0.08157	52.86519
	Responsive	G1_intercept02	4.72400	0.08679	54.43096
	Helpful	G1_intercept03	3.92100	0.07958	49.27201
	Delivery	G1_intercept04	4.35700	0.09484	45.93968
	Pricing	G1_intercept05	6.14400	0.07882	77.94992
	Availability	G1_intercept06	4.99400	0.07674	65.07315
	Quality	G1_intercept07	5.97100	0.08500	70.24543
Model 2. Means and Intercepts					
Type	Variable	Parameter	Estimate	Standard Error	t Value
Intercept	Spend02	G2_InterSpend02	156.25000	0.18511	844.09015
	Spend03	G2_InterSpend03	299.68311	5.77478	51.89515
	Courtesy	G2_intercept01	2.41200	0.07709	31.28628
	Responsive	G2_intercept02	2.72700	0.08203	33.24350
	Helpful	G2_intercept03	5.22400	0.07522	69.45319
	Delivery	G2_intercept04	6.37600	0.08964	71.12697
	Pricing	G2_intercept05	7.14700	0.07450	95.93427
	Availability	G2_intercept06	3.23300	0.07254	44.57020
	Quality	G2_intercept07	5.11900	0.08034	63.71500

All the mean and intercept estimates are statistically significant at $\alpha = 0.01$. Except for the fixed zero means for Service and Product, a quick glimpse of these mean and intercepts estimates shows a quite different pattern for the two models. Do these estimates truly differ beyond chance? The simultaneous tests of these parameter estimates shown in [Output 27.28.10](#) can confirm this.

Output 27.28.10 shows two simultaneous tests, as requested in the original statements.

Output 27.28.10 Simultaneous Tests

Simultaneous Tests					
Simultaneous Test	Parametric Function	Function Value	DF	Chi-Square	p Value
SpendDiff			2	10458	<.0001
	Spend02Diff	-27.25000	1	10225	<.0001
	Spend03Diff	14.18831	1	185.86725	<.0001
MeasurementDiff			7	1610	<.0001
	CourtesyDiff	-1.90000	1	286.58605	<.0001
	ResponsiveDiff	-1.99700	1	279.63659	<.0001
	HelpfulDiff	1.30300	1	141.59942	<.0001
	DeliveryDiff	2.01900	1	239.35318	<.0001
	PricingDiff	1.00300	1	85.52567	<.0001
	AvailabilityDiff	-1.76100	1	278.09360	<.0001
	QualityDiff	-0.85200	1	53.06240	<.0001

The first one is SpendDiff, which tests simultaneously the following hypotheses:

$$H_0 : G2_InterSpend02 - G1_InterSpend02 = 0$$

$$H_0 : G2_InterSpend03 - G1_InterSpend03 = 0$$

The exceedingly large chi-square value 10,460 suggests the composite null hypothesis is false. Individual tests for these hypotheses suggest that each of these hypotheses should be rejected. The chi-square values for individual tests are 10,227 and 185.84, respectively.

Similarly, the simultaneous and individual tests of the intercepts in the measurement model suggest that the two models (groups) differ significantly in the means of the measured variables. Region 2 has significantly higher means in variables Helpful, Delivery, and Pricing, but significantly lower means in variables Courtesy, Responsive, Availability, and Quality.

Now you are ready to answer the main research questions. The overall customer service (Service) does affect the future purchase (Spend03), but not the current purchase (Spend02), because the corresponding path coefficient (_Parm01) is only marginally significant. Perhaps this is an artifact because the rating was done after the purchases in 2002. That is, purchases in 2002 had been done before the impression about customer service was fully formed. However, this argument cannot explain why overall customer service (Service) also shows a strong and significant relationship with purchases in 2002 (Spend02). Nonetheless, customer service and product quality do affect the future purchases (Spend03) in an expected way, even after partialling out the effect of the previous purchase amount (Spend02). Apart from the mean differences of the variables, the common measurement and prediction (or structural) models fit the two regions very well.

Because the current model fits well and most parts of fitting meet your expectations, you might accept this model without looking for further improvement. Nonetheless, for illustration purposes, it would be useful to consider the LM test results. In [Output 27.28.11](#), ranked LM statistics for the path coefficients in Model 1 and Model 2 are shown.

Output 27.28.11 LM Tests for Path Coefficients

Model 1. Rank Order of the 10 Largest LM Stat for Path Relations				
To	From	LM Stat	Pr > ChiSq	Parm Change
Service	Courtesy	11.15249	0.0008	-0.17145
Service	Helpful	3.09038	0.0788	0.09431
Service	Delivery	2.59511	0.1072	0.07504
Courtesy	Responsive	1.75943	0.1847	-0.07730
Delivery	Courtesy	1.66721	0.1966	0.08669
Helpful	Courtesy	1.62005	0.2031	0.07277
Courtesy	Product	1.48928	0.2223	-0.14815
Service	Product	0.83498	0.3608	-0.12327
Responsive	Helpful	0.76664	0.3813	-0.05625
Product	Helpful	0.53020	0.4665	-0.03831
Model 2. Rank Order of the 10 Largest LM Stat for Path Relations				
To	From	LM Stat	Pr > ChiSq	Parm Change
Delivery	Courtesy	16.91167	<.0001	-0.26641
Service	Courtesy	9.11235	0.0025	0.15430
Courtesy	Delivery	8.12091	0.0044	-0.12989
Courtesy	Responsive	8.03954	0.0046	0.16215
Pricing	Responsive	5.48406	0.0192	0.10424
Courtesy	Product	4.39347	0.0361	0.24412
Courtesy	Quality	3.52147	0.0606	0.08672
Service	Delivery	3.20160	0.0736	-0.08281
Service	Helpful	2.97015	0.0848	-0.09198
Responsive	Pricing	2.91498	0.0878	0.08943

Path coefficients that lead to better improvement (larger chi-square decrease) are shown first in the tables. For example, the first path coefficient that is suggested to be freed in Model 1 is the Service <==== Courtesy path. The associated *p*-value is 0.0008 and the estimated change of parameter value is -0.171. The second path coefficient is for the Service <==== Helpful path, but it is not significant at the 0.05 level. So, is it good to add the Service <==== Courtesy path to Model 1, based on the LM test results? The answer is that it depends on your application and the theoretical and practical implications. For example, the Service <====> Courtesy path, which is a part of the measurement model, is already specified in Model 1. Even though the LM test statistic shows a significant decrease of model fit chi-square, adding the Service <==== Courtesy path might destroy the measurement model and lead to problematic interpretations. In this case, it is wise not to add the Service <==== Courtesy path, which is suggested by the LM test results.

LM tests for the path coefficients in Model 2 are shown at the bottom of [Output 27.28.11](#). Quite a few of these tests suggest significant improvements in model fit. Again, you are cautioned against adding these paths blindly.

LM tests for the error variances and covariances are shown in [Output 27.28.12](#).

Output 27.28.12 LM Tests for Error Covariances

Model 1. Rank Order of the 10 Largest LM Stat for Error Variances and Covariances				
Error of	Error of	LM Stat	Pr > ChiSq	Parm Change
Responsive	Helpful	1.26589	0.2605	-0.15774
Delivery	Courtesy	0.70230	0.4020	0.12577
Helpful	Courtesy	0.50167	0.4788	0.09103
Quality	Availability	0.47993	0.4885	-0.09739
Quality	Pricing	0.45925	0.4980	0.09449
Responsive	Availability	0.25734	0.6120	0.05965
Helpful	Availability	0.24811	0.6184	-0.05413
Responsive	Pricing	0.23748	0.6260	-0.05911
Spend02	Availability	0.19634	0.6577	-0.13200
Responsive	Courtesy	0.18212	0.6696	0.06201
Model 2. Rank Order of the 10 Largest LM Stat for Error Variances and Covariances				
Error of	Error of	LM Stat	Pr > ChiSq	Parm Change
Delivery	Courtesy	16.00996	<.0001	-0.57408
Responsive	Pricing	4.89190	0.0270	0.25403
Helpful	Delivery	3.33480	0.0678	0.25299
Delivery	Availability	2.79513	0.0946	0.20656
Responsive	Availability	2.16944	0.1408	-0.16421
Quality	Courtesy	2.14952	0.1426	0.17094
Responsive	Courtesy	2.12832	0.1446	0.20604
Quality	Pricing	2.00978	0.1563	-0.19154
Quality	Availability	1.99477	0.1578	0.19459
Responsive	Quality	1.88736	0.1695	-0.16963

Using $\alpha = 0.05$, you might consider adding two pairs of correlated errors in Model 2. The first pair is for Delivery and Courtesy, which has a p -value less than 0.0001. The second pair is Pricing and Responsive, which has a p -value of 0.027. Again, adding correlated errors (in the PCOV statement) should not be a pure statistical consideration. You should also consider theoretical and practical implications.

LM tests for other subsets of parameters are also conducted. Some subsets do not have parameters that can be freed, and so they are not shown here. Other subsets are not shown here simply for conserving space.

PROC CALIS ranks and outputs the LM test results for some default subsets of parameters. You have seen the subsets for path coefficients and correlated errors in the two previous outputs. Some other LM test results are not shown. With this kind of default LM output, there could be a huge amount of modification indices to look at. Fortunately, you can limit the LM test results to any subsets of potential parameters that you might be interested in. With your substantive knowledge, you can define such meaningful subsets of potential parameters by using the LMTESTS statement. The LM test indices and rankings are then done for each predefined subset of potential parameters. With these customized LM results, you can limit your attention to consider only those meaningful parameters to be added. See the LMTESTS statement on page 1166 for details.

The next group of LM tests is for releasing implicit equality constraints in your model, as shown in Output 27.28.13.

Output 27.28.13 LM Tests for Equality Constraints

Lagrange Multiplier Statistics for Releasing Equality Constraints								
-----Released Parameter-----							-----Changes-----	
Parm	Model	Type	Var1	Var2	LM Stat	Pr > ChiSq	Original Parm	Released Parm
_Parm01	1	DV_IV	Spend02	Service	0.01554	0.9008	-0.0213	0.0238
	2	DV_IV	Spend02	Service	0.01554	0.9008	0.0238	-0.0213
_Parm02	1	DV_IV	Spend03	Service	0.01763	0.8944	-0.0222	0.0248
	2	DV_IV	Spend03	Service	0.01763	0.8944	0.0248	-0.0222
_Parm03	1	DV_IV	Spend02	Product	0.0003403	0.9853	-0.00321	0.00355
	2	DV_IV	Spend02	Product	0.0003403	0.9853	0.00355	-0.00321
_Parm04	1	DV_IV	Spend03	Product	0.00176	0.9665	0.00714	-0.00802
	2	DV_IV	Spend03	Product	0.00176	0.9665	-0.00802	0.00714
_Parm05	1	DV_DV	Spend03	Spend02	0.0009698	0.9752	-0.00100	0.00112
	2	DV_DV	Spend03	Spend02	0.0009698	0.9752	0.00112	-0.00100
_Parm06	1	DV_IV	Courtesy	Service	19.17225	<.0001	0.2851	-0.3191
	2	DV_IV	Courtesy	Service	19.17225	<.0001	-0.3191	0.2851
_Parm07	1	DV_IV	Responsive	Service	0.21266	0.6447	-0.0304	0.0341
	2	DV_IV	Responsive	Service	0.21266	0.6447	0.0341	-0.0304
_Parm08	1	DV_IV	Helpful	Service	4.60629	0.0319	-0.1389	0.1555
	2	DV_IV	Helpful	Service	4.60629	0.0319	0.1555	-0.1389
_Parm09	1	DV_IV	Delivery	Service	3.59763	0.0579	-0.1508	0.1687
	2	DV_IV	Delivery	Service	3.59763	0.0579	0.1687	-0.1508
_Parm10	1	DV_IV	Pricing	Product	0.50974	0.4753	0.0468	-0.0524
	2	DV_IV	Pricing	Product	0.50974	0.4753	-0.0524	0.0468
_Parm11	1	DV_IV	Availability	Product	0.57701	0.4475	-0.0457	0.0512
	2	DV_IV	Availability	Product	0.57701	0.4475	0.0512	-0.0457
_Parm12	1	DV_IV	Quality	Product	0.00566	0.9400	-0.00511	0.00574
	2	DV_IV	Quality	Product	0.00566	0.9400	0.00574	-0.00511
_Parm13	1	COVERR	Courtesy	Courtesy	45.24725	<.0001	0.7204	-0.8064
	2	COVERR	Courtesy	Courtesy	45.24725	<.0001	-0.8064	0.7204
_Parm14	1	COVERR	Responsive	Responsive	1.73499	0.1878	-0.1555	0.1740
	2	COVERR	Responsive	Responsive	1.73499	0.1878	0.1740	-0.1555
_Parm15	1	COVERR	Helpful	Helpful	11.13266	0.0008	-0.3448	0.3860
	2	COVERR	Helpful	Helpful	11.13266	0.0008	0.3860	-0.3448
_Parm16	1	COVERR	Delivery	Delivery	4.99097	0.0255	-0.3364	0.3766
	2	COVERR	Delivery	Delivery	4.99097	0.0255	0.3766	-0.3364
_Parm17	1	COVERR	Pricing	Pricing	2.86428	0.0906	0.1729	-0.1936
	2	COVERR	Pricing	Pricing	2.86428	0.0906	-0.1936	0.1729
_Parm18	1	COVERR	Availability	Availability	2.53147	0.1116	-0.1494	0.1672
	2	COVERR	Availability	Availability	2.53147	0.1116	0.1672	-0.1494
_Parm19	1	COVERR	Quality	Quality	0.07328	0.7866	-0.0315	0.0352
	2	COVERR	Quality	Quality	0.07328	0.7866	0.0352	-0.0315
_Parm20	1	COVERR	Spend02	Spend02	0.00214	0.9631	0.0304	-0.0340
	2	COVERR	Spend02	Spend02	0.00214	0.9631	-0.0340	0.0304
_Parm21	1	COVERR	Spend03	Spend03	0.0001773	0.9894	-0.00842	0.00946
	2	COVERR	Spend03	Spend03	0.0001773	0.9894	0.00946	-0.00842
_Parm22	1	COVEXOG	Service	Product	0.87147	0.3505	0.0605	-0.0678
	2	COVEXOG	Service	Product	0.87147	0.3505	-0.0678	0.0605

Recall that the measurement and the prediction models for the two regions are constrained to be the same by model referencing (that is, the `REFMODEL` statement). Output 27.28.13 shows you which parameter can be unconstrained so that your overall model fit might improve. For example, if you unconstrain the

first parameter `_Parm01`, which is for the path effect of `Spend02 <=== Service`, for the two models, the expected chi-square decrease (LM Stat) is about 0.0158, which is not significant ($p = .9001$). The associated parameter changes are small too. However, if you consider unconstraining parameter `_Parm06`, which is for the path effect of `Courtesy <=== Service`, the expected decrease of chi-square is 19.22 ($p < 0.0001$). There are two rows for this parameter. Each row represents a parameter location to be released from the equality constraint. Consider the first row first. If you rename the coefficient for the `Courtesy <=== Service` path in Model 1 to a new parameter, say “new” (while keeping `_Parm06` as the parameter for the `Courtesy <=== Service` path in Model 2) and fit the model again, the new estimate of `_Parm06` is 0.2852 greater than the previous `_Parm06` estimate. The estimate of “new” is 0.3196 less than the previous `_Parm06` estimate. The second row for the `_Parm06` parameter shows similar but reflected results. It is for renaming the parameter location in Model 2. For this example each equality constraint has exactly two locations, one for Model 1 and one for Model 2. That is the reason why you always observe reflected results for freeing the locations successively. Reflected results are not the case if you have equality constraints with more than two parameter locations.

Another example of a large expected improvement of model fit is the result of freeing the constrained variances of `Courtesy` among the two models. The corresponding row to look at is the row with parameter `_Parm13`, where the parameter type is labeled “COVERR” and the values for `Var1` and `Var2` are both “`Courtesy`.” The LM statistic is 45.255, which is a significant chi-square decrease if you free either parameter location. If you choose to rename the error variance for `Courtesy` in Model 1, the new `_Parm13` estimate is 0.8052 smaller than the original `_Parm13` estimate. The new estimate of the error variance for `Courtesy` in Model 2 is 0.7211 greater than the previous `_Parm13` estimate. Finally, the constrained parameter `_Parm15`, which is the error variance parameter for `Helpful` in both models, is also a potential constraint that can be released with a significant model fit improvement.

In addition to the LM statistics for suggesting ways to improve model fit, PROC CALIS also computes the Wald tests to show which parameters can be constrained to zero without jeopardizing the model fit significantly. The Wald test results are shown in [Output 27.28.14](#).

Output 27.28.14 Wald Tests

Stepwise Multivariate Wald Test					
Parm	-----Cumulative Statistics-----			--Univariate Increment--	
	Chi-Square	DF	Pr > ChiSq	Chi-Square	Pr > ChiSq
<code>_Parm01</code>	3.09039	1	0.0788	3.09039	0.0788

In [Output 27.28.14](#), you see that `_Parm01`, which is for the path effect of `Spend02 <=== Service`, is suggested to be a fixed zero parameter (eliminated from the model) by the Wald test. Fixing this parameter to zero (or dropping the `Spend02 <=== Service` path from the model) is expected to increase the model fit chi-square by 3.085 ($p = .079$), which is only marginally significant at $\alpha = 0.05$.

As is the case for the LM test statistics, you should not automatically adhere to the suggestions by the Wald statistics. Substantive and theoretical considerations should always be considered when determining whether a parameter should be added or dropped.

Example 27.29: Fitting the RAM and EQS Models by the COSAN Modeling Language

The COSAN modeling language in PROC CALIS enables you to specify the direct or implied mean and covariance structures for the data in terms of matrix formulas. It is a very general modeling language, and all other modeling languages in PROC CALIS are special cases of the COSAN modeling language. This example shows how you can apply the COSAN modeling language to situations where you might usually use the “easier” modeling languages. Therefore, the purpose of this example is not to recommend the use of the COSAN modeling specification to the specific application. Rather, through its connections with other more well-known model types, this example intends to help you understand the basics of the COSAN modeling language.

In [Example 27.17](#), you fit a path model to the Wheaton data (Wheaton et al. 1977) by using the PATH modeling language. The mathematical basis of the PATH modeling language is the RAM model. In [Example 27.23](#), you use the RAM and LINEQS statements to specify the same path model. In all these different types of specifications, you specify the functional relationships of the variables and the variance and covariance parameters in the model. PROC CALIS then generates the implied covariance structures for analysis internally. The COSAN modeling language is quite different. In the COSAN statement, you specify the covariance structures directly as a matrix formula. This example shows how you can do that in two different ways. One specification emulates the RAM model (McDonald 1978, 1980) covariance structures and the other emulates the EQS model (Bentler 1995) covariance structures.

Emulating the RAM model by the COSAN Modeling Language

In the RAM model, you specify all information regarding the path effects or coefficients (that is, single-headed arrows in the path diagram) in the so-called **A** (`_A_`) matrix. You specify all the information regarding the variances and covariances (that is, the double-headed arrows in the path diagram) in the **P** (`_P_`) matrix. See the section “[The RAM Model](#)” on page 1294 for more details about the mathematical model for RAM. Once you define these two matrices, the implied covariance structures for the observed variables are derived by the formula

$$\Sigma = \mathbf{J} * (\mathbf{I} - \mathbf{A})^{-1} * \mathbf{P} * (\mathbf{I} - \mathbf{A})^{-1'} * \mathbf{J}'$$

where **I** is an identity matrix and **J** is a selection matrix that contains 0 or 1 as its elements for selecting the covariance structures elements for the observed variables.

For example, in the RAM model specification in [Example 27.23](#), you essentially use the following RAM model specification:

```

proc calis nobs=932 data=Wheaton primat nose;
  ram
    var =  Anomie67      /* 1 */
          Powerless67   /* 2 */
          Anomie71      /* 3 */
          Powerless71   /* 4 */
          Education     /* 5 */
          SEI           /* 6 */
          Alien67       /* 7 */
          Alien71       /* 8 */
          SES,          /* 9 */

    _A_  1  7  1.0,
    _A_  2  7  0.833,
    _A_  3  8  1.0,
    _A_  4  8  0.833,
    _A_  5  9  1.0,
    _A_  6  9  lambda,
    _A_  7  9  gamma1,
    _A_  8  9  gamma2,
    _A_  8  7  beta,
    _P_  1  1  theta1,
    _P_  2  2  theta2,
    _P_  3  3  theta1,
    _P_  4  4  theta2,
    _P_  5  5  theta3,
    _P_  6  6  theta4,
    _P_  7  7  psi1,
    _P_  8  8  psi2,
    _P_  9  9  phi,
    _P_  1  3  theta5,
    _P_  2  4  theta5;
run;

```

In the RAM statement, you specify all the parameters in the `_A_` and `_P_` matrices, and PROC CALIS generates the corresponding covariance structures for analysis. However, with the COSAN modeling language, in addition to the parameter in the model matrices, you need to supply the matrix formula for the covariance structures, as shown in the preceding formula for Σ .

Before discussing how you can specify the COSAN model that corresponds to this RAM model specification, it is useful to look at the initial model matrices that are generated by the preceding RAM model specification. To do this, you use the `PRIMAT` option in the PROC CALIS statement.

Output 27.29.1 and Output 27.29.2 show the initial *_A_* and *_P_* matrices, respectively, for the RAM model.

Output 27.29.1 Initial *_A_* Matrix of the RAM Model

Initial RAM <i>_A_</i> Matrix						
	Anomie67	Powerless67	Anomie71	Powerless71	Education	
Anomie67	0	0	0	0	0	
Powerless67	0	0	0	0	0	
Anomie71	0	0	0	0	0	
Powerless71	0	0	0	0	0	
Education	0	0	0	0	0	
SEI	0	0	0	0	0	
Alien67	0	0	0	0	0	
Alien71	0	0	0	0	0	
SES	0	0	0	0	0	

Output 27.29.1 *continued*

Initial RAM _A_ Matrix				
	SEI	Alien67	Alien71	SES
Anomie67	0	1.0000	0	0
Powerless67	0	0.8330	0	0
Anomie71	0	0	1.0000	0
Powerless71	0	0	0.8330	0
Education	0	0	0	1.0000
SEI	0	0	0	. [lambda]
Alien67	0	0	0	. [gamma1]
Alien71	0	. [beta]	0	. [gamma2]
SES	0	0	0	0

Output 27.29.2 Initial _P_ Matrix of the RAM Model

Initial RAM _P_ Matrix					
	Anomie67	Powerless67	Anomie71	Powerless71	Education
Anomie67	.	0	.	0	0
	[theta1]		[theta5]		
Powerless67	0	.	0	.	0
		[theta2]		[theta5]	
Anomie71	.	0	.	0	0
	[theta5]		[theta1]		
Powerless71	0	.	0	.	0
		[theta5]		[theta2]	
Education	0	0	0	0	.
					[theta3]
SEI	0	0	0	0	0
Alien67	0	0	0	0	0
Alien71	0	0	0	0	0
SES	0	0	0	0	0

Output 27.29.2 *continued*

Initial RAM _P_ Matrix				
	SEI	Alien67	Alien71	SES
Anomie67	0	0	0	0
Powerless67	0	0	0	0
Anomie71	0	0	0	0
Powerless71	0	0	0	0
Education	0	0	0	0
SEI	.	0	0	0
	[theta4]			
Alien67	0	.	0	0
		[psi1]		
Alien71	0	0	.	0
			[psi2]	
SES	0	0	0	.
				[phi]

Essentially, to specify the same model by the COSAN modeling language, you need to provide the same information in these two initial model matrices and the covariance structure formula for Σ in the COSAN model specification, which is shown in the following statements:


```

proc calis data=Wheaton nobs=932 nose;
  cosan
    var= Anomie67 Powerless67 Anomie71 Powerless71 Education SEI,
    J(9, IDE) * A(9, GEN, IMI) * P(9, SYM);
  matrix A
    [1 2 8 , 7] = 1.0 0.833 beta,
    [3 4 , 8] = 1.0 0.833 ,
    [5 6 7 8 , 9] = 1. lambda gamma1 gamma2;
  matrix P
    [1,1] = theta1-theta2 theta1-theta4 ,
    [7,7] = psi1 psi2 phi,
    [3,1] = theta5 ,
    [4,2] = theta5 ;
  vnames
    J = [Anomie67 Powerless67 Anomie71 Powerless71
        Education SEI Alien67 Alien71 SES],
    A = J,
    P = A;
run;

```

In the PROC CALIS statement, you provide the data set in the DATA= option and the number of observations in the NOBS= option. You use the NOSE option to turn off the computation of the standard error estimates.

In the VAR= option of the COSAN statement, you provide the list of observed variables for the analysis. You do not specify the latent variables in the VAR= option in the COSAN statement as you do in the VAR= option in the RAM statement. Then, you specify the formula for the covariance structures for the set of variables in the VAR= list. Because the covariance structure formula is symmetric, you only need to specify “half” of it. That is, the specification $J(9, IDE) * A(9, GEN, IMI) * P(9, SYM)$ in the COSAN statement automatically expands to

$$J * (I - A)^{-1} * P * (I - A)^{-1'} * J'$$

which is the required covariance structures. The arguments in the matrices represent the number of columns, the matrix type, and the transformation type (optional), respectively. For example, the notation $A(9, GEN, IMI)$ means that matrix A has nine columns and it is a general (GEN) rectangular or square matrix. You do not specify the number of rows for matrix A explicitly, but PROC CALIS can deduce that because matrix A follows matrix J in the multiplication. To make matrix multiplication conformable, the number of rows for matrix A must be the same as the number of columns for matrix J , which is nine. The IMI notation means the identity-minus-inverse transformation, which results in putting $(I - A)^{-1}$ in the expression. Matrix P in the covariance structure formula is a 9×9 symmetric matrix. It does not have any transformation in the formula. Matrix J in the covariance structure formula is a so-called generalized identity matrix (IDE), which has six rows and nine columns. Basically, you use this matrix to select the observed variables in the covariance structure formula. The exact form of this matrix will become clear when the PROC CALIS output is shown.

Next, you use two MATRIX statements to specify the parameters in the model matrices A and P , for RAM model matrices $_A_$ and $_P_$, respectively. For example, in the first entry of the MATRIX statement for the A matrix, you specify the elements $[1, 7]$, $[2, 7]$, and $[8, 7]$ by 1.0, 0.833, and beta, respectively. The first two elements are fixed constants, while the last one is a free parameter named beta. Similarly, you specify all the fixed or free parameters in matrix A , which reflects the same pattern you specify for the $_A_$ matrix of the RAM model, as shown in [Output 27.29.1](#).

For the **P** matrix, you specify the parameters in the same fashion. Because **P** is defined as a symmetric matrix, you need to specify only the lower triangular elements. In the first entry of the **MATRIX** statement for the **P** matrix, you specify the **[1, 1]** element, but the trailing parameter list has six parameters. The **[1, 1]** notation here is interpreted as the starting location of the matrix. It proceeds to **[2, 2]**, **[3, 3]**, **[4, 4]** and so on. The length of the trailing parameter list determines the number of elements being specified. Therefore, the last parameter in this entry is for **P[6, 6]**, which is a free parameter **theta4**. Similarly, you define all other parameters in the **P** matrix, which reflects the same pattern you specify for the **_P_** matrix of the RAM model, as shown in [Output 27.29.2](#).

In the **VNAMES** statement, you can specify the column variable names for the model matrices. You provide a set of nine variable names for the column of matrix **J** in the pairs of brackets. The first six names are those of the observed variables in the COSAN model, while the last six names are for latent factors. How about the row variable names for matrix **J**? Because matrix **J** is the first matrix in the covariance structure formula, its row names are automatically the same as the names of the observed variables in the **VAR=** list of the COSAN statement. Next, you specify the column variable names of matrix **A**. You equate that to matrix **J**, meaning that the column variable names in matrix **A** are the same those for matrix **J**. How about the row variable names for matrix **A**? Because matrix **A** follows matrix **J** in the covariance structure formula, its row names are automatically same as the column names for matrix **J**. Lastly, you define that the column names for matrix **P** are the same as those for matrix **A**.

Notice that column names serve only as labels. PROC CALIS does not know the identities of the row and column variables. For example, the first column of matrix **A** is **Anomie67**, which is also a name for an observed variable in the COSAN model. Keeping other specifications intact, you could name this column by any other name without affecting the model estimation. It is recommended that you use sensible names that help you remember the identities of the row and column variables, such as this example shows.

[Output 27.29.3](#) shows the modeling information and the observed variables in the COSAN model. PROC CALIS analyzed the covariance structures of the six observed variables listed in [Output 27.29.3](#).

Output 27.29.3 Modeling Information of the COSAN Model for the Wheaton Data: RAM Emulation

Modeling Information					
Maximum Likelihood Estimation					
Data Set	WORK.WHEATON				
N Obs	932				
Model Type	COSAN				
Analysis	Covariances				
Observed Variables (N = 6) in the Model					
Anomie67	Powerless67	Anomie71	Powerless71	Education	SEI

[Output 27.29.4](#) shows the covariance structures and some properties of the model matrices. The covariance structure formula for Sigma is defined as required. You can also check the matrix properties in this output to see if they are what you intend them to be.

Output 27.29.4 The Covariance Structures and Model Matrices of the COSAN Model for the Wheaton Data: RAM Emulation

COSAN Model Structures			
Sigma = J*inv(_I_-A)*P*(inv(_I_-A))`*J`			
Summary of Model Matrices			
Matrix	N Row	N Col	Matrix Type
A	9	9	GEN: Square
J	6	9	IDE: (I 0)
P	9	9	SYM: Symmetric

Output 27.29.4 shows that **J** is a 6×9 “identity” matrix ($I||0$). Essentially, **J** is a selection matrix that contains either 0 or 1 as its elements. The role of matrix **J** in the covariance structure formula is to extract first six rows and columns in the inner covariance structures $(\mathbf{I} - \mathbf{A})^{-1} * \mathbf{P} * (\mathbf{I} - \mathbf{A})^{-1'}$ (which is 9×9) to form the covariance structures only for the observed variables (which is 6×6). But how can this identity matrix have more columns (9) than rows (6)? In common mathematical notation, an identity matrix must always be a square matrix. However, for convenience in notation, PROC CALIS generalizes it to the IDE type. An IDE matrix that has the same numbers of columns and rows is a square identity matrix. If an IDE matrix has more columns than rows, it denotes an identity matrix concatenated (to the right) by a null matrix (that is, the $(I||0)$ notation). If an IDE matrix has more rows than columns, it denotes an identity matrix appended (to the bottom) by a null matrix (that is, the $(I//0)$ notation). The generalized definition for the IDE matrix offers an efficient way to define selection matrix, such as the **J** matrix shown in this example.

Output 27.29.5 shows the model fit chi-square of the COSAN model. This is the same model fit as in Output 27.17.6 of Example 27.17, as expected.

Output 27.29.5 Model Fit of the COSAN Model for the Wheaton Data: RAM Emulation

Fit Summary	
Chi-Square	13.4851
Chi-Square DF	9
Pr > Chi-Square	0.1419

Output 27.29.6 shows the estimates in the A matrix.

Output 27.29.6 Estimate of the A Matrix by the COSAN Model Specification

Model Matrix A (9 x 9 General Square Matrix)						
	Anomie67	Powerless67	Anomie71	Powerless71	Education	
Anomie67	0	0	0	0	0	0
Powerless67	0	0	0	0	0	0
Anomie71	0	0	0	0	0	0
Powerless71	0	0	0	0	0	0
Education	0	0	0	0	0	0
SEI	0	0	0	0	0	0
Alien67	0	0	0	0	0	0
Alien71	0	0	0	0	0	0
SES	0	0	0	0	0	0

Output 27.29.6 *continued*

Model Matrix A (9 x 9 General Square Matrix)				
	SEI	Alien67	Alien71	SES
Anomie67	0	1.0000	0	0
Powerless67	0	0.8330	0	0
Anomie71	0	0	1.0000	0
Powerless71	0	0	0.8330	0
Education	0	0	0	1.0000
SEI	0	0	0	5.3689 [lambda]
Alien67	0	0	0	-0.6299 [gamma1]
Alien71	0	0.5931 [beta]	0	-0.2409 [gamma2]
SES	0	0	0	0

The estimates in [Output 27.29.6](#) from the COSAN model specification are essentially the same as those from the RAM model specification, as shown in the matrix form in [Output 27.29.7](#).

Output 27.29.7 Estimate of the A Matrix by the RAM Model Specification

RAM _A_ Matrix						
	Anomie67	Powerless67	Anomie71	Powerless71	Education	
Anomie67	0	0	0	0	0	0
Powerless67	0	0	0	0	0	0
Anomie71	0	0	0	0	0	0
Powerless71	0	0	0	0	0	0
Education	0	0	0	0	0	0
SEI	0	0	0	0	0	0
Alien67	0	0	0	0	0	0
Alien71	0	0	0	0	0	0
SES	0	0	0	0	0	0

Output 27.29.7 continued

RAM _A_ Matrix				
	SEI	Alien67	Alien71	SES
Anomie67	0	1.0000	0	0
Powerless67	0	0.8330	0	0
Anomie71	0	0	1.0000	0
Powerless71	0	0	0.8330	0
Education	0	0	0	1.0000
SEI	0	0	0	5.3688 [lambda]
Alien67	0	0	0	-0.6299 [gamma1]
Alien71	0	0.5931 [beta]	0	-0.2409 [gamma2]
SES	0	0	0	0

Output 27.29.8 shows the estimates in the **P** matrix.

Output 27.29.8 Estimate of the **P** Matrix by the COSAN Model Specification

Model Matrix P (9 x 9 Symmetric Matrix)					
	Anomie67	Powerless67	Anomie71	Powerless71	Education
Anomie67	3.6078 [theta1]	0	0.9058 [theta5]	0	0
Powerless67	0	3.5950 [theta2]	0	0.9058 [theta5]	0
Anomie71	0.9058 [theta5]	0	3.6078 [theta1]	0	0
Powerless71	0	0.9058 [theta5]	0	3.5950 [theta2]	0
Education	0	0	0	0	2.9938 [theta3]
SEI	0	0	0	0	0
Alien67	0	0	0	0	0
Alien71	0	0	0	0	0
SES	0	0	0	0	0

Output 27.29.8 continued

Model Matrix P (9 x 9 Symmetric Matrix)				
	SEI	Alien67	Alien71	SES
Anomie67	0	0	0	0
Powerless67	0	0	0	0
Anomie71	0	0	0	0
Powerless71	0	0	0	0
Education	0	0	0	0
SEI	259.5738 [theta4]	0	0	0
Alien67	0	5.6705 [psi1]	0	0
Alien71	0	0	4.5148 [psi2]	0
SES	0	0	0	6.6162 [phi]

Again, aside from very minor numerical differences, the estimates shown in [Output 27.29.8](#) from the COSAN model specification are essentially the same as those from the RAM model specification, as shown in the matrix form in [Output 27.29.9](#).

Output 27.29.9 Estimate of the P Matrix by the RAM Model Specification

RAM _P_ Matrix					
	Anomie67	Powerless67	Anomie71	Powerless71	Education
Anomie67	3.6080 [theta1]	0	0.9058 [theta5]	0	0
Powerless67	0	3.5949 [theta2]	0	0.9058 [theta5]	0
Anomie71	0.9058 [theta5]	0	3.6080 [theta1]	0	0
Powerless71	0	0.9058 [theta5]	0	3.5949 [theta2]	0
Education	0	0	0	0	2.9937 [theta3]
SEI	0	0	0	0	0
Alien67	0	0	0	0	0
Alien71	0	0	0	0	0
SES	0	0	0	0	0

Output 27.29.9 *continued*

RAM _P_ Matrix				
	SEI	Alien67	Alien71	SES
Anomie67	0	0	0	0
Powerless67	0	0	0	0
Anomie71	0	0	0	0
Powerless71	0	0	0	0
Education	0	0	0	0
SEI	259.5764 [theta4]	0	0	0
Alien67	0	5.6705 [psi1]	0	0
Alien71	0	0	4.5148 [psi2]	0
SES	0	0	0	6.6163 [phi]

Emulating the EQS model by the COSAN Modeling Language

The LINEQS modeling language in PROC CALIS enables you to specify the functional relationships among variables by using the equation input, much the same way that you can do with the EQS software (Bentler 1995). The covariance structure formula for the observed variables in the EQS model is

$$\Sigma = \mathbf{J} * (\mathbf{I} - \mathbf{Beta})^{-1} * \mathbf{Gamma} * \mathbf{Phi} * \mathbf{Gamma}' * (\mathbf{I} - \mathbf{Beta})^{-1'} * \mathbf{J}'$$

where \mathbf{I} is an identity matrix, \mathbf{J} is a selection matrix that contains 0 or 1 as its elements for selecting the covariance structures elements for the observed variables, \mathbf{Beta} is a square matrix for specifying relationships among the endogenous variables, \mathbf{Gamma} is a matrix for specifying relationships between the endogenous variables and the exogenous variables, and \mathbf{Phi} is a matrix for specifying the variances and covariances of the exogenous variables. Notice that in the EQS model, error or disturbance variables are counted as exogenous variables in the model.

In [Example 27.23](#), you use the following LINEQS specification for the Wheaton data:

```
proc calis nob=932 data=Wheaton primat nose;
  lineqs
    Anomie67      = 1.0      * f_Alien67 + e1,
    Powerless67   = 0.833    * f_Alien67 + e2,
    Anomie71      = 1.0      * f_Alien71 + e3,
    Powerless71   = 0.833    * f_Alien71 + e4,
    Education     = 1.0      * f_SES      + e5,
    SEI           = lambda   * f_SES      + e6,
    f_Alien67     = gamma1   * f_SES      + d1,
    f_Alien71     = gamma2   * f_SES      + beta * f_Alien67 + d2;
  variance
    E1            = theta1,
    E2            = theta2,
    E3            = theta1,
    E4            = theta2,
    E5            = theta3,
    E6            = theta4,
    D1            = psi1,
    D2            = psi2,
    f_SES         = phi;
  cov
    E1 E3        = theta5,
    E2 E4        = theta5;
run;
```

In the LINEQS statement, you specify all the functional relationships among variables. In the VARIANCE and COV statements, you specify all the variance and covariance parameters in the model. None of the parameters is specified as a matrix element in the LINEQS model. The default output by PROC CALIS does not print the EQS model matrices. To print these model matrices, you use the PRIMAT option in the PROC CALIS statement. [Output 27.29.10](#), [Output 27.29.11](#), and [Output 27.29.12](#) show the initial specification of these model matrices:

Output 27.29.10 The Initial _EQSBETA_ Matrix by the LINEQS Model Specification

Initial _EQSBETA_ Matrix				
	Anomie67	Anomie71	Education	Powerless67
Anomie67	0	0	0	0
Anomie71	0	0	0	0
Education	0	0	0	0
Powerless67	0	0	0	0
Powerless71	0	0	0	0
SEI	0	0	0	0
f_Alien67	0	0	0	0
f_Alien71	0	0	0	0

Initial _EQSBETA_ Matrix				
	Powerless71	SEI	f_Alien67	f_Alien71
Anomie67	0	0	1.0000	0
Anomie71	0	0	0	1.0000
Education	0	0	0	0
Powerless67	0	0	0.8330	0
Powerless71	0	0	0	0.8330
SEI	0	0	0	0
f_Alien67	0	0	0	0
f_Alien71	0	0	.	0
			[beta]	

Output 27.29.11 The Initial `_EQSGAMMA_` Matrix by the LINEQS Model Specification

Initial <code>_EQSGAMMA_</code> Matrix					
	f_SES	e1	e3	e5	e2
Anomie67	0	1.0000	0	0	0
Anomie71	0	0	1.0000	0	0
Education	1.0000	0	0	1.0000	0
Powerless67	0	0	0	0	1.0000
Powerless71	0	0	0	0	0
SEI	. [lambda]	0	0	0	0
f_Alien67	. [gamma1]	0	0	0	0
f_Alien71	. [gamma2]	0	0	0	0

Initial <code>_EQSGAMMA_</code> Matrix				
	e4	e6	d1	d2
Anomie67	0	0	0	0
Anomie71	0	0	0	0
Education	0	0	0	0
Powerless67	0	0	0	0
Powerless71	1.0000	0	0	0
SEI	0	1.0000	0	0
f_Alien67	0	0	1.0000	0
f_Alien71	0	0	0	1.0000

Output 27.29.12 The Initial _EQSPHI_ Matrix by the LINEQS Model Specification

Initial _EQSPHI_ Matrix						
	f_SES	e1	e3	e5	e2	
f_SES	.	0	0	0	0	
	[phi]					
e1	0	.	.	0	0	
		[theta1]	[theta5]			
e3	0	.	.	0	0	
		[theta5]	[theta1]			
e5	0	0	0	.	0	
				[theta3]		
e2	0	0	0	0	.	
					[theta2]	
e4	0	0	0	0	.	
					[theta5]	
e6	0	0	0	0	0	
d1	0	0	0	0	0	
d2	0	0	0	0	0	

Output 27.29.12 *continued*

Initial _EQSPHI_ Matrix				
	e4	e6	d1	d2
f_SES	0	0	0	0
e1	0	0	0	0
e3	0	0	0	0
e5	0	0	0	0
e2	.	0	0	0
	[theta5]			
e4	.	0	0	0
	[theta2]			
e6	0	.	0	0
		[theta4]		
d1	0	0	.	0
			[psi1]	
d2	0	0	0	.
				[psi2]

In the COSAN modeling language, you need to provide the three initial model matrices and the covariance structure formula for Σ , which is shown in the following statements:

```
proc calis cov data=Wheaton nobs=932 nose;
  cosan
    var = Anomie67 Anomie71 Education Powerless67 Powerless71 SEI,
        J(8, IDE) * Beta(8, GEN, IMI) * Gamma(9, GEN) * Phi(9, SYM);
  matrix Beta
    [1 4 8 , 7] = 1.0 0.833 beta,
    [2 5 , 8] = 1.0 0.833 ;
  matrix Gamma
    [3 6 7 8 , 1] = 1.0 lambda gamma1 gamma2,
    [1,2] = 8 * 1.0;
  matrix Phi
    [1,1] = phi 2*theta1 theta3 2*theta2 theta4 psi1 psi2,
    [3,2] = theta5 ,
    [6,5] = theta5 ;
  vnames J = [Anomie67 Anomie71 Education Powerless67 Powerless71 SEI
             f_Alien67 f_Alien71],
    Beta = J,
    Gamma = [f_SES e1 e3 e5 e2 e4 e6 d1 d2],
    Phi = Gamma;
run;
```

In the PROC CALIS statement, you provide the data set in the DATA= option and the number of observations in the NOBS= option. You use the NOSE option to turn off the computation of the standard error estimates.

In the VAR= option of the COSAN statement, you provide the list of observed variables for the analysis. You arrange the observed variables in such a way that they are in the same order as in [Output 27.29.10](#), [Output 27.29.10](#), and [Output 27.29.12](#). This is useful for comparing the results from the LINEQS and COSAN model specifications. After the specification of the observed variables, you specify the covariance structure model in the COSAN statement. Again, you only need to specify “half” of it. That is, the specification $J(8, IDE) * Beta(8, GEN, IMI) * Gamma(9, GEN) * Phi(9, SYM)$ in the COSAN statement automatically expands to

$$\Sigma = J * (I - Beta)^{-1} * Gamma * Phi * Gamma' * (I - Beta)^{-1'} * J'$$

which is the required covariance structures. Matrix properties and transformation types are defined in the arguments for the matrices.

Next, you use three matrix statements to specify the parameters in the matrix elements. The specifications here reflect exactly the initial specifications for the LINEQS model matrices as shown in [Output 27.29.10](#), [Output 27.29.10](#), and [Output 27.29.12](#).

In the V NAMES statement, you specify the column variable names for the matrices. The column variable names of the J matrix include all the observed variable names and the names of the intended endogenous latent factors f_Alien67 and f_Alien71. The column variable names for the Beta matrix are the same as those for matrix J. The column variables for the Gamma matrix include the intended latent factor f_SES and error variable names e1–e6 and d1–d2, which are arranged in such a way that they match the order of the error variables in the LINEQS output shown in [Output 27.29.12](#).

[Output 27.29.13](#) shows the covariance structures and some properties of the model matrices. The covariance structure formula for Sigma is defined as required. You can also check the matrix properties in this output to see if they are what you intend them to be.

Output 27.29.13 The Covariance Structures and Model Matrices of the COSAN Model for the Wheaton Data: EQS Emulation

COSAN Model Structures			
Sigma = J*inv(_I_-Beta)*Gamma*Phi*Gamma`*(inv(_I_-Beta))`*J`			
Summary of Model Matrices			
Matrix	N Row	N Col	Matrix Type
Beta	8	8	GEN: Square
Gamma	8	9	GEN: Rectangular
J	6	8	IDE: (I 0)
Phi	9	9	SYM: Symmetric

Output 27.29.14 shows the model fit chi-square of the current COSAN model. As expected, this is the same model fit as in Output 27.17.6 of Example 27.17 and in Output 27.29.5.

Output 27.29.14 Model Fit of the COSAN Model for the Wheaton Data: EQS Emulation

Fit Summary	
Chi-Square	13.4851
Chi-Square DF	9
Pr > Chi-Square	0.1419

Output 27.29.15 shows the estimates of the Beta matrix by the COSAN model specification. These estimates are essentially the same as the estimates of the _EQSBETA_ matrix obtained from the LINEQS model specification, as shown in Output 27.29.16.

Output 27.29.15 Estimate of the Beta Matrix by the COSAN Model Specification

Model Matrix Beta (8 x 8 General Square Matrix)				
	Anomie67	Anomie71	Education	Powerless67
Anomie67	0	0	0	0
Anomie71	0	0	0	0
Education	0	0	0	0
Powerless67	0	0	0	0
Powerless71	0	0	0	0
SEI	0	0	0	0
f_Alien67	0	0	0	0
f_Alien71	0	0	0	0

Model Matrix Beta (8 x 8 General Square Matrix)				
	Powerless71	SEI	f_Alien67	f_Alien71
Anomie67	0	0	1.0000	0
Anomie71	0	0	0	1.0000
Education	0	0	0	0
Powerless67	0	0	0.8330	0
Powerless71	0	0	0	0.8330
SEI	0	0	0	0
f_Alien67	0	0	0	0
f_Alien71	0	0	0.5931	0

[beta]

Output 27.29.16 Estimate of the `_EQSBETA_` Matrix by the LINEQS Model Specification

<code>_EQSBETA_</code> Matrix				
	<code>Anomie67</code>	<code>Anomie71</code>	<code>Education</code>	<code>Powerless67</code>
<code>Anomie67</code>	0	0	0	0
<code>Anomie71</code>	0	0	0	0
<code>Education</code>	0	0	0	0
<code>Powerless67</code>	0	0	0	0
<code>Powerless71</code>	0	0	0	0
<code>SEI</code>	0	0	0	0
<code>f_Alien67</code>	0	0	0	0
<code>f_Alien71</code>	0	0	0	0

<code>_EQSBETA_</code> Matrix				
	<code>Powerless71</code>	<code>SEI</code>	<code>f_Alien67</code>	<code>f_Alien71</code>
<code>Anomie67</code>	0	0	1.0000	0
<code>Anomie71</code>	0	0	0	1.0000
<code>Education</code>	0	0	0	0
<code>Powerless67</code>	0	0	0.8330	0
<code>Powerless71</code>	0	0	0	0.8330
<code>SEI</code>	0	0	0	0
<code>f_Alien67</code>	0	0	0	0
<code>f_Alien71</code>	0	0	0.5931 [beta]	0

Output 27.29.17 shows the estimates of the **Gamma** matrix by the COSAN model specification. Again, these estimates are essentially the same as the estimates of the `_EQSGAMMA_` matrix obtained from the LINEQS model specification, as shown in Output 27.29.18.

Output 27.29.17 Estimate of the Gamma Matrix by the COSAN Model Specification

Model Matrix Gamma (8 x 9 General Rectangular Matrix)					
	f_SES	e1	e3	e5	e2
Anomie67	0	1.0000	0	0	0
Anomie71	0	0	1.0000	0	0
Education	1.0000	0	0	1.0000	0
Powerless67	0	0	0	0	1.0000
Powerless71	0	0	0	0	0
SEI	5.3689 [lambda]	0	0	0	0
f_Alien67	-0.6299 [gamma1]	0	0	0	0
f_Alien71	-0.2409 [gamma2]	0	0	0	0

Model Matrix Gamma (8 x 9 General Rectangular Matrix)				
	e4	e6	d1	d2
Anomie67	0	0	0	0
Anomie71	0	0	0	0
Education	0	0	0	0
Powerless67	0	0	0	0
Powerless71	1.0000	0	0	0
SEI	0	1.0000	0	0
f_Alien67	0	0	1.0000	0
f_Alien71	0	0	0	1.0000

Output 27.29.18 Estimate of the `_EQSGAMMA_` Matrix by the LINEQS Model Specification

<u>_EQSGAMMA_ Matrix</u>					
	f_SES	e1	e3	e5	e2
Anomie67	0	1.0000	0	0	0
Anomie71	0	0	1.0000	0	0
Education	1.0000	0	0	1.0000	0
Powerless67	0	0	0	0	1.0000
Powerless71	0	0	0	0	0
SEI	5.3688 [lambda]	0	0	0	0
f_Alien67	-0.6299 [gamma1]	0	0	0	0
f_Alien71	-0.2409 [gamma2]	0	0	0	0
<u>_EQSGAMMA_ Matrix</u>					
	e4	e6	d1	d2	
Anomie67	0	0	0	0	
Anomie71	0	0	0	0	
Education	0	0	0	0	
Powerless67	0	0	0	0	
Powerless71	1.0000	0	0	0	
SEI	0	1.0000	0	0	
f_Alien67	0	0	1.0000	0	
f_Alien71	0	0	0	1.0000	

Finally, [Output 27.29.19](#) shows the estimates of the **Phi** matrix by the COSAN model specification. These estimates are essentially the same as the estimates of the `_EQSPHI_` matrix obtained from the LINEQS model specification, as shown in [Output 27.29.20](#).

Output 27.29.19 Estimate of the **Phi** Matrix by the COSAN Model Specification

		Model Matrix Phi (9 x 9 Symmetric Matrix)				
	f_SES	e1	e3	e5	e2	
f_SES	6.6162 [phi]	0	0	0	0	
e1	0	3.6078 [theta1]	0.9058 [theta5]	0	0	
e3	0	0.9058 [theta5]	3.6078 [theta1]	0	0	
e5	0	0	0	2.9938 [theta3]	0	
e2	0	0	0	0	3.5950 [theta2]	
e4	0	0	0	0	0.9058 [theta5]	
e6	0	0	0	0	0	
d1	0	0	0	0	0	
d2	0	0	0	0	0	

Output 27.29.19 *continued*

Model Matrix Phi (9 x 9 Symmetric Matrix)				
	e4	e6	d1	d2
f_SES	0	0	0	0
e1	0	0	0	0
e3	0	0	0	0
e5	0	0	0	0
e2	0.9058 [theta5]	0	0	0
e4	3.5950 [theta2]	0	0	0
e6	0	259.5738 [theta4]	0	0
d1	0	0	5.6705 [psi1]	0
d2	0	0	0	4.5148 [psi2]

Output 27.29.20 Estimate of the `_EQSPHI_` Matrix by the LINEQS Model Specification

		<code>_EQSPHI_</code> Matrix				
	<code>f_SES</code>	<code>e1</code>	<code>e3</code>	<code>e5</code>	<code>e2</code>	
<code>f_SES</code>	6.6163 [phi]	0	0	0	0	
<code>e1</code>	0	3.6080 [theta1]	0.9058 [theta5]	0	0	
<code>e3</code>	0	0.9058 [theta5]	3.6080 [theta1]	0	0	
<code>e5</code>	0	0	0	2.9937 [theta3]	0	
<code>e2</code>	0	0	0	0	3.5949 [theta2]	
<code>e4</code>	0	0	0	0	0.9058 [theta5]	
<code>e6</code>	0	0	0	0	0	
<code>d1</code>	0	0	0	0	0	
<code>d2</code>	0	0	0	0	0	

Output 27.29.20 *continued*

<u>_EQSPHI_ Matrix</u>				
	e4	e6	d1	d2
f_SES	0	0	0	0
e1	0	0	0	0
e3	0	0	0	0
e5	0	0	0	0
e2	0.9058 [theta5]	0	0	0
e4	3.5949 [theta2]	0	0	0
e6	0	259.5764 [theta4]	0	0
d1	0	0	5.6705 [psi1]	0
d2	0	0	0	4.5148 [psi2]

Example 27.30: Second-Order Confirmatory Factor Analysis

A second-order confirmatory factor analysis model is applied to a correlation matrix of Thurstone reported by McDonald (1985). The data set is shown in the following DATA step:

```
data Thurst (TYPE=CORR);
title "Example of THURSTONE resp. McDONALD (1985, p.57, p.105)";
  _TYPE_ = 'CORR'; Input _NAME_ $ Obs1-Obs9;
  label obs1='Sentences' obs2='Vocabulary' obs3='Sentence Completion'
        obs4='First Letters' obs5='Four-letter Words' obs6='Suffices'
        obs7='Letter series' obs8='Pedigrees' obs9='Letter Grouping';
  datalines;
obs1  1.      .      .      .      .      .      .      .      .
obs2  .828    1.      .      .      .      .      .      .      .
obs3  .776    .779    1.      .      .      .      .      .      .
obs4  .439    .493    .460    1.      .      .      .      .      .
obs5  .432    .464    .425    .674    1.      .      .      .      .
obs6  .447    .489    .443    .590    .541    1.      .      .      .
obs7  .447    .432    .401    .381    .402    .288    1.      .      .
obs8  .541    .537    .534    .350    .367    .320    .555    1.      .
obs9  .380    .358    .359    .424    .446    .325    .598    .452    1.
;

```

Using the LINEQS modeling language, you specify the three-term second-order factor analysis model in the following statements:

```
proc calis data=Thurst nobs=213 corr nose;
lineqs
  obs1 = x1 * f1 + e1,
  obs2 = x2 * f1 + e2,
  obs3 = x3 * f1 + e3,
  obs4 = x4 * f2 + e4,
  obs5 = x5 * f2 + e5,
  obs6 = x6 * f2 + e6,
  obs7 = x7 * f3 + e7,
  obs8 = x8 * f3 + e8,
  obs9 = x9 * f3 + e9,
  f1   = x10 * f4 + e10,
  f2   = x11 * f4 + e11,
  f3   = x12 * f4 + e12;
variance
  f4    = 1.,
  e1-e9 = u1-u9,
  e10-e12 = 3 * 1.;
bounds
  0. <= u1-u9;
run;

```

In the PROC CALIS statement, you specify the data set in the DATA= option and the number of observations in the NOBS= option. With the CORR option, you request the correlations be analyzed. You use the NOSE option to suppress the computation of standard error estimates.

In the LINEQS statement, the first-order loadings for the three factors, f1, f2, and f3, each refer to three variables, X1–X3, X4–X6, and X7–X9, respectively. One second-order factor, f4, reflects the correlations among the three first-order factors, f1, f2, and f3.

In the VARIANCE statement, you fix the variance of f4 to 1.0 for identification. The variances of error terms e1–e9 are free parameters u1–u9. The error variances for the three first-order factors are also fixed at 1.0 for identification purposes.

You also specify the boundary constraints for the error variance parameters u1–u9. You require them to be positive in the estimation.

Output 27.30.1 shows the estimation results.

Output 27.30.1 Estimation Results of the Second-Order Factor Model for Thurstone Data: LINEQS Model

Linear Equations	
Obs1 =	0.5151*f1 + 1.0000 e1 x1
Obs2 =	0.5203*f1 + 1.0000 e2 x2
Obs3 =	0.4874*f1 + 1.0000 e3 x3
Obs4 =	0.5211*f2 + 1.0000 e4 x4
Obs5 =	0.4971*f2 + 1.0000 e5 x5
Obs6 =	0.4381*f2 + 1.0000 e6 x6
Obs7 =	0.4524*f3 + 1.0000 e7 x7
Obs8 =	0.4173*f3 + 1.0000 e8 x8
Obs9 =	0.4076*f3 + 1.0000 e9 x9
f1 =	1.4438*f4 + 1.0000 e10 x10
f2 =	1.2538*f4 + 1.0000 e11 x11
f3 =	1.4065*f4 + 1.0000 e12 x12

Output 27.30.1 *continued*

Estimates for Variances of Exogenous Variables			
Variable Type	Variable	Parameter	Estimate
Latent	f4		1.00000
Error	e1	u1	0.18150
	e2	u2	0.16493
	e3	u3	0.26713
	e4	u4	0.30150
	e5	u5	0.36450
	e6	u6	0.50642
	e7	u7	0.39033
	e8	u8	0.48138
	e9	u9	0.50509
Disturbance	e10		1.00000
	e11		1.00000
	e12		1.00000

Alternatively, you can use the COSAN model specification for analyzing the same data set. First, under the second-order factor model, the covariance structures of the observed variables can be derived as

$$\Sigma = \mathbf{F1} * \mathbf{F2} * \mathbf{P} * \mathbf{F2}' * \mathbf{F1}' + \mathbf{F1} * \mathbf{U2} * \mathbf{F1}' + \mathbf{U1}$$

where $\mathbf{F1}$ is the 9×3 first-order loading matrix for the observed variables, $\mathbf{F2}$ is the 3×1 second-order loading matrix for the first-order factors, \mathbf{P} is the 1×1 covariance matrix for the second-order factor f4, $\mathbf{U2}$ is the 3×3 error covariance matrix of the first-order factors f1–f3 (or the covariance matrix of the error terms e10–12), and $\mathbf{U1}$ is the 9×9 error covariance matrix for the observed variables (or the covariance matrix of the error terms e1–9).

Matrix $\mathbf{F1}$ contains the loading parameters x1–x9 and matrix $\mathbf{F2}$ contains the loading parameters x10–x12. Because there is only one second-order factor f4 in the model, matrix \mathbf{P} is a scalar, which is a fixed constant 1 in the LINEQS model. Matrix $\mathbf{U2}$ is an identity matrix because all error variances are fixed at 1 and they are not correlated. Matrix $\mathbf{U2}$ is a diagonal matrix that contains the parameters u1–u9. Given this information, you can use the following statements to specify the second-order factor model as a COSAN model:

```

proc calis data=Thurst nobs=213 corr nose;
  cosan
    var = obs1-obs9,
    F1(3) * F2(1) * P(1,IDE) + F1(3) * U2(3,IDE) + U1(9,DIA);
  matrix F1
    [1 , @1] = x1-x3,
    [4 , @2] = x4-x6,
    [7 , @3] = x7-x9;
  matrix F2
    [ ,1] = x10-x12;
  matrix U1
    [1,1] = u1-u9;
  bounds
    0. <= u1-u9;
  vnames
    F1 = [f1 f2 f3],
    F2 = [f4],
    U1 = [e1-e9];
run;

```

In the PROC CALIS statement, you specify the observed variables in the VAR= option and the covariance structures for the observed variables. In the terms of the covariance structure formula, you need to specify the expressions only up the central symmetric matrices. The latter parts of these expressions are redundant and can be generated automatically by PROC CALIS, as shown in [Output 27.30.2](#).

Output 27.30.2 The Covariance Structures and Model Matrices of the Second-Order Factor Model: COSAN Model

COSAN Model Structures			
Sigma = F1*F2*P*F2`*F1` + F1*U2*F1` + U1			
Summary of Model Matrices			
Matrix	N Row	N Col	Matrix Type
F1	9	3	GEN: Rectangular
F2	3	1	GEN: Vector
P	1	1	IDE: Identity
U1	9	9	DIA: Diagonal
U2	3	3	IDE: Identity

[Output 27.30.2](#) shows that the intended covariance structures for the observed variables are being analyzed. The matrix types are shown next. Matrix **F1** is a rectangular matrix and matrix **F2** is a vector, although they have the default general (GEN) matrix type. Matrices **P** and **U2** are fixed identity (IDE) matrices in the model. For these two matrices, you do not need to specify any of their elements by using the MATRIX statement because they are already well-defined with the IDE type. Lastly, matrix **U1** is a diagonal (DIA) matrix in the model.

Output 27.30.3 shows the estimates of the first-order factor loading matrix **F1**.

Output 27.30.3 Estimation of the **F1** Matrix of the Second-Order Factor Model: COSAN Model

Model Matrix F1 (9 x 3 General Rectangular Matrix)			
	f1	f2	f3
Obs1 [x1]	0.5151	0	0
Obs2 [x2]	0.5203	0	0
Obs3 [x3]	0.4874	0	0
Obs4 [x4]	0	0.5211	0
Obs5 [x5]	0	0.4971	0
Obs6 [x6]	0	0.4381	0
Obs7 [x7]	0	0	0.4524
Obs8 [x8]	0	0	0.4173
Obs9 [x9]	0	0	0.4076

In the **MATRIX** statement for **F1**, you specify the pattern of the loadings. In the first entry of the **MATRIX** statement, you specify the loadings in the following elements: [1, 1], [2, 1], and [3, 1]. They are free parameters x1–x3, respectively. Notice that the @ sign is necessary in the first entry because the elements being defined would have been [1, 1], [2, 2], and [3, 3] otherwise. The @ sign fixes the column number to 1. See the **MATRIX** statement for more details about the notation. Similarly, you define the other clusters of loading in the second and third entries in the **MATRIX** statement for **F1**. This explains the pattern of factor loadings in Output 27.30.3. These loading estimates x1–x9 match those by the **LINEQS** model specification, as shown in Output 27.30.1.

Output 27.30.3 shows the estimates of the second-order factor loading matrix **F2**.

Output 27.30.4 Estimation of the **F2** Matrix of the Second-Order Factor Model: COSAN Model

Model Matrix F2 (3 x 1 Column Vector)	
	f4
f1	1.4438 [x10]
f2	1.2538 [x11]
f3	1.4066 [x12]

In the **MATRIX** statement for **F2**, you do not specify the row numbers in the [, 1] specification. PROC CALIS interprets this as stating that all the valid elements in the first column are being specified in the parameter list. In the current example, this means that elements **F2**[1, 1], **F2**[2, 1], and **F2**[3, 1] are filled with the free parameters x10, x11, and x12, respectively. Output 27.30.3 shows these specification and the corresponding estimates, which match those of the LINEQS model specification, as shown in Output 27.30.1.

Output 27.30.5 shows the estimates of the error covariance matrix $U1$.

Output 27.30.5 Estimation of the $U1$ Matrix of the Second-Order Factor Model: COSAN Model

Model Matrix U1 (9 x 9 Diagonal Matrix)					
	e1	e2	e3	e4	e5
e1	0.1815 [u1]	0	0	0	0
e2	0	0.1649 [u2]	0	0	0
e3	0	0	0.2671 [u3]	0	0
e4	0	0	0	0.3015 [u4]	0
e5	0	0	0	0	0.3645 [u5]
e6	0	0	0	0	0
e7	0	0	0	0	0
e8	0	0	0	0	0
e9	0	0	0	0	0

Output 27.30.5 *continued*

Model Matrix U1 (9 x 9 Diagonal Matrix)				
	e6	e7	e8	e9
e1	0	0	0	0
e2	0	0	0	0
e3	0	0	0	0
e4	0	0	0	0
e5	0	0	0	0
e6	0.5064 [u6]	0	0	0
e7	0	0.3903 [u7]	0	0
e8	0	0	0.4814 [u8]	0
e9	0	0	0	0.5051 [u9]

In the MATRIX statement for U1, you specify the diagonal elements of the matrix by using the starting element at [1, 1]. The parameter assignment proceeds to [2, 2], [3, 3] and so on such that all the trailing parameters u1–u9 are filled. This means that the last element U1[9, 9] is a free parameter named u9. Output 27.30.5 confirms this intended pattern. Again, all these error variance estimates match those by the LINEQS model specification, as shown in Output 27.30.1.

Example 27.31: Linear Relations among Factor Loadings: COSAN Model Specification

This example reanalyzes the models in Example 27.27 by using the COSAN modeling language. The correlation matrix of six variables from Kinzer and Kinzer (N=326) is used (see Guttman 1957). McDonald (1980) uses this data set to demonstrate the fitting of a factor analysis model with linear constraints on factor loadings. Two factors are assumed for the data. The factor loading matrix \mathbf{B} is shown in the following:

$$\mathbf{B} = \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \\ b_{31} & b_{32} \\ b_{41} & b_{42} \\ b_{51} & b_{52} \\ b_{61} & b_{62} \end{pmatrix}$$

The loadings on the second factor are linearly related to the loadings on the first factor, as described by the following formula:

$$b_{j2} = \alpha - b_{j1}, \quad j = 1, \dots, 6$$

The correlation structures are represented by

$$\mathbf{P} = \mathbf{B}\mathbf{B}' + \mathbf{\Psi}$$

where $\mathbf{\Psi} = \text{diag}(\psi_{11}, \psi_{22}, \psi_{33}, \psi_{44}, \psi_{55}, \psi_{66})$ represents the diagonal matrix of unique variances for the variables. Because matrix \mathbf{P} is a correlation matrix, its diagonal elements are fixed constants 1. This means that the diagonal elements of the correlation structures must also satisfy the following condition:

$$\Psi_{jj} = 1 - b_{j1}^2 - b_{j2}^2, \quad j = 1, \dots, 6$$

To analyze the correlation structures by using PROC CALIS, you formulate a covariance structure model with such correlation structures embedded in the model. That is, you want to fit the following covariance structure model to the Kinzer data:

$$\mathbf{\Sigma} = \mathbf{D}\mathbf{P}\mathbf{D}' = \mathbf{D}(\mathbf{B}\mathbf{B}' + \mathbf{\Psi})\mathbf{D}' = \mathbf{D}\mathbf{B}\mathbf{B}'\mathbf{D}' + \mathbf{D}\mathbf{\Psi}\mathbf{D}'$$

where \mathbf{D} is a 6 x 6 diagonal matrix that contains the population standard deviations of the observed variables.

The following statements use the COSAN modeling language to specify this covariance structure model:

```

proc calis data=Kinzer nobs=326 nose;
  cosan
    var= var1-var6,
    D(6,DIA) * B(2,GEN) + D(6,DIA) * Psi(6,DIA);
  matrix B
    [ ,1] = b11 b21 b31 b41 b51 b61,
    [ ,2] = b12 b22 b32 b42 b52 b62;
  matrix Psi
    [1,1] = psi1-psi6;
  matrix D
    [1,1] = d1-d6;
  parameters alpha (1.);

  /* SAS Programming Statements to Define Dependent Parameters*/
  /* 6 constraints on the factor loadings */
  b12 = alpha - b11;
  b22 = alpha - b21;
  b32 = alpha - b31;
  b42 = alpha - b41;
  b52 = alpha - b51;
  b62 = alpha - b61;

  /* 6 Constraints on Correlation structures */
  psi1 = 1. - b11 * b11 - b12 * b12;
  psi2 = 1. - b21 * b21 - b22 * b22;
  psi3 = 1. - b31 * b31 - b32 * b32;
  psi4 = 1. - b41 * b41 - b42 * b42;
  psi5 = 1. - b51 * b51 - b52 * b52;
  psi6 = 1. - b61 * b61 - b62 * b62;
  vnames
    D = [var1-var6],
    B = [factor1 factor2],
    Psi = D;
run;

```

In the PROC CALIS statement, you specify the data set by the DATA= option and the number of observations by the NOBS= option. You also use the NOSE option to suppress the printing of the standard error estimates.

In the COSAN statement, you specify the variables for the covariance structure analysis in the VAR= option. Next, you specify the covariance structure formula for the variables. When generating the covariance structure expressions for the terms, PROC CALIS examines the matrix type of the last matrix in each term to determine how the expression is generated. If the last matrix in a term is not a symmetric matrix (including diagonal or identity matrix), the transpose of the last matrix would be included in the expression. This ensures that a symmetric matrix expression is formed for the covariance structures. For example, the first term in the current covariance structure formula is $D(6, DIA) * B(2, GEN)$. Because **B** is not a symmetric matrix, the expression generated by PROC CALIS is

$$D * B * B' * D'$$

However, for the second term $D(6, DIA) * Psi(6, DIA)$, matrix **Psi** is a symmetric matrix so that the expression generated by PROC CALIS is

$$D * Psi * D'$$

Output 27.31.1 shows the covariance structure model and the model matrices. With **Psi** representing the unique variance matrix Ψ , the printed covariance structure formula for **Sigma** is clearly what you intend to specify.

Output 27.31.1 The Covariance Structures and Model Matrices: Linearly Constrained Loadings

COSAN Model Structures			
Sigma = D*B*B`*D` + D*Psi*D`			
Summary of Model Matrices			
Matrix	N Row	N Col	Matrix Type
B	6	2	GEN: Rectangular
D	6	6	DIA: Diagonal
Psi	6	6	DIA: Diagonal

In the MATRIX statements, you specify the parameters in the model matrices. You use parameters with the **b** prefix to name the two columns of loadings of the factor matrix **B**. You use free parameters **psi1–psi6** for the diagonal elements of the **Psi** matrix, and free parameters **d1–d6** for the diagonal elements of the **D** matrix. Next, you use a PARAMETERS statement to define an independent parameter **alpha** in the model. This parameter takes an initial value of 1.0. Using this independent parameter and six SAS programming statements, you define the loadings in the second column of matrix **B** as functions of the loadings in the first column of the same matrix.

You use six more SAS programming statements to define the unique variance parameters **psi1–psi6** as dependent parameters of the factor loadings. These constraints ensure that the embedded correlation structures have diagonal elements fixed at 1.0.

Lastly, you use the VNAMEs statement to label the column names of the model matrices. The column names of the diagonal matrix **D** are the same as the observed variables. The column names of matrix **B** are for the factor names.

As compared with the covariance structure specification (that is, the second specification) by the LINEQS model in Example 27.27, the current COSAN specification seems to be more direct and concise in specifying the parameter constraints. Because of the direct references to the matrix elements in the COSAN modeling language, you can set the required 12 constraints in a very straightforward way as the 12 SAS programming statements in the preceding specification. However, with the LINEQS model specification language in Example 27.27, you need 18 more SAS programming statements to define the correct constraints for the same covariance structure model.

Output 27.31.2 shows the fit summary table. The chi-square test statistic is 14.63 with $df = 8$ ($p = 0.067$). These are the same model fitting results as using the LINEQS model specification, as shown in Output 27.27.4 of Example 27.27.

Output 27.31.2 Model Fit: Linearly Constrained Loadings with Embedded Correlation Structures

Fit Summary	
Chi-Square	14.6269
Chi-Square DF	8
Pr > Chi-Square	0.0668

Output 27.31.3 shows the estimation of the loading matrix **B**. These estimates of factor loadings are essentially the same as those obtained from the LINEQS model specification, as shown in Output 27.27.6, except that the two columns of the loading matrix **B** are switched. The column switching is not a concern because the factor labels are arbitrary.

Output 27.31.3 Estimation of the B Matrix by the COSAN Model Specification

Model Matrix B (6 x 2 General Rectangular Matrix)		
	factor1	factor2
var1	0.6318 [b11]	0.3422 [b12]
var2	0.6531 [b21]	0.3210 [b22]
var3	0.4822 [b31]	0.4918 [b32]
var4	0.3985 [b41]	0.5755 [b42]
var5	0.1971 [b51]	0.7769 [b52]
var6	0.3074 [b61]	0.6666 [b62]

Output 27.31.4 shows the estimation of the scaling matrix **D**. All these standard deviation estimates for the observed variables match those obtained from the LINEQS model specification, as shown in Output 27.27.6.

Output 27.31.4 Estimation of the D Matrix by the COSAN Model Specification

Model Matrix D (6 x 6 Diagonal Matrix)						
	var1	var2	var3	var4	var5	var6
var1	1.0077 [d1]	0	0	0	0	0
var2	0	0.9971 [d2]	0	0	0	0
var3	0	0	0.9908 [d3]	0	0	0
var4	0	0	0	0.9909 [d4]	0	0
var5	0	0	0	0	0.9964 [d5]	0
var6	0	0	0	0	0	1.0169 [d6]

Output 27.31.5 shows the estimation of the unique covariance matrix Ψ . All these unique variance parameter estimates match those obtained from the LINEQS model specification, as shown in Output 27.27.6.

Output 27.31.5 Estimation of the Psi Matrix by the COSAN Model Specification

Model Matrix Psi (6 x 6 Diagonal Matrix)						
	var1	var2	var3	var4	var5	var6
var1	0.4837 [psi1]	0	0	0	0	0
var2	0	0.4705 [psi2]	0	0	0	0
var3	0	0	0.5256 [psi3]	0	0	0
var4	0	0	0	0.5100 [psi4]	0	0
var5	0	0	0	0	0.3576 [psi5]	0
var6	0	0	0	0	0	0.4612 [psi6]

Finally, Output 27.31.6 shows the estimation of the independent parameter alpha. The same estimate of alpha is shown in Output 27.27.6.

Output 27.31.6 Estimation of the Independent Parameter alpha by the COSAN Model Specification

Additional Parameters		
Type	Parameter	Estimate
Independent	alpha	0.97400

Example 27.32: Ordinal Relations among Factor Loadings

The same data set as in Example 27.31 is used in McDonald (1980) for analysis with ordinally constrained factor loadings. In Example 27.27, the results of the linearly constrained factor analysis show that the loadings of the two factors are ordered as 2, 1, 3, 4, 6, 5. McDonald (1980) then tests the hypothesis that the factor loadings are all nonnegative and can be ordered in the following manner:

$$b_{11} \geq b_{21} \geq b_{31} \geq b_{41} \geq b_{51} \geq b_{61}$$

$$b_{12} \leq b_{22} \leq b_{32} \leq b_{42} \leq b_{52} \leq b_{62}$$

In this example, you implement these ordinal relationships by using the LINCON statement in the following COSAN model specification:

```
proc calis data=Kinzer nobs=326 nose;
  cosan
    var= var1-var6,
    D(6,DIA) * B(2,GEN) + D(6,DIA) * Psi(6,DIA);
  matrix B
    [ ,1]= b11 b21 b31 b41 b51 b61,
    [ ,2]= 0. b22 b32 b42 b52 b62;
  matrix Psi
    [1,1]= psi1-psi6;
  matrix D
    [1,1]= d1-d6 ;
  lincon
    b61 <= b51,
    b51 <= b41,
    b41 <= b31,
    b31 <= b21,
    b21 <= b11,
    0. <= b22,
    b22 <= b32,
    b32 <= b42,
    b42 <= b52,
    b52 <= b62;

  /* SAS Programming Statements */
  /* 6 Constraints on Correlation structures */
  psi1 = 1. - b11 * b11;
  psi2 = 1. - b21 * b21 - b22 * b22;
  psi3 = 1. - b31 * b31 - b32 * b32;
  psi4 = 1. - b41 * b41 - b42 * b42;
  psi5 = 1. - b51 * b51 - b52 * b52;
  psi6 = 1. - b61 * b61 - b62 * b62;
  vnames
    B = [factor1 factor2],
    Psi = [var1-var6],
    D = Psi;
run;
```

As in Example 27.31, correlation structures are analyzed in the current example so that the unique variance parameters psi1–psi6 are defined as functions of the loadings in the SAS programming statements. However,

the loading parameters are no longer not constrained in the current model. Instead, you impose ordinal constraints on the loading parameters. First, b21 is fixed at 0 for identification purposes. Then, you use the LINCON statement to specify the ordinal relations of the factor loadings.

As shown in [Output 27.32.1](#), the solution converges in 12 iterations. In the fit summary table, the chi-square test statistic is 8.48 ($df = 6, p = 0.20$). This indicates a good fit. However, in the model there are 11 loading parameters (the b's) and 6 population standard deviation parameters (the d's). The degrees of freedom should have been $4 = 21 - 11 - 6$, but why is this number 6 in the fit summary table?

Output 27.32.1 Final Iteration Status and Fit

Optimization Results			
Iterations	12	Function Calls	29
Jacobian Calls	14	Active Constraints	2
Objective Function	0.0260990149	Max Abs Gradient Element	2.7626747E-6
Lambda	0	Actual Over Pred Change	1.1572072766
Radius	0.0000851592		
Convergence criterion (ABSGCONV=0.00001) satisfied.			
Fit Summary			
Chi-Square	8.4822		
Chi-Square DF	6		
Pr > Chi-Square	0.2049		

The reason is that there are two active constraints in the solution, resulting in two free parameters fewer in the final solution than originally specified. Active constraints are those inequality constraints that are fulfilled on the boundary equalities. As shown in the “Optimization Results” table, the number of active constraints for the current fitting is two. The default treatment in PROC CALIS is to treat these active constraints as if they were going to happen for all possible repeated sampling. This might as well be seen as fitting the active equality constraints on every possible repeated sample. This results in an increase of the degrees of freedom for model fit, as adjusted in the current fit summary table in [Output 27.32.1](#). To warn you about the degrees-of-freedom adjustment, the following messages are also printed with the output:

WARNING: There are 2 active boundary or linear inequality constraints at the solution. The standard errors and chi-square test statistic assume that the solution is located in the interior of the parameter space; hence, they do not apply if it is likely that some different set of inequality a constraints could be active.

NOTE: The degrees of freedom are increased by the number of active constraints. The number of parameters in calculating fit indices is decreased by the number of active constraints. To turn off the adjustment, use the NOADJDF option.

When active constraints are encountered, you need to be cautious about two implications. First, the estimates fall on the boundary of the parameter space originally specified. As shown in [Output 27.32.2](#), estimates for b_{11} and b_{21} are the same, and so are the pair of estimates for b_{52} and b_{62} . These pairs of parameters were originally constrained by inequalities in the model. For example, b_{62} was constrained to be at least as large as b_{52} . The fact that this constraint is honored only on the bound means that a better model fit might exist with b_{62} being smaller than b_{52} . Similarly, a better model fit might result without requiring b_{11} to be at least as large as b_{21} . Therefore, solutions with active boundary constraints might imply that the original strict inequality constraints are not appropriate for the data.

Output 27.32.2 Estimation of the Factor Loading Matrix B

Model Matrix B (6 x 2 General Rectangular Matrix)		
	factor1	factor2
var1	0.7100 [b11]	0
var2	0.7100 [b21]	0.0393 [b22]
var3	0.6799 [b31]	0.2463 [b32]
var4	0.6561 [b41]	0.3295 [b42]
var5	0.5541 [b51]	0.5432 [b52]
var6	0.4733 [b61]	0.5432 [b62]

Output 27.32.3 Estimation of the Scaling Matrix D and Unique Covariance Matrix Psi

Model Matrix D (6 x 6 Diagonal Matrix)						
	var1	var2	var3	var4	var5	var6
var1	1.0022 [d1]	0	0	0	0	0
var2	0	0.9985 [d2]	0	0	0	0
var3	0	0	1.0004 [d3]	0	0	0
var4	0	0	0	1.0004 [d4]	0	0
var5	0	0	0	0	0.9990 [d5]	0
var6	0	0	0	0	0	1.0021 [d6]
Model Matrix Psi (6 x 6 Diagonal Matrix)						
	var1	var2	var3	var4	var5	var6
var1	0.4959 [psi1]	0	0	0	0	0
var2	0	0.4944 [psi2]	0	0	0	0
var3	0	0	0.4771 [psi3]	0	0	0
var4	0	0	0	0.4610 [psi4]	0	0
var5	0	0	0	0	0.3979 [psi5]	0
var6	0	0	0	0	0	0.4809 [psi6]

The second implication for the presence of active constraints is that the chi-square test statistic and the standard error estimates are computed as if repeated samples were fitted by the model with the presence of the active equality constraints. The degrees-of-freedom adjustment by PROC CALIS is based on this assumption. However, if the particular active constraints reflect only a rare sampling event, the degrees-of-freedom adjustment (or even the computation of the chi-square statistic and standard error estimates) might not be justified. Unfortunately, whether the active constraints are reflecting the truth of the model or pure sampling fluctuation is usually difficult to determine.

Example 27.33: Longitudinal Factor Analysis

The following example (McDonald 1980) illustrates both the ability of PROC CALIS to formulate complex covariance structure analysis problems by the generalized COSAN matrix model and the use of programming statements to impose nonlinear constraints on the parameters. The example is a longitudinal factor analysis that uses the Swaminathan (1974) model. For $m = 3$ tests, $k = 3$ occasions, and $r = 2$ factors, the covariance structure model is formulated as follows:

$$\Sigma = \mathbf{F}_1 \mathbf{F}_2 \mathbf{F}_3 \mathbf{L} \mathbf{F}_3^{-1} \mathbf{F}_2^{-1} \mathbf{P} (\mathbf{F}_2^{-1})' (\mathbf{F}_3^{-1})' \mathbf{L}' \mathbf{F}_3' \mathbf{F}_2' \mathbf{F}_1' + \mathbf{U}^2$$

$$\mathbf{F}_1 = \begin{pmatrix} \mathbf{B}_1 & & \\ & \mathbf{B}_2 & \\ & & \mathbf{B}_3 \end{pmatrix}, \quad \mathbf{F}_2 = \begin{pmatrix} \mathbf{I}_2 & & \\ & \mathbf{D}_2 & \\ & & \mathbf{D}_2 \end{pmatrix}, \quad \mathbf{F}_3 = \begin{pmatrix} \mathbf{I}_2 & & \\ & \mathbf{I}_2 & \\ & & \mathbf{D}_3 \end{pmatrix}$$

$$\mathbf{L} = \begin{pmatrix} \mathbf{I}_2 & 0 & 0 \\ \mathbf{I}_2 & \mathbf{I}_2 & 0 \\ \mathbf{I}_2 & \mathbf{I}_2 & \mathbf{I}_2 \end{pmatrix}, \quad \mathbf{P} = \begin{pmatrix} \mathbf{I}_2 & & \\ & \mathbf{S}_2 & \\ & & \mathbf{S}_3 \end{pmatrix}, \quad \mathbf{U} = \begin{pmatrix} \mathbf{U}_{11} & \mathbf{U}_{12} & \mathbf{U}_{13} \\ \mathbf{U}_{21} & \mathbf{U}_{22} & \mathbf{U}_{23} \\ \mathbf{U}_{31} & \mathbf{U}_{32} & \mathbf{U}_{33} \end{pmatrix}$$

$$\mathbf{S}_2 = \mathbf{I}_2 - \mathbf{D}_2^2, \quad \mathbf{S}_3 = \mathbf{I}_2 - \mathbf{D}_3^2$$

The Swaminathan longitudinal factor model assumes that the factor scores for each (m) common factor change from occasion to occasion (k) according to a first-order autoregressive scheme. The matrix \mathbf{F}_1 contains the k factor loading matrices \mathbf{B}_1 , \mathbf{B}_2 , and \mathbf{B}_3 (each is $n \times m$). The matrices \mathbf{D}_2 , \mathbf{D}_3 , \mathbf{S}_2 , \mathbf{S}_3 and U_{ij} , $i, j = 1, \dots, k$, are diagonal, and the matrices \mathbf{D}_i and \mathbf{S}_i , $i = 2, \dots, k$, are subjected to the constraint

$$\mathbf{S}_i + \mathbf{D}_i^2 = \mathbf{I}$$

Although the covariance structure model looks pretty complicated, it poses no problem for the COSAN model specifications. Since the constructed correlation matrix given by McDonald (1980) is singular, only unweighted least squares (METHOD=LS) estimates can be computed. The following statements specify the COSAN model for the correlation structures.

```
Title "Swaminathan's Longitudinal Factor Model, Data: McDONALD(1980)";
Title2 "Constructed Singular Correlation Matrix, GLS & ML not possible";
data Mcdon(TYPE=CORR);
    _TYPE_ = 'CORR'; INPUT _NAME_ $ obs1-obs9;
    datalines;
obs1  1.000      .      .      .      .      .      .      .      .
obs2  .100  1.000      .      .      .      .      .      .      .
```

```

obs3  .250  .400  1.000  .      .      .      .      .      .
obs4  .720  .108  .270  1.000  .      .      .      .      .
obs5  .135  .740  .380  .180  1.000  .      .      .      .
obs6  .270  .318  .800  .360  .530  1.000  .      .      .
obs7  .650  .054  .135  .730  .090  .180  1.000  .      .
obs8  .108  .690  .196  .144  .700  .269  .200  1.000  .
obs9  .189  .202  .710  .252  .336  .760  .350  .580  1.000
;

proc calis data=Mcdon method=ls nobs=100 corr;
  cosan
    var = obs1-obs9,
    F1(6,GEN) * F2(6,DIA) * F3(6,DIA) * L(6,LOW) * F3(6,DIA,INV)
      * F2(6,DIA,INV) * P(6,DIA) + U(9,SYM);
  matrix F1
    [1 , @1] = x1-x3,
    [2 , @2] = x4-x5,
    [4 , @3] = x6-x8,
    [5 , @4] = x9-x10,
    [7 , @5] = x11-x13,
    [8 , @6] = x14-x15;
  matrix F2
    [1,1]= 2 * 1. x16 x17 x16 x17;
  matrix F3
    [1,1]= 4 * 1. x18 x19;
  matrix L
    [1,1]= 6 * 1.,
    [3,1]= 4 * 1.,
    [5,1]= 2 * 1.;
  matrix P
    [1,1]= 2 * 1. x20-x23;
  matrix U
    [1,1]= x24-x32,
    [4,1]= x33-x38,
    [7,1]= x39-x41;
  bounds 0. <= x24-x32,
    -1. <= x16-x19 <= 1.;
  /* SAS programming statements for dependent parameters */
  x20 = 1. - x16 * x16;
  x21 = 1. - x17 * x17;
  x22 = 1. - x18 * x18;
  x23 = 1. - x19 * x19;
run;

```

In the PROC CALIS statement, you use the NOBS= option to specify the number of observations. The CORR option requests the analysis of the correlation matrix.

In the COSAN statement, you list the observed variables for the analysis in the VAR= option. Then you specify the formula for the covariance structures. Notice that in the covariance structure formula, some matrices are specified twice. That is, matrix **F2** and **F3** appear in two different places. Matrices with the same name means that they are identical—which certainly makes sense. In addition, you can apply different transformations to the same matrix in different locations of the matrix formula. For example, you do not transform matrix **F2** in the first location, but the same matrix is inverted (INV) later in the expression. Similarly for matrix **F3**.

Next, you define the parameters in the six distinct model matrices by six MATRIX statements. Each matrix has some specific patterns under the covariance structure model. For the **F1** matrix, it has the following pattern for the free parameters in the model:

	col1	col2	col3	col4	col5	col6
row1	x					
row2	x	x				
row3	x	x				
row4			x			
row5			x	x		
row6			x	x		
row7					x	
row8					x	x
row9					x	x

To specify these parameters, you can use some shorthand notation in the MATRIX statement. For example, in the first entry of the MATRIX statement for matrix **F1**, you use the notation `[1, @1]`. This means that the parameter specification starts with the `[1, 1]` element and proceeds to the next element while fixing the column number at 1. Hence, parameters `x1–x3` are specified for the `F1[1, 1]`, `F1[2, 1]`, and `F1[3, 1]` elements, respectively. Similarly, you specify other parameters in the **F1** matrix in a column by column fashion.

If you do not use the `@` sign in the specification, the parameters are assigned differently. For example, in the specification of the **L** matrix, the first entry in the corresponding MATRIX statement also starts with the `[1, 1]` element. But it proceeds down to `[2, 2]`, `[3, 3]`, and so on because the `@` sign is not used to fix any column or row number. As a result, the MATRIX statement for **L** specifies the following pattern:

	col1	col2	col3	col4	col5	col6
row1	1					
row2		1				
row3	1		1			
row4		1		1		
row5	1		1		1	
row6		1		1		1

The unspecified elements are fixed zeros in the model.

Similarly, you specify the diagonal matrices **F2**, **F3**, and **P**, and the symmetric matrix **U**.

You also set bounds for some parameters in the BOUNDS statement and some dependent parameters in the SAS programming statements.

Output 27.33.1 shows the correlation structures and the model matrices in the analysis. All appear to be intended.

Output 27.33.1 The Correlation Structures and Model Matrices of the Longitudinal Factor Model

COSAN Model Structures	
Sigma =	$F1 * F2 * F3 * L * \text{inv}(F3) * \text{inv}(F2) * P * (\text{inv}(F2))' * (\text{inv}(F3))' * L' * F3' * F2' * F1' + U$

Output 27.33.1 *continued*

Summary of Model Matrices			
Matrix	N Row	N Col	Matrix Type
F1	9	6	GEN: Rectangular
F2	6	6	DIA: Diagonal
F3	6	6	DIA: Diagonal
L	6	6	LOW: L Triangular
P	6	6	DIA: Diagonal
U	9	9	SYM: Symmetric

PROC CALIS finds a converged solution for the estimation problem. [Output 27.33.2](#), [Output 27.33.3](#), and [Output 27.33.4](#) show the estimation results of the F1, F2, and F3 matrices, respectively.

Output 27.33.2 Estimation of the F1 Matrix of the Longitudinal Factor Model

Model Matrix F1 (9 x 6 General Rectangular Matrix)						
	Col1	Col2	Col3	Col4	Col5	Col6
obs1	0.3515 [x1]	0	0	0	0	0
obs2	0.2871 [x2]	0.9528 [x4]	0	0	0	0
obs3	0.7101 [x3]	0.2059 [x5]	0	0	0	0
obs4	0	0	0.4204 [x6]	0	0	0
obs5	0	0	0.4303 [x7]	0.9027 [x9]	0	0
obs6	0	0	0.8591 [x8]	0.1772 [x10]	0	0
obs7	0	0	0	0	0.3487 [x11]	0
obs8	0	0	0	0	0.5924 [x12]	-0.1971 [x14]
obs9	0	0	0	0	0.9987 [x13]	0.0871 [x15]

Output 27.33.3 Estimation of the F2 Matrix of the Longitudinal Factor Model

Model Matrix F2 (6 x 6 Diagonal Matrix)						
	Col1	Col2	Col3	Col4	Col5	Col6
Row1	1.0000	0	0	0	0	0
Row2	0	1.0000	0	0	0	0
Row3	0	0	0.8939 [x16]	0	0	0
Row4	0	0	0	0.5806 [x17]	0	0
Row5	0	0	0	0	0.8939 [x16]	0
Row6	0	0	0	0	0	0.5806 [x17]

Output 27.33.4 Estimation of the F3 Matrix of the Longitudinal Factor Model

Model Matrix F3 (6 x 6 Diagonal Matrix)						
	Col1	Col2	Col3	Col4	Col5	Col6
Row1	1.0000	0	0	0	0	0
Row2	0	1.0000	0	0	0	0
Row3	0	0	1.0000	0	0	0
Row4	0	0	0	1.0000	0	0
Row5	0	0	0	0	0.5963 [x18]	0
Row6	0	0	0	0	0	1.0000 [x19]

Output 27.33.5 shows the estimation results of the **L** matrix, which is a fixed matrix that contains only 0 or 1 for its elements.

Output 27.33.5 Estimation of the **L** Matrix of the Longitudinal Factor Model

Model Matrix L (6 x 6 Lower Triangular Matrix)						
	Col1	Col2	Col3	Col4	Col5	Col6
Row1	1.0000	0	0	0	0	0
Row2	0	1.0000	0	0	0	0
Row3	1.0000	0	1.0000	0	0	0
Row4	0	1.0000	0	1.0000	0	0
Row5	1.0000	0	1.0000	0	1.0000	0
Row6	0	1.0000	0	1.0000	0	1.0000

Output 27.33.6 shows the estimation results of the **P** matrix. Notice that parameter estimate **x23** falls on the lower boundary at zero.

Output 27.33.6 Estimation of the **P** Matrix of the Longitudinal Factor Model

Model Matrix P (6 x 6 Diagonal Matrix)						
	Col1	Col2	Col3	Col4	Col5	Col6
Row1	1.0000	0	0	0	0	0
Row2	0	1.0000	0	0	0	0
Row3	0	0	0.2010 [x20]	0	0	0
Row4	0	0	0	0.6629 [x21]	0	0
Row5	0	0	0	0	0.6444 [x22]	0
Row6	0	0	0	0	0	0 [x23]

In fact, PROC CALIS routinely checks for zero values for the estimates on the diagonal of the central symmetric matrices. In this case, you get the following messages regarding the estimation of matrix **P**:

WARNING: Although all predicted variances for the observed variables are positive, the corresponding predicted covariance matrix is not positive definite. It has one negative eigenvalue.
 WARNING: The estimated variance of variable 6 is essentially zero in the central matrix P of term 1 of the COSAN model.
 WARNING: The central matrix P of term 1 of the COSAN model is not positive definite. It has one zero eigenvalue.

Output 27.33.7 shows the estimation results of the U matrix. Parameter estimates x28 and x32 fall on the lower boundary at zero. PROC CALIS issues the following messages regarding the estimation of matrix U:

WARNING: The estimated variance of obs5 is essentially zero in the central matrix U of term 2 of the COSAN model.
 WARNING: The estimated variance of obs9 is essentially zero in the central matrix U of term 2 of the COSAN model.
 WARNING: The central matrix U of term 2 of the COSAN model is not positive definite. It has 3 negative eigenvalues.

Output 27.33.7 Estimation of the U Matrix of the Longitudinal Factor Model

Model Matrix U (9 x 9 Symmetric Matrix)					
	obs1	obs2	obs3	obs4	obs5
obs1	0.8764 [x24]	0	0	0.5879 [x33]	0
obs2	0	0.009683 [x25]	0	0	0.1302 [x34]
obs3	0	0	0.4533 [x26]	0	0
obs4	0.5879 [x33]	0	0	0.8233 [x27]	0
obs5	0	0.1302 [x34]	0	0	0 [x28]
obs6	0	0	0.2335 [x35]	0	0
obs7	0.5847 [x39]	0	0	0.6426 [x36]	0
obs8	0	0.7084 [x40]	0	0	0.7259 [x37]
obs9	0	0	0.3215 [x41]	0	0

Output 27.33.7 continued

Model Matrix U (9 x 9 Symmetric Matrix)				
	obs6	obs7	obs8	obs9
obs1	0	0.5847 [x39]	0	0
obs2	0	0	0.7084 [x40]	0
obs3	0.2335 [x35]	0	0	0.3215 [x41]
obs4	0	0.6426 [x36]	0	0
obs5	0	0	0.7259 [x37]	0
obs6	0.2305 [x29]	0	0	0.2329 [x38]
obs7	0	0.8784 [x30]	0	0
obs8	0	0	0.6102 [x31]	0
obs9	0.2329 [x38]	0	0	0 [x32]

Because this formulation of Swaminathan's model in general leads to an unidentified problem, the results given here are different from those reported by McDonald (1980). The displayed output of PROC CALIS also indicates that the fitted central model matrices \mathbf{P} and \mathbf{U} are not positive-definite. The BOUNDS statement constrains the diagonals of the matrices \mathbf{P} and \mathbf{U} to be nonnegative, but this cannot prevent \mathbf{U} from having three negative eigenvalues. The fact that many of the published results for more complex models in covariance structure analysis are connected to unidentified problems implies that more theoretical work should be done to study the general features of such models.

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Chapter 28

The CANCORR Procedure

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Overview: CANCORR Procedure

The CANCORR procedure performs canonical correlation, partial canonical correlation, and canonical redundancy analysis.

Canonical correlation is a generalization of multiple correlation for analyzing the relationship between two sets of variables. In multiple correlation, you examine the relationship between a linear combination of a set of explanatory variables, X , and a *single* response variable, Y . In canonical correlation, you examine the relationship between linear combinations of the set of X variables and linear combinations of a *set* of Y variables. These linear combinations are called *canonical variables* or *canonical variates*. Either set of variables can be considered explanatory or response variables, since the statistical model is symmetric in the two sets of variables. Simple and multiple correlation are special cases of canonical correlation in which one or both sets contain a single variable.

The CANCELL procedure tests a series of hypotheses that each canonical correlation and all smaller canonical correlations are zero in the population. PROC CANCELL uses an F approximation (Rao 1973; Kshirsagar 1972) that gives better small sample results than the usual χ^2 approximation. At least one of the two sets of variables should have an approximate multivariate normal distribution in order for the probability levels to be valid.

Both standardized and unstandardized canonical coefficients are computed, as well as the four *canonical structure* matrices showing correlations between the two sets of canonical variables and the two sets of original variables. A canonical redundancy analysis (Stewart and Love 1968; Cooley and Lohnes 1971) can also be done. PROC CANCELL provides multiple regression analysis options to aid in interpreting the canonical correlation analysis. You can examine the linear regression of each variable on the opposite set of variables.

PROC CANCELL can produce a data set containing the scores of each observation on each canonical variable, and you can use the PRINT procedure to list these values. A plot of each canonical variable against its counterpart in the other group is often useful, and you can use PROC SGLOT with the output data set to produce these plots. A second output data set contains the canonical correlations, coefficients, and most other statistics computed by the procedure.

Background

Canonical correlation was developed by Hotelling (1935, 1936).

The application of canonical correlation is discussed by Cooley and Lohnes (1971); Tatsuoka (1971); Mardia, Kent, and Bibby (1979). One of the best theoretical treatments is given by Kshirsagar (1972).

Given a set of p X variables and q Y variables, the CANCELL procedure finds the linear combinations

$$\begin{aligned}w_1 &= a_{11}x_1 + a_{21}x_2 + \cdots + a_{p1}x_p \\v_1 &= b_{11}y_1 + b_{21}y_2 + \cdots + b_{q1}y_q\end{aligned}$$

such that the two canonical variables, w_1 and v_1 , have the largest possible correlation. This maximized correlation between the two canonical variables is the first canonical correlation. The coefficients of the linear combinations are canonical coefficients or canonical weights. It is customary to normalize the canonical coefficients so that each canonical variable has a variance of 1.

PROC CANCELL continues by finding a second set of canonical variables, uncorrelated with the first pair, that produces the second-highest correlation coefficient. That is, the second pair of canonical variables is

$$\begin{aligned}w_2 &= a_{12}x_1 + a_{22}x_2 + \cdots + a_{p2}x_p \\v_2 &= b_{12}y_1 + b_{22}y_2 + \cdots + b_{q2}y_q\end{aligned}$$

such that w_2 is uncorrelated with w_1 and v_1 , v_2 is uncorrelated with w_1 and v_1 , and w_2 and v_2 have the largest possible correlation subject to these constraints. The process of constructing canonical variables continues until the number of pairs of canonical variables is $\min(p, q)$, the number of variables in the smaller group.

Each canonical variable is uncorrelated with all the other canonical variables of either set except for the one corresponding canonical variable in the opposite set. The canonical coefficients are not generally orthogonal, however, so the canonical variables do not represent jointly perpendicular directions through the space of the original variables.

The first canonical correlation is at least as large as the multiple correlation between any variable and the opposite set of variables. It is possible for the first canonical correlation to be very large while all the multiple correlations for predicting one of the original variables from the opposite set of canonical variables are small. Canonical redundancy analysis (Stewart and Love 1968; Cooley and Lohnes 1971; van den Wollenberg 1977) examines how well the original variables can be predicted from the canonical variables.

PROC CANCERR can also perform partial canonical correlation, which is a multivariate generalization of ordinary partial correlation (Cooley and Lohnes 1971; Timm 1975). Most commonly used parametric statistical methods, ranging from t tests to multivariate analysis of covariance, are special cases of partial canonical correlation.

Getting Started: CANCERR Procedure

The following example demonstrates how you can use the CANCERR procedure to calculate and test canonical correlations between two sets of variables.

Suppose you want to determine the degree of correspondence between a set of job characteristics and measures of employee satisfaction. Using a survey instrument for employees, you calculate three measures of job satisfaction. With another instrument designed for supervisors, you calculate the corresponding job characteristics profile.

Your three variables associated with job satisfaction are as follows:

- career track satisfaction: employee satisfaction with career direction and the possibility of future advancement, expressed as a percent
- management and supervisor satisfaction: employee satisfaction with supervisor's communication and management style, expressed as a percent
- financial satisfaction: employee satisfaction with salary and other benefits, using a scale measurement from 1 to 10 (1=unsatisfied, 10=satisfied)

The three variables associated with job characteristics are as follows:

- task variety: degree of variety involved in tasks, expressed as a percent
- feedback: degree of feedback required in job tasks, expressed as a percent
- autonomy: degree of autonomy required in job tasks, expressed as a percent

The following statements create the SAS data set Jobs and request a canonical correlation analysis:

```

data Jobs;
  input Career Supervisor Finance Variety Feedback Autonomy;
  label Career      ='Career Satisfaction' Variety ='Task Variety'
        Supervisor='Supervisor Satisfaction' Feedback='Amount of Feedback'
        Finance     ='Financial Satisfaction' Autonomy='Degree of Autonomy';
  datalines;
72 26 9          10 11 70
63 76 7          85 22 93
96 31 7          83 63 73
96 98 6          82 75 97
84 94 6          36 77 97
66 10 5          28 24 75
31 40 9          64 23 75
45 14 2          19 15 50
42 18 6          33 13 70
79 74 4          23 14 90
39 12 2          37 13 70
54 35 3          23 74 53
60 75 5          45 58 83
63 45 5          22 67 53
;

proc cancorr data=Jobs
  vprefix=Satisfaction wprefix=Characteristics
  vname='Satisfaction Areas' wname='Job Characteristics';
  var Career Supervisor Finance;
  with Variety Feedback Autonomy;
run;

```

The DATA= option in the PROC CANCELL statement specifies Jobs as the SAS data set to be analyzed. The VPREFIX and WPREFIX options specify the prefixes for naming the canonical variables from the VAR statement and the WITH statement, respectively. The VNAME option specifies 'Satisfaction Areas' to refer to the set of variables from the VAR statement. Similarly, the WNAME option specifies 'Job Characteristics' to refer to the set of variables from the WITH statement.

The VAR statement defines the first of the two sets of variables to be analyzed as Career, Supervisor, and Finance. The WITH statement defines the second set of variables to be Variety, Feedback, and Autonomy. The results of this analysis are displayed in [Figure 28.1](#) to [Figure 28.4](#).

[Figure 28.1](#) displays the canonical correlation, adjusted canonical correlation, approximate standard error, and squared canonical correlation for each pair of canonical variables. The first canonical correlation (the correlation between the first pair of canonical variables) is 0.9194. This value represents the highest possible correlation between any linear combination of the job satisfaction variables and any linear combination of the job characteristics variables.

[Figure 28.1](#) also lists the likelihood ratio and associated statistics for testing the hypothesis that the canonical correlations in the current row and all that follow are zero.

Figure 28.1 Canonical Correlations, Eigenvalues, and Likelihood Tests

The CANCERR Procedure					
Canonical Correlation Analysis					
	Canonical Correlation	Adjusted Canonical Correlation	Approximate Standard Error	Squared Canonical Correlation	
1	0.919412	0.898444	0.042901	0.845318	
2	0.418649	0.276633	0.228740	0.175267	
3	0.113366	.	0.273786	0.012852	
Eigenvalues of Inv(E) * H = CanRsqr / (1 - CanRsqr)					
	Eigenvalue	Difference	Proportion	Cumulative	
1	5.4649	5.2524	0.9604	0.9604	
2	0.2125	0.1995	0.0373	0.9977	
3	0.0130		0.0023	1.0000	
Test of H0: The canonical correlations in the current row and all that follow are zero					
	Likelihood Ratio	Approximate F Value	Num DF	Den DF	Pr > F
1	0.12593148	2.93	9	19.621	0.0223
2	0.81413359	0.49	4	18	0.7450
3	0.98714819	0.13	1	10	0.7257

The first approximate F value of 2.93 corresponds to the test that all three canonical correlations are zero. Since the p -value is small (0.0223), you would reject the null hypothesis at the 0.05 level. The second approximate F value of 0.49 corresponds to the test that both the second and the third canonical correlations are zero. Since the p -value is large (0.7450), you would fail to reject the hypothesis and conclude that only the first canonical correlation is significant.

Figure 28.2 lists several multivariate statistics and tests that use approximations based on the F distribution for the null hypothesis that all canonical correlations are zero. Alternatively, you can specify `MSTAT=EXACT` to compute exact p -values for three of the four tests (Wilks' Lambda, the Hotelling-Lawley Trace, and Roy's greatest root) and an improved F approximation for the fourth (Pillai's Trace). These statistics are described in the section "Multivariate Tests" on page 92 in Chapter 4, "Introduction to Regression Procedures."

Figure 28.2 Multivariate Statistics and *F* Approximations

Multivariate Statistics and F Approximations					
	S=3	M=-0.5	N=3		
Statistic	Value	F Value	Num DF	Den DF	Pr > F
Wilks' Lambda	0.12593148	2.93	9	19.621	0.0223
Pillai's Trace	1.03343732	1.75	9	30	0.1204
Hotelling-Lawley Trace	5.69042615	4.76	9	9.8113	0.0119
Roy's Greatest Root	5.46489324	18.22	3	10	0.0002

NOTE: F Statistic for Roy's Greatest Root is an upper bound.

The small *p*-values for these tests (< 0.05), except for Pillai's trace, suggest rejecting the null hypothesis that all canonical correlations are zero in the population, confirming the results of the preceding likelihood ratio test (Figure 28.1). With only one of the tests resulting in a *p*-value larger than 0.05, you can assume that the first canonical correlation is significant. The next step is to interpret or identify the two canonical variables corresponding to this significant correlation.

Even though canonical variables are artificial, they can often be "identified" in terms of the original variables. This is done primarily by inspecting the standardized coefficients of the canonical variables and the correlations between the canonical variables and their original variables. Since only the first canonical correlation is significant, only the first pair of canonical variables (Satisfaction1 and Characteristics1) need to be identified.

PROC CANCERR calculates and displays the raw canonical coefficients for the job satisfaction variables and the job characteristic variables. However, since the original variables do not necessarily have equal variance and are not measured in the same units, the raw coefficients must be standardized to allow interpretation. The coefficients are standardized by multiplying the raw coefficients with the standard deviation of the associated variable.

The standardized canonical coefficients in Figure 28.3 show that the first canonical variable for the Satisfaction group is a weighted sum of the variables Supervisor (0.7854) and Career (0.3028), with the emphasis on Supervisor. The coefficient for the variable Finance is near 0. Thus, a person satisfied with his or her supervisor and with a large degree of career satisfaction would score high on the canonical variable Satisfaction1.

Figure 28.3 Standardized Canonical Coefficients from the CANCERR Procedure

Standardized Canonical Coefficients for the Satisfaction Areas				
		Satisfaction1	Satisfaction2	Satisfaction3
Career	Career Satisfaction	0.3028	-0.5416	1.0408
Supervisor	Supervisor Satisfaction	0.7854	0.1305	-0.9085
Finance	Financial Satisfaction	0.0538	0.9754	0.3329

Figure 28.3 continued

Standardized Canonical Coefficients for the Job Characteristics			
		Characteristics1	Characteristics2
Variety	Task Variety	-0.1108	0.8095
Feedback	Amount of Feedback	0.5520	-0.7722
Autonomy	Degree of Autonomy	0.8403	0.1020
Standardized Canonical Coefficients for the Job Characteristics			
		Characteristics3	
Variety	Task Variety	0.9071	
Feedback	Amount of Feedback	0.4194	
Autonomy	Degree of Autonomy	-0.8297	

The coefficients for the job characteristics variables show that degree of autonomy (Autonomy) and amount of feedback (Feedback) contribute heavily to the Characteristics1 canonical variable (0.8403 and 0.5520, respectively).

Figure 28.4 shows the table of correlations between the canonical variables and the original variables.

Figure 28.4 Canonical Structure Correlations from the CANCORR Procedure

The CANCORR Procedure				
Canonical Structure				
Correlations Between the Satisfaction Areas and Their Canonical Variables				
		Satisfaction1	Satisfaction2	Satisfaction3
Career	Career Satisfaction	0.7499	-0.2503	0.6123
Supervisor	Supervisor Satisfaction	0.9644	0.0362	-0.2618
Finance	Financial Satisfaction	0.2873	0.8814	0.3750
Correlations Between the Job Characteristics and Their Canonical Variables				
		Characteristics1	Characteristics2	
Variety	Task Variety	0.4863	0.6592	
Feedback	Amount of Feedback	0.6216	-0.5452	
Autonomy	Degree of Autonomy	0.8459	0.4451	
Correlations Between the Job Characteristics and Their Canonical Variables				
		Characteristics3		
Variety	Task Variety	0.5736		
Feedback	Amount of Feedback	0.5625		
Autonomy	Degree of Autonomy	-0.2938		

Figure 28.4 continued

Correlations Between the Satisfaction Areas and the Canonical Variables of the Job Characteristics				
		Characteristics1	Characteristics2	
Career	Career Satisfaction	0.6895	-0.1048	
Supervisor	Supervisor Satisfaction	0.8867	0.0152	
Finance	Financial Satisfaction	0.2642	0.3690	
Correlations Between the Satisfaction Areas and the Canonical Variables of the Job Characteristics				
		Characteristics3		
Career	Career Satisfaction	0.0694		
Supervisor	Supervisor Satisfaction	-0.0297		
Finance	Financial Satisfaction	0.0425		
Correlations Between the Job Characteristics and the Canonical Variables of the Satisfaction Areas				
		Satisfaction1	Satisfaction2	Satisfaction3
Variety	Task Variety	0.4471	0.2760	0.0650
Feedback	Amount of Feedback	0.5715	-0.2283	0.0638
Autonomy	Degree of Autonomy	0.7777	0.1863	-0.0333

Although these univariate correlations must be interpreted with caution since they do not indicate how the original variables contribute *jointly* to the canonical analysis, they are often useful in the identification of the canonical variables.

Figure 28.4 shows that the supervisor satisfaction variable Supervisor is strongly associated with the Satisfaction1 canonical variable, with a correlation of 0.9644. Slightly less influential is the variable Career, which has a correlation with the canonical variable of 0.7499. Thus, the canonical variable Satisfaction1 seems to represent satisfaction with supervisor and career track.

The correlations for the job characteristics variables show that the canonical variable Characteristics1 seems to represent all three measured variables, with degree of autonomy variable (Autonomy) being the most influential (0.8459).

Hence, you can interpret these results to mean that job characteristics and job satisfaction are related—jobs that possess a high degree of autonomy and level of feedback are associated with workers who are more satisfied with their supervisor and their career. While financial satisfaction is a factor in job satisfaction, it is not as important as the other measured satisfaction-related variables.

Syntax: CANCERR Procedure

The following statements are available in the CANCERR procedure:

```

PROC CANCERR < options > ;
  WITH variables ;
  BY variables ;
  FREQ variable ;
  PARTIAL variables ;
  VAR variables ;
  WEIGHT variable ;

```

The PROC CANCERR statement and the WITH statement are required. The rest of this section provides detailed syntax information for each of the preceding statements, beginning with the PROC CANCERR statement. The remaining statements are covered in alphabetical order.

PROC CANCERR Statement

```

PROC CANCERR < options > ;

```

The PROC CANCERR statement invokes the CANCERR procedure. Optionally, it also identifies input and output data sets, specifies the analyses performed, and controls displayed output. [Table 28.1](#) summarizes the options available in the PROC CANCERR statement.

Table 28.1 Summary of PROC CANCERR Statement Options

Option	Description
Specify computational details	
EDF=	Specifies error degrees of freedom if input observations are regression residuals
MSTAT=	Specifies the method of evaluating the multivariate test statistics
NOINT	Omits intercept from canonical correlation and regression models
RDF=	Specifies regression degrees of freedom if input observations are regression residuals
SINGULAR=	Specifies the singularity criterion
Specify input and output data sets	
DATA=	Specifies input data set name
OUT=	Specifies output data set name
OUTSTAT=	Specifies output data set name containing various statistics
Specify labeling options	
PARPREFIX=	Specifies a prefix for naming residual variables
VNAME=	Specifies a name to refer to VAR statement variables
VPREFIX=	Specifies a prefix for naming VAR statement canonical variables
WNAME=	Specifies a name to refer to WITH statement variables
WPREFIX=	Specifies a prefix for naming WITH statement canonical variables

Table 28.1 *continued*

Option	Description
Control amount of output	
ALL	Produces simple statistics, input variable correlations, and canonical redundancy analysis
CORR	Produces input variable correlations
NCAN=	Specifies number of canonical variables for which full output is desired
NOPRINT	Suppresses all displayed output
REDUNDANCY	Produces canonical redundancy analysis
SHORT	Suppresses default output from canonical analysis
SIMPLE	Produces means and standard deviations
Request regression analyses	
VDEP	Requests multiple regression analyses with the VAR variables as dependents and the WITH variables as regressors
VREG	Requests multiple regression analyses with the VAR variables as regressors and the WITH variables as dependents
WDEP	Same as VREG
WREG	Same as VDEP
Specify regression statistics	
ALL	Produces all regression statistics and includes these statistics in the OUTSTAT= data set
B	Produces raw regression coefficients
CLB	Produces 95% confidence interval limits for the regression coefficients
CORRB	Produces correlations among regression coefficients
INT	Requests statistics for the intercept when you specify the B, CLB, SEB, T, or PROBT option
PCORR	Displays partial correlations between regressors and dependents
PROBT	Displays probability levels for <i>t</i> statistics
SEB	Displays standard errors of regression coefficients
SMC	Displays squared multiple correlations and <i>F</i> tests
SPCORR	Displays semipartial correlations between regressors and dependents
SQPCORR	Displays squared partial correlations between regressors and dependents
SQSPCORR	Displays squared semipartial correlations between regressors and dependents
STB	Displays standardized regression coefficients
T	Displays <i>t</i> statistics for regression coefficients

Following are explanations of the options that can be used in the PROC CANCELL statement (in alphabetic order).

ALL

displays simple statistics, correlations among the input variables, the confidence limits for the regression coefficients, and the canonical redundancy analysis. If you specify the VDEP or WDEP option, the ALL option displays all related regression statistics (unless the NOPRINT option is specified) and includes these statistics in the OUTSTAT= data set.

B

produces raw regression coefficients from the regression analyses.

CLB

produces the 95% confidence limits for the regression coefficients from the regression analyses.

CORR**C**

produces correlations among the original variables. If you include a PARTIAL statement, the CORR option produces a correlation matrix for all variables in the analysis, the regression statistics (R square, RMSE), the standardized regression coefficients for both the VAR and WITH variables as predicted from the PARTIAL statement variables, and partial correlation matrices.

CORRB

produces correlations among the regression coefficient estimates.

DATA=SAS-data-set

names the SAS data set to be analyzed by PROC CANCORR. It can be an ordinary SAS data set or a TYPE=CORR, COV, FACTOR, SSCP, UCORR, or UCOV data set. By default, the procedure uses the most recently created SAS data set.

EDF=error-df

specifies the error degrees of freedom if the input observations are residuals from a regression analysis. The effective number of observations is the EDF= value plus one. If you have 100 observations, then specifying EDF=99 has the same effect as omitting the EDF= option.

INT

requests that statistics for the intercept be included when B, CLB, SEB, T, or PROBT is specified for the regression analyses.

MSTAT=FAPPROX | EXACT

specifies the method of evaluating the multivariate test statistics. The default is MSTAT=FAPPROX, which specifies that the multivariate tests are evaluated using the usual approximations based on the F distribution, as discussed in the section “[Multivariate Tests](#)” on page 92 in Chapter 4, “[Introduction to Regression Procedures](#).” Alternatively, you can specify MSTAT=EXACT to compute exact p -values for three of the four tests (Wilks’ lambda, the Hotelling-Lawley trace, and Roy’s greatest root) and an improved F approximation for the fourth (Pillai’s trace). While MSTAT=EXACT provides better control of the significance probability for the tests, especially for Roy’s greatest root, computations for the exact p -values can be appreciably more demanding, and are in fact infeasible for large problems (many dependent variables). Thus, although MSTAT=EXACT is more accurate for most data, it is not the default method.

NCAN=number

specifies the number of canonical variables for which full output is desired. The *number* must be less than or equal to the number of canonical variables in the analysis.

The value of the NCAN= option specifies the number of canonical variables for which canonical coefficients and canonical redundancy statistics are displayed, and the number of variables shown in the canonical structure matrices. The NCAN= option does not affect the number of displayed canonical correlations.

If an OUTSTAT= data set is requested, the NCAN= option controls the number of canonical variables for which statistics are output. If an OUT= data set is requested, the NCAN= option controls the number of canonical variables for which scores are output.

NOINT

omits the intercept from the canonical correlation and regression models. Standard deviations, variances, covariances, and correlations are not corrected for the mean. If you use a TYPE=SSCP data set as input to the CANCELL procedure and list the variable Intercept in the VAR or WITH statement, the procedure runs as if you also specified the NOINT option. If you use NOINT and also create an OUTSTAT= data set, the data set is TYPE=UCORR.

NOPRINT

suppresses the display of all output. Note that this option temporarily disables the Output Delivery System (ODS). For more information, see Chapter 20, “Using the Output Delivery System.”

OUT=SAS-data-set

creates an output SAS data set to contain all the original data plus scores on the canonical variables. The OUT= option cannot be used when the DATA= data set is TYPE=CORR, COV, FACTOR, SSCP, UCORR, or UCOV. For details about OUT= data sets, see the section “Output Data Sets” on page 1729. If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*.

OUTSTAT=SAS-data-set

creates an output SAS data set containing various statistics, including the canonical correlations and coefficients and the multiple regression statistics you request. For details about OUTSTAT= data sets, see the section “Output Data Sets” on page 1729. If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*.

PCORR

produces partial correlations between regressors and dependent variables, removing from each dependent variable and regressor the effects of all other regressors.

PROBT

produces probability levels for the t statistics in the regression analyses.

RDF=regression-df

specifies the regression degrees of freedom if the input observations are residuals from a regression analysis. The effective number of observations is the actual number minus the RDF= value. The degrees of freedom for the intercept should not be included in the RDF= option.

REDUNDANCY**RED**

produces canonical redundancy statistics.

PARPREFIX=*name*

PPREFIX=*name*

specifies a prefix for naming the residual variables in the OUT= data set and the OUTSTAT= data set. By default, the prefix is R_. The number of characters in the prefix plus the maximum length of the variable names should not exceed the current name length defined by the VALIDVARNAME= system option.

SEB

produces standard errors of the regression coefficients.

SHORT

suppresses all default output from the canonical analysis except the tables of canonical correlations and multivariate statistics.

SIMPLE

S

produces means and standard deviations.

SINGULAR=*p*

SING=*p*

specifies the singularity criterion, where $0 < p < 1$. If a variable in the PARTIAL statement has an R square as large as $1 - p$ (where p is the value of the SINGULAR= option) when predicted from the variables listed before it in the statement, the variable is assigned a standardized regression coefficient of 0, and the SAS log generates a linear dependency warning message. By default, SINGULAR=1E-8.

SMC

produces squared multiple correlations and F tests for the regression analyses.

SPCORR

produces semipartial correlations between regressors and dependent variables, removing from each regressor the effects of all other regressors.

SQPCORR

produces squared partial correlations between regressors and dependent variables, removing from each dependent variable and regressor the effects of all other regressors.

SQSPCORR

produces squared semipartial correlations between regressors and dependent variables, removing from each regressor the effects of all other regressors.

STB

produces standardized regression coefficients.

T

produces t statistics for the regression coefficients.

VDEP**WREG**

requests multiple regression analyses with the VAR variables as dependent variables and the WITH Variables as regressors.

VNAME=*label*

VN=*label*

specifies a character constant to refer to variables from the VAR statement in the output. Enclose the constant in single or double quotes. If you omit the VNAME= option, these variables are referred to as the VAR variables. The number of characters in the label should not exceed the label length defined by the VALIDVARNAME= system option. For more information about the VALIDVARNAME= system option, see *SAS System Options: Reference*.

VPREFIX=*name*

VP=*name*

specifies a prefix for naming canonical variables from the VAR statement. By default, these canonical variables are given the names V1, V2, and so on. If you specify VPREFIX=ABC, the names are ABC1, ABC2, and so on. The number of characters in the prefix plus the number of digits required to designate the variables should not exceed the name length defined by the VALIDVARNAME= system option. For more information about the VALIDVARNAME= system option, see *SAS System Options: Reference*.

WDEP**VREG**

requests multiple regression analyses with the WITH variables as dependent variables and the VAR variables as regressors.

WNAME=*label*

WN=*label*

specifies a character constant to refer to variables in the WITH statement in the output. Enclose the constant in single or double quotes. If you omit the WNAME= option, these variables are referred to as the WITH variables. The number of characters in the label should not exceed the label length defined by the VALIDVARNAME= system option. For more information about the VALIDVARNAME= system option, see *SAS System Options: Reference*.

WPREFIX=*name*

WP=*name*

specifies a prefix for naming canonical variables from the WITH statement. By default, these canonical variables are given the names W1, W2, and so on. If you specify WPREFIX=XYZ, the names are XYZ1, XYZ2, and so on. The number of characters in the prefix plus the number of digits required to designate the variables should not exceed the label length defined by the VALIDVARNAME= system option. For more information about the VALIDVARNAME= system option, see *SAS System Options: Reference*.

BY Statement

BY variables ;

You can specify a BY statement with PROC CANCORR to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the CANCORR procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

FREQ Statement

FREQ variable ;

If one variable in your input data set represents the frequency of occurrence for other values in the observation, specify the variable's name in a FREQ statement. PROC CANCORR then treats the data set as if each observation appeared n times, where n is the value of the FREQ variable for the observation. If the value of the FREQ variable is less than one, the observation is not used in the analysis. Only the integer portion of the value is used. The total number of observations is considered to be equal to the sum of the FREQ variable when PROC CANCORR calculates significance probabilities.

PARTIAL Statement

PARTIAL variables ;

You can use the PARTIAL statement to base the canonical analysis on partial correlations. The variables in the PARTIAL statement are partialled out of the VAR and WITH variables. If you request an OUT= or OUTSTAT= data set, the residual variables are named by prefixing the characters R_ by default or the string specified in the RPREFIX= option to the VAR variables.

VAR Statement

VAR *variables* ;

The VAR statement lists the variables in the first of the two sets of variables to be analyzed. The variables must be numeric. If you omit the VAR statement, all numeric variables not mentioned in other statements make up the first set of variables. If, however, the DATA= data set is TYPE=SSCP, the default set of variables used as VAR variables does not include the variable Intercept.

WEIGHT Statement

WEIGHT *variable* ;

If you want to compute weighted product-moment correlation coefficients, specify the name of the weighting variable in a WEIGHT statement. The WEIGHT and FREQ statements have a similar effect, except the WEIGHT statement does not alter the degrees of freedom or number of observations. An observation is used in the analysis only if the WEIGHT variable is greater than zero.

WITH Statement

WITH *variables* ;

The WITH statement lists the variables in the second set of variables to be analyzed. The variables must be numeric. The WITH statement is required.

Details: CANCERR Procedure

Missing Values

If an observation has a missing value for any of the variables in the analysis, that observation is omitted from the analysis.

Formulas

Assume without loss of generality that the two sets of variables, \mathbf{X} with p variables and \mathbf{Y} with q variables, have means of zero. Let n be the number of observations, and let m be $n - 1$.

Note that the scales of eigenvectors and canonical coefficients are arbitrary. PROC CANCERR follows the usual procedure of rescaling the canonical coefficients so that each canonical variable has a variance of one.

There are several different sets of formulas that can be used to compute the canonical correlations, ρ_i , $i = 1, \dots, \min(p, q)$, and unscaled canonical coefficients:

1. Let $S_{XX} = X'X/m$ be the covariance matrix of X , $S_{YY} = Y'Y/m$ be the covariance matrix of Y , and $S_{XY} = X'Y/m$ be the covariance matrix between X and Y . Then the eigenvalues of $S_{YY}^{-1}S'_{XY}S_{XX}^{-1}S_{XY}$ are the squared canonical correlations, and the right eigenvectors are raw canonical coefficients for the Y variables. The eigenvalues of $S_{XX}^{-1}S_{XY}S_{YY}^{-1}S'_{XY}$ are the squared canonical correlations, and the right eigenvectors are raw canonical coefficients for the X variables.
2. Let $T = Y'Y$ and $H = Y'X(X'X)^{-1}X'Y$. The eigenvalues ξ_i of $T^{-1}H$ are the squared canonical correlations, ρ_i^2 , and the right eigenvectors are raw canonical coefficients for the Y variables. Interchange X and Y in the preceding formulas, and the eigenvalues remain the same, but the right eigenvectors are raw canonical coefficients for the X variables.
3. Let $E = T - H$. The eigenvalues of $E^{-1}H$ are $\lambda_i = \rho_i^2/(1 - \rho_i^2)$. The right eigenvectors of $E^{-1}H$ are the same as the right eigenvectors of $T^{-1}H$.
4. Canonical correlation can be viewed as a principal component analysis of the predicted values of one set of variables from a regression on the other set of variables, in the metric of the error covariance matrix. For example, regress the Y variables on the X variables. Call the predicted values $P = X(X'X)^{-1}X'Y$ and the residuals $R = Y - P = (I - X(X'X)^{-1}X')Y$. The error covariance matrix is $R'R/m$. Choose a transformation Q that converts the error covariance matrix to an identity—that is, $(RQ)'(RQ) = Q'R'RQ = mI$. Apply the same transformation to the predicted values to yield, say, $Z = PQ$. Now do a principal component analysis on the covariance matrix of Z , and you get the eigenvalues of $E^{-1}H$. Repeat with X and Y variables interchanged, and you get the same eigenvalues.

To show this relationship between canonical correlation and principal components, note that $P'P = H$, $R'R = E$, and $QQ' = mE^{-1}$. Let the covariance matrix of Z be G . Then $G = Z'Z/m = (PQ)'PQ/m = Q'P'PQ/m = Q'HQ/m$. Let u be an eigenvector of G and κ be the corresponding eigenvalue. Then by definition, $Gu = \kappa u$; hence $Q'HQu/m = \kappa u$. Premultiplying both sides by Q yields $QQ'HQu/m = \kappa Qu$ and thus $E^{-1}HQu = \kappa Qu$. Hence Qu is an eigenvector of $E^{-1}H$ and κ is also an eigenvalue of $E^{-1}H$.
5. If the covariance matrices are replaced by correlation matrices, the preceding formulas yield standardized canonical coefficients instead of raw canonical coefficients.

The formulas for multivariate test statistics are shown in the section “[Multivariate Tests](#)” on page 92 in Chapter 4, “[Introduction to Regression Procedures](#).” Formulas for linear regression are provided in other sections of that chapter.

Output Data Sets

OUT= Data Set

The OUT= data set contains all the variables in the original data set plus new variables containing the canonical variable scores. The number of new variables is twice that specified by the NCAN= option. The names of the new variables are formed by concatenating the values given by the VPREFIX= and WPREFIX= options (the defaults are V and W) with the numbers 1, 2, 3, and so on. The new variables have mean 0 and variance equal to 1. An OUT= data set cannot be created if the DATA= data set is TYPE=CORR, COV, FACTOR, SSCP, UCORR, or UCOV.

If you use a PARTIAL statement, the OUT= data set also contains the residuals from predicting the VAR variables from the PARTIAL variables. The names of the residual variables are formed by concatenating the values given by the PARPREFIX= option (the default is R_) with the numbers 1, 2, 3, and so on.

OUTSTAT= Data Set

The OUTSTAT= data set is similar to the TYPE=CORR or TYPE=UCORR data set produced by the CORR procedure, but it contains several results in addition to those produced by PROC CORR.

The new data set contains the following variables:

- the BY variables, if any
- two new character variables, _TYPE_ and _NAME_
- Intercept, if the INT option is used
- the variables analyzed (those in the VAR statement and the WITH statement)

Each observation in the new data set contains some type of statistic as indicated by the _TYPE_ variable. The values of the _TYPE_ variable are as follows.

TYPE	Contents
MEAN	means
STD	standard deviations
USTD	uncorrected standard deviations. When you specify the NOINT option in the PROC CANCELL statement, the OUTSTAT= data set contains standard deviations not corrected for the mean (_TYPE_='USTD').
N	number of observations on which the analysis is based. This value is the same for each variable.
SUMWGT	sum of the weights if a WEIGHT statement is used. This value is the same for each variable.
CORR	correlations. The _NAME_ variable contains the name of the variable corresponding to each row of the correlation matrix.
UCORR	uncorrected correlation matrix. When you specify the NOINT option in the PROC CANCELL statement, the OUTSTAT= data set contains a matrix of correlations not corrected for the means.
CORRB	correlations among the regression coefficient estimates
STB	standardized regression coefficients. The _NAME_ variable contains the name of the dependent variable.

B	raw regression coefficients
SEB	standard errors of the regression coefficients
LCLB	95% lower confidence limits for the regression coefficients
UCLB	95% upper confidence limits for the regression coefficients
T	<i>t</i> statistics for the regression coefficients
PROBT	probability levels for the <i>t</i> statistics
SPCORR	semipartial correlations between regressors and dependent variables
SQSPCORR	squared semipartial correlations between regressors and dependent variables
PCORR	partial correlations between regressors and dependent variables
SQPCORR	squared partial correlations between regressors and dependent variables
RSQUARED	R squares for the multiple regression analyses
ADJRSQ	adjusted R squares
LCLRSQ	approximate 95% lower confidence limits for the R squares
UCLRSQ	approximate 95% upper confidence limits for the R squares
F	<i>F</i> statistics for the multiple regression analyses
PROBF	probability levels for the <i>F</i> statistics
CANCORR	canonical correlations
SCORE	standardized canonical coefficients. The <code>_NAME_</code> variable contains the name of the canonical variable. To obtain the canonical variable scores, these coefficients should be multiplied by the standardized data, using means obtained from the observation with <code>_TYPE_='MEAN'</code> and standard deviations obtained from the observation with <code>_TYPE_='STD'</code> .
RAWSCORE	raw canonical coefficients. To obtain the canonical variable scores, these coefficients should be multiplied by the raw data centered by means obtained from the observation with <code>_TYPE_='MEAN'</code> .
USCORE	scoring coefficients to be applied without subtracting the mean from the raw variables. These are standardized canonical coefficients computed under a NOINT model. To obtain the canonical variable scores, these coefficients should be multiplied by the data that are standardized by the uncorrected standard deviations obtained from the observation with <code>_TYPE_='USTD'</code> .
STRUCTUR	canonical structure.

Computational Resources

Notation

Let

n = number of observations

v = number of variables

w = number of WITH variables

p = $\max(v, w)$

q = $\min(v, w)$

b = $v + w$

t = total number of variables (VAR, WITH, and PARTIAL)

Time Requirements

The time required to compute the correlation matrix is roughly proportional to

$$n(p + q)^2$$

The time required for the canonical analysis is roughly proportional to

$$\frac{1}{6}p^3 + p^2q + \frac{3}{2}pq^2 + 5q^3$$

but the coefficient for q^3 varies depending on the number of QR iterations in the singular value decomposition.

Memory Requirements

The minimum memory required is approximately

$$4(v^2 + w^2 + t^2)$$

bytes. Additional memory is required if you request the VDEP or WDEP option.

Displayed Output

If the SIMPLE option is specified, PROC CANCORR produces means and standard deviations for each input variable. If the CORR option is specified, PROC CANCORR produces correlations among the input variables. Unless the NOPRINT option is specified, PROC CANCORR displays a table of canonical correlations containing the following:

- Canonical Correlations. These are always nonnegative.
- Adjusted Canonical Correlations (Lawley 1959), which are asymptotically less biased than the raw correlations and can be negative. The adjusted canonical correlations might not be computable, and they are displayed as missing values if two canonical correlations are nearly equal or if some are close to zero. A missing value is also displayed if an adjusted canonical correlation is larger than a previous adjusted canonical correlation.
- Approx Standard Errors, which are the approximate standard errors of the canonical correlations
- Squared Canonical Correlations
- Eigenvalues of $INV(E)*H$, which are equal to $CanRsq/(1-CanRsq)$, where $CanRsq$ is the corresponding squared canonical correlation. Also displayed for each eigenvalue is the Difference from the next eigenvalue, the Proportion of the sum of the eigenvalues, and the Cumulative proportion.
- Likelihood Ratio for the hypothesis that the current canonical correlation and all smaller ones are zero in the population. The likelihood ratio for all canonical correlations equals Wilks' lambda.
- Approx F statistic based on Rao's approximation to the distribution of the likelihood ratio (Rao 1973, p. 556; Kshirsagar 1972, p. 326)
- Num DF and Den DF (numerator and denominator degrees of freedom) and $Pr > F$ (probability level) associated with the F statistic

Unless you specify the NOPRINT option, PROC CANCORR produces a table of multivariate statistics for the null hypothesis that all canonical correlations are zero in the population. These statistics, as described in the section "[Multivariate Tests](#)" on page 92 in Chapter 4, "[Introduction to Regression Procedures](#)," are as follows:

- Wilks' lambda
- Pillai's trace
- Hotelling-Lawley trace
- Roy's greatest root

For each of the preceding statistics, PROC CANCORR displays the following, depending on the specification of the MSTAT= option.

If you specify MSTAT=FAPPROX (also the default value), the following statistics are displayed:

- an F approximation or upper bound
- Num DF, the numerator degrees of freedom

- Den DF, the denominator degrees of freedom
- Pr > F, the probability level

If you specify MSTAT=EXACT, the following statistic is displayed:

- a *t* value

Unless you specify the SHORT or NOPRINT option, PROC CANCELL displays the following:

- both Raw (unstandardized) and Standardized Canonical Coefficients normalized to give canonical variables with unit variance. Standardized coefficients can be used to compute canonical variable scores from the standardized (zero mean and unit variance) input variables. Raw coefficients can be used to compute canonical variable scores from the input variables without standardizing them.
- all four Canonical Structure matrices, giving Correlations Between the canonical variables and the original variables

If you specify the REDUNDANCY option, PROC CANCELL displays the following:

- the Canonical Redundancy Analysis (Stewart and Love 1968; Cooley and Lohnes 1971), including Raw (unstandardized) and Standardized Variance and Cumulative Proportion of the Variance of each set of variables Explained by Their Own Canonical Variables and Explained by The Opposite Canonical Variables
- the Squared Multiple Correlations of each variable with the first *m* canonical variables of the opposite set, where *m* varies from 1 to the number of canonical correlations

If you specify the VDEP option, PROC CANCELL performs multiple regression analyses with the VAR variables as dependent variables and the WITH variables as regressors. If you specify the WDEP option, PROC CANCELL performs multiple regression analyses with the WITH variables as dependent variables and the VAR variables as regressors. If you specify the VDEP or WDEP option and also specify the ALL option, PROC CANCELL displays the following items. You can also specify individual options to request a subset of the output generated by the ALL option; or you can suppress the output by specifying the NOPRINT option.

SMC	Squared Multiple Correlations and <i>F</i> Tests. For each regression model, identified by its dependent variable name, PROC CANCELL displays the R square, Adjusted R square (Wherry 1931), <i>F</i> Statistic, and Pr > <i>F</i> . Also for each regression model, PROC CANCELL displays an Approximate 95% Confidence Interval for the population R square Helland (1987). These confidence limits are valid only when the regressors are random and when the regressors and dependent variables are approximately distributed according to a multivariate normal distribution. The average R squares for the models considered, unweighted and weighted by variance, are also given.
CORRB	Correlations Among the Regression Coefficient Estimates
STB	Standardized Regression Coefficients
B	Raw Regression Coefficients

SEB	Standard Errors of the Regression Coefficients
CLB	95% confidence limits for the regression coefficients
T	T Statistics for the Regression Coefficients
PROBT	Probability > T for the Regression Coefficients
SPCORR	Semipartial Correlations between regressors and dependent variables, Removing from Each Regressor the Effects of All Other Regressors
SQSPCORR	Squared Semipartial Correlations between regressors and dependent variables, Removing from Each Regressor the Effects of All Other Regressors
PCORR	Partial Correlations between regressors and dependent variables, Removing the Effects of All Other Regressors from Both Regressor and Criterion
SQPCORR	Squared Partial Correlations between regressors and dependent variables, Removing the Effects of All Other Regressors from Both Regressor and Criterion

ODS Table Names

PROC CANCORR assigns a name to each table it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in [Table 28.2](#).

For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

All of the tables in [Table 28.2](#) are created with the specification of the PROC CANCORR statement; a few tables need an additional PARTIAL statement.

Table 28.2 ODS Tables Produced by PROC CANCORR

ODS Table Name	Description	Statement and Option
AvgRSquare	Average R squares (weighted and unweighted)	VDEP, WDEP, SMC, or ALL
CanCorr	Canonical correlations	default
CanStructureVCan	Correlations between the VAR canonical variables and the VAR and WITH variables	default (if SHORT is not specified)
CanStructureWCan	Correlations between the WITH canonical variables and the WITH and VAR variables	default (if SHORT is not specified)
ConfidenceLimits	95% confidence limits for the regression coefficients	VDEP, WDEP, CLB, or ALL
Corr	Correlations among the original variables	CORR or ALL
CorrOnPartial	Partial correlations	PARTIAL statement with CORR or ALL
CorrRegCoefEst	Correlations among the regression coefficient estimates	VDEP, WDEP, CORRB, or ALL
MultStat	Multivariate statistics	default

Table 28.2 continued

ODS Table Name	Description	Statement and Option
NObsNVar	Number of observations and variables	SIMPLE or ALL
ParCorr	Partial correlations	VDEP, WDEP, PCORR, or ALL
ProbtRegCoef	Prob > t for the regression coefficients	VDEP, WDEP, PROBT, or ALL
RawCanCoefV	Raw canonical coefficients for the VAR variables	default (if SHORT is not specified)
RawCanCoefW	Raw canonical coefficients for the WITH variables	default (if SHORT is not specified)
RawRegCoef	Raw regression coefficients	VDEP, WDEP, B, or ALL
Redundancy	Canonical redundancy analysis	REDUNDANCY or ALL
Regression	Squared multiple correlations and F tests	VDEP, WDEP, SMC, or ALL
RSquareRMSEOnPartial	R squares and RMSEs on PARTIAL variables	PARTIAL statement with CORR or ALL
SemiParCorr	Semipartial correlations	VDEP, WDEP, SPCORR, or ALL
SimpleStatistics	Simple statistics	SIMPLE or ALL
SqMultCorr	Canonical redundancy analysis: squared multiple correlations	REDUNDANCY or ALL
SqParCorr	Squared partial correlations	VDEP, WDEP, SQPCORR, or ALL
SqSemiParCorr	Squared semipartial correlations	VDEP, WDEP, SQSPCORR, or ALL
StdCanCoefV	Standardized canonical coefficients for the VAR variables	default (if SHORT is not specified)
StdCanCoefW	Standardized canonical coefficients for the WITH variables	default (if SHORT is not specified)
StdErrRawRegCoef	Standard errors of the raw regression coefficients	VDEP, WDEP, SEB, or ALL
StdRegCoef	Standardized regression coefficients	VDEP, WDEP, STB, or ALL
StdRegCoefOnPartial	Standardized regression coefficients on PARTIAL variables	PARTIAL statement with CORR or ALL
tValueRegCoef	t values for the regression coefficients	VDEP, WDEP, T, or ALL

Example: CANCERR Procedure

Example 28.1: Canonical Correlation Analysis of Fitness Club Data

Three physiological and three exercise variables are measured on 20 middle-aged men in a fitness club. You can use the CANCERR procedure to determine whether the physiological variables are related in any way to the exercise variables. The following statements create the SAS data set Fit and produce [Output 28.1.1](#) through [Output 28.1.5](#):

```

data Fit;
  input Weight Waist Pulse Chins Situps Jumps;
  datalines;
191 36 50 5 162 60
189 37 52 2 110 60
193 38 58 12 101 101
162 35 62 12 105 37
189 35 46 13 155 58
182 36 56 4 101 42
211 38 56 8 101 38
167 34 60 6 125 40
176 31 74 15 200 40
154 33 56 17 251 250
169 34 50 17 120 38
166 33 52 13 210 115
154 34 64 14 215 105
247 46 50 1 50 50
193 36 46 6 70 31
202 37 62 12 210 120
176 37 54 4 60 25
157 32 52 11 230 80
156 33 54 15 225 73
138 33 68 2 110 43
;

proc cancorr data=Fit all
  vprefix=Physiological vname='Physiological Measurements'
  wprefix=Exercises wname='Exercises';
  var Weight Waist Pulse;
  with Chins Situps Jumps;
  title 'Middle-Aged Men in a Health Fitness Club';
  title2 'Data Courtesy of Dr. A. C. Linnerud, NC State Univ';
run;

```

Output 28.1.1 Correlations among the Original Variables

Middle-Aged Men in a Health Fitness Club Data Courtesy of Dr. A. C. Linnerud, NC State Univ			
The CANCERR Procedure			
Correlations Among the Original Variables			
Correlations Among the Physiological Measurements			
	Weight	Waist	Pulse
Weight	1.0000	0.8702	-0.3658
Waist	0.8702	1.0000	-0.3529
Pulse	-0.3658	-0.3529	1.0000
Correlations Among the Exercises			
	Chins	Situps	Jumps
Chins	1.0000	0.6957	0.4958
Situps	0.6957	1.0000	0.6692
Jumps	0.4958	0.6692	1.0000
Correlations Between the Physiological Measurements and the Exercises			
	Chins	Situps	Jumps
Weight	-0.3897	-0.4931	-0.2263
Waist	-0.5522	-0.6456	-0.1915
Pulse	0.1506	0.2250	0.0349

Output 28.1.1 displays the correlations among the original variables. The correlations between the physiological and exercise variables are moderate, the largest being -0.6456 between Waist and Situps. There are larger within-set correlations: 0.8702 between Weight and Waist, 0.6957 between Chins and Situps, and 0.6692 between Situps and Jumps.

Output 28.1.2 Canonical Correlations and Multivariate Statistics

Middle-Aged Men in a Health Fitness Club Data Courtesy of Dr. A. C. Linnerud, NC State Univ					
The CANCERR Procedure					
Canonical Correlation Analysis					
	Canonical Correlation	Adjusted Canonical Correlation	Approximate Standard Error	Squared Canonical Correlation	
1	0.795608	0.754056	0.084197	0.632992	
2	0.200556	-.076399	0.220188	0.040223	
3	0.072570	.	0.228208	0.005266	
Eigenvalues of Inv(E)*H = CanRsqr/(1-CanRsqr)					
	Eigenvalue	Difference	Proportion	Cumulative	
1	1.7247	1.6828	0.9734	0.9734	
2	0.0419	0.0366	0.0237	0.9970	
3	0.0053		0.0030	1.0000	
Test of H0: The canonical correlations in the current row and all that follow are zero					
	Likelihood Ratio	Approximate F Value	Num DF	Den DF	Pr > F
1	0.35039053	2.05	9	34.223	0.0635
2	0.95472266	0.18	4	30	0.9491
3	0.99473355	0.08	1	16	0.7748
Multivariate Statistics and F Approximations					
	S=3	M=-0.5	N=6		
Statistic	Value	F Value	Num DF	Den DF	Pr > F
Wilks' Lambda	0.35039053	2.05	9	34.223	0.0635
Pillai's Trace	0.67848151	1.56	9	48	0.1551
Hotelling-Lawley Trace	1.77194146	2.64	9	19.053	0.0357
Roy's Greatest Root	1.72473874	9.20	3	16	0.0009
NOTE: F Statistic for Roy's Greatest Root is an upper bound.					

As **Output 28.1.2** shows, the first canonical correlation is 0.7956, which would appear to be substantially larger than any of the between-set correlations. The probability level for the null hypothesis that all the canonical correlations are zero in the population is only 0.0635, so no firm conclusions can be drawn. The remaining canonical correlations are not worthy of consideration, as can be seen from the probability levels and especially from the negative adjusted canonical correlations.

Because the variables are not measured in the same units, the standardized coefficients rather than the raw coefficients should be interpreted. The correlations given in the canonical structure matrices should also be examined.

Output 28.1.3 Raw and Standardized Canonical Coefficients

Raw Canonical Coefficients for the Physiological Measurements			
	Physiological1	Physiological2	Physiological3
Weight	-0.031404688	-0.076319506	-0.007735047
Waist	0.4932416756	0.3687229894	0.1580336471
Pulse	-0.008199315	-0.032051994	0.1457322421

Raw Canonical Coefficients for the Exercises			
	Exercises1	Exercises2	Exercises3
Chins	-0.066113986	-0.071041211	-0.245275347
Situps	-0.016846231	0.0019737454	0.0197676373
Jumps	0.0139715689	0.0207141063	-0.008167472

Standardized Canonical Coefficients for the Physiological Measurements			
	Physiological1	Physiological2	Physiological3
Weight	-0.7754	-1.8844	-0.1910
Waist	1.5793	1.1806	0.5060
Pulse	-0.0591	-0.2311	1.0508

Standardized Canonical Coefficients for the Exercises			
	Exercises1	Exercises2	Exercises3
Chins	-0.3495	-0.3755	-1.2966
Situps	-1.0540	0.1235	1.2368
Jumps	0.7164	1.0622	-0.4188

The first canonical variable for the physiological variables, displayed in [Output 28.1.3](#), is a weighted difference of *Waist* (1.5793) and *Weight* (-0.7754), with more emphasis on *Waist*. The coefficient for *Pulse* is near 0. The correlations between *Waist* and *Weight* and the first canonical variable are both positive, 0.9254 for *Waist* and 0.6206 for *Weight*. *Weight* is therefore a suppressor variable, meaning that its coefficient and its correlation have opposite signs.

The first canonical variable for the exercise variables also shows a mixture of signs, subtracting *Situps* (-1.0540) and *Chins* (-0.3495) from *Jumps* (0.7164), with the most weight on *Situps*. All the correlations are negative, indicating that *Jumps* is also a suppressor variable.

It might seem contradictory that a variable should have a coefficient of opposite sign from that of its correlation with the canonical variable. In order to understand how this can happen, consider a simplified situation: predicting *Situps* from *Waist* and *Weight* by multiple regression. In informal terms, it seems plausible that obese people should do fewer sit-ups than skinny people. Assume that the men in the sample do

not vary much in height, so there is a strong correlation between Waist and Weight (0.8702). Examine the relationships between obesity and the independent variables:

- People with large waists tend to be more obese than people with small waists. Hence, the correlation between Waist and Situps should be negative.
- People with high weights tend to be more obese than people with low weights. Therefore, Weight should correlate negatively with Situps.
- For a fixed value of Weight, people with large waists tend to be shorter and more obese. Thus, the multiple regression coefficient for Waist should be negative.
- For a fixed value of Waist, people with higher weights tend to be taller and skinnier. The multiple regression coefficient for Weight should therefore be positive, of opposite sign from the correlation between Weight and Situps.

Therefore, the general interpretation of the first canonical correlation is that Weight and Jumps act as suppressor variables to enhance the correlation between Waist and Situps. This canonical correlation might be strong enough to be of practical interest, but the sample size is not large enough to draw definite conclusions.

The canonical redundancy analysis (Output 28.1.4) shows that neither of the first pair of canonical variables is a good overall predictor of the opposite set of variables, the proportions of variance explained being 0.2854 and 0.2584. The second and third canonical variables add virtually nothing, with cumulative proportions for all three canonical variables being 0.2969 and 0.2767.

Output 28.1.4 Canonical Redundancy Analysis

Middle-Aged Men in a Health Fitness Club Data Courtesy of Dr. A. C. Linnerud, NC State Univ					
The CANCELL Procedure					
Canonical Redundancy Analysis					
Canonical Variable Number	Standardized Variance of the Physiological Measurements Explained by Their Own Canonical Variables			The Opposite Canonical Variables	
	Proportion	Cumulative Proportion	Canonical R-Square	Proportion	Cumulative Proportion
1	0.4508	0.4508	0.6330	0.2854	0.2854
2	0.2470	0.6978	0.0402	0.0099	0.2953
3	0.3022	1.0000	0.0053	0.0016	0.2969

Output 28.1.4 *continued*

Canonical Variable Number	Standardized Variance of the Exercises Explained by Their Own Canonical Variables			The Opposite Canonical Variables	
	Proportion	Cumulative Proportion	Canonical R-Square	Proportion	Cumulative Proportion
1	0.4081	0.4081	0.6330	0.2584	0.2584
2	0.4345	0.8426	0.0402	0.0175	0.2758
3	0.1574	1.0000	0.0053	0.0008	0.2767

The squared multiple correlations ([Output 28.1.5](#)) indicate that the first canonical variable of the physiological measurements has some predictive power for Chins (0.3351) and Situps (0.4233) but almost none for Jumps (0.0167). The first canonical variable of the exercises is a fairly good predictor of Waist (0.5421), a poorer predictor of Weight (0.2438), and nearly useless for predicting Pulse (0.0701).

Output 28.1.5 Canonical Redundancy Analysis

Squared Multiple Correlations Between the Physiological Measurements and the First M Canonical Variables of the Exercises			
M	1	2	3
Weight	0.2438	0.2678	0.2679
Waist	0.5421	0.5478	0.5478
Pulse	0.0701	0.0702	0.0749
Squared Multiple Correlations Between the Exercises and the First M Canonical Variables of the Physiological Measurements			
M	1	2	3
Chins	0.3351	0.3374	0.3396
Situps	0.4233	0.4365	0.4365
Jumps	0.0167	0.0536	0.0539

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Chapter 29

The CANDISC Procedure

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Overview: CANDISC Procedure

Canonical discriminant analysis is a dimension-reduction technique related to principal component analysis and canonical correlation. The methodology used in deriving the canonical coefficients parallels that of a one-way MANOVA. MANOVA tests for equality of the mean vector across class levels. Canonical discriminant analysis finds linear combinations of the quantitative variables that provide maximal separation between classes or groups. Given a classification variable and several quantitative variables, the CANDISC procedure derives *canonical variables*, linear combinations of the quantitative variables that summarize between-class variation in much the same way that principal components summarize total variation.

The CANDISC procedure performs a canonical discriminant analysis, computes squared Mahalanobis distances between class means, and performs both univariate and multivariate one-way analyses of variance. Two output data sets can be produced: one containing the canonical coefficients and another containing, among other things, scored canonical variables. The canonical coefficients output data set can be rotated

by the FACTOR procedure. It is customary to standardize the canonical coefficients so that the canonical variables have means that are equal to zero and pooled within-class variances that are equal to one. PROC CANDISC displays both standardized and unstandardized canonical coefficients. Correlations between the canonical variables and the original variables as well as the class means for the canonical variables are also displayed; these correlations, sometimes known as loadings, are called canonical structures. To aid the visual interpretation of group differences, you can use ODS Graphics to display graphs of pairs of canonical variables from the scored canonical variables output data set.

Given two or more groups of observations with measurements on several quantitative variables, canonical discriminant analysis derives a linear combination of the variables that has the highest possible multiple correlation with the groups. This maximal multiple correlation is called the *first canonical correlation*. The coefficients of the linear combination are the *canonical coefficients* or *canonical weights*. The variable defined by the linear combination is the *first canonical variable* or *canonical component*. The second canonical correlation is obtained by finding the linear combination uncorrelated with the first canonical variable that has the highest possible multiple correlation with the groups. The process of extracting canonical variables can be repeated until the number of canonical variables equals the number of original variables or the number of classes minus one, whichever is smaller.

The first canonical correlation is at least as large as the multiple correlation between the groups and any of the original variables. If the original variables have high within-group correlations, the first canonical correlation can be large even if all the multiple correlations are small. In other words, the first canonical variable can show substantial differences between the classes, even if none of the original variables do. Canonical variables are sometimes called *discriminant functions*, but this usage is ambiguous because the DISCRIM procedure produces very different functions for classification that are also called discriminant functions.

For each canonical correlation, PROC CANDISC tests the hypothesis that it and all smaller canonical correlations are zero in the population. An F approximation (Rao 1973; Kshirsagar 1972) is used that gives better small-sample results than the usual chi-square approximation. The variables should have an approximate multivariate normal distribution within each class, with a common covariance matrix in order for the probability levels to be valid.

Canonical discriminant analysis is equivalent to canonical correlation analysis between the quantitative variables and a set of dummy variables coded from the class variable. Canonical discriminant analysis is also equivalent to performing the following steps:

1. Transform the variables so that the pooled within-class covariance matrix is an identity matrix.
2. Compute class means on the transformed variables.
3. Perform a principal component analysis on the means, weighting each mean by the number of observations in the class. The eigenvalues are equal to the ratio of between-class variation to within-class variation in the direction of each principal component.
4. Back-transform the principal components into the space of the original variables, obtaining the canonical variables.

An interesting property of the canonical variables is that they are uncorrelated whether the correlation is calculated from the total sample or from the pooled within-class correlations. The canonical coefficients are not orthogonal, however, so the canonical variables do not represent perpendicular directions through the space of the original variables.

Getting Started: CANDISC Procedure

The data in this example are measurements of 159 fish caught in Finland's lake Laengelmavesi; this data set is available from the Puranen. For each of the seven species (bream, roach, whitefish, parkki, perch, pike, and smelt) the weight, length, height, and width of each fish are tallied. Three different length measurements are recorded: from the nose of the fish to the beginning of its tail, from the nose to the notch of its tail, and from the nose to the end of its tail. The height and width are recorded as percentages of the third length variable. The fish data set is available from the Sashelp library.

The following step uses PROC CANDISC to find the three canonical variables that best separate the species of fish in the Sashelp.Fish data and create the output data set outcan. With the NCAN=3 option, only the first three canonical variables are displayed. The ODS EXCLUDE statement is specified to exclude the canonical structure tables and most of the canonical coefficient tables in order to obtain a more compact set of results. The TEMPLATE and SGRENDER procedures are used to create a plot of the first two canonical variables. The following statements produce [Figure 29.1](#) through [Figure 29.6](#):

```

title 'Fish Measurement Data';

proc candisc data=sashelp.fish ncan=3 out=outcan;
  ods exclude tstruc bstruc pstruc tcoef pcoef;
  class Species;
  var Weight Length1 Length2 Length3 Height Width;
run;

proc template;
  define statgraph scatter;
    begingraph;
    entrytitle 'Fish Measurement Data';
    layout overlayequated / equatetype=fit
      xaxisopts=(label='Canonical Variable 1')
      yaxisopts=(label='Canonical Variable 2');
    scatterplot x=Can1 y=Can2 / group=species name='fish';
    layout gridded / autoalign=(topright);
      discretelegend 'fish' / border=false opaque=false;
    endlayout;
  endlayout;
endgraph;
end;
run;

proc sgrender data=outcan template=scatter;
run;

```

PROC CANDISC begins by displaying summary information about the variables in the analysis. This information includes the number of observations, the number of quantitative variables in the analysis (specified with the VAR statement), and the number of classes in the classification variable (specified with the CLASS statement). The frequency of each class is also displayed.

Figure 29.1 Summary Information

Fish Measurement Data				
The CANDISC Procedure				
Total Sample Size	158	DF Total		157
Variables	6	DF Within Classes		151
Classes	7	DF Between Classes		6
Number of Observations Read		159		
Number of Observations Used		158		
Class Level Information				
Species	Variable Name	Frequency	Weight	Proportion
Bream	Bream	34	34.0000	0.215190
Parkki	Parkki	11	11.0000	0.069620
Perch	Perch	56	56.0000	0.354430
Pike	Pike	17	17.0000	0.107595
Roach	Roach	20	20.0000	0.126582
Smelt	Smelt	14	14.0000	0.088608
Whitefish	Whitefish	6	6.0000	0.037975

PROC CANDISC performs a multivariate one-way analysis of variance (one-way MANOVA) and provides four multivariate tests of the hypothesis that the class mean vectors are equal. These tests, shown in Figure 29.2, indicate that not all of the mean vectors are equal ($p < .0001$).

Figure 29.2 MANOVA and Multivariate Tests

Fish Measurement Data					
The CANDISC Procedure					
Multivariate Statistics and F Approximations					
	S=6	M=-0.5	N=72		
Statistic	Value	F Value	Num DF	Den DF	Pr > F
Wilks' Lambda	0.00036325	90.71	36	643.89	<.0001
Pillai's Trace	3.10465132	26.99	36	906	<.0001
Hotelling-Lawley Trace	52.05799676	209.24	36	413.64	<.0001
Roy's Greatest Root	39.13499776	984.90	6	151	<.0001
NOTE: F Statistic for Roy's Greatest Root is an upper bound.					

The first canonical correlation is the greatest possible multiple correlation with the classes that can be achieved by using a linear combination of the quantitative variables. The first canonical correlation, displayed in Figure 29.3, is 0.987463. A likelihood ratio test is displayed of the hypothesis that the current canonical correlation and all smaller ones are zero. The first line is equivalent to Wilks' lambda multivariate test.

Figure 29.3 Canonical Correlations

Fish Measurement Data					
The CANDISC Procedure					
	Canonical Correlation	Adjusted Canonical Correlation	Approximate Standard Error	Squared Canonical Correlation	
1	0.987463	0.986671	0.001989	0.975084	
2	0.952349	0.950095	0.007425	0.906969	
3	0.838637	0.832518	0.023678	0.703313	
4	0.633094	0.623649	0.047821	0.400809	
5	0.344157	0.334170	0.070356	0.118444	
6	0.005701	.	0.079806	0.000033	
Eigenvalues of Inv(E)*H = CanRsqr/(1-CanRsqr)					
	Eigenvalue	Difference	Proportion	Cumulative	
1	39.1350	29.3859	0.7518	0.7518	
2	9.7491	7.3786	0.1873	0.9390	
3	2.3706	1.7016	0.0455	0.9846	
4	0.6689	0.5346	0.0128	0.9974	
5	0.1344	0.1343	0.0026	1.0000	
6	0.0000		0.0000	1.0000	
Test of H0: The canonical correlations in the current row and all that follow are zero					
	Likelihood Ratio	Approximate F Value	Num DF	Den DF	Pr > F
1	0.00036325	90.71	36	643.89	<.0001
2	0.01457896	46.46	25	547.58	<.0001
3	0.15671134	23.61	16	452.79	<.0001
4	0.52820347	12.09	9	362.78	<.0001
5	0.88152702	4.88	4	300	0.0008
6	0.99996749	0.00	1	151	0.9442

The first canonical variable, Can1, shows that the linear combination of the centered variables $\text{Can1} = -0.0006 \times \text{Weight} - 0.33 \times \text{Length1} + 2.49 \times \text{Length2} + 2.60 \times \text{Length3} + 1.12 \times \text{Height} - 1.45 \times \text{Width}$ separates the species most effectively (see Figure 29.4).

Figure 29.4 Raw Canonical Coefficients

Fish Measurement Data			
The CANDISC Procedure			
Raw Canonical Coefficients			
Variable	Can1	Can2	Can3
Weight	-0.000648508	-0.005231659	-0.005596192
Length1	-0.329435762	-0.626598051	-2.934324102
Length2	-2.486133674	-0.690253987	4.045038893
Length3	2.595648437	1.803175454	-1.139264914
Height	1.121983854	-0.714749340	0.283202557
Width	-1.446386704	-0.907025481	0.741486686

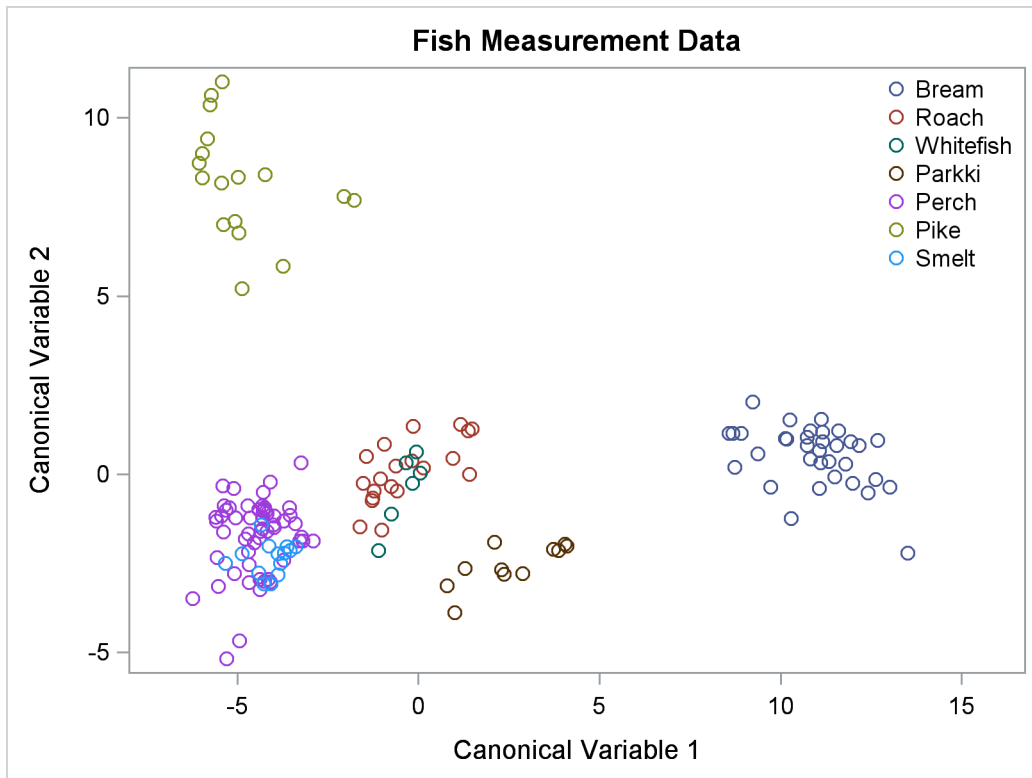
PROC CANDISC computes the means of the canonical variables for each class. The first canonical variable is the linear combination of the variables Weight, Length1, Length2, Length3, Height, and Width that provides the greatest difference (in terms of a univariate F test) between the class means. The second canonical variable provides the greatest difference between class means while being uncorrelated with the first canonical variable.

Figure 29.5 Class Means for Canonical Variables

Class Means on Canonical Variables			
Species	Can1	Can2	Can3
Bream	10.94142464	0.52078394	0.23496708
Parkki	2.58903743	-2.54722416	-0.49326158
Perch	-4.47181389	-1.70822715	1.29281314
Pike	-4.89689441	8.22140791	-0.16469132
Roach	-0.35837149	0.08733611	-1.10056438
Smelt	-4.09136653	-2.35805841	-4.03836098
Whitefish	-0.39541755	-0.42071778	1.06459242

A plot of the first two canonical variables (Figure 29.6) shows that Can1 discriminates between three groups: 1) bream; 2) whitefish, roach, and parkki; and 3) smelt, pike, and perch. Can2 best discriminates between pike and the other species.

Figure 29.6 Plot of First Two Canonical Variables



Syntax: CANDISC Procedure

The following statements are available in the CANDISC procedure:

```

PROC CANDISC < options > ;
  CLASS variable ;
  BY variables ;
  FREQ variable ;
  VAR variables ;
  WEIGHT variable ;

```

The BY, CLASS, FREQ, VAR, and WEIGHT statements are described after the PROC CANDISC statement.

PROC CANDISC Statement

PROC CANDISC < options > ;

The PROC CANDISC statement invokes the CANDISC procedure. Table 29.1 summarizes the options available in the PROC CANDISC statement.

Table 29.1 CANDISC Procedure Options

Option	Description
Input Data Set	
DATA=	Specifies input SAS data set
Output Data Sets	
OUT=	Specifies output data set with canonical scores
OUTSTAT=	Specifies output statistics data set
Method Details	
NCAN=	Specifies the number of canonical variables
PREFIX=	Specifies a prefix for naming the canonical variables
SINGULAR=	Specifies the singularity criterion
Control Displayed Output	
ALL	Displays all output
ANOVA	Displays univariate statistics
BCORR	Displays between correlations
BCOV	Displays between covariances
BSSCP	Displays between SSCPs
DISTANCE	Displays squared Mahalanobis distances
NOPRINT	Suppresses all displayed output
PCORR	Displays pooled correlations
PCOV	Displays pooled covariances
PSSCP	Displays pooled SSCPs
SHORT	Suppresses some displayed output
SIMPLE	Displays simple descriptive statistics
STDMEAN	Displays standardized class means
TCORR	Displays total correlations
TCOV	Displays total covariances
TSSCP	Displays total SSCPs
WCORR	Displays within correlations
WCOV	Displays within covariances
WSSCP	Displays within SSCPs

ALL

activates all of the display options.

ANOVA

displays univariate statistics for testing the hypothesis that the class means are equal in the population for each variable.

BCORR

displays between-class correlations.

BCOV

displays between-class covariances. The between-class covariance matrix equals the between-class SSCP matrix divided by $n(c - 1)/c$, where n is the number of observations and c is the number of classes. The between-class covariances should be interpreted in comparison with the total-sample and within-class covariances, not as formal estimates of population parameters.

BSSCP

displays the between-class SSCP matrix.

DATA=SAS-data-set

specifies the data set to be analyzed. The data set can be an ordinary SAS data set or one of several specially structured data sets created by SAS statistical procedures. These specially structured data sets include TYPE=CORR, COV, CSSCP, and SSCP. If you omit the DATA= option, the procedure uses the most recently created SAS data set.

DISTANCE**MAHALANOBIS**

displays squared Mahalanobis distances between the group means, F statistics, and the corresponding probabilities of greater squared Mahalanobis distances between the group means.

NCAN= n

specifies the number of canonical variables to be computed. The value of n must be less than or equal to the number of variables. If you specify NCAN=0, the procedure displays the canonical correlations, but not the canonical coefficients, structures, or means. A negative value suppresses the canonical analysis entirely. Let v be the number of variables in the VAR statement, and let c be the number of classes. If you omit the NCAN= option, only $\min(v, c - 1)$ canonical variables are generated; if you also specify an OUT= output data set, v canonical variables are generated, and the last $v - (c - 1)$ canonical variables have missing values.

NOPRINT

suppresses the normal display of results. Note that this option temporarily disables the Output Delivery System (ODS); see Chapter 20, “Using the Output Delivery System,” for more information.

OUT=SAS-data-set

creates an output SAS data set containing the original data and the canonical variable scores. If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*.

OUTSTAT=SAS-data-set

creates a TYPE=CORR output SAS data set that contains various statistics, including class means, standard deviations, correlations, canonical correlations, canonical structures, canonical coefficients, and means of canonical variables for each class. If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*.

PCORR

displays pooled within-class correlations (partial correlations based on the pooled within-class covariances).

PCOV

displays pooled within-class covariances.

PREFIX=name

specifies a prefix for naming the canonical variables. By default the names are Can1, Can2, Can3, and so forth. If you specify PREFIX=Abc, the components are named Abc1, Abc2, and so on. The number of characters in the prefix plus the number of digits required to designate the canonical variables should not exceed 32. The prefix is truncated if the combined length exceeds 32.

PSSCP

displays the pooled within-class corrected SSCP matrix.

SHORT

suppresses the display of canonical structures, canonical coefficients, and class means on canonical variables; only tables of canonical correlations and multivariate test statistics are displayed.

SIMPLE

displays simple descriptive statistics for the total sample and within each class.

SINGULAR= ρ

specifies the criterion for determining the singularity of the total-sample correlation matrix and the pooled within-class covariance matrix, where $0 < \rho < 1$. The default is SINGULAR=1E-8.

Let S be the total-sample correlation matrix. If the R square for predicting a quantitative variable in the VAR statement from the variables preceding it exceeds $1 - \rho$, then S is considered singular. If S is singular, the probability levels for the multivariate test statistics and canonical correlations are adjusted for the number of variables with R square exceeding $1 - \rho$.

If S is considered singular and the inverse of S (squared Mahalanobis distances) is required, a quasi inverse is used instead. For details see the section “[Quasi-inverse](#)” on page 2083 in Chapter 33, “[The DISCRIM Procedure](#).”

STDMEAN

displays total-sample and pooled within-class standardized class means.

TCORR

displays total-sample correlations.

TCOV

displays total-sample covariances.

TSSCP

displays the total-sample corrected SSCP matrix.

WCORR

displays within-class correlations for each class level.

WCOV

displays within-class covariances for each class level.

WSSCP

displays the within-class corrected SSCP matrix for each class level.

BY Statement

BY *variables* ;

You can specify a BY statement with PROC CANDISC to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the CANDISC procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

CLASS Statement

CLASS *variable* ;

The values of the CLASS variable define the groups for analysis. Class levels are determined by the formatted values of the CLASS variable. The CLASS variable can be numeric or character. A CLASS statement is required.

FREQ Statement

FREQ *variable* ;

If a variable in the data set represents the frequency of occurrence for the other values in the observation, include the name of the variable in a FREQ statement. The procedure then treats the data set as if each observation appears n times, where n is the value of the FREQ variable for the observation. The total number of observations is considered to be equal to the sum of the FREQ variable when the procedure determines degrees of freedom for significance probabilities.

If the value of the FREQ variable is missing or is less than one, the observation is not used in the analysis. If the value is not an integer, the value is truncated to an integer.

VAR Statement

VAR *variables* ;

You specify the quantitative variables to include in the analysis by using a VAR statement. If you do not use a VAR statement, the analysis includes all numeric variables not listed in other statements.

WEIGHT Statement

WEIGHT *variable* ;

To use relative weights for each observation in the input data set, place the weights in a variable in the data set and specify the name in a WEIGHT statement. This is often done when the variance associated with each observation is different and the values of the WEIGHT variable are proportional to the reciprocals of the variances. If the value of the WEIGHT variable is missing or is less than zero, then a value of zero for the weight is assumed.

The WEIGHT and FREQ statements have a similar effect except that the WEIGHT statement does not alter the degrees of freedom.

Details: CANDISC Procedure

Missing Values

If an observation has a missing value for any of the quantitative variables, it is omitted from the analysis. If an observation has a missing CLASS value but is otherwise complete, it is not used in computing the canonical correlations and coefficients; however, canonical variable scores are computed for that observation for the OUT= data set.

Computational Details

General Formulas

Canonical discriminant analysis is equivalent to canonical correlation analysis between the quantitative variables and a set of dummy variables coded from the class variable. In the following notation the dummy variables are denoted by \mathbf{y} and the quantitative variables by \mathbf{x} . The total sample covariance matrix for the \mathbf{x} and \mathbf{y} variables is

$$\mathbf{S} = \begin{bmatrix} \mathbf{S}_{xx} & \mathbf{S}_{xy} \\ \mathbf{S}_{yx} & \mathbf{S}_{yy} \end{bmatrix}$$

When c is the number of groups, n_t is the number of observations in group t , and \mathbf{S}_t is the sample covariance matrix for the \mathbf{x} variables in group t , the within-class pooled covariance matrix for the \mathbf{x} variables is

$$\mathbf{S}_p = \frac{1}{\sum n_t - c} \sum (n_t - 1) \mathbf{S}_t$$

The canonical correlations, ρ_i , are the square roots of the eigenvalues, λ_i , of the following matrix. The corresponding eigenvectors are \mathbf{v}_i .

$$\mathbf{S}_p^{-1/2} \mathbf{S}_{xy} \mathbf{S}_{yy}^{-1} \mathbf{S}_{yx} \mathbf{S}_p^{-1/2}$$

Let \mathbf{V} be the matrix with the eigenvectors \mathbf{v}_i that correspond to nonzero eigenvalues as columns. The raw canonical coefficients are calculated as follows:

$$\mathbf{R} = \mathbf{S}_p^{-1/2} \mathbf{V}$$

The pooled within-class standardized canonical coefficients are

$$\mathbf{P} = \text{diag}(\mathbf{S}_p)^{1/2} \mathbf{R}$$

The total sample standardized canonical coefficients are

$$\mathbf{T} = \text{diag}(\mathbf{S}_{xx})^{1/2} \mathbf{R}$$

Let \mathbf{X}_c be the matrix with the centered x variables as columns. The canonical scores can be calculated by any of the following:

$$\mathbf{X}_c \mathbf{R}$$

$$\mathbf{X}_c \text{diag}(\mathbf{S}_p)^{-1/2} \mathbf{P}$$

$$\mathbf{X}_c \text{diag}(\mathbf{S}_{xx})^{-1/2} \mathbf{T}$$

For the multivariate tests based on $\mathbf{E}^{-1} \mathbf{H}$,

$$\mathbf{E} = (n - 1)(\mathbf{S}_{yy} - \mathbf{S}_{yx} \mathbf{S}_{xx}^{-1} \mathbf{S}_{xy})$$

$$\mathbf{H} = (n - 1) \mathbf{S}_{yx} \mathbf{S}_{xx}^{-1} \mathbf{S}_{xy}$$

where n is the total number of observations.

Input Data Set

The input DATA= data set can be an ordinary SAS data set or one of several specially structured data sets created by statistical procedures available with SAS/STAT software. For more information about special types of data sets, see Appendix A, “[Special SAS Data Sets](#).” The BY variable in these data sets becomes the CLASS variable in PROC CANDISC. These specially structured data sets include the following:

- TYPE=CORR data sets created by PROC CORR by using a BY statement
- TYPE=COV data sets created by PROC PRINCOMP by using both the COV option and a BY statement
- TYPE=CSSCP data sets created by PROC CORR by using the CSSCP option and a BY statement, where the OUT= data set is assigned TYPE=CSSCP with the TYPE= data set option
- TYPE=SSCP data sets created by PROC REG by using both the OUTSSCP= option and a BY statement.

When the input data set is TYPE=CORR, TYPE=COV, or TYPE=CSSCP, then PROC CANDISC reads the number of observations for each class from the observations with `_TYPE_='N'` and the variable means in each class from the observations with `_TYPE_='MEAN'`. The CANDISC procedure then reads the within-class correlations from the observations with `_TYPE_='CORR'`, the standard deviations from the observations with `_TYPE_='STD'` (data set TYPE=CORR), the within-class covariances from the observations with `_TYPE_='COV'` (data set TYPE=COV), or the within-class corrected sums of squares and crossproducts from the observations with `_TYPE_='CSSCP'` (data set TYPE=CSSCP).

When the data set does not include any observations with `_TYPE_='CORR'` (data set `TYPE=CORR`), `_TYPE_='COV'` (data set `TYPE=COV`), or `_TYPE_='CSSCP'` (data set `TYPE=CSSCP`) for each class, PROC CANDISC reads the pooled within-class information from the data set. In this case, PROC CANDISC reads the pooled within-class correlations from the observations with `_TYPE_='PCORR'`, the pooled within-class standard deviations from the observations with `_TYPE_='PSTD'` (data set `TYPE=CORR`), the pooled within-class covariances from the observations with `_TYPE_='PCOV'` (data set `TYPE=COV`), or the pooled within-class corrected SSCP matrix from the observations with `_TYPE_='PSSCP'` (data set `TYPE=CSSCP`).

When the input data set is `TYPE=SSCP`, then PROC CANDISC reads the number of observations for each class from the observations with `_TYPE_='N'`, the sum of weights of observations from the variable `INTERCEPT` in observations with `_TYPE_='SSCP'` and `_NAME_='INTERCEPT'`, the variable sums from the analysis variables in observations with `_TYPE_='SSCP'` and `_NAME_='INTERCEPT'`, and the uncorrected sums of squares and crossproducts from the analysis variables in observations with `_TYPE_='SSCP'` and `_NAME_=variablenames`.

Output Data Sets

OUT= Data Set

The `OUT=` data set contains all the variables in the original data set plus new variables containing the canonical variable scores. You determine the number of new variables by using the `NCAN=` option. The names of the new variables are formed as described in the `PREFIX=` option. The new variables have means equal to zero and pooled within-class variances equal to one. An `OUT=` data set cannot be created if the `DATA=` data set is not an ordinary SAS data set.

OUTSTAT= Data Set

The `OUTSTAT=` data set is similar to the `TYPE=CORR` data set produced by the `CORR` procedure but contains many results in addition to those produced by the `CORR` procedure.

The `OUTSTAT=` data set is `TYPE=CORR`, and it contains the following variables:

- the `BY` variables, if any
- the `CLASS` variable
- `_TYPE_`, a character variable of length 8 that identifies the type of statistic
- `_NAME_`, a character variable of length 32 that identifies the row of the matrix or the name of the canonical variable
- the quantitative variables (those in the `VAR` statement, or if there is no `VAR` statement, all numeric variables not listed in any other statement)

The observations, as identified by the variable `_TYPE_`, have the following `_TYPE_` values:

<code>_TYPE_</code>	Contents
N	number of observations both for the total sample (CLASS variable missing) and within each class (CLASS variable present)
SUMWGT	sum of weights both for the total sample (CLASS variable missing) and within each class (CLASS variable present) if a WEIGHT statement is specified
MEAN	means both for the total sample (CLASS variable missing) and within each class (CLASS variable present)
STDMEAN	total-standardized class means
PSTDMEAN	pooled within-class standardized class means
STD	standard deviations both for the total sample (CLASS variable missing) and within each class (CLASS variable present)
PSTD	pooled within-class standard deviations
BSTD	between-class standard deviations
RSQUARED	univariate R squares

The following kinds of observations are identified by the combination of the variables `_TYPE_` and `_NAME_`. When the `_TYPE_` variable has one of the following values, the `_NAME_` variable identifies the row of the matrix:

<code>_TYPE_</code>	Contents
CSSCP	corrected SSCP matrix for the total sample (CLASS variable missing) and within each class (CLASS variable present)
PSSCP	pooled within-class corrected SSCP matrix
BSSCP	between-class SSCP matrix
COV	covariance matrix for the total sample (CLASS variable missing) and within each class (CLASS variable present)
PCOV	pooled within-class covariance matrix
BCOV	between-class covariance matrix
CORR	correlation matrix for the total sample (CLASS variable missing) and within each class (CLASS variable present)
PCORR	pooled within-class correlation matrix
BCORR	between-class correlation matrix

When the `_TYPE_` variable has one of the following values, the `_NAME_` variable identifies the canonical variable:

<code>_TYPE_</code>	Contents
CANCORR	canonical correlations
STRUCTUR	canonical structure

BSTRUCT	between canonical structure
PSTRUCT	pooled within-class canonical structure
SCORE	total sample standardized canonical coefficients
PSCORE	pooled within-class standardized canonical coefficients
RAWSCORE	raw canonical coefficients
CANMEAN	means of the canonical variables for each class

You can use this data set with PROC SCORE to get scores on the canonical variables for new data by using one of the following forms:

```
* The CLASS variable C is numeric;
proc score data=NewData score=Coef (where=(c = . )) out=Scores;
run;

* The CLASS variable C is character;
proc score data=NewData score=Coef (where=(c = ' ')) out=Scores;
run;
```

The WHERE clause is used to exclude the within-class means and standard deviations. PROC SCORE standardizes the new data by subtracting the original variable means that are stored in the `_TYPE_='MEAN'` observations, and dividing by the original variable standard deviations from the `_TYPE_='STD'` observations. Then PROC SCORE multiplies the standardized variables by the coefficients from the `_TYPE_='SCORE'` observations to get the canonical scores.

Computational Resources

In the following discussion, let

- n = number of observations
- c = number of class levels
- v = number of variables in the VAR list
- l = length of the CLASS variable

Memory Requirements

The amount of memory in bytes for temporary storage needed to process the data is

$$c(4v^2 + 28v + 4l + 68) + 16v^2 + 96v + 4l$$

With the ANOVA option, the temporary storage must be increased by $16v$ bytes. The DISTANCE option requires an additional temporary storage of $4v^2 + 4v$ bytes.

Time Requirements

The following factors determine the time requirements of the CANDISC procedure:

- The time needed for reading the data and computing covariance matrices is proportional to nv^2 . PROC CANDISC must also look up each class level in the list. This is faster if the data are sorted by the CLASS variable. The time for looking up class levels is proportional to a value ranging from n to $n \log(c)$.
- The time for inverting a covariance matrix is proportional to v^3 .
- The time required for the canonical discriminant analysis is proportional to v^3 .

Each of the preceding factors has a different constant of proportionality.

Displayed Output

The displayed output from PROC CANDISC includes the class level information table. For each level of the classification variable, the following information is provided: the output data set variable name, frequency sum, weight sum, and the proportion of the total sample.

The optional output from PROC CANDISC includes the following:

- Within-class SSCP matrices for each group
- Pooled within-class SSCP matrix
- Between-class SSCP matrix
- Total-sample SSCP matrix
- Within-class covariance matrices for each group
- Pooled within-class covariance matrix
- Between-class covariance matrix, equal to the between-class SSCP matrix divided by $n(c - 1)/c$, where n is the number of observations and c is the number of classes
- Total-sample covariance matrix
- Within-class correlation coefficients and $\text{Pr} > |r|$ to test the hypothesis that the within-class population correlation coefficients are zero
- Pooled within-class correlation coefficients and $\text{Pr} > |r|$ to test the hypothesis that the partial population correlation coefficients are zero
- Between-class correlation coefficients and $\text{Pr} > |r|$ to test the hypothesis that the between-class population correlation coefficients are zero
- Total-sample correlation coefficients and $\text{Pr} > |r|$ to test the hypothesis that the total population correlation coefficients are zero

- Simple statistics, including N (the number of observations), sum, mean, variance, and standard deviation both for the total sample and within each class
- Total-sample standardized class means, obtained by subtracting the grand mean from each class mean and dividing by the total sample standard deviation
- Pooled within-class standardized class means, obtained by subtracting the grand mean from each class mean and dividing by the pooled within-class standard deviation
- Pairwise squared distances between groups
- Univariate test statistics, including total-sample standard deviations, pooled within-class standard deviations, between-class standard deviations, R square, $R^2/(1 - R^2)$, F , and $\text{Pr} > F$ (univariate F values and probability levels for one-way analyses of variance)

By default, PROC CANDISC displays these statistics:

- Multivariate statistics and F approximations including Wilks' lambda, Pillai's trace, Hotelling-Lawley trace, and Roy's greatest root with F approximations, numerator and denominator degrees of freedom (Num DF and Den DF), and probability values ($\text{Pr} > F$). Each of these four multivariate statistics tests the hypothesis that the class means are equal in the population. See the section "[Multivariate Tests](#)" on page 92 in Chapter 4, "[Introduction to Regression Procedures](#)," for more information.
- Canonical correlations
- Adjusted canonical correlations (Lawley 1959). These are asymptotically less biased than the raw correlations and can be negative. The adjusted canonical correlations might not be computable and are displayed as missing values if two canonical correlations are nearly equal or if some are close to zero. A missing value is also displayed if an adjusted canonical correlation is larger than a previous adjusted canonical correlation.
- Approximate standard error of the canonical correlations
- Squared canonical correlations
- Eigenvalues of $\mathbf{E}^{-1}\mathbf{H}$. Each eigenvalue is equal to $\rho^2/(1 - \rho^2)$, where ρ^2 is the corresponding squared canonical correlation and can be interpreted as the ratio of between-class variation to pooled within-class variation for the corresponding canonical variable. The table includes Eigenvalues, Differences between successive eigenvalues, the Proportion of the sum of the eigenvalues, and the Cumulative proportion.
- Likelihood ratio for the hypothesis that the current canonical correlation and all smaller ones are zero in the population. The likelihood ratio for the hypothesis that all canonical correlations equal zero is Wilks' lambda.
- Approx F statistic based on Rao's approximation to the distribution of the likelihood ratio (Rao 1973, p. 556; Kshirsagar 1972, p. 326)
- Numerator degrees of freedom (Num DF), denominator degrees of freedom (Den DF), and $\text{Pr} > F$, the probability level associated with the F statistic

The following statistics can be suppressed with the SHORT option:

- Total canonical structure, giving total-sample correlations between the canonical variables and the original variables
- Between canonical structure, giving between-class correlations between the canonical variables and the original variables
- Pooled within canonical structure, giving pooled within-class correlations between the canonical variables and the original variables
- Total-sample standardized canonical coefficients, standardized to give canonical variables with zero mean and unit pooled within-class variance when applied to the total-sample standardized variables
- Pooled within-class standardized canonical coefficients, standardized to give canonical variables with zero mean and unit pooled within-class variance when applied to the pooled within-class standardized variables
- Raw canonical coefficients, standardized to give canonical variables with zero mean and unit pooled within-class variance when applied to the centered variables
- Class means on the canonical variables

ODS Table Names

PROC CANDISC assigns a name to each table it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in Table 29.2. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

Table 29.2 ODS Tables Produced by PROC CANDISC

ODS Table Name	Description	PROC CANDISC Option
ANOVA	Univariate statistics	ANOVA
AveRSquare	Average R square	ANOVA
BCorr	Between-class correlations	BCORR
BCov	Between-class covariances	BCOV
BSSCP	Between-class SSCP matrix	BSSCP
BStruc	Between canonical structure	default
CanCorr	Canonical correlations	default
CanonicalMeans	Class means on canonical variables	default
Counts	Number of observations, variables, classes, df	default
CovDF	DF for covariance matrices, not printed	any *COV option
Dist	Squared distances	DISTANCE
DistFValues	F statistics based on squared distances	DISTANCE
DistProb	Probabilities for F statistics from squared distances	DISTANCE

Table 29.2 continued

ODS Table Name	Description	PROC CANDISC Option
Levels	Class level information	default
MultStat	MANOVA	default
NObs	Number of observations	default
PCoef	Pooled standard canonical coefficients	default
PCorr	Pooled within-class correlations	PCORR
PCov	Pooled within-class covariances	PCOV
PSSCP	Pooled within-class SSCP matrix	PSSCP
PStdMeans	Pooled standardized class means	STDMEAN
PStruc	Pooled within canonical structure	default
RCoef	Raw canonical coefficients	default
SimpleStatistics	Simple statistics	SIMPLE
TCoef	Total-sample standard canonical coefficients	default
TCorr	Total-sample correlations	TCORR
TCov	Total-sample covariances	TCOV
TSSCP	Total-sample SSCP matrix	TSSCP
TStdMeans	Total standardized class means	STDMEAN
TStruc	Total canonical structure	default
WCorr	Within-class correlations	WCORR
WCov	Within-class covariances	WCOV
WSSCP	Within-class SSCP matrices	WSSCP

Example: CANDISC Procedure

Example 29.1: Analysis of Iris Data With PROC CANDISC

The iris data published by Fisher (1936) have been widely used for examples in discriminant analysis and cluster analysis. The sepal length, sepal width, petal length, and petal width are measured in millimeters on 50 iris specimens from each of three species: *Iris setosa*, *I. versicolor*, and *I. virginica*. The iris data set is available from the Sashelp library.

This example is a canonical discriminant analysis that creates an output data set containing scores on the canonical variables and plots the canonical variables.

The following statements produce [Output 29.1.1](#) through [Output 29.1.6](#):

```

title 'Fisher (1936) Iris Data';

proc candisc data=sashelp.iris out=outcan distance anova;
  class Species;
  var SepalLength SepalWidth PetalLength PetalWidth;
run;

```

PROC CANDISC first displays information about the observations and the classes in the data set in [Output 29.1.1](#).

Output 29.1.1 Iris Data: Summary Information

Fisher (1936) Iris Data				
The CANDISC Procedure				
Total Sample Size	150	DF Total		149
Variables	4	DF Within Classes		147
Classes	3	DF Between Classes		2
Number of Observations Read		150		
Number of Observations Used		150		
Class Level Information				
Species	Variable Name	Frequency	Weight	Proportion
Setosa	Setosa	50	50.0000	0.333333
Versicolor	Versicolor	50	50.0000	0.333333
Virginica	Virginica	50	50.0000	0.333333

The DISTANCE option in the PROC CANDISC statement displays squared Mahalanobis distances between class means. Results from the DISTANCE option are shown in [Output 29.1.2](#).

Output 29.1.2 Iris Data: Squared Mahalanobis Distances and Distance Statistics

Fisher (1936) Iris Data				
The CANDISC Procedure				
Squared Distance to Species				
From Species	Setosa	Versicolor	Virginica	
Setosa	0	89.86419	179.38471	
Versicolor	89.86419	0	17.20107	
Virginica	179.38471	17.20107	0	

Output 29.1.2 *continued*

F Statistics, NDF=4, DDF=144 for Squared Distance to Species			
From Species	Setosa	Versicolor	Virginica
Setosa	0	550.18889	1098
Versicolor	550.18889	0	105.31265
Virginica	1098	105.31265	0

Prob > Mahalanobis Distance for Squared Distance to Species			
From Species	Setosa	Versicolor	Virginica
Setosa	1.0000	<.0001	<.0001
Versicolor	<.0001	1.0000	<.0001
Virginica	<.0001	<.0001	1.0000

The ANOVA option uses univariate statistics to test the hypothesis that the class means are equal. The resulting R-square values (see [Output 29.1.3](#)) range from 0.4008 for SepalWidth to 0.9414 for PetalLength, and each variable is significant at the 0.0001 level. The multivariate test for differences between the classes (which is displayed by default) is also significant at the 0.0001 level; you would expect this from the highly significant univariate test results.

Output 29.1.3 Iris Data: Univariate and Multivariate Statistics

Fisher (1936) Iris Data								
The CANDISC Procedure								
Univariate Test Statistics								
F Statistics, Num DF=2, Den DF=147								
Variable	Label	Total Standard Deviation	Pooled Standard Deviation	Between Standard Deviation	R-Square	R-Square / (1-RSq)	F Value	Pr > F
Sepal Length	Sepal Length (mm)	8.2807	5.1479	7.9506	0.6187	1.6226	119.26	<.0001
Sepal Width	Sepal Width (mm)	4.3587	3.3969	3.3682	0.4008	0.6688	49.16	<.0001
Petal Length	Petal Length (mm)	17.6530	4.3033	20.9070	0.9414	16.0566	1180.16	<.0001
Petal Width	Petal Width (mm)	7.6224	2.0465	8.9673	0.9289	13.0613	960.01	<.0001

Output 29.1.3 continued

Average R-Square					
Unweighted					0.7224358
Weighted by Variance					0.8689444
Multivariate Statistics and F Approximations					
	S=2	M=0.5	N=71		
Statistic	Value	F Value	Num DF	Den DF	Pr > F
Wilks' Lambda	0.02343863	199.15	8	288	<.0001
Pillai's Trace	1.19189883	53.47	8	290	<.0001
Hotelling-Lawley Trace	32.47732024	582.20	8	203.4	<.0001
Roy's Greatest Root	32.19192920	1166.96	4	145	<.0001
NOTE: F Statistic for Roy's Greatest Root is an upper bound.					
NOTE: F Statistic for Wilks' Lambda is exact.					

The R square between Can1 and the class variable, 0.969872, is much larger than the corresponding R square for Can2, 0.222027. This is displayed in [Output 29.1.4](#).

Output 29.1.4 Iris Data: Canonical Correlations and Eigenvalues

Fisher (1936) Iris Data					
The CANDISC Procedure					
	Canonical Correlation	Adjusted Canonical Correlation	Approximate Standard Error	Squared Canonical Correlation	
1	0.984821	0.984508	0.002468	0.969872	
2	0.471197	0.461445	0.063734	0.222027	
Eigenvalues of $\text{Inv}(E) * H$ = $\text{CanRsqr} / (1 - \text{CanRsqr})$					
	Eigenvalue	Difference	Proportion	Cumulative	
1	32.1919	31.9065	0.9912	0.9912	
2	0.2854		0.0088	1.0000	
Test of H0: The canonical correlations in the current row and all that follow are zero					
	Likelihood Ratio	Approximate F Value	Num DF	Den DF	Pr > F
1	0.02343863	199.15	8	288	<.0001
2	0.77797337	13.79	3	145	<.0001

Output 29.1.5 Iris Data: Correlations between Canonical and Original Variables

Fisher (1936) Iris Data			
The CANDISC Procedure			
Total Canonical Structure			
Variable	Label	Can1	Can2
SepalLength	Sepal Length (mm)	0.791888	0.217593
SepalWidth	Sepal Width (mm)	-0.530759	0.757989
PetalLength	Petal Length (mm)	0.984951	0.046037
PetalWidth	Petal Width (mm)	0.972812	0.222902

Between Canonical Structure			
Variable	Label	Can1	Can2
SepalLength	Sepal Length (mm)	0.991468	0.130348
SepalWidth	Sepal Width (mm)	-0.825658	0.564171
PetalLength	Petal Length (mm)	0.999750	0.022358
PetalWidth	Petal Width (mm)	0.994044	0.108977

Pooled Within Canonical Structure			
Variable	Label	Can1	Can2
SepalLength	Sepal Length (mm)	0.222596	0.310812
SepalWidth	Sepal Width (mm)	-0.119012	0.863681
PetalLength	Petal Length (mm)	0.706065	0.167701
PetalWidth	Petal Width (mm)	0.633178	0.737242

The raw canonical coefficients (shown in [Output 29.1.6](#)) for the first canonical variable, Can1, show that the classes differ most widely on the linear combination of the centered variables: $-0.0829378 \times \text{SepalLength} - 0.153447 \times \text{SepalWidth} + 0.220121 \times \text{PetalLength} + 0.281046 \times \text{PetalWidth}$.

Output 29.1.6 Iris Data: Canonical Coefficients

Fisher (1936) Iris Data			
The CANDISC Procedure			
Total-Sample Standardized Canonical Coefficients			
Variable	Label	Can1	Can2
SepalLength	Sepal Length (mm)	-0.686779533	0.019958173
SepalWidth	Sepal Width (mm)	-0.668825075	0.943441829
PetalLength	Petal Length (mm)	3.885795047	-1.645118866
PetalWidth	Petal Width (mm)	2.142238715	2.164135931

Output 29.1.6 continued

Pooled Within-Class Standardized Canonical Coefficients			
Variable	Label	Can1	Can2
SepalLength	Sepal Length (mm)	-.4269548486	0.0124075316
SepalWidth	Sepal Width (mm)	-.5212416758	0.7352613085
PetalLength	Petal Length (mm)	0.9472572487	-.4010378190
PetalWidth	Petal Width (mm)	0.5751607719	0.5810398645

Raw Canonical Coefficients			
Variable	Label	Can1	Can2
SepalLength	Sepal Length (mm)	-.0829377642	0.0024102149
SepalWidth	Sepal Width (mm)	-.1534473068	0.2164521235
PetalLength	Petal Length (mm)	0.2201211656	-.0931921210
PetalWidth	Petal Width (mm)	0.2810460309	0.2839187853

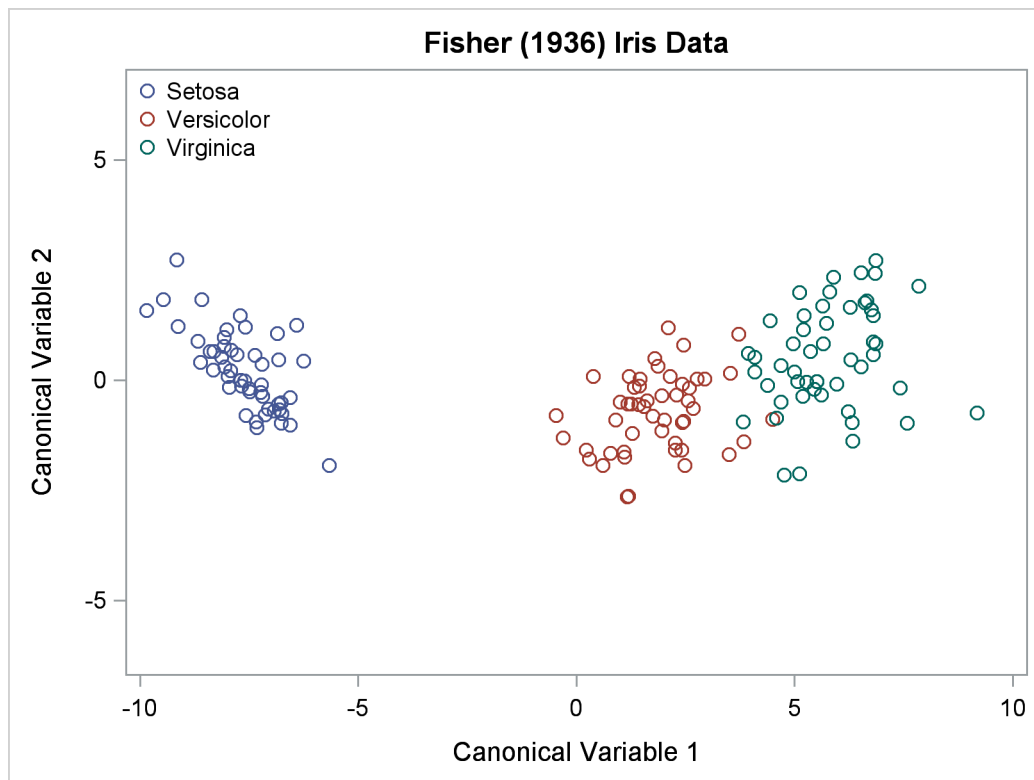
Output 29.1.7 Iris Data: Canonical Means

Class Means on Canonical Variables			
Species		Can1	Can2
Setosa		-7.607599927	0.215133017
Versicolor		1.825049490	-0.727899622
Virginica		5.782550437	0.512766605

The TEMPLATE and SGRENDER procedures are used to create a plot of the first two canonical variables. The following statements produce [Output 29.1.8](#):

```
proc template;
  define statgraph scatter;
    begingraph;
      entrytitle 'Fisher (1936) Iris Data';
      layout overlayequated / equatetype=fit
        xaxisopts=(label='Canonical Variable 1')
        yaxisopts=(label='Canonical Variable 2');
      scatterplot x=Can1 y=Can2 / group=species name='iris';
      layout gridded / autoalign=(topleft);
      discretelegend 'iris' / border=false opaque=false;
    endlayout;
  endgraph;
end;
run;

proc sgrender data=outcan template=scatter;
run;
```

Output 29.1.8 Iris Data: Plot of First Two Canonical Variables

The plot of canonical variables in [Output 29.1.8](#) shows that of the two canonical variables, Can1 has more discriminatory power.

References

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Chapter 30

The CATMOD Procedure

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Overview: CATMOD Procedure

The CATMOD procedure performs categorical data modeling of data that can be represented by a contingency table. PROC CATMOD fits linear models to functions of response frequencies, and it can be used for linear modeling, log-linear modeling, logistic regression, and repeated measurement analysis. PROC CATMOD uses the following estimation methods:

- weighted least squares (WLS) estimation of parameters for a wide range of general linear models
- maximum likelihood (ML) estimation of parameters for log-linear models and the analysis of generalized logits

The CATMOD procedure provides a wide variety of categorical data analyses, many of which are generalizations of continuous data analysis methods. For example, analysis of variance, in the traditional sense, refers to the analysis of means and the partitioning of variation among the means into various sources. Here, the term *analysis of variance* is used in a generalized sense to denote the analysis of response functions and the partitioning of variation among those functions into various sources. The response functions might be mean scores if the dependent variables are ordinally scaled. But they can also be marginal probabilities, cumulative logits, or other functions that incorporate the essential information from the dependent variables.

NOTE: PROC CATMOD specializes in WLS modeling and analysis of a wide range of models on contingency tables. For ML modeling on standard models, especially with continuous predictors, it might be more appropriate to use a procedure such as PROC GENMOD or PROC LOGISTIC; see Chapter 40, “The GENMOD Procedure,” and Chapter 54, “The LOGISTIC Procedure,” for more information.

Types of Input Data

The data that PROC CATMOD analyzes are usually supplied in one of two ways. First, you can supply raw data, where each observation is a subject. Second, you can supply cell count data, where each observation is a cell in a contingency table. (A third way, which uses direct input of the covariance matrix, is also available; details are given in the section “[Inputting Response Functions and Covariances Directly](#)” on page 1820.)

Suppose detergent brand preference is related to three other categorical variables: water softness, water temperature, and previous use of a brand of detergent. In the raw data case, each observation in the input data set identifies a given respondent in the study and contains information about all four variables. The data set contains the same number of observations as the survey had respondents. In the cell count case, each observation identifies a given cell in the four-way table of water softness, water temperature, previous use of brand, and brand preference. A fifth variable contains the number of respondents in the cell. In the analysis, this fifth variable is identified in a **WEIGHT** statement. The data set contains the same number of observations as the number of cross-classifications formed by the four categorical variables. For more about this particular example, see [Example 30.1](#). For additional details, see the section “[Input Data Sets](#)” on page 1818.

Most of the examples in this chapter use cell counts as input and use a **WEIGHT** statement.

Types of Statistical Analyses

This section illustrates, by example, the wide variety of categorical data analyses that PROC CATMOD provides. For each type of analysis, a brief description of the statistical problem and the SAS statements to provide the analysis are given. For each analysis, assume that the input data set consists of a set of cell counts from a contingency table. The variable specified in the **WEIGHT** statement contains these counts. In all these analyses, both the dependent and independent variables are categorical.

Linear Model Analysis

Suppose you want to analyze the relationship between the dependent variables (r_1 , r_2) and the independent variables (a , b). Analyze the marginal probabilities of the dependent variables, and use a main-effects model:

```
proc catmod;
  weight wt;
  response marginals;
  model r1*r2=a b;
quit;
```

Log-Linear Model Analysis

Suppose you want to analyze the nominal dependent variables (r_1 , r_2 , r_3) with a log-linear model. Use maximum likelihood analysis, include the main effects and the r_1*r_2 interaction in the model, and obtain the predicted cell frequencies:

```
proc catmod;
  weight wt;
  model r1*r2*r3=_response_ / pred=freq;
  loglin r1|r2 r3;
quit;
```

Logistic Regression

Suppose you want to analyze the relationship between the nominal dependent variable (r) and the independent variables (x_1 , x_2) with a logistic regression analysis. Use maximum likelihood estimation:

```
proc catmod;
  weight wt;
  direct x1 x2;
  model r=x1 x2;
quit;
```

If x_1 and x_2 are continuous so that each observation has a unique value of these two variables, then it might be more appropriate to use the [LOGISTIC](#) or [GENMOD](#) procedure. (See the section “[Logistic Regression](#)” on page 1826.)

Repeated Measures Analysis

Suppose the dependent variables (r_1 , r_2 , r_3) represent the same type of measurement taken at three different times. Analyze the relationship among the dependent variables, the repeated measurement factor (time), and the independent variable (a):

```
proc catmod;
  weight wt;
  response marginals;
  model r1*r2*r3=_response_|a;
  repeated time 3 / _response_=time;
quit;
```

Analysis of Variance

Suppose you want to investigate the relationship between the dependent variable (r) and the independent variables (a , b). Analyze the mean of the dependent variable, and include all main effects and interactions in the model:

```
proc catmod;
  weight wt;
  response mean;
  model r=a|b;
quit;
```

Linear Regression

PROC CATMOD can analyze the relationship between the dependent variables (r_1 , r_2) and the independent variables (x_1 , x_2). Use a linear regression analysis to analyze the marginal probabilities of the dependent variables:

```
proc catmod;
  weight wt;
  direct x1 x2;
  response marginals;
  model r1*r2=x1 x2;
quit;
```

Logistic Analysis of Ordinal Data

Suppose you want to analyze the relationship between the ordinally scaled dependent variable (r) and the independent variable (a). Use cumulative logits to take into account the ordinal nature of the dependent variable, and use weighted least squares estimation:

```
proc catmod;
  weight wt;
  response clogits;
  model r=_response_ a;
quit;
```

Sample Survey Analysis

Suppose the data set contains estimates of a vector of four functions and their covariance matrix, estimated in such a way as to correspond to the sampling process that is used. Analyze the functions with respect to the independent variables (a , b), and use a main-effects model:

```
proc catmod;
  response read b1-b10;
  model _f=_response_;
  factors a 2 , b 5 / _response_=a b;
quit;
```

Background: The Underlying Model

The CATMOD procedure analyzes data that can be represented by a two-dimensional contingency table. The rows of the table correspond to populations (or samples) formed on the basis of one or more independent variables. The columns of the table correspond to observed responses formed on the basis of one or more dependent variables. The frequency in the (i, j) cell is the number of subjects in the i th population that have the j th response. The frequencies in the table are assumed to follow a product multinomial distribution, corresponding to a sampling design in which a simple random sample is taken for each population. The contingency table can be represented as shown in [Table 30.1](#).

Table 30.1 Contingency Table Representation

Sample	Response				Total
	1	2	...	<i>r</i>	
1	n_{11}	n_{12}	...	n_{1r}	n_1
2	n_{21}	n_{22}	...	n_{2r}	n_2
⋮	⋮	⋮	⋮	⋮	⋮
<i>s</i>	n_{s1}	n_{s2}	...	n_{sr}	n_s

For each sample i , the probability of the j th response (π_{ij}) is estimated by the sample proportion, $p_{ij} = n_{ij}/n_i$. The vector (\mathbf{p}) of all such proportions is then transformed into a vector of functions, denoted by $\mathbf{F} = \mathbf{F}(\mathbf{p})$. If $\boldsymbol{\pi}$ denotes the vector of true probabilities for the entire table, then the functions of the true probabilities, denoted by $\mathbf{F}(\boldsymbol{\pi})$, are assumed to follow a linear model

$$\mathbf{E}_A(\mathbf{F}) = \mathbf{F}(\boldsymbol{\pi}) = \mathbf{X}\boldsymbol{\beta}$$

where \mathbf{E}_A denotes asymptotic expectation, \mathbf{X} is the design matrix containing fixed constants, and $\boldsymbol{\beta}$ is a vector of parameters to be estimated.

PROC CATMOD provides two estimation methods:

- The weighted least squares method minimizes the weighted residual sum of squares for the model. The weights are contained in the inverse covariance matrix of the functions $\mathbf{F}(\mathbf{p})$. According to central limit theory, if the sample sizes within populations are sufficiently large, the elements of \mathbf{F} and \mathbf{b} (the estimate of $\boldsymbol{\beta}$) are distributed approximately as multivariate normal. This allows the computation of statistics for testing the goodness of fit of the model and the significance of other sources of variation. For details of the theory, see Grizzle, Starmer, and Koch (1969) or Koch et al. (1977, Appendix 1). Weighted least squares estimation is available for all types of response functions.
- The maximum likelihood method estimates the parameters of the linear model so as to maximize the value of the joint multinomial likelihood function of the responses. Maximum likelihood estimation is available only for the standard response functions, logits and generalized logits, which are used for logistic regression analysis and log-linear model analysis. Two methods of maximization are available: Newton-Raphson and iterative proportional fitting. For details of the theory, see Bishop, Fienberg, and Holland (1975).

Following parameter estimation, hypotheses about linear combinations of the parameters can be tested. For that purpose, PROC CATMOD computes generalized Wald (1943) statistics, which are approximately chi-square distributed if the sample sizes are sufficiently large and the null hypotheses are true.

Linear Models Contrasted with Log-Linear Models

Linear model methods typified by the Grizzle, Starmer, and Koch (1969) approach make a very clear distinction between independent and dependent variables. The emphasis of these methods is estimation and hypothesis testing of the model parameters. Therefore, it is easy to test for differences among probabilities,

perform repeated measures analysis, and test for marginal homogeneity, but it is difficult to test for independence and generalized independence. These methods are a natural extension of the usual ANOVA approach for continuous data.

In contrast, log-linear model methods typified by the Bishop, Fienberg, and Holland (1975) approach do not make an a priori distinction between independent and dependent variables, although model specifications that allow for the distinction can be made. The emphasis of these methods is on model building, goodness-of-fit tests, and estimation of cell frequencies or probabilities for the underlying contingency table. With these methods, it is easy to test independence and generalized independence, but it is difficult to test for differences among probabilities, do repeated measures analysis, and test for marginal homogeneity.

Using PROC CATMOD Interactively

You can use the CATMOD procedure interactively. After specifying a model with a MODEL statement and running PROC CATMOD with a RUN statement, you can execute any statement without reinvoking PROC CATMOD. You can execute the statements singly or in groups by following the single statement or group of statements with a RUN statement. Note that you can use more than one MODEL statement; this is an important difference from the GLM procedure.

If you use PROC CATMOD interactively, you can end the CATMOD procedure with a DATA step, another PROC step, an ENDSAS statement, or a QUIT statement. The syntax of the QUIT statement is as follows:

```
quit;
```

When you are using PROC CATMOD interactively, additional RUN statements do not end the procedure run but tell the procedure to execute additional statements.

When the CATMOD procedure detects a BY statement, it disables interactive processing; that is, once the BY statement and the next RUN statement are encountered, processing proceeds for each BY group in the data set, and no additional statements are accepted by the procedure. For example, the following statements perform three analyses: one for the entire data set, one for males, and one for females:

```
proc catmod;
  weight wt;
  response marginals;
  model r1*r2=a|b;
run;
  by sex;
run;
```

Note that the BY statement can appear after the first RUN statement; this is an important difference from PROC GLM, which requires that the BY statement appear before the first RUN statement.

Getting Started: CATMOD Procedure

The CATMOD procedure is a general modeling procedure for categorical data analysis, and it can be used for sophisticated analyses that require matrix specification of the response function and the design matrix.

It can also be used to perform basic analysis-of-variance-type analyses that require only a few statements. The following is a basic example.

Weighted Least Squares Analysis of Mean Response

Consider the data in Table 30.2 (Stokes, Davis, and Koch 2000).

Table 30.2 Colds in Children

Sex	Residence	Periods with Colds			Total
		0	1	2	
Female	Rural	45	64	71	180
Female	Urban	80	104	116	300
Male	Rural	84	124	82	290
Male	Urban	106	117	87	310

For male and female children in rural and urban counties, the number of periods (of two) in which subjects report cold symptoms are recorded. So 45 subjects who are female and in rural counties report no cold symptoms, and 71 subjects who are female and from rural counties report colds in both periods.

The question of interest is whether the mean number of periods with colds reported is associated with gender or type of county. There is no reason to believe that the mean number of periods with colds is normally distributed, so a weighted least squares analysis of these data is performed with PROC CATMOD instead of an analysis of variance with PROC ANOVA or PROC GLM.

The input data for categorical data are often recorded in frequency form, with the counts for each particular profile being the input values. For the colds data, the input SAS data set colds is created with the following statements. The variable count contains the frequency of observations that have the particular profile described by the values of the other variables in that input line.

```
data colds;
  input sex $ residence $ periods count @@;
  datalines;
female rural 0 45 female rural 1 64 female rural 2 71
female urban 0 80 female urban 1 104 female urban 2 116
male rural 0 84 male rural 1 124 male rural 2 82
male urban 0 106 male urban 1 117 male urban 2 87
;
```

In order to fit a model to the mean number of periods with colds, you have to specify the response function in PROC CATMOD. The default response function is the logit if the response variable has two values, and it is generalized logits if the response variable has more than two values. If you want a different response function, then you specify that function in the RESPONSE statement. To request the mean number of periods with colds, you specify the MEANS option in the RESPONSE statement.

You can request a model consisting of the main effects and interaction of the variables sex and residence just as you would in the GLM procedure. Unlike the GLM procedure, PROC CATMOD does not require you to use a CLASS statement to treat a variable as a classification variable. In the CATMOD procedure, all variables in the MODEL statement are treated as classification variables unless you specify otherwise with

a **DIRECT** statement. To verify that your model is specified correctly, you can specify the **DESIGN** option in the **MODEL** statement to display the design matrix.

The PROC CATMOD statements needed to model mean periods of colds with a main-effects and interaction model are as follows:

```
proc catmod data=colds;
  weight count;
  response means;
  model periods = sex residence sex*residence / design;
run;
```

The results of this analysis are shown in [Figure 30.1](#) through [Figure 30.3](#).

In [Figure 30.1](#), the CATMOD procedure first displays a summary of the contingency table you are analyzing. The “Population Profiles” table lists the values of the explanatory variables that define each population, or row of the underlying contingency table, and labels each group with a sample number. The number of observations in each population is also displayed. The “Response Profiles” table lists the variable levels that define the response, or columns of the underlying contingency table.

Figure 30.1 Model Information and Profile Tables

The CATMOD Procedure			
Data Summary			
Response	periods	Response Levels	3
Weight Variable	count	Populations	4
Data Set	COLDS	Total Frequency	1080
Frequency Missing	0	Observations	12
Population Profiles			
Sample	sex	residence	Sample Size
1	female	rural	180
2	female	urban	300
3	male	rural	290
4	male	urban	310
Response Profiles			
Response	periods		
1	0		
2	1		
3	2		

The “Response Functions and Design Matrix” table in [Figure 30.2](#) contains the observed response functions—in this case, the mean number of periods with colds for each of the populations—and the design matrix. The first column of the design matrix contains the coefficients for the intercept parameter. The second column contains the coefficients for the sex parameter. (Note that the sum-to-zero constraint of the

default full-rank parameterization `PARAM=EFFECT` implies that the coefficient for males is the negative of that for females; the parameter is called the *differential effect* for females.) The third column is similarly set up for residence, and the last column is for the interaction.

Figure 30.2 Observed Response Functions and Design Matrix

Response Functions and Design Matrix					
Sample	Response Function	Design Matrix			
		1	2	3	4
1	1.14444	1	1	1	1
2	1.12000	1	1	-1	-1
3	0.99310	1	-1	1	-1
4	0.93871	1	-1	-1	1

The model-fitting results are displayed in the “Analysis of Variance” table (Figure 30.3), which is similar to an ANOVA table. The effects from the right side of the MODEL statement are listed in the Source column.

Figure 30.3 ANOVA Table for the Saturated Model

Analysis of Variance			
Source	DF	Chi-Square	Pr > ChiSq
Intercept	1	1841.13	<.0001
sex	1	11.57	0.0007
residence	1	0.65	0.4202
sex*residence	1	0.09	0.7594
Residual	0	.	.

You can see in Figure 30.3 that the interaction effect is nonsignificant, so the data are reanalyzed using a main-effects model. Since PROC CATMOD is an interactive procedure, you can analyze the main-effects model by simply submitting the new MODEL statement as follows. The resulting tables are displayed in Figure 30.4 and Figure 30.5.

```
model periods = sex residence / design;
run;
```

From the ANOVA table in Figure 30.4, you can see that the goodness-of-fit chi-square statistic is 0.09 with one degree of freedom and a p -value of 0.7594; hence, the model fits the data. Note that the chi-square tests in Figure 30.4 check whether all the parameters for a given effect are zero. In this model, each effect has only one parameter and therefore only one degree of freedom.

Figure 30.4 Main-Effects Model

The CATMOD Procedure			
Data Summary			
Response	periods	Response Levels	3
Weight Variable	count	Populations	4
Data Set	COLDS	Total Frequency	1080
Frequency Missing	0	Observations	12

Population Profiles			
Sample	sex	residence	Sample Size
1	female	rural	180
2	female	urban	300
3	male	rural	290
4	male	urban	310

Response Profiles		
Response	periods	
1	0	
2	1	
3	2	

Response Functions and Design Matrix				
Sample	Response Function	Design Matrix		
		1	2	3
1	1.14444	1	1	1
2	1.12000	1	1	-1
3	0.99310	1	-1	1
4	0.93871	1	-1	-1

Analysis of Variance			
Source	DF	Chi-Square	Pr > ChiSq
Intercept	1	1882.77	<.0001
sex	1	12.08	0.0005
residence	1	0.76	0.3839
Residual	1	0.09	0.7594

The “Analysis of Weighted Least Squares Estimates” table in [Figure 30.5](#) lists the parameters and their estimates for the model, as well as the standard errors, Wald statistics, and *p*-values. These chi-square tests are one-degree-of-freedom tests that the individual parameter is equal to zero. They are equal to the tests shown in [Figure 30.4](#) since each effect is composed of exactly one parameter.

Figure 30.5 Parameter Estimates for the Main-Effects Model

Analysis of Weighted Least Squares Estimates				
Parameter	Estimate	Standard Error	Chi-Square	Pr > ChiSq
Intercept	1.0501	0.0242	1882.77	<.0001
sex female	0.0842	0.0242	12.08	0.0005
residence rural	0.0210	0.0241	0.76	0.3839

You can compute the mean number of periods with colds for the first population (Sample 1, females in rural residences) from Table 30.2 as follows:

$$\text{mean colds} = 0 \times \frac{45}{180} + 1 \times \frac{64}{180} + 2 \times \frac{71}{180} = 1.1444$$

This is the same value reported in the Response Function column for Sample 1 in the “Response Functions and Design Matrix” table displayed in Figure 30.4.

PROC CATMOD is fitting a model to the mean number of colds in each population as follows:

$$\begin{bmatrix} \text{Expected number of colds for rural females} \\ \text{urban females} \\ \text{rural males} \\ \text{urban males} \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & -1 \\ 1 & -1 & 1 \\ 1 & -1 & -1 \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix}$$

where the design matrix is the same one displayed in Figure 30.4, β_0 is the mean number of colds averaged over all the populations, β_1 is the differential effect for females, and β_2 is the differential effect for rural residences. The parameter estimates are shown in Figure 30.5; the expected number of periods with colds for rural females from this model is computed as

$$1 \times 1.0501 + 1 \times 0.0842 + 1 \times 0.0210 = 1.1553$$

and the expected number for rural males from this model is

$$1 \times 1.0501 - 1 \times 0.0842 + 1 \times 0.0210 = 0.9869$$

Notice also, in Figure 30.5, that the differential effect for residence is nonsignificant ($p = 0.3839$). If you continue the analysis by fitting a single-effect model (sex), you need to include a POPULATION statement to maintain the same underlying contingency table:

```
population sex residence;
model periods = sex;
run;
```

Generalized Logits Model

Over the course of one school year, third-graders from three different schools are exposed to three different styles of mathematics instruction: a self-paced computer-learning style, a team approach, and a traditional

class approach. The students are asked which style they prefer, and their responses, classified by the type of program they are in (a regular school day versus a regular school day supplemented with an afternoon school program), are displayed in Table 30.3. The data set is from Stokes, Davis, and Koch (2000), and it is also analyzed in the section “Example 54.4: Nominal Response Data: Generalized Logits Model” on page 4327 of Chapter 54, “The LOGISTIC Procedure.”

Table 30.3 School Program Data

School	Program	Learning Style Preference		
		Self	Team	Class
1	Regular	10	17	26
1	Afternoon	5	12	50
2	Regular	21	17	26
2	Afternoon	16	12	36
3	Regular	15	15	16
3	Afternoon	12	12	20

The levels of the response variable (self, team, and class) have no essential ordering, so a logistic regression is performed on the generalized logits. The model to be fit is

$$\log\left(\frac{\pi_{hij}}{\pi_{hir}}\right) = \alpha_j + \mathbf{x}'_{hi} \boldsymbol{\beta}_j$$

where π_{hij} is the probability that a student in school h and program i prefers teaching style j , $j \neq r$, and style r is the class style. There are separate sets of intercept parameters α_j and regression parameters β_j for each logit, and the matrix \mathbf{x}_{hi} is the set of explanatory variables for the hi population. Thus, two logits are modeled for each school and program combination (population): the logit comparing self to class and the logit comparing team to class.

The following statements create the data set `school` and request the analysis. Generalized logits are the default response functions, and maximum likelihood estimation is the default method for analyzing generalized logits, so only the `WEIGHT` and `MODEL` statements are required. The option `ORDER=DATA` means that the response variable levels are ordered as they exist in the data set: self, team, and class; the logits are formed by comparing self to class and by comparing team to class. The results of this analysis are shown in Figure 30.6 and Figure 30.7.

```
data school;
  length Program $ 9;
  input School Program $ Style $ Count @@;
  datalines;
1 regular self 10 1 regular team 17 1 regular class 26
1 afternoon self 5 1 afternoon team 12 1 afternoon class 50
2 regular self 21 2 regular team 17 2 regular class 26
2 afternoon self 16 2 afternoon team 12 2 afternoon class 36
3 regular self 15 3 regular team 15 3 regular class 16
3 afternoon self 12 3 afternoon team 12 3 afternoon class 20
;
```

```
proc catmod order=data;
  weight Count;
  model Style=School Program School*Program;
run;
```

A summary of the data set is displayed in Figure 30.6; the variable levels that form the three responses and six populations are listed in the “Response Profiles” and “Population Profiles” tables, respectively.

Figure 30.6 Model Information and Profile Tables

The CATMOD Procedure			
Data Summary			
Response	Style	Response Levels	3
Weight Variable	Count	Populations	6
Data Set	SCHOOL	Total Frequency	338
Frequency Missing	0	Observations	18
Population Profiles			
Sample	School	Program	Sample Size
1	1	regular	53
2	1	afternoon	67
3	2	regular	64
4	2	afternoon	64
5	3	regular	46
6	3	afternoon	44
Response Profiles			
Response	Style		
1	self		
2	team		
3	class		

The analysis of variance table is displayed in Figure 30.7. Since this is a saturated model, there are no degrees of freedom remaining for a likelihood ratio test, and missing values are displayed in the table. The interaction effect is clearly nonsignificant, so a main-effects model is fit.

Figure 30.7 Saturated Model: ANOVA Table

Maximum Likelihood Analysis of Variance			
Source	DF	Chi-Square	Pr > ChiSq
Intercept	2	40.05	<.0001
School	4	14.55	0.0057
Program	2	10.48	0.0053
School*Program	4	1.74	0.7827
Likelihood Ratio	0	.	.

Since PROC CATMOD is an interactive procedure, you can analyze the main-effects model by simply submitting the new MODEL statement as follows:

```
model Style=School Program;
run;
```

You can check the population and response profiles (not shown) to confirm that they are the same as those in Figure 30.6. The analysis of variance table is shown in Figure 30.8. The likelihood ratio chi-square statistic is 1.78 with a *p*-value of 0.7766, indicating a good fit; the Wald chi-square tests for the school and program effects are also significant. Since School has three levels, two parameters are estimated for each of the two logits they modeled, for a total of four degrees of freedom. Since Program has two levels, one parameter is estimated for each of the two logits, for a total of two degrees of freedom.

Figure 30.8 Main-Effects Model: ANOVA Table

Maximum Likelihood Analysis of Variance			
Source	DF	Chi-Square	Pr > ChiSq
Intercept	2	39.88	<.0001
School	4	14.84	0.0050
Program	2	10.92	0.0043
Likelihood Ratio	4	1.78	0.7766

The parameter estimates and tests for individual parameters are displayed in Figure 30.9. The order of the parameters corresponds to the order of the population and response variables as shown in the profile tables (see Figure 30.6), with the levels of the response variables varying most rapidly. The first response function is the logit that compares self to class, and the corresponding parameters have Function Number=1. The second logit (Function Number=2) compares team to class. The School=1 parameters are the differential effects versus School=3 for their respective logits, and the School=2 parameters are likewise differential effects versus School=3. The Program parameters are the differential effects of 'regular' versus 'afternoon' for the two response functions.

Figure 30.9 Parameter Estimates

Analysis of Maximum Likelihood Estimates						
Parameter		Function Number	Estimate	Standard Error	Chi-Square	Pr > ChiSq
Intercept		1	-0.7979	0.1465	29.65	<.0001
		2	-0.6589	0.1367	23.23	<.0001
School	1	1	-0.7992	0.2198	13.22	0.0003
		2	-0.2786	0.1867	2.23	0.1356
	2	1	0.2836	0.1899	2.23	0.1352
		2	-0.0985	0.1892	0.27	0.6028
Program	regular	1	0.3737	0.1410	7.03	0.0080
	regular	2	0.3713	0.1353	7.53	0.0061

The Program variable has nearly the same effect on both logits, while School=1 has the largest effect of the schools.

Syntax: CATMOD Procedure

The following statements are available in the CATMOD procedure:

```

PROC CATMOD < options > ;
DIRECT < variables > ;
MODEL response-effect = design-effects < / options > ;
CONTRAST 'label' row-description < , ... , row-description > < / options > ;
BY variables ;
FACTORS factor-description < , ... , factor-description > < / options > ;
LOGLIN effects < / option > ;
POPULATION variables ;
REPEATED factor-description < , ... , factor-description > < / options > ;
RESPONSE < function > < / options > ;
RESTRICT parameter=value < ... parameter=value > ;
WEIGHT variable ;

```

You can use all of the statements in PROC CATMOD interactively. The first RUN statement executes all of the previous statements. Any subsequent RUN statement executes only those statements that appear between the previous RUN statement and the current one. However, if you specify a BY statement, interactive processing is disabled. That is, all statements through the following RUN statement are processed for each BY group in the data set, but no additional statements are accepted by the procedure.

If more than one CONTRAST statement appears between two RUN statements, all the CONTRAST statements are processed. If more than one RESPONSE statement appears between two RUN statements, then analyses associated with each RESPONSE statement are produced. For all other statements, there can be only one occurrence of the statement between any two RUN statements. For example, if there are two LOGLIN statements between two RUN statements, the first LOGLIN statement is ignored.

The PROC CATMOD and MODEL statements are required. If specified, the DIRECT statement must precede the MODEL statement. As a result, if you use the DIRECT statement interactively, you need to specify a MODEL statement in the same RUN group. See the section “DIRECT Statement” on page 1795 for an example.

The CONTRAST statements, if any, must follow the MODEL statement.

You can specify only one of the LOGLIN, REPEATED, and FACTORS statements between any two RUN statements, because they all specify the same information: how to partition the variation among the response functions within a population.

A QUIT statement executes any statements that have not been processed and then ends the CATMOD procedure run.

The purpose of each statement, other than the PROC CATMOD statement, is summarized in the following list:

BY	determines groups in which data are to be processed separately.
CONTRAST	specifies a hypothesis to test.
DIRECT	specifies independent variables that are to be treated quantitatively (like continuous variables) rather than qualitatively (like classification or discrete variables). These variables also help to determine the rows of the contingency table and distinguish response functions in one population from those in other populations.
FACTORS	specifies (1) the factors that distinguish response functions from others in the same population and (2) model effects, based on these factors, which help to determine the design matrix.
LOGLIN	specifies log-linear model effects.
MODEL	specifies (1) dependent variables, which determine the columns of the contingency table, (2) independent variables, which distinguish response functions in one population from those in other populations, and (3) model effects, which determine the design matrix and the way in which total variation among the response functions is partitioned.
POPULATION	specifies variables that determine the rows of the contingency table and distinguish response functions in one population from those in other populations.
REPEATED	specifies (1) the repeated measurement factors that distinguish response functions from others in the same population and (2) model effects, based on these factors, which help to determine the design matrix.
RESPONSE	determines the response functions that are to be modeled.
RESTRICT	restricts values of parameters to the values you specify.
WEIGHT	specifies a variable containing frequency counts.

PROC CATMOD Statement

PROC CATMOD < options > ;

The PROC CATMOD statement invokes the CATMOD procedure. Table 30.4 summarizes the options available in the PROC CATMOD statement.

Table 30.4 PROC CATMOD Statement Options

Option	Description
DATA=	Names the input SAS data set
NAMELEN=	Specifies the length of effect names
NOPRINT	Suppresses the normal display of results
ORDER=	Specifies the sort order for the levels of classification variables

You can specify the following options.

DATA=SAS-data-set

names the SAS data set containing the data to be analyzed. By default, the CATMOD procedure uses the most recently created SAS data set. For details, see the section “[Input Data Sets](#)” on page 1818.

NAMELEN=*n*

specifies the length of effect names in tables and output data sets to be *n* characters long, where *n* is a value between 24 and 200. The default length is 24 characters.

NOPRINT

suppresses the normal display of results. The NOPRINT option is useful when you only want to create output data sets with the **OUT=** or **OUTEST=** option in the **RESPONSE** statement. A **NOPRINT** option is also available in the **MODEL** statement. Note that this option temporarily disables the Output Delivery System (ODS); see Chapter 20, “[Using the Output Delivery System](#),” for more information.

ORDER=DATA | FORMATTED | FREQ | INTERNAL

specifies the sort order for the levels of classification variables. This affects the ordering of the populations, responses, and parameters, as well as the definitions of the parameters. The default, **ORDER=INTERNAL**, orders the variable levels by their unformatted values (for example, numeric order or alphabetical order).

The following table shows how PROC CATMOD interprets values of the **ORDER=** option.

Value of ORDER=	Levels Sorted By
DATA	Order of appearance in the input data set
FORMATTED	External formatted value, except for numeric variables with no explicit format, which are sorted by their unformatted (internal) value
FREQ	Descending frequency count; levels with the most observations come first in the order
INTERNAL	Unformatted value

By default, **ORDER=INTERNAL**. For **ORDER=FORMATTED** and **ORDER=INTERNAL**, the sort order is machine dependent. See the section “[Ordering of Populations and Responses](#)” on page 1821 for more information and examples. For more information about sort order, see the chapter on the **SORT** procedure in the *Base SAS Procedures Guide* and the discussion of BY-group processing in *SAS Language Reference: Concepts*.

BY Statement

BY *variables* ;

You can specify a BY statement with PROC CATMOD to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the CATMOD procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

You can specify one or more *variables* in the input data set on the BY statement.

When you specify a BY statement with PROC CATMOD, no further interactive processing is possible. In other words, once the BY statement appears, all statements up to the associated RUN statement are executed for each BY group in the data set. After the RUN statement, no further statements are accepted by the procedure.

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

CONTRAST Statement

CONTRAST *'label'* *row-description* <, ..., *row-description*> </ *options* > ;

where a *row-description* is defined as follows:

< @*n* > *effect values* < ... < @*n* > *effect values* >

The CONTRAST statement constructs and tests linear functions of the parameters in the MODEL statement or effects listed in the LOGLIN statement. Each set of effects (separated by commas) specifies one row or set of rows of the matrix C that PROC CATMOD uses to test the hypothesis $C\beta = 0$.

CONTRAST statements must be preceded by the MODEL statement, and by the LOGLIN statement, if one is used. You can specify the following terms in the CONTRAST statement.

'label' specifies up to 256 characters of identifying information displayed with the test. The *'label'* is required.

effect is one of the effects specified in the MODEL or LOGLIN statement, INTERCEPT (for the intercept parameter), or ALL_PARDS (for the complete set of parameters).

The ALL_PARDS option is regarded as an effect with the same number of parameters as the number of columns in the design matrix. This is particularly useful when the design matrix is input directly, as in the following example:

```

model y=(1 0 0 0,
         1 0 1 0,
         1 1 0 0,
         1 1 1 1);
contrast 'Main Effect of B' all_pards 0 1 0 0;
contrast 'Main Effect of C' all_pards 0 0 1 0;
contrast 'B*C Interaction ' all_pards 0 0 0 1;

```

values are numbers that form the coefficients of the parameters associated with the given effect. If there are fewer values than parameters for an effect, the remaining coefficients become zero. For example, if you specify two values and the effect actually has five parameters, the final three are set to zero.

@n points to the parameters in the *n*th set when the model has a separate set of parameters for each of the response functions. The *@n* notation is seldom needed. It enables you to test the variation among response functions in the same population. However, it is usually easier to model and test such variation by using the `_RESPONSE_` effect in the MODEL statement or by using the ALL_PARDS designation. Usually, contrasts are performed with respect to all of the response functions, and this is what the CONTRAST statement does by default (in this case, do not use the *@n* notation).

For example, if there are three response functions per population, then the following contrast results in a three-degree-of-freedom test comparing the first two levels of A simultaneously on the three response functions.

```

contrast 'Level 1 vs. Level 2' A 1 -1 0;

```

If, however, you want to specify a contrast with respect to the parameters in the *n*th set only, then use a single *@n* in a *row-description*. For example, the following statement tests that the first parameter of A and the first parameter of B are zero in the third response function:

```

contrast 'A=0, B=0, Function 3' @3 A 1 B 1;

```

To specify a contrast with respect to parameters in two or more different sets of effects, use *@n* with each effect. For example:

```

contrast 'Average over Functions' @1 A 1 0 -1
                                @2 A 1 1 -2;

```

When the model does not have a separate set of parameters for each of the response functions, the *@n* notation is invalid. This type of model is called AVERAGED. For details, see the description of the AVERAGED option and the section “Generation of the Design Matrix” on page 1832.

You can specify the following options in the CONTRAST statement after a slash.

ALPHA=*value*

specifies the significance level of the confidence interval for each contrast when the **ESTIMATE=** option is specified. The default is ALPHA=0.05, resulting in a 95% confidence interval for each contrast.

ESTIMATE=*keyword*

EST=*keyword*

requests that each individual contrast (that is, each row, $c_i\beta$, of $C\beta$) or exponentiated contrast ($\exp(c_i\beta)$) be estimated and tested. PROC CATMOD displays the point estimate, its standard error, a Wald confidence interval, and a Wald chi-square test for each contrast. The significance level of the confidence interval is controlled by the **ALPHA=** option.

You can estimate the contrast or the exponentiated contrast, or both, by specifying one of the following keywords:

PARM	specifies that the contrast itself be estimated.
EXP	specifies that the exponentiated contrast be estimated.
BOTH	specifies that both the contrast and the exponentiated contrast be estimated.

Specifying Contrasts

PROC CATMOD is parameterized differently than PROC GLM, so you must be careful not to use the same contrasts that you would with PROC GLM. Since PROC CATMOD uses full-rank parameterizations, all estimable parameters are directly estimable without involving other parameters.

For example, suppose a classification variable A has four levels and uses the default parameterization (**PARAM=**EFFECT). Then there are four parameters ($\alpha_1, \alpha_2, \alpha_3, \alpha_4$), of which PROC CATMOD uses only the first three. The fourth parameter is related to the others by the equation

$$\alpha_4 = -\alpha_1 - \alpha_2 - \alpha_3$$

To test the first versus the fourth level of A, you would test $\alpha_1 = \alpha_4$, which is

$$\alpha_1 = -\alpha_1 - \alpha_2 - \alpha_3$$

or, equivalently,

$$2\alpha_1 + \alpha_2 + \alpha_3 = 0$$

Therefore, you would use the following CONTRAST statement:

```
contrast '1 vs. 4' A 2 1 1;
```

To contrast the third level with the average of the first two levels, you would test

$$\frac{\alpha_1 + \alpha_2}{2} = \alpha_3$$

or, equivalently,

$$\alpha_1 + \alpha_2 - 2\alpha_3 = 0$$

Therefore, you would use the following CONTRAST statement:

```
contrast '1&2 vs. 3' A 1 1 -2;
```

Other CONTRAST statements are constructed similarly. For example:

```
contrast '1 vs. 2' A 1 -1 0;
contrast '1&2 vs. 4' A 3 3 2;
contrast '1&2 vs. 3&4' A 2 2 0;
contrast 'Main Effect' A 1 0 0,
                    A 0 1 0,
                    A 0 0 1;
```

The actual form of the C matrix depends on the effects in the model. The remaining examples in this section assume a single response function for each population.

Recall that the statements to test the first versus the fourth level of A are as follows:

```
proc catmod;
  model y=a;
  contrast '1 vs. 4' A 2 1 1;
run;
```

Since the first parameter corresponds to the intercept, the C matrix for the preceding statements is

$$C = [0 \ 2 \ 1 \ 1]$$

But suppose you have a variable B with three levels and you use the following statements:

```
proc catmod;
  model y=b a;
  contrast '1 vs. 4' A 2 1 1;
run;
```

Then the CONTRAST statement produces the C matrix

$$C = [0 \ 0 \ 0 \ 2 \ 1 \ 1]$$

since the first parameter corresponds to the intercept and the next two correspond to the B main effect.

You can also use the CONTRAST statement to test the joint effect of two or more effects in the MODEL statement. For example, the joint effect of A and B in the previous model has five degrees of freedom and is obtained by specifying the following:

```
contrast 'Joint Effect of A&B' A 1 0 0,
                                A 0 1 0,
                                A 0 0 1,
                                B 1 0,
                                B 0 1;
```

The ordering of variable levels is determined by the `ORDER=` option in the PROC CATMOD statement. Whenever you specify a contrast that depends on the order of the variable levels, you should verify the order from the “Population Profiles” table, the “Response Profiles” table, or the “One-Way Frequencies” table.

DIRECT Statement

DIRECT *variables* ;

The DIRECT statement lists numeric independent variables to be treated in a quantitative, rather than qualitative, way. The DIRECT statement is useful for logistic regression, which is described in the section “Logistic Regression” on page 1826. For limitations of models involving continuous variables, see the section “Continuous Variables” on page 1827.

CAUTION: If a DIRECT variable is formatted, then the unformatted (internal) values are used in the analysis and the formatted values are displayed. If you use a format to group the internal values into one formatted value, then the first internal value is used in the analysis. If specified, the DIRECT statement must precede the MODEL statement. For example:

```
proc catmod;
  direct X;
  model Y=X;
run;
```

Suppose *X* has five levels. Then the main effect *X* adds only one column to the design matrix rather than four. The values inserted into the design matrix are the actual values of *X*.

You can interactively change the variables declared as DIRECT variables by using the statement without listing any variables. The following statements are valid:

```
proc catmod;
  direct X;
  model Y=X;
  weight wt;
run;
  direct;
  model Y=X;
run;
```

The first MODEL statement uses the actual values of *X*, and the second MODEL statement uses the four variables created when PROC CATMOD generates the design matrix. Note that the preceding statements can be run without a WEIGHT statement if the input data are raw data rather than cell counts.

For more details, see the discussions of main and direct effects in the section “Generation of the Design Matrix” on page 1832.

FACTORS Statement

FACTORS *factor-description* < , . . . , *factor-description* > < / *options* > ;

where a *factor-description* is defined as follows:

factor-name < \$ > < *levels* >

and *factor-descriptions* are separated from each other by a comma. The \$ is required for character-valued factors. The value of *levels* provides the number of levels of the factor identified by a given *factor-name*. For only one factor, *levels* is optional; for two or more factors, it is required.

The FACTORS statement identifies factors that distinguish response functions from others in the same population. It also specifies how those factors are incorporated into the model. You can use the FACTORS statement whenever there is more than one response function per population and the keyword `_RESPONSE_` is specified in the MODEL statement. You can specify the name, type, and number of levels of each factor and the identification of each level.

The FACTORS statement is most useful when the response functions and their covariance matrix are read directly from the input data set. In this case, PROC CATMOD reads the response functions as though they are from one population (this poses no problem in the multiple-population case because the appropriately constructed covariance matrix is also read directly). Thus, you can use the FACTORS statement to partition the variation among the response functions into appropriate sources, even when the functions actually represent separate populations.

The format of the FACTORS statement is identical to that of the REPEATED statement. In fact, repeated measurement factors are simply special cases of factors in which some of the response functions correspond to multiple dependent variables that are measurements on the same experimental (or sampling) units.

You cannot specify the FACTORS statement for an analysis that also contains the REPEATED or LOGLIN statement since all of them specify the same information: how to partition the variation among the response functions within a population.

You can specify the following terms in the FACTORS statement:

- factor-name* names a factor that corresponds to two or more response functions. This name must be a valid SAS variable name, and it should not be the same as the name of a variable that already exists in the data set being analyzed.
- \$ indicates that the factor is character-valued. If the \$ is omitted, then the CATMOD procedure assumes that the factor is numeric. The type of the factor is relevant only when you use the PROFILE= option or when the _RESPONSE_= option (described later in this section) specifies nested-by-value effects.
- levels* specifies the number of levels of the corresponding factor. If there is only one such factor, and the number is omitted, then PROC CATMOD assumes that the number of levels is equal to the number of response functions per population (*q*). Unless you specify the PROFILE= option, the number *q* must either be equal to or be a multiple of the product of the number of levels of all the factors.

You can specify the following options in the FACTORS statement after a slash.

PROFILE=(matrix)

specifies the values assumed by the factors for each response function. There should be one column for each factor, and the values in a given column (character or numeric) should match the type of the corresponding factor. Character values are restricted to 16 characters or less. If there are q response functions per population, then the matrix must have i rows, where q must either be equal to or be a multiple of i . Adjacent rows of the matrix should be separated by a comma.

The values in the PROFILE matrix are useful for specifying models in those situations where the study design is not a full factorial with respect to the factors. They can also be used to specify nested-by-value effects in the `_RESPONSE_` option. If you specify character values in both places (the PROFILE= option and the `_RESPONSE_` option), then the values must match with respect to whether or not they are enclosed in quotes (that is, enclosed in quotes in both places or in neither place).

For an example of using the PROFILE= option, see [Example 30.10](#).

RESPONSE=effects

specifies design effects. The variables named in the effects must be *factor-names* that appear in the FACTORS statement. If the `_RESPONSE_` option is omitted, then PROC CATMOD builds a full factorial `_RESPONSE_` effect with respect to the factors.

TITLE='title'

displays the *title* at the top of certain pages of output that correspond to the current FACTORS statement.

For an example of how the FACTORS statement is useful, consider the case where the response functions and their covariance matrix are read directly from the input data set. The TYPE=EST data set might be created in the following manner:

```
data direct (type=est);
  input b1-b4 _type_ $ _name_ $8.;
  datalines;
0.590463 0.384720 0.273269 0.136458 parms .
0.001690 0.000911 0.000474 0.000432 cov b1
0.000911 0.001823 0.000031 0.000102 cov b2
0.000474 0.000031 0.001056 0.000477 cov b3
0.000432 0.000102 0.000477 0.000396 cov b4
;
```

Suppose the response functions correspond to four populations that represent the cross-classification of age (two groups) by sex. You can use the FACTORS statement to identify these two factors and to name the effects in the model. The statements required to fit a main-effects model to these data are as follows:

```
proc catmod data=direct;
  response read b1-b4;
  model _f=_response_;
  factors age 2, sex 2 / _response_=age sex;
run;
```


If you want to specify some nested-by-value effects, you can change the FACTORS statement to the following:

```
factors age $ 2, sex $ 2 /
  _response_=age sex(age='under 30') sex(age='30 & over')
  profile=('under 30'   male,
          'under 30'   female,
          '30 & over'  male,
          '30 & over'  female);
```

If, by design or by chance, the study contains no male subjects under 30 years of age, then there are only three response functions, and you can specify a main-effects model as follows:

```
proc catmod data=direct;
  response read b2-b4;
  model _f=_response_;
  factors age $ 2, sex $ 2 / _response_=age sex
    profile=('under 30'   female,
            '30 & over'  male,
            '30 & over'  female);
run;
```

When you specify two or more factors and omit the PROFILE= option, PROC CATMOD presumes that the response functions are ordered so that the levels of the rightmost factor change most rapidly. For the preceding example, the order implied by the FACTORS statement is as follows:

Response Function	Dependent Variable	Age	Sex
1	b1	1	1
2	b2	1	2
3	b3	2	1
4	b4	2	2

For additional examples of how to use the FACTORS statement, see the section “[Repeated Measures Analysis](#)” on page 1830. All of the examples in that section are applicable, with the REPEATED statement replaced by the FACTORS statement.

LOGLIN Statement

LOGLIN *effects* </option> ;

The LOGLIN statement is used to define log-linear model effects. It can be used whenever the default response functions (generalized logits) are used.

In the LOGLIN statement, *effects* are design effects that contain dependent variables in the MODEL statement, including interaction, nested, and nested-by-value effects. You can use the bar (|) and at (@) operators as well. The following lists of effects are equivalent:

a b c a*b a*c b*c

and

```
a|b|c @2
```

When you use the LOGLIN statement, the keyword `_RESPONSE_` should be specified in the MODEL statement. For further information about log-linear model analysis, see the section “[Log-Linear Model Analysis](#)” on page 1827.

You cannot specify the LOGLIN statement for an analysis that also contains the [REPEATED](#) or [FACTORS](#) statement since all of them specify the same information: how to partition the variation among the response functions within a population.

You can specify the following option in the LOGLIN statement after a slash.

TITLE=*'title'*

displays the *title* at the top of certain pages of output that correspond to this LOGLIN statement.

The following statements give an example of how to use the LOGLIN statement:

```
proc catmod;
  model a*b*c=_response_;
  loglin a|b|c @ 2;
run;
```

These statements yield a log-linear model analysis that contains all main effects and two-variable interactions. For more examples of log-linear model analysis, see the section “[Log-Linear Model Analysis](#)” on page 1827.

MODEL Statement

MODEL *response-effect* = < *design-effects* > < / *options* > ;

PROC CATMOD requires a MODEL statement. You can specify the following in a MODEL statement:

response-effect can be either a single variable, a crossed effect with two or more variables joined by asterisks, or `_F_`. The `_F_` specification indicates that the response functions and their estimated covariance matrix are to be read directly into the procedure (see the section “[Inputting Response Functions and Covariances Directly](#)” on page 1820 for details). The *response-effect* indicates the dependent variables that determine the response categories (the columns of the underlying contingency table).

design-effects specify potential sources of variation (such as main effects and interactions) in the model. These effects determine the number of model parameters, as well as the interpretation of such parameters. In addition, if there is no [POPULATION](#) statement, PROC CATMOD uses these variables to determine the populations (the rows of the underlying contingency table). When fitting the model, PROC CATMOD adjusts the independent effects in the model for all other independent effects in the model.

Design-effects can be any of those described in the section “[Specification of Effects](#)” on page 1822, or they can be defined by specifying the actual design matrix, enclosed in

parentheses (see the section “Specifying the Design Matrix Directly” on page 1806). In addition, you can use the keyword `_RESPONSE_` alone or as part of an effect. Effects cannot be nested within `_RESPONSE_`, so effects of the form `A(_RESPONSE_)` are invalid.

For more information, see the section “Log-Linear Model Analysis” on page 1827 and the section “Repeated Measures Analysis” on page 1830.

Some example MODEL statements are shown in the following table:

Example	Result
<code>model r=a b;</code>	Main effects only
<code>model r=a b a*b;</code>	Main effects with interaction
<code>model r=a b(a);</code>	Nested effect
<code>model r=a b;</code>	Complete factorial
<code>model r=a b(a=1) b(a=2);</code>	Nested-by-value effects
<code>model r*s=_response_;</code>	Log-linear model
<code>model r*s=a _response_(a);</code>	Nested repeated measurement factor
<code>model _f=_response_;</code>	Direct input of the response functions

The relationship between these specifications and the structure of the design matrix **X** is described in the section “Generation of the Design Matrix” on page 1832.

Table 30.5 summarizes the options available in the MODEL statement.

Table 30.5 MODEL Statement Options

Options	Task
Specify details of computation	
<code>ML=</code>	Generates the maximum likelihood estimates
<code>GLS</code>	Generates the weighted least squares estimates
<code>WLS</code>	
<code>NOINT</code>	Omits the intercept term from the model
<code>PARAM=</code>	Specifies the parameterization of classification variables
<code>ADDCELL=</code>	Adds a number to each cell frequency
<code>AVERAGED</code>	Averages the main effects across response functions
<code>EPSILON=</code>	Specifies the convergence criterion for maximum likelihood
<code>MAXITER=</code>	Specifies the number of iterations for maximum likelihood
<code>MISSING=</code>	Specifies how missing cells are treated
<code>ZERO=</code>	Specifies how zero cells are treated

Table 30.5 continued

Options	Task
Request additional computation and tables	
ALPHA=	Specifies the significance level of confidence intervals
CLPARM	Displays the Wald confidence intervals of estimates
CORRB	Displays the estimated correlation matrix of estimates
COV	Displays the covariance matrix of response functions
COVB	Displays the estimated covariance matrix of estimates
DESIGN	Displays the design and <code>_RESPONSE_</code> matrix
FREQ	Displays the two-way frequency tables
ITPRINT	Displays the iterations for maximum likelihood
ONEWAY	Displays the one-way frequency tables
PRED=	Displays the predicted values
PREDICT	
PROB	Displays the probability estimates
PROFILE	Displays the population profiles
XPX	Displays the crossproducts matrix
TITLE=	Specifies the title
Suppress output	
NODESIGN	Suppresses the design matrix
NOPARM	Suppresses the parameter estimates
NOPREDVAR	Suppresses the variable levels
NOPROFILE	Suppresses the population and response profiles
NORESPONSE	Suppresses the <code>_RESPONSE_</code> matrix

The following list describes these options in alphabetical order.

ADDCELL=number

adds *number* to the frequency count in each cell, where *number* is any positive number. This option has no effect on maximum likelihood analysis; it is used only for weighted least squares analysis.

ALPHA=number

sets the significance level for the Wald confidence intervals for parameter estimates. The value must be between 0 and 1. The default value of 0.05 results in the calculation of a 95% confidence interval. This option has no effect unless the **CLPARM** option is also specified.

AVERAGED

specifies that dependent variable effects can be modeled and that independent variable main effects are averaged across the response functions in a population. For further information about the effect of using (or not using) the **AVERAGED** option, see the section “[Generation of the Design Matrix](#)” on page 1832. Direct input of the design matrix or specification of the `_RESPONSE_` keyword in the MODEL statement automatically uses an **AVERAGED** model type.

CLPARM

produces Wald confidence limits for the parameter estimates. The confidence coefficient can be specified with the **ALPHA=** option.

CORRB

displays the estimated correlation matrix of the parameter estimates.

COV

displays S_j , which is the covariance matrix of the response functions for each population.

COVB

displays the estimated covariance matrix of the parameter estimates.

DESIGN

displays the design matrix X for WLS and ML analyses, and also displays the `_RESPONSE_` matrix for log-linear models. For further information, see the section “[Generation of the Design Matrix](#)” on page 1832.

EPSILON=number

specifies the convergence criterion for the maximum likelihood estimation of the parameters. The iterative estimation process stops when the proportional change in the log likelihood is less than *number*, or after the number of iterations specified by the `MAXITER=` option, whichever comes first. By default, `EPSILON=1E-8`.

FREQ

produces the two-way frequency table for the cross-classification of populations by responses.

ITPRINT

displays parameter estimates and other information at each iteration of a maximum likelihood analysis.

MAXITER=number

specifies the maximum number of iterations used for the maximum likelihood estimation of the parameters. By default, `MAXITER=20`.

ML <= NR | IPF<(ipf-options)>

computes maximum likelihood estimates (MLE) by using either a Newton-Raphson algorithm (NR) or an iterative proportional fitting algorithm (IPF).

The option `ML=NR` (or simply `ML`) is available when you use generalized logits, and also when you perform binary logistic regression with logits, cumulative logits, or adjacent category logits. For generalized logits (the default response functions), `ML=NR` is the default estimation method.

The option `ML=IPF` is available for fitting a hierarchical log-linear model with one population (no independent variables and no population variables). The use of bar notation to express the log-linear effects guarantees that the model is hierarchical (the presence of any interaction term in the model requires the presence of all its lower-order terms). If your table is *incomplete* (that is, your table has a zero or missing entry in at least one cell), then all missing cells and all cells with zero weight are treated as structural zeros by default; this behavior can be modified with the `ZERO=` and `MISSING=` options in the `MODEL` statement.

You can control the convergence of the two algorithms with the `EPSILON=` and `MAXITER=` options in the `MODEL` statement. You can select the convergence criterion for the IPF algorithm with the `CONVCRT=` option.

NOTE: The `RESTRICT` statement is not available with the `ML=IPF` option.

You can specify the following *ipf-options* within parentheses after the `ML=IPF` option.

CONVCRT=keyword

specifies the method that determines when convergence of the IPF algorithm occurs. You can specify one of the following *keywords*:

- CELL** termination requires the maximum absolute difference between consecutive cell estimates to be less than 0.001 (or the value of the **EPSILON=** option, if specified).
- LOGL** termination requires the relative difference between consecutive estimates of the log likelihood to be less than $1E-8$ (or the value of the **EPSILON=** option, if specified). This is the default.
- MARGIN** termination requires the maximum absolute difference between consecutive margin estimates to be less than 0.001 (or the value of the **EPSILON=** option, if specified).

DF=keyword

specifies the method used to compute the degrees of freedom for the goodness-of-fit G^2 test (labeled “Likelihood Ratio” in the “Estimates” table).

For a *complete* table (a table having nonzero entries in every cell), the degrees of freedom are calculated as the number of cells in the table (n_c) minus the number of independent parameters specified in the model (n_p). For incomplete tables, these degrees of freedom can be adjusted by the number of fitted zeros (n_z , which includes the number of structural zeros) and the number of nonestimable parameters due to the zeros (n_n). If you are analyzing an incomplete table, you should verify that the degrees of freedom are correct.

You can specify one of the following *keywords*:

- UNADJ** computes the unadjusted degrees of freedom as $n_c - n_p$. These are the same degrees of freedom you would get if all cells in the table were positive.
- ADJ** computes the degrees of freedom as $(n_c - n_p) - (n_z - n_n)$ (Bishop, Fienberg, and Holland 1975), which adjusts for fitted zeros and nonestimable parameters. This is the default, and for complete tables it gives the same results as the UNADJ option.
- ADJEST** computes the degrees of freedom as $(n_c - n_p) - n_z$, which adjusts for fitted zeros only. This gives a lower bound on the true degrees of freedom.

PARM

computes parameter estimates, generates the “ANOVA,” “Parameter Estimates,” and “Predicted Values of Response Functions” tables, and includes the predicted standard errors in the “Predicted Values of Frequencies and Probabilities” tables.

When you specify the PARM option, the algorithm used to obtain the maximum likelihood parameter estimates is weighted least squares on the IPF-predicted frequencies. This algorithm can be much faster than the Newton-Raphson algorithm that is used if you specify the **ML=NR** option. In the resulting ANOVA table, the likelihood ratio is computed from the initial IPF fit while the degrees of freedom are generated from the WLS analysis; the **DF=** option can override this. Also, the initial response function, which the WLS method usually computes from the raw data, is computed from the IPF-predicted frequencies.

If there are any zero marginals in the configurations that define the model, then there are predicted cell frequencies of zero and WLS cannot be used to compute the estimates. In this case, PROC CATMOD automatically changes the algorithm from ML=IPF to ML=NR and prints a note in the log.

MISSING=*keyword*

MISS=*keyword*

specifies whether a missing cell is treated as a sampling or structural zero.

Structural zero cells are removed from the analysis since their expected values are zero, while sampling zero cells can have nonzero expected value and might be estimable. For a single population, the missing cells are treated as structural zeros by default. For multiple populations, as long as some population has a nonzero count for a given population and response profile, the missing values are treated as sampling zeros by default.

The following table displays the available *keywords* and summarizes how PROC CATMOD treats missing values for one or more populations:

MISSING=	One Population	Multiple Populations
STRUCTURAL (default)	Structural zeros	Sampling zeros
SAMP SAMPLING <i>value</i>	Sampling zeros Sets missing weights and cells to <i>value</i>	Sampling zeros Sets missing weights and cells to <i>value</i>

NODESIGN

suppresses the display of the design matrix **X** when the **DESIGN** option is also specified. This enables you to display only the **_RESPONSE_** matrix for log-linear models.

NOINT

suppresses the intercept term in the model.

NOPARM

suppresses the display of the estimated parameters and the statistics for testing that each parameter is zero.

NOPREDVAR

suppresses the display of the variable levels in tables requested with the **PRED=** option and in the “Estimates” table. Population profiles are replaced with the sample number, classification variable levels are suppressed, and response profiles are replaced with a function number.

NOPRINT

suppresses the normal display of results. The **NOPRINT** option is useful when you only want to create output data sets with the **OUT=** or **OUTEST=** option in the **RESPONSE** statement. A **NOPRINT** option is also available in the PROC CATMOD statement. Note that this option temporarily disables the Output Delivery System (ODS); see Chapter 20, “Using the Output Delivery System,” for more information.

NOPROFILE

suppresses the display of the population profiles and the response profiles.

NORESPONSE

suppresses the display of the `_RESPONSE_` matrix for log-linear models when the `DESIGN` option is also specified. This enables you to display only the design matrix for log-linear models.

ONEWAY

produces a one-way table of frequencies for each variable used in the analysis. This table is useful in determining the order of the observed levels for each variable.

PARAM=EFFECT | REFERENCE

specifies the parameterization method for the classification variable or variables. The default is `PARAM=EFFECT`. Both the effect and reference parameterizations are full rank. See the section “[Generation of the Design Matrix](#)” on page 1832 for further details.

PREDICT**PRED=FREQ | PROB**

displays the observed and predicted values of the response functions for each population, together with their standard errors and the residuals (observed minus predicted). In addition, if the response functions are the standard ones (generalized logits), then the `PRED=FREQ` option specifies the computation and display of predicted cell frequencies, while `PRED=PROB` (or just `PREDICT`) specifies the computation and display of predicted cell probabilities.

The `OUT=` data set always contains the predicted probabilities. If the response functions are the generalized logits, the predicted cell probabilities are output unless the option `PRED=FREQ` is specified, in which case the predicted cell frequencies are output.

PROB

produces the two-way table of probability estimates for the cross-classification of populations by responses. These estimates sum to one across the response categories for each population.

PROFILE

displays all of the population profiles. If you have more than 60 populations, then by default only the first 40 profiles are displayed; the `PROFILE` option overrides this default behavior.

TITLE='title'

displays the *title* at the top of certain pages of output that correspond to this `MODEL` statement.

WLS**GLS**

computes weighted least squares estimates. This type of estimation is also called generalized least squares estimation. For response functions other than the default (of generalized logits), `WLS` is the default estimation method.

XPX

displays $X'S^{-1}X$, the crossproducts matrix for the normal equations.

ZERO=keyword

specifies whether a nonmissing cell with zero weight in the data set is treated as a sampling or structural zero.

Structural zero cells are removed from the analysis since their expected values are zero, while sampling zero cells have nonzero expected value and might be estimable. For a single population, the zero

The preceding statements are appropriate when Group and Time each have three levels and R is dichotomous. The **POPULATION** statement produces nine populations, and $q = 1$ (since R is dichotomous), so $q \times s = 1 \times 9 = 9$.

If you input the design matrix directly but do not specify any subsets of the parameters to be tested, then PROC CATMOD tests the effect of MODEL | MEAN, which represents the significance of the model beyond what is explained by an overall mean. For the previous example, the MODEL | MEAN effect is the same as that obtained by specifying the following at the end of the MODEL statement:

```
(2 3 4='model|mean');
```

POPULATION Statement

POPULATION *variables* ;

The POPULATION statement specifies that populations are to be based only on cross-classifications of the specified *variables*. If you do not specify the POPULATION statement, then populations are based only on cross-classifications of the independent variables in the MODEL statement.

The POPULATION statement has two major uses:

- When you enter the design matrix directly, there are no independent variables in the MODEL statement; therefore, the POPULATION statement is the only way to produce more than one population.
- When you fit a reduced model, the POPULATION statement might be necessary if you want to form the same number of populations as there are for the saturated model.

To illustrate the first use, suppose you specify the following statements:

```
data one;
  input A $ B $ wt @@;
  datalines;
yes yes 23   yes no 31   no yes 47   no no 50
;

proc catmod;
  weight wt;
  population B;
  model A=(1 0,
           1 1);
run;
```

Since the dependent variable A has two levels, there is one response function per population. Since the variable B has two levels, there are two populations. The MODEL statement is valid since the number of rows in the design matrix (2) is the same as the total number of response functions. If the POPULATION statement is omitted, there would be only one population and one response function, and the MODEL statement would be invalid.

To illustrate the second use, suppose you specify the following statements:

```

data two;
  input A $ B $ Y wt @@;
  datalines;
yes  yes  1  23      yes  yes  2  63
yes  no   1  31      yes  no   2  70
no   yes  1  47      no   yes  2  80
no   no   1  50      no   no   2  84
;

proc catmod;
  weight wt;
  model Y=A B A*B / wls;
run;

```

These statements form four populations and produce the following design matrix and analysis of variance table:

$$X = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix}$$

Source	DF	Chi-Square	Pr > ChiSq
Intercept	1	48.10	<.0001
A	1	3.47	0.0625
B	1	0.25	0.6186
A*B	1	0.19	0.6638
Residual	0		

Since the B and A*B effects are nonsignificant ($p > 0.10$), fit the reduced model that contains only the A effect:

```

proc catmod;
  weight wt;
  model Y=A / wls;
run;

```

Now only two populations are formed, and the design matrix and the analysis of variance table are as follows:

$$X = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

Source	DF	Chi-Square	Pr > ChiSq
Intercept	1	47.94	<.0001
A	1	3.33	0.0678
Residual	0		

However, you can form four populations by adding the POPULATION statement to the analysis:

```

proc catmod;
  weight wt;
  population A B;
  model Y=A / wls;
run;

```

The design matrix and the analysis of variance table resulting from these statements are as follows:

Source	DF	Chi-Square	Pr > ChiSq
Intercept	1	47.76	<.0001
A	1	3.30	0.0694
Residual	2	0.35	0.8374

The advantage of the latter analysis is that it retains four populations for the reduced model, thereby creating a built-in goodness-of-fit test: the residual chi-square. Such a test is important because the cumulative (or joint) effect of deleting two or more effects from the model can be significant, even if the individual effects are not.

The resulting differences between the two analyses are due to the fact that the latter analysis uses pure weighted least squares estimates with respect to the four populations that are actually sampled. The former analysis pools populations and therefore uses parameter estimates that can be regarded as weighted least squares estimates of maximum likelihood predicted cell frequencies. In any case, the estimation methods are asymptotically equivalent; therefore, the results are very similar. If you specify the **ML** option (instead of the **WLS** option) in the preceding **MODEL** statements, then the parameter estimates are identical for the two analyses.

CAUTION: If your model has different covariate profiles within any population, then the first profile is used in the analysis.

REPEATED Statement

REPEATED *factor-description* <, ..., *factor-description*> </ *options*> ;

where a *factor-description* is defined as follows:

factor-name <\$> < *levels*>

and *factor-descriptions* are separated from each other by a comma. The \$ is required for character-valued factors. The value of *levels* provides the number of levels of the repeated measurement factor identified by a given *factor-name*. For only one repeated measurement factor, *levels* is optional; for two or more repeated measurement factors, it is required. The **REPEATED** statement incorporates repeated measurement factors into the model. You can use this statement whenever there is more than one dependent variable and the keyword **_RESPONSE_** is specified in the **MODEL** statement. If the dependent variables correspond to one or more repeated measurement factors, you can use the **REPEATED** statement to define **_RESPONSE_** in terms of those factors. You can specify the name, type, and number of levels of each factor, as well as the identification of each level.

You cannot specify the **REPEATED** statement for an analysis that also contains the **FACTORS** or **LOGLIN** statement since all of them specify the same information: how to partition the variation among the response functions within a population.

You can specify the following terms in the REPEATED statement:

- factor-name* names a repeated measurement factor that corresponds to two or more response functions. This name must be a valid SAS variable name, and it should not be the same as the name of a variable that already exists in the data set being analyzed.
- \$ indicates that the factor is character-valued. If the \$ is omitted, then the CATMOD procedure assumes that the factor is numeric. The type of the factor is relevant only when you use the PROFILE= option or when the _RESPONSE= option specifies nested-by-value effects.
- levels* specifies the number of levels of the corresponding repeated measurement factor. If there is only one such factor and the number is omitted, then PROC CATMOD assumes that the number of levels is equal to the number of response functions per population (q). Unless you specify the PROFILE= option, the number q must either be equal to or be a multiple of the product of the number of levels of all the factors.

You can specify the following options in the REPEATED statement after a slash.

PROFILE=(matrix)

specifies the values assumed by the factors for each response function. There should be one column for each factor, and the values in a given column should match the type (character or numeric) of the corresponding factor. Character values are restricted to 16 characters or less. If there are q response functions per population, then the matrix must have i rows, where q must either be equal to or be a multiple of i . Adjacent rows of the matrix should be separated by a comma.

The values in the PROFILE matrix are useful for specifying models in those situations where the study design is not a full factorial with respect to the factors. They can also be used to specify nested-with-value effects in the _RESPONSE= option. If you specify character values in both the PROFILE= option and the _RESPONSE= option, then the values must match with respect to whether or not they are enclosed in quotes (that is, they must be enclosed in quotes in both places or in neither place).

RESPONSE=effects

specifies design effects. The variables named in the effects must be *factor-names* that appear in the REPEATED statement. If the _RESPONSE= option is omitted, then PROC CATMOD builds a full factorial _RESPONSE_ effect with respect to the repeated measurement factors. For example, the following two statements are equivalent in that they produce the same parameter estimates:

```
repeated Time 2, Treatment 2;
repeated Time 2, Treatment 2 / _response_=Time|Treatment;
```

However, the second statement produces tests of the Time, Treatment, and Time*Treatment effects in the “Analysis of Variance” table, whereas the first statement produces a single test for the combined effects in _RESPONSE_.

TITLE='title'

displays the *title* at the top of certain pages of output that correspond to this REPEATED statement.

For further information and numerous examples of the REPEATED statement, see the section “Repeated Measures Analysis” on page 1830.

RESPONSE Statement

RESPONSE < *function* > < / *options* > ;

The RESPONSE statement specifies functions of the response probabilities. The procedure models these response functions as linear combinations of the parameters.

By default, PROC CATMOD uses the standard response functions (generalized logits, which are explained in detail in the section “[Understanding the Standard Response Functions](#)” on page 1817). With these standard response functions, the default estimation method is maximum likelihood, but you can use the **WLS** option in the MODEL statement to request weighted least squares estimation. With other response functions (specified in the RESPONSE statement), the default (and only) estimation method is weighted least squares.

You can specify more than one RESPONSE statement, in which case each RESPONSE statement produces a separate analysis. If the computed response functions for any population are linearly dependent (yielding a singular covariance matrix), then PROC CATMOD displays an error message and stops processing. See the section “[Cautions](#)” on page 1842 for methods of dealing with this.

The *function* specification can be any of the items in the following list. For an example of response functions generated and formulas for q (the number of response functions), see the section “[More on Response Functions](#)” on page 1813.

Table 30.6 summarizes the options available in the RESPONSE statement.

Table 30.6 RESPONSE Statement Options

Option	Description
ALOGIT	Specifies response functions as adjacent-category logits
CLOGIT	Specifies that the response functions are cumulative logits
JOINT	Specifies that the response functions are the joint response probabilities
LOGIT	Specifies that the response functions are generalized logits
MARGINAL	Specifies that the response functions are marginal probabilities
MEAN	Specifies that the response functions are the means dependent variables
READ	Directly reads the response functions and their covariance matrix from the input data set
OUT=	Produces a SAS data set that contains predicted values, standard errors and residuals
OUTEST=	Produces a SAS data set that contains the estimated parameter vector and its estimated covariance matrix
TITLE=	Displays the <i>title</i>

ALOGIT

ALOGITS

specifies response functions as adjacent-category logits of the marginal probabilities for each of the dependent variables. For each dependent variable, the response functions are a set of linearly independent adjacent-category logits, obtained by taking the logarithms of the ratios of two probabilities. The denominator of the k th ratio is the marginal probability corresponding to the k th level of the vari-

able, and the numerator is the marginal probability corresponding to the $(k + 1)$ level. If a dependent variable has two levels, then the adjacent-category logit is the negative of the generalized logit.

CLOGIT

CLOGITS

specifies that the response functions are cumulative logits of the marginal probabilities for each of the dependent variables. For each dependent variable, the response functions are a set of linearly independent cumulative logits, obtained by taking the logarithms of the ratios of two probabilities. The denominator of the k th ratio is the cumulative probability, c_k , corresponding to the k th level of the variable, and the numerator is $1 - c_k$ (Agresti 1984, 113–114). If a dependent variable has two levels, then PROC CATMOD computes its cumulative logit as the negative of its generalized logit. You should use cumulative logits only when the dependent variables are ordinally scaled.

JOINT

specifies that the response functions are the joint response probabilities. A linearly independent set is created by deleting the last response probability. For the case of one dependent variable, the JOINT and [MARGINALS](#) specifications are equivalent.

LOGIT

LOGITS

specifies that the response functions are generalized logits of the marginal probabilities for each of the dependent variables. For each dependent variable, the response functions are a set of linearly independent generalized logits, obtained by taking the logarithms of the ratios of two probabilities. The denominator of each ratio is the marginal probability corresponding to the last observed level of the variable, and the numerators are the marginal probabilities corresponding to each of the other levels. If there is one dependent variable, then specifying LOGIT is equivalent to using the standard response functions.

MARGINAL

MARGINALS

specifies that the response functions are marginal probabilities for each of the dependent variables in the MODEL statement. For each dependent variable, the response functions are a set of linearly independent marginals, obtained by deleting the marginal probability corresponding to the last level.

MEAN

MEANS

specifies that the response functions are the means of the dependent variables in the MODEL statement. This specification requires that all of the dependent variables be numeric.

READ *variables*

specifies that the response functions and their covariance matrix are to be read directly from the input data set with one response function for each variable named. See the section “[Inputting Response Functions and Covariances Directly](#)” on page 1820 for more information.

transformation

specifies response functions that can be expressed by using successive applications of the four operations: LOG, EXP, * matrix literal, or + matrix literal. The operations are described in detail in the section “[Using a Transformation to Specify Response Functions](#)” on page 1815.

You can specify the following options in the RESPONSE statement after a slash.

OUT=SAS-data-set

produces a SAS data set that contains, for each population, the observed and predicted values of the response functions, their standard errors, and the residuals. Moreover, if you use the standard response functions, the data set also includes observed and predicted values of the cell frequencies or the cell probabilities. For further information, see the section “Output Data Sets” on page 1824.

OUTEST=SAS-data-set

produces a SAS data set that contains the estimated parameter vector and its estimated covariance matrix. For further information, see the section “Output Data Sets” on page 1824.

TITLE='title'

displays the *title* at the top of certain pages of output that correspond to this RESPONSE statement.

More on Response Functions

Suppose the dependent variable *A* has three levels and is the only *response-effect* in the MODEL statement. The following table shows the proportions upon which the response functions are defined:

Value of A:	1	2	3
Proportions:	p_1	p_2	p_3

Note that $\sum_j p_j = 1$. The following table shows the response functions generated for each population:

Function Specification	Value of q	Response Function
none*	2	$\ln\left(\frac{p_1}{p_3}\right), \ln\left(\frac{p_2}{p_3}\right)$
ALOGITS	2	$\ln\left(\frac{p_2}{p_1}\right), \ln\left(\frac{p_3}{p_2}\right)$
CLOGITS	2	$\ln\left(\frac{1-p_1}{p_1}\right), \ln\left(\frac{1-(p_1+p_2)}{p_1+p_2}\right)$
JOINT	2	p_1, p_2
LOGITS	2	$\ln\left(\frac{p_1}{p_3}\right), \ln\left(\frac{p_2}{p_3}\right)$
MARGINAL	2	p_1, p_2
MEAN	1	$1p_1 + 2p_2 + 3p_3$

*Without a function specification, the default response functions are generalized logits.

Now, suppose the dependent variables *A* and *B* each have three levels (valued 1, 2, and 3 each) and the *response-effect* in the MODEL statement is *A*B*. The following table shows the proportions upon which the response functions are defined:

Value of A:	1	1	1	2	2	2	3	3	3
Value of B:	1	2	3	1	2	3	1	2	3
Proportions:	p_1	p_2	p_3	p_4	p_5	p_6	p_7	p_8	p_9

The marginal totals for the preceding table are defined as follows:

$$\begin{aligned} p_{1\cdot} &= p_1 + p_2 + p_3 & p_{\cdot 1} &= p_1 + p_4 + p_7 \\ p_{2\cdot} &= p_4 + p_5 + p_6 & p_{\cdot 2} &= p_2 + p_5 + p_8 \\ p_{3\cdot} &= p_7 + p_8 + p_9 & p_{\cdot 3} &= p_3 + p_6 + p_9 \end{aligned}$$

where $\sum_j p_j = 1$. The following table shows the response functions generated for each population:

Function Specification	Value of q	Response Function
none*	8	$\ln\left(\frac{p_1}{p_9}\right), \ln\left(\frac{p_2}{p_9}\right), \ln\left(\frac{p_3}{p_9}\right), \dots, \ln\left(\frac{p_8}{p_9}\right)$
ALOGITS	4	$\ln\left(\frac{p_{2\cdot}}{p_{1\cdot}}\right), \ln\left(\frac{p_{3\cdot}}{p_{2\cdot}}\right), \ln\left(\frac{p_{\cdot 2}}{p_{\cdot 1}}\right), \ln\left(\frac{p_{\cdot 3}}{p_{\cdot 2}}\right)$
CLOGITS	4	$\ln\left(\frac{1-p_{1\cdot}}{p_{1\cdot}}\right), \ln\left(\frac{1-(p_{1\cdot}+p_{2\cdot})}{p_{1\cdot}+p_{2\cdot}}\right), \ln\left(\frac{1-p_{\cdot 1}}{p_{\cdot 1}}\right), \ln\left(\frac{1-(p_{\cdot 1}+p_{\cdot 2})}{p_{\cdot 1}+p_{\cdot 2}}\right)$
JOINT	8	$p_1, p_2, p_3, p_4, p_5, p_6, p_7, p_8$
LOGITS	4	$\ln\left(\frac{p_{1\cdot}}{p_{3\cdot}}\right), \ln\left(\frac{p_{2\cdot}}{p_{3\cdot}}\right), \ln\left(\frac{p_{\cdot 1}}{p_{\cdot 3}}\right), \ln\left(\frac{p_{\cdot 2}}{p_{\cdot 3}}\right)$
MARGINAL	4	$p_{1\cdot}, p_{2\cdot}, p_{\cdot 1}, p_{\cdot 2}$
MEAN	2	$1p_{1\cdot} + 2p_{2\cdot} + 3p_{3\cdot}, 1p_{\cdot 1} + 2p_{\cdot 2} + 3p_{\cdot 3}$

* Without a function specification, the default response functions are generalized logits.

The READ and *transformation* function specifications are not shown in the preceding table. For these two situations, there is not a general response function; the response functions that are generated depend on what you specify.

Another important aspect of the function specification is the number of response functions generated per population, q . Let m_i represent the number of levels for the i th dependent variable in the MODEL statement, and let d represent the number of dependent variables in the MODEL statement. Then, if the function specification is ALOGITS, CLOGITS, LOGITS, or MARGINALS, the number of response functions is

$$q = \sum_{i=1}^d (m_i - 1)$$

If the function specification is JOINT or the default (generalized logits), the number of response functions per population is

$$q = r - 1$$

where r is the number of response profiles. If every possible cross-classification of the dependent variables is observed in the samples, then

$$r = \prod_{i=1}^d m_i$$

Otherwise, r is the number of cross-classifications actually observed.

If the function specification is MEANS, the number of response functions per population is $q = d$.

Response Statement Examples

Some example response statements are shown in the following table:

Example	Result
<code>response marginals;</code>	Marginals for each dependent variable
<code>response means;</code>	The mean of each dependent variable
<code>response logits;</code>	Generalized logits of the marginal probabilities
<code>response clogits;</code>	Cumulative logits of the marginal probabilities
<code>response alogits;</code>	Adjacent-category logits of the marginal probabilities
<code>response joint;</code>	The joint probabilities
<code>response 1 -1 log;</code>	The logit
<code>response;</code>	Generalized logits
<code>response 1 2 3;</code>	The mean score, with scores of 1, 2, and 3 corresponding to the three response levels
<code>response read b1-b4;</code>	Four response functions and their covariance matrix, read directly from the input data set

Using a Transformation to Specify Response Functions

If you specify a *transformation*, it is applied to the vector that contains the sample proportions in each population. The *transformation* can be any combination of the following four operations:

Operation	Specification
linear combination	* matrix literal
linear combination	matrix literal
logarithm	LOG
exponential	EXP
adding constant	+ matrix literal

If more than one operation is specified, then PROC CATMOD applies the operations consecutively from right to left.

A matrix literal is a matrix of numbers with each row of the matrix separated from the next by a comma. If you specify a linear combination, in most cases the * is not needed. The following statement defines the response function $p_1 + 1$. The * is needed to separate the two matrix literals '1' and '1 0'.

```
response + 1 * 1 0;
```

The **LOG** of a vector transforms each element of the vector into its natural logarithm; the **EXP** of a vector transforms each element into its exponential function (antilogarithm).

In order to specify a linear response function for data that have $r = 3$ response categories, you can specify either of the following RESPONSE statements:

```
response * 1 0 0 , 0 1 0;
response 1 0 0 , 0 1 0;
```

The matrix literal in the preceding statements specifies a 2×3 matrix, which is applied to each population as follows:

$$\begin{bmatrix} F_1 \\ F_2 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} * \begin{bmatrix} p_1 \\ p_2 \\ p_3 \end{bmatrix}$$

where p_1 , p_2 , and p_3 are sample proportions for the three response categories in a population, and F_1 and F_2 are the two response functions computed for that population. Therefore, this response function sets $F_1 = p_1$ and $F_2 = p_2$ in each population.

As another example of the linear response function, suppose you have two dependent variables corresponding to two observers who evaluate the same subjects. If the observers grade on the same three-point scale and if all nine possible responses are observed, then the following RESPONSE statement would compute the probability that the observers agree on their assessments:

```
response 1 0 0 0 1 0 0 0 1;
```

This response function is then computed as

$$F = p_{11} + p_{22} + p_{33} = \begin{bmatrix} 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \end{bmatrix} * \begin{bmatrix} p_{11} \\ p_{12} \\ p_{13} \\ p_{21} \\ p_{22} \\ p_{23} \\ p_{31} \\ p_{32} \\ p_{33} \end{bmatrix}$$

where p_{ij} denotes the probability that a subject gets a grade of i from the first observer and j from the second observer.

If the function is a compound function, requiring more than one operation to specify it, then the operations should be listed so that the first operation to be applied is on the right and the last operation to be applied is on the left. For example, if there are two response levels, you can have the following response function:

```
response 1 -1 log;
```

This is equivalent to the matrix expression

$$F = \begin{bmatrix} 1 & -1 \end{bmatrix} * \begin{bmatrix} \log(p_1) \\ \log(p_2) \end{bmatrix} = \log(p_1) - \log(p_2) = \log\left(\frac{p_1}{p_2}\right)$$

which is the logit response function since $p_2 = 1 - p_1$ when there are only two response levels.

The following statement specifies another example of a compound response function:

```
response exp 1 -1 * 1 0 0 1, 0 1 1 0 log;
```

This is equivalent to the matrix expression

$$F = \text{EXP}(A * B * \text{LOG}(P))$$

where P is the vector of sample proportions for some population,

$$A = \begin{bmatrix} 1 & -1 \end{bmatrix} \text{ and } B = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix}$$

If the four responses are based on two dependent variables, each with two levels, then the function can also be written as

$$F = \frac{p_{11}p_{22}}{p_{12}p_{21}}$$

which is the odds (crossproduct) ratio for a 2×2 table.

Understanding the Standard Response Functions

If no RESPONSE statement is specified, PROC CATMOD computes the standard response functions, which contrast the log of each response probability with the log of the probability for the last response category. If there are r response categories, then there are $r - 1$ standard response functions. For example, if there are four response categories, using no RESPONSE statement is equivalent to specifying the following:

```
response 1 0 0 -1,
          0 1 0 -1,
          0 0 1 -1 log;
```

This results in three response functions:

$$F = \begin{bmatrix} F_1 \\ F_2 \\ F_3 \end{bmatrix} = \begin{bmatrix} \log(p_1/p_4) \\ \log(p_2/p_4) \\ \log(p_3/p_4) \end{bmatrix}$$

If there are only two response levels, the resulting response function would be a logit, which is why the standard response functions are called generalized logits. They are useful in dealing with the log-linear model:

$$\pi = \text{EXP}(X\beta)$$

If C denotes the matrix in the preceding RESPONSE statement, then because of the restriction that the probabilities sum to 1, it follows that an equivalent model is

$$C * \text{LOG}(\pi) = (CX)\beta$$

But $C * \text{LOG}(P)$ is simply the vector of standard response functions. Thus, fitting a log-linear model on the cell probabilities is equivalent to fitting a linear model on the generalized logits.

RESTRICT Statement

RESTRICT *parameter=value* <...*parameter=value*> ;

where *parameter* is the letter B followed by a number; for example, B3 specifies the third parameter in the model. The *value* is the value to which the parameter is restricted. The RESTRICT statement restricts values of parameters to the values you specify, so that the estimation of the remaining parameters is subject to these restrictions. Consider the following statement:

```
restrict b1=1 b4=0 b6=0;
```

This restricts the values of three parameters. The first parameter is set to 1, and the fourth and sixth parameters are set to zero.

The RESTRICT statement is interactive. A new RESTRICT statement replaces any previous ones. In addition, if you submit two or more MODEL, LOGLIN, FACTORS, or REPEATED statements, then the subsequent occurrences of these statements also delete the previous RESTRICT statement.

WEIGHT Statement

WEIGHT *variable* ;

You can use a WEIGHT statement to refer to a variable containing the cell frequencies, which do not need to be integers. The WEIGHT statement lets you use summary data sets containing a count variable. See the section “Input Data Sets” on page 1818 for further information about the WEIGHT statement.

Details: CATMOD Procedure

Missing Values

Observations with missing values for any variable listed in the MODEL or POPULATION statement are omitted from the analysis.

If the WEIGHT variable for an observation has a missing value, the observation is by default omitted from the analysis. You can modify this behavior by specifying the MISSING= option in the MODEL statement. The option MISSING=*value* sets all missing weights to *value* and all missing cells to *value*. The option MISSING=SAMPLING causes all missing cells in a contingency table to be treated as sampling zeros.

Any observation with nonpositive weight is also, by default, omitted from the analysis. If it has zero weight, then you can specify the ZERO= option in the MODEL statement.

Input Data Sets

Data to be analyzed by PROC CATMOD must be in a SAS data set containing one of the following:

- raw data values (variable values for every subject)
- frequency counts and the corresponding variable values
- response function values and their covariance matrix

If you specify a **WEIGHT** statement, then PROC CATMOD uses the values of the WEIGHT variable as the frequency counts. If the **READ** function is specified in the **RESPONSE** statement, then the procedure expects the input data set to contain the values of response functions and their covariance matrix. Otherwise, PROC CATMOD assumes that the SAS data set contains raw data values.

Raw Data Values

If you use raw data, PROC CATMOD first counts the number of observations having each combination of values for all variables specified in the **MODEL** or **POPULATION** statement. For example, suppose the variables A and B each take on the values 1 and 2, and their frequencies can be represented as follows:

		A	
		1	2
B	1	2	1
	2	3	1

The SAS data set Raw containing the raw data might be as follows:

Observation	A	B
1	1	1
2	1	1
3	1	2
4	1	2
5	1	2
6	2	1
7	2	2

And the statements for PROC CATMOD are as follows:

```
proc catmod data=Raw;
  model A=B;
run;
```

For discussions of how to handle structural and random zeros with raw data as input data, see the section “Zero Frequencies” on page 1843 and [Example 30.5](#).

Frequency Counts

If your data set contains frequency counts, then use the **WEIGHT** statement to specify the variable containing the frequencies. For example, you could create and analyze the Summary data set as follows:

```
data Summary;
  input A B Count;
  datalines;
1 1 2
1 2 3
2 1 1
```

```

2 2 1
;

proc catmod data=Summary;
  weight Count;
  model A=B;
run;

```

The data set Summary can also be created from the data set Raw by using the FREQ procedure:

```

proc freq data=Raw;
  tables A*B / out=Summary;
run;

```

Inputting Response Functions and Covariances Directly

If you want to read in the response functions and their covariance matrix, rather than have PROC CATMOD compute them, create a TYPE=EST data set. In addition to having one variable name for each function, the data set should have two additional variables: `_TYPE_` and `_NAME_`, both character variables of length 8. The variable `_TYPE_` should have the value 'PARMS' when the observation contains the response functions; it should have the value 'COV' when the observation contains elements of the covariance matrix of the response functions. The variable `_NAME_` is used only when `_TYPE_=COV`, in which case it should contain the name of the variable that has its covariance elements stored in that observation. In the following data set, for example, the covariance between the second and fourth response functions is 0.000102:

```

data direct(type=est);
  input b1-b4 _type_ $ _name_ $8.;
  datalines;
0.590463  0.384720  0.273269  0.136458  PARMS  .
0.001690  0.000911  0.000474  0.000432  COV    B1
0.000911  0.001823  0.000031  0.000102  COV    B2
0.000474  0.000031  0.001056  0.000477  COV    B3
0.000432  0.000102  0.000477  0.000396  COV    B4
;

```

In order to tell PROC CATMOD that the input data set contains the values of response functions and their covariance matrix, do the following:

- specify the `READ` function in the `RESPONSE` statement
- specify `_F_` as the dependent variable in the `MODEL` statement

For example, suppose the response functions correspond to four populations that represent the cross-classification of two age groups by two race groups. You can use the `FACTORS` statement to identify these two factors and to name the effects in the model. The following statements are required to fit a main-effects model to these data:

```

proc catmod data=direct;
  response read b1-b4;
  model _f_=_response_;
  factors age 2, race 2 / _response_=age race;
run;

```

Ordering of Populations and Responses

By default, populations and responses are sorted in standard SAS order as follows:

- alphabetical order for character variables
- increasing numeric order for numeric variables

Suppose you specify the following statements:

```
data one;
  length A B $ 6;
  input A $ B $ wt @@;
  datalines;
low      low  23  low   medium  31  low   high  38
medium   low  40  medium medium  42  medium high  50
high     low  52  high   medium  54  high   high  61
;

proc catmod;
  weight wt;
  model A=B / oneway;
run;
```

The ordering of populations and responses corresponds to the alphabetical order of the levels of the character variables. You can specify the **ONEWAY** option to display the ordering of the variables, while the “Population Profiles” and “Response Profiles” tables display the ordering of the populations and the responses, respectively.

Population Profiles		Response Profiles	
Sample	B	Response	A
1	high	1	high
2	low	2	low
3	medium	3	medium

In this example, if you want to have the levels ordered in the natural order of ‘low,’ ‘medium,’ ‘high,’ you can specify the **ORDER=DATA** option:

```
proc catmod order=data;
  weight wt;
  model a=b / oneway;
run;
```

The resulting ordering of populations and responses is as follows:

Population Profiles		Response Profiles	
Sample	B	Response	A
1	low	1	low
2	medium	2	medium
3	high	3	high

You can use the `ORDER=DATA` option to ensure that populations and responses are ordered in a specific way. But since this also affects the definitions and the ordering of the parameters, you must exercise caution when using the `_RESPONSE_` effect, the `CONTRAST` statement, or direct input of the design matrix.

An alternative method of ensuring that populations and responses are ordered in a specific way is to assign a format to your variables and specify the `ORDER=FORMATTED` option. The levels are then ordered according to their formatted values.

Another method is to replace any character variables with numeric variables and to assign formatted values such as ‘yes’ and ‘no’ to the numeric levels. Since `ORDER=INTERNAL` is the default ordering, PROC CATMOD orders the populations and responses according to the numeric values but displays the formatted values.

Specification of Effects

By default, the CATMOD procedure treats all variables as classification variables. As a result, there is no `CLASS` statement in PROC CATMOD. The values of a classification variable can be numeric or character. PROC CATMOD builds a set of effects-coded variables to represent the levels of the classification variable and then uses these to fit the model (for details, see the section “[Generation of the Design Matrix](#)” on page 1832). You can modify the default by using the `DIRECT` statement to treat numeric independent continuous variables as continuous variables. The classification variables, combinations of classification variables, and continuous variables are then used in fitting linear models to data.

The parameters of a linear model are generally divided into subsets that correspond to meaningful sources of variation in the response functions. These sources, called *effects*, can be specified in the `MODEL`, `LOGLIN`, `FACTORS`, `REPEATED`, and `CONTRAST` statements. Effects can be specified in any of the following ways:

- A main effect is a single classification variable (that is, it produces class levels): `A B C`.
- A crossed effect (or interaction) is two or more classification variables joined by asterisks—for example: `A*B A*B*C`.
- A nested effect is a main effect or an interaction, followed by a parenthetical field containing a main effect or an interaction. Multiple variables within the parentheses are assumed to form a crossed effect even when the asterisk is absent. In the following list, the last two effects are identical: `B(A) C(A*B) A*B(C*D) A*B(C D)`.
- A nested-by-value effect is the same as a nested effect except that any variable in the parentheses can be followed by an equal sign and a value: `B(A=1) C(A B=1) C*D(A=1 B=1) A(C='low')`.
- A direct effect is a variable specified in a `DIRECT` statement: `X Y`.
- Direct effects can be crossed with other effects: `X*Y X*X*X X*A*B(C D=1)`.

The variables for crossed and nested effects remain in the order in which they are first encountered. For example, in the following model, the effect `A*B` is reported as `B*A` since `B` appears before `A` in the statement:

```
model R=B A A*B C(A B);
```

Also, C(A B) is interpreted as C(A*B) and is therefore reported as C(B*A).

Bar Notation

You can shorten the specification of multiple effects by using bar notation. For example, the following statements illustrate two methods of writing a full three-way factorial model:

```
proc catmod;
  model y=a b c a*b a*c b*c a*b*c;
run;
```

```
proc catmod;
  model y=a|b|c;
run;
```

When you use the bar (|) notation, the right and left sides become effects, and the interaction between them becomes an effect. Multiple bars are permitted. The expressions are expanded from left to right, using rules 1 through 4 given in Searle (1971, p. 390):

- Multiple bars are evaluated left to right. For example, A|B|C is evaluated as follows:

$$\begin{aligned} A|B|C &\rightarrow \{A|B\}|C \\ &\rightarrow \{A B A*B\}|C \\ &\rightarrow A B A*B C A*C B*C A*B*C \end{aligned}$$
- Crossed and nested groups of variables are combined. For example, A(B)|C(D) generates A*C(B D), among other terms.
- Duplicate variables are removed. For example, A(C)|B(C) generates A*B(C C), among other terms, and the extra C is removed.
- Effects are discarded if a variable occurs on both the crossed and nested sides of an effect. For instance, A(B)|B(D E) generates A*B(B D E), but this effect is deleted.

You can also specify the maximum number of variables involved in any effect that results from bar evaluation by specifying that maximum number, preceded by an @ sign, at the end of the bar effect. For example, the specification A|B|C @ 2 would result in only those effects that contain two or fewer variables; in this case, the effects A, B, A*B, C, A*C, and B*C are generated.

Other examples of the bar notation follow:

A C(B)	is equivalent to	A C(B) A*C(B)
A(B) C(B)	is equivalent to	A(B) C(B) A*C(B)
A(B) B(D E)	is equivalent to	A(B) B(D E)
A B(A) C	is equivalent to	A B(A) C A*C B*C(A)
A B(A) C@2	is equivalent to	A B(A) C A*C
A B C D@2	is equivalent to	A B A*B C A*C B*C D A*D B*D C*D

For details about how the effects specified lead to a design matrix, see the section “[Generation of the Design Matrix](#)” on page 1832.

Output Data Sets

OUT= Data Set

For each population, the **OUT=** data set contains the observed and predicted values of the response functions, their standard errors, the residuals, and variables that describe the population and response profiles. In addition, if you use the standard response functions, the data set includes observed and predicted values for the cell frequencies or the cell probabilities, together with their standard errors and residuals.

Number of Observations

For the standard response functions, there are $s \times (2q - 1)$ observations in the data set for each BY group, where s is the number of populations and q is the number of response functions per population. Otherwise, there are $s \times q$ observations in the data set for each BY group.

Variables in the OUT= Data Set

The data set contains the following variables:

BY variables	If you use a BY statement, the BY variables are included in the OUT= data set.
dependent variables	If the response functions are the default ones (generalized logits), then the dependent variables, which describe the response profiles, are included in the OUT= data set. When <code>_TYPE_=FUNCTION</code> , the values of these variables are missing.
independent variables	The independent variables, which describe the population profiles, are included in the OUT= data set.
<code>_NUMBER_</code>	the sequence number of the response function or the cell probability or the cell frequency
<code>_OBS_</code>	the observed value
<code>_PRED_</code>	the predicted value
<code>_RESID_</code>	the residual (observed minus predicted)
<code>_SAMPLE_</code>	the population number. This matches the sample number in the “Population Profile” section of the output.
<code>_SEOBS_</code>	the standard error of the observed value
<code>_SEPRED_</code>	the standard error of the predicted value
<code>_TYPE_</code>	specifies a character variable with three possible values. When <code>_TYPE_=FUNCTION</code> , the observed and predicted values are values of the response functions. When <code>_TYPE_=PROB</code> , they are values of the cell probabilities. When <code>_TYPE_=FREQ</code> , they are values of the cell frequencies. Cell probabilities or frequencies are provided only when the default response functions are modeled. In this case, cell probabilities are provided by default, and cell frequencies are provided if you specify the option <code>PRED=FREQ</code> .

OUTEST= Data Set

This TYPE=EST output data set contains the estimated parameter vector and its estimated covariance matrix. If you specify both the **ML** and **WLS** options in the MODEL statement, the **OUTEST=** data set contains both sets of estimates. For each BY group, there are $p + 1$ observations in the data set for each estimation method, where p is the number of estimated parameters. The data set contains the following variables:

B1, B2, and so on	variables for the estimated parameters. The OUTEST= data set contains one variable for each estimated parameter.
BY variables	If you use a BY statement, the BY variables are included in the OUT= data set.
<code>_METHOD_</code>	the method used to obtain parameter estimates. For weighted least squares estimation, <code>_METHOD_=WLS</code> , and for maximum likelihood estimation, <code>_METHOD_=ML</code> .
<code>_NAME_</code>	identifies parameter names. When <code>_TYPE_=PARMS</code> , <code>_NAME_</code> is blank, but when <code>_TYPE_=COV</code> , <code>_NAME_</code> has one of the values B1, B2, and so on, corresponding to the parameter names.
<code>_STATUS_</code>	indicates whether the estimates have converged
<code>_TYPE_</code>	identifies the statistics contained in the variables for parameter estimates (B1, B2, and so on). When <code>_TYPE_=PARMS</code> , the variables contain parameter estimates; when <code>_TYPE_=COV</code> , they contain covariance estimates.

The variables `_METHOD_`, `_NAME_`, and `_TYPE_` are character variables; the BY variables can be either character or numeric; and the variables for estimated parameters are numeric.

See Appendix A, “[Special SAS Data Sets](#),” for more information about special SAS data sets.

Logistic Analysis

In a logistic analysis, the response functions are the logits of the dependent variable.

PROC CATMOD can compute the three following types of logits with the use of keywords in the **RESPONSE** statement. Note that other types of response functions can be generated by specifying appropriate transformations in the **RESPONSE** statement.

- Generalized logits are used primarily for nominally scaled dependent variables, but they can also be used for ordinal data modeling. Maximum likelihood estimation is available for the analysis of these logits.
- Cumulative logits are used for ordinal scaled dependent variables. Except for dependent variables with two response levels, only weighted least squares estimation is available for the analysis of these logits.
- Adjacent-category logits are equivalent to generalized logits, but they have some advantages for ordinal data analysis because they automatically incorporate integer scores for the levels of the dependent variable. Except for dependent variables with two response levels, only weighted least squares estimation is available for the analysis of these logits.

If the dependent variable has only two responses, then the cumulative logit and the adjacent-category logit are the negative of the generalized logit, as computed by PROC CATMOD. Consequently, parameter estimates obtained by using these logits are the negative of those obtained from using generalized logits. A simple logistic analysis of variance uses statements like the following:

```
proc catmod;
  model r=a|b;
run;
```

Logistic Regression

If the independent variables are treated quantitatively (like continuous variables), then a logistic analysis is known as a *logistic regression*. If you want PROC CATMOD to treat the independent variables as quantitative variables, specify them in both the **DIRECT** and **MODEL** statements, as follows:

```
proc catmod;
  direct x1 x2 x3;
  model r=x1 x2 x3;
run;
```

Since the preceding statements do not include a **RESPONSE** statement, generalized logits are computed. See [Example 30.3](#) for another example.

The parameter estimates from the CATMOD procedure are the same as those from a logistic regression program such as PROC LOGISTIC (see Chapter 54, “[The LOGISTIC Procedure](#)”). The chi-square statistics and the predicted values are also identical. In the binary response case, PROC CATMOD can be made to model the probability of the maximum value by either (1) organizing the input data so that the maximum value occurs first and specifying **ORDER=DATA** in the PROC CATMOD statement or (2) specifying cumulative logits (CLOGITS) in the **RESPONSE** statement.

CAUTION: Computational difficulties might occur if you use a continuous variable with a large number of unique values in a **DIRECT** statement. See the section “[Continuous Variables](#)” on page 1827 for more details.

Cumulative Logits

If your dependent variable is ordinally scaled, you can specify the analysis of cumulative logits that take into account the ordinal nature of the dependent variable:

```
proc catmod;
  response clogits;
  direct x;
  model r=a x;
run;
```

The preceding statements correspond to a simple analysis that addresses the question of existence of an association between the independent variables and the ordinal dependent variable. However, there are some commonly used models for the analysis of ordinal data (Agresti 1984) that address the structure of association (in terms of odds ratios), as well as its existence.

If the independent variables are classification variables, a typical analysis for such a model uses the following statements:

```
proc catmod;
  weight wt;
  response clogits;
  model r=_response_ a b;
run;
```

On the other hand, if the independent variables are ordinally scaled, you might specify numeric scores in variables *x1* and *x2*, and use the following statements:

```
proc catmod;
  weight wt;
  direct x1 x2;
  response clogits;
  model r=_response_ x1 x2;
run;
```

See Agresti (1984) for additional details of estimation, testing, and interpretation.

Continuous Variables

Computational difficulties might occur if you have a continuous variable with a large number of unique values and you use this variable in a **DIRECT** statement, since an observation often represents a separate population of size one. At this extreme of sparseness, the weighted least squares method is inappropriate since there are too many zero frequencies. Therefore, you should use the maximum likelihood method. PROC CATMOD is not designed optimally for continuous variables; therefore, it might be less efficient and unable to allocate sufficient memory to handle this problem, as compared with a procedure designed specifically to handle continuous data. In these situations, consider using the **LOGISTIC** or **GENMOD** procedure to analyze your data.

Log-Linear Model Analysis

When the response functions are the default generalized logits, then inclusion of the keyword **_RESPONSE_** in every effect in the right side of the MODEL statement fits a log-linear model. The keyword **_RESPONSE_** tells PROC CATMOD that you want to model the variation among the dependent variables. You then specify the actual model in the **LOGLIN** statement.

When you perform log-linear model analysis, you can request weighted least squares estimates, maximum likelihood estimates, or both. By default, PROC CATMOD calculates maximum likelihood estimates when the default response functions are used. The following table provides appropriate MODEL statements for the combinations of types of estimates:

Estimation Desired	MODEL Statement
Maximum likelihood (Newton-Raphson)	<code>model a*b=_response_;</code>
Maximum likelihood (Iterative Proportional Fitting)	<code>model a*b=_response_ / ml=ipf;</code>
Weighted least squares	<code>model a*b=_response_ / wls;</code>
Maximum likelihood and weighted least squares	<code>model a*b=_response_ / wls ml;</code>

CAUTION: Sampling zeros in the input data set should be specified with the `ZERO=` option to ensure that these sampling zeros are not treated as structural zeros. Alternatively, you can replace cell counts for sampling zeros with some positive number close to zero (such as $1E-20$) in a DATA step. Data containing sampling zeros should be analyzed with maximum likelihood estimation. See the section “Cautions” on page 1842 and [Example 30.5](#) for further information and an illustration that uses both cell count data and raw data.

One Population

The usual log-linear model analysis has one population, which means that all of the variables are dependent variables. For example, the following statements yield a maximum likelihood analysis of a saturated log-linear model for the dependent variables `r1` and `r2`:

```
proc catmod;
  weight wt;
  model r1*r2=_response_;
  loglin r1|r2;
run;
```

If you want to fit a reduced model with respect to the dependent variables (for example, a model of independence or conditional independence), specify the reduced model in the `LOGLIN` statement. For example, the following statements yield a main-effects log-linear model analysis of the factors `r1` and `r2`:

```
proc catmod;
  weight wt;
  model r1*r2=_response_ / pred;
  loglin r1 r2;
run;
```

The output includes Wald statistics for the individual effects `r1` and `r2`, as well as predicted cell probabilities. Moreover, the goodness-of-fit statistic is the likelihood ratio test for the hypothesis of independence between `r1` and `r2` or, equivalently, a test of `r1*r2`.

Multiple Populations

You can do log-linear model analysis with multiple populations by using a `POPULATION` statement or by including effects on the right side of the MODEL statement that contain independent variables. Each effect must include the `_RESPONSE_` keyword.

For example, suppose the dependent variables `r1` and `r2` are dichotomous, and the independent variable group has three levels. Then the following statements specify a saturated model (three degrees of freedom for `_RESPONSE_` and six degrees of freedom for the interaction between `_RESPONSE_` and `group`):

```
proc catmod;
  weight wt;
  model r1*r2=_response_ group*_response_;
  loglin r1|r2;
run;
```

From another point of view, `_RESPONSE_*group` can be regarded as a main effect for `group` with respect to the three response functions, while `_RESPONSE_` can be regarded as an intercept effect with respect to the functions. In other words, the following statements give essentially the same results as the logistic analysis:

```
proc catmod;
  weight wt;
  model r1*r2=group;
run;
```

The ability to model the interaction between the independent and the dependent variables becomes particularly useful when a reduced model is specified for the dependent variables. For example, the following statements specify a model with two degrees of freedom for `_RESPONSE_` (one for `r1` and one for `r2`) and four degrees of freedom for the interaction of `_RESPONSE_*group`:

```
proc catmod;
  weight wt;
  model r1*r2=_response_ group*_response_;
  loglin r1 r2;
run;
```

The likelihood ratio goodness-of-fit statistic (three degrees of freedom) tests the hypothesis that `r1` and `r2` are independent in each of the three groups.

Iterative Proportional Fitting

You can use the iterative proportional fitting (IPF) algorithm to fit a hierarchical log-linear model with no independent variables and no population variables.

The advantage of IPF over the Newton-Raphson (NR) algorithm and over the weighted least squares (WLS) method is that, when the contingency table has several dimensions and the parameter vector is large, you can obtain the log likelihood, the goodness-of-fit G^2 , and the predicted frequencies or probabilities without performing potentially expensive parameter estimation and covariance matrix calculations. This enables you to do the following:

- compare two models by computing the likelihood ratio statistics to test the significance of the contribution of the variables in one model that are not in the other model
- compute predicted values of the cell probabilities or frequencies for the final model

Each iteration of the IPF algorithm is generally faster than an iteration of the NR algorithm; however, the IPF algorithm converges to the MLEs more slowly than the NR algorithm. Both NR and WLS are more general methods that are able to perform more complex analyses than IPF can.

Repeated Measures Analysis

If there are multiple dependent variables and the variables represent repeated measurements of the same observational unit, then the variation among the dependent variables can be attributed to one or more repeated measurement factors. The factors can be included in the model by specifying `_RESPONSE_` on the right side of the MODEL statement and by using a **REPEATED** statement to identify the factors.

To perform a repeated measures analysis, you also need to specify a **RESPONSE** statement, since the standard response functions (generalized logits) cannot be used. Typically, the **MEANS** or **MARGINALS** response functions are specified in a repeated measures analysis, but other response functions can also be reasonable.

One Population

Consider an experiment in which each subject is measured at three times, and the response functions are marginal probabilities for each of the dependent variables. If the dependent variables each have k levels, then PROC CATMOD computes $k-1$ response functions for each time. Differences among the response functions with respect to these times could be attributed to the repeated measurement factor Time. To incorporate the Time variation into the model, specify the following statements:

```
proc catmod;
  response marginals;
  model t1*t2*t3=_response_;
  repeated Time 3 / _response_=Time;
run;
```

These statements produce a Time effect that has $2(k-1)$ degrees of freedom since there are $k-1$ response functions at each time point. For a dichotomous variable, the Time effect has two degrees of freedom.

Now suppose that at each time point, each subject has X-rays taken, and the X-rays are read by two different radiologists. This creates six dependent variables that represent the 3×2 cross-classification of the repeated measurement factors Time and Reader. A saturated model with respect to these factors can be obtained by specifying the following statements:

```
proc catmod;
  response marginals;
  model r11*r12*r21*r22*r31*r32=_response_;
  repeated Time 3, Reader 2
    / _response_=Time Reader Time*Reader;
run;
```

If you want to fit a main-effects model with respect to Time and Reader, then change the **REPEATED** statement to the following:

```
repeated Time 3, Reader 2 / _response_=Time Reader;
```

If you want to fit a main-effects model for Time but for only one of the readers, the **REPEATED** statement might look like the following:

```

repeated Time $ 3, Reader $ 2
  /_response_=Time(Reader=Smith)
  profile =('1' Smith,
            '1' Jones,
            '2' Smith,
            '2' Jones,
            '3' Smith,
            '3' Jones);

```

If Jones had been unavailable for a reading at time 3, then there would be only $5(k - 1)$ response functions, even though PROC CATMOD would be expecting some multiple of 6 ($= 3 \times 2$). In that case, the **PROFILE=** option would be necessary to indicate which repeated measurement profiles were actually represented:

```

repeated Time $ 3, Reader $ 2
  /_response_=Time(Reader=Smith)
  profile =('1' Smith,
            '1' Jones,
            '2' Smith,
            '2' Jones,
            '3' Smith);

```

When two or more repeated measurement factors are specified, PROC CATMOD presumes that the response functions are ordered so that the levels of the rightmost factor change most rapidly. This means that the dependent variables should be specified in the same order. For this example, the order implied by the **REPEATED** statement is as follows, where the variable r_{ij} corresponds to Time i and Reader j :

Response Function	Dependent Variable	Time	Reader
1	r_{11}	1	1
2	r_{12}	1	2
3	r_{21}	2	1
4	r_{22}	2	2
5	r_{31}	3	1
6	r_{32}	3	2

The order of dependent variables in the **MODEL** statement must agree with the order implied by the **REPEATED** statement.

Multiple Populations

When there are variables specified in the **POPULATION** statement or on the right side of the **MODEL** statement, these variables produce multiple populations. PROC CATMOD can then model these independent variables, the repeated measurement factors, and the interactions between the two.

For example, suppose that there are five groups of subjects, that each subject in the study is measured at three different times, and that the dichotomous dependent variables are labeled t_1 , t_2 , and t_3 . The following statements compute three response functions for each population:

```
proc catmod;
  weight wt;
  population Group;
  response marginals;
  model t1*t2*t3=_response_;
  repeated Time / _response_=Time;
run;
```

PROC CATMOD then regards `_RESPONSE_` as a variable with three levels corresponding to the three response functions in each population and forms an effect with two degrees of freedom. The `MODEL` and `REPEATED` statements tell PROC CATMOD to fit the main effect of Time.

In general, the `MODEL` statement tells PROC CATMOD how to integrate the independent variables and the repeated measurement factors into the model. For example, again suppose that there are five groups of subjects, that each subject is measured at three times, and that the dichotomous independent variables are labeled t1, t2, and t3. If you use the same `WEIGHT`, `POPULATION`, `RESPONSE`, and `REPEATED` statements as in the preceding program, the following `MODEL` statements result in the indicated analyses:

<code>model t1*t2*t3=Group / averaged;</code>	Specifies the Group main effect (with 4 degrees of freedom)
<code>model t1*t2*t3=_response_;</code>	Specifies the Time main effect (with 2 degrees of freedom)
<code>model t1*t2*t3=_response_*Group;</code>	Specifies the interaction between Time and Group (with 8 degrees of freedom)
<code>model t1*t2*t3=_response_ Group;</code>	Specifies both main effects, and the interaction between Time and Group (with a total of 14 degrees of freedom)
<code>model t1*t2*t3=_response_(Group);</code>	Specifies a Time main effect within each Group (with 10 degrees of freedom)

However, the following `MODEL` statement is invalid since effects cannot be nested within `_RESPONSE_`:

```
model t1*t2*t3=Group(_response_);
```

Generation of the Design Matrix

Each row of the design matrix (corresponding to a population) is generated by a unique combination of independent variable values. Each column of the design matrix corresponds to a model parameter. The columns are produced from the effect specifications in the `MODEL`, `LOGLIN`, `FACTORS`, and `REPEATED` statements. For details about effect specifications, see the section “[Specification of Effects](#)” on page 1822.

This section is divided into three parts:

- one response function per population
- [two or more](#) response functions per population (excluding log-linear models), beginning on page 1835
- [log-linear models](#), beginning on page 1839

This section assumes that the default effect parameterization is used. Specifying the [reference parameterization](#) replaces the “-1”s with zeros in the design matrix for the main effects of classification variables, and makes appropriate changes to interaction terms.

You can display the design matrix by specifying the [DESIGN](#) option in the MODEL statement.

One Response Function per Population

Intercept

When there is one response function per population, all design matrices start with a column of 1s for the intercept unless the [NOINT](#) option is specified or the design matrix is input directly.

Main Effects

If a classification variable A has k levels, then its main effect has $k - 1$ degrees of freedom, and the design matrix has $k - 1$ columns that correspond to the first $k - 1$ levels of A. The i th column contains a 1 in the i th row, a -1 in the last row, and 0s everywhere else. If α_i denotes the parameter that corresponds to the i th level of variable A, then the $k - 1$ columns yield estimates of the independent parameters, $\alpha_1, \alpha_2, \dots, \alpha_{k-1}$. The last parameter is not needed because PROC CATMOD constrains the k parameters to sum to zero. In other words, PROC CATMOD uses a full-rank center-point parameterization to build design matrices. Here are two examples:

Variable	Data Levels	Effect Parameterization	
		Design Matrix	
A	1	1	0
	2	0	1
	3	-1	-1
B	1		-1
	2		-1

For an effect with three levels, such as A, PROC CATMOD produces two parameter estimates for each response function. By default, the first (corresponding to the first row in the design columns) estimates the effect of level 1 of A compared to the average effect of the three levels of A. The second (corresponding to the second row in the design columns) estimates the effect of level 2 of A compared to the average effect of the three levels of A. The sum-to-zero constraint requires the effect of level 3 of A to be the negative of the sum of the level 1 and 2 effects (as shown by the third row in the design columns).

Crossed Effects (Interactions)

Crossed effects (such as A*B) are formed by the horizontal direct products of main effects, as illustrated in the following table:

Data Levels		Design Matrix				
A	B	A	B	A*B		
1	1	1	0	1	1	0
1	2	1	0	-1	-1	0
2	1	0	1	1	0	1
2	2	0	1	-1	0	-1
3	1	-1	-1	1	-1	-1
3	2	-1	-1	-1	1	1

The number of degrees of freedom for a crossed effect (that is, the number of design matrix columns) is equal to the product of the numbers of degrees of freedom for the separate effects.

Nested Effects

The effect A(B) is read “A within B” and is the same as specifying an A main effect for every value of B. If n_a and n_b are the number of levels in A and B, respectively, then the number of columns for A(B) is $(n_a - 1)n_b$ when every combination of levels exists in the data. The following table gives an example:

Data Levels		Design Matrix			
B	A	A(B)			
1	1	1	0	0	0
1	2	0	1	0	0
1	3	-1	-1	0	0
2	1	0	0	1	0
2	2	0	0	0	1
2	3	0	0	-1	-1

CAUTION: PROC CATMOD actually allocates a column for all possible combinations of values even though some combinations are not present in the data. This can be of particular concern if the data are not balanced with respect to the nested levels.

Nested-by-Value Effects

Instead of nesting an effect within all values of the main effect, you can nest an effect within specified values of the nested variable (A(B=1), for example). The four degrees of freedom for the A(B) effect shown in the preceding section can also be obtained by specifying the two separate nested effects with values, as the following table shows:

Data Levels		Design Matrix			
B	A	A(B=1)		A(B=2)	
1	1	1	0	0	0
1	2	0	1	0	0
1	3	-1	-1	0	0
2	1	0	0	1	0
2	2	0	0	0	1
2	3	0	0	-1	-1

Each effect has $n_a - 1$ degrees of freedom, assuming a complete combination, so each effect in this example has two degrees of freedom.

The procedure compares nested values to data values on the basis of formatted values. If a format is not specified for the variable, the procedure formats internal data values to BEST16, left-justified. The nested values specified in nested-by-value effects are also converted to a BEST16 formatted value, left-justified.

For example, if the numeric variable B has internal data values 1 and 2, then A(B=1), A(B=1.0), and A(B=1E0) are all valid nested-by-value effects. However, if the data value 1 is formatted as ‘one’, then A(B=‘one’) is a valid effect, but A(B=1) is not since the formatted nested value (1) does not match the formatted data value (one).

To ensure correct nested-by-value effects, look at the tables of population and response profiles. These are displayed by default, and they contain the formatted data values. In addition, the population and response profiles are displayed when you specify the **ONEWAY** option in the **MODEL** statement.

Direct Effects

To request that the actual values of a variable be inserted into the design matrix, declare the variable in a **DIRECT** statement, and specify the effect by the variable name. For example, specifying the effects **X1** and **X2** in both the **MODEL** and **DIRECT** statements results in the following:

Data Levels		Design Columns	
X1	X2	X1	X2
1	1	1	1
2	4	2	4
3	9	3	9

Unless there is a **POPULATION** statement that excludes the direct variables, the direct variables help to define the sample populations. In general, the variables should not be continuous in the sense that every subject has a different value because this would create a separate population for each subject (note, however, that such a strategy is used purposely for logistic regression).

If there is a **POPULATION** statement that omits mention of the direct variables, then the values of the direct variables must be identical for all subjects in a given population since there can be only one independent variable profile for each population.

Two or More Response Functions per Population

When there is more than one response function per population, the structure of the design matrix depends on whether or not the model type is **AVERAGED** (see the **AVERAGED** option in the **MODEL** statement). The model type is **AVERAGED** if independent variable effects are averaged over the multiple responses within a population rather than being nested in them.

The following subsections illustrate the effect of specifying (or not specifying) an **AVERAGED** model type. This section does not apply to log-linear models; for these models, see the section “**Log-Linear Model Design Matrices**” on page 1839.

Model Type Not AVERAGED

Suppose the variable **A** has two levels, and you specify the following statements:

```
proc catmod;
  model Y=A / design;
run;
```

If the variable **Y** has two levels, then there is only one response function per population, and the design matrix is as follows:

Sample	Design Matrix	
	Intercept	A
1	1	1
2	1	-1

But if the variable Y has three levels, then there are two response functions per population, and the preceding design matrix is assumed to hold for each of the two response functions. The response functions are always ordered so that the multiple response functions within a population are grouped together. For this example, the design matrix would be as follows:

Sample	Response	Design Matrix			
	Function	Intercept	A		
	Number				
1	1	1	0	1	0
1	2	0	1	0	1
2	1	1	0	-1	0
2	2	0	1	0	-1

Since the same submatrix applies to each of the multiple response functions, PROC CATMOD displays only the submatrix (that is, the one it would create if there were only one response function per population) rather than the entire design matrix. PROC CATMOD displays

$$\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

Ordering of Parameters

This grouping of multiple response functions within populations also has an effect in the table of parameter estimates displayed by PROC CATMOD. The following table shows some parameter estimates, where the four rows of the table correspond to the four columns in the preceding design matrix:

Effect	Parameter	Estimate
Intercept	1	1.4979
	2	0.8404
A	3	0.1116
	4	-0.3296

Notice that the intercept and the A effect each have two parameter estimates associated with them. The first estimate in each pair is associated with the first response function, and the second in each pair is associated with the second response function. Consequently, 0.1116 is the effect of the first level of A on the first response function. In any table of parameter estimates displayed by PROC CATMOD, as you read down the column of estimates, the response function level changes before levels of the variables making up the effect.

Model Type AVERAGED

When the model type is *AVERAGED* (for example, when the *AVERAGED* option is specified in the MODEL statement, when *_RESPONSE_* is used in the MODEL statement, or when the design matrix is input directly in the MODEL statement), PROC CATMOD does not assume that the same submatrix applies to each of the q response functions per population. Rather, it averages any independent variable effects across the functions, and it enables you to study variation among the q functions. The first column of the design matrix is always a column of 1s corresponding to the intercept, unless the *NOINT* option is specified in the MODEL statement or the design matrix is input directly. Also, since the design matrix does not have any special submatrix structure, PROC CATMOD displays the entire matrix.

For example, suppose the dependent variable *Y* has three levels, the independent variable *A* has two levels, and you specify the following statements:

```
proc catmod;
  response marginals;
  model y=a / averaged design;
run;
```

Then there are two response functions per population, and the response functions are always ordered so that the multiple response functions within a population are grouped together. For this example, the design matrix would be as follows:

Sample	Response Function Number	Design Matrix	
		Intercept	A
1	1	1	1
1	2	1	1
2	1	1	-1
2	2	1	-1

Note that the model now has only two degrees of freedom. The remaining two degrees of freedom in the residual correspond to variation among the three levels of the dependent variable. Generally, that variation tends to be statistically significant and therefore should not be left out of the model. You can include it in the model by including the two effects, `_RESPONSE_` and `_RESPONSE_*A`, but if the study is not a repeated measures study, those sources of variation tend to be uninteresting. The usual solution for this type of study (one dependent variable) is to exclude the `AVERAGED` option from the `MODEL` statement.

An `AVERAGED` model type is automatically used whenever you use the `_RESPONSE_` keyword in the `MODEL` statement. The `_RESPONSE_` effect models variation among the q response functions per population. If there is no `REPEATED`, `FACTORS`, or `LOGLIN` statement, then `PROC CATMOD` builds a main effect with $q - 1$ degrees of freedom. For example, three response functions would produce the following design columns:

Response Function Number	Design Columns	
	<code>_RESPONSE_</code>	
1	1	0
2	0	1
3	-1	-1

If there is more than one population, then the `_RESPONSE_` effect is averaged over the populations. Also, the `_RESPONSE_` effect can be crossed with any other effect, or it can be nested within an effect.

If there is a `REPEATED` statement that contains only one repeated measurement factor, then `PROC CATMOD` builds the design columns for `_RESPONSE_` in the same way, except that the output labels the main effect with the factor name rather than with the word `_RESPONSE_`. For example, suppose an independent variable *A* has two levels, and the input statements are as follows:


```

proc catmod;
  response marginals;
  model Time1*Time2=A _response_ A*_response_ / design;
  repeated Time 2 / _response_=Time;
run;

```

If Time1 and Time2 each have two levels (so that they each have one independent marginal probability), then the **RESPONSE** statement makes PROC CATMOD compute two response functions per population. The design matrix is as follows:

Sample	Response Function Number	Design Matrix			
		Intercept	A	Time	A*Time
1	1	1	1	1	1
1	2	1	1	-1	-1
2	1	1	-1	1	-1
2	2	1	-1	-1	1

However, if Time1 and Time2 each have three levels (so that they each have two independent marginal probabilities), then the **RESPONSE** statement causes PROC CATMOD to compute four response functions per population. In that case, since Time has two levels, PROC CATMOD groups the functions into sets of 2 (= 4/2) and constructs the preceding submatrix for each function in the set. This results in the following design matrix, which is obtained from the previous one by multiplying each element by an identity matrix of order two:

Sample	Response Function	Design Matrix							
		Intercept		A		Time		A*Time	
1	P(Time1=1)	1	0	1	0	1	0	1	0
1	P(Time1=2)	0	1	0	1	0	1	0	1
1	P(Time2=1)	1	0	1	0	-1	0	-1	0
1	P(Time2=2)	0	1	0	1	0	-1	0	-1
2	P(Time1=1)	1	0	-1	0	1	0	-1	0
2	P(Time1=2)	0	1	0	-1	0	1	0	-1
2	P(Time2=1)	1	0	-1	0	-1	0	1	0
2	P(Time2=2)	0	1	0	-1	0	-1	0	1

If there is a **REPEATED** statement that contains two or more repeated measurement factors, then PROC CATMOD builds the design columns for **_RESPONSE_** according to the definition of **_RESPONSE_** in the **REPEATED** statement. For example, suppose you specify the following statements:

```

proc catmod;
  response marginals;
  model R11*R12*R21*R22=_response_ / design;
  repeated Time 2, Place 2 / _response_=Time Place;
run;

```

If each of the dependent variables has two levels, then PROC CATMOD builds four response functions. The **_RESPONSE_** effect generates a main-effects model with respect to Time and Place, and the design matrix is as follows:

Response Function Number	Variable	Time	Place	Design Matrix		
				Intercept	_RESPONSE_	
1	R11	1	1	1	1	1
2	R12	1	2	1	1	-1
3	R21	2	1	1	-1	1
4	R22	2	2	1	-1	-1

Log-Linear Model Design Matrices

When the response functions are the standard ones (generalized logits), then inclusion of the keyword `_RESPONSE_` in every design effect fits a log-linear model. The design matrix for a log-linear model looks different from a standard design matrix because the standard one is transformed by the same linear transformation that converts the r response probabilities to $r - 1$ generalized logits. For example, suppose the dependent variables X and Y each have two levels, and you specify a saturated log-linear model analysis:

```
proc catmod;
  model X*Y=_response_ / design;
  loglin X Y X*Y;
run;
```

Then the cross-classification of X and Y yields four response probabilities, p_{11} , p_{12} , p_{21} , and p_{22} , which are then reduced to three generalized logit response functions, $F_1 = \log(p_{11}/p_{22})$, $F_2 = \log(p_{12}/p_{22})$, and $F_3 = \log(p_{21}/p_{22})$.

Since the saturated log-linear model implies that

$$\begin{aligned} \begin{bmatrix} \log(p_{11}) \\ \log(p_{12}) \\ \log(p_{21}) \\ \log(p_{22}) \end{bmatrix} &= \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix} \boldsymbol{\gamma} - \lambda \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \\ &= \begin{bmatrix} 1 & 1 & 1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ -1 & -1 & 1 \end{bmatrix} \boldsymbol{\beta} - \delta \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \end{aligned}$$

where $\boldsymbol{\gamma}$ and $\boldsymbol{\beta}$ are parameter vectors, and λ and δ are normalizing constants required by the restriction that the probabilities sum to 1, it follows that the MODEL statement yields

$$\begin{aligned} \begin{bmatrix} F_1 \\ F_2 \\ F_3 \end{bmatrix} &= \begin{bmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & 0 & -1 \\ 0 & 0 & 1 & -1 \end{bmatrix} \times \begin{bmatrix} \log(p_{11}) \\ \log(p_{12}) \\ \log(p_{21}) \\ \log(p_{22}) \end{bmatrix} \\ &= \begin{bmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & 0 & -1 \\ 0 & 0 & 1 & -1 \end{bmatrix} \times \begin{bmatrix} 1 & 1 & 1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ -1 & -1 & 1 \end{bmatrix} \boldsymbol{\beta} \\ &= \begin{bmatrix} 2 & 2 & 0 \\ 2 & 0 & -2 \\ 0 & 2 & -2 \end{bmatrix} \boldsymbol{\beta} \end{aligned}$$

The design matrix is as follows:

Sample	Response Function Number	Design Matrix		
		X	Y	X*Y
1	1	2	2	0
1	2	2	0	-2
1	3	0	2	-2

Design matrices for reduced models are constructed similarly. For example, suppose you request a main-effects log-linear model analysis of the factors X and Y:

```
proc catmod;
  model X*Y=_response_ / design;
  loglin X Y;
run;
```

Since the main-effects log-linear model implies that

$$\begin{aligned} \begin{bmatrix} \log(p_{11}) \\ \log(p_{12}) \\ \log(p_{21}) \\ \log(p_{22}) \end{bmatrix} &= \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & -1 \\ 1 & -1 & 1 \\ 1 & -1 & -1 \end{bmatrix} \boldsymbol{\gamma} - \lambda \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \\ &= \begin{bmatrix} 1 & 1 \\ 1 & -1 \\ -1 & 1 \\ -1 & -1 \end{bmatrix} \boldsymbol{\beta} - \delta \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \end{aligned}$$

it follows that the MODEL statement yields

$$\begin{aligned} \begin{bmatrix} F_1 \\ F_2 \\ F_3 \end{bmatrix} &= \begin{bmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & 0 & -1 \\ 0 & 0 & 1 & -1 \end{bmatrix} \times \begin{bmatrix} \log(p_{11}) \\ \log(p_{12}) \\ \log(p_{21}) \\ \log(p_{22}) \end{bmatrix} \\ &= \begin{bmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & 0 & -1 \\ 0 & 0 & 1 & -1 \end{bmatrix} \times \begin{bmatrix} 1 & 1 \\ 1 & -1 \\ -1 & 1 \\ -1 & -1 \end{bmatrix} \boldsymbol{\beta} \\ &= \begin{bmatrix} 2 & 2 \\ 2 & 0 \\ 0 & 2 \end{bmatrix} \boldsymbol{\beta} \end{aligned}$$

Therefore, the corresponding design matrix is as follows:

Sample	Response	Design Matrix	
	Function Number	X	Y
1	1	2	2
1	2	2	0
1	3	0	2

Since it is difficult to tell from the final design matrix whether PROC CATMOD used the parameterization that you intended, the procedure displays the untransformed `_RESPONSE_` matrix for log-linear models. For example, specifying the main-effects model in the preceding example displays the following matrix:

Response	<code>_RESPONSE_</code> Matrix	
	Function Number	1
1	1	1
2	1	-1
3	-1	1
4	-1	-1

You can suppress the display of this matrix by specifying the `NORESPONSE` option in the MODEL statement.

Cautions

Effective Sample Size

Since the method depends on asymptotic approximations, you need to be careful that the sample sizes are sufficiently large to support the asymptotic normal distributions of the response functions. A general guideline is that you would like to have an effective sample size of at least 25 to 30 for each response function that is being analyzed. For example, if you have one dependent variable and $r = 4$ response levels, and you use the standard response functions to compute three generalized logits for each population, then you would like the sample size of each population to be at least 75. Moreover, the subjects should be dispersed throughout the table so that less than 20 percent of the response functions have an effective sample size less than 5. For example, if each population had less than 5 subjects in the first response category, then it would be wiser to pool this category with another category rather than to assume the asymptotic normality of the first response function. Or, if the dependent variable is ordinally scaled, an alternative is to request the mean score response function rather than three generalized logits.

If there is more than one dependent variable, and you specify **RESPONSE MEANS**, then the effective sample size for each response function is the same as the actual sample size. Thus, a sample size of 30 could be sufficient to support four response functions, provided that the functions are the means of four dependent variables.

A Singular Covariance Matrix

If there is a singular (noninvertible) covariance matrix for the response functions in any population, then PROC CATMOD writes an error message and stops processing. You have several options available to correct this problem:

- You can reduce the number of response functions according to how many can be supported by the populations with the smallest sample sizes.
- If there are three or more levels for any independent variable, you can pool the levels into a fewer number of categories, thereby reducing the number of populations. However, your interpretation of results must be done more cautiously since such pooling implies a different sampling scheme and masks any differences that existed among the pooled categories.
- If there are two or more independent variables, you can delete at least one of them from the model. However, this is just another form of pooling, and the same cautions that apply to the previous option also apply here.
- If there is one independent variable, then, in some situations, you might simply eliminate the populations that are causing the covariance matrices to be singular.
- You can use the **ADDCELL=** option in the MODEL statement to add a small amount (for example, 0.5) to every cell frequency, but this can seriously bias the results if the cell frequencies are small.

Zero Frequencies

There are two types of zero cells in a contingency table: structural and sampling. A structural zero cell has an expected value of zero, while a sampling zero cell can have nonzero expected value and can be estimable.

If you use the standard response functions and there are zero frequencies, you should use maximum likelihood estimation (the default is `ML=NR`) rather than weighted least squares to analyze the data. For weighted least squares analysis, the `CATMOD` procedure always computes the observed response functions and might need to take the logarithm of a zero proportion. In this case, `PROC CATMOD` issues a warning and then takes the log of a small value ($0.5/n_i$ for the probability) in order to continue, but this can produce invalid results if the cells contain too few observations. Maximum likelihood analysis, on the other hand, does not require computation of the observed response functions and therefore yields valid results for the parameter estimates and all of the predicted values.

For a log-linear model analysis with `WLS` or `ML=NR`, `PROC CATMOD` creates response profiles only for the observed profiles. For any log-linear model analysis with one population (the usual case), the contingency table does not contain zeros, which means that all zero frequencies are treated as structural zeros. If there is more than one population, then a zero in the body of the contingency table is treated as a sampling zero (as long as some population has a nonzero count for that profile). If you fit the log-linear model by using `ML=IPF`, the contingency table is incomplete and the zeros are treated like structural zeros. If you want zero frequencies that `PROC CATMOD` would normally treat as structural zeros to be interpreted as sampling zeros, you can specify the `ZERO=SAMPLING` and `MISSING=SAMPLING` options in the `MODEL` statement. Alternatively, you can specify `ZERO=1E-20` and `MISSING=1E-20`.

See Bishop, Fienberg, and Holland (1975) for a discussion of the issues and [Example 30.5](#) for an illustration of a log-linear model analysis of data that contain both structural and sampling zeros.

If you perform a weighted least squares analysis on a contingency table that contains zero cell frequencies, then avoid using the `LOG` transformation as the first transformation on the observed proportions. In general, it is better to change the response functions or to pool some of the response categories than to settle for the 0.5 correction or to use the `ADDCELL=` option.

Testing the Wrong Hypothesis

If you use the keyword `_RESPONSE_` in the `MODEL` statement, and you specify `MARGINALS`, `LOGITS`, `ALOGITS`, or `CLOGITS` in your `RESPONSE` statement, you might receive the following warning message:

```
Warning: The _RESPONSE_ effect may be testing the wrong
         hypothesis since the marginal levels of the
         dependent variables do not coincide. Consult the
         response profiles and the CATMOD documentation.
```

The following examples illustrate situations in which the `_RESPONSE_` effect tests the wrong hypothesis.

Zeros in the Marginal Frequencies

Suppose you specify the following statements:

```

data A1;
  input Time1 Time2 @@;
  datalines;
1 2    2 3    1 3
;

proc catmod;
  response marginals;
  model Time1*Time2=_response_;
  repeated Time 2 / _response_=Time;
run;

```

One marginal probability is computed for each dependent variable, resulting in two response functions. The model is a saturated one: one degree of freedom for the intercept and one for the main effect of Time. Except for the warning message, PROC CATMOD produces an analysis with no apparent errors, but the “Response Profiles” table displayed by PROC CATMOD is as follows:

Response Profiles		
Response	Time1	Time2
1	1	2
2	1	3
3	2	3

Since **RESPONSE MARGINALS** yields marginal probabilities for every level but the last, the two response functions being analyzed are $\text{Prob}(\text{Time1}=1)$ and $\text{Prob}(\text{Time2}=2)$. The Time effect is testing the hypothesis that $\text{Prob}(\text{Time1}=1)=\text{Prob}(\text{Time2}=2)$. What it *should* be testing is the hypothesis that

```

Prob(Time1=1) = Prob(Time2=1)
Prob(Time1=2) = Prob(Time2=2)
Prob(Time1=3) = Prob(Time2=3)

```

but there are not enough data to support the test (assuming that none of the probabilities are structural zeros by the design of the study).

The ORDER=DATA Option

Suppose you specify the following statements:

```

data a1;
  input Time1 Time2 @@;
  datalines;
2 1    2 2    1 1    1 2    2 1
;

proc catmod order=data;
  response marginals;
  model Time1*Time2=_response_;
  repeated Time 2 / _response_=Time;
run;

```

As in the preceding example, one marginal probability is computed for each dependent variable, resulting in two response functions. The model is also the same: one degree of freedom for the intercept and one for the main effect of Time. PROC CATMOD issues the warning message and displays the following “Response Profiles” table:

Response Profiles		
Response	Time1	Time2
1	2	1
2	2	2
3	1	1
4	1	2

Although the marginal levels are the same for the two dependent variables, they are not in the same order because the `ORDER=DATA` option specified that they be ordered according to their appearance in the input stream. Since `RESPONSE MARGINALS` yields marginal probabilities for every level except the last, the two response functions being analyzed are $\text{Prob}(\text{Time1}=2)$ and $\text{Prob}(\text{Time2}=1)$. The Time effect is testing the hypothesis that $\text{Prob}(\text{Time1}=2)=\text{Prob}(\text{Time2}=1)$. What it *should* be testing is the hypothesis that

$$\begin{aligned} \text{Prob}(\text{Time1}=1) &= \text{Prob}(\text{Time2}=1) \\ \text{Prob}(\text{Time1}=2) &= \text{Prob}(\text{Time2}=2) \end{aligned}$$

Whenever the warning message appears, look at the “Response Profiles” table or the “One-Way Frequencies” table to determine what hypothesis is actually being tested. For the latter example, a correct analysis can be obtained by deleting the `ORDER=DATA` option or by reordering the data so that the (1,1) observation is first.

Computational Method

The notation used in PROC CATMOD differs slightly from that used in the literature. The following table provides a summary of the basic dimensions and the notation for a contingency table. See the section “Computational Formulas” on page 1846 for a complete description.

Summary of Basic Dimensions

- s = number of populations or samples (= number of rows in the underlying contingency table)
- r = number of response categories (= number of columns in the underlying contingency table)
- q = number of response functions computed for each population
- d = number of parameters

Notation

- \mathbf{j} Denotes a column vector of 1s.
- \mathbf{J} Denotes a square matrix of 1s.
- \sum_k Denotes the sum over all the possible values of k .
- n_i Denotes the row sum $\sum_j n_{ij}$.
- $\text{DIAG}_n(\mathbf{p})$ Denotes the diagonal matrix formed from the first n elements of the vector \mathbf{p} .
- $\text{DIAG}_n^{-1}(\mathbf{p})$ Denotes the inverse of $\text{DIAG}_n(\mathbf{p})$.
- $\text{DIAG}(\mathbf{A}_1, \mathbf{A}_2, \dots, \mathbf{A}_k)$ Denotes a block diagonal matrix with the \mathbf{A} matrices on the main diagonal.

Input data can be represented by a contingency table, as shown in Table 30.7.

Table 30.7 Input Data Represented by a Contingency Table

Population	Response				Total
	1	2	...	r	
1	n_{11}	n_{12}	...	n_{1r}	n_1
2	n_{21}	n_{22}	...	n_{2r}	n_2
\vdots	\vdots	\vdots	\ddots	\vdots	\vdots
s	n_{s1}	n_{s2}	...	n_{sr}	n_s

Computational Formulas

The following formulas are shown for each population and for all populations combined.

Source	Formula	Dimension
Probability Estimates		
jth response	$p_{ij} = \frac{n_{ij}}{n_i}$	1×1
ith population	$\mathbf{p}_i = \begin{bmatrix} p_{i1} \\ p_{i2} \\ \vdots \\ p_{ir} \end{bmatrix}$	$r \times 1$
all populations	$\mathbf{p} = \begin{bmatrix} \mathbf{p}_1 \\ \mathbf{p}_2 \\ \vdots \\ \mathbf{p}_s \end{bmatrix}$	$sr \times 1$

Source	Formula	Dimension
Variance of Probability Estimates		
<i>i</i> th population	$V_i = \frac{1}{n_i}(\text{DIAG}(\mathbf{p}_i) - \mathbf{p}_i\mathbf{p}_i')$	$r \times r$
all populations	$V = \text{DIAG}(V_1, V_2, \dots, V_s)$	$sr \times sr$
Response Functions		
<i>i</i> th population	$F_i = F(\mathbf{p}_i)$	$q \times 1$
all populations	$F = \begin{bmatrix} F_1 \\ F_2 \\ \vdots \\ F_s \end{bmatrix}$	$sq \times 1$
Derivative of Function with Respect to Probability Estimates		
<i>i</i> th population	$H_i = \frac{\partial F(\mathbf{p}_i)}{\partial \mathbf{p}_i}$	$q \times r$
all populations	$H = \text{DIAG}(H_1, H_2, \dots, H_s)$	$sq \times sr$
Variance of Functions		
<i>i</i> th population	$S_i = H_i V_i H_i'$	$q \times q$
all populations	$S = \text{DIAG}(S_1, S_2, \dots, S_s)$	$sq \times sq$
Inverse Variance of Functions		
<i>i</i> th population	$S^i = (S_i)^{-1}$	$q \times q$
all populations	$S^{-1} = \text{DIAG}(S^1, S^2, \dots, S^s)$	$sq \times sq$

Derivative Table for Compound Functions: Y=F(G(p))

In the following table, let $G(\mathbf{p})$ be a vector of functions of \mathbf{p} , and let D denote $\partial G/\partial \mathbf{p}$, which is the first derivative matrix of G with respect to \mathbf{p} :

Function	$Y = F(G)$	Derivative ($\partial Y/\partial \mathbf{p}$)
Multiply matrix	$Y = A * G$	$A * D$
Logarithm	$Y = \text{LOG}(G)$	$\text{DIAG}^{-1}(G) * D$
Exponential	$Y = \text{EXP}(G)$	$\text{DIAG}(Y) * D$
Add constant	$Y = G + A$	D

Default Response Functions: Generalized Logits

In the following table, subscripts i for the population are suppressed. Also denote $f_j = \log\left(\frac{p_j}{p_r}\right)$ for $j = 1, \dots, r - 1$ for each population $i = 1, \dots, s$.

Formula
Inverse of Response Functions for a Population
$p_j = \frac{\exp(f_j)}{1 + \sum_k \exp(f_k)} \text{ for } j = 1, \dots, r - 1$
$p_r = \frac{1}{1 + \sum_k \exp(f_k)}$
Form of F and Derivative for a Population
$\mathbf{F} = \mathbf{KLOG}(\mathbf{p}) = (\mathbf{I}_{r-1}, -\mathbf{j}) \mathbf{LOG}(\mathbf{p})$
$\mathbf{H} = \frac{\partial \mathbf{F}}{\partial \mathbf{p}} = \left(\mathbf{DIAG}_{r-1}^{-1}(\mathbf{p}), \frac{-1}{p_r} \mathbf{j} \right)$
Covariance Results for a Population
$\mathbf{S} = \mathbf{H}\mathbf{V}\mathbf{H}'$
$= \frac{1}{n} \left(\mathbf{DIAG}_{r-1}^{-1}(\mathbf{p}) + \frac{1}{p_r} \mathbf{J}_{r-1} \right)$
where \mathbf{V} , \mathbf{H} , and \mathbf{J} are as previously defined.
$\mathbf{S}^{-1} = n(\mathbf{DIAG}_{r-1}(\mathbf{p}) - \mathbf{q}\mathbf{q}') \text{ , where } \mathbf{q} = \mathbf{DIAG}_{r-1}(\mathbf{p}) \mathbf{j}$
$\mathbf{S}^{-1}\mathbf{F} = n\mathbf{DIAG}_{r-1}(\mathbf{p})\mathbf{F} - (n \sum_j p_j f_j) \mathbf{q}$
$\mathbf{F}'\mathbf{S}^{-1}\mathbf{F} = n \sum_j p_j f_j^2 - n \left(\sum_j p_j f_j \right)^2$

The following calculations are shown for each population and then for all populations combined:

Source	Formula	Dimension
Design Matrix		
ith population	\mathbf{X}_i	$q \times d$
all populations	$\mathbf{X} = \begin{bmatrix} \mathbf{X}_1 \\ \mathbf{X}_2 \\ \vdots \\ \mathbf{X}_s \end{bmatrix}$	$sq \times d$

Source	Formula	Dimension
Crossproduct of Design Matrix		
<i>i</i> th population	$C_i = \mathbf{X}_i' \mathbf{S}^i \mathbf{X}_i$	$d \times d$
all populations	$\mathbf{C} = \mathbf{X}' \mathbf{S}^{-1} \mathbf{X} = \sum_i C_i$	$d \times d$

In the following table, z_p is the 100 p th percentile of the standard normal distribution:

Formula	Dimension
Crossproduct of Design Matrix with Function	
$\mathbf{R} = \mathbf{X}' \mathbf{S}^{-1} \mathbf{F} = \sum_i \mathbf{X}_i' \mathbf{S}^i \mathbf{F}_i$	$d \times 1$
Weighted Least Squares Estimates	
$\mathbf{b} = \mathbf{C}^{-1} \mathbf{R} = (\mathbf{X}' \mathbf{S}^{-1} \mathbf{X})^{-1} (\mathbf{X}' \mathbf{S}^{-1} \mathbf{F})$	$d \times 1$
Covariance of Weighted Least Squares Estimates	
$\text{COV}(\mathbf{b}) = \mathbf{C}^{-1}$	$d \times d$
Wald Confidence Limits for Parameter Estimates	
$b_k \pm z_{1-\alpha/2} C_{kk}^{-1}$	$k = 1, \dots, d$
Predicted Response Functions	
$\hat{\mathbf{F}} = \mathbf{X} \mathbf{b}$	$sq \times 1$
Covariance of Predicted Response Functions	
$\mathbf{V}_{\hat{\mathbf{F}}} = \mathbf{X} \mathbf{C}^{-1} \mathbf{X}'$	$sq \times sq$
Residual Chi-Square	
$\text{RSS} = \mathbf{F}' \mathbf{S}^{-1} \mathbf{F} - \hat{\mathbf{F}}' \mathbf{S}^{-1} \hat{\mathbf{F}}$	1×1
Chi-Square for $H_0: \mathbf{L} \boldsymbol{\beta} = 0$	
$\mathbf{Q} = (\mathbf{L} \mathbf{b})' (\mathbf{L} \mathbf{C}^{-1} \mathbf{L}')^{-1} (\mathbf{L} \mathbf{b})$	1×1

Maximum Likelihood Method

Let \mathbf{C} be the Hessian matrix and \mathbf{G} be the gradient of the log-likelihood function (both functions of $\boldsymbol{\pi}$ and the parameters $\boldsymbol{\beta}$). Let \mathbf{p}_i^* denote the vector containing the first $r - 1$ sample proportions from population i , and let $\boldsymbol{\pi}_i^*$ denote the corresponding vector of probability estimates from the current iteration. Starting with the least squares estimates \mathbf{b}_0 of $\boldsymbol{\beta}$ (if you use the **ML** and **WLS** options; with the **ML** option alone, the procedure starts with $\mathbf{0}$), the probabilities $\boldsymbol{\pi}(\mathbf{b})$ are computed, and \mathbf{b} is calculated iteratively by the Newton-Raphson method until it converges (see the **EPSILON=** option). The factor λ is a step-halving factor that equals one at the start of each iteration. For any iteration in which the likelihood decreases, PROC CATMOD uses a series of subiterations in which λ is iteratively divided by two. The subiterations continue until the likelihood is greater than that of the previous iteration. If the likelihood has not reached that point after 10 subiterations, then convergence is assumed, and a warning message is displayed.

Sometimes, infinite parameters are present in the model, either because of the presence of one or more zero frequencies or because of a poorly specified model with collinearity among the estimates. If an estimate is tending toward infinity, then PROC CATMOD flags the parameter as infinite and holds the estimate fixed in subsequent iterations. PROC CATMOD regards a parameter to be infinite when two conditions apply:

- The absolute value of its estimate exceeds five divided by the range of the corresponding variable.
- The standard error of its estimate is at least three times greater than the estimate itself.

The estimator of the asymptotic covariance matrix of the maximum likelihood predicted probabilities is given by Imrey, Koch, and Stokes (1981, eq. 2.18).

The following equations summarize the method:

$$\mathbf{b}_{k+1} = \mathbf{b}_k - \lambda \mathbf{C}^{-1} \mathbf{G}$$

where

$$\mathbf{C} = \mathbf{X}'\mathbf{S}^{-1}(\boldsymbol{\pi})\mathbf{X}$$

$$\mathbf{N} = \begin{bmatrix} n_1(\mathbf{p}_1^* - \boldsymbol{\pi}_1^*) \\ \vdots \\ n_s(\mathbf{p}_s^* - \boldsymbol{\pi}_s^*) \end{bmatrix}$$

$$\mathbf{G} = \mathbf{X}'\mathbf{N}$$

Iterative Proportional Fitting

The algorithm used by PROC CATMOD for iterative proportional fitting is described in Bishop, Fienberg, and Holland (1975); Haberman (1972); Agresti (2002). To illustrate the method, consider the observed three-dimensional table $\{n_{ijk}\}$ for the variables X , Y , and Z , and the following hierarchical model:

$$\log(m_{ijk}) = \mu + \lambda_i^X + \lambda_j^Y + \lambda_k^Z + \lambda_{ij}^{XY} + \lambda_{ik}^{XZ} + \lambda_{jk}^{YZ}$$

The following statements request that PROC CATMOD use IPF to fit the preceding model:

```

model X*Y*Z = _response_ / ml=ipf;
loglin X|Y|Z@2;

```

Begin with a table of initial cell estimates $\{\hat{m}_{ijk}^{(0)}\}$. PROC CATMOD produces the initial estimates by setting the n_{sz} structural zero cells to 0 and all other cells to $n/(n_c - n_{sz})$, where n is the total weight of the table and n_c is the total number of cells in the table. Iteratively adjust the estimates at step $s - 1$ to the observed marginal tables specified in the model by cycling through the following three-stage process to produce the estimates at step s :

$$\begin{aligned} \hat{m}_{ijk}^{(s_1)} &= \hat{m}_{ijk}^{(s-1)} \frac{n_{ij\cdot}}{\hat{m}_{ij\cdot}^{(s-1)}} \\ \hat{m}_{ijk}^{(s_2)} &= \hat{m}_{ijk}^{(s_1)} \frac{n_{i\cdot k}}{\hat{m}_{i\cdot k}^{(s_1)}} \\ \hat{m}_{ijk}^{(s)} &= \hat{m}_{ijk}^{(s_2)} \frac{n_{\cdot jk}}{\hat{m}_{\cdot jk}^{(s_2)}} \end{aligned}$$

The subscript “.” indicates summation over the missing subscript. The log-likelihood l_s is estimated at each step s by

$$l_s = \sum_{i,j,k} n_{ijk} \log \left(\frac{\hat{m}_{ijk}^{(s)}}{n} \right)$$

When the function $|(l_{s-1} - l_s)/l_{s-1}|$ is less than 10^{-8} , the iterations terminate. You can change the comparison value with the **EPSILON=** option, and you can change the convergence criterion with the **CONVCRT=** option. The option **CONVCRT=CELL** uses the maximum cell difference

$$\max_{i,j,k} |\hat{m}_{ijk}^{(s-1)} - \hat{m}_{ijk}^{(s)}|$$

as the criterion while the option **CONVCRT=MARGIN** computes the maximum difference of the margins

$$\text{Maximum of } \left\{ \max_{i,j} |\hat{m}_{ij\cdot}^{(s-1)} - \hat{m}_{ij\cdot}^{(s)}|, \max_{i,k} |\hat{m}_{i\cdot k}^{(s-1)} - \hat{m}_{i\cdot k}^{(s)}|, \max_{j,k} |\hat{m}_{\cdot jk}^{(s-1)} - \hat{m}_{\cdot jk}^{(s)}| \right\}$$

Memory and Time Requirements

The memory and time required by PROC CATMOD are proportional to the number of parameters in the model.

Displayed Output

PROC CATMOD displays the following information in the “Data Summary” table:

- the response effect
- the weight variable, if one is specified
- the data set name
- the number of response levels
- the number of samples or populations
- the total frequency, which is the total sample size
- the number of observations from the data set (the number of data records)
- the frequency of missing observations, labeled as “Frequency Missing”

Except for the analysis of variance table, all of the following items can be displayed or suppressed, depending on your specification of statements and options.

- The **ONEWAY** option produces the “One-Way Frequencies” table, which displays the frequencies of each variable value used in the analysis.
- The populations (or samples) are defined in a table labeled “Population Profiles.” The sample size and the values of the defining variables are displayed for each sample. This table is suppressed if the **NOPROFILE** option is specified.
- The observed responses are defined in a table labeled “Response Profiles.” The values of the defining variables are displayed for each response. This table is suppressed if the **NOPROFILE** option is specified.
- If the **FREQ** option is specified, then the “Response Frequencies” table is displayed, which shows the frequency of each response for each population.
- If the **PROB** option is specified, then the “Response Probabilities” table is produced. This table displays the probability of each response for each population.
- If the **COV** option is specified, the “Response Functions, Covariance Matrix” table, which shows the covariance matrix of the response functions for each sample, is displayed.
- If the **DESIGN** option is specified, the response functions are displayed in the “Response Functions, Design Matrix” table. If the **COV** option is also specified, the response functions are displayed in the “Response Functions, Covariance Matrix” table.
- If the **DESIGN** option is specified, the design matrix is displayed in the “Response Functions, Design Matrix” table, and if a log-linear model is being fit, the `_RESPONSE_` matrix is displayed in the “`_Response_ Matrix`” table. If the model type is **AVERAGED**, then the design matrix is displayed with $q * s$ rows, assuming q response functions for each of s populations. Otherwise, the design matrix is displayed with only s rows since the model is the same for each of the q response functions.

- The “ $X' \text{Inv}(S) X$ ” matrix is displayed for weighted least squares analyses if the **XPX** option is specified.
- The “Analysis of Variance” table for the weighted least squares analysis reports the results of significance tests for each of the *design-effects* on the right side of the MODEL statement. If **_RESPONSE_** is a *design-effect* and is defined explicitly in the **LOGLIN**, **FACTORS**, or **REPEATED** statement, then the table contains test statistics for the individual effects constituting the **_RESPONSE_** effect. If the design matrix is input directly, then the content of the displayed output depends on whether you specify any subsets of the parameters to be tested. If you specify one or more subsets, then the table contains one test for each subset. Otherwise, the table contains one test for the effect **MODEL | MEAN**. In every case, the table also contains the residual goodness-of-fit test. Produced for each test of significance are the source of variation, the number of degrees of freedom (DF), the Wald chi-square value, and the significance probability ($\text{Pr} > \text{ChiSq}$).

- The “Analysis of Weighted Least Squares Estimates” table lists, for each parameter in the model, the least squares estimate, the estimated standard error of the parameter estimate, the Wald chi-square value (calculated as $((\text{parameter estimate})/(\text{standard error}))^2$) for testing that the parameter is zero, and the significance probability ($\text{Pr} > \text{ChiSq}$) of the test. If the **CLPARM** option is specified, then 95% Wald confidence intervals are displayed.

Each row in the table is labeled with the parameter (the model effect and the class levels) and the response function number; however, if the **NOPREDVAR** option or a **REPEATED** or **FACTORS** statement is specified or if the design matrix is directly input, the rows are labeled by the effect in the model for which parameters are formed and the parameter number.

- The “Covariance Matrix of the Parameter Estimates” table for the weighted least squares analysis displays the estimated covariance matrix of the least squares estimates of the parameters, provided that the **COVB** option is specified.
- The “Correlation Matrix of the Parameter Estimates” table for the weighted least squares analysis displays the estimated correlation matrix of the least squares estimates of the parameters, provided that the **CORRB** option is specified.
- The “Maximum Likelihood Analysis” table is produced when the **ML** and **ITPRINT** options are specified for the standard response functions. It displays the iteration number, the number of step-halving sub-iterations, $-2 \log$ likelihood for that iteration, the convergence criterion, and the parameter estimates for each iteration.
- The “Maximum Likelihood Analysis of Variance” table, displayed when the **ML** option is specified for the standard response functions, is similar to the table produced for the least squares analysis. The Wald chi-square test for each effect is based on the information matrix from the likelihood calculations. The likelihood ratio statistic compares the specified model with the unrestricted (saturated) model and is an appropriate goodness-of-fit test for the model.
- The “Analysis of Maximum Likelihood Estimates” table, displayed when the **ML** option is specified for the standard response functions, is similar to the one produced for the least squares analysis. The table includes the maximum likelihood estimates, the estimated standard errors based on the information matrix, and the Wald chi-square statistics based on estimated standard errors.
- The “Covariance Matrix of the Maximum Likelihood Estimates” table displays the estimated covariance matrix of the maximum likelihood estimates of the parameters, provided that the **COVB** and **ML** options are specified for the standard response functions.

- The “Correlation Matrix of the Maximum Likelihood Estimates” table displays the estimated correlation matrix of the maximum likelihood estimates of the parameters, provided that the **CORRB** and **ML** options are specified for the standard response functions.
- For each source of variation specified in a **CONTRAST** statement, the “Contrasts” table lists the label for the source (Contrast), the number of degrees of freedom (DF), the Wald chi-square value, and the significance probability ($\text{Pr} > \text{ChiSq}$). If the **ESTIMATE=** option is specified, the “Analysis of Contrasts” table displays, for each row of the contrast, the label (Contrast), the type (PARM or EXP), the row of the contrast, the estimate and its standard error, a Wald confidence interval, the Wald chi-square, and the p -value ($\text{Pr} > \text{ChiSq}$) for 1 degree of freedom.
- Specification of the **PREDICT** option in the MODEL statement has the following effect. Produced for each response function within each population are the observed and predicted function values, their standard errors, and the residual (observed minus predicted). If the response functions are the default ones (generalized logits), additional information displayed for each response within each population includes the observed and predicted cell probabilities, their standard errors, and the residual. However, specifying **PRED=FREQ** in the MODEL statement results in the display of the predicted cell frequencies rather than the predicted cell probabilities. The displayed output includes the population profiles and, for the response function table, the function number, while the probability and frequency tables display the response profiles. If the **NOPREDVAR** option is specified in the MODEL statement, the population profiles are replaced with the sample numbers, and the response profiles are replaced with the labels “ P_n ” for the n th cell probability, and “ F_n ” for the n th cell frequency.
- When there are multiple **RESPONSE** statements, the output for each statement starts on a new page. For each **RESPONSE** statement, the corresponding title, if specified, is displayed at the top of each page.
- If the **ADDCELL=** option is specified in the MODEL statement, and if there is a weighted least squares analysis specified, the adjusted sample size for each population (with number added to each cell) is labeled “Adjusted Sample Size” in the “Population Profiles” table. Similarly, the adjusted response frequencies and probabilities are displayed in the “Adjusted Response Frequencies” and “Adjusted Response Probabilities” tables, respectively.
- If **_RESPONSE_** is defined explicitly in the **LOGLIN**, **FACTORS**, or **REPEATED** statement, then the definition is displayed as a note whenever **_RESPONSE_** appears in the output.

ODS Table Names

PROC CATMOD assigns a name to each table it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in the following table. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

Table 30.12 ODS Tables Produced by PROC CATMOD

ODS Table Name	Description	Statement	Option
ANOVA	Analysis of variance	MODEL	default
Contrasts	Contrasts	CONTRAST	default
ContrastEstimates	Analysis of contrasts	CONTRAST	ESTIMATE=
ConvergenceStatus	Convergence status	MODEL	ML
CorrB	Correlation matrix of the estimates	MODEL	CORRB
CovB	Covariance matrix of the estimates	MODEL	COVB
DataSummary	Data summary	PROC	default
Estimates	Analysis of estimates	MODEL	default, unless NOPARM
MaxLikelihood	Maximum likelihood analysis	MODEL	ML and ITPRINT
OneWayFreqs	One-way frequencies	MODEL	ONEWAY
PopProfiles	Population profiles	MODEL	default, unless NOPROFILE
PredictedFreqs	Predicted frequencies	MODEL	PRED=FREQ
PredictedProbs	Predicted probabilities	MODEL	PREDICT or PRED=PROB
PredictedValues	Predicted values	MODEL	PREDICT or PRED=
ResponseCov	Response functions, covariance matrix	MODEL	COV
ResponseDesign	Response functions, design matrix	MODEL	DESIGN, unless NODESIGN
ResponseFreqs	Response frequencies	MODEL	FREQ
ResponseMatrix	_RESPONSE_ matrix	MODEL and LOGLIN	DESIGN, unless NORESPONSE
ResponseProbs	Response probabilities	MODEL	PROB
ResponseProfiles	Response profiles	MODEL	default, unless NOPROFILE
XPX	$\mathbf{X}' * \text{Inv}(\mathbf{S}) * \mathbf{X}$ matrix	MODEL	XPX, for WLS*

* WLS estimation is the default for response functions other than the default (generalized logits).

Examples: CATMOD Procedure

Example 30.1: Linear Response Function, $r=2$ Responses

In an example from Ries and Smith (1963), the choice of detergent brand (Brand = M or X) is related to three other categorical variables: the softness of the laundry water (Softness = soft, medium, or hard), the temperature of the water (Temperature = high or low), and whether the subject was a previous user of Brand M (Previous = yes or no). The linear response function, which could also be specified as **RESPONSE MARGINALS**, yields one probability, $\text{Pr}(\text{brand preference}=\text{M})$, as the response function to be analyzed. Two models are fit in this example: the first model is a saturated one, containing all of the main effects and interactions, while the second is a reduced model containing only the main effects. The following statements produce [Output 30.1.1](#) through [Output 30.1.4](#):

```
data detergent;
  input Softness $ Brand $ Previous $ Temperature $ Count @@;
  datalines;
soft X yes high 19    soft X yes low 57
soft X no high 29     soft X no low 63
soft M yes high 29    soft M yes low 49
soft M no high 27     soft M no low 53
med X yes high 23     med X yes low 47
med X no high 33      med X no low 66
med M yes high 47     med M yes low 55
med M no high 23      med M no low 50
hard X yes high 24    hard X yes low 37
hard X no high 42     hard X no low 68
hard M yes high 43    hard M yes low 52
hard M no high 30     hard M no low 42
;

title 'Detergent Preference Study';
proc catmod data=detergent;
  response 1 0;
  weight Count;
  model Brand=Softness|Previous|Temperature / freq prob;
  title2 'Saturated Model';
run;
```

The “Data Summary” table ([Output 30.1.1](#)) indicates that you have two response levels and twelve populations.

Output 30.1.1 Detergent Preference Study: Linear Model Analysis

Detergent Preference Study			
Saturated Model			
The CATMOD Procedure			
Data Summary			
Response	Brand	Response Levels	2
Weight Variable	Count	Populations	12
Data Set	DETERGENT	Total Frequency	1008
Frequency Missing	0	Observations	24

The “Population Profiles” table in [Output 30.1.2](#) displays the ordering of independent variable levels as used in the table of parameter estimates.

Output 30.1.2 Population Profiles

Population Profiles				
Sample	Softness	Previous	Temperature	Sample Size
1	hard	no	high	72
2	hard	no	low	110
3	hard	yes	high	67
4	hard	yes	low	89
5	med	no	high	56
6	med	no	low	116
7	med	yes	high	70
8	med	yes	low	102
9	soft	no	high	56
10	soft	no	low	116
11	soft	yes	high	48
12	soft	yes	low	106

Since Brand M is the first level in the “Response Profiles” table ([Output 30.1.3](#)), the `RESPONSE` statement causes $\text{Pr}(\text{Brand}=\text{M})$ to be the single response function modeled.

Output 30.1.3 Response Profiles, Frequencies, and Probabilities

Response Profiles	
Response	Brand
1	M
2	X

Output 30.1.3 *continued*

Response Frequencies		
Sample	Response Number	
	1	2
1	30	42
2	42	68
3	43	24
4	52	37
5	23	33
6	50	66
7	47	23
8	55	47
9	27	29
10	53	63
11	29	19
12	49	57

Response Probabilities		
Sample	Response Number	
	1	2
1	0.41667	0.58333
2	0.38182	0.61818
3	0.64179	0.35821
4	0.58427	0.41573
5	0.41071	0.58929
6	0.43103	0.56897
7	0.67143	0.32857
8	0.53922	0.46078
9	0.48214	0.51786
10	0.45690	0.54310
11	0.60417	0.39583
12	0.46226	0.53774

The “Analysis of Variance” table in [Output 30.1.4](#) shows that all of the interactions are nonsignificant.

Output 30.1.4 Analysis of Variance

Analysis of Variance			
Source	DF	Chi-Square	Pr > ChiSq
Intercept	1	983.13	<.0001
Softness	2	0.09	0.9575
Previous	1	22.68	<.0001
Softness*Previous	2	3.85	0.1457
Temperature	1	3.67	0.0555
Softness*Temperature	2	0.23	0.8914
Previous*Temperature	1	2.26	0.1324
Softnes*Previou*Temperat	2	0.76	0.6850
Residual	0	.	.

Therefore, a main-effects model is fit with the following statements:

```

model Brand=Softness Previous Temperature
      / clparm noprofile design;
title2 'Main-Effects Model';
run;
quit;

```

The PROC CATMOD statement is not required due to the interactive capability of the CATMOD procedure. The NOPROFILE option suppresses the redisplay of the “Response Profiles” table. The CLPARM option produces 95% confidence limits for the parameter estimates. Output 30.1.5 through Output 30.1.7 are produced.

The design matrix in Output 30.1.5 displays the results of the differential-effects modeling used in PROC CATMOD.

Output 30.1.5 Main-Effects Design Matrix

Detergent Preference Study			
Main-Effects Model			
The CATMOD Procedure			
Data Summary			
Response	Brand	Response Levels	2
Weight Variable	Count	Populations	12
Data Set	DETERGENT	Total Frequency	1008
Frequency Missing	0	Observations	24

Output 30.1.5 continued

Response Functions and Design Matrix						
Sample	Response Function	Design Matrix				
		1	2	3	4	5
1	0.41667	1	1	0	1	1
2	0.38182	1	1	0	1	-1
3	0.64179	1	1	0	-1	1
4	0.58427	1	1	0	-1	-1
5	0.41071	1	0	1	1	1
6	0.43103	1	0	1	1	-1
7	0.67143	1	0	1	-1	1
8	0.53922	1	0	1	-1	-1
9	0.48214	1	-1	-1	1	1
10	0.45690	1	-1	-1	1	-1
11	0.60417	1	-1	-1	-1	1
12	0.46226	1	-1	-1	-1	-1

The analysis of variance table in [Output 30.1.6](#) shows that previous use of Brand M, together with the temperature of the laundry water, is a significant factor in whether a subject prefers Brand M laundry detergent. The table also shows that the additive model fits since the goodness-of-fit statistic (the residual chi-square) is nonsignificant.

Output 30.1.6 ANOVA Table for the Main-Effects Model

Analysis of Variance			
Source	DF	Chi-Square	Pr > ChiSq
Intercept	1	1004.93	<.0001
Softness	2	0.24	0.8859
Previous	1	20.96	<.0001
Temperature	1	3.95	0.0468
Residual	7	8.26	0.3100

The chi-square test in [Output 30.1.7](#) shows that the Softness parameters are not significantly different from zero; as expected, the Wald confidence limits for these two estimates contain zero. So softness of the water is not a factor in choosing Brand M.

Output 30.1.7 WLS Estimates for the Main-Effects Model

Analysis of Weighted Least Squares Estimates						
Parameter		Estimate	Standard Error	Chi-Square	Pr > ChiSq	95% Confidence Limits
Intercept		0.5080	0.0160	1004.93	<.0001	0.4766 0.5394
Softness	hard	-0.00256	0.0218	0.01	0.9066	-0.0454 0.0402
	med	0.0104	0.0218	0.23	0.6342	-0.0323 0.0530
Previous	no	-0.0711	0.0155	20.96	<.0001	-0.1015 -0.0407
Temperature	high	0.0319	0.0161	3.95	0.0468	0.000446 0.0634

The negative coefficient for Previous (-0.0711) indicates that the first level of Previous (which is shown to be ‘no’) is associated with a smaller probability of preferring Brand M than the second level of Previous (with coefficient constrained to be 0.0711 since the parameter estimates for a given effect must sum to zero). In other words, previous users of Brand M are much more likely to prefer it than those who have never used it before.

Similarly, the positive coefficient for Temperature indicates that the first level of Temperature (which, from the “Population Profiles” table, is ‘high’) has a larger probability of preferring Brand M than the second level of Temperature. In other words, those who do their laundry in hot water are more likely to prefer Brand M than those who do their laundry in cold water.

Example 30.2: Mean Score Response Function, r=3 Responses

Four surgical operations for duodenal ulcers are compared in a clinical trial at four hospitals. The operations performed are as follows: Treatment = a, drainage and vagotomy; Treatment = b, 25% resection and vagotomy; Treatment = c, 50% resection and vagotomy; and Treatment = d, 75% resection. The response is severity of an undesirable complication called “dumping syndrome.” The data in the following statements are from Grizzle, Starmer, and Koch (1969, pp. 489–504).

```
data operate;
  input Hospital Treatment $ Severity $ wt @@;
  datalines;
1 a none 23    1 a slight 7    1 a moderate 2
1 b none 23    1 b slight 10   1 b moderate 5
1 c none 20    1 c slight 13   1 c moderate 5
1 d none 24    1 d slight 10   1 d moderate 6
2 a none 18    2 a slight 6    2 a moderate 1
2 b none 18    2 b slight 6    2 b moderate 2
2 c none 13    2 c slight 13   2 c moderate 2
2 d none 9     2 d slight 15   2 d moderate 2
3 a none 8     3 a slight 6    3 a moderate 3
3 b none 12    3 b slight 4    3 b moderate 4
3 c none 11    3 c slight 6    3 c moderate 2
3 d none 7     3 d slight 7    3 d moderate 4
4 a none 12    4 a slight 9    4 a moderate 1
4 b none 15    4 b slight 3    4 b moderate 2
```



```

4 c none 14      4 c slight  8      4 c moderate 3
4 d none 13      4 d slight  6      4 d moderate 4
;

```

The response variable (Severity) is ordinally scaled with three levels, so assignment of scores is appropriate (0 = none, 0.5 = slight, 1 = moderate). For these scores, the response function yields the mean score. The following statements produce [Output 30.2.1](#) through [Output 30.2.3](#):

```

title 'Dumping Syndrome Data';
proc catmod data=operate order=data ;
  weight wt;
  response 0 0.5 1;
  model Severity=Treatment Hospital / freq oneway design;
  title2 'Main-Effects Model';
quit;

```

The `ORDER=` option is specified so that the levels of the response variable remain in the correct order. A main-effects model is fit. The `ONEWAY` option produces a table of the number of subjects within each variable level, and the `FREQ` option displays the frequency of each response within each sample ([Output 30.2.1](#)).

Output 30.2.1 Surgical Data: Analysis of Mean Scores

Dumping Syndrome Data			
Main-Effects Model			
The CATMOD Procedure			
Data Summary			
Response	Severity	Response Levels	3
Weight Variable	wt	Populations	16
Data Set	OPERATE	Total Frequency	417
Frequency Missing	0	Observations	48
One-Way Frequencies			
Variable	Value	Frequency	
Severity	none	240	
	slight	129	
	moderate	48	
Treatment	a	96	
	b	104	
	c	110	
	d	107	
Hospital	1	148	
	2	105	
	3	74	
	4	90	

Output 30.2.1 *continued*

Population Profiles			
Sample	Treatment	Hospital	Sample Size
1	a	1	32
2	a	2	25
3	a	3	17
4	a	4	22
5	b	1	38
6	b	2	26
7	b	3	20
8	b	4	20
9	c	1	38
10	c	2	28
11	c	3	19
12	c	4	25
13	d	1	40
14	d	2	26
15	d	3	18
16	d	4	23

Response Profiles	
Response	Severity
1	none
2	slight
3	moderate

Response Frequencies			
Sample	Response Number		
	1	2	3
1	23	7	2
2	18	6	1
3	8	6	3
4	12	9	1
5	23	10	5
6	18	6	2
7	12	4	4
8	15	3	2
9	20	13	5
10	13	13	2
11	11	6	2
12	14	8	3
13	24	10	6
14	9	15	2
15	7	7	4
16	13	6	4

You can use the one-way frequencies and the response profiles from [Output 30.2.1](#) to verify that the response levels are in the desired order (none, slight, moderate) so that the response scores (0, 0.5, 1.0) are applied appropriately. If the `ORDER=DATA` option had not been used, the levels would have been in a different order.

The analysis of variance table ([Output 30.2.2](#)) shows that the additive model fits (since the residual chi-square is not significant), that the Treatment effect is significant, and that the Hospital effect is not significant.

Output 30.2.2 Surgical Data: Analysis of Mean Scores

Response Functions and Design Matrix								
Sample	Response Function	Design Matrix						
		1	2	3	4	5	6	7
1	0.17188	1	1	0	0	1	0	0
2	0.16000	1	1	0	0	0	1	0
3	0.35294	1	1	0	0	0	0	1
4	0.25000	1	1	0	0	-1	-1	-1
5	0.26316	1	0	1	0	1	0	0
6	0.19231	1	0	1	0	0	1	0
7	0.30000	1	0	1	0	0	0	1
8	0.17500	1	0	1	0	-1	-1	-1
9	0.30263	1	0	0	1	1	0	0
10	0.30357	1	0	0	1	0	1	0
11	0.26316	1	0	0	1	0	0	1
12	0.28000	1	0	0	1	-1	-1	-1
13	0.27500	1	-1	-1	-1	1	0	0
14	0.36538	1	-1	-1	-1	0	1	0
15	0.41667	1	-1	-1	-1	0	0	1
16	0.30435	1	-1	-1	-1	-1	-1	-1

Analysis of Variance			
Source	DF	Chi-Square	Pr > ChiSq
Intercept	1	248.77	<.0001
Treatment	3	8.90	0.0307
Hospital	3	2.33	0.5065
Residual	9	6.33	0.7069

The coefficients of Treatment in [Output 30.2.3](#) show that the first two treatments (with negative coefficients) have lower mean scores than the last two treatments (the fourth coefficient, not shown, must be positive since the four coefficients must sum to zero). In other words, the less severe treatments (the first two) cause significantly less severe dumping syndrome complications.

Output 30.2.3 Surgical Data: Analysis of Mean Scores

Analysis of Weighted Least Squares Estimates				
Parameter	Estimate	Standard Error	Chi-Square	Pr > ChiSq
Intercept	0.2724	0.0173	248.77	<.0001
Treatment a	-0.0552	0.0270	4.17	0.0411
b	-0.0365	0.0289	1.59	0.2073
c	0.0248	0.0280	0.78	0.3757
Hospital 1	-0.0204	0.0264	0.60	0.4388
2	-0.0178	0.0268	0.44	0.5055
3	0.0531	0.0352	2.28	0.1312

Example 30.3: Logistic Regression, Standard Response Function

In this data set, from Cox and Snell (1989), ingots are prepared with different heating and soaking times and tested for their readiness to be rolled. The following DATA step creates a response variable Y with value 1 for ingots that are not ready and value 0 otherwise. The explanatory variables are Heat and Soak.

```
data ingots;
  input Heat Soak nready ntotal @@;
  Count=nready;
  Y=1;
  output;
  Count=ntotal-nready;
  Y=0;
  output;
  drop nready ntotal;
  datalines;
7 1.0 0 10   14 1.0 0 31   27 1.0 1 56   51 1.0 3 13
7 1.7 0 17   14 1.7 0 43   27 1.7 4 44   51 1.7 0 1
7 2.2 0 7    14 2.2 2 33   27 2.2 0 21   51 2.2 0 1
7 2.8 0 12   14 2.8 0 31   27 2.8 1 22   51 4.0 0 1
7 4.0 0 9    14 4.0 0 19   27 4.0 1 16
;
```

Logistic regression analysis is often used to investigate the relationship between discrete response variables and continuous explanatory variables. For logistic regression, the continuous *design-effects* are declared in a DIRECT statement. The following statements produce Output 30.3.1 through Output 30.3.6:

```
title 'Maximum Likelihood Logistic Regression';
proc catmod data=ingots;
  weight Count;
  direct Heat Soak;
  model Y=Heat Soak / freq covb corrb itprint design;
quit;
```

You can verify that the populations are defined as you intended by looking at the “Population Profiles” table in Output 30.3.1.

Output 30.3.1 Maximum Likelihood Logistic Regression

Maximum Likelihood Logistic Regression			
The CATMOD Procedure			
Data Summary			
Response	Y	Response Levels	2
Weight Variable	Count	Populations	19
Data Set	INGOTS	Total Frequency	387
Frequency Missing	0	Observations	25
Population Profiles			
Sample	Heat	Soak	Sample Size
1	7	1	10
2	7	1.7	17
3	7	2.2	7
4	7	2.8	12
5	7	4	9
6	14	1	31
7	14	1.7	43
8	14	2.2	33
9	14	2.8	31
10	14	4	19
11	27	1	56
12	27	1.7	44
13	27	2.2	21
14	27	2.8	22
15	27	4	16
16	51	1	13
17	51	1.7	1
18	51	2.2	1
19	51	4	1

Since the “Response Profiles” table in [Output 30.3.2](#) shows the response level ordering as 0, 1, the default response function, the logit, is defined as $\log\left(\frac{p_{Y=0}}{p_{Y=1}}\right)$.

Output 30.3.2 Response Summaries

Response Profiles	
Response	Y
1	0
2	1

Output 30.3.2 *continued*

Response Frequencies		
Sample	Response Number	
	1	2
1	10	0
2	17	0
3	7	0
4	12	0
5	9	0
6	31	0
7	43	0
8	31	2
9	31	0
10	19	0
11	55	1
12	40	4
13	21	0
14	21	1
15	15	1
16	10	3
17	1	0
18	1	0
19	1	0

The values of the continuous variable are inserted into the design matrix (Output 30.3.3).

Output 30.3.3 Design Matrix

Response Functions and Design Matrix				
Sample	Response Function	Design Matrix		
		1	2	3
1	2.99573	1	7	1
2	3.52636	1	7	1.7
3	2.63906	1	7	2.2
4	3.17805	1	7	2.8
5	2.89037	1	7	4
6	4.12713	1	14	1
7	4.45435	1	14	1.7
8	2.74084	1	14	2.2
9	4.12713	1	14	2.8
10	3.63759	1	14	4
11	4.00733	1	27	1
12	2.30259	1	27	1.7
13	3.73767	1	27	2.2
14	3.04452	1	27	2.8
15	2.70805	1	27	4
16	1.20397	1	51	1
17	0.69315	1	51	1.7
18	0.69315	1	51	2.2
19	0.69315	1	51	4

Seven Newton-Raphson iterations are required to find the maximum likelihood estimates (Output 30.3.4).

Output 30.3.4 Iteration History

Maximum Likelihood Analysis						
Iteration	Sub Iteration	-2 Log Likelihood	Convergence Criterion	Parameter Estimates		
				1	2	3
0	0	536.49592	1.0000	0	0	0
1	0	152.58961	0.7156	2.1594	-0.0139	-0.003733
2	0	106.76066	0.3003	3.5334	-0.0363	-0.0120
3	0	96.692171	0.0943	4.7489	-0.0640	-0.0299
4	0	95.383825	0.0135	5.4138	-0.0790	-0.0498
5	0	95.345659	0.000400	5.5539	-0.0819	-0.0564
6	0	95.345613	4.8289E-7	5.5592	-0.0820	-0.0568
7	0	95.345613	7.728E-13	5.5592	-0.0820	-0.0568

Maximum likelihood computations converged.

The analysis of variance table (Output 30.3.5) shows that the model fits since the likelihood ratio goodness-of-fit test is nonsignificant. It also shows that the length of heating time is a significant factor with respect to readiness but that length of soaking time is not.

Output 30.3.5 Analysis of Variance Table

Maximum Likelihood Analysis of Variance			
Source	DF	Chi-Square	Pr > ChiSq
Intercept	1	24.65	<.0001
Heat	1	11.95	0.0005
Soak	1	0.03	0.8639
Likelihood Ratio	16	13.75	0.6171

From the table of maximum likelihood estimates in Output 30.3.6, the fitted model is

$$E(\logit(p)) = 5.559 - 0.082(\text{Heat}) - 0.057(\text{Soak})$$

For example, for Sample 1 with Heat = 7 and Soak = 1, the estimate is

$$E(\logit(p)) = 5.559 - 0.082(7) - 0.057(1) = 4.9284$$

Output 30.3.6 Maximum Likelihood Estimates, Covariances, and Correlations

Analysis of Maximum Likelihood Estimates				
Parameter	Estimate	Standard Error	Chi-Square	Pr > ChiSq
Intercept	5.5592	1.1197	24.65	<.0001
Heat	-0.0820	0.0237	11.95	0.0005
Soak	-0.0568	0.3312	0.03	0.8639

Covariance Matrix of the Maximum Likelihood Estimates				
Row	Parameter	Col1	Col2	Col3
1	Intercept	1.2537133	-0.0215664	-0.2817648
2	Heat	-0.0215664	0.0005633	0.0026243
3	Soak	-0.2817648	0.0026243	0.1097020

Correlation Matrix of the Maximum Likelihood Estimates				
Row	Parameter	Col1	Col2	Col3
1	Intercept	1.00000	-0.81152	-0.75977
2	Heat	-0.81152	1.00000	0.33383
3	Soak	-0.75977	0.33383	1.00000

Predicted values of the logits, as well as the probabilities of readiness, could be obtained by specifying `PRED=PROB` in the `MODEL` statement. For the example of Sample 1 with `Heat = 7` and `Soak = 1`, `PRED=PROB` would give an estimate of the probability of readiness equal to 0.9928 since

$$4.9284 = \log\left(\frac{\hat{p}}{1 - \hat{p}}\right)$$

implies that

$$\hat{p} = \frac{e^{4.9284}}{1 + e^{4.9284}} = 0.9928$$

As another consideration, since soaking time is nonsignificant, you could fit another model that deleted the variable `Soak`.

Example 30.4: Log-Linear Model, Three Dependent Variables

This analysis reproduces the predicted cell frequencies for Bartlett's data by using a log-linear model of no three-variable interaction (Bishop, Fienberg, and Holland 1975, p. 89). Cuttings of two different lengths (Length=short or long) are planted at one of two time points (Time=now or spring), and their survival status (Status=dead or alive) is recorded.

As in the text, the variable levels are simply labeled 1 and 2. The following statements produce [Output 30.4.1](#) through [Output 30.4.3](#):


```

data bartlett;
  input Length Time Status wt @@;
  datalines;
1 1 1 156    1 1 2 84      1 2 1 84      1 2 2 156
2 1 1 107    2 1 2 133     2 2 1 31      2 2 2 209
;

title 'Bartlett's Data';
proc catmod data=bartlett;
  weight wt;
  model Length*Time*Status=_response_
    / noparm pred=freq;
  loglin Length|Time|Status @ 2;
  title2 'Model with No 3-Variable Interaction';
quit;

```

Output 30.4.1 Analysis of Bartlett's Data: Log-Linear Model

Bartlett's Data			
Model with No 3-Variable Interaction			
The CATMOD Procedure			
Data Summary			
Response	Length*Time*Status	Response Levels	8
Weight Variable	wt	Populations	1
Data Set	BARTLETT	Total Frequency	960
Frequency Missing	0	Observations	8
Population Profiles			
Sample	Sample Size		

1	960		
Response Profiles			
Response	Length	Time	Status

1	1	1	1
2	1	1	2
3	1	2	1
4	1	2	2
5	2	1	1
6	2	1	2
7	2	2	1
8	2	2	2
Maximum Likelihood Analysis			
Maximum likelihood computations converged.			

Output 30.4.1 *continued*

Maximum Likelihood Analysis of Variance			
Source	DF	Chi-Square	Pr > ChiSq
Length	1	2.64	0.1041
Time	1	5.25	0.0220
Length*Time	1	5.25	0.0220
Status	1	48.94	<.0001
Length*Status	1	48.94	<.0001
Time*Status	1	95.01	<.0001
Likelihood Ratio	1	2.29	0.1299

The analysis of variance table shows that the model fits since the likelihood ratio test for the three-variable interaction is nonsignificant. All of the two-variable interactions, however, are significant; this shows that there is mutual dependence among all three variables.

The predicted values table (Output 30.4.2) displays observed and predicted values for the generalized logits.

Output 30.4.2 Response Function Predicted Values

Maximum Likelihood Predicted Values for Response Functions					
Function Number	-----Observed-----		-----Predicted-----		Residual
	Function	Standard Error	Function	Standard Error	
1	-0.29248	0.105806	-0.23565	0.098486	-0.05683
2	-0.91152	0.129188	-0.94942	0.129948	0.037901
3	-0.91152	0.129188	-0.94942	0.129948	0.037901
4	-0.29248	0.105806	-0.23565	0.098486	-0.05683
5	-0.66951	0.118872	-0.69362	0.120172	0.024113
6	-0.45199	0.110921	-0.3897	0.102267	-0.06229
7	-1.90835	0.192465	-1.73146	0.142969	-0.17688

The predicted frequencies table (Output 30.4.3) displays observed and predicted cell frequencies, their standard errors, and residuals.

Output 30.4.3 Predicted Frequencies

Maximum Likelihood Predicted Values for Frequencies							
Length	Time	Status	-----Observed-----		-----Predicted-----		Residual
			Frequency	Standard Error	Frequency	Standard Error	
1	1	1	156	11.43022	161.0961	11.07379	-5.09614
1	1	2	84	8.754999	78.90386	7.808613	5.096139
1	2	1	84	8.754999	78.90386	7.808613	5.096139
1	2	2	156	11.43022	161.0961	11.07379	-5.09614
2	1	1	107	9.750588	101.9039	8.924304	5.096139
2	1	2	133	10.70392	138.0961	10.33434	-5.09614
2	2	1	31	5.47713	36.09614	4.826315	-5.09614
2	2	2	209	12.78667	203.9039	12.21285	5.09614

Example 30.5: Log-Linear Model, Structural and Sampling Zeros

This example illustrates a log-linear model of independence, by using data that contain structural zero frequencies as well as sampling (random) zero frequencies.

In a population of six squirrel monkeys, the joint distribution of genital display with respect to active or passive role was observed. The data are from Fienberg (1980, Table 8-2). Since a monkey cannot have both the active and passive roles in the same interaction, the diagonal cells of the table are structural zeros. See Agresti (2002) for more information about the quasi-independence model.

The DATA step replaces the structural zeros with missing values, and the `MISSING=STRUCTURAL` option is specified in the MODEL statement to remove these zeros from the analysis. The `ZERO=SAMPLING` option treats the off-diagonal zeros as sampling zeros. Also, the row for Monkey 't' is deleted since it contains all zeros; therefore, the cell frequencies predicted by a model of independence are also zero. In addition, the `CONTRAST` statement compares the behavior of the two monkeys labeled 'u' and 'v'. See the section "Structural and Sampling Zeros with Raw Data" on page 1877 for information about how to perform this analysis when you have raw data. The following statements produce Output 30.5.1 through Output 30.5.8:

```
data Display;
  input Active $ Passive $ wt @@;
  if Active ne 't';
  if Active eq Passive then wt=.;
  datalines;
r r 0   r s 1   r t 5   r u 8   r v 9   r w 0
s r 29  s s 0   s t 14  s u 46  s v 4   s w 0
t r 0   t s 0   t t 0   t u 0   t v 0   t w 0
u r 2   u s 3   u t 1   u u 0   u v 38  u w 2
v r 0   v s 0   v t 0   v u 0   v v 0   v w 1
w r 9   w s 25  w t 4   w u 6   w v 13  w w 0
;
```

```

title 'Behavior of Squirrel Monkeys';
proc catmod data=Display;
  weight wt;
  model Active*Passive=_response_ /
    missing=structural zero=sampling
    freq pred=freq noparm oneway;
  loglin Active Passive;
  contrast 'Passive, U vs. V' Passive 0 0 0 1 -1;
  contrast 'Active, U vs. V' Active 0 0 1 -1;
  title2 'Test Quasi-Independence for the Incomplete Table';
quit;

```

Output 30.5.1 Log-Linear Model Analysis with Zero Frequencies

Behavior of Squirrel Monkeys			
Test Quasi-Independence for the Incomplete Table			
The CATMOD Procedure			
Data Summary			
Response	Active*Passive	Response Levels	25
Weight Variable	wt	Populations	1
Data Set	DISPLAY	Total Frequency	220
Frequency Missing	0	Observations	25

The results of the **ONEWAY** option are shown in [Output 30.5.2](#). Monkey ‘t’ does not show up as a value for the Active variable since that row was removed.

Output 30.5.2 Output from the **ONEWAY** option

One-Way Frequencies		
Variable	Value	Frequency
Active	r	23
	s	93
	u	46
	v	1
	w	57
Passive	r	40
	s	29
	t	24
	u	60
	v	64
	w	3

Sampling zeros are displayed as 0 in [Output 30.5.4](#). The Response Number column corresponds to the value displayed in the “Response Profiles” table in [Output 30.5.3](#).

Output 30.5.3 Profiles

Population Profiles		
Sample	Sample Size	

1	220	

Response Profiles		
Response	Active	Passive

1	r	s
2	r	t
3	r	u
4	r	v
5	r	w
6	s	r
7	s	t
8	s	u
9	s	v
10	s	w
11	u	r
12	u	s
13	u	t
14	u	v
15	u	w
16	v	r
17	v	s
18	v	t
19	v	u
20	v	w
21	w	r
22	w	s
23	w	t
24	w	u
25	w	v

Output 30.5.4 Frequency of Response by Response Number

Response Frequencies								
Sample	Response Number							
	1	2	3	4	5	6	7	8
1	1	5	8	9	0	29	14	46

Response Frequencies								
Sample	Response Number							
	9	10	11	12	13	14	15	16
1	4	0	2	3	1	38	2	0

Response Frequencies								
Sample	Response Number							
	17	18	19	20	21	22	23	24
1	0	0	0	1	9	25	4	6

Response Frequencies	
Sample	Response Number
1	25
1	13

The analysis of variance table (Output 30.5.5) shows that the model of independence does not fit since the likelihood ratio test for the interaction is significant. In other words, active and passive behaviors of the squirrel monkeys are dependent behavior roles.

Output 30.5.5 Analysis of Variance Table

Maximum Likelihood Analysis of Variance			
Source	DF	Chi-Square	Pr > ChiSq
Active	4	56.58	<.0001
Passive	5	47.94	<.0001
Likelihood Ratio	15	135.17	<.0001

If the model fit these data, then the contrasts in Output 30.5.6 show that monkeys ‘u’ and ‘v’ appear to have similar passive behavior patterns but very different active behavior patterns.

Output 30.5.6 Contrasts between Monkeys 'u' and 'v'

Contrasts of Maximum Likelihood Estimates			
Contrast	DF	Chi-Square	Pr > ChiSq
Passive, U vs. V	1	1.31	0.2524
Active, U vs. V	1	14.87	0.0001

Output 30.5.7 displays the predicted response functions and Output 30.5.8 displays predicted cell frequencies (from the PRED=FREQ option), but since the model does not fit, these should be ignored. Note that, since the response function is the generalized logit with the 25th response as the baseline, the observed response functions for the sampling zeros are missing.

Output 30.5.7 Response Function Predicted Values

Maximum Likelihood Predicted Values for Response Functions					
Function Number	-----Observed-----		-----Predicted-----		Residual
	Function	Standard Error	Function	Standard Error	
1	-2.56495	1.037749	-0.97355	0.339019	-1.5914
2	-0.95551	0.526235	-1.72504	0.345438	0.769529
3	-0.48551	0.449359	-0.52751	0.309254	0.042007
4	-0.36772	0.433629	-0.73927	0.249006	0.371543
5	.	.	-3.56052	0.634104	.
6	0.802346	0.333775	0.320589	0.26629	0.481758
7	0.074108	0.385164	-0.29934	0.295634	0.37345
8	1.263692	0.314105	0.898184	0.250857	0.365508
9	-1.17865	0.571772	0.686431	0.173396	-1.86509
10	.	.	-2.13482	0.608071	.
11	-1.8718	0.759555	-0.2415	0.287218	-1.63031
12	-1.46634	0.640513	-0.10994	0.303568	-1.3564
13	-2.56495	1.037749	-0.86143	0.314794	-1.70352
14	1.072637	0.321308	0.124346	0.204345	0.94829
15	-1.8718	0.759555	-2.6969	0.617433	0.8251
16	.	.	-4.14787	1.024508	.
17	.	.	-4.01632	1.030062	.
18	.	.	-4.76781	1.032457	.
19	.	.	-3.57028	1.020794	.
20	-2.56495	1.037749	-6.60328	1.161289	4.038332
21	-0.36772	0.433629	-0.36584	0.202959	-0.00188
22	0.653926	0.34194	-0.23429	0.232794	0.888212
23	-1.17865	0.571772	-0.98577	0.239408	-0.19288
24	-0.77319	0.493548	0.211754	0.185007	-0.98494

Output 30.5.8 Predicted Frequencies

Maximum Likelihood Predicted Values for Frequencies						
Active	Passive	-----Observed-----		-----Predicted-----		Residual
		Frequency	Standard Error	Frequency	Standard Error	
r	s	1	0.997725	5.259508	1.36156	-4.25951
r	t	5	2.210512	2.480726	0.691066	2.519274
r	u	8	2.776525	8.215948	1.855146	-0.21595
r	v	9	2.937996	6.648049	1.50932	2.351951
r	w	0	0	0.395769	0.240268	-0.39577
s	r	29	5.017696	19.18599	3.147915	9.814007
s	t	14	3.620648	10.32172	2.169599	3.678284
s	u	46	6.031734	34.18463	4.428706	11.81537
s	v	4	1.981735	27.66096	3.722788	-23.661
s	w	0	0	1.6467	0.952712	-1.6467
u	r	2	1.407771	10.9364	2.12322	-8.9364
u	s	3	1.720201	12.47407	2.554336	-9.47407
u	t	1	0.997725	5.883583	1.380655	-4.88358
u	v	38	5.606814	15.7673	2.684692	22.2327
u	w	2	1.407771	0.938652	0.551645	1.061348
v	r	0	0	0.219966	0.221779	-0.21997
v	s	0	0	0.250893	0.253706	-0.25089
v	t	0	0	0.118338	0.120314	-0.11834
v	u	0	0	0.391924	0.393255	-0.39192
v	w	1	0.997725	0.018879	0.021728	0.981121
w	r	9	2.937996	9.657645	1.808656	-0.65765
w	s	25	4.707344	11.01553	2.275019	13.98447
w	t	4	1.981735	5.195638	1.184452	-1.19564
w	u	6	2.415857	17.2075	2.772098	-11.2075
w	v	13	3.497402	13.92369	2.24158	-0.92369

Structural and Sampling Zeros with Raw Data

The preceding PROC CATMOD step uses cell count data as input. Prior to invoking the CATMOD procedure, structural and sampling zeros are easily identified and manipulated in a single DATA step. For the situation where structural or sampling zeros (or both) exist and the input data set is raw data, use the following steps:

1. Run PROC FREQ on the raw data (see Chapter 38, “The FREQ Procedure”). In the TABLES statement, list all dependent and independent variables, separated by asterisks, and use the SPARSE option and the OUT= option. This creates an output data set that contains all possible zero frequencies. Since the tabled output can be huge, you should also specify the NOPRINT option in the TABLES statement.
2. Use a DATA step to change the zero frequencies associated with either sampling zeros or structural zeros to missing.
3. Use the resulting data set as input to PROC CATMOD, specify the statement WEIGHT COUNT to use adjusted frequencies, and specify the ZERO= and MISSING= options to define your sampling and structural zeros.

For example, suppose the data set RawDisplay contains the raw data for the squirrel monkey data. The following statements show how to obtain the same analysis as shown previously:

```
proc freq data=RawDisplay;
  tables Active*Passive / sparse out=Combos noprint;
run;

data Combos2;
  set Combos;
  if Active ne 't';
  if Active eq Passive then count=.;
run;

proc catmod data=Combos2;
  weight count;
  model Active*Passive=_response_ /
    zero=sampling missing=structural
    freq pred=freq noparm noresponse;
  loglin Active Passive;
quit;
```

The first IF statement in the DATA step is needed only for this particular example; since observations for Monkey 't' were deleted from the Display data set, they also need to be deleted from Combos2.

Example 30.6: Repeated Measures, 2 Response Levels, 3 Populations

In this multiple-population repeated measures example, from Guthrie (1981), subjects from three groups have their responses (0 or 1) recorded in each of four trials. The analysis of the marginal probabilities is directed at assessing the main effects of the repeated measurement factor (Trial) and the independent variable (Group), as well as their interaction. Although the contingency table is incomplete (only 13 of the 16 possible responses are observed), this poses no problem in the computation of the marginal probabilities. The following statements produce [Output 30.6.1](#):

```
data group;
  input a b c d Group wt @@;
  datalines;
1 1 1 1 2 2      0 0 0 0 2 2      0 0 1 0 1 2      0 0 1 0 2 2
0 0 0 1 1 4      0 0 0 1 2 1      0 0 0 1 3 3      1 0 0 1 2 1
0 0 1 1 1 1      0 0 1 1 2 2      0 0 1 1 3 5      0 1 0 0 1 4
0 1 0 0 2 1      0 1 0 1 2 1      0 1 0 1 3 2      0 1 1 0 3 1
1 0 0 0 1 3      1 0 0 0 2 1      0 1 1 1 2 1      0 1 1 1 3 2
1 0 1 0 1 1      1 0 1 1 2 1      1 0 1 1 3 2
;
```

```

title 'Multiple-Population Repeated Measures';
proc catmod data=group;
  weight wt;
  response marginals;
  model a*b*c*d=Group _response_ Group*_response_
    / freq;
  repeated Trial 4;
  title2 'Saturated Model';
run;

```

Output 30.6.1 Analysis of Multiple-Population Repeated Measures

Multiple-Population Repeated Measures				
Saturated Model				
The CATMOD Procedure				
Data Summary				
Response	a*b*c*d	Response Levels	13	
Weight Variable	wt	Populations	3	
Data Set	GROUP	Total Frequency	45	
Frequency Missing	0	Observations	23	
Population Profiles				
Sample	Group	Sample Size		
1	1	15		
2	2	15		
3	3	15		
Response Profiles				
Response	a	b	c	d
1	0	0	0	0
2	0	0	0	1
3	0	0	1	0
4	0	0	1	1
5	0	1	0	0
6	0	1	0	1
7	0	1	1	0
8	0	1	1	1
9	1	0	0	0
10	1	0	0	1
11	1	0	1	0
12	1	0	1	1
13	1	1	1	1

Output 30.6.1 continued

Response Frequencies								
Sample	Response Number							
	1	2	3	4	5	6	7	8
1	0	4	2	1	4	0	0	0
2	2	1	2	2	1	1	0	1
3	0	3	0	5	0	2	1	2

Response Frequencies					
Sample	Response Number				
	9	10	11	12	13
1	3	0	1	0	0
2	1	1	0	1	2
3	0	0	0	2	0

Analysis of Variance			
Source	DF	Chi-Square	Pr > ChiSq
Intercept	1	354.88	<.0001
Group	2	24.79	<.0001
Trial	3	21.45	<.0001
Group*Trial	6	18.71	0.0047
Residual	0	.	.

Analysis of Weighted Least Squares Estimates					
Effect	Parameter	Estimate	Standard Error	Chi-Square	Pr > ChiSq
Intercept	1	0.5833	0.0310	354.88	<.0001
Group	2	0.1333	0.0335	15.88	<.0001
	3	-0.0333	0.0551	0.37	0.5450
	4	0.1722	0.0557	9.57	0.0020
Trial	5	0.1056	0.0647	2.66	0.1028
	6	-0.0722	0.0577	1.57	0.2107
	7	-0.1556	0.0852	3.33	0.0679
Group*Trial	8	-0.0556	0.0800	0.48	0.4877
	9	-0.0889	0.0953	0.87	0.3511
	10	0.0111	0.0866	0.02	0.8979
	11	0.0889	0.0822	1.17	0.2793
	12	-0.0111	0.0824	0.02	0.8927

The analysis of variance table in Output 30.6.1 shows that there is a significant interaction between the independent variable Group and the repeated measurement factor Trial. An intermediate model (not shown) is fit in which the effects Trial and Group* Trial are replaced by Trial(Group=1), Trial(Group=2), and Trial(Group=3). Of these three effects, only the last is significant, so it is retained in the final model. The following statements produce Output 30.6.2 and Output 30.6.3:

```

model a*b*c*d=Group _response_(Group=3)
  / noprofile noparm design;
title2 'Trial Nested within Group 3';
quit;

```

Output 30.6.2 displays the design matrix resulting from retaining the nested effect.

Output 30.6.2 Final Model: Design Matrix

Multi-Population Repeated Measures Trial Nested within Group 3								
The CATMOD Procedure								
Data Summary								
Response		a*b*c*d	Response Levels	13				
Weight Variable		wt	Populations	3				
Data Set		GROUP	Total Frequency	45				
Frequency Missing		0	Observations	23				
Response Functions and Design Matrix								
Sample	Function Number	Response Function	Design Matrix					
			1	2	3	4	5	6
1	1	0.73333	1	1	0	0	0	0
	2	0.73333	1	1	0	0	0	0
	3	0.73333	1	1	0	0	0	0
	4	0.66667	1	1	0	0	0	0
2	1	0.66667	1	0	1	0	0	0
	2	0.66667	1	0	1	0	0	0
	3	0.46667	1	0	1	0	0	0
	4	0.40000	1	0	1	0	0	0
3	1	0.86667	1	-1	-1	1	0	0
	2	0.66667	1	-1	-1	0	1	0
	3	0.33333	1	-1	-1	0	0	1
	4	0.06667	1	-1	-1	-1	-1	-1

The residual goodness-of-fit statistic tests the joint effect of Trial(Group=1) and Trial(Group=2). The analysis of variance table in Output 30.6.3 shows that the final model fits, that there is a significant Group effect, and that there is a significant Trial effect in Group 3.

Output 30.6.3 ANOVA Table

Analysis of Variance			
Source	DF	Chi-Square	Pr > ChiSq
Intercept	1	386.94	<.0001
Group	2	25.42	<.0001
Trial (Group=3)	3	75.07	<.0001
Residual	6	5.09	0.5319

Example 30.7: Repeated Measures, 4 Response Levels, 1 Population

This example illustrates a repeated measures analysis in which there are more than two levels of response. In this study, from Grizzle, Starmer, and Koch (1969, p. 493), 7,477 women aged 30–39 are tested for vision in both right and left eyes. Since there are four response levels for each dependent variable, the **RESPONSE** statement computes three marginal probabilities for each dependent variable, resulting in six response functions for analysis. Since the model contains a repeated measurement factor (**Side**) with two levels (**Right**, **Left**), PROC CATMOD groups the functions into sets of three ($=6/2$). Therefore, the **Side** effect has three degrees of freedom (one for each marginal probability), and it is the appropriate test of marginal homogeneity. The following statements produce [Output 30.7.1](#):

```

title 'Vision Symmetry';
data vision;
  input Right Left count @@;
  datalines;
1 1 1520   1 2 266   1 3 124   1 4 66
2 1 234   2 2 1512   2 3 432   2 4 78
3 1 117   3 2 362   3 3 1772   3 4 205
4 1 36   4 2 82   4 3 179   4 4 492
;

proc catmod data=vision;
  weight count;
  response marginals;
  model Right*Left=_response_ / freq design;
  repeated Side 2;
  title2 'Test of Marginal Homogeneity';
quit;

```

Output 30.7.1 Vision Study: Analysis of Marginal Homogeneity

Vision Symmetry Test of Marginal Homogeneity								
The CATMOD Procedure								
Data Summary								
Response	Right*Left	Response Levels	16					
Weight Variable	count	Populations	1					
Data Set	VISION	Total Frequency	7477					
Frequency Missing	0	Observations	16					
Population Profiles								
Sample	Sample Size							
-----	-----							
1	7477							
Response Profiles								
Response	Right	Left						
-----	-----	-----						
1	1	1						
2	1	2						
3	1	3						
4	1	4						
5	2	1						
6	2	2						
7	2	3						
8	2	4						
9	3	1						
10	3	2						
11	3	3						
12	3	4						
13	4	1						
14	4	2						
15	4	3						
16	4	4						
Response Frequencies								
Sample	Response Number							
-----	-----	-----	-----	-----	-----	-----	-----	-----
1	1520	266	124	66	234	1512	432	78
Response Frequencies								
Sample	Response Number							
-----	-----	-----	-----	-----	-----	-----	-----	-----
1	117	362	1772	205	36	82	179	492

Output 30.7.1 *continued*

Response Functions and Design Matrix								
Sample	Function Number	Response Function	Design Matrix					
			1	2	3	4	5	6
1	1	0.26428	1	0	0	1	0	0
	2	0.30173	0	1	0	0	1	0
	3	0.32847	0	0	1	0	0	1
	4	0.25505	1	0	0	-1	0	0
	5	0.29718	0	1	0	0	-1	0
	6	0.33529	0	0	1	0	0	-1

Analysis of Variance			
Source	DF	Chi-Square	Pr > ChiSq
Intercept	3	78744.17	<.0001
Side	3	11.98	0.0075
Residual	0	.	.

Analysis of Weighted Least Squares Estimates					
Effect	Parameter	Estimate	Standard Error	Chi-Square	Pr > ChiSq
Intercept	1	0.2597	0.00468	3073.03	<.0001
	2	0.2995	0.00464	4160.17	<.0001
	3	0.3319	0.00483	4725.25	<.0001
Side	4	0.00461	0.00194	5.65	0.0174
	5	0.00227	0.00255	0.80	0.3726
	6	-0.00341	0.00252	1.83	0.1757

The analysis of variance table in [Output 30.7.1](#) shows that the Side effect is significant, so there is not marginal homogeneity between left-eye vision and right-eye vision. In other words, the distribution of the quality of right-eye vision differs significantly from the distribution of the quality of left-eye vision in the same subjects. The test of the Side effect is equivalent to Bhapkar's test (Agresti 1990).

Example 30.8: Repeated Measures, Logistic Analysis of Growth Curve

The following data, from a longitudinal study reported in Koch et al. (1977), are from patients in four populations (2 diagnostic groups \times 2 treatments) who are measured at three times to assess their response (n=normal or a=abnormal) to treatment:

```

title 'Growth Curve Analysis';
data growth2;
  input Diagnosis $ Treatment $ week1 $ week2 $ week4 $ count @@;
  datalines;

```

```

mild std n n n 16      severe std n n n 2
mild std n n a 13      severe std n n a 2
mild std n a n 9       severe std n a n 8
mild std n a a 3       severe std n a a 9
mild std a n n 14      severe std a n n 9
mild std a n a 4       severe std a n a 15
mild std a a n 15      severe std a a n 27
mild std a a a 6       severe std a a a 28
mild new n n n 31      severe new n n n 7
mild new n n a 0       severe new n n a 2
mild new n a n 6       severe new n a n 5
mild new n a a 0       severe new n a a 2
mild new a n n 22      severe new a n n 31
mild new a n a 2       severe new a n a 5
mild new a a n 9       severe new a a n 32
mild new a a a 0       severe new a a a 6
;

```

The analysis is directed at assessing the effect of the repeated measurement factor, Time, as well as the independent variables, Diagnosis (mild or severe) and Treatment (std or new). The **RESPONSE** statement is used to compute the logits of the marginal probabilities. The times used in the design matrix (0, 1, 2) correspond to the logarithms (base 2) of the actual times (1, 2, 4). The following statements produce Output 30.8.1 through Output 30.8.4:

```

proc catmod data=growth2 order=data;
  title2 'Reduced Logistic Model';
  weight count;
  population Diagnosis Treatment;
  response logit;
  model week1*week2*week4=(1 0 0 0, /* mild, std */
                           1 0 1 0,
                           1 0 2 0,
                           1 0 0 0, /* mild, new */
                           1 0 0 1,
                           1 0 0 2,
                           0 1 0 0, /* severe, std */
                           0 1 1 0,
                           0 1 2 0,
                           0 1 0 0, /* severe, new */
                           0 1 0 1,
                           0 1 0 2)
    (1='Mild diagnosis, week 1',
     2='Severe diagnosis, week 1',
     3='Time effect for std trt',
     4='Time effect for new trt')
    / freq design;
  contrast 'Diagnosis effect, week 1' all_parms 1 -1 0 0;
  contrast 'Equal time effects' all_parms 0 0 1 -1;
quit;

```


The samples and the response numbers are defined in [Output 30.8.1](#), and the frequency distribution of the response numbers within the samples is displayed.

Output 30.8.1 Logistic Analysis of Growth Curve

Growth Curve Analysis			
Reduced Logistic Model			
The CATMOD Procedure			
Data Summary			
Response	week1*week2*week4	Response Levels	8
Weight Variable	count	Populations	4
Data Set	GROWTH2	Total Frequency	340
Frequency Missing	0	Observations	29
Population Profiles			
Sample	Diagnosis	Treatment	Sample Size
1	mild	std	80
2	mild	new	70
3	severe	std	100
4	severe	new	90
Response Profiles			
Response	week1	week2	week4
1	n	n	n
2	n	n	a
3	n	a	n
4	n	a	a
5	a	n	n
6	a	n	a
7	a	a	n
8	a	a	a

[Output 30.8.2](#) displays the design matrix specified in the MODEL statement, and the observed logits of the marginal probabilities are displayed in the Response Function column.

Output 30.8.2 Response Frequencies

Response Frequencies								
Sample	Response Number							
	1	2	3	4	5	6	7	8
1	16	13	9	3	14	4	15	6
2	31	0	6	0	22	2	9	0
3	2	2	8	9	9	15	27	28
4	7	2	5	2	31	5	32	6

Response Functions and Design Matrix						
Sample	Function Number	Response Function	Design Matrix			
			1	2	3	4
1	1	0.05001	1	0	0	0
	2	0.35364	1	0	1	0
	3	0.73089	1	0	2	0
2	1	0.11441	1	0	0	0
	2	1.29928	1	0	0	1
	3	3.52636	1	0	0	2
3	1	-1.32493	0	1	0	0
	2	-0.94446	0	1	1	0
	3	-0.16034	0	1	2	0
4	1	-1.53148	0	1	0	0
	2	0.00000	0	1	0	1
	3	1.60944	0	1	0	2

The analysis of variance table in [Output 30.8.3](#) shows that the data can be adequately modeled by two parameters that represent diagnosis effects at week 1 and two log-linear time effects (one for each treatment). Both of the time effects are significant.

Since the estimate of the logit for the severe diagnosis effect (parameter 2) is more negative than it is for the mild diagnosis effect (parameter 1), there is a smaller predicted probability of the first response (normal) for the severe diagnosis group.

Output 30.8.3 ANOVA and Parameter Estimates

Analysis of Variance			
Source	DF	Chi-Square	Pr > ChiSq
Mild diagnosis, week 1	1	0.28	0.5955
Severe diagnosis, week 1	1	100.48	<.0001
Time effect for std trt	1	26.35	<.0001
Time effect for new trt	1	125.09	<.0001
Residual	8	4.20	0.8387

Output 30.8.3 continued

Analysis of Weighted Least Squares Estimates					
Effect	Parameter	Estimate	Standard Error	Chi-Square	Pr > ChiSq
Model	1	-0.0716	0.1348	0.28	0.5955
	2	-1.3529	0.1350	100.48	<.0001
	3	0.4944	0.0963	26.35	<.0001
	4	1.4552	0.1301	125.09	<.0001

The analysis of contrasts (Output 30.8.4) shows that the diagnosis effect at week 1 is highly significant. In other words, those subjects with a severe diagnosis have a significantly higher probability of abnormal response at week 1 than those subjects with a mild diagnosis.

Output 30.8.4 Contrasts

Analysis of Contrasts			
Contrast	DF	Chi-Square	Pr > ChiSq
Diagnosis effect, week 1	1	77.02	<.0001
Equal time effects	1	59.12	<.0001

The analysis of contrasts (Output 30.8.4) also shows that the time effect for the standard treatment is significantly different from the one for the new treatment. The table of parameter estimates (Output 30.8.3) shows that the time effect for the new treatment (parameter 4) is stronger than it is for the standard treatment (parameter 3).

Example 30.9: Repeated Measures, Two Repeated Measurement Factors

This example, from MacMillan et al. (1981), illustrates a repeated measures analysis in which there are two repeated measurement factors. Two diagnostic procedures (standard and test) are performed on each subject, and the results of both are evaluated at each of two times as being positive or negative. In the following DATA step, `std1` and `std2` are the two measurements of the standard procedure, and `test1` and `test2` are the two measurements of the test procedure:

```
data a;
  input std1 $ test1 $ std2 $ test2 $ wt @@;
  datalines;
neg neg neg neg 509 neg neg neg pos 4 neg neg pos neg 17
neg neg pos pos 3 neg pos neg neg 13 neg pos neg pos 8
neg pos pos pos 8 pos neg neg neg 14 pos neg neg pos 1
pos neg pos neg 17 pos neg pos pos 9 pos pos neg neg 7
pos pos neg pos 4 pos pos pos neg 9 pos pos pos pos 170
;
```

For the initial model, the response functions are marginal probabilities, and the repeated measurement factors are Time and Treatment. The model is a saturated one, containing effects for Time, Treatment, and Time*Treatment. The following statements produce [Output 30.9.1](#):

```
proc catmod data=a;
  title2 'Marginal Symmetry, Saturated Model';
  weight wt;
  response marginals;
  model std1*test1*std2*test2=_response_ / freq design noparm;
  repeated Time 2, Treatment 2 / _response_=Time Treatment
    Time*Treatment;
run;
```

The analysis of variance table in [Output 30.9.1](#) shows that there is no significant effect of Time, either by itself or in its interaction with Treatment. The second model includes only the Treatment effect. Again, the response functions are marginal probabilities, and the repeated measurement factors are Time and Treatment.

Output 30.9.1 Diagnosis Data: Two Repeated Measurement Factors

Diagnostic Procedure Comparison			
Marginal Symmetry, Saturated Model			
The CATMOD Procedure			
Data Summary			
Response	std1*test1*std2*test2	Response Levels	15
Weight Variable	wt	Populations	1
Data Set	A	Total Frequency	793
Frequency Missing	0	Observations	15
Population Profiles			
Sample	Sample Size		

1	793		

Output 30.9.1 continued

Response Profiles					
Response	std1	test1	std2	test2	
1	neg	neg	neg	neg	
2	neg	neg	neg	pos	
3	neg	neg	pos	neg	
4	neg	neg	pos	pos	
5	neg	pos	neg	neg	
6	neg	pos	neg	pos	
7	neg	pos	pos	pos	
8	pos	neg	neg	neg	
9	pos	neg	neg	pos	
10	pos	neg	pos	neg	
11	pos	neg	pos	pos	
12	pos	pos	neg	neg	
13	pos	pos	neg	pos	
14	pos	pos	pos	neg	
15	pos	pos	pos	pos	

Response Frequencies								
Sample	Response Number							
	1	2	3	4	5	6	7	8
1	509	4	17	3	13	8	8	14

Response Frequencies							
Sample	Response Number						
	9	10	11	12	13	14	15
1	1	17	9	7	4	9	170

Response Functions and Design Matrix						
Sample	Function Number	Response Function	Design Matrix			
			1	2	3	4
1	1	0.70870	1	1	1	1
	2	0.72383	1	1	-1	-1
	3	0.70618	1	-1	1	-1
	4	0.73897	1	-1	-1	1

Output 30.9.1 *continued*

Analysis of Variance			
Source	DF	Chi-Square	Pr > ChiSq
Intercept	1	2385.34	<.0001
Time	1	0.85	0.3570
Treatment	1	8.20	0.0042
Time*Treatment	1	2.40	0.1215
Residual	0	.	.

A main effect model with respect to Treatment is fit. The following statements produces [Output 30.9.2](#):

```

title2 'Marginal Symmetry, Reduced Model';
model std1*test1*std2*test2=_response_ / corrb design noprofile;
repeated Time 2, Treatment 2 / _response_=Treatment;
run;
    
```

The analysis of variance table for the reduced model ([Output 30.9.2](#)) shows that the model fits (since the residual chi-square is nonsignificant) and that the treatment effect is significant. The negative parameter estimate for Treatment shows that the first level of treatment (std) has a smaller probability of the first response level (neg) than the second level of treatment (test). In other words, the standard diagnostic procedure gives a significantly higher probability of a positive response than the test diagnostic procedure.

Output 30.9.2 Diagnosis Data: Reduced Model

Diagnostic Procedure Comparison				
Marginal Symmetry, Reduced Model				
The CATMOD Procedure				
Data Summary				
Response	std1*test1*std2*test2	Response Levels	15	
Weight Variable	wt	Populations	1	
Data Set	A	Total Frequency	793	
Frequency Missing	0	Observations	15	
Response Functions and Design Matrix				
Sample	Function Number	Response Function	Design Matrix	
			1	2
1	1	0.70870	1	1
	2	0.72383	1	-1
	3	0.70618	1	1
	4	0.73897	1	-1

Output 30.9.2 continued

Analysis of Variance			
Source	DF	Chi-Square	Pr > ChiSq
Intercept	1	2386.97	<.0001
Treatment	1	9.55	0.0020
Residual	2	3.51	0.1731

Analysis of Weighted Least Squares Estimates					
Effect	Parameter	Estimate	Standard Error	Chi-Square	Pr > ChiSq
Intercept	1	0.7196	0.0147	2386.97	<.0001
Treatment	2	-0.0128	0.00416	9.55	0.0020

Correlation Matrix of the Parameter Estimates			
Row	Col1	Col2	
1	1.00000	0.04194	
2	0.04194	1.00000	

The next example illustrates a **RESPONSE** statement that, at each time, computes the sensitivity and specificity of the test diagnostic procedure with respect to the standard procedure. Since these are measures of the relative accuracy of the two diagnostic procedures, the repeated measurement factors in this case are labeled Time and Accuracy. Only 15 of the 16 possible responses are observed, so additional care must be taken in formulating the **RESPONSE** statement for computation of sensitivity and specificity.

The following statements produce **Output 30.9.3** and **Output 30.9.4**:

```

title2 'Sensitivity and Specificity Analysis, '
      'Main-Effects Model';
model std1*test1*std2*test2=_response_ / covb design noprofile;
repeated Time 2, Accuracy 2 / _response_=Time Accuracy;
response exp 1 -1 0 0 0 0 0 0,
             0 0 1 -1 0 0 0 0,
             0 0 0 0 1 -1 0 0,
             0 0 0 0 0 0 1 -1

      log 0 0 0 0 0 0 0 0 1 1 1 1,
           0 0 0 0 0 0 0 1 1 1 1 1 1,
           1 1 1 1 0 0 0 0 0 0 0 0,
           1 1 1 1 1 1 1 0 0 0 0 0 0,
           0 0 0 1 0 0 1 0 0 0 1 0 0 0 1,
           0 0 1 1 0 0 1 0 0 1 1 0 0 1 1,
           1 0 0 0 1 0 0 1 0 0 0 1 0 0 0,
           1 1 0 0 1 1 0 1 1 0 0 1 1 0 0;

quit;

```

For the sensitivity and specificity analysis, the four response functions displayed next to the design matrix (Output 30.9.3) represent the following:

1. sensitivity, time 1
2. specificity, time 1
3. sensitivity, time 2
4. specificity, time 2

The sensitivities and specificities are for the test diagnostic procedure relative to the standard procedure.

Output 30.9.3 Diagnosis Data: Sensitivity and Specificity Analysis

Diagnostic Procedure Comparison					
Sensitivity and Specificity Analysis, Main-Effects Model					
The CATMOD Procedure					
Data Summary					
Response	std1*test1*std2*test2	Response Levels	15		
Weight Variable	wt	Populations	1		
Data Set	A	Total Frequency	793		
Frequency Missing	0	Observations	15		
Response Functions and Design Matrix					
Sample	Function Number	Response Function	Design Matrix		
			1	2	3
1	1	0.82251	1	1	1
	2	0.94840	1	1	-1
	3	0.81545	1	-1	1
	4	0.96964	1	-1	-1
Analysis of Variance					
Source	DF	Chi-Square	Pr > ChiSq		
Intercept	1	6448.79	<.0001		
Time	1	4.10	0.0428		
Accuracy	1	38.81	<.0001		
Residual	1	1.00	0.3178		

The ANOVA table in Output 30.9.3 shows that an additive model fits, that there is a significant effect of time, and that the sensitivity is significantly different from the specificity.

Output 30.9.4 shows that the predicted sensitivities and specificities are lower for time 1 (since parameter 2 is negative). It also shows that the sensitivity is significantly less than the specificity.

Output 30.9.4 Parameter Estimates

Analysis of Weighted Least Squares Estimates					
Effect	Parameter	Estimate	Standard Error	Chi-Square	Pr > ChiSq
Intercept	1	0.8892	0.0111	6448.79	<.0001
Time	2	-0.00932	0.00460	4.10	0.0428
Accuracy	3	-0.0702	0.0113	38.81	<.0001

Covariance Matrix of the Parameter Estimates			
Row	Col1	Col2	Col3
1	0.00012260	0.00000229	0.00010137
2	0.00000229	0.00002116	-.00000587
3	0.00010137	-.00000587	0.00012697

Example 30.10: Direct Input of Response Functions and Covariance Matrix

This example illustrates the ability of PROC CATMOD to operate on an existing vector of functions and the corresponding covariance matrix. The estimates under investigation are composite indices summarizing the responses to 18 psychological questions pertaining to general well-being. These estimates are computed for domains corresponding to an age-by-sex cross-classification, and the covariance matrix is calculated using the method of balanced repeated replications. The analysis is directed at obtaining a description of the variation among these domain estimates. The data are from Koch and Stokes (1979).

In the following statements, the first row of the `fbeing` data set contains the response functions for the variables `b1–b10`, while the remaining rows contain the covariance matrix. From the PROC CATMOD statements, the `READ` option in the `RESPONSE` statement says that you are inputting the response functions and their covariance matrix, while the `PROFILE=` option in the `FACTORS` statement tells you that the variables `b1–b5` correspond to the effects for `sex='male'` at the five different age groupings, and `b6–b10` likewise correspond to the effects for `sex='female'`. See the section “[Inputting Response Functions and Covariances Directly](#)” on page 1820 for more information about using the `READ` option.

```

data fbeing(type=est);
  input  b1-b5  _type_ $  _name_ $  b6-b10 #2;
  datalines;
7.93726  7.92509  7.82815  7.73696  8.16791  parms  .
7.24978  7.18991  7.35960  7.31937  7.55184
0.00739  0.00019  0.00146  -0.00082  0.00076  cov    b1
0.00189  0.00118  0.00140  -0.00140  0.00039
0.00019  0.01172  0.00183  0.00029  0.00083  cov    b2
-0.00123 -0.00629 -0.00088 -0.00232  0.00034
0.00146  0.00183  0.01050 -0.00173  0.00011  cov    b3
0.00434 -0.00059 -0.00055  0.00023  -0.00013
-0.00082  0.00029 -0.00173  0.01335  0.00140  cov    b4
0.00158  0.00212  0.00211  0.00066  0.00240
0.00076  0.00083  0.00011  0.00140  0.01430  cov    b5
-0.00050 -0.00098  0.00239 -0.00010  0.00213
0.00189 -0.00123  0.00434  0.00158  -0.00050  cov    b6
0.01110  0.00101  0.00177 -0.00018  -0.00082
0.00118 -0.00629 -0.00059  0.00212  -0.00098  cov    b7
0.00101  0.02342  0.00144  0.00369  0.00253
0.00140 -0.00088 -0.00055  0.00211  0.00239  cov    b8
0.00177  0.00144  0.01060  0.00157  0.00226
-0.00140 -0.00232  0.00023  0.00066  -0.00010  cov    b9
-0.00018  0.00369  0.00157  0.02298  0.00918
0.00039  0.00034 -0.00013  0.00240  0.00213  cov    b10
-0.00082  0.00253  0.00226  0.00918  0.01921
;

```

The following statements produce [Output 30.10.1](#):

```

proc catmod data=fbeing;
  title 'Complex Sample Survey Analysis';
  response read b1-b10;
  factors sex $ 2, age $ 5 / _response_=sex age
                          profile=(male   '25-34',
                                       male   '35-44',
                                       male   '45-54',
                                       male   '55-64',
                                       male   '65-74',
                                       female '25-34',
                                       female '35-44',
                                       female '45-54',
                                       female '55-64',
                                       female '65-74');
  model _f=_response_
        / design title='Main Effects for Sex and Age';
run;

```


The analysis of the contrast shows that there is no significant difference among the four age groups that are under age 65.

Output 30.10.2 Health Survey Data: Age<65 Contrast

Complex Sample Survey Analysis			
Main Effects for Sex and Age			
The CATMOD Procedure			
Analysis of Contrasts			
Contrast	DF	Chi-Square	Pr > ChiSq
No Age Effect for Age<65	3	0.72	0.8678

The next model contains a binary age effect (under 65 versus 65 and over). The following statements produce [Output 30.10.3](#):

```

model _f_=(1 1 1,
           1 1 1,
           1 1 1,
           1 1 1,
           1 1 -1,
           1 -1 1,
           1 -1 1,
           1 -1 1,
           1 -1 1,
           1 -1 -1)
           (1='Intercept' ,
           2='Sex' ,
           3='Age (25-64 vs. 65-74)')
/ design title='Binary Age Effect (25-64 vs. 65-74)' ;

run;
quit;

```

Output 30.10.3 Health Survey Data: Age<65 Model

Complex Sample Survey Analysis					
Binary Age Effect (25-64 vs. 65-74)					
The CATMOD Procedure					
Response Functions and Design Matrix					
Sample	Function Number	Response Function	Design Matrix		
			1	2	3
1	1	7.93726	1	1	1
	2	7.92509	1	1	1
	3	7.82815	1	1	1
	4	7.73696	1	1	1
	5	8.16791	1	1	-1
	6	7.24978	1	-1	1
	7	7.18991	1	-1	1
	8	7.35960	1	-1	1
	9	7.31937	1	-1	1
	10	7.55184	1	-1	-1

Analysis of Variance			
Source	DF	Chi-Square	Pr > ChiSq
Intercept	1	19087.16	<.0001
Sex	1	72.64	<.0001
Age (25-64 vs. 65-74)	1	8.49	0.0036
Residual	7	3.64	0.8198

Analysis of Weighted Least Squares Estimates					
Effect	Parameter	Estimate	Standard Error	Chi-Square	Pr > ChiSq
Model	1	7.7183	0.0559	19087.16	<.0001
	2	0.2800	0.0329	72.64	<.0001
	3	-0.1304	0.0448	8.49	0.0036

The analysis of variance table in [Output 30.10.3](#) shows that the model fits (note that the goodness-of-fit statistic is the sum of the previous one ([Output 30.10.1](#)) plus the chi-square for the contrast matrix in [Output 30.10.2](#)). The age and sex effects are significant. Since the second parameter in the table of estimates is positive, males (the first level for the sex variable) have a higher predicted index of well-being than females. Since the third parameter estimate is negative, those younger than age 65 (the first level of age) have a lower predicted index of well-being than those 65 and older.

Example 30.11: Predicted Probabilities

Suppose you have collected marketing research data to examine the relationship between a prospect's likelihood of buying your product and the person's education and income. Specifically, the variables are as follows:

Variable	Levels	Interpretation
Education	high, low	Prospect's education level
Income	high, low	Prospect's income level
Purchase	yes, no	Did prospect purchase product?

The following statements first create a data set, `loan`, that contains the marketing research data. Then the `CATMOD` procedure fits a model, obtains the parameter estimates, and obtains the predicted probabilities of interest. These statements produce [Output 30.11.1](#) and [Output 30.11.2](#).

```
data loan;
  input Education $ Income $ Purchase $ wt;
  datalines;
high high yes 54
high high no 23
high low yes 41
high low no 12
low high yes 35
low high no 42
low low yes 19
low low no 8
;

ods output PredictedValues=Predicted (keep=Education Income PredFunction);
proc catmod data=loan order=data;
  weight wt;
  response marginals;
  model Purchase=Education Income / pred design;
run;

proc sort data=Predicted;
  by descending PredFunction;
run;
proc print data=Predicted;
run;
```

Notice that the preceding statements use the Output Delivery System (ODS) to output the parameter estimates instead of the `OUT=` option, though either can be used.

Output 30.11.1 Marketing Research Data: Obtaining Predicted Probabilities

Complex Sample Survey Analysis				
The CATMOD Procedure				
Data Summary				
Response	Purchase	Response Levels	2	
Weight Variable	wt	Populations	4	
Data Set	LOAN	Total Frequency	234	
Frequency Missing	0	Observations	8	
Population Profiles				
Sample	Education	Income	Sample Size	
1	high	high	77	
2	high	low	53	
3	low	high	77	
4	low	low	27	
Response Profiles				
Response	Purchase			
1	yes			
2	no			
Response Functions and Design Matrix				
Sample	Response Function	Design Matrix		
		1	2	3
1	0.70130	1	1	1
2	0.77358	1	1	-1
3	0.45455	1	-1	1
4	0.70370	1	-1	-1
Analysis of Variance				
Source	DF	Chi-Square	Pr > ChiSq	
Intercept	1	418.36	<.0001	
Education	1	8.85	0.0029	
Income	1	4.70	0.0302	
Residual	1	1.84	0.1745	

Output 30.11.1 *continued*

Analysis of Weighted Least Squares Estimates				
Parameter	Estimate	Standard Error	Chi-Square	Pr > ChiSq
Intercept	0.6481	0.0317	418.36	<.0001
Education high	0.0924	0.0311	8.85	0.0029
Income high	-0.0675	0.0312	4.70	0.0302

Predicted Values for Response Functions							
		Function	-----Observed-----	Standard	-----Predicted-----	Standard	
Education	Income	Number	Function	Error	Function	Error	Residual
high	high	1	0.701299	0.052158	0.67294	0.047794	0.028359
high	low	1	0.773585	0.057487	0.808034	0.051586	-0.03445
low	high	1	0.454545	0.056744	0.48811	0.051077	-0.03356
low	low	1	0.703704	0.087877	0.623204	0.064867	0.080499

Output 30.11.2 Predicted Probabilities Data Set

Complex Sample Survey Analysis			
Obs	Education	Income	Pred Function
1	high	low	0.808034
2	high	high	0.67294
3	low	low	0.623204
4	low	high	0.48811

You can use the predicted values (values of PredFunction in [Output 30.11.2](#)) as scores representing the likelihood that a randomly chosen subject from one of these populations will purchase the product. Notice that the “Response Profiles” table in [Output 30.11.1](#) shows you that the first sorted level of Purchase is ‘yes’, indicating that the predicted probabilities are for Pr(Purchase=‘yes’). For example, someone with high education and low income has an estimated probability of purchase of 0.808. Like any response function estimate given by PROC CATMOD, this estimate can be obtained by cross-multiplying the row from the design matrix corresponding to the sample (sample number 2 in this case) with the vector of parameter estimates: $(1 * 0.6481) + (1 * 0.0924) + (-1 * (-0.0675))$.

This ranking of scores can help in decision making (for example, with respect to allocation of advertising dollars, choice of advertising media, choice of print media, and so on).

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Chapter 31

The CLUSTER Procedure

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Overview: CLUSTER Procedure

The CLUSTER procedure hierarchically clusters the observations in a SAS data set by using one of 11 methods. The data can be coordinates or distances. If the data are coordinates, PROC CLUSTER computes (possibly squared) Euclidean distances. If you want non-Euclidean distances, use the DISTANCE procedure (see Chapter 34) to compute an appropriate distance data set that can then be used as input to PROC CLUSTER.

The clustering methods are: average linkage, the centroid method, complete linkage, density linkage (including Wong's hybrid and k th-nearest-neighbor methods), maximum likelihood for mixtures of spherical multivariate normal distributions with equal variances but possibly unequal mixing proportions, the flexible-beta method, McQuitty's similarity analysis, the median method, single linkage, two-stage density linkage, and Ward's minimum-variance method. Each method is described in the section "Clustering Methods" on page 1926.

All methods are based on the usual agglomerative hierarchical clustering procedure. Each observation begins in a cluster by itself. The two closest clusters are merged to form a new cluster that replaces the two old clusters. Merging of the two closest clusters is repeated until only one cluster is left. The various clustering methods differ in how the distance between two clusters is computed.

The CLUSTER procedure is not practical for very large data sets because the CPU time is roughly proportional to the square or cube of the number of observations. The FASTCLUS procedure (see Chapter 36) requires time proportional to the number of observations and thus can be used with much larger data sets than PROC CLUSTER. If you want to cluster a very large data set hierarchically, use PROC FASTCLUS for a preliminary cluster analysis to produce a large number of clusters. Then use PROC CLUSTER to cluster the preliminary clusters hierarchically. This method is illustrated in Example 31.3.

PROC CLUSTER displays a history of the clustering process, showing statistics useful for estimating the number of clusters in the population from which the data are sampled. It creates a dendrogram when ODS Graphics is enabled. PROC CLUSTER also creates an output data set that can be used by the TREE procedure to output the cluster membership at any desired level. For example, to obtain the six-cluster solution, you could first use PROC CLUSTER with the OUTTREE= option, and then use this output data set as the input data set to the TREE procedure. With PROC TREE, specify the NCLUSTERS=6 and the OUT= options to obtain the six-cluster solution. For an example, see Example 98.1 in Chapter 98, "The TREE Procedure."

For coordinate data, Euclidean distances are computed from differences between coordinate values. The use of differences has several important consequences:

- For differences to be valid, the variables must have an interval or stronger scale of measurement. Ordinal or ranked data are generally not appropriate for cluster analysis.
- For Euclidean distances to be comparable, equal differences should have equal practical importance. You might need to transform the variables linearly or nonlinearly to satisfy this condition. For example, if one variable is measured in dollars and one in euros, you might need to convert to the same currency. Or, if ratios are more meaningful than differences, take logarithms.

- Variables with large variances tend to have more effect on the resulting clusters than variables with small variances. If you consider all variables to be equally important, you can use the STD option in PROC CLUSTER to standardize the variables to mean 0 and standard deviation 1. However, standardization is not always appropriate. See Milligan and Cooper (1987) for a Monte Carlo study on various methods of variable standardization. You should remove outliers before using PROC CLUSTER with the STD option unless you specify the TRIM= option. The STDIZE procedure (see Chapter 87) provides additional methods for standardizing variables and imputing missing values.

The ACECLUS procedure (see Chapter 23) is useful for linear transformations of the variables if any of the following conditions hold:

- You have no idea how the variables should be scaled.
- You want to detect natural clusters regardless of whether some variables have more influence than others.
- You want to use a clustering method designed for finding compact clusters, but you want to be able to detect elongated clusters.

Agglomerative hierarchical clustering is discussed in all standard references on cluster analysis, such as Anderberg (1973); Sneath and Sokal (1973); Hartigan (1975); Everitt (1980); Spath (1980). An especially good introduction is given by Massart and Kaufman (1983). Anyone considering doing a hierarchical cluster analysis should study the Monte Carlo results of Milligan (1980); Milligan and Cooper (1985); Cooper and Milligan (1988).

Other essential, though more advanced, references on hierarchical clustering include Hartigan (1977, pp. 60–68; 1981), Wong (1982); Wong and Schaack (1982); Wong and Lane (1983). For a discussion of the confusing terminology in hierarchical cluster analysis, see Blashfield and Aldenderfer (1978).

Getting Started: CLUSTER Procedure

This example shows how you can use the CLUSTER procedure to compute hierarchical clusters of observations in a SAS data set.

Suppose you want to determine whether national figures for birth rates, death rates, and infant death rates can be used to categorize countries. Previous studies indicate that the clusters computed from this type of data can be elongated and elliptical. Thus, you need to perform a linear transformation on the raw data before the cluster analysis.

The following data¹ from Rouncefield (1995) are birth rates, death rates, and infant death rates for 97 countries. The DATA step creates the SAS data set Poverty:

```
data Poverty;
  input Birth Death InfantDeath Country $20. @@;
  datalines;
24.7  5.7  30.8 Albania                12.5 11.9  14.4 Bulgaria
13.4 11.7  11.3 Czechoslovakia        12   12.4   7.6 Former E. Germany
11.6 13.4  14.8 Hungary                14.3 10.2   16 Poland
13.6 10.7  26.9 Romania                14    9  20.2 Yugoslavia

... more lines ...

41.7 10.3   66 Zimbabwe
;
```

The data set Poverty contains the character variable Country and the numeric variables Birth, Death, and InfantDeath, which represent the birth rate per thousand, death rate per thousand, and infant death rate per thousand. The \$20. in the INPUT statement specifies that the variable Country is a character variable with a length of 20. The double trailing at sign (@@) in the INPUT statement holds the input line for further iterations of the DATA step, specifying that observations are input from each line until all values are read.

Because the variables in the data set do not have equal variance, you must perform some form of scaling or transformation. One method is to standardize the variables to mean zero and variance one. However, when you suspect that the data contain elliptical clusters, you can use the ACECLUS procedure to transform the data such that the resulting within-cluster covariance matrix is spherical. The procedure obtains approximate estimates of the pooled within-cluster covariance matrix and then computes canonical variables to be used in subsequent analyses.

The following statements perform the ACECLUS transformation by using the SAS data set Poverty. The OUT= option creates an output SAS data set called Ace that contains the canonical variable scores:

```
proc aceclus data=Poverty out=Ace p=.03 noprint;
  var Birth Death InfantDeath;
run;
```

The P= option specifies that approximately 3% of the pairs are included in the estimation of the within-cluster covariance matrix. The NOPRINT option suppresses the display of the output. The VAR statement specifies that the variables Birth, Death, and InfantDeath are used in computing the canonical variables.

The following statements invoke the CLUSTER procedure, using the SAS data set Ace created in the previous PROC ACECLUS run:

```
ods graphics on;

proc cluster data=Ace method=ward ccc pseudo print=15 out=tree
  plots=den(height=rsq);
  var can1-can3;
  id country;
run;

ods graphics off;
```

¹ These data have been compiled from the *United Nations Demographic Yearbook 1990* (United Nations publications, Sales No. E/F.91.XII.1, copyright 1991, United Nations, New York) and are reproduced with the permission of the United Nations.

The ODS GRAPHICS ON statement enables ODS Graphics. Ward's minimum-variance clustering method is specified by the METHOD= option. The CCC option displays the cubic clustering criterion, and the PSEUDO option displays pseudo F and t^2 statistics. The PRINT=15 option displays only the last 15 generations of the cluster history. By default, when ODS Graphics is enabled, a dendrogram displaying the semipartial R square is displayed on the X axis. The option PLOTS=DEN(HEIGHT=RSQ) requests a dendrogram with R square displayed instead.

The VAR statement specifies that the canonical variables computed in the ACECLUS procedure are used in the cluster analysis. The ID statement selects the variable Country as the Y axis variable in the dendrogram and also specifies that Country should be added to the Tree output data set.

PROC CLUSTER first displays the table of eigenvalues of the covariance matrix (Figure 31.1). These eigenvalues are used in the computation of the cubic clustering criterion. The first two columns list each eigenvalue and the difference between the eigenvalue and its successor. The last two columns display the individual and cumulative proportion of variation associated with each eigenvalue.

Figure 31.1 Table of Eigenvalues of the Covariance Matrix

The CLUSTER Procedure				
Ward's Minimum Variance Cluster Analysis				
Eigenvalues of the Covariance Matrix				
	Eigenvalue	Difference	Proportion	Cumulative
1	64.5500051	54.7313223	0.8091	0.8091
2	9.8186828	4.4038309	0.1231	0.9321
3	5.4148519		0.0679	1.0000
Root-Mean-Square Total-Sample Standard Deviation				5.156987
Root-Mean-Square Distance Between Observations				12.63199

Figure 31.2 displays the last 15 generations of the cluster history. First listed are the number of clusters and the names of the clusters joined. The observations are identified either by the ID value or by CL_n , where n is the number of the cluster. Next, PROC CLUSTER displays the number of observations in the new cluster and the semipartial R square. The latter value represents the decrease in the proportion of variance accounted for by joining the two clusters.

Figure 31.2 Cluster History

Cluster History									
NCL	-----Clusters	Joined-----	Freq	SpRSq	RSq	ERSq	CCC	Ps F	T i e
15	Oman	CL37	5	0.0039	.957	.933	6.03	132	12.1
14	CL31	CL22	13	0.0040	.953	.928	5.81	131	9.7
13	CL41	CL17	32	0.0041	.949	.922	5.70	131	13.1
12	CL19	CL21	10	0.0045	.945	.916	5.65	132	6.4
11	CL39	CL15	9	0.0052	.940	.909	5.60	134	6.3
10	CL76	CL27	6	0.0075	.932	.900	5.25	133	18.1
9	CL23	CL11	15	0.0130	.919	.890	4.20	125	12.4
8	CL10	Afghanistan	7	0.0134	.906	.879	3.55	122	7.3
7	CL9	CL25	17	0.0217	.884	.864	2.26	114	11.6
6	CL8	CL20	14	0.0239	.860	.846	1.42	112	10.5
5	CL14	CL13	45	0.0307	.829	.822	0.65	112	59.2
4	CL16	CL7	28	0.0323	.797	.788	0.57	122	14.8
3	CL12	CL6	24	0.0323	.765	.732	1.84	153	11.6
2	CL3	CL4	52	0.1782	.587	.613	-.82	135	48.9
1	CL5	CL2	97	0.5866	.000	.000	0.00	.	135

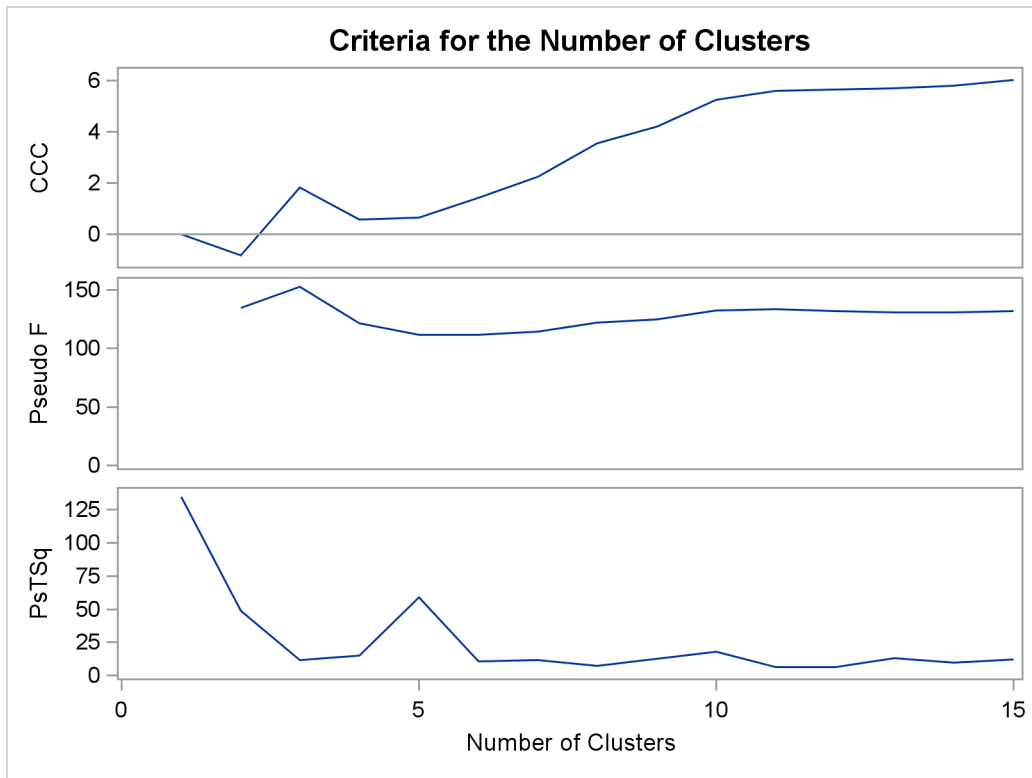
Next listed is the squared multiple correlation, R square, which is the proportion of variance accounted for by the clusters. Figure 31.2 shows that, when the data are grouped into three clusters, the proportion of variance accounted for by the clusters (R square) is just under 77%. The approximate expected value of R square is given in the ERSq column. This expectation is approximated under the null hypothesis that the data have a uniform distribution instead of forming distinct clusters.

The next three columns display the values of the cubic clustering criterion (CCC), pseudo F (PSF), and t^2 (PST2) statistics. These statistics are useful for estimating the number of clusters in the data.

The final column in Figure 31.2 lists ties for minimum distance; a blank value indicates the absence of a tie. A tie means that the clusters are indeterminate and that changing the order of the observations might change the clusters. See Example 31.4 for ways to investigate the effects of ties.

Figure 31.3 plots the three statistics for estimating the number of clusters. Peaks in the plot of the cubic clustering criterion with values greater than 2 or 3 indicate good clusters; peaks with values between 0 and 2 indicate possible clusters. Large negative values of the CCC can indicate outliers. In Figure 31.3, there is a local peak of the CCC when the number of clusters is three. The CCC drops at four clusters and then steadily increases, leveling off at eleven clusters.

Another method of judging the number of clusters in a data set is to look at the pseudo F statistic (PSF). Relatively large values indicate good numbers of clusters. In Figure 31.3, the pseudo F statistic suggests three clusters or eleven clusters.

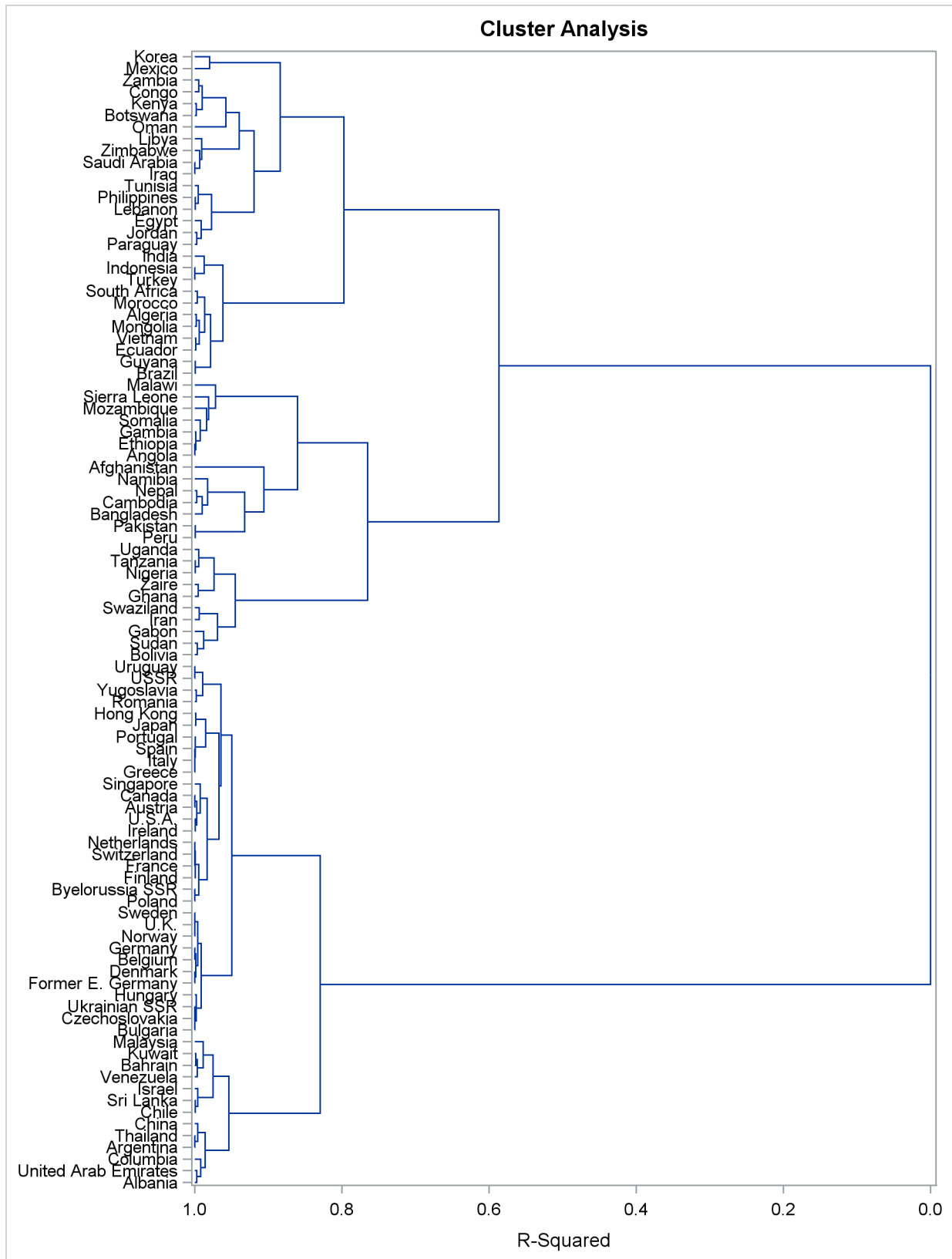
Figure 31.3 Plot of Statistics for Estimating the Number of Clusters

To interpret the values of the pseudo t^2 statistic, look down the column or look at the plot from right to left until you find the first value that is markedly larger than the previous value, then move back up the column or to the right in the plot by one step in the cluster history. In Figure 31.3, you can see possibly good clustering levels at eleven clusters, six clusters, three clusters, and two clusters.

Considered together, these statistics suggest that the data can be clustered into eleven clusters or three clusters. The following statements examine the results of clustering the data into three clusters.

Figure 31.4 displays the dendrogram. The figure provides a graphical view of the information in Figure 31.2. As the number of branches grows to the left from the root, the R square approaches 1; the first three clusters (branches of the tree) account for over half of the variation (about 77%, from Figure 31.4). In other words, only three clusters are necessary to explain over three-fourths of the variation.

Figure 31.4 Dendrogram of Clusters versus R-Square Values



You can use PROC TREE and the output data set from PROC CLUSTER to create a new data set that contains information about cluster membership as follows:

```
proc tree data=Tree out=New nclusters=3 noprint;
  height _rsq_;
  copy can1 can2;
  id country;
run;
```

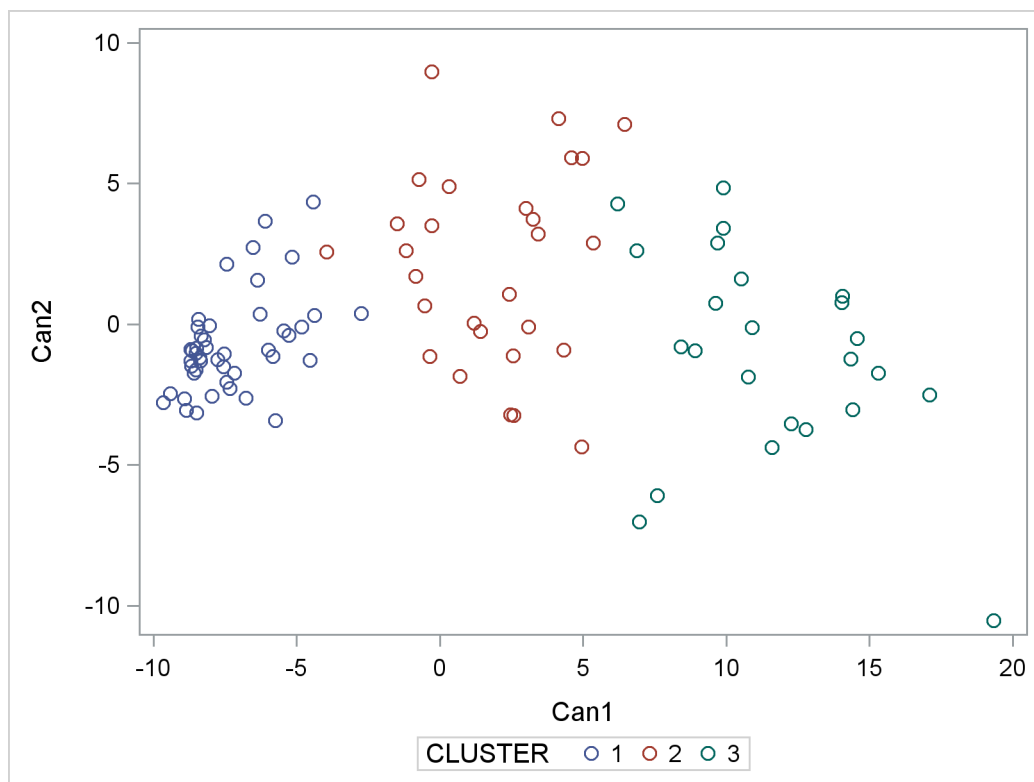
The SAS data set Tree is input. The OUT= option creates an output SAS data set named New that contains information about cluster membership. The NCLUSTERS= option specifies the number of clusters desired in the data set New. The results can be displayed in a scatter plot.

The following statements use the SGPLOT procedure to display the results that are in the SAS data set New:

```
proc sgplot data=New;
  scatter y=can2 x=can1 / group=cluster;
run;
```

The SCATTER statement requests a plot of the two canonical variables, using the value of the variable cluster, which is produced by PROC TREE as the identification variable. The results are displayed in Figure 31.5.

Figure 31.5 Plot of Canonical Variables and Cluster for Three Clusters



The statistics in Figure 31.2 and Figure 31.3, the dendrogram in Figure 31.4, and the plot of the canonical variables in Figure 31.5 assist in the estimation of the number of clusters in the data. There seems to be reasonable separation in the clusters. However, you must use this information, along with experience and knowledge of the field, to help in deciding the correct number of clusters.

Syntax: CLUSTER Procedure

The following statements are available in the CLUSTER procedure:

```
PROC CLUSTER METHOD=name < options > ;
  BY variables ;
  COPY variables ;
  FREQ variable ;
  ID variable ;
  RMSSTD variable ;
  VAR variables ;
```

Only the PROC CLUSTER statement is required, except that the FREQ statement is required when the RMSSTD statement is used; otherwise the FREQ statement is optional. Usually only the VAR statement and possibly the ID and COPY statements are needed in addition to the PROC CLUSTER statement. The rest of this section provides detailed syntax information for each of the preceding statements, beginning with the PROC CLUSTER statement. The remaining statements are covered in alphabetical order.

PROC CLUSTER Statement

```
PROC CLUSTER METHOD=name < options > ;
```

The PROC CLUSTER statement invokes the CLUSTER procedure. It also specifies a clustering method, and optionally specifies details for clustering methods, data sets, data processing, and displayed output.

Table 31.1 summarizes the options available in the PROC CLUSTER statement.

Table 31.1 PROC CLUSTER Statement Options

Option	Description
Specify input and output data sets	
DATA=	Specifies input data set
OUTTREE=	Creates output data set
Specify clustering methods	
BETA=	Specifies beta value for flexible beta method
HYBRID	Specifies Wong's hybrid clustering method
METHOD=	Specifies clustering method
MODE=	Specifies the minimum number of members for modal clusters
PENALTY=	Specifies the penalty coefficient for maximum likelihood
Control data processing prior to clustering	
NOEIGEN	Suppresses computation of eigenvalues
NONORM	Suppresses normalizing of distances
NOSQUARE	Suppresses squaring of distances
STANDARD	Standardizes variables
TRIM=	Omits points with low probability densities
Control density estimation	
K=	Specifies number of neighbors for <i>k</i> th-nearest-neighbor density estimation

Table 31.1 *continued*

Option	Description
R=	Specifies radius of sphere of support for uniform-kernel density estimation
Ties	
NOTIE	Suppresses checking for ties
Control display of the cluster history	
CCC	Displays cubic clustering criterion
NOID	Suppresses display of ID values
PRINT=	Specifies number of generations to display
PSEUDO	Displays pseudo F and t^2 statistics
RMSSTD	Displays root mean square standard deviation
RSQUARE	Displays R square and semipartial R square
Control other aspects of output	
NOPRINT	Suppresses display of all output
PLOTS=	Specifies ODS graphics details
SIMPLE	Displays simple summary statistics

METHOD=*name*

The METHOD= specification determines the clustering method used by the procedure. Any one of the following 11 methods can be specified for *name*:

AVERAGE AVE	requests average linkage (group average, unweighted pair-group method using arithmetic averages, UPGMA). Distance data are squared unless you specify the NOSQUARE option.
CENTROID CEN	requests the centroid method (unweighted pair-group method using centroids, UPGMC, centroid sorting, weighted-group method). Distance data are squared unless you specify the NOSQUARE option.
COMPLETE COM	requests complete linkage (furthest neighbor, maximum method, diameter method, rank order typal analysis). To reduce distortion of clusters by outliers, the TRIM= option is recommended.
DENSITY DEN	requests density linkage, which is a class of clustering methods using non-parametric probability density estimation. You must also specify either the K=, R=, or HYBRID option to indicate the type of density estimation to be used. See also the MODE= and DIM= options in this section.
EML	requests maximum-likelihood hierarchical clustering for mixtures of spherical multivariate normal distributions with equal variances but possibly unequal mixing proportions. Use METHOD=EML only with coordinate data. See the PENALTY= option for details. The NONORM option does not affect the reported likelihood values but does affect other unrelated criteria. The EML method is much slower than the other methods in the CLUSTER procedure.
FLEXIBLE FLE	requests the Lance-Williams flexible-beta method. See the BETA= option in this section.

MCQUITTY MCQ	requests McQuitty's similarity analysis (weighted average linkage, weighted pair-group method using arithmetic averages, WPGMA).
MEDIAN MED	requests Gower's median method (weighted pair-group method using centroids, WPGMC). Distance data are squared unless you specify the NOSQUARE option.
SINGLE SIN	requests single linkage (nearest neighbor, minimum method, connectedness method, elementary linkage analysis, or dendritic method). To reduce chaining, you can use the TRIM= option with METHOD=SINGLE.
TWOSTAGE TWO	requests two-stage density linkage. You must also specify the K=, R=, or HYBRID option to indicate the type of density estimation to be used. See also the MODE= and DIM= options in this section.
WARD WAR	requests Ward's minimum-variance method (error sum of squares, trace W). Distance data are squared unless you specify the NOSQUARE option. To reduce distortion by outliers, the TRIM= option is recommended. See the NONORM option.

The following list provides details about the other options.

BETA=*n*

specifies the beta parameter for METHOD=FLEXIBLE. The value of *n* should be less than 1, usually between 0 and -1. By default, BETA=-0.25. Milligan (1987) suggests a somewhat smaller value, perhaps -0.5, for data with many outliers.

CCC

displays the cubic clustering criterion and approximate expected R square under the uniform null hypothesis (Sarle 1983). The statistics associated with the RSQUARE option, R square and semipartial R square, are also displayed. The CCC option applies only to coordinate data. The CCC option is not appropriate with METHOD=SINGLE because of the method's tendency to chop off tails of distributions. Computation of the CCC requires the eigenvalues of the covariance matrix. If the number of variables is large, computing the eigenvalues requires much computer time and memory.

DATA=SAS-*data-set*

names the input data set that contains observations to be clustered. By default, the procedure uses the most recently created SAS data set. If the data set is TYPE=DISTANCE, the data are interpreted as a distance matrix; the number of variables must equal the number of observations in the data set or in each BY group. The distances are assumed to be Euclidean, but the procedure accepts other types of distances or dissimilarities. If the data set is not TYPE=DISTANCE, the data are interpreted as coordinates in a Euclidean space, and Euclidean distances are computed. For more about TYPE=DISTANCE data sets, see Chapter A, "[Special SAS Data Sets](#)."

Data set types (such as TYPE=DISTANCE) do not persist when you copy or modify a data set. You must specify the TYPE= data set option for the new data set, as in the following example:

```
data dist2(type=distance);
  set dist;
run;
```

If you do not specify the TYPE=DISTANCE data set option, the new data set is the default TYPE=DATA. If you use the new data set in a procedure that accepts both TYPE=DATA or TYPE=DISTANCE data sets (such as PROC CLUSTER or PROC MODECLUS), the results will be incorrect.

You cannot use a TYPE=CORR data set as input to PROC CLUSTER, since the procedure uses dissimilarity measures. Instead, you can use a DATA step or the IML procedure to extract the correlation matrix from a TYPE=CORR data set and transform the values to dissimilarities such as $1 - r$ or $1 - r^2$, where r is the correlation.

All methods produce the same results when used with coordinate data as when used with Euclidean distances computed from the coordinates. However, the DIM= option must be used with distance data if you specify METHOD=TWOSTAGE or METHOD=DENSITY or if you specify the TRIM= option.

Certain methods that are most naturally defined in terms of coordinates require *squared* Euclidean distances to be used in the combinatorial distance formulas (Lance and Williams 1967). For this reason, distance data are automatically squared when used with METHOD=AVERAGE, METHOD=CENTROID, METHOD=MEDIAN, or METHOD=WARD. If you want the combinatorial formulas to be applied to the (unsquared) distances with these methods, use the NOSQUARE option.

DIM= n

specifies the dimensionality used when computing density estimates with the TRIM= option, METHOD=DENSITY, or METHOD=TWOSTAGE. The values of n must be greater than or equal to 1. The default is the number of variables if the data are coordinates; the default is 1 if the data are distances.

HYBRID

requests the Wong (1982) hybrid clustering method in which density estimates are computed from a preliminary cluster analysis using the k -means method. The DATA= data set must contain means, frequencies, and root mean square standard deviations of the preliminary clusters (see the FREQ and RMSSTD statements). To use HYBRID, you must use either a FREQ statement or a DATA= data set that contains a _FREQ_ variable, and you must also use either an RMSSTD statement or a DATA= data set that contains an _RMSSTD_ variable.

The MEAN= data set produced by the FASTCLUS procedure is suitable for input to the CLUSTER procedure for hybrid clustering. Since this data set contains _FREQ_ and _RMSSTD_ variables, you can use it as input and then omit the FREQ and RMSSTD statements.

You must specify either METHOD=DENSITY or METHOD=TWOSTAGE with the HYBRID option. You cannot use this option in combination with the TRIM=, K=, or R= option.

K= n

specifies the number of neighbors to use for k th-nearest-neighbor density estimation (Silverman 1986, pp. 19–21 and 96–99). The number of neighbors (n) must be at least two but less than the number of observations. See the MODE= option, which follows.

Density estimation is used with the TRIM=, METHOD=DENSITY, and METHOD=TWOSTAGE options.

MODE=*n*

specifies that, when two clusters are joined, each must have at least n members in order for either cluster to be designated a modal cluster. If you specify `MODE=1`, each cluster must also have a maximum density greater than the fusion density in order for either cluster to be designated a modal cluster.

Use the `MODE=` option only with `METHOD=DENSITY` or `METHOD=TWOSTAGE`. With `METHOD=TWOSTAGE`, the `MODE=` option affects the number of modal clusters formed. With `METHOD=DENSITY`, the `MODE=` option does not affect the clustering process but does determine the number of modal clusters reported on the output and identified by the `_MODE_` variable in the output data set.

If you specify the `K=` option, the default value of `MODE=` is the same as the value of `K=` because the use of k th-nearest-neighbor density estimation limits the resolution that can be obtained for clusters with fewer than k members. If you do not specify the `K=` option, the default is `MODE=2`.

If you specify `MODE=0`, the default value is used instead of 0.

If you specify a `FREQ` statement or if a `_FREQ_` variable appears in the input data set, the `MODE=` value is compared with the number of actual observations in the clusters being joined, not with the sum of the frequencies in the clusters.

NOEIGEN

suppresses computation of the eigenvalues of the covariance matrix and substitutes the variances of the variables for the eigenvalues when computing the cubic clustering criterion. The `NOEIGEN` option saves time if the number of variables is large, but it should be used only if the variables are nearly uncorrelated. If you specify the `NOEIGEN` option and the variables are highly correlated, the cubic clustering criterion might be very liberal. The `NOEIGEN` option applies only to coordinate data.

NOID

suppresses the display of ID values for the clusters joined at each generation of the cluster history.

NONORM

prevents the distances from being normalized to unit mean or unit root mean square with most methods. With `METHOD=WARD`, the `NONORM` option prevents the between-cluster sum of squares from being normalized by the total sum of squares to yield a squared semipartial correlation. The `NONORM` option does not affect the reported likelihood values with `METHOD=EML`, but it does affect other unrelated criteria, such as the `_DIST_` variable.

NOPRINT

suppresses the display of all output. Note that this option temporarily disables the Output Delivery System (ODS). For more information, see Chapter 20, “Using the Output Delivery System.”

NOSQUARE

prevents input distances from being squared with `METHOD=AVERAGE`, `METHOD=CENTROID`, `METHOD=MEDIAN`, or `METHOD=WARD`.

If you specify the `NOSQUARE` option with distance data, the data are assumed to be squared Euclidean distances for computing R-square and related statistics defined in a Euclidean coordinate system.

If you specify the `NOSQUARE` option with coordinate data with `METHOD=CENTROID`, `METHOD=MEDIAN`, or `METHOD=WARD`, then the combinatorial formula is applied to un-

squared Euclidean distances. The resulting cluster distances do not have their usual Euclidean interpretation and are therefore labeled “False” in the output.

NOTIE

prevents PROC CLUSTER from checking for ties for minimum distance between clusters at each generation of the cluster history. If your data are measured with such precision that ties are unlikely, then you can specify the NOTIE option to reduce slightly the time and space required by the procedure. See the section “[Ties](#)” on page 1937 for more information.

OUTTREE=*SAS-data-set*

creates an output data set that can be used by the TREE procedure to draw a tree diagram. If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*. If you omit the OUTTREE= option, the data set is named by using the DATA n convention and is not permanently saved. If you do not want to create an output data set, use OUTTREE=_NULL_.

PENALTY= p

specifies the penalty coefficient used with METHOD=EML. See the section “[Clustering Methods](#)” on page 1926 for more information. Values for p must be greater than zero. By default, PENALTY=2.

PLOTS <(global-plot-options)> <= plot-request >

PLOTS <(global-plot-options)> <= (plot-request <... plot-request >)>

controls the plots produced through ODS Graphics.

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;

proc cluster method=ward plots=all;
run;

ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS](#).”

By default, PROC CLUSTER produces a dendrogram. PROC CLUSTER can also produce plots of the cubic clustering criterion, the pseudo F statistic, and the pseudo t^2 statistic from the cluster history table. These statistics are useful for estimating the number of clusters. Each statistic is plotted against the number of clusters. You can request that PROC CLUSTER create these graphs by specifying the CCC or PSEUDO options, or by specifying the statistics in a *plot-request* in the PLOT option. PROC CLUSTER might be unable to compute the statistics in some cases; for details, see the CCC and PSEUDO options. If a statistic cannot be computed, it cannot be plotted. PROC CLUSTER plots all of these statistics that are computed unless you tell it specifically what to plot using PLOTS=.

PROC CLUSTER has a CCC and PSEUDO option as well as CCC and PSEUDO plot requests. All four options are illustrated in the following step:

```
ods graphics on;

proc cluster ccc pseudo plots=(ccc pseudo);
run;

ods graphics off;
```

The maximum number of clusters shown in all the plots is the minimum of the following quantities:

- the number of observations
- the value of the PRINT= option, if that option is specified
- the maximum number of clusters for which CCC is computed, if the CCC is plotted

The *global-plot-options* apply to all plots generated by the CLUSTER procedure. The *global-plot-options* are as follows:

MAXCLUS=*n*

right-truncates the CCC, PSF, and PST2 plots at the *n* value. This prevents these plots from losing resolution when a large number of clusters are plotted. The default is MAXCLUS=200.

MAXPOINTS=*n*

MAXPTS=*n*

suppresses the dendrogram when the number of clusters exceeds the *n* value. This prevents an unreadable plot from being produced. The default is MAXPOINTS=200.

UNPACKPANEL

UNPACK

breaks a plot that is otherwise paneled into separate plots for each statistic.

ONLY

suppresses the default plots. Only plots specifically requested are displayed.

The following *plot-requests* can be specified:

ALL

generates all possible plots. The CCC and PSEUDO options must be specified to obtain the CCC, PSF and PST2 plots in addition to the dendrogram.

CCC

implicitly specifies the CCC option and, if possible, plots the cubic clustering criterion against the number of clusters.

DENDROGRAM <(*dendrogram-options*)>

requests a dendrogram and specifies *dendrogram-options*. A dendrogram is created by default unless the ONLY *global-plot-option* is requested.

Unlike most graphs, the size of the dendrogram can vary as a function of the number of objects that appear in the dendrogram. You can specify the following *dendrogram-options* to control the size and appearance of the dendrogram:

COMPUTEHEIGHT=*a b***CH=*a b***

specifies the constants for computing the height of the dendrogram. For n points being clustered, intercept a , and slope b , the height is based in part on $a + bn$. For a horizontal dendrogram, the default (given in pixels) is COMPUTEHEIGHT=100 12, the default height in pixels is $\max(100 + 12n, 480)$, the default height in inches is $\max(1.04167 + 0.125n, 5)$, and the default height in centimeters is $\max(2.64583 + 0.3175n, 12.7)$. For a vertical dendrogram, the default height is 480 pixels. The default unit is pixels, and you can use the UNIT= *dendrogram-option* to change the unit to inches or centimeters for this option. Inches equals pixels divided by 96, and centimeters equals inches times 2.54.

COMPUTEWIDTH=*a b***CW=*a b***

specifies the constants for computing the width of the dendrogram. For n points being clustered, intercept a , and slope b , the width is based in part on $a + bn$. For a vertical dendrogram, the default (given in pixels) is COMPUTEWIDTH=100 12, the default width in pixels is $\max(100 + 12n, 640)$, the default width in inches is $\max(1.04167 + 0.125n, 6.66667)$, and the default width in centimeters is $\max(2.64583 + 0.3175n, 16.933)$. For a horizontal dendrogram, the default width is 640 pixels. The default unit is pixels, and you can use the UNIT= *dendrogram-option* to change the unit to inches or centimeters for this option. Inches equals pixels divided by 96, and centimeters equals inches times 2.54.

HEIGHT=HEIGHT | MODE | NCL | RSQ**H=H | M | N | R**

specifies the method for drawing the height of the dendrogram. HEIGHT=HEIGHT is the default.

HEIGHT=HEIGHT specifies the distance or similarity between the last clusters joined, as defined in the section “Clustering Methods” on page 1926.

HEIGHT=MODE pertains to the modal clusters. With METHOD=DENSITY, the mode indicates the number of modal clusters contained by the current cluster. With METHOD=TWOSTAGE, the mode gives the maximum density in each modal cluster and the fusion density, d^* , for clusters containing two or more modal clusters; for clusters that contain no modal clusters, that value of the `_MODE_` variable is missing.

HEIGHT=NCL specifies that the number of clusters is used.

HEIGHT=RSQ specifies that the squared multiple correlation is used.

HORIZONTAL | VERTICAL

specifies either a horizontal dendrogram with the objects on the vertical axis (HORIZONTAL) or a vertical dendrogram with the objects on the horizontal axis (VERTICAL). The default is HORIZONTAL.

SETHEIGHT=*height***SH=*height***

specifies the height of the dendrogram. By default, the height is based on the COMPUTEHEIGHT= option. The default unit is pixels, and you can use the UNIT= *dendrogram-option* to change the unit to inches or centimeters for this *dendrogram-option*.

SETWIDTH=width

SW=width

specifies the width of the dendrogram. By default, the width is based on the COMPUTEWIDTH= option. The default unit is pixels, and you can use the UNIT= *dendrogram-option* to change the unit to inches or centimeters for this *dendrogram-option*.

UNIT=PX | IN | CM

specifies the unit (pixels, inches, or centimeters) for the SETHEIGHT=, SETWIDTH=, COMPUTEHEIGHT=, and COMPUTEWIDTH= *dendrogram-options*.

NONE

suppresses all plots.

PSEUDO

implicitly specifies the PSEUDO option and, if possible, plots the pseudo F statistic and the pseudo t^2 statistic against the number of clusters.

PSF

implicitly specifies the PSEUDO option and, if possible, plots the pseudo F statistic against the number of clusters.

PST2

implicitly specifies the PSEUDO option and, if possible, plots the pseudo t^2 statistic against the number of clusters.

You can specify one or more of the plot requests in the same PLOT option. For example, all of the following are valid:

```
proc cluster plots=(ccc pst2);
proc cluster plots=(psf);
proc cluster plots=psf;
```

The first statement plots both the cubic clustering criterion and the pseudo t^2 statistic, while the second and third statements plot the pseudo F statistic only. When you specify only one plot request, you can omit the parentheses around the plot request. When you specify more than one plot request, you must specify parentheses. Otherwise the second and subsequent plot requests are options. Since CCC and PSEUDO are both options as well as plot requests, the following three statements are valid, but they are not equivalent:

```
proc cluster plots(only)=ccc pseudo;
proc cluster plots(only)=pseudo ccc;
proc cluster plots(only)=(ccc pseudo);
```

The first two examples have one plot request and one procedure option. The third example has two plot requests.

The names of the graphs that PROC CLUSTER generates are listed in [Table 31.5](#), along with the required statements and options.

PRINT=*n* | P=*n*

specifies the number of generations of the cluster history to display. The PRINT= option displays the latest *n* generations; for example, PRINT=5 displays the cluster history from one cluster through five clusters. The value of PRINT= must be a nonnegative integer. The default is to display all generations. Specify PRINT=0 to suppress the cluster history.

PSEUDO

displays pseudo *F* and t^2 statistics. This option is effective only when the data are coordinates or when METHOD=AVERAGE, METHOD=CENTROID, or METHOD=WARD is specified. See the section “Miscellaneous Formulas” on page 1933 for more information. The PSEUDO option is not appropriate with METHOD=SINGLE because of the method’s tendency to chop off tails of distributions.

R=*n*

specifies the radius of the sphere of support for uniform-kernel density estimation (Silverman 1986, pp. 11–13 and 75–94).

The value of R= must be greater than zero.

Density estimation is used with the TRIM=, METHOD=DENSITY, and METHOD=TWOSTAGE options.

RMSSTD

displays the root mean square standard deviation of each cluster. This option is effective only when the data are coordinates or when METHOD=AVERAGE, METHOD=CENTROID, or METHOD=WARD is specified.

See the section “Miscellaneous Formulas” on page 1933 for more information.

RSQUARE | RSQ

displays the R square and semipartial R square. This option is effective only when the data are coordinates or when METHOD=AVERAGE or METHOD=CENTROID is specified. The R square and semipartial R square statistics are always displayed with METHOD=WARD. See the section “Miscellaneous Formulas” on page 1933 for more information..

SIMPLE | S

displays means, standard deviations, skewness, kurtosis, and a coefficient of bimodality. The SIMPLE option applies only to coordinate data. See the section “Miscellaneous Formulas” on page 1933 for more information.

STANDARD | STD

standardizes the variables to mean 0 and standard deviation 1. The STANDARD option applies only to coordinate data.

TRIM=*p*

omits points with low estimated probability densities from the analysis. Valid values for the TRIM= option are $0 \leq p < 100$. If $p < 1$, then *p* is the proportion of observations omitted. If $p \geq 1$, then *p* is interpreted as a percentage. A specification of TRIM=10, which trims 10% of the points, is a reasonable value for many data sets. Densities are estimated by the *k*th-nearest-neighbor or uniform-kernel method. Trimmed points are indicated by a negative value of the _FREQ_ variable in the OUTTREE= data set.

You must use either the K= or R= option when you use TRIM=. You cannot use the HYBRID option in combination with TRIM=, so you might want to use the DIM= option instead. If you specify the STANDARD option in combination with TRIM=, the variables are standardized both before and after trimming.

The TRIM= option is useful for removing outliers and reducing chaining. Trimming is highly recommended with METHOD=WARD or METHOD=COMPLETE because clusters from these methods can be severely distorted by outliers. Trimming is also valuable with METHOD=SINGLE since single linkage is the method most susceptible to chaining. Most other methods also benefit from trimming. However, trimming is unnecessary with METHOD=TWOSTAGE or METHOD=DENSITY when *k*th-nearest-neighbor density estimation is used.

Use of the TRIM= option can spuriously inflate the cubic clustering criterion and the pseudo *F* and t^2 statistics. Trimming only outliers improves the accuracy of the statistics, but trimming saddle regions between clusters yields excessively large values.

BY Statement

BY variables ;

You can specify a BY statement with PROC CLUSTER to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the CLUSTER procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

COPY Statement

COPY variables ;

The variables in the COPY statement are copied from the input data set to the OUTTREE= data set. Observations in the OUTTREE= data set that represent clusters of more than one observation from the input data set have missing values for the COPY variables.

FREQ Statement

FREQ *variable* ;

If one variable in the input data set represents the frequency of occurrence for other values in the observation, specify the variable's name in a FREQ statement. PROC CLUSTER then treats the data set as if each observation appeared n times, where n is the value of the FREQ variable for the observation. Noninteger values of the FREQ variable are truncated to the largest integer less than the FREQ value.

If you omit the FREQ statement but the DATA= data set contains a variable called `_FREQ_`, then frequencies are obtained from the `_FREQ_` variable. If neither a FREQ statement nor an `_FREQ_` variable is present, each observation is assumed to have a frequency of one.

If each observation in the DATA= data set represents a cluster (for example, clusters formed by PROC FASTCLUS), the variable specified in the FREQ statement should give the number of original observations in each cluster.

If you specify the RMSSTD statement, a FREQ statement is required. A FREQ statement or `_FREQ_` variable is required when you specify the HYBRID option.

With most clustering methods, the same clusters are obtained from a data set with a FREQ variable as from a similar data set without a FREQ variable, if each observation is repeated as many times as the value of the FREQ variable in the first data set. The FLEXIBLE method can yield different results due to the nature of the combinatorial formula. The DENSITY and TWOSTAGE methods are also exceptions because two identical observations can be absorbed one at a time by a cluster with a higher density. If you are using a FREQ statement with either the DENSITY or TWOSTAGE method, see the [MODE=option](#) for details.

ID Statement

ID *variable* ;

The values of the ID variable identify observations in the displayed cluster history and in the OUTTREE= data set. If the ID statement is omitted, each observation is denoted by `OB n` , where n is the observation number.

RMSSTD Statement

RMSSTD *variable* ;

If the coordinates in the DATA= data set represent cluster means (for example, formed by the FASTCLUS procedure), you can obtain accurate statistics in the cluster histories for `METHOD=AVERAGE`, `METHOD=CENTROID`, or `METHOD=WARD` if the data set contains both of the following:

- a variable giving the number of original observations in each cluster (see the discussion of the FREQ statement earlier in this chapter)
- a variable giving the root mean squared standard deviation of each cluster

Specify the name of the variable containing root mean squared standard deviations in the RMSSTD statement. If you specify the RMSSTD statement, you must also specify a FREQ statement.

If you omit the RMSSTD statement but the DATA= data set contains a variable called `_RMSSTD_`, then the root mean squared standard deviations are obtained from the `_RMSSTD_` variable.

An RMSSTD statement or `_RMSSTD_` variable is required when you specify the HYBRID option.

A data set created by PROC FASTCLUS, using the MEAN= option, contains `_FREQ_` and `_RMSSTD_` variables, so you do not have to use FREQ and RMSSTD statements when using such a data set as input to the CLUSTER procedure.

VAR Statement

VAR *variables* ;

The VAR statement lists numeric variables to be used in the cluster analysis. If you omit the VAR statement, all numeric variables not listed in other statements are used.

Details: CLUSTER Procedure

Clustering Methods

The following notation is used, with lowercase symbols generally pertaining to observations and uppercase symbols pertaining to clusters:

n	number of observations
v	number of variables if data are coordinates
G	number of clusters at any given level of the hierarchy
x_i or \mathbf{x}_i	i th observation (row vector if coordinate data)
C_K	K th cluster, subset of $\{1, 2, \dots, n\}$
N_K	number of observations in C_K
$\bar{\mathbf{x}}$	sample mean vector
$\bar{\mathbf{x}}_K$	mean vector for cluster C_K
$\ \mathbf{x}\ $	Euclidean length of the vector \mathbf{x} —that is, the square root of the sum of the squares of the elements of \mathbf{x}
T	$\sum_{i=1}^n \ \mathbf{x}_i - \bar{\mathbf{x}}\ ^2$
W_K	$\sum_{i \in C_K} \ \mathbf{x}_i - \bar{\mathbf{x}}_K\ ^2$
P_G	$\sum W_J$, where summation is over the G clusters at the G th level of the hierarchy
B_{KL}	$W_M - W_K - W_L$ if $C_M = C_K \cup C_L$
$d(\mathbf{x}, \mathbf{y})$	any distance or dissimilarity measure between observations or vectors \mathbf{x} and \mathbf{y}
D_{KL}	any distance or dissimilarity measure between clusters C_K and C_L

The distance between two clusters can be defined either directly or combinatorially (Lance and Williams 1967)—that is, by an equation for updating a distance matrix when two clusters are joined. In all of the following combinatorial formulas, it is assumed that clusters C_K and C_L are merged to form C_M , and the formula gives the distance between the new cluster C_M and any other cluster C_J .

For an introduction to most of the methods used in the CLUSTER procedure, see Massart and Kaufman (1983).

Average Linkage

The following method is obtained by specifying METHOD=AVERAGE. The distance between two clusters is defined by

$$D_{KL} = \frac{1}{N_K N_L} \sum_{i \in C_K} \sum_{j \in C_L} d(x_i, x_j)$$

If $d(\mathbf{x}, \mathbf{y}) = \|\mathbf{x} - \mathbf{y}\|^2$, then

$$D_{KL} = \|\bar{\mathbf{x}}_K - \bar{\mathbf{x}}_L\|^2 + \frac{W_K}{N_K} + \frac{W_L}{N_L}$$

The combinatorial formula is

$$D_{JM} = \frac{N_K D_{JK} + N_L D_{JL}}{N_M}$$

In average linkage the distance between two clusters is the average distance between pairs of observations, one in each cluster. Average linkage tends to join clusters with small variances, and it is slightly biased toward producing clusters with the same variance.

Average linkage was originated by Sokal and Michener (1958).

Centroid Method

The following method is obtained by specifying METHOD=CENTROID. The distance between two clusters is defined by

$$D_{KL} = \|\bar{\mathbf{x}}_K - \bar{\mathbf{x}}_L\|^2$$

If $d(\mathbf{x}, \mathbf{y}) = \|\mathbf{x} - \mathbf{y}\|^2$, then the combinatorial formula is

$$D_{JM} = \frac{N_K D_{JK} + N_L D_{JL}}{N_M} - \frac{N_K N_L D_{KL}}{N_M^2}$$

In the centroid method, the distance between two clusters is defined as the (squared) Euclidean distance between their centroids or means. The centroid method is more robust to outliers than most other hierarchical methods but in other respects might not perform as well as Ward's method or average linkage (Milligan 1980).

The centroid method was originated by Sokal and Michener (1958).

Complete Linkage

The following method is obtained by specifying METHOD=COMPLETE. The distance between two clusters is defined by

$$D_{KL} = \max_{i \in C_K} \max_{j \in C_L} d(x_i, x_j)$$

The combinatorial formula is

$$D_{JM} = \max(D_{JK}, D_{JL})$$

In complete linkage, the distance between two clusters is the maximum distance between an observation in one cluster and an observation in the other cluster. Complete linkage is strongly biased toward producing clusters with roughly equal diameters, and it can be severely distorted by moderate outliers (Milligan 1980).

Complete linkage was originated by Sorensen (1948).

Density Linkage

The phrase *density linkage* is used here to refer to a class of clustering methods that use nonparametric probability density estimates (for example, Hartigan 1975, pp. 205–212; Wong 1982; Wong and Lane 1983). Density linkage consists of two steps:

1. A new dissimilarity measure, d^* , based on density estimates and adjacencies is computed. If x_i and x_j are adjacent (the definition of *adjacency* depends on the method of density estimation), then $d^*(x_i, x_j)$ is the reciprocal of an estimate of the density midway between x_i and x_j ; otherwise, $d^*(x_i, x_j)$ is infinite.
2. A single linkage cluster analysis is performed using d^* .

The CLUSTER procedure supports three types of density linkage: the k th-nearest-neighbor method, the uniform-kernel method, and Wong's hybrid method. These are obtained by using METHOD=DENSITY and the K=, R=, and HYBRID options, respectively.

*k*th-Nearest-Neighbor Method

The k th-nearest-neighbor method (Wong and Lane 1983) uses k th-nearest-neighbor density estimates. Let $r_k(x)$ be the distance from point x to the k th-nearest observation, where k is the value specified for the K= option. Consider a closed sphere centered at x with radius $r_k(x)$. The estimated density at x , $f(x)$, is the proportion of observations within the sphere divided by the volume of the sphere. The new dissimilarity measure is computed as

$$d^*(x_i, x_j) = \begin{cases} \frac{1}{2} \left(\frac{1}{f(x_i)} + \frac{1}{f(x_j)} \right) & \text{if } d(x_i, x_j) \leq \max(r_k(x_i), r_k(x_j)) \\ \infty & \text{otherwise} \end{cases}$$

Wong and Lane (1983) show that k th-nearest-neighbor density linkage is strongly set consistent for high-density (density-contour) clusters if k is chosen such that $k/n \rightarrow 0$ and $k/\ln(n) \rightarrow \infty$ as $n \rightarrow \infty$. Wong and Schaack (1982) discuss methods for estimating the number of population clusters by using k th-nearest-neighbor clustering.

Uniform-Kernel Method

The uniform-kernel method uses uniform-kernel density estimates. Let r be the value specified for the R= option. Consider a closed sphere centered at point x with radius r . The estimated density at x , $f(x)$, is the proportion of observations within the sphere divided by the volume of the sphere. The new dissimilarity measure is computed as

$$d^*(x_i, x_j) = \begin{cases} \frac{1}{2} \left(\frac{1}{f(x_i)} + \frac{1}{f(x_j)} \right) & \text{if } d(x_i, x_j) \leq r \\ \infty & \text{otherwise} \end{cases}$$

Wong's Hybrid Method

The Wong (1982) hybrid clustering method uses density estimates based on a preliminary cluster analysis by the k -means method. The preliminary clustering can be done by the FASTCLUS procedure, by using the MEAN= option to create a data set containing cluster means, frequencies, and root mean squared standard deviations. This data set is used as input to the CLUSTER procedure, and the HYBRID option is specified with METHOD=DENSITY to request the hybrid analysis. The hybrid method is appropriate for very large data sets but should not be used with small data sets—say, than those with fewer than 100 observations in the original data. The term *preliminary cluster* refers to an observation in the DATA= data set.

For preliminary cluster C_K , N_K and W_K are obtained from the input data set, as are the cluster means or the distances between the cluster means. Preliminary clusters C_K and C_L are considered adjacent if the midpoint between \bar{x}_K and \bar{x}_L is closer to either \bar{x}_K or \bar{x}_L than to any other preliminary cluster mean or, equivalently, if $d^2(\bar{x}_K, \bar{x}_L) < d^2(\bar{x}_K, \bar{x}_M) + d^2(\bar{x}_L, \bar{x}_M)$ for all other preliminary clusters C_M , $M \neq K$ or L . The new dissimilarity measure is computed as

$$d^*(\bar{x}_K, \bar{x}_L) = \begin{cases} \frac{(W_K + W_L + \frac{1}{4}(N_K + N_L)d^2(\bar{x}_K, \bar{x}_L))^{\frac{v}{2}}}{(N_K + N_L)^{1 + \frac{v}{2}}} & \text{if } C_K \text{ and } C_L \text{ are adjacent} \\ \infty & \text{otherwise} \end{cases}$$

Using the K= and R= Options

The values of the K= and R= options are called *smoothing parameters*. Small values of K= or R= produce jagged density estimates and, as a consequence, many modes. Large values of K= or R= produce smoother density estimates and fewer modes. In the hybrid method, the smoothing parameter is the number of clusters in the preliminary cluster analysis. The number of modes in the final analysis tends to increase as the number of clusters in the preliminary analysis increases. Wong (1982) suggests using $n^{0.3}$ preliminary clusters, where n is the number of observations in the original data set. There is no rule of thumb for selecting K= values. For all types of density linkage, you should repeat the analysis with several different values of the smoothing parameter (Wong and Schaack 1982).

There is no simple answer to the question of which smoothing parameter to use (Silverman 1986, pp. 43–61, 84–88, and 98–99). It is usually necessary to try several different smoothing parameters. A reasonable first guess for the R= option in many coordinate data sets is given by

$$\left[\frac{2^{v+2}(v+2)\Gamma(\frac{v}{2}+1)}{nv^2} \right]^{\frac{1}{v+4}} \sqrt{\sum_{l=1}^v s_l^2}$$

where s_l^2 is the standard deviation of the l th variable. The estimate for R= can be computed in a DATA step by using the GAMMA function for Γ . This formula is derived under the assumption that the data are

sampled from a multivariate normal distribution and tends, therefore, to be too large (oversmooth) if the true distribution is multimodal. Robust estimates of the standard deviations can be preferable if there are outliers. If the data are distances, the factor $\sum s_i^2$ can be replaced by an average (mean, trimmed mean, median, root mean square, and so on) distance divided by $\sqrt{2}$. To prevent outliers from appearing as separate clusters, you can also specify $K=2$, or more generally $K=m$, $m \geq 2$, which in most cases forces clusters to have at least m members.

If the variables all have unit variance (for example, if the STANDARD option is used), Table 31.2 can be used to obtain an initial guess for the R= option.

Since infinite d^* values occur in density linkage, the final number of clusters can exceed one when there are wide gaps between the clusters or when the smoothing parameter results in little smoothing.

Density linkage applies no constraints to the shapes of the clusters and, unlike most other hierarchical clustering methods, is capable of recovering clusters with elongated or irregular shapes. Since density linkage uses less prior knowledge about the shape of the clusters than do methods restricted to compact clusters, density linkage is less effective at recovering compact clusters from small samples than are methods that always recover compact clusters, regardless of the data.

Table 31.2 Reasonable First Guess for the R= Option for Standardized Data

Number of Observations	Number of Variables									
	1	2	3	4	5	6	7	8	9	10
20	1.01	1.36	1.77	2.23	2.73	3.25	3.81	4.38	4.98	5.60
35	0.91	1.24	1.64	2.08	2.56	3.08	3.62	4.18	4.77	5.38
50	0.84	1.17	1.56	1.99	2.46	2.97	3.50	4.06	4.64	5.24
75	0.78	1.09	1.47	1.89	2.35	2.85	3.38	3.93	4.50	5.09
100	0.73	1.04	1.41	1.82	2.28	2.77	3.29	3.83	4.40	4.99
150	0.68	0.97	1.33	1.73	2.18	2.66	3.17	3.71	4.27	4.85
200	0.64	0.93	1.28	1.67	2.11	2.58	3.09	3.62	4.17	4.75
350	0.57	0.85	1.18	1.56	1.98	2.44	2.93	3.45	4.00	4.56
500	0.53	0.80	1.12	1.49	1.91	2.36	2.84	3.35	3.89	4.45
750	0.49	0.74	1.06	1.42	1.82	2.26	2.74	3.24	3.77	4.32
1000	0.46	0.71	1.01	1.37	1.77	2.20	2.67	3.16	3.69	4.23
1500	0.43	0.66	0.96	1.30	1.69	2.11	2.57	3.06	3.57	4.11
2000	0.40	0.63	0.92	1.25	1.63	2.05	2.50	2.99	3.49	4.03

EML

The following method is obtained by specifying METHOD=EML. The distance between two clusters is given by

$$D_{KL} = nv \ln \left(1 + \frac{B_{KL}}{P_G} \right) - 2 (N_M \ln(N_M) - N_K \ln(N_K) - N_L \ln(N_L))$$

The EML method joins clusters to maximize the likelihood at each level of the hierarchy under the following assumptions:

- multivariate normal mixture
- equal spherical covariance matrices
- unequal sampling probabilities

The EML method is similar to Ward's minimum-variance method but removes the bias toward equal-sized clusters. Practical experience has indicated that EML is somewhat biased toward unequal-sized clusters. You can specify the `PENALTY=` option to adjust the degree of bias. If you specify `PENALTY=p`, the formula is modified to

$$D_{KL} = nv \ln \left(1 + \frac{B_{KL}}{P_G} \right) - p (N_M \ln(N_M) - N_K \ln(N_K) - N_L \ln(N_L))$$

The EML method was derived by W. S. Sarle of SAS Institute from the maximum likelihood formula obtained by Symons (1981, p. 37, Equation 8) for disjoint clustering. There are currently no other published references on the EML method.

Flexible-Beta Method

The following method is obtained by specifying `METHOD=FLEXIBLE`. The combinatorial formula is

$$D_{JM} = (D_{JK} + D_{JL}) \frac{1-b}{2} + D_{KL}b$$

where b is the value of the `BETA=` option, or -0.25 by default.

The flexible-beta method was developed by Lance and Williams (1967); see also Milligan (1987).

McQuitty's Similarity Analysis

The following method is obtained by specifying `METHOD=MCQUITTY`. The combinatorial formula is

$$D_{JM} = \frac{D_{JK} + D_{JL}}{2}$$

The method was independently developed by Sokal and Michener (1958) and McQuitty (1966).

Median Method

The following method is obtained by specifying `METHOD=MEDIAN`. If $d(\mathbf{x}, \mathbf{y}) = \|\mathbf{x} - \mathbf{y}\|^2$, then the combinatorial formula is

$$D_{JM} = \frac{D_{JK} + D_{JL}}{2} - \frac{D_{KL}}{4}$$

The median method was developed by Gower (1967).

Single Linkage

The following method is obtained by specifying METHOD=SINGLE. The distance between two clusters is defined by

$$D_{KL} = \min_{i \in C_K} \min_{j \in C_L} d(x_i, x_j)$$

The combinatorial formula is

$$D_{JM} = \min(D_{JK}, D_{JL})$$

In single linkage, the distance between two clusters is the minimum distance between an observation in one cluster and an observation in the other cluster. Single linkage has many desirable theoretical properties (Jardine and Sibson 1971; Fisher and Van Ness 1971; Hartigan 1981) but has fared poorly in Monte Carlo studies (for example, Milligan 1980). By imposing no constraints on the shape of clusters, single linkage sacrifices performance in the recovery of compact clusters in return for the ability to detect elongated and irregular clusters. You must also recognize that single linkage tends to chop off the tails of distributions before separating the main clusters (Hartigan 1981). The notorious chaining tendency of single linkage can be alleviated by specifying the TRIM= option (Wishart 1969, pp. 296–298).

Density linkage and two-stage density linkage retain most of the virtues of single linkage while performing better with compact clusters and possessing better asymptotic properties (Wong and Lane 1983).

Single linkage was originated by Florek et al. (1951b, a) and later reinvented by McQuitty (1957) and Sneath (1957).

Two-Stage Density Linkage

If you specify METHOD=DENSITY, the modal clusters often merge before all the points in the tails have clustered. The option METHOD=TWOSTAGE is a modification of density linkage that ensures that all points are assigned to modal clusters before the modal clusters are permitted to join. The CLUSTER procedure supports the same three varieties of two-stage density linkage as of ordinary density linkage: *k*th-nearest neighbor, uniform kernel, and hybrid.

In the first stage, disjoint modal clusters are formed. The algorithm is the same as the single linkage algorithm ordinarily used with density linkage, with one exception: two clusters are joined only if at least one of the two clusters has fewer members than the number specified by the MODE= option. At the end of the first stage, each point belongs to one modal cluster.

In the second stage, the modal clusters are hierarchically joined by single linkage. The final number of clusters can exceed one when there are wide gaps between the clusters or when the smoothing parameter is small.

Each stage forms a tree that can be plotted by the TREE procedure. By default, the TREE procedure plots the tree from the first stage. To obtain the tree for the second stage, use the option HEIGHT=MODE in the PROC TREE statement. You can also produce a single tree diagram containing both stages, with the number of clusters as the height axis, by using the option HEIGHT=N in the PROC TREE statement. To produce an output data set from PROC TREE containing the modal clusters, use _HEIGHT_ for the HEIGHT variable (the default) and specify LEVEL=0.

Two-stage density linkage was developed by W. S. Sarle of SAS Institute. There are currently no other published references on two-stage density linkage.

Ward's Minimum-Variance Method

The following method is obtained by specifying METHOD=WARD. The distance between two clusters is defined by

$$D_{KL} = B_{KL} = \frac{\|\bar{\mathbf{x}}_K - \bar{\mathbf{x}}_L\|^2}{\frac{1}{N_K} + \frac{1}{N_L}}$$

If $d(\mathbf{x}, \mathbf{y}) = \frac{1}{2}\|\mathbf{x} - \mathbf{y}\|^2$, then the combinatorial formula is

$$D_{JM} = \frac{(N_J + N_K)D_{JK} + (N_J + N_L)D_{JL} - N_J D_{KL}}{N_J + N_M}$$

In Ward's minimum-variance method, the distance between two clusters is the ANOVA sum of squares between the two clusters added up over all the variables. At each generation, the within-cluster sum of squares is minimized over all partitions obtainable by merging two clusters from the previous generation. The sums of squares are easier to interpret when they are divided by the total sum of squares to give proportions of variance (squared semipartial correlations).

Ward's method joins clusters to maximize the likelihood at each level of the hierarchy under the following assumptions:

- multivariate normal mixture
- equal spherical covariance matrices
- equal sampling probabilities

Ward's method tends to join clusters with a small number of observations, and it is strongly biased toward producing clusters with roughly the same number of observations. It is also very sensitive to outliers (Milligan 1980).

Ward (1963) describes a class of hierarchical clustering methods including the minimum variance method.

Miscellaneous Formulas

The root mean squared standard deviation of a cluster C_K is

$$\text{RMSSTD} = \sqrt{\frac{W_K}{v(N_K - 1)}}$$

The R-square statistic for a given level of the hierarchy is

$$R^2 = 1 - \frac{P_G}{T}$$

The squared semipartial correlation for joining clusters C_K and C_L is

$$\text{semipartial } R^2 = \frac{B_{KL}}{T}$$

The bimodality coefficient is

$$b = \frac{m_3^2 + 1}{m_4 + \frac{3(n-1)^2}{(n-2)(n-3)}}$$

where m_3 is skewness and m_4 is kurtosis. Values of b greater than 0.555 (the value for a uniform population) can indicate bimodal or multimodal marginal distributions. The maximum of 1.0 (obtained for the Bernoulli distribution) is obtained for a population with only two distinct values. Very heavy-tailed distributions have small values of b regardless of the number of modes.

Formulas for the cubic-clustering criterion and approximate expected R square are given in Sarle (1983).

The pseudo F statistic for a given level is

$$\text{pseudo } F = \frac{\frac{T - P_G}{G - 1}}{\frac{P_G}{n - G}}$$

The pseudo t^2 statistic for joining C_K and C_L is

$$\text{pseudo } t^2 = \frac{B_{KL}}{\frac{W_K + W_L}{N_K + N_L - 2}}$$

The pseudo F and t^2 statistics can be useful indicators of the number of clusters, but they are *not* distributed as F and t^2 random variables. If the data are independently sampled from a multivariate normal distribution with a scalar covariance matrix and if the clustering method allocates observations to clusters randomly (which no clustering method actually does), then the pseudo F statistic is distributed as an F random variable with $v(G - 1)$ and $v(n - G)$ degrees of freedom. Under the same assumptions, the pseudo t^2 statistic is distributed as an F random variable with v and $v(N_K + N_L - 2)$ degrees of freedom. The pseudo t^2 statistic differs computationally from Hotelling's T^2 in that the latter uses a general symmetric covariance matrix instead of a scalar covariance matrix. The pseudo F statistic was suggested by Calinski and Harabasz (1974). The pseudo t^2 statistic is related to the $J_e(2)/J_e(1)$ statistic of Duda and Hart (1973) by

$$\frac{J_e(2)}{J_e(1)} = \frac{W_K + W_L}{W_M} = \frac{1}{1 + \frac{t^2}{N_K + N_L - 2}}$$

See Milligan and Cooper (1985) and Cooper and Milligan (1988) regarding the performance of these statistics in estimating the number of population clusters. Conservative tests for the number of clusters using the pseudo F and t^2 statistics can be obtained by the Bonferroni approach (Hawkins, Muller, and ten Krooden 1982, pp. 337–340).

Ultrametrics

A dissimilarity measure $d(x, y)$ is called an *ultrametric* if it satisfies the following conditions:

- $d(x, x) = 0$ for all x
- $d(x, y) \geq 0$ for all x, y
- $d(x, y) = d(y, x)$ for all x, y
- $d(x, y) \leq \max(d(x, z), d(y, z))$ for all x, y , and z

Any hierarchical clustering method induces a dissimilarity measure on the observations—say, $h(x_i, x_j)$. Let C_M be the cluster with the fewest members that contains both x_i and x_j . Assume C_M was formed by joining C_K and C_L . Then define $h(x_i, x_j) = D_{KL}$.

If the fusion of C_K and C_L reduces the number of clusters from g to $g - 1$, then define $D_{(g)} = D_{KL}$. Johnson (1967) shows that if

$$0 \leq D_{(n)} \leq D_{(n-1)} \leq \cdots \leq D_{(2)}$$

then $h(\cdot, \cdot)$ is an ultrametric. A method that always satisfies this condition is said to be a *monotonic* or *ultrametric clustering method*. All methods implemented in PROC CLUSTER except CENTROID, EML, and MEDIAN are ultrametric (Milligan 1979; Batagelj 1981).

Algorithms

Anderberg (1973) describes three algorithms for implementing agglomerative hierarchical clustering: stored data, stored distance, and sorted distance. The algorithms used by PROC CLUSTER for each method are indicated in Table 31.3. For METHOD=AVERAGE, METHOD=CENTROID, or METHOD=WARD, either the stored data or the stored distance algorithm can be used. For these methods, if the data are distances or if you specify the NOSQUARE option, the stored distance algorithm is used; otherwise, the stored data algorithm is used.

Table 31.3 Three Algorithms for Implementing Agglomerative Hierarchical Clustering

Clustering Method	Algorithm		
	Stored Data	Stored Distance	Sorted Distance
AVERAGE	x	x	
CENTROID	x	x	
COMPLETE		x	
DENSITY			x
EML	x		
FLEXIBLE		x	
MCQUITTY		x	
MEDIAN		x	
SINGLE		x	
TWOSTAGE			x
WARD	x	x	

Note: All of the hierarchical methods accept coordinate data. Methods that require stored or sorted distances automatically calculate distances from the coordinates.

Computational Resources

The CLUSTER procedure stores the data (including the COPY and ID variables) in memory or, if necessary, on disk. If eigenvalues are computed, the covariance matrix is stored in memory. If the stored distance or sorted distance algorithm is used, the distances are stored in memory or, if necessary, on disk.

With coordinate data, the increase in CPU time is roughly proportional to the number of variables. The VAR statement should list the variables in order of decreasing variance for greatest efficiency.

For both coordinate and distance data, the dominant factor determining CPU time is the number of observations. For density methods with coordinate data, the asymptotic time requirements are somewhere between $n \ln(n)$ and n^2 , depending on how the smoothing parameter increases. For other methods except EML, time is roughly proportional to n^2 . For the EML method, time is roughly proportional to n^3 .

PROC CLUSTER runs much faster if the data can be stored in memory and, when the stored distance algorithm is used, if the distance matrix can be stored in memory as well. To estimate the bytes of memory needed for the data, use the following formula and round up to the nearest multiple of d .

$$\begin{array}{ll}
 n(vd & + 8d + i \\
 & + i & \text{if density estimation or the} \\
 & & \text{sorted distance algorithm is used} \\
 & + 3d & \text{if stored data algorithm is used} \\
 & + 3d & \text{if density estimation is used} \\
 & + \max(8, \text{length of ID variable}) & \text{if ID variable is used} \\
 & + \text{length of ID variable} & \text{if ID variable is used} \\
 & + \text{sum of lengths of COPY variables}) & \text{if COPY variables is used}
 \end{array}$$

where

- n is the number of observations
- v is the number of variables
- d is the size of a C variable of type *double*. For most computers, $d = 8$.
- i is the size of a C variable of type *int*. For most computers, $i = 4$.

The number of bytes needed for the distance matrix is $dn(n + 1)/2$.

Missing Values

If the data are coordinates, observations with missing values are excluded from the analysis. If the data are distances, missing values are not permitted in the lower triangle of the distance matrix. The upper triangle is ignored. For more about TYPE=DISTANCE data sets, see Chapter A, “Special SAS Data Sets.”

Ties

At each level of the clustering algorithm, PROC CLUSTER must identify the pair of clusters with the minimum distance. Sometimes, usually when the data are discrete, there can be two or more pairs with the same minimum distance. In such cases the tie must be broken in some arbitrary way. If there are ties, then the results of the cluster analysis depend on the order of the observations in the data set. The presence of ties is reported in the SAS log and in the column of the cluster history labeled “Tie” unless the NOTIE option is specified.

PROC CLUSTER breaks ties as follows. Each cluster is identified by the smallest observation number among its members. For each pair of clusters, there is a smaller identification number and a larger identification number. If two or more pairs of clusters are tied for minimum distance between clusters, the pair that has the minimum larger identification number is merged. If there is a tie for minimum larger identification number, the pair that has the minimum smaller identification number is merged.

A tie means that the level in the cluster history at which the tie occurred and possibly some of the subsequent levels are not uniquely determined. Ties that occur early in the cluster history usually have little effect on the later stages. Ties that occur in the middle part of the cluster history are cause for further investigation. Ties that occur late in the cluster history indicate important indeterminacies.

The importance of ties can be assessed by repeating the cluster analysis for several different random permutations of the observations. The discrepancies at a given level can be examined by crosstabulating the clusters obtained at that level for all of the permutations. See [Example 31.4](#) for details.

Size, Shape, and Correlation

In some biological applications, the organisms that are being clustered can be at different stages of growth. Unless it is the growth process itself that is being studied, differences in size among such organisms are not of interest. Therefore, distances among organisms should be computed in such a way as to control for differences in size while retaining information about differences in shape.

If coordinate data are measured on an interval scale, you can control for size by subtracting a measure of the overall size of each observation from each data item. For example, if no other direct measure of size is available, you could subtract the mean of each row of the data matrix, producing a row-centered coordinate matrix. An easy way to subtract the mean of each row is to use PROC STANDARD on the transposed coordinate matrix:

```
proc transpose data= coordinate-datatype;
run;

proc standard m=0;
run;

proc transpose out=row-centered-coordinate-data;
run;
```

Another way to remove size effects from interval-scale coordinate data is to do a principal component analysis and discard the first component (Blackith and Reyment 1971).

If the data are measured on a ratio scale, you can control for size by dividing each observation by a measure of overall size; in this case, the geometric mean is a more natural measure of size than the arithmetic mean. However, it is often more meaningful to analyze the logarithms of ratio-scaled data, in which case you can subtract the arithmetic mean after taking logarithms. You must also consider the dimensions of measurement. For example, if you have measures of both length and weight, you might need to cube the measures of length or take the cube root of the weights. Various other complications can also arise in real applications, such as different growth rates for different parts of the body (Sneath and Sokal 1973).

Issues of size and shape are pertinent to many areas besides biology (for example, Hamer and Cunningham 1981). Suppose you have data consisting of subjective ratings made by several different raters. Some raters tend to give higher overall ratings than other raters. Some raters also tend to spread out their ratings over more of the scale than other raters. If it is impossible for you to adjust directly for rater differences, then distances should be computed in such a way as to control for differences both in size and variability. For example, if the data are considered to be measured on an interval scale, you can subtract the mean of each observation and divide by the standard deviation, producing a row-standardized coordinate matrix. With some clustering methods, analyzing squared Euclidean distances from a row-standardized coordinate matrix is equivalent to analyzing the matrix of correlations among rows, since squared Euclidean distance is an affine transformation of the correlation (Hartigan 1975, p. 64).

If you do an analysis of row-centered or row-standardized data, you need to consider whether the columns (variables) should be standardized before centering or standardizing the rows, after centering or standardizing the rows, or both before and after. If you standardize the columns after standardizing the rows, then strictly speaking you are not analyzing shape because the profiles are distorted by standardizing the columns; however, this type of double standardization might be necessary in practice to get reasonable results. It is not clear whether iterating the standardization of rows and columns can be of any benefit.

The choice of distance or correlation measure should depend on the meaning of the data and the purpose of the analysis. Simulation studies that compare distance and correlation measures are useless unless the data are generated to mimic data from your field of application. Conclusions drawn from artificial data cannot be generalized, because it is possible to generate data such that distances that include size effects work better or such that correlations work better.

You can standardize the rows of a data set by using a DATA step or by using the TRANSPOSE and STANDARD procedures. You can also use PROC TRANSPOSE and then have PROC CORR create a TYPE=CORR data set containing a correlation matrix. If you want to analyze a TYPE=CORR data set with PROC CLUSTER, you must use a DATA step to perform the following steps:

1. Set the data set TYPE= to DISTANCE.
2. Convert the correlations to dissimilarities by computing $1-r$, $\sqrt{1-r}$, $1-r^2$, or some other decreasing function.
3. Delete observations for which the variable `_TYPE_` does not have the value 'CORR'.

Output Data Set

The OUTTREE= data set contains one observation for each observation in the input data set, plus one observation for each cluster of two or more observations (that is, one observation for each node of the

cluster tree). The total number of output observations is usually $2n - 1$, where n is the number of input observations. The density methods can produce fewer output observations when the number of clusters cannot be reduced to one.

The label of the OUTTREE= data set identifies the type of cluster analysis performed and is automatically displayed when the TREE procedure is invoked.

The variables in the OUTTREE= data set are as follows:

- the BY variables, if you use a BY statement
- the ID variable, if you use an ID statement
- the COPY variables, if you use a COPY statement
- `_NAME_`, a character variable giving the name of the node. If the node is a cluster, the name is CL_n , where n is the number of the cluster. If the node is an observation, the name is OB_n , where n is the observation number. If the node is an observation and the ID statement is used, the name is the formatted value of the ID variable.
- `_PARENT_`, a character variable giving the value of `_NAME_` of the parent of the node
- `_NCL_`, the number of clusters
- `_FREQ_`, the number of observations in the current cluster
- `_HEIGHT_`, the distance or similarity between the last clusters joined, as defined in the section “[Clustering Methods](#)” on page 1926. The variable `_HEIGHT_` is used by the TREE procedure as the default height axis. The label of the `_HEIGHT_` variable identifies the between-cluster distance measure. For `METHOD=TWOSTAGE`, the `_HEIGHT_` variable contains the densities at which clusters joined in the first stage; for clusters formed in the second stage, `_HEIGHT_` is a very small negative number.

If the input data set contains coordinates, the following variables appear in the output data set:

- the variables containing the coordinates used in the cluster analysis. For output observations that correspond to input observations, the values of the coordinates are the same in both data sets except for some slight numeric error possibly introduced by standardizing and unstandardizing if the STANDARD option is used. For output observations that correspond to clusters of more than one input observation, the values of the coordinates are the cluster means.
- `_ERSQ_`, the approximate expected value of R square under the uniform null hypothesis
- `_RATIO_`, equal to $(1 - \text{ERSQ}) / (1 - \text{RSQ})$
- `_LOGR_`, natural logarithm of `_RATIO_`
- `_CCC_`, the cubic clustering criterion

The variables `_ERSQ_`, `_RATIO_`, `_LOGR_`, and `_CCC_` have missing values when the number of clusters is greater than one-fifth the number of observations.

If the input data set contains coordinates and `METHOD=AVERAGE`, `METHOD=CENTROID`, or `METHOD=WARD`, then the following variables appear in the output data set:

- `_DIST_`, the Euclidean distance between the means of the last clusters joined
- `_AVLINK_`, the average distance between the last clusters joined

If the input data set contains coordinates or `METHOD=AVERAGE`, `METHOD=CENTROID`, or `METHOD=WARD`, then the following variables appear in the output data set:

- `_RMSSTD_`, the root mean squared standard deviation of the current cluster
- `_SPRSQ_`, the semipartial squared multiple correlation or the decrease in the proportion of variance accounted for due to joining two clusters to form the current cluster
- `_RSQ_`, the squared multiple correlation
- `_PSF_`, the pseudo F statistic
- `_PST2_`, the pseudo t^2 statistic

If `METHOD=EML`, then the following variable appears in the output data set:

- `_LNLR_`, the log-likelihood ratio

If `METHOD=TWOSTAGE` or `METHOD=DENSITY`, the following variable appears in the output data set:

- `_MODE_`, pertaining to the modal clusters. With `METHOD=DENSITY`, the `_MODE_` variable indicates the number of modal clusters contained by the current cluster. With `METHOD=TWOSTAGE`, the `_MODE_` variable gives the maximum density in each modal cluster and the fusion density, d^* , for clusters containing two or more modal clusters; for clusters containing no modal clusters, `_MODE_` is missing.

If nonparametric density estimates are requested (when `METHOD=DENSITY` or `METHOD=TWOSTAGE` and the `HYBRID` option is not used; or when any of the `TRIM=`, `K=` or `R=` options are used), the output data set contains the following:

- `_DENS_`, the maximum density in the current cluster

Displayed Output

If you specify the `SIMPLE` option and the data are coordinates, `PROC CLUSTER` produces simple descriptive statistics for each variable:

- the Mean
- the standard deviation, Std Dev

- the Skewness
- the Kurtosis
- a coefficient of Bimodality

If the data are coordinates and you do not specify the NOEIGEN option, PROC CLUSTER displays the following:

- the Eigenvalues of the Correlation or Covariance Matrix
- the Difference between successive eigenvalues
- the Proportion of variance explained by each eigenvalue
- the Cumulative proportion of variance explained

If the data are coordinates, PROC CLUSTER displays the Root Mean Squared Total-Sample Standard Deviation of the variables

If the distances are normalized, PROC CLUSTER displays one of the following, depending on whether squared or unsquared distances are used:

- the Root Mean Squared Distance Between Observations
- the Mean Distance Between Observations

For the generations in the clustering process specified by the PRINT= option, PROC CLUSTER displays the following:

- the Number of Clusters or NCL
- the names of the Clusters Joined. The observations are identified by the formatted value of the ID variable, if any; otherwise, the observations are identified by OBn , where n is the observation number. The CLUSTER procedure displays the entire value of the ID variable in the cluster history instead of truncating at 16 characters. Long ID values might be split onto several lines. Clusters of two or more observations are identified as CLn , where n is the number of clusters existing after the cluster in question is formed.
- the number of observations in the new cluster, Frequency of New Cluster or FREQ

If you specify the RMSSTD option and the data are coordinates, or if you specify METHOD=AVERAGE, METHOD=CENTROID, or METHOD=WARD, then PROC CLUSTER displays the root mean squared standard deviation of the new cluster, RMS Std of New Cluster or RMS Std.

PROC CLUSTER displays the following items if you specify METHOD=WARD. It also displays them if you specify the RSQUARE option and either the data are coordinates or you specify METHOD=AVERAGE or METHOD=CENTROID.

- the decrease in the proportion of variance accounted for resulting from joining the two clusters, Semi-partial R-Square or SPRSQ. This equals the between-cluster sum of squares divided by the corrected total sum of squares.
- the squared multiple correlation, R-Square or RSQ. R square is the proportion of variance accounted for by the clusters.

If you specify the CCC option and the data are coordinates, PROC CLUSTER displays the following:

- Approximate Expected R-Square or ERSQ, the approximate expected value of R square under the uniform null hypothesis
- the Cubic Clustering Criterion or CCC. The cubic clustering criterion and approximate expected R square are given missing values when the number of clusters is greater than one-fifth the number of observations.

If you specify the PSEUDO option and the data are coordinates, or if you specify METHOD=AVERAGE, METHOD=CENTROID, or METHOD=WARD, then PROC CLUSTER displays the following:

- Pseudo F or PSF, the pseudo F statistic measuring the separation among all the clusters at the current level
- Pseudo t^2 or PST2, the pseudo t^2 statistic measuring the separation between the two clusters most recently joined

If you specify the NOSQUARE option and METHOD=AVERAGE, PROC CLUSTER displays the (Normalized) Average Distance or (Norm) Aver Dist, the average distance between pairs of objects in the two clusters joined with one object from each cluster.

If you do not specify the NOSQUARE option and METHOD=AVERAGE, PROC CLUSTER displays the (Normalized) RMS Distance or (Norm) RMS Dist, the root mean squared distance between pairs of objects in the two clusters joined with one object from each cluster.

If METHOD=CENTROID, PROC CLUSTER displays the (Normalized) Centroid Distance or (Norm) Cent Dist, the distance between the two cluster centroids.

If METHOD=COMPLETE, PROC CLUSTER displays the (Normalized) Maximum Distance or (Norm) Max Dist, the maximum distance between the two clusters.

If METHOD=DENSITY or METHOD=TWOSTAGE, PROC CLUSTER displays the following:

- Normalized Fusion Density or Normalized Fusion Dens, the value of d^* as defined in the section “Clustering Methods” on page 1926
- the Normalized Maximum Density in Each Cluster joined, including the Lesser or Min, and the Greater or Max, of the two maximum density values

If METHOD=EML, PROC CLUSTER displays the following:

- Log Likelihood Ratio or LNLR
- Log Likelihood or LNLIKE

If METHOD=FLEXIBLE, PROC CLUSTER displays the (Normalized) Flexible Distance or (Norm) Flex Dist, the distance between the two clusters based on the Lance-Williams flexible formula.

If METHOD=MEDIAN, PROC CLUSTER displays the (Normalized) Median Distance or (Norm) Med Dist, the distance between the two clusters based on the median method.

If METHOD=MCQUITTY, PROC CLUSTER displays the (Normalized) McQuitty's Similarity or (Norm) MCQ, the distance between the two clusters based on McQuitty's similarity method.

If METHOD=SINGLE, PROC CLUSTER displays the (Normalized) Minimum Distance or (Norm) Min Dist, the minimum distance between the two clusters.

If you specify the NONORM option and METHOD=WARD, PROC CLUSTER displays the Between-Cluster Sum of Squares or BSS, the ANOVA sum of squares between the two clusters joined.

If you specify neither the NOTIE option nor METHOD=TWOSTAGE or METHOD=DENSITY, PROC CLUSTER displays Tie, where a T in the column indicates a tie for minimum distance and a blank indicates the absence of a tie.

After the cluster history, if METHOD=TWOSTAGE or METHOD=DENSITY, PROC CLUSTER displays the number of modal clusters.

ODS Table Names

PROC CLUSTER assigns a name to each table it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in Table 31.4. For more information about ODS, see Chapter 20, "Using the Output Delivery System."

Table 31.4 ODS Tables Produced by PROC CLUSTER

ODS Table Name	Description	Statement	Option
ClusterHistory	Observation or clusters joined, frequencies and other cluster statistics	PROC	default
SimpleStatistics	Simple statistics, before or after trimming	PROC	SIMPLE
EigenvalueTable	Eigenvalues of the CORR or COV matrix	PROC	default
RMSStd	Root mean square total sample standard deviation	PROC	default
AvDist	Root mean square distance between observations	PROC	default

ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “Statistical Graphics Using ODS.”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “A Primer on ODS Statistical Graphics” on page 599 in Chapter 21, “Statistical Graphics Using ODS.”

PROC CLUSTER can produce plots of the cubic clustering criterion, pseudo F , and pseudo t^2 statistics, and a dendrogram. To plot a statistic, you must ask for it to be computed via one or more of the CCC, PSEUDO, or PLOT options.

You can reference every graph produced through ODS Graphics with a name. The names of the graphs that PROC CLUSTER generates are listed in Table 31.5, along with the required statements and options.

Table 31.5 Graphs Produced by PROC CLUSTER

ODS Graph Name	Plot Description	Statement & Option
CubicClusCritPlot	Cubic clustering criterion for the number of clusters	PROC CLUSTER PLOTS=CCC
PseudoFPlot	Pseudo F criterion for the number of clusters	PROC CLUSTER PLOTS=PSF
PseudoTSqPlot	Pseudo t^2 criterion for the number of clusters	PROC CLUSTER PLOTS=PST2
CccAndPsTSqPlot	Cubic clustering criterion and pseudo t^2	PROC CLUSTER PLOTS=(CCC PST2)
CccAndPsfPlot	Cubic clustering criterion and pseudo F	PROC CLUSTER PLOTS=(CCC PSF)
CccPsfAndPsTSqPlot	Cubic clustering criterion, pseudo F , and pseudo t^2	PROC CLUSTER PLOTS=ALL
Dendrogram	Dendrogram (tree diagram)	PROC CLUSTER PLOTS=DENDROGRAM

Examples: CLUSTER Procedure

Example 31.1: Cluster Analysis of Flying Mileages between 10 American Cities

This example clusters 10 American cities based on the flying mileages between them. Six clustering methods are shown with corresponding dendrograms. The EML method cannot be used because it requires coordinate data. The other omitted methods produce the same clusters, although not the same distances between clusters, as one of the illustrated methods: complete linkage and the flexible-beta method yield the same clusters as Ward's method, McQuitty's similarity analysis produces the same clusters as average linkage, and the median method corresponds to the centroid method.

All of the methods suggest a division of the cities into two clusters along the east-west dimension. There is disagreement, however, about which cluster Denver should belong to. Some of the methods indicate a possible third cluster that contains Denver and Houston.

The following step displays the city mileage SAS data set, which is available in the Sashelp library and is designated as a TYPE=DISTANCE data set when it is used by PROC CLUSTER:

```
proc print noobs data=sashelp.mileages;
run;
```

Output 31.1.1 City Mileage Data Set

Atlanta	Chicago	Denver	Houston	Los Angeles	Miami	New York	San Francisco	Seattle	Washington DC	City
0	Atlanta
587	0	Chicago
1212	920	0	Denver
701	940	879	0	Houston
1936	1745	831	1374	0	Los Angeles
604	1188	1726	968	2339	0	Miami
748	713	1631	1420	2451	1092	0	.	.	.	New York
2139	1858	949	1645	347	2594	2571	0	.	.	San Francisco
2182	1737	1021	1891	959	2734	2408	678	0	.	Seattle
543	597	1494	1220	2300	923	205	2442	2329	0	Washington D.C.

A partial listing from the following statements include [Output 31.1.2](#) and [Output 31.1.3](#):

```
title 'Cluster Analysis of Flying Mileages Between 10 American Cities';
ods graphics on;

title2 'Using METHOD=AVERAGE';
proc cluster data=sashelp.mileages (type=distance) method=average pseudo;
  id City;
run;
```

Output 31.1.2 Cluster History Using METHOD=AVERAGE

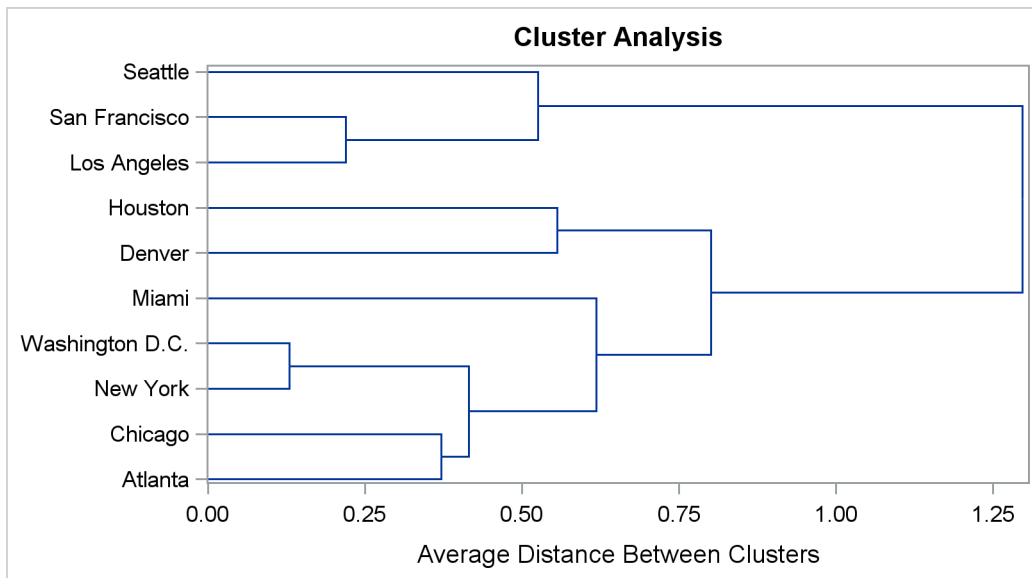
Cluster Analysis of Flying Mileages Between 10 American Cities
Using METHOD=AVERAGE

The CLUSTER Procedure
Average Linkage Cluster Analysis

Cluster History

NCL	-----Clusters Joined-----	Freq	Ps F	PsT2	Norm T RMS i Dist e
9	New York Washington D.C.	2	66.7	.	0.1297
8	Los Angeles San Francisco	2	39.2	.	0.2196
7	Atlanta Chicago	2	21.7	.	0.3715
6	CL7 CL9	4	14.5	3.4	0.4149
5	CL8 Seattle	3	12.4	7.3	0.5255
4	Denver Houston	2	13.9	.	0.5562
3	CL6 Miami	5	15.5	3.8	0.6185
2	CL3 CL4	7	16.0	5.3	0.8005
1	CL2 CL5	10	.	16.0	1.2967

Output 31.1.3 Dendrogram Using METHOD=AVERAGE



A partial listing from the following statements include [Output 31.1.4](#) and [Output 31.1.5](#):

```

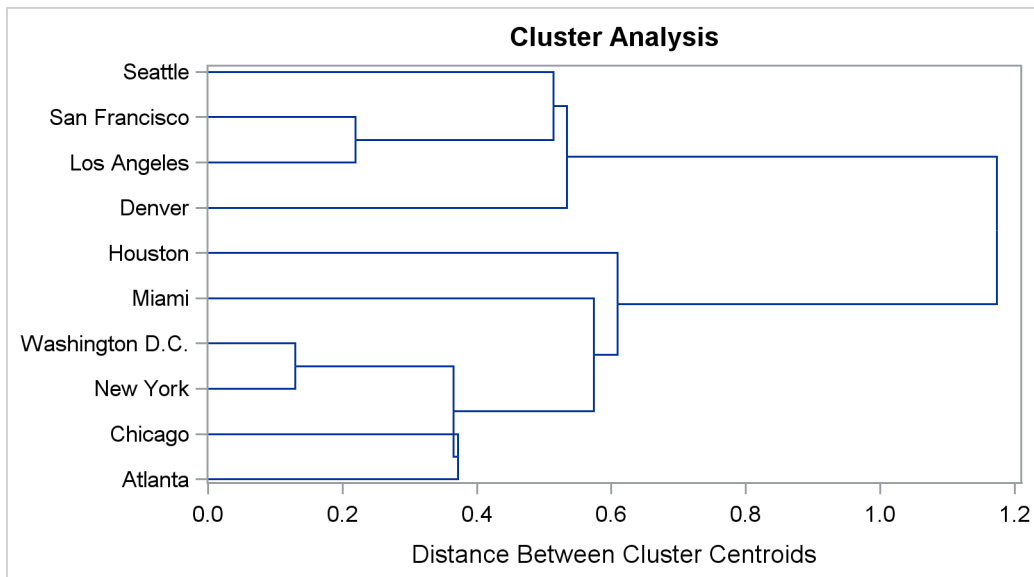
title2 'Using METHOD=CENTROID';
proc cluster data=sashelp.mileages (type=distance) method=centroid pseudo;
  id City;
run;

```

Output 31.1.4 Cluster History Using METHOD=CENTROID

Cluster Analysis of Flying Mileages Between 10 American Cities Using METHOD=CENTROID					
The CLUSTER Procedure					
Centroid Hierarchical Cluster Analysis					
Cluster History					
NCL	-----Clusters Joined-----	Freq	Ps F	PsT2	Norm T Cent i Dist e
9	New York Washington D.C.	2	66.7	.	0.1297
8	Los Angeles San Francisco	2	39.2	.	0.2196
7	Atlanta Chicago	2	21.7	.	0.3715
6	CL7 CL9	4	14.5	3.4	0.3652
5	CL8 Seattle	3	12.4	7.3	0.5139
4	Denver CL5	4	12.4	2.1	0.5337
3	CL6 Miami	5	14.2	3.8	0.5743
2	CL3 Houston	6	22.1	2.6	0.6091
1	CL2 CL4	10	.	22.1	1.173

Output 31.1.5 Dendrogram Using METHOD=CENTROID



A partial listing from the following statements include [Output 31.1.6](#) and [Output 31.1.7](#):

```

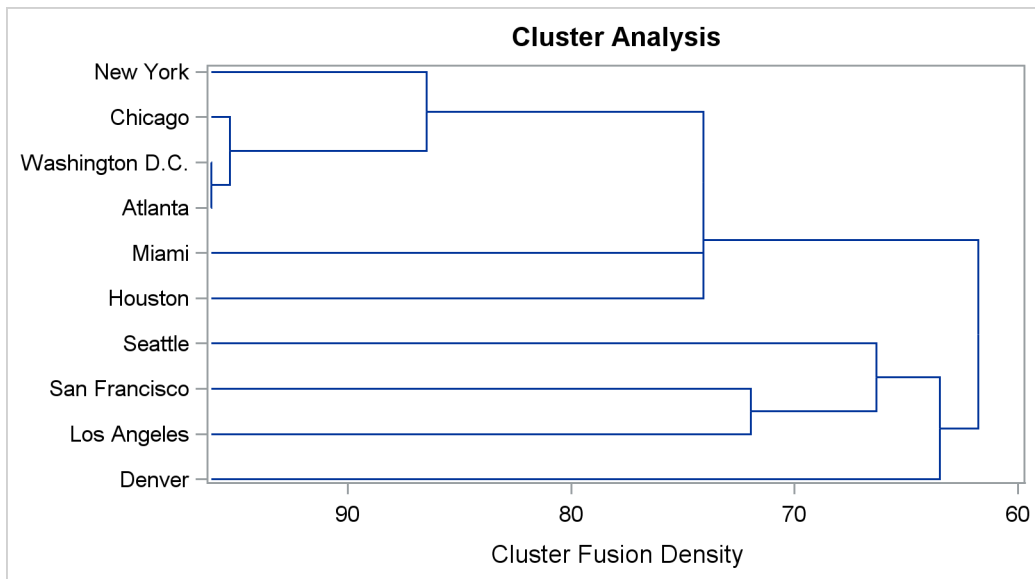
title2 'Using METHOD=DENSITY K=3';
proc cluster data=sashelp.mileages (type=distance) method=density k=3;
  id City;
run;

```

Output 31.1.6 Cluster History Using METHOD=DENSITY K=3

Cluster Analysis of Flying Mileages Between 10 American Cities Using METHOD=DENSITY K=3						
The CLUSTER Procedure						
Density Linkage Cluster Analysis						
Cluster History						
NCL	-----Clusters Joined-----	Freq	Normalized Fusion Density	Maximum Density		T i e
				Lesser	Greater	
9	Atlanta Washington	2	96.106	92.5043	100.0	
8	CL9 Chicago	3	95.263	90.9548	100.0	
7	CL8 New York	4	86.465	76.1571	100.0	
6	CL7 Miami	5	74.079	58.8299	100.0	T
5	CL6 Houston	6	74.079	61.7747	100.0	
4	Los Angeles San Francisco	2	71.968	65.3430	80.0885	
3	CL4 Seattle	3	66.341	56.6215	80.0885	
2	CL3 Denver	4	63.509	61.7747	80.0885	
1	CL5 CL2	10	61.775 *	80.0885	100.0	

Output 31.1.7 Dendrogram Using METHOD=DENSITY K=3



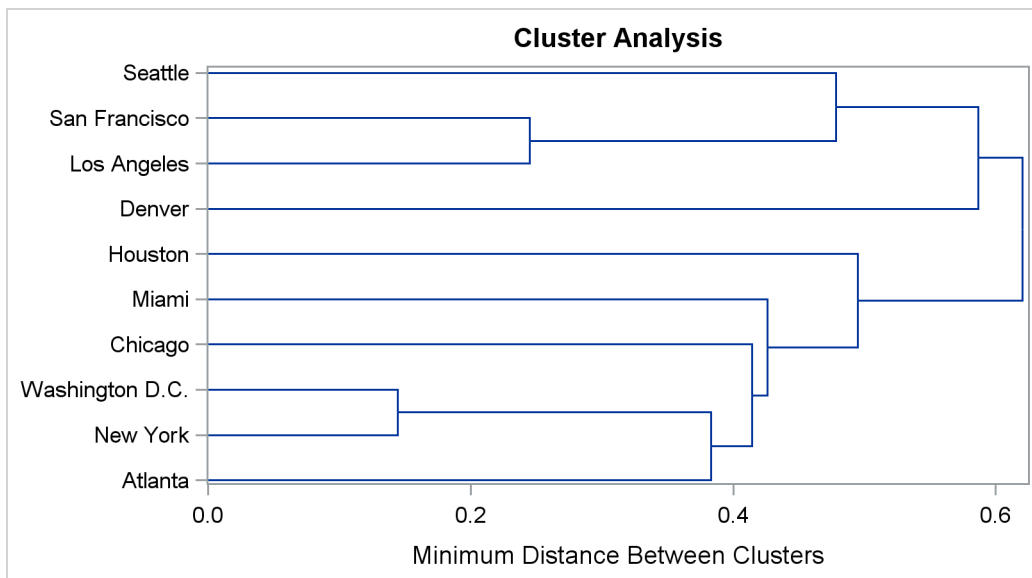
A partial listing from the following statements include [Output 31.1.8](#) and [Output 31.1.9](#):

```
title2 'Using METHOD=SINGLE';
proc cluster data=sashelp.mileages (type=distance) method=single;
  id City;
run;
```

Output 31.1.8 Cluster History Using METHOD=SINGLE

Cluster Analysis of Flying Mileages Between 10 American Cities Using METHOD=SINGLE					
The CLUSTER Procedure					
Single Linkage Cluster Analysis					
Cluster History					
Number of Clusters	-----Clusters Joined-----		Freq	Norm Minimum Distance	Tie
9	New York	Washington D.C.	2	0.1447	
8	Los Angeles	San Francisco	2	0.2449	
7	Atlanta	CL9	3	0.3832	
6	CL7	Chicago	4	0.4142	
5	CL6	Miami	5	0.4262	
4	CL8	Seattle	3	0.4784	
3	CL5	Houston	6	0.4947	
2	Denver	CL4	4	0.5864	
1	CL3	CL2	10	0.6203	

Output 31.1.9 Dendrogram Using METHOD=SINGLE



A partial listing from the following statements include [Output 31.1.10](#) and [Output 31.1.11](#):

```

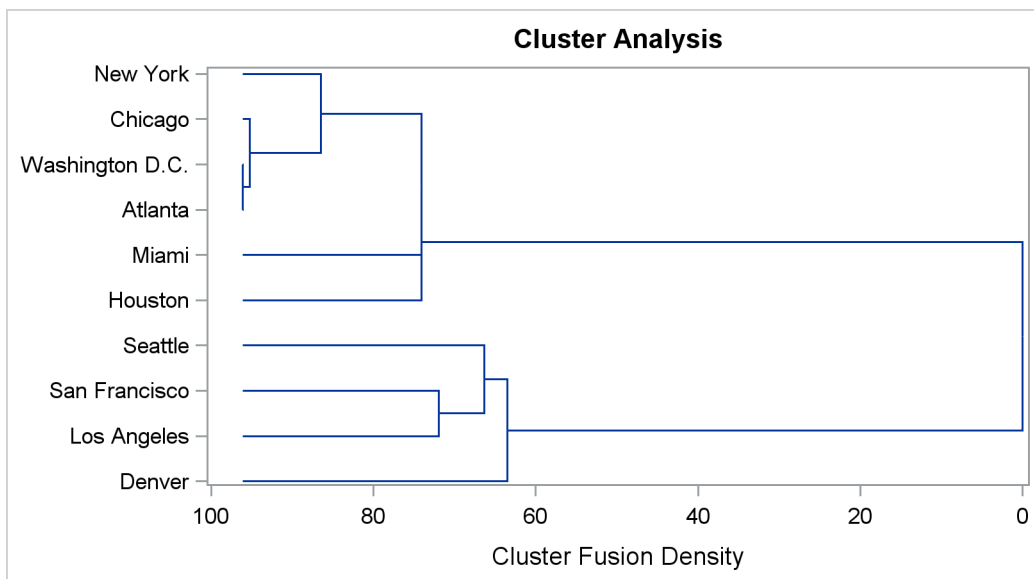
title2 'Using METHOD=TWOSTAGE K=3';
proc cluster data=sashelp.mileages (type=distance) method=twostage k=3;
  id City;
run;

```

Output 31.1.10 Cluster History Using METHOD=TWOSTAGE K=3

Cluster Analysis of Flying Mileages Between 10 American Cities Using METHOD=TWOSTAGE K=3						
The CLUSTER Procedure Two-Stage Density Linkage Clustering						
Cluster History						
NCL	-----Clusters Joined-----	Freq	Normalized Fusion Density	Maximum Density in Each Cluster		T i e
				Lesser	Greater	
9	Atlanta Washington D.C.	2	96.106	92.5043	100.0	
8	CL9 Chicago	3	95.263	90.9548	100.0	
7	CL8 New York	4	86.465	76.1571	100.0	
6	CL7 Miami	5	74.079	58.8299	100.0	T
5	CL6 Houston	6	74.079	61.7747	100.0	
4	Los Angeles San Francisco	2	71.968	65.3430	80.0885	
3	CL4 Seattle	3	66.341	56.6215	80.0885	
2	CL3 Denver	4	63.509	61.7747	80.0885	
1	CL5 CL2	10	61.775	80.0885	100.0	

Output 31.1.11 Dendrogram Using METHOD=TWOSTAGE K=3



A partial listing from the following statements include [Output 31.1.12](#) and [Output 31.1.13](#):

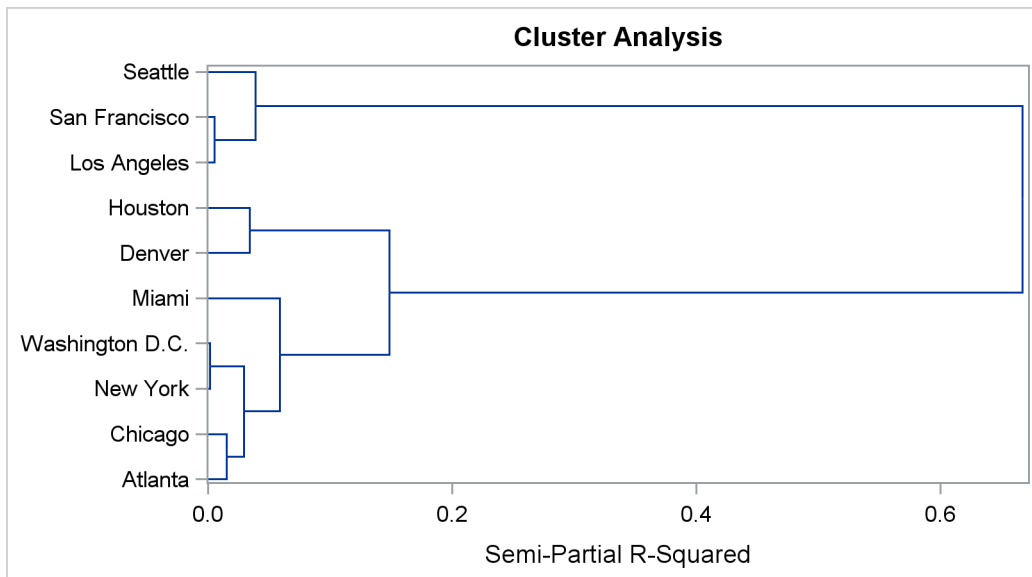
```

title2 'Using METHOD=WARD';
proc cluster data=sashelp.mileages (type=distance) method=ward pseudo;
  id City;
run;
    
```

Output 31.1.12 Cluster History Using METHOD=WARD

Cluster Analysis of Flying Mileages Between 10 American Cities Using METHOD=WARD						
The CLUSTER Procedure						
Ward's Minimum Variance Cluster Analysis						
Cluster History						
NCL	-----Clusters Joined-----	Freq	SpRSq	RSq	Ps F	PsT2 e
9	New York Washington D.C.	2	0.0019	.998	66.7	.
8	Los Angeles San Francisco	2	0.0054	.993	39.2	.
7	Atlanta Chicago	2	0.0153	.977	21.7	.
6	CL7 CL9	4	0.0296	.948	14.5	3.4
5	Denver Houston	2	0.0344	.913	13.2	.
4	CL8 Seattle	3	0.0391	.874	13.9	7.3
3	CL6 Miami	5	0.0586	.816	15.5	3.8
2	CL3 CL5	7	0.1488	.667	16.0	5.3
1	CL2 CL4	10	0.6669	.000	.	16.0

Output 31.1.13 Dendrogram Using METHOD=WARD



Example 31.2: Crude Birth and Death Rates

This example uses the SAS data set `Poverty` created in the section “Getting Started: CLUSTER Procedure” on page 1907. The data, from Rouncefield (1995), are birth rates, death rates, and infant death rates for 97 countries. Six cluster analyses are performed with eight methods. Scatter plots showing cluster membership at selected levels are produced instead of tree diagrams.

Each cluster analysis is performed by a macro called `ANALYZE`. The macro takes two arguments. The first, `&METHOD`, specifies the value of the `METHOD=` option to be used in the `PROC CLUSTER` statement. The second, `&NCL`, must be specified as a list of integers, separated by blanks, indicating the number of clusters desired in each scatter plot. For example, the first invocation of `ANALYZE` specifies the `AVERAGE` method and requests plots of three and eight clusters. When two-stage density linkage is used, the `K=` and `R=` options are specified as part of the first argument.

The `ANALYZE` macro first invokes the `CLUSTER` procedure with `METHOD=&METHOD`, where `&METHOD` represents the value of the first argument to `ANALYZE`. This part of the macro produces the `PROC CLUSTER` output shown.

The `%DO` loop processes `&NCL`, the list of numbers of clusters to plot. The macro variable `&K` is a counter that indexes the numbers within `&NCL`. The `%SCAN` function picks out the k th number in `&NCL`, which is then assigned to the macro variable `&N`. When `&K` exceeds the number of numbers in `&NCL`, `%SCAN` returns a null string. Thus, the `%DO` loop executes while `&N` is not equal to a null string. In the `%WHILE` condition, a null string is indicated by the absence of any nonblank characters between the comparison operator (`NE`) and the right parenthesis that terminates the condition.

Within the `%DO` loop, the `TREE` procedure creates an output data set containing `&N` clusters. The `SGPLOT` procedure then produces a scatter plot in which each observation is identified by the number of the cluster to which it belongs. The `TITLE2` statement uses double quotes so that `&N` and `&METHOD` can be used within the title. At the end of the loop, `&K` is incremented by 1, and the next number is extracted from `&NCL` by `%SCAN`.

```

title 'Cluster Analysis of Birth and Death Rates';
ods graphics on;

%macro analyze(method,ncl);
  proc cluster data=poverty outtree=tree method=&method print=15 ccc pseudo;
    var birth death;
    title2;
  run;

  %let k=1;
  %let n=%scan(&ncl,&k);
  %do %while(&n NE);

    proc tree data=tree noprint out=out ncl=&n;
      copy birth death;
    run;

```

```

proc sgplot;
  scatter y=death x=death / group=cluster;
  title2 "Plot of &n Clusters from METHOD=&METHOD";
run;

%let k=%eval(&k+1);
%let n=%scan(&ncl, &k);
%end;
%mend;

```

The following statement produces [Output 31.2.1](#), [Output 31.2.3](#), and [Output 31.2.4](#):

```
%analyze(average, 3 8)
```

For average linkage, the CCC has peaks at three, eight, ten, and twelve clusters, but the three-cluster peak is lower than the eight-cluster peak. The pseudo F statistic has peaks at three, eight, and twelve clusters. The pseudo t^2 statistic drops sharply at three clusters, continues to fall at four clusters, and has a particularly low value at twelve clusters. However, there are not enough data to seriously consider as many as twelve clusters. Scatter plots are given for three and eight clusters. The results are shown in [Output 31.2.1](#) through [Output 31.2.4](#). In [Output 31.2.4](#), the eighth cluster consists of the two outlying observations, Mexico and Korea.

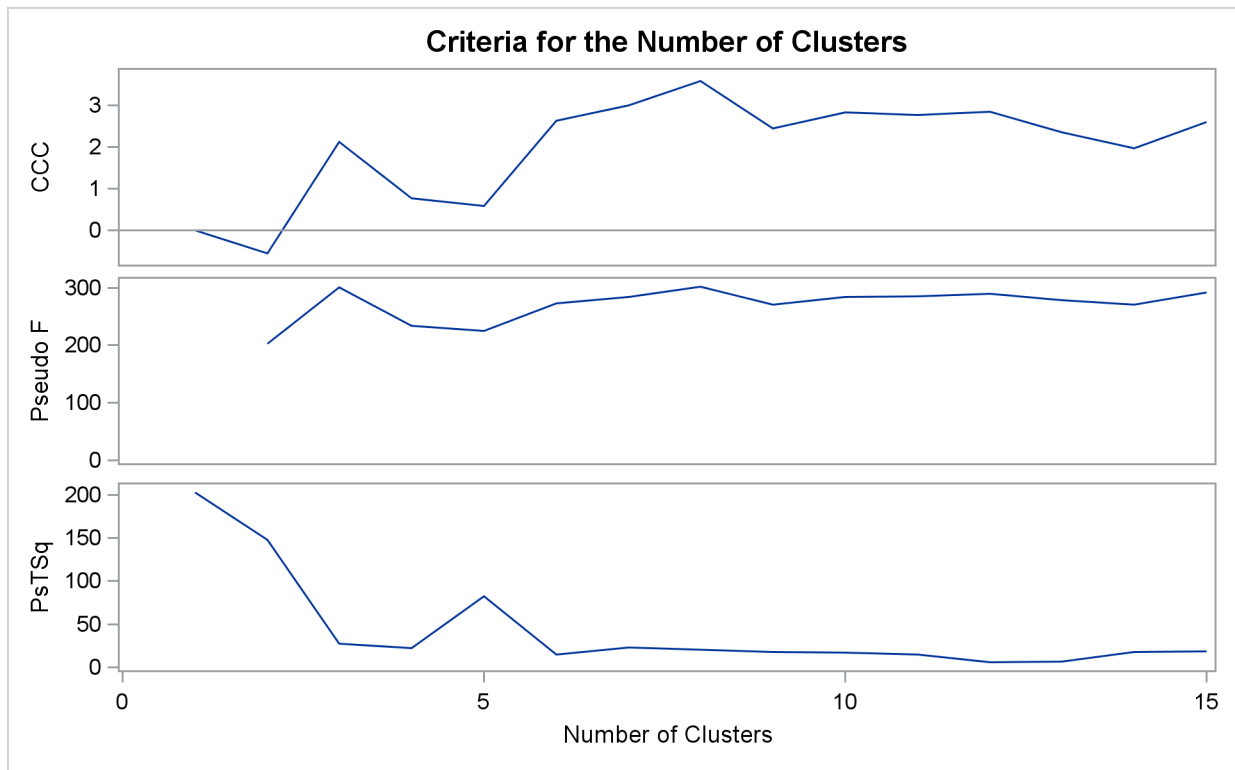
Output 31.2.1 Cluster Analysis for Birth and Death Rates: METHOD=AVERAGE

Cluster Analysis of Birth and Death Rates				
The CLUSTER Procedure				
Average Linkage Cluster Analysis				
Eigenvalues of the Covariance Matrix				
	Eigenvalue	Difference	Proportion	Cumulative
1	189.106588	173.101020	0.9220	0.9220
2	16.005568		0.0780	1.0000
Root-Mean-Square Total-Sample Standard Deviation				10.127
Root-Mean-Square Distance Between Observations				20.25399

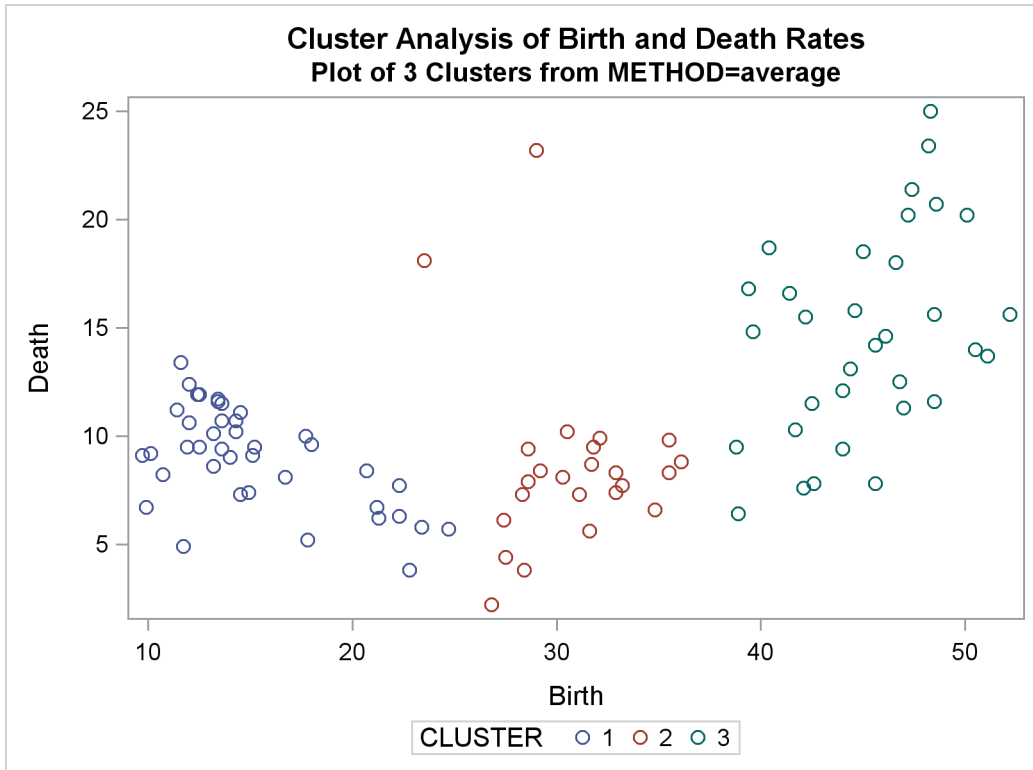
Output 31.2.1 continued

Cluster History										
NCL	---Clusters Joined---		Freq	SpRSq	RSq	ERSq	CCC	Ps F	Pst2	Norm T RMS i Dist e
15	CL27	CL20	18	0.0035	.980	.975	2.61	292	18.6	0.2325
14	CL23	CL17	28	0.0034	.977	.972	1.97	271	17.7	0.2358
13	CL18	CL54	8	0.0015	.975	.969	2.35	279	7.1	0.2432
12	CL21	CL26	8	0.0015	.974	.966	2.85	290	6.1	0.2493
11	CL19	CL24	12	0.0033	.971	.962	2.78	285	14.8	0.2767
10	CL22	CL16	12	0.0036	.967	.957	2.84	284	17.4	0.2858
9	CL15	CL28	22	0.0061	.961	.951	2.45	271	17.5	0.3353
8	OB23	OB61	2	0.0014	.960	.943	3.59	302	.	0.3703
7	CL25	CL11	17	0.0098	.950	.933	3.01	284	23.3	0.4033
6	CL7	CL12	25	0.0122	.938	.920	2.63	273	14.8	0.4132
5	CL10	CL14	40	0.0303	.907	.902	0.59	225	82.7	0.4584
4	CL13	CL6	33	0.0244	.883	.875	0.77	234	22.2	0.5194
3	CL9	CL8	24	0.0182	.865	.827	2.13	300	27.7	0.735
2	CL5	CL3	64	0.1836	.681	.697	-.55	203	148	0.8402
1	CL2	CL4	97	0.6810	.000	.000	0.00	.	203	1.3348

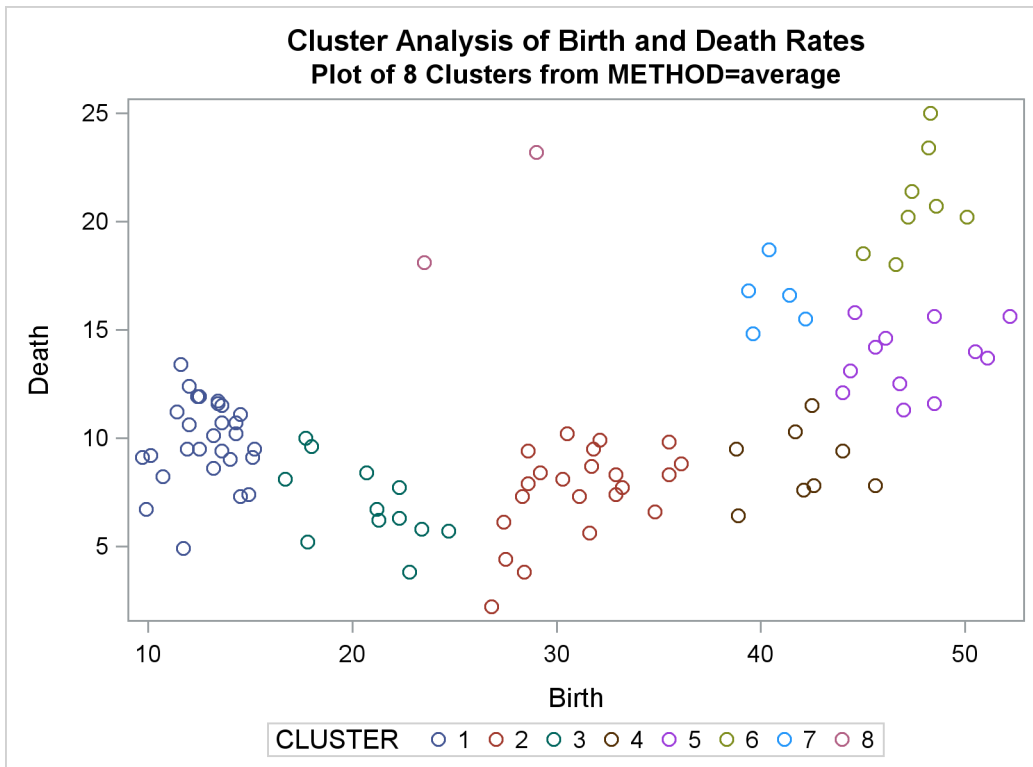
Output 31.2.2 Criteria for the Number of Clusters: METHOD=AVERAGE



Output 31.2.3 Plot of Three Clusters: METHOD=AVERAGE



Output 31.2.4 Plot of Eight Clusters: METHOD=AVERAGE



The following statement produces [Output 31.2.5](#) and [Output 31.2.7](#):

```
%analyze(complete, 3)
```

Complete linkage shows CCC peaks at three, eight and twelve clusters. The pseudo F statistic peaks at three and twelve clusters. The pseudo t^2 statistic indicates three clusters.

The scatter plot for three clusters is shown.

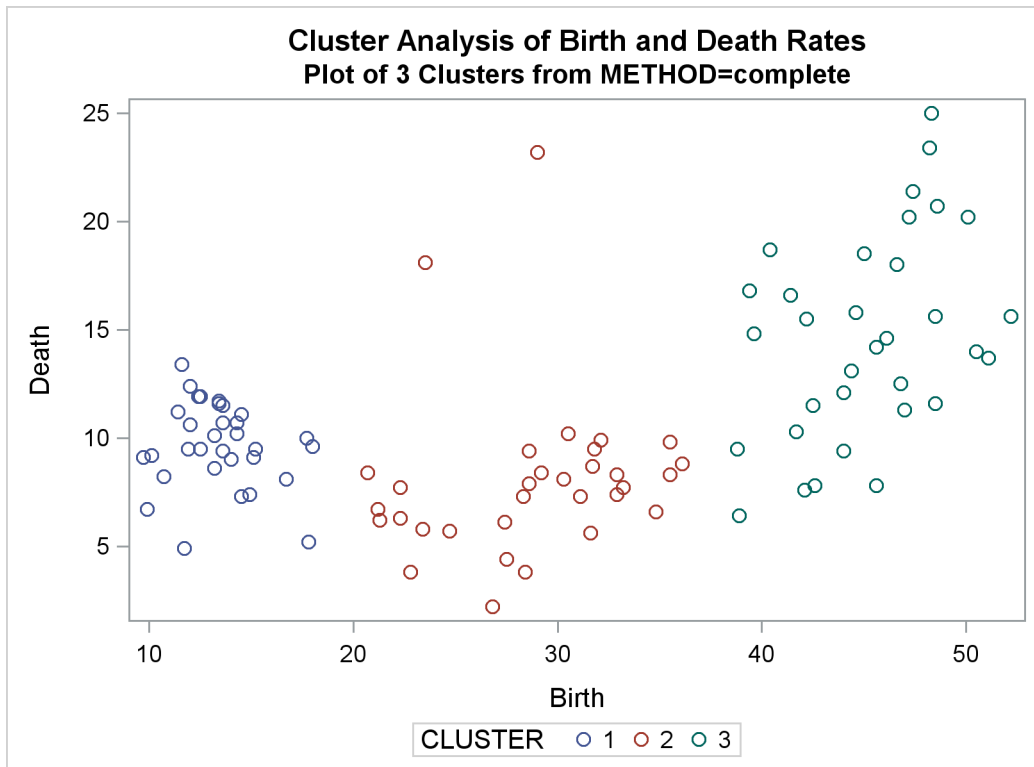
Output 31.2.5 Cluster History for Birth and Death Rates: METHOD=COMPLETE

Cluster Analysis of Birth and Death Rates									
The CLUSTER Procedure									
Complete Linkage Cluster Analysis									
Eigenvalues of the Covariance Matrix									
	Eigenvalue	Difference	Proportion	Cumulative					
1	189.106588	173.101020	0.9220	0.9220					
2	16.005568		0.0780	1.0000					
Root-Mean-Square Total-Sample Standard Deviation				10.127					
Mean Distance Between Observations			17.13099						
Cluster History									
NCL	---Clusters Joined---	Freq	SpRSq	RSq	ERSq	CCC	Ps F	Pst2	Norm T Max i Dist e
15	CL22 CL33	8	0.0015	.983	.975	3.80	329	6.1	0.4092
14	CL56 CL18	8	0.0014	.981	.972	3.97	331	6.6	0.4255
13	CL30 CL44	8	0.0019	.979	.969	4.04	330	19.0	0.4332
12	OB23 OB61	2	0.0014	.978	.966	4.45	340	.	0.4378
11	CL19 CL24	24	0.0034	.974	.962	4.17	327	24.1	0.4962
10	CL17 CL28	12	0.0033	.971	.957	4.18	325	14.8	0.5204
9	CL20 CL13	16	0.0067	.964	.951	3.38	297	25.2	0.5236
8	CL11 CL21	32	0.0054	.959	.943	3.44	297	19.7	0.6001
7	CL26 CL15	13	0.0096	.949	.933	2.93	282	28.9	0.7233
6	CL14 CL10	20	0.0128	.937	.920	2.46	269	27.7	0.8033
5	CL9 CL16	30	0.0237	.913	.902	1.29	241	47.1	0.8993
4	CL6 CL7	33	0.0240	.889	.875	1.38	248	21.7	1.2165
3	CL5 CL12	32	0.0178	.871	.827	2.56	317	13.6	1.2326
2	CL3 CL8	64	0.1900	.681	.697	- .55	203	167	1.5412
1	CL2 CL4	97	0.6810	.000	.000	0.00	.	203	2.5233

Output 31.2.6 Criteria for the Number of Clusters: METHOD=COMPLETE



Output 31.2.7 Plot of Clusters for METHOD=COMPLETE



The following statement produces [Output 31.2.8](#) and [Output 31.2.10](#):

```
%analyze(single, 7 10)
```

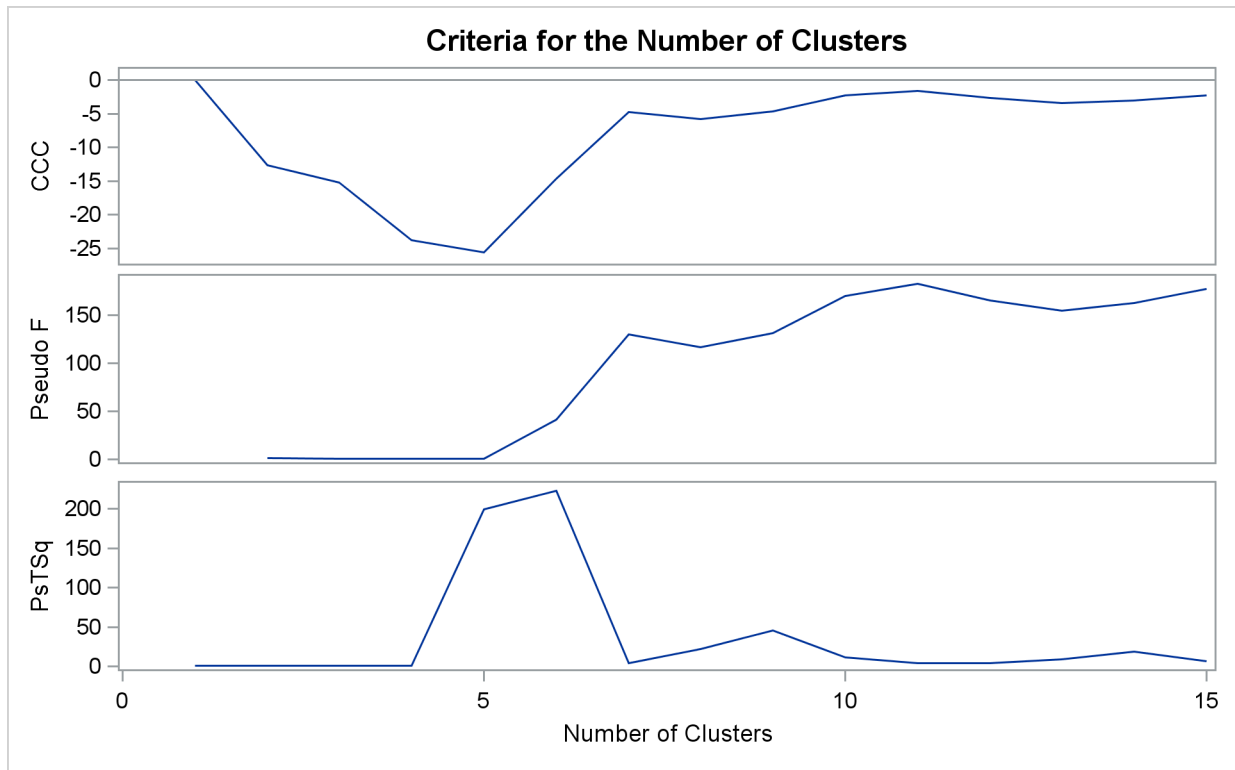
The CCC and pseudo F statistics are not appropriate for use with single linkage because of the method's tendency to chop off tails of distributions. The pseudo t^2 statistic can be used by looking for *large* values and taking the number of clusters to be one greater than the level at which the large pseudo t^2 value is displayed. For these data, there are large values at levels 6 and 9, suggesting seven or ten clusters.

The scatter plots for seven and ten clusters are shown.

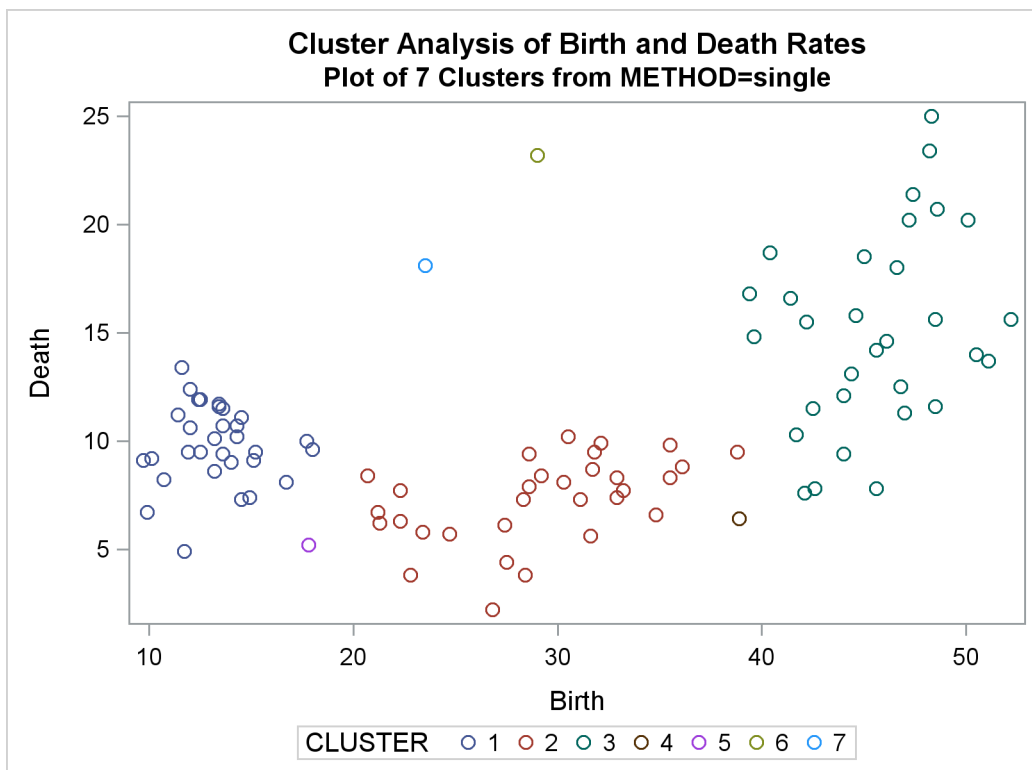
Output 31.2.8 Cluster History for Birth and Death Rates: METHOD=SINGLE

Cluster Analysis of Birth and Death Rates									
The CLUSTER Procedure									
Single Linkage Cluster Analysis									
Eigenvalues of the Covariance Matrix									
	Eigenvalue	Difference	Proportion	Cumulative					
1	189.106588	173.101020	0.9220	0.9220					
2	16.005568		0.0780	1.0000					
Root-Mean-Square Total-Sample Standard Deviation				10.127					
Mean Distance Between Observations			17.13099						
Cluster History									
NCL	---Clusters Joined---	Freq	SpRSq	RSq	ERSq	CCC	Ps F	PsT2	Norm T Min i Dist e
15	CL37 CL19	8	0.0014	.968	.975	-2.3	178	6.6	0.1331
14	CL20 CL23	15	0.0059	.962	.972	-3.1	162	18.7	0.1412
13	CL14 CL16	19	0.0054	.957	.969	-3.4	155	8.8	0.1442
12	CL26 OB58	31	0.0014	.955	.966	-2.7	165	4.0	0.1486
11	OB86 CL18	4	0.0003	.955	.962	-1.6	183	3.8	0.1495
10	CL13 CL11	23	0.0088	.946	.957	-2.3	170	11.3	0.1518
9	CL22 CL17	30	0.0235	.923	.951	-4.7	131	45.7	0.1593 T
8	CL15 CL10	31	0.0210	.902	.943	-5.8	117	21.8	0.1593
7	CL9 OB75	31	0.0052	.897	.933	-4.7	130	4.0	0.1628
6	CL7 CL12	62	0.2023	.694	.920	-15	41.3	223	0.1725
5	CL6 CL8	93	0.6681	.026	.902	-26	0.6	199	0.1756
4	CL5 OB48	94	0.0056	.021	.875	-24	0.7	0.5	0.1811 T
3	CL4 OB67	95	0.0083	.012	.827	-15	0.6	0.8	0.1811
2	OB23 OB61	2	0.0014	.011	.697	-13	1.0	.	0.4378
1	CL3 CL2	97	0.0109	.000	.000	0.00	.	1.0	0.5815

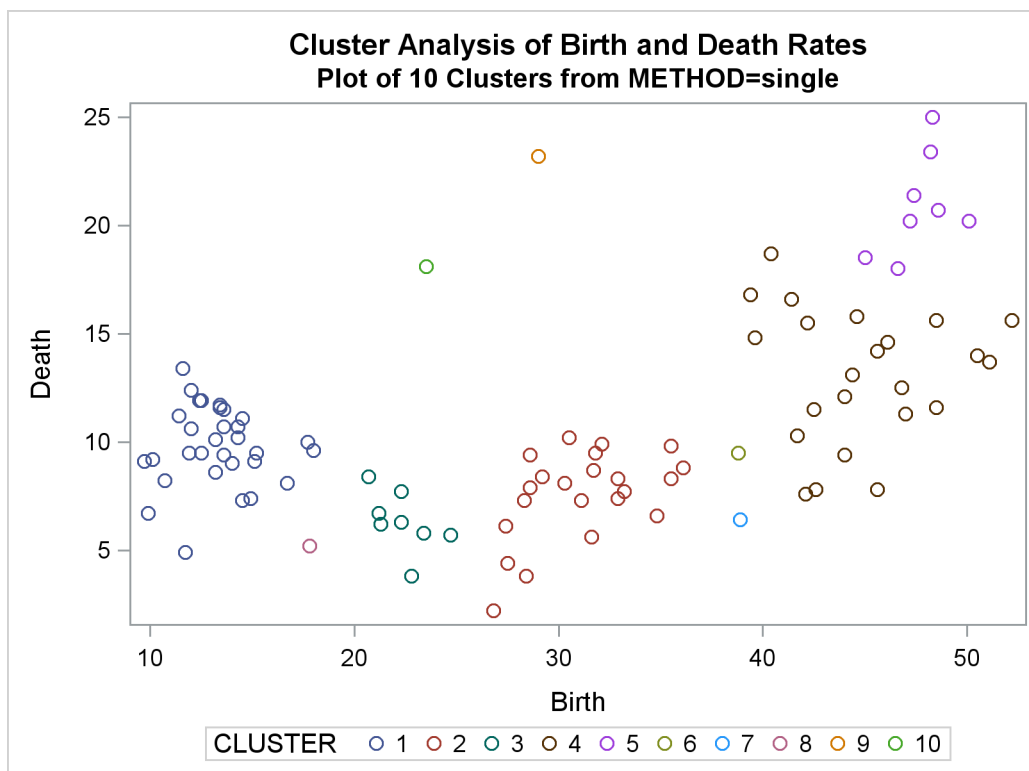
Output 31.2.9 Criteria for the Number of Clusters: METHOD=SINGLE



Output 31.2.10 Plot of Clusters for METHOD=SINGLE



Output 31.2.10 continued



The following statements produce [Output 31.2.11](#) through [Output 31.2.14](#):

```
%analyze(two k=10, 3)
```

```
%analyze(two k=18, 2)
```

For k th-nearest-neighbor density linkage, the number of modes as a function of k is as follows (not all of these analyses are shown):

k	Modes
3	13
4	6
5-7	4
8-15	3
16-21	2
22+	1

Thus, there is strong evidence of three modes and an indication of the possibility of two modes. Uniform-kernel density linkage gives similar results. For K=10 (10th-nearest-neighbor density linkage), the scatter plot for three clusters is shown; and for K=18, the scatter plot for two clusters is shown.

Output 31.2.11 Cluster History for Birth and Death Rates: METHOD=TWOSTAGE K=10

Cluster Analysis of Birth and Death Rates												
The CLUSTER Procedure												
Two-Stage Density Linkage Clustering												
Eigenvalues of the Covariance Matrix												
		Eigenvalue	Difference	Proportion	Cumulative							
1		189.106588	173.101020	0.9220	0.9220							
2		16.005568		0.0780	1.0000							
K = 10												
Root-Mean-Square Total-Sample Standard Deviation										10.127		
Cluster History												
NCL ---Clusters Joined---		Freq	SpRSq	RSq	ERSq	CCC	Ps F	PsT2	Normalized Fusion Density	Maximum Density in Each Cluster T i e		
									Lesser	Greater	e	
15	CL16	OB94	22	0.0015	.921	.975	-11	68.4	1.4	9.2234	6.7927	15.3069
14	CL19	OB49	28	0.0021	.919	.972	-11	72.4	1.8	8.7369	5.9334	33.4385
13	CL15	OB52	23	0.0024	.917	.969	-10	76.9	2.3	8.5847	5.9651	15.3069
12	CL13	OB96	24	0.0018	.915	.966	-9.3	83.0	1.6	7.9252	5.4724	15.3069
11	CL12	OB93	25	0.0025	.912	.962	-8.5	89.5	2.2	7.8913	5.4401	15.3069
10	CL11	OB78	26	0.0031	.909	.957	-7.7	96.9	2.5	7.787	5.4082	15.3069
9	CL10	OB76	27	0.0026	.907	.951	-6.7	107	2.1	7.7133	5.4401	15.3069
8	CL9	OB77	28	0.0023	.904	.943	-5.5	120	1.7	7.4256	4.9017	15.3069
7	CL8	OB43	29	0.0022	.902	.933	-4.1	138	1.6	6.927	4.4764	15.3069
6	CL7	OB87	30	0.0043	.898	.920	-2.7	160	3.1	4.932	2.9977	15.3069
5	CL6	OB82	31	0.0055	.892	.902	-1.1	191	3.7	3.7331	2.1560	15.3069
4	CL22	OB61	37	0.0079	.884	.875	0.93	237	10.6	3.1713	1.6308	100.0
3	CL14	OB23	29	0.0126	.872	.827	2.60	320	10.4	2.0654	1.0744	33.4385
2	CL4	CL3	66	0.2129	.659	.697	-1.3	183	172	12.409	33.4385	100.0
1	CL2	CL5	97	0.6588	.000	.000	0.00	.	183	10.071	15.3069	100.0
3 modal clusters have been formed.												

Output 31.2.12 Cluster History for Birth and Death Rates: METHOD=TWOSTAGE K=18

Cluster Analysis of Birth and Death Rates

The CLUSTER Procedure
Two-Stage Density Linkage Clustering

Eigenvalues of the Covariance Matrix

	Eigenvalue	Difference	Proportion	Cumulative
1	189.106588	173.101020	0.9220	0.9220
2	16.005568		0.0780	1.0000

K = 18

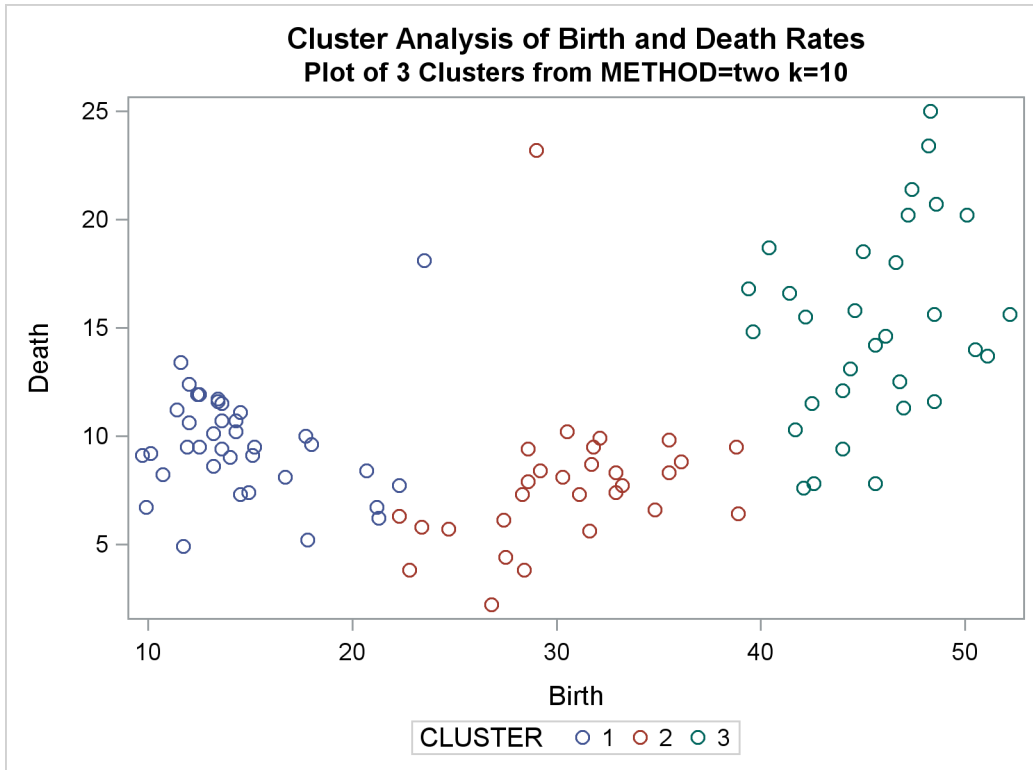
Root-Mean-Square Total-Sample Standard Deviation 10.127

Cluster History

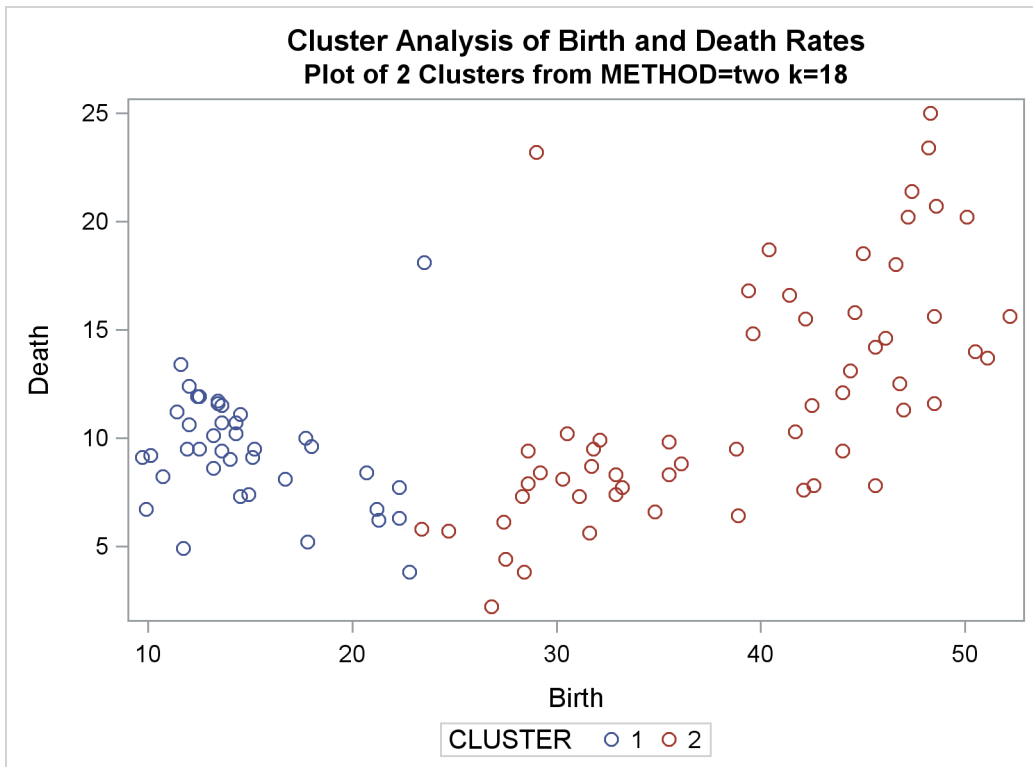
NCL	---Clusters Joined---	Freq	SpRSq	RSq	ERSq	CCC	Ps F	PsT2	Normalized Fusion Density	Maximum Density in Each Cluster		T i e
										Lesser	Greater	
15	CL16 OB72	46	0.0107	.799	.975	-21	23.3	3.0	10.118	7.7445	23.4457	
14	CL15 OB94	47	0.0098	.789	.972	-21	23.9	2.7	9.676	7.1257	23.4457	
13	CL14 OB51	48	0.0037	.786	.969	-20	25.6	1.0	9.409	6.8398	23.4457	T
12	CL13 OB96	49	0.0099	.776	.966	-19	26.7	2.6	9.409	6.8398	23.4457	
11	CL12 OB76	50	0.0114	.764	.962	-19	27.9	2.9	8.8136	6.3138	23.4457	
10	CL11 OB77	51	0.0021	.762	.957	-18	31.0	0.5	8.6593	6.0751	23.4457	
9	CL10 OB78	52	0.0103	.752	.951	-17	33.3	2.5	8.6007	6.0976	23.4457	
8	CL9 OB43	53	0.0034	.748	.943	-16	37.8	0.8	8.4964	5.9160	23.4457	
7	CL8 OB93	54	0.0109	.737	.933	-15	42.1	2.6	8.367	5.7913	23.4457	
6	CL7 OB88	55	0.0110	.726	.920	-13	48.3	2.6	7.916	5.3679	23.4457	
5	CL6 OB87	56	0.0120	.714	.902	-12	57.5	2.7	6.6917	4.3415	23.4457	
4	CL20 OB61	39	0.0077	.707	.875	-9.8	74.7	8.3	6.2578	3.2882	100.0	
3	CL5 OB82	57	0.0138	.693	.827	-5.0	106	3.0	5.3605	3.2834	23.4457	
2	CL3 OB23	58	0.0117	.681	.697	-5.4	203	2.5	3.2687	1.7568	23.4457	
1	CL2 CL4	97	0.6812	.000	.000	0.00	.	203	13.764	23.4457	100.0	

2 modal clusters have been formed.

Output 31.2.13 Plot of Clusters for METHOD=TWOSTAGE K=10



Output 31.2.14 Plot of Clusters for METHOD=TWOSTAGE K=18



In summary, most of the clustering methods indicate three or eight clusters. Most methods agree at the three-cluster level, but at the other levels, there is considerable disagreement about the composition of the clusters. The presence of numerous ties also complicates the analysis; see [Example 31.4](#).

Example 31.3: Cluster Analysis of Fisher's Iris Data

The iris data published by Fisher (1936) have been widely used for examples in discriminant analysis and cluster analysis. The sepal length, sepal width, petal length, and petal width are measured in millimeters on 50 iris specimens from each of three species, *Iris setosa*, *I. versicolor*, and *I. virginica*. Mezzich and Solomon (1980) discuss a variety of cluster analyses of the iris data.

The following step displays the iris SAS data set, which is available in the Sashelp library:

```
title 'Cluster Analysis of Fisher (1936) Iris Data';

proc print data=sashelp.iris;
run;
```

The results of this step are not shown.

This example analyzes the iris data by using Ward's method and two-stage density linkage and then illustrates how the FASTCLUS procedure can be used in combination with PROC CLUSTER to analyze large data sets.

The following macro, SHOW, is used in the subsequent analyses to display cluster results. It invokes the FREQ procedure to crosstabulate clusters and species. The CANDISC procedure computes canonical variables for discriminating among the clusters, and the first two canonical variables are plotted to show cluster membership. See Chapter 29, “[The CANDISC Procedure](#),” for a canonical discriminant analysis of the iris species.

```
/*--- Define macro show ---*/
%macro show;
  proc freq;
    tables cluster*species / nopercent norow nocol plot=none;
  run;

  proc candisc noprint out=can;
    class cluster;
    var petal: sepal:;
  run;

  proc sgplot data=can;
    scatter y=can2 x=can1 / group=cluster;
  run;
%mend;
```

The first analysis clusters the iris data by using Ward's method (see [Output 31.3.1](#)) and plots the CCC and pseudo F and t^2 statistics (see [Output 31.3.2](#)). The CCC has a local peak at three clusters but a higher peak at five clusters. The pseudo F statistic indicates three clusters, while the pseudo t^2 statistic suggests three or six clusters.

The TREE procedure creates an output data set containing the three-cluster partition for use by the SHOW macro. The FREQ procedure reveals 16 misclassifications. The results are shown in [Output 31.3.3](#).

```

title2 'By Ward's Method';
ods graphics on;

proc cluster data=sashelp.iris method=ward print=15 ccc pseudo;
  var petal: sepal:;
  copy species;
run;

proc tree noprint ncl=3 out=out;
  copy petal: sepal: species;
run;

%show;

```

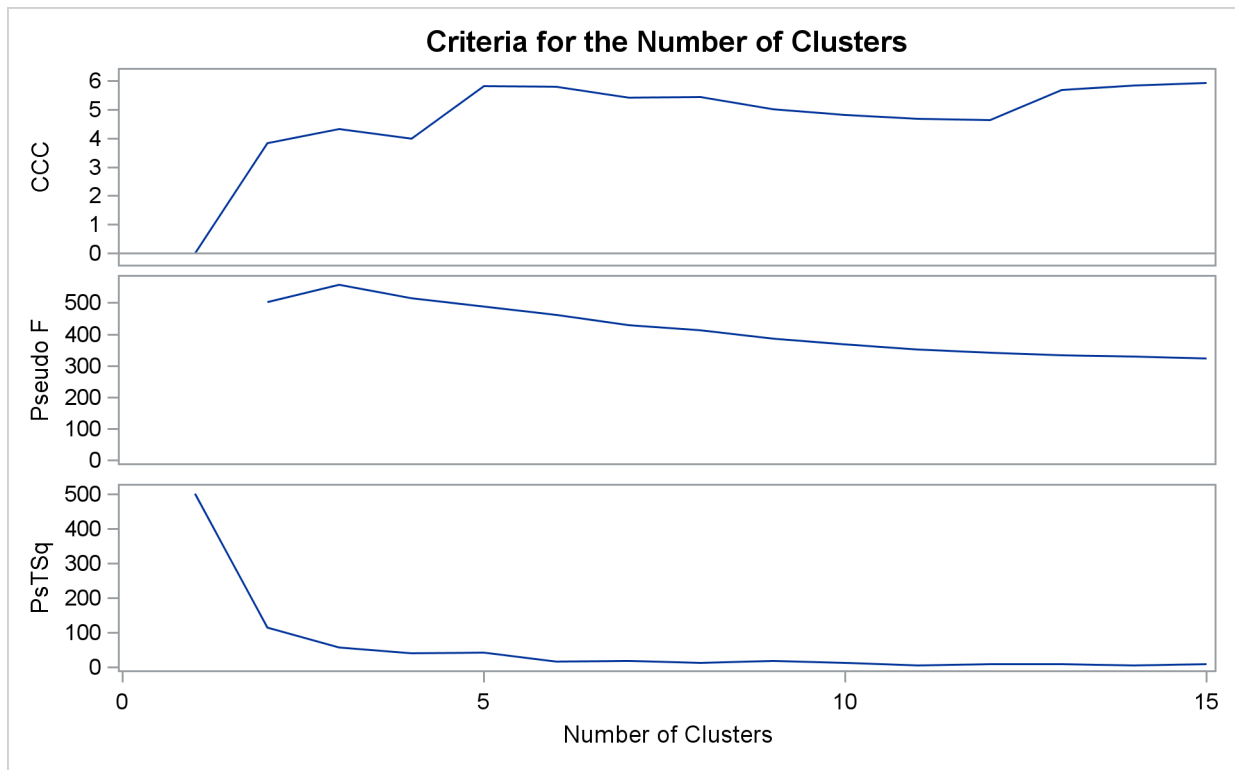
Output 31.3.1 Cluster Analysis of Fisher's Iris Data: PROC CLUSTER with METHOD=WARD

Cluster Analysis of Fisher (1936) Iris Data				
By Ward's Method				
The CLUSTER Procedure				
Ward's Minimum Variance Cluster Analysis				
Eigenvalues of the Covariance Matrix				
	Eigenvalue	Difference	Proportion	Cumulative
1	422.824171	398.557096	0.9246	0.9246
2	24.267075	16.446125	0.0531	0.9777
3	7.820950	5.437441	0.0171	0.9948
4	2.383509		0.0052	1.0000
Root-Mean-Square Total-Sample Standard Deviation				10.69224
Root-Mean-Square Distance Between Observations				30.24221

Output 31.3.1 continued

Cluster History										
NCL	---Clusters Joined---		Freq	SpRSq	RSq	ERSq	CCC	Ps F	PsTSq	T i e
15	CL24	CL28	15	0.0016	.971	.958	5.93	324	9.8	
14	CL21	CL53	7	0.0019	.969	.955	5.85	329	5.1	
13	CL18	CL48	15	0.0023	.967	.953	5.69	334	8.9	
12	CL16	CL23	24	0.0023	.965	.950	4.63	342	9.6	
11	CL14	CL43	12	0.0025	.962	.946	4.67	353	5.8	
10	CL26	CL20	22	0.0027	.959	.942	4.81	368	12.9	
9	CL27	CL17	31	0.0031	.956	.936	5.02	387	17.8	
8	CL35	CL15	23	0.0031	.953	.930	5.44	414	13.8	
7	CL10	CL47	26	0.0058	.947	.921	5.43	430	19.1	
6	CL8	CL13	38	0.0060	.941	.911	5.81	463	16.3	
5	CL9	CL19	50	0.0105	.931	.895	5.82	488	43.2	
4	CL12	CL11	36	0.0172	.914	.872	3.99	515	41.0	
3	CL6	CL7	64	0.0301	.884	.827	4.33	558	57.2	
2	CL3	CL4	100	0.1110	.773	.697	3.83	503	116	
1	CL5	CL2	150	0.7726	.000	.000	0.00	.	503	

Output 31.3.2 Criteria for the Number of Clusters with METHOD=WARD



Output 31.3.3 Crosstabulation of Clusters for METHOD=WARD

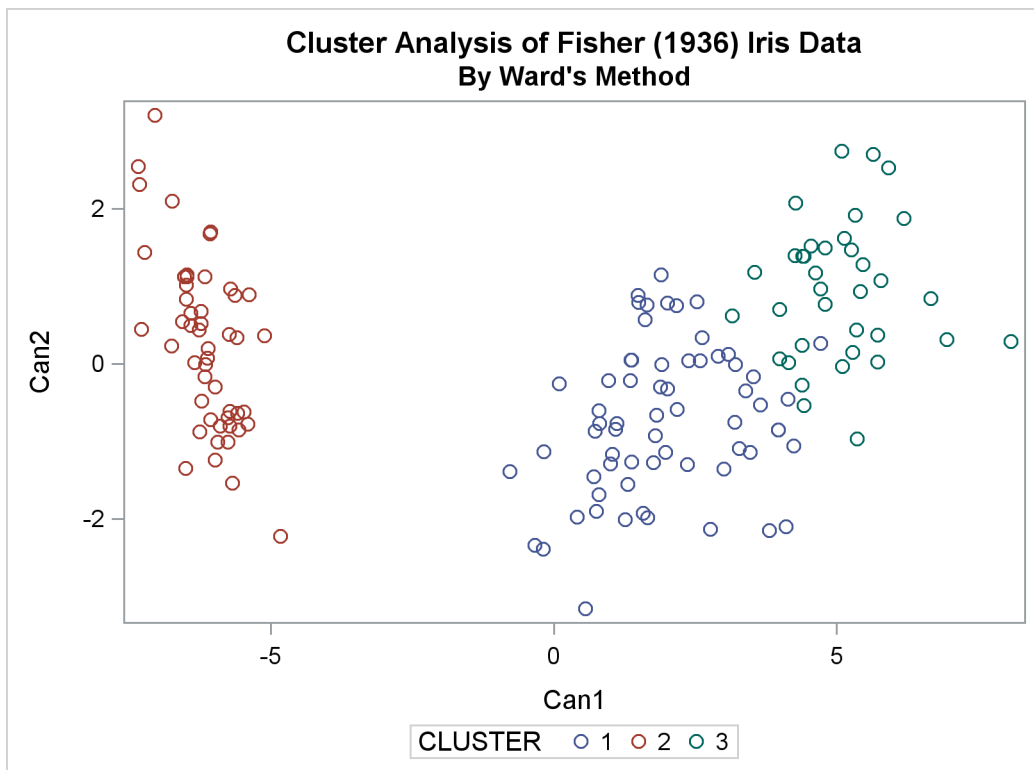
Cluster Analysis of Fisher (1936) Iris Data
By Ward's Method

The FREQ Procedure

Table of CLUSTER by Species

CLUSTER	Species(Iris Species)			Total
	Setosa	Versicol or	Virginic a	
1	0	49	15	64
2	50	0	0	50
3	0	1	35	36
Total	50	50	50	150

Output 31.3.4 Scatter Plot of Clusters for METHOD=WARD



The second analysis uses two-stage density linkage. The raw data suggest two or six modes instead of three:

<i>k</i>	Modes
3	12
4-6	6
7	4
8	3
9-50	2
51+	1

The following analysis uses $K=8$ to produce three clusters for comparison with other analyses. There are only six misclassifications. The results are shown in [Output 31.3.5](#) and [Output 31.3.6](#).

```

title2 'By Two-Stage Density Linkage';
ods graphics on;

proc cluster data=sashelp.iris method=twostage k=8 print=15 ccc pseudo;
  var petal: sepal;;
  copy species;
run;

proc tree noprint ncl=3 out=out;
  copy petal: sepal: species;
run;

%show;

```

Output 31.3.5 Cluster Analysis of Fisher's Iris Data: PROC CLUSTER with METHOD=TWOSTAGE

```

Cluster Analysis of Fisher (1936) Iris Data
By Two-Stage Density Linkage

The CLUSTER Procedure
Two-Stage Density Linkage Clustering

Eigenvalues of the Covariance Matrix

Eigenvalue   Difference   Proportion   Cumulative
1    422.824171   398.557096     0.9246     0.9246
2     24.267075    16.446125     0.0531     0.9777
3     7.820950     5.437441     0.0171     0.9948
4     2.383509

```

K = 8

```

Root-Mean-Square Total-Sample Standard Deviation    10.69224

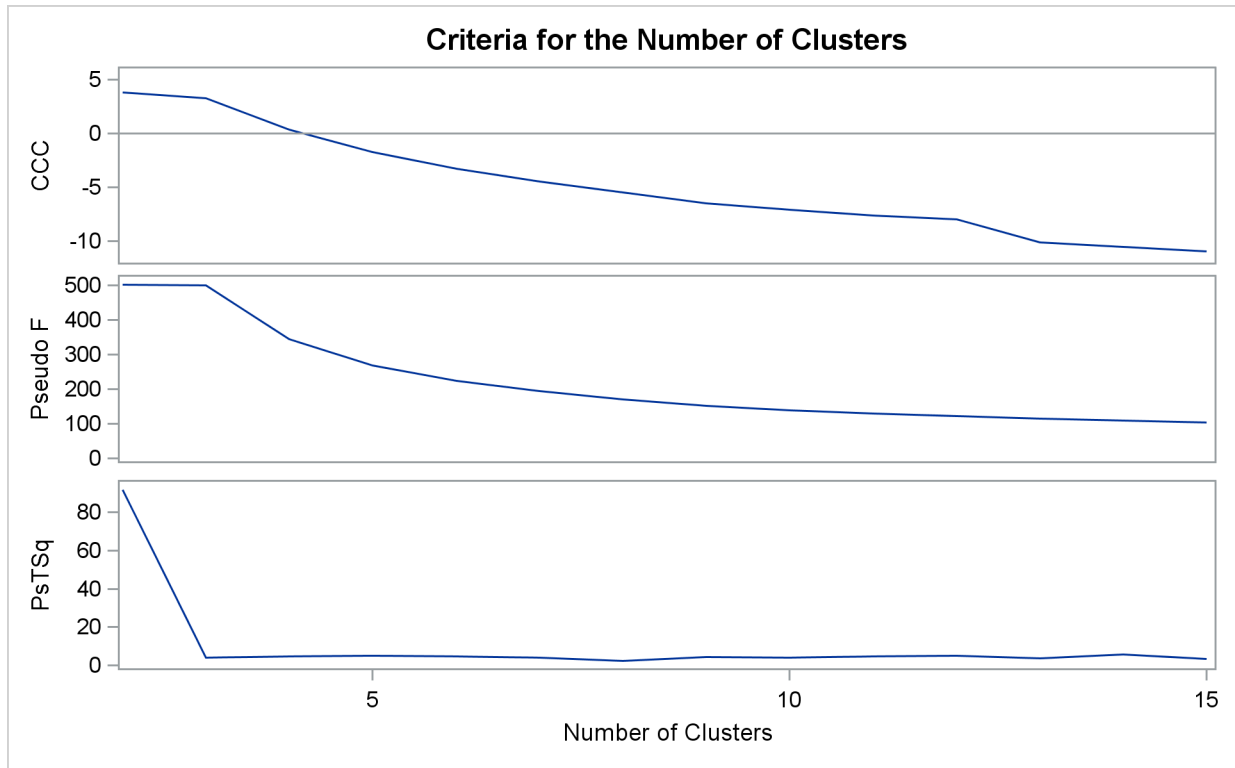
```

Output 31.3.5 continued

Cluster History										Maximum Density		
NCL	---Clusters Joined---	Freq	SpRSq	RSq	ERSq	CCC	Ps F	PsT2	Normalized Fusion Density	in Each Cluster		T i e
										Lesser	Greater	
15	CL17 OB144	44	0.0025	.916	.958	-11	105	3.4	0.3903	0.2066	3.5156	
14	CL16 OB44	50	0.0023	.913	.955	-11	110	5.6	0.3637	0.1837	100.0	
13	CL15 OB127	45	0.0029	.910	.953	-10	116	3.7	0.3553	0.2130	3.5156	
12	CL28 OB66	46	0.0036	.907	.950	-8.0	122	5.2	0.3223	0.1736	8.3678	T
11	CL12 OB73	47	0.0036	.903	.946	-7.6	130	4.8	0.3223	0.1736	8.3678	
10	CL11 OB79	48	0.0033	.900	.942	-7.1	140	4.1	0.2879	0.1479	8.3678	
9	CL13 OB112	46	0.0037	.896	.936	-6.5	152	4.4	0.2802	0.2005	3.5156	
8	CL10 OB113	49	0.0019	.894	.930	-5.5	171	2.2	0.2699	0.1372	8.3678	
7	CL8 OB91	50	0.0035	.891	.921	-4.5	194	4.0	0.2586	0.1372	8.3678	
6	CL9 OB120	47	0.0042	.886	.911	-3.3	225	4.6	0.1412	0.0832	3.5156	
5	CL6 OB118	48	0.0049	.882	.895	-1.7	270	5.0	0.107	0.0605	3.5156	
4	CL5 OB110	49	0.0049	.877	.872	0.35	346	4.7	0.0969	0.0541	3.5156	
3	CL4 OB135	50	0.0047	.872	.827	3.28	500	4.1	0.0715	0.0370	3.5156	
2	CL7 CL3	100	0.0993	.773	.697	3.83	503	91.9	2.6277	3.5156	8.3678	

3 modal clusters have been formed.

Output 31.3.6 Criteria for the Number of Clusters with METHOD=TWOSTAGE



Output 31.3.7 Crosstabulation of Clusters for METHOD=TWOSTAGE

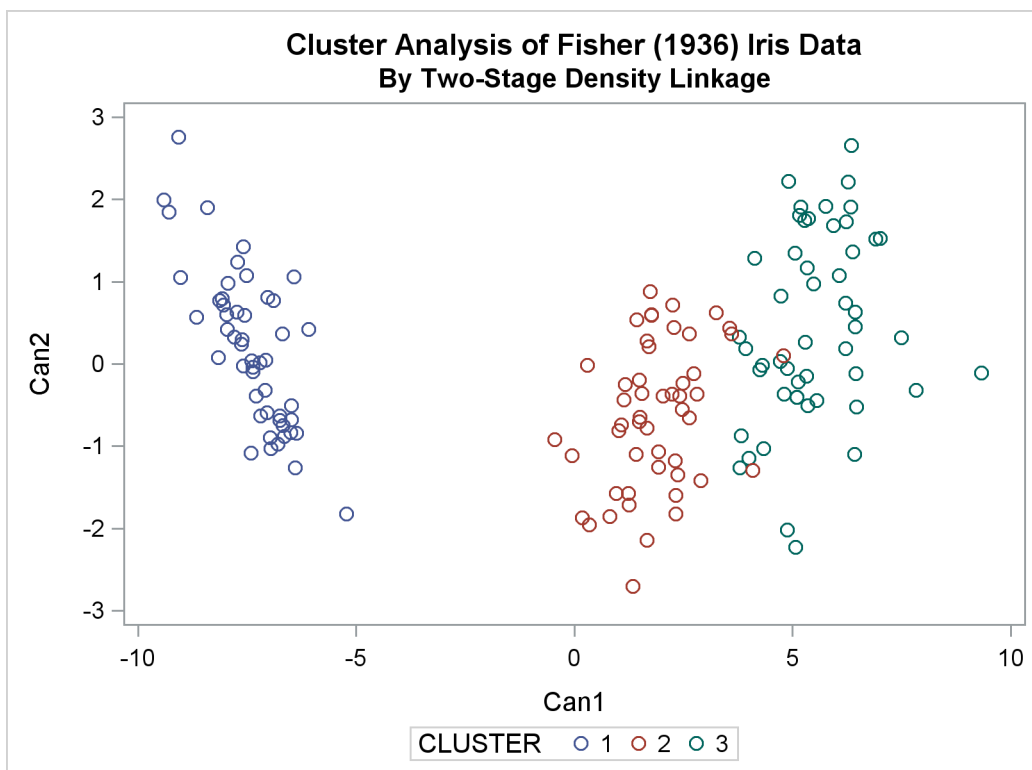
Cluster Analysis of Fisher (1936) Iris Data
By Two-Stage Density Linkage

The FREQ Procedure

Table of CLUSTER by Species

CLUSTER	Species(Iris Species)			Total
	Setosa	Versicol or	Virginic a	
1	50	0	0	50
2	0	47	3	50
3	0	3	47	50
Total	50	50	50	150

Output 31.3.8 Scatter Plot of Clusters for METHOD=TWOSTAGE



The CLUSTER procedure is not practical for very large data sets because, with most methods, the CPU time is roughly proportional to the square or cube of the number of observations. The FASTCLUS procedure requires time proportional to the number of observations and can therefore be used with much larger data sets than PROC CLUSTER. If you want to hierarchically cluster a very large data set, you can use PROC FASTCLUS for a preliminary cluster analysis to produce a large number of clusters and then use PROC CLUSTER to hierarchically cluster the preliminary clusters.

FASTCLUS automatically creates the variables `_FREQ_` and `_RMSSTD_` in the `MEAN=` output data set. These variables are then automatically used by PROC CLUSTER in the computation of various statistics.

The following SAS code uses the iris data to illustrate the process of clustering clusters. In the preliminary analysis, PROC FASTCLUS produces ten clusters, which are then crosstabulated with species. The data set containing the preliminary clusters is sorted in preparation for later merges. The results are shown in [Output 31.3.9](#) and [Output 31.3.10](#).

```

title2 'Preliminary Analysis by FASTCLUS';
proc fastclus data=sashelp.iris summary maxc=10 maxiter=99 converge=0
              mean=mean out=prelim cluster=preclus;
  var petal: sepal;;
run;

proc freq;
  tables preclus*species / nopercnt norow nocol plot=none;
run;

proc sort data=prelim;
  by preclus;
run;

```

Output 31.3.9 Preliminary Analysis of Fisher's Iris Data: FASTCLUS Procedure

```

Cluster Analysis of Fisher (1936) Iris Data
Preliminary Analysis by FASTCLUS

The FASTCLUS Procedure
Replace=FULL Radius=0 Maxclusters=10 Maxiter=99 Converge=0

Convergence criterion is satisfied.

Criterion Based on Final Seeds = 2.1271

```

Output 31.3.9 continued

Cluster Summary					
Cluster	Frequency	RMS Std Deviation	Maximum Distance from Seed to Observation	Radius Exceeded	Nearest Cluster
1	14	2.3258	6.6047		10
2	16	2.0402	6.7373		3
3	23	1.6115	6.3775		8
4	24	2.4329	8.3178		6
5	10	3.1829	7.9517		4
6	18	2.2628	7.1135		7
7	12	1.9824	7.0833		1
8	11	1.7123	7.0435		3
9	10	2.5155	6.1335		10
10	12	2.0207	7.9390		1

Cluster Summary	
Cluster	Distance Between Cluster Centroids
1	5.6068
2	6.2977
3	5.4185
4	9.3274
5	12.4281
6	8.2685
7	7.6733
8	5.4185
9	8.4783
10	5.6068

Pseudo F Statistic = 374.89

Observed Over-All R-Squared = 0.96016

Approximate Expected Over-All R-Squared = 0.82928

Cubic Clustering Criterion = 27.285

WARNING: The two values above are invalid for correlated variables.

Output 31.3.10 Crosstabulation of Species and Cluster From the FASTCLUS Procedure

```

Cluster Analysis of Fisher (1936) Iris Data
Preliminary Analysis by FASTCLUS

The FREQ Procedure

Table of preclus by Species

preclus (Cluster)      Species (Iris Species)

Frequency|Setosa  |Versicol|Virginic|  Total
         |         |or      |a       |
-----+-----+-----+-----+
         1 |      0 |    14 |      0 |      14
-----+-----+-----+-----+
         2 |     16 |      0 |      0 |      16
-----+-----+-----+-----+
         3 |     23 |      0 |      0 |      23
-----+-----+-----+-----+
         4 |      0 |      0 |     24 |      24
-----+-----+-----+-----+
         5 |      0 |      0 |     10 |      10
-----+-----+-----+-----+
         6 |      0 |      3 |     15 |      18
-----+-----+-----+-----+
         7 |      0 |     12 |      0 |      12
-----+-----+-----+-----+
         8 |     11 |      0 |      0 |      11
-----+-----+-----+-----+
         9 |      0 |     10 |      0 |      10
-----+-----+-----+-----+
        10 |      0 |     11 |      1 |      12
-----+-----+-----+-----+
Total          50      50      50      150
    
```

The following macro, CLUS, clusters the preliminary clusters. There is one argument to choose the METHOD= specification to be used by PROC CLUSTER. The TREE procedure creates an output data set containing the three-cluster partition, which is sorted and merged with the OUT= data set from PROC FASTCLUS to determine which cluster each of the original 150 observations belongs to. The SHOW macro is then used to display the results. In this example, the CLUS macro is invoked using Ward's method, which produces 16 misclassifications, and Wong's hybrid method, which produces 22 misclassifications.


```

/*--- Define macro clus ---*/
%macro clus(method);
  proc cluster data=mean method=&method ccc pseudo;
    var petal: sepal:;
    copy preclus;
  run;

  proc tree noprint ncl=3 out=out;
    copy petal: sepal: preclus;
  run;

  proc sort data=out;
    by preclus;
  run;

  data clus;
    merge out prelim;
    by preclus;
  run;

  %show;
%mend;

```

The following statements produce [Output 31.3.11](#) through [Output 31.3.14](#).

```

title2 'Clustering Clusters by Ward' 's Method';
%clus(ward);

```

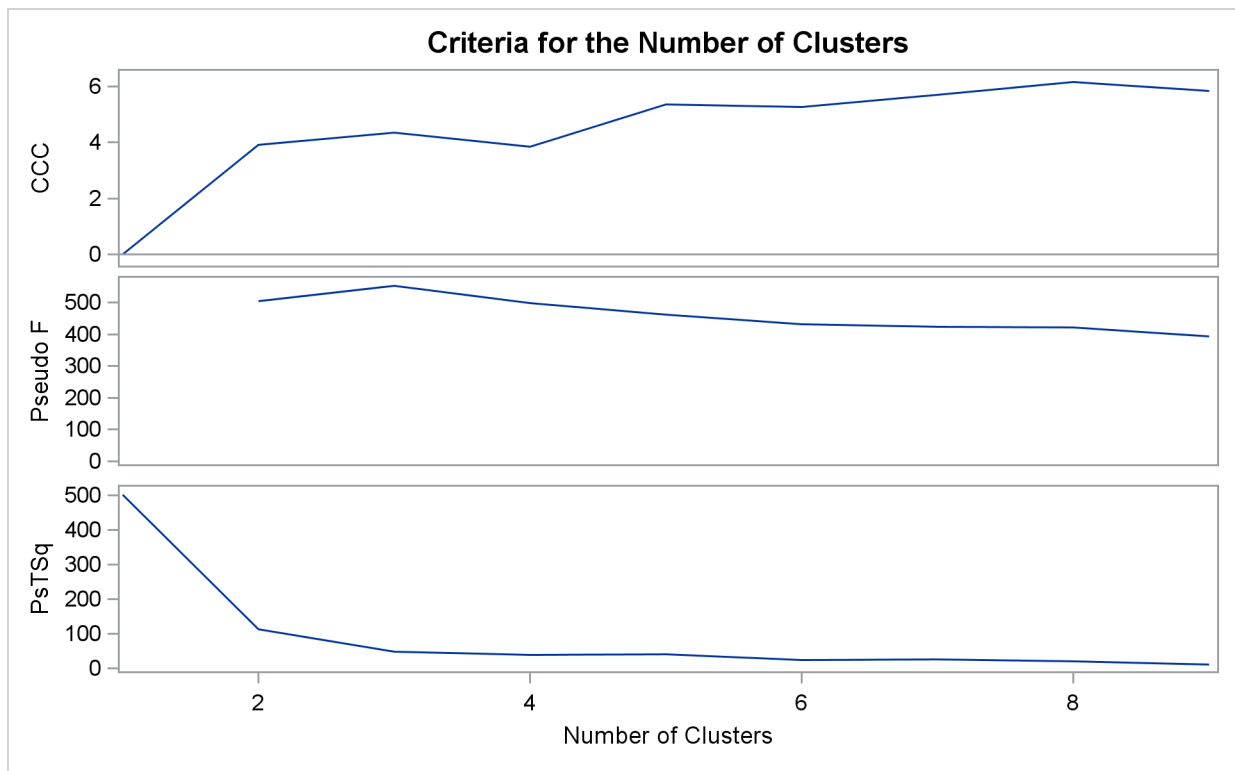
Output 31.3.11 Clustering Clusters by Ward's Method

Cluster Analysis of Fisher (1936) Iris Data				
Clustering Clusters by Ward's Method				
The CLUSTER Procedure				
Ward's Minimum Variance Cluster Analysis				
Eigenvalues of the Covariance Matrix				
	Eigenvalue	Difference	Proportion	Cumulative
1	417.301104	398.455363	0.9504	0.9504
2	18.845742	16.244505	0.0429	0.9933
3	2.601236	2.272553	0.0059	0.9993
4	0.328684		0.0007	1.0000
Root-Mean-Square Total-Sample Standard Deviation				10.69224
Root-Mean-Square Distance Between Observations				30.24221

Output 31.3.11 continued

Cluster History								T	
NCL	---Clusters Joined---		Freq	SpRSq	RSq	ERSq	CCC	Ps F	PsT2 e
9	OB1	OB10	26	0.0030	.957	.934	5.84	394	10.6
8	OB3	OB8	34	0.0032	.954	.927	6.16	420	20.2
7	OB6	OB7	30	0.0072	.947	.919	5.70	424	26.5
6	CL9	OB9	36	0.0094	.937	.908	5.26	431	24.5
5	OB2	CL8	50	0.0103	.927	.893	5.36	461	41.3
4	OB4	OB5	34	0.0160	.911	.870	3.84	498	38.4
3	CL6	CL7	66	0.0285	.883	.825	4.36	552	48.8
2	CL3	CL4	100	0.1099	.773	.695	3.91	503	113
1	CL2	CL5	150	0.7726	.000	.000	0.00	.	503

Output 31.3.12 Criteria for the Number of Clusters for Clustering Clusters from Ward's Method



Output 31.3.13 Crosstabulation for Clustering Clusters from Ward's Method

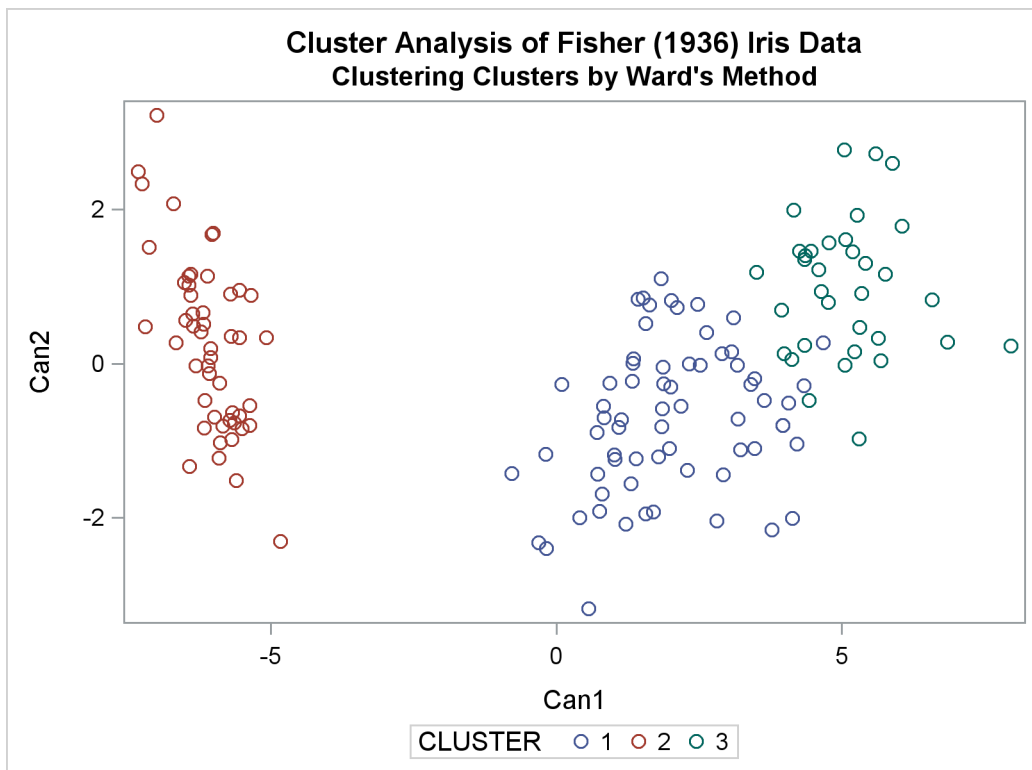
Cluster Analysis of Fisher (1936) Iris Data
Clustering Clusters by Ward's Method

The FREQ Procedure

Table of CLUSTER by Species

CLUSTER	Species(Iris Species)			Total
	Setosa	Versicol or	Virginic a	
1	0	50	16	66
2	50	0	0	50
3	0	0	34	34
Total	50	50	50	150

Output 31.3.14 Scatter Plot for Clustering Clusters using Ward's Method



The following statements produce Output 31.3.15 through Output 31.3.17.

```
title2 "Clustering Clusters by Wong's Hybrid Method";
%clus (twostage hybrid);
```

Output 31.3.15 Clustering Clusters by Wong's Hybrid Method

Cluster Analysis of Fisher (1936) Iris Data											
Clustering Clusters by Wong's Hybrid Method											
The CLUSTER Procedure											
Two-Stage Density Linkage Clustering											
Eigenvalues of the Covariance Matrix											
	Eigenvalue	Difference	Proportion	Cumulative							
1	417.301104	398.455363	0.9504	0.9504							
2	18.845742	16.244505	0.0429	0.9933							
3	2.601236	2.272553	0.0059	0.9993							
4	0.328684		0.0007	1.0000							
Root-Mean-Square Total-Sample Standard Deviation				10.69224							
Cluster History											
NCL	---Clusters Joined---	Freq	SpRSq	RSq	ERSq	CCC	Ps F	PsT2	Normalized Fusion Density	Maximum Density in Each Cluster	Greater e
9	OB3 OB8	34	0.0032	.957	.934	5.77	392	20.2	47.595	41.5390	100.0
8	CL9 OB2	50	0.0103	.947	.927	4.19	360	41.3	34.03	28.1852	100.0
7	OB1 OB10	26	0.0030	.944	.919	4.94	399	10.6	17.044	14.8854	22.9763
6	OB6 OB7	30	0.0072	.936	.908	5.07	424	26.5	10.842	20.6497	24.8051
5	CL6 OB4	54	0.0169	.920	.893	4.00	415	38.4	9.7472	20.0098	24.8051
4	CL7 OB9	36	0.0094	.910	.870	3.74	493	24.5	7.0911	8.2711	22.9763
3	CL5 OB5	64	0.0347	.875	.825	3.72	517	47.7	3.4164	3.2270	24.8051
2	CL3 CL4	100	0.1029	.773	.695	3.91	503	98.5	10.77	22.9763	24.8051
1	CL2 CL8	150	0.7726	.000	.000	0.00	.	503	0.5153	24.8051	100.0
3 modal clusters have been formed.											

Output 31.3.16 Crosstabulation for Clustering Clusters from Wong's Hybrid Method

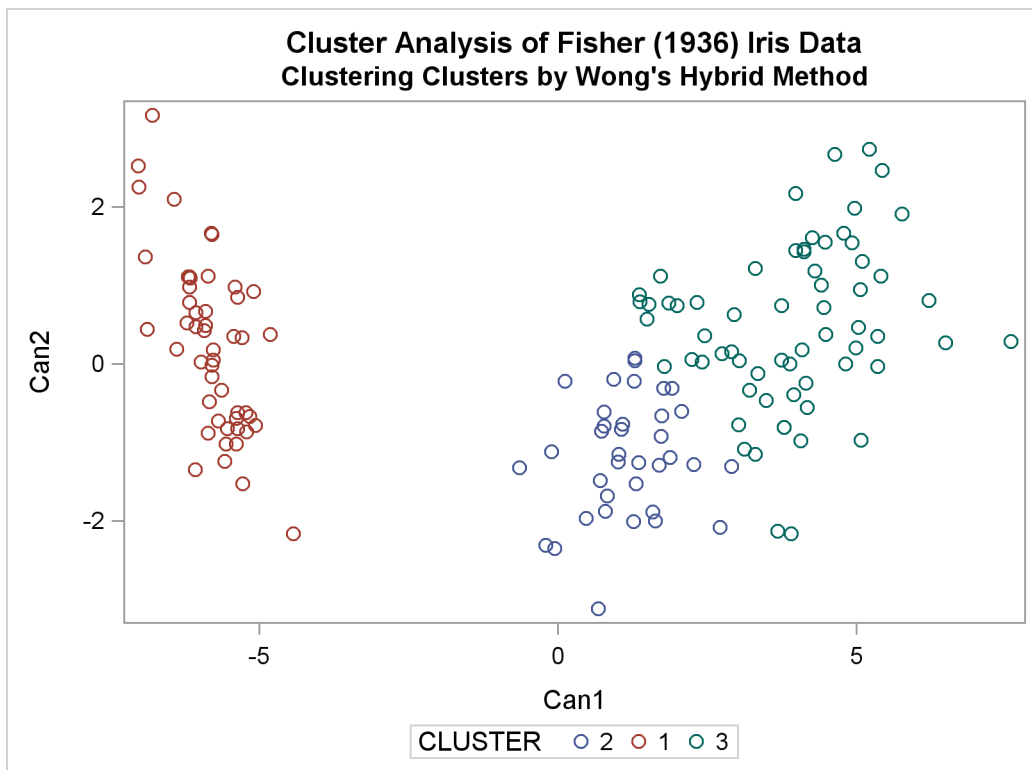
**Cluster Analysis of Fisher (1936) Iris Data
Clustering Clusters by Wong's Hybrid Method**

The FREQ Procedure

Table of CLUSTER by Species

CLUSTER	Species(Iris Species)			Total
	Setosa	Versicol or	Virginic a	
1	50	0	0	50
2	0	35	1	36
3	0	15	49	64
Total	50	50	50	150

Output 31.3.17 Scatter Plot for Clustering Clusters using Wong's Hybrid Method



Example 31.4: Evaluating the Effects of Ties

If, at some level of the cluster history, there is a tie for minimum distance between clusters, then one or more levels of the sample cluster tree are not uniquely determined. This example shows how the degree of indeterminacy can be assessed.

Mammals have four kinds of teeth: incisors, canines, premolars, and molars. The following data set gives the number of teeth of each kind on one side of the top and bottom jaws for 32 mammals.

Since all eight variables are measured in the same units, it is not strictly necessary to rescale the data. However, the canines have much less variance than the other kinds of teeth and, therefore, have little effect on the analysis if the variables are not standardized. An average linkage cluster analysis is run with and without standardization to enable comparison of the results.

```

title 'Hierarchical Cluster Analysis of Mammals' 'Teeth Data';
title2 'Evaluating the Effects of Ties';
data teeth;
  input Mammal & $16. v1-v8 @@;
  label v1='Top incisors'
        v2='Bottom incisors'
        v3='Top canines'
        v4='Bottom canines'
        v5='Top premolars'
        v6='Bottom premolars'
        v7='Top molars'
        v8='Bottom molars';
  datalines;
Brown Bat      2 3 1 1 3 3 3 3   Mole           3 2 1 0 3 3 3 3
Silver Hair Bat 2 3 1 1 2 3 3 3   Pigmy Bat     2 3 1 1 2 2 3 3
House Bat      2 3 1 1 1 2 3 3   Red Bat       1 3 1 1 2 2 3 3
Pika           2 1 0 0 2 2 3 3   Rabbit        2 1 0 0 3 2 3 3
Beaver         1 1 0 0 2 1 3 3   Groundhog     1 1 0 0 2 1 3 3
Gray Squirrel  1 1 0 0 1 1 3 3   House Mouse   1 1 0 0 0 0 3 3
Porcupine      1 1 0 0 1 1 3 3   Wolf          3 3 1 1 4 4 2 3
Bear           3 3 1 1 4 4 2 3   Raccoon       3 3 1 1 4 4 3 2
Marten         3 3 1 1 4 4 1 2   Weasel        3 3 1 1 3 3 1 2
Wolverine      3 3 1 1 4 4 1 2   Badger        3 3 1 1 3 3 1 2
River Otter    3 3 1 1 4 3 1 2   Sea Otter     3 2 1 1 3 3 1 2
Jaguar         3 3 1 1 3 2 1 1   Cougar        3 3 1 1 3 2 1 1
Fur Seal       3 2 1 1 4 4 1 1   Sea Lion      3 2 1 1 4 4 1 1
Grey Seal      3 2 1 1 3 3 2 2   Elephant Seal 2 1 1 1 4 4 1 1
Reindeer       0 4 1 0 3 3 3 3   Elk           0 4 1 0 3 3 3 3
Deer           0 4 0 0 3 3 3 3   Moose         0 4 0 0 3 3 3 3
;

```

The following statements produce Output 31.4.1:

```

title3 'Raw Data';
proc cluster data=teeth method=average nonorm noeigen;
  var v1-v8;
  id mammal;
run;

```

Output 31.4.1 Average Linkage Analysis of Mammals' Teeth Data: Raw Data

Hierarchical Cluster Analysis of Mammals' Teeth Data					
Evaluating the Effects of Ties					
Raw Data					
The CLUSTER Procedure					
Average Linkage Cluster Analysis					
Root-Mean-Square Total-Sample Standard Deviation				0.898027	
Cluster History					
Number of Clusters	-----Clusters Joined-----		Freq	RMS Distance	Tie
31	Beaver	Groundhog	2	0	T
30	Gray Squirrel	Porcupine	2	0	T
29	Wolf	Bear	2	0	T
28	Marten	Wolverine	2	0	T
27	Weasel	Badger	2	0	T
26	Jaguar	Cougar	2	0	T
25	Fur Seal	Sea Lion	2	0	T
24	Reindeer	Elk	2	0	T
23	Deer	Moose	2	0	
22	Brown Bat	Silver Hair Bat	2	1	T
21	Pigmy Bat	House Bat	2	1	T
20	Pika	Rabbit	2	1	T
19	CL31	CL30	4	1	T
18	CL28	River Otter	3	1	T
17	CL27	Sea Otter	3	1	T
16	CL24	CL23	4	1	
15	CL21	Red Bat	3	1.2247	
14	CL17	Grey Seal	4	1.291	
13	CL29	Raccoon	3	1.4142	T
12	CL25	Elephant Seal	3	1.4142	
11	CL18	CL14	7	1.5546	
10	CL22	CL15	5	1.5811	
9	CL20	CL19	6	1.8708	T
8	CL11	CL26	9	1.9272	
7	CL8	CL12	12	2.2278	
6	Mole	CL13	4	2.2361	
5	CL9	House Mouse	7	2.4833	
4	CL6	CL7	16	2.5658	
3	CL10	CL16	9	2.8107	
2	CL3	CL5	16	3.7054	
1	CL2	CL4	32	4.2939	

The following statements produce [Output 31.4.2](#):

```
title3 'Standardized Data';  
proc cluster data=teeth std method=average nonorm noeigen;  
  var v1-v8;  
  id mammal;  
run;
```

Output 31.4.2 Average Linkage Analysis of Mammals' Teeth Data: Standardized Data

```

      Hierarchical Cluster Analysis of Mammals' Teeth Data
      Evaluating the Effects of Ties
      Standardized Data

      The CLUSTER Procedure
      Average Linkage Cluster Analysis

The data have been standardized to mean 0 and variance 1

Root-Mean-Square Total-Sample Standard Deviation           1
```


Output 31.4.2 continued

Number of Clusters	Cluster History		Freq	RMS Distance	Tie
	-----Clusters	Joined-----			
31	Beaver	Groundhog	2	0	T
30	Gray Squirrel	Porcupine	2	0	T
29	Wolf	Bear	2	0	T
28	Marten	Wolverine	2	0	T
27	Weasel	Badger	2	0	T
26	Jaguar	Cougar	2	0	T
25	Fur Seal	Sea Lion	2	0	T
24	Reindeer	Elk	2	0	T
23	Deer	Moose	2	0	
22	Pigmy Bat	Red Bat	2	0.9157	
21	CL28	River Otter	3	0.9169	
20	CL31	CL30	4	0.9428	T
19	Brown Bat	Silver Hair Bat	2	0.9428	T
18	Pika	Rabbit	2	0.9428	
17	CL27	Sea Otter	3	0.9847	
16	CL22	House Bat	3	1.1437	
15	CL21	CL17	6	1.3314	
14	CL25	Elephant Seal	3	1.3447	
13	CL19	CL16	5	1.4688	
12	CL15	Grey Seal	7	1.6314	
11	CL29	Raccoon	3	1.692	
10	CL18	CL20	6	1.7357	
9	CL12	CL26	9	2.0285	
8	CL24	CL23	4	2.1891	
7	CL9	CL14	12	2.2674	
6	CL10	House Mouse	7	2.317	
5	CL11	CL7	15	2.6484	
4	CL13	Mole	6	2.8624	
3	CL4	CL8	10	3.5194	
2	CL3	CL6	17	4.1265	
1	CL2	CL5	32	4.7753	

There are ties at 16 levels for the raw data but at only 10 levels for the standardized data. There are more ties for the raw data because the increments between successive values are the same for all of the raw variables but different for the standardized variables.

One way to assess the importance of the ties in the analysis is to repeat the analysis on several random permutations of the observations and then to see to what extent the results are consistent at the interesting levels of the cluster history. Three macros are presented to facilitate this process, as follows.

```

/* ----- */
/*
/* The macro CLUSPERM randomly permutes observations and
/* does a cluster analysis for each permutation.
/* The arguments are as follows:
/*
/* data data set name
/* var list of variables to cluster
/* id id variable for proc cluster
/* method clustering method (and possibly other options)
/* nperm number of random permutations.
/* ----- */
%macro CLUSPERM(data,var,id,method,nperm);

/* -----CREATE TEMPORARY DATA SET WITH RANDOM NUMBERS----- */
data _temp_;
  set &data;
  array _random_ _ran_1-_ran_&nperm;
  do over _random_;
    _random_=ranuni(835297461);
  end;
run;

/* -----PERMUTE AND CLUSTER THE DATA----- */
%do n=1 %to &nperm;
  proc sort data=_temp_ (keep=_ran_&n &var &id) out=_perm_;
    by _ran_&n;
  run;

  proc cluster method=&method noprint outtree=_tree_&n;
    var &var;
    id &id;
  run;
%end;
%mend;

```

```

/* ----- */
/*
/* The macro PLOTPERM plots various cluster statistics
/* against the number of clusters for each permutation.
/* The arguments are as follows:
/*
/* nclus maximum number of clusters to be plotted
/* nperm number of random permutations.
/*
/* ----- */
%macro PLOTPERM(nclus,nperm);

/* ---CONCATENATE TREE DATA SETS FOR 20 OR FEWER CLUSTERS--- */
data _plot_;
  set %do n=1 %to &nperm; _tree_&n(in=_in_&n) %end;;
  if _ncl_<=&nclus;
  %do n=1 %to &nperm;
    if _in_&n then _perm_=&n;
  %end;
  label _perm_='permutation number';
  keep _ncl_ _psf_ _pst2_ _ccc_ _perm_;
run;

/* ---PLOT THE REQUESTED STATISTICS BY NUMBER OF CLUSTERS--- */
proc sgscatter;
  compare y=( _ccc_ _psf_ _pst2_ ) x=_ncl_ /group=_perm_;
  label _ccc_ = 'CCC' _psf_ = 'Pseudo F' _pst2_ = 'Pseudo T-Squared';
run;
%mend;

/* ----- */
/*
/* The macro TABPERM generates cluster-membership variables
/* for a specified number of clusters for each permutation.
/* PROC TABULATE gives the frequencies and means.
/* The arguments are as follows:
/*
/* var list of variables to cluster
/* (no "-" or ":" allowed)
/* id id variable for proc cluster
/* meanfmt format for printing means in PROC TABULATE
/* nclus number of clusters desired
/* nperm number of random permutations.
/*
/* ----- */
%macro TABPERM(var,id,meanfmt,nclus,nperm);

/* -----CREATE DATA SETS GIVING CLUSTER MEMBERSHIP----- */
%do n=1 %to &nperm;
  proc tree data=_tree_&n noprint n=&nclus
    out=_out_&n(drop=clusname
              rename=(cluster=_clus_&n));
    copy &var;
    id &id;
  run;

```

```

proc sort;
  by &id &var;
run;
%end;

/* -----MERGE THE CLUSTER VARIABLES----- */
data _merge_;
merge
  %do n=1 %to &nperm;
    _out_&n
  %end;;
by &id &var;
length all_clus $ %eval(3*&nperm);
%do n=1 %to &nperm;
  substr( all_clus, %eval(1+(&n-1)*3), 3) =
    put( _clus_&n, 3.);
%end;
run;

/*----- TABULATE CLUSTER COMBINATIONS----- */
proc sort;
  by _clus_;;
run;
proc tabulate order=data formchar='          ';
  class all_clus;
  var &var;
  table all_clus, n='FREQ'*f=5. mean*f=&meanfmt*(&var) /
    rts=%eval(&nperm*3+1);
run;
%mend;

```

To use these macros, it is first convenient to define a macro variable, `VLIST`, listing the teeth variables, since the forms `V1-V8` or `V:` cannot be used with the `TABULATE` procedure in the `TABPERM` macro:

```

/* -TABULATE does not accept hyphens or colons in VAR lists- */
%let vlist=v1 v2 v3 v4 v5 v6 v7 v8;

```

The `CLUSPERM` macro is then called to analyze 10 random permutations. The `PLOTPERM` macro plots the pseudo F and t^2 statistics and the cubic clustering criterion. Since the data are discrete, the pseudo F statistic and the cubic clustering criterion can be expected to increase as the number of clusters increases, so local maxima or large jumps in these statistics are more relevant than the global maximum in determining the number of clusters. For the raw data, only the pseudo t^2 statistic indicates the possible presence of clusters, with the four-cluster level being suggested. Hence, the macros are used as follows to analyze the results at the four-cluster level:

```

title3 'Raw Data';

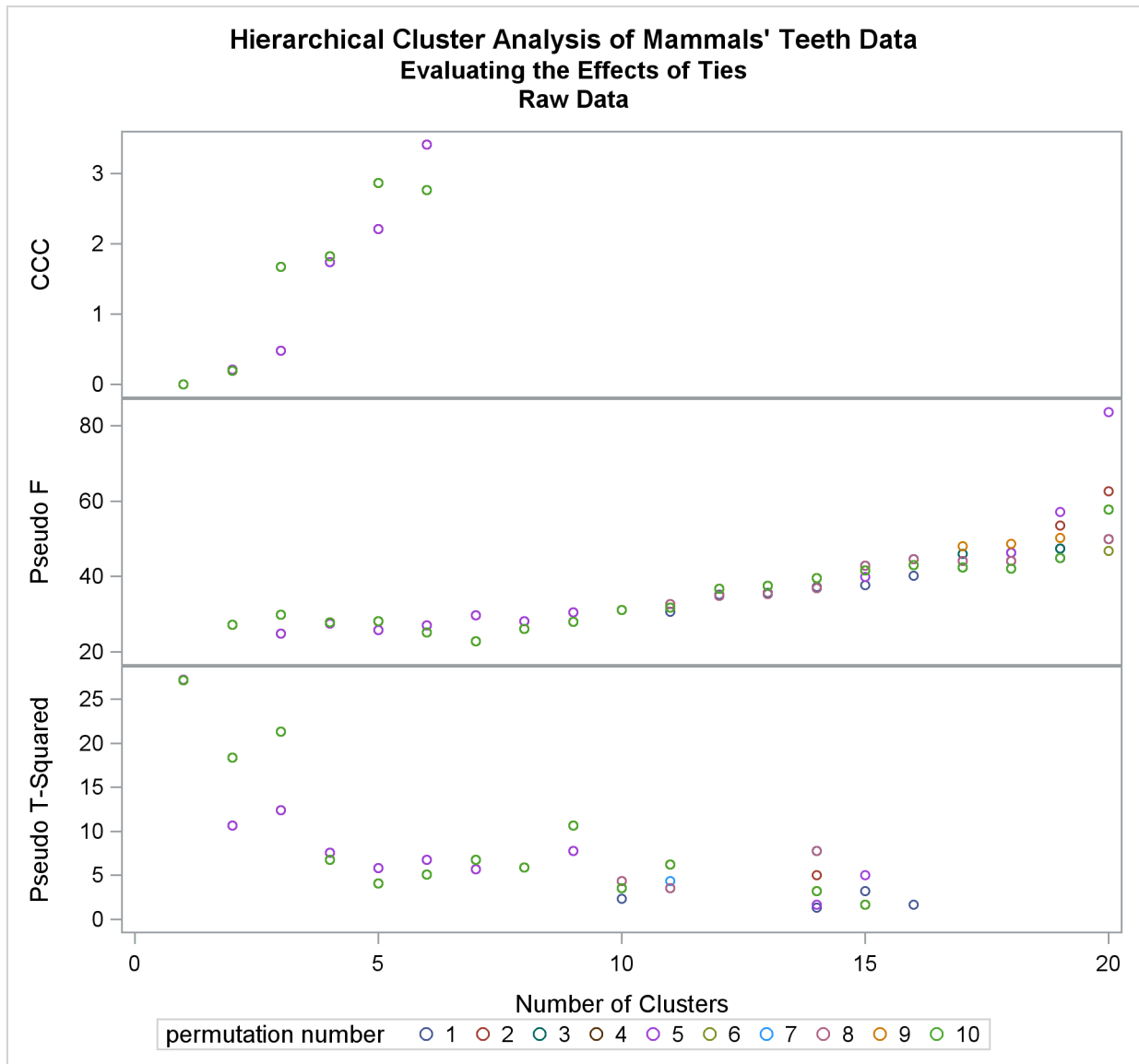
/* -----CLUSTER RAW DATA WITH AVERAGE LINKAGE----- */
%clusperm( teeth, &vlist, mammal, average, 10);

```

The following statements produce Output 31.4.3.

```
/* -----PLOT STATISTICS FOR THE LAST 20 LEVELS----- */
%plotperm(20, 10);
```

Output 31.4.3 Analysis of 10 Random Permutations of Raw Mammals' Teeth Data



The following statements produce Output 31.4.4.

```
/* -----ANALYZE THE 4-CLUSTER LEVEL----- */
%tabperm( &vlist, mammal, 9.1, 4, 10);
```

Output 31.4.4 Raw Mammals' Teeth Data: Indeterminacy at the Four-Cluster Level

Hierarchical Cluster Analysis of Mammals' Teeth Data														
Evaluating the Effects of Ties														
Raw Data														

										Mean				

										Top Bottom Top Bottom				
										FREQ incisors incisors canines canines				

all_clus														

1	3	1	1	1	3	3	3	2	3	4	0.0	4.0	0.5	0.0
2	2	2	2	2	2	1	2	1	1	15	2.9	2.6	1.0	1.0
2	4	2	2	4	2	1	2	1	1	1	3.0	2.0	1.0	0.0
3	1	3	3	3	1	2	1	3	2	5	1.0	1.0	0.0	0.0
3	4	3	3	4	1	2	1	3	2	2	2.0	1.0	0.0	0.0
4	4	4	4	4	4	4	4	4	4	5	1.8	3.0	1.0	1.0

(Continued)

Hierarchical Cluster Analysis of Mammals' Teeth Data													
Evaluating the Effects of Ties													
Raw Data													

										Mean			

										Top Bottom Top Bottom			
										premolars premolars molars molars			

all_clus													

1	3	1	1	1	3	3	3	2	3	3.0	3.0	3.0	3.0
2	2	2	2	2	2	1	2	1	1	3.6	3.4	1.3	1.8
2	4	2	2	4	2	1	2	1	1	3.0	3.0	3.0	3.0
3	1	3	3	3	1	2	1	3	2	1.2	0.8	3.0	3.0
3	4	3	3	4	1	2	1	3	2	2.5	2.0	3.0	3.0
4	4	4	4	4	4	4	4	4	4	2.0	2.4	3.0	3.0

From the TABULATE output, you can see that two types of clustering are obtained. In one case, the mole is grouped with the carnivores, while the pika and rabbit are grouped with the rodents. In the other case, both the mole and the lagomorphs are grouped with the bats.

Next, the analysis is repeated with the standardized data as shown in the following statements. The pseudo F and t^2 statistics indicate three or four clusters, while the cubic clustering criterion shows a sharp rise up to four clusters and then levels off up to six clusters. So the TABPERM macro is used again at the four-cluster level. In this case, there is no indeterminacy, because the same four clusters are obtained with every permutation, although in different orders. It must be emphasized, however, that lack of indeterminacy in no way indicates validity.

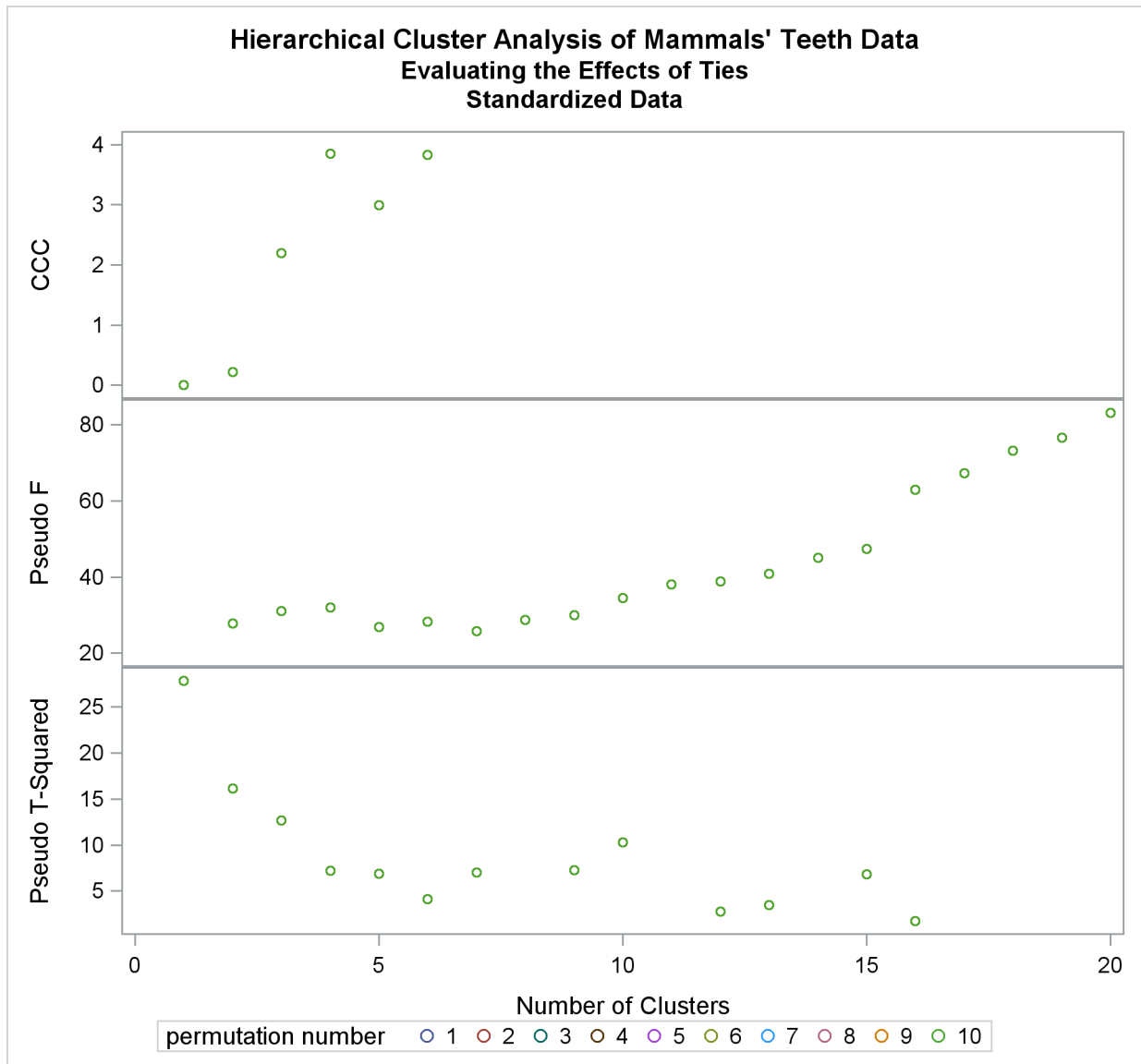
```
title3 'Standardized Data';

/*-----CLUSTER STANDARDIZED DATA WITH AVERAGE LINKAGE-----*/
%clusperm( teeth, &vlist, mammal, average std, 10);
```

The following statements produce [Output 31.4.5](#).

```
/* -----PLOT STATISTICS FOR THE LAST 20 LEVELS----- */
%plotperm(20, 10);
```

Output 31.4.5 Analysis of 10 Random Permutations of Standardized Mammals' Teeth Data



The following statements produce Output 31.4.6.

```
/* -----ANALYZE THE 4-CLUSTER LEVEL----- */
%tabperm( &vlist, mammal, 9.1, 4, 10);
```

Output 31.4.6 Standardized Mammals' Teeth Data: No Indeterminacy at the Four-Cluster Level

Hierarchical Cluster Analysis of Mammals' Teeth Data														
Evaluating the Effects of Ties														
Standardized Data														

										Mean				

										Top	Bottom	Top	Bottom	
										incisors	incisors	canines	canines	
										-----	-----	-----	-----	
all_clus														

1	3	1	1	1	3	3	3	2	3	4	0.0	4.0	0.5	0.0
2	2	2	2	2	2	1	2	1	1	15	2.9	2.6	1.0	1.0
3	1	3	3	3	1	2	1	3	2	7	1.3	1.0	0.0	0.0
4	4	4	4	4	4	4	4	4	4	6	2.0	2.8	1.0	0.8

(Continued)														
Hierarchical Cluster Analysis of Mammals' Teeth Data														
Evaluating the Effects of Ties														
Standardized Data														

										Mean				

										Top	Bottom	Top	Bottom	
										premolars	premolars	molars	molars	
										-----	-----	-----	-----	
all_clus														

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Chapter 32

The CORRESP Procedure

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Overview: CORRESP Procedure

The CORRESP procedure performs simple correspondence analysis and multiple correspondence analysis (MCA). You can use correspondence analysis to find a low-dimensional graphical representation of the rows and columns of a crosstabulation or contingency table. Each row and column is represented by a point in a plot determined from the cell frequencies. PROC CORRESP can also compute coordinates for supplementary rows and columns.

PROC CORRESP can read two kinds of input: raw categorical responses on two or more classification variables or a two-way contingency table. The correspondence analysis plot is displayed with ODS Graphics. For more information about ODS Graphics, see the section “[ODS Graphics](#)” on page 2038.

Background

Correspondence analysis is a popular data analysis method in France and Japan. In France, correspondence analysis was developed under the influence of Jean-Paul Benzécri; in Japan, it was developed under Chikio Hayashi. The name *correspondence analysis* is a translation of the French *analyse des correspondances*. The technique apparently has many independent beginnings (for example, Richardson and Kuder 1933; Hirshfield 1935; Horst 1935; Fisher 1940; Guttman 1941; Burt 1950; Hayashi 1950). It has had many other names, including optimal scaling, reciprocal averaging, optimal scoring, and appropriate scoring in the United States; quantification method in Japan; homogeneity analysis in the Netherlands; dual scaling in Canada; and scalogram analysis in Israel.

Correspondence analysis is described in more detail in French in Benzécri (1973) and Lebart, Morineau, and Tabard (1977). In Japanese, the subject is described in Komazawa (1982); Nishisato (1982); Kobayashi (1981). In English, correspondence analysis is described in Lebart, Morineau, and Warwick (1984); Greenacre (1984); Nishisato (1980); Tenenhaus and Young (1985); Gifi (1990); Greenacre and Hastie (1987), and many other sources. Hoffman and Franke (1986) offer a short, introductory treatment that uses examples from the field of market research.

Getting Started: CORRESP Procedure

Data are available containing the numbers of Ph.D.’s awarded in the United States during the years 1973 through 1978 (U.S. Bureau of the Census 1979). The table has six rows, one for each of six academic disciplines, and six columns for the six years.

The following DATA step reads the complete table into a SAS data set, and PROC CORRESP displays correspondence analysis results including the inertia decomposition and coordinates:

```

title "Number of Ph.D.'s Awarded from 1973 to 1978";

data PhD;
  input Science $ 1-19 y1973-y1978;
  label y1973 = '1973'
        y1974 = '1974'
        y1975 = '1975'
        y1976 = '1976'
        y1977 = '1977'
        y1978 = '1978';
  datalines;
Life Sciences      4489 4303 4402 4350 4266 4361
Physical Sciences  4101 3800 3749 3572 3410 3234
Social Sciences    3354 3286 3344 3278 3137 3008
Behavioral Sciences 2444 2587 2749 2878 2960 3049
Engineering        3338 3144 2959 2791 2641 2432
Mathematics        1222 1196 1149 1003  959  959
;

ods graphics on;

proc corresp data=PhD out=Results short;
  var y1973-y1978;
  id Science;
run;

```

The results are displayed in Figure 32.1 and Figure 32.2.

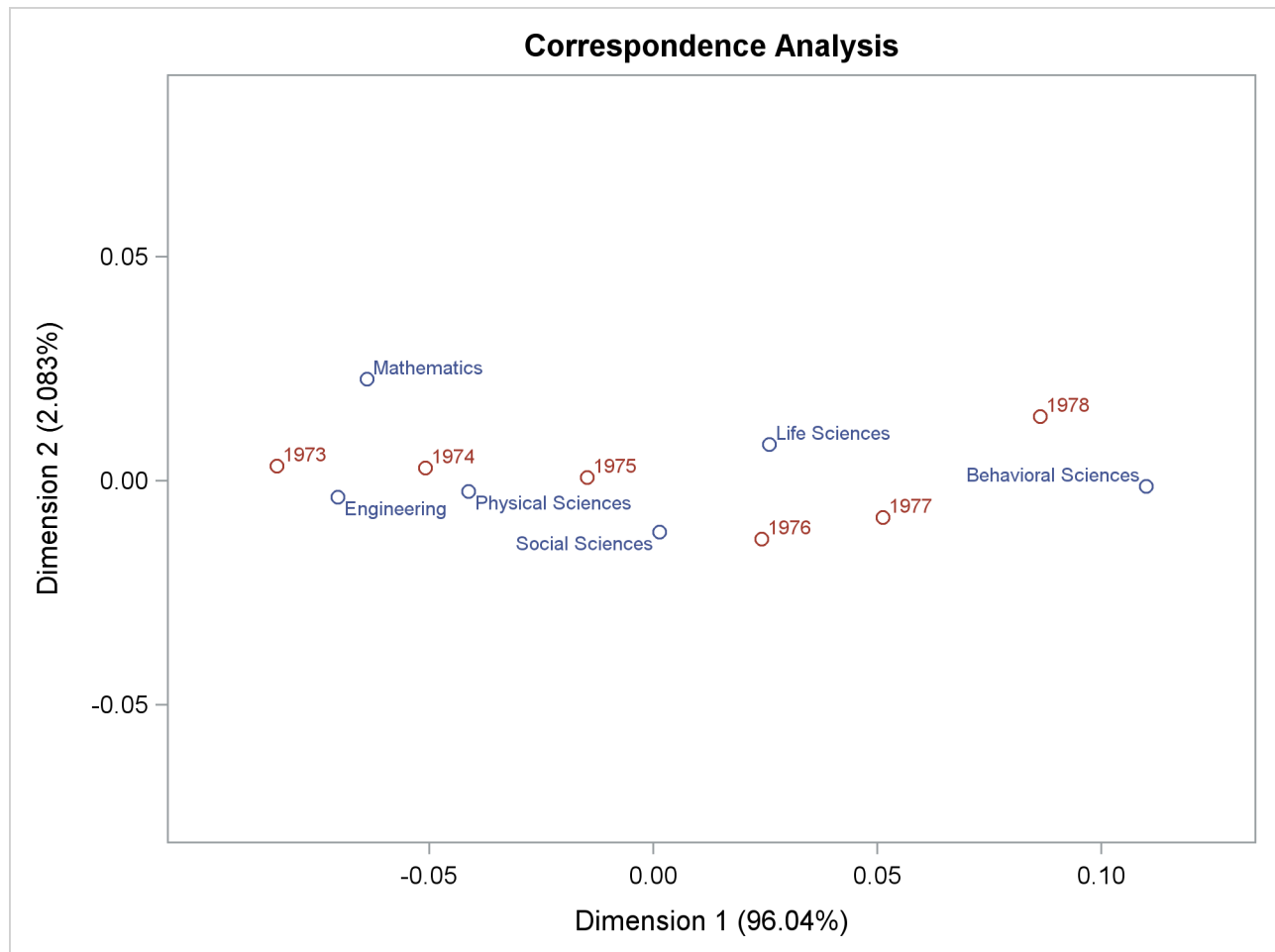
Figure 32.1 Inertia and Chi-Square Decomposition

Number of Ph.D.'s Awarded from 1973 to 1978									
The CORRESP Procedure									
Inertia and Chi-Square Decomposition									
Singular Value	Principal Inertia	Chi-Square	Percent	Cumulative Percent	19	38	57	76	95
0.05845	0.00342	368.653	96.04	96.04	-----+-----+-----+-----+-----	*****			
0.00861	0.00007	7.995	2.08	98.12	*				
0.00694	0.00005	5.197	1.35	99.48					
0.00414	0.00002	1.852	0.48	99.96					
0.00122	0.00000	0.160	0.04	100.00					
Total	0.00356	383.856	100.00						
Degrees of Freedom = 25									

The concept of *inertia* in correspondence analysis is analogous to the concept of variance in principal component analysis, and it is proportional to the chi-square information.

The total chi-square statistic in Figure 32.1, which is a measure of the association between the rows and columns in the full five dimensions of the (centered) table, is 383.856. The maximum number of dimensions (or axes) is the minimum of the number of rows and columns, minus one. More than 96% of the total chi-square and inertia is explained by the first dimension, indicating that the association between the row and column categories is essentially one-dimensional. The plot in Figure 32.2 shows how the number of doctorates in the different disciplines changes over time. The plot shows that the number of doctorates in the behavioral sciences is associated with later years, and the number of doctorates in mathematics and engineering is associated with earlier years. This is consistent with the data that show that the number of doctorates in the behavioral sciences is increasing, the number of doctorates in every other discipline is decreasing, and the rate of decrease is greatest for mathematics and engineering.

Figure 32.2 Correspondence Analysis of Ph.D. Data



Syntax: CORRESP Procedure

The following statements are available in the CORRESP procedure.

```

PROC CORRESP < options > ;
  TABLES < row-variables, > column-variables ;
  VAR variables ;
  BY variables ;
  ID variable ;
  SUPPLEMENTARY variables ;
  WEIGHT variable ;

```

There are two separate forms of input to PROC CORRESP. One form is specified in the TABLES statement, the other in the VAR statement. You must specify either the TABLES or the VAR statement, but not both, each time you run PROC CORRESP.

Specify the TABLES statement if you are using raw, categorical data, the levels of which define the rows and columns of a table.

Specify the VAR statement if your data are already in tabular form. PROC CORRESP is generally more efficient with VAR statement input than with TABLES statement input.

The other statements are optional. All of the statements are explained, in alphabetical order, following the PROC CORRESP statement. All of the options in PROC CORRESP can be abbreviated to their first three letters, except for the OUTF= option. This is a special feature of PROC CORRESP and is not generally true of SAS/STAT procedures.

PROC CORRESP Statement

```

PROC CORRESP < options > ;

```

The PROC CORRESP statement invokes the CORRESP procedure. [Table 32.1](#) summarizes the options available in the PROC CORRESP statement. These options are described following the table.

Table 32.1 Summary of PROC CORRESP Statement Options

Option	Description
Data Set Options	
DATA=	Specifies input SAS data set
OUTC=	Specifies output coordinate SAS data set
OUTF=	Specifies output frequency SAS data set
Row and Column Coordinates	
DIMENS=	Specifies the number of dimensions or axes
MCA	Performs multiple correspondence analysis
PROFILE=	Standardizes the row and column coordinates
Table Construction	
BINARY	Specifies binary table

Table 32.1 *continued*

Option	Description
CROSS=	Specifies cross levels of TABLES variables
FREQOUT	Specifies input data in PROC FREQ output
MISSING	Includes observations with missing values
Control Displayed Output	
ALL	Displays all output
BENZECRI	Displays inertias adjusted by Benzécri's method
CELLCHI2	Displays cell contributions to chi-square
CP	Displays column profile matrix
DEVIATION	Displays observed minus expected values
EXPECTED	Displays chi-square expected values
GREENACRE	Displays inertias adjusted by Greenacre's method
NOCOLUMN=	Suppresses the display of column coordinates
NOPRINT	Suppresses the display of all output
NOROW=	Suppresses the display of row coordinates
OBSERVED	Displays contingency table of observed frequencies
PLOTS=	Specifies ODS Graphics details
PRINT=	Displays percentages or frequencies
RP	Displays row profile matrix
SHORT	Suppresses all point and coordinate statistics
UNADJUSTED	Displays unadjusted inertias
Other Options	
COLUMN=	Specifies esoteric column coordinate standardizations
MININERTIA=	Specifies minimum inertia
NVARS=	Specifies number of classification variables
ROW=	Specifies esoteric row coordinate standardizations
SINGULAR=	Specifies effective zero
SOURCE	Includes level source in the OUTC= data set

The display options control the amount of displayed output. The CELLCHI2, EXPECTED, and DEVIATION options display additional chi-square information. See the “[Details: CORRESP Procedure](#)” section for more information. The unit of the matrices displayed by the CELLCHI2, CP, DEVIATION, EXPECTED, OBSERVED, and RP options depends on the value of the PRINT= option. The table construction options control the construction of the contingency table; these options are valid only when you also specify a TABLES statement.

You can specify the following options in the PROC CORRESP statement. They are given in alphabetical order.

ALL

is equivalent to specifying the OBSERVED, RP, CP, CELLCHI2, EXPECTED, and DEVIATION options. Specifying the ALL option does not affect the PRINT= option. Therefore, only frequencies (not percentages) for these options are displayed unless you specify otherwise with the PRINT= option.

BENZECRI**BEN**

displays adjusted inertias when performing multiple correspondence analysis. By default, unadjusted inertias, the usual inertias from multiple correspondence analysis, are displayed. However, adjusted inertias that use a method proposed by Benzécri (1979) and described by Greenacre (1984, p. 145) can be displayed by specifying the **BENZECRI** option. Specify the **UNADJUSTED** option to output the usual table of unadjusted inertias as well. See the section “[MCA Adjusted Inertias](#)” on page 2031 for more information.

BINARY

enables you to create binary tables easily. When you specify the **BINARY** option, specify only column variables in the **TABLES** statement. Each input data set observation forms a single row in the constructed table.

CELLCHI2**CEL**

displays the contribution to the total chi-square test statistic for each cell. See also the descriptions of the **DEVIATION**, **EXPECTED**, and **OBSERVED** options.

COLUMN=B | BD | DB | DBD | DBD1/2 | DBID1/2**COL=B | BD | DB | DBD | DBD1/2 | DBID1/2**

provides other standardizations of the column coordinates. The **COLUMN=** option is rarely needed. Typically, you should use the **PROFILE=** option instead (see the section “[The PROFILE=, ROW=, and COLUMN= Options](#)” on page 2028). By default, **COLUMN=DBD**.

CP

displays the column profile matrix. Column profiles contain the observed conditional probabilities of row membership given column membership. See also the **RP** option.

CROSS=BOTH | COLUMN | NONE | ROW**CRO=BOT | COL | NON | ROW**

specifies the method of crossing (factorially combining) the levels of the **TABLES** variables. The default is **CROSS=NONE**.

NONE causes each level of every row variable to become a row label and each level of every column variable to become a column label.

ROW causes each combination of levels for all row variables to become a row label, whereas each level of every column variable becomes a column label.

COLUMN causes each combination of levels for all column variables to become a column label, whereas each level of every row variable becomes a row label.

BOTH causes each combination of levels for all row variables to become a row label and each combination of levels for all column variables to become a column label.

The section “[TABLES Statement](#)” on page 2008 provides a more detailed description of this option.

DATA=SAS-data-set

specifies the SAS data set to be used by PROC CORRESP. If you do not specify the DATA= option, PROC CORRESP uses the most recently created SAS data set.

DEVIATION**DEV**

displays the matrix of deviations between the observed frequency matrix and the product of its row marginals and column marginals divided by its grand frequency. For ordinary two-way contingency tables, these are the observed minus expected frequencies under the hypothesis of row and column independence and are components of the chi-square test statistic. See also the CELLCHI2, EXPECTED, and OBSERVED options.

DIMENS=*n***DIM=*n***

specifies the number of dimensions or axes to use. The default is DIMENS=2. The maximum value of the DIMENS= option in an ($n_r \times n_c$) table is $n_r - 1$ or $n_c - 1$, whichever is smaller. For example, in a table with 4 rows and 5 columns, the maximum specification is DIMENS=3. If your table has 2 rows or 2 columns, specify DIMENS=1.

EXPECTED**EXP**

displays the product of the row marginals and the column marginals divided by the grand frequency of the observed frequency table. For ordinary two-way contingency tables, these are the expected frequencies under the hypothesis of row and column independence and are components of the chi-square test statistic. In other situations, this interpretation is not strictly valid. See also the CELLCHI2, DEVIATION, and OBSERVED options.

FREQOUT**FRE**

indicates that the PROC CORRESP input data set has the same form as an output data set from the PROC FREQ procedure, even if it was not directly produced by PROC FREQ. The FREQOUT option enables PROC CORRESP to take shortcuts in constructing the contingency table.

When you specify the FREQOUT option, you must also specify a WEIGHT statement. The cell frequencies in a PROC FREQ output data set are contained in a variable called COUNT, so specify COUNT in a WEIGHT statement with PROC CORRESP. The FREQOUT option might produce unexpected results if the DATA= data set is structured incorrectly. Each of the two variable lists specified in the TABLES statement must consist of a single variable, and observations must be grouped by the levels of the row variable and then by the levels of the column variable. It is not required that the observations be sorted by the row variable and column variable, but they must be grouped consistently. There must be as many observations in the input data set (or BY group) as there are cells in the completed contingency table. Zero cells must be specified with zero weights. When you use PROC FREQ to create the PROC CORRESP input data set, you must specify the SPARSE option in the FREQ procedure's TABLES statement so that the zero cells are written to the output data set.

GREENACRE**GRE**

displays adjusted inertias when you are performing multiple correspondence analysis. By default,

unadjusted inertias, the usual inertias from multiple correspondence analysis, are displayed. However, adjusted inertias that use a method proposed by Greenacre (1984, p. 156) can be displayed by specifying the GREENACRE option. Specify the UNADJUSTED option to output the usual table of unadjusted inertias as well. See the section “[MCA Adjusted Inertias](#)” on page 2031 for more information.

MCA

requests a multiple correspondence analysis. This option requires that the input table be a Burt table, which is a symmetric matrix of crosstabulations among several categorical variables. If you specify the MCA option and a VAR statement, you must also specify the NVAR= option, which gives the number of categorical variables that were used to create the table. With raw categorical data, if you want results for the individuals as well as the categories, use the BINARY option instead.

MININERTIA=*n*

MIN=*n*

specifies the minimum inertia ($0 \leq n \leq 1$) used to create the “best” tables—the indicator of which points best explain the inertia of each dimension. By default, MININERTIA=0.8. See the section “[Algorithm and Notation](#)” on page 2026 for more information.

MISSING

MIS

specifies that observations with missing values for the TABLES statement variables are included in the analysis. Missing values are treated as a distinct level of each categorical variable. By default, observations with missing values are excluded from the analysis.

NOCOLUMN <= BOTH | DATA | PRINT >

NOC <= BOT | DAT | PRI >

suppresses the display of the column coordinates and statistics and omits them from the output coordinate data set.

BOTH suppresses all column information from both the SAS listing and the output data set. The NOCOLUMN option is equivalent to the option NOCOLUMN=BOTH.

DATA suppresses all column information from the output data set.

PRINT suppresses all column information from the SAS listing.

NOPRINT

NOP

suppresses the display of all output. This option is useful when you need only an output data set. This option disables the Output Delivery System (ODS), including ODS Graphics, for the duration of the PROC. For more information, see Chapter 20, “[Using the Output Delivery System.](#)”

NOROW <= BOTH | DATA | PRINT >

NOR <= BOT | DAT | PRI >

suppresses the display of the row coordinates and statistics and omits them from the output coordinate data set.

BOTH	suppresses all row information from both the SAS listing and the output data set. The NOROW option is equivalent to the option NOROW=BOTH.
DATA	suppresses all row information from the output data set.
PRINT	suppresses all row information from the SAS listing.

The NOROW option can be useful when the rows of the contingency table are replications.

NVARS=*n*

NVA=*n*

specifies the number of classification variables that were used to create the Burt table. For example, suppose the Burt table was originally created with the following statement:

```
tables a b c;
```

You must specify NVARS=3 to read the table with a VAR statement.

The NVARS= option is required when you specify both the MCA option and a VAR statement. (See the section “[VAR Statement](#)” on page 2008 for an example.)

OBSERVED

OBS

displays the contingency table of observed frequencies and its row, column, and grand totals. If you do not specify the OBSERVED or ALL option, the contingency table is not displayed.

OUTC=*SAS-data-set*

OUT=*SAS-data-set*

creates an output coordinate SAS data set to contain the row, column, supplementary observation, and supplementary variable coordinates. This data set also contains the masses, squared cosines, quality of each point’s representation in the DIMENS=*n* dimensional display, relative inertias, partial contributions to inertia, and best indicators.

OUTF=*SAS-data-set*

creates an output frequency SAS data set to contain the contingency table, row, and column profiles, the expected values, and the observed minus expected values and contributions to the chi-square statistic.

PLOTS< (*global-plot-options*) > <= *plot-request* < (*options*) > >

PLOTS< (*global-plot-options*) > <= (*plot-request* < (*options*) > < ... *plot-request* < (*options*) > > >

specifies options that control the details of the plots. When you specify only one plot request, you can omit the parentheses around the plot request.

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;

proc corresp;
  tables Marital, Origin;
run;

ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS](#).”

By default, for simple correspondence analysis, PROC CORRESP prints the configuration of points consisting of the row coordinates and column coordinates. With MCA, only column coordinates are printed. The default plots ($y * x$) are Dim2 * Dim1, Dim3 * Dim1, Dim3 * Dim2, and so on. When you specify PLOTS(FILIP), the plots are Dim1 * Dim2, Dim1 * Dim3, Dim2 * Dim3, and so on.

The global plot option is as follows:

FLIP

FLI

flips or interchanges the X-axis and Y-axis dimensions.

The plot requests include the following:

ALL

produces all appropriate plots.

NONE

NON

suppresses all plots.

PRINT=BOTH | FREQ | PERCENT

PRI=BOT | FRE | PER

affects the OBSERVED, RP, CP, CELLCHI2, EXPECTED, and DEVIATION options. The default is PRINT=FREQ.

- The PRINT=FREQ option displays output in the appropriate raw or natural units. (That is, PROC CORRESP displays raw frequencies for the OBSERVED option, relative frequencies with row marginals of 1.0 for the RP option, and so on.)
- The PRINT=PERCENT option scales results to percentages for the display of the output. (All elements in the OBSERVED matrix sum to 100.0, the row marginals are 100.0 for the RP option, and so on.)
- The PRINT=BOTH option displays both percentages and frequencies.

PROFILE=BOTH | COLUMN | NONE | ROW

PRO=BOT | COL | NON | ROW

specifies the standardization for the row and column coordinates. The default is PROFILE=BOTH.

BOTH specifies a standard correspondence analysis, which jointly displays the principal row and column coordinates. Row coordinates are computed from the row profile matrix, and column coordinates are computed from the column profile matrix.

ROW specifies a correspondence analysis of the row profile matrix. The row coordinates are weighted centroids of the column coordinates.

COLUMN specifies a correspondence analysis of the column profile matrix. The column coordinates are weighted centroids of the row coordinates.

NONE is rarely needed. Row and column coordinates are the generalized singular vectors, without the customary standardizations.

ROW=A | AD | DA | DAD | DAD1/2 | DAID1/2

provides other standardizations of the row coordinates. The ROW= option is rarely needed. Typically, you should use the PROFILE= option instead (see the section “The PROFILE=, ROW=, and COLUMN= Options” on page 2028). By default, ROW=DAD.

RP

displays the row profile matrix. Row profiles contain the observed conditional probabilities of column membership given row membership. See also the CP option.

SHORT**SHO**

suppresses the display of all point and coordinate statistics except the coordinates. The following information is suppressed: each point’s mass, relative contribution to the total inertia, and quality of representation in the DIMENS=*n* dimensional display; the squared cosines of the angles between each axis and a vector from the origin to the point; the partial contributions of each point to the inertia of each dimension; and the best indicators.

SINGULAR=*n***SIN=*n***

specifies the largest value that is considered to be within rounding error of zero. The default value is 1E–8. This parameter is used in checking for zero rows and columns, in checking Burt table diagonal sums for equality, in checking denominators before dividing, and so on. Typically, you should not assign a value outside the range 1E–6 to 1E–12.

SOURCE**SOU**

adds the variable `_VAR_`, which contains the name or label of the variable corresponding to the current level, to the OUTC= and OUTF= data sets.

UNADJUSTED**UNA**

displays unadjusted inertias when performing multiple correspondence analysis. By default, unadjusted inertias, the usual inertias from multiple correspondence analysis, are displayed. However, if adjusted inertias are requested by either the GREENACRE option or the BENZECRI option, then the unadjusted inertia table is not displayed unless the UNADJUSTED option is specified. See the section “MCA Adjusted Inertias” on page 2031 for more information.

BY Statement

BY *variables* ;

You can specify a BY statement with PROC CORRESP to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the CORRESP procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

ID Statement

ID *variable* ;

You specify the ID statement only in conjunction with the VAR statement. You cannot specify the ID statement when you use the TABLES statement or the MCA option. When you specify an ID variable, PROC CORRESP labels the rows of the tables with the ID values and places the ID variable in the output data set.

SUPPLEMENTARY Statement

SUPPLEMENTARY *variables* ;

SUP *variables* ;

The SUPPLEMENTARY statement specifies variables that are to be represented as points in the joint row and column space but that are not used in determining the locations of the other, active row and column points of the contingency table. Supplementary observations on supplementary variables are ignored in simple correspondence analysis but are needed to compute the squared cosines for multiple correspondence analysis. Variables that are specified in the SUPPLEMENTARY statement must also be specified in the TABLES or VAR statement.

When you specify a VAR statement, each SUPPLEMENTARY variable indicates one supplementary column of the table. Supplementary variables must be numeric with VAR statement input.

When you specify a TABLES statement, each SUPPLEMENTARY variable indicates a set of rows or columns of the table that is supplementary. Supplementary variables can be either character or numeric with TABLES statement input.

TABLES Statement

TABLES < row-variables, > column-variables ;

The TABLES statement instructs PROC CORRESP to create a contingency table, Burt table, or binary table from the values of two or more categorical variables. The TABLES statement specifies classification variables that are used to construct the rows and columns of the contingency table. The variables can be either numeric or character. The variable lists in the TABLES statement and the CROSS= option together determine the row and column labels of the contingency table.

You can specify both row variables and column variables separated by a comma, or you can specify only column variables and no comma. If you do not specify row variables (that is, if you list variables but do not use the comma as a delimiter), then you should specify either the MCA or the BINARY option. With the MCA option, PROC CORRESP creates a Burt table, which is a crosstabulation of each variable with itself and every other variable. The Burt table is symmetric. With the BINARY option, PROC CORRESP creates a binary table, which consists of one row for each input data set observation and one column for each category of each TABLES statement variable. If the binary matrix is Z , then the Burt table is $Z'Z$. Specifying the BINARY option with the NOROWS option produces the same results as specifying the MCA option (except for the chi-square statistics).

See [Figure 32.6](#) for an example or see the section “[The MCA Option](#)” on page 2030 for a detailed description of Burt tables.

You can use the WEIGHT statement with the TABLES statement to read category frequencies. Specify the SUPPLEMENTARY statement to name variables with categories that are supplementary rows or columns. You cannot specify the ID or VAR statement with the TABLES statement. See the section “[Using the TABLES Statement](#)” on page 2010 for an example.

VAR Statement

VAR variables ;

You should specify the VAR statement when your data are in tabular form. The VAR variables must be numeric. The VAR statement instructs PROC CORRESP to read an existing contingency table, binary indicator matrix, fuzzy-coded indicator matrix, or Burt table, rather than raw data. See the section “[Algorithm and Notation](#)” on page 2026 for a description of a binary indicator matrix and a fuzzy-coded indicator matrix.

You can specify the WEIGHT statement with the VAR statement to read category frequencies and designate supplementary rows. Specify the SUPPLEMENTARY statement to name supplementary variables. You cannot specify the TABLES statement with the VAR statement.

WEIGHT Statement

WEIGHT *variable* ;

The WEIGHT statement specifies weights for each observation and indicates supplementary observations for simple correspondence analyses with VAR statement input. You can include only one WEIGHT statement, and the weight variable must be numeric.

If you omit the WEIGHT statement, each observation contributes a value of 1 to the frequency count for its category. That is, each observation represents one subject. When you specify a WEIGHT statement, each observation contributes the value of the weighting variable for that observation. For example, a weight of 3 means that the observation represents three subjects. Weight values are not required to be integers.

You can specify the WEIGHT statement with a TABLES statement to indicate category frequencies, as in the following example:

```
proc freq;
  tables a*b / out=outfreq sparse;
run;

proc corresp freqout;
  tables a, b;
  weight count;
run;
```

If you specify a VAR statement, you can specify the WEIGHT statement to indicate supplementary observations and to weight some rows of the table more heavily than others. When the value of the WEIGHT variable is negative, the observation is treated as supplementary, and the absolute value of the weight is used as the weighting value.

You cannot specify a WEIGHT statement with a VAR statement and the MCA option, because the table must be symmetric. Supplementary variables are indicated with the SUPPLEMENTARY statement, so differential weighting of rows is inappropriate.

Details: CORRESP Procedure

Input Data Set

PROC CORRESP can read two kinds of input:

- raw category responses on two or more classification variables with the TABLES statement
- a two-way contingency table with the VAR statement

You can use output from PROC FREQ as input for PROC CORRESP.

The classification variables referred to by the TABLES statement can be either numeric or character variables. Normally, all observations for a given variable that have the same formatted value are placed in the same level, and observations with different values are placed in different levels.

The variables in the VAR statement must be numeric. The values of the observations specify the cell frequencies. These values are not required to be integers, but only those observations with all nonnegative, nonmissing values are used in the correspondence analysis. Observations with one or more negative values are removed from the analysis.

The WEIGHT variable must be numeric. Observations with negative weights are treated as supplementary observations. The absolute values of the weights are used to weight the observations.

Using the TABLES Statement

This section explains some of the choices for the correspondence analysis input data table and illustrates some table-construction capabilities of PROC CORRESP. The SAS data set Neighbor, which follows, will be used throughout this section to illustrate various ways in which PROC CORRESP can read and process data. This data set consists of one observation for each resident in a fictitious neighborhood along with some personal information.

```
title 'PROC CORRESP Table Construction';

data Neighbor;
  input Name $ 1-10 Age $ 12-18 Sex $ 19-25
        Height $ 26-30 Hair $ 32-37;
  datalines;
Jones      Old      Male      Short White
Smith     Young    Female    Tall  Brown
Kasavitz  Old      Male      Short Brown
Ernst     Old      Female    Tall  White
Zannoria  Old      Female    Short Brown
Spangel   Young    Male      Tall  Blond
```

```

Myers      Young  Male  Tall  Brown
Kasinski   Old    Male  Short Blond
Colman     Young  Female Short Blond
Delafave   Old    Male  Tall  Brown
Singer     Young  Male  Tall  Brown
Igor       Old                    Short
;

```

This first step creates a simple contingency table or crosstabulation. In the TABLES statement, each variable list consists of a single variable. The following statements produce the table in [Figure 32.3](#).

```

proc corresp data=Neighbor dimens=1 observed short;
  title2 'Simple Crosstabulation';
  ods select observed;
  tables Sex, Age;
run;

```

These statements create a contingency table with two rows (**Female** and **Male**) and two columns (**Old** and **Young**) and show the neighbors categorized by age and sex. The DIMENS=1 option specifies the number of dimensions in the correspondence analysis. Typically, you do not have to specify this option, because typically your tables will be larger than two by two. The default is DIMENS=2, which is too large for a table with a two-level factor. The OBSERVED option displays the contingency table. The SHORT option limits the displayed output. Because it contains missing values, the observation where Name='Igor' is omitted from the analysis. The table is shown in [Figure 32.3](#).

Figure 32.3 Contingency Table for Sex, Age

PROC CORRESP Table Construction			
Simple Crosstabulation			
The CORRESP Procedure			
Contingency Table			
	Old	Young	Sum
Female	2	2	4
Male	4	3	7
Sum	6	5	11

The preceding example showed how to make a two-way contingency table based on the levels of two categorical variables, which, if it were larger, would be a very typical form of data for a correspondence analysis. However, many other types of tables, N , can be used as input to a correspondence analysis, and all tables can be defined based on a binary matrix, Z . The BINARY option enables you to directly compute and display this matrix. The TABLES statement consists of a single list of all the categorical variables. The following statements produce [Figure 32.4](#).

```

proc corresp data=neighbor observed short binary;
  title2 'Binary Coding';
  ods select binary;
  tables Hair Height Sex Age;
run;

```

Figure 32.4 Binary Table Using the BINARY Option

PROC CORRESP Table Construction									
Binary Coding									
The CORRESP Procedure									
Binary Table									
	Blond	Brown	White	Short	Tall	Female	Male	Old	Young
1	0	0	1	1	0	0	1	1	0
2	0	1	0	0	1	1	0	0	1
3	0	1	0	1	0	0	1	1	0
4	0	0	1	0	1	1	0	1	0
5	0	1	0	1	0	1	0	1	0
6	1	0	0	0	1	0	1	0	1
7	0	1	0	0	1	0	1	0	1
8	1	0	0	1	0	0	1	1	0
9	1	0	0	1	0	1	0	0	1
10	0	1	0	0	1	0	1	1	0
11	0	1	0	0	1	0	1	0	1

In this case, $N = Z$ is directly analyzed. The binary matrix has one row for each individual or case and one column for each category. A binary table constructed from m categorical variables has m partitions. This binary table has four partitions, one for each of the four categorical variables. Each partition has a 1 in each row, and each row contains exactly four 1s since there are four categorical variables. More generally, the binary design matrix has exactly m 1s in each row. The 1s indicate the categories to which the observation applies. For example, the categorical variable Sex, with two levels (**Female** and **Male**), is coded using two indicator variables. For the variable Sex, a male would be coded Female=0 and Male=1, and a female would be coded Female=1 and Male=0. This is the same kind of coding that procedures like GLM and TRANSREG use for CLASS variables.

Implicitly, the binary table has an automatic row variable that is equal to the observation number. Alternatively, when there is a row ID variable, as there is in this case, you can use it as a row variable in the TABLES statement, and the resulting ordinary observed frequency table is the binary table. This example uses two variable lists: Name for the row variable, and Hair Height Sex Age for the column variables. Since two lists were provided, the BINARY option was not specified. The following statements produce Figure 32.5.

```
proc corresp data=neighbor observed short;
  title2 'Binary Coding';
  ods select observed;
  tables Name, Hair Height Sex Age;
run;
```

Figure 32.5 Binary Table Using a Row Variable

PROC CORRESP Table Construction										
Binary Coding										
The CORRESP Procedure										
Contingency Table										
	Blond	Brown	White	Short	Tall	Female	Male	Old	Young	Sum
Colman	1	0	0	1	0	1	0	0	1	4
Delafave	0	1	0	0	1	0	1	1	0	4
Ernst	0	0	1	0	1	1	0	1	0	4
Jones	0	0	1	1	0	0	1	1	0	4
Kasavitz	0	1	0	1	0	0	1	1	0	4
Kasinski	1	0	0	1	0	0	1	1	0	4
Myers	0	1	0	0	1	0	1	0	1	4
Singer	0	1	0	0	1	0	1	0	1	4
Smith	0	1	0	0	1	1	0	0	1	4
Spangel	1	0	0	0	1	0	1	0	1	4
Zannoria	0	1	0	1	0	1	0	1	0	4
Sum	3	6	2	5	6	4	7	6	5	44

With the MCA option, the Burt table ($Z'Z$) is analyzed. A Burt table is a partitioned symmetric matrix containing all pairs of crosstabulations among a set of categorical variables. Each diagonal partition is a diagonal matrix containing marginal frequencies (a crosstabulation of a variable with itself). Each off-diagonal partition is an ordinary contingency table. The following statements produce Figure 32.6.

```
proc corresp data=neighbor observed short mca;
  title2 'MCA Burt Table';
  ods select burt;
  tables Hair Height Sex Age;
run;
```

Note that there is a single variable list in the TABLES statement, since the row and column variable lists are the same.

Figure 32.6 MCA Burt Table

PROC CORRESP Table Construction									
MCA Burt Table									
The CORRESP Procedure									
Burt Table									
	Blond	Brown	White	Short	Tall	Female	Male	Old	Young
Blond	3	0	0	2	1	1	2	1	2
Brown	0	6	0	2	4	2	4	3	3
White	0	0	2	1	1	1	1	2	0
Short	2	2	1	5	0	2	3	4	1
Tall	1	4	1	0	6	2	4	2	4
Female	1	2	1	2	2	4	0	2	2
Male	2	4	1	3	4	0	7	4	3
Old	1	3	2	4	2	2	4	6	0
Young	2	3	0	1	4	2	3	0	5

This Burt table is composed of all pairs of crosstabulations among the variables Hair, Height, Sex, and Age. It is composed of sixteen individual subtables—the number of variables squared. Both the rows and the columns have the same nine categories (in this case Blond, Brown, White, Short, Tall, Female, Male, Old, and Young). Below the diagonal (from left to right, top to bottom) are the following crosstabulations: Height * Hair, Sex * Hair, Sex * Height, Age * Hair, Age * Height, and Age * Sex. Each crosstabulation below the diagonal has a transposed counterpart above the diagonal. The diagonal contains the crosstabulations: Hair * Hair, Height * Height, Sex * Sex, and Age * Age. The diagonal elements of the diagonal partitions contain marginal frequencies of the off-diagonal partitions. The table Hair * Height, for example, has three rows for Hair and two columns for Height. The values of the Hair * Height table, summed across rows, sum to the diagonal values of the Height * Height table, as displayed in the following results. The following statements produce Figure 32.7.

```
proc corresp data=neighbor observed short dimens=1;
  title2 'Part of the Burt Table';
  ods output observed=o;
  tables Hair Height, Height;
run;

proc print data=o(drop=sum) label noobs;
  where label ne 'Sum';
  label label = '00'x;
run;
```

Figure 32.7 Part of the Burt Table

PROC CORRESP Table Construction Part of the Burt Table		
	Short	Tall
Blond	2	1
Brown	2	4
White	1	1
Short	5	0
Tall	0	6

A simple crosstabulation of Hair \times Height is $N = Z_{\text{Hair}}'Z_{\text{Height}}$. Tables such as $(N = Z_{\text{Hair}}'Z_{\text{Height,Sex}})$, made up of several crosstabulations, can also be analyzed in simple correspondence analysis. The following statements produce Figure 32.8.

```
proc corresp data=neighbor observed short dimens=1;
  title2 'Multiple Crosstabulations';
  ods select observed;
  tables Hair, Height Sex;
run;
```

Figure 32.8 Hair \times (Height Sex) Crosstabulation

PROC CORRESP Table Construction Multiple Crosstabulations					
The CORRESP Procedure					
Contingency Table					
	Short	Tall	Female	Male	Sum
Blond	2	1	1	2	6
Brown	2	4	2	4	12
White	1	1	1	1	4
Sum	5	6	4	7	22

The following statements create a table with six rows (**Blond*Short**, **Blond*Tall**, **Brown*Short**, **Brown*Tall**, **White*Short**, and **White*Tall**) and four columns (**Female**, **Male**, **Old**, and **Young**). The levels of the row variables are crossed by the **CROSS=ROW** option, forming mutually exclusive categories. Hence each individual fits into exactly one row category, but two column categories. The following statements produce Figure 32.9.

```
proc corresp data=Neighbor cross=row observed short;
  title2 'Multiple Crosstabulations with Crossed Rows';
  ods select observed;
  tables Hair Height, Sex Age;
run;
```

Figure 32.9 Contingency Table for Hair * Height, Sex Age

PROC CORRESP Table Construction					
Multiple Crosstabulations with Crossed Rows					
The CORRESP Procedure					
Contingency Table					
	Female	Male	Old	Young	Sum
Blond * Short	1	1	1	1	4
Blond * Tall	0	1	0	1	2
Brown * Short	1	1	2	0	4
Brown * Tall	1	3	1	3	8
White * Short	0	1	1	0	2
White * Tall	1	0	1	0	2
Sum	4	7	6	5	22

You can enter supplementary variables with TABLES input by including a SUPPLEMENTARY statement. Variables named in the SUPPLEMENTARY statement indicate TABLES variables with categories that are supplementary. In other words, the categories of the variable Age are represented in the row and column space, but they are not used in determining the scores of the categories of the variables Hair, Height, and Sex. The variable used in the SUPPLEMENTARY statement must be listed in the TABLES statement as well. For example, the following statements create a Burt table with seven active rows and columns (**Blond, Brown, White, Short, Tall, Female, Male**) and two supplementary rows and columns (**Old** and **Young**). The following statements produce [Figure 32.10](#).

```
proc corresp data=Neighbor observed short mca;
  title2 'MCA with Supplementary Variables';
  ods select burt supcols;
  tables Hair Height Sex Age;
  supplementary Age;
run;
```

Figure 32.10 Burt Table from PROC CORRESP with Supplementary Variables

PROC CORRESP Table Construction							
MCA with Supplementary Variables							
The CORRESP Procedure							
Burt Table							
	Blond	Brown	White	Short	Tall	Female	Male
Blond	3	0	0	2	1	1	2
Brown	0	6	0	2	4	2	4
White	0	0	2	1	1	1	1
Short	2	2	1	5	0	2	3
Tall	1	4	1	0	6	2	4
Female	1	2	1	2	2	4	0
Male	2	4	1	3	4	0	7

Figure 32.10 continued

Supplementary Columns		
	Old	Young
Blond	1	2
Brown	3	3
White	2	0
Short	4	1
Tall	2	4
Female	2	2
Male	4	3

The following statements create a binary table with 7 active columns (**Blond**, **Brown**, **White**, **Short**, **Tall**, **Female**, **Male**), 2 supplementary columns (**Old** and **Young**), and 11 rows for the 11 observations with nonmissing values. The following statements produce Figure 32.11.

```
proc corresp data=Neighbor observed short binary;
  title2 'Supplementary Binary Variables';
  ods select binary supcols;
  tables Hair Height Sex Age;
  supplementary Age;
run;
```

Figure 32.11 Binary Table from PROC CORRESP with Supplementary Variables

PROC CORRESP Table Construction Supplementary Binary Variables							
The CORRESP Procedure							
Binary Table							
	Blond	Brown	White	Short	Tall	Female	Male
1	0	0	1	1	0	0	1
2	0	1	0	0	1	1	0
3	0	1	0	1	0	0	1
4	0	0	1	0	1	1	0
5	0	1	0	1	0	1	0
6	1	0	0	0	1	0	1
7	0	1	0	0	1	0	1
8	1	0	0	1	0	0	1
9	1	0	0	1	0	1	0
10	0	1	0	0	1	0	1
11	0	1	0	0	1	0	1

Figure 32.11 continued

Supplementary Columns		
	Old	Young
1	1	0
2	0	1
3	1	0
4	1	0
5	1	0
6	0	1
7	0	1
8	1	0
9	0	1
10	1	0
11	0	1

Using the VAR Statement

With VAR statement input, the rows of the contingency table correspond to the observations of the input data set, and the columns correspond to the VAR statement variables. The values of the variables typically contain the table frequencies. The table in Figure 32.3 could be created with VAR statement input by using the following statements:

```
data Ages;
  input Sex $ Old Young;
  datalines;
Female  2 2
Male    4 3
;

proc corresp data=Ages dimens=1 observed short;
  var Old Young;
  id Sex;
run;
```

Only nonnegative values are accepted. Negative values are treated as missing, causing the observation to be excluded from the analysis. The values are not required to be integers. Row labels for the table are specified with an ID variable. Column labels are constructed from the variable name or variable label if one is specified. When you specify multiple correspondence analysis (MCA), the row and column labels are the same and are constructed from the variable names or labels, so you cannot include an ID statement. With MCA, the VAR statement must list the variables in the order in which the rows occur. An example is the table in Figure 32.6, which was created with the following TABLES statement.

```
tables Hair Height Sex Age;
```

This table could have been created with a VAR statement as follows:

```
proc corresp data=table nvars=4 mca;
  var Blond Brown White Short Tall Female Male Old Young;
run;
```

You must specify the NVAR= option in order to specify the number of original categorical variables with the MCA option. The option NVAR= n is needed to find boundaries between the subtables of the Burt table. If f is the sum of all elements in the Burt table $Z'Z$, then fn^{-2} is the number of rows in the binary matrix Z . The sum of all elements in each diagonal subtable of the Burt table must be fn^{-2} .

To enter supplementary observations, include a WEIGHT statement with negative weights for those observations. Specify the SUPPLEMENTARY statement to include supplementary variables. You must list supplementary variables in both the VAR and SUPPLEMENTARY statements.

Missing and Invalid Data

With VAR statement input, observations with missing or negative frequencies are excluded from the analysis. Supplementary variables and supplementary observations with missing or negative frequencies are also excluded. Negative weights are valid with VAR statement input.

With TABLES statement input, observations with negative weights are excluded from the analysis. With this form of input, missing cell frequencies cannot occur. Observations with missing values on the categorical variables are excluded unless you specify the MISSING option. If you specify the MISSING option, ordinary missing values and special missing values are treated as additional levels of a categorical variable. In all cases, if any row or column of the constructed table contains only zeros, that row or column is excluded from the analysis.

Observations with missing weights are excluded from the analysis.

Coding, Fuzzy Coding, and Doubling

Sometimes, binary data such as Yes/No data are available—for example, 1 means “Yes, I have bought this brand in the last month” and 0 means “No, I have not bought this brand in the last month”. The following statements read a data set with Yes/No purchase data for three hypothetical brands.

```
title 'Doubling Yes/No Data';

proc format;
  value yn 0 = 'No ' 1 = 'Yes';
run;

data BrandChoice;
  input a b c;
  label a = 'Brand A' b = 'Brand B' c = 'Brand B';
```

```

format a b c yn.;
datalines;
0 0 1
1 1 0
0 1 1
0 1 0
1 0 0
;

```

Data such as these cannot be analyzed directly because the raw data do not consist of partitions, each with one column per level and exactly one 1 in each row. (See the section “Using the TABLES Statement” on page 2010.) The data must be *doubled* so that both Yes and No are represented by a column in the data matrix. The TRANSREG procedure provides one way of doubling. In the following statements, the DESIGN option specifies that PROC TRANSREG is being used only for coding, not analysis. The option SEPARATORS=': ' specifies that labels for the coded columns are constructed from input variable labels, followed by a colon and space, followed by the formatted value. The variables are designated in the MODEL statement as CLASS variables, and the ZERO=NONE option creates binary variables for all levels. The OUTPUT statement specifies the output data set and drops the _NAME_, _TYPE_, and Intercept variables. PROC TRANSREG stores a list of coded variable names in a macro variable &_TRGIND, which in this case has the value “aNo aYes bNo bYes cNo cYes”. This macro variable can be used directly in the VAR statement in PROC CORRESP. The following statements produce Figure 32.12. Only the input table is displayed.

```

proc transreg data=BrandChoice design separators=': ';
  model class(a b c / zero=none);
  output out=Doubled(drop=_: Intercept);
run;

proc print label;
run;

proc corresp data=Doubled norow short;
  var &_trgind;
run;

```

Figure 32.12 Doubling Yes/No Data

Doubling Yes/No Data									
Obs	Brand A: No	Brand A: Yes	Brand B: No	Brand B: Yes	Brand B: No	Brand B: Yes	Brand A	Brand B	Brand B
1	1	0	1	0	0	1	No	No	Yes
2	0	1	0	1	1	0	Yes	Yes	No
3	1	0	0	1	0	1	No	Yes	Yes
4	1	0	0	1	1	0	No	Yes	No
5	0	1	1	0	1	0	Yes	No	No

A fuzzy-coded indicator also sums to 1.0 across levels of the categorical variable, but it is coded with fractions rather than with 0 and 1. The fractions represent the distribution of the attribute across several levels of the categorical variable.

Ordinal variables, such as survey responses of 1 to 3, can be represented as two fuzzy-coded variables, as shown in [Table 32.2](#).

Table 32.2 Coding an Ordinal Variable

Ordinal Values	Coding	
1	0.25	0.75
2	0.50	0.50
3	0.75	0.25

The values of the coding sum to one across the two coded variables.

These next steps illustrate the use of binary and fuzzy-coded indicator variables. Fuzzy-coded indicators are used to represent missing data. Note that the missing values in the observation Igor are coded with equal proportions. The following statements produce [Figure 32.13](#).

```

title 'Fuzzy Coding of Missing Values';

proc transreg data=Neighbor design cprefix=0;
  model class(Age Sex Height Hair / zero=none);
  output out=Neighbor2(drop=_: Intercept);
  id Name;
run;

data Neighbor3;
  set Neighbor2;
  if Sex = ' ' then do;
    Female = 0.5;
    Male   = 0.5;
  end;
  if Hair = ' ' then do;
    White = 1/3;
    Brown = 1/3;
    Blond = 1/3;
  end;
run;

proc print label noobs data=Neighbor3(drop=age--name);
  format _numeric_ best4.;
run;

```


Figure 32.13 Fuzzy Coding of Missing Values

Fuzzy Coding of Missing Values								
Age Old	Age Young	Sex Female	Sex Male	Height Short	Height Tall	Hair Blond	Hair Brown	Hair White
1	0	0	1	1	0	0	0	1
0	1	1	0	0	1	0	1	0
1	0	0	1	1	0	0	1	0
1	0	1	0	0	1	0	0	1
1	0	1	0	1	0	0	1	0
0	1	0	1	0	1	1	0	0
0	1	0	1	0	1	0	1	0
1	0	0	1	1	0	1	0	0
0	1	1	0	1	0	1	0	0
1	0	0	1	0	1	0	1	0
0	1	0	1	0	1	0	1	0
1	0	0.5	0.5	1	0	0.33	0.33	0.33

There is one set of coded variables for each input categorical variable. If observation 12 is excluded, each set is a binary design matrix. Each design matrix has one column for each category and exactly one 1 in each row. Fuzzy coding is shown in the final observation, which corresponds to Igor. The observation for Igor has missing values for the variables Sex and Hair. The design matrix variables are coded with fractions that sum to one within each categorical variable.

An alternative way to represent missing data is to treat missing values as an additional level of the categorical variable. This alternative is available with the MISSING option in the PROC CORRESP statement. This approach yields coordinates for missing responses, allowing the comparison of “missing” along with the other levels of the categorical variables.

Greenacre and Hastie (1987) discuss additional coding schemes, including one for continuous variables. Continuous variables can be coded with PROC TRANSREG by specifying BSPLINE(*variables* / degree=1) in the MODEL statement.

Creating a Data Set Containing the Crosstabulation

The CORRESP procedure can read or create a contingency or Burt table. PROC CORRESP is generally more efficient with VAR statement input than with TABLES statement input. TABLES statement input requires that the table be created from raw categorical variables, whereas the VAR statement is used to read an existing table. For extremely large problems, if PROC CORRESP runs out of memory, it might be possible to use some other method to create the table and then use VAR statement input with PROC CORRESP.

The following example uses the CORRESP, FREQ, and TRANSPOSE procedures to create rectangular tables from a SAS data set WORK.A that contains the categorical variables V1–V5. The Burt table examples assume that no categorical variable has a value found in any of the other categorical variables (that is, that each row and column label is unique).

You can use PROC CORRESP and the ODS OUTPUT statement as follows to create a rectangular two-way contingency table from two categorical variables:

```
proc corresp data=a observed short;
  ods output Observed=Obs (drop=Sum where=(Label ne 'Sum'));
  tables v1, v2;
run;
```

You can use PROC FREQ and PROC TRANSPOSE to create a rectangular two-way contingency table from two categorical variables, as in the following statements:

```
proc freq data=a;
  tables v1 * v2 / sparse noprint out=freqs;
run;

proc transpose data=freqs out=rfreqs(drop=_:);
  id v2;
  var count;
  by v1;
run;
```

You can use PROC CORRESP and the ODS OUTPUT statement as follows to create a Burt table from five categorical variables:

```
proc corresp data=a observed short mca;
  ods output Burt=Obs;
  tables v1-v5;
run;
```

You can use a DATA step, PROC FREQ, and PROC TRANSPOSE to create a Burt table from five categorical variables, as in the following statements:

```
data b;
  set a;
  array v[5] $ v1-v5;
  do i = 1 to 5;
    row = v[i];
    do j = 1 to 5;
      column = v[j];
      output;
    end;
  end;
  keep row column;
run;

proc freq data=b;
  tables row * column / sparse noprint out=freqs;
run;

proc transpose data=freqs out=rfreqs(drop=_:);
  id column;
  var count;
  by row;
run;
```

Output Data Sets

PROC CORRESP has two output data sets. The OUTC= data set contains coordinates and the results of the correspondence analysis. The OUTF= data set contains frequencies and other cross-tabulation results.

The OUTC= Data Set

The OUTC= data set contains two or three character variables and $4n + 4$ numeric variables, where n is the number of axes from DIMENS= n (two by default). The OUTC= data set contains one observation for each row, column, supplementary row, and supplementary column point, and one observation for inertias.

The first variable is named `_TYPE_` and identifies the type of observation. The values of `_TYPE_` are as follows:

- The 'INERTIA' observation contains the total inertia in the INERTIA variable, and each dimension's inertia in the Contr1–Contr n variables.
- The 'OBS' observations contain the coordinates and statistics for the rows of the table.
- The 'SUPOBS' observations contain the coordinates and statistics for the supplementary rows of the table.
- The 'VAR' observations contain the coordinates and statistics for the columns of the table.
- The 'SUPVAR' observations contain the coordinates and statistics for the supplementary columns of the table.

If you specify the SOURCE option, then the data set also contains a variable `_VAR_` containing the name or label of the input variable from which that row originates. The name of the next variable is either `_NAME_` or (if you specify an ID statement) the name of the ID variable.

For observations with a value of 'OBS' or 'SUPOBS' for the `_TYPE_` variable, the values of the second variable are constructed as follows:

- When you use a VAR statement without an ID statement, the values are 'Row1', 'Row2', and so on.
- When you specify a VAR statement with an ID statement, the values are set equal to the values of the ID variable.
- When you specify a TABLES statement, the `_NAME_` variable has values formed from the appropriate row variable values.

For observations with a value of 'VAR' or 'SUPVAR' for the `_TYPE_` variable, the values of the second variable are equal to the names or labels of the VAR (or SUPPLEMENTARY) variables. When you specify a TABLES statement, the values are formed from the appropriate column variable values.

The third and subsequent variables contain the numerical results of the correspondence analysis.

- Quality contains the quality of each point's representation in the DIMENS= n dimensional display, which is the sum of squared cosines over the first n dimensions.
- Mass contains the masses or marginal sums of the relative frequency matrix.
- Inertia contains each point's relative contribution to the total inertia.

- Dim1–Dim n contain the point coordinates.
- Contr1–Contr n contain the partial contributions to inertia.
- SqCos1–SqCos n contain the squared cosines.
- Best1–Best n and Best contain the summaries of the partial contributions to inertia.

The OUTF= Data Set

The OUTF= data set contains frequencies and percentages. It is similar to a PROC FREQ output data set. The OUTF= data set begins with a variable called `_TYPE_`, which contains the observation type. If the SOURCE option is specified, the data set contains two variables, `_ROWVAR_` and `_COLVAR_`, that contain the names or labels of the row and column input variables from which each cell originates. The next two variables are classification variables that contain the row and column levels. If you use TABLES statement input and each variable list consists of a single variable, the names of the first two variables match the names of the input variables; otherwise, these variables are named Row and Column. The next two variables are Count and Percent, which contain frequencies and percentages.

The `_TYPE_` variable can have the following values:

- ‘OBSERVED’ observations contain the contingency table.
- ‘SUPOBS’ observations contain the supplementary rows.
- ‘SUPVAR’ observations contain the supplementary columns.
- ‘EXPECTED’ observations contain the product of the row marginals and the column marginals divided by the grand frequency of the observed frequency table. For ordinary two-way contingency tables, these are the expected frequency matrix under the hypothesis of row and column independence.
- ‘DEVIATION’ observations contain the matrix of deviations between the observed frequency matrix and the product of its row marginals and column marginals divided by its grand frequency. For ordinary two-way contingency tables, these are the observed minus expected frequencies under the hypothesis of row and column independence.
- ‘CELLCHI2’ observations contain contributions to the total chi-square test statistic.
- ‘RP’ observations contain the row profiles.
- ‘SUPRP’ observations contain supplementary row profiles.
- ‘CP’ observations contain the column profiles.
- ‘SUPCP’ observations contain supplementary column profiles.

Computational Resources

Let

n_r = number of rows in the table

n_c = number of columns in the table

n = number of observations

v = number of VAR statement variables

t = number of TABLES statement variables

$c = \max(n_r, n_c)$

$d = \min(n_r, n_c)$

For TABLES statement input, more than

$$32(t + 1) + 8(\max(2tn, (n_r + 3)(n_c + 3)))$$

bytes of array space are required.

For VAR statement input, more than

$$16(v + 2) + 8(n_r + 3)(n_c + 3)$$

bytes of array space are required.

Memory

The computational resources formulas are underestimates of the amounts of memory needed to handle most problems. If you use a utility data set, and if memory could be used with perfect efficiency, then roughly the stated amount of memory would be needed. In reality, most problems require at least two or three times the minimum.

PROC CORRESP tries to store the raw data (TABLES input) and the contingency table in memory. If there is not enough memory, a utility data set is used, potentially resulting in a large increase in execution time.

Time

The time required to perform the generalized singular value decomposition is roughly proportional to $2cd^2 + 5d^3$. Overall computation time increases with table size at a rate roughly proportional to $(n_r n_c)^{\frac{3}{2}}$.

Algorithm and Notation

This section is primarily based on the theory of correspondence analysis found in Greenacre (1984). If you are interested in other references, see the section “[Background](#)” on page 1996.

Let \mathbf{N} be the contingency table formed from those observations and variables that are not supplementary and from those observations that have no missing values and have a positive weight. This table is an $(n_r \times n_c)$

rank q matrix of nonnegative numbers with nonzero row and column sums. If \mathbf{Z}_a is the binary coding for variable A, and \mathbf{Z}_b is the binary coding for variable B, then $\mathbf{N} = \mathbf{Z}'_a \mathbf{Z}_b$ is a contingency table. Similarly, if $\mathbf{Z}_{b,c}$ contains the binary coding for both variables B and C, then $\mathbf{N} = \mathbf{Z}'_a \mathbf{Z}_{b,c}$ can also be input to a correspondence analysis. With the BINARY option, $\mathbf{N} = \mathbf{Z}$, and the analysis is based on a binary table. In multiple correspondence analysis, the analysis is based on a Burt table, $\mathbf{Z}'\mathbf{Z}$.

Let $\mathbf{1}$ be a vector of 1s of the appropriate order, let \mathbf{I} be an identity matrix, and let $\text{diag}(\cdot)$ be a matrix-valued function that creates a diagonal matrix from a vector. Let

$$\begin{aligned} f &= \mathbf{1}'\mathbf{N}\mathbf{1} \\ \mathbf{P} &= \frac{1}{f}\mathbf{N} \\ \mathbf{r} &= \mathbf{P}\mathbf{1} \\ \mathbf{c} &= \mathbf{P}'\mathbf{1} \\ \mathbf{D}_r &= \text{diag}(\mathbf{r}) \\ \mathbf{D}_c &= \text{diag}(\mathbf{c}) \\ \mathbf{R} &= \mathbf{D}_r^{-1}\mathbf{P} \\ \mathbf{C}' &= \mathbf{D}_c^{-1}\mathbf{P}' \end{aligned}$$

The scalar f is the sum of all elements in \mathbf{N} . The matrix \mathbf{P} is a matrix of relative frequencies. The vector \mathbf{r} contains row marginal proportions or row “masses.” The vector \mathbf{c} contains column marginal proportions or column masses. The matrices \mathbf{D}_r and \mathbf{D}_c are diagonal matrices of marginals.

The rows of \mathbf{R} contain the “row profiles.” The elements of each row of \mathbf{R} sum to one. Each (i, j) element of \mathbf{R} contains the observed probability of being in column j given membership in row i . Similarly, the columns of \mathbf{C} contain the column profiles. The coordinates in correspondence analysis are based on the generalized singular value decomposition of \mathbf{P} ,

$$\mathbf{P} = \mathbf{A}\mathbf{D}_u\mathbf{B}'$$

where

$$\mathbf{A}'\mathbf{D}_r^{-1}\mathbf{A} = \mathbf{B}'\mathbf{D}_c^{-1}\mathbf{B} = \mathbf{I}$$

In multiple correspondence analysis,

$$\mathbf{P} = \mathbf{B}\mathbf{D}_u^2\mathbf{B}'$$

The matrix \mathbf{A} , which is the rectangular matrix of left generalized singular vectors, has n_r rows and q columns; the matrix \mathbf{D}_u , which is a diagonal matrix of singular values, has q rows and columns; and the matrix \mathbf{B} , which is the rectangular matrix of right generalized singular vectors, has n_c rows and q columns. The columns of \mathbf{A} and \mathbf{B} define the principal axes of the column and row point clouds, respectively.

The generalized singular value decomposition of $\mathbf{P} - \mathbf{r}\mathbf{c}'$, discarding the last singular value (which is zero) and the last left and right singular vectors, is exactly the same as a generalized singular value decomposition of \mathbf{P} , discarding the first singular value (which is one), the first left singular vector, \mathbf{r} , and the first right singular vector, \mathbf{c} . The first (trivial) column of \mathbf{A} and \mathbf{B} and the first singular value in \mathbf{D}_u are discarded

before any results are displayed. You can obtain the generalized singular value decomposition of $\mathbf{P} - \mathbf{rc}'$ from the ordinary singular value decomposition of $\mathbf{D}_r^{-1/2}(\mathbf{P} - \mathbf{rc}')\mathbf{D}_c^{-1/2}$:

$$\begin{aligned}\mathbf{D}_r^{-1/2}(\mathbf{P} - \mathbf{rc}')\mathbf{D}_c^{-1/2} &= \mathbf{U}\mathbf{D}_u\mathbf{V}' = (\mathbf{D}_r^{-1/2}\mathbf{A})\mathbf{D}_u(\mathbf{D}_c^{-1/2}\mathbf{B})' \\ \mathbf{P} - \mathbf{rc}' &= \mathbf{D}_r^{1/2}\mathbf{U}\mathbf{D}_u\mathbf{V}'\mathbf{D}_c^{1/2} = (\mathbf{D}_r^{1/2}\mathbf{U})\mathbf{D}_u(\mathbf{D}_c^{1/2}\mathbf{V})' = \mathbf{A}\mathbf{D}_u\mathbf{B}'\end{aligned}$$

Hence, $\mathbf{A} = \mathbf{D}_r^{1/2}\mathbf{U}$ and $\mathbf{B} = \mathbf{D}_c^{1/2}\mathbf{V}$.

The default row coordinates are $\mathbf{D}_r^{-1}\mathbf{A}\mathbf{D}_u$, and the default column coordinates are $\mathbf{D}_c^{-1}\mathbf{B}\mathbf{D}_u$. Typically the first two columns of $\mathbf{D}_r^{-1}\mathbf{A}\mathbf{D}_u$ and $\mathbf{D}_c^{-1}\mathbf{B}\mathbf{D}_u$ are plotted to display graphical associations between the row and column categories. The plot consists of two overlaid plots, one for rows and one for columns. The row points are row profiles, and the column points are column profiles, both rescaled so that distances between profiles can be displayed as ordinary Euclidean distances, then orthogonally rotated to a principal axes orientation. Distances between row points and other row points have meaning, as do distances between column points and other column points. However, distances between column points and row points are not interpretable.

The PROFILE=, ROW=, and COLUMN= Options

The PROFILE=, ROW=, and COLUMN= options standardize the coordinates before they are displayed and placed in the output data set. The options PROFILE=BOTH, PROFILE=ROW, and PROFILE=COLUMN provide the standardizations that are typically used in correspondence analysis. There are six choices each for row and column coordinates (see Table 32.3). However, most of the combinations of the ROW= and COLUMN= options are not useful. The ROW= and COLUMN= options are provided for completeness, but they are not intended for general use.

Table 32.3 Coordinates

ROW=	Matrix Formula
A	\mathbf{A}
AD	$\mathbf{A}\mathbf{D}_u$
DA	$\mathbf{D}_r^{-1}\mathbf{A}$
DAD	$\mathbf{D}_r^{-1}\mathbf{A}\mathbf{D}_u$
DAD1/2	$\mathbf{D}_r^{-1}\mathbf{A}\mathbf{D}_u^{1/2}$
DAID1/2	$\mathbf{D}_r^{-1}\mathbf{A}(\mathbf{I} + \mathbf{D}_u)^{1/2}$
COLUMN=	Matrix Formula
B	\mathbf{B}
BD	$\mathbf{B}\mathbf{D}_u$
DB	$\mathbf{D}_c^{-1}\mathbf{B}$
DBD	$\mathbf{D}_c^{-1}\mathbf{B}\mathbf{D}_u$
DBD1/2	$\mathbf{D}_c^{-1}\mathbf{B}\mathbf{D}_u^{1/2}$
DBID1/2	$\mathbf{D}_c^{-1}\mathbf{B}(\mathbf{I} + \mathbf{D}_u)^{1/2}$

When PROFILE=ROW (ROW=DAD and COLUMN=DB), the row coordinates $\mathbf{D}_r^{-1}\mathbf{A}\mathbf{D}_u$ and column coordinates $\mathbf{D}_c^{-1}\mathbf{B}$ provide a correspondence analysis based on the row profile matrix. The row profile (conditional probability) matrix is defined as $\mathbf{R} = \mathbf{D}_r^{-1}\mathbf{P} = \mathbf{D}_r^{-1}\mathbf{A}\mathbf{D}_u\mathbf{B}'$. The elements of each row of \mathbf{R} sum to

one. Each (i, j) element of \mathbf{R} contains the observed probability of being in column j given membership in row i . The “principal” row coordinates $\mathbf{D}_r^{-1}\mathbf{A}\mathbf{D}_u$ and “standard” column coordinates $\mathbf{D}_c^{-1}\mathbf{B}$ provide a decomposition of $\mathbf{D}_r^{-1}\mathbf{A}\mathbf{D}_u\mathbf{B}'\mathbf{D}_c^{-1} = \mathbf{D}_r^{-1}\mathbf{P}\mathbf{D}_c^{-1} = \mathbf{R}\mathbf{D}_c^{-1}$. Since $\mathbf{D}_r^{-1}\mathbf{A}\mathbf{D}_u = \mathbf{R}\mathbf{D}_c^{-1}\mathbf{B}$, the row coordinates are weighted centroids of the column coordinates. Each column point, with coordinates scaled to standard coordinates, defines a vertex in $(n_c - 1)$ -dimensional space. All of the principal row coordinates are located in the space defined by the standard column coordinates. Distances among row points have meaning, but distances among column points and distances between row and column points are not interpretable.

The option PROFILE=COLUMN can be described as applying the PROFILE=ROW formulas to the transpose of the contingency table. When PROFILE=COLUMN (ROW=DA and COLUMN=DBD), the principal column coordinates $\mathbf{D}_c^{-1}\mathbf{B}\mathbf{D}_u$ are weighted centroids of the standard row coordinates $\mathbf{D}_r^{-1}\mathbf{A}$. Each row point, with coordinates scaled to standard coordinates, defines a vertex in $(n_r - 1)$ -dimensional space. All of the principal column coordinates are located in the space defined by the standard row coordinates. Distances among column points have meaning, but distances among row points and distances between row and column points are not interpretable.

The usual sets of coordinates are given by the default PROFILE=BOTH (ROW=DAD and COLUMN=DBD). All of the summary statistics, such as the squared cosines and contributions to inertia, apply to these two sets of points. One advantage to using these coordinates is that both sets ($\mathbf{D}_r^{-1}\mathbf{A}\mathbf{D}_u$ and $\mathbf{D}_c^{-1}\mathbf{B}\mathbf{D}_u$) are postmultiplied by the diagonal matrix \mathbf{D}_u , which has diagonal values that are all less than or equal to one. When \mathbf{D}_u is a part of the definition of only one set of coordinates, that set forms a tight cluster near the centroid, whereas the other set of points is more widely dispersed. Including \mathbf{D}_u in both sets makes a better graphical display. However, care must be taken in interpreting such a plot. No correct interpretation of distances between row points and column points can be made.

Another property of this choice of coordinates concerns the geometry of distances between points within each set. The default row coordinates can be decomposed into $\mathbf{D}_r^{-1}\mathbf{A}\mathbf{D}_u = \mathbf{D}_r^{-1}\mathbf{A}\mathbf{D}_u\mathbf{B}'\mathbf{D}_c^{-1}\mathbf{B} = (\mathbf{D}_r^{-1}\mathbf{P})(\mathbf{D}_c^{-1/2})(\mathbf{D}_c^{-1/2}\mathbf{B})$. The row coordinates are row profiles ($\mathbf{D}_r^{-1}\mathbf{P}$), rescaled by $\mathbf{D}_c^{-1/2}$ (rescaled so that distances between profiles are transformed from a chi-square metric to a Euclidean metric), then orthogonally rotated (with $\mathbf{D}_c^{-1/2}\mathbf{B}$) to a principal axes orientation. Similarly, the column coordinates are column profiles rescaled to a Euclidean metric and orthogonally rotated to a principal axes orientation.

The rationale for computing distances between row profiles by using the non-Euclidean chi-square metric is as follows. Each row of the contingency table can be viewed as a realization of a multinomial distribution conditional on its row marginal frequency. The null hypothesis of row and column independence is equivalent to the hypothesis of homogeneity of the row profiles. A significant chi-square statistic is geometrically interpreted as a significant deviation of the row profiles from their centroid, \mathbf{c}' . The chi-square metric is the Mahalanobis metric between row profiles based on their estimated covariance matrix under the homogeneity assumption (Greenacre and Hastie 1987). A parallel argument can be made for the column profiles.

When ROW=DAD1/2 and COLUMN=DBD1/2 (Gifi 1990; van der Heijden and de Leeuw 1985), the row coordinates $\mathbf{D}_r^{-1}\mathbf{A}\mathbf{D}_u^{1/2}$ and column coordinates $\mathbf{D}_c^{-1}\mathbf{B}\mathbf{D}_u^{1/2}$ are a decomposition of $\mathbf{D}_r^{-1}\mathbf{P}\mathbf{D}_c^{-1}$.

In all of the preceding pairs, distances between row and column points are not meaningful. This prompted Carroll, Green, and Schaffer (1986) to propose that row coordinates $\mathbf{D}_r^{-1}\mathbf{A}(\mathbf{I} + \mathbf{D}_u)^{1/2}$ and column coordinates $\mathbf{D}_c^{-1}\mathbf{B}(\mathbf{I} + \mathbf{D}_u)^{1/2}$ be used. These coordinates are (except for a constant scaling) the coordinates from a multiple correspondence analysis of a Burt table created from two categorical variables. This standardization is available with ROW=DAID1/2 and COLUMN=DBID1/2. However, this approach has been criticized on both theoretical and empirical grounds by Greenacre (1989). The Carroll, Green, and Schaffer standardization relies on the assumption that the chi-square metric is an appropriate metric for measuring the distance between the columns of a bivariate indicator matrix. See the section

“Using the TABLES Statement” on page 2010 for a description of indicator matrices. Greenacre (1989) showed that this assumption cannot be justified.

The MCA Option

The MCA option performs a multiple correspondence analysis (MCA). This option requires a Burt table. You can specify the MCA option with a table created from a design matrix with fuzzy coding schemes as long as every row of every partition of the design matrix has the same marginal sum. For example, each row of each partition could contain the probabilities that the observation is a member of each level. Then the Burt table constructed from this matrix no longer contains all integers, and the diagonal partitions are no longer diagonal matrices, but MCA is still valid.

A TABLES statement with a single variable list creates a Burt table. Thus, you can always specify the MCA option with this type of input. If you use the MCA option when reading an existing table with a VAR statement, you must ensure that the table is a Burt table.

If you perform MCA on a table that is not a Burt table, the results of the analysis are invalid. If the table is not symmetric, or if the sums of all elements in each diagonal partition are not equal, PROC CORRESP displays an error message and quits.

A subset of the columns of a Burt table is not necessarily a Burt table, so in MCA it is not appropriate to designate arbitrary columns as supplementary. You can, however, designate all columns from one or more categorical variables as supplementary.

The results of a multiple correspondence analysis of a Burt table $Z'Z$ are the same as the column results from a simple correspondence analysis of the binary (or fuzzy) matrix Z . Multiple correspondence analysis is not a simple correspondence analysis of the Burt table. It is not appropriate to perform a simple correspondence analysis of a Burt table. The MCA option is based on $P = BD_u^2B'$, whereas a simple correspondence analysis of the Burt table would be based on $P = BD_uB'$.

Since the rows and columns of the Burt table are the same, no row information is displayed or written to the output data sets. The resulting inertias and the default (COLUMN=DBD) column coordinates are the appropriate inertias and coordinates for an MCA. The supplementary column coordinates, cosines, and quality of representation formulas for MCA differ from the simple correspondence analysis formulas because the design matrix column profiles and left singular vectors are not available.

The following statements create a Burt table and perform a multiple correspondence analysis:

```
proc corresp data=Neighbor observed short mca;
  tables Hair Height Sex Age;
run;
```

Both the rows and the columns have the same nine categories (Blond, Brown, White, Short, Tall, Female, Male, Old, and Young).

MCA Adjusted Inertias

The usual principal inertias of a Burt table constructed from m categorical variables in MCA are the eigenvalues u_k from D_u^2 . The problem with these inertias is that they provide a pessimistic indication of fit. Benzécri (1979) proposed the following inertia adjustment, which is also described by Greenacre (1984, p. 145):

$$\left(\frac{m}{m-1}\right)^2 \times \left(u_k - \frac{1}{m}\right)^2 \quad \text{for } u_k > \frac{1}{m}$$

This adjustment computes the percent of adjusted inertia relative to the sum of the adjusted inertias for all inertias greater than $\frac{1}{m}$. The Benzécri adjustment is available with the BENZECRI option.

Greenacre (1994, p. 156) argues that the Benzécri adjustment overestimates the quality of fit. Greenacre proposes instead to compute the percentage of adjusted inertia relative to

$$\frac{m}{m-1} \left(\text{trace}(D_u^4) - \frac{n_c - m}{m^2} \right)$$

for all inertias greater than $\frac{1}{m}$, where $\text{trace}(D_u^4)$ is the sum of squared inertias. The Greenacre adjustment is available with the GREENACRE option.

Ordinary unadjusted inertias are printed by default with MCA when neither the BENZECRI nor the GREENACRE option is specified. However, the unadjusted inertias are not printed by default when either the BENZECRI or the GREENACRE option is specified. To display both adjusted and unadjusted inertias, specify the UNADJUSTED option in addition to the relevant adjusted inertia option (BENZECRI, GREENACRE, or both).

Supplementary Rows and Columns

Supplementary rows and columns are represented as points in the joint row and column space, but they are not used in determining the locations of the other active rows and columns of the table. The formulas that are used to compute coordinates for the supplementary rows and columns depend on the PROFILE= option or the ROW= and COLUMN= options. Let S_o be a matrix with rows that contain the supplementary observations, and let S_v be a matrix with rows that contain the supplementary variables. Note that S_v is defined to be the transpose of the supplementary variable partition of the table. Let $R_s = \text{diag}(S_o \mathbf{1})^{-1} S_o$ be the supplementary observation profile matrix, and let $C_s = \text{diag}(S_v \mathbf{1})^{-1} S_v$ be the supplementary variable profile matrix. Note that the notation $\text{diag}(\cdot)^{-1}$ means to convert the vector to a diagonal matrix, then invert the diagonal matrix. The coordinates for the supplementary observations and variables are shown in Table 32.4.

Table 32.4 Coordinates for Supplementary Observations

ROW=	Matrix Formula
A	$\frac{1}{f} S_o D_c^{-1} B D_u^{-1}$
AD	$\frac{1}{f} S_o D_c^{-1} B$
DA	$R_s D_c^{-1} B D_u^{-1}$
DAD	$R_s D_c^{-1} B$
DAD1/2	$R_s D_c^{-1} B D_u^{-1/2}$
DAID1/2	$R_s D_c^{-1} B D_u^{-1} (I + D_u)^{1/2}$
COLUMN=	Matrix Formula
B	$\frac{1}{f} S_v D_r^{-1} A D_u^{-1}$
BD	$\frac{1}{f} S_v D_r^{-1} A$
DB	$C_s D_r^{-1} A D_u^{-1}$
DBD	$C_s D_r^{-1} A$
DBD1/2	$C_s D_r^{-1} A D_u^{-1/2}$
DBID1/2	$C_s D_r^{-1} A D_u^{-1} (I + D_u)^{1/2}$
MCA COLUMN=	Matrix Formula
B	not allowed
BD	not allowed
DB	$C_s D_r^{-1} B D_u^{-2}$
DBD	$C_s D_r^{-1} B D_u^{-1}$
DBD1/2	$C_s D_r^{-1} B D_u^{-3/2}$
DBID1/2	$C_s D_r^{-1} B D_u^{-2} (I + D_u)^{1/2}$

Statistics That Aid Interpretation

The partial contributions to inertia, squared cosines, quality of representation, inertia, and mass provide additional information about the coordinates. These statistics are displayed by default. Include the SHORT or NOPRINT option in the PROC CORRESP statement to avoid having these statistics displayed.

These statistics pertain to the default PROFILE=BOTH coordinates, no matter what values you specify for the ROW=, COLUMN=, or PROFILE= option. Let $\text{sq}(\cdot)$ be a matrix-valued function denoting element-wise squaring of the argument matrix. Let t be the total inertia (the sum of the elements in D_u^2).

In MCA, let D_s be the Burt table partition containing the intersection of the supplementary columns and the supplementary rows. The matrix D_s is a diagonal matrix of marginal frequencies of the supplemental columns of the binary matrix Z . Let p be the number of rows in this design matrix. The statistics are defined in Table 32.5.

Table 32.5 Statistics That Aid Interpretation

Statistic	Matrix Formula
Row partial contributions to inertia	$\mathbf{D}_r^{-1}\text{sq}(\mathbf{A})$
Column partial contributions to inertia	$\mathbf{D}_c^{-1}\text{sq}(\mathbf{B})$
Row squared cosines	$\text{diag}(\text{sq}(\mathbf{A}\mathbf{D}_u)\mathbf{1})^{-1}\text{sq}(\mathbf{A}\mathbf{D}_u)$
Column squared cosines	$\text{diag}(\text{sq}(\mathbf{B}\mathbf{D}_u)\mathbf{1})^{-1}\text{sq}(\mathbf{B}\mathbf{D}_u)$
Row mass	\mathbf{r}
Column mass	\mathbf{c}
Row inertia	$\frac{1}{t}\mathbf{D}_r^{-1}\text{sq}(\mathbf{A}\mathbf{D}_u)\mathbf{1}$
Column inertia	$\frac{1}{t}\mathbf{D}_c^{-1}\text{sq}(\mathbf{B}\mathbf{D}_u)\mathbf{1}$
Supplementary row squared cosines	$\text{diag}(\text{sq}(\mathbf{R}_s - \mathbf{1}\mathbf{c}')\mathbf{D}_c^{-1}\mathbf{1})^{-1}\text{sq}(\mathbf{R}_s\mathbf{D}_c^{-1}\mathbf{B})$
Supplementary column squared cosines	$\text{diag}(\text{sq}(\mathbf{C}_s - \mathbf{1}\mathbf{r}')\mathbf{D}_r^{-1}\mathbf{1})^{-1}\text{sq}(\mathbf{C}_s\mathbf{D}_r^{-1}\mathbf{A})$
MCA supplementary column squared cosines	$\mathbf{D}_s(p\mathbf{I} - \mathbf{D}_s)^{-1}\text{sq}(\mathbf{C}_s\mathbf{D}_r^{-1}\mathbf{B}\mathbf{D}_u^{-1})$

The quality of representation in the DIMENS= n dimensional display of any point is the sum of its squared cosines over only the n dimensions. Inertia and mass are not defined for supplementary points.

A table that summarizes the partial contributions to inertia table is also computed. The points that best explain the inertia of each dimension and the dimension to which each point contributes the most inertia are indicated. The output data set variable names for this table are Best1–Best n (where DIMENS= n) and Best. The Best column contains the dimension number of the largest partial contribution to inertia for each point (the index of the maximum value in each row of $\mathbf{D}_r^{-1}\text{sq}(\mathbf{A})$ or $\mathbf{D}_c^{-1}\text{sq}(\mathbf{B})$).

For each row, the Best1–Best n columns contain either the corresponding value of Best, if the point is one of the biggest contributors to the dimension's inertia, or 0 if it is not. Specifically, Best1 contains the value of Best for the point with the largest contribution to dimension one's inertia. A cumulative proportion sum is initialized to this point's partial contribution to the inertia of dimension one. If this sum is less than the value for the MININERTIA= option, then Best1 contains the value of Best for the point with the second-largest contribution to dimension one's inertia. Otherwise, this point's Best1 is 0. This point's partial contribution to inertia is added to the sum. This process continues for the point with the third-largest partial contribution, and so on, until adding a point's contribution to the sum increases the sum beyond the value of the MININERTIA= option. This same algorithm is then used for Best2, and so on.

For example, the following table contains contributions to inertia and the corresponding Best variables. The contribution to inertia variables are proportions that sum to 1 within each column. The first point makes its greatest contribution to the inertia of dimension two, so Best for point one is set to 2, and Best1–Best3 for point one must all be 0 or 2. The second point also makes its greatest contribution to the inertia of dimension two, so Best for point two is set to 2, and Best1–Best3 for point two must all be 0 or 2, and so on.

Assume MININERTIA=0.8, the default. Table 32.6 shows some contributions to inertia. In dimension one, the largest contribution is 0.41302 for the fourth point, so Best1 is set to 1, the value of Best for the fourth point. Because this value is less than 0.8, the second-largest value (0.36456 for point five) is found and its Best1 is set to its Best's value of 1. Because $0.41302 + 0.36456 = 0.77758$ is less than 0.8, the third point (0.0882 at point eight) is found and Best1 is set to 3, since the contribution to dimension three for that point is greater than the contribution to dimension one. This increases the sum of the partial contributions to greater than 0.8, so the remaining Best1 values are all 0.

Table 32.6 Best Statistics

Contr1	Contr2	Contr3	Best1	Best2	Best3	Best
0.01593	0.32178	0.07565	0	2	2	2
0.03014	0.24826	0.07715	0	2	2	2
0.00592	0.02892	0.02698	0	0	0	2
0.41302	0.05191	0.05773	1	0	0	1
0.36456	0.00344	0.15565	1	0	1	1
0.03902	0.30966	0.11717	0	2	2	2
0.00019	0.01840	0.00734	0	0	0	2
0.08820	0.00527	0.16555	3	0	3	3
0.01447	0.00024	0.03851	0	0	0	3
0.02855	0.01213	0.27827	0	0	3	3

Displayed Output

The display options control the amount of displayed output. By default, the following information is displayed:

- an inertia and chi-square decomposition table including the total inertia, the principal inertias of each dimension (eigenvalues), the singular values (square roots of the eigenvalues), each dimension's percentage of inertia, a horizontal bar chart of the percentages, and the total chi-square with its degrees of freedom and decomposition. The chi-square statistics and degrees of freedom are valid only when the constructed table is an ordinary two-way contingency table.
- the coordinates of the rows and columns on the dimensions
- the mass, relative contribution to the total inertia, and quality of representation in the DIMENS= n dimensional display of each row and column
- the squared cosines of the angles between each axis and a vector from the origin to the point
- the partial contributions of each point to each dimension's inertia
- the table of indicators of which points best explain the inertia of each dimension

Specific display options and combinations of options display output as follows.

If you specify the OBSERVED or ALL option and you do not specify PRINT=PERCENT, PROC CORRESP displays the following:

- the contingency table, including the row and column marginal frequencies; or with BINARY, the binary table; or the Burt table in MCA
- the supplementary rows
- the supplementary columns

If you specify the OBSERVED or ALL option, with the PRINT=PERCENT or PRINT=BOTH option, PROC CORRESP displays the following:

- the contingency table or Burt table in MCA, scaled to percentages, including the row and column marginal percentages
- the supplementary rows, scaled to percentages
- the supplementary columns, scaled to percentages

If you specify the EXPECTED or ALL option and you do not specify PRINT=PERCENT, PROC CORRESP displays the product of the row marginals and the column marginals divided by the grand frequency of the observed frequency table. For ordinary two-way contingency tables, these are the expected frequencies under the hypothesis of row and column independence.

If you specify the EXPECTED or ALL option with the PRINT=PERCENT or PRINT=BOTH option, PROC CORRESP displays the product of the row marginals and the column marginals divided by the grand frequency of the observed percentages table. For ordinary two-way contingency tables, these are the expected percentages under the hypothesis of row and column independence.

If you specify the DEVIATION or ALL option and you do not specify PRINT=PERCENT, PROC CORRESP displays the observed minus expected frequencies. For ordinary two-way contingency tables, these are the expected frequencies under the hypothesis of row and column independence.

If you specify the DEVIATION or ALL option with the PRINT=PERCENT or PRINT=BOTH option, PROC CORRESP displays the observed minus expected percentages. For ordinary two-way contingency tables, these are the expected percentages under the hypothesis of row and column independence.

If you specify the CELLCHI2 or ALL option and you do not specify PRINT=PERCENT, PROC CORRESP displays contributions to the total chi-square test statistic, including the row and column marginals. The intersection of the marginals contains the total chi-square statistic.

If you specify the CELLCHI2 or ALL option with the PRINT=PERCENT or the PRINT=BOTH option, PROC CORRESP displays contributions to the total chi-square, scaled to percentages, including the row and column marginals.

If you specify the RP or ALL option and you do not specify PRINT=PERCENT, PROC CORRESP displays the row profiles and the supplementary row profiles.

If you specify the RP or ALL option with the PRINT=PERCENT or the PRINT=BOTH option, PROC CORRESP displays the row profiles (scaled to percentages) and the supplementary row profiles (scaled to percentages).

If you specify the CP or ALL option and you do not specify PRINT=PERCENT, PROC CORRESP displays the column profiles and the supplementary column profiles.

If you specify the CP or ALL option with the PRINT=PERCENT or PRINT=BOTH option, PROC CORRESP displays the column profiles (scaled to percentages) and the supplementary column profiles (scaled to percentages).

If you do not specify the NOPRINT option, PROC CORRESP displays the inertia and chi-square decomposition table. This includes the nonzero singular values of the contingency table (or, in MCA, the binary matrix Z used to create the Burt table), the nonzero principal inertias (or eigenvalues) for each dimension, the total inertia, the total chi-square, the decomposition of chi-square, the chi-square degrees of freedom (appropriate only when the table is an ordinary two-way contingency table), the percentage of the total chi-square and inertia for each dimension, and a bar chart of the percentages.

If you specify the MCA option and you do not specify the NOPRINT option, PROC CORRESP displays the adjusted inertias. This includes the nonzero adjusted inertias, percentages, cumulative percentages, and a bar chart of the percentages.

If you do not specify the NOROW, NOPRINT, or MCA option, PROC CORRESP displays the row coordinates and the supplementary row coordinates (displayed when there are supplementary row points).

If you do not specify the NOROW, NOPRINT, MCA, or SHORT option, PROC CORRESP displays the following:

- the summary statistics for the row points, including the quality of representation of the row points in the n -dimensional display, the mass, and the relative contributions to inertia
- the quality of representation of the supplementary row points in the n -dimensional display (displayed when there are supplementary row points)
- the partial contributions to inertia for the row points
- the table of indicators of which row points best explain the inertia of each dimension
- the squared cosines for the row points
- the squared cosines for the supplementary row points (displayed when there are supplementary row points)

If you do not specify the NOCOLUMN or NOPRINT option, PROC CORRESP displays the column coordinates and the supplementary column coordinates (displayed when there are supplementary column points).

If you do not specify the NOCOLUMN, NOPRINT, or SHORT option, PROC CORRESP displays the following:

- the summary statistics for the column points, including the quality of representation of the column points in the n -dimensional display, the mass, and the relative contributions to inertia for the supplementary column points
- the quality of representation of the supplementary column points in the n -dimensional display (displayed when there are supplementary column points)
- the partial contributions to inertia for the column points
- the table of indicators of which column points best explain the inertia of each dimension

- the squared cosines for the column points
- the squared cosines for the supplementary column points

ODS Table Names

PROC CORRESP assigns a name to each table it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in Table 32.7 along with the PROC CORRESP statement options needed to produce the table. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

Table 32.7 ODS Tables Produced by PROC CORRESP

ODS Table Name	Description	Option
AdjInGreenacre	Greenacre Inertia Adjustment	GREENACRE
AdjInBenzecri	Benzécri Inertia Adjustment	BENZECRI
Binary	Binary table	OBSERVED, BINARY
BinaryPct	Binary table percentages	OBSERVED, BINARY*
Burt	Burt table	OBSERVED, MCA
BurtPct	Burt table percentages	OBSERVED, MCA*
CellChiSq	Contributions to chi-square	CELLCHI2
CellChiSqPct	Contributions, percentages	CELLCHI2*
ColBest	Col best indicators	default
ColContr	Col contributions to inertia	default
ColCoors	Col coordinates	default
ColProfiles	Col profiles	CP
ColProfilesPct	Col profiles, percentages	CP*
ColQualMassIn	Col quality, mass, inertia	default
ColSqCos	Col squared cosines	default
DF	DF, chi-square (not displayed)	default
Deviations	Observed - expected freqs	DEVIATIONS
DeviationsPct	Observed - expected percentages	DEVIATIONS*
Expected	Expected frequencies	EXPECTED
ExpectedPct	Expected percentages	EXPECTED*
Inertias	Inertia decomposition table	default
Observed	Observed frequencies	OBSERVED
ObservedPct	Observed percentages	OBSERVED*
RowBest	Row best indicators	default
RowContr	Row contributions to inertia	default
RowCoors	Row coordinates	default
RowProfiles	Row profiles	RP
RowProfilesPct	Row profiles, percentages	RP*
RowQualMassIn	Row quality, mass, inertia	default
RowSqCos	Row squared cosines	default
SupColCoors	Supp col coordinates	default
SupColProfiles	Supp col profiles	CP
SupColProfilesPct	Supp col profiles, percentages	CP*

Table 32.7 *continued*

ODS Table Name	Description	Option
SupColQuality	Supp col quality	default
SupCols	Supplementary col freq	OBSERVED
SupColsPct	Supplementary col percentages	OBSERVED*
SupColSqCos	Supp col squared cosines	default
SupRows	Supplementary row freqs	OBSERVED
SupRowCoors	Supp row coordinates	default
SupRowProfiles	Supp row profiles	RP
SupRowProfilesPct	Supp row profiles, percentages	RP*
SupRowQuality	Supp row quality	default
SupRowsPct	Supplementary row percentages	OBSERVED*
SupRowSqCos	Supp row squared cosines	default

*Percentages are displayed when you specify the PRINT=PERCENT or PRINT=BOTH option.

ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “Statistical Graphics Using ODS.”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “A Primer on ODS Statistical Graphics” on page 599 in Chapter 21, “Statistical Graphics Using ODS.”

You can reference every graph produced through ODS Graphics with a name. The names of the graph that PROC CORRESP generates is listed in Table 32.8. It is displayed by default when ODS graphics is enabled.

Table 32.8 Graphs Produced by PROC CORRESP

ODS Graph Name	Plot Description
ConfigPlot	Correspondence analysis plot

Examples: CORRESP Procedure

Example 32.1: Simple and Multiple Correspondence Analysis of Automobiles and Their Owners

In this example, PROC CORRESP creates a contingency table from categorical data and performs a simple correspondence analysis. The data are from a sample of individuals who were asked to provide informa-

tion about themselves and their automobiles. The questions included origin of the automobile (American, Japanese, European) and family status (single, married, single and living with children, married living with children).

The first steps read the input data and assign formats. PROC CORRESP is used to perform the simple correspondence analysis. The ALL option displays all tables, including the contingency table, chi-square information, profiles, and all results of the correspondence analysis. The OUTC= option creates an output coordinate data set. The TABLES statement specifies the row and column categorical variables. The results are displayed with ODS Graphics.

The following statements produce [Output 32.1.1](#):

```

title1 'Automobile Owners and Auto Attributes';
title2 'Simple Correspondence Analysis';

proc format;
  value Origin  1 = 'American' 2 = 'Japanese' 3 = 'European';
  value Size    1 = 'Small'    2 = 'Medium'  3 = 'Large';
  value Type    1 = 'Family'   2 = 'Sporty'  3 = 'Work';
  value Home    1 = 'Own'      2 = 'Rent';
  value Sex     1 = 'Male'     2 = 'Female';
  value Income  1 = '1 Income' 2 = '2 Incomes';
  value Marital 1 = 'Single with Kids' 2 = 'Married with Kids'
                3 = 'Single'          4 = 'Married';
run;

data Cars;
  missing a;
  input (Origin Size Type Home Income Marital Kids Sex) (1.) @@;
  * Check for End of Line;
  if n(of Origin -- Sex) eq 0 then do; input; return; end;
  marital = 2 * (kids le 0) + marital;
  format Origin Origin. Size Size. Type Type. Home Home.
           Sex Sex. Income Income. Marital Marital.;
  output;
  datalines;
131112212121110121112201131211011211221122112121131122123211222212212201
121122023121221232211101122122022121110122112102131112211121110112311101
211112113211223121122202221122111311123131211102321122223221220221221101
122122022121220211212201221122021122110132112202213112111331226122221101

... more lines ...

212122011211122131221101121211022212220212121101
;

ods graphics on;

* Perform Simple Correspondence Analysis;
proc corresp all data=Cars outc=Coor;
  tables Marital, Origin;
run;

```

Correspondence analysis locates all the categories in a Euclidean space. The first two dimensions of this space are plotted to examine the associations among the categories. Since the smallest dimension of this table is three, there is no loss of information when only two dimensions are plotted. The plot should be thought of as two different overlaid plots, one for each categorical variable. Distances between points within a variable have meaning, but distances between points from different variables do not.

Output 32.1.1 Simple Correspondence Analysis

Automobile Owners and Auto Attributes				
Simple Correspondence Analysis				
The CORRESP Procedure				
Contingency Table				
	American	European	Japanese	Sum
Married	37	14	51	102
Married with Kids	52	15	44	111
Single	33	15	63	111
Single with Kids	6	1	8	15
Sum	128	45	166	339
Chi-Square Statistic Expected Values				
	American	European	Japanese	
Married	38.5133	13.5398	49.9469	
Married with Kids	41.9115	14.7345	54.3540	
Single	41.9115	14.7345	54.3540	
Single with Kids	5.6637	1.9912	7.3451	
Observed Minus Expected Values				
	American	European	Japanese	
Married	-1.5133	0.4602	1.0531	
Married with Kids	10.0885	0.2655	-10.3540	
Single	-8.9115	0.2655	8.6460	
Single with Kids	0.3363	-0.9912	0.6549	
Contributions to the Total Chi-Square Statistic				
	American	European	Japanese	Sum
Married	0.05946	0.01564	0.02220	0.09730
Married with Kids	2.42840	0.00478	1.97235	4.40553
Single	1.89482	0.00478	1.37531	3.27492
Single with Kids	0.01997	0.49337	0.05839	0.57173
Sum	4.40265	0.51858	3.42825	8.34947

Output 32.1.1 continued

Row Profiles			
	American	European	Japanese
Married	0.362745	0.137255	0.500000
Married with Kids	0.468468	0.135135	0.396396
Single	0.297297	0.135135	0.567568
Single with Kids	0.400000	0.066667	0.533333

Column Profiles			
	American	European	Japanese
Married	0.289063	0.311111	0.307229
Married with Kids	0.406250	0.333333	0.265060
Single	0.257813	0.333333	0.379518
Single with Kids	0.046875	0.022222	0.048193

Automobile Owners and Auto Attributes
Simple Correspondence Analysis

The CORRESP Procedure

Inertia and Chi-Square Decomposition

Singular Value	Principal Inertia	Chi-Square	Percent	Cumulative Percent	19	38	57	76	95
0.15122	0.02287	7.75160	92.84	92.84	*****				
0.04200	0.00176	0.59787	7.16	100.00	**				
Total	0.02463	8.34947	100.00						

Degrees of Freedom = 6

Row Coordinates

	Dim1	Dim2
Married	-0.0278	0.0134
Married with Kids	0.1991	0.0064
Single	-0.1716	0.0076
Single with Kids	-0.0144	-0.1947

Summary Statistics for the Row Points

	Quality	Mass	Inertia
Married	1.0000	0.3009	0.0117
Married with Kids	1.0000	0.3274	0.5276
Single	1.0000	0.3274	0.3922
Single with Kids	1.0000	0.0442	0.0685

Output 32.1.1 continued

Partial Contributions to Inertia for the Row Points

	Dim1	Dim2
Married	0.0102	0.0306
Married with Kids	0.5678	0.0076
Single	0.4217	0.0108
Single with Kids	0.0004	0.9511

Indices of the Coordinates That Contribute Most to Inertia for the Row Points

	Dim1	Dim2	Best
Married	0	0	2
Married with Kids	1	0	1
Single	1	0	1
Single with Kids	0	2	2

Squared Cosines for the Row Points

	Dim1	Dim2
Married	0.8121	0.1879
Married with Kids	0.9990	0.0010
Single	0.9980	0.0020
Single with Kids	0.0054	0.9946

Column Coordinates

	Dim1	Dim2
American	0.1847	-0.0166
European	0.0013	0.1073
Japanese	-0.1428	-0.0163

Summary Statistics for the Column Points

	Quality	Mass	Inertia
American	1.0000	0.3776	0.5273
European	1.0000	0.1327	0.0621
Japanese	1.0000	0.4897	0.4106

Partial Contributions to Inertia for the Column Points

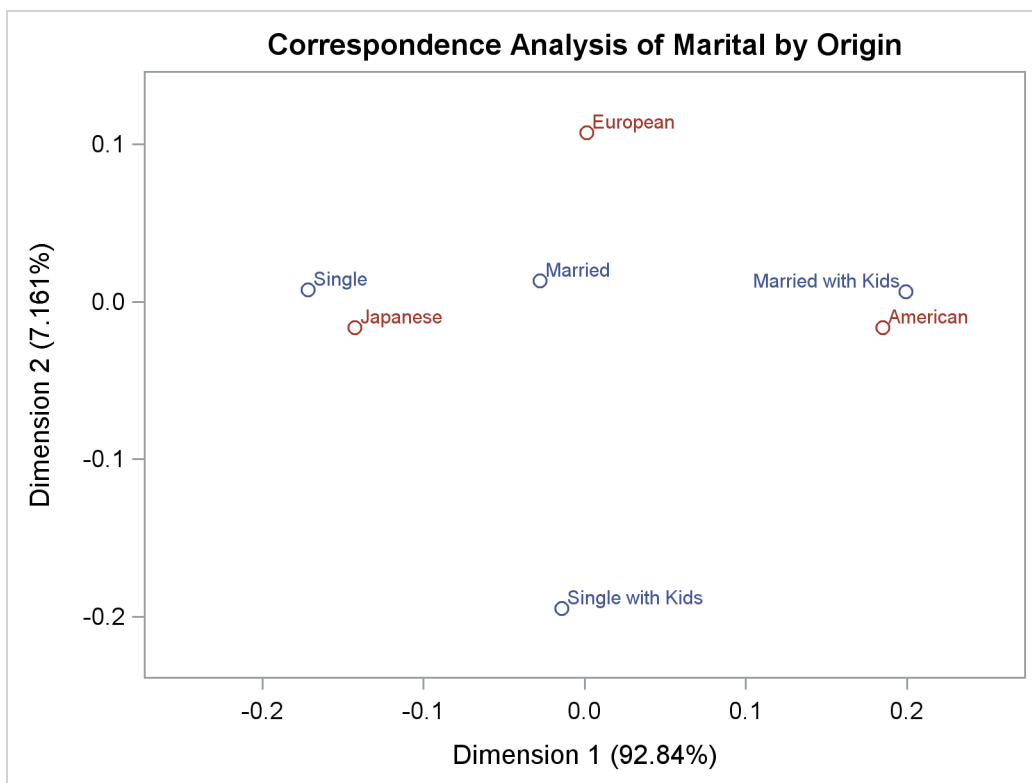
	Dim1	Dim2
American	0.5634	0.0590
European	0.0000	0.8672
Japanese	0.4366	0.0737

Output 32.1.1 *continued*

Indices of the Coordinates That Contribute Most to Inertia for the Column Points			
	Dim1	Dim2	Best
American	1	0	1
European	0	2	2
Japanese	1	0	1

Squared Cosines for the Column Points		
	Dim1	Dim2
American	0.9920	0.0080
European	0.0001	0.9999
Japanese	0.9871	0.0129

Output 32.1.1 *continued*



To interpret the plot, start by interpreting the row points separately from the column points. The European point is near and to the left of the centroid, so it makes a relatively small contribution to the chi-square statistic (because it is near the centroid), it contributes almost nothing to the inertia of dimension one (since its coordinate on dimension one has a small absolute value relative to the other column points), and it makes a relatively large contribution to the inertia of dimension two (since its coordinate on dimension two has a large absolute value relative to the other column points). Its squared cosines for dimension one and two, approximately 0 and 1, respectively, indicate that its position is almost completely determined by its location on dimension two. Its quality of display is 1.0, indicating perfect quality, since the table is two-dimensional after the centering. The American and Japanese points are far from the centroid, and they lie along dimension one. They make relatively large contributions to the chi-square statistic and the inertia of dimension one. The horizontal dimension seems to be largely determined by Japanese versus American automobile ownership.

In the row points, the Married point is near the centroid, and the Single with Kids point has a small coordinate on dimension one that is near zero. The horizontal dimension seems to be largely determined by the Single versus the Married with Kids points. The two interpretations of dimension one show the association with being Married with Kids and owning an American auto, and being single and owning a Japanese auto. The fact that the Married with Kids point is close to the American point and the fact that the Japanese point is near the Single point should be ignored. Distances between row and column points are not defined. The plot shows that more people who are married with kids than you would expect if the rows and columns were independent drive an American auto, and more people who are single than you would expect if the rows and columns were independent drive a Japanese auto.

In the second part of this example, PROC CORRESP creates a Burt table from categorical data and performs a multiple correspondence analysis. The variables used in this example are Origin, Size, Type, Income, Home, Marital, and Sex. MCA specifies multiple correspondence analysis, OBSERVED displays the Burt table, and the OUTC= option creates an output coordinate data set. The TABLES statement with only a single variable list and no comma creates the Burt table.

The following statements produce [Output 32.1.2](#):

```

title2 'Multiple Correspondence Analysis';

* Perform Multiple Correspondence Analysis;
proc corresp mca observed data=Cars outc=Coor;
    tables Origin Size Type Income Home Marital Sex;
run;

```

Output 32.1.2 Multiple Correspondence Analysis

Automobile Owners and Auto Attributes
Multiple Correspondence Analysis

The CORRESP Procedure

Burt Table

	American	European	Japanese	Large	Medium	Small	Family	Sporty	Work
American	125	0	0	36	60	29	81	24	20
European	0	44	0	4	20	20	17	23	4
Japanese	0	0	165	2	61	102	76	59	30
Large	36	4	2	42	0	0	30	1	11
Medium	60	20	61	0	141	0	89	39	13
Small	29	20	102	0	0	151	55	66	30
Family	81	17	76	30	89	55	174	0	0
Sporty	24	23	59	1	39	66	0	106	0
Work	20	4	30	11	13	30	0	0	54
1 Income	58	18	74	20	57	73	69	55	26
2 Incomes	67	26	91	22	84	78	105	51	28
Own	93	38	111	35	106	101	130	71	41
Rent	32	6	54	7	35	50	44	35	13
Married	37	13	51	9	42	50	50	35	16
Married with Kids	50	15	44	21	51	37	79	12	18
Single	32	15	62	11	40	58	35	57	17
Single with Kids	6	1	8	1	8	6	10	2	3
Female	58	21	70	17	70	62	83	44	22
Male	67	23	95	25	71	89	91	62	32

Burt Table

	1	2	Married			Single		Female	Male	
	Income	Incomes	Own	Rent	Married	with Kids	with Single			
American	58	67	93	32	37	50	32	6	58	67
European	18	26	38	6	13	15	15	1	21	23
Japanese	74	91	111	54	51	44	62	8	70	95
Large	20	22	35	7	9	21	11	1	17	25
Medium	57	84	106	35	42	51	40	8	70	71
Small	73	78	101	50	50	37	58	6	62	89
Family	69	105	130	44	50	79	35	10	83	91
Sporty	55	51	71	35	35	12	57	2	44	62
Work	26	28	41	13	16	18	17	3	22	32
1 Income	150	0	80	70	10	27	99	14	47	103
2 Incomes	0	184	162	22	91	82	10	1	102	82
Own	80	162	242	0	76	106	52	8	114	128
Rent	70	22	0	92	25	3	57	7	35	57
Married	10	91	76	25	101	0	0	0	53	48
Married with Kids	27	82	106	3	0	109	0	0	48	61
Single	99	10	52	57	0	0	109	0	35	74
Single with Kids	14	1	8	7	0	0	0	15	13	2
Female	47	102	114	35	53	48	35	13	149	0
Male	103	82	128	57	48	61	74	2	0	185

Output 32.1.2 continued

Automobile Owners and Auto Attributes
Multiple Correspondence Analysis

The CORRESP Procedure

Inertia and Chi-Square Decomposition

Singular Value	Principal Inertia	Chi-Square	Percent	Cumulative Percent	4	8	12	16	20
					-----+-----+-----+-----+-----	-----+-----+-----+-----+-----	-----+-----+-----+-----+-----	-----+-----+-----+-----+-----	-----+-----+-----+-----+-----
0.56934	0.32415	970.77	18.91	18.91	*****	*****	*****	*****	*****
0.48352	0.23380	700.17	13.64	32.55	*****	*****	*****	*****	*****
0.42716	0.18247	546.45	10.64	43.19	*****	*****	*****	*****	*****
0.41215	0.16987	508.73	9.91	53.10	*****	*****	*****	*****	*****
0.38773	0.15033	450.22	8.77	61.87	*****	*****	*****	*****	*****
0.38520	0.14838	444.35	8.66	70.52	*****	*****	*****	*****	*****
0.34066	0.11605	347.55	6.77	77.29	*****	*****	*****	*****	*****
0.32983	0.10879	325.79	6.35	83.64	*****	*****	*****	*****	*****
0.31517	0.09933	297.47	5.79	89.43	*****	*****	*****	*****	*****
0.28069	0.07879	235.95	4.60	94.03	*****	*****	*****	*****	*****
0.26115	0.06820	204.24	3.98	98.01	*****	*****	*****	*****	*****
0.18477	0.03414	102.24	1.99	100.00	**	**	**	**	**
Total	1.71429	5133.92	100.00						

Degrees of Freedom = 324

Column Coordinates

	Dim1	Dim2
American	-0.4035	0.8129
European	-0.0568	-0.5552
Japanese	0.3208	-0.4678
Large	-0.6949	1.5666
Medium	-0.2562	0.0965
Small	0.4326	-0.5258
Family	-0.4201	0.3602
Sporty	0.6604	-0.6696
Work	0.0575	0.1539
1 Income	0.8251	0.5472
2 Incomes	-0.6727	-0.4461
Own	-0.3887	-0.0943
Rent	1.0225	0.2480
Married	-0.4169	-0.7954
Married with Kids	-0.8200	0.3237
Single	1.1461	0.2930
Single with Kids	0.4373	0.8736
Female	-0.3365	-0.2057
Male	0.2710	0.1656

Output 32.1.2 *continued*

Summary Statistics for the Column Points

	Quality	Mass	Inertia
American	0.4925	0.0535	0.0521
European	0.0473	0.0188	0.0724
Japanese	0.3141	0.0706	0.0422
Large	0.4224	0.0180	0.0729
Medium	0.0548	0.0603	0.0482
Small	0.3825	0.0646	0.0457
Family	0.3330	0.0744	0.0399
Sporty	0.4112	0.0453	0.0569
Work	0.0052	0.0231	0.0699
1 Income	0.7991	0.0642	0.0459
2 Incomes	0.7991	0.0787	0.0374
Own	0.4208	0.1035	0.0230
Rent	0.4208	0.0393	0.0604
Married	0.3496	0.0432	0.0581
Married with Kids	0.3765	0.0466	0.0561
Single	0.6780	0.0466	0.0561
Single with Kids	0.0449	0.0064	0.0796
Female	0.1253	0.0637	0.0462
Male	0.1253	0.0791	0.0372

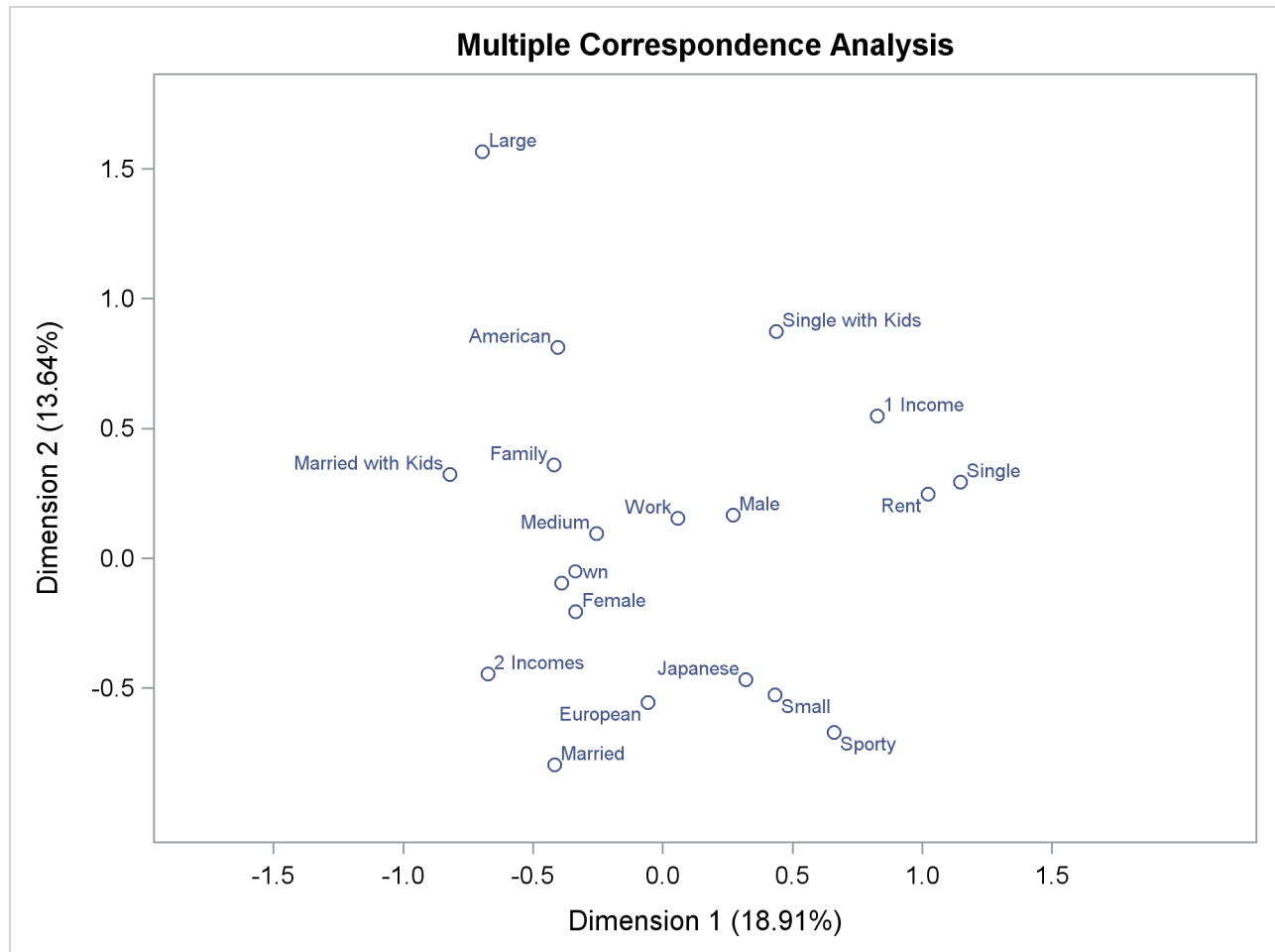
Partial Contributions to Inertia for the Column Points

	Dim1	Dim2
American	0.0268	0.1511
European	0.0002	0.0248
Japanese	0.0224	0.0660
Large	0.0268	0.1886
Medium	0.0122	0.0024
Small	0.0373	0.0764
Family	0.0405	0.0413
Sporty	0.0610	0.0870
Work	0.0002	0.0023
1 Income	0.1348	0.0822
2 Incomes	0.1099	0.0670
Own	0.0482	0.0039
Rent	0.1269	0.0103
Married	0.0232	0.1169
Married with Kids	0.0967	0.0209
Single	0.1889	0.0171
Single with Kids	0.0038	0.0209
Female	0.0223	0.0115
Male	0.0179	0.0093

Output 32.1.2 continued

Indices of the Coordinates That Contribute Most to Inertia for the Column Points			
	Dim1	Dim2	Best
American	0	2	2
European	0	0	2
Japanese	0	2	2
Large	0	2	2
Medium	0	0	1
Small	0	2	2
Family	2	0	2
Sporty	2	2	2
Work	0	0	2
1 Income	1	1	1
2 Incomes	1	1	1
Own	1	0	1
Rent	1	0	1
Married	0	2	2
Married with Kids	1	0	1
Single	1	0	1
Single with Kids	0	0	2
Female	0	0	1
Male	0	0	1

Squared Cosines for the Column Points		
	Dim1	Dim2
American	0.0974	0.3952
European	0.0005	0.0468
Japanese	0.1005	0.2136
Large	0.0695	0.3530
Medium	0.0480	0.0068
Small	0.1544	0.2281
Family	0.1919	0.1411
Sporty	0.2027	0.2085
Work	0.0006	0.0046
1 Income	0.5550	0.2441
2 Incomes	0.5550	0.2441
Own	0.3975	0.0234
Rent	0.3975	0.0234
Married	0.0753	0.2742
Married with Kids	0.3258	0.0508
Single	0.6364	0.0416
Single with Kids	0.0090	0.0359
Female	0.0912	0.0341
Male	0.0912	0.0341

Output 32.1.2 *continued*

Multiple correspondence analysis locates all the categories in a Euclidean space. The first two dimensions of this space are plotted to examine the associations among the categories. The top-right quadrant of the plot shows that the categories Single, Single with Kids, 1 Income, and Rent are associated. Proceeding clockwise, the categories Sporty, Small, and Japanese are associated. The bottom-left quadrant shows the association between being married, owning your own home, and having two incomes. Having children is associated with owning a large American family auto. Such information could be used in market research to identify target audiences for advertisements.

This interpretation is based on points found in approximately the same direction from the origin and in approximately the same region of the space. Distances between points do not have a straightforward interpretation in multiple correspondence analysis. The geometry of multiple correspondence analysis is not a simple generalization of the geometry of simple correspondence analysis (Greenacre and Hastie 1987; Greenacre 1988).

If you want to perform a multiple correspondence analysis and get scores for the individuals, you can specify the `BINARY` option to analyze the binary table, as in the following statements. In the interest of space, only the first 10 rows of coordinates are printed in [Output 32.1.3](#).

```

title2 'Binary Table';

* Perform Multiple Correspondence Analysis;
proc corresp data=Cars binary;
ods select RowCoors;
tables Origin Size Type Income Home Marital Sex;
run;

```

Output 32.1.3 Correspondence Analysis of a Binary Table

Automobile Owners and Auto Attributes Binary Table		
The CORRESP Procedure		
Row Coordinates		
	Dim1	Dim2
1	-0.4093	1.0878
2	0.8198	-0.2221
3	-0.2193	-0.5328
4	0.4382	1.1799
5	-0.6750	0.3600
6	-0.1778	0.1441
7	-0.9375	0.6846
8	-0.7405	-0.1539
9	-0.3027	-0.2749
10	-0.7263	-0.0803

Example 32.2: Simple Correspondence Analysis of U.S. Population

In this example, PROC CORRESP reads an existing contingency table with supplementary observations and performs a simple correspondence analysis. The data are populations of the 50 U.S. states, grouped into regions, for each of the census years from 1920 to 1970 (U.S. Bureau of the Census 1979). Alaska and Hawaii are treated as supplementary regions, because they were not states during this entire period and are not physically connected to the other 48 states. Consequently, it is reasonable to expect that population changes in these two states operate differently from population changes in the other states. The correspondence analysis is performed giving the supplementary points negative weight, and then the coordinates for the supplementary points are computed in the solution defined by the other points.

The initial DATA step reads the table, provides labels for the years, flags the supplementary rows with negative weights, and specifies absolute weights of 1000 for all observations since the data were originally reported in units of 1000 people.

In the PROC CORRESP statement, PRINT=PERCENT and the display options display the table of cell percentages (OBSERVED), cell contributions to the total chi-square scaled to sum to 100 (CELLCHI2), row profile rows that sum to 100 (RP), and column profile columns that sum to 100 (CP). The SHORT option specifies that the correspondence analysis summary statistics, contributions to inertia, and squared

cosines should not be displayed. The option OUTC=COOR creates the output coordinate data set. Since the data are already in table form, a VAR statement is used to read the table. Row labels are specified with the ID statement, and column labels come from the variable labels. The WEIGHT statement flags the supplementary observations and restores the table values to populations.

The following statements produce [Output 32.2.1](#):

```

title 'United States Population, 1920-1970';

data USPop;

  * Regions:
  * New England      - ME, NH, VT, MA, RI, CT.
  * Great Lakes      - OH, IN, IL, MI, WI.
  * South Atlantic   - DE, MD, DC, VA, WV, NC, SC, GA, FL.
  * Mountain         - MT, ID, WY, CO, NM, AZ, UT, NV.
  * Pacific          - WA, OR, CA.
  *
  * Note: Multiply data values by 1000 to get populations.;

input Region $14. y1920 y1930 y1940 y1950 y1960 y1970;

label y1920 = '1920'    y1930 = '1930'    y1940 = '1940'
      y1950 = '1950'    y1960 = '1960'    y1970 = '1970';

if region = 'Hawaii' or region = 'Alaska'
  then w = -1000;      /* Flag Supplementary Observations */
  else w = 1000;

  datalines;
New England      7401  8166  8437  9314 10509 11842
NY, NJ, PA      22261 26261 27539 30146 34168 37199
Great Lakes     21476 25297 26626 30399 36225 40252
Midwest         12544 13297 13517 14061 15394 16319
South Atlantic  13990 15794 17823 21182 25972 30671
KY, TN, AL, MS  8893  9887 10778 11447 12050 12803
AR, LA, OK, TX  10242 12177 13065 14538 16951 19321
Mountain        3336  3702  4150  5075  6855  8282
Pacific         5567  8195  9733 14486 20339 25454
Alaska          55    59    73   129   226   300
Hawaii          256   368   423   500   633   769
;

ods graphics on;

* Perform Simple Correspondence Analysis;
proc corresp data=uspop print=percent observed cellchi2 rp cp
  short outc=Coor plot(flip);
  var y1920 -- y1970;
  id Region;
  weight w;
run;

```

The contingency table shows that the population of all regions increased over this time period. The row profiles show that population increased at a different rate for the different regions. There was a small increase in population in the Midwest, for example, but the population more than quadrupled in the Pacific region over the same period. The column profiles show that in 1920, the U.S. population was concentrated in the NY, NJ, PA, Great Lakes, Midwest, and South Atlantic regions. With time, the population shifted more to the South Atlantic, Mountain, and Pacific regions. This is also clear from the correspondence analysis. The inertia and chi-square decomposition table shows that there are five nontrivial dimensions in the table, but the association between the rows and columns is almost entirely one-dimensional.

Output 32.2.1 United States Population, 1920–1970

United States Population, 1920–1970							
The CORRESP Procedure							
Contingency Table							
Percents	1920	1930	1940	1950	1960	1970	Sum
New England	0.830	0.916	0.946	1.045	1.179	1.328	6.245
NY, NJ, PA	2.497	2.946	3.089	3.382	3.833	4.173	19.921
Great Lakes	2.409	2.838	2.987	3.410	4.064	4.516	20.224
Midwest	1.407	1.492	1.516	1.577	1.727	1.831	9.550
South Atlantic	1.569	1.772	1.999	2.376	2.914	3.441	14.071
KY, TN, AL, MS	0.998	1.109	1.209	1.284	1.352	1.436	7.388
AR, LA, OK, TX	1.149	1.366	1.466	1.631	1.902	2.167	9.681
Mountain	0.374	0.415	0.466	0.569	0.769	0.929	3.523
Pacific	0.625	0.919	1.092	1.625	2.282	2.855	9.398
Sum	11.859	13.773	14.771	16.900	20.020	22.677	100.000
Supplementary Rows							
Percents	1920	1930	1940	1950	1960	1970	
Alaska	0.006170	0.006619	0.008189	0.014471	0.025353	0.033655	
Hawaii	0.028719	0.041283	0.047453	0.056091	0.071011	0.086268	
Contributions to the Total Chi-Square Statistic							
Percents	1920	1930	1940	1950	1960	1970	Sum
New England	0.937	0.314	0.054	0.009	0.352	0.469	2.135
NY, NJ, PA	0.665	1.287	0.633	0.006	0.521	2.265	5.378
Great Lakes	0.004	0.085	0.000	0.001	0.005	0.094	0.189
Midwest	5.749	2.039	0.684	0.072	1.546	4.472	14.563
South Atlantic	0.509	1.231	0.259	0.000	0.285	1.688	3.973
KY, TN, AL, MS	1.454	0.711	1.098	0.087	0.946	2.945	7.242
AR, LA, OK, TX	0.000	0.069	0.077	0.001	0.059	0.030	0.238
Mountain	0.391	0.868	0.497	0.098	0.498	1.834	4.187
Pacific	18.591	9.380	5.458	0.074	7.346	21.248	62.096
Sum	28.302	15.986	8.761	0.349	11.558	35.046	100.000

Output 32.2.1 continued

Row Profiles						
Percents	1920	1930	1940	1950	1960	1970
New England	13.2947	14.6688	15.1557	16.7310	18.8777	21.2722
NY, NJ, PA	12.5362	14.7888	15.5085	16.9766	19.2416	20.9484
Great Lakes	11.9129	14.0325	14.7697	16.8626	20.0943	22.3281
Midwest	14.7348	15.6193	15.8777	16.5167	18.0825	19.1691
South Atlantic	11.1535	12.5917	14.2093	16.8872	20.7060	24.4523
KY, TN, AL, MS	13.5033	15.0126	16.3655	17.3813	18.2969	19.4403
AR, LA, OK, TX	11.8687	14.1111	15.1401	16.8471	19.6433	22.3897
Mountain	10.6242	11.7898	13.2166	16.1624	21.8312	26.3758
Pacific	6.6453	9.7823	11.6182	17.2918	24.2784	30.3841

Supplementary Row Profiles						
Percents	1920	1930	1940	1950	1960	1970
Alaska	6.5321	7.0071	8.6698	15.3207	26.8409	35.6295
Hawaii	8.6809	12.4788	14.3438	16.9549	21.4649	26.0766

Column Profiles						
Percents	1920	1930	1940	1950	1960	1970
New England	7.0012	6.6511	6.4078	6.1826	5.8886	5.8582
NY, NJ, PA	21.0586	21.3894	20.9155	20.0109	19.1457	18.4023
Great Lakes	20.3160	20.6042	20.2221	20.1788	20.2983	19.9126
Midwest	11.8664	10.8303	10.2660	9.3337	8.6259	8.0730
South Atlantic	13.2343	12.8641	13.5363	14.0606	14.5532	15.1729
KY, TN, AL, MS	8.4126	8.0529	8.1857	7.5985	6.7521	6.3336
AR, LA, OK, TX	9.6888	9.9181	9.9227	9.6503	9.4983	9.5581
Mountain	3.1558	3.0152	3.1519	3.3688	3.8411	4.0971
Pacific	5.2663	6.6748	7.3921	9.6158	11.3968	12.5921

United States Population, 1920-1970

The CORRESP Procedure

Inertia and Chi-Square Decomposition

Singular Value	Principal Inertia	Chi-Square	Percent	Cumulative Percent	20	40	60	80	100
0.10664	0.01137	1.014E7	98.16	98.16	*****	*****	*****	*****	*****
0.01238	0.00015	136586	1.32	99.48					
0.00658	0.00004	38540	0.37	99.85					
0.00333	0.00001	9896.6	0.10	99.95					
0.00244	0.00001	5309.9	0.05	100.00					
Total	0.01159	1.033E7	100.00						

Degrees of Freedom = 40

Output 32.2.1 *continued***Row Coordinates**

	Dim1	Dim2
New England	0.0611	0.0132
NY, NJ, PA	0.0546	-0.0117
Great Lakes	0.0074	-0.0028
Midwest	0.1315	0.0186
South Atlantic	-0.0553	0.0105
KY, TN, AL, MS	0.1044	-0.0144
AR, LA, OK, TX	0.0131	-0.0067
Mountain	-0.1121	0.0338
Pacific	-0.2766	-0.0070

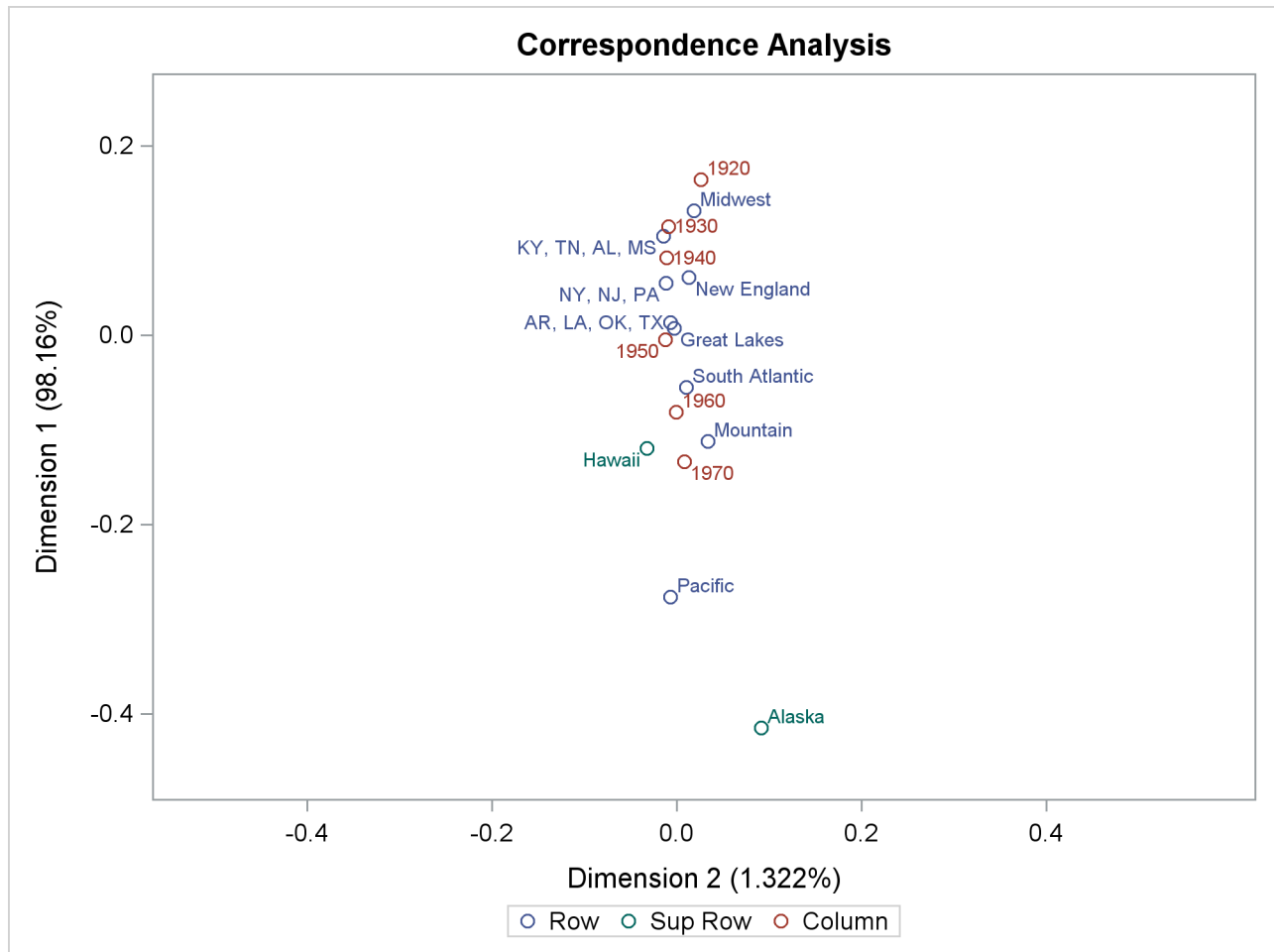
Supplementary Row Coordinates

	Dim1	Dim2
Alaska	-0.4152	0.0912
Hawaii	-0.1198	-0.0321

Column Coordinates

	Dim1	Dim2
1920	0.1642	0.0263
1930	0.1149	-0.0089
1940	0.0816	-0.0108
1950	-0.0046	-0.0125
1960	-0.0815	-0.0007
1970	-0.1335	0.0086

Output 32.2.1 continued



ODS Graphics is used to plot the results. The data are essentially one-dimensional. For data such as these, it is better to plot the first dimension vertically, as opposed to the default, which is horizontally. The vertical orientation has fewer opportunities for label collisions. Specifying PLOTS(FILIP) on the PROC CORRESP statement switches the vertical and horizontal axes to improve the graphical display.

The plot shows that the first dimension correctly orders the years. There is nothing in the correspondence analysis that forces this to happen; the analysis has no information about the inherent ordering of the column categories. The ordering of the regions and the ordering of the years reflect the shift over time of the U.S. population from the Northeast quadrant of the country to the South and to the West. The results show that the West and Southeast grew faster than the rest of the contiguous 48 states during this period.

The plot also shows that the growth pattern for Hawaii was similar to the growth pattern for the mountain states and that Alaska's growth was even more extreme than the Pacific states' growth. The row profiles confirm this interpretation.

The Pacific region is farther from the origin than all other active points. The Midwest is the extreme region in the other direction. The table of contributions to the total chi-square shows that 62% of the total chi-square statistic is contributed by the Pacific region, which is followed by the Midwest at over 14%. Similarly the two extreme years, 1920 and 1970, together contribute over 63% to the total chi-square, whereas the years nearer the origin of the plot contribute less.

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Chapter 33

The DISCRIM Procedure

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Overview: DISCRIM Procedure

For a set of observations containing one or more quantitative variables and a classification variable defining groups of observations, the DISCRIM procedure develops a discriminant criterion to classify each observation into one of the groups. The derived discriminant criterion from this data set can be applied to a second data set during the same execution of PROC DISCRIM. The data set that PROC DISCRIM uses to derive the discriminant criterion is called the *training* or *calibration* data set.

When the distribution within each group is assumed to be multivariate normal, a parametric method can be used to develop a discriminant function. The discriminant function, also known as a classification criterion, is determined by a measure of generalized squared distance (Rao 1973). The classification criterion can be based on either the individual within-group covariance matrices (yielding a quadratic function) or the pooled covariance matrix (yielding a linear function); it also takes into account the prior probabilities of the groups. The calibration information can be stored in a special SAS data set and applied to other data sets.

When no assumptions can be made about the distribution within each group, or when the distribution is assumed not to be multivariate normal, nonparametric methods can be used to estimate the group-specific densities. These methods include the kernel and k -nearest-neighbor methods (Rosenblatt 1956; Parzen 1962). The DISCRIM procedure uses uniform, normal, Epanechnikov, biweight, or triweight kernels for density estimation.

Either Mahalanobis or Euclidean distance can be used to determine proximity. Mahalanobis distance can be based on either the full covariance matrix or the diagonal matrix of variances. With a k -nearest-neighbor method, the pooled covariance matrix is used to calculate the Mahalanobis distances. With a kernel method, either the individual within-group covariance matrices or the pooled covariance matrix can be used to calculate the Mahalanobis distances. With the estimated group-specific densities and their associated prior probabilities, the posterior probability estimates of group membership for each class can be evaluated.

Canonical discriminant analysis is a dimension-reduction technique related to principal component analysis and canonical correlation. Given a classification variable and several quantitative variables, PROC DISCRIM derives canonical variables (linear combinations of the quantitative variables) that summarize between-class variation in much the same way that principal components summarize total variation. (See Chapter 29, “[The CANDISC Procedure](#),” for more information about canonical discriminant analysis.) A discriminant criterion is always derived in PROC DISCRIM. If you want canonical discriminant analysis without the use of a discriminant criterion, you should use the CANDISC procedure.

The DISCRIM procedure can produce an output data set containing various statistics such as means, standard deviations, and correlations. If a parametric method is used, the discriminant function is also stored in the data set to classify future observations. When canonical discriminant analysis is performed, the output data set includes canonical coefficients that can be rotated by the FACTOR procedure. PROC DISCRIM can also create a second type of output data set containing the classification results for each observation. When canonical discriminant analysis is performed, this output data set also includes canonical variable scores. A third type of output data set containing the group-specific density estimates at each observation can also be produced.

PROC DISCRIM evaluates the performance of a discriminant criterion by estimating error rates (probabilities of misclassification) in the classification of future observations. These error-rate estimates include error-count estimates and posterior probability error-rate estimates. When the input data set is an ordinary SAS data set, the error rate can also be estimated by cross validation.

Do not confuse discriminant analysis with cluster analysis. All varieties of discriminant analysis require prior knowledge of the classes, usually in the form of a sample from each class. In cluster analysis, the data do not include information about class membership; the purpose is to construct a classification.

See Chapter 10, “Introduction to Discriminant Procedures,” for a discussion of discriminant analysis.

Getting Started: DISCRIM Procedure

The data in this example are measurements of 159 fish caught in Finland’s lake Laengelma-vesi; this data set is available from the Puranen. For each of the seven species (bream, roach, whitefish, parkki, perch, pike, and smelt) the weight, length, height, and width of each fish are tallied. Three different length measurements are recorded: from the nose of the fish to the beginning of its tail, from the nose to the notch of its tail, and from the nose to the end of its tail. The height and width are recorded as percentages of the third length variable. The fish data set is available from the Sashelp library. The goal now is to find a discriminant function based on these six variables that best classifies the fish into species.

First, assume that the data are normally distributed within each group with equal covariances across groups. The following statements use PROC DISCRIM to analyze the Sashelp.Fish data and create [Figure 33.1](#) through [Figure 33.5](#):

```
title 'Fish Measurement Data';

proc discrim data=sashelp.fish;
  class Species;
run;
```

The DISCRIM procedure begins by displaying summary information about the variables in the analysis (see [Figure 33.1](#)). This information includes the number of observations, the number of quantitative variables in the analysis (specified with the VAR statement), and the number of classes in the classification variable (specified with the CLASS statement). The frequency of each class, its weight, the proportion of the total sample, and the prior probability are also displayed. Equal priors are assigned by default.

Figure 33.1 Summary Information

Fish Measurement Data					
The DISCRIM Procedure					
Total Sample Size	158	DF Total	157		
Variables	6	DF Within Classes	151		
Classes	7	DF Between Classes	6		
Number of Observations Read		159			
Number of Observations Used		158			
Class Level Information					
Species	Variable Name	Frequency	Weight	Proportion	Prior Probability
Bream	Bream	34	34.0000	0.215190	0.142857
Parkki	Parkki	11	11.0000	0.069620	0.142857
Perch	Perch	56	56.0000	0.354430	0.142857
Pike	Pike	17	17.0000	0.107595	0.142857
Roach	Roach	20	20.0000	0.126582	0.142857
Smelt	Smelt	14	14.0000	0.088608	0.142857
Whitefish	Whitefish	6	6.0000	0.037975	0.142857

The natural log of the determinant of the pooled covariance matrix is displayed in [Figure 33.2](#).

Figure 33.2 Pooled Covariance Matrix Information

Pooled Covariance Matrix Information	
Covariance Matrix Rank	Natural Log of the Determinant of the Covariance Matrix
6	4.17613

The squared distances between the classes are shown in [Figure 33.3](#).

Figure 33.3 Squared Distances

Fish Measurement Data							
The DISCRIM Procedure							
Generalized Squared Distance to Species							
From Species	Bream	Parkki	Perch	Pike	Roach	Smelt	Whitefish
Bream	0	83.32523	243.66688	310.52333	133.06721	252.75503	132.05820
Parkki	83.32523	0	57.09760	174.20918	27.00096	60.52076	26.54855
Perch	243.66688	57.09760	0	101.06791	29.21632	29.26806	20.43791
Pike	310.52333	174.20918	101.06791	0	92.40876	127.82177	99.90673
Roach	133.06721	27.00096	29.21632	92.40876	0	33.84280	6.31997
Smelt	252.75503	60.52076	29.26806	127.82177	33.84280	0	46.37326
Whitefish	132.05820	26.54855	20.43791	99.90673	6.31997	46.37326	0

The coefficients of the linear discriminant function are displayed (in [Figure 33.4](#)) with the default options METHOD=NORMAL and POOL=YES.

Figure 33.4 Linear Discriminant Function

Linear Discriminant Function for Species							
Variable	Bream	Parkki	Perch	Pike	Roach	Smelt	Whitefish
Constant	-185.91682	-64.92517	-48.68009	-148.06402	-62.65963	-19.70401	-67.44603
Weight	-0.10912	-0.09031	-0.09418	-0.13805	-0.09901	-0.05778	-0.09948
Length1	-23.02273	-13.64180	-19.45368	-20.92442	-14.63635	-4.09257	-22.57117
Length2	-26.70692	-5.38195	17.33061	6.19887	-7.47195	-3.63996	3.83450
Length3	50.55780	20.89531	5.25993	22.94989	25.00702	10.60171	21.12638
Height	13.91638	8.44567	-1.42833	-8.99687	-0.26083	-1.84569	0.64957
Width	-23.71895	-13.38592	1.32749	-9.13410	-3.74542	-3.43630	-2.52442

A summary of how the discriminant function classifies the data used to develop the function is displayed last. In [Figure 33.5](#), you see that only three of the observations are misclassified. The error-count estimates give the proportion of misclassified observations in each group. Since you are classifying the same data that are used to derive the discriminant function, these error-count estimates are biased.

Figure 33.5 Resubstitution Misclassification Summary

Fish Measurement Data								
The DISCRIM Procedure								
Classification Summary for Calibration Data: SASHELP.FISH								
Resubstitution Summary using Linear Discriminant Function								
Number of Observations and Percent Classified into Species								
From Species	Bream	Parkki	Perch	Pike	Roach	Smelt	Whitefish	Total
Bream	34 100.00	0 0.00	0 0.00	0 0.00	0 0.00	0 0.00	0 0.00	34 100.00
Parkki	0 0.00	11 100.00	0 0.00	0 0.00	0 0.00	0 0.00	0 0.00	11 100.00
Perch	0 0.00	0 0.00	53 94.64	0 0.00	0 0.00	3 5.36	0 0.00	56 100.00
Pike	0 0.00	0 0.00	0 0.00	17 100.00	0 0.00	0 0.00	0 0.00	17 100.00
Roach	0 0.00	0 0.00	0 0.00	0 0.00	20 100.00	0 0.00	0 0.00	20 100.00
Smelt	0 0.00	0 0.00	0 0.00	0 0.00	0 0.00	14 100.00	0 0.00	14 100.00
Whitefish	0 0.00	0 0.00	0 0.00	0 0.00	0 0.00	0 0.00	6 100.00	6 100.00
Total	34 21.52	11 6.96	53 33.54	17 10.76	20 12.66	17 10.76	6 3.80	158 100.00
Priors	0.14286	0.14286	0.14286	0.14286	0.14286	0.14286	0.14286	
Error Count Estimates for Species								
	Bream	Parkki	Perch	Pike	Roach	Smelt	Whitefish	Total
Rate	0.0000	0.0000	0.0536	0.0000	0.0000	0.0000	0.0000	0.0077
Priors	0.1429	0.1429	0.1429	0.1429	0.1429	0.1429	0.1429	

One way to reduce the bias of the error-count estimates is to split your data into two sets. One set is used to derive the discriminant function, and the other set is used to run validation tests. [Example 33.4](#) shows how to analyze a test data set. Another method of reducing bias is to classify each observation by using a discriminant function computed from all of the other observations; this method is invoked with the CROSSVALIDATE option.

Syntax: DISCRIM Procedure

The following statements are available in the DISCRIM procedure:

```

PROC DISCRIM < options > ;
  CLASS variable ;
  BY variables ;
  FREQ variable ;
  ID variable ;
  PRIORS probabilities ;
  TESTCLASS variable ;
  TESTFREQ variable ;
  TESTID variable ;
  VAR variables ;
  WEIGHT variable ;

```

Only the PROC DISCRIM and CLASS statements are required.

The following sections describe the PROC DISCRIM statement and then describe the other statements in alphabetical order.

PROC DISCRIM Statement

```

PROC DISCRIM < options > ;

```

The PROC DISCRIM statement invokes the DISCRIM procedure. [Table 33.1](#) summarizes the options available in the PROC DISCRIM statement.

Table 33.1 Options Available in the PROC DISCRIM Statement

Option	Description
Input Data Sets	
DATA=	Specifies input SAS data set
TESTDATA=	Specifies input SAS data set to classify
Output Data Sets	
OUTSTAT=	Specifies output statistics data set
OUT=	Specifies output data set with classification results
OUTCROSS=	Specifies output data set with cross validation results
OUTD=	Specifies output data set with densities
SCORES=	Outputs discriminant scores to the OUT= data set
TESTOUT=	Specifies output data set with TEST= results
TESTOUTD=	Specifies output data set with TEST= densities
Method Details	
METHOD=	Specifies parametric or nonparametric method
POOL=	Specifies whether to pool the covariance matrices
SINGULAR=	Specifies the singularity criterion

Table 33.1 *continued*

Option	Description
SLPOOL=	Specifies significance level homogeneity test
THRESHOLD=	Specifies the minimum threshold for classification
Nonparametric Methods	
K=	Specifies k value for k nearest neighbors
KPROP=	Specifies proportion, p , for computing k
R=	Specifies radius for kernel density estimation
KERNEL=	Specifies a kernel density to estimate
METRIC=	Specifies metric in for squared distances
Canonical Discriminant Analysis	
CANONICAL	Performs canonical discriminant analysis
CANPREFIX=	Specifies a prefix for naming the canonical variables
NCAN=	Specifies the number of canonical variables
Resubstitution Classification	
LIST	Displays the classification results
LISTERR	Displays the misclassified observations
NOCLASSIFY	Suppresses the classification
TESTLIST	Displays the classification results of TEST=
TESTLISTERR	Displays the misclassified observations of TEST=
Cross Validation Classification	
CROSSLIST	Displays the cross validation results
CROSSLISTERR	Displays the misclassified cross validation results
CROSSVALIDATE	Specifies cross validation
Control Displayed Output	
ALL	Displays all output
ANOVA	Displays univariate statistics
BCORR	Displays between correlations
BCOV	Displays between covariances
BSSCP	Displays between SSCPs
DISTANCE	Displays squared Mahalanobis distances
FORMULA	Displays formulas in destinations other than LISTING
MANOVA	Displays multivariate ANOVA results
NOPRINT	Suppresses all displayed output
PCORR	Displays pooled correlations
PCOV	Displays pooled covariances
POSTERR	Displays posterior probability error-rate estimates
PSSCP	Displays pooled SSCPs
SHORT	Suppresses some displayed output
SIMPLE	Displays simple descriptive statistics
STDMEAN	Displays standardized class means
TCORR	Displays total correlations
TCOV	Displays total covariances
TSSCP	Displays total SSCPs

Table 33.1 *continued*

Option	Description
WCORR	Displays within correlations
WCOV	Displays within covariances
WSSCP	Displays within SSCPs

ALL

activates all options that control displayed output. When the derived classification criterion is used to classify observations, the ALL option also activates the **POSTERR** option.

ANOVA

displays univariate statistics for testing the hypothesis that the class means are equal in the population for each variable.

BCORR

displays between-class correlations.

BCOV

displays between-class covariances. The between-class covariance matrix equals the between-class SSCP matrix divided by $n(c - 1)/c$, where n is the number of observations and c is the number of classes. You should interpret the between-class covariances in comparison with the total-sample and within-class covariances, not as formal estimates of population parameters.

BSSCP

displays the between-class SSCP matrix.

CANONICAL**CAN**

performs canonical discriminant analysis.

CANPREFIX=*name*

specifies a prefix for naming the canonical variables. By default, the names are Can1, Can2, ..., Can*n*. If you specify CANPREFIX=ABC, the components are named ABC1, ABC2, ABC3, and so on. The number of characters in the prefix, plus the number of digits required to designate the canonical variables, should not exceed 32. The prefix is truncated if the combined length exceeds 32.

The CANONICAL option is activated when you specify either the NCAN= or the CANPREFIX= option. A discriminant criterion is always derived in PROC DISCRIM. If you want canonical discriminant analysis without the use of discriminant criteria, you should use PROC CANDISC.

CROSSLIST

displays the cross validation classification results for each observation.

CROSSLISTERR

displays the cross validation classification results for misclassified observations only.

CROSSVALIDATE

specifies the cross validation classification of the input DATA= data set. When a parametric method is used, PROC DISCRIM classifies each observation in the DATA= data set by using a discriminant function computed from the other observations in the DATA= data set, excluding the observation being classified. When a nonparametric method is used, the covariance matrices used to compute the distances are based on all observations in the data set and do not exclude the observation being classified. However, the observation being classified is excluded from the nonparametric density estimation (if you specify the R= option) or the k nearest neighbors (if you specify the K= or KPROP= option) of that observation. The CROSSVALIDATE option is set when you specify the CROSSLIST, CROSSLISTERR, or OUTCROSS= option. With these options, cross validation information is displayed or output in addition to the usual resubstitution classification results. Cross validation classification results are written to the OUTCROSS= data set, and resubstitution classification results are written to the OUT= data set.

DATA=SAS-data-set

specifies the data set to be analyzed. The data set can be an ordinary SAS data set or one of several specially structured data sets created by SAS/STAT procedures. These specially structured data sets include TYPE=CORR, TYPE=COV, TYPE=CSSCP, TYPE=SSCP, TYPE=LINEAR, TYPE=QUAD, and TYPE=MIXED. The input data set must be an ordinary SAS data set if you specify METHOD=NP. If you omit the DATA= option, the procedure uses the most recently created SAS data set.

DISTANCE**MAHALANOBIS**

displays the squared Mahalanobis distances between the group means, F statistics, and the corresponding probabilities of greater Mahalanobis squared distances between the group means. The squared distances are based on the specification of the POOL= and METRIC= options.

FORMULA

displays formulas in destinations other than LISTING. See the section “Formulas” on page 2097 for more information.

K= k

specifies a k value for the k -nearest-neighbor rule. An observation x is classified into a group based on the information from the k nearest neighbors of x . Do not specify the K= option with the KPROP= or R= option.

KPROP= p

specifies a proportion, p , for computing the k value for the k -nearest-neighbor rule: $k = \max(1, \text{floor}(np))$, where n is the number of valid observations. When there is a FREQ statement, n is the sum of the FREQ variable for the observations used in the analysis (those without missing or invalid values). An observation x is classified into a group based on the information from the k nearest neighbors of x . Do not specify the KPROP= option with the K= or R= option.

KERNEL=BIWEIGHT | BIW

KERNEL=EPANECHNIKOV | EPA

KERNEL=NORMAL | NOR

KERNEL=TRIWEIGHT | TRI

KERNEL=UNIFORM | UNI

specifies a kernel density to estimate the group-specific densities. You can specify the **KERNEL=** option only when the **R=** option is specified. The default is **KERNEL=UNIFORM**.

LIST

displays the resubstitution classification results for each observation. You can specify this option only when the input data set is an ordinary SAS data set.

LISTERR

displays the resubstitution classification results for misclassified observations only. You can specify this option only when the input data set is an ordinary SAS data set.

MANOVA

displays multivariate statistics for testing the hypothesis that the class means are equal in the population.

METHOD=NORMAL | NPAR

determines the method to use in deriving the classification criterion. When you specify **METHOD=NORMAL**, a parametric method based on a multivariate normal distribution within each class is used to derive a linear or quadratic discriminant function. The default is **METHOD=NORMAL**. When you specify **METHOD=NPAR**, a nonparametric method is used and you must also specify either the **K=** or **R=** option.

METRIC=DIAGONAL | FULL | IDENTITY

specifies the metric in which the computations of squared distances are performed. If you specify **METRIC=FULL**, then PROC DISCRIM uses either the pooled covariance matrix (**POOL=YES**) or individual within-group covariance matrices (**POOL=NO**) to compute the squared distances. If you specify **METRIC=DIAGONAL**, then PROC DISCRIM uses either the diagonal matrix of the pooled covariance matrix (**POOL=YES**) or diagonal matrices of individual within-group covariance matrices (**POOL=NO**) to compute the squared distances. If you specify **METRIC=IDENTITY**, then PROC DISCRIM uses Euclidean distance. The default is **METRIC=FULL**. When you specify **METHOD=NORMAL**, the option **METRIC=FULL** is used.

NCAN=number

specifies the number of canonical variables to compute. The value of *number* must be less than or equal to the number of variables. If you specify the option **NCAN=0**, the procedure displays the canonical correlations but not the canonical coefficients, structures, or means. Let v be the number of variables in the VAR statement, and let c be the number of classes. If you omit the **NCAN=** option, only $\min(v, c - 1)$ canonical variables are generated. If you request an output data set (**OUT=**, **OUTCROSS=**, **TESTOUT=**), v canonical variables are generated. In this case, the last $v - (c - 1)$ canonical variables have missing values.

The **CANONICAL** option is activated when you specify either the **NCAN=** or the **CANPREFIX=** option. A discriminant criterion is always derived in PROC DISCRIM. If you want canonical discriminant analysis without the use of discriminant criterion, you should use PROC CANDISC.

NOCLASSIFY

suppresses the resubstitution classification of the input DATA= data set. You can specify this option only when the input data set is an ordinary SAS data set.

NOPRINT

suppresses the normal display of results. Note that this option temporarily disables the Output Delivery System (ODS); see Chapter 20, “Using the Output Delivery System,” for more information.

OUT=SAS-data-set

creates an output SAS data set containing all the data from the DATA= data set, plus the posterior probabilities and the class into which each observation is classified by resubstitution. When you specify the CANONICAL option, the data set also contains new variables with canonical variable scores. See the section “OUT= Data Set” on page 2089 for more information.

OUTCROSS=SAS-data-set

creates an output SAS data set containing all the data from the DATA= data set, plus the posterior probabilities and the class into which each observation is classified by cross validation. When you specify the CANONICAL option, the data set also contains new variables with canonical variable scores. See the section “OUT= Data Set” on page 2089 for more information.

OUTD=SAS-data-set

creates an output SAS data set containing all the data from the DATA= data set, plus the group-specific density estimates for each observation. See the section “OUT= Data Set” on page 2089 for more information.

OUTSTAT=SAS-data-set

creates an output SAS data set containing various statistics such as means, standard deviations, and correlations. When the input data set is an ordinary SAS data set or when TYPE=CORR, TYPE=COV, TYPE=CSSCP, or TYPE=SSCP, this option can be used to generate discriminant statistics. When you specify the CANONICAL option, canonical correlations, canonical structures, canonical coefficients, and means of canonical variables for each class are included in the data set. If you specify METHOD=NORMAL, the output data set also includes coefficients of the discriminant functions, and the output data set is TYPE=LINEAR (POOL=YES), TYPE=QUAD (POOL=NO), or TYPE=MIXED (POOL=TEST). If you specify METHOD=NPART, this output data set is TYPE=CORR. This data set also holds calibration information that can be used to classify new observations. See the sections “Saving and Using Calibration Information” on page 2086 and “OUT= Data Set” on page 2089 for more information.

PCORR

displays pooled within-class correlations.

PCOV

displays pooled within-class covariances.

POOL=NO | TEST | YES

determines whether the pooled or within-group covariance matrix is the basis of the measure of the squared distance. If you specify POOL=YES, then PROC DISCRIM uses the pooled covariance matrix in calculating the (generalized) squared distances. Linear discriminant functions are computed. If you specify POOL=NO, the procedure uses the individual within-group covariance matrices in calculating the distances. Quadratic discriminant functions are computed. The default is POOL=YES.

The k -nearest-neighbor method assumes the default of POOL=YES, and the POOL=TEST option cannot be used with the METHOD=NPART option.

When you specify METHOD=NORMAL, the option POOL=TEST requests Bartlett's modification of the likelihood ratio test (Morrison 1976; Anderson 1984) of the homogeneity of the within-group covariance matrices. The test is unbiased (Perlman 1980). However, it is not robust to nonnormality. If the test statistic is significant at the level specified by the SLPOOL= option, the within-group covariance matrices are used. Otherwise, the pooled covariance matrix is used. The discriminant function coefficients are displayed only when the pooled covariance matrix is used.

POSTERR

displays the posterior probability error-rate estimates of the classification criterion based on the classification results.

PSSCP

displays the pooled within-class corrected SSCP matrix.

R= r

specifies a radius r value for kernel density estimation. With uniform, Epanechnikov, biweight, or triweight kernels, an observation \mathbf{x} is classified into a group based on the information from observations \mathbf{y} in the training set within the radius r of \mathbf{x} —that is, the group t observations \mathbf{y} with squared distance $d_t^2(\mathbf{x}, \mathbf{y}) \leq r^2$. When a normal kernel is used, the classification of an observation \mathbf{x} is based on the information of the estimated group-specific densities from all observations in the training set. The matrix $r^2 \mathbf{V}_t$ is used as the group t covariance matrix in the normal-kernel density, where \mathbf{V}_t is the matrix used in calculating the squared distances. Do not specify the K= or KPROP= option with the R= option. For more information about selecting r , see the section “Nonparametric Methods” on page 2079.

SCORES<= prefix >

computes and outputs discriminant scores to the OUT= and TESTOUT= data sets with the default options METHOD=NORMAL and POOL=YES (or with METHOD=NORMAL, POOL=TEST, and a nonsignificant chi-square test). Otherwise, or if no OUT= or TESTOUT= data set is specified, this option is ignored. The scores are computed by a matrix multiplication of an intercept term and the raw data or test data by the coefficients in the linear discriminant function. One score variable is created for each level of the CLASS variable. By default, the variables are named “Sc_” followed by the formatted class level. You can specify SCORES=prefix to use a prefix other than “Sc_”. The specifications SCORES and SCORES=Sc_ are equivalent.

SHORT

suppresses the display of certain items in the default output. If you specify METHOD=NORMAL, then PROC DISCRIM suppresses the display of determinants, generalized squared distances between-class means, and discriminant function coefficients. When you specify the CANONICAL option, PROC DISCRIM suppresses the display of canonical structures, canonical coefficients, and class means on canonical variables; only tables of canonical correlations are displayed.

SIMPLE

displays simple descriptive statistics for the total sample and within each class.

SINGULAR= p

specifies the criterion for determining the singularity of a matrix, where $0 < p < 1$. The default is `SINGULAR=1E-8`.

Let S be the total-sample correlation matrix. If the R square for predicting a quantitative variable in the VAR statement from the variables preceding it exceeds $1 - p$, then S is considered singular. If S is singular, the probability levels for the multivariate test statistics and canonical correlations are adjusted for the number of variables with R square exceeding $1 - p$.

Let S_t be the group t covariance matrix, and let S_p be the pooled covariance matrix. In group t , if the R square for predicting a quantitative variable in the VAR statement from the variables preceding it exceeds $1 - p$, then S_t is considered singular. Similarly, if the partial R square for predicting a quantitative variable in the VAR statement from the variables preceding it, after controlling for the effect of the CLASS variable, exceeds $1 - p$, then S_p is considered singular.

If PROC DISCRIM needs to compute either the inverse or the determinant of a matrix that is considered singular, then it uses a quasi inverse or a quasi determinant. For details, see the section “Quasi-inverse” on page 2083.

SLPOOL= p

specifies the significance level for the test of homogeneity. You can specify the SLPOOL= option only when POOL=TEST is also specified. If you specify POOL= TEST but omit the SLPOOL= option, PROC DISCRIM uses 0.10 as the significance level for the test.

STDMEAN

displays total-sample and pooled within-class standardized class means.

TCORR

displays total-sample correlations.

TCOV

displays total-sample covariances.

TESTDATA=*SAS-data-set*

names an ordinary SAS data set with observations that are to be classified. The quantitative variable names in this data set must match those in the DATA= data set. When you specify the TESTDATA= option, you can also specify the `TESTCLASS`, `TESTFREQ`, and `TESTID` statements. When you specify the TESTDATA= option, you can use the `TESTOUT=` and `TESTOUTD=` options to generate classification results and group-specific density estimates for observations in the test data set. Note that if the CLASS variable is not present in the TESTDATA= data set, the output will not include misclassification statistics.

TESTLIST

lists classification results for all observations in the TESTDATA= data set.

TESTLISTERR

lists only misclassified observations in the TESTDATA= data set but only if a `TESTCLASS` statement is also used.

TESTOUT=SAS-data-set

creates an output SAS data set containing all the data from the **TESTDATA=** data set, plus the posterior probabilities and the class into which each observation is classified. When you specify the **CANONICAL** option, the data set also contains new variables with canonical variable scores. See the section “**OUT= Data Set**” on page 2089 for more information.

TESTOUTD=SAS-data-set

creates an output SAS data set containing all the data from the **TESTDATA=** data set, plus the group-specific density estimates for each observation. See the section “**OUT= Data Set**” on page 2089 for more information.

THRESHOLD= ρ

specifies the minimum acceptable posterior probability for classification, where $0 \leq \rho \leq 1$. If the largest posterior probability of group membership is less than the **THRESHOLD** value, the observation is labeled as 'Other'. The default is **THRESHOLD=0**. In some cases, you might want to specify a **THRESHOLD=** value slightly smaller than the desired ρ so that observations with posterior probabilities within rounding error of ρ are classified. For example, you can specify **threshold=%sysevalf(0.5 - 1e-8)** instead of **THRESHOLD=0.5** so that observations with posterior probabilities within $1E-8$ of 0.5 and larger are classified.

TSSCP

displays the total-sample corrected SSCP matrix.

WCORR

displays within-class correlations for each class level.

WCOV

displays within-class covariances for each class level.

WSSCP

displays the within-class corrected SSCP matrix for each class level.

BY Statement

BY variables ;

You can specify a **BY** statement with **PROC DISCRIM** to obtain separate analyses of observations in groups that are defined by the **BY** variables. When a **BY** statement appears, the procedure expects the input data set to be sorted in order of the **BY** variables. If you specify more than one **BY** statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the **SORT** procedure with a similar **BY** statement.
- Specify the **NOTSORTED** or **DESCENDING** option in the **BY** statement for the **DISCRIM** procedure. The **NOTSORTED** option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the **BY** variables) and that these groups are not necessarily in alphabetical or increasing numeric order.

- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

If you specify the TESTDATA= option and the TESTDATA= data set does not contain any of the BY variables, then the entire TESTDATA= data set is classified according to the discriminant functions computed in each BY group in the DATA= data set.

If the TESTDATA= data set contains some but not all of the BY variables, or if some BY variables do not have the same type or length in the TESTDATA= data set as in the DATA= data set, then PROC DISCRIM displays an error message and stops.

If all BY variables appear in the TESTDATA= data set with the same type and length as in the DATA= data set, then each BY group in the TESTDATA= data set is classified by the discriminant function from the corresponding BY group in the DATA= data set. The BY groups in the TESTDATA= data set must be in the same order as in the DATA= data set. If you specify the NOTSORTED option in the BY statement, there must be exactly the same BY groups in the same order in both data sets. If you omit the NOTSORTED option, some BY groups can appear in one data set but not in the other. If some BY groups appear in the TESTDATA= data set but not in the DATA= data set, and you request an output test data set by using the TESTOUT= or TESTOUTD= option, these BY groups are not included in the output data set.

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

CLASS Statement

CLASS *variable* ;

The values of the classification variable define the groups for analysis. Class levels are determined by the formatted values of the CLASS variable. The specified variable can be numeric or character. A CLASS statement is required.

FREQ Statement

FREQ *variable* ;

If a variable in the data set represents the frequency of occurrence for the other values in the observation, include the variable's name in a FREQ statement. The procedure then treats the data set as if each observation appears n times, where n is the value of the FREQ variable for the observation. The total number of observations is considered to be equal to the sum of the FREQ variable when the procedure determines degrees of freedom for significance probabilities.

If the value of the FREQ variable is missing or is less than one, the observation is not used in the analysis. If the value is not an integer, it is truncated to an integer.

ID Statement

ID *variable* ;

The ID statement is effective only when you specify the LIST or LISTERR option in the PROC DISCRIM statement. When the DISCRIM procedure displays the classification results, the ID variable (rather than the observation number) is displayed for each observation.

PRIORS Statement

PRIORS EQUAL ;

PRIORS PROPORTIONAL | PROP ;

PRIORS *probabilities* ;

The PRIORS statement specifies the prior probabilities of group membership. To set the prior probabilities equal, use the following statement:

```
priors equal;
```

To set the prior probabilities proportional to the sample sizes, use the following statement:

```
priors proportional;
```

For other than equal or proportional priors, specify the prior probability for each level of the classification variable. Each class level can be written as either a SAS name or a quoted string, and it must be followed by an equal sign and a numeric constant between zero and one. A SAS name begins with a letter or an underscore and can contain digits as well. Lowercase character values and data values with leading blanks must be enclosed in quotes. For example, to define prior probabilities for each level of Grade, where Grade's values are A, B, C, and D, the PRIORS statement can be specified as follows:

```
priors A=0.1 B=0.3 C=0.5 D=0.1;
```

If Grade's values are 'a', 'b', 'c', and 'd', each class level must be written as a quoted string as follows:

```
priors 'a'=0.1 'b'=0.3 'c'=0.5 'd'=0.1;
```

If Grade is numeric, with formatted values of '1', '2', and '3', the PRIORS statement can be written as follows:

```
priors '1'=0.3 '2'=0.6 '3'=0.1;
```

The specified class levels must exactly match the formatted values of the CLASS variable. For example, if a CLASS variable C has the format 4.2 and a value 5, the PRIORS statement must specify '5.00', not '5.0' or '5'. If the prior probabilities do not sum to one, these probabilities are scaled proportionally to have the sum equal to one. The default is PRIORS EQUAL.

TESTCLASS Statement

TESTCLASS *variable* ;

The TESTCLASS statement names the variable in the TESTDATA= data set that is used to determine whether an observation in the TESTDATA= data set is misclassified. The TESTCLASS variable should have the same type (character or numeric) and length as the variable given in the CLASS statement. PROC

DISCRIM considers an observation misclassified when the formatted value of the TESTCLASS variable does not match the group into which the TESTDATA= observation is classified. When the TESTCLASS statement is missing and the TESTDATA= data set contains the variable given in the CLASS statement, the CLASS variable is used as the TESTCLASS variable. Note that if the CLASS variable is not present in the TESTDATA= data set, the output will not include misclassification statistics.

TESTFREQ Statement

TESTFREQ *variable* ;

If a variable in the TESTDATA= data set represents the frequency of occurrence of the other values in the observation, include the variable's name in a TESTFREQ statement. The procedure then treats the data set as if each observation appears n times, where n is the value of the TESTFREQ variable for the observation.

If the value of the TESTFREQ variable is missing or is less than one, the observation is not used in the analysis. If the value is not an integer, it is truncated to an integer.

TESTID Statement

TESTID *variable* ;

The TESTID statement is effective only when you specify the TESTLIST or TESTLISTERR option in the PROC DISCRIM statement. When the DISCRIM procedure displays the classification results for the TESTDATA= data set, the TESTID variable (rather than the observation number) is displayed for each observation. The variable given in the TESTID statement must be in the TESTDATA= data set.

VAR Statement

VAR *variables* ;

The VAR statement specifies the quantitative variables to be included in the analysis. The default is all numeric variables not listed in other statements.

WEIGHT Statement

WEIGHT *variable* ;

To use relative weights for each observation in the input data set, place the weights in a variable in the data set and specify the name in a WEIGHT statement. This is often done when the variance associated with each observation is different and the values of the weight variable are proportional to the reciprocals of the variances. If the value of the WEIGHT variable is missing or is less than zero, then a value of zero for the weight is used.

The WEIGHT and FREQ statements have a similar effect except that the WEIGHT statement does not alter the degrees of freedom.

Details: DISCRIM Procedure

Missing Values

Observations with missing values for variables in the analysis are excluded from the development of the classification criterion. When the values of the classification variable are missing, the observation is excluded from the development of the classification criterion, but if no other variables in the analysis have missing values for that observation, the observation is classified and displayed with the classification results.

Background

The following notation is used to describe the classification methods:

\mathbf{x}	a p -dimensional vector containing the quantitative variables of an observation
\mathbf{S}_p	the pooled covariance matrix
t	a subscript to distinguish the groups
n_t	the number of training set observations in group t
\mathbf{m}_t	the p -dimensional vector containing variable means in group t
\mathbf{S}_t	the covariance matrix within group t
$ \mathbf{S}_t $	the determinant of \mathbf{S}_t
q_t	the prior probability of membership in group t
$p(t \mathbf{x})$	the posterior probability of an observation \mathbf{x} belonging to group t
f_t	the probability density function for group t
$f_t(\mathbf{x})$	the group-specific density estimate at \mathbf{x} from group t
$f(\mathbf{x})$	$\sum_t q_t f_t(\mathbf{x})$, the estimated unconditional density at \mathbf{x}
e_t	the classification error rate for group t

Bayes' Theorem

Assuming that the prior probabilities of group membership are known and that the group-specific densities at \mathbf{x} can be estimated, PROC DISCRIM computes $p(t|\mathbf{x})$, the probability of \mathbf{x} belonging to group t , by applying Bayes' theorem:

$$p(t|\mathbf{x}) = \frac{q_t f_t(\mathbf{x})}{f(\mathbf{x})}$$

PROC DISCRIM partitions a p -dimensional vector space into regions R_t , where the region R_t is the subspace containing all p -dimensional vectors \mathbf{y} such that $p(t|\mathbf{y})$ is the largest among all groups. An observation is classified as coming from group t if it lies in region R_t .

Parametric Methods

Assuming that each group has a multivariate normal distribution, PROC DISCRIM develops a discriminant function or classification criterion by using a measure of generalized squared distance. The classification criterion is based on either the individual within-group covariance matrices or the pooled covariance matrix; it also takes into account the prior probabilities of the classes. Each observation is placed in the class from which it has the smallest generalized squared distance. PROC DISCRIM also computes the posterior probability of an observation belonging to each class.

The squared Mahalanobis distance from \mathbf{x} to group t is

$$d_t^2(\mathbf{x}) = (\mathbf{x} - \mathbf{m}_t)' \mathbf{V}_t^{-1} (\mathbf{x} - \mathbf{m}_t)$$

where $\mathbf{V}_t = \mathbf{S}_t$ if the within-group covariance matrices are used, or $\mathbf{V}_t = \mathbf{S}_p$ if the pooled covariance matrix is used.

The group-specific density estimate at \mathbf{x} from group t is then given by

$$f_t(\mathbf{x}) = (2\pi)^{-\frac{p}{2}} |\mathbf{V}_t|^{-\frac{1}{2}} \exp(-0.5d_t^2(\mathbf{x}))$$

Using Bayes' theorem, the posterior probability of \mathbf{x} belonging to group t is

$$p(t|\mathbf{x}) = \frac{q_t f_t(\mathbf{x})}{\sum_u q_u f_u(\mathbf{x})}$$

where the summation is over all groups.

The generalized squared distance from \mathbf{x} to group t is defined as

$$D_t^2(\mathbf{x}) = d_t^2(\mathbf{x}) + g_1(t) + g_2(t)$$

where

$$g_1(t) = \begin{cases} \ln |\mathbf{S}_t| & \text{if the within-group covariance matrices are used} \\ 0 & \text{if the pooled covariance matrix is used} \end{cases}$$

and

$$g_2(t) = \begin{cases} -2 \ln(q_t) & \text{if the prior probabilities are not all equal} \\ 0 & \text{if the prior probabilities are all equal} \end{cases}$$

The posterior probability of \mathbf{x} belonging to group t is then equal to

$$p(t|\mathbf{x}) = \frac{\exp(-0.5D_t^2(\mathbf{x}))}{\sum_u \exp(-0.5D_u^2(\mathbf{x}))}$$

The discriminant scores are $-0.5D_u^2(\mathbf{x})$. An observation is classified into group u if setting $t = u$ produces the largest value of $p(t|\mathbf{x})$ or the smallest value of $D_t^2(\mathbf{x})$. If this largest posterior probability is less than the threshold specified, \mathbf{x} is labeled as 'Other'.

Nonparametric Methods

Nonparametric discriminant methods are based on nonparametric estimates of group-specific probability densities. Either a kernel method or the k -nearest-neighbor method can be used to generate a nonparametric density estimate in each group and to produce a classification criterion. The kernel method uses uniform, normal, Epanechnikov, biweight, or triweight kernels in the density estimation.

Either Mahalanobis distance or Euclidean distance can be used to determine proximity. When the k -nearest-neighbor method is used, the Mahalanobis distances are based on the pooled covariance matrix. When a kernel method is used, the Mahalanobis distances are based on either the individual within-group covariance matrices or the pooled covariance matrix. Either the full covariance matrix or the diagonal matrix of variances can be used to calculate the Mahalanobis distances.

The squared distance between two observation vectors, \mathbf{x} and \mathbf{y} , in group t is given by

$$d_t^2(\mathbf{x}, \mathbf{y}) = (\mathbf{x} - \mathbf{y})' \mathbf{V}_t^{-1} (\mathbf{x} - \mathbf{y})$$

where \mathbf{V}_t has one of the following forms:

$$\mathbf{V}_t = \begin{cases} \mathbf{S}_p & \text{the pooled covariance matrix} \\ \text{diag}(\mathbf{S}_p) & \text{the diagonal matrix of the pooled covariance matrix} \\ \mathbf{S}_t & \text{the covariance matrix within group } t \\ \text{diag}(\mathbf{S}_t) & \text{the diagonal matrix of the covariance matrix within group } t \\ \mathbf{I} & \text{the identity matrix} \end{cases}$$

The classification of an observation vector \mathbf{x} is based on the estimated group-specific densities from the training set. From these estimated densities, the posterior probabilities of group membership at \mathbf{x} are evaluated. An observation \mathbf{x} is classified into group u if setting $t = u$ produces the largest value of $p(t|\mathbf{x})$. If there is a tie for the largest probability or if this largest probability is less than the threshold specified, \mathbf{x} is labeled as 'Other'.

The kernel method uses a fixed radius, r , and a specified kernel, K_t , to estimate the group t density at each observation vector \mathbf{x} . Let \mathbf{z} be a p -dimensional vector. Then the volume of a p -dimensional unit sphere bounded by $\mathbf{z}'\mathbf{z} = 1$ is

$$v_0 = \frac{\pi^{\frac{p}{2}}}{\Gamma(\frac{p}{2} + 1)}$$

where Γ represents the gamma function (see *SAS Functions and CALL Routines: Reference*).

Thus, in group t , the volume of a p -dimensional ellipsoid bounded by $\{\mathbf{z} \mid \mathbf{z}'\mathbf{V}_t^{-1}\mathbf{z} = r^2\}$ is

$$v_r(t) = r^p |\mathbf{V}_t|^{-\frac{1}{2}} v_0$$

The kernel method uses one of the following densities as the kernel density in group t :

Uniform Kernel

$$K_t(\mathbf{z}) = \begin{cases} \frac{1}{v_r(t)} & \text{if } \mathbf{z}'\mathbf{V}_t^{-1}\mathbf{z} \leq r^2 \\ 0 & \text{elsewhere} \end{cases}$$

Normal Kernel (with mean zero, variance $r^2\mathbf{V}_t$)

$$K_t(\mathbf{z}) = \frac{1}{c_0(t)} \exp\left(-\frac{1}{2r^2}\mathbf{z}'\mathbf{V}_t^{-1}\mathbf{z}\right)$$

where $c_0(t) = (2\pi)^{\frac{p}{2}} r^p |\mathbf{V}_t|^{-\frac{1}{2}}$.

Epanechnikov Kernel

$$K_t(\mathbf{z}) = \begin{cases} c_1(t) \left(1 - \frac{1}{r^2}\mathbf{z}'\mathbf{V}_t^{-1}\mathbf{z}\right) & \text{if } \mathbf{z}'\mathbf{V}_t^{-1}\mathbf{z} \leq r^2 \\ 0 & \text{elsewhere} \end{cases}$$

where $c_1(t) = \frac{1}{v_r(t)} \left(1 + \frac{p}{2}\right)$.

Biweight Kernel

$$K_t(\mathbf{z}) = \begin{cases} c_2(t) \left(1 - \frac{1}{r^2}\mathbf{z}'\mathbf{V}_t^{-1}\mathbf{z}\right)^2 & \text{if } \mathbf{z}'\mathbf{V}_t^{-1}\mathbf{z} \leq r^2 \\ 0 & \text{elsewhere} \end{cases}$$

where $c_2(t) = \left(1 + \frac{p}{4}\right) c_1(t)$.

Triweight Kernel

$$K_t(\mathbf{z}) = \begin{cases} c_3(t) \left(1 - \frac{1}{r^2}\mathbf{z}'\mathbf{V}_t^{-1}\mathbf{z}\right)^3 & \text{if } \mathbf{z}'\mathbf{V}_t^{-1}\mathbf{z} \leq r^2 \\ 0 & \text{elsewhere} \end{cases}$$

where $c_3(t) = \left(1 + \frac{p}{6}\right) c_2(t)$.

The group t density at \mathbf{x} is estimated by

$$f_t(\mathbf{x}) = \frac{1}{n_t} \sum_{\mathbf{y}} K_t(\mathbf{x} - \mathbf{y})$$

where the summation is over all observations \mathbf{y} in group t , and K_t is the specified kernel function. The posterior probability of membership in group t is then given by

$$p(t|\mathbf{x}) = \frac{q_t f_t(\mathbf{x})}{f(\mathbf{x})}$$

where $f(\mathbf{x}) = \sum_u q_u f_u(\mathbf{x})$ is the estimated unconditional density. If $f(\mathbf{x})$ is zero, the observation \mathbf{x} is labeled as 'Other'.

The uniform-kernel method treats $K_t(\mathbf{z})$ as a multivariate uniform function with density uniformly distributed over $\mathbf{z}'\mathbf{V}_t^{-1}\mathbf{z} \leq r^2$. Let k_t be the number of training set observations \mathbf{y} from group t within the closed ellipsoid centered at \mathbf{x} specified by $d_t^2(\mathbf{x}, \mathbf{y}) \leq r^2$. Then the group t density at \mathbf{x} is estimated by

$$f_t(\mathbf{x}) = \frac{k_t}{n_t v_r(t)}$$

When the identity matrix or the pooled within-group covariance matrix is used in calculating the squared distance, $v_r(t)$ is a constant, independent of group membership. The posterior probability of \mathbf{x} belonging to group t is then given by

$$p(t|\mathbf{x}) = \frac{\frac{q_t k_t}{n_t}}{\sum_u \frac{q_u k_u}{n_u}}$$

If the closed ellipsoid centered at \mathbf{x} does not include any training set observations, $f(\mathbf{x})$ is zero and \mathbf{x} is labeled as 'Other'. When the prior probabilities are equal, $p(t|\mathbf{x})$ is proportional to k_t/n_t and \mathbf{x} is classified into the group that has the highest proportion of observations in the closed ellipsoid. When the prior probabilities are proportional to the group sizes, $p(t|\mathbf{x}) = k_t / \sum_u k_u$, \mathbf{x} is classified into the group that has the largest number of observations in the closed ellipsoid.

The nearest-neighbor method fixes the number, k , of training set points for each observation \mathbf{x} . The method finds the radius $r_k(\mathbf{x})$ that is the distance from \mathbf{x} to the k th-nearest training set point in the metric \mathbf{V}_t^{-1} . Consider a closed ellipsoid centered at \mathbf{x} bounded by $\{\mathbf{z} \mid (\mathbf{z} - \mathbf{x})'\mathbf{V}_t^{-1}(\mathbf{z} - \mathbf{x}) = r_k^2(\mathbf{x})\}$; the nearest-neighbor method is equivalent to the uniform-kernel method with a location-dependent radius $r_k(\mathbf{x})$. Note that, with ties, more than k training set points might be in the ellipsoid.

Using the k -nearest-neighbor rule, the k_n (or more with ties) smallest distances are saved. Of these k distances, let k_t represent the number of distances that are associated with group t . Then, as in the uniform-kernel method, the estimated group t density at \mathbf{x} is

$$f_t(\mathbf{x}) = \frac{k_t}{n_t v_k(\mathbf{x})}$$

where $v_k(\mathbf{x})$ is the volume of the ellipsoid bounded by $\{\mathbf{z} \mid (\mathbf{z} - \mathbf{x})'\mathbf{V}_t^{-1}(\mathbf{z} - \mathbf{x}) = r_k^2(\mathbf{x})\}$. Since the pooled within-group covariance matrix is used to calculate the distances used in the nearest-neighbor method, the volume $v_k(\mathbf{x})$ is a constant independent of group membership. When $k = 1$ is used in the nearest-neighbor rule, \mathbf{x} is classified into the group associated with the \mathbf{y} point that yields the smallest squared distance $d_t^2(\mathbf{x}, \mathbf{y})$. Prior probabilities affect nearest-neighbor results in the same way that they affect uniform-kernel results.

With a specified squared distance formula (METRIC=, POOL=), the values of r and k determine the degree of irregularity in the estimate of the density function, and they are called smoothing parameters. Small values of r or k produce jagged density estimates, and large values of r or k produce smoother density estimates. Various methods for choosing the smoothing parameters have been suggested, and there is as yet no simple solution to this problem.

For a fixed kernel shape, one way to choose the smoothing parameter r is to plot estimated densities with different values of r and to choose the estimate that is most in accordance with the prior information about the density. For many applications, this approach is satisfactory.

Another way of selecting the smoothing parameter r is to choose a value that optimizes a given criterion. Different groups might have different sets of optimal values. Assume that the unknown density has bounded

and continuous second derivatives and that the kernel is a symmetric probability density function. One criterion is to minimize an approximate mean integrated square error of the estimated density (Rosenblatt 1956). The resulting optimal value of r depends on the density function and the kernel. A reasonable choice for the smoothing parameter r is to optimize the criterion with the assumption that group t has a normal distribution with covariance matrix \mathbf{V}_t . Then, in group t , the resulting optimal value for r is given by

$$\left(\frac{A(K_t)}{n_t} \right)^{1/(p+4)}$$

where the optimal constant $A(K_t)$ depends on the kernel K_t (Epanechnikov 1969). For some useful kernels, the constants $A(K_t)$ are given by the following:

$$A(K_t) = \frac{1}{p} 2^{p+1} (p+2) \Gamma\left(\frac{p}{2}\right) \quad \text{with a uniform kernel}$$

$$A(K_t) = \frac{4}{2p+1} \quad \text{with a normal kernel}$$

$$A(K_t) = \frac{2^{p+2} p^2 (p+2)(p+4)}{2p+1} \Gamma\left(\frac{p}{2}\right) \quad \text{with an Epanechnikov kernel}$$

These selections of $A(K_t)$ are derived under the assumption that the data in each group are from a multivariate normal distribution with covariance matrix \mathbf{V}_t . However, when the Euclidean distances are used in calculating the squared distance ($\mathbf{V}_t = \mathbf{I}$), the smoothing constant should be multiplied by s , where s is an estimate of standard deviations for all variables. A reasonable choice for s is

$$s = \left(\frac{1}{p} \sum s_{jj} \right)^{\frac{1}{2}}$$

where s_{jj} are group t marginal variances.

The DISCRIM procedure uses only a single smoothing parameter for all groups. However, the selection of the matrix in the distance formula (from the METRIC= or POOL= option), enables individual groups and variables to have different scalings. When \mathbf{V}_t , the matrix used in calculating the squared distances, is an identity matrix, the kernel estimate at each data point is scaled equally for all variables in all groups. When \mathbf{V}_t is the diagonal matrix of a covariance matrix, each variable in group t is scaled separately by its variance in the kernel estimation, where the variance can be the pooled variance ($\mathbf{V}_t = \mathbf{S}_p$) or an individual within-group variance ($\mathbf{V}_t = \mathbf{S}_t$). When \mathbf{V}_t is a full covariance matrix, the variables in group t are scaled simultaneously by \mathbf{V}_t in the kernel estimation.

In nearest-neighbor methods, the choice of k is usually relatively uncritical (Hand 1982). A practical approach is to try several different values of the smoothing parameters within the context of the particular application and to choose the one that gives the best cross validated estimate of the error rate.

Classification Error-Rate Estimates

A classification criterion can be evaluated by its performance in the classification of future observations. PROC DISCRIM uses two types of error-rate estimates to evaluate the derived classification criterion based on parameters estimated by the training sample:

- error-count estimates
- posterior probability error-rate estimates

The error-count estimate is calculated by applying the classification criterion derived from the training sample to a test set and then counting the number of misclassified observations. The group-specific error-count estimate is the proportion of misclassified observations in the group. When the test set is independent of the training sample, the estimate is unbiased. However, the estimate can have a large variance, especially if the test set is small.

When the input data set is an ordinary SAS data set and no independent test sets are available, the same data set can be used both to define and to evaluate the classification criterion. The resulting error-count estimate has an optimistic bias and is called an *apparent error rate*. To reduce the bias, you can split the data into two sets—one set for deriving the discriminant function and the other set for estimating the error rate. Such a split-sample method has the unfortunate effect of reducing the effective sample size.

Another way to reduce bias is cross validation (Lachenbruch and Mickey 1968). Cross validation treats $n - 1$ out of n training observations as a training set. It determines the discriminant functions based on these $n - 1$ observations and then applies them to classify the one observation left out. This is done for each of the n training observations. The misclassification rate for each group is the proportion of sample observations in that group that are misclassified. This method achieves a nearly unbiased estimate but with a relatively large variance.

To reduce the variance in an error-count estimate, smoothed error-rate estimates are suggested (Glick 1978). Instead of summing terms that are either zero or one as in the error-count estimator, the smoothed estimator uses a continuum of values between zero and one in the terms that are summed. The resulting estimator has a smaller variance than the error-count estimate. The posterior probability error-rate estimates provided by the POSTERR option in the PROC DISCRIM statement (see the section “[Posterior Probability Error-Rate Estimates](#)” on page 2085) are smoothed error-rate estimates. The posterior probability estimates for each group are based on the posterior probabilities of the observations classified into that same group. The posterior probability estimates provide good estimates of the error rate when the posterior probabilities are accurate. When a parametric classification criterion (linear or quadratic discriminant function) is derived from a nonnormal population, the resulting posterior probability error-rate estimators might not be appropriate.

The overall error rate is estimated through a weighted average of the individual group-specific error-rate estimates, where the prior probabilities are used as the weights.

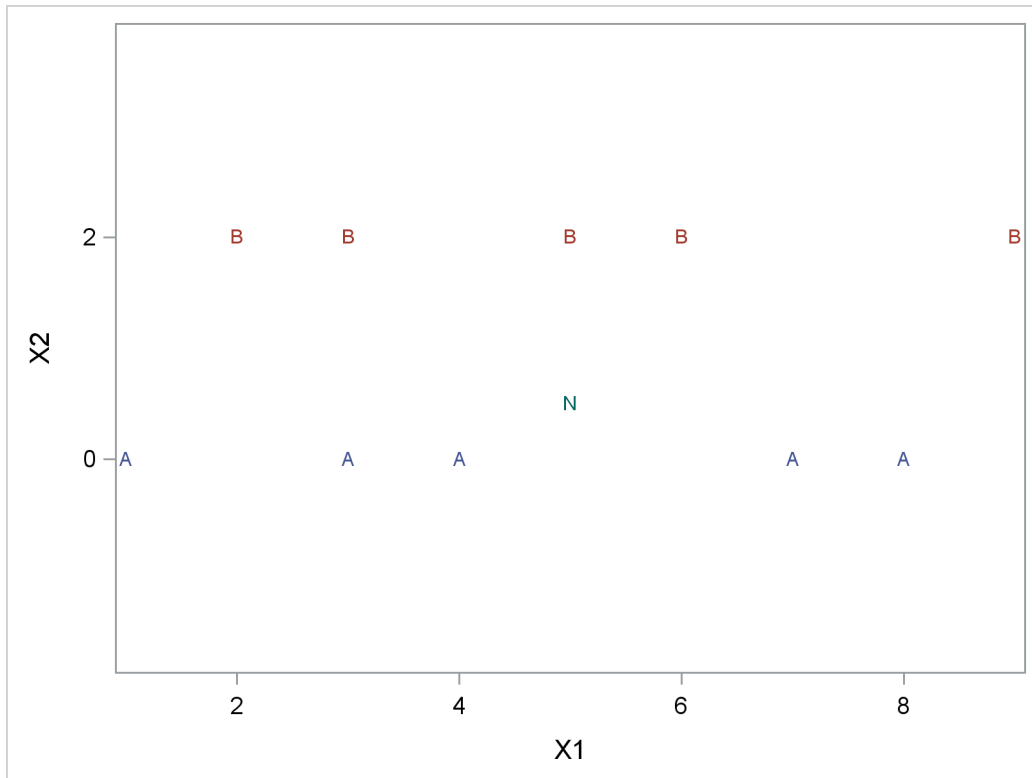
To reduce both the bias and the variance of the estimator, Hora and Wilcox (1982) compute the posterior probability estimates based on cross validation. The resulting estimates are intended to have both low variance from using the posterior probability estimate and low bias from cross validation. They use Monte Carlo studies on two-group multivariate normal distributions to compare the cross validation posterior probability estimates with three other estimators: the apparent error rate, cross validation estimator, and posterior probability estimator. They conclude that the cross validation posterior probability estimator has a lower mean squared error in their simulations.

Quasi-inverse

Consider the plot shown in [Figure 33.6](#) with two variables, X1 and X2, and two classes, A and B. The within-class covariance matrix is diagonal, with a positive value for X1 but zero for X2. Using a Moore-Penrose pseudo-inverse would effectively ignore X2 in doing the classification, and the two classes would have a

zero generalized distance and could not be discriminated at all. The quasi inverse used by PROC DISCRIM replaces the zero variance for X2 with a small positive number to remove the singularity. This permits X2 to be used in the discrimination and results correctly in a large generalized distance between the two classes and a zero error rate. It also permits new observations, such as the one indicated by N, to be classified in a reasonable way. PROC CANDISC also uses a quasi inverse when the total-sample covariance matrix is considered to be singular and Mahalanobis distances are requested. This problem with singular within-class covariance matrices is discussed in Ripley (1996, p. 38). The use of the quasi inverse is an innovation introduced by SAS.

Figure 33.6 Plot of Data with Singular Within-Class Covariance Matrix



Let \mathbf{S} be a singular covariance matrix. The matrix \mathbf{S} can be either a within-group covariance matrix, a pooled covariance matrix, or a total-sample covariance matrix. Let v be the number of variables in the VAR statement, and let the nullity n be the number of variables among them with (partial) R square exceeding $1 - p$. If the determinant of \mathbf{S} (Testing of Homogeneity of Within Covariance Matrices) or the inverse of \mathbf{S} (Squared Distances and Generalized Squared Distances) is required, a quasi determinant or quasi inverse is used instead. With raw data input, PROC DISCRIM scales each variable to unit total-sample variance before calculating this quasi inverse. The calculation is based on the spectral decomposition $\mathbf{S} = \mathbf{\Gamma}\mathbf{\Lambda}\mathbf{\Gamma}'$, where $\mathbf{\Lambda}$ is a diagonal matrix of eigenvalues λ_j , $j = 1, \dots, v$, where $\lambda_i \geq \lambda_j$ when $i < j$, and $\mathbf{\Gamma}$ is a matrix with the corresponding orthonormal eigenvectors of \mathbf{S} as columns. When the nullity n is less than v , set $\lambda_j^0 = \lambda_j$ for $j = 1, \dots, v - n$, and $\lambda_j^0 = p\bar{\lambda}$ for $j = v - n + 1, \dots, v$, where

$$\bar{\lambda} = \frac{1}{v - n} \sum_{k=1}^{v-n} \lambda_k$$

When the nullity n is equal to v , set $\lambda_j^0 = p$, for $j = 1, \dots, v$. A quasi determinant is then defined as the product of λ_j^0 , $j = 1, \dots, v$. Similarly, a quasi inverse is then defined as $S^* = \Gamma \Lambda^* \Gamma'$, where Λ^* is a diagonal matrix of values $1/\lambda_j^0$, $j = 1, \dots, v$.

Posterior Probability Error-Rate Estimates

The posterior probability error-rate estimates (Fukunaga and Kessel 1973; Glick 1978; Hora and Wilcox 1982) for each group are based on the posterior probabilities of the observations classified into that same group.

A sample of observations with classification results can be used to estimate the posterior error rates. The following notation is used to describe the sample:

- \mathcal{S} the set of observations in the (training) sample
- n the number of observations in \mathcal{S}
- n_t the number of observations in \mathcal{S} in group t
- \mathcal{R}_t the set of observations such that the posterior probability belonging to group t is the largest
- \mathcal{R}_{ut} the set of observations from group u such that the posterior probability belonging to group t is the largest

The classification error rate for group t is defined as

$$e_t = 1 - \int_{\mathcal{R}_t} f_t(\mathbf{x}) d\mathbf{x}$$

The posterior probability of \mathbf{x} for group t can be written as

$$p(t|\mathbf{x}) = \frac{q_t f_t(\mathbf{x})}{f(\mathbf{x})}$$

where $f(\mathbf{x}) = \sum_u q_u f_u(\mathbf{x})$ is the unconditional density of \mathbf{x} .

Thus, if you replace $f_t(\mathbf{x})$ with $p(t|\mathbf{x})f(\mathbf{x})/q_t$, the error rate is

$$e_t = 1 - \frac{1}{q_t} \int_{\mathcal{R}_t} p(t|\mathbf{x})f(\mathbf{x})d\mathbf{x}$$

An estimator of e_t , unstratified over the groups from which the observations come, is then given by

$$\hat{e}_t \text{ (unstratified)} = 1 - \frac{1}{nq_t} \sum_{\mathcal{R}_t} p(t|\mathbf{x})$$

where $p(t|\mathbf{x})$ is estimated from the classification criterion, and the summation is over all sample observations of \mathcal{S} classified into group t . The true group membership of each observation is not required in the estimation. The term nq_t is the number of observations that are expected to be classified into group t , given the priors. If more observations than expected are classified into group t , then \hat{e}_t can be negative.

Further, if you replace $f(\mathbf{x})$ with $\sum_u q_u f_u(\mathbf{x})$, the error rate can be written as

$$e_t = 1 - \frac{1}{q_t} \sum_u q_u \int_{\mathcal{R}_{ut}} p(t|\mathbf{x})f_u(\mathbf{x})d\mathbf{x}$$

and an estimator stratified over the group from which the observations come is given by

$$\hat{e}_t \text{ (stratified)} = 1 - \frac{1}{q_t} \sum_u q_u \frac{1}{n_u} \left(\sum_{\mathcal{R}_{ut}} p(t|\mathbf{x}) \right)$$

The inner summation is over all sample observations of \mathcal{S} coming from group u and classified into group t , and n_u is the number of observations originally from group u . The stratified estimate uses only the observations with known group membership. When the prior probabilities of the group membership are proportional to the group sizes, the stratified estimate is the same as the unstratified estimator.

The estimated group-specific error rates can be less than zero, usually due to a large discrepancy between prior probabilities of group membership and group sizes. To have a reliable estimate for group-specific error rate estimates, you should use group sizes that are at least approximately proportional to the prior probabilities of group membership.

A total error rate is defined as a weighted average of the individual group error rates

$$e = \sum_t q_t e_t$$

and can be estimated from

$$\hat{e} \text{ (unstratified)} = \sum_t q_t \hat{e}_t \text{ (unstratified)}$$

or

$$\hat{e} \text{ (stratified)} = \sum_t q_t \hat{e}_t \text{ (stratified)}$$

The total unstratified error-rate estimate can also be written as

$$\hat{e} \text{ (unstratified)} = 1 - \frac{1}{n} \sum_t \sum_{\mathcal{R}_t} p(t|\mathbf{x})$$

which is one minus the average value of the maximum posterior probabilities for each observation in the sample. The prior probabilities of group membership do not appear explicitly in this overall estimate.

Saving and Using Calibration Information

When you specify METHOD=NORMAL to derive a linear or quadratic discriminant function, you can save the calibration information developed by the DISCRIM procedure in a SAS data set by using the OUTSTAT= option in the procedure. PROC DISCRIM then creates a specially structured SAS data set of TYPE=LINEAR, TYPE=QUAD, or TYPE=MIXED that contains the calibration information. For more information about these data sets, see Appendix A, “[Special SAS Data Sets](#).” Calibration information cannot be saved when METHOD=NPART, but you can classify a TESTDATA= data set in the same step. For an example of this, see [Example 33.1](#).

To use this calibration information to classify observations in another data set, specify both of the following:

- the name of the calibration data set after the DATA= option in the PROC DISCRIM statement

- the name of the data set to be classified after the TESTDATA= option in the PROC DISCRIM statement

Here is an example:

```
data original;
    input position x1 x2;
    datalines;
...[data lines]
;

proc discrim outstat=info;
    class position;
run;

data check;
    input position x1 x2;
    datalines;
...[second set of data lines]
;

proc discrim data=info testdata=check testlist;
    class position;
run;
```

The first DATA step creates the SAS data set Original, which the DISCRIM procedure uses to develop a classification criterion. Specifying OUTSTAT=INFO in the PROC DISCRIM statement causes the DISCRIM procedure to store the calibration information in a new data set called Info. The next DATA step creates the data set Check. The second PROC DISCRIM statement specifies DATA=INFO and TESTDATA=CHECK so that the classification criterion developed earlier is applied to the Check data set. Note that if the CLASS variable is not present in the TESTDATA= data set, the output will not include misclassification statistics.

Input Data Sets

DATA= Data Set

When you specify METHOD=NPAR, an ordinary SAS data set is required as the input DATA= data set. When you specify METHOD=NORMAL, the DATA= data set can be an ordinary SAS data set or one of several specially structured data sets created by SAS/STAT procedures. These specially structured data sets include the following:

- TYPE=CORR data sets created by PROC CORR by using a BY statement
- TYPE=COV data sets created by PROC PRINCOMP by using both the COV option and a BY statement
- TYPE=CSSCP data sets created by PROC CORR by using the CSSCP option and a BY statement, where the OUT= data set is assigned TYPE=CSSCP with the TYPE= data set option
- TYPE=SSCP data sets created by PROC REG by using both the OUTSSCP= option and a BY statement

- TYPE=LINEAR, TYPE=QUAD, and TYPE=MIXED data sets produced by previous runs of PROC DISCRIM that used both METHOD=NORMAL and OUTSTAT= options

When the input data set is TYPE=CORR, TYPE=COV, TYPE=CSSCP, or TYPE=SSCP, the BY variable in these data sets becomes the CLASS variable in the DISCRIM procedure.

When the input data set is TYPE=CORR, TYPE=COV, or TYPE=CSSCP, then PROC DISCRIM reads the number of observations for each class from the observations with `_TYPE_='N'` and reads the variable means in each class from the observations with `_TYPE_='MEAN'`. Then PROC DISCRIM reads the within-class correlations from the observations with `_TYPE_='CORR'` and reads the standard deviations from the observations with `_TYPE_='STD'` (data set TYPE=CORR), the within-class covariances from the observations with `_TYPE_='COV'` (data set TYPE=COV), or the within-class corrected sums of squares and crossproducts from the observations with `_TYPE_='CSSCP'` (data set TYPE=CSSCP).

When you specify POOL=YES and the data set does not include any observations with `_TYPE_='CSSCP'` (data set TYPE=CSSCP), `_TYPE_='COV'` (data set TYPE=COV), or `_TYPE_='CORR'` (data set TYPE=CORR) for each class, PROC DISCRIM reads the pooled within-class information from the data set. In this case, PROC DISCRIM reads the pooled within-class covariances from the observations with `_TYPE_='PCOV'` (data set TYPE=COV) or reads the pooled within-class correlations from the observations with `_TYPE_='PCORR'` and the pooled within-class standard deviations from the observations with `_TYPE_='PSTD'` (data set TYPE=CORR) or the pooled within-class corrected SSCP matrix from the observations with `_TYPE_='PSSCP'` (data set TYPE=CSSCP).

When the input data set is TYPE=SSCP, the DISCRIM procedure reads the number of observations for each class from the observations with `_TYPE_='N'`, the sum of weights of observations for each class from the variable INTERCEP in observations with `_TYPE_='SSCP'` and `_NAME_='INTERCEPT'`, the variable sums from the analysis variables in observations with `_TYPE_='SSCP'` and `_NAME_='INTERCEPT'`, and the uncorrected sums of squares and crossproducts from the analysis variables in observations with `_TYPE_='SSCP'` and `_NAME_='variablenames'`.

When the input data set is TYPE=LINEAR, TYPE=QUAD, or TYPE=MIXED, then PROC DISCRIM reads the prior probabilities for each class from the observations with variable `_TYPE_='PRIOR'`.

When the input data set is TYPE=LINEAR, then PROC DISCRIM reads the coefficients of the linear discriminant functions from the observations with variable `_TYPE_='LINEAR'`.

When the input data set is TYPE=QUAD, then PROC DISCRIM reads the coefficients of the quadratic discriminant functions from the observations with variable `_TYPE_='QUAD'`.

When the input data set is TYPE=MIXED, then PROC DISCRIM reads the coefficients of the linear discriminant functions from the observations with variable `_TYPE_='LINEAR'`. If there are no observations with `_TYPE_='LINEAR'`, then PROC DISCRIM reads the coefficients of the quadratic discriminant functions from the observations with variable `_TYPE_='QUAD'`.

TESTDATA= Data Set

The TESTDATA= data set is an ordinary SAS data set with observations that are to be classified. The quantitative variable names in this data set must match those in the DATA= data set. The TESTCLASS statement can be used to specify the variable containing group membership information of the TESTDATA= data set observations. When the TESTCLASS statement is missing and the TESTDATA= data set contains the variable given in the CLASS statement, this variable is used as the TESTCLASS variable. The TESTCLASS

variable should have the same type (character or numeric) and length as the variable given in the CLASS statement. PROC DISCRIM considers an observation misclassified when the value of the TESTCLASS variable does not match the group into which the TESTDATA= observation is classified.

Output Data Sets

When an output data set includes variables containing the posterior probabilities of group membership (OUT=, OUTCROSS=, or TESTOUT= data sets) or group-specific density estimates (OUTD= or TESTOUTD= data sets), the names of these variables are constructed from the formatted values of the class levels converted to valid SAS variable names.

OUT= Data Set

The OUT= data set contains all the variables in the DATA= data set, plus new variables containing the posterior probabilities and the resubstitution classification results. The names of the new variables containing the posterior probabilities are constructed from the formatted values of the class levels converted to SAS names. A new variable, `_INTO_`, with the same attributes as the CLASS variable, specifies the class to which each observation is assigned. If an observation is labeled as 'Other', the variable `_INTO_` has a missing value. When you specify the CANONICAL option, the data set also contains new variables with canonical variable scores. The NCAN= option determines the number of canonical variables. The names of the canonical variables are constructed as described in the CANPREFIX= option. The canonical variables have means equal to zero and pooled within-class variances equal to one.

An OUT= data set cannot be created if the DATA= data set is not an ordinary SAS data set.

OUTD= Data Set

The OUTD= data set contains all the variables in the DATA= data set, plus new variables containing the group-specific density estimates. The names of the new variables containing the density estimates are constructed from the formatted values of the class levels.

An OUTD= data set cannot be created if the DATA= data set is not an ordinary SAS data set.

OUTCROSS= Data Set

The OUTCROSS= data set contains all the variables in the DATA= data set, plus new variables containing the posterior probabilities and the classification results of cross validation. The names of the new variables containing the posterior probabilities are constructed from the formatted values of the class levels. A new variable, `_INTO_`, with the same attributes as the CLASS variable, specifies the class to which each observation is assigned. When an observation is labeled as 'Other', the variable `_INTO_` has a missing value. When you specify the CANONICAL option, the data set also contains new variables with canonical variable scores. The NCAN= option determines the number of new variables. The names of the new variables are constructed as described in the CANPREFIX= option. The new variables have mean zero and pooled within-class variance equal to one.

An OUTCROSS= data set cannot be created if the DATA= data set is not an ordinary SAS data set.

TESTOUT= Data Set

The TESTOUT= data set contains all the variables in the TESTDATA= data set, plus new variables containing the posterior probabilities and the classification results. The names of the new variables containing the posterior probabilities are formed from the formatted values of the class levels. A new variable, `_INTO_`, with the same attributes as the CLASS variable, gives the class to which each observation is assigned. If an observation is labeled as 'Other', the variable `_INTO_` has a missing value. When you specify the CANONICAL option, the data set also contains new variables with canonical variable scores. The NCAN= option determines the number of new variables. The names of the new variables are formed as described in the CANPREFIX= option.

TESTOUTD= Data Set

The TESTOUTD= data set contains all the variables in the TESTDATA= data set, plus new variables containing the group-specific density estimates. The names of the new variables containing the density estimates are formed from the formatted values of the class levels.

OUTSTAT= Data Set

The OUTSTAT= data set is similar to the TYPE=CORR data set produced by the CORR procedure. The data set contains various statistics such as means, standard deviations, and correlations. For an example of an OUTSTAT= data set, see [Example 33.3](#). When you specify the CANONICAL option, canonical correlations, canonical structures, canonical coefficients, and means of canonical variables for each class are included in the data set.

If you specify METHOD=NORMAL, the output data set also includes coefficients of the discriminant functions, and the data set is TYPE=LINEAR (POOL=YES), TYPE=QUAD (POOL=NO), or TYPE=MIXED (POOL=TEST). If you specify METHOD=NPART, this output data set is TYPE=CORR.

The OUTSTAT= data set contains the following variables:

- the BY variables, if any
- the CLASS variable
- `_TYPE_`, a character variable of length 8 that identifies the type of statistic
- `_NAME_`, a character variable of length 32 that identifies the row of the matrix, the name of the canonical variable, or the type of the discriminant function coefficients
- the quantitative variables—that is, those in the VAR statement, or, if there is no VAR statement, all numeric variables not listed in any other statement

The observations, as identified by the variable `_TYPE_`, have the following values:

<code>_TYPE_</code>	Contents
N	number of observations both for the total sample (CLASS variable missing) and within each class (CLASS variable present)
SUMWGT	sum of weights both for the total sample (CLASS variable missing) and within each class (CLASS variable present), if a WEIGHT statement is specified
MEAN	means both for the total sample (CLASS variable missing) and within each class (CLASS variable present)
PRIOR	prior probability for each class
STDMEAN	total-standardized class means
PSTDMEAN	pooled within-class standardized class means
STD	standard deviations both for the total sample (CLASS variable missing) and within each class (CLASS variable present)
PSTD	pooled within-class standard deviations
BSTD	between-class standard deviations
RSQUARED	univariate R squares
LNDETERM	the natural log of the determinant or the natural log of the quasi determinant of the within-class covariance matrix either pooled (CLASS variable missing) or not pooled (CLASS variable present)

The following kinds of observations are identified by the combination of the variables `_TYPE_` and `_NAME_`. When the `_TYPE_` variable has one of the following values, the `_NAME_` variable identifies the row of the matrix:

<code>_TYPE_</code>	Contents
CSSCP	corrected SSCP matrix both for the total sample (CLASS variable missing) and within each class (CLASS variable present)
PSSCP	pooled within-class corrected SSCP matrix
BSSCP	between-class SSCP matrix
COV	covariance matrix both for the total sample (CLASS variable missing) and within each class (CLASS variable present)
PCOV	pooled within-class covariance matrix
BCOV	between-class covariance matrix
CORR	correlation matrix both for the total sample (CLASS variable missing) and within each class (CLASS variable present)
PCORR	pooled within-class correlation matrix
BCORR	between-class correlation matrix

When you request canonical discriminant analysis, the `_NAME_` variable identifies a canonical variable, and `_TYPE_` variable can have one of the following values:

<code>_TYPE_</code>	Contents
CANCORR	canonical correlations
STRUCTUR	canonical structure
BSTRUCT	between canonical structure
PSTRUCT	pooled within-class canonical structure
SCORE	standardized canonical coefficients
RAWSCORE	raw canonical coefficients
CANMEAN	means of the canonical variables for each class

When you specify `METHOD=NORMAL`, the `_NAME_` variable identifies different types of coefficients in the discriminant function, and the `_TYPE_` variable can have one of the following values:

<code>_TYPE_</code>	Contents
LINEAR	coefficients of the linear discriminant functions
QUAD	coefficients of the quadratic discriminant functions

The values of the `_NAME_` variable are as follows:

<code>_NAME_</code>	Contents
<i>variable names</i>	quadratic coefficients of the quadratic discriminant functions (a symmetric matrix for each class)
<code>_LINEAR_</code>	linear coefficients of the discriminant functions
<code>_CONST_</code>	constant coefficients of the discriminant functions

Computational Resources

In the following discussion, let

- n = number of observations in the training data set
- v = number of variables
- c = number of class levels
- k = number of canonical variables
- l = length of the CLASS variable

Memory Requirements

The amount of temporary storage required depends on the discriminant method used and the options specified. The least amount of temporary storage in bytes needed to process the data is approximately

$$c(32v + 3l + 128) + 8v^2 + 104v + 4l$$

A parametric method (METHOD=NORMAL) requires an additional temporary memory of $12v^2 + 100v$ bytes. When you specify the CROSSVALIDATE option, this temporary storage must be increased by $4v^2 + 44v$ bytes. When a nonparametric method (METHOD=NPARG) is used, an additional temporary storage of $10v^2 + 94v$ bytes is needed if you specify METRIC=FULL to evaluate the distances.

With the MANOVA option, the temporary storage must be increased by $8v^2 + 96v$ bytes. The CANONICAL option requires a temporary storage of $2v^2 + 94v + 8k(v + c)$ bytes. The POSTERR option requires a temporary storage of $8c^2 + 64c + 96$ bytes. Additional temporary storage is also required for classification summary and for each output data set.

Consider the following statements:

```
proc discrim manova;
  class gp;
  var x1 x2 x3;
run;
```

If the CLASS variable gp has a length of 8 and the input data set contains two class levels, the procedure requires a temporary storage of 1992 bytes. This includes 1104 bytes for processing data, 480 bytes for using a parametric method, and 408 bytes for specifying the MANOVA option.

Time Requirements

The following factors determine the time requirements of discriminant analysis:

- The time needed for reading the data and computing covariance matrices is proportional to nv^2 . PROC DISCRIM must also look up each class level in the list. This is faster if the data are sorted by the CLASS variable. The time for looking up class levels is proportional to a value ranging from n to $n \ln(c)$.
- The time for inverting a covariance matrix is proportional to v^3 .
- With a parametric method, the time required to classify each observation is proportional to cv for a linear discriminant function and cv^2 for a quadratic discriminant function. When you specify the CROSSVALIDATE option, the discriminant function is updated for each observation in the classification. A substantial amount of time is required.
- With a nonparametric method, the data are stored in a tree structure (Friedman, Bentley, and Finkel 1977). The time required to organize the observations into the tree structure is proportional to $nv \ln(n)$. The time for performing each tree search is proportional to $\ln(n)$. When you specify the normal KERNEL= option, all observations in the training sample contribute to the density estimation and more computer time is needed.
- The time required for the canonical discriminant analysis is proportional to v^3 .

Each of the preceding factors has a different machine-dependent constant of proportionality.

Displayed Output

The displayed output from PROC DISCRIM includes the class level information table. For each level of the classification variable, the following information is provided: the output data set variable name, frequency sum, weight sum, proportion of the total sample, and prior probability.

The optional output from PROC DISCRIM includes the following:

- Within-class SSCP matrices for each group
- Pooled within-class SSCP matrix
- Between-class SSCP matrix
- Total-sample SSCP matrix
- Within-class covariance matrices, S_t , for each group
- Pooled within-class covariance matrix, S_p
- Between-class covariance matrix, equal to the between-class SSCP matrix divided by $n(c - 1)/c$, where n is the number of observations and c is the number of classes
- Total-sample covariance matrix
- Within-class correlation coefficients and $\text{Pr} > |r|$ to test the hypothesis that the within-class population correlation coefficients are zero
- Pooled within-class correlation coefficients and $\text{Pr} > |r|$ to test the hypothesis that the partial population correlation coefficients are zero
- Between-class correlation coefficients and $\text{Pr} > |r|$ to test the hypothesis that the between-class population correlation coefficients are zero
- Total-sample correlation coefficients and $\text{Pr} > |r|$ to test the hypothesis that the total population correlation coefficients are zero
- Simple statistics, including N (the number of observations), sum, mean, variance, and standard deviation both for the total sample and within each class
- Total-sample standardized class means, obtained by subtracting the grand mean from each class mean and dividing by the total-sample standard deviation
- Pooled within-class standardized class means, obtained by subtracting the grand mean from each class mean and dividing by the pooled within-class standard deviation
- Pairwise squared distances between groups
- Univariate test statistics, including total-sample standard deviations, pooled within-class standard deviations, between-class standard deviations, R square, $R^2/(1 - R^2)$, F , and $\text{Pr} > F$ (univariate F values and probability levels for one-way analyses of variance)

- Multivariate statistics and F approximations, including Wilks' lambda, Pillai's trace, Hotelling-Lawley trace, and Roy's greatest root with F approximations, numerator and denominator degrees of freedom (Num DF and Den DF), and probability values ($\text{Pr} > F$). Each of these four multivariate statistics tests the hypothesis that the class means are equal in the population. See the section "Multivariate Tests" on page 92 in Chapter 4, "Introduction to Regression Procedures," for more information.

If you specify METHOD=NORMAL, the following three statistics are displayed:

- Covariance matrix information, including covariance matrix rank and natural log of determinant of the covariance matrix for each group (POOL=TEST, POOL=NO) and for the pooled within-group (POOL=TEST, POOL=YES)
- Optionally, test of homogeneity of within covariance matrices (the results of a chi-square test of homogeneity of the within-group covariance matrices) (Morrison 1976; Kendall, Stuart, and Ord 1983; Anderson 1984)
- Pairwise generalized squared distances between groups

If the CANONICAL option is specified, the displayed output contains these statistics:

- Canonical correlations
- Adjusted canonical correlations (Lawley 1959). These are asymptotically less biased than the raw correlations and can be negative. The adjusted canonical correlations might not be computable and are displayed as missing values if two canonical correlations are nearly equal or if some are close to zero. A missing value is also displayed if an adjusted canonical correlation is larger than a previous adjusted canonical correlation.
- Approximate standard error of the canonical correlations
- Squared canonical correlations
- Eigenvalues of $\mathbf{E}^{-1}\mathbf{H}$. Each eigenvalue is equal to $\rho^2/(1 - \rho^2)$, where ρ^2 is the corresponding squared canonical correlation and can be interpreted as the ratio of between-class variation to within-class variation for the corresponding canonical variable. The table includes eigenvalues, differences between successive eigenvalues, proportion of the sum of the eigenvalues, and cumulative proportion.
- Likelihood ratio for the hypothesis that the current canonical correlation and all smaller ones are zero in the population. The likelihood ratio for all canonical correlations equals Wilks' lambda.
- Approximate F statistic based on Rao's approximation to the distribution of the likelihood ratio (Rao 1973, p. 556; Kshirsagar 1972, p. 326)
- Numerator degrees of freedom (Num DF), denominator degrees of freedom (Den DF), and $\text{Pr} > F$, the probability level associated with the F statistic

The following statistic concerns the classification criterion:

- the linear discriminant function, but only if you specify `METHOD=NORMAL` and the pooled covariance matrix is used to calculate the (generalized) squared distances

When the input `DATA=` data set is an ordinary SAS data set, the displayed output includes the following:

- Optionally, the resubstitution results including the observation number (if an `ID` statement is included, the values of the `ID` variable are displayed instead of the observation number), the actual group for the observation, the group into which the developed criterion would classify it, and the posterior probability of membership in each group
- Resubstitution summary, a summary of the performance of the classification criterion based on resubstitution classification results
- Error count estimate of the resubstitution classification results
- Optionally, posterior probability error rate estimates of the resubstitution classification results

If you specify the `CROSSVALIDATE` option, the displayed output contains these statistics:

- Optionally, the cross validation results including the observation number (if an `ID` statement is included, the values of the `ID` variable are displayed instead of the observation number), the actual group for the observation, the group into which the developed criterion would classify it, and the posterior probability of membership in each group
- Cross validation summary, a summary of the performance of the classification criterion based on cross validation classification results
- Error count estimate of the cross validation classification results
- Optionally, posterior probability error rate estimates of the cross validation classification results

If you specify the `TESTDATA=` option, the displayed output contains these statistics:

- Optionally, the classification results including the observation number (if a `TESTID` statement is included, the values of the `ID` variable are displayed instead of the observation number), the actual group for the observation (if a `TESTCLASS` statement is included), the group into which the developed criterion would classify it, and the posterior probability of membership in each group
- Classification summary, a summary of the performance of the classification criterion
- Error count estimate of the test data classification results
- Optionally, posterior probability error rate estimates of the test data classification results

Formulas

By default, PROC DISCRIM displays formulas such as the following in the LISTING destination:

$$D(i|j) = \sum_i \sum_j (X_i - \bar{X}_j)' \text{DIAG}(\text{COV}_j)^{-1} (X_i - \bar{X}_j)$$

$$\text{RHO} = 1.0 - \frac{\sum_i \frac{1}{N(i)} - \frac{1}{N}}{\frac{2P + 3P - 1}{6(P+1)(K-1)}}$$

$$D(X) = \sum_j (X - \bar{X}_j)' \text{COV}_j^{-1} (X - \bar{X}_j) + \ln |\text{COV}_j| - 2 \ln \text{PRIOR}_j$$

These formulas are properly displayed only with uniform fonts. Formulas are not displayed by default in destinations such as HTML, RTF, and PDF, because destinations other than LISTING typically use proportional fonts. You can use the FORMULA option to display formulas in destinations other than LISTING.

In the LISTING destination, formulas are displayed as notes. In other destinations, formulas are displayed with batch capture (which provides uniform fonts). Therefore, the names that are used to select and exclude formulas from the LISTING destination are different from the names that are used with other destinations.

By default, batch capture results are displayed in a box. You can remove the box and change the color and font of the formulas as follows:

```
proc template;
  define style styles.batch; parent=styles.htmlblue;
    style fonts from fonts / "BatchFixedFont" =
      ("SAS Monospace, <monospace>, Courier, monospace", 2, bold);
    style batch from batch / frame=void foreground=colors('notefg');
  end;
run;

ods listing;
ods html style=batch body='dis.html';
ods rtf style=batch body='dis.rtf';
ods pdf style=batch body='dis.pdf';

proc discrim data=sashelp.iris formula;
  class Species;
  var Peta;;
run;

ods _all_ close;
```

The results of these steps are not displayed.

ODS Table Names

PROC DISCRIM assigns a name to each table it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in Table 33.2. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

Table 33.2 ODS Tables Produced by PROC DISCRIM

ODS Table Name	Description	PROC DISCRIM Option
ANOVA	Univariate statistics	ANOVA
AvePostCrossVal	Average posterior probabilities, cross validation	POSTERR & CROSSVALIDATE
AvePostResub	Average posterior probabilities, resubstitution	POSTERR
AvePostTestClass	Average posterior probabilities, test classification	POSTERR & TEST=
AveRSquare	Average R-square	ANOVA
BCorr	Between-class correlations	BCORR
BCov	Between-class covariances	BCOV
BSSCP	Between-class SSCP matrix	BSSCP
BStruc	Between canonical structure	CANONICAL
CanCorr	Canonical correlations	CANONICAL
CanonicalMeans	Class means on canonical variables	CANONICAL
ChiSq	Chi-square information	POOL=TEST
ClassifiedCrossVal	Number of observations and percent classified, cross validation	CROSSVALIDATE
ClassifiedResub	Number of observations and percent classified, resubstitution	default
ClassifiedTestClass	Number of observations and percent classified, test classification	TEST=
Counts	Number of observations, variables, classes, df	default
CovDF	DF for covariance matrices, not displayed	any *COV option
Dist	Squared distances	DISTANCE
DistFValues	F values based on squared distances	DISTANCE
DistGeneralized	Generalized squared distances	default
DistProb	Probabilities for F values from squared distances	DISTANCE
ErrorCrossVal	Error count estimates, cross validation	CROSSVALIDATE
ErrorResub	Error count estimates, resubstitution	default
ErrorTestClass	Error count estimates, test classification	TEST=

Table 33.2 *continued*

ODS Table Name	Description	PROC DISCRIM Option
Levels	Class level information	default
LinearDiscFunc	Linear discriminant function	POOL=YES
LogDet	Log determinant of the covariance matrix	default
MultStat	MANOVA	MANOVA
PCoef	Pooled standard canonical coefficients	CANONICAL
PCorr	Pooled within-class correlations	PCORR
PCov	Pooled within-class covariances	PCOV
PSSCP	Pooled within-class SSCP matrix	PSSCP
PStdMeans	Pooled standardized class means	STDMEAN
PStruc	Pooled within canonical structure	CANONICAL
PostCrossVal	Posterior probabilities, cross validation	CROSSLIST or CROSSLISTERR
PostErrCrossVal	Posterior error estimates, cross validation	POSTERR & CROSSVALIDATE
PostErrResub	Posterior error estimates, resubstitution	POSTERR
PostErrTestClass	Posterior error estimates, test classification	POSTERR & TEST=
PostResub	Posterior probabilities, resubstitution	LIST or LISTERR
PostTestClass	Posterior probabilities, test classification	TESTLIST or TESTLISTERR
RCoef	Raw canonical coefficients	CANONICAL
SimpleStatistics	Simple statistics	SIMPLE
TCoef	Total-sample standard canonical coefficients	CANONICAL
TCorr	Total-sample correlations	TCORR
TCov	Total-sample covariances	TCOV
TSSCP	Total-sample SSCP matrix	TSSCP
TStdMeans	Total standardized class means	STDMEAN
TStruc	Total canonical structure	CANONICAL
WCorr	Within-class correlations	WCORR
WCov	Within-class covariances	WCOV
WSSCP	Within-class SSCP matrices	WSSCP

Examples: DISCRIM Procedure

The iris data published by Fisher (1936) are widely used for examples in discriminant analysis and cluster analysis. The sepal length, sepal width, petal length, and petal width are measured in millimeters on 50 iris specimens from each of three species: *Iris setosa*, *I. versicolor*, and *I. virginica*. The iris data set is available from the Sashelp library.

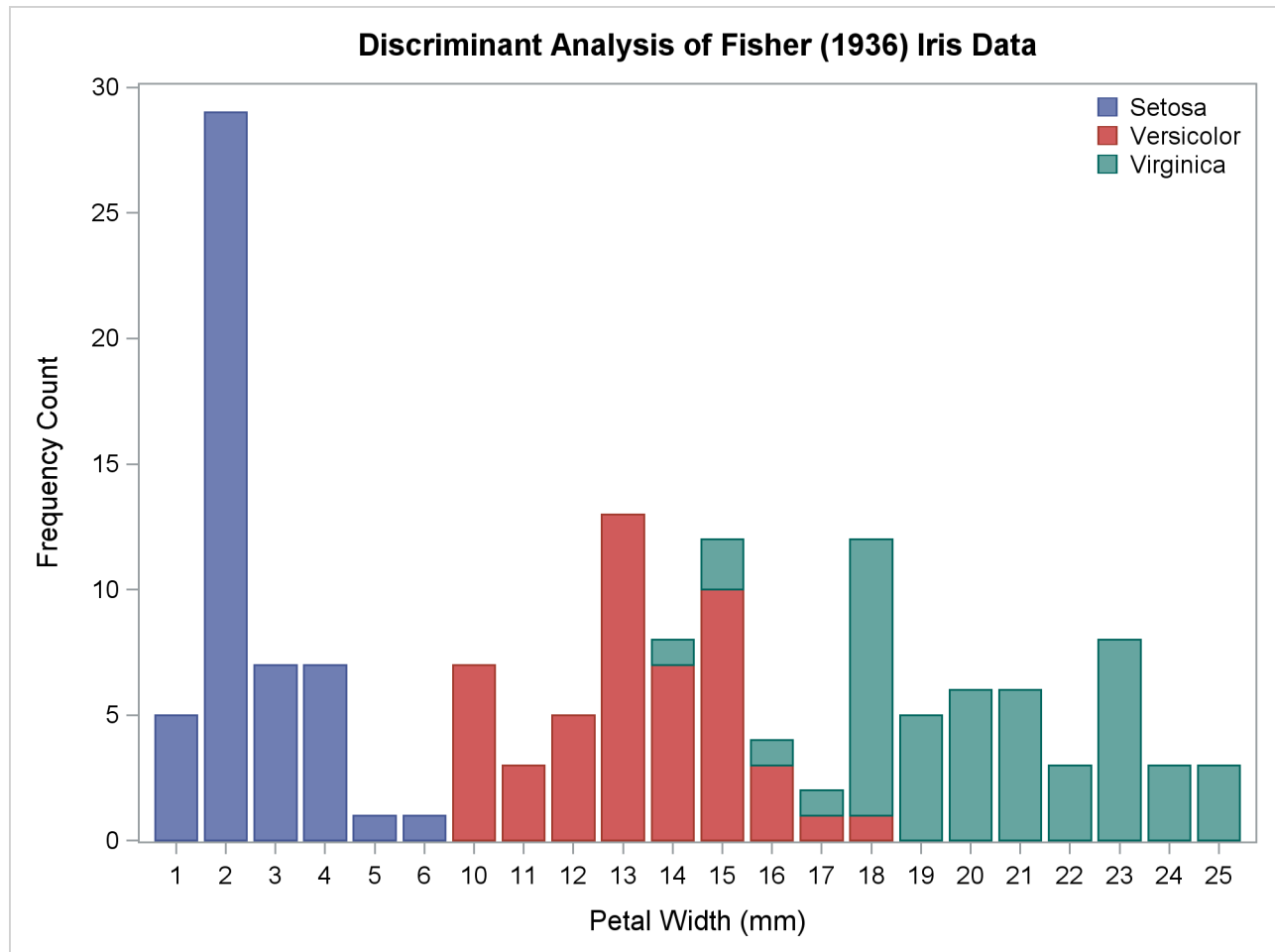
Example 33.1: Univariate Density Estimates and Posterior Probabilities

In this example, several discriminant analyses are run with a single quantitative variable, petal width, so that density estimates and posterior probabilities can be plotted easily. The example produces [Output 33.1.1](#) through [Output 33.1.5](#). ODS Graphics is used to display the sample distribution of petal width in the three species. For general information about ODS Graphics, see Chapter 21, “Statistical Graphics Using ODS.” Note the overlap between the species *I. versicolor* and *I. virginica* that the bar chart shows. The following statements produce [Output 33.1.1](#):

```
title 'Discriminant Analysis of Fisher (1936) Iris Data';

proc freq data=sashelp.iris noprint;
  tables petalwidth * species / out=freqout;
run;

proc sgplot data=freqout;
  vbar petalwidth / response=count group=species;
  keylegend / location=inside position=ne noborder across=1;
run;
```

Output 33.1.1 Sample Distribution of Petal Width in Three Species

In order to plot the density estimates and posterior probabilities, a data set called `plotdata` is created containing equally spaced values from -5 to 30 , covering the range of petal width with a little to spare on each end. The `plotdata` data set is used with the `TESTDATA=` option in `PROC DISCRIM`. The following statements make the data set:

```
data plotdata;
  do PetalWidth=-5 to 30 by 0.5;
    output;
  end;
run;
```

The same plots are produced after each discriminant analysis, so macros are used to reduce the amount of typing required. The macros use two data sets. The data set `pltd`, containing density estimates, is created by the `TESTOUTD=` option in `PROC DISCRIM`. The data set `plotp`, containing posterior probabilities, is created by the `TESTOUT=` option. For each data set, the macros remove uninteresting values (near zero) and create an overlay plot showing all three species in a single plot.

The following statements create the macros:

```
%macro plotden;
  title3 'Plot of Estimated Densities';

  data plotd2;
    set plotd;
    if setosa      < .002 then setosa      = .;
    if versicolor < .002 then versicolor = .;
    if virginica  < .002 then virginica  = .;
    g = 'Setosa   '; Density = setosa;      output;
    g = 'Versicolor'; Density = versicolor; output;
    g = 'Virginica '; Density = virginica;  output;
    label PetalWidth='Petal Width in mm.';
  run;

  proc sgplot data=plotd2;
    series y=Density x=PetalWidth / group=g;
    discretelegend;
  run;
%mend;

%macro plotprob;
  title3 'Plot of Posterior Probabilities';

  data plotp2;
    set plotp;
    if setosa      < .01 then setosa      = .;
    if versicolor < .01 then versicolor = .;
    if virginica  < .01 then virginica  = .;
    g = 'Setosa   '; Probability = setosa;      output;
    g = 'Versicolor'; Probability = versicolor; output;
    g = 'Virginica '; Probability = virginica;  output;
    label PetalWidth='Petal Width in mm.';
  run;

  proc sgplot data=plotp2;
    series y=Probability x=PetalWidth / group=g;
    discretelegend;
  run;
%mend;
```

The first analysis uses normal-theory methods (METHOD=NORMAL) assuming equal variances (POOL=YES) in the three classes. The NOCLASSIFY option suppresses the resubstitution classification results of the input data set observations. The CROSSLISTERR option lists the observations that are misclassified under cross validation and displays cross validation error-rate estimates. The following statements produce [Output 33.1.2](#):

```

title2 'Using Normal Density Estimates with Equal Variance';

proc discrim data=sashelp.iris method=normal pool=yes
            testdata=plotdata testout=plotp testoutd=plotd
            short noclassify crosslisterr;
    class Species;
    var PetalWidth;
run;

%plotden;
%plotprob;

```

Output 33.1.2 Normal Density Estimates with Equal Variance

Discriminant Analysis of Fisher (1936) Iris Data Using Normal Density Estimates with Equal Variance					
The DISCRIM Procedure					
Total Sample Size	150	DF Total		149	
Variables	1	DF Within Classes		147	
Classes	3	DF Between Classes		2	
Number of Observations Read				150	
Number of Observations Used				150	
Class Level Information					
Species	Variable Name	Frequency	Weight	Proportion	Prior Probability
Setosa	Setosa	50	50.0000	0.333333	0.333333
Versicolor	Versicolor	50	50.0000	0.333333	0.333333
Virginica	Virginica	50	50.0000	0.333333	0.333333

Output 33.1.2 continued

Discriminant Analysis of Fisher (1936) Iris Data
Using Normal Density Estimates with Equal Variance

The DISCRIM Procedure
Classification Results for Calibration Data: SASHELP.IRIS
Cross-validation Results using Linear Discriminant Function

Posterior Probability of Membership in Species

Obs	From Species	Classified into Species	Setosa	Versicolor	Virginica
53	Versicolor	Virginica *	0.0000	0.0952	0.9048
100	Versicolor	Virginica *	0.0000	0.3828	0.6172
103	Virginica	Versicolor *	0.0000	0.9610	0.0390
124	Virginica	Versicolor *	0.0000	0.9940	0.0060
130	Virginica	Versicolor *	0.0000	0.8009	0.1991
136	Virginica	Versicolor *	0.0000	0.9610	0.0390

* Misclassified observation

Discriminant Analysis of Fisher (1936) Iris Data
Using Normal Density Estimates with Equal Variance

The DISCRIM Procedure
Classification Summary for Calibration Data: SASHELP.IRIS
Cross-validation Summary using Linear Discriminant Function

Number of Observations and Percent Classified into Species

From Species	Setosa	Versicolor	Virginica	Total
Setosa	50 100.00	0 0.00	0 0.00	50 100.00
Versicolor	0 0.00	48 96.00	2 4.00	50 100.00
Virginica	0 0.00	4 8.00	46 92.00	50 100.00
Total	50 33.33	52 34.67	48 32.00	150 100.00
Priors	0.33333	0.33333	0.33333	

Error Count Estimates for Species

	Setosa	Versicolor	Virginica	Total
Rate	0.0000	0.0400	0.0800	0.0400
Priors	0.3333	0.3333	0.3333	

Output 33.1.2 *continued*

**Discriminant Analysis of Fisher (1936) Iris Data
Using Normal Density Estimates with Equal Variance**

The DISCRIM Procedure

Classification Summary for Test Data: WORK.PLOTDATA
Classification Summary using Linear Discriminant Function

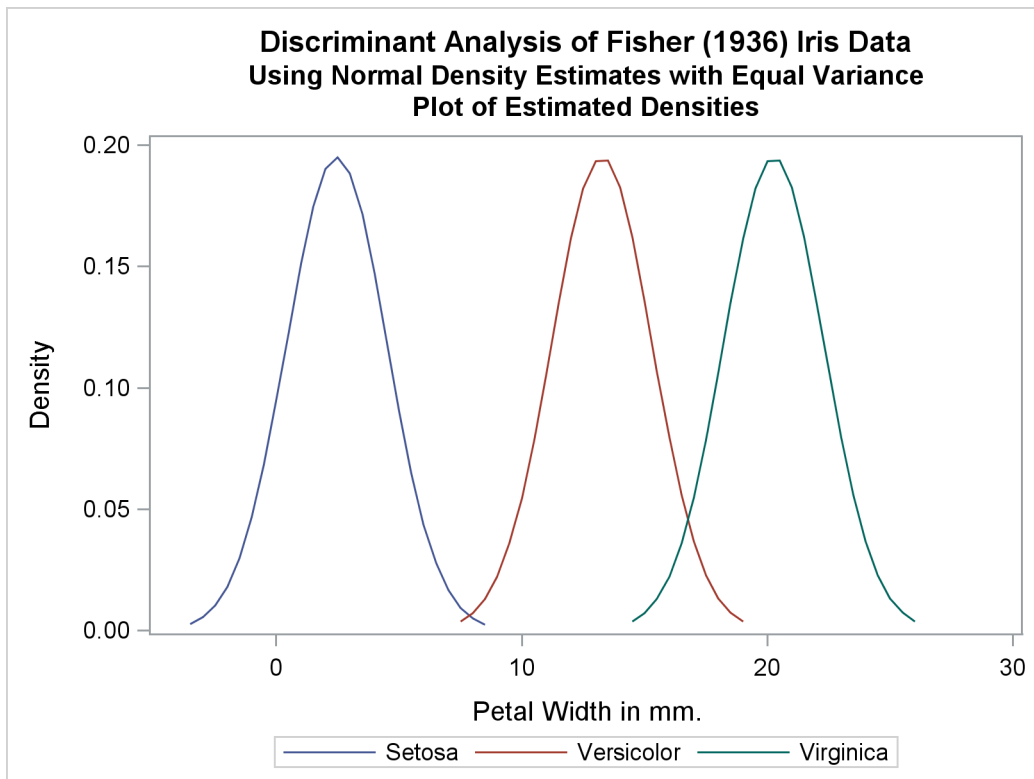
Observation Profile for Test Data

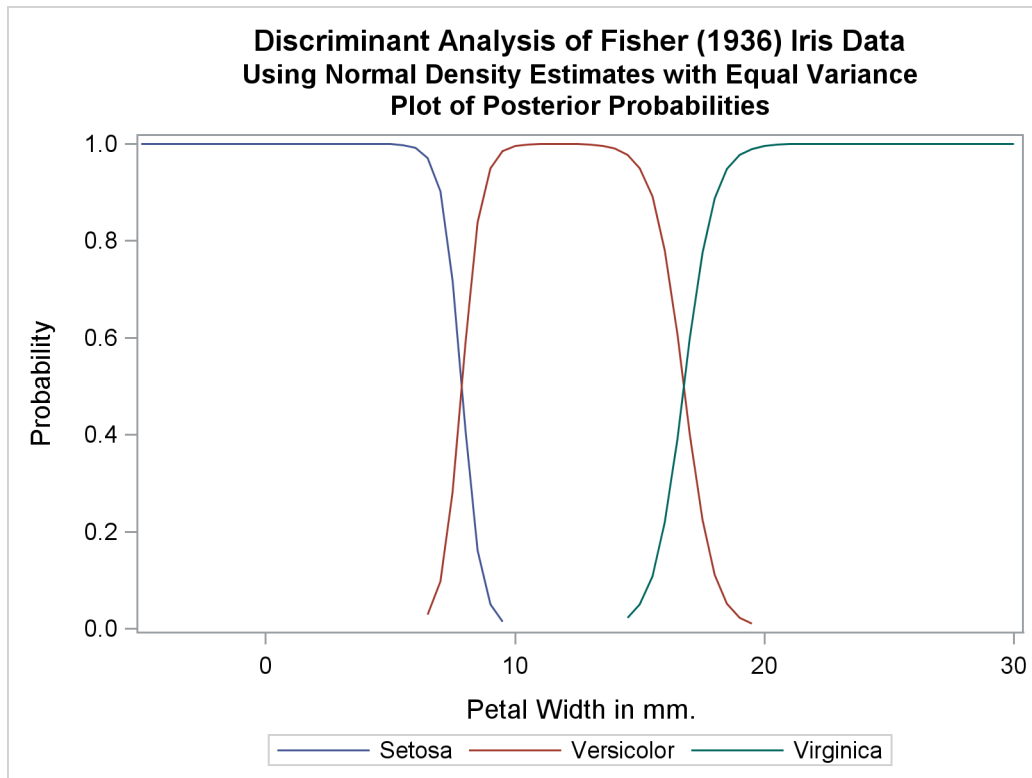
Number of Observations Read	71
Number of Observations Used	71

Number of Observations and Percent Classified into Species

	Setosa	Versicolor	Virginica	Total
Total	26	18	27	71
	36.62	25.35	38.03	100.00
Priors	0.33333	0.33333	0.33333	

Output 33.1.2 *continued*



Output 33.1.2 *continued*

The next analysis uses normal-theory methods assuming unequal variances (POOL=NO) in the three classes. The following statements produce **Output 33.1.3**:

```

title2 'Using Normal Density Estimates with Unequal Variance';

proc discrim data=sashelp.iris method=normal pool=no
  testdata=plotdata testout=plotp testoutd=plotd
  short noclassify crosslisterr;
  class Species;
  var PetalWidth;
run;

%plotden;
%plotprob;

```

Output 33.1.3 Normal Density Estimates with Unequal Variance

Discriminant Analysis of Fisher (1936) Iris Data Using Normal Density Estimates with Unequal Variance			
The DISCRIM Procedure			
Total Sample Size	150	DF Total	149
Variables	1	DF Within Classes	147
Classes	3	DF Between Classes	2

Output 33.1.3 *continued*

	Number of Observations Read	150			
	Number of Observations Used	150			
Class Level Information					
Species	Variable Name	Frequency	Weight	Proportion	Prior Probability
Setosa	Setosa	50	50.0000	0.333333	0.333333
Versicolor	Versicolor	50	50.0000	0.333333	0.333333
Virginica	Virginica	50	50.0000	0.333333	0.333333
Discriminant Analysis of Fisher (1936) Iris Data Using Normal Density Estimates with Unequal Variance					
The DISCRIM Procedure					
Classification Results for Calibration Data: SASHELP.IRIS					
Cross-validation Results using Quadratic Discriminant Function					
Posterior Probability of Membership in Species					
Obs	From Species	Classified into Species	Setosa	Versicolor	Virginica
10	Setosa	Versicolor *	0.4923	0.5073	0.0004
53	Versicolor	Virginica *	0.0000	0.0686	0.9314
100	Versicolor	Virginica *	0.0000	0.2871	0.7129
103	Virginica	Versicolor *	0.0000	0.8740	0.1260
124	Virginica	Versicolor *	0.0000	0.9602	0.0398
130	Virginica	Versicolor *	0.0000	0.6558	0.3442
136	Virginica	Versicolor *	0.0000	0.8740	0.1260
* Misclassified observation					

Output 33.1.3 continued

Discriminant Analysis of Fisher (1936) Iris Data
Using Normal Density Estimates with Unequal Variance

The DISCRIM Procedure
Classification Summary for Calibration Data: SASHELP.IRIS
Cross-validation Summary using Quadratic Discriminant Function

Number of Observations and Percent Classified into Species

From Species	Setosa	Versicolor	Virginica	Total
Setosa	49 98.00	1 2.00	0 0.00	50 100.00
Versicolor	0 0.00	48 96.00	2 4.00	50 100.00
Virginica	0 0.00	4 8.00	46 92.00	50 100.00
Total	49 32.67	53 35.33	48 32.00	150 100.00
Priors	0.33333	0.33333	0.33333	

Error Count Estimates for Species

	Setosa	Versicolor	Virginica	Total
Rate	0.0200	0.0400	0.0800	0.0467
Priors	0.3333	0.3333	0.3333	

Discriminant Analysis of Fisher (1936) Iris Data
Using Normal Density Estimates with Unequal Variance

The DISCRIM Procedure
Classification Summary for Test Data: WORK.PLOTDATA
Classification Summary using Quadratic Discriminant Function

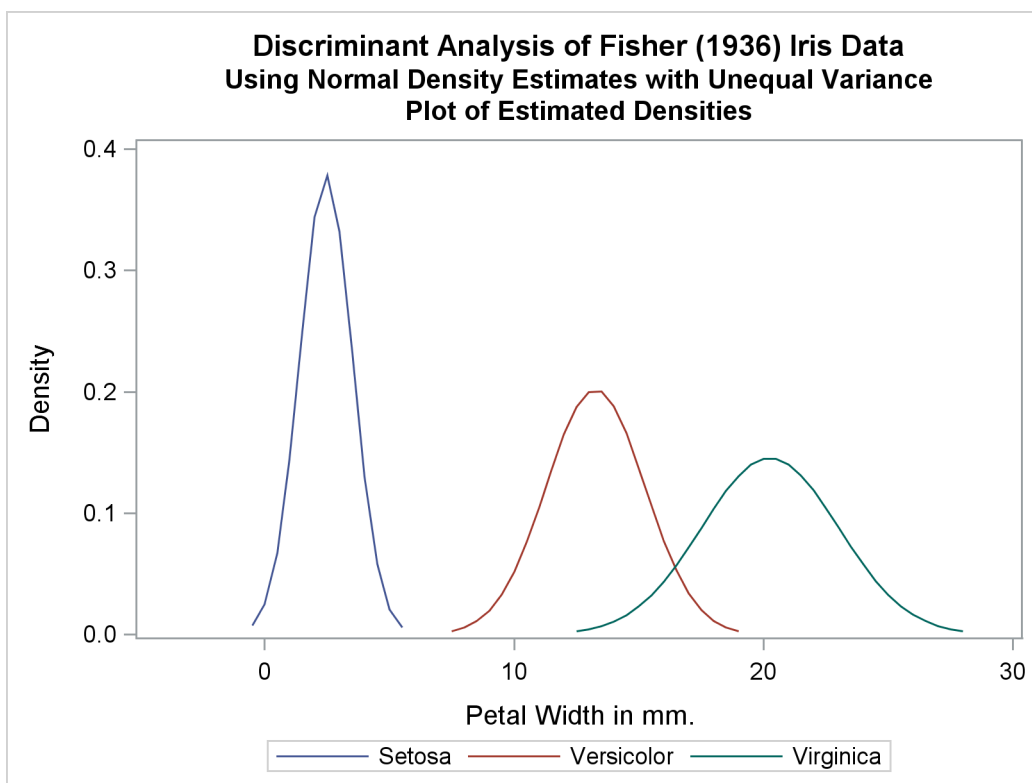
Observation Profile for Test Data

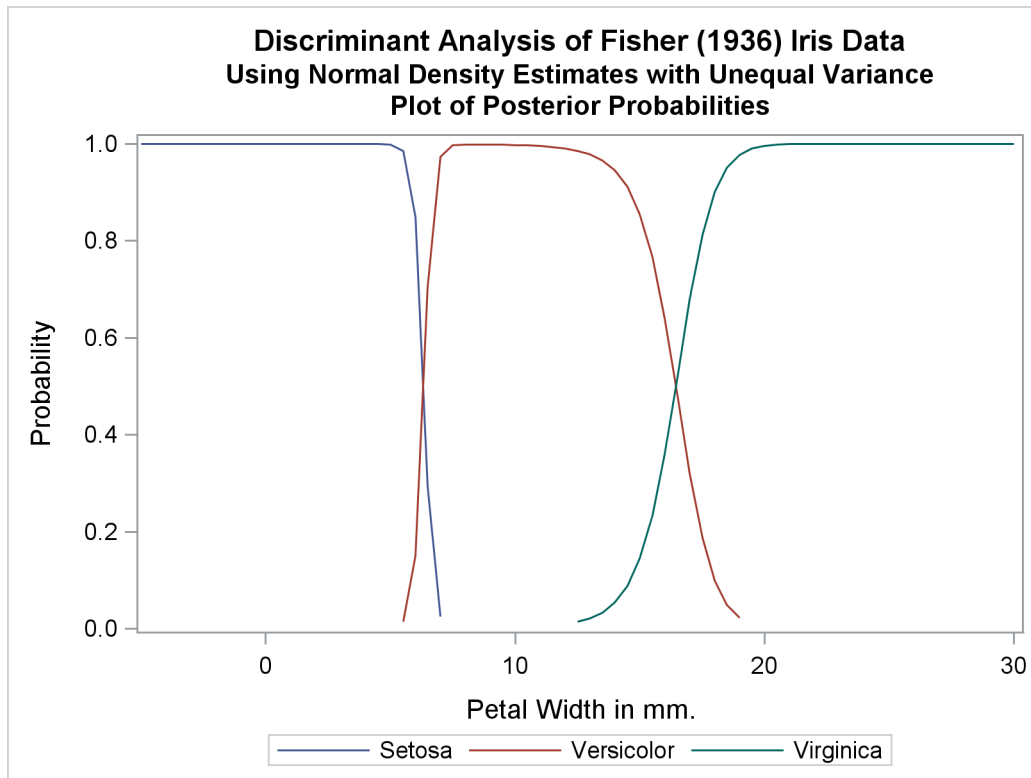
Number of Observations Read	71
Number of Observations Used	71

Output 33.1.3 *continued*

Number of Observations and Percent Classified into Species				
	Setosa	Versicolor	Virginica	Total
Total	23	20	28	71
	32.39	28.17	39.44	100.00
Priors	0.33333	0.33333	0.33333	

Output 33.1.3 *continued*



Output 33.1.3 *continued*

Two more analyses are run with nonparametric methods (METHOD=NPAR), specifically kernel density estimates with normal kernels (KERNEL=NORMAL). The first of these uses equal bandwidths (smoothing parameters) (POOL=YES) in each class. The use of equal bandwidths does not constrain the density estimates to be of equal variance. The value of the radius parameter that, assuming normality, minimizes an approximate mean integrated square error is 0.48 (see the section “Nonparametric Methods” on page 2079). Choosing $r = 0.4$ gives a more detailed look at the irregularities in the data. The following statements produce Output 33.1.4:

```

title2 'Using Kernel Density Estimates with Equal Bandwidth';

proc discrim data=sashelp.iris method=npar kernel=normal
    r=.4 pool=yes
    testdata=plotdata testout=plotp
    testoutd=plotd
    short noclassify crosslisterr;
    class Species;
    var PetalWidth;
run;

%plotden;
%plotprob;

```

Output 33.1.4 Kernel Density Estimates with Equal Bandwidth

```

Discriminant Analysis of Fisher (1936) Iris Data
Using Kernel Density Estimates with Equal Bandwidth

The DISCRIM Procedure

Total Sample Size      150          DF Total          149
Variables              1          DF Within Classes 147
Classes                3          DF Between Classes  2

Number of Observations Read      150
Number of Observations Used      150

Class Level Information

Species      Variable
            Name      Frequency      Weight      Proportion      Prior
            Probability

Setosa      Setosa      50          50.0000     0.333333      0.333333
Versicolor  Versicolor  50          50.0000     0.333333      0.333333
Virginica   Virginica   50          50.0000     0.333333      0.333333

Discriminant Analysis of Fisher (1936) Iris Data
Using Kernel Density Estimates with Equal Bandwidth

The DISCRIM Procedure
Classification Results for Calibration Data: SASHELP.IRIS
Cross-validation Results using Normal Kernel Density

Posterior Probability of Membership in Species

Obs      From      Classified
         Species  into Species      Setosa      Versicolor      Virginica

53      Versicolor  Virginica *      0.0000     0.0438      0.9562
100     Versicolor  Virginica *      0.0000     0.2586      0.7414
103     Virginica   Versicolor *     0.0000     0.8827      0.1173
124     Virginica   Versicolor *     0.0000     0.9472      0.0528
130     Virginica   Versicolor *     0.0000     0.8061      0.1939
136     Virginica   Versicolor *     0.0000     0.8827      0.1173

* Misclassified observation
    
```

Output 33.1.4 continued

Discriminant Analysis of Fisher (1936) Iris Data
Using Kernel Density Estimates with Equal Bandwidth

The DISCRIM Procedure
Classification Summary for Calibration Data: SASHELP.IRIS
Cross-validation Summary using Normal Kernel Density

Number of Observations and Percent Classified into Species

From Species	Setosa	Versicolor	Virginica	Total
Setosa	50 100.00	0 0.00	0 0.00	50 100.00
Versicolor	0 0.00	48 96.00	2 4.00	50 100.00
Virginica	0 0.00	4 8.00	46 92.00	50 100.00
Total	50 33.33	52 34.67	48 32.00	150 100.00
Priors	0.33333	0.33333	0.33333	

Error Count Estimates for Species

	Setosa	Versicolor	Virginica	Total
Rate	0.0000	0.0400	0.0800	0.0400
Priors	0.3333	0.3333	0.3333	

Discriminant Analysis of Fisher (1936) Iris Data
Using Kernel Density Estimates with Equal Bandwidth

The DISCRIM Procedure
Classification Summary for Test Data: WORK.PLOTDATA
Classification Summary using Normal Kernel Density

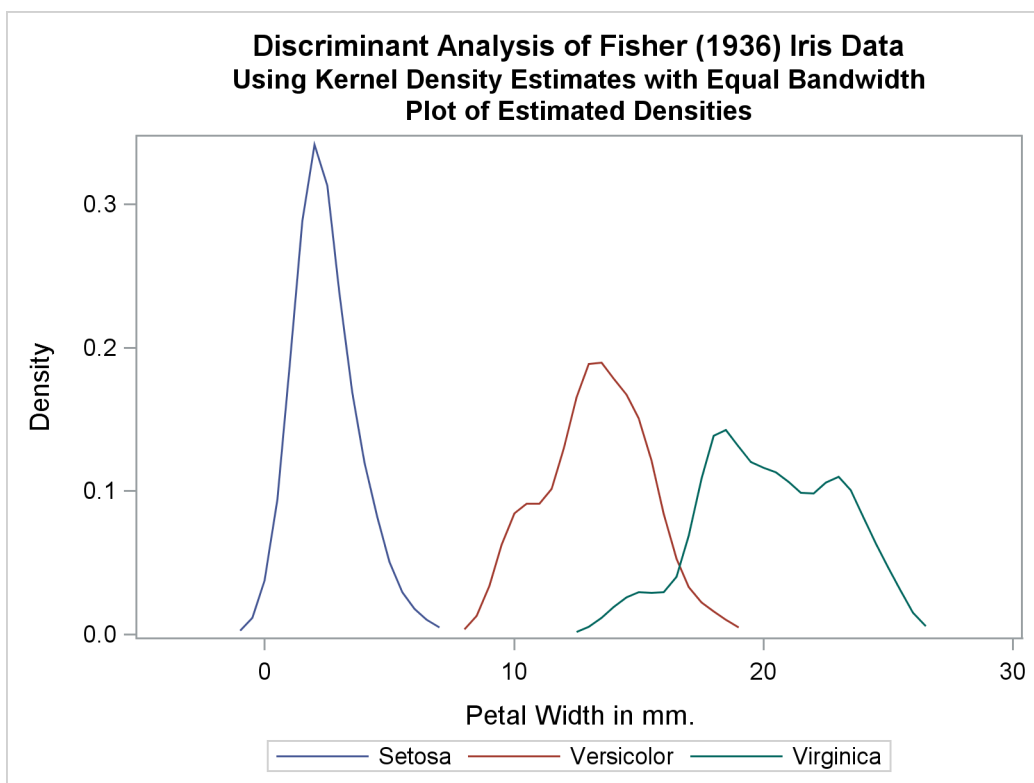
Observation Profile for Test Data

Number of Observations Read	71
Number of Observations Used	71

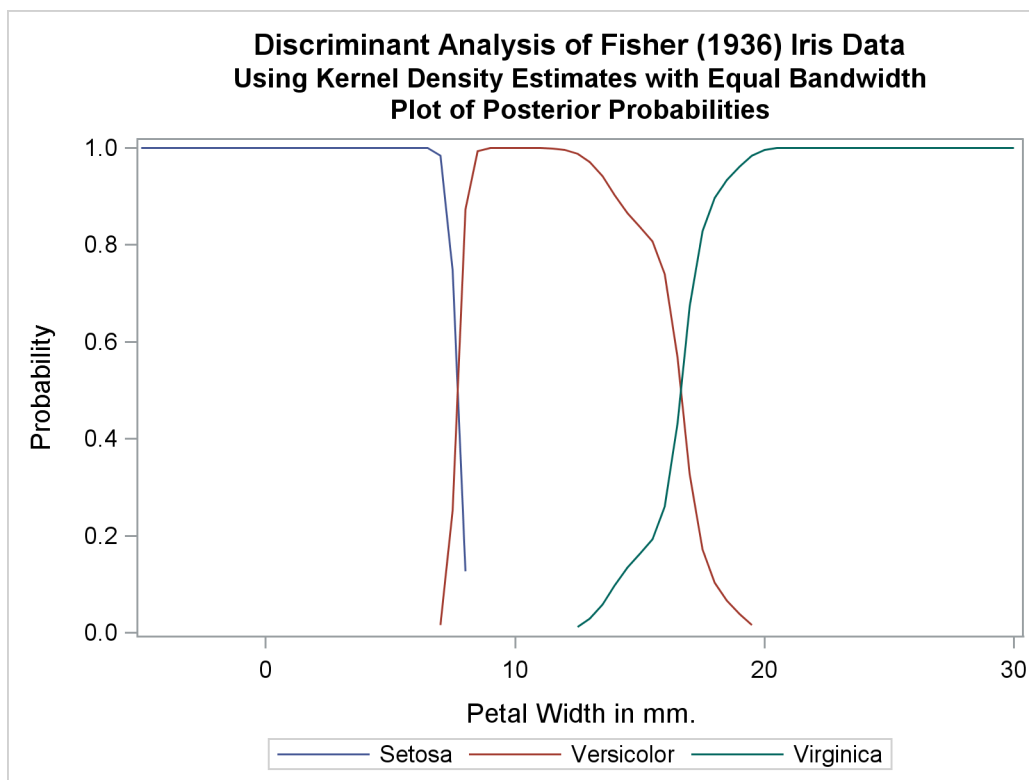
Output 33.1.4 *continued*

Number of Observations and Percent Classified into Species				
	Setosa	Versicolor	Virginica	Total
Total	26	18	27	71
	36.62	25.35	38.03	100.00
Priors	0.33333	0.33333	0.33333	

Output 33.1.4 *continued*



Output 33.1.4 continued



Another nonparametric analysis is run with unequal bandwidths (POOL=NO). The following statements produce [Output 33.1.5](#):

```

title2 'Using Kernel Density Estimates with Unequal Bandwidth';

proc discrim data=sashelp.iris method=npar kernel=normal
    r=.4 pool=no
    testdata=plotdata testout=plotp
    testoutd=plotd
    short noclassify crosslisterr;
    class Species;
    var PetalWidth;
run;

%plotden;
%plotprob;

```

Output 33.1.5 Kernel Density Estimates with Unequal Bandwidth

```

Discriminant Analysis of Fisher (1936) Iris Data
Using Kernel Density Estimates with Unequal Bandwidth

The DISCRIM Procedure

Total Sample Size      150          DF Total          149
Variables              1          DF Within Classes 147
Classes                3          DF Between Classes  2

Number of Observations Read      150
Number of Observations Used      150

Class Level Information

Species      Variable
            Name      Frequency      Weight      Proportion      Prior
            Probability

Setosa      Setosa      50          50.0000     0.333333      0.333333
Versicolor  Versicolor  50          50.0000     0.333333      0.333333
Virginica   Virginica   50          50.0000     0.333333      0.333333

Discriminant Analysis of Fisher (1936) Iris Data
Using Kernel Density Estimates with Unequal Bandwidth

The DISCRIM Procedure
Classification Results for Calibration Data: SASHELP.IRIS
Cross-validation Results using Normal Kernel Density

Posterior Probability of Membership in Species

Obs      From      Classified
         Species  into Species      Setosa      Versicolor      Virginica

53      Versicolor  Virginica *      0.0000     0.0475     0.9525
100     Versicolor  Virginica *      0.0000     0.2310     0.7690
103     Virginica   Versicolor *     0.0000     0.8805     0.1195
124     Virginica   Versicolor *     0.0000     0.9394     0.0606
130     Virginica   Versicolor *     0.0000     0.7193     0.2807
136     Virginica   Versicolor *     0.0000     0.8805     0.1195

* Misclassified observation
    
```

Output 33.1.5 continued

Discriminant Analysis of Fisher (1936) Iris Data
Using Kernel Density Estimates with Unequal Bandwidth

The DISCRIM Procedure
Classification Summary for Calibration Data: SASHELP.IRIS
Cross-validation Summary using Normal Kernel Density

Number of Observations and Percent Classified into Species

From Species	Setosa	Versicolor	Virginica	Total
Setosa	50 100.00	0 0.00	0 0.00	50 100.00
Versicolor	0 0.00	48 96.00	2 4.00	50 100.00
Virginica	0 0.00	4 8.00	46 92.00	50 100.00
Total	50 33.33	52 34.67	48 32.00	150 100.00
Priors	0.33333	0.33333	0.33333	

Error Count Estimates for Species

	Setosa	Versicolor	Virginica	Total
Rate	0.0000	0.0400	0.0800	0.0400
Priors	0.3333	0.3333	0.3333	

Discriminant Analysis of Fisher (1936) Iris Data
Using Kernel Density Estimates with Unequal Bandwidth

The DISCRIM Procedure
Classification Summary for Test Data: WORK.PLOTDATA
Classification Summary using Normal Kernel Density

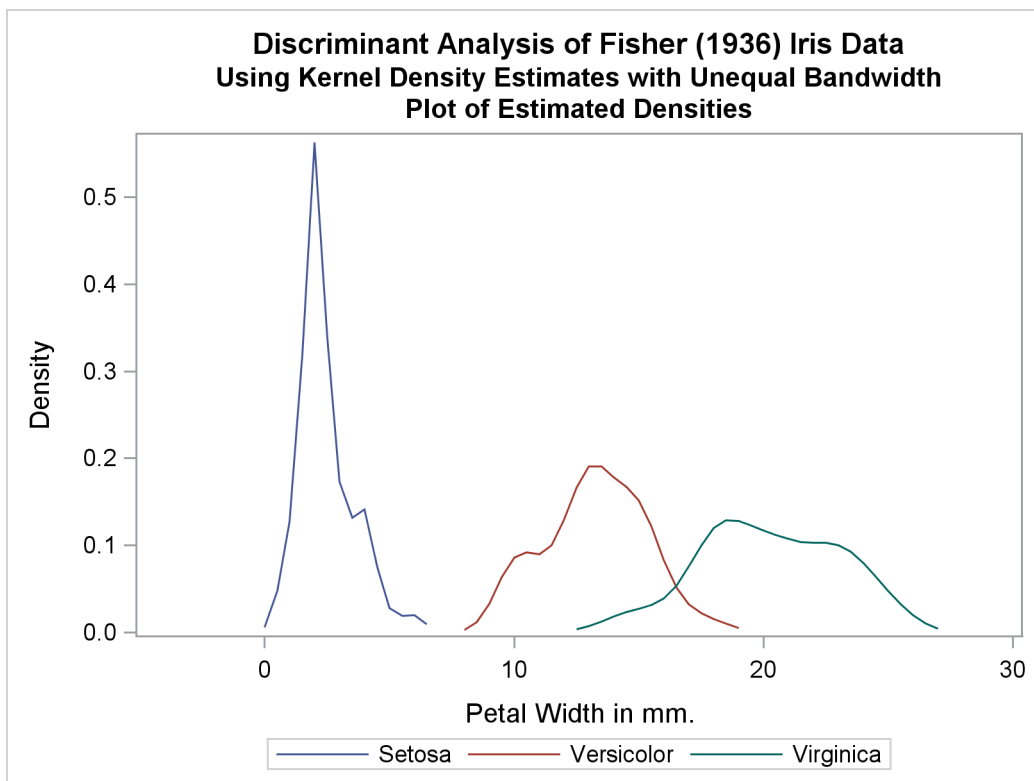
Observation Profile for Test Data

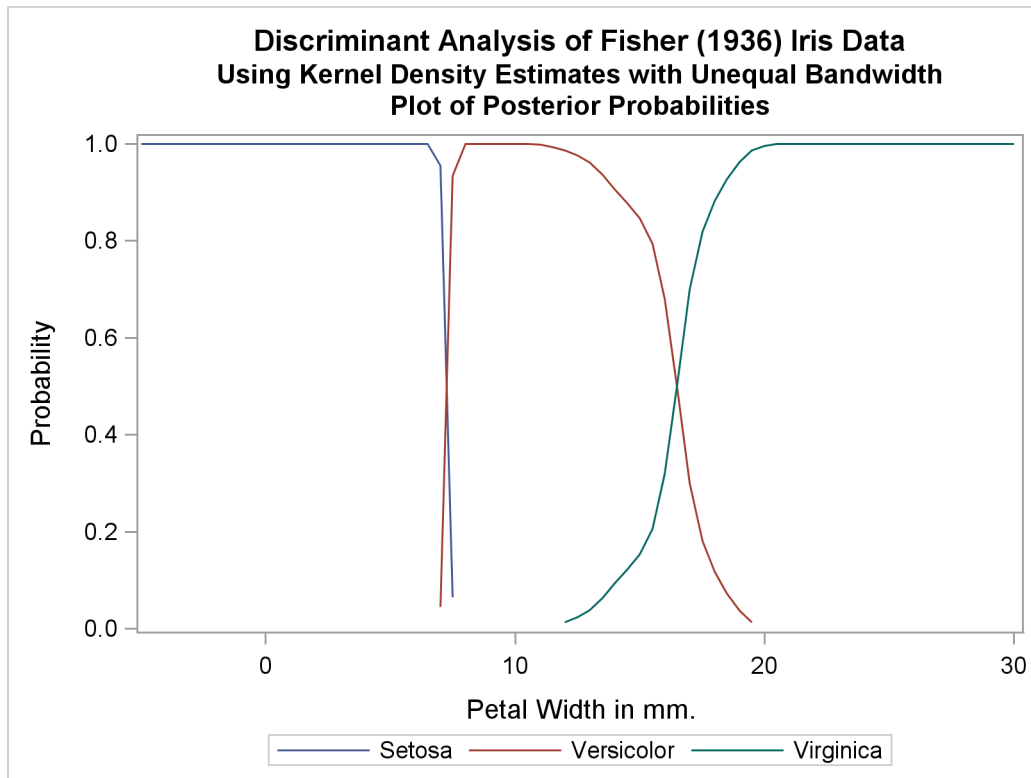
Number of Observations Read	71
Number of Observations Used	71

Output 33.1.5 *continued*

Number of Observations and Percent Classified into Species				
	Setosa	Versicolor	Virginica	Total
Total	25	18	28	71
	35.21	25.35	39.44	100.00
Priors	0.33333	0.33333	0.33333	

Output 33.1.5 *continued*



Output 33.1.5 *continued***Example 33.2: Bivariate Density Estimates and Posterior Probabilities**

In this example, four more discriminant analyses of iris data are run with two quantitative variables: petal width and petal length. The following statements produce [Output 33.2.1](#) through [Output 33.2.5](#):

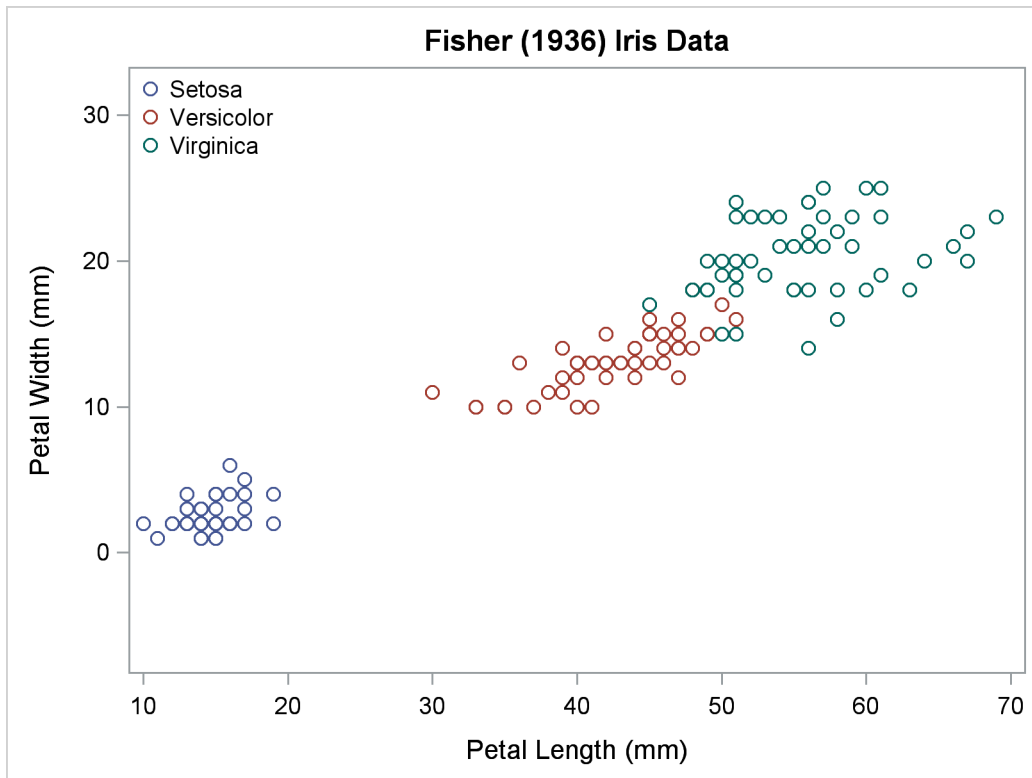
```

title 'Discriminant Analysis of Fisher (1936) Iris Data';
proc template;
  define statgraph scatter;
    begingraph;
      entrytitle 'Fisher (1936) Iris Data';
      layout overlayequated / equatetype=fit;
      scatterplot x=petalength y=petalwidth /
        group=species name='iris';
      layout gridded / autoalign=(topleft);
      discretelegend 'iris' / border=false opaque=false;
    endlayout;
  endgraph;
end;
run;

proc sgrender data=sashelp.iris template=scatter;
run;

```

The scatter plot in [Output 33.2.1](#) shows the joint sample distribution.

Output 33.2.1 Joint Sample Distribution of Petal Width and Petal Length in Three Species

Another data set is created for plotting, containing a grid of points suitable for contour plots. The following statements create the data set:

```
data plotdata;
  do PetalLength = -2 to 72 by 0.5;
    do PetalWidth= - 5 to 32 by 0.5;
      output;
    end;
  end;
end;
run;
```

Three macros are defined as follows to make contour plots of density estimates, posterior probabilities, and classification results:

```

%let close = thresholdmin=0 thresholdmax=0 offsetmin=0 offsetmax=0;
%let close = xaxisopts=(&close) yaxisopts=(&close);

proc template;
  define statgraph contour;
    begingraph;
      layout overlayequated / equatetype=equate &close;
      contourplotparm x=petalength y=petalwidth z=z /
        contourtype=fill nhint=30;
      scatterplot x=pl y=pw / group=species name='iris'
        includemissinggroup=false primary=true;
      layout gridded / autoalign=(topleft);
      discretelegend 'iris' / border=false opaque=false;
    endlayout;
  endlayout;
endgraph;
end;
run;

%macro contden;
  data contour(keep=PetalWidth PetalLength species z pl pw);
    merge plotd(in=d) sashelp.iris(keep=PetalWidth PetalLength species
      rename=(PetalWidth=pw PetalLength=pl));
    if d then z = max(setosa,versicolor,virginica);
  run;

  title3 'Plot of Estimated Densities';

  proc sgrender data=contour template=contour;
  run;
%mend;

%macro contprob;
  data posterior(keep=PetalWidth PetalLength species z pl pw into);
    merge plotp(in=d) sashelp.iris(keep=PetalWidth PetalLength species
      rename=(PetalWidth=pw PetalLength=pl));
    if d then z = max(setosa,versicolor,virginica);
    into = 1 * (_into_ =: 'Set') + 2 * (_into_ =: 'Ver') +
      3 * (_into_ =: 'Vir');
  run;

  title3 'Plot of Posterior Probabilities ';

  proc sgrender data=posterior template=contour;
  run;
%mend;

```

```
%macro contclass;
  title3 'Plot of Classification Results';

  proc sgrender data=posterior(drop=z rename=(into=z)) template=contour;
  run;
%mend;
```

A normal-theory analysis (METHOD=NORMAL) assuming equal covariance matrices (POOL=YES) illustrates the linearity of the classification boundaries. These statements produce [Output 33.2.2](#):

```
title2 'Using Normal Density Estimates with Equal Variance';

proc discrim data=sashelp.iris method=normal pool=yes
  testdata=plotdata testout=plotp testoutd=plotd
  short noclassify crosslisterr;
  class Species;
  var Petal;;
run;

%contden
%contprob
%contclass
```

Output 33.2.2 Normal Density Estimates with Equal Variance

Discriminant Analysis of Fisher (1936) Iris Data Using Normal Density Estimates with Equal Variance					
The DISCRIM Procedure					
Total Sample Size	150	DF Total	149		
Variables	2	DF Within Classes	147		
Classes	3	DF Between Classes	2		
Number of Observations Read		150			
Number of Observations Used		150			
Class Level Information					
Species	Variable Name	Frequency	Weight	Proportion	Prior Probability
Setosa	Setosa	50	50.0000	0.333333	0.333333
Versicolor	Versicolor	50	50.0000	0.333333	0.333333
Virginica	Virginica	50	50.0000	0.333333	0.333333

Output 33.2.2 continued

Discriminant Analysis of Fisher (1936) Iris Data
Using Normal Density Estimates with Equal Variance

The DISCRIM Procedure
Classification Results for Calibration Data: SASHELP.IRIS
Cross-validation Results using Linear Discriminant Function

Posterior Probability of Membership in Species

Obs	From Species	Classified into Species	Setosa	Versicolor	Virginica
53	Versicolor	Virginica *	0.0000	0.2130	0.7870
100	Versicolor	Virginica *	0.0000	0.3118	0.6882
103	Virginica	Versicolor *	0.0000	0.8453	0.1547
113	Virginica	Versicolor *	0.0000	0.8322	0.1678
124	Virginica	Versicolor *	0.0000	0.8057	0.1943
136	Virginica	Versicolor *	0.0000	0.8903	0.1097

* Misclassified observation

Discriminant Analysis of Fisher (1936) Iris Data
Using Normal Density Estimates with Equal Variance

The DISCRIM Procedure
Classification Summary for Calibration Data: SASHELP.IRIS
Cross-validation Summary using Linear Discriminant Function

Number of Observations and Percent Classified into Species

From Species	Setosa	Versicolor	Virginica	Total
Setosa	50 100.00	0 0.00	0 0.00	50 100.00
Versicolor	0 0.00	48 96.00	2 4.00	50 100.00
Virginica	0 0.00	4 8.00	46 92.00	50 100.00
Total	50 33.33	52 34.67	48 32.00	150 100.00
Priors	0.33333	0.33333	0.33333	

Error Count Estimates for Species

	Setosa	Versicolor	Virginica	Total
Rate	0.0000	0.0400	0.0800	0.0400
Priors	0.3333	0.3333	0.3333	

Output 33.2.2 *continued*

Discriminant Analysis of Fisher (1936) Iris Data
Using Normal Density Estimates with Equal Variance

The DISCRIM Procedure
Classification Summary for Test Data: WORK.PLOTDATA
Classification Summary using Linear Discriminant Function

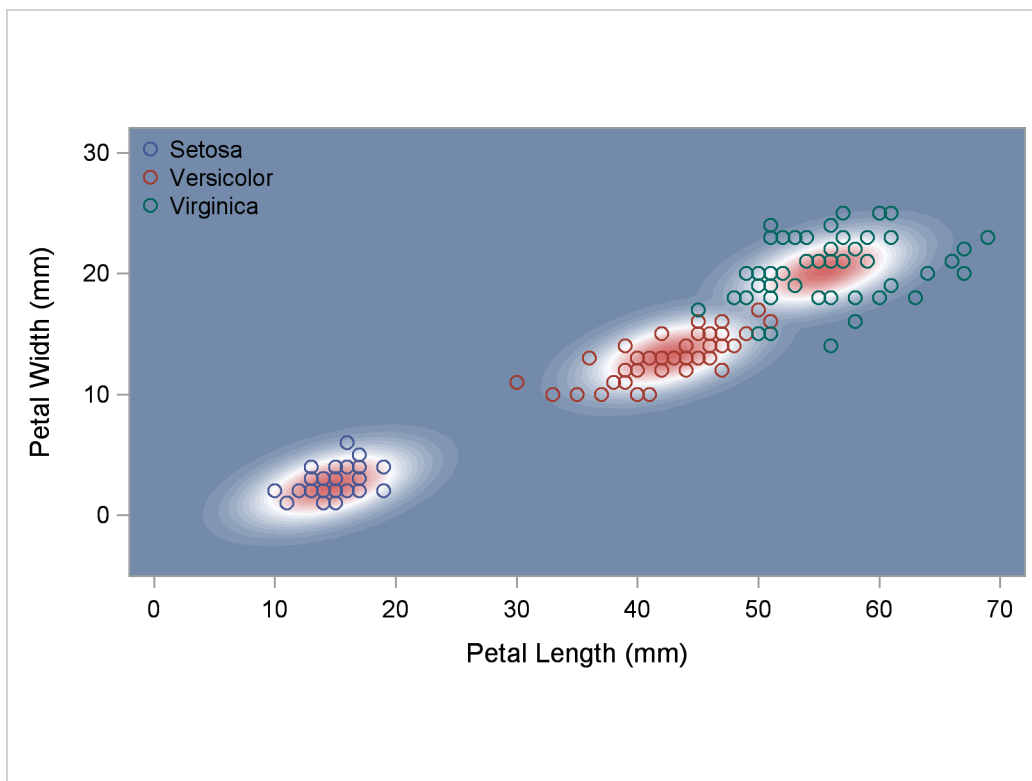
Observation Profile for Test Data

Number of Observations Read	11175
Number of Observations Used	11175

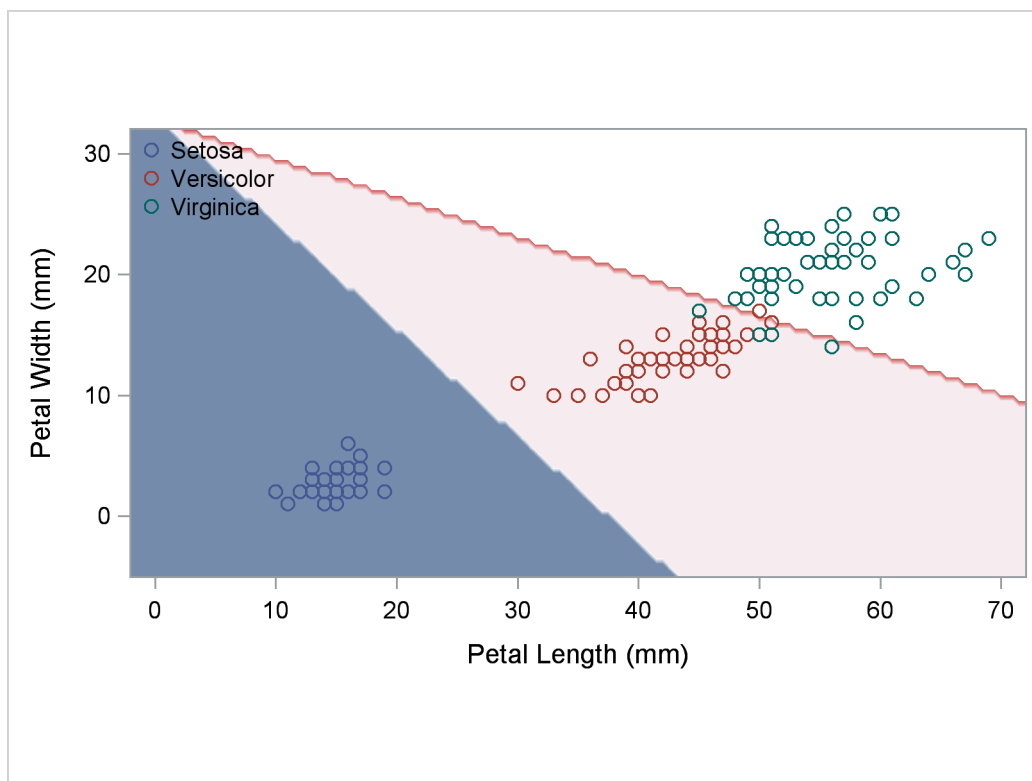
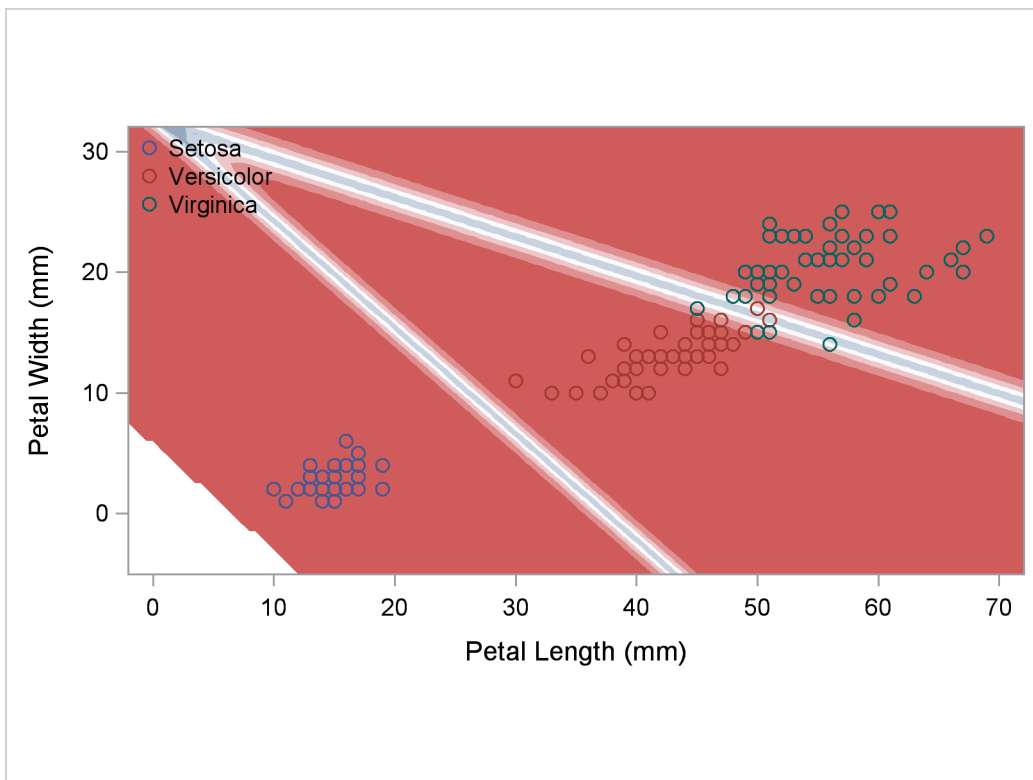
Number of Observations and Percent Classified into Species

	Setosa	Versicolor	Virginica	Total
Total	3670	4243	3262	11175
	32.84	37.97	29.19	100.00
Priors	0.33333	0.33333	0.33333	

Output 33.2.2 *continued*



Output 33.2.2 continued



A normal-theory analysis assuming unequal covariance matrices (POOL=NO) illustrates quadratic classification boundaries. These statements produce [Output 33.2.3](#):

```

title2 'Using Normal Density Estimates with Unequal Variance';

proc discrim data=sashelp.iris method=normal pool=no
      testdata=plotdata testout=plotp testoutd=plotd
      short noclassify crosslisterr;
  class Species;
  var Petal;;
run;

%contden
%contprob
%contclass
    
```

Output 33.2.3 Normal Density Estimates with Unequal Variance

Discriminant Analysis of Fisher (1936) Iris Data Using Normal Density Estimates with Unequal Variance					
The DISCRIM Procedure					
Total Sample Size	150	DF Total		149	
Variables	2	DF Within Classes		147	
Classes	3	DF Between Classes		2	
Number of Observations Read		150			
Number of Observations Used		150			
Class Level Information					
Species	Variable Name	Frequency	Weight	Proportion	Prior Probability
Setosa	Setosa	50	50.0000	0.333333	0.333333
Versicolor	Versicolor	50	50.0000	0.333333	0.333333
Virginica	Virginica	50	50.0000	0.333333	0.333333

Output 33.2.3 continued

Discriminant Analysis of Fisher (1936) Iris Data
Using Normal Density Estimates with Unequal Variance

The DISCRIM Procedure
Classification Results for Calibration Data: SASHELP.IRIS
Cross-validation Results using Quadratic Discriminant Function

Posterior Probability of Membership in Species

Obs	From Species	Classified into Species	Setosa	Versicolor	Virginica
53	Versicolor	Virginica *	0.0000	0.0903	0.9097
100	Versicolor	Virginica *	0.0000	0.4675	0.5325
103	Virginica	Versicolor *	0.0000	0.7288	0.2712
113	Virginica	Versicolor *	0.0000	0.5196	0.4804
136	Virginica	Versicolor *	0.0000	0.8335	0.1665

* Misclassified observation

Discriminant Analysis of Fisher (1936) Iris Data
Using Normal Density Estimates with Unequal Variance

The DISCRIM Procedure
Classification Summary for Calibration Data: SASHELP.IRIS
Cross-validation Summary using Quadratic Discriminant Function

Number of Observations and Percent Classified into Species

From Species	Setosa	Versicolor	Virginica	Total
Setosa	50 100.00	0 0.00	0 0.00	50 100.00
Versicolor	0 0.00	48 96.00	2 4.00	50 100.00
Virginica	0 0.00	3 6.00	47 94.00	50 100.00
Total	50 33.33	51 34.00	49 32.67	150 100.00
Priors	0.33333	0.33333	0.33333	

Error Count Estimates for Species

	Setosa	Versicolor	Virginica	Total
Rate	0.0000	0.0400	0.0600	0.0333
Priors	0.3333	0.3333	0.3333	

Output 33.2.3 *continued*

Discriminant Analysis of Fisher (1936) Iris Data
Using Normal Density Estimates with Unequal Variance

The DISCRIM Procedure
Classification Summary for Test Data: WORK.PLOTDATA
Classification Summary using Quadratic Discriminant Function

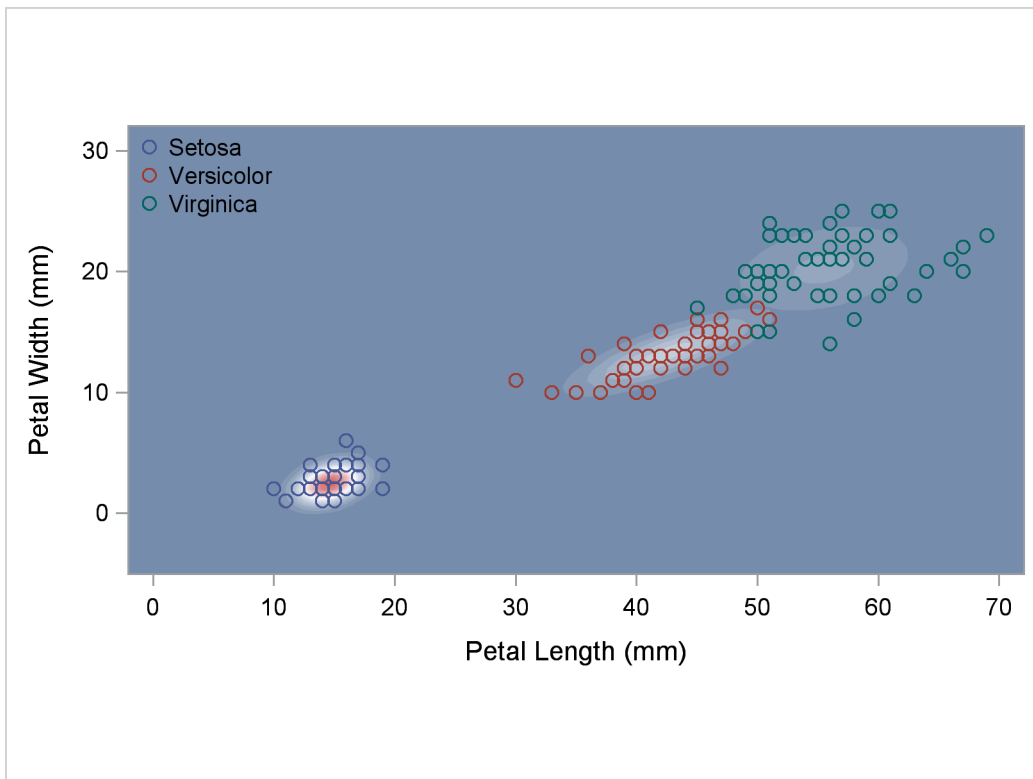
Observation Profile for Test Data

Number of Observations Read	11175
Number of Observations Used	11175

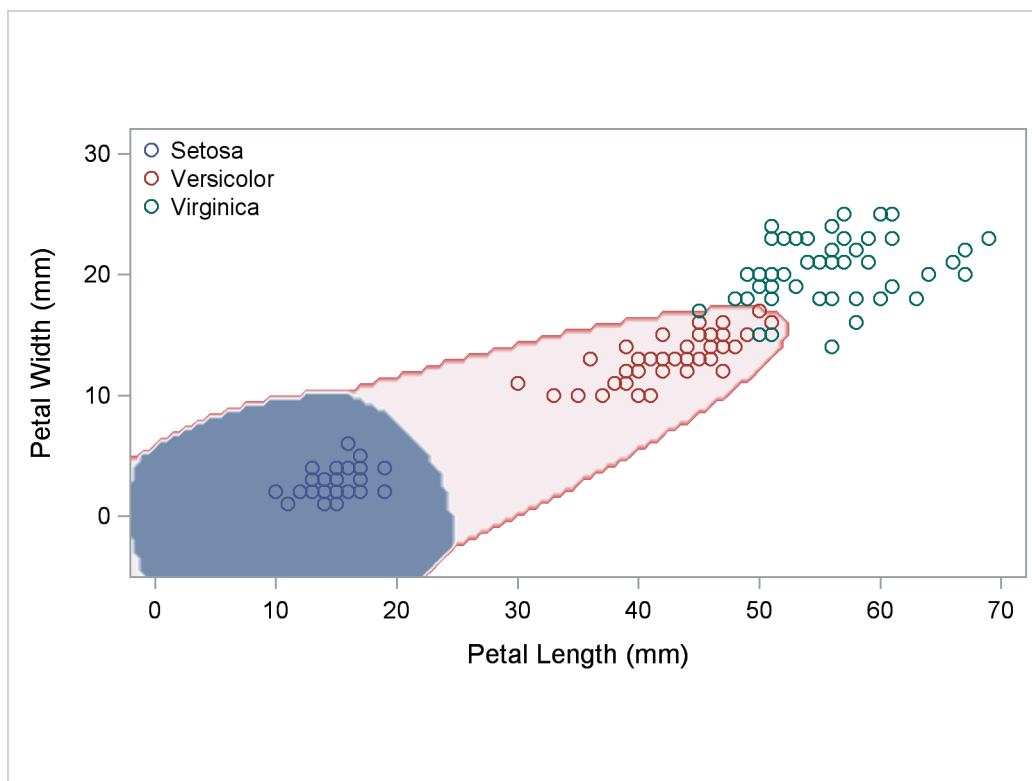
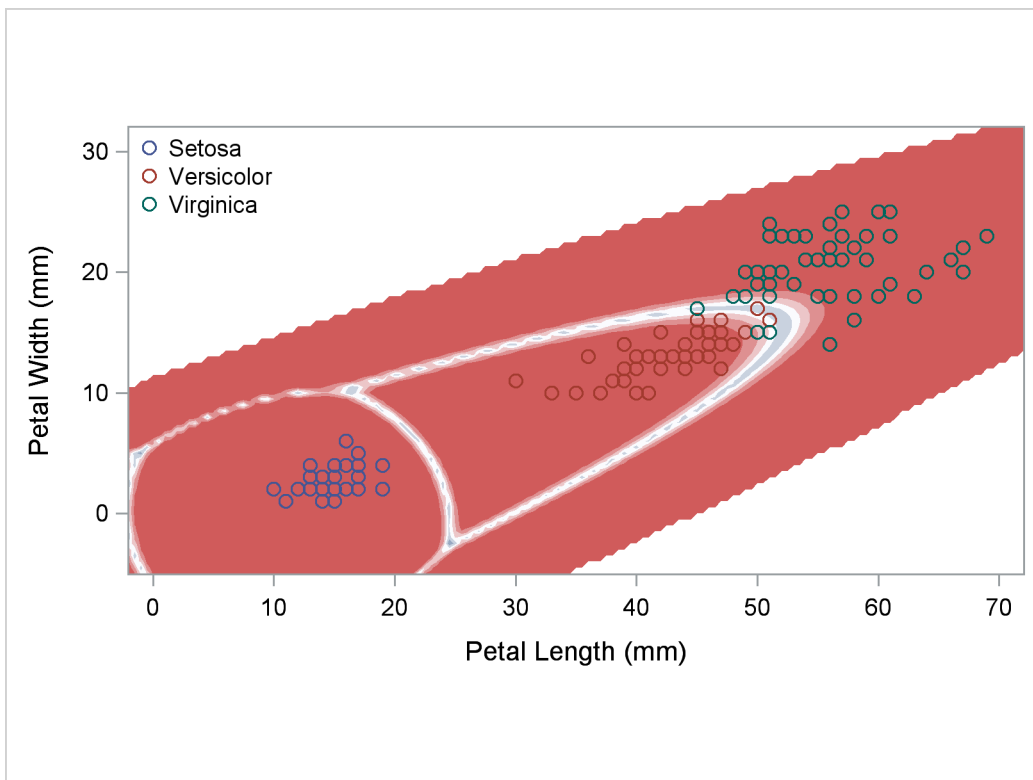
Number of Observations and Percent Classified into Species

	Setosa	Versicolor	Virginica	Total
Total	1382	1345	8448	11175
	12.37	12.04	75.60	100.00
Priors	0.33333	0.33333	0.33333	

Output 33.2.3 *continued*



Output 33.2.3 continued



A nonparametric analysis (METHOD=NPARG) follows, using normal kernels (KERNEL=NORMAL) and equal bandwidths (POOL=YES) in each class. The value of the radius parameter r that, assuming normality, minimizes an approximate mean integrated square error is 0.50 (see the section “Nonparametric Methods” on page 2079). These statements produce [Output 33.2.4](#):

```

title2 'Using Kernel Density Estimates with Equal Bandwidth';

proc discrim data=sashelp.iris method=nparg kernel=normal
    r=.5 pool=yes testoutd=plotd
    testdata=plotdata testout=plotp
    short noclassify crosslisterr;
    class Species;
    var Petal;;
run;

%contden
%contprob
%contclass
    
```

Output 33.2.4 Kernel Density Estimates with Equal Bandwidth

Discriminant Analysis of Fisher (1936) Iris Data Using Kernel Density Estimates with Equal Bandwidth					
The DISCRIM Procedure					
Total Sample Size	150	DF Total		149	
Variables	2	DF Within Classes		147	
Classes	3	DF Between Classes		2	
Number of Observations Read				150	
Number of Observations Used				150	
Class Level Information					
Species	Variable Name	Frequency	Weight	Proportion	Prior Probability
Setosa	Setosa	50	50.0000	0.333333	0.333333
Versicolor	Versicolor	50	50.0000	0.333333	0.333333
Virginica	Virginica	50	50.0000	0.333333	0.333333

Output 33.2.4 continued

Discriminant Analysis of Fisher (1936) Iris Data
Using Kernel Density Estimates with Equal Bandwidth

The DISCRIM Procedure
Classification Results for Calibration Data: SASHELP.IRIS
Cross-validation Results using Normal Kernel Density

Posterior Probability of Membership in Species

Obs	From Species	Classified into Species	Setosa	Versicolor	Virginica
53	Versicolor	Virginica *	0.0000	0.0800	0.9200
100	Versicolor	Virginica *	0.0000	0.4123	0.5877
103	Virginica	Versicolor *	0.0000	0.7474	0.2526
113	Virginica	Versicolor *	0.0000	0.5863	0.4137
136	Virginica	Versicolor *	0.0000	0.8358	0.1642

* Misclassified observation

Discriminant Analysis of Fisher (1936) Iris Data
Using Kernel Density Estimates with Equal Bandwidth

The DISCRIM Procedure
Classification Summary for Calibration Data: SASHELP.IRIS
Cross-validation Summary using Normal Kernel Density

Number of Observations and Percent Classified into Species

From Species	Setosa	Versicolor	Virginica	Total
Setosa	50 100.00	0 0.00	0 0.00	50 100.00
Versicolor	0 0.00	48 96.00	2 4.00	50 100.00
Virginica	0 0.00	3 6.00	47 94.00	50 100.00
Total	50 33.33	51 34.00	49 32.67	150 100.00
Priors	0.33333	0.33333	0.33333	

Error Count Estimates for Species

	Setosa	Versicolor	Virginica	Total
Rate	0.0000	0.0400	0.0600	0.0333
Priors	0.3333	0.3333	0.3333	

Output 33.2.4 *continued*

Discriminant Analysis of Fisher (1936) Iris Data
Using Kernel Density Estimates with Equal Bandwidth

The DISCRIM Procedure
Classification Summary for Test Data: WORK.PLOTDATA
Classification Summary using Normal Kernel Density

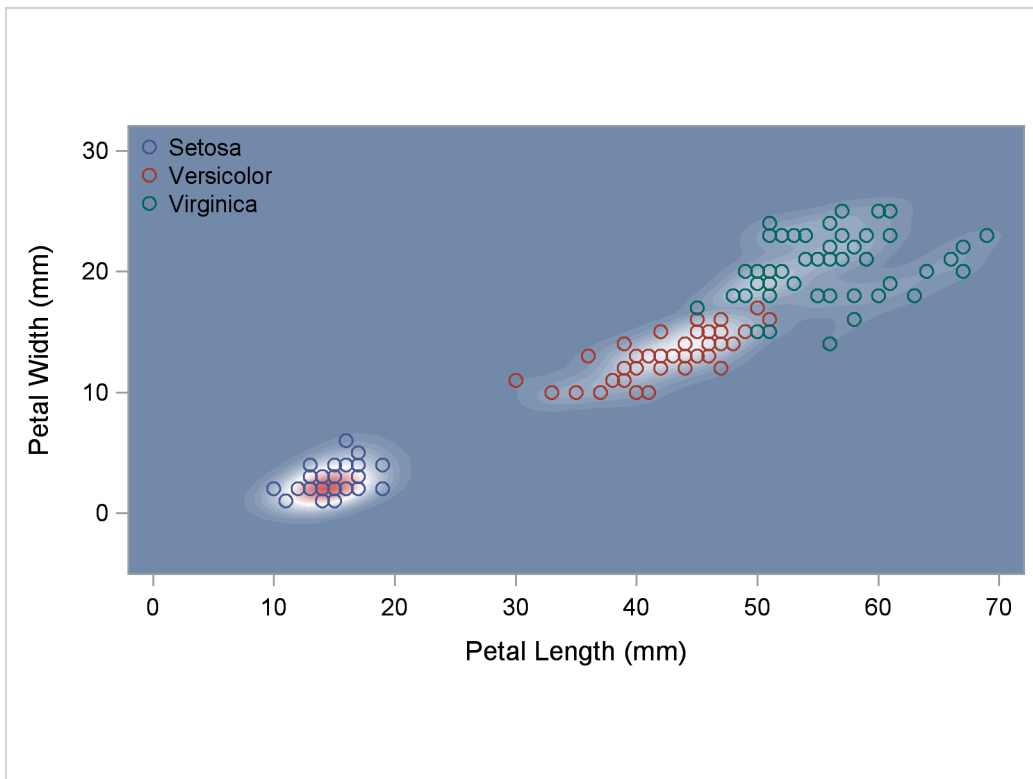
Observation Profile for Test Data

Number of Observations Read	11175
Number of Observations Used	11175

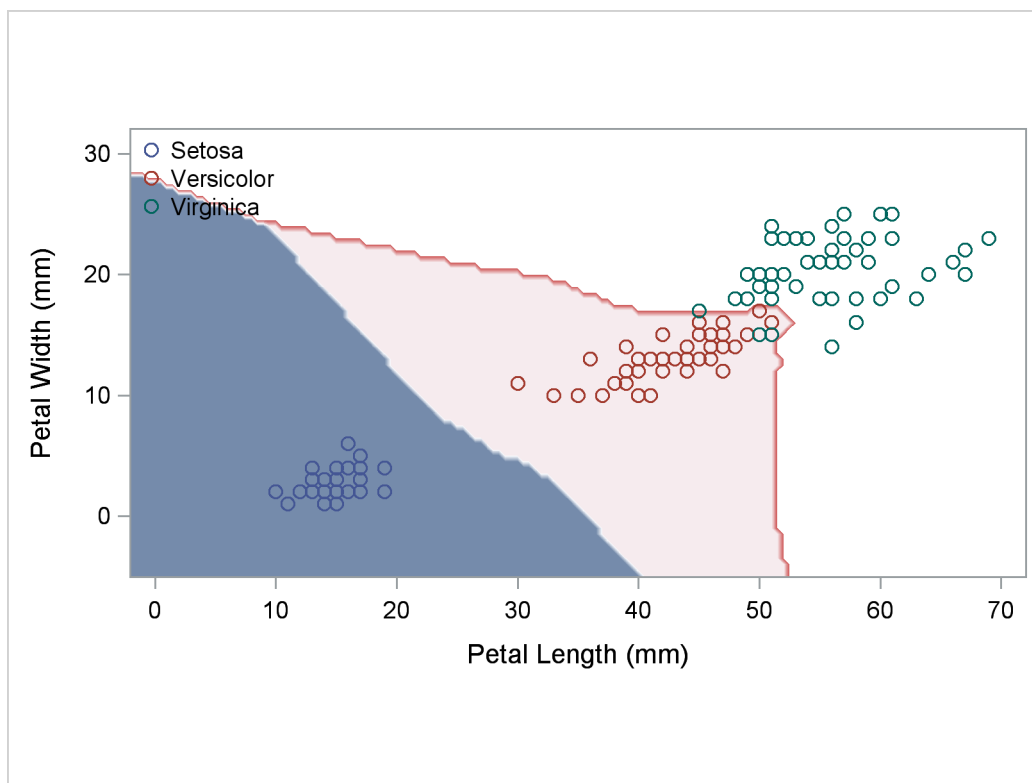
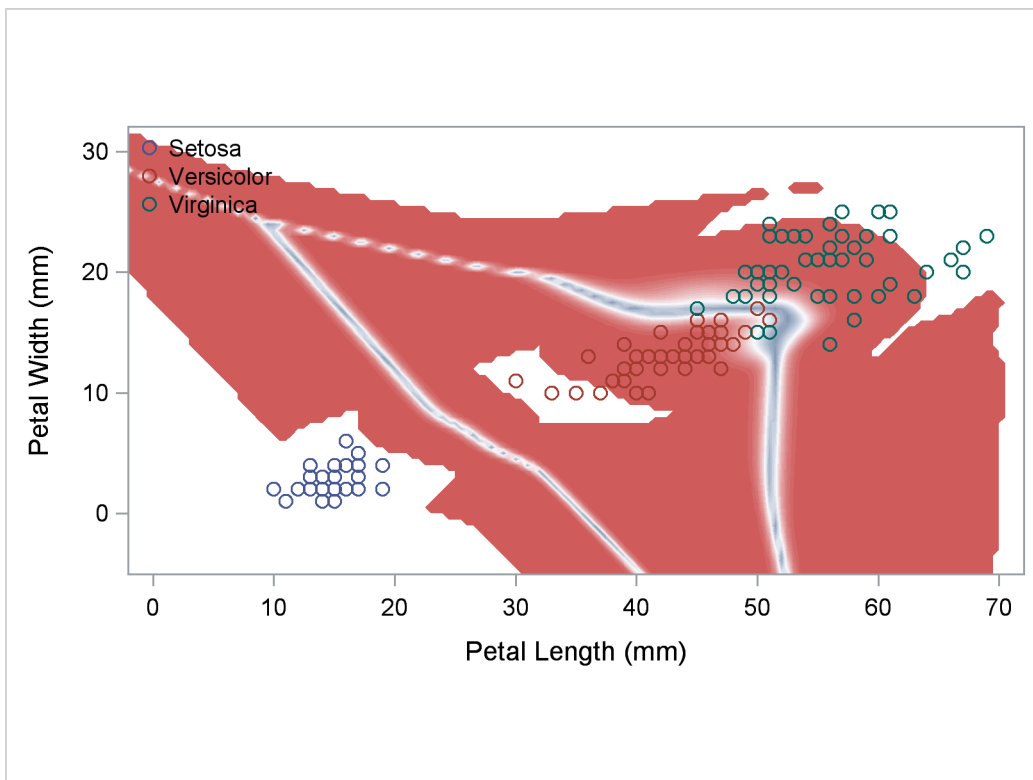
Number of Observations and Percent Classified into Species

	Setosa	Versicolor	Virginica	Total
Total	3195	2492	5488	11175
	28.59	22.30	49.11	100.00
Priors	0.33333	0.33333	0.33333	

Output 33.2.4 *continued*



Output 33.2.4 continued



Another nonparametric analysis is run with unequal bandwidths (POOL=NO). These statements produce Output 33.2.5:

```

title2 'Using Kernel Density Estimates with Unequal Bandwidth';

proc discrim data=sashelp.iris method=npnr kernel=normal
    r=.5 pool=no testoutd=plotd
    testdata=plotdata testout=plotp
    short noclassify crosslisterr;
    class Species;
    var Petal;;
run;

%contden
%contprob
%contclass
    
```

Output 33.2.5 Kernel Density Estimates with Unequal Bandwidth

Discriminant Analysis of Fisher (1936) Iris Data Using Kernel Density Estimates with Unequal Bandwidth					
The DISCRIM Procedure					
Total Sample Size	150	DF Total		149	
Variables	2	DF Within Classes		147	
Classes	3	DF Between Classes		2	
Number of Observations Read		150			
Number of Observations Used		150			
Class Level Information					
Species	Variable Name	Frequency	Weight	Proportion	Prior Probability
Setosa	Setosa	50	50.0000	0.333333	0.333333
Versicolor	Versicolor	50	50.0000	0.333333	0.333333
Virginica	Virginica	50	50.0000	0.333333	0.333333

Output 33.2.5 continued

Discriminant Analysis of Fisher (1936) Iris Data
Using Kernel Density Estimates with Unequal Bandwidth

The DISCRIM Procedure
Classification Results for Calibration Data: SASHELP.IRIS
Cross-validation Results using Normal Kernel Density

Posterior Probability of Membership in Species

Obs	From Species	Classified into Species	Setosa	Versicolor	Virginica
53	Versicolor	Virginica *	0.0000	0.0516	0.9484
100	Versicolor	Virginica *	0.0000	0.3773	0.6227
103	Virginica	Versicolor *	0.0000	0.7826	0.2174
136	Virginica	Versicolor *	0.0000	0.8802	0.1198

* Misclassified observation

Discriminant Analysis of Fisher (1936) Iris Data
Using Kernel Density Estimates with Unequal Bandwidth

The DISCRIM Procedure
Classification Summary for Calibration Data: SASHELP.IRIS
Cross-validation Summary using Normal Kernel Density

Number of Observations and Percent Classified into Species

From Species	Setosa	Versicolor	Virginica	Total
Setosa	50 100.00	0 0.00	0 0.00	50 100.00
Versicolor	0 0.00	48 96.00	2 4.00	50 100.00
Virginica	0 0.00	2 4.00	48 96.00	50 100.00
Total	50 33.33	50 33.33	50 33.33	150 100.00
Priors	0.33333	0.33333	0.33333	

Error Count Estimates for Species

	Setosa	Versicolor	Virginica	Total
Rate	0.0000	0.0400	0.0400	0.0267
Priors	0.3333	0.3333	0.3333	

Output 33.2.5 *continued*

Discriminant Analysis of Fisher (1936) Iris Data
Using Kernel Density Estimates with Unequal Bandwidth

The DISCRIM Procedure
Classification Summary for Test Data: WORK.PLOTDATA
Classification Summary using Normal Kernel Density

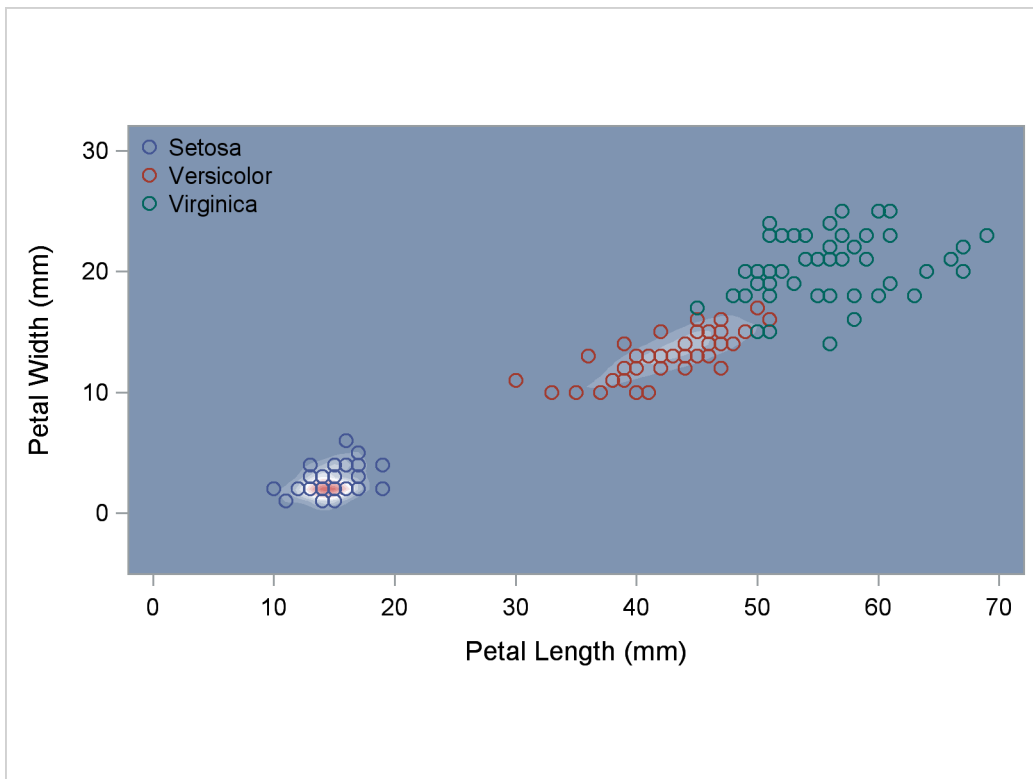
Observation Profile for Test Data

Number of Observations Read	11175
Number of Observations Used	11175

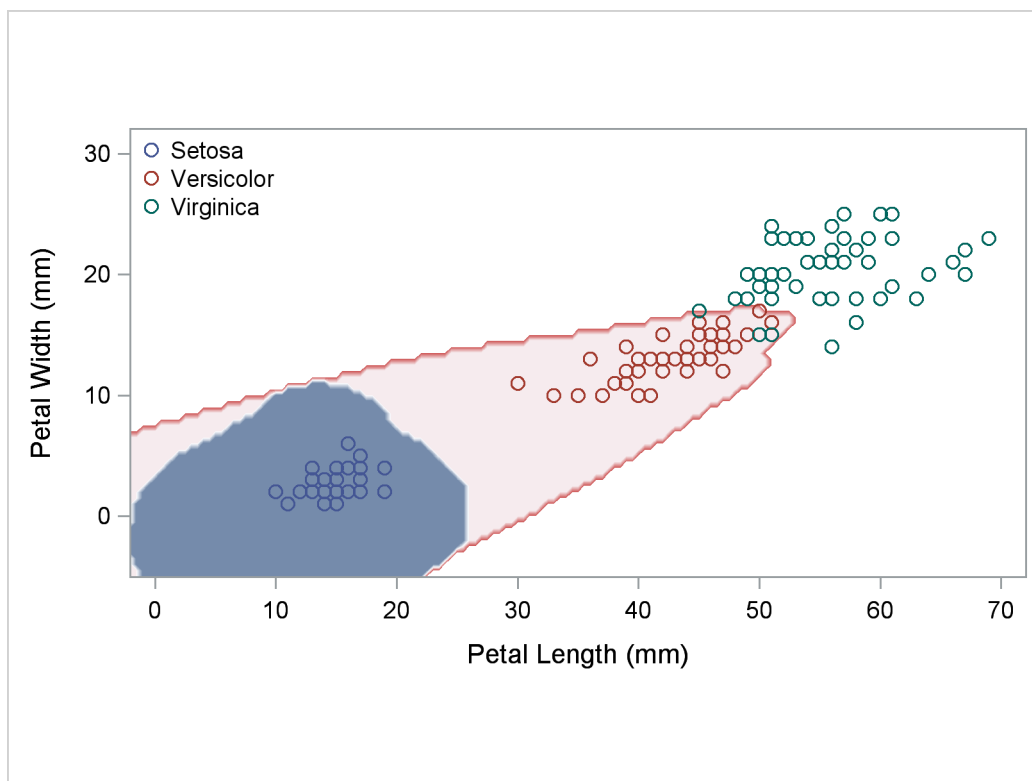
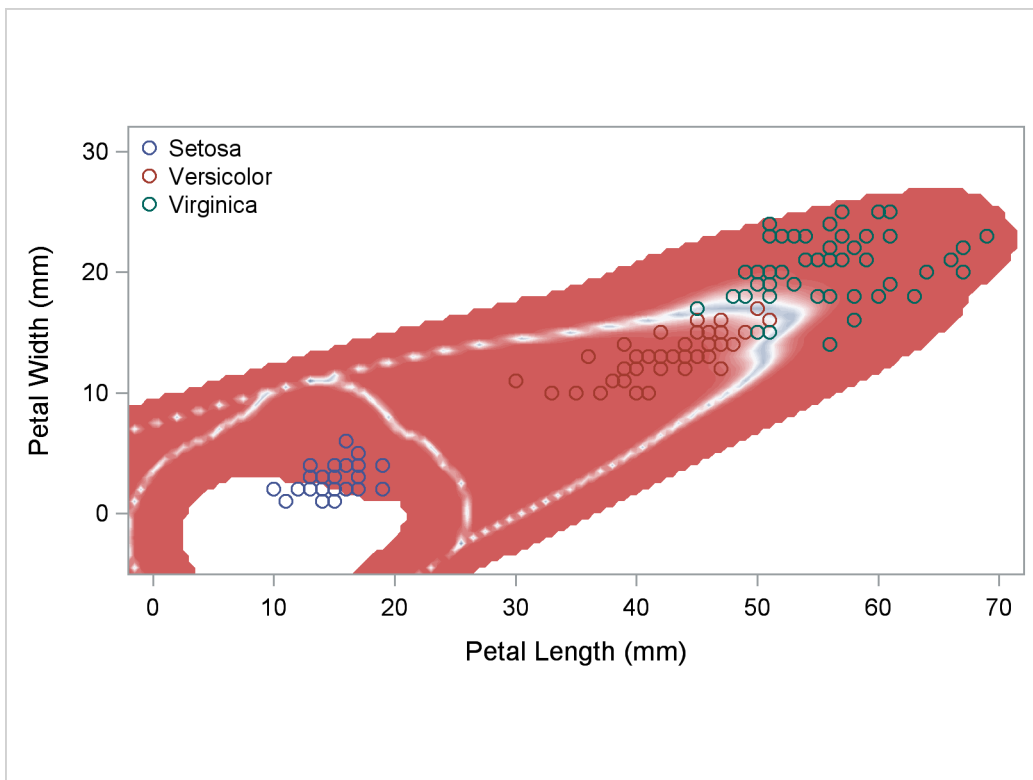
Number of Observations and Percent Classified into Species

	Setosa	Versicolor	Virginica	Total
Total	1370	1505	8300	11175
	12.26	13.47	74.27	100.00
Priors	0.33333	0.33333	0.33333	

Output 33.2.5 *continued*



Output 33.2.5 continued



Example 33.3: Normal-Theory Discriminant Analysis of Iris Data

In this example, PROC DISCRIM uses normal-theory methods to classify the iris data used in Example 33.1. The POOL=TEST option tests the homogeneity of the within-group covariance matrices (Output 33.3.3). Since the resulting test statistic is significant at the 0.10 level, the within-group covariance matrices are used to derive the quadratic discriminant criterion. The WCOV and PCOV options display the within-group covariance matrices and the pooled covariance matrix (Output 33.3.2). The DISTANCE option displays squared distances between classes (Output 33.3.4). The ANOVA and MANOVA options test the hypothesis that the class means are equal, by using univariate statistics and multivariate statistics; all statistics are significant at the 0.0001 level (Output 33.3.5). The LISTERR option lists the misclassified observations under resubstitution (Output 33.3.6). The CROSSLISTERR option lists the observations that are misclassified under cross validation and displays cross validation error-rate estimates (Output 33.3.7). The resubstitution error count estimate, 0.02, is not larger than the cross validation error count estimate, 0.0267, as would be expected because the resubstitution estimate is optimistically biased. The OUTSTAT= option generates a TYPE=MIXED (because POOL=TEST) output data set containing various statistics such as means, covariances, and coefficients of the discriminant function (Output 33.3.8).

The following statements produce Output 33.3.1 through Output 33.3.8:

```

title 'Discriminant Analysis of Fisher (1936) Iris Data';
title2 'Using Quadratic Discriminant Function';

proc discrim data=sashelp.iris outstat=irisstat
            wcov pcov method=normal pool=test
            distance anova manova listerr crosslisterr;
  class Species;
  var SepalLength SepalWidth PetalLength PetalWidth;
run;

proc print data=irisstat;
  title2 'Output Discriminant Statistics';
run;

```

Output 33.3.1 Quadratic Discriminant Analysis of Iris Data

Discriminant Analysis of Fisher (1936) Iris Data Using Quadratic Discriminant Function			
The DISCRIM Procedure			
Total Sample Size	150	DF Total	149
Variables	4	DF Within Classes	147
Classes	3	DF Between Classes	2
Number of Observations Read		150	
Number of Observations Used		150	

Output 33.3.1 continued

Class Level Information					
Species	Variable Name	Frequency	Weight	Proportion	Prior Probability
Setosa	Setosa	50	50.0000	0.333333	0.333333
Versicolor	Versicolor	50	50.0000	0.333333	0.333333
Virginica	Virginica	50	50.0000	0.333333	0.333333

Output 33.3.2 Covariance Matrices

Discriminant Analysis of Fisher (1936) Iris Data Using Quadratic Discriminant Function					
The DISCRIM Procedure Within-Class Covariance Matrices					
Species = Setosa, DF = 49					
Variable	Label	SepalLength	SepalWidth	PetalLength	PetalWidth
Sepal Length	Sepal Length (mm)	12.42489796	9.92163265	1.63551020	1.03306122
SepalWidth	Sepal Width (mm)	9.92163265	14.36897959	1.16979592	0.92979592
Petal Length	Petal Length (mm)	1.63551020	1.16979592	3.01591837	0.60693878
PetalWidth	Petal Width (mm)	1.03306122	0.92979592	0.60693878	1.11061224

Species = Versicolor, DF = 49					
Variable	Label	SepalLength	SepalWidth	PetalLength	PetalWidth
Sepal Length	Sepal Length (mm)	26.64326531	8.51836735	18.28979592	5.57795918
SepalWidth	Sepal Width (mm)	8.51836735	9.84693878	8.26530612	4.12040816
Petal Length	Petal Length (mm)	18.28979592	8.26530612	22.08163265	7.31020408
PetalWidth	Petal Width (mm)	5.57795918	4.12040816	7.31020408	3.91061224

Output 33.3.2 *continued*

```

-----
                                Species = Virginica,      DF = 49
Variable  Label                SepalLength  SepalWidth  PetalLength  PetalWidth
Sepal     Sepal Length        40.43428571  9.37632653  30.32897959  4.90938776
Length   (mm)
SepalWidth Sepal Width (mm)    9.37632653  10.40040816  7.13795918  4.76285714
Petal     Petal Length        30.32897959  7.13795918  30.45877551  4.88244898
Length   (mm)
PetalWidth Petal Width (mm)    4.90938776  4.76285714  4.88244898  7.54326531
-----

Discriminant Analysis of Fisher (1936) Iris Data
Using Quadratic Discriminant Function

The DISCRIM Procedure

Pooled Within-Class Covariance Matrix,      DF = 147
Variable  Label                SepalLength  SepalWidth  PetalLength  PetalWidth
Sepal     Sepal Length        26.50081633  9.27210884  16.75142857  3.84013605
Length   (mm)
SepalWidth Sepal Width (mm)    9.27210884  11.53877551  5.52435374  3.27102041
Petal     Petal Length        16.75142857  5.52435374  18.51877551  4.26653061
Length   (mm)
PetalWidth Petal Width (mm)    3.84013605  3.27102041  4.26653061  4.18816327
    
```

Output 33.3.2 *continued*

```

Within Covariance Matrix Information

Species      Covariance Matrix Rank      Natural Log of the
Determinant of the
Covariance Matrix

Setosa              4              5.35332
Versicolor          4              7.54636
Virginica           4              9.49362
Pooled              4              8.46214
    
```

Output 33.3.3 Homogeneity Test

Discriminant Analysis of Fisher (1936) Iris Data
Using Quadratic Discriminant Function

The DISCRIM Procedure
Test of Homogeneity of Within Covariance Matrices

Chi-Square	DF	Pr > ChiSq
140.943050	20	<.0001

Since the Chi-Square value is significant at the 0.1 level, the within covariance matrices will be used in the discriminant function.

Reference: Morrison, D.F. (1976) Multivariate Statistical Methods p252.

Output 33.3.4 Squared Distances

Discriminant Analysis of Fisher (1936) Iris Data
Using Quadratic Discriminant Function

The DISCRIM Procedure

Squared Distance to Species

From Species	Setosa	Versicolor	Virginica
Setosa	0	103.19382	168.76759
Versicolor	323.06203	0	13.83875
Virginica	706.08494	17.86670	0

Generalized Squared Distance to Species

From Species	Setosa	Versicolor	Virginica
Setosa	5.35332	110.74017	178.26121
Versicolor	328.41535	7.54636	23.33238
Virginica	711.43826	25.41306	9.49362

Output 33.3.5 Tests of Equal Class Means

```

Discriminant Analysis of Fisher (1936) Iris Data
Using Quadratic Discriminant Function

The DISCRIM Procedure

Univariate Test Statistics

F Statistics,      Num DF=2,      Den DF=147

      Total      Pooled      Between
Variable Label  Standard  Standard  Standard  R-Square / (1-RSq) F Value Pr > F
Deviation      Deviation      Deviation
Sepal Length (mm)  8.2807      5.1479      7.9506      0.6187      1.6226      119.26 <.0001
Sepal Width (mm)   4.3587      3.3969      3.3682      0.4008      0.6688      49.16 <.0001
Petal Length (mm) 17.6530      4.3033      20.9070     0.9414      16.0566     1180.16 <.0001
Petal Width (mm)   7.6224      2.0465      8.9673      0.9289      13.0613     960.01 <.0001

Average R-Square

Unweighted          0.7224358
Weighted by Variance 0.8689444

Multivariate Statistics and F Approximations

      S=2      M=0.5      N=71

Statistic          Value      F Value      Num DF      Den DF      Pr > F
Wilks' Lambda      0.02343863      199.15      8      288      <.0001
Pillai's Trace     1.19189883      53.47      8      290      <.0001
Hotelling-Lawley Trace 32.47732024      582.20      8      203.4      <.0001
Roy's Greatest Root 32.19192920      1166.96      4      145      <.0001

NOTE: F Statistic for Roy's Greatest Root is an upper bound.
NOTE: F Statistic for Wilks' Lambda is exact.
    
```


Output 33.3.6 Misclassified Observations: Resubstitution

Discriminant Analysis of Fisher (1936) Iris Data Using Quadratic Discriminant Function					
The DISCRIM Procedure					
Classification Results for Calibration Data: SASHELP.IRIS					
Resubstitution Results using Quadratic Discriminant Function					
Posterior Probability of Membership in Species					
Obs	From Species	Classified into Species	Setosa	Versicolor	Virginica
53	Versicolor	Virginica *	0.0000	0.3359	0.6641
55	Versicolor	Virginica *	0.0000	0.1543	0.8457
103	Virginica	Versicolor *	0.0000	0.6050	0.3950
* Misclassified observation					
Discriminant Analysis of Fisher (1936) Iris Data Using Quadratic Discriminant Function					
The DISCRIM Procedure					
Classification Summary for Calibration Data: SASHELP.IRIS					
Resubstitution Summary using Quadratic Discriminant Function					
Number of Observations and Percent Classified into Species					
From Species	Setosa	Versicolor	Virginica	Total	
Setosa	50 100.00	0 0.00	0 0.00	50 100.00	
Versicolor	0 0.00	48 96.00	2 4.00	50 100.00	
Virginica	0 0.00	1 2.00	49 98.00	50 100.00	
Total	50 33.33	49 32.67	51 34.00	150 100.00	
Priors	0.33333	0.33333	0.33333		
Error Count Estimates for Species					
	Setosa	Versicolor	Virginica	Total	
Rate	0.0000	0.0400	0.0200	0.0200	
Priors	0.3333	0.3333	0.3333		

Output 33.3.7 Misclassified Observations: Cross Validation

Discriminant Analysis of Fisher (1936) Iris Data Using Quadratic Discriminant Function					
The DISCRIM Procedure					
Classification Results for Calibration Data: SASHELP.IRIS					
Cross-validation Results using Quadratic Discriminant Function					
Posterior Probability of Membership in Species					
Obs	From Species	Classified into Species	Setosa	Versicolor	Virginica
52	Versicolor	Virginica *	0.0000	0.3134	0.6866
53	Versicolor	Virginica *	0.0000	0.1616	0.8384
55	Versicolor	Virginica *	0.0000	0.0713	0.9287
103	Virginica	Versicolor *	0.0000	0.6632	0.3368
* Misclassified observation					
Discriminant Analysis of Fisher (1936) Iris Data Using Quadratic Discriminant Function					
The DISCRIM Procedure					
Classification Summary for Calibration Data: SASHELP.IRIS					
Cross-validation Summary using Quadratic Discriminant Function					
Number of Observations and Percent Classified into Species					
From Species	Setosa	Versicolor	Virginica	Total	
Setosa	50 100.00	0 0.00	0 0.00	50 100.00	
Versicolor	0 0.00	47 94.00	3 6.00	50 100.00	
Virginica	0 0.00	1 2.00	49 98.00	50 100.00	
Total	50 33.33	48 32.00	52 34.67	150 100.00	
Priors	0.33333	0.33333	0.33333		
Error Count Estimates for Species					
	Setosa	Versicolor	Virginica	Total	
Rate	0.0000	0.0600	0.0200	0.0267	
Priors	0.3333	0.3333	0.3333		

Output 33.3.8 Output Statistics from Iris Data

Discriminant Analysis of Fisher (1936) Iris Data							
Output Discriminant Statistics							
Obs	Species	_TYPE_	_NAME_	Sepal Length	Sepal Width	Petal Length	Petal Width
1		N		150.00	150.00	150.00	150.00
2	Setosa	N		50.00	50.00	50.00	50.00
3	Versicolor	N		50.00	50.00	50.00	50.00
4	Virginica	N		50.00	50.00	50.00	50.00
5		MEAN		58.43	30.57	37.58	11.99
6	Setosa	MEAN		50.06	34.28	14.62	2.46
7	Versicolor	MEAN		59.36	27.70	42.60	13.26
8	Virginica	MEAN		65.88	29.74	55.52	20.26
9	Setosa	PRIOR		0.33	0.33	0.33	0.33
10	Versicolor	PRIOR		0.33	0.33	0.33	0.33
11	Virginica	PRIOR		0.33	0.33	0.33	0.33
12	Setosa	CSSCP	SepalLength	608.82	486.16	80.14	50.62
13	Setosa	CSSCP	SepalWidth	486.16	704.08	57.32	45.56
14	Setosa	CSSCP	PetalLength	80.14	57.32	147.78	29.74
15	Setosa	CSSCP	PetalWidth	50.62	45.56	29.74	54.42
16	Versicolor	CSSCP	SepalLength	1305.52	417.40	896.20	273.32
17	Versicolor	CSSCP	SepalWidth	417.40	482.50	405.00	201.90
18	Versicolor	CSSCP	PetalLength	896.20	405.00	1082.00	358.20
19	Versicolor	CSSCP	PetalWidth	273.32	201.90	358.20	191.62
20	Virginica	CSSCP	SepalLength	1981.28	459.44	1486.12	240.56
21	Virginica	CSSCP	SepalWidth	459.44	509.62	349.76	233.38
22	Virginica	CSSCP	PetalLength	1486.12	349.76	1492.48	239.24
23	Virginica	CSSCP	PetalWidth	240.56	233.38	239.24	369.62
24		PSSCP	SepalLength	3895.62	1363.00	2462.46	564.50
25		PSSCP	SepalWidth	1363.00	1696.20	812.08	480.84
26		PSSCP	PetalLength	2462.46	812.08	2722.26	627.18
27		PSSCP	PetalWidth	564.50	480.84	627.18	615.66
28		BSSCP	SepalLength	6321.21	-1995.27	16524.84	7127.93
29		BSSCP	SepalWidth	-1995.27	1134.49	-5723.96	-2293.27
30		BSSCP	PetalLength	16524.84	-5723.96	43710.28	18677.40
31		BSSCP	PetalWidth	7127.93	-2293.27	18677.40	8041.33
32		CSSCP	SepalLength	10216.83	-632.27	18987.30	7692.43
33		CSSCP	SepalWidth	-632.27	2830.69	-4911.88	-1812.43
34		CSSCP	PetalLength	18987.30	-4911.88	46432.54	19304.58
35		CSSCP	PetalWidth	7692.43	-1812.43	19304.58	8656.99
36		RSQUARED		0.62	0.40	0.94	0.93
37	Setosa	COV	SepalLength	12.42	9.92	1.64	1.03
38	Setosa	COV	SepalWidth	9.92	14.37	1.17	0.93
39	Setosa	COV	PetalLength	1.64	1.17	3.02	0.61
40	Setosa	COV	PetalWidth	1.03	0.93	0.61	1.11
41	Versicolor	COV	SepalLength	26.64	8.52	18.29	5.58
42	Versicolor	COV	SepalWidth	8.52	9.85	8.27	4.12
43	Versicolor	COV	PetalLength	18.29	8.27	22.08	7.31
44	Versicolor	COV	PetalWidth	5.58	4.12	7.31	3.91
45	Virginica	COV	SepalLength	40.43	9.38	30.33	4.91
46	Virginica	COV	SepalWidth	9.38	10.40	7.14	4.76
47	Virginica	COV	PetalLength	30.33	7.14	30.46	4.88
48	Virginica	COV	PetalWidth	4.91	4.76	4.88	7.54

Output 33.3.8 continued

Discriminant Analysis of Fisher (1936) Iris Data							
Output Discriminant Statistics							
Obs	Species	_TYPE_	_NAME_	Sepal Length	Sepal Width	Petal Length	Petal Width
49		PCOV	SepalLength	26.501	9.2721	16.751	3.840
50		PCOV	SepalWidth	9.272	11.5388	5.524	3.271
51		PCOV	PetalLength	16.751	5.5244	18.519	4.267
52		PCOV	PetalWidth	3.840	3.2710	4.267	4.188
53		BCOV	SepalLength	63.212	-19.9527	165.248	71.279
54		BCOV	SepalWidth	-19.953	11.3449	-57.240	-22.933
55		BCOV	PetalLength	165.248	-57.2396	437.103	186.774
56		BCOV	PetalWidth	71.279	-22.9327	186.774	80.413
57		COV	SepalLength	68.569	-4.2434	127.432	51.627
58		COV	SepalWidth	-4.243	18.9979	-32.966	-12.164
59		COV	PetalLength	127.432	-32.9656	311.628	129.561
60		COV	PetalWidth	51.627	-12.1639	129.561	58.101
61	Setosa	STD		3.525	3.7906	1.737	1.054
62	Versicolor	STD		5.162	3.1380	4.699	1.978
63	Virginica	STD		6.359	3.2250	5.519	2.747
64		PSTD		5.148	3.3969	4.303	2.047
65		BSTD		7.951	3.3682	20.907	8.967
66		STD		8.281	4.3587	17.653	7.622
67	Setosa	CORR	SepalLength	1.000	0.7425	0.267	0.278
68	Setosa	CORR	SepalWidth	0.743	1.0000	0.178	0.233
69	Setosa	CORR	PetalLength	0.267	0.1777	1.000	0.332
70	Setosa	CORR	PetalWidth	0.278	0.2328	0.332	1.000
71	Versicolor	CORR	SepalLength	1.000	0.5259	0.754	0.546
72	Versicolor	CORR	SepalWidth	0.526	1.0000	0.561	0.664
73	Versicolor	CORR	PetalLength	0.754	0.5605	1.000	0.787
74	Versicolor	CORR	PetalWidth	0.546	0.6640	0.787	1.000
75	Virginica	CORR	SepalLength	1.000	0.4572	0.864	0.281
76	Virginica	CORR	SepalWidth	0.457	1.0000	0.401	0.538
77	Virginica	CORR	PetalLength	0.864	0.4010	1.000	0.322
78	Virginica	CORR	PetalWidth	0.281	0.5377	0.322	1.000
79		PCORR	SepalLength	1.000	0.5302	0.756	0.365
80		PCORR	SepalWidth	0.530	1.0000	0.378	0.471
81		PCORR	PetalLength	0.756	0.3779	1.000	0.484
82		PCORR	PetalWidth	0.365	0.4705	0.484	1.000
83		BCORR	SepalLength	1.000	-0.7451	0.994	1.000
84		BCORR	SepalWidth	-0.745	1.0000	-0.813	-0.759
85		BCORR	PetalLength	0.994	-0.8128	1.000	0.996
86		BCORR	PetalWidth	1.000	-0.7593	0.996	1.000
87		CORR	SepalLength	1.000	-0.1176	0.872	0.818
88		CORR	SepalWidth	-0.118	1.0000	-0.428	-0.366
89		CORR	PetalLength	0.872	-0.4284	1.000	0.963
90		CORR	PetalWidth	0.818	-0.3661	0.963	1.000
91	Setosa	STDMEAN		-1.011	0.8504	-1.301	-1.251
92	Versicolor	STDMEAN		0.112	-0.6592	0.284	0.166
93	Virginica	STDMEAN		0.899	-0.1912	1.016	1.085
94	Setosa	PSTDMEAN		-1.627	1.0912	-5.335	-4.658
95	Versicolor	PSTDMEAN		0.180	-0.8459	1.167	0.619
96	Virginica	PSTDMEAN		1.447	-0.2453	4.169	4.039

Output 33.3.8 continued

Discriminant Analysis of Fisher (1936) Iris Data							
Output Discriminant Statistics							
Obs	Species	_TYPE_	_NAME_	Sepal Length	Sepal Width	Petal Length	Petal Width
97		LNDETERM		8.462	8.462	8.462	8.462
98	Setosa	LNDETERM		5.353	5.353	5.353	5.353
99	Versicolor	LNDETERM		7.546	7.546	7.546	7.546
100	Virginica	LNDETERM		9.494	9.494	9.494	9.494
101	Setosa	QUAD	SepalLength	-0.095	0.062	0.023	0.024
102	Setosa	QUAD	SepalWidth	0.062	-0.078	-0.006	0.011
103	Setosa	QUAD	PetalLength	0.023	-0.006	-0.194	0.090
104	Setosa	QUAD	PetalWidth	0.024	0.011	0.090	-0.530
105	Setosa	QUAD	_LINEAR_	4.455	-0.762	3.356	-3.126
106	Setosa	QUAD	_CONST_	-121.826	-121.826	-121.826	-121.826
107	Versicolor	QUAD	SepalLength	-0.048	0.018	0.043	-0.032
108	Versicolor	QUAD	SepalWidth	0.018	-0.099	-0.011	0.097
109	Versicolor	QUAD	PetalLength	0.043	-0.011	-0.099	0.135
110	Versicolor	QUAD	PetalWidth	-0.032	0.097	0.135	-0.436
111	Versicolor	QUAD	_LINEAR_	1.801	1.596	0.327	-1.471
112	Versicolor	QUAD	_CONST_	-76.549	-76.549	-76.549	-76.549
113	Virginica	QUAD	SepalLength	-0.053	0.017	0.050	-0.009
114	Virginica	QUAD	SepalWidth	0.017	-0.079	-0.006	0.042
115	Virginica	QUAD	PetalLength	0.050	-0.006	-0.067	0.014
116	Virginica	QUAD	PetalWidth	-0.009	0.042	0.014	-0.097
117	Virginica	QUAD	_LINEAR_	0.737	1.325	0.623	0.966
118	Virginica	QUAD	_CONST_	-75.821	-75.821	-75.821	-75.821

Example 33.4: Linear Discriminant Analysis of Remote-Sensing Data on Crops

In this example, the remote-sensing data are used. In this data set, the observations are grouped into five crops: clover, corn, cotton, soybeans, and sugar beets. Four measures called x1 through x4 make up the descriptive variables.

In the first PROC DISCRIM statement, the DISCRIM procedure uses normal-theory methods (METHOD=NORMAL) assuming equal variances (POOL=YES) in five crops. The PRIORS statement, PRIORS PROP, sets the prior probabilities proportional to the sample sizes. The LIST option lists the resubstitution classification results for each observation (Output 33.4.2). The CROSSVALIDATE option displays cross validation error-rate estimates (Output 33.4.3). The OUTSTAT= option stores the calibration information in a new data set to classify future observations. A second PROC DISCRIM statement uses this calibration information to classify a test data set. Note that the values of the identification variable, xvalues, are obtained by rereading the x1 through x4 fields in the data lines as a single character variable. The following statements produce Output 33.4.1 through Output 33.4.3:

```

title 'Discriminant Analysis of Remote Sensing Data on Five Crops';

data crops;
  input Crop $ 1-10 x1-x4 xvalues $ 11-21;
  datalines;
Corn      16 27 31 33
Corn      15 23 30 30
Corn      16 27 27 26
Corn      18 20 25 23
Corn      15 15 31 32
Corn      15 32 32 15
Corn      12 15 16 73
Soybeans  20 23 23 25
Soybeans  24 24 25 32
Soybeans  21 25 23 24
Soybeans  27 45 24 12
Soybeans  12 13 15 42
Soybeans  22 32 31 43
Cotton    31 32 33 34
Cotton    29 24 26 28
Cotton    34 32 28 45
Cotton    26 25 23 24
Cotton    53 48 75 26
Cotton    34 35 25 78
Sugarbeets22 23 25 42
Sugarbeets25 25 24 26
Sugarbeets34 25 16 52
Sugarbeets54 23 21 54
Sugarbeets25 43 32 15
Sugarbeets26 54 2 54
Clover    12 45 32 54
Clover    24 58 25 34
Clover    87 54 61 21
Clover    51 31 31 16
Clover    96 48 54 62
Clover    31 31 11 11
Clover    56 13 13 71
Clover    32 13 27 32
Clover    36 26 54 32
Clover    53 08 06 54
Clover    32 32 62 16
;

title2 'Using the Linear Discriminant Function';

proc discrim data=crops outstat=cropstat method=normal pool=yes
  list crossvalidate;
  class Crop;
  priors prop;
  id xvalues;
  var x1-x4;
run;

```

Output 33.4.1 Linear Discriminant Function on Crop Data

Discriminant Analysis of Remote Sensing Data on Five Crops Using the Linear Discriminant Function					
The DISCRIM Procedure					
Total Sample Size	36	DF Total	35		
Variables	4	DF Within Classes	31		
Classes	5	DF Between Classes	4		
Number of Observations Read		36			
Number of Observations Used		36			
Class Level Information					
Crop	Variable Name	Frequency	Weight	Proportion	Prior Probability
Clover	Clover	11	11.0000	0.305556	0.305556
Corn	Corn	7	7.0000	0.194444	0.194444
Cotton	Cotton	6	6.0000	0.166667	0.166667
Soybeans	Soybeans	6	6.0000	0.166667	0.166667
Sugarbeets	Sugarbeets	6	6.0000	0.166667	0.166667
Pooled Covariance Matrix Information					
Covariance Matrix Rank		Natural Log of the Determinant of the Covariance Matrix			
4		21.30189			
Discriminant Analysis of Remote Sensing Data on Five Crops Using the Linear Discriminant Function					
The DISCRIM Procedure					
Generalized Squared Distance to Crop					
From Crop	Clover	Corn	Cotton	Soybeans	Sugarbeets
Clover	2.37125	7.52830	4.44969	6.16665	5.07262
Corn	6.62433	3.27522	5.46798	4.31383	6.47395
Cotton	3.23741	5.15968	3.58352	5.01819	4.87908
Soybeans	4.95438	4.00552	5.01819	3.58352	4.65998
Sugarbeets	3.86034	6.16564	4.87908	4.65998	3.58352

Output 33.4.1 *continued*

Linear Discriminant Function for Crop					
Variable	Clover	Corn	Cotton	Soybeans	Sugarbeets
Constant	-10.98457	-7.72070	-11.46537	-7.28260	-9.80179
x1	0.08907	-0.04180	0.02462	0.0000369	0.04245
x2	0.17379	0.11970	0.17596	0.15896	0.20988
x3	0.11899	0.16511	0.15880	0.10622	0.06540
x4	0.15637	0.16768	0.18362	0.14133	0.16408

Output 33.4.2 Misclassified Observations: Resubstitution

Discriminant Analysis of Remote Sensing Data on Five Crops
Using the Linear Discriminant Function

The DISCRIM Procedure
Classification Results for Calibration Data: WORK.CROPS
Resubstitution Results using Linear Discriminant Function

Posterior Probability of Membership in Crop

xvalues	From Crop	Classified into Crop	Clover	Corn	Cotton	Soybeans	Sugarbeets
16 27 31 33	Corn	Corn	0.0894	0.4054	0.1763	0.2392	0.0897
15 23 30 30	Corn	Corn	0.0769	0.4558	0.1421	0.2530	0.0722
16 27 27 26	Corn	Corn	0.0982	0.3422	0.1365	0.3073	0.1157
18 20 25 23	Corn	Corn	0.1052	0.3634	0.1078	0.3281	0.0955
15 15 31 32	Corn	Corn	0.0588	0.5754	0.1173	0.2087	0.0398
15 32 32 15	Corn	Soybeans *	0.0972	0.3278	0.1318	0.3420	0.1011
12 15 16 73	Corn	Corn	0.0454	0.5238	0.1849	0.1376	0.1083
20 23 23 25	Soybeans	Soybeans	0.1330	0.2804	0.1176	0.3305	0.1385
24 24 25 32	Soybeans	Soybeans	0.1768	0.2483	0.1586	0.2660	0.1502
21 25 23 24	Soybeans	Soybeans	0.1481	0.2431	0.1200	0.3318	0.1570
27 45 24 12	Soybeans	Sugarbeets *	0.2357	0.0547	0.1016	0.2721	0.3359
12 13 15 42	Soybeans	Corn *	0.0549	0.4749	0.0920	0.2768	0.1013
22 32 31 43	Soybeans	Cotton *	0.1474	0.2606	0.2624	0.1848	0.1448
31 32 33 34	Cotton	Clover *	0.2815	0.1518	0.2377	0.1767	0.1523
29 24 26 28	Cotton	Soybeans *	0.2521	0.1842	0.1529	0.2549	0.1559
34 32 28 45	Cotton	Clover *	0.3125	0.1023	0.2404	0.1357	0.2091
26 25 23 24	Cotton	Soybeans *	0.2121	0.1809	0.1245	0.3045	0.1780
53 48 75 26	Cotton	Clover *	0.4837	0.0391	0.4384	0.0223	0.0166
34 35 25 78	Cotton	Cotton	0.2256	0.0794	0.3810	0.0592	0.2548
22 23 25 42	Sugarbeets	Corn *	0.1421	0.3066	0.1901	0.2231	0.1381
25 25 24 26	Sugarbeets	Soybeans *	0.1969	0.2050	0.1354	0.2960	0.1667
34 25 16 52	Sugarbeets	Sugarbeets	0.2928	0.0871	0.1665	0.1479	0.3056
54 23 21 54	Sugarbeets	Clover *	0.6215	0.0194	0.1250	0.0496	0.1845
25 43 32 15	Sugarbeets	Soybeans *	0.2258	0.1135	0.1646	0.2770	0.2191
26 54 2 54	Sugarbeets	Sugarbeets	0.0850	0.0081	0.0521	0.0661	0.7887
12 45 32 54	Clover	Cotton *	0.0693	0.2663	0.3394	0.1460	0.1789
24 58 25 34	Clover	Sugarbeets *	0.1647	0.0376	0.1680	0.1452	0.4845
87 54 61 21	Clover	Clover	0.9328	0.0003	0.0478	0.0025	0.0165
51 31 31 16	Clover	Clover	0.6642	0.0205	0.0872	0.0959	0.1322
96 48 54 62	Clover	Clover	0.9215	0.0002	0.0604	0.0007	0.0173
31 31 11 11	Clover	Sugarbeets *	0.2525	0.0402	0.0473	0.3012	0.3588
56 13 13 71	Clover	Clover	0.6132	0.0212	0.1226	0.0408	0.2023
32 13 27 32	Clover	Clover	0.2669	0.2616	0.1512	0.2260	0.0943
36 26 54 32	Clover	Cotton *	0.2650	0.2645	0.3495	0.0918	0.0292
53 08 06 54	Clover	Clover	0.5914	0.0237	0.0676	0.0781	0.2392
32 32 62 16	Clover	Cotton *	0.2163	0.3180	0.3327	0.1125	0.0206

* Misclassified observation

Output 33.4.2 *continued*

**Discriminant Analysis of Remote Sensing Data on Five Crops
Using the Linear Discriminant Function**

The DISCRIM Procedure
 Classification Summary for Calibration Data: WORK.CROPS
 Resubstitution Summary using Linear Discriminant Function

Number of Observations and Percent Classified into Crop

From Crop	Clover	Corn	Cotton	Soybeans	Sugarbeets	Total
Clover	6 54.55	0 0.00	3 27.27	0 0.00	2 18.18	11 100.00
Corn	0 0.00	6 85.71	0 0.00	1 14.29	0 0.00	7 100.00
Cotton	3 50.00	0 0.00	1 16.67	2 33.33	0 0.00	6 100.00
Soybeans	0 0.00	1 16.67	1 16.67	3 50.00	1 16.67	6 100.00
Sugarbeets	1 16.67	1 16.67	0 0.00	2 33.33	2 33.33	6 100.00
Total	10 27.78	8 22.22	5 13.89	8 22.22	5 13.89	36 100.00
Priors	0.30556	0.19444	0.16667	0.16667	0.16667	

Error Count Estimates for Crop

	Clover	Corn	Cotton	Soybeans	Sugarbeets	Total
Rate	0.4545	0.1429	0.8333	0.5000	0.6667	0.5000
Priors	0.3056	0.1944	0.1667	0.1667	0.1667	

Output 33.4.3 Misclassified Observations: Cross Validation

Discriminant Analysis of Remote Sensing Data on Five Crops Using the Linear Discriminant Function						
The DISCRIM Procedure						
Classification Summary for Calibration Data: WORK.CROPS						
Cross-validation Summary using Linear Discriminant Function						
Number of Observations and Percent Classified into Crop						
From Crop	Clover	Corn	Cotton	Soybeans	Sugarbeets	Total
Clover	4 36.36	3 27.27	1 9.09	0 0.00	3 27.27	11 100.00
Corn	0 0.00	4 57.14	1 14.29	2 28.57	0 0.00	7 100.00
Cotton	3 50.00	0 0.00	0 0.00	2 33.33	1 16.67	6 100.00
Soybeans	0 0.00	1 16.67	1 16.67	3 50.00	1 16.67	6 100.00
Sugarbeets	2 33.33	1 16.67	0 0.00	2 33.33	1 16.67	6 100.00
Total	9 25.00	9 25.00	3 8.33	9 25.00	6 16.67	36 100.00
Priors	0.30556	0.19444	0.16667	0.16667	0.16667	
Error Count Estimates for Crop						
	Clover	Corn	Cotton	Soybeans	Sugarbeets	Total
Rate	0.6364	0.4286	1.0000	0.5000	0.8333	0.6667
Priors	0.3056	0.1944	0.1667	0.1667	0.1667	

Next, you can use the calibration information stored in the Cropstat data set to classify a test data set. The TESTLIST option lists the classification results for each observation in the test data set. The following statements produce [Output 33.4.4](#) and [Output 33.4.5](#):

```
data test;
  input Crop $ 1-10 x1-x4 xvalues $ 11-21;
  datalines;
Corn      16 27 31 33
Soybeans  21 25 23 24
Cotton    29 24 26 28
Sugarbeets54 23 21 54
Clover    32 32 62 16
;
```

```

title2 'Classification of Test Data';

proc discrim data=cropstat testdata=test testout=tout testlist;
  class Crop;
  testid xvalues;
  var x1-x4;
run;

proc print data=tout;
  title 'Discriminant Analysis of Remote Sensing Data on Five Crops';
  title2 'Output Classification Results of Test Data';
run;

```

Output 33.4.4 Classification of Test Data

Discriminant Analysis of Remote Sensing Data on Five Crops Classification of Test Data						
The DISCRIM Procedure						
Classification Results for Test Data: WORK.TEST						
Classification Results using Linear Discriminant Function						
Posterior Probability of Membership in Crop						
xvalues	From Crop	Classified into Crop	Clover Sugarbeets	Corn	Cotton	Soybeans
16 27 31 33	Corn	Corn	0.0894 0.0897	0.4054	0.1763	0.2392
21 25 23 24	Soybeans	Soybeans	0.1481 0.1570	0.2431	0.1200	0.3318
29 24 26 28	Cotton	Soybeans *	0.2521 0.1559	0.1842	0.1529	0.2549
54 23 21 54	Sugarbeets	Clover *	0.6215 0.1845	0.0194	0.1250	0.0496
32 32 62 16	Clover	Cotton *	0.2163 0.0206	0.3180	0.3327	0.1125
* Misclassified observation						
Discriminant Analysis of Remote Sensing Data on Five Crops Classification of Test Data						
The DISCRIM Procedure						
Classification Summary for Test Data: WORK.TEST						
Classification Summary using Linear Discriminant Function						
Observation Profile for Test Data						
Number of Observations Read				5		
Number of Observations Used				5		

Output 33.4.4 continued

Number of Observations and Percent Classified into Crop						
From Crop	Clover	Corn	Cotton	Soybeans	Sugarbeets	Total
Clover	0 0.00	0 0.00	1 100.00	0 0.00	0 0.00	1 100.00
Corn	0 0.00	1 100.00	0 0.00	0 0.00	0 0.00	1 100.00
Cotton	0 0.00	0 0.00	0 0.00	1 100.00	0 0.00	1 100.00
Soybeans	0 0.00	0 0.00	0 0.00	1 100.00	0 0.00	1 100.00
Sugarbeets	1 100.00	0 0.00	0 0.00	0 0.00	0 0.00	1 100.00
Total	1 20.00	1 20.00	1 20.00	2 40.00	0 0.00	5 100.00
Priors	0.30556	0.19444	0.16667	0.16667	0.16667	
Error Count Estimates for Crop						
	Clover	Corn	Cotton	Soybeans	Sugarbeets	Total
Rate	1.0000	0.0000	1.0000	0.0000	1.0000	0.6389
Priors	0.3056	0.1944	0.1667	0.1667	0.1667	

Output 33.4.5 Output Data Set of the Classification Results for Test Data

Discriminant Analysis of Remote Sensing Data on Five Crops									
Output Classification Results of Test Data									
Obs	Crop	x1	x2	x3	x4	xvalues	Clover	Corn	
1	Corn	16	27	31	33	16 27 31 33	0.08935	0.40543	
2	Soybeans	21	25	23	24	21 25 23 24	0.14811	0.24308	
3	Cotton	29	24	26	28	29 24 26 28	0.25213	0.18420	
4	Sugarbeets	54	23	21	54	54 23 21 54	0.62150	0.01937	
5	Clover	32	32	62	16	32 32 62 16	0.21633	0.31799	
Obs	Cotton	Soybeans	Sugarbeets	_INTO_					
1	0.17632	0.23918	0.08972	Corn					
2	0.11999	0.33184	0.15698	Soybeans					
3	0.15294	0.25486	0.15588	Soybeans					
4	0.12498	0.04962	0.18452	Clover					
5	0.33266	0.11246	0.02056	Cotton					

In this next example, PROC DISCRIM uses normal-theory methods (METHOD=NORMAL) assuming unequal variances (POOL=NO) for the remote-sensing data. The PRIORS statement, PRIORS PROP, sets the prior probabilities proportional to the sample sizes. The CROSSVALIDATE option displays cross validation error-rate estimates. Note that the total error count estimate by cross validation (0.5556) is much larger than the total error count estimate by resubstitution (0.1111). The following statements produce Output 33.4.6:

```

title2 'Using Quadratic Discriminant Function';

proc discrim data=crops method=normal pool=no crossvalidate;
  class Crop;
  priors prop;
  id xvalues;
  var x1-x4;
run;

```

Output 33.4.6 Quadratic Discriminant Function on Crop Data

Discriminant Analysis of Remote Sensing Data on Five Crops Using Quadratic Discriminant Function					
The DISCRIM Procedure					
Total Sample Size	36	DF Total		35	
Variables	4	DF Within Classes		31	
Classes	5	DF Between Classes		4	
Number of Observations Read				36	
Number of Observations Used				36	
Class Level Information					
Crop	Variable Name	Frequency	Weight	Proportion	Prior Probability
Clover	Clover	11	11.0000	0.305556	0.305556
Corn	Corn	7	7.0000	0.194444	0.194444
Cotton	Cotton	6	6.0000	0.166667	0.166667
Soybeans	Soybeans	6	6.0000	0.166667	0.166667
Sugarbeets	Sugarbeets	6	6.0000	0.166667	0.166667
Within Covariance Matrix Information					
Crop	Covariance Matrix Rank	Natural Log of the Determinant of the Covariance Matrix			
Clover	4	23.64618			
Corn	4	11.13472			
Cotton	4	13.23569			
Soybeans	4	12.45263			
Sugarbeets	4	17.76293			

Output 33.4.6 *continued*

Discriminant Analysis of Remote Sensing Data on Five Crops Using Quadratic Discriminant Function					
The DISCRIM Procedure					
Generalized Squared Distance to Crop					
From Crop	Clover	Corn	Cotton	Soybeans	Sugarbeets
Clover	26.01743	1320	104.18297	194.10546	31.40816
Corn	27.73809	14.40994	150.50763	38.36252	25.55421
Cotton	26.38544	588.86232	16.81921	52.03266	37.15560
Soybeans	27.07134	46.42131	41.01631	16.03615	23.15920
Sugarbeets	26.80188	332.11563	43.98280	107.95676	21.34645

Discriminant Analysis of Remote Sensing Data on Five Crops Using Quadratic Discriminant Function						
The DISCRIM Procedure						
Classification Summary for Calibration Data: WORK.CROPS Resubstitution Summary using Quadratic Discriminant Function						
Number of Observations and Percent Classified into Crop						
From Crop	Clover	Corn	Cotton	Soybeans	Sugarbeets	Total
Clover	9	0	0	0	2	11
	81.82	0.00	0.00	0.00	18.18	100.00
Corn	0	7	0	0	0	7
	0.00	100.00	0.00	0.00	0.00	100.00
Cotton	0	0	6	0	0	6
	0.00	0.00	100.00	0.00	0.00	100.00
Soybeans	0	0	0	6	0	6
	0.00	0.00	0.00	100.00	0.00	100.00
Sugarbeets	0	0	1	1	4	6
	0.00	0.00	16.67	16.67	66.67	100.00
Total	9	7	7	7	6	36
	25.00	19.44	19.44	19.44	16.67	100.00
Priors	0.30556	0.19444	0.16667	0.16667	0.16667	

Error Count Estimates for Crop						
	Clover	Corn	Cotton	Soybeans	Sugarbeets	Total
Rate	0.1818	0.0000	0.0000	0.0000	0.3333	0.1111
Priors	0.3056	0.1944	0.1667	0.1667	0.1667	

Output 33.4.6 *continued*

Discriminant Analysis of Remote Sensing Data on Five Crops Using Quadratic Discriminant Function						
The DISCRIM Procedure						
Classification Summary for Calibration Data: WORK.CROPS						
Cross-validation Summary using Quadratic Discriminant Function						
Number of Observations and Percent Classified into Crop						
From Crop	Clover	Corn	Cotton	Soybeans	Sugarbeets	Total
Clover	9 81.82	0 0.00	0 0.00	0 0.00	2 18.18	11 100.00
Corn	3 42.86	2 28.57	0 0.00	0 0.00	2 28.57	7 100.00
Cotton	3 50.00	0 0.00	2 33.33	0 0.00	1 16.67	6 100.00
Soybeans	3 50.00	0 0.00	0 0.00	2 33.33	1 16.67	6 100.00
Sugarbeets	3 50.00	0 0.00	1 16.67	1 16.67	1 16.67	6 100.00
Total	21 58.33	2 5.56	3 8.33	3 8.33	7 19.44	36 100.00
Priors	0.30556	0.19444	0.16667	0.16667	0.16667	
Error Count Estimates for Crop						
	Clover	Corn	Cotton	Soybeans	Sugarbeets	Total
Rate	0.1818	0.7143	0.6667	0.6667	0.8333	0.5556
Priors	0.3056	0.1944	0.1667	0.1667	0.1667	

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Chapter 34

The DISTANCE Procedure

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Overview: DISTANCE Procedure

The DISTANCE procedure computes various measures of distance, dissimilarity, or similarity between the observations (rows) of an input SAS data set, which can contain numeric or character variables, or both, depending on which proximity measure is used.

The proximity measures are stored as a lower triangular matrix or a square matrix (depending on the SHAPE= option) in an output data set that can then be used as input to the CLUSTER, MDS, and MOD-ECLUS procedures.

The number of rows and columns in the output data set equals the number of observations in the input data set. If the input data set contains BY groups, an output matrix is computed for each BY group with the size determined by the maximum number of observations in any BY group.

The output data set is of type TYPE=DISTANCE or TYPE=SIMILAR, depending on the value of the METHOD= option. See the METHOD= option for more information about the association between the method and the output data set type.

Data set types do not persist when you copy or modify a data set. You must specify the TYPE= data set option for the new data set, as in the following example:

```
data dist2(type=distance);
  set dist;
run;
```

See the OUT= option for more information about data set type persistence.

PROC DISTANCE also provides various nonparametric and parametric methods for standardizing variables. Different variables can be standardized with different methods.

Distance matrices are used frequently in data mining, genomics, marketing, financial analysis, management science, education, chemistry, psychology, biology, and various other fields.

Levels of Measurement

Measurement of some attribute of a set of objects is the process of assigning numbers or other symbols to the objects in such a way that properties of the numbers or symbols reflect properties of the attribute being measured. There are different *levels* of measurement that involve different properties (relations and operations) of the numbers or symbols. Associated with each level of measurement is a set of transformations of the measurements that preserve the relevant properties; these transformations are called *permissible* transformations. A particular way of assigning numbers or symbols to measure something is called a *scale* of measurement.

The most commonly discussed levels of measurement are as follows:

Nominal	Two objects are assigned the same symbol if they have the same value of the attribute. Permissible transformations are any one-to-one or many-to-one transformation, although a many-to-one transformation loses information.
Ordinal	Objects are assigned numbers such that the order of the numbers reflects an order relation defined on the attribute. Two objects x and y with attribute values $a(x)$ and $a(y)$ are assigned numbers $m(x)$ and $m(y)$ such that if $m(x) > m(y)$, then $a(x) > a(y)$. Permissible transformations are any monotone increasing transformation, although a transformation that is not strictly increasing loses information.
Interval	Objects are assigned numbers such that differences between the numbers reflect differences of the attribute. If $m(x) - m(y) > m(u) - m(v)$, then $a(x) - a(y) > a(u) - a(v)$. Permissible transformations are any affine transformation $t(m) = c * m + d$, where c and d are constants; another way of saying this is that the origin and unit of measurement are arbitrary.

Log-interval	Objects are assigned numbers such that ratios between the numbers reflect ratios of the attribute. If $m(x)/m(y) > m(u)/m(v)$, then $a(x)/a(y) > a(u)/a(v)$. Permissible transformations are any power transformation $t(m) = c * m^d$, where c and d are constants.
Ratio	Objects are assigned numbers such that differences and ratios between the numbers reflect differences and ratios of the attribute. Permissible transformations are any linear (similarity) transformation $t(m) = c * m$, where c is a constant; another way of saying this is that the unit of measurement is arbitrary.
Absolute	Objects are assigned numbers such that all properties of the numbers reflect analogous properties of the attribute. The only permissible transformation is the identity transformation.

Proximity measures provided in the DISTANCE procedure accept four levels of measurement: nominal, ordinal, interval, and ratio. Ordinal variables are transformed to interval variables before processing. This is done by replacing the data with their rank scores, and by assuming that the classes of an ordinal variable are spaced equally along the interval scale. See the RANKSCORE= option in the section “PROC DISTANCE Statement” on page 2168 for choices on assigning scores to ordinal variables. There are also different approaches for how to transform an ordinal variable to an interval variable. See Anderberg (1973) for alternatives.

Symmetric versus Asymmetric Nominal Variables

A binary variable contains two possible outcomes: 1 (positive/present) or 0 (negative/absent). If there is no preference for which outcome should be coded as 0 and which as 1, the binary variable is called *symmetric*. For example, the binary variable “is evergreen?” for a plant has the possible states “loses leaves in winter” and “does not lose leaves in winter.” Both are equally valuable and carry the same weight when a proximity measure is computed. Commonly used measures that accept symmetric binary variables include the Simple Matching, Hamann, Roger and Tanimoto, Sokal and Sneath 1, and Sokal and Sneath 3 coefficients.

If the outcomes of a binary variable are not equally important, the binary variable is called *asymmetric*. An example of such a variable is the presence or absence of a relatively rare attribute, such as “is color-blind” for a human being. While you say that two people who are color-blind have something in common, you cannot say that people who are not color-blind have something in common. The most important outcome is usually coded as 1 (present) and the other is coded as 0 (absent). The agreement of two 1’s (a present-present match or a positive match) is more significant than the agreement of two 0’s (an absent-absent match or a negative match). Usually, the negative match is treated as irrelevant. Commonly used measures that accept asymmetric binary variables include Jaccard, Dice, Russell and Rao, Binary Lance and Williams nonmetric, and Kulczynski coefficients.

When nominal variables are employed, the comparison of one data unit with another can only be in terms of whether the data units score the same or different on the variables. If a variable is defined as an asymmetric nominal variable and two data units score the same but fall into the absent category, the absent-absent match is excluded from the computation of the proximity measure.

Standardization

Since variables with large variances tend to have more effect on the proximity measure than those with small variances, it is recommended that you standardize the variables before the computation of the proximity measure. The DISTANCE procedure provides a convenient way to standardize each variable with its own method before the proximity measures are computed. You can also perform the standardization by using the STDIZE procedure, with the limitation that all variables must be standardized with the same method.

Mandatory Standardization

Variable standardization is not required if any of the following conditions is true:

- if there is only one level of measurement
- if only asymmetric nominal and nominal levels are specified
- if the NOSTD option is specified in the PROC DISTANCE statement

Otherwise, standardization is mandatory.

When standardization is mandatory and no standardization method is specified, a default method of standardization will be used. This default method is determined by the measurement level. In general, the default method is STD for interval variables and is MAXABS for ratio variables except when METHOD=GOWER or METHOD=DGOWER is specified. See the STD= option in the section “VAR Statement” on page 2174 for the default methods for GOWER and DGOWER as well as methods available for standardizing variables.

When standardization is mandatory, PROC DISTANCE ignores the REONLY option, if it is specified.

Getting Started: DISTANCE Procedure

Creating a Distance Matrix as Input for a Subsequent Cluster Analysis

The following example demonstrates how you can use the DISTANCE procedure to obtain a distance matrix that will be used as input to a subsequent clustering procedure.

The following data, originated by A. Weber and cited in Hand et al. (1994, p. 297), measure the amount of protein consumed for nine food groups in 25 European countries. The nine food groups are red meat (RedMeat), white meat (WhiteMeat), eggs (Eggs), milk (Milk), fish (Fish), cereal (Cereal), starch (Starch), nuts (Nuts), and fruits and vegetables (FruitVeg). Suppose you want to determine whether national figures in protein consumption can be used to determine certain types or categories of countries; specifically, you want to perform a cluster analysis to determine whether these 25 countries can be formed into groups suggested by the data.

The following DATA step creates the SAS data set Protein:

```

data Protein;
  input Country $14. RedMeat WhiteMeat Eggs Milk
          Fish Cereal Starch Nuts FruitVeg;
  datalines;
Albania      10.1  1.4  0.5   8.9  0.2  42.3  0.6  5.5  1.7
Austria      8.9 14.0  4.3  19.9  2.1  28.0  3.6  1.3  4.3
Belgium     13.5  9.3  4.1  17.5  4.5  26.6  5.7  2.1  4.0
Bulgaria     7.8  6.0  1.6   8.3  1.2  56.7  1.1  3.7  4.2
Czechoslovakia 9.7 11.4  2.8  12.5  2.0  34.3  5.0  1.1  4.0
Denmark     10.6 10.8  3.7  25.0  9.9  21.9  4.8  0.7  2.4
E Germany    8.4 11.6  3.7  11.1  5.4  24.6  6.5  0.8  3.6
Finland     9.5  4.9  2.7  33.7  5.8  26.3  5.1  1.0  1.4
France     18.0  9.9  3.3  19.5  5.7  28.1  4.8  2.4  6.5
Greece     10.2  3.0  2.8  17.6  5.9  41.7  2.2  7.8  6.5
Hungary     5.3 12.4  2.9   9.7  0.3  40.1  4.0  5.4  4.2
Ireland    13.9 10.0  4.7  25.8  2.2  24.0  6.2  1.6  2.9
Italy      9.0  5.1  2.9  13.7  3.4  36.8  2.1  4.3  6.7
Netherlands 9.5 13.6  3.6  23.4  2.5  22.4  4.2  1.8  3.7
Norway     9.4  4.7  2.7  23.3  9.7  23.0  4.6  1.6  2.7
Poland     6.9 10.2  2.7  19.3  3.0  36.1  5.9  2.0  6.6
Portugal   6.2  3.7  1.1   4.9 14.2  27.0  5.9  4.7  7.9
Romania    6.2  6.3  1.5  11.1  1.0  49.6  3.1  5.3  2.8
Spain     7.1  3.4  3.1   8.6  7.0  29.2  5.7  5.9  7.2
Sweden    9.9  7.8  3.5   4.7  7.5  19.5  3.7  1.4  2.0
Switzerland 13.1 10.1  3.1  23.8  2.3  25.6  2.8  2.4  4.9
UK       17.4  5.7  4.7  20.6  4.3  24.3  4.7  3.4  3.3
USSR     9.3  4.6  2.1  16.6  3.0  43.6  6.4  3.4  2.9
W Germany 11.4 12.5  4.1  18.8  3.4  18.6  5.2  1.5  3.8
Yugoslavia 4.4  5.0  1.2   9.5  0.6  55.9  3.0  5.7  3.2
;

```

The data set Protein contains the character variable Country and the nine numeric variables representing the food groups. The \$14. in the INPUT statement specifies that the variable Country has a length of 14.

The following statements create the distance matrix and display part of it:

```

title 'Protein Consumption in Europe';
proc distance data=Protein out=Dist method=Euclid;
  var interval(RedMeat--FruitVeg / std=Std);
  id Country;
run;

proc print data=Dist (obs=10);
  title2 'First 10 Observations in Output Data Set from PROC DISTANCE';
run;
title2;

```

An output SAS data set called `Dist`, which contains the distance matrix, is created through the `OUT=` option. The `METHOD=EUCLID` option requests that Euclidean distances (which is the default) should be computed and produces an output data set of `TYPE=DISTANCE`.¹

The `VAR` statement lists the variables (`RedMeat—FruitVeg`) along with their measurement level to be used in the analysis. An interval level of measurement is assigned to those variables. Since variables with large variances tend to have more effect on the proximity measure than those with small variances, each variable is standardized by the `STD` method to have a mean of 0 and a standard deviation of 1. This is done by adding “/ `STD=STD`” at the end of the variables list.

The `ID` statement specifies that the variable `Country` should be copied to the `OUT=` data set and used to generate names for the distance variables. The distance variables in the output data set are named by the values in the `ID` variable, and the maximum length for the names of these variables is 14.

There are 25 observations in the input data set; therefore, the output data set `Dist` contains a 25-by-25 lower triangular matrix.

The `PROC PRINT` statement displays the first 10 observations in the output data set `Dist` as shown in [Figure 34.1](#).

¹Data set types do not persist when you copy or modify a data set. You must specify the `TYPE=` data set option for the new data set. See the `METHOD=` and `OUT=` options for more information about data set types.

Figure 34.1 First 10 Observations in the Output Data Set from PROC DISTANCE

Protein Consumption in Europe							
First 10 Observations in Output Data Set from PROC DISTANCE							
	C	A	A	B	B	C	D
	o	l	u	e	u	z	e
	n	b	s	l	l	e	n
	t	a	t	g	a	h	a
	r	n	r	i	r	o	m
	i	i	i	u	i	s	a
	a	a	a	m	a	a	k
1	Albania	0.00000
2	Austria	6.12388	0.00000
3	Belgium	5.94109	2.44987	0.00000	.	.	.
4	Bulgaria	2.76446	4.88331	5.22711	0.00000	.	.
5	Czechoslovakia	5.13959	2.11498	2.21330	3.94761	0.00000	.
6	Denmark	6.61002	3.01392	2.52541	6.00803	3.34049	0.00000
7	E Germany	6.39178	2.56341	2.10211	5.40824	1.87962	2.72112
8	Finland	5.81458	4.04271	3.45779	5.74882	3.91378	2.61570
9	France	6.29601	3.58891	2.19329	5.54675	3.36011	3.65772
10	Greece	4.24495	5.16330	4.69515	3.74849	4.86684	5.59084

	E	F	H	I	N	P	R	S	Y
	—	i	r	r	e	o	R	w	W
	G	n	e	e	I	l	o	i	u
	e	l	g	l	l	o	o	t	g
	r	a	r	t	a	r	t	m	—
	m	n	r	a	r	l	u	S	G
	a	a	a	a	a	u	a	w	e
	n	n	c	c	r	n	a	n	r
	y	d	e	e	y	d	y	d	l
1
2
3
4
5
6
7	0.00000
8	3.99426	0.00000
9	3.78184	4.56796	0.00000
10	5.61496	5.47453	4.54456	0

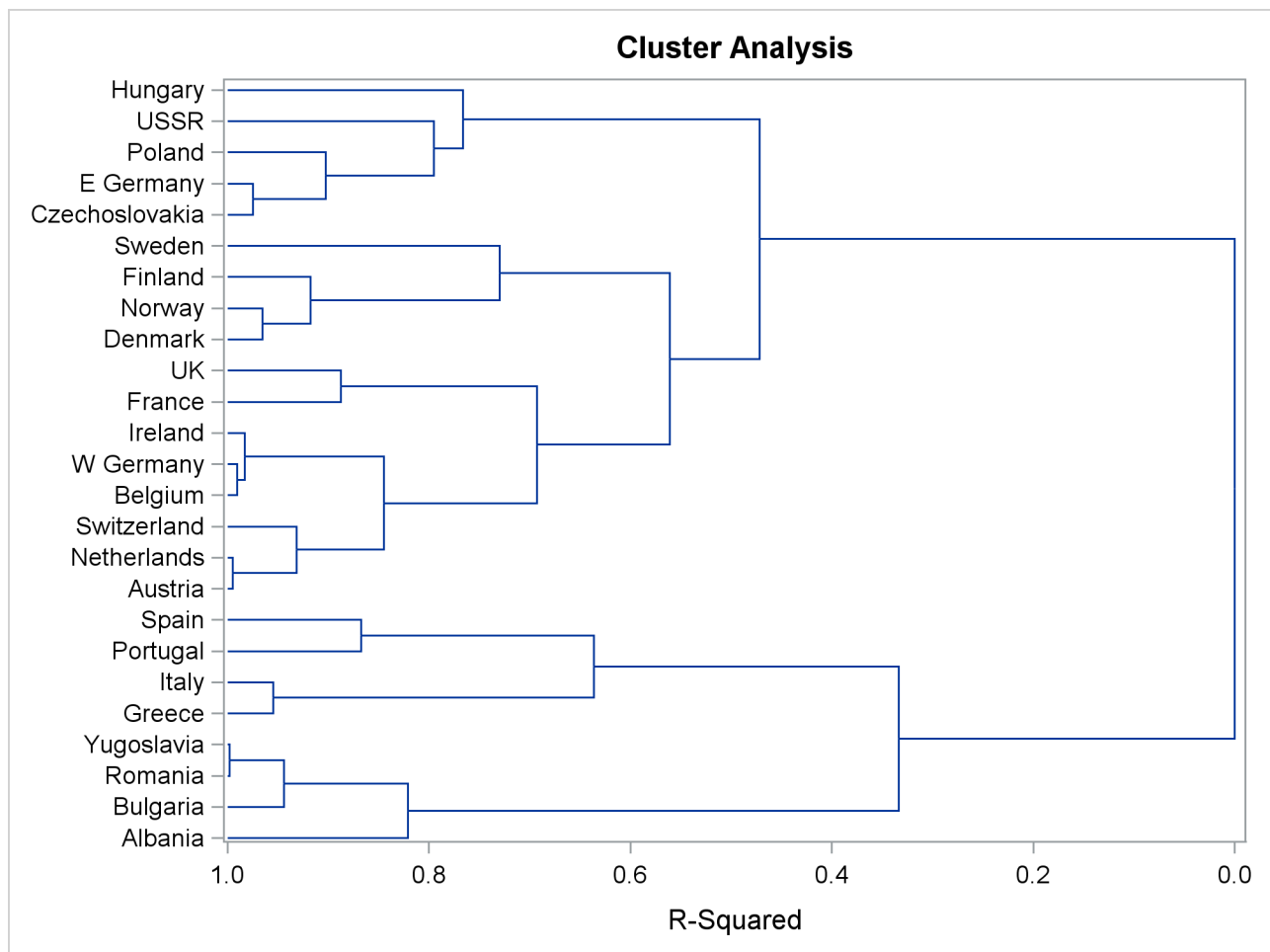
The following statements produce the dendrogram in Figure 34.2:

```
ods graphics on;

proc cluster data=Dist method=Ward plots=dendrogram(height=rsq);
  id Country;
run;
```

The CLUSTER procedure performs a Ward's minimum-variance cluster analysis based on the distance matrix created by PROC DISTANCE. PROC CLUSTER, along with ODS Graphics, produces the dendrogram shown in Figure 34.2. The option PLOTS=DENDROGRAM(HEIGHT=RSQ) specifies the squared multiple correlation as the height variable in the dendrogram.

Figure 34.2 Dendrogram of R Square



After inspecting the dendrogram in [Figure 34.2](#), you will see that when the countries are grouped into six clusters, the proportion of variance accounted for by these clusters is slightly less than 70% (69.3%). The 25 countries are clustered as follows:

- Balkan countries: Albania, Bulgaria, Romania, and Yugoslavia
- Mediterranean countries: Greece and Italy
- Iberian countries: Portugal and Spain
- Western European countries: Austria, Netherlands, Switzerland, Belgium, former West Germany, Ireland, France, and U.K.
- Scandinavian countries: Denmark, Norway, Finland, and Sweden
- Eastern European countries: former Czechoslovakia, former East Germany, Poland, former U.S.S.R., and Hungary

Syntax: DISTANCE Procedure

The following statements are available in the DISTANCE procedure:

```
PROC DISTANCE < options > ;  
  BY variables ;  
  COPY variables ;  
  FREQ variable ;  
  ID variable ;  
  VAR level (variables < / options >) ;  
  WEIGHT variable ;
```

Both the PROC DISTANCE statement and the VAR statement are required.

PROC DISTANCE Statement

PROC DISTANCE < options > ;

The PROC DISTANCE statement invokes the DISTANCE procedure. Table 34.1 summarizes the options available in the PROC DISTANCE statement. These options are discussed in the following section.

Table 34.1 Summary of PROC DISTANCE Statement Options

Option	Description
Standardize variables	
ADD=	Specifies the constant to add to each value after standardizing and multiplying by the value specified in the MULT= option
FUZZ=	Specifies the relative fuzz factor for writing the output
INITIAL=	Specifies the method for computing initial estimates for the A-estimates
MULT=	Specifies the constant to multiply each value by after standardizing
NORM	Normalizes the scale estimator to be consistent for the standard deviation of a normal distribution
NOSTD	Suppresses standardization
SNORM	Normalizes the scale estimator to have an expectation of approximately 1 for a standard normal distribution
STDONLY	Standardizes variables only (suppresses computation of the distance matrix)
VARDEF=	Specifies the variances divisor
Generate distance matrix	
ABSENT=	Specifies the value to be used as an absence value for all the asymmetric nominal variables
METHOD=	Specifies the method for computing proximity measures
PREFIX=	Specifies a prefix for naming the distance variables in the OUT= data set
RANKSCORE=	Specifies the method of assigning scores to ordinal variables
SHAPE=	Specifies the shape of the proximity matrix to be stored in the OUT= data set
UNDEF=	Specifies the numeric constant used to replace undefined distances
Replace missing values	
NOMISS	Omits observations with missing values from computation of the location and scale measures, if standardization applies; outputs missing values to the distance matrix for observations with missing values
REPLACE	Replaces missing data with zero in the standardized data
REONLY	Replaces missing data with the location measure (does not standardize the data)
Specify data set details	
DATA=	Specifies the input data set
OUT=	Specifies the output data set
OUTSDZ=	Specifies the output data set for standardized scores

These options and their abbreviations are described (in alphabetical order) in the remainder of this section.

ABSENT=*number* | *qs*

specifies the value to be used as an absence value in an irrelevant absent-absent match for *all* of the asymmetric nominal variables. If you want to specify a different absence value for a particular variable, use the ABSENT= option in the VAR statement. See the ABSENT= option in the section “[VAR Statement](#)” on page 2174 for details.

An absence value for a variable can be either a numeric value or a quoted string consisting of combinations of characters. For instance, ., -999, and “NA” are legal values for the ABSENT= option.

The default absence value for a character variable is “NONE” (notice that a blank value is considered a missing value), and the default absence value for a numeric variable is 0.

ADD=*c*

specifies a constant, *c*, to add to each value after standardizing and multiplying by the value you specify in the MULT= option. The default value is 0.

DATA=*SAS-data-set*

specifies the input data set containing observations from which the proximity is computed. If you omit the DATA= option, the most recently created SAS data set is used.

FUZZ=*c*

specifies the relative fuzz factor for computing the standardized scores. The default value is 1E-14. For the OUTSDZ= data set, the score is computed as follows:

$$\text{if } |\text{standardized scores}| < m \times c, \text{ then standardized scores} = 0$$

where *m* is the numeric constant specified in the MULT= option, or 1 if MULT= option is not specified.

INITIAL=*method*

specifies the method of computing initial estimates for the A-estimates (ABW, AWAVE, and AHUBER). The following methods are not allowed for the INITIAL= option: ABW, AHUBER, AWAVE, and IN.

The default value is INITIAL=MAD.

METHOD=*method*

specifies the method of computing proximity measures.

For use in PROC CLUSTER, distance or dissimilarity measures such as METHOD=EUCLID or METHOD=DGOWER should be chosen.

The following six tables outline the proximity measures available for the METHOD= option. These tables are classified by levels of measurement accepted by each method. Each table contains four or five columns: the Method column shows the proximity measures, one or two Range columns show the upper and lower bounds, and the TYPE= column shows the type of proximity. The TYPE= column contains SIMILAR if a method generates similarity measures or DISTANCE if a method generates distance or dissimilarity measures. The output data set is of the type shown. For more information about the output data set, see the [OUT=](#) option.

For formulas and descriptions of these methods, see the section “[Details: DISTANCE Procedure](#)” on page 2181.

Table 34.2 shows the range and output matrix type of the GOWER and DGOWER methods. These two methods accept all measurement levels including ratio, interval, ordinal, nominal, and asymmetric nominal. METHOD=GOWER or METHOD=DGOWER always implies standardization. Assuming all the numeric (ordinal, interval, and ratio) variables are standardized by their corresponding default methods, the possible range values for both methods are from 0 and 1, inclusive. For more information about the default methods of standardization for METHOD=GOWER or METHOD=DGOWER, see the STD= option in the section “VAR Statement” on page 2174.

Table 34.2 Methods That Accept All Measurement Levels

Method	Description	Range	TYPE=
GOWER	Gower and Legendre (1986) similarity	0 to 1	SIMILAR
DGOWER	1 minus GOWER	0 to 1	DISTANCE

Table 34.3 shows methods that accept ratio, interval, and ordinal variables.

Table 34.3 Methods That Accept Ratio, Interval, and Ordinal Variables

Method	Description	Range	TYPE=
EUCLID	Euclidean distance	≥ 0	DISTANCE
SQEUCLID	Squared Euclidean distance	≥ 0	DISTANCE
SIZE	Size distance	≥ 0	DISTANCE
SHAPE	Shape distance	≥ 0	DISTANCE
COV	Covariance	≥ 0	SIMILAR
CORR	Correlation	-1 to 1	SIMILAR
DCORR	Correlation transformed to Euclidean distance	0 to 2	DISTANCE
SQCORR	Squared correlation	0 to 1	SIMILAR
DSQCORR	One minus squared correlation	0 to 1	DISTANCE
L(<i>p</i>)	Minkowski (L_p) distance, where <i>p</i> is a positive numeric value	≥ 0	DISTANCE
CITYBLOCK	L_1 , city-block, or Manhattan distance	≥ 0	DISTANCE
CHEBYCHEV	L_∞	≥ 0	DISTANCE
POWER(<i>p</i> , <i>r</i>)	Generalized Euclidean distance where <i>p</i> is a positive numeric value and <i>r</i> is a nonnegative numeric value. The distance between two observations is the <i>r</i> th root of sum of the absolute differences to the <i>p</i> th power between the values for the observations.	≥ 0	DISTANCE

Table 34.4 shows methods that accept ratio variables. Notice that all possible range values are non-negative, because ratio variables are assumed to be positive.

Table 34.4 Methods That Accept Ratio Variables

Method	Description	Range	TYPE=
SIMRATIO	Similarity ratio (if variables are binary, this is the Jaccard coefficient)	0 to 1	SIMILAR
DISRATIO	One minus similarity ratio	0 to 1	DISTANCE
NONMETRIC	Lance and Williams nonmetric coefficient	0 to 1	DISTANCE
CANBERRA	Canberra metric distance coefficient	0 to 1	DISTANCE
COSINE	Cosine coefficient	0 to 1	SIMILAR
DOT	Dot (inner) product coefficient	≥ 0	SIMILAR
OVERLAP	Overlap similarity	≥ 0	SIMILAR
DOVERLAP	Overlap dissimilarity	≥ 0	DISTANCE
CHISQ	Chi-square coefficient	≥ 0	DISTANCE
CHI	Square root of chi-square coefficient	≥ 0	DISTANCE
PHISQ	Phi-square coefficient	≥ 0	DISTANCE
PHI	Square root of phi-square coefficient	≥ 0	DISTANCE

Table 34.5 shows methods that accept nominal variables.

Table 34.5 Methods That Accept Nominal Variables

Method	Description	Range	TYPE=
HAMMING	Hamming distance	0 to ν	DISTANCE
MATCH	Simple matching coefficient	0 to 1	SIMILAR
DMATCH	Simple matching coefficient transformed to Euclidean distance	0 to 1	DISTANCE
DSQMATCH	Simple matching coefficient transformed to squared Euclidean distance	0 to 1	DISTANCE
HAMANN	Hamann coefficient	-1 to 1	SIMILAR
RT	Roger and Tanimoto	0 to 1	SIMILAR
SS1	Sokal and Sneath 1	0 to 1	SIMILAR
SS3	Sokal and Sneath 3	0 to 1	SIMILAR

Note that ν denotes the number of variables (dimensionality).

Table 34.6 shows methods that accept asymmetric nominal variables. Use the ABSENT= option to create a value to be considered absent.

Table 34.6 Methods That Accept Asymmetric Nominal Variables

Method	Description	Range	TYPE=
DICE	Dice coefficient or Czekanowski/Sorensen similarity coefficient	0 to 1	SIMILAR
RR	Russell and Rao	0 to 1	SIMILAR
BLWNM	Binary Lance and Williams nonmetric, or Bray-Curtis coefficient	0 to 1	DISTANCE
K1	Kulczynski 1	≥ 0	SIMILAR

Table 34.7 shows methods that accept asymmetric nominal and ratio variables. Use the ABSENT= option to create a value to be considered absent. The table contains five columns. The third column contains possible range values if only one level of measurement (either ratio or asymmetric nominal but not both) is specified; the fourth column contains possible range values if both levels are specified.

The JACCARD method is equivalent to the SIMRATIO method if there is no asymmetric nominal variable; if both ratio and asymmetric nominal variables are present, the coefficient is computed as the sum of the coefficient from the ratio variables and the coefficient from the asymmetric nominal variables. See “Proximity Measures” in the section “Details: DISTANCE Procedure” on page 2181 for the formula and descriptions of the JACCARD method.

Table 34.7 Methods That Accept Asymmetric Nominal and Ratio Variables

Method	Description	Range (One Level)	Range (Two Levels)	TYPE=
JACCARD	Jaccard similarity coefficient	0 to 1	0 to 2	SIMILAR
DJACCARD	Jaccard dissimilarity coefficient	0 to 1	0 to 2	DISTANCE

MULT=c

specifies a numeric constant, *c*, by which to multiply each value after standardizing. The default value is 1.

NOMISS

omits observations with missing values from computation of the location and scale measures when standardizing; generates undefined (missing) distances for observations with missing values when computing distances. Use the UNDEF= option to specify the undefined values.

If a distance matrix is created to be used as an input to PROC CLUSTER, the NOMISS option should not be used because PROC CLUSTER does not accept distance matrices with missing values.

NORM

normalizes the scale estimator to be consistent for the standard deviation of a normal distribution when you specify the option STD=AGK, STD=IQR, STD=MAD, or STD=SPACING in the VAR statement.

NOSTD

suppresses standardization of the variables. The NOSTD option should not be specified with the STDONLY option or with the REPLACE option.

OUT=SAS-data-set

specifies the name of the SAS data set created by PROC DISTANCE. The output data set contains the BY variables, the ID variable, computed distance variables, the COPY variables, the FREQ variable, and the WEIGHT variables.

If you omit the OUT= option, PROC DISTANCE creates an output data set named according to the DATA n convention.

The output data set is of type TYPE=DISTANCE or TYPE=SIMILAR. See the METHOD= option for more information about the association between the method and the output data set type. Data set types do not persist when you copy or modify a data set. You must specify the TYPE= data set option for the new data set, as in the following example:

```
data dist2 (type=distance);
  set dist;
run;
```

If you do not specify the TYPE=DISTANCE data set option, the new data set is the default TYPE=DATA. If you use the new data set in a procedure that accepts both TYPE=DATA or TYPE=DISTANCE data sets (such as PROC CLUSTER or PROC MODECLUS), the results will be incorrect.

OUTSDZ=SAS-data-set

specifies the name of the SAS data set containing the standardized scores. The output data set contains a copy of the DATA= data set, except that the analyzed variables have been standardized. Analyzed variables are those listed in the VAR statement.

PREFIX=name

specifies a prefix for naming the distance variables in the OUT= data set. By default, the names are Dist1, Dist2, ..., Dist*n*. If you specify PREFIX=ABC, the variables are named ABC1, ABC2, ..., ABC*n*. If the ID statement is also specified, the variables are named by appending the value of the ID variable to the prefix.

RANKSCORE=MIDRANK | INDEX

specifies the method of assigning scores to ordinal variables. The available methods are listed as follows:

MIDRANK assigns consecutive integers to each category with consideration of the frequency value. This is the default method.

INDEX assigns consecutive integers to each category regardless of frequencies.

The following example explains how each method assigns the rank scores. Suppose the data contain an ordinal variable ABC with values A, B, C. There are two ways to assign numbers. One is to use midranks, which depend on the frequencies of each category. Another is to assign consecutive integers to each category, regardless of frequencies.

Table 34.8 Example of Assigning Rank Scores

ABC	MIDRANK	INDEX
A	1.5	1
A	1.5	1
B	4	2
B	4	2
B	4	2
C	6	3

REPLACE

replaces missing data with zero in the standardized data (to correspond to the location measure before standardizing). To replace missing data with something else, use the MISSING= option in the VAR statement. The REPLACE option implies standardization.

You cannot specify the following options together:

- both the REPLACE and the REONLY options
- both the REPLACE and the NOSTD options

REONLY

measure specified by the MISSING= option or the STD= option (if the MISSING= option is not specified), but does *not* standardize the data. If the MISSING= option is not specified and METHOD=GOWER is specified, missing values are replaced by the location measure from the RANGE method (the minimum value), no matter what the value of the STD= option is.

You cannot specify both the REPLACE and the REONLY options.

SHAPE=TRIANGLE | TRI | SQUARE | SQU | SQR

specifies the shape of the proximity matrix to be stored in the OUT= data set. SHAPE=TRIANGLE requests the matrix to be stored as a lower triangular matrix; SHAPE=SQUARE requests that the matrix be stored as a square matrix. Use SHAPE=SQUARE if the output data set is to be used as input to the MODECLUS procedures. The default is TRIANGLE.

SNORM

normalizes the scale estimator to have an expectation of approximately 1 for a standard normal distribution when the STD=SPACING option is specified.

STDONLY

standardizes variables only and computes no distance matrix. You must use the OUTSDZ= option to save the standardized scores. You cannot specify both the STDONLY option and the NOSTD option.

UNDEF=*n*

specifies the numeric constant used to replace undefined distances, such as when an observation has all missing values, or if a divisor is zero.

VARDEF=DF | N | WDF | WEIGHT | WGT

specifies the divisor to be used in the calculation of distance, dissimilarity, or similarity measures, and for standardizing variables whenever a variance or covariance is computed. By default, VARDEF=DF. The values and associated divisors are as follows:

Value	Divisor	Formula
DF	degrees of freedom	$n - 1$
N	number of observations	n
WDF	sum of weights minus 1	$(\sum_i w_i) - 1$
WEIGHT WGT	sum of weights	$\sum_i w_i$

VAR Statement

```
VAR level (variables </ options>)< level (variables </ options>)... > ;
```

where the syntax for the *options* is as follows:

ABSENT=*value*

MISSING=*miss-method* | *value*

ORDER=*order-option*

STD=*std-method*

WEIGHTS=*weight-list*

The VAR statement lists variables from which distances are to be computed. The VAR statement is required. The variables can be numeric or character depending on their measurement levels. A variable cannot appear more than once in either the same list or a different list.

level is required. It declares the levels of measurement for those variables specified within the parentheses. Available values for *level* are as follows:

ANOMINAL	variables are asymmetric nominal and can be either numeric or character.
NOMINAL	variables are symmetric nominal and can be either numeric or character.
ORDINAL	variables are ordinal and can be either numeric or character. Values of ordinal variables are replaced by their corresponding rank scores. If standardization is required, the standardized rank scores are output to the data set specified in the OUTSDZ= option. See the RANKSCORE= option in the PROC DISTANCE statement for methods available for assigning rank scores to ordinal variables. After being replaced by scores, ordinal variables are considered interval.
INTERVAL	variables are interval and numeric.
RATIO	variables are ratio and numeric. Ratio variables should always contain positive measurements.

Each variable list can be followed by an option list. Use “/” after the list of variables to start the option list. An option list contains options that are applied to the variables. The following options are available in the option list:

ABSENT=	specifies the value to be used as an absence value in an irrelevant absent-absent match for asymmetric nominal variables.
MISSING=	specifies the method (or numeric value) with which to replace missing data.
ORDER=	selects the order for assigning scores to ordinal variables.
STD=	selects the standardization method.
WEIGHTS=	assigns weights to the variables in the list.

If an option is missing from the current attribute list, PROC DISTANCE provides default values for all the variables in the current list.

For example, in the VAR statement

```
var ratio(x1-x4/std= mad weights= .5 .5 .1 .5 missing= -99)
  interval(x5/std= range)
  ordinal(x6/order= desc);
```

the first option list defines x1–x4 as ratio variables to be standardized by the MAD method. Also, any missing values in x1–x4 should be replaced by –99. x1 is given a weight of 0.5, x2 is given a weight of 0.5, x3 is given a weight of 0.1, and x4 is given a weight of 0.5.

The second option list defines x5 as an interval variable to be standardized by the RANGE method. If the REPLACE option is specified in the PROC DISTANCE statement, missing values in x5 are replaced by the location estimate from the RANGE method. By default, x5 is given a weight of 1.

The last option list defines x6 as an ordinal variable. The scores are assigned from highest to lowest by its unformatted values. Although the STD= option is not specified, x6 is standardized by the default method

(STD) because there is more than one level of measurements (ratio, interval, and ordinal) in the VAR statement. Again, if the REPLACE option is specified, missing values in x_6 are replaced by the location estimate from the STD method. Finally, by default, x_6 is given a weight of 1.

More details for the options are explained as follows.

STD=std-method

specifies the standardization method. Valid values for *std-method* are MEAN, MEDIAN, SUM, EUCLLEN, USTD, STD, RANGE, MIDRANGE, MAXABS, IQR, MAD, ABW, AHUBER, AWAVE, AGK, SPACING, and L. Table 34.9 lists available methods of standardization as well as their corresponding location and scale measures.

Table 34.9 Available Standardization Methods

Method	Scale	Location
MEAN	1	mean
MEDIAN	1	median
SUM	sum	0
EUCLLEN	Euclidean length	0
USTD	standard deviation about origin	0
STD	standard deviation	mean
RANGE	range	minimum
MIDRANGE	range/2	midrange
MAXABS	maximum absolute value	0
IQR	interval quartile range	median
MAD	median absolute deviation from median	median
ABW(<i>c</i>)	biweight A-estimate	biweight 1-step M-estimate
AHUBER(<i>c</i>)	Huber A-estimate	Huber 1-step M-estimate
AWAVE(<i>c</i>)	Wave 1-step M-estimate	Wave A-estimate
AGK(<i>p</i>)	AGK estimate (ACECLUS)	mean
SPACING(<i>p</i>)	minimum spacing	mid minimum-spacing
L(<i>p</i>)	L_p	L_p

These standardization methods are further documented in the section on the METHOD= option in the PROC STDIZE statement of the STDIZE procedure (see the section “Standardization Methods” on page 7468 in Chapter 87, “The STDIZE Procedure”).

Standardization is not required if there is only one level of measurement, or if only asymmetric nominal and nominal levels are specified; otherwise, standardization is mandatory. When standardization is mandatory, a default method is provided when the STD= option is not specified. You can suppress the mandatory standardization by using the NOSTD option in the PROC DISTANCE statement. See the NOSTD option in the section “PROC DISTANCE Statement” on page 2168 and the section “Mandatory Standardization” on page 2162 for details.

The default method is STD for standardizing interval variables and MAXABS for standardizing ratio variables unless METHOD=GOWER or METHOD=DGOWER is specified. If METHOD=GOWER is specified, interval variables are standardized by the RANGE method, and whatever is specified in the STD= option is ignored; if METHOD=DGOWER is specified, the RANGE method is the default

standardization method for interval variables. The MAXABS method is the default standardization method for ratio variables for both the GOWER and DGOWER methods.

Notice that a ratio variable should always be positive.

Table 34.10 lists standardization methods and the levels of measurement that can be accepted by each method. For example, the SUM method can be used to standardize ratio variables but not interval or ordinal variables. Also, the AGK and SPACING methods should not be used to standardize ordinal variables. If you apply AGK and SPACING to ranks, the results are degenerate because all the spacings of a given order are equal.

Table 34.10 Legitimate Levels of Measurements for Each Method

Standardization Method	Legitimate Levels of Measurement
MEAN	ratio, interval, ordinal
MEDIAN	ratio, interval, ordinal
SUM	ratio
EUCLEN	ratio
USTD	ratio
STD	ratio, interval, ordinal
RANGE	ratio, interval, ordinal
MIDRANGE	ratio, interval, ordinal
MAXABS	ratio
IQR	ratio, interval, ordinal
MAD	ratio, interval, ordinal
ABW(<i>c</i>)	ratio, interval, ordinal
AHUBER(<i>c</i>)	ratio, interval, ordinal
AWAVE(<i>c</i>)	ratio, interval, ordinal
AGK(<i>p</i>)	ratio, interval
SPACING(<i>p</i>)	ratio, interval
L(<i>p</i>)	ratio, interval, ordinal

ABSENT=*numner* | *qs*

specifies the value to be used as an absence value in an irrelevant absent-absent match for asymmetric nominal variables. The absence value specified here overwrites the absence value specified through the ABSENT= option in the PROC DISTANCE statement for those variables in the current variable list.

An absence value for a variable can be either a numeric value or a quoted string consisting of combinations of characters. For instance, ., -999, "NA" are legal values for the ABSENT= option.

The default for an absence value for a character variable is "NONE" (notice that a blank value is considered a missing value), and the default for an absence value for a numeric variable is 0.

MISSING=*miss-method* | *value*

specifies the method or a numeric value for replacing missing values. If you omit the MISSING= option, the REPLACE option replaces missing values with the location measure given by the STD= option. Specify the MISSING= option when you want to replace missing values with a different

value. You can specify any method that is valid in the STD= option. The corresponding location measure is used to replace missing values.

If a numeric value is given, the value replaces missing values after standardizing the data. However, when standardization is not mandatory, you can specify the REONLY option with the MISSING= option to suppress standardization for cases in which you want only to replace missing values.

If the NOSTD option is specified, there is no standardization, but missing values are replaced by the corresponding location measures or by the numeric value of the MISSING= option. See the section “Missing Values” on page 2187 for details about missing values replacement with and without standardization.

ORDER=ASCENDING | DESCENDING | ASCFORMATTED | DESFORMATTED | DSORDER

ORDER=ASC | DESC | ASCFMT | DESFMT | DATA

specifies the order for assigning score to ordinal variables. The value for the ORDER= option can be one of the following:

ASCENDING	scores are assigned in lowest-to-highest order of unformatted values.
DESCENDING	scores are assigned in highest-to-lowest order of unformatted values.
ASCFORMATTED	scores are assigned in ascending order by their formatted values. This option can be applied to character variables only, since unformatted values are always used for numeric variables.
DESFORMATTED	scores are assigned in descending order by their formatted values. This option can be applied to character variables only, since unformatted values are always used for numeric variables.
DSORDER	scores are assigned according to the order of their appearance in the input data set.

The default value is ASCENDING.

WEIGHTS=weight-list

specifies a list of values for weighting individual variables while computing the proximity. Values in this list can be separated by blanks or commas. You can include one or more items of the form *start TO stop BY increment*. This list should contain at least one weight. The maximum number of weights you can list is equal to the number of variables. If the number of weights is less than the number of variables, the last value in the *weight-list* is used for the rest of the variables; conversely, if the number of weights is greater than the number of variables, the trailing weights are discarded.

The default value is 1.

ID Statement

ID variable ;

The ID statement specifies a single variable to be copied to the OUT= data set and used to generate names for the distance variables. The ID variable must be character.

Typically, each ID value occurs only once in the input data set or, if you use a BY statement, only once within a BY group.

If you specify both the ID and BY statements, the ID variable must have the same values in the same order in each BY group.

COPY Statement

COPY *variables* ;

The COPY statement specifies a list of additional variables to be copied to the OUT= data set.

BY Statement

BY *variables* ;

You can specify a BY statement with PROC DISTANCE to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the DISTANCE procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

FREQ Statement

FREQ | **FREQUENCY** *variable* ;

The frequency variable is used for either standardizing variables or assigning rank scores to the ordinal variables. It has no direct effect on computing the distances.

For standardizing variables and assigning rank scores, PROC DISTANCE treats the data set as if each observation appeared n times, where n is the value of the FREQ variable for the observation. Nonintegral values of the FREQ variable are truncated to the largest integer less than the FREQ value. If the FREQ variable has a value that is less than 1 or is missing, the observation is not used in the analysis.

WEIGHT Statement

WGT | WEIGHT *variable* ;

The WEIGHT statement specifies a numeric variable in the input data set with values that are used to weight each observation. This weight variable is used for standardizing variables rather than computing the distances. Only one variable can be specified.

The WEIGHT variable values can be nonintegers. An observation is used in the analysis only if the value of the WEIGHT variable is greater than zero. The WEIGHT variable applies to variables that are standardized by the following options: STD=MEAN, STD=SUM, STD=EUCLEN, STD=USTD, STD=STD, STD=AGK, or STD=L.

PROC DISTANCE uses the value of the WEIGHT variable w_i to compute the sample mean, uncorrected sample variances, and sample variances as follows:

$$\bar{x}_w = \frac{\sum_i w_i x_i}{\sum_i w_i}$$

$$u_w^2 = \frac{\sum_i w_i x_i^2}{d}$$

$$s_w^2 = \frac{\sum_i w_i (x_i - \bar{x}_w)^2}{d}$$

w_i is the weight value of the i th observation, x_i is the value of the i th observation, and d is the divisor controlled by the VARDEF= option (see the VARDEF= option in the PROC DISTANCE statement for details).

PROC DISTANCE uses the value of the WEIGHT variable to calculate the following statistics for standardization:

MEAN	the weighted mean, \bar{x}_w
SUM	the weighted sum, $\sum_i w_i x_i$
USTD	the weighted uncorrected standard deviation, $\sqrt{u_w^2}$
STD	the weighted standard deviation, $\sqrt{s_w^2}$
EUCLEN	the weighted Euclidean length, computed as the square root of the weighted uncorrected sum of squares:

$$\sqrt{\sum_i w_i x_i^2}$$

AGK	the AGK estimate. This estimate is documented further in the ACECLUS procedure as the METHOD=COUNT option. See the discussion of the WEIGHT statement in Chapter 23, “ The ACECLUS Procedure ,” for information about how the WEIGHT variable is applied to the AGK estimate.
-----	---

L the L_p estimate. This estimate is documented further in the FASTCLUS procedure as the LEAST= option. See the discussion of the WEIGHT statement in Chapter 36, “The FASTCLUS Procedure,” for information about how the WEIGHT variable is used to compute weighted cluster means. Note that the number of clusters is always 1.

Details: DISTANCE Procedure

Proximity Measures

The following notation is used in this section:

v	the number of variables or the dimensionality
x_j	data for observation x and the j th variable, where $j = 1$ to v
y_j	data for observation y and the j th variable, where $j = 1$ to v
w_j	weight for the j th variable from the WEIGHTS= option in the VAR statement. $w_j = 0$ when either x_j or y_j is missing.
W	the sum of total weights. No matter if the observation is missing or not, its weight is added to this metric.
\bar{x}	mean for observation x $\bar{x} = \sum_{j=1}^v w_j x_j / \sum_{j=1}^v w_j$
\bar{y}	mean for observation y $\bar{y} = \sum_{j=1}^v w_j y_j / \sum_{j=1}^v w_j$
$d(x, y)$	the distance or dissimilarity between observations x and y
$s(x, y)$	the similarity between observations x and y

The factor $W / \sum_{j=1}^v w_j$ is used to adjust some of the proximity measures for missing values.

Methods That Accept All Measurement Levels

GOWER	Gower's similarity $s_1(x, y) = \sum_{j=1}^v w_j \delta_{x,y}^j d_{x,y}^j / \sum_{j=1}^v w_j \delta_{x,y}^j$ $\delta_{x,y}^j$ is computed as follows: For nominal, ordinal, interval, or ratio variable, $\delta_{x,y}^j = 1$ For asymmetric nominal variable, $\delta_{x,y}^j = 1, \text{ if either } x_j \text{ or } y_j \text{ is present}$ $\delta_{x,y}^j = 0, \text{ if both } x_j \text{ and } y_j \text{ are absent}$
-------	--

For nominal or asymmetric nominal variable,

$$d_{x,y}^j = 1, \text{ if } x_j = y_j$$

$$d_{x,y}^j = 0, \text{ if } x_j \neq y_j$$

For ordinal, interval, or ratio variable,

$$d_{x,y}^j = 1 - |x_j - y_j|$$

DGOWER 1 minus Gower
 $d_2(x, y) = 1 - s_1(x, y)$

Methods That Accept Ratio, Interval, and Ordinal Variables

EUCLID Euclidean distance
 $d_3(x, y) = \sqrt{(\sum_{j=1}^v w_j (x_j - y_j)^2)W / (\sum_{j=1}^v w_j)}$

SQEUCLID squared Euclidean distance
 $d_4(x, y) = (\sum_{j=1}^v w_j (x_j - y_j)^2)W / (\sum_{j=1}^v w_j)$

SIZE size distance
 $d_5(x, y) = |\sum_{j=1}^v w_j (x_j - y_j)|\sqrt{W} / (\sum_{j=1}^v w_j)$

SHAPE shape distance
 $d_6(x, y) = \sqrt{(\sum_{j=1}^v w_j [(x_j - \bar{x}) - (y_j - \bar{y})]^2)W / (\sum_{j=1}^v w_j)}$

NOTE: squared shape distance plus squared size distance equals squared Euclidean distance.

COV covariance similarity coefficient
 $s_7(x, y) = \sum_{j=1}^v w_j (x_j - \bar{x})(y_j - \bar{y}) / \text{vardiv}$, where
 $\text{vardiv} = v$ if VARDEF = N
 $= v - 1$ if VARDEF = DF
 $= \sum_{j=1}^v w_j$ if VARDEF = WEIGHT
 $= \sum_{j=1}^v w_j - 1$ if VARDEF = WDF

CORR correlation similarity coefficient
 $s_8(x, y) = \frac{\sum_{j=1}^v w_j (x_j - \bar{x})(y_j - \bar{y})}{\sqrt{\sum_{j=1}^v w_j (x_j - \bar{x})^2 \sum_{j=1}^v w_j (y_j - \bar{y})^2}}$

DCORR correlation transformed to Euclidean distance as $\text{sqrt}(1 - \text{CORR})$
 $d_9(x, y) = \sqrt{1 - s_8(x, y)}$

SQCORR squared correlation
 $s_{10}(x, y) = \frac{[\sum_{j=1}^v w_j (x_j - \bar{x})(y_j - \bar{y})]^2}{\sum_{j=1}^v w_j (x_j - \bar{x})^2 \sum_{j=1}^v w_j (y_j - \bar{y})^2}$

DSQCORR squared correlation transformed to squared Euclidean distance as (1–SQCORR)

$$d_{11}(x, y) = 1 - s_{10}(x, y)$$

L(*p*) Minkowski (L_p) distance, where *p* is a positive numeric value

$$d_{12}(x, y) = [(\sum_{j=1}^v w_j |x_j - y_j|^p)W / (\sum_{j=1}^v w_j)]^{1/p}$$

CITYBLOCK L_1

$$d_{13}(x, y) = (\sum_{j=1}^v w_j |x_j - y_j|)W / (\sum_{j=1}^v w_j)$$

CHEBYCHEV L_∞

$$d_{14}(x, y) = \max_{j=1}^v w_j |x_j - y_j|$$

POWER(*p*,*r*) generalized Euclidean distance, where *p* is a nonnegative numeric value and *r* is a positive numeric value. The distance between two observations is the *r*th root of sum of the absolute differences to the *p*th power between the values for the observations:

$$d_{15}(x, y) = [(\sum_{j=1}^v w_j |x_j - y_j|^p)W / (\sum_{j=1}^v w_j)]^{1/r}$$

Methods That Accept Ratio Variables

SIMRATIO similarity ratio

$$s_{16}(x, y) = \frac{\sum_{j=1}^v w_j (x_j y_j)}{\sum_{j=1}^v w_j (x_j y_j) + \sum_{j=1}^v w_j (x_j - y_j)^2}$$

DISRATIO one minus similarity ratio

$$d_{17}(x, y) = 1 - s_{16}(x, y)$$

NONMETRIC Lance-Williams nonmetric coefficient

$$d_{18}(x, y) = \frac{\sum_{j=1}^v w_j |x_j - y_j|}{\sum_{j=1}^v w_j (x_j + y_j)}$$

CANBERRA Canberra metric coefficient. See Sneath and Sokal (1973, pp. 125–126)

$$d_{19}(x, y) = \sum_{j=1}^v \frac{w_j |x_j - y_j|}{w_j (x_j + y_j)}$$

COSINE cosine coefficient

$$s_{20}(x, y) = \frac{\sum_{j=1}^v w_j (x_j y_j)}{\sqrt{\sum_{j=1}^v w_j x_j^2 \sum_{j=1}^v w_j y_j^2}}$$

DOT dot (inner) product coefficient

$$s_{21}(x, y) = [\sum_{j=1}^v w_j (x_j y_j)] / \sum_{j=1}^v w_j$$

OVERLAP sum of the minimum values

$$s_{22}(x, y) = \sum_{j=1}^v w_j [\min(x_j, y_j)]$$

DOVERLAP maximum of the sum of the x and the sum of y minus overlap
 $d_{23}(x, y) = \max(\sum_{j=1}^v w_j x_j, \sum_{j=1}^v w_j y_j) - s_{22}(x, y)$

CHISQ chi-square
 If the data represent the frequency counts, chi-square dissimilarity between two sets of frequencies can be computed. A 2-by- v contingency table is illustrated to explain how the chi-square dissimilarity is computed as follows:

	Variable				Row
Observation	Var 1	Var 2	...	Var v	Sum
X	x_1	x_2	...	x_v	r_x
Y	y_1	y_2	...	y_v	r_y
Column Sum	c_1	c_2	...	c_v	T

where

$$r_x = \sum_{j=1}^v w_j x_j$$

$$r_y = \sum_{j=1}^v w_j y_j$$

$$c_j = w_j(x_j + y_j)$$

$$T = r_x + r_y = \sum_{j=1}^v c_j$$

The chi-square measure is computed as follows:

$$d_{24}(x, y) = (\sum_{j=1}^v \frac{(w_j x_j - E(x_j))^2}{E(x_j)} + \sum_{j=1}^v \frac{(w_j y_j - E(y_j))^2}{E(y_j)}) / (\sum_{j=1}^v w_j)$$

where for $j= 1, 2, \dots, v$

$$E(x_j) = r_x c_j / T$$

$$E(y_j) = r_y c_j / T$$

CHI square root of chi-square
 $d_{25}(x, y) = \sqrt{d_{24}(x, y)}$

PHISQ phi-square
 This is the CHISQ dissimilarity normalized by the sum of weights
 $d_{26}(x, y) = d_{24}(x, y) / (\sum_{j=1}^v w_j)$

PHI square root of phi-square
 $d_{27}(x, y) = \sqrt{d_{26}(x, y)}$

Methods That Accept Symmetric Nominal Variables

The following notation is used for computing $d_{28}(x, y)$ to $s_{35}(x, y)$. Notice that only the nonmissing pairs are discussed below; all the pairs with at least one missing value will be excluded from any of the computations in the following section because $w_j = 0$, if either x_j or y_j is missing.

M	nonmissing matches $M = \sum_{j=1}^v w_j \delta_{x,y}^j$, where $\delta_{x,y}^j = 1$, if $x_j = y_j$ $\delta_{x,y}^j = 0$, otherwise
X	nonmissing mismatches $X = \sum_{j=1}^v w_j \delta_{x,y}^j$, where $\delta_{x,y}^j = 1$, if $x_j \neq y_j$ $\delta_{x,y}^j = 0$, otherwise
N	total nonmissing pairs $N = \sum_{j=1}^v w_j$
HAMMING	Hamming distance $d_{28}(x, y) = X$
MATCH	simple matching coefficient $s_{29}(x, y) = M/N$
DMATCH	simple matching coefficient transformed to Euclidean distance $d_{30}(x, y) = \sqrt{1 - M/N} = \sqrt{(X/N)}$
DSQMATCH	simple matching coefficient transformed to squared Euclidean distance $d_{31}(x, y) = 1 - M/N = X/N$
HAMANN	Hamann coefficient $s_{32}(x, y) = (M - X)/N$
RT	Roger and Tanimoto $s_{33}(x, y) = M/(M + 2X)$
SS1	Sokal and Sneath 1 $s_{34}(x, y) = 2M/(2M + X)$
SS3	Sokal and Sneath 3. The coefficient between an observation and itself is always indeterminate (missing) since there is no mismatch. $s_{35}(x, y) = M/X$

The following notation is used for computing $s_{36}(x, y)$ to $d_{41}(x, y)$. Notice that only the nonmissing pairs are discussed in the following section; all the pairs with at least one missing value are excluded from any of the computations in the following section because $w_j = 0$, if either x_j or y_j is missing.

Also, the observed nonmissing data of an asymmetric binary variable can have only two possible outcomes: presence or absence. Therefore, the notation, PX (present mismatches), always has a value of zero for an asymmetric binary variable.

The following methods distinguish between the presence and absence of attributes.

X	mismatches with at least one present $X = \sum_{j=1}^v w_j \delta_{x,y}^j$, where $\delta_{x,y}^j = 1$, if $x_j \neq y_j$ and not both x_j and y_j are absent $\delta_{x,y}^j = 0$, otherwise
PM	present matches $PM = \sum_{j=1}^v w_j \delta_{x,y}^j$, where $\delta_{x,y}^j = 1$, if $x_j = y_j$ and both x_j and y_j are present $\delta_{x,y}^j = 0$, otherwise
PX	present mismatches $PX = \sum_{j=1}^v w_j \delta_{x,y}^j$, where $\delta_{x,y}^j = 1$, if $x_j \neq y_j$ and both x_j and y_j are present $\delta_{x,y}^j = 0$, otherwise
PP	both present = $PM + PX$
P	at least one present = $PM + X$
PAX	present-absent mismatches $PAX = \sum_{j=1}^v w_j \delta_{x,y}^j$, where $\delta_{x,y}^j = 1$, if $x_j \neq y_j$ and either x_j is present and y_j is absent or x_j is absent and y_j is present $\delta_{x,y}^j = 0$ otherwise
N	total nonmissing pairs $N = \sum_{j=1}^v w_j$

Methods That Accept Asymmetric Nominal and Ratio Variables

JACCARD Jaccard similarity coefficient

The JACCARD method is equivalent to the SIMRATIO method if there are only ratio variables; if there are both ratio and asymmetric nominal variables, the coefficient is computed as sum of the coefficient from the ratio variables (SIMRATIO) and the coefficient from the asymmetric nominal variables.

$$s_{36}(x, y) = s_{16}(x, y) + PM/P$$

DJACCARD Jaccard dissimilarity coefficient

The DJACCARD method is equivalent to the DISRATIO method if there are only ratio variables; if there are both ratio and asymmetric nominal variables, the coefficient is computed as sum of the coefficient from the ratio variables (DISRATIO) and the coefficient from the asymmetric nominal variables.

$$d_{37}(x, y) = d_{17}(x, y) + X/P$$

Methods That Accept Asymmetric Nominal Variables

DICE Dice coefficient or Czekanowski/Sorensen similarity coefficient

$$s_{38}(x, y) = 2PM/(P + PM)$$

RR Russell and Rao. This is the binary equivalent of the dot product coefficient.

$$s_{39}(x, y) = PM/N$$

BLWNM | BRAYCURTIS Binary Lance and Williams, also known as Bray and Curtis coefficient

$$d_{40}(x, y) = X/(PAX + 2PP)$$

K1 Kulczynski 1. The coefficient between an observation and itself is always indeterminate (missing) since there is no mismatch.

$$d_{41}(x, y) = PM/X$$

Missing Values

Standardization versus No Standardization

You can replace the missing values with or without standardization. Missing values are replaced after standardization by specifying either the REPLACE option in the PROC DISTANCE statement or the MISSING= option in the VAR statement.

To replace missing values without standardization, use the following two options:

- the NOSTD option in the PROC DISTANCE statement. The NOSTD option suppresses standardization but still replaces the missing values with the location of the method or the numeric value specified in the MISSING= option in the VAR statement.
- the REONLY option in the PROC DISTANCE statement. PROC DISTANCE replaces missing values with the location of the standardization method or with the numeric value specified in the MISSING= option in the VAR statement. This approach assumes that standardization is not mandatory (see the section “[Standardization](#)” on page 2162).

Eliminating Observations with Missing Values

If you specify the NOMISS option, PROC DISTANCE omits observations with any missing values in the analyzed variables from computation of the location and scale measures.

Distance Measures

If you specify the NOMISS option, PROC DISTANCE generates missing distance for observations with missing values. If the NOMISS option is not specified, the sum of total weights, no matter if an observation is missing or not, is incorporated into the computation of some of the proximity measures. See the section “Details: DISTANCE Procedure” on page 2181 for the formulas and descriptions.

Formatted versus Unformatted Values

PROC DISTANCE uses the formatted values from a character variable, if the variable has a format—for example, one assigned by a format statement. PROC DISTANCE uses the unformatted values from a numeric variable, even if it has a format.

Output Data Sets

OUT= Data Set

The DISTANCE procedure always produces an output data set, regardless of whether you specify the OUT= option in the PROC DISTANCE statement. PROC DISTANCE displays no output. Use PROC PRINT to display the output data set.

The output data set contains the following variables:

- the ID variable, if any
- the BY variables, if any
- the COPY variables, if any
- the FREQ variable, if any
- the WEIGHT variable, if any
- the new distance variables, named from PREFIX= options along with the ID values, or from the default values

The output data set is of type TYPE=DISTANCE or TYPE=SIMILAR. See the METHOD= option for more information about the output data set types. Data set types do not persist when you copy or modify a data set. You must specify the TYPE= data set option for the new data set, as in the following example:

```
data dist2(type=distance);
  set dist;
run;
```

See the OUT= option for more information about data set type persistence.

OUTSDZ= Data Set

The output data set is a copy of the DATA= data set except that the analyzed variables have been standardized. Analyzed variables are those listed in the VAR statement.

Examples: DISTANCE Procedure

Example 34.1: Divorce Grounds – the Jaccard Coefficient

A wide variety of distance and similarity measures are used in cluster analysis (Anderberg 1973; Sneath and Sokal 1973). If your data are in coordinate form and you want to use a non-Euclidean distance for clustering, you can compute a distance matrix by using the DISTANCE procedure.

Similarity measures must be converted to dissimilarities before being used in PROC CLUSTER. Such conversion can be done in a variety of ways, such as taking reciprocals or subtracting from a large value. The choice of conversion method depends on the application and the similarity measure. If applicable, PROC DISTANCE provides a corresponding dissimilarity measure for each similarity measure.

In the following example, the observations are states. Binary-valued variables correspond to various grounds for divorce and indicate whether the grounds for divorce apply in each of the U.S. states. A value of “1” indicates that the ground for divorce applies, and a value of “0” indicates the opposite. The 0-0 matches are treated as totally irrelevant; therefore, each variable has an asymmetric nominal level of measurement. The absence value is 0.

The DISTANCE procedure is used to compute the Jaccard coefficient (Anderberg 1973, pp. 89, 115, and 117) between each pair of states. The Jaccard coefficient is defined as the number of variables that are coded as 1 for both states divided by the number of variables that are coded as 1 for either or both states. Since dissimilarity measures are required by PROC CLUSTER, the DJACCARD coefficient is selected. [Output 34.1.1](#) displays the distance matrix between the first 10 states.

The CENTROID method is used to perform the cluster analysis, and the resulting tree diagram from PROC CLUSTER is saved into the tree output data set. [Output 34.1.2](#) displays the cluster history.

The TREE procedure generates nine clusters in the output data set out. After being sorted by the state, the out data set is then merged with the input data set divorce. After being sorted by the state, the merged data set is printed to display the cluster membership as shown in [Output 34.1.3](#).

The following statements produce [Output 34.1.1](#) through [Output 34.1.3](#):

```
data divorce;
  input State $15.
        (Incompatibility Cruelty Desertion Non_Support Alcohol
         Felony Impotence Insanity Separation) (1.) @@;
  if mod(_n_,2) then input +4 @@; else input;
  datalines;
Alabama      111111111      Alaska      111011110
Arizona      100000000      Arkansas    011111111
California   100000010      Colorado    100000000
Connecticut  111111011      Delaware    100000001
```



```
... more lines ...

Wisconsin      100000001    Wyoming      100000011
;

title 'Grounds for Divorce';
proc distance data=divorce method=djaccard absent=0 out=distjacc;
  var anominal(Incompatibility--Separation);
  id state;
run;

proc print data=distjacc(obs=10);
  id state; var alabama--georgia;
  title2 'First 10 States';
run;
title2;

proc cluster data=distjacc method=centroid
  pseudo outtree=tree;
  id state;
  var alabama--wyoming;
run;

proc tree data=tree noprint n=9 out=out;
  id state;
run;

proc sort;
  by state;
run;

data clus;
  merge divorce out;
  by state;
run;

proc sort;
  by cluster;
run;

proc print;
  id state;
  var Incompatibility--Separation;
  by cluster;
run;
```

Output 34.1.1 Distance Matrix Based on the Jaccard Coefficient

Grounds for Divorce						
First 10 States						
State	Alabama	Alaska	Arizona	Arkansas	California	Colorado
Alabama	0.00000
Alaska	0.22222	0.00000
Arizona	0.88889	0.85714	0.00000	.	.	.
Arkansas	0.11111	0.33333	1.00000	0.00000	.	.
California	0.77778	0.71429	0.50000	0.88889	0.00000	.
Colorado	0.88889	0.85714	0.00000	1.00000	0.50000	0.00000
Connecticut	0.11111	0.33333	0.87500	0.22222	0.75000	0.87500
Delaware	0.77778	0.87500	0.50000	0.88889	0.66667	0.50000
Florida	0.77778	0.71429	0.50000	0.88889	0.00000	0.50000
Georgia	0.22222	0.00000	0.85714	0.33333	0.71429	0.85714

State	Connecticut	Delaware	Florida	Georgia
Alabama
Alaska
Arizona
Arkansas
California
Colorado
Connecticut	0.00000	.	.	.
Delaware	0.75000	0.00000	.	.
Florida	0.75000	0.66667	0.00000	.
Georgia	0.33333	0.87500	0.71429	0

Output 34.1.2 Clustering History

Grounds for Divorce	
The CLUSTER Procedure	
Centroid Hierarchical Cluster Analysis	
Root-Mean-Square Distance Between Observations	0.694873

Output 34.1.2 continued

Cluster History					Norm T
NCL	-----Clusters Joined-----	Freq	Ps F	PsT2	Cent i Dist e
49	Arizona Colorado	2	.	.	0 T
48	California Florida	2	.	.	0 T
47	Alaska Georgia	2	.	.	0 T
46	Delaware Hawaii	2	.	.	0 T
45	Connecticut Idaho	2	.	.	0 T
44	CL49 Iowa	3	.	.	0 T
43	CL47 Kansas	3	.	.	0 T
42	CL44 Kentucky	4	.	.	0 T
41	CL42 Michigan	5	.	.	0 T
40	CL41 Minnesota	6	.	.	0 T
39	CL43 Mississippi	4	.	.	0 T
38	CL40 Missouri	7	.	.	0 T
37	CL38 Montana	8	.	.	0 T
36	CL37 Nebraska	9	.	.	0 T
35	North Dakota Oklahoma	2	.	.	0 T
34	CL36 Oregon	10	.	.	0 T
33	Massachusetts Rhode Island	2	.	.	0 T
32	New Hampshire Tennessee	2	.	.	0 T
31	CL46 Washington	3	.	.	0 T
30	CL31 Wisconsin	4	.	.	0 T
29	Nevada Wyoming	2	.	.	0
28	Alabama Arkansas	2	1561	.	0.1599 T
27	CL33 CL32	4	479	.	0.1799 T
26	CL39 CL35	6	265	.	0.1799 T
25	CL45 West Virginia	3	231	.	0.1799
24	Maryland Pennsylvania	2	199	.	0.2399
23	CL28 Utah	3	167	3.2	0.2468
22	CL27 Ohio	5	136	5.4	0.2698
21	CL26 Maine	7	111	8.9	0.2998
20	CL23 CL21	10	75.2	8.7	0.3004
19	CL25 New Jersey	4	71.8	6.5	0.3053 T
18	CL19 Texas	5	69.1	2.5	0.3077
17	CL20 CL22	15	48.7	9.9	0.3219
16	New York Virginia	2	50.1	.	0.3598
15	CL18 Vermont	6	49.4	2.9	0.3797
14	CL17 Illinois	16	47.0	3.2	0.4425
13	CL14 CL15	22	29.2	15.3	0.4722
12	CL48 CL29	4	29.5	.	0.4797 T
11	CL13 CL24	24	27.6	4.5	0.5042
10	CL11 South Dakota	25	28.4	2.4	0.5449
9	Louisiana CL16	3	30.3	3.5	0.5844
8	CL34 CL30	14	23.3	.	0.7196
7	CL8 CL12	18	19.3	15.0	0.7175
6	CL10 South Carolina	26	21.4	4.2	0.7384
5	CL6 New Mexico	27	24.0	4.7	0.8303
4	CL5 Indiana	28	28.9	4.1	0.8343
3	CL4 CL9	31	31.7	10.9	0.8472
2	CL3 North Carolina	32	55.1	4.1	1.0017
1	CL2 CL7	50	.	55.1	1.0663

Output 34.1.3 continued

Grounds for Divorce									
----- CLUSTER=2 -----									
	I n c o m p a r i b l e t t e	C r i t i c a l	D e s e r t i o n	N o n - S u p p o r t l y	A l t e r n a t i v e	F o l l o w i n g	I m p o n e n t	I n s e r t i o n	S e p a r a t i o n
California	1	0	0	0	0	0	0	1	0
Florida	1	0	0	0	0	0	0	1	0
Nevada	1	0	0	0	0	0	0	1	1
Wyoming	1	0	0	0	0	0	0	1	1
----- CLUSTER=3 -----									
	I n c o m p a r i b l e t t e	C r i t i c a l	D e s e r t i o n	N o n - S u p p o r t l y	A l t e r n a t i v e	F o l l o w i n g	I m p o n e n t	I n s e r t i o n	S e p a r a t i o n
Alabama	1	1	1	1	1	1	1	1	1
Alaska	1	1	1	0	1	1	1	1	0
Arkansas	0	1	1	1	1	1	1	1	1
Connecticut	1	1	1	1	1	1	0	1	1
Georgia	1	1	1	0	1	1	1	1	0

Output 34.1.3 continued

Grounds for Divorce									
----- CLUSTER=3 -----									
(continued)									
	I n c o m p a r i s o n	C s u r r o r y	D e s e r t o r y	N o n _ S e p a r a t e	A l c o h o l i c m i s t e r y	F e l o n c y	I m p o s s i b l e	I n j u r y	S e p a r a t e
Idaho	1	1	1	1	1	1	0	1	1
Illinois	0	1	1	0	1	1	1	0	0
Kansas	1	1	1	0	1	1	1	1	0
Maine	1	1	1	1	1	0	1	1	0
Maryland	0	1	1	0	0	1	1	1	1
Massachusetts	1	1	1	1	1	1	1	0	1
Mississippi	1	1	1	0	1	1	1	1	0
New Hampshire	1	1	1	1	1	1	1	0	0
New Jersey	0	1	1	0	1	1	0	1	1
North Dakota	1	1	1	1	1	1	1	1	0
Ohio	1	1	1	0	1	1	1	0	1
Oklahoma	1	1	1	1	1	1	1	1	0
Pennsylvania	0	1	1	0	0	1	1	1	0
Rhode Island	1	1	1	1	1	1	1	0	1
South Dakota	0	1	1	1	1	1	0	0	0
Tennessee	1	1	1	1	1	1	1	0	0
Texas	1	1	1	0	0	1	0	1	1
Utah	0	1	1	1	1	1	1	1	0
Vermont	0	1	1	1	0	1	0	1	1
West Virginia	1	1	1	0	1	1	0	1	1

Output 34.1.3 continued

Grounds for Divorce									
----- CLUSTER=4 -----									
	I n c o m p a r i b l e t t e	C r i t i c a l l y	D e s e r v i t y	N o n - S u p e r i o r t y	A l t e r n a t i v e	F e l o n y	I m p o n e n t	I n s e r t i o n	S e p a r a t i o n
Delaware	1	0	0	0	0	0	0	0	1
Hawaii	1	0	0	0	0	0	0	0	1
Washington	1	0	0	0	0	0	0	0	1
Wisconsin	1	0	0	0	0	0	0	0	1
----- CLUSTER=5 -----									
	I n c o m p a r i b l e t t e	C r i t i c a l l y	D e s e r v i t y	N o n - S u p e r i o r t y	A l t e r n a t i v e	F e l o n y	I m p o n e n t	I n s e r t i o n	S e p a r a t i o n
Louisiana	0	0	0	0	0	1	0	0	1
New York	0	1	1	0	0	1	0	0	1
Virginia	0	1	0	0	0	1	0	0	1

Output 34.1.3 continued

Grounds for Divorce									
----- CLUSTER=6 -----									
	I n c o m p a r i b l e t t e y	C r i l l t y	D e s e r t o r n	N o n - S u p p o r t	A l c o h o l i c	F e l o n c y	I m p o n e n c e	I n s e n s i b l e	S e p a r a t i o n
South Carolina	0	1	1	0	1	0	0	0	1
----- CLUSTER=7 -----									
	I n c o m p a r i b l e t t e y	C r i l l t y	D e s e r t o r n	N o n - S u p p o r t	A l c o h o l i c	F e l o n c y	I m p o n e n c e	I n s e n s i b l e	S e p a r a t i o n
New Mexico	1	1	1	0	0	0	0	0	0

Output 34.1.3 continued

Grounds for Divorce									
----- CLUSTER=8 -----									
	I n c o m p a r t i b l e t t e y	C r i t i c l e t t e y	D e s e r t o r n	N o n - S u p p o r t	A l t e r n a t i v e	F e l o n c y	I m p o r t a n c e	I n s e p a r a t i o n	S e p a r a t i o n
Indiana	1	0	0	0	0	1	1	1	0
----- CLUSTER=9 -----									
	I n c o m p a r t i b l e t t e y	C r i t i c l e t t e y	D e s e r t o r n	N o n - S u p p o r t	A l t e r n a t i v e	F e l o n c y	I m p o r t a n c e	I n s e p a r a t i o n	S e p a r a t i o n
North Carolina	0	0	0	0	0	0	1	1	1

Example 34.2: Financial Data – Stock Dividends

The following data set contains the average dividend yields for 15 utility stocks in the United States. The observations are names of the companies, and the variables correspond to the annual dividend yields for the period 1986–1990. The objective is to group similar stocks into clusters.

Before the cluster analysis is performed, the correlation similarity is chosen for measuring the closeness between each observation. Since distance type of measures are required by PROC CLUSTER, METHOD=DCORR is used in the PROC DISTANCE statement to transform the correlation measures to the distance measures. Notice that in [Output 34.2.1](#), all the values in the distance matrix are between 0 and 2.

PROC CLUSTER performs hierarchical clustering by using agglomerative methods based on the distance data created from the previous PROC DISTANCE statement. Since the cubic clustering criterion is not suitable for distance data, only the pseudo F statistic is requested to identify the number of clusters.

The two clustering methods are Ward's and the average linkage methods. Since the results of the pseudo t^2 statistic from both Ward's and the average linkage methods contain many missing values, only the plot of the pseudo F statistic versus the number of clusters is requested along with the dendrogram by specifying PLOTS(ONLY)=(PSF DENDROGRAM) in the PROC CLUSTER statement.

Both [Output 34.2.2](#) and [Output 34.2.3](#) suggest four clusters. Both methods produce the same clustering result, as shown in [Output 34.2.4](#) and [Output 34.2.5](#). The four clusters are as follows:

- Cincinnati G&E and Detroit Edison
- Texas Utilities and Pennsylvania Power & Light
- Union Electric, Iowa-Ill Gas & Electric, Oklahoma Gas & Electric, and Wisconsin Energy
- Orange & Rockland Utilities, Kentucky Utilities, Kansas Power & Light, Allegheny Power, Green Mountain Power, Dominion Resources, and Minnesota Power & Light

```

title 'Stock Dividends';

data stock;
  input Company $27.  Div_1986 Div_1987 Div_1988 Div_1989 Div_1990;
  datalines;
Cincinnati G&E           8.4    8.2    8.4    8.1    8.0
Texas Utilities          7.9    8.9   10.4    8.9    8.3
Detroit Edison           9.7   10.7   11.4    7.8    6.5
Orange & Rockland Utilities 6.5    7.2    7.3    7.7    7.9
Kentucky Utilities       6.5    6.9    7.0    7.2    7.5
Kansas Power & Light     5.9    6.4    6.9    7.4    8.0
Union Electric           7.1    7.5    8.4    7.8    7.7
Dominion Resources       6.7    6.9    7.0    7.0    7.4
Allegheny Power          6.7    7.3    7.8    7.9    8.3
Minnesota Power & Light  5.6    6.1    7.2    7.0    7.5
Iowa-Ill Gas & Electric  7.1    7.5    8.5    7.8    8.0
Pennsylvania Power & Light 7.2    7.6    7.7    7.4    7.1
Oklahoma Gas & Electric  6.1    6.7    7.4    6.7    6.8
Wisconsin Energy         5.1    5.7    6.0    5.7    5.9
Green Mountain Power    7.1    7.4    7.8    7.8    8.3
;

proc distance data=stock method=dcorr out=distdcorr;
  var interval(div_1986 div_1987 div_1988 div_1989 div_1990);
  id company;
run;

proc print data=distdcorr;
  id company;
  title2 'Distance Matrix for 15 Utility Stocks';
run;
title2;

ods graphics on;

/* compute pseudo statistic versus number of clusters and create plot */
proc cluster data=distdcorr method=ward pseudo plots(only)=(psf dendrogram);
  id company;
run;

/* compute pseudo statistic versus number of clusters and create plot */
proc cluster data=distdcorr method=average pseudo plots(only)=(psf dendrogram);
  id company;
run;

ods graphics off;

```

Output 34.2.1 Distance Matrix Based on the DCORR Coefficient

Stock Dividends Distance Matrix for 15 Utility Stocks						
	Cincinnati_ G_E	Texas_ Utilities	Detroit_ Edison	Orange_ Rockland_ Utilities		
Company						
Cincinnati G&E	0.00000	.	.	.		
Texas Utilities	0.82056	0.00000	.	.		
Detroit Edison	0.40511	0.65453	0.00000	.		
Orange & Rockland Utilities	1.35380	0.88583	1.27306	0.00000		
Kentucky Utilities	1.35581	0.92539	1.29382	0.12268		
Kansas Power & Light	1.34227	0.94371	1.31696	0.19905		
Union Electric	0.98516	0.29043	0.89048	0.68798		
		Kansas_ Kentucky_ Utilities	Power_ Light	Union_ Electric	Dominion_ Resources	Allegheny_ Power
Company						
Cincinnati G&E
Texas Utilities
Detroit Edison
Orange & Rockland Utilities
Kentucky Utilities	0.00000
Kansas Power & Light	0.12874	0.00000
Union Electric	0.71824	0.72082	0.00000	.	.	.
		Minnesota_ Power_ Light	Iowa_Ill_ Gas_ Electric	Pennsylvania_ Power_ Light	Oklahoma_ Gas_ Electric	
Company						
Cincinnati G&E
Texas Utilities
Detroit Edison
Orange & Rockland Utilities
Kentucky Utilities
Kansas Power & Light
Union Electric
		Wisconsin_ Energy	Green_ Mountain_ Power			
Company						
Cincinnati G&E
Texas Utilities
Detroit Edison
Orange & Rockland Utilities
Kentucky Utilities
Kansas Power & Light
Union Electric

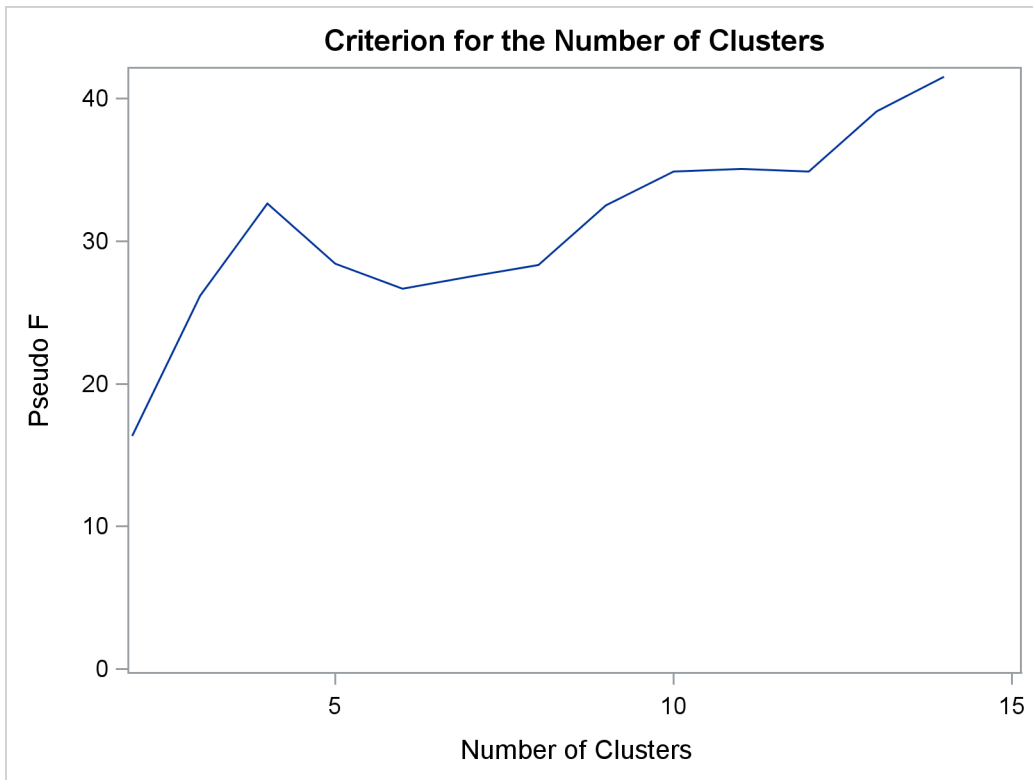
Output 34.2.1 continued

Stock Dividends				
Distance Matrix for 15 Utility Stocks				
	Cincinnati_	Texas_	Detroit_	Orange_
Company	G_E	Utilities	Edison	Rockland_
				Utilities
Dominion Resources	1.32945	0.96853	1.29016	0.33290
Allegheny Power	1.30492	0.81666	1.24565	0.17844
Minnesota Power & Light	1.24069	0.74082	1.20432	0.32581
Iowa-Ill Gas & Electric	1.04924	0.43100	0.97616	0.61166
Pennsylvania Power & Light	0.74931	0.37821	0.44256	1.03566
Oklahoma Gas & Electric	1.00604	0.30141	0.86200	0.68021
Wisconsin Energy	1.17988	0.54830	1.03081	0.45013
		Kansas_		
Company	Kentucky_	Power_	Union_	Dominion_
	Utilities	Light	Electric	Resources
				Allegheny_
				Power
Dominion Resources	0.21510	0.24189	0.76587	0.00000
Allegheny Power	0.15759	0.17029	0.58452	0.27819
Minnesota Power & Light	0.30462	0.27231	0.48372	0.35733
Iowa-Ill Gas & Electric	0.61760	0.61736	0.16923	0.63545
Pennsylvania Power & Light	1.08878	1.12876	0.63285	1.14354
Oklahoma Gas & Electric	0.70259	0.73158	0.17122	0.72977
Wisconsin Energy	0.47184	0.53381	0.37405	0.51969
Company	Minnesota_	Iowa_Ill_		Oklahoma_
	Power_	Gas_	Pennsylvania_	Gas_
	Light	Electric	Power_Light	Electric
Dominion Resources
Allegheny Power
Minnesota Power & Light	0.00000	.	.	.
Iowa-Ill Gas & Electric	0.36368	0.00000	.	.
Pennsylvania Power & Light	0.99384	0.75596	0.00000	.
Oklahoma Gas & Electric	0.50744	0.19673	0.60216	0.00000
Wisconsin Energy	0.36319	0.30259	0.76085	0.28070
Company	Wisconsin_	Green_		
	Energy	Mountain_		
		Power		
Dominion Resources	.	.		
Allegheny Power	.	.		
Minnesota Power & Light	.	.		
Iowa-Ill Gas & Electric	.	.		
Pennsylvania Power & Light	.	.		
Oklahoma Gas & Electric	.	.		
Wisconsin Energy	0.00000	.		

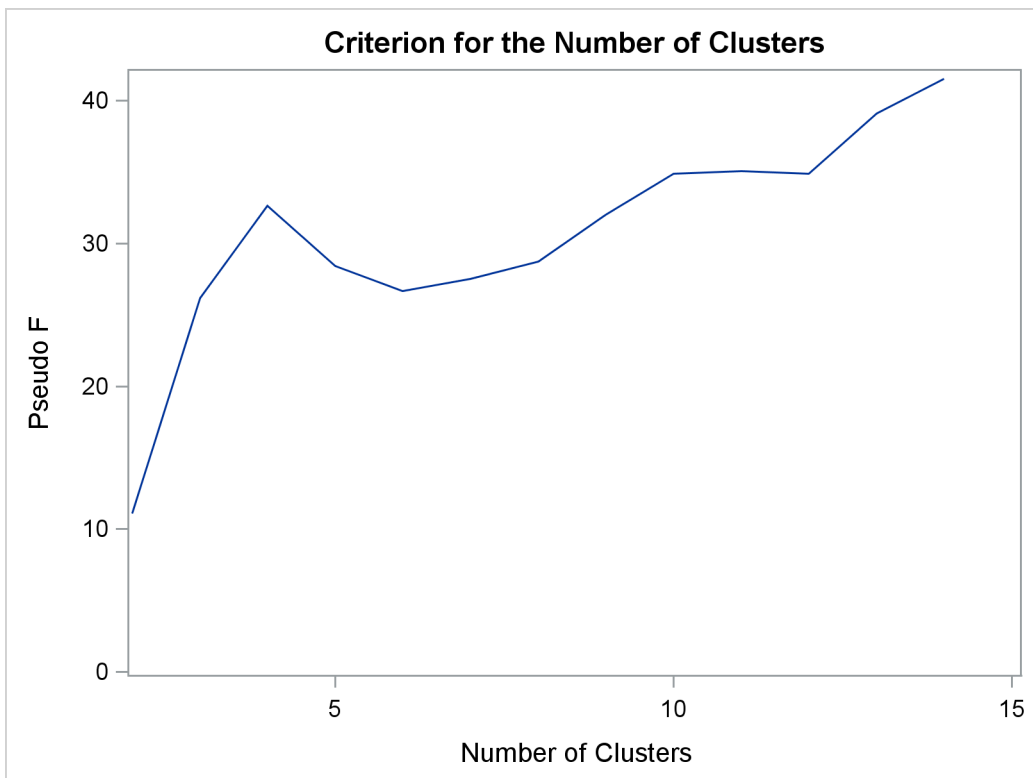
Output 34.2.1 continued

Stock Dividends					
Distance Matrix for 15 Utility Stocks					
Company	Cincinnati_ G_E	Texas_ Utilities	Detroit_ Edison	Orange_ Rockland_ Utilities	
Green Mountain Power	1.30397	0.88063	1.27176	0.26948	
Company	Kentucky_ Utilities	Kansas_ Power_ Light	Union_ Electric	Dominion_ Resources	Allegheny_ Power
Green Mountain Power	0.17909	0.15377	0.64869	0.17360	0.13958
Company	Minnesota_ Power_ Light	Iowa_ Ill_ Gas_ Electric	Pennsylvania_ Power_ Light	Oklahoma_ Gas_ Electric	
Green Mountain Power	0.19370	0.52083	1.09269	0.64175	
Company	Wisconsin_ Energy	Green_ Mountain_ Power			
Green Mountain Power	0.44814	0			

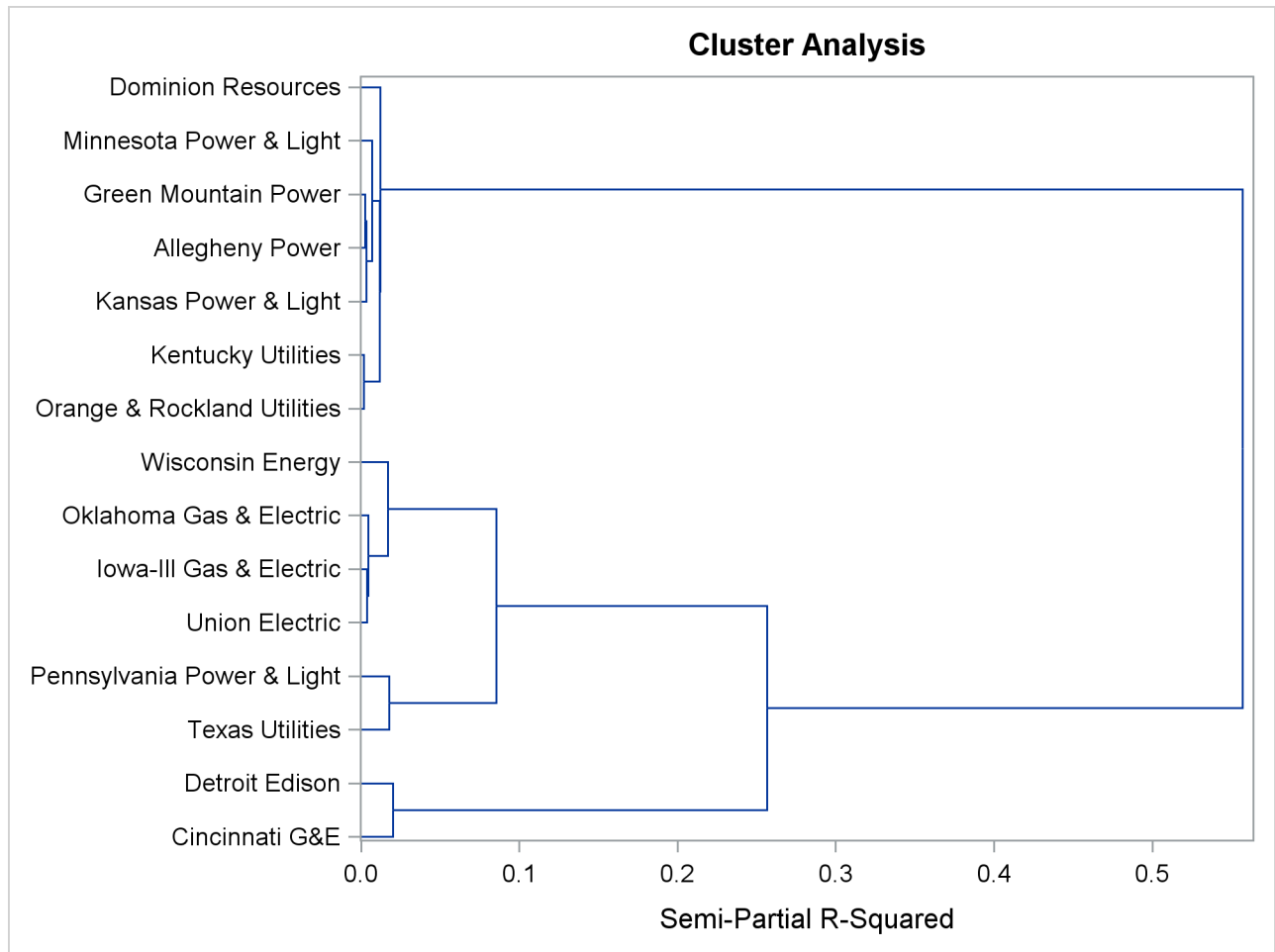
Output 34.2.2 Pseudo F versus Number of Clusters When METHOD=WARD

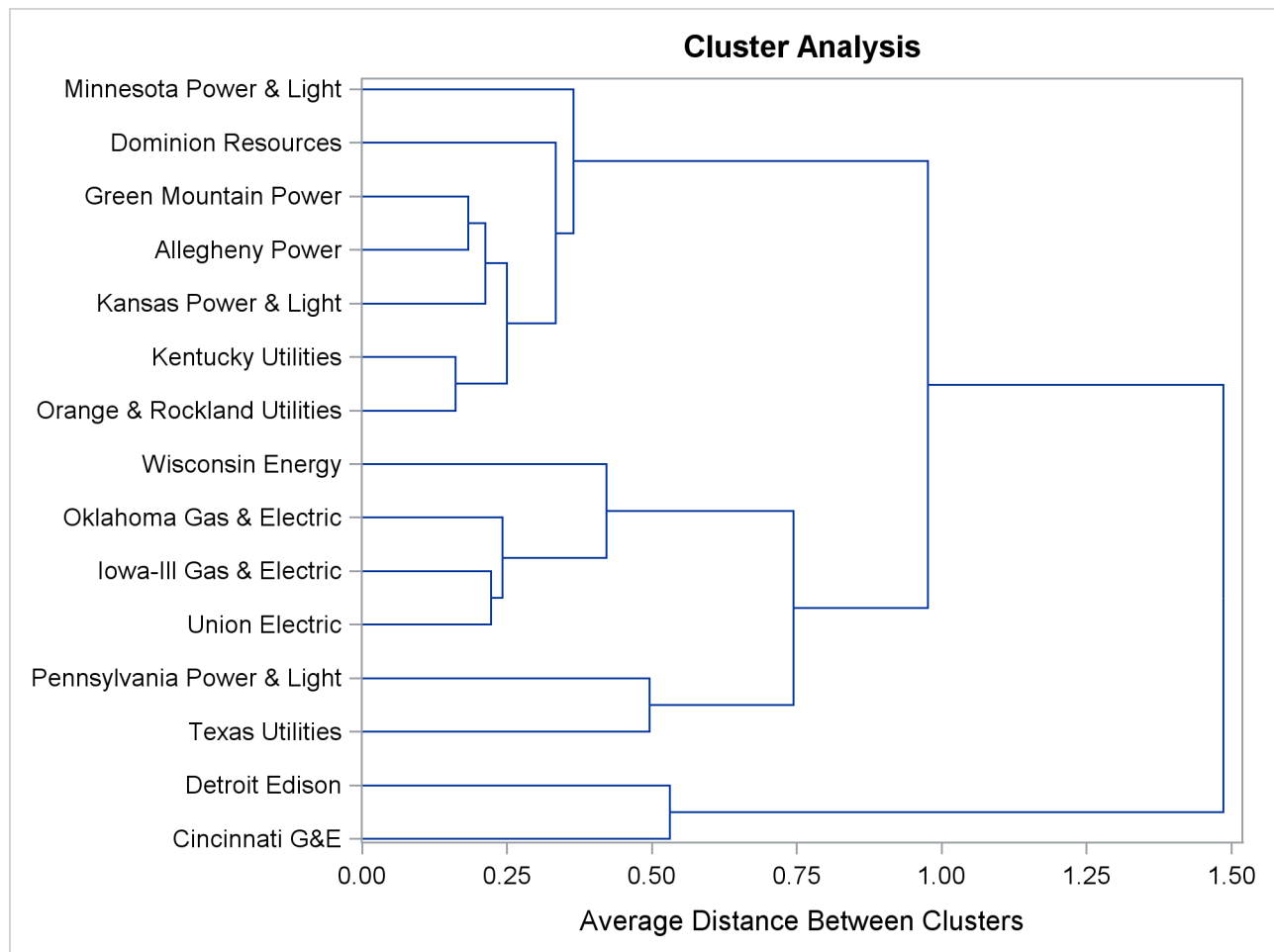


Output 34.2.3 Pseudo F versus Number of Clusters When METHOD=AVERAGE



Output 34.2.4 Dendrogram of Semipartial R-Square Values When METHOD=WARD



Output 34.2.5 Dendrogram of Average Distance between Clusters When METHOD=AVERAGE

References

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- Hand, D. J., Daly, F., Lunn, A. D., McConway, K. J., and Ostrowski, E. (1994), *A Handbook of Small Data Sets*, London: Chapman & Hall.
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Chapter 35

The FACTOR Procedure

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Overview: FACTOR Procedure

The FACTOR procedure performs a variety of common factor and component analyses and rotations. Input can be multivariate data, a correlation matrix, a covariance matrix, a factor pattern, or a matrix of scoring coefficients. The procedure can factor either the correlation or covariance matrix, and you can save most results in an output data set.

PROC FACTOR can process output from other procedures. For example, it can rotate the canonical coefficients from multivariate analyses in the GLM procedure.

The methods for factor extraction are principal component analysis, principal factor analysis, iterated principal factor analysis, unweighted least squares factor analysis, maximum likelihood (canonical) factor analysis, alpha factor analysis, image component analysis, and Harris component analysis. A variety of methods for prior communality estimation is also available.

Specific methods for orthogonal rotation are varimax, quartimax, biquartimax, equamax, parsimax, and factor parsimax. Oblique versions of these methods are also available. In addition, quartimin, biquartimin, and covarimin methods for (direct) oblique rotation are available. General methods for orthogonal rotation are orthomax with user-specified gamma, Crawford-Ferguson family with user-specified weights on variable parsimony and factor parsimony, and generalized Crawford-Ferguson family with user-specified weights. General methods for oblique rotation are direct oblimin with user-specified tau, Crawford-Ferguson family with user-specified weights on variable parsimony and factor parsimony, generalized Crawford-Ferguson family with user-specified weights, promax with user-specified exponent, Harris-Kaiser case II with user-specified exponent, and Procrustes with a user-specified target pattern.

Output includes means, standard deviations, correlations, Kaiser's measure of sampling adequacy, eigenvalues, a scree plot, eigenvectors, prior and final communality estimates, the unrotated factor pattern, residual and partial correlations, the rotated primary factor pattern, the primary factor structure, interfactor correlations, the reference structure, reference axis correlations, the variance explained by each factor both ignoring and eliminating other factors, plots of both rotated and unrotated factors, squared multiple correlation of each factor with the variables, standard error estimates, confidence limits, coverage displays, and scoring coefficients.

The FACTOR procedure uses ODS Graphics to create graphs as part of its output. For general information about ODS Graphics, see Chapter 21, "Statistical Graphics Using ODS."

Any topics that are not given explicit references are discussed in Mulaik (1972) or Harman (1976).

Background

See Chapter 73, "The PRINCOMP Procedure," for a discussion of principal component analysis. See Chapter 27, "The CALIS Procedure," for a discussion of confirmatory factor analysis.

Common factor analysis was invented by Spearman (1904). Kim and Mueller (1978a, b) provide a very elementary discussion of the common factor model. Gorsuch (1974) presents a broad survey of factor analysis, and Gorsuch (1974) and Cattell (1978) are useful as guides to practical research methodology. Harman (1976) gives a lucid discussion of many of the more technical aspects of factor analysis, especially oblique rotation. Morrison (1976) and Mardia, Kent, and Bibby (1979) provide excellent statistical treatments of common factor analysis. Mulaik (1972) provides the most thorough and authoritative general reference on

factor analysis and is highly recommended to anyone familiar with matrix algebra. Stewart (1981) gives a nontechnical presentation of some issues to consider when deciding whether or not a factor analysis might be appropriate.

A frequent source of confusion in the field of factor analysis is the term *factor*. It sometimes refers to a hypothetical, unobservable variable, as in the phrase *common factor*. In this sense, *factor analysis* must be distinguished from component analysis since a component is an observable linear combination. *Factor* is also used in the sense of *matrix factor*, in that one matrix is a factor of a second matrix if the first matrix multiplied by its transpose equals the second matrix. In this sense, *factor analysis* refers to all methods of data analysis that use matrix factors, including component analysis and common factor analysis.

A *common factor* is an unobservable, hypothetical variable that contributes to the variance of at least two of the observed variables. The unqualified term “factor” often refers to a common factor. A *unique factor* is an unobservable, hypothetical variable that contributes to the variance of only one of the observed variables. The model for common factor analysis posits one unique factor for each observed variable.

The equation for the common factor model is

$$y_{ij} = x_{i1}b_{1j} + x_{i2}b_{2j} + \cdots + x_{iq}b_{qj} + e_{ij}$$

where

y_{ij}	is the value of the i th observation on the j th variable
x_{ik}	is the value of the i th observation on the k th common factor
b_{kj}	is the regression coefficient of the k th common factor for predicting the j th variable
e_{ij}	is the value of the i th observation on the j th unique factor
q	is the number of common factors

It is assumed, for convenience, that all variables have a mean of 0. In matrix terms, these equations reduce to

$$\mathbf{Y} = \mathbf{XB} + \mathbf{E}$$

In the preceding equation, \mathbf{X} is the matrix of factor scores, and \mathbf{B}' is the factor pattern.

There are two critical assumptions:

- The unique factors are uncorrelated with each other.
- The unique factors are uncorrelated with the common factors.

In principal component analysis, the residuals are generally correlated with each other. In common factor analysis, the unique factors play the role of residuals and are defined to be uncorrelated both with each other and with the common factors. Each common factor is assumed to contribute to at least two variables; otherwise, it would be a unique factor.

When the factors are initially extracted, it is also assumed, for convenience, that the common factors are uncorrelated with each other and have unit variance. In this case, the common factor model implies that the covariance s_{jk} between the j th and k th variables, $j \neq k$, is given by

$$s_{jk} = b_{1j}b_{1k} + b_{2j}b_{2k} + \cdots + b_{qj}b_{qk}$$

or

$$\mathbf{S} = \mathbf{B}'\mathbf{B} + \mathbf{U}^2$$

where \mathbf{S} is the covariance matrix of the observed variables, and \mathbf{U}^2 is the diagonal covariance matrix of the unique factors.

If the original variables are standardized to unit variance, the preceding formula yields correlations instead of covariances. It is in this sense that common factors explain the correlations among the observed variables. When considering the diagonal elements of standardized \mathbf{S} , the variance of the j th variable is expressed as

$$s_{jj} = 1 = b_{1j}^2 + b_{2j}^2 + \cdots + b_{qj}^2 + [\mathbf{U}^2]_{jj}$$

where $b_{1j}^2 + b_{2j}^2 + \cdots + b_{qj}^2$ and $[\mathbf{U}^2]_{jj}$ are the communality and uniqueness, respectively, of the j th variable. The communality represents the extent of the overlap with the common factors. In other words, it is the proportion of variance accounted for by the common factors.

The difference between the correlation predicted by the common factor model and the actual correlation is the *residual correlation*. A good way to assess the goodness of fit of the common factor model is to examine the residual correlations.

The common factor model implies that the partial correlations among the variables, removing the effects of the common factors, must all be zero. When the common factors are removed, only unique factors, which are by definition uncorrelated, remain.

The assumptions of common factor analysis imply that the common factors are, in general, not linear combinations of the observed variables. In fact, even if the data contain measurements on the entire population of observations, you cannot compute the scores of the observations on the common factors. Although the common factor scores cannot be computed directly, they can be estimated in a variety of ways.

The problem of factor score indeterminacy has led several factor analysts to propose methods yielding components that can be considered approximations to common factors. Since these components are defined as linear combinations, they are computable. The methods include Harris component analysis and image component analysis. The advantage of producing determinate component scores is offset by the fact that, even if the data fit the common factor model perfectly, component methods do not generally recover the correct factor solution. You should not use any type of component analysis if you really want a common factor analysis (Dziuban and Harris 1973; Lee and Comrey 1979).

After the factors are estimated, it is necessary to interpret them. Interpretation usually means assigning to each common factor a name that reflects the *salience* of the factor in predicting each of the observed variables—that is, the coefficients in the pattern matrix corresponding to the factor. Factor interpretation is a subjective process. It can sometimes be made less subjective by *rotating* the common factors—that is, by applying a nonsingular linear transformation. A rotated pattern matrix in which all the coefficients are close to 0 or ± 1 is easier to interpret than a pattern with many intermediate elements. Therefore, most rotation methods attempt to optimize a simplicity function of the rotated pattern matrix that measures, in some sense, how close the elements are to 0 or ± 1 . Because the loading estimates are subject to sampling variability, it is useful to obtain the standard error estimates for the loadings for assessing the uncertainty due to random sampling. Notice that the *salience* of a factor loading refers to the magnitude of the loading, while statistical *significance* refers to the statistical evidence against a particular hypothetical value. A loading significantly different from 0 does not automatically mean it must be salient. For example, if salience is defined as a

magnitude larger than 0.4 while the entire 95% confidence interval for a loading lies between 0.1 and 0.3, the loading is statistically significant larger than 0 but it is not salient. Under the maximum likelihood method, you can obtain standard errors and confidence intervals for judging the salience of factor loadings.

After the initial factor extraction, the common factors are uncorrelated with each other. If the factors are rotated by an *orthogonal transformation*, the rotated factors are also uncorrelated. If the factors are rotated by an *oblique transformation*, the rotated factors become correlated. Oblique rotations often produce more useful patterns than do orthogonal rotations. However, a consequence of correlated factors is that there is no single unambiguous measure of the importance of a factor in explaining a variable. Thus, for oblique rotations, the pattern matrix does not provide all the necessary information for interpreting the factors; you must also examine the *factor structure* and the *reference structure*.

Rotating a set of factors does not change the statistical explanatory power of the factors. You cannot say that any rotation is better than any other rotation from a statistical point of view; all rotations, orthogonal or oblique, are equally good statistically. Therefore, the choice among different rotations must be based on nonstatistical grounds. For most applications, the preferred rotation is that which is most easily interpretable, or most compatible with substantive theories.

If two rotations give rise to different interpretations, those two interpretations must not be regarded as conflicting. Rather, they are two different ways of looking at the same thing, two different points of view in the common-factor space. Any conclusion that depends on one and only one rotation being correct is invalid.

Outline of Use

Principal Component Analysis

One important type of analysis performed by the FACTOR procedure is principal component analysis. The following statements result in a principal component analysis:

```
proc factor;
run;
```

The output includes all the eigenvalues and the pattern matrix for eigenvalues greater than one.

Most applications require additional output. For example, you might want to compute principal component scores for use in subsequent analyses or obtain a graphical aid to help decide how many components to keep. You can save the results of the analysis in a permanent SAS data library by using the **OUTSTAT=** option. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*. Assuming that your SAS data library has the libref `save` and that the data are in a SAS data set called `raw`, you could do a principal component analysis as follows:

```
proc factor data=raw method=principal scree mineigen=0 score
      outstat=save.fact_all;
run;
```

The **SCREE** option produces a plot of the eigenvalues that is helpful in deciding how many components to use. Alternatively, you can use the **PLOTS=SCREE** option to produce high-quality scree plots. The **MINEIGEN=0** option causes all components with variance greater than zero to be retained. The **SCORE** option requests that scoring coefficients be computed. The **OUTSTAT=** option saves the results in a specially

structured SAS data set. The name of the data set, in this case `fact_all`, is arbitrary. To compute principal component scores, use the SCORE procedure:

```
proc score data=raw score=save.fact_all out=save.scores;
run;
```

The SCORE procedure uses the data and the scoring coefficients that are saved in `save.fact_all` to compute principal component scores. The component scores are placed in variables named `Factor1`, `Factor2`, ..., `Factor n` and are saved in the data set `save.scores`. If you know ahead of time how many principal components you want to use, you can obtain the scores directly from PROC FACTOR by specifying the `NFACTORS=` and `OUT=` options. To get scores from three principal components, specify the following:

```
proc factor data=raw method=principal
  nfactors=3 out=save.scores;
run;
```

To plot the scores for the first three components, use the SGSCATTER procedure:

```
proc sgscatter;
  matrix factor1-factor3;
run;
```

Principal Factor Analysis

The simplest and computationally most efficient method of common factor analysis is principal factor analysis, which is obtained in the same way as principal component analysis except for the use of the `PRIORS=` option. The usual form of the initial analysis is as follows:

```
proc factor data=raw method=principal scree
  mineigen=0 priors=smc outstat=save.fact_all;
run;
```

The squared multiple correlations (SMC) of each variable with all the other variables are used as the prior communality estimates. If your correlation matrix is singular, you should specify `PRIORS=MAX` instead of `PRIORS=SMC`. The `SCREE` and `MINEIGEN=` options serve the same purpose as in the preceding principal component analysis. Saving the results with the `OUTSTAT=` option enables you to examine the eigenvalues and scree plot before deciding how many factors to rotate and to try several different rotations without re-extracting the factors. The `OUTSTAT=` data set is automatically marked `TYPE=FACTOR`, so the FACTOR procedure realizes that it contains statistics from a previous analysis instead of raw data.

After looking at the eigenvalues to estimate the number of factors, you can try some rotations. Two and three factors can be rotated with the following statements:

```
proc factor data=save.fact_all method=principal n=2
  rotate=promax reorder score outstat=save.fact_2;
run;
proc factor data=save.fact_all method=principal n=3
  rotate=promax reorder score outstat=save.fact_3;
run;
```

The output data set from the previous run is used as input for these analyses. The options `N=2` and `N=3` specify the number of factors to be rotated. The specification `ROTATE=PROMAX` requests a promax rotation, which has the advantage of providing both orthogonal and oblique rotations with only one invocation of

PROC FACTOR. The **REORDER** option causes the variables to be reordered in the output so that variables associated with the same factor appear next to each other.

You can now compute and plot factor scores for the two-factor promax-rotated solution as follows:

```
proc score data=raw score=save.fact_2 out=save.scores;
run;

proc sgplot;
  scatter y=factor2 x=factor1;
run;
```

Maximum Likelihood Factor Analysis

Although principal factor analysis is perhaps the most commonly used method of common factor analysis, most statisticians prefer maximum likelihood (ML) factor analysis (Lawley and Maxwell 1971). The ML method of estimation has desirable asymptotic properties (Bickel and Doksum 1977) and produces better estimates than principal factor analysis in large samples. You can test hypotheses about the number of common factors by using the ML method. You can also obtain standard error and confidence interval estimates for many classes of rotated or unrotated factor loadings, factor correlations, and structure loadings under the ML theory.

The unrotated ML solution is equivalent to Rao's canonical factor solution (Rao 1955) and Howe's solution maximizing the determinant of the partial correlation matrix (Morrison 1976). Thus, as a descriptive method, ML factor analysis does not require a multivariate normal distribution. The validity of Bartlett's χ^2 test for the number of factors does require approximate normality plus additional regularity conditions that are usually satisfied in practice (Geweke and Singleton 1980). Bartlett's test of sphericity in the context of factor analysis is equivalent to Bartlett's χ^2 test for zero common factors. This test is routinely displayed in the maximum likelihood factor analysis output.

Lawley and Maxwell (1971) derive the standard error formulas for unrotated loadings, while Archer and Jennrich (1973) and Jennrich (1973, 1974) derive the standard error formulas for several classes of rotated solutions. Extended formulas for computing standard errors in various situations appear in Browne et al. (2008); Hayashi and Yung (1999); Yung and Hayashi (2001). A combination of these methods is used in PROC FACTOR to compute standard errors in an efficient manner. Confidence intervals are computed by using the asymptotic normality of the estimates. To ensure that the confidence intervals fall within the admissible parameter range, transformation methods due to Browne (1982) are used. The validity of the standard error estimates and confidence limits requires the assumptions of multivariate normality and a fixed number of factors.

The ML method is more computationally demanding than principal factor analysis for two reasons. First, the communalities are estimated iteratively, and each iteration takes about as much computer time as principal factor analysis. The number of iterations typically ranges from about five to twenty. Second, if you want to extract different numbers of factors, as is often the case, you must run the FACTOR procedure once for each number of factors. Therefore, an ML analysis can take 100 times as long as a principal factor analysis. This does not include the time for computing standard error estimates, which is even more computationally demanding. For analyses with fewer than 35 variables, the computing time for the ML method, including the computation of standard errors, usually ranges from a few seconds to well under a minute. This seems to be a reasonable performance.

You can use principal factor analysis to get a rough idea of the number of factors before doing an ML analysis. If you think that there are between one and three factors, you can use the following statements for the ML analysis:

```
proc factor data=raw method=ml n=1
    outstat=save.fact1;
run;
proc factor data=raw method=ml n=2 rotate=promax
    outstat=save.fact2;
run;
proc factor data=raw method=ml n=3 rotate=promax
    outstat=save.fact3;
run;
```

The output data sets can be used for trying different rotations, computing scoring coefficients, or restarting the procedure in case it does not converge within the allotted number of iterations.

If you can determine how many factors should be retained before an analysis, as in the following statements, you can get the standard errors and confidence limits to aid interpretations for the ML analysis:

```
proc factor data=raw method=ml n=3 rotate=quartimin se
    cover=.4;
run;
```

In this analysis, you specify the quartimin rotation in the **ROTATE=** option. The **SE** option requests the computation of standard error estimates. In the **COVER=** option, you require absolute values of 0.4 or greater in order for loadings to be salient. In the output of coverage display, loadings that are salient would have their entire confidence intervals spanning beyond the 0.4 mark (or the -0.4 mark in the opposite direction). Only those salient loadings should be used for interpreting the factors. See the section “[Confidence Intervals and the Salience of Factor Loadings](#)” on page 2243 for more details.

The ML method cannot be used with a singular correlation matrix, and it is especially prone to Heywood cases. See the section “[Heywood Cases and Other Anomalies about Communality Estimates](#)” on page 2248 for a discussion of Heywood cases. If you have problems with ML, the best alternative is to use the **METHOD=ULS** option for unweighted least squares factor analysis.

Factor Rotation

After the initial factor extraction, the factors are uncorrelated with each other. If the factors are rotated by an *orthogonal transformation*, the rotated factors are also uncorrelated. If the factors are rotated by an *oblique transformation*, the rotated factors become correlated. Oblique rotations often produce more useful patterns than orthogonal rotations do. However, a consequence of correlated factors is that there is no single unambiguous measure of the importance of a factor in explaining a variable. Thus, for oblique rotations, the pattern matrix does not provide all the necessary information for interpreting the factors; you must also examine the *factor structure* and the *reference structure*.

Nowadays, most rotations are done analytically. There are many choices for orthogonal and oblique rotations. An excellent summary of a wide class of analytic rotations is in Crawford and Ferguson (1970). The Crawford-Ferguson family of orthogonal rotations includes the orthomax rotation as a subclass and the popular varimax rotation as a special case. To illustrate these relationships, the following four specifications for orthogonal rotations with different **ROTATE=** options will give the same results for a data set with nine observed variables:

```

/* Orthogonal Crawford-Ferguson Family with
   variable parsimony weight = nvar - 1 = 8, and
   factor parsimony weight = 1 */
proc factor data=raw n=3 rotate=orthcf(8,1);
run;

/* Orthomax without the GAMMA= option */
proc factor data=raw n=3 rotate=orthomax(1);
run;

/* Orthomax with the GAMMA= option */
proc factor data=raw n=3 rotate=orthomax gamma=1;
run;

/* Varimax */
proc factor data=raw n=3 rotate=varimax;
run;

```

You can also get the oblique versions of the varimax in two equivalent ways:

```

/* Oblique Crawford-Ferguson Family with
   variable parsimony weight = nvar - 1 = 8, and
   factor parsimony weight = 1; */
proc factor data=raw n=3 rotate=oblicf(8,1);
run;

/* Oblique Varimax */
proc factor data=raw n=3 rotate=obvarimax;
run;

```

Jennrich (1973) proposes a generalized Crawford-Ferguson family that includes the Crawford-Ferguson family and the (direct) oblimin family (see Harman 1976) as subclasses. The better-known quartimin rotation is a special case of the oblimin class, and hence a special case of the generalized Crawford-Ferguson family. For example, the following four specifications of oblique rotations are equivalent:

```

/* Oblique generalized Crawford-Ferguson Family
   with weights 0, 1, 0, -1 */
proc factor data=raw n=3 rotate=obligencf(0,1,0,-1);
run;

/* Oblimin family without the TAU= option */
proc factor data=raw n=3 rotate=oblimin(0);
run;

/* Oblimin family with the TAU= option */
proc factor data=raw n=3 rotate=oblimin tau=0;
run;

/* Quartimin */
proc factor data=raw n=3 rotate=quartimin;
run;

```

In addition to the generalized Crawford-Ferguson family, the available oblique rotation methods in PROC FACTOR include Harris-Kaiser, promax, and Procrustes. See the section “Simplicity Functions for Rotations” on page 2244 for details about the definitions of various rotations. See Harman (1976) and Mulaik (1972) for further information.

Getting Started: FACTOR Procedure

The following example demonstrates how you can use the FACTOR procedure to perform common factor analysis and factor rotation.

In this example, 103 police officers were rated by their supervisors on 14 scales (variables). You conduct a common factor analysis on these variables to see what latent factors are operating behind these ratings. The overall rating variable is excluded from the factor analysis.

The following DATA step creates the SAS data set jobratings:

```
options validvarname=any;
data jobratings;
  input ('Communication Skills'n
        'Problem Solving'n
        'Learning Ability'n
        'Judgment Under Pressure'n
        'Observational Skills'n
        'Willingness to Confront Problems'n
        'Interest in People'n
        'Interpersonal Sensitivity'n
        'Desire for Self-Improvement'n
        'Appearance'n
        'Dependability'n
        'Physical Ability'n
        'Integrity'n
        'Overall Rating'n) (1.);
  datalines;
26838853879867
74758876857667
56757863775875
67869777988997
99997798878888
89897899888799
89999889899798
87794798468886

... more lines ...

99899899899899
76656399567486
;
```

The following statements invoke the FACTOR procedure:

```
proc factor data=jobratings(drop='Overall Rating'n) priors=smc
  rotate=varimax;
run;
```

The **DATA=** option in PROC FACTOR specifies the SAS data set jobratings as the input data set. The **DROP=** option drops the Overall Rating variable from the analysis. To conduct a common factor analysis, you need to set the prior communality estimate to less than one for each variable. Otherwise, the factor solution would simply be a recast of the principal components solution, in which “factors” are linear combinations of observed variables. However, in the common factor model you always assume that observed variables are functions of underlying factors. In this example, the **PRIORS=** option specifies that the squared multiple correlations (SMC) of each variable with all the other variables are used as the prior communality estimates. Note that squared multiple correlations are usually less than one. By default, the principal factor extraction is used if the **METHOD=** option is not specified. To facilitate interpretations, the **ROTATE=** option specifies the VARIMAX orthogonal factor rotation to be used.

The output from the factor analysis is displayed in Figure 35.1 through Figure 35.5.

As displayed in Figure 35.1, the prior communality estimates are set to the squared multiple correlations. Figure 35.1 also displays the table of eigenvalues (the variances of the principal factors) of the reduced correlation matrix. Each row of the table pertains to a single eigenvalue. Following the column of eigenvalues are three measures of each eigenvalue’s relative size and importance. The first of these displays the difference between the eigenvalue and its successor. The last two columns display the individual and cumulative proportions that the corresponding factor contributes to the total variation. The last line displayed in Figure 35.1 states that three factors are retained, as determined by the PROPORTION criterion.

Figure 35.1 Table of Eigenvalues from PROC FACTOR

The FACTOR Procedure				
Initial Factor Method: Principal Factors				
Prior Communality Estimates: SMC				
Communication Skills	Problem Solving	Learning Ability	Judgment Under Pressure	Observational Skills
0.62981394	0.58657431	0.61009871	0.63766021	0.67187583
Willingness to Confront Problems	Interest in People	Interpersonal Sensitivity	Desire for Self-Improvement	
0.64779805	0.75641519	0.75584891	0.57460176	
Appearance	Dependability	Physical Ability	Integrity	
0.45505304	0.63449045	0.42245324	0.68195454	

Figure 35.1 continued

Eigenvalues of the Reduced Correlation Matrix:				
Total = 8.06463816 Average = 0.62035678				
	Eigenvalue	Difference	Proportion	Cumulative
1	6.17760549	4.71531946	0.7660	0.7660
2	1.46228602	0.90183348	0.1813	0.9473
3	0.56045254	0.28093933	0.0695	1.0168
4	0.27951322	0.04766016	0.0347	1.0515
5	0.23185305	0.16113428	0.0287	1.0802
6	0.07071877	0.07489624	0.0088	1.0890
7	-0.00417747	0.03387533	-0.0005	1.0885
8	-0.03805279	0.04776534	-0.0047	1.0838
9	-0.08581814	0.02438060	-0.0106	1.0731
10	-0.11019874	0.01452741	-0.0137	1.0595
11	-0.12472615	0.02356465	-0.0155	1.0440
12	-0.14829080	0.05823605	-0.0184	1.0256
13	-0.20652684		-0.0256	1.0000

3 factors will be retained by the PROPORTION criterion.

Figure 35.2 displays the initial factor pattern matrix. The factor pattern matrix represents standardized regression coefficients for predicting the variables by using the extracted factors. Because the initial factors are uncorrelated, the pattern matrix is also equal to the correlations between variables and the common factors.

Figure 35.2 Factor Pattern Matrix from PROC FACTOR

Factor Pattern			
	Factor1	Factor2	Factor3
Communication Skills	0.75441	0.07707	-0.25551
Problem Solving	0.68590	0.08026	-0.34788
Learning Ability	0.65904	0.34808	-0.25249
Judgment Under Pressure	0.73391	-0.21405	-0.23513
Observational Skills	0.69039	0.45292	0.10298
Willingness to Confront Problems	0.66458	0.47460	0.09210
Interest in People	0.70770	-0.53427	0.10979
Interpersonal Sensitivity	0.64668	-0.61284	-0.07582
Desire for Self-Improvement	0.73820	0.12506	0.09062
Appearance	0.57188	0.20052	0.16367
Dependability	0.79475	-0.04516	0.16400
Physical Ability	0.51285	0.10251	0.34860
Integrity	0.74906	-0.35091	0.18656

The pattern matrix suggests that Factor1 represents general ability. All loadings for Factor1 in the Factor Pattern are at least 0.5. Factor2 consists of high positive loadings on certain task-related skills (Willingness to Confront Problems, Observational Skills, and Learning Ability) and high negative loadings on some interpersonal skills (Interpersonal Sensitivity, Interest in People, and Integrity). This factor measures individuals' relative strength in these skills. Theoretically, individuals with high positive scores on this factor would exhibit better task-related skills than interpersonal skills. Individuals with high negative scores would exhibit better interpersonal skills than task-related skills. Individuals with scores near zero would have those skills balanced. Factor3 does not have a cluster of very high or very low factor loadings. Therefore, interpreting this factor is difficult.

Figure 35.3 displays the proportion of variance explained by each factor and the final communality estimates, including the total communality. The final communality estimates are the proportion of variance of the variables accounted for by the common factors. When the factors are orthogonal, the final communalities are calculated by taking the sum of squares of each row of the factor pattern matrix.

Figure 35.3 Variance Explained and Final Communality Estimates

Variance Explained by Each Factor				
	Factor1	Factor2	Factor3	
	6.1776055	1.4622860	0.5604525	
Final Communality Estimates: Total = 8.200344				
Communication Skills	Problem Solving	Learning Ability	Judgment Under Pressure	Observational Skills
0.64036292	0.59791844	0.61924167	0.63972863	0.69237485
Willingness to Confront Problems	Interest in People	Interpersonal Sensitivity	Desire for Self-Improvement	
0.67538695	0.79833968	0.79951357	0.56879171	
Appearance	Dependability	Physical Ability	Integrity	
0.39403630	0.66056907	0.39504805	0.71903222	

Figure 35.4 displays the results of the VARIMAX rotation of the three extracted factors and the corresponding orthogonal transformation matrix. The rotated factor pattern matrix is calculated by postmultiplying the original factor pattern matrix (Figure 35.4) by the transformation matrix.

Figure 35.4 Transformation Matrix and Rotated Factor Pattern

Orthogonal Transformation Matrix			
	1	2	3
1	0.59125	0.59249	0.54715
2	-0.80080	0.51170	0.31125
3	0.09557	0.62219	-0.77701

Rotated Factor Pattern			
	Factor1	Factor2	Factor3
Communication Skills	0.35991	0.32744	0.63530
Problem Solving	0.30802	0.23102	0.67058
Learning Ability	0.08679	0.41149	0.66512
Judgment Under Pressure	0.58287	0.17901	0.51764
Observational Skills	0.05533	0.70488	0.43870
Willingness to Confront Problems	0.02168	0.69391	0.43978
Interest in People	0.85677	0.21422	0.13562
Interpersonal Sensitivity	0.86587	0.02239	0.22200
Desire for Self-Improvement	0.34498	0.55775	0.37242
Appearance	0.19319	0.54327	0.24814
Dependability	0.52174	0.54981	0.29337
Physical Ability	0.25445	0.57321	0.04165
Integrity	0.74172	0.38033	0.15567

The rotated factor pattern matrix is somewhat simpler to interpret. If a magnitude of at least 0.5 is required to indicate a salient variable-factor relationship, Factor1 now represents interpersonal skills (Interpersonal Sensitivity, Interest in People, Integrity, Judgment Under Pressure, and Dependability). Factor2 measures physical skills and job enthusiasm (Observational Skills, Willingness to Confront Problems, Physical Ability, Desire for Self-Improvement, Dependability, and Appearance). Factor3 measures cognitive skills (Communication Skills, Problem Solving, Learning Ability, and Judgment Under Pressure).

However, using 0.5 for determining a salient variable-factor relationship does not take sampling variability into account. If the underlying assumptions for the maximum likelihood estimation are approximately satisfied, you can output standard error estimates and the confidence intervals with `METHOD=ML`. You can then determine the salience of the variable-factor relationship by using the coverage displays. See the section “[Confidence Intervals and the Salience of Factor Loadings](#)” on page 2243 for more details.

Figure 35.5 displays the variance explained by each factor and the final communality estimates after the orthogonal rotation. Even though the variances explained by the rotated factors are different from that of the unrotated factor (compare with Figure 35.3), the cumulative variance explained by the common factors remains the same. Note also that the final communalities for variables, as well as the total communality, remain unchanged after rotation. Although rotating a factor solution will not increase or decrease the statistical quality of the factor model, it can simplify the interpretations of the factors and redistribute the variance explained by the factors.

Figure 35.5 Variance Explained and Final Communality Estimates after Rotation

Variance Explained by Each Factor				
	Factor1	Factor2	Factor3	
	3.1024330	2.7684489	2.3294622	
Final Communality Estimates: Total = 8.200344				
Communication Skills	Problem Solving	Learning Ability	Judgment Under Pressure	Observational Skills
0.64036292	0.59791844	0.61924167	0.63972863	0.69237485
Willingness to Confront Problems	Interest in People	Interpersonal Sensitivity	Desire for Self-Improvement	
0.67538695	0.79833968	0.79951357	0.56879171	
Appearance	Dependability	Physical Ability	Integrity	
0.39403630	0.66056907	0.39504805	0.71903222	

Syntax: FACTOR Procedure

The following statements are available in the FACTOR procedure:

```

PROC FACTOR < options > ;
  VAR variables ;
  PRIORS communalities ;
  PARTIAL variables ;
  FREQ variable ;
  WEIGHT variable ;
  BY variables ;

```

Usually only the VAR statement is needed in addition to the PROC FACTOR statement. The descriptions of the BY, FREQ, PARTIAL, PRIORS, VAR, and WEIGHT statements follow the description of the PROC FACTOR statement in alphabetical order.

PROC FACTOR Statement

```

PROC FACTOR < options > ;

```

The PROC FACTOR statement invokes the FACTOR procedure. The options listed in [Table 35.1](#) are available in the PROC FACTOR statement.

Table 35.1 Options Available in the PROC FACTOR Statement

Option	Description
Data Set Options	
DATA=	Specifies input SAS data set
OUT=	Specifies output SAS data set
OUTSTAT=	Specifies output data set containing statistical results
TARGET=	Specifies input data set containing the target pattern for rotation
Factor Extraction and Communalities	
HEYWOOD	Sets to 1 any communality greater than 1
METHOD=	Specifies the estimation method
PRIORS=	Specifies the method for computing prior communality estimates
RANDOM=	Specifies the seed for pseudo-random number generation
ULTRAHEYWOOD	Allows communalities to exceed 1
Number of Factors	
MINEIGEN=	Specifies the smallest eigenvalue for retaining a factor
NFACTORS=	Specifies the number of factors to retain
PROPORTION=	Specifies the proportion of common variance in extracted factors
Data Analysis Options	
ALPHA=	Specifies the confidence level for interval construction
COVARIANCE	Requests factoring of the covariance matrix
COVER=	Computes the confidence interval and specifies the coverage reference point
NOINT	Omits the intercept from computing covariances or correlations
SE	Requests the standard error estimates in ML estimation
VARDEF=	Specifies the divisor used in calculating covariances or correlations
WEIGHT	Factors a weighted correlation or covariance matrix
Rotation Method and Properties	
GAMMA=	Specifies the orthomax weight
HKPOWER=	Specifies the power in Harris-Kaiser rotation
NORM=	Specifies the method for row normalization in rotation
NOPROMAXNORM	Turns off row normalization in promax rotation
POWER=	Specifies the power to be used in promax rotation
PREROTATE=	Specifies the prerotation method in promax rotation
RCONVERGE=	Specifies the convergence criterion for rotation cycles
RITER=	Specifies the maximum number of cycles for rotation
ROTATE=	Specifies the rotation method
TAU=	Specifies the oblimin weight

Table 35.1 *continued*

Option	Description
ODS Graphics	
PLOTS=	Specifies ODS Graphics selection
Control Display Output	
ALL	Displays all optional output except plots
CORR	Displays the (partial) correlation matrix
EIGENVECTORS	Displays the eigenvectors of the reduced correlation matrix
FLAG=	Specifies the minimum absolute value to be flagged in the correlation and loading matrices
FUZZ=	Specifies the maximum absolute value to be displayed as missing in the correlation and loading matrices
MSA	Computes Kaiser's measure of sampling adequacy and the related partial correlations
NOPRINT	Suppresses the display of all output
NPLOT=	Specifies the number of factors to be plotted
PLOT	Plots the rotated factor pattern
PLOTREF	Plots the reference structure
PREPLOT	Plots the factor pattern before rotation
PRINT	Displays the input factor pattern or scoring coefficients and related statistics
REORDER	Reorders the rows (variables) of various factor matrices
RESIDUALS	Displays the residual correlation matrix and the associated partial correlation matrix
ROUND	Prints correlation and loading matrices with rounded values
SCORE	Displays the factor scoring coefficients
SCREE	Displays the scree plot of the eigenvalues
SIMPLE	Displays means, standard deviations, and number of observations
Numerical Properties	
CONVERGE=	Specifies the convergence criterion
MAXITER=	Specifies the maximum number of iterations
SINGULAR=	Specifies the singularity criterion
Miscellaneous	
NOCORR	Excludes the correlation matrix from the OUTSTAT= data set
NOBS=	Specifies the number of observations
PARPREFIX=	Specifies the prefix for the residual variables in the output data sets
PREFIX=	Specifies the prefix for naming factors

ALL

displays all optional output except plots. When the input data set is TYPE=CORR, TYPE=UCORR, TYPE=COV, TYPE=UCOV, or TYPE=FACTOR, simple statistics, correlations, and MSA are not displayed.

ALPHA= p

specifies the level of confidence $1 - p$ for interval construction. By default, $p = 0.05$, corresponding to $1 - p = 95\%$ confidence intervals. If p is greater than one, it is interpreted as a percentage and divided by 100. With multiple confidence intervals to be constructed, the ALPHA= value is applied to each interval construction one at a time. This will not control the coverage probability of the intervals simultaneously. To control familywise coverage probability, you might consider supplying a nonconventional p by using methods such as Bonferroni adjustment.

CONVERGE= p **CONV= p**

specifies the convergence criterion for the METHOD=PRINIT, METHOD=ULS, METHOD=ALPHA, or METHOD=ML option. Iteration stops when the maximum change in the communalities is less than the value of the CONVERGE= option. The default value is 0.001. Negative values are not allowed.

CORR**C**

displays the correlation matrix or partial correlation matrix.

COVARIANCE**COV**

requests factoring of the covariance matrix instead of the correlation matrix. The COV option is effective only with the METHOD=PRINCIPAL, METHOD=PRINIT, METHOD=ULS, or METHOD=IMAGE option. For other methods, PROC FACTOR produces the same results with or without the COV option.

COVER <= p >**CI <= p >**

computes the confidence intervals and optionally specifies the value of factor loading for coverage detection. By default, $p = 0$. The specified value is represented by an asterisk (*) in the coverage display. This is useful for determining the salience of loadings. For example, if COVER=0.4, a display '0*[]' indicates that the entire confidence interval is above 0.4, implying strong evidence for the salience of the loading. See the section “[Confidence Intervals and the Salience of Factor Loadings](#)” on page 2243 for more details.

DATA=SAS-data-set

specifies the input data set, which can be an ordinary SAS data set or a specially structured SAS data set as described in the section “[Input Data Set](#)” on page 2239. If the DATA= option is omitted, the most recently created SAS data set is used.

EIGENVECTORS**EV**

displays the eigenvectors of the reduced correlation matrix, of which the diagonal elements are replaced with the communality estimates. When **METHOD=ML**, the eigenvectors are for the weighted reduced correlation matrix. PROC FACTOR chooses the solution that makes the sum of the elements of each eigenvector nonnegative. If the sum of the elements is equal to zero, then the sign depends on how the number is rounded off.

FLAG= p

flags absolute values larger than p with an asterisk in the correlation and loading matrices. Negative values are not allowed for p . Values printed in the matrices are multiplied by 100 and rounded to the nearest integer (see the **ROUND** option). The **FLAG=** option has no effect when standard errors or confidence intervals are also printed.

FUZZ= p

prints correlations and factor loadings with absolute values less than p printed as missing. For partial correlations, the **FUZZ=** value is divided by 2. For residual correlations, the **FUZZ=** value is divided by 4. The exact values in any matrix can be obtained from the **OUTSTAT=** and ODS output data sets. Negative values are not allowed. The **FUZZ=** option has no effect when standard errors or confidence intervals are also printed.

GAMMA= p

specifies the orthomax weight used with the option **ROTATE=ORTHOMAX** or **PRE-ROTATE=ORTHOMAX**. Alternatively, you can use **ROTATE=ORTHOMAX(p)** with p representing the orthomax weight. There is no restriction on valid values for the orthomax weight, although the most common values are between zero and the number of variables. The default **GAMMA=** value is one, resulting in the varimax rotation. See the section “**Simplicity Functions for Rotations**” on page 2244 for more details.

HEYWOOD**HEY**

sets to 1 any communality greater than 1, allowing iterations to proceed. See the section “**Heywood Cases and Other Anomalies about Communality Estimates**” on page 2248 for a discussion of Heywood cases.

HKPOWER= p **HKP= p**

specifies the power of the square roots of the eigenvalues used to rescale the eigenvectors for Harris-Kaiser (**ROTATE=HK**) rotation, assuming that the factors are extracted by the principal factor method. If the principal factor method is not used for factor extraction, the eigenvectors are replaced by the normalized columns of the unrotated factor matrix, and the eigenvalues are replaced by the column normalizing constants. **HKPOWER=** values between 0.0 and 1.0 are reasonable. The default value is 0.0, yielding the independent cluster solution, in which each variable tends to have a large loading on only one factor. An **HKPOWER=** value of 1.0 is equivalent to an orthogonal rotation, with the varimax rotation as the default. You can also specify the **HKPOWER=** option with **ROTATE=QUARTIMAX**, **ROTATE=BIQUARTIMAX**, **ROTATE=EQUAMAX**, or **ROTATE=ORTHOMAX**, and so on. The only restriction is that the Harris-Kaiser rotation must be associated with an orthogonal rotation.

MAXITER=*n*

specifies the maximum number of iterations for factor extraction. You can use the MAXITER= option with the PRINIT, ULS, ALPHA, or ML method. The default is 30.

METHOD=*name***M=*name***

specifies the method for extracting factors. The default is METHOD=PRINCIPAL unless the DATA= data set is TYPE=FACTOR, in which case the default is METHOD=PATTERN. Valid values for *name* are as follows:

ALPHA A	produces alpha factor analysis.
HARRIS H	yields Harris component analysis of $S^{-1}RS^{-1}$ (Harris 1962), a noniterative approximation to canonical component analysis.
IMAGE I	yields principal component analysis of the image covariance matrix, not the image analysis of Kaiser (1963, 1970) or Kaiser and Rice (1974). A nonsingular correlation matrix is required.
ML M	performs maximum likelihood factor analysis with an algorithm due, except for minor details, to Fuller (1987). The option METHOD=ML requires a nonsingular correlation matrix.
PATTERN	reads a factor pattern from a TYPE=FACTOR, TYPE=CORR, TYPE=UCORR, TYPE=COV, or TYPE=UCOV data set. If you create a TYPE=FACTOR data set in a DATA step, only observations containing the factor pattern (<code>_TYPE_='PATTERN'</code>) and, if the factors are correlated, the interfactor correlations (<code>_TYPE_='FCORR'</code>) are required.
PRINCIPAL PRIN P	yields principal component analysis if no PRIORS option or statement is used or if you specify PRIORS=ONE; if you specify a PRIORS statement or a PRIORS= value other than PRIORS=ONE, a principal factor analysis is performed.
PRINIT	yields iterated principal factor analysis.
SCORE	reads scoring coefficients (<code>_TYPE_='SCORE'</code>) from a TYPE=FACTOR, TYPE=CORR, TYPE=UCORR, TYPE=COV, or TYPE=UCOV data set. The data set must also contain either a correlation or a covariance matrix. Scoring coefficients are also displayed if you specify the OUT= option.
ULS U	produces unweighted least squares factor analysis.

MINEIGEN=*p***MIN=*p***

specifies the smallest eigenvalue for which a factor is retained. If you specify two or more of the MINEIGEN=, NFACTORS=, and PROPORTION= options, the number of factors retained is the minimum number satisfying any of the criteria. The MINEIGEN= option cannot be used with either the METHOD=PATTERN or the METHOD=SCORE option. Negative values are not allowed. The default is 0 unless you omit both the NFACTORS= and the PROPORTION= options and one of the following conditions holds:

- If you specify the METHOD=ALPHA or METHOD=HARRIS option, then MINEIGEN=1.

- If you specify the **METHOD=IMAGE** option, then

$$\text{MINEIGEN} = \frac{\text{total image variance}}{\text{number of variables}}$$

- For any other **METHOD=** specification, if prior communality estimates of 1.0 are used, then

$$\text{MINEIGEN} = \frac{\text{total weighted variance}}{\text{number of variables}}$$

When an unweighted correlation matrix is factored, this value is 1.

MSA

produces the partial correlations between each pair of variables controlling for all other variables (the negative anti-image correlations) and Kaiser's measure of sampling adequacy (Kaiser 1970; Kaiser and Rice 1974; Cerny and Kaiser 1977).

NFACTORS=*n*

NFACT=*n*

N=*n*

specifies the maximum number of factors to be extracted and determines the amount of memory to be allocated for factor matrices. The default is the number of variables. Specifying a number that is small relative to the number of variables can substantially decrease the amount of memory required to run PROC FACTOR, especially with oblique rotations. If you specify two or more of the **NFACTORS=**, **MINEIGEN=**, and **PROPORTION=** options, the number of factors retained is the minimum number satisfying any of the criteria. If you specify the option **NFACTORS=0**, eigenvalues are computed, but no factors are extracted. If you specify the option **NFACTORS=-1**, neither eigenvalues nor factors are computed. You can use the **NFACTORS=** option with the **METHOD=PATTERN** or **METHOD=SCORE** option to specify a smaller number of factors than are present in the data set.

NOBS=*n*

specifies the number of observations. If the **DATA=** input data set is a raw data set, *nobs* is defined by default to be the number of observations in the raw data set. The **NOBS=** option overrides this default definition. If the **DATA=** input data set contains a covariance, correlation, or scalar product matrix, the number of observations can be specified either by using the **NOBS=** option in the PROC FACTOR statement or by including a **_TYPE_='N'** observation in the **DATA=** input data set.

NOCORR

prevents the correlation matrix from being transferred to the **OUTSTAT=** data set when you specify the **METHOD=PATTERN** option. The **NOCORR** option greatly reduces memory requirements when there are many variables but few factors. The **NOCORR** option is not effective if the correlation matrix is required for other requested output; for example, if the scores or the residual correlations are displayed (for example, by using the **SCORE**, **RESIDUALS**, or **ALL** option).

NOINT

omits the intercept from the analysis; covariances or correlations are not corrected for the mean.

NOPRINT

suppresses the display of all output. Note that this option temporarily disables the Output Delivery System (ODS). For more information, see Chapter 20, "Using the Output Delivery System."

NOPROMAXNORM | NOPMAXNORM

turns off the default row normalization of the prerotated factor pattern, which is used in computing the promax target matrix.

NORM=COV | KAISER | NONE | RAW | WEIGHT

specifies the method for normalizing the rows of the factor pattern for rotation. If you specify the option **NORM=KAISER**, Kaiser's normalization is used ($\sum_j p_{ij}^2 = 1$). If you specify the option **NORM=WEIGHT**, the rows are weighted by the Cureton-Mulaik technique (Cureton and Mulaik 1975). If you specify the option **NORM=COV**, the rows of the pattern matrix are rescaled to represent covariances instead of correlations. If you specify the option **NORM=NONE** or **NORM=RAW**, normalization is not performed. The default is **NORM=KAISER**.

NPLOTS | NPLOT=*n*

specifies the number of factors to be plotted. The default is to plot all factors. The smallest allowable value is 2. If you specify the option **NPLOTS=*n***, all pairs of the first *n* factors are plotted, producing a total of $n(n - 1)/2$ plots.

OUT=SAS-data-set

creates a data set containing all the data from the **DATA=** data set plus variables called Factor1, Factor2, and so on, containing estimated factor scores. The **DATA=** data set must contain multivariate data, not correlations or covariances. You must also specify the **NFACTORS=** option to determine the number of factor score variables. If you specify partial variables in the **PARTIAL** statement, the **OUT=** data set will also contain the residual variables that are used for factor analysis. The output data set is described in detail in the section “**Output Data Sets**” on page 2241. If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*.

OUTSTAT=SAS-data-set

specifies an output data set containing most of the results of the analysis. The output data set is described in detail in the section “**Output Data Sets**” on page 2241. If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*.

PARPREFIX=name

specifies the prefix for the residual variables in the **OUT=** and the **OUTSTAT=** data sets when partial variables are specified in the **PARTIAL** statement.

PLOT

plots the factor pattern after rotation. This option produces printer plots. High-quality ODS graphical plots for factor patterns can be requested with the **PLOTS=LOADINGS** or **PLOTS=INITLOADINGS** option.

PLOTREF

plots the reference structure instead of the default factor pattern after oblique rotation.

PLOTS <(global-plot-options)> = plot-request <(options)>

PLOTS <(global-plot-options)> = (plot-request <(options)> <...plot-request <(options)> >)

specifies one or more ODS graphical plots in PROC FACTOR. When you specify only one *plot-request*, you can omit the parentheses around the *plot-request*. Here are some examples:


```
plots=all
plots(flip)=loadings
plots=(loadings(flip) scree(unpack))
```

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;
proc factor plots=all;
run;
ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS](#).”

For an example containing graphical displays of factor analysis results, see [Example 35.2](#).

The following table shows the available *plot-requests* and their available suboptions:

<i>Plot-Request</i>	Plot Description	Suboptions
ALL	all available plots	all
INITLOADINGS	unrotated factor loadings	CIRCLE=, FLIP, NPLOTS=, PLOTREF, and VECTOR
LOADINGS	rotated factor loadings	CIRCLE=, FLIP, NPLOTS=, PLOTREF, and VECTOR
NONE	no ODS graphical plots	
PRELOADINGS	prerotated factor loadings	CIRCLE=, FLIP, NPLOTS=, PLOTREF, and VECTOR
SCREE	scree and variance explained	UNPACK

The following are the available *global-plot-options* or *options* for plots:

CIRCLE | CIRCLES *< = numbers >* draws circular reference lines in scatter plots or vector plots of factor loadings. You can specify the locations of the circular reference lines in the *numbers* list. Each number indicates the proportion or percentage of area of the unit circle that is enclosed by the specified circle. Each of the *numbers* must lie between 0 and 100, inclusively. When a number is between 0 and 1 (inclusively), it is interpreted as a proportion; otherwise, it is interpreted as a percentage. The maximum number of circles is 5.

The CIRCLE option applies to the scatter or vector plots requested by the INITLOADINGS, LOADINGS, and PRELOADINGS options. By default, a unit-circle, which represents 100% of the total area, is drawn for the vector plots. However, no circle will be drawn for scatter plots unless the CIRCLE option is specified. Two special cases for this option are: (1) With no *numbers* following the CIRCLE option, a 100% circle will be drawn. (2) With CIRCLE=0, no circle will be drawn. This special case is primarily used to turn off the default unit-circle in vector plots.

FLIP switches the X and Y axes. It applies to the INITLOADINGS, LOADINGS, and PRELOADINGS *plot-requests*.

NPLOT | NPLOTS=*n* specifies the number of factors *n* ($n \geq 2$) to be plotted. It applies to the INITLOADINGS, LOADINGS, and PRELOADINGS *plot-requests*. Since this option can also be specified in the PROC FACTOR statement, the final value of *n* is determined by the following steps. The NPLOTS= value of the PROC FACTOR is read first. If the NPLOTS= option is specified as a *global-plot-option*, the value of *n* will be updated. Then, if the NPLOTS= option is again specified in an individual *plot-request*, the value will be updated again for that individual *plot-request*. For example, in the following statement, four factors are extracted with the N=4 option:

```
proc factor n=4 nplots=3 plots(nplots=4)=
      (loadings preloadings(nplots=2));
```

Initially, plots of the first three factors are specified with the NPLOTS=3 option. When you are producing ODS graphical plots, the *global-plot-option* NPLOTS=4 is used. As a result, the LOADINGS *plot-request* will produce plots for all pairs of the first 4 factors. However, because the NPLOTS=2 is specified locally for the PRELOADINGS *plot-request*, it will produce a prerotated factor loading plot for the first two factors only.

The default NPLOTS= value is 5 or the total number of factors (*m*), whichever is smaller. If you specify an NPLOTS= value that is greater than *m*, NPLOTS=*m* will be used.

- PLOTREF** plots the reference structures rather than the factor pattern loadings. It applies to the INITLOADINGS, LOADINGS, and PRELOADINGS *plot-requests* when the factor solution is oblique. This option can also be set globally as an option in the PROC FACTOR statement.
- UNPACK** plots component graphs separately. It applies to the SCREE *plot-request* only.
- VECTOR** plots loadings in vector form. It applies to the INITLOADINGS, LOADINGS, and PRELOADINGS *plot-requests* when the factor solution is orthogonal. For oblique solutions, the VECTOR option is ignored and the default scatter plots for factor loadings or reference structures are displayed.

Be aware that the **PLOT** option in the PROC FACTOR statement requests only the printer plots of factor loadings. The current option PLOTS= or PLOT=, however, is for ODS graphical plots.

You can specify options for the requested ODS graphical plots as *global-plot-options* or as local *options*. *Global-plot-options* apply to all appropriate individual *plot-requests* specified. For example, because the SCREE plot is not subject to axes flipping, the following two specifications are equivalent:

```
plots(flip)=(loadings preloadings scree)
plots=(loadings(flip) preloadings(flip) scree)
```

Options specified locally after each *plot-request* apply to that plot-request only. For example, consider the following specification:

plots=(scree (unpack) loadings (plotref) preloadings (flip))

The FLIP option applies to the PRELOADINGS *plot-request* but not the LOADINGS *plot-request*; the PLOTREF option applies to the LOADINGS *plot-request* but not the PRELOADINGS *plot-request*; and the UNPACK option applies to the SCREE *plot-request* only.

POWER=*n*

specifies the power to be used in computing the target pattern for the option ROTATE=PROMAX. Valid values must be integers ≥ 1 . The default value is 3. You can also specify the POWER= value in the ROTATE= option—for example, ROTATE=PROMAX(4).

PREFIX=*name*

specifies a prefix for naming the factors. By default, the names are Factor1, Factor2, . . . , Factor*n*. If you specify PREFIX=ABC, the factors are named ABC1, ABC2, ABC3, and so on. The number of characters in the prefix plus the number of digits required to designate the variables should not exceed the current name length defined by the VALIDVARNAME= system option.

PREPLOT

plots the factor pattern before rotation. This option produces printer plots. High-quality ODS graphical plots for factor patterns can be requested with the PLOTS=PRELOADINGS option.

PREROTATE=*name*

PRE=*name*

specifies the prerotation method for the option ROTATE=PROMAX. Any rotation method other than PROMAX or PROCUSTES can be used. The default is PREROTATE=VARIMAX. If a previously rotated pattern is read using the option METHOD=PATTERN, you should specify the PREROTATE=NONE option.

PRINT

displays the input factor pattern or scoring coefficients and related statistics. In oblique cases, the reference and factor structures are computed and displayed. The PRINT option is effective only with the option METHOD=PATTERN or METHOD=SCORE.

PRIORS=*name*

specifies a method for computing prior communality estimates. You can specify numeric values for the prior communality estimates by using the PRIORS statement. Valid values for *name* are as follows:

ASMC A	sets the prior communality estimates proportional to the squared multiple correlations but adjusted so that their sum is equal to that of the maximum absolute correlations (Cureton 1968).
INPUT I	reads the prior communality estimates from the first observation with either <code>_TYPE_='PRIORS'</code> or <code>_TYPE_='COMMUNAL'</code> in the DATA= data set (which cannot be TYPE=DATA).
MAX M	sets the prior communality estimate for each variable to its maximum absolute correlation with any other variable.
ONE O	sets all prior communalities to 1.0.

RANDOM R	sets the prior communality estimates to pseudo-random numbers uniformly distributed between 0 and 1.
SMC S	sets the prior communality estimate for each variable to its squared multiple correlation with all other variables.

The default prior communality estimates are as follows:

METHOD=	PRIORS=
PRINCIPAL	ONE
PRINIT	ONE
ALPHA	SMC
ULS	SMC
ML	SMC
HARRIS	(not applicable)
IMAGE	(not applicable)
PATTERN	(not applicable)
SCORE	(not applicable)

By default, the options `METHOD=PRINIT`, `METHOD=ULS`, `METHOD=ALPHA`, and `METHOD=ML` stop iterating and set the number of factors to 0 if an estimated communality exceeds 1. The options `HEYWOOD` and `ULTRAHEYWOOD` allow processing to continue.

PROPORTION=*p*

PERCENT=*p*

P=*p*

specifies the proportion of common variance to be accounted for by the retained factors. The proportion of common variance is computed using the total prior communality estimates as the basis. If the value is greater than one, it is interpreted as a percentage and divided by 100. The options `PROPORTION=0.75` and `PERCENT=75` are equivalent. The default value is 1.0 or 100%. You cannot specify the `PROPORTION=` option with the `METHOD=PATTERN` or `METHOD=SCORE` option. If you specify two or more of the `PROPORTION=`, `NFACTORS=`, and `MINEIGEN=` options, the number of factors retained is the minimum number satisfying any of the criteria.

RANDOM=*n*

specifies a positive integer as a starting value for the pseudo-random number generator for use with the option `PRIORS=RANDOM`. If you do not specify the `RANDOM=` option, the time of day is used to initialize the pseudo-random number sequence. Valid values must be integers ≥ 1 .

RCONVERGE=*p*

RCONV=*p*

specifies the convergence criterion for rotation cycles. Rotation stops when the scaled change of the simplicity function value is less than the `RCONVERGE=` value. The default convergence criterion is

$$|f_{new} - f_{old}|/K < \epsilon$$

where f_{new} and f_{old} are simplicity function values of the current cycle and the previous cycle, respectively, $K = \max(1, |f_{old}|)$ is a scaling factor, and ϵ is 1E-9 by default and is modified by the RCONVERGE= value.

REORDER

RE

causes the rows (variables) of various factor matrices to be reordered on the output. Variables with their highest absolute loading (reference structure loading for oblique rotations) on the first factor are displayed first, from largest to smallest loading, followed by variables with their highest absolute loading on the second factor, and so on. The order of the variables in the output data set is not affected. The factors are not reordered.

RESIDUALS

RES

displays the residual correlation matrix and the associated partial correlation matrix. The diagonal elements of the residual correlation matrix are the unique variances.

RITER= n

specifies the maximum number of cycles n for factor rotation. Except for promax and Procrustes, you can use the RITER= option with all rotation methods. The default n is the maximum between 10 times the number of variables and 100.

ROTATE= $name$

R= $name$

specifies the rotation method. The default is ROTATE=NONE.

Valid *names* for orthogonal rotations are as follows:

BIQUARTIMAX | BIQMAX specifies orthogonal biquartimax rotation. This corresponds to the specification ROTATE=ORTHOMAX(.5).

EQUAMAX | E specifies orthogonal equamax rotation. This corresponds to the specification ROTATE=ORTHOMAX with GAMMA=*number of factors*/2.

FACTORPARSIMAX | FPA specifies orthogonal factor parsimax rotation. This corresponds to the specification ROTATE=ORTHOMAX with GAMMA=*number of variables*.

NONE | N specifies that no rotation be performed, leaving the original orthogonal solution.

ORTHCF($p1,p2$) | ORCF($p1,p2$) specifies the orthogonal Crawford-Ferguson rotation with the weights $p1$ and $p2$ for variable parsimony and factor parsimony, respectively. See the definitions of weights in the section “Simplicity Functions for Rotations” on page 2244.

ORTHGENCF($p1,p2,p3,p4$) | ORGENCF($p1,p2,p3,p4$) specifies the orthogonal generalized Crawford-Ferguson rotation with the four weights $p1$, $p2$, $p3$, and $p4$. See the definitions of weights in the section “Simplicity Functions for Rotations” on page 2244.

ORTHOMAX< p > | ORMAX< p > specifies the orthomax rotation with orthomax weight p . If ROTATE=ORTHOMAX is used, the default p value is 1 unless specified otherwise in the GAMMA= option. Alternatively, ROTATE=ORTHOMAX(p) specifies p as the orthomax weight or the GAMMA= value. See the definition of the orthomax weight in the section “Simplicity Functions for Rotations” on page 2244.

PARSIMAX | PA specifies orthogonal parsimax rotation. This corresponds to the specification ROTATE=ORTHOMAX with

$$\text{GAMMA} = \frac{nvar \times (nfact - 1)}{nvar + nfact - 2}$$

where *nvar* is the number of variables and *nfact* is the number of factors.

QUARTIMAX | QMAX | Q specifies orthogonal quartimax rotation. This corresponds to the specification ROTATE=ORTHOMAX(0).

VARIMAX | V specifies orthogonal varimax rotation. This corresponds to the specification ROTATE=ORTHOMAX with GAMMA=1.

Valid *names* for oblique rotations are as follows:

BIQUARTIMIN | BIQMIN specifies biquartimin rotation. It corresponds to the specification ROTATE=OBLIMIN(.5) or ROTATE=OBLIMIN with TAU=0.5.

COVARIMIN | CVMIN specifies covarimin rotation. It corresponds to the specification ROTATE=OBLIMIN(1) or ROTATE=OBLIMIN with TAU=1.

HK<(p)> | H<(p)> specifies Harris-Kaiser case II orthoblique rotation. When specifying this option, you can use the HKPOWER= option to set the power of the square roots of the eigenvalues by which the eigenvectors are scaled, assuming that the factors are extracted by the principal factor method. For other extraction methods, the unrotated factor pattern is column normalized. The power is then applied to the column normalizing constants, instead of the eigenvalues. You can also use ROTATE=HK(p), with *p* representing the HKPOWER= value. The default associated orthogonal rotation with ROTATE=HK is the varimax rotation without Kaiser normalization. You might associate the Harris-Kaiser with other orthogonal rotations by using the ROTATE= option together with the HKPOWER= option.

OBBIQUARTIMAX | OBIQMAX specifies oblique biquartimax rotation.

OBEQUAMAX | OE specifies oblique equamax rotation.

OBFACORPARSIMAX | OFPA specifies oblique factor parsimax rotation.

OBLICF(*p1,p2*) | OBCF(*p1,p2*) specifies the oblique Crawford-Ferguson rotation with the weights *p1* and *p2* for variable parsimony and factor parsimony, respectively. See the definitions of weights in the section “Simplicity Functions for Rotations” on page 2244.

OBLIGENCF(*p1,p2,p3,p4*) | OBGENCF(*p1,p2,p3,p4*) specifies the oblique generalized Crawford-Ferguson rotation with the four weights *p1*, *p2*, *p3*, and *p4*. See the definitions of weights in the section “Simplicity Functions for Rotations” on page 2244.

OBLIMIN<(p)> | OBLMIN<(p)> specifies the oblimin rotation with oblimin weight *p*. If ROTATE=OBLIMIN is used, the default *p* value is zero unless specified otherwise in the TAU= option. Alternatively, ROTATE=OBLIMIN(*p*) specifies *p* as the oblimin weight or the TAU= value. See the definition of the oblimin weight in the section “Simplicity Functions for Rotations” on page 2244.

OBPARSIMAX | OPA specifies oblique parsimax rotation.

OBQUARTIMAX | OQMAX specifies oblique quartimax rotation. This is the same as the **QUARTIMIN** method.

OBVARIMAX | OV specifies oblique varimax rotation.

PROCRUSTES specifies oblique Procrustes rotation with the target pattern provided by the **TARGET=** data set. The unrestricted least squares method is used with factors scaled to unit variance after rotation.

PROMAX<(p)> | P<(p)> specifies oblique promax rotation. You can use the **PREROTATE=** option to set the desirable prerotation method, orthogonal or oblique. When used with **ROTATE=PROMAX**, the **POWER=** option lets you specify the power for forming the target. You can also use **ROTATE=PROMAX(p)**, where p represents the **POWER=** value.

QUARTIMIN | QMIN specifies quartimin rotation. It is the same as the oblique quartimax method. It also corresponds to the specification **ROTATE=OBLIMIN(0)** or **ROTATE=OBLIMIN** with **TAU=0**.

ROUND

prints correlation and loading matrices with entries multiplied by 100 and rounded to the nearest integer. The exact values can be obtained from the **OUTSTAT=** and ODS output data sets. The **ROUND** option also flags absolute values larger than the **FLAG=** value with an asterisk in correlation and loading matrices (see the **FLAG=** option). If the **FLAG=** option is not specified, the root mean square of all the values in the matrix printed is used as the default **FLAG=** value. The **ROUND** option has no effect when standard errors or confidence intervals are also printed.

SCORE

displays the factor scoring coefficients. The squared multiple correlation of each factor with the variables is also displayed except in the case of unrotated principal components. The **SCORE** option also outputs the factor scoring coefficients in the **_TYPE_=SCORE** or **_TYPE_=USCORE** observations in the **OUTSTAT=** data set. Unless you specify the **NOINT** option in **PROC FACTOR**, the scoring coefficients should be applied to standardized variables—variables that are centered by subtracting the original variable means and then divided by the original variable standard deviations. With the **NOINT** option, the scoring coefficients should be applied to data without centering.

SCREE

displays a scree plot of the eigenvalues (Cattell 1966, 1978; Cattell and Vogelman 1977; Horn and Engstrom 1979). This option produces printer plots. High-quality scree plots can be requested with the **PLOTS=SCREE** option.

SE

STDERR

computes standard errors for various classes of unrotated and rotated solutions under the maximum likelihood estimation.

SIMPLE

S

displays means, standard deviations, and the number of observations.

SINGULAR= p **SING= p**

specifies the singularity criterion, where $0 < p < 1$. The default value is 1E-8.

TARGET=*SAS-data-set*

specifies an input data set containing the target pattern for Procrustes rotation (see the description of the **ROTATE=** option). The **TARGET=** data set must contain variables with the same names as those being factored. Each observation in the **TARGET=** data set becomes one column of the target factor pattern. Missing values are treated as zeros. The **_NAME_** and **_TYPE_** variables are not required and are ignored if present.

TAU= p

specifies the oblimin weight used with the option **ROTATE=OBLIMIN** or **PREROTATE=OBLIMIN**. Alternatively, you can use **ROTATE=OBLIMIN(p)** with p representing the oblimin weight. There is no restriction on valid values for the oblimin weight, although for practical purposes a negative or zero value is recommended. The default **TAU=** value is 0, resulting in the quartimin rotation. See the section “[Simplicity Functions for Rotations](#)” on page 2244 for more details.

ULTRAHEYWOOD**ULTRA**

allows communalities to exceed 1. The **ULTRAHEYWOOD** option can cause convergence problems because communalities can become extremely large, and ill-conditioned Hessians might occur. See the section “[Heywood Cases and Other Anomalies about Communality Estimates](#)” on page 2248 for a discussion of Heywood cases.

VARDEF=DF | N | WDF | WEIGHT | WGT

specifies the divisor used in the calculation of variances and covariances. The default value is **VARDEF=DF**. The values and associated divisors are displayed in the following table where $i=0$ if the **NOINT** option is used and $i=1$ otherwise, and where k is the number of partial variables specified in the **PARTIAL** statement.

Value	Description	Divisor
DF	degrees of freedom	$n - k - i$
N	number of observations	$n - k$
WDF	sum of weights DF	$\sum_i w_i - k - i$
WEIGHT WGT	sum of weights	$\sum_i w_i - k$

WEIGHT

factors a weighted correlation or covariance matrix. The **WEIGHT** option can be used only with the **METHOD=PRINCIPAL**, **METHOD=PRINIT**, **METHOD=ULS**, or **METHOD=IMAGE** option. The input data set must be of type **CORR**, **UCORR**, **COV**, **UCOV**, or **FACTOR**, and the variable weights are obtained from an observation with **_TYPE_='WEIGHT'**.

BY Statement

BY variables ;

You can specify a BY statement with PROC FACTOR to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the FACTOR procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

If you specify the **TARGET=** option and the **TARGET=** data set does not contain any of the BY variables, then the entire **TARGET=** data set is used as a Procrustean target for each BY group in the **DATA=** data set.

If the **TARGET=** data set contains some but not all of the BY variables, or if some BY variables do not have the same type or length in the **TARGET=** data set as in the **DATA=** data set, then PROC FACTOR displays an error message and stops.

If all the BY variables appear in the **TARGET=** data set with the same type and length as in the **DATA=** data set, then each BY group in the **TARGET=** data set is used as a Procrustean target for the corresponding BY group in the **DATA=** data set. The BY groups in the **TARGET=** data set must be in the same order as in the **DATA=** data set. If you specify the NOTSORTED option in the BY statement, there must be identical BY groups in the same order in both data sets. If you do not specify the NOTSORTED option, some BY groups can appear in one data set but not in the other.

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

FREQ Statement

FREQ variable ;

If a variable in the data set represents the frequency of occurrence for the other values in the observation, include the variable's name in a FREQ statement. The procedure then treats the data set as if each observation appears n times, where n is the value of the FREQ variable for the observation. The total number of observations is considered to be equal to the sum of the FREQ variable when the procedure determines degrees of freedom for significance probabilities.

If the value of the FREQ variable is missing or is less than one, the observation is not used in the analysis. If the value is not an integer, the value is truncated to an integer.

The WEIGHT and FREQ statements have a similar effect, except in determining the number of observations for significance tests.

PARTIAL Statement

PARTIAL *variables* ;

If you want the analysis to be based on a partial correlation or covariance matrix, use the PARTIAL statement to list the variables that are used to partial out the variables in the analysis.

PRIORS Statement

PRIORS *communalities* ;

The PRIORS statement specifies numeric values between 0.0 and 1.0 for the prior communality estimates for each variable. The first numeric value corresponds to the first variable in the VAR statement, the second value to the second variable, and so on. The number of numeric values must equal the number of variables. For example:

```
proc factor;
  var      x y z;
  priors .7 .8 .9;
run;
```

You can specify various methods for computing prior communality estimates with the PRIORS= option in the PROC FACTOR statement. See the description of that option for more information about the default prior communality estimates.

VAR Statement

VAR *variables* ;

The VAR statement specifies the numeric variables to be analyzed. If the VAR statement is omitted, all numeric variables not specified in other statements are analyzed.

WEIGHT Statement

WEIGHT *variable* ;

If you want to use relative weights for each observation in the input data set, specify a variable containing weights in a WEIGHT statement. This is often done when the variance associated with each observation is different and the values of the weight variable are proportional to the reciprocals of the variances. If a variable value is negative or is missing, it is excluded from the analysis.

Details: FACTOR Procedure

Input Data Set

The FACTOR procedure can read an ordinary SAS data set containing raw data or a special data set specified as a TYPE=CORR, TYPE=UCORR, TYPE=SSCP, TYPE=COV, TYPE=UCOV, or TYPE=FACTOR data set containing previously computed statistics. A TYPE=CORR data set can be created by the CORR procedure or various other procedures such as the PRINCOMP procedure. It contains means, standard deviations, the sample size, the correlation matrix, and possibly other statistics if it is created by some procedure other than PROC CORR. A TYPE=COV data set is similar to a TYPE=CORR data set but contains a covariance matrix. A TYPE=UCORR or TYPE=UCOV data set contains a correlation or covariance matrix that is not corrected for the mean. The default VAR variable list does not include Intercept if the DATA= data set is TYPE=SSCP. If the Intercept variable is explicitly specified in the VAR statement with a TYPE=SSCP data set, the NOINT option is activated. A TYPE=FACTOR data set can be created by the FACTOR procedure and is described in the section “Output Data Sets” on page 2241.

If your data set has many observations and you plan to run FACTOR several times, you can save computer time by first creating a TYPE=CORR data set and using it as input to PROC FACTOR, as in the following statements:

```
proc corr data=raw out=correl;      /* create TYPE=CORR data set */
proc factor data=correl method=ml; /* maximum likelihood      */
proc factor data=correl;           /* principal components   */
```

The data set created by the CORR procedure is automatically given the TYPE=CORR data set option, so you do not have to specify TYPE=CORR. However, if you use a DATA step with a SET statement to modify the correlation data set, you must use the TYPE=CORR attribute in the new data set. You can use a VAR statement with PROC FACTOR when reading a TYPE=CORR data set to select a subset of the variables or change the order of the variables.

Problems can arise from using the CORR procedure when there are missing data. By default, PROC CORR computes each correlation from all observations that have values present for the pair of variables involved (pairwise deletion). The resulting correlation matrix might have negative eigenvalues. If you specify the NOMISS option with the CORR procedure, observations with any missing values are completely omitted from the calculations (listwise deletion), and there is no danger of negative eigenvalues.

PROC FACTOR can also create a TYPE=FACTOR data set, which includes all the information in a TYPE=CORR data set, and use it for repeated analyses. For a TYPE=FACTOR data set, the default value of the METHOD= option is PATTERN. The following PROC FACTOR statements produce the same results as the previous example:

```
proc factor data=raw method=ml outstat=fact; /* max. likelihood */
proc factor data=fact method=prin;         /* principal components */
```

You can use a TYPE=FACTOR data set to try several different rotation methods on the same data without repeatedly extracting the factors. In the following example, the second and third PROC FACTOR statements use the data set fact created by the first PROC FACTOR statement:

```
proc factor data=raw outstat=fact; /* principal components */
proc factor rotate=varimax;      /* varimax rotation      */
proc factor rotate=quartimax;    /* quartimax rotation  */
```

You can create a TYPE=CORR, TYPE=UCORR, or TYPE=FACTOR data set in a DATA step for PROC FACTOR to read as input. For example, in the following a TYPE=CORR data set is created and is read as input data set by the subsequent PROC FACTOR statement:

```
data correl(type=corr);
  _TYPE_='CORR';
  input _NAME_ $ x y z;
  datalines;
x 1.0 . .
y .7 1.0 .
z .5 .4 1.0
;
proc factor;
run;
```

Be sure to specify the TYPE= option in parentheses after the data set name in the DATA statement and include the _TYPE_ and _NAME_ variables. In a TYPE=CORR data set, only the correlation matrix (_TYPE_='CORR') is necessary. It can contain missing values as long as every pair of variables has at least one nonmissing value.

You can also create a TYPE=FACTOR data set containing only a factor pattern (_TYPE_='PATTERN') and use the FACTOR procedure to rotate it, as these statements show:

```
data pat(type=factor);
  _TYPE_='PATTERN';
  input _NAME_ $ x y z;
  datalines;
factor1 .5 .7 .3
factor2 .8 .2 .8
;
proc factor rotate=promax prerotate=none;
run;
```

If the input factors are oblique, you must also include the interfactor correlation matrix with _TYPE_='FCORR', as shown here:

```
data pat(type=factor);
  input _TYPE_ $ _NAME_ $ x y z;
  datalines;
pattern factor1 .5 .7 .3
pattern factor2 .8 .2 .8
fcorr factor1 1.0 .2 .
fcorr factor2 .2 1.0 .
;
proc factor rotate=promax prerotate=none;
run;
```

Some procedures, such as the PRINCOMP and CANDISC procedures, produce TYPE=CORR or TYPE=UCORR data sets containing scoring coefficients (_TYPE_='SCORE' or _TYPE_='USCORE'). These coefficients can be input to PROC FACTOR and rotated by using the METHOD=SCORE option, as in the following statements:

```
proc princomp data=raw n=2 outstat=prin;
run;
proc factor data=prin method=score rotate=varimax;
run;
```

Notice that the input data set prin must contain the correlation matrix as well as the scoring coefficients.

Output Data Sets

The OUT= Data Set

The **OUT=** data set contains all the data in the **DATA=** data set plus new variables called Factor1, Factor2, and so on, containing estimated factor scores. Each estimated factor score is computed as a linear combination of the standardized values of the variables that are factored. The coefficients are always displayed if the **OUT=** option is specified, and they are labeled “Standardized Scoring Coefficients.”

If partial variables are specified in the **PARTIAL** statement, the factor analysis is on the residuals of the variables, which are regressed on the partial variables. In this case, the **OUT=** data set also contains the (unstandardized) residuals, which are prefixed by **R_** by default. For example, the residual of variable **X** is named **R_X** in the **OUT=** data set. You might also assign the prefix by the **PARPREFIX=** option. Because the residuals are factor-analyzed, the estimated factor scores are computed as linear combinations of the standardized values of the residuals, but not the original variables.

The OUTSTAT= Data Set

The **OUTSTAT=** data set is similar to the **TYPE=CORR** or **TYPE=UCORR** data set produced by the **CORR** procedure, but it is a **TYPE=FACTOR** data set and it contains many results in addition to those produced by **PROC CORR**. The **OUTSTAT=** data set contains observations with **_TYPE_='UCORR'** and **_TYPE_='USTD'** if you specify the **NOINT** option.

The output data set contains the following variables:

- the **BY** variables, if any
- two new character variables, **_TYPE_** and **_NAME_**
- the variables analyzed—those in the **VAR** statement, or, if there is no **VAR** statement, all numeric variables not listed in any other statement. If partial variables are specified in the **PARTIAL** statement, the residuals are included instead. By default, the residual variable names are prefixed by **R_**, unless you specify something different in the **PARPREFIX=** option.

Each observation in the output data set contains some type of statistic as indicated by the **_TYPE_** variable. The **_NAME_** variable is blank except where otherwise indicated. The values of the **_TYPE_** variable are as follows:

MEAN	means
STD	standard deviations
USTD	uncorrected standard deviations

N	sample size
CORR	correlations. The <code>_NAME_</code> variable contains the name of the variable corresponding to each row of the correlation matrix.
UCORR	uncorrected correlations. The <code>_NAME_</code> variable contains the name of the variable corresponding to each row of the uncorrected correlation matrix.
IMAGE	image coefficients. The <code>_NAME_</code> variable contains the name of the variable corresponding to each row of the image coefficient matrix.
IMAGECOV	image covariance matrix. The <code>_NAME_</code> variable contains the name of the variable corresponding to each row of the image covariance matrix.
COMMUNAL	final communality estimates
PRIORS	prior communality estimates, or estimates from the last iteration for iterative methods
WEIGHT	variable weights
SUMWGT	sum of the variable weights
EIGENVAL	eigenvalues
UNROTATE	unrotated factor pattern. The <code>_NAME_</code> variable contains the name of the factor.
SE_UNROT	standard error estimates for the unrotated loadings. The <code>_NAME_</code> variable contains the name of the factor.
RESIDUAL	residual correlations. The <code>_NAME_</code> variable contains the name of the variable corresponding to each row of the residual correlation matrix.
PRETRANS	transformation matrix from prerotation. The <code>_NAME_</code> variable contains the name of the factor.
PREFCORR	prerotated interfactor correlations. The <code>_NAME_</code> variable contains the name of the factor.
SE_PREFC	standard error estimates for prerotated interfactor correlations. The <code>_NAME_</code> variable contains the name of the factor.
PREROTAT	prerotated factor pattern. The <code>_NAME_</code> variable contains the name of the factor.
SE_PREPA	standard error estimates for the prerotated loadings. The <code>_NAME_</code> variable contains the name of the factor.
PRERCORR	prerotated reference axis correlations. The <code>_NAME_</code> variable contains the name of the factor.
PREREFER	prerotated reference structure. The <code>_NAME_</code> variable contains the name of the factor.
PRESTRUC	prerotated factor structure. The <code>_NAME_</code> variable contains the name of the factor.
SE_PREST	standard error estimates for prerotated structure loadings. The <code>_NAME_</code> variable contains the name of the factor.
PRESCORE	prerotated scoring coefficients. The <code>_NAME_</code> variable contains the name of the factor.
TRANSFOR	transformation matrix from rotation. The <code>_NAME_</code> variable contains the name of the factor.
FCORR	interfactor correlations. The <code>_NAME_</code> variable contains the name of the factor.
SE_FCORR	standard error estimates for interfactor correlations. The <code>_NAME_</code> variable contains the name of the factor.

PATTERN	factor pattern. The <code>_NAME_</code> variable contains the name of the factor.
SE_PAT	standard error estimates for the rotated loadings. The <code>_NAME_</code> variable contains the name of the factor.
RCORR	reference axis correlations. The <code>_NAME_</code> variable contains the name of the factor.
REFERENC	reference structure. The <code>_NAME_</code> variable contains the name of the factor.
STRUCTUR	factor structure. The <code>_NAME_</code> variable contains the name of the factor.
SE_STRUC	standard error estimates for structure loadings. The <code>_NAME_</code> variable contains the name of the factor.
SCORE	scoring coefficients to be applied to standardized variables if the SCORE option is specified on the PROC FACTOR statement. The <code>_NAME_</code> variable contains the name of the factor.
USCORE	scoring coefficients to be applied without subtracting the mean from the raw variables if the SCORE option is specified on the PROC FACTOR statement. The <code>_NAME_</code> variable contains the name of the factor.

Confidence Intervals and the Saliency of Factor Loadings

The traditional approach to determining salient loadings (loadings that are considered large in absolute values) employs rules of thumb such as 0.3 or 0.4. However, this does not use the statistical evidence efficiently. The asymptotic normality of the distribution of factor loadings enables you to construct confidence intervals to gauge the saliency of factor loadings. To guarantee the range-respecting properties of confidence intervals, a transformation procedure such as in CEFA (Browne et al. 2008) is used. For example, because the orthogonal rotated factor loading θ must be bounded between -1 and $+1$, the Fisher transformation

$$\varphi = \frac{1}{2} \log\left(\frac{1 + \theta}{1 - \theta}\right)$$

is employed so that φ is an unbounded parameter. Assuming the asymptotic normality of $\hat{\varphi}$, a symmetric confidence interval for φ is constructed. Then, a back-transformation on the confidence limits yields an asymmetric confidence interval for θ . Applying the results of Browne (1982), a $(1-\alpha)100\%$ confidence interval for the orthogonal factor loading θ is

$$(\hat{\theta}_l = \frac{a/b - 1}{a/b + 1}, \hat{\theta}_u = \frac{a \times b - 1}{a \times b + 1})$$

where

$$a = \frac{1 + \hat{\theta}}{1 - \hat{\theta}}, \quad b = \exp(z_{\alpha/2} \times \frac{2\hat{\theta}}{1 - \hat{\theta}^2})$$

and $\hat{\theta}$ is the estimated factor loading, $\hat{\sigma}$ is the standard error estimate of the factor loading, and $z_{\alpha/2}$ is the $(1 - \alpha/2)100$ percentile point of a standard normal distribution.

Once the confidence limits are constructed, you can use the corresponding coverage displays for determining the salience of the variable-factor relationship. In a coverage display, the **COVER=** value is represented by an asterisk (*). The following table summarizes various displays and their interpretations.

Table 35.2 Interpretations of the Coverage Displays

Positive Estimate	Negative Estimate	COVER=0 Specified	Interpretation
[0]*	*[0]		The estimate is not significantly different from zero, and the CI covers a region of values that are smaller in magnitude than the COVER= value. This is strong statistical evidence for the nonsalience of the variable-factor relationship.
0[]*	*[]0		The estimate is significantly different from zero, but the CI covers a region of values that are smaller in magnitude than the COVER= value. This is strong statistical evidence for the nonsalience of the variable-factor relationship.
[0*]	[*0]	[0]	The estimate is not significantly different from zero or the COVER= value. The population value might have been larger or smaller in magnitude than the COVER= value. There is no statistical evidence for the salience of the variable-factor relationship.
0[*]	[*]0		The estimate is significantly different from zero but not from the COVER= value. This is marginal statistical evidence for the salience of the variable-factor relationship.
0*[]	[]*0	0[] or []0	The estimate is significantly different from zero, and the CI covers a region of values that are larger in magnitude than the COVER= value. This is strong statistical evidence for the salience of the variable-factor relationship.

See [Example 35.4](#) for an illustration of the use of confidence intervals for interpreting factors.

Simplicity Functions for Rotations

To rotate a factor pattern is to apply a nonsingular linear transformation to the unrotated factor pattern matrix. An optimal transformation is usually defined as a minimum or maximum point of a simplicity function. Different rotation methods are based on different simplicity functions employed.

For the promax or the Procrustes rotation, the simplicity function used is the sum of squared differences between the rotated factor pattern and the target matrix. The optimal transformation is obtained by minimizing this simplicity function with respect to the choices of all possible transformation.

For the class of the generalized Crawford-Ferguson family Jennrich (1973), the simplicity function being optimized is

$$f = k_1 Z + k_2 H + k_3 V + k_4 Q$$

where

$$Z = \left(\sum_j \sum_i b_{ij}^2 \right)^2, \quad H = \sum_i \left(\sum_j b_{ij}^2 \right)^2$$

$$V = \sum_j \left(\sum_i b_{ij}^2 \right)^2, \quad Q = \sum_j \sum_i b_{ij}^4$$

k_1, k_2, k_3 , and k_4 are constants, and b_{ij} represents an element of the rotated pattern matrix. Except for specialized research purposes, it is uncommon in practice to use this simplicity function directly for rotation. However, this simplicity function reduces to many well-known classes of rotations. One of these is the Crawford-Ferguson family Crawford and Ferguson (1970), which minimizes

$$f_{cf} = c_1(H - Q) + c_2(V - Q)$$

where c_1 and c_2 are constants, $(H - Q)$ represents variable (row) parsimony, and $(V - Q)$ represents factor (column) parsimony. Therefore, the relative importance of both the variable parsimony and of the factor parsimony is adjusted using the constants c_1 and c_2 . The orthomax class (see Harman 1976) maximizes the function

$$f_{or} = pQ - \gamma V$$

where γ is the orthomax weight and is usually between 0 and the number of variables p . The oblimin class minimizes the function

$$f_{ob} = p(H - Q) - \tau(Z - V)$$

where τ is the oblimin weight. For practical purposes, a negative or zero value for τ is recommended.

All of the preceding definitions are for rotations without row normalization. For rotations with Kaiser normalization, the definition of b_{ij} is replaced by b_{ij}/h_i , where h_i is the communality estimate of variable i .

Missing Values

If the `DATA=` data set contains data (rather than a matrix or factor pattern), then observations with missing values for any variables in the analysis are omitted from the computations. If a correlation or covariance matrix is read, it can contain missing values as long as every pair of variables has at least one nonmissing entry. Missing values in a pattern or scoring coefficient matrix are treated as zeros.

Cautions

- The amount of time that FACTOR takes is roughly proportional to the cube of the number of variables. Factoring 100 variables, therefore, takes about 1,000 times as long as factoring 10 variables. Iterative methods (PRINIT, ALPHA, ULS, ML) can also take 100 times as long as noniterative methods (PRINCIPAL, IMAGE, HARRIS).
- No computer program is capable of reliably determining the optimal number of factors, since the decision is ultimately subjective. You should not blindly accept the number of factors obtained by default; instead, use your own judgment to make a decision.
- Singular correlation matrices cause problems with the options **PRIORS=SMC** and **METHOD=ML**. Singularities can result from using a variable that is the sum of other variables, coding too many dummy variables from a classification variable, or having more variables than observations.
- If you use the CORR procedure to compute the correlation matrix and there are missing data and the NOMISS option is not specified, then the correlation matrix might have negative eigenvalues.
- If a TYPE=CORR, TYPE=UCORR, or TYPE=FACTOR data set is copied or modified using a DATA step, the new data set does not automatically have the same TYPE as the old data set. You must specify the TYPE= data set option in the DATA statement. If you try to analyze a data set that has lost its TYPE=CORR attribute, PROC FACTOR displays a warning message saying that the data set contains `_NAME_` and `_TYPE_` variables but analyzes the data set as an ordinary SAS data set.
- For a TYPE=FACTOR data set, the default is **METHOD=PATTERN**, not **METHOD=PRIN**.

Factor Scores

The FACTOR procedure can compute estimated factor scores directly if you specify the **NFACTORS=** and **OUT=** options, or indirectly using the SCORE procedure. The latter method is preferable if you use the FACTOR procedure interactively to determine the number of factors, the rotation method, or various other aspects of the analysis. To compute factor scores for each observation by using the SCORE procedure, do the following:

- Use the **SCORE** option in the PROC FACTOR statement.
- Create a TYPE=FACTOR output data set with the **OUTSTAT=** option.
- Use the SCORE procedure with both the raw data and the TYPE=FACTOR data set.
- Do not use the TYPE= option in the PROC SCORE statement.

For example, the following statements could be used:

```
proc factor data=raw score outstat=fact;
run;
proc score data=raw score=fact out=scores;
run;
```

or

```
proc corr data=raw out=correl;
run;
proc factor data=correl score outstat=fact;
run;
proc score data=raw score=fact out=scores;
run;
```

For a more detailed example, see [Example 82.1](#) in Chapter 82, “The SCORE Procedure.”

A component analysis (principal, image, or Harris) produces scores with mean zero and variance one. If you have done a common factor analysis, the true factor scores have mean zero and variance one, but the computed factor scores are only estimates of the true factor scores. These estimates have mean zero but variance equal to the squared multiple correlation of the factor with the variables. The estimated factor scores might have small nonzero correlations even if the true factors are uncorrelated.

Variable Weights and Variance Explained

A principal component analysis of a correlation matrix treats all variables as equally important. A principal component analysis of a covariance matrix gives more weight to variables with larger variances. A principal component analysis of a covariance matrix is equivalent to an analysis of a weighted correlation matrix, where the weight of each variable is equal to its variance. Variables with large weights tend to have larger loadings on the first component and smaller residual correlations than variables with small weights.

You might want to give weights to variables by using values other than their variances. Mulaik (1972) explains how to obtain a maximally reliable component by means of a weighted principal component analysis. With the FACTOR procedure, you can indirectly give arbitrary weights to the variables by using the COV option and rescaling the variables to have variance equal to the desired weight, or you can give arbitrary weights directly by using the WEIGHT option and including the weights in a TYPE=CORR data set.

Arbitrary variable weights can be used with the METHOD=PRINCIPAL, METHOD=PRINT, METHOD=ULS, or METHOD=IMAGE option. Alpha and ML factor analyses compute variable weights based on the communalities (Harman 1976, pp. 217–218). For alpha factor analysis, the weight of a variable is the reciprocal of its communality. In ML factor analysis, the weight is the reciprocal of the uniqueness. Harris component analysis uses weights equal to the reciprocal of one minus the squared multiple correlation of each variable with the other variables.

For uncorrelated factors, the variance explained by a factor can be computed with or without taking the weights into account. The usual method for computing variance accounted for by a factor is to take the sum of squares of the corresponding column of the factor pattern, yielding an unweighted result. If the square of each loading is multiplied by the weight of the variable before the sum is taken, the result is the weighted variance explained, which is equal to the corresponding eigenvalue except in image analysis. Whether the weighted or unweighted result is more important depends on the purpose of the analysis.

In the case of correlated factors, the variance explained by a factor can be computed with or without taking the other factors into account. If you want to ignore the other factors, the variance explained is given by the weighted or unweighted sum of squares of the appropriate column of the factor structure since the factor structure contains simple correlations. If you want to subtract the variance explained by the other factors from the amount explained by the factor in question (the Type II variance explained), you can take the weighted or unweighted sum of squares of the appropriate column of the reference structure because the reference structure contains semipartial correlations. There are other ways of measuring the variance explained. For example, given a prior ordering of the factors, you can eliminate from each factor the variance explained by previous factors and compute a Type I variance explained. Harman (1976, pp. 268–270) provides another method, which is based on direct and joint contributions.

Heywood Cases and Other Anomalies about Community Estimates

Since communalities are squared correlations, you would expect them always to lie between 0 and 1. It is a mathematical peculiarity of the common factor model, however, that final communality estimates might exceed 1. If a communality equals 1, the situation is referred to as a Heywood case, and if a communality exceeds 1, it is an ultra-Heywood case. An ultra-Heywood case implies that some unique factor has negative variance, a clear indication that something is wrong. Possible causes include the following:

- bad prior communality estimates
- too many common factors
- too few common factors
- not enough data to provide stable estimates
- the common factor model is not an appropriate model for the data

An ultra-Heywood case renders a factor solution invalid. Factor analysts disagree about whether or not a factor solution with a Heywood case can be considered legitimate.

With `METHOD=PRINIT`, `METHOD=ULS`, `METHOD=ALPHA`, or `METHOD=ML`, the FACTOR procedure, by default, stops iterating and sets the number of factors to 0 if an estimated communality exceeds 1. To enable processing to continue with a Heywood or ultra-Heywood case, you can use the `HEYWOOD` or `ULTRAHEYWOOD` option in the PROC FACTOR statement. The `HEYWOOD` option sets the upper bound of any communality to 1, while the `ULTRAHEYWOOD` option allows communalities to exceed 1.

Theoretically, the communality of a variable should not exceed its reliability. Violation of this condition is called a quasi-Heywood case and should be regarded with the same suspicion as an ultra-Heywood case.

Elements of the factor structure and reference structure matrices can exceed 1 only in the presence of an ultra-Heywood case. On the other hand, an element of the factor pattern might exceed 1 in an oblique rotation.

The maximum likelihood method is especially susceptible to quasi- or ultra-Heywood cases. During the iteration process, a variable with high communality is given a high weight; this tends to increase its communality, which increases its weight, and so on.

It is often stated that the squared multiple correlation of a variable with the other variables is a lower bound to its communality. This is true if the common factor model fits the data perfectly, but it is not generally the case with real data. A final communality estimate that is less than the squared multiple correlation can, therefore, indicate poor fit, possibly due to not enough factors. It is by no means as serious a problem as an ultra-Heywood case. Factor methods that use the Newton-Raphson method can actually produce communalities less than 0, a result even more disastrous than an ultra-Heywood case.

The squared multiple correlation of a factor with the variables might exceed 1, even in the absence of ultra-Heywood cases. This situation is also cause for alarm. Alpha factor analysis seems to be especially prone to this problem, but it does not occur with maximum likelihood. If a squared multiple correlation is negative, there are too many factors retained.

With data that do not fit the common factor model perfectly, you can expect some of the eigenvalues to be negative. If an iterative factor method converges properly, the sum of the eigenvalues corresponding to rejected factors should be 0; hence, some eigenvalues are positive and some negative. If a principal factor analysis fails to yield any negative eigenvalues, the prior communality estimates are probably too large. Negative eigenvalues cause the cumulative proportion of variance explained to exceed 1 for a sufficiently large number of factors. The cumulative proportion of variance explained by the retained factors should be approximately 1 for principal factor analysis and should converge to 1 for iterative methods. Occasionally, a single factor can explain more than 100 percent of the common variance in a principal factor analysis, indicating that the prior communality estimates are too low.

If a squared canonical correlation or a coefficient alpha is negative, there are too many factors retained.

Principal component analysis, unlike common factor analysis, has none of these problems if the covariance or correlation matrix is computed correctly from a data set with no missing values. Various methods for missing value correlation or severe rounding of the correlations can produce negative eigenvalues in principal components.

Time Requirements

- n = number of observations
- v = number of variables
- f = number of factors
- i = number of iterations during factor extraction
- r = length of iterations during factor rotation

The time required to compute. . .	is roughly proportional to
an overall factor analysis	iv^3
the correlation matrix	nv^2
PRIORS=SMC or ASMC	v^3
PRIORS=MAX	v^2
eigenvalues	v^3
final eigenvectors	fv^2
generalized Crawford-Ferguson family of rotations, PROMAX, or HK	rvf^2
ROTATE=PROCRUSTES	vf^2

Each iteration in the PRINIT or ALPHA method requires computation of eigenvalues and f eigenvectors.

Each iteration in the ML or ULS method requires computation of eigenvalues and $v - f$ eigenvectors.

The amount of time that PROC FACTOR takes is roughly proportional to the cube of the number of variables. Factoring 100 variables, therefore, takes about 1000 times as long as factoring 10 variables. Iterative methods (PRINIT, ALPHA, ULS, ML) can also take 100 times as long as noniterative methods (PRINCIPAL, IMAGE, HARRIS).

Displayed Output

PROC FACTOR output includes the following.

- Input data type, numbers of records read and used for raw data input, number of observations (NOBS=) set in the PROC FACTOR statements, and the number of observations used in significance tests
- Mean and Std Dev (standard deviation) of each variable and the number of observations, if you specify the SIMPLE option
- Correlations, if you specify the CORR option
- Inverse Correlation Matrix, if you specify the ALL option
- Partial Correlations Controlling all other Variables (negative anti-image correlations), if you specify the MSA option. If the data are appropriate for the common factor model, the partial correlations should be small.
- Kaiser's Measure of Sampling Adequacy (Kaiser 1970; Kaiser and Rice 1974; Cerny and Kaiser 1977), both overall and for each variable, if you specify the MSA option. The MSA is a summary of how small the partial correlations are relative to the ordinary correlations. Values greater than 0.8 can be considered good. Values less than 0.5 require remedial action, either by deleting the offending variables or by including other variables related to the offenders.

- Prior Communality Estimates, unless 1.0s are used or unless you specify the **METHOD=IMAGE**, **METHOD=HARRIS**, **METHOD=PATTERN**, or **METHOD=SCORE** option
- Squared Multiple Correlations of each variable with all the other variables, if you specify the **METHOD=IMAGE** or **METHOD=HARRIS** option
- Image Coefficients, if you specify the **METHOD=IMAGE** option
- Image Covariance Matrix, if you specify the **METHOD=IMAGE** option
- Preliminary Eigenvalues based on the prior communalities, if you specify the **METHOD=PRINIT**, **METHOD=ALPHA**, **METHOD=ML**, or **METHOD=ULS** option. The table produced includes the Total and the Average of the eigenvalues, the Difference between successive eigenvalues, the Proportion of variation represented, and the Cumulative proportion of variation.
- the number of factors that are retained, unless you specify the **METHOD=PATTERN** or **METHOD=SCORE** option
- the Scree Plot of Eigenvalues, if you specify the **SCREE** option. The preliminary eigenvalues are used if you specify the **METHOD=PRINIT**, **METHOD=ALPHA**, **METHOD=ML**, or **METHOD=ULS** option.
- the iteration history, if you specify the **METHOD=PRINIT**, **METHOD=ALPHA**, **METHOD=ML**, or **METHOD=ULS** option. The table produced contains the iteration number (Iter); the Criterion being optimized (Jöreskog 1977); the Ridge value for the iteration if you specify the **METHOD=ML** or **METHOD=ULS** option; the maximum Change in any communality estimate; and the Communalities.
- Significance tests, if you specify the option **METHOD=ML**, including Bartlett's chi-square, df, and Prob > χ^2 for H_0 : No common factors and H_0 : factors retained are sufficient to explain the correlations. The H_0 test for no common factors is equivalent to Bartlett's test of sphericity. The variables should have an approximate multivariate normal distribution for the probability levels to be valid. Lawley and Maxwell (1971) suggest that the number of observations should exceed the number of variables by 50 or more, although Geweke and Singleton (1980) claim that as few as 10 observations are adequate with five variables and one common factor. Certain regularity conditions must also be satisfied for Bartlett's χ^2 test to be valid (Geweke and Singleton 1980), but in practice these conditions usually are satisfied. The notation Prob>chi**2 means "the probability under the null hypothesis of obtaining a greater χ^2 statistic than that observed." The chi-square value is displayed with and without Bartlett's correction.
- Akaike's Information Criterion, if you specify the **METHOD=ML** option. Akaike's information criterion (AIC) (Akaike 1973, 1974, 1987) is a general criterion for estimating the best number of parameters to include in a model when maximum likelihood estimation is used. The number of factors that yields the smallest value of AIC is considered best. Like the chi-square test, AIC tends to include factors that are statistically significant but inconsequential for practical purposes.
- Schwarz's Bayesian Criterion, if you specify the **METHOD=ML** option. Schwarz's Bayesian Criterion (SBC) (Schwarz 1978) is another criterion, similar to AIC, for determining the best number of parameters. The number of factors that yields the smallest value of SBC is considered best; SBC seems to be less inclined to include trivial factors than either AIC or the chi-square test.
- Tucker and Lewis's Reliability Coefficient, if you specify the **METHOD=ML** option (Tucker and Lewis 1973)

- Squared Canonical Correlations, if you specify the `METHOD=ML` option. These are the same as the squared multiple correlations for predicting each factor from the variables.
- Coefficient Alpha for Each Factor, if you specify the `METHOD=ALPHA` option
- Eigenvectors, if you specify the `EIGENVECTORS` or `ALL` option, unless you also specify the `METHOD=PATTERN` or `METHOD=SCORE` option
- Eigenvalues of the (Weighted) (Reduced) (Image) Correlation or Covariance Matrix, unless you specify the `METHOD=PATTERN` or `METHOD=SCORE` option. Included are the Total and the Average of the eigenvalues, the Difference between successive eigenvalues, the Proportion of variation represented, and the Cumulative proportion of variation.
- the Factor Pattern, which is equal to both the matrix of standardized regression coefficients for predicting variables from common factors and the matrix of correlations between variables and common factors since the extracted factors are uncorrelated. Standard error estimates are included if the `SE` option is specified with `METHOD=ML`. Confidence limits and coverage displays are included if `COVER=` option is specified with `METHOD=ML`.
- Variance explained by each factor, both Weighted and Unweighted, if variable weights are used
- Final Community Estimates, including the Total communality; or Final Community Estimates and Variable Weights, including the Total communality, both Weighted and Unweighted, if variable weights are used. Final communality estimates are the squared multiple correlations for predicting the variables from the estimated factors, and they can be obtained by taking the sum of squares of each row of the factor pattern, or a weighted sum of squares if variable weights are used.
- Residual Correlations with Uniqueness on the Diagonal, if you specify the `RESIDUAL` or `ALL` option
- Root Mean Square Off-diagonal Residuals, both Over-all and for each variable, if you specify the `RESIDUAL` or `ALL` option
- Partial Correlations Controlling Factors, if you specify the `RESIDUAL` or `ALL` option
- Root Mean Square Off-diagonal Partials, both Over-all and for each variable, if you specify the `RESIDUAL` or `ALL` option
- Plots of Factor Pattern for unrotated factors, if you specify the `PREPLOT` option. The number of plots is determined by the `NPLOT=` option.
- Variable Weights for Rotation, if you specify the `NORM=WEIGHT` option
- Factor Weights for Rotation, if you specify the `HKPOWER=` option
- Orthogonal Transformation Matrix, if you request an orthogonal rotation
- Rotated Factor Pattern, if you request an orthogonal rotation. Standard error estimates are included if the `SE` option is specified with `METHOD=ML`. Confidence limits and coverage displays are included if `COVER=` option is specified with `METHOD=ML`.
- Variance explained by each factor after rotation. If you request an orthogonal rotation and if variable weights are used, both weighted and unweighted values are produced.

- Target Matrix for Procrustean Transformation, if you specify the `ROTATE=PROMAX` or `ROTATE=PROCRUSTES` option
- the Procrustean Transformation Matrix, if you specify the `ROTATE=PROMAX` or `ROTATE=PROCRUSTES` option
- the Normalized Oblique Transformation Matrix, if you request an oblique rotation, which, for the option `ROTATE=PROMAX`, is the product of the prerotation and the Procrustes rotation
- Inter-factor Correlations, if you specify an oblique rotation. Standard error estimates are included if the `SE` option is specified with `METHOD=ML`. Confidence limits and coverage displays are included if `COVER=` option is specified with `METHOD=ML`.
- Rotated Factor Pattern (Std Reg Coefs), if you specify an oblique rotation, giving standardized regression coefficients for predicting the variables from the factors. Standard error estimates are included if the `SE` option is specified with `METHOD=ML`. Confidence limits and coverage displays are included if `COVER=` option is specified with `METHOD=ML`.
- Reference Axis Correlations if you specify an oblique rotation. These are the partial correlations between the primary factors when all factors other than the two being correlated are partialled out.
- Reference Structure (Semipartial Correlations), if you request an oblique rotation. The reference structure is the matrix of semipartial correlations (Kerlinger and Pedhazur 1973) between variables and common factors, removing from each common factor the effects of other common factors. If the common factors are uncorrelated, the reference structure is equal to the factor pattern.
- Variance explained by each factor eliminating the effects of all other factors, if you specify an oblique rotation. Both Weighted and Unweighted values are produced if variable weights are used. These variances are equal to the (weighted) sum of the squared elements of the reference structure corresponding to each factor.
- Factor Structure (Correlations), if you request an oblique rotation. The (primary) factor structure is the matrix of correlations between variables and common factors. If the common factors are uncorrelated, the factor structure is equal to the factor pattern. Standard error estimates are included if the `SE` option is specified with `METHOD=ML`. Confidence limits and coverage displays are included if `COVER=` option is specified with `METHOD=ML`.
- Variance explained by each factor ignoring the effects of all other factors, if you request an oblique rotation. Both Weighted and Unweighted values are produced if variable weights are used. These variances are equal to the (weighted) sum of the squared elements of the factor structure corresponding to each factor.
- Final Communality Estimates for the rotated factors if you specify the `ROTATE=` option. The estimates should equal the unrotated communalities.
- Squared Multiple Correlations of the Variables with Each Factor, if you specify the `SCORE` or `ALL` option, except for unrotated principal components
- Standardized Scoring Coefficients, if you specify the `SCORE` or `ALL` option
- Plots of the Factor Pattern for rotated factors, if you specify the `PLOT` option and you request an orthogonal rotation. The number of plots is determined by the `NPLOT=` option.

- Plots of the Reference Structure for rotated factors, if you specify the **PLOT** option and you request an oblique rotation. The number of plots is determined by the **NPLOT=** option. Included are the Reference Axis Correlation and the Angle between the Reference Axes for each pair of factors plotted.

If you specify the **ROTATE=PROMAX** option, the output includes results for both the prerotation and the Procrustes rotation.

ODS Table Names

PROC FACTOR assigns a name to each table it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in Table 35.3. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

Table 35.3 ODS Tables Produced by PROC FACTOR

ODS Table Name	Description	Option
AlphaCoef	Coefficient alpha for each factor	METHOD=ALPHA
CanCorr	Squared canonical correlations	METHOD=ML
CondStdDev	Conditional standard deviations	SIMPLE with PARTIAL
ConvergenceStatus	Convergence status	METHOD=PRINIT, ALPHA, ML, or ULS
Corr	Correlations	CORR
Eigenvalues	Eigenvalues	default, SCREE
Eigenvectors	Eigenvectors	EIGENVECTORS
FactorWeightRotate	Factor weights for rotation	HKPOWER=
FactorPattern	Factor pattern	default
FactorStructure	Factor structure	ROTATE= any oblique rotation
FinalCommun	Final communalities	default
FinalCommunWgt	Final communalities with weights	METHOD=ML or ALPHA
FitMeasures	Measures of fit	METHOD=ML
ImageCoef	Image coefficients	METHOD=IMAGE
ImageCov	Image covariance matrix	METHOD=IMAGE
ImageFactors	Image factor matrix	METHOD=IMAGE
InputFactorPattern	Input factor pattern	METHOD=PATTERN with PRINT or ALL
InputScoreCoef	Standardized input scoring coefficients	METHOD=SCORE with PRINT or ALL
InterFactorCorr	Interfactor correlations	ROTATE= any oblique rotation
InvCorr	Inverse correlation matrix	ALL
IterHistory	Iteration history	METHOD=PRINIT, ALPHA, ML, or ULS
MultipleCorr	Squared multiple correlations	METHOD=IMAGE or METHOD=HARRIS
NObs	Number of records and observations, input data type	default

Table 35.3 *continued*

ODS Table Name	Description	Option
NormObliqueTrans	Normalized oblique transformation matrix	ROTATE= any oblique rotation
ObliqueRotFactPat	Rotated factor pattern	ROTATE= any oblique rotation
ObliqueTrans	Oblique transformation matrix	HKPOWER=
OrthRotFactPat	Rotated factor pattern	ROTATE= any orthogonal rotation
OrthTrans	Orthogonal transformation matrix	ROTATE= any orthogonal rotation
ParCorrControlFactor	Partial correlations controlling factors	RESIDUAL
ParCorrControlVar	Partial correlations controlling other variables	MSA
PartialCorr	Partial correlations	MSA, CORR with PARTIAL
PriorCommunalEst	Prior communality estimates	PRIORS=, METHOD=ML or ALPHA
ProcrustesTarget	Target matrix for Procrustean transformation	ROTATE=PROCRUSTES, ROTATE=PROMAX
ProcrustesTrans	Procrustean transformation matrix	ROTATE=PROCRUSTES, ROTATE=PROMAX
RMSOffDiagPartials	Root mean square off-diagonal partials	RESIDUAL
RMSOffDiagResids	Root mean square off-diagonal residuals	RESIDUAL
ReferenceAxisCorr	Reference axis correlations	ROTATE= any oblique rotation
ReferenceStructure	Reference structure	ROTATE= any oblique rotation
ResCorrUniqueDiag	Residual correlations with uniqueness on the diagonal	RESIDUAL
SamplingAdequacy	Kaiser's measure of sampling adequacy	MSA
SignifTests	Significance tests	METHOD=ML
SimpleStatistics	Simple statistics	SIMPLE
StdScoreCoef	Standardized scoring coefficients	SCORE
VarExplain	Variance explained	default
VarExplainWgt	Variance explained with weights	METHOD=ML, or ALPHA
VarFactorCorr	Squared multiple correlations of the variables with each factor	SCORE
VarWeightRotate	Variable weights for rotation	NORM=WEIGHT, ROTATE=

ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “Statistical Graphics Using ODS.”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “A Primer on ODS Statistical Graphics” on page 599 in Chapter 21, “Statistical Graphics Using ODS.”

The names of the graphs that PROC FACTOR generates are listed in Table 35.4, along with the required statements and options.

Table 35.4 Graphs Produced by PROC FACTOR

ODS Graph Name	Plot Description	Option
PatternPlot	Rotated factor pattern	PLOTS=LOADINGS
InitPatternPlot	Initial factor pattern	PLOTS=INITLOADINGS
InitRefStructurePlot	Initial reference structures	PLOTS=INITLOADINGS and PLOTREF
PrePatternPlot	Prerotated factor pattern	PLOTS=PRELOADINGS
PreRefStructurePlot	Prerotated reference structures	PLOTS=PRELOADINGS and PLOTREF
RefStructurePlot	Rotated reference structures	PLOTS=LOADINGS and PLOTREF
ScreePlot	Scree and variance explained plots	PLOTS=SCREE
VariancePlot	Plot of explained variance	PLOTS=SCREE(UNPACK)

Examples: FACTOR Procedure

Example 35.1: Principal Component Analysis

This example analyzes socioeconomic data provided by Harman (1976). The five variables represent total population (Population), median school years (School), total employment (Employment), miscellaneous professional services (Services), and median house value (HouseValue). Each observation represents one of twelve census tracts in the Los Angeles Standard Metropolitan Statistical Area.

You conduct a principal component analysis by using the following statements:

```

data SocioEconomics;
  input Population School Employment Services HouseValue;
  datalines;
5700    12.8    2500    270    25000
1000    10.9    600     10    10000
3400    8.8     1000    10    9000
3800    13.6    1700    140   25000
4000    12.8    1600    140   25000
8200    8.3     2600    60    12000
1200    11.4    400     10    16000
9100    11.5    3300    60    14000
9900    12.5    3400    180   18000
9600    13.7    3600    390   25000
9600    9.6     3300    80    12000
9400    11.4    4000    100   13000
;

proc factor data=SocioEconomics simple corr;
run;

```

You begin with the specification of the raw data set with 12 observations. Then you use the `DATA=` option in the `PROC FACTOR` statement to specify the data set in the analysis. You also set the `SIMPLE` and `CORR` options for additional output results, which are shown in [Output 35.1.2](#) and [Output 35.1.3](#), respectively.

By default, `PROC FACTOR` assumes that all initial communalities are 1, which is the case for the current principal component analysis. If you intend to find common factors instead, use the `PRIORS=` option or the `PRIORS` statement to set initial communalities to values less than 1, which results in extracting the principal factors rather than the principal components. See [Example 35.2](#) for the specification of a principal factor analysis.

For the current principal component analysis, the first output table is displayed in the [Output 35.1.1](#).

Output 35.1.1 Principal Component Analysis: Number of Observations

Five Socioeconomic Variables	
See Page 14 of Harman: Modern Factor Analysis, 3rd Ed	
Principal Component Analysis	
The FACTOR Procedure	
Input Data Type	Raw Data
Number of Records Read	12
Number of Records Used	12
N for Significance Tests	12

In [Output 35.1.1](#), the input data type is shown to be raw data. `PROC FACTOR` also accepts other data type such as correlations and covariances. See [Example 35.4](#) for the use of correlations as input data. For the current raw data set, `PROC FACTOR` reads in 12 records and all these 12 records are used. When there are missing values in the data set, these two numbers might not match due to the dropping of the records with missing values. The last row of the table shows that $N = 12$ is used in the significance tests conducted in the analysis.

The **SIMPLE** option specified in the PROC FACTOR statement generates the means and standard deviations of all observed variables in the analysis, as shown in [Output 35.1.2](#).

Output 35.1.2 Principal Component Analysis: Simple Statistics

Means and Standard Deviations from 12 Observations		
Variable	Mean	Std Dev
Population	6241.667	3439.9943
School	11.442	1.7865
Employment	2333.333	1241.2115
Services	120.833	114.9275
HouseValue	17000.000	6367.5313

The ranges of means and standard deviations for the analysis are quite large. Variables are measured on quite different scales. However, this is not an issue because PROC FACTOR basically analyzes the standardized scales (that is, the correlations) of the variables.

The **CORR** option specified in the PROC FACTOR statement generates the output of the observed correlations in [Output 35.1.3](#).

Output 35.1.3 Principal Component Analysis: Correlations

	Correlations				
	Population	School	Employment	Services	HouseValue
Population	1.00000	0.00975	0.97245	0.43887	0.02241
School	0.00975	1.00000	0.15428	0.69141	0.86307
Employment	0.97245	0.15428	1.00000	0.51472	0.12193
Services	0.43887	0.69141	0.51472	1.00000	0.77765
HouseValue	0.02241	0.86307	0.12193	0.77765	1.00000

The correlation matrix shown in [Output 35.1.3](#) is analyzed by PROC FACTOR.

The first step of principal component analysis is to look at the eigenvalues of the correlation matrix. The larger eigenvalues are extracted first. Because there are five observed variables, five eigenvalues can be extracted, as shown in [Output 35.1.4](#).

Output 35.1.4 Principal Component Analysis: Eigenvalues

Eigenvalues of the Correlation Matrix: Total = 5 Average = 1				
	Eigenvalue	Difference	Proportion	Cumulative
1	2.87331359	1.07665350	0.5747	0.5747
2	1.79666009	1.58182321	0.3593	0.9340
3	0.21483689	0.11490283	0.0430	0.9770
4	0.09993405	0.08467868	0.0200	0.9969
5	0.01525537		0.0031	1.0000

In [Output 35.1.4](#), the two largest eigenvalues are 2.8733 and 1.7967, which together account for 93.4% of the standardized variance. Thus, the first two principal components provide an adequate summary of the data for most purposes. Three components, which explain 97.7% of the variation, should be sufficient for almost any application. PROC FACTOR retains the first two components on the basis of the eigenvalues-greater-than-one rule since the third eigenvalue is only 0.2148.

To express the observed variables as functions of the components (or factors, in general), you consult the factor loading matrix as shown in [Output 35.1.5](#).

Output 35.1.5 Principal Component Analysis: Factor Pattern

Factor Pattern		
	Factor1	Factor2
Population	0.58096	0.80642
School	0.76704	-0.54476
Employment	0.67243	0.72605
Services	0.93239	-0.10431
HouseValue	0.79116	-0.55818

The factor pattern is often referred to as the factor loading matrix in factor analysis. The elements in the loading matrix are called factor loadings. There are at least two ways you can interpret these factor loadings. First, you can use this table to express the observed variables as functions of the extracted factors (or components, as in the current analysis). Each row of the factor loadings tells you the linear combination of the factor or component scores that would yield the expected value of the associated variable. Second, you can interpret each loading as a correlation between an observed variable and a factor or component, provided that the factor solution is an orthogonal one (that is, factors are uncorrelated), such as the current initial factor solution. Hence, the factor loadings indicate how strongly the variables and the factors or components are related.

In [Output 35.1.5](#), the first component (labeled “Factor1”) has large positive loadings for all five variables. Its correlation with Services (0.9324) is especially high. The second component is basically a contrast of Population (0.8064) and Employment (0.7261) against School (-0.5448) and HouseValue (-0.5582), with a very small loading on Services (-0.1043).

The total variance explained by the two components are shown in [Output 35.1.6](#).

Output 35.1.6 Principal Component Analysis: Total Variance Explained by Factors

Variance Explained by Each Factor	
Factor1	Factor2
2.8733136	1.7966601

The first and second component account for 2.8733 and 1.7967, respectively, of the total variance of 5. In the initial factor solution, the total variance explained by the factors or components are the same as the eigenvalues extracted. (Compare the total variance with the eigenvalues shown in [Output 35.1.4](#).) Due to the dropping of the less important components, the sum of these two numbers is 4.6700, which is only a little bit less than total variance 5 of the original correlation matrix.

You can also look at the variance explained by the two components for each observed variables in [Output 35.1.7](#).

Output 35.1.7 Principal Component Analysis: Final Community Estimates

Final Community Estimates: Total = 4.669974				
Population	School	Employment	Services	HouseValue
0.98782629	0.88510555	0.97930583	0.88023562	0.93750041

In [Output 35.1.7](#), the final communality estimates show that all the variables are well accounted for by the two components, with final communality estimates ranging from 0.8802 for Services to 0.9878 for Population. The sum of the communalities is 4.6700, which is the same as the sum of the variance explained by the two components, as shown in [Output 35.1.6](#).

Principal Component Analysis by PROC FACTOR and PROC PRINCOMP

The principal component analysis by PROC FACTOR emphasizes how the principal components explain the observed variables. The factor loadings in the factor pattern as shown in [Output 35.1.5](#) are the coefficients for combining the factor/component scores to yield the observed variable scores when the expected error residuals are zero. For example, the predicted standardized value of Population given the factor/component scores for Factor1 and Factor2 is given by:

$$\text{Population} = 0.58096 \times \text{Factor1} + 0.80642 \times \text{Factor2}$$

If you are primarily interested in getting the component scores as linear combinations of the observed variables, the factor loading matrix table is not the right one for you. However, you might request the standardized scoring coefficients by adding the `SCORE` option in the FACTOR statement:

```
proc factor data=SocioEconomics n=5 score;
run;
```

In the preceding PROC FACTOR statement, N=5 is specified for retaining all five components. This is done for comparing the PROC FACTOR results with those of PROC PRINCOMP, which is described later.

The **SCORE** option requests the display of the standardized scoring coefficients, which are shown in [Output 35.1.8](#).

Output 35.1.8 Principal Component Analysis: Scoring Coefficients for Computing Component Scores

Standardized Scoring Coefficients					
	Factor1	Factor2	Factor3	Factor4	Factor5
Population	0.20219065	0.44884459	0.1284067	0.64542101	5.58240225
School	0.26695219	-0.3032049	1.48611655	-1.1184573	1.41573501
Employment	0.23402646	0.40410834	0.53496241	0.07255759	-5.6513542
Services	0.32450082	-0.0580552	-1.432726	-1.5828806	-0.0010006
HouseValue	0.27534803	-0.3106762	-0.3012889	2.41418899	-0.6673445

In [Output 35.1.8](#), each factor/component is expressed as a linear combination of the standardized observed variables. For example, the first principal component or Factor1 is computed as:

$$0.2022 \times \text{Population} + 0.2670 \times \text{School} + 0.2340 \times \text{Employment} + 0.3245 \times \text{Services} + 0.2753 \times \text{HouseValue}$$

Again, when applying this formula you must use the standardized observed variables (with means 0 and standard deviations 1), but not the raw data.

Apart from some scaling differences, the set of scoring coefficients obtained from PROC FACTOR are equivalent to those obtained from PROC PRINCOMP, as specified by the following statement:

```
proc princomp data=SocioEconomics;
run;
```

PROC PRINCOMP displays the scoring coefficients as eigenvectors, which are shown in [Output 35.1.9](#).

Output 35.1.9 Principal Component Analysis by PROC PRINCOMP: Eigenvectors

Eigenvectors					
	Prin1	Prin2	Prin3	Prin4	Prin5
Population	0.342730	0.601629	0.059517	0.204033	0.689497
School	0.452507	-0.406414	0.688822	-0.353571	0.174861
Employment	0.396695	0.541665	0.247958	0.022937	-0.698014
Services	0.550057	-0.077817	-0.664076	-0.500386	-0.000124
HouseValue	0.466738	-0.416429	-0.139649	0.763182	-0.082425

For example, to get the first principal component score, you use the following formula:

$$0.3427 \times \text{Population} + 0.4525 \times \text{School} + 0.3967 \times \text{Employment} + 0.5500 \times \text{Services} + 0.4667 \times \text{HouseValue}$$

This formula is not exactly the same as the one shown by using PROC FACTOR. All scoring coefficients in PROC FACTOR are smaller, approximately a factor of 0.59 to those coefficients obtained from PROC PRINCOMP. The reason for the scalar difference is that PROC FACTOR assumes all factors/components to

have variance of 1, while PROC PRINCOMP creates components that have variances equal to the eigenvalues. You can do a simple rescaling of the standardized scoring coefficients obtained from PROC FACTOR so that they match the associated eigenvectors from the PROC PRINCOMP. Basically, you need to rescale each column of the standardized scoring coefficients obtained from PROC FACTOR to have the sum of squares equaling one, which is a defining characteristic of eigenvectors. This could be accomplished by dividing each coefficient by the square root of the corresponding column sum of squares.

For the present example, you can use PROC STDIZE to do the rescaling, as shown in the following statements:

```
proc factor data=SocioEconomics n=5 score;
  ods output StdScoreCoef=Coef;
run;

proc stdize method=ustd mult=.44721 data=Coef out=eigenvectors;
  Var Factor1-Factor5;
run;

proc print data=eigenvectors;
run;
```

First, you create an output set Coef for the standardized scoring coefficients by the ODS OUTPUT statement. Note that “StdScoreCoef” is the ODS table that contains the standardized scoring coefficients as shown in [Output 35.1.8](#). (See [Table 35.3](#) for all ODS table names for PROC FACTOR.) Next, you use METHOD=USTD in the PROC STDIZE statement to divide the output coefficients by the corresponding uncorrected (for mean) standard deviations. The following formula shows the relationship between the uncorrected standard deviation and the sum of squares:

$$\text{uncorrected standard deviation} = \sqrt{\text{sum of squares}/N}$$

Recall that what you intend to divide from each coefficient is its square root of the corresponding column sum of squares. Therefore, to adjust for what PROC STDIZE does using METHOD=USTD, you have to multiply each variable by a constant term of $1/\sqrt{N}$ in the standardization. For the current example, this constant term is 0.44721 ($= 1/\sqrt{5}$) and is specified through the MULT= option in the PROC STDIZE statement. With the OUT= option, the rescaled scoring coefficients are saved in the SAS data set eigenvectors. The printout of the data set in [Output 35.1.10](#) shows the rescaled standardized scoring coefficients obtained from PROC FACTOR.

Output 35.1.10 Rescaled Standardized Scoring Coefficients

Obs	Variable	Factor1	Factor2	Factor3	Factor4	Factor5
1	Population	0.34272761	0.60162443	0.05951667	0.20403109	0.68949172
2	School	0.45250304	-0.4064112	0.68881691	-0.3535678	0.17485977
3	Employment	0.39669158	0.54166065	0.24795576	0.02293697	-0.6980081
4	Services	0.5500521	-0.0778162	-0.6640703	-0.5003817	-0.0001236
5	HouseValue	0.4667346	-0.4164256	-0.1396478	0.76317568	-0.0824248

As you can see, these standardized scoring coefficients are essentially the same as those obtained from PROC PRINCOMP, as shown in [Output 35.1.9](#). This example shows that principal component analyses by PROC FACTOR and PROC PRINCOMP are indeed equivalent. PROC PRINCOMP emphasizes more the linear combinations of the variables to form the components, while PROC FACTOR expresses variables as linear combinations of the components in the output. If a principal component analysis of the data is all you need in a particular application, there is no reason to use PROC FACTOR instead of PROC PRINCOMP. Therefore, the following examples focus on common factor analysis for which that you can apply only PROC FACTOR, but not PROC PRINCOMP.

Example 35.2: Principal Factor Analysis

This example uses the data presented in [Example 35.1](#) and performs a principal factor analysis with squared multiple correlations for the prior communality estimates. Unlike [Example 35.1](#), which analyzes the principal components (with default `PRIORS=ONE`), the current analysis is based on a common factor model. To use a common factor model, you specify `PRIORS=SMC` in the PROC FACTOR statement, as shown in the following:

```
ods graphics on;

proc factor data=SocioEconomics
  priors=smc msa residual
  rotate=promax reorder
  outstat=fact_all
  plots=(scree initloadings preloadings loadings);
run;

ods graphics off;
```

In the PROC FACTOR statement, you include several other options to help you analyze the results. To help determine whether the common factor model is appropriate, you request the Kaiser's measure of sampling adequacy with the `MSA` option. You specify the `RESIDUALS` option to compute the residual correlations and partial correlations.

The `ROTATE=` and `REORDER` options are specified to enhance factor interpretability. The `ROTATE=PROMAX` option produces an orthogonal varimax prerotation (default) followed by an oblique Procrustes rotation, and the `REORDER` option reorders the variables according to their largest factor loadings. An `OUTSTAT=` data set is created by PROC FACTOR and displayed in [Output 35.2.15](#).

PROC FACTOR can produce high-quality graphs that are very useful for interpreting the factor solutions. To request these graphs, ODS Graphics must be enabled. All ODS graphs in PROC FACTOR are requested with the `PLOTS=` option. In this example, you request a scree plot (`SCREE`) and loading plots for the factor matrix during the following three stages: initial unrotated solution (`INITLOADINGS`), prerotated (varimax) solution (`PRELOADINGS`), and promax-rotated solution (`LOADINGS`). The scree plot helps you determine the number of factors, and the loading plots help you visualize the patterns of factor loadings during various stages of analyses.

Principal Factor Analysis: Kaiser's MSA and Factor Extraction Results

Output 35.2.1 displays the results of the partial correlations and Kaiser's measure of sampling adequacy.

Output 35.2.1 Principal Factor Analysis: Partial Correlations and Kaiser's MSA

Partial Correlations Controlling all other Variables					
	Population	School	Employment	Services	HouseValue
Population	1.00000	-0.54465	0.97083	0.09612	0.15871
School	-0.54465	1.00000	0.54373	0.04996	0.64717
Employment	0.97083	0.54373	1.00000	0.06689	-0.25572
Services	0.09612	0.04996	0.06689	1.00000	0.59415
HouseValue	0.15871	0.64717	-0.25572	0.59415	1.00000
Kaiser's Measure of Sampling Adequacy: Overall MSA = 0.57536759					
	Population	School	Employment	Services	HouseValue
	0.47207897	0.55158839	0.48851137	0.80664365	0.61281377

If the data are appropriate for the common factor model, the partial correlations (controlling all other variables) should be small compared to the original correlations. For example, the partial correlation between the variables School and HouseValue is 0.65, slightly less than the original correlation of 0.86 (see [Output 35.1.3](#)). The partial correlation between Population and School is -0.54 , which is much larger in absolute value than the original correlation; this is an indication of trouble. Kaiser's *MSA* is a summary, for each variable and for all variables together, of how much smaller the partial correlations are than the original correlations. Values of 0.8 or 0.9 are considered good, while MSAs below 0.5 are unacceptable. The variables Population, School, and Employment have very poor MSAs. Only the Services variable has a good MSA. The overall MSA of 0.58 is sufficiently poor that additional variables should be included in the analysis to better define the common factors. A commonly used rule is that there should be at least three variables per factor. In the following analysis, you determine that there are two common factors in these data. Therefore, more variables are needed for a reliable analysis.

Output 35.2.2 displays the results of the principal factor extraction.

Output 35.2.2 Principal Factor Analysis: Factor Extraction

Prior Communality Estimates: SMC					
	Population	School	Employment	Services	HouseValue
	0.96859160	0.82228514	0.96918082	0.78572440	0.84701921

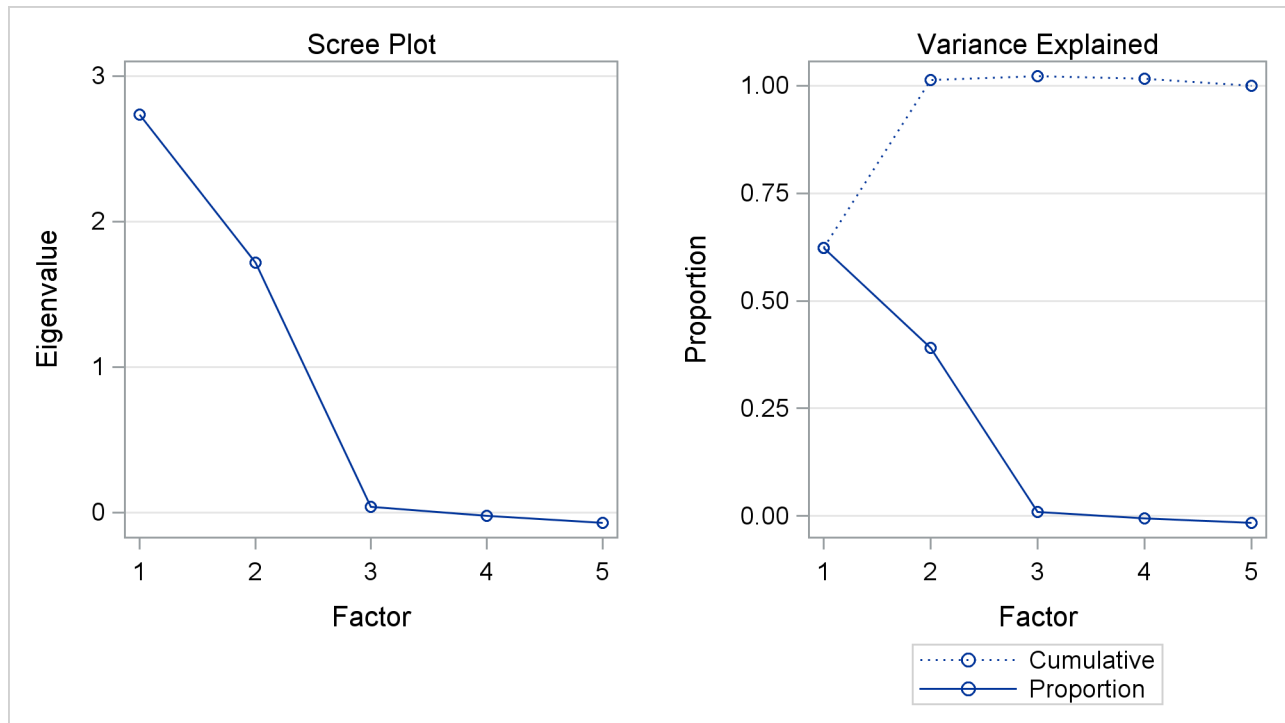
Output 35.2.2 *continued*

Eigenvalues of the Reduced Correlation Matrix:				
Total = 4.39280116 Average = 0.87856023				
	Eigenvalue	Difference	Proportion	Cumulative
1	2.73430084	1.01823217	0.6225	0.6225
2	1.71606867	1.67650586	0.3907	1.0131
3	0.03956281	0.06408626	0.0090	1.0221
4	-.02452345	0.04808427	-0.0056	1.0165
5	-.07260772		-0.0165	1.0000

The square multiple correlations are shown as prior communality estimates in [Output 35.2.2](#). The **PRIORS=SMC** option basically replaces the diagonal of the original observed correlation matrix by these square multiple correlations. Because the square multiple correlations are usually less than one, the resulting correlation matrix for factoring is called the reduced correlation matrix. In the current example, the SMCs are all fairly large; hence, you expect the results of the principal factor analysis to be similar to those in the principal component analysis.

The first two largest positive eigenvalues of the reduced correlation matrix account for 101.31% of the common variance. This is possible because the reduced correlation matrix, in general, is not necessarily positive definite, and negative eigenvalues for the matrix are possible. A pattern like this suggests that you might not need more than two common factors. The scree and variance explained plots of [Output 35.2.3](#) clearly support the conclusion that two common factors are present. Showing in the left panel of [Output 35.2.3](#) is the scree plot of the eigenvalues of the reduced correlation matrix. A sharp bend occurs at the third eigenvalue, reinforcing the conclusion that two common factors are present. These cumulative proportions of common variance explained by factors are plotted in the right panel of [Output 35.2.3](#), which shows that the curve essentially flattens out after the second factor.

Output 35.2.3 Scree and Variance Explained Plots



Principal Factor Analysis: Initial Factor Solution

For the current analysis, PROC FACTOR retains two factors by certain default criteria. This decision agrees with the conclusion drawn by inspecting the scree plot. The principal factor pattern with the two factors is displayed in Output 35.2.4. This factor pattern is similar to the principal component pattern seen in Output 35.1.5 of Example 35.1. For example, the variable Services has the largest loading on the first factor, and the Population variable has the smallest. The variables Population and Employment have large positive loadings on the second factor, and the HouseValue and School variables have large negative loadings.

Output 35.2.4 Initial Factor Pattern Matrix and Communalities

Factor Pattern		
	Factor1	Factor2
Services	0.87899	-0.15847
HouseValue	0.74215	-0.57806
Employment	0.71447	0.67936
School	0.71370	-0.55515
Population	0.62533	0.76621
Variance Explained by Each Factor		
	Factor1	Factor2
	2.7343008	1.7160687

Output 35.2.4 *continued*

Final Communality Estimates: Total = 4.450370				
Population	School	Employment	Services	HouseValue
0.97811334	0.81756387	0.97199928	0.79774304	0.88494998

Comparing the current factor loading matrix in [Output 35.2.4](#) with that in [Output 35.1.5](#) in [Example 35.1](#), you notice that the variables are arranged differently in the two output tables. This is due to the use of the **REORDER** option in the current analysis. The advantage of using this option might not be very obvious in [Output 35.2.4](#), but you can see its value when looking at the rotated solutions, as shown in [Output 35.2.7](#) and [Output 35.2.11](#).

The final communality estimates are all fairly close to the priors (shown in [Output 35.2.2](#)). Only the communality for the variable `HouseValue` increased appreciably, from 0.847 to 0.885. Therefore, you are sure that all the common variance is accounted for.

[Output 35.2.5](#) shows that the residual correlations (off-diagonal elements) are low, the largest being 0.03. The partial correlations are not quite as impressive, since the uniqueness values are also rather small. These results indicate that the squared multiple correlations are good but not quite optimal communality estimates.

Output 35.2.5 Residual and Partial Correlations

Residual Correlations With Uniqueness on the Diagonal					
	Population	School	Employment	Services	HouseValue
Population	0.02189	-0.01118	0.00514	0.01063	0.00124
School	-0.01118	0.18244	0.02151	-0.02390	0.01248
Employment	0.00514	0.02151	0.02800	-0.00565	-0.01561
Services	0.01063	-0.02390	-0.00565	0.20226	0.03370
HouseValue	0.00124	0.01248	-0.01561	0.03370	0.11505

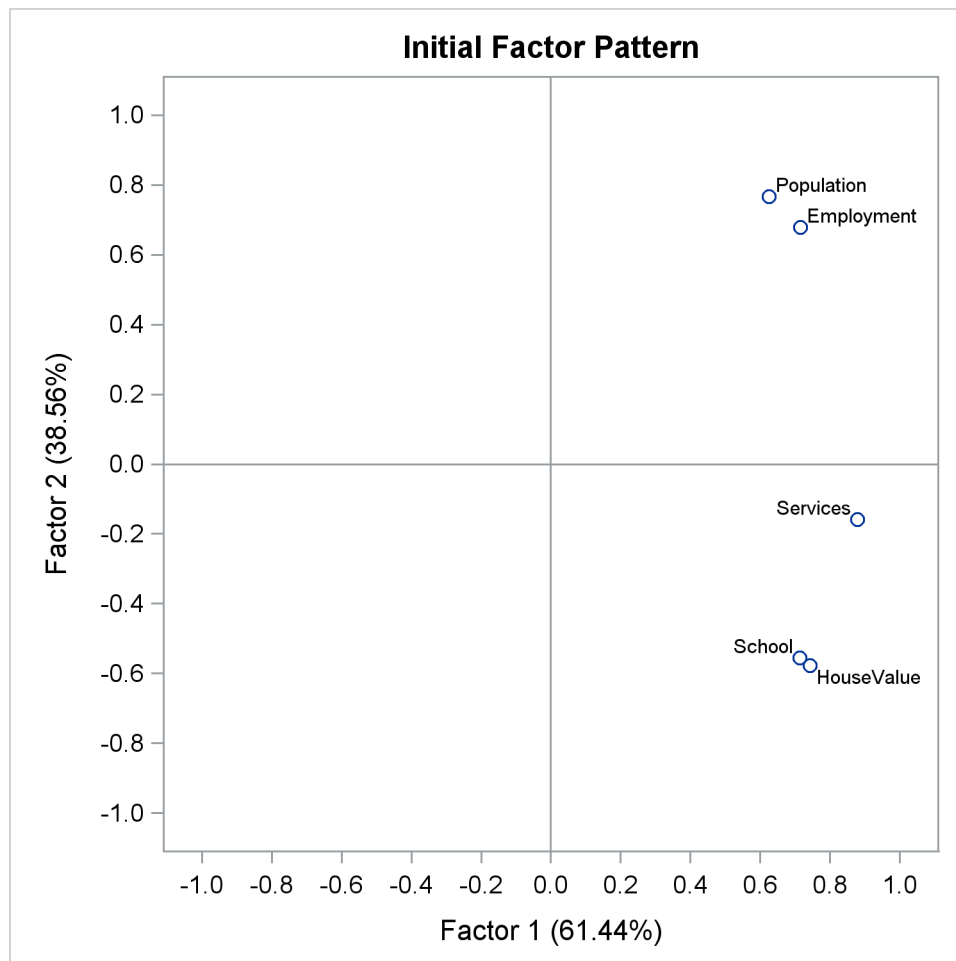
Root Mean Square Off-Diagonal Residuals: Overall = 0.01693282					
	Population	School	Employment	Services	HouseValue
	0.00815307	0.01813027	0.01382764	0.02151737	0.01960158

Partial Correlations Controlling Factors					
	Population	School	Employment	Services	HouseValue
Population	1.00000	-0.17693	0.20752	0.15975	0.02471
School	-0.17693	1.00000	0.30097	-0.12443	0.08614
Employment	0.20752	0.30097	1.00000	-0.07504	-0.27509
Services	0.15975	-0.12443	-0.07504	1.00000	0.22093
HouseValue	0.02471	0.08614	-0.27509	0.22093	1.00000

Output 35.2.5 *continued*

Root Mean Square Off-Diagonal Partial: Overall = 0.18550132				
Population	School	Employment	Services	HouseValue
0.15850824	0.19025867	0.23181838	0.15447043	0.18201538

As displayed in [Output 35.2.6](#), the unrotated factor pattern reveals two tight clusters of variables, with the variables HouseValue and School at the negative end of Factor2 axis and the variables Employment and Population at the positive end. The Services variable is in between but closer to the HouseValue and School variables. A good rotation would place the axes so that most variables would have zero loadings on most factors. As a result, the axes would appear as though they are put through the variable clusters.

Output 35.2.6 Unrotated Factor Loading Plot

Principal Factor Analysis: Varimax Prerotation

In Output 35.2.7, the results of the varimax prerotation are shown. To yield the varimax-rotated factor loading (pattern), the initial factor loading matrix is postmultiplied by an orthogonal transformation matrix. This orthogonal transformation matrix is shown in Output 35.2.7, followed by the varimax-rotated factor pattern. This rotation or transformation leads to small loadings of Population and Employment on the first factor and small loadings of HouseValue and School on the second factor. Services appears to have a larger loading on the first factor than it has on the second factor, although both loadings are substantial. Hence, Services appears to be factorially complex.

With the REORDER option in effect, you can see the variable clusters clearly in the factor pattern. The first factor is associated more with the first three variables (first three rows of variables): HouseValue, School, and Services. The second factor is associated more with the last two variables (last two rows of variables): Population and Employment.

For orthogonal factor solutions such as the current varimax-rotated solution, you can also interpret the values in the factor loading (pattern) matrix as correlations. For example, HouseValue and Factor 1 have a high correlation at 0.94, while Population and Factor 1 have a low correlation at 0.02.

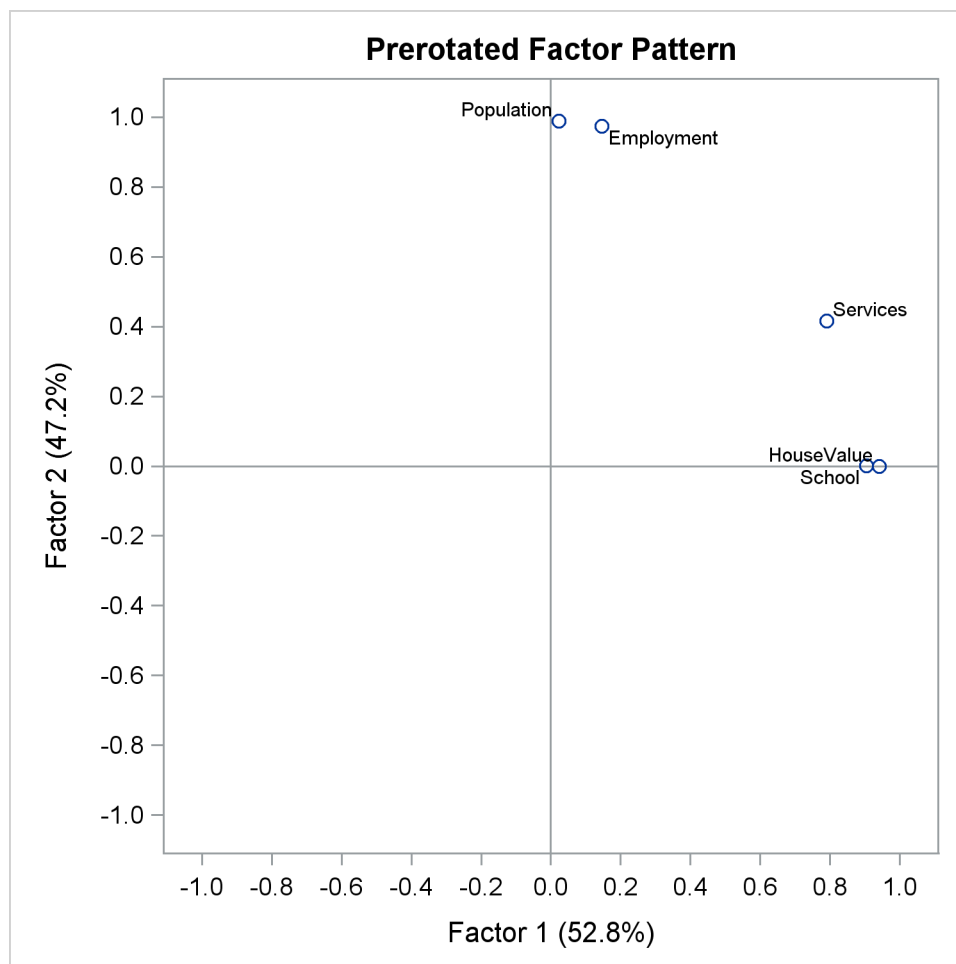
Output 35.2.7 Varimax Rotation: Transform Matrix and Rotated Pattern

Orthogonal Transformation Matrix				
	1	2		
1	0.78895	0.61446		
2	-0.61446	0.78895		
Rotated Factor Pattern				
	Factor1	Factor2		
HouseValue	0.94072	-0.00004		
School	0.90419	0.00055		
Services	0.79085	0.41509		
Population	0.02255	0.98874		
Employment	0.14625	0.97499		
Variance Explained by Each Factor				
	Factor1	Factor2		
	2.3498567	2.1005128		
Final Communality Estimates: Total = 4.450370				
Population	School	Employment	Services	HouseValue
0.97811334	0.81756387	0.97199928	0.79774304	0.88494998

The variance explained by the factors are more evenly distributed in the varimax-rotated solution, as compared with that of the unrotated solution. Indeed, this is a typical fact for any kinds of factor rotation. In the current example, before the varimax rotation the two factors explain 2.73 and 1.72, respectively, of the common variance (see [Output 35.2.4](#)). After the varimax rotation the two rotated factors explain 2.35 and 2.10, respectively, of the common variance. However, the total variance accounted for by the factors remains unchanged after the varimax rotation. This invariance property is also observed for the communalities of the variables after the rotation, as evidenced by comparing the current communality estimates in [Output 35.2.7](#) with those in [Output 35.2.4](#).

[Output 35.2.8](#) shows the graphical plot of the varimax-rotated factor loadings. Clearly, HouseValue and School cluster together on the Factor 1 axis, while Population and Employment cluster together on the Factor 2 axis. Service is closer to the cluster of HouseValue and School.

Output 35.2.8 Varimax-Rotated Factor Loadings

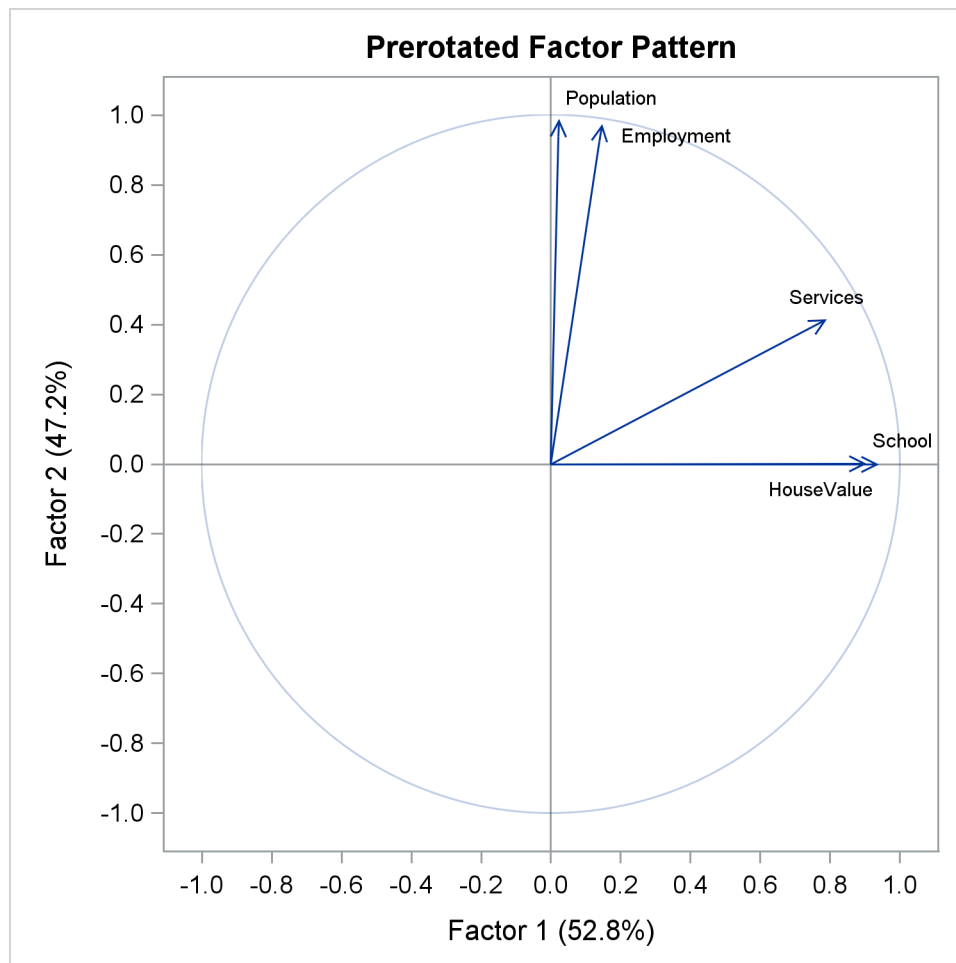


An alternative to the scatter plot of factor loadings is the so-called vector plot of loadings, which is shown in [Output 35.2.9](#). The vector plot is requested with the suboption VECTOR in the `PLOTS=` option. That is:

```
plots=preloadings(vector)
```

This generates the vector plot of loadings in [Output 35.2.9](#).

Output 35.2.9 Varimax-Rotated Factor Loadings: Vector Plot



Principal Factor Analysis: Oblique Promax Rotation

For some researchers, the varimax-rotated factor solution in the preceding section might be good enough to provide them useful and interpretable results. For others who believe that common factors are seldom orthogonal, an obliquely rotated factor solution might be more desirable, or at least should be attempted.

PROC FACTOR provides a very large class of oblique factor rotations. The current example shows a particular one—namely, the promax rotation as requested by the `ROTATE=PROMAX` option.

The results of the promax rotation are shown in [Output 35.2.10](#) and [Output 35.2.11](#). The corresponding plot of factor loadings is shown in [Output 35.2.12](#).

Output 35.2.10 Promax Rotation: Procrustean Target and Transformation

Target Matrix for Procrustean Transformation		
	Factor1	Factor2
HouseValue	1.00000	-0.00000
School	1.00000	0.00000
Services	0.69421	0.10045
Population	0.00001	1.00000
Employment	0.00326	0.96793

Procrustean Transformation Matrix		
	1	2
1	1.04116598	-0.0986534
2	-0.1057226	0.96303019

Normalized Oblique Transformation Matrix		
	1	2
1	0.73803	0.54202
2	-0.70555	0.86528

Output 35.2.10 shows the Procrustean target, to which the varimax factor pattern is rotated, followed by the display of the Procrustean transformation matrix. This is the matrix that transforms the varimax factor pattern so that the rotated pattern is as close as possible to the Procrustean target. However, because the variances of factors have to be fixed at 1 during the oblique transformation, a normalized version of the Procrustean transformation matrix is the one that is actually used in the transformation. This normalized transformation matrix is shown at the bottom of Output 35.2.10. Using this transformation matrix leads to the promax-rotated factor solution, as shown in Output 35.2.11.

Output 35.2.11 Promax Rotation: Factor Correlations and Factor Pattern

Inter-Factor Correlations		
	Factor1	Factor2
Factor1	1.00000	0.20188
Factor2	0.20188	1.00000

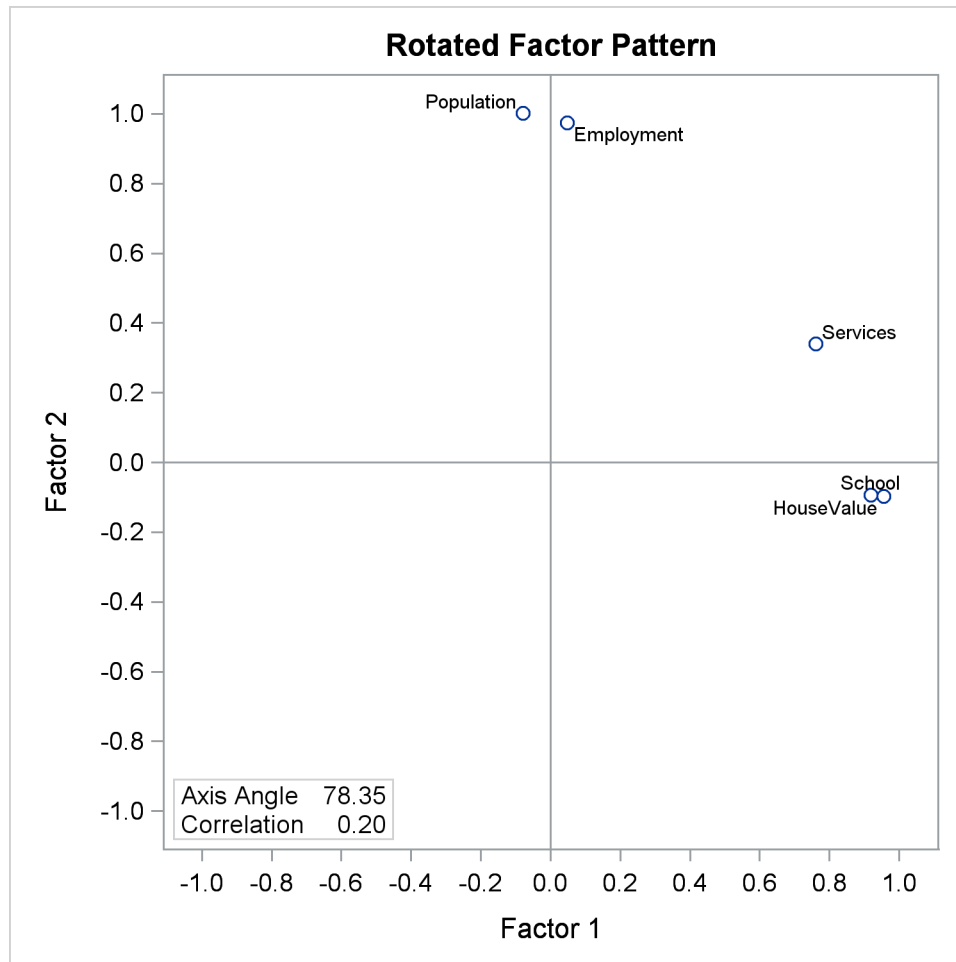
Output 35.2.11 *continued*

Rotated Factor Pattern (Standardized Regression Coefficients)		
	Factor1	Factor2
HouseValue	0.95558485	-0.0979201
School	0.91842142	-0.0935214
Services	0.76053238	0.33931804
Population	-0.0790832	1.00192402
Employment	0.04799	0.97509085

After the promax rotation, the factors are no longer uncorrelated. As shown in [Output 35.2.11](#), the correlation of the two factors is now 0.20. In the (initial) unrotated and the varimax solutions, the two factors are not correlated.

In addition to allowing the factors to be correlated, in an oblique factor solution you seek a pattern of factor loadings that is more “differentiated” (referred to as the “simple structures” in the literature). The more differentiated the loadings, the easier the interpretation of the factors.

For example, factor loadings of Services and Population on Factor 2 are 0.415 and 0.989, respectively, in the (orthogonal) varimax-rotated factor pattern (see [Output 35.2.7](#)). With the (oblique) promax rotation (see [Output 35.2.11](#)), these two loadings become even more differentiated with values 0.339 and 1.002, respectively. Overall, however, the factor patterns before and after the promax rotation do not seem to differ too much. This fact is confirmed by comparing the graphical plots of factor loadings. The plots in [Output 35.2.12](#) (promax-rotated factor loadings) and [Output 35.2.8](#) (varimax-rotated factor loadings) show very similar patterns.

Output 35.2.12 Promax Rotation: Factor Loading Plot

Unlike the orthogonal factor solutions where you can interpret the factor loadings as correlations between variables and factors, in oblique factor solutions such as the promax solution, you have to turn to the factor structure matrix for examining the correlations between variables and factors. [Output 35.2.13](#) shows the factor structures of the promax-rotated solution.

Output 35.2.13 Promax Rotation: Factor Structures and Final Communalities

Factor Structure (Correlations)		
	Factor1	Factor2
HouseValue	0.93582	0.09500
School	0.89954	0.09189
Services	0.82903	0.49286
Population	0.12319	0.98596
Employment	0.24484	0.98478

Output 35.2.13 *continued*

Variance Explained by Each Factor Ignoring Other Factors				
	Factor1	Factor2		
	2.4473495	2.2022803		
Final Communality Estimates: Total = 4.450370				
Population	School	Employment	Services	HouseValue
0.97811334	0.81756387	0.97199928	0.79774304	0.88494998

Basically, the factor structure matrix shown in [Output 35.2.13](#) reflects a similar pattern to the factor pattern matrix shown in [Output 35.2.11](#). The critical difference is that you can have the correlation interpretation only by using the factor structure matrix. For example, in the factor structure matrix shown in [Output 35.2.13](#), the correlation between Population and Factor 2 is 0.986. The corresponding value shown in the factor pattern matrix in [Output 35.2.11](#) is 1.002, which certainly cannot be interpreted as a correlation coefficient.

Common variance explained by the promax-rotated factors are 2.447 and 2.202, respectively, for the two factors. Unlike the orthogonal factor solutions (for example, the prerotated varimax solution), variance explained by these promax-rotated factors do not sum up to the total communality estimate 4.45. In oblique factor solutions, variance explained by oblique factors cannot be partitioned for the factors. Variance explained by a common factor is computed while ignoring the contributions from the other factors.

However, the communalities for the variables, as shown in the bottom of [Output 35.2.13](#), do not change from rotation to rotation. They are still the same set of communalities in the initial, varimax-rotated, and promax-rotated solutions. This is a basic fact about factor rotations: they only redistribute the variance explained by the factors; the total variance explained by the factors for any variable (that is, the communality of the variable) remains unchanged.

In the literature of exploratory factor analysis, reference axes had been an important tool in factor rotation. Nowadays, rotations are seldom done through the uses of the reference axes. Despite that, results about reference axes do provide additional information for interpreting factor analysis results. For the current example of the promax rotation, PROC FACTOR shows the relevant results about the reference axes in [Output 35.2.14](#).

Output 35.2.14 Promax Rotation: Reference Axis Correlations and Reference Structures

Reference Axis Correlations		
	Factor1	Factor2
Factor1	1.00000	-0.20188
Factor2	-0.20188	1.00000

Output 35.2.14 *continued*

Reference Structure (Semipartial Correlations)		
	Factor1	Factor2
HouseValue	0.93591	-0.09590
School	0.89951	-0.09160
Services	0.74487	0.33233
Population	-0.07745	0.98129
Employment	0.04700	0.95501

Variance Explained by Each Factor Eliminating Other Factors		
	Factor1	Factor2
	2.2480892	2.0030200

To explain the results in the reference-axis system, some geometric interpretations of the factor axes are needed. Consider a single factor in a system of n common factors in an oblique factor solution. Taking away the factor under consideration, the remaining $n - 1$ factors span a hyperplane in the factor space of $n - 1$ dimensions. The vector that is orthogonal to this hyperplane is the reference axis (reference vector) of the factor under consideration. Using the same definition for the remaining factors, you have n reference vectors for n factors.

A factor in an oblique factor solution can be considered as the sum of two independent components: its associated reference vector and a component that is overlapped with all other factors. In other words, the reference vector of a factor is a unique part of the factor that is not predictable from all other factors. Thus, the loadings on a reference vector are the unique effects of the corresponding factor, partialling out the effects from all other factors. The variances explained by a reference vector are the unique variances explained by the corresponding factor, partialling out the variances explained by all other factors.

Output 35.2.14 shows the reference axis correlations. The correlation between the reference vectors is -0.20 . Next, Output 35.2.14 shows the loadings on the reference vectors in the table entitled “Reference Structure (Semipartial Correlations).” As explained previously, loadings on a reference vector are also the unique effects of the corresponding factor, partialling out the effects from the all other factors. For example, the unique effect of Factor 1 on HouseValue is 0.936. Another important property of the reference vector system is that loadings on a reference vector are also correlations between the variables and the corresponding factor, partialling out the correlations between the variables and other factors. This means that the loading 0.936 in the reference structure table is the unique correlation between HouseValue and Factor 1, partialling out the correlation between HouseValue with Factor 2. Hence, as suggested by the title of table, all loadings reported in the “Reference Structure (Semipartial Correlations)” can be interpreted as semipartial correlations between variables and factors.

The last table shown in [Output 35.2.14](#) are the variances explained by the reference vectors. As explained previously, these are also unique variances explained by the factors, partialling out the variances explained by all other factors (or eliminating all other factors, as suggested by the title of the table). In the current example, Factor 1 explains 2.248 of the variable variances, partialling out all variable variances explained by Factor 2.

Notice that factor pattern (shown in [Output 35.2.11](#)), factor structures (correlations, shown in [Output 35.2.13](#)), and reference structures (semipartial correlations, shown in [Output 35.2.14](#)) give you different information about the oblique factor solutions such as the promax-rotated solution. However, for orthogonal factor solutions such as the varimax-rotated solution, factor structures and reference structures are all the same as the factor pattern.

Principal Factor Analysis: Factor Rotations with Factor Pattern Input

The promax rotation is one of the many rotations that PROC FACTOR provides. You can specify many different rotation algorithms by using the `ROTATE=` options. In this section, you explore different rotated factor solutions from the initial principal factor solution. Specifically, you want to examine the factor patterns yielded by the quartimax transformation (an orthogonal transformation) and the Harris-Kaiser (an oblique transformation), respectively.

Rather than analyzing the entire problem again with new rotations, you can simply use the `OUTSTAT=` data set from the preceding factor analysis results.

First, the `OUTSTAT=` data set is printed using the following statements:

```
proc print data=fact_all;
run;
```

The output data set is displayed in [Output 35.2.15](#).

Output 35.2.15 Output Data Set

Factor Output Data Set							
Obs	_TYPE_	_NAME_	Population	School	Employment	Services	House Value
1	MEAN		6241.67	11.4417	2333.33	120.833	17000.00
2	STD		3439.99	1.7865	1241.21	114.928	6367.53
3	N		12.00	12.0000	12.00	12.000	12.00
4	CORR	Population	1.00	0.0098	0.97	0.439	0.02
5	CORR	School	0.01	1.0000	0.15	0.691	0.86
6	CORR	Employment	0.97	0.1543	1.00	0.515	0.12
7	CORR	Services	0.44	0.6914	0.51	1.000	0.78
8	CORR	HouseValue	0.02	0.8631	0.12	0.778	1.00
9	COMMUNAL		0.98	0.8176	0.97	0.798	0.88
10	PRIORS		0.97	0.8223	0.97	0.786	0.85
11	EIGENVAL		2.73	1.7161	0.04	-0.025	-0.07
12	UNROTATE	Factor1	0.63	0.7137	0.71	0.879	0.74
13	UNROTATE	Factor2	0.77	-0.5552	0.68	-0.158	-0.58
14	RESIDUAL	Population	0.02	-0.0112	0.01	0.011	0.00
15	RESIDUAL	School	-0.01	0.1824	0.02	-0.024	0.01
16	RESIDUAL	Employment	0.01	0.0215	0.03	-0.006	-0.02
17	RESIDUAL	Services	0.01	-0.0239	-0.01	0.202	0.03
18	RESIDUAL	HouseValue	0.00	0.0125	-0.02	0.034	0.12
19	PRETRANS	Factor1	0.79	-0.6145	.	.	.
20	PRETRANS	Factor2	0.61	0.7889	.	.	.
21	PREROTAT	Factor1	0.02	0.9042	0.15	0.791	0.94
22	PREROTAT	Factor2	0.99	0.0006	0.97	0.415	-0.00
23	TRANSFOR	Factor1	0.74	-0.7055	.	.	.
24	TRANSFOR	Factor2	0.54	0.8653	.	.	.
25	FCORR	Factor1	1.00	0.2019	.	.	.
26	FCORR	Factor2	0.20	1.0000	.	.	.
27	PATTERN	Factor1	-0.08	0.9184	0.05	0.761	0.96
28	PATTERN	Factor2	1.00	-0.0935	0.98	0.339	-0.10
29	RCORR	Factor1	1.00	-0.2019	.	.	.
30	RCORR	Factor2	-0.20	1.0000	.	.	.
31	REFERENC	Factor1	-0.08	0.8995	0.05	0.745	0.94
32	REFERENC	Factor2	0.98	-0.0916	0.96	0.332	-0.10
33	STRUCTUR	Factor1	0.12	0.8995	0.24	0.829	0.94
34	STRUCTUR	Factor2	0.99	0.0919	0.98	0.493	0.09

Various results from the previous factor analysis are saved in this data set, including the initial unrotated solution (its factor pattern is saved in observations with `_TYPE_=UNROTATE`), the prerotated varimax solution (its factor pattern is saved in observations with `_TYPE_=PREROTAT`), and the oblique promax solution (its factor pattern is saved in observations with `_TYPE_=PATTERN`).

When PROC FACTOR reads in an input data set with `TYPE=FACTOR`, the observations with `_TYPE_=PATTERN` are treated as the initial factor pattern to be rotated by PROC FACTOR. Hence, it is important that you provide the correct initial factor pattern for PROC FACTOR to read in.

In the current example, you need to provide the unrotated solution from the preceding analysis as the input factor pattern. The following statements create a TYPE=FACTOR data set fact2 from the preceding OUTSTAT= data set fact_all:

```
data fact2(type=factor);
  set fact_all;
  if _TYPE_ in('PATTERN' 'FCORR') then delete;
  if _TYPE_='UNROTATE' then _TYPE_='PATTERN';
run;
```

In these statements, you delete observations with _TYPE_=PATTERN or _TYPE_=FCORR, which are for the promax-rotated factor solution, and change observations with _TYPE_=UNROTATE to _TYPE_=PATTERN in the new data set fact2. In this way, the initial orthogonal factor pattern matrix is saved in the observations with _TYPE_=PATTERN.

You use this new data set and rotate the initial solution to another oblique solution with the ROTATE=QUARTIMAX option, as shown in the following statements:

```
proc factor data=fact2 rotate=quartimax reorder;
run;
```

As shown in [Output 35.2.16](#), the input data set is of the FACTOR type for the new rotation.

Output 35.2.16 Quartimax Rotation With Input Factor Pattern

Quartimax Rotation From a TYPE=FACTOR Data Set	
The FACTOR Procedure	
Input Data Type	FACTOR
N Set/Assumed in Data Set	12
N for Significance Tests	12

The quartimax-rotated factor pattern is displayed in [Output 35.2.17](#).

Output 35.2.17 Quartimax-Rotated Factor Pattern

Orthogonal Transformation Matrix		
	1	2
1	0.80138	0.59815
2	-0.59815	0.80138

Output 35.2.17 *continued*

Rotated Factor Pattern		
	Factor1	Factor2
HouseValue	0.94052	-0.01933
School	0.90401	-0.01799
Services	0.79920	0.39878
Population	0.04282	0.98807
Employment	0.16621	0.97179

Variance Explained by Each Factor	
Factor1	Factor2
2.3699941	2.0803754

The quartimax rotation produces an orthogonal transformation matrix shown at the top of [Output 35.2.17](#). After the transformation, the factor pattern is shown next. Compared with the varimax-rotated factor pattern (see [Output 35.2.7](#)), the quartimax-rotated factor pattern shows some differences. The loadings of HouseValue and School on Factor 1 drop only slightly in the quartimax factor pattern, while the loadings of Services, Population, and Employment on Factor 1 gain relatively larger amounts. The total variance explained by Factor 1 in the varimax-rotated solution (see [Output 35.2.7](#)) is 2.350, while it is 2.370 after the quartimax-rotation. In other words, more variable variances are explained by the first factor in the quartimax factor pattern than in the varimax factor pattern. Although not very strongly demonstrated in the current example, this illustrates a well-known property about the quartimax rotation: it tends to produce a general factor for all variables.

Another oblique rotation is now explored. The Harris-Kaiser transformation weighted by the Cureton-Mulaik technique is applied to the initial factor pattern. To achieve this, you use the `ROTATE=HK` and `NORM=WEIGHT` options in the following PROC FACTOR statement:

```
ods graphics on;

proc factor data=fact2 rotate=hk norm=weight reorder
  plots=loadings;
run;

ods graphics off;
```

[Output 35.2.18](#) shows the variable weights in the rotation.

Output 35.2.18 Harris-Kaiser Rotation: Weights

Variable Weights for Rotation				
Population	School	Employment	Services	HouseValue
0.95982747	0.93945424	0.99746396	0.12194766	0.94007263

While all other variables have weights at least as large as 0.93, the weight for *Services* is only 0.12. This means that due to its small weight, *Services* is not as important as the other variables for determining the rotation (transformation). This makes sense when you look at the initial unrotated factor pattern plot in [Output 35.2.6](#). In the plot, there are two main clusters of variables, and *Services* does not seem to fall into either of the clusters. In order to yield a Harris-Kaiser rotation (transformation) that would gear towards two clusters, the Cureton-Mulaik weighting essentially downweights the contribution from *Services* in the factor rotation.

The results of the Harris-Kaiser factor solution are displayed in [Output 35.2.19](#), with a graphical plot of rotated loadings displayed in [Output 35.2.20](#).

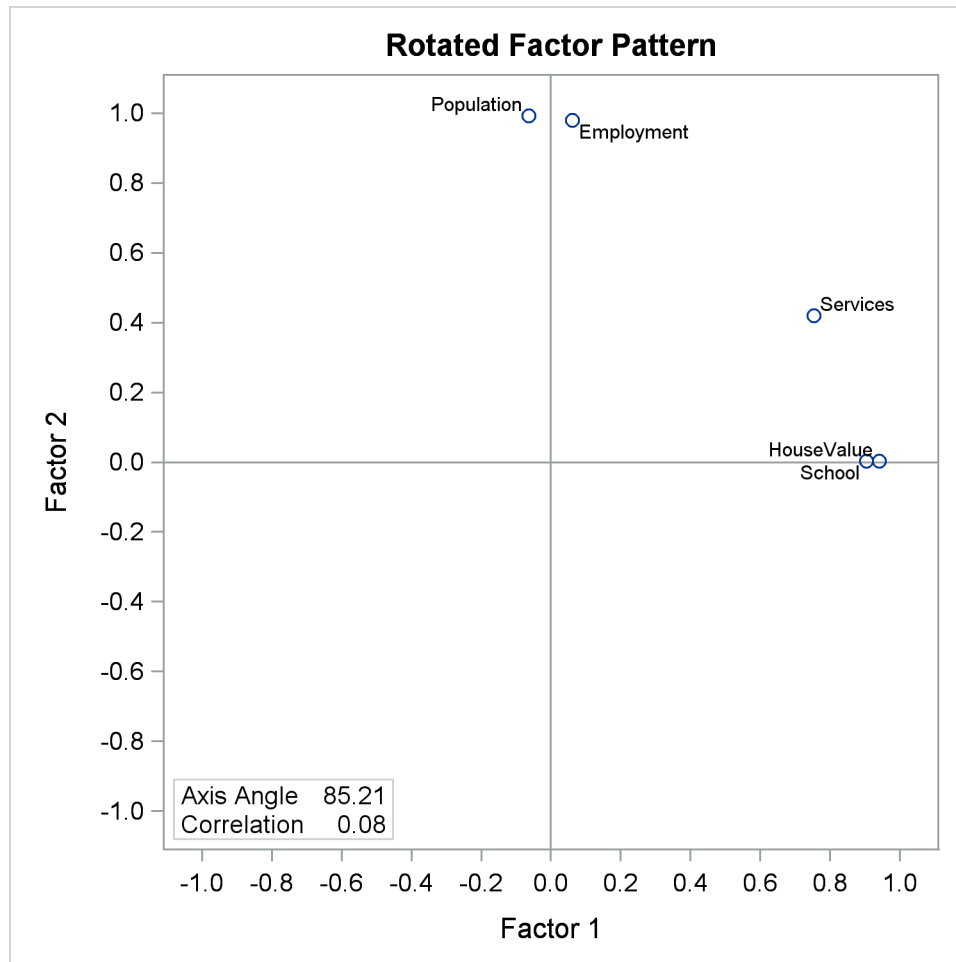
Output 35.2.19 Harris-Kaiser Rotation: Factor Correlations and Factor Pattern

Inter-Factor Correlations		
	Factor1	Factor2
Factor1	1.00000	0.08358
Factor2	0.08358	1.00000
Rotated Factor Pattern (Standardized Regression Coefficients)		
	Factor1	Factor2
HouseValue	0.94048	0.00279
School	0.90391	0.00327
Services	0.75459	0.41892
Population	-0.06335	0.99227
Employment	0.06152	0.97885

Because the Harris-Kaiser produces an oblique factor solution, you compare the current results with that of the promax (see [Output 35.2.11](#)), which also produces an oblique factor solution. The correlation between the factors in the Harris-Kaiser solution is 0.084; this value is much smaller than the same correlation in the promax solution, which is 0.201. However, the Harris-Kaiser rotated factor pattern shown in [Output 35.2.19](#) is more or less the same as that of the promax-rotated factor pattern shown in [Output 35.2.11](#). Which solution would you consider to be more reasonable or interpretable?

From the statistical point of view, the Harris-Kaiser and promax factor solutions are equivalent. They explain the observed variable relationships equally well. From the simplicity point of view, however, you might prefer to interpret the Harris-Kaiser solution because the factor correlation is smaller. In other words, the factors in the Harris-Kaiser solution do not overlap that much conceptually; hence they should be more distinctive to interpret. However, in practice simplicity in factor correlations might not be the only principle to consider. Researchers might actually expect to have some factors to be highly correlated based on theoretical or substantive grounds.

Although the Harris-Kaiser and the promax factor patterns are very similar, the graphical plots of the loadings from the two solutions paint slightly different pictures. The plot of the promax-rotated loadings is shown in [Output 35.2.12](#), while the plot of the loadings for the current Harris-Kaiser solution is shown in [Output 35.2.20](#).

Output 35.2.20 Harris-Kaiser Rotation: Factor Loading Plot

The two factor axes in the Harris-Kaiser rotated pattern ([Output 35.2.20](#)) clearly cut through the centers of the two variable clusters, while the Factor 1 axis in the promax solution lies above a variable cluster ([Output 35.2.12](#)). The reason for this subtle difference is that in the Harris-Kaiser rotation, the Services is a “loner” that has been downweighted by the Cureton-Mulaik technique (see its relatively small weight in [Output 35.2.18](#)). As a result, the rotated axes are basically determined by the two variable clusters in the Harris-Kaiser rotation.

As far as the current discussion goes, it is not recommending one rotation method over another. Rather, it simply illustrates how you could control certain types of characteristics of factor rotation through the many options supported by PROC FACTOR. Should you prefer an orthogonal rotation to an oblique rotation? Should you choose the oblique factor solution with the smallest factor correlations? Should you use a weighting scheme that would enable you to find independent variable clusters? While PROC FACTOR enables you to explore all these alternatives, you must consult advanced textbooks and published articles to get satisfactory and complete answers to these questions.

Example 35.3: Maximum Likelihood Factor Analysis

This example uses maximum likelihood factor analyses for one, two, and three factors. It is already apparent from the principal factor analysis that the best number of common factors is almost certainly two. The one- and three-factor ML solutions reinforce this conclusion and illustrate some of the numerical problems that can occur. The following statements produce [Output 35.3.1](#) through [Output 35.3.3](#):

```

title3 'Maximum Likelihood Factor Analysis with One Factor';
proc factor data=SocioEconomics method=ml heywood n=1;
run;

title3 'Maximum Likelihood Factor Analysis with Two Factors';
proc factor data=SocioEconomics method=ml heywood n=2;
run;

title3 'Maximum Likelihood Factor Analysis with Three Factors';
proc factor data=SocioEconomics method=ml heywood n=3;
run;

```

[Output 35.3.1](#) displays the results of the analysis with one factor.

Output 35.3.1 Maximum Likelihood Factor Analysis

Maximum Likelihood Factor Analysis with One Factor				
The FACTOR Procedure				
Input Data Type		Raw Data		
Number of Records Read		12		
Number of Records Used		12		
N for Significance Tests		12		
Maximum Likelihood Factor Analysis with One Factor				
The FACTOR Procedure				
Initial Factor Method: Maximum Likelihood				
Prior Communality Estimates: SMC				
Population	School	Employment	Services	HouseValue
0.96859160	0.82228514	0.96918082	0.78572440	0.84701921

Output 35.3.1 *continued*

Preliminary Eigenvalues: Total = 76.1165859 Average = 15.2233172

	Eigenvalue	Difference	Proportion	Cumulative
1	63.7010086	50.6462895	0.8369	0.8369
2	13.0547191	12.7270798	0.1715	1.0084
3	0.3276393	0.6749199	0.0043	1.0127
4	-0.3472805	0.2722202	-0.0046	1.0081
5	-0.6195007		-0.0081	1.0000

1 factor will be retained by the NFACTOR criterion.

Iteration	Criterion	Ridge	Change	Communalities			
1	6.5429218	0.0000	0.1033	0.93828	0.72227	1.00000	0.71940
				0.74371			
2	3.1232699	0.0000	0.7288	0.94566	0.02380	1.00000	0.26493
				0.01487			

Convergence criterion satisfied.

Significance Tests Based on 12 Observations

Test	DF	Chi-Square	Pr > ChiSq
H0: No common factors	10	54.2517	<.0001
HA: At least one common factor			
H0: 1 Factor is sufficient	5	24.4656	0.0002
HA: More factors are needed			

Chi-Square without Bartlett's Correction	34.355969
Akaike's Information Criterion	24.355969
Schwarz's Bayesian Criterion	21.931436
Tucker and Lewis's Reliability Coefficient	0.120231

Squared Canonical Correlations

Factor1

1.0000000

Output 35.3.1 *continued*

Eigenvalues of the Weighted Reduced Correlation Matrix: Total = 0 Average = 0		
	Eigenvalue	Difference
1	Infty	Infty
2	1.92716032	2.15547340
3	-.22831308	0.56464322
4	-.79295630	0.11293464
5	-.90589094	

Factor Pattern	
	Factor1
Population	0.97245
School	0.15428
Employment	1.00000
Services	0.51472
HouseValue	0.12193

Variance Explained by Each Factor		
Factor	Weighted	Unweighted
Factor1	17.8010629	2.24926004

Final Community Estimates and Variable Weights		
Total Community: Weighted = 17.801063 Unweighted = 2.249260		
Variable	Community	Weight
Population	0.94565561	18.4011648
School	0.02380349	1.0243839
Employment	1.00000000	Infty
Services	0.26493499	1.3604239
HouseValue	0.01486595	1.0150903

The solution on the second iteration is so close to the optimum that PROC FACTOR cannot find a better solution; hence you receive this message:

Convergence criterion satisfied.

When this message appears, you should try rerunning PROC FACTOR with different prior communality estimates to make sure that the solution is correct. In this case, other prior estimates lead to the same solution or possibly to worse local optima, as indicated by the information criteria or the chi-square values.

The variable Employment has a communality of 1.0 and, therefore, an infinite weight that is displayed next to the final communality estimate as a missing/infinite value. The first eigenvalue is also infinite. Infinite values are ignored in computing the total of the eigenvalues and the total final communality.

Output 35.3.2 displays the results of the analysis with two factors. The analysis converges without incident. This time, however, the Population variable is a Heywood case.

Output 35.3.2 Maximum Likelihood Factor Analysis: Two Factors

Input Data Type		Raw Data					
Number of Records Read		12					
Number of Records Used		12					
N for Significance Tests		12					
Prior Communality Estimates: SMC							
Population	School	Employment	Services	HouseValue			
0.96859160	0.82228514	0.96918082	0.78572440	0.84701921			
Preliminary Eigenvalues: Total = 76.1165859 Average = 15.2233172							
	Eigenvalue	Difference	Proportion	Cumulative			
1	63.7010086	50.6462895	0.8369	0.8369			
2	13.0547191	12.7270798	0.1715	1.0084			
3	0.3276393	0.6749199	0.0043	1.0127			
4	-0.3472805	0.2722202	-0.0046	1.0081			
5	-0.6195007		-0.0081	1.0000			
2 factors will be retained by the NFACTOR criterion.							
Iteration	Criterion	Ridge	Change	Communalities			
1	0.3431221	0.0000	0.0471	1.00000	0.80672	0.95058	0.79348
				0.89412			
2	0.3072178	0.0000	0.0307	1.00000	0.80821	0.96023	0.81048
				0.92480			
3	0.3067860	0.0000	0.0063	1.00000	0.81149	0.95948	0.81677
				0.92023			
4	0.3067373	0.0000	0.0022	1.00000	0.80985	0.95963	0.81498
				0.92241			
5	0.3067321	0.0000	0.0007	1.00000	0.81019	0.95955	0.81569
				0.92187			
Convergence criterion satisfied.							

Output 35.3.2 *continued*

Significance Tests Based on 12 Observations				
Test	DF	Chi-Square	Pr > ChiSq	
H0: No common factors	10	54.2517	<.0001	
HA: At least one common factor				
H0: 2 Factors are sufficient	1	2.1982	0.1382	
HA: More factors are needed				
Chi-Square without Bartlett's Correction		3.3740530		
Akaike's Information Criterion		1.3740530		
Schwarz's Bayesian Criterion		0.8891463		
Tucker and Lewis's Reliability Coefficient		0.7292200		
Squared Canonical Correlations				
	Factor1	Factor2		
	1.0000000	0.9518891		
Eigenvalues of the Weighted Reduced Correlation Matrix: Total = 19.7853157 Average = 4.94632893				
	Eigenvalue	Difference	Proportion	Cumulative
1	Infty	Infty		
2	19.7853143	19.2421292	1.0000	1.0000
3	0.5431851	0.5829564	0.0275	1.0275
4	-0.0397713	0.4636411	-0.0020	1.0254
5	-0.5034124		-0.0254	1.0000
Factor Pattern				
		Factor1	Factor2	
	Population	1.00000	0.00000	
	School	0.00975	0.90003	
	Employment	0.97245	0.11797	
	Services	0.43887	0.78930	
	HouseValue	0.02241	0.95989	
Variance Explained by Each Factor				
Factor	Weighted	Unweighted		
Factor1	24.4329707	2.13886057		
Factor2	19.7853143	2.36835294		

Output 35.3.2 *continued*

Final Commuality Estimates and Variable Weights		
Total Commuality: Weighted = 44.218285 Unweighted = 4.507214		
Variable	Commuality	Weight
Population	1.0000000	Infty
School	0.81014489	5.2682940
Employment	0.95957142	24.7246669
Services	0.81560348	5.4256462
HouseValue	0.92189372	12.7996793

The results of the three-factor analysis are shown in [Output 35.3.3](#).

Output 35.3.3 Maximum Likelihood Factor Analysis: Three Factors

Input Data Type		Raw Data		
Number of Records Read		12		
Number of Records Used		12		
N for Significance Tests		12		
Prior Commuality Estimates: SMC				
Population	School	Employment	Services	HouseValue
0.96859160	0.82228514	0.96918082	0.78572440	0.84701921
Preliminary Eigenvalues: Total = 76.1165859 Average = 15.2233172				
	Eigenvalue	Difference	Proportion	Cumulative
1	63.7010086	50.6462895	0.8369	0.8369
2	13.0547191	12.7270798	0.1715	1.0084
3	0.3276393	0.6749199	0.0043	1.0127
4	-0.3472805	0.2722202	-0.0046	1.0081
5	-0.6195007		-0.0081	1.0000

Output 35.3.3 *continued*

3 factors will be retained by the NFACTOR criterion.

WARNING: Too many factors for a unique solution.

Iteration	Criterion	Ridge	Change	Communalities			
1	0.1798029	0.0313	0.0501	0.96081 0.89716	0.84184	1.00000	0.80175
2	0.0016405	0.0313	0.0678	0.98081 0.96500	0.88713	1.00000	0.79559
3	0.0000041	0.0313	0.0094	0.98195 0.96751	0.88603	1.00000	0.80498
4	0.0000000	0.0313	0.0006	0.98202 0.96735	0.88585	1.00000	0.80561

ERROR: Converged, but not to a proper optimum.

Try a different 'PRIORS' statement.

Significance Tests Based on 12 Observations

Test	DF	Chi-Square	Pr > ChiSq
H0: No common factors	10	54.2517	<.0001
HA: At least one common factor			
H0: 3 Factors are sufficient	-2	0.0000	.
HA: More factors are needed			

Chi-Square without Bartlett's Correction	0.0000003
Akaike's Information Criterion	4.0000003
Schwarz's Bayesian Criterion	4.9698136
Tucker and Lewis's Reliability Coefficient	0.0000000

Squared Canonical Correlations

Factor1	Factor2	Factor3
1.0000000	0.9751895	0.6894465

Output 35.3.3 *continued*

Eigenvalues of the Weighted Reduced Correlation				
Matrix: Total = 41.5254193 Average = 10.3813548				
	Eigenvalue	Difference	Proportion	Cumulative
1	Infty	Infty		
2	39.3054826	37.0854258	0.9465	0.9465
3	2.2200568	2.2199693	0.0535	1.0000
4	0.0000875	0.0002949	0.0000	1.0000
5	-0.0002075		-0.0000	1.0000

Factor Pattern			
	Factor1	Factor2	Factor3
Population	0.97245	-0.11233	-0.15409
School	0.15428	0.89108	0.26083
Employment	1.00000	0.00000	0.00000
Services	0.51472	0.72416	-0.12766
HouseValue	0.12193	0.97227	-0.08473

Variance Explained by Each Factor		
Factor	Weighted	Unweighted
Factor1	54.6115241	2.24926004
Factor2	39.3054826	2.27634375
Factor3	2.2200568	0.11525433

Final Communality Estimates and Variable Weights		
Total Communality: Weighted = 96.137063 Unweighted = 4.640858		
Variable	Communality	Weight
Population	0.98201660	55.6066901
School	0.88585165	8.7607194
Employment	1.00000000	Infty
Services	0.80564301	5.1444261
HouseValue	0.96734687	30.6251078

In the results, a warning message is displayed:

WARNING: Too many factors for a unique solution.

The number of parameters in the model exceeds the number of elements in the correlation matrix from which they can be estimated, so an infinite number of different perfect solutions can be obtained. The criterion approaches zero at an improper optimum, as indicated by this message:

Converged, but not to a proper optimum.

The degrees of freedom for the chi-square test are -2 , so a probability level cannot be computed for three factors. Note also that the variable Employment is a Heywood case again.

The probability levels for the chi-square test are 0.0001 for the hypothesis of no common factors, 0.0002 for one common factor, and 0.1382 for two common factors. Therefore, the two-factor model seems to be an adequate representation. Akaike's information criterion and Schwarz's Bayesian criterion attain their minimum values at two common factors, so there is little doubt that two factors are appropriate for these data.

Example 35.4: Using Confidence Intervals to Locate Salient Factor Loadings

This example illustrates how you can use the standard errors and confidence intervals to understand the pattern of factor loadings under the maximum likelihood estimation. There are nine tests and you want a three-factor solution ($N=3$) for a correlation matrix based on 200 observations. The following statements define the input data set and specify the desirable analysis by the FACTOR procedure:

```
data test(type=corr);
  title 'Quartimin-Rotated Factor Solution with Standard Errors';
  input _name_ $ test1-test9;
  _type_ = 'corr';
  datalines;
Test1      1  .561  .602  .290  .404  .328  .367  .179  -.268
Test2    .561  1  .743  .414  .526  .442  .523  .289  -.399
Test3    .602  .743  1  .286  .343  .361  .679  .456  -.532
Test4    .290  .414  .286  1  .677  .446  .412  .400  -.491
Test5    .404  .526  .343  .677  1  .584  .408  .299  -.466
Test6    .328  .442  .361  .446  .584  1  .333  .178  -.306
Test7    .367  .523  .679  .412  .408  .333  1  .711  -.760
Test8    .179  .289  .456  .400  .299  .178  .711  1  -.725
Test9   -.268 -.399 -.532 -.491 -.466 -.306 -.760 -.725  1
;

title2 'A nine-variable-three-factor example';
proc factor data=test method=ml reorder rotate=quartimin
  nobs=200 n=3 se cover=.45 alpha=.1;
run;
```

In the PROC FACTOR statement, you apply quartimin rotation with (default) Kaiser normalization. You define loadings with magnitudes greater than 0.45 to be salient ($COVER=0.45$) and use 90% confidence intervals ($ALPHA=0.1$) to judge the salience. The REORDER option is specified so that variables that have similar loadings with factors are clustered together.

After the quartimin rotation, the correlation matrix for factors is shown in [Output 35.4.1](#).

Output 35.4.1 Quartimin-Rotated Factor Solution with Standard Errors

Inter-Factor Correlations			
With 90% confidence limits			
Estimate/StdErr/LowerCL/UpperCL			
	Factor1	Factor2	Factor3
Factor1	1.00000	0.41283	0.38304
	0.00000	0.06267	0.06060
	.	0.30475	0.27919
	.	0.51041	0.47804
Factor2	0.41283	1.00000	0.47006
	0.06267	0.00000	0.05116
	0.30475	.	0.38177
	0.51041	.	0.54986
Factor3	0.38304	0.47006	1.00000
	0.06060	0.05116	0.00000
	0.27919	0.38177	.
	0.47804	0.54986	.

The factors are medium to highly correlated. The confidence intervals seem to be very wide, suggesting that the estimation of factor correlations might not be very accurate for this sample size. For example, the 90% confidence interval for the correlation between Factor1 and Factor2 is (0.30, 0.51), a range of 0.21. You might need a larger sample to get a narrower interval, or you might need a better estimation.

Next, coverage displays for factor loadings are shown in [Output 35.4.2](#).

Output 35.4.2 Using the Rotated Factor Pattern to Interpret the Factors

Rotated Factor Pattern (Standardized Regression Coefficients)			
With 90% confidence limits; Cover * = 0.45?			
Estimate/StdErr/LowerCL/UpperCL/Coverage Display			
	Factor1	Factor2	Factor3
test8	0.86810	-0.05045	0.00114
	0.03282	0.03185	0.03087
	0.80271	-0.10265	-0.04959
	0.91286	0.00204	0.05187
	0*[]	*[0]	[0]*
test7	0.73204	0.27296	0.01098
	0.04434	0.05292	0.03838
	0.65040	0.18390	-0.05211
	0.79697	0.35758	0.07399
	0*[]	0[]*	[0]*
test9	-0.79654	-0.01230	-0.17307
	0.03948	0.04225	0.04420
	-0.85291	-0.08163	-0.24472
	-0.72180	0.05715	-0.09955
	[]*0	*[0]	*[]0
test3	0.27715	0.91156	-0.19727
	0.05489	0.04877	0.02981
	0.18464	0.78650	-0.24577
	0.36478	0.96481	-0.14778
	0[]*	0*[]	*[]0
test2	0.01063	0.71540	0.20500
	0.05060	0.05148	0.05496
	-0.07248	0.61982	0.11310
	0.09359	0.79007	0.29342
	[0]*	0*[]	0[]*
test1	-0.07356	0.63815	0.13983
	0.04245	0.05380	0.05597
	-0.14292	0.54114	0.04682
	-0.00348	0.71839	0.23044
	[]0	0[]	0[]*
test5	0.00863	0.03234	0.91282
	0.04394	0.04387	0.04509
	-0.06356	-0.03986	0.80030
	0.08073	0.10421	0.96323
	[0]*	[0]*	0*[]
test4	0.22357	-0.07576	0.67925
	0.05956	0.03640	0.05434
	0.12366	-0.13528	0.57955
	0.31900	-0.01569	0.75891
	0[]*	*[]0	0*[]
test6	-0.04295	0.21911	0.53183
	0.05114	0.07481	0.06905
	-0.12656	0.09319	0.40893
	0.04127	0.33813	0.63578
	[0]	0[]	0[*]

The coverage displays in [Output 35.4.2](#) show that Test8, Test7, and Test9 have salient relationships with Factor1. The coverage displays are either '0*[]' or '[]*0', indicating that the entire 90% confidence intervals for the corresponding loadings are beyond the salience value at 0.45. On the other hand, the coverage display for Test3 on Factor1 is '0[]*'. This indicates that even though the loading estimate is significantly larger than zero, it is not large enough to be salient. Similarly, Test3, Test2, and Test1 have salient relationships with Factor2, while Test5 and Test4 have salient relationships with Factor3. For Test6, its relationship with Factor3 is a little bit ambiguous; the 90% confidence interval approximately covers values between 0.40 and 0.64. This means that the population value might have been smaller or larger than 0.45. It is marginal evidence for a salient relationship.

For oblique factor solutions, some researchers prefer to examine the factor structure loadings, which represent correlations, for determining salient relationships. In [Output 35.4.3](#), the factor structure loadings and the associated standard error estimates and coverage displays are shown.

Output 35.4.3 Using the Factor Structure to Interpret the Factors

Factor Structure (Correlations)			
With 90% confidence limits; Cover * = 0.45?			
Estimate/StdErr/LowerCL/UpperCL/Coverage Display			
	Factor1	Factor2	Factor3
test8	0.84771	0.30847	0.30994
	0.02871	0.06593	0.06263
	0.79324	0.19641	0.20363
	0.88872	0.41257	0.40904
	0*[]	0[]*	0[]*
test7	0.84894	0.58033	0.41970
	0.02688	0.05265	0.06060
	0.79834	0.48721	0.31523
	0.88764	0.66041	0.51412
	0*[]	0*[]	0[*]
test9	-0.86791	-0.42248	-0.48396
	0.02522	0.06187	0.05504
	-0.90381	-0.51873	-0.56921
	-0.81987	-0.31567	-0.38841
	[]*0	[*]0	[*]0
test3	0.57790	0.93325	0.33738
	0.05069	0.02953	0.06779
	0.48853	0.86340	0.22157
	0.65528	0.96799	0.44380
	0*[]	0*[]	0[]*
test2	0.38449	0.81615	0.54535
	0.06143	0.03106	0.05456
	0.27914	0.75829	0.44946
	0.48070	0.86126	0.62883
	0[*]	0*[]	0[*]
test1	0.24345	0.67351	0.41162
	0.06864	0.04284	0.05995
	0.12771	0.59680	0.30846
	0.35264	0.73802	0.50522
	0[]*	0*[]	0[*]
test5	0.37163	0.46498	0.93132
	0.06092	0.04979	0.03277
	0.26739	0.37923	0.85159
	0.46727	0.54282	0.96894
	0[*]	0[*]	0*[]
test4	0.45248	0.33583	0.72927
	0.05876	0.06289	0.04061
	0.35072	0.22867	0.65527
	0.54367	0.43494	0.78941
	0[*]	0[]*	0*[]
test6	0.25122	0.45137	0.61837
	0.07140	0.05858	0.05051
	0.13061	0.34997	0.52833
	0.36450	0.54232	0.69465
	0[]*	0[*]	0*[]

The interpretations based on the factor structure matrix do not change much from that based on the factor loadings except for Test3 and Test9. Test9 now has a salient correlation with Factor3. For Test3, it has salient correlations with both Factor1 and Factor2. Fortunately, there are still tests that have salient correlations only with either Factor1 or Factor2 (but not both). This would make interpretations of factors less problematic.

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Chapter 36

The FASTCLUS Procedure

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Overview: FASTCLUS Procedure

The FASTCLUS procedure performs a disjoint cluster analysis on the basis of distances computed from one or more quantitative variables. The observations are divided into clusters such that every observation belongs to one and only one cluster; the clusters do not form a tree structure as they do in the CLUSTER procedure. If you want separate analyses for different numbers of clusters, you can run PROC FASTCLUS once for each analysis. Alternatively, to do hierarchical clustering on a large data set, use PROC FASTCLUS to find initial clusters, and then use those initial clusters as input to PROC CLUSTER.

By default, the FASTCLUS procedure uses Euclidean distances, so the cluster centers are based on least squares estimation. This kind of clustering method is often called a *k-means model*, since the cluster centers

are the means of the observations assigned to each cluster when the algorithm is run to complete convergence. Each iteration reduces the least squares criterion until convergence is achieved.

Often there is no need to run the FASTCLUS procedure to convergence. PROC FASTCLUS is designed to find good clusters (but not necessarily the best possible clusters) with only two or three passes through the data set. The initialization method of PROC FASTCLUS guarantees that, if there exist clusters such that all distances between observations in the same cluster are less than all distances between observations in different clusters, and if you tell PROC FASTCLUS the correct number of clusters to find, it can always find such a clustering without iterating. Even with clusters that are not as well separated, PROC FASTCLUS usually finds initial seeds that are sufficiently good that few iterations are required. Hence, by default, PROC FASTCLUS performs only one iteration.

The initialization method used by the FASTCLUS procedure makes it sensitive to outliers. PROC FASTCLUS can be an effective procedure for detecting outliers because outliers often appear as clusters with only one member.

The FASTCLUS procedure can use an L_p (least p th powers) clustering criterion (Spath 1985, pp. 62–63) instead of the least squares (L_2) criterion used in k -means clustering methods. The LEAST= p option specifies the power p to be used. Using the LEAST= option increases execution time since more iterations are usually required, and the default iteration limit is increased when you specify LEAST= p . Values of p less than 2 reduce the effect of outliers on the cluster centers compared with least squares methods; values of p greater than 2 increase the effect of outliers.

The FASTCLUS procedure is intended for use with large data sets, with 100 or more observations. With small data sets, the results can be highly sensitive to the order of the observations in the data set.

PROC FASTCLUS uses algorithms that place a larger influence on variables with larger variance, so it might be necessary to standardize the variables before performing the cluster analysis. See the “Using PROC FASTCLUS” section for standardization details.

PROC FASTCLUS produces brief summaries of the clusters it finds. For more extensive examination of the clusters, you can request an output data set containing a cluster membership variable.

Background

The FASTCLUS procedure combines an effective method for finding initial clusters with a standard iterative algorithm for minimizing the sum of squared distances from the cluster means. The result is an efficient procedure for disjoint clustering of large data sets. PROC FASTCLUS was directly inspired by the Hartigan (1975) *leader algorithm* and the MacQueen (1967) *k-means algorithm*. PROC FASTCLUS uses a method that Anderberg (1973) calls *nearest centroid sorting*. A set of points called *cluster seeds* is selected as a first guess of the means of the clusters. Each observation is assigned to the nearest seed to form temporary clusters. The seeds are then replaced by the means of the temporary clusters, and the process is repeated until no further changes occur in the clusters. Similar techniques are described in most references on clustering (Anderberg 1973; Hartigan 1975; Everitt 1980; Spath 1980).

The FASTCLUS procedure differs from other nearest centroid sorting methods in the way the initial cluster seeds are selected. The importance of initial seed selection is demonstrated by Milligan (1980).

The clustering is done on the basis of Euclidean distances computed from one or more numeric variables. If there are missing values, PROC FASTCLUS computes an adjusted distance by using the nonmissing values. Observations that are very close to each other are usually assigned to the same cluster, while observations that are far apart are in different clusters.

The FASTCLUS procedure operates in four steps:

1. Observations called *cluster seeds* are selected.
2. If you specify the DRIFT option, temporary clusters are formed by assigning each observation to the cluster with the nearest seed. Each time an observation is assigned, the cluster seed is updated as the current mean of the cluster. This method is sometimes called *incremental, on-line, or adaptive training*.
3. If the maximum number of iterations is greater than zero, clusters are formed by assigning each observation to the nearest seed. After all observations are assigned, the cluster seeds are replaced by either the cluster means or other location estimates (cluster centers) appropriate to the LEAST= p option. This step can be repeated until the changes in the cluster seeds become small or zero (MAXITER= $n \geq 1$).
4. Final clusters are formed by assigning each observation to the nearest seed.

If PROC FASTCLUS runs to complete convergence, the final cluster seeds will equal the cluster means or cluster centers. If PROC FASTCLUS terminates before complete convergence, which often happens with the default settings, the final cluster seeds might not equal the cluster means or cluster centers. If you want complete convergence, specify CONVERGE=0 and a large value for the MAXITER= option.

The initial cluster seeds must be observations with no missing values. You can specify the maximum number of seeds (and, hence, clusters) by using the MAXCLUSTERS= option. You can also specify a minimum distance by which the seeds must be separated by using the RADIUS= option.

PROC FASTCLUS always selects the first complete (no missing values) observation as the first seed. The next complete observation that is separated from the first seed by at least the distance specified in the RADIUS= option becomes the second seed. Later observations are selected as new seeds if they are separated from all previous seeds by at least the radius, as long as the maximum number of seeds is not exceeded.

If an observation is complete but fails to qualify as a new seed, PROC FASTCLUS considers using it to replace one of the old seeds. Two tests are made to see if the observation can qualify as a new seed.

First, an old seed is replaced if the distance between the observation and the closest seed is greater than the minimum distance between seeds. The seed that is replaced is selected from the two seeds that are closest to each other. The seed that is replaced is the one of these two with the shortest distance to the closest of the remaining seeds when the other seed is replaced by the current observation.

If the observation fails the first test for seed replacement, a second test is made. The observation replaces the nearest seed if the smallest distance from the observation to all seeds other than the nearest one is greater than the shortest distance from the nearest seed to all other seeds. If the observation fails this test, PROC FASTCLUS goes on to the next observation.

You can specify the REPLACE= option to limit seed replacement. You can omit the second test for seed replacement (REPLACE=PART), causing PROC FASTCLUS to run faster, but the seeds selected might not be as widely separated as those obtained by the default method. You can also suppress seed replacement entirely by specifying REPLACE=NONE. In this case, PROC FASTCLUS runs much faster, but you must choose a good value for the RADIUS= option in order to get good clusters. This method is similar to the Hartigan (1975, pp. 74–78) leader algorithm and the *simple cluster seeking algorithm* described by Tou and Gonzalez (1974, pp. 90–92).

Getting Started: FASTCLUS Procedure

The following example demonstrates how to use the FASTCLUS procedure to compute disjoint clusters of observations in a SAS data set.

The data in this example are measurements taken on 159 freshwater fish caught from the same lake (Laengelmavesi) near Tampere in Finland. This data set is available from Puranen.

The species (bream, parkki, pike, perch, roach, smelt, and whitefish), weight, three different length measurements (measured from the nose of the fish to the beginning of its tail, the notch of its tail, and the end of its tail), height, and width of each fish are tallied. The height and width are recorded as percentages of the third length variable.

Suppose that you want to group empirically the fish measurements into clusters and that you want to associate the clusters with the species. You can use the FASTCLUS procedure to perform a cluster analysis.

The following DATA step creates the SAS data set Fish:

```
proc format;
  value specfmt
    1='Bream'
    2='Roach'
    3='Whitefish'
    4='Parkki'
    5='Perch'
    6='Pike'
    7='Smelt';
run;

data fish (drop=HtPct WidthPct);
  title 'Fish Measurement Data';
  input Species Weight Length1 Length2 Length3 HtPct WidthPct @@;

  *** transform variables;
  if Weight <= 0 or Weight =. then delete;
  Weight3=Weight**(1/3);
  Height=HtPct*Length3/(Weight3*100);
  Width=WidthPct*Length3/(Weight3*100);
  Length1=Length1/Weight3;
  Length2=Length2/Weight3;
  Length3=Length3/Weight3;
  logLengthRatio=log(Length3/Length1);

  format Species specfmt.;
  symbol = put(Species, specfmt2.);
  datalines;
1 242.0 23.2 25.4 30.0 38.4 13.4 1 290.0 24.0 26.3 31.2 40.0 13.8
1 340.0 23.9 26.5 31.1 39.8 15.1 1 363.0 26.3 29.0 33.5 38.0 13.3
1 430.0 26.5 29.0 34.0 36.6 15.1 1 450.0 26.8 29.7 34.7 39.2 14.2
1 500.0 26.8 29.7 34.5 41.1 15.3 1 390.0 27.6 30.0 35.0 36.2 13.4
1 450.0 27.6 30.0 35.1 39.9 13.8 1 500.0 28.5 30.7 36.2 39.3 13.7
1 475.0 28.4 31.0 36.2 39.4 14.1 1 500.0 28.7 31.0 36.2 39.7 13.3
1 500.0 29.1 31.5 36.4 37.8 12.0 1 . 29.5 32.0 37.3 37.3 13.6
```

```

1  600.0 29.4 32.0 37.2 40.2 13.9 1  600.0 29.4 32.0 37.2 41.5 15.0
1  700.0 30.4 33.0 38.3 38.8 13.8 1  700.0 30.4 33.0 38.5 38.8 13.5
... more lines ...

7  19.7 13.2 14.3 15.2 18.9 13.6 7  19.9 13.8 15.0 16.2 18.1 11.6
;
```

The double trailing at sign (@@) in the INPUT statement specifies that observations are input from each line until all values are read. The variables are rescaled in order to adjust for dimensionality. Because the new variables Weight3–logLengthRatio depend on the variable Weight, observations with missing values for Weight are not added to the data set. Consequently, there are 157 observations in the SAS data set Fish.

In the Fish data set, the variables are not measured in the same units and cannot be assumed to have equal variance. Therefore, it is necessary to standardize the variables before performing the cluster analysis.

The following statements standardize the variables and perform a cluster analysis on the standardized data:

```

proc stdize data=Fish out=Stand method=std;
  var Length1 logLengthRatio Height Width Weight3;
run;

proc fastclus data=Stand out=Clust
  maxclusters=7 maxiter=100;
  var Length1 logLengthRatio Height Width Weight3;
run;
```

The STDIZE procedure is first used to standardize all the analytical variables to a mean of 0 and standard deviation of 1. The procedure creates the output data set Stand to contain the transformed variables (for detailed information, see Chapter 87, “[The STDIZE Procedure](#)”).

The FASTCLUS procedure then uses the data set Stand as input and creates the data set Clust. This output data set contains the original variables and two new variables, Cluster and Distance. The variable Cluster contains the cluster number to which each observation has been assigned. The variable Distance gives the distance from the observation to its cluster seed.

It is usually desirable to try several values of the MAXCLUSTERS= option. A reasonable beginning for this example is to use MAXCLUSTERS=7, since there are seven species of fish represented in the data set Fish.

The VAR statement specifies the variables used in the cluster analysis.

The results from this analysis are displayed in the following figures.

Figure 36.1 Initial Seeds Used in the FASTCLUS Procedure

Fish Measurement Data					
The FASTCLUS Procedure					
Replace=FULL Radius=0 Maxclusters=7 Maxiter=100 Converge=0.02					
Initial Seeds					
Cluster	Length1	logLength Ratio	Height	Width	Weight3
1	1.388338414	-0.979577858	-1.594561848	-2.254050655	2.103447062
2	-1.117178039	-0.877218192	-0.336166276	2.528114070	1.170706464
3	2.393997461	-0.662642015	-0.930738701	-2.073879107	-1.839325419
4	-0.495085516	-0.964041012	-0.265106856	-0.028245072	1.536846394
5	-0.728772773	0.540096664	1.130501398	-1.207930053	-1.107018207
6	-0.506924177	0.748211648	1.762482687	0.211507596	1.368987826
7	1.573996573	-0.796593995	-0.824217424	1.561715851	-1.607942726

Criterion Based on Final Seeds = 0.3979

the [Figure 36.1](#) displays the table of initial seeds used for each variable and cluster. The first line in the figure displays the option settings for REPLACE, RADIUS, MAXCLUSTERS, and MAXITER. These options, with the exception of MAXCLUSTERS and MAXITER, are set at their respective default values (REPLACE=FULL, RADIUS=0). Both the MAXCLUSTERS= and MAXITER= options are set in the PROC FASTCLUS statement.

Next, PROC FASTCLUS produces a table of summary statistics for the clusters. [Figure 36.2](#) displays the number of observations in the cluster (frequency) and the root mean squared standard deviation. The next two columns display the largest Euclidean distance from the cluster seed to any observation within the cluster and the number of the nearest cluster.

The last column of the table displays the distance between the centroid of the nearest cluster and the centroid of the current cluster. A centroid is the point having coordinates that are the means of all the observations in the cluster.

Figure 36.2 Cluster Summary Table from the FASTCLUS Procedure

Cluster Summary					
Cluster	Frequency	RMS Std Deviation	Maximum Distance from Seed to Observation	Radius Exceeded	Nearest Cluster
1	17	0.5064	1.7781		4
2	19	0.3696	1.5007		4
3	13	0.3803	1.7135		1
4	13	0.4161	1.3976		7
5	11	0.2466	0.6966		6
6	34	0.3563	1.5443		5
7	50	0.4447	2.3915		4

Cluster Summary	
Cluster	Distance Between Cluster Centroids
1	2.5106
2	1.5510
3	2.6704
4	1.4266
5	1.7301
6	1.7301
7	1.4266

Figure 36.3 displays the table of statistics for the variables. The table lists for each variable the total standard deviation, the pooled within-cluster standard deviation and the R-square value for predicting the variable from the cluster. The ratio of between-cluster variance to within-cluster variance (R^2 to $1 - R^2$) appears in the last column.

Figure 36.3 Statistics for Variables Used in the FASTCLUS Procedure

Statistics for Variables				
Variable	Total STD	Within STD	R-Square	RSQ/(1-RSQ)
Length1	1.00000	0.31428	0.905030	9.529606
logLengthRatio	1.00000	0.39276	0.851676	5.741989
Height	1.00000	0.20917	0.957929	22.769295
Width	1.00000	0.55558	0.703200	2.369270
Weight3	1.00000	0.47251	0.785323	3.658162
OVER-ALL	1.00000	0.40712	0.840631	5.274764

Pseudo F Statistic = 131.87

Approximate Expected Over-All R-Squared = 0.57420

Cubic Clustering Criterion = 37.808

The pseudo F statistic, approximate expected overall R square, and cubic clustering criterion (CCC) are listed at the bottom of the figure. You can compare values of these statistics by running PROC FASTCLUS with different values for the MAXCLUSTERS= option. The R square and CCC values are not valid for correlated variables.

Values of the cubic clustering criterion greater than 2 or 3 indicate good clusters. Values between 0 and 2 indicate potential clusters, but they should be taken with caution; large negative values can indicate outliers.

PROC FASTCLUS next produces the within-cluster means and standard deviations of the variables, displayed in Figure 36.4.

Figure 36.4 Cluster Means and Standard Deviations from the FASTCLUS Procedure

Cluster Means					
Cluster	Length1	logLength Ratio	Height	Width	Weight3
1	1.747808245	-0.868605685	-1.327226832	-1.128760946	0.806373599
2	-0.405231510	-0.979113021	-0.281064162	1.463094486	1.060450065
3	2.006796315	-0.652725165	-1.053213440	-1.224020795	-1.826752838
4	-0.136820952	-1.039312574	-0.446429482	0.162596336	0.278560318
5	-0.850130601	0.550190242	1.245156076	-0.836585750	-0.567022647
6	-0.843912827	1.522291347	1.511408739	-0.380323563	0.763114370
7	-0.165570970	-0.048881276	-0.353723615	0.546442064	-0.668780782

Cluster Standard Deviations					
Cluster	Length1	logLength Ratio	Height	Width	Weight3
1	0.3418476428	0.3544065543	0.1666302451	0.6172880027	0.7944227150
2	0.3129902863	0.3592350778	0.1369052680	0.5467406493	0.3720119097
3	0.2962504486	0.1740941675	0.1736086707	0.7528475622	0.0905232968
4	0.3254364840	0.2836681149	0.1884592934	0.4543390702	0.6612055341
5	0.1781837609	0.0745984121	0.2056932592	0.2784540794	0.3832002850
6	0.2273744242	0.3385584051	0.2046010964	0.5143496067	0.4025849044
7	0.3734733622	0.5275768119	0.2551130680	0.5721303628	0.4223181710

It is useful to study further the clusters calculated by the FASTCLUS procedure. One method is to look at a frequency tabulation of the clusters with other classification variables. The following statements invoke the FREQ procedure to crosstabulate the empirical clusters with the variable Species:

```
proc freq data=Clust;
  tables Species*Cluster;
run;
```

Figure 36.5 displays the marked division between clusters.

Figure 36.5 Frequency Table of Cluster versus Species

Fish Measurement Data					
The FREQ Procedure					
Table of Species by CLUSTER					
Species	CLUSTER(Cluster)				
Frequency					
Percent					
Row Pct					
Col Pct	1	2	3	4	Total
Bream	0	0	0	0	34
	0.00	0.00	0.00	0.00	21.66
	0.00	0.00	0.00	0.00	
	0.00	0.00	0.00	0.00	
Roach	0	0	0	0	19
	0.00	0.00	0.00	0.00	12.10
	0.00	0.00	0.00	0.00	
	0.00	0.00	0.00	0.00	
Whitefish	0	2	0	1	6
	0.00	1.27	0.00	0.64	3.82
	0.00	33.33	0.00	16.67	
	0.00	10.53	0.00	7.69	
Parkki	0	0	0	0	11
	0.00	0.00	0.00	0.00	7.01
	0.00	0.00	0.00	0.00	
	0.00	0.00	0.00	0.00	
Perch	0	17	0	12	56
	0.00	10.83	0.00	7.64	35.67
	0.00	30.36	0.00	21.43	
	0.00	89.47	0.00	92.31	
Pike	17	0	0	0	17
	10.83	0.00	0.00	0.00	10.83
	100.00	0.00	0.00	0.00	
	100.00	0.00	0.00	0.00	
Smelt	0	0	13	0	14
	0.00	0.00	8.28	0.00	8.92
	0.00	0.00	92.86	0.00	
	0.00	0.00	100.00	0.00	
Total	17	19	13	13	157
	10.83	12.10	8.28	8.28	100.00

(Continued)

Figure 36.5 continued

Fish Measurement Data				
The FREQ Procedure				
Table of Species by CLUSTER				
Species	CLUSTER(Cluster)			
Frequency	5	6	7	Total
Percent				
Row Pct				
Col Pct				
Bream	0	34	0	34
	0.00	21.66	0.00	21.66
	0.00	100.00	0.00	
	0.00	100.00	0.00	
Roach	0	0	19	19
	0.00	0.00	12.10	12.10
	0.00	0.00	100.00	
	0.00	0.00	38.00	
Whitefish	0	0	3	6
	0.00	0.00	1.91	3.82
	0.00	0.00	50.00	
	0.00	0.00	6.00	
Parkki	11	0	0	11
	7.01	0.00	0.00	7.01
	100.00	0.00	0.00	
	100.00	0.00	0.00	
Perch	0	0	27	56
	0.00	0.00	17.20	35.67
	0.00	0.00	48.21	
	0.00	0.00	54.00	
Pike	0	0	0	17
	0.00	0.00	0.00	10.83
	0.00	0.00	0.00	
	0.00	0.00	0.00	
Smelt	0	0	1	14
	0.00	0.00	0.64	8.92
	0.00	0.00	7.14	
	0.00	0.00	2.00	
Total	11	34	50	157
	7.01	21.66	31.85	100.00

For cases in which you have three or more clusters, you can use the CANDISC and SGPLOT procedures to obtain a graphical check on the distribution of the clusters. In the following statements, the CANDISC and SGPLOT procedures are used to compute canonical variables and plot the clusters:

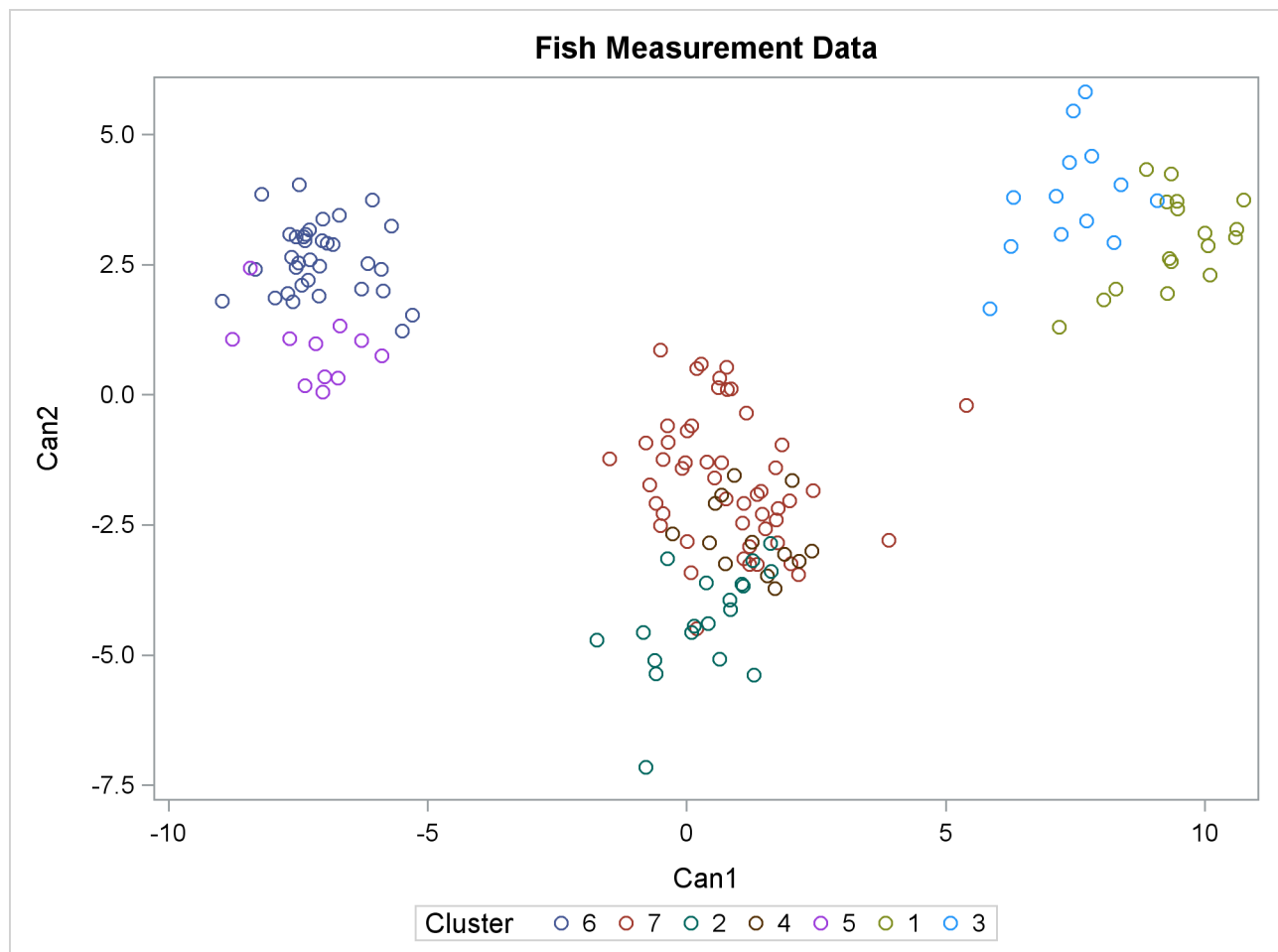
```
proc candisc data=Clust out=Can noprint;
  class Cluster;
  var Length1 logLengthRatio Height Width Weight3;
run;

proc sgplot data=Can;
  scatter y=Can2 x=Can1 / group=Cluster;
run;
```

First, the CANDISC procedure is invoked to perform a canonical discriminant analysis by using the data set Clust and creating the output SAS data set Can. The NOPRINT option suppresses display of the output. The CLASS statement specifies the variable Cluster to define groups for the analysis. The VAR statement specifies the variables used in the analysis.

Next, the SGPLOT procedure plots the two canonical variables from PROC CANDISC, Can1 and Can2. The SCATTER statement specifies the variable Cluster as the group identification variable. The resulting plot (Figure 36.6) illustrates the spatial separation of the clusters calculated in the FASTCLUS procedure.

Figure 36.6 Plot of Canonical Variables and Cluster Value



Syntax: FASTCLUS Procedure

The following statements are available in the FASTCLUS procedure:

```
PROC FASTCLUS < MAXCLUSTERS=n> < RADIUS=t> < options> ;  
  VAR variables ;  
  ID variables ;  
  FREQ variable ;  
  WEIGHT variable ;  
  BY variables ;
```

Usually you need only the VAR statement in addition to the PROC FASTCLUS statement. The BY, FREQ, ID, VAR, and WEIGHT statements are described in alphabetical order after the PROC FASTCLUS statement.

PROC FASTCLUS Statement

```
PROC FASTCLUS < MAXCLUSTERS=n> < RADIUS=t> < options> ;
```

The PROC FASTCLUS statement invokes the FASTCLUS procedure. You must specify the MAXCLUSTERS= option or RADIUS= option or both in the PROC FASTCLUS statement.

MAXCLUSTERS=*n*

MAXC=*n*

specifies the maximum number of clusters permitted. If you omit the MAXCLUSTERS= option, a value of 100 is assumed.

RADIUS=*t*

R=*t*

establishes the minimum distance criterion for selecting new seeds. No observation is considered as a new seed unless its minimum distance to previous seeds exceeds the value given by the RADIUS= option. The default value is 0. If you specify the REPLACE=RANDOM option, the RADIUS= option is ignored.

You can specify the following options in the PROC FASTCLUS statement. Table 36.1 summarizes the options available in the PROC FASTCLUS statement.

Table 36.1 PROC FASTCLUS Statement Options

Option	Description
Specify input and output data sets	
DATA=	Specifies input data set
INSTAT=	Specifies input SAS data set previously created by the OUTSTAT= option
SEED=	Specifies input SAS data set for selecting initial cluster seeds
VARDEF=	Specifies divisor for variances
Output Data Processing	
CLUSTER=	Specifies name for cluster membership variable in OUTSEED= and OUT= data sets
CLUSTERLABEL=	Specifies label for cluster membership variable in OUTSEED= and OUT= data sets
OUT=	Specifies output SAS data set containing original data and cluster assignments
OUTITER	Specifies writing to OUTSEED= data set on every iteration
OUTSEED= or MEAN=	Specifies output SAS data set containing cluster centers
OUTSTAT=	Specifies output SAS data set containing statistics
Initial Clusters	
DRIFT	Permits cluster to seeds to drift during initialization
MAXCLUSTERS=	Specifies maximum number of clusters
RADIUS=	Specifies minimum distance for selecting new seeds
RANDOM=	Specifies seed to initializes pseudo-random number generator
REPLACE=	Specifies seed replacement method
Clustering Methods	
CONVERGE=	Specifies convergence criterion
DELETE=	Deletes cluster seeds with few observations
LEAST=	Optimizes an L_p criterion, where $1 \leq p \leq \infty$
MAXITER=	Specifies maximum number of iterations
STRICT	Prevents an observation from being assigned to a cluster if its distance to the nearest cluster seed is large

Table 36.1 continued

Option	Description
Arcane Algorithmic Options	
BINS=	Specifies number of bins used for computing medians for LEAST=1
HC=	Specifies criterion for updating the homotopy parameter
HP=	Specifies initial value of the homotopy parameter
IRLS	Uses an iteratively reweighted least squares method instead of the modified Ekblom-Newton method for $1 < p < 2$
Missing Values	
IMPUTE	Imputes missing values after final cluster assignment
NOMISS	Excludes observations with missing values
Control Displayed Output	
DISTANCE	Displays distances between cluster centers
LIST	Displays cluster assignments for all observations
NOPRINT	Suppresses displayed output
SHORT	Suppresses display of large matrices
SUMMARY	Suppresses display of all results except for the cluster summary
VARIABLESAREUNCORRELATED	Suppresses warning in output

The following list provides details on these options. The list is in alphabetical order.

BINS=*n*

specifies the number of bins used in the bin-sort algorithm for computing medians for LEAST=1. By default, PROC FASTCLUS uses from 10 to 100 bins, depending on the amount of memory available. Larger values use more memory and make each iteration somewhat slower, but they can reduce the number of iterations. Smaller values have the opposite effect. The minimum value of *n* is 5.

CLUSTER=*name*

specifies a name for the variable in the OUTSEED= and OUT= data sets that indicates cluster membership. The default name for this variable is CLUSTER.

CLUSTERLABEL=*name*

specifies a label for the variable CLUSTER in the OUTSEED= and OUT= data sets. By default this variable has no label.

CONVERGE=*c***CONV=*c***

specifies the convergence criterion. Any nonnegative value is permitted. The default value is 0.0001 for all values of *p* if LEAST=*p* is explicitly specified; otherwise, the default value is 0.02. Iterations stop when the maximum relative change in the cluster seeds is less than or equal to the convergence criterion and additional conditions on the homotopy parameter, if any, are satisfied (see the HP= option). The relative change in a cluster seed is the distance between the old seed and the new seed divided by a scaling factor. If you do not specify the LEAST= option, the scaling factor is the minimum distance between the initial seeds. If you specify the LEAST= option, the scaling factor is an L_1 scale estimate and is recomputed on each iteration. Specify the CONVERGE= option only if you specify a MAXITER= value greater than 1.

DATA=SAS-data-set

specifies the input data set containing observations to be clustered. If you omit the DATA= option, the most recently created SAS data set is used. The data must be coordinates, not distances, similarities, or correlations.

DELETE=*n*

deletes cluster seeds to which *n* or fewer observations are assigned. Deletion occurs after processing for the DRIFT option is completed and after each iteration specified by the MAXITER= option. Cluster seeds are not deleted after the final assignment of observations to clusters, so in rare cases a final cluster might not have more than *n* members. The DELETE= option is ineffective if you specify MAXITER=0 and do not specify the DRIFT option. By default, no cluster seeds are deleted.

DISTANCE | DIST

computes distances between the cluster means.

DRIFT

executes the second of the four steps described in the section “Background” on page 2300. After initial seed selection, each observation is assigned to the cluster with the nearest seed. After an observation is processed, the seed of the cluster to which it is assigned is recalculated as the mean of the observations currently assigned to the cluster. Thus, the cluster seeds drift about rather than remaining fixed for the duration of the pass.

HC=*c***HP=*p*₁ < *p*₂ >**

pertains to the homotopy parameter for LEAST=*p*, where $1 < p < 2$. You should specify these options only if you encounter convergence problems when you use the default values.

For $1 < p < 2$, PROC FASTCLUS tries to optimize a perturbed variant of the L_p clustering criterion (Gonin and Money 1989, pp. 5–6).

When the homotopy parameter is 0, the optimization criterion is equivalent to the clustering criterion. For a large homotopy parameter, the optimization criterion approaches the least squares criterion and is therefore easy to optimize. Beginning with a large homotopy parameter, PROC FASTCLUS gradually decreases it by a factor in the range [0.01,0.5] over the course of the iterations. When both the homotopy parameter and the convergence measure are sufficiently small, the optimization process is declared to have converged.

If the initial homotopy parameter is too large or if it is decreased too slowly, the optimization can require many iterations. If the initial homotopy parameter is too small or if it is decreased too quickly, convergence to a local optimum is likely. The following list gives details on setting the homotopy parameter.

HC=*c* specifies the criterion for updating the homotopy parameter. The homotopy parameter is updated when the maximum relative change in the cluster seeds is less than or equal to *c*. The default is the minimum of 0.01 and 100 times the value of the CONVERGE= option.

HP=*p*₁ specifies *p*₁ as the initial value of the homotopy parameter. The default is 0.05 if the modified Eklom-Newton method is used; otherwise, it is 0.25.

HP=*p*₁ *p*₂ also specifies *p*₂ as the minimum value for the homotopy parameter, which must be reached for convergence. The default is the minimum of *p*₁ and 0.01 times the value of the CONVERGE= option.

IMPUTE

requests imputation of missing values after the final assignment of observations to clusters. If an observation that is assigned (or would have been assigned) to a cluster has a missing value for variables used in the cluster analysis, the missing value is replaced by the corresponding value in the cluster seed to which the observation is assigned (or would have been assigned). If the observation cannot be assigned to a cluster, missing value replacement depends on whether or not the NOMISS option is specified. If NOMISS is not specified, missing values are replaced by the mean of all observations in the DATA= data set having a value for that variable. If NOMISS is specified, missing values are replaced by the mean of only observations used in the analysis. (A weighted mean is used if a variable is specified in the WEIGHT statement.) For information about cluster assignment see the section “OUT= Data Set” on page 2320. If you specify the IMPUTE option, the imputed values are not used in computing cluster statistics.

If you also request an OUT= data set, it contains the imputed values.

INSTAT=SAS-data-set

reads a SAS data set previously created with the FASTCLUS procedure by using the OUTSTAT= option. If you specify the INSTAT= option, no clustering iterations are performed and no output is displayed. Only cluster assignment and imputation are performed as an OUT= data set is created.

IRLS

causes PROC FASTCLUS to use an iteratively reweighted least squares method instead of the modified Eklblom-Newton method. If you specify the IRLS option, you must also specify LEAST= p , where $1 < p < 2$. Use the IRLS option only if you encounter convergence problems with the default method.

LEAST= p | MAX**L= p | MAX**

causes PROC FASTCLUS to optimize an L_p criterion, where $1 \leq p \leq \infty$ (Spath 1985, pp. 62–63). Infinity is indicated by LEAST=MAX. The value of this clustering criterion is displayed in the iteration history.

If you do not specify the LEAST= option, PROC FASTCLUS uses the least squares (L_2) criterion. However, the default number of iterations is only 1 if you omit the LEAST= option, so the optimization of the criterion is generally not completed. If you specify the LEAST= option, the maximum number of iterations is increased to permit the optimization process a chance to converge. See the MAXITER= n option for details.

Specifying the LEAST= option also changes the default convergence criterion from 0.02 to 0.0001. See the CONVERGE= c for details.

When LEAST=2, PROC FASTCLUS tries to minimize the root mean squared difference between the data and the corresponding cluster means.

When LEAST=1, PROC FASTCLUS tries to minimize the mean absolute difference between the data and the corresponding cluster medians.

When LEAST=MAX, PROC FASTCLUS tries to minimize the maximum absolute difference between the data and the corresponding cluster midranges.

For general values of p , PROC FASTCLUS tries to minimize the p th root of the mean of the p th powers of the absolute differences between the data and the corresponding cluster seeds.

The divisor in the clustering criterion is either the number of nonmissing data used in the analysis or, if there is a WEIGHT statement, the sum of the weights corresponding to all the nonmissing data used in the analysis (that is, an observation with n nonmissing data contributes n times the observation weight to the divisor). The divisor is not adjusted for degrees of freedom.

The method for updating cluster seeds during iteration depends on the LEAST= p option, as follows (Gonin and Money 1989).

LEAST= p	Algorithm for Computing Cluster Seeds
$p = 1$	bin sort for median
$1 < p < 2$	modified Merle-Spath if you specify IRLS; otherwise modified Ekblom-Newton
$p = 2$	arithmetic mean
$2 < p < \infty$	Newton
$p = \infty$	midrange

During the final pass, a modified Merle-Spath step is taken to compute the cluster centers for $1 \leq p < 2$ or $2 < p < \infty$.

If you specify the LEAST= p option with a value other than 2, PROC FASTCLUS computes pooled scale estimates analogous to the root mean squared standard deviation but based on p th power deviations instead of squared deviations.

LEAST= p	Scale Estimate
$p = 1$	mean absolute deviation
$1 < p < \infty$	root mean p th-power absolute deviation
$p = \infty$	maximum absolute deviation

The divisors for computing the mean absolute deviation or the root mean p th-power absolute deviation are adjusted for degrees of freedom just like the divisors for computing standard deviations. This adjustment can be suppressed by the VARDEF= option.

LIST

lists all observations, giving the value of the ID variable (if any), the number of the cluster to which the observation is assigned, and the distance between the observation and the final cluster seed.

MAXITER= n

specifies the maximum number of iterations for recomputing cluster seeds. When the value of the MAXITER= option is greater than zero, PROC FASTCLUS executes the third of the four steps described in the section “[Background](#)” on page 2300. In each iteration, each observation is assigned to the nearest seed, and the seeds are recomputed as the means of the clusters.

The default value of the MAXITER= option depends on the LEAST= p option.

LEAST= p	MAXITER=
not specified	1
$p = 1$	20
$1 < p < 1.5$	50
$1.5 \leq p < 2$	20
$p = 2$	10
$2 < p \leq \infty$	20

MEAN=SAS-data-set

creates an output data set to contain the cluster means and other statistics for each cluster. If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*.

NOMISS

excludes observations with missing values from the analysis. However, if you also specify the **IMPUTE** option, observations with missing values are included in the final cluster assignments.

NOPRINT

suppresses the display of all output. Note that this option temporarily disables the Output Delivery System (ODS). For more information, see Chapter 20, “Using the Output Delivery System.”

OUT=SAS-data-set

creates an output data set to contain all the original data, plus the new variables **CLUSTER** and **DISTANCE**. If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*.

OUTITER

outputs information from the iteration history to the **OUTSEED=** data set, including the cluster seeds at each iteration.

OUTSEED=SAS-data-set**OUTS=SAS-data-set**

is another name for the **MEAN=** data set, provided because the data set can contain location estimates other than means. The **MEAN=** option is still accepted.

OUTSTAT=SAS-data-set

creates an output data set to contain various statistics, especially those not included in the **OUTSEED=** data set. Unlike the **OUTSEED=** data set, the **OUTSTAT=** data set is not suitable for use as a **SEED=** data set in a subsequent **PROC FASTCLUS** step.

RANDOM=n

specifies a positive integer as a starting value for the pseudo-random number generator for use with **REPLACE=RANDOM**. If you do not specify the **RANDOM=** option, the time of day is used to initialize the pseudo-random number sequence.

REPLACE=FULL | PART | NONE | RANDOM

specifies how seed replacement is performed, as follows:

FULL	requests default seed replacement as described in the section “Background” on page 2300.
PART	requests seed replacement only when the distance between the observation and the closest seed is greater than the minimum distance between seeds.
NONE	suppresses seed replacement.
RANDOM	selects a simple pseudo-random sample of complete observations as initial cluster seeds.

SEED=SAS-data-set

specifies an input data set from which initial cluster seeds are to be selected. If you do not specify the SEED= option, initial seeds are selected from the DATA= data set. The SEED= data set must contain the same variables that are used in the data analysis.

SHORT

suppresses the display of the initial cluster seeds, cluster means, and standard deviations.

STRICT**STRICT=s**

prevents an observation from being assigned to a cluster if its distance to the nearest cluster seed exceeds the value of the STRICT= option. If you specify the STRICT option without a numeric value, you must also specify the RADIUS= option, and its value is used instead. In the OUT= data set, observations that are not assigned due to the STRICT= option are given a negative cluster number, the absolute value of which indicates the cluster with the nearest seed.

SUMMARY

suppresses the display of the initial cluster seeds, statistics for variables, cluster means, and standard deviations.

VARDEF=DF | N | WDF | WEIGHT | WGT

specifies the divisor to be used in the calculation of variances and covariances. The default value is VARDEF=DF. The possible values of the VARDEF= option and associated divisors are as follows.

Value	Description	Divisor
DF	error degrees of freedom	$n - c$
N	number of observations	n
WDF	sum of weights DF	$(\sum_i w_i) - c$
WEIGHT WGT	sum of weights	$\sum_i w_i$

In the preceding definitions, c represents the number of clusters.

VARIABLESAREUNCORRELATED

suppresses the warning, displayed in the listing when there are two or more VAR variables, concerning the validity of the Approximate Expected Over-All R-Squared and the Cubic Clustering Criterion when the variables used in clustering are correlated. Note that the FASTCLUS procedure does not compute correlations; the warning is for a potential problem.

BY Statement

BY variables ;

You can specify a BY statement with PROC FASTCLUS to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the FASTCLUS procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

If you specify the SEED= option and the SEED= data set does not contain any of the BY variables, then the entire SEED= data set is used to obtain initial cluster seeds for each BY group in the DATA= data set.

If the SEED= data set contains some but not all of the BY variables, or if some BY variables do not have the same type or length in the SEED= data set as in the DATA= data set, then PROC FASTCLUS displays an error message and stops.

If all the BY variables appear in the SEED= data set with the same type and length as in the DATA= data set, then each BY group in the SEED= data set is used to obtain initial cluster seeds for the corresponding BY group in the DATA= data set. All BY groups in the DATA= data set must also appear in the SEED= data set. The BY groups in the SEED= data set must be in the same order as in the DATA= data set. If you specify the NOTSORTED option in the BY statement, both data sets must contain exactly the same BY groups in the same order. If you do not specify NOTSORTED, some BY groups can appear in the SEED= data set but not in the DATA= data set; such BY groups are not used in the analysis.

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

FREQ Statement

FREQ *variable* ;

If a variable in the data set represents the frequency of occurrence for the other values in the observation, include the variable's name in a FREQ statement. The procedure then treats the data set as if each observation appears n times, where n is the value of the FREQ variable for the observation.

If the value of the FREQ variable is missing or less than or equal to zero, the observation is not used in the analysis. The exact values of the FREQ variable are used in computations: frequency values are not truncated to integers. The total number of observations is considered to be equal to the sum of the FREQ variable when the procedure determines degrees of freedom for significance probabilities.

The WEIGHT and FREQ statements have a similar effect, except in determining the number of observations for significance tests.

ID Statement

ID *variable* ;

The ID variable, which can be character or numeric, identifies observations on the output when you specify the LIST option.

VAR Statement

VAR *variables* ;

The VAR statement lists the numeric variables to be used in the cluster analysis. If you omit the VAR statement, all numeric variables not listed in other statements are used.

WEIGHT Statement

WEIGHT *variable* ;

The values of the WEIGHT variable are used to compute weighted cluster means. The WEIGHT and FREQ statements have a similar effect, except the WEIGHT statement does not alter the degrees of freedom or the number of observations. The WEIGHT variable can take nonintegral values. An observation is used in the analysis only if the value of the WEIGHT variable is greater than zero.

Details: FASTCLUS Procedure

Updates in the FASTCLUS Procedure

Some FASTCLUS procedure options and statements have changed from previous versions. The differences are as follows:

- Values of the FREQ variable are no longer truncated to integers. Noninteger variables specified in the FREQ statement produce results different from those in previous releases.
- The IMPUTE option produces different cluster standard deviations and related statistics. When you specify the IMPUTE option, imputed values are no longer used in computing cluster statistics. This change causes the cluster standard deviations and other statistics computed from the standard deviations to be different from those in previous releases.
- The INSTAT= option reads a SAS data set previously created with the FASTCLUS procedure by using the OUTSTAT= option. If you specify the INSTAT= option, no clustering iterations are performed and no output is produced. Only cluster assignment and imputation are performed as an OUT= data set is created.
- The OUTSTAT= data set contains additional information used for imputation. `_TYPE_=SEED` corresponds to values that are cluster seeds. Observations previously designated `_TYPE_='SCALE'` are now `_TYPE_='DISPERSION'`.

Missing Values

Observations with all missing values are excluded from the analysis. If you specify the NOMISS option, observations with any missing values are excluded. Observations with missing values cannot be cluster seeds.

The distance between an observation with missing values and a cluster seed is obtained by computing the squared distance based on the nonmissing values, multiplying by the ratio of the number of variables, n , to the number of variables having nonmissing values, m , and taking the square root:

$$\sqrt{\left(\frac{n}{m}\right) \sum (x_i - s_i)^2}$$

where

- n = number of variables
- m = number of variables with nonmissing values
- x_i = value of the i th variable for the observation
- s_i = value of the i th variable for the seed

If you specify the LEAST= p option with a power p other than 2 (the default), the distance is computed using

$$\left(\left(\frac{n}{m}\right) \sum (x_i - s_i)^p\right)^{\frac{1}{p}}$$

The summation is taken over variables with nonmissing values.

The IMPUTE option fills in missing values in the OUT= output data set.

Output Data Sets

OUT= Data Set

The OUT= data set contains the following:

- the original variables
- a new variable indicating the cluster assignment status of each observation. The value will be less than the permitted number of clusters (see the MAXCLUSTERS= option) if the procedure detects fewer clusters than the maximum. A positive value indicates the cluster to which the observation was assigned. A negative value indicates that the observation was not assigned to a cluster (see the STRICT option), and the absolute value indicates the cluster to which the observation would have been assigned. If the value is missing, the observation cannot be assigned to any cluster. You can specify the variable name with the CLUSTER= option. The default name is CLUSTER.
- a new variable, DISTANCE, giving the distance from the observation to its cluster seed

If you specify the IMPUTE option, the OUT= data set also contains a new variable, _IMPUTE_, giving the number of imputed values in each observation.

OUTSEED= Data Set

The OUTSEED= data set contains one observation for each cluster. The variables are as follows:

- the BY variables, if any
- a new variable giving the cluster number. You can specify the variable name with the CLUSTER= option. The default name is CLUSTER.
- either the FREQ variable or a new variable called `_FREQ_` giving the number of observations in the cluster
- the WEIGHT variable, if any
- a new variable, `_RMSSTD_`, giving the root mean squared standard deviation for the cluster. See Chapter 31, “The CLUSTER Procedure,” for details.
- a new variable, `_RADIUS_`, giving the maximum distance between any observation in the cluster and the cluster seed
- a new variable, `_GAP_`, containing the distance between the current cluster mean and the nearest other cluster mean. The value is the centroid distance given in the output.
- a new variable, `_NEAR_`, specifying the cluster number of the nearest cluster
- the VAR variables giving the cluster means

If you specify the `LEAST=p` option with a value other than 2, the `_RMSSTD_` variable is replaced by the `_SCALE_` variable, which contains the pooled scale estimate analogous to the root mean squared standard deviation but based on *p*th-power deviations instead of squared deviations:

<code>LEAST=1</code>	mean absolute deviation
<code>LEAST=<i>p</i></code>	root mean <i>p</i> -th-power absolute deviation
<code>LEAST=MAX</code>	maximum absolute deviation

If you specify the OUTITER option, there is one set of observations in the OUTSEED= data set for each pass through the data set (that is, one set for initial seeds, one for each iteration, and one for the final clusters). Also, several additional variables appear:

<code>_ITER_</code>	is the iteration number. For the initial seeds, the value is 0. For the final cluster means or centers, the <code>_ITER_</code> variable is one greater than the last iteration reported in the iteration history.
<code>_CRIT_</code>	is the clustering criterion as described under the <code>LEAST=</code> option.
<code>_CHANGE_</code>	is the maximum over clusters of the relative change in the cluster seed from the previous iteration. The relative change in a cluster seed is the distance between the old seed and the new seed divided by a scaling factor. If you do not specify the <code>LEAST=</code> option, the scaling factor is the minimum distance between the initial seeds. If you specify the <code>LEAST=</code> option, the scaling factor is an L_1 scale estimate and is recomputed on each iteration.

- `_HOMPAR_` is the value of the homotopy parameter. This variable appears only for `LEAST= p` with $1 < p < 2$.
- `_BINSIZ_` is the maximum bin size used for estimating medians. This variable appears only for `LEAST=1`.

If you specify the `OUTITER` option, the variables `_SCALE_` or `_RMSSTD_`, `_RADIUS_`, `_NEAR_`, and `_GAP_` have missing values except for the last pass.

You can use the `OUTSEED=` data set as a `SEED=` input data set for a subsequent analysis.

OUTSTAT= Data Set

The variables in the `OUTSTAT=` data set are as follows:

- BY variables, if any
- a new character variable, `_TYPE_`, specifying the type of statistic given by other variables (see [Table 36.2](#) and [Table 36.3](#))
- a new numeric variable giving the cluster number. You can specify the variable name with the `CLUSTER=` option. The default name is `CLUSTER`.
- a new numeric variable, `OVER_ALL`, containing statistics that apply over all of the `VAR` variables
- the `VAR` variables giving statistics for particular variables

The values of `_TYPE_` for all `LEAST=` options are given in [Table 36.2](#).

Table 36.2 `_TYPE_`

<code>_TYPE_</code>	Contents of <code>VAR</code> Variables	Contents of <code>OVER_ALL</code>
INITIAL	Initial seeds	Missing
CRITERION	Missing	Optimization criterion (see the <code>LEAST=</code> option); this value is displayed just before the “Cluster Summary” table.
CENTER	Cluster centers (see the <code>LEAST=</code> option)	Missing
SEED	Cluster seeds: additional information used for imputation	
DISPERSION	Dispersion estimates for each cluster (see the <code>LEAST=</code> option); these values are displayed in a separate row with title depending on the <code>LEAST=</code> option	Dispersion estimates pooled over variables (see the <code>LEAST=</code> option); these values are displayed in the “Cluster Summary” table with label depending on the <code>LEAST=</code> option.

Table 36.2 *continued*

TYPE	Contents of VAR variables	Contents of OVER_ALL
FREQ	Frequency of each cluster omitting observations with missing values for the VAR variable; these values are not displayed	Frequency of each cluster based on all observations with any nonmissing value; these values are displayed in the “Cluster Summary” table.
WEIGHT	Sum of weights for each cluster omitting observations with missing values for the VAR variable; these values are not displayed	Sum of weights for each cluster based on all observations with any nonmissing value; these values are displayed in the “Cluster Summary” table.

Observations with `_TYPE_='WEIGHT'` are included only if you specify the `WEIGHT` statement.

The `_TYPE_` values included only for least squares clustering are given Table 36.3. Least squares clustering is obtained by omitting the `LEAST=` option or by specifying `LEAST=2`.

Table 36.3 `_TYPE_`

TYPE	Contents of VAR Variables	Contents of OVER_ALL
MEAN	Mean for the total sample; this is not displayed	Missing
STD	Standard deviation for the total sample; labeled “Total STD” in the output	Standard deviation pooled over all the VAR variables; labeled “Total STD” in the output
WITHIN_STD	Pooled within-cluster standard deviation	Within cluster standard deviation pooled over clusters and all the VAR variables
RSQ	R square for predicting the variable from the clusters; labeled “R-Squared” in the output	R square pooled over all the VAR variables; labeled “R-Squared” in the output
RSQ_RATIO	$\frac{R^2}{1-R^2}$; labeled “RSQ/(1-RSQ)” in the output	$\frac{R^2}{1-R^2}$; labeled “RSQ/(1-RSQ)” in the output
PSEUDO_F	Missing	Pseudo <i>F</i> statistic

Table 36.3 continued

TYPE	Contents of VAR variables	Contents of OVER_ALL
ESRQ	Missing	Approximate expected value of R square under the null hypothesis of a single uniform cluster
CCC	Missing	Cubic clustering criterion

Computational Resources

Let

- n = number of observations
- v = number of variables
- c = number of clusters
- p = number of passes over the data set

Memory

The memory required is approximately $4(19v + 12cv + 10c + 2 \max(c + 1, v))$ bytes.

If you request the DISTANCE option, an additional $4c(c + 1)$ bytes of space is needed.

Time

The overall time required by PROC FASTCLUS is roughly proportional to $nvc p$ if c is small with respect to n .

Initial seed selection requires one pass over the data set. If the observations are in random order, the time required is roughly proportional to

$$nvc + vc^2$$

unless you specify REPLACE=NONE. In that case, a complete pass might not be necessary, and the time is roughly proportional to mvc , where $c \leq m \leq n$.

The DRIFT option, each iteration, and the final assignment of cluster seeds each require one pass, with time for each pass roughly proportional to nvc .

For greatest efficiency, you should list the variables in the VAR statement in order of decreasing variance.

Using PROC FASTCLUS

Before using PROC FASTCLUS, decide whether your variables should be standardized in some way, since variables with large variances tend to have more effect on the resulting clusters than those with small variances. If all variables are measured in the same units, standardization might not be necessary. Otherwise, some form of standardization is strongly recommended. The STDIZE procedure provides a variety of standardization methods, including robust scale estimators (for detailed information, see Chapter 87, “The STDIZE Procedure”).

The FACTOR or PRINCOMP procedure can compute standardized principal component scores. The ACECLUS procedure can transform the variables according to an estimated within-cluster covariance matrix.

Nonlinear transformations of the variables can change the number of population clusters and should therefore be approached with caution. For most applications, the variables should be transformed so that equal differences are of equal practical importance. An interval scale of measurement is required. Ordinal or ranked data are generally not appropriate.

PROC FASTCLUS produces relatively little output. In most cases you should create an output data set and use another procedure such as PRINT, SGPLOT, MEANS, DISCRIM, or CANDISC to study the clusters. It is usually desirable to try several values of the MAXCLUSTERS= option. Macros are useful for running PROC FASTCLUS repeatedly with other procedures.

A simple application of PROC FASTCLUS with two variables to examine the 2- and 3-cluster solutions can proceed as follows:

```
proc stdize method=std out=stan;
  var v1 v2;
run;

proc fastclus data=stan out=clust maxclusters=2;
  var v1 v2;
run;

proc sgplot;
  scatter y=v2 x=v1 / markerchar=cluster;
run;

proc fastclus data=stan out=clust maxclusters=3;
  var v1 v2;
run;

proc sgplot;
  scatter y=v2 x=v1 / markerchar=cluster;
run;
```

If you have more than two variables, you can use the CANDISC procedure to compute canonical variables for plotting the clusters. For example:


```

proc stdize method=std out=stan;
  var v1-v10;
run;

proc fastclus data=stan out=clust maxclusters=3;
  var v1-v10;
run;

proc candisc out=can;
  var v1-v10;
  class cluster;
run;

proc sgplot;
  scatter y=can2 x=can1 / markerchar=cluster;
run;

```

If the data set is not too large, it might also be helpful to use the following to list the clusters:

```

proc sort;
  by cluster distance;
run;

proc print;
  by cluster;
run;

```

By examining the values of `DISTANCE`, you can determine if any observations are unusually far from their cluster seeds.

It is often advisable, especially if the data set is large or contains outliers, to make a preliminary PROC FASTCLUS run with a large number of clusters, perhaps 20 to 100. Use `MAXITER=0` and `OUTSEED=SAS-data-set`. You can save time on subsequent runs if you select cluster seeds from this output data set by using the `SEED=` option.

You should check the preliminary clusters for outliers, which often appear as clusters with only one member. Use a `DATA` step to delete outliers from the data set created by the `OUTSEED=` option before using it as a `SEED=` data set in later runs. If there are severe outliers, you should specify the `STRICT` option in the subsequent PROC FASTCLUS runs to prevent the outliers from distorting the clusters.

You can use the `OUTSEED=` data set with the `SGPLOT` procedure to plot `_GAP_` by `_FREQ_`. An overlay of `_RADIUS_` by `_FREQ_` provides a baseline against which to compare the values of `_GAP_`. Outliers appear in the upper-left area of the plot, with large `_GAP_` values and small `_FREQ_` values. Good clusters appear in the upper-right area, with large values of both `_GAP_` and `_FREQ_`. Good potential cluster seeds appear in the lower right, as well as in the upper-right, since large `_FREQ_` values indicate high-density regions. Small `_FREQ_` values in the left part of the plot indicate poor cluster seeds because the points are in low-density regions. It often helps to remove all clusters with small frequencies even though the clusters might not be remote enough to be considered outliers. Removing points in low-density regions improves cluster separation and provides visually sharper cluster outlines in scatter plots.

Displayed Output

Unless the `SHORT` or `SUMMARY` option is specified, PROC FASTCLUS displays the following:

- Initial Seeds, cluster seeds selected after one pass through the data
- Change in Cluster Seeds for each iteration, if you specify `MAXITER= $n > 1$`

If you specify the `LEAST= p` option, with $(1 < p < 2)$, and you omit the `IRLS` option, an additional column is displayed in the Iteration History table. This column contains a character to identify the method used in each iteration. PROC FASTCLUS chooses the most efficient method to cluster the data at each iterative step, given the condition of the data. Thus, the method chosen is data dependent. The possible values are described as follows:

Value	Method
N	Newton's Method
I or L	iteratively weighted least squares (IRLS)
1	IRLS step, halved once
2	IRLS step, halved twice
3	IRLS step, halved three times

PROC FASTCLUS displays a Cluster Summary, giving the following for each cluster:

- Cluster number
- Frequency, the number of observations in the cluster
- Weight, the sum of the weights of the observations in the cluster, if you specify the `WEIGHT` statement
- RMS Std Deviation, the root mean squared across variables of the cluster standard deviations, which is equal to the root mean square distance between observations in the cluster
- Maximum Distance from Seed to Observation, the maximum distance from the cluster seed to any observation in the cluster
- Nearest Cluster, the number of the cluster with mean closest to the mean of the current cluster
- Centroid Distance, the distance between the centroids (means) of the current cluster and the nearest other cluster

A table of statistics for each variable is displayed unless you specify the `SUMMARY` option. The table contains the following:

- Total STD, the total standard deviation
- Within STD, the pooled within-cluster standard deviation

- R-Square, the R square for predicting the variable from the cluster
- RSQ/(1 - RSQ), the ratio of between-cluster variance to within-cluster variance ($R^2/(1 - R^2)$)
- OVER-ALL, all of the previous quantities pooled across variables

PROC FASTCLUS also displays the following:

- Pseudo F Statistic,

$$\frac{\frac{R^2}{c-1}}{\frac{1-R^2}{n-c}}$$

where R square is the observed overall R square, c is the number of clusters, and n is the number of observations. The pseudo F statistic was suggested by Calinski and Harabasz (1974). See Milligan and Cooper (1985) and Cooper and Milligan (1988) regarding the use of the pseudo F statistic in estimating the number of clusters. See Example 31.2 in Chapter 31, “The CLUSTER Procedure,” for a comparison of pseudo F statistics.

- Observed Overall R-Square, if you specify the SUMMARY option
- Approximate Expected Overall R-Square, the approximate expected value of the overall R square under the uniform null hypothesis assuming that the variables are uncorrelated. The value is missing if the number of clusters is greater than one-fifth the number of observations.
- Cubic Clustering Criterion, computed under the assumption that the variables are uncorrelated. The value is missing if the number of clusters is greater than one-fifth the number of observations.

If you are interested in the approximate expected R square or the cubic clustering criterion but your variables are correlated, you should cluster principal component scores from the PRINCOMP procedure. Both of these statistics are described by Sarle (1983). The performance of the cubic clustering criterion in estimating the number of clusters is examined by Milligan and Cooper (1985) and Cooper and Milligan (1988).

- Distances Between Cluster Means, if you specify the DISTANCE option

Unless you specify the SHORT or SUMMARY option, PROC FASTCLUS displays the following:

- Cluster Means for each variable
- Cluster Standard Deviations for each variable

ODS Table Names

PROC FASTCLUS assigns a name to each table it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in Table 36.4. For more information on ODS, see Chapter 20, “Using the Output Delivery System.”

Table 36.4 ODS Tables Produced by PROC FASTCLUS

ODS Table Name	Description	Statement	Option
ApproxExpOverAllRSq	Approximate expected overall R-square, single number	PROC	default
CCC	CCC, Cubic Clustering Criterion, single number	PROC	default
ClusterList	Cluster listing, obs, id, and distances	PROC	LIST
ClusterSum	Cluster summary, cluster number, distances	PROC	PRINTALL
ClusterCenters	Cluster centers	PROC	default
ClusterDispersion	Cluster dispersion	PROC	default
ConvergenceStatus	Convergence status	PROC	PRINTALL
Criterion	Criterion based on final seeds, single number	PROC	default
DistBetweenClust	Distance between clusters	PROC	default
InitialSeeds	Initial seeds	PROC	default
IterHistory	Iteration history, various statistics for each iteration	PROC	PRINTALL
MinDist	Minimum distance between initial seeds, single number	PROC	PRINTALL
NumberOfBins	Number of bins	PROC	default
ObsOverAllRSquare	Observed overall R-square, single number	PROC	SUMMARY
PrelScaleEst	Preliminary L(1) scale estimate, single number	PROC	PRINTALL
PseudoFStat	Pseudo F statistic, single number	PROC	default
SimpleStatistics	Simple statistics for input variables	PROC	default
VariableStat	Statistics for variables within clusters	PROC	default

Examples: FASTCLUS Procedure

Example 36.1: Fisher's Iris Data

The iris data published by Fisher (1936) have been widely used for examples in discriminant analysis and cluster analysis. The sepal length, sepal width, petal length, and petal width are measured in millimeters on 50 iris specimens from each of three species, *Iris setosa*, *I. versicolor*, and *I. virginica*. Mezzich and Solomon (1980) discuss a variety of cluster analyses of the iris data.

In this example, the FASTCLUS procedure is used to find two and then three clusters. In the following code, an output data set is created, and PROC FREQ is invoked to compare the clusters with the species classification. See [Output 36.1.1](#) and [Output 36.1.2](#) for these results.

For three clusters, you can use the CANDISC procedure to compute canonical variables for plotting the clusters. See [Output 36.1.3](#) and [Output 36.1.4](#) for the results.

```
title 'Fisher (1936) Iris Data';
proc fastclus data=sashelp.iris maxc=2 maxiter=10 out=clus;
  var SepalLength SepalWidth PetalLength PetalWidth;
run;

proc freq;
  tables cluster*species;
run;

proc fastclus data=sashelp.iris maxc=3 maxiter=10 out=clus;
  var SepalLength SepalWidth PetalLength PetalWidth;
run;

proc freq;
  tables cluster*Species;
run;

proc candisc anova out=can;
  class cluster;
  var SepalLength SepalWidth PetalLength PetalWidth;
  title2 'Canonical Discriminant Analysis of Iris Clusters';
run;

proc sgplot data=Can;
  scatter y=Can2 x=Can1 / group=Cluster;
  title2 'Plot of Canonical Variables Identified by Cluster';
run;
```

Output 36.1.1 Fisher's Iris Data: PROC FASTCLUS with MAXC=2 and PROC FREQ

```

Fisher (1936) Iris Data

The FASTCLUS Procedure
Replace=FULL Radius=0 Maxclusters=2 Maxiter=10 Converge=0.02

Initial Seeds

Cluster      SepalLength      SepalWidth      PetalLength      PetalWidth
-----
1            77.00000000      26.00000000      69.00000000      23.00000000
2            45.00000000      23.00000000      13.00000000      3.00000000

Minimum Distance Between Initial Seeds = 67.59438

Iteration History

Iteration      Criterion      Relative Change
                in Cluster Seeds
                1          2
-----
1             11.0045      0.3169      0.2164
2              5.6161      0.0379      0.0791
3              5.1042      0.0133      0.0306
4              5.0417      0.00348     0.00679

Convergence criterion is satisfied.

Criterion Based on Final Seeds = 5.0390

Cluster Summary

Cluster      Frequency      RMS Std      Maximum Distance
                Deviation      from Seed
                to Observation      Radius      Nearest
                Exceeded      Cluster
-----
1             97            5.6779      24.8448
2             53            3.7050      21.6197

Cluster Summary

Cluster      Distance Between
                Cluster Centroids
-----
1             39.2879
2             39.2879
    
```

Output 36.1.1 continued

Statistics for Variables				
Variable	Total STD	Within STD	R-Square	RSQ/(1-RSQ)
SepalLength	8.28066	5.49313	0.562896	1.287784
SepalWidth	4.35866	3.70393	0.282710	0.394137
PetalLength	17.65298	6.80331	0.852470	5.778291
PetalWidth	7.62238	3.57200	0.781868	3.584390
OVER-ALL	10.69224	5.07291	0.776410	3.472463

Pseudo F Statistic = 513.92

Approximate Expected Over-All R-Squared = 0.51539

Cubic Clustering Criterion = 14.806

WARNING: The two values above are invalid for correlated variables.

Cluster Means				
Cluster	SepalLength	SepalWidth	PetalLength	PetalWidth
1	63.01030928	28.86597938	49.58762887	16.95876289
2	50.05660377	33.69811321	15.60377358	2.90566038

Cluster Standard Deviations				
Cluster	SepalLength	SepalWidth	PetalLength	PetalWidth
1	6.336887455	3.267991438	7.800577673	4.155612484
2	3.427350930	4.396611045	4.404279486	2.105525249

Output 36.1.1 *continued*

```

Fisher (1936) Iris Data

The FREQ Procedure

Table of CLUSTER by Species

CLUSTER(Cluster)      Species(Iris Species)

Frequency|
Percent   |
Row Pct   |
Col Pct   |Setosa  |Versicol|Virginic|  Total
          |   or   |   a    |
-----+-----+-----+-----+
          1 |     0  |    47  |    50  |    97
          |  0.00 |  31.33 |  33.33 |  64.67
          |  0.00 |  48.45 |  51.55 |
          |  0.00 |  94.00 | 100.00 |
-----+-----+-----+-----+
          2 |    50  |     3  |     0  |    53
          | 33.33 |    2.00 |    0.00 |  35.33
          | 94.34 |    5.66 |    0.00 |
          |100.00 |    6.00 |    0.00 |
-----+-----+-----+-----+
Total      50      50      50      150
          33.33  33.33  33.33  100.00
    
```

Output 36.1.2 Fisher's Iris Data: PROC FASTCLUS with MAXC=3 and PROC FREQ

```

Fisher (1936) Iris Data

The FASTCLUS Procedure

Replace=FULL Radius=0 Maxclusters=3 Maxiter=10 Converge=0.02

Initial Seeds

Cluster      SepalLength      SepalWidth      PetalLength      PetalWidth
-----+-----+-----+-----+
1            77.00000000      38.00000000      67.00000000      22.00000000
2            57.00000000      44.00000000      15.00000000      4.00000000
3            49.00000000      25.00000000      45.00000000      17.00000000

Minimum Distance Between Initial Seeds = 38.23611

Iteration History

Iteration      Criterion      Relative Change in Cluster Seeds
          1          2          3
-----+-----+-----+-----+
1            7.0151      0.3205      0.3151      0.2985
2            3.7097      0.0459      0          0.0317
3            3.6427      0.0182      0          0.0124
    
```


Output 36.1.2 continued

Convergence criterion is satisfied.

Criterion Based on Final Seeds = 3.6289

Cluster Summary

Cluster	Frequency	RMS Std Deviation	Maximum Distance from Seed to Observation	Radius Exceeded	Nearest Cluster
1	38	4.0168	14.9736		3
2	50	2.7803	12.4803		3
3	62	4.0398	16.9272		1

Cluster Summary

Cluster	Distance Between Cluster Centroids
1	17.9718
2	33.5693
3	17.9718

Statistics for Variables

Variable	Total STD	Within STD	R-Square	RSQ/(1-RSQ)
SepalLength	8.28066	4.39488	0.722096	2.598359
SepalWidth	4.35866	3.24816	0.452102	0.825156
PetalLength	17.65298	4.21431	0.943773	16.784895
PetalWidth	7.62238	2.45244	0.897872	8.791618
OVER-ALL	10.69224	3.66198	0.884275	7.641194

Pseudo F Statistic = 561.63

Approximate Expected Over-All R-Squared = 0.62728

Cubic Clustering Criterion = 25.021

WARNING: The two values above are invalid for correlated variables.

Cluster Means

Cluster	SepalLength	SepalWidth	PetalLength	PetalWidth
1	68.5000000	30.73684211	57.42105263	20.71052632
2	50.0600000	34.28000000	14.62000000	2.46000000
3	59.01612903	27.48387097	43.93548387	14.33870968

Output 36.1.2 *continued*

Cluster Standard Deviations				
Cluster	SepalLength	SepalWidth	PetalLength	PetalWidth
1	4.941550255	2.900924461	4.885895746	2.798724562
2	3.524896872	3.790643691	1.736639965	1.053855894
3	4.664100551	2.962840548	5.088949673	2.974997167

Fisher (1936) Iris Data

The FREQ Procedure

Table of CLUSTER by Species

CLUSTER(Cluster)	Species(Iris Species)			Total
Frequency	Setosa	Versicol	Virginic	
Percent		or	a	
Row Pct				
Col Pct	Setosa	Versicol	Virginic	Total
		or	a	
1	0	2	36	38
	0.00	1.33	24.00	25.33
	0.00	5.26	94.74	
	0.00	4.00	72.00	
2	50	0	0	50
	33.33	0.00	0.00	33.33
	100.00	0.00	0.00	
	100.00	0.00	0.00	
3	0	48	14	62
	0.00	32.00	9.33	41.33
	0.00	77.42	22.58	
	0.00	96.00	28.00	
Total	50	50	50	150
	33.33	33.33	33.33	100.00

Output 36.1.3 Fisher's Iris Data using PROC CANDISC

Fisher (1936) Iris Data
Canonical Discriminant Analysis of Iris Clusters

The CANDISC Procedure

Total Sample Size	150	DF Total	149
Variables	4	DF Within Classes	147
Classes	3	DF Between Classes	2

Output 36.1.3 continued

Number of Observations Read		150					
Number of Observations Used		150					
Class Level Information							
CLUSTER	Variable Name	Frequency	Weight	Proportion			
1	_1	38	38.0000	0.253333			
2	_2	50	50.0000	0.333333			
3	_3	62	62.0000	0.413333			
Fisher (1936) Iris Data Canonical Discriminant Analysis of Iris Clusters							
The CANDISC Procedure							
Univariate Test Statistics							
F Statistics, Num DF=2, Den DF=147							
Variable Label	Total Standard Deviation	Pooled Standard Deviation	Between Standard Deviation	R-Square	R-Square / (1-RSq)	F Value	Pr > F
Sepal Length (mm)	8.2807	4.3949	8.5893	0.7221	2.5984	190.98	<.0001
Sepal Width (mm)	4.3587	3.2482	3.5774	0.4521	0.8252	60.65	<.0001
Petal Length (mm)	17.6530	4.2143	20.9336	0.9438	16.7849	1233.69	<.0001
Petal Width (mm)	7.6224	2.4524	8.8164	0.8979	8.7916	646.18	<.0001
Average R-Square							
Unweighted			0.7539604				
Weighted by Variance			0.8842753				

Output 36.1.3 continued

Multivariate Statistics and F Approximations					
S=2 M=0.5 N=71					
Statistic	Value	F Value	Num DF	Den DF	Pr > F
Wilks' Lambda	0.03222337	164.55	8	288	<.0001
Pillai's Trace	1.25669612	61.29	8	290	<.0001
Hotelling-Lawley Trace	21.06722883	377.66	8	203.4	<.0001
Roy's Greatest Root	20.63266809	747.93	4	145	<.0001
NOTE: F Statistic for Roy's Greatest Root is an upper bound.					
NOTE: F Statistic for Wilks' Lambda is exact.					
Fisher (1936) Iris Data					
Canonical Discriminant Analysis of Iris Clusters					
The CANDISC Procedure					
	Canonical Correlation	Adjusted Canonical Correlation	Approximate Standard Error	Squared Canonical Correlation	
1	0.976613	0.976123	0.003787	0.953774	
2	0.550384	0.543354	0.057107	0.302923	
Eigenvalues of Inv(E)*H = CanRsqr/(1-CanRsqr)					
	Eigenvalue	Difference	Proportion	Cumulative	
1	20.6327	20.1981	0.9794	0.9794	
2	0.4346		0.0206	1.0000	
Test of H0: The canonical correlations in the current row and all that follow are zero					
	Likelihood Ratio	Approximate F Value	Num DF	Den DF	Pr > F
1	0.03222337	164.55	8	288	<.0001
2	0.69707749	21.00	3	145	<.0001

Output 36.1.3 continued

Fisher (1936) Iris Data
 Canonical Discriminant Analysis of Iris Clusters

The CANDISC Procedure

Total Canonical Structure

Variable	Label	Can1	Can2
SepalLength	Sepal Length (mm)	0.831965	0.452137
SepalWidth	Sepal Width (mm)	-0.515082	0.810630
PetalLength	Petal Length (mm)	0.993520	0.087514
PetalWidth	Petal Width (mm)	0.966325	0.154745

Between Canonical Structure

Variable	Label	Can1	Can2
SepalLength	Sepal Length (mm)	0.956160	0.292846
SepalWidth	Sepal Width (mm)	-0.748136	0.663545
PetalLength	Petal Length (mm)	0.998770	0.049580
PetalWidth	Petal Width (mm)	0.995952	0.089883

Pooled Within Canonical Structure

Variable	Label	Can1	Can2
SepalLength	Sepal Length (mm)	0.339314	0.716082
SepalWidth	Sepal Width (mm)	-0.149614	0.914351
PetalLength	Petal Length (mm)	0.900839	0.308136
PetalWidth	Petal Width (mm)	0.650123	0.404282

Fisher (1936) Iris Data
 Canonical Discriminant Analysis of Iris Clusters

The CANDISC Procedure

Total-Sample Standardized Canonical Coefficients

Variable	Label	Can1	Can2
SepalLength	Sepal Length (mm)	0.047747341	1.021487262
SepalWidth	Sepal Width (mm)	-0.577569244	0.864455153
PetalLength	Petal Length (mm)	3.341309573	-1.283043758
PetalWidth	Petal Width (mm)	0.996451144	0.900476563

Output 36.1.3 *continued*

Pooled Within-Class Standardized Canonical Coefficients

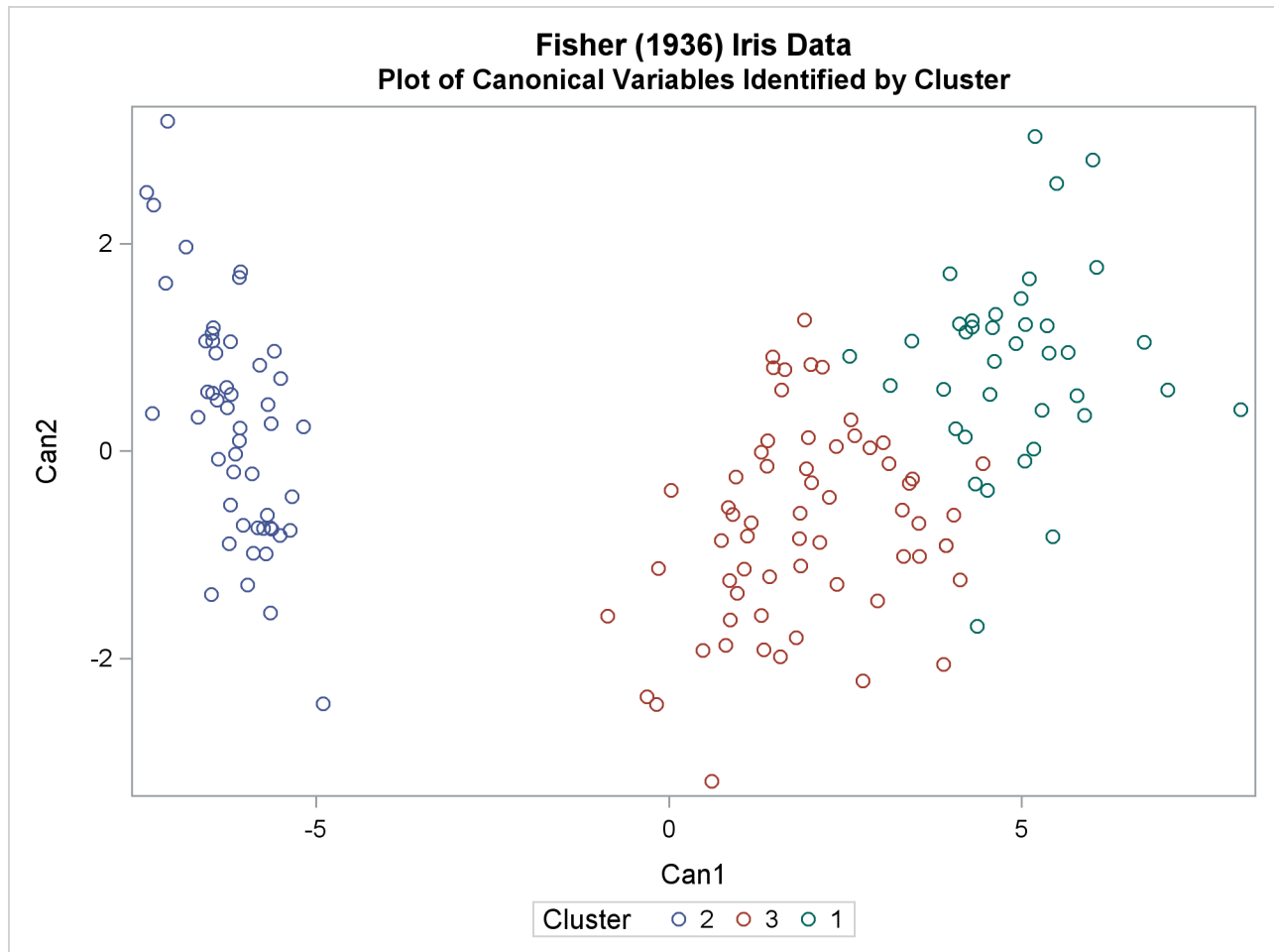
Variable	Label	Can1	Can2
SepalLength	Sepal Length (mm)	0.0253414487	0.5421446856
SepalWidth	Sepal Width (mm)	-.4304161258	0.6442092294
PetalLength	Petal Length (mm)	0.7976741592	-.3063023132
PetalWidth	Petal Width (mm)	0.3205998034	0.2897207865

Raw Canonical Coefficients

Variable	Label	Can1	Can2
SepalLength	Sepal Length (mm)	0.0057661265	0.1233581748
SepalWidth	Sepal Width (mm)	-.1325106494	0.1983303556
PetalLength	Petal Length (mm)	0.1892773419	-.0726814163
PetalWidth	Petal Width (mm)	0.1307270927	0.1181359305

Class Means on Canonical Variables

CLUSTER	Can1	Can2
1	4.931414018	0.861972277
2	-6.131527227	0.244761516
3	1.922300462	-0.725693908

Output 36.1.4 Plot of Fisher's Iris Data using PROC CANDISC

Example 36.2: Outliers

This example involves data artificially generated to contain two clusters and several severe outliers. A preliminary analysis specifies 20 clusters and outputs an `OUTSEED=` data set to be used for a diagnostic plot. The exact number of initial clusters is not important; similar results could be obtained with 10 or 50 initial clusters. Examination of the plot suggests that clusters with more than five (again, the exact number is not important) observations can yield good seeds for the main analysis. A `DATA` step deletes clusters with five or fewer observations, and the remaining cluster means provide seeds for the next PROC FASTCLUS analysis.

Two clusters are requested; the `LEAST=` option specifies the mean absolute deviation criterion (`LEAST=1`). Values of the `LEAST=` option less than 2 reduce the effect of outliers on cluster centers.

The next analysis also requests two clusters; the `STRICT=` option is specified to prevent outliers from distorting the results. The `STRICT=` value is chosen to be close to the `_GAP_` and `_RADIUS_` values of the larger clusters in the diagnostic plot; the exact value is not critical.

A final PROC FASTCLUS run assigns the outliers to clusters.

The following SAS statements implement these steps, and the results are displayed in [Output 36.2.3](#) through [Output 36.2.8](#). First, an artificial data set is created with two clusters and some outliers. Then PROC FASTCLUS is run with many clusters to produce an OUTSEED= data set. A diagnostic plot using the variables `_GAP_` and `_RADIUS_` is then produced using the SGSCATTER procedure. The results from these steps are shown in [Output 36.2.1](#) and [Output 36.2.2](#).

```

title 'Using PROC FASTCLUS to Analyze Data with Outliers';
data x;
  drop n;
  do n=1 to 100;
    x=rannor(12345)+2;
    y=rannor(12345);
    output;
  end;
  do n=1 to 100;
    x=rannor(12345)-2;
    y=rannor(12345);
    output;
  end;
  do n=1 to 10;
    x=10*rannor(12345);
    y=10*rannor(12345);
    output;
  end;
run;

title2 'Preliminary PROC FASTCLUS Analysis with 20 Clusters';
proc fastclus data=x outseed=mean1 maxc=20 maxiter=0 summary;
  var x y;
run;

proc sgscatter data=mean1;
  compare y=( _gap_ _radius_ ) x=_freq_;
run;

```

Output 36.2.1 Preliminary Analysis of Data with Outliers Using PROC FASTCLUS

```

Using PROC FASTCLUS to Analyze Data with Outliers
Preliminary PROC FASTCLUS Analysis with 20 Clusters

The FASTCLUS Procedure
Replace=FULL Radius=0 Maxclusters=20 Maxiter=0

Criterion Based on Final Seeds = 0.6873

```


Output 36.2.1 continued

Cluster Summary					
Cluster	Frequency	RMS Std Deviation	Maximum Distance from Seed to Observation	Radius Exceeded	Nearest Cluster
1	8	0.4753	1.1924		19
2	1	.	0		6
3	44	0.6252	1.6774		5
4	1	.	0		20
5	38	0.5603	1.4528		3
6	2	0.0542	0.1085		2
7	1	.	0		14
8	2	0.6480	1.2961		1
9	1	.	0		7
10	1	.	0		18
11	1	.	0		16
12	20	0.5911	1.6291		16
13	5	0.6682	1.4244		3
14	1	.	0		7
15	5	0.4074	1.2678		3
16	22	0.4168	1.5139		19
17	8	0.4031	1.4794		5
18	1	.	0		10
19	45	0.6475	1.6285		16
20	3	0.5719	1.3642		15

Cluster Summary	
Cluster	Distance Between Cluster Centroids
1	1.7205
2	6.2847
3	1.4386
4	5.2130
5	1.4386
6	6.2847
7	2.5094
8	1.8450
9	9.4534
10	4.2514
11	4.7582
12	1.5601
13	1.9553
14	2.5094
15	1.7609
16	1.4936
17	1.5564
18	4.2514
19	1.4936
20	1.8999

Pseudo F Statistic = 207.58

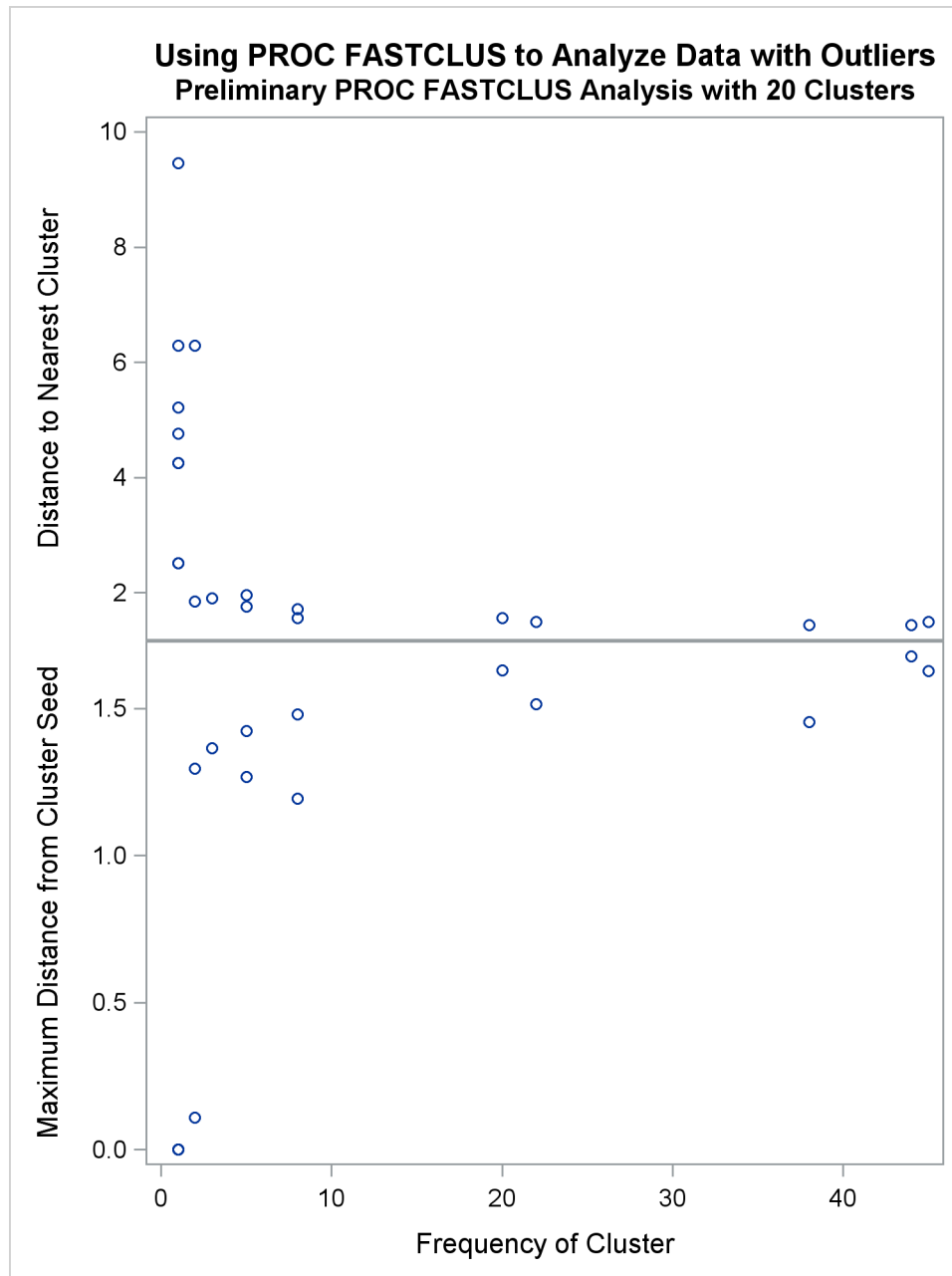
Output 36.2.1 *continued*

Observed Over-All R-Squared = 0.95404

Approximate Expected Over-All R-Squared = 0.96103

Cubic Clustering Criterion = -2.503

WARNING: The two values above are invalid for correlated variables.

Output 36.2.2 Preliminary Analysis of Data with Outliers: Plot Using and PROC SGSCATGTER

In the following SAS statements, a DATA step is used to remove low frequency clusters, then the FASTCLUS procedure is run again, selecting seeds from the high frequency clusters in the previous analysis using LEAST=1 clustering criterion. The results are shown in [Output 36.2.3](#) and [Output 36.2.4](#).

```

data seed;
  set mean1;
  if _freq_>5;
run;

title2 'PROC FASTCLUS Analysis Using LEAST= Clustering Criterion';

```

```

title3 'Values < 2 Reduce Effect of Outliers on Cluster Centers';
proc fastclus data=x seed=seed maxc=2 least=1 out=out;
  var x y;
run;

proc sgplot data=out;
  scatter y=y x=x / group=cluster;
run;

```

Output 36.2.3 Analysis of Data with Outliers Using the LEAST= Option

```

Using PROC FASTCLUS to Analyze Data with Outliers
PROC FASTCLUS Analysis Using LEAST= Clustering Criterion
Values < 2 Reduce Effect of Outliers on Cluster Centers

The FASTCLUS Procedure
Replace=FULL Radius=0 Maxclusters=2 Maxiter=20 Converge=0.0001 Least=1

Initial Seeds

Cluster          x          y
-----
1          2.794174248      -0.065970836
2          -2.027300384      -2.051208579

Minimum Distance Between Initial Seeds = 6.806712

Preliminary L(1) Scale Estimate =          2.796579

Number of Bins =          100

Iteration History

Iteration  Criterion  Maximum  Relative Change
          Bin Size  in Cluster Seeds
          1          2
-----
1          1.3983    0.2263    0.4091    0.6696
2          1.0776    0.0226    0.00511   0.0452
3          1.0771    0.00226   0.00229   0.00234
4          1.0771    0.000396  0.000253  0.000144
5          1.0771    0.000396          0          0

Convergence criterion is satisfied.

Criterion Based on Final Seeds = 1.0771

```

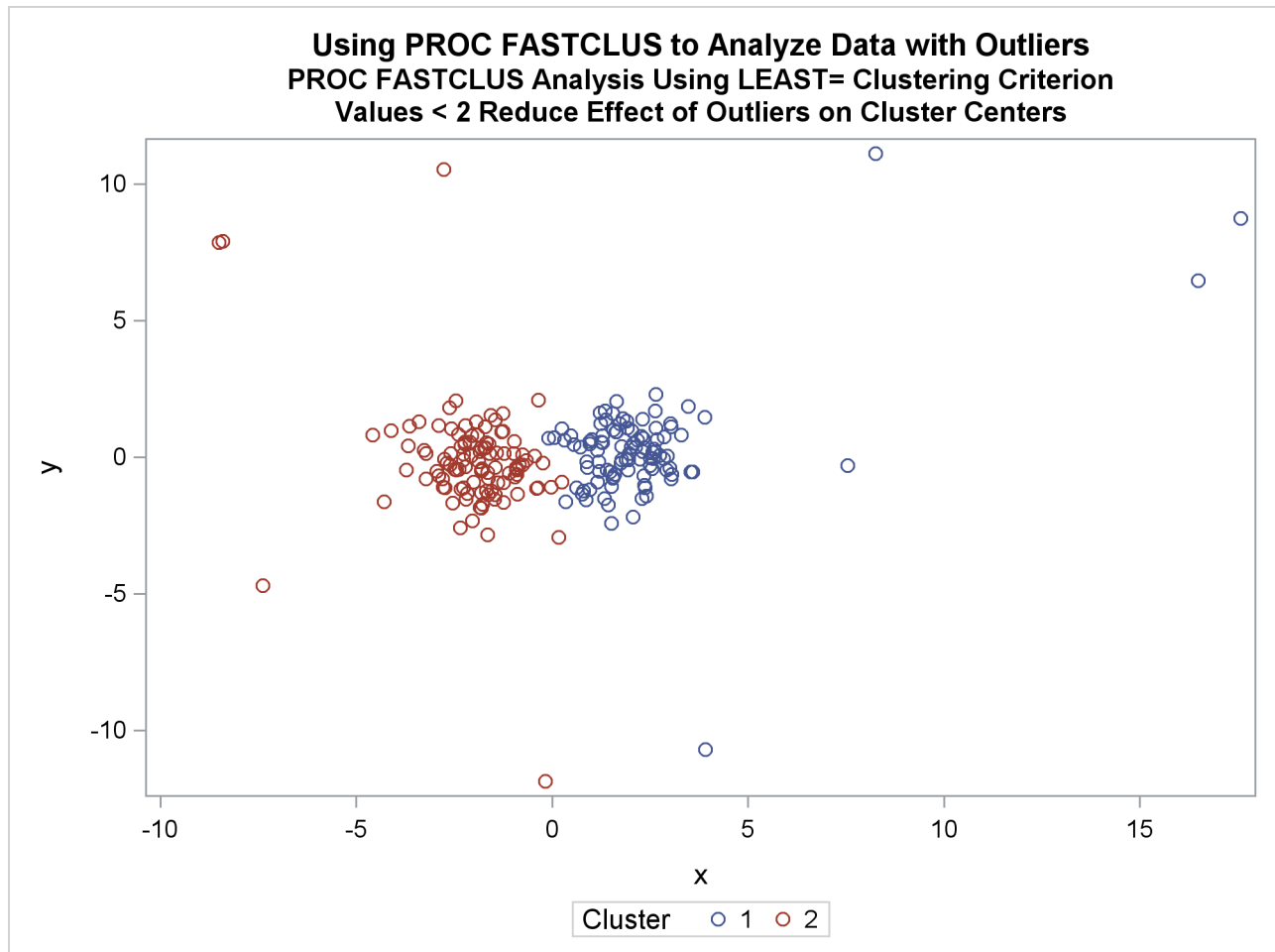
Output 36.2.3 continued

Cluster Summary					
Cluster	Frequency	Mean Absolute Deviation	Maximum Distance from Seed to Observation	Radius Exceeded	Nearest Cluster
1	102	1.1278	24.1622		2
2	108	1.0494	14.8292		1

Cluster Summary	
Cluster	Distance Between Cluster Medians
1	4.2585
2	4.2585

Cluster Medians		
Cluster	x	y
1	1.923023887	0.222482918
2	-1.826721743	-0.286253041

Mean Absolute Deviations from Final Seeds		
Cluster	x	y
1	1.113465261	1.142120480
2	0.890331835	1.208370913

Output 36.2.4 Analysis Plot of Data with Outliers

The FASTCLUS procedure is run again, selecting seeds from high frequency clusters in the previous analysis. `STRICT=` prevents outliers from distorting the results. The results are shown in [Output 36.2.5](#) and [Output 36.2.6](#).

```

title2 'PROC FASTCLUS Analysis Using STRICT= to Omit Outliers';
proc fastclus data=x seed=seed
    maxc=2 strict=3.0 out=out outseed=mean2;
    var x y;
run;

proc sgplot data=out;
    scatter y=y x=x / group=cluster;
run;

```

Output 36.2.5 Cluster Analysis with Outliers Omitted: PROC FASTCLUS SGPLOT

```

Using PROC FASTCLUS to Analyze Data with Outliers
PROC FASTCLUS Analysis Using STRICT= to Omit Outliers

The FASTCLUS Procedure
Replace=FULL Radius=0 Strict=3 Maxclusters=2 Maxiter=1

Initial Seeds

Cluster          x          y
-----
1          2.794174248      -0.065970836
2          -2.027300384      -2.051208579

Criterion Based on Final Seeds = 0.9515

Cluster Summary

Cluster          Frequency          RMS Std          Maximum Distance
                   Deviation          from Seed
                   to Observation          Radius          Nearest
                   Exceeded          Cluster
-----
1              99          0.9501          2.9589          2
2              99          0.9290          2.8011          1

Cluster Summary

Cluster          Distance Between
                   Cluster Centroids
-----
1              3.7666
2              3.7666

12 Observation(s) were not assigned to a cluster
because the minimum distance to a cluster seed exceeded the STRICT= value.

Statistics for Variables

Variable          Total STD          Within STD          R-Square          RSQ/(1-RSQ)
-----
x              2.06854          0.87098          0.823609          4.669219
y              1.02113          1.00352          0.039093          0.040683
OVER-ALL          1.63119          0.93959          0.669891          2.029303

Pseudo F Statistic = 397.74

Approximate Expected Over-All R-Squared = 0.60615

Cubic Clustering Criterion = 3.197

```

Output 36.2.5 continued

WARNING: The two values above are invalid for correlated variables.

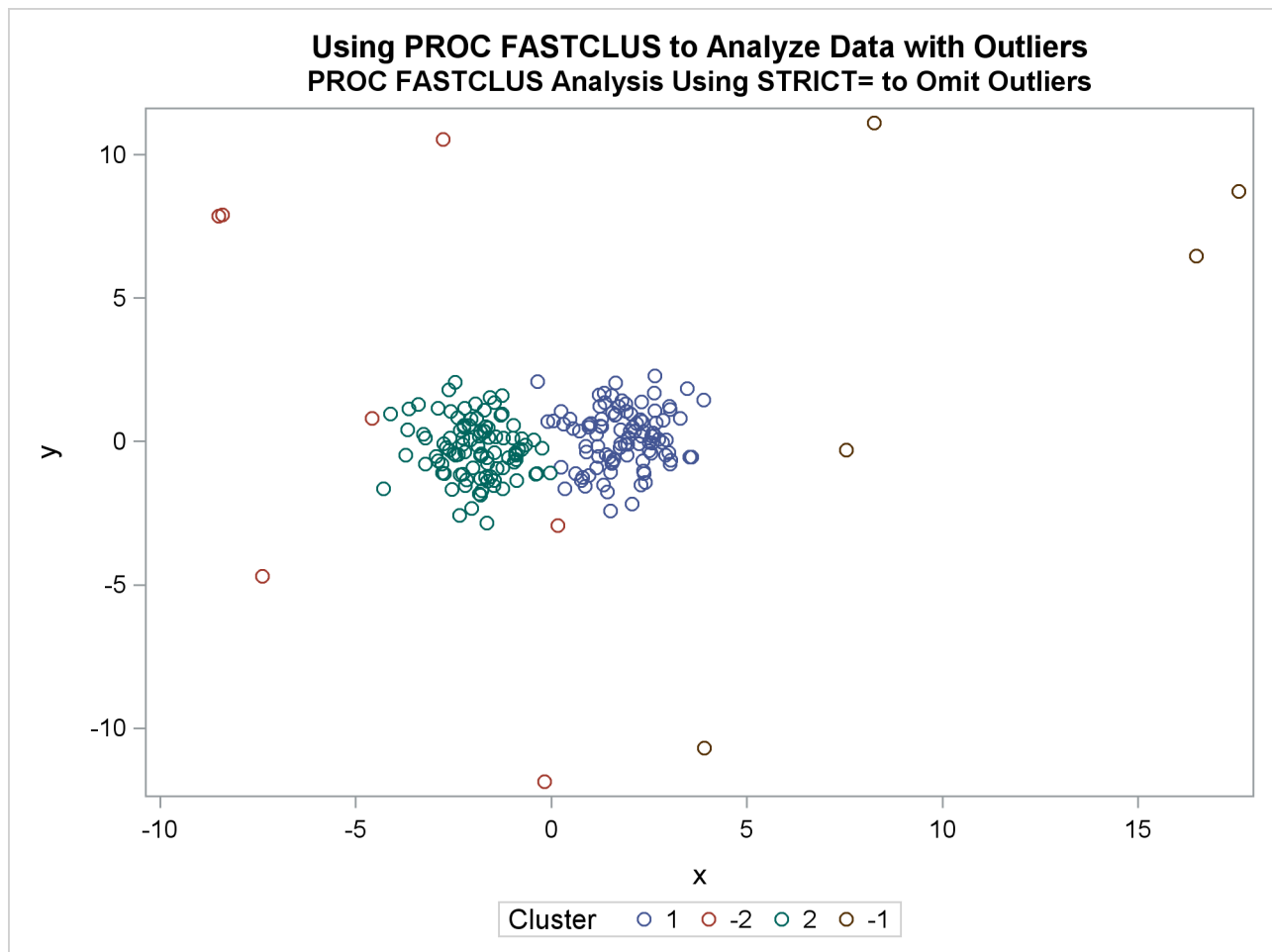
Cluster Means

Cluster	x	y
1	1.825111432	0.141211701
2	-1.919910712	-0.261558725

Cluster Standard Deviations

Cluster	x	y
1	0.889549271	1.006965219
2	0.852000588	1.000062579

Output 36.2.6 Cluster Analysis with Outliers Omitted: Plot Using PROC SGPLOT



Finally, the FASTCLUS procedure is run one more time with zero iterations to assign outliers and tails to clusters. The results are shown in [Output 36.2.7](#) and [Output 36.2.8](#).

```

title2 'Final PROC FASTCLUS Analysis Assigning Outliers to Clusters';
proc fastclus data=x seed=mean2 maxc=2 maxiter=0 out=out;
  var x y;
run;

proc sgplot data=out;
  scatter y=y x=x / group=cluster;
run;

```

Output 36.2.7 Cluster Analysis with Outliers Omitted: PROC FASTCLUS

Using PROC FASTCLUS to Analyze Data with Outliers					
Final PROC FASTCLUS Analysis Assigning Outliers to Clusters					
The FASTCLUS Procedure					
Replace=FULL Radius=0 Maxclusters=2 Maxiter=0					
Initial Seeds					
Cluster	x	y			
1	1.825111432	0.141211701			
2	-1.919910712	-0.261558725			
Criterion Based on Final Seeds = 2.0594					
Cluster Summary					
Cluster	Frequency	RMS Std Deviation	Maximum Distance from Seed to Observation	Radius Exceeded	Nearest Cluster
1	103	2.2569	17.9426		2
2	107	1.8371	11.7362		1
Cluster Summary					
Cluster	Distance Between Cluster Centroids				
1	4.3753				
2	4.3753				
Statistics for Variables					
Variable	Total STD	Within STD	R-Square	RSQ/(1-RSQ)	
x	2.92721	1.95529	0.555950	1.252000	
y	2.15248	2.14754	0.009347	0.009435	
OVER-ALL	2.56922	2.05367	0.364119	0.572621	

Output 36.2.7 *continued*

Pseudo F Statistic = 119.11

Approximate Expected Over-All R-Squared = 0.49090

Cubic Clustering Criterion = -5.338

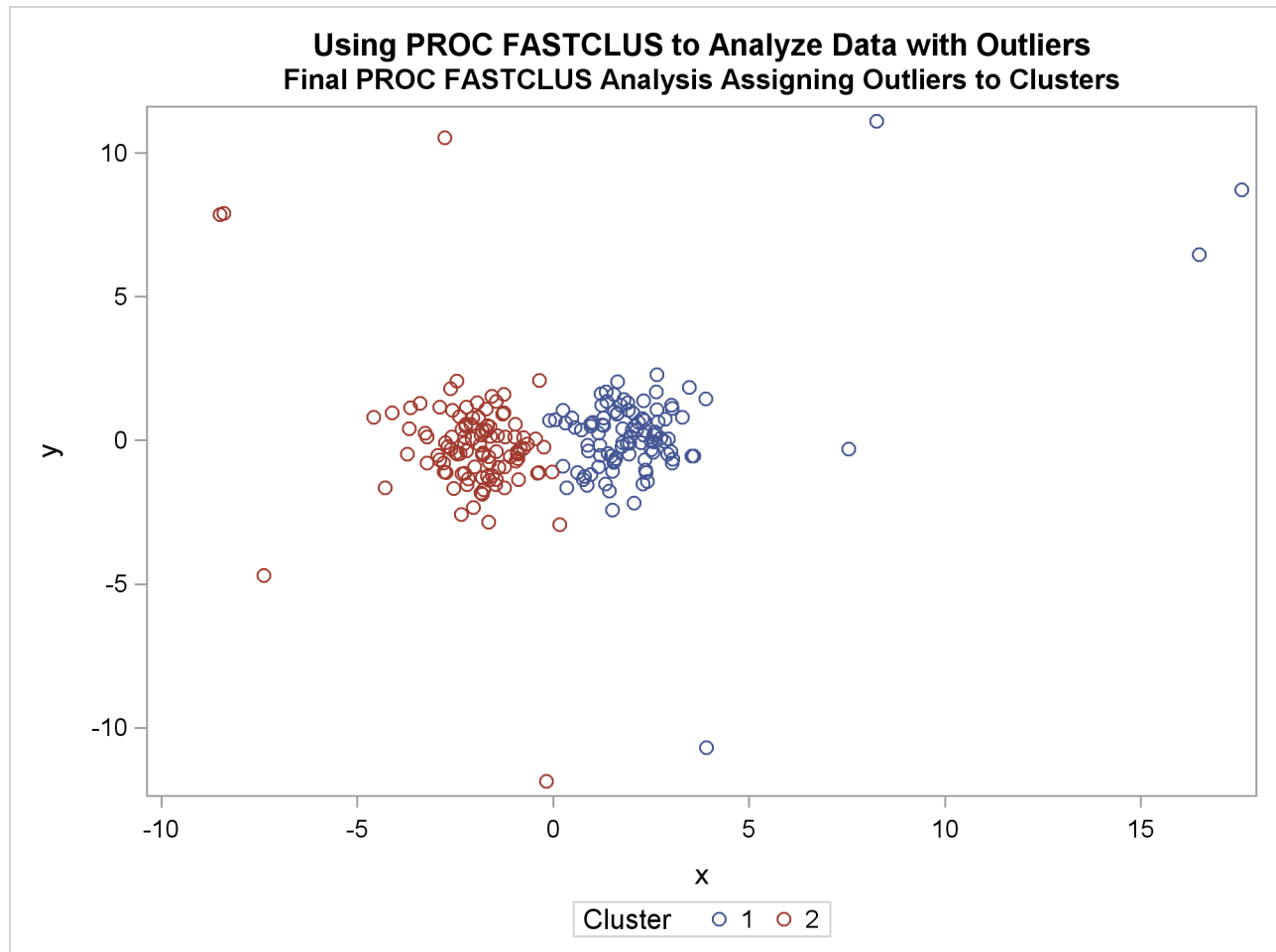
WARNING: The two values above are invalid for correlated variables.

Cluster Means

Cluster	x	y
1	2.280017469	0.263940765
2	-2.075547895	-0.151348765

Cluster Standard Deviations

Cluster	x	y
1	2.412264861	2.089922815
2	1.379355878	2.201567557

Output 36.2.8 Cluster Analysis with Outliers Omitted: Plot Using PROC SGPLOT

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Chapter 37

The FMM Procedure

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Overview: FMM Procedure

The FMM procedure fits statistical models to data for which the distribution of the response is a finite mixture of univariate distributions—that is, each response comes from one of several random univariate distributions with unknown probabilities. You can use PROC FMM to model the component distributions in addition to the mixing probabilities; see “A Gentle Introduction to Finite Mixture Models” on page 2423 for more precise definitions and discussion of similar but distinct modeling methodologies.

Classical statistical models are a special case of the finite mixture models in which the distribution of the data has only a single component.

Finite mixture models are useful for the following applications:

- estimating multimodal or heavy-tailed densities
- fitting zero-inflated or hurdle models to count data with excess zeros
- modeling overdispersed data
- fitting regression models with complex error distributions
- classifying observations based on predicted component probabilities
- accounting for unobservable, omitted variables
- estimating switching regressions

The FMM procedure is designed to fit finite mixtures of regression models or finite mixtures of generalized linear models in which the covariates and regression structure can be the same across components or might be different. You can fit finite mixture models by maximum likelihood or Bayesian methods.

For more information about the differences between the FMM procedure and other statistical modeling procedures in SAS/STAT software, see the section “[PROC FMM Contrasted with Other SAS Procedures](#)” on page 2359.

Basic Features

The FMM procedure estimates the parameters in univariate finite mixture models and produces various statistics to evaluate parameters and model fit. The following list summarizes some basic features of the FMM procedure:

- maximum likelihood estimation for all models
- Markov chain Monte Carlo estimation for many models, including zero-inflated Poisson models
- many built-in link and distribution functions for modeling, including the beta, shifted t , Weibull, beta-binomial, and generalized Poisson distributions, in addition to many standard members of the exponential family of distributions
- specialized built-in mixture models such as the binomial cluster model (Morel and Nagaraj 1993; Morel and Neerchal 1997; Neerchal and Morel 1998)
- acceptance of multiple **MODEL** statements to build mixture models in which the model effects, distributions, or link functions vary across mixture components
- model-building syntax using **CLASS** and effect-based **MODEL** statements familiar from many other SAS/STAT procedures (for example, the GLM, GLIMMIX, and MIXED procedures)
- evaluation of sequences of mixture models when you specify ranges for the number of components
- simple syntax to impose linear equality and inequality constraints among parameters
- ability to model regression and classification effects in the mixing probabilities through the **PROB-MODEL** statement
- ability to incorporate full or partially known component membership into the analysis through the **PARTIAL=** option in the **PROC FMM** statement
- **OUTPUT** statement that produces a SAS data set with important statistics for interpreting mixture models, such as component log likelihoods and prior and posterior probabilities
- ability to add zero-inflation to any model
- output data set with posterior parameter values for the Markov chain
- high degree of multithreading for high-performance optimization and Monte Carlo sampling

The FMM procedure uses ODS Graphics to create graphs as part of its output. For general information about ODS Graphics, see Chapter 21, “[Statistical Graphics Using ODS](#).” For specific information about the statistical graphics available with the FMM procedure, see the **PLOTS** options in the **PROC FMM** statement.

Assumptions

The FMM procedure makes the following assumptions in fitting statistical models:

- The number of components k in the finite mixture is known a priori and is not a parameter to be estimated.
- The parameters of the components are distinct a priori.
- The observations are uncorrelated.

Notation for the Finite Mixture Model

The general expression for the finite mixture model fitted with the FMM procedure is as follows:

$$f(y) = \sum_{j=1}^k \pi_j(\mathbf{z}, \boldsymbol{\alpha}_j) p_j(y; \mathbf{x}'_j \boldsymbol{\beta}_j, \phi_j)$$

The number of components in the mixture is denoted as k . The mixture probabilities π_j can depend on regressor variables \mathbf{z} and parameters $\boldsymbol{\alpha}_j$. By default, the FMM procedure models these probabilities using a logit transform if $k = 2$ and as a generalized logit model if $k > 2$. The component distributions p_j can also depend on regressor variables in \mathbf{x}_j , regression parameters $\boldsymbol{\beta}_j$, and possibly scale parameters ϕ_j . Notice that the component distributions p_j are indexed by j since the distributions might belong to different families. For example, in a two-component model, you might model one component as a normal (Gaussian) variable and the second component as a variable with a t distribution with low degrees of freedom to manage overdispersion.

The mixture probabilities π_j satisfy $\pi_j \geq 0$, for all j , and

$$\sum_{j=1}^k \pi_j(\mathbf{z}, \boldsymbol{\alpha}_j) = 1$$

Homogeneous Mixtures

If the component distributions are of the same distributional form, the mixture is called homogeneous. In most applications of homogeneous mixtures, the mixing probabilities do not depend on regression parameters. The general model then simplifies to

$$f(y) = \sum_{j=1}^k \pi_j p(y; \mathbf{x}'_j \boldsymbol{\beta}_j, \phi_j)$$

Since the component distributions depend on regression parameters β_j , this model is known as a homogeneous regression mixture. A homogeneous regression mixture assumes that the regression effects are the same across the components, although the FMM procedure does not impose such a restriction. If the component distributions do not contain regression effects, the model

$$f(y) = \sum_{j=1}^k \pi_j p(y; \mu_j, \phi_j)$$

is *the* homogeneous mixture model. A classical case is the estimation of a continuous density as a k -component mixture of normal distributions.

Special Mixtures

The FMM procedure enables you to fit several special mixture models. The Morel-Neerchal binomial cluster model (Morel and Nagaraj 1993; Morel and Neerchal 1997; Neerchal and Morel 1998) is a mixture of binomial distributions in which the success probabilities depend on the mixing probabilities.

Zero-inflated count models are obtained as two-component mixtures where one component is a classical count model—such as the Poisson or negative binomial model—and the other component is a distribution that is concentrated at zero. If the nondegenerate part of this special mixture is a zero-truncated model, the resulting two-component mixture is known as a hurdle model (Cameron and Trivedi 1998).

PROC FMM Contrasted with Other SAS Procedures

Since the FMM procedure fits finite mixtures of generalized linear models, it can also fit standard forms of these models in which the distribution of the data does not follow a mixture. This enables you to use the FMM procedure to estimate parameters in models that can be fit with the CATMOD, LOGISTIC, GENMOD, or GLIMMIX procedures. However, the FMM procedure does not fit models for multinomial data or models with random effects.

The FMM procedure has limited postprocessing capabilities compared to some other statistical procedures that are based on linear models. Concepts that are well understood and commonplace in linear models, such as (linear) estimable functions, estimability, and least squares means, do not apply to mixture models in the same way. For example, even the computation of a predicted value is not without ambiguity. You can estimate the means in the component distributions in addition to the overall mean of the mixture.

The FMM procedure provides a limited number of built-in distributions and link functions. User-defined distributions or link functions are not supported. Mixture models with component distributions that are not supported by the FMM procedure can be fit with the NLMIXED procedure.

For Bayesian estimation, the FMM procedure implements a small number of highly specialized sampling algorithms. These algorithms are very efficient and specifically designed for generalized linear models and their mixtures. This limits, for example, the allowable specifications for prior distributions of the model parameters. Models that do not fit the targeted algorithms of the FMM procedure can be fit with the MCMC procedure.

Getting Started: FMM Procedure

Mixture Modeling for Binomial Overdispersion: “Student,” Pearson, Beer, and Yeast

The following example demonstrates how you can model a complicated, two-component binomial mixture distribution, either with maximum likelihood or with Bayesian methods, with a few simple PROC FMM statements.

William Sealy Gosset, a chemist at the Arthur Guinness Son and Company brewery in Dublin, joined the statistical laboratory of Karl Pearson in 1906–1907 to study statistics. At first Gosset—who published all but one paper under the pseudonym “Student” because his employer forbade publications by employees after a co-worker had disclosed trade secrets—worked on the Poisson limit to the binomial distribution, using haemocytometer yeast cell counts. Gosset’s interest in studying small-sample (and limit) problems was motivated by the small sample sizes he typically saw in his work at the brewery.

Subsequently, Gosset’s yeast count data have been examined and revisited by many authors. In 1915, Karl Pearson undertook his own examination and realized that the variability in “Student’s” data exceeded that consistent with a Poisson distribution. Pearson (1915) bemoans the fact that if this were so, “it is certainly most unfortunate that such material should have been selected to illustrate Poisson’s limit to the binomial.”

Using a count of Gosset’s yeast cell counts on the 400 squares of a haemocytometer (Table 37.1), Pearson argues that a mixture process would explain the heterogeneity (beyond the Poisson).

Table 37.1 “Student’s” Yeast Cell Counts

Number of Cells	0	1	2	3	4	5
Frequency	213	128	37	18	3	1

Pearson fits various models to these data, chief among them a mixture of two binomial series

$$v_1(p_1 + q_1)^\theta + v_2(p_2 + q_2)^\theta$$

where θ is real-valued and thus the binomial series expands to

$$(p + q)^\theta = \sum_{k=0}^{\infty} \frac{\Gamma(\theta + 1)}{\Gamma(k + 1)\Gamma(\theta - k + 1)} p^k q^{\theta - k}$$

Pearson’s fitted model has $\theta = 4.89997$, $v_1 = 356.986$, $v_2 = 43.014$ (corresponding to a mixing proportion of $356.986/(43.014 + 356.986) = 0.892$), and estimated success probabilities in the binomial components of 0.1017 and 0.4514, respectively. The success probabilities indicate that although the data have about a 90% chance of coming from a distribution with small success probability of about 0.1, there is a 10% chance of coming from a distribution with a much larger success probability of about 0.45.

If θ is an integer, the binomial series is the cumulative mass function of a binomial random variable. The value of θ suggests that a suitable model for these data could also be constructed as a two-component mixture of binomial random variables as follows:

$$f(y) = \pi \text{binomial}(5, \mu_1) + (1 - \pi) \text{binomial}(5, \mu_2)$$

The binomial sample size $n=5$ is suggested by Pearson's estimate of $\theta = 4.89997$ and the fact that the largest cell count in Table 37.1 is 5.

The following DATA step creates a SAS data set from the data in Table 37.1.

```
data yeast;
  input count f;
  n = 5;
  datalines;
  0      213
  1      128
  2       37
  3       18
  4        3
  5        1
  ;
```

The two-component binomial model is fit with the FMM procedure with the following statements:

```
proc fmm data=yeast;
  model count/n = / k=2;
  freq f;
run;
```

Because the events/trials syntax is used in the MODEL statement, PROC FMM defaults to the binomial distribution. The $K=2$ option specifies that the number of components is fixed and known to be two. The FREQ statement indicates that the data are grouped; for example, the first observation represents 213 squares on the haemacytometer where no yeast cells were found.

The "Model Information" and "Number of Observations" tables in Figure 37.1 convey that the fitted model is a two-component homogeneous binomial mixture with a logit link function. The mixture is *homogeneous* because there are no model effects in the MODEL statement and because both component distributions belong to the same distributional family. By default, PROC FMM estimates the model parameters by maximum likelihood.

Although only six observations are read from the data set, the data represent 400 observations (squares on the haemacytometer). Since a constant binomial sample size of 5 is assumed, the data represent 273 successes (finding a yeast cell) out of 2,000 Bernoulli trials.

Figure 37.1 Model Information for Yeast Cell Model

The FMM Procedure	
Model Information	
Data Set	WORK.YEAST
Response Variable (Events)	count
Response Variable (Trials)	n
Frequency Variable	f
Type of Model	Homogeneous Mixture
Distribution	Binomial
Components	2
Link Function	Logit
Estimation Method	Maximum Likelihood

Figure 37.1 continued

Number of Observations Read	6
Number of Observations Used	6
Sum of Frequencies Read	400
Sum of Frequencies Used	400
Number of Events	273
Number of Trials	2000

The estimated intercepts (on the logit scale) for the two binomial means are -2.2316 and -0.2974 , respectively. These values correspond to binomial success probabilities of 0.09695 and 0.4262 , respectively (Figure 37.2). The two components mix with probabilities 0.8799 and $1 - 0.8799 = 0.1201$. These values are generally close to the values found by Pearson (1915) using infinite binomial series instead of binomial mass functions.

Figure 37.2 Maximum Likelihood Estimates

Parameter Estimates for 'Binomial' Model						
Component	Parameter	Estimate	Standard Error	z Value	Pr > z	Inverse Linked Estimate
1	Intercept	-2.2316	0.1522	-14.66	<.0001	0.09695
2	Intercept	-0.2974	0.3655	-0.81	0.4158	0.4262
Parameter Estimates for Mixing Probabilities						
-----Linked Scale-----						
Parameter	Estimate	Standard Error	z Value	Pr > z	Probability	
Probability	1.9913	0.5725	3.48	0.0005	0.8799	

To obtain fitted values and other observationwise statistics under the stipulated two-component model, you can add the **OUTPUT** statement to the previous PROC FMM run. The following statements request componentwise predicted values and the posterior probabilities:

```
proc fmm data=yeast;
  model count/n = / k=2;
  freq f;
  output out=fmmout pred(components) posterior;
run;
data fmmout;
  set fmmout;
  PredCount_1 = post_1 * f;
  PredCount_2 = post_2 * f;
run;
proc print data=fmmout;
run;
```

The DATA step following the PROC FMM step computes the predicted cell counts in each component (Figure 37.3). The predicted means in the components, 0.48476 and 2.13099, are close to the values determined by Pearson (0.4983 and 2.2118), as are the predicted cell counts.

Figure 37.3 Predicted Cell Counts

Obs	count	f	n	Pred_1	Pred_2	Post_1	Post_2	Pred Count_1	Pred Count_2
1	0	213	5	0.096951	0.42620	0.98606	0.01394	210.030	2.9698
2	1	128	5	0.096951	0.42620	0.91089	0.08911	116.594	11.4058
3	2	37	5	0.096951	0.42620	0.59638	0.40362	22.066	14.9341
4	3	18	5	0.096951	0.42620	0.17598	0.82402	3.168	14.8323
5	4	3	5	0.096951	0.42620	0.02994	0.97006	0.090	2.9102
6	5	1	5	0.096951	0.42620	0.00444	0.99556	0.004	0.9956

Gosset, who was interested in small-sample statistical problems, investigated the use of prior knowledge in mathematical-statistical analysis—for example, deriving the sampling distribution of the correlation coefficient after having assumed a uniform prior distribution for the coefficient in the population (Aldrich 1997). Pearson also was not opposed to using prior information, especially uniform priors that reflect “equal distribution of ignorance.” Fisher, on the other hand, would not have any of it: the best estimator in his opinion is obtained by a criterion that is absolutely independent of prior assumptions about probabilities of particular values. He objected to the insinuation that his derivations in the work on the correlation were deduced from Bayes theorem (Fisher 1921).

The preceding analysis of the yeast cell count data uses maximum likelihood methods that are free of prior assumptions. The following analysis takes instead a Bayesian approach, assuming a beta prior distribution for the binomial success probabilities and a uniform prior distribution for the mixing probabilities. The changes from the previous FMM run are the addition of the ODS GRAPHICS, PERFORMANCE, and BAYES statements and the SEED=12345 option.

```
ods graphics on;
proc fmm data=yeast seed=12345;
  model count/n = / k=2;
  freq f;
  performance cpucount=2;
  bayes;
run;
ods graphics off;
```

With ODS Graphics enabled, PROC FMM produces diagnostic trace plots for the posterior samples. Bayesian analyses are sensitive to the random number seed and thread count; the SEED= and CPUCOUNT= options ensure consistent results for the purposes of this example. The SEED=12345 option in the PROC FMM statement determines the random number seed for the random number generator used in the analysis. The CPUCOUNT=2 option in the PERFORMANCE statement sets the number of available processors to two. The BAYES statement requests a Bayesian analysis.

The “Bayes Information” table in Figure 37.4 provides basic information about the Markov chain Monte Carlo sampler. Because the model is a homogeneous mixture, the FMM procedure applies an efficient conjugate sampling algorithm with a posterior sample size of 10,000 samples after a burn-in size of 2,000

samples. The “Prior Distributions” table displays the prior distribution for each parameter along with its mean and variance and the initial value in the chain. Notice that in this situation all three prior distributions reduce to a uniform distribution on (0, 1).

Figure 37.4 Basic Information about MCMC Sampler

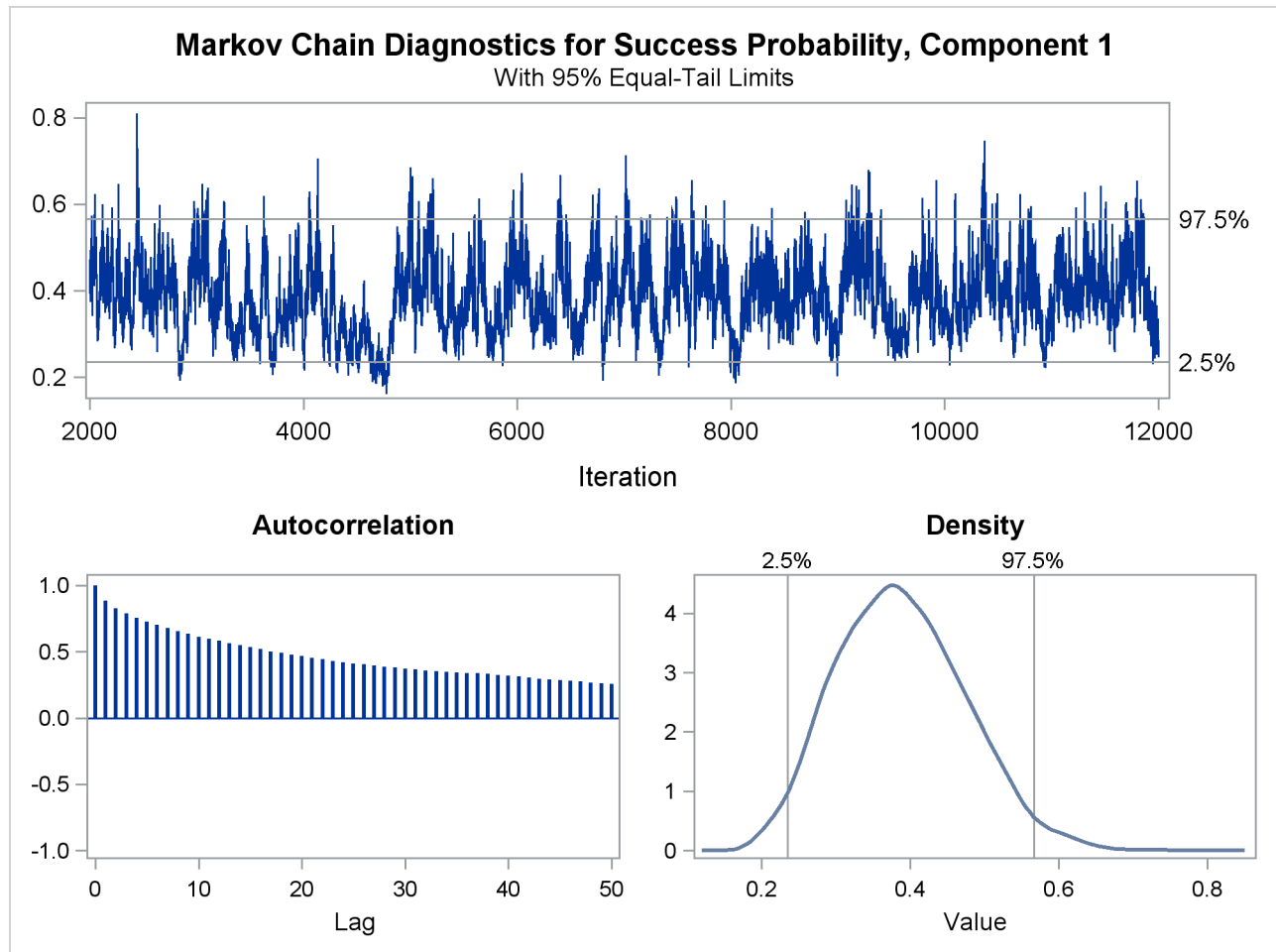
The FMM Procedure					
Bayes Information					
Sampling Algorithm	Conjugate				
Data Augmentation	Latent Variable				
Initial Values of Chain	Data Based				
Burn-In Size	2000				
MC Sample Size	10000				
MC Thinning	1				
Parameters in Sampling	3				
Mean Function Parameters	2				
Scale Parameters	0				
Mixing Prob Parameters	1				
Number of Threads	2				
Prior Distributions					
Component	Parameter	Distribution	Mean	Variance	Initial Value
1	Success Probability	Beta(1, 1)	0.5000	0.08333	0.1365
2	Success Probability	Beta(1, 1)	0.5000	0.08333	0.1365
1	Probability	Dirichlet(1, 1)	0.5000	0.08333	0.6180

The FMM procedure produces a log note for this model, indicating that the sampled quantities are not the linear predictors on the logit scale, but are the actual population parameters (on the data scale):

NOTE: Bayesian results for this model (no regressor variables, non-identity link) are displayed on the data scale, not the linked scale. You can obtain results on the linked (=linear) scale by requesting a Metropolis-Hastings sampling algorithm.

The trace panel for the success probability in the first binomial component is shown in [Figure 37.5](#). Note that the first component in this Bayesian analysis corresponds to the second component in the MLE analysis. The graphics in this panel can be used to diagnose the convergence of the Markov chain. If the chain has not converged, inferences cannot be made based on quantities derived from the chain. You generally look for the following:

- a smooth unimodal distribution of the posterior estimates in the density plot displayed on the lower right
- good mixing of the posterior samples in the trace plot at the top of the panel (good mixing is indicated when the trace traverses the support of the distribution and appears to have reached a stationary distribution)

Figure 37.5 Trace Panel for Success Probability in First Component

The autocorrelation plot in [Figure 37.5](#) shows fairly high and sustained autocorrelation among the posterior estimates. While this is generally not a problem, you can affect the degree of autocorrelation among the posterior estimates by running a longer chain and thinning the posterior estimates; see the `NMC=` and `THIN=` options in the `BAYES` statement.

Both the trace plot and the density plot in [Figure 37.5](#) are indications of successful convergence.

[Figure 37.6](#) reports selected results that summarize the 10,000 posterior samples. The arithmetic means of the success probabilities in the two components are 0.3884 and 0.0905, respectively. The posterior mean of the mixing probability is 0.1771. These values are similar to the maximum likelihood parameter estimates in [Figure 37.2](#) (after swapping components).

Figure 37.6 Summaries for Posterior Estimates

Posterior Summaries				
Component	Parameter	N	Mean	Standard Deviation
1	Success Probability	10000	0.3884	0.0861
2	Success Probability	10000	0.0905	0.0162
1	Probability	10000	0.1771	0.0978

Posterior Summaries				
Component	Parameter	25%	Percentiles	
			50%	75%
1	Success Probability	0.3254	0.3835	0.4457
2	Success Probability	0.0811	0.0923	0.1017
1	Probability	0.1073	0.1534	0.2227

Posterior Intervals					
Component	Parameter	Alpha	Equal-Tail Interval		HPD Interval
			Lower	Upper	
1	Success Probability	0.050	0.2355	0.5663	0.2224 0.5494
2	Success Probability	0.050	0.0538	0.1171	0.0572 0.1187
1	Probability	0.050	0.0564	0.4311	0.0424 0.3780

Note that the standard errors in Figure 37.2 are not comparable to those in Figure 37.6, since the standard errors for the MLEs are expressed on the logit scale and the Bayes estimates are expressed on the data scale. You can add the `METROPOLIS` option in the `BAYES` statement to sample the quantities on the logit scale.

The “Posterior Intervals” table in Figure 37.6 displays 95% credible intervals (equal-tail intervals and intervals of highest posterior density). It can be concluded that the component with the higher success probability contributes less than 40% to the process.

Modeling Zero-Inflation: Is it Better to Fish Poorly or Not to Have Fished At All?

The following example shows how you can use PROC FMM to model data with more zero values than expected.

Many count data show an excess of zeros relative to the frequency of zeros expected under a reference model. An excess of zeros leads to overdispersion since the process is more variable than a standard count data model. Different mechanisms can lead to excess zeros. For example, suppose that the data are generated from two processes with different distribution functions—one process generates the zero counts, and the other process generates nonzero counts. In the vernacular of Cameron and Trivedi (1998), such a model is called a *hurdle* model. With a certain probability—the probability of a nonzero count—a hurdle is crossed, and events are being generated. Hurdle models are useful, for example, to model the number of doctor

visits per year. Once the decision to see a doctor has been made—the hurdle has been overcome—a certain number of visits follow.

Hurdle models are closely related to zero-inflated models. Both can be expressed as two-component mixtures in which one component has a degenerate distribution at zero and the other component is a count model. In a hurdle model, the count model follows a zero-truncated distribution. In a zero-inflated model, the count model has a nonzero probability of generating zeros. Formally, a zero-inflated model can be written as

$$\Pr(Y = y) = \pi p_1 + (1 - \pi) p_2(y, \mu)$$

$$p_1 = \begin{cases} 1 & y = 0 \\ 0 & \text{otherwise} \end{cases}$$

where $p_2(y, \mu)$ is a standard count model with mean μ and support $y \in \{0, 1, 2, \dots\}$.

The following data illustrates the use of a zero-inflated model. In a survey of park attendees, randomly selected individuals were asked about the number of fish they caught in the last six months. Along with that count, the gender and age of each sampled individual was recorded. The following DATA step displays the data for the analysis:

```
data catch;
  input gender $ age count @@;
  datalines;
  F 54 18 M 37 0 F 48 12 M 27 0
  M 55 0 M 32 0 F 49 12 F 45 11
  M 39 0 F 34 1 F 50 0 M 52 4
  M 33 0 M 32 0 F 23 1 F 17 0
  F 44 5 M 44 0 F 26 0 F 30 0
  F 38 0 F 38 0 F 52 18 M 23 1
  F 23 0 M 32 0 F 33 3 M 26 0
  F 46 8 M 45 5 M 51 10 F 48 5
  F 31 2 F 25 1 M 22 0 M 41 0
  M 19 0 M 23 0 M 31 1 M 17 0
  F 21 0 F 44 7 M 28 0 M 47 3
  M 23 0 F 29 3 F 24 0 M 34 1
  F 19 0 F 35 2 M 39 0 M 43 6
  ;
```

At first glance, the prevalence of zeros in the DATA set is apparent. Many park attendees did not catch any fish. These zero counts are made up of two populations: attendees who do not fish and attendees who fish poorly. A zero-inflation mechanism thus appears reasonable for this application since a zero count can be produced by two separate distributions.

The following statements fit a standard Poisson regression model to these data. A common intercept is assumed for men and women, and the regression slope varies with gender.

```
proc fmm data=catch;
  class gender;
  model count = gender*age / dist=Poisson;
run;
```

Figure 37.7 displays information about the model and data set. The “Model Information” table conveys that the model is a single-component Poisson model (a Poisson GLM) and that parameters are estimated by maximum likelihood. There are two levels in the CLASS variable gender, with females preceding males.

Figure 37.7 Model Information and Class Levels in Poisson Regression

The FMM Procedure		
Model Information		
Data Set	WORK.CATCH	
Response Variable	count	
Type of Model	Generalized Linear (GLM)	
Distribution	Poisson	
Components	1	
Link Function	Log	
Estimation Method	Maximum Likelihood	
Class Level Information		
Class	Levels	Values
gender	2	F M
Number of Observations Read	52	
Number of Observations Used	52	

The “Fit Statistics” and “Parameter Estimates” tables from the maximum likelihood estimation of the Poisson GLM are shown in Figure 37.8. If the model is not overdispersed, the Pearson statistic should roughly equal the number of observations in the data set minus the number of parameters. With $n=52$, there is evidence of overdispersion in these data.

Figure 37.8 Fit Results in Poisson Regression

Fit Statistics					
-2 Log Likelihood			182.7		
AIC (smaller is better)			188.7		
AICC (smaller is better)			189.2		
BIC (smaller is better)			194.6		
Pearson Statistic			85.9573		
Parameter Estimates for 'Poisson' Model					
Effect	gender	Estimate	Standard Error	z Value	Pr > z
Intercept		-3.9811	0.5439	-7.32	<.0001
age*gender	F	0.1278	0.01149	11.12	<.0001
age*gender	M	0.1044	0.01224	8.53	<.0001

Suppose that the cause of overdispersion is zero-inflation of the count data. The following statements fit a zero-inflated Poisson model.

```
proc fmm data=catch;
  class gender;
  model count = gender*age / dist=Poisson ;
  model      +           / dist=Constant;
run;
```

There are two **MODEL** statements, one for each component of the mixture. Because the distributions are different for the components, you cannot specify the mixture model with a single **MODEL** statement. The first **MODEL** statement identifies the response variable for the model (count) and defines a Poisson model with intercept and gender-specific slopes. The second **MODEL** statement uses the continuation operator (“+”) and adds a model with a degenerate distribution by using **DIST=CONSTANT**. Because the mass of the constant is placed by default at zero, the second **MODEL** statement adds a zero-inflation component to the model. It is sufficient to specify the response variable in one of the **MODEL** statements; you use the “=” sign in that statement to separate the response variable from the model effects.

Figure 37.9 displays the “Model Information” and “Optimization Information” tables for this run of the FMM procedure. The model is now identified as a zero-inflated Poisson (ZIP) model with two components, and the parameters continue to be estimated by maximum likelihood. The “Optimization Information” table shows that there are four parameters in the optimization (compared to three parameters in the Poisson GLM model). The four parameters correspond to three parameters in the mean function (intercept and two gender-specific slopes) and the mixing probability.

Figure 37.9 Model and Optimization Information in the ZIP Model

The FMM Procedure	
Model Information	
Data Set	WORK.CATCH
Response Variable	count
Type of Model	Zero-inflated Poisson
Components	2
Estimation Method	Maximum Likelihood
Optimization Information	
Optimization Technique	Dual Quasi-Newton
Parameters in Optimization	4
Mean Function Parameters	3
Scale Parameters	0
Mixing Prob Parameters	1
Number of Threads	2

Results from fitting the ZIP model by maximum likelihood are shown in Figure 37.10. The $-2 \log$ likelihood and the information criteria suggest a much-improved fit over the single-component Poisson model (compare Figure 37.10 to Figure 37.8). The Pearson statistic is reduced by factor 2 compared to the Poisson model and suggests a better fit than the standard Poisson model.

Figure 37.10 Maximum Likelihood Results for the ZIP model

Fit Statistics						
	-2 Log Likelihood					145.6
	AIC (smaller is better)					153.6
	AICC (smaller is better)					154.5
	BIC (smaller is better)					161.4
	Pearson Statistic					43.4467
	Effective Parameters					4
	Effective Components					2
Parameter Estimates for 'Poisson' Model						
Component	Effect	gender	Estimate	Standard Error	z Value	Pr > z
1	Intercept		-3.5215	0.6448	-5.46	<.0001
1	age*gender	F	0.1216	0.01344	9.04	<.0001
1	age*gender	M	0.1056	0.01394	7.58	<.0001
Parameter Estimates for Mixing Probabilities						
-----Linked Scale-----						
Effect	Estimate	Standard Error	z Value	Pr > z	Probability	
Intercept	0.8342	0.4768	1.75	0.0802	0.6972	

The number of effective parameters and components shown in Figure 37.8 equals the values from Figure 37.9. This is not always the case because components can collapse (for example, when the mixing probability approaches zero or when two components have identical parameter estimates). In this example, both components and all four parameters are identifiable. The Poisson regression and the zero process mix, with a probability of approximately 0.6972 attributed to the Poisson component.

The FMM procedure enables you to fit some mixture models by Bayesian techniques. The following statements add the `BAYES` statement to the previous PROC FMM statements:

```
proc fmm data=catch seed=12345;
  class gender;
  model count = gender*age / dist=Poisson;
  model      +           / dist=constant;
  performance cpubcount=2;
  bayes;
run;
```

The “Model Information” table indicates that the model parameters are estimated by Markov chain Monte Carlo techniques, and it displays the random number seed (Figure 37.11). This is useful if you did not specify a seed to identify the seed value that reproduces the current analysis. The “Bayes Information” table provides basic information about the Monte Carlo sampling scheme. The sampling method uses a data augmentation scheme to impute component membership and then the Gamerman (1997) algorithm to

sample the component-specific parameters. The 2,000 burn-in samples are followed by 10,000 Monte Carlo samples without thinning.

Figure 37.11 Model, Bayes, and Prior Information in the ZIP Model

The FMM Procedure						
Model Information						
Data Set	WORK.CATCH					
Response Variable	count					
Type of Model	Zero-inflated Poisson					
Components	2					
Estimation Method	Markov Chain Monte Carlo					
Random Number Seed	12345					
Bayes Information						
Sampling Algorithm	Gamerman					
Data Augmentation	Latent Variable					
Initial Values of Chain	ML Estimates					
Burn-In Size	2000					
MC Sample Size	10000					
MC Thinning	1					
Parameters in Sampling	4					
Mean Function Parameters	3					
Scale Parameters	0					
Mixing Prob Parameters	1					
Number of Threads	2					
Prior Distributions						
Component	Effect	gender	Distribution	Mean	Variance	Initial Value
1	Intercept		Normal(0, 1000)	0	1000.00	-3.5215
1	age*gender	F	Normal(0, 1000)	0	1000.00	0.1216
1	age*gender	M	Normal(0, 1000)	0	1000.00	0.1056
1	Probability		Dirichlet(1, 1)	0.5000	0.08333	0.6972

The “Prior Distributions” table identifies the prior distributions, their parameters for the sampled quantities, and their initial values. The prior distribution of parameters associated with model effects is a normal distribution with mean 0 and variance 1,000. The prior distribution for the mixing probability is a Dirichlet(1,1), which is identical to a uniform distribution (Figure 37.11). Since the second mixture component is a degeneracy at zero with no associated parameters, it does not appear in the “Prior Distributions” table in Figure 37.11.

Figure 37.12 displays descriptive statistics about the 10,000 posterior samples. Recall from Figure 37.10 that the maximum likelihood estimates were -3.5215 , 0.1216 , 0.1056 , and 0.6972 , respectively. With this choice of prior, the means of the posterior samples are generally close to the MLEs in this example. The “Posterior Intervals” table displays 95% intervals of equal-tail probability and 95% intervals of highest posterior density (HPD) intervals.

Figure 37.12 Posterior Summaries and Intervals in the ZIP Model

Posterior Summaries						
Component	Effect	gender	N	Mean	Standard Deviation	
1	Intercept		10000	-3.5524	0.6509	
1	age*gender	F	10000	0.1220	0.0136	
1	age*gender	M	10000	0.1058	0.0140	
1	Probability		10000	0.6938	0.0945	

Posterior Summaries						
Component	Effect	gender	25%	50%	Percentiles 75%	
1	Intercept		-3.9922	-3.5359	-3.0875	
1	age*gender	F	0.1124	0.1218	0.1314	
1	age*gender	M	0.0961	0.1055	0.1153	
1	Probability		0.6293	0.6978	0.7605	

Posterior Intervals							
Component	Effect	gender	Alpha	Equal-Tail Interval		HPD Interval	
1	Intercept		0.050	-4.8693	-2.3222	-4.8927	-2.3464
1	age*gender	F	0.050	0.0960	0.1494	0.0961	0.1494
1	age*gender	M	0.050	0.0792	0.1339	0.0796	0.1341
1	Probability		0.050	0.5041	0.8688	0.5025	0.8666

You can generate trace plots for the posterior parameter estimates by enabling ODS Graphics:

```
ods graphics on;
ods select TADPanel;
proc fmm data=catch seed=12345;
  class gender;
  model count = gender*age / dist=Poisson;
  model      +           / dist=constant;
  performance cpubcount=2;
  bayes;
run;
ods graphics off;
```

A separate trace panel is produced for each sampled parameter, and the panels for the gender-specific slopes are shown in Figure 37.13. There is good mixing in the chains: the modest autocorrelation that diminishes after about 10 successive samples. By default, the FMM procedure transfers the credible intervals for each parameter from the “Posterior Intervals” table to the trace plot and the density plot in the trace panel.

Figure 37.13 Trace Panels for Gender-Specific Slopes

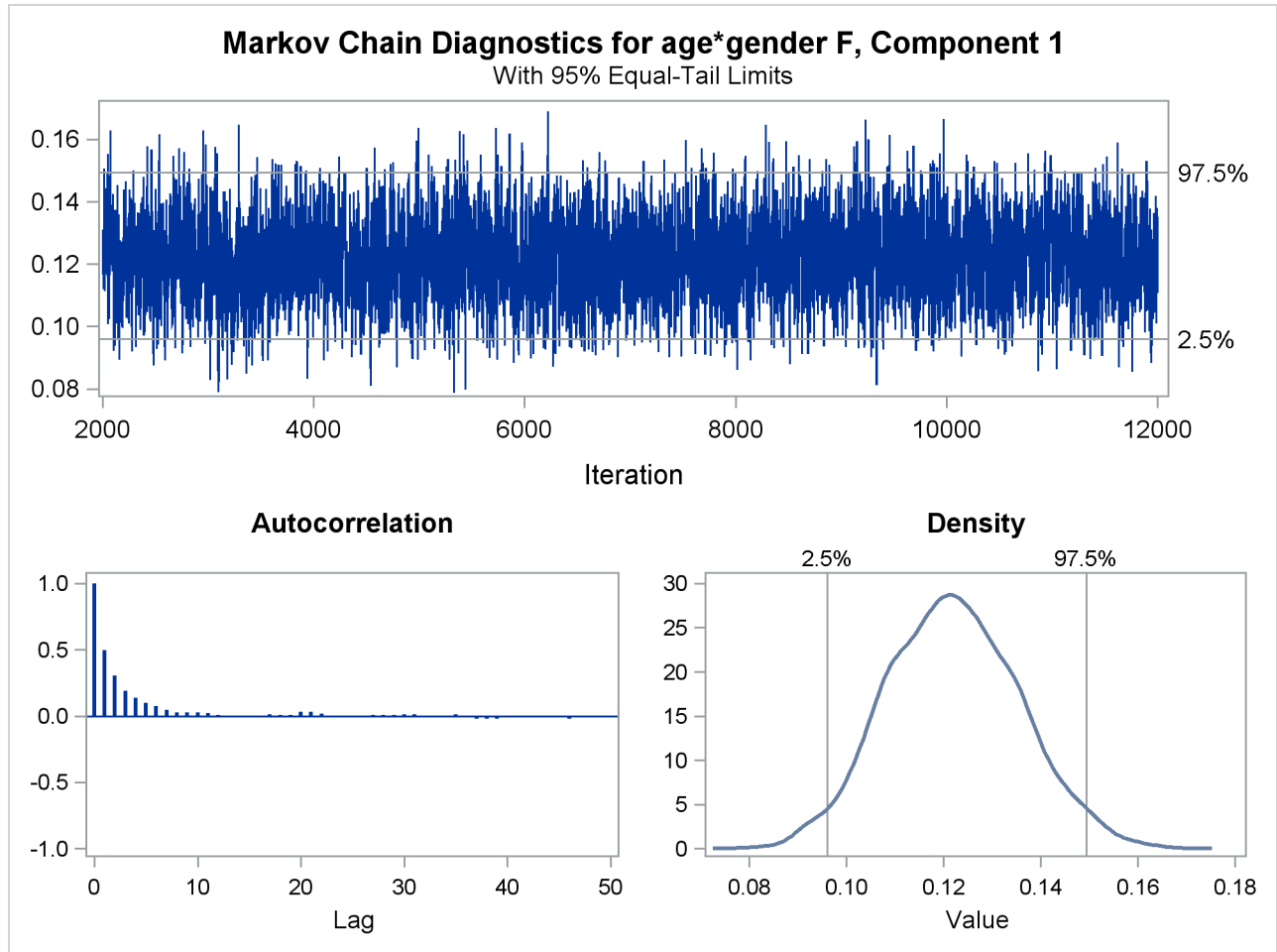
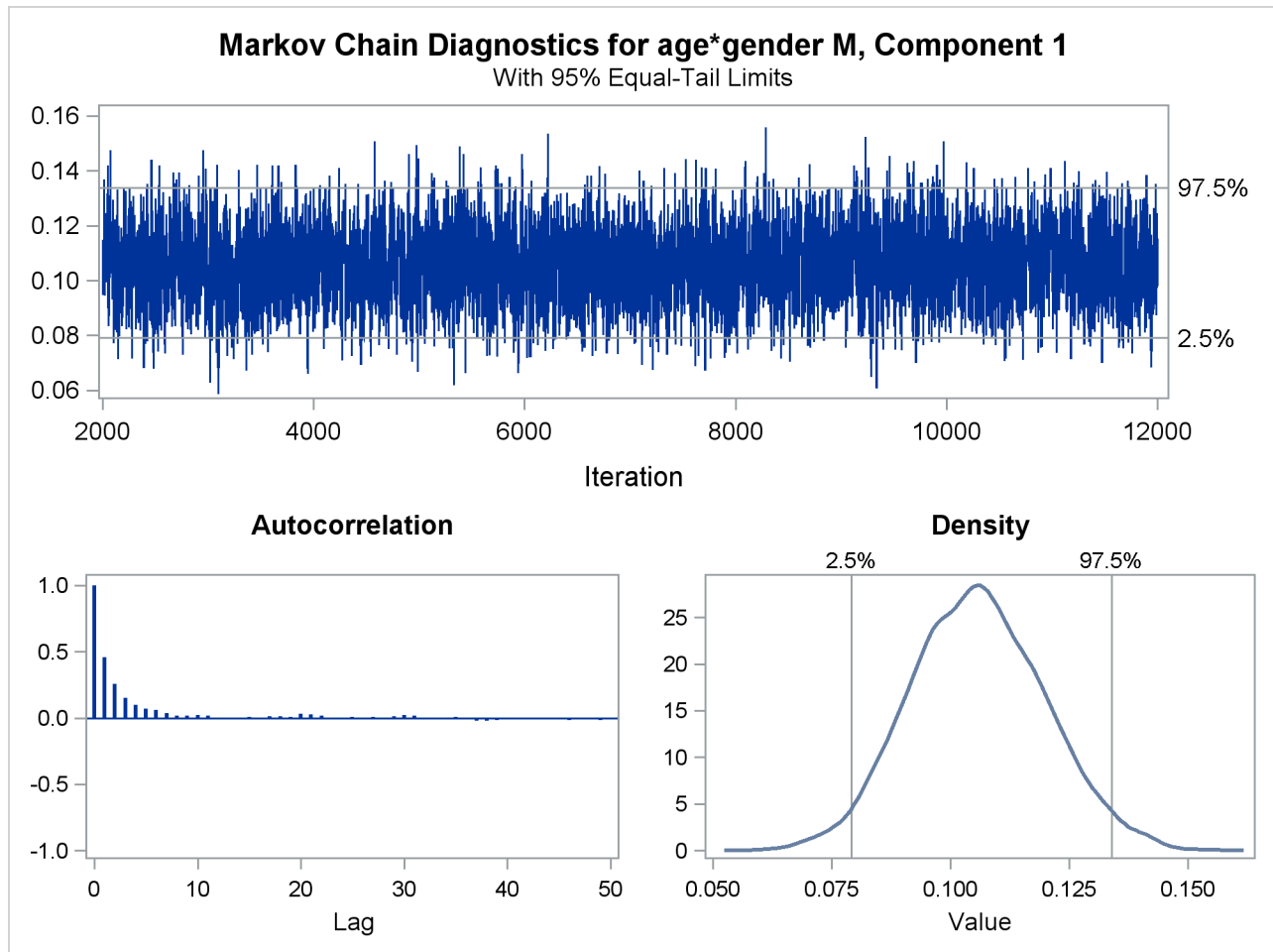


Figure 37.13 continued



Looking for Multiple Modes: Are Galaxies Clustered?

Mixture modeling is essentially a generalized form of one-dimensional cluster analysis. The following example shows how you can use PROC FMM to explore the number and nature of Gaussian clusters in univariate data.

Roeder (1990) presents data from the Corona Borealis sky survey with the velocities of 82 galaxies in a narrow slice of the sky. Cosmological theory suggests that the observed velocity of each galaxy is proportional to its distance from the observer. Thus, the presence of multiple modes in the density of these velocities could indicate a clustering of the galaxies at different distances.

The following DATA step recreates the data set in Roeder (1990). The computed variable *v* represents the measured velocity in thousands of kilometers per second.

```

title "FMM Analysis of Galaxies Data";
data galaxies;
  input velocity @@;
  v = velocity / 1000;

```

```

datalines;
9172 9350 9483 9558 9775 10227 10406 16084 16170 18419
18552 18600 18927 19052 19070 19330 19343 19349 19440 19473
19529 19541 19547 19663 19846 19856 19863 19914 19918 19973
19989 20166 20175 20179 20196 20215 20221 20415 20629 20795
20821 20846 20875 20986 21137 21492 21701 21814 21921 21960
22185 22209 22242 22249 22314 22374 22495 22746 22747 22888
22914 23206 23241 23263 23484 23538 23542 23666 23706 23711
24129 24285 24289 24366 24717 24990 25633 26960 26995 32065
32789 34279
;

```

Analysis of potentially multimodal data is a natural application of finite mixture models. In this case, the modeling is complicated by the question of the variance for each of the components. Using identical variances for each component could obscure underlying structure, but the additional flexibility granted by component-specific variances might introduce spurious features.

You can use PROC FMM to prepare analyses for equal and unequal variances and use one of the available fit statistics to compare the resulting models. You can use the model selection facility to explore models with varying numbers of mixture components—say, from three to seven as investigated in Roeder (1990). The following statements select the best unequal-variance model using Akaike’s information criterion (AIC), which has a built-in penalty for model complexity:

```

title2 "Three to Seven Components, Unequal Variances";
ods graphics on;
ods select DensityPlot;
proc fmm data=galaxies criterion=AIC;
  model v = / kmin=3 kmax=7;
  ods exclude IterHistory OptInfo ComponentInfo;
run;

```

The `KMIN=` and `KMAX=` options indicate the smallest and largest number of components to consider. The `ODS GRAPHICS` and `ODS SELECT` statements request a density plot. The output for unequal variances is shown in Figure 37.14 and Figure 37.15.

Figure 37.14 Model Selection for Galaxy Data Assuming Unequal Variances

FMM Analysis of Galaxies Data	
Three to Seven Components, Unequal Variances	
The FMM Procedure	
Model Information	
Data Set	WORK.GALAXIES
Response Variable	v
Type of Model	Homogeneous Mixture
Distribution	Normal
Min Components	3
Max Components	7
Link Function	Identity
Estimation Method	Maximum Likelihood

Figure 37.14 continued

Component Evaluation for Mixture Models								
Model ID	----- Number of -----		-----		-2 Log L	AIC	AICC	BIC
	-Components- Total	Eff.	-Parameters- Total	Eff.				
1	3	3	8	8	406.96	422.96	424.94	442.22
2	4	4	11	11	406.96	428.96	432.74	455.44
3	5	5	14	14	406.96	434.96	441.23	468.66
4	6	6	17	17	406.96	440.96	450.53	481.88
5	7	7	20	20	406.96	446.96	460.73	495.10

Component Evaluation for Mixture Models							
Model ID	----- Number of -----		-----		Pearson	Max Gradient	
	-Components- Total	Eff.	-Parameters- Total	Eff.			
1	3	3	8	8	82.00	0.000024	
2	4	4	11	11	82.00	0.00012	
3	5	5	14	14	82.00	0.000039	
4	6	6	17	17	82.00	0.00012	
5	7	7	20	20	82.00	0.00024	

The model with 3 components (ID=1) was selected as 'best' based on the AIC statistic.

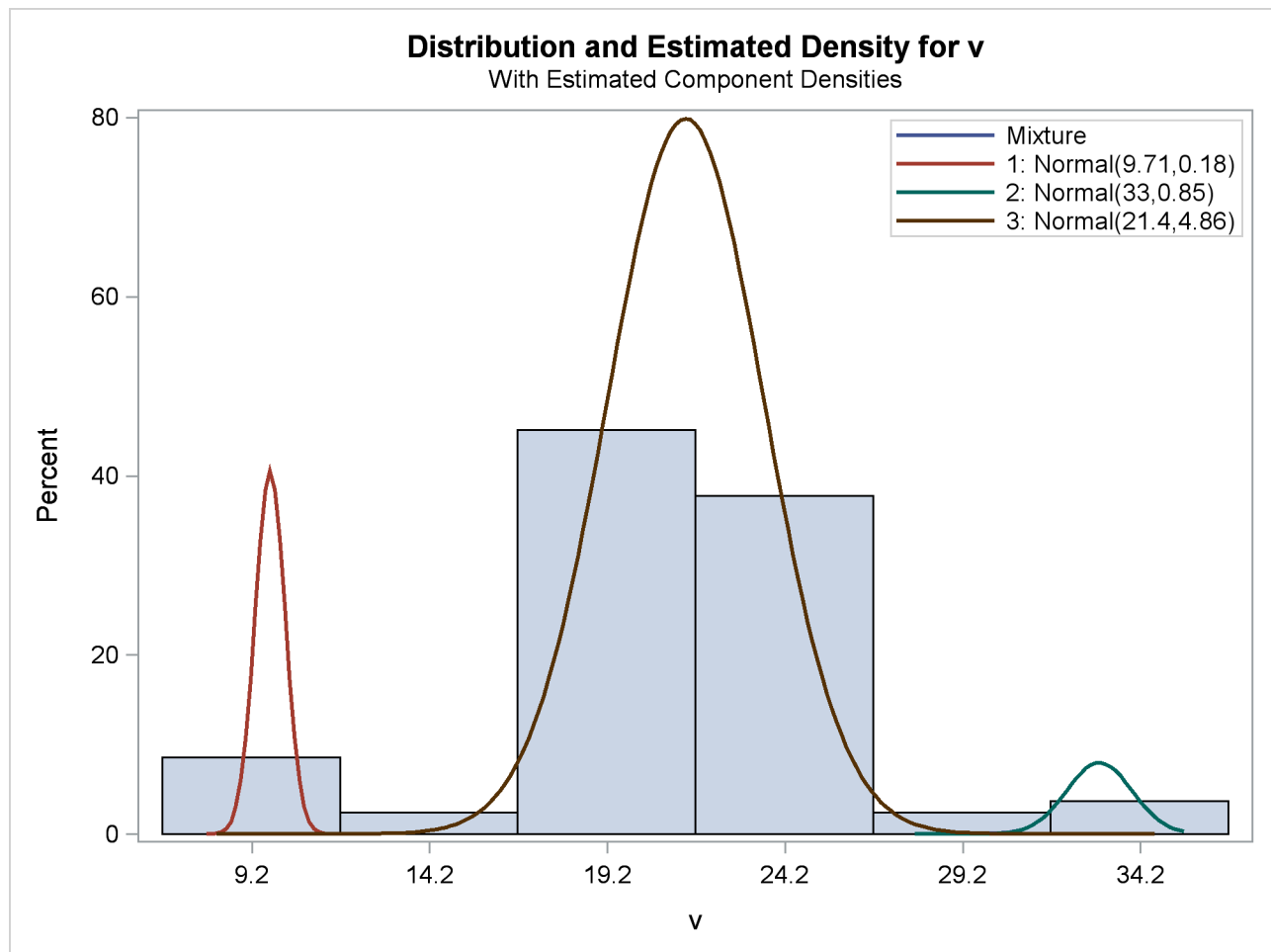
Fit Statistics	
-2 Log Likelihood	407.0
AIC (smaller is better)	423.0
AICC (smaller is better)	424.9
BIC (smaller is better)	442.2
Pearson Statistic	82.0002
Effective Parameters	8
Effective Components	3

Parameter Estimates for 'Normal' Model					
Component	Parameter	Estimate	Standard Error	z Value	Pr > z
1	Intercept	9.7101	0.1597	60.80	<.0001
2	Intercept	33.0444	0.5322	62.09	<.0001
3	Intercept	21.4039	0.2597	82.41	<.0001
1	Variance	0.1785	0.09542		
2	Variance	0.8496	0.6937		
3	Variance	4.8567	0.8098		

Figure 37.14 continued

Parameter Estimates for Mixing Probabilities						
Component	Parameter	Estimate	-----Linked Scale-----		Pr > z	Probability
			Standard Error	z Value		
1	Probability	-2.3308	0.3959	-5.89	<.0001	0.0854
2	Probability	-3.1781	0.5893	-5.39	<.0001	0.0366

Figure 37.15 Density Plot for Best (Three-Component) Model Assuming Unequal Variances



To require that the separate components have identical variances, add the `EQUATE=SCALE` option in the `MODEL` statement:

```

title2 "Three to Seven Components, Equal Variances";
ods select DensityPlot;
proc fmm data=galaxies criterion=AIC gconv=0;
  model v = / kmin=3 kmax=7 equate=scale;
  ods exclude IterHistory OptInfo ComponentInfo;
run;

```

The `GCONV=` convergence criterion is turned off in this PROC FMM run to avoid the early stoppage of the iterations when the relative gradient changes little between iterations. Turning the criterion off usually ensures that convergence is achieved with a small absolute gradient of the objective function.

The output for equal variances is shown in Figure 37.16 and Figure 37.17.

Figure 37.16 Model Selection for Galaxy Data Assuming Equal Variances

```

FMM Analysis of Galaxies Data
Three to Seven Components, Equal Variances

The FMM Procedure

Model Information

Data Set          WORK.GALAXIES
Response Variable v
Type of Model     Homogeneous Mixture
Distribution       Normal
Min Components    3
Max Components    7
Link Function     Identity
Estimation Method Maximum Likelihood

Component Evaluation for Mixture Models

----- Number of -----
Model  -Components-  -Parameters-
  ID   Total    Eff.   Total    Eff.   -2 Log L      AIC      AICC      BIC
-----
  1     3      3      6      6     478.74     490.74     491.86     505.18
  2     4      4      8      8     416.49     432.49     434.47     451.75
  3     5      5     10     10     416.49     436.49     439.59     460.56
  4     6      6     12     12     416.49     440.49     445.02     469.37
  5     7      7     14     14     416.49     444.49     450.76     478.19

Component Evaluation for Mixture Models

----- Number of -----
Model  -Components-  -Parameters-
  ID   Total    Eff.   Total    Eff.   Pearson      Max
                          Gradient
-----
  1     3      3      6      6     82.00     1.197E-6
  2     4      4      8      8     82.00     6.967E-7
  3     5      5     10     10     82.00     4.31E-6
  4     6      6     12     12     82.00     3.03E-6
  5     7      7     14     14     82.00     4.896E-6

The model with 4 components (ID=2) was selected as 'best' based on the AIC
statistic.

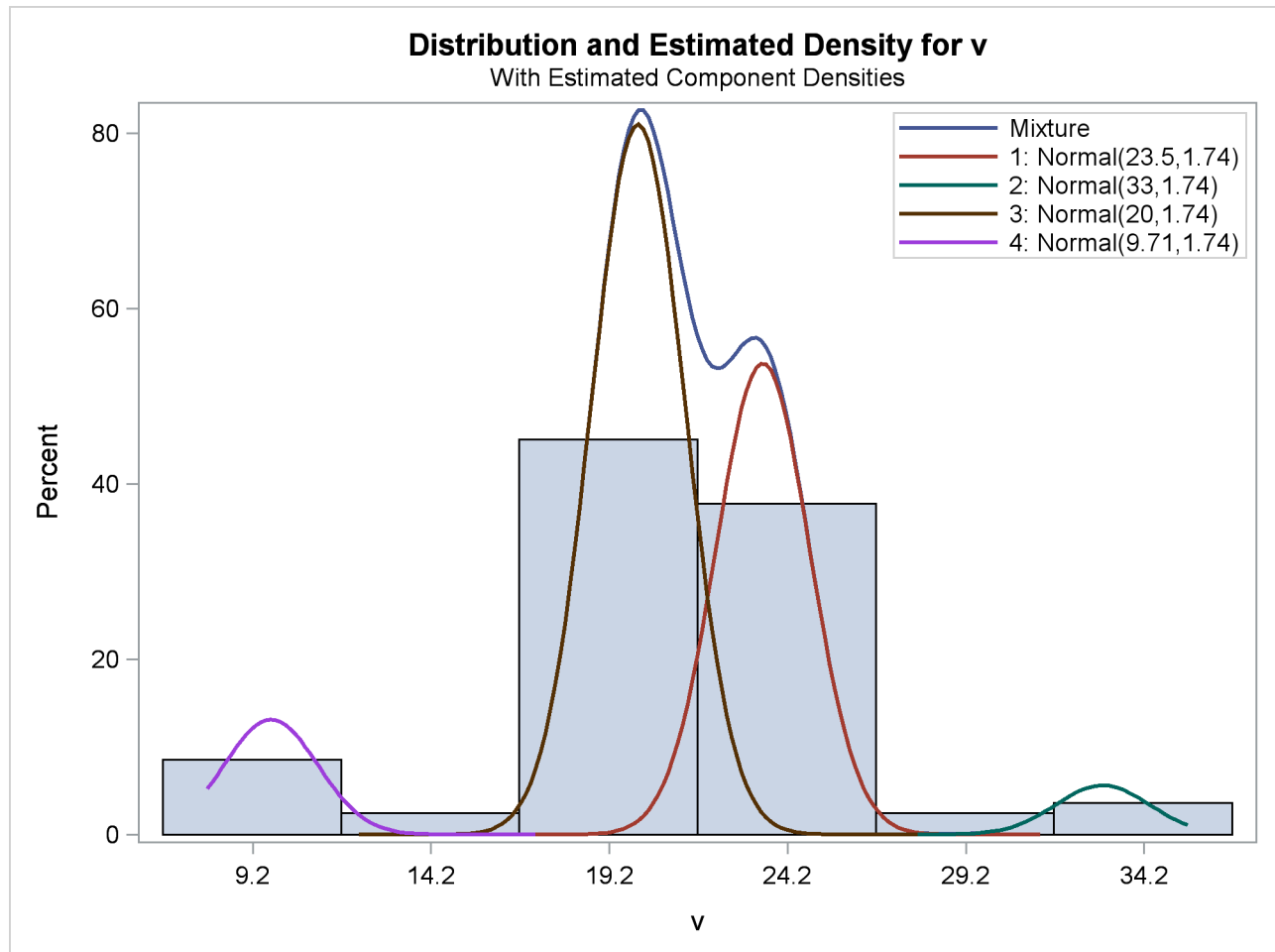
```

Figure 37.16 continued

Fit Statistics					
-2 Log Likelihood					416.5
AIC (smaller is better)					432.5
AICC (smaller is better)					434.5
BIC (smaller is better)					451.7
Pearson Statistic					82.0000
Effective Parameters					8
Effective Components					4

Parameter Estimates for 'Normal' Model					
Component	Parameter	Estimate	Standard Error	z Value	Pr > z
1	Intercept	23.5058	0.3460	67.93	<.0001
2	Intercept	33.0440	0.7610	43.42	<.0001
3	Intercept	20.0086	0.3029	66.06	<.0001
4	Intercept	9.7103	0.4981	19.50	<.0001
1	Variance	1.7354	0.3905		
2	Variance	1.7354	0.3905		
3	Variance	1.7354	0.3905		
4	Variance	1.7354	0.3905		

Parameter Estimates for Mixing Probabilities						
-----Linked Scale-----						
Component	Parameter	Estimate	Standard Error	z Value	Pr > z	Probability
1	Probability	1.4118	0.4497	3.14	0.0017	0.3503
2	Probability	-0.8473	0.6901	-1.23	0.2195	0.0366
3	Probability	1.8216	0.4205	4.33	<.0001	0.5277

Figure 37.17 Density Plot for Best (Six-Component) Model Assuming Equal Variances

Not surprisingly, the two variance specifications produce different optimal models. The unequal variance specification favors a three-component model while the equal variance specification favors a four-component model. Comparison of the AIC fit statistics, 423.0 and 432.5, indicates that the three-component, unequal variance model provides the best overall fit.

Comparison with Roeder's Method

It is important to note that Roeder's original analysis proceeds in a different manner than the finite mixture modeling presented here. The technique presented by Roeder first develops a "best" range of scale parameters based on a specific criterion. Roeder then uses fixed scale parameters taken from this range to develop optimal equal-scale Gaussian mixture models.

You can reproduce Roeder's point estimate for the density by specifying a five-component Gaussian mixture. In addition, use the `EQUATE=SCALE` option in the `MODEL` statement and a `RESTRICT` statement fixing the first component's scale parameter at 0.9025 (Roeder's $h = 0.95$, $\text{scale} = h^2$). The combination of these options produces a mixture of five Gaussian components, each with variance 0.9025. The following statements conduct this analysis:

```

title2 "Five Components, Equal Variances = 0.9025";
ods select DensityPlot;
proc fmm data=galaxies;
  model v = / K=5 equate=scale;
  restrict int 0 (scale 1) = 0.9025;
  ods exclude IterHistory OptInfo ComponentInfo;
run;
ods graphics off;

```

The output is shown in [Figure 37.18](#) and [Figure 37.19](#).

Figure 37.18 Reproduction of Roeder's Five-Component Analysis of Galaxy Data

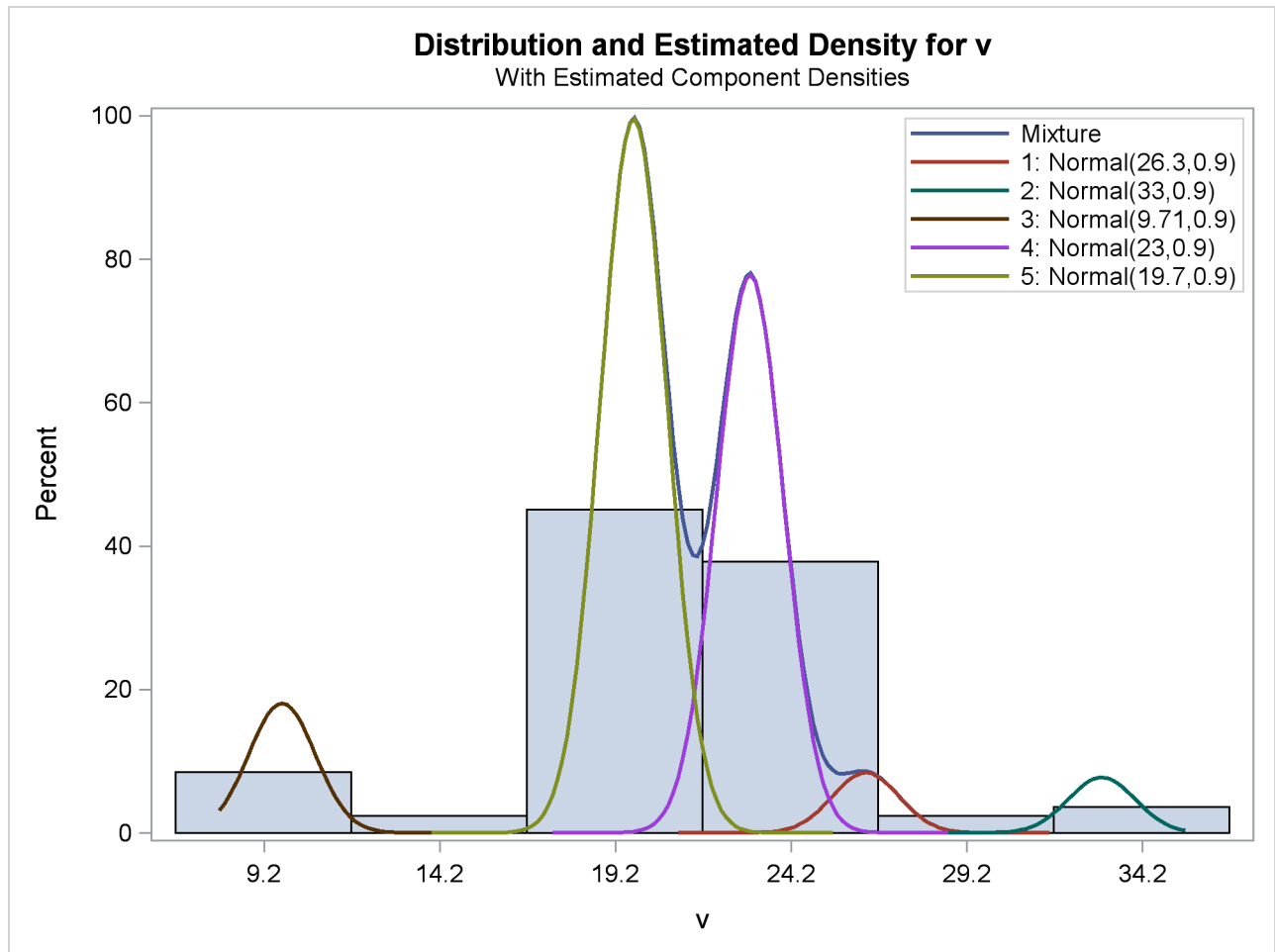
FMM Analysis of Galaxies Data			
Five Components, Equal Variances = 0.9025			
The FMM Procedure			
Model Information			
Data Set		WORK.GALAXIES	
Response Variable		v	
Type of Model		Homogeneous Mixture	
Distribution		Normal	
Components		5	
Link Function		Identity	
Estimation Method		Maximum Likelihood	
Fit Statistics			
-2 Log Likelihood		412.2	
AIC (smaller is better)		430.2	
AICC (smaller is better)		432.7	
BIC (smaller is better)		451.9	
Pearson Statistic		82.5549	
Effective Parameters		9	
Effective Components		5	
Linear Constraints at Solution			
			Constraint
k = 1			Active
Variance	=	0.90	Yes

Figure 37.18 continued

Parameter Estimates for 'Normal' Model					
Component	Parameter	Estimate	Standard Error	z Value	Pr > z
1	Intercept	26.3266	0.7778	33.85	<.0001
2	Intercept	33.0443	0.5485	60.25	<.0001
3	Intercept	9.7101	0.3591	27.04	<.0001
4	Intercept	23.0295	0.2294	100.38	<.0001
5	Intercept	19.7187	0.1784	110.55	<.0001
1	Variance	0.9025	0		
2	Variance	0.9025	0		
3	Variance	0.9025	0		
4	Variance	0.9025	0		
5	Variance	0.9025	0		

Parameter Estimates for Mixing Probabilities						
-----Linked Scale-----						
Component	Parameter	Estimate	Standard Error	z Value	Pr > z	Probability
1	Probability	-2.4739	0.7084	-3.49	0.0005	0.0397
2	Probability	-2.5544	0.6016	-4.25	<.0001	0.0366
3	Probability	-1.7071	0.4141	-4.12	<.0001	0.0854
4	Probability	-0.2466	0.2699	-0.91	0.3609	0.3678

Figure 37.19 Density Plot for Roeder's Analysis



Syntax: FMM Procedure

The following statements are available in the FMM procedure:

```

PROC FMM < options > ;
  BAYES bayes-options ;
  BY variables ;
  CLASS variables < / TRUNCATE > ;
  FREQ variable ;
  ID variables ;
  MODEL response< (response-options) > = < effects > < / model-options > ;
  MODEL events/trials = < effects > < / model-options > ;
  MODEL          + < effects > < / model-options > ;
  OUTPUT < OUT=SAS-data-set >
    < keyword< (keyword-options) > < =name > > ...
    < keyword< (keyword-options) > < =name > > < / options > ;
  PERFORMANCE performance-options ;
  PROBMODEL < effects > < / probmodel-options > ;
  RESTRICT < 'label' > constraint-specification < , ... , constraint-specification >
    < operator < value > > < / option > ;
  WEIGHT variable ;

```

The **PROC FMM** statement and at least one **MODEL** statement is required. The **CLASS**, **RESTRICT** and **MODEL** statements can appear multiple times. If a **CLASS** statement is specified, it must precede the **MODEL** statements. The **RESTRICT** statements must appear after the **MODEL** statements.

PROC FMM Statement

```
PROC FMM < options > ;
```

The **PROC FMM** statement invokes the FMM procedure. [Table 37.2](#) summarizes the options available in the **PROC FMM** statement. These and other options in the **PROC FMM** statement are then described fully in alphabetical order.

Table 37.2 PROC FMM Statement Options

Option	Description
Basic Options	
DATA=	Specifies the input data set
EXCLUSION=	Specifies how the procedure responds to support violations in the data
NAMELEN=	Specifies the length of effect names
ORDER=	Determines the sort order of CLASS variables
SEED=	Specifies the random number seed for analyses that require random number draws

Table 37.2 *continued*

Option	Description
Displayed Output	
COMPONENTINFO	Displays information about the mixture components
CORR	Displays the asymptotic correlation matrix of the maximum likelihood parameter estimates or the empirical correlation matrix of the Bayesian posterior estimates
COV	Displays the asymptotic covariance matrix of the maximum likelihood parameter estimates or the empirical covariance matrix of the Bayesian posterior estimates
COVI	Displays the inverse of the covariance matrix of the parameter estimates
FITDETAILS	Displays fit information for all examined models
ITDETAILS	Adds estimates and gradients to the “Iteration History” table
NOCLPRINT	Suppresses the “Class Level Information” table completely or partially
NOITPRINT	Suppresses the “Iteration History Information” table
NOPRINT	Suppresses tabular and graphical output
PARMSTYLE=	Specifies how parameters are displayed in ODS tables
PLOTS	Produces ODS statistical graphics
Computational Options	
CRITERION=	Specifies the criterion used in model selection
NOCENTER	Prevents centering and scaling of the regressor variables
PARTIAL=	Specifies a variable that defines a partial classification
Options Related to Optimization	
ABSCONV=	Tunes an absolute function convergence criterion
ABSFCONV=	Tunes an absolute function difference convergence criterion
ABSGCONV=	Tunes the absolute gradient convergence criterion
FCONV=	Specifies a relative function convergence criterion that is based on a relative change of the function value
FCONV2=	Specifies a relative function convergence criterion that is based on a predicted reduction of the objective function
GCONV=	Tunes the relative gradient convergence criterion
MAXITER=	Specifies the maximum number of iterations in any optimization
MAXFUNC=	Specifies the maximum number of function evaluations in any optimization
MAXTIME=	Specifies the upper limit of CPU time in seconds for any optimization
MINITER=	Specifies the minimum number of iterations in any optimization
TECHNIQUE=	Selects the optimization technique
Singularity Tolerances	
INVALIDLOGL=	Tunes the value assigned to an invalid component log likelihood
SINGCHOL=	Tunes singularity for Cholesky decompositions

Table 37.2 *continued*

Option	Description
SINGRES=	Tunes singularity for the residual variance
SINGULAR=	Tunes general singularity criterion

You can specify the following *options* in the PROC FMM statement.

ABSCONV=*r***ABSTOL=*r***

specifies an absolute function convergence criterion. For minimization, the termination criterion is $f(\boldsymbol{\psi}^{(k)}) \leq r$, where $\boldsymbol{\psi}$ is the vector of parameters in the optimization and $f(\cdot)$ is the objective function. The default value of r is the negative square root of the largest double-precision value, which serves only as a protection against overflows.

ABSFCONV=*r* < *n* >**ABSFTOL=*r* < *n* >**

specifies an absolute function difference convergence criterion. For all techniques except NMSIMP, the termination criterion is a small change of the function value in successive iterations:

$$|f(\boldsymbol{\psi}^{(k-1)}) - f(\boldsymbol{\psi}^{(k)})| \leq r$$

Here, $\boldsymbol{\psi}$ denotes the vector of parameters that participate in the optimization, and $f(\cdot)$ is the objective function. The same formula is used for the NMSIMP technique, but $\boldsymbol{\psi}^{(k)}$ is defined as the vertex with the lowest function value, and $\boldsymbol{\psi}^{(k-1)}$ is defined as the vertex with the highest function value in the simplex. The default value is $r=0$. The optional integer value n specifies the number of successive iterations for which the criterion must be satisfied before the process can be terminated.

ABSGCONV=*r* < *n* >**ABSGTOL=*r* < *n* >**

specifies an absolute gradient convergence criterion. The termination criterion is a small maximum absolute gradient element:

$$\max_j |g_j(\boldsymbol{\psi}^{(k)})| \leq r$$

Here, $\boldsymbol{\psi}$ denotes the vector of parameters that participate in the optimization, and $g_j(\cdot)$ is the gradient of the objective function with respect to the j th parameter. This criterion is not used by the NMSIMP technique. The default value is $r=1E-5$. The optional integer value n specifies the number of successive iterations for which the criterion must be satisfied before the process can be terminated.

COMPONENTINFO**COMPINFO****CINFO**

produces a table with additional details about the fitted model components.

COV

produces the covariance matrix of the parameter estimates. For maximum likelihood estimation, this matrix is based on the inverse (projected) Hessian matrix. For Bayesian estimation, it is the empirical covariance matrix of the posterior estimates. The covariance matrix is shown for all parameters, even if they did not participate in the optimization or sampling.

COVI

produces the inverse of the covariance matrix of the parameter estimates. For maximum likelihood estimation, the covariance matrix is based on the inverse (projected) Hessian matrix. For Bayesian estimation, it is the empirical covariance matrix of the posterior estimates. This matrix is then inverted by sweeping, and rows and columns that correspond to linear dependencies or singularities are zeroed.

CORR

produces the correlation matrix of the parameter estimates. For maximum likelihood estimation this matrix is based on the inverse (projected) Hessian matrix. For Bayesian estimation, it is based on the empirical covariance matrix of the posterior estimates.

CRITERION=keyword**CRIT=keyword**

specifies the criterion by which the FMM procedure ranks models when multiple models are evaluated during maximum likelihood estimation. You can choose from the following *keywords* to rank models:

AIC	based on Akaike's information criterion
AICC	based on the bias-corrected AIC criterion
BIC	based on the Bayesian information criterion
GRADIENT	based on the largest element of the gradient (in absolute value)
LOGL LL	based on the mixture log likelihood
PEARSON	based on the Pearson statistic

The default is CRITERION=BIC.

DATA=SAS-data-set

names the SAS data set to be used by PROC FMM. The default is the most recently created data set.

EXCLUSION=NONE | ANY | ALL**EXCLUDE=NONE | ANY | ALL**

specifies how the FMM procedure handles support violations of observations. For example, in a mixture of two Poisson variables, negative response values are not possible. However, in a mixture of a Poisson and a normal variable, negative values are possible, and their likelihood contribution to the Poisson component is zero. An observation that violates the support of one component distribution of the model might be a valid response with respect to one or more other component distributions. This requires some nuanced handling of support violations in mixture models.

The default exclusion technique, EXCLUSION=ALL, removes an observation from the analysis only if it violates the support of all component distributions. The other extreme, EXCLUSION=NONE, permits an observation into the analysis regardless of support violations. EXCLUSION=ANY removes observations from the analysis if the response violates the support of any component distributions. In the single-component case, EXCLUSION=ALL and EXCLUSION=ANY are identical.

FCONV= $r < n >$ **FTOL**= $r < n >$

specifies a relative function convergence criterion that is based on the relative change of the function value. For all techniques except NMSIMP, PROC FMM terminates when there is a small relative change of the function value in successive iterations:

$$\frac{|f(\boldsymbol{\psi}^{(k)}) - f(\boldsymbol{\psi}^{(k-1)})|}{|f(\boldsymbol{\psi}^{(k-1)})|} \leq r$$

Here, $\boldsymbol{\psi}$ denotes the vector of parameters that participate in the optimization, and $f(\cdot)$ is the objective function. The same formula is used for the NMSIMP technique, but $\boldsymbol{\psi}^{(k)}$ is defined as the vertex with the lowest function value, and $\boldsymbol{\psi}^{(k-1)}$ is defined as the vertex with the highest function value in the simplex.

The default is $r = 10^{-\text{FDIGITS}}$, where FDIGITS is by default $-\log_{10}\{\epsilon\}$, and ϵ is the machine precision. The optional integer value n specifies the number of successive iterations for which the criterion must be satisfied before the process terminates.

FCONV2= $r < n >$ **FTOL2**= $r < n >$

specifies a relative function convergence criterion that is based on the predicted reduction of the objective function. For all techniques except NMSIMP, the termination criterion is a small predicted reduction

$$df^{(k)} \approx f(\boldsymbol{\theta}^{(k)}) - f(\boldsymbol{\theta}^{(k)} + \mathbf{s}^{(k)})$$

of the objective function. The predicted reduction

$$\begin{aligned} df^{(k)} &= -\mathbf{g}^{(k)'} \mathbf{s}^{(k)} - \frac{1}{2} \mathbf{s}^{(k)'} \mathbf{H}^{(k)} \mathbf{s}^{(k)} \\ &= -\frac{1}{2} \mathbf{s}^{(k)'} \mathbf{g}^{(k)} \\ &\leq r \end{aligned}$$

is computed by approximating the objective function f by the first two terms of the Taylor series and substituting the Newton step:

$$\mathbf{s}^{(k)} = -[\mathbf{H}^{(k)}]^{-1} \mathbf{g}^{(k)}$$

For the NMSIMP technique, the termination criterion is a small standard deviation of the function values of the $n + 1$ simplex vertices $\boldsymbol{\theta}_l^{(k)}$, $l = 0, \dots, n$,

$$\sqrt{\frac{1}{n+1} \sum_l \left[f(\boldsymbol{\theta}_l^{(k)}) - \bar{f}(\boldsymbol{\theta}^{(k)}) \right]^2} \leq r$$

where $\bar{f}(\boldsymbol{\theta}^{(k)}) = \frac{1}{n+1} \sum_l f(\boldsymbol{\theta}_l^{(k)})$. If there are n_{act} boundary constraints active at $\boldsymbol{\theta}^{(k)}$, the mean and standard deviation are computed only for the $n + 1 - n_{act}$ unconstrained vertices.

The default value is $r = 1\text{E-}6$ for the NMSIMP technique and $r = 0$ otherwise. The optional integer value n specifies the number of successive iterations for which the criterion must be satisfied before the process terminates.

FITDETAILS

requests that the “Optimization Information,” “Iteration History,” and “Fit Statistics” tables be produced for all optimizations when models with different number of components are evaluated. For example, the following statements fit a binomial regression model with up to three components and produces fit and optimization information for all three:

```
proc fmm fitdetails;
  model y/n = x / kmax=3;
run;
```

Without the FITDETAILS option, only the “Fit Statistics” table for the selected model is displayed.

GCONV=*r*<*n*>**GTOL=*r*<*n*>**

specifies a relative gradient convergence criterion. For all techniques except CONGRA and NMSIMP, the termination criterion is a small normalized predicted function reduction:

$$\frac{\mathbf{g}(\boldsymbol{\psi}^{(k)})'[\mathbf{H}^{(k)}]^{-1}\mathbf{g}(\boldsymbol{\psi}^{(k)})}{|f(\boldsymbol{\psi}^{(k)})|} \leq r$$

Here, $\boldsymbol{\psi}$ denotes the vector of parameters that participate in the optimization, $f(\cdot)$ is the objective function, and $\mathbf{g}(\cdot)$ is the gradient. For the CONGRA technique (where a reliable Hessian estimate \mathbf{H} is not available), the following criterion is used:

$$\frac{\|\mathbf{g}(\boldsymbol{\psi}^{(k)})\|_2 \|\mathbf{s}(\boldsymbol{\psi}^{(k)})\|_2}{\|\mathbf{g}(\boldsymbol{\psi}^{(k)}) - \mathbf{g}(\boldsymbol{\psi}^{(k-1)})\|_2 |f(\boldsymbol{\psi}^{(k)})|} \leq r$$

This criterion is not used by the NMSIMP technique. The default value is $r=1\text{E}-8$. The optional integer value n specifies the number of successive iterations for which the criterion must be satisfied before the process can terminate.

HESSIAN

displays the Hessian matrix of the model. This option is not available for Bayesian estimation.

INVALIDLOGL=*r*

specifies the value assumed by the FMM procedure if a log likelihood cannot be computed (for example, because the value of the response variable falls outside of the response distribution’s support). The default value is $-1\text{E}20$.

ITDETAILS

adds parameter estimates and gradients to the “Iteration History” table. If the FMM procedure centers or scales the model variables (or both), the parameter estimates and gradients reported during the iteration refer to that scale. You can suppress centering and scaling with the [NOCENTER](#) option.

MAXFUNC=*n***MAXFU=*n***

specifies the maximum number of function calls in the optimization process. The default values are as follows, depending on the optimization technique:

- TRUREG, NRRIDG, and NEWRAP: 125
- QUANEW and DBLDOG: 500
- CONGRA: 1000
- NMSIMP: 3000

The optimization can terminate only after completing a full iteration. Therefore, the number of function calls that are actually performed can exceed the number that is specified by the `MAXFUNC=` option. You can choose the optimization technique with the `TECHNIQUE=` option.

MAXITER=*n***MAXIT=*n***

specifies the maximum number of iterations in the optimization process. The default values are as follows, depending on the optimization technique:

- TRUREG, NRRIDG, and NEWRAP: 50
- QUANEW and DBLDOG: 200
- CONGRA: 400
- NMSIMP: 1000

These default values also apply when *n* is specified as a missing value. You can choose the optimization technique with the `TECHNIQUE=` option.

MAXTIME=*r*

specifies an upper limit of *r* seconds of CPU time for the optimization process. The default value is the largest floating-point double representation of your computer. The time specified by the `MAXTIME=` option is checked only once at the end of each iteration. Therefore, the actual running time can be longer than that specified by the `MAXTIME=` option.

MINITER=*n***MINIT=*n***

specifies the minimum number of iterations. The default value is 0. If you request more iterations than are actually needed for convergence to a stationary point, the optimization algorithms can behave strangely. For example, the effect of rounding errors can prevent the algorithm from continuing for the required number of iterations.

NAMELEN=*number*

specifies the length to which long effect names are shortened. The default and minimum value is 20.

NOCENTER

requests that regressor variables not be centered or scaled. By default the FMM procedure centers and scales columns of the **X** matrix if the models contain intercepts. If `NOINT` options in `MODEL` statements are in effect, the columns of **X** are scaled but not centered. Centering and scaling can help with the stability of estimation and sampling algorithms. The FMM procedure does not produce a table of the centered and scaled coefficients and provides no user control over the type of centering and scaling that is applied. The `NOCENTER` option turns any centering and scaling off and processes the raw values of the continuous variables.

NOCLPRINT<=*number*>

suppresses the display of the “Class Level Information” table if you do not specify *number*. If you specify *number*, the values of the classification variables are displayed for only those variables whose number of levels is less than *number*. Specifying a *number* helps to reduce the size of the “Class Level Information” table if some classification variables have a large number of levels.

NOITPRINT

suppresses the display of the “Iteration History Information” table.

NOPRINT

suppresses the normal display of tabular and graphical results. The NOPRINT option is useful when you want to create only one or more output data sets with the procedure. This option temporarily disables the Output Delivery System (ODS); see Chapter 20, “Using the Output Delivery System,” for more information.

ORDER=*order-type*

specifies the sort order for the levels of **CLASS** variables. This ordering determines which parameters in the model correspond to each level in the data.

You can specify the following values for *order-type*:

DATA

sorts the levels by order of appearance in the input data set.

FORMATTED

sorts the levels by external formatted value, except for numeric variables with no explicit format, which are sorted by their unformatted (internal) value.

FREQ

sorts the levels by descending frequency count; levels with the most observations come first in the order.

INTERNAL

sorts the levels by unformatted value.

FREQDATA

sorts the levels by order of descending frequency count, and within counts by order of appearance in the input data set when counts are tied.

FREQFORMATTED

sorts the levels by order of descending frequency count, and within counts by formatted value (as above) when counts are tied.

FREQINTERNAL

sorts the levels by order of descending frequency count, and within counts by unformatted value when counts are tied.

When the default ORDER=FORMATTED is in effect for numeric variables for which you have supplied no explicit format, the levels are ordered by their internal values. To order numeric class levels with no explicit format by their BEST12. formatted values, you can specify this format explicitly for the **CLASS** variables.

When FORMATTED and INTERNAL values are involved, the sort order is machine-dependent.

When the response variable appears in a CLASS statement, the ORDER= option in the PROC FMM statement applies to its sort order. For example, in the following statements the sort order of the wheeze variable is determined by the order of appearance in the input data set because the response variable appears in the CLASS statement:

```
proc fmm order=data;
  class city wheeze;
  model wheeze = city age / dist=binary s;
run;
```

However, in the following statements the sort order of the wheeze variable is determined by the formatted value (the default *response-option* in the MODEL statement):

```
proc fmm order=data;
  class city;
  model wheeze = city age / dist=binary s;
run;
```

The ORDER= option in the PROC FMM statement has no effect on the sort order of the wheeze variable because it does not appear in the CLASS statement.

When you specify a *response-option* in the MODEL statement, it overrides the ORDER= option in the PROC FMM statement.

For more information about sort order, see the chapter on the SORT procedure in the *Base SAS Procedures Guide* and the discussion of BY-group processing in *SAS Language Reference: Concepts*.

PARAMSTYLE=EFFECT | LABEL

specifies the display style for parameters and effects. The FMM procedure can display parameters in two styles:

- The EFFECT style (which is used by the MIXED and GLIMMIX procedure, for example) identifies a parameter with an “Effect” column and adds separate columns for the CLASS variables in the model.
- The LABEL style creates one column, named Parameter, that combines the relevant information about a parameter into a single column. If your model contains multiple CLASS variables, the LABEL style might use space more economically.

The EFFECT style is the default for models that contain effects; otherwise the LABEL style is used (for example, in homogeneous mixtures). You can change the display style with the PARAMSTYLE= option. Regardless of the display style, ODS output data sets that contain information about parameter estimates contain columns for both styles.

PARTIAL=*variable*

MEMBERSHIP=*variable*

specifies a variable in the input data set that identifies component membership. You can specify missing values for observations whose component membership is undetermined; this is known as a partial classification (McLachlan and Peel 2000, p. 75). For observations with known membership,

the likelihood contribution is no longer a mixture. If observation i is known to be a member of component m , then its log likelihood contribution is

$$\log \{ \pi_m(\mathbf{z}, \boldsymbol{\alpha}_m) p_m(y; \mathbf{x}'_m \boldsymbol{\beta}_m, \phi_m) \}$$

Otherwise, if membership is undetermined, it is

$$\log \left\{ \sum_{j=1}^k \pi_j(\mathbf{z}, \boldsymbol{\alpha}_j) p_j(y; \mathbf{x}'_j \boldsymbol{\beta}_j, \phi_j) \right\}$$

The variable specified in the PARTIAL= option can be numeric or character. In case of a character variable, the variable must appear in the CLASS statement. If the PARTIAL= variable appears in the CLASS statement, the membership assignment is made based on the levelized values of the variable, as shown in the “Class Level Information” table. Invalid values of the PARTIAL= variable are ignored.

In a model in which label switching is a problem, the switching can sometimes be avoided by assigning just a few observations to categories. For example, in a three-component model, switches might be prevented by assigning the observation with the smallest response value to the first component and the observation with the largest response value to the last component.

PLOTS <(global-plot-options)> <= plot-request <(options)>>

PLOTS <(global-plot-options)> <= (plot-request <(options)> <... plot-request <(options)>>>

controls the plots produced through ODS Graphics.

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;
proc fmm data=yeast seed=12345;
  model count/n = / k=2;
  freq f;
  performance cpucount=2;
  bayes;
run;
ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS](#).”

Global Plot Options

The *global-plot-options* apply to all relevant plots generated by the FMM procedure. The *global-plot-options* supported by the FMM procedure are as follows:

UNPACKPANEL**UNPACK**

displays each graph separately. (By default, some graphs can appear together in a single panel.)

ONLY

produces only the specified plots. This option is useful if you do not want the procedure to generate all default graphics, but only the ones specified.

Specific Plot Options

The following listing describes the specific plots and their options.

ALL

requests that all plots appropriate for the analysis be produced.

NONE

requests that no ODS graphics be produced.

DENSITY <(density-options)>

requests a plot of the data histogram and mixture density function. This graphic is a default graphic in models without effects in the **MODEL** statements and is available only in these models. Furthermore, all distributions involved in the mixture must be continuous. You can specify the following *density-options* to modify the plot:

CUMULATIVE**CDF**

displays the histogram and densities in cumulative form.

NBINS=*n***BINS**=*n*

specifies the number of bins in the histogram; *n* is greater than or equal to 0. By default, the FMM procedure computes a suitable bin width and number of bins, based on the range of the response and the number of usable observations. The option has no effect for binary data.

NOCOMPONENTS**NOCOMP**

suppresses the component densities from the plot. If the component densities are displayed, they are scaled so that their sum equals the mixture density at any point on the graph. In single-component models, this option has no effect.

NODENSITY**NODENS**

suppresses the computation of the mixture density (and the component densities if the **COMPONENTS** suboption is specified). If you specify the **NOHISTOGRAM** and the **NODENSITY** option, no graphic is produced.

NOLABEL

suppresses the component identification with labels. By default, the FMM procedure labels component densities in the legend of the plot. If you do not specify a model label with the **LABEL=** option in the **MODEL** statement, an identifying label is constructed from the parameter estimates that are associated with the component. In this case the parameter values are not necessarily the mean and variance of the distribution; the values used to identify the densities on the plot are chosen to simplify linking between graphical and tabular results.

NOHISTOGRAM**NOHIST**

suppresses the computation of the histogram of the raw values. If you specify the **NOHISTOGRAM** and the **NODENSITY** option, no graphic is produced.

NPOINTS=*n***N=*n***

specifies the number of values used to compute the density functions; *n* is greater than or equal to 0. The default is N=200.

WIDTH=*value***BINWIDTH=*value***

specifies the bin width for the histogram. The *value* is specified in units of the response variable and must be positive. The option has no effect for binary data.

TRACE <(tadpanel-options)>

requests a trace panel with posterior diagnostics for a Bayesian analysis. If a **BAYES** statement is present, the trace panel plots are generated by default, one for each sampled parameter. You can specify the following *tadpanel-options* to modify the graphic:

BOX**BOXPLOT**

replaces the autocorrelation plot with a box plot of the posterior sample.

SMOOTH=NONE | MEAN | SPLINE

adds a reference estimate to the trace plot. By default, **SMOOTH=NONE**. **SMOOTH=MEAN** uses the arithmetic mean of the trace as the reference. **SMOOTH=SPLINE** adds a penalized B-spline.

REFERENCE= *reference-style*

adds vertical reference lines to the density plot, trace plot, and box plot. The available options for the *reference-style* are:

NONE	suppresses the reference lines
EQT	requests equal-tail intervals
HPD	requests intervals of highest posterior density. The level for the credible or HPD intervals is chosen based on the “Posterior Interval Statistics” table.
PERCENTILES (or PERC)	for percentiles. Up to three percentiles can be displayed, as based on the “Posterior Summary Statistics” table.

The default is **REFERENCE=CREDIBLE**.

UNPACK

unpacks the panel graphic and displays its elements as separate plots.

SEED=*n*

determines the random number seed for analyses that depend on a random number stream. If you do not specify a seed or if you specify a value less than or equal to zero, the seed is generated from reading the time of day from the computer clock. The largest possible value for the seed is $2^{31} - 1$. The seed value is reported in the “Model Information” table.

You can use the `SYSRANDOM` and `SYSRANEND` macro variables after a PROC FMM run to query the initial and final seed values. However, using the final seed value as the starting seed for a subsequent analysis does not continue the random number stream where the previous analysis left off. The `SYSRANEND` macro variable provides a mechanism to pass on seed values to ensure that the sequence of random numbers is the same every time you run an entire program.

Analyses that use the same (nonzero) seed are not completely reproducible if they are executed with a different number of threads since the random number streams in separate threads are independent. You can control the number of threads used by the FMM procedure with system options or through the `PERFORMANCE` statement in the FMM procedure.

SINGCHOL=*number*

tunes the singularity criterion in Cholesky decompositions. The default is 1E4 times the machine epsilon; this product is approximately 1E-12 on most computers.

SINGRES=*number*

sets the tolerance for which the residual variance or scale parameter is considered to be zero. The default is 1E4 times the machine epsilon; this product is approximately 1E-12 on most computers.

SINGULAR=*number*

tunes the general singularity criterion applied by the FMM procedure in sweeps and inversions. The default is 1E4 times the machine epsilon; this product is approximately 1E-12 on most computers.

TECHNIQUE=*keyword***TECH=*keyword***

specifies the optimization technique to obtain maximum likelihood estimates. You can choose from the following techniques by specifying the appropriate *keyword*:

CONGRA	performs a conjugate-gradient optimization.
DBLDOG	performs a version of double-dogleg optimization.
NEWRAP	performs a Newton-Raphson optimization combining a line-search algorithm with ridging.
NMSIMP	performs a Nelder-Mead simplex optimization.
NONE	performs no optimization.
NRRIDG	performs a Newton-Raphson optimization with ridging.
QUANEW	performs a dual quasi-Newton optimization.
TRUREG	performs a trust-region optimization.

The default is TECH=QUANEW.

For more details about these optimization methods, see the section “Choosing an Optimization Algorithm” on page 494 of Chapter 19, “Shared Concepts and Topics.”

BAYES Statement

BAYES *bayes-options* ;

The BAYES statement requests that the parameters of the model be estimated by Markov chain Monte Carlo sampling techniques. The FMM procedure can estimate by maximum likelihood the parameters of all models supported by the procedure. Bayes estimation, on the other hand, is available for only a subset of these models.

In Bayesian analysis, it is essential to examine the convergence of the Markov chains before you proceed with posterior inference. With ODS Graphics turned on, the FMM procedure produces graphs at the end of the procedure output; these graphs enable you to visually examine the convergence of the chain. Inferences cannot be made if the Markov chain has not converged.

The output produced for a Bayesian analysis is markedly different from that for a frequentist (maximum likelihood) analysis for the following reasons:

- Parameter estimates do not have the same interpretation in the two analyses. Parameters are fixed unknown constants in the frequentist context and random variables in a Bayesian analysis.
- The results of a Bayesian analysis are summarized through chain diagnostics and posterior summary statistics and intervals.
- The FMM procedure samples the mixing probabilities in Bayesian models directly, rather than mapping them onto a logistic (or other) scale.

The FMM procedure applies highly specialized sampling algorithms in Bayesian models. For single-component models without effects, a conjugate sampling algorithm is used where possible. For models in the exponential family that contain effects, the sampling algorithm is based on Gamerman (1997). For the normal and t distributions, a conjugate sampler is the default sampling algorithm for models with and without effects. In multi-component models, the sampling algorithm is based on latent variable sampling through data augmentation (Frühwirth-Schnatter 2006) and the Gamerman or conjugate sampler. Because of this specialization, the options for controlling the prior distributions of the parameters are limited.

Table 37.3 summarizes the *bayes-options* available in the BAYES statement. The full assortment of options is then described in alphabetical order.

Table 37.3 BAYES Statement Options

Option	Description
Options Related to Sampling	
INITIAL=	Specifies how to construct initial values
NBI=	Specifies the number of burn-in samples
NMC=	Specifies the number of samples after burn-in

Table 37.3 *continued*

Option	Description
METROPOLIS	Forces a Metropolis-Hastings sampling algorithm even if conjugate sampling is possible
OUTPOST=	Generates a data set that contains the posterior estimates
THIN=	Controls the thinning of the Markov chain
Specification of Prior Information	
MIXPRIORPARMS	Specifies the prior parameters for the Dirichlet distribution of the mixing probabilities
BETAPRIORPARMS=	Specifies the parameters of the normal prior distribution for individual parameters in the β vector
MUPRIORPARMS=	Specifies the parameters of the prior distribution for the means in homogeneous mixtures without effects
PHIPRIORPARMS=	Specifies the parameters of the inverse gamma prior distribution for the scale parameters in homogeneous mixtures
PRIOROPTIONS	Specifies additional options used in the determination of the prior distribution
Posterior Summary Statistics and Convergence Diagnostics	
DIAGNOSTICS=	Displays convergence diagnostics for the Markov chain
STATISTICS	Displays posterior summary information for the Markov chain
Other Options	
ESTIMATE=	Specifies which estimate is used for the computation of OUTPUT statistics and graphics
TIMEINC=	Specifies the time interval to report on sampling progress (in seconds)

You can specify the following *bayes-options* in the BAYES statement.

BETAPRIORPARMS=*pair-specification*

BETAPRIORPARMS(*pair-specification ... pair-specification*)

specifies the parameters for the normal prior distribution of the parameters that are associated with model effects (β s). The *pair-specification* is of the form (a, b), and the values a and b are the mean and variance of the normal distribution, respectively. This option overrides the **PRIOROPTIONS** option.

The form of the **BETAPRIORPARMS** with an equal sign and a single pair is used to specify one pair of prior parameters that applies to all components in the mixture. In the following example, the two intercepts and the two regression coefficients all have a $N(0, 100)$ prior distribution:

```
proc fmm;
  model y = x / k=2;
  bayes betapriorparms=(0,100);
run;
```

You can also provide a list of pairs to specify different sets of prior parameters for the various regression parameters and components. For example:

```
proc fmm;
  model y = x/ k=2;
  bayes betapriorparms( (0,10) (0,20) (.,.) (3,100) );
run;
```

The simple linear regression in the first component has a $N(0, 10)$ prior for the intercept and a $N(0, 20)$ prior for the slope. The prior for the intercept in the second component uses the FMM default, whereas the prior for the slope is $N(3, 100)$.

DIAGNOSTICS=ALL | NONE | (*keyword-list*)

DIAG=ALL | NONE | (*keyword-list*)

controls the computation of diagnostics for the posterior chain. You can request all posterior diagnostics by specifying **DIAGNOSTICS=ALL** or suppress the computation of posterior diagnostics by specifying **DIAGNOSTICS=NONE**. The following *keywords* enable you to select subsets of posterior diagnostics; the default is **DIAGNOSTICS=(AUTOCORR)**.

AUTOCORR <(LAGS= *numeric-list*)>

computes for each sampled parameter the autocorrelations of lags specified in the **LAGS=** list. Elements in the list are truncated to integers, and repeated values are removed. If the **LAGS=** option is not specified, autocorrelations are computed by default for lags 1, 5, 10, and 50. See the section “[Autocorrelations](#)” on page 152 for details.

ESS

computes an estimate of the effective sample size (Kass et al. 1998), the correlation time, and the efficiency of the chain for each parameter. See the section “[Effective Sample Size](#)” on page 152 for details.

GEWEKE <(geweke-options)>

computes the Geweke spectral density diagnostics (Geweke 1992), which are essentially a two-sample t test between the first f_1 portion and the last f_2 portion of the chain. The default is $f_1 = 0.1$ and $f_2 = 0.5$, but you can choose other fractions by using the following *geweke-options*:

FRAC1=value

specifies the fraction f_1 for the first window.

FRAC2=value

specifies the fraction f_2 for the second window.

See the section “[Geweke Diagnostics](#)” on page 146 for details.

HEIDELBERGER <(Heidel-options)>

HEIDEL <(Heidel-options)>

computes the Heidelberg and Welch diagnostic (which consists of a stationarity test and a half-width test) for each variable. The stationary diagnostic test tests the null hypothesis that the posterior samples are generated from a stationary process. If the stationarity test is passed, a half-width test is then carried out. See the section “[Heidelberg and Welch Diagnostics](#)” on page 148 for more details.

These diagnostics are not performed by default. You can specify the `DIAGNOSTICS=HEIDELBERGER` option to request these diagnostics, and you can also specify suboptions, such as `DIAGNOSTICS=HEIDELBERGER(EPS=0.05)`, as follows:

SALPHA=*value*

specifies the α level ($0 < \alpha < 1$) for the stationarity test. By default, `SALPHA=0.05`.

HALPHA=*value*

specifies the α level ($0 < \alpha < 1$) for the half-width test. By default, `HALPHA=0.05`.

EPS=*value*

specifies a small positive number ϵ such that if the half-width is less than ϵ times the sample mean of the retaining iterates, the half-width test is passed. By default, `EPS=0.1`.

MCERROR

MCSE

computes an estimate of the Monte Carlo standard error for each sampled parameter. See the section “[Standard Error of the Mean Estimate](#)” on page 153 for details.

MAXLAG=*n*

specifies the largest lag used in computing the effective sample size and the Monte Carlo standard error. Specifying this option implies the `ESS` and `MCERROR` options. The default is `MAXLAG=250`.

RAFTERY <(Raftery-options)>

RL <(Raftery-options)>

computes the Raftery and Lewis diagnostics, which evaluate the accuracy of the estimated quantile ($\hat{\theta}_Q$ for a given $Q \in (0, 1)$) of a chain. $\hat{\theta}_Q$ can achieve any degree of accuracy when the chain is allowed to run for a long time. The algorithm stops when the estimated probability $\hat{P}_Q = \Pr(\theta \leq \hat{\theta}_Q)$ reaches within $\pm R$ of the value Q with probability S ; that is, $\Pr(Q - R \leq \hat{P}_Q \leq Q + R) = S$. See the section “[Raftery and Lewis Diagnostics](#)” on page 149 for more details. The *Raftery-options* enable you to specify Q , R , S , and a precision level ϵ for a stationary test.

These diagnostics are not performed by default. You can specify the `DIAGNOSTICS=RAFERTY` option to request these diagnostics, and you can also specify suboptions, such as `DIAGNOSTICS=RAFERTY(QUANTILE=0.05)`, as follows:

QUANTILE=*value*

Q=*value*

specifies the order (a value between 0 and 1) of the quantile of interest. By default, `QUANTILE=0.025`.

ACCURACY=*value*

R=*value*

specifies a small positive number as the margin of error for measuring the accuracy of estimation of the quantile. By default, ACCURACY=0.005.

PROB=*value*

S=*value*

specifies the probability of attaining the accuracy of the estimation of the quantile. By default, PROB=0.95.

EPS=*value*

specifies the tolerance level (a small positive number between 0 and 1) for the stationary test. By default, EPS=0.001.

MIXPRIORPARMS=K

MIXPRIORPARMS(*value-list*)

specifies the parameters used in constructing the Dirichlet prior distribution for the mixing parameters. If you specify MIXPRIORPARMS=K, the parameters of the k -dimensional Dirichlet distribution are a vector that contains the number of components in the model (k), whatever that might be. You can specify an explicit list of parameters in *value-list*. If the MIXPRIORPARMS option is not specified, the default Dirichlet parameter vector is a vector of length k of ones. This results in a uniform prior over the unit simplex; for $k=2$, this is the uniform distribution. See the section “[Prior Distributions](#)” on page 2435 for the distribution function of the Dirichlet as used by the FMM procedure.

ESTIMATE=MEAN | MAP

determines which overall estimate is used, based on the posterior sample, in the computation of **OUTPUT** statistics and certain ODS graphics. By default, the arithmetic average of the (thinned) posterior sample is used. If you specify ESTIMATE=MAP, the parameter vector is used that corresponds to the maximum log posterior density in the posterior sample. In any event, a message is written to the SAS log if postprocessing results depend on a summary estimate of the posterior sample.

INITIAL=DATA | MLE | MODE | RANDOM

determines how initial values for the Markov chain are obtained. The default when a conjugate sampler is used is INITIAL=DATA, in which case the FMM procedure uses the same algorithm to obtain data-dependent starting values as it uses for maximum likelihood estimation. If no conjugate sampler is available or if you use the METROPOLIS option to explicitly request that it not be used, then the default is INITIAL=MLE, in which case the maximum likelihood estimates are used as the initial values. If the maximum likelihood optimization fails, the FMM procedure switches to the default INITIAL=DATA.

The options INITIAL=MODE and INITIAL=RANDOM use the mode and random draws from the prior distribution, respectively, to obtain initial values. If the mode does not exist or if it falls on the boundary of the parameter space, the prior mean is used instead.

METROPOLIS

requests that the FMM procedure use the Metropolis-Hastings sampling algorithm based on Geman (1997), even in situations where a conjugate sampler is available.

MUPRIORPARMS=*pair-specification*

MUPRIORPARMS(*pair-specification* ... *pair-specification*)

specifies the parameters for the means in homogeneous mixtures without regression coefficients. The *pair-specification* is of the form (a, b) , where a and b are the two parameters of the prior distribution, optionally delimited with a comma. The actual distribution of the parameter is implied by the distribution selected in the **MODEL** statement. For example, it is a normal distribution for a mixture of normals, a gamma distribution for a mixture of Poisson variables, a beta distribution for a mixture of binary variables, and an inverse gamma distribution for a mixture of exponential variables. This option overrides the **PRIOROPTIONS** option.

The parameters correspond as follows:

Beta:	The parameters correspond to the α and β parameters of the beta prior distribution such that its mean is $\mu = \alpha/(\alpha + \beta)$ and its variance is $\mu(1 - \mu)/(\alpha + \beta + 1)$.
Normal:	The parameters correspond to the mean and variance of the normal prior distribution.
Gamma:	The parameters correspond to the α and β parameters of the gamma prior distribution such that its mean is α/β and its variance is α/β^2 .
Inverse gamma:	The parameters correspond to the α and β parameters of the inverse gamma prior distribution such that its mean is $\mu = \beta/(\alpha - 1)$ and its variance is $\mu^2/(\alpha - 2)$.

The two techniques for specifying the prior parameters with the **MUPRIORPARMS** option are as follows:

- Specify an equal sign and a single pair of values:

```
proc fmm seed=12345;
  model y = / k=2;
  bayes mupriorparms=(0,50);
run;
```

- Specify a list of parameter pairs within parentheses:

```
proc fmm seed=12345;
  model y = / k=2;
  bayes mupriorparms( (.,.) (1.4,10.5) );
run;
```

If you specify an invalid value (outside of the parameter space for the prior distribution), the FMM procedure chooses the default value and writes a message to the SAS log. If you want to use the default values for a particular parameter, you can also specify missing values in the *pair-specification*. For example, the preceding list specification assigns default values for the first component and uses the values 1.4 and 10.5 for the mean and variance of the normal prior distribution in the second component. The first example assigns a $N(0, 50)$ prior distribution to the means in both components.

NBI=*n*

specifies the number of burn-in samples. During the burn-in phase, chains are not saved. The default is NBI=2000.

NMC=*n***SAMPLE=*n***

specifies the number of Monte Carlo samples after the burn-in. Samples after the burn-in phase are saved unless they are thinned with the THIN= option. The default is NMC=10000.

OUTPOST< (*outpost-options*) >=*data-set*

requests that the posterior sample be saved to a SAS data set. In addition to variables that contain log likelihood and log posterior values, the OUTPOST data set contains variables for the parameters. The variable names for the parameters are generic (Parm_1, Parm_2, ..., Parm_p). The labels of the parameters are descriptive and correspond to the “Parameter Mapping” table that is produced when the OUTPOST= option is in effect.

You can specify the following *outpost-options* in parentheses:

LOGPRIOR

adds the value of the log prior distribution to the data set.

NONSINGULAR | NONSING | COMPRESS

eliminates parameters that correspond to singular columns in the design matrix (and were not sampled) from the posterior data set. This is the default.

SINGULAR | SING

adds columns of zeros to the data set in positions that correspond to singularities in the model or to parameters that were not sampled for other reasons. By default, these columns of zeros are not written to the posterior data set.

PHIPRIORPARMS=*pair-specification***PHIPRIORPARMS**(*pair-specification* ... *pair-specification*)

specifies the parameters for the inverse gamma prior distribution of the scale parameters (ϕ 's) in the model. The *pair-specification* is of the form (*a*, *b*), and the values are chosen such that the prior distribution has mean $\mu = b/(a - 1)$ and variance $\mu^2/(a - 2)$.

The form of the PHIPRIORPARMS with an equal sign and a single pair is used to specify one pair of prior parameters that applies to all components in the mixture. For example:

```
proc fmm seed=12345;
  model y = / k=2;
  bayes phipriorparms=(2.001,1.001);
run;
```

The form with a list of pairs is used to specify different prior parameters for the scale parameters in different components. For example:

```
proc fmm seed=12345;
  model y = / k=2;
  bayes phipriorparms( (.,1.001) (3.001,2.001) );
run;
```

If you specify an invalid value (outside of the parameter space for the prior distribution), the FMM procedure chooses the default value and writes a message to the SAS log. If you want to use the default values for a particular parameter, you can also specify missing values in the *pair-specification*. For example, the preceding list specification assigns default values for the first component a prior parameter and uses the value 1.001 for the b prior parameter. The second pair assigns 3.001 and 2.001 for the a and b prior parameters, respectively.

PRIOROPTIONS $\langle = \rangle$ (*prior-options*)

PRIOROPTS $\langle = \rangle$ (*prior-options*)

specifies options related to the construction of the prior distribution and the choice of their parameters. Some *prior-options* apply only in particular models. The **BETAPRIORPARMS=** and **MUPRIORPARMS=** options override this option.

You can specify the following *prior-options*:

CONDITIONAL | COND

chooses a conditional prior specification for the homogeneous normal and t distribution response components. The default prior specification in these models is an independence prior where the mean of the h th component has prior $\mu_h \sim N(a, b)$. The conditional prior is characterized by $\mu_h \sim N(a, \sigma_h^2/b)$.

DEPENDENT | DEP

chooses a data-dependent prior for the homogeneous models without effects. The prior parameters a and b are chosen as follows, based on the distribution in the **MODEL** statement:

Binary and binomial: $a = \bar{y}/(1-\bar{y})$, $b=1$, and the prior distribution for the success probability is $\text{beta}(a, b)$.

Poisson: $a = 1$, $b = 1/\bar{y}$, and the prior distribution for μ is $\text{gamma}(a, b)$. See Frühwirth-Schnatter (2006, p. 280) and Viallefont, Richardson, and Greene (2002).

Exponential: $a = 3$, $b = 2\bar{y}$, and the prior distribution for μ is inverse gamma with parameters a and b .

Normal and t : Under the default independence prior, the prior distribution for μ is $N(\bar{y}, fs^2)$ where f is the variance factor from the **VAR=** option and

$$s^2 = \frac{1}{n} \sum_{i=1}^n (y_i - \bar{y})^2$$

Under the default conditional prior specification, the prior for μ_h is $N(a, \sigma_h^2/b)$ where $a = \bar{y}$ and $b = 2.6/(\max\{y\} - \min\{y\})$. The prior for the scale parameter is inverse gamma with parameters 1.28 and $0.36s^2$. For further details, see Raftery (1996) and Frühwirth-Schnatter (2006, p. 179).

VAR=f

specifies the variance for normal prior distributions. The default is **VAR=1000**. This factor is used, for example, in determining the prior variance of regression coefficients or in determining the prior variance of means in homogeneous mixtures of t or normal distributions (unless a data-dependent prior is used).

MLE=<r>

specifies that the prior distribution for regression variables be based on a multivariate normal distribution centered at the MLEs and whose dispersion is a multiple r of the asymptotic MLE covariance matrix. The default is MLE=10. In other words, if you specify PRIOROPTIONS(MLE), the FMM procedure chooses the prior distribution for the regression variables as $N(\hat{\beta}, 10\text{Var}[\hat{\beta}])$ where $\hat{\beta}$ is the vector of maximum likelihood estimates. The prior for the scale parameter is inverse gamma with parameters 1.28 and $0.36s^2$ where

$$s^2 = \frac{1}{n} \sum_{i=1}^n (y_i - \bar{y})^2$$

For further details, see Raftery (1996) and Frühwirth-Schnatter (2006, p. 179). If you specify PRIOROPTIONS(MLE) for the regression parameters, then the data-dependent prior is used for the scale parameter; see the PRIOROPTIONS(DEPENDENT) option above.

The MLE option is not available for mixture models in which the parameters are estimated directly on the data scale, such as homogeneous mixture models or mixtures of distributions without model effects for which a conjugate sampler is available. By using the METROPOLIS option, you can always force the FMM procedure to abandon a conjugate sampler in favor of a Metropolis-Hastings sampling algorithm to which the MLE option applies.

STATISTICS < (*global-options*) > = **ALL** | **NONE** | *keyword* | (*keyword-list*)

SUMMARIES < (*global-options*) > = **ALL** | **NONE** | *keyword* | (*keyword-list*)

controls the number of posterior statistics produced. Specifying STATISTICS=ALL is equivalent to specifying STATISTICS=(SUMMARY INTERVAL). To suppress the computation of posterior statistics, specify STATISTICS=NONE. The default is STATISTICS=(SUMMARY INTERVAL). See the section “[Summary Statistics](#)” on page 153 for more details.

The *global-options* include the following:

ALPHA=*numeric-list*

controls the coverage levels of the equal-tail credible intervals and the credible intervals of highest posterior density (HPD) credible intervals. The ALPHA= values must be between 0 and 1. Each ALPHA= value produces a pair of $100(1-\alpha)\%$ equal-tail and HPD credible intervals for each sampled parameter. The default is ALPHA=0.05, which results in 95% credible intervals for the parameters.

PERCENT=*numeric-list*

requests the percentile points of the posterior samples. The values in *numeric-list* must be between 0 and 100. The default is PERCENT=(25 50 75), which yields for each parameter the 25th, 50th, and 75th percentiles, respectively.

The list of *keywords* includes the following:

SUMMARY

produces the means, standard deviations, and percentile points for the posterior samples. The default is to produce the 25th, 50th, and 75th percentiles; you can modify this list with the global PERCENT= option.

INTERVAL

produces equal-tail and HPD credible intervals. The default is to produce the 95% equal-tail credible intervals and 95% HPD credible intervals, but you can use the `ALPHA= global-option` to request credible intervals for any probabilities.

THIN=*n***THINNING=*n***

controls the thinning of the Markov chain after the burn-in. Only one in every k samples is used when `THIN= k` , and if `NBI= n_0` and `NMC= n` , the number of samples kept is

$$\left[\frac{n_0 + n}{k} \right] - \left[\frac{n_0}{k} \right]$$

where $[a]$ represents the integer part of the number a . The default is `THIN=1`—that is, all samples are kept after the burn-in phase.

TIMEINC=*n*

specifies a time interval in seconds to report progress during the burn-in and sampling phase. The time interval is approximate, since the minimum time interval in which the FMM procedure can respond depends on the multithreading configuration.

BY Statement

BY variables ;

You can specify a BY statement with PROC FMM to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the `NOTSORTED` or `DESCENDING` option in the BY statement for the FMM procedure. The `NOTSORTED` option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

Because sorting the data changes the order in which PROC FMM reads observations, the sort order for the levels of the `CLASS` variable might be affected if you have specified `ORDER=DATA` in the PROC FMM statement.

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

CLASS Statement

CLASS *variables* </ **TRUNCATE** > ;

The CLASS statement names the classification variables to be used in the model. Typical classification variables are Treatment, Sex, Race, Group, and Replication. If you use the CLASS statement, it must appear before the MODEL statement.

Classification variables can be either character or numeric. By default, class levels are determined from the entire set of formatted values of the CLASS variables.

NOTE: Prior to SAS 9, class levels were determined by using no more than the first 16 characters of the formatted values. To revert to this previous behavior, you can use the TRUNCATE option in the CLASS statement.

In any case, you can use formats to group values into levels. See the discussion of the FORMAT procedure in the *Base SAS Procedures Guide* and the discussions of the FORMAT statement and SAS formats in *SAS Formats and Informats: Reference*. You can adjust the order of CLASS variable levels with the ORDER= option in the PROC FMM statement. You can specify the following option in the CLASS statement after a slash (/):

TRUNCATE

specifies that class levels should be determined by using only up to the first 16 characters of the formatted values of CLASS variables. When formatted values are longer than 16 characters, you can use this option to revert to the levels as determined in releases prior to SAS 9.

FREQ Statement

FREQ *variable* ;

The *variable* in the FREQ statement identifies a numeric variable in the data set that contains the frequency of occurrence for each observation. PROC FMM treats each observation as if it appears f times, where f is the value of the FREQ variable for the observation. If it is not an integer, the frequency value is truncated to an integer. If the frequency value is less than 1 or missing, the observation is not used in the analysis. When the FREQ statement is not specified, each observation is assigned a frequency of 1.

ID Statement

ID *variables* ;

The ID statement specifies a list of variables that are included in the OUT= data set of the OUTPUT statement. If no ID statement is specified, all variables from the input data set are copied into the output data set.

MODEL Statement

```
MODEL response <(response-options)> = <effects> </model-options>;
```

```
MODEL events/trials = <effects> </model-options>;
```

```
MODEL          + <effects> </model-options>;
```

The MODEL statement defines elements of the mixture model, such as the model effects, the distribution, and the link function. At least one MODEL statement is required. You can specify more than one MODEL statement. Each MODEL statement identifies one or more components of a mixture. For example, if components differ in their distributions, link functions, or regressor variables, then you can use separate MODEL statements to define the components. If the finite mixture model is homogeneous—in the sense that all components share the same regressors, distribution, and link function—then you can specify the mixture model with a single MODEL statement by using the **K=** option.

An intercept is included in each model by default. It can be removed with the **NOINT** option.

The dependent variable can be specified by using either the *response* syntax or the *events/trials* syntax. The *events/trials* syntax is specific to models for binomial-type data. A binomial(n, π) variable is the sum of n independent Bernoulli trials with event probability π . Each Bernoulli trial results in either an event or a nonevent (with probability $1 - \pi$). The value of the second variable, *trials*, gives the number n of Bernoulli trials. The value of the first variable, *events*, is the number of events out of n . The values of both *events* and (*trials*–*events*) must be nonnegative, and the value of *trials* must be positive. Other distributions that allow the *events/trials* syntax are the beta-binomial distribution and the binomial cluster model.

If the *events/trials* syntax is used, the FMM procedure defaults to the binomial distribution. If you use the *response* syntax, the procedure defaults to the normal distribution unless the response variable is a character variable or listed in the **CLASS** statement.

The FMM procedure supports a continuation-style syntax in MODEL statements. Since a mixture has only one response variable, it is sufficient to specify the response variable in one MODEL statement. Other MODEL statements can use the continuation symbol “+” before the specification of effects. For example, the following statements fit a three-component binomial mixture model:

```
class A;
model y/n = x / k=2;
model      + A;
```

The first MODEL statement uses the “=” sign to separate response from effect information and specifies the response variable by using the *events/trials* syntax. This determines the distribution as binomial. This MODEL statement adds two components to the mixture models with different intercepts and regression slopes. The second MODEL statement adds another component to the mixture where the mean is a function of the classification main effect for variable A. The response is also binomial; it is a continuation from the previous MODEL statement.

There are two sets of options in the MODEL statement. The *response-options* determine how the FMM procedure models probabilities for binary data. The *model-options* control other aspects of model formation and inference. Table 37.4 summarizes the *response-options* and *model-options* available in the MODEL statement. These are subsequently discussed in detail in alphabetical order by option category.

Table 37.4 Summary of MODEL Statement Options

Option	Description
Response Variable Options	
DESCENDING	Reverses the order of response categories
EVENT=	Specifies the event category in binary models
ORDER=	Specifies the sort order for the response variable
REFERENCE=	Specifies the reference category in categorical models
Model Building	
DIST=	Specifies the response distribution
LINK=	Specifies the link function
K=	Specifies the number of mixture components
KMAX=	Specifies the maximum number of mixture components
KMIN=	Specifies the minimum number of mixture components
KRESTART	Requests that the starting values for each analysis be determined separately instead of sequentially
NOINT	Excludes fixed-effect intercept from model
OFFSET=	Specifies the offset variable for linear predictor
Statistical Computations and Output	
ALPHA= α	Determines the confidence level ($1 - \alpha$)
CL	Displays confidence limits for fixed-effects parameter estimates
EQUATE=	Imposes simple equality constraints on parameters in this model
LABEL=	Identifies the model
PARMS	Provides starting values for the parameters in this model

Response Variable Options

Response variable options determine how the FMM procedure models probabilities for binary data.

You can specify the following *response-options* by enclosing them in parentheses after the *response* variable. The default is ORDER=FORMATTED.

DESCENDING

DESC

reverses the order of the response categories. If both the DESCENDING and ORDER= options are specified, PROC FMM orders the response categories according to the ORDER= option and then reverses that order.

EVENT=*'category'* | *keyword*

specifies the event category for the binary response model. PROC FMM models the probability of the event category. You can specify the value (formatted, if a format is applied) of the event category in quotes, or you can specify one of the following keywords:

FIRST

designates the first ordered category as the event. This is the default.

LAST

designates the last ordered category as the event.

ORDER=*order-type*

specifies the sort order for the levels of the response variable. You can specify the following values for *order-type*:

DATA

sorts the levels by order of appearance in the input data set.

FORMATTED

sorts the levels by external formatted value, except for numeric variables with no explicit format, which are sorted by their unformatted (internal) value.

FREQ

sorts the levels by descending frequency count; levels with the most observations come first in the order.

INTERNAL

sorts the levels by unformatted value.

FREQDATA

sorts the levels by order of descending frequency count, and within counts by order of appearance in the input data set when counts are tied.

FREQFORMATTED

sorts the levels by order of descending frequency count, and within counts by formatted value (as above) when counts are tied.

FREQINTERNAL

sorts the levels by order of descending frequency count, and within counts by unformatted value when counts are tied.

When ORDER=FORMATTED (the default) for numeric variables for which you have supplied no explicit format (that is, for which there is no corresponding FORMAT statement in the current PROC FMM run or in the DATA step that created the data set), the levels are ordered by their internal (numeric) value. If you specify the ORDER= option in the MODEL statement and the ORDER= option in the PROC FMM statement, the former takes precedence.

By default, ORDER=FORMATTED. For the FORMATTED and INTERNAL values, the sort order is machine-dependent.

For more information about sort order, see the chapter on the SORT procedure in the *Base SAS Procedures Guide* and the discussion of BY-group processing in *SAS Language Reference: Concepts*.

REFERENCE='category' | *keyword***REF=**'category' | *keyword*

specifies the reference category for categorical models. For the binary response model, specifying one response category as the reference is the same as specifying the other response category as the event category. You can specify the value (formatted if a format is applied) of the reference category in quotes, or you can specify one of the following *keywords*:

FIRST

designates the first ordered category as the reference category.

LAST

designates the last ordered category as the reference category. This is the default.

Model Options**ALPHA=number**

requests that confidence intervals be constructed for each of the parameters with confidence level $1 - \text{number}$. The value of *number* must be between 0 and 1; the default is 0.05.

CL

requests that confidence limits be constructed for each of the parameter estimates. The confidence level is 0.95 by default; this can be changed with the **ALPHA=** option.

DISTRIBUTION=keyword**DIST=keyword**

specifies the probability distribution for a mixture component.

If you specify the **DIST=** option and you do not specify a link function with the **LINK=** option, a default link function is chosen according to [Table 37.5](#). If you do not specify a distribution, the FMM procedure defaults to the normal distribution for continuous response variables and to the binary distribution for classification or character variables, unless the *events/trial* syntax is used in the MODEL statement. If you choose the *events/trial* syntax, the FMM procedure defaults to the binomial distribution.

[Table 37.5](#) lists *keywords* that you can specify for the **DISTRIBUTION=** option and the corresponding default link functions. For generalized linear models with these distributions, you can find expressions for the log-likelihood functions in the section “[Log-Likelihood Functions for Response Distributions](#)” on page 2427.

Table 37.5 Keyword Values of the **DIST=** Option

<i>keyword</i>	Alias	Distribution	Default Link Function
BETA		Beta	Logit
BETABINOMIAL	BETABIN	Beta-binomial	Logit
BINARY	BERNOULLI	Binary	Logit
BINOMIAL	BIN	Binomial	Logit
BINOMCLUSTER	BINOMCLUS	Binomial cluster	Logit
CONSTANT <(c)>	DEGENERATE <(c)>	Degenerate	N/A
EXPONENTIAL	EXPO	Exponential	Log
FOLDEDNORMAL	FNORMAL	Folded normal	Identity
GAMMA	GAM	Gamma	Log
GAUSSIAN	NORMAL	Normal	Identity
GENPOISSON	GPOISSON	Generalized Poisson	Log
GEOMETRIC	GEOM	Geometric	Log
INVGAUSS	IGAUSSIAN, IG	Inverse Gaussian	Inverse squared (power(-2))

Table 37.5 continued

DIST=	Alias	Distribution	Default Link Function
LOGNORMAL	LOGN	Lognormal	Identity
NEGBINOMIAL	NEGBIN, NB	Negative binomial	Log
POISSON	POI	Poisson	Log
T <(v)>	STUDENT <(v)>	<i>t</i>	Identity
TRUNCEXPO <(a,b)>	TEXPO <(a,b)>	Truncated exponential	Log
TRUNCLOGN <(a,b)>	TLOGN <(a,b)>	Lognormal	Identity
TRUNCNEGBIN	TNEGBIN, TNB	Negative binomial	Log
TRUNCNORMAL <(a,b)>	TNORMAL <(a,b)>	Truncated normal	Identity
TRUNCPOISSON	TPOISSON, TPOI	Truncated Poisson	Log
UNIFORM <(a,b)>	UNIF <(a,b)>	Uniform	N/A
WEIBULL		Weibull	Log

Note that the PROC FMM default link for the gamma or exponential distribution is not the canonical link (the reciprocal link).

The binomial cluster model is a two-component model described in Morel and Nagaraj (1993); Morel and Neerchal (1997); Neerchal and Morel (1998). See [Example 37.1](#) for an application of the binomial cluster model in a teratological experiment.

If the *events/trials* syntax is used, the default distribution is the binomial and only the following choices are available: DIST=BINOMIAL, DIST=BETABINOMIAL, and DIST=BINOMCLUSTER. The *trials* variable is ignored for all other distributions. This enables you to fit models in which some components have a binomial or binomial-like distribution. For example, suppose that variable *n* is a binomial denominator and variable *logn* is its logarithm. Then the following statements model a two-component mixture of a binomial and Poisson count model:

```
model y/n = ;
model      + / dist=Poisson offset=logn;
```

The **OFFSET=** option is used in the second MODEL statement to specify that the Poisson counts refer to different base counts, since the trial variable *n* is ignored in the second model.

If DIST=BINOMIAL is specified without the *events/trials* syntax, then *n*=1 is used for the default number of trials.

DIST=TRUNCNEGBIN and DIST=TRUNCPOISSON are zero-truncated versions of DIST=NEGBINOMIAL and DIST=POISSON, respectively—that is, only the value of 0 is excluded from the support.

For DIST=TRUNCEXPO, DIST=TRUNCLOGN, and DIST=TRUNCNORMAL, you must specify the lower (*a*) and upper (*b*) truncation points of the distribution. For example:

```
DIST=TRUNCEXPO<(a,b)>
DIST=TRUNCLOGN<(a,b)>
DIST=TRUNCNORMAL<(a,b)>
```

Each of these distributions is the conditional version of its corresponding nontruncated distribution that is confined to the support $[a, b]$ (inclusive). You can specify a missing value (.) for either a or b to truncate only on the other side; that is, $a=.$ indicates a right-truncated distribution, and $b=.$ indicates a left-truncated distribution.

For several distribution specifications you can provide additional optional parameters to further define the distribution. These optional parameters are listed in the following:

DIST=CONSTANT<(c)> The number c specifies the value where the mass is concentrated. The default is **DIST=CONSTANT**(0), so you can add zero-inflation to any model by adding a **MODEL** statement with **DIST=CONSTANT**.

DIST=T<(v)> The number v specifies the degrees of freedom for the (shifted) t distribution. The default is **DIST=T**(3); this leads to a heavy-tailed distribution for which the variance is defined. See the section “[Log-Likelihood Functions for Response Distributions](#)” on page 2427 for the density function of the shifted t_v distribution.

DIST=UNIFORM<(a,b)> The values a and b define the support of the uniform distribution, $a < b$. By default, $a = 0$ and $b = 1$.

EQUATE=MEAN | SCALE | NONE

EQUATE=EFFECTS(*effect-list*)

specifies simple sets of parameter constraints across the components in a **MODEL** statement; the default is **EQUATE=NONE**. This option is available only for maximum likelihood estimation. If you specify **EQUATE=MEAN**, the parameters that determine the mean are reduced to a single set that is applicable to all components in the **MODEL** statement. If you specify **EQUATE=SCALE**, a single parameter represents the common scale for all components in the **MODEL** statement. The **EFFECTS** option enables you to force the parameters for the chosen model effects to be equal across components; however, the number of parameters is unaffected.

For example, the following statements fit a two-component multiple regression model in which the coefficients for variable `logd` vary by component and the intercepts and coefficients for variable `dose` are the same for the two components:

```
proc fmm;
  model num = dose logd / equate=effects(int dose) k=2;
run;
```

To fix all coefficients across the two components, you can write the **MODEL** statement as

```
model num = dose logd / equate=effects(int dose logd) k=2;
```

or

```
model num = dose logd / equate=mean k=2;
```

If you restrict all parameters in a k -component **MODEL** statement to be equal, the **FMM** procedure reduces the model to $k=1$.

K=*n***NUMBER=*n***

specifies the number of components the MODEL statement contributes to the overall mixture. For the binomial cluster model, this option is not available, since this model is a two-component model by definition.

KMAX=*n*

specifies the maximum number of components the MODEL statement contributes to the overall mixture.

If the maximum number of components in the mixture, as determined by all KMAX= options, is larger than the minimum number of components, the FMM procedure fits all possible models and displays summary fit information for the sequence of evaluated models. The “best” model according to the CRITERION= option in the PROC FMM statement is then chosen, and the remaining output and analyses performed by PROC FMM pertain to this “best” model.

The KMAX= option is available only for maximum likelihood estimation. When you estimate the parameters of a mixture by MCMC methods, you need to ensure that the chain for a given value of *k* has converged; otherwise, comparisons among models with varying number of components might not be meaningful.

If you specify the KMIN= option but not the KMAX= option, then the default value for the KMAX= option is the value of the KMIN= option (unless KMIN=0, in which case the KMAX= option is set to 1).

KMIN=*n*

specifies the minimum number of components the MODEL statement contributes to the overall mixture. This option is available only for maximum likelihood estimation. When you estimate the parameters of a mixture by MCMC methods, you need to ensure that the chain for a given value of *k* has converged; otherwise comparisons among models with varying number of components might not be meaningful.

KRESTART

requests that the starting values for each analysis (that is, for each unique number of components as determined by the KMIN= and KMAX= options) be determined separately, in the same way as if no other analyses were performed. If you do not specify the KRESTART option, then the starting values for each analysis are based on results from the previous analysis with one less component.

LABEL=*'label'*

specifies an optional label for the model that is used to identify the model in printed output, on graphics, and in data sets created from ODS tables.

LINK=*keyword*

specifies the link function in the model. The keywords and expressions for the associated link functions are shown in [Table 37.6](#).

Table 37.6 Link Functions in MODEL Statement of the FMM Procedure

LINK=	Alias	Link Function	$g(\mu) = \eta =$
CLOGLOG	CLL	Complementary log-log	$\log(-\log(1 - \mu))$
IDENTITY	ID	Identity	μ
LOG		Log	$\log(\mu)$
LOGIT		Logit	$\log(\mu/(1 - \mu))$
LOGLOG		Log-log	$-\log(-\log(\mu))$
PROBIT	NORMIT	Probit	$\Phi^{-1}(\mu)$
POWER(λ)	POW(λ)	Power with exponent $\lambda = \text{number}$	$\begin{cases} \mu^\lambda & \text{if } \lambda \neq 0 \\ \log(\mu) & \text{if } \lambda = 0 \end{cases}$
POWERMINUS2		Power with exponent -2	$1/\mu^2$
RECIPROCAL	INVERSE	Reciprocal	$1/\mu$

The default link functions for the various distributions are shown in [Table 37.5](#).

NOINT

requests that no intercept be included in the model. An intercept is included by default, unless the distribution is **DIST=CONSTANT** or **DIST=UNIFORM**.

OFFSET=variable

specifies the offset variable function for the linear predictor in the model. An offset variable can be thought of as a regressor variable whose regression coefficient is known to be 1. For example, you can use an offset in a Poisson model when counts have been obtained in time intervals of different lengths. With a log link function, you can model the counts as Poisson variables with the logarithm of the time interval as the offset variable.

PARAMETERS(parameter-specification)**PARMS(parameter-specification)**

specifies starting values for the model parameters. If no PARMS option is given, the FMM procedure determines starting values by a data-dependent algorithm. To determine initial values for the Markov chain with Bayes estimation, see also the **INITIAL=** option in the **BAYES** statement. The specification of the parameters takes the following form: parameters in the mean function precede the scale parameters, and parameters for different components are separated by commas.

The following statements specify starting parameters for a two-component normal model. The initial values for the intercepts are 1 and -3; the initial values for the variances are 0.5 and 4.

```
proc fmm;
  model y = / k=2 parms (1 0.5, -3 4);
run;
```

You can specify missing values for parameters whose starting values are to be determined by the default method. Only values for parameters that participate in the optimization are specified. The values for model effects are specified on the linear (linked) scale.

OUTPUT Statement

```
OUTPUT < OUT=SAS-data-set >
  < keyword<(keyword-options) > <=name>> ...
  < keyword<(keyword-options) > <=name>> </options> ;
```

The OUTPUT statement creates a data set that contains observationwise statistics that are computed after fitting the model. By default, all variables in the original data set are included in the output data set. You can use the ID statement to limit the variables copied from the input data set to the output data set.

The output statistics are computed based on the parameter estimates of the converged model if the parameters are estimated by maximum likelihood. If a Bayesian analysis is performed, the output statistics are computed based on the arithmetic mean in the posterior sample. You can change to the maximum posterior estimate with the ESTIMATE=MAP option in the BAYES statement.

You can specify the following syntax elements in the OUTPUT statement before the slash (/).

OUT=SAS-data-set

specifies the name of the output data set. If the OUT= option is omitted, the procedure uses the DATA n convention to name the output data set.

keyword<(keyword-options) > <=name>

specifies a statistic to include in the output data set and optionally assigns the variable the name *name*. If you do not provide a name, the FMM procedure assigns a default name based on the type of statistic requested. If you provide a name for a statistic that leads to multiple output statistics, the name is modified to index the associated component number.

You can use the *keyword-options* to control which type of a particular statistic is computed. The following are valid values for *keyword* and *keyword-options*:

PREDICTED<(COMPONENT | OVERALL)>

PRED<(COMPONENT | OVERALL)>

MEAN<(COMPONENT | OVERALL)>

requests predicted values (predicted means) for the response variable. The predictions in the output data set are mapped onto the data scale in all cases except for a binomial or binary response with *events/trials* syntax and when PREDTYPE=COUNT has not been specified. In that case the predictions are predicted success probabilities.

The default is to compute the predicted value for the mixture (OVERALL). You can request predictions for the means of the component distributions by adding the COMPONENT suboption in parentheses. The predicted values for some distributions are not identical to the parameter modeled as μ . For example, in the lognormal distribution the predicted mean is $\exp\{\mu + 0.5\phi\}$ where μ and ϕ are the parameters of an underlying normal process; see the section “Log-Likelihood Functions for Response Distributions” on page 2427 for details.

RESIDUAL<(COMPONENT | OVERALL)>

RESID<(COMPONENT | OVERALL)>

requests residuals for the response or residuals in the component distributions. Only “raw” residuals on the data scale are computed (observed minus predicted).

VARIANCE<(COMPONENT | OVERALL)>**VAR<(COMPONENT | OVERALL)>**

requests variances for the mixture or the component distributions.

LOGLIKE<(COMPONENT | OVERALL)>**LOGL<(COMPONENT | OVERALL)>**

requests values of the log-likelihood function for the mixture or the components. For observations used in the analysis, the overall computed value is the observations' contribution to the log likelihood; if a **FREQ** statement is present, the frequency is accounted for in the computed value. In other words, if all observations in the input data set have been used in the analysis, adding the value of the log-likelihood contributions in the OUTPUT data set produces the negative of the final objective function value in the "Iteration History" table. By default, the log-likelihood contribution to the mixture is computed. You can request the individual mixture component contributions with the **COMPONENT** suboption.

MIXPROBS<(COMPONENT | MAX)>**MIXPROB<(COMPONENT | MAX)>****PRIOR<(COMPONENT | MAX)>****MIXWEIGHTS<(COMPONENT | MAX)>**

requests that the prior weights $\pi_j(\mathbf{z}, \boldsymbol{\alpha}_j)$ be added to the OUTPUT data set. By default, the probabilities are output for all components. You can limit the output to a single statistic, the largest mixing probability, with the **MAX** suboption.

NOTE: The keyword "prior" is used here because of long-standing practice to refer to the mixing probabilities as prior weights. This must not be confused with the prior distribution and its parameters in a Bayesian analysis.

POSTERIOR<(COMPONENT | MAX)>**POST<(COMPONENT | MAX)>****PROB<(COMPONENT | MAX)>**

requests that the posterior weights

$$\frac{\pi_j(\mathbf{z}, \boldsymbol{\alpha}_j) p_j(y; \mathbf{x}'_j \boldsymbol{\beta}_j, \phi_j)}{\sum_{j=1}^k \pi_j(\mathbf{z}, \boldsymbol{\alpha}_j) p_j(y; \mathbf{x}'_j \boldsymbol{\beta}_j, \phi_j)}$$

be added to the OUTPUT data set. By default, the probabilities are output for all components. You can limit the output to a single statistic, the largest posterior probability, with the **MAX** suboption.

NOTE: The keyword "posterior" is used here because of long-standing practice to refer to these probabilities as posterior probabilities. This must not be confused with the posterior distribution in a Bayesian analysis.

LINP**XBETA**

requests that the linear predictors for the models be added to the OUTPUT data set.

CLASS | CATEGORY | GROUP

adds the estimated component membership to the OUTPUT data set. An observation is associated with the component that has the highest posterior probability.

MAXPOST | MAXPROB

adds the highest posterior probability to the OUTPUT data set.

A *keyword* can appear multiple times. For example, the following OUTPUT statement requests predicted values for the mixture in addition to the predicted means in the individual components:

```
output out=fmmout pred=MixtureMean pred(component)=CompMean;
```

In a three-component model, this produces four variables in the fmmout data set: MixtureMean, CompMean_1, CompMean_2, and CompMean_3.

You can specify the following *options* in the OUTPUT statement after a slash (/).

ALLSTATS

requests that all statistics are computed. If you do not use a keyword to assign a name, the FMM procedure uses the default name.

NOVAR

requests that variables from the input data set not be added to the output data set. This option does not apply to variables listed in the **BY** statement or to variables listed in the **ID** statement.

PREDTYPE=PROB | COUNT

specifies the type of predicted values that are produced for a binomial or binary response with *events/trials* syntax. If PREDTYPE=PROB, the predicted values are success probabilities. If PREDTYPE=COUNT, the predicted values are success counts. The default is PREDTYPE=PROB.

PERFORMANCE Statement

```
PERFORMANCE < performance-options > ;
```

The PERFORMANCE statement enables you to control the performance characteristics of the FMM procedure (for example, the number of CPUs, the number of threads for multithreading, and so on). By default, the FMM procedure performs many analyses in multiple threads, and the number of threads equals the number of CPUs. Certain system and configuration options also can control the number of CPUs available to a SAS session or whether multithreaded computations are permissible. For example, you can set the number of available processors to two with

```
options cpucount=2;
```

The FMM procedure then acts as though two processors were available, regardless of the number of physically available processors.

The FMM procedure applies multithreading to the following analytical tasks:

Starting values: all starting value computations that require a pass through the data.

Optimization: all evaluations of objective function, gradient, and Hessian; computation of covariance matrix.

Bayesian analysis: all sample passes through the data, formation of cross-product matrices, sampling of latent variables, and posterior diagnostics.

Scoring and ODS Graphics: computation of all output statistics and statistics for the construction of graphics that require passes through the data.

You can specify the following *performance-options*:

CPUCOUNT=*n*

CPUCOUNT=ACTUAL

specifies the number of processors available to the FMM procedure; the number *n* must be between 1 and 1024. CPUCOUNT=ACTUAL sets the number of available processors equal to the number of physical processors.

DETAILS

requests a table with timing detail for the tasks performed by the FMM procedure.

NOTHEADS

disables multithreaded computations.

THREADS=YES

THREADS=NO

enables or disables multithreaded processing. The number of threads used by the FMM procedure is displayed in the “Bayes Information” or “Optimization Information” table. It typically equals the number of available CPUs, which can be different from the number of physical CPUs, and can be modified with the global CPUCOUNT SAS option or with the CPUCOUNT= option in the PERFORMANCE statement.

PROBMODEL Statement

PROBMODEL < *effects* > < / *probmodel-options* > ;

The PROBMODEL statement defines the model effects for the mixing probabilities and their link function and starting values. Model effects (other than the implied intercept) are not supported with Bayesian estimation. By default, the FMM procedure models mixing probabilities on the logit scale for two-component models and as generalized logit models in situations with more than two components. The PROBMODEL statement is not required.

The generalized logit model with *k* categories has a common vector of regressor or design variables, *z*, *k* – 1 parameter vectors that vary with category, and one linear predictor whose value is constant. The constant linear predictor is assigned by the FMM procedure to the last component in the model, and its value is zero ($\alpha_k = 0$). The probability of observing category $1 \leq j \leq k$ is then

$$\pi_j(\mathbf{z}, \boldsymbol{\alpha}_j) = \frac{\exp\{\mathbf{z}'\boldsymbol{\alpha}_j\}}{\sum_{i=1}^k \exp\{\mathbf{z}'\boldsymbol{\alpha}_i\}}$$

For $k=2$, the generalized logit model reduces to a model with the logit link (a logistic model); hence the attribute *generalized* logit.

By default, an intercept is included in the model for the mixing probabilities. If you suppress the intercept with the **NOINT** option, you must specify at least one effect in the statement.

You can specify the following *probmodel-options* in the **PROBMODEL** statement after the slash (/):

ALPHA=number

requests that confidence intervals be constructed for the parameters in the probability model with confidence level $1 - \text{number}$. The value of *number* must be between 0 and 1; the default is 0.05. If the probability model is simple—that is, it does not contain any effects, the confidence intervals are produced for the estimated parameters (on the logit scale) as well as for the mixing probabilities.

CL

requests that confidence limits be constructed for each of the parameter estimates. The confidence level is 0.95 by default; this can be changed with the **ALPHA=** option.

LINK=keyword

specifies the link function in the model for the mixing probabilities. The default is a logit link for models with two components. For models with more than two components, only the generalized logit link is available. The *keywords* and expressions for the associated link functions for two-component models are shown in [Table 37.7](#).

Table 37.7 Link Functions in the **PROBMODEL** Statement

LINK=	Link Function	$g(\mu) = \eta =$
CLOGLOG CLL	Complementary log-log	$\log(-\log(1 - \mu))$
LOGIT	Logit	$\log(\mu/(1 - \mu))$
LOGLOG	Log-log	$-\log(-\log(\mu))$
PROBIT NORMIT	Probit	$\Phi^{-1}(\mu)$

NOINT

requests that no intercept be included in the model for the mixing probabilities. An intercept is included by default. If you suppress the intercept with the **NOINT** option, you must specify at least one other effect for the mixing probabilities—since an empty probability model is not meaningful.

PARAMETERS(*parameter-specification*)

PARMS(*parameter-specification*)

specifies starting values for the parameters. The specification of the parameters takes the following form: parameters in the mean function appear in a list, and parameters for different components are separated by commas. Starting values are given on the linked scale, not in terms of probabilities. Also, you need to specify starting values for only up to the first $k - 1$ components in a k -component model. The linear predictor for the last component is always assumed to be zero.

The following statements specify a three-component mixture of multiple regression models. The **PROBMODEL** statement does not list any effects, a standard “intercept-only” generalized logit model is used to model the mixing probabilities.

```
proc fmm;
  model y = x1 x2 / k=3;
  probmodel / parms(2, 1);
run;
```

There are three linear predictors in the model for the mixing probabilities, α_1 , α_2 , and α_3 . With starting values of $\alpha_1 = 2$, $\alpha_2 = 1$, and $\alpha_3 = 0$, this leads to initial mixing probabilities of

$$\pi_1 = \frac{e^2}{e^2 + e^1 + e^0} = 0.24$$

$$\pi_2 = \frac{e^1}{e^2 + e^1 + e^0} = 0.66$$

$$\pi_3 = \frac{e^0}{e^2 + e^1 + e^0} = 0.1$$

You can specify missing values for parameters whose starting values are to be determined by the default method.

RESTRICT Statement

RESTRICT < 'label' > *constraint-specification* < , ... , *constraint-specification* >
 < operator < value > > < / option > ;

The RESTRICT statement enables you to specify linear equality or inequality constraints among the parameters of a mixture model. These restrictions are incorporated into the maximum likelihood analysis. The RESTRICT statement is not available for a Bayesian analysis with the FMM procedure.

Following are reasons why you might want to place constraints and restrictions on the model parameters:

- to fix a parameter at a particular value
- to equate parameters in different components in a mixture
- to impose order conditions on the parameters in a model
- to specify contrasts among the parameters that the fitted model should honor

A restriction is composed of a left-hand side and a right-hand side, separated by an operator. If the operator and right-hand side are not specified, the restriction is assumed to be an equality constraint against zero. If the right-hand side is not specified, the value is assumed to be zero.

An individual *constraint-specification* is written in (nearly) the same form as estimable linear functions are specified in the ESTIMATE statement of the GLM, MIXED, or GLIMMIX procedure. The *constraint-specification* takes the form

model-effect value-list < ... *model-effect value-list* > < (**SCALE=** value) >

At least one *model-effect* must be specified followed by one or more values in the *value-list*. The values in the list correspond to the multipliers of the corresponding parameter that is associated with the position in the model effect. If you specify more values in the *value-list* than the *model-effect* occupies in the model design matrix, the extra coefficients are ignored.

To specify restrictions for effects in specific components in the model, separate the *constraint-specification* by commas. The following statements provide an example:

```
proc fmm;
  class A;
  model y/n = A x / k = 2;
  restrict A 1 0 -1;
  restrict x 2, x -1 >= 0.5;
run;
```

The linear predictors for this two-component model can be written as

$$\begin{aligned}\eta_1 &= \beta_{10} + \alpha_{11}A_1 + \cdots + \alpha_{1a}A_a + x\beta_{11} \\ \eta_2 &= \beta_{20} + \alpha_{21}A_1 + \cdots + \alpha_{2a}A_a + x\beta_{21}\end{aligned}$$

where A_k is the binary variable associated with the k th level of A .

The first RESTRICT statement applies only to the first component and specifies that the parameter estimates that are associated with the first and third level of the A effect are identical. In terms of the linear predictor, the restriction can be written as

$$\alpha_{11} - \alpha_{13} = 0$$

Now suppose that A has only two levels. Then the FMM procedure ignores the value -1 in the first RESTRICT statement and imposes the restriction

$$\alpha_{11} = 0$$

on the fitted model.

The second RESTRICT statement involves parameters in two different components of the model. In terms of the linear predictors, the restriction can be written as

$$2\beta_{11} - \beta_{21} \geq \frac{1}{2}$$

When restrictions are specified explicitly through the RESTRICT statement or implied through the EQUATE=EFFECTS option in the MODEL statement, the FMM procedure lists all restrictions after the model fit in a table of linear constraints and indicates whether a particular constraint is active at the converged solution.

The following operators can be specified to separate the left- and right-hand sides of the restriction: =, >, <, >=, <=.

Some distributions involve scale parameters (the parameter ϕ in the expressions of the log likelihood) and you can also use the *constraint-specification* to involve a component's scale parameter in a constraint. To this end, assign a value to the keyword SCALE, separated from the model effects and value lists with parentheses. The following statements fit a two-component normal model and restrict the component variances to be equal:

```
proc fmm;
  model y = / k=2;
  restrict int 0 (scale 1),
           int 0 (scale -1);
run;
```

The intercept specification is necessary because each *constraint-specification* requires at least one model effect. The zero coefficient ensures that the intercepts are not involved in the restriction. Instead, the RESTRICT statement leads to $\phi_1 - \phi_2 = 0$.

You can specify the following *option* in the RESTRICT statement after a slash (/).

DIVISOR=value

specifies a *value* by which all coefficients on the right-hand side and left-hand side of the restriction are divided.

WEIGHT Statement

WEIGHT variable ;

The WEIGHT statement is used to perform a weighted analysis. Consult the section “[Log-Likelihood Functions for Response Distributions](#)” on page 2427 for expressions on how weight variables are included in the log-likelihood functions. Because the probability structure of a mixture model is different from that of a classical statistical model, the presence of a weight variable in a mixture model *cannot* be interpreted as altering the variance of an observation.

Observations with nonpositive or missing weights are not included in the PROC FMM analysis. If a WEIGHT statement is not included, all observations used in the analysis are assigned a weight of 1.

Details: FMM Procedure

A Gentle Introduction to Finite Mixture Models

The Form of the Finite Mixture Model

Suppose that you observe realizations of a random variable Y , the distribution of which depends on an unobservable random variable S that has a discrete distribution. S can occupy one of k states, the number of which might be unknown but is at least known to be finite. Since S is not observable, it is frequently referred to as a latent variable.

Let π_j denote the probability that S takes on state j . Conditional on $S = j$, the distribution of the response Y is assumed to be $f_j(y; \alpha_j, \beta_j | S = j)$. In other words, each distinct state j of the random variable S leads to a particular distributional form f_j and set of parameters $\{\alpha_j, \beta_j\}$ for Y .

Let $\{\alpha, \beta\}$ denote the collection of α_j and β_j parameters across all $j = 1$ to k . The marginal distribution of Y is obtained by summing the joint distribution of Y and S over the states in the support of S :

$$\begin{aligned} f(y; \alpha, \beta) &= \sum_{j=1}^k \Pr(S = j) f(y; \alpha_j, \beta_j | S = j) \\ &= \sum_{j=1}^k \pi_j f(y; \alpha_j, \beta_j | S = j) \end{aligned}$$

This is a mixture of distributions, and the π_j are called the mixture (or prior) probabilities. Because the number of states k of the latent variable S is finite, the entire model is termed a finite mixture (of distributions) model.

The finite mixture model can be expressed in a more general form by representing α and β in terms of regressor variables and parameters with optional additional scale parameters for β . The section “Notation for the Finite Mixture Model” on page 2358 develops this in detail.

Mixture Models Contrasted with Mixing and Mixed Models: Untangling the Terminology

Web

Statistical terminology can have its limitations. The terms mixture, mixing, and mixed models are sometimes used interchangeably, causing confusion. Even worse, the terms arise in related situations. One application needs to be eliminated from the discussion in this documentation: mixture experiments, where design factors are the proportions with which components contribute to a blend, are not mixture models and do not fall under the purview of the FMM procedure. However, the data from a mixture experiment might be analyzed with a mixture model, a mixing model, or a mixed model, besides other types of statistical models.

Suppose that you observe realizations of random variable Y and assume that Y follows some distribution $f(y; \alpha, \beta)$ that depends on parameters α and β . Furthermore, suppose that the model is found to be deficient in the sense that the variability implied by the fitted model is less than the observed variability in the data, a condition known as overdispersion (see the section “Overdispersion” on page 2426). To tackle the problem the statistical model needs to be modified to allow for more variability. Clearly, one way of doing this is to introduce additional random variables into the process. Mixture, mixing, and mixed models are simply different ways of adding such random variables. The section “The Form of the Finite Mixture Model” on page 2423 explains how mixture models add a discrete state variable S . The following two subsections explain how mixing and mixed models instead assume variation for a natural parameter or in the mean function.

Mixing Models

Suppose that the model is modified to allow for some random quantity U , which might be one of the parameters of the model or a quantity related to the parameters. Now there are two distributions to cope with: the conditional distribution of the response given the random effect U ,

$$f(y; \alpha, \beta | u)$$

and the marginal distribution of the data. If U is continuous, the marginal distribution is obtained by integration:

$$f(y; \alpha, \beta) = \int f(y; \alpha, \beta | u) f(u) du$$

Otherwise, it is obtained by summation over the support of U :

$$f(y; \boldsymbol{\alpha}, \boldsymbol{\beta}) = \sum_u \Pr(U = u) f(y; \boldsymbol{\alpha}, \boldsymbol{\beta}|u)$$

The important entity for statistical estimation is the marginal distribution $f(y; \boldsymbol{\alpha}, \boldsymbol{\beta})$; the conditional distribution is often important for model description, genesis, and interpretation.

In a mixing model the marginal distribution is known and is typically of a well-known form. For example, if $Y|n$ has a binomial(n, μ) distribution and n follows a Poisson distribution, then the marginal distribution of Y is Poisson. The preceding operation is called *mixing* a binomial distribution with a Poisson distribution. Similarly, when mixing a Poisson(λ) distribution with a gamma(a, b) distribution for λ , a negative binomial distribution results as the marginal distribution. Other important mixing models involve mixing a binomial(n, μ) random variable with a beta(a, b) distribution for the binomial success probability μ . This results in a distribution known as the beta-binomial.

The finite mixtures have in common with the mixing models the introduction of random effects into the model to vary some or all of the parameters at random.

Mixed Models

The difference between a mixing and a mixed model is that the conditional distribution is not that important in the mixing model. It matters to motivate the overdispersed reference model and to arrive at the marginal distribution. Inferences with respect to the conditional distribution, such as predicting the random variable U , are not performed in mixing models. In a mixed model the random variable U typically follows a continuous distribution—almost always a normal distribution. The random effects usually do not model the natural parameters of the distribution; instead, they are involved in linear predictors that relate to the conditional mean. For example, a linear mixed model is a model in which the response and the random effects are normally distributed, and the random effects enter the conditional mean function linearly:

$$\begin{aligned} \mathbf{Y} &= \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\mathbf{U} + \boldsymbol{\epsilon} \\ \mathbf{U} &\sim N(\mathbf{0}, \mathbf{G}) \\ \boldsymbol{\epsilon} &\sim N(\mathbf{0}, \mathbf{R}) \\ \text{Cov}[\mathbf{U}, \boldsymbol{\epsilon}] &= \mathbf{0} \end{aligned}$$

The conditional and marginal distributions are then

$$\begin{aligned} \mathbf{Y}|\mathbf{U} &\sim N(\mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\mathbf{U} + \boldsymbol{\epsilon}, \mathbf{R}) \\ \mathbf{Y} &\sim N(\mathbf{X}\boldsymbol{\beta}, \mathbf{Z}\mathbf{G}\mathbf{Z}' + \mathbf{R}) \end{aligned}$$

For this model, because of the linearity in the mean and the normality of the random effects, you could also refer to mixing the normal vector \mathbf{Y} with the normal vector \mathbf{U} , since the marginal distribution is known. The linear mixed model can be fit with the MIXED procedure. When the conditional distribution is not normal and the random effects are normal, the marginal distribution does not have a closed form. In this class of mixed models, called generalized linear mixed models, model approximations and numerical integration methods are commonly used in model fitting; see for example, those models fit by the GLIMMIX and NLMIXED procedures. Chapter 6, “Introduction to Mixed Modeling Procedures,” contains details about the various classes of mixed models and about the relevant SAS/STAT procedures.

The previous expression for the marginal variance in the linear mixed model, $\text{var}[\mathbf{Y}] = \mathbf{Z}\mathbf{G}\mathbf{Z}' + \mathbf{R}$, emphasizes again that the variability in the marginal distribution of a model that contains random effects exceeds the variability in a model without the random effects (\mathbf{R}).

The finite mixtures have in common with the mixed models that the marginal distribution is not necessarily a well-known model, but is expressed through a formal integration over the random-effects distribution. In contrast to the mixed models, in particular those involving nonnormal distributions or nonlinear elements, this integration is rather trivial; it reduces to a weighted and finite sum of densities or mass functions.

Overdispersion

Overdispersion is the condition by which the data are more dispersed than is permissible under a reference model. Overdispersion arises only if the variability a model can capture is limited (for example, because of a functional relationship between mean and variance). For example, a model for normal data can never be overdispersed in this sense, although the reasons that lead to overdispersion also negatively affect a misspecified model for normal data. For example, omitted variables increase the residual variance estimate because variability that should have been modeled through changes in the mean is now “picked up” as error variability.

Overdispersion is important because an overdispersed model can lead to misleading inferences and conclusions. However, diagnosing and remedying overdispersion is complicated. In order to handle it appropriately, the source of overdispersion must be identified. For example, overdispersion can arise from any of the following conditions alone or in combination:

- omitted variables and model effects
- omitted random effects (a source of random variation is not being modeled or is modeled as a fixed effect)
- correlation among the observations
- incorrect distributional assumptions
- incorrectly specified mean-variance relationships
- outliers in the data

As discussed in the previous section, introducing randomness into a system increases its variability. Mixture, mixed, and mixing models have thus been popular in modeling data that appear overdispersed. Finite mixture models are particularly powerful in this regard, because even low-order mixtures of basic, symmetric distributions (such as two- or three-component mixtures of normal or t distributions) enable you to model data with multiple modes, heavy tails, and skewness. In addition, the latent variable S provides a natural way to accommodate omitted, unobservable variables into the model.

One approach to remedy overdispersion is to apply simple modifications of the variance function of the reference model. For example, with binomial-type data this approach replaces the variance of the binomial count variable $Y \sim \text{Binomial}(n, \mu)$, $\text{Var}[Y] = n \times \mu(1 - \mu)$ with a scaled version, $\phi n \times \mu(1 - \mu)$, where ϕ is called an overdispersion parameter, $\phi > 0$.

In addressing overdispersion problems, it is important to tackle the problem at its root. A missing scale factor on the variance function is hardly ever the root cause of overdispersion; it is only the easiest remedy.

Log-Likelihood Functions for Response Distributions

The FMM procedure calculates the log likelihood that corresponds to a particular response distribution according to the following formulas. The response distribution is the distribution specified (or chosen by default) through the `DIST=` option in the `MODEL` statement. The parameterizations used for log-likelihood functions of these distributions were chosen to facilitate expressions in terms of mean parameters that are modeled through an (inverse) link functions and in terms of scale parameters. These are not necessarily the parameterizations in which parameters of prior distributions are specified in a Bayesian analysis of homogeneous mixtures. See the section “Prior Distributions” on page 2435 for details about the parameterizations of prior distributions.

The FMM procedure includes all constant terms in the computation of densities or mass functions. In the expressions that follow, l denotes the log-likelihood function, ϕ denotes a general scale parameter, μ_i is the “mean”, and w_i is a weight from the use of a `WEIGHT` statement.

For some distributions (for example, the Weibull distribution) μ_i is not the mean of the distribution. The parameter μ_i is the quantity that is modeled as $g^{-1}(\mathbf{x}'\boldsymbol{\beta})$, where $g^{-1}(\cdot)$ is the inverse link function and the \mathbf{x} vector is constructed based on the effects in the `MODEL` statement. Situations in which the parameter μ does not represent the mean of the distribution are explicitly mentioned in the list that follows.

The parameter ϕ is frequently labeled as a “Scale” parameter in output from the FMM procedure. It is not necessarily the scale parameter of the particular distribution.

Beta(μ, ϕ)

$$l(\mu_i, \phi; y_i, w_i) = \log \left\{ \frac{\Gamma(\phi/w_i)}{\Gamma(\mu_i\phi/w_i)\Gamma((1-\mu_i)\phi/w_i)} \right\} \\ + (\mu_i\phi/w_i - 1) \log\{y_i\} \\ + ((1-\mu_i)\phi/w_i - 1) \log\{1-y_i\}$$

This parameterization of the beta distribution is due to Ferrari and Cribari-Neto (2004) and has properties $E[Y] = \mu$, $\text{Var}[Y] = \mu(1-\mu)/(1+\phi)$, $\phi > 0$.

Beta-binomial($n; \mu, \phi$)

$$\phi = (1 - \rho^2)/\rho^2 \\ l(\mu_i, \rho; y_i) = \log\{\Gamma(n_i + 1)\} - \log\{\Gamma(y_i + 1)\} \\ - \log\{\Gamma(n_i - y_i + 1)\} \\ + \log\{\Gamma(\phi)\} - \log\{\Gamma(n_i + \phi)\} + \log\{\Gamma(y_i + \phi\mu_i)\} \\ + \log\{\Gamma(n_i - y_i + \phi(1 - \mu_i))\} - \log\{\Gamma(\phi\mu_i)\} \\ - \log\{\Gamma(\phi(1 - \mu_i))\} \\ l(\mu_i, \rho; y_i, w_i) = w_i l(\mu_i, \rho; y_i)$$

where y_i and n_i are the *events* and *trials* in the *events/trials* syntax and $0 < \mu < 1$. This parameterization of the beta-binomial model presents the distribution as a special case of the Dirichlet-Multinomial distribution—see, for example, Neerchal and Morel (1998). In this parameterization, $E[Y] = n\mu$ and $\text{Var}[Y] = n\mu(1-\mu)(1+(n-1)/(\phi+1))$, $0 \leq \rho \leq 1$. The FMM procedure models the parameter ϕ and labels it “Scale” on the procedure output. For other parameterizations of the beta-binomial model, see Griffiths (1973) or Williams (1975).

Binomial($n; \mu$)

$$\begin{aligned}
l(\mu_i; y_i) &= y_i \log\{\mu_i\} + (n_i - y_i) \log\{1 - \mu_i\} \\
&\quad + \log\{\Gamma(n_i + 1)\} - \log\{\Gamma(y_i + 1)\} \\
&\quad - \log\{\Gamma(n_i - y_i + 1)\} \\
l(\mu_i; y_i, w_i) &= w_i l(\mu_i; y_i)
\end{aligned}$$

where y_i and n_i are the *events* and *trials* in the *events/trials* syntax and $0 < \mu < 1$. In this parameterization $E[Y] = n\mu$, $\text{Var}[Y] = n\mu(1 - \mu)$.

Binomial cluster($n; \mu, \pi$)

$$\begin{aligned}
z &= \log\{\Gamma(n_i + 1)\} - \log\{\Gamma(y_i + 1)\} - \log\{\Gamma(n_i - y_i + 1)\} \\
\mu_i^* &= (1 - \mu_i)\pi \\
l(\mu_i, \pi; y_i) &= \log\{\pi\} + z + y_i \log\{\mu_i^* + \mu_i\} \\
&\quad + (n_i - y_i) \log\{1 - \mu_i^* - \mu_i\} \\
&\quad + \log\{1 - \pi\} + z + y_i \log\{\mu_i^*\} \\
&\quad + (n_i - y_i) \log\{1 - \mu_i^*\} \\
l(\mu_i, \pi; y_i, w_i) &= w_i l(\mu_i, \pi; y_i)
\end{aligned}$$

In this parameterization, $E[Y] = n\pi$ and $\text{Var}[Y] = n\pi(1 - \pi) \{1 + \mu^2(n - 1)\}$. The binomial cluster model is a two-component mixture of a binomial($n, \mu^* + \mu$) and a binomial(n, μ^*) random variable. This mixture is unusual in that it fixes the number of components and because the mixing probability π appears in the moments of the mixture components. For further details, see Morel and Nagaraj (1993); Morel and Neerchal (1997); Neerchal and Morel (1998) and [Example 37.1](#) in this chapter. The expressions for the mean and variance in the binomial cluster model are identical to those of the beta-binomial model shown previously, with $\pi_{bc} = \mu_{bb}$, $\mu_{bc} = \rho_{bb}$.

The FMM procedure models the parameter μ through the **MODEL** statement and the parameter π through the **PROBMODEL** statement.

Constant(c)

$$l(y_i) = \begin{cases} 0 & y_i = c \\ -1E20 & y_i \neq c \end{cases}$$

The extreme value when $y_i \neq c$ is chosen so that $\exp\{l(y_i)\}$ yields a likelihood of zero. You can change this value with the **INVALIDLOGL=** option in the **PROC FMM** statement. The constant distribution is useful for modeling overdispersion due to zero-inflation (or inflation of the process at support c).

Exponential(μ)

$$l(\mu_i; y_i, w_i) = \begin{cases} -\log\{\mu_i\} - y_i/\mu_i & w_i = 1 \\ w_i \log\left\{\frac{w_i y_i}{\mu_i}\right\} - \frac{w_i y_i}{\mu_i} - \log\{y_i \Gamma(w_i)\} & w_i \neq 1 \end{cases}$$

In this parameterization, $E[Y] = \mu$ and $\text{Var}[Y] = \mu^2$.

Folded normal(μ, ϕ)

$$l(\mu_i, \phi; y_i, w_i) = -\frac{1}{2} \log\{2\pi\} - \frac{1}{2} \log\{\phi/w_i\} + \log \left\{ \exp \left\{ \frac{-w_i(y_i - \mu_i)^2}{2\phi} \right\} + \exp \left\{ \frac{-w_i(y_i + \mu_i)^2}{2\phi} \right\} \right\}$$

If X has a normal distribution with mean μ and variance ϕ , then $Y = |X|$ has a folded normal distribution and log-likelihood function $l(\mu, \phi; y, w)$ for $y \geq 0$. The folded normal distribution arises, for example, when normally distributed measurements are observed, but their signs are not observed. The mean and variance of the folded normal in terms of the underlying $N(\mu, \phi)$ distribution are

$$E[Y] = \frac{1}{\sqrt{2\pi\phi}} \exp \left\{ -\frac{\mu^2}{2\phi} \right\} + \mu \left(1 - 2\Phi \left(-\mu/\sqrt{\phi} \right) \right)$$

$$\text{Var}[Y] = \phi + \mu^2 - E[Y]^2$$

The FMM procedure models the folded normal distribution through the mean μ and variance ϕ of the underlying normal distribution. When the FMM procedure computes output statistics for the response variable (for example when you use the OUTPUT statement), the mean and variance of the response Y are reported. Similarly, the fit statistics apply to the distribution of $Y = |X|$, not the distribution of X . When you model a folded normal variable, the response input variable should be positive; the FMM procedure treats negative values of Y as a support violation.

Gamma(μ, ϕ)

$$l(\mu_i, \phi; y_i, w_i) = w_i \phi \log \left\{ \frac{w_i y_i \phi}{\mu_i} \right\} - \frac{w_i y_i \phi}{\mu_i} - \log\{y_i\} - \log \{ \Gamma(w_i \phi) \}$$

In this parameterization, $E[Y] = \mu$ and $\text{Var}[Y] = \mu^2/\phi$, $\phi > 0$. This parameterization of the gamma distribution differs from that in the GLIMMIX procedure, which expresses the log-likelihood function in terms of $1/\phi$ in order to achieve a variance function suitable for mixed model analysis.

Geometric(μ)

$$l(\mu_i; y_i, w_i) = y_i \log \left\{ \frac{\mu_i}{w_i} \right\} - (y_i + w_i) \log \left\{ 1 + \frac{\mu_i}{w_i} \right\} + \log \left\{ \frac{\Gamma(y_i + w_i)}{\Gamma(w_i)\Gamma(y_i + 1)} \right\}$$

In this parameterization, $E[Y] = \mu$ and $\text{Var}[Y] = \mu + \mu^2$. The geometric distribution is a special case of the negative binomial distribution with $\phi = 1$.

Generalized Poisson(μ, ϕ)

$$\xi_i = (1 - \exp\{-\phi\})/w_i$$

$$\mu_i^* = \mu_i - \xi(\mu_i - y_i)$$

$$l(\mu_i^*, \xi_i; y_i, w_i) = \log\{\mu_i^* - \xi_i y_i\} + (y_i - 1) \log\{\mu_i^*\} - \mu_i^* - \log\{\Gamma(y_i + 1)\}$$

In this parameterization, $E[Y] = \mu$, $\text{Var}[Y] = \mu/(1 - \xi)^2$, and $\phi \geq 0$. The FMM procedure models the mean μ through the effects in the **MODEL** statement and applies a log link by default. The generalized Poisson distribution provides an overdispersed alternative to the Poisson distribution; $\phi = \xi_i = 0$ produces the mass function of a regular Poisson random variable. For details about the generalized Poisson distribution and a comparison with the negative binomial distribution, see Joe and Zhu (2005).

Inverse Gaussian(μ, ϕ)

$$l(\mu_i, \phi; y_i, w_i) = -\frac{1}{2} \left[\frac{w_i (y_i - \mu_i)^2}{y_i \phi \mu_i^2} + \log \left\{ \frac{\phi y_i^3}{w_i} \right\} + \log\{2\pi\} \right]$$

The variance is $\text{Var}[Y] = \phi \mu^3$, $\phi > 0$.

Lognormal(μ, ϕ)

$$z_i = \log\{y_i\} - \mu_i$$

$$l(\mu_i, \phi; y_i, w_i) = -\frac{1}{2} \left(2 \log\{y_i\} + \log \left\{ \frac{\phi}{w_i} \right\} + \log\{2\pi\} + \frac{w_i z_i^2}{\phi} \right)$$

If $X = \log\{Y\}$ has a normal distribution with mean μ and variance ϕ , then Y has the log-likelihood function $l(\mu_i, \phi; y_i, w_i)$. The FMM procedure models the lognormal distribution and not the “shortcut” version you can obtain by taking the logarithm of a random variable and modeling that as normally distributed. The two approaches are not equivalent, and the approach taken by PROC FMM is the actual lognormal distribution. Although the lognormal model is a member of the exponential family of distributions, it is not in the “natural” exponential family because it cannot be written in canonical form.

In terms of the parameters μ and ϕ of the underlying normal process for X , the mean and variance of Y are $E[Y] = \exp\{\mu\}\sqrt{\omega}$ and $\text{Var}[Y] = \exp\{2\mu\}\omega(\omega - 1)$, respectively, where $\omega = \exp\{\phi\}$. When you request predicted values with the **OUTPUT** statement, the FMM procedure computes $E[Y]$ and not μ .

Negative binomial(μ, ϕ)

$$l(\mu_i, \phi; y_i, w_i) = y_i \log \left\{ \frac{\phi \mu_i}{w_i} \right\} - (y_i + w_i/\phi) \log \left\{ 1 + \frac{\phi \mu_i}{w_i} \right\}$$

$$+ \log \left\{ \frac{\Gamma(y_i + w_i/\phi)}{\Gamma(w_i/\phi)\Gamma(y_i + 1)} \right\}$$

The variance is $\text{Var}[Y] = \mu + \phi \mu^2$, $\phi > 0$.

For a given ϕ , the negative binomial distribution is a member of the exponential family. The parameter ϕ is related to the scale of the data because it is part of the variance function. However, it cannot be factored from the variance, as is the case with the ϕ parameter in many other distributions.

Normal(μ, ϕ)

$$l(\mu_i, \phi; y_i, w_i) = -\frac{1}{2} \left[\frac{w_i (y_i - \mu_i)^2}{\phi} + \log \left\{ \frac{\phi}{w_i} \right\} + \log\{2\pi\} \right]$$

The mean and variance are $E[Y] = \mu$ and $\text{Var}[Y] = \phi$, respectively, $\phi > 0$

Poisson(μ)

$$l(\mu_i; y_i, w_i) = w_i(y_i \log\{\mu_i\} - \mu_i - \log\{\Gamma(y_i + 1)\})$$

The mean and variance are $E[Y] = \mu$ and $\text{Var}[Y] = \mu$.

(Shifted) $T(v; \mu, \phi)$

$$z_i = -0.5 \log\{\phi/\sqrt{w_i}\} + \log\{\Gamma(0.5(v + 1))\} - \log\{\Gamma(0.5v)\} - 0.5 \times \log\{\pi v\}$$

$$l(\mu_i, \phi; y_i, w_i) = -\left(\frac{v + 1}{2}\right) \log\left\{1 + \frac{w_i(y_i - \mu_i)^2}{v\phi}\right\} + z_i$$

In this parameterization $E[Y] = \mu$ and $\text{Var}[Y] = \phi v/(v - 2)$, $\phi > 0, v > 0$. Note that this form of the t distribution is not a non-central distribution, but that of a shifted central t random variable.

Truncated Exponential($\mu; a, b$)

$$l(\mu_i; a, b, y_i, w_i) = w_i \log\left\{\frac{w_i y_i}{\mu_i}\right\} - \frac{w_i y_i}{\mu_i} - \log\{y_i \Gamma(w_i)\} - \log\left[\frac{\gamma\left(w_i, \frac{w_i b}{\mu_i}\right)}{\Gamma(w_i)} - \frac{\gamma\left(w_i, \frac{w_i a}{\mu_i}\right)}{\Gamma(w_i)}\right]$$

where

$$\gamma(c_1, c_2) = \int_0^{c_2} t^{c_1-1} \exp(-t) dt$$

is the lower incomplete gamma function. The mean and variance are

$$E[Y] = \frac{(a + \mu_i) \exp(-a/\mu_i) - (b + \mu_i) \exp(-b/\mu_i)}{\exp(-a/\mu_i) - \exp(-b/\mu_i)}$$

$$\text{Var}[Y] = \frac{(a^2 + 2a\mu_i + 2\mu_i^2) \exp(-a/\mu_i) - (b^2 + 2b\mu_i + 2\mu_i^2) \exp(-b/\mu_i)}{\exp(-a/\mu_i) - \exp(-b/\mu_i)} - (E[Y])^2$$

Truncated Lognormal($\mu, \phi; a, b$)

$$z_i = \log\{y_i\} - \mu_i$$

$$l(\mu_i, \phi; a, b, y_i, w_i) = -\frac{1}{2} \left(2 \log\{y_i\} + \log\left\{\frac{\phi}{w_i}\right\} + \log\{2\pi\} + \frac{w_i z_i^2}{\phi} \right) - \log\left\{\Phi\left[\sqrt{w_i/\phi}(\log b - \mu_i)\right] - \Phi\left[\sqrt{w_i/\phi}(\log a - \mu_i)\right]\right\}$$

where $\Phi(\cdot)$ is the cumulative distribution function of the standard normal distribution. The mean and variance are

$$E[Y] = \exp(\mu_i + 0.5\phi) \frac{\Phi\left(\sqrt{\phi} - \frac{\log a - \mu_i}{\sqrt{\phi}}\right) - \Phi\left(\sqrt{\phi} - \frac{\log b - \mu_i}{\sqrt{\phi}}\right)}{\Phi\left(\frac{\log b - \mu_i}{\sqrt{\phi}}\right) - \Phi\left(\frac{\log a - \mu_i}{\sqrt{\phi}}\right)}$$

$$\text{Var}[Y] = \exp(2\mu_i + 2\phi) \frac{\Phi\left(2\sqrt{\phi} - \frac{\log a - \mu_i}{\sqrt{\phi}}\right) - \Phi\left(2\sqrt{\phi} - \frac{\log b - \mu_i}{\sqrt{\phi}}\right)}{\Phi\left(\frac{\log b - \mu_i}{\sqrt{\phi}}\right) - \Phi\left(\frac{\log a - \mu_i}{\sqrt{\phi}}\right)} - (E[Y])^2$$

Truncated Negative binomial(μ, ϕ)

$$l(\mu_i, \phi; y_i, w_i) = y_i \log \left\{ \frac{\phi \mu_i}{w_i} \right\} - (y_i + w_i/\phi) \log \left\{ 1 + \frac{\phi \mu_i}{w_i} \right\} \\ + \log \left\{ \frac{\Gamma(y_i + w_i/\phi)}{\Gamma(w_i/\phi) \Gamma(y_i + 1)} \right\} \\ - \log \left\{ 1 - \left(\frac{\phi \mu_i}{w_i} + 1 \right)^{-w_i/\phi} \right\}$$

The mean and variance are

$$E[Y] = \mu_i \left\{ 1 - (\phi \mu_i + 1)^{-1/\phi} \right\}^{-1} \\ \text{Var}[Y] = (1 + \phi \mu_i + \mu_i) E[Y] - (E[Y])^2$$

Truncated Normal($\mu, \phi; a, b$)

$$l(\mu_i, \phi; a, b, y_i, w_i) = -\frac{1}{2} \left[\frac{w_i (y_i - \mu_i)^2}{\phi} + \log \left\{ \frac{\phi}{w_i} \right\} + \log \{2\pi\} \right] \\ - \log \left\{ \Phi \left[\sqrt{w_i/\phi} (b - \mu_i) \right] - \Phi \left[\sqrt{w_i/\phi} (a - \mu_i) \right] \right\}$$

where $\Phi(\cdot)$ is the cumulative distribution function of the standard normal distribution.

The mean and variance are

$$E[Y] = \mu_i + \sqrt{\phi} \frac{\text{phi} \left(\frac{a - \mu_i}{\sqrt{\phi}} \right) - \text{phi} \left(\frac{b - \mu_i}{\sqrt{\phi}} \right)}{\Phi \left(\frac{b - \mu_i}{\sqrt{\phi}} \right) - \Phi \left(\frac{a - \mu_i}{\sqrt{\phi}} \right)} \\ \text{Var}[Y] = \phi \left[1 + \frac{\frac{a - \mu_i}{\sqrt{\phi}} \text{phi} \left(\frac{a - \mu_i}{\sqrt{\phi}} \right) - \frac{b - \mu_i}{\sqrt{\phi}} \text{phi} \left(\frac{b - \mu_i}{\sqrt{\phi}} \right)}{\Phi \left(\frac{b - \mu_i}{\sqrt{\phi}} \right) - \Phi \left(\frac{a - \mu_i}{\sqrt{\phi}} \right)} \right. \\ \left. - \left\{ \frac{\text{phi} \left(\frac{a - \mu_i}{\sqrt{\phi}} \right) - \text{phi} \left(\frac{b - \mu_i}{\sqrt{\phi}} \right)}{\Phi \left(\frac{b - \mu_i}{\sqrt{\phi}} \right) - \Phi \left(\frac{a - \mu_i}{\sqrt{\phi}} \right)} \right\}^2 \right]$$

where $\text{phi}(\cdot)$ is the probability density function of the standard normal distribution.

Truncated Poisson(μ)

$$l(\mu_i; y_i, w_i) = w_i (y_i \log \{\mu_i\} - \log \{\exp(\mu_i) - 1\} - \log \{\Gamma(y_i + 1)\})$$

The mean and variance are

$$E[Y] = \frac{\mu}{1 - \exp(-\mu)} \\ \text{Var}[Y] = \frac{\mu [1 - \exp(-\mu) - \mu \exp(-\mu)]}{[1 - \exp(-\mu)]^2}$$

Uniform(a, b)

$$l(\mu_i; y_i, w_i) = -\log \{b - a\}$$

The mean and variance are $E[Y] = 0.5(a + b)$ and $\text{Var}[Y] = (b - a)^2/12$.

Weibull(μ, ϕ)

$$l(\mu_i, \phi; y_i) = -\frac{\phi - 1}{\phi} \log \left\{ \frac{y_i}{\mu_i} \right\} - \log\{\mu_i \phi\} - \exp \left\{ \log \left\{ \frac{y_i}{\mu_i} \right\} / \phi \right\}$$

In this particular parameterization of the two-parameter Weibull distribution, the mean and variance of the random variable Y are $E[Y] = \mu\Gamma(1 + \phi)$ and $\text{Var}[Y] = \mu^2 \{ \Gamma(1 + 2\phi) - \Gamma^2(1 + \phi) \}$.

Bayesian Analysis

Conjugate Sampling

The FMM procedure uses Bayesian analysis via a conjugate Gibbs sampler if the model belongs to a small class of mixture models for which a conjugate sampler is available. See the section “[Gibbs Sampler](#)” on page 135 for a general discussion of Gibbs sampling. [Table 37.8](#) summarizes the models for which conjugate and Metropolis-Hastings samplers are available.

Table 37.8 Availability of Conjugate and Metropolis Samplers in the FMM Procedure

Effects (exclusive of intercept)	Distributions	Available Samplers
No	Normal or T	Conjugate or Metropolis-Hastings
Yes	Normal or T	Conjugate or Metropolis-Hastings
No	Binomial, binary, Poisson, exponential	Conjugate or Metropolis-Hastings
Yes	Binomial, binary, Poisson, exponential	Metropolis-Hastings only

The conjugate sampler enjoys greater efficiency than the Metropolis-Hastings sampler and has the advantage of sampling in terms of the natural parameters of the distribution.

You can always switch to the Metropolis-Hastings sampling algorithm in any model by adding the `METROPOLIS` option in the `BAYES` statement.

Metropolis-Hastings Algorithm

If Metropolis-Hastings is the only sampler available for the specified model (see [Table 37.8](#)) or if the `METROPOLIS` option is specified in the `BAYES` statement, PROC FMM uses the Metropolis-Hastings approach of Gamerman (1997). See the section “[Metropolis and Metropolis-Hastings Algorithms](#)” on page 134 for a general discussion of the Metropolis-Hastings algorithm.

The Gamerman (1997) algorithm derives a specific density that is used to generate proposals for the component-specific parameters β_j . The form of this proposal density is multivariate normal, with mean \mathbf{m}_j and covariance matrix \mathbf{C}_j derived as follows.

Suppose β_j is the vector of model coefficients in the j th component and suppose that β_j has prior distribution $N(\mathbf{a}, \mathbf{R})$. Consider a generalized linear model (GLM) with link function $g(\mu) = \eta = \mathbf{x}'\boldsymbol{\beta}$ and variance

function $a(\mu)$. The pseudo-response and weight in the GLM for a weighted least squares step are

$$y^* = \eta + (y - \mu) / \frac{\partial \mu}{\partial \eta}$$

$$w = \frac{\partial \mu}{\partial \eta} / a(\mu)$$

If the model contains offsets or **FREQ** or **WEIGHT** statements, or if a *trials* variable is involved, suitable adjustments are made to these quantities.

In each component, $j = 1, \dots, k$, form an adjusted cross-product matrix with a “pseudo” border

$$\begin{bmatrix} \mathbf{X}'_j \mathbf{W}_j \mathbf{X}_j + \mathbf{R}^{-1} & \mathbf{X}'_j \mathbf{W}_j \mathbf{y}_j^* + \mathbf{R}^{-1} \mathbf{a} \\ \mathbf{y}_j^{*'} \mathbf{W}_j \mathbf{X}_j + \mathbf{a}' \mathbf{R}^{-1} & c \end{bmatrix}$$

where \mathbf{W}_j is a diagonal matrix formed from the pseudo-weights w , \mathbf{y}^* is a vector of pseudo-responses, and c is arbitrary. This is basically a system of normal equations with ridging, and the degree of ridging is governed by the precision and mean of the normal prior distribution of the coefficients. Sweeping on the leading partition leads to

$$\mathbf{C}_j = (\mathbf{X}'_j \mathbf{W}_j \mathbf{X}_j + \mathbf{R}^{-1})^{-}$$

$$\mathbf{m}_j = \mathbf{C}_j (\mathbf{X}'_j \mathbf{W}_j \mathbf{y}_j^* + \mathbf{R}^{-1} \mathbf{a})$$

where the generalized inverse is a reflexive, g_2 -inverse (see the section “Linear Model Theory” on page 55 of Chapter 3, “Introduction to Statistical Modeling with SAS/STAT Software,” for details).

PROC FMM then generates a proposed parameter vector from the resulting multivariate normal distribution, and then accepts or rejects this proposal according to the appropriate Metropolis-Hastings thresholds.

Latent Variables via Data Augmentation

In order to fit finite Bayesian mixture models, the FMM procedure treats the mixture model as a missing data problem and introduces an assignment variable \mathbf{S} as in Dempster, Laird, and Rubin (1977). Since \mathbf{S} is not observable, it is frequently referred to as a latent variable. The unobservable variable \mathbf{S} assigns an observation to a component in the mixture model. The number of states, k , might be unknown, but it is known to be finite. Conditioning on the latent variable \mathbf{S} , the component memberships of each observation is assumed to be known, and Bayesian estimation is straightforward for each component in the finite mixture model. That is, conditional on $S = j$, the distribution of the response is now assumed to be $f(y; \alpha_j, \beta_j | S = j)$. In other words, each distinct state of the random variable \mathbf{S} leads to a distinct set of parameters. The parameters in each component individually are then updated using a conjugate Gibbs sampler (where available) or a Metropolis-Hastings sampling algorithm.

The FMM procedure assumes that the random variable \mathbf{S} has a discrete multinomial distribution with probability π_j of belonging to a component j ; it can occupy one of k states. The distribution for the latent variable \mathbf{S} is

$$f(S_i = j | \pi_1, \dots, \pi_k) = \text{multinomial}(1, \pi_1, \dots, \pi_k)$$

where $f(\cdot | \cdot)$ denotes a conditional probability density. The parameters in the density π_j denote the probability that S takes on state j .

The FMM procedure assumes a conjugate Dirichlet prior distribution on the mixture proportions π_j written as:

$$p(\boldsymbol{\pi}) = \text{Dirichlet}(a_1, \dots, a_k)$$

where $p(\cdot)$ indicates a prior distribution.

Using Bayes' theorem, the likelihood function and prior distributions determine a conditionally conjugate posterior distribution of \mathbf{S} and $\boldsymbol{\pi}$ from the multinomial distribution and Dirichlet distribution, respectively.

Prior Distributions

The following list displays the parameterization of prior distributions for situations in which the FMM procedure uses a conjugate sampler in mixture models without model effects and certain basic distributions (binary, binomial, exponential, Poisson, normal, and t). You specify the parameters a and b in the formulas below in the `MUPRIORPARMS=` and `PHIPRIORPARMS=` options in the `BAYES` statement in these models.

Beta(a, b)

$$f(y) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} y^{a-1} (1-y)^{b-1}$$

where $a > 0, b > 0$. In this parameterization, the mean and variance of the distribution are $\mu = a/(a+b)$ and $\mu(1-\mu)/(a+b+1)$, respectively. The beta distribution is the prior distribution for the success probability in binary and binomial distributions when conjugate sampling is used.

Dirichlet(a_1, \dots, a_k)

$$f(\mathbf{y}) = \frac{\Gamma\left(\sum_{i=1}^k a_i\right)}{\prod_{i=1}^k \Gamma(a_i)} y_1^{a_1-1} \dots y_k^{a_k-1}$$

where $\sum_{i=1}^k y_i = 1$ and the parameters $a_i > 0$. If any a_i were zero, an improper density would result. The Dirichlet density is the prior distribution for the mixture probabilities. You can affect the choice of the a_i through the `MIXPRIORPARMS` option in the `BAYES` statement. If $k=2$, the Dirichlet is the same as the beta(a, b) distribution.

Gamma(a, b)

$$f(y) = \frac{b^a}{\Gamma(a)} y^{a-1} \exp\{-by\}$$

where $a > 0, b > 0$. In this parameterization, the mean and variance of the distribution are $\mu = a/b$ and μ/b , respectively. The gamma distribution is the prior distribution for the mean parameter of the Poisson distribution when conjugate sampling is used.

Inverse gamma(a, b)

$$f(y) = \frac{b^a}{\Gamma(a)} y^{-a-1} \exp\{-b/y\}$$

where $a > 0$, $b > 0$. In this parameterization, the mean and variance of the distribution are $\mu = b/(a - 1)$ if $a > 1$ and $\mu^2/(a - 2)$ if $a > 2$, respectively. The inverse gamma distribution is the prior distribution for the mean parameter of the exponential distribution when conjugate sampling is used. It is also the prior distribution for the scale parameter ϕ in all models.

Multinomial(1, π_1, \dots, π_k)

$$f(\mathbf{y}) = \frac{1}{y_1! \cdots y_k!} \pi_1^{y_1} \cdots \pi_k^{y_k}$$

where $\sum_{j=1}^k y_j = n$, $y_j \geq 0$, $\sum_{j=1}^k \pi_j = 1$, and n is the number of observations included in the analysis. The multinomial density is the prior distribution for the mixture proportions. The mean and variance of Y_j are $\mu_j = \pi_j$ and $\mu_j(1 - \mu_j)$, respectively.

Normal(a, b)

$$f(y) = \frac{a}{\sqrt{2\pi b}} \exp \left\{ -\frac{1}{2} \frac{(y - a)^2}{b} \right\}$$

where $b > 0$. The mean and variance of the distribution are $\mu = a$ and b , respectively. The normal distribution is the prior distribution for the mean parameter of the normal and t distribution when conjugate sampling is used.

When a **MODEL** statement contains effects or if you specify the **METROPOLIS** option, the prior distribution for the regression parameters is multivariate normal, and you can specify the means and variances of the parameters in the **BETAPRIORPARMS=** option in the **BAYES** statement.

Parameterization of Model Effects

PROC FMM constructs a finite mixture model according to the specifications in the **CLASS**, **MODEL**, and **PROBMODEL** statements. Each effect in the **MODEL** statement generates one or more columns in the matrix **X** for that model. The same **X** matrix applies to all components that are associated with the **MODEL** statement. Each effect in the **PROBMODEL** statement generates one or more columns in the matrix **Z** from which the linear predictors in the model for the mixture probability models is formed. The same **Z** matrix applies to all components.

The formation of effects from continuous and classification variables in the FMM procedure follows the same general rules and techniques as for other linear modeling procedures. See the section “GLM Parameterization of Classification Variables and Effects” on page 383 of Chapter 19, “Shared Concepts and Topics.”

Default Output

The following sections describe the output that PROC FMM produces by default. The output is organized into various tables, which are discussed in the order of appearance for maximum likelihood and Bayes estimation, respectively.

Model Information

The “Model Information” table displays basic information about the model, such as the response variable, frequency variable, link function, and the model category that the FMM procedure determined based on your input and options. The “Model Information” table is one of a few tables that are produced irrespective of estimation technique. Most other tables are specific to Bayes or maximum likelihood estimation.

If the analysis depends on generated random numbers, the “Model Information” table also displays the random number seed used to initialize the random number generators. If you repeat the analysis and pass this seed value in the `SEED=` option in the `PROC FMM` statement, an identical stream of random numbers results.

Class Level Information

The “Class Level Information” table lists the levels of every variable specified in the `CLASS` statement. You should check this information to make sure that the data are correct. You can adjust the order of the `CLASS` variable levels with the `ORDER=` option in the `PROC FMM` statement. You can suppress the “Class Level Information” table completely or partially with the `NOCLPRINT` option in the `PROC FMM` statement.

Number of Observations

The “Number of Observations” table displays the number of observations read from the input data set and the number of observations used in the analysis. If you specify a `FREQ` statement, the table also displays the sum of frequencies read and used. If the `events/trials` syntax is used for the response, the table also displays the number of events and trials used in the analysis.

Note that the number of observations “used” in the analysis is not unambiguous in a mixture model. An observation that is “unusable” for one component distribution (because the response value is outside of the support of the distribution) might still be usable in the mixture model when the response value is in the support of another component distribution. You can affect the way in which `PROC FMM` handles exclusion of observations due to support violations with the `EXCLUSION=` option in the `PROC FMM` statement.

Response Profile

For binary data, the “Response Profile” table displays the ordered value from which the FMM procedure determines the probability being modeled as an event for binary data. For each response category level, the frequency used in the analysis is reported.

Default Output for Maximum Likelihood

Optimization Information

The “Optimization Information” table displays basic information about the optimization setup to determine the maximum likelihood estimates, such as the optimization technique, the parameters that participate in the optimization, and the number of threads used for the calculations. This table is not produced during model selection—that is, if the `KMAX=` option is specified in the `MODEL` statement.

Iteration History

The “Iteration History” table displays for each iteration of the optimization the number of function evaluations (including gradient and Hessian evaluations), the value of the objective function, the change in the objective function from the previous iteration, and the absolute value of the largest (projected) gradient

element. The objective function used in the optimization in the FMM procedure is the negative of the mixture log likelihood; consequently, PROC FMM performs a minimization. This table is not produced if the `KMAX=` option is specified in the `MODEL` statement.

Convergence Status

The convergence status table is a small ODS table that follows the “Iteration History” table in the default output. In the listing, it appears as a message that identifies whether the optimization succeeded and which convergence criterion was met. If the optimization fails, the message indicates the reason for the failure. If you save the “Convergence Status” table to an output data set, a numeric `Status` variable is added that allows you to assess convergence programmatically. The values of the `Status` variable encode the following:

- | | |
|---|---|
| 0 | Convergence was achieved or an optimization was not performed (because of <code>TECHNIQUE=NONE</code>). |
| 1 | The objective function could not be improved. |
| 2 | Convergence was not achieved because of a user interrupt or because a limit was exceeded, such as the maximum number of iterations or the maximum number of function evaluations. To modify these limits, see the <code>MAXITER=</code> , <code>MAXFUNC=</code> , and <code>MAXTIME=</code> options in the <code>PROC FMM</code> statement. |
| 3 | Optimization failed to converge because function or derivative evaluations failed at the starting values or during the iterations or because a feasible point that satisfies the parameter constraints could not be found in the parameter space. |

Fit Statistics

The “Fit Statistics” table displays a variety of fit measures based on the mixture log likelihood in addition to the Pearson statistic. All statistics are presented in “smaller is better” form. If you are fitting a single-component normal, gamma, or inverse gaussian model, the table also contains the unscaled Pearson statistic. If you are fitting a mixture model or the model has been fitted under restrictions, the table also contains the number of effective components and the number of effective parameters.

The calculation of the information criteria uses the following formulas, where p denotes the number of effective parameters, n denotes the number of observations used (or the sum of the frequencies used if a `FREQ` statement is present), and l is the log likelihood of the mixture evaluated at the converged estimates:

$$\begin{aligned} \text{AIC} &= -2l + 2p \\ \text{AICC} &= \begin{cases} -2l + 2pn/(n - p - 1) & n > p + 2 \\ -2l + 2p(p + 2) & \text{otherwise} \end{cases} \\ \text{BIC} &= -2l + p \log(n) \end{aligned}$$

The Pearson statistic is computed simply as

$$\text{Pearson statistic} = \sum_{i=1}^n f_i \frac{(y_i - \hat{\mu}_i)^2}{\widehat{\text{Var}}[Y_i]}$$

where n denotes the number of observations used in the analysis, f_i is the frequency associated with the i th observation (or 1 if no frequency is specified), μ_i is the mean of the mixture, and the denominator is the

variance of the i th observation in the mixture. Note that the mean and variance in this expression are not those of the component distributions, but the mean and variance of the mixture:

$$\mu_i = E[Y_i] = \sum_{j=1}^k \pi_{ij} \mu_{ij}$$

$$\text{Var}[Y_i] = -\mu_i^2 + \sum_{j=1}^k \pi_{ij} (\sigma_{ij}^2 + \mu_{ij}^2)$$

where μ_{ij} and σ_{ij}^2 are the mean and variance, respectively, for observation i in the j th component distribution and π_{ij} is the mixing probability for observation i in component j .

The unscaled Pearson statistic is computed with the same expression as the Pearson statistic with n , f_i , and μ_i as previously defined, but the scale parameter ϕ is set to 1 in the $\widehat{\text{Var}}[Y_i]$ expression.

The number of effective components and the number of effective parameters are determined by examining the converged solution for the parameters that are associated with model effects and the mixing probabilities. For example, if a component has an estimated mixing probability of zero, the values of its parameter estimates are immaterial. You might argue that all parameters should be counted towards the penalty in the information criteria. But a component with zero mixing probability in a k -component model effectively reduces the model to a $(k - 1)$ -component model. A situation of an overfit model, for which a parameter penalty needs to be taken when calculating the information criteria, is a different situation; here the mixing probability might be small, possibly close to zero.

Parameter Estimates

The parameter estimates, their estimated (asymptotic) standard errors, and p -values for the hypothesis that the parameter is zero are presented in the “Parameter Estimates” table. A separate table is produced for each **MODEL** statement, and the components that are associated with a **MODEL** statement are identified with an overall component count variable that counts across **MODEL** statements. If you assign a label to a model with the **LABEL=** option in the **MODEL** statement, the label appears in the title of the “Parameter Estimates” table. Otherwise, the internal label generated by the FMM procedure is used.

If the **MODEL** statement does not contain effects and the link function is not the identity, the inversely linked estimate is also displayed in the table. For many distributions, the inverse linked estimate is the estimated mean on the data scale. For example, in a binomial or binary model, it represents the estimated probability of an event. For some distributions (for example, the Weibull distribution), the inverse linked estimate is not the component distribution mean.

If you request confidence intervals with the **CL** or **ALPHA=** option in the **MODEL** statement, confidence limits are produced for the estimate on the linear scale. If the inverse linked estimate is displayed, confidence intervals for that estimate are also produced by inversely linking the confidence bounds on the linear scale.

Mixing Probabilities

If you fit a model with more than one component, the table of mixing probabilities is produced. If there are no effects in the **PROBMODEL** statement or if there is no **PROBMODEL** statement, the parameters are reported on the linear scale and as mixing probabilities. If model effects are present, only the linear parameters (on the scale of the logit, generalized logit, probit, and so on) are displayed.

Default Output for Bayes Estimation

Bayes Information

This table provides basic information about the sampling algorithm. The FMM procedure uses either a conjugate sampler or a Metropolis-Hastings sampling algorithm based on Gamerman (1997). The table reveals, for example, how many model parameters are sampled, how many parameters associated with mixing probabilities are sampled, and how many threads are used to perform multithreaded analysis.

Prior Distributions

The “Prior Distributions” table lists for each sampled parameter the prior distribution and its parameters. The mean and variance (if they exist) for those values of the parameters are also displayed, along with the initial value for the parameter in the Markov chain. The Component column in this table identifies the mixture component to which a particular parameter belongs. You can control how the FMM procedure determines initial values with the `INITIAL=` option in the `BAYES` statement.

Posterior Summaries

The arithmetic mean, standard deviation, and percentiles of the posterior distribution of the parameter estimates are displayed in the “Posterior Summaries” table. By default, the FMM procedure computes the 25th, 50th (median), and 75th percentiles of the sampling distribution. You can modify the percentiles through suboptions of the `STATISTICS` option in the `BAYES` statement. If a parameter corresponds to a singularity in the design and was removed from sampling for that purpose, it is also displayed in the table of posterior summaries (and in other tables that relate to output from the `BAYES` statement). The posterior sample size for such a parameter is shown as $N = 0$.

Posterior Intervals

The table of “Posterior Intervals” displays equal-tail intervals and intervals of highest posterior density for each parameter. By default, intervals are computed for an α -level of 0.05, which corresponds to 95% intervals. You can modify this confidence level by providing one or more α values in the `ALPHA=` suboption of the `STATISTICS` option in the `BAYES` statement. The computation of these intervals is detailed in section “Summary Statistics” on page 153 of Chapter 7, “Introduction to Bayesian Analysis Procedures.”

Posterior Autocorrelations

Autocorrelations for the posterior estimates are computed by default for autocorrelation lags 1, 5, 10, and 50, provided that a sufficient number of posterior samples is available. See the section “Assessing Markov Chain Convergence” on page 139 of Chapter 7, “Introduction to Bayesian Analysis Procedures,” for the computation of posterior autocorrelations and their utility in diagnosing convergence of Markov chains. You can modify the list of lags for which posterior autocorrelations are calculated with the `AUTOCORR` suboption of the `DIAGNOSTICS=` option in the `BAYES` statement.

ODS Table Names

Each table created by PROC FMM has a name associated with it, and you must use this name to reference the table when you use ODS statements. These names are listed in [Table 37.9](#).

Table 37.9 ODS Tables Produced by PROC FMM

Table Name	Description	Required Statement / Option
Autocorr	Autocorrelation among posterior estimates	BAYES
BayesInfo	Basic information about Bayesian estimation	BAYES
ClassLevels	Level information from the CLASS statement	CLASS
CompDescription	Component description in models with varying number of components	KMAX= in MODEL with ML estimation
CompEvaluation	Comparison of mixture models with varying number of components	KMAX= in MODEL with ML estimation
CompInfo	Component information	COMPONENTINFO option in PROC FMM statement
ConvergenceStatus	Status of optimization at conclusion of optimization	Default output
Constraints	Linear equality and inequality constraints	RESTRICT statement or EQUATE=EFFECTS option in MODEL statement
Corr	Asymptotic correlation matrix of parameter estimates (ML) or empirical correlation matrix of the Bayesian posterior estimates	CORR option in PROC FMM statement
Cov	Asymptotic covariance matrix of parameter estimates (ML) or empirical covariance matrix of the Bayesian posterior estimates	COV option in PROC FMM statement
CovI	Inverse of the covariance matrix of the parameter estimates	COVI option in PROC FMM statement
ESS	Effective sample size	DIAG=ESS option in BAYES statement
FitStatistics	Fit statistics	Default output
Geweke	Geweke diagnostics (Geweke 1992) for Markov chain	DIAG=GEWEKE option in BAYES statement
Hessian	Hessian matrix from the maximum likelihood optimization, evaluated at the converged estimates	HESSIAN
IterHistory	Iteration history	Default output for ML estimation
MCSE	Monte Carlo standard errors	DIAG=MCERROR in BAYES statement

Table 37.9 continued

Table Name	Description	Required Statement / Option
MixingProbs	Solutions for the parameter estimates associated with effects in PROBMODEL statements	Default output for ML estimation if number of components is greater than 1
ModelInfo	Model information	Default output
NObs	Number of observations read and used, number of trials and events	Default output
OptInfo	Optimization information	Default output for ML estimation
ParameterEstimates	Solutions for the parameter estimates associated with effects in MODEL statements	Default output for ML estimation
ParameterMap	Mapping of parameter names to OUTPOST= data set	OUTPOST= option in BAYES statement
PriorInfo	Prior distributions and initial value of Markov chain	BAYES
PostSummaries	Summary statistics for posterior estimates	BAYES
PostIntervals	Equal-tail and highest posterior density intervals for posterior estimates	BAYES
ResponseProfile	Response categories and category modeled	Default output in models with binary response

ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “[Statistical Graphics Using ODS](#).”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the **ODS GRAPHICS ON** statement). For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS](#).”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “[A Primer on ODS Statistical Graphics](#)” on page 599 in Chapter 21, “[Statistical Graphics Using ODS](#).”

You can reference every graph produced through ODS Graphics with a name. The names of the graphs that PROC FMM generates are listed in [Table 37.10](#), along with the required statements and options.

Table 37.10 Graphs Produced by PROC FMM

ODS Graph Name	Plot Description	Option
TADPanel	Panel of diagnostic graphics to assess convergence of Markov chains	BAYES
DensityPlot	Histogram and density with component distributions	Default plot for homogeneous mixtures

Examples: FMM Procedure

Example 37.1: Modeling Mixing Probabilities: All Mice Are Created Equal, but Some Are More Equal

This example demonstrates how you can model the means and mixture proportions separately in a binomial cluster model. It also compares the binomial cluster model to the beta-binomial model.

In a typical teratological experiment, the offspring of animals that were exposed to a toxin during pregnancy are studied for malformation. If you count the number of malformed offspring in a litter of size n , then this count is typically not binomially distributed. The responses of the offspring from the same litter are not independent; hence their sum does not constitute a binomial random variable. Relative to a binomial model, data from teratological experiments exhibit overdispersion because ignoring positive correlation among the responses tends to overstate the precision of the parameter estimates. Overdispersion mechanisms are briefly discussed in the section “[Overdispersion](#)” on page 2426.

In this application, the focus is on mixtures and models that involve a mixing mechanism. The mixing approach (Williams 1975; Haseman and Kupper 1979) supposes that the binomial success probability is a random variable that follows a $\text{beta}(\alpha, \beta)$ distribution:

$$\begin{aligned}
 Y|\mu &\sim \text{Binomial}(n, \mu) \\
 \mu &\sim \text{Beta}(\alpha, \beta) \\
 Y &\sim \text{Beta-binomial}(n, \mu, \phi) \\
 E[Y] &= n\pi \\
 \text{Var}[Y] &= n\pi(1 - \pi) \{1 + \mu^2(n - 1)\}
 \end{aligned}$$

If $\mu = 0$, then the beta-binomial distribution reduces to a standard binomial model with success probability π . The parameterization of the beta-binomial distribution used by the FMM procedure is based on Neerchal and Morel (1998), see the section “[Log-Likelihood Functions for Response Distributions](#)” on page 2427 for details.

Morel and Nagaraj (1993); Morel and Neerchal (1997); Neerchal and Morel (1998) propose a different model to capture dependency within binomial clusters. Their model is a two-component mixture that gives rise to the same mean and variance function as the beta-binomial model. The genesis is different, however.

In the binomial cluster model of Morel and Neerchal, suppose there is a cluster of n Bernoulli outcomes with success probability π . The number of responses in the cluster decomposes into $N \leq n$ outcomes that all respond with either “success” or “failure”; the important aspect is that they all respond identically. The remaining $n - N$ Bernoulli outcomes respond independently, so the sum of successes in this group is a binomial($n - N, \pi$) random variable. Denote the probability with which cluster members fall into the group of identical respondents as μ . Then $1 - \mu$ is the probability that a response belongs to the group of independent Bernoulli outcomes.

It is easy to see how this process of dividing the individual Bernoulli outcomes creates clustering. The binomial cluster model can be written as the two-component mixture

$$\Pr(Y = y) = \pi \Pr(U = y) + (1 - \pi) \Pr(V = y)$$

where $U \sim \text{Binomial}(n, \mu^* + \mu)$, $V \sim \text{Binomial}(n, \mu^*)$, and $\mu^* = (1 - \mu)\pi$. This mixture model is somewhat unusual because the mixing probability π appears as a parameter in the component distributions. The two probabilities involved, π and μ , have the following interpretation: π is the unconditional probability of success for any observation, and μ is the probability with which the Bernoulli observations respond identically. The complement of this probability, $1 - \mu$, is the probability with which the Bernoulli outcomes respond independently. If $\mu = 0$, then the two-component mixture reduces to a standard Binomial model with success probability π . Since both π and μ are involved in the success probabilities of the two Binomial variables in the mixture, you can affect these binomial means by specifying effects in the **PROBMODEL** statement (for the π s) or the **MODEL** statement (for the μ s). In a “straight” two-component Binomial mixture,

$$\pi \text{Binomial}(n, \mu_1) + (1 - \pi) \text{Binomial}(n, \mu_2)$$

you would vary the success probabilities μ_1 and μ_2 through the **MODEL** statement.

With the FMM procedure, you can fit the beta-binomial model by specifying **DIST=BETABIN** and the binomial cluster model by specifying **DIST=BINOMCLUS** in the **MODEL** statement.

Morel and Neerchal (1997) report data from a completely randomized design that studies the teratogenicity of phenytoin in 81 pregnant mice. The treatment structure of the experiment is an augmented factorial. In addition to an untreated control, mice received 60 mg/kg of phenytoin (PHT), 100 mg/kg of trichloropropene oxide (TCPO), and their combination. The design was augmented with a control group that was treated with water. As in Morel and Neerchal (1997), the two control groups are combined here into a single group.

The following **DATA** step creates the data for this analysis as displayed in Table 1 of Morel and Neerchal (1997). The second **DATA** step creates continuous variables x_1 – x_3 to match the parameterization of these authors.

```
data ossi;
  length tx $8;
  input tx$ n @@;
  do i=1 to n;
    input y m @@;
    output;
  end;
  drop i;
  datalines;
Control 18 8 8 9 9 7 9 0 5 3 3 5 8 9 10 5 8 5 8 1 6 0 5
          8 8 9 10 5 5 4 7 9 10 6 6 3 5
```

```

Control  17 8 9 7 10 10 10 1  6 6  6 1 9 8  9 6 7 5 5 7 9
          2 5 5  6  2  8 1  8 0  2 7 8 5  7
PHT      19 1 9 4  9  3  7 4  7 0  7 0 4 1  8 1 7 2 7 2 8 1 7
          0 2 3 10  3  7 2  7 0  8 0 8 1 10 1 1
TCPO     16 0 5 7 10  4  4 8 11 6 10 6 9 3  4 2 8 0 6 0 9
          3 6 2  9  7  9 1 10 8  8 6 9
PHT+TCPO 11 2 2 0  7  1  8 7  8 0 10 0 4 0  6 0 7 6 6 1 6 1 7
;

```

```

data ossi;
  set ossi;
  array xx{3} x1-x3;
  do i=1 to 3; xx{i}=0; end;
  pht = 0;
  tcpo = 0;
  if (tx='TCPO') then do;
    xx{1} = 1;
    tcpo = 100;
  end; else if (tx='PHT') then do;
    xx{2} = 1;
    pht = 60;
  end; else if (tx='PHT+TCPO') then do;
    pht = 60;
    tcpo = 100;
    xx{1} = 1; xx{2} = 1; xx{3}=1;
  end;
run;

```

The FMM procedure models the mean parameters μ through the **MODEL** statement and the mixing proportions π through the **PROBMODEL** statement. In the binomial cluster model, you can place a regression structure on either set of probabilities, and the regression structure does not need to be the same. In the following statements, the unconditional probability of ossification is modeled as a two-way factorial, whereas the intralitter effect—the propensity to group within a cluster—is assumed to be constant:

```

proc fmm data=ossi;
  class pht tcpo;
  model y/m = / dist=binomcluster;
  probmodel pht tcpo pht*tcpo;
run;

```

The **CLASS** statement declares the PHT and TCPO variables as classification variables. They affect the analysis through their levels, not through their numeric values. The **MODEL** statement declares the distribution of the data to follow a binomial cluster model. The FMM procedure then automatically assumes that the model is a two-component mixture. An intercept is included by default. The **PROBMODEL** statement declares the effect structure for the mixing probabilities. The unconditional probability of ossification of a fetus depends on the main effects and the interaction in the factorial.

The “Model Information” table displays important details about the model fit with the FMM procedure (Output 37.1.1). Although no **K=** option was specified in the **MODEL** statement, the FMM procedure recognizes the model as a two-component model. The “Class Level Information” table displays the levels and values of the PHT and TCPO variables. Eighty-one observations are read from the data and are used in the analysis. These observations comprise 287 events and 585 total outcomes.

Output 37.1.1 Model Information in Binomial Cluster Model with Constant Clustering Probability

The FMM Procedure		
Model Information		
Data Set		WORK.OSSI
Response Variable (Events)		y
Response Variable (Trials)		m
Type of Model		Binomial Cluster
Distribution		Binomial Cluster
Components		2
Link Function		Logit
Estimation Method		Maximum Likelihood
Class Level Information		
Class	Levels	Values
pht	2	0 60
tcpo	2	0 100
Number of Observations Read		81
Number of Observations Used		81
Number of Events		287
Number of Trials		585

The “Optimization Information” table in [Output 37.1.2](#) gives details about the maximum likelihood optimization. By default, the FMM procedure uses a quasi-Newton algorithm. The model contains five parameters, four of which are part of the model for the mixing probabilities. The fifth parameter is the intercept in the model for μ .

Output 37.1.2 Optimization in Binomial Cluster Model with Constant Clustering Probability

Optimization Information	
Optimization Technique	Dual Quasi-Newton
Parameters in Optimization	5
Mean Function Parameters	1
Scale Parameters	0
Mixing Prob Parameters	4
Number of Threads	2

Output 37.1.2 *continued*

Iteration History				
Iteration	Evaluations	Objective Function	Change	Max Gradient
0	5	174.92723892	.	43.78769
1	2	154.13180744	20.79543149	11.2346
2	3	153.26693611	0.86487133	6.888215
3	2	152.84974281	0.41719329	3.541977
4	3	152.61756033	0.23218248	2.783556
5	3	152.54795303	0.06960730	1.146807
6	3	152.52684929	0.02110374	0.034367
7	3	152.52671214	0.00013715	0.011511
8	3	152.52670799	0.00000415	0.000202
9	3	152.52670799	0.00000000	4.001E-6

Convergence criterion (GCONV=1E-8) satisfied.

Fit Statistics	
-2 Log Likelihood	305.1
AIC (smaller is better)	315.1
AICC (smaller is better)	315.9
BIC (smaller is better)	327.0
Pearson Statistic	89.2077
Effective Parameters	5
Effective Components	2

After nine iterations, the iterative optimization converges. The -2 log likelihood at the converged solution is 305.1, and the Pearson statistic is 89.2077. The FMM procedure computes the Pearson statistic as a general goodness-of-fit measure that expresses the closeness of the fitted model to the data.

The estimates of the parameters in the conditional probability μ and in the unconditional probability π are given in Output 37.1.3. The intercept estimate in the model for μ is 0.3356. Since the default link in the binomial cluster model is the logit link, the estimate of the conditional probability is

$$\hat{\mu} = \frac{1}{1 + \exp\{-0.3356\}} = 0.5831$$

This value is displayed in the “Inverse Linked Estimate” column. There is greater than a 50% chance that the individual fetuses in a litter provide the same response. The clustering tendency is substantial.

Output 37.1.3 Parameter Estimates in Binomial Cluster Model with Constant Clustering Probability

Parameter Estimates for 'Binomial Cluster' Model						
Component	Effect	Estimate	Standard Error	z Value	Pr > z	Inverse Linked Estimate
1	Intercept	0.3356	0.1714	1.96	0.0503	0.5831

Parameter Estimates for Mixing Probabilities						
Effect	pht	tcpo	Estimate	Standard Error	z Value	Pr > z
Intercept			-1.2194	0.4690	-2.60	0.0093
pht	0		0.9129	0.5608	1.63	0.1036
pht	60		0	.	.	.
tcpo		0	0.3295	0.5534	0.60	0.5516
tcpo		100	0	.	.	.
pht*tcpo	0	0	0.6162	0.6678	0.92	0.3561
pht*tcpo	0	100	0	.	.	.
pht*tcpo	60	0	0	.	.	.
pht*tcpo	60	100	0	.	.	.

The “Mixing Probabilities” table displays the estimates of the parameters in the model for π on the logit scale (Output 37.1.3). Table 37.11 constructs the estimates of the unconditional probabilities of ossification.

Table 37.11 Estimates of Ossification Probabilities

PHT	TCPO	$\hat{\eta}$	$\hat{\pi}$
0	0	$-1.2194 + 0.9129 + 0.3295 + 0.6162 = 0.6392$	0.6546
60	0	$-1.2194 + 0.3295 = -0.8899$	0.2911
0	100	$-1.2194 + 0.9129 = -0.3065$	0.4240
60	100	-1.2194	0.2280

Morel and Neerchal (1997) considered a model in which the intralitter effects also depend on the treatments. This model is fit with the FMM procedure with the following statements:

```
proc fmm data=ossi;
  class pht tcpo;
  model y/m = pht tcpo pht*tcpo / dist=binomcluster;
  probmodel pht tcpo pht*tcpo;
run;
```

The -2 log likelihood of this model is much reduced compared to the previous model with constant conditional probability (compare 287.8 in Output 37.1.4 with 305.1 in Output 37.1.2). The likelihood-ratio statistic of 17.3 is significant, $\Pr(\chi^2_3 > 17.3 = 0.0006)$. Varying the conditional probabilities by treatment improved the model fit significantly.

Output 37.1.4 Fit Statistics and Parameter Estimates in Binomial Cluster Model

The FMM Procedure							
Fit Statistics							
		-2 Log Likelihood		287.8			
		AIC (smaller is better)		303.8			
		AICC (smaller is better)		305.8			
		BIC (smaller is better)		323.0			
		Pearson Statistic		85.5998			
		Effective Parameters		8			
		Effective Components		2			
Parameter Estimates for 'Binomial Cluster' Model							
Component	Effect	pht	tcpo	Estimate	Standard Error	z Value	Pr > z
1	Intercept			1.8213	0.5889	3.09	0.0020
1	pht	0		-1.4962	0.6630	-2.26	0.0240
1	pht	60		0	.	.	.
1	tcpo		0	-3.1828	1.1261	-2.83	0.0047
1	tcpo		100	0	.	.	.
1	pht*tcpo	0	0	3.3736	1.1953	2.82	0.0048
1	pht*tcpo	0	100	0	.	.	.
1	pht*tcpo	60	0	0	.	.	.
1	pht*tcpo	60	100	0	.	.	.
Parameter Estimates for Mixing Probabilities							
Effect	pht	tcpo	Estimate	Standard Error	z Value	Pr > z	
Intercept			-0.7394	0.5395	-1.37	0.1705	
pht	0		0.4351	0.6203	0.70	0.4830	
pht	60		0	.	.	.	
tcpo		0	-0.5342	0.5893	-0.91	0.3646	
tcpo		100	0	.	.	.	
pht*tcpo	0	0	1.4055	0.7080	1.99	0.0471	
pht*tcpo	0	100	0	.	.	.	
pht*tcpo	60	0	0	.	.	.	
pht*tcpo	60	100	0	.	.	.	

Table 37.12 computes the conditional probabilities in the four treatment groups. Recall that the previous model estimated a constant clustering probability of 0.5831.

Table 37.12 Estimates of Clustering Probabilities

PHT	TCPO	$\hat{\eta}$	$\hat{\mu}$
0	0	$1.8213 - 1.4962 - 3.1828 + 3.3736 = 0.5159$	0.6262
60	0	$1.8213 - 3.1828 = -1.3615$	0.2040
0	100	$1.8213 - 1.4962 = 0.3251$	0.5806
60	100	1.8213	0.8607

The presence of phenytoin alone reduces the probability of response clustering within the litter. The presence of trichloropropene oxide alone does not have a strong effect on the clustering. The simultaneous presence of both agents substantially increases the probability of clustering.

The following statements fit the binomial cluster model in the parameterization of Morel and Neerchal (1997).

```
proc fmm data=ossi;
  model y/m = x1-x3 / dist=binomcluster;
  probmodel x1-x3;
run;
```

The model fit is the same as in the previous model (compare the “Fit Statistics” tables in [Output 37.1.5](#) and [Output 37.1.4](#)). The parameter estimates change due to the reparameterization of the treatment effects and match the results in Table III of Morel and Neerchal (1997).

Output 37.1.5 Fit Statistics and Estimates (Morel and Neerchal Parameterization)

The FMM Procedure					
Fit Statistics					
		-2 Log Likelihood			287.8
		AIC (smaller is better)			303.8
		AICC (smaller is better)			305.8
		BIC (smaller is better)			323.0
		Pearson Statistic			85.5999
		Effective Parameters			8
		Effective Components			2
Parameter Estimates for 'Binomial Cluster' Model					
Component	Effect	Estimate	Standard Error	z Value	Pr > z
1	Intercept	0.5159	0.2603	1.98	0.0475
1	x1	-0.1908	0.4006	-0.48	0.6339
1	x2	-1.8774	0.9946	-1.89	0.0591
1	x3	3.3736	1.1953	2.82	0.0048

Output 37.1.5 *continued*

Parameter Estimates for Mixing Probabilities				
Effect	Estimate	Standard Error	z Value	Pr > z
Intercept	0.5669	0.2455	2.31	0.0209
x1	-0.8712	0.3924	-2.22	0.0264
x2	-1.8405	0.3413	-5.39	<.0001
x3	1.4055	0.7080	1.99	0.0471

The following sets of statements fit the binomial and beta-binomial models, respectively, as single-component mixtures in the parameterization akin to the first binomial cluster model. Note that the model effects that affect the underlying Bernoulli success probabilities are specified in the **MODEL** statement, in contrast to the binomial cluster model.

```
proc fmm data=ossi;
  model y/m = x1-x3 / dist=binomial;
run;

proc fmm data=ossi;
  model y/m = x1-x3 / dist=betabinomial;
run;
```

The Pearson statistic for the beta-binomial model (Output 37.1.6) indicates a much better fit compared to the single-component binomial model (Output 37.1.7). This is not surprising since these data are obviously overdispersed relative to a binomial model because the Bernoulli outcomes are not independent. The difference between the binomial cluster and the beta-binomial model lies in the mechanism by which the correlations are induced:

- a mixing mechanism in the beta-binomial model that leads to a common shared random effect among all offspring in a cluster
- a mixture specification in the binomial cluster model that divides the offspring in a litter into identical and independent responders

Output 37.1.6 Fit Statistics in Binomial Model

The FMM Procedure	
Fit Statistics	
-2 Log Likelihood	401.8
AIC (smaller is better)	409.8
AICC (smaller is better)	410.3
BIC (smaller is better)	419.4
Pearson Statistic	252.1

Output 37.1.7 Fit Statistics in Beta-Binomial Model

The FMM Procedure	
Fit Statistics	
-2 Log Likelihood	306.6
AIC (smaller is better)	316.6
AICC (smaller is better)	317.4
BIC (smaller is better)	328.5
Pearson Statistic	87.5379

Example 37.2: The Usefulness of Custom Starting Values: When Do Cows Eat?

This example with a mixture of normal and Weibull distributions illustrates the benefits of specifying starting values for some of the components.

The data for this example were generously provided by Dr. Luciano A. Gonzalez of the Lethbridge Research Centre of Agriculture and Agri-Food Canada and his collaborator, Dr. Bert Tolcamp, from the Scottish Agricultural College.

The outcome variable of interest is the logarithm of a time interval between consecutive visits by cattle to feeders. The intervals fall into three categories:

- short breaks within meals—such as when an animal stops eating for a moment and resumes shortly thereafter
- somewhat longer breaks when eating is interrupted to go have a drink of water
- long breaks between meals

Modeling such time interval data is important to understand the feeding behavior and biology of the animals and to derive other biological parameters such as the probability of an animal to stop eating after it has consumed a certain amount of a given food. Because there are three distinct biological categories, data of this nature are frequently modeled as three-component mixtures. The point at which the second and third components cross over is used to separate feeding events into meals.

The original data set comprises 141,414 observations of log feeding intervals. For the purpose of presentation in this document, where space is limited, the data have been rounded to precision 0.05 and grouped by frequency. The following DATA step displays the modified data used in this example. A comparison with the raw data and the results obtained in a full analysis of the original data show that the grouping does not alter the presentation or conclusions in a way that matters for the purpose of this example.

```

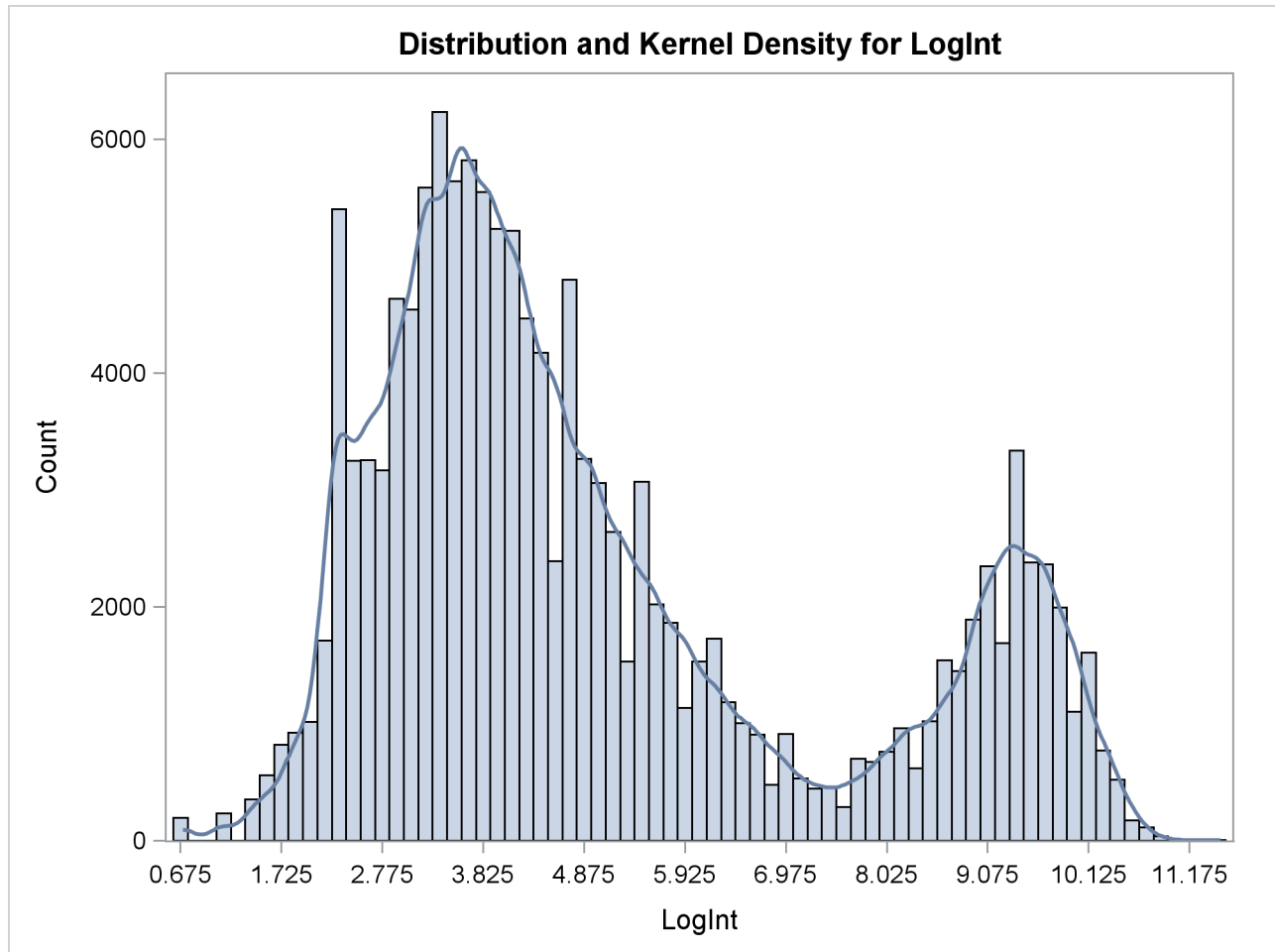
data cattle;
  input LogInt Count @@;
  datalines;
0.70 195 1.10 233 1.40 355 1.60 563
1.80 822 1.95 926 2.10 1018 2.20 1712
2.30 3190 2.40 2212 2.50 1692 2.55 1558
2.65 1622 2.70 1637 2.75 1568 2.85 1599
2.90 1575 2.95 1526 3.00 1537 3.05 1561
3.10 1555 3.15 1427 3.20 2852 3.25 1396
3.30 1343 3.35 2473 3.40 1310 3.45 2453
3.50 1168 3.55 2300 3.60 2174 3.65 2050
3.70 1926 3.75 1849 3.80 1687 3.85 2416
3.90 1449 3.95 2095 4.00 1278 4.05 1864
4.10 1672 4.15 2104 4.20 1443 4.25 1341
4.30 1685 4.35 1445 4.40 1369 4.45 1284
4.50 1523 4.55 1367 4.60 1027 4.65 1491
4.70 1057 4.75 1155 4.80 1095 4.85 1019
4.90 1158 4.95 1088 5.00 1075 5.05 912
5.10 1073 5.15 803 5.20 924 5.25 916
5.30 784 5.35 751 5.40 766 5.45 833
5.50 748 5.55 725 5.60 674 5.65 690
5.70 659 5.75 695 5.80 529 5.85 639
5.90 580 5.95 557 6.00 524 6.05 473
6.10 538 6.15 444 6.20 456 6.25 453
6.30 374 6.35 406 6.40 409 6.45 371
6.50 320 6.55 334 6.60 353 6.65 305
6.70 302 6.75 301 6.80 263 6.85 218
6.90 255 6.95 240 7.00 219 7.05 202
7.10 192 7.15 180 7.20 162 7.25 126
7.30 148 7.35 173 7.40 142 7.45 163
7.50 152 7.55 149 7.60 139 7.65 161
7.70 174 7.75 179 7.80 188 7.85 239
7.90 225 7.95 213 8.00 235 8.05 256
8.10 272 8.15 290 8.20 320 8.25 355
8.30 307 8.35 311 8.40 317 8.45 335
8.50 369 8.55 365 8.60 365 8.65 396
8.70 419 8.75 467 8.80 468 8.85 515
8.90 558 8.95 623 9.00 712 9.05 716
9.10 829 9.15 803 9.20 834 9.25 856
9.30 838 9.35 842 9.40 826 9.45 834
9.50 798 9.55 801 9.60 780 9.65 849
9.70 779 9.75 737 9.80 683 9.85 686
9.90 626 9.95 582 10.00 522 10.05 450
10.10 443 10.15 375 10.20 342 10.25 285
10.30 254 10.35 231 10.40 195 10.45 186
10.50 143 10.55 100 10.60 73 10.65 49
10.70 28 10.75 36 10.80 16 10.85 9
10.90 5 10.95 6 11.00 4 11.05 1
11.15 1 11.25 4 11.30 2 11.35 5
11.40 4 11.45 3 11.50 1
;

```


If you scan the columns for the Count variable in the DATA step, the prevalence of values between 2 and 5 units of LogInt is apparent, as is a long right tail. To explore these data graphically, the following statements produce a histogram of the data and a kernel density estimate of the density of the LogInt variable.

```
ods graphics on;
proc kde data=cattle;
  univar LogInt / bwm=4;
  freq count;
run;
```

Output 37.2.1 Histogram and Kernel Density for LogInt



Two modes are clearly visible in [Output 37.2.1](#). Given the biological background, one would expect that three components contribute to the mixture. The histogram would suggest either a two-component mixture with modes near 4 and 9, or a three-component mixture with modes near 3, 5, and 9.

Following Dr. Gonzalez' suggestion, the process is modeled as a three-component mixture of two normal distributions and a Weibull distribution. The Weibull distribution is chosen because it can have long left and right tails and it is popular in modeling data that relate to time intervals.

```

proc fmm data=cattle gconv=0;
  model LogInt = / dist=normal k=2 parms(3 1, 5 1);
  model      + / dist=weibull;
  freq count;
run;

```

The `GCONV=` convergence criterion is turned off in this PROC FMM run to avoid the early stoppage of the iterations when the relative gradient changes little between iterations. Turning the criterion off usually ensures that convergence is achieved with a small absolute gradient of the objective function. The `PARMS` option in the first `MODEL` statement provides starting values for the means and variances for the parameters of the normal distributions. The means for the two components are started at $\mu = 3$ and $\mu = 5$, respectively. Specifying starting values is generally not necessary. However, the choice of starting values can play an important role in modeling finite mixture models; the importance of the choice of starting values in this example is discussed further below.

The “Model Information” table shows that the model is a three-component mixture and that the FMM procedure considers the estimation of a density to be the purpose of modeling. The procedure draws this conclusion from the absence of effects in the `MODEL` statements. There are 187 observations in the data set, but these actually represent 141,414 measurements (Output 37.2.2).

Output 37.2.2 Model Information and Number of Observations

The FMM Procedure	
Model Information	
Data Set	WORK.CATTLE
Response Variable	LogInt
Frequency Variable	Count
Type of Model	Density Estimation
Components	3
Estimation Method	Maximum Likelihood
Number of Observations Read	187
Number of Observations Used	187
Sum of Frequencies Read	141414
Sum of Frequencies Used	141414

There are eight parameters in the optimization: the means and variances of the two normal distributions, the μ and ϕ parameter of the Weibull distribution, and the two mixing probabilities (Output 37.2.3). At the converged solution, the $-2 \log$ likelihood is 563,153 and all parameters and components are effective—that is, the model is not overspecified in the sense that components have collapsed during the model fitting. The Pearson statistic is close to the number of observations in the data set, indicating a good fit.

Output 37.2.3 Optimization Information and Fit Statistics

Optimization Information	
Optimization Technique	Dual Quasi-Newton
Parameters in Optimization	8
Mean Function Parameters	3
Scale Parameters	3
Mixing Prob Parameters	2
Lower Boundaries	3
Upper Boundaries	0
Number of Threads	2

Fit Statistics	
-2 Log Likelihood	563153
AIC (smaller is better)	563169
AICC (smaller is better)	563169
BIC (smaller is better)	563248
Pearson Statistic	141458
Effective Parameters	8
Effective Components	3

Output 37.2.4 displays the parameter estimates for the three models and for the mixing probabilities. The order in which the “Parameter Estimates” tables appear in the output corresponds to the order in which the MODEL statements were specified.

Output 37.2.4 Optimization Information and Fit Statistics

Parameter Estimates for 'Normal' Model					
Component	Parameter	Estimate	Standard Error	z Value	Pr > z
1	Intercept	3.3415	0.01260	265.16	<.0001
2	Intercept	4.8940	0.05447	89.84	<.0001
1	Variance	0.6718	0.01287		
2	Variance	1.4497	0.05247		

Parameter Estimates for 'Weibull' Model						
Component	Parameter	Estimate	Standard Error	z Value	Pr > z	Inverse Linked Estimate
3	Intercept	2.2531	0.000506	4452.11	<.0001	9.5174
3	Scale	0.06848	0.000427			

Output 37.2.4 continued

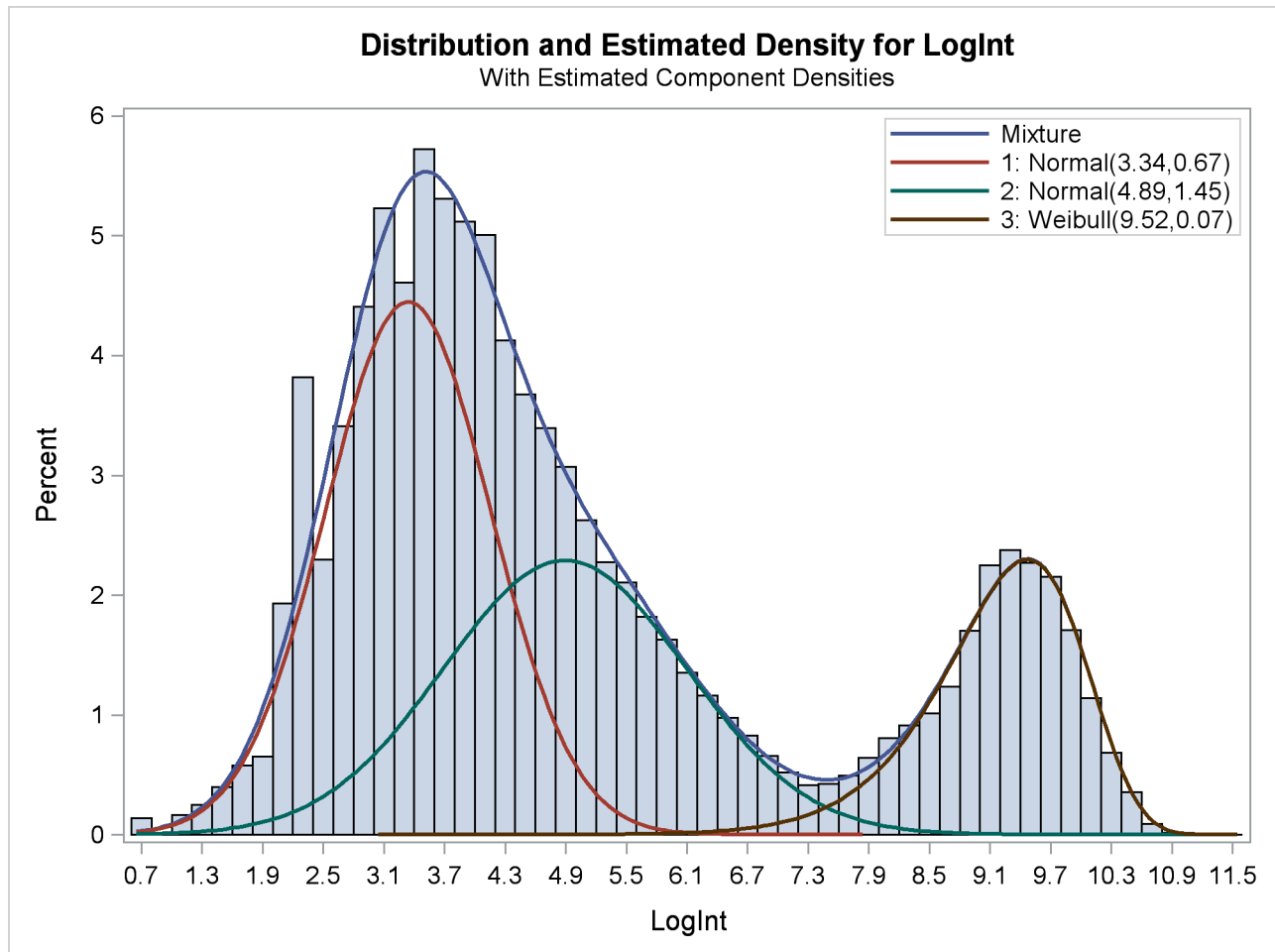
Parameter Estimates for Mixing Probabilities						
Component	Parameter	Estimate	-----Linked Scale-----		Pr > z	Probability
			Standard Error	z Value		
1	Probability	0.8106	0.03409	23.78	<.0001	0.4545
2	Probability	0.5305	0.04640	11.43	<.0001	0.3435

The estimated means of the two normal components are 3.3415 and 4.8940, respectively. Note that the means are displayed here as Intercept. The inverse linked estimate is not produced because the default link for the normal distribution is the identity link; hence the Estimate column represents the means of the component distributions. The parameter estimates in the Weibull model are $\hat{\beta}_0 = 2.2531$, $\hat{\phi} = 0.06848$, and $\hat{\mu} = \exp\{\hat{\beta}_0\} = 9.5174$. In the Weibull distribution, the μ parameter does not estimate the mean of the distribution, the maximum likelihood estimate of the distribution's mean is $\hat{\mu}\Gamma(\hat{\phi} + 1) = 9.1828$.

The estimated mixing probabilities are $\hat{\pi}_1 = 0.4545$, $\hat{\pi}_2 = 0.3435$, and $\hat{\pi}_3 = 1 - \hat{\pi}_1 - \hat{\pi}_2 = 0.2020$. In other words, the estimated distribution of log feeding intervals is a 45:35:20 mixture of an N(3.3415, 0.6718), a N(4.8940, 1.4497), and a Weibull(9.5174, 0.06848) distribution.

You can obtain a graphical display of the observed and estimated distribution of these data by enabling ODS Graphics. The **PLOTS** option in the **PROC FMM** statement modifies the default density plot by adding the densities of the mixture components:

```
ods select DensityPlot;
proc fmm data=cattle gconv=0;
  model LogInt = / dist=normal k=2 parms(3 1, 5 1);
  model          + / dist=weibull;
  freq count;
run;
```

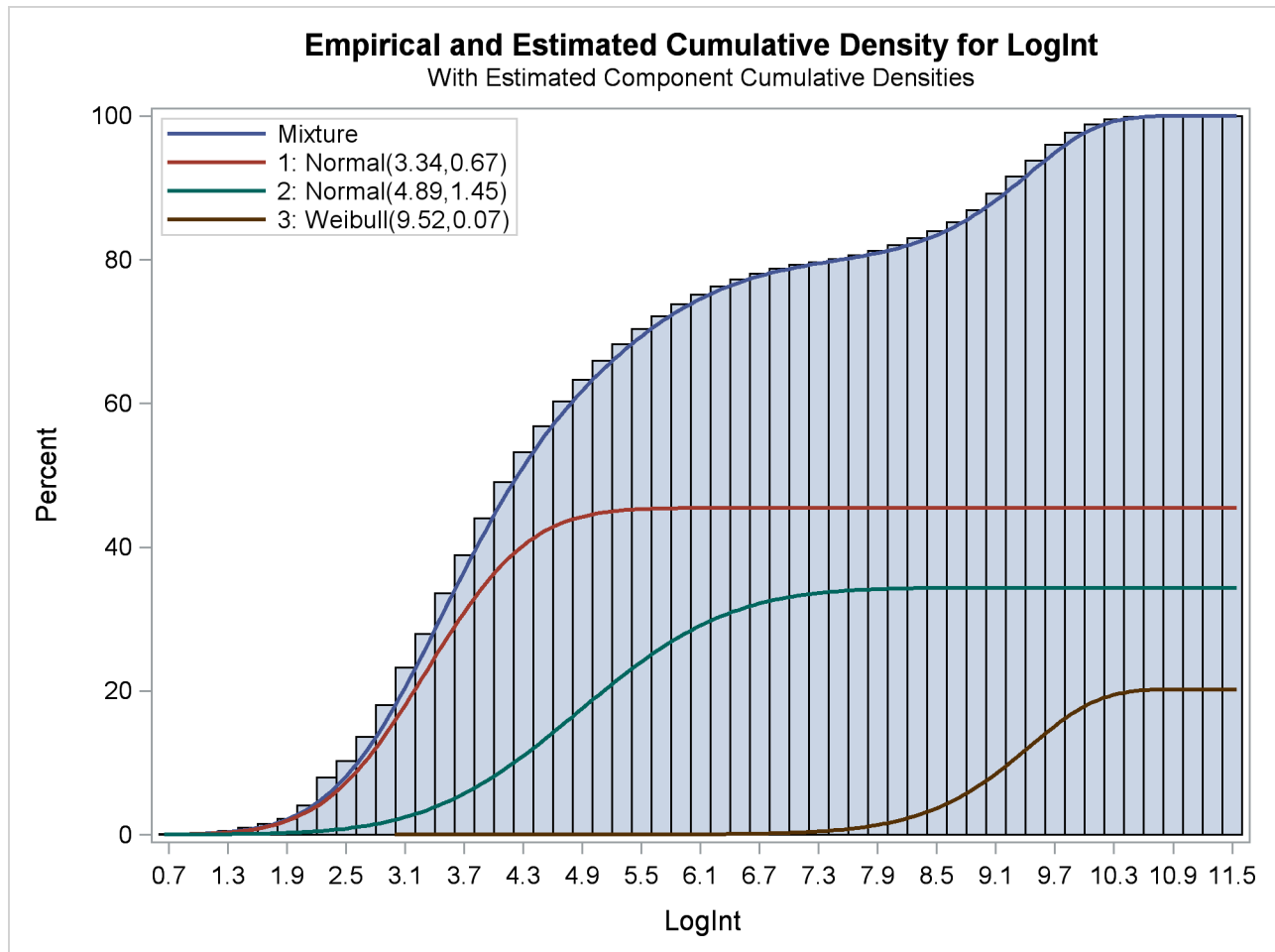
Output 37.2.5 Observed and Estimated Densities in the Three-Component Model

The estimated mixture density matches the histogram of the observed data closely (Output 37.2.5). The component densities are displayed in such a way that, at each point in the support of the LogInt variable, their sum combines to the overall mixture density. The three components in the mixtures are well separated.

The excellent quality of the fit is even more evident when the distributions are displayed cumulatively by adding the CUMULATIVE option in the DENSITY option (Output 37.2.6):

```
ods select DensityPlot;
proc fmm data=cattle plot=density(cumulative) gconv=0;
  model LogInt = / dist=normal k=2 parms(3 1, 5 1);
  model      + / dist=weibull;
  freq count;
run;
```

The component cumulative distribution functions are again scaled so that their sum produces the overall mixture cumulative distribution function. Because of this scaling, the percentage reached at the maximum value of LogInt corresponds to the mixing probabilities in Output 37.2.4.

Output 37.2.6 Observed and Estimated Cumulative Densities in the Three-Component Model

The importance of starting values for the parameter estimates was mentioned previously. Suppose that different starting values are selected for the three components (for example, the default starting values).

```
proc fmm data=cattle gconv=0;
  model LogInt = / dist=normal k=2;
  model      + / dist=weibull;
  freq count;
run;
ods graphics off;
```

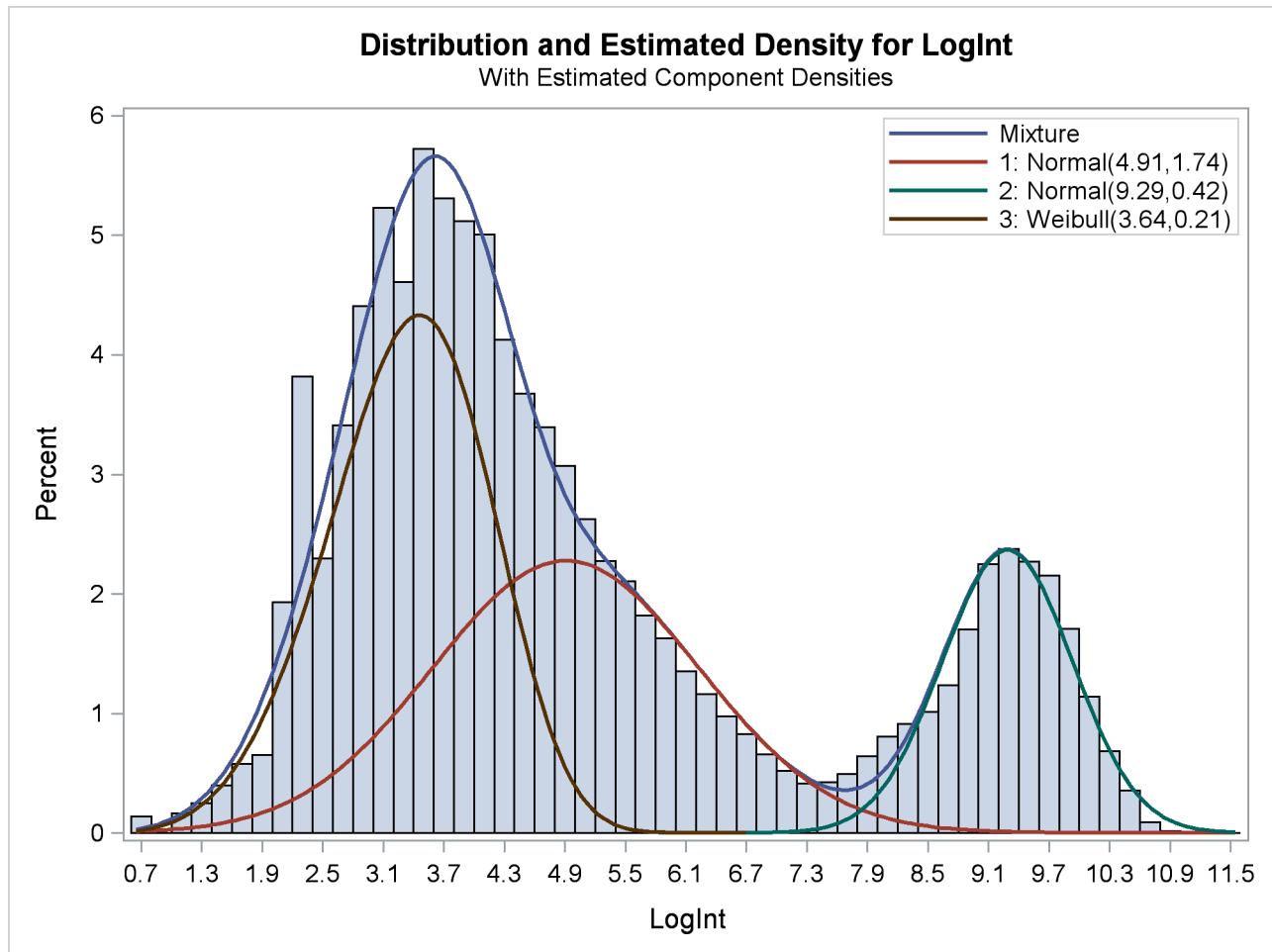
The fit statistics and parameter estimates from this run are displayed in [Output 37.2.7](#), and the density plot is shown in [Output 37.2.8](#).

Output 37.2.7 Fit Statistics and Parameter Estimates

The FMM Procedure						
Fit Statistics						
	-2 Log Likelihood					564431
	AIC (smaller is better)					564447
	AICC (smaller is better)					564447
	BIC (smaller is better)					564526
	Pearson Statistic					141228
	Effective Parameters					8
	Effective Components					3
Parameter Estimates for 'Normal' Model						
Component	Parameter	Estimate	Standard Error	z Value	Pr > z	
1	Intercept	4.9106	0.02604	188.56	<.0001	
2	Intercept	9.2883	0.005031	1846.28	<.0001	
1	Variance	1.7410	0.02753			
2	Variance	0.4158	0.005086			
Parameter Estimates for 'Weibull' Model						
Component	Parameter	Estimate	Standard Error	z Value	Pr > z	Inverse Linked Estimate
3	Intercept	1.2908	0.002790	462.71	<.0001	3.6358
3	Scale	0.2093	0.001311			
Parameter Estimates for Mixing Probabilities						
-----Linked Scale-----						
Component	Parameter	Estimate	Standard Error	z Value	Pr > z	Probability
1	Probability	-0.1505	0.03678	-4.09	<.0001	0.3745
2	Probability	-0.8280	0.01922	-43.08	<.0001	0.1902

All components are active; no collapsing of components occurred. However, a closer look at the “Parameter Estimates” tables in [Output 37.2.7](#) shows an important difference from the tables in [Output 37.2.4](#). The means of the two normal distributions are now 4.9106 and 9.2883. Previously, the means were 3.3415 and 4.8940. The “position” of the Weibull distribution has moved from right to left, and the third component is now modeled by a symmetric normal distribution ([Output 37.2.8](#)). The mixture probabilities have also changed—in particular, for the first and third component.

Output 37.2.8 Three-Component Model with Default Starting Values



Such switching is not uncommon in mixture modeling. As judged by the information criteria, the model in which the Weibull distribution is the component with the smallest mean does not fit the data as well as the first model in which the specification of the starting values guided the optimization towards placing the normal distributions first. The converged solution found in the last FMM run represents a local minimum of the log-likelihood surface. There are other local minima—for example, when components are removed from the model, which is tantamount to estimating the associated mixture probabilities as zero.

Example 37.3: Enforcing Homogeneity Constraints: Count and Dispersion—It Is All Over!

The following example demonstrates how you can use either the `EQUATE=` option in the `MODEL` statement or the `RESTRICT` statement to impose homogeneity constraints on chosen model effects.

The data for this example were presented by Margolin, Kaplan, and Zeiger (1981) and analyzed by various authors applying a number of techniques. The following `DATA` step shows the number of revertant salmonella colonies (variable `num`) at six levels of quinoline dosing (variable `dose`). There are three replicate plates at each dose of quinoline.


```

data assay;
  label dose = 'Dose of quinoline (microg/plate)'
        num = 'Observed number of colonies';
  input dose @;
  logd = log(dose+10);
  do i=1 to 3; input num@; output; end;
  datalines;
  0 15 21 29
 10 16 18 21
 33 16 26 33
100 27 41 60
333 33 38 41
1000 20 27 42
;

```

The basic notion is that the data are overdispersed relative to a Poisson distribution in which the logarithm of the mean count is modeled as a linear regression in dose (in $\mu\text{g}/\text{plate}$) and in the derived variable $\log\{\text{dose} + 10\}$ (Lawless 1987). The log of the expected count of revertants is thus

$$\beta_0 + \beta_1 \text{dose} + \beta_2 \log\{\text{dose} + 10\}$$

The following statements fit a standard Poisson regression model to these data:

```

proc fmm data=assay;
  model num = dose logd / dist=Poisson;
run;

```

The Pearson statistic for this model is rather large compared to the number of degrees of freedom ($18 - 3 = 15$). The ratio $46.2707/15 = 3.08$ indicates an overdispersion problem in the Poisson model (Output 37.3.1).

Output 37.3.1 Result of Fitting Poisson Regression Models

The FMM Procedure	
Number of Observations Read	18
Number of Observations Used	18
Fit Statistics	
-2 Log Likelihood	136.3
AIC (smaller is better)	142.3
AICC (smaller is better)	144.0
BIC (smaller is better)	144.9
Pearson Statistic	46.2707

Output 37.3.1 continued

Parameter Estimates for 'Poisson' Model				
Effect	Estimate	Standard Error	z Value	Pr > z
Intercept	2.1728	0.2184	9.95	<.0001
dose	-0.00101	0.000245	-4.13	<.0001
logd	0.3198	0.05700	5.61	<.0001

Breslow (1984) accounts for overdispersion by including a random effect in the predictor for the log rate and applying a quasi-likelihood technique to estimate the parameters. Wang et al. (1996) examine these data using mixtures of Poisson regression models. They fit several two- and three-component Poisson regression mixtures. Examining the log likelihoods, AIC, and BIC criteria, they eventually settle on a two-component model in which the intercepts vary by category and the regression coefficients are the same. This mixture model can be written as

$$f(y) = \pi \frac{1}{y!} \lambda_1^y \exp\{-\lambda_1\} + (1 - \pi) \frac{1}{y!} \lambda_2^y \exp\{-\lambda_2\}$$

$$\lambda_1 = \exp\{\beta_{01} + \beta_1 \text{dose} + \beta_2 \log\{\text{dose} + 10\}\}$$

$$\lambda_2 = \exp\{\beta_{02} + \beta_1 \text{dose} + \beta_2 \log\{\text{dose} + 10\}\}$$

This model is fit with the FMM procedure with the following statements:

```
proc fmm data=assay;
  model num = dose logd / dist=Poisson k=2
          equate=effects(dose logd);
run;
```

The `EQUATE=` option in the `MODEL` statement places constraints on the optimization and makes the coefficients for `dose` and `logd` homogeneous across components in the model. [Output 37.3.2](#) displays the “Fit Statistics” and parameter estimates in the mixture. The Pearson statistic is drastically reduced compared to the Poisson regression model in [Output 37.3.1](#). With $18 - 5 = 13$ degrees of freedom, the ratio of the Pearson and the degrees of freedom is now $16.1573/13 = 1.2429$. Note that the effective number of parameters was used to compute the degrees of freedom, not the total number of parameters, because of the equality constraints.

Output 37.3.2 Result for Two-Component Poisson Regression Mixture

The FMM Procedure					
Fit Statistics					
	-2 Log Likelihood				121.8
	AIC (smaller is better)				131.8
	AICC (smaller is better)				136.8
	BIC (smaller is better)				136.3
	Pearson Statistic				16.1573
	Effective Parameters				5
	Effective Components				2
Parameter Estimates for 'Poisson' Model					
Component	Effect	Estimate	Standard Error	z Value	Pr > z
1	Intercept	1.9097	0.2654	7.20	<.0001
1	dose	-0.00126	0.000273	-4.62	<.0001
1	logd	0.3639	0.06602	5.51	<.0001
2	Intercept	2.4770	0.2731	9.07	<.0001
2	dose	-0.00126	0.000273	-4.62	<.0001
2	logd	0.3639	0.06602	5.51	<.0001
Parameter Estimates for Mixing Probabilities					
-----Linked Scale-----					
Effect	Estimate	Standard Error	z Value	Pr > z	Probability
Intercept	1.4984	0.6875	2.18	0.0293	0.8173

You could also have used **RESTRICT** statements to impose the homogeneity constraints on the model fit, as shown in the following statements:

```
proc fmm data=assay;
  model num = dose logd / dist=Poisson k=2;
  restrict 'common dose' dose 1, dose -1;
  restrict 'common logd' logd 1, logd -1;
run;
```

The first **RESTRICT** statement equates the coefficients for the dose variable in the two components, and the second **RESTRICT** statement accomplishes the same for the coefficients of the logd variable. If the right-hand side of a restriction is not specified, PROC FMM defaults to equating the left-hand side of the restriction to zero. The “Linear Constraints” table in [Output 37.3.3](#) shows that both linear equality constraints are active. The parameter estimates match the previous FMM run.

Output 37.3.3 Result for Two-Component Mixture with RESTRICT Statements

The FMM Procedure					
Linear Constraints at Solution					
Label	k =				Constraint
	1	k = 2			Active
common dose	dose	- dose	=	0	Yes
common logd	logd	- logd	=	0	Yes
Parameter Estimates for 'Poisson' Model					
Component	Effect	Estimate	Standard Error	z Value	Pr > z
1	Intercept	1.9097	0.2654	7.20	<.0001
1	dose	-0.00126	0.000273	-4.62	<.0001
1	logd	0.3639	0.06602	5.51	<.0001
2	Intercept	2.4770	0.2731	9.07	<.0001
2	dose	-0.00126	0.000273	-4.62	<.0001
2	logd	0.3639	0.06602	5.51	<.0001
Parameter Estimates for Mixing Probabilities					
-----Linked Scale-----					
Effect	Estimate	Standard Error	z Value	Pr > z	Probability
Intercept	1.4984	0.6875	2.18	0.0293	0.8173

Wang et al. (1996) note that observation 12 with a revertant colony count of 60 is comparably high. The following statements remove the observation from the analysis and fit their selected model:

```
proc fmm data=assay(where=(num ne 60));
  model num = dose logd / dist=Poisson k=2
          equate=effects(dose logd);
run;
```

Output 37.3.4 Result for Two-Component Model without Outlier

The FMM Procedure					
Fit Statistics					
-2 Log Likelihood					111.5
AIC (smaller is better)					121.5
AICC (smaller is better)					126.9
BIC (smaller is better)					125.6
Pearson Statistic					16.5987
Effective Parameters					5
Effective Components					2
Parameter Estimates for 'Poisson' Model					
Component	Effect	Estimate	Standard Error	z Value	Pr > z
1	Intercept	2.2272	0.3022	7.37	<.0001
1	dose	-0.00065	0.000445	-1.46	0.1440
1	logd	0.2432	0.1045	2.33	0.0199
2	Intercept	2.5477	0.3331	7.65	<.0001
2	dose	-0.00065	0.000445	-1.46	0.1440
2	logd	0.2432	0.1045	2.33	0.0199
Parameter Estimates for Mixing Probabilities					
-----Linked Scale-----					
Effect	Estimate	Standard Error	z Value	Pr > z	Probability
Intercept	0.3134	1.7261	0.18	0.8559	0.5777

The ratio of Pearson Statistic over degrees of freedom (12) is only slightly worse than in the previous model; the loss of 5% of the observations carries a price ([Output 37.3.4](#)). The parameter estimates for the two intercepts are now fairly close. If the intercepts were identical, then the two-component model would collapse to the Poisson regression model:

```
proc fmm data=assay(where=(num ne 60));
  model num = dose logd / dist=Poisson;
run;
```

Output 37.3.5 Result of Fitting Poisson Regression Model without Outlier

The FMM Procedure				
Number of Observations Read				17
Number of Observations Used				17
Fit Statistics				
-2 Log Likelihood				114.1
AIC (smaller is better)				120.1
AICC (smaller is better)				121.9
BIC (smaller is better)				122.5
Pearson Statistic				27.8008
Parameter Estimates for 'Poisson' Model				
Effect	Estimate	Standard Error	z Value	Pr > z
Intercept	2.3164	0.2244	10.32	<.0001
dose	-0.00072	0.000258	-2.78	0.0055
logd	0.2603	0.05996	4.34	<.0001

Compared to the same model applied to the full data, the Pearson statistic is much reduced (compare 46.2707 in [Output 37.3.1](#) to 27.8008 in [Output 37.3.5](#)). The outlier—or *overcount*, if you will—induces at least some of the *overdispersion*.

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Chapter 38

The FREQ Procedure

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Overview: FREQ Procedure

The FREQ procedure produces one-way to n -way frequency and contingency (crosstabulation) tables. For two-way tables, PROC FREQ computes tests and measures of association. For n -way tables, PROC FREQ provides stratified analysis by computing statistics across, as well as within, strata.

For one-way frequency tables, PROC FREQ computes goodness-of-fit tests for equal proportions or specified null proportions. For one-way tables, PROC FREQ also provides confidence limits and tests for binomial proportions, including tests for noninferiority and equivalence.

For contingency tables, PROC FREQ can compute various statistics to examine the relationships between two classification variables. For some pairs of variables, you might want to examine the existence or strength of any association between the variables. To determine if an association exists, chi-square tests are computed. To estimate the strength of an association, PROC FREQ computes measures of association that tend to be close to zero when there is no association and close to the maximum (or minimum) value when there is perfect association. The statistics for contingency tables include the following:

- chi-square tests and measures
- measures of association
- risks (binomial proportions) and risk differences for 2×2 tables
- odds ratios and relative risks for 2×2 tables
- tests for trend
- tests and measures of agreement
- Cochran-Mantel-Haenszel statistics

PROC FREQ computes asymptotic standard errors, confidence intervals, and tests for measures of association and measures of agreement. Exact p -values and confidence intervals are available for many test statistics and measures. PROC FREQ also performs analyses that adjust for any stratification variables by computing statistics across, as well as within, strata for n -way tables. These statistics include Cochran-Mantel-Haenszel statistics and measures of agreement.

In choosing measures of association to use in analyzing a two-way table, you should consider the study design (which indicates whether the row and column variables are dependent or independent), the measurement scale of the variables (nominal, ordinal, or interval), the type of association that each measure is designed to detect, and any assumptions required for valid interpretation of a measure. You should exercise care in selecting measures that are appropriate for your data.

Similar comments apply to the choice and interpretation of test statistics. For example, the Mantel-Haenszel chi-square statistic requires an ordinal scale for both variables and is designed to detect a linear association. The Pearson chi-square, on the other hand, is appropriate for all variables and can detect any kind of association, but it is less powerful for detecting a linear association because its power is dispersed over a greater number of degrees of freedom (except for 2×2 tables).

For more information about selecting the appropriate statistical analyses, see Agresti (2007) and Stokes, Davis, and Koch (2012).

Several SAS procedures produce frequency counts; only PROC FREQ computes chi-square tests for one-way to n -way tables and measures of association and agreement for contingency tables. Other procedures to consider for counting include the TABULATE and UNIVARIATE procedures. When you want to produce contingency tables and tests of association for sample survey data, use PROC SURVEYFREQ. See Chapter 14, “[Introduction to Survey Procedures](#),” for more information. When you want to fit models to categorical data, use a procedure such as CATMOD, GENMOD, GLIMMIX, LOGISTIC, PROBIT, or SURVEYLOGISTIC. See Chapter 8, “[Introduction to Categorical Data Analysis Procedures](#),” for more information.

PROC FREQ uses the Output Delivery System (ODS), a SAS subsystem that provides capabilities for displaying and controlling the output from SAS procedures. ODS enables you to convert any of the output from PROC FREQ into a SAS data set. See the section “[ODS Table Names](#)” on page 2617 for more information.

PROC FREQ uses ODS Graphics to create graphs as part of its output. For general information about ODS Graphics, see Chapter 21, “[Statistical Graphics Using ODS](#).” For specific information about the statistical graphics available with the FREQ procedure, see the PLOTS= option in the TABLES statement and the section “[ODS Graphics](#)” on page 2621.

Getting Started: FREQ Procedure

Frequency Tables and Statistics

The FREQ procedure provides easy access to statistics for testing for association in a crosstabulation table.

In this example, high school students applied for courses in a summer enrichment program; these courses included journalism, art history, statistics, graphic arts, and computer programming. The students accepted were randomly assigned to classes with and without internships in local companies. Table 38.1 contains counts of the students who enrolled in the summer program by gender and whether they were assigned an internship slot.

Table 38.1 Summer Enrichment Data

Gender	Internship	Enrollment		
		Yes	No	Total
boys	yes	35	29	64
boys	no	14	27	41
girls	yes	32	10	42
girls	no	53	23	76

The SAS data set SummerSchool is created by inputting the summer enrichment data as cell count data, or providing the frequency count for each combination of variable values. The following DATA step statements create the SAS data set SummerSchool:

```
data SummerSchool;
  input Gender $ Internship $ Enrollment $ Count @@;
  datalines;
boys yes yes 35   boys yes no 29
boys no yes 14   boys no no 27
girls yes yes 32   girls yes no 10
girls no yes 53   girls no no 23
;
```

The variable Gender takes the values ‘boys’ or ‘girls,’ the variable Internship takes the values ‘yes’ and ‘no,’ and the variable Enrollment takes the values ‘yes’ and ‘no.’ The variable Count contains the number of students that correspond to each combination of data values. The double at sign (@@) indicates that more than one observation is included on a single data line. In this DATA step, two observations are included on each line.

Researchers are interested in whether there is an association between internship status and summer program enrollment. The Pearson chi-square statistic is an appropriate statistic to assess the association in the corresponding 2×2 table. The following PROC FREQ statements specify this analysis.

You specify the table for which you want to compute statistics with the TABLES statement. You specify the statistics you want to compute with options after a slash (/) in the TABLES statement.

```
proc freq data=SummerSchool order=data;
  tables Internship*Enrollment / chisq;
  weight Count;
run;
```

The ORDER= option controls the order in which variable values are displayed in the rows and columns of the table. By default, the values are arranged according to the alphanumeric order of their unformatted values. If you specify ORDER=DATA, the data are displayed in the same order as they occur in the input data set. Here, because ‘yes’ appears before ‘no’ in the data, ‘yes’ appears first in any table. Other options for controlling order include ORDER=FORMATTED, which orders according to the formatted values, and ORDER=FREQUENCY, which orders by descending frequency count.

In the TABLES statement, Internship*Enrollment specifies a table where the rows are internship status and the columns are program enrollment. The CHISQ option requests chi-square statistics for assessing association between these two variables. Because the input data are in cell count form, the WEIGHT statement is required. The WEIGHT statement names the variable Count, which provides the frequency of each combination of data values.

Figure 38.1 presents the crosstabulation of Internship and Enrollment. In each cell, the values printed under the cell count are the table percentage, row percentage, and column percentage, respectively. For example, in the first cell, 63.21 percent of the students offered courses with internships accepted them and 36.79 percent did not.

Figure 38.1 Crosstabulation Table

The FREQ Procedure				
Table of Internship by Enrollment				
Internship	Enrollment			
	yes	no	Total	
yes	67	39	106	
	30.04	17.49	47.53	
	63.21	36.79		
	50.00	43.82		
no	67	50	117	
	30.04	22.42	52.47	
	57.26	42.74		
	50.00	56.18		
Total	134	89	223	
	60.09	39.91	100.00	

Figure 38.2 displays the statistics produced by the CHISQ option. The Pearson chi-square statistic is labeled 'Chi-Square' and has a value of 0.8189 with 1 degree of freedom. The associated p -value is 0.3655, which means that there is no significant evidence of an association between internship status and program enrollment. The other chi-square statistics have similar values and are asymptotically equivalent. The other statistics (phi coefficient, contingency coefficient, and Cramér's V) are measures of association derived from the Pearson chi-square. For Fisher's exact test, the two-sided p -value is 0.4122, which also shows no association between internship status and program enrollment.

Figure 38.2 Statistics Produced with the CHISQ Option

Statistic	DF	Value	Prob
Chi-Square	1	0.8189	0.3655
Likelihood Ratio Chi-Square	1	0.8202	0.3651
Continuity Adj. Chi-Square	1	0.5899	0.4425
Mantel-Haenszel Chi-Square	1	0.8153	0.3666
Phi Coefficient		0.0606	
Contingency Coefficient		0.0605	
Cramer's V		0.0606	
Fisher's Exact Test			

Cell (1,1) Frequency (F)		67	
Left-sided Pr <= F		0.8513	
Right-sided Pr >= F		0.2213	
Table Probability (P)		0.0726	
Two-sided Pr <= P		0.4122	

The analysis, so far, has ignored gender. However, it might be of interest to ask whether program enrollment is associated with internship status after adjusting for gender. You can address this question by doing an analysis of a set of tables (in this case, by analyzing the set consisting of one for boys and one for girls). The Cochran-Mantel-Haenszel (CMH) statistic is appropriate for this situation: it addresses whether rows and columns are associated after controlling for the stratification variable. In this case, you would be stratifying by gender.

The PROC FREQ statements for this analysis are very similar to those for the first analysis, except that there is a third variable, Gender, in the TABLES statement. When you cross more than two variables, the two rightmost variables construct the rows and columns of the table, respectively, and the leftmost variables determine the stratification.

The following PROC FREQ statements also request frequency plots for the crosstabulation tables. PROC FREQ produces these plots by using ODS Graphics to create graphs as part of the procedure output. ODS Graphics must be enabled before producing plots. The PLOTS(ONLY)=FREQPLOT option requests frequency plots. The TWOWAY=CLUSTER *plot-option* specifies a cluster layout for the two-way frequency plots.

```
ods graphics on;
proc freq data=SummerSchool;
  tables Gender*Internship*Enrollment /
         chisq cmh plots(only)=freqplot(twoway=cluster);
  weight Count;
run;
ods graphics off;
```

This execution of PROC FREQ first produces two individual crosstabulation tables of Internship by Enrollment: one for boys and one for girls. Frequency plots and chi-square statistics are produced for each individual table. Figure 38.3, Figure 38.4, and Figure 38.5 show the results for boys. Note that the chi-square statistic for boys is significant at the $\alpha = 0.05$ level of significance. Boys offered a course with an internship are more likely to enroll than boys who are not.

Figure 38.4 displays the frequency plot of Internship by Enrollment for boys. By default, frequency plots are displayed as bar charts. You can use PLOTS= options to request dot plots instead of bar charts, to change the orientation of the bars from vertical to horizontal, and to change the scale from frequencies to percents. You can also use PLOTS= options to specify other two-way layouts (stacked, vertical groups, or horizontal groups) and to change the primary grouping from column levels to row levels.

Figure 38.6, Figure 38.7, and Figure 38.8 display the crosstabulation table, frequency plot, and chi-square statistics for girls. You can see that there is no evidence of association between internship offers and program enrollment for girls.

Figure 38.3 Crosstabulation Table for Boys

The FREQ Procedure			
Table 1 of Internship by Enrollment Controlling for Gender=boys			
Internship	Enrollment		
	no	yes	Total
Frequency			
Percent			
Row Pct			
Col Pct			
	no	yes	Total
no	27	14	41
	25.71	13.33	39.05
	65.85	34.15	
	48.21	28.57	
yes	29	35	64
	27.62	33.33	60.95
	45.31	54.69	
	51.79	71.43	
Total	56	49	105
	53.33	46.67	100.00

Figure 38.4 Frequency Plot for Boys

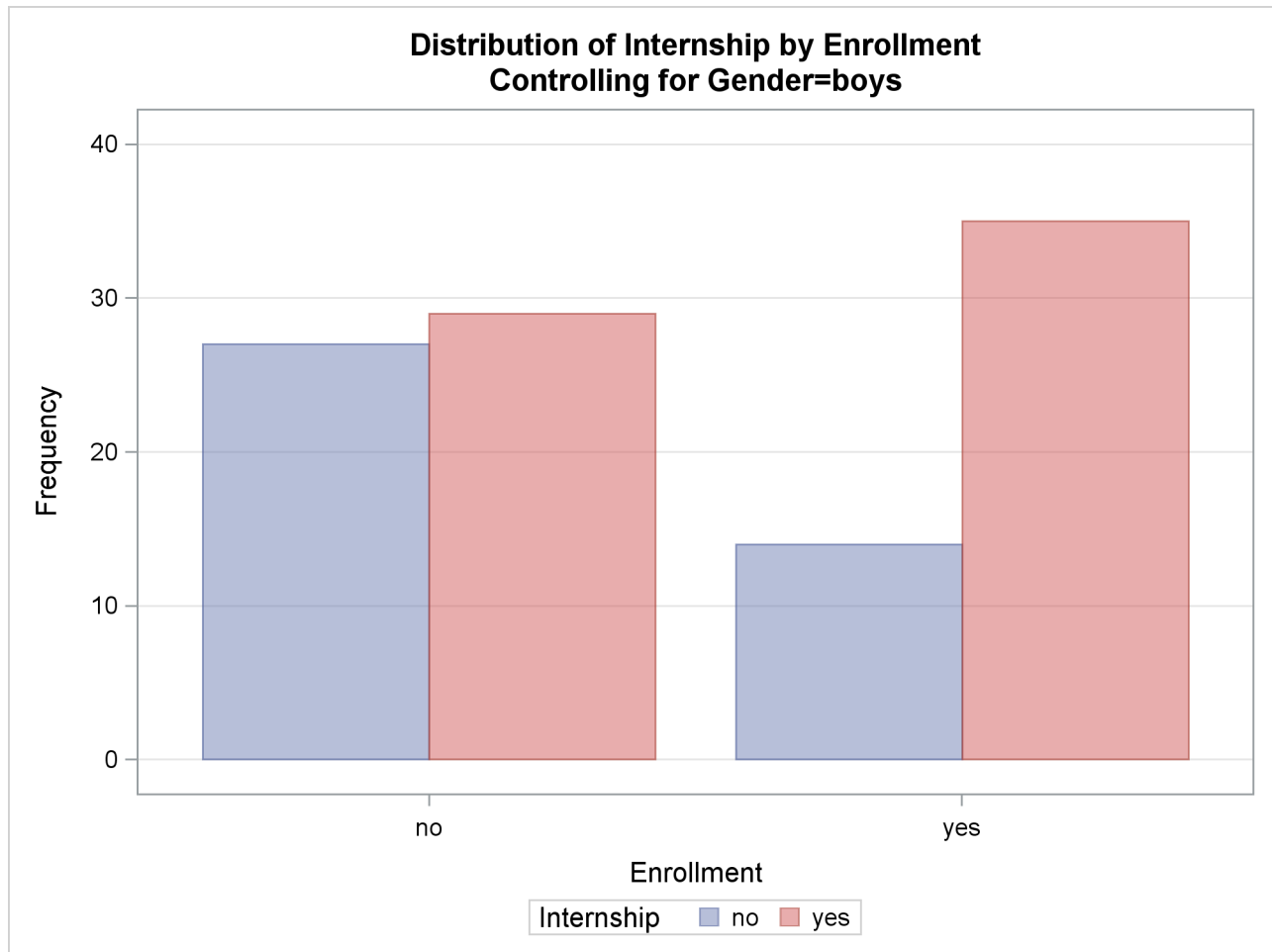


Figure 38.5 Chi-Square Statistics for Boys

Statistic	DF	Value	Prob
Chi-Square	1	4.2366	0.0396
Likelihood Ratio Chi-Square	1	4.2903	0.0383
Continuity Adj. Chi-Square	1	3.4515	0.0632
Mantel-Haenszel Chi-Square	1	4.1963	0.0405
Phi Coefficient		0.2009	
Contingency Coefficient		0.1969	
Cramer's V		0.2009	
Fisher's Exact Test			
Cell (1,1) Frequency (F)		27	
Left-sided Pr <= F		0.9885	
Right-sided Pr >= F		0.0311	
Table Probability (P)		0.0196	
Two-sided Pr <= P		0.0467	

Figure 38.6 Crosstabulation Table for Girls

Internship		Enrollment		
Frequency	Percent	Row Pct	Col Pct	Total
		no	yes	
no		23	53	76
		19.49	44.92	64.41
		30.26	69.74	
		69.70	62.35	
yes		10	32	42
		8.47	27.12	35.59
		23.81	76.19	
		30.30	37.65	
Total		33	85	118
		27.97	72.03	100.00

Figure 38.7 Frequency Plot for Girls

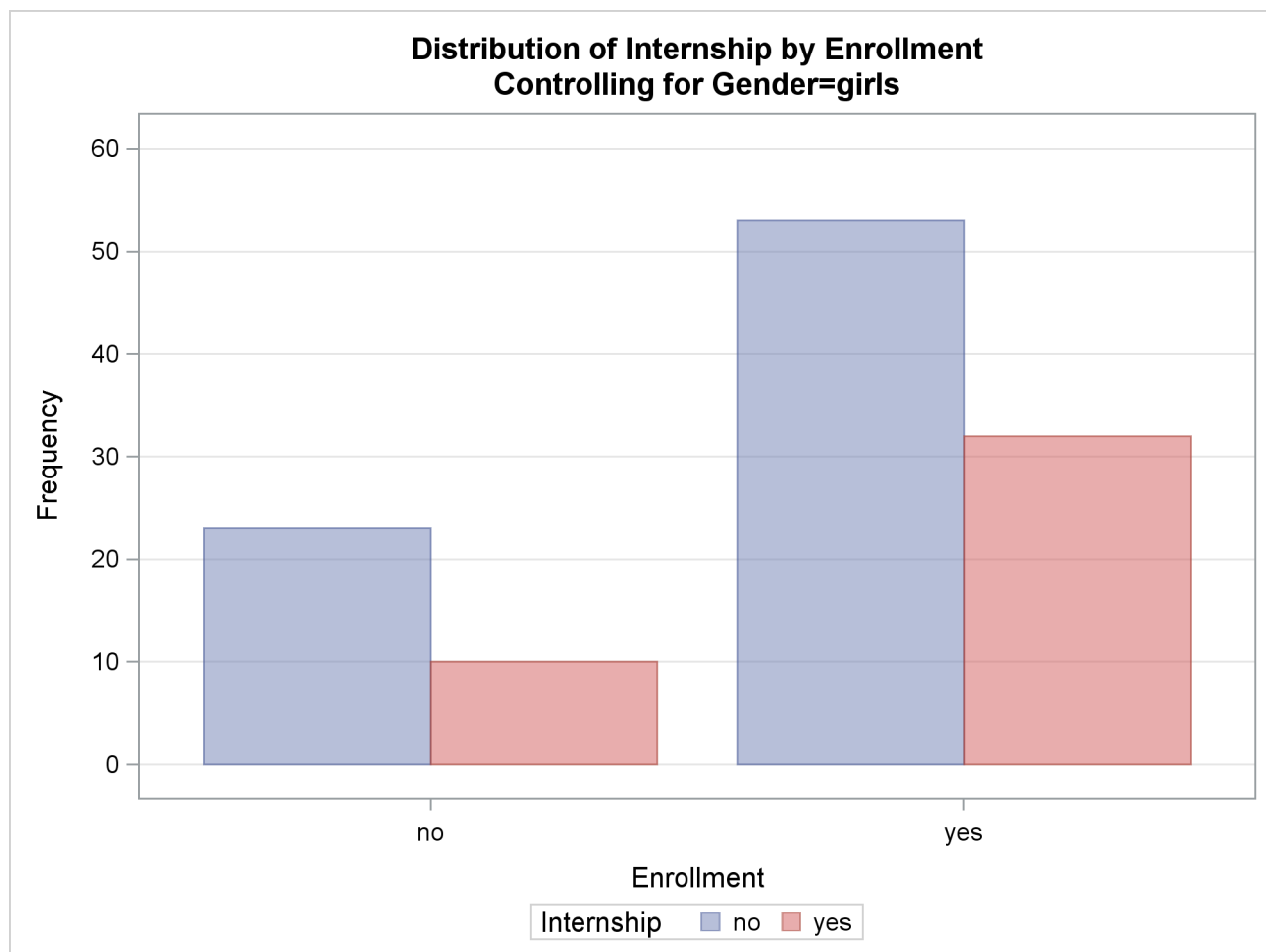


Figure 38.8 Chi-Square Statistics for Girls

Statistic	DF	Value	Prob
Chi-Square	1	0.5593	0.4546
Likelihood Ratio Chi-Square	1	0.5681	0.4510
Continuity Adj. Chi-Square	1	0.2848	0.5936
Mantel-Haenszel Chi-Square	1	0.5545	0.4565
Phi Coefficient		0.0688	
Contingency Coefficient		0.0687	
Cramer's V		0.0688	
Fisher's Exact Test			
Cell (1,1) Frequency (F)		23	
Left-sided Pr <= F		0.8317	
Right-sided Pr >= F		0.2994	
Table Probability (P)		0.1311	
Two-sided Pr <= P		0.5245	

These individual table results demonstrate the occasional problems with combining information into one table and not accounting for information in other variables such as Gender. Figure 38.9 contains the CMH results. There are three summary (CMH) statistics; which one you use depends on whether your rows and/or columns have an order in $r \times c$ tables. However, in the case of 2×2 tables, ordering does not matter and all three statistics take the same value. The CMH statistic follows the chi-square distribution under the hypothesis of no association, and here, it takes the value 4.0186 with 1 degree of freedom. The associated p -value is 0.0450, which indicates a significant association at the $\alpha = 0.05$ level.

Thus, when you adjust for the effect of gender in these data, there is an association between internship and program enrollment. But, if you ignore gender, no association is found. Note that the CMH option also produces other statistics, including estimates and confidence limits for relative risk and odds ratios for 2×2 tables and the Breslow-Day Test. These results are not displayed here.

Figure 38.9 Test for the Hypothesis of No Association

Cochran-Mantel-Haenszel Statistics (Based on Table Scores)				
Statistic	Alternative Hypothesis	DF	Value	Prob
1	Nonzero Correlation	1	4.0186	0.0450
2	Row Mean Scores Differ	1	4.0186	0.0450
3	General Association	1	4.0186	0.0450

Agreement Study

Medical researchers are interested in evaluating the efficacy of a new treatment for a skin condition. Dermatologists from participating clinics were trained to conduct the study and to evaluate the condition. After the training, two dermatologists examined patients with the skin condition from a pilot study and rated the same patients. The possible evaluations are terrible, poor, marginal, and clear. Table 38.2 contains the data.

Table 38.2 Skin Condition Data

Dermatologist 1	Dermatologist 2			
	Terrible	Poor	Marginal	Clear
Terrible	10	4	1	0
Poor	5	10	12	2
Marginal	2	4	12	5
Clear	0	2	6	13

The following DATA step statements create the SAS dataset SkinCondition. The dermatologists' evaluations of the patients are contained in the variables Derm1 and Derm2; the variable Count is the number of patients given a particular pair of ratings.

```
data SkinCondition;
  input Derm1 $ Derm2 $ Count;
  datalines;
  terrible terrible 10
  terrible    poor 4
  terrible marginal 1
  terrible    clear 0
  poor        terrible 5
  poor        poor 10
  poor        marginal 12
  poor        clear 2
  marginal terrible 2
  marginal    poor 4
  marginal marginal 12
  marginal    clear 5
  clear       terrible 0
  clear       poor 2
  clear       marginal 6
  clear       clear 13
  ;
```

The following PROC FREQ statements request an agreement analysis of the skin condition data. In order to evaluate the agreement of the diagnoses (a possible contribution to measurement error in the study), the *kappa coefficient* is computed.

The TABLES statement requests a crosstabulation of the variables Derm1 and Derm2. The AGREE option in the TABLES statement requests the kappa coefficient, together with its standard error and confidence limits. The KAPPA option in the TEST statement requests a test for the null hypothesis that kappa equals zero, or that the agreement is purely by chance. The NOPRINT option in the TABLES statement suppresses the display of the two-way table. The PLOTS= option requests an agreement plot for the two dermatologists. ODS Graphics must be enabled before producing plots.

```
ods graphics on;
proc freq data=SkinCondition order=data;
  tables Derm1*Derm2 /
    agree noprint plots=agreeplot;
  test kappa;
  weight Count;
run;
ods graphics off;
```

Figure 38.10 and Figure 38.11 show the results. The kappa coefficient has the value 0.3449, which indicates some agreement between the dermatologists, and the hypothesis test confirms that you can reject the null hypothesis of no agreement. This conclusion is further supported by the confidence interval of (0.2030, 0.4868), which suggests that the true kappa is greater than zero. The AGREE option also produces Bowker's test for symmetry and the weighted kappa coefficient, but that output is not shown here. Figure 38.11 displays the agreement plot for the ratings of the two dermatologists.

Figure 38.10 Agreement Study

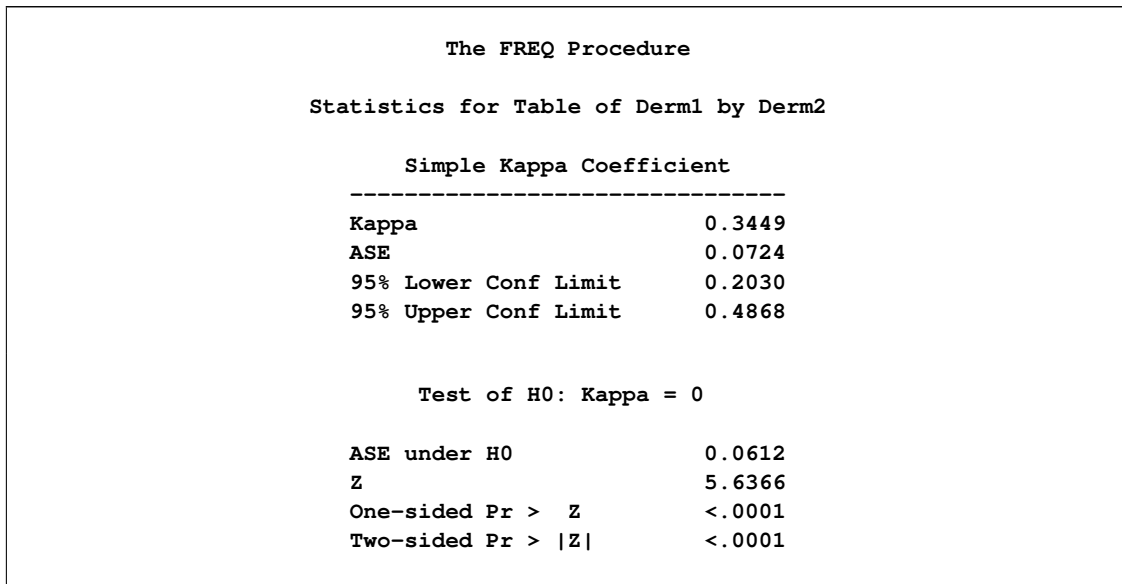
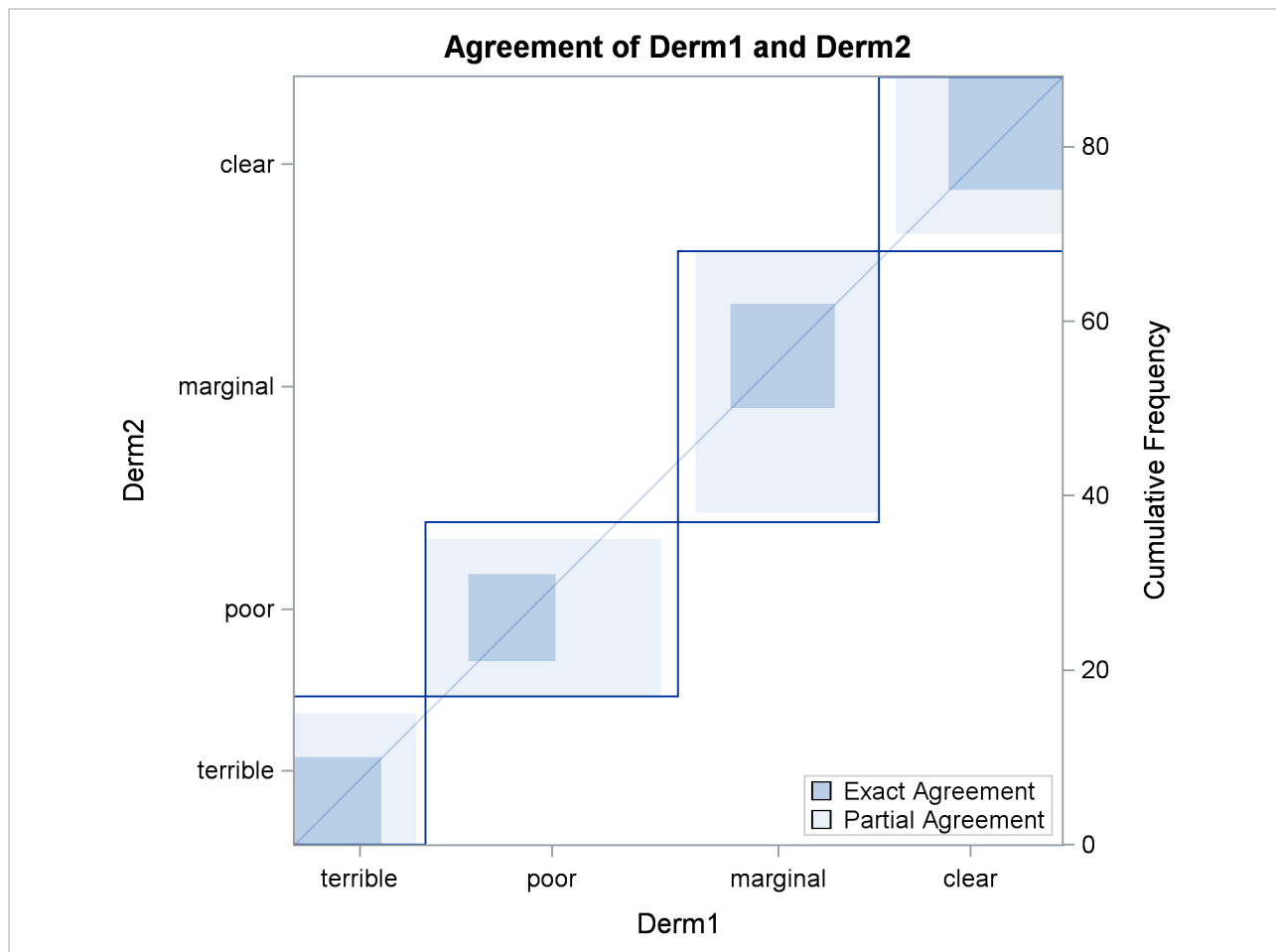


Figure 38.11 Agreement Plot



Syntax: FREQ Procedure

The following statements are available in the FREQ procedure:

```
PROC FREQ < options > ;
  BY variables ;
  EXACT statistic-options < / computation-options > ;
  OUTPUT < OUT=SAS-data-set > output-options ;
  TABLES requests < / options > ;
  TEST options ;
  WEIGHT variable < / option > ;
```

The PROC FREQ statement is the only required statement for the FREQ procedure. If you specify the following statements, PROC FREQ produces a one-way frequency table for each variable in the most recently created data set.

```
proc freq;
run;
```

The rest of this section gives detailed syntax information for the BY, EXACT, OUTPUT, TABLES, TEST, and WEIGHT statements in alphabetical order after the description of the PROC FREQ statement. Table 38.3 summarizes the basic function of each PROC FREQ statement.

Table 38.3 Summary of PROC FREQ Statements

Statement	Description
BY	Provides separate analyses for each BY group
EXACT	Requests exact tests
OUTPUT	Requests an output data set
TABLES	Specifies tables and requests analyses
TEST	Requests tests for measures of association and agreement
WEIGHT	Identifies a weight variable

PROC FREQ Statement

```
PROC FREQ < options > ;
```

The PROC FREQ statement invokes the FREQ procedure. Optionally, it also identifies the input data set. By default, the procedure uses the most recently created SAS data set.

Table 38.4 lists the *options* available in the PROC FREQ statement. Descriptions of the *options* follow in alphabetical order.

Table 38.4 PROC FREQ Statement Options

Option	Description
COMPRESS	Begins the next one-way table on the current page
DATA=	Names the input data set
FORMCHAR=	Specifies the outline and cell divider characters for crosstabulation tables
NLEVELS	Displays the number of levels for all TABLES variables
NOPRINT	Suppresses all displayed output
ORDER=	Specifies the order for reporting variable values
PAGE	Displays one table per page

You can specify the following *options* in the PROC FREQ statement.

COMPRESS

begins display of the next one-way frequency table on the same page as the preceding one-way table if there is enough space to begin the table. By default, the next one-way table begins on the current page only if the entire table fits on that page. The COMPRESS option is not valid with the PAGE option.

DATA=SAS-data-set

names the SAS data set to be analyzed by PROC FREQ. If you omit the DATA= option, the procedure uses the most recently created SAS data set.

FORMCHAR(1,2,7)= 'formchar-string'

defines the characters to be used for constructing the outlines and dividers for the cells of crosstabulation table displays. The *formchar-string* should be three characters long. The characters are used to draw the vertical separators (1), the horizontal separators (2), and the vertical-horizontal intersections (7). If you do not specify the FORMCHAR= option, PROC FREQ uses FORMCHAR(1,2,7)='|-+' by default. Table 38.5 summarizes the formatting characters used by PROC FREQ.

Table 38.5 Formatting Characters Used by PROC FREQ

Position	Default	Used to Draw
1		Vertical separators
2	-	Horizontal separators
7	+	Intersections of vertical and horizontal separators

The FORMCHAR= option can specify 20 different SAS formatting characters used to display output; however, PROC FREQ uses only the first, second, and seventh formatting characters. Therefore, the proper specification for PROC FREQ is FORMCHAR(1,2,7)= '*formchar-string*'.

Specifying all blanks for *formchar-string* produces crosstabulation tables with no outlines or dividers—for example, FORMCHAR(1,2,7)=' '. You can use any character in *formchar-string*, including hexadecimal characters. If you use hexadecimal characters, you must put an *x* after the closing quote. For information about which hexadecimal codes to use for which characters, see the documentation for your hardware.

See the CALENDAR, PLOT, and TABULATE procedures in the *Base SAS Procedures Guide* for more information about form characters.

NLEVELS

displays the “Number of Variable Levels” table, which provides the number of levels for each variable named in the TABLES statements. See the section “[Number of Variable Levels Table](#)” on page 2609 for details. PROC FREQ determines the variable levels from the formatted variable values, as described in the section “[Grouping with Formats](#)” on page 2544.

NOPRINT

suppresses the display of all output. You can use the NOPRINT option when you only want to create an output data set. See the section “[Output Data Sets](#)” on page 2606 for information about the output data sets produced by PROC FREQ. Note that the NOPRINT option temporarily disables the Output Delivery System (ODS). For more information, see Chapter 20, “[Using the Output Delivery System](#).”

NOTE: A NOPRINT option is also available in the TABLES statement. It suppresses display of the crosstabulation tables but allows display of the requested statistics.

ORDER=DATA | FORMATTED | FREQ | INTERNAL

specifies the order of the variable levels in the frequency and crosstabulation tables, which you request in the TABLES statement.

The ORDER= option can take the following values:

Value of ORDER=	Levels Ordered By
DATA	Order of appearance in the input data set
FORMATTED	External formatted value, except for numeric variables with no explicit format, which are sorted by their unformatted (internal) value
FREQ	Descending frequency count; levels with the most observations come first in the order
INTERNAL	Unformatted value

By default, ORDER=INTERNAL. The FORMATTED and INTERNAL orders are machine-dependent. The ORDER= option does not apply to missing values, which are always ordered first.

For more information about sort order, see the chapter on the SORT procedure in the *Base SAS Procedures Guide* and the discussion of BY-group processing in *SAS Language Reference: Concepts*.

PAGE

displays only one table per page. Otherwise, PROC FREQ displays multiple tables per page as space permits. The PAGE option is not valid with the COMPRESS option.

BY Statement

BY variables ;

You can specify a BY statement with PROC FREQ to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the FREQ procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

EXACT Statement

EXACT *statistic-options* < / *computation-options* > ;

The EXACT statement requests exact tests and confidence limits for selected statistics. The *statistic-options* identify which statistics to compute, and the *computation-options* specify options for computing exact statistics. See the section “Exact Statistics” on page 2601 for details.

NOTE: PROC FREQ computes exact tests by using fast and efficient algorithms that are superior to direct enumeration. Exact tests are appropriate when a data set is small, sparse, skewed, or heavily tied. For some large problems, computation of exact tests might require a considerable amount of time and memory. Consider using asymptotic tests for such problems. Alternatively, when asymptotic methods might not be sufficient for such large problems, consider using Monte Carlo estimation of exact *p*-values. You can request Monte Carlo estimation by specifying the **MC** *computation-option* in the EXACT statement. See the section “Computational Resources” on page 2604 for more information.

Statistic Options

The *statistic-options* specify which exact tests and confidence limits to compute. Table 38.6 lists the available *statistic-options* and the exact statistics that are computed. Descriptions of the *statistic-options* follow the table in alphabetical order.

For one-way tables, exact *p*-values are available for binomial proportion tests, the chi-square goodness-of-fit test, and the likelihood ratio chi-square test. Exact (Clopper-Pearson) confidence limits are available for the binomial proportion.

For two-way tables, exact *p*-values are available for the following tests: Pearson chi-square test, likelihood ratio chi-square test, Mantel-Haenszel chi-square test, Fisher’s exact test, Jonckheere-Terpstra test, and Cochran-Armitage test for trend. Exact *p*-values are also available for tests of the following statistics: Pearson correlation coefficient, Spearman correlation coefficient, Kendall’s tau-*b*, Stuart’s tau-*c*, Somers’ $D(C|R)$, Somers’ $D(R|C)$, simple kappa coefficient, and weighted kappa coefficient.

For 2×2 tables, PROC FREQ provides the exact McNemar’s test, exact confidence limits for the odds ratio, and Barnard’s unconditional exact test for the risk (proportion) difference. PROC FREQ also provides exact

unconditional confidence limits for the risk difference and for the relative risk (ratio of proportions). For stratified 2×2 tables, PROC FREQ provides Zelen's exact test for equal odds ratios, exact confidence limits for the common odds ratio, and an exact test for the common odds ratio.

Most of the *statistic-option* names listed in Table 38.6 are identical to the corresponding option names in the TABLES and OUTPUT statements. You can request exact computations for groups of statistics by using *statistic-options* that are identical to the TABLES statement options CHISQ, MEASURES, and AGREE. For example, when you specify the CHISQ *statistic-option* in the EXACT statement, PROC FREQ computes exact p -values for the Pearson chi-square, likelihood ratio chi-square, and Mantel-Haenszel chi-square tests for two-way tables. You can request an exact test for an individual statistic by specifying the corresponding *statistic-option* from the list in Table 38.6.

Using the EXACT Statement with the TABLES Statement

You must use a TABLES statement with the EXACT statement. If you use only one TABLES statement, you do not need to specify the same options in both the TABLES and EXACT statements; when you specify a *statistic-option* in the EXACT statement, PROC FREQ automatically invokes the corresponding TABLES statement option. However, when you use an EXACT statement with multiple TABLES statements, you must specify options in the TABLES statements to request statistics. PROC FREQ then provides exact tests or confidence limits for those statistics that you also specify in the EXACT statement.

Table 38.6 EXACT Statement Statistic Options

Statistic Option	Exact Statistics
AGREE	McNemar's test (for 2×2 tables), simple kappa test, weighted kappa test
BARNARD	Barnard's test (for 2×2 tables)
BINOMIAL	Binomial proportion tests for one-way tables
CHISQ	Chi-square goodness-of-fit test for one-way tables; Pearson chi-square, likelihood ratio chi-square, and Mantel-Haenszel chi-square tests for two-way tables
COMOR	Confidence limits for the common odds ratio, common odds ratio test (for $h \times 2 \times 2$ tables)
EQOR ZELLEN	Zelen's test for equal odds ratios (for $h \times 2 \times 2$ tables)
FISHER	Fisher's exact test
JT	Jonckheere-Terpstra test
KAPPA	Test for the simple kappa coefficient
KENTB	Test for Kendall's tau- b
LRCHI	Likelihood ratio chi-square test (one-way or two-way tables)
MCNEM	McNemar's test (for 2×2 tables)
MEASURES	Tests for the Pearson correlation and Spearman correlation, confidence limits for the odds ratio (for 2×2 tables)
MHCHI	Mantel-Haenszel chi-square test
OR	Confidence limits for the odds ratio (for 2×2 tables)
PCHI	Pearson chi-square test
PCORR	Test for the Pearson correlation coefficient
RELRIK	Confidence limits for the relative risk (for 2×2 tables)
RISKDIFF	Confidence limits for the proportion difference (for 2×2 tables)
SCORR	Test for the Spearman correlation coefficient

Table 38.6 *continued*

Statistic Option	Exact Statistics
SMDCR	Test for Somers' $D(C R)$
SMDRC	Test for Somers' $D(R C)$
STUTC	Test for Stuart's tau- c
TREND	Cochran-Armitage test for trend
WTKAP	Test for the weighted kappa coefficient

You can specify the following *statistic-options* in the EXACT statement.

AGREE

requests the exact McNemar's test and exact tests for the simple and weighted kappa coefficients. See the sections "Tests and Measures of Agreement" on page 2588 and "Exact Statistics" on page 2601 for details.

The **AGREE** option in the TABLES statement provides the asymptotic McNemar's test and the kappa estimates, standard errors, and confidence limits. The **AGREE** option in the TEST statement provides asymptotic tests for the kappa coefficients.

Kappa coefficients are defined only for square tables, where the number of rows equals the number of columns. McNemar's test is available for 2×2 tables.

BARNARD

requests Barnard's exact unconditional test for the risk (proportion) difference for 2×2 tables. See the section "Barnard's Unconditional Exact Test" on page 2581 for details. The **RISKDIFF** option in the TABLES statement provides risk difference estimates, confidence limits, and asymptotic tests. See the section "Risks and Risk Differences" on page 2572 for more information.

BINOMIAL

requests exact tests for the binomial proportion (for one-way tables). See the section "Binomial Tests" on page 2568 for details. The **BINOMIAL** option in the TABLES statement provides confidence limits and asymptotic tests for the binomial proportion. See the section "Binomial Proportion" on page 2565 for more information.

CHISQ

requests exact tests for the Pearson chi-square, likelihood ratio chi-square, and Mantel-Haenszel chi-square for two-way tables. See the section "Chi-Square Tests and Statistics" on page 2550 for details. The **CHISQ** option in the TABLES statement provides asymptotic tests for these statistics.

For one-way tables, the **CHISQ** option requests the exact chi-square goodness-of-fit test. See the section "Chi-Square Test for One-Way Tables" on page 2551 for details.

COMOR

requests an exact test and exact confidence limits for the common odds ratio for multiway 2×2 tables. See the section "Exact Confidence Limits for the Common Odds Ratio" on page 2599 for details. The **CMH** option in the TABLES statement provides Mantel-Haenszel and logit estimates and asymptotic confidence limits for the common odds ratio.

EQOR

requests Zelen's exact test for equal odds ratios, which is available for multiway 2×2 tables. See the section “Zelen's Exact Test for Equal Odds Ratios” on page 2598 for details. The **CMH** option in the **TABLES** statement provides the asymptotic Breslow-Day test for homogeneity of odds ratios.

FISHER

request Fisher's exact test. See the sections “Fisher's Exact Test” on page 2554 and “Exact Statistics” on page 2601 for details. For 2×2 tables, the **CHISQ** option in the **TABLES** statement provides Fisher's exact test. For general $R \times C$ tables, Fisher's exact test is also known as the Freeman-Halton test.

JT

requests the exact Jonckheere-Terpstra test. See the sections “Jonckheere-Terpstra Test” on page 2586 and “Exact Statistics” on page 2601 for details. The **JT** option in the **TABLES** statement provides the asymptotic Jonckheere-Terpstra test.

KAPPA

requests an exact test for the simple kappa coefficient. See the sections “Simple Kappa Coefficient” on page 2589 and “Exact Statistics” on page 2601 for details. The **AGREE** option in the **TABLES** statement provides the simple kappa estimate, standard error, and confidence limits. The **KAPPA** option in the **TEST** statement provides the asymptotic test for the simple kappa coefficient.

Kappa coefficients are defined only for square tables, where the number of rows equals the number of columns. PROC FREQ does not compute kappa coefficients for tables that are not square.

KENTB

requests an exact test for Kendall's tau-*b*. See the sections “Kendall's Tau-*b*” on page 2558 and “Exact Statistics” on page 2601 for details. The **MEASURES** option in the **TABLES** statement provides the Kendall's tau-*b* estimate and standard error. The **KENTB** option in the **TEST** statement provides an asymptotic test for Kendall's tau-*b*.

LRCHI

requests an exact test for the likelihood ratio chi-square for two-way tables. See the sections “Likelihood Ratio Chi-Square Test” on page 2553 and “Exact Statistics” on page 2601 for details. For one-way tables, the **LRCHI** option requests an exact likelihood ratio goodness-of-fit test. See the section “Likelihood Ratio Chi-Square Test for One-Way Tables” on page 2552 for details.

The **CHISQ** option in the **TABLES** statement provides asymptotic likelihood ratio chi-square tests.

MCNEM

requests the exact McNemar's test. See the sections “McNemar's Test” on page 2588 and “Exact Statistics” on page 2601 for details. The **AGREE** option in the **TABLES** statement provides the asymptotic McNemar's test.

MEASURES

requests exact tests for the Pearson and Spearman correlations. See the sections “Pearson Correlation Coefficient” on page 2559, “Spearman Rank Correlation Coefficient” on page 2560, and “Exact Statistics” on page 2601 for details. The **PCORR** and **SCORR** options in the **TEST** statement provide asymptotic tests for the Pearson and Spearman correlations, respectively.

The **MEASURES** option also requests exact confidence limits for the odds ratio for 2×2 tables. See the sections “Odds Ratio (Case-Control Studies)” on page 2582 and “Exact Confidence Limits for the Odds Ratio” on page 2583 for details. The **MEASURES** and **RELRISK** options in the **TABLES** statement provide asymptotic confidence limits for the odds ratio.

MHCHI

requests an exact test for the Mantel-Haenszel chi-square. See the sections “[Mantel-Haenszel Chi-Square Test](#)” on page 2553 and “[Exact Statistics](#)” on page 2601 for details. The **CHISQ** option in the **TABLES** statement provides the asymptotic Mantel-Haenszel chi-square test.

OR

requests exact confidence limits for the odds ratio for 2×2 tables. See the sections “[Odds Ratio \(Case-Control Studies\)](#)” on page 2582 and “[Exact Confidence Limits for the Odds Ratio](#)” on page 2583 for details. The **MEASURES** and **RELRISK** options in the **TABLES** statement provide asymptotic confidence limits for the odds ratio.

PCHI

requests an exact test for the Pearson chi-square for two-way tables. See the sections “[Pearson Chi-Square Test for Two-Way Tables](#)” on page 2551 and “[Exact Statistics](#)” on page 2601 for details. For one-way tables, the **PCHI** option requests an exact chi-square goodness-of-fit test. See the section “[Chi-Square Test for One-Way Tables](#)” on page 2551 for details. The **CHISQ** option in the **TABLES** statement provides asymptotic chi-square tests.

PCORR

requests an exact test for the Pearson correlation coefficient. See the sections “[Pearson Correlation Coefficient](#)” on page 2559 and “[Exact Statistics](#)” on page 2601 for details. The **MEASURES** option in the **TABLES** statement provides the Pearson correlation estimate and standard error. The **PCORR** option in the **TEST** statement provides an asymptotic test for the Pearson correlation.

RELRISK < (options) >

requests exact unconditional confidence limits for the relative risk for 2×2 tables. **PROC FREQ** computes the confidence limits by inverting two separate one-sided exact tests (Santner and Snell 1980). By default, this computation uses the unstandardized relative risk as the test statistic. If you specify the **RELRISK(METHOD=SCORE)** option, the computation uses the score statistic (Chan and Zhang 1999). See the section “[Exact Unconditional Confidence Limits for the Relative Risk](#)” on page 2584 for more information.

You can set the confidence level by specifying the **ALPHA=** option in the **TABLES** statement. The default of **ALPHA=0.5** produces 95% confidence limits.

The **RELRISK** option in the **TABLES** statement provides asymptotic confidence limits for the relative risk. See the section “[Relative Risks \(Cohort Studies\)](#)” on page 2583 for more information.

You can specify the following *options* in parentheses after the **RELRISK** *statistic-option*:

COLUMN=1 | 2 | BOTH

specifies the 2×2 table column for which to compute the relative risk. The default is **COLUMN=1**, which provides exact confidence limits for the column 1 relative risk. If you specify **COLUMN=BOTH**, **PROC FREQ** provides exact confidence limits for both column 1 and column 2 relative risks.

METHOD=SCORE

requests exact unconditional confidence limits that are based on the score statistic (Chan and Zhang 1999). See the section “[Exact Unconditional Confidence Limits for the Relative Risk](#)” on page 2584 for more information. If you do not specify **METHOD=SCORE**, by default the exact confidence limit computations are based on the unstandardized relative risk.

RISKDIFF <(options)>

requests exact unconditional confidence limits for the risk difference for 2×2 tables. PROC FREQ computes the confidence limits by inverting two separate one-sided exact tests (Santner and Snell 1980). By default, this computation uses the unstandardized risk difference as the test statistic. If you specify the **RISKDIFF(METHOD=SCORE)** option, the computation uses the score statistic (Chan and Zhang 1999). See the section “Exact Unconditional Confidence Limits for the Risk Difference” on page 2580 for more information.

You can set the confidence level by specifying the **ALPHA=** option in the **TABLES** statement. The default of **ALPHA=0.5** produces 95% confidence limits.

The **RISKDIFF** option in the **TABLES** statement provides asymptotic confidence limits for the risk difference, including Wald, Newcombe, and Miettinen-Nurminen confidence limits. See the section “Risk Difference Confidence Limits” on page 2574 for more information.

You can specify the following *options* in parentheses after the **RISKDIFF** *statistic-option*:

COLUMN=1 | 2 | BOTH

specifies the 2×2 table column for which to compute the risk difference. The default is **COLUMN=BOTH**, which provides exact confidence limits for both column 1 and column 2 risk differences.

METHOD=SCORE

requests exact unconditional confidence limits that are based on the score statistic (Chan and Zhang 1999). See the section “Exact Unconditional Confidence Limits for the Risk Difference” on page 2580 for more information. If you do not specify **METHOD=SCORE**, by default the exact confidence limit computations are based on the unstandardized risk difference.

SCORR

requests an exact test for the Spearman correlation coefficient. See the sections “Spearman Rank Correlation Coefficient” on page 2560 and “Exact Statistics” on page 2601 for details. The **MEASURES** option in the **TABLES** statement provides the Spearman correlation estimate and standard error. The **SCORR** option in the **TEST** statement provides an asymptotic test for the Spearman correlation.

SMDCR

requests an exact test for Somers’ $D(C|R)$. See the sections “Somers’ D ” on page 2559 and “Exact Statistics” on page 2601 for details. The **MEASURES** option in the **TABLES** statement provides Somers’ $D(C|R)$ estimate and the standard error. The **SMDCR** option in the **TEST** statement provides an asymptotic test for Somers’ $D(C|R)$.

SMDRC

requests an exact test for Somers’ $D(R|C)$. See the sections “Somers’ D ” on page 2559 and “Exact Statistics” on page 2601 for details. The **MEASURES** option in the **TABLES** statement provides Somers’ $D(R|C)$ estimate and the standard error. The **SMDRC** option in the **TEST** statement requests an asymptotic test for Somers’ $D(C|R)$.

STUTC

requests an exact test for Stuart’s tau- c . See the sections “Stuart’s Tau- c ” on page 2558 and “Exact Statistics” on page 2601 for details. The **MEASURES** option in the **TABLES** statement provides Stuart’s tau- c estimate and the standard error. The **STUTC** option in the **TEST** statement provides an asymptotic test for Stuart’s tau- c .

TREND

requests the exact Cochran-Armitage test for trend. See the sections “[Cochran-Armitage Test for Trend](#)” on page 2585 and “[Exact Statistics](#)” on page 2601 for details. The **TREND** option in the TABLES statement provides the asymptotic Cochran-Armitage trend test. The trend test is available for tables of dimensions $2 \times C$ or $R \times 2$.

WTKAP

requests an exact test for the weighted kappa coefficient. See the sections “[Weighted Kappa Coefficient](#)” on page 2590 and “[Exact Statistics](#)” on page 2601 for details. The **AGREE** option in the TABLES statement provides the weighted kappa estimate, standard error, and confidence limits. The **WTKAP** option in the TEST statement provides the asymptotic test for the weighted kappa coefficient.

Kappa coefficients are defined only for square tables, where the number of rows equals the number of columns. PROC FREQ does not compute kappa coefficients for tables that are not square. For 2×2 tables, the weighted kappa coefficient equals the simple kappa coefficient, and PROC FREQ does not present separate results for the weighted kappa coefficient.

Computation Options

The *computation-options* specify options for computing exact statistics. You can specify the following *computation-options* in the EXACT statement after a slash (/).

ALPHA= α

specifies the level of the confidence limits for Monte Carlo p -value estimates. The value of α must be between 0 and 1, and the default is 0.01. A confidence level of α produces $100(1 - \alpha)\%$ confidence limits. The default of ALPHA=.01 produces 99% confidence limits for the Monte Carlo estimates.

The ALPHA= option invokes the **MC** option.

MAXTIME=*value*

specifies the maximum clock time (in seconds) that PROC FREQ can use to compute an exact p -value. If the procedure does not complete the computation within the specified time, the computation terminates. The value of MAXTIME= must be a positive number. The MAXTIME= option is valid for Monte Carlo estimation of exact p -values as well as for direct exact p -value computation. See the section “[Computational Resources](#)” on page 2604 for more information.

MC

6 requests Monte Carlo estimation of exact p -values instead of direct exact p -value computation. Monte Carlo estimation can be useful for large problems that require a considerable amount of time and memory for exact computations but for which asymptotic approximations might not be sufficient. See the section “[Monte Carlo Estimation](#)” on page 2604 for more information.

The MC option is available for all EXACT *statistic-options* except the BINOMIAL option and the following options that apply only to 2×2 or $h \times 2 \times 2$ tables: BARNARD, COMOR, EQOR, MCNEM, OR, RELRISK, and RISKDIFF. PROC FREQ computes only exact tests or confidence limits for these statistics.

The ALPHA=, N=, and SEED= options also invoke the MC option.

N=*n*

specifies the number of samples for Monte Carlo estimation. The value of *n* must be a positive integer, and the default is 10,000. Larger values of *n* produce more precise estimates of exact *p*-values. Because larger values of *n* generate more samples, the computation time increases.

The N= option invokes the MC option.

POINT

requests exact point probabilities for the test statistics.

The POINT option is available for all EXACT statement *statistic-options* except BARNARD, OR, RELRISK, and RISKDIFF. The POINT option is not available with the MC option.

SEED=*number*

specifies the initial seed for random number generation for Monte Carlo estimation. The value of the SEED= option must be an integer. If you do not specify the SEED= option or if the SEED= value is negative or zero, PROC FREQ uses the time of day from the computer's clock to obtain the initial seed.

The SEED= option invokes the MC option.

OUTPUT Statement

OUTPUT < **OUT=** *SAS-data-set* > *output-options* ;

The OUTPUT statement creates a SAS data set that contains statistics that are computed by PROC FREQ. Table 38.7 lists the statistics that can be stored in the output data set. You identify which statistics to include by specifying *output-options*.

You must use a TABLES statement with the OUTPUT statement. The OUTPUT statement stores statistics for only one table request. If you use multiple TABLES statements, the contents of the output data set correspond to the last TABLES statement. If you use multiple table requests in a single TABLES statement, the contents of the output data set correspond to the last table request. Only one OUTPUT statement is allowed in a single invocation of the procedure.

For a one-way or two-way table, the output data set contains one observation that stores the requested statistics for the table. For a multiway table, the output data set contains an observation for each two-way table (stratum) of the multiway crosstabulation. If you request summary statistics for the multiway table, the output data set also contains an observation that stores the across-strata summary statistics. If you use a BY statement, the output data set contains an observation or set of observations for each BY group. For more information about the contents of the output data set, see the section “Contents of the OUTPUT Statement Output Data Set” on page 2608.

The output data set that is created by the OUTPUT statement is not the same as the output data set that is created by the OUT= option in the TABLES statement. The OUTPUT statement creates a data set that contains statistics (such as the Pearson chi-square and its *p*-value), and the OUT= option in the TABLES statement creates a data set that contains frequency table counts and percentages. See the section “Output Data Sets” on page 2606 for more information.

As an alternative to the OUTPUT statement, you can use the Output Delivery System (ODS) to store statistics that PROC FREQ computes. ODS can create a SAS data set from any table that PROC FREQ produces. See the section “ODS Table Names” on page 2617 for more information.

You can specify the following *options* in the OUTPUT statement:

OUT=SAS-data-set

specifies the name of the output data set. When you use an OUTPUT statement but do not use the OUT= option, PROC FREQ creates a data set and names it by using the *DATA*n** convention.

output-options

specify the statistics to include in the output data set. Table 38.7 lists the *output-options* that are available in the OUTPUT statement, together with the TABLES statement options that are required to produce the statistics. Descriptions of the *output-options* follow the table in alphabetical order.

You can specify *output-options* to request individual statistics, or you can request groups of statistics by using *output-options* that are identical to the group options in the TABLES statement (for example, the CHISQ, MEASURES, CMH, AGREE, and ALL options).

When you specify an *output-option*, the output data set includes statistics from the corresponding analysis. In addition to the estimate or test statistic, the output data set includes associated values such as standard errors, confidence limits, *p*-values, and degrees of freedom. See the section “Contents of the OUTPUT Statement Output Data Set” on page 2608 for details.

To store a statistic in the output data set, you must also request computation of that statistic with the appropriate TABLES, EXACT, or TEST statement option. For example, the PCHI *output-option* includes the Pearson chi-square in the output data set. You must also request computation of the Pearson chi-square by specifying the CHISQ option in the TABLES statement. Or, if you use only one TABLES statement, you can request computation of the Pearson chi-square by specifying the PCHI or CHISQ option in the EXACT statement. Table 38.7 lists the TABLES statement options that are required to produce the OUTPUT data set statistics.

Table 38.7 OUTPUT Statement Output Options

Output Option	Output Data Set Statistics	Required TABLES Statement Option
AGREE	McNemar’s test (2×2 tables), Bowker’s test, simple and weighted kappas; for multiple strata, overall simple and weighted kappas, tests for equal kappas, and Cochran’s <i>Q</i> ($h \times 2 \times 2$ tables)	AGREE
AJCHI	Continuity-adjusted chi-square (2×2 tables)	CHISQ
ALL	CHISQ, MEASURES, and CMH statistics; N (number of nonmissing observations)	ALL
BDCHI BD	Breslow-Day test ($h \times 2 \times 2$ tables)	CMH, CMH1, or CMH2
BINOMIAL	Binomial statistics (one-way tables)	BINOMIAL
CHISQ	For one-way tables, goodness-of-fit test; for two-way tables, Pearson, likelihood ratio, continuity-adjusted, and Mantel-Haenszel chi-squares, Fisher’s exact test (2×2 tables), phi and contingency coefficients, Cramér’s <i>V</i>	CHISQ
CMH	Cochran-Mantel-Haenszel (CMH) correlation, row mean scores (ANOVA), and general association statistics; for 2×2 tables, logit and Mantel-Haenszel common odds ratios and relative risks, Breslow-Day test	CMH

Table 38.7 continued

Output Option	Output Data Set Statistics	Required TABLES Statement Option
CMH1	CMH statistics, except row mean scores (ANOVA) and general association statistics	CMH or CMH1
CMH2	CMH statistics, except general association statistic	CMH or CMH2
CMHCOR	CMH correlation statistic	CMH, CMH1, or CMH2
CMHGA	CMH general association statistic	CMH
CMHRMS	CMH row mean scores (ANOVA) statistic	CMH or CMH2
COCHQ	Cochran's Q ($h \times 2 \times 2$ tables)	AGREE
CONTGY	Contingency coefficient	CHISQ
CRAMV	Cramér's V	CHISQ
EQKAP	Test for equal simple kappas	AGREE
EQOR ZELEN	Zelen's test for equal odds ratios ($h \times 2 \times 2$ tables)	CMH and EXACT EQOR
EQWKP	Test for equal weighted kappas	AGREE
FISHER	Fisher's exact test	CHISQ or FISHER ¹
GAILSIMON GS	Gail-Simon test	CMH(GAILSIMON)
GAMMA	Gamma	MEASURES
JT	Jonckheere-Terpstra test	JT
KAPPA	Simple kappa coefficient	AGREE
KENTB TAUB	Kendall's tau- b	MEASURES
LAMCR	Lambda asymmetric ($C R$)	MEASURES
LAMDAS	Lambda symmetric	MEASURES
LAMRC	Lambda asymmetric ($R C$)	MEASURES
LGOR	Logit common odds ratio	CMH, CMH1, or CMH2
LGRRC1	Logit common relative risk, column 1	CMH, CMH1, or CMH2
LGRRC2	Logit common relative risk, column 2	CMH, CMH1, or CMH2
LRCHI	Likelihood ratio chi-square	CHISQ
MCNEM	McNemar's test (2×2 tables)	AGREE
MEASURES	Gamma, Kendall's tau- b , Stuart's tau- c , Somers' $D(C R)$ and $D(R C)$, Pearson and Spearman correlations, lambda asymmetric ($C R$) and ($R C$), lambda symmetric, uncertainty coefficients ($C R$) and ($R C$), symmetric uncertainty coefficient; odds ratio and relative risks (2×2 tables)	MEASURES
MHCHI	Mantel-Haenszel chi-square	CHISQ
MHOR COMOR	Mantel-Haenszel common odds ratio	CMH, CMH1, or CMH2
MHRRC1	Mantel-Haenszel common relative risk, column 1	CMH, CMH1, or CMH2
MHRRC2	Mantel-Haenszel common relative risk, column 2	CMH, CMH1, or CMH2
N	Number of nonmissing observations	
NMISS	Number of missing observations	
OR	Odds ratio (2×2 tables)	MEASURES or RELRISK

¹CHISQ computes Fisher's exact test for 2×2 tables. Use the FISHER option to compute Fisher's exact test for general $r \times c$ tables.

Table 38.7 continued

Output Option	Output Data Set Statistics	Required TABLES Statement Option
PCHI	Chi-square goodness-of-fit test (one-way tables), Pearson chi-square (two-way tables)	CHISQ
PCORR	Pearson correlation coefficient	MEASURES
PHI	Phi coefficient	CHISQ
PLCORR	Polychoric correlation coefficient	PLCORR
RDIF1	Column 1 risk difference (row 1 – row 2)	RISKDIFF
RDIF2	Column 2 risk difference (row 1 – row 2)	RISKDIFF
RELRISK	Odds ratio and relative risks (2×2 tables)	MEASURES or RELRISK
RISKDIFF	Risks and risk differences (2×2 tables)	RISKDIFF
RISKDIFF1	Risks and risk difference, column 1	RISKDIFF
RISKDIFF2	Risks and risk difference, column 2	RISKDIFF
RRC1 RELRISK1	Relative risk, column 1	MEASURES or RELRISK
RRC2 RELRISK2	Relative risk, column 2	MEASURES or RELRISK
RSK1 RISK1	Column 1 overall risk	RISKDIFF
RSK11 RISK11	Column 1 risk for row 1	RISKDIFF
RSK12 RISK12	Column 2 risk for row 1	RISKDIFF
RSK2 RISK2	Column 2 overall risk	RISKDIFF
RSK21 RISK21	Column 1 risk for row 2	RISKDIFF
RSK22 RISK22	Column 2 risk for row 2	RISKDIFF
SCORR	Spearman correlation coefficient	MEASURES
SMDCR	Somers' $D(C R)$	MEASURES
SMDRC	Somers' $D(R C)$	MEASURES
STUTC TAUC	Stuart's tau- c	MEASURES
TREND	Cochran-Armitage test for trend	TREND
TSYMM BOWKER	Bowker's test of symmetry	AGREE
U	Symmetric uncertainty coefficient	MEASURES
UCR	Uncertainty coefficient ($C R$)	MEASURES
URC	Uncertainty coefficient ($R C$)	MEASURES
WTKAP	Weighted kappa coefficient	AGREE

You can specify the following *output-options* in the OUTPUT statement.

AGREE

includes the following tests and measures of agreement in the output data set: McNemar's test (for 2×2 tables), Bowker's test of symmetry, the simple kappa coefficient, and the weighted kappa coefficient. For multiway tables, the AGREE option also includes the following statistics in the output data set: overall simple and weighted kappa coefficients, tests for equal simple and weighted kappa coefficients, and Cochran's Q test.

The AGREE option in the TABLES statement requests computation of tests and measures of agreement. See the section "Tests and Measures of Agreement" on page 2588 for details about these statistics.

AGREE statistics are computed only for square tables, where the number of rows equals the number of columns. PROC FREQ provides Bowker's test of symmetry and weighted kappa coefficients only

for tables larger than 2×2 . (For 2×2 tables, Bowker's test is identical to McNemar's test, and the weighted kappa coefficient equals the simple kappa coefficient.) Cochran's Q is available for multiway 2×2 tables.

AJCHI

includes the continuity-adjusted chi-square in the output data set. The continuity-adjusted chi-square is available for 2×2 tables and is provided by the **CHISQ** option in the **TABLES** statement. See the section “Continuity-Adjusted Chi-Square Test” on page 2553 for details.

ALL

includes all statistics that are requested by the **CHISQ**, **MEASURES**, and **CMH** *output-options* in the output data set. **ALL** also includes the number of nonmissing observations, which you can request individually by specifying the **N** *output-option*.

BDCHI | BD

includes the Breslow-Day test in the output data set. The Breslow-Day test for homogeneity of odds ratios is computed for multiway 2×2 tables and is provided by the **CMH**, **CMH1**, and **CMH2** options in the **TABLES** statement. See the section “Breslow-Day Test for Homogeneity of the Odds Ratios” on page 2598 for details.

BINOMIAL

includes the binomial proportion estimate, confidence limits, and tests in the output data set. The **BINOMIAL** option in the **TABLES** statement requests computation of binomial statistics, which are available for one-way tables. See the section “Binomial Proportion” on page 2565 for details.

CHISQ

includes the following chi-square tests and measures in the output data set for two-way tables: Pearson chi-square, likelihood ratio chi-square, Mantel-Haenszel chi-square, phi coefficient, contingency coefficient, and Cramér's V . For 2×2 tables, **CHISQ** also includes Fisher's exact test and the continuity-adjusted chi-square in the output data set. See the section “Chi-Square Tests and Statistics” on page 2550 for details. For one-way tables, **CHISQ** includes the chi-square goodness-of-fit test in the output data set. See the section “Chi-Square Test for One-Way Tables” on page 2551 for details. The **CHISQ** option in the **TABLES** statement requests computation of these statistics.

If you specify the **CHISQ(WARN=OUTPUT)** option in the **TABLES** statement, the **CHISQ** option also includes the variable **WARN_PCHI** in the output data set. This variable indicates the validity warning for the asymptotic Pearson chi-square test.

CMH

includes the following Cochran-Mantel-Haenszel statistics in the output data set: correlation, row mean scores (ANOVA), and general association. For 2×2 tables, the **CMH** option also includes the Mantel-Haenszel and logit estimates of the common odds ratio and relative risks. For multiway (stratified) 2×2 tables, the **CMH** option includes the Breslow-Day test for homogeneity of odds ratios. The **CMH** option in the **TABLES** statement requests computation of these statistics. See the section “Cochran-Mantel-Haenszel Statistics” on page 2592 for details.

If you specify the **CMH(MF)** option in the **TABLES** statement, the **CMH** option includes the Mantel-Fleiss analysis in the output data set. The variables **MF_CMH** and **WARN_CMH** contain the Mantel-Fleiss criterion and the warning indicator, respectively.

CMH1

includes the **CMH** statistics in the output data set, with the exception of the row mean scores (ANOVA) statistic and the general association statistic. The **CMH1** option in the **TABLES** statement requests computation of these statistics. See the section “Cochran-Mantel-Haenszel Statistics” on page 2592 for details.

CMH2

includes the **CMH** statistics in the output data set, with the exception of the general association statistic. The **CMH2** option in the **TABLES** statement requests computation of these statistics. See the section “Cochran-Mantel-Haenszel Statistics” on page 2592 for details.

CMHCOR

includes the Cochran-Mantel-Haenszel correlation statistic in the output data set. The **CMH** option in the **TABLES** statement requests computation of this statistic. See the section “Correlation Statistic” on page 2594 for details.

CMHGA

includes the Cochran-Mantel-Haenszel general association statistic in the output data set. The **CMH** option in the **TABLES** statement requests computation of this statistic. See the section “General Association Statistic” on page 2595 for details.

CMHRMS

includes the Cochran-Mantel-Haenszel row mean scores (ANOVA) statistic in the output data set. The **CMH** option in the **TABLES** statement requests computation of this statistic. See the section “ANOVA (Row Mean Scores) Statistic” on page 2594 for details.

COCHQ

includes Cochran’s Q test in the output data set. The **AGREE** option in the **TABLES** statement requests computation of this test, which is available for multiway 2×2 tables. See the section “Cochran’s Q Test” on page 2592 for details.

CONTGY

includes the contingency coefficient in the output data set. The **CHISQ** option in the **TABLES** statement requests computation of the contingency coefficient. See the section “Contingency Coefficient” on page 2555 for details.

GRAMV

includes Cramér’s V in the output data set. The **CHISQ** option in the **TABLES** statement requests computation of Cramér’s V . See the section “Cramér’s V ” on page 2555 for details.

EQKAP

includes the test for equal simple kappa coefficients in the output data set. The **AGREE** option in the **TABLES** statement requests computation of this test, which is available for multiway, square ($h \times r \times r$) tables. See the section “Tests for Equal Kappa Coefficients” on page 2591 for details.

EQOR | ZELEN

includes Zelen’s exact test for equal odds ratios in the output data set. The **EQOR** option in the **EXACT** statement requests computation of this test, which is available for multiway 2×2 tables. See the section “Zelen’s Exact Test for Equal Odds Ratios” on page 2598 for details.

EQWKP

includes the test for equal weighted kappa coefficients in the output data set. The **AGREE** option in the **TABLES** statement requests computation of this test. The test for equal weighted kappas is available for multiway, square ($h \times r \times r$) tables where $r > 2$. See the section “Tests for Equal Kappa Coefficients” on page 2591 for details.

FISHER

includes Fisher’s exact test in the output data set. For 2×2 tables, the **CHISQ** option in the **TABLES** statement provides Fisher’s exact test. For tables larger than 2×2 , the **FISHER** option in the **EXACT** statement provides Fisher’s exact test. See the section “Fisher’s Exact Test” on page 2554 for details.

GAILSIMON | GS

includes the Gail-Simon test for qualitative interaction in the output data set. The **CMH(GAILSIMON)** option in the **TABLES** statement requests computation of this test. See the section “Gail-Simon Test for Qualitative Interactions” on page 2601 for details.

GAMMA

includes the gamma statistic in the output data set. The **MEASURES** option in the **TABLES** statement requests computation of the gamma statistic. See the section “Gamma” on page 2557 for details.

JT

includes the Jonckheere-Terpstra test in the output data set. The **JT** option in the **TABLES** statement requests the Jonckheere-Terpstra test. See the section “Jonckheere-Terpstra Test” on page 2586 for details.

KAPPA

includes the simple kappa coefficient in the output data set. The **AGREE** option in the **TABLES** statement requests computation of kappa, which is available for square tables (where the number of rows equals the number of columns). For multiway square tables, the **KAPPA** option also includes the overall kappa coefficient in the output data set. See the sections “Simple Kappa Coefficient” on page 2589 and “Overall Kappa Coefficient” on page 2591 for details.

KENTB | TAUB

includes Kendall’s tau- b in the output data set. The **MEASURES** option in the **TABLES** statement requests computation of Kendall’s tau- b . See the section “Kendall’s Tau- b ” on page 2558 for details.

LAMCR

includes the asymmetric lambda $\lambda(C|R)$ in the output data set. The **MEASURES** option in the **TABLES** statement requests computation of lambda. See the section “Lambda (Asymmetric)” on page 2563 for details.

LAMDAS

includes the symmetric lambda in the output data set. The **MEASURES** option in the **TABLES** statement requests computation of lambda. See the section “Lambda (Symmetric)” on page 2563 for details.

LAMRC

includes the asymmetric lambda $\lambda(R|C)$ in the output data set. The **MEASURES** option in the **TABLES** statement requests computation of lambda. See the section “Lambda (Asymmetric)” on page 2563 for details.

LGOR

includes the logit estimate of the common odds ratio in the output data set. The **CMH** option in the **TABLES** statement requests computation of this statistic, which is available for 2×2 tables. See the section “Adjusted Odds Ratio and Relative Risk Estimates” on page 2596 for details.

LGRRC1

includes the logit estimate of the common relative risk (column 1) in the output data set. The **CMH** option in the **TABLES** statement requests computation of this statistic, which is available for 2×2 tables. See the section “Adjusted Odds Ratio and Relative Risk Estimates” on page 2596 for details.

LGRRC2

includes the logit estimate of the common relative risk (column 2) in the output data set. The **CMH** option in the **TABLES** statement requests computation of this statistic, which is available for 2×2 tables. See the section “Adjusted Odds Ratio and Relative Risk Estimates” on page 2596 for details.

LRCHI

includes the likelihood ratio chi-square in the output data set. The **CHISQ** option in the **TABLES** statement requests computation of the likelihood ratio chi-square. See the section “Likelihood Ratio Chi-Square Test” on page 2553 for details.

MCNEM

includes McNemar’s test (for 2×2 tables) in the output data set. The **AGREE** option in the **TABLES** statement requests computation of McNemar’s test. See the section “McNemar’s Test” on page 2588 for details.

MEASURES

includes the following measures of association in the output data set: gamma, Kendall’s tau-*b*, Stuart’s tau-*c*, Somers’ $D(C|R)$, Somers’ $D(R|C)$, Pearson and Spearman correlation coefficients, lambda (symmetric and asymmetric), and uncertainty coefficients (symmetric and asymmetric). For 2×2 tables, the **MEASURES** option also includes the odds ratio, column 1 relative risk, and column 2 relative risk. The **MEASURES** option in the **TABLES** statement requests computation of these statistics. See the section “Measures of Association” on page 2556 for details.

MHCHI

includes the Mantel-Haenszel chi-square in the output data set. The **CHISQ** option in the **TABLES** statement requests computation of the Mantel-Haenszel chi-square. See the section “Mantel-Haenszel Chi-Square Test” on page 2553 for details.

MHOR | COMOR

includes the Mantel-Haenszel estimate of the common odds ratio in the output data set. The **CMH** option in the **TABLES** statement requests computation of this statistic, which is available for 2×2 tables. See the section “Adjusted Odds Ratio and Relative Risk Estimates” on page 2596 for details.

MHRC1

includes the Mantel-Haenszel estimate of the common relative risk (column 1) in the output data set. The **CMH** option in the **TABLES** statement requests computation of this statistic, which is available for 2×2 tables. See the section “Adjusted Odds Ratio and Relative Risk Estimates” on page 2596 for details.

MHRRC2

includes the Mantel-Haenszel estimate of the common relative risk (column 2) in the output data set. The **CMH** option in the **TABLES** statement requests computation of this statistic, which is available for 2×2 tables. See the section “[Adjusted Odds Ratio and Relative Risk Estimates](#)” on page 2596 for details.

N

includes the number of nonmissing observations in the output data set.

NMISS

includes the number of missing observations in the output data set. See the section “[Missing Values](#)” on page 2545 for details about how PROC FREQ handles missing values.

OR

includes the odds ratio (for 2×2 tables) in the output data set. The **MEASURES** and **REL RISK** options in the **TABLES** statement request this statistic. See the section “[Odds Ratio and Relative Risks for 2 x 2 Tables](#)” on page 2582 for details.

PCHI

includes the Pearson chi-square in the output data set for two-way tables. See the section “[Pearson Chi-Square Test for Two-Way Tables](#)” on page 2551 for details. For one-way tables, the **PCHI** option includes the chi-square goodness-of-fit test in the output data set. See the section “[Chi-Square Test for One-Way Tables](#)” on page 2551 for details. The **CHISQ** option in the **TABLES** statement requests computation of these statistics.

If you specify the **CHISQ(WARN=OUTPUT)** option in the **TABLES** statement, the **PCHI** option also includes the variable **WARN_PCHI** in the output data set. This variable indicates the validity warning for the asymptotic Pearson chi-square test.

PCORR

includes the Pearson correlation coefficient in the output data set. The **MEASURES** option in the **TABLES** statement requests computation of the Pearson correlation. See the section “[Pearson Correlation Coefficient](#)” on page 2559 for details.

PHI

includes the phi coefficient in the output data set. The **CHISQ** option in the **TABLES** statement requests computation of the phi coefficient. See the section “[Phi Coefficient](#)” on page 2555 for details.

PLCORR

includes the polychoric correlation coefficient in the output data set. For 2×2 tables, this statistic is known as the tetrachoric correlation coefficient. The **PLCORR** option in the **TABLES** statement requests computation of the polychoric correlation. See the section “[Polychoric Correlation](#)” on page 2562 for details.

RDIF1

includes the column 1 risk difference (row 1 – row 2) in the output data set. The **RISKDIFF** option in the **TABLES** statement requests computation of risks and risk differences, which are available for 2×2 tables. See the section “[Risks and Risk Differences](#)” on page 2572 for details.

RDIF2

includes the column 2 risk difference (row 1 – row 2) in the output data set. The **RISKDIFF** option in the **TABLES** statement requests computation of risks and risk differences, which are available for 2×2 tables. See the section “[Risks and Risk Differences](#)” on page 2572 for details.

RELRIK

includes the column 1 and column 2 relative risks (for 2×2 tables) in the output data set. The **MEASURES** and **RELRIK** options in the **TABLES** statement request these statistics. See the section “[Odds Ratio and Relative Risks for 2 x 2 Tables](#)” on page 2582 for details.

RISKDIFF

includes risks (binomial proportions) and risk differences for 2×2 tables in the output data set. These statistics include the row 1 risk, row 2 risk, total (overall) risk, and risk difference (row 1 – row 2) for column 1 and column 2. The **RISKDIFF** option in the **TABLES** statement requests computation of these statistics. See the section “[Risks and Risk Differences](#)” on page 2572 for details.

RISKDIFF1

includes column 1 risks (binomial proportions) and risk differences for 2×2 tables in the output data set. These statistics include the row 1 risk, row 2 risk, total (overall) risk, and risk difference (row 1 – row 2). The **RISKDIFF** option in the **TABLES** statement requests computation of these statistics. See the section “[Risks and Risk Differences](#)” on page 2572 for details.

RISKDIFF2

includes column 2 risks (binomial proportions) and risk differences for 2×2 tables in the output data set. These statistics include the row 1 risk, row 2 risk, total (overall) risk, and risk difference (row 1 – row 2). The **RISKDIFF** option in the **TABLES** statement requests computation of these statistics. See the section “[Risks and Risk Differences](#)” on page 2572 for details.

RRC1 | RELRIK1

includes the column 1 relative risk in the output data set. The **MEASURES** and **RELRIK** options in the **TABLES** statement request relative risks, which are available for 2×2 tables. See the section “[Odds Ratio and Relative Risks for 2 x 2 Tables](#)” on page 2582 for details.

RRC2 | RELRIK2

includes the column 2 relative risk in the output data set. The **MEASURES** and **RELRIK** options in the **TABLES** statement request relative risks, which are available for 2×2 tables. See the section “[Odds Ratio and Relative Risks for 2 x 2 Tables](#)” on page 2582 for details.

RSK1 | RISK1

includes the overall column 1 risk in the output data set. The **RISKDIFF** option in the **TABLES** statement requests computation of risks and risk differences, which are available for 2×2 tables. See the section “[Risks and Risk Differences](#)” on page 2572 for details.

RSK11 | RISK11

includes the column 1 risk for row 1 in the output data set. The **RISKDIFF** option in the **TABLES** statement requests computation of risks and risk differences, which are available for 2×2 tables. See the section “[Risks and Risk Differences](#)” on page 2572 for details.

RSK12 | RISK12

includes the column 2 risk for row 1 in the output data set. The **RISKDIFF** option in the **TABLES** statement requests computation of risks and risk differences, which are available for 2×2 tables. See the section “[Risks and Risk Differences](#)” on page 2572 for details.

RSK2 | RISK2

includes the overall column 2 risk in the output data set. The **RISKDIFF** option in the **TABLES** statement requests computation of risks and risk differences. See the section “[Risks and Risk Differences](#)” on page 2572 for details.

RSK21 | RISK21

includes the column 1 risk for row 2 in the output data set. The **RISKDIFF** option in the **TABLES** statement requests computation of risks and risk differences, which are available for 2×2 tables. See the section “[Risks and Risk Differences](#)” on page 2572 for details.

RSK22 | RISK22

includes the column 2 risk for row 2 in the output data set. The **RISKDIFF** option in the **TABLES** statement requests computation of risks and risk differences, which are available for 2×2 tables. See the section “[Risks and Risk Differences](#)” on page 2572 for details.

SCORR

includes the Spearman correlation coefficient in the output data set. The **MEASURES** option in the **TABLES** statement requests computation of the Spearman correlation. See the section “[Spearman Rank Correlation Coefficient](#)” on page 2560 for details.

SMDCR

includes Somers’ $D(C|R)$ in the output data set. The **MEASURES** option in the **TABLES** statement requests computation of Somers’ D . See the section “[Somers’ \$D\$](#) ” on page 2559 for details.

SMDRC

includes Somers’ $D(R|C)$ in the output data set. The **MEASURES** option in the **TABLES** statement requests computation of Somers’ D . See the section “[Somers’ \$D\$](#) ” on page 2559 for details.

STUTC | TAUC

includes Stuart’s tau- c in the output data set. The **MEASURES** option in the **TABLES** statement requests computation of tau- c . See the section “[Stuart’s Tau- \$c\$](#) ” on page 2558 for details.

TREND

includes the Cochran-Armitage test for trend in the output data set. The **TREND** option in the **TABLES** statement requests computation of the trend test. This test is available for tables of dimension $2 \times C$ or $R \times 2$. See the section “[Cochran-Armitage Test for Trend](#)” on page 2585 for details.

TSYMM | BOWKER

includes Bowker’s test of symmetry in the output data set. The **AGREE** option in the **TABLES** statement requests computation of Bowker’s test. See the section “[Bowker’s Test of Symmetry](#)” on page 2588 for details.

U

includes the uncertainty coefficient (symmetric) in the output data set. The **MEASURES** option in the **TABLES** statement requests computation of the uncertainty coefficient. See the section “[Uncertainty Coefficient \(Symmetric\)](#)” on page 2565 for details.

UCR

includes the asymmetric uncertainty coefficient $U(C|R)$ in the output data set. The **MEASURES** option in the **TABLES** statement requests computation of the uncertainty coefficient. See the section “[Uncertainty Coefficients \(Asymmetric\)](#)” on page 2564 for details.

URC

includes the asymmetric uncertainty coefficient $U(R|C)$ in the output data set. The **MEASURES** option in the **TABLES** statement requests computation of the uncertainty coefficient. See the section “[Uncertainty Coefficients \(Asymmetric\)](#)” on page 2564 for details.

WTKAP

includes the weighted kappa coefficient in the output data set. The **AGREE** option in the **TABLES** statement requests computation of weighted kappa, which is available for square tables larger than 2×2 . For multiway tables, the **WTKAP** option also includes the overall weighted kappa coefficient in the output data set. See the sections “[Weighted Kappa Coefficient](#)” on page 2590 and “[Overall Kappa Coefficient](#)” on page 2591 for details.

TABLES Statement

TABLES *requests* </ options > ;

The **TABLES** statement requests one-way to n -way frequency and crosstabulation tables and statistics for those tables.

If you omit the **TABLES** statement, **PROC FREQ** generates one-way frequency tables for all data set variables that are not listed in the other statements.

The following argument is required in the **TABLES** statement.

requests

specify the frequency and crosstabulation tables to produce. A request is composed of one variable name or several variable names separated by asterisks. To request a one-way frequency table, use a single variable. To request a two-way crosstabulation table, use an asterisk between two variables. To request a multiway table (an n -way table, where $n > 2$), separate the desired variables with asterisks. The unique values of these variables form the rows, columns, and strata of the table. You can include up to 50 variables in a single multiway table request.

For two-way to multiway tables, the values of the last variable form the crosstabulation table columns, while the values of the next-to-last variable form the rows. Each level (or combination of levels) of the other variables forms one stratum. **PROC FREQ** produces a separate crosstabulation table for each stratum. For example, a specification of **A*B*C*D** in a **TABLES** statement produces k tables, where k is the number of different combinations of values for **A** and **B**. Each table lists the values for **C** down the side and the values for **D** across the top.

You can use multiple TABLES statements in the PROC FREQ step. PROC FREQ builds all the table requests in one pass of the data, so that there is essentially no loss of efficiency. You can also specify any number of table requests in a single TABLES statement. To specify multiple table requests quickly, use a grouping syntax by placing parentheses around several variables and joining other variables or variable combinations. For example, the statements shown in Table 38.8 illustrate grouping syntax.

Table 38.8 Grouping Syntax

TABLES Request	Equivalent to
A*(B C)	A*B A*C
(A B)*(C D)	A*C B*C A*D B*D
(A B C)*D	A*D B*D C*D
A -- C	A B C
(A -- C)*D	A*D B*D C*D

The TABLES statement variables are one or more variables from the DATA= input data set. These variables can be either character or numeric, but the procedure treats them as categorical variables. PROC FREQ uses the formatted values of the TABLES variable to determine the categorical variable levels. So if you assign a format to a variable with a FORMAT statement, PROC FREQ formats the values before dividing observations into the levels of a frequency or crosstabulation table. See the FORMAT procedure in the *Base SAS Procedures Guide* and the FORMAT statement and SAS formats in *SAS Formats and Informats: Reference*.

If you use PROC FORMAT to create a user-written format that combines missing and nonmissing values into one category, PROC FREQ treats the entire category of formatted values as missing. See the discussion in the section “[Grouping with Formats](#)” on page 2544 for more information.

By default, the frequency or crosstabulation table lists the values of both character and numeric variables in ascending order based on internal (unformatted) variable values. You can change the order of the values in the table by specifying the ORDER= option in the PROC FREQ statement. To list the values in ascending order by formatted value, use ORDER=FORMATTED.

Without Options

If you request a one-way frequency table for a variable without specifying options, PROC FREQ produces frequencies, cumulative frequencies, percentages of the total frequency, and cumulative percentages for each value of the variable. If you request a two-way or an n -way crosstabulation table without specifying options, PROC FREQ produces crosstabulation tables that include cell frequencies, cell percentages of the total frequency, cell percentages of row frequencies, and cell percentages of column frequencies. The procedure excludes observations with missing values from the table but displays the total frequency of missing observations below each table.

Options

Table 38.9 lists the *options* available in the TABLES statement. Descriptions of the *options* follow in alphabetical order.

Table 38.9 TABLES Statement Options

Option	Description
Control Statistical Analysis	
AGREE	Requests tests and measures of classification agreement
ALL	Requests tests and measures of association produced by the CHISQ, MEASURES, and CMH options
ALPHA=	Sets the confidence level for confidence limits
BINOMIAL	Requests binomial proportions, confidence limits, and tests for one-way tables
CHISQ	Requests chi-square tests and measures based on chi-square
CL	Requests confidence limits for MEASURES statistics
CMH	Requests all Cochran-Mantel-Haenszel statistics
CMH1	Requests CMH correlation statistic, adjusted odds ratios, and adjusted relative risks
CMH2	Requests CMH correlation and row mean scores (ANOVA) statistics, adjusted odds ratios, and adjusted relative risks
CONVERGE=	Specifies convergence criterion for polychoric correlation
FISHER	Requests Fisher's exact test for tables larger than 2×2
GAILSIMON	Requests Gail-Simon test for qualitative interactions
JT	Requests Jonckheere-Terpstra test
MAXITER=	Specifies maximum number of iterations for polychoric correlation
MEASURES	Requests measures of association
MISSING	Treats missing values as nonmissing
PLCORR	Requests polychoric correlation
RELRISK	Requests odds ratios and relative risks for 2×2 tables
RISKDIFF	Requests risks and risk differences for 2×2 tables
SCORES=	Specifies the type of row and column scores
TREND	Requests Cochran-Armitage test for trend
Control Additional Table Information	
CELLCHI2	Displays cell contributions to the Pearson chi-square statistic
CUMCOL	Displays cumulative column percentages
DEVIATION	Displays deviations of cell frequencies from expected values
EXPECTED	Displays expected cell frequencies
MISSPRINT	Displays missing value frequencies
SPARSE	Includes all possible combinations of variable levels in the LIST table and OUT= data set
STDRES	Displays standardized residuals in the CROSSLIST table
TOTPCT	Displays percentages of total frequency for n -way tables ($n > 2$)
Control Displayed Output	
CONTENTS=	Specifies the contents label for crosstabulation tables
CROSSLIST	Displays crosstabulation tables in ODS column format
FORMAT=	Formats the frequencies in crosstabulation tables
LIST	Displays two-way to n -way tables in list format
MAXLEVELS=	Specifies maximum number of levels to display in one-way tables
NOCOL	Suppresses display of column percentages

Table 38.9 continued

Option	Description
NOCUM	Suppresses display of cumulative frequencies and percentages
NOFREQ	Suppresses display of frequencies
NOPERCENT	Suppresses display of percentages
NOPRINT	Suppresses display of crosstabulation tables but displays statistics
NOROW	Suppresses display of row percentages
NOSPARSE	Suppresses zero frequency levels in the CROSSLIST table, LIST table, and OUT= data set
NOWARN	Suppresses log warning message for the chi-square test
PRINTKWT	Displays kappa coefficient weights
SCOROUT	Displays row and column scores
Produce Statistical Graphics	
PLOTS=	Requests plots from ODS Graphics
Create an Output Data Set	
OUT=	Names an output data set to contain frequency counts
OUTCUM	Includes cumulative frequencies and percentages in the output data set for one-way tables
OUTEXPECT	Includes expected frequencies in the output data set
OUTPCT	Includes row, column, and two-way table percentages in the output data set

You can specify the following *options* in a TABLES statement.

AGREE <(WT=FC)>

requests tests and measures of classification agreement for square tables. The AGREE option provides McNemar's test for 2×2 tables and Bowker's test of symmetry for square tables with more than two response categories. The AGREE option also produces the simple kappa coefficient, the weighted kappa coefficient, their asymptotic standard errors, and their confidence limits. When there are multiple strata, the AGREE option provides overall simple and weighted kappas as well as tests for equal kappas among strata. When there are multiple strata and two response categories, PROC FREQ computes Cochran's Q test. See the section "[Tests and Measures of Agreement](#)" on page 2588 for details about these statistics.

If you specify the WT=FC option in parentheses after the AGREE option, PROC FREQ uses Fleiss-Cohen weights to compute the weighted kappa coefficient. By default, PROC FREQ uses Cicchetti-Allison weights. See the section "[Weighted Kappa Coefficient](#)" on page 2590 for details. You can specify the **PRINTKWT** option to display the kappa coefficient weights.

AGREE statistics are computed only for square tables, where the number of rows equals the number of columns. If your table is not square due to observations with zero weights, you can specify the **ZEROS** option in the WEIGHT statement to include these observations. For more details, see the section "[Tables with Zero Rows and Columns](#)" on page 2592.

You can use the **TEST** statement to request asymptotic tests for the simple and weighted kappa coefficients. You can request exact p -values for the simple and weighted kappa coefficient tests, as well

as for McNemar's test, by specifying the corresponding options in the **EXACT** statement. See the section “[Exact Statistics](#)” on page 2601 for more information.

ALL

requests all tests and measures that are produced by the **CHISQ**, **MEASURES**, and **CMH** options. You can control the number of CMH statistics to compute by specifying the **CMH1** or **CMH2** option.

ALPHA= α

specifies the level of confidence limits. The value of α must be between 0 and 1, and the default is 0.05. A confidence level of α produces $100(1 - \alpha)\%$ confidence limits. The default of ALPHA=0.05 produces 95% confidence limits.

ALPHA= applies to confidence limits that are requested by TABLES statement options. There is a separate ALPHA= option in the EXACT statement that sets the level of confidence limits for Monte Carlo estimates of exact p -values, which you request by specifying the **MC** option in the EXACT statement.

BINOMIAL <(binomial-options)>

requests the binomial proportion for one-way tables. When you specify the BINOMIAL option, by default PROC FREQ also provides the asymptotic standard error, asymptotic Wald and exact (Clopper-Pearson) confidence limits, and the asymptotic equality test for the binomial proportion.

You can specify *binomial-options* in parentheses after the BINOMIAL option. The **LEVEL=** *binomial-option* identifies the variable level for which to compute the proportion. If you do not specify LEVEL=, PROC FREQ computes the proportion for the first level that appears in the output. The **P=** *binomial-option* specifies the null proportion for the binomial tests. If you do not specify P=, PROC FREQ uses P=0.5 by default.

You can also specify *binomial-options* to request additional tests and confidence limits for the binomial proportion. The **EQUIV**, **NONINF**, and **SUP** *binomial-options* request tests of equivalence, noninferiority, and superiority, respectively. The **CL=** *binomial-option* requests confidence limits for the binomial proportion. [Table 38.10](#) summarizes the *binomial-options*.

Available confidence limits for the binomial proportion include Agresti-Coull, exact (Clopper-Pearson), Jeffreys, Wald, and Wilson (score) confidence limits. You can specify more than one type of binomial confidence limits in the same analysis. If you do not specify any confidence limit requests, PROC FREQ computes Wald asymptotic confidence limits and exact (Clopper-Pearson) confidence limits by default. The ALPHA= option determines the confidence level, and the default of ALPHA=0.05 produces 95% confidence limits for the binomial proportion.

As part of the noninferiority, superiority, and equivalence analyses, PROC FREQ provides test-based confidence limits that have a confidence coefficient of $100(1 - 2\alpha)\%$ (Schuirmann 1999). The ALPHA= option determines the confidence level, and the default of ALPHA=0.05 produces 90% confidence limits. See the sections “[Noninferiority Test](#)” on page 2569 and “[Equivalence Test](#)” on page 2570 for details.

To request exact tests for the binomial proportion, specify the **BINOMIAL** option in the **EXACT** statement. PROC FREQ then computes exact p -values for all binomial tests that you request with *binomial-options*, which can include tests of noninferiority, superiority, and equivalence, in addition to the test of equality.

See the section “[Binomial Proportion](#)” on page 2565 for details.

Table 38.10 BINOMIAL Options

Option	Description
LEVEL=	Specifies the variable level
P=	Specifies the null proportion
CORRECT	Requests continuity correction
Request Confidence Limits	
CL=AGRESTICOULL AC	Requests Agresti-Coull confidence limits
CL=ALL	Requests all confidence limits
CL=EXACT CLOPPERPEARSON	Requests Clopper-Pearson confidence limits
CL=JEFFREYS J	Requests Jeffreys confidence limits
CL=WALD	Requests Wald confidence limits
CL=WILSON W	Requests Wilson (score) confidence limits
Request Tests	
EQUIV EQUIVALENCE	Requests an equivalence test
NONINF NONINFERIORITY	Requests a noninferiority test
SUP SUPERIORITY	Requests a superiority test
MARGIN=	Specifies the test margin
VAR=SAMPLE NULL	Specifies the test variance

You can specify the following *binomial-options* in parentheses after the BINOMIAL option:

CL=type | (types)

requests confidence limits for the binomial proportion. You can specify one or more *types* of confidence limits. When you specify only one *type*, you can omit the parentheses around the request.

PROC FREQ displays the confidence limits in the “Binomial Confidence Limits” table. The ALPHA= option determines the level of the confidence limits that the CL= *binomial-option* provides. The default of ALPHA=0.05 produces 95% confidence limits for the binomial proportion. This differs from the test-based confidence limits that are provided with the equivalence, noninferiority, and superiority tests (EQUIV, NONINF, and SUP), which have a confidence coefficient of $100(1-2\alpha)\%$ (Schuirmann 1999). See the sections “Equivalence Test” on page 2570 and “Noninferiority Test” on page 2569 for details.

You can specify the CL= *binomial-option* with or without requests for binomial tests. The confidence limits that CL= produces do not depend on the tests that you request and do not use the value of the test margin (which you specify by using the MARGIN= *binomial-option*).

The following *types* of binomial confidence limits are available:

AGRESTICOULL | AC

requests Agresti-Coull confidence limits for the binomial proportion. See the section “Agresti-Coull Confidence Limits” on page 2566 for details.

ALL

requests all available types of confidence limits for the binomial proportion. These include the following: Agresti-Coull, exact (Clopper-Pearson), Jeffreys, Wald, and Wilson (score) confidence limits.

EXACT | CLOPPERPEARSON

requests exact (Clopper-Pearson) confidence limits for the binomial proportion. See the section “[Exact \(Clopper-Pearson\) Confidence Limits](#)” on page 2567 for details. If you do not request any binomial confidence limits by specifying the `CL= binomial-option`, PROC FREQ produces Wald and exact (Clopper-Pearson) confidence limits by default. To request exact tests for the binomial proportion, specify the `BINOMIAL` option in the `EXACT` statement.

JEFFREYS | J

requests Jeffreys confidence limits for the binomial proportion. See the section “[Jeffreys Confidence Limits](#)” on page 2566 for details.

WALD < (CORRECT) >

requests Wald confidence limits for the binomial proportion. See the section “[Wald Confidence Limits](#)” on page 2566 for details. If you do not request any binomial confidence limits by specifying the `CL= binomial-option`, PROC FREQ produces Wald and exact (Clopper-Pearson) confidence limits by default.

If you specify `CL=WALD(CORRECT)`, the Wald confidence limits include a continuity correction. If you specify the `CORRECT binomial-option`, the Wald confidence limits and the Wald tests include continuity corrections.

WILSON | W | SCORE < (CORRECT) >

requests Wilson confidence limits for the binomial proportion. These are also known as *score* confidence limits. See the section “[Wilson \(Score\) Confidence Limits](#)” on page 2567 for details.

If you specify `CL=WILSON(CORRECT)` or the `CORRECT binomial-option`, the Wilson confidence limits include a continuity correction.

CORRECT

includes a continuity correction in the Wald confidence limits, Wald tests, and Wilson confidence limits.

You can request continuity corrections individually for Wald or Wilson confidence limits by specifying the `CL=WALD(CORRECT)` or `CL=WILSON(CORRECT) binomial-option`, respectively.

EQUIV | EQUIVALENCE

requests a test of equivalence for the binomial proportion. See the section “[Equivalence Test](#)” on page 2570 for details. You can specify the equivalence test margins, the null proportion, and the variance type with the `MARGIN=`, `P=`, and `VAR= binomial-options`, respectively. To request an exact equivalence test, specify the `BINOMIAL` option in the `EXACT` statement.

LEVEL=level-number | 'level-value'

specifies the variable level for the binomial proportion. By default, PROC FREQ computes the proportion of observations for the first variable level that appears in the output. To request a different level, use `LEVEL=level-number` or `LEVEL='level-value'`, where *level-number* is the variable level's number or order in the output, and *level-value* is the formatted value of the variable level. The value of *level-number* must be a positive integer. You must enclose *level-value* in single quotes.

MARGIN=*value* | (*lower,upper*)

specifies the margin for the noninferiority, superiority, and equivalence tests, which you request with the **NONINF**, **SUP**, and **EQUIV** *binomial-options*, respectively. If you do not specify **MARGIN=**, PROC FREQ uses a margin of 0.2 by default.

For noninferiority and superiority tests, specify a single *value* for the **MARGIN=** option. The **MARGIN=** *value* must be a positive number. You can specify *value* as a number between 0 and 1. Or you can specify *value* in percentage form as a number between 1 and 100, and PROC FREQ converts that number to a proportion. The procedure treats the value 1 as 1%.

For noninferiority and superiority tests, the test limits must be between 0 and 1. The limits are determined by the null proportion value (which you can specify with the **P=** *binomial-option*) and by the margin value. The noninferiority limit equals the null proportion minus the margin. By default, the null proportion equals 0.5 and the margin equals 0.2, which gives a noninferiority limit of 0.3. The superiority limit equals the null proportion plus the margin, which is 0.7 by default.

For an equivalence test, you can specify a single **MARGIN=** *value*, or you can specify both *lower* and *upper* values. If you specify a single **MARGIN=** *value*, it must be a positive number, as described previously. If you specify a single **MARGIN=** *value* for an equivalence test, PROC FREQ uses $-value$ as the lower margin and *value* as the upper margin for the test. If you specify both *lower* and *upper* values for an equivalence test, you can specify them in proportion form as numbers between -1 or 1. Or you can specify them in percentage form as numbers between -100 and 100, and PROC FREQ converts the numbers to proportions. The value of *lower* must be less than the value of *upper*.

The equivalence limits must be between 0 and 1. The equivalence limits are determined by the null proportion value (which you can specify with the **P=** *binomial-option*) and by the margin values. The lower equivalence limit equals the null proportion plus the lower margin. By default, the null proportion equals 0.5 and the lower margin equals -0.2 , which gives a lower equivalence limit of 0.3. The upper equivalence limit equals the null proportion plus the upper margin, which is 0.7 by default.

See the sections “[Noninferiority Test](#)” on page 2569 and “[Equivalence Test](#)” on page 2570 for details.

NONINF | **NONINFERIORITY**

requests a test of noninferiority for the binomial proportion. See the section “[Noninferiority Test](#)” on page 2569 for details. You can specify the noninferiority test margin, the null proportion, and the variance type with the **MARGIN=**, **P=**, and **VAR=** *binomial-options*, respectively. To request an exact noninferiority test, specify the **BINOMIAL** option in the **EXACT** statement.

P=*value*

specifies the null hypothesis proportion for the binomial tests. If you omit the **P=** option, PROC FREQ uses 0.5 as the null proportion. The null proportion *value* must be a positive number. You can specify *value* as a number between 0 and 1. Or you can specify *value* in percentage form as a number between 1 and 100, and PROC FREQ converts that number to a proportion. The procedure treats the value 1 as 1%.

SUP | SUPERIORITY

requests a test of superiority for the binomial proportion. See the section “[Superiority Test](#)” on page 2570 for details. You can specify the superiority test margin, the null proportion, and the variance type with the **MARGIN=**, **P=**, and **VAR=** *binomial-options*, respectively. To request an exact superiority test, specify the **BINOMIAL** option in the **EXACT** statement.

VAR=SAMPLE | NULL

specifies the type of variance estimate to use in the Wald tests of noninferiority, superiority, and equivalence. The default is **VAR=SAMPLE**, which estimates the variance from the sample proportion. **VAR=NULL** uses a test-based variance that is computed from the null hypothesis proportion (which is specified by the **P=** *binomial-option*). See the sections “[Noninferiority Test](#)” on page 2569 and “[Equivalence Test](#)” on page 2570 for details.

CELLCHI2

displays each crosstabulation table cell’s contribution to the total Pearson chi-square statistic. The cell contribution is computed as

$$(frequency - expected)^2 / expected$$

where *frequency* is the table cell frequency or count and *expected* is the expected cell frequency, which is computed under the null hypothesis that the row and column variables are independent. See the section “[Pearson Chi-Square Test for Two-Way Tables](#)” on page 2551 for details.

The **CELLCHI2** option has no effect for one-way tables or for tables that are displayed with the **LIST** option.

CHISQ <(chisq-options)>

requests chi-square tests of homogeneity or independence and measures of association that are based on the chi-square statistic. For two-way tables, the chi-square tests include the Pearson chi-square, likelihood ratio chi-square, and Mantel-Haenszel chi-square tests. The chi-square measures include the phi coefficient, contingency coefficient, and Cramér’s *V*. For 2×2 tables, the **CHISQ** option also provides Fisher’s exact test and the continuity-adjusted chi-square test. See the section “[Chi-Square Tests and Statistics](#)” on page 2550 for details.

For one-way tables, the **CHISQ** option provides the Pearson chi-square goodness-of-fit test. You can also request the likelihood ratio goodness-of-fit test for one-way tables by specifying the **LRCHISQ** *chisq-option* in parentheses after the **CHISQ** option. By default, the one-way chi-square tests are based on the null hypothesis of equal proportions. Alternatively, you can provide null hypothesis proportions or frequencies by specifying the **TESTP=** or **TESTF=** *chisq-option*, respectively. See the section “[Chi-Square Test for One-Way Tables](#)” on page 2551 for more information.

To request Fisher’s exact test for tables larger than 2×2 , specify the **FISHER** option in the **EXACT** statement. Exact *p*-values are also available for the Pearson, likelihood ratio, and Mantel-Haenszel chi-square tests. See the description of the **EXACT** statement for more information.

You can specify the following *chisq-options* in parentheses after the **CHISQ** option:

DF=df

specifies the degrees of freedom for the chi-square tests. The value of *df* must not be zero. If the value of *df* is positive, PROC FREQ uses *df* as the degrees of freedom for the chi-square tests. If the value of *df* is negative, PROC FREQ uses *df* to adjust the default degrees of freedom for the chi-square tests.

By default for one-way tables, the value of *df* is $(n - 1)$, where n is the number of variable levels in the table. By default for two-way tables, the value of *df* is $(r - 1)(c - 1)$, where r is the number of rows in the table and c is the number of columns. See the sections “[Chi-Square Test for One-Way Tables](#)” on page 2551 and “[Chi-Square Tests and Statistics](#)” on page 2550 for more information.

If you specify a negative value of *df*, PROC FREQ adjusts the default degrees of freedom by adding the (negative) value of *df* to the default value to produce the adjusted degrees of freedom. The adjusted degrees of freedom must be positive.

The `DF= chisq-option` specifies or adjusts the degrees of freedom for the following chi-square tests: the Pearson and likelihood ratio goodness-of-fit tests for one-way tables; and the Pearson, likelihood ratio, and Mantel-Haenszel chi-square tests for two-way tables.

LRCHISQ

requests the likelihood ratio goodness-of-fit test for one-way tables. See the section “[Likelihood Ratio Chi-Square Test for One-Way Tables](#)” on page 2552 for more information.

By default, this test is based on the null hypothesis of equal proportions. You can provide null hypothesis proportions or frequencies by specifying the `TESTP=` or `TESTF= chisq-option`, respectively. You can request an exact likelihood ratio goodness-of-fit test by specifying the `LRCHI` option in the EXACT statement.

TESTF=(*values*) | SAS-data-set

specifies null hypothesis frequencies for the one-way chi-square goodness-of-fit tests. See the section “[Chi-Square Test for One-Way Tables](#)” on page 2551 for details. You can list the null frequencies as *values* in parentheses after `TESTF=`. Or you can provide the null frequencies in a secondary input data set by specifying `TESTF=SAS-data-set`. The `TESTF=SAS-data-set` cannot be the same data set that you specify in the `DATA=` option. You can specify only one `TESTF=` or `TESTP=` data set in a single invocation of the procedure.

If you list the null frequencies as *values*, you can separate the *values* with blanks or commas. The *values* must be positive numbers. The number of *values* must equal the number of variable levels in the one-way table. The sum of the *values* must equal the total frequency for the one-way table. Order the *values* to match the order in which the corresponding variable levels appear in the one-way frequency table.

If you provide the null frequencies in a secondary input data set (`TESTF=SAS-data-set`), the variable that contains the null frequencies should be named `_TESTF_`, `TestFrequency`, or `Frequency`. The null frequencies must be positive numbers. The number of frequencies must equal the number of levels in the one-way frequency table, and the sum of the frequencies must equal the total frequency for the one-way table. Order the null frequencies in the data set to match the order in which the corresponding variable levels appear in the one-way frequency table.

TESTP=(*values*) | SAS-data-set

specifies null hypothesis proportions for the one-way chi-square goodness-of-fit tests. See the section “[Chi-Square Test for One-Way Tables](#)” on page 2551 for details. You can list the null proportions as *values* in parentheses after `TESTP=`. Or you can provide the null proportions in a secondary input data set by specifying `TESTP=SAS-data-set`. The `TESTP=SAS-data-set` cannot be the same data set that you specify in the `DATA=` option. You can specify only one `TESTF=` or `TESTP=` data set in a single invocation of the procedure.

If you list the null proportions as *values*, you can separate the *values* with blanks or commas. The *values* must be positive numbers. The number of *values* must equal the number of variable levels in the one-way table. Order the *values* to match the order in which the corresponding variable levels appear in the one-way frequency table. You can specify *values* in probability form as numbers between 0 and 1, where the proportions sum to 1. Or you can specify *values* in percentage form as numbers between 0 and 100, where the percentages sum to 100.

If you provide the null proportions in a secondary input data set (TESTP=*SAS-data-set*), the variable that contains the null proportions should be named `_TESTP_`, `TestPercent`, or `Percent`. The null proportions must be positive numbers. The number of proportions must equal the number of levels in the one-way frequency table. You can provide the proportions in probability form as numbers between 0 and 1, where the proportions sum to 1. Or you can provide the proportions in percentage form as numbers between 0 and 100, where the percentages sum to 100. Order the null proportions in the data set to match the order in which the corresponding variable levels appear in the one-way frequency table.

WARN=*value* | (*values*)

controls the warning message for the validity of the asymptotic Pearson chi-square test. By default, PROC FREQ displays a warning message when more than 20% of the table cells have expected frequencies that are less than 5. If you specify the **NOPRINT** option in the **PROC FREQ** statement, the procedure displays the warning in the log; otherwise, the procedure displays the warning as a footnote in the chi-square table. You can use the **WARN=** option to suppress the warning and to include a warning indicator in the output data set.

The **WARN=** option can take one or more of the following values. If you specify more than one value, enclose the values in parentheses after **WARN=**. For example, **warn = (output noprint)**.

Value of WARN=	Description
OUTPUT	Adds a warning indicator variable to the output data set
NOLOG	Suppresses the chi-square warning message in the log
NOPRINT	Suppresses the chi-square warning message in the display
NONE	Suppresses the chi-square warning message entirely

If you specify the **WARN=OUTPUT** option, the ODS output data set `ChiSq` contains a variable named `Warning` that equals 1 for the Pearson chi-square observation when more than 20% of the table cells have expected frequencies that are less than 5 and equals 0 otherwise. If you specify **WARN=OUTPUT** and also specify the **CHISQ** option in the **OUTPUT** statement, the statistics output data set contains a variable named `WARN_PCHI` that indicates the warning.

The **WARN=NOLOG** option has the same effect as the **NOWARN** option in the **TABLES** statement.

CL

requests confidence limits for the **MEASURES** statistics. If you omit the **MEASURES** option, the **CL** option invokes **MEASURES**. You can set the level of the confidence limits by using the **ALPHA=** option. The default of **ALPHA=0.5** produces 95% confidence limits. See the sections “**Measures of Association**” on page 2556 and “**Confidence Limits**” on page 2556 for more information.

CMH <(cmh-options)>

requests Cochran-Mantel-Haenszel statistics, which test for association between the row and column variables after adjusting for the remaining variables in a multiway table. The Cochran-Mantel-Haenszel statistics include the nonzero correlation statistic, the row mean scores (ANOVA) statistic, and the general association statistic. In addition, for 2×2 tables, the CMH option provides the adjusted Mantel-Haenszel and logit estimates of the odds ratio and relative risks, together with their confidence limits. For stratified 2×2 tables, the CMH option provides the Breslow-Day test for homogeneity of odds ratios. (To request Tarone's adjustment for the Breslow-Day test, specify the **BDT** *cmh-option*.) See the section "Cochran-Mantel-Haenszel Statistics" on page 2592 for details.

You can use the **CMH1** or **CMH2** option to control the number of CMH statistics that PROC FREQ computes.

For stratified 2×2 tables, you can request Zelen's exact test for equal odds ratios by specifying the EQOR option in the **EXACT** statement. See the section "Zelen's Exact Test for Equal Odds Ratios" on page 2598 for details. You can request exact confidence limits for the common odds ratio by specifying the COMOR option in the EXACT statement. This option also provides a common odds ratio test. See the section "Exact Confidence Limits for the Common Odds Ratio" on page 2599 for details.

You can specify the following *cmh-options* in parentheses after the CMH option. These *cmh-options*, which apply to stratified 2×2 tables, are also available with the **CMH1** or **CMH2** option.

BDT

requests Tarone's adjustment in the Breslow-Day test for homogeneity of odds ratios. See the section "Breslow-Day Test for Homogeneity of the Odds Ratios" on page 2598 for details.

GAILSIMON | GS <(COLUMN=1 | 2)>

requests the Gail-Simon test for qualitative interaction, which applies to stratified 2×2 tables. See the section "Gail-Simon Test for Qualitative Interactions" on page 2601 for details.

The COLUMN= option specifies the column of the risk differences to use in computing the Gail-Simon test. By default, PROC FREQ uses column 1 risk differences. If you specify COLUMN=2, PROC FREQ uses column 2 risk differences.

The GAILSIMON *cmh-option* has the same effect as the **GAILSIMON** option in the TABLES statement.

MANTELFLEISS | MF

requests the Mantel-Fleiss criterion for the Mantel-Haenszel statistic for stratified 2×2 tables. See the section "Mantel-Fleiss Criterion" on page 2595 for details.

CMH1 <(cmh-options)>

requests the Cochran-Mantel-Haenszel correlation statistic. This option does not provide the CMH row mean scores (ANOVA) statistic or the general association statistic, which are provided by the **CMH** option. For tables larger than 2×2 , the CMH1 option requires less memory than the CMH option, which can require an enormous amount of memory for large tables.

For 2×2 tables, the CMH1 option also provides the adjusted Mantel-Haenszel and logit estimates of the odds ratio and relative risks, together with their confidence limits. For stratified 2×2 tables, the CMH1 option provides the Breslow-Day test for homogeneity of odds ratios.

The *cmh-options* for CMH1 are the same as the *cmh-options* that are available with the CMH option. See the description of the **CMH** option for details.

CMH2 < (*cmh-options*) >

requests the Cochran-Mantel-Haenszel correlation statistic and the row mean scores (ANOVA) statistic. This option does not provide the CMH general association statistic, which is provided by the **CMH** option. For tables larger than 2×2 , the CMH2 option requires less memory than the CMH option, which can require an enormous amount of memory for large tables.

For 2×2 tables, the CMH1 option also provides the adjusted Mantel-Haenszel and logit estimates of the odds ratio and relative risks, together with their confidence limits. For stratified 2×2 tables, the CMH1 option provides the Breslow-Day test for homogeneity of odds ratios.

The *cmh-options* for CMH2 are the same as the *cmh-options* that are available with the CMH option. See the description of the **CMH** option for details.

CONTENTS= 'string'

specifies the label to use for crosstabulation tables in the contents file, the Results window, and the trace record. For information about output presentation, see the *SAS Output Delivery System: User's Guide*.

If you omit the CONTENTS= option, the contents label for crosstabulation tables is "Cross-Tabular Freq Table" by default.

Note that contents labels for all crosstabulation tables that are produced by a single TABLES statement use the same text. To specify different contents labels for different crosstabulation tables, request the tables in separate TABLES statements and use the CONTENTS= option in each TABLES statement.

To remove the crosstabulation table entry from the contents file, you can specify a null label with CONTENTS="".

The CONTENTS= option affects only contents labels for crosstabulation tables. It does not affect contents labels for other PROC FREQ tables.

To specify the contents label for any PROC FREQ table, you can use PROC TEMPLATE to create a customized table definition. The CONTENTS_LABEL attribute in the DEFINE TABLE statement of PROC TEMPLATE specifies the contents label for the table. See the chapter "The TEMPLATE Procedure" in the *SAS Output Delivery System: User's Guide* for more information.

CONVERGE= *value*

specifies the convergence criterion for computing the polychoric correlation, which you request by specifying the **PLCORR** option. The CONVERGE= *value* must be a positive number. By default, CONVERGE=0.0001. Iterative computation of the polychoric correlation stops when the convergence measure falls below *value* or when the number of iterations exceeds the **MAXITER=** value, whichever happens first. For parameter values that are less than 0.01, the procedure evaluates convergence by using the absolute difference instead of the relative difference. See the section "Polychoric Correlation" on page 2562 for details.

CROSSLIST < **STDRES** >

displays crosstabulation tables in ODS column format instead of the default crosstabulation cell format. In the CROSSLIST table display, the rows correspond to the crosstabulation table cells, and the columns correspond to descriptive statistics such as Frequency and Percent. The CROSSLIST table displays the same information as the default crosstabulation table, but it uses an ODS column format instead of the table cell format. See the section "Multiway Tables" on page 2611 for details about the contents of the CROSSLIST table.

You can control the contents of a CROSSLIST table by specifying the same options available for the default crosstabulation table. These include the **NOFREQ**, **NOPERCENT**, **NOROW**, and **NOCOL** options. You can request additional information in a CROSSLIST table by specifying the **CELLCHI2**,

DEVIATION, EXPECTED, MISSPRINT, and TOTPCT options. You can also display standardized residuals in a CROSSLIST table by specifying the CROSSLIST(STDRES) option (which is not available for the default crosstabulation table).

The FORMAT= and CUMCOL options have no effect on CROSSLIST tables. You cannot specify both the LIST option and the CROSSLIST option in the same TABLES statement.

For CROSSLIST tables, you can use the NOSPARSE option to suppress display of variable levels that have zero frequencies. By default, PROC FREQ displays all levels of the column variable within each level of the row variable, including any levels that have zero frequencies. By default for multiway tables displayed as CROSSLIST tables, the procedure displays all levels of the row variable for each stratum of the table, including any row levels with zero frequencies in the stratum.

You can specify the following *option* in parentheses after the CROSSLIST option:

STDRES

displays the standardized residuals of the table cells in the CROSSLIST table. The standardized residual is the ratio of (*frequency* – *expected*) to its standard error, where *frequency* is the table cell frequency and *expected* is the expected table cell frequency, which is computed under the null hypothesis that the row and column variables are independent. See the section “Standardized Residuals” on page 2552 for more information.

CUMCOL

displays the cumulative column percentages in the cells of the crosstabulation table. The CUMCOL option does not apply to crosstabulation tables produced with the LIST or CROSSLIST option.

DEVIATION

displays the deviation of the frequency from the expected frequency for each cell of the crosstabulation table. See the section “Pearson Chi-Square Test for Two-Way Tables” on page 2551 for details. The DEVIATION option does not apply to crosstabulation tables produced with the LIST option.

EXPECTED

displays the expected cell frequencies under the hypothesis of independence (or homogeneity) for crosstabulation tables. See the section “Pearson Chi-Square Test for Two-Way Tables” on page 2551 for details. The EXPECTED option does not apply to tables produced with the LIST option.

FISHER | EXACT

requests Fisher’s exact test for tables that are larger than 2×2 . (For 2×2 tables, the CHISQ option provides Fisher’s exact test.) This test is also known as the Freeman-Halton test. See the sections “Fisher’s Exact Test” on page 2554 and “Exact Statistics” on page 2601 for more information.

If you omit the CHISQ option in the TABLES statement, the FISHER option invokes CHISQ. You can also request Fisher’s exact test by specifying the FISHER option in the EXACT statement.

NOTE: PROC FREQ computes exact tests by using fast and efficient algorithms that are superior to direct enumeration. Exact tests are appropriate when a data set is small, sparse, skewed, or heavily tied. For some large problems, computation of exact tests might require a substantial amount of time and memory. Consider using asymptotic tests for such problems. Alternatively, when asymptotic methods might not be sufficient for such large problems, consider using Monte Carlo estimation of exact *p*-values. You can request Monte Carlo estimation by specifying the MC *computation-option* in the EXACT statement. See the section “Computational Resources” on page 2604 for more information.

FORMAT=*format-name*

specifies a format for the following crosstabulation table cell values: frequency, expected frequency, and deviation. PROC FREQ also uses the specified format to display the row and column total frequencies and the overall total frequency in crosstabulation tables.

You can specify any standard SAS numeric format or a numeric format defined with the FORMAT procedure. The format length must not exceed 24. If you omit the FORMAT= option, by default PROC FREQ uses the BEST6. format to display frequencies less than 1E6, and the BEST7. format otherwise.

The FORMAT= option applies only to crosstabulation tables displayed in the default format. It does not apply to crosstabulation tables produced with the LIST or CROSSLIST option.

To change display formats in any FREQ table, you can use PROC TEMPLATE. See the chapter “The TEMPLATE Procedure” in the *SAS Output Delivery System: User’s Guide* for more information.

GAILSIMON | GS <(COLUMN=1 | 2)>

requests the Gail-Simon test for qualitative interaction, which applies to stratified 2×2 tables. See the section “[Gail-Simon Test for Qualitative Interactions](#)” on page 2601 for details.

The COLUMN= option specifies the column of the risk differences to use in computing the Gail-Simon test. By default, PROC FREQ uses column 1 risk differences. If you specify COLUMN=2, PROC FREQ uses column 2 risk differences.

JT

requests the Jonckheere-Terpstra test. See the section “[Jonckheere-Terpstra Test](#)” on page 2586 for details. To request exact p -values for the Jonckheere-Terpstra test, specify the JT option in the EXACT statement. See the section “[Exact Statistics](#)” on page 2601 for more information.

LIST

displays two-way to n -way crosstabulation tables in a list format instead of the default crosstabulation cell format. The LIST option displays the entire multiway table in one table, instead of displaying a separate two-way table for each stratum. See the section “[Multiway Tables](#)” on page 2611 for details.

The LIST option is not available when you also specify statistical options. You must use the standard crosstabulation table display or the CROSSLIST display when you request statistical tests or measures.

MAXITER=*number*

specifies the maximum number of iterations for computing the polychoric correlation, which you request by specifying the PLCORR option. The value of *number* must be a positive integer. By default MAXITER=20. Iterative computation of the polychoric correlation stops when the number of iterations exceeds the MAXITER= value or when the convergence measure falls below the CONVERGE= value, whichever happens first. See the section “[Polychoric Correlation](#)” on page 2562 for details.

MAXLEVELS=*n*

specifies the maximum number of variable levels to display in one-way frequency tables. The value of n must be a positive integer. PROC FREQ displays the first n variable levels, matching the order in which the levels appear in the one-way frequency table. (The ORDER= option controls the order of the variable levels. By default, ORDER=INTERNAL, which orders the variable levels by unformatted value.)

The `MAXLEVELS=` option also applies to one-way frequency plots, which you can request by specifying the `PLOTS=FREQPLOT` option when ODS Graphics is enabled.

If you specify the `MISSPRINT` option to display missing levels in the frequency table, the `MAXLEVELS=` option displays the first n nonmissing levels.

The `MAXLEVELS=` option does not apply to the `OUT=` output data set, which includes all variable levels. The `MAXLEVELS=` option does not affect the computation of percentages, statistics, or tests for the one-way table; these values are based on the complete table.

MEASURES

requests measures of association. The `MEASURES` option provides the following statistics and their asymptotic standard errors: gamma, Kendall's tau- b , Stuart's tau- c , Somers' $D(C|R)$, Somers' $D(R|C)$, Pearson and Spearman correlation coefficients, lambda (symmetric and asymmetric), and uncertainty coefficients (symmetric and asymmetric). To request confidence limits for these measures of association, you can specify the `CL` option.

For 2×2 tables, the `MEASURES` option also provides the odds ratio, column 1 relative risk, column 2 relative risk, and the corresponding confidence limits. Alternatively, you can request the odds ratio and relative risks separately (without the other measures of association), by specifying the `REL RISK` option.

See the section “[Measures of Association](#)” on page 2556 for details.

You can use the `TEST` statement to request asymptotic tests for the following measures of association: gamma, Kendall's tau- b , Stuart's tau- c , Somers' $D(C|R)$, Somers' $D(R|C)$, and Pearson and Spearman correlation coefficients. You can use the `EXACT` statement to request exact confidence limits for the odds ratio, exact unconditional confidence limits for the relative risks, and exact tests for the following measures of association: Kendall's tau- b , Stuart's tau- c , Somers' $D(C|R)$ and $D(R|C)$, and Pearson and Spearman correlation coefficients. See the descriptions of the `TEST` and `EXACT` statements for more information.

MISSING

treats missing values as a valid nonmissing level for all `TABLES` variables. The `MISSING` option displays the missing levels in frequency and crosstabulation tables and includes them in all calculations of percentages, tests, and measures.

By default, if you do not specify the `MISSING` or `MISSPRINT` option, an observation is excluded from a table if it has a missing value for any of the variables in the `TABLES` request. When PROC FREQ excludes observations with missing values, it displays the total frequency of missing observations below the table. See the section “[Missing Values](#)” on page 2545 for more information.

MISSPRINT

displays missing value frequencies in frequency and crosstabulation tables but does not include the missing value frequencies in any computations of percentages, tests, or measures.

By default, if you do not specify the `MISSING` or `MISSPRINT` option, an observation is excluded from a table if it has a missing value for any of the variables in the `TABLES` request. When PROC FREQ excludes observations with missing values, it displays the total frequency of missing observations below the table. See the section “[Missing Values](#)” on page 2545 for more information.

NOCOL

suppresses the display of column percentages in crosstabulation table cells.

NOCUM

suppresses the display of cumulative frequencies and percentages in one-way frequency tables. The NOCUM option also suppresses the display of cumulative frequencies and percentages in crosstabulation tables in list format, which you request with the **LIST** option.

NOFREQ

suppresses the display of cell frequencies in crosstabulation tables. The NOFREQ option also suppresses row total frequencies. This option has no effect for one-way tables or for crosstabulation tables in list format, which you request with the **LIST** option.

NOPERCENT

suppresses the display of overall percentages in crosstabulation tables. These percentages include the cell percentages of the total (two-way) table frequency, as well as the row and column percentages of the total table frequency. To suppress the display of cell percentages of row or column totals, use the **NOROW** or **NOCOL** option, respectively.

For one-way frequency tables and crosstabulation tables in list format, the NOPERCENT option suppresses the display of percentages and cumulative percentages.

NOPRINT

suppresses the display of frequency and crosstabulation tables but displays all requested tests and statistics. To suppress the display of all output, including tests and statistics, use the **NOPRINT** option in the PROC FREQ statement.

NOROW

suppresses the display of row percentages in crosstabulation table cells.

NOSPARSE

suppresses the display of cells with a zero frequency count in **LIST** output and omits them from the **OUT=** data set. The NOSPARSE option applies when you specify the **ZEROS** option in the **WEIGHT** statement to include observations with zero weights. By default, the **ZEROS** option invokes the **SPARSE** option, which displays table cells with a zero frequency count in the **LIST** output and includes them in the **OUT=** data set. See the description of the **ZEROS** option for more information.

The NOSPARSE option also suppresses the display of variable levels with zero frequency in **CROSSLIST** tables. By default for **CROSSLIST** tables, PROC FREQ displays all levels of the column variable within each level of the row variable, including any column variable levels with zero frequency for that row. For multiway tables displayed with the **CROSSLIST** option, the procedure displays all levels of the row variable for each stratum of the table by default, including any row variable levels with zero frequency for the stratum.

NOWARN

suppresses the log warning message for the validity of the asymptotic Pearson chi-square test. By default, PROC FREQ provides a validity warning for the asymptotic Pearson chi-square test when more than 20 cells have expected frequencies that are less than 5. This warning message appears in the log if you specify the **NOPRINT** option in the PROC FREQ statement,

The NOWARN option is equivalent to the **CHISQ(WARN=NOLOG)** option. You can also use the **CHISQ(WARN=)** option to suppress the warning message in the display and to request a warning variable in the chi-square ODS output data set or in the **OUTPUT** data set.

OUT=SAS-data-set

names an output data set that contains frequency or crosstabulation table counts and percentages. If more than one table request appears in the TABLES statement, the contents of the OUT= data set correspond to the last table request in the TABLES statement. The OUT= data set variable COUNT contains the frequencies and the variable PERCENT contains the percentages. See the section “[Output Data Sets](#)” on page 2606 for details. You can specify the following options to include additional information in the OUT= data set: [OUTCUM](#), [OUTEXPECT](#), and [OUTPCT](#).

OUTCUM

includes cumulative frequencies and cumulative percentages in the OUT= data set for one-way tables. The variable CUM_FREQ contains the cumulative frequencies, and the variable CUM_PCT contains the cumulative percentages. See the section “[Output Data Sets](#)” on page 2606 for details. The OUTCUM option has no effect for two-way or multiway tables.

OUTEXPECT

includes expected cell frequencies in the OUT= data set for crosstabulation tables. The variable EXPECTED contains the expected cell frequencies. See the section “[Output Data Sets](#)” on page 2606 for details. The EXPECTED option has no effect for one-way tables.

OUTPCT

includes the following additional variables in the OUT= data set for crosstabulation tables:

PCT_COL	percentage of column frequency
PCT_ROW	percentage of row frequency
PCT_TABL	percentage of stratum (two-way table) frequency, for $n > 2$

See the section “[Output Data Sets](#)” on page 2606 for details. The OUTPCT option has no effect for one-way tables.

PLCORR

requests the polychoric correlation coefficient. For 2×2 tables, this statistic is more commonly known as the tetrachoric correlation coefficient, and it is labeled as such in the displayed output. See the section “[Polychoric Correlation](#)” on page 2562 for details.

The PLCORR option provides the polychoric correlation coefficient and its asymptotic standard error. If you also specify the [CL](#) option, PROC FREQ provides confidence limits for the polychoric correlation. You can specify the [PLCORR](#) option in the TEST statement, to request Wald and likelihood ratio tests for the polychoric correlation. If you omit the [MEASURES](#) option, the PLCORR option invokes the MEASURES option.

The [CONVERGE=](#) and [MAXITER=](#) options control the iterative computation of the polychoric correlation coefficient. The [CONVERGE=](#) option specifies the convergence criterion and the [MAXITER=](#) option specifies the maximum number of iterations. By default [CONVERGE=0.0001](#) and [MAXITER=20](#). Iterative computation of the polychoric correlation stops when the number of iterations exceeds the [MAXITER=](#) value or when the convergence measures falls below the [CONVERGE=](#) value, whichever happens first.

PLOTS < (*global-plot-options*) > < = *plot-request* < (*plot-options*) > >

PLOTS < (*global-plot-options*) >

< = (*plot-request* < (*plot-options*) > < ... *plot-request* < (*plot-options*) > >) >

controls the plots that are produced through ODS Graphics. *Plot-requests* identify the plots, and *plot-options* control the appearance and content of the plots. You can specify *plot-options* in parentheses after a *plot-request*. A *global-plot-option* applies to all plots for which it is available unless it is altered by a specific *plot-option*. You can specify *global-plot-options* in parentheses after the PLOTS option.

When you specify only one *plot-request*, you can omit the parentheses around the request. For example:

```
plots=all
plots=freqplot
plots=(freqplot oddsrationplot)
plots(only)=(cumfreqplot deviationplot)
```

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;
proc freq;
  tables treatment*response / chisq plots=freqplot;
  weight wt;
run;
ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

If ODS Graphics is enabled but you do not specify the PLOTS= option, PROC FREQ produces all plots that are associated with the analyses that you request with the exception of the frequency, cumulative frequency, and mosaic plots. To produce a frequency plot or cumulative frequency plot when ODS Graphics is enabled, you must specify the **FREQPLOT** or **CUMFREQPLOT** *plot-request*, respectively, in the PLOTS= option, or you must specify the **PLOTS=ALL** option. To produce a mosaic plot when ODS Graphics is enabled, you must specify the **MOSAICPLOT** *plot-request* in the PLOTS= option, or you must specify the **PLOTS=ALL** option.

PROC FREQ produces the remaining plots (listed in Table 38.11) by default when you request the corresponding TABLES statement options. You can suppress default plots and request specific plots by using the **PLOTS(ONLY)=** option; **PLOTS(ONLY)=(*plot-requests*)** produces only the plots that are specified as *plot-requests*. You can suppress all plots by specifying the **PLOTS=NONE** option. The PLOTS= option has no effect when you specify the **NOPRINT** option in the PROC FREQ statement.

Plot Requests

Table 38.11 lists the available *plot-requests* together with their required TABLES statement options. Descriptions of the *plot-requests* follow the table in alphabetical order.

Table 38.11 Plot Requests

Plot Request	Description	Required TABLES Statement Option
AGREEPLOT	Agreement plot	AGREE ($r \times r$ table)
ALL	All plots	None
CUMFREQPLOT	Cumulative frequency plot	One-way table request
DEVIATIONPLOT	Deviation plot	CHISQ (one-way table)
FREQPLOT	Frequency plot	Any table request
KAPPAPLOT	Kappa plot	AGREE ($h \times r \times r$ table)
MOSAICPLOT	Mosaic plot	Two-way or multiway table request
NONE	No plots	None
ODDSRATIOPLOT	Odds ratio plot	MEASURES or RELRISK ($h \times 2 \times 2$ table)
RELRIKSPLOT	Relative risk plot	MEASURES or RELRISK ($h \times 2 \times 2$ table)
RISKDIFFPLOT	Risk difference plot	RISKDIFF ($h \times 2 \times 2$ table)
WTKAPPAPLOT	Weighted kappa plot	AGREE ($h \times r \times r$ table, $r > 2$)

The following *plot-requests* are available with the PLOTS= option:

AGREEPLOT < (*plot-options*) >

requests an agreement plot (Bangdiwala and Bryan 1987). An agreement plot displays the strength of agreement in a two-way table, where the row and column variables represent two independent ratings of n subjects. For information about agreement plots, see Bangdiwala (1988); Bangdiwala et al. (2008), and Friendly (2000, Section 3.7.2).

To produce an agreement plot, you must also specify the **AGREE** option in the TABLES statement. Agreement statistics and plots are available for two-way square tables, where the number of rows equals the number of columns.

Table 38.12 lists the *plot-options* that are available for agreement plots. See the subsection “Plot Options” for descriptions of the *plot-options*.

Table 38.12 Plot Options for AGREEPLOT

Plot Option	Description	Values
LEGEND=	Legend	YES* or NO
PARTIAL=	Partial agreement	YES* or NO
SHOWSCALE=	Frequency scale	YES* or NO
STATS	Statistics	None

*Default

ALL

requests all plots that are associated with the specified analyses. If you specify the PLOTS=ALL option, PROC FREQ produces the frequency, cumulative frequency, and mosaic plots that are associated with the tables that you request. (PROC FREQ does not produce these plots by default when ODS Graphics is enabled.)

CUMFREQPLOT < (*plot-options*) >

requests a plot of cumulative frequencies. Cumulative frequency plots are available for one-way frequency tables.

To produce a cumulative frequency plot, you must specify the CUMFREQPLOT *plot-request* in the PLOTS= option, or you must specify the PLOTS=ALL option. PROC FREQ does not produce cumulative frequency plots by default when ODS Graphics is enabled.

Table 38.13 lists the *plot-options* that are available for cumulative frequency plots. See the subsection “Plot Options” for descriptions of the *plot-options*.

Table 38.13 Plot Options for CUMFREQPLOT

Plot Option	Description	Values
ORIENT=	Orientation	VERTICAL* or HORIZONTAL
SCALE=	Scale	FREQ* or PERCENT
TYPE=	Type	BARCHART* or DOTPLOT

*Default

DEVIATIONPLOT < (*plot-options*) >

requests a plot of relative deviations from expected frequencies. Deviation plots are available for chi-square analysis of one-way frequency tables. To produce a deviation plot, you must also specify the CHISQ option in the TABLES statement for a one-way frequency table.

Table 38.14 lists the *plot-options* that are available for deviation plots. See the subsection “Plot Options” for descriptions of the *plot-options*.

Table 38.14 Plot Options for DEVIATIONPLOT

Plot Option	Description	Values
NOSTAT	No statistic	None
ORIENT=	Orientation	VERTICAL* or HORIZONTAL
TYPE=	Type	BARCHART* or DOTPLOT

*Default

FREQPLOT < (*plot-options*) >

requests a frequency plot. Frequency plots are available for frequency and crosstabulation tables. For multiway crosstabulation tables, PROC FREQ provides a two-way frequency plot for each stratum (two-way table).

To produce a frequency plot, you must specify the FREQPLOT *plot-request* in the PLOTS= option, or you must specify the PLOTS=ALL option. PROC FREQ does not produce frequency plots by default when ODS Graphics is enabled.

By default, PROC FREQ displays frequency plots as bar charts. You can specify the TYPE=DOTPLOT *plot-option* to display frequency plots as dot plots. You can plot percentages instead of frequencies by specifying the SCALE=PERCENT *plot-option*. There are four frequency plot layouts available, which you can request by specifying the TWOWAY= *plot-option*. See the subsection “Plot Options” for more information.

By default, the primary grouping of graph cells in a two-way layout is by column variable. Row variable levels are then displayed within column variable levels. You can specify the `GROUPBY=ROW` *plot-option* to group first by row variable.

Table 38.15 lists the *plot-options* that are available for frequency plots. See the subsection “Plot Options” for descriptions of the *plot-options*.

The following *plot-options* are available for all frequency plots: `ORIENT=`, `SCALE=`, and `TYPE=`. The following *plot-options* are available for frequency plots of two-way (and multi-way) tables: `GROUPBY=`, `NPANELPOS=`, and `TWOWAY=`. The `NPANELPOS=` *plot-option* is not available with the `TWOWAY=CLUSTER` or `TWOWAY=STACKED` layout, which is always displayed in a single panel.

Table 38.15 Plot Options for FREQPLOT

Plot Option	Description	Values
<code>GROUPBY=**</code>	Primary group	COLUMN* or ROW
<code>NPANELPOS=**</code>	Sections per panel	Number (4*)
<code>ORIENT=</code>	Orientation	VERTICAL* or HORIZONTAL
<code>SCALE=</code>	Scale	FREQ* or PERCENT
<code>TWOWAY=**</code>	Two-way layout	CLUSTER, GROUPHORIZONTAL, GROUPVERTICAL*, or STACKED
<code>TYPE=</code>	Type	BARCHART* or DOTPLOT

*Default

**For two-way tables

KAPPAPLOT < (*plot-options*) >

requests a plot of kappa statistics with confidence limits. Kappa plots are available for multiway square tables and display the kappa statistic (with confidence limits) for each two-way table (stratum). Kappa plots also display the overall kappa statistic unless you specify the `COMMON=NO` *plot-option*. To produce a kappa plot, you must specify the `AGREE` option in the TABLES statement to compute kappa statistics.

Table 38.16 lists the *plot-options* that are available for kappa plots. See the subsection “Plot Options” for descriptions of the *plot-options*.

Table 38.16 Plot Options for KAPPAPLOT and WTKAPPAPLOT

Plot Option	Description	Values
<code>CLDISPLAY=</code>	Error bar type	SERIF*, LINE, or BAR
<code>COMMON=</code>	Overall kappa	YES* or NO
<code>NPANELPOS=</code>	Statistics per graphic	Number
<code>ORDER=</code>	Order of two-way levels	ASCENDING or DESCENDING
<code>RANGE=</code>	Range to display	Values or CLIP
<code>STATS</code>	Statistics	None

*Default

MOSAICPLOT < (*plot-option*) >

requests a mosaic plot. Mosaic plots are available for crosstabulation tables. For multiway tables, PROC FREQ provides a mosaic plot for each two-way table (stratum).

To produce a mosaic plot, you must specify the MOSAICPLOT *plot-request* in the PLOTS= option, or you must specify the PLOTS=ALL option. PROC FREQ does not produce mosaic plots by default when ODS Graphics is enabled.

Mosaic plots display tiles that correspond to the crosstabulation table cells. The areas of the tiles are proportional to the frequencies of the table cells. The column variable is displayed on the X axis, and the tile widths are proportional to the relative frequencies of the column variable levels. The row variable is displayed on the Y axis, and the tile heights are proportional to the relative frequencies of the row levels within column levels. The colors of the tiles correspond to the row variable levels. See Friendly (2000) for more information.

You can specify the following *plot-option* in parentheses after the MOSAICPLOT *plot-request*:

SQUARE

produces a square mosaic plot, where the height of the Y axis equals the width of the X axis. In a square mosaic plot, the scale of the relative frequencies is the same on both axes. By default, PROC FREQ produces a rectangular mosaic plot.

NONE

suppresses all plots.

ODDSRATIOPLOT < (*plot-options*) >

requests a plot of odds ratios with confidence limits. Odds ratio plots are available for multiway 2×2 tables and display the odds ratio (with confidence limits) for each 2×2 table (stratum). To produce an odds ratio plot, you must also specify the MEASURES or RELRISK option in the TABLES statement to compute odds ratios.

If you specify the CMH option in the TABLES statement to compute the common odds ratio for the multiway table, by default the plot displays the common odds ratio. The COMMON=NO *plot-option* suppresses display of the common odds ratio. If you do not specify the CMH option, the common odds ratio is not available to be displayed in the plot.

By default, odds ratio plots display asymptotic confidence limits. You can specify the CL=EXACT *plot-option* to display exact confidence limits for the odds ratios. You must also request computation of exact confidence limits by specifying the OR option in the EXACT statement. To display the common odds ratio with exact confidence limits, you must also specify the COMOR option in the EXACT statement.

Table 38.17 lists the *plot-options* that are available for odds ratio plots. See the subsection “Plot Options” for descriptions of the *plot-options*.

Table 38.17 Plot Options for *ODDSRATIO*PLOT, *RELRISK*PLOT, and *RISKDIFF*PLOT

Plot Option	Description	Values
<i>CL</i> =	Confidence limit type	Type
<i>CLDISPLAY</i> =	Error bar type	SERIF*, LINE, or BAR
<i>COLUMN</i> =**	Risk column	1* or 2
<i>LOGBASE</i> =***	Axis scale	2, E, or 10
<i>NPANELPOS</i> =	Statistics per graphic	Number (All*)
<i>ORDER</i> =	Order of two-way levels	ASCENDING or DESCENDING
<i>RANGE</i> =	Range to display	Values or CLIP
<i>STATS</i>	Statistics	None

*Default

** Available for *RELRISK*PLOT and *RISKDIFF*PLOT*** Available for *ODDSRATIO*PLOT and *RELRISK*PLOT**RELRISK**PLOT <(plot-options)>

requests a plot of relative risks with confidence limits. Relative risk plots are available for multiway 2×2 tables and display the relative risk (with confidence limits) for each 2×2 table (stratum). To produce a relative risk plot, you must also specify the *MEASURES* or *RELRISK* option in the *TABLES* statement to compute relative risks.

If you specify the *CMH* option in the *TABLES* statement to compute the common relative risk for the multiway table, by default the plot displays the common relative risk. The *COMMON=NO* plot-option suppresses display of the common relative risk. If you do not specify the *CMH* option, the common relative risk is not available to be displayed in the plot.

By default, relative risk plots display asymptotic confidence limits. You can specify the *CL=EXACT* plot-option to display exact confidence limits for the relative risks. You must also request computation of exact confidence limits by specifying the *RELRISK* option in the *EXACT* statement. When you specify the *CL=EXACT* plot-option, the relative risk plot does not display the common relative risk.

Table 38.17 lists the plot-options that are available for relative risk plots. See the subsection “Plot Options” for descriptions of the plot-options.

RISKDIFFPLOT <(plot-options)>

requests a plot of risk (proportion) differences with confidence limits. Risk difference plots are available for multiway 2×2 tables and display the risk difference (with confidence limits) for each 2×2 table (stratum). To produce a risk difference plot, you must also specify the *RISKDIFF* option in the *TABLES* statement to compute risk differences.

By default, risk difference plots display asymptotic Wald confidence limits. You can specify the *CL=EXACT* plot-option to display exact confidence limits for the risk differences. You must also request computation of exact confidence limits by specifying the *RISKDIFF* option in the *EXACT* statement.

In addition to Wald and exact confidence limits, you can display the following confidence limit types in a risk difference plot: Agresti-Caffo, Hauck-Anderson, Miettinen-Nurminen, and Newcombe. See the descriptions of the *CL=EXACT* plot-option and the *RISKDIFF* option for more information.

Table 38.17 lists the plot-options that are available for risk difference plots. See the subsection “Plot Options” for descriptions of the plot-options.

WTKAPPAPLOT <(plot-options)>

requests a plot of weighted kappa statistics with confidence limits. Weighted kappa plots are available for multiway square tables and display the weighted kappa statistic (with confidence limits) for each two-way table (stratum). Weighted kappa plots also display the overall weighted kappa statistic unless you specify the **COMMON=NO** *plot-option*.

To produce a weighted kappa plot, you must also specify the **AGREE** option in the TABLES statement to compute weighted kappa statistics. Simple kappa and weighted kappa statistics are equal for 2×2 tables; therefore, PROC FREQ displays weighted kappa statistics and plots only for tables that are larger than 2×2 .

Table 38.16 lists the *plot-options* that are available for weighted kappa plots. See the subsection “Plot Options” for descriptions of the *plot-options*.

Global Plot Options

A *global-plot-option* applies to all plots for which the option is available unless it is altered by an individual *plot-option*. You can specify *global-plot-options* in parentheses after the PLOTS option. For example:

```
plots(order=ascending stats)=(riskdiffplot oddsratioplot)
plots(only)=freqplot
```

The following *plot-options* are available as *global-plot-options*: **CLDISPLAY=**, **COLUMN=**, **COMMON=**, **EXACT**, **LOGBASE=**, **NPANELPOS=**, **ORDER=**, **ORIENT=**, **RANGE=**, **SCALE=**, **STATS**, and **TYPE=**. See the subsection “Plot Options” for description of these *plot-options*.

In addition to these *plot-options*, you can specify the following *global-plot-option* in parentheses after the PLOTS option:

ONLY

suppresses the default plots and requests only the plots that are specified as *plot-requests*.

Plot Options

You can specify the following *plot-options* in parentheses after a *plot-request*:

CL=type

specifies the type of confidence limits to display. The **CL=** *plot-option* is available for the following plots: **ODDSRATIOPLOT**, **RELRIKSPLOT**, and **RISKDIFFPLOT**.

For odds ratio and relative risk plots, the available confidence limit types are asymptotic and exact, which you can request by specifying **CL=ASYMPTOTIC** and **CL=EXACT**, respectively. By default, these plots display asymptotic confidence limits. When you specify **CL=EXACT** to display exact confidence limits, you must also request computation of exact confidence limits by specifying the corresponding option (**OR** or **RELRIKSPLOT**) in the EXACT statement. See the sections “Exact Confidence Limits for the Odds Ratio” on page 2583 and “Exact Unconditional Confidence Limits for the Relative Risk” on page 2584 for more information.

For risk difference plots, the available confidence limit types include the following: **CL=AC** (Agresti-Caffo), **CL=EXACT** (exact unconditional), **CL=HA** (Hauck-Anderson), **CL=MN**

(Miettinen-Nurminen), CL=NEWCOMBE (Newcombe), and CL=WALD (Wald). See the description of the CL= *riskdiff-option* and see the section “Risk Difference Confidence Limits” on page 2574 for more information. If you specify CL=EXACT to display exact confidence limits in the plot, you must also request computation of exact confidence limits by specifying the RISKDIFF option in the EXACT statement.

CLDISPLAY=SERIF | LINE | BAR < width >

controls the appearance of the confidence limit error bars. The CLDISPLAY= *plot-option* is available for the following plots: KAPPAPLOT, ODDSRATIO PLOT, RELRISK PLOT, RISKDIFF PLOT, and WTKAPPAPLOT.

The default value is CLDISPLAY=SERIF, which displays the confidence limits as lines with serifs. CLDISPLAY=LINE displays the confidence limits as plain lines without serifs.

CLDISPLAY=BAR displays the confidence limits as bars. By default, the width of the bars equals the size of the marker for the estimate. You can control the width of the bars and the size of the marker by specifying the value of *width* as a percentage of the distance between bars, $0 < width \leq 1$. The bar might disappear when the value of *width* is very small.

COLUMN=1 | 2

specifies the 2×2 table column to use to compute the risk (proportion). The COLUMN= *plot-option* is available for the relative risk plot (RELRISK PLOT) and the risk difference plot (RISKDIFF PLOT). If you specify COLUMN=1, the plot displays the column 1 relative risks or the column 1 risk difference. Similarly, if you specify COLUMN=2, the plot displays the column 2 relative risks or risk difference. The default is COLUMN=1.

COMMON=YES | NO

controls the display of the common (overall) statistic in plots that display stratum (two-way table) statistics for a multiway table. The COMMON= *plot-option* is available for the following plots: KAPPAPLOT, ODDSRATIO PLOT, RELRISK PLOT, and WTKAPPAPLOT.

By default, COMMON=YES and the plots display the common value when it is available. When you specify the AGREE option in the TABLES statement for a multiway table, PROC FREQ computes overall kappa statistics in addition to kappa statistics for each stratum. When you specify the MEASURES or RELRISK option in the TABLES statement, PROC FREQ computes only stratum-level odds ratios and relative risks; to compute common odds ratios and relative risks, you must also specify the CMH option in the TABLES statement.

COMMON=YES is not available for relative risk plots when you specify the CL=EXACT *plot-option* to display exact confidence limits.

EXACT

requests display of exact confidence limits instead of asymptotic confidence limits. The EXACT *plot-option* is available for the odds ratio plot (ODDSRATIO PLOT), relative risk plot (RELRISK PLOT), and risk difference plot (RISKDIFF PLOT). The EXACT *plot-option* is equivalent to the CL=EXACT *plot-option*.

When you specify the EXACT *plot-option*, you must also request computation of exact confidence limits by specifying the appropriate *statistic-option* in the EXACT statement.

GROUPBY=COLUMN | ROW

specifies the primary grouping for two-way frequency plots. The default is `GROUPBY=COLUMN`, which groups graph cells first by column variable and displays row variable levels within column variable levels. You can specify `GROUPBY=ROW` to group first by row variable. In two-way and multiway table requests, the column variable is the last variable specified and forms the columns of the crosstabulation table. The row variable is the next-to-last variable specified and forms the rows of the table.

By default for a bar chart that is displayed in the `TWOWAY=STACKED` layout, bars correspond to the column variable levels, and row levels are displayed (stacked) within each column bar. By default for a bar chart that is displayed in the `TWOWAY=CLUSTER` layout, bars are first grouped by column variable levels, and row levels are displayed as adjacent bars within each column-level group. You can reverse the default row and column variable grouping by specifying `GROUPBY=ROW`.

LOGBASE=2 | E | 10

applies to the odds ratio plot (`ODDSRATIOPLOT`) and the relative risk plot (`RELRIKSPLOT`). `LOGBASE=` displays the odds ratio or relative risk axis on the log scale that you specify.

LEGEND=YES | NO

applies to the agreement plot (`AGREEPLOT`). `LEGEND=NO` suppresses the legend that identifies the areas of exact and partial agreement. The default is `LEGEND=YES`.

NOSTAT

applies to the deviation plot (`DEVIATIONPLOT`). `NOSTAT` suppresses the chi-square p -value that deviation plot displays by default.

NPANELPOS= n

applies to the following plots: `FREQPLOT` (for two-way and multiway tables), `KAPPAPLOT`, `ODDSRATIOPLOT`, `RELRIKSPLOT`, `RISKDIFFPLOT`, and `WTKAPPAPLOT`.

For kappa, odds ratio, relative risk, risk difference, and weighted kappa plots, `NPANELPOS=` divides the plot into multiple panels that display at most $|n|$ statistics per panel. If n is positive, the number of statistics per panel is balanced; if n is negative, the number of statistics per panel is not balanced. For example, suppose you want to display 21 odds ratios. `NPANELPOS=20` displays two panels, the first with 11 odds ratios and the second with 10 odds ratios; `NPANELPOS=-20` displays 20 odds ratios in the first panel but only one in the second panel. By default, $n = 0$ and all statistics are displayed in a single panel.

For two-way frequency plots, the `NPANELPOS= plot-option` divides the plot into multiple panels that display at most $|n|$ sections per panel. Sections correspond to row or column variable levels, depending on the type of plot and the grouping.

The `NPANELPOS= plot-option` applies to two-way plots that are displayed in the `TWOWAY=GROUPVERTICAL` or `TWOWAY=GROUPHORIZONTAL` layout. The `NPANELPOS= plot-option` does not apply to the `TWOWAY=CLUSTER` and `TWOWAY=STACKED` layouts, which are always displayed in a single panel.

If n is positive, the number of sections per panel is balanced; if n is negative, the number of sections per panel is not balanced. By default for frequency plots, $n = 4$ and each panel includes at most four sections.

ORDER=ASCENDING | DESCENDING

displays the statistics in sorted order. By default, the statistics are displayed in the order in which the two-way table strata appear in the multiway table display. The ORDER= *plot-option* applies to the following plots: [KAPPAPLOT](#), [ODDSRATIO PLOT](#), [REL RISK PLOT](#), [RISKDIFF PLOT](#), and [WTKAPPAPLOT](#).

ORIENT=HORIZONTAL | VERTICAL

controls the orientation of the plot. The ORIENT= *plot-option* applies to the following plots: [CUMFREQ PLOT](#), [DEVIATION PLOT](#), and [FREQ PLOT](#).

ORIENT=HORIZONTAL places the variable levels on the Y axis and the frequencies, percentages, or statistic values on the X axis. ORIENT=VERTICAL places the variable levels on the X axis. The default orientation is ORIENT=VERTICAL for bar charts ([TYPE=BAR CHART](#)) and ORIENT=HORIZONTAL for dot plots ([TYPE=DOT PLOT](#)).

PARTIAL=YES | NO

controls the display of partial agreement in the agreement plot ([AGREE PLOT](#)). PARTIAL=NO suppresses the display of partial agreement. When you specify PARTIAL=NO, the agreement plot displays only exact agreement. Exact agreement includes the diagonal cells of the square table, where the row and column variable levels are the same. Partial agreement includes the adjacent off-diagonal table cells, where the row and column values are within one level of exact agreement. The default is PARTIAL=YES.

RANGE=(*< min >* *< ,max >*) | CLIP

specifies the range of values to display. The RANGE= *plot-option* applies to the following plots: [KAPPAPLOT](#), [ODDSRATIO PLOT](#), [REL RISK PLOT](#), [RISKDIFF PLOT](#), and [WTKAPPAPLOT](#). If you specify RANGE=CLIP, the confidence limits are clipped and the display range is determined by the minimum and maximum values of the statistics. By default, the display range includes all confidence limits.

SCALE=FREQ | LOG | PERCENT | SQRT

specifies the scale of the frequencies to display. The SCALE= *plot-option* applies to the frequency plot ([FREQ PLOT](#)) and the cumulative frequency plot ([CUMFREQ PLOT](#)).

The default is SCALE=FREQ, which displays unscaled frequencies. SCALE=LOG displays log (base 10) frequencies. SCALE=PERCENT displays percentages (relative frequencies). SCALE=SQRT displays square roots of the frequencies, which produces a plot known as a *rootogram*.

SHOWSCALE=YES | NO

controls the display of the cumulative frequency scale on the right side of the agreement plot ([AGREE PLOT](#)). SHOWSCALE=NO suppresses the display of the scale. The default is SHOWSCALE=YES.

SQUARE

requests a square mosaic plot ([MOSAIC PLOT](#)), where the height of the Y axis equals the width of the X axis. In a square mosaic plot, the scale of the relative frequencies is the same on both axes. By default, the mosaic plot area is rectangular.

STATS

displays statistic values in the plot. For the following plots, the *STATS plot-option* displays the statistics and their confidence limits on the right side of the plot: **KAPPAPLOT**, **ODDSRATIOPLOT**, **RELRISKPLOT**, **RISKDIFFPLOT**, and **WTKAPPAPLOT**.

For the agreement plot (**AGREEPLOT**), *STATS* displays the values of the kappa statistic, the weighted kappa statistic, and the B_n measure (Bangdiwala and Bryan 1987).

If you do not request the *STATS plot-option*, these plots do not display the statistic values.

TWOWAY=CLUSTER | GROUPTHORIZONTAL | GROUPVERTICAL | STACKED

specifies the layout for two-way frequency plots.

All **TWOWAY=** layouts are available for bar charts (**TYPE=BARCHART**). All **TWOWAY=** layouts except **TWOWAY=CLUSTER** are available for dot plots (**TYPE=DOTPLOT**). The **ORIENT=** and **GROUPBY=** *plot-options* are available for all **TWOWAY=** layouts.

The default two-way layout is **TWOWAY=GROUPVERTICAL**, which produces a grouped plot that has a vertical common baseline. By default for bar charts (**TYPE=BARCHART**, **ORIENT=VERTICAL**), the X axis displays column variable levels, and the Y axis displays frequencies. The plot includes a vertical (Y-axis) block for each row variable level. The relative positions of the graph cells in this plot layout are the same as the relative positions of the table cells in the crosstabulation table. You can reverse the default row and column grouping by specifying the **GROUPBY=ROW** *plot-option*.

The **TWOWAY=GROUPTHORIZONTAL** layout produces a grouped plot that has a horizontal common baseline. By default (**GROUPBY=COLUMN**), the plot displays a block on the X axis for each column variable level. Within each column-level block, the plot displays row variable levels.

The **TWOWAY=STACKED** layout produces stacked displays of frequencies. By default (**GROUPBY=COLUMN**) in a stacked bar chart, the bars correspond to column variable levels, and row levels are stacked within each column level. By default in a stacked dot plot, the dotted lines correspond to column levels, and cell frequencies are plotted as data dots on the corresponding column line. The dot color identifies the row level.

The **TWOWAY=CLUSTER** layout, which is available only for bar charts, displays groups of adjacent bars. By default, the primary grouping is by column variable level, and row levels are displayed within each column level.

You can reverse the default row and column grouping in any layout by specifying the **GROUPBY=ROW** *plot-option*. The default is **GROUPBY=COLUMN**, which groups first by column variable.

TYPE=BARCHART | DOTPLOT

specifies the plot type for frequency (**FREQPLOT**), cumulative frequency (**CUMFREQPLOT**), and deviation plots (**DEVIATIONPLOT**). **TYPE=BARCHART** produces a bar chart and **TYPE=DOTPLOT** produces a dot plot. The default is **TYPE=BARCHART**.

PRINTKWT

displays the weights that PROC FREQ uses to compute the weighted kappa coefficient. You must also specify the **AGREE** option to request the weighted kappa coefficient. You can specify (WT=FC) with the **AGREE** option to request Fleiss-Cohen weights. By default, PROC FREQ uses Cicchetti-Allison weights to compute the weighted kappa coefficient. See the section “[Weighted Kappa Coefficient](#)” on page 2590 for details.

RELRISK | OR

requests relative risk measures and their confidence limits for 2×2 tables. These measures include the odds ratio and the column 1 and 2 relative risks. See the section “[Odds Ratio and Relative Risks for \$2 \times 2\$ Tables](#)” on page 2582 for details.

You can also obtain the RELRISK measures by specifying the **MEASURES** option, which produces other measures of association in addition to the relative risks.

You can request exact confidence limits for the odds ratio by specifying the **OR** option in the **EXACT** statement. You can request exact unconditional confidence limits for the relative risks by specifying the **RELRISK** option in the **EXACT** statement. See the sections “[Exact Confidence Limits for the Odds Ratio](#)” on page 2583 and “[Exact Unconditional Confidence Limits for the Relative Risk](#)” on page 2584 for more information.

RISKDIFF < (*riskdiff-options*) >

requests risks (binomial proportions) and risk differences for 2×2 tables. When you specify the **RISKDIFF** option, PROC FREQ provides the row 1 risk, row 2 risk, total (overall) risk, and risk difference (row 1 – row 2), together with their asymptotic standard errors and Wald confidence limits. PROC FREQ also provides exact (Clopper-Pearson) confidence limits for the row 1, row 2, and total risks by default. You can request exact unconditional confidence limits for the risk difference by specifying the **RISKDIFF** option in the **EXACT** statement. See the section “[Risks and Risk Differences](#)” on page 2572 for details. PROC FREQ displays these results in the column 1 and column 2 “Risk Estimates” tables.

You can specify *riskdiff-options* in parentheses after the **RISKDIFF** option to request tests and additional confidence limits for the risk difference. [Table 38.18](#) summarizes the *riskdiff-options*.

The **EQUIV**, **NONINF**, and **SUP** *riskdiff-options* request tests of equivalence, noninferiority, and superiority, respectively, for the risk difference. Available test methods include Farrington-Manning (score), Hauck-Anderson, and Newcombe (hybrid-score), in addition to the Wald test.

As part of the noninferiority, superiority, and equivalence analyses, PROC FREQ provides test-based confidence limits that have a confidence coefficient of $100(1 - 2\alpha)\%$ (Schuirmann 1999). The **ALPHA=** option determines the confidence level, and the default of **ALPHA=0.05** produces 90% confidence limits. See the sections “[Noninferiority Tests](#)” on page 2577 and “[Equivalence Tests](#)” on page 2580 for details.

The **CL=** *riskdiff-option* requests confidence limits for the risk difference. Available confidence limit types include Agresti-Caffo, exact unconditional, Hauck-Anderson, Miettinen-Nurminen, Newcombe, and Wald. Continuity-corrected Newcombe and Wald confidence limits are also available. You can request more than one type of confidence limits in the same analysis. PROC FREQ displays the confidence limits in the “Proportion (Risk) Difference Confidence Limits” table.

The **ALPHA=** option determines the level of the confidence limits that the **CL= riskdiff-option** provides. The default of **ALPHA=0.05** produces 95% confidence limits for the risk difference.

The **CL=EXACT riskdiff-option** displays exact unconditional confidence limits in the “Proportion (Risk) Difference Confidence Limits” table. When you use **CL=EXACT**, you must also request computation of the exact confidence limits by specifying the **RISKDIFF** option in the **EXACT** statement.

Table 38.18 RISKDIFF (Proportion Difference) Options

Option	Description
COLUMN=1 2	Specifies the risk column
CORRECT	Requests continuity correction
NORISKS	Suppresses default risk tables
Request Confidence Limits	
CL=AC	Requests Agresti-Caffo confidence limits
CL=EXACT	Displays exact confidence limits
CL=HA	Requests Hauck-Anderson confidence limits
CL=MN	Requests Miettinen-Nurminen confidence limits
CL=NEWCOMBE	Requests Newcombe confidence limits
CL=WALD	Requests Wald confidence limits
Request Tests	
EQUAL	Requests an equality test
EQUIV EQUIVALENCE	Requests an equivalence test
NONINF NONINFERIORITY	Requests a noninferiority test
SUP SUPERIORITY	Requests a superiority test
MARGIN=	Specifies the test margin
METHOD=	Specifies the test method
VAR=SAMPLE NULL	Specifies the test variance

You can specify the following *riskdiff-options* in parentheses after the **RISKDIFF** option:

CL=type | (types)

requests confidence limits for the risk difference. You can specify one or more *types* of confidence limits. When you specify only one *type*, you can omit the parentheses around the request. PROC FREQ displays the confidence limits in the “Proportion (Risk) Difference Confidence Limits” table.

The **ALPHA=** option determines the confidence level, and the default of **ALPHA=0.05** produces 95% confidence limits for the risk difference. This differs from the test-based confidence limits that are provided with the equivalence, noninferiority, and superiority tests (**EQUIV**, **NONINF**, and **SUP**), which have a confidence coefficient of $100(1 - 2\alpha)\%$ (Schuirmann 1999).

You can specify **CL=** with or without requests for risk difference tests. The confidence limits produced by **CL=** do not depend on the tests that you request and do not use the value of the test margin (which you specify by using **MARGIN= riskdiff-option**).

You can control the risk column for the confidence limits by specifying the **COLUMN= riskdiff-option**. If you do not specify **COLUMN=**, PROC FREQ provides confidence limits for the column 1 risk difference by default.

The following *types* of confidence limits are available:

AC | AGRESTICAFFO

requests Agresti-Caffo confidence limits for the risk difference. See the subsection “Agresti-Caffo Confidence Limits” in the section “Risk Difference Confidence Limits” on page 2574 for details.

EXACT

displays exact unconditional confidence limits for the risk difference in the “Proportion (Risk) Difference Confidence Limits” table. You must also request computation of the exact confidence limits by specifying the **RISKDIFF** option in the **EXACT** statement.

PROC FREQ computes the confidence limits by inverting two separate one-sided exact tests (tail method), where the tests are based on the unstandardized risk difference by default. If you specify the **RISKDIFF(METHOD=SCORE)** option in the **EXACT** statement, the tests are based on the score statistic. See the **RISKDIFF** option in the **EXACT** statement and the section “Exact Unconditional Confidence Limits for the Risk Difference” on page 2580 for more information.

By default, PROC FREQ also displays these exact confidence limits in the “Risk Estimates” table. You can suppress this table by specifying the **NORISKS** *riskdiff-option*.

HA

requests Hauck-Anderson confidence limits for the risk difference. See the subsection “Hauck-Anderson Confidence Limits” in the section “Risk Difference Confidence Limits” on page 2574 for details.

MN < (CORRECT=NO | MEE) >

requests Miettinen-Nurminen confidence limits for the risk difference. See the subsection “Miettinen-Nurminen Confidence Limits” in the section “Risk Difference Confidence Limits” on page 2574 for details. By default, the Miettinen-Nurminen confidence limits include a bias correction factor (Miettinen and Nurminen 1985; Newcombe and Nurminen 2011). If you specify **CL=MN(CORRECT=NO)**, PROC FREQ provides the uncorrected form of the confidence limits (Mee 1984).

NEWCOMBE | SCORE | WILSON < (CORRECT) >

requests Newcombe hybrid-score confidence limits for the risk difference. If you specify **CL=NEWCOMBE(CORRECT)** or the **CORRECT** *riskdiff-option*, the Newcombe confidence limits include a continuity correction. See the subsection “Newcombe Confidence Limits” in the section “Risk Difference Confidence Limits” on page 2574 for details.

WALD < (CORRECT) >

requests Wald confidence limits for the risk difference. If you specify **CL=WALD(CORRECT)** or the **CORRECT** *riskdiff-option*, the Wald confidence limits include a continuity correction. See the subsection “Wald Confidence Limits” in the section “Risk Difference Confidence Limits” on page 2574 for details.

COLUMN=1 | 2 | BOTH

specifies the table column for which to compute the risk difference tests (**EQUAL**, **EQUIV**, **NONINF**, and **SUP**) and the risk difference confidence limits (which are requested by the **CL=** *riskdiff-option*).

If you do not specify `COLUMN=`, PROC FREQ provides the risk difference tests and confidence limits for column 1 by default. The `COLUMN=` option has no effect on the “Risk Estimates” table, which is produced for both column 1 and column 2. You can suppress the “Risk Estimates” table by specifying the `NORISKS riskdiff-option`.

CORRECT

includes a continuity correction in the Wald confidence limits, Wald tests, and Newcombe confidence limits. See the section “Risks and Risk Differences” on page 2572 for details.

EQUAL

requests a test of the null hypothesis that the risk difference equals zero. PROC FREQ provides an asymptotic Wald test of equality. If you specify the `CORRECT riskdiff-option`, the Wald test includes a continuity correction. If you specify the `VAR=NULL riskdiff-option`, the test uses the null (test-based) variance instead of the sample-based variance. See the section “Equality Test” on page 2576 for details.

EQUIV | EQUIVALENCE

requests a test of equivalence for the risk difference. See the section “Equivalence Tests” on page 2580 for details. You can specify the equivalence test margins with the `MARGIN= riskdiff-option` and the test method with the `METHOD= riskdiff-option`. PROC FREQ uses `METHOD=WALD` by default.

MARGIN=value | (lower,upper)

specifies the margin for the noninferiority, superiority, and equivalence tests, which you request with the `NONINF`, `SUP`, and `EQUIV riskdiff-options`, respectively. If you do not specify `MARGIN=`, PROC FREQ uses a margin of 0.2 by default.

For noninferiority and superiority tests, specify a single *value* for `MARGIN=`. The `MARGIN=value` must be a positive number. You can specify *value* as a number between 0 and 1. Or you can specify *value* in percentage form as a number between 1 and 100, and PROC FREQ converts that number to a proportion. The procedure treats the value 1 as 1%.

For an equivalence test, you can specify a single `MARGIN= value`, or you can specify both *lower* and *upper* values. If you specify a single `MARGIN= value`, it must be a positive number, as described previously. If you specify a single `MARGIN= value` for an equivalence test, PROC FREQ uses $-value$ as the lower margin and *value* as the upper margin for the test. If you specify both *lower* and *upper* values for an equivalence test, you can specify them in proportion form as numbers between -1 or 1 . Or you can specify them in percentage form as numbers between -100 and 100 , and PROC FREQ converts the numbers to proportions. The value of *lower* must be less than the value of *upper*.

METHOD=method

specifies the method for the noninferiority, superiority, and equivalence analyses, which you request with the `NONINF`, `SUP`, and `EQUIV riskdiff-options`, respectively. If you do not specify the `METHOD= riskdiff-option`, PROC FREQ uses `METHOD=WALD` by default.

The following *methods* are available:

FM

requests Farrington-Manning (score) tests and test-based confidence limits for the equivalence, noninferiority, and superiority analyses. See the subsection “Farrington-Manning Test” in the section “Noninferiority Tests” on page 2577 for details.

HA

requests Hauck-Anderson tests and confidence limits for the equivalence, noninferiority, and superiority analyses. See the subsection “Hauck-Anderson Test” in the section “Noninferiority Tests” on page 2577 for details.

NEWCOMBE | SCORE | WILSON

requests Newcombe (hybrid-score) confidence limits for the equivalence, noninferiority, and superiority analyses. If you specify the **CORRECT** *riskdiff-option*, the Newcombe confidence limits include a continuity correction. See the subsection “Newcombe Noninferiority Analysis” in the section “Noninferiority Tests” on page 2577 for details.

WALD

requests Wald tests and confidence limits for the equivalence, noninferiority, and superiority analyses. If you specify the **CORRECT** *riskdiff-option*, the Wald confidence limits include a continuity correction. If you specify the **VAR=NULL** *riskdiff-option*, the tests and confidence limits use the null (test-based) variance instead of the sample-based variance. See the subsection “Wald Test” in the section “Noninferiority Tests” on page 2577 for details.

NONINF | NONINFERIORITY

requests a test of noninferiority for the risk difference. See the section “Noninferiority Tests” on page 2577 for details. You can specify the test margin with the **MARGIN=** *riskdiff-option* and the test method with the **METHOD=** *riskdiff-option*. PROC FREQ uses **METHOD=WALD** by default.

NORISKS

suppresses display of the “Risk Estimates” tables, which the **RISKDIFF** option produces by default for column 1 and column 2. The “Risk Estimates” tables contain the risks and risk differences, together with their asymptotic standard errors, Wald confidence limits, and exact confidence limits.

SUP | SUPERIORITY

requests a test of superiority for the binomial proportion. See the section “Superiority Test” on page 2579 for details. You can specify the test margin with the **MARGIN=** *riskdiff-option* and the test method with the **METHOD=** *riskdiff-option*. PROC FREQ uses **METHOD=WALD** by default.

VAR=SAMPLE | NULL

specifies the type of variance estimate to use in the Wald tests of noninferiority, superiority, equivalence, and equality. The default is **VAR=SAMPLE**, which uses the sample-based variance. **VAR=NULL** uses a test-based variance that is computed from the null hypothesis risk difference value. See the sections “Equality Test” on page 2576 and “Noninferiority Tests” on page 2577 for details.

SCORES=type

specifies the type of row and column scores that PROC FREQ uses to compute the following statistics: Mantel-Haenszel chi-square, Pearson correlation, Cochran-Armitage test for trend, weighted kappa coefficient, and Cochran-Mantel-Haenszel statistics. The value of *type* can be one of the following:

- MODRIDIT
- RANK
- RIDIT
- TABLE

See the section “[Scores](#)” on page 2549 for descriptions of these score types.

If you do not specify the SCORES= option, PROC FREQ uses SCORES=TABLE by default. For character variables, the row and column TABLE scores are the row and column numbers. That is, the TABLE score is 1 for row 1, 2 for row 2, and so on. For numeric variables, the row and column TABLE scores equal the variable values. See the section “[Scores](#)” on page 2549 for details. Using MODRIDIT, RANK, or RIDIT scores yields nonparametric analyses.

You can use the [SCOROUT](#) option to display the row and column scores.

SCOROUT

displays the row and column scores that PROC FREQ uses to compute score-based tests and statistics. You can specify the score type with the SCORES= option. See the section “[Scores](#)” on page 2549 for details.

The scores are computed and displayed only when PROC FREQ computes statistics for two-way tables. You can use ODS to store the scores in an output data set. See the section “[ODS Table Names](#)” on page 2617 for more information.

SPARSE

reports all possible combinations of the variable values for an n -way table when $n > 1$, even if a combination does not occur in the data. The SPARSE option applies only to crosstabulation tables displayed in LIST format and to the OUT= output data set. If you do not use the LIST or OUT= option, the SPARSE option has no effect.

When you specify the SPARSE and LIST options, PROC FREQ displays all combinations of variable values in the table listing, including those with a frequency count of zero. By default, without the SPARSE option, PROC FREQ does not display zero-frequency levels in LIST output. When you use the SPARSE and OUT= options, PROC FREQ includes empty crosstabulation table cells in the output data set. By default, PROC FREQ does not include zero-frequency table cells in the output data set.

See the section “[Missing Values](#)” on page 2545 for more information.

TOTPCT

displays the percentage of the total multiway table frequency in crosstabulation tables for n -way tables, where $n > 2$. By default, PROC FREQ displays the percentage of the individual two-way table frequency but does not display the percentage of the total frequency for multiway crosstabulation tables. See the section “[Multiway Tables](#)” on page 2611 for more information.

The percentage of total multiway table frequency is displayed by default when you specify the LIST option. It is also provided by default in the PERCENT variable in the OUT= output data set.

TREND

requests the Cochran-Armitage test for trend. The table must be $2 \times C$ or $R \times 2$ to compute the trend test. See the section “[Cochran-Armitage Test for Trend](#)” on page 2585 for details. To request exact p -values for the trend test, specify the TREND option in the EXACT statement. See the section “[Exact Statistics](#)” on page 2601 for more information.

TEST Statement

TEST *test-options* ;

The TEST statement requests asymptotic tests for measures of association and measures of agreement. The *test-options* identify which tests to compute. Table 38.19 lists the available *test-options*, together with their corresponding TABLES statement options. Descriptions of the *test-options* follow the table in alphabetical order.

For each measure of association or agreement that you request in the TEST statement, PROC FREQ provides an asymptotic test that the measure equals zero. The procedure displays the asymptotic standard error under the null hypothesis, the test statistic, and the one-sided and two-sided *p*-values. Additionally, PROC FREQ reports the confidence limits for the measure. The ALPHA= option in the TABLES statement determines the confidence level, which by default equals 0.05 and provides 95% confidence limits. See the sections “Asymptotic Tests” on page 2556 and “Confidence Limits” on page 2556 for details. Also see the sections “Measures of Association” on page 2556 and “Tests and Measures of Agreement” on page 2588 for information about the individual measures.

You can also request exact tests for selected measures of association and agreement by using the EXACT statement. See the section “Exact Statistics” on page 2601 for more information.

Using the TEST Statement with the TABLES Statement

You must use a TABLES statement with the TEST statement. If you use only one TABLES statement, you do not need to specify the same options in both the TABLES and TEST statements; when you specify an option in the TEST statement, PROC FREQ automatically invokes the corresponding TABLES statement option. However, when you use the TEST statement with multiple TABLES statements, you must specify options in the TABLES statements to request statistics. PROC FREQ then provides asymptotic tests for those statistics that you also specify in the TEST statement.

Table 38.19 TEST Statement Options

Test Option	Asymptotic Tests	Required TABLES Statement Option
AGREE	Simple and weighted kappa coefficients	AGREE
GAMMA	Gamma	ALL or MEASURES
KAPPA	Simple kappa coefficient	AGREE
KENTB	Kendall's tau- <i>b</i>	ALL or MEASURES
MEASURES	Gamma, Kendall's tau- <i>b</i> , Stuart's tau- <i>c</i> , Somers' $D(C R)$, Somers' $D(R C)$, Pearson and Spearman correlations	ALL or MEASURES
PCORR	Pearson correlation coefficient	ALL or MEASURES
PLCORR	Polychoric correlation	PLCORR
SCORR	Spearman correlation coefficient	ALL or MEASURES
SMDCR	Somers' $D(C R)$	ALL or MEASURES
SMDRC	Somers' $D(R C)$	ALL or MEASURES
STUTC	Stuart's tau- <i>c</i>	ALL or MEASURES
WTKAP	Weighted kappa coefficient	AGREE

You can specify the following *test-options* in the TEST statement.

AGREE

requests asymptotic tests for the simple kappa coefficient and the weighted kappa coefficient. See the sections “[Simple Kappa Coefficient](#)” on page 2589 and “[Weighted Kappa Coefficient](#)” on page 2590 for details.

The **AGREE** option in the TABLES statement provides estimates, standard errors, and confidence limits for kappa coefficients. You can request exact tests for kappa coefficients by using the **EXACT** statement.

Kappa coefficients are defined only for square tables, where the number of rows equals the number of columns. Kappa coefficients are not computed for tables that are not square. For 2×2 tables, the weighted kappa coefficient is identical to the simple kappa coefficient, and PROC FREQ presents only the simple kappa coefficient.

GAMMA

requests an asymptotic test for the gamma statistic. See the section “[Gamma](#)” on page 2557 for details. The **MEASURES** option in the TABLES statement provides the gamma statistic and its asymptotic standard error.

KAPPA

requests an asymptotic test for the simple kappa coefficient. See the section “[Simple Kappa Coefficient](#)” on page 2589 for details.

The **AGREE** option in the TABLES statement provides the kappa statistic, its standard error, and its confidence limits. You can request an exact test for the simple kappa coefficient by specifying the **KAPPA** option in the EXACT statement.

Kappa coefficients are defined only for square tables, where the number of rows equals the number of columns. PROC FREQ does not compute kappa coefficients for tables that are not square.

KENTB | TAUB

requests an asymptotic test for Kendall’s tau-*b*. See the section “[Kendall’s Tau-b](#)” on page 2558 for details.

The **MEASURES** option in the TABLES statement provides Kendall’s tau-*b* and its standard error. You can request an exact test for Kendall’s tau-*b* by specifying the **KENTB** option in the EXACT statement.

MEASURES

requests asymptotic tests for the following measures of association: gamma, Kendall’s tau-*b*, Pearson correlation coefficient, Somers’ $D(C|R)$, Somers’ $D(R|C)$, Spearman correlation coefficient, and Stuart’s tau-*c*. See the section “[Measures of Association](#)” on page 2556 for details.

The **MEASURES** option in the TABLES statement provides measures of association and their asymptotic standard errors. You can request exact tests for selected measures by using the **EXACT** statement.

PCORR

requests an asymptotic test for the Pearson correlation coefficient. See the section “[Pearson Correlation Coefficient](#)” on page 2559 for details.

The **MEASURES** option in the TABLES statement provides the Pearson correlation and its standard error. You can request an exact test for the Pearson correlation by specifying the **PCORR** option in the EXACT statement.

PLCORR

requests Wald and likelihood ratio tests for the polychoric correlation coefficient. See the section “[Polychoric Correlation](#)” on page 2562 for details.

The **PLCORR** option in the TABLES statement provides the polychoric correlation and its standard error.

SCORR

requests an asymptotic test for the Spearman correlation coefficient. See the section “[Spearman Rank Correlation Coefficient](#)” on page 2560 for details.

The **MEASURES** option in the TABLES statement provides the Spearman correlation and its standard error. You can request an exact test for the Spearman correlation by specifying the **SCORR** option in the EXACT statement.

SMDCR

requests an asymptotic test for Somers’ $D(C|R)$. See the section “[Somers’ D](#)” on page 2559 for details.

The **MEASURES** option in the TABLES statement provides Somers’ $D(C|R)$ and its standard error. You can request an exact test for Somers’ $D(C|R)$ by specifying the **SMDCR** option in the EXACT statement.

SMDRC

requests an asymptotic test for Somers’ $D(R|C)$. See the section “[Somers’ D](#)” on page 2559 for details.

The **MEASURES** option in the TABLES statement provides Somers’ $D(R|C)$ and its standard error. You can request an exact test for Somers’ $D(R|C)$ by specifying the **SMDRC** option in the EXACT statement.

STUTC | TAUC

requests an asymptotic test for Stuart’s tau- c . See the section “[Stuart’s Tau-c](#)” on page 2558 for details.

The **MEASURES** option in the TABLES statement provides Stuart’s tau- c and its standard error. You can request an exact test for Stuart’s tau- c by specifying the **STUTC** option in the EXACT statement.

WTKAP

requests an asymptotic test for the weighted kappa coefficient. See the section “[Weighted Kappa Coefficient](#)” on page 2590 for details.

The **AGREE** option in the TABLES statement provides the weighted kappa statistic, its standard error, and its confidence limits. You can request an exact test for weighted kappa by specifying the **WTKAP** option in the EXACT statement.

Kappa coefficients are defined only for square tables, where the number of rows equals the number of columns. PROC FREQ does not compute kappa coefficients for tables that are not square. For 2×2 tables, the weighted kappa coefficient is identical to the simple kappa coefficient, and PROC FREQ presents only the simple kappa coefficient.

WEIGHT Statement

WEIGHT *variable* </ *option* > ;

The WEIGHT statement names a numeric variable that provides a weight for each observation in the input data set. The WEIGHT statement is most commonly used to input cell count data. See the section “[Inputting Frequency Counts](#)” on page 2544 for more information. If you use a WEIGHT statement, PROC FREQ assumes that an observation represents n observations, where n is the value of *variable*. The value of the WEIGHT variable is not required to be an integer.

If the value of the WEIGHT variable is missing, PROC FREQ does not use that observation in the analysis. If the value of the WEIGHT variable is zero, PROC FREQ ignores the observation unless you specify the **ZEROS** option, which includes observations with zero weights. If you do not specify a WEIGHT statement, PROC FREQ assigns a weight of one to each observation. The sum of the WEIGHT variable values represents the total number of observations.

If any value of the WEIGHT variable is negative, PROC FREQ displays the frequencies computed from the weighted values but does not compute percentages and statistics. If you create an output data set by using the **OUT=** option in the TABLES statement, PROC FREQ assigns missing values to the PERCENT variable. PROC FREQ also assigns missing values to the variables that the OUTEXPECT and OUTPCT options provide. If any value of the WEIGHT variable is negative, you cannot create an output data set by using the **OUTPUT** statement because statistics are not computed when there are negative weights.

You can specify the following *option* in the WEIGHT statement:

ZEROS

includes observations with zero weight values. By default, PROC FREQ ignores observations with zero weights.

If you specify the ZEROS option, frequency and crosstabulation tables display any levels corresponding to observations with zero weights. Without the ZEROS option, PROC FREQ does not process observations with zero weights, and so does not display levels that contain only observations with zero weights.

With the ZEROS option, PROC FREQ includes levels with zero weights in the chi-square goodness-of-fit test for one-way tables. Also, PROC FREQ includes any levels with zero weights in binomial computations for one-way tables. This makes it possible to compute binomial tests and estimates when the specified level contains no observations with positive weights.

For two-way tables, the ZEROS option enables computation of kappa statistics when there are levels that contain no observations with positive weight. For more information, see the section “[Tables with Zero Rows and Columns](#)” on page 2592.

Note that even with the ZEROS option, PROC FREQ does not compute the **CHISQ** or **MEASURES** statistics for two-way tables when the table has a zero row or zero column because most of these statistics are undefined in this case.

The ZEROS option invokes the **SPARSE** option in the TABLES statement, which includes table cells with a zero frequency count in the **LIST** output and in the **OUT=** data set. By default, without the SPARSE option, PROC FREQ does not include zero frequency cells in the LIST output or in the **OUT=** data set. If you specify the ZEROS option in the WEIGHT statement but do not want the SPARSE option, you can specify the **NOSPARSE** option in the TABLES statement.

Details: FREQ Procedure

Inputting Frequency Counts

PROC FREQ can use either raw data or cell count data to produce frequency and crosstabulation tables. *Raw data*, also known as case-record data, report the data as one record for each subject or sample member. *Cell count data* report the data as a table, listing all possible combinations of data values along with the frequency counts. This way of presenting data often appears in published results.

The following DATA step statements store raw data in a SAS data set:

```
data Raw;
  input Subject $ R C @@;
  datalines;
01 1 1  02 1 1  03 1 1  04 1 1  05 1 1
06 1 2  07 1 2  08 1 2  09 2 1  10 2 1
11 2 1  12 2 1  13 2 2  14 2 2  14 2 2
;
```

You can store the same data as cell counts by using the following DATA step statements:

```
data CellCounts;
  input R C Count @@;
  datalines;
 1 1 5   1 2 3
 2 1 4   2 2 3
;
```

The variable *R* contains the values for the rows, and the variable *C* contains the values for the columns. The variable *Count* contains the cell count for each row and column combination.

Both the *Raw* data set and the *CellCounts* data set produce identical frequency counts, two-way tables, and statistics. When using the *CellCounts* data set, you must include a *WEIGHT* statement to specify that the variable *Count* contains cell counts. For example, the following PROC FREQ statements create a two-way crosstabulation table by using the *CellCounts* data set:

```
proc freq data=CellCounts;
  tables R*C;
  weight Count;
run;
```

Grouping with Formats

PROC FREQ groups a variable's values according to its formatted values. If you assign a format to a variable with a *FORMAT* statement, PROC FREQ formats the variable values before dividing observations into the levels of a frequency or crosstabulation table.

For example, suppose that variable X has the values 1.1, 1.4, 1.7, 2.1, and 2.3. Each of these values appears as a level in the frequency table. If you decide to round each value to a single digit, include the following statement in the PROC FREQ step:

```
format X 1.;
```

Now the table lists the frequency count for formatted level 1 as two and for formatted level 2 as three.

PROC FREQ treats formatted character variables in the same way. The formatted values are used to group the observations into the levels of a frequency table or crosstabulation table. PROC FREQ uses the entire value of a character format to classify an observation.

You can also use the FORMAT statement to assign formats that were created with the FORMAT procedure to the variables. User-written formats determine the number of levels for a variable and provide labels for a table. If you use the same data with different formats, then you can produce frequency counts and statistics for different classifications of the variable values.

When you use PROC FORMAT to create a user-written format that combines missing and nonmissing values into one category, PROC FREQ treats the entire category of formatted values as missing. For example, a questionnaire codes 1 as yes, 2 as no, and 8 as a no answer. The following PROC FORMAT statements create a user-written format:

```
proc format;
  value Questfmt 1   ='Yes'
                2   ='No'
                8,. ='Missing';
run;
```

When you use a FORMAT statement to assign Questfmt. to a variable, the variable's frequency table no longer includes a frequency count for the response of 8. You must use the MISSING or MISSPRINT option in the TABLES statement to list the frequency for no answer. The frequency count for this level includes observations with either a value of 8 or a missing value (.).

The frequency or crosstabulation table lists the values of both character and numeric variables in ascending order based on internal (unformatted) variable values unless you change the order with the ORDER= option. To list the values in ascending order by formatted values, use ORDER=FORMATTED in the PROC FREQ statement.

For more information about the FORMAT statement, see *SAS Formats and Informats: Reference*.

Missing Values

When the value of the WEIGHT variable is missing, PROC FREQ does not include that observation in the analysis.

PROC FREQ treats missing BY variable values like any other BY variable value. The missing values form a separate BY group.

If an observation has a missing value for a variable in a TABLES request, by default PROC FREQ does not include that observation in the frequency or crosstabulation table. Also by default, PROC FREQ does not include observations with missing values in the computation of percentages and statistics. The procedure displays the number of missing observations below each table.

PROC FREQ also reports the number of missing values in output data sets. The TABLES statement OUT= data set includes an observation that contains the missing value frequency. The NMISS option in the OUTPUT statement provides an output data set variable that contains the missing value frequency.

The following options change the way in which PROC FREQ handles missing values of TABLES variables:

- MISSPRINT** displays missing value frequencies in frequency or crosstabulation tables but does not include them in computations of percentages or statistics.
- MISSING** treats missing values as a valid nonmissing level for all TABLES variables. Displays missing levels in frequency and crosstabulation tables and includes them in computations of percentages and statistics.

This example shows the three ways that PROC FREQ can handle missing values of TABLES variables. The following DATA step statements create a data set with a missing value for the variable A:

```
data one;
  input A Freq;
  datalines;
1 2
2 2
. 2
;
```

The following PROC FREQ statements request a one-way frequency table for the variable A. The first request does not specify a missing value option. The second request specifies the MISSPRINT option in the TABLES statement. The third request specifies the MISSING option in the TABLES statement.

```
proc freq data=one;
  tables A;
  weight Freq;
  title 'Default';
run;
proc freq data=one;
  tables A / missprint;
  weight Freq;
  title 'MISSPRINT Option';
run;
proc freq data=one;
  tables A / missing;
  weight Freq;
  title 'MISSING Option';
run;
```

Figure 38.12 displays the frequency tables produced by this example. The first table shows PROC FREQ's default behavior for handling missing values. The observation with a missing value of the TABLES variable A is not included in the table, and the frequency of missing values is displayed below the table. The second table, for which the MISSPRINT option is specified, displays the missing observation but does not include its frequency when computing the total frequency and percentages. The third table shows that PROC FREQ treats the missing level as a valid nonmissing level when the MISSING option is specified. The table displays the missing level, and PROC FREQ includes this level when computing frequencies and percentages.

Figure 38.12 Missing Values in Frequency Tables

Default				
The FREQ Procedure				
A	Frequency	Percent	Cumulative Frequency	Cumulative Percent
1	2	50.00	2	50.00
2	2	50.00	4	100.00
Frequency Missing = 2				
MISSPRINT Option				
The FREQ Procedure				
A	Frequency	Percent	Cumulative Frequency	Cumulative Percent
.	2	.	.	.
1	2	50.00	2	50.00
2	2	50.00	4	100.00
Frequency Missing = 2				
MISSING Option				
The FREQ Procedure				
A	Frequency	Percent	Cumulative Frequency	Cumulative Percent
.	2	33.33	2	33.33
1	2	33.33	4	66.67
2	2	33.33	6	100.00

When a combination of variable values for a two-way table is missing, PROC FREQ assigns zero to the frequency count for the table cell. By default, PROC FREQ does not display missing combinations in LIST format. Also, PROC FREQ does not include missing combinations in the OUT= output data set by default. To include missing combinations, you can specify the SPARSE option with the LIST or OUT= option in the TABLES statement.

In-Database Computation

The FREQ procedure can use in-database computation to construct frequency and crosstabulation tables when the `DATA=` input data set is stored as a table in a supported database management system (DBMS). Supported databases include Teradata, DB2 under UNIX, and Oracle. In-database computation can provide the advantages of faster processing and reduced data transfer between the database and SAS software. For information about in-database computation, see the section “In-Database Procedures” in *SAS/ACCESS for Relational Databases: Reference*.

PROC FREQ performs in-database computation by using SQL implicit pass-through. The procedure generates SQL queries that are based on the tables that you request in the `TABLES` statement. The database executes these SQL queries to construct initial summary tables, which are then transmitted to PROC FREQ. The procedure uses this summary information to perform the remaining analyses and tasks in the usual way (out of the database). So instead of transferring the entire data set over the network between the database and SAS software, the in-database method transfers only the summary tables. This can substantially reduce processing time when the dimensions of the summary tables (in terms of rows and columns) are much smaller than the dimensions of the entire database table (in terms of individual observations). Additionally, in-database summarization uses efficient parallel processing, which can also provide performance advantages.

In-database computation is controlled by the `SQLGENERATION` option, which you can specify in either a `LIBNAME` statement or an `OPTIONS` statement. See the section “In-Database Procedures” in *SAS/ACCESS for Relational Databases: Reference* for details about the `SQLGENERATION` option and other options that affect in-database computation. By default, PROC FREQ uses in-database computation when possible. There are no FREQ procedure options that control in-database computation.

PROC FREQ uses formatted values to group observations into the levels of frequency and crosstabulation tables. See the section “Grouping with Formats” on page 2544 for more information. If formats are available in the database, then in-database summarization uses the formats. If formats are not available in the database, then in-database summarization is based on the raw data values, and PROC FREQ performs the final, formatted classification (out of the database). For more information, see the section “Deploying and Using SAS Formats in Teradata” in *SAS/ACCESS for Relational Databases: Reference*.

The order of observations is not inherently defined for DBMS tables. The following options relate to the order of observations and therefore should not be specified for PROC FREQ in-database computation:

- If you specify the `FIRSTOBS=` or `OBS=` data set option, PROC FREQ does not perform in-database computation.
- If you specify the `NOTSORTED` option in the `BY` statement, PROC FREQ in-database computation ignores it and uses the default `ASCENDING` order for `BY` variables.
- If you specify the `ORDER=DATA` option for input data in a DBMS table, PROC FREQ computation might produce different results for separate runs of the same analysis. In addition to determining the order of variable levels in crosstabulation table displays, the `ORDER=` option can also affect the values of many of the test statistics and measures that PROC FREQ computes.

Statistical Computations

Definitions and Notation

A two-way table represents the crosstabulation of row variable X and column variable Y . Let the table row values or levels be denoted by $X_i, i = 1, 2, \dots, R$, and the column values by $Y_j, j = 1, 2, \dots, C$. Let n_{ij} denote the frequency of the table cell in the i th row and j th column and define the following notation:

$$n_{i.} = \sum_j n_{ij} \quad (\text{row totals})$$

$$n_{.j} = \sum_i n_{ij} \quad (\text{column totals})$$

$$n = \sum_i \sum_j n_{ij} \quad (\text{overall total})$$

$$p_{ij} = n_{ij}/n \quad (\text{cell percentages})$$

$$p_{i.} = n_{i.}/n \quad (\text{row percentages of total})$$

$$p_{.j} = n_{.j}/n \quad (\text{column percentages of total})$$

$$R_i = \text{score for row } i$$

$$C_j = \text{score for column } j$$

$$\bar{R} = \sum_i n_{i.} R_i / n \quad (\text{average row score})$$

$$\bar{C} = \sum_j n_{.j} C_j / n \quad (\text{average column score})$$

$$A_{ij} = \sum_{k>i} \sum_{l>j} n_{kl} + \sum_{k<i} \sum_{l<j} n_{kl}$$

$$D_{ij} = \sum_{k>i} \sum_{l<j} n_{kl} + \sum_{k<i} \sum_{l>j} n_{kl}$$

$$P = \sum_i \sum_j n_{ij} A_{ij} \quad (\text{twice the number of concordances})$$

$$Q = \sum_i \sum_j n_{ij} D_{ij} \quad (\text{twice the number of discordances})$$

Scores

PROC FREQ uses scores of the variable values to compute the Mantel-Haenszel chi-square, Pearson correlation, Cochran-Armitage test for trend, weighted kappa coefficient, and Cochran-Mantel-Haenszel statistics. The SCORES= option in the TABLES statement specifies the score type that PROC FREQ uses. The available score types are TABLE, RANK, RIDIT, and MODRIDIT scores. The default score type is TABLE. Using MODRIDIT, RANK, or RIDIT scores yields nonparametric analyses.

For numeric variables, table scores are the values of the row and column levels. If the row or column variable is formatted, then the table score is the internal numeric value corresponding to that level. If two or more numeric values are classified into the same formatted level, then the internal numeric value for that

level is the smallest of these values. For character variables, table scores are defined as the row numbers and column numbers (that is, 1 for the first row, 2 for the second row, and so on).

Rank scores, which you request with the SCORES=RANK option, are defined as

$$R_i^1 = \sum_{k < i} n_k + (n_i + 1)/2 \quad i = 1, 2, \dots, R$$

$$C_j^1 = \sum_{l < j} n_l + (n_j + 1)/2 \quad j = 1, 2, \dots, C$$

where R_i^1 is the rank score of row i , and C_j^1 is the rank score of column j . Note that rank scores yield midranks for tied values.

Ridit scores, which you request with the SCORES=RIDIT option, are defined as rank scores standardized by the sample size (Bross 1958; Mack and Skillings 1980). Ridit scores are derived from the rank scores as

$$R_i^2 = R_i^1/n \quad i = 1, 2, \dots, R$$

$$C_j^2 = C_j^1/n \quad j = 1, 2, \dots, C$$

Modified ridit scores (SCORES=MODRIDIT) represent the expected values of the order statistics of the uniform distribution on (0,1) (van Elteren 1960; Lehmann 2006). Modified ridit scores are derived from rank scores as

$$R_i^3 = R_i^1/(n + 1) \quad i = 1, 2, \dots, R$$

$$C_j^3 = C_j^1/(n + 1) \quad j = 1, 2, \dots, C$$

Chi-Square Tests and Statistics

The CHISQ option provides chi-square tests of homogeneity or independence and measures of association that are based on the chi-square statistic. When you specify the CHISQ option in the TABLES statement, PROC FREQ computes the following chi-square tests for each two-way table: Pearson chi-square, likelihood ratio chi-square, and Mantel-Haenszel chi-square tests. PROC FREQ provides the following measures of association that are based on the Pearson chi-square statistic: phi coefficient, contingency coefficient, and Cramér's V . For 2×2 tables, the CHISQ option also provides Fisher's exact test and the continuity-adjusted chi-square statistic. You can request Fisher's exact test for general $R \times C$ tables by specifying the FISHER option in the TABLES or EXACT statement.

If you specify the CHISQ option for one-way tables, PROC FREQ provides a one-way Pearson chi-square goodness-of-fit test. If you specify the CHISQ(LRCHISQ) option for one-way tables, PROC FREQ also provides a one-way likelihood ratio chi-square test. The other tests and statistics that the CHISQ option produces are available only for two-way tables.

For two-way tables, the null hypothesis for the chi-square tests is no association between the row variable and the column variable. When the sample size n is large, the test statistics have asymptotic chi-square distributions under the null hypothesis. When the sample size is not large, or when the data set is sparse or heavily tied, exact tests might be more appropriate than asymptotic tests. PROC FREQ provides exact p -values for the Pearson chi-square, likelihood ratio chi-square, and Mantel-Haenszel chi-square tests, in addition to Fisher's exact test. For one-way tables, PROC FREQ provides exact p -values for the Pearson and likelihood ratio chi-square goodness-of-fit tests. You can request these exact tests by specifying the

corresponding options in the EXACT statement. See the section “Exact Statistics” on page 2601 for more information.

The Mantel-Haenszel chi-square statistic is appropriate only when both variables lie on an ordinal scale. The other chi-square tests and statistics in this section are appropriate for either nominal or ordinal variables. The following sections give the formulas that PROC FREQ uses to compute the chi-square tests and statistics. For more information about these statistics, see Agresti (2007) and Stokes, Davis, and Koch (2012), and the other references cited.

Chi-Square Test for One-Way Tables

For one-way frequency tables, the CHISQ option in the TABLES statement provides a chi-square goodness-of-fit test. Let C denote the number of classes, or levels, in the one-way table. Let f_i denote the frequency of class i (or the number of observations in class i) for $i = 1, 2, \dots, C$. Then PROC FREQ computes the one-way chi-square statistic as

$$Q_P = \sum_{i=1}^C (f_i - e_i)^2 / e_i$$

where e_i is the expected frequency for class i under the null hypothesis.

In the test for equal proportions, which is the default for the CHISQ option, the null hypothesis specifies equal proportions of the total sample size for each class. Under this null hypothesis, the expected frequency for each class equals the total sample size divided by the number of classes,

$$e_i = n / C \quad \text{for } i = 1, 2, \dots, C$$

In the test for specified frequencies, which PROC FREQ computes when you input null hypothesis frequencies by using the TESTF= option, the expected frequencies are the TESTF= values that you specify. In the test for specified proportions, which PROC FREQ computes when you input null hypothesis proportions by using the TESTP= option, the expected frequencies are determined from the specified TESTP= proportions p_i as

$$e_i = p_i \times n \quad \text{for } i = 1, 2, \dots, C$$

Under the null hypothesis (of equal proportions, specified frequencies, or specified proportions), Q_P has an asymptotic chi-square distribution with $C-1$ degrees of freedom.

In addition to the asymptotic test, you can request an exact one-way chi-square test by specifying the CHISQ option in the EXACT statement. See the section “Exact Statistics” on page 2601 for more information.

Pearson Chi-Square Test for Two-Way Tables

The Pearson chi-square for two-way tables involves the differences between the observed and expected frequencies, where the expected frequencies are computed under the null hypothesis of independence. The Pearson chi-square statistic is computed as

$$Q_P = \sum_i \sum_j (n_{ij} - e_{ij})^2 / e_{ij}$$

where n_{ij} is the observed frequency in table cell (i, j) and e_{ij} is the expected frequency for table cell (i, j) . The expected frequency is computed under the null hypothesis that the row and column variables are independent,

$$e_{ij} = (n_{i.} n_{.j}) / n$$

When the row and column variables are independent, Q_P has an asymptotic chi-square distribution with $(R-1)(C-1)$ degrees of freedom. For large values of Q_P , this test rejects the null hypothesis in favor of the alternative hypothesis of general association.

In addition to the asymptotic test, you can request an exact Pearson chi-square test by specifying the PCHI or CHISQ option in the EXACT statement. See the section “Exact Statistics” on page 2601 for more information.

For 2×2 tables, the Pearson chi-square is also appropriate for testing the equality of two binomial proportions. For $R \times 2$ and $2 \times C$ tables, the Pearson chi-square tests the homogeneity of proportions. See Fienberg (1980) for details.

Standardized Residuals

When you specify the CROSSLIST(STDRES) option in the TABLES statement for two-way or multiway tables, PROC FREQ displays the standardized residuals in the CROSSLIST table.

The standardized residual of a crosstabulation table cell is the ratio of (*frequency* – *expected*) to its standard error, where *frequency* is the table cell frequency and *expected* is the estimated expected cell frequency. The expected frequency is computed under the null hypothesis that the row and column variables are independent. See the section “Pearson Chi-Square Test for Two-Way Tables” on page 2551 for more information.

PROC FREQ computes the standardized residual of table cell (i, j) as

$$(n_{ij} - e_{ij}) / \sqrt{e_{ij}(1 - p_{i.})(1 - p_{.j})}$$

where n_{ij} is the observed frequency of table cell (i, j) , e_{ij} is the expected frequency of the table cell, $p_{i.}$ is the proportion in row i ($n_{i.}/n$), and $p_{.j}$ is the proportion in column j ($n_{.j}/n$). The expected frequency of table cell (i, j) is computed as

$$e_{ij} = (n_{i.} n_{.j}) / n$$

Under the null hypothesis of independence, each standardized residual has an asymptotic standard normal distribution. See section 2.4.5 of Agresti (2007) for more information.

Likelihood Ratio Chi-Square Test for One-Way Tables

For one-way frequency tables, the CHISQ(LRCHISQ) option in the TABLES statement provides a likelihood ratio chi-square goodness-of-fit test. By default, the likelihood ratio test is based on the null hypothesis of equal proportions in the C classes (levels) of the one-way table. If you specify null hypothesis proportions or frequencies by using the CHISQ(TESTP=) or CHISQ(TESTF=) option, respectively, the likelihood ratio test is based on the null hypothesis values that you specify.

PROC FREQ computes the one-way likelihood ratio test as

$$G^2 = 2 \sum_{i=1}^C f_i \ln(f_i/e_i)$$

where f_i is the observed frequency of class i , and e_i is the expected frequency of class i under the null hypothesis.

For the null hypothesis of equal proportions, the expected frequency of each class equals the total sample size divided by the number of classes,

$$e_i = n / C \quad \text{for } i = 1, 2, \dots, C$$

If you provide null hypothesis frequencies by specifying the CHISQ(TESTF=) option in the TABLES statement, the expected frequencies are the TESTF= values that you specify. If you provide null hypothesis proportions by specifying the CHISQ(TESTP=) option in the TABLES statement, PROC FREQ computes the expected frequencies as

$$e_i = p_i \times n \quad \text{for } i = 1, 2, \dots, C$$

where the proportions p_i are the TESTP= values that you specify.

Under the null hypothesis (of equal proportions, specified frequencies, or specified proportions), the likelihood ratio statistic G^2 has an asymptotic chi-square distribution with $C-1$ degrees of freedom.

In addition to the asymptotic test, you can request an exact one-way likelihood ratio chi-square test by specifying the LRCHISQ option in the EXACT statement. See the section “Exact Statistics” on page 2601 for more information.

Likelihood Ratio Chi-Square Test

The likelihood ratio chi-square involves the ratios between the observed and expected frequencies. The likelihood ratio chi-square statistic is computed as

$$G^2 = 2 \sum_i \sum_j n_{ij} \ln(n_{ij}/e_{ij})$$

where n_{ij} is the observed frequency in table cell (i, j) and e_{ij} is the expected frequency for table cell (i, j) .

When the row and column variables are independent, G^2 has an asymptotic chi-square distribution with $(R-1)(C-1)$ degrees of freedom.

In addition to the asymptotic test, you can request an exact likelihood ratio chi-square test by specifying the LRCHI or CHISQ option in the EXACT statement. See the section “Exact Statistics” on page 2601 for more information.

Continuity-Adjusted Chi-Square Test

The continuity-adjusted chi-square for 2×2 tables is similar to the Pearson chi-square, but it is adjusted for the continuity of the chi-square distribution. The continuity-adjusted chi-square is most useful for small sample sizes. The use of the continuity adjustment is somewhat controversial; this chi-square test is more conservative (and more like Fisher’s exact test) when the sample size is small. As the sample size increases, the continuity-adjusted chi-square becomes more like the Pearson chi-square.

The continuity-adjusted chi-square statistic is computed as

$$Q_C = \sum_i \sum_j (\max(0, |n_{ij} - e_{ij}| - 0.5))^2 / e_{ij}$$

Under the null hypothesis of independence, Q_C has an asymptotic chi-square distribution with $(R-1)(C-1)$ degrees of freedom.

Mantel-Haenszel Chi-Square Test

The Mantel-Haenszel chi-square statistic tests the alternative hypothesis that there is a linear association between the row variable and the column variable. Both variables must lie on an ordinal scale. The Mantel-Haenszel chi-square statistic is computed as

$$Q_{MH} = (n - 1)r^2$$

where r is the Pearson correlation between the row variable and the column variable. For a description of the Pearson correlation, see the “[Pearson Correlation Coefficient](#)” on page 2559. The Pearson correlation and thus the Mantel-Haenszel chi-square statistic use the scores that you specify in the SCORES= option in the TABLES statement. See Mantel and Haenszel (1959) and Landis, Heyman, and Koch (1978) for more information.

Under the null hypothesis of no association, Q_{MH} has an asymptotic chi-square distribution with one degree of freedom.

In addition to the asymptotic test, you can request an exact Mantel-Haenszel chi-square test by specifying the MHCHI or CHISQ option in the EXACT statement. See the section “[Exact Statistics](#)” on page 2601 for more information.

Fisher’s Exact Test

Fisher’s exact test is another test of association between the row and column variables. This test assumes that the row and column totals are fixed, and then uses the hypergeometric distribution to compute probabilities of possible tables conditional on the observed row and column totals. Fisher’s exact test does not depend on any large-sample distribution assumptions, and so it is appropriate even for small sample sizes and for sparse tables.

2 × 2 Tables For 2 × 2 tables, PROC FREQ gives the following information for Fisher’s exact test: table probability, two-sided p -value, left-sided p -value, and right-sided p -value. The table probability equals the hypergeometric probability of the observed table, and is in fact the value of the test statistic for Fisher’s exact test.

Where p is the hypergeometric probability of a specific table with the observed row and column totals, Fisher’s exact p -values are computed by summing probabilities p over defined sets of tables,

$$\text{Prob} = \sum_A p$$

The two-sided p -value is the sum of all possible table probabilities (conditional on the observed row and column totals) that are less than or equal to the observed table probability. For the two-sided p -value, the set A includes all possible tables with hypergeometric probabilities less than or equal to the probability of the observed table. A small two-sided p -value supports the alternative hypothesis of association between the row and column variables.

For 2 × 2 tables, one-sided p -values for Fisher’s exact test are defined in terms of the frequency of the cell in the first row and first column of the table, the (1,1) cell. Denoting the observed (1,1) cell frequency by n_{11} , the left-sided p -value for Fisher’s exact test is the probability that the (1,1) cell frequency is less than or equal to n_{11} . For the left-sided p -value, the set A includes those tables with a (1,1) cell frequency less than or equal to n_{11} . A small left-sided p -value supports the alternative hypothesis that the probability of an observation being in the first cell is actually less than expected under the null hypothesis of independent row and column variables.

Similarly, for a right-sided alternative hypothesis, A is the set of tables where the frequency of the (1,1) cell is greater than or equal to that in the observed table. A small right-sided p -value supports the alternative that the probability of the first cell is actually greater than that expected under the null hypothesis.

Because the (1,1) cell frequency completely determines the 2 × 2 table when the marginal row and column sums are fixed, these one-sided alternatives can be stated equivalently in terms of other cell probabilities or

ratios of cell probabilities. The left-sided alternative is equivalent to an odds ratio less than 1, where the odds ratio equals $(n_{11}n_{22}/n_{12}n_{21})$. Additionally, the left-sided alternative is equivalent to the column 1 risk for row 1 being less than the column 1 risk for row 2, $p_{1|1} < p_{1|2}$. Similarly, the right-sided alternative is equivalent to the column 1 risk for row 1 being greater than the column 1 risk for row 2, $p_{1|1} > p_{1|2}$. See Agresti (2007) for details.

R × C Tables Fisher's exact test was extended to general $R \times C$ tables by Freeman and Halton (1951), and this test is also known as the Freeman-Halton test. For $R \times C$ tables, the two-sided p -value definition is the same as for 2×2 tables. The set A contains all tables with p less than or equal to the probability of the observed table. A small p -value supports the alternative hypothesis of association between the row and column variables. For $R \times C$ tables, Fisher's exact test is inherently two-sided. The alternative hypothesis is defined only in terms of general, and not linear, association. Therefore, Fisher's exact test does not have right-sided or left-sided p -values for general $R \times C$ tables.

For $R \times C$ tables, PROC FREQ computes Fisher's exact test by using the network algorithm of Mehta and Patel (1983), which provides a faster and more efficient solution than direct enumeration. See the section "Exact Statistics" on page 2601 for more details.

Phi Coefficient

The phi coefficient is a measure of association derived from the Pearson chi-square. The range of the phi coefficient is $-1 \leq \phi \leq 1$ for 2×2 tables. For tables larger than 2×2 , the range is $0 \leq \phi \leq \min(\sqrt{R-1}, \sqrt{C-1})$ (Liebetrau 1983). The phi coefficient is computed as

$$\phi = (n_{11}n_{22} - n_{12}n_{21}) / \sqrt{n_{1.}n_{2.}n_{.1}n_{.2}} \quad \text{for } 2 \times 2 \text{ tables}$$

$$\phi = \sqrt{Q_P/n} \quad \text{otherwise}$$

See Fleiss, Levin, and Paik (2003, pp. 98–99) for more information.

Contingency Coefficient

The contingency coefficient is a measure of association derived from the Pearson chi-square. The range of the contingency coefficient is $0 \leq P \leq \sqrt{(m-1)/m}$, where $m = \min(R, C)$ (Liebetrau 1983). The contingency coefficient is computed as

$$P = \sqrt{Q_P / (Q_P + n)}$$

See Kendall and Stuart (1979, pp. 587–588) for more information.

Cramér's V

Cramér's V is a measure of association derived from the Pearson chi-square. It is designed so that the attainable upper bound is always 1. The range of Cramér's V is $-1 \leq V \leq 1$ for 2×2 tables; for tables larger than 2×2 , the range is $0 \leq V \leq 1$. Cramér's V is computed as

$$V = \phi \quad \text{for } 2 \times 2 \text{ tables}$$

$$V = \sqrt{\frac{Q_P/n}{\min(R-1, C-1)}} \quad \text{otherwise}$$

See Kendall and Stuart (1979, p. 588) for more information.

Measures of Association

When you specify the MEASURES option in the TABLES statement, PROC FREQ computes several statistics that describe the association between the row and column variables of the contingency table. The following are measures of ordinal association that consider whether the column variable Y tends to increase as the row variable X increases: gamma, Kendall's tau- b , Stuart's tau- c , and Somers' D . These measures are appropriate for ordinal variables, and they classify pairs of observations as *concordant* or *discordant*. A pair is concordant if the observation with the larger value of X also has the larger value of Y . A pair is discordant if the observation with the larger value of X has the smaller value of Y . See Agresti (2007) and the other references cited for the individual measures of association.

The Pearson correlation coefficient and the Spearman rank correlation coefficient are also appropriate for ordinal variables. The Pearson correlation describes the strength of the linear association between the row and column variables, and it is computed by using the row and column scores specified by the SCORES= option in the TABLES statement. The Spearman correlation is computed with rank scores. The polychoric correlation (requested by the PLCORR option) also requires ordinal variables and assumes that the variables have an underlying bivariate normal distribution. The following measures of association do not require ordinal variables and are appropriate for nominal variables: lambda asymmetric, lambda symmetric, and the uncertainty coefficients.

PROC FREQ computes estimates of the measures according to the formulas given in the following sections. For each measure, PROC FREQ computes an asymptotic standard error (ASE), which is the square root of the asymptotic variance denoted by Var in the following sections.

Confidence Limits

If you specify the CL option in the TABLES statement, PROC FREQ computes asymptotic confidence limits for all MEASURES statistics. The confidence coefficient is determined according to the value of the ALPHA= option, which, by default, equals 0.05 and produces 95% confidence limits.

The confidence limits are computed as

$$\text{Est} \pm (z_{\alpha/2} \times \text{ASE})$$

where Est is the estimate of the measure, $z_{\alpha/2}$ is the $100(1 - \alpha/2)$ percentile of the standard normal distribution, and ASE is the asymptotic standard error of the estimate.

Asymptotic Tests

For each measure that you specify in the TEST statement, PROC FREQ computes an asymptotic test of the null hypothesis that the measure equals zero. Asymptotic tests are available for the following measures of association: gamma, Kendall's tau- b , Stuart's tau- c , Somers' $D(C|R)$, Somers' $D(R|C)$, the Pearson correlation coefficient, and the Spearman rank correlation coefficient. To compute an asymptotic test, PROC FREQ uses a standardized test statistic z , which has an asymptotic standard normal distribution under the null hypothesis. The test statistic is computed as

$$z = \text{Est} / \sqrt{\text{Var}_0(\text{Est})}$$

where Est is the estimate of the measure and $\text{Var}_0(\text{Est})$ is the variance of the estimate under the null hypothesis. Formulas for $\text{Var}_0(\text{Est})$ for the individual measures of association are given in the following sections.

Note that the ratio of Est to $\sqrt{\text{Var}_0(\text{Est})}$ is the same for the following measures: gamma, Kendall's tau-*b*, Stuart's tau-*c*, Somers' $D(C|R)$, and Somers' $D(R|C)$. Therefore, the tests for these measures are identical. For example, the p -values for the test of H_0 : gamma = 0 equal the p -values for the test of H_0 : tau-*b* = 0.

PROC FREQ computes one-sided and two-sided p -values for each of these tests. When the test statistic z is greater than its null hypothesis expected value of zero, PROC FREQ displays the right-sided p -value, which is the probability of a larger value of the statistic occurring under the null hypothesis. A small right-sided p -value supports the alternative hypothesis that the true value of the measure is greater than zero. When the test statistic is less than or equal to zero, PROC FREQ displays the left-sided p -value, which is the probability of a smaller value of the statistic occurring under the null hypothesis. A small left-sided p -value supports the alternative hypothesis that the true value of the measure is less than zero. The one-sided p -value P_1 can be expressed as

$$P_1 = \begin{cases} \text{Prob}(Z > z) & \text{if } z > 0 \\ \text{Prob}(Z < z) & \text{if } z \leq 0 \end{cases}$$

where Z has a standard normal distribution. The two-sided p -value P_2 is computed as

$$P_2 = \text{Prob}(|Z| > |z|)$$

Exact Tests

Exact tests are available for the following measures of association: Kendall's tau-*b*, Stuart's tau-*c*, Somers' $D(C|R)$ and $(R|C)$, the Pearson correlation coefficient, and the Spearman rank correlation coefficient. If you request an exact test for a measure of association in the EXACT statement, PROC FREQ computes the exact test of the hypothesis that the measure equals zero. See the section "Exact Statistics" on page 2601 for details.

Gamma

The gamma (Γ) statistic is based only on the number of concordant and discordant pairs of observations. It ignores tied pairs (that is, pairs of observations that have equal values of X or equal values of Y). Gamma is appropriate only when both variables lie on an ordinal scale. The range of gamma is $-1 \leq \Gamma \leq 1$. If the row and column variables are independent, then gamma tends to be close to zero. Gamma is computed as

$$G = (P - Q) / (P + Q)$$

and the asymptotic variance is

$$\text{Var}(G) = \frac{16}{(P + Q)^4} \sum_i \sum_j n_{ij} (QA_{ij} - PD_{ij})^2$$

For 2×2 tables, gamma is equivalent to Yule's Q . See Goodman and Kruskal (1979) and Agresti (2002) for more information.

The variance under the null hypothesis that gamma equals zero is computed as

$$\text{Var}_0(G) = \frac{4}{(P + Q)^2} \left(\sum_i \sum_j n_{ij} (A_{ij} - D_{ij})^2 - (P - Q)^2/n \right)$$

See Brown and Benedetti (1977) for details.

Kendall's Tau-b

Kendall's tau- b (τ_b) is similar to gamma except that tau- b uses a correction for ties. Tau- b is appropriate only when both variables lie on an ordinal scale. The range of tau- b is $-1 \leq \tau_b \leq 1$. Kendall's tau- b is computed as

$$t_b = (P - Q) / \sqrt{w_r w_c}$$

and the asymptotic variance is

$$\text{Var}(t_b) = \frac{1}{w^4} \left(\sum_i \sum_j n_{ij} (2w d_{ij} + t_b v_{ij})^2 - n^3 t_b^2 (w_r + w_c)^2 \right)$$

where

$$\begin{aligned} w &= \sqrt{w_r w_c} \\ w_r &= n^2 - \sum_i n_i^2 \\ w_c &= n^2 - \sum_j n_{.j}^2 \\ d_{ij} &= A_{ij} - D_{ij} \\ v_{ij} &= n_{i \cdot} w_c + n_{\cdot j} w_r \end{aligned}$$

See Kendall (1955) for more information.

The variance under the null hypothesis that tau- b equals zero is computed as

$$\text{Var}_0(t_b) = \frac{4}{w_r w_c} \left(\sum_i \sum_j n_{ij} (A_{ij} - D_{ij})^2 - (P - Q)^2 / n \right)$$

See Brown and Benedetti (1977) for details.

PROC FREQ also provides an exact test for the Kendall's tau- b . You can request this test by specifying the KENTB option in the EXACT statement. See the section "Exact Statistics" on page 2601 for more information.

Stuart's Tau-c

Stuart's tau- c (τ_c) makes an adjustment for table size in addition to a correction for ties. Tau- c is appropriate only when both variables lie on an ordinal scale. The range of tau- c is $-1 \leq \tau_c \leq 1$. Stuart's tau- c is computed as

$$t_c = m(P - Q) / n^2(m - 1)$$

and the asymptotic variance is

$$\text{Var}(t_c) = \frac{4m^2}{(m - 1)^2 n^4} \left(\sum_i \sum_j n_{ij} d_{ij}^2 - (P - Q)^2 / n \right)$$

where $m = \min(R, C)$ and $d_{ij} = A_{ij} - D_{ij}$. The variance under the null hypothesis that tau- c equals zero is the same as the asymptotic variance Var,

$$\text{Var}_0(t_c) = \text{Var}(t_c)$$

See Brown and Benedetti (1977) for details.

PROC FREQ also provides an exact test for the Stuart's tau- c . You can request this test by specifying the STUTC option in the EXACT statement. See the section "Exact Statistics" on page 2601 for more information.

Somers' D

Somers' $D(C|R)$ and Somers' $D(R|C)$ are asymmetric modifications of tau- b . $C|R$ indicates that the row variable X is regarded as the independent variable and the column variable Y is regarded as dependent. Similarly, $R|C$ indicates that the column variable Y is regarded as the independent variable and the row variable X is regarded as dependent. Somers' D differs from tau- b in that it uses a correction only for pairs that are tied on the independent variable. Somers' D is appropriate only when both variables lie on an ordinal scale. The range of Somers' D is $-1 \leq D \leq 1$. Somers' $D(C|R)$ is computed as

$$D(C|R) = (P - Q) / w_r$$

and its asymptotic variance is

$$\text{Var}(D(C|R)) = \frac{4}{w_r^4} \sum_i \sum_j n_{ij} (w_r d_{ij} - (P - Q)(n - n_{i.}))^2$$

where $d_{ij} = A_{ij} - D_{ij}$ and

$$w_r = n^2 - \sum_i n_i^2.$$

For more information, see Somers (1962); Goodman and Kruskal (1979); Liebetrau (1983).

The variance under the null hypothesis that $D(C|R)$ equals zero is computed as

$$\text{Var}_0(D(C|R)) = \frac{4}{w_r^2} \left(\sum_i \sum_j n_{ij} (A_{ij} - D_{ij})^2 - (P - Q)^2 / n \right)$$

See Brown and Benedetti (1977) for details.

Formulas for Somers' $D(R|C)$ are obtained by interchanging the indices.

PROC FREQ also provides exact tests for Somers' $D(C|R)$ and $(R|C)$. You can request these tests by specifying the SMDCR and SMDCR options in the EXACT statement. See the section "Exact Statistics" on page 2601 for more information.

Pearson Correlation Coefficient

The Pearson correlation coefficient (ρ) is computed by using the scores specified in the SCORES= option. This measure is appropriate only when both variables lie on an ordinal scale. The range of the Pearson correlation is $-1 \leq \rho \leq 1$. The Pearson correlation coefficient is computed as

$$r = v/w = ss_{rc} / \sqrt{ss_r ss_c}$$

and its asymptotic variance is

$$\text{Var}(r) = \frac{1}{w^4} \sum_i \sum_j n_{ij} \left(w(R_i - \bar{R})(C_j - \bar{C}) - \frac{b_{ij}v}{2w} \right)^2$$

where R_i and C_j are the row and column scores and

$$ss_r = \sum_i \sum_j n_{ij} (R_i - \bar{R})^2$$

$$ss_c = \sum_i \sum_j n_{ij} (C_j - \bar{C})^2$$

$$ss_{rc} = \sum_i \sum_j n_{ij} (R_i - \bar{R})(C_j - \bar{C})$$

$$b_{ij} = (R_i - \bar{R})^2 ss_c + (C_j - \bar{C})^2 ss_r$$

$$v = ss_{rc}$$

$$w = \sqrt{ss_r ss_c}$$

See Snedecor and Cochran (1989) for more information.

The SCORES= option in the TABLES statement determines the type of row and column scores used to compute the Pearson correlation (and other score-based statistics). The default is SCORES=TABLE. See the section “Scores” on page 2549 for details about the available score types and how they are computed.

The variance under the null hypothesis that the correlation equals zero is computed as

$$\text{Var}_0(r) = \left(\sum_i \sum_j n_{ij} (R_i - \bar{R})^2 (C_j - \bar{C})^2 - ss_{rc}^2 / n \right) / ss_r ss_c$$

Note that this expression for the variance is derived for multinomial sampling in a contingency table framework, and it differs from the form obtained under the assumption that both variables are continuous and normally distributed. See Brown and Benedetti (1977) for details.

PROC FREQ also provides an exact test for the Pearson correlation coefficient. You can request this test by specifying the PCORR option in the EXACT statement. See the section “Exact Statistics” on page 2601 for more information.

Spearman Rank Correlation Coefficient

The Spearman correlation coefficient (ρ_s) is computed by using rank scores, which are defined in the section “Scores” on page 2549. This measure is appropriate only when both variables lie on an ordinal scale. The range of the Spearman correlation is $-1 \leq \rho_s \leq 1$. The Spearman correlation coefficient is computed as

$$r_s = v / w$$

and its asymptotic variance is

$$\text{Var}(r_s) = \frac{1}{n^2 w^4} \sum_i \sum_j n_{ij} (z_{ij} - \bar{z})^2$$

where R_i^1 and C_j^1 are the row and column rank scores and

$$v = \sum_i \sum_j n_{ij} R(i)C(j)$$

$$w = \frac{1}{12} \sqrt{FG}$$

$$F = n^3 - \sum_i n_{i.}^3$$

$$G = n^3 - \sum_j n_{.j}^3$$

$$R(i) = R_i^1 - n/2$$

$$C(j) = C_j^1 - n/2$$

$$\bar{z} = \frac{1}{n} \sum_i \sum_j n_{ij} z_{ij}$$

$$z_{ij} = wv_{ij} - vw_{ij}$$

$$v_{ij} = n \left(R(i)C(j) + \frac{1}{2} \sum_l n_{il} C(l) + \frac{1}{2} \sum_k n_{kj} R(k) + \sum_l \sum_{k>i} n_{kl} C(l) + \sum_k \sum_{l>j} n_{kl} R(k) \right)$$

$$w_{ij} = \frac{-n}{96w} (Fn_{.j}^2 + Gn_{i.}^2)$$

See Snedecor and Cochran (1989) for more information.

The variance under the null hypothesis that the correlation equals zero is computed as

$$\text{Var}_0(r_s) = \frac{1}{n^2 w^2} \sum_i \sum_j n_{ij} (v_{ij} - \bar{v})^2$$

where

$$\bar{v} = \sum_i \sum_j n_{ij} v_{ij} / n$$

Note that the asymptotic variance is derived for multinomial sampling in a contingency table framework, and it differs from the form obtained under the assumption that both variables are continuous and normally distributed. See Brown and Benedetti (1977) for details.

PROC FREQ also provides an exact test for the Spearman correlation coefficient. You can request this test by specifying the SCORR option in the EXACT statement. See the section “Exact Statistics” on page 2601 for more information.

Polychoric Correlation

When you specify the PLCORR option in the TABLES statement, PROC FREQ computes the polychoric correlation and its standard error. The polychoric correlation is based on the assumption that the two ordinal, categorical variables of the frequency table have an underlying bivariate normal distribution. The polychoric correlation coefficient is the maximum likelihood estimate of the product-moment correlation between the underlying normal variables. The range of the polychoric correlation is from -1 to 1 . For 2×2 tables, the polychoric correlation is also known as the tetrachoric correlation (and it is labeled as such in the displayed output). See Drasgow (1986) for an overview of polychoric correlation coefficient.

Olsson (1979) gives the likelihood equations and the asymptotic standard errors for estimating the polychoric correlation. The underlying continuous variables relate to the observed crosstabulation table through thresholds, which define a range of numeric values that correspond to each categorical (table) level. PROC FREQ uses Olsson’s maximum likelihood method for simultaneous estimation of the polychoric correlation and the thresholds. (Olsson also presents a two-step method that estimates the thresholds first.)

PROC FREQ iteratively solves the likelihood equations by using a Newton-Raphson algorithm. The initial estimates of the thresholds are computed from the inverse of the normal distribution function at the cumulative marginal proportions of the table. Iterative computation of the polychoric correlation stops when the convergence measure falls below the convergence criterion or when the maximum number of iterations is reached, whichever occurs first. For parameter values that are less than 0.01, the procedure evaluates convergence by using the absolute difference instead of the relative difference. The PLCORR(CONVERGE=) option specifies the convergence criterion, which is 0.0001 by default. The PLCORR(MAXITER=) option specifies the maximum number of iterations, which is 20 by default.

If you specify the CL option in the TABLES statement, PROC FREQ provides confidence limits for the polychoric correlation. The confidence limits are computed as

$$\hat{\rho} \pm (z_{\alpha/2} \times SE(\hat{\rho}))$$

where $\hat{\rho}$ is the estimate of the polychoric correlation, $z_{\alpha/2}$ is the $100(1 - \alpha/2)$ percentile of the standard normal distribution, and $SE(\hat{\rho})$ is the standard error of the polychoric correlation estimate.

If you specify the PLCORR option in the TEST statement, PROC FREQ provides Wald and likelihood ratio tests of the null hypothesis that the polychoric correlation equals 0. The Wald test statistic is computed as

$$z = \hat{\rho} / SE(\hat{\rho})$$

which has a standard normal distribution under the null hypothesis. PROC FREQ computes one-sided and two-sided p -values for the Wald test. When the test statistic z is greater than its null expected value of 0, PROC FREQ displays the right-sided p -value. When the test statistic is less than or equal to 0, PROC FREQ displays the left-sided p -value.

The likelihood ratio statistic for the polychoric correlation is computed as

$$G^2 = -2 \ln(L_0/L_1)$$

where L_0 is the value of the likelihood function (Olsson 1979) when the polychoric correlation is 0, and L_1 is the value of the likelihood function at the maximum (where all parameters are replaced by their maximum likelihood estimates). Under the null hypothesis, the likelihood ratio statistic has an asymptotic chi-square distribution with one degree of freedom.

Lambda (Asymmetric)

Asymmetric lambda, $\lambda(C|R)$, is interpreted as the probable improvement in predicting the column variable Y given knowledge of the row variable X . The range of asymmetric lambda is $0 \leq \lambda(C|R) \leq 1$. Asymmetric lambda $(C|R)$ is computed as

$$\lambda(C|R) = \frac{\sum_i r_i - r}{n - r}$$

and its asymptotic variance is

$$\text{Var}(\lambda(C|R)) = \frac{n - \sum_i r_i}{(n - r)^3} \left(\sum_i r_i + r - 2 \sum_i (r_i | l_i = l) \right)$$

where

$$r_i = \max_j(n_{ij})$$

$$r = \max_j(n_{.j})$$

$$c_j = \max_i(n_{ij})$$

$$c = \max_i(n_{i.})$$

The values of l_i and l are determined as follows. Denote by l_i the unique value of j such that $r_i = n_{ij}$, and let l be the unique value of j such that $r = n_{.j}$. Because of the uniqueness assumptions, ties in the frequencies or in the marginal totals must be broken in an arbitrary but consistent manner. In case of ties, l is defined as the smallest value of j such that $r = n_{.j}$.

For those columns containing a cell (i, j) for which $n_{ij} = r_i = c_j$, cs_j records the row in which c_j is assumed to occur. Initially cs_j is set equal to -1 for all j . Beginning with $i=1$, if there is at least one value j such that $n_{ij} = r_i = c_j$, and if $cs_j = -1$, then l_i is defined to be the smallest such value of j , and cs_j is set equal to i . Otherwise, if $n_{il} = r_i$, then l_i is defined to be equal to l . If neither condition is true, then l_i is taken to be the smallest value of j such that $n_{ij} = r_i$.

The formulas for lambda asymmetric $(R|C)$ can be obtained by interchanging the indices.

See Goodman and Kruskal (1979) for more information.

Lambda (Symmetric)

The nondirectional lambda is the average of the two asymmetric lambdas, $\lambda(C|R)$ and $\lambda(R|C)$. Its range is $0 \leq \lambda \leq 1$. Lambda symmetric is computed as

$$\lambda = \frac{\sum_i r_i + \sum_j c_j - r - c}{2n - r - c} = \frac{w - v}{w}$$

and its asymptotic variance is computed as

$$\text{Var}(\lambda) = \frac{1}{w^4} \left(wvy - 2w^2 \left(n - \sum_i \sum_j (n_{ij} | j = l_i, i = k_j) \right) - 2v^2(n - n_{kl}) \right)$$

where

$$r_i = \max_j(n_{ij})$$

$$r = \max_j(n_{.j})$$

$$c_j = \max_i(n_{ij})$$

$$c = \max_i(n_{i.})$$

$$w = 2n - r - c$$

$$v = 2n - \sum_i r_i - \sum_j c_j$$

$$x = \sum_i (r_i | l_i = l) + \sum_j (c_j | k_j = k) + r_k + c_l$$

$$y = 8n - w - v - 2x$$

The definitions of l_i and l are given in the previous section. The values k_j and k are defined in a similar way for lambda asymmetric ($R|C$).

See Goodman and Kruskal (1979) for more information.

Uncertainty Coefficients (Asymmetric)

The uncertainty coefficient $U(C|R)$ measures the proportion of uncertainty (entropy) in the column variable Y that is explained by the row variable X . Its range is $0 \leq U(C|R) \leq 1$. The uncertainty coefficient is computed as

$$U(C|R) = (H(X) + H(Y) - H(XY)) / H(Y) = v/w$$

and its asymptotic variance is

$$\text{Var}(U(C|R)) = \frac{1}{n^2 w^4} \sum_i \sum_j n_{ij} \left(H(Y) \ln \left(\frac{n_{ij}}{n_{i.}} \right) + (H(X) - H(XY)) \ln \left(\frac{n_{.j}}{n} \right) \right)^2$$

where

$$\begin{aligned}
 v &= H(X) + H(Y) - H(XY) \\
 w &= H(Y) \\
 H(X) &= -\sum_i \left(\frac{n_{i\cdot}}{n}\right) \ln\left(\frac{n_{i\cdot}}{n}\right) \\
 H(Y) &= -\sum_j \left(\frac{n_{\cdot j}}{n}\right) \ln\left(\frac{n_{\cdot j}}{n}\right) \\
 H(XY) &= -\sum_i \sum_j \left(\frac{n_{ij}}{n}\right) \ln\left(\frac{n_{ij}}{n}\right)
 \end{aligned}$$

The formulas for the uncertainty coefficient $U(R|C)$ can be obtained by interchanging the indices.

See Theil (1972, pp. 115–120) and Goodman and Kruskal (1979) for more information.

Uncertainty Coefficient (Symmetric)

The uncertainty coefficient U is the symmetric version of the two asymmetric uncertainty coefficients. Its range is $0 \leq U \leq 1$. The uncertainty coefficient is computed as

$$U = 2(H(X) + H(Y) - H(XY)) / (H(X) + H(Y))$$

and its asymptotic variance is

$$\text{Var}(U) = 4 \sum_i \sum_j \frac{n_{ij} \left(H(XY) \ln\left(\frac{n_{i\cdot} n_{\cdot j}}{n^2}\right) - (H(X) + H(Y)) \ln\left(\frac{n_{ij}}{n}\right) \right)^2}{n^2 (H(X) + H(Y))^4}$$

where $H(X)$, $H(Y)$, and $H(XY)$ are defined in the previous section. See Goodman and Kruskal (1979) for more information.

Binomial Proportion

If you specify the BINOMIAL option in the TABLES statement, PROC FREQ computes the binomial proportion for one-way tables. By default, this is the proportion of observations in the first variable level that appears in the output. (You can use the LEVEL= option to specify a different level for the proportion.) The binomial proportion is computed as

$$\hat{p} = n_1 / n$$

where n_1 is the frequency of the first (or designated) level and n is the total frequency of the one-way table. The standard error of the binomial proportion is computed as

$$\text{se}(\hat{p}) = \sqrt{\hat{p}(1 - \hat{p}) / n}$$

Binomial Confidence Limits

By default, PROC FREQ provides Wald and exact (Clopper-Pearson) confidence limits for the binomial proportion. If you do not specify any confidence limit requests with the `CL= binomial-option`, PROC FREQ computes Wald asymptotic confidence limits. You can also request Agresti-Coull, Jeffreys, and Wilson (score) confidence limits for the binomial proportion. For details about these binomial confidence limits, including comparisons of their performance, see Brown, Cai, and DasGupta (2001); Agresti and Coull (1998); Newcombe (1998b).

Wald Confidence Limits Wald asymptotic confidence limits are based on the normal approximation to the binomial distribution. PROC FREQ computes the Wald confidence limits for the binomial proportion as

$$\hat{p} \pm (z_{\alpha/2} \times \text{se}(\hat{p}))$$

where $z_{\alpha/2}$ is the $100(1 - \alpha/2)$ percentile of the standard normal distribution. The confidence level α is determined by the `ALPHA=` option, which, by default, equals 0.05 and produces 95% confidence limits.

If you specify `CL=WALD(CORRECT)` or the `CORRECT binomial-option`, PROC FREQ includes a continuity correction of $1/2n$ in the Wald asymptotic confidence limits. The purpose of this correction is to adjust for the difference between the normal approximation and the discrete binomial distribution. See Fleiss, Levin, and Paik (2003) for more information. The continuity-corrected Wald confidence limits for the binomial proportion are computed as

$$\hat{p} \pm (z_{\alpha/2} \times \text{se}(\hat{p}) + (1/2n))$$

Agresti-Coull Confidence Limits If you specify the `CL=AGRESTICOULL binomial-option`, PROC FREQ computes Agresti-Coull confidence limits for the binomial proportion as

$$\tilde{p} \pm (z_{\alpha/2} \times \sqrt{\tilde{p}(1 - \tilde{p}) / \tilde{n}})$$

where

$$\begin{aligned} \tilde{n}_1 &= n_1 + z_{\alpha/2}^2 / 2 \\ \tilde{n} &= n + z_{\alpha/2}^2 \\ \tilde{p} &= \tilde{n}_1 / \tilde{n} \end{aligned}$$

The Agresti-Coull confidence interval has the same general form as the standard Wald interval but uses \tilde{p} in place of \hat{p} . For $\alpha = 0.05$, the value of $z_{\alpha/2}$ is close to 2, and this interval is the “add 2 successes and 2 failures” adjusted Wald interval of Agresti and Coull (1998).

Jeffreys Confidence Limits If you specify the `CL=JEFFREYS binomial-option`, PROC FREQ computes Jeffreys confidence limits for the binomial proportion as

$$(\beta(\alpha/2, n_1 + 1/2, n - n_1 + 1/2), \beta(1 - \alpha/2, n_1 + 1/2, n - n_1 + 1/2))$$

where $\beta(\alpha, b, c)$ is the α percentile of the beta distribution with shape parameters b and c . The lower confidence limit is set to 0 when $n_1 = 0$, and the upper confidence limit is set to 1 when $n_1 = n$. This is an equal-tailed interval based on the noninformative Jeffreys prior for a binomial proportion. See Brown, Cai, and DasGupta (2001) for details. See Berger (1985) for information about using beta priors for inference on the binomial proportion.

Wilson (Score) Confidence Limits If you specify the CL=WILSON *binomial-option*, PROC FREQ computes Wilson confidence limits for the binomial proportion. These are also known as score confidence limits (Wilson 1927). The confidence limits are based on inverting the normal test that uses the null proportion in the variance (the score test). Wilson confidence limits are the roots of

$$|p - \hat{p}| = z_{\alpha/2} \sqrt{p(1-p)/n}$$

and are computed as

$$\left(\hat{p} + z_{\alpha/2}^2/2n \pm z_{\alpha/2} \sqrt{\left(\hat{p}(1-\hat{p}) + z_{\alpha/2}^2/4n \right) / n} \right) / \left(1 + z_{\alpha/2}^2/n \right)$$

If you specify CL=WILSON(CORRECT) or the CORRECT *binomial-option*, PROC FREQ provides continuity-corrected Wilson confidence limits, which are computed as the roots of

$$|p - \hat{p}| - 1/2n = z_{\alpha/2} \sqrt{p(1-p)/n}$$

The Wilson interval has been shown to have better performance than the Wald interval and the exact (Clopper-Pearson) interval. For more information, see Agresti and Coull (1998); Brown, Cai, and DasGupta (2001); Newcombe (1998b).

Exact (Clopper-Pearson) Confidence Limits Exact (Clopper-Pearson) confidence limits for the binomial proportion are constructed by inverting the equal-tailed test based on the binomial distribution. This method is attributed to Clopper and Pearson (1934). The exact confidence limits p_L and p_U satisfy the following equations, for $n_1 = 1, 2, \dots, n-1$:

$$\sum_{x=n_1}^n \binom{n}{x} p_L^x (1-p_L)^{n-x} = \alpha/2$$

$$\sum_{x=0}^{n_1} \binom{n}{x} p_U^x (1-p_U)^{n-x} = \alpha/2$$

The lower confidence limit equals 0 when $n_1 = 0$, and the upper confidence limit equals 1 when $n_1 = n$.

PROC FREQ computes the exact (Clopper-Pearson) confidence limits by using the F distribution as

$$p_L = \left(1 + \frac{n - n_1 + 1}{n_1 F(\alpha/2, 2n_1, 2(n - n_1 + 1))} \right)^{-1}$$

$$p_U = \left(1 + \frac{n - n_1}{(n_1 + 1) F(1 - \alpha/2, 2(n_1 + 1), 2(n - n_1))} \right)^{-1}$$

where $F(\alpha/2, b, c)$ is the $\alpha/2$ percentile of the F distribution with b and c degrees of freedom. See Leemis and Trivedi (1996) for a derivation of this expression. Also see Collett (1991) for more information about exact binomial confidence limits.

Because this is a discrete problem, the confidence coefficient (coverage probability) of the exact (Clopper-Pearson) interval is not exactly $(1 - \alpha)$ but is at least $(1 - \alpha)$. Thus, this confidence interval is conservative. Unless the sample size is large, the actual coverage probability can be much larger than the target value. For more information about the performance of these confidence limits, see Agresti and Coull (1998); Brown, Cai, and DasGupta (2001); Leemis and Trivedi (1996).

Binomial Tests

The BINOMIAL option provides an asymptotic equality test for the binomial proportion by default. You can also specify *binomial-options* to request tests of noninferiority, superiority, and equivalence for the binomial proportion. If you specify the BINOMIAL option in the EXACT statement, PROC FREQ also computes exact p -values for the tests that you request with the *binomial-options*.

Equality Test PROC FREQ computes an asymptotic test of the hypothesis that the binomial proportion equals p_0 , where you can specify the value of p_0 with the $P=$ *binomial-option*. If you do not specify a null value with $P=$, PROC FREQ uses $p_0 = 0.5$ by default. The binomial test statistic is computed as

$$z = (\hat{p} - p_0)/se$$

By default, the standard error is based on the null hypothesis proportion as

$$se = \sqrt{p_0(1 - p_0)/n}$$

If you specify the VAR=SAMPLE *binomial-option*, the standard error is computed from the sample proportion as

$$se = \sqrt{\hat{p}(1 - \hat{p})/n}$$

If you specify the CORRECT *binomial-option*, PROC FREQ includes a continuity correction in the asymptotic test statistic, towards adjusting for the difference between the normal approximation and the discrete binomial distribution. See Fleiss, Levin, and Paik (2003) for details. The continuity correction of $(1/2n)$ is subtracted from the numerator of the test statistic if $(\hat{p} - p_0)$ is positive; otherwise, the continuity correction is added to the numerator.

PROC FREQ computes one-sided and two-sided p -values for this test. When the test statistic z is greater than zero (its expected value under the null hypothesis), PROC FREQ computes the right-sided p -value, which is the probability of a larger value of the statistic occurring under the null hypothesis. A small right-sided p -value supports the alternative hypothesis that the true value of the proportion is greater than p_0 . When the test statistic is less than or equal to zero, PROC FREQ computes the left-sided p -value, which is the probability of a smaller value of the statistic occurring under the null hypothesis. A small left-sided p -value supports the alternative hypothesis that the true value of the proportion is less than p_0 . The one-sided p -value P_1 can be expressed as

$$P_1 = \begin{cases} \text{Prob}(Z > z) & \text{if } z > 0 \\ \text{Prob}(Z < z) & \text{if } z \leq 0 \end{cases}$$

where Z has a standard normal distribution. The two-sided p -value is computed as $P_2 = 2 \times P_1$.

If you specify the BINOMIAL option in the EXACT statement, PROC FREQ also computes an exact test of the null hypothesis $H_0: p = p_0$. To compute the exact test, PROC FREQ uses the binomial probability function,

$$\text{Prob}(X = x | p_0) = \binom{n}{x} p_0^x (1 - p_0)^{(n-x)} \quad \text{for } x = 0, 1, 2, \dots, n$$

where the variable X has a binomial distribution with parameters n and p_0 . To compute the left-sided p -value, $\text{Prob}(X \leq n_1)$, PROC FREQ sums the binomial probabilities over x from zero to n_1 . To compute

the right-sided p -value, $\text{Prob}(X \geq n_1)$, PROC FREQ sums the binomial probabilities over x from n_1 to n . The exact one-sided p -value is the minimum of the left-sided and right-sided p -values,

$$P_1 = \min(\text{Prob}(X \leq n_1 | p_0), \text{Prob}(X \geq n_1 | p_0))$$

and the exact two-sided p -value is computed as $P_2 = 2 \times P_1$.

Noninferiority Test If you specify the NONINF *binomial-option*, PROC FREQ provides a noninferiority test for the binomial proportion. The null hypothesis for the noninferiority test is

$$H_0: p - p_0 \leq -\delta$$

versus the alternative

$$H_a: p - p_0 > -\delta$$

where δ is the noninferiority margin and p_0 is the null proportion. Rejection of the null hypothesis indicates that the binomial proportion is not inferior to the null value. See Chow, Shao, and Wang (2003) for more information.

You can specify the value of δ with the MARGIN= *binomial-option*, and you can specify p_0 with the P= *binomial-option*. By default, $\delta = 0.2$ and $p_0 = 0.5$.

PROC FREQ provides an asymptotic Wald test for noninferiority. The test statistic is computed as

$$z = (\hat{p} - p_0^*) / \text{se}$$

where p_0^* is the noninferiority limit,

$$p_0^* = p_0 - \delta$$

By default, the standard error is computed from the sample proportion as

$$\text{se} = \sqrt{\hat{p}(1 - \hat{p})/n}$$

If you specify the VAR=NULL *binomial-option*, the standard error is based on the noninferiority limit (determined by the null proportion and the margin) as

$$\text{se} = \sqrt{p_0^*(1 - p_0^*)/n}$$

If you specify the CORRECT *binomial-option*, PROC FREQ includes a continuity correction in the asymptotic test statistic z . The continuity correction of $(1/2n)$ is subtracted from the numerator of the test statistic if $(\hat{p} - p_0^*)$ is positive; otherwise, the continuity correction is added to the numerator.

The p -value for the noninferiority test is

$$P_z = \text{Prob}(Z > z)$$

where Z has a standard normal distribution.

As part of the noninferiority analysis, PROC FREQ provides asymptotic Wald confidence limits for the binomial proportion. These confidence limits are computed as described in the section “[Wald Confidence Limits](#)” on page 2566 but use the same standard error (VAR=NULL or VAR=SAMPLE) as the noninferiority

test statistic z . The confidence coefficient is $100(1 - 2\alpha)\%$ (Schuirmann 1999). By default, if you do not specify the ALPHA= option, the noninferiority confidence limits are 90% confidence limits. You can compare the confidence limits to the noninferiority limit, $p_0^* = p_0 - \delta$.

If you specify the BINOMIAL option in the EXACT statement, PROC FREQ provides an exact noninferiority test for the binomial proportion. The exact p -value is computed by using the binomial probability function with parameters p_0^* and n ,

$$P_x = \sum_{k=n_1}^{k=n} \binom{n}{k} (p_0^*)^k (1 - p_0^*)^{(n-k)}$$

See Chow, Shao, and Wang (2003, p. 116) for details. If you request exact binomial statistics, PROC FREQ also includes exact (Clopper-Pearson) confidence limits for the binomial proportion in the equivalence analysis display. See the section “Exact (Clopper-Pearson) Confidence Limits” on page 2567 for details.

Superiority Test If you specify the SUP *binomial-option*, PROC FREQ provides a superiority test for the binomial proportion. The null hypothesis for the superiority test is

$$H_0: p - p_0 \leq \delta$$

versus the alternative

$$H_a: p - p_0 > \delta$$

where δ is the superiority margin and p_0 is the null proportion. Rejection of the null hypothesis indicates that the binomial proportion is superior to the null value. You can specify the value of δ with the MARGIN= *binomial-option*, and you can specify the value of p_0 with the P= *binomial-option*. By default, $\delta = 0.2$ and $p_0 = 0.5$.

The superiority analysis is identical to the noninferiority analysis but uses a positive value of the margin δ in the null hypothesis. The superiority limit equals $p_0 + \delta$. The superiority computations follow those in the section “Noninferiority Test” on page 2569 but replace $-\delta$ with δ . See Chow, Shao, and Wang (2003) for more information.

Equivalence Test If you specify the EQUIV *binomial-option*, PROC FREQ provides an equivalence test for the binomial proportion. The null hypothesis for the equivalence test is

$$H_0: p - p_0 \leq \delta_L \quad \text{or} \quad p - p_0 \geq \delta_U$$

versus the alternative

$$H_a: \delta_L < p - p_0 < \delta_U$$

where δ_L is the lower margin, δ_U is the upper margin, and p_0 is the null proportion. Rejection of the null hypothesis indicates that the binomial proportion is equivalent to the null value. See Chow, Shao, and Wang (2003) for more information.

You can specify the value of the margins δ_L and δ_U with the MARGIN= *binomial-option*. If you do not specify MARGIN=, PROC FREQ uses lower and upper margins of -0.2 and 0.2 by default. If you specify a single margin value δ , PROC FREQ uses lower and upper margins of $-\delta$ and δ . You can specify the null proportion p_0 with the P= *binomial-option*. By default, $p_0 = 0.5$.

PROC FREQ computes two one-sided tests (TOST) for equivalence analysis (Schuirmann 1987). The TOST approach includes a right-sided test for the lower margin and a left-sided test for the upper margin. The overall p -value is taken to be the larger of the two p -values from the lower and upper tests.

For the lower margin, the asymptotic Wald test statistic is computed as

$$z_L = (\hat{p} - p_L^*) / se$$

where the lower equivalence limit is

$$p_L^* = p_0 + \delta_L$$

By default, the standard error is computed from the sample proportion as

$$se = \sqrt{\hat{p}(1 - \hat{p})/n}$$

If you specify the VAR=NULL *binomial-option*, the standard error is based on the lower equivalence limit (determined by the null proportion and the lower margin) as

$$se = \sqrt{p_L^*(1 - p_L^*)/n}$$

If you specify the CORRECT *binomial-option*, PROC FREQ includes a continuity correction in the asymptotic test statistic z_L . The continuity correction of $(1/2n)$ is subtracted from the numerator of the test statistic $(\hat{p} - p_L^*)$ if the numerator is positive; otherwise, the continuity correction is added to the numerator.

The p -value for the lower margin test is

$$P_{z,L} = \text{Prob}(Z > z_L)$$

The asymptotic test for the upper margin is computed similarly. The Wald test statistic is

$$z_U = (\hat{p} - p_U^*) / se$$

where the upper equivalence limit is

$$p_U^* = p_0 + \delta_U$$

By default, the standard error is computed from the sample proportion. If you specify the VAR=NULL *binomial-option*, the standard error is based on the upper equivalence limit as

$$se = \sqrt{p_U^*(1 - p_U^*)/n}$$

If you specify the CORRECT *binomial-option*, PROC FREQ includes a continuity correction of $(1/2n)$ in the asymptotic test statistic z_U .

The p -value for the upper margin test is

$$P_{z,U} = \text{Prob}(Z < z_U)$$

Based on the two one-sided tests (TOST), the overall p -value for the test of equivalence equals the larger p -value from the lower and upper margin tests, which can be expressed as

$$P_z = \max(P_{z,L}, P_{z,U})$$

As part of the equivalence analysis, PROC FREQ provides asymptotic Wald confidence limits for the binomial proportion. These confidence limits are computed as described in the section “[Wald Confidence Limits](#)” on page 2566, but use the same standard error (VAR=NULL or VAR=SAMPLE) as the equivalence test statistics and have a confidence coefficient of $100(1 - 2\alpha)\%$ (Schuirmann 1999). By default, if you do not specify the ALPHA= option, the equivalence confidence limits are 90% limits. If you specify VAR=NULL, separate standard errors are computed for the lower and upper margin tests, each based on the null proportion and the corresponding (lower or upper) margin. The confidence limits are computed by using the maximum of these two standard errors. You can compare the confidence limits to the equivalence limits, $(p_0 + \delta_L, p_0 + \delta_U)$.

If you specify the BINOMIAL option in the EXACT statement, PROC FREQ also provides an exact equivalence test by using two one-sided exact tests (TOST). The procedure computes lower and upper margin exact tests by using the binomial probability function as described in the section “[Noninferiority Test](#)” on page 2569. The overall exact p -value for the equivalence test is taken to be the larger p -value from the lower and upper margin exact tests. If you request exact statistics, PROC FREQ also includes exact (Clopper-Pearson) confidence limits in the equivalence analysis display. The confidence coefficient is $100(1 - 2\alpha)\%$ (Schuirmann 1999). See the section “[Exact \(Clopper-Pearson\) Confidence Limits](#)” on page 2567 for details.

Risks and Risk Differences

The RISKDIFF option in the TABLES statement provides estimates of risks (binomial proportions) and risk differences for 2×2 tables. This analysis might be appropriate when comparing the proportion of some characteristic for two groups, where row 1 and row 2 correspond to the two groups, and the columns correspond to two possible characteristics or outcomes. For example, the row variable might be a treatment or dose, and the column variable might be the response. For more information, see Collett (1991); Fleiss, Levin, and Paik (2003); Stokes, Davis, and Koch (2012).

Let the frequencies of the 2×2 table be represented as follows.

	Column 1	Column 2	Total
Row 1	n_{11}	n_{12}	$n_{1\cdot}$
Row 2	n_{21}	n_{22}	$n_{2\cdot}$
Total	$n_{\cdot 1}$	$n_{\cdot 2}$	n

By default when you specify the RISKDIFF option, PROC FREQ provides estimates of the row 1 risk (proportion), the row 2 risk, the overall risk, and the risk difference for column 1 and for column 2 of the 2×2 table. The risk difference is defined as the row 1 risk minus the row 2 risk. The risks are binomial proportions of their rows (row 1, row 2, or overall), and the computation of their standard errors and Wald confidence limits follow the binomial proportion computations, which are described in the section “[Binomial Proportion](#)” on page 2565.

The column 1 risk for row 1 is the proportion of row 1 observations classified in column 1,

$$\hat{p}_1 = n_{11} / n_{1\cdot}$$

which estimates the conditional probability of the column 1 response, given the first level of the row variable. The column 1 risk for row 2 is the proportion of row 2 observations classified in column 1,

$$\hat{p}_2 = n_{21} / n_{2\cdot}$$

The overall column 1 risk is the proportion of all observations classified in column 1,

$$\hat{p} = n_{.1} / n$$

The column 1 risk difference compares the risks for the two rows, and it is computed as the column 1 risk for row 1 minus the column 1 risk for row 2,

$$\hat{d} = \hat{p}_1 - \hat{p}_2$$

The standard error of the column 1 risk for row i is computed as

$$se(\hat{p}_i) = \sqrt{\hat{p}_i (1 - \hat{p}_i) / n_{i.}}$$

The standard error of the overall column 1 risk is computed as

$$se(\hat{p}) = \sqrt{\hat{p} (1 - \hat{p}) / n}$$

Where the two rows represent independent binomial samples, the standard error of the column 1 risk difference is computed as

$$se(\hat{d}) = \sqrt{\hat{p}_1(1 - \hat{p}_1) + \hat{p}_2(1 - \hat{p}_2)}$$

The computations are similar for the column 2 risks and risk difference.

Confidence Limits

By default, the RISKDIFF option provides Wald asymptotic confidence limits for the risks (row 1, row 2, and overall) and the risk difference. By default, the RISKDIFF option also provides exact (Clopper-Pearson) confidence limits for the risks. You can suppress the display of this information by specifying the NORISKS *riskdiff-option*. You can specify *riskdiff-options* to request tests and other types of confidence limits for the risk difference. See the sections “Risk Difference Confidence Limits” on page 2574 and “Risk Difference Tests” on page 2576 for more information.

The risks are equivalent to the binomial proportions of their corresponding rows. This section describes the Wald confidence limits that are provided by default when you specify the RISKDIFF option. The BINOMIAL option provides additional confidence limit types and tests for risks (binomial proportions). See the sections “Binomial Confidence Limits” on page 2566 and “Binomial Tests” on page 2568 for details.

The Wald confidence limits are based on the normal approximation to the binomial distribution. PROC FREQ computes the Wald confidence limits for the risks and risk differences as

$$\text{Est} \pm (z_{\alpha/2} \times se(\text{Est}))$$

where Est is the estimate, $z_{\alpha/2}$ is the $100(1 - \alpha/2)$ percentile of the standard normal distribution, and $se(\text{Est})$ is the standard error of the estimate. The confidence level α is determined by the value of the ALPHA= option; the default of ALPHA=0.5 produces 95% confidence limits.

If you specify the CORRECT *riskdiff-option*, PROC FREQ includes continuity corrections in the Wald confidence limits for the risks and risk differences. The purpose of a continuity correction is to adjust for the difference between the normal approximation and the binomial distribution, which is discrete. See Fleiss, Levin, and Paik (2003) for more information. The continuity-corrected Wald confidence limits are computed as

$$\text{Est} \pm (z_{\alpha/2} \times se(\text{Est}) + cc)$$

where cc is the continuity correction. For the row 1 risk, $cc = (1/2n_{1.})$; for the row 2 risk, $cc = (1/2n_{2.})$; for the overall risk, $cc = (1/2n)$; and for the risk difference, $cc = ((1/n_{1.} + 1/n_{2.})/2)$. The column 1 and column 2 risks use the same continuity corrections.

By default when you specify the RISKDIFF option, PROC FREQ also provides exact (Clopper-Pearson) confidence limits for the column 1, column 2, and overall risks. These confidence limits are constructed by inverting the equal-tailed test that is based on the binomial distribution. See the section “Exact (Clopper-Pearson) Confidence Limits” on page 2567 for details.

Risk Difference Confidence Limits You can request additional confidence limits for the risk difference by specifying the `CL= riskdiff-option`. Available confidence limit types include Agresti-Caffo, exact unconditional, Hauck-Anderson, Miettinen-Nurminen, Newcombe (hybrid-score), and Wald confidence limits. Continuity-corrected Newcombe and Wald confidence limits are also available.

The confidence coefficient for the confidence limits produced by the `CL= riskdiff-option` is $100(1 - \alpha)\%$, where the value of α is determined by the `ALPHA=` option. The default of `ALPHA=0.05` produces 95% confidence limits. This differs from the test-based confidence limits that are provided with the equivalence, noninferiority, and superiority tests, which have a confidence coefficient of $100(1 - 2\alpha)\%$ (Schuurmann 1999). See the section “Risk Difference Tests” on page 2576 for details.

The section “Exact Unconditional Confidence Limits for the Risk Difference” on page 2580 describes the computation of the exact confidence limits. The confidence limits are constructed by inverting two separate one-sided exact tests (tail method). By default, the tests are based on the unstandardized risk difference. If you specify the `RISKDIFF(METHOD=SCORE)` option, the tests are based on the score statistic.

The following sections describe the computation of the Agresti-Coull, Hauck-Anderson, Miettinen-Nurminen, Newcombe (hybrid-score), and Wald confidence limits for the risk difference.

Agresti-Caffo Confidence Limits The Agresti-Caffo confidence limits for the risk difference are computed as

$$\tilde{d} \pm (z_{\alpha/2} \times \text{se}(\tilde{d}))$$

where $\tilde{d} = \tilde{p}_1 - \tilde{p}_2$, $\tilde{p}_i = (n_{i1} + 1)/(n_{i.} + 2)$,

$$\text{se}(\tilde{d}) = \sqrt{\tilde{p}_1(1 - \tilde{p}_1)/(n_{1.} + 2) + \tilde{p}_2(1 - \tilde{p}_2)/(n_{2.} + 2)}$$

and $z_{\alpha/2}$ is the $100(1 - \alpha/2)$ percentile of the standard normal distribution.

The Agresti-Caffo interval adjusts the Wald interval for the risk difference by adding a pseudo-observation of each type (success and failure) to each sample. See Agresti and Caffo (2000) and Agresti and Coull (1998) for more information.

Hauck-Anderson Confidence Limits The Hauck-Anderson confidence limits for the risk difference are computed as

$$\hat{d} \pm (cc + z_{\alpha/2} \times \text{se}(\hat{d}))$$

where $\hat{d} = \hat{p}_1 - \hat{p}_2$ and $z_{\alpha/2}$ is the $100(1 - \alpha/2)$ percentile of the standard normal distribution. The standard error is computed from the sample proportions as

$$\text{se}(\hat{d}) = \sqrt{\hat{p}_1(1 - \hat{p}_1)/(n_{1.} - 1) + \hat{p}_2(1 - \hat{p}_2)/(n_{2.} - 1)}$$

The Hauck-Anderson continuity correction cc is computed as

$$cc = 1 / (2 \min(n_{1.}, n_{2.}))$$

See Hauck and Anderson (1986) for more information. The subsection “[Hauck-Anderson Test](#)” in the section “[Noninferiority Tests](#)” on page 2577 describes the corresponding noninferiority test.

Miettinen-Nurminen Confidence Limits The Miettinen-Nurminen confidence limits for the risk difference (Miettinen and Nurminen 1985; Newcombe and Nurminen 2011) are based on the likelihood score test for the null hypothesis that the risk difference is zero. The test statistic is

$$T(\delta) = (\hat{d} - \delta) / \sqrt{\widetilde{\text{Var}}(\delta)}$$

where \hat{d} is the observed value of the risk difference ($\hat{p}_1 - \hat{p}_2$),

$$\widetilde{\text{Var}}(\delta) = (n/(n-1)) (\tilde{p}_1(\delta)(1 - \tilde{p}_1(\delta))/n_1 + \tilde{p}_2(\delta)(1 - \tilde{p}_2(\delta))/n_2)$$

and $\tilde{p}_1(\delta)$ and $\tilde{p}_2(\delta)$ are the maximum likelihood estimates of the risks (proportions) when the risk difference is δ . PROC FREQ computes the maximum likelihood estimates $\tilde{p}_1(\delta)$ and $\tilde{p}_2(\delta)$ as described in the subsection “[Farrington-Manning Test](#)” in the section “[Noninferiority Tests](#)” on page 2577.

The $100(1 - \alpha)\%$ confidence interval for the risk difference consists of all values of δ for which the score test statistic $T(\delta)$ falls in the acceptance region,

$$\{\delta : T(\delta) < z_{\alpha/2}\}$$

PROC FREQ finds the confidence limits by iterative computation, which stops when the iteration increment falls below the convergence criterion or when the maximum number of iterations is reached, whichever occurs first. By default, the convergence criterion is 0.00000001 and the maximum number of iterations is 100.

By default, the Miettinen-Nurminen confidence limits include the bias correction factor $n/(n-1)$ in the computation of $\widetilde{\text{Var}}(\delta)$, as given by Miettinen and Nurminen (1985, p. 216). See Newcombe and Nurminen (2011) for more information. If you specify the `CL=MN(CORRECT=NO) riskdiff-option`, PROC FREQ does not include the bias correction factor in the computation of the confidence limits (Mee 1984). See also Agresti (2002, p. 77). The uncorrected confidence limits are labeled as “Miettinen-Nurminen-Mee” confidence limits in the displayed output.

Newcombe Confidence Limits Newcombe (hybrid-score) confidence limits for the risk difference are constructed from the Wilson score confidence limits for each of the two individual proportions. The confidence limits for the individual proportions are used in the standard error terms of the Wald confidence limits for the proportion difference. See Newcombe (1998a) and Barker et al. (2001) for more information.

Wilson score confidence limits for p_1 and p_2 are the roots of

$$|p_i - \hat{p}_i| = z_{\alpha/2} \sqrt{p_i(1 - p_i)/n_i}$$

for $i = 1, 2$. The confidence limits are computed as

$$\left(\hat{p}_i + z_{\alpha/2}^2/2n_i \pm z_{\alpha/2} \sqrt{(\hat{p}_i(1 - \hat{p}_i) + z_{\alpha/2}^2/4n_i)/n_i} \right) / \left(1 + z_{\alpha/2}^2/n_i \right)$$

See the section “[Wilson \(Score\) Confidence Limits](#)” on page 2567 for details.

Denote the lower and upper Wilson score confidence limits for p_1 as L_1 and U_1 , and denote the lower and upper confidence limits for p_2 as L_2 and U_2 . The Newcombe confidence limits for the proportion difference ($d = p_1 - p_2$) are computed as

$$d_L = (\hat{p}_1 - \hat{p}_2) - \sqrt{(\hat{p}_1 - L_1)^2 + (U_2 - \hat{p}_2)^2}$$

$$d_U = (\hat{p}_1 - \hat{p}_2) + \sqrt{(U_1 - \hat{p}_1)^2 + (\hat{p}_2 - L_2)^2}$$

If you specify the CORRECT *riskdiff-option*, PROC FREQ provides continuity-corrected Newcombe confidence limits. By including a continuity correction of $1/2n_i$, the Wilson score confidence limits for the individual proportions are computed as the roots of

$$|p_i - \hat{p}_i| - 1/2n_i = z_{\alpha/2} \sqrt{p_i(1 - p_i)/n_i}$$

The continuity-corrected confidence limits for the individual proportions are then used to compute the proportion difference confidence limits d_L and d_U .

Wald Confidence Limits The Wald confidence limits for the risk difference are computed as

$$\hat{d} \pm (z_{\alpha/2} \times \text{se}(\hat{d}))$$

where $\hat{d} = \hat{p}_1 - \hat{p}_2$, $z_{\alpha/2}$ is the $100(1 - \alpha/2)$ percentile of the standard normal distribution, and the standard error is computed from the sample proportions as

$$\text{se}(\hat{d}) = \sqrt{\hat{p}_1(1 - \hat{p}_1)/n_1 + \hat{p}_2(1 - \hat{p}_2)/n_2}$$

If you specify the CORRECT *riskdiff-option*, the Wald confidence limits include a continuity correction cc ,

$$\hat{d} \pm (cc + z_{\alpha/2} \times \text{se}(\hat{d}))$$

where $cc = (1/n_1 + 1/n_2)/2$.

The subsection “Wald Test” in the section “Noninferiority Tests” on page 2577 describes the corresponding noninferiority test.

Risk Difference Tests

You can specify *riskdiff-options* to request tests of the risk (proportion) difference. You can request tests of equality, noninferiority, superiority, and equivalence for the risk difference. The test of equality is a standard Wald asymptotic test, available with or without a continuity correction. For noninferiority, superiority, and equivalence tests of the risk difference, the following test methods are provided: Wald (with and without continuity correction), Hauck-Anderson, Farrington-Manning (score), and Newcombe (with and without continuity correction). You can specify the test method with the METHOD= *riskdiff-option*. By default, PROC FREQ uses METHOD=WALD.

Equality Test If you specify the EQUAL *riskdiff-option*, PROC FREQ computes a test of equality, or a test of the null hypothesis that the risk difference equals zero. For the column 1 (or 2) risk difference, this test can be expressed as $H_0: d = 0$ versus the alternative $H_a: d \neq 0$, where $d = p_1 - p_2$ denotes the column 1 (or 2) risk difference. PROC FREQ provides a Wald asymptotic test of equality. The test statistic is computed as

$$z = \hat{d}/\text{se}(\hat{d})$$

By default, the standard error is computed from the sample proportions as

$$se(\hat{d}) = \sqrt{\hat{p}_1(1 - \hat{p}_1)/n_{1.} + \hat{p}_2(1 - \hat{p}_2)/n_{2.}}$$

If you specify the VAR=NULL *riskdiff-option*, the standard error is based on the null hypothesis that the row 1 and row 2 risks are equal,

$$se(\hat{d}) = \sqrt{\hat{p}(1 - \hat{p}) \times (1/n_{1.} + 1/n_{2.})}$$

where $\hat{p} = n_{.1}/n$ estimates the overall column 1 risk.

If you specify the CORRECT *riskdiff-option*, PROC FREQ includes a continuity correction in the test statistic. If $\hat{d} > 0$, the continuity correction is subtracted from \hat{d} in the numerator of the test statistic; otherwise, the continuity correction is added to the numerator. The value of the continuity correction is $(1/n_{1.} + 1/n_{2.})/2$.

PROC FREQ computes one-sided and two-sided p -values for this test. When the test statistic z is greater than 0, PROC FREQ displays the right-sided p -value, which is the probability of a larger value occurring under the null hypothesis. The one-sided p -value can be expressed as

$$P_1 = \begin{cases} \text{Prob}(Z > z) & \text{if } z > 0 \\ \text{Prob}(Z < z) & \text{if } z \leq 0 \end{cases}$$

where Z has a standard normal distribution. The two-sided p -value is computed as $P_2 = 2 \times P_1$.

Noninferiority Tests If you specify the NONINF *riskdiff-option*, PROC FREQ provides a noninferiority test for the risk difference, or the difference between two proportions. The null hypothesis for the noninferiority test is

$$H_0: p_1 - p_2 \leq -\delta$$

versus the alternative

$$H_a: p_1 - p_2 > -\delta$$

where δ is the noninferiority margin. Rejection of the null hypothesis indicates that the row 1 risk is not inferior to the row 2 risk. See Chow, Shao, and Wang (2003) for more information.

You can specify the value of δ with the MARGIN= *riskdiff-option*. By default, $\delta = 0.2$. You can specify the test method with the METHOD= *riskdiff-option*. The following methods are available for the risk difference noninferiority analysis: Wald (with and without continuity correction), Hauck-Anderson, Farrington-Manning (score), and Newcombe (with and without continuity correction). The Wald, Hauck-Anderson, and Farrington-Manning methods provide tests and corresponding test-based confidence limits; the Newcombe method provides only confidence limits. If you do not specify METHOD=, PROC FREQ uses the Wald test by default.

The confidence coefficient for the test-based confidence limits is $100(1 - 2\alpha)\%$ (Schuirmann 1999). By default, if you do not specify the ALPHA= option, these are 90% confidence limits. You can compare the confidence limits to the noninferiority limit, $-\delta$.

The following sections describe the noninferiority analysis methods for the risk difference.

Wald Test If you specify the METHOD=WALD *riskdiff-option*, PROC FREQ provides an asymptotic Wald test of noninferiority for the risk difference. This is also the default method. The Wald test statistic is computed as

$$z = (\hat{d} + \delta) / \text{se}(\hat{d})$$

where $\hat{d} = \hat{p}_1 - \hat{p}_2$ estimates the risk difference and δ is the noninferiority margin.

By default, the standard error for the Wald test is computed from the sample proportions as

$$\text{se}(\hat{d}) = \sqrt{\hat{p}_1(1 - \hat{p}_1)/n_1 + \hat{p}_2(1 - \hat{p}_2)/n_2}$$

If you specify the VAR=NULL *riskdiff-option*, the standard error is based on the null hypothesis that the risk difference equals $-\delta$ (Dunnett and Gent 1977). The standard error is computed as

$$\text{se}(\hat{d}) = \sqrt{\tilde{p}(1 - \tilde{p})/n_2 + (\tilde{p} - \delta)(1 - \tilde{p} + \delta)/n_1}$$

where

$$\tilde{p} = (n_{11} + n_{21} + \delta n_{1.})/n$$

If you specify the CORRECT *riskdiff-option*, the test statistic includes a continuity correction. The continuity correction is subtracted from the numerator of the test statistic if the numerator is greater than zero; otherwise, the continuity correction is added to the numerator. The value of the continuity correction is $(1/n_1 + 1/n_2)/2$.

The p -value for the Wald noninferiority test is $P_z = \text{Prob}(Z > z)$, where Z has a standard normal distribution.

Hauck-Anderson Test If you specify the METHOD=HA *riskdiff-option*, PROC FREQ provides the Hauck-Anderson test for noninferiority. The Hauck-Anderson test statistic is computed as

$$z = (\hat{d} + \delta \pm cc) / \text{se}(\hat{d})$$

where $\hat{d} = \hat{p}_1 - \hat{p}_2$ and the standard error is computed from the sample proportions as

$$\text{se}(\hat{d}) = \sqrt{\hat{p}_1(1 - \hat{p}_1)/(n_1 - 1) + \hat{p}_2(1 - \hat{p}_2)/(n_2 - 1)}$$

The Hauck-Anderson continuity correction cc is computed as

$$cc = 1 / (2 \min(n_{1.}, n_{2.}))$$

The p -value for the Hauck-Anderson noninferiority test is $P_z = \text{Prob}(Z > z)$, where Z has a standard normal distribution. See Hauck and Anderson (1986) and Schuirmann (1999) for more information.

Farrington-Manning Test If you specify the METHOD=FM *riskdiff-option*, PROC FREQ provides the Farrington-Manning (score) test of noninferiority for the risk difference. The score test statistic is computed as

$$z = (\hat{d} + \delta) / \text{se}(\hat{d})$$

where $\hat{d} = \hat{p}_1 - \hat{p}_2$ and

$$\text{se}(\hat{d}) = \sqrt{\tilde{p}_1(1 - \tilde{p}_1)/n_1 + \tilde{p}_2(1 - \tilde{p}_2)/n_2}$$

where \tilde{p}_1 and \tilde{p}_2 are the maximum likelihood estimators of p_1 and p_2 under the null hypothesis that the risk difference equals $-\delta$ (Miettinen and Nurminen 1985; Farrington and Manning 1990; Dann and Koch 2005). The p -value for the noninferiority test is then $P_z = \text{Prob}(Z > z)$, where Z has a standard normal distribution.

From Farrington and Manning (1990, p. 1453), the solution to the maximum likelihood equation is

$$\tilde{p}_1 = 2u \cos(w) - b/3a \quad \text{and} \quad \tilde{p}_2 = \tilde{p}_1 + \delta$$

where

$$\begin{aligned} w &= (\pi + \cos^{-1}(v/u^3))/3 \\ v &= b^3/(3a)^3 - bc/6a^2 + d/2a \\ u &= \text{sign}(v) \sqrt{b^2/(3a)^2 - c/3a} \\ a &= 1 + \theta \\ b &= -(1 + \theta + \hat{p}_1 + \theta \hat{p}_2 - \delta(\theta + 2)) \\ c &= \delta^2 - \delta(2\hat{p}_1 + \theta + 1) + \hat{p}_1 + \theta \hat{p}_2 \\ d &= \hat{p}_1 \delta(1 - \delta) \\ \theta &= n_2./n_1. \end{aligned}$$

Newcombe Noninferiority Analysis If you specify the `METHOD=NEWCOMBE riskdiff-option`, PROC FREQ provides a noninferiority analysis that is based on Newcombe hybrid-score confidence limits for the risk difference. The confidence coefficient for the confidence limits is $100(1 - 2\alpha)\%$ (Schuirmann 1999). By default, if you do not specify the `ALPHA=` option, these are 90% confidence limits. You can compare the confidence limits with the noninferiority limit, $-\delta$. If you specify the `CORRECT riskdiff-option`, the confidence limits includes a continuity correction. See the subsection “Newcombe Confidence Limits” in the section “Risk Difference Confidence Limits” on page 2574 for more information.

Superiority Test If you specify the `SUP riskdiff-option`, PROC FREQ provides a superiority test for the risk difference. The null hypothesis is

$$H_0: p_1 - p_2 \leq \delta$$

versus the alternative

$$H_a: p_1 - p_2 > \delta$$

where δ is the superiority margin. Rejection of the null hypothesis indicates that the row 1 proportion is superior to the row 2 proportion. You can specify the value of δ with the `MARGIN= riskdiff-option`. By default, $\delta = 0.2$.

The superiority analysis is identical to the noninferiority analysis but uses a positive value of the margin δ in the null hypothesis. The superiority computations follow those in the section “Noninferiority Tests” on page 2577 by replacing $-\delta$ by δ . See Chow, Shao, and Wang (2003) for more information.

Equivalence Tests If you specify the *EQUIV riskdiff-option*, PROC FREQ provides an equivalence test for the risk difference, or the difference between two proportions. The null hypothesis for the equivalence test is

$$H_0: p_1 - p_2 \leq -\delta_L \quad \text{or} \quad p_1 - p_2 \geq \delta_U$$

versus the alternative

$$H_a: \delta_L < p_1 - p_2 < \delta_U$$

where δ_L is the lower margin and δ_U is the upper margin. Rejection of the null hypothesis indicates that the two binomial proportions are equivalent. See Chow, Shao, and Wang (2003) for more information.

You can specify the value of the margins δ_L and δ_U with the *MARGIN= riskdiff-option*. If you do not specify *MARGIN=*, PROC FREQ uses lower and upper margins of -0.2 and 0.2 by default. If you specify a single margin value δ , PROC FREQ uses lower and upper margins of $-\delta$ and δ . You can specify the test method with the *METHOD= riskdiff-option*. The following methods are available for the risk difference equivalence analysis: Wald (with and without continuity correction), Hauck-Anderson, Farrington-Manning, and Newcombe (with and without continuity correction). The Wald, Hauck-Anderson, and Farrington-Manning methods provide tests and corresponding test-based confidence limits; the Newcombe method provides only confidence limits. If you do not specify *METHOD=*, PROC FREQ uses the Wald test by default.

PROC FREQ computes two one-sided tests (TOST) for equivalence analysis (Schuirmann 1987). The TOST approach includes a right-sided test for the lower margin δ_L and a left-sided test for the upper margin δ_U . The overall p -value is taken to be the larger of the two p -values from the lower and upper tests.

The section “**Noninferiority Tests**” on page 2577 gives details about the Wald, Hauck-Anderson, Farrington-Manning and Newcombe methods for the risk difference. The lower margin equivalence test statistic takes the same form as the noninferiority test statistic but uses the lower margin value δ_L in place of $-\delta$. The upper margin equivalence test statistic take the same form as the noninferiority test statistic but uses the upper margin value δ_U in place of $-\delta$.

The test-based confidence limits for the risk difference are computed according to the equivalence test method that you select. If you specify *METHOD=WALD* with *VAR=NULL*, or *METHOD=FM*, separate standard errors are computed for the lower and upper margin tests. In this case, the test-based confidence limits are computed by using the maximum of these two standard errors. The confidence limits have a confidence coefficient of $100(1 - 2\alpha)\%$ (Schuirmann 1999). By default, if you do not specify the *ALPHA=* option, these are 90% confidence limits. You can compare the confidence limits to the equivalence limits, (δ_L, δ_U) .

Exact Unconditional Confidence Limits for the Risk Difference

If you specify the *RISKDIFF* option in the *EXACT* statement, PROC FREQ provides exact unconditional confidence limits for the risk difference. PROC FREQ computes the confidence limits by inverting two separate one-sided tests (tail method), where the size of each test is at most $\alpha/2$ and the confidence coefficient is at least $(1 - \alpha)$. Exact conditional methods, described in the section “**Exact Statistics**” on page 2601, do not apply to the risk difference due to the presence of a nuisance parameter (Agresti 1992). The unconditional approach eliminates the nuisance parameter by maximizing the p -value over all possible values of the parameter (Santner and Snell 1980).

By default, PROC FREQ uses the unstandardized risk difference as the test statistic in the confidence limit computations. If you specify the *RISKDIFF(METHOD=SCORE)* option, the procedure uses the score

statistic (Chan and Zhang 1999). The score statistic is a less discrete statistic than the raw risk difference and produces less conservative confidence limits (Agresti and Min 2001). See also Santner et al. (2007) for comparisons of methods for computing exact confidence limits for the risk difference.

PROC FREQ computes the confidence limits as follows. The risk difference is defined as the difference between the row 1 and row 2 risks (proportions), $d = p_1 - p_2$, and n_1 and n_2 denote the row totals of the 2×2 table. The joint probability function for the table can be expressed in terms of the table cell frequencies, the risk difference, and the nuisance parameter p_2 as

$$f(n_{11}, n_{21}; n_1, n_2, d, p_2) = \binom{n_1}{n_{11}} (d + p_2)^{n_{11}} (1 - d - p_2)^{n_1 - n_{11}} \times \binom{n_2}{n_{21}} p_2^{n_{21}} (1 - p_2)^{n_2 - n_{21}}$$

The $100(1 - \alpha/2)\%$ confidence limits for the risk difference are computed as

$$\begin{aligned} d_L &= \sup (d_* : P_U(d_*) > \alpha/2) \\ d_U &= \inf (d_* : P_L(d_*) > \alpha/2) \end{aligned}$$

where

$$\begin{aligned} P_U(d_*) &= \sup_{p_2} \left(\sum_{A, T(a) \geq t_0} f(n_{11}, n_{21}; n_1, n_2, d_*, p_2) \right) \\ P_L(d_*) &= \sup_{p_2} \left(\sum_{A, T(a) \leq t_0} f(n_{11}, n_{21}; n_1, n_2, d_*, p_2) \right) \end{aligned}$$

The set A includes all 2×2 tables with row sums equal to n_1 and n_2 , and $T(a)$ denotes the value of the test statistic for table a in A . To compute $P_U(d_*)$, the sum includes probabilities of those tables for which $(T(a) \geq t_0)$, where t_0 is the value of the test statistic for the observed table. For a fixed value of d_* , $P_U(d_*)$ is taken to be the maximum sum over all possible values of p_2 .

By default, PROC FREQ uses the unstandardized risk difference as the test statistic T . If you specify the RISKDIFF(METHOD=SCORE) option, the procedure uses the risk difference score statistic as the test statistic (Chan and Zhang 1999). The computation of the risk difference score statistic is described in the subsection “Farrington-Manning Test” in the section “Noninferiority Tests” on page 2577. See Miettinen and Nurminen (1985) and Farrington and Manning (1990) for more information.

Barnard’s Unconditional Exact Test

The BARNARD option in the EXACT statement provides an unconditional exact test for the risk (proportion) difference for 2×2 tables. The reference set for the unconditional exact test consists of all 2×2 tables that have the same row sums as the observed table (Barnard 1945, 1947, 1949). This differs from the reference set for exact conditional inference, which is restricted to the set of tables that have the same row sums and the same column sums as the observed table. See the sections “Fisher’s Exact Test” on page 2554 and “Exact Statistics” on page 2601 for more information.

The test statistic is the standardized risk difference, which is computed as

$$T = d / \sqrt{p_{\cdot 1}(1 - p_{\cdot 1})(1/n_1 + 1/n_2)}$$

where the risk difference d is defined as the difference between the row 1 and row 2 risks (proportions), $d = (n_{11}/n_1 - n_{21}/n_2)$; n_1 and n_2 are the row 1 and row 2 totals, respectively; and $p_{.1}$ is the overall proportion in column 1, $(n_{11} + n_{21})/n$.

Under the null hypothesis that the risk difference is 0, the joint probability function for a table can be expressed in terms of the table cell frequencies, the row totals, and the unknown parameter π as

$$f(n_{11}, n_{21}; n_1, n_2, \pi) = \binom{n_1}{n_{11}} \binom{n_2}{n_{21}} \pi^{n_{11} + n_{21}} (1 - \pi)^{n - n_{11} - n_{21}}$$

where π is the common value of the risk (proportion).

PROC FREQ sums the table probabilities over the reference set for those tables where the test statistic is greater than or equal to the observed value of the test statistic. This sum can be expressed as

$$\text{Prob}(\pi) = \sum_{A, T(a) \geq t_0} f(n_{11}, n_{21}; n_1, n_2, \pi)$$

where the set A contains all 2×2 tables with row sums equal to n_1 and n_2 , and $T(a)$ denotes the value of the test statistic for table a in A . The sum includes probabilities of those tables for which $(T(a) \geq t_0)$, where t_0 is the value of the test statistic for the observed table.

The sum $\text{Prob}(\pi)$ depends on the unknown value of π . To compute the exact p -value, PROC FREQ eliminates the nuisance parameter π by taking the maximum value of $\text{Prob}(\pi)$ over all possible values of π ,

$$\text{Prob} = \sup_{(0 \leq \pi \leq 1)} (\text{Prob}(\pi))$$

See Suissa and Shuster (1985) and Mehta and Senchaudhuri (2003).

Odds Ratio and Relative Risks for 2 x 2 Tables

Odds Ratio (Case-Control Studies)

The odds ratio is a useful measure of association for a variety of study designs. For a retrospective design called a *case-control study*, the odds ratio can be used to estimate the relative risk when the probability of positive response is small (Agresti 2002). In a case-control study, two independent samples are identified based on a binary (yes-no) response variable, and the conditional distribution of a binary explanatory variable is examined, within fixed levels of the response variable. See Stokes, Davis, and Koch (2012) and Agresti (2007).

The odds of a positive response (column 1) in row 1 is n_{11}/n_{12} . Similarly, the odds of a positive response in row 2 is n_{21}/n_{22} . The odds ratio is formed as the ratio of the row 1 odds to the row 2 odds. The odds ratio for a 2×2 table is defined as

$$OR = \frac{n_{11}/n_{12}}{n_{21}/n_{22}} = \frac{n_{11} n_{22}}{n_{12} n_{21}}$$

The odds ratio can be any nonnegative number. When the row and column variables are independent, the true value of the odds ratio equals 1. An odds ratio greater than 1 indicates that the odds of a positive response are higher in row 1 than in row 2. Values less than 1 indicate the odds of positive response are higher in row 2. The strength of association increases with the deviation from 1.

The transformation $G = (OR - 1)/(OR + 1)$ transforms the odds ratio to the range $(-1, 1)$ with $G = 0$ when $OR = 1$; $G = -1$ when $OR = 0$; and G approaches 1 as OR approaches infinity. G is the gamma statistic, which PROC FREQ computes when you specify the MEASURES option.

The asymptotic $100(1 - \alpha)\%$ confidence limits for the odds ratio are

$$(OR \times \exp(-z\sqrt{v}), OR \times \exp(z\sqrt{v}))$$

where

$$v = \text{Var}(\ln OR) = \frac{1}{n_{11}} + \frac{1}{n_{12}} + \frac{1}{n_{21}} + \frac{1}{n_{22}}$$

and z is the $100(1 - \alpha/2)$ percentile of the standard normal distribution. If any of the four cell frequencies are zero, the estimates are not computed.

Exact Confidence Limits for the Odds Ratio When you specify the OR option in the EXACT statement, PROC FREQ computes exact confidence limits for the odds ratio. Because this is a discrete problem, the confidence coefficient for the exact confidence interval is not exactly $(1 - \alpha)$ but is at least $(1 - \alpha)$. Thus, these confidence limits are conservative. See Agresti (1992) for more information.

PROC FREQ computes exact confidence limits for the odds ratio by using an algorithm based on Thomas (1971). See also Gart (1971). The following two equations are solved iteratively to determine the lower and upper confidence limits, ϕ_1 and ϕ_2 :

$$\sum_{i=n_{11}}^{n_{1\cdot}} \binom{n_{1\cdot}}{i} \binom{n_{2\cdot}}{n_{1\cdot} - i} \phi_1^i / \sum_{i=0}^{n_{1\cdot}} \binom{n_{1\cdot}}{i} \binom{n_{2\cdot}}{n_{1\cdot} - i} \phi_1^i = \alpha/2$$

$$\sum_{i=0}^{n_{11}} \binom{n_{1\cdot}}{i} \binom{n_{2\cdot}}{n_{1\cdot} - i} \phi_2^i / \sum_{i=0}^{n_{1\cdot}} \binom{n_{1\cdot}}{i} \binom{n_{2\cdot}}{n_{1\cdot} - i} \phi_2^i = \alpha/2$$

When the odds ratio equals zero, which occurs when either $n_{11} = 0$ or $n_{22} = 0$, PROC FREQ sets the lower exact confidence limit to zero and determines the upper limit with level α . Similarly, when the odds ratio equals infinity, which occurs when either $n_{12} = 0$ or $n_{21} = 0$, PROC FREQ sets the upper exact confidence limit to infinity and determines the lower limit with level α .

Relative Risks (Cohort Studies)

These measures of relative risk are useful in *cohort* (prospective) study designs, where two samples are identified based on the presence or absence of an explanatory factor. The two samples are observed in future time for the binary (yes-no) response variable under study. Relative risk measures are also useful in cross-sectional studies, where two variables are observed simultaneously. See Stokes, Davis, and Koch (2012) and Agresti (2007) for more information.

The column 1 relative risk is the ratio of the column 1 risk for row 1 to row 2. The column 1 risk for row 1 is the proportion of the row 1 observations classified in column 1,

$$p_1 = n_{11} / n_{1\cdot}$$

Similarly, the column 1 risk for row 2 is

$$p_2 = n_{21} / n_{2\cdot}$$

The column 1 relative risk is computed as

$$RR_1 = p_1 / p_2$$

A relative risk greater than 1 indicates that the probability of positive response is greater in row 1 than in row 2. Similarly, a relative risk less than 1 indicates that the probability of positive response is less in row 1 than in row 2. The strength of association increases with the deviation from 1.

Asymptotic $100(1 - \alpha)\%$ confidence limits for the column 1 relative risk are computed as

$$(RR_1 \times \exp(-z\sqrt{v}), RR_1 \times \exp(z\sqrt{v}))$$

where

$$v = \text{Var}(\ln RR_1) = ((1 - p_1)/n_{11}) + ((1 - p_2)/n_{21})$$

and z is the $100(1 - \alpha/2)$ percentile of the standard normal distribution. If either n_{11} or n_{21} is zero, the estimates are not computed.

PROC FREQ computes the column 2 relative risks in the same way.

Exact Unconditional Confidence Limits for the Relative Risk If you specify the RELRISK option in the EXACT statement, PROC FREQ provides exact unconditional confidence limits for the relative risk. PROC FREQ computes the confidence limits by inverting two separate one-sided tests (tail method), where the size of each test is at most $\alpha/2$ and the confidence coefficient is at least $(1 - \alpha)$. Exact conditional methods, described in the section “Exact Statistics” on page 2601, do not apply to the relative risk due to the presence of a nuisance parameter (Agresti 1992). The unconditional approach eliminates the nuisance parameter by maximizing the p -value over all possible values of the parameter (Santner and Snell 1980).

By default, PROC FREQ uses the unstandardized relative risk as the test statistic in the confidence limit computations. If you specify the RELRISK(METHOD=SCORE) option, the procedure uses the relative risk score statistic (Chan and Zhang 1999). The score statistic is a less discrete statistic than the raw relative risk and produces less conservative confidence limits (Agresti and Min 2001). See also Santner et al. (2007) for comparisons of methods for computing exact confidence limits.

See the section “Exact Unconditional Confidence Limits for the Risk Difference” on page 2580 for a description of the method that PROC FREQ uses to compute confidence limits for the relative risk. The test statistic for the relative risk computation is either the unstandardized relative risk (by default) or the relative risk score statistic (if you specify the RELRISK(METHOD=SCORE) option). PROC FREQ uses the following form of the unstandardized relative risk, which adds 0.05 to each frequency, to ensure that the statistic is defined when there are zero table cells (Gart and Nam 1988):

$$rr = \frac{(n_{11} + 0.5) / (n_{1\cdot} + 0.5)}{(n_{21} + 0.5) / (n_{2\cdot} + 0.5)}$$

If you specify the RELRISK(METHOD=SCORE) option, PROC FREQ uses the relative risk score statistic (Miettinen and Nurminen 1985; Farrington and Manning 1990). This test statistic is computed as

$$z = (\hat{p}_1 - R_0 \hat{p}_2) / se(rr)$$

where

$$se(rr) = \sqrt{\tilde{p}_1(1 - \tilde{p}_1)/n_1 + R_0^2 \tilde{p}_2(1 - \tilde{p}_2)/n_2}$$

where \tilde{p}_1 and \tilde{p}_2 are the maximum likelihood estimators of p_1 and p_2 under the null hypothesis that the relative risk equals R_0 . From Farrington and Manning (1990, p. 1454), the maximum likelihood solution is

$$\tilde{p}_1 = (-b - \sqrt{b^2 - 4ac})/2a \quad \text{and} \quad \tilde{p}_2 = \tilde{p}_1/R_0$$

where

$$\begin{aligned} a &= 1 + \theta \\ b &= -(R_0(1 + \theta \hat{p}_2) + \theta + \hat{p}_1) \\ c &= R_0(\hat{p}_1 + \theta \hat{p}_2) \\ \theta &= n_2./n_1. \end{aligned}$$

Cochran-Armitage Test for Trend

The TREND option in the TABLES statement provides the Cochran-Armitage test for trend, which tests for trend in binomial proportions across levels of a single factor or covariate. This test is appropriate for a two-way table where one variable has two levels and the other variable is ordinal. The two-level variable represents the response, and the other variable represents an explanatory variable with ordered levels. When the two-way has two columns and R rows, PROC FREQ tests for trend across the R levels of the row variable, and the binomial proportion is computed as the proportion of observations in the first column. When the table has two rows and C columns, PROC FREQ tests for trend across the C levels of the column variable, and the binomial proportion is computed as the proportion of observations in the first row.

The trend test is based on the regression coefficient for the weighted linear regression of the binomial proportions on the scores of the explanatory variable levels. See Margolin (1988) and Agresti (2002) for details. If the table has two columns and R rows, the trend test statistic is computed as

$$T = \sum_{i=1}^R n_{i1}(R_i - \bar{R}) / \sqrt{p_{.1}(1 - p_{.1}) s^2}$$

where R_i is the score of row i , \bar{R} is the average row score, and

$$s^2 = \sum_{i=1}^R n_{i.}(R_i - \bar{R})^2$$

The SCORES= option in the TABLES statement determines the type of row scores used in computing the trend test (and other score-based statistics). The default is SCORES=TABLE. See the section “Scores” on page 2549 for details. For character variables, the table scores for the row variable are the row numbers (for example, 1 for the first row, 2 for the second row, and so on). For numeric variables, the table score for each row is the numeric value of the row level. When you perform the trend test, the explanatory variable might be numeric (for example, dose of a test substance), and the variable values might be appropriate scores. If

the explanatory variable has ordinal levels that are not numeric, you can assign meaningful scores to the variable levels. Sometimes equidistant scores, such as the table scores for a character variable, might be appropriate. For more information on choosing scores for the trend test, see Margolin (1988).

The null hypothesis for the Cochran-Armitage test is no trend, which means that the binomial proportion $p_{i1} = n_{i1}/n_i$ is the same for all levels of the explanatory variable. Under the null hypothesis, the trend statistic has an asymptotic standard normal distribution.

PROC FREQ computes one-sided and two-sided p -values for the trend test. When the test statistic is greater than its null hypothesis expected value of zero, PROC FREQ displays the right-sided p -value, which is the probability of a larger value of the statistic occurring under the null hypothesis. A small right-sided p -value supports the alternative hypothesis of increasing trend in proportions from row 1 to row R . When the test statistic is less than or equal to zero, PROC FREQ displays the left-sided p -value. A small left-sided p -value supports the alternative of decreasing trend.

The one-sided p -value for the trend test is computed as

$$P_1 = \begin{cases} \text{Prob}(Z > T) & \text{if } T > 0 \\ \text{Prob}(Z < T) & \text{if } T \leq 0 \end{cases}$$

where Z has a standard normal distribution. The two-sided p -value is computed as

$$P_2 = \text{Prob}(|Z| > |T|)$$

PROC FREQ also provides exact p -values for the Cochran-Armitage trend test. You can request the exact test by specifying the TREND option in the EXACT statement. See the section “Exact Statistics” on page 2601 for more information.

Jonckheere-Terpstra Test

The JT option in the TABLES statement provides the Jonckheere-Terpstra test, which is a nonparametric test for ordered differences among classes. It tests the null hypothesis that the distribution of the response variable does not differ among classes. It is designed to detect alternatives of ordered class differences, which can be expressed as $\tau_1 \leq \tau_2 \leq \dots \leq \tau_R$ (or $\tau_1 \geq \tau_2 \geq \dots \geq \tau_R$), with at least one of the inequalities being strict, where τ_i denotes the effect of class i . For such ordered alternatives, the Jonckheere-Terpstra test can be preferable to tests of more general class difference alternatives, such as the Kruskal-Wallis test (produced by the WILCOXON option in the NPAR1WAY procedure). See Pirie (1983) and Hollander and Wolfe (1999) for more information about the Jonckheere-Terpstra test.

The Jonckheere-Terpstra test is appropriate for a two-way table in which an ordinal column variable represents the response. The row variable, which can be nominal or ordinal, represents the classification variable. The levels of the row variable should be ordered according to the ordering you want the test to detect. The order of variable levels is determined by the ORDER= option in the PROC FREQ statement. The default is ORDER=INTERNAL, which orders by unformatted values. If you specify ORDER=DATA, PROC FREQ orders values according to their order in the input data set. For more information about how to order variable levels, see the ORDER= option.

The Jonckheere-Terpstra test statistic is computed by first forming $R(R-1)/2$ Mann-Whitney counts $M_{i,i'}$, where $i < i'$, for pairs of rows in the contingency table,

$$M_{i,i'} = \left\{ \begin{array}{l} \text{number of times } X_{i,j} < X_{i',j'}, \quad j = 1, \dots, n_i; \quad j' = 1, \dots, n_{i'} \end{array} \right\} \\ + \frac{1}{2} \left\{ \begin{array}{l} \text{number of times } X_{i,j} = X_{i',j'}, \quad j = 1, \dots, n_i; \quad j' = 1, \dots, n_{i'} \end{array} \right\}$$

where $X_{i,j}$ is response j in row i . The Jonckheere-Terpstra test statistic is computed as

$$J = \sum_{1 \leq i < i' \leq R} \sum M_{i,i'}$$

This test rejects the null hypothesis of no difference among classes for large values of J . Asymptotic p -values for the Jonckheere-Terpstra test are obtained by using the normal approximation for the distribution of the standardized test statistic. The standardized test statistic is computed as

$$J^* = (J - E_0(J)) / \sqrt{\text{Var}_0(J)}$$

where $E_0(J)$ and $\text{Var}_0(J)$ are the expected value and variance of the test statistic under the null hypothesis,

$$E_0(J) = \left(n^2 - \sum_i n_{i.}^2 \right) / 4$$

$$\text{Var}_0(J) = A/72 + B/(36n(n-1)(n-2)) + C/(8n(n-1))$$

where

$$A = n(n-1)(2n+5) - \sum_i n_{i.}(n_{i.}-1)(2n_{i.}+5) - \sum_j n_{.j}(n_{.j}-1)(2n_{.j}+5)$$

$$B = \left(\sum_i n_{i.}(n_{i.}-1)(n_{i.}-2) \right) \left(\sum_j n_{.j}(n_{.j}-1)(n_{.j}-2) \right)$$

$$C = \left(\sum_i n_{i.}(n_{i.}-1) \right) \left(\sum_j n_{.j}(n_{.j}-1) \right)$$

PROC FREQ computes one-sided and two-sided p -values for the Jonckheere-Terpstra test. When the standardized test statistic is greater than its null hypothesis expected value of zero, PROC FREQ displays the right-sided p -value, which is the probability of a larger value of the statistic occurring under the null hypothesis. A small right-sided p -value supports the alternative hypothesis of increasing order from row 1 to row R . When the standardized test statistic is less than or equal to zero, PROC FREQ displays the left-sided p -value. A small left-sided p -value supports the alternative of decreasing order from row 1 to row R .

The one-sided p -value for the Jonckheere-Terpstra test, P_1 , is computed as

$$P_1 = \begin{cases} \text{Prob}(Z > J^*) & \text{if } J^* > 0 \\ \text{Prob}(Z < J^*) & \text{if } J^* \leq 0 \end{cases}$$

where Z has a standard normal distribution. The two-sided p -value, P_2 , is computed as

$$P_2 = \text{Prob}(|Z| > |J^*|)$$

PROC FREQ also provides exact p -values for the Jonckheere-Terpstra test. You can request the exact test by specifying the JT option in the EXACT statement. See the section “Exact Statistics” on page 2601 for more information.

Tests and Measures of Agreement

When you specify the AGREE option in the TABLES statement, PROC FREQ computes tests and measures of agreement for square tables (that is, for tables where the number of rows equals the number of columns). For two-way tables, these tests and measures include McNemar's test for 2×2 tables, Bowker's test of symmetry, the simple kappa coefficient, and the weighted kappa coefficient. For multiple strata (n -way tables, where $n > 2$), PROC FREQ also computes the overall simple kappa coefficient and the overall weighted kappa coefficient, as well as tests for equal kappas (simple and weighted) among strata. Cochran's Q is computed for multiway tables when each variable has two levels, that is, for $h \times 2 \times 2$ tables.

PROC FREQ computes the kappa coefficients (simple and weighted), their asymptotic standard errors, and their confidence limits when you specify the AGREE option in the TABLES statement. If you also specify the KAPPA option in the TEST statement, then PROC FREQ computes the asymptotic test of the hypothesis that simple kappa equals zero. Similarly, if you specify the WTKAP option in the TEST statement, PROC FREQ computes the asymptotic test for weighted kappa.

In addition to the asymptotic tests described in this section, PROC FREQ provides exact p -values for McNemar's test, the simple kappa coefficient test, and the weighted kappa coefficient test. You can request these exact tests by specifying the corresponding options in the EXACT statement. See the section "Exact Statistics" on page 2601 for more information.

The following sections provide the formulas that PROC FREQ uses to compute the AGREE statistics. For information about the use and interpretation of these statistics, see Agresti (2002, 2007); Fleiss, Levin, and Paik (2003), and the other references cited for each statistic.

McNemar's Test

PROC FREQ computes McNemar's test for 2×2 tables when you specify the AGREE option. McNemar's test is appropriate when you are analyzing data from matched pairs of subjects with a dichotomous (yes-no) response. It tests the null hypothesis of marginal homogeneity, or $p_{1.} = p_{.1}$. McNemar's test is computed as

$$Q_M = (n_{12} - n_{21})^2 / (n_{12} + n_{21})$$

Under the null hypothesis, Q_M has an asymptotic chi-square distribution with one degree of freedom. See McNemar (1947), as well as the general references cited in the preceding section. In addition to the asymptotic test, PROC FREQ also computes the exact p -value for McNemar's test when you specify the MCNEM option in the EXACT statement.

Bowker's Test of Symmetry

For Bowker's test of symmetry, the null hypothesis is that the cell proportions are symmetric, or that $p_{ij} = p_{ji}$ for all pairs of table cells. For 2×2 tables, Bowker's test is identical to McNemar's test, and so PROC FREQ provides Bowker's test for square tables larger than 2×2 .

Bowker's test of symmetry is computed as

$$Q_B = \sum_{i < j} \sum (n_{ij} - n_{ji})^2 / (n_{ij} + n_{ji})$$

For large samples, Q_B has an asymptotic chi-square distribution with $R(R-1)/2$ degrees of freedom under the null hypothesis of symmetry. See Bowker (1948) for details.

Simple Kappa Coefficient

The simple kappa coefficient, introduced by Cohen (1960), is a measure of interrater agreement. PROC FREQ computes the simple kappa coefficient as

$$\hat{\kappa} = (P_o - P_e) / (1 - P_e)$$

where $P_o = \sum_i p_{ii}$ and $P_e = \sum_i p_{i.}p_{.i}$. If the two response variables are viewed as two independent ratings of the n subjects, the kappa coefficient equals +1 when there is complete agreement of the raters. When the observed agreement exceeds chance agreement, kappa is positive, with its magnitude reflecting the strength of agreement. Although this is unusual in practice, kappa is negative when the observed agreement is less than chance agreement. The minimum value of kappa is between -1 and 0, depending on the marginal proportions.

The asymptotic variance of the simple kappa coefficient is computed as

$$\text{Var}(\hat{\kappa}) = (A + B - C) / (1 - P_e)^2 n$$

where

$$A = \sum_i p_{ii} (1 - (p_{i.} + p_{.i})(1 - \hat{\kappa}))^2$$

$$B = (1 - \hat{\kappa})^2 \sum_{i \neq j} p_{ij} (p_{.i} + p_{.j})^2$$

$$C = (\hat{\kappa} - P_e(1 - \hat{\kappa}))^2$$

See Fleiss, Cohen, and Everitt (1969) for details.

PROC FREQ computes confidence limits for the simple kappa coefficient as

$$\hat{\kappa} \pm (z_{\alpha/2} \times \sqrt{\text{Var}(\hat{\kappa})})$$

where $z_{\alpha/2}$ is the $100(1 - \alpha/2)$ percentile of the standard normal distribution. The value of α is determined by the value of the ALPHA= option, which, by default, equals 0.05 and produces 95% confidence limits.

To compute an asymptotic test for the kappa coefficient, PROC FREQ uses the standardized test statistic $\hat{\kappa}^*$, which has an asymptotic standard normal distribution under the null hypothesis that kappa equals zero. The standardized test statistic is computed as

$$\hat{\kappa}^* = \hat{\kappa} / \sqrt{\text{Var}_0(\hat{\kappa})}$$

where $\text{Var}_0(\hat{\kappa})$ is the variance of the kappa coefficient under the null hypothesis,

$$\text{Var}_0(\hat{\kappa}) = \left(P_e + P_e^2 - \sum_i p_{i.}p_{.i}(p_{i.} + p_{.i}) \right) / (1 - P_e)^2 n$$

See Fleiss, Levin, and Paik (2003) for details.

PROC FREQ also provides an exact test for the simple kappa coefficient. You can request the exact test by specifying the KAPPA or AGREE option in the EXACT statement. See the section “Exact Statistics” on page 2601 for more information.

Weighted Kappa Coefficient

The weighted kappa coefficient is a generalization of the simple kappa coefficient that uses weights to quantify the relative difference between categories. For 2×2 tables, the weighted kappa coefficient equals the simple kappa coefficient. PROC FREQ displays the weighted kappa coefficient only for tables larger than 2×2 . PROC FREQ computes the kappa weights from the column scores, by using either Cicchetti-Allison weights or Fleiss-Cohen weights, both of which are described in the following section. The weights w_{ij} are constructed so that $0 \leq w_{ij} < 1$ for all $i \neq j$, $w_{ii} = 1$ for all i , and $w_{ij} = w_{ji}$. The weighted kappa coefficient is computed as

$$\hat{\kappa}_w = (P_{o(w)} - P_{e(w)}) / (1 - P_{e(w)})$$

where

$$P_{o(w)} = \sum_i \sum_j w_{ij} p_{ij}$$

$$P_{e(w)} = \sum_i \sum_j w_{ij} p_{i \cdot} p_{\cdot j}$$

The asymptotic variance of the weighted kappa coefficient is

$$\text{Var}(\hat{\kappa}_w) = \left(\sum_i \sum_j p_{ij} (w_{ij} - (\bar{w}_{i \cdot} + \bar{w}_{\cdot j})) (1 - \hat{\kappa}_w) \right)^2 - (\hat{\kappa}_w - P_{e(w)} (1 - \hat{\kappa}_w))^2 \Big/ (1 - P_{e(w)})^2 n$$

where

$$\bar{w}_{i \cdot} = \sum_j p_{\cdot j} w_{ij}$$

$$\bar{w}_{\cdot j} = \sum_i p_{i \cdot} w_{ij}$$

See Fleiss, Cohen, and Everitt (1969) for details.

PROC FREQ computes confidence limits for the weighted kappa coefficient as

$$\hat{\kappa}_w \pm (z_{\alpha/2} \times \sqrt{\text{Var}(\hat{\kappa}_w)})$$

where $z_{\alpha/2}$ is the $100(1 - \alpha/2)$ percentile of the standard normal distribution. The value of α is determined by the value of the ALPHA= option, which, by default, equals 0.05 and produces 95% confidence limits.

To compute an asymptotic test for the weighted kappa coefficient, PROC FREQ uses the standardized test statistic $\hat{\kappa}_w^*$, which has an asymptotic standard normal distribution under the null hypothesis that weighted kappa equals zero. The standardized test statistic is computed as

$$\hat{\kappa}_w^* = \hat{\kappa}_w / \sqrt{\text{Var}_0(\hat{\kappa}_w)}$$

where $\text{Var}_0(\hat{\kappa}_w)$ is the variance of the weighted kappa coefficient under the null hypothesis,

$$\text{Var}_0(\hat{\kappa}_w) = \left(\sum_i \sum_j p_{i \cdot} p_{\cdot j} (w_{ij} - (\bar{w}_{i \cdot} + \bar{w}_{\cdot j})) \right)^2 - P_{e(w)}^2 \Big/ (1 - P_{e(w)})^2 n$$

See Fleiss, Levin, and Paik (2003) for details.

PROC FREQ also provides an exact test for the weighted kappa coefficient. You can request the exact test by specifying the WTKAPPA or AGREE option in the EXACT statement. See the section “Exact Statistics” on page 2601 for more information.

Weights PROC FREQ computes kappa coefficient weights by using the column scores and one of the two available weight types. The column scores are determined by the SCORES= option in the TABLES statement. The two available types of kappa weights are Cicchetti-Allison and Fleiss-Cohen weights. By default, PROC FREQ uses Cicchetti-Allison weights. If you specify (WT=FC) with the AGREE option, then PROC FREQ uses Fleiss-Cohen weights to compute the weighted kappa coefficient.

PROC FREQ computes Cicchetti-Allison kappa coefficient weights as

$$w_{ij} = 1 - \frac{|C_i - C_j|}{C_C - C_1}$$

where C_i is the score for column i and C is the number of categories or columns. See Cicchetti and Allison (1971) for details.

The SCORES= option in the TABLES statement determines the type of column scores used to compute the kappa weights (and other score-based statistics). The default is SCORES=TABLE. See the section “Scores” on page 2549 for details. For numeric variables, table scores are the values of the variable levels. You can assign numeric values to the levels in a way that reflects their level of similarity. For example, suppose you have four levels and order them according to similarity. If you assign them values of 0, 2, 4, and 10, the Cicchetti-Allison kappa weights take the following values: $w_{12} = 0.8$, $w_{13} = 0.6$, $w_{14} = 0$, $w_{23} = 0.8$, $w_{24} = 0.2$, and $w_{34} = 0.4$. Note that when there are only two categories (that is, $C = 2$), the weighted kappa coefficient is identical to the simple kappa coefficient.

If you specify (WT=FC) with the AGREE option in the TABLES statement, PROC FREQ computes Fleiss-Cohen kappa coefficient weights as

$$w_{ij} = 1 - \frac{(C_i - C_j)^2}{(C_C - C_1)^2}$$

See Fleiss and Cohen (1973) for details.

For the preceding example, the Fleiss-Cohen kappa weights are: $w_{12} = 0.96$, $w_{13} = 0.84$, $w_{14} = 0$, $w_{23} = 0.96$, $w_{24} = 0.36$, and $w_{34} = 0.64$.

Overall Kappa Coefficient

When there are multiple strata, PROC FREQ combines the stratum-level estimates of kappa into an overall estimate of the supposed common value of kappa. Assume there are q strata, indexed by $h = 1, 2, \dots, q$, and let $\text{Var}(\hat{\kappa}_h)$ denote the variance of $\hat{\kappa}_h$. The estimate of the overall kappa coefficient is computed as

$$\hat{\kappa}_T = \frac{\sum_{h=1}^q \hat{\kappa}_h}{\sum_{h=1}^q \frac{1}{\text{Var}(\hat{\kappa}_h)}}$$

See Fleiss, Levin, and Paik (2003) for details.

PROC FREQ computes an estimate of the overall weighted kappa in the same way.

Tests for Equal Kappa Coefficients

When there are multiple strata, the following chi-square statistic tests whether the stratum-level values of kappa are equal:

$$Q_K = \sum_{h=1}^q (\hat{\kappa}_h - \hat{\kappa}_T)^2 / \text{Var}(\hat{\kappa}_h)$$

Under the null hypothesis of equal kappas for the q strata, Q_K has an asymptotic chi-square distribution with $q-1$ degrees of freedom. See Fleiss, Levin, and Paik (2003) for more information. PROC FREQ computes a test for equal weighted kappa coefficients in the same way.

Cochran's Q Test

Cochran's Q is computed for multiway tables when each variable has two levels, that is, for $2 \times 2 \cdots \times 2$ tables. Cochran's Q statistic is used to test the homogeneity of the one-dimensional margins. Let m denote the number of variables and N denote the total number of subjects. Cochran's Q statistic is computed as

$$Q_C = m(m-1) \left(\sum_{j=1}^m T_j^2 - T^2 \right) / \left(mT - \sum_{k=1}^N S_k^2 \right)$$

where T_j is the number of positive responses for variable j , T is the total number of positive responses over all variables, and S_k is the number of positive responses for subject k . Under the null hypothesis, Cochran's Q has an asymptotic chi-square distribution with $m-1$ degrees of freedom. See Cochran (1950) for details. When there are only two binary response variables ($m=2$), Cochran's Q simplifies to McNemar's test. When there are more than two response categories, you can test for marginal homogeneity by using the repeated measures capabilities of the CATMOD procedure.

Tables with Zero Rows and Columns

The AGREE statistics are defined only for square tables, where the number of rows equals the number of columns. If the table is not square, PROC FREQ does not compute AGREE statistics. In the kappa statistic framework, where two independent raters assign ratings to each of n subjects, suppose one of the raters does not use all possible r rating levels. If the corresponding table has r rows but only $r-1$ columns, then the table is not square and PROC FREQ does not compute AGREE statistics. To create a square table in this situation, use the ZEROS option in the WEIGHT statement, which requests that PROC FREQ include observations with zero weights in the analysis. Include zero-weight observations in the input data set to represent any rating levels that are not used by a rater, so that the input data set has at least one observation for each possible rater and rating combination. The analysis then includes all rating levels, even when all levels are not actually assigned by both raters. The resulting table (of rater 1 by rater 2) is a square table, and AGREE statistics can be computed.

For more information, see the description of the ZEROS option. By default, PROC FREQ does not process observations that have zero weights, because these observations do not contribute to the total frequency count, and because any resulting zero-weight row or column causes many of the tests and measures of association to be undefined. However, kappa statistics are defined for tables with a zero-weight row or column, and the ZEROS option makes it possible to input zero-weight observations and construct the tables needed to compute kappas.

Cochran-Mantel-Haenszel Statistics

The CMH option in the TABLES statement gives a stratified statistical analysis of the relationship between the row and column variables after controlling for the strata variables in a multiway table. For example, for the table request A*B*C*D, the CMH option provides an analysis of the relationship between C and D, after controlling for A and B. The stratified analysis provides a way to adjust for the possible confounding effects of A and B without being forced to estimate parameters for them.

The CMH analysis produces Cochran-Mantel-Haenszel statistics, which include the correlation statistic, the ANOVA (row mean scores) statistic, and the general association statistic. For 2×2 tables, the CMH option

also provides Mantel-Haenszel and logit estimates of the common odds ratio and the common relative risks, as well as the Breslow-Day test for homogeneity of the odds ratios.

Exact statistics are also available for stratified 2×2 tables. If you specify the EQOR option in the EXACT statement, PROC FREQ provides Zelen's exact test for equal odds ratios. If you specify the COMOR option in the EXACT statement, PROC FREQ provides exact confidence limits for the common odds ratio and an exact test that the common odds ratio equals one.

Let the number of strata be denoted by q , indexing the strata by $h = 1, 2, \dots, q$. Each stratum contains a contingency table with X representing the row variable and Y representing the column variable. For table h , denote the cell frequency in row i and column j by n_{hij} , with corresponding row and column marginal totals denoted by $n_{hi\cdot}$ and $n_{h\cdot j}$, and the overall stratum total by n_h .

Because the formulas for the Cochran-Mantel-Haenszel statistics are more easily defined in terms of matrices, the following notation is used. Vectors are presumed to be column vectors unless they are transposed ($'$).

$$\begin{aligned} \mathbf{n}'_{hi} &= (n_{hi1}, n_{hi2}, \dots, n_{hiC}) && (1 \times C) \\ \mathbf{n}'_h &= (\mathbf{n}'_{h1}, \mathbf{n}'_{h2}, \dots, \mathbf{n}'_{hR}) && (1 \times RC) \\ p_{hi\cdot} &= n_{hi\cdot} / n_h && (1 \times 1) \\ p_{h\cdot j} &= n_{h\cdot j} / n_h && (1 \times 1) \\ \mathbf{P}'_{h*} &= (p_{h1\cdot}, p_{h2\cdot}, \dots, p_{hR\cdot}) && (1 \times R) \\ \mathbf{P}'_{h\cdot*} &= (p_{h\cdot 1}, p_{h\cdot 2}, \dots, p_{h\cdot C}) && (1 \times C) \end{aligned}$$

Assume that the strata are independent and that the marginal totals of each stratum are fixed. The null hypothesis, H_0 , is that there is no association between X and Y in any of the strata. The corresponding model is the multiple hypergeometric; this implies that, under H_0 , the expected value and covariance matrix of the frequencies are, respectively,

$$\begin{aligned} \mathbf{m}_h &= \mathbf{E}[\mathbf{n}_h | H_0] = n_h(\mathbf{P}_{h\cdot*} \otimes \mathbf{P}_{h*}) \\ \text{Var}[\mathbf{n}_h | H_0] &= c \left((\mathbf{D}_{\mathbf{P}_{h\cdot*}} - \mathbf{P}_{h\cdot*}\mathbf{P}'_{h\cdot*}) \otimes (\mathbf{D}_{\mathbf{P}_{h*}} - \mathbf{P}_{h*}\mathbf{P}'_{h*}) \right) \end{aligned}$$

where

$$c = n_h^2 / (n_h - 1)$$

and where \otimes denotes Kronecker product multiplication and \mathbf{D}_a is a diagonal matrix with the elements of \mathbf{a} on the main diagonal.

The generalized CMH statistic (Landis, Heyman, and Koch 1978) is defined as

$$Q_{CMH} = \mathbf{G}'\mathbf{V}_G^{-1}\mathbf{G}$$

where

$$\begin{aligned} \mathbf{G} &= \sum_h \mathbf{B}_h(\mathbf{n}_h - \mathbf{m}_h) \\ \mathbf{V}_G &= \sum_h \mathbf{B}_h (\text{Var}[\mathbf{n}_h | H_0]) \mathbf{B}'_h \end{aligned}$$

and where

$$\mathbf{B}_h = \mathbf{C}_h \otimes \mathbf{R}_h$$

is a matrix of fixed constants based on column scores \mathbf{C}_h and row scores \mathbf{R}_h . When the null hypothesis is true, the CMH statistic has an asymptotic chi-square distribution with degrees of freedom equal to the rank of \mathbf{B}_h . If \mathbf{V}_G is found to be singular, PROC FREQ prints a message and sets the value of the CMH statistic to missing.

PROC FREQ computes three CMH statistics by using this formula for the generalized CMH statistic, with different row and column score definitions for each statistic. The CMH statistics that PROC FREQ computes are the correlation statistic, the ANOVA (row mean scores) statistic, and the general association statistic. These statistics test the null hypothesis of no association against different alternative hypotheses. The following sections describe the computation of these CMH statistics.

CAUTION: The CMH statistics have low power for detecting an association in which the patterns of association for some of the strata are in the opposite direction of the patterns displayed by other strata. Thus, a nonsignificant CMH statistic suggests either that there is no association or that no pattern of association has enough strength or consistency to dominate any other pattern.

Correlation Statistic

The correlation statistic, popularized by Mantel and Haenszel, has one degree of freedom and is known as the Mantel-Haenszel statistic (Mantel and Haenszel 1959; Mantel 1963).

The alternative hypothesis for the correlation statistic is that there is a linear association between X and Y in at least one stratum. If either X or Y does not lie on an ordinal (or interval) scale, then this statistic is not meaningful.

To compute the correlation statistic, PROC FREQ uses the formula for the generalized CMH statistic with the row and column scores determined by the SCORES= option in the TABLES statement. See the section “Scores” on page 2549 for more information about the available score types. The matrix of row scores \mathbf{R}_h has dimension $1 \times R$, and the matrix of column scores \mathbf{C}_h has dimension $1 \times C$.

When there is only one stratum, this CMH statistic reduces to $(n - 1)r^2$, where r is the Pearson correlation coefficient between X and Y. When nonparametric (RANK or RIDIT) scores are specified, the statistic reduces to $(n - 1)r_s^2$, where r_s is the Spearman rank correlation coefficient between X and Y. When there is more than one stratum, this CMH statistic becomes a stratum-adjusted correlation statistic.

ANOVA (Row Mean Scores) Statistic

The ANOVA statistic can be used only when the column variable Y lies on an ordinal (or interval) scale so that the mean score of Y is meaningful. For the ANOVA statistic, the mean score is computed for each row of the table, and the alternative hypothesis is that, for at least one stratum, the mean scores of the R rows are unequal. In other words, the statistic is sensitive to location differences among the R distributions of Y.

The matrix of column scores \mathbf{C}_h has dimension $1 \times C$, and the column scores are determined by the SCORES= option.

The matrix of row scores \mathbf{R}_h has dimension $(R - 1) \times R$ and is created internally by PROC FREQ as

$$\mathbf{R}_h = [\mathbf{I}_{R-1}, -\mathbf{J}_{R-1}]$$

where \mathbf{I}_{R-1} is an identity matrix of rank $R - 1$ and \mathbf{J}_{R-1} is an $(R - 1) \times 1$ vector of ones. This matrix has the effect of forming $R - 1$ independent contrasts of the R mean scores.

When there is only one stratum, this CMH statistic is essentially an analysis of variance (ANOVA) statistic in the sense that it is a function of the variance ratio F statistic that would be obtained from a one-way ANOVA on the dependent variable Y . If nonparametric scores are specified in this case, then the ANOVA statistic is a Kruskal-Wallis test.

If there is more than one stratum, then this CMH statistic corresponds to a stratum-adjusted ANOVA or Kruskal-Wallis test. In the special case where there is one subject per row and one subject per column in the contingency table of each stratum, this CMH statistic is identical to Friedman's chi-square. See [Example 38.9](#) for an illustration.

General Association Statistic

The alternative hypothesis for the general association statistic is that, for at least one stratum, there is some kind of association between X and Y . This statistic is always interpretable because it does not require an ordinal scale for either X or Y .

For the general association statistic, the matrix \mathbf{R}_h is the same as the one used for the ANOVA statistic. The matrix \mathbf{C}_h is defined similarly as

$$\mathbf{C}_h = [\mathbf{I}_{C-1}, -\mathbf{J}_{C-1}]$$

PROC FREQ generates both score matrices internally. When there is only one stratum, then the general association CMH statistic reduces to $Q_P(n-1)/n$, where Q_P is the Pearson chi-square statistic. When there is more than one stratum, then the CMH statistic becomes a stratum-adjusted Pearson chi-square statistic. Note that a similar adjustment can be made by summing the Pearson chi-squares across the strata. However, the latter statistic requires a large sample size in each stratum to support the resulting chi-square distribution with $q(R-1)(C-1)$ degrees of freedom. The CMH statistic requires only a large overall sample size because it has only $(R-1)(C-1)$ degrees of freedom.

See Cochran (1954); Mantel and Haenszel (1959); Mantel (1963); Birch (1965); Landis, Heyman, and Koch (1978).

Mantel-Fleiss Criterion

If you specify the CMH(MANTELFLISS) option in the TABLES statement, PROC FREQ computes the Mantel-Fleiss criterion for stratified 2×2 tables. The Mantel-Fleiss criterion can be used to assess the validity of the chi-square approximation for the distribution of the Mantel-Haenszel statistic for 2×2 tables. For details, see Mantel and Fleiss (1980); Mantel and Haenszel (1959); Stokes, Davis, and Koch (2012); Dmitrienko et al. (2005).

The Mantel-Fleiss criterion is computed as

$$MF = \min \left(\left[\sum_h m_{h11} - \sum_h (n_{h11})_L \right], \left[\sum_h (n_{h11})_U - \sum_h m_{h11} \right] \right)$$

where m_{h11} is the expected value of n_{h11} under the hypothesis of no association between the row and column variables in table h , $(n_{h11})_L$ is the minimum possible value of the table cell frequency, and $(n_{h11})_U$ is the maximum possible value,

$$m_{h11} = n_{h1\cdot} \cdot n_{h\cdot 1} / n_h$$

$$(n_{h11})_L = \max(0, n_{h1\cdot} - n_{h\cdot 2})$$

$$(n_{h11})_U = \min(n_{h\cdot 1}, n_{h1\cdot})$$

The Mantel-Fleiss guideline accepts the validity of the Mantel-Haenszel approximation when the value of the criterion is at least 5. When the criterion is less than 5, PROC FREQ displays a warning.

Adjusted Odds Ratio and Relative Risk Estimates

The CMH option provides adjusted odds ratio and relative risk estimates for stratified 2×2 tables. For each of these measures, PROC FREQ computes a Mantel-Haenszel estimate and a logit estimate. These estimates apply to n -way table requests in the TABLES statement, when the row and column variables both have two levels.

For example, for the table request $A*B*C*D$, if the row and column variables C and D both have two levels, PROC FREQ provides odds ratio and relative risk estimates, adjusting for the confounding variables A and B .

The choice of an appropriate measure depends on the study design. For case-control (retrospective) studies, the odds ratio is appropriate. For cohort (prospective) or cross-sectional studies, the relative risk is appropriate. See the section “Odds Ratio and Relative Risks for 2×2 Tables” on page 2582 for more information on these measures.

Throughout this section, z denotes the $100(1 - \alpha/2)$ percentile of the standard normal distribution.

Odds Ratio, Case-Control Studies PROC FREQ provides Mantel-Haenszel and logit estimates for the common odds ratio for stratified 2×2 tables.

Mantel-Haenszel Estimator The Mantel-Haenszel estimate of the common odds ratio is computed as

$$OR_{MH} = \left(\sum_h n_{h11} n_{h22} / n_h \right) / \left(\sum_h n_{h12} n_{h21} / n_h \right)$$

It is always computed unless the denominator is zero. See Mantel and Haenszel (1959) and Agresti (2002) for details.

To compute confidence limits for the common odds ratio, PROC FREQ uses the Robins, Breslow, and Greenland (1986) variance estimate for $\ln(OR_{MH})$. The $100(1 - \alpha/2)\%$ confidence limits for the common odds ratio are

$$\left(OR_{MH} \times \exp(-z\hat{\sigma}), OR_{MH} \times \exp(z\hat{\sigma}) \right)$$

where

$$\begin{aligned} \hat{\sigma}^2 &= \widehat{\text{Var}}(\ln(OR_{MH})) \\ &= \frac{\sum_h (n_{h11} + n_{h22})(n_{h11} n_{h22}) / n_h^2}{2 \left(\sum_h n_{h11} n_{h22} / n_h \right)^2} \\ &\quad + \frac{\sum_h [(n_{h11} + n_{h22})(n_{h12} n_{h21}) + (n_{h12} + n_{h21})(n_{h11} n_{h22})] / n_h^2}{2 \left(\sum_h n_{h11} n_{h22} / n_h \right) \left(\sum_h n_{h12} n_{h21} / n_h \right)} \\ &\quad + \frac{\sum_h (n_{h12} + n_{h21})(n_{h12} n_{h21}) / n_h^2}{2 \left(\sum_h n_{h12} n_{h21} / n_h \right)^2} \end{aligned}$$

Note that the Mantel-Haenszel odds ratio estimator is less sensitive to small n_h than the logit estimator.

Logit Estimator The adjusted logit estimate of the common odds ratio (Woolf 1955) is computed as

$$OR_L = \exp\left(\frac{\sum_h w_h \ln(OR_h)}{\sum_h w_h}\right)$$

and the corresponding $100(1 - \alpha)\%$ confidence limits are

$$\left(OR_L \times \exp\left(-z / \sqrt{\sum_h w_h}\right), OR_L \times \exp\left(z / \sqrt{\sum_h w_h}\right) \right)$$

where OR_h is the odds ratio for stratum h , and

$$w_h = 1/\text{Var}(\ln(OR_h))$$

If any table cell frequency in a stratum h is zero, PROC FREQ adds 0.5 to each cell of the stratum before computing OR_h and w_h (Haldane 1955) for the logit estimate. The procedure prints a warning when this occurs.

Relative Risks, Cohort Studies PROC FREQ provides Mantel-Haenszel and logit estimates of the common relative risks for stratified 2×2 tables.

Mantel-Haenszel Estimator The Mantel-Haenszel estimate of the common relative risk for column 1 is computed as

$$RR_{MH} = \left(\sum_h n_{h11} n_{h2\cdot} / n_h\right) / \left(\sum_h n_{h21} n_{h1\cdot} / n_h\right)$$

It is always computed unless the denominator is zero. See Mantel and Haenszel (1959) and Agresti (2002) for more information.

To compute confidence limits for the common relative risk, PROC FREQ uses the Greenland and Robins (1985) variance estimate for $\log(RR_{MH})$. The $100(1 - \alpha/2)\%$ confidence limits for the common relative risk are

$$(RR_{MH} \times \exp(-z\hat{\sigma}), RR_{MH} \times \exp(z\hat{\sigma}))$$

where

$$\hat{\sigma}^2 = \widehat{\text{Var}}(\ln(RR_{MH})) = \frac{\sum_h (n_{h1\cdot} n_{h2\cdot} n_{h\cdot 1} - n_{h11} n_{h21} n_h) / n_h^2}{(\sum_h n_{h11} n_{h2\cdot} / n_h) (\sum_h n_{h21} n_{h1\cdot} / n_h)}$$

Logit Estimator The adjusted logit estimate of the common relative risk for column 1 is computed as

$$RR_L = \exp\left(\frac{\sum_h w_h \ln(RR_h)}{\sum_h w_h}\right)$$

and the corresponding $100(1 - \alpha)\%$ confidence limits are

$$\left(RR_L \times \exp\left(-z / \sqrt{\sum_h w_h}\right), RR_L \times \exp\left(z / \sqrt{\sum_h w_h}\right) \right)$$

where RR_h is the column 1 relative risk estimate for stratum h and

$$w_h = 1 / \text{Var}(\ln(RR_h))$$

If n_{h11} or n_{h21} is zero, then PROC FREQ adds 0.5 to each cell of the stratum before computing RR_h and w_h for the logit estimate. The procedure prints a warning when this occurs. See Kleinbaum, Kupper, and Morgenstern (1982, Sections 17.4 and 17.5) for details.

Breslow-Day Test for Homogeneity of the Odds Ratios

When you specify the CMH option, PROC FREQ computes the Breslow-Day test for stratified 2×2 tables. It tests the null hypothesis that the odds ratios for the q strata are equal. When the null hypothesis is true, the statistic has approximately a chi-square distribution with $q-1$ degrees of freedom. See Breslow and Day (1980) and Agresti (2007) for more information.

The Breslow-Day statistic is computed as

$$Q_{BD} = \sum_h (n_{h11} - E(n_{h11} | OR_{MH}))^2 / \text{Var}(n_{h11} | OR_{MH})$$

where E and Var denote expected value and variance, respectively. The summation does not include any table with a zero row or column. If OR_{MH} equals zero or if it is undefined, then PROC FREQ does not compute the statistic and prints a warning message.

For the Breslow-Day test to be valid, the sample size should be relatively large in each stratum, and at least 80% of the expected cell counts should be greater than 5. Note that this is a stricter sample size requirement than the requirement for the Cochran-Mantel-Haenszel test for $q \times 2 \times 2$ tables, in that each stratum sample size (not just the overall sample size) must be relatively large. Even when the Breslow-Day test is valid, it might not be very powerful against certain alternatives, as discussed in Breslow and Day (1980).

If you specify the BDT option, PROC FREQ computes the Breslow-Day test with Tarone's adjustment, which subtracts an adjustment factor from Q_{BD} to make the resulting statistic asymptotically chi-square. The Breslow-Day-Tarone statistic is computed as

$$Q_{BDT} = Q_{BD} - \left(\sum_h (n_{h11} - E(n_{h11} | OR_{MH})) \right)^2 / \sum_h \text{Var}(n_{h11} | OR_{MH})$$

See Tarone (1985); Jones et al. (1989); Breslow (1996) for more information.

Zelen's Exact Test for Equal Odds Ratios

If you specify the EQOR option in the EXACT statement, PROC FREQ computes Zelen's exact test for equal odds ratios for stratified 2×2 tables. Zelen's test is an exact counterpart to the Breslow-Day asymptotic test for equal odds ratios. The reference set for Zelen's test includes all possible $q \times 2 \times 2$ tables with the same row, column, and stratum totals as the observed multiway table and with the same sum of cell (1,1) frequencies as the observed table. The test statistic is the probability of the observed $q \times 2 \times 2$ table conditional on the fixed margins, which is a product of hypergeometric probabilities.

The p -value for Zelen's test is the sum of all table probabilities that are less than or equal to the observed table probability, where the sum is computed over all tables in the reference set determined by the fixed margins and the observed sum of cell (1,1) frequencies. This test is similar to Fisher's exact test for two-way tables. For more information, see Zelen (1971); Hirji (2006); Agresti (1992). PROC FREQ computes Zelen's exact test by using the polynomial multiplication algorithm of Hirji et al. (1996).

Exact Confidence Limits for the Common Odds Ratio

If you specify the COMOR option in the EXACT statement, PROC FREQ computes exact confidence limits for the common odds ratio for stratified 2×2 tables. This computation assumes that the odds ratio is constant over all the 2×2 tables. Exact confidence limits are constructed from the distribution of $S = \sum_h n_{h11}$, conditional on the marginal totals of the 2×2 tables.

Because this is a discrete problem, the confidence coefficient for these exact confidence limits is not exactly $(1 - \alpha)$ but is at least $(1 - \alpha)$. Thus, these confidence limits are conservative. See Agresti (1992) for more information.

PROC FREQ computes exact confidence limits for the common odds ratio by using an algorithm based on Vollset, Hirji, and Elashoff (1991). See also Mehta, Patel, and Gray (1985).

Conditional on the marginal totals of 2×2 table h , let the random variable S_h denote the frequency of table cell (1,1). Given the row totals $n_{h1\cdot}$ and $n_{h2\cdot}$ and column totals $n_{\cdot 1}$ and $n_{\cdot 2}$, the lower and upper bounds for S_h are l_h and u_h ,

$$l_h = \max(0, n_{h1\cdot} - n_{h2\cdot})$$

$$u_h = \min(n_{h1\cdot}, n_{\cdot 1})$$

Let C_{s_h} denote the hypergeometric coefficient,

$$C_{s_h} = \binom{n_{h1\cdot}}{s_h} \binom{n_{h2\cdot}}{n_{h1\cdot} - s_h}$$

and let ϕ denote the common odds ratio. Then the conditional distribution of S_h is

$$P(S_h = s_h | n_{1\cdot}, n_{\cdot 1}, n_{\cdot 2}) = C_{s_h} \phi^{s_h} / \sum_{x=l_h}^{x=u_h} C_x \phi^x$$

Summing over all the 2×2 tables, $S = \sum_h S_h$, and the lower and upper bounds of S are l and u ,

$$l = \sum_h l_h \quad \text{and} \quad u = \sum_h u_h$$

The conditional distribution of the sum S is

$$P(S = s | n_{h1\cdot}, n_{h\cdot 1}, n_{h\cdot 2}; h = 1, \dots, q) = C_s \phi^s / \sum_{x=l}^{x=u} C_x \phi^x$$

where

$$C_s = \sum_{s_1 + \dots + s_q = s} \left(\prod_h C_{s_h} \right)$$

Let s_0 denote the observed sum of cell (1,1) frequencies over the q tables. The following two equations are solved iteratively for lower and upper confidence limits for the common odds ratio, ϕ_1 and ϕ_2 :

$$\sum_{x=s_0}^{x=u} C_x \phi_1^x / \sum_{x=l}^{x=u} C_x \phi_1^x = \alpha/2$$

$$\sum_{x=l}^{x=s_0} C_x \phi_2^x / \sum_{x=l}^{x=u} C_x \phi_2^x = \alpha/2$$

When the observed sum s_0 equals the lower bound l , PROC FREQ sets the lower confidence limit to zero and determines the upper limit with level α . Similarly, when the observed sum s_0 equals the upper bound u , PROC FREQ sets the upper confidence limit to infinity and determines the lower limit with level α .

When you specify the COMOR option in the EXACT statement, PROC FREQ also computes the exact test that the common odds ratio equals one. Setting $\phi = 1$, the conditional distribution of the sum S under the null hypothesis becomes

$$P_0(S = s \mid n_{h1\cdot}, n_{h\cdot 1}, n_{h\cdot 2}; h = 1, \dots, q) = C_s / \sum_{x=l}^{x=u} C_x$$

The point probability for this exact test is the probability of the observed sum s_0 under the null hypothesis, conditional on the marginals of the stratified 2×2 tables, and is denoted by $P_0(s_0)$. The expected value of S under the null hypothesis is

$$E_0(S) = \sum_{x=l}^{x=u} x C_x / \sum_{x=l}^{x=u} C_x$$

The one-sided exact p -value is computed from the conditional distribution as $P_0(S \geq s_0)$ or $P_0(S \leq s_0)$, depending on whether the observed sum s_0 is greater or less than $E_0(S)$,

$$P_1 = P_0(S \geq s_0) = \sum_{x=s_0}^{x=u} C_x / \sum_{x=l}^{x=u} C_x \quad \text{if } s_0 > E_0(S)$$

$$P_1 = P_0(S \leq s_0) = \sum_{x=l}^{x=s_0} C_x / \sum_{x=l}^{x=u} C_x \quad \text{if } s_0 \leq E_0(S)$$

PROC FREQ computes two-sided p -values for this test according to three different definitions. A two-sided p -value is computed as twice the one-sided p -value, setting the result equal to one if it exceeds one,

$$P_2^a = 2 \times P_1$$

Additionally, a two-sided p -value is computed as the sum of all probabilities less than or equal to the point probability of the observed sum s_0 , summing over all possible values of s , $l \leq s \leq u$,

$$P_2^b = \sum_{l \leq s \leq u: P_0(s) \leq P_0(s_0)} P_0(s)$$

Also, a two-sided p -value is computed as the sum of the one-sided p -value and the corresponding area in the opposite tail of the distribution, equidistant from the expected value,

$$P_2^c = P_0(|S - E_0(S)| \geq |s_0 - E_0(S)|)$$

Gail-Simon Test for Qualitative Interactions

The GAILSIMON option in the TABLES statement provides the Gail-Simon test for qualitative interaction for stratified 2×2 tables. For details, see Gail and Simon (1985); Silvapulle (2001); Dmitrienko et al. (2005).

The Gail-Simon test is based on the risk differences in stratified 2×2 tables, where the risk difference is defined as the row 1 risk (proportion in column 1) minus the row 2 risk. See the section “Risks and Risk Differences” on page 2572 for details. By default, the procedure uses column 1 risks to compute the Gail-Simon test. If you specify the GAILSIMON(COLUMN=2) option, the procedure uses column 2 risks.

PROC FREQ computes the Gail-Simon test statistics as described in Gail and Simon (1985),

$$Q- = \sum_h (d_h/s_h)^2 I(d_h > 0)$$

$$Q+ = \sum_h (d_h/s_h)^2 I(d_h < 0)$$

$$Q = \min(Q-, Q+)$$

where d_h is the risk difference in table h , s_h is the standard error of the risk difference, and $I(d_h > 0)$ equals 1 if $d_h > 0$ and 0 otherwise. Similarly, $I(d_h < 0)$ equals 1 if $d_h < 0$ and 0 otherwise. The q 2×2 tables (strata) are indexed by $h = 1, 2, \dots, q$.

The p -values for the Gail-Simon statistics are computed as

$$p(Q-) = \sum_h (1 - F_h(Q-)) B(h; n = q, p = 0.5)$$

$$p(Q+) = \sum_h (1 - F_h(Q+)) B(h; n = q, p = 0.5)$$

$$p(Q) = \sum_{h=1}^{q-1} (1 - F_h(Q)) B(h; n = (q - 1), p = 0.5)$$

where $F_h(\cdot)$ is the cumulative chi-square distribution function with h degrees of freedom and $B(h; n, p)$ is the binomial probability function with parameters n and p . The statistic Q tests the null hypothesis of no qualitative interaction. The statistic $Q-$ tests the null hypothesis of positive risk differences. A small p -value for $Q-$ indicates negative differences; similarly, a small p -value for $Q+$ indicates positive risk differences.

Exact Statistics

Exact statistics can be useful in situations where the asymptotic assumptions are not met, and so the asymptotic p -values are not close approximations for the true p -values. Standard asymptotic methods involve the assumption that the test statistic follows a particular distribution when the sample size is sufficiently large. When the sample size is not large, asymptotic results might not be valid, with the asymptotic p -values

differing perhaps substantially from the exact p -values. Asymptotic results might also be unreliable when the distribution of the data is sparse, skewed, or heavily tied. See Agresti (2007) and Bishop, Fienberg, and Holland (1975) for more information. Exact computations are based on the statistical theory of exact conditional inference for contingency tables, reviewed by Agresti (1992).

In addition to computation of exact p -values, PROC FREQ provides the option of estimating exact p -values by Monte Carlo simulation. This can be useful for problems that are so large that exact computations require a great amount of time and memory, but for which asymptotic approximations might not be sufficient.

Exact statistics are available for many PROC FREQ tests. For one-way tables, PROC FREQ provides exact p -values for the binomial proportion tests and the chi-square goodness-of-fit test. Exact (Clopper-Pearson) confidence limits are available for the binomial proportion. For two-way tables, PROC FREQ provides exact p -values for the following tests: Pearson chi-square test, likelihood ratio chi-square test, Mantel-Haenszel chi-square test, Fisher's exact test, Jonckheere-Terpstra test, and Cochran-Armitage test for trend. PROC FREQ also computes exact p -values for tests of the following statistics: Kendall's tau- b , Stuart's tau- c , Somers' $D(C|R)$, Somers' $D(R|C)$, Pearson correlation coefficient, Spearman correlation coefficient, simple kappa coefficient, and weighted kappa coefficient. For 2×2 tables, PROC FREQ provides McNemar's exact test and exact confidence limits for the odds ratio. PROC FREQ also provides exact unconditional confidence limits for the proportion (risk) difference and for the relative risk. For stratified 2×2 tables, PROC FREQ provides Zelen's exact test for equal odds ratios, exact confidence limits for the common odds ratio, and an exact test for the common odds ratio.

The following sections summarize the exact computational algorithms, define the exact p -values that PROC FREQ computes, discuss the computational resource requirements, and describe the Monte Carlo estimation option.

Computational Algorithms

PROC FREQ computes exact p -values for general $R \times C$ tables by using the network algorithm developed by Mehta and Patel (1983). This algorithm provides a substantial advantage over direct enumeration, which can be very time-consuming and feasible only for small problems. See Agresti (1992) for a review of algorithms for computation of exact p -values, and see Mehta, Patel, and Tsiatis (1984) and Mehta, Patel, and Senchaudhuri (1991) for information about the performance of the network algorithm.

The reference set for a given contingency table is the set of all contingency tables with the observed marginal row and column sums. Corresponding to this reference set, the network algorithm forms a directed acyclic network consisting of nodes in a number of stages. A path through the network corresponds to a distinct table in the reference set. The distances between nodes are defined so that the total distance of a path through the network is the corresponding value of the test statistic. At each node, the algorithm computes the shortest and longest path distances for all the paths that pass through that node. For statistics that can be expressed as a linear combination of cell frequencies multiplied by increasing row and column scores, PROC FREQ computes shortest and longest path distances by using the algorithm of Agresti, Mehta, and Patel (1990). For statistics of other forms, PROC FREQ computes an upper bound for the longest path and a lower bound for the shortest path by following the approach of Valz and Thompson (1994).

The longest and shortest path distances or bounds for a node are compared to the value of the test statistic to determine whether all paths through the node contribute to the p -value, none of the paths through the node contribute to the p -value, or neither of these situations occurs. If all paths through the node contribute, the p -value is incremented accordingly, and these paths are eliminated from further analysis. If no paths contribute, these paths are eliminated from the analysis. Otherwise, the algorithm continues, still processing this node and the associated paths. The algorithm finishes when all nodes have been accounted for.

In applying the network algorithm, PROC FREQ uses full numerical precision to represent all statistics, row and column scores, and other quantities involved in the computations. Although it is possible to use rounding to improve the speed and memory requirements of the algorithm, PROC FREQ does not do this because it can result in reduced accuracy of the p -values.

For one-way tables, PROC FREQ computes the exact chi-square goodness-of-fit test by the method of Radlow and Alf (1975). PROC FREQ generates all possible one-way tables with the observed total sample size and number of categories. For each possible table, PROC FREQ compares its chi-square value with the value for the observed table. If the table's chi-square value is greater than or equal to the observed chi-square, PROC FREQ increments the exact p -value by the probability of that table, which is calculated under the null hypothesis by using the multinomial frequency distribution. By default, the null hypothesis states that all categories have equal proportions. If you specify null hypothesis proportions or frequencies by using the TESTP= or TESTF= option in the TABLES statement, then PROC FREQ calculates the exact chi-square test based on that null hypothesis.

Other exact computations are described in sections about the individual statistics. See the section “[Binomial Proportion](#)” on page 2565 for details about how PROC FREQ computes exact confidence limits and tests for the binomial proportion. See the section “[Odds Ratio and Relative Risks for 2 x 2 Tables](#)” on page 2582 for information about computation of exact confidence limits for the odds ratio for 2×2 tables. Also, see the sections “[Exact Unconditional Confidence Limits for the Risk Difference](#)” on page 2580, “[Exact Confidence Limits for the Common Odds Ratio](#)” on page 2599, and “[Zelen's Exact Test for Equal Odds Ratios](#)” on page 2598.

Definition of p -Values

For several tests in PROC FREQ, the test statistic is nonnegative, and large values of the test statistic indicate a departure from the null hypothesis. Such nondirectional tests include the Pearson chi-square, the likelihood ratio chi-square, the Mantel-Haenszel chi-square, Fisher's exact test for tables larger than 2×2 , McNemar's test, and the one-way chi-square goodness-of-fit test. The exact p -value for a nondirectional test is the sum of probabilities for those tables having a test statistic greater than or equal to the value of the observed test statistic.

There are other tests where it might be appropriate to test against either a one-sided or a two-sided alternative hypothesis. For example, when you test the null hypothesis that the true parameter value equals 0 ($T = 0$), the alternative of interest might be one-sided ($T \leq 0$, or $T \geq 0$) or two-sided ($T \neq 0$). Such tests include the Pearson correlation coefficient, Spearman correlation coefficient, Jonckheere-Terpstra test, Cochran-Armitage test for trend, simple kappa coefficient, and weighted kappa coefficient. For these tests, PROC FREQ displays the right-sided p -value when the observed value of the test statistic is greater than its expected value. The right-sided p -value is the sum of probabilities for those tables for which the test statistic is greater than or equal to the observed test statistic. Otherwise, when the observed test statistic is less than or equal to the expected value, PROC FREQ displays the left-sided p -value. The left-sided p -value is the sum of probabilities for those tables for which the test statistic is less than or equal to the one observed. The one-sided p -value P_1 can be expressed as

$$P_1 = \begin{cases} \text{Prob}(\text{Test Statistic} \geq t) & \text{if } t > E_0(T) \\ \text{Prob}(\text{Test Statistic} \leq t) & \text{if } t \leq E_0(T) \end{cases}$$

where t is the observed value of the test statistic and $E_0(T)$ is the expected value of the test statistic under the null hypothesis. PROC FREQ computes the two-sided p -value as the sum of the one-sided p -value and the corresponding area in the opposite tail of the distribution of the statistic, equidistant from the expected

value. The two-sided p -value P_2 can be expressed as

$$P_2 = \text{Prob} (|\text{Test Statistic} - E_0(T)| \geq |t - E_0(T)|)$$

If you specify the POINT option in the EXACT statement, PROC FREQ also displays exact point probabilities for the test statistics. The exact point probability is the exact probability that the test statistic equals the observed value.

Computational Resources

PROC FREQ uses relatively fast and efficient algorithms for exact computations. These recently developed algorithms, together with improvements in computer power, now make it feasible to perform exact computations for data sets where previously only asymptotic methods could be applied. Nevertheless, there are still large problems that might require a prohibitive amount of time and memory for exact computations, depending on the speed and memory available on your computer. For large problems, consider whether exact methods are really needed or whether asymptotic methods might give results quite close to the exact results, while requiring much less computer time and memory. When asymptotic methods might not be sufficient for such large problems, consider using Monte Carlo estimation of exact p -values, as described in the section “[Monte Carlo Estimation](#)” on page 2604.

A formula does not exist that can predict in advance how much time and memory are needed to compute an exact p -value for a certain problem. The time and memory required depend on several factors, including which test is being performed, the total sample size, the number of rows and columns, and the specific arrangement of the observations into table cells. Generally, larger problems (in terms of total sample size, number of rows, and number of columns) tend to require more time and memory. Additionally, for a fixed total sample size, time and memory requirements tend to increase as the number of rows and columns increases, because this corresponds to an increase in the number of tables in the reference set. Also for a fixed sample size, time and memory requirements increase as the marginal row and column totals become more homogeneous. See Agresti, Mehta, and Patel (1990) and Gail and Mantel (1977) for more information.

At any time while PROC FREQ is computing exact p -values, you can terminate the computations by pressing the system interrupt key sequence (see the *SAS Companion* for your system) and choosing to stop computations. After you terminate exact computations, PROC FREQ completes all other remaining tasks. The procedure produces the requested output and reports missing values for any exact p -values that were not computed by the time of termination.

You can also use the MAXTIME= option in the EXACT statement to limit the amount of time PROC FREQ uses for exact computations. You specify a MAXTIME= value that is the maximum amount of clock time (in seconds) that PROC FREQ can use to compute an exact p -value. If PROC FREQ does not finish computing an exact p -value within that time, it terminates the computation and completes all other remaining tasks.

Monte Carlo Estimation

If you specify the option MC in the EXACT statement, PROC FREQ computes Monte Carlo estimates of the exact p -values instead of directly computing the exact p -values. Monte Carlo estimation can be useful for large problems that require a great amount of time and memory for exact computations but for which asymptotic approximations might not be sufficient. To describe the precision of each Monte Carlo estimate, PROC FREQ provides the asymptotic standard error and $100(1 - \alpha)\%$ confidence limits. The confidence level α is determined by the ALPHA= option in the EXACT statement, which, by default, equals 0.01 and produces 99% confidence limits. The N= n option in the EXACT statement specifies the number of samples that PROC FREQ uses for Monte Carlo estimation; the default is 10000 samples. You can specify a larger value for n to improve the precision of the Monte Carlo estimates. Because larger values of n generate more

samples, the computation time increases. Alternatively, you can specify a smaller value of n to reduce the computation time.

To compute a Monte Carlo estimate of an exact p -value, PROC FREQ generates a random sample of tables with the same total sample size, row totals, and column totals as the observed table. PROC FREQ uses the algorithm of Agresti, Wackerly, and Boyett (1979), which generates tables in proportion to their hypergeometric probabilities conditional on the marginal frequencies. For each sample table, PROC FREQ computes the value of the test statistic and compares it to the value for the observed table. When estimating a right-sided p -value, PROC FREQ counts all sample tables for which the test statistic is greater than or equal to the observed test statistic. Then the p -value estimate equals the number of these tables divided by the total number of tables sampled.

$$\begin{aligned}\hat{P}_{MC} &= M / N \\ M &= \text{number of samples with (Test Statistic} \geq t) \\ N &= \text{total number of samples} \\ t &= \text{observed Test Statistic}\end{aligned}$$

PROC FREQ computes left-sided and two-sided p -value estimates in a similar manner. For left-sided p -values, PROC FREQ evaluates whether the test statistic for each sampled table is less than or equal to the observed test statistic. For two-sided p -values, PROC FREQ examines the sample test statistics according to the expression for P_2 given in the section “Definition of p -Values” on page 2603.

The variable M is a binomially distributed variable with N trials and success probability p . It follows that the asymptotic standard error of the Monte Carlo estimate is

$$se(\hat{P}_{MC}) = \sqrt{\hat{P}_{MC} (1 - \hat{P}_{MC}) / (N - 1)}$$

PROC FREQ constructs asymptotic confidence limits for the p -values according to

$$\hat{P}_{MC} \pm (z_{\alpha/2} \times se(\hat{P}_{MC}))$$

where $z_{\alpha/2}$ is the $100(1 - \alpha/2)$ percentile of the standard normal distribution and the confidence level α is determined by the ALPHA= option in the EXACT statement.

When the Monte Carlo estimate \hat{P}_{MC} equals 0, PROC FREQ computes the confidence limits for the p -value as

$$(0, 1 - \alpha^{(1/N)})$$

When the Monte Carlo estimate \hat{P}_{MC} equals 1, PROC FREQ computes the confidence limits as

$$(\alpha^{(1/N)}, 1)$$

Computational Resources

For each variable in a table request, PROC FREQ stores all of the levels in memory. If all variables are numeric and not formatted, this requires about 84 bytes for each variable level. When there are character variables or formatted numeric variables, the memory that is required depends on the formatted variable lengths, with longer formatted lengths requiring more memory. The number of levels for each variable is limited only by the largest integer that your operating environment can store.

For any single crosstabulation table requested, PROC FREQ builds the entire table in memory, regardless of whether the table has zero cell counts. Thus, if the numeric variables A, B, and C each have 10 levels, PROC FREQ requires 2520 bytes to store the variable levels for the table request A*B*C, as follows:

```
3 variables * 10 levels/variable * 84 bytes/level
```

In addition, PROC FREQ requires 8000 bytes to store the table cell frequencies

```
1000 cells * 8 bytes/cell
```

even though there might be only 10 observations.

When the variables have many levels or when there are many multiway tables, your computer might not have enough memory to construct the tables. If PROC FREQ runs out of memory while constructing tables, it stops collecting levels for the variable with the most levels and returns the memory that is used by that variable. The procedure then builds the tables that do not contain the disabled variables.

If there is not enough memory for your table request and if increasing the available memory is impractical, you can reduce the number of multiway tables or variable levels. If you are not using the CMH or AGREE option in the TABLES statement to compute statistics across strata, reduce the number of multiway tables by using PROC SORT to sort the data set by one or more of the variables or by using the DATA step to create an index for the variables. Then remove the sorted or indexed variables from the TABLES statement and include a BY statement that uses these variables. You can also reduce memory requirements by using a FORMAT statement in the PROC FREQ step to reduce the number of levels. Additionally, reducing the formatted variable lengths reduces the amount of memory that is needed to store the variable levels. For more information about using formats, see the section “[Grouping with Formats](#)” on page 2544.

Output Data Sets

PROC FREQ produces two types of output data sets that you can use with other statistical and reporting procedures. You can request these data sets as follows:

- Specify the OUT= option in a TABLES statement. This creates an output data set that contains frequency or crosstabulation table counts and percentages
- Specify an OUTPUT statement. This creates an output data set that contains statistics.

PROC FREQ does not display the output data sets. Use PROC PRINT, PROC REPORT, or any other SAS reporting tool to display an output data set.

In addition to these two output data sets, you can create a SAS data set from any piece of PROC FREQ output by using the Output Delivery System. See the section “ODS Table Names” on page 2617 for more information.

Contents of the TABLES Statement Output Data Set

The OUT= option in the TABLES statement creates an output data set that contains one observation for each combination of variable values (or table cell) in the last table request. By default, each observation contains the frequency and percentage for the table cell. When the input data set contains missing values, the output data set also contains an observation with the frequency of missing values. The output data set includes the following variables:

- BY variables
- table request variables, such as A, B, C, and D in the table request A*B*C*D
- COUNT, which contains the table cell frequency
- PERCENT, which contains the table cell percentage

If you specify the OUTEXPECT option in the TABLES statement for a two-way or multiway table, the output data set also includes expected frequencies. If you specify the OUTPCT option for a two-way or multiway table, the output data set also includes row, column, and table percentages. The additional variables are as follows:

- EXPECTED, which contains the expected frequency
- PCT_TABL, which contains the percentage of two-way table frequency, for n -way tables where $n > 2$
- PCT_ROW, which contains the percentage of row frequency
- PCT_COL, which contains the percentage of column frequency

If you specify the OUTCUM option in the TABLES statement for a one-way table, the output data set also includes cumulative frequencies and cumulative percentages. The additional variables are as follows:

- CUM_FREQ, which contains the cumulative frequency
- CUM_PCT, which contains the cumulative percentage

The OUTCUM option has no effect for two-way or multiway tables.

The following PROC FREQ statements create an output data set of frequencies and percentages:

```
proc freq;
  tables A A*B / out=D;
run;
```

The output data set D contains frequencies and percentages for the table of A by B, which is the last table request listed in the TABLES statement. If A has two levels (1 and 2), B has three levels (1,2, and 3), and no table cell count is zero or missing, then the output data set D includes six observations, one for each combination of A and B levels. The first observation corresponds to A=1 and B=1; the second observation corresponds to A=1 and B=2; and so on. The data set includes the variables COUNT and PERCENT. The value of COUNT is the number of observations with the given combination of A and B levels. The value of PERCENT is the percentage of the total number of observations with that A and B combination.

When PROC FREQ combines different variable values into the same formatted level, the output data set contains the smallest internal value for the formatted level. For example, suppose a variable X has the values 1.1., 1.4, 1.7, 2.1, and 2.3. When you submit the statement

```
format X 1.;
```

in a PROC FREQ step, the formatted levels listed in the frequency table for X are 1 and 2. If you create an output data set with the frequency counts, the internal values of the levels of X are 1.1 and 1.7. To report the internal values of X when you display the output data set, use a format of 3.1 for X.

Contents of the OUTPUT Statement Output Data Set

The **OUTPUT** statement creates a SAS data set that contains statistics computed by PROC FREQ. [Table 38.7](#) lists the statistics that can be stored in the output data set. You identify which statistics to include by specifying *output-options*. See the description of the OUTPUT statement for details.

If you specify multiple **TABLES** statements or multiple table requests in a single TABLES statement, the contents of the output data set correspond to the last table request.

For a one-way table or a two-way table, the output data set contains one observation that stores the requested statistics for the table. For a multiway table, the output data set contains an observation for each two-way table (stratum) of the multiway crosstabulation. If you request summary statistics for the multiway table, the output data set also contains an observation that stores the across-strata summary statistics. If you use a BY statement, the output data set contains an observation (for one-way or two-way tables) or set of observations (for multiway tables) for each BY group.

The OUTPUT data set can include the following variables:

- BY variables
- Variables that identify the stratum for multiway tables, such as A and B in the table request A*B*C*D
- Variables that contain the specified statistics

In addition to the specified estimate or test statistic, the output data set includes associated values such as standard errors, confidence limits, *p*-values, and degrees of freedom.

PROC FREQ constructs variable names for the statistics in the output data set by enclosing the *output-option* names in underscores. Variable names for the corresponding standard errors, confidence limits, *p*-values, and degrees of freedom are formed by combining the *output-option* names with prefixes that identify the associated values. [Table 38.20](#) lists the prefixes and their descriptions.

Table 38.20 Output Data Set Variable Name Prefixes

Prefix	Description
E_	Asymptotic standard error (ASE)
L_	Lower confidence limit
U_	Upper confidence limit
E0_	Null hypothesis ASE
Z_	Standardized value
DF_	Degrees of freedom
P_	<i>p</i> -value
P2_	Two-sided <i>p</i> -value
PL_	Left-sided <i>p</i> -value
PR_	Right-sided <i>p</i> -value
XP_	Exact <i>p</i> -value
XP2_	Exact two-sided <i>p</i> -value
XPL_	Exact left-sided <i>p</i> -value
XPR_	Exact right-sided <i>p</i> -value
XPT_	Exact point probability
XL_	Exact lower confidence limit
XU_	Exact upper confidence limit

For example, the *PCHI* *output-option* in the *OUTPUT* statement includes the Pearson chi-square test in the output data set. The variable names for the Pearson chi-square statistic, its degrees of freedom, and the corresponding *p*-value are *_PCHI_*, *DF_PCHI*, and *P_PCHI*, respectively. If the length of the prefix plus the *output-option* name exceeds eight characters, PROC FREQ truncates the variable name to eight characters.

Displayed Output

Number of Variable Levels Table

If you specify the *NLEVELS* option in the PROC FREQ statement, PROC FREQ displays the “Number of Variable Levels” table. This table provides the number of levels for all variables named in the TABLES statements. PROC FREQ determines the variable levels from the formatted variable values. See “[Grouping with Formats](#)” on page 2544 for details. The “Number of Variable Levels” table contains the following information:

- Variable name
- Levels, which is the total number of levels of the variable
- Number of Nonmissing Levels, if there are missing levels for any of the variables
- Number of Missing Levels, if there are missing levels for any of the variables

One-Way Frequency Tables

PROC FREQ displays one-way frequency tables for all one-way table requests in the TABLES statements, unless you specify the NOPRINT option in the PROC FREQ statement or the NOPRINT option in the TABLES statement. For a one-way table showing the frequency distribution of a single variable, PROC FREQ displays the name of the variable and its values. For each variable value or level, PROC FREQ displays the following information:

- Frequency count, which is the number of observations in the level
- Test Frequency count, if you specify the CHISQ and TESTF= options to request a chi-square goodness-of-fit test for specified frequencies
- Percent, which is the percentage of the total number of observations. (The NOPERCENT option suppresses this information.)
- Test Percent, if you specify the CHISQ and TESTP= options to request a chi-square goodness-of-fit test for specified percents. (The NOPERCENT option suppresses this information.)
- Cumulative Frequency count, which is the sum of the frequency counts for that level and all other levels listed above it in the table. The last cumulative frequency is the total number of nonmissing observations. (The NOCUM option suppresses this information.)
- Cumulative Percent, which is the percentage of the total number of observations in that level and in all other levels listed above it in the table. (The NOCUM or the NOPERCENT option suppresses this information.)

The one-way table also displays the Frequency Missing, which is the number of observations with missing values.

Statistics for One-Way Frequency Tables

For one-way tables, two statistical options are available in the TABLES statement. The CHISQ option provides a chi-square goodness-of-fit test, and the BINOMIAL option provides binomial proportion statistics and tests. PROC FREQ displays the following information, unless you specify the NOPRINT option in the PROC FREQ statement:

- If you specify the CHISQ option for a one-way table, PROC FREQ provides a chi-square goodness-of-fit test, displaying the Chi-Square statistic, the degrees of freedom (DF), and the probability value ($Pr > ChiSq$). If you specify the CHISQ option in the EXACT statement, PROC FREQ also displays the exact probability value for this test. If you specify the POINT option with the CHISQ option in the EXACT statement, PROC FREQ displays the exact point probability for the test statistic.
- If you specify the BINOMIAL option for a one-way table, PROC FREQ displays the estimate of the binomial Proportion, which is the proportion of observations in the first class listed in the one-way table. PROC FREQ also displays the asymptotic standard error (ASE) and the asymptotic (Wald) and exact (Clopper-Pearson) confidence limits by default. For the binomial proportion test, PROC FREQ displays the asymptotic standard error under the null hypothesis (ASE Under H0), the standardized test statistic (Z), and the one-sided and two-sided probability values.

If you specify the `BINOMIAL` option in the `EXACT` statement, PROC FREQ also displays the exact one-sided and two-sided probability values for this test. If you specify the `POINT` option with the `BINOMIAL` option in the `EXACT` statement, PROC FREQ displays the exact point probability for the test.

- If you request additional binomial confidence limits by specifying *binomial-options*, PROC FREQ provides a table that displays the lower and upper confidence limits for each type that you request. In addition to the Wald and exact (Clopper-Pearson) confidence limits, you can request Agresti-Coull, Jeffreys, and Wilson (score) confidence limits for the binomial proportion.
- If you request a binomial noninferiority or superiority test by specifying the `NONINF` or `SUP` *binomial-option*, PROC FREQ displays the following information: the binomial Proportion, the test ASE (under H0 or Sample), the test statistic Z, the probability value, the noninferiority or superiority limit, and the test confidence limits. If you specify the `BINOMIAL` option in the `EXACT` statement, PROC FREQ also provides the exact probability value for the test, and exact test confidence limits.
- If you request a binomial equivalence test by specifying the `EQUIV` *binomial-option*, PROC FREQ displays the binomial Proportion and the test ASE (under H0 or Sample). PROC FREQ displays two one-sided tests (TOST) for equivalence, which include test statistics (Z) and probability values for the Lower and Upper tests, together with the Overall probability value. PROC FREQ also displays the equivalence limits and the test-based confidence limits. If you specify the `BINOMIAL` option in the `EXACT` statement, PROC FREQ provides exact probability values for the TOST and exact test-based confidence limits.

Multiway Tables

PROC FREQ displays all multiway table requests in the `TABLES` statements, unless you specify the `NO-PRINT` option in the `PROC FREQ` statement or the `NOPRINT` option in the `TABLES` statement.

For two-way to multiway crosstabulation tables, the values of the last variable in the table request form the table columns. The values of the next-to-last variable form the rows. Each level (or combination of levels) of the other variables forms one stratum.

There are three ways to display multiway tables in PROC FREQ. By default, PROC FREQ displays multiway tables as separate two-way crosstabulation tables for each stratum of the multiway table. Also by default, PROC FREQ displays these two-way crosstabulation tables in table cell format. Alternatively, if you specify the `CROSSLIST` option, PROC FREQ displays the two-way crosstabulation tables in ODS column format. If you specify the `LIST` option, PROC FREQ displays multiway tables in list format, which presents the entire multiway crosstabulation in a single table.

Crosstabulation Tables

By default, PROC FREQ displays two-way crosstabulation tables in table cell format. The row variable values are listed down the side of the table, the column variable values are listed across the top of the table, and each row and column variable level combination forms a table cell.

Each cell of a crosstabulation table can contain the following information:

- Frequency, which is the number of observations in the table cell. (The `NOFREQ` option suppresses this information.)

- Expected frequency under the hypothesis of independence, if you specify the **EXPECTED** option
- Deviation of the cell frequency from the expected value, if you specify the **DEVIATION** option
- Cell Chi-Square, which is the cell's contribution to the total chi-square statistic, if you specify the **CELLCHI2** option
- Tot Pct, which is the cell's percentage of the total multiway table frequency, for n -way tables when $n > 2$, if you specify the **TOTPCT** option
- Percent, which is the cell's percentage of the total (two-way table) frequency. (The **NOPERCENT** option suppresses this information.)
- Row Pct, or the row percentage, which is the cell's percentage of the total frequency for its row. (The **NOROW** option suppresses this information.)
- Col Pct, or column percentage, which is the cell's percentage of the total frequency for its column. (The **NOCOL** option suppresses this information.)
- Cumulative Col%, or cumulative column percentage, if you specify the **CUMCOL** option

The table also displays the Frequency Missing, which is the number of observations with missing values.

CROSSLIST Tables

If you specify the **CROSSLIST** option, PROC FREQ displays two-way crosstabulation tables in ODS column format. The **CROSSLIST** column format is different from the default crosstabulation table cell format, but the **CROSSLIST** table provides the same information (frequencies, percentages, and other statistics) as the default crosstabulation table.

In the **CROSSLIST** table format, the rows of the display correspond to the crosstabulation table cells, and the columns of the display correspond to descriptive statistics such as frequencies and percentages. Each table cell is identified by the values of its **TABLES** row and column variable levels, with all column variable levels listed within each row variable level. The **CROSSLIST** table also provides row totals, column totals, and overall table totals.

For a crosstabulation table in **CROSSLIST** format, PROC FREQ displays the following information:

- the row variable name and values
- the column variable name and values
- Frequency, which is the number of observations in the table cell. (The **NOFREQ** option suppresses this information.)
- Expected cell frequency under the hypothesis of independence, if you specify the **EXPECTED** option
- Deviation of the cell frequency from the expected value, if you specify the **DEVIATION** option
- Cell Chi-Square, which is the cell's contribution to the total chi-square statistic, if you specify the **CELLCHI2** option
- Total Percent, which is the cell's percentage of the total multiway table frequency, for n -way tables when $n > 2$, if you specify the **TOTPCT** option

- Percent, which is the cell's percentage of the total (two-way table) frequency. (The `NOPERCENT` option suppresses this information.)
- Row Percent, which is the cell's percentage of the total frequency for its row. (The `NOROW` option suppresses this information.)
- Column Percent, the cell's percentage of the total frequency for its column. (The `NOCOL` option suppresses this information.)

The table also displays the Frequency Missing, which is the number of observations with missing values.

LIST Tables

If you specify the `LIST` option in the `TABLES` statement, `PROC FREQ` displays multiway tables in a list format rather than as crosstabulation tables. The `LIST` option displays the entire multiway table in one table, instead of displaying a separate two-way table for each stratum. The `LIST` option is not available when you also request statistical options. Unlike the default crosstabulation output, the `LIST` output does not display row percentages, column percentages, and optional information such as expected frequencies and cell chi-squares.

For a multiway table in list format, `PROC FREQ` displays the following information:

- the variable names and values
- Frequency, which is the number of observations in the level (with the indicated variable values)
- Percent, which is the level's percentage of the total number of observations. (The `NOPERCENT` option suppresses this information.)
- Cumulative Frequency, which is the accumulated frequency of the level and all other levels listed above it in the table. The last cumulative frequency in the table is the total number of nonmissing observations. (The `NOCUM` option suppresses this information.)
- Cumulative Percent, which is the accumulated percentage of the level and all other levels listed above it in the table. (The `NOCUM` or the `NOPERCENT` option suppresses this information.)

The table also displays the Frequency Missing, which is the number of observations with missing values.

Statistics for Multiway Tables

`PROC FREQ` computes statistical tests and measures for crosstabulation tables, depending on which statements and options you specify. You can suppress the display of these results by specifying the `NOPRINT` option in the `PROC FREQ` statement. With any of the following information, `PROC FREQ` also displays the Sample Size and the Frequency Missing.

- If you specify the `SCOROUT` option in the `TABLES` statement, `PROC FREQ` displays the Row Scores and Column Scores that it uses for statistical computations. The Row Scores table displays the row variable values and the Score corresponding to each value. The Column Scores table displays the column variable values and the corresponding Scores. `PROC FREQ` also identifies the score type used to compute the row and column scores. You can specify the score type with the `SCORES=` option in the `TABLES` statement.

- If you specify the **CHISQ** option, PROC FREQ displays the following statistics for each two-way table: Pearson Chi-Square, Likelihood Ratio Chi-Square, Continuity-Adjusted Chi-Square (for 2×2 tables), Mantel-Haenszel Chi-Square, the Phi Coefficient, the Contingency Coefficient, and Cramér's V. For each test statistic, PROC FREQ also displays the degrees of freedom (DF) and the probability value (Prob).
- If you specify the **CHISQ** option for 2×2 tables, PROC FREQ also displays Fisher's exact test. The test output includes the cell (1,1) frequency (F), the exact left-sided and right-sided probability values, the table probability (P), and the exact two-sided probability value.
- If you specify the **FISHER** option in the TABLES statement (or, equivalently, the FISHER option in the **EXACT** statement), PROC FREQ displays Fisher's exact test for tables larger than 2×2 . The test output includes the table probability (P) and the probability value. In addition, PROC FREQ displays the CHISQ output listed earlier, even if you do not also specify the CHISQ option.
- If you specify the **PCHI**, **LRCHI**, or **MHCHI** option in the **EXACT** statement, PROC FREQ displays the corresponding exact test: Pearson Chi-Square, Likelihood Ratio Chi-Square, or Mantel-Haenszel Chi-Square, respectively. The test output includes the test statistic, the degrees of freedom (DF), and the asymptotic and exact probability values. If you also specify the **POINT** option in the **EXACT** statement, PROC FREQ displays the point probability for each exact test requested. If you specify the **CHISQ** option in the **EXACT** statement, PROC FREQ displays exact probability values for all three of these chi-square tests.
- If you specify the **MEASURES** option, PROC FREQ displays the following statistics and their asymptotic standard errors (ASE) for each two-way table: Gamma, Kendall's Tau-*b*, Stuart's Tau-*c*, Somers' $D(C|R)$, Somers' $D(R|C)$, Pearson Correlation, Spearman Correlation, Lambda Asymmetric ($C|R$), Lambda Asymmetric ($R|C$), Lambda Symmetric, Uncertainty Coefficient ($C|R$), Uncertainty Coefficient ($R|C$), and Uncertainty Coefficient Symmetric. If you specify the **CL** option, PROC FREQ also displays confidence limits for these measures.
- If you specify the **PLCORR** option, PROC FREQ displays the tetrachoric correlation for 2×2 tables or the polychoric correlation for larger tables. In addition, PROC FREQ displays the MEASURES output listed earlier, even if you do not also specify the MEASURES option.
- If you specify the **GAMMA**, **KENTB**, **STUTC**, **SMDCR**, **SMDRC**, **PCORR**, or **SCORR** option in the **TEST** statement, PROC FREQ displays asymptotic tests for Gamma, Kendall's Tau-*b*, Stuart's Tau-*c*, Somers' $D(C|R)$, Somers' $D(R|C)$, the Pearson Correlation, or the Spearman Correlation, respectively. If you specify the **MEASURES** option in the **TEST** statement, PROC FREQ displays all these asymptotic tests. The test output includes the statistic, its asymptotic standard error (ASE), Confidence Limits, the ASE under the null hypothesis H_0 , the standardized test statistic (Z), and the one-sided and two-sided probability values.
- If you specify the **KENTB**, **STUTC**, **SMDCR**, **SMDRC**, **PCORR**, or **SCORR** option in the **EXACT** statement, PROC FREQ displays asymptotic and exact tests for the corresponding measure of association: Kendall's Tau-*b*, Stuart's Tau-*c*, Somers' $D(C|R)$, Somers' $D(R|C)$, the Pearson Correlation, or the Spearman correlation, respectively. The test output includes the correlation, its asymptotic standard error (ASE), Confidence Limits, the ASE under the null hypothesis H_0 , the standardized test statistic (Z), and the asymptotic and exact one-sided and two-sided probability values. If you also specify the **POINT** option in the **EXACT** statement, PROC FREQ displays the point probability for each exact test requested.

- If you specify the **RISKDIFF** option for 2×2 tables, PROC FREQ displays the Column 1 and Column 2 Risk Estimates. For each column, PROC FREQ displays the Row 1 Risk, Row 2 Risk, Total Risk, and Risk Difference, together with their asymptotic standard errors (ASE) and Asymptotic Confidence Limits. PROC FREQ also displays Exact Confidence Limits for the Row 1 Risk, Row 2 Risk, and Total Risk. If you specify the **RISKDIFF** option in the **EXACT** statement, PROC FREQ provides unconditional Exact Confidence Limits for the Risk Difference.
- If you specify the **RISKDIFF(CL=)** option for 2×2 tables, PROC FREQ displays the Proportion Difference Confidence Limits. For each confidence limit Type that you request (Exact, Farrington-Manning, Hauck-Anderson, Newcombe Score, or Wald), PROC FREQ displays the Lower and Upper Confidence Limits.
- If you request a noninferiority or superiority test for the proportion difference (**RISKDIFF**) by specifying the **NONINF** or **SUP** *riskdiff-option*, and if you specify **METHOD=HA** (Hauck-Anderson), **METHOD=FM** (Farrington-Manning), or **METHOD=WALD** (Wald), PROC FREQ displays the following information: the Proportion Difference, the test ASE (H0, Sample, Sample H-A, or FM, depending on the method you specify), the test statistic Z, the probability value, the Noninferiority or Superiority Limit, and the test-based Confidence Limits. If you specify **METHOD=NEWCOMBE** (Newcombe score), PROC FREQ displays the Proportion Difference, the Noninferiority or Superiority Limit, and the Newcombe Confidence Limits.
- If you request an equivalence test for the proportion difference (**RISKDIFF**) by specifying the **EQUIV** *riskdiff-option*, and if you specify **METHOD=HA** (Hauck-Anderson), **METHOD=FM** (Farrington-Manning), or **METHOD=WALD** (Wald), PROC FREQ displays the following information: the Proportion Difference and the test ASE (H0, Sample, Sample H-A, or FM, depending on the method you specify). PROC FREQ displays a two one-sided test (TOST) for equivalence, which includes test statistics (Z) and probability values for the Lower and Upper tests, together with the Overall probability value. PROC FREQ also displays the Equivalence Limits and the test-based Confidence Limits. If you specify **METHOD=NEWCOMBE** (Newcombe), PROC FREQ displays the Proportion Difference, the Equivalence Limits, and the score Confidence Limits.
- If you request an equality test for the proportion difference (**RISKDIFF**) by specifying the **EQUAL** *riskdiff-option*, PROC FREQ displays the following information: the Proportion Difference and the test ASE (H0 or Sample), the test statistic Z, the One-Sided probability value ($\Pr > Z$ or $\Pr < Z$), and the Two-Sided probability value, $\Pr > |Z|$.
- If you specify the **MEASURES** option or the **RELRISK** option for 2×2 tables, PROC FREQ displays Estimates of the Relative Risk for Case-Control and Cohort studies, together with their Confidence Limits. These measures are also known as the Odds Ratio and the Column 1 and 2 Relative Risks. If you specify the **OR** option in the **EXACT** statement, PROC FREQ also displays Exact Confidence Limits for the Odds Ratio. If you specify the **RELRISK** option in the **EXACT** statement, PROC FREQ displays unconditional Exact Confidence Limits for the Relative Risk.
- If you specify the **TREND** option, PROC FREQ displays the Cochran-Armitage Trend Test for tables that are $2 \times C$ or $R \times 2$. For this test, PROC FREQ gives the Statistic (Z) and the one-sided and two-sided probability values. If you specify the **TREND** option in the **EXACT** statement, PROC FREQ also displays the exact one-sided and two-sided probability values for this test. If you specify the **POINT** option with the **TREND** option in the **EXACT** statement, PROC FREQ displays the exact point probability for the test statistic.

- If you specify the **JT** option, PROC FREQ displays the Jonckheere-Terpstra Test, showing the Statistic (JT), the standardized test statistic (Z), and the one-sided and two-sided probability values. If you specify the JT option in the **EXACT** statement, PROC FREQ also displays the exact one-sided and two-sided probability values for this test. If you specify the **POINT** option with the JT option in the **EXACT** statement, PROC FREQ displays the exact point probability for the test statistic.
- If you specify the **AGREE** option and the **PRINTKWT** option, PROC FREQ displays the Kappa Coefficient Weights for square tables larger than 2×2 .
- If you specify the **AGREE** option, for two-way tables PROC FREQ displays McNemar's Test and the Simple Kappa Coefficient for 2×2 tables. For square tables larger than 2×2 , PROC FREQ displays Bowker's Test of Symmetry, the Simple Kappa Coefficient, and the Weighted Kappa Coefficient. For McNemar's Test and Bowker's Test of Symmetry, PROC FREQ displays the Statistic (S), the degrees of freedom (DF), and the probability value ($\text{Pr} > S$). If you specify the **MCNEM** option in the **EXACT** statement, PROC FREQ also displays the exact probability value for McNemar's test. If you specify the **POINT** option with the **MCNEM** option in the **EXACT** statement, PROC FREQ displays the exact point probability for the test statistic. For the simple and weighted kappa coefficients, PROC FREQ displays the kappa values, asymptotic standard errors (ASE), and Confidence Limits.
- If you specify the **KAPPA** or **WTKAP** option in the **TEST** statement, PROC FREQ displays asymptotic tests for the simple kappa coefficient or the weighted kappa coefficient, respectively. If you specify the **AGREE** option in the **TEST** statement, PROC FREQ displays both these asymptotic tests. The test output includes the kappa coefficient, its asymptotic standard error (ASE), Confidence Limits, the ASE under the null hypothesis H_0 , the standardized test statistic (Z), and the one-sided and two-sided probability values.
- If you specify the **KAPPA** or **WTKAP** option in the **EXACT** statement, PROC FREQ displays asymptotic and exact tests for the simple kappa coefficient or the weighted kappa coefficient, respectively. The test output includes the kappa coefficient, its asymptotic standard error (ASE), Confidence Limits, the ASE under the null hypothesis H_0 , the standardized test statistic (Z), and the asymptotic and exact one-sided and two-sided probability values. If you specify the **POINT** option in the **EXACT** statement, PROC FREQ displays the point probability for each exact test requested.
- If you specify the **MC** option in the **EXACT** statement, PROC FREQ displays Monte Carlo estimates for all exact p -values requested by *statistic-options* in the **EXACT** statement. The Monte Carlo output includes the p -value Estimate, its Confidence Limits, the Number of Samples used to compute the Monte Carlo estimate, and the Initial Seed for random number generation.
- If you specify the **AGREE** option, for multiple strata PROC FREQ displays Overall Simple and Weighted Kappa Coefficients, with their asymptotic standard errors (ASE) and Confidence Limits. PROC FREQ also displays Tests for Equal Kappa Coefficients, giving the Chi-Squares, degrees of freedom (DF), and probability values ($\text{Pr} > \text{ChiSq}$) for the Simple Kappa and Weighted Kappa. For multiple strata of 2×2 tables, PROC FREQ displays Cochran's Q , giving the Statistic (Q), the degrees of freedom (DF), and the probability value ($\text{Pr} > Q$).
- If you specify the **CMH** option, PROC FREQ displays Cochran-Mantel-Haenszel Statistics for the following three alternative hypotheses: Nonzero Correlation, Row Mean Scores Differ (ANOVA Statistic), and General Association. For each of these statistics, PROC FREQ gives the degrees of freedom (DF) and the probability value (Prob). If you specify the **MANTELFLEISS** option, PROC FREQ displays the Mantel-Fleiss Criterion for 2×2 tables. For 2×2 tables, PROC FREQ also

displays Estimates of the Common Relative Risk for Case-Control and Cohort studies, together with their confidence limits. These include both Mantel-Haenszel and Logit stratum-adjusted estimates of the common Odds Ratio, Column 1 Relative Risk, and Column 2 Relative Risk. Also for 2×2 tables, PROC FREQ displays the Breslow-Day Test for Homogeneity of the Odds Ratios. For this test, PROC FREQ gives the Chi-Square, the degrees of freedom (DF), and the probability value ($\text{Pr} > \text{ChiSq}$).

- If you specify the **CMH** option in the TABLES statement and also specify the COMOR option in the EXACT statement, PROC FREQ displays exact confidence limits for the Common Odds Ratio for multiple strata of 2×2 tables. PROC FREQ also displays the Exact Test of H_0 : Common Odds Ratio = 1. The test output includes the Cell (1,1) Sum (S), Mean of S Under H_0 , One-sided $\text{Pr} \leq S$, and Point $\text{Pr} = S$. PROC FREQ also provides exact two-sided probability values for the test, computed according to the following three methods: 2 * One-sided, Sum of probabilities \leq Point probability, and $\text{Pr} \geq |S - \text{Mean}|$.
- If you specify the **CMH** option in the TABLES statement and also specify the EQOR option in the EXACT statement, PROC FREQ computes Zelen's exact test for equal odds ratios for $h \times 2 \times 2$ tables. PROC FREQ displays Zelen's test along with the asymptotic Breslow-Day test produced by the CMH option. PROC FREQ displays the test statistic, Zelen's Exact Test (P), and the probability value, Exact $\text{Pr} \leq P$.
- If you specify the **GAILSIMON** option in the TABLES statement for a multiway 2×2 tables, PROC FREQ displays the Gail-Simon test for qualitative interactions. The display include the following statistics and their p -values: Q+ (Positive Risk Differences), Q- (Negative Risk Differences), and Q (Two-Sided).

ODS Table Names

PROC FREQ assigns a name to each table that it creates. You can use these names to refer to tables when you use the Output Delivery System (ODS) to select tables and create output data sets. For more information about ODS, see Chapter 20, "Using the Output Delivery System."

Table 38.21 lists the ODS table names together with their descriptions and the options required to produce the tables. Note that the ALL option in the TABLES statement invokes the CHISQ, MEASURES, and CMH options.

Table 38.21 ODS Tables Produced by PROC FREQ

ODS Table Name	Description	Statement	Option
BarnardsTest	Barnard's exact test	EXACT	BARNARD
BinomialCLs	Binomial confidence limits	TABLES	BINOMIAL(AC J W)
BinomialEquiv	Binomial equivalence analysis	TABLES	BINOMIAL(EQUIV)
BinomialEquivLimits	Binomial equivalence limits	TABLES	BINOMIAL(EQUIV)
BinomialEquivTest	Binomial equivalence test	TABLES	BINOMIAL(EQUIV)
BinomialNoninf	Binomial noninferiority test	TABLES	BINOMIAL(NONINF)
BinomialProp	Binomial proportion	TABLES	BINOMIAL
BinomialPropTest	Binomial proportion test	TABLES	BINOMIAL
BinomialSup	Binomial superiority test	TABLES	BINOMIAL(SUP)

Table 38.21 continued

ODS Table Name	Description	Statement	Option
BreslowDayTest	Breslow-Day test	TABLES	CMH ($h \times 2 \times 2$ table)
CMH	Cochran-Mantel-Haenszel statistics	TABLES	CMH
ChiSq	Chi-square tests	TABLES	CHISQ
CochransQ	Cochran's Q	TABLES	AGREE ($h \times 2 \times 2$ table)
ColScores	Column scores	TABLES	SCOROUT
CommonOdds- RatioCl	Exact confidence limits for the common odds ratio	EXACT	COMOR ($h \times 2 \times 2$ table)
CommonOdds- RatioTest	Common odds ratio exact test	EXACT	COMOR ($h \times 2 \times 2$ table)
CommonRelRisks	Common relative risks	TABLES	CMH ($h \times 2 \times 2$ table)
CrossList	Crosstabulation table in column format	TABLES	CROSSLIST (n -way table, $n > 1$)
CrossTabFreqs	Crosstabulation table	TABLES	(n -way table, $n > 1$)
EqualKappaTest	Test for equal simple kappas	TABLES	AGREE ($h \times 2 \times 2$ table)
EqualKappaTests	Tests for equal kappas	TABLES	AGREE ($h \times r \times r$, $r > 2$)
EqualOddsRatios	Tests for equal odds ratios	EXACT	EQOR ($h \times 2 \times 2$ table)
GailSimon	Gail-Simon test	TABLES	GAILSIMON ($h \times 2 \times 2$ table)
FishersExact	Fisher's exact test	EXACT or TABLES or TABLES	FISHER FISHER or EXACT CHISQ (2×2 table)
FishersExactMC	Monte Carlo estimates for Fisher's exact test	EXACT	FISHER / MC
Gamma	Gamma	TEST	GAMMA
GammaTest	Gamma test	TEST	GAMMA
JTTest	Jonckheere-Terpstra test	TABLES	JT
JTTestMC	Monte Carlo estimates for Jonckheere-Terpstra exact test	EXACT	JT / MC
KappaStatistics	Kappa statistics	TABLES	AGREE, no TEST or EXACT ($r \times r$ table, $r > 2$)
KappaWeights	Kappa weights	TABLES	AGREE and PRINTKWT
List	List format multiway table	TABLES	LIST
LRChiSq	Likelihood ratio chi-square exact test	EXACT	LRCHI
LRChiSqMC	Monte Carlo exact test for likelihood ratio chi-square	EXACT	LRCHI / MC

Table 38.21 continued

ODS Table Name	Description	Statement	Option
MantelFleiss	Mantel-Fleiss criterion	TABLES	CMH(MF) ($h \times 2 \times 2$ table)
McNemarsTest	McNemar's test	TABLES	AGREE (2×2 table)
Measures	Measures of association	TABLES	MEASURES
MHChiSq	Mantel-Haenszel chi-square exact test	EXACT	MHCHI
MHChiSqMC	Monte Carlo exact test for Mantel-Haenszel chi-square	EXACT	MHCHI / MC
NLevels	Number of variable levels	PROC	NLEVELS
OddsRatioCL	Exact confidence limits for the odds ratio	EXACT	OR (2×2 table)
OneWayChiSq	One-way chi-square test	TABLES	CHISQ (one-way table)
OneWayChiSqMC	Monte Carlo exact test for one-way chi-square	EXACT	CHISQ / MC (one-way table)
OneWayFreqs	One-way frequencies	PROC or TABLES	(no TABLES stmt) (one-way table)
OneWayLRChiSq	One-way likelihood ratio chi-square test	TABLES	CHISQ(LRCHISQ) (one-way table)
OverallKappa	Overall simple kappa	TABLES	AGREE ($h \times 2 \times 2$ table)
OverallKappas	Overall kappa coefficients	TABLES	AGREE ($h \times r \times r, r > 2$)
PdiffCLs	Proportion difference confidence limits	TABLES	RISKDIFF(CL=) (2×2 table)
PdiffEquiv	Equivalence analysis for the proportion difference	TABLES	RISKDIFF(EQUIV) (2×2 table)
PdiffEquivLimits	Equivalence limits for the proportion difference	TABLES	RISKDIFF(EQUIV) (2×2 table)
PdiffEquivTest	Equivalence test for the proportion difference	TABLES	RISKDIFF(EQUIV) (2×2 table)
PdiffNoninf	Noninferiority test for the proportion difference	TABLES	RISKDIFF(NONINF) (2×2 table)
PdiffSup	Superiority test for the proportion difference	TABLES	RISKDIFF(SUP) (2×2 table)
PdiffTest	Proportion difference test	TABLES	RISKDIFF(EQUAL) (2×2 table)
PearsonChiSq	Pearson chi-square exact test	EXACT	PCHI
PearsonChiSqMC	Monte Carlo exact test for Pearson chi-square	EXACT	PCHI / MC
PearsonCorr	Pearson correlation	TEST or EXACT	PCORR PCORR
PearsonCorrMC	Monte Carlo exact test for Pearson correlation	EXACT	PCORR / MC

Table 38.21 continued

ODS Table Name	Description	Statement	Option
PearsonCorrTest	Pearson correlation test	TEST or EXACT	PCORR PCORR
PICorr	Polychoric correlation	TEST	PLCORR
PICorrTest	Polychoric correlation test	TEST	PLCORR
RelativeRisks	Relative risk estimates	TABLES	RELRIK or MEASURES (2 × 2 table)
RelRisk1CL	Exact confidence limits for column 1 relative risk	EXACT	RELRIK (2 × 2 table)
RelRisk2CL	Exact confidence limits for column 2 relative risk	EXACT	RELRIK (2 × 2 table)
RiskDiffCol1	Column 1 risk estimates	TABLES	RISKDIFF (2 × 2 table)
RiskDiffCol2	Column 2 risk estimates	TABLES	RISKDIFF (2 × 2 table)
RowScores	Row scores	TABLES	SCOROUT
SimpleKappa	Simple kappa coefficient	TEST or EXACT	KAPPA KAPPA
SimpleKappaMC	Monte Carlo exact test for simple kappa	EXACT	KAPPA / MC
SimpleKappaTest	Simple kappa test	TEST or EXACT	KAPPA KAPPA
SomersDCR	Somers' $D(C R)$	TEST or EXACT	SMDCR SMDCR
SomersDCRMC	Monte Carlo exact test for Somers' $D(C R)$	EXACT	SMDCR / MC
SomersDCRTest	Somers' $D(C R)$ test	TEST or EXACT	SMDCR SMDCR
SomersDRC	Somers' $D(R C)$	TEST or EXACT	SMDRC SMDRC
SomersDRCMC	Monte Carlo exact test for Somers' $D(R C)$	EXACT	SMDRC / MC
SomersDRCTest	Somers' $D(R C)$ test	TEST or EXACT	SMDRC SMDRC
SpearmanCorr	Spearman correlation	TEST or EXACT	SCORR SCORR
SpearmanCorrMC	Monte Carlo exact test for Spearman correlation	EXACT	SCORR / MC
SpearmanCorrTest	Spearman correlation test	TEST or EXACT	SCORR SCORR
SymmetryTest	Test of symmetry	TABLES	AGREE
TauB	Kendall's tau- b	TEST or EXACT	KENTB KENTB
TauBMC	Monte Carlo exact test for Kendall's tau- b	EXACT	KENTB / MC

Table 38.21 *continued*

ODS Table Name	Description	Statement	Option
TauBTest	Kendall's tau- <i>b</i> test	TEST or EXACT	KENTB KENTB
TauC	Stuart's tau- <i>c</i>	TEST or EXACT	STUTC STUTC
TauCMC	Monte Carlo exact test for Stuart's tau- <i>c</i>	EXACT	STUTC / MC
TauCTest	Stuart's tau- <i>c</i> test	TEST or EXACT	STUTC STUTC
TrendTest	Cochran-Armitage trend test	TABLES	TREND
TrendTestMC	Monte Carlo exact test for trend	EXACT	TREND / MC
WeightedKappa	Weighted kappa	TEST or EXACT	WTKAP WTKAP
WeightedKappaMC	Monte Carlo exact test for weighted kappa	EXACT	WTKAP / MC
WeightedKappaTest	Weighted kappa test	TEST or EXACT	WTKAP WTKAP

ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “[Statistical Graphics Using ODS.](#)”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS.](#)”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “[A Primer on ODS Statistical Graphics](#)” on page 599 in Chapter 21, “[Statistical Graphics Using ODS.](#)”

When ODS Graphics is enabled, you can request specific plots with the PLOTS= option in the TABLES statement. To produce a frequency plot or cumulative frequency plot, you must specify the [FREQPLOT](#) or [CUMFREQPLOT](#) *plot-request*, respectively, in the PLOTS= option. To produce a mosaic plot, you must specify the [MOSAICPLOT](#) *plot-request* in the PLOTS= option. You can also produce frequency, cumulative frequency, and mosaic plots by specifying the PLOTS=ALL option. By default, PROC FREQ produces all other plots that are associated with the analyses that you request in the TABLES statement. You can suppress the default plots and request specific plots by using the PLOTS(ONLY)= option. See the description of the PLOTS= option for details.

PROC FREQ assigns a name to each graph that it creates with ODS Graphics. You can use these names to refer to the graphs. [Table 38.22](#) lists the names of the graphs that PROC FREQ generates together with their descriptions, their PLOTS= options (*plot-requests*), and the TABLES statement options that are required to produce the graphs.

Table 38.22 Graphs Produced by PROC FREQ

ODS Graph Name	Description	PLOTS= Option	TABLES Statement Option
AgreePlot	Agreement plot	AGREEPLOT	AGREE ($r \times r$ table)
CumFreqPlot	Cumulative frequency plot	CUMFREQPLOT	One-way table request
DeviationPlot	Deviation plot	DEVIATIONPLOT	CHISQ (one-way table)
FreqPlot	Frequency plot	FREQPLOT	Any table request
KappaPlot	Kappa plot	KAPPAPLOT	AGREE ($h \times r \times r$ table)
MosaicPlot	Mosaic plot	MOSAICPLOT	Two-way or multiway table request
ORPlot	Odds ratio plot	ODDSRATIOPLOT	MEASURES or RELRISK ($h \times 2 \times 2$ table)
RelRiskPlot	Relative risk plot	RELRIKSPLOT	MEASURES or RELRISK ($h \times 2 \times 2$ table)
RiskDiffPlot	Risk difference plot	RISKDIFFPLOT	RISKDIFF ($h \times 2 \times 2$ table)
WtKappaPlot	Weighted kappa plot	WTKAPPAPLOT	AGREE ($h \times r \times r$ table, $r > 2$)

Examples: FREQ Procedure

Example 38.1: Output Data Set of Frequencies

The eye and hair color of children from two different regions of Europe are recorded in the data set Color. Instead of recording one observation per child, the data are recorded as cell counts, where the variable Count contains the number of children exhibiting each of the 15 eye and hair color combinations. The data set does not include missing combinations.

The following DATA step statements create the SAS data set Color:

```

data Color;
  input Region Eyes $ Hair $ Count @@;
  label Eyes = 'Eye Color'
        Hair = 'Hair Color'
        Region = 'Geographic Region';
  datalines;
1 blue fair 23 1 blue red 7 1 blue medium 24
1 blue dark 11 1 green fair 19 1 green red 7
1 green medium 18 1 green dark 14 1 brown fair 34
1 brown red 5 1 brown medium 41 1 brown dark 40
1 brown black 3 2 blue fair 46 2 blue red 21
2 blue medium 44 2 blue dark 40 2 blue black 6
2 green fair 50 2 green red 31 2 green medium 37
2 green dark 23 2 brown fair 56 2 brown red 42
2 brown medium 53 2 brown dark 54 2 brown black 13
;

```

The following PROC FREQ statements read the Color data set and create an output data set that contains the frequencies, percentages, and expected cell frequencies of the two-way table of Eyes by Hair. The TABLES

statement requests three tables: a frequency table for Eyes, a frequency table for Hair, and a crosstabulation table for Eyes by Hair. The OUT= option creates the FreqCount data set, which contains the crosstabulation table frequencies. The OUTEXPECT option outputs the expected table cell frequencies to FreqCount, and the SPARSE option includes zero cell frequencies in the output data set. The WEIGHT statement specifies that the variable Count contains the observation weights. These statements create [Output 38.1.1](#) through [Output 38.1.3](#).

```
proc freq data=Color;
  tables Eyes Hair Eyes*Hair / out=FreqCount outexpect sparse;
  weight Count;
  title 'Eye and Hair Color of European Children';
run;

proc print data=FreqCount noobs;
  title2 'Output Data Set from PROC FREQ';
run;
```

[Output 38.1.1](#) displays the two frequency tables produced by PROC FREQ: one showing the distribution of eye color, and one showing the distribution of hair color. By default, PROC FREQ lists the variables values in alphabetical order. The 'Eyes*Hair' specification produces a crosstabulation table, shown in [Output 38.1.2](#), with eye color defining the table rows and hair color defining the table columns. A zero cell frequency for green eyes and black hair indicates that this eye and hair color combination does not occur in the data.

The output data set FreqCount ([Output 38.1.3](#)) contains frequency counts and percentages for the last table requested in the TABLES statement, Eyes by Hair. Because the SPARSE option is specified, the data set includes the observation with a zero frequency. The variable Expected contains the expected frequencies, as requested by the OUTEXPECT option.

Output 38.1.1 Frequency Tables

Eye and Hair Color of European Children				
The FREQ Procedure				
Eye Color				
Eyes	Frequency	Percent	Cumulative Frequency	Cumulative Percent
blue	222	29.13	222	29.13
brown	341	44.75	563	73.88
green	199	26.12	762	100.00
Hair Color				
Hair	Frequency	Percent	Cumulative Frequency	Cumulative Percent
black	22	2.89	22	2.89
dark	182	23.88	204	26.77
fair	228	29.92	432	56.69
medium	217	28.48	649	85.17
red	113	14.83	762	100.00

Output 38.1.2 Crosstabulation Table

Table of Eyes by Hair						
Eyes(Eye Color)	Hair(Hair Color)					
Frequency						
Percent						
Row Pct						
Col Pct	black	dark	fair	medium	red	Total
blue	6	51	69	68	28	222
	0.79	6.69	9.06	8.92	3.67	29.13
	2.70	22.97	31.08	30.63	12.61	
	27.27	28.02	30.26	31.34	24.78	
brown	16	94	90	94	47	341
	2.10	12.34	11.81	12.34	6.17	44.75
	4.69	27.57	26.39	27.57	13.78	
	72.73	51.65	39.47	43.32	41.59	
green	0	37	69	55	38	199
	0.00	4.86	9.06	7.22	4.99	26.12
	0.00	18.59	34.67	27.64	19.10	
	0.00	20.33	30.26	25.35	33.63	
Total	22	182	228	217	113	762
	2.89	23.88	29.92	28.48	14.83	100.00

Output 38.1.3 Output Data Set of Frequencies

Eye and Hair Color of European Children				
Output Data Set from PROC FREQ				
Eyes	Hair	COUNT	EXPECTED	PERCENT
blue	black	6	6.409	0.7874
blue	dark	51	53.024	6.6929
blue	fair	69	66.425	9.0551
blue	medium	68	63.220	8.9239
blue	red	28	32.921	3.6745
brown	black	16	9.845	2.0997
brown	dark	94	81.446	12.3360
brown	fair	90	102.031	11.8110
brown	medium	94	97.109	12.3360
brown	red	47	50.568	6.1680
green	black	0	5.745	0.0000
green	dark	37	47.530	4.8556
green	fair	69	59.543	9.0551
green	medium	55	56.671	7.2178
green	red	38	29.510	4.9869

Example 38.2: Frequency Dot Plots

This example produces frequency dot plots for the children's eye and hair color data from [Example 38.1](#).

PROC FREQ produces plots by using ODS Graphics to create graphs as part of the procedure output. Frequency plots are available for any frequency or crosstabulation table request. You can display frequency plots as bar charts or dot plots. You can use *plot-options* to specify the orientation (vertical or horizontal), scale, and layout of the plots.

The following PROC FREQ statements request frequency tables and dot plots. The first TABLES statement requests a one-way frequency table of Hair and a crosstabulation table of Eyes by Hair. The PLOTS= option requests frequency plots for the tables, and the TYPE=DOTPLOT *plot-option* specifies dot plots. By default, frequency plots are produced as bar charts. ODS Graphics must be enabled before producing plots.

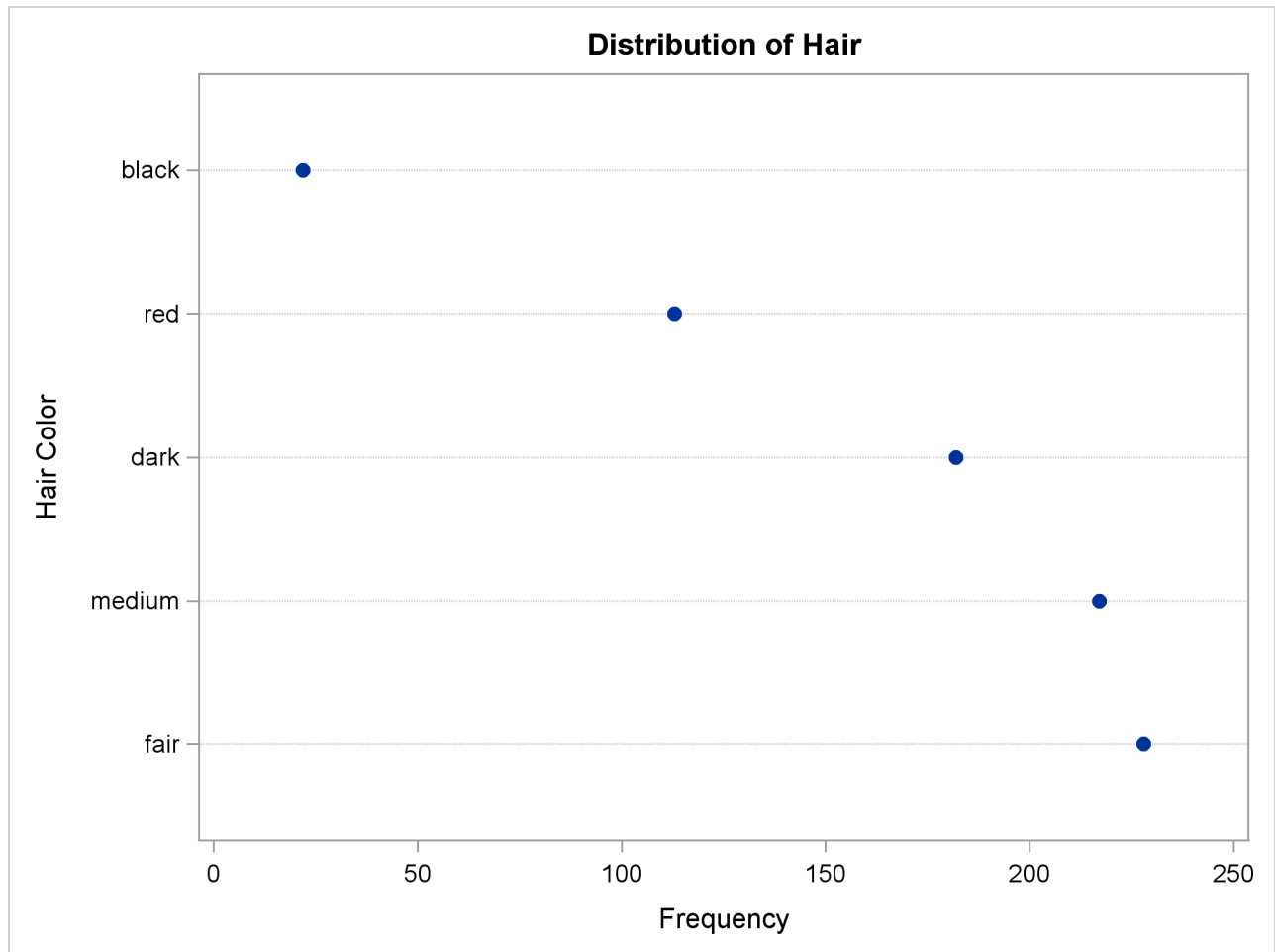
The second TABLES statement requests a crosstabulation table of Region by Hair and a frequency dot plot for this table. The SCALE=PERCENT *plot-option* plots percentages instead of frequency counts. SCALE=LOG and SCALE=SQRT *plot-options* are also available to plot log frequencies and square roots of frequencies, respectively.

The ORDER=FREQ option in the PROC FREQ statement orders the variable levels by frequency. This order applies to the frequency and crosstabulation table displays and also to the corresponding frequency plots.

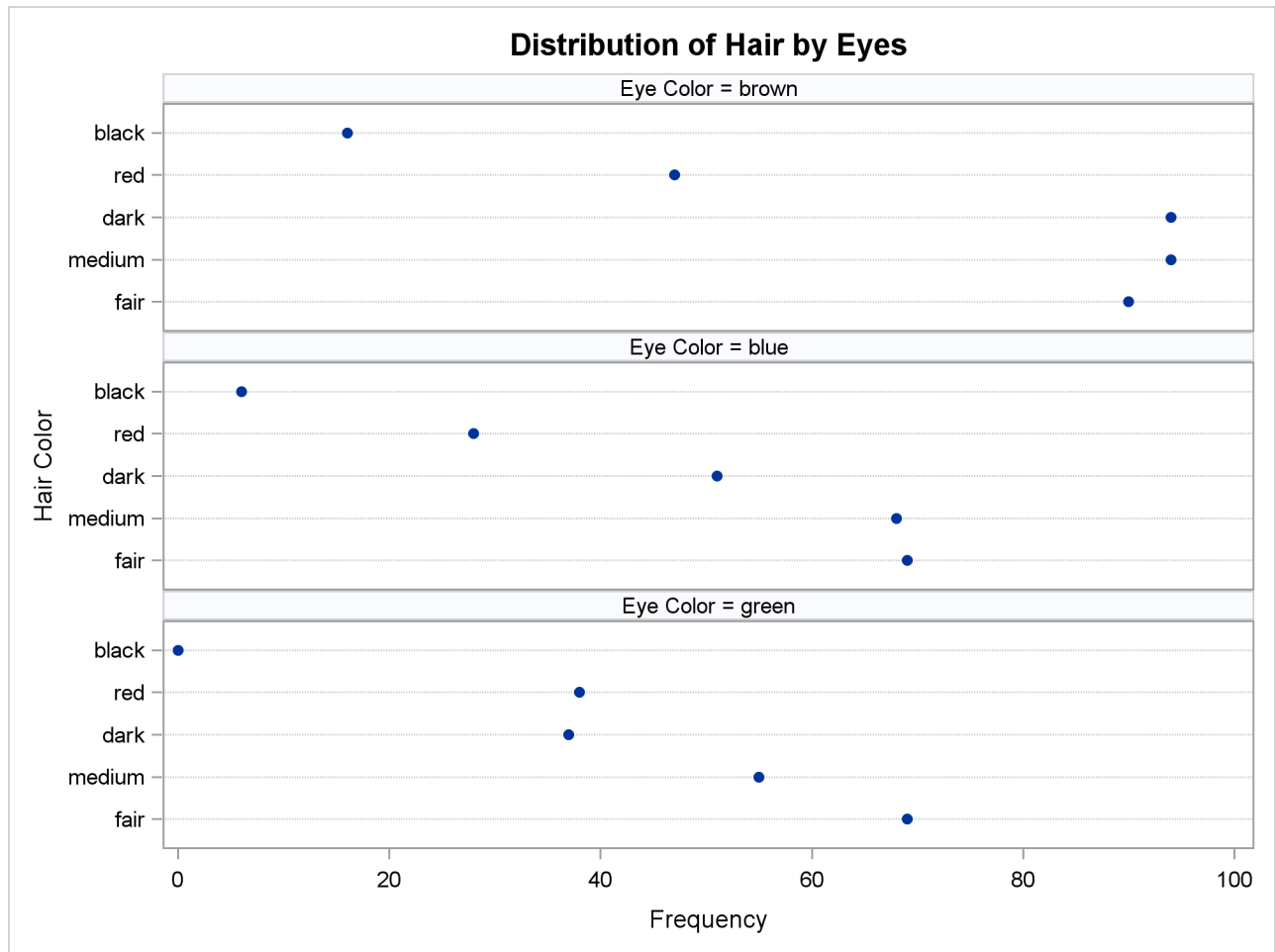
```
ods graphics on;
proc freq data=Color order=freq;
  tables Hair Hair*Eyes / plots=freqplot(type=dotplot);
  tables Hair*Region / plots=freqplot(type=dotplot scale=percent);
  weight Count;
  title 'Eye and Hair Color of European Children';
run;
ods graphics off;
```

Output 38.2.1, Output 38.2.2, and Output 38.2.3 display the dot plots produced by PROC FREQ. By default, the orientation of dot plots is horizontal, which places the variable levels on the Y axis. You can specify the ORIENT=VERTICAL *plot-option* to request a vertical orientation. For two-way plots, you can use the TWOWAY= *plot-option* to specify the plot layout. The default layout (shown in [Output 38.2.2](#) and [Output 38.2.3](#)) is GROUPVERTICAL. Two-way layouts STACKED and GROUPTHORIZONTAL are also available.

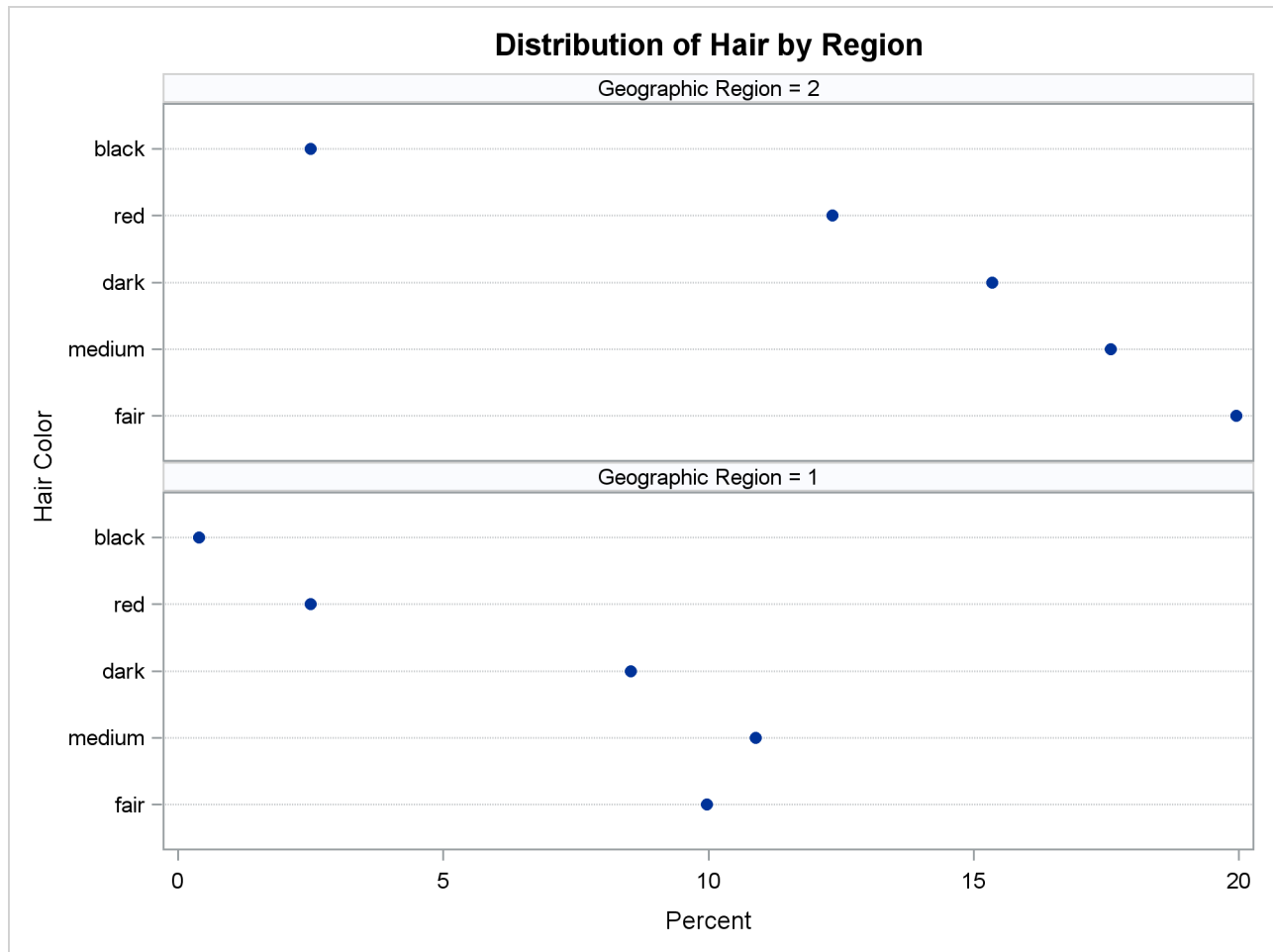
Output 38.2.1 One-Way Frequency Dot Plot



Output 38.2.2 Two-Way Frequency Dot Plot



Output 38.2.3 Two-Way Percent Dot Plot



Example 38.3: Chi-Square Goodness-of-Fit Tests

This example examines whether the children's hair color (from [Example 38.1](#)) has a specified multinomial distribution for the two geographical regions. The hypothesized distribution of hair color is 30% fair, 12% red, 30% medium, 25% dark, and 3% black.

In order to test the hypothesis for each region, the data are first sorted by Region. Then the FREQ procedure uses a BY statement to produce a separate table for each BY group (Region). The option ORDER=DATA orders the variable values (hair color) in the frequency table by their order in the input data set. The TABLES statement requests a frequency table for hair color, and the option NOCUM suppresses the display of the cumulative frequencies and percentages.

The CHISQ option requests a chi-square goodness-of-fit test for the frequency table of Hair. The TESTP= option specifies the hypothesized (or test) percentages for the chi-square test; the number of percentages listed equals the number of table levels, and the percentages sum to 100%. The TESTP= percentages are listed in the same order as the corresponding variable levels appear in frequency table.

The PLOTS= option requests a deviation plot, which is associated with the CHISQ option and displays the relative deviations from the test frequencies. The TYPE=DOTPLOT *plot-option* requests a dot plot instead

of the default type, which is a bar chart. ODS Graphics must be enabled before producing plots. These statements produce [Output 38.3.1](#) through [Output 38.3.4](#).

```
proc sort data=Color;
  by Region;
run;

ods graphics on;
proc freq data=Color order=data;
  tables Hair / nocum chisq testp=(30 12 30 25 3)
           plots(only)=deviationplot(type=dotplot);
  weight Count;
  by Region;
  title 'Hair Color of European Children';
run;
ods graphics off;
```

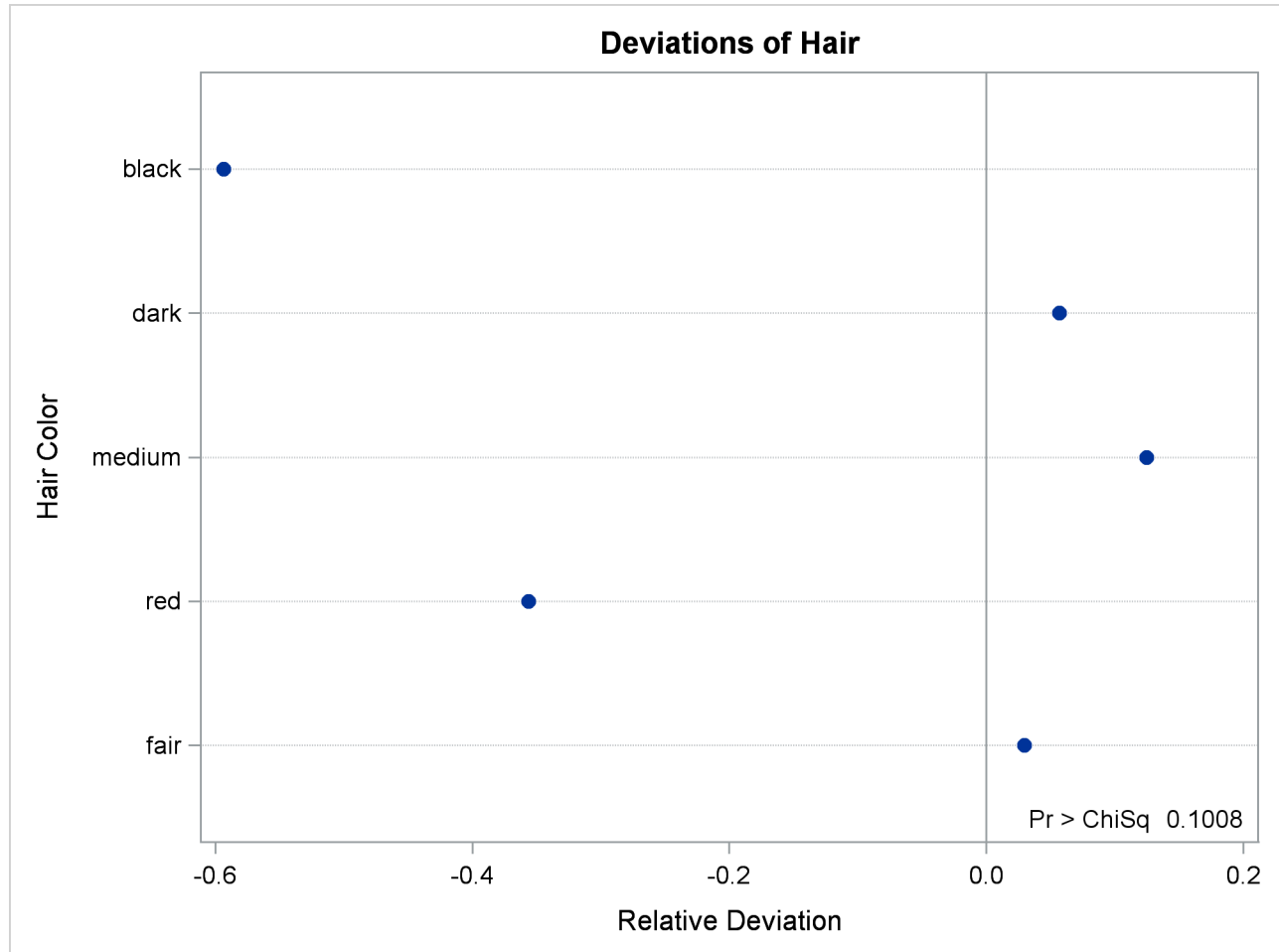
Output 38.3.1 Frequency Table and Chi-Square Test for Region 1

Hair Color of European Children				
----- Geographic Region=1 -----				
The FREQ Procedure				
Hair Color				
Hair	Frequency	Percent		Test Percent
fair	76	30.89		30.00
red	19	7.72		12.00
medium	83	33.74		30.00
dark	65	26.42		25.00
black	3	1.22		3.00
----- Geographic Region=1 -----				
Chi-Square Test for Specified Proportions				
	Chi-Square	7.7602		
	DF	4		
	Pr > ChiSq	0.1008		

[Output 38.3.1](#) shows the frequency table and chi-square test for Region 1. The frequency table lists the variable values (hair color) in the order in which they appear in the data set. The “Test Percent” column lists the hypothesized percentages for the chi-square test. Always check that you have ordered the TESTP= percentages to correctly match the order of the variable levels.

Output 38.3.2 shows the deviation plot for Region 1, which displays the relative deviations from the hypothesized values. The relative deviation for a level is the difference between the observed and hypothesized (test) percentage divided by the test percentage. You can suppress the chi-square p -value that is displayed by default in the deviation plot by specifying the NOSTATS *plot-option*.

Output 38.3.2 Deviation Plot for Region 1

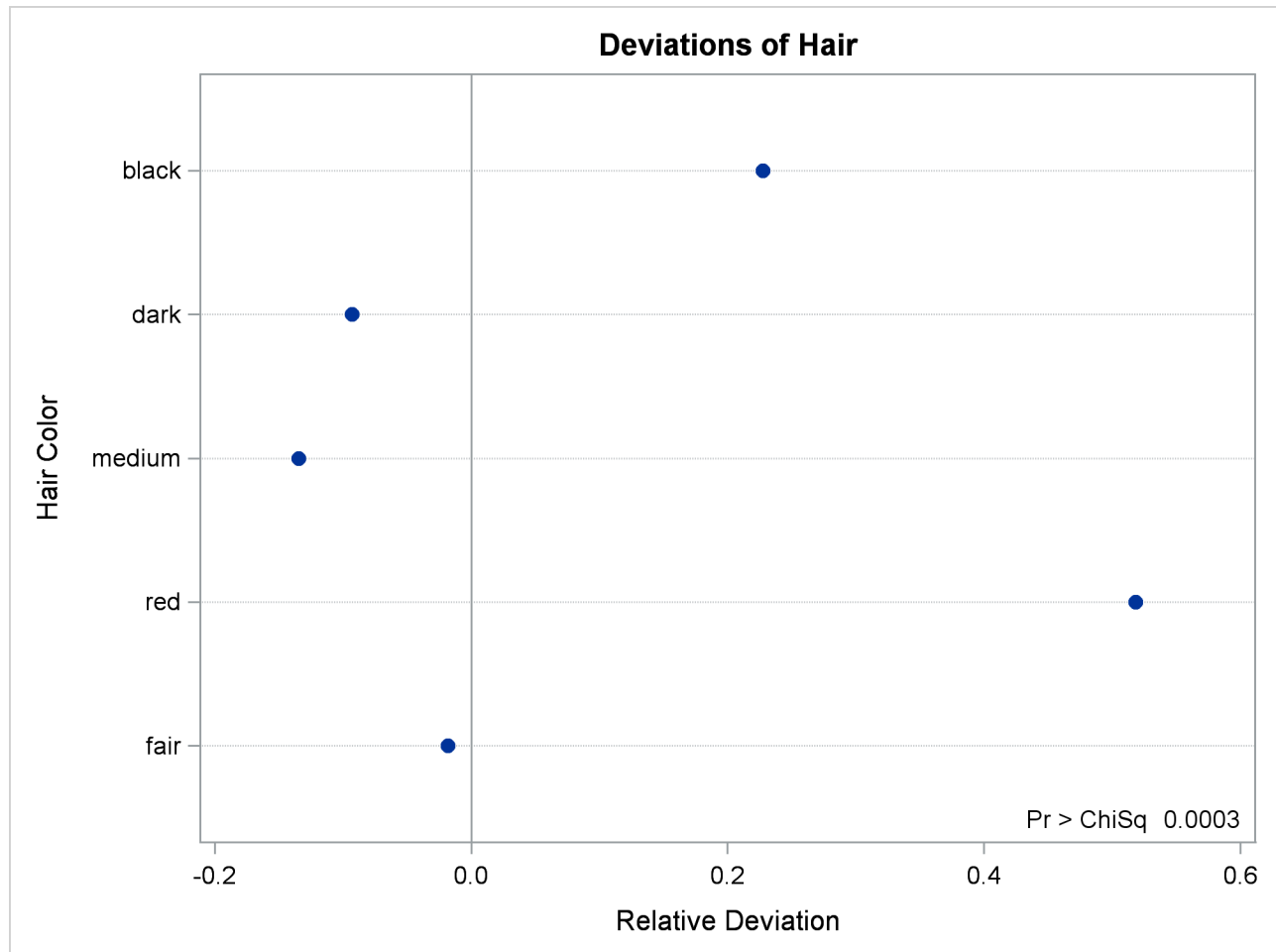


Output 38.3.3 and Output 38.3.4 show the results for Region 2. PROC FREQ computes a chi-square statistic for each region. The chi-square statistic is significant at the 0.05 level for Region 2 ($p=0.0003$) but not for Region 1. This indicates a significant departure from the hypothesized percentages in Region 2.

Output 38.3.3 Frequency Table and Chi-Square Test for Region 2

Hair Color of European Children			
----- Geographic Region=2 -----			
The FREQ Procedure			
Hair Color			
Hair	Frequency	Percent	Test Percent
fair	152	29.46	30.00
red	94	18.22	12.00
medium	134	25.97	30.00
dark	117	22.67	25.00
black	19	3.68	3.00
----- Geographic Region=2 -----			
Chi-Square Test for Specified Proportions			
Chi-Square	21.3824		
DF	4		
Pr > ChiSq	0.0003		

Output 38.3.4 Deviation Plot for Region 2



Example 38.4: Binomial Proportions

In this example, PROC FREQ computes binomial proportions, confidence limits, and tests. The example uses the eye and hair color data from Example 38.1. By default, PROC FREQ computes the binomial proportion as the proportion of observations in the first level of the one-way table. You can designate a different level by using the `LEVEL= binomial-option`.

The following PROC FREQ statements compute the proportion of children with brown eyes (from the data set in Example 38.1) and test the null hypothesis that the population proportion equals 50%. These statements also compute an equivalence for the proportion of children with fair hair.

The first TABLES statement requests a one-way frequency table for the variable Eyes. The BINOMIAL option requests the binomial proportion, confidence limits, and test. PROC FREQ computes the proportion with Eyes = 'brown', which is the first level displayed in the table. The AC, WILSON, and EXACT *binomial-options* request the following confidence limits types: Agresti-Coull, Wilson (score), and exact (Clopper-Pearson). By default, PROC FREQ provides Wald and exact (Clopper-Pearson) confidence limits for the binomial proportion. The BINOMIAL option also produces an asymptotic Wald test that the proportion equals 0.5. You can specify a different test proportion with the `P= binomial-option`. The ALPHA=0.1 option specifies that $\alpha = 10\%$, which produces 90% confidence limits.

The second TABLES statement requests a one-way frequency table for the variable Hair. The BINOMIAL option requests the proportion for the first level, Hair = 'fair'. The EQUIV *binomial-option* requests an equivalence test for the binomial proportion. The P=.28 option specifies 0.28 as the null hypothesis proportion, and the MARGIN=.1 option specifies 0.1 as the equivalence test margin.

```
proc freq data=Color order=freq;
  tables Eyes / binomial(ac wilson exact) alpha=.1;
  tables Hair / binomial(equiv p=.28 margin=.1);
  weight Count;
  title 'Hair and Eye Color of European Children';
run;
```

Output 38.4.1 displays the results for eye color, and Output 38.4.2 displays the results for hair color.

Output 38.4.1 Binomial Proportion for Eye Color

Hair and Eye Color of European Children				
The FREQ Procedure				
Eye Color				
Eyes	Frequency	Percent	Cumulative Frequency	Cumulative Percent
brown	341	44.75	341	44.75
blue	222	29.13	563	73.88
green	199	26.12	762	100.00
Binomial Proportion				
Eyes = brown				
	Proportion	0.4475		
	ASE	0.0180		
Type	90% Confidence Limits			
Wilson	0.4181		0.4773	
Agresti-Coull	0.4181		0.4773	
Clopper-Pearson (Exact)	0.4174		0.4779	
Test of H0: Proportion = 0.5				
	ASE under H0	0.0181		
	Z	-2.8981		
	One-sided Pr < Z	0.0019		
	Two-sided Pr > Z	0.0038		

The frequency table in Output 38.4.1 displays the values of Eyes in order of descending frequency count. PROC FREQ computes the proportion of children in the first level displayed in the frequency table, Eyes = 'brown'. Output 38.4.1 displays the binomial proportion confidence limits and test. The confidence

limits are 90% confidence limits. If you do not specify the ALPHA= option, PROC FREQ computes 95% confidence limits by default. Because the value of Z is less than zero, PROC FREQ displays the left-sided p -value (0.0019). This small p -value supports the alternative hypothesis that the true value of the proportion of children with brown eyes is less than 50%.

Output 38.4.2 displays the equivalence test results produced by the second TABLES statement. The null hypothesis proportion is 0.28 and the equivalence margins are -0.1 and 0.1 , which yield equivalence limits of 0.18 and 0.38. PROC FREQ provides two one-sided tests (TOST) for equivalence. The small p -value indicates rejection of the null hypothesis in favor of the alternative that the proportion is equivalent to the null value.

Output 38.4.2 Binomial Proportion for Hair Color

Hair Color				
Hair	Frequency	Percent	Cumulative Frequency	Cumulative Percent
fair	228	29.92	228	29.92
medium	217	28.48	445	58.40
dark	182	23.88	627	82.28
red	113	14.83	740	97.11
black	22	2.89	762	100.00

Equivalence Analysis				
H0: $P - p_0 \leq \text{Lower Margin}$ or $\geq \text{Upper Margin}$				
Ha: $\text{Lower Margin} < P - p_0 < \text{Upper Margin}$				
$p_0 = 0.28$	Lower Margin = -0.1	Upper Margin = 0.1		
Proportion	ASE (Sample)			
0.2992	0.0166			
Two One-Sided Tests (TOST)				
Test	Z	P-Value		
Lower Margin	7.1865	Pr > Z	<.0001	
Upper Margin	-4.8701	Pr < Z	<.0001	
Overall			<.0001	
Equivalence Limits		90% Confidence Limits		
0.1800	0.3800	0.2719	0.3265	

Example 38.5: Analysis of a 2x2 Contingency Table

This example computes chi-square tests and Fisher's exact test to compare the probability of coronary heart disease for two types of diet. It also estimates the relative risks and computes exact confidence limits for the odds ratio.

The data set `FatComp` contains hypothetical data for a case-control study of high fat diet and the risk of coronary heart disease. The data are recorded as cell counts, where the variable `Count` contains the frequencies for each exposure and response combination. The data set is sorted in descending order by the variables `Exposure` and `Response`, so that the first cell of the 2×2 table contains the frequency of positive exposure and positive response. The `FORMAT` procedure creates formats to identify the type of exposure and response with character values.

```
proc format;
  value ExpFmt 1='High Cholesterol Diet'
              0='Low Cholesterol Diet';
  value RspFmt 1='Yes'
              0='No';
run;

data FatComp;
  input Exposure Response Count;
  label Response='Heart Disease';
  datalines;
0 0 6
0 1 2
1 0 4
1 1 11
;

proc sort data=FatComp;
  by descending Exposure descending Response;
run;
```

In the following `PROC FREQ` statements, `ORDER=DATA` option orders the contingency table values by their order in the input data set. The `TABLES` statement requests a two-way table of `Exposure` by `Response`. The `CHISQ` option produces several chi-square tests, while the `RELRISK` option produces relative risk measures. The `EXACT` statement requests the exact Pearson chi-square test and exact confidence limits for the odds ratio.

```
proc freq data=FatComp order=data;
  format Exposure ExpFmt. Response RspFmt.;
  tables Exposure*Response / chisq relrisk;
  exact pchi or;
  weight Count;
  title 'Case-Control Study of High Fat/Cholesterol Diet';
run;
```

The contingency table in [Output 38.5.1](#) displays the variable values so that the first table cell contains the frequency for the first cell in the data set (the frequency of positive exposure and positive response).

Output 38.5.1 Contingency Table

Case-Control Study of High Fat/Cholesterol Diet			
The FREQ Procedure			
Table of Exposure by Response			
Exposure	Response (Heart Disease)		
	Yes	No	Total
Frequency			
Percent			
Row Pct			
Col Pct			
High Cholesterol Diet	11	4	15
	47.83	17.39	65.22
	73.33	26.67	
	84.62	40.00	
Low Cholesterol Diet	2	6	8
	8.70	26.09	34.78
	25.00	75.00	
	15.38	60.00	
Total	13	10	23
	56.52	43.48	100.00

[Output 38.5.2](#) displays the chi-square statistics. Because the expected counts in some of the table cells are small, PROC FREQ gives a warning that the asymptotic chi-square tests might not be appropriate. In this case, the exact tests are appropriate. The alternative hypothesis for this analysis states that coronary heart disease is more likely to be associated with a high fat diet, so a one-sided test is desired. Fisher's exact right-sided test analyzes whether the probability of heart disease in the high fat group exceeds the probability of heart disease in the low fat group; because this p -value is small, the alternative hypothesis is supported.

The odds ratio, displayed in [Output 38.5.3](#), provides an estimate of the relative risk when an event is rare. This estimate indicates that the odds of heart disease is 8.25 times higher in the high fat diet group; however, the wide confidence limits indicate that this estimate has low precision.

Output 38.5.2 Chi-Square Statistics

Statistic	DF	Value	Prob
Chi-Square	1	4.9597	0.0259
Likelihood Ratio Chi-Square	1	5.0975	0.0240
Continuity Adj. Chi-Square	1	3.1879	0.0742
Mantel-Haenszel Chi-Square	1	4.7441	0.0294
Phi Coefficient		0.4644	
Contingency Coefficient		0.4212	
Cramer's V		0.4644	

WARNING: 50% of the cells have expected counts less than 5.
(Asymptotic) Chi-Square may not be a valid test.

Pearson Chi-Square Test

Chi-Square	4.9597
DF	1
Asymptotic Pr > ChiSq	0.0259
Exact Pr >= ChiSq	0.0393

Fisher's Exact Test

Cell (1,1) Frequency (F)	11
Left-sided Pr <= F	0.9967
Right-sided Pr >= F	0.0367
Table Probability (P)	0.0334
Two-sided Pr <= P	0.0393

Output 38.5.3 Relative Risk

Estimates of the Relative Risk (Row1/Row2)

Type of Study	Value	95% Confidence Limits	
Case-Control (Odds Ratio)	8.2500	1.1535	59.0029
Cohort (Col1 Risk)	2.9333	0.8502	10.1204
Cohort (Col2 Risk)	0.3556	0.1403	0.9009

Odds Ratio (Case-Control Study)

Odds Ratio	8.2500
Asymptotic Conf Limits	
95% Lower Conf Limit	1.1535
95% Upper Conf Limit	59.0029
Exact Conf Limits	
95% Lower Conf Limit	0.8677
95% Upper Conf Limit	105.5488

Example 38.6: Output Data Set of Chi-Square Statistics

This example uses the Color data from Example 38.1 to output the Pearson chi-square and the likelihood ratio chi-square statistics to a SAS data set. The following PROC FREQ statements create a two-way table of eye color versus hair color.

```
proc freq data=Color order=data;
  tables Eyes*Hair / expected cellchi2 norow nocol chisq;
  output out=ChiSqData n nmiss pchi lrchi;
  weight Count;
  title 'Chi-Square Tests for 3 by 5 Table of Eye and Hair Color';
run;

proc print data=ChiSqData noobs;
  title1 'Chi-Square Statistics for Eye and Hair Color';
  title2 'Output Data Set from the FREQ Procedure';
run;
```

The EXPECTED option displays expected cell frequencies in the crosstabulation table, and the CELLCHI2 option displays the cell contribution to the overall chi-square. The NOROW and NOCOL options suppress the display of row and column percents in the crosstabulation table. The CHISQ option produces chi-square tests.

The OUTPUT statement creates the ChiSqData output data set and specifies the statistics to include. The N option requests the number of nonmissing observations, the NMISS option stores the number of missing observations, and the PCHI and LRCHI options request Pearson and likelihood ratio chi-square statistics, respectively, together with their degrees of freedom and p -values.

The preceding statements produce Output 38.6.1 and Output 38.6.2. The contingency table in Output 38.6.1 displays eye and hair color in the order in which they appear in the Color data set. The Pearson chi-square statistic in Output 38.6.2 provides evidence of an association between eye and hair color ($p=0.0073$). The cell chi-square values show that most of the association is due to more green-eyed children with fair or red hair and fewer with dark or black hair. The opposite occurs with the brown-eyed children.

Output 38.6.3 displays the output data set created by the OUTPUT statement. It includes one observation that contains the sample size, the number of missing values, and the chi-square statistics and corresponding degrees of freedom and p -values as in Output 38.6.2.

Output 38.6.1 Contingency Table

Chi-Square Tests for 3 by 5 Table of Eye and Hair Color

The FREQ Procedure

Table of Eyes by Hair

Eyes (Eye Color)	Hair (Hair Color)					Total
Frequency	fair	red	medium	dark	black	
Expected						
Cell Chi-Square						
Percent						
blue	69	28	68	51	6	222
	66.425	32.921	63.22	53.024	6.4094	
	0.0998	0.7357	0.3613	0.0772	0.0262	
	9.06	3.67	8.92	6.69	0.79	29.13
green	69	38	55	37	0	199
	59.543	29.51	56.671	47.53	5.7454	
	1.5019	2.4422	0.0492	2.3329	5.7454	
	9.06	4.99	7.22	4.86	0.00	26.12
brown	90	47	94	94	16	341
	102.03	50.568	97.109	81.446	9.8451	
	1.4187	0.2518	0.0995	1.935	3.8478	
	11.81	6.17	12.34	12.34	2.10	44.75
Total	228	113	217	182	22	762
	29.92	14.83	28.48	23.88	2.89	100.00

Output 38.6.2 Chi-Square Statistics

Statistic	DF	Value	Prob
Chi-Square	8	20.9248	0.0073
Likelihood Ratio Chi-Square	8	25.9733	0.0011
Mantel-Haenszel Chi-Square	1	3.7838	0.0518
Phi Coefficient		0.1657	
Contingency Coefficient		0.1635	
Cramer's V		0.1172	

Output 38.6.3 Output Data Set

Chi-Square Statistics for Eye and Hair Color

Output Data Set from the FREQ Procedure

N	NMISS	_PCHI_	DF_PCHI	P_PCHI	_LRCHI_	DF_LRCHI	P_LRCHI
762	0	20.9248	8	.007349898	25.9733	8	.001061424

Example 38.7: Cochran-Mantel-Haenszel Statistics

The data set `Migraine` contains hypothetical data for a clinical trial of migraine treatment. Subjects of both genders receive either a new drug therapy or a placebo. Their response to treatment is coded as ‘Better’ or ‘Same’. The data are recorded as cell counts, and the number of subjects for each treatment and response combination is recorded in the variable `Count`.

```
data Migraine;
  input Gender $ Treatment $ Response $ Count @@;
  datalines;
female Active Better 16   female Active Same 11
female Placebo Better 5   female Placebo Same 20
male Active Better 12    male Active Same 16
male Placebo Better 7    male Placebo Same 19
;
```

The following PROC FREQ statements create a multiway table stratified by Gender, where Treatment forms the rows and Response forms the columns. The RELRISK option in the TABLES statement requests the odds ratio and relative risks for the two-way tables of Treatment by Response. The PLOTS= option requests a relative risk plot, which shows the relative risk and its confidence limits for each level of Gender and overall. The CMH option requests Cochran-Mantel-Haenszel statistics for the multiway table. For this stratified 2×2 table, the CMH option also produces estimates of the common relative risk and the Breslow-Day test for homogeneity of the odds ratios. The NOPRINT option suppresses the display of the crosstabulation tables.

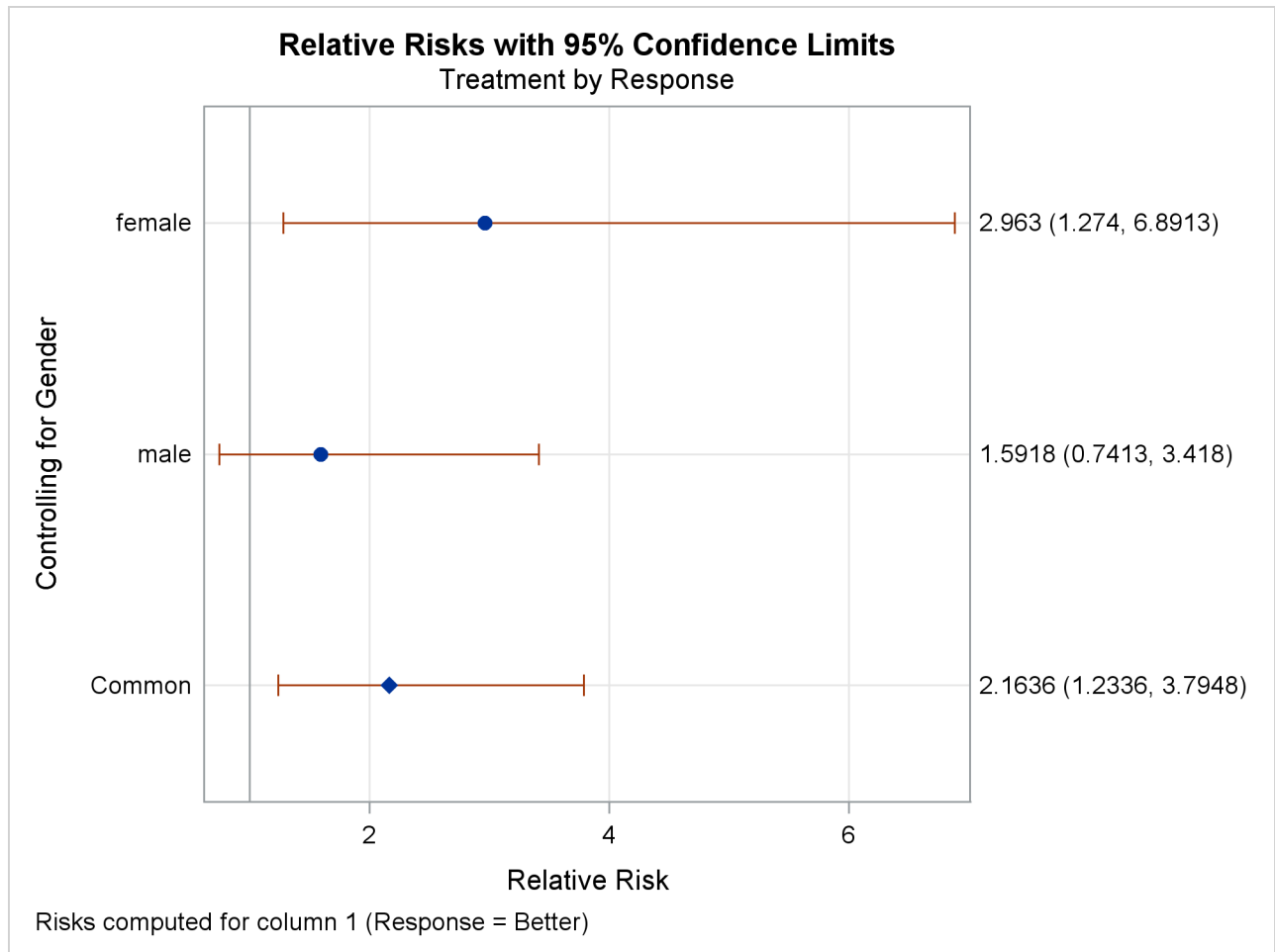
```
ods graphics on;
proc freq data=Migraine;
  tables Gender*Treatment*Response /
         relrisk plots(only)=relriskplot(stats) cmh noprint;
  weight Count;
  title 'Clinical Trial for Treatment of Migraine Headaches';
run;
ods graphics off;
```

Output 38.7.1 through Output 38.7.4 show the results of the analysis. The relative risk plot (Output 38.7.1) displays the relative risks and confidence limits for the two levels of Gender and for the overall (common) relative risk. Output 38.7.2 displays the CMH statistics. For a stratified 2×2 table, the three CMH statistics test the same hypothesis. The significant p -value (0.004) indicates that the association between treatment and response remains strong after adjusting for gender.

The CMH option also produces a table of overall relative risks, as shown in Output 38.7.3. Because this is a prospective study, the relative risk estimate assesses the effectiveness of the new drug; the “Cohort (Coll Risk)” values are the appropriate estimates for the first column (the risk of improvement). The probability of migraine improvement with the new drug is just over two times the probability of improvement with the placebo.

The large p -value for the Breslow-Day test (0.2218) in Output 38.7.4 indicates no significant gender difference in the odds ratios.

Output 38.7.1 Relative Risk Plot



Output 38.7.2 Cochran-Mantel-Haenszel Statistics

Cochran-Mantel-Haenszel Statistics (Based on Table Scores)				
Statistic	Alternative Hypothesis	DF	Value	Prob
1	Nonzero Correlation	1	8.3052	0.0040
2	Row Mean Scores Differ	1	8.3052	0.0040
3	General Association	1	8.3052	0.0040

Output 38.7.3 CMH Option: Common Relative Risks

Estimates of the Common Relative Risk (Row1/Row2)				
Type of Study	Method	Value	95% Confidence Limits	
Case-Control (Odds Ratio)	Mantel-Haenszel	3.3132	1.4456	7.5934
	Logit	3.2941	1.4182	7.6515
Cohort (Col1 Risk)	Mantel-Haenszel	2.1636	1.2336	3.7948
	Logit	2.1059	1.1951	3.7108
Cohort (Col2 Risk)	Mantel-Haenszel	0.6420	0.4705	0.8761
	Logit	0.6613	0.4852	0.9013

Output 38.7.4 CMH Option: Breslow-Day Test

Breslow-Day Test for Homogeneity of the Odds Ratios	
Chi-Square	1.4929
DF	1
Pr > ChiSq	0.2218

Example 38.8: Cochran-Armitage Trend Test

The data set Pain contains hypothetical data for a clinical trial of a drug therapy to control pain. The clinical trial investigates whether adverse responses increase with larger drug doses. Subjects receive either a placebo or one of four drug doses. An adverse response is recorded as Adverse='Yes'; otherwise, it is recorded as Adverse='No'. The number of subjects for each drug dose and response combination is contained in the variable Count.

```
data pain;
  input Dose Adverse $ Count @@;
  datalines;
0 No 26  0 Yes  6
1 No 26  1 Yes  7
2 No 23  2 Yes  9
3 No 18  3 Yes 14
4 No  9  4 Yes 23
;
```

The following PROC FREQ statements provide a trend analysis. The TABLES statement requests a table of Adverse by Dose. The MEASURES option produces measures of association, and the CL option produces confidence limits for these measures. The TREND option tests for a trend across the ordinal values of the variable Dose with the Cochran-Armitage test. The PLOTS= option requests a mosaic plot of Adverse by Dose.

The EXACT statement produces exact p -values for this test, and the MAXTIME= option terminates the exact computations if they do not complete within 60 seconds. The TEST statement computes an asymptotic test for Somers' $D(R|C)$.

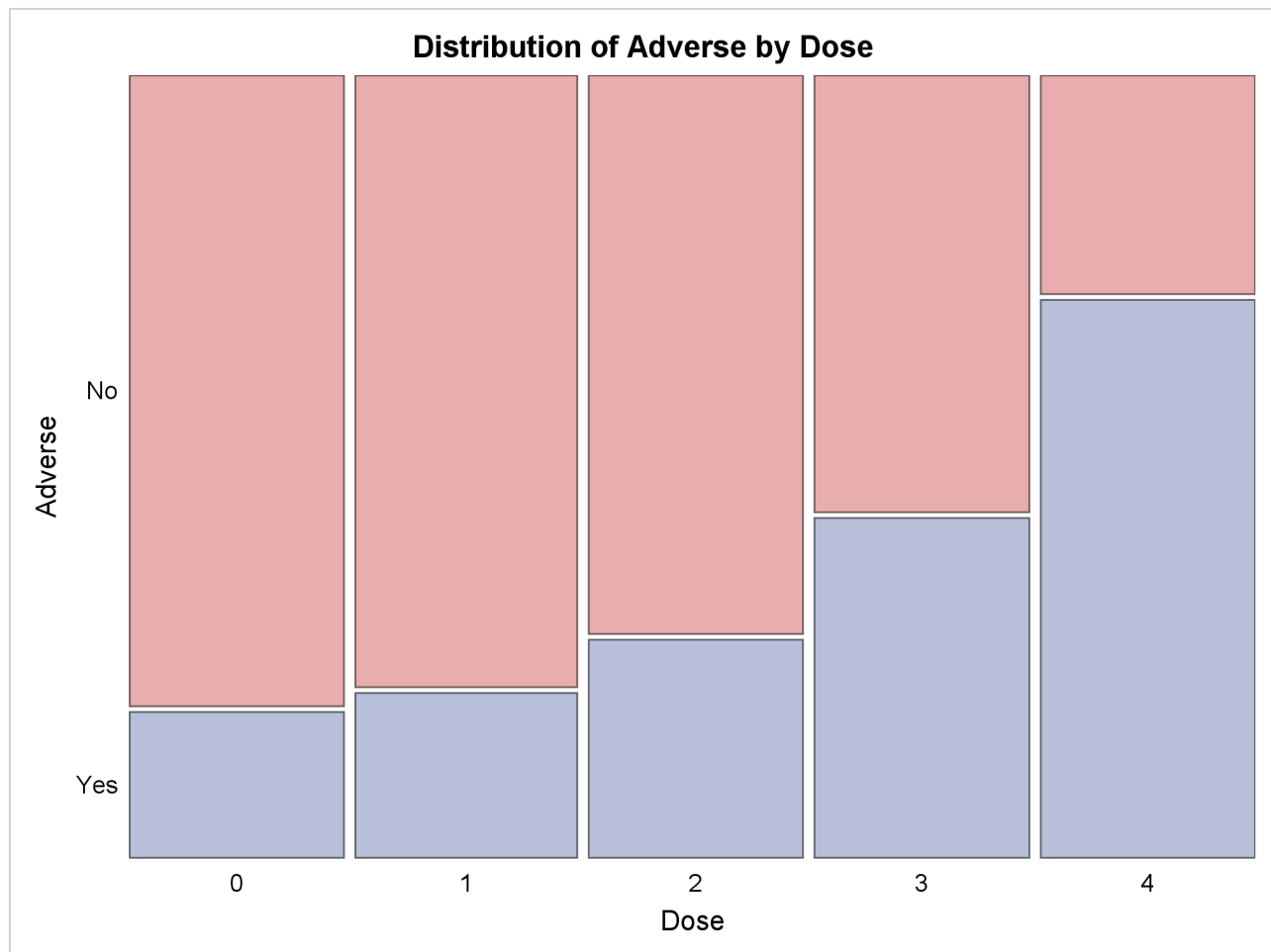
```
ods graphics on;
proc freq data=Pain;
  tables Adverse*Dose / trend measures cl
    plots=mosaicplot;
  test smdrc;
  exact trend / maxtime=60;
  weight Count;
  title 'Clinical Trial for Treatment of Pain';
run;
ods graphics off;
```

Output 38.8.1 through Output 38.8.4 display the results of the analysis. The “Col Pct” values in Output 38.8.1 show the expected increasing trend in the proportion of adverse effects with the increasing dosage (from 18.75% to 71.88%). The corresponding mosaic plot (Output 38.8.2) also shows this increasing trend.

Output 38.8.1 Contingency Table

Clinical Trial for Treatment of Pain						
The FREQ Procedure						
Table of Adverse by Dose						
Adverse	Dose					
Frequency						
Percent						
Row Pct						
Col Pct	0	1	2	3	4	Total
No	26	26	23	18	9	102
	16.15	16.15	14.29	11.18	5.59	63.35
	25.49	25.49	22.55	17.65	8.82	
	81.25	78.79	71.88	56.25	28.13	
Yes	6	7	9	14	23	59
	3.73	4.35	5.59	8.70	14.29	36.65
	10.17	11.86	15.25	23.73	38.98	
	18.75	21.21	28.13	43.75	71.88	
Total	32	33	32	32	32	161
	19.88	20.50	19.88	19.88	19.88	100.00

Output 38.8.2 Mosaic Plot



Output 38.8.3 displays the measures of association produced by the MEASURES option. Somers' $D(R|C)$ measures the association treating the row variable (Adverse) as the response and the column variable (Dose) as a predictor. Because the asymptotic 95% confidence limits do not contain zero, this indicates a strong positive association. Similarly, the Pearson and Spearman correlation coefficients show evidence of a strong positive association, as hypothesized.

The Cochran-Armitage test (Output 38.8.4) supports the trend hypothesis. The small left-sided p -values for the Cochran-Armitage test indicate that the probability of the Row 1 level (Adverse='No') decreases as Dose increases or, equivalently, that the probability of the Row 2 level (Adverse='Yes') increases as Dose increases. The two-sided p -value tests against either an increasing or decreasing alternative. This is an appropriate hypothesis when you want to determine whether the drug has progressive effects on the probability of adverse effects but the direction is unknown.

Output 38.8.3 Measures of Association

Statistic	Value	ASE	95% Confidence Limits	
Gamma	0.5313	0.0935	0.3480	0.7146
Kendall's Tau-b	0.3373	0.0642	0.2114	0.4631
Stuart's Tau-c	0.4111	0.0798	0.2547	0.5675
Somers' D C R	0.4427	0.0837	0.2786	0.6068
Somers' D R C	0.2569	0.0499	0.1592	0.3547
Pearson Correlation	0.3776	0.0714	0.2378	0.5175
Spearman Correlation	0.3771	0.0718	0.2363	0.5178
Lambda Asymmetric C R	0.1250	0.0662	0.0000	0.2547
Lambda Asymmetric R C	0.2373	0.0837	0.0732	0.4014
Lambda Symmetric	0.1604	0.0621	0.0388	0.2821
Uncertainty Coefficient C R	0.0515	0.0191	0.0140	0.0890
Uncertainty Coefficient R C	0.1261	0.0467	0.0346	0.2175
Uncertainty Coefficient Symmetric	0.0731	0.0271	0.0199	0.1262

Somers' D R C	
Somers' D R C	0.2569
ASE	0.0499
95% Lower Conf Limit	0.1592
95% Upper Conf Limit	0.3547

Test of H0: Somers' D R|C = 0

ASE under H0	0.0499
Z	5.1511
One-sided Pr > Z	<.0001
Two-sided Pr > Z	<.0001

Output 38.8.4 Trend Test

Cochran-Armitage Trend Test	
Statistic (Z)	-4.7918
Asymptotic Test	
One-sided Pr < Z	<.0001
Two-sided Pr > Z	<.0001
Exact Test	
One-sided Pr <= Z	7.237E-07
Two-sided Pr >= Z	1.324E-06

Example 38.9: Friedman's Chi-Square Test

Friedman's test is a nonparametric test for treatment differences in a randomized complete block design. Each block of the design might be a subject or a homogeneous group of subjects. If blocks are groups of subjects, the number of subjects in each block must equal the number of treatments. Treatments are randomly assigned to subjects within each block. If there is one subject per block, then the subjects are repeatedly measured once under each treatment. The order of treatments is randomized for each subject.

In this setting, Friedman's test is identical to the ANOVA (row means scores) CMH statistic when the analysis uses rank scores (SCORES=RANK). The three-way table uses subject (or subject group) as the stratifying variable, treatment as the row variable, and response as the column variable. PROC FREQ handles ties by assigning midranks to tied response values. If there are multiple subjects per treatment in each block, the ANOVA CMH statistic is a generalization of Friedman's test.

The data set Hypnosis contains data from a study investigating whether hypnosis has the same effect on skin potential (measured in millivolts) for four emotions (Lehmann 2006, p. 264). Eight subjects are asked to display fear, joy, sadness, and calmness under hypnosis. The data are recorded as one observation per subject for each emotion.

```
data Hypnosis;
  length Emotion $ 10;
  input Subject Emotion $ SkinResponse @@;
  datalines;
1 fear 23.1 1 joy 22.7 1 sadness 22.5 1 calmness 22.6
2 fear 57.6 2 joy 53.2 2 sadness 53.7 2 calmness 53.1
3 fear 10.5 3 joy 9.7 3 sadness 10.8 3 calmness 8.3
4 fear 23.6 4 joy 19.6 4 sadness 21.1 4 calmness 21.6
5 fear 11.9 5 joy 13.8 5 sadness 13.7 5 calmness 13.3
6 fear 54.6 6 joy 47.1 6 sadness 39.2 6 calmness 37.0
7 fear 21.0 7 joy 13.6 7 sadness 13.7 7 calmness 14.8
8 fear 20.3 8 joy 23.6 8 sadness 16.3 8 calmness 14.8
;
```

In the following PROC FREQ statements, the TABLES statement creates a three-way table stratified by Subject and a two-way table; the variables Emotion and SkinResponse form the rows and columns of each table. The CMH2 option produces the first two Cochran-Mantel-Haenszel statistics, the option SCORES=RANK specifies that rank scores are used to compute these statistics, and the NOPRINT option suppresses the contingency tables. These statements produce [Output 38.9.1](#) and [Output 38.9.2](#).

```
proc freq data=Hypnosis;
  tables Subject*Emotion*SkinResponse /
         cmh2 scores=rank noprint;
run;

proc freq data=Hypnosis;
  tables Emotion*SkinResponse /
         cmh2 scores=rank noprint;
run;
```

Because the CMH statistics in [Output 38.9.1](#) are based on rank scores, the Row Mean Scores Differ statistic is identical to Friedman's chi-square ($Q = 6.45$). The p -value of 0.0917 indicates that differences in skin potential response for different emotions are significant at the 10% level but not at the 5% level.

When you do not stratify by subject, the Row Mean Scores Differ CMH statistic is identical to a Kruskal-Wallis test and is not significant ($p = 0.9038$ in [Output 38.9.2](#)). Thus, adjusting for subject is critical to reducing the background variation due to subject differences.

Output 38.9.1 CMH Statistics: Stratifying by Subject

```

Clinical Trial for Treatment of Pain

The FREQ Procedure

Summary Statistics for Emotion by SkinResponse
Controlling for Subject

Cochran-Mantel-Haenszel Statistics (Based on Rank Scores)

```

Statistic	Alternative Hypothesis	DF	Value	Prob
1	Nonzero Correlation	1	0.2400	0.6242
2	Row Mean Scores Differ	3	6.4500	0.0917

Output 38.9.2 CMH Statistics: No Stratification

```

Clinical Trial for Treatment of Pain

The FREQ Procedure

Summary Statistics for Emotion by SkinResponse

Cochran-Mantel-Haenszel Statistics (Based on Rank Scores)

```

Statistic	Alternative Hypothesis	DF	Value	Prob
1	Nonzero Correlation	1	0.0001	0.9933
2	Row Mean Scores Differ	3	0.5678	0.9038

Example 38.10: Cochran's Q Test

When a binary response is measured several times or under different conditions, Cochran's Q tests that the marginal probability of a positive response is unchanged across the times or conditions. When there are more than two response categories, you can use the CATMOD procedure to fit a repeated-measures model.

The data set `Drugs` contains data for a study of three drugs to treat a chronic disease (Agresti 2002). Forty-six subjects receive drugs A, B, and C. The response to each drug is either favorable ('F') or unfavorable ('U').

```

proc format;
  value $ResponseFmt 'F'='Favorable'
                    'U'='Unfavorable';
run;

```

```

data drugs;
  input Drug_A $ Drug_B $ Drug_C $ Count @@;
  datalines;
F F F 6   U F F 2
F F U 16  U F U 4
F U F 2   U U F 6
F U U 4   U U U 6
;

```

The following statements create one-way frequency tables of the responses to each drug. The AGREE option produces Cochran's Q and other measures of agreement for the three-way table. These statements produce [Output 38.10.1](#) through [Output 38.10.5](#).

```

proc freq data=Drugs;
  tables Drug_A Drug_B Drug_C / nocum;
  tables Drug_A*Drug_B*Drug_C / agree noprint;
  format Drug_A Drug_B Drug_C $ResponseFmt.;
  weight Count;
  title 'Study of Three Drug Treatments for a Chronic Disease';
run;

```

The one-way frequency tables in [Output 38.10.1](#) provide the marginal response for each drug. For drugs A and B, 61% of the subjects reported a favorable response while 35% of the subjects reported a favorable response to drug C. [Output 38.10.2](#) and [Output 38.10.3](#) display measures of agreement for the 'Favorable' and 'Unfavorable' levels of drug A, respectively. McNemar's test shows a strong discordance between drugs B and C when the response to drug A is favorable.

Output 38.10.1 One-Way Frequency Tables

Study of Three Drug Treatments for a Chronic Disease		
The FREQ Procedure		
Drug_A	Frequency	Percent

Favorable	28	60.87
Unfavorable	18	39.13
Drug_B	Frequency	Percent

Favorable	28	60.87
Unfavorable	18	39.13
Drug_C	Frequency	Percent

Favorable	16	34.78
Unfavorable	30	65.22

Output 38.10.2 Measures of Agreement for Drug A Favorable

McNemar's Test	
Statistic (S)	10.8889
DF	1
Pr > S	0.0010

Simple Kappa Coefficient	
Kappa	-0.0328
ASE	0.1167
95% Lower Conf Limit	-0.2615
95% Upper Conf Limit	0.1960

Output 38.10.3 Measures of Agreement for Drug A Unfavorable

McNemar's Test	
Statistic (S)	0.4000
DF	1
Pr > S	0.5271

Simple Kappa Coefficient	
Kappa	-0.1538
ASE	0.2230
95% Lower Conf Limit	-0.5909
95% Upper Conf Limit	0.2832

Output 38.10.4 displays the overall kappa coefficient. The small negative value of kappa indicates no agreement between drug B response and drug C response.

Output 38.10.4 Overall Measures of Agreement

Overall Kappa Coefficient	
Kappa	-0.0588
ASE	0.1034
95% Lower Conf Limit	-0.2615
95% Upper Conf Limit	0.1439

Test for Equal Kappa Coefficients	
Chi-Square	0.2314
DF	1
Pr > ChiSq	0.6305

Cochran's Q is statistically significant ($p=0.0145$ in **Output 38.10.5**), which leads to rejection of the hypothesis that the probability of favorable response is the same for the three drugs.

Output 38.10.5 Cochran's Q Test

Cochran's Q, for Drug_A by Drug_B by Drug_C	

Statistic (Q)	8.4706
DF	2
Pr > Q	0.0145

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Chapter 39

The GAM Procedure

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Overview: GAM Procedure

The GAM procedure fits generalized additive models as defined by Hastie and Tibshirani (1990). This procedure provides powerful tools for nonparametric regression and smoothing.

Nonparametric regression relaxes the usual assumption of linearity and enables you to uncover relationships between the independent variables and the dependent variable that might otherwise be missed. SAS provides many procedures for nonparametric regression, such as the LOESS procedure for local regression and the TPSPLINE procedure for thin-plate smoothing splines. The generalized additive models fit by the GAM procedure combine the following:

- an additivity assumption (Stone 1985) that enables relatively many nonparametric relationships to be explored simultaneously
- the distributional flexibility of generalized linear models (Nelder and Wedderburn 1972)

Thus, you can use the GAM procedure when you have multiple independent variables whose effect you want to model nonparametrically, or when the dependent variable is not normally distributed. See the section “[Nonparametric Regression](#)” on page 2672 for more details on the form of generalized additive models.

The GAM procedure does the following:

- provides nonparametric estimates for additive models
- supports the use of multidimensional data
- supports multiple SCORE statements
- fits both generalized semiparametric additive models and generalized additive models
- enables you to choose a particular model by specifying the model degrees of freedom or smoothing parameter
- produces graphs with ODS Graphics

Getting Started: GAM Procedure

The following example illustrates the use of the GAM procedure to explore in a nonparametric way how two factors affect a response. The data come from a study of the factors affecting patterns of insulin-dependent diabetes mellitus in children (Sochett et al. 1987). The objective is to investigate the dependence of the level of serum C-peptide on various other factors in order to understand the patterns of residual insulin secretion. The response measurement is the logarithm of C-peptide concentration (pmol/ml) at diagnosis, and the predictor measurements are age and base deficit (a measure of acidity).

```

title 'Patterns of Diabetes';
data diabetes;
  input Age BaseDeficit CPeptide @@;
  logCP = log(CPeptide);
  datalines;
5.2   -8.1  4.8   8.8  -16.1  4.1  10.5  -0.9  5.2
10.6  -7.8  5.5  10.4  -29.0  5.0   1.8  -19.2  3.4
12.7 -18.9  3.4  15.6  -10.6  4.9   5.8  -2.8  5.6
1.9  -25.0  3.7   2.2   -3.1  3.9   4.8  -7.8  4.5
7.9  -13.9  4.8   5.2   -4.5  4.9   0.9 -11.6  3.0
11.8  -2.1  4.6   7.9   -2.0  4.8  11.5  -9.0  5.5
10.6 -11.2  4.5   8.5   -0.2  5.3  11.1  -6.1  4.7
12.8  -1.0  6.6  11.3   -3.6  5.1   1.0  -8.2  3.9
14.5  -0.5  5.7  11.9   -2.0  5.1   8.1  -1.6  5.2
13.8 -11.9  3.7  15.5   -0.7  4.9   9.8  -1.2  4.8
11.0 -14.3  4.4  12.4   -0.8  5.2  11.1 -16.8  5.1
5.1   -5.1  4.6   4.8   -9.5  3.9   4.2 -17.0  5.1
6.9   -3.3  5.1  13.2   -0.7  6.0   9.9  -3.3  4.9
12.5 -13.6  4.1  13.2   -1.9  4.6   8.9 -10.0  4.9
10.8 -13.5  5.1
;

```

The following statements perform the desired analysis. The PROC GAM statement invokes the procedure and specifies the diabetes data set as input. The MODEL statement specifies logCP as the response variable and names Age and BaseDeficit as independent variables with univariate smoothing splines and the default of four degrees of freedom.

```

ods graphics on;
proc gam data=diabetes;
  model logCP = spline(Age) spline(BaseDeficit);
run;

```

The results are shown in Figure 39.1 and Figure 39.2.

Figure 39.1 Summary Statistics

Patterns of Diabetes	
The GAM Procedure	
Dependent Variable: logCP	
Smoothing Model Component(s): spline(Age) spline(BaseDeficit)	
Summary of Input Data Set	
Number of Observations	43
Number of Missing Observations	0
Distribution	Gaussian
Link Function	Identity

Figure 39.1 continued

Iteration Summary and Fit Statistics	
Final Number of Backfitting Iterations	5
Final Backfitting Criterion	5.542745E-10
The Deviance of the Final Estimate	0.4180791724

Figure 39.1 shows two tables. The first table summarizes the input data set and the distributional family used for the model; the second table summarizes the convergence criterion for backfitting.

Figure 39.2 Analysis of Model

Regression Model Analysis Parameter Estimates				
Parameter	Parameter Estimate	Standard Error	t Value	Pr > t
Intercept	1.48141	0.05120	28.93	<.0001
Linear (Age)	0.01437	0.00437	3.28	0.0024
Linear (BaseDeficit)	0.00807	0.00247	3.27	0.0025

Smoothing Model Analysis Fit Summary for Smoothing Components				
Component	Smoothing Parameter	DF	GCV	Num Unique Obs
Spline (Age)	0.995582	3.000000	0.011675	37
Spline (BaseDeficit)	0.995299	3.000000	0.012437	39

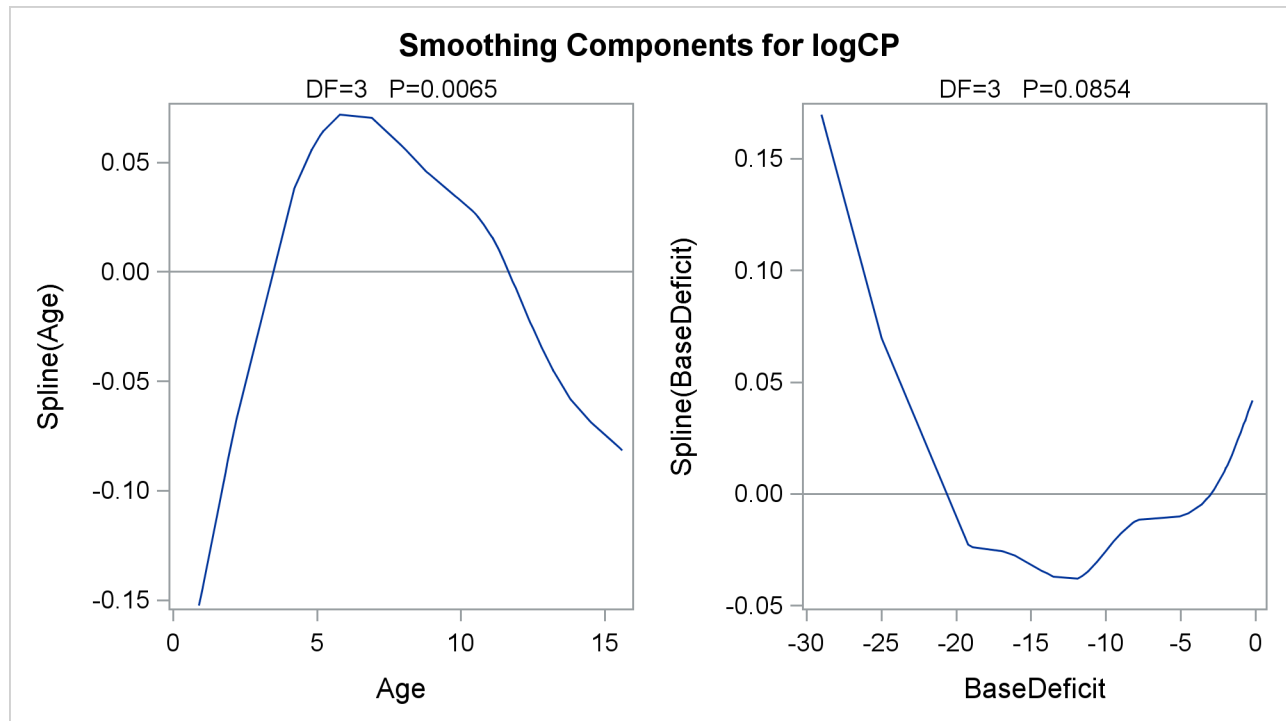
Smoothing Model Analysis Analysis of Deviance				
Source	DF	Sum of Squares	Chi-Square	Pr > ChiSq
Spline (Age)	3.00000	0.150761	12.2605	0.0065
Spline (BaseDeficit)	3.00000	0.081273	6.6095	0.0854

Figure 39.2 displays summary statistics for the model. It consists of three tables. The first is the “Parameter Estimates” table for the parametric part of the model. It indicates that the linear trends for both Age and BaseDeficit are highly significant. The second table is the summary of smoothing components of the nonparametric part of the model. This table presents the smoothing parameter and degrees of freedom (DF) for each component. By default, each smoothing component has approximately 4 DF. For univariate spline components, one DF is taken up by the (parametric) linear part of the model, so the remaining approximate DF is 3. Finally, the third table is the “Analysis of Deviance” table for the nonparametric component of the model.

With ODS Graphics enabled, PROC GAM produces by default a panel of plots of partial prediction curves of smoothing components. In these plots, the partial prediction for a predictor such as Age is its nonparametric contribution to the model, $s(\text{Age})$. For general information about ODS Graphics, see Chapter 21, “Statistical Graphics Using ODS.” For specific information about the graphics available in the GAM procedure, see the section “ODS Graphics” on page 2686.

Plots for both predictors (Figure 39.3) show a strong quadratic pattern, with a possible indication of higher-order behavior. Further investigation is required to determine whether these patterns are real or not.

Figure 39.3 Partial Predictions for Each Predictor



Syntax: GAM Procedure

The following statements are available in the GAM procedure:

```
PROC GAM < options > ;
  CLASS variable < (options) > < variable < (options) > ... < / options > ;
  MODEL dependent < (options) > = < PARAM(effects) > < smoothing-effects > < / options > ;
  SCORE DATA= SAS-data-set OUT= SAS-data-set ;
  OUTPUT OUT= SAS-data-set < keyword< =prefix > ... keyword< =prefix > > ;
  BY variables ;
  FREQ variable ;
```


The syntax of the GAM procedure is similar to that of other regression procedures in the SAS System. The PROC GAM and MODEL statements are required. The CLASS statement, if specified, must precede the MODEL statement. The CLASS and SCORE statements can appear multiple times; all other statements must appear only once.

The syntax for PROC GAM is described in the following sections in alphabetical order after the description of the PROC GAM statement.

PROC GAM Statement

PROC GAM < options > ;

The PROC GAM statement invokes the procedure. Table 39.1 summarizes the options available in the PROC GAM statement.

Table 39.1 PROC GAM Statement Options

Option	Description
DATA=	Specifies the input SAS data set
DESCENDING	Reverses the sort order of all CLASS variables
ORDER=	Specifies the sort order for CLASS variables
PLOTS	Controls plots produced through ODS Graphics

You can specify the following options.

DATA=SAS-data-set

specifies the SAS data set to be read by PROC GAM. The default value is the most recently created data set.

DESCENDING

DESC

reverses the sort order of all classification variables (specified in the CLASS statement). If both the DESCENDING and ORDER= options are specified, PROC GAM orders the categories according to the ORDER= option and then reverses that order. This option has the same effect as the classification variable option DESCENDING in the CLASS statement and the response variable option DESCENDING in the MODEL statement.

ORDER=DATA | FORMATTED | FREQ | INTERNAL

specifies the sort order for the levels of all classification variables (specified in the CLASS statement). This ordering determines which parameters in the model correspond to each level in the data. Note that the ORDER= option in the CLASS statement and the ORDER= response variable option in the MODEL statement override the ORDER= option in the PROC GAM statement.

PLOTS < (global-plot-options) > < = plot-request < (options) > >

PLOTS < (global-plot-options) > < =(plot-request < (options) > < . . . plot-request < (options) > > >

controls the plots produced through ODS Graphics. When you specify only one plot-request, you can omit the parentheses around the plot-request. Here are some examples:

```
plots=all

plots=components (commonaxes)

plots (unpack)=components (commonaxes clm)
```

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;

proc gam data=test plots (unpack)=components (commonaxes clm);
  model z=spline(x) spline(y);
run;

ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS](#).”

With ODS Graphics enabled, PROC GAM produces by default a panel of plots of partial prediction curves of smoothing components.

Global Plot Options

The *global-plot-options* apply to all plots generated by the GAM procedure, unless altered by a *specific-plot-option*.

UNPACK

separately displays the smoothing component plots that are by default presented in panels. Use this option if you want to access individual smoothing component plots within the panel.

Specific Plot Options

The following listing describes the specific plots and their options.

ALL

requests that all plots be produced.

NONE

suppresses all plots.

COMPONENTS | COMPONENT <(components-options)>

displays a panel of smoothing component plots. The following *components-options* are available:

ADDITIVE

produces the additive component plots for spline and loess effects. The additive component plots combine the linear trend and the nonparametric prediction for each spline or loess effect.

CLM

includes confidence limits in the smoothing component plots. By default, 95% confidence limits are produced, but you can change the significance level by specifying the ALPHA= option in the MODEL statement. Note that producing these limits can be computationally intensive for large data sets.

COMMONAXES

specifies that smoothing component plots use a common vertical axis. This enables you to visually judge relative effect size.

UNPACK

displays the smoothing components individually.

BY Statement

BY *variables* ;

You can specify a BY statement with PROC GAM to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the GAM procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

CLASS Statement

CLASS *variable* <(options)> <*variable* <(options)> ... > </options> ;

The CLASS statement names the classification variables to be used in the analysis. The CLASS statement must precede the MODEL statement. You can specify various *options* for each variable by enclosing them in parentheses after the variable name. You can also specify global *options* for the CLASS statement by placing them after a slash (/). Global *options* are applied to all the variables specified in the CLASS statement. If you specify more than one CLASS statement, the global *options* specified on any one CLASS statement apply to all CLASS statements. However, individual CLASS variable *options* override the global *options*.

DESCENDING**DESC**

reverses the sort order of the classification variable. If both the **DESCENDING** and **ORDER=** options are specified, PROC GAM orders the categories according to the **ORDER=** option and then reverses that order.

ORDER=DATA | FORMATTED | FREQ | INTERNAL

specifies the sort order for the categories of categorical variables. This ordering determines which parameters in the model correspond to each level in the data. When the default **ORDER=FORMATTED** is in effect for numeric variables for which you have supplied no explicit format, the levels are ordered by their internal values. The following table shows how PROC GAM interprets values of the **ORDER=** option.

Value of ORDER=	Levels Sorted By
DATA	Order of appearance in the input data set
FORMATTED	External formatted value, except for numeric variables with no explicit format, which are sorted by their unformatted (internal) value
FREQ	Descending frequency count; levels with the most observations come first in the order
INTERNAL	Unformatted value

By default, **ORDER=FORMATTED**. For **FORMATTED** and **INTERNAL**, the sort order is machine-dependent. For more information on sort order, see the chapter on the **SORT** procedure in the *Base SAS Procedures Guide* and the discussion of **BY**-group processing in *SAS Language Reference: Concepts*.

TRUNCATE<=n>

specifies the length n of **CLASS** variable values to use in determining **CLASS** variable levels. If you specify **TRUNCATE** without the length n , the first 16 characters of the formatted values are used. When formatted values are longer than 16 characters, you can use this option to revert to the levels as determined in releases previous to SAS 9. The default is to use the full formatted length of the **CLASS** variable. The **TRUNCATE** option is available only as a global option.

FREQ Statement

FREQ *variable* ;

The **FREQ** statement names a variable that provides frequencies for each observation in the **DATA=** data set. Specifically, if n is the value of the **FREQ** variable for a given observation, then that observation is used n times.

The analysis produced by using a **FREQ** statement reflects the expanded number of observations. You can produce the same analysis (without the **FREQ** statement) by first creating a new data set that contains the expanded number of observations. For example, if the value of the **FREQ** variable is 5 for the first

observation, the first five observations in the new data set are identical. Each observation in the old data set is replicated n_i times in the new data set, where n_i is the value of the FREQ variable for that observation.

If the value of the FREQ variable is missing or is less than 1, the observation is not used in the analysis. If the value is not an integer, only the integer portion is used.

The FREQ statement is not available when a loess smoother is included in the model.

MODEL Statement

MODEL *dependent* < (*options*) > = < **PARAM**(*effects*) > < *smoothing-effects* > < / *options* > ;

MODEL *event/trials* = < **PARAM**(*effects*) > < *smoothing-effects* > < / *options* > ;

The MODEL statement specifies the dependent variable and the independent effects you want to use in the model. Specify the independent parametric variables inside the parentheses of PARAM(). The parametric variables can be either classification variables or continuous variables. Classification variables must be declared in a CLASS statement. Interactions between variables can also be included as parametric effects. Multiple PARAM() specifications are allowed in the MODEL statement. The syntax for the specification of effects is the same as for the GLM procedure (Chapter 42, “The GLM Procedure”).

Only continuous variables can be specified in smoothing effects. Any number of smoothing effects can be specified, as follows:

Smoothing Effect	Meaning
SPLINE(<i>variable</i> < , DF= <i>number</i> >)	Fits a smoothing spline with the variable and with DF= <i>number</i>
LOESS(<i>variable</i> < , DF= <i>number</i> >)	Fits a local regression with the variable and with DF= <i>number</i>
SPLINE2(<i>variable1</i> , <i>variable2</i> < ,DF= <i>number</i> >)	Fits a bivariate thin-plate smoothing spline with <i>variable1</i> and <i>variable2</i> and with DF= <i>number</i>

The number specified in the DF= option must be positive. If you specify neither the DF= option nor the **METHOD=GCV** in the MODEL statement, then the default is DF=4. Note that for univariate spline and loess components, a degree of freedom is used by default to account for the linear portion of the model, so the value displayed in the “Fit Summary” and “Analysis of Deviance” tables will be one less than the value you specify.

Both parametric effects and smoothing effects are optional. If none are specified, a model that contains only an intercept is fitted.

If only parametric variables are present, PROC GAM fits a parametric linear model by using the terms inside the parentheses of PARAM(). If only smoothing effects are present, PROC GAM fits a nonparametric additive model. If both types of effect are present, PROC GAM fits a semiparametric model by using the parametric effects as the linear part of the model.

Table 39.2 shows how to specify various models for a dependent variable y and independent variables x , x_1 , and x_2 . $s_i(\cdot)$, $i = 1, 2$ are nonparametric smooth functions.

Table 39.2 Syntax for Common GAM Models

Type of Model	Syntax for model	Mathematical Form
Parametric	<code>y=param(x1 x2)</code>	$E(Y X = x) = \beta_0 + \beta_1x_1 + \beta_2x_2$
Nonparametric	<code>y=spline(x)</code>	$E(Y X = x) = \beta_0 + \beta_1x + s(x)$
Nonparametric	<code>y=loess(x)</code>	$E(Y X = x) = \beta_0 + \beta_1x + s(x)$
Semiparametric	<code>y=spline(x1) param(x2)</code>	$E(Y X = x) = \beta_0 + \beta_1x_1 + \beta_2x_2 + s(x_1)$
Additive	<code>y=spline(x1) spline(x2)</code>	$E(Y X = x) = \beta_0 + \beta_1x_1 + \beta_2x_2 + s_1(x_1) + s_2(x_2)$
Thin-plate spline	<code>y=spline2(x1, x2)</code>	$E(Y X = x) = \beta_0 + s(x_1, x_2)$

Table 39.3 summarizes the options available in the MODEL statement.

Table 39.3 MODEL Statement Options

Option	Description
Response Variable Options	
DESCENDING	Reverses the order of the response categories
EVENT=	Specifies the event category for the binary response model
ORDER=	Specifies the sort order for the response variable
Model Options	
ALPHA=	Specifies the significance level
ANODEV=	Specifies the method used to analyze smoothing effects
DIST=	Specifies the distribution family
EPSILON=	Specifies the convergence criterion for the backfitting algorithm
EPSSCORE=	Specifies the convergence criterion for the local scoring algorithm
ITPRINT	Produces an iteration summary table for the smoothing effects
MAXITER=	Specifies the maximum number of iterations for the backfitting algorithm
MAXITSCORE=	Specifies the maximum number of iterations for the local scoring algorithm
METHOD=	Specifies the method for selecting the value of the smoothing parameter
OFFSET=	Specifies an offset for the linear predictor

Response Variable Options

Response variable options determine how the GAM procedure models probabilities for binary data.

You can specify the following options by enclosing them in parentheses after the response variable. See the section “CLASS Statement” on page 2664 for more detail.

DESCENDING

DESC

reverses the order of the response categories. If both the DESCENDING and ORDER= options are specified, PROC GAM orders the response categories according to the ORDER= option and then reverses that order.

EVENT=*'category' | keyword*

specifies the event category for the binary response model. PROC GAM models the probability of the event category. You can specify the value (formatted, if a format is applied) of the event category in quotes, or you can specify one of the following keywords. The default is EVENT=FIRST.

FIRST

designates the first ordered category as the event.

LAST

designates the last ordered category as the event.

One of the most common sets of response levels is $\{0, 1\}$, with 1 representing the event for which the probability is to be modeled. Consider the example where Y takes the value 1 and 0 for event and nonevent, respectively, and X is the explanatory variable. By default, PROC GAM models the probability that $Y = 0$. To model the probability that $Y = 1$, specify the following MODEL statement:

```
model Y (event='1') = X;
```

ORDER=*DATA | FORMATTED | FREQ | INTERNAL*

specifies the sort order for the levels of the response variable. By default, ORDER=FORMATTED. When ORDER=FORMATTED, the values of numeric variables for which you have supplied no explicit format (that is, for which there is no corresponding FORMAT statement in the current PROC GAM run or in the DATA step that created the data set), are ordered by their internal (numeric) value. If you specify the ORDER= option in the MODEL statement and the ORDER= option in the CLASS statement, the former takes precedence. The following table shows the interpretation of the ORDER= values:

Value of ORDER=	Levels Sorted By
DATA	Order of appearance in the input data set
FORMATTED	External formatted value, except for numeric variables with no explicit format, which are sorted by their unformatted (internal) value
FREQ	Descending frequency count; levels with the most observations come first in the order
INTERNAL	Unformatted value

For the FORMATTED and INTERNAL values, the sort order is machine-dependent.

For more information about sort order, see the chapter on the SORT procedure in the *Base SAS Procedures Guide* and the discussion of BY-group processing in *SAS Language Reference: Concepts*.

Model Options

ALPHA=*number*

specifies the significance level α of the confidence limits on the final nonparametric component estimates when you request confidence limits to be included in the output data set. Specify *number* as a value between 0 and 1. The default value is 0.05. See the section “OUTPUT Statement” on page 2670 for more information about the OUTPUT statement.

ANODEV=*type*

specifies the *type* of method to be used to produce the “Analysis of Deviance” table for smoothing effects. The available choices are as follows:

- REFIT** specifies that PROC GAM perform χ^2 tests by fitting nested GAM models. This is the default choice if you do not specify the ANODEV= option. This choice requires fitting separate GAM models where one smoothing term is omitted from each model.
- NOREFIT** specifies that PROC GAM perform approximate tests of smoothing effects. To test each smoothing effect, a weighted least squares model is fitted to the remaining parametric part of the model while keeping other nonlinear smoothers fixed. For details, see Hastie (1991). This choice requires only a single GAM fitting to be performed, which reduces the time of the procedure.
- NONE** requests that the procedure not produce the “Analysis of Deviance” table for smoothing effects.

DIST=*distribution-id***LINK=***distribution-id*

specifies the distribution family used in the model. The choices for *distribution-id* are displayed in Table 39.4. See “Distribution Family and Canonical Link” on page 2682 for more information.

Table 39.4 Distribution Families for GAM Models

DIST=	Distribution	Link Function	Response Data Type
GAUSSIAN GAUS NORM	Normal (Gaussian)	Identity	Continuous variables
BINOMIAL LOGI BIN	Binomial	Logit	Binary variables
POISSON POIS LOGL	Poisson	Log	Nonnegative discrete variables
GAMMA GAMM	Gamma	Negative reciprocal	Positive continuous variables
IGAUSSIAN IGAU INVG	Inverse Gaussian	Squared reciprocal	Positive continuous variables

Canonical link functions are used with those distributions. Although alternative links are possible theoretically, the final fit of nonparametric regression models is relatively insensitive to the precise choice of link functions. Therefore, only the canonical link for each distribution family is implemented in PROC GAM. The loess smoother is not available for DIST=BINOMIAL when the number of trials is greater than 1.

EPSILON=*number*

specifies the convergence criterion for the backfitting algorithm. The default value is 1E–8.

EPSSCORE=*number*

specifies the convergence criterion for the local scoring algorithm. The default value is 1E–8.

ITPRINT

produces an iteration summary table for the smoothing effects when doing backfitting and local scoring.

MAXITER=number

specifies the maximum number of iterations for the backfitting algorithm. The default value is 50.

MAXITSCORE=number

specifies the maximum number of iterations for the local scoring algorithm. The default value is 100.

METHOD=GCV

specifies that the value of the smoothing parameter should be selected by generalized cross validation. If you specify both METHOD=GCV and the DF= option for the smoothing effects, the user-specified DF is used, and the METHOD=GCV option is ignored. See the section “[Selection of Smoothing Parameters](#)” on page 2679 for more details on the GCV method.

OFFSET=variable

specifies an offset for the linear predictor. An offset plays the role of a predictor whose coefficient is known to be 1. For example, you can use an offset in a Poisson model when counts have been obtained in time intervals of different lengths. With a log link function, you can model the counts as Poisson variables with the logarithm of the time interval as the offset variable. The offset variable cannot appear in the CLASS statement or elsewhere in the MODEL statement.

OUTPUT Statement

OUTPUT OUT= SAS-data-set < keyword< =prefix> ... keyword< =prefix> > ;

The OUTPUT statement creates a new SAS data set that contains diagnostic measures calculated after fitting the model.

All the variables in the original data set are included in the new data set, along with new variables that are created with *keywords* specified in the OUTPUT statement. These new variables contain the values of a variety of statistics and diagnostic measures that are calculated for each observation in the data set. If no *keywords* are present, the OUT= data set contains only the original data set and predicted values. The predicted values include the linear predictor for the response and the prediction for each smoothing term in the model. When you specify a distribution family with the DIST= or LINK= option in the MODEL statement, predicted response values after applying the inverse link function are also included. Predicted values are computed for observations that have missing response values, nonmissing values in the explanatory variables, and values of the smoothing variables that are within the smoothing ranges of the fitted model.

You can specify the following options in the OUTPUT statement:

OUT=SAS-data-set

specifies the name of the new data set to contain the diagnostic measures. This option is required.

keyword < =prefix >

specifies the statistics to include in the output data set. The keywords and the statistics they represent are as follows:

PREDICTED

predicted values for each smoothing component and overall predicted values on the response scale at design points. The prediction for each spline or loess term is only for the nonlinear component of each smoother.

LINP	linear prediction values on the link scale at design points
UCLM	upper confidence limits for each predicted smoothing component
LCLM	lower confidence limits for each predicted smoothing component
ADIAG	diagonal element of the hat matrix associated with the observation for each smoothing spline component
RESIDUAL	residual standardized by its weights
STD	standard deviation of the prediction for each smoothing component
ALL	all statistics in this list

The names of the new variables that contain the statistics are formed by concatenating a *prefix* and the corresponding variable names. If you do not specify a *prefix*, the names are formed by using default prefixes listed in the following table:

Keyword	Prefix
PRED	P_
LINP	LINP_
UCLM	UCLM_
LCLM	LCLM_
ADIAG	ADIAG_
RESID	R_
STD	STD_ (for spline) STDP_ (for loess)

For example, suppose that you have a dependent variable y and an independent smoothing variable x . If you specify the keywords `PRED=MyP_` and `ADIAG=MyA_`, the new variables in the output SAS data set are `MyP_y`, `MyP_x`, and `MyA_x`. If you specify the keywords `PRED` and `ADIAG` without prefixes, the new variables are `P_y`, `P_x`, and `ADIAG_x`.

SCORE Statement

SCORE DATA= *SAS-data-set* **OUT=** *SAS-data-set* ;

The SCORE statement calculates predicted values for a new data set. All the variables in the DATA= data set are included in the OUT= data set, along with the predicted values. The predicted values consist of predicted responses after the inverse link function transformation, predicted values of all smoothing terms, and predicted values on the link scale. Predicted values are computed for observations with missing response values whose values of the specified explanatory variables are nonmissing, and whose values of the specified smoothing variables are within the smoothing ranges of the fitted model. The predicted variables use the same naming convention as the OUTPUT statement. If you have multiple data sets to score, you can specify multiple SCORE statements.

The following options must be specified in the SCORE statement:

DATA=SAS-data-set

specifies an input SAS data set containing all the variables included in independent effects in the MODEL statement. The predicted response is computed for each observation in the SCORE DATA=data set.

OUT=SAS-data-set

specifies the name of the SAS data set to contain the predictions.

Details: GAM Procedure

Missing Values

When fitting a model, PROC GAM excludes any observation with missing values for an explanatory variable, offset variable, or dependent variable. However, if only the response is missing, predicted values can be computed and output to a data set by using the OUTPUT or SCORE statement.

Nonparametric Regression

Nonparametric regression relaxes the usual assumption of linearity and enables you to explore the data more flexibly, uncovering structure in the data that might otherwise be missed.

However, many forms of nonparametric regression do not perform well when the number of independent variables in the model is large. The sparseness of data in this setting causes the variances of the estimates to be unacceptably large unless the sample size is extremely large. The problem of rapidly increasing variance for increasing dimensionality is sometimes referred to as the “curse of dimensionality.” Interpretability is another problem with nonparametric regression based on kernel and smoothing spline estimates. These estimates contain information about the relationship between the dependent and independent variables, and the information is often difficult to comprehend.

To overcome these difficulties, additive models were proposed by some researchers, for example, Stone (1985). These models estimate an additive approximation to the multivariate regression function. The benefits of an additive approximation are at least twofold. First, since each of the individual additive terms is estimated by using a univariate smoother, the curse of dimensionality is avoided, at the cost of not being able to approximate universally. Second, estimates of the individual terms explain how the dependent variable changes with the corresponding independent variables.

To extend the additive model to a wide range of distribution families, Hastie and Tibshirani (1990) proposed generalized additive models. These models enable the mean of the dependent variable to depend on an additive predictor through a nonlinear link function. The models permit the response probability distribution to be any member of the exponential family of distributions. Many widely used statistical models belong to this general class; they include additive models for Gaussian data, nonparametric logistic models for binary data, and nonparametric log-linear models for Poisson data.

Additive Models and Generalized Additive Models

This section describes the methodology and the fitting procedure behind generalized additive models.

Let Y be a response random variable and X_1, X_2, \dots, X_p be a set of predictor variables. A regression procedure can be viewed as a method for estimating the expected value of Y given the values of X_1, X_2, \dots, X_p . The standard linear regression model assumes a linear form for the dependency of Y on X :

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_p X_p + \epsilon$$

where $E(\epsilon) = 0$ and $\text{Var}(\epsilon) = \sigma^2$. Given a sample, estimates of $\beta_0, \beta_1, \dots, \beta_p$ are usually obtained by the least squares method.

The additive model generalizes the linear model by modeling the dependency as

$$Y = s_0 + s_1(X_1) + s_2(X_2) + \dots + s_p(X_p) + \epsilon$$

where $s_j(X)$, $j = 1, 2, \dots, p$, are smooth functions, $E(\epsilon) = 0$ and $\text{Var}(\epsilon) = \sigma^2$.

In order to be estimable, the smooth functions s_i have to satisfy standardized conditions such as $E(s_j(X_j)) = 0$. These functions are not given a parametric form but instead are estimated in a non-parametric fashion.

While traditional linear models and additive models can be used in most statistical data analysis, there are types of problems for which they are not appropriate. For example, the normal distribution might not be adequate for modeling discrete responses such as counts or bounded responses such as proportions.

Generalized additive models address these difficulties, extending additive models to many other distributions besides just the normal. Thus, generalized additive models can be applied to a much wider range of data analysis problems.

Like generalized linear models, generalized additive models consist of a random component, an additive component, and a link function relating the two components. The response Y , the random component, is assumed to have exponential family density

$$f_Y(y; \theta, \phi) = \exp \left\{ \frac{y\theta - b(\theta)}{a(\phi)} + c(y, \phi) \right\}$$

where θ is called the natural parameter and ϕ is the scale parameter. The mean of the response variable μ is related to the set of covariates X_1, X_2, \dots, X_p by a link function g . The quantity

$$\eta = s_0 + \sum_{j=1}^p s_j(X_j)$$

defines the additive component, where $s_1(\cdot), \dots, s_p(\cdot)$ are smooth functions, and the relationship between μ and η is defined by $g(\mu) = \eta$. The most commonly used link function is the canonical link, for which $\eta = \theta$.

Generalized additive models and generalized linear models can be applied in similar situations, but they serve different analytic purposes. Generalized linear models emphasize estimation and inference for the parameters of the model, while generalized additive models focus on exploring data nonparametrically. Generalized additive models are more suitable for exploring the data and visualizing the relationship between the dependent variable and the independent variables.

Forms of Additive Models

Suppose that y is a continuous variable and x_1 and x_2 are two explanatory variables of interest. To fit an additive model, you can use a MODEL statement similar to that used in many regression procedures in the SAS System:

```
model y = spline(x1) spline(x2);
```

This model statement requires the procedure to fit the following model:

$$\eta(x_1, x_2) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + s_1(x_1) + s_2(x_2)$$

where the $s_i(\cdot)$ terms denote nonparametric spline functions of the respective explanatory variables.

The GAM procedure can fit semiparametric models. The following MODEL statement assumes a linear relation with x_1 and an unknown functional relation with x_2 :

```
model y = param(x1) spline(x2);
```

If you want to fit a model containing a functional two-way interaction between x_1 and x_2 , you can use the following MODEL statement:

```
model y = spline2(x1, x2);
```

In this case, the GAM procedure fits a model equivalent to that of PROC TPSPLINE.

Estimates from PROC GAM

PROC GAM provides the capability to fit both nonparametric and semiparametric models. So that you can better understand the underlying trend of any given factor, PROC GAM separates the linear trend from any general nonparametric trend during the fitting as well as in the final report. This makes it easy to determine whether the significance of a smoothing variable is associated with a simple linear trend or a more complicated pattern.

For example, suppose you want to fit a semiparametric model as

$$y = \alpha_0 + \alpha_1 z + f_1(x_1) + f_2(x_2)$$

The GAM estimate for this model is

$$y = \hat{\alpha}_0 + \hat{\alpha}_1 z + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \hat{s}_1(x_1) + \hat{s}_2(x_2)$$

where \hat{s}_1 and \hat{s}_2 are linear-adjusted nonparametric estimates of the f_1 and f_2 effects. The p -values for $\hat{\alpha}_0$, $\hat{\alpha}_1$, $\hat{\beta}_1$, and $\hat{\beta}_2$ are reported in the parameter estimates table. $\hat{\beta}_1$ and $\hat{\beta}_2$ are the estimates labeled Linear(x1) and Linear(x2) in the table. The p -values for \hat{s}_1 and \hat{s}_2 are reported in the analysis of deviance table.

Only \hat{s}_1 , \hat{s}_2 , and \hat{y} are output to the output data set, with the corresponding variable names P_x1, P_x2, and P_y. For Gaussian data, the complete marginal prediction for variable x_1 is:

$$\hat{\beta}_1 x_1 + P_x1$$

If the additive component plots are requested by the ADDITIVE suboption, the additive component for variable x_2 is computed as:

$$\widehat{\beta}_2(x_2 - \bar{x}_2) + P_{x_2}$$

where \bar{x}_2 is the mean for variable x_2 .

Backfitting and Local Scoring Algorithms

Much of the development and notation in this section follows Hastie and Tibshirani (1986).

Additive Models

Consider the estimation of the smoothing terms $s_0, s_1(), \dots, s_p()$ in the additive model

$$\eta(X) = s_0 + \sum_{j=1}^p s_j(X_j)$$

where $E(s_j(X_j)) = 0$ for every j . Since the algorithm for additive models is the basis for fitting generalized additive models, the algorithm for additive models is discussed first.

Many ways are available to approach the formulation and estimation of additive models. The backfitting algorithm is a general algorithm that can fit an additive model with any regression-type fitting mechanisms.

Define the k th set of partial residuals as

$$R_k = Y - s_0 - \sum_{j \neq k} s_j(X_j)$$

then $E(R_k|X_k) = s_k(X_k)$. This observation provides a way to estimate each smoothing function $s_k()$ given estimates $\{\hat{s}_j(), j \neq k\}$ for all the others. The resulting iterative procedure is known as the backfitting algorithm (Friedman and Stuetzle 1981). The following formulation is taken from Hastie and Tibshirani (1986).

The Backfitting Algorithm

The unweighted form of the backfitting algorithm is as follows:

1. **Initialization:**

$$s_0 = E(Y), s_1^{(1)} = s_2^{(1)} = \dots = s_p^{(1)} = 0, m = 0$$

2. **Iterate:**

$$m = m + 1;$$

for $j = 1$ to p do:

$$R_j = Y - s_0 - \sum_{k=1}^{j-1} s_k^{(m)}(X_k) - \sum_{k=j+1}^p s_k^{(m-1)}(X_k);$$

$$s_j^{(m)} = E(R_j|X_j);$$

3. **Until:**

$$\text{RSS} = \frac{1}{n} \left\| Y - s_0 - \sum_{j=1}^p s_j^{(m)}(X_j) \right\|^2 \text{ fails to decrease, or satisfies the convergence criterion.}$$

In the preceding notation, $s_j^{(m)}(\cdot)$ denotes the estimate of $s_j(\cdot)$ at the m th iteration. It can be shown that with many smoothers (including linear regression, univariate and bivariate splines, and combinations of these), RSS never increases at any step. This implies that the algorithm always converges (Hastie and Tibshirani 1986). Note, however, that for distributions other than Gaussian, numerical instabilities with weights can cause convergence problems. Even when the algorithm converges, the individual functions need not be unique, since dependence among the covariates can lead to more than one representation for the same fitted surface.

A weighted backfitting algorithm has the same form as for the unweighted case, except that the smoothers are weighted. In PROC GAM, weights are used with non-Gaussian data in the local scoring procedure described later in this section.

The GAM procedure uses the following condition as the convergence criterion for the backfitting algorithm:

$$\frac{\sum_{i=1}^n \sum_{j=1}^p \left(s_j^{(m-1)}(\mathbf{X}_{ij}) - s_j^{(m)}(\mathbf{X}_{ij}) \right)^2}{1 + \sum_{i=1}^n \sum_{j=1}^p \left(s_j^{(m-1)}(\mathbf{X}_{ij}) \right)^2} \leq \epsilon$$

where $\epsilon = 10^{-8}$ by default; you can change this with the EPSILON= option in the MODEL statement.

Generalized Additive Models

The algorithm described so far fits only additive models. The algorithm for generalized additive models is a little more complicated. Generalized additive models extend generalized linear models in the same manner that additive models extend linear regression models—that is, by replacing the form $\alpha + \sum_j \beta_j \mathbf{x}_j$ with the additive form $\alpha + \sum_j f_j(\mathbf{x}_j)$. See “Generalized Linear Models Theory” on page 2799 in Chapter 40, “The GENMOD Procedure,” for more information.

PROC GAM fits generalized additive models by using a modified form of adjusted dependent variable regression, as described for generalized linear models in McCullagh and Nelder (1989), with the additive predictor taking the role of the linear predictor. Hastie and Tibshirani (1986) call this the *local scoring algorithm*. Important components of this algorithm depend on the link function for each distribution, as shown in the following table.

Distribution	Link	Adjusted Dependent (z)	Weights (w)
Normal	μ	y	1
Binomial	$\log\left(\frac{\mu}{n-\mu}\right)$	$\eta + (y - \mu)/n\mu(1 - \mu)$	$n\mu(1 - \mu)$
Gamma	$-1/\mu$	$\eta + (y - \mu)/\mu^2$	μ^2
Poisson	$\log(\mu)$	$\eta + (y - \mu)/\mu$	μ
Inverse Gaussian	$1/\mu^2$	$\eta - 2(y - \mu)/\mu^3$	$\mu^3/4$

Once the distribution and hence these quantities are defined, the local scoring algorithm proceeds as follows.

The General Local Scoring Algorithm

1. Initialization:

$$s_i = g(E(y)), s_1^0 = s_2^0 = \dots = s_p^0 = 0, m = 0$$

2. Iterate:

$$m = m + 1;$$

Form the predictor η , mean μ , weights \mathbf{w} , and adjusted dependent variable \mathbf{z} based on their corresponding values from the previous iteration:

$$\eta_i^{(m-1)} = s_0 + \sum_{j=1}^p s_j^{(m-1)}(x_{ij})$$

$$\mu_i^{(m-1)} = g^{-1}(\eta_i^{(m-1)})$$

$$w_i = \left(V_i^{(m-1)}\right)^{-1} \cdot \left[\left(\frac{\partial \mu}{\partial \eta}\right)_i^{(m-1)}\right]^2$$

$$z_i = \eta_i^{(m-1)} + \left(y_i - \mu_i^{(m-1)}\right) \cdot \left(\frac{\partial \mu}{\partial \eta}\right)_i^{(m-1)}$$

where $V_i^{(m-1)}$ is the variance of Y at $\mu_i^{(m-1)}$. Fit an additive model to \mathbf{z} by using the backfitting algorithm with weights \mathbf{w} to obtain estimated functions $s_j^{(m)}(\cdot)$, $j = 1, \dots, p$;

3. Until:

The convergence criterion is satisfied or the deviance fails to decrease. The deviance is an extension to generalized linear models of the RSS; see “[Goodness of Fit](#)” on page 2806 in Chapter 40, “[The GENMOD Procedure](#),” for a definition.

The GAM procedure uses the following condition as the convergence criterion for local scoring:

$$\frac{\sum_{i=1}^n w_i \sum_{j=1}^p \left(s_j^{(m-1)}(\mathbf{X}_{ij}) - s_j^{(m)}(\mathbf{X}_{ij})\right)^2}{\sum_{i=1}^n w_i \left(1 + \sum_{j=1}^p \left(s_j^{(m-1)}(\mathbf{X}_{ij})\right)^2\right)} \leq \epsilon^s$$

where $\epsilon^s = 10^{-8}$ by default; you can change this with the EPSSCORE= option in the MODEL statement.

The estimating procedure for generalized additive models consists of two loops. Inside each step of the local scoring algorithm (outer loop), a weighted backfitting algorithm (inner loop) is used until convergence or until the RSS fails to decrease. Then, based on the estimates from this weighted backfitting algorithm, a new set of weights is calculated and the next iteration of the scoring algorithm starts. The scoring algorithm stops when the convergence criterion is satisfied or the deviance of the estimates stops decreasing.

Smoother

You can specify three types of smoothers in the MODEL statement:

- SPLINE(x) specifies a cubic smoothing spline term for variable x
- LOESS(x) specifies a loess term for variable x
- SPLINE2(x1, x2) specifies a thin-plate smoothing spline term for variables x1 and x2

A smoother is a tool for summarizing the trend of a response measurement Y as a function of one or more predictor measurements X_1, \dots, X_p . It produces an estimate of the trend that is less variable than Y itself. An important property of a smoother is its nonparametric nature. It does not assume a rigid form for the dependence of Y on X_1, \dots, X_p . This section gives a brief overview of the smoothers that can be used with the GAM procedure.

Cubic Smoothing Spline

A smoothing spline is the solution to the following optimization problem: among all functions $\eta(x)$ with two continuous derivatives, find one that minimizes the penalized least square

$$\sum_{i=1}^n (y_i - \eta(x_i))^2 + \lambda \int_a^b (\eta''(t))^2 dt$$

where λ is a fixed constant and $a \leq x_1 \leq \dots \leq x_n \leq b$. The first term measures closeness to the data while the second term penalizes curvature in the function. It can be shown that there exists an explicit, unique minimizer, and that minimizer is a natural cubic spline with knots at the unique values of x_i .

The value $\lambda/(1 + \lambda)$ is the *smoothing parameter*. When λ is large, the smoothing parameter is close to 1, producing a smoother curve; small values of λ , corresponding to smoothing parameters near 0, are apt to produce rougher curves, more nearly interpolating the data.

Local Regression

Local regression was proposed by Cleveland, Devlin, and Grosse (1988). The idea of local regression is that at a predictor x , the regression function $\eta(x)$ can be locally approximated by the value of a function in some specified parametric class. Such a local approximation is obtained by fitting a regression surface to the data points within a chosen neighborhood of the point x . A weighted least squares algorithm is used to fit linear functions of the predictors at the centers of neighborhoods. The radius of each neighborhood is chosen so that the neighborhood contains a specified percentage of the data points. The smoothing parameter for the local regression procedure, which controls the smoothness of the estimated curve, is the fraction of the data in each local neighborhood. Data points in a given local neighborhood are weighted by a smooth decreasing function of their distance from the center of the neighborhood. See Chapter 53, “[The LOESS Procedure](#),” for more details.

Thin-Plate Smoothing Spline

The thin-plate smoothing spline is a multivariate version of the cubic smoothing spline. The theoretical foundations for the thin-plate smoothing spline are described in Duchon (1976, 1977); Meinguet (1979). The smoothing parameter for the thin-plate smoothing spline smoother is the parameter that controls the smoothness penalty. When the smoothing parameter is close to 0, the fit is close to an interpolation. When the smoothing parameter is very large, the fit is a smooth surface. Further results and applications are given in Wahba and Wendelberger (1980). See Chapter 96, “[The TPSPLINE Procedure](#),” for more details.

Selection of Smoothing Parameters

CV and GCV

The smoothers discussed here have a single smoothing parameter. In choosing the smoothing parameter, cross validation can be used. Cross validation works by leaving points (x_i, y_i) out one at a time, estimating the squared residual for smooth function at x_i based on the remaining $n - 1$ data points, and choosing the smoother to minimize the sum of those squared residuals. This mimics the use of training and test samples for prediction. The cross validation function is defined as

$$\text{CV}(\lambda) = \frac{1}{n} \sum_{i=1}^n \left(y_i - \hat{\eta}_{\lambda}^{(-i)}(x_i) \right)^2$$

where $\hat{\eta}_{\lambda}^{(-i)}(x_i)$ indicates the fit at x_i , computed by leaving out the i th data point. The quantity $n\text{CV}(\lambda)$ is sometimes called the prediction sum of squares, or PRESS (Allen 1974).

All of the smoothers fit by the GAM procedure can be formulated as a linear combination of the sample responses

$$\hat{\eta}(x) = \mathbf{A}(\lambda)\mathbf{y}$$

for some matrix $\mathbf{A}(\lambda)$, which depends on λ . (The matrix $\mathbf{A}(\lambda)$ depends on x and the sample data as well, but this dependence is suppressed in the preceding equation.) Let a_{ii} be the i th diagonal element of $\mathbf{A}(\lambda)$. Then the CV function can be expressed as

$$\text{CV}(\lambda) = \frac{1}{n} \sum_{i=1}^n \left(\frac{y_i - \hat{\eta}_{\lambda}(x_i)}{1 - a_{ii}} \right)^2$$

In most cases, it is very time-consuming to compute the quantity a_{ii} individually. To solve this computational problem, Wahba (1990) has proposed the generalized cross validation function (GCV) that can be used to solve a wide variety of problems involving selection of a parameter to minimize the prediction risk.

The GCV function is defined as

$$\text{GCV}(\lambda) = \frac{n \sum_{i=1}^n (y_i - \hat{\eta}_{\lambda}(x_i))^2}{(n - \text{Trace}(\mathbf{A}(\lambda)))^2}$$

The GCV formula simply replaces the a_{ii} with $\text{Trace}(\mathbf{A}(\lambda))/n$. Therefore, it can be viewed as a weighted version of CV. In most of the cases of interest, GCV is closely related to CV but much easier to compute. Specify the **METHOD=GCV** option in the MODEL statement in order to use the GCV function to choose the smoothing parameters.

Degrees of Freedom

The estimated GAM model can be expressed as

$$\hat{\eta}(X) = \hat{s}_0 + \sum_{j=1}^p \mathbf{A}_j(\lambda_j)Y$$

Because the weights are calculated based on previous iteration during the local scoring iteration, the matrices \mathbf{A}_j might depend on Y for non-Gaussian data. However, for the final iteration, the \mathbf{A}_j matrix for the spline smoothers has the same role as the projection matrix in linear regression; therefore, nonparametric degrees of freedom (DF) for the j th spline smoother can be defined as

$$\text{DF}(j \text{ th spline smoother}) = \text{Trace}(\mathbf{A}_j(\lambda_j))$$

For loess smoothers \mathbf{A}_j is not symmetric and so is not a projection matrix. In this case PROC GAM uses

$$\text{DF}(j \text{ th loess smoother}) = \text{Trace}(\mathbf{A}_j(\lambda_j)' \mathbf{A}_j(\lambda_j))$$

The GAM procedure gives you the option of specifying the degrees of freedom for each individual smoothing component. If you choose a particular value for the degrees of freedom, then during every local scoring iteration the procedure will search for a corresponding smoothing parameter lambda that yields the specified value or comes as close as possible. The final estimate for the smoother during this local scoring iteration will be based on this lambda. Note that for univariate spline and loess components, an additional degree of freedom is used by default to account for the linear portion of the model, so the value displayed in the “Fit Summary” and “Analysis of Deviance” tables will be one less than the value you specify.

Confidence Intervals for Smoothers

Buja, Hastie, and Tibshirani (1989) showed that each smoothing function estimate from the backfitting algorithm is the result of a linear mapping applied to the working response, if the backfitting algorithm converges.

The smoothing function estimate can be expressed as

$$\hat{s}_j(\mathbf{x}_j) = \mathbf{H}_j \mathbf{z}$$

where \mathbf{x}_j is the j th covariate and \mathbf{z} is the adjusted dependent variable that is formed in the local scoring algorithm. If the errors are independent and identically distributed, then

$$\text{Cov}(\hat{s}_j) = \sigma^2 \mathbf{H}_j \mathbf{H}_j'$$

where $\sigma^2 = \text{Var}(\mathbf{z})$.

However, direct computation of \mathbf{H}_j is formidable within the backfitting framework. Hastie and Tibshirani (1990) proposed using each individual smoothing matrix $\mathbf{A}_j(\lambda_j)$ as a substitute for the linear operator \mathbf{H}_j when computing confidence intervals. In the GAM procedure, curvewise confidence intervals for smoothing splines and pointwise confidence intervals for loess are provided in the output data set.

Curvewise Confidence Interval for Smoothing Spline Smoothers

Viewing the spline model as a Bayesian model, Wahba (1983) proposes Bayesian confidence intervals for smoothing spline estimates as:

$$\hat{s}_\lambda(x_i) \pm z_{\alpha/2} \sqrt{\hat{\mathbf{V}}_{ii}(\lambda)}$$

where $\hat{\mathbf{V}}_{ii}(\lambda)$ is the i th diagonal element of the Bayesian posterior covariance matrix $\hat{\mathbf{V}}$ and $z_{\alpha/2}$ is the $1 - \alpha/2$ quantile of the standard normal distribution. The confidence intervals are interpreted as intervals “across the function” as opposed to pointwise intervals.

Suppose that you fit a spline estimate to experimental data that consist of a true function f and a random error term ϵ_i . In repeated experiments, it is likely that about $100(1 - \alpha)\%$ of the confidence intervals cover the corresponding true values, although some values are covered every time and other values are not covered by the confidence intervals most of the time. This effect is more pronounced when the true response curve or surface has small regions of particularly rapid change.

In the GAM procedure, let the smoothing matrix for the nonlinear part of the j th spline term be $\tilde{\mathbf{A}}_j$ after the linear part is separated out from $\mathbf{A}_j(\lambda)$. The Bayesian posterior variance for the nonlinear part is computed as

$$\hat{\mathbf{V}}_j = \hat{\phi} \tilde{\mathbf{A}}_j \mathbf{W}^{-1}$$

where $\hat{\phi}$ is the dispersion parameter estimate and \mathbf{W} is the weight matrix from the final local scoring iteration. If you specify UCLM, LCLM, ADIAG, and STD options in the OUTPUT statement, the statistics are derived based on $\hat{\mathbf{V}}_j$.

When you request both the ADDITIVE and CLM suboptions in the PLOTS=COMPONENTS option, each of the smoothing component plots displays a confidence band for the total contribution of each smoothing spline smoother. The confidence band is derived from the total variance that is contributed by both linear and nonlinear parts by the j th term

$$\hat{\phi} \left(\mathbf{x}'_j (\mathbf{X}'\mathbf{W}\mathbf{X})^{-1} \mathbf{x}_j + \tilde{\mathbf{A}}_j \mathbf{W}^{-1} \right)$$

Pointwise Confidence Interval for Loess Smoothers

As shown in Cleveland, Devlin, and Grosse (1988), the smoothing matrix $\mathbf{A}(\lambda)$ for a loess smoother is asymmetric. The confidence intervals are computed as follows:

$$\hat{s}_\lambda(x_i) \pm z_{\alpha/2} \sqrt{\hat{\mathbf{V}}_{ii}(\lambda)}$$

where $\hat{\mathbf{V}}_{ii}(\lambda)$ is the i th diagonal element of the covariance matrix $\hat{\mathbf{V}}$ and $z_{\alpha/2}$ is the $1 - \alpha/2$ quantile of the standard normal distribution.

In the GAM procedure, let the smoothing matrix for the nonlinear part of the j th loess term be $\tilde{\mathbf{A}}_j$ after the linear part is separated out from $\mathbf{A}_j(\lambda)$. The covariance matrix for the nonlinear part is then

$$\hat{\mathbf{V}}_j = \hat{\phi} \tilde{\mathbf{A}}_j \mathbf{W}^{-1} \tilde{\mathbf{A}}'_j$$

where $\hat{\phi}$ is the dispersion parameter estimate and \mathbf{W} is the weight matrix from the final local scoring iteration. If you specify UCLM, LCLM, and STD options in the OUTPUT statement, the statistics are derived based on $\hat{\mathbf{V}}_j$.

When you request both the ADDITIVE and CLM suboptions in the PLOTS=COMPONENTS option, each of the smoothing component plots displays confidence intervals for total prediction of each loess smoother. The confidence intervals are derived from the total variance that is contributed by both the linear and nonlinear parts by the j th term

$$\hat{\phi} \left(\mathbf{x}'_j (\mathbf{X}'\mathbf{W}\mathbf{X})^{-1} \mathbf{x}_j + \tilde{\mathbf{A}}_j \mathbf{W}^{-1} \tilde{\mathbf{A}}'_j \right)$$

Distribution Family and Canonical Link

In general, there is not just one reasonable link function for a given response variable distribution. For parametric models, the choice of link function can lead to substantively different estimates and tests. However, the inherent flexibility of nonparametric models makes them less likely to be sensitive to the precise choice of link function. Thus, for simplicity and computational efficiency, the GAM procedure uses only the canonical link for each distribution, as discussed in the following sections.

The Gaussian Model

For a Gaussian model, the link function is the identity function, and the generalized additive model is the same as the additive model. The Gaussian model is selected by default or when you specify the `DIST=GAUSSIAN` option in the `MODEL` statement.

The Binomial Model

The binomial model is selected by specifying the `DIST=BINOMIAL` option in the `MODEL` statement. A binomial response model assumes that the proportion of successes Y is such that Y has a $\text{Bi}(n, p(x))$ distribution. $\text{Bi}(n, p(x))$ refers to the binomial distribution with the parameters n and $p(x)$. Often the data are binary, in which case $n = 1$. The canonical link is

$$g(p) = \log \frac{p}{n - p} = \eta$$

By default, PROC GAM models the probability of the response level with the *lower ordered value*. Ordered values are assigned to response levels in ascending sorted order and are displayed in the “Response Profiles” table. For binary data, if your event category has a higher Ordered Value, then by default the nonevent is modeled. The effect of modeling the nonevent is to change the signs of the estimated coefficients for linear terms in the model for the event. You can change which probability is modeled by specifying the `EVENT=`, `DESCENDING`, or `ORDER=` response variable options in the `MODEL` statement.

The Poisson Model

The Poisson model is selected by specifying the `DIST=POISSON` option in the `MODEL` statement. The link function for the Poisson model is the log function. Assuming that the mean of the Poisson distribution is $\mu(x)$, the dependence of $\mu(x)$ and independent variables x_1, \dots, x_k is

$$g(\mu) = \log(\mu) = \eta$$

The Gamma Model

The gamma model is selected by specifying the `DIST=GAMMA` option in the `MODEL` statement. Let the mean of the gamma distribution be $\mu(x)$. The canonical link function for the gamma distribution is $-1/\mu(x)$. Note that this link function is the negative of the default link function in PROC GENMOD for a gamma model. The relationship between $\mu(x)$ and the independent variables x_1, \dots, x_k is

$$g(\mu) = -\frac{1}{\mu} = \eta$$

The Inverse Gaussian Model

The inverse Gaussian model is selected by specifying the DIST=IGAUSSIAN option in the MODEL statement. Let the mean of the inverse Gaussian distribution be $\mu(x)$. The canonical link function for inverse Gaussian distribution is $1/\mu^2$. Therefore, the relationship between $\mu(x)$ and the independent variables x_1, \dots, x_k is

$$g(\mu) = \frac{1}{\mu^2} = \eta$$

Dispersion Parameter

Continuous distributions in the exponential family (Gaussian, gamma, and inverse Gaussian) have a dispersion parameter that can be estimated by the scaled deviance. For these continuous response distributions, PROC GAM incorporates this dispersion parameter estimate into standard errors of the parameter estimates, prediction standard errors of spline and loess components, and chi-square statistics. The discrete distributions used in GAM (binomial and Poisson) do not have a dispersion parameter. For more details on the distributions, dispersion parameter, and deviance, see “Generalized Linear Models Theory” on page 2799 in Chapter 40, “The GENMOD Procedure.”

Computational Resources

Since PROC GAM implements a doubly iterative method (inner backfitting iterations within each local scoring iteration), data are accessed multiple times in performing a fit. To expedite the data access, PROC GAM keeps the data used in the analysis in memory.

Let

- n = number of observations used in the analysis
- p_r = number of parametric variables
- p_s = number of univariate spline smoothers
- p_l = number of loess smoothers
- p_b = number of bivariate thin-plate spline smoothers
- p = $p_r + p_s + p_l + p_b$
- p_n = $p_s + p_l + p_b$
- m = maximum number of iterations for the backfitting algorithm

In addition to the space to store the data ($8np$ bytes), the minimum working space (in bytes) needed for fitting a model using PROC GAM is

$$(16 + 8p_r)(n + 2p_r) + (160 + 48p + 16p_s + 8p_b + 8p_l)n + 8p + 32p_b + 32p_s + 8m + 8n + (4n + 4)p_s + 4.$$

For fitting bivariate thin-plate smoothing spline variables, an extra $80 + 120n + 8n^2 + 8p_b$ bytes of memory are needed. For fitting loess variables, an extra $48n + 16p_l$ bytes of memory are needed. If model inference or confidence limits are requested, additional memory is required.

It is difficult to provide accurate estimates of the time required to fit a GAM model. Both the backfitting algorithm and the local scoring algorithm are iterative techniques whose convergence rates depend on the particular data being analyzed. Furthermore, the time required depends on the types of smoothers that you specify, as well as on the inferential information you request.

You can estimate the time required for problems with a larger number of observations by observing the time required for smaller problems and then using the following growth rules (obtained using by simulations) that show that the time required grows proportionally with the following:

- n^3 when at least one bivariate thin-plate spline is used
- $n^{3/2}$ when only loess smoothers are used
- n when only univariate smoothing splines are used

For additive models (models with Gaussian response distribution) with a fixed number of observations, the time required is roughly proportional to $p_n^{3/2}$. For generalized additive models (models with non-Gaussian distributions), the computation time grows more rapidly as p_n increases. This is harder to quantify as it depends on the distribution family and the number of iterations required for the local scoring algorithm to converge.

Figure 39.4 Feasible Problem Sizes for Different Smoothers

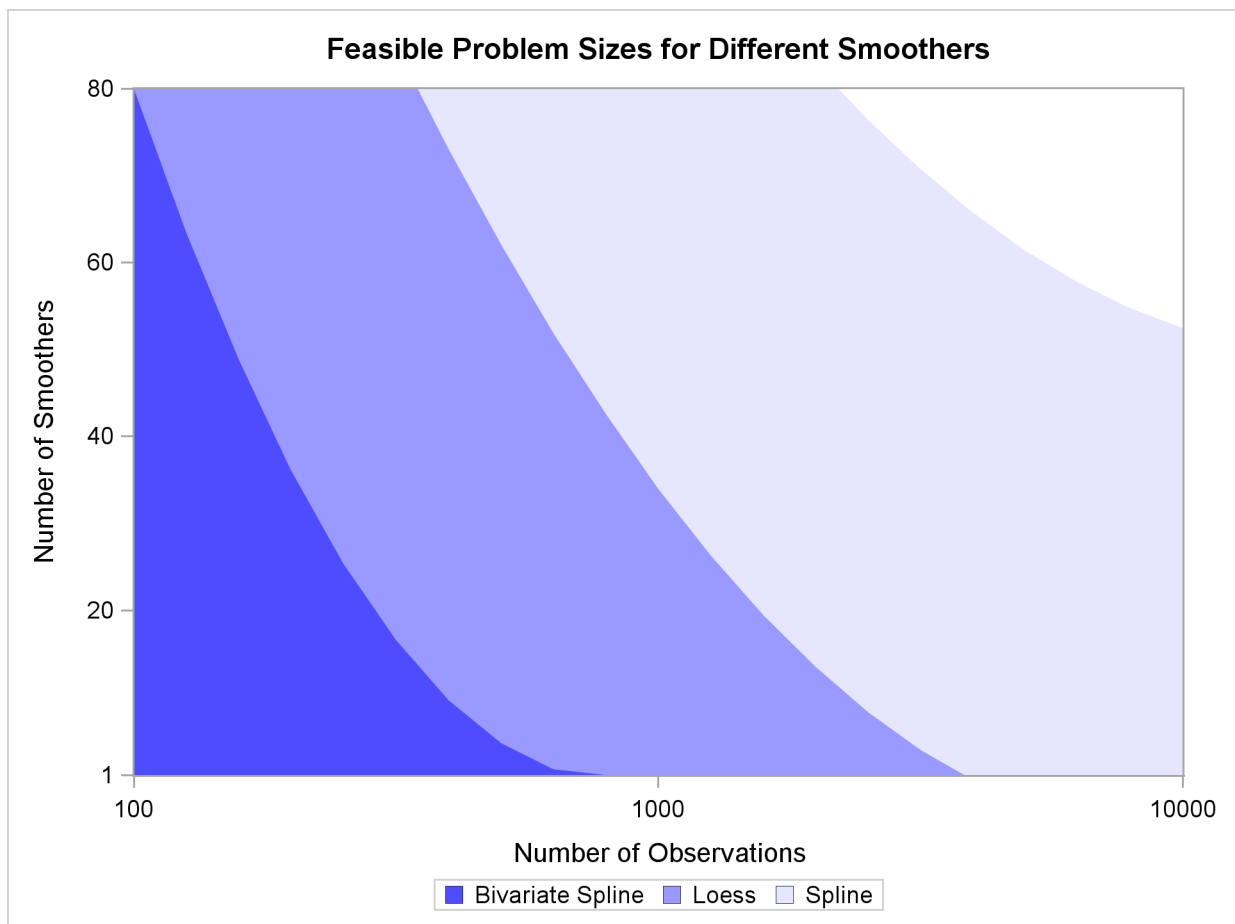


Figure 39.4 shows a rough estimation of feasible sizes for the smoothers that you can use, as a function of the number of observations and number of smoothing components. This figure depicts the regions where you can expect a single fit of an additive model to finish within a few minutes on a typical Pentium 4 system.

Note that the times reflected in Figure 39.4 are based on fitting additive models (no local scoring iterations) when no analysis of deviance or confidence limits are computed. The time required for fitting generalized additive models grows proportionally with the number of the local scoring iterations. Furthermore, analysis of deviance (if you do not request the fast approximations with the ANODEV option) requires fitting multiple GAM models as each smoothing component is omitted sequentially, and so the time estimates need to be multiplied by the number of smoothing components when analysis of deviance is performed. Finally computation of confidence limits for each individual smoother increases the time required, especially when loess smoothers are utilized.

For univariate spline smoothers, subject to the aforementioned caveats, problems that correspond to all shaded regions in Figure 39.4 can be completed within a few minutes. For univariate loess smoothers, the two darkest regions are feasible. For bivariate spline smoothers, problems that correspond to only the darkest shading can be completed in the order of a few minutes. The problems that correspond to the upper right unshaded region might be possible, but they require long computation times.

ODS Table Names

PROC GAM assigns a name to each table it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in the following table. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

Table 39.5 ODS Tables Produced by PROC GAM

ODS Table Name	Description	Statement	Option
ANODEV	Analysis of deviance table for smoothing variables	PROC	Default
ClassSummary	Summary of classification variables	PROC	Default
ConvergenceStatus	Convergence status of the local scoring algorithm	PROC	Default
InputSummary	Input data summary	PROC	Default
IterHistory	Iteration history table	MODEL	ITPRINT
IterSummary	Iteration summary	PROC	Default
FitSummary	Fit parameters and fit summary	PROC	Default
ParameterEstimates	Parameter estimation for regression variables	PROC	Default
ResponseProfile	Frequency counts for binary models	MODEL	DIST=BINOMIAL

By referring to the names of such tables, you can use the ODS OUTPUT statement to place one or more of these tables in output data sets.

ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “Statistical Graphics Using ODS.”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “A Primer on ODS Statistical Graphics” on page 599 in Chapter 21, “Statistical Graphics Using ODS.”

When ODS Graphics is enabled, the GAM procedure by default produces plots of the partial predictions for each nonparametric predictor in the model. Use the PLOTS option in the PROC GAM statement to control aspects of these plots.

ODS Graph Names

PROC GAM assigns a name to each graph it creates by using ODS. You can use these names to reference the graphs when using ODS. The names are listed in Table 39.6.

Table 39.6 Graphs Produced by PROC GAM

ODS Graph Name	Plot Description	PLOTS= Option
SmoothingComponentPlot	Panel of multiple partial prediction curves	COMPONENTS
SmoothingComponentPlot	Unpacked partial prediction curves	COMPONENTS(UNPACK)

By default, partial prediction plots for each component are displayed in panels containing at most six plots. If you specify more than six smoothing components, multiple panels are used. Use the PLOTS(UNPACK) option in the PROC GAM statement to display these plots individually.

Examples: GAM Procedure

Example 39.1: Generalized Additive Model with Binary Data

This example illustrates the capabilities of the GAM procedure and compares it to the GENMOD procedure. From this example, you can see that PROC GAM is very useful in visualizing the data and detecting the nonlinearity among the variables.

The data used in this example are based on a study by Bell et al. (1994). Bell and his associates studied the result of multiple-level thoracic and lumbar laminectomy, a corrective spinal surgery commonly performed on children. The data in the study consist of retrospective measurements on 83 patients. The specific outcome of interest is the presence (1) or absence (0) of kyphosis, defined as a forward flexion of the

spine of at least 40 degrees from vertical. The available predictor variables are age in months at time of the operation (Age), the starting of vertebrae levels involved in the operation (StartVert), and the number of levels involved (NumVert). The goal of this analysis is to identify risk factors for kyphosis. PROC GENMOD can be used to investigate the relationship among kyphosis and the predictors. The following statements create the data kyphosis and fit a logistic model specifying linear effects for the three predictors:

```

title 'Comparing PROC GAM with PROC GENMOD';
data kyphosis;
  input Age StartVert NumVert Kyphosis @@;
  datalines;
71 5 3 0      158 14 3 0      128 5 4 1
2 1 5 0      1 15 4 0      1 16 2 0
61 17 2 0     37 16 3 0     113 16 2 0
59 12 6 1     82 14 5 1     148 16 3 0
18 2 5 0      1 12 4 0     243 8 8 0
168 18 3 0    1 16 3 0     78 15 6 0
175 13 5 0    80 16 5 0     27 9 4 0
22 16 2 0    105 5 6 1     96 12 3 1
131 3 2 0    15 2 7 1     9 13 5 0
12 2 14 1    8 6 3 0     100 14 3 0
4 16 3 0    151 16 2 0     31 16 3 0
125 11 2 0   130 13 5 0     112 16 3 0
140 11 5 0   93 16 3 0     1 9 3 0
52 6 5 1    20 9 6 0     91 12 5 1
73 1 5 1    35 13 3 0     143 3 9 0
61 1 4 0    97 16 3 0     139 10 3 1
136 15 4 0   131 13 5 0     121 3 3 1
177 14 2 0   68 10 5 0     9 17 2 0
139 6 10 1   2 17 2 0     140 15 4 0
72 15 5 0   2 13 3 0     120 8 5 1
51 9 7 0    102 13 3 0     130 1 4 1
114 8 7 1   81 1 4 0     118 16 3 0
118 16 4 0   17 10 4 0     195 17 2 0
159 13 4 0   18 11 4 0     15 16 5 0
158 15 4 0   127 12 4 0     87 16 4 0
206 10 4 0   11 15 3 0     178 15 4 0
157 13 3 1   26 13 7 0     120 13 2 0
42 6 7 1    36 13 4 0
;

proc genmod data=kyphosis descending;
  model Kyphosis = Age StartVert NumVert/link=logit dist=binomial;
run;

```

The GENMOD analysis of the independent variable effects is shown in [Output 39.1.1](#). Based on these results, the only significant factor is StartVert with a log odds ratio of -0.1972 . The variable NumVert has a p -value of 0.0904 with a log odds ratio of 0.3031.

Output 39.1.1 GENMOD Analysis: Partial Output

Comparing PROC GAM with PROC GENMOD							
The GENMOD Procedure							
Analysis Of Maximum Likelihood Parameter Estimates							
Parameter	DF	Estimate	Standard Error	Wald	95% Confidence Limits	Wald Chi-Square	Pr > ChiSq
Intercept	1	-1.2497	1.2424	-3.6848	1.1853	1.01	0.3145
Age	1	0.0061	0.0055	-0.0048	0.0170	1.21	0.2713
StartVert	1	-0.1972	0.0657	-0.3260	-0.0684	9.01	0.0027
NumVert	1	0.3031	0.1790	-0.0477	0.6540	2.87	0.0904
Scale	0	1.0000	0.0000	1.0000	1.0000		

NOTE: The scale parameter was held fixed.

The GENMOD procedure assumes a strict linear relationship between the predictors and the response function, which is the logit (log odds) in this model. The following SAS statements use PROC GAM to investigate a less restrictive model, with moderately flexible spline terms for each of the predictors:

```

title 'Comparing PROC GAM with PROC GENMOD';
proc gam data=kyphosis;
  model Kyphosis (event='1') = spline(Age      ,df=3)
                               spline(StartVert,df=3)
                               spline(NumVert  ,df=3) / dist=binomial;
run;

```

The MODEL statement requests an additive model with a univariate smoothing spline for each term. The response variable option `EVENT=` chooses `Kyphosis= 1` (presence) as the event so that the probability of presence of kyphosis is modeled. The option `DIST=BINOMIAL` with binary responses specifies a logistic model. Each term is fit by using a univariate smoothing spline with three degrees of freedom. Of these three degrees of freedom, one is taken up by the linear portion of the fit and two are left for the nonlinear spline portion. Although this might seem to be an unduly modest amount of flexibility, it is better to be conservative with a data set this small.

Output 39.1.2 and Output 39.1.3 list the output from PROC GAM.

Output 39.1.2 Summary Statistics

```

Comparing PROC GAM with PROC GENMOD

The GAM Procedure
Dependent Variable: Kyphosis
Smoothing Model Component(s): spline(Age) spline(StartVert) spline(NumVert)

Summary of Input Data Set

Number of Observations           83
Number of Missing Observations   0
Distribution                      Binomial
Link Function                     Logit

Response Profile

Ordered Value      Kyphosis      Total
                    Frequency

1                   0           65
2                   1           18

NOTE: PROC GAM is modeling the probability that Kyphosis=1. One way to change
this to model the probability that Kyphosis=0 is to specify the response
variable option EVENT='0'.

Iteration Summary and Fit Statistics

Number of local scoring iterations           9
Local scoring convergence criterion         2.6635661E-9
Final Number of Backfitting Iterations      1
Final Backfitting Criterion                 5.2326593E-9
The Deviance of the Final Estimate         46.610922438
    
```

Output 39.1.3 Model Fit Statistics

```

Regression Model Analysis
Parameter Estimates

Parameter      Parameter Estimate      Standard Error      t Value      Pr > |t|

Intercept      -2.01533                1.45620             -1.38        0.1706
Linear (Age)    0.01213                 0.00794             1.53         0.1308
Linear (StartVert) -0.18615              0.07628            -2.44        0.0171
Linear (NumVert) 0.38347                0.19102             2.01         0.0484
    
```


Output 39.1.4 Approximate Analysis of Deviance Table

PROC GAM with Approximate Analysis of Deviance			
The GAM Procedure			
Dependent Variable: Kyphosis			
Smoothing Model Component(s): spline(Age) spline(StartVert) spline(NumVert)			
Smoothing Model Analysis			
Approximate Analysis of Deviance			
Source	DF	Chi-Square	Pr > ChiSq
Spline(Age)	2.00000	7.0888	0.0289
Spline(StartVert)	2.00000	5.0431	0.0803
Spline(NumVert)	2.00000	2.2471	0.3251

The “Approximate Analysis of Deviance” table shown in [Output 39.1.4](#) yields similar conclusions to those of the “Analysis of Deviance” table ([Output 39.1.3](#)). In addition to fitting the model using all the specified smoothing effects, the default ANODEV=REFIT option requires fitting p additional subset models to p smoothing effects. Each submodel is fit by omitting one smoothing term from the model. By contrast, the ANODEV=NOREFIT option keeps the nonparametric terms fixed and requires a weighted least squares fit for only the parametric part of the model. Hence, GAM with the ANODEV=NOREFIT option is computationally inexpensive and is useful for obtaining approximate analysis of deviance results for models with many smoothing effects. This option assumes that the remaining nonparametric terms do not change much with the deletion of one nonparametric component. It should be used with caution when a model contains highly correlated predictors.

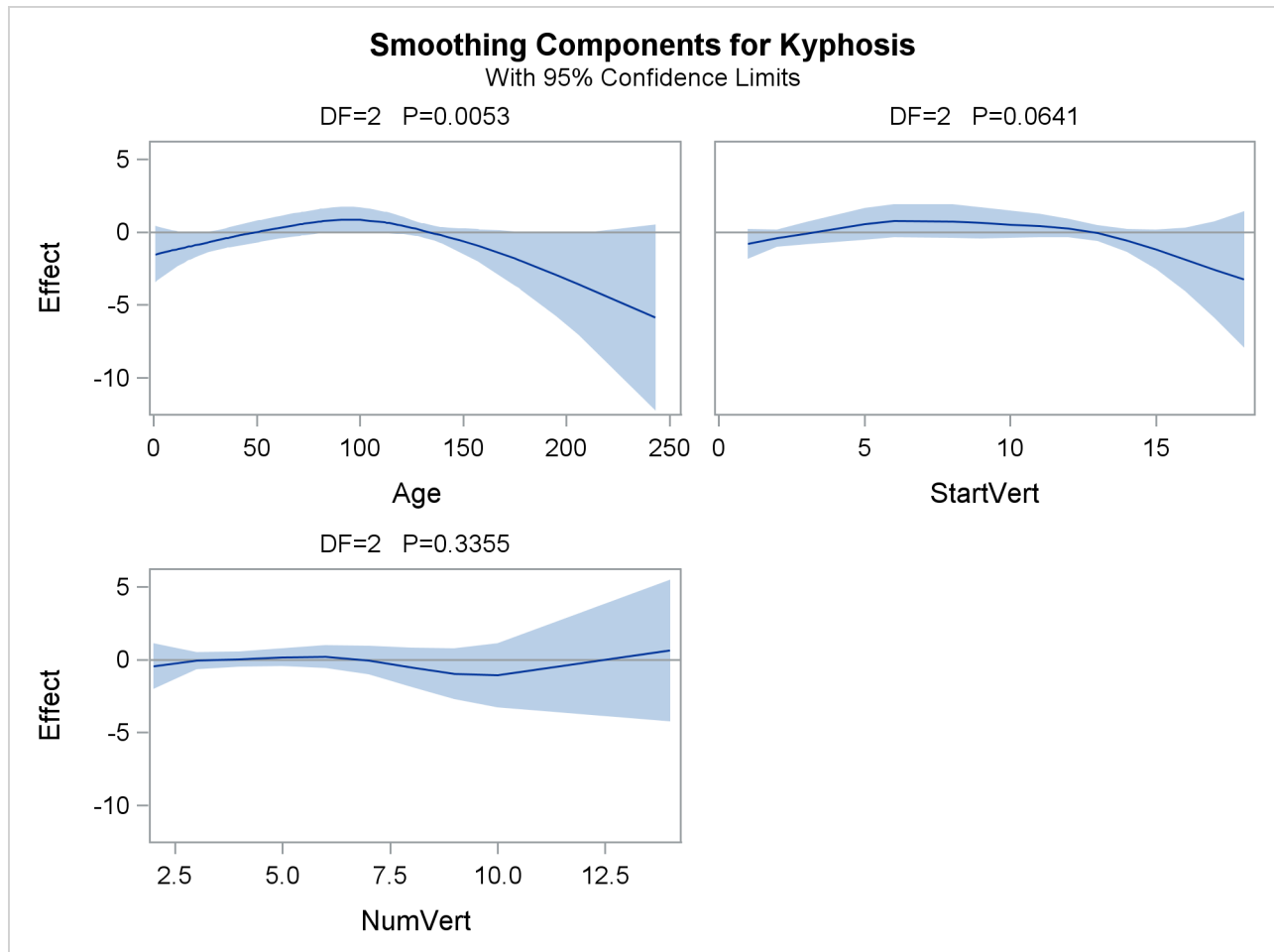
Plots of the partial predictions for each predictor can be used to investigate why PROC GAM and PROC GENMOD produce different results. The following statements use ODS Graphics to produce plots of the individual smoothing components. The CLM suboption in the PLOTS=COMPONENTS option adds a curvewise Bayesian confidence band to each smoothing component, while the COMMONAXES suboption forces all three smoothing component plots to share the same vertical axis limits, allowing a visual judgment of the relative nonparametric effect sizes.

```
ods graphics on;

proc gam data=kyphosis plots=components(clm commonaxes);
  model Kyphosis (event='1') = spline(Age      ,df=3)
                               spline(StartVert,df=3)
                               spline(NumVert  ,df=3) / dist=binomial;
run;

ods graphics off;
```

For general information about ODS Graphics, see Chapter 21, “[Statistical Graphics Using ODS](#).” For specific information about the graphics available in the GAM procedure, see the section “[ODS Graphics](#)” on page 2686. The smoothing component plots are displayed in [Output 39.1.5](#).

Output 39.1.5 Partial Prediction for Each Predictor

The plots show that the partial predictions corresponding to both Age and StartVert have a quadratic pattern, while NumVert has a more complicated but ultimately nonsignificant pattern.

An important difference between the first analysis of these data with PROC GENMOD and the subsequent analysis with PROC GAM is that PROC GAM indicates that Age has a significant but nonlinear association with kyphosis. The difference is due to the fact that the generalized linear model includes only the linear effect of Age whereas the generalized additive model allows a more complex relationship, which the plots indicate is nearly quadratic. Having used the GAM procedure to discover an appropriate form of the dependence of Kyphosis on each of the three independent variables, you can use the GENMOD procedure to fit and assess the corresponding parametric model. The following statements fit a generalized linear model with quadratic terms for all three variables. The parameter estimates are shown in [Output 39.1.6](#).

```

title 'Comparing PROC GAM with PROC GENMOD';
proc genmod data=kyphosis descending;
  model kyphosis = Age      Age      *Age
                StartVert StartVert*StartVert
                NumVert   NumVert  *NumVert /
                link=logit dist=binomial;
run;

```

Output 39.1.6 Logistic Model with Quadratic Terms

Comparing PROC GAM with PROC GENMOD						
The GENMOD Procedure						
Analysis Of Maximum Likelihood Parameter Estimates						
Parameter	DF	Estimate	Standard Error	Wald	95% Confidence Limits	Wald Chi-Square
Intercept	1	-5.8134	2.5618	-10.8345	-0.7923	5.15
Age	1	0.0819	0.0345	0.0143	0.1496	5.63
Age*Age	1	-0.0004	0.0002	-0.0008	-0.0000	4.32
StartVert	1	0.4394	0.3234	-0.1944	1.0733	1.85
StartVert*StartVert	1	-0.0396	0.0202	-0.0791	-0.0001	3.86
NumVert	1	0.3798	0.5988	-0.7939	1.5535	0.40
NumVert*NumVert	1	0.0020	0.0420	-0.0803	0.0843	0.00
Scale	0	1.0000	0.0000	1.0000	1.0000	

Analysis Of Maximum Likelihood Parameter Estimates	
Parameter	Pr > ChiSq
Intercept	0.0233
Age	0.0176
Age*Age	0.0376
StartVert	0.1742
StartVert*StartVert	0.0495
NumVert	0.5259
NumVert*NumVert	0.9621
Scale	

NOTE: The scale parameter was held fixed.

The p -value for the χ^2 test is 0.0376 for dropping the quadratic term of Age, 0.0495 for dropping the quadratic term of StartVert, and 0.9621 for dropping this quadratic term of NumVert. The results for the quadratic GENMOD model are consistent with the GAM results.

Example 39.2: Poisson Regression Analysis of Component Reliability

In this example, the number of maintenance repairs on a complex system are modeled as realizations of Poisson random variables. The system under investigation has a large number of components, which occasionally break down and are replaced or repaired. During a four-year period, the system was observed to be in a state of steady operation, meaning that the rate of operation remained approximately constant. A monthly maintenance record is available for that period, which tracks the number of components removed for maintenance each month. The data are listed in the following statements, which create a SAS data set:


```

title 'Analysis of Component Reliability';
data equip;
  input year month removals @@;
  datalines;
1987  1  2 1987  2  4 1987  3  3
1987  4  3 1987  5  3 1987  6  8
1987  7  2 1987  8  6 1987  9  3
1987 10  9 1987 11  4 1987 12 10
1988  1  4 1988  2  6 1988  3  4
1988  4  4 1988  5  3 1988  6  5
1988  7  3 1988  8  4 1988  9  5
1988 10  3 1988 11  6 1988 12  3
1989  1  2 1989  2  6 1989  3  1
1989  4  5 1989  5  5 1989  6  4
1989  7  2 1989  8  2 1989  9  2
1989 10  5 1989 11  1 1989 12 10
1990  1  3 1990  2  8 1990  3 12
1990  4  7 1990  5  3 1990  6  2
1990  7  4 1990  8  3 1990  9  0
1990 10  6 1990 11  6 1990 12  6
;

```

For planning purposes, it is of interest to understand the long- and short-term trends in the maintenance needs of the system. Over the long term, it is suspected that the quality of new components and repair work improves over time, so the number of component removals would tend to decrease from year to year. It is not known whether the robustness of the system is affected by seasonal variations in the operating environment, but this possibility is also of interest.

Because the maintenance record is in the form of counts, the number of removals are modeled as realizations of Poisson random variables. Denote by λ_{ij} the unobserved component removal rate for year i and month j . Since the data were recorded at regular intervals (from a system operating at a constant rate), each λ_{ij} is assumed to be a function of year and month only.

A preliminary two-way analysis is performed by using PROC GENMOD to make broad inferences on repair trends. A log-link is specified for the model

$$\log \lambda_{ij} = \mu + \alpha_i^Y + \alpha_j^M$$

where μ is a grand mean, α_i^Y is the effect of the i th year, and α_j^M is the effect of the j th month.

In the following statements, the CLASS statement declares the variables year and month as categorical. Type III sum of squares are requested to test whether there is an overall effect of year and/or month.

```

title2 'Two-way model';
proc genmod data=equip;
  class year month;
  model removals=year month / dist=Poisson link=log type3;
run;

```

Output 39.2.1 displays the listed Type III statistics for the fitted model. With the test for year effects yielding a p -value of 0.4527, there is no evidence of a long-term trend in maintenance rates. Apparently, the quality of new or repaired components did not change between 1987 and 1990. However, the test for monthly trends does yield a small p -value of 0.0321, indicating that seasonal trends are significant at the $\alpha = 0.05$ level.

Output 39.2.1 PROC GENMOD Listing for Type III Analysis

Analysis of Component Reliability			
Two-way model			
The GENMOD Procedure			
LR Statistics For Type 3 Analysis			
Source	DF	Chi-Square	Pr > ChiSq
year	3	2.63	0.4527
month	11	21.12	0.0321

If `year` is dropped from the model, the focus of the analysis is now on identifying the form of the underlying seasonal trend, which is a task that PROC GAM is especially suited for. PROC GAM will be used to fit both a reduced categorical model, with `year` eliminated, and a nonparametric spline model. Although PROC GENMOD also has the capability to fit categorical models, as demonstrated earlier, PROC GAM will be used here to fit both models for a better comparison.

The following PROC GAM statements specify the reduced categorical model and write predicted values to a data set. For this part of the analysis, a CLASS statement is again used to specify that `month` is a categorical variable. In the follow-up, the seasonal effect will be treated as a nonparametric function of `month`.

```

title2 'One-way model';
proc gam data=equip;
  class month;
  model removals=param(month) / dist=Poisson;
  output out=est p;
run;

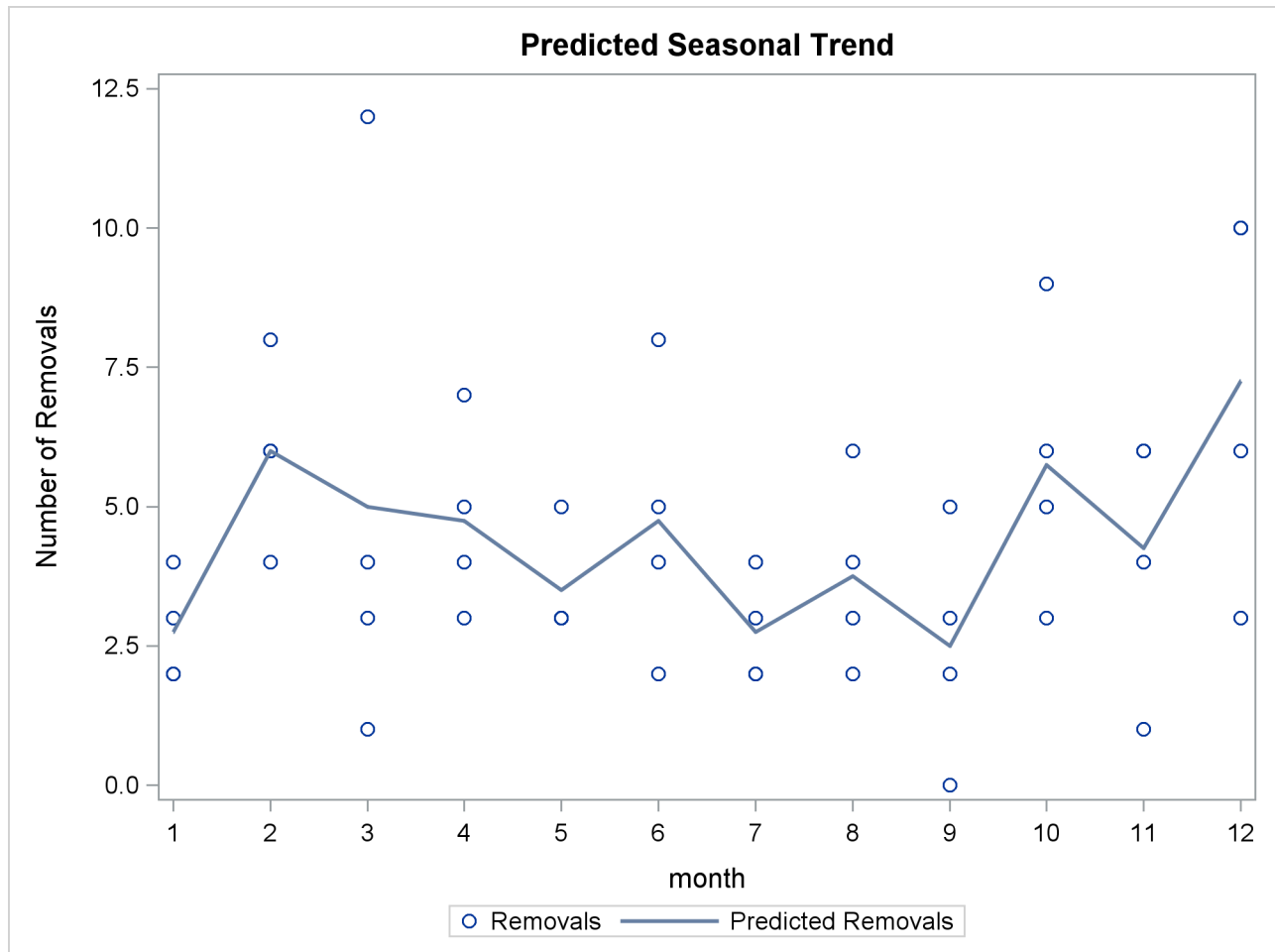
```

The following statements use the SGPLOT procedure to generate a plot of the estimated seasonal trend. The plot is displayed in [Output 39.2.2](#).

```

proc sort data=est;by month;run;
proc sgplot data=est;
  title "Predicted Seasonal Trend";
  yaxis label="Number of Removals";
  xaxis integer values=(1 to 12);
  scatter x=Month y=Removals / name="points"
          legendLabel="Removals";
  series x=Month y=p_Removals / name="line"
         legendLabel="Predicted Removals"
         lineattrs = GRAPHFIT;
  discretelegend "points" "line";
run;

```

Output 39.2.2 Predicted Seasonal Trend from a Parametric Model Fit Using a CLASS Statement

The predicted repair rates shown in [Output 39.2.2](#) form a jagged seasonal pattern. Ignoring the month-to-month fluctuations, which are difficult to explain and can be artifacts of random noise, the general removal rate trend is high in winter and low in summer.

One advantage of nonparametric regression is its ability to highlight general trends in the data, such as those described earlier, and to attribute local fluctuations to unexplained random noise. The nonparametric regression model used by PROC GAM specifies that the underlying removal rates λ_j are of the form

$$\log \lambda_j = \beta_0 + \beta_1 \text{Month}_j + s(\text{Month}_j)$$

where β_1 is a linear coefficient and $s(\cdot)$ is a nonparametric regression function. β_1 and $s(\cdot)$ define the linear and nonparametric parts, respectively, of the seasonal trend.

The following statements request that PROC GAM fit a cubic spline model to the monthly repair data. The output listing is displayed in [Output 39.2.3](#) and [Output 39.2.4](#).

```

title 'Analysis of Component Reliability';
title2 'Spline model';
proc gam data=equip;
  model removals=spline(month) / dist=Poisson method=gcv;
run;

```

The `METHOD=GCV` option is used to determine an appropriate level of smoothing.

Output 39.2.3 PROC GAM Listing for Cubic Spline Regression Using the **METHOD=GCV** Option

```

Analysis of Component Reliability
      Spline model

      The GAM Procedure
      Dependent Variable: removals
      Smoothing Model Component(s): spline(month)

      Summary of Input Data Set

      Number of Observations           48
      Number of Missing Observations   0
      Distribution                      Poisson
      Link Function                    Log
    
```

Output 39.2.4 Model Fit Statistics

```

Regression Model Analysis
      Parameter Estimates

      Parameter           Parameter Estimate      Standard Error      t Value      Pr > |t|

      Intercept           1.34594           0.14509           9.28         <.0001
      Linear(month)       0.02274           0.01893           1.20         0.2362

      Smoothing Model Analysis
      Fit Summary for Smoothing Components

      Component           Smoothing Parameter      DF           GCV           Num Unique Obs

      Spline(month)       0.901512           1.879980      0.115848      12

      Smoothing Model Analysis
      Analysis of Deviance

      Source           DF           Sum of Squares      Chi-Square      Pr > ChiSq

      Spline(month)     1.87998      8.877764           8.8778         0.0103
    
```

Notice in the listing in **Output 39.2.4** that the DF value chosen for the nonlinear portion of the spline by minimizing GCV is about 1.88, which is smaller than the default value of 3. This indicates that the spline model of the seasonal trend is relatively simple. As indicated by the “Analysis of Deviance” table, it is a significant feature of the data. The table lists a *p*-value of 0.0103 for the hypothesis of no seasonal trend. Note also that the “Parameter Estimates” table lists a *p*-value of 0.2362 for the hypothesis of no linear factor in the seasonal trend indicating no significant linear trend.

The following statements use ODS Graphics to plot the smoothing component for the effect of Month on predicted repair rates. The CLM suboption for the PLOTS=COMPONENTS option adds a 95% confidence band to the fit.

```
ods graphics on;

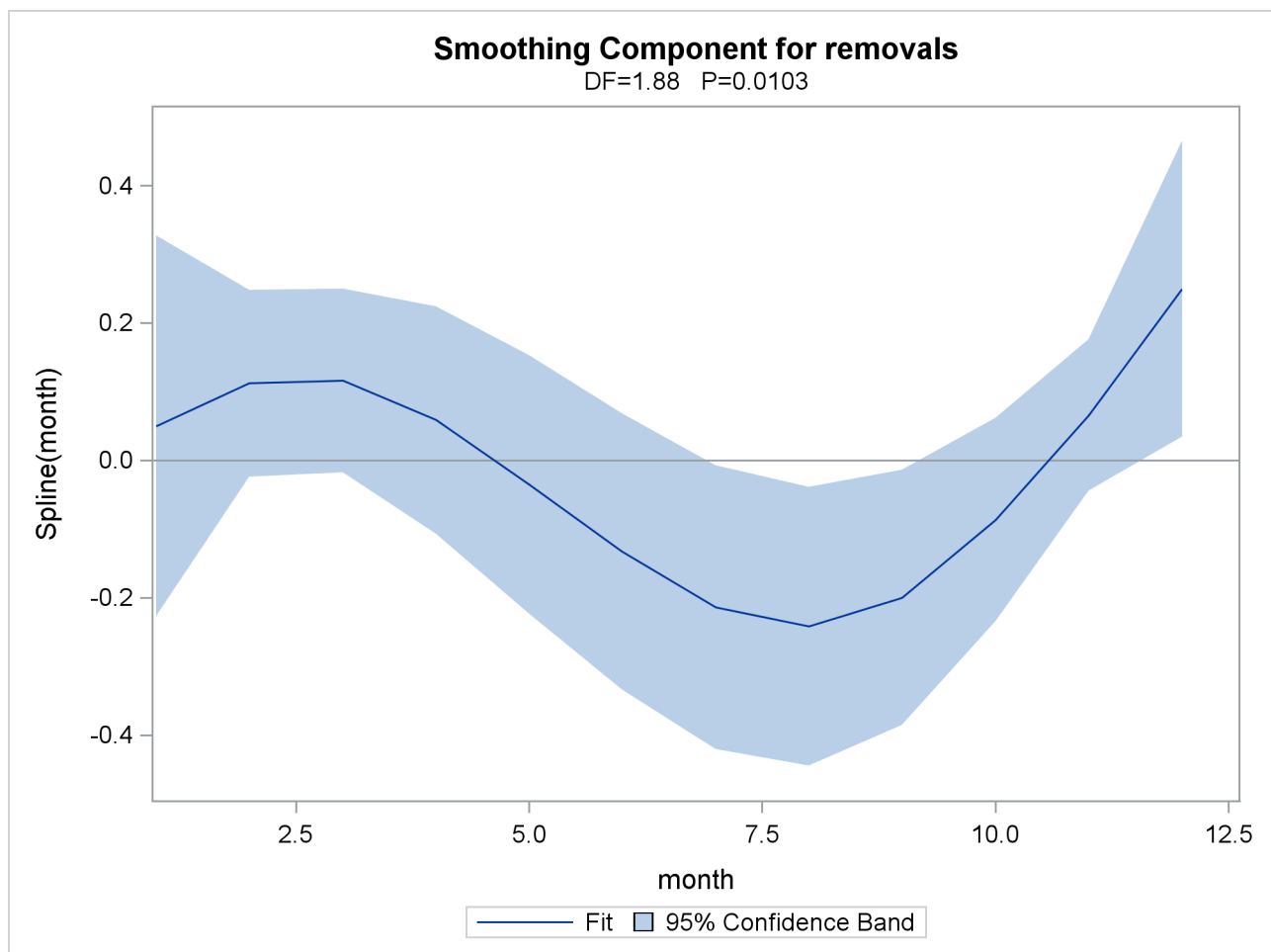
proc gam data=equip plots=components(clm);
  model removals=spline(month) / dist=Poisson method=gcv;
run;

ods graphics off;
```

For general information about ODS graphics, see Chapter 21, “Statistical Graphics Using ODS.” For specific information about the graphics available in the GAM procedure, see the section “ODS Graphics” on page 2686. The smoothing component plot is displayed in [Output 39.2.5](#).

In [Output 39.2.5](#), it is apparent that the pattern of repair rates follows the general pattern observed in [Output 39.2.2](#). However, the plot in [Output 39.2.5](#) is much cleaner because the month-to-month fluctuations are smoothed out to reveal the broader seasonal trend.

Output 39.2.5 Estimated Nonparametric Factor of Seasonal Trend, Along with 95% Confidence Bounds



In [Output 39.2.1](#) the small p -value ($p = 0.0321$) for the hypothesis of no seasonal trend indicates that the data exhibit significant seasonal structure. [Output 39.2.5](#) is a graphical illustration of the seasonality of the number of removals.

Example 39.3: Comparing PROC GAM with PROC LOESS

In an analysis of simulated data from a hypothetical chemistry experiment, additive nonparametric regression performed by PROC GAM is compared to the unrestricted multidimensional procedure of PROC LOESS.

In each repetition of the experiment, a catalyst is added to a chemical solution, thereby inducing synthesis of a new material. The data are measurements of the temperature of the solution, the amount of catalyst added, and the yield of the chemical reaction. The following statements read and plots the raw data.

```
data ExperimentA;
  format Temperature f4.0 Catalyst f6.3 Yield f8.3;
  input Temperature Catalyst Yield @@;
  datalines;
80 0.005 6.039 80 0.010 4.719 80 0.015 6.301
80 0.020 4.558 80 0.025 5.917 80 0.030 4.365
80 0.035 6.540 80 0.040 5.063 80 0.045 4.668
80 0.050 7.641 80 0.055 6.736 80 0.060 7.255
80 0.065 5.515 80 0.070 5.260 80 0.075 4.813
80 0.080 4.465 90 0.005 4.540 90 0.010 3.553
90 0.015 5.611 90 0.020 4.586 90 0.025 6.503
90 0.030 4.671 90 0.035 4.919 90 0.040 6.536
90 0.045 4.799 90 0.050 6.002 90 0.055 6.988
90 0.060 6.206 90 0.065 5.193 90 0.070 5.783
90 0.075 6.482 90 0.080 5.222 100 0.005 5.042
100 0.010 5.551 100 0.015 4.804 100 0.020 5.313
100 0.025 4.957 100 0.030 6.177 100 0.035 5.433
100 0.040 6.139 100 0.045 6.217 100 0.050 6.498
100 0.055 7.037 100 0.060 5.589 100 0.065 5.593
100 0.070 7.438 100 0.075 4.794 100 0.080 3.692
110 0.005 6.005 110 0.010 5.493 110 0.015 5.107
110 0.020 5.511 110 0.025 5.692 110 0.030 5.969
110 0.035 6.244 110 0.040 7.364 110 0.045 6.412
110 0.050 6.928 110 0.055 6.814 110 0.060 8.071
110 0.065 6.038 110 0.070 6.295 110 0.075 4.308
110 0.080 7.020 120 0.005 5.409 120 0.010 7.009
120 0.015 6.160 120 0.020 7.408 120 0.025 7.123
120 0.030 7.009 120 0.035 7.708 120 0.040 5.278
120 0.045 8.111 120 0.050 8.547 120 0.055 8.279
120 0.060 8.736 120 0.065 6.988 120 0.070 6.283
120 0.075 7.367 120 0.080 6.579 130 0.005 7.629
130 0.010 7.171 130 0.015 5.997 130 0.020 6.587
130 0.025 7.335 130 0.030 7.209 130 0.035 8.259
130 0.040 6.530 130 0.045 8.400 130 0.050 7.218
130 0.055 9.167 130 0.060 9.082 130 0.065 7.680
130 0.070 7.139 130 0.075 7.275 130 0.080 7.544
140 0.005 4.860 140 0.010 5.932 140 0.015 3.685
```

```

140 0.020 5.581 140 0.025 4.935 140 0.030 5.197
140 0.035 5.559 140 0.040 4.836 140 0.045 5.795
140 0.050 5.524 140 0.055 7.736 140 0.060 5.628
140 0.065 6.644 140 0.070 3.785 140 0.075 4.853
140 0.080 6.006
;

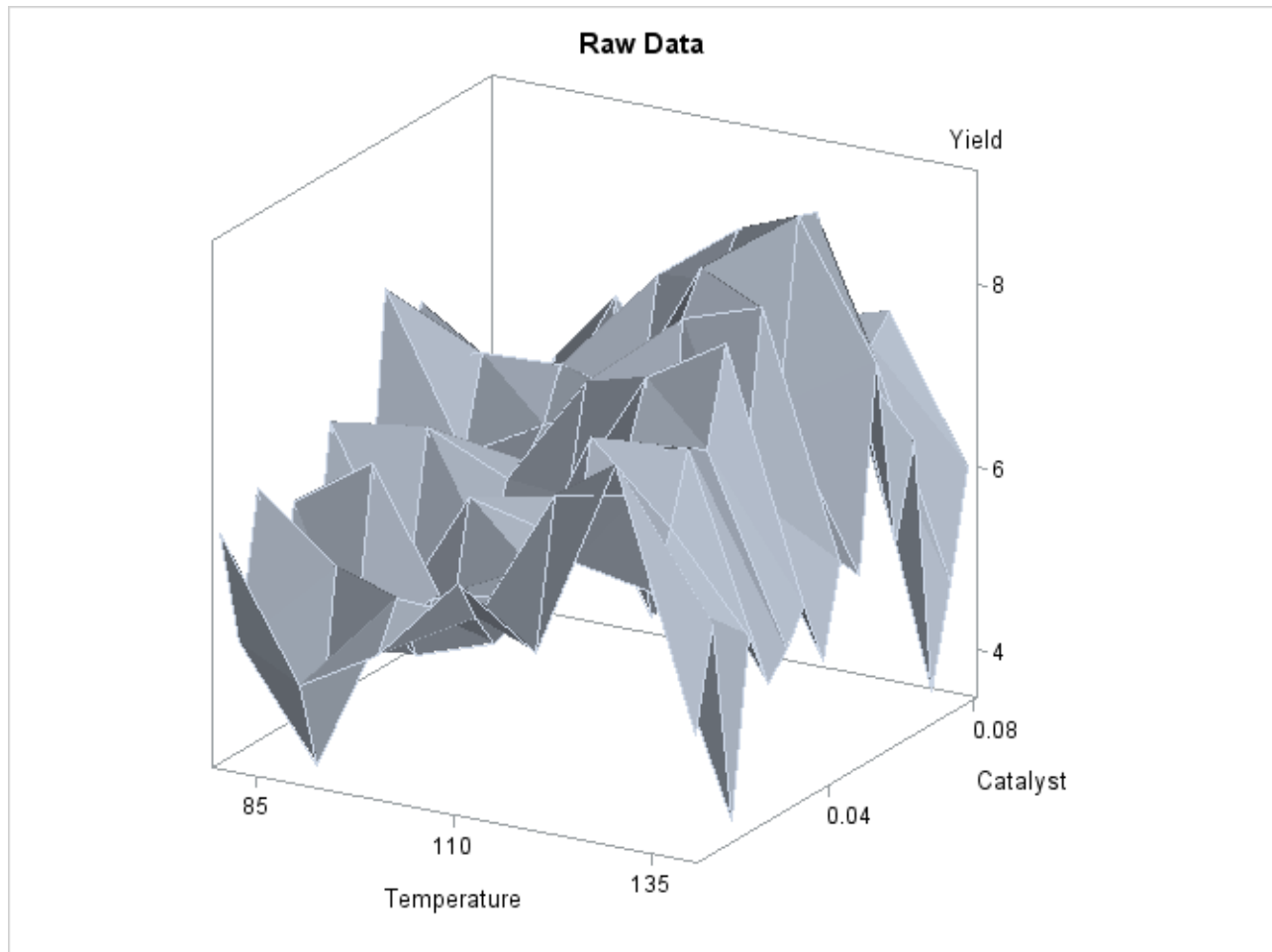
proc sort data=ExperimentA;
  by Temperature Catalyst;
run;

proc template;
  define statgraph surface;
    dynamic _X _Y _Z _T;
    begingraph;
    entrytitle _T;
    layout overlay3d/
      xaxisopts=(linearopts=(tickvaluesequence=
        (start=85 end=135 increment=25)))
      yaxisopts=(linearopts=(tickvaluesequence=
        (start=0 end=0.08 increment=0.04)))
      rotate=30 cube=false;
      surfaceplotparm x=_X y=_Y z=_Z;
    endlayout;
  endgraph;
end;
run;

ods graphics on;
proc sgrender data=ExperimentA template=surface;
  dynamic _X='Temperature' _Y='Catalyst' _Z='Yield' _T='Raw Data';
run;

```

The plot is displayed in [Output 39.3.1](#). A surface fitted to the plot of [Output 39.3.1](#) by PROC LOESS will be of a very general (and flexible) type, since the procedure requires only weak assumptions about the structure of the dependencies among the data. PROC GAM, on the other hand, makes stronger structural assumptions by restricting the fitted surface to an additive form. These differences will be demonstrated in this example.

Output 39.3.1 Surface Plot of Yield by Temperature and Amount of Catalyst

The following statements request that both PROC LOESS and PROC GAM fit surfaces to the data:

```
ods output ScoreResults=PredLOESS;
proc loess data=ExperimentA;
  model Yield = Temperature Catalyst
           / scale=sd select=gcv degree=2;
  score;
run;

proc gam data=PredLoess;
  model Yield = loess(Temperature) loess(Catalyst) / method=gcv;
  output out=PredGAM p=Gam_p_;
run;
```

In both cases the smoothing parameter was chosen as the value that minimizes GCV. This is performed automatically by PROC LOESS and PROC GAM.

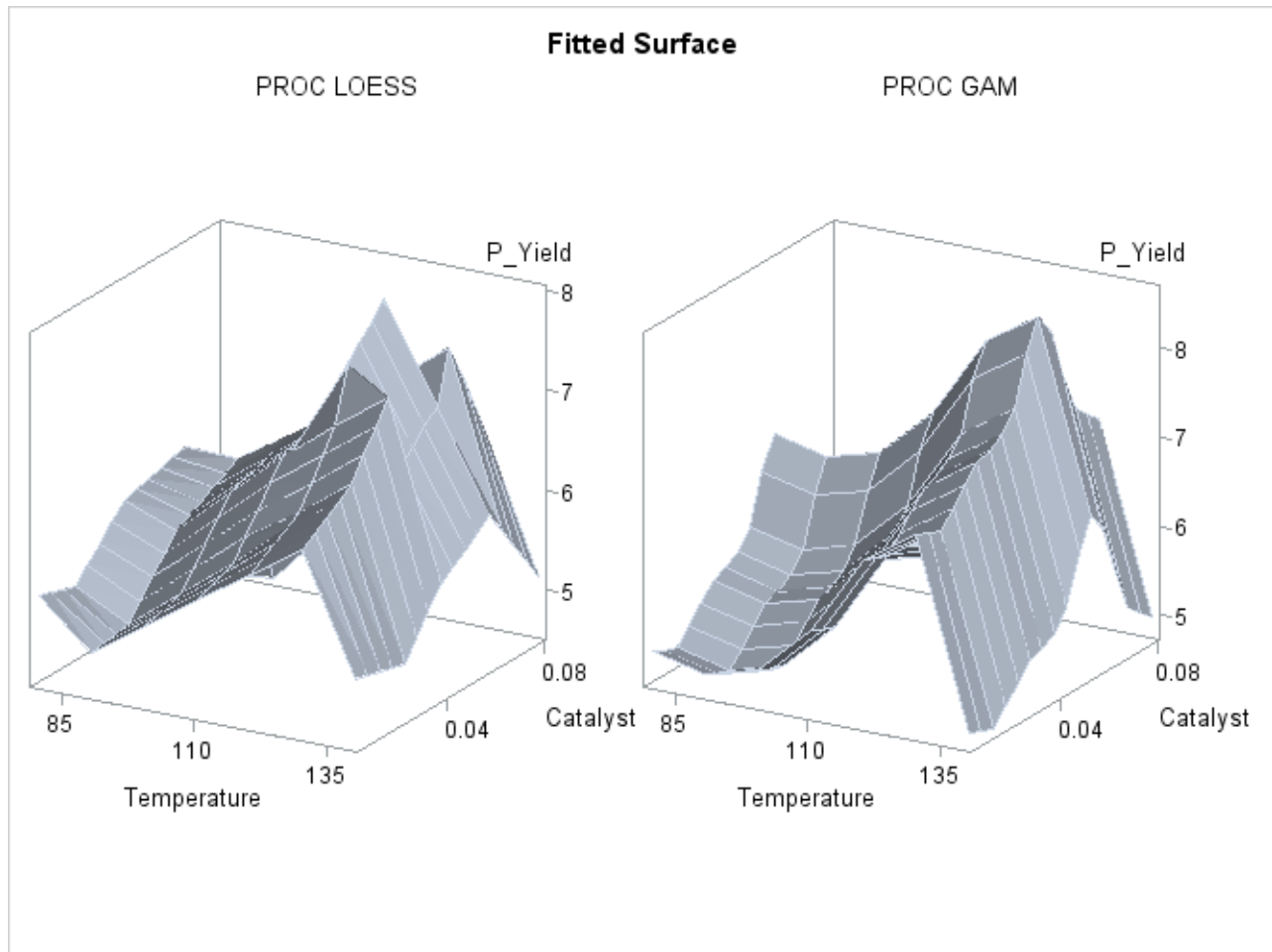
The following statements generate plots of the predicted yields, which are displayed in [Output 39.3.2](#):

```

proc template;
  define statgraph surfacel;
    begingraph;
      entrytitle "Fitted Surface";
      layout lattice/columns=2;
      layout
        overlay3d/xaxisopts=(linearopts=(tickvaluesequence=
          (start=85 end=135 increment=25)))
          yaxisopts=(linearopts=(tickvaluesequence=
            (start=0 end=0.08 increment=0.04)))
          zaxisopts=(label="P_Yield")
          rotate=30 cube=0;
      entry "PROC LOESS"/location=outside valign=top
        textattrs=graphlabeltext;
      surfaceplotparm x=Temperature y=Catalyst z=p_Yield;
    endlayout;
    layout
      overlay3d/xaxisopts=(linearopts=(tickvaluesequence=
        (start=85 end=135 increment=25)))
        yaxisopts=(linearopts=(tickvaluesequence=
          (start=0 end=0.08 increment=0.04)))
        rotate=30 cube=0
        zaxisopts=(label="P_Yield")
        rotate=30 cube=0;
      entry "PROC GAM"/location=outside valign=top
        textattrs=graphlabeltext;
      surfaceplotparm x=Temperature y=Catalyst z=Gam_p_Yield;
    endlayout;
  endlayout;
endgraph;
end;
run;

proc sgrender data=PredGAM template=surfacel;
run;

```

Output 39.3.2 Fitted Regression Surfaces

Though both PROC LOESS and PROC GAM use the statistical technique loess, it is apparent from [Output 39.3.2](#) that the manner in which it is applied is very different. By smoothing out the data in local neighborhoods, PROC LOESS essentially fits a surface to the data in pieces, one neighborhood at a time. The local regions are treated independently, so separate areas of the fitted surface are only weakly related. PROC GAM imposes additive structure, requiring that cross sections of the fitted surface always have the same shape and thereby relating regions that have a common value of the same individual regressor variable. Under that restriction, the loess technique need not be applied to the entire multidimensional scatter plot, but only to one-dimensional cross sections of the data.

The advantage of using additive model fitting is that its statistical power is directed toward univariate smoothing, and so it is able to discern the finer details of any underlying structure in the data. Regression data can be very sparse when viewed in the context of multidimensional space, even when every individual set of regressor values densely covers its range. This is the familiar curse of dimensionality. Sparse data greatly restrict the effectiveness of nonparametric procedures, but additive model fitting, when appropriate, is one way to overcome this limitation.

To examine these properties, you can use ODS Graphics to generate plots of cross sections of the unrestricted (PROC LOESS) and additive (PROC GAM) fitted surfaces for the variable Catalyst, as shown in the following statements:

```
proc template;
  define statgraph projection;
    beginingraph;
      entrytitle "Cross Sections of Fitted Surfaces";
      layout lattice/rows=2 columndatarange=unionall
        columngutter=10;
      columnAxes;
        columnAxis / display=all griddisplay=auto_on;
      endColumnAxes;

      layout overlay/
        xaxisopts=(display=none)
        yaxisopts=(label="LOESS Prediction"
          linearopts=(viewmin=2 viewmax=10));
        seriesplot x=Catalyst y=p_Yield /
          group=temperature
          name="Temperature";
      endlayout;

      layout overlay/
        xaxisopts=(display=none)
        yaxisopts=(label="GAM Prediction"
          linearopts=(viewmin=2 viewmax=10));
        seriesplot x=Catalyst y=Gam_p_Yield /
          group=temperature
          name="Temperature";
      endlayout;

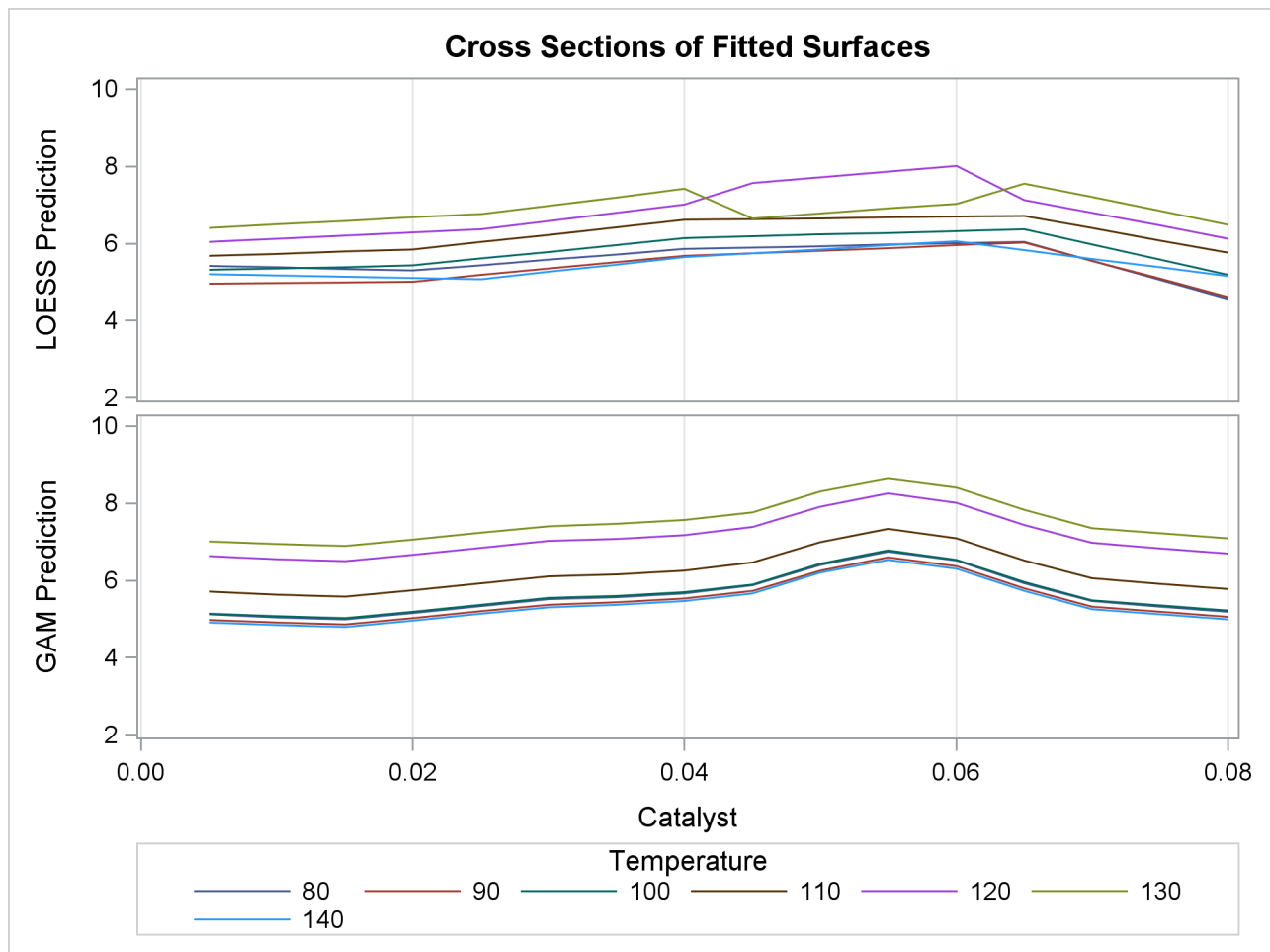
      columnheaders;
        discreteLegend "Temperature" / title = "Temperature";
      endcolumnheaders;

      endlayout;
    endgraph;
  end;
run;

proc sgrender data=PredGAM template=projection;
run;
```

The plots are displayed in Output 39.3.3.

Output 39.3.3 Cross Sections of Fitted Regression Surfaces



Notice that the cross sections in the top panel (PROC LOESS) of Output 39.3.3 have varying shapes, while every cross section in the bottom panel (PROC GAM) is the same curve shifted vertically. This illustrates precisely the kind of structural differences that distinguish additive models. A second important comparison to make between Output 39.3.2 and Output 39.3.3 is the level of detail in the fitted regression surfaces. Cross sections of the PROC LOESS surface are rather flat, but those of the additive surface have a clear shape. In particular, the ridge near Catalyst=0.055 is only vaguely evident in the PROC LOESS surface, but it is plainly revealed by the additive procedure.

For an example of a situation where unrestricted multidimensional fitting is preferred over additive regression, consider the following simulated data from a similar experiment. The following statements create another SAS data set and plot.

```

data ExperimentB;
  format Temperature f4.0 Catalyst f6.3 Yield f8.3;
  input Temperature Catalyst Yield @@;
  datalines;
80 0.005 9.115 80 0.010 9.275 80 0.015 9.160
80 0.020 7.065 80 0.025 6.054 80 0.030 4.899
80 0.035 4.504 80 0.040 4.238 80 0.045 3.232
80 0.050 3.135 80 0.055 5.100 80 0.060 4.802
80 0.065 8.218 80 0.070 7.679 80 0.075 9.669
80 0.080 9.071 90 0.005 7.085 90 0.010 6.814
90 0.015 4.009 90 0.020 4.199 90 0.025 3.377
90 0.030 2.141 90 0.035 3.500 90 0.040 5.967
90 0.045 5.268 90 0.050 6.238 90 0.055 7.847
90 0.060 7.992 90 0.065 7.904 90 0.070 10.184
90 0.075 7.914 90 0.080 6.842 100 0.005 4.497
100 0.010 2.565 100 0.015 2.637 100 0.020 2.436
100 0.025 2.525 100 0.030 4.474 100 0.035 6.238
100 0.040 7.029 100 0.045 8.183 100 0.050 8.939
100 0.055 9.283 100 0.060 8.246 100 0.065 6.927
100 0.070 7.062 100 0.075 5.615 100 0.080 4.687
110 0.005 3.706 110 0.010 3.154 110 0.015 3.726
110 0.020 4.634 110 0.025 5.970 110 0.030 8.219
110 0.035 8.590 110 0.040 9.097 110 0.045 7.887
110 0.050 8.480 110 0.055 6.818 110 0.060 7.666
110 0.065 4.375 110 0.070 3.994 110 0.075 3.630
110 0.080 2.685 120 0.005 4.697 120 0.010 4.268
120 0.015 6.507 120 0.020 7.747 120 0.025 9.412
120 0.030 8.761 120 0.035 8.997 120 0.040 7.538
120 0.045 7.003 120 0.050 6.010 120 0.055 3.886
120 0.060 4.897 120 0.065 2.562 120 0.070 2.714
120 0.075 3.141 120 0.080 5.081 130 0.005 8.729
130 0.010 7.460 130 0.015 9.549 130 0.020 10.049
130 0.025 8.131 130 0.030 7.553 130 0.035 6.191
130 0.040 6.272 130 0.045 4.649 130 0.050 3.884
130 0.055 2.522 130 0.060 4.366 130 0.065 3.272
130 0.070 4.906 130 0.075 6.538 130 0.080 7.380
140 0.005 8.991 140 0.010 8.029 140 0.015 8.417
140 0.020 8.049 140 0.025 4.608 140 0.030 5.025
140 0.035 2.795 140 0.040 3.123 140 0.045 3.407
140 0.050 4.183 140 0.055 3.750 140 0.060 6.316
140 0.065 5.799 140 0.070 7.992 140 0.075 7.835
140 0.080 8.985
;

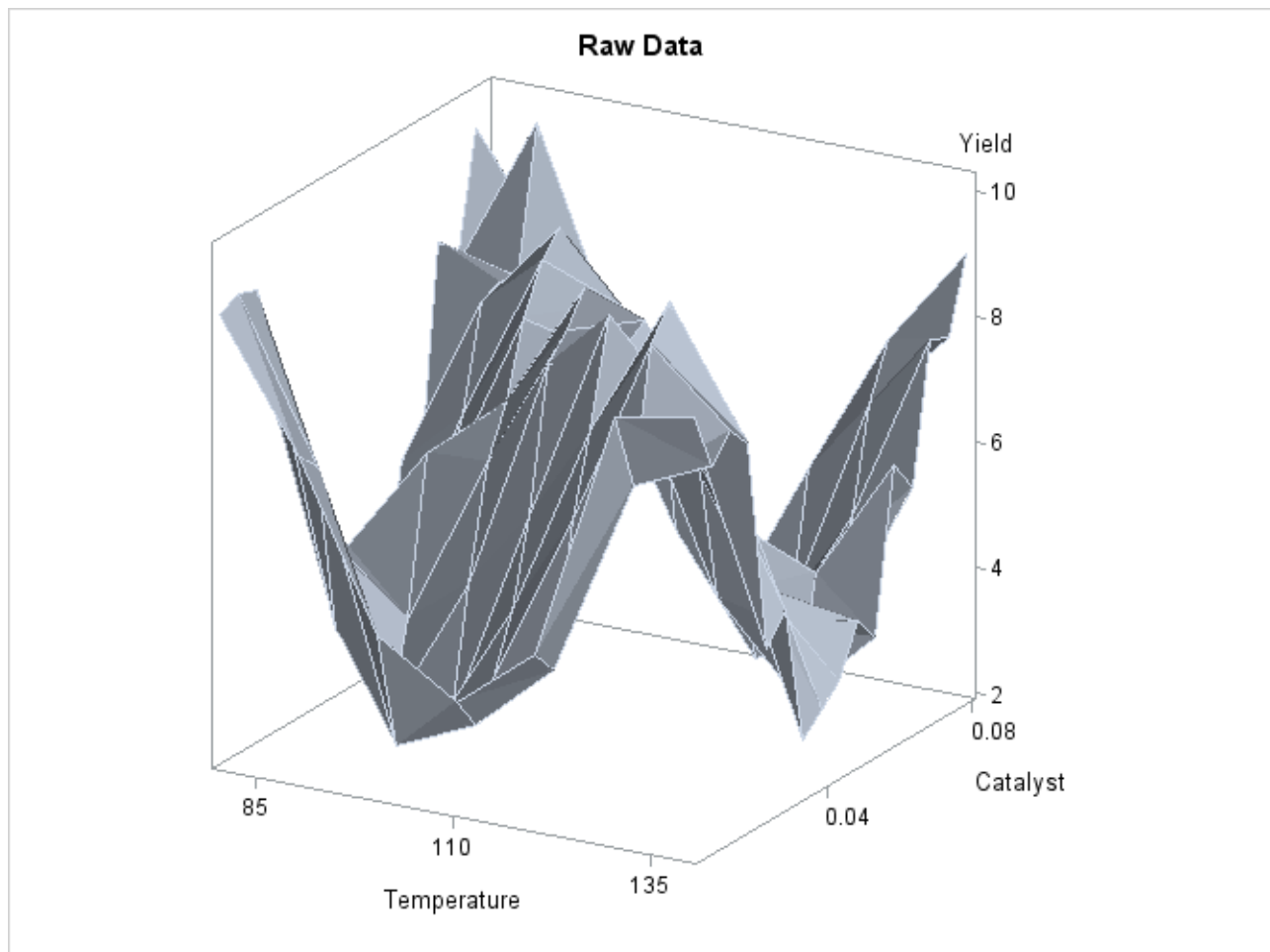
proc sort data=ExperimentB;
  by Temperature Catalyst;
run;

proc sgrender data=ExperimentB template=surface;
  dynamic _X='Temperature' _Y='Catalyst' _Z='Yield' _T='Raw Data';
run;

```

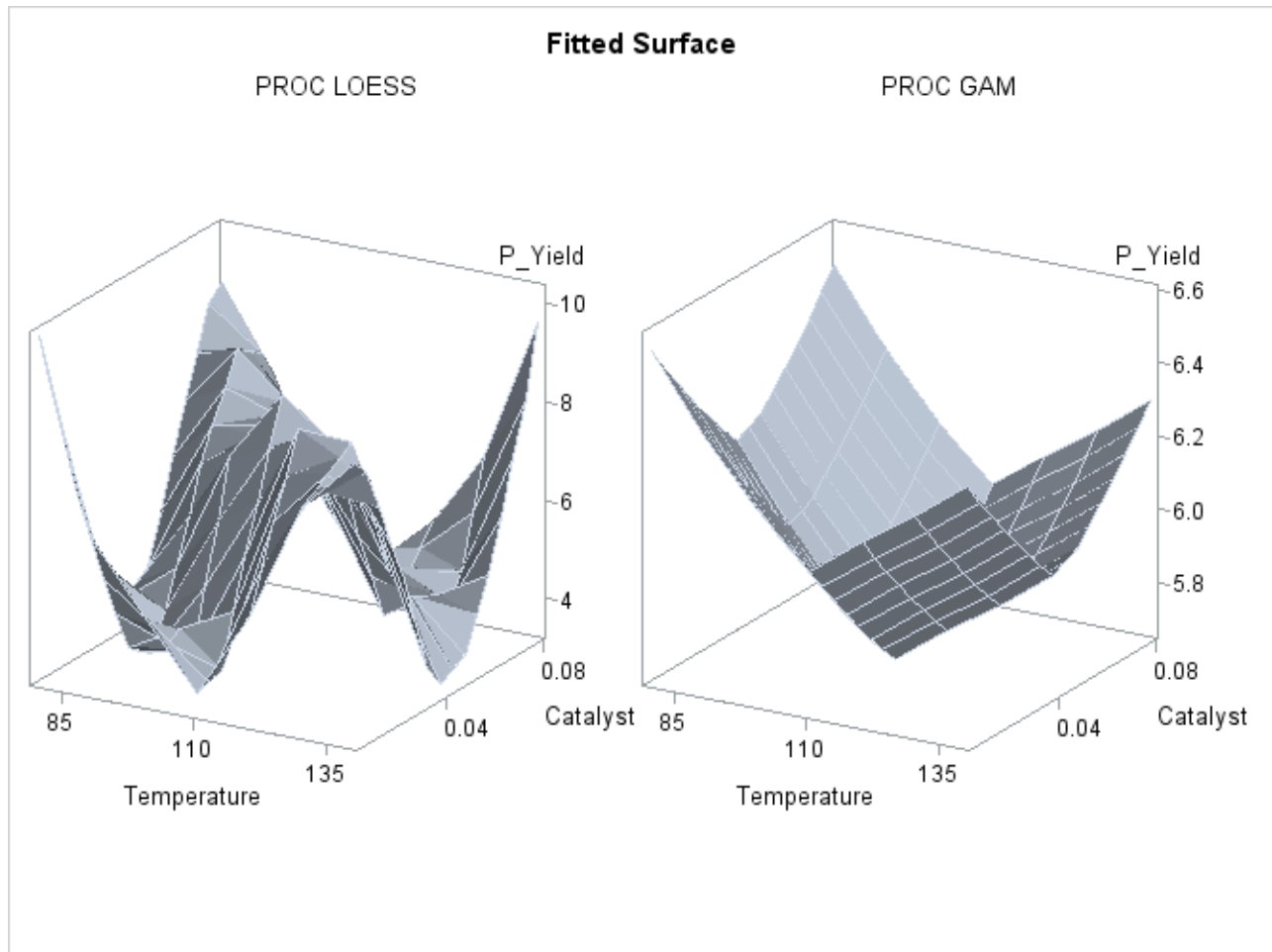
A plot of the raw data is displayed in [Output 39.3.4](#).

Output 39.3.4 Raw Data from Experiment B



Though the surface displayed in [Output 39.3.4](#) is quite jagged, a distinct feature of the plot is a large ridge that runs diagonally across its surface. One would expect that the ridge would appear in the fitted regression surface of an appropriate nonparametric procedure. Nevertheless, between PROC LOESS and PROC GAM, only PROC LOESS is able to capture this significant feature.

The SAS program for fitting the new data is essentially the same as that for the data set from the first experiment and produces output data set `PredGAMb` for this experiment. As in [Output 39.3.2](#), multivariate and additive fitted surfaces for these data are displayed in [Output 39.3.5](#).

Output 39.3.5 Fitted Regression Surfaces

It is clear from [Output 39.3.5](#) that the results of PROC LOESS and PROC GAM are completely different. While the plot in the left panel resembles the raw data plot in [Output 39.3.4](#), the plot in the right panel is essentially featureless.

To understand what is happening, compare the scatter plots of Yield by Catalyst for the two data sets in this example. These are generated by the following statements and displayed in [Output 39.3.6](#).

```
data PredGAM;
  set PredGAM;
  rename Yield=Yield_a;
run;

data PredGAMb;
  set PredGAMb;
  set PredGAM(keep=Yield_a);
run;
```

```

proc template;
  define statgraph scatter2;
    dynamic _X _Y1 _Y2;
    begingraph;
      entrytitle "Scatter Plots of Yield by Catalyst";
      layout lattice/rows=2 columndatarange=unionall
        rowdatarange=unionall
        columngutter=15;
      columnAxes;
        columnAxis / display=all griddisplay=auto_on;
      endColumnAxes;

      layout overlay/
        xaxisopts=(display=none)
        yaxisopts=(label="Yield of Experiment A"
          lineartopts=(viewmin=2 viewmax=10));
        scatterplot x=_X y=_Y1;
      endlayout;

      layout overlay/
        xaxisopts=(display=none)
        yaxisopts=(label="Yield of Experiment B"
          lineartopts=(viewmin=2 viewmax=10));
        scatterplot x=_X y=_Y2;
      endlayout;

    endlayout;
  endgraph;
end;
run;

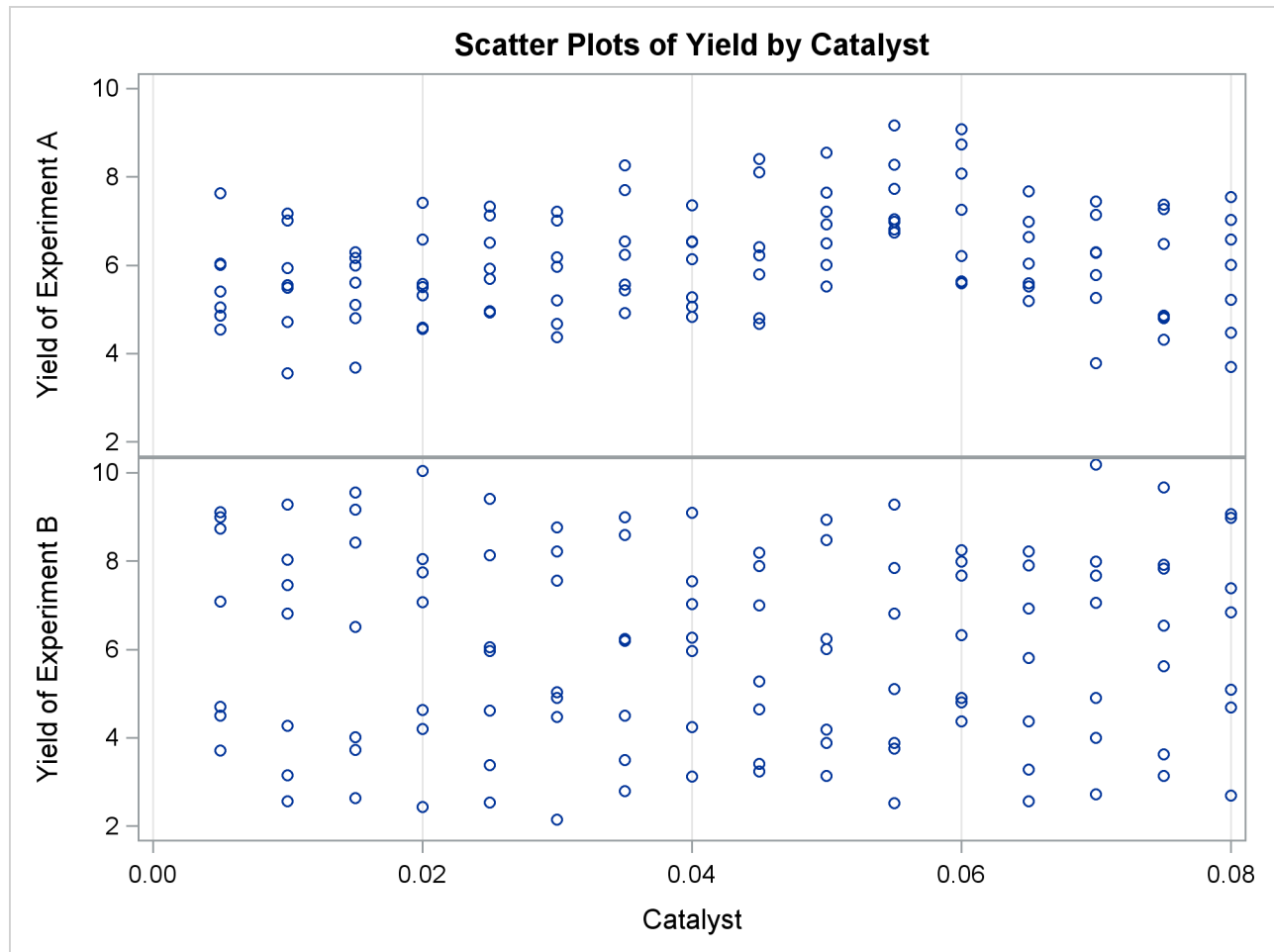
proc sgrender data=PredGAMb template=scatter2;
  dynamic _X='Catalyst' _Y1='Yield_a' _Y2='Yield';
run;

ods graphics off;

```

The top panel of [Output 39.3.6](#) hints at the same kind of structure exhibited in the fitted cross sections of [Output 39.3.3](#). In PROC GAM, the additive model component corresponding to Catalyst is fit to a similar scatter plot, with the partial residuals computed in the backfitting algorithm, so it is able to capture the trend seen here. In contrast, when the second data set is viewed from the perspective of [Output 39.3.6](#), the diagonal ridge apparent in [Output 39.3.4](#) is washed out, and no clear structure shows up in the scatter plot. As a result, the additive model fit produced by PROC GAM is relatively featureless.

Output 39.3.6 Scatter Plots of Yield by Catalyst



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Chapter 40

The GENMOD Procedure

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Overview: GENMOD Procedure

The GENMOD procedure fits generalized linear models, as defined by Nelder and Wedderburn (1972). The class of generalized linear models is an extension of traditional linear models that allows the mean of a population to depend on a *linear predictor* through a nonlinear *link function* and allows the response probability distribution to be any member of an exponential family of distributions. Many widely used statistical models are generalized linear models. These include classical linear models with normal errors, logistic and probit models for binary data, and log-linear models for multinomial data. Many other useful statistical models can be formulated as generalized linear models by the selection of an appropriate link function and response probability distribution.

See McCullagh and Nelder (1989) for a discussion of statistical modeling using generalized linear models. The books by Aitkin et al. (1989) and Dobson (1990) are also excellent references with many examples of applications of generalized linear models. Firth (1991) provides an overview of generalized linear models. Myers, Montgomery, and Vining (2002) provide applications of generalized linear models in the engineering and physical sciences. Collett (2003) and Hilbe (2009) provide comprehensive accounts of generalized linear models when the responses are binary.

The analysis of correlated data arising from repeated measurements when the measurements are assumed to be multivariate normal has been studied extensively. However, the normality assumption might not always be reasonable; for example, different methodology must be used in the data analysis when the responses are discrete and correlated. Generalized estimating equations (GEEs) provide a practical method with reasonable statistical efficiency to analyze such data.

Liang and Zeger (1986) introduced GEEs as a method of dealing with correlated data when, except for the correlation among responses, the data can be modeled as a generalized linear model. For example, correlated binary and count data in many cases can be modeled in this way.

The GENMOD procedure can fit models to correlated responses by the GEE method. You can use PROC GENMOD to fit models with most of the correlation structures from Liang and Zeger (1986) by using GEEs. For more details on GEEs, see Hardin and Hilbe (2003); Diggle, Liang, and Zeger (1994); Lipsitz et al. (1994).

Bayesian analysis of generalized linear models can be requested by using the BAYES statement in the GENMOD procedure. In Bayesian analysis, the model parameters are treated as random variables, and inference about parameters is based on the posterior distribution of the parameters, given the data. The posterior distribution is obtained using Bayes' theorem as the likelihood function of the data weighted with a prior distribution. The prior distribution enables you to incorporate knowledge or experience of the likely range of values of the parameters of interest into the analysis. If you have no prior knowledge of the parameter values, you can use a noninformative prior distribution, and the results of the Bayesian analysis will be very similar to a classical analysis based on maximum likelihood. A closed form of the posterior distribution is often not feasible, and a Markov chain Monte Carlo method by Gibbs sampling is used to simulate samples from the posterior distribution. See Chapter 7, "[Introduction to Bayesian Analysis Procedures](#)," for an introduction to the basic concepts of Bayesian statistics. Also see the section "[Bayesian Analysis: Advantages and Disadvantages](#)" on page 132 for a discussion of the advantages and disadvantages of Bayesian analysis. See Ibrahim, Chen, and Sinha (2001) for a detailed description of Bayesian analysis.

In a Bayesian analysis, a Gibbs chain of samples from the posterior distribution is generated for the model parameters. Summary statistics (mean, standard deviation, quartiles, HPD and credible intervals, correlation matrix) and convergence diagnostics (autocorrelations; Gelman-Rubin, Geweke, Raftery-Lewis, and

Heidelberger and Welch tests; the effective sample size; and Monte Carlo standard errors) are computed for each parameter, as well as the correlation matrix and the covariance matrix of the posterior sample. Trace plots, posterior density plots, and autocorrelation function plots that are created using ODS Graphics are also provided for each parameter.

The GENMOD procedure enables you to perform exact logistic regression, also called exact conditional binary logistic regression, and exact Poisson regression, also called exact conditional Poisson regression, by specifying one or more **EXACT** statements. You can test individual parameters or conduct a joint test for several parameters. The procedure computes two exact tests: the exact conditional score test and the exact conditional probability test. You can request exact estimation of specific parameters and corresponding odds ratios where appropriate. Point estimates, standard errors, and confidence intervals are provided.

The GENMOD procedure uses ODS Graphics to create graphs as part of its output. For general information about ODS Graphics, see Chapter 21, “[Statistical Graphics Using ODS](#).”

What Is a Generalized Linear Model?

A traditional linear model is of the form

$$y_i = \mathbf{x}_i' \boldsymbol{\beta} + \varepsilon_i$$

where y_i is the response variable for the i th observation. The quantity \mathbf{x}_i is a column vector of covariates, or explanatory variables, for observation i that is known from the experimental setting and is considered to be fixed, or nonrandom. The vector of unknown coefficients $\boldsymbol{\beta}$ is estimated by a least squares fit to the data \mathbf{y} . The ε_i are assumed to be independent, normal random variables with zero mean and constant variance. The expected value of y_i , denoted by μ_i , is

$$\mu_i = \mathbf{x}_i' \boldsymbol{\beta}$$

While traditional linear models are used extensively in statistical data analysis, there are types of problems such as the following for which they are not appropriate.

- It might not be reasonable to assume that data are normally distributed. For example, the normal distribution (which is continuous) might not be adequate for modeling counts or measured proportions that are considered to be discrete.
- If the mean of the data is naturally restricted to a range of values, the traditional linear model might not be appropriate, since the linear predictor $\mathbf{x}_i' \boldsymbol{\beta}$ can take on any value. For example, the mean of a measured proportion is between 0 and 1, but the linear predictor of the mean in a traditional linear model is not restricted to this range.
- It might not be realistic to assume that the variance of the data is constant for all observations. For example, it is not unusual to observe data where the variance increases with the mean of the data.

A generalized linear model extends the traditional linear model and is therefore applicable to a wider range of data analysis problems. A generalized linear model consists of the following components:

- The linear component is defined just as it is for traditional linear models:

$$\eta_i = \mathbf{x}_i' \boldsymbol{\beta}$$

- A monotonic differentiable link function g describes how the expected value of y_i is related to the linear predictor η_i :

$$g(\mu_i) = \mathbf{x}_i' \boldsymbol{\beta}$$

- The response variables y_i are independent for $i = 1, 2, \dots$ and have a probability distribution from an exponential family. This implies that the variance of the response depends on the mean μ through a *variance function* V :

$$\text{Var}(y_i) = \frac{\phi V(\mu_i)}{w_i}$$

where ϕ is a constant and w_i is a known weight for each observation. The *dispersion parameter* ϕ is either known (for example, for the binomial or Poisson distribution, $\phi = 1$) or must be estimated.

See the section “[Response Probability Distributions](#)” on page 2799 for the form of a probability distribution from the exponential family of distributions.

As in the case of traditional linear models, fitted generalized linear models can be summarized through statistics such as parameter estimates, their standard errors, and goodness-of-fit statistics. You can also make statistical inference about the parameters by using confidence intervals and hypothesis tests. However, specific inference procedures are usually based on asymptotic considerations, since exact distribution theory is not available or is not practical for all generalized linear models.

Examples of Generalized Linear Models

You construct a generalized linear model by deciding on response and explanatory variables for your data and choosing an appropriate link function and response probability distribution. Some examples of generalized linear models follow. Explanatory variables can be any combination of continuous variables, classification variables, and interactions.

Traditional Linear Model

- response variable: a continuous variable
- distribution: normal
- link function: identity, $g(\mu) = \mu$

Logistic Regression

- response variable: a proportion
- distribution: binomial
- link function: logit, $g(\mu) = \log\left(\frac{\mu}{1-\mu}\right)$

Poisson Regression in Log-Linear Model

- response variable: a count
- distribution: Poisson
- link function: $\log, g(\mu) = \log(\mu)$

Gamma Model with Log Link

- response variable: a positive, continuous variable
- distribution: gamma
- link function: $\log, g(\mu) = \log(\mu)$

The GENMOD Procedure

The GENMOD procedure fits a generalized linear model to the data by maximum likelihood estimation of the parameter vector β . There is, in general, no closed form solution for the maximum likelihood estimates of the parameters. The GENMOD procedure estimates the parameters of the model numerically through an iterative fitting process. The dispersion parameter ϕ is also estimated by maximum likelihood or, optionally, by the residual deviance or by Pearson's chi-square divided by the degrees of freedom. Covariances, standard errors, and p -values are computed for the estimated parameters based on the asymptotic normality of maximum likelihood estimators. A number of popular link functions and probability distributions are available in the GENMOD procedure. The built-in link functions are as follows:

- identity: $g(\mu) = \mu$
- logit: $g(\mu) = \log(\mu/(1 - \mu))$
- probit: $g(\mu) = \Phi^{-1}(\mu)$, where Φ is the standard normal cumulative distribution function
- power: $g(\mu) = \begin{cases} \mu^\lambda & \text{if } \lambda \neq 0 \\ \log(\mu) & \text{if } \lambda = 0 \end{cases}$
- log: $g(\mu) = \log(\mu)$
- complementary log-log: $g(\mu) = \log(-\log(1 - \mu))$

The available distributions and associated variance functions are as follows:

- normal: $V(\mu) = 1$
- binomial (proportion): $V(\mu) = \mu(1 - \mu)$
- Poisson: $V(\mu) = \mu$
- gamma: $V(\mu) = \mu^2$

- inverse Gaussian: $V(\mu) = \mu^3$
- negative binomial: $V(\mu) = \mu + k\mu^2$
- geometric: $V(\mu) = \mu + \mu^2$
- multinomial
- zero-inflated Poisson
- zero-inflated negative binomial

The negative binomial and zero-inflated negative binomial are distributions with an additional parameter k in the variance function. PROC GENMOD estimates k by maximum likelihood, or you can optionally set it to a constant value. For discussions of the negative binomial distribution, see McCullagh and Nelder (1989); Hilbe (1994, 2007); Long (1997); Cameron and Trivedi (1998); Lawless (1987).

The multinomial distribution is sometimes used to model a response that can take values from a number of categories. The binomial is a special case of the multinomial with two categories. See the section “[Multinomial Models](#)” on page 2817 and McCullagh and Nelder (1989, Chapter 5) for a description of the multinomial distribution.

The zero-inflated Poisson and zero-inflated negative binomial are included in PROC GENMOD even though they are not generalized linear models. They are useful extensions of generalized linear models. See the section “[Zero-Inflated Models](#)” on page 2818 for information about the zero-inflated distributions. Models for data with correlated responses fit by the GEE method are not available for zero-inflated distributions.

In addition, you can easily define your own link functions or distributions through DATA step programming statements used within the procedure.

An important aspect of generalized linear modeling is the selection of explanatory variables in the model. Changes in goodness-of-fit statistics are often used to evaluate the contribution of subsets of explanatory variables to a particular model. The deviance, defined to be twice the difference between the maximum attainable log likelihood and the log likelihood of the model under consideration, is often used as a measure of goodness of fit. The maximum attainable log likelihood is achieved with a model that has a parameter for every observation. See the section “[Goodness of Fit](#)” on page 2806 for formulas for the deviance.

One strategy for variable selection is to fit a sequence of models, beginning with a simple model with only an intercept term, and then to include one additional explanatory variable in each successive model. You can measure the importance of the additional explanatory variable by the difference in deviances or fitted log likelihoods between successive models. Asymptotic tests computed by the GENMOD procedure enable you to assess the statistical significance of the additional term.

The GENMOD procedure enables you to fit a sequence of models, up through a maximum number of terms specified in a MODEL statement. A table summarizes twice the difference in log likelihoods between each successive pair of models. This is called a *Type I* analysis in the GENMOD procedure, because it is analogous to Type I (sequential) sums of squares in the GLM procedure. As with the PROC GLM Type I sums of squares, the results from this process depend on the order in which the model terms are fit.

The GENMOD procedure also generates a *Type 3* analysis analogous to Type III sums of squares in the GLM procedure. A Type 3 analysis does not depend on the order in which the terms for the model are specified. A GENMOD procedure Type 3 analysis consists of specifying a model and computing likelihood ratio statistics for Type III contrasts for each term in the model. The contrasts are defined in the same way

as they are in the GLM procedure. The GENMOD procedure optionally computes Wald statistics for Type III contrasts. This is computationally less expensive than likelihood ratio statistics, but it is thought to be less accurate because the specified significance level of hypothesis tests based on the Wald statistic might not be as close to the actual significance level as it is for likelihood ratio tests.

A Type 3 analysis generalizes the use of Type III estimable functions in linear models. Briefly, a Type III estimable function (contrast) for an effect is a linear function of the model parameters that involves the parameters of the effect and any interactions with that effect. A test of the hypothesis that the Type III contrast for a main effect is equal to 0 is intended to test the significance of the main effect in the presence of interactions. See Chapter 42, “The GLM Procedure,” and Chapter 15, “The Four Types of Estimable Functions,” for more information about Type III estimable functions. Also see Littell, Freund, and Spector (1991).

Additional features of the GENMOD procedure include the following:

- likelihood ratio statistics for user-defined contrasts—that is, linear functions of the parameters and p -values based on their asymptotic chi-square distributions
- estimated values, standard errors, and confidence limits for user-defined contrasts and least squares means
- ability to create a SAS data set corresponding to most tables displayed by the procedure (see [Table 40.12](#) and [Table 40.13](#))
- confidence intervals for model parameters based on either the profile likelihood function or asymptotic normality
- syntax similar to that of PROC GLM for the specification of the response and model effects, including interaction terms and automatic coding of classification variables
- ability to fit GEE models for clustered response data
- ability to perform Bayesian analysis by Gibbs sampling

Getting Started: GENMOD Procedure

Poisson Regression

You can use the GENMOD procedure to fit a variety of statistical models. A typical use of PROC GENMOD is to perform Poisson regression.

You can use the Poisson distribution to model the distribution of cell counts in a multiway contingency table. Aitkin et al. (1989) have used this method to model insurance claims data. Suppose the following hypothetical insurance claims data are classified by two factors: age group (with two levels) and car type (with three levels).

```

data insure;
  input n c car$ age;
  ln = log(n);
  datalines;
500  42  small  1
1200 37  medium 1
100   1  large  1
400 101  small  2
500  73  medium 2
300  14  large  2
;

```

In the preceding data set, the variable *n* represents the number of insurance policyholders and the variable *c* represents the number of insurance claims. The variable *car* is the type of car involved (classified into three groups) and the variable *age* is the age group of a policyholder (classified into two groups).

You can use PROC GENMOD to perform a Poisson regression analysis of these data with a log link function. This type of model is sometimes called a *log-linear model*.

Assume that the number of claims *c* has a Poisson probability distribution and that its mean, μ_i , is related to the factors *car* and *age* for observation *i* by

$$\begin{aligned}
 \log(\mu_i) &= \log(n_i) + \mathbf{x}'_i \boldsymbol{\beta} \\
 &= \log(n_i) + \beta_0 + \\
 &\quad \text{car}_i(1)\beta_1 + \text{car}_i(2)\beta_2 + \text{car}_i(3)\beta_3 + \\
 &\quad \text{age}_i(1)\beta_4 + \text{age}_i(2)\beta_5
 \end{aligned}$$

The indicator variables $\text{car}_i(j)$ and $\text{age}_i(j)$ are associated with the *j*th level of the variables *car* and *age* for observation *i*

$$\text{car}_i(j) = \begin{cases} 1 & \text{if } \text{car} = j \\ 0 & \text{if } \text{car} \neq j \end{cases}$$

The β s are unknown parameters to be estimated by the procedure. The logarithm of the variable *n* is used as an *offset*—that is, a regression variable with a constant coefficient of 1 for each observation. A log-linear relationship between the mean and the factors *car* and *age* is specified by the log link function. The log link function ensures that the mean number of insurance claims for each car and age group predicted from the fitted model is positive.

The following statements invoke the GENMOD procedure to perform this analysis:

```

proc genmod data=insure;
  class car age;
  model c = car age / dist = poisson
                    link = log
                    offset = ln;
run;

```

The variables `car` and `age` are specified as CLASS variables so that PROC GENMOD automatically generates the indicator variables associated with `car` and `age`.

The MODEL statement specifies `c` as the response variable and `car` and `age` as explanatory variables. An intercept term is included by default. Thus, the model matrix \mathbf{X} (the matrix that has as its i th row the transpose of the covariate vector for the i th observation) consists of a column of 1s representing the intercept term and columns of 0s and 1s derived from indicator variables representing the levels of the `car` and `age` variables.

That is, the model matrix is

$$\mathbf{X} = \left[\begin{array}{c|ccc|cc} 1 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 & 1 \end{array} \right]$$

where the first column corresponds to the intercept, the next three columns correspond to the variable `car`, and the last two columns correspond to the variable `age`.

The response distribution is specified as Poisson, and the link function is chosen to be log. That is, the Poisson mean parameter μ is related to the linear predictor by

$$\log(\mu) = \mathbf{x}'_i \boldsymbol{\beta}$$

The logarithm of n is specified as an offset variable, as is common in this type of analysis. In this case, the offset variable serves to normalize the fitted cell means to a per-policyholder basis, since the total number of claims, not individual policyholder claims, is observed. PROC GENMOD produces the following default output from the preceding statements.

Figure 40.1 Model Information

The GENMOD Procedure	
Model Information	
Data Set	WORK.INSURE
Distribution	Poisson
Link Function	Log
Dependent Variable	c
Offset Variable	ln

The “Model Information” table displayed in Figure 40.1 provides information about the specified model and the input data set.

Figure 40.2 Class Level Information

Class Level Information				
Class	Levels	Values		
car	3	large	medium	small
age	2	1	2	

Figure 40.2 displays the “Class Level Information” table, which identifies the levels of the classification variables that are used in the model. Note that car is a character variable, and the values are sorted in alphabetical order. This is the default sort order, but you can select different sort orders with the `ORDER=` option in the PROC GENMOD statement.

Figure 40.3 Goodness of Fit

Criteria For Assessing Goodness Of Fit			
Criterion	DF	Value	Value/DF
Deviance	2	2.8207	1.4103
Scaled Deviance	2	2.8207	1.4103
Pearson Chi-Square	2	2.8416	1.4208
Scaled Pearson X2	2	2.8416	1.4208
Log Likelihood		837.4533	
Full Log Likelihood		-16.4638	
AIC (smaller is better)		40.9276	
AICC (smaller is better)		80.9276	
BIC (smaller is better)		40.0946	

The “Criteria For Assessing Goodness Of Fit” table displayed in Figure 40.3 contains statistics that summarize the fit of the specified model. These statistics are helpful in judging the adequacy of a model and in comparing it with other models under consideration. If you compare the deviance of 2.8207 with its asymptotic chi-square with 2 degrees of freedom distribution, you find that the p -value is 0.24. This indicates that the specified model fits the data reasonably well.

Figure 40.4 Analysis of Parameter Estimates

Analysis Of Maximum Likelihood Parameter Estimates							
Parameter		DF	Estimate	Standard Error	Wald 95% Confidence Limits		Wald Chi-Square
Intercept		1	-1.3168	0.0903	-1.4937	-1.1398	212.73
car	large	1	-1.7643	0.2724	-2.2981	-1.2304	41.96
car	medium	1	-0.6928	0.1282	-0.9441	-0.4414	29.18
car	small	0	0.0000	0.0000	0.0000	0.0000	.
age	1	1	-1.3199	0.1359	-1.5863	-1.0536	94.34
age	2	0	0.0000	0.0000	0.0000	0.0000	.
Scale		0	1.0000	0.0000	1.0000	1.0000	

Analysis Of Maximum Likelihood Parameter Estimates		
Parameter		Pr > ChiSq
Intercept		<.0001
car	large	<.0001
car	medium	<.0001
car	small	.
age	1	<.0001
age	2	.
Scale		

NOTE: The scale parameter was held fixed.

Figure 40.4 displays the “Analysis Of Parameter Estimates” table, which summarizes the results of the iterative parameter estimation process. For each parameter in the model, PROC GENMOD displays columns with the parameter name, the degrees of freedom associated with the parameter, the estimated parameter value, the standard error of the parameter estimate, the confidence intervals, and the Wald chi-square statistic and associated p -value for testing the significance of the parameter to the model. If a column of the model matrix corresponding to a parameter is found to be linearly dependent, or *aliased*, with columns corresponding to parameters preceding it in the model, PROC GENMOD assigns it zero degrees of freedom and displays a value of zero for both the parameter estimate and its standard error.

This table includes a row for a scale parameter, even though there is no free scale parameter in the Poisson distribution. See the section “[Response Probability Distributions](#)” on page 2799 for the form of the Poisson probability distribution. PROC GENMOD allows the specification of a scale parameter to fit overdispersed Poisson and binomial distributions. In such cases, the SCALE row indicates the value of the overdispersion scale parameter used in adjusting output statistics. See the section “[Overdispersion](#)” on page 2809 for more about overdispersion and the meaning of the SCALE parameter output by the GENMOD procedure. PROC GENMOD displays a note indicating that the scale parameter is fixed—that is, not estimated by the iterative fitting process.

It is usually of interest to assess the importance of the main effects in the model. Type 1 and Type 3 analyses generate statistical tests for the significance of these effects.

You can request these analyses with the TYPE1 and TYPE3 options in the MODEL statement, as follows:

```

proc genmod data=insure;
  class car age;
  model c = car age / dist = poisson
          link = log
          offset = ln
          type1
          type3;
run;

```

The results of these analyses are summarized in the figures that follow.

Figure 40.5 Type 1 Analysis

The GENMOD Procedure				
LR Statistics For Type 1 Analysis				
Source	Deviance	DF	Chi-Square	Pr > ChiSq
Intercept	175.1536			
car	107.4620	2	67.69	<.0001
age	2.8207	1	104.64	<.0001

In the table for Type 1 analysis displayed in [Figure 40.5](#), each entry in the deviance column represents the deviance for the model containing the effect for that row and all effects preceding it in the table. For example, the deviance corresponding to car in the table is the deviance of the model containing an intercept and car. As more terms are included in the model, the deviance decreases.

Entries in the chi-square column are likelihood ratio statistics for testing the significance of the effect added to the model containing all the preceding effects. The chi-square value of 67.69 for car represents twice the difference in log likelihoods between fitting a model with only an intercept term and a model with an intercept and car. Since the scale parameter is set to 1 in this analysis, this is equal to the difference in deviances. Since two additional parameters are involved, this statistic can be compared with a chi-square distribution with two degrees of freedom. The resulting p -value (labeled Pr>Chi) of less than 0.0001 indicates that this variable is highly significant. Similarly, the chi-square value of 104.64 for age represents the difference in log likelihoods between the model with the intercept and car and the model with the intercept, car, and age. This effect is also highly significant, as indicated by the small p -value.

Figure 40.6 Type 3 Analysis

LR Statistics For Type 3 Analysis				
Source	DF	Chi-Square	Pr > ChiSq	
car	2	72.82	<.0001	
age	1	104.64	<.0001	

The Type 3 analysis results in the same conclusions as the Type 1 analysis. The Type 3 chi-square value for the car variable, for example, is twice the difference between the log likelihood for the model with the variables Intercept, car, and age included and the log likelihood for the model with the car variable excluded. The hypothesis tested in this case is the significance of the variable car given that the variable age is in the model. In other words, it tests the additional contribution of car in the model.

The values of the Type 3 likelihood ratio statistics for the car and age variables indicate that both of these factors are highly significant in determining the claims performance of the insurance policyholders.

Bayesian Analysis of a Linear Regression Model

Neter et al. (1996) describe a study of 54 patients undergoing a certain kind of liver operation in a surgical unit. The data set Surg contains survival time and certain covariates for each patient. Observations for the first 20 patients in the data set Surg are shown in Figure 40.7.

Figure 40.7 Surgical Unit Data

Obs	x1	x2	x3	x4	y	logy	Logx1
1	6.7	62	81	2.59	200	2.3010	1.90211
2	5.1	59	66	1.70	101	2.0043	1.62924
3	7.4	57	83	2.16	204	2.3096	2.00148
4	6.5	73	41	2.01	101	2.0043	1.87180
5	7.8	65	115	4.30	509	2.7067	2.05412
6	5.8	38	72	1.42	80	1.9031	1.75786
7	5.7	46	63	1.91	80	1.9031	1.74047
8	3.7	68	81	2.57	127	2.1038	1.30833
9	6.0	67	93	2.50	202	2.3054	1.79176
10	3.7	76	94	2.40	203	2.3075	1.30833
11	6.3	84	83	4.13	329	2.5172	1.84055
12	6.7	51	43	1.86	65	1.8129	1.90211
13	5.8	96	114	3.95	830	2.9191	1.75786
14	5.8	83	88	3.95	330	2.5185	1.75786
15	7.7	62	67	3.40	168	2.2253	2.04122
16	7.4	74	68	2.40	217	2.3365	2.00148
17	6.0	85	28	2.98	87	1.9395	1.79176
18	3.7	51	41	1.55	34	1.5315	1.30833
19	7.3	68	74	3.56	215	2.3324	1.98787
20	5.6	57	87	3.02	172	2.2355	1.72277

Consider the model

$$Y = \beta_0 + \beta_1 \text{LogX1} + \beta_2 X2 + \beta_3 X3 + \beta_4 X4 + \epsilon$$

where Y is the survival time, LogX1 is log(blood-clotting score), X2 is a prognostic index, X3 is an enzyme function test score, X4 is a liver function test score, and ϵ is an $N(0, \sigma^2)$ error term.

A question of scientific interest is whether blood clotting score has a positive effect on survival time. Using PROC GENMOD, you can obtain a maximum likelihood estimate of the coefficient and construct a null point hypothesis to test whether β_1 is equal to 0. However, if you are interested in finding the probability that the coefficient is positive, Bayesian analysis offers a convenient alternative. You can use Bayesian analysis to directly estimate the conditional probability, $\Pr(\beta_1 > 0|Y)$, using the posterior distribution samples, which are produced as part of the output by PROC GENMOD.

The example that follows shows how to use PROC GENMOD to carry out a Bayesian analysis of the linear model with a normal error term. The SEED= option is specified to maintain reproducibility; no other options are specified in the BAYES statement. By default, a uniform prior distribution is assumed on the regression coefficients. The uniform prior is a flat prior on the real line with a distribution that reflects ignorance of the location of the parameter, placing equal likelihood on all possible values the regression coefficient can take. Using the uniform prior in the following example, you would expect the Bayesian estimates to resemble the classical results of maximizing the likelihood. If you can elicit an informative prior distribution for the regression coefficients, you should use the COEFFPRIOR= option to specify it. A default noninformative gamma prior is used for the scale parameter σ .

You should make sure that the posterior distribution samples have achieved convergence before using them for Bayesian inference. PROC GENMOD produces three convergence diagnostics by default. If ODS Graphics is enabled as specified in the following SAS statements, diagnostic plots are also displayed. See the section “[Assessing Markov Chain Convergence](#)” on page 139 for more information about convergence diagnostics and their interpretation.

Summary statistics of the posterior distribution samples are produced by default. However, these statistics might not be sufficient for carrying out your Bayesian inference, and further processing of the posterior samples might be necessary. The following SAS statements request the Bayesian analysis, and the OUTPOST= option saves the samples in the SAS data set PostSurg for further processing:

```
proc genmod data=Surg;
  model y = Logx1 X2 X3 X4 / dist=normal;
  bayes seed=1 OutPost=PostSurg;
run;
```

The results of this analysis are shown in the following figures.

The “Model Information” table in [Figure 40.8](#) summarizes information about the model you fit and the size of the simulation.

Figure 40.8 Model Information

The GENMOD Procedure		
Bayesian Analysis		
Model Information		
Data Set	WORK.SURG	
Burn-In Size	2000	
MC Sample Size	10000	
Thinning	1	
Sampling Algorithm	Conjugate	
Distribution	Normal	
Link Function	Identity	
Dependent Variable	y	Survival Time

The “Analysis of Maximum Likelihood Parameter Estimates” table in [Figure 40.9](#) summarizes maximum likelihood estimates of the model parameters.

Figure 40.9 Maximum Likelihood Parameter Estimates

Analysis Of Maximum Likelihood Parameter Estimates					
Parameter	DF	Estimate	Standard Error	Wald	95% Confidence Limits
Intercept	1	-730.559	85.4333	-898.005	-563.112
Logx1	1	171.8758	38.2250	96.9561	246.7954
x2	1	4.3019	0.5566	3.2109	5.3929
x3	1	4.0309	0.4996	3.0517	5.0100
x4	1	18.1377	12.0721	-5.5232	41.7986
Scale	1	59.8591	5.7599	49.5705	72.2832

NOTE: The scale parameter was estimated by maximum likelihood.

Since no prior distributions for the regression coefficients were specified, the default noninformative uniform distributions shown in the “Uniform Prior for Regression Coefficients” table in [Figure 40.10](#) are used. Noninformative priors are appropriate if you have no prior knowledge of the likely range of values of the parameters, and if you want to make probability statements about the parameters or functions of the parameters. See, for example, Ibrahim, Chen, and Sinha (2001) for more information about choosing prior distributions.

Figure 40.10 Regression Coefficient Priors

The GENMOD Procedure	
Bayesian Analysis	
Uniform Prior for Regression Coefficients	
Parameter	Prior
Intercept	Constant
Logx1	Constant
x2	Constant
x3	Constant
x4	Constant

The default noninformative improper prior distribution for the normal dispersion parameter is shown in the “Independent Prior Distributions for Model Parameters” table in [Figure 40.11](#).

Figure 40.11 Scale Parameter Prior

Independent Prior Distributions for Model Parameters	
Parameter	Prior Distribution
Dispersion	Improper

By default, the maximum likelihood estimates of the regression parameters are used as the starting values for the simulation when noninformative prior distributions are used. These are listed in the “Initial Values and Seeds” table in [Figure 40.12](#).

Figure 40.12 MCMC Initial Values and Seeds

Initial Values of the Chain						
Chain	Seed	Intercept	Logx1	x2	x3	x4
1	1	-730.559	171.8758	4.301896	4.030878	18.1377
Initial Values of the Chain						
Dispersion						
3449.176						

Summary statistics for the posterior sample are displayed in the “Fit Statistics,” “Descriptive Statistics for the Posterior Sample,” “Interval Statistics for the Posterior Sample,” and “Posterior Correlation Matrix” tables in Figure 40.13, Figure 40.14, Figure 40.15, and Figure 40.16, respectively.

Figure 40.13 Fit Statistics

Fit Statistics	
DIC (smaller is better)	607.796
pD (effective number of parameters)	6.062

Figure 40.14 Descriptive Statistics

The GENMOD Procedure						
Bayesian Analysis						
Posterior Summaries						
Parameter	N	Mean	Standard Deviation	Percentiles		
				25%	50%	75%
Intercept	10000	-730.0	91.2102	-789.6	-729.6	-670.5
Logx1	10000	171.7	40.6455	144.2	171.6	198.6
x2	10000	4.2988	0.5952	3.9029	4.2919	4.6903
x3	10000	4.0308	0.5359	3.6641	4.0267	4.3921
x4	10000	18.0858	12.9123	9.4471	18.1230	26.8141
Dispersion	10000	4113.1	867.7	3497.2	3995.9	4606.4

Figure 40.15 Interval Statistics

Posterior Intervals					
Parameter	Alpha	Equal-Tail Interval		HPD Interval	
Intercept	0.050	-908.6	-549.8	-906.9	-549.1
Logx1	0.050	91.9723	252.5	94.1279	254.0
x2	0.050	3.1091	5.4778	3.1705	5.5167
x3	0.050	2.9803	5.1031	2.9227	5.0343
x4	0.050	-7.3043	43.6387	-8.8440	41.8229
Dispersion	0.050	2741.5	6096.6	2540.1	5810.0

Figure 40.16 Posterior Sample Correlation Matrix

Posterior Correlation Matrix						
Parameter	Intercept	Logx1	x2	x3	x4	Dispersion
Intercept	1.000	-0.857	-0.579	-0.712	0.582	0.000
Logx1	-0.857	1.000	0.286	0.491	-0.640	0.007
x2	-0.579	0.286	1.000	0.302	-0.489	-0.009
x3	-0.712	0.491	0.302	1.000	-0.618	-0.006
x4	0.582	-0.640	-0.489	-0.618	1.000	0.003
Dispersion	0.000	0.007	-0.009	-0.006	0.003	1.000

Since noninformative prior distributions were used, the posterior sample means, standard deviations, and interval statistics shown in [Figure 40.13](#) and [Figure 40.14](#) are consistent with the maximum likelihood estimates shown in [Figure 40.9](#).

By default, PROC GENMOD computes three convergence diagnostics: the lag1, lag5, lag10, and lag50 autocorrelations ([Figure 40.17](#)); Geweke diagnostic statistics ([Figure 40.18](#)); and effective sample sizes ([Figure 40.19](#)). There is no indication that the Markov chain has not converged. See the section “Assessing Markov Chain Convergence” on page 139 for more information about convergence diagnostics and their interpretation.

Figure 40.17 Posterior Sample Autocorrelations

The GENMOD Procedure				
Bayesian Analysis				
Posterior Autocorrelations				
Parameter	Lag 1	Lag 5	Lag 10	Lag 50
Intercept	-0.0059	-0.0037	-0.0152	0.0010
Logx1	-0.0002	-0.0064	-0.0066	-0.0054
x2	-0.0120	-0.0026	-0.0267	-0.0168
x3	0.0036	0.0033	-0.0035	0.0004
x4	0.0034	-0.0064	0.0083	-0.0124
Dispersion	-0.0011	0.0091	-0.0279	0.0037

Figure 40.18 Geweke Diagnostic Statistics

Geweke Diagnostics		
Parameter	z	Pr > z
Intercept	-1.0815	0.2795
Logx1	1.6667	0.0956
x2	0.0977	0.9222
x3	0.2506	0.8021
x4	-1.1082	0.2678
Dispersion	0.2451	0.8064

Figure 40.19 Effective Sample Sizes

Parameter	ESS	Autocorrelation	
		Time	Efficiency
Intercept	10000.0	1.0000	1.0000
Logx1	10000.0	1.0000	1.0000
x2	10245.2	0.9761	1.0245
x3	10000.0	1.0000	1.0000
x4	10000.0	1.0000	1.0000
Dispersion	10000.0	1.0000	1.0000

Trace, autocorrelation, and density plots for the seven model parameters, shown in [Figure 40.20](#) through [Figure 40.25](#), are useful in diagnosing whether the Markov chain of posterior samples has converged. These plots show no evidence that the chain has not converged. See the section “[Visual Analysis via Trace Plots](#)” on page 139 for help with interpreting these diagnostic plots.

Figure 40.20 Diagnostic Plots for Intercept

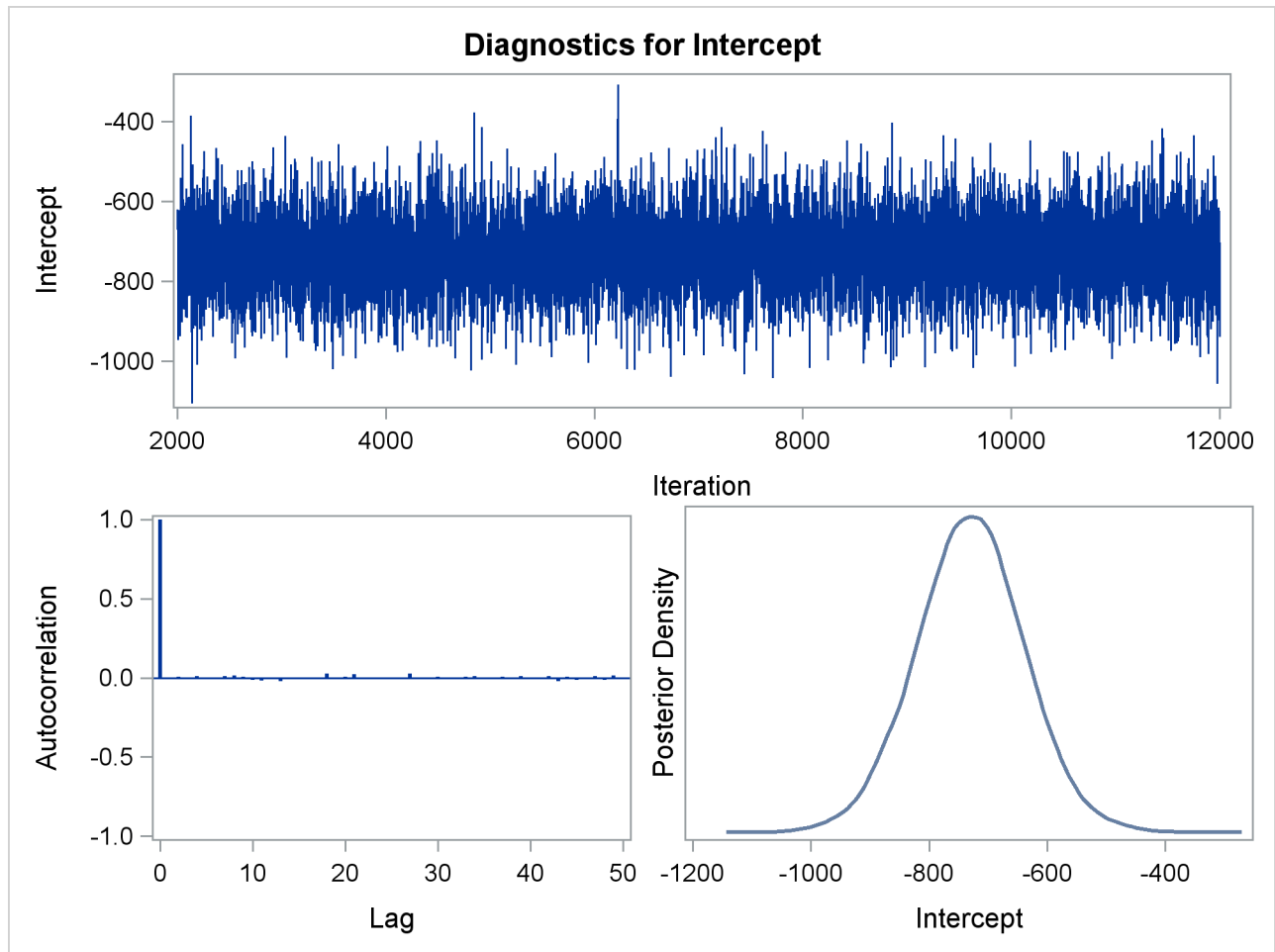


Figure 40.21 Diagnostic Plots for logX1

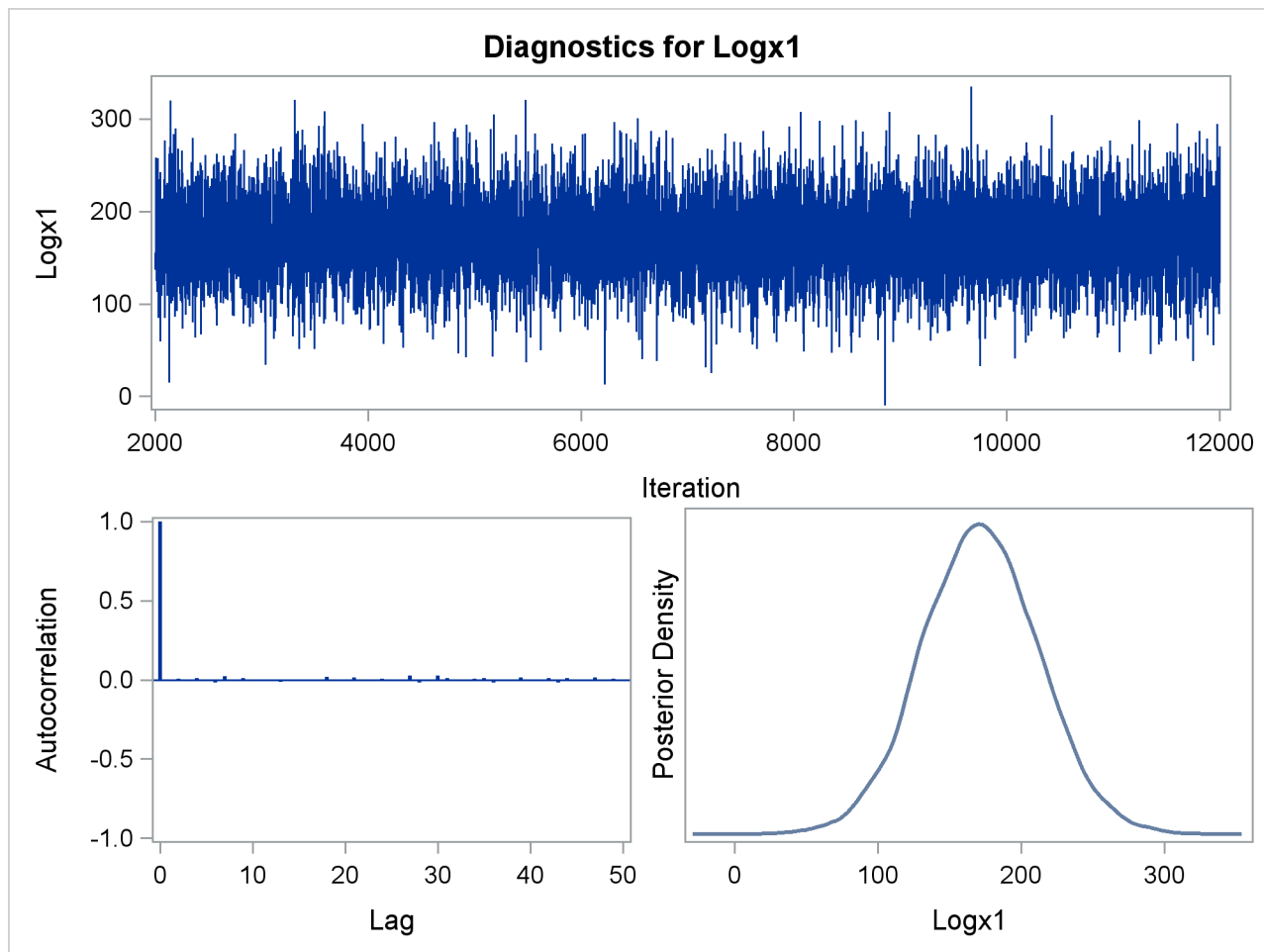


Figure 40.22 Diagnostic Plots for X2

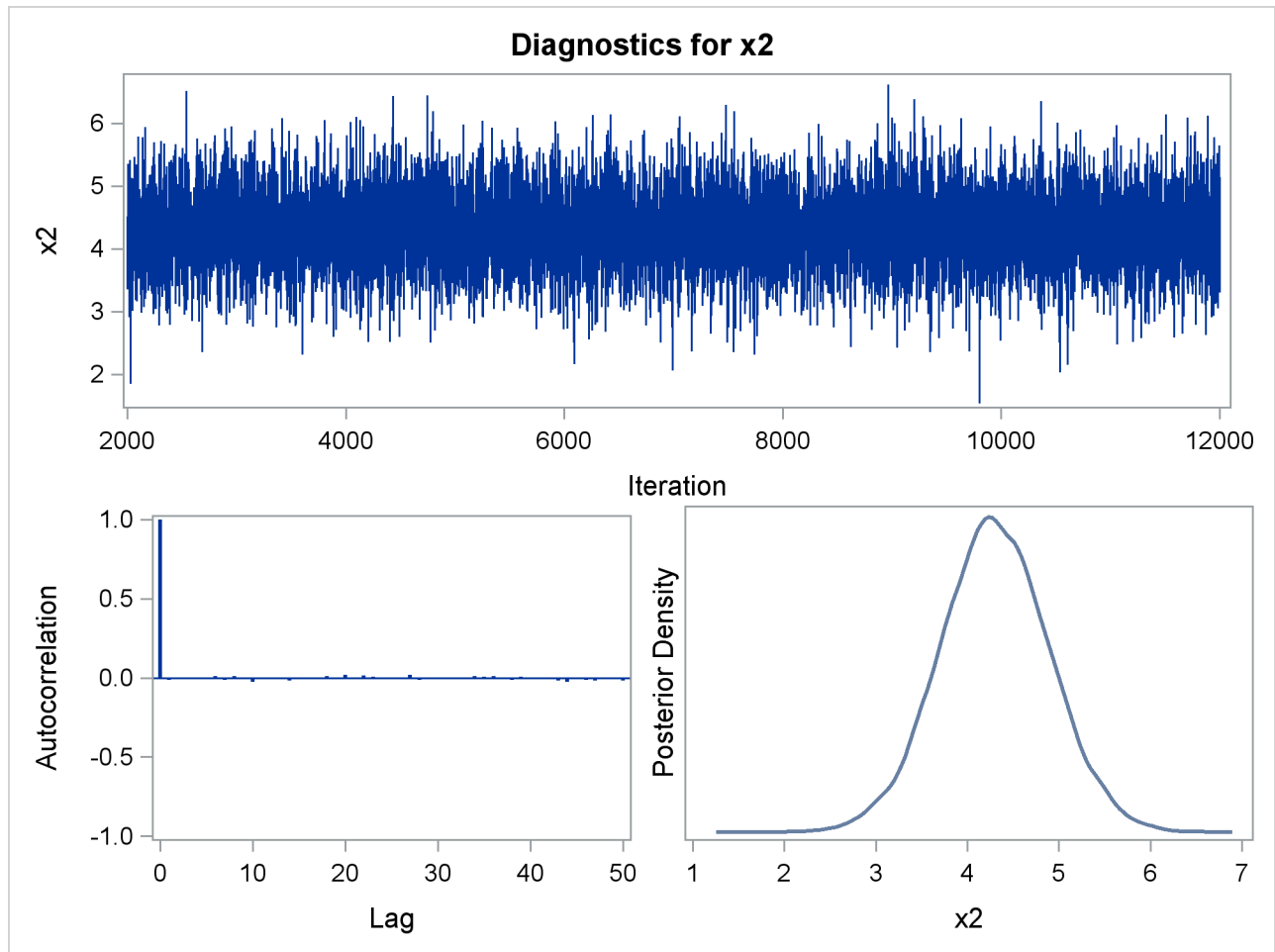


Figure 40.23 Diagnostic Plots for X3

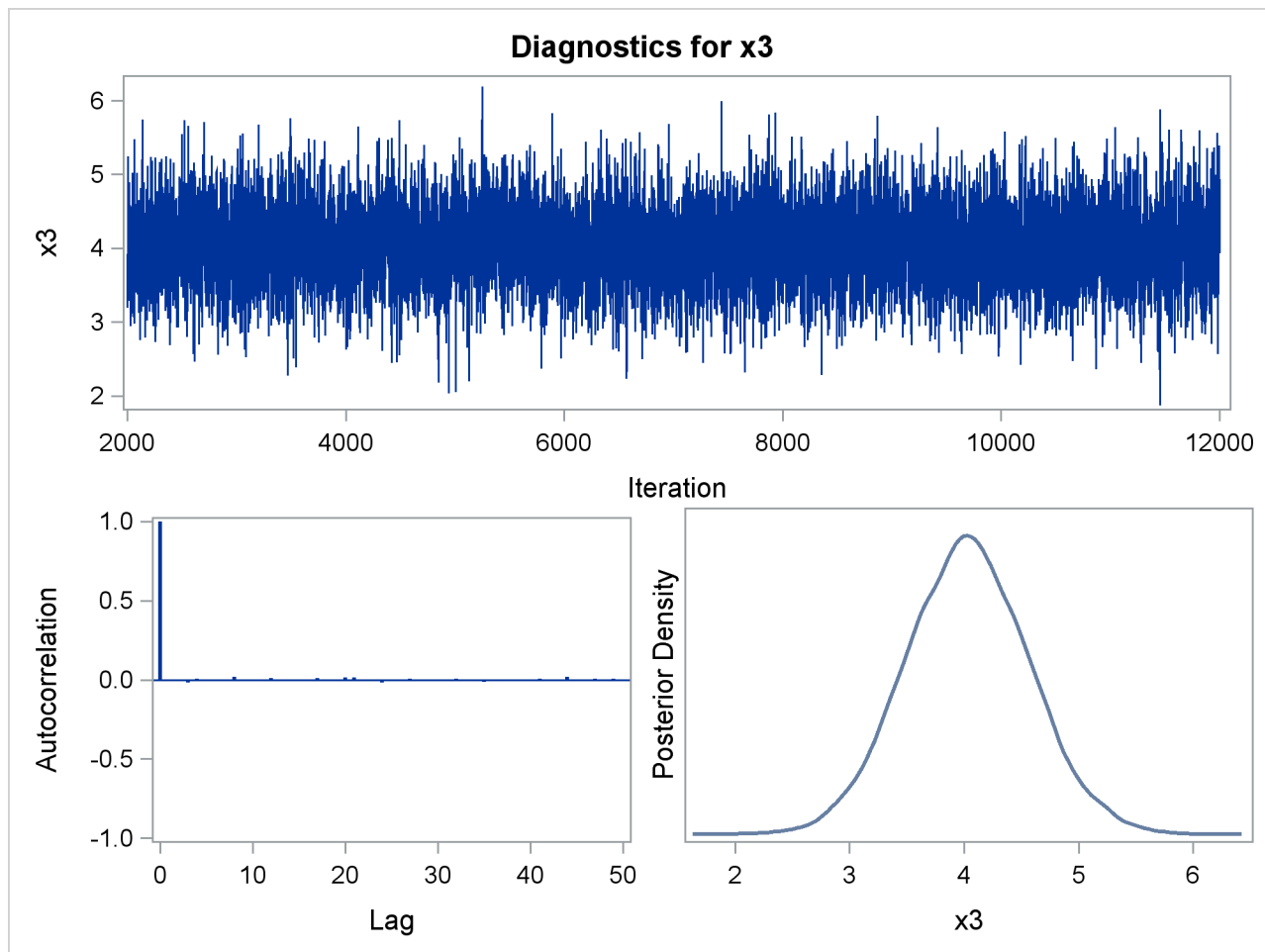


Figure 40.24 Diagnostic Plots for X4

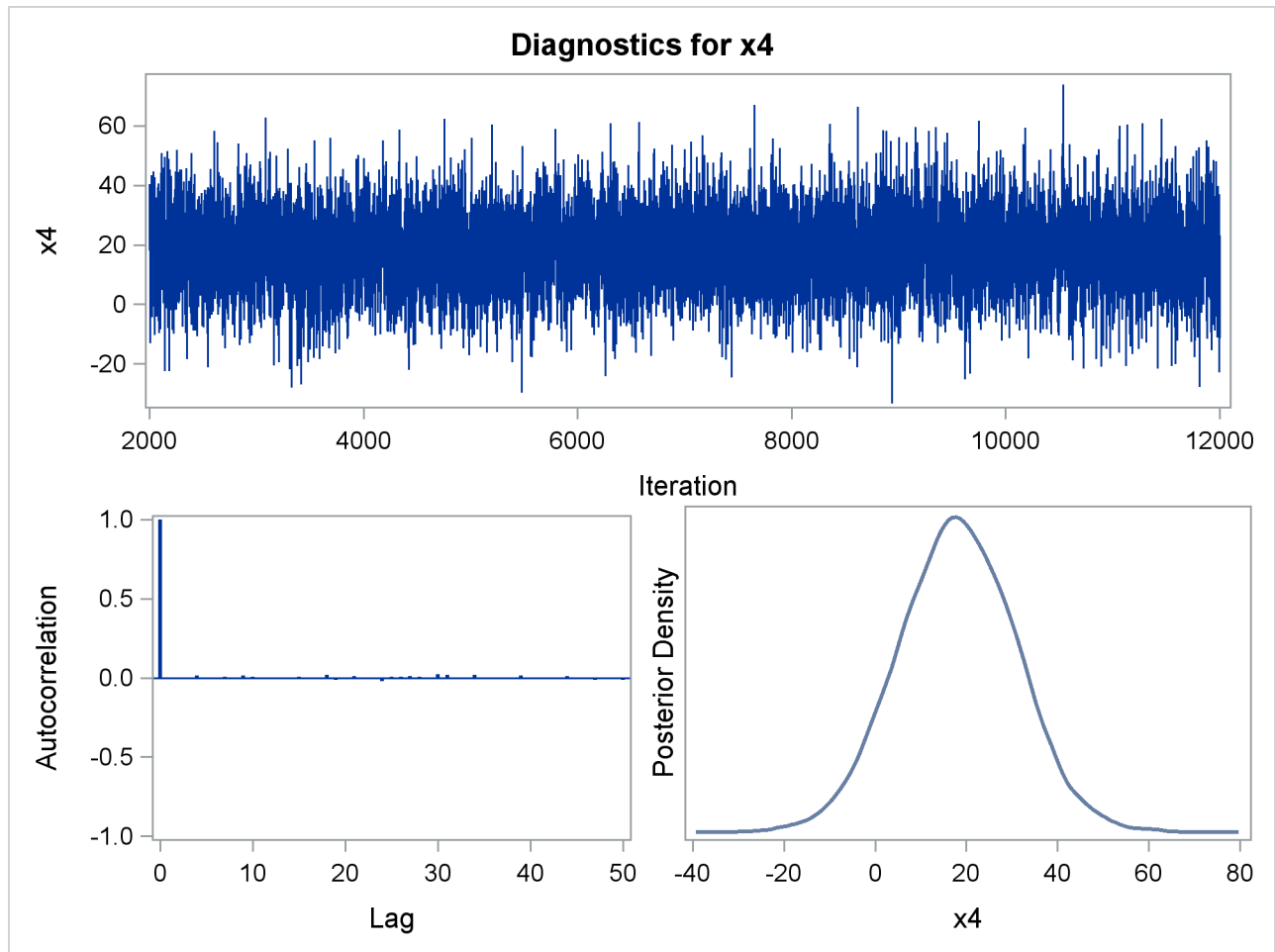
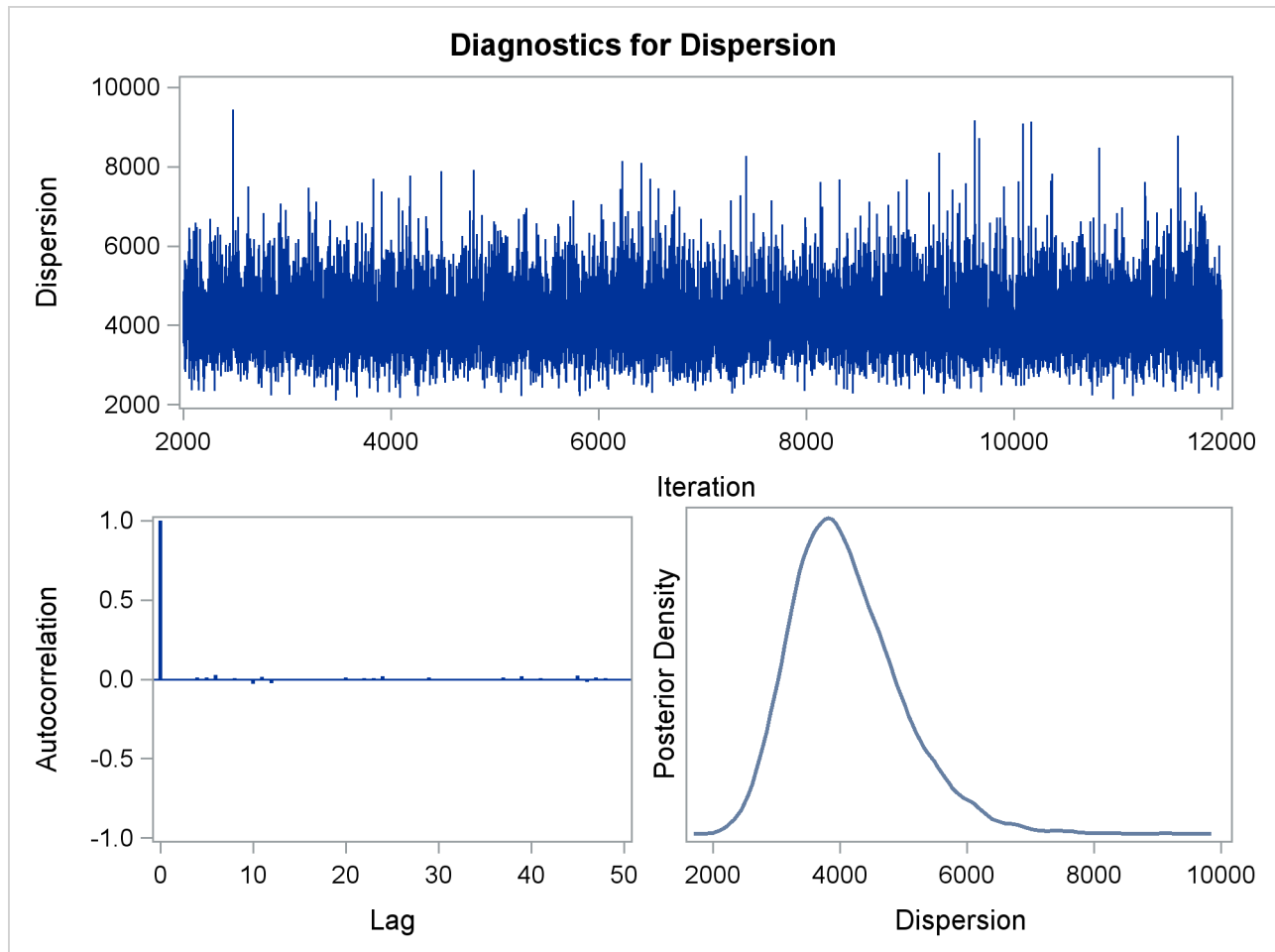


Figure 40.25 Diagnostic Plots for X5



Suppose, for illustration, a question of scientific interest is whether blood clotting score has a positive effect on survival time. Since the model parameters are regarded as random quantities in a Bayesian analysis, you can answer this question by estimating the conditional probability of β_1 being positive, given the data, $\Pr(\beta_1 > 0 | \mathbf{Y})$, from the posterior distribution samples. The following SAS statements compute the estimate of the probability of β_1 being positive:

```
data Prob;
  set PostSurg;
  Indicator = (logX1 > 0);
  label Indicator= 'log(Blood Clotting Score) > 0';
run;

proc Means data = Prob(keep=Indicator) n mean;
run;
```

As shown in Figure 40.26, there is a 1.00 probability of a positive relationship between the logarithm of a blood clotting score and survival time, adjusted for the other covariates.

Figure 40.26 Probability That $\beta_1 > 0$

The MEANS Procedure	
Analysis Variable : Indicator log(Blood Clotting Score) > 0	
N	Mean
10000	0.9999000

Generalized Estimating Equations

This section illustrates the use of the REPEATED statement to fit a GEE model, using repeated measures data from the “Six Cities” study of the health effects of air pollution (Ware et al. 1984). The data analyzed are the 16 selected cases in Lipsitz et al. (1994). The binary response is the wheezing status of 16 children at ages 9, 10, 11, and 12 years. The mean response is modeled as a logistic regression model by using the explanatory variables city of residence, age, and maternal smoking status at the particular age. The binary responses for individual children are assumed to be equally correlated, implying an exchangeable correlation structure.

The data set and SAS statements that fit the model by the GEE method are as follows:

```
data six;
  input case city$ @@;
  do i=1 to 4;
    input age smoke wheeze @@;
    output;
  end;
  datalines;
1 portage 9 0 1 10 0 1 11 0 1 12 0 0
2 kingston 9 1 1 10 2 1 11 2 0 12 2 0
3 kingston 9 0 1 10 0 0 11 1 0 12 1 0
4 portage 9 0 0 10 0 1 11 0 1 12 1 0
5 kingston 9 0 0 10 1 0 11 1 0 12 1 0
6 portage 9 0 0 10 1 0 11 1 0 12 1 0
7 kingston 9 1 0 10 1 0 11 0 0 12 0 0
8 portage 9 1 0 10 1 0 11 1 0 12 2 0
9 portage 9 2 1 10 2 0 11 1 0 12 1 0
10 kingston 9 0 0 10 0 0 11 0 0 12 1 0
11 kingston 9 1 1 10 0 0 11 0 1 12 0 1
12 portage 9 1 0 10 0 0 11 0 0 12 0 0
13 kingston 9 1 0 10 0 1 11 1 1 12 1 1
14 portage 9 1 0 10 2 0 11 1 0 12 2 1
15 kingston 9 1 0 10 1 0 11 1 0 12 2 1
16 portage 9 1 1 10 1 1 11 2 0 12 1 0
;
```

```

proc genmod data=six;
  class case city;
  model wheeze = city age smoke / dist=bin;
  repeated subject=case / type=exch covb corrw;
run;

```

The CLASS statement and the MODEL statement specify the model for the mean of the wheeze variable response as a logistic regression with city, age, and smoke as independent variables, just as for an ordinary logistic regression.

The REPEATED statement invokes the GEE method, specifies the correlation structure, and controls the displayed output from the GEE model. The option SUBJECT=CASE specifies that individual subjects be identified in the input data set by the variable case. The SUBJECT= variable case must be listed in the CLASS statement. Measurements on individual subjects at ages 9, 10, 11, and 12 are in the proper order in the data set, so the WITHINSUBJECT= option is not required. The TYPE=EXCH option specifies an exchangeable working correlation structure, the COVB option specifies that the parameter estimate covariance matrix be displayed, and the CORRW option specifies that the final working correlation be displayed.

Initial parameter estimates for iterative fitting of the GEE model are computed as in an ordinary generalized linear model, as described previously. Results of the initial model fit displayed as part of the generated output are not shown here. Statistics for the initial model fit such as parameter estimates, standard errors, deviances, and Pearson chi-squares do not apply to the GEE model and are valid only for the initial model fit. The following figures display information that applies to the GEE model fit.

Figure 40.27 displays general information about the GEE model fit.

Figure 40.27 GEE Model Information

The GENMOD Procedure	
GEE Model Information	
Correlation Structure	Exchangeable
Subject Effect	case (16 levels)
Number of Clusters	16
Correlation Matrix Dimension	4
Maximum Cluster Size	4
Minimum Cluster Size	4

Figure 40.28 displays the parameter estimate covariance matrices specified by the COVB option. Both model-based and empirical covariances are produced.

Figure 40.28 GEE Parameter Estimate Covariance Matrices

Covariance Matrix (Model-Based)				
	Prm1	Prm2	Prm4	Prm5
Prm1	5.74947	-0.22257	-0.53472	0.01655
Prm2	-0.22257	0.45478	-0.002410	0.01876
Prm4	-0.53472	-0.002410	0.05300	-0.01658
Prm5	0.01655	0.01876	-0.01658	0.19104

Covariance Matrix (Empirical)				
	Prm1	Prm2	Prm4	Prm5
Prm1	9.33994	-0.85104	-0.83253	-0.16534
Prm2	-0.85104	0.47368	0.05736	0.04023
Prm4	-0.83253	0.05736	0.07778	-0.002364
Prm5	-0.16534	0.04023	-0.002364	0.13051

The exchangeable working correlation matrix specified by the CORRW option is displayed in [Figure 40.29](#).

Figure 40.29 GEE Working Correlation Matrix

Working Correlation Matrix				
	Col1	Col2	Col3	Col4
Row1	1.0000	0.1648	0.1648	0.1648
Row2	0.1648	1.0000	0.1648	0.1648
Row3	0.1648	0.1648	1.0000	0.1648
Row4	0.1648	0.1648	0.1648	1.0000

The parameter estimates table, displayed in [Figure 40.30](#), contains parameter estimates, standard errors, confidence intervals, Z scores, and p -values for the parameter estimates. Empirical standard error estimates are used in this table. A table that displays model-based standard errors can be created by using the REPEATED statement option MODELSE.

Figure 40.30 GEE Parameter Estimates Table

Analysis Of GEE Parameter Estimates Empirical Standard Error Estimates							
Parameter		Estimate	Standard Error	95% Confidence Limits		Z	Pr > Z
Intercept		-1.2751	3.0561	-7.2650	4.7148	-0.42	0.6765
city	kingston	-0.1223	0.6882	-1.4713	1.2266	-0.18	0.8589
city	portage	0.0000	0.0000	0.0000	0.0000	.	.
age		0.2036	0.2789	-0.3431	0.7502	0.73	0.4655
smoke		0.0935	0.3613	-0.6145	0.8016	0.26	0.7957

Syntax: GENMOD Procedure

The following statements are available in the GENMOD procedure. Items within the < > are optional.

```

PROC GENMOD < options > ;
  ASSESS | ASSESSMENT VAR=(effect) | LINK < / options > ;
  BAYES < options > ;
  BY variables ;
  CLASS variable < (options) > ... < variable < (options) > > < / options > ;
  CODE < options > ;
  CONTRAST 'label' contrast-specification < / options > ;
  DEVIANCE variable = expression ;
  EFFECTPLOT < plot-type < (plot-definition-options) > > < / options > ;
  ESTIMATE 'label' effect values < , ... effect values > < / options > ;
  EXACT < 'label' > < INTERCEPT > < effects > < / options > ;
  EXACTOPTIONS options ;
  FREQ | FREQUENCY variable ;
  FWDLINK variable = expression ;
  INVLINK variable = expression ;
  LSMEANS < model-effects > < / options > ;
  LSMESTIMATE model-effect < 'label' > values < divisor=n > < , ... < 'label' > values < divisor=n > >
    < / options > ;
  MODEL response = < effects > < / options > ;
  OUTPUT < OUT=SAS-data-set > < keyword=name ... keyword=name > ;
  Programming statements ;
  REPEATED SUBJECT=subject-effect < / options > ;
  SLICE model-effect < / options > ;
  STORE < OUT= > item-store-name < / LABEL='label' > ;
  STRATA variable < (option) > ... < variable < (option) > > < / options > ;
  WEIGHT | SCWGT variable ;
  VARIANCE variable = expression ;
  ZEROMODEL < effects > < / options > ;

```

The **ASSESS**, **BAYES**, **BY**, **CLASS**, **CODE**, **CONTRAST**, **DEVIANCE**, **ESTIMATE**, **FREQUENCY**, **FWDLINK**, **INVLINK**, **MODEL**, **OUTPUT**, programming statements, **REPEATED**, **VARIANCE**, **WEIGHT**, and **ZEROMODEL** statements are described in full after the **PROC GENMOD** statement in alphabetical order. The **EFFECTPLOT**, **LSMEANS**, **LSMESTIMATE**, **SLICE**, and **STORE** statements are common to many procedures. Summary descriptions of functionality and syntax for these statements are also given after the **PROC GENMOD** statement in alphabetical order, and full documentation about them is available in Chapter 19, “Shared Concepts and Topics.”

The **PROC GENMOD** statement invokes the **GENMOD** procedure. All statements other than the **MODEL** statement are optional. The **CLASS** statement, if present, must precede the **MODEL** statement, and the **CONTRAST** and **EXACT** statements must come after the **MODEL** statement.

PROC GENMOD Statement

PROC GENMOD < options > ;

The **PROC GENMOD** statement invokes the **GENMOD** procedure. Table 40.1 summarizes the options available in the **PROC GENMOD** statement.

Table 40.1 PROC GENMOD Statement Options

Option	Description
DATA=	Specifies the input data set
DESCENDING	Sorts response variable in the reverse of the default order
EXACTONLY	Requests only the exact analyses
NAMELEN=	Specifies the length of effect names
ORDER=	Specifies the sort order of CLASS variable
PLOTS	Controls the plots produced through ODS Graphics
RORDER=	Specifies the sort order for the levels of the response variable

You can specify the following options.

DATA=SAS-data-set

specifies the SAS data set containing the data to be analyzed. If you omit the **DATA=** option, the procedure uses the most recently created SAS data set.

DESCENDING

DESCEND

DESC

specifies that the levels of the response variable for the ordinal multinomial model and the binomial model with single variable response syntax be sorted in the reverse of the default order. For example, if **RORDER=FORMATTED** (the default), the **DESCENDING** option causes the levels to be sorted from highest to lowest instead of from lowest to highest. If **RORDER=FREQ**, the **DESCENDING** option causes the levels to be sorted from lowest frequency count to highest instead of from highest to lowest.

EXACTONLY

requests only the exact analyses. The asymptotic analysis that PROC GENMOD usually performs is suppressed.

NAMELEN=*n*

specifies the length of effect names in tables and output data sets to be *n* characters long, where *n* is a value between 20 and 200 characters. The default length is 20 characters.

ORDER=DATA | FORMATTED | FREQ | INTERNAL

specifies the sort order for the levels of the classification variables (which are specified in the **CLASS** statement). The ORDER= option can be useful when you use the CONTRAST or ESTIMATE statement because it determines which parameters in the model correspond to each level in the data.

This option applies to the levels for all classification variables, except when you use the (default) ORDER=FORMATTED option with numeric classification variables that have no explicit format. With this option, the levels of such variables are ordered by their internal value.

The ORDER= option can take the following values:

Value of ORDER=	Levels Sorted By
DATA	Order of appearance in the input data set
FORMATTED	External formatted value, except for numeric variables with no explicit format, which are sorted by their unformatted (internal) value
FREQ	Descending frequency count; levels with the most observations come first in the order
INTERNAL	Unformatted value

By default, ORDER=FORMATTED. For ORDER=FORMATTED and ORDER=INTERNAL, the sort order is machine-dependent. For more information about sort order, see the chapter on the SORT procedure in the *Base SAS Procedures Guide* and the discussion of BY-group processing in *SAS Language Reference: Concepts*.

PLOTS <(global-plot-option) >= plot-request <(options) >

PLOTS <(global-plot-options) > <= (plot-request <(options) > <...plot-request <(options) > > >

specifies plots to be created using ODS Graphics. Many of the observational statistics in the output data set can be plotted using this option. You are not required to create an output data set in order to produce a plot. When you specify only one plot request, you can omit the parentheses around the plot request. Here are some examples:

```
plots=all
plots=predicted
plots=(predicted reschi)
plots(unpack)=dfbeta
```

ODS Graphics must be enabled before plots can be requested. For example:

```
proc genmod plots=all;
  model y = x;
run;
```

For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS](#).”

Any specified global plot options apply to all plots that are specified with plot requests. The following global plot options are available.

CLUSTERLABEL

displays formatted levels of the SUBJECT= effect instead of plot symbols. This option applies only to diagnostic statistics for models fit by GEEs that are plotted against cluster number, and provides a way to identify cluster level names with corresponding ordered cluster numbers.

UNPACK

displays multiple plots individually. The default is to display related multiple plots in a panel.

See the section “[OUTPUT Statement](#)” on page 2787 for definitions of the statistics specified with the plot requests. The plot requests include the following:

ALL

produces all available plots.

COOKSD

DOBS

plots the Cook’s distance statistic as a function of observation number.

DFBETA

plots the β deletion statistic as a function of observation number for each regression parameter in the model.

DFBETAS

plots the standardized β deletion statistic as a function of observation number for each regression parameter in the model.

LEVERAGE

plots the leverage as a function of observation number.

PREDICTED< (option) >

plots predicted values with confidence limits as a function of observation number. The PREDICTED plot request has the following *option*:

CLM

includes confidence limits in the predicted value plot.

PZERO

plots the zero inflation probability for zero-inflated Poisson and negative binomial models as a function of observation number.

RESCHI<(*options*)>

The RESCHI plot request has the following *options*:

INDEX

plots as a function of observation number.

XBETA

plots as a function of linear predictor.

If you do not specify an option, Pearson residuals are plotted as a function of observation number.

RESDEV<(*options*)>

plots deviance residuals. The RESDEV plot request has the following *options*:

INDEX

plots as a function of observation number.

XBETA

plots as a function of linear predictor.

If you do not specify an option, deviance residuals are plotted as a function of observation number.

RESLIK<(*options*)>

plots likelihood residuals. The RESLIK plot request has the following *options*:

INDEX

plots as a function of observation number.

XBETA

plots as a function of linear predictor.

If you do not specify an option, likelihood residuals are plotted as a function of observation number.

RESRAW<(*options*)>

plots raw residuals. The RESRAW plot request has the following *options*:

INDEX

plots as a function of observation number.

XBETA

plots as a function of linear predictor.

If you do not specify an option, raw residuals are plotted as a function of observation number.

STDRESCHI<(*options*)>

plots standardized Pearson residuals. The STDRESCHI plot request has the following *options*:

INDEX

plots as a function of observation number.

XBETA

plots as a function of linear predictor.

If you do not specify an option, standardized Pearson residuals are plotted as a function of observation number.

STDRESDEV< (*options*) >

plots standardized deviance residuals. The STDRESDEV plot request has the following *options*:

INDEX

plots as a function of observation number.

XBETA

plots as a function of linear predictor.

If you do not specify an option, standardized deviance residuals are plotted as a function of observation number.

If you fit a model by using generalized estimating equations (GEEs), the following additional plot requests are available:

CLEVERAGE

plots the cluster leverage as a function of ordered cluster.

CLUSTERCOOKSD**DCLS**

plots the cluster Cook's distance statistic as a function of ordered cluster.

CLUSTERDFIT**MCLS**

plots the studentized cluster Cook's distance statistic as a function of ordered cluster.

DFBETAC

plots the cluster deletion statistic as a function of ordered cluster for each regression parameter in the model.

DFBETACS

plots the standardized cluster deletion statistic as a function of ordered cluster for each regression parameter in the model.

RORDER=*keyword*

specifies the sort order for the levels of the response variable. This order determines which intercept parameter in the model corresponds to each level in the data. If RORDER=FORMATTED for numeric variables for which you have supplied no explicit format, the levels are ordered by their internal values. The following table displays the valid *keywords* and describes how PROC GENMOD interprets them.

RORDER=keyword	Levels Sorted by
DATA	Order of appearance in the input data set
FORMATTED	External formatted value, except for numeric variables with no explicit format, which are sorted by their unformatted (internal) value
FREQ	Descending frequency count; levels with the most observations come first in the order
INTERNAL	Unformatted value

By default, RORDER=FORMATTED. For RORDER=FORMATTED and RORDER=INTERNAL, the sort order is machine dependent. The DESCENDING option in the PROC GENMOD statement causes the response variable to be sorted in the reverse of the order displayed in the previous table. For more information about sort order, see the chapter on the SORT procedure in the *Base SAS Procedures Guide*.

The NOPRINT option, which suppresses displayed output in other SAS procedures, is not available in the PROC GENMOD statement. However, you can use the Output Delivery System (ODS) to suppress all displayed output, store all output on disk for further analysis, or create SAS data sets from selected output. You can suppress all displayed output with the statement `ODS SELECT NONE;` and turn displayed output back on with the statement `ODS SELECT ALL;`. See Table 40.12 and Table 40.13 for the names of output tables available from PROC GENMOD. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

ASSESS Statement

ASSESS VAR=(effect)| LINK </ options > ;

ASSESSMENT VAR=(effect)| LINK </ options > ;

The ASSESS statement computes and plots, using ODS Graphics, model-checking statistics based on aggregates of residuals. See the section “Assessment of Models Based on Aggregates of Residuals” on page 2827 for details about the model assessment methods available in GENMOD.

The types of aggregates available are cumulative residuals, moving sums of residuals, and loess smoothed residuals. If you do not specify which aggregate to use, the assessments are based on cumulative sums. PROC GENMOD uses ODS Graphics for graphical displays. For specific information about the graphics available in PROC GENMOD, see the section “ODS Graphics” on page 2856.

You must specify either LINK or VAR= in order to create an analysis.

LINK requests the assessment of the link function by performing the analysis with respect to the linear predictor.

VAR=(effect) specifies that the functional form of a covariate be checked by performing the analysis with respect to the variable identified by the effect. The effect must be specified in the MODEL statement and must contain only continuous variables (variables not listed in a CLASS statement).

You can specify the following options after the slash (/).

CRPANEL

requests that a plot with four panels showing just a few of the paths from the default aggregate plot to make it easier to compare simulated and observed paths. The plot in each panel contains aggregates of the observed residuals and two simulated curves (fewer if `NPATHS=` is less than 8).

LOESS< (*number*) >**LOWESS**< (*number*) >

requests model assessment based on loess smoothed residuals with optional *number* the fraction of data used; *number* must be between zero and one. If *number* is not specified, the default value one-third is used.

NPATHS=*number***NPATH**=*number***PATHS**=*number***PATH**=*number*

specifies the number of simulated paths to plot in the default aggregate residuals plot. The default value of *number* is twenty.

RESAMPLE< =*number* >**RESAMPLES**< =*number* >

specifies that a *p*-value be computed based on 1,000 simulated paths, or *number* paths, if *number* is specified.

SEED=*number*

specifies a seed for the normal random number generator used in creating simulated realizations of aggregates of residuals for plots and estimating *p*-values. Specifying a seed enables you to produce identical graphs and *p*-values from one run of the procedure to the next run. If a seed is not specified, or if *number* is negative or zero, a random number seed is derived from the time of day.

WINDOW< (*number*) >

requests assessment based on a moving sum window of width *number*. If *number* is not specified, a value of one-half of the range of the *x*-coordinate is used.

BAYES Statement

BAYES < *options* > ;

The BAYES statement requests a Bayesian analysis of the regression model by using Gibbs sampling. The Bayesian posterior samples (also known as the chain) for the regression parameters are not tabulated. The Bayesian posterior samples (also known as the chain) for the regression parameters can be output to a SAS data set. Table 40.2 summarizes the options available in the BAYES statement.

Table 40.2 BAYES Statement Options

Option	Description
Monte Carlo Options	
INITIAL=	Specifies the initial values of the chain

Table 40.2 (continued)

Option	Description
INITIALMLE	Specifies that maximum likelihood estimates be used as initial values of the chain
METROPOLIS=	Specifies the use of a Metropolis step in the ARMS algorithm
NBI=	Specifies the number of burn-in iterations
NMC=	Specifies the number of iterations after burn-in
SAMPLING=	Specifies the algorithm used to sample the posterior distribution
SEED=	Specifies the random number generator seed
THINNING=	Controls the thinning of the Markov chain
Model and Prior Options	
COEFFPRIOR=	Specifies the prior of the regression coefficients
DISPERSIONPRIOR=	Specifies the prior of the dispersion parameter
PRECISIONPRIOR=	Specifies the prior of the precision parameter
SCALEPRIOR=	Specifies the prior of the scale parameter
Summary Statistics and Convergence Diagnostics	
DIAGNOSTICS=	Displays convergence diagnostics
PLOTS=	Displays diagnostic plots
STATISTICS=	Displays summary statistics of the posterior samples
Posterior Samples	
OUTPOST=	Names a SAS data set for the posterior samples

The following list describes these options and their suboptions.

COEFFPRIOR=JEFFREYS< (option) > | **NORMAL**< (options) > | **UNIFORM**

COEFF=JEFFREYS< (options) > | **NORMAL**< (options) > | **UNIFORM**

CPRIOR=JEFFREYS< (options) > | **NORMAL**< (options) > | **UNIFORM**

specifies the prior distribution for the regression coefficients. The default is **COEFFPRIOR=UNIFORM**, which specifies the noninformative and improper prior of a constant.

Jeffreys' prior is specified by **COEFFPRIOR=JEFFREYS**, which can be followed by the following option in parentheses. Jeffreys' prior is proportional to $|I(\boldsymbol{\beta})|^{-\frac{1}{2}}$, where $I(\boldsymbol{\beta})$ is the Fisher information matrix. See the section "Jeffreys' Prior" on page 2837 and Ibrahim and Laud (1991) for more details.

CONDITIONAL

specifies that the Jeffreys' prior, conditional on the current Markov chain value of the generalized linear model precision parameter τ , is proportional to $|\tau I(\boldsymbol{\beta})|^{-\frac{1}{2}}$.

The normal prior is specified by **COEFFPRIOR=NORMAL**, which can be followed by one of the following options enclosed in parentheses. However, if you do not specify an option, the normal prior $N(\mathbf{0}, 10^6\mathbf{I})$, where \mathbf{I} is the identity matrix, is used. See the section "Normal Prior" on page 2837 for more details.

CONDITIONAL

specifies that the normal prior, conditional on the current Markov chain value of the generalized linear model precision parameter τ , is $N(\boldsymbol{\mu}, \tau^{-1} \boldsymbol{\Sigma})$, where $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ are the mean and covariance of the normal prior specified by other normal options.

INPUT=SAS-data-set

specifies a SAS data set containing the mean and covariance information of the normal prior. The data set must have a `_TYPE_` variable to represent the type of each observation and a variable for each regression coefficient. If the data set also contains a `_NAME_` variable, the values of this variable are used to identify the covariances for the `_TYPE_='COV'` observations; otherwise, the `_TYPE_='COV'` observations are assumed to be in the same order as the explanatory variables in the MODEL statement. PROC GENMOD reads the mean vector from the observation with `_TYPE_='MEAN'` and reads the covariance matrix from observations with `_TYPE_='COV'`. For an independent normal prior, the variances can be specified with `_TYPE_='VAR'`; alternatively, the precisions (inverse of the variances) can be specified with `_TYPE_='PRECISION'`.

RELVAR<=c>

specifies the normal prior $N(\mathbf{0}, c\mathbf{J})$, where \mathbf{J} is a diagonal matrix with diagonal elements equal to the variances of the corresponding ML estimator. By default, $c = 10^6$.

VAR<=c>

specifies the normal prior $N(\mathbf{0}, c\mathbf{I})$, where \mathbf{I} is the identity matrix.

DIAGNOSTICS=ALL | NONE | (keyword-list)**DIAG=ALL | NONE | (keyword-list)**

controls the number of diagnostics produced. You can request all the following diagnostics by specifying `DIAGNOSTICS=ALL`. If you do not want any of these diagnostics, specify `DIAGNOSTICS=NONE`. If you want some but not all of the diagnostics, or if you want to change certain settings of these diagnostics, specify a subset of the following keywords. The default is `DIAGNOSTICS=(AUTOCORR ESS GEWEKE)`.

AUTOCORR <(LAGS= numeric-list)>

computes the autocorrelations of lags given by `LAGS=` list for each parameter. Elements in the list are truncated to integers and repeated values are removed. If the `LAGS=` option is not specified, autocorrelations of lags 1, 5, 10, and 50 are computed for each variable. See the section “[Autocorrelations](#)” on page 152 for details.

ESS

computes Carlin’s estimate of the effective sample size, the correlation time, and the efficiency of the chain for each parameter. See the section “[Effective Sample Size](#)” on page 152 for details.

GELMAN <(gelman-options)>

computes the Gelman and Rubin convergence diagnostics. You can specify one or more of the following *gelman-options*:

NCHAIN | N=number

specifies the number of parallel chains used to compute the diagnostic, and must be 2 or larger. The default is `NCHAIN=3`. If an `INITIAL=` data set is used, `NCHAIN` defaults to the number of rows in the `INITIAL=` data set. If any number other than this is specified with the `NCHAIN=` option, the `NCHAIN=` value is ignored.

ALPHA=*value*

specifies the significance level for the upper bound. The default is ALPHA=0.05, resulting in a 97.5% bound.

See the section “[Gelman and Rubin Diagnostics](#)” on page 145 for details.

GEWEKE < (*geweke-options*) >

computes the Geweke spectral density diagnostics, which are essentially a two-sample t test between the first f_1 portion and the last f_2 portion of the chain. The default is $f_1 = 0.1$ and $f_2 = 0.5$, but you can choose other fractions by using the following *geweke-options*:

FRAC1=*value*

specifies the fraction f_1 for the first window.

FRAC2=*value*

specifies the fraction f_2 for the second window.

See the section “[Geweke Diagnostics](#)” on page 146 for details.

HEIDELBERGER < (*heidel-options*) >

computes the Heidelberg and Welch diagnostic for each variable, which consists of a stationarity test of the null hypothesis that the sample values form a stationary process. If the stationarity test is not rejected, a halfwidth test is then carried out. Optionally, you can specify one or more of the following *heidel-options*:

SALPHA=*value*

specifies the α level ($0 < \alpha < 1$) for the stationarity test.

HALPHA=*value*

specifies the α level ($0 < \alpha < 1$) for the halfwidth test.

EPS=*value*

specifies a positive number ϵ such that if the halfwidth is less than ϵ times the sample mean of the retained iterates, the halfwidth test is passed.

See the section “[Heidelberg and Welch Diagnostics](#)” on page 148 for details.

MCSE**MCERROR**

computes the Monte Carlo standard error for each parameter. The Monte Carlo standard error, which measures the simulation accuracy, is the standard error of the posterior mean estimate and is calculated as the posterior standard deviation divided by the square root of the effective sample size. See the section “[Standard Error of the Mean Estimate](#)” on page 153 for details.

RAFTERY < (*raftery-options*) >

computes the Raftery and Lewis diagnostics that evaluate the accuracy of the estimated quantile ($\hat{\theta}_Q$ for a given $Q \in (0, 1)$) of a chain. $\hat{\theta}_Q$ can achieve any degree of accuracy when the chain is allowed to run for a long time. A stopping criterion is when the estimated probability $\hat{P}_Q = \Pr(\theta \leq \hat{\theta}_Q)$ reaches within $\pm R$ of the value Q with probability S ; that is, $\Pr(Q - R \leq \hat{P}_Q \leq Q + R) = S$. The following *raftery-options* enable you to specify Q , R , S , and a precision level ϵ for the test:

QUANTILE | Q=value

specifies the order (a value between 0 and 1) of the quantile of interest. The default is 0.025.

ACCURACY | R=value

specifies a small positive number as the margin of error for measuring the accuracy of estimation of the quantile. The default is 0.005.

PROBABILITY | S=value

specifies the probability of attaining the accuracy of the estimation of the quantile. The default is 0.95.

EPSILON | EPS=value

specifies the tolerance level (a small positive number) for the stationary test. The default is 0.001.

See the section “Raftery and Lewis Diagnostics” on page 149 for details.

DISPERSIONPRIOR=GAMMA< (options)> | IGAMMA< (options)> | IMPROPER**DPRIOR=GAMMA< (options)> | IGAMMA< (options)> | IMPROPER**

specifies that Gibbs sampling be performed on the generalized linear model dispersion parameter and the prior distribution for the dispersion parameter, if there is a dispersion parameter in the model. For models that do not have a dispersion parameter (the Poisson and binomial), this option is ignored. Note that you can specify Gibbs sampling on either the dispersion parameter ϕ , the scale parameter $\sigma = \phi^{\frac{1}{2}}$, or the precision parameter $\tau = \phi^{-1}$, with the DPRIOR=, SPRIOR=, and PPRIOR= options, respectively. These three parameters are transformations of one another, and you should specify Gibbs sampling for only one of them.

A gamma prior $G(a, b)$ with density $f(t) = \frac{b(bt)^{a-1}e^{-bt}}{\Gamma(a)}$ is specified by DISPERSIONPRIOR=GAMMA, which can be followed by one of the following *gamma-options* enclosed in parentheses. The hyperparameters a and b are the shape and inverse-scale parameters of the gamma distribution, respectively. See the section “Gamma Prior” on page 2836 for details. The default is $G(10^{-4}, 10^{-4})$.

RELSHAPE<=c>

specifies independent $G(c\hat{\phi}, c)$ distribution, where $\hat{\phi}$ is the MLE of the dispersion parameter. With this choice of hyperparameters, the mean of the prior distribution is $\hat{\phi}$ and the variance is $\frac{\hat{\phi}}{c}$. By default, $c=10^{-4}$.

SHAPE=a**ISCALE=b**

when both specified, results in a $G(a, b)$ prior.

SHAPE=c

when specified alone, results in a $G(c, c)$ prior.

ISCALE=c

when specified alone, results in a $G(c, c)$ prior.

An inverse gamma prior $IG(a, b)$ with density $f(t) = \frac{b^a}{\Gamma(a)}t^{-(a+1)}e^{-b/t}$ is specified by DISPERSIONPRIOR=IGAMMA, which can be followed by one of the following *inverse gamma-options*

enclosed in parentheses. The hyperparameters a and b are the shape and scale parameters of the inverse gamma distribution, respectively. See the section “[Inverse Gamma Prior](#)” on page 2837 for details. The default is $IG(2.001, 0.001)$.

RELSHAPE=<c>

specifies independent $IG(\frac{c+\hat{\phi}}{\hat{\phi}}, c)$ distribution, where $\hat{\phi}$ is the MLE of the dispersion parameter.

With this choice of hyperparameters, the mean of the prior distribution is $\hat{\phi}$. By default, $c=10^{-4}$.

SHAPE=a**SCALE=b**

when both specified, results in a $IG(a, b)$ prior.

SHAPE=c

when specified alone, results in an $IG(c, c)$ prior.

SCALE=c

when specified alone, results in an $IG(c, c)$ prior.

An improper prior with density $f(t)$ proportional to t^{-1} is specified with `DISPERSION-PRIOR=IMPROPER`.

INITIAL=SAS-data-set

specifies the SAS data set that contains the initial values of the Markov chains. The `INITIAL=` data set must contain all the variables of the model. You can specify multiple rows as the initial values of the parallel chains for the Gelman-Rubin statistics, but posterior summaries, diagnostics, and plots are computed only for the first chain. If the data set also contains the variable `_SEED_`, the value of the `_SEED_` variable is used as the seed of the random number generator for the corresponding chain.

INITIALMLE

specifies that maximum likelihood estimates of the model parameters be used as initial values of the Markov chain. If this option is not specified, estimates of the mode of the posterior distribution obtained by optimization are used as initial values.

METROPOLIS=YES**METROPOLIS=NO**

specifies the use of a Metropolis step to generate Gibbs samples for posterior distributions that are not log concave. The default value is `METROPOLIS=YES`.

NBI=number

specifies the number of burn-in iterations before the chains are saved. The default is 2000.

NMC=number

specifies the number of iterations after the burn-in. The default is 10000.

OUTPOST=SAS-data-set**OUT=SAS-data-set**

names the SAS data set that contains the posterior samples. See the sections “[OUTPOST= Output Data Set](#)” on page 2839 and “[Posterior Samples Output Data Set](#)” on page 2836 for more information. Alternatively, you can create the output data set by specifying an `ODS OUTPUT` statement as follows:

ODS OUTPUT POSTERIORSAMPLE=SAS-data-set

PRECISIONPRIOR=GAMMA< (options) > | **IMPROPER****PPRIOR=GAMMA**< (options) > | **IMPROPER**

specifies that Gibbs sampling be performed on the generalized linear model precision parameter and the prior distribution for the precision parameter, if there is a precision parameter in the model. For models that do not have a precision parameter (the Poisson and binomial), this option is ignored. Note that you can specify Gibbs sampling on either the dispersion parameter ϕ , the scale parameter $\sigma = \phi^{\frac{1}{2}}$, or the precision parameter $\tau = \phi^{-1}$, with the DPRIOR=, SPRIOR=, and PPRIOR= options, respectively. These three parameters are transformations of one another, and you should specify Gibbs sampling for only one of them.

A gamma prior $G(a, b)$ with density $f(t) = \frac{b(bt)^{a-1}e^{-bt}}{\Gamma(a)}$ is specified by PRECISIONPRIOR=GAMMA, which can be followed by one of the following *gamma-options* enclosed in parentheses. The hyperparameters a and b are the shape and inverse-scale parameters of the gamma distribution, respectively. See the section “Gamma Prior” on page 2836 for details. The default is $G(10^{-4}, 10^{-4})$.

RELSHAPE<=c>

specifies independent $G(c\hat{\tau}, c)$ distribution, where $\hat{\tau}$ is the MLE of the dispersion parameter. With this choice of hyperparameters, the mean of the prior distribution is $\hat{\tau}$ and the variance is $\frac{\hat{\tau}}{c}$. By default, $c = 10^{-4}$.

SHAPE=a**ISCALE**=b

when both specified, results in a $G(a, b)$ prior.

SHAPE=c

when specified alone, results in an $G(c, c)$ prior.

ISCALE=c

when specified alone, results in an $G(c, c)$ prior.

An improper prior with density $f(t)$ proportional to t^{-1} is specified with PRECISIONPRIOR=IMPROPER.

PLOTS< (global-plot-options) >= plot-request**PLOTS**< (global-plot-options) >= (plot-request < ... plot-request >)

controls the display of diagnostic plots. Three types of plots can be requested: trace plots, autocorrelation function plots, and kernel density plots. By default, the plots are displayed in panels unless the global plot option UNPACK is specified. Also, when you are specifying more than one type of plots, the plots are displayed by parameters unless the global plot option GROUPBY is specified. When you specify only one plot request, you can omit the parentheses around the plot request. For example:

```
plots=none
plots(unpack)=trace
plots=(trace autocorr)
```

ODS Graphics must be enabled before requesting plots. For example, the following SAS statements enable ODS Graphics:

```
ods graphics on;
proc genmod;
  model y=x;
  bayes plots=trace;
run;
ods graphics off;
```

The global plot options are as follows:

FRINGE

creates a fringe plot on the X axis of the density plot.

GROUPBY=PARAMETER

GROUPBY=TYPE

specifies how the plots are grouped when there is more than one type of plot.

GROUPBY=TYPE

specifies that the plots be grouped by type.

GROUPBY=PARAMETER

specifies that the plots be grouped by parameter.

GROUPBY=PARAMETER is the default.

LAGS=*n*

specifies that autocorrelations be plotted up to lag *n*. If this option is not specified, autocorrelations are plotted up to lag 50.

SMOOTH

displays a fitted penalized B-spline curve for each trace plot.

UNPACKPANEL

UNPACK

specifies that all paneled plots be unpacked, meaning that each plot in a panel is displayed separately.

The plot requests include the following:

ALL

specifies all types of plots. PLOTS=ALL is equivalent to specifying PLOTS=(TRACE AUTOCORR DENSITY).

AUTOCORR

displays the autocorrelation function plots for the parameters.

DENSITY

displays the kernel density plots for the parameters.

NONE

suppresses all diagnostic plots.

TRACE

displays the trace plots for the parameters. See the section “[Visual Analysis via Trace Plots](#)” on page 139 for details.

SAMPLING=option

specifies an algorithm used to sample the posterior distribution. The following options are available:

ARMS**GIBBS**

use the ARMS algorithm. This is the default method except for the normal distribution with a conjugate prior. In this case a closed form for the posterior distribution is available, and samples are obtained directly from the posterior distribution.

GAMERMAN**GAM**

use the Gaman algorithm.

IM

Use the independent Metropolis algorithm.

SCALEPRIOR=GAMMA< options > | IMPROPER**SPRIOR=GAMMA< options > | IMPROPER**

specifies that Gibbs sampling be performed on the generalized linear model scale parameter and the prior distribution for the scale parameter, if there is a scale parameter in the model. For models that do not have a scale parameter (the Poisson and binomial), this option is ignored. Note that you can specify Gibbs sampling on either the dispersion parameter ϕ , the scale parameter $\sigma = \phi^{1/2}$, or the precision parameter $\tau = \phi^{-1}$, with the DPRIOR=, SPRIOR=, and PPRIOR= options, respectively. These three parameters are transformations of one another, and you should specify Gibbs sampling for only one of them.

A gamma prior $G(a, b)$ with density $f(t) = \frac{b(bt)^{a-1}e^{-bt}}{\Gamma(a)}$ is specified by SCALEPRIOR=GAMMA, which can be followed by one of the following *gamma-options* enclosed in parentheses. The hyperparameters a and b are the shape and inverse-scale parameters of the gamma distribution, respectively. See the section “[Gamma Prior](#)” on page 2836 for details. The default is $G(10^{-4}, 10^{-4})$.

RELSHAPE<=c>

specifies independent $G(c\hat{\sigma}, c)$ distribution, where $\hat{\sigma}$ is the MLE of the dispersion parameter. With this choice of hyperparameters, the mean of the prior distribution is $\hat{\sigma}$ and the variance is $\frac{\hat{\sigma}}{c}$. By default, $c = 10^{-4}$.

SHAPE=a**ISCALE=b**

when both specified, results in a $G(a, b)$ prior.

SHAPE=*c*

when specified alone, results in an $G(c, c)$ prior.

ISCALE=*c*

when specified alone, results in an $G(c, c)$ prior.

An improper prior with density $f(t)$ proportional to t^{-1} is specified with SCALEPRIOR=IMPROPER.

SEED=*number*

specifies an integer seed in the range 1 to $2^{31} - 1$ for the random number generator in the simulation. Specifying a seed enables you to reproduce identical Markov chains for the same specification. If the SEED= option is not specified, or if you specify a nonpositive seed, a random seed is derived from the time of day.

STATISTICS < (*global-options*) > = ALL | NONE | *keyword* | (*keyword-list*)**STATS < (*global-options*) > = ALL | NONE | *keyword* | (*keyword-list*)**

controls the number of posterior statistics produced. Specifying STATISTICS=ALL is equivalent to specifying STATISTICS= (SUMMARY INTERVAL COV CORR). If you do not want any posterior statistics, you specify STATISTICS=NONE. The default is STATISTICS=(SUMMARY INTERVAL). See the section “[Summary Statistics](#)” on page 153 for details. The *global-options* include the following:

ALPHA=*numeric-list*

controls the probabilities of the credible intervals. The ALPHA= values must be between 0 and 1. Each ALPHA= value produces a pair of $100(1-\text{ALPHA})\%$ equal-tail and HPD intervals for each parameters. The default is the value of the ALPHA= option in the MODEL statement, or 0.05 if that option is not specified (yielding the 95% credible intervals for each parameter).

PERCENT=*numeric-list*

requests the percentile points of the posterior samples. The PERCENT= values must be between 0 and 100. The default is PERCENT=25, 50, 75, which yield the 25th, 50th, and 75th percentile points, respectively, for each parameter.

The list of *keywords* includes the following:

CORR

produces the posterior correlation matrix.

COV

produces the posterior covariance matrix.

SUMMARY

produces the means, standard deviations, and percentile points for the posterior samples. The default is to produce the 25th, 50th, and 75th percentile points, but you can use the global PERCENT= option to request specific percentile points.

INTERVAL

produces equal-tail credible intervals and HPD intervals. The default is to produce the 95% equal-tail credible intervals and 95% HPD intervals, but you can use the global ALPHA= option to request intervals of any probabilities.

THINNING=*number*

THIN=*number*

controls the thinning of the Markov chain. Only one in every k samples is used when **THINNING**= k , and if **NBI**= n_0 and **NMC**= n , the number of samples kept is

$$\left[\frac{n_0 + n}{k} \right] - \left[\frac{n_0}{k} \right]$$

where $[a]$ represents the integer part of the number a . The default is **THINNING**=1.

BY Statement

BY *variables* ;

You can specify a **BY** statement with PROC GENMOD to obtain separate analyses of observations in groups that are defined by the **BY** variables. When a **BY** statement appears, the procedure expects the input data set to be sorted in order of the **BY** variables. If you specify more than one **BY** statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar **BY** statement.
- Specify the **NOTSORTED** or **DESCENDING** option in the **BY** statement for the GENMOD procedure. The **NOTSORTED** option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the **BY** variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the **BY** variables by using the DATASETS procedure (in Base SAS software).

For more information about **BY**-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

CLASS Statement

CLASS *variable* < (*options*) > ... < *variable* < (*options*) > > < / *global-options* > ;

The **CLASS** statement names the classification variables to be used as explanatory variables in the analysis. Response variables do not need to be specified in the **CLASS** statement.

The **CLASS** statement must precede the **MODEL** statement. Most options can be specified either as individual variable *options* or as *global-options*. You can specify *options* for each variable by enclosing the options in parentheses after the variable name. You can also specify *global-options* for the **CLASS** statement by placing them after a slash (/). *Global-options* are applied to all the variables specified in the **CLASS**

statement. If you specify more than one CLASS statement, the *global-options* specified in any one CLASS statement apply to all CLASS statements. However, individual CLASS variable *options* override the *global-options*. You can specify the following values for either an *option* or a *global-option*:

CPREFIX=*n*

specifies that, at most, the first *n* characters of a CLASS variable name be used in creating names for the corresponding design variables. The default is $32 - \min(32, \max(2, f))$, where *f* is the formatted length of the CLASS variable.

DESCENDING**DESC**

reverses the sort order of the classification variable. If both the DESCENDING and ORDER= options are specified, PROC GENMOD orders the categories according to the ORDER= option and then reverses that order.

LPREFIX=*n*

specifies that, at most, the first *n* characters of a CLASS variable label be used in creating labels for the corresponding design variables. The default is $256 - \min(256, \max(2, f))$, where *f* is the formatted length of the CLASS variable.

MISSING

treats missing values ('.', '._', '.A', ..., '.Z' for numeric variables and blanks for character variables) as valid values for the CLASS variable.

ORDER=DATA | FORMATTED | FREQ | INTERNAL

specifies the sort order for the levels of classification variables. This ordering determines which parameters in the model correspond to each level in the data, so the ORDER= option can be useful when you use the CONTRAST statement. By default, ORDER=FORMATTED. For ORDER=FORMATTED and ORDER=INTERNAL, the sort order is machine-dependent. When ORDER=FORMATTED is in effect for numeric variables for which you have supplied no explicit format, the levels are ordered by their internal values.

The following table shows how PROC GENMOD interprets values of the ORDER= option.

Value of ORDER=	Levels Sorted By
DATA	Order of appearance in the input data set
FORMATTED	External formatted values, except for numeric variables with no explicit format, which are sorted by their unformatted (internal) values
FREQ	Descending frequency count; levels with more observations come earlier in the order
INTERNAL	Unformatted value

For more information about sort order, see the chapter on the SORT procedure in the *Base SAS Procedures Guide* and the discussion of BY-group processing in *SAS Language Reference: Concepts*.

PARAM=keyword

specifies the parameterization method for the classification variable or variables. You can specify any of the *keywords* shown in the following table; Design matrix columns are created from CLASS variables according to the corresponding coding schemes:

Value of PARAM=	Coding
EFFECT	Effect coding
GLM	Less-than-full-rank reference cell coding (this <i>keyword</i> can be used only in a global option)
ORDINAL THERMOMETER	Cumulative parameterization for an ordinal CLASS variable
POLYNOMIAL POLY	Polynomial coding
REFERENCE REF	Reference cell coding
ORTHEFFECT	Orthogonalizes PARAM=EFFECT coding
ORTHORDINAL ORTHOTHERM	Orthogonalizes PARAM=ORDINAL coding
ORTHPOLY	Orthogonalizes PARAM=POLYNOMIAL coding
ORTHREF	Orthogonalizes PARAM=REFERENCE coding

All parameterizations are full rank, except for the GLM parameterization. The **REF=** option in the CLASS statement determines the reference level for EFFECT and REFERENCE coding and for their orthogonal parameterizations. It also indirectly determines the reference level for a singular GLM parameterization through the order of levels.

If PARAM=ORTHPOLY or PARAM=POLY and the classification variable is numeric, then the **ORDER=** option in the CLASS statement is ignored, and the internal unformatted values are used. See the section “Other Parameterizations” on page 387 of Chapter 19, “Shared Concepts and Topics,” for further details.

REF= '*level*' | *keyword*

specifies the reference level for **PARAM=EFFECT**, **PARAM=REFERENCE**, and their orthogonalizations. For **PARAM=GLM**, the **REF=** option specifies a level of the classification variable to be put at the end of the list of levels. This level thus corresponds to the reference level in the usual interpretation of the linear estimates with a singular parameterization.

For an individual variable **REF=** option (but not for a global **REF=** option), you can specify the *level* of the variable to use as the reference level. Specify the formatted value of the variable if a format is assigned. For a global or individual variable **REF=** option, you can use one of the following *keywords*. The default is **REF=LAST**.

FIRST designates the first ordered level as reference.

LAST designates the last ordered level as reference.

TRUNCATE $\langle =n \rangle$

specifies the length n of CLASS variable values to use in determining CLASS variable levels. The default is to use the full formatted length of the CLASS variable. If you specify TRUNCATE without the length n , the first 16 characters of the formatted values are used. When formatted values are longer than 16 characters, you can use this option to revert to the levels as determined in releases before SAS 9. The TRUNCATE option is available only as a global option.

Class Variable Default Parameterization

If you do not specify the PARAM= option, the default PARAM=GLM parameterization is used.

Class Variable Naming Convention

Parameter names for a CLASS predictor variable are constructed by concatenating the CLASS variable name with the CLASS levels. However, for the POLYNOMIAL and orthogonal parameterizations, parameter names are formed by concatenating the CLASS variable name and keywords that reflect the parameterization. See the section “Other Parameterizations” on page 387 in Chapter 19, “Shared Concepts and Topics,” for examples and further details.

Class Variable Parameterization with Unbalanced Designs

PROC GENMOD initially parameterizes the CLASS variables by looking at the levels of the variables across the complete data set. If you have an *unbalanced* replication of levels across variables or BY groups, then the design matrix and the parameter interpretation might be different from what you expect. For instance, suppose you have a model with one CLASS variable A with three levels (1, 2, and 3), and another CLASS variable B with two levels (1 and 2). If the third level of A occurs only with the first level of B, if you use the EFFECT parameterization, and if your model contains the effect A(B) and an intercept, then the design for A within the second level of B is not a differential effect. In particular, the design looks like the following:

		Design Matrix			
		A(B=1)		A(B=2)	
B	A	A1	A2	A1	A2
1	1	1	0	0	0
1	2	0	1	0	0
1	3	-1	-1	0	0
2	1	0	0	1	0
2	2	0	0	0	1

PROC GENMOD detects linear dependency among the last two design variables and sets the parameter for A2(B=2) to zero, resulting in an interpretation of these parameters as if they were reference- or dummy-coded. The REFERENCE or GLM parameterization might be more appropriate for such problems.

CODE Statement

CODE $\langle options \rangle$;

The CODE statement enables you to write SAS DATA step code for computing predicted values of the fitted model either to a file or to a catalog entry. This code can then be included in a DATA step to score new data.

Table 40.3 summarizes the *options* available in the CODE statement.

Table 40.3 CODE Statement Options

Option	Description
CATALOG=	Names the catalog entry where the generated code is saved
DUMMIES	Retains the dummy variables in the data set
ERROR	Computes the error function
FILE=	Names the file where the generated code is saved
FORMAT=	Specifies the numeric format for the regression coefficients
GROUP=	Specifies the group identifier for array names and statement labels
IMPUTE	Imputes predicted values for observations with missing or invalid covariates
LINESIZE=	Specifies the line size of the generated code
LOOKUP=	Specifies the algorithm for looking up CLASS levels
RESIDUAL	Computes residuals

For details about the syntax of the CODE statement, see the section “CODE Statement” on page 390 in Chapter 19, “Shared Concepts and Topics.”

CONTRAST Statement

CONTRAST *'label' contrast-specification* </ options > ;

The CONTRAST statement provides a means of obtaining a test of a specified hypothesis concerning the model parameters. This is accomplished by specifying a matrix L for testing the hypothesis $L'\beta = 0$. You must be familiar with the details of the model parameterization that PROC GENMOD uses. For more information, see the section “Parameterization Used in PROC GENMOD” on page 2811 and the section “CLASS Statement” on page 2759. Computed statistics are based on the asymptotic chi-square distribution of the likelihood ratio statistic, or the generalized score statistic for GEE models, with degrees of freedom determined by the number of linearly independent rows in the L' matrix. You can request Wald chi-square statistics with the Wald option in the CONTRAST statement.

There is no limit to the number of CONTRAST statements that you can specify, but they must appear after the MODEL statement and after the ZEROMODEL statement for zero-inflated models. Statistics for multiple CONTRAST statements are displayed in a single table.

The elements of the CONTRAST statement are as follows:

label identifies the contrast on the output. A label is required for every contrast specified. Labels can be up to 20 characters and must be enclosed in single quotes.

contrast-specification identifies the effects and their coefficients from which the L matrix is formed. The *contrast-specification* can be specified in two different ways. The first method applies to all models except the zero-inflated (ZI) distributions (zero-inflated Poisson and zero-inflated negative binomial), and the syntax is:

effect values <,... *effect values*>

The second method of specifying a contrast applies only to ZI models, and the syntax is:

effect values <,... *effect values*> **@ZERO** *effect values* <,... *effect values*>

where

effect identifies an effect that appears in the MODEL statement. The value INTERCEPT or intercept can be used as an effect when an intercept is included in the model. You do not need to include all effects that are included in the MODEL statement.

values are constants that are elements of the **L** vector associated with the effect.

options specifies CONTRAST statement options.

Specification of sets of *effect values* before the @ZERO separator results in a row of the **L'** matrix with coefficients for *effects* in the regression part of the model set to *values* and with the coefficients for the zero-inflation part of the model set to zero. Specification of sets of *effect values* after the @ZERO separator results in a row of the **L** matrix with the coefficients for the regression part of the model set to zero and with the coefficients of *effects* in the zero-inflation part of the model set to *values*.

For example, the statements

```
class a;
model y=a;
contrast 'Label1' A 1 -1;
```

specify an **L'** matrix with one row with coefficients 1 for the first level of A and -1 for the second level of A.

The statements

```
class a b;
model y=a / dist=zip;
zeromodel b;
contrast 'Label2' A 1 -1 @zero B 1 -1;
```

specify an **L'** matrix with two rows: the first row has coefficients 1 for the first level of A, -1 for the second level of A, and zeros for all levels of B; the second row has coefficients 0 for all levels of A, 1 for the first level of B, and -1 for the second level of B.

The rows of **L'** are specified in order and are separated by commas.

If you use the default less-than-full-rank PROC GLM CLASS variable parameterization, each row of the **L'** matrix is checked for estimability. If PROC GENMOD finds a contrast to be nonestimable, it displays missing values in corresponding rows in the results. See Searle (1971) for a discussion of estimable functions. If the elements of **L'** are not specified for an effect that contains a specified effect, then the elements of the specified effect are distributed over the levels of the higher-order effect just as the GLM procedure does for its CONTRAST and ESTIMATE statements. For example, suppose that the model contains effects A and B and their interaction A*B. If you specify a CONTRAST statement involving A alone, the **L'** matrix contains nonzero terms for both A and A*B, since A*B contains A.

When you use any of the full-rank PARAM= CLASS variable options, all parameters are directly estimable, and rows of **L'** are not checked for estimability.

If an effect is not specified in the CONTRAST statement, all of its coefficients in the L' matrix are set to 0. If too many values are specified for an effect, the extra ones are ignored. If too few values are specified, the remaining ones are set to 0.

PROC GENMOD handles missing level combinations of classification variables in the same manner as the GLM and MIXED procedures. Parameters corresponding to missing level combinations are not included in the model. This convention can affect the way in which you specify the L matrix in your CONTRAST statement.

If you specify the WALD option, the test of hypothesis is based on a Wald chi-square statistic. If you omit the WALD option, the test statistic computed depends on whether an ordinary generalized linear model or a GEE-type model is specified.

For an ordinary generalized linear model, the CONTRAST statement computes the likelihood ratio statistic. This is defined to be twice the difference between the log likelihood of the model unconstrained by the contrast and the log likelihood with the model fitted under the constraint that the linear function of the parameters defined by the contrast is equal to 0. A p -value is computed based on the asymptotic chi-square distribution of the chi-square statistic.

If you specify a GEE model with the REPEATED statement, the test is based on a score statistic. The GEE model is fit under the constraint that the linear function of the parameters defined by the contrast is equal to 0. The score chi-square statistic is computed based on the generalized score function. See the section “Generalized Score Statistics” on page 2827 for more information.

The degrees of freedom is the number of linearly independent constraints implied by the CONTRAST statement—that is, the rank of L .

You can specify the following options after a slash (/).

E

requests that the L matrix be displayed.

SINGULAR=*number*

EPSILON=*number*

tunes the estimability checking. If \mathbf{v} is a vector, define $ABS(\mathbf{v})$ to be the absolute value of the element of \mathbf{v} with the largest absolute value. Let \mathbf{K}' be any row in the contrast matrix L . Define C to be equal to $ABS(\mathbf{K}')$ if $ABS(\mathbf{K}')$ is greater than 0; otherwise, C equals 1. If $ABS(\mathbf{K}' - \mathbf{K}'\mathbf{T})$ is greater than $C * \textit{number}$, then \mathbf{K} is declared nonestimable. \mathbf{T} is the Hermite form matrix $(\mathbf{X}'\mathbf{X})^{-}(\mathbf{X}'\mathbf{X})$, and $(\mathbf{X}'\mathbf{X})^{-}$ represents a generalized inverse of the matrix $\mathbf{X}'\mathbf{X}$. The value for *number* must be between 0 and 1; the default value is $1E-4$. The SINGULAR= option in the MODEL statement affects the computation of the generalized inverse of the matrix $\mathbf{X}'\mathbf{X}$. It might also be necessary to adjust this value for some data.

WALD

requests that a Wald chi-square statistic be computed for the contrast rather than the default likelihood ratio or score statistic. The Wald statistic for testing $L'\beta = \mathbf{0}$ is defined by

$$S = (L'\hat{\beta})'(L'\Sigma L)^{-}(L'\hat{\beta})$$

where $\hat{\beta}$ is the maximum likelihood estimate and Σ is its estimated covariance matrix. The asymptotic distribution of S is χ_r^2 , where r is the rank of L . Computed p -values are based on this distribution.

If you specify a GEE model with the REPEATED statement, Σ is the empirical covariance matrix estimate.

DEVIANCE Statement

DEVIANCE *variable=expression* ;

You can specify a probability distribution other than those available in PROC GENMOD by using the DEVIANCE and VARIANCE statements. You do not need to specify the DEVIANCE or VARIANCE statement if you use the DIST= MODEL statement option to specify a probability distribution. The *variable* identifies the deviance contribution from a single observation to the procedure, and it must be a valid SAS variable name that does not appear in the input data set. The *expression* can be any arithmetic expression supported by the DATA step language, and it is used to define the functional dependence of the deviance on the mean and the response. You use the automatic variables `_MEAN_` and `_RESP_` to represent the mean and response in the *expression*.

Alternatively, the deviance function can be defined using programming statements (see the section “Programming Statements” on page 2790) and assigned to a variable, which is then listed as the *expression*. This form is convenient for using complex statements such as IF-THEN/ELSE clauses.

The DEVIANCE statement is ignored unless the VARIANCE statement is also specified.

EFFECTPLOT Statement

EFFECTPLOT *< plot-type <(plot-definition-options)>> </ options>* ;

The EFFECTPLOT statement produces a display of the fitted model and provides options for changing and enhancing the displays. Table 40.4 describes the available *plot-types* and their *plot-definition-options*.

Table 40.4 *Plot-Types and Plot-Definition-Options*

Plot-Type and Description	Plot-Definition-Options
<p>BOX Displays a box plot of continuous response data at each level of a CLASS effect, with predicted values superimposed and connected by a line. This is an alternative to the INTERACTION <i>plot-type</i>.</p>	<p>PLOTBY= variable or CLASS effect X= CLASS variable or effect</p>
<p>CONTOUR Displays a contour plot of predicted values against two continuous covariates.</p>	<p>PLOTBY= variable or CLASS effect X= continuous variable Y= continuous variable</p>
<p>FIT Displays a curve of predicted values versus a continuous variable.</p>	<p>PLOTBY= variable or CLASS effect X= continuous variable</p>
<p>INTERACTION Displays a plot of predicted values (possibly with error bars) versus the levels of a CLASS effect. The predicted values are connected with lines and can be grouped by the levels of another CLASS effect.</p>	<p>PLOTBY= variable or CLASS effect SLICEBY= variable or CLASS effect X= CLASS variable or effect</p>

Table 40.4 continued

Plot-Type and Description	Plot-Definition-Options
SLICEFIT Displays a curve of predicted values versus a continuous variable grouped by the levels of a CLASS effect.	PLOTBY= variable or CLASS effect SLICEBY= variable or CLASS effect X= continuous variable

For full details about the syntax and options of the EFFECTPLOT statement, see the section “EFFECTPLOT Statement” on page 411 in Chapter 19, “Shared Concepts and Topics.”

ESTIMATE Statement

```
ESTIMATE 'label' contrast-specification </ options> ;
```

The ESTIMATE statement is similar to a CONTRAST statement, except only one-row L' matrices are permitted.

The elements of the ESTIMATE statement are as follows:

label identifies the contrast on the output. A label is required for every contrast specified. Labels can be up to 20 characters and must be enclosed in single quotes.

contrast-specification identifies the effects and their coefficients from which the L matrix is formed. The *contrast-specification* can be specified in two different ways. The first method applies to all models except the zero-inflated (ZI) distributions (zero-inflated Poisson and zero-inflated negative binomial), and the syntax is:

```
effect values < ... effect values >
```

The second method of specifying a contrast applies only to ZI models, and the syntax is:

```
effect values < ... effect values > @ZERO effect values < ... effect values >
```

where

effect identifies an effect that appears in the MODEL statement. The value INTERCEPT or intercept can be used as an effect when an intercept is included in the model. You do not need to include all effects that are included in the MODEL statement.

values are constants that are elements of the L vector associated with the effect.

options specifies options for the ESTIMATE statement.

For ZI models, sets of *effects values* before the @ZERO separator correspond to the regression part of the model with regression parameters β , and *effects values* after the @ZERO separator correspond to the zero-inflation part of the model with regression parameters γ . In the case of ZI models, a one-row L' matrix is created for the regression part of the model, another one-row L' matrix is created for the zero-inflation part of the model, and separate estimates for the two L matrices are computed and displayed.

If you use the default less-than-full-rank GLM CLASS variable parameterization, each row is checked for estimability. If PROC GENMOD finds a contrast to be nonestimable, it displays missing values in corresponding rows in the results. See Searle (1971) for a discussion of estimable functions.

The actual estimate, $L'\beta$ (and $L'\gamma$ for ZI models), its approximate standard error, and confidence limits are displayed. Additionally, the corresponding estimate on the mean scale (defined as the inverse link function applied to $L'\beta$), and confidence limits are displayed. Wald chi-square tests that $L'\beta = 0$ and $L'\gamma = 0$ are also displayed.

The approximate standard error of the estimate is computed as the square root of $L'\hat{\Sigma}L$, where $\hat{\Sigma}$ is the estimated covariance matrix of the parameter estimates. If you specify a GEE model in the REPEATED statement, $\hat{\Sigma}$ is the empirical covariance matrix estimate.

If you specify the EXP option, then $\exp(L'\beta)$, its standard error, and its confidence limits are also displayed.

The construction of the L vector and the checking for estimability for an ESTIMATE statement follow the same rules as listed under the CONTRAST statement.

You can specify the following options in the ESTIMATE statement after a slash (/).

ALPHA=number

requests that a confidence interval be constructed with confidence level $1 - \text{number}$. The value of *number* must be between 0 and 1; the default value is 0.05.

DIVISOR=number

specifies a value by which to divide all coefficients so that fractional coefficients can be entered as integer numerators. For example, you can use

```
estimate '1/3(A1+A2) - 2/3A3' a 1 1 -2 / divisor=3;
```

instead of

```
estimate '1/3(A1+A2) - 2/3A3' a 0.33333 0.33333 -0.66667;
```

E

requests that the L matrix coefficients be displayed.

EXP

requests that $\exp(L'\beta)$, its standard error, and its confidence limits be computed. If you specify the EXP option, standard errors are computed using the delta method. Confidence limits are computed by exponentiating the confidence limits for $L'\beta$.

SINGULAR=number

EPSILON=number

tunes the estimability checking as described for the CONTRAST statement.

EXACT Statement

```
EXACT <'label'> <INTERCEPT> <effects> </options>;
```

The EXACT statement performs exact tests of the parameters for the specified *effects* and optionally estimates the parameters and outputs the exact conditional distributions. You can specify the keyword INTERCEPT and any effects in the MODEL statement. Inference on the parameters of the specified effects is

performed by conditioning on the sufficient statistics of all the other model parameters (possibly including the intercept).

You can specify several EXACT statements, but they must follow the **MODEL** statement. Each statement can optionally include an identifying *label*. If several EXACT statements are specified, any statement without a label is assigned a label of the form “Exact n ,” where n indicates the n th EXACT statement. The label is included in the headers of the displayed exact analysis tables.

If a **STRATA** statement is also specified, then a stratified exact logistic regression or a stratified exact Poisson regression is performed. The model contains a different intercept for each stratum, and these intercepts are conditioned out of the model along with any other nuisance parameters (parameters for effects specified in the **MODEL** statement that are not in the EXACT statement).

The **ASSESSMENT**, **BAYES**, **CONTRAST**, **EFFECTPLOT**, **ESTIMATE**, **LSMEANS**, **LSMESTIMATE**, **OUTPUT**, **SLICE**, and **STORE** statements are not available with an exact analysis. Exact analyses are not performed when you specify a **WEIGHT** statement, or a model other than **LINK=LOGIT** with **DIST=BIN** or **LINK=LOG** with **DIST=POISSON**. An **OFFSET=** variable is not available with exact logistic regression. Exact estimation is not available for ordinal response models.

For classification variables, use of the reference parameterization is recommended.

The following options can be specified in each EXACT statement after a slash (/):

ALPHA=number

specifies the level of significance α for $100(1 - \alpha)\%$ confidence limits for the parameters or odds ratios. The value of *number* must be between 0 and 1. By default, *number* is equal to the value of the **ALPHA=** option in the **MODEL** statement, or 0.05 if that option is not specified.

CLTYPE=EXACT | MIDP

requests either the exact or mid- p confidence intervals for the parameter estimates. By default, the exact intervals are produced. The confidence coefficient can be specified with the **ALPHA=** option. The mid- p interval can be modified with the **MIDPFACTOR=** option. See the section “Exact Logistic and Exact Poisson Regression” on page 2839 for details.

ESTIMATE <=keyword>

estimates the individual parameters (conditioned on all other parameters) for the effects specified in the EXACT statement. For each parameter, a point estimate, a standard error, a confidence interval, and a p -value for a two-sided test that the parameter is zero are displayed. Note that the two-sided p -value is twice the one-sided p -value. You can optionally specify one of the following keywords:

PARAM specifies that the parameters be estimated. This is the default.

ODDS specifies that the odds ratios be estimated. If you have classification variables, then you must also specify the **PARAM=REF** option in the **CLASS** statement.

BOTH specifies that both the parameters and odds ratios be estimated.

JOINT

performs the joint test that all of the parameters are simultaneously equal to zero, performs individual hypothesis tests for the parameter of each continuous variable, and performs joint tests for the parameters of each classification variable. The joint test is indicated in the “Conditional Exact Tests” table by the label “Joint.”

JOINTONLY

performs only the joint test of the parameters. The test is indicated in the “Conditional Exact Tests” table by the label “Joint.” When this option is specified, individual tests for the parameters of each continuous variable and joint tests for the parameters of the classification variables are not performed.

MIDPFACTOR= δ_1 | (δ_1, δ_2)

sets the tie factors used to produce the mid- p hypothesis statistics and the mid- p confidence intervals. δ_1 modifies both the hypothesis tests and confidence intervals, while δ_2 affects only the hypothesis tests. By default, $\delta_1 = 0.5$ and $\delta_2 = 1.0$. See the section “Exact Logistic and Exact Poisson Regression” on page 2839 for details.

ONESIDED

requests one-sided confidence intervals and p -values for the individual parameter estimates and odds ratios. The one-sided p -value is the smaller of the left- and right-tail probabilities for the observed sufficient statistic of the parameter under the null hypothesis that the parameter is zero. The two-sided p -values (default) are twice the one-sided p -values. See the section “Exact Logistic and Exact Poisson Regression” on page 2839 for more details.

OUTDIST=*SAS-data-set*

names the SAS data set that contains the exact conditional distributions. This data set contains all of the exact conditional distributions that are required to process the corresponding EXACT statement. This data set contains the possible sufficient statistics for the parameters of the effects specified in the EXACT statement, the counts, and, when hypothesis tests are performed on the parameters, the probability of occurrence and the score value for each sufficient statistic. When you request an OUTDIST= data set, the observed sufficient statistics are displayed in the “Sufficient Statistics” table. See the section “OUTDIST= Output Data Set” on page 2840 for more information.

EXACT Statement Examples

In the following example, two exact tests are computed: one for x_1 and the other for x_2 . The test for x_1 is based on the exact conditional distribution of the sufficient statistic for the x_1 parameter given the observed values of the sufficient statistics for the intercept, x_2 , and x_3 parameters; likewise, the test for x_2 is conditional on the observed sufficient statistics for the intercept, x_1 , and x_3 .

```
proc genmod;
  model y= x1 x2 x3/d=b;
  exact x1 x2;
run;
```

PROC GENMOD determines, from all the specified EXACT statements, the distinct conditional distributions that need to be evaluated. For example, there is only one exact conditional distribution for the following two EXACT statements:

```
exact 'One' x1 / estimate=parm;
exact 'Two' x1 / estimate=parm onesided;
```

For each EXACT statement, individual tests for the parameters of the specified effects are computed unless the **JOINTONLY** option is specified. Consider the following EXACT statements:

```

exact 'E12' x1 x2 / estimate;
exact 'E1'  x1    / estimate;
exact 'E2'  x2    / estimate;
exact 'J12' x1 x2 / joint;

```

In the E12 statement, the parameters for x1 and x2 are estimated and tested separately. Specifying the E12 statement is equivalent to specifying both the E1 and E2 statements. In the J12 statement, the joint test for the parameters of x1 and x2 is computed in addition to the individual tests for x1 and x2.

EXACTOPTIONS Statement

EXACTOPTIONS *options* ;

The EXACTOPTIONS statement specifies options that apply to every **EXACT** statement in the program. The following *options* are available:

ABSFCNV=*value*

specifies the absolute function convergence criterion. Convergence requires a small change in the log-likelihood function in subsequent iterations,

$$|l_i - l_{i-1}| < \textit{value}$$

where l_i is the value of the log-likelihood function at iteration i .

By default, ABSFCNV=1E-12. You can also specify the **FCNV=** and **XCONV=** criteria; optimizations are terminated as soon as one criterion is satisfied.

ADDTOBS

adds the observed sufficient statistic to the sampled exact distribution if the statistic was not sampled. This option has no effect unless the **METHOD=NETWORKMC** option is specified and the **ESTIMATE** option is specified in the **EXACT** statement. If the observed statistic has not been sampled, then the parameter estimate does not exist; by specifying this option, you can produce (biased) estimates.

BUILDSUBSETS

builds every distribution for sampling. By default, some exact distributions are created by taking a subset of a previously generated exact distribution. When the **METHOD=NETWORKMC** option is invoked, this subsetting behavior has the effect of using fewer than the desired n samples; see the **N=** option for more details. Use the **BUILDSUBSETS** option to suppress this subsetting.

EPSILON=*value*

controls how the partial sums $\sum_{i=1}^j y_i x_i$ are compared. *value* must be between 0 and 1; by default, *value*=1E-8.

FCNV=*value*

specifies the relative function convergence criterion. Convergence requires a small relative change in the log-likelihood function in subsequent iterations,

$$\frac{|l_i - l_{i-1}|}{|l_{i-1}| + 1\text{E-}6} < \textit{value}$$

where l_i is the value of the log likelihood at iteration i .

By default, FCONV=1E-8. You can also specify the ABSFCONV= and XCONV= criteria; if more than one criterion is specified, then optimizations are terminated as soon as one criterion is satisfied.

MAXTIME=seconds

specifies the maximum clock time (in seconds) that PROC GENMOD can use to calculate the exact distributions. If the limit is exceeded, the procedure halts all computations and prints a note to the LOG. The default maximum clock time is seven days.

METHOD=keyword

specifies which exact conditional algorithm to use for every EXACT statement specified. You can specify one of the following keywords:

DIRECT invokes the multivariate shift algorithm of Hirji, Mehta, and Patel (1987). This method directly builds the exact distribution, but it can require an excessive amount of memory in its intermediate stages. METHOD=DIRECT is invoked by default when you are conditioning out at most the intercept.

NETWORK invokes an algorithm described in Mehta, Patel, and Senchaudhuri (1992). This method builds a network for each parameter that you are conditioning out, combines the networks, then uses the multivariate shift algorithm to create the exact distribution. The NETWORK method can be faster and require less memory than the DIRECT method. The NETWORK method is invoked by default for most analyses.

NETWORKMC invokes the hybrid network and Monte Carlo algorithm of Mehta, Patel, and Senchaudhuri (1992). This method creates a network, then samples from that network; this method does not reject any of the samples at the cost of using a large amount of memory to create the network. METHOD=NETWORKMC is most useful for producing parameter estimates for problems that are too large for the DIRECT and NETWORK methods to handle and for which asymptotic methods are invalid—for example, for sparse data on a large grid.

N=n

specifies the number of Monte Carlo samples to take when the METHOD=NETWORKMC option is specified. By default, $n = 10,000$. If the procedure cannot obtain n samples due to a lack of memory, then a note is printed in the SAS log (the number of valid samples is also reported in the listing) and the analysis continues.

The number of samples used to produce any particular statistic might be smaller than n . For example, let $X1$ and $X2$ be continuous variables, denote their joint distribution by $f(X1,X2)$, and let $f(X1 | X2 = x2)$ denote the marginal distribution of $X1$ conditioned on the observed value of $X2$. If you request the JOINT test of $X1$ and $X2$, then n samples are used to generate the estimate $\hat{f}(X1,X2)$ of $f(X1,X2)$, from which the test is computed. However, the parameter estimate for $X1$ is computed from the subset of $\hat{f}(X1,X2)$ that has $X2 = x2$, and this subset need not contain n samples. Similarly, the distribution for each level of a classification variable is created by extracting the appropriate subset from the joint distribution for the CLASS variable.

In some cases, the marginal sample size can be too small to admit accurate estimation of a particular statistic; a note is printed in the SAS log when a marginal sample size is less than 100. Increasing n increases the number of samples used in a marginal distribution; however, if you want to control the sample size exactly, you can either specify the BUILDSUBSETS option or do both of the following:

- Remove the **JOINT** option from the **EXACT** statement.
- Create dummy variables in a **DATA** step to represent the levels of a **CLASS** variable, and specify them as independent variables in the **MODEL** statement.

NOLOGSCALE

specifies that computations for the exact conditional models be computed by using normal scaling. Log scaling can handle numerically larger problems than normal scaling; however, computations in the log scale are slower than computations in normal scale.

ONDISK

uses disk space instead of random access memory to build the exact conditional distribution. Use this option to handle larger problems at the cost of slower processing.

SEED=seed

specifies the initial seed for the random number generator used to take the Monte Carlo samples when the **METHOD=NETWORKMC** option is specified. The value of the **SEED=** option must be an integer. If you do not specify a seed, or if you specify a value less than or equal to zero, then **PROC GENMOD** uses the time of day from the computer's clock to generate an initial seed.

STATUSN=number

prints a status line in the SAS log after every *number* of Monte Carlo samples when the **METHOD=NETWORKMC** option is specified. The number of samples taken and the current exact *p*-value for testing the significance of the model are displayed. You can use this status line to track the progress of the computation of the exact conditional distributions.

STATUSTIME=seconds

specifies the time interval (in seconds) for printing a status line in the LOG. You can use this status line to track the progress of the computation of the exact conditional distributions. The time interval you specify is approximate; the actual time interval varies. By default, no status reports are produced.

XCONV=value

specifies the relative parameter convergence criterion. Convergence requires a small relative parameter change in subsequent iterations,

$$\max_j |\delta_j^{(i)}| < value$$

where

$$\delta_j^{(i)} = \begin{cases} \frac{\beta_j^{(i)} - \beta_j^{(i-1)}}{\beta_j^{(i-1)}} & |\beta_j^{(i-1)}| < 0.01 \\ \beta_j^{(i)} - \beta_j^{(i-1)} & \text{otherwise} \end{cases}$$

and $\beta_j^{(i)}$ is the estimate of the *j*th parameter at iteration *i*.

By default, **XCONV=1E-4**. You can also specify the **ABSFCNV=** and **FCONV=** criteria; if more than one criterion is specified, then optimizations are terminated as soon as one criterion is satisfied.

FREQ Statement

FREQ *variable* ;

FREQUENCY *variable* ;

The *variable* in the FREQ statement identifies a variable in the input data set containing the frequency of occurrence of each observation. PROC GENMOD treats each observation as if it appears n times, where n is the value of the FREQ variable for the observation. If it is not an integer, the frequency value is truncated to an integer. If it is less than 1 or missing, the observation is not used. In the case of models fit with generalized estimating equations (GEEs), the frequencies apply to the subject/cluster and therefore must be the same for all observations within each subject.

FWDLINK Statement

FWDLINK *variable=expression* ;

You can define a link function other than a built-in link function by using the FWDLINK statement. If you use the MODEL statement option LINK= to specify a link function, you do not need to use the FWDLINK statement. The *variable* identifies the link function to the procedure. The *expression* can be any arithmetic expression supported by the DATA step language, and it is used to define the functional dependence on the mean.

Alternatively, the link function can be defined by using programming statements (see the section “[Programming Statements](#)” on page 2790) and assigned to a variable, which is then listed as the *expression*. The second form is convenient for using complex statements such as IF-THEN/ELSE clauses. The GENMOD procedure automatically computes derivatives of the link function required for iterative fitting. You must specify the inverse of the link function in the INVLINK statement when you specify the FWDLINK statement to define the link function. You use the automatic variable `_MEAN_` to represent the mean in the preceding *expression*.

INVLINK Statement

INVLINK *variable=expression* ;

If you define a link function in the FWDLINK statement, then you must define the inverse link function by using the INVLINK statement. If you use the MODEL statement option LINK= to specify a link function, you do not need to use the INVLINK statement. The *variable* identifies the inverse link function to the procedure. The *expression* can be any arithmetic expression supported by the DATA step language, and it is used to define the functional dependence on the linear predictor.

Alternatively, the inverse link function can be defined using programming statements (see the section “[Programming Statements](#)” on page 2790) and assigned to a variable, which is then listed as the *expression*. The second form is convenient for using complex statements such as IF-THEN/ELSE clauses. The automatic variable `_XBETA_` represents the linear predictor in the preceding *expression*.

LSMEANS Statement

LSMEANS < *model-effects* > < / *options* > ;

The LSMEANS statement computes and compares least squares means (LS-means) of fixed effects. LS-means are *predicted population margins*—that is, they estimate the marginal means over a balanced population. In a sense, LS-means are to unbalanced designs as class and subclass arithmetic means are to balanced designs.

Table 40.5 summarizes the options available in the LSMEANS statement. If you specify the BAYES statement, the ADJUST=, STEPDOWN, and LINES options are ignored. The PLOTS= option is not available for a maximum likelihood analysis; it is available only for a Bayesian analysis.

If you specify a zero-inflated model (that is, a model for either the zero-inflated Poisson or the zero-inflated negative binomial distribution), then the least squares means are computed only for effects in the model for the distribution mean, and not for effects in the zero-inflation probability part of the model.

Table 40.5 LSMEANS Statement Options

Option	Description
Construction and Computation of LS-Means	
AT	Modifies the covariate value in computing LS-means
BYLEVEL	Computes separate margins
DIFF	Requests differences of LS-means
OM=	Specifies the weighting scheme for LS-means computation as determined by the input data set
SINGULAR=	Tunes estimability checking
Degrees of Freedom and p-values	
ADJUST=	Determines the method for multiple-comparison adjustment of LS-means differences
ALPHA= α	Determines the confidence level ($1 - \alpha$)
STEPDOWN	Adjusts multiple-comparison p -values further in a step-down fashion
Statistical Output	
CL	Constructs confidence limits for means and mean differences
CORR	Displays the correlation matrix of LS-means
COV	Displays the covariance matrix of LS-means
E	Prints the L matrix
LINES	Produces a “Lines” display for pairwise LS-means differences
MEANS	Prints the LS-means
PLOTS=	Requests graphs of means and mean comparisons
SEED=	Specifies the seed for computations that depend on random numbers

Table 40.5 *continued*

Option	Description
Generalized Linear Modeling	
EXP	Exponentiates and displays estimates of LS-means or LS-means differences
ILINK	Computes and displays estimates and standard errors of LS-means (but not differences) on the inverse linked scale
ODDSRATIO	Reports (simple) differences of least squares means in terms of odds ratios if permitted by the link function

For details about the syntax of the LSMEANS statement, see the section “LSMEANS Statement” on page 453 of Chapter 19, “Shared Concepts and Topics.”

LSMESTIMATE Statement

```
LSMESTIMATE model-effect <'label'> values <divisor=n>
             < , ... <'label'> values <divisor=n> >
             </options> ;
```

The LSMESTIMATE statement provides a mechanism for obtaining custom hypothesis tests among least squares means.

Table 40.6 summarizes the options available in the LSMESTIMATE statement.

Table 40.6 LSMESTIMATE Statement Options

Option	Description
Construction and Computation of LS-Means	
AT	Modifies covariate values in computing LS-means
BYLEVEL	Computes separate margins
DIVISOR=	Specifies a list of values to divide the coefficients
OM=	Specifies the weighting scheme for LS-means computation as determined by a data set
SINGULAR=	Tunes estimability checking
Degrees of Freedom and p-values	
ADJUST=	Determines the method for multiple-comparison adjustment of LS-means differences
ALPHA= α	Determines the confidence level ($1 - \alpha$)
LOWER	Performs one-sided, lower-tailed inference
STEPDOWN	Adjusts multiple-comparison p -values further in a step-down fashion
TESTVALUE=	Specifies values under the null hypothesis for tests
UPPER	Performs one-sided, upper-tailed inference

Table 40.6 *continued*

Option	Description
Statistical Output	
CL	Constructs confidence limits for means and mean differences
CORR	Displays the correlation matrix of LS-means
COV	Displays the covariance matrix of LS-means
E	Prints the L matrix
ELSM	Prints the K matrix
JOINT	Produces a joint <i>F</i> or chi-square test for the LS-means and LS-means differences
PLOTS=	Requests graphs of means and mean comparisons
SEED=	Specifies the seed for computations that depend on random numbers
Generalized Linear Modeling	
CATEGORY=	Specifies how to construct estimable functions with multinomial data
EXP	Exponentiates and displays LS-means estimates
ILINK	Computes and displays estimates and standard errors of LS-means (but not differences) on the inverse linked scale

For details about the syntax of the LSMESTIMATE statement, see the section “[LSMESTIMATE Statement](#)” on page 470 in Chapter 19, “[Shared Concepts and Topics](#).”

MODEL Statement

MODEL *response* = < *effects* > < / *options* > ;

MODEL *events/trials* = < *effects* > < / *options* > ;

The MODEL statement specifies the response, or dependent variable, and the effects, or explanatory variables. If you omit the explanatory variables, the procedure fits an intercept-only model. An intercept term is included in the model by default. The intercept can be removed with the NOINT option.

You can specify the response in the form of a single variable or in the form of a ratio of two variables denoted *events/trials*. The first form is applicable to all responses. The second form is applicable only to summarized binomial response data. When each observation in the input data set contains the number of events (for example, successes) and the number of trials from a set of binomial trials, use the *events/trials* syntax.

In the *events/trials* model syntax, you specify two variables that contain the event and trial counts. These two variables are separated by a slash (/). The values of both *events* and (*trials*–*events*) must be nonnegative, and the value of the *trials* variable must be greater than 0 for an observation to be valid. The variable *events* or *trials* can take noninteger values.

When each observation in the input data set contains a single trial from a binomial or multinomial experiment, use the first form of the preceding MODEL statements. The response variable can be numeric or

character. The ordering of response levels is critical in these models. You can use the RORDER= option in the PROC GENMOD statement to specify the response level ordering.

Responses for the Poisson distribution must be all nonnegative, but they can be noninteger values.

The effects in the MODEL statement consist of an explanatory variable or combination of variables. Explanatory variables can be continuous or classification variables. Classification variables can be character or numeric. Explanatory variables representing nominal, or classification, data must be declared in a CLASS statement. Interactions between variables can also be included as effects. Columns of the design matrix are automatically generated for classification variables and interactions. The syntax for specification of effects is the same as for the GLM procedure. See the section “Specification of Effects” on page 2810 for more information. Also see Chapter 42, “The GLM Procedure.”

Table 40.7 summarizes the options available in the MODEL statement.

Table 40.7 MODEL Statement Options

Option	Description
AGGREGATE=	Specifies the subpopulations
ALPHA=	Sets the confidence coefficient
CICONV=	Sets the convergence criterion for profile likelihood confidence intervals
CL	Displays confidence limits for predicted values
CODING=	Uses effect coding for all classification variables
CONVERGE=	Sets the convergence criterion
CONVH=	Sets the relative Hessian convergence criterion
CORRB	Displays the parameter estimate correlation matrix
COVB	Displays the parameter estimate covariance matrix
DIAGNOSTICS	Displays case deletion diagnostic statistics
DIST=	Specifies the built-in probability distribution
EXACTMAX	Names a variable used for performing an exact Poisson regression
EXPECTED	Computes covariances and associated statistics using the expected Fisher information matrix
ID=	Displays the values of <i>variable</i> in the input data set in the OBSTATS table
INITIAL=	Sets initial values for parameter estimates
INTERCEPT=	Initializes the intercept term
ITPRINT	Displays the iteration history for all iterative processes
LINK=	Specifies the link function
LOGNB	Computes the maximum likelihood estimate and confidence limits of k based $\log(k)$
LRCI	Computes two-sided confidence intervals for the partially likelihood function
MAXITER=	Sets the maximum allowable number of iterations for all iterative computation processes
NOINT	Requests that no intercept term
NOLOGNB	Computes the maximum likelihood estimate and confidence limits of k based on k
NOSCALE	Holds the scale parameter fixed
OBSTATS	Displays an additional table of statistics
OFFSET=	Specifies a variable in the input data set to be used as an offset

Table 40.7 *continued*

Option	Description
PREDICTED	Displays predicted values and associated statistics
RESIDUALS	Displays residuals and standardized residuals
SCALE=	Sets the value used for the scale
SCORING=	Computes the Hessian matrix using the Fisher scoring method
SINGULAR=	Sets the tolerance for testing singularity
TYPE1	Performs a Type 1 analysis
TYPE3	Computes statistics for Type 3 contrasts
WALD	Requests Wald statistics for Type 3 contrasts
WALDCI	Computes two-sided Wald confidence intervals
XVARS	Includes the regression variables in the OBSTATS table

You can specify the following options in the MODEL statement after a slash (/).

AGGREGATE= *(variable-list)*

AGGREGATE= *variable*

AGGREGATE

specifies the subpopulations on which the Pearson chi-square and the deviance are calculated. This option applies only to the multinomial distribution or the binomial distribution with binary (single trial syntax) response. It is ignored if specified for other cases. Observations with common values in the given list of variables are regarded as coming from the same subpopulation. This affects the computation of the deviance and Pearson chi-square statistics. Variables in the list can be any variables in the input data set. Specifying the AGGREGATE option is equivalent to specifying the AGGREGATE= option with a variable list that includes all explanatory variables in the MODEL statement. Pearson chi-square and deviance statistics are not computed for multinomial models unless this option is specified.

ALPHA=*number*

ALPH=*number*

A=*number*

sets the confidence coefficient for parameter confidence intervals to $1 - \textit{number}$. The value of *number* must be between 0 and 1. The default value of *number* is 0.05.

CICONV=*number*

sets the convergence criterion for profile likelihood confidence intervals. See the section “[Confidence Intervals for Parameters](#)” on page 2813 for the definition of convergence. The value of *number* must be between 0 and 1. By default, CICONV=1E-4.

CL

requests that confidence limits for predicted values be displayed (see the OBSTATS option).

CODING=EFFECT

CODING=FULLRANK

specifies that effect coding be used for all classification variables in the model. This is the same as specifying PARAM=EFFECT as a CLASS statement option.

CONVERGE=number

sets the convergence criterion. The value of *number* must be between 0 and 1. The iterations are considered to have converged when the maximum change in the parameter estimates between iteration steps is less than the value specified. The change is a relative change if the parameter is greater than 0.01 in absolute value; otherwise, it is an absolute change. By default, CONVERGE=1E-4. This convergence criterion is used in parameter estimation for a single model fit, Type 1 statistics, and likelihood ratio statistics for Type 3 analyses and CONTRAST statements.

CONVH=number

sets the relative Hessian convergence criterion. The value of *number* must be between 0 and 1. After convergence is determined with the change in parameter criterion specified with the CONVERGE= option, the quantity $tc = \frac{\mathbf{g}'\mathbf{H}^{-1}\mathbf{g}}{|f|}$ is computed and compared to *number*, where \mathbf{g} is the gradient vector, \mathbf{H} is the Hessian matrix for the model parameters, and f is the log-likelihood function. If tc is greater than *number*, a warning that the relative Hessian convergence criterion has been exceeded is printed. This criterion detects the occasional case where the change in parameter convergence criterion is satisfied, but a maximum in the log-likelihood function has not been attained. By default, CONVH=1E-4.

CORRB

requests that the parameter estimate correlation matrix be displayed.

COVB

requests that the parameter estimate covariance matrix be displayed.

DIAGNOSTICS**INFLUENCE**

requests that case deletion diagnostic statistics be displayed (see the OBSTATS option).

DIST=keyword**D=keyword****ERROR=keyword****ERR=keyword**

specifies the built-in probability distribution to use in the model. If you specify the DIST= option and you omit a user-defined link function, a default link function is chosen as displayed in the following table. If you specify no distribution and no link function, then the GENMOD procedure defaults to the normal distribution with the identity link function. Models for data with correlated responses fit by the GEE method are not available for the zero-inflated distributions.

DIST=	Distribution	Default Link Function
BINOMIAL BIN B	Binomial	Logit
GAMMA GAM G	Gamma	Inverse (power(-1))
GEOMETRIC GEOM	Geometric	Log
IGAUSSIAN IG	Inverse Gaussian	Inverse squared (power(-2))
MULTINOMIAL MULT	Multinomial	Cumulative logit
NEGBIN NB	Negative binomial	Log
NORMAL NOR N	Normal	Identity
POISSON POI P	Poisson	Log
ZIP	Zero-inflated Poisson	Log/logit
ZINB	Zero-inflated negative binomial	Log/logit

EXACTMAX<=*variable*>

names a variable used for performing an exact Poisson regression. For each observation, the integer part of the EXACTMAX value should be nonnegative and at least as large as the response value. If the EXACTMAX option is specified without a variable, then default values are computed. See the section “Exact Logistic and Exact Poisson Regression” on page 2839 for information about using this option.

EXPECTED

requests that the expected Fisher information matrix be used to compute parameter estimate covariances and the associated statistics. The default action is to use the observed Fisher information matrix. This option does not affect the model fitting, only the way in which the covariance matrix is computed (see the SCORING= option.)

ID=*variable*

causes the values of *variable* in the input data set to be displayed in the OBSTATS table. If an explicit format for *variable* has been defined, the formatted values are displayed. If the OBSTATS option is not specified, this option has no effect.

INITIAL=*numbers*

sets initial values for parameter estimates in the model. The default initial parameter values are weighted least squares estimates based on using the response data as the initial mean estimate. This option can be useful in case of convergence difficulty. The intercept parameter is initialized with the INTERCEPT= option and is not included here. The values are assigned to the variables in the MODEL statement in the same order in which they appear in the MODEL statement. The order of levels for CLASS variables is determined by the ORDER= option. Note that some levels of classification variables can be aliased; that is, they correspond to linearly dependent parameters that are not estimated by the procedure. Initial values must be assigned to all levels of classification variables, regardless of whether they are aliased or not. The procedure ignores initial values corresponding to parameters not being estimated. If you specify a BY statement, all classification variables must take on the same number of levels in each BY group. Otherwise, classification variables in some of the BY groups are assigned incorrect initial values. Types of INITIAL= specifications are illustrated in the following table.

Type of List	Specification
List separated by blanks	INITIAL = 3 4 5
List separated by commas	INITIAL = 3, 4, 5
x to y	INITIAL = 3 to 5
x to y by z	INITIAL = 3 to 5 by 1
Combination of list types	INITIAL = 1, 3 to 5, 9

INTERCEPT=*number***INTERCEPT**=*number-list*

initializes the intercept term to *number* for parameter estimation. If you specify both the INTERCEPT= and the NOINT options, the intercept term is not estimated, but an intercept term of *number* is included in the model. If you specify a multinomial model for ordinal data, you can specify a *number-list* for the multiple intercepts in the model.

ITPRINT

displays the iteration history for all iterative processes: parameter estimation, fitting constrained models for contrasts and Type 3 analyses, and profile likelihood confidence intervals. The last evaluation of the gradient and the negative of the Hessian (second derivative) matrix are also displayed for parameter estimation. If you perform a Bayesian analysis by specifying the BAYES statement, the iteration history for computing the mode of the posterior distribution is also displayed.

This option might result in a large amount of displayed output, especially if some of the optional iterative processes are selected.

LINK=keyword

specifies the link function to use in the model. The keywords and their associated built-in link functions are as follows.

LINK=	Link Function
CUMCLL	
CCLL	Cumulative complementary log-log
CUMLOGIT	
CLOGIT	Cumulative logit
CUMPROBIT	
CPROBIT	Cumulative probit
CLOGLOG	
CLL	Complementary log-log
IDENTITY	
ID	Identity
LOG	Log
LOGIT	Logit
PROBIT	Probit
POWER(<i>number</i>) POW(<i>number</i>)	Power with $\lambda = \textit{number}$

If no LINK= option is supplied and there is a user-defined link function, the user-defined link function is used. If you specify neither the LINK= option nor a user-defined link function, then the default canonical link function is used if you specify the DIST= option. Otherwise, if you omit the DIST= option, the identity link function is used.

The cumulative link functions are appropriate only for the multinomial distribution.

LOGNB

specifies that the maximum likelihood estimate and confidence limits of the negative binomial dispersion parameter k be computed based $\log(k)$. This is the default method used for the negative binomial dispersion parameter, so that specifying no option or specifying the LOGNB option have the same effect. The GENMOD procedure computes the maximum likelihood estimate of $\log(k)$ and computes confidence limits based on the asymptotic normality of $\log(k)$ rather than of k . The results are always reported in terms of k rather than of $\log(k)$. This method ensures that the estimate and confidence limits for k are positive. See Meeker and Escobar (1998, p. 163) for details about this method of computing confidence limits.

LRCI

requests that two-sided confidence intervals for all model parameters be computed based on the profile likelihood function. This is sometimes called the partially maximized likelihood function. See the section “[Confidence Intervals for Parameters](#)” on page 2813 for more information about the profile likelihood function. This computation is iterative and can consume a relatively large amount of CPU time. The confidence coefficient can be selected with the `ALPHA=number` option. The resulting confidence coefficient is $1 - \text{number}$. The default confidence coefficient is 0.95.

MAXITER=number**MAXIT=number**

sets the maximum allowable number of iterations for all iterative computation processes in PROC GENMOD. By default, MAXITER=50.

NOINT

requests that no intercept term be included in the model. An intercept is included unless this option is specified.

NOLOGNB

specifies that the maximum likelihood estimate and confidence limits of the negative binomial dispersion parameter k be computed based on k rather than $\log(k)$. If this option is not specified, then the GENMOD procedure computes the maximum likelihood estimate of $\log(k)$ and computes confidence limits based on the asymptotic normality of $\log(k)$ rather than of k . The results are always reported in terms of k rather than of $\log(k)$. This method ensures that the estimate and confidence limits for k are positive. See Meeker and Escobar (1998, p. 163) for details about this method of computing confidence limits.

NOSCALE

holds the scale parameter fixed. Otherwise, for the normal, inverse Gaussian, and gamma distributions, the scale parameter is estimated by maximum likelihood. If you omit the SCALE= option, the scale parameter is fixed at the value 1.

OBSTATS

specifies that an additional table of statistics be displayed. Formulas for the statistics are given in the section “[Predicted Values of the Mean](#)” on page 2815, the section “[Residuals](#)” on page 2816, and the section “[Case Deletion Diagnostic Statistics](#)” on page 2831. Residuals and fit diagnostics are not computed for multinomial models.

For each observation, the following items are displayed:

- the value of the response variable (variables if the data are binomial), frequency, and weight variables
- the values of the regression variables
- predicted mean, $\hat{\mu} = g^{-1}(\eta)$, where $\eta = \mathbf{x}'_i \hat{\boldsymbol{\beta}}$ is the linear predictor and g is the link function. If there is an offset, it is included in $\mathbf{x}'_i \hat{\boldsymbol{\beta}}$.
- estimate of the linear predictor $\mathbf{x}'_i \hat{\boldsymbol{\beta}}$. If there is an offset, it is included in $\mathbf{x}'_i \hat{\boldsymbol{\beta}}$.
- standard error of the linear predictor $\mathbf{x}'_i \hat{\boldsymbol{\beta}}$
- the value of the Hessian weight at the final iteration

- lower confidence limit of the predicted value of the mean. The confidence coefficient is specified with the ALPHA= option. See the section “Confidence Intervals on Predicted Values” on page 2815 for the computational method.
- upper confidence limit of the predicted value of the mean
- raw residual, defined as $Y - \mu$
- Pearson, or chi residual, defined as the square root of the contribution for the observation to the Pearson chi-square—that is,

$$\frac{Y - \mu}{\sqrt{V(\mu)/w}}$$

where Y is the response, μ is the predicted mean, w is the value of the prior weight variable specified in a WEIGHT statement, and $V(\mu)$ is the variance function evaluated at μ .

- the standardized Pearson residual
- deviance residual, defined as the square root of the deviance contribution for the observation, with sign equal to the sign of the raw residual
- the standardized deviance residual
- the likelihood residual
- a Cook distance type statistic for assessing the influence of individual observations on overall model fit
- observation leverage
- DFBETA, defined as an approximation to $\hat{\beta} - \hat{\beta}_{[i]}$ for each parameter estimate $\hat{\beta}$, where $\hat{\beta}_{[i]}$ is the parameter estimate with the i th observation deleted
- standardized DFBETA, defined as DFBETA, normalized by its standard deviation
- zero inflation probability for zero-inflated models
- the mean of a zero-inflated response

The following additional cluster deletion diagnostic statistics are created and displayed for each cluster if a REPEATED statement is specified:

- a Cook distance type statistic for assessing the influence of entire clusters on overall model fit
- a studentized Cook distance for assessing influence of clusters
- cluster leverage
- cluster DFBETA for assessing the influence of entire clusters on individual parameter estimates
- cluster DFBETA normalized by its standard deviation

If you specify the multinomial distribution, only regression variable values, response values, predicted values, confidence limits for the predicted values, and the linear predictor are displayed in the table. Residuals and other diagnostic statistics are not available for the multinomial distribution.

The RESIDUALS, DIAGNOSTICS | INFLUENCE, PREDICTED, XVARS, and CL options cause only subgroups of the observation statistics to be displayed. You can specify more than one of these options to include different subgroups of statistics.

The `ID=variable` option causes the values of *variable* in the input data set to be displayed in the table. If an explicit format for *variable* has been defined, the formatted values are displayed.

If a REPEATED statement is present, a table is displayed for the GEE model specified in the REPEATED statement. Regression variables, response values, predicted values, confidence limits for the predicted values, linear predictor, raw residuals, Pearson residuals for each observation in the input data set are available. Case deletion diagnostic statistics are available for each observation and for each cluster.

OFFSET=variable

specifies a variable in the input data set to be used as an offset variable. This variable cannot be a CLASS variable, and it cannot be the response variable or one of the explanatory variables.

When you perform an exact Poisson regression with an OFFSET= variable but the EXACTMAX= option is not specified, then if o_i is the offset for the i th observation, $\text{floor}(\exp(o_i))$ should be greater than or equal to the response value. See the section “Exact Logistic and Exact Poisson Regression” on page 2839 for information about the use of the offset in the exact Poisson model.

PREDICTED

PRED

P

requests that predicted values, the linear predictor, its standard error, and the Hessian weight be displayed (see the OBSTATS option).

RESIDUALS

R

requests that residuals and standardized residuals be displayed. Residuals and other diagnostic statistics are not available for the multinomial distribution (see the OBSTATS option).

SCALE=number

SCALE=PEARSON

SCALE=P

PSCALE

SCALE=DEVIANCE

SCALE=D

DSCALE

sets the value used for the scale parameter where the NOSCALE option is used. For the binomial and Poisson distributions, which have no free scale parameter, this can be used to specify an *overdispersed* model. In this case, the parameter covariance matrix and the likelihood function are adjusted by the scale parameter. See the section “Dispersion Parameter” on page 2808 and the section “Overdispersion” on page 2809 for more information. If the NOSCALE option is not specified, then *number* is used as an initial estimate of the scale parameter.

Specifying SCALE=PEARSON or SCALE=P is the same as specifying the PSCALE option. This fixes the scale parameter at the value 1 in the estimation procedure. After the parameter estimates are determined, the exponential family dispersion parameter is assumed to be given by Pearson’s chi-square statistic divided by the degrees of freedom, and all statistics such as standard errors and likelihood ratio statistics are adjusted appropriately.

Specifying SCALE=DEVIANCE or SCALE=D is the same as specifying the DSCALE option. This fixes the scale parameter at a value of 1 in the estimation procedure.

After the parameter estimates are determined, the exponential family dispersion parameter is assumed to be given by the deviance divided by the degrees of freedom. All statistics such as standard errors and likelihood ratio statistics are adjusted appropriately.

SCORING=number

requests that on iterations up to *number*, the Hessian matrix be computed using the Fisher scoring method. For further iterations, the full Hessian matrix is computed. The default value is 1. A value of 0 causes all iterations to use the full Hessian matrix, and a value greater than or equal to the value of the MAXITER option causes all iterations to use Fisher scoring. The value of the SCORING= option must be 0 or a positive integer.

SINGULAR=number

sets the tolerance for testing singularity of the information matrix and the crossproducts matrix. Roughly, the test requires that a pivot be at least this number times the original diagonal value. By default, *number* is 10^7 times the machine epsilon. The default *number* is approximately 10^{-9} on most machines. This value also controls the check on estimability for ESTIMATE and CONTRAST statements.

TYPE1

requests that a Type 1, or sequential, analysis be performed. This consists of sequentially fitting models, beginning with the null (intercept term only) model and continuing up to the model specified in the MODEL statement. The likelihood ratio statistic between each successive pair of models is computed and displayed in a table.

A Type 1 analysis is not available for GEE models, since there is no associated likelihood.

TYPE3

requests that statistics for Type 3 contrasts be computed for each effect specified in the MODEL statement. The default analysis is to compute likelihood ratio statistics for the contrasts or score statistics for GEEs. Wald statistics are computed if the WALD option is also specified.

WALD

requests Wald statistics for Type 3 contrasts. You must also specify the TYPE3 option in order to compute Type 3 Wald statistics.

WALDCI

requests that two-sided Wald confidence intervals for all model parameters be computed based on the asymptotic normality of the parameter estimators. This computation is not as time-consuming as the LRCI method, since it does not involve an iterative procedure. However, it is thought to be less accurate, especially for small sample sizes. The confidence coefficient can be selected with the ALPHA= option in the same way as for the LRCI option.

XVARS

requests that the regression variables be included in the OBSTATS table.

OUTPUT Statement

OUTPUT < **OUT=SAS-data-set** > < *keyword=name* . . . *keyword=name* > ;

The OUTPUT statement creates a new SAS data set that contains all the variables in the input data set and, optionally, the estimated linear predictors (XBETA) and their standard error estimates, the weights for the Hessian matrix, predicted values of the mean, confidence limits for predicted values, residuals, and case deletion diagnostics. Residuals and diagnostic statistics are not computed for multinomial models.

You can also request these statistics with the OBSTATS, PREDICTED, RESIDUALS, DIAGNOSTICS | INFLUENCE, CL, or XVARS option in the MODEL statement. You can then create a SAS data set containing them with ODS OUTPUT commands.

You might prefer to specify the OUTPUT statement for requesting these statistics since the following are true:

- The OUTPUT statement produces no tabular output.
- The OUTPUT statement creates a SAS data set more efficiently than ODS. This can be an advantage for large data sets.
- You can specify the individual statistics to be included in the SAS data set.

If you use the multinomial distribution with one of the cumulative link functions for ordinal data, the data set also contains variables named `_ORDER_` and `_LEVEL_` that indicate the levels of the ordinal response variable and the values of the variable in the input data set corresponding to the sorted levels. These variables indicate that the predicted value for a given observation is the probability that the response variable is as large as the value of the `_LEVEL_` variable. Residuals and other diagnostic statistics are not available for the multinomial distribution.

The estimated linear predictor, its standard error estimate, and the predicted values and their confidence intervals are computed for all observations in which the explanatory variables are all nonmissing, even if the response is missing. By adding observations with missing response values to the input data set, you can compute these statistics for new observations or for settings of the explanatory variables not present in the data without affecting the model fit.

The following list explains specifications in the OUTPUT statement.

OUT=SAS-data-set

specifies the output data set. If you omit the OUT=option, the output data set is created and given a default name that uses the `DATA n` convention.

keyword=name

specifies the statistics to be included in the output data set and names the new variables that contain the statistics. Specify a keyword for each desired statistic (see the following list of keywords), an equal sign, and the name of the new variable or variables to contain the statistic. You can list only one variable after the equal sign for all the statistics, except for the case deletion diagnostics for individual parameter estimates, `DFBETA`, `DFBETAS`, `DFBETAC`, and `DFBETACS`. You can list variables enclosed in parentheses to correspond to the variables in the model, or you can specify the keyword `_all_`, without parentheses, to include deletion diagnostics for all of the parameters in the model.

Although you can use the OUTPUT statement without any *keyword=name* specifications, the output data set then contains only the original variables and, possibly, the variables Level and Value (if you use the multinomial model with ordinal data). Note that the residuals and deletion diagnostics are not available for the multinomial model with ordinal data. Some of the case deletion diagnostic statistics apply only to models for correlated data specified with a REPEATED statement. If you request these statistics for ordinary generalized linear models, the values of the corresponding variables are set to missing in the output data set. Formulas for the statistics are given in the section “Predicted Values of the Mean” on page 2815, the section “Residuals” on page 2816, and the section “Case Deletion Diagnostic Statistics” on page 2831.

The keywords allowed and the statistics they represent are as follows:

- DFBETA | DBETA represents the effect of deleting an observation on parameter estimates. If you specify the keyword *_all_* after the equal sign, variables named *DFBETA_ParameterName* will be included in the output data set to contain the values of the diagnostic statistic to measure the influence of deleting a single observation on the individual parameter estimates. *ParameterName* is the name of the regression model parameter formed from the input variable names concatenated with the appropriate levels, if classification variables are involved.
- DFBETAS | DBETAS represents the effect of deleting an observation on standardized parameter estimates. If you specify the keyword *_all_* after the equal sign, variables named *DFBETAS_ParameterName* will be included in the output data set to contain the values of the diagnostic statistic to measure the influence of deleting a single observation on the individual parameter estimates. *ParameterName* is the name of the regression model parameter formed from the input variable names concatenated with the appropriate levels, if classification variables are involved.
- DOBS | COOKD | COOKSD represents the Cook distance type statistic to measure the influence of deleting a single observation on the overall model fit.
- HESSWGT represents the diagonal element of the weight matrix used in computing the Hessian matrix.
- H | LEVERAGE represents the leverage of a single observation.
- LOWER | L represents the lower confidence limit for the predicted value of the mean, or the lower confidence limit for the probability that the response is less than or equal to the value of Level or Value. The confidence coefficient is determined by the *ALPHA=number* option in the MODEL statement as $(1 - \textit{number}) \times 100\%$. The default confidence coefficient is 95%.
- PREDICTED | PRED | PROB | P represents the predicted value of the mean of the response or the predicted probability that the response variable is less than or equal to the value of *_LEVEL_* if the multinomial model for ordinal data is used (in other words, $\Pr(Y \leq \textit{_LEVEL_})$, where Y is the response variable).
- PZERO represents the [zero-inflation probability](#) for zero-inflated models.
- RESCHI represents the Pearson (chi) residual for identifying observations that are poorly accounted for by the model.
- RESDEV represents the deviance residual for identifying poorly fitted observations.
- RESLIK represents the likelihood residual for identifying poorly fitted observations.

RESRAW	represents the raw residual for identifying poorly fitted observations.
STDRESCHI	represents the standardized Pearson (chi) residual for identifying observations that are poorly accounted for by the model.
STDRESDEV	represents the standardized deviance residual for identifying poorly fitted observations.
STDXBETA	represents the standard error estimate of XBETA (see the XBETA keyword).
UPPER U	represents the upper confidence limit for the predicted value of the mean, or the upper confidence limit for the probability that the response is less than or equal to the value of Level or Value. The confidence coefficient is determined by the ALPHA= <i>number</i> option in the MODEL statement as $(1 - \textit{number}) \times 100\%$. The default confidence coefficient is 95%.
XBETA	represents the estimate of the linear predictor $\mathbf{x}'_i\boldsymbol{\beta}$ for observation <i>i</i> , or $\alpha_j + \mathbf{x}'_i\boldsymbol{\beta}$, where <i>j</i> is the corresponding ordered value of the response variable for the multinomial model with ordinal data. If there is an offset, it is included in $\mathbf{x}'_i\boldsymbol{\beta}$.

The keywords in the following list apply only to models specified with a REPEATED statement, fit by generalized estimating equations (GEEs).

CH CLUSTERH CLEVERAGE	represents the leverage of a cluster.
CLUSTER	represents the numerical cluster index, in order of sorted clusters.
DCLS CLUSTERCOOKD CLUSTERCOOKSD	represents the Cook distance type statistic to measure the influence of deleting an entire cluster on the overall model fit.
DFBETAC DBETAC	represents the effect of deleting an entire cluster on parameter estimates. If you specify the keyword <i>_all_</i> after the equal sign, variables named DFBETAC_ <i>ParameterName</i> will be included in the output data set to contain the values of the diagnostic statistic to measure the influence of deleting the cluster on the individual parameter estimates. <i>ParameterName</i> is the name of the regression model parameter formed from the input variable names concatenated with the appropriate levels, if classification variables are involved.
DFBETACS DBETACS	represents the effect of deleting an entire cluster on normalized parameter estimates. If you specify the keyword <i>_all_</i> after the equal sign, variables named DFBETACS_ <i>ParameterName</i> will be included in the output data set to contain the values of the diagnostic statistic to measure the influence of deleting the cluster on the individual parameter estimates, normalized by their standard errors. <i>ParameterName</i> is the name of the regression model parameter formed from the input variable names concatenated with the appropriate levels, if classification variables are involved.
MCLS CLUSTERDFIT	represents the studentized Cook distance type statistic to measure the influence of deleting an entire cluster on the overall model fit.

Programming Statements

Although the most commonly used link and probability distributions are available as built-in functions, the GENMOD procedure enables you to define your own link functions and response probability distributions by using the FWDLINK, INVLINK, VARIANCE, and DEVIANCE statements. The variables assigned in these statements can have values computed in programming statements.

These programming statements can occur anywhere between the PROC GENMOD statement and the RUN statement. Variable names used in programming statements must be unique. Variables from the input data set can be referenced in programming statements. The mean, linear predictor, and response are represented by the automatic variables `_MEAN_`, `_XBETA_`, and `_RESP_`, respectively, which can be referenced in your programming statements. Programming statements are used to define the functional dependencies of the link function, the inverse link function, the variance function, and the deviance function on the mean, linear predictor, and response variable.

The following statements illustrate the use of programming statements. Even though you usually request the Poisson distribution by specifying `DIST=POISSON` as a MODEL statement option, you can define the variance and deviance functions for the Poisson distribution by using the VARIANCE and DEVIANCE statements. For example, the following statements perform the same analysis as the Poisson regression example in the section “Getting Started: GENMOD Procedure” on page 2720.

The statements must be in logical order for computation, just as in a DATA step.

```
proc genmod;
  class car age;
  a = _MEAN_;
  y = _RESP_;
  d = 2 * ( y * log( y / a ) - ( y - a ) );
  variance var = a;
  deviance dev = d;
  model c = car age / link = log offset = ln;
run;
```

The variables `var` and `dev` are dummy variables used internally by the procedure to identify the variance and deviance functions. Any valid SAS variable names can be used.

Similarly, the log link function and its inverse could be defined with the FWDLINK and INVLINK statements, as follows:

```
fwmlink link = log(_MEAN_);
invlink ilink = exp(_XBETA_);
```

These statements are for illustration, and they work well for most Poisson regression problems. If, however, in the iterative fitting process, the mean parameter becomes too close to 0, or a 0 response value occurs, an error condition occurs when the procedure attempts to evaluate the log function. You can circumvent this kind of problem by using IF-THEN/ELSE clauses or other conditional statements to check for possible error conditions and appropriately define the functions for these cases.

Data set variables can be referenced in user definitions of the link function and response distributions by using programming statements and the FWDLINK, INVLINK, DEVIANCE, and VARIANCE statements.

See the DEVIANCE, VARIANCE, FWDLINK, and INVLINK statements for more information.

The syntax of programming statements used in PROC GENMOD is identical to that used in the NLMIXED procedure and the GLIMMIX procedure (see Chapter 64, “The NLMIXED Procedure,” and Chapter 41, “The GLIMMIX Procedure,”) and the MODEL procedure (see the *SAS/ETS User’s Guide*). Most of the programming statements that can be used in the DATA step can also be used in the GENMOD procedure. See *SAS Statements: Reference* for a description of SAS programming statements. The following are some commonly used programming statements.

```

ABORT;
ARRAY arrayname < [ dimensions ] > < $ > < variables-and-constants >;
CALL name < (expression < , expression ... >) >;
DELETE;
DO < variable = expression < TO expression > < BY expression > >
    < , expression < TO expression > < BY expression > > ...
    < WHILE expression > < UNTIL expression >;
END;
GOTO statement-label;
IF expression;
IF expression THEN program-statement;
    ELSE program-statement;
variable = expression;
variable + expression;
LINK statement-label;
PUT < variable > < = > ...;
RETURN;
SELECT < (expression) >;
STOP;
SUBSTR(variable, index, length)= expression;
WHEN (expression)program-statement;
    OTHERWISE program-statement;

```

REPEATED Statement

REPEATED SUBJECT=subject-effect < / options > ;

The REPEATED statement specifies the covariance structure of multivariate responses for GEE model fitting in the GENMOD procedure. In addition, the REPEATED statement controls the iterative fitting algorithm used in GEEs and specifies optional output. Other GENMOD procedure statements, such as the MODEL and CLASS statements, are used in the same way as they are for ordinary generalized linear models to specify the regression model for the mean of the responses.

Table 40.8 summarizes the options available in the REPEATED statement.

Table 40.8 REPEATED Statement Options

Option	Description
ALPHAINIT=	Specifies initial values for log odds ratio regression parameters
CONVERGE=	Specifies the convergence criterion for GEE parameter estimation
CORRB	Displays the estimated correlation matrix
CORRW	Displays the estimated working correlation matrix

Table 40.8 *continued*

Option	Description
COVB	Displays the estimated covariance matrix
ECORRB	Displays the estimated empirical correlation matrix
ECOV	Displays the estimated empirical covariance matrix
INITIAL=	Specifies initial values of the regression parameters estimation
INTERCEPT=	Specifies either an initial or a fixed value of the intercept
LOGOR=	Specifies the regression structure of the log odds ratio
MAXITER=	Specifies the maximum number of iterations
MCORRB	Displays the estimated model-based correlation matrix
MCOVB	Displays the estimated model-based covariance matrix
MODELSE	Displays an analysis of parameter estimates table
PRINTMLE	Displays an analysis of maximum likelihood parameter estimates table
RUPDATE=	Specifies the number of iterations between updates of the working correlation matrix
SORTED	Groups by subject and sorts within subject
SUBCLUSTER=	Specifies a variable defining subclusters
SUBJECT=	Identifies a different subject, or cluster
TYPE=	Specifies the working correlation matrix structure
V6CORR	Uses the SAS 'Version 6' method of computing normalized Pearson chi-square
WITHIN=	Specifies the order of measurements within subjects
YPAIR=	Specifies the pairs of responses
ZDATA=	Specifies the full z matrix
ZROW=	Specifies the rows of the z matrix

SUBJECT=*subject-effect*

identifies subjects in the input data set. The *subject-effect* can be a single variable, an interaction effect, a nested effect, or a combination. Each distinct value, or level, of the effect identifies a different subject, or cluster. Responses from different subjects are assumed to be statistically independent, and responses within subjects are assumed to be correlated. A *subject-effect* must be specified, and variables used in defining the *subject-effect* must be listed in the CLASS statement. The input data set does not need to be sorted by subject (see the SORTED option).

The *options* control how the model is fit and what output is produced. You can specify the following options after a slash (/).

ALPHAINIT=*numbers*

specifies initial values for log odds ratio regression parameters if the LOGOR= option is specified for binary data. If this option is not specified, an initial value of 0.01 is used for all the parameters.

CONVERGE=*number*

specifies the convergence criterion for GEE parameter estimation. If the maximum absolute difference between regression parameter estimates is less than the value of *number* on two successive iterations, convergence is declared. If the absolute value of a regression parameter estimate is greater than 0.08, then the absolute difference normalized by the regression parameter value is used instead of the absolute difference. The default value of *number* is 0.0001.

CORRW

displays the estimated working correlation matrix. If you specify an exchangeable working correlation structure with the `CORR=EXCH` option, the `CORRW` option is not needed to view the estimated correlation, since a table is printed by default that contains the single estimated correlation.

CORRB

displays the estimated regression parameter correlation matrix. Both model-based and empirical correlations are displayed.

COVB

displays the estimated regression parameter covariance matrix. Both model-based and empirical covariances are displayed.

ECORRB

displays the estimated regression parameter empirical correlation matrix.

ECOV

displays the estimated regression parameter empirical covariance matrix.

INTERCEPT=number

specifies either an initial or a fixed value of the intercept regression parameter in the GEE model. If you specify the `NOINT` option in the `MODEL` statement, then the intercept is fixed at the value of *number*.

INITIAL=numbers

specifies initial values of the regression parameters estimation, other than the intercept parameter, for GEE estimation. If this option is not specified, the estimated regression parameters assuming independence for all responses are used for the initial values.

LOGOR=log-odds-ratio-structure-keyword

specifies the regression structure of the log odds ratio used to model the association of the responses from subjects for binary data. The response syntax must be of the single variable type, the distribution must be binomial, and the data must be binary. [Table 40.9](#) displays the log odds ratio structure keywords and the corresponding log odds ratio regression structures. See the section “[Alternating Logistic Regressions](#)” on page 2823 for definitions of the log odds ratio types and examples of specifying log odds ratio models. You should specify either the `LOGOR=` or the `TYPE=` option, but not both.

Table 40.9 Log Odds Ratio Regression Structures

Keyword	Log Odds Ratio Regression Structure
EXCH	Exchangeable
FULLCLUST	Fully parameterized clusters
LOGORVAR(<i>variable</i>)	Indicator variable for specifying block effects
NESTK	<i>k</i> -nested
NEST1	1-nested
ZFULL	Fully specified <i>z</i> matrix specified in <code>ZDATA=</code> data set
ZREP	Single cluster specification for replicated <i>z</i> matrix specified in <code>ZDATA=</code> data set
ZREP(matrix)	Single cluster specification for replicated <i>z</i> matrix

MAXITER=number**MAXIT=number**

specifies the maximum number of iterations allowed in the iterative GEE estimation process. The default number is 50.

MCORRB

displays the estimated regression parameter model-based correlation matrix.

MCOVB

displays the estimated regression parameter model-based covariance matrix.

MODELSE

displays an analysis of parameter estimates table that uses model-based standard errors for inference. By default, an “Analysis of Parameter Estimates” table based on empirical standard errors is displayed.

PRINTMLE

displays an analysis of maximum likelihood parameter estimates table. The maximum likelihood estimates are not displayed unless this option is specified.

RUPDATE=number

specifies the number of iterations between updates of the working correlation matrix. For example, RUPDATE=5 specifies that the working correlation is updated once for every five regression parameter updates. The default value of *number* is 1; that is, the working correlation is updated every time the regression parameters are updated.

SORTED

specifies that the input data are grouped by subject and sorted within subject. If this option is not specified, then the procedure internally sorts by *subject-effect* and *within subject-effect*, if a *within subject-effect* is specified.

SUBCLUSTER=variable**SUBCLUST=variable**

specifies a variable defining subclusters for the 1-nested or *k*-nested log odds ratio association modeling structures. This variable must be listed in the CLASS statement.

TYPE=correlation-structure keyword**CORR=correlation-structure keyword**

specifies the structure of the working correlation matrix used to model the correlation of the responses from subjects. Table 40.10 displays the correlation structure keywords and the corresponding correlation structures. The default working correlation type is the independent (CORR=IND). See the section “[Details: GENMOD Procedure](#)” on page 2799 for definitions of the correlation matrix types. You should specify LOGOR= or TYPE= but not both.

Table 40.10 Correlation Structure Types

Keyword	Correlation Matrix Type
AR	
AR(1)	Autoregressive(1)
EXCH	
CS	Exchangeable
IND	Independent
MDEP(number)	<i>m</i> -dependent with <i>m</i> =number
UNSTR	
UN	Unstructured
USER	
FIXED (matrix)	Fixed, user-specified correlation matrix

For example, you can specify a fixed 4×4 correlation matrix with the following option:

```
type=user( 1.0  0.9  0.8  0.6
           0.9  1.0  0.9  0.8
           0.8  0.9  1.0  0.9
           0.6  0.8  0.9  1.0 )
```

V6CORR

specifies that the SAS ‘Version 6’ method of computing the normalized Pearson chi-square be used for working correlation estimation and for model-based covariance matrix scale factor.

WITHINSUBJECT | WITHIN=*within subject-effect*

defines an effect specifying the order of measurements within subjects. Each distinct level of the *within subject-effect* defines a different response from the same subject. If the data are in proper order within each subject, you do not need to specify this option.

If some measurements do not appear in the data for some subjects, this option properly orders the existing measurements and treats the omitted measurements as missing values. If the WITHINSUBJECT= option is not used in this situation, measurements might be improperly ordered and missing values assumed for the last measurements in a cluster.

Variables used in defining the *within subject-effect* must be listed in the CLASS statement.

YPAIR=*variable-list*

specifies the variables in the ZDATA= data set corresponding to pairs of responses for log odds ratio association modeling.

ZDATA=*SAS-data-set*

specifies a SAS data set containing either the full *z* matrix for log odds ratio association modeling or the *z* matrix for a single complete cluster to be replicated for all clusters.

ZROW=*variable-list*

specifies the variables in the ZDATA= data set corresponding to rows of the z matrix for log odds ratio association modeling.

SLICE Statement

SLICE *model-effect* </ *options* > ;

The SLICE statement provides a general mechanism for performing a partitioned analysis of the LS-means for an interaction. This analysis is also known as an analysis of simple effects.

The SLICE statement uses the same options as the LSMEANS statement, which are summarized in Table 19.21. For details about the syntax of the SLICE statement, see the section “SLICE Statement” on page 498 in Chapter 19, “Shared Concepts and Topics.”

STORE Statement

STORE < **OUT=** > *item-store-name* </ **LABEL=** 'label' > ;

The STORE statement requests that the procedure save the context and results of the statistical analysis. The resulting item store has a binary file format that cannot be modified. The contents of the item store can be processed with the PLM procedure.

For details about the syntax of the STORE statement, see the section “STORE Statement” on page 501 in Chapter 19, “Shared Concepts and Topics.”

STRATA Statement

STRATA *variable* < (*option*) > . . . < *variable* < (*option*) > > </ *options* > ;

The STRATA statement names the *variables* that define *strata* or *matched sets* to use in *stratified exact* logistic regression of binary response data, or a *stratified exact* Poisson regression of count data. An **EXACT** statement must also be specified.

Observations that have the same *variable* values are in the same matched set. For a stratified logistic model, you can analyze 1: 1, 1: n , m : n , and general m_i : n_i matched sets where the number of cases and controls varies across strata. For a stratified Poisson model, you can have any number of observations in each stratum. At least one variable must be specified to invoke the stratified analysis, and the usual unconditional asymptotic analysis is not performed. The stratified logistic model has the form

$$\text{logit}(\pi_{hi}) = \alpha_h + \mathbf{x}'_{hi} \boldsymbol{\beta}$$

where π_{hi} is the event probability for the i th observation in stratum h with covariates \mathbf{x}_{hi} and where the stratum-specific intercepts α_h are the nuisance parameters that are to be conditioned out.

STRATA variables can also be specified in the **MODEL** statement as classification or continuous covariates; however, the effects are nondegenerate only when crossed with a nonstratification variable. Specifying

several STRATA statements is the same as specifying one STRATA statement that contains all the strata variables. The STRATA variables can be either character or numeric, and the formatted values of the STRATA variables determine the levels. Thus, you can also use formats to group values into levels; see the discussion of the FORMAT procedure in the *Base SAS Procedures Guide*.

The “Strata Summary” table is displayed by default. For an exact logistic regression, it displays the number of strata that have a specific number of events and non-events. For example, if you are analyzing a 1: 5 matched study, this table enables you to verify that every stratum in the analysis has exactly one event and five non-events. Strata that contain only events or only non-events are reported in this table, but such strata are uninformative and are not used in the analysis. For an exact Poisson regression, the “Strata Summary” table displays the number of strata that contain a specific number of observations, which enables you to check whether every stratum in the analysis has the same number of observations.

The ASSESSMENT, BAYES, CONTRAST, EFFECTPLOT, ESTIMATE, LSMEANS, LSMESTIMATE, OUTPUT, REPEATED, SLICE, and STORE statements are not available with a STRATA statement. Exact analyses are not performed when you specify a WEIGHT statement, or a model other than LINK=LOGIT with DIST=BIN or LINK=LOG with DIST=POISSON. An OFFSET= variable is not available with exact logistic regression.

The following *option* can be specified for a stratification variable by enclosing the option in parentheses after the variable name, or it can be specified globally for all STRATA variables after a slash (/).

MISSING

treats missing values (‘.’, ‘._’, ‘.A’, . . . , ‘.Z’ for numeric variables and blanks for character variables) as valid STRATA variable values.

The following strata *options* are also available after the slash:

CHECKDEPENDENCY | CHECK=*keyword*

specifies which variables are to be tested for dependency before the analysis is performed. The available *keywords* are as follows:

NONE performs no dependence checking. Typically, a message about a singular information matrix is displayed if you have dependent variables. Dependent variables can be identified after the analysis by noting any missing parameter estimates.

COVARIATES checks dependence between covariates and an added intercept. Dependent covariates are removed from the analysis. However, covariates that are linear functions of the strata variable might not be removed, which results in a singular information matrix message being displayed in the SAS log. This is the default.

ALL checks dependence between all the strata and covariates. This option can adversely affect performance if you have a large number of strata.

NOSUMMARY

suppresses the display of the “Strata Summary” table.

INFO

displays the “Strata Information” table, which includes the stratum number, levels of the STRATA variables that define the stratum, and the total frequency for each stratum. Since the number of strata can be very large, this table is displayed only by request.

VARIANCE Statement

VARIANCE *variable* = *expression* ;

You can specify a probability distribution other than the built-in distributions by using the VARIANCE and DEVIANCE statements. The variable name *variable* identifies the variance function to the procedure. The *expression* is used to define the functional dependence on the mean, and it can be any arithmetic expression supported by the DATA step language. You use the automatic variable `_MEAN_` to represent the mean in the expression.

Alternatively, you can define the variance function with programming statements, as detailed in the section “Programming Statements” on page 2790. This form is convenient for using complex statements such as IF-THEN/ELSE clauses. Derivatives of the variance function for use during optimization are computed automatically. The DEVIANCE statement must also appear when the VARIANCE statement is used to define the variance function.

WEIGHT Statement

WEIGHT | **SCWGT** *variable* ;

The WEIGHT statement identifies a *variable* in the input data set to be used as the exponential family dispersion parameter weight for each observation. The exponential family dispersion parameter is divided by the WEIGHT variable value for each observation. This is true regardless of whether the parameter is estimated by the procedure or specified in the MODEL statement with the SCALE= option. It is also true for distributions such as the Poisson and binomial that are not usually defined to have a dispersion parameter. For these distributions, a WEIGHT variable weights the overdispersion parameter, which has the default value of 1.

The WEIGHT variable does not have to be an integer; if it is less than or equal to 0 or if it is missing, the corresponding observation is not used.

ZEROMODEL Statement

ZEROMODEL *effects* </ *options*> ;

The ZEROMODEL statement enables you to perform zero-inflated Poisson regression or zero-inflated negative binomial regression when those respective distributions are specified by the DIST= option in the MODEL statement. The effects in the ZEROMODEL statement consist of explanatory variables or combinations of variables for the zero-inflation probability regression model in a zero-inflated model. The same effects can be used in both the ZEROMODEL statement and the MODEL statement, or effects can be used in one statement or the other separately. Explanatory variables can be continuous or classification variables. Classification variables can be character or numeric. Explanatory variables representing nominal, or classification, data must be declared in a CLASS statement. Interactions between variables can also be included as effects. Columns of the design matrix are automatically generated for classification variables and interactions. The syntax for specification of effects is the same as for the GLM procedure. See the section “Specification of Effects” on page 2810 for more information. Also see Chapter 42, “The GLM Procedure.”

You can specify the following option in the ZEROMODEL statement after a slash (/).

LINK=keyword

specifies the link function to use in the model. The keywords and their associated link functions are as follows.

LINK=	Link Function
CLOGLOG	
CLL	Complementary log-log
LOGIT	Logit
PROBIT	Probit

If no LINK= option is supplied, the LOGIT link is used. User-defined link functions are not allowed.

Details: GENMOD Procedure

Generalized Linear Models Theory

This is a brief introduction to the theory of generalized linear models.

Response Probability Distributions

In generalized linear models, the response is assumed to possess a probability distribution of the exponential form. That is, the probability density of the response Y for continuous response variables, or the probability function for discrete responses, can be expressed as

$$f(y) = \exp \left\{ \frac{y\theta - b(\theta)}{a(\phi)} + c(y, \phi) \right\}$$

for some functions a , b , and c that determine the specific distribution. For fixed ϕ , this is a one-parameter exponential family of distributions. The functions a and c are such that $a(\phi) = \phi/w$ and $c = c(y, \phi/w)$, where w is a known weight for each observation. A variable representing w in the input data set can be specified in the WEIGHT statement. If no WEIGHT statement is specified, $w_i = 1$ for all observations.

Standard theory for this type of distribution gives expressions for the mean and variance of Y :

$$\begin{aligned} E(Y) &= b'(\theta) \\ \text{Var}(Y) &= \frac{b''(\theta)\phi}{w} \end{aligned}$$

where the primes denote derivatives with respect to θ . If μ represents the mean of Y , then the variance expressed as a function of the mean is

$$\text{Var}(Y) = \frac{V(\mu)\phi}{w}$$

where V is the *variance function*.

Probability distributions of the response Y in generalized linear models are usually parameterized in terms of the mean μ and dispersion parameter ϕ instead of the *natural parameter* θ . The probability distributions that are available in the GENMOD procedure are shown in the following list. The zero-inflated Poisson and zero-inflated negative binomial distributions are not generalized linear models. However, the zero-inflated distributions are included in PROC GENMOD since they are useful extensions of generalized linear models. See Long (1997) for a discussion of the zero-inflated Poisson and zero-inflated negative binomial distributions. The PROC GENMOD scale parameter and the variance of Y are also shown.

- Normal:

$$\begin{aligned} f(y) &= \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{1}{2}\left(\frac{y-\mu}{\sigma}\right)^2\right] \quad \text{for } -\infty < y < \infty \\ \phi &= \sigma^2 \\ \text{scale} &= \sigma \\ \text{Var}(Y) &= \sigma^2 \end{aligned}$$

- Inverse Gaussian:

$$\begin{aligned} f(y) &= \frac{1}{\sqrt{2\pi y^3}\sigma} \exp\left[-\frac{1}{2y}\left(\frac{y-\mu}{\mu\sigma}\right)^2\right] \quad \text{for } 0 < y < \infty \\ \phi &= \sigma^2 \\ \text{scale} &= \sigma \\ \text{Var}(Y) &= \sigma^2\mu^3 \end{aligned}$$

- Gamma:

$$\begin{aligned} f(y) &= \frac{1}{\Gamma(v)y} \left(\frac{yv}{\mu}\right)^v \exp\left(-\frac{yv}{\mu}\right) \quad \text{for } 0 < y < \infty \\ \phi &= v^{-1} \\ \text{scale} &= v \\ \text{Var}(Y) &= \frac{\mu^2}{v} \end{aligned}$$

- Geometric: This is a special case of the negative binomial with $k = 1$.

$$\begin{aligned} f(y) &= \frac{(\mu)^y}{(1+\mu)^{y+1}} \quad \text{for } y = 0, 1, 2, \dots \\ \phi &= 1 \\ \text{Var}(Y) &= \mu(1+\mu) \end{aligned}$$

- Negative binomial:

$$\begin{aligned}
 f(y) &= \frac{\Gamma(y + 1/k)}{\Gamma(y + 1)\Gamma(1/k)} \frac{(k\mu)^y}{(1 + k\mu)^{y+1/k}} \text{ for } y = 0, 1, 2, \dots \\
 \phi &= 1 \\
 \text{dispersion} &= k \\
 \text{Var}(Y) &= \mu + k\mu^2
 \end{aligned}$$

- Poisson:

$$\begin{aligned}
 f(y) &= \frac{\mu^y e^{-\mu}}{y!} \text{ for } y = 0, 1, 2, \dots \\
 \phi &= 1 \\
 \text{Var}(Y) &= \mu
 \end{aligned}$$

- Binomial:

$$\begin{aligned}
 f(y) &= \binom{n}{r} \mu^r (1 - \mu)^{n-r} \text{ for } y = \frac{r}{n}, r = 0, 1, 2, \dots, n \\
 \phi &= 1 \\
 \text{Var}(Y) &= \frac{\mu(1 - \mu)}{n}
 \end{aligned}$$

- Multinomial:

$$\begin{aligned}
 f(y_1, y_2, \dots, y_k) &= \frac{m!}{y_1! y_2! \dots y_k!} p_1^{y_1} p_2^{y_2} \dots p_k^{y_k} \\
 \phi &= 1
 \end{aligned}$$

- Zero-inflated Poisson:

$$\begin{aligned}
 f(y) &= \begin{cases} \omega + (1 - \omega)e^{-\lambda} & \text{for } y = 0 \\ (1 - \omega) \frac{\lambda^y e^{-\lambda}}{y!} & \text{for } y = 1, 2, \dots \end{cases} \\
 \phi &= 1 \\
 \mu = E(Y) &= (1 - \omega)\lambda \\
 \text{Var}(Y) &= (1 - \omega)\lambda(1 + \omega\lambda) \\
 &= \mu + \frac{\omega}{1 - \omega} \mu^2
 \end{aligned}$$

- Zero-inflated negative binomial:

$$\begin{aligned}
 f(y) &= \begin{cases} \omega + (1 - \omega)(1 + k\lambda)^{-\frac{1}{k}} & \text{for } y = 0 \\ (1 - \omega) \frac{\Gamma(y+1/k)}{\Gamma(y+1)\Gamma(1/k)} \frac{(k\lambda)^y}{(1+k\lambda)^{y+1/k}} & \text{for } y = 1, 2, \dots \end{cases} \\
 \phi &= 1 \\
 \text{dispersion} &= k \\
 \mu = E(Y) &= (1 - \omega)\lambda \\
 \text{Var}(Y) &= (1 - \omega)\lambda(1 + \omega\lambda + k\lambda) \\
 &= \mu + \left(\frac{\omega}{1 - \omega} + \frac{k}{1 - \omega} \right) \mu^2
 \end{aligned}$$

The negative binomial and the zero-inflated negative binomial distributions contain a parameter k , called the negative binomial dispersion parameter. This is not the same as the generalized linear model dispersion ϕ , but it is an additional distribution parameter that must be estimated or set to a fixed value.

For the binomial distribution, the response is the binomial proportion $Y = \text{events}/\text{trials}$. The variance function is $V(\mu) = \mu(1 - \mu)$, and the binomial trials parameter n is regarded as a weight w .

If a weight variable is present, ϕ is replaced with ϕ/w , where w is the weight variable.

PROC GENMOD works with a scale parameter that is related to the exponential family dispersion parameter ϕ instead of working with ϕ itself. The scale parameters are related to the dispersion parameter as shown previously with the probability distribution definitions. Thus, the scale parameter output in the “Analysis of Parameter Estimates” table is related to the exponential family dispersion parameter. If you specify a constant scale parameter with the SCALE= option in the MODEL statement, it is also related to the exponential family dispersion parameter in the same way.

Link Function

For distributions other than the zero-inflated Poisson or zero-inflated negative binomial, the mean μ_i of the response in the i th observation is related to a linear predictor through a monotonic differentiable link function g .

$$g(\mu_i) = \mathbf{x}_i' \boldsymbol{\beta}$$

Here, \mathbf{x}_i is a fixed known vector of explanatory variables, and $\boldsymbol{\beta}$ is a vector of unknown parameters.

There are two link functions and linear predictors associated with zero-inflated distributions: one for the zero inflation probability ω , and another for the mean parameter λ . See the section “Zero-Inflated Models” on page 2818 for more details about zero-inflated distributions.

Log-Likelihood Functions

Log-likelihood functions for the distributions that are available in the procedure are parameterized in terms of the means μ_i and the dispersion parameter ϕ . Zero-inflated log likelihoods are parameterized in terms two parameters, λ and ω . The parameter ω is the zero-inflation probability, and λ is a function of the distribution mean. The relationship between the mean of the zero-inflated Poisson and zero-inflated negative binomial distributions and the parameter λ is defined in the section “Response Probability Distributions”

on page 2799. The term y_i represents the response for the i th observation, and w_i represents the known dispersion weight. The log-likelihood functions are of the form

$$L(\mathbf{y}, \boldsymbol{\mu}, \phi) = \sum_i \log(f(y_i, \mu_i, \phi))$$

where the sum is over the observations. The forms of the individual contributions

$$l_i = \log(f(y_i, \mu_i, \phi))$$

are shown in the following list; the parameterizations are expressed in terms of the mean and dispersion parameters.

For the discrete distributions (binomial, multinomial, negative binomial, and Poisson), the functions computed as the sum of the l_i terms are not proper log-likelihood functions, since terms involving binomial coefficients or factorials of the observed counts are dropped from the computation of the log likelihood, and a dispersion parameter ϕ is included in the computation. Deletion of factorial terms and inclusion of a dispersion parameter do not affect parameter estimates or their estimated covariances for these distributions, and this is the function used in maximum likelihood estimation. The value of ϕ used in computing the reported log-likelihood function is either the final estimated value, or the fixed value, if the dispersion parameter is fixed. Even though it is not a proper log-likelihood function in all cases, the function computed as the sum of the l_i terms is reported in the output as the *log likelihood*. The proper log-likelihood function is also computed as the sum of the ll_i terms in the following list, and it is reported as the *full log likelihood* in the output.

- Normal:

$$ll_i = l_i = -\frac{1}{2} \left[\frac{w_i (y_i - \mu_i)^2}{\phi} + \log\left(\frac{\phi}{w_i}\right) + \log(2\pi) \right]$$

- Inverse Gaussian:

$$ll_i = l_i = -\frac{1}{2} \left[\frac{w_i (y_i - \mu_i)^2}{y_i \mu_i^2 \phi} + \log\left(\frac{\phi y_i^3}{w_i}\right) + \log(2\pi) \right]$$

- Gamma:

$$ll_i = l_i = \frac{w_i}{\phi} \log\left(\frac{w_i y_i}{\phi \mu_i}\right) - \frac{w_i y_i}{\phi \mu_i} - \log(y_i) - \log\left(\Gamma\left(\frac{w_i}{\phi}\right)\right)$$

- Negative binomial:

$$l_i = y_i \log\left(\frac{k\mu}{w_i}\right) - (y_i + w_i/k) \log\left(1 + \frac{k\mu}{w_i}\right) + \log\left(\frac{\Gamma(y_i + w_i/k)}{\Gamma(w_i/k)}\right)$$

$$ll_i = y_i \log\left(\frac{k\mu}{w_i}\right) - (y_i + w_i/k) \log\left(1 + \frac{k\mu}{w_i}\right) + \log\left(\frac{\Gamma(y_i + w_i/k)}{\Gamma(y_i + 1)\Gamma(w_i/k)}\right)$$

- Poisson:

$$l_i = \frac{w_i}{\phi} [y_i \log(\mu_i) - \mu_i]$$

$$ll_i = w_i [y_i \log(\mu_i) - \mu_i - \log(y_i!)]$$

- Binomial:

$$l_i = \frac{w_i}{\phi} [r_i \log(p_i) + (n_i - r_i) \log(1 - p_i)]$$

$$ll_i = w_i \left[\log \binom{n_i}{r_i} + r_i \log(p_i) + (n_i - r_i) \log(1 - p_i) \right]$$

- Multinomial (k categories):

$$l_i = \frac{w_i}{\phi} \sum_{j=1}^k y_{ij} \log(\mu_{ij})$$

$$ll_i = w_i \left[\log(m_i!) + \sum_{j=1}^k (y_{ij} \log(\mu_{ij}) - \log(y_{ij}!)) \right]$$

- Zero-inflated Poisson:

$$l_i = ll_i = \begin{cases} w_i \log[\omega_i + (1 - \omega_i) \exp(-\lambda_i)] & y_i = 0 \\ w_i [\log(1 - \omega_i) + y_i \log(\lambda_i) - \lambda_i - \log(y_i!)] & y_i > 0 \end{cases}$$

- Zero-inflated negative binomial:

$$l_i = ll_i = \begin{cases} \log[\omega_i + (1 - \omega_i) (1 + \frac{k}{w_i} \lambda)^{-\frac{1}{k}}] & y_i = 0 \\ \log(1 - \omega_i) + y_i \log\left(\frac{k\lambda}{w_i}\right) \\ - (y_i + \frac{w_i}{k}) \log\left(1 + \frac{k\lambda}{w_i}\right) \\ + \log\left(\frac{\Gamma(y_i + \frac{w_i}{k})}{\Gamma(y_i + 1) \Gamma(\frac{w_i}{k})}\right) & y_i > 0 \end{cases}$$

Maximum Likelihood Fitting

The GENMOD procedure uses a ridge-stabilized Newton-Raphson algorithm to maximize the log-likelihood function $L(\mathbf{y}, \boldsymbol{\mu}, \phi)$ with respect to the regression parameters. By default, the procedure also produces maximum likelihood estimates of the scale parameter as defined in the section “Response Probability Distributions” on page 2799 for the normal, inverse Gaussian, negative binomial, and gamma distributions.

On the r th iteration, the algorithm updates the parameter vector $\boldsymbol{\beta}_r$ with

$$\boldsymbol{\beta}_{r+1} = \boldsymbol{\beta}_r - \mathbf{H}^{-1}\mathbf{s}$$

where \mathbf{H} is the Hessian (second derivative) matrix, and \mathbf{s} is the gradient (first derivative) vector of the log-likelihood function, both evaluated at the current value of the parameter vector. That is,

$$\mathbf{s} = [s_j] = \left[\frac{\partial L}{\partial \beta_j} \right]$$

and

$$\mathbf{H} = [h_{ij}] = \left[\frac{\partial^2 L}{\partial \beta_i \partial \beta_j} \right]$$

In some cases, the scale parameter is estimated by maximum likelihood. In these cases, elements corresponding to the scale parameter are computed and included in \mathbf{s} and \mathbf{H} .

If $\eta_i = \mathbf{x}'_i \boldsymbol{\beta}$ is the linear predictor for observation i and g is the link function, then $\eta_i = g(\mu_i)$, so that $\mu_i = g^{-1}(\mathbf{x}'_i \boldsymbol{\beta})$ is an estimate of the mean of the i th observation, obtained from an estimate of the parameter vector $\boldsymbol{\beta}$.

The gradient vector and Hessian matrix for the regression parameters are given by

$$\begin{aligned} \mathbf{s} &= \sum_i \frac{w_i(y_i - \mu_i)\mathbf{x}_i}{V(\mu_i)g'(\mu_i)\phi} \\ \mathbf{H} &= -\mathbf{X}'\mathbf{W}_o\mathbf{X} \end{aligned}$$

where \mathbf{X} is the design matrix, \mathbf{x}_i is the transpose of the i th row of \mathbf{X} , and V is the variance function. The matrix \mathbf{W}_o is diagonal with its i th diagonal element

$$w_{oi} = w_{ei} + w_i(y_i - \mu_i) \frac{V(\mu_i)g''(\mu_i) + V'(\mu_i)g'(\mu_i)}{(V(\mu_i))^2(g'(\mu_i))^3\phi}$$

where

$$w_{ei} = \frac{w_i}{\phi V(\mu_i)(g'(\mu_i))^2}$$

The primes denote derivatives of g and V with respect to μ . The negative of \mathbf{H} is called the observed information matrix. The expected value of \mathbf{W}_o is a diagonal matrix \mathbf{W}_e with diagonal values w_{ei} . If you replace \mathbf{W}_o with \mathbf{W}_e , then the negative of \mathbf{H} is called the expected information matrix. \mathbf{W}_e is the weight matrix for the Fisher scoring method of fitting. Either \mathbf{W}_o or \mathbf{W}_e can be used in the update equation. The GENMOD procedure uses Fisher scoring for iterations up to the number specified by the SCORING option in the MODEL statement, and it uses the observed information matrix on additional iterations.

Covariance and Correlation Matrix

The estimated covariance matrix of the parameter estimator is given by

$$\Sigma = -\mathbf{H}^{-1}$$

where \mathbf{H} is the Hessian matrix evaluated using the parameter estimates on the last iteration. Note that the dispersion parameter, whether estimated or specified, is incorporated into \mathbf{H} . Rows and columns corresponding to aliased parameters are not included in Σ .

The correlation matrix is the normalized covariance matrix. That is, if σ_{ij} is an element of Σ , then the corresponding element of the correlation matrix is $\sigma_{ij}/\sigma_i\sigma_j$, where $\sigma_i = \sqrt{\sigma_{ii}}$.

Goodness of Fit

Two statistics that are helpful in assessing the goodness of fit of a given generalized linear model are the scaled deviance and Pearson's chi-square statistic. For a fixed value of the dispersion parameter ϕ , the scaled deviance is defined to be twice the difference between the maximum achievable log likelihood and the log likelihood at the maximum likelihood estimates of the regression parameters.

Note that these statistics are not valid for GEE models.

If $l(\mathbf{y}, \boldsymbol{\mu})$ is the log-likelihood function expressed as a function of the predicted mean values $\boldsymbol{\mu}$ and the vector \mathbf{y} of response values, then the scaled deviance is defined by

$$D^*(\mathbf{y}, \boldsymbol{\mu}) = 2(l(\mathbf{y}, \hat{\boldsymbol{\mu}}) - l(\mathbf{y}, \boldsymbol{\mu}))$$

For specific distributions, this can be expressed as

$$D^*(\mathbf{y}, \boldsymbol{\mu}) = \frac{D(\mathbf{y}, \boldsymbol{\mu})}{\phi}$$

where D is the deviance. The following table displays the deviance for each of the probability distributions available in PROC GENMOD. The deviance cannot be directly calculated for zero-inflated models. Twice the negative of the log likelihood is reported instead of the proper deviance for the zero-inflated Poisson and zero-inflated negative binomial.

Distribution	Deviance
Normal	$\sum_i w_i (y_i - \mu_i)^2$
Poisson	$2 \sum_i w_i \left[y_i \log \left(\frac{y_i}{\mu_i} \right) - (y_i - \mu_i) \right]$
Binomial	$2 \sum_i w_i m_i \left[y_i \log \left(\frac{y_i}{\mu_i} \right) + (1 - y_i) \log \left(\frac{1 - y_i}{1 - \mu_i} \right) \right]$
Gamma	$2 \sum_i w_i \left[-\log \left(\frac{y_i}{\mu_i} \right) + \frac{y_i - \mu_i}{\mu_i} \right]$
Inverse Gaussian	$\sum_i \frac{w_i (y_i - \mu_i)^2}{\mu_i^2 y_i}$
Multinomial	$\sum_i \sum_j w_i y_{ij} \log \left(\frac{y_{ij}}{p_{ij} m_i} \right)$
Negative binomial	$2 \sum_i \left[y \log(y/\mu) - (y + w_i/k) \log \left(\frac{y + w_i/k}{\mu + w_i/k} \right) \right]$
Zero-inflated Poisson	$-2 \sum_i \begin{cases} w_i \log[\omega_i + (1 - \omega_i) \exp(-\mu_i)] & y_i = 0 \\ w_i [\log(1 - \omega_i) + y_i \log(\mu_i) - \mu_i - \log(y_i!)] & y_i > 0 \end{cases}$
Zero-inflated negative binomial	$-2 \sum_i \begin{cases} \log[\omega_i + (1 - \omega_i)(1 + \frac{k}{w_i} \lambda)] & y_i = 0 \\ \log(1 - \omega_i) + y_i \log \left(\frac{k\lambda}{w_i} \right) - (y_i + \frac{w_i}{k}) \log \left(1 + \frac{k\lambda}{w_i} \right) + \log \left(\frac{\Gamma(y_i + \frac{w_i}{k})}{\Gamma(y_i + 1) \Gamma(\frac{w_i}{k})} \right) & y_i > 0 \end{cases}$

In the binomial case, $y_i = r_i/m_i$, where r_i is a binomial count and m_i is the binomial number of trials parameter.

In the multinomial case, y_{ij} refers to the observed number of occurrences of the j th category for the i th subpopulation defined by the AGGREGATE= variable, m_i is the total number in the i th subpopulation, and p_{ij} is the category probability.

Pearson’s chi-square statistic is defined as

$$X^2 = \sum_i \frac{w_i (y_i - \mu_i)^2}{V(\mu_i)}$$

and the scaled Pearson’s chi-square is X^2/ϕ .

The scaled version of both of these statistics, under certain regularity conditions, has a limiting chi-square distribution, with degrees of freedom equal to the number of observations minus the number of parameters estimated. The scaled version can be used as an approximate guide to the goodness of fit of a given model. Use caution before applying these statistics to ensure that all the conditions for the asymptotic distributions hold. McCullagh and Nelder (1989) advise that differences in deviances for nested models can be better approximated by chi-square distributions than the deviances can themselves.

In cases where the dispersion parameter is not known, an estimate can be used to obtain an approximation to the scaled deviance and Pearson’s chi-square statistic. One strategy is to fit a model that contains a sufficient

number of parameters so that all systematic variation is removed, estimate ϕ from this model, and then use this estimate in computing the scaled deviance of submodels. The deviance or Pearson's chi-square divided by its degrees of freedom is sometimes used as an estimate of the dispersion parameter ϕ . For example, since the limiting chi-square distribution of the scaled deviance $D^* = D/\phi$ has $n - p$ degrees of freedom, where n is the number of observations and p is the number of parameters, equating D^* to its mean and solving for ϕ yields $\hat{\phi} = D/(n - p)$. Similarly, an estimate of ϕ based on Pearson's chi-square X^2 is $\hat{\phi} = X^2/(n - p)$. Alternatively, a maximum likelihood estimate of ϕ can be computed by the procedure, if desired. See the discussion in the section “Type 1 Analysis” on page 2811 for more about the estimation of the dispersion parameter.

Other Fit Statistics

The Akaike information criterion (AIC) is a measure of goodness of model fit that balances model fit against model simplicity. AIC has the form

$$\text{AIC} = -2\text{LL} + 2p$$

where p is the number of parameters estimated in the model, and LL is the log likelihood evaluated at the value of the estimated parameters. An alternative form is the corrected AIC given by

$$\text{AICC} = -2\text{LL} + 2p \frac{n}{n - p - 1}$$

where n is the total number of observations used.

The Bayesian information criterion (BIC) is a similar measure. BIC is defined by

$$\text{BIC} = -2\text{LL} + p \log(n)$$

See Akaike (1981, 1979) for details of AIC and BIC. See Simonoff (2003) for a discussion of using AIC, AICC, and BIC with generalized linear models. These criteria are useful in selecting among regression models, with smaller values representing better model fit. PROC GENMOD uses the full log likelihoods defined in the section “Log-Likelihood Functions” on page 2802, with all terms included, for computing all of the criteria.

Dispersion Parameter

There are several options available in PROC GENMOD for handling the exponential distribution dispersion parameter. The NOSCALE and SCALE options in the MODEL statement affect the way in which the dispersion parameter is treated. If you specify the SCALE=DEVIANANCE option, the dispersion parameter is estimated by the deviance divided by its degrees of freedom. If you specify the SCALE=PEARSON option, the dispersion parameter is estimated by Pearson's chi-square statistic divided by its degrees of freedom.

Otherwise, values of the SCALE and NOSCALE options and the resultant actions are displayed in the following table.

NOSCALE	SCALE=value	Action
Present	Present	Scale fixed at <i>value</i>
Present	Not present	Scale fixed at 1
Not present	Not present	Scale estimated by ML
Not present	Present	Scale estimated by ML, starting point at <i>value</i>
Present (negative binomial)	Not present	<i>k</i> fixed at 0

The meaning of the scale parameter displayed in the “Analysis Of Parameter Estimates” table is different for the gamma distribution than for the other distributions. The relation of the scale parameter as used by PROC GENMOD to the exponential family dispersion parameter ϕ is displayed in the following table. For the binomial and Poisson distributions, ϕ is the overdispersion parameter, as defined in the “Overdispersion” section, which follows.

Distribution	Scale
Normal	$\sqrt{\phi}$
Inverse Gaussian	$\sqrt{\phi}$
Gamma	$1/\phi$
Binomial	$\sqrt{\phi}$
Poisson	$\sqrt{\phi}$

In the case of the negative binomial distribution, PROC GENMOD reports the “dispersion” parameter estimated by maximum likelihood. This is the negative binomial parameter k defined in the section “Response Probability Distributions” on page 2799.

Overdispersion

Overdispersion is a phenomenon that sometimes occurs in data that are modeled with the binomial or Poisson distributions. If the estimate of dispersion after fitting, as measured by the deviance or Pearson’s chi-square, divided by the degrees of freedom, is not near 1, then the data might be *overdispersed* if the dispersion estimate is greater than 1 or *underdispersed* if the dispersion estimate is less than 1. A simple way to model this situation is to allow the variance functions of these distributions to have a multiplicative overdispersion factor ϕ :

- Binomial: $V(\mu) = \phi\mu(1 - \mu)$
- Poisson: $V(\mu) = \phi\mu$

An alternative method to allow for overdispersion in the Poisson distribution is to fit a negative binomial distribution, where $V(\mu) = \mu + k\mu^2$, instead of the Poisson. The parameter k can be estimated by maximum likelihood, thus allowing for overdispersion of a specific form. This is different from the multiplicative overdispersion factor ϕ , which can accommodate many forms of overdispersion.

The models are fit in the usual way, and the parameter estimates are not affected by the value of ϕ . The covariance matrix, however, is multiplied by ϕ , and the scaled deviance and log likelihoods used in likelihood ratio tests are divided by ϕ . The profile likelihood function used in computing confidence intervals is also divided by ϕ . If you specify a WEIGHT statement, ϕ is divided by the value of the WEIGHT variable for each observation. This has the effect of multiplying the contributions of the log-likelihood function, the gradient, and the Hessian by the value of the WEIGHT variable for each observation.

The SCALE= option in the MODEL statement enables you to specify a value of $\sigma = \sqrt{\phi}$ for the binomial and Poisson distributions. If you specify the SCALE=DEVIANC option in the MODEL statement, the procedure uses the deviance divided by degrees of freedom as an estimate of ϕ , and all statistics are adjusted appropriately. You can use Pearson’s chi-square instead of the deviance by specifying the SCALE=PEARSON option.

The function obtained by dividing a log-likelihood function for the binomial or Poisson distribution by a dispersion parameter is not a legitimate log-likelihood function. It is an example of a *quasi-likelihood*

function. Most of the asymptotic theory for log likelihoods also applies to quasi-likelihoods, which justifies computing standard errors and likelihood ratio statistics by using quasi-likelihoods instead of proper log likelihoods. For details on quasi-likelihood functions, see McCullagh and Nelder (1989, Chapter 9), McCullagh (1983); Hardin and Hilbe (2003).

Although the estimate of the dispersion parameter is often used to indicate overdispersion or underdispersion, this estimate might also indicate other problems such as an incorrectly specified model or outliers in the data. You should carefully assess whether this type of model is appropriate for your data.

Specification of Effects

Each term in a model is called an effect. Effects are specified in the MODEL statement. You specify effects with a special notation that uses variable names and operators. There are two types of variables, *classification* (or CLASS) variables and *continuous* variables. There are two primary types of operators, *crossing* and *nesting*. A third type, the *bar* operator, is used to simplify effect specification. Crossing is the type of operator most commonly used in generalized linear models.

Variables that identify classification levels are called CLASS variables in SAS and are identified in a CLASS statement. These might also be called *categorical*, *qualitative*, *discrete*, or *nominal* variables. CLASS variables can be either character or numeric. The values of CLASS variables are called *levels*. For example, the CLASS variable Sex could have the levels ‘male’ and ‘female’.

In a model, an explanatory variable that is not declared in a CLASS statement is assumed to be continuous. Continuous variables must be numeric. For example, the heights and weights of subjects in an experiment are continuous variables.

The types of effects most useful in generalized linear models are shown in the following list. Assume that A, B, and C are classification variables and that X1 and X2 are continuous variables.

- Regressor effects are specified by writing continuous variables by themselves: X1, X2.
- Polynomial effects are specified by joining two or more continuous variables with asterisks: X1*X2.
- Main effects are specified by writing classification variables by themselves: A, B, C.
- Crossed effects (interactions) are specified by joining two or more classification variables with asterisks: A*B, B*C, A*B*C.
- Nested effects are specified by following a main effect or crossed effect with a classification variable or list of classification variables enclosed in parentheses: B(A), C(B A), A*B(C). In the preceding example, B(A) is “B nested within A.”
- Combinations of continuous and classification variables can be specified in the same way by using the crossing and nesting operators.

The bar operator consists of two effects joined with a vertical bar (|). It is shorthand notation for including the left-hand side, the right-hand side, and the cross between them as effects in the model. For example, A | B is equivalent to A B A*B. The effects in the bar operator can be classification variables, continuous variables, or combinations of effects defined using operators. Multiple bars are permitted. For example, A | B | C means A B C A*B A*C B*C A*B*C.

You can specify the maximum number of variables in any effect that results from bar evaluation by specifying the maximum number, preceded by an @ sign. For example, A | B | C@2 results in effects that involve two or fewer variables: A B C A*B A*C B*C.

Parameterization Used in PROC GENMOD

Design Matrix

The linear predictor part of a generalized linear model is

$$\eta = \mathbf{X}\boldsymbol{\beta}$$

where $\boldsymbol{\beta}$ is an unknown parameter vector and \mathbf{X} is a known design matrix. By default, all models automatically contain an intercept term; that is, the first column of \mathbf{X} contains all 1s. Additional columns of \mathbf{X} are generated for classification variables, regression variables, and any interaction terms included in the model. It is important to understand the ordering of classification variable parameters when you use the ESTIMATE or CONTRAST statement. The ordering of these parameters is displayed in the “[CLASS Level Information](#)” table and in tables displaying the parameter estimates of the fitted model.

When you specify an overparameterized model with the [PARAM=GLM](#) option in the CLASS statement, some columns of \mathbf{X} can be linearly dependent on other columns. For example, when you specify a model consisting of an intercept term and a classification variable, the column corresponding to any one of the levels of the classification variable is linearly dependent on the other columns of \mathbf{X} . The columns of $\mathbf{X}'\mathbf{X}$ are checked in the order in which the model is specified for dependence on preceding columns. If a dependency is found, the parameter corresponding to the dependent column is set to 0 along with its standard error to indicate that it is not estimated. The order in which the levels of a classification variable are checked for dependencies can be set by the [ORDER=](#) option in the PROC GENMOD statement or by the [ORDER=](#) option in the CLASS statement. For full-rank parameterizations, the columns of the \mathbf{X} matrix are designed to be linearly independent.

You can exclude the intercept term from the model by specifying the NOINT option in the MODEL statement.

Missing Level Combinations

All levels of interaction terms involving classification variables might not be represented in the data. In that case, PROC GENMOD does not include parameters in the model for the missing levels.

Type 1 Analysis

A Type 1 analysis consists of fitting a sequence of models, beginning with a simple model with only an intercept term, and continuing through a model of specified complexity, fitting one additional effect on each step. Likelihood ratio statistics—that is, twice the difference of the log likelihoods—are computed between successive models. This type of analysis is sometimes called an analysis of deviance since, if the dispersion parameter is held fixed for all models, it is equivalent to computing differences of scaled deviances. The asymptotic distribution of the likelihood ratio statistics, under the hypothesis that the additional parameters included in the model are equal to 0, is a chi-square with degrees of freedom equal to the difference in the

number of parameters estimated in the successive models. Thus, these statistics can be used in a test of hypothesis of the significance of each additional term fit.

This type of analysis is not available for GEE models, since the deviance is not computed for this type of model.

If the dispersion parameter ϕ is known, it can be included in the models; if it is unknown, there are two strategies allowed by PROC GENMOD. The dispersion parameter can be estimated from a maximal model by the deviance or Pearson's chi-square divided by degrees of freedom, as discussed in the section "Goodness of Fit" on page 2806, and this value can be used in all models. An alternative is to consider the dispersion to be an additional unknown parameter for each model and estimate it by maximum likelihood on each step. By default, PROC GENMOD estimates scale by maximum likelihood at each step.

A table of likelihood ratio statistics is produced, along with associated p -values based on the asymptotic chi-square distributions.

If you specify either the SCALE=DEVIANCE or the SCALE=PEARSON option in the MODEL statement, the dispersion parameter is estimated using the deviance or Pearson's chi-square statistic, and F statistics are computed in addition to the chi-square statistics for assessing the significance of each additional term in the Type 1 analysis. See the section " F Statistics" on page 2814 for a definition of F statistics.

This Type 1 analysis has the general property that the results depend on the order in which the terms of the model are fitted. The terms are fitted in the order in which they are specified in the MODEL statement.

Type 3 Analysis

A Type 3 analysis is similar to the Type III sums of squares used in PROC GLM, except that likelihood ratios are used instead of sums of squares. First, a Type III estimable function is defined for an effect of interest in exactly the same way as in PROC GLM. Then maximum likelihood estimates are computed under the constraint that the Type III function of the parameters is equal to 0, by using constrained optimization. Let the resulting constrained parameter estimates be $\tilde{\beta}$ and the log likelihood be $l(\tilde{\beta})$. Then the likelihood ratio statistic

$$S = 2(l(\hat{\beta}) - l(\tilde{\beta}))$$

where $\hat{\beta}$ is the unconstrained estimate, has an asymptotic chi-square distribution under the hypothesis that the Type III contrast is equal to 0, with degrees of freedom equal to the number of parameters associated with the effect.

When a Type 3 analysis is requested, PROC GENMOD produces a table that contains the likelihood ratio statistics, degrees of freedom, and p -values based on the limiting chi-square distributions for each effect in the model. If you specify either the DSCALE or PSCALE option in the MODEL statement, F statistics are also computed for each effect.

Options for handling the dispersion parameter are the same as for a Type 1 analysis. The dispersion parameter can be specified to be a known value, estimated from the deviance or Pearson's chi-square divided by degrees of freedom, or estimated by maximum likelihood individually for the unconstrained and constrained models. By default, PROC GENMOD estimates scale by maximum likelihood for each model fit.

The results of this type of analysis do not depend on the order in which the terms are specified in the MODEL statement.

A Type 3 analysis can consume considerable computation time since a constrained model is fitted for each effect. Wald statistics for Type 3 contrasts are computed if you specify the WALS option. Wald statistics for contrasts use less computation time than likelihood ratio statistics but might be less accurate indicators of the significance of the effect of interest. The Wald statistic for testing $L'\beta = 0$, where L is the contrast matrix, is defined by

$$S = (L'\hat{\beta})'(L'\hat{\Sigma}L)^{-1}(L'\hat{\beta})$$

where β is the maximum likelihood estimate and Σ is its estimated covariance matrix. The asymptotic distribution of S is chi-square with r degrees of freedom, where r is the rank of L .

See Chapter 42, “The GLM Procedure,” and Chapter 15, “The Four Types of Estimable Functions,” for more information about Type III estimable functions. Also see Littell, Freund, and Spector (1991).

Generalized score tests for Type III contrasts are computed for GEE models if you specify the TYPE3 option in the MODEL statement when a REPEATED statement is also used. See the section “Generalized Score Statistics” on page 2827 for more information about generalized score statistics. Wald tests are also available with the Wald option in the CONTRAST statement. In this case, the robust covariance matrix estimate is used for Σ in the Wald statistic.

Confidence Intervals for Parameters

Likelihood Ratio-Based Confidence Intervals

PROC GENMOD produces likelihood ratio-based confidence intervals, also known as profile likelihood confidence intervals, for parameter estimates for generalized linear models. These are not computed for GEE models, since there is no likelihood for this type of model. Suppose that the parameter vector is $\beta = [\beta_0, \beta_1, \dots, \beta_p]'$ and that you want a confidence interval for β_j . The profile likelihood function for β_j is defined as

$$l^*(\beta_j) = \max_{\tilde{\beta}} l(\beta)$$

where $\tilde{\beta}$ is the vector β with the j th element fixed at β_j and l is the log-likelihood function. If $l = l(\hat{\beta})$ is the log likelihood evaluated at the maximum likelihood estimate $\hat{\beta}$, then $2(l - l^*(\beta_j))$ has a limiting chi-square distribution with one degree of freedom if β_j is the true parameter value. A $(1 - \alpha)100\%$ confidence interval for β_j is

$$\{\beta_j : l^*(\beta_j) \geq l_0 = l - 0.5\chi_{1-\alpha,1}^2\}$$

where $\chi_{1-\alpha,1}^2$ is the $100(1 - \alpha)$ th percentile of the chi-square distribution with one degree of freedom. The endpoints of the confidence interval can be found by solving numerically for values of β_j that satisfy equality in the preceding relation. PROC GENMOD solves this by starting at the maximum likelihood estimate of β . The log-likelihood function is approximated with a quadratic surface, for which an exact solution is possible. The process is iterated until convergence to an endpoint is attained. The process is repeated for the other endpoint.

Convergence is controlled by the CICONV= option in the MODEL statement. Suppose ϵ is the number specified in the CICONV= option. The default value of ϵ is 10^{-4} . Let the parameter of interest be β_j ,

and define $\mathbf{r} = \mathbf{u}_j$, the unit vector with a 1 in position j and 0s elsewhere. Convergence is declared on the current iteration if the following two conditions are satisfied:

$$|l^*(\beta_j) - l_0| \leq \epsilon$$

$$(\mathbf{s} + \lambda \mathbf{r})' \mathbf{H}^{-1} (\mathbf{s} + \lambda \mathbf{r}) \leq \epsilon$$

where $l^*(\beta_j)$, \mathbf{s} , and \mathbf{H} are the log likelihood, the gradient, and the Hessian evaluated at the current parameter vector and λ is a constant computed by the procedure. The first condition for convergence means that the log-likelihood function must be within ϵ of the correct value, and the second condition means that the gradient vector must be proportional to the restriction vector \mathbf{r} .

When you specify the LRCI option in the MODEL statement, PROC GENMOD computes profile likelihood confidence intervals for all parameters in the model, including the scale parameter, if there is one. The interval endpoints are displayed in a table as well as the values of the remaining parameters at the solution.

Wald Confidence Intervals

You can request that PROC GENMOD produce Wald confidence intervals for the parameters. The $(1 - \alpha)100\%$ Wald confidence interval for a parameter β is defined as

$$\hat{\beta} \pm z_{1-\alpha/2} \hat{\sigma}$$

where z_p is the 100 p percentile of the standard normal distribution, $\hat{\beta}$ is the parameter estimate, and $\hat{\sigma}$ is the estimate of its standard error.

F Statistics

Suppose that D_0 is the deviance resulting from fitting a generalized linear model and that D_1 is the deviance from fitting a submodel. Then, under appropriate regularity conditions, the asymptotic distribution of $(D_1 - D_0)/\phi$ is chi-square with r degrees of freedom, where r is the difference in the number of parameters between the two models and ϕ is the dispersion parameter. If ϕ is unknown, and $\hat{\phi}$ is an estimate of ϕ based on the deviance or Pearson's chi-square divided by degrees of freedom, then, under regularity conditions, $(n-p)\hat{\phi}/\phi$ has an asymptotic chi-square distribution with $n-p$ degrees of freedom. Here, n is the number of observations and p is the number of parameters in the model that is used to estimate ϕ . Thus, the asymptotic distribution of

$$F = \frac{D_1 - D_0}{r\hat{\phi}}$$

is the F distribution with r and $n-p$ degrees of freedom, assuming that $(D_1 - D_0)/\phi$ and $(n-p)\hat{\phi}/\phi$ are approximately independent.

This F statistic is computed for the Type 1 analysis, Type 3 analysis, and hypothesis tests specified in CONTRAST statements when the dispersion parameter is estimated by either the deviance or Pearson's chi-square divided by degrees of freedom, as specified by the DSCALE or PSCALE option in the MODEL statement. In the case of a Type 1 analysis, model 0 is the higher-order model obtained by including one additional effect in model 1. For a Type 3 analysis and hypothesis tests, model 0 is the full specified model and model 1 is the submodel obtained from constraining the Type III contrast or the user-specified contrast to be 0.

Lagrange Multiplier Statistics

When you select the NOINT or NOSCALE option, restrictions are placed on the intercept or scale parameters. Lagrange multiplier, or score, statistics are computed in these cases. These statistics assess the validity of the restrictions, and they are computed as

$$\chi^2 = \frac{s^2}{V}$$

where s is the component of the score vector evaluated at the restricted maximum corresponding to the restricted parameter and $V = \mathbf{I}_{11} - \mathbf{I}_{12}\mathbf{I}_{22}^{-1}\mathbf{I}_{21}$. The matrix \mathbf{I} is the information matrix, 1 refers to the restricted parameter, and 2 refers to the rest of the parameters.

Under regularity conditions, this statistic has an asymptotic chi-square distribution with one degree of freedom, and p -values are computed based on this limiting distribution.

If you set $k = 0$ in a negative binomial model, s is the score statistic of Cameron and Trivedi (1998) for testing for overdispersion in a Poisson model against alternatives of the form $V(\mu) = \mu + k\mu^2$.

See Rao (1973, p. 417) for more details.

Predicted Values of the Mean

Predicted Values

A predicted value, or fitted value, of the mean μ_i corresponding to the vector of covariates \mathbf{x}_i is given by

$$\hat{\mu}_i = g^{-1}(\mathbf{x}_i' \hat{\boldsymbol{\beta}})$$

where g is the link function, regardless of whether \mathbf{x}_i corresponds to an observation or not. That is, the response variable can be missing and the predicted value is still computed for valid \mathbf{x}_i . In the case where \mathbf{x}_i does not correspond to a valid observation, \mathbf{x}_i is not checked for estimability. You should check the estimability of \mathbf{x}_i in this case in order to ensure the uniqueness of the predicted value of the mean. If there is an offset, it is included in the predicted value computation.

Confidence Intervals on Predicted Values

Approximate confidence intervals for predicted values of the mean can be computed as follows. The variance of the linear predictor $\eta_i = \mathbf{x}_i' \hat{\boldsymbol{\beta}}$ is estimated by

$$\sigma_x^2 = \mathbf{x}_i' \boldsymbol{\Sigma} \mathbf{x}_i$$

where $\boldsymbol{\Sigma}$ is the estimated covariance of $\hat{\boldsymbol{\beta}}$. The robust estimate of the covariance is used for $\boldsymbol{\Sigma}$ in the case of models fit with GEEs.

Approximate $100(1 - \alpha)\%$ confidence intervals are computed as

$$g^{-1} \left(\mathbf{x}_i' \hat{\boldsymbol{\beta}} \pm z_{1-\alpha/2} \sigma_x \right)$$

where z_p is the $100p$ th percentile of the standard normal distribution and g is the link function. If either endpoint in the argument is outside the valid range of arguments for the inverse link function, the corresponding confidence interval endpoint is set to missing.

Residuals

The GENMOD procedure computes three kinds of residuals. Residuals are available for all generalized linear models except multinomial models for ordinal response data, for which residuals are not available. Raw residuals and Pearson residuals are available for models fit with generalized estimating equations (GEEs).

The raw residual is defined as

$$r_i = y_i - \mu_i$$

where y_i is the i th response and μ_i is the corresponding predicted mean. You can request raw residuals in an output data set with the keyword **RESRAW** in the OUTPUT statement.

The Pearson residual is the square root of the i th contribution to the Pearson's chi-square:

$$r_{Pi} = (y_i - \mu_i) \sqrt{\frac{w_i}{V(\mu_i)}}$$

You can request Pearson residuals in an output data set with the keyword **RESCHI** in the OUTPUT statement.

Finally, the deviance residual is defined as the square root of the contribution of the i th observation to the deviance, with the sign of the raw residual:

$$r_{Di} = \sqrt{d_i}(\text{sign}(y_i - \mu_i))$$

You can request deviance residuals in an output data set with the keyword **RESDEV** in the OUTPUT statement.

The adjusted Pearson, deviance, and likelihood residuals are defined by Agresti (2002); Williams (1987); Davison and Snell (1991). These residuals are useful for outlier detection and for assessing the influence of single observations on the fitted model.

For the generalized linear model, the variance of the i th individual observation is given by

$$v_i = \frac{\phi V(\mu_i)}{w_i}$$

where ϕ is the dispersion parameter, w_i is a user-specified prior weight (if not specified, $w_i = 1$), μ_i is the mean, and $V(\mu_i)$ is the variance function. Let

$$w_{ei} = v_i^{-1} (g'(\mu_i))^{-2}$$

for the i th observation, where $g'(\mu_i)$ is the derivative of the link function, evaluated at μ_i . Let \mathbf{W}_e be the diagonal matrix with w_{ei} denoting the i th diagonal element. The weight matrix \mathbf{W}_e is used in computing the expected information matrix.

Define h_i as the i th diagonal element of the matrix

$$\mathbf{W}_e^{\frac{1}{2}} \mathbf{X} (\mathbf{X}' \mathbf{W}_e \mathbf{X})^{-1} \mathbf{X}' \mathbf{W}_e^{\frac{1}{2}}$$

The Pearson residuals, standardized to have unit asymptotic variance, are given by

$$r_{Pi} = \frac{y_i - \mu_i}{\sqrt{v_i(1 - h_i)}}$$

You can request standardized Pearson residuals in an output data set with the keyword **STDRESCHI** in the **OUTPUT** statement. The deviance residuals, standardized to have unit asymptotic variance, are given by

$$r_{Di} = \frac{\text{sign}(y_i - \mu_i)\sqrt{d_i}}{\sqrt{\phi(1 - h_i)}}$$

where d_i is the contribution to the total deviance from observation i , and $\text{sign}(y_i - \mu_i)$ is 1 if $y_i - \mu_i$ is positive and -1 if $y_i - \mu_i$ is negative. You can request standardized deviance residuals in an output data set with the keyword **STDRESDEV** in the **OUTPUT** statement. The likelihood residuals are defined by

$$r_{Gi} = \text{sign}(y_i - \mu_i)\sqrt{(1 - h_i)r_{Di}^2 + h_i r_{Pi}^2}$$

You can request likelihood residuals in an output data set with the keyword **RESLIK** in the **OUTPUT** statement.

Multinomial Models

This type of model applies to cases where an observation can fall into one of k categories. Binary data occur in the special case where $k = 2$. If there are m_i observations in a subpopulation i , then the probability distribution of the number falling into the k categories $y_i = (y_{i1}, y_{i2}, \dots, y_{ik})$ can be modeled by the multinomial distribution, defined in the section “[Response Probability Distributions](#)” on page 2799, with $\sum_j y_{ij} = m_i$. The multinomial model is an *ordinal* model if the categories have a natural order.

Residuals are not available in the **OBSTATS** table or the output data set for multinomial models.

By default, and consistently with binomial models, the **GENMOD** procedure orders the response categories for ordinal multinomial models from lowest to highest and models the probabilities of the lower response levels. You can change the way **PROC GENMOD** orders the response levels with the **RORDER=** option in the **PROC GENMOD** statement. The order that **PROC GENMOD** uses is shown in the “[Response Profiles](#)” output table described in the section “[Response Profile](#)” on page 2843.

The **GENMOD** procedure supports only the ordinal multinomial model. If $(p_{i1}, p_{i2}, \dots, p_{ik})$ are the category probabilities, the cumulative category probabilities are modeled with the same link functions used for binomial data. Let $P_{ir} = \sum_{j=1}^r p_{ij}$, $r = 1, 2, \dots, k - 1$, be the cumulative category probabilities (note that $P_{ik} = 1$). The ordinal model is

$$g(P_{ir}) = \mu_r + \mathbf{x}'\boldsymbol{\beta} \quad \text{for } r = 1, 2, \dots, k - 1$$

where $\mu_1, \mu_2, \dots, \mu_{k-1}$ are intercept terms that depend only on the categories and \mathbf{x}_i is a vector of covariates that does not include an intercept term. The logit, probit, and complementary log-log link functions g are available. These are obtained by specifying the **MODEL** statement options **DIST=MULTINOMIAL** and **LINK=CUMLOGIT** (cumulative logit), **LINK=CUMPROBIT** (cumulative probit), or **LINK=CUMCLL** (cumulative complementary log-log). Alternatively,

$$P_{ir} = F(\mu_r + \mathbf{x}'\boldsymbol{\beta}) \quad \text{for } r = 1, 2, \dots, k - 1$$

where $F = g^{-1}$ is a cumulative distribution function for the logistic, normal, or extreme-value distribution.

PROC GENMOD estimates the intercept parameters $\mu_1, \mu_2, \dots, \mu_{k-1}$ and regression parameters $\boldsymbol{\beta}$ by maximum likelihood.

The subpopulations i are defined by constant values of the **AGGREGATE=** variable. This has no effect on the parameter estimates, but it does affect the deviance and Pearson chi-square statistics; it also affects parameter estimate standard errors if you specify the **SCALE=DEVIANANCE** or **SCALE=PEARSON** option.

Zero-Inflated Models

Count data that have an incidence of zeros greater than expected for the underlying probability distribution of counts can be modeled with a zero-inflated distribution. In GENMOD, the underlying distribution can be either Poisson or negative binomial. See Lambert (1992), Long (1997) and Cameron and Trivedi (1998) for more information about zero-inflated models. The population is considered to consist of two types of individuals. The first type gives Poisson or negative binomial distributed counts, which might contain zeros. The second type always gives a zero count. Let λ be the underlying distribution mean and ω be the probability of an individual being of the second type. The parameter ω is called here the *zero-inflation probability*, and is the probability of zero counts in excess of the frequency predicted by the underlying distribution. You can request that the zero inflation probability be displayed in an output data set with the **PZERO** keyword. The probability distribution of a zero-inflated Poisson random variable Y is given by

$$\Pr(Y = y) = \begin{cases} \omega + (1 - \omega)e^{-\lambda} & \text{for } y = 0 \\ (1 - \omega)\frac{\lambda^y e^{-\lambda}}{y!} & \text{for } y = 1, 2, \dots \end{cases}$$

and the probability distribution of a zero-inflated negative binomial random variable Y is given by

$$\Pr(Y = y) = \begin{cases} \omega + (1 - \omega)(1 + k\lambda)^{-\frac{1}{k}} & \text{for } y = 0 \\ (1 - \omega)\frac{\Gamma(y+1/k)}{\Gamma(y+1)\Gamma(1/k)}\frac{(k\lambda)^y}{(1+k\lambda)^{y+1/k}} & \text{for } y = 1, 2, \dots \end{cases}$$

where k is the negative binomial dispersion parameter.

You can model the parameters ω and λ in GENMOD with the regression models:

$$\begin{aligned} h(\omega_i) &= \mathbf{z}'_i \boldsymbol{\gamma} \\ g(\lambda_i) &= \mathbf{x}'_i \boldsymbol{\beta} \end{aligned}$$

where h is one of the binary link functions: logit, probit, or complementary log-log. The link function h is the logit link by default, or the link function option specified in the **ZEROMODEL** statement. The link function g is the log link function by default, or the link function specified in the **MODEL** statement, for both the Poisson and the negative binomial. The covariates \mathbf{z}_i for observation i are determined by the model specified in the **ZEROMODEL** statement, and the covariates \mathbf{x}_i are determined by the model specified in the **MODEL** statement. The regression parameters $\boldsymbol{\gamma}$ and $\boldsymbol{\beta}$ are estimated by maximum likelihood.

The mean and variance of Y for the zero-inflated Poisson are given by

$$\begin{aligned} E(Y) &= \mu = (1 - \omega)\lambda \\ \text{Var}(Y) &= \mu + \frac{\omega}{1 - \omega}\mu^2 \end{aligned}$$

and for the zero-inflated negative binomial by

$$\begin{aligned} E(Y) &= \mu = (1 - \omega)\lambda \\ \text{Var}(Y) &= \mu + \left(\frac{\omega}{1 - \omega} + \frac{k}{1 - \omega} \right) \mu^2 \end{aligned}$$

You can request that the mean of Y be displayed for each observation in an output data set with the **PRED** keyword.

Generalized Estimating Equations

Let y_{ij} , $j = 1, \dots, n_i$, $i = 1, \dots, K$, represent the j th measurement on the i th subject. There are n_i measurements on subject i and $\sum_{i=1}^K n_i$ total measurements.

Correlated data are modeled using the same link function and linear predictor setup (systematic component) as the independence case. The random component is described by the same variance functions as in the independence case, but the covariance structure of the correlated measurements must also be modeled. Let the vector of measurements on the i th subject be $\mathbf{Y}_i = [y_{i1}, \dots, y_{in_i}]'$ with corresponding vector of means $\boldsymbol{\mu}_i = [\mu_{i1}, \dots, \mu_{in_i}]'$, and let \mathbf{V}_i be the covariance matrix of \mathbf{Y}_i . Let the vector of independent, or explanatory, variables for the j th measurement on the i th subject be

$$\mathbf{x}_{ij} = [x_{ij1}, \dots, x_{ijp}]'$$

The generalized estimating equation of Liang and Zeger (1986) for estimating the $p \times 1$ vector of regression parameters $\boldsymbol{\beta}$ is an extension of the independence estimating equation to correlated data and is given by

$$\mathbf{S}(\boldsymbol{\beta}) = \sum_{i=1}^K \mathbf{D}_i' \mathbf{V}_i^{-1} (\mathbf{Y}_i - \boldsymbol{\mu}_i(\boldsymbol{\beta})) = \mathbf{0}$$

where

$$\mathbf{D}_i = \frac{\partial \boldsymbol{\mu}_i}{\partial \boldsymbol{\beta}}$$

Since

$$g(\mu_{ij}) = \mathbf{x}_{ij}' \boldsymbol{\beta}$$

where g is the link function, the $p \times n_i$ matrix of partial derivatives of the mean with respect to the regression parameters for the i th subject is given by

$$\mathbf{D}_i' = \frac{\partial \boldsymbol{\mu}_i'}{\partial \boldsymbol{\beta}} = \begin{bmatrix} \frac{x_{i11}}{g'(\mu_{i1})} & \cdots & \frac{x_{in_i1}}{g'(\mu_{in_i})} \\ \vdots & & \vdots \\ \frac{x_{i1p}}{g'(\mu_{i1})} & \cdots & \frac{x_{in_ip}}{g'(\mu_{in_i})} \end{bmatrix}$$

Working Correlation Matrix

Let $\mathbf{R}_i(\boldsymbol{\alpha})$ be an $n_i \times n_i$ “working” correlation matrix that is fully specified by the vector of parameters $\boldsymbol{\alpha}$. The covariance matrix of \mathbf{Y}_i is modeled as

$$\mathbf{V}_i = \phi \mathbf{A}_i^{\frac{1}{2}} \mathbf{W}_i^{-\frac{1}{2}} \mathbf{R}_i(\boldsymbol{\alpha}) \mathbf{W}_i^{-\frac{1}{2}} \mathbf{A}_i^{\frac{1}{2}}$$

where \mathbf{A}_i is an $n_i \times n_i$ diagonal matrix with $v(\mu_{ij})$ as the j th diagonal element and \mathbf{W}_i is an $n_i \times n_i$ diagonal matrix with w_{ij} as the j th diagonal, where w_{ij} is a weight specified with the WEIGHT statement. If there is no WEIGHT statement, $w_{ij} = 1$ for all i and j . If $\mathbf{R}_i(\boldsymbol{\alpha})$ is the true correlation matrix of \mathbf{Y}_i , then \mathbf{V}_i is the true covariance matrix of \mathbf{Y}_i .

The working correlation matrix is usually unknown and must be estimated. It is estimated in the iterative fitting process by using the current value of the parameter vector $\boldsymbol{\beta}$ to compute appropriate functions of the Pearson residual

$$e_{ij} = \frac{y_{ij} - \mu_{ij}}{\sqrt{v(\mu_{ij})/w_{ij}}}$$

If you specify the working correlation as $\mathbf{R}_0 = \mathbf{I}$, which is the identity matrix, the GEE reduces to the independence estimating equation.

Following are the structures of the working correlation supported by the GENMOD procedure and the estimators used to estimate the working correlations.

Working Correlation Structure	Estimator
<p>Fixed</p> <p>$\text{Corr}(Y_{ij}, Y_{ik}) = r_{jk}$ where r_{jk} is the jkth element of a constant, user-specified correlation matrix \mathbf{R}_0.</p>	<p>The working correlation is not estimated in this case.</p>
<p>Independent</p> <p>$\text{Corr}(Y_{ij}, Y_{ik}) = \begin{cases} 1 & j = k \\ 0 & j \neq k \end{cases}$</p>	<p>The working correlation is not estimated in this case.</p>
<p>m-dependent</p> <p>$\text{Corr}(Y_{ij}, Y_{i,j+t}) = \begin{cases} 1 & t = 0 \\ \alpha_t & t = 1, 2, \dots, m \\ 0 & t > m \end{cases}$</p>	<p>$\hat{\alpha}_t = \frac{1}{(K_t - p)\phi} \sum_{i=1}^K \sum_{j \leq n_i - t} e_{ij} e_{i,j+t}$ $K_t = \sum_{i=1}^K (n_i - t)$</p>
<p>Exchangeable</p> <p>$\text{Corr}(Y_{ij}, Y_{ik}) = \begin{cases} 1 & j = k \\ \alpha & j \neq k \end{cases}$</p>	<p>$\hat{\alpha} = \frac{1}{(N^* - p)\phi} \sum_{i=1}^K \sum_{j < k} e_{ij} e_{ik}$ $N^* = 0.5 \sum_{i=1}^K n_i (n_i - 1)$</p>
<p>Unstructured</p> <p>$\text{Corr}(Y_{ij}, Y_{ik}) = \begin{cases} 1 & j = k \\ \alpha_{jk} & j \neq k \end{cases}$</p>	<p>$\hat{\alpha}_{jk} = \frac{1}{(K - p)\phi} \sum_{i=1}^K e_{ij} e_{ik}$</p>
<p>Autoregressive AR(1)</p> <p>$\text{Corr}(Y_{ij}, Y_{i,j+t}) = \alpha^t$ for $t = 0, 1, 2, \dots, n_i - j$</p>	<p>$\hat{\alpha} = \frac{1}{(K_1 - p)\phi} \sum_{i=1}^K \sum_{j \leq n_i - 1} e_{ij} e_{i,j+1}$ $K_1 = \sum_{i=1}^K (n_i - 1)$</p>

Dispersion Parameter

The dispersion parameter ϕ is estimated by

$$\hat{\phi} = \frac{1}{N - p} \sum_{i=1}^K \sum_{j=1}^{n_i} e_{ij}^2$$

where $N = \sum_{i=1}^K n_i$ is the total number of measurements and p is the number of regression parameters.

The square root of $\hat{\phi}$ is reported by PROC GENMOD as the scale parameter in the “Analysis of GEE Parameter Estimates Model-Based Standard Error Estimates” output table. If a fixed scale parameter is specified with the NOSCALE option in the MODEL statement, then the fixed value is used in estimating the model-based covariance matrix and standard errors.

Fitting Algorithm

The following is an algorithm for fitting the specified model by using GEEs. Note that this is not in general a likelihood-based method of estimation, so that inferences based on likelihoods are not possible for GEE methods.

1. Compute an initial estimate of $\boldsymbol{\beta}$ with an ordinary generalized linear model assuming independence.
2. Compute the working correlations \mathbf{R} based on the standardized residuals, the current $\boldsymbol{\beta}$, and the assumed structure of \mathbf{R} .
3. Compute an estimate of the covariance:

$$\mathbf{V}_i = \phi \mathbf{A}_i^{\frac{1}{2}} \mathbf{W}_i^{-\frac{1}{2}} \hat{\mathbf{R}}(\boldsymbol{\alpha}) \mathbf{W}_i^{-\frac{1}{2}} \mathbf{A}_i^{\frac{1}{2}}$$

4. Update $\boldsymbol{\beta}$:

$$\boldsymbol{\beta}_{r+1} = \boldsymbol{\beta}_r + \left[\sum_{i=1}^K \frac{\partial \boldsymbol{\mu}_i'}{\partial \boldsymbol{\beta}} \mathbf{V}_i^{-1} \frac{\partial \boldsymbol{\mu}_i}{\partial \boldsymbol{\beta}} \right]^{-1} \left[\sum_{i=1}^K \frac{\partial \boldsymbol{\mu}_i'}{\partial \boldsymbol{\beta}} \mathbf{V}_i^{-1} (\mathbf{Y}_i - \boldsymbol{\mu}_i) \right]$$

5. Repeat steps 2-4 until convergence.

Missing Data

See Diggle, Liang, and Zeger (1994, Chapter 11) for a discussion of missing values in longitudinal data. Suppose that you intend to take measurements Y_{i1}, \dots, Y_{in} for the i th unit. Missing values for which Y_{ij} are missing whenever Y_{ik} is missing for all $j \geq k$ are called *dropouts*. Otherwise, missing values that occur intermixed with nonmissing values are *intermittent* missing values. The GENMOD procedure can estimate the working correlation from data containing both types of missing values by using the *all available pairs* method, in which all nonmissing pairs of data are used in the moment estimators of the working correlation parameters defined previously. The resulting covariances and standard errors are valid under the missing completely at random (MCAR) assumption.

For example, for the unstructured working correlation model,

$$\hat{\alpha}_{jk} = \frac{1}{(K' - p)\phi} \sum e_{ij} e_{ik}$$

where the sum is over the units that have nonmissing measurements at times j and k , and K' is the number of units with nonmissing measurements at j and k . Estimates of the parameters for other working correlation types are computed in a similar manner, using available nonmissing pairs in the appropriate moment estimators.

The contribution of the i th unit to the parameter update equation is computed by omitting the elements of $(\mathbf{Y}_i - \boldsymbol{\mu}_i)$, the columns of $\mathbf{D}'_i = \frac{\partial \boldsymbol{\mu}'_i}{\partial \boldsymbol{\beta}}$, and the rows and columns of \mathbf{V}_i corresponding to missing measurements.

Parameter Estimate Covariances

The *model-based* estimator of $\text{Cov}(\hat{\boldsymbol{\beta}})$ is given by

$$\boldsymbol{\Sigma}_m(\hat{\boldsymbol{\beta}}) = \mathbf{I}_0^{-1}$$

where

$$\mathbf{I}_0 = \sum_{i=1}^K \frac{\partial \boldsymbol{\mu}'_i}{\partial \boldsymbol{\beta}} \mathbf{V}_i^{-1} \frac{\partial \boldsymbol{\mu}_i}{\partial \boldsymbol{\beta}}$$

This is the GEE equivalent of the inverse of the Fisher information matrix that is often used in generalized linear models as an estimator of the covariance estimate of the maximum likelihood estimator of $\boldsymbol{\beta}$. It is a consistent estimator of the covariance matrix of $\hat{\boldsymbol{\beta}}$ if the mean model and the working correlation matrix are correctly specified.

The estimator

$$\boldsymbol{\Sigma}_e = \mathbf{I}_0^{-1} \mathbf{I}_1 \mathbf{I}_0^{-1}$$

is called the *empirical*, or *robust*, estimator of the covariance matrix of $\hat{\boldsymbol{\beta}}$, where

$$\mathbf{I}_1 = \sum_{i=1}^K \frac{\partial \boldsymbol{\mu}'_i}{\partial \boldsymbol{\beta}} \mathbf{V}_i^{-1} \text{Cov}(\mathbf{Y}_i) \mathbf{V}_i^{-1} \frac{\partial \boldsymbol{\mu}_i}{\partial \boldsymbol{\beta}}$$

It has the property of being a consistent estimator of the covariance matrix of $\hat{\boldsymbol{\beta}}$, even if the working correlation matrix is misspecified—that is, if $\text{Cov}(\mathbf{Y}_i) \neq \mathbf{V}_i$. For further information about the robust variance estimate, see Zeger, Liang, and Albert (1988); Royall (1986); White (1982). In computing $\boldsymbol{\Sigma}_e$, $\boldsymbol{\beta}$ and ϕ are replaced by estimates, and $\text{Cov}(\mathbf{Y}_i)$ is replaced by the estimate

$$(\mathbf{Y}_i - \boldsymbol{\mu}_i(\hat{\boldsymbol{\beta}}))(\mathbf{Y}_i - \boldsymbol{\mu}_i(\hat{\boldsymbol{\beta}}))'$$

Multinomial GEEs

Lipsitz, Kim, and Zhao (1994) and Miller, Davis, and Landis (1993) describe how to extend GEEs to multinomial data. Currently, only the independent working correlation is available for multinomial models in PROC GENMOD.

Alternating Logistic Regressions

If the responses are binary (that is, they take only two values), then there is an alternative method to account for the association among the measurements. The alternating logistic regressions (ALR) algorithm of Carey, Zeger, and Diggle (1993) models the association between pairs of responses with log odds ratios, instead of with correlations, as ordinary GEEs do.

For binary data, the correlation between the j th and k th response is, by definition,

$$\text{Corr}(Y_{ij}, Y_{ik}) = \frac{\Pr(Y_{ij} = 1, Y_{ik} = 1) - \mu_{ij}\mu_{ik}}{\sqrt{\mu_{ij}(1 - \mu_{ij})\mu_{ik}(1 - \mu_{ik})}}$$

The joint probability in the numerator satisfies the following bounds, by elementary properties of probability, since $\mu_{ij} = \Pr(Y_{ij} = 1)$:

$$\max(0, \mu_{ij} + \mu_{ik} - 1) \leq \Pr(Y_{ij} = 1, Y_{ik} = 1) \leq \min(\mu_{ij}, \mu_{ik})$$

The correlation, therefore, is constrained to be within limits that depend in a complicated way on the means of the data.

The odds ratio, defined as

$$\text{OR}(Y_{ij}, Y_{ik}) = \frac{\Pr(Y_{ij} = 1, Y_{ik} = 1) \Pr(Y_{ij} = 0, Y_{ik} = 0)}{\Pr(Y_{ij} = 1, Y_{ik} = 0) \Pr(Y_{ij} = 0, Y_{ik} = 1)}$$

is not constrained by the means and is preferred, in some cases, to correlations for binary data.

The ALR algorithm seeks to model the logarithm of the odds ratio, $\gamma_{ijk} = \log(\text{OR}(Y_{ij}, Y_{ik}))$, as

$$\gamma_{ijk} = \mathbf{z}'_{ijk} \boldsymbol{\alpha}$$

where $\boldsymbol{\alpha}$ is a $q \times 1$ vector of regression parameters and \mathbf{z}_{ijk} is a fixed, specified vector of coefficients.

The parameter γ_{ijk} can take any value in $(-\infty, \infty)$ with $\gamma_{ijk} = 0$ corresponding to no association.

The log odds ratio, when modeled in this way with a regression model, can take different values in subgroups defined by \mathbf{z}_{ijk} . For example, \mathbf{z}_{ijk} can define subgroups within clusters, or it can define “block effects” between clusters.

You specify a GEE model for binary data that uses log odds ratios by specifying a model for the mean, as in ordinary GEEs, and a model for the log odds ratios. You can use any of the link functions appropriate for binary data in the model for the mean, such as logistic, probit, or complementary log-log. The ALR algorithm alternates between a GEE step to update the model for the mean and a logistic regression step to update the log odds ratio model. Upon convergence, the ALR algorithm provides estimates of the regression parameters for the mean, $\boldsymbol{\beta}$, the regression parameters for the log odds ratios, $\boldsymbol{\alpha}$, their standard errors, and their covariances.

Specifying Log Odds Ratio Models

Specifying a regression model for the log odds ratio requires you to specify rows of the \mathbf{z} matrix \mathbf{z}_{ijk} for each cluster i and each unique within-cluster pair (j, k) . The GENMOD procedure provides several methods of specifying \mathbf{z}_{ijk} . These are controlled by the `LOGOR=keyword` and associated options in the REPEATED statement. The supported keywords and the resulting log odds ratio models are described as follows.

EXCH specifies exchangeable log odds ratios. In this model, the log odds ratio is a constant for all clusters i and pairs (j, k) . The parameter α is the common log odds ratio.

$$z_{ijk} = 1 \quad \text{for all } i, j, k$$

FULLCLUST specifies fully parameterized clusters. Each cluster is parameterized in the same way, and there is a parameter for each unique pair within clusters. If a complete cluster is of size n , then there are $\frac{n(n-1)}{2}$ parameters in the vector α . For example, if a full cluster is of size 4, then there are $\frac{4 \times 3}{2} = 6$ parameters, and the \mathbf{z} matrix is of the form

$$\mathbf{Z} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

The elements of α correspond to log odds ratios for cluster pairs in the following order:

Pair	Parameter
(1,2)	Alpha1
(1,3)	Alpha2
(1,4)	Alpha3
(2,3)	Alpha4
(2,4)	Alpha5
(3,4)	Alpha6

LOGORVAR(variable) specifies log odds ratios by cluster. The argument *variable* is a variable name that defines the “block effects” between clusters. The log odds ratios are constant within clusters, but they take a different value for each different value of the *variable*. For example, if *Center* is a variable in the input data set taking a different value for k treatment centers, then specifying **LOGOR=LOGORVAR(Center)** requests a model with different log odds ratios for each of the k centers, constant within center.

NESTK specifies k -nested log odds ratios. You must also specify the **SUBCLUST=variable** option to define subclusters within clusters. Within each cluster, PROC GENMOD computes a log odds ratio parameter for pairs having the same value of *variable* for both members of the pair and one log odds ratio parameter for each unique combination of different values of *variable*.

NEST1 specifies 1-nested log odds ratios. You must also specify the **SUBCLUST=variable** option to define subclusters within clusters. There are two log odds ratio parameters for this model. Pairs having the same value of *variable* correspond to one parameter; pairs having different values of *variable* correspond to the other parameter. For example, if clusters are hospitals and subclusters are wards within hospitals, then patients within the same ward have

one log odds ratio parameter, and patients from different wards have the other parameter.

ZFULL

specifies the full \mathbf{z} matrix. You must also specify a SAS data set containing the \mathbf{z} matrix with the ZDATA=*data-set-name* option. Each observation in the data set corresponds to one row of the \mathbf{z} matrix. You must specify the ZDATA data set as if all clusters are complete—that is, as if all clusters are the same size and there are no missing observations. The ZDATA data set has $K[n_{max}(n_{max} - 1)/2]$ observations, where K is the number of clusters and n_{max} is the maximum cluster size. If the members of cluster i are ordered as $1, 2, \dots, n$, then the rows of the \mathbf{z} matrix must be specified for pairs in the order $(1, 2), (1, 3), \dots, (1, n), (2, 3), \dots, (2, n), \dots, (n - 1, n)$. The variables specified in the REPEATED statement for the SUBJECT effect must also be present in the ZDATA= data set to identify clusters. You must specify variables in the data set that define the columns of the \mathbf{z} matrix by the ZROW=*variable-list* option. If there are q columns (q variables in *variable-list*), then there are q log odds ratio parameters. You can optionally specify variables indicating the cluster pairs corresponding to each row of the \mathbf{z} matrix with the YPAIR=(*variable1*, *variable2*) option. If you specify this option, the data from the ZDATA data set are sorted within each cluster by *variable1* and *variable2*. See Example 40.6 for an example of specifying a full \mathbf{z} matrix.

ZREP

specifies a replicated \mathbf{z} matrix. You specify \mathbf{z} matrix data exactly as you do for the ZFULL case, except that you specify only one complete cluster. The \mathbf{z} matrix for the one cluster is replicated for each cluster. The number of observations in the ZDATA data set is $\frac{n_{max}(n_{max}-1)}{2}$, where n_{max} is the size of a complete cluster (a cluster with no missing observations).

ZREP(matrix)

specifies direct input of the replicated \mathbf{z} matrix. You specify the \mathbf{z} matrix for one cluster with the syntax LOGOR=ZREP ((y_1 y_2) z_1 $z_2 \dots z_q, \dots$), where y_1 and y_2 are numbers representing a pair of observations and the values z_1, z_2, \dots, z_q make up the corresponding row of the \mathbf{z} matrix. The number of rows specified is $\frac{n_{max}(n_{max}-1)}{2}$, where n_{max} is the size of a complete cluster (a cluster with no missing observations). For example,

```
logor = zrep((1 2) 1 0,
             (1 3) 1 0,
             (1 4) 1 0,
             (2 3) 1 1,
             (2 4) 1 1,
             (3 4) 1 1)
```

specifies the $\frac{4 \times 3}{2} = 6$ rows of the \mathbf{z} matrix for a cluster of size 4 with $q = 2$ log odds ratio parameters. The log odds ratio for the pairs (1 2), (1 3), (1 4) is α_1 , and the log odds ratio for the pairs (2 3), (2 4), (3 4) is $\alpha_1 + \alpha_2$.

Quasi-likelihood Information Criterion

The quasi-likelihood information criterion (QIC) was developed by Pan (2001) as a modification of the Akaike information criterion (AIC) to apply to models fit by GEEs.

Define the quasi-likelihood under the independence working correlation assumption, evaluated with the parameter estimates under the working correlation of interest as

$$Q(\hat{\beta}(R), \phi) = \sum_{i=1}^K \sum_{j=1}^{n_i} Q(\hat{\beta}(R), \phi; (Y_{ij}, \mathbf{X}_{ij}))$$

where the quasi-likelihood contribution of the j th observation in the i th cluster is defined in the section “Quasi-likelihood Functions” on page 2826 and $\hat{\beta}(R)$ are the parameter estimates obtained from GEEs with the working correlation of interest R .

QIC is defined as

$$\text{QIC}(R) = -2Q(\hat{\beta}(R), \phi) + 2\text{trace}(\hat{\Omega}_I \hat{V}_R)$$

where \hat{V}_R is the robust covariance estimate and $\hat{\Omega}_I$ is the inverse of the model-based covariance estimate under the independent working correlation assumption, evaluated at $\hat{\beta}(R)$, the parameter estimates obtained from GEEs with the working correlation of interest R .

PROC GENMOD also computes an approximation to $\text{QIC}(R)$ defined by Pan (2001) as

$$\text{QIC}_u(R) = -2Q(\hat{\beta}(R), \phi) + 2p$$

where p is the number of regression parameters.

Pan (2001) notes that QIC is appropriate for selecting regression models and working correlations, whereas QIC_u is appropriate only for selecting regression models.

Quasi-likelihood Functions

See McCullagh and Nelder (1989) and Hardin and Hilbe (2003) for discussions of quasi-likelihood functions. The contribution of observation j in cluster i to the quasi-likelihood function evaluated at the regression parameters β is given by $Q(\beta, \phi; (Y_{ij}, \mathbf{X}_{ij})) = \frac{Q_{ij}}{\phi}$, where Q_{ij} is defined in the following list. These are used in the computation of the quasi-likelihood information criteria (QIC) for goodness of fit of models fit with GEEs. The w_{ij} are prior weights, if any, specified with the WEIGHT or FREQ statements. Note that the definition of the quasi-likelihood for the negative binomial differs from that given in McCullagh and Nelder (1989). The definition used here allows the negative binomial quasi-likelihood to approach the Poisson as $k \rightarrow 0$.

- Normal:

$$Q_{ij} = -\frac{1}{2}w_{ij}(y_{ij} - \mu_{ij})^2$$

- Inverse Gaussian:

$$Q_{ij} = \frac{w_{ij}(\mu_{ij} - .5y_{ij})}{\mu_{ij}^2}$$

- Gamma:

$$Q_{ij} = -w_{ij} \left[\frac{y_{ij}}{\mu_{ij}} + \log(\mu_{ij}) \right]$$

- Negative binomial:

$$Q_{ij} = w_{ij} \left[\log \Gamma \left(y_{ij} + \frac{1}{k} \right) - \log \Gamma \left(\frac{1}{k} \right) + y_{ij} \log \left(\frac{k\mu_{ij}}{1 + k\mu_{ij}} \right) + \frac{1}{k} \log \left(\frac{1}{1 + k\mu_{ij}} \right) \right]$$

- Poisson:

$$Q_{ij} = w_{ij}(y_{ij} \log(\mu_{ij}) - \mu_{ij})$$

- Binomial:

$$Q_{ij} = w_{ij}[r_{ij} \log(p_{ij}) + (n_{ij} - r_{ij}) \log(1 - p_{ij})]$$

- Multinomial (s categories):

$$Q_{ij} = w_{ij} \sum_{k=1}^s y_{ijk} \log(\mu_{ijk})$$

Generalized Score Statistics

Boos (1992) and Rotnitzky and Jewell (1990) describe score tests applicable to testing $\mathbf{L}'\boldsymbol{\beta} = \mathbf{0}$ in GEEs, where \mathbf{L}' is a user-specified $r \times p$ contrast matrix or a contrast for a Type 3 test of hypothesis.

Let $\tilde{\boldsymbol{\beta}}$ be the regression parameters resulting from solving the GEE under the restricted model $\mathbf{L}'\boldsymbol{\beta} = \mathbf{0}$, and let $\mathbf{S}(\tilde{\boldsymbol{\beta}})$ be the generalized estimating equation values at $\tilde{\boldsymbol{\beta}}$.

The generalized score statistic is

$$T = \mathbf{S}(\tilde{\boldsymbol{\beta}})' \boldsymbol{\Sigma}_m \mathbf{L} (\mathbf{L}' \boldsymbol{\Sigma}_e \mathbf{L})^{-1} \mathbf{L}' \boldsymbol{\Sigma}_m \mathbf{S}(\tilde{\boldsymbol{\beta}})$$

where $\boldsymbol{\Sigma}_m$ is the model-based covariance estimate and $\boldsymbol{\Sigma}_e$ is the empirical covariance estimate. The p -values for T are computed based on the chi-square distribution with r degrees of freedom.

Assessment of Models Based on Aggregates of Residuals

Lin, Wei, and Ying (2002) present graphical and numerical methods for model assessment based on the cumulative sums of residuals over certain coordinates (such as covariates or linear predictors) or some related aggregates of residuals. The distributions of these stochastic processes under the assumed model can be approximated by the distributions of certain zero-mean Gaussian processes whose realizations can be generated by simulation. Each observed residual pattern can then be compared, both graphically and numerically, with a number of realizations from the null distribution. Such comparisons enable you to assess objectively whether the observed residual pattern reflects anything beyond random fluctuation. These procedures are useful in determining appropriate functional forms of covariates and link function. You use the ASSESS|ASSESSMENT statement to perform this kind of model-checking with cumulative sums of

residuals, moving sums of residuals, or LOESS smoothed residuals. See Example 40.8 and Example 40.9 for examples of model assessment.

Let the model for the mean be

$$g(\mu_i) = \mathbf{x}'_i \boldsymbol{\beta}$$

where μ_i is the mean of the response y_i and \mathbf{x}_i is the vector of covariates for the i th observation. Denote the raw residual resulting from fitting the model as

$$e_i = y_i - \hat{\mu}_i$$

and let x_{ij} be the value of the j th covariate in the model for observation i . Then to check the functional form of the j th covariate, consider the cumulative sum of residuals with respect to x_{ij} ,

$$W_j(x) = \frac{1}{\sqrt{n}} \sum_{i=1}^n I(x_{ij} \leq x) e_i$$

where $I()$ is the indicator function. For any x , $W_j(x)$ is the sum of the residuals with values of x_j less than or equal to x .

Denote the score, or gradient vector, by

$$U(\boldsymbol{\beta}) = \sum_{i=1}^n h(\mathbf{x}'_i \boldsymbol{\beta}) \mathbf{x}_i (y_i - v(\mathbf{x}'_i \boldsymbol{\beta}))$$

where $v(r) = g^{-1}(r)$, and

$$h(r) = \frac{1}{g'(v(r))V(v(r))}$$

Let \mathbf{J} be the Fisher information matrix

$$\mathbf{J}(\boldsymbol{\beta}) = -\frac{\partial U(\boldsymbol{\beta})}{\partial \boldsymbol{\beta}'}$$

Define

$$\hat{W}_j(x) = \frac{1}{\sqrt{n}} \sum_{i=1}^n [I(x_{ij} \leq x) + \boldsymbol{\eta}'(x; \hat{\boldsymbol{\beta}}) \mathbf{J}^{-1}(\hat{\boldsymbol{\beta}}) \mathbf{x}_i h(\mathbf{x}'_i \hat{\boldsymbol{\beta}})] e_i Z_i$$

where

$$\boldsymbol{\eta}(x; \boldsymbol{\beta}) = -\sum_{i=1}^n I(x_{ij} \leq x) \frac{\partial v(\mathbf{x}'_i \boldsymbol{\beta})}{\partial \boldsymbol{\beta}}$$

and Z_i are independent $N(0, 1)$ random variables. Then the conditional distribution of $\hat{W}_j(x)$, given (y_i, \mathbf{x}_i) , $i = 1, \dots, n$, under the null hypothesis H_0 that the model for the mean is correct, is the same asymptotically as $n \rightarrow \infty$ as the unconditional distribution of $W_j(x)$ (Lin, Wei, and Ying 2002).

You can approximate realizations from the null hypothesis distribution of $W_j(x)$ by repeatedly generating normal samples Z_i , $i = 1, \dots, n$, while holding (y_i, \mathbf{x}_i) , $i = 1, \dots, n$, at their observed values and computing $\hat{W}_j(x)$ for each sample.

You can assess the functional form of covariate j by plotting a few realizations of $\hat{W}_j(x)$ on the same plot as the observed $W_j(x)$ and visually comparing to see how typical the observed $W_j(x)$ is of the null distribution samples.

You can supplement the graphical inspection method with a Kolmogorov-type supremum test. Let s_j be the observed value of $S_j = \sup_x |W_j(x)|$. The p -value $\Pr[S_j \geq s_j]$ is approximated by $\Pr[\hat{S}_j \geq s_j]$, where $\hat{S}_j = \sup_x |\hat{W}_j(x)|$. $\Pr[\hat{S}_j \geq s_j]$ is estimated by generating realizations of $\hat{W}_j(\cdot)$ (1,000 is the default number of realizations).

You can check the link function instead of the j th covariate by using values of the linear predictor $\mathbf{x}'_i \hat{\boldsymbol{\beta}}$ in place of values of the j th covariate x_{ij} . The graphical and numerical methods described previously are then sensitive to inadequacies in the link function.

An alternative aggregate of residuals is the moving sum statistic

$$W_j(x, b) = \frac{1}{\sqrt{n}} \sum_{i=1}^n I(x - b \leq x_{ij} \leq x) e_i$$

If you specify the keyword WINDOW(b), then the moving sum statistic with window size b is used instead of the cumulative sum of residuals, with $I(x - b \leq x_{ij} \leq x)$ replacing $I(x_{ij} \leq x)$ in the earlier equation.

If you specify the keyword LOESS(f), loess smoothed residuals are used in the preceding formulas, where f is the fraction of the data to be used at a given point. If f is not specified, $f = \frac{1}{3}$ is used. For data $(Y_i, X_i), i = 1, \dots, n$, define r as the nearest integer to nf and h as the r th smallest among $|X_i - x|, i = 1, \dots, n$. Let

$$K_i(x) = K\left(\frac{X_i - x}{h}\right)$$

where

$$K(t) = \frac{70}{81}(1 - |t|^3)^3 I(-1 \leq t \leq 1)$$

Define

$$w_i(x) = K_i(x)[S_2(x) - (X_i - x)S_1(x)]$$

where

$$S_1(x) = \sum_{i=1}^n K_i(x)(X_i - x)$$

$$S_2(x) = \sum_{i=1}^n K_i(x)(X_i - x)^2$$

Then the loess estimate of Y at x is defined by

$$\hat{Y}(x) = \sum_{i=1}^n \frac{w_i(x)}{\sum_{i=1}^n w_i(x)} Y_i$$

Loess smoothed residuals for checking the functional form of the j th covariate are defined by replacing Y_i with e_i and X_i with x_{ij} . To implement the graphical and numerical assessment methods, $I(x_{ij} \leq x)$ is replaced with $\frac{w_i(x)}{\sum_{i=1}^n w_i(x)}$ in the formulas for $W_j(x)$ and $\hat{W}_j(x)$.

You can perform the model checking described earlier for marginal models for dependent responses fit by generalized estimating equations (GEEs). Let y_{ik} denote the k th measurement on the i th cluster, $i = 1, \dots, K$, $k = 1, \dots, n_i$, and let \mathbf{x}_{ik} denote the corresponding vector of covariates. The marginal mean of the response $\mu_{ik} = E(y_{ik})$ is assumed to depend on the covariate vector by

$$g(\mu_{ik}) = \mathbf{x}'_{ik} \boldsymbol{\beta}$$

where g is the link function.

Define the vector of residuals for the i th cluster as

$$\mathbf{e}_i = (e_{i1}, \dots, e_{in_i})' = (y_{i1} - \hat{\mu}_{i1}, \dots, y_{in_i} - \hat{\mu}_{in_i})'$$

You use the following extension of $W_j(x)$ defined earlier to check the functional form of the j th covariate:

$$W_j(x) = \frac{1}{\sqrt{K}} \sum_{i=1}^K \sum_{k=1}^{n_i} I(x_{ikj} \leq x) e_{ik}$$

where x_{ikj} is the j th component of \mathbf{x}_{ik} .

The null distribution of $W_j(x)$ can be approximated by the conditional distribution of

$$\hat{W}_j(x) = \frac{1}{\sqrt{K}} \sum_{i=1}^K \left\{ \sum_{k=1}^{n_i} I(x_{ikj} \leq x) e_{ik} + \boldsymbol{\eta}'(x, \hat{\boldsymbol{\beta}}) \mathbf{I}_0^{-1} \hat{\mathbf{D}}_i' \hat{\mathbf{V}}_i^{-1} \mathbf{e}_i \right\} Z_i$$

where $\hat{\mathbf{D}}_i$ and $\hat{\mathbf{V}}_i$ are defined as in the section “Generalized Estimating Equations” on page 2819 with the unknown parameters replaced by their estimated values,

$$\boldsymbol{\eta}(x, \boldsymbol{\beta}) = - \sum_{i=1}^K \sum_{k=1}^{n_i} I(x_{ikj} \leq x) \frac{\partial \mu_{ik}}{\partial \boldsymbol{\beta}}$$

$$\mathbf{I}_0 = \sum_{i=1}^K \hat{\mathbf{D}}_i' \hat{\mathbf{V}}_i^{-1} \hat{\mathbf{D}}_i$$

and Z_i , $i = 1, \dots, K$, are independent $N(0, 1)$ random variables. You replace x_{ikj} with the linear predictor $\mathbf{x}'_{ik} \hat{\boldsymbol{\beta}}$ in the preceding formulas to check the link function.

Case Deletion Diagnostic Statistics

For ordinary generalized linear models, regression diagnostic statistics developed by Williams (1987) can be requested in an output data set or in the OBSTATS table by specifying the DIAGNOSTICS | INFLUENCE option in the MODEL statement. These diagnostics measure the influence of an individual observation on model fit, and generalize the one-step diagnostics developed by Pregibon (1981) for the logistic regression model for binary data.

Preisser and Qaqish (1996) further generalized regression diagnostics to apply to models for correlated data fit by generalized estimating equations (GEEs), where the influence of entire clusters of correlated observations, or the influence of individual observations within a cluster, is measured. These diagnostic statistics can be requested in an output data set or in the OBSTATS table if a model for correlated data is specified with a REPEATED statement.

The next two sections use the following notation:

- $\hat{\boldsymbol{\beta}}$ is the maximum likelihood estimate of the regression parameters $\boldsymbol{\beta}$, or, in the case of correlated data, the solution of the GEEs.
- $\hat{\boldsymbol{\beta}}_{[i]}$ is the corresponding estimate evaluated with the i th observation deleted, or, in the case of correlated data, with the i th cluster deleted.
- p is the dimension of the regression parameter vector $\boldsymbol{\beta}$.
- r_{pi} is the standardized Pearson residual $\frac{y_i - \mu_i}{\sqrt{v_i(1-h_i)}}$, where v_i is the variance of the i th response and h_i is the leverage defined in the section “H | LEVERAGE” on page 2832.
- v_i is the variance of response i , $\text{Var}(Y_i) = \phi V(\mu_i)$, where $V(\mu)$ is the variance function and ϕ is the dispersion parameter.
- w_i is the prior weight of the i th observation specified with the WEIGHT statement. If there is no WEIGHT statement, $w_i = 1$ for all i .

All unknown quantities are replaced by their estimated values in the following two sections.

Diagnostics for Ordinary Generalized Linear Models

The following statistics are available for generalized linear models.

DFBETA

The DFBETA statistic for measuring the influence of the i th observation is defined as the one-step approximation to the difference in the MLE of the regression parameter vector and the MLE of the regression parameter vector without the i th observation. This one-step approximation assumes a Fisher scoring step, and is given by

$$\hat{\boldsymbol{\beta}} - \hat{\boldsymbol{\beta}}_{[i]} \approx \text{DFBETA}_i = (\mathbf{X}'\mathbf{W}\mathbf{X})^{-1}\mathbf{X}'_i\mathbf{W}_i^{\frac{1}{2}}(1-h_i)^{-\frac{1}{2}}r_{pi}$$

where h_i is the leverage defined in the section “H | LEVERAGE” on page 2832.

DFBETAS

The standardized DFBETA statistic for assessing the influence of the i th observation on the j th regression parameter is defined as the DFBETA statistic for the j th parameter divided by its estimated standard deviation, where the standard deviation is estimated from all the data.

$$\text{DFBETAS}_{ij} = \text{DFBETA}_{ij} / \hat{\sigma}(\beta_j)$$

DOBS / COOKD / COOKSD

In normal linear regression, the influence of observation i can be measured by Cook's distance (Cook and Weisberg 1982). A measure of influence of observation i for generalized linear models that is equivalent to Cook's distance for normal linear regression is given by

$$\text{DOBS}_i = p^{-1} h_i (1 - h_i)^{-1} r_{pi}^2$$

where h_i is the leverage defined in the section “**H | LEVERAGE**” on page 2832. This measure is the one-step approximation to $2p^{-1}[L(\hat{\boldsymbol{\beta}}) - L(\hat{\boldsymbol{\beta}}_{[i]})]$, where $L(\boldsymbol{\beta})$ is the log likelihood evaluated at $\boldsymbol{\beta}$.

H | LEVERAGE

The Fisher scores, or expected, weight for observation i is $w_{ei} = \frac{w_i}{\phi V(\mu_i)(g'(\mu_i))^2}$. Let \mathbf{W} be the diagonal matrix with w_{ei} as the i th diagonal. The leverage h_i of the i th observation is defined as the i th diagonal element of the hat matrix

$$\mathbf{H} = \mathbf{W}^{\frac{1}{2}} \mathbf{X}(\mathbf{X}'\mathbf{W}\mathbf{X})^{-1} \mathbf{X}'\mathbf{W}^{\frac{1}{2}}$$

Diagnostics for Models Fit by Generalized Estimating Equations (GEEs)

The diagnostic statistics in this section were developed by Preisser and Qaqish (1996). See the section “**Generalized Estimating Equations**” on page 2819 for further information and notation for generalized estimating equations (GEEs). The following additional notation is used in this section.

Partition the design matrix \mathbf{X} and response vector \mathbf{Y} by cluster; that is, let $\mathbf{X} = (X'_1, \dots, X'_K)'$, and $\mathbf{Y} = (Y'_1, \dots, Y'_K)'$ corresponding to the K clusters.

Let n_i be the number of responses for cluster i , and denote by $N = \sum_{i=1}^K n_i$ the total number of observations. Denote by A_i the $n_i \times n_i$ diagonal matrix with $V(\mu_{ij})$ as the j th diagonal element. If there is a WEIGHT statement, the diagonal element of A_i is $V(\mu_{ij})/w_{ij}$, where w_{ij} is the specified weight of the j th observation in the i th cluster. Let \mathbf{B} the $N \times N$ diagonal matrix with $g'(\mu_{ij})$ as diagonal elements, $i = 1, \dots, K, j = 1, \dots, n_i$. Let \mathbf{B}_i the $n_i \times n_i$ diagonal matrix corresponding to cluster i with $g'(\mu_{ij})$ as the j th diagonal element.

Let \mathbf{W} be the $N \times N$ block diagonal weight matrix whose i th block, corresponding to the i th cluster, is the $n_i \times n_i$ matrix

$$\mathbf{W}_{ei} = \mathbf{B}_i^{-1} \mathbf{A}_i^{-\frac{1}{2}} \mathbf{R}_i^{-1}(\hat{\boldsymbol{\alpha}}) \mathbf{A}_i^{-\frac{1}{2}} \mathbf{B}_i^{-1}$$

where \mathbf{R}_i is the working correlation matrix for cluster i .

Let

$$Q_i = \mathbf{X}_i (\mathbf{X}' \mathbf{W} \mathbf{X})^{-1} \mathbf{X}_i'$$

where \mathbf{X}_i is the $n_i \times p$ design matrix corresponding to cluster i .

Define the adjusted residual vector as

$$\mathbf{E} = \mathbf{B}(\mathbf{Y} - \hat{\boldsymbol{\mu}})$$

and $\mathbf{E}_i = \mathbf{B}_i(\mathbf{Y}_i - \hat{\boldsymbol{\mu}}_i)$, the estimated residual for the i th cluster.

Let the subscript $[i]$ denote estimates evaluated without the i th cluster, $[it]$ estimates evaluated using all the data except the t th observation of the i th cluster, and let $i[t]$ denote matrices corresponding to the i th cluster without the t th observation.

The following statistics are available for generalized estimating equation models.

CH / CLUSTERH / CLEVERAGE

The leverage of cluster i is contained in the matrix $\mathbf{H}_i = \mathbf{Q}_i \mathbf{W}_{ei}$, and is summarized by the trace of \mathbf{H}_i ,

$$ch_i = \text{tr}(\mathbf{H}_i)$$

The leverage h_{it} of the t th observation in the i th cluster is the t th diagonal element of \mathbf{H}_i .

DFBETAC

The effect of deleting cluster i on the estimated parameter vector is given by the following one-step approximation for $\hat{\boldsymbol{\beta}} - \hat{\boldsymbol{\beta}}_{[i]}$:

$$\text{DBETAC}_i = (\mathbf{X}' \mathbf{W} \mathbf{X})^{-1} \mathbf{X}_i' (\mathbf{W}_{ei}^{-1} - \mathbf{Q}_i)^{-1} \mathbf{E}_i$$

DFBETACS

The cluster deletion statistic DFBETAC can be standardized using the variances of $\hat{\boldsymbol{\beta}}$ based on the complete data. The standardized one-step approximation for the change in $\hat{\beta}_j$ due to deletion of cluster i is

$$\text{DBETACS}_{ij} = \frac{\text{DBETAC}_{ij}}{\hat{\phi}[(\mathbf{X}' \mathbf{W} \mathbf{X})^{-1}]_{jj}^{\frac{1}{2}}}$$

DFBETAO

Partition the matrices \mathbf{W}_{ei} and \mathbf{V}_i as

$$\mathbf{W}_{ei} = \begin{pmatrix} W_{eit} & \mathbf{W}_{eit[t]} \\ \mathbf{W}_{ei[t]t} & \mathbf{W}_{ei[t]} \end{pmatrix}$$

$$\mathbf{V}_i = \mathbf{W}_{ei}^{-1} = \begin{pmatrix} \mathbf{V}_{it} & \mathbf{V}_{it[t]} \\ \mathbf{V}_{i[t]t} & \mathbf{V}_{i[t]} \end{pmatrix}$$

and let $\mathbf{E}_{it} = \mathbf{B}_{it}(\mathbf{Y}_{it} - \hat{\boldsymbol{\mu}}_{it})$ and $\mathbf{E}_{i[t]} = \mathbf{B}_{i[t]}(\mathbf{Y}_{i[t]} - \hat{\boldsymbol{\mu}}_{i[t]})$.

The effect of deleting the t th observation from the i th cluster is given by the following one-step approximation to $\hat{\boldsymbol{\beta}} - \hat{\boldsymbol{\beta}}_{[it]}$:

$$\text{DBETAO}_{it} = (\mathbf{X}'\mathbf{W}\mathbf{X})^{-1}\tilde{\mathbf{X}}'_{it}\frac{\tilde{E}_{it}}{W_{eit}^{-1} - \tilde{Q}_{it}}$$

where $\tilde{\mathbf{X}}_{it} = \mathbf{X}_{it} - \mathbf{V}_{it[t]}\mathbf{V}_{i[t]}^{-1}\mathbf{X}_{i[t]}$, $\tilde{Q}_{it} = \tilde{\mathbf{X}}_{it}(\mathbf{X}'\mathbf{W}\mathbf{X})^{-1}\tilde{\mathbf{X}}'_{it}$, and $\tilde{E}_{it} = \mathbf{E}_{it} - \mathbf{V}_{it[t]}\mathbf{V}_{i[t]}^{-1}\mathbf{E}_{i[t]}$. Note that W_{eit} , \tilde{Q}_{it} , and \tilde{E}_{it} are scalars.

DFBETAOS

The observation deletion statistic DFBETAO can be standardized using the variances of $\hat{\boldsymbol{\beta}}$ based on the complete data. The standardized one-step approximation for the change in $\hat{\beta}_j$ due to deletion of observation t in cluster i is

$$\text{DBETAOS}_{itj} = \frac{\text{DBETAO}_{itj}}{\hat{\phi}[(\mathbf{X}'\mathbf{W}\mathbf{X})^{-1}]_{jj}^{1/2}}$$

DCLS | CLUSTERCOOKD | CLUSTERCOOKSD

A measure of the standardized influence of the subset m of observations on the overall fit is $(\hat{\boldsymbol{\beta}} - \hat{\boldsymbol{\beta}}_{[m]})'(\mathbf{X}'\mathbf{W}\mathbf{X})(\hat{\boldsymbol{\beta}} - \hat{\boldsymbol{\beta}}_{[m]})/p\hat{\phi}$. For deletion of cluster i , this is approximated by

$$\text{DCLS}_i = \mathbf{E}'_i(\mathbf{W}_{ei}^{-1} - \mathbf{Q}_i)^{-1}\mathbf{Q}_i(\mathbf{W}_{ei}^{-1} - \mathbf{Q}_i)^{-1}\mathbf{E}_i/p\hat{\phi}$$

DOBS | COOKD | COOKSD

The measure of overall fit in the section “DCLS | CLUSTERCOOKD | CLUSTERCOOKSD” on page 2834 for the deletion of the t th observation in the i th cluster is approximated by

$$\text{DOBS}_{it} = \frac{\tilde{E}_{it}^2\tilde{Q}_{it}}{p\hat{\phi}(W_{eit}^{-1} - \tilde{Q}_{it})^2}$$

where \tilde{E}_{it} , \tilde{Q}_{it} , and W_{eit} are defined in the section “DFBETAO” on page 2833. In the case of the independence working correlation, this is equal to the measure for ordinary generalized linear models defined in the section “DOBS | COOKD | COOKSD” on page 2832.

MCLS | CLUSTERDFIT

A studentized distance measure of the type defined in the section “DCLS | CLUSTERCOOKD | CLUSTERCOOKSD” on page 2834 of the influence of the i th cluster is given by

$$\text{MCLS}_i = \mathbf{E}'_i(\mathbf{W}_{ei}^{-1} - \mathbf{Q}_i)^{-1}\mathbf{H}_i\mathbf{E}_i/p\hat{\phi}$$

Bayesian Analysis

In generalized linear models, the response has a probability distribution from a family of distributions of the exponential form. That is, the probability density of the response Y for continuous response variables, or the probability function for discrete responses, can be expressed as

$$f(y) = \exp\left\{\frac{y\theta - b(\theta)}{a(\phi)} + c(y, \phi)\right\}$$

for some functions a , b , and c that determine the specific distribution. The canonical parameters θ depend only on the means of the response μ_i , which are related to the regression parameters β through the link function $g(\mu_i) = x'\beta$. The additional parameter ϕ is the dispersion parameter. The GENMOD procedure estimates the regression parameters and the scale parameter $\sigma = \phi^{\frac{1}{2}}$ by maximum likelihood. However, the GENMOD procedure can also provide Bayesian estimates of the regression parameters and either the scale σ , the dispersion ϕ , or the precision $\tau = \phi^{-1}$ by sampling from the posterior distribution. Except where noted, the following discussion applies to either σ , ϕ , or τ , although ϕ is used to illustrate the formulas. Note that the Poisson and binomial distributions do not have a dispersion parameter, and the dispersion is considered to be fixed at $\phi = 1$. The ASSESS, CONTRAST, ESTIMATE, OUTPUT, and REPEATED statements, if specified, are ignored. Also ignored are the PLOTS= option in the PROC GENMOD statement and the following options in the MODEL statement: ALPHA=, CORRB, COVB, TYPE1, TYPE3, SCALE=DEVIANC (DSCALE), SCALE=PEARSON (PSCALE), OBSTATS, RESIDUALS, XVAR, PREDICTED, DIAGNOSTICS, and SCALE= for Poisson and binomial distributions. The multinomial and zero-inflated Poisson distributions are not available for Bayesian analysis.

See the section “Assessing Markov Chain Convergence” on page 139 for information about assessing the convergence of the chain of posterior samples.

Several algorithms, specified with the SAMPLING= option in the BAYES statement, are available in GENMOD for drawing samples from the posterior distribution.

ARMS Algorithm for Gibbs Sampling

This section provides details for Bayesian analysis by Gibbs sampling in generalized linear models. See the section “Gibbs Sampler” on page 135 for a general discussion of Gibbs sampling. See Gilks, Richardson, and Spiegelhalter (1996) for a discussion of applications of Gibbs sampling to a number of different models, including generalized linear models.

Let $\theta = (\theta_1, \dots, \theta_k)'$ be the parameter vector. For generalized linear models, the θ_i s are the regression coefficients β_i s and the dispersion parameter ϕ . Let $L(D|\theta)$ be the likelihood function, where D is the observed data. Let $\pi(\theta)$ be the prior distribution. The full conditional distribution of $[\theta_i|\theta_j, i \neq j]$ is proportional to the joint distribution; that is,

$$\pi(\theta_i|\theta_j, i \neq j, D) \propto L(D|\theta)p(\theta)$$

For instance, the one-dimensional conditional distribution of θ_1 given $\theta_j = \theta_j^*, 2 \leq j \leq k$, is computed as

$$\pi(\theta_1|\theta_j = \theta_j^*, 2 \leq j \leq k, D) = L(D|(\theta = (\theta_1, \theta_2^*, \dots, \theta_k^*)'))p(\theta = (\theta_1, \theta_2^*, \dots, \theta_k^*)')$$

Suppose you have a set of arbitrary starting values $\{\theta_1^{(0)}, \dots, \theta_k^{(0)}\}$. Using the ARMS (adaptive rejection Metropolis sampling) algorithm (Gilks and Wild 1992; Gilks, Best, and Tan 1995), you can do the following:

```
draw  $\theta_1^{(1)}$  from  $[\theta_1|\theta_2^{(0)}, \dots, \theta_k^{(0)}]$ 
draw  $\theta_2^{(1)}$  from  $[\theta_2|\theta_1^{(1)}, \theta_3^{(0)}, \dots, \theta_k^{(0)}]$ 
...
draw  $\theta_k^{(1)}$  from  $[\theta_k|\theta_1^{(1)}, \dots, \theta_{k-1}^{(1)}]$ 
```

This completes one iteration of the Gibbs sampler. After one iteration, you have $\{\theta_1^{(1)}, \dots, \theta_k^{(1)}\}$. After n iterations, you have $\{\theta_1^{(n)}, \dots, \theta_k^{(n)}\}$. PROC GENMOD implements the ARMS algorithm provided by Gilks (2003) to draw a sample from a full conditional distribution. See the section “[Adaptive Rejection Sampling Algorithm](#)” on page 136 for more information about the ARMS algorithm. The ARMS algorithm is the default method used to sample from the posterior distribution, except in the case of a normal distribution with a conjugate prior, in which case a closed form is available for the posterior distribution. See any of the introductory references in Chapter 7, “[Introduction to Bayesian Analysis Procedures](#),” for a discussion of conjugate prior distributions for a linear model with the normal distribution.

Gamerman Algorithm

The Gamerman algorithm, unlike a Gibbs sampling algorithm, samples parameters from their multivariate posterior conditional distribution. The algorithm uses the structure of generalized linear models to efficiently sample from the posterior distribution of the model parameters. For a detailed description and explanation of the algorithm, see Gamerman (1997) and the section “[Gamerman Algorithm](#)” on page 138.

Independence Metropolis Algorithm

The independence Metropolis algorithm is another sampling algorithm that draws multivariate samples from the posterior distribution. See the section “[Independence Sampler](#)” on page 137 for more details.

Posterior Samples Output Data Set

You can output posterior samples into a SAS data set through ODS. The following SAS statement outputs the posterior samples into the SAS data set Post:

```
ODS OUTPUT POSTERIORSAMPLE=Post
```

You can alternatively create the SAS data set Post with the **OUTPOST=Post** option in the **BAYES** statement.

The data set also includes the variables LogPost and LogLike, which represent the log of the posterior likelihood and the log of the likelihood, respectively.

Priors for Model Parameters

The model parameters are the regression coefficients and the dispersion parameter (or the precision or scale), if the model has one. The priors for the dispersion parameter and the priors for the regression coefficients are assumed to be independent, while you can have a joint multivariate normal prior for the regression coefficients.

Dispersion, Precision, or Scale Parameter

Gamma Prior The gamma distribution $G(a, b)$ has a probability density function

$$f(u) = \frac{b(bu)^{a-1}e^{-bu}}{\Gamma(a)}, \quad u > 0$$

where a is the shape parameter and b is the inverse-scale parameter. The mean is $\frac{a}{b}$ and the variance is $\frac{a}{b^2}$.

Improper Prior The joint prior density is given by

$$p(u) \propto u^{-1}, \quad u > 0$$

Inverse Gamma Prior The inverse gamma distribution $IG(a, b)$ has a probability density function

$$f(u) = \frac{b^a}{\Gamma(a)} u^{-(a+1)} e^{-b/u}, \quad u > 0$$

where a is the shape parameter and b is the scale parameter. The mean is $\frac{b}{a-1}$ if $a > 1$, and the variance is $\frac{b^2}{(a-1)^2(a-2)}$ if $a > 2$.

Regression Coefficients

Let $\boldsymbol{\beta}$ be the regression coefficients.

Jeffreys' Prior The joint prior density is given by

$$p(\boldsymbol{\beta}) \propto |\mathbf{I}(\boldsymbol{\beta})|^{-\frac{1}{2}}$$

where $\mathbf{I}(\boldsymbol{\beta})$ is the Fisher information matrix for the model. If the underlying model has a scale parameter (for example, a normal linear regression model), then the Fisher information matrix is computed with the scale parameter set to a fixed value of one.

If you specify the CONDITIONAL option, then Jeffreys' prior, conditional on the current Markov chain value of the generalized linear model precision parameter τ , is given by

$$|\tau \mathbf{I}(\boldsymbol{\beta})|^{-\frac{1}{2}}$$

where τ is the model precision parameter.

See Ibrahim and Laud (1991) for a full discussion, with examples, of Jeffreys' prior for generalized linear models.

Normal Prior Assume $\boldsymbol{\beta}$ has a multivariate normal prior with mean vector $\boldsymbol{\beta}_0$ and covariance matrix $\boldsymbol{\Sigma}_0$. The joint prior density is given by

$$p(\boldsymbol{\beta}) \propto e^{-\frac{1}{2}(\boldsymbol{\beta}-\boldsymbol{\beta}_0)' \boldsymbol{\Sigma}_0^{-1}(\boldsymbol{\beta}-\boldsymbol{\beta}_0)}$$

If you specify the CONDITIONAL option, then, conditional on the current Markov chain value of the generalized linear model precision parameter τ , the joint prior density is given by

$$p(\boldsymbol{\beta}) \propto e^{-\frac{1}{2}(\boldsymbol{\beta}-\boldsymbol{\beta}_0)' \tau \boldsymbol{\Sigma}_0^{-1}(\boldsymbol{\beta}-\boldsymbol{\beta}_0)}$$

Uniform Prior The joint prior density is given by

$$p(\boldsymbol{\beta}) \propto 1$$

Deviance Information Criterion

Let θ_i be the model parameters at iteration i of the Gibbs sampler and let $LL(\theta_i)$ be the corresponding model log likelihood. PROC GENMOD computes the following fit statistics defined by Spiegelhalter et al. (2002):

- Effective number of parameters:

$$p_D = \overline{\text{LL}(\theta)} - \text{LL}(\bar{\theta})$$

- Deviance information criterion (DIC):

$$\text{DIC} = \overline{\text{LL}(\theta)} + p_D$$

where

$$\overline{\text{LL}(\theta)} = \frac{1}{n} \sum_{i=1}^n \text{LL}(\theta_i)$$

$$\bar{\theta} = \frac{1}{n} \sum_{i=1}^n \theta_i$$

PROC GENMOD uses the full log likelihoods defined in the section “Log-Likelihood Functions” on page 2802, with all terms included, for computing the DIC.

Posterior Distribution

Denote the observed data by D .

The posterior distribution is

$$\pi(\boldsymbol{\beta}|D) \propto L_P(D|\boldsymbol{\beta})p(\boldsymbol{\beta})$$

where $L_P(D|\boldsymbol{\beta})$ is the likelihood function with regression coefficients $\boldsymbol{\beta}$ as parameters.

Starting Values of the Markov Chains

When the BAYES statement is specified, PROC GENMOD generates one Markov chain containing the approximate posterior samples of the model parameters. Additional chains are produced when the Gelman-Rubin diagnostics are requested. Starting values (or initial values) can be specified in the INITIAL= data set in the BAYES statement. If INITIAL= option is not specified, PROC GENMOD picks its own initial values for the chains.

Denote $[x]$ as the integral value of x . Denote $\hat{s}(X)$ as the estimated standard error of the estimator X .

Regression Coefficients

For the first chain that the summary statistics and regression diagnostics are based on, the default initial values are estimates of the mode of the posterior distribution. If the INITIALMLE option is specified, the initial values are the maximum likelihood estimates; that is,

$$\beta_i^{(0)} = \hat{\beta}_i$$

Initial values for the r th chain ($r \geq 2$) are given by

$$\beta_i^{(0)} = \hat{\beta}_i \pm \left(2 + \left\lceil \frac{r}{2} \right\rceil\right) \hat{s}(\hat{\beta}_i)$$

with the plus sign for odd r and minus sign for even r .

Dispersion, Scale, or Precision Parameter λ

Let λ be the generalized linear model parameter you choose to sample, either the dispersion, scale, or precision parameter. Note that the Poisson and binomial distributions do not have this additional parameter.

For the first chain that the summary statistics and regression diagnostics are based on, the default initial values are estimates of the mode of the posterior distribution. If the INITIALMLE option is specified, the initial values are the maximum likelihood estimates; that is,

$$\lambda^{(0)} = \hat{\lambda}$$

The initial values of the r th chain ($r \geq 2$) are given by

$$\lambda^{(0)} = \hat{\lambda} e^{\pm \left(\left[\frac{r}{2} \right] + 2 \right) \hat{s}(\hat{\lambda})}$$

with the plus sign for odd r and minus sign for even r .

OUTPOST= Output Data Set

The OUTPOST= data set contains the generated posterior samples. There are $3+n$ variables, where n is the number of model parameters. The variable Iteration represents the iteration number, the variable LogLike contains the log of the likelihood, and the variable LogPost contains the log of the posterior. The other n variables represent the draws of the Markov chain for the model parameters.

Exact Logistic and Exact Poisson Regression

The theory of exact logistic regression, also called exact conditional logistic regression, is described in the section “Exact Conditional Logistic Regression” on page 4274 of Chapter 54, “The LOGISTIC Procedure.” The following discussion of exact Poisson regression, also called exact conditional Poisson regression, uses the notation given in that section.

Note that in exact logistic regression, the coefficients $C(\mathbf{t})$ are the number of possible response vectors \mathbf{y} that generate \mathbf{t} : $C(\mathbf{t}) = ||\{\mathbf{y} : \mathbf{y}'\mathbf{X} = \mathbf{t}'\}||$. However, when performing an exact Poisson regression, this value is replaced by

$$C(\mathbf{t}) = \sum_{\Omega} \prod_{i=1}^n \frac{N_i^{y_i}}{y_i!}$$

where $\Omega = \{\mathbf{y} : \mathbf{y}'\mathbf{X} = \mathbf{t}'\}$ and $N_i = \exp(o_i)$ is the exponential of the offset o_i for observation i . If an offset variable is not specified, then $N_i = 1$.

The probability density function (PDF) for \mathbf{T} is created by summing over all candidate sequences \mathbf{y} that generate an observable \mathbf{t}

$$\Pr(\mathbf{T} = \mathbf{t}) = \frac{C(\mathbf{t}) \exp(\mathbf{t}'\boldsymbol{\beta})}{\prod_{i=1}^n \exp(N_i e^{\mathbf{x}'_i \boldsymbol{\beta}})}$$

However, the conditional likelihood of \mathbf{T}_I given $\mathbf{T}_N = \mathbf{t}_N$ has the same form as that for exact logistic regression.

For details about hypothesis testing and estimation, see the sections “Hypothesis Tests” on page 4276 and “Inference for a Single Parameter” on page 4277 of Chapter 54, “The LOGISTIC Procedure.” See the section “Computational Resources for Exact Logistic Regression” on page 4284 of Chapter 54, “The LOGISTIC Procedure,” for some computational notes about exact analyses.

In exact logistic binary regression, each component $y_i, i = 1, \dots, n$, of \mathbf{y} can take a value of 0 or 1, so there are a finite number, 2^n , of candidate \mathbf{y} vectors to be considered. Since a Poisson-distributed response variable can take an infinite number of values, exact Poisson regression should evaluate an infinite number of \mathbf{y} vectors. However, by identifying the maximum value of y_i to check, S_i , for each observation i , the number of candidate \mathbf{y} vectors to check is reduced to $\prod_{i=1}^n S_i$. On a practical level, as S_i becomes large the probability of the Poisson random variable achieving this value drops to zero, so S_i can be thought of as the point at which the value does not matter. You can provide these maxima by specifying either an **OFFSET=** variable, o_i , or an **EXACTMAX=** variable, e_i , or you can let the algorithm choose a maximum for you. The way these two options interact to provide a maximum is described in the following list:

1. If an **EXACTMAX=** variable is specified, then $S_i = e_i$.
2. If the **EXACTMAX** option is specified without a variable, or if neither the **EXACTMAX=** nor **OFFSET=** options are specified, then you must also condition out the intercept or you must specify the **STRATA** statement. If you are conditioning out the intercept, then every S_i has an effective maximum of $\sum_{i=1}^n f_i y_{0i}$, where y_0 is the observed response and f_i is the frequency of the observation; this is the sufficient statistic for the intercept term. If you are performing a stratified analysis, these sums are computed within each stratum.
3. If an **offset** variable is specified and the **EXACTMAX** option is not specified (you are modeling proportions), then $N_i = \exp(o_i)$ must be a positive integer, and $S_i = N_i$ is the maximum possible value for each observation in the experiment; for example, if you are counting the number of rats in a cage that acquire a disease, then N_i is the number of rats in cage i .

OUTDIST= Output Data Set

The **OUTDIST=** data set contains every exact conditional distribution necessary to process the corresponding **EXACT** statement. For example, the following statements create one distribution for the **x1** parameter and another for the **x2** parameters, and produce the data set **dist** shown in Table 40.11:

```
data test;
  input y x1 x2 count;
  datalines;
0 0 0 1
1 0 0 1
0 1 1 2
1 1 1 1
1 0 2 3
1 1 2 1
1 2 0 3
1 2 1 2
1 2 2 1
;
```

```

proc genmod data=test exactonly;
  class x2 / param=ref;
  model y=x1 x2 / d=b;
  exact x1 x2/ outdist=dist;
run;
proc print data=dist;
run;

```

Table 40.11 OUTDIST= Data Set

Obs	x1	x20	x21	Count	Score	Prob
1	.	0	0	3	5.81151	0.03333
2	.	0	1	15	1.66031	0.16667
3	.	0	2	9	3.12728	0.10000
4	.	1	0	15	1.46523	0.16667
5	.	1	1	18	0.21675	0.20000
6	.	1	2	6	4.58644	0.06667
7	.	2	0	19	1.61869	0.21111
8	.	2	1	2	3.27293	0.02222
9	.	3	0	3	6.27189	0.03333
10	2	.	.	6	3.03030	0.12000
11	3	.	.	12	0.75758	0.24000
12	4	.	.	11	0.00000	0.22000
13	5	.	.	18	0.75758	0.36000
14	6	.	.	3	3.03030	0.06000

The first nine observations in the `dist` data set contain an exact distribution for the parameters of the `x2` effect (hence the values for the `x1` parameter are missing), and the remaining five observations are for the `x1` parameter. If a joint distribution was created, there would be observations with values for both the `x1` and `x2` parameters. For **CLASS** variables, the corresponding parameters in the `dist` data set are identified by concatenating the variable name with the appropriate classification level.

The data set contains the possible sufficient statistics of the parameters for the effects specified in the **EXACT** statement, and the `Count` variable contains the number of different responses that yield these statistics. In particular, there are six possible response vectors y for which the dot product $y'x_1$ was equal to 2, and for which $y'x_{20}$, $y'x_{21}$, and $y'1$ were equal to their actual observed values (displayed in the “Sufficient Statistics” table).

NOTE: If you are performing an exact Poisson analysis, then the `Count` variable is replaced by a variable named `Weight`.

When hypothesis tests are performed on the parameters, the `Prob` variable contains the probability of obtaining that statistic (which is just the count divided by the total count), and the `Score` variable contains the score for that statistic.

The `OUTDIST=` data set can contain a different exact conditional distribution for each specified **EXACT** statement. For example, consider the following **EXACT** statements:

```

exact 'O1'   x1   /                   outdist=o1;
exact 'OJ12' x1 x2 / jointonly outdist=oj12;
exact 'OA12' x1 x2 / joint      outdist=oa12;
exact 'OE12' x1 x2 / estimate  outdist=oe12;

```

The O1 statement outputs a single exact conditional distribution. The OJ12 statement outputs only the joint distribution for x1 and x2. The OA12 statement outputs three conditional distributions: one for x1, one for x2, and one jointly for x1 and x2. The OE12 statement outputs two conditional distributions: one for x1 and the other for x2. Data set oe12 contains both the x1 and x2 variables; the distribution for x1 has missing values in the x2 column while the distribution for x2 has missing values in the x1 column.

Missing Values

For generalized linear models, PROC GENMOD ignores any observation with a missing value for any variable involved in the model. You can score an observation in an output data set by setting only the response value to missing. For models fit with generalized estimating equations (GEEs), observations with missing values within a cluster are not used, and all available pairs are used in estimating the working correlation matrix. Clusters with fewer observations than the full cluster size are treated as having missing observations occurring at the end of the cluster. You can specify the order of missing observations with the `WITHINSUBJECT=` option. See the section “Missing Data” on page 2821 for more information about missing values in GEEs.

Displayed Output for Classical Analysis

The following output is produced by the GENMOD procedure. Note that some of the tables are optional and appear only in conjunction with the REPEATED statement and its options or with options in the MODEL statement. For details, see the section “ODS Table Names” on page 2852.

Model Information

The “Model Information” table displays the two-level data set name, the response distribution, the link function, the response variable name, the offset variable name, the frequency variable name, the scale weight variable name, the number of observations used, the number of events if events/trials format is used for response, the number of trials if events/trials format is used for response, the sum of frequency weights, the number of missing values in data set, and the number of invalid observations (for example, negative or 0 response values with gamma distribution or number of observations with events greater than trials with binomial distribution).

Class Level Information

If you use classification variables in the model, PROC GENMOD displays the levels of classification variables specified in the CLASS statement and in the MODEL statement. The levels are displayed in the same sorted order used to generate columns in the design matrix.

Response Profile

If you specify an ordinal model for the multinomial distribution, a table titled “Response Profile” is displayed containing the ordered values of the response variable and the number of occurrences of the values used in the model.

Iteration History for Parameter Estimates

If you specify the ITPRINT model option, PROC GENMOD displays a table containing the following for each iteration in the Newton-Raphson procedure for model fitting: the iteration number, the ridge value, the log likelihood, and values of all parameters in the model.

Criteria for Assessing Goodness of Fit

In the “Criteria for Assessing Goodness of Fit” table, PROC GENMOD displays the degrees of freedom for deviance and Pearson’s chi-square, equal to the number of observations minus the number of regression parameters estimated, the deviance, the deviance divided by degrees of freedom, the scaled deviance, the scaled deviance divided by degrees of freedom, Pearson’s chi-square, Pearson’s chi-square divided by degrees of freedom, the scaled Pearson’s chi-square, the scaled Pearson’s chi-square divided by degrees of freedom, the log likelihood (excludes factorial terms) the full log likelihood, the Akaike information criterion, the corrected Akaike information criterion, and the Bayesian information criterion. The information in this table is valid only for maximum likelihood model fitting, and the table is not printed if the REPEATED statement is specified.

Last Evaluation of the Gradient

If you specify the model option ITPRINT, the GENMOD procedure displays the last evaluation of the gradient vector.

Last Evaluation of the Hessian

If you specify the model option ITPRINT, the GENMOD procedure displays the last evaluation of the Hessian matrix.

Analysis of (Initial) Parameter Estimates

The “Analysis of (Initial) Parameter Estimates” table contains the results from fitting a generalized linear model to the data. If you specify the REPEATED statement, these GLM parameter estimates are used as initial values for the GEE solution, and are displayed only if the PRINTMLE option in the REPEATED statement is specified. For each parameter in the model, PROC GENMOD displays the parameter name, as follows:

- the variable name for continuous regression variables
- the variable name and level for classification variables and interactions involving classification variables
- SCALE for the scale variable related to the dispersion parameter

In addition, PROC GENMOD displays the degrees of freedom for the parameter, the estimate value, the standard error, the Wald chi-square value, the p -value based on the chi-square distribution, and the confidence limits (Wald or profile likelihood) for parameters.

Lagrange Multiplier Statistics

If you specify that either the model intercept or the scale parameter is fixed, for those distributions that have a distribution scale parameter, the GENMOD procedure displays a table of Lagrange multiplier, or score, statistics for testing the validity of the constrained parameter that contains the test statistic, and the p -value.

Estimated Covariance Matrix

If you specify the model option COVB, the GENMOD procedure displays the estimated covariance matrix, defined as the inverse of the information matrix at the final iteration. This is based on the expected information matrix if the EXPECTED option is specified in the MODEL statement. Otherwise, it is based on the Hessian matrix used at the final iteration. This is, by default, the observed Hessian unless altered by the SCORING option in the MODEL statement.

Estimated Correlation Matrix

If you specify the CORRB model option, PROC GENMOD displays the estimated correlation matrix. This is based on the expected information matrix if the EXPECTED option is specified in the MODEL statement. Otherwise, it is based on the Hessian matrix used at the final iteration. This is, by default, the observed Hessian unless altered by the SCORING option in the MODEL statement.

Iteration History for LR Confidence Intervals

If you specify the ITPRINT and LRCI model options, PROC GENMOD displays an iteration history table for profile likelihood-based confidence intervals. For each parameter in the model, PROC GENMOD displays the parameter identification number, the iteration number, the log-likelihood value, parameter values.

Likelihood Ratio-Based Confidence Intervals for Parameters

If you specify the LRCI and the ITPRINT options in the MODEL statement, a table is displayed that summarizes profile likelihood-based confidence intervals for all parameters. For each parameter in the model, the table displays the confidence coefficient, the parameter identification number, lower and upper endpoints of confidence intervals for the parameter, and values of all other parameters at the solution.

LR Statistics for Type 1 Analysis

If you specify the TYPE1 model option, a table is displayed that contains the name of the effect, the deviance for the model including the effect and all previous effects, the degrees of freedom for the effect, the likelihood ratio statistic for testing the significance of the effect, and the p -value computed from the chi-square distribution with the effect's degrees of freedom.

If you specify either the SCALE=DEVIANCE or SCALE=PEARSON option in the MODEL statement, columns are displayed that contain the name of the effect, the deviance for the model including the effect and all previous effects, the numerator degrees of freedom, the denominator degrees of freedom, the chi-square statistic for testing the significance of the effect, the p -value computed from the chi-square distribution with

numerator degrees of freedom, the F statistic for testing the significance of the effect, and the p -value based on the F distribution.

Iteration History for Type 3 Contrasts

If you specify the model options `ITPRINT` and `TYPE3`, an iteration history table is displayed for fitting the model with Type 3 contrast constraints for each effect that contains the effect name, the iteration number, the ridge value, the log likelihood, and values of all parameters.

LR Statistics for Type 3 Analysis

If you specify the `TYPE3` model option, a table is displayed that contains, for each effect in the model, the name of the effect, the likelihood ratio statistic for testing the significance of the effect, the degrees of freedom for the effect, and the p -value computed from the chi-square distribution.

If you specify either the `SCALE=DEVIANCE` or `SCALE=PEARSON` option in the `MODEL` statement, columns are displayed that contain the name of the effect, the likelihood ratio statistic for testing the significance of the effect, the F statistic for testing the significance of the effect, the numerator degrees of freedom, the denominator degrees of freedom, the p -value based on the F distribution, and the p -value computed from the chi-square distribution with the numerator's degrees of freedom.

Wald Statistics for Type 3 Analysis

If you specify the `TYPE3` and `WALD` model options, a table is displayed that contains the name of the effect, the degrees of freedom of the effect, the Wald statistic for testing the significance of the effect, and the p -value computed from the chi-square distribution.

Parameter Information

If you specify the `ITPRINT`, `COVB`, `CORRB`, `WALDCI`, or `LRCI` option in the `MODEL` statement, or if you specify a `CONTRAST` statement, a table is displayed that identifies parameters with numbers, rather than names, for use in tables and matrices where a compact identifier for parameters is helpful. For each parameter, the table contains an index number that identifies the parameter, and the parameter name, including level information for effects containing classification variables.

Observation Statistics

If you specify the `OBSTATS` option in the `MODEL` statement, `PROC GENMOD` displays a table containing miscellaneous statistics. Residuals and case deletion diagnostic statistics are not available for the multinomial distribution. Case deletion diagnostics are not available for zero-inflated models.

For each observation in the input data set, the following are displayed:

- the value of the response variable
- the predicted value of the mean
- the value of the linear predictor The value of an `OFFSET` variable is added to the linear predictor.
- the estimated standard error of the linear predictor

- the value of the negative of the weight in the Hessian matrix at the final iteration. This is the expected weight if the EXPECTED option is specified in the MODEL statement. Otherwise, it is the weight used in the final iteration. That is, it is the observed weight unless the SCORING= option has been specified.
- approximate lower and upper endpoints for a confidence interval for the predicted value of the mean
- raw residual
- Pearson residual
- deviance residual
- standardized Pearson residual
- standardized deviance residual
- likelihood residual
- leverage
- Cook's distance statistic
- DFBETA statistic, for each parameter
- standardized DFBETA statistic, for each parameter
- zero-inflation probability for zero-inflated models
- response mean for zero-inflated models

ESTIMATE Statement Results

If you specify a REPEATED statement, the ESTIMATE statement results apply to the specified GEE model. Otherwise, they apply to the specified generalized linear model.

For each ESTIMATE statement, the table contains the contrast label, the estimated value of the contrast, the standard error of the estimate, the significance level α , $(1 - \alpha) \times 100\%$ confidence intervals for contrast, the Wald chi-square statistic for the contrast, and the p -value computed from the chi-square distribution. The mean of the contrast, defined as the inverse link function applied to the contrast, and $(1 - \alpha) \times 100\%$ confidence intervals for the mean are also displayed.

If you specify the EXP option, an additional row is displayed with statistics for the exponentiated value of the contrast.

CONTRAST Coefficients

If you specify the CONTRAST or ESTIMATE statement and you specify the E option, a table titled "Coefficients For Contrast *label*" is displayed, where *label* is the label specified in the CONTRAST statement. The table contains the contrast label, and the rows of the contrast matrix.

Iteration History for Contrasts

If you specify the ITPRINT option, an iteration history table is displayed for fitting the model with contrast constraints for each effect. The table contains the contrast label, the iteration number, the ridge value, the log likelihood, and values of all parameters.

CONTRAST Statement Results

If you specify a REPEATED statement, the CONTRAST statement results apply to the specified GEE model. Otherwise, they apply to the specified generalized linear model.

A table is displayed that contains the contrast label, the degrees of freedom for the contrast, and the likelihood ratio, score, or Wald statistic for testing the significance of the contrast. Score statistics are used in GEE models, likelihood ratio statistics are used in generalized linear models, and Wald statistics are used in both. Also displayed are the p -value computed from the chi-square distribution, and the type of statistic computed for this contrast: Wald, LR, or score.

If you specify either the SCALE=DEVIANCE or SCALE=PEARSON option for generalized linear models, columns are displayed that contain the contrast label, the likelihood ratio statistic for testing the significance of the contrast, the F statistic for testing the significance of the contrast, the numerator degrees of freedom, the denominator degrees of freedom, the p -value based on the F distribution, and the p -value computed from the chi-square distribution with numerator degrees of freedom.

LSMEANS Coefficients

If you specify the LSMEANS statement and you specify the E option, the “Coefficients for *effect* Least Squares Means” table is displayed, where *effect* is the effect specified in the LSMEANS statement. The table contains the effect names and the rows of least squares means coefficients.

Least Squares Means

If you specify the LSMEANS statement, the “Least Squares Means” table is displayed. The table contains for each effect the following: the effect name, and for each level of each effect the following:

- the least squares mean estimate
- standard error
- chi-square value
- p -value computed from the chi-square distribution

If you specify the DIFF option, a table titled “Differences of Least Squares Means” is displayed containing corresponding statistics for the differences between the least squares means for the levels of each effect.

GEE Model Information

If you specify the REPEATED statement, the “GEE Model Information” table displays the correlation structure of the working correlation matrix or the log odds ratio structure, the within-subject effect, the subject effect, the number of clusters, the correlation matrix dimension, and the minimum and maximum cluster size.

Log Odds Ratio Parameter Information

If you specify the REPEATED statement and specify a log odds ratio model for binary data with the LOGOR= option, then the “Log Odds Ratio Parameter Information” table is displayed showing the correspondence between data pairs and log odds ratio model parameters.

Iteration History for GEE Parameter Estimates

If you specify the REPEATED statement and the MODEL statement option ITPRINT, the “Iteration History For GEE Parameter Estimates” table is displayed. The table contains the parameter identification number, the iteration number, and values of all parameters.

Last Evaluation of the Generalized Gradient and Hessian

If you specify the REPEATED statement and select ITPRINT as a model option, PROC GENMOD displays the “Last Evaluation Of The Generalized Gradient And Hessian” table.

GEE Parameter Estimate Covariance Matrices

If you specify the REPEATED statement and the COVB option, PROC GENMOD displays the “Covariance Matrix (Model-Based)” and “Covariance Matrix (Empirical)” tables.

GEE Parameter Estimate Correlation Matrices

If you specify the REPEATED statement and the CORRB option, PROC GENMOD displays the “Correlation Matrix (Model-Based)” and “Correlation Matrix (Empirical)” tables.

GEE Working Correlation Matrix

If you specify the REPEATED statement and the CORRW option, PROC GENMOD displays the “Working Correlation Matrix” table.

GEE Fit Criteria

If you specify the REPEATED statement, PROC GENMOD displays the quasi-likelihood information criteria for model fit QIC and QIC_u in the “GEE Fit Criteria” table.

Analysis of GEE Parameter Estimates

If you specify the REPEATED statement, PROC GENMOD uses empirical standard error estimates to compute and display the “Analysis Of GEE Parameter Estimates Empirical Standard Error Estimates” table that contains the parameter names as follows:

- the variable name for continuous regression variables
- the variable name and level for classification variables and interactions involving classification variables
- “Scale” for the scale variable related to the dispersion parameter

In addition, the parameter estimate, the empirical standard error, a 95% confidence interval, and the Z score and p -value are displayed for each parameter.

If you specify the MODELSE option in the REPEATED statement, the “Analysis Of GEE Parameter Estimates Model-Based Standard Error Estimates” table based on model-based standard errors is also produced.

GEE Observation Statistics

If you specify the OBSTATS option in the REPEATED statement, PROC GENMOD displays a table containing miscellaneous statistics. For each observation in the input data set, the following are displayed:

- the value of the response variable and all other variables in the model, denoted by the variable names
- the predicted value of the mean
- the value of the linear predictor
- the standard error of the linear predictor
- confidence limits for the predicted values
- raw residual
- Pearson residual
- cluster number
- leverage
- cluster leverage
- cluster Cook’s distance statistic
- studentized cluster Cook’s distance statistic
- individual observation Cook’s distance statistic
- cluster DFBETA statistic for each parameter
- cluster standardized DFBETA statistic for each parameter
- individual observation DFBETA statistic for each parameter
- individual observation standardized DFBETA statistic for each parameter

Displayed Output for Bayesian Analysis

If a Bayesian analysis is requested with a BAYES statement, the displayed output includes the following.

Model Information

The “Model Information” table displays the two-level data set name, the number of burn-in iterations, the number of iterations after the burn-in, the number of thinning iterations, the response distribution, the link function, the response variable name, the offset variable name, the frequency variable name, the scale weight variable name, the number of observations used, the number of events if events/trials format is used for response, the number of trials if events/trials format is used for response, the sum of frequency weights, the number of missing values in data set, and the number of invalid observations (for example, negative or 0 response values with gamma distribution or number of observations with events greater than trials with binomial distribution).

Class Level Information

The “Class Level Information” table displays the levels of classification variables if you specify a CLASS statement.

Maximum Likelihood Estimates

The “Analysis of Maximum Likelihood Parameter Estimates” table displays the maximum likelihood estimate of each parameter, the estimated standard error of the parameter estimator, and confidence limits for each parameter.

Coefficient Prior

The “Coefficient Prior” table displays the prior distribution of the regression coefficients.

Independent Prior Distributions for Model Parameters

The “Independent Prior Distributions for Model Parameters” table displays the prior distributions of additional model parameters (scale, exponential scale, Weibull scale, Weibull shape, gamma shape).

Initial Values and Seeds

The “Initial Values and Seeds” table displays the initial values and random number generator seeds for the Gibbs chains.

Fit Statistics

The “Fit Statistics” table displays the deviance information criterion (DIC) and the effective number of parameters.

Descriptive Statistics of the Posterior Samples

The “Descriptive Statistics of the Posterior Sample” table contains the size of the sample, the mean, the standard deviation, and the quartiles for each model parameter.

Interval Estimates for Posterior Sample

The “Interval Estimates for Posterior Sample” table contains the HPD intervals and the credible intervals for each model parameter.

Correlation Matrix of the Posterior Samples

The “Correlation Matrix of the Posterior Samples” table is produced if you include the CORR suboption in the SUMMARY= option in the BAYES statement. This table displays the sample correlation of the posterior samples.

Covariance Matrix of the Posterior Samples

The “Covariance Matrix of the Posterior Samples” table is produced if you include the COV suboption in the SUMMARY= option in the BAYES statement. This table displays the sample covariance of the posterior samples.

Autocorrelations of the Posterior Samples

The “Autocorrelations of the Posterior Samples” table displays the lag1, lag5, lag10, and lag50 autocorrelations for each parameter.

Gelman and Rubin Diagnostics

The “Gelman and Rubin Diagnostics” table is produced if you include the GELMAN suboption in the DIAGNOSTIC= option in the BAYES statement. This table displays the estimate of the potential scale reduction factor and its 97.5% upper confidence limit for each parameter.

Geweke Diagnostics

The “Geweke Diagnostics” table displays the Geweke statistic and its p -value for each parameter.

Raftery and Lewis Diagnostics

The “Raftery Diagnostics” tables is produced if you include the RAFTERY suboption in the DIAGNOSTIC= option in the BAYES statement. This table displays the Raftery and Lewis diagnostics for each variable.

Heidelberger and Welch Diagnostics

The “Heidelberger and Welch Diagnostics” table is displayed if you include the HEIDELBERGER suboption in the DIAGNOSTIC= option in the BAYES statement. This table shows the results of a stationary test and a halfwidth test for each parameter.

Effective Sample Size

The “Effective Sample Size” table displays, for each parameter, the effective sample size, the correlation time, and the efficiency.

Monte Carlo Standard Errors

The “Monte Carlo Standard Errors” table displays, for each parameter, the Monte Carlo standard error, the posterior sample standard deviation, and the ratio of the two.

Displayed Output for Exact Analysis

If an exact analysis is requested with an `EXACT` statement, the displayed output includes the following tables. If the `METHOD=NETWORKMC` option is specified, the test and estimate tables are renamed “Monte Carlo” tables and a Monte Carlo standard error column ($\sqrt{p(1-p)/n}$) is displayed.

Sufficient Statistics

Displays if you request an `OUTDIST=` data set in an `EXACT` statement. The table lists the parameters and their observed sufficient statistics.

(Monte Carlo) Conditional Exact Tests

This table tests the hypotheses that the parameters of interest are insignificant. See the section “Exact Logistic and Exact Poisson Regression” on page 2839 for details.

(Monte Carlo) Exact Parameter Estimates

Displays if you specify the `ESTIMATE` option in the `EXACT` statement. This table gives individual parameter estimates for each variable (conditional on the values of all the other parameters in the model), confidence limits, and a two-sided p -value (twice the one-sided p -value) for testing that the parameter is zero. See the section “Exact Logistic and Exact Poisson Regression” on page 2839 for details.

(Monte Carlo) Exact Odds Ratios

Displays if you specify the `ESTIMATE=ODDS` or `ESTIMATE=BOTH` option in the `EXACT` statement. See the section “Exact Logistic and Exact Poisson Regression” on page 2839 for details.

Strata Summary

Displays if a `STRATA` statement is also specified. Shows the pattern of the number of events and the number of nonevents, or of the number of observations, in a stratum. See the section “STRATA Statement” on page 2796 for more information.

Strata Information

Displays if a `STRATA` statement is specified with the `INFO` option.

ODS Table Names

PROC GENMOD assigns a name to each table that it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed separately in Table 40.12 for a maximum likelihood analysis, in Table 40.13 for a Bayesian analysis, and in Table 40.14 for an Exact analysis. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

Table 40.12 ODS Tables Produced in PROC GENMOD for a Classical Analysis

ODS Table Name	Description	Statement	Option
AssessmentSummary	Model assessment summary	ASSESS	Default
ClassLevels	Classification variable levels	CLASS	Default
Contrasts	Tests of contrasts	CONTRAST	Default
ContrastCoef	Contrast coefficients	CONTRAST	E
ConvergenceStatus	Convergence status	MODEL	Default
CorrB	Parameter estimate correlation matrix	MODEL	CORRB
CovB	Parameter estimate covariance matrix	MODEL	COVB
Estimates	Estimates of contrasts	ESTIMATE	Default
EstimateCoef	Contrast coefficients	ESTIMATE	E
GEEEmpPEst	GEE parameter estimates with empirical standard errors	REPEATED	Default
GEEFitCriteria	GEE QIC fit criteria	REPEATED	Default
GEELogORInfo	GEE log odds ratio model information	REPEATED	LOGOR=
GEEModInfo	GEE model information	REPEATED	Default
GEEModPEst	GEE parameter estimates with model-based standard errors	REPEATED	MODELSE
GEENCorr	GEE model-based correlation matrix	REPEATED	MCORRB
GEENCov	GEE model-based covariance matrix	REPEATED	MCOVB
GEERCorr	GEE empirical correlation matrix	REPEATED	ECORRB
GEERCov	GEE empirical covariance matrix	REPEATED	ECOV
GEEWCorr	GEE working correlation matrix	REPEATED	CORRW
IterContrasts	Iteration history for contrasts	MODEL CONTRAST	ITPRINT
IterLRCI	Iteration history for likelihood ratio confidence intervals	MODEL	LRCI ITPRINT
IterParms	Iteration history for parameter estimates	MODEL	ITPRINT
IterParmsGEE	Iteration history for GEE parameter estimates	MODEL REPEATED	ITPRINT
IterType3	Iteration history for Type 3 statistics	MODEL	TYPE3 ITPRINT

Table 40.12 *continued*

ODS Table Name	Description	Statement	Option
LRCI	Likelihood ratio confidence intervals	MODEL	LRCI ITPRINT
LSMeanCoef	Coefficients for least squares means	LSMEANS	E
LSMeanDiffs	Least squares means differences	LSMEANS	DIFF
LSMeans	Least squares means	LSMEANS	Default
LagrangeStatistics	Lagrange statistics	MODEL	NOINT NOSCALE
LastGEEGrad	Last evaluation of the generalized gradient and Hessian	MODEL	ITPRINT
LastGradHess	Last evaluation of the gradient and Hessian	MODEL	ITPRINT
LinDep	Linearly dependent rows of contrasts	CONTRAST	Default
ModelInfo	Model information	MODEL	Default
Modelfit	Goodness-of-fit statistics	MODEL	Default without REPEATED
NObs	Number of observations summary		Default
NonEst	Nonestimable rows of contrasts	CONTRAST	Default
ObStats	Observation-wise statistics	MODEL	OBSTATS CL PREDICTED RESIDUALS XVARs
ParameterEstimates	Parameter estimates	MODEL	Default without REPEATED PRINTMLE with REPEATED
ParmInfo	Parameter indices	MODEL	Default
ResponseProfile	Frequency counts for multinomial and binary models	MODEL	DIST=MULTINOMIAL DIST=BINOMIAL
Type1	Type 1 tests	MODEL	TYPE1
Type3	Type 3 tests	MODEL	TYPE3
ZeroParameterEstimates	Parameter estimates for zero-inflated model	ZEROMODEL	Default

Table 40.13 ODS Tables Produced in PROC GENMOD for a Bayesian Analysis

ODS Table Name	Description	Statement	Option
AutoCorr	Autocorrelations of the posterior samples	BAYES	Default
ClassLevels	Classification variable levels	CLASS	Default
CoeffPrior	Prior distribution of the regression coefficients	BAYES	Default
ConvergenceStatus	Convergence status of maximum likelihood estimation	MODEL	Default

Table 40.13 *continued*

ODS Table Name	Description	Statement	Option
Corr	Correlation matrix of the posterior samples	BAYES	SUMMARY=CORR
ESS	Effective sample size	BAYES	Default
FitStatistics	Fit statistics	BAYES	Default
Gelman	Gelman and Rubin convergence diagnostics	BAYES	DIAG=GELMAN
Geweke	Geweke convergence diagnostics	BAYES	Default
Heidelberger	Heidelberger and Welch convergence diagnostics	BAYES	DIAG=HEIDELBERGER
InitialValues	Initial values of the Markov chains	BAYES	Default
IterParms	Iteration history for parameter estimates	MODEL	ITPRINT
LastGradHess	Last evaluation of the gradient and Hessian for maximum likelihood estimation	MODEL	ITPRINT
MCErr	Monte Carlo standard errors	BAYES	DIAG=MCSE
ModelInfo	Model information	PROC	Default
NObs	Number of observations		Default
ParameterEstimates	Maximum likelihood estimates of model parameters	MODEL	Default
ParmInfo	Parameter indices	MODEL	Default
ParmPrior	Prior distribution for scale and shape	BAYES	Default
PostIntervals	HPD and equal-tail intervals of the posterior samples	BAYES	Default
PosteriorSample	Posterior samples (for ODS output data set only)	BAYES	
PostSummaries	Summary statistics of the posterior samples	BAYES	Default
Raftery	Raftery and Lewis convergence diagnostics	BAYES	DIAG=RAFTERY

Table 40.14 ODS Tables Produced in PROC GENMOD for an Exact Analysis

ODS Table Name	Description	Statement	Option
ExactOddsRatio	Exact odds ratios	EXACT	ESTIMATE=ODDS, ESTIMATE=BOTH
ExactParmEst	Parameter estimates	EXACT	ESTIMATE, ESTIMATE=PARAM, ESTIMATE=BOTH
ExactTests	Conditional exact tests	EXACT	Default

Table 40.14 *continued*

ODS Table Name	Description	Statement	Option
NStrataIgnored	Number of uninformative strata	STRATA	Default
StrataSummary	Number of strata with specific response frequencies	STRATA	Default
StrataInfo	Event and nonevent frequencies for each stratum	STRATA	INFO
SuffStats	Sufficient statistics	EXACT	OUTDIST=

ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “Statistical Graphics Using ODS.”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “A Primer on ODS Statistical Graphics” on page 599 in Chapter 21, “Statistical Graphics Using ODS.”

Some graphs are produced by default; other graphs are produced by using statements and options. You can reference every graph produced through ODS Graphics with a name. The names of the graphs that PROC GENMOD generates are listed in Table 40.15, along with the required statements and options.

ODS Graph Names

PROC GENMOD assigns a name to each graph it creates using ODS. You can use these names to reference the graphs when using ODS. The names are listed in Table 40.15.

To request these graphs, ODS Graphics must be enabled and you must specify the statement and options indicated in Table 40.15.

Table 40.15 Graphs Produced by PROC GENMOD

ODS Graph Name	Description	Statement	Option
ADPanel	Autocorrelation function and density panel	BAYES	PLOTS=(AUTOCORR DENSITY)
AutocorrPanel	Autocorrelation function panel	BAYES	PLOTS= AUTOCORR
AutocorrPlot	Autocorrelation function plot	BAYES	PLOTS(UNPACK)=AUTOCORR
ClusterCooksDPlot	Cluster Cook’s D by cluster number	PROC	PLOTS=

Table 40.15 continued

ODS Table Name	Description	Statement	Option
ClusterDFFITPlot	Cluster DFFIT by cluster number	PROC	PLOTS=
ClusterLeveragePlot	Cluster leverage by cluster number	PROC	PLOTS=
CooksDPlot	Cook's distance	PROC	PLOTS=
CumResidPanel	Panel of aggregates of residuals	ASSESS	CRPANEL
CumulativeResiduals	Model assessment based on aggregates of residuals	ASSESS	Default
DevianceResidByXBeta	Deviance residuals by linear predictor	PROC	PLOTS=
DevianceResidualPlot	Deviance values	PROC	PLOTS=
DFBETAByCluster	Cluster DFBeta by cluster number	PROC	PLOTS=
DFBETAPlot	DFBeta	PROC	PLOTS=
DiagnosticPlot	Panel of residuals, influence, and diagnostic statistics	PROC MODEL RE- PEATED	PLOTS=
LeveragePlot	Leverage	PROC	PLOTS=
LikeResidByXBeta	Likelihood residuals by linear predictor	PROC	PLOTS=
LikeResidualPlot	Likelihood residuals	PROC	PLOTS=
PearsonResidByXBeta	Pearson residuals by linear predictor	PROC	PLOTS=
PearsonResidualPlot	Pearson residuals	PROC	PLOTS=
PredictedByObservation	Predicted values	PROC	PLOTS=
RawResidByXBeta	Raw residuals by linear predictor	PROC	PLOTS=
RawResidualPlot	Raw residuals	PROC	PLOTS=
StdDevianceResidByXBeta	Standardized deviance residuals by linear predictor	PROC	PLOTS=
StdDevianceResidualPlot	Standardized deviance residuals	PROC	PLOTS=
StdDFBETAByCluster	Standardized cluster DFBeta by cluster number	PROC	PLOTS=
StdDFBETAPlot	Standardized DFBeta	PROC	PLOTS=
StdPearsonResidByXBeta	Standardized Pearson residuals by linear predictor	PROC	PLOTS=
StdPearsonResidualPlot	Standardized Pearson residuals	PROC	PLOTS=

Table 40.15 *continued*

ODS Table Name	Description	Statement	Option
TAPanel	Trace and autocorrelation function panel	BAYES	PLOTS=(TRACE AUTOCORR)
TADPanel	Trace, autocorrelation, and density function panel	BAYES	Default
TDPanel	Trace and density panel	BAYES	PLOTS=(TRACE DENSITY)
TracePanel	Trace panel	BAYES	PLOTS=TRACE
TracePlot	Trace plot	BAYES	PLOTS(UNPACK)=TRACE
ZeroInflationProbPlot	Zero-inflation probabilities	PROC	PLOTS=

Examples: GENMOD Procedure

The following examples illustrate some of the capabilities of the GENMOD procedure. These are not intended to represent definitive analyses of the data sets presented here. You should refer to the texts cited in the references for guidance on complete analysis of data by using generalized linear models.

Example 40.1: Logistic Regression

In an experiment comparing the effects of five different drugs, each drug is tested on a number of different subjects. The outcome of each experiment is the presence or absence of a positive response in a subject. The following artificial data represent the number of responses r in the n subjects for the five different drugs, labeled A through E. The response is measured for different levels of a continuous covariate x for each drug. The drug type and the continuous covariate x are explanatory variables in this experiment. The number of responses r is modeled as a binomial random variable for each combination of the explanatory variable values, with the binomial number of trials parameter equal to the number of subjects n and the binomial probability equal to the probability of a response.

The following DATA step creates the data set:

```
data drug;
  input drug$ x r n @@;
  datalines;
A .1 1 10 A .23 2 12 A .67 1 9
B .2 3 13 B .3 4 15 B .45 5 16 B .78 5 13
C .04 0 10 C .15 0 11 C .56 1 12 C .7 2 12
D .34 5 10 D .6 5 9 D .7 8 10
E .2 12 20 E .34 15 20 E .56 13 15 E .8 17 20
;
```

A logistic regression for these data is a generalized linear model with response equal to the binomial proportion r/n . The probability distribution is binomial, and the link function is logit. For these data, drug and x are explanatory variables. The probit and the complementary log-log link functions are also appropriate for binomial data.

PROC GENMOD performs a logistic regression on the data in the following SAS statements:

```
proc genmod data=drug;
  class drug;
  model r/n = x drug / dist = bin
                    link = logit
                    lrci;
run;
```

Since these data are binomial, you use the events/trials syntax to specify the response in the MODEL statement. Profile likelihood confidence intervals for the regression parameters are computed using the LRCI option.

General model and data information is produced in [Output 40.1.1](#).

Output 40.1.1 Model Information

The GENMOD Procedure	
Model Information	
Data Set	WORK.DRUG
Distribution	Binomial
Link Function	Logit
Response Variable (Events)	r
Response Variable (Trials)	n

The five levels of the CLASS variable DRUG are displayed in [Output 40.1.2](#).

Output 40.1.2 CLASS Variable Levels

Class Level Information		
Class	Levels	Values
drug	5	A B C D E

In the “Criteria For Assessing Goodness Of Fit” table displayed in [Output 40.1.3](#), the value of the deviance divided by its degrees of freedom is less than 1. A p -value is not computed for the deviance; however, a deviance that is approximately equal to its degrees of freedom is a possible indication of a good model fit. Asymptotic distribution theory applies to binomial data as the number of binomial trials parameter n becomes large for each combination of explanatory variables. McCullagh and Nelder (1989) caution against the use of the deviance alone to assess model fit. The model fit for each observation should be assessed by examination of residuals. The OBSTATS option in the MODEL statement produces a table of residuals and other useful statistics for each observation.

Output 40.1.3 Goodness-of-Fit Criteria

Criteria For Assessing Goodness Of Fit			
Criterion	DF	Value	Value/DF
Deviance	12	5.2751	0.4396
Scaled Deviance	12	5.2751	0.4396
Pearson Chi-Square	12	4.5133	0.3761
Scaled Pearson X2	12	4.5133	0.3761
Log Likelihood		-114.7732	
Full Log Likelihood		-23.7343	
AIC (smaller is better)		59.4686	
AICC (smaller is better)		67.1050	
BIC (smaller is better)		64.8109	

In the “Analysis Of Parameter Estimates” table displayed in [Output 40.1.4](#), chi-square values for the explanatory variables indicate that the parameter values other than the intercept term are all significant. The scale parameter is set to 1 for the binomial distribution. When you perform an overdispersion analysis, the value of the overdispersion parameter is indicated here. See the section “[Overdispersion](#)” on page 2809 for a discussion of overdispersion.

Output 40.1.4 Parameter Estimates

Analysis Of Maximum Likelihood Parameter Estimates							
Parameter	DF	Estimate	Standard Error	Likelihood Ratio		Wald Chi-Square	Pr > ChiSq
				95% Confidence Limits			
Intercept	1	0.2792	0.4196	-0.5336	1.1190	0.44	0.5057
x	1	1.9794	0.7660	0.5038	3.5206	6.68	0.0098
drug A	1	-2.8955	0.6092	-4.2280	-1.7909	22.59	<.0001
drug B	1	-2.0162	0.4052	-2.8375	-1.2435	24.76	<.0001
drug C	1	-3.7952	0.6655	-5.3111	-2.6261	32.53	<.0001
drug D	1	-0.8548	0.4838	-1.8072	0.1028	3.12	0.0773
drug E	0	0.0000	0.0000	0.0000	0.0000	.	.
Scale	0	1.0000	0.0000	1.0000	1.0000	.	.

NOTE: The scale parameter was held fixed.

The preceding table contains the profile likelihood confidence intervals for the explanatory variable parameters requested with the LRCI option. Wald confidence intervals are displayed by default. Profile likelihood confidence intervals are considered to be more accurate than Wald intervals (see Aitkin et al. (1989)), especially with small sample sizes. You can specify the confidence coefficient with the ALPHA= option in the MODEL statement. The default value of 0.05, corresponding to 95% confidence limits, is used here. See the section “[Confidence Intervals for Parameters](#)” on page 2813 for a discussion of profile likelihood confidence intervals.

Example 40.2: Normal Regression, Log Link

Consider the following data, where x is an explanatory variable and y is the response variable. It appears that y varies nonlinearly with x and that the variance is approximately constant. A normal distribution with a log link function is chosen to model these data; that is, $\log(\mu_i) = \mathbf{x}'_i\boldsymbol{\beta}$ so that $\mu_i = \exp(\mathbf{x}'_i\boldsymbol{\beta})$.

```
data nor;
  input x y;
  datalines;
0 5
0 7
0 9
1 7
1 10
1 8
2 11
2 9
3 16
3 13
3 14
4 25
4 24
5 34
5 32
5 30
;
```

The following SAS statements produce the analysis with the normal distribution and log link:

```
proc genmod data=nor;
  model y = x / dist = normal
          link = log;
  output out      = Residuals
         pred     = Pred
         resraw   = Resraw
         reschi   = Reschi
         resdev   = Resdev
         stdreschi = Stdreschi
         stdresdev = Stdresdev
         reslik   = Reslik;
run;
```

The OUTPUT statement is specified to produce a data set that contains predicted values and residuals for each observation. This data set can be useful for further analysis, such as residual plotting.

The results from these statements are displayed in [Output 40.2.1](#).

Output 40.2.1 Log-Linked Normal Regression

The GENMOD Procedure							
Model Information							
Data Set	WORK.NOR						
Distribution	Normal						
Link Function	Log						
Dependent Variable	y						
Criteria For Assessing Goodness Of Fit							
Criterion	DF	Value	Value/DF				
Deviance	14	52.3000	3.7357				
Scaled Deviance	14	16.0000	1.1429				
Pearson Chi-Square	14	52.3000	3.7357				
Scaled Pearson X2	14	16.0000	1.1429				
Log Likelihood		-32.1783					
Full Log Likelihood		-32.1783					
AIC (smaller is better)		70.3566					
AICC (smaller is better)		72.3566					
BIC (smaller is better)		72.6743					
Analysis Of Maximum Likelihood Parameter Estimates							
Parameter	DF	Estimate	Standard Error	Wald 95% Confidence Limits		Wald Chi-Square	Pr > ChiSq
Intercept	1	1.7214	0.0894	1.5461	1.8966	370.76	<.0001
x	1	0.3496	0.0206	0.3091	0.3901	286.64	<.0001
Scale	1	1.8080	0.3196	1.2786	2.5566		
NOTE: The scale parameter was estimated by maximum likelihood.							

The PROC GENMOD scale parameter, in the case of the normal distribution, is the standard deviation. By default, the scale parameter is estimated by maximum likelihood. You can specify a fixed standard deviation by using the NOSCALE and SCALE= options in the MODEL statement.

```
proc print data=Residuals;
run;
```

Output 40.2.2 Data Set of Predicted Values and Residuals

Obs	x	y	Pred	Reschi	Resraw	Resdev	Stdreschi	Stdresdev	Reslik
1	0	5	5.5921	-0.59212	-0.59212	-0.59212	-0.34036	-0.34036	-0.34036
2	0	7	5.5921	1.40788	1.40788	1.40788	0.80928	0.80928	0.80928
3	0	9	5.5921	3.40788	3.40788	3.40788	1.95892	1.95892	1.95892
4	1	7	7.9324	-0.93243	-0.93243	-0.93243	-0.54093	-0.54093	-0.54093
5	1	10	7.9324	2.06757	2.06757	2.06757	1.19947	1.19947	1.19947
6	1	8	7.9324	0.06757	0.06757	0.06757	0.03920	0.03920	0.03920
7	2	11	11.2522	-0.25217	-0.25217	-0.25217	-0.14686	-0.14686	-0.14686
8	2	9	11.2522	-2.25217	-2.25217	-2.25217	-1.31166	-1.31166	-1.31166
9	3	16	15.9612	0.03878	0.03878	0.03878	0.02249	0.02249	0.02249
10	3	13	15.9612	-2.96122	-2.96122	-2.96122	-1.71738	-1.71738	-1.71738
11	3	14	15.9612	-1.96122	-1.96122	-1.96122	-1.13743	-1.13743	-1.13743
12	4	25	22.6410	2.35897	2.35897	2.35897	1.37252	1.37252	1.37252
13	4	24	22.6410	1.35897	1.35897	1.35897	0.79069	0.79069	0.79069
14	5	34	32.1163	1.88366	1.88366	1.88366	1.22914	1.22914	1.22914
15	5	32	32.1163	-0.11634	-0.11634	-0.11634	-0.07592	-0.07592	-0.07592
16	5	30	32.1163	-2.11634	-2.11634	-2.11634	-1.38098	-1.38098	-1.38098

The data set of predicted values and residuals (Output 40.2.2) is created by the OUTPUT statement. You can use the PLOTS= option in the PROC GENMOD statement to create plots of predicted values and residuals. Note that raw, Pearson, and deviance residuals are equal in this example. This is a characteristic of the normal distribution and is not true in general for other distributions.

Example 40.3: Gamma Distribution Applied to Life Data

Life data are sometimes modeled with the gamma distribution. Although PROC GENMOD does not analyze censored data or provide other useful lifetime distributions such as the Weibull or lognormal, it can be used for modeling complete (uncensored) data with the gamma distribution, and it can provide a statistical test for the exponential distribution against other gamma distribution alternatives. See Lawless (2003) or Nelson (1982) for applications of the gamma distribution to life data.

The following data represent failure times of machine parts, some of which are manufactured by manufacturer A and some by manufacturer B.

```

data A;
  input lifetime @@;
  mfg = 'A';
  datalines;
620 470 260 89 388 242
103 100 39 460 284 1285
218 393 106 158 152 477
403 103 69 158 818 947
399 1274 32 12 134 660
548 381 203 871 193 531
317 85 1410 250 41 1101
32 421 32 343 376 1512
1792 47 95 76 515 72
1585 253 6 860 89 1055

```

```

537 101 385 176 11 565
164 16 1267 352 160 195
1279 356 751 500 803 560
151 24 689 1119 1733 2194
763 555 14 45 776 1
;

data B;
  input lifetime @@;
  mfg = 'B';
  datalines;
1747 945 12 1453 14 150
20 41 35 69 195 89
1090 1868 294 96 618 44
142 892 1307 310 230 30
403 860 23 406 1054 1935
561 348 130 13 230 250
317 304 79 1793 536 12
9 256 201 733 510 660
122 27 273 1231 182 289
667 761 1096 43 44 87
405 998 1409 61 278 407
113 25 940 28 848 41
646 575 219 303 304 38
195 1061 174 377 388 10
246 323 198 234 39 308
55 729 813 1216 1618 539
6 1566 459 946 764 794
35 181 147 116 141 19
380 609 546
;

data lifdat;
  set A B;
run;

```

The following SAS statements use PROC GENMOD to compute Type 3 statistics to test for differences between the two manufacturers in machine part life. Type 3 statistics are identical to Type 1 statistics in this case, since there is only one effect in the model. The log link function is selected to ensure that the mean is positive.

```

proc genmod data = lifdat;
  class mfg;
  model lifetime = mfg / dist=gamma
                        link=log
                        type3;
run;

```

The output from these statements is displayed in [Output 40.3.1](#).

Output 40.3.1 Gamma Model of Life Data

```

The GENMOD Procedure

Model Information

Data Set           WORK.LIFDAT
Distribution        Gamma
Link Function      Log
Dependent Variable lifetime

Class Level Information

Class      Levels  Values
mfg        2      A B

Criteria For Assessing Goodness Of Fit

Criterion          DF          Value          Value/DF
Deviance           199          287.0591         1.4425
Scaled Deviance    199          237.5335         1.1936
Pearson Chi-Square 199          211.6870         1.0638
Scaled Pearson X2  199          175.1652         0.8802
Log Likelihood                    -1432.4177
Full Log Likelihood                -1432.4177
AIC (smaller is better)            2870.8353
AICC (smaller is better)           2870.9572
BIC (smaller is better)            2880.7453

Analysis Of Maximum Likelihood Parameter Estimates

Parameter      DF      Estimate      Standard      Wald 95%      Wald
                DF      Estimate      Error      Confidence Limits  Chi-Square  Pr > ChiSq
Intercept      1      6.1302      0.1043      5.9257      6.3347      3451.61      <.0001
mfg            A      1      0.0199      0.1559      -0.2857      0.3255      0.02      0.8985
mfg            B      0      0.0000      0.0000      0.0000      0.0000      .          .
Scale          1      0.8275      0.0714      0.6987      0.9800

NOTE: The scale parameter was estimated by maximum likelihood.

LR Statistics For Type 3 Analysis

Source          DF          Chi-Square      Pr > ChiSq
mfg              1           0.02           0.8985
    
```

The p -value of 0.8985 for the chi-square statistic in the Type 3 table indicates that there is no significant difference in the part life between the two manufacturers.

Using the following statements, you can refit the model without using the manufacturer as an effect. The LRCI option in the MODEL statement is specified to compute profile likelihood confidence intervals for the mean life and scale parameters.

```
proc genmod data = lifdat;
  model lifetime = / dist=gamma
                  link=log
                  lrci;
run;
```

Output 40.3.2 displays the results of fitting the model with the mfg effect omitted.

Output 40.3.2 Refitting of the Gamma Model: Omitting the mfg Effect

The GENMOD Procedure							
Analysis Of Maximum Likelihood Parameter Estimates							
Parameter	DF	Estimate	Standard Error	Likelihood Ratio		Wald Chi-Square	Pr > ChiSq
				95% Confidence Limits			
Intercept	1	6.1391	0.0775	5.9904	6.2956	6268.10	<.0001
Scale	1	0.8274	0.0714	0.6959	0.9762		

NOTE: The scale parameter was estimated by maximum likelihood.

The intercept is the estimated log mean of the fitted gamma distribution, so that the mean life of the parts is

$$\mu = \exp(\text{INTERCEPT}) = \exp(6.1391) = 463.64$$

The SCALE parameter used in PROC GENMOD is the inverse of the gamma dispersion parameter, and it is sometimes called the gamma *index parameter*. See the section “Response Probability Distributions” on page 2799 for the definition of the gamma probability density function. A value of 1 for the index parameter corresponds to the exponential distribution. The estimated value of the scale parameter is 0.8274. The 95% profile likelihood confidence interval for the scale parameter is (0.6959, 0.9762), which does not contain 1. The hypothesis of an exponential distribution for the data is, therefore, rejected at the 0.05 level. A confidence interval for the mean life is

$$(\exp(5.99), \exp(6.30)) = (399.57, 542.18)$$

Example 40.4: Ordinal Model for Multinomial Data

This example illustrates how you can use the GENMOD procedure to fit a model to data measured on an ordinal scale. The following statements create a SAS data set called `Icecream`. The data set contains the results of a hypothetical taste test of three brands of ice cream. The three brands are rated for taste on a five-point scale from very good (vg) to very bad (vb). An analysis is performed to assess the differences in the ratings of the three brands. The variable `taste` contains the ratings, and the variable `brand` contains the brands tested. The variable `count` contains the number of testers rating each brand in each category.

The following statements create the `Icecream` data set:

```

data Icecream;
  input count brand$ taste$;
  datalines;
70  ice1  vg
71  ice1  g
151 ice1  m
30  ice1  b
46  ice1  vb
20  ice2  vg
36  ice2  g
130 ice2  m
74  ice2  b
70  ice2  vb
50  ice3  vg
55  ice3  g
140 ice3  m
52  ice3  b
50  ice3  vb
;

```

The following statements fit a cumulative logit model to the ordinal data with the variable taste as the response and the variable brand as a covariate. The variable count is used as a FREQ variable.

```

proc genmod data=Icecream rorder=data;
  freq count;
  class brand;
  model taste = brand / dist=multinomial
                    link=cumlogit
                    aggregate=brand
                    type1;
  estimate 'LogOR12' brand 1 -1 / exp;
  estimate 'LogOR13' brand 1  0 -1 / exp;
  estimate 'LogOR23' brand 0  1 -1 / exp;
run;

```

The AGGREGATE=BRAND option in the MODEL statement specifies the variable brand as defining multinomial populations for computing deviances and Pearson chi-squares. The RORDER=DATA option specifies that the taste variable levels be ordered by their order of appearance in the input data set—that is, from very good (vg) to very bad (vb). By default, the response is sorted in increasing ASCII order. Always check the “Response Profiles” table to verify that response levels are appropriately ordered. The TYPE1 option requests a Type 1 test for the significance of the covariate brand.

If $\gamma_j(\mathbf{x}) = \Pr(\text{taste} \leq j)$ is the cumulative probability of the j th or lower taste category, then the odds ratio comparing \mathbf{x}_1 to \mathbf{x}_2 is as follows:

$$\frac{\gamma_j(\mathbf{x}_1)/(1 - \gamma_j(\mathbf{x}_1))}{\gamma_j(\mathbf{x}_2)/(1 - \gamma_j(\mathbf{x}_2))} = \exp[(\mathbf{x}_1 - \mathbf{x}_2)' \boldsymbol{\beta}]$$

See McCullagh and Nelder (1989, Chapter 5) for details on the cumulative logit model. The ESTIMATE statements compute log odds ratios comparing each of brands. The EXP option in the ESTIMATE statements exponentiates the log odds ratios to form odds ratio estimates. Standard errors and confidence intervals are also computed.

Output 40.4.1 displays general information about the model and data, the levels of the CLASS variable brand, and the total number of occurrences of the ordered levels of the response variable taste.

Output 40.4.1 Ordinal Model Information

The GENMOD Procedure			
Model Information			
Data Set	WORK.ICECREAM		
Distribution	Multinomial		
Link Function	Cumulative Logit		
Dependent Variable	taste		
Frequency Weight Variable	count		
Class Level Information			
Class	Levels	Values	
brand	3	ice1	ice2 ice3
Response Profile			
Ordered Value	taste	Total Frequency	
1	vg	140	
2	g	162	
3	m	421	
4	b	156	
5	vb	166	

Output 40.4.2 displays estimates of the intercept terms and covariates and associated statistics. The intercept terms correspond to the four cumulative logits defined on the taste categories in the order shown in Output 40.4.1. That is, Intercept1 is the intercept for the first cumulative logit, $\log\left(\frac{p_1}{1-p_1}\right)$, Intercept2 is the intercept for the second cumulative logit, $\log\left(\frac{p_1+p_2}{1-(p_1+p_2)}\right)$, and so forth.

Output 40.4.2 Parameter Estimates

Analysis Of Maximum Likelihood Parameter Estimates						
Parameter	DF	Estimate	Standard Error	Wald 95% Confidence Limits		Wald Chi-Square
Intercept1	1	-1.8578	0.1219	-2.0967	-1.6189	232.35
Intercept2	1	-0.8646	0.1056	-1.0716	-0.6576	67.02
Intercept3	1	0.9231	0.1060	0.7154	1.1308	75.87
Intercept4	1	1.8078	0.1191	1.5743	2.0413	230.32
brand ice1	1	0.3847	0.1370	0.1162	0.6532	7.89
brand ice2	1	-0.6457	0.1397	-0.9196	-0.3719	21.36
brand ice3	0	0.0000	0.0000	0.0000	0.0000	.
Scale	0	1.0000	0.0000	1.0000	1.0000	

Analysis Of Maximum Likelihood Parameter Estimates		
Parameter	Pr > ChiSq	
Intercept1	<.0001	
Intercept2	<.0001	
Intercept3	<.0001	
Intercept4	<.0001	
brand ice1	0.0050	
brand ice2	<.0001	
brand ice3	.	
Scale		

NOTE: The scale parameter was held fixed.

The Type 1 test displayed in [Output 40.4.3](#) indicates that Brand is highly significant; that is, there are significant differences among the brands. The log odds ratios and odds ratios in the “ESTIMATE Statement Results” table indicate the relative differences among the brands. For example, the odds ratio of 2.8 in the “Exp(LogOR12)” row indicates that the odds of brand 1 being in lower taste categories is 2.8 times the odds of brand 2 being in lower taste categories. Since, in this ordering, the lower categories represent the more favorable taste results, this indicates that brand 1 scored significantly better than brand 2. This is also apparent from the data in this example.

Output 40.4.3 Type 1 Tests and Odds Ratios

LR Statistics For Type 1 Analysis				
Source	Deviance	DF	Chi-Square	Pr > ChiSq
Intercepts	65.9576			
brand	9.8654	2	56.09	<.0001

Output 40.4.3 continued

Contrast Estimate Results						
Label	Mean Estimate	Mean Confidence Limits		L'Beta Estimate	Standard Error	Alpha
LogOR12	0.7370	0.6805	0.7867	1.0305	0.1401	0.05
Exp (LogOR12)				2.8024	0.3926	0.05
LogOR13	0.5950	0.5290	0.6577	0.3847	0.1370	0.05
Exp (LogOR13)				1.4692	0.2013	0.05
LogOR23	0.3439	0.2850	0.4081	-0.6457	0.1397	0.05
Exp (LogOR23)				0.5243	0.0733	0.05

Contrast Estimate Results				
Label	L'Beta Confidence Limits		Chi-Square	Pr > ChiSq
LogOR12	0.7559	1.3050	54.11	<.0001
Exp (LogOR12)	2.1295	3.6878		
LogOR13	0.1162	0.6532	7.89	0.0050
Exp (LogOR13)	1.1233	1.9217		
LogOR23	-0.9196	-0.3719	21.36	<.0001
Exp (LogOR23)	0.3987	0.6894		

Example 40.5: GEE for Binary Data with Logit Link Function

Output 40.5.1 displays a partial listing of a SAS data set of clinical trial data comparing two treatments for a respiratory disorder. See “Gee Model for Binary Data” in the SAS/STAT Sample Program Library for the complete data set. These data are from Stokes, Davis, and Koch (2000).

Patients in each of two centers are randomly assigned to groups receiving the active treatment or a placebo. During treatment, respiratory status, represented by the variable *outcome* (coded here as 0=poor, 1=good), is determined for each of four visits. The variables *center*, *treatment*, *sex*, and *baseline* (baseline respiratory status) are classification variables with two levels. The variable *age* (age at time of entry into the study) is a continuous variable.

Explanatory variables in the model are Intercept (x_{ij1}), treatment (x_{ij2}), center (x_{ij3}), sex (x_{ij4}), age (x_{ij5}), and baseline (x_{ij6}), so that $x' = [x_{ij1}, x_{ij2}, \dots, x_{ij6}]$ is the vector of explanatory variables. Indicator variables for the classification explanatory variables can be automatically generated by listing them in the CLASS statement in PROC GENMOD. To be consistent with the analysis in Stokes, Davis, and Koch (2000), the four classification explanatory variables are coded as follows via options in the CLASS statement:

$$x_{ij2} = \begin{cases} 0 & \text{placebo} \\ 1 & \text{active} \end{cases} \quad x_{ij3} = \begin{cases} 0 & \text{center 1} \\ 1 & \text{center 2} \end{cases}$$

$$x_{ij4} = \begin{cases} 0 & \text{male} \\ 1 & \text{female} \end{cases} \quad x_{ij6} = \begin{cases} 0 & 0 \\ 1 & 1 \end{cases}$$

Suppose y_{ij} represents the respiratory status of patient i at the j th visit, $j = 1, \dots, 4$, and $\mu_{ij} = E(y_{ij})$ represents the mean of the respiratory status. Since the response data are binary, you can use the variance function for the binomial distribution $v(\mu_{ij}) = \mu_{ij}(1 - \mu_{ij})$ and the logit link function $g(\mu_{ij}) = \log(\mu_{ij}/(1 - \mu_{ij}))$. The model for the mean is $g(\mu_{ij}) = \mathbf{x}_{ij}'\boldsymbol{\beta}$, where $\boldsymbol{\beta}$ is a vector of regression parameters to be estimated.

Output 40.5.1 Respiratory Disorder Data

	c		t		a		b				o	
	e		r		s		v				u	
	n		e		a		i				t	
O	t		s		g		s				i	
b	e		e		e		s				c	
s	r		x		e		s				o	
							1	2	3	4	t	e
1	1	1	P	M	46	0	0	0	0	0	1	0
2	1	1	P	M	46	0	0	0	0	0	2	0
3	1	1	P	M	46	0	0	0	0	0	3	0
4	1	1	P	M	46	0	0	0	0	0	4	0
5	1	2	P	M	28	0	0	0	0	0	1	0
6	1	2	P	M	28	0	0	0	0	0	2	0
7	1	2	P	M	28	0	0	0	0	0	3	0
8	1	2	P	M	28	0	0	0	0	0	4	0
9	1	3	A	M	23	1	1	1	1	1	1	1
10	1	3	A	M	23	1	1	1	1	1	2	1
11	1	3	A	M	23	1	1	1	1	1	3	1
12	1	3	A	M	23	1	1	1	1	1	4	1
13	1	4	P	M	44	1	1	1	1	0	1	1
14	1	4	P	M	44	1	1	1	1	0	2	1
15	1	4	P	M	44	1	1	1	1	0	3	1
16	1	4	P	M	44	1	1	1	1	0	4	0
17	1	5	P	F	13	1	1	1	1	1	1	1
18	1	5	P	F	13	1	1	1	1	1	2	1
19	1	5	P	F	13	1	1	1	1	1	3	1
20	1	5	P	F	13	1	1	1	1	1	4	1

The GEE solution is requested with the REPEATED statement in the GENMOD procedure. The option SUBJECT=ID(CENTER) specifies that the observations in a single cluster be uniquely identified by center and id within center. The option TYPE=UNSTR specifies the unstructured working correlation structure. The MODEL statement specifies the regression model for the mean with the binomial distribution variance function. The following SAS statements perform the GEE model fit:

```
proc genmod data=resp descend;
  class id treatment(ref="P") center(ref="1") sex(ref="M")
    baseline(ref="0") / param=ref;
  model outcome=treatment center sex age baseline / dist=bin;
  repeated subject=id(center) / corr=unstr corrw;
run;
```

These statements first fit the generalized linear (GLM) model specified in the MODEL statement. The parameter estimates from the generalized linear model fit are not shown in the output, but they are used

as initial values for the GEE solution. The DESCEND option in the PROC GENMOD statement specifies that the probability that outcome = 1 be modeled. If the DESCEND option had not been specified, the probability that outcome = 0 would be modeled by default.

Information about the GEE model is displayed in [Output 40.5.2](#). The results of GEE model fitting are displayed in [Output 40.5.3](#). Model goodness-of-fit criteria are displayed in [Output 40.5.4](#). If you specify no other options, the standard errors, confidence intervals, Z scores, and *p*-values are based on empirical standard error estimates. You can specify the MODELSE option in the REPEATED statement to create a table based on model-based standard error estimates.

Output 40.5.2 Model Fitting Information

The GENMOD Procedure	
GEE Model Information	
Correlation Structure	Unstructured
Subject Effect	id(center) (111 levels)
Number of Clusters	111
Correlation Matrix Dimension	4
Maximum Cluster Size	4
Minimum Cluster Size	4

Output 40.5.3 Results of Model Fitting

Working Correlation Matrix				
	Col1	Col2	Col3	Col4
Row1	1.0000	0.3351	0.2140	0.2953
Row2	0.3351	1.0000	0.4429	0.3581
Row3	0.2140	0.4429	1.0000	0.3964
Row4	0.2953	0.3581	0.3964	1.0000

Analysis Of GEE Parameter Estimates						
Empirical Standard Error Estimates						
Parameter	Estimate	Standard Error	95% Confidence Limits		Z	Pr > Z
Intercept	-0.8882	0.4568	-1.7835	0.0071	-1.94	0.0519
treatment A	1.2442	0.3455	0.5669	1.9214	3.60	0.0003
center 2	0.6558	0.3512	-0.0326	1.3442	1.87	0.0619
sex F	0.1128	0.4408	-0.7512	0.9768	0.26	0.7981
age	-0.0175	0.0129	-0.0427	0.0077	-1.36	0.1728
baseline 1	1.8981	0.3441	1.2237	2.5725	5.52	<.0001

Output 40.5.4 Model Fit Criteria

GEE Fit Criteria	
QIC	512.3416
QICu	499.6081

The nonsignificance of age and sex make them candidates for omission from the model.

Example 40.6: Log Odds Ratios and the ALR Algorithm

Since the respiratory data in [Example 40.5](#) are binary, you can use the ALR algorithm to model the log odds ratios instead of using working correlations to model associations. In this example, a “fully parameterized cluster” model for the log odds ratio is fit. That is, there is a log odds ratio parameter for each unique pair of responses within clusters, and all clusters are parameterized identically. The following statements fit the same regression model for the mean as in [Example 40.5](#) but use a regression model for the log odds ratios instead of a working correlation. The LOGOR=FULLCLUST option specifies a fully parameterized log odds ratio model.

```
proc genmod data=resp descend;
  class id treatment(ref="P") center(ref="1") sex(ref="M")
    baseline(ref="0") / param=ref;
  model outcome=treatment center sex age baseline / dist=bin;
  repeated subject=id(center) / logor=fullclust;
run;
```

The results of fitting the model are displayed in [Output 40.6.1](#) along with a table that shows the correspondence between the log odds ratio parameters and the within-cluster pairs. Model goodness-of-fit criteria are shown in [Output 40.6.2](#). The QIC for the ALR model shown in [Output 40.6.2](#) is 511.86, whereas the QIC for the unstructured working correlation model shown in [Output 40.5.4](#) is 512.34, indicating that the ALR model is a slightly better fit.

Output 40.6.1 Results of Model Fitting

The GENMOD Procedure	
Log Odds Ratio Parameter Information	
Parameter	Group
Alpha1	(1, 2)
Alpha2	(1, 3)
Alpha3	(1, 4)
Alpha4	(2, 3)
Alpha5	(2, 4)
Alpha6	(3, 4)

Output 40.6.1 *continued*

Analysis Of GEE Parameter Estimates Empirical Standard Error Estimates						
Parameter	Estimate	Standard Error	95% Confidence Limits		Z	Pr > Z
Intercept	-0.9266	0.4513	-1.8111	-0.0421	-2.05	0.0400
treatment A	1.2611	0.3406	0.5934	1.9287	3.70	0.0002
center 2	0.6287	0.3486	-0.0545	1.3119	1.80	0.0713
sex F	0.1024	0.4362	-0.7526	0.9575	0.23	0.8144
age	-0.0162	0.0125	-0.0407	0.0084	-1.29	0.1977
baseline 1	1.8980	0.3404	1.2308	2.5652	5.58	<.0001
Alpha1	1.6109	0.4892	0.6522	2.5696	3.29	0.0010
Alpha2	1.0771	0.4834	0.1297	2.0246	2.23	0.0259
Alpha3	1.5875	0.4735	0.6594	2.5155	3.35	0.0008
Alpha4	2.1224	0.5022	1.1381	3.1068	4.23	<.0001
Alpha5	1.8818	0.4686	0.9634	2.8001	4.02	<.0001
Alpha6	2.1046	0.4949	1.1347	3.0745	4.25	<.0001

Output 40.6.2 Model Fit Criteria

GEE Fit Criteria	
QIC	511.8589
QICu	499.6516

You can fit the same model by fully specifying the z matrix. The following statements create a data set containing the full z matrix:

```

data zin;
  keep id center z1-z6 y1 y2;
  array zin(6) z1-z6;
  set resp;
  by center id;
  if first.id
  then do;
    t = 0;
    do m = 1 to 4;
      do n = m+1 to 4;
        do j = 1 to 6;
          zin(j) = 0;
        end;
        y1 = m;
        y2 = n;
        t + 1;
        zin(t) = 1;
        output;
      end;
    end;
  end;
run;

```

```
proc print data=zin (obs=12);
run;
```

Output 40.6.3 displays the full z matrix for the first two clusters. The z matrix is identical for all clusters in this example.

Output 40.6.3 Full z Matrix Data Set

Obs	z1	z2	z3	z4	z5	z6	center	id	y1	y2
1	1	0	0	0	0	0	1	1	1	2
2	0	1	0	0	0	0	1	1	1	3
3	0	0	1	0	0	0	1	1	1	4
4	0	0	0	1	0	0	1	1	2	3
5	0	0	0	0	1	0	1	1	2	4
6	0	0	0	0	0	1	1	1	3	4
7	1	0	0	0	0	0	1	2	1	2
8	0	1	0	0	0	0	1	2	1	3
9	0	0	1	0	0	0	1	2	1	4
10	0	0	0	1	0	0	1	2	2	3
11	0	0	0	0	1	0	1	2	2	4
12	0	0	0	0	0	1	1	2	3	4

The following statements fit the model for fully parameterized clusters by fully specifying the z matrix. The results are identical to those shown previously.

```
proc genmod data=resp descend;
  class id treatment(ref="P") center(ref="1") sex(ref="M")
    baseline(ref="0") / param=ref;
  model outcome=treatment center sex age baseline / dist=bin;
  repeated subject=id(center) / logor=zfull
    zdata=zin
    zrow =(z1-z6)
    ypair=(y1 y2);
run;
```

Example 40.7: Log-Linear Model for Count Data

In this example the data, from Thall and Vail (1990), concern the treatment of people suffering from epileptic seizure episodes. These data are also analyzed in Diggle, Liang, and Zeger (1994). The data consist of the number of epileptic seizures in an eight-week baseline period, before any treatment, and in each of four two-week treatment periods, in which patients received either a placebo or the drug Progabide in addition to other therapy. A portion of the data is displayed in Table 40.16. See “Gee Model for Count Data, Exchangeable Correlation” in the SAS/STAT Sample Program Library for the complete data set.

Table 40.16 Epileptic Seizure Data

Patient ID	Treatment	Baseline	Visit1	Visit2	Visit3	Visit4
104	Placebo	11	5	3	3	3
106	Placebo	11	3	5	3	3
107	Placebo	6	2	4	0	5
.						
.						
.						
101	Progabide	76	11	14	9	8
102	Progabide	38	8	7	9	4
103	Progabide	19	0	4	3	0
.						
.						
.						

Model the data as a log-linear model with $V(\mu) = \mu$ (the Poisson variance function) and

$$\log(E(Y_{ij})) = \beta_0 + x_{i1}\beta_1 + x_{i2}\beta_2 + x_{i1}x_{i2}\beta_3 + \log(t_{ij})$$

where

Y_{ij} = number of epileptic seizures in interval j

t_{ij} = length of interval j

$$x_{i1} = \begin{cases} 1 & \text{weeks 8–16 (treatment)} \\ 0 & \text{weeks 0–8 (baseline)} \end{cases}$$

$$x_{i2} = \begin{cases} 1 & \text{progabide group} \\ 0 & \text{placebo group} \end{cases}$$

The correlations between the counts are modeled as $r_{ij} = \alpha$, $i \neq j$ (exchangeable correlations). For comparison, the correlations are also modeled as independent (identity correlation matrix). In this model, the regression parameters have the interpretation in terms of the log seizure rate displayed in Table 40.17.

Table 40.17 Interpretation of Regression Parameters

Treatment	Visit	$\log(E(Y_{ij})/t_{ij})$
Placebo	Baseline	β_0
	1–4	$\beta_0 + \beta_1$
Progabide	Baseline	$\beta_0 + \beta_2$
	1–4	$\beta_0 + \beta_1 + \beta_2 + \beta_3$

The difference between the log seizure rates in the pretreatment (baseline) period and the treatment periods is β_1 for the placebo group and $\beta_1 + \beta_3$ for the Progabide group. A value of $\beta_3 < 0$ indicates a reduction in the seizure rate.

Output 40.7.1 lists the first 14 observations of the data, which are arranged as one visit per observation:

Output 40.7.1 Partial Listing of the Seizure Data

Obs	id	y	visit	trt	bline	age
1	104	5	1	0	11	31
2	104	3	2	0	11	31
3	104	3	3	0	11	31
4	104	3	4	0	11	31
5	106	3	1	0	11	30
6	106	5	2	0	11	30
7	106	3	3	0	11	30
8	106	3	4	0	11	30
9	107	2	1	0	6	25
10	107	4	2	0	6	25
11	107	0	3	0	6	25
12	107	5	4	0	6	25
13	114	4	1	0	8	36
14	114	4	2	0	8	36

Some further data manipulations create an observation for the baseline measures, a log time interval variable for use as an offset, and an indicator variable for whether the observation is for a baseline measurement or a visit measurement. Patient 207 is deleted as an outlier, as in the Diggle, Liang, and Zeger (1994) analysis. The following statements prepare the data for analysis with PROC GENMOD:

```
data new;
  set thall;
  output;
  if visit=1 then do;
    y=bline;
    visit=0;
    output;
  end;
run;
```

```
data new;
  set new;
  if id ne 207;
  if visit=0 then do;
    x1=0;
    ltime=log(8);
  end;
  else do;
    x1=1;
    ltime=log(2);
  end;
run;
```

For comparison with the GEE results, an ordinary Poisson regression is first fit. The results are shown in Output 40.7.2.

Output 40.7.2 Maximum Likelihood Estimates

The GENMOD Procedure							
Analysis Of Maximum Likelihood Parameter Estimates							
Parameter	DF	Estimate	Standard Error	Wald 95% Confidence Limits		Wald Chi-Square	Pr > ChiSq
Intercept	1	1.3476	0.0341	1.2809	1.4144	1565.44	<.0001
x1	1	0.1108	0.0469	0.0189	0.2027	5.58	0.0181
trt	1	-0.1080	0.0486	-0.2034	-0.0127	4.93	0.0264
x1*trt	1	-0.3016	0.0697	-0.4383	-0.1649	18.70	<.0001
Scale	0	1.0000	0.0000	1.0000	1.0000		

NOTE: The scale parameter was held fixed.

The GEE solution is requested with the REPEATED statement in the GENMOD procedure. The SUBJECT=ID option indicates that the variable id describes the observations for a single cluster, and the CORRW option displays the working correlation matrix. The TYPE= option specifies the correlation structure; the value EXCH indicates the exchangeable structure.

The following statements perform the analysis:

```
proc genmod data=new;
  class id;
  model y=x1 | trt / d=poisson offset=ltime;
  repeated subject=id / corrw covb type=exch;
run;
```

These statements first fit a generalized linear model (GLM) to these data by maximum likelihood. The estimates are not shown in the output, but are used as initial values for the GEE solution.

Information about the GEE model is displayed in [Output 40.7.3](#). The results of fitting the model are displayed in [Output 40.7.4](#). Compare these with the model of independence displayed in [Output 40.7.2](#). The parameter estimates are nearly identical, but the standard errors for the independence case are underestimated. The coefficient of the interaction term, β_3 , is highly significant under the independence model and marginally significant with the exchangeable correlations model.

Output 40.7.3 GEE Model Information

The GENMOD Procedure	
GEE Model Information	
Correlation Structure	Exchangeable
Subject Effect	id (58 levels)
Number of Clusters	58
Correlation Matrix Dimension	5
Maximum Cluster Size	5
Minimum Cluster Size	5

Output 40.7.4 GEE Parameter Estimates

Analysis Of GEE Parameter Estimates						
Empirical Standard Error Estimates						
Parameter	Estimate	Standard Error	95% Confidence Limits		Z	Pr > Z
Intercept	1.3476	0.1574	1.0392	1.6560	8.56	<.0001
x1	0.1108	0.1161	-0.1168	0.3383	0.95	0.3399
trt	-0.1080	0.1937	-0.4876	0.2716	-0.56	0.5770
x1*trt	-0.3016	0.1712	-0.6371	0.0339	-1.76	0.0781

Table 40.18 displays the regression coefficients, standard errors, and normalized coefficients that result from fitting the model with independent and exchangeable working correlation matrices.

Table 40.18 Results of Model Fitting

Variable	Correlation Structure	Coef.	Std. Error	Coef./S.E.
Intercept	Exchangeable	1.35	0.16	8.56
	Independent	1.35	0.03	39.52
Visit (x_1)	Exchangeable	0.11	0.12	0.95
	Independent	0.11	0.05	2.36
Treat (x_2)	Exchangeable	-0.11	0.19	-0.56
	Independent	-0.11	0.05	-2.22
$x_1 * x_2$	Exchangeable	-0.30	0.17	-1.76
	Independent	-0.30	0.07	-4.32

The fitted exchangeable correlation matrix is specified with the CORRW option and is displayed in Output 40.7.5.

Output 40.7.5 Working Correlation Matrix

Working Correlation Matrix					
	Col1	Col2	Col3	Col4	Col5
Row1	1.0000	0.5941	0.5941	0.5941	0.5941
Row2	0.5941	1.0000	0.5941	0.5941	0.5941
Row3	0.5941	0.5941	1.0000	0.5941	0.5941
Row4	0.5941	0.5941	0.5941	1.0000	0.5941
Row5	0.5941	0.5941	0.5941	0.5941	1.0000

If you specify the COVB option, you produce both the model-based (naive) and the empirical (robust) covariance matrices. Output 40.7.6 contains these estimates.

Output 40.7.6 Covariance Matrices

Covariance Matrix (Model-Based)				
	Prm1	Prm2	Prm3	Prm4
Prm1	0.01223	0.001520	-0.01223	-0.001520
Prm2	0.001520	0.01519	-0.001520	-0.01519
Prm3	-0.01223	-0.001520	0.02495	0.005427
Prm4	-0.001520	-0.01519	0.005427	0.03748

Covariance Matrix (Empirical)				
	Prm1	Prm2	Prm3	Prm4
Prm1	0.02476	-0.001152	-0.02476	0.001152
Prm2	-0.001152	0.01348	0.001152	-0.01348
Prm3	-0.02476	0.001152	0.03751	-0.002999
Prm4	0.001152	-0.01348	-0.002999	0.02931

The two covariance estimates are similar, indicating an adequate correlation model.

Example 40.8: Model Assessment of Multiple Regression Using Aggregates of Residuals

This example illustrates the use of cumulative residuals to assess the adequacy of a normal linear regression model. Neter et al. (1996, Section 8.2) describe a study of 54 patients undergoing a certain kind of liver operation in a surgical unit. The data consist of the survival time and certain covariates. After a model selection procedure, they arrived at the following model:

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 + \epsilon$$

where Y is the logarithm (base 10) of the survival time; X_1 , X_2 , X_3 are *blood-clotting score*, *prognostic index*, and *enzyme function*, respectively; and ϵ is a normal error term. A listing of the SAS data set containing the data is shown in [Output 40.8.1](#). The variables Y , X_1 , X_2 , and X_3 correspond to Y , X_1 , X_2 , and X_3 , and $\text{Log}X_1$ is $\log(X_1)$. The PROC GENMOD fit of the model is shown in [Output 40.8.2](#). The analysis first focuses on the adequacy of the functional form of X_1 , *blood-clotting score*.

Output 40.8.1 Surgical Unit Example Data

Obs	Y	X1	X2	X3	LogX1
1	2.3010	6.7	62	81	0.82607
2	2.0043	5.1	59	66	0.70757
3	2.3096	7.4	57	83	0.86923
4	2.0043	6.5	73	41	0.81291
5	2.7067	7.8	65	115	0.89209
6	1.9031	5.8	38	72	0.76343
7	1.9031	5.7	46	63	0.75587
8	2.1038	3.7	68	81	0.56820
9	2.3054	6.0	67	93	0.77815
10	2.3075	3.7	76	94	0.56820
11	2.5172	6.3	84	83	0.79934
12	1.8129	6.7	51	43	0.82607
13	2.9191	5.8	96	114	0.76343
14	2.5185	5.8	83	88	0.76343
15	2.2253	7.7	62	67	0.88649
16	2.3365	7.4	74	68	0.86923
17	1.9395	6.0	85	28	0.77815
18	1.5315	3.7	51	41	0.56820
19	2.3324	7.3	68	74	0.86332
20	2.2355	5.6	57	87	0.74819
21	2.0374	5.2	52	76	0.71600
22	2.1335	3.4	83	53	0.53148
23	1.8451	6.7	26	68	0.82607
24	2.3424	5.8	67	86	0.76343
25	2.4409	6.3	59	100	0.79934
26	2.1584	5.8	61	73	0.76343
27	2.2577	5.2	52	86	0.71600
28	2.7589	11.2	76	90	1.04922
29	1.8573	5.2	54	56	0.71600
30	2.2504	5.8	76	59	0.76343
31	1.8513	3.2	64	65	0.50515
32	1.7634	8.7	45	23	0.93952
33	2.0645	5.0	59	73	0.69897
34	2.4698	5.8	72	93	0.76343
35	2.0607	5.4	58	70	0.73239
36	2.2648	5.3	51	99	0.72428
37	2.0719	2.6	74	86	0.41497
38	2.0792	4.3	8	119	0.63347
39	2.1790	4.8	61	76	0.68124
40	2.1703	5.4	52	88	0.73239
41	1.9777	5.2	49	72	0.71600
42	1.8751	3.6	28	99	0.55630
43	2.6840	8.8	86	88	0.94448
44	2.1847	6.5	56	77	0.81291
45	2.2810	3.4	77	93	0.53148
46	2.0899	6.5	40	84	0.81291
47	2.4928	4.5	73	106	0.65321
48	2.5999	4.8	86	101	0.68124
49	2.1987	5.1	67	77	0.70757
50	2.4914	3.9	82	103	0.59106
51	2.0934	6.6	77	46	0.81954
52	2.0969	6.4	85	40	0.80618
53	2.2967	6.4	59	85	0.80618
54	2.4955	8.8	78	72	0.94448

In order to assess the adequacy of the fitted multiple regression model, the ASSESS statement in the following SAS statements is used to create the plots of cumulative residuals against X1 shown in [Output 40.8.3](#) and [Output 40.8.4](#) and the summary table in [Output 40.8.5](#):

```
ods graphics on;

proc genmod data=Surg;
  model Y = X1 X2 X3 / scale=Pearson;
  assess var=(X1) / resample=10000
              seed=603708000
              crpanel;
run;
```

Output 40.8.2 Regression Model for Linear X1

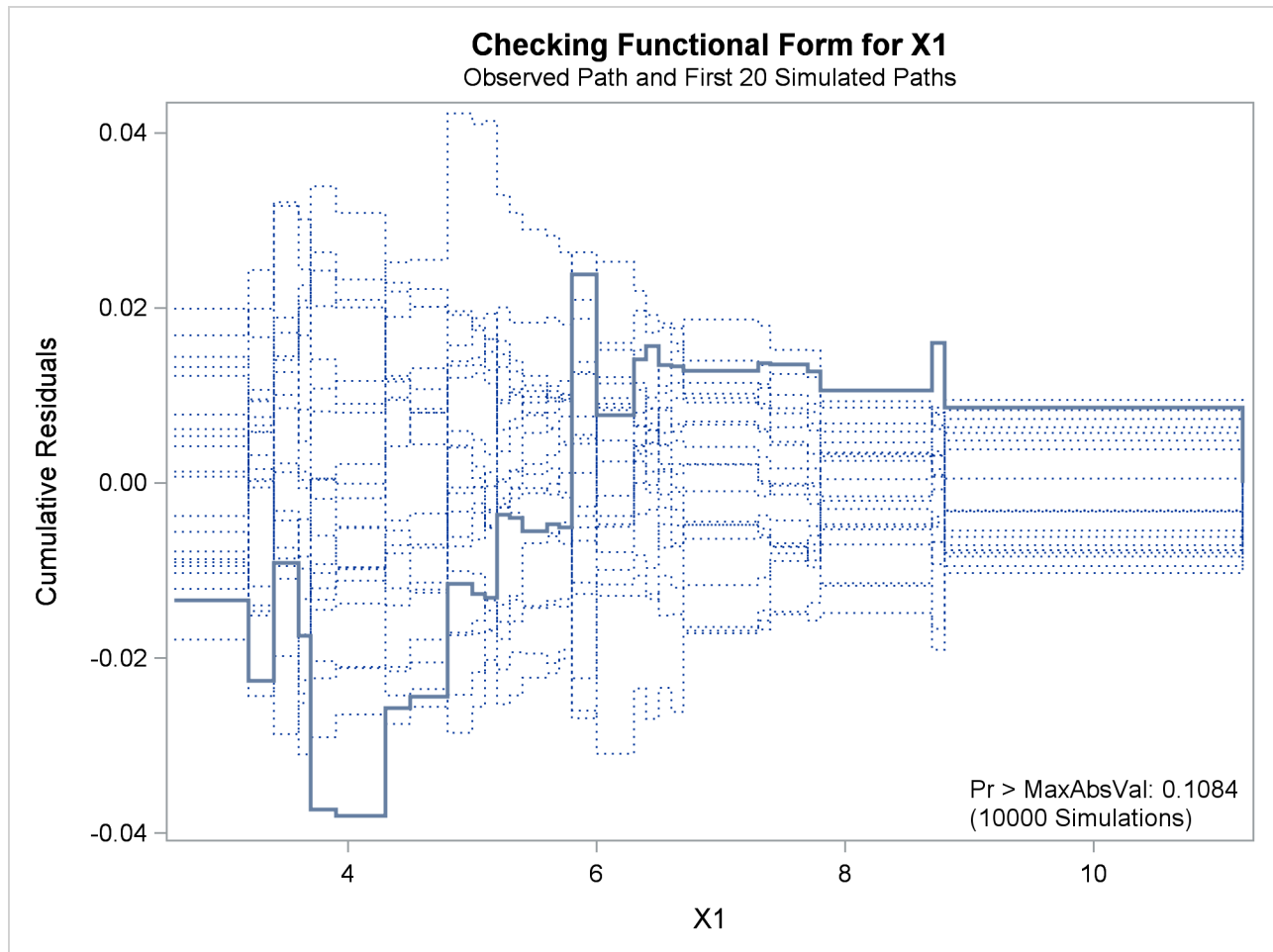
The GENMOD Procedure							
Analysis Of Maximum Likelihood Parameter Estimates							
Parameter	DF	Estimate	Standard Error	Wald 95% Confidence Limits	Wald Chi-Square	Pr >	ChiSq
Intercept	1	0.4836	0.0426	0.4001 0.5672	128.71	<.0001	
X1	1	0.0692	0.0041	0.0612 0.0772	288.17	<.0001	
X2	1	0.0093	0.0004	0.0085 0.0100	590.45	<.0001	
X3	1	0.0095	0.0003	0.0089 0.0101	966.07	<.0001	
Scale	0	0.0469	0.0000	0.0469 0.0469			

NOTE: The scale parameter was estimated by the square root of Pearson's Chi-Square/DOF.

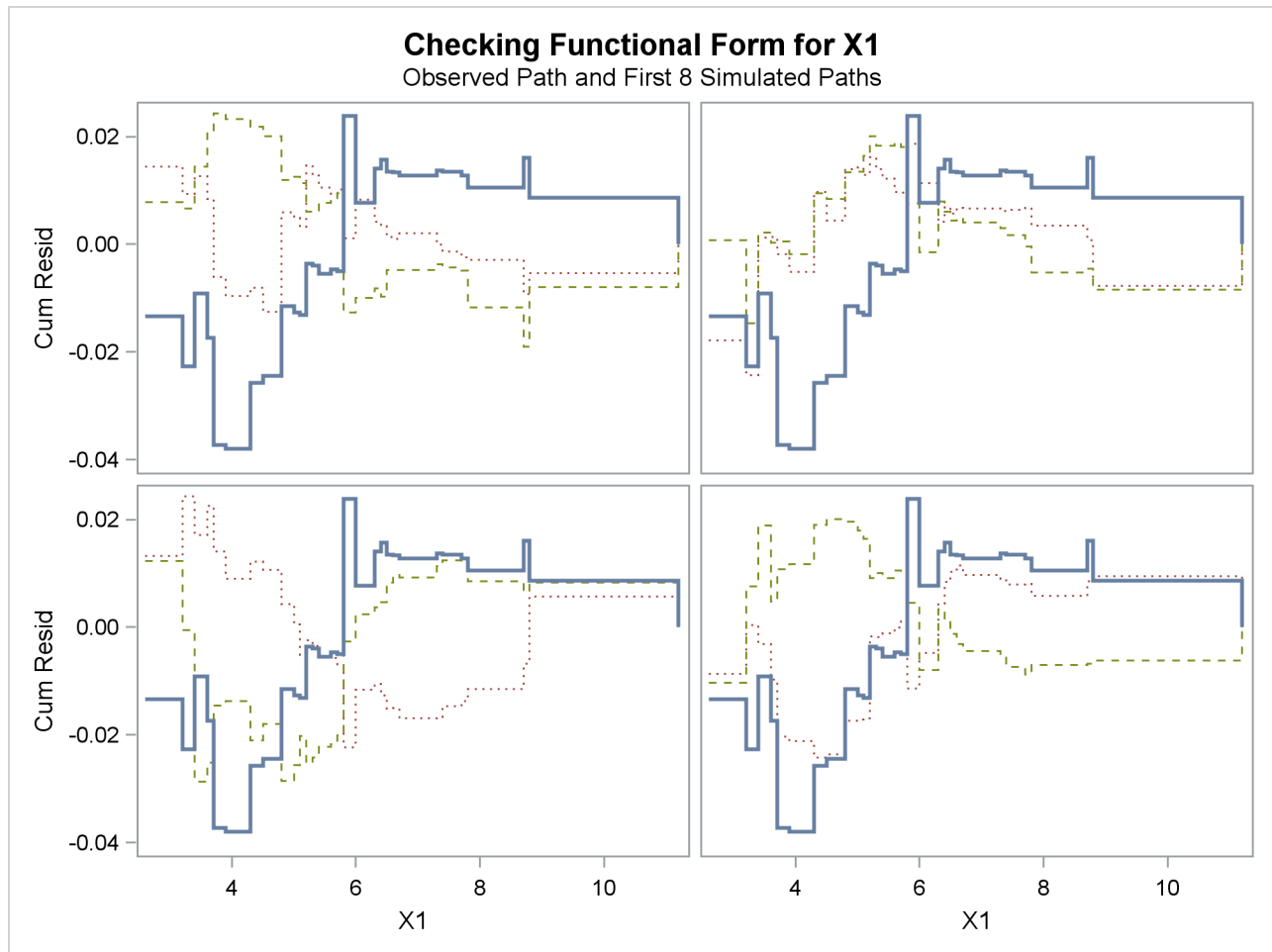
See Lin, Wei, and Ying (2002) for details about model assessment that uses cumulative residual plots. The RESAMPLE= keyword specifies that a p -value be computed based on a sample of 10,000 simulated residual paths. A random number seed is specified by the SEED= keyword for reproducibility. If you do not specify the seed, one is derived from the time of day. The keyword CRPANEL specifies that the panel of four cumulative residual plots shown in [Output 40.8.4](#) be created, each with two simulated paths. The single residual plot with 20 simulated paths in [Output 40.8.3](#) is created by default.

To request these graphs, ODS Graphics must be enabled and you must specify the ASSESS statement. For general information about ODS Graphics, see Chapter 21, “[Statistical Graphics Using ODS](#).” For specific information about the graphics available in the GENMOD procedure, see the section “[ODS Graphics](#)” on page 2856.

Output 40.8.3 Cumulative Residual Plot for Linear X1 Fit



Output 40.8.4 Cumulative Residual Panel Plot for Linear X1 Fit



Output 40.8.5 Summary of Model Assessment

Assessment Summary				
Assessment Variable	Maximum Absolute Value	Replications	Seed	Pr > MaxAbsVal
x1	0.0380	10000	603708000	0.1084

The p -value of 0.1084 reported on [Output 40.8.3](#) and [Output 40.8.5](#) suggests that a more adequate model might be possible. The observed cumulative residuals in [Output 40.8.3](#) and [Output 40.8.4](#), represented by the heavy lines, seem atypical of the simulated curves, represented by the light lines, reinforcing the conclusion that a more appropriate functional form for X1 is possible.

The cumulative residual plots in [Output 40.8.6](#) provide guidance in determining a more appropriate functional form. The four curves were created from simple forms of model misspecification by using simulated data. The mean models of the data and the fitted model are shown in [Table 40.19](#).

Output 40.8.6 Typical Cumulative Residual Patterns

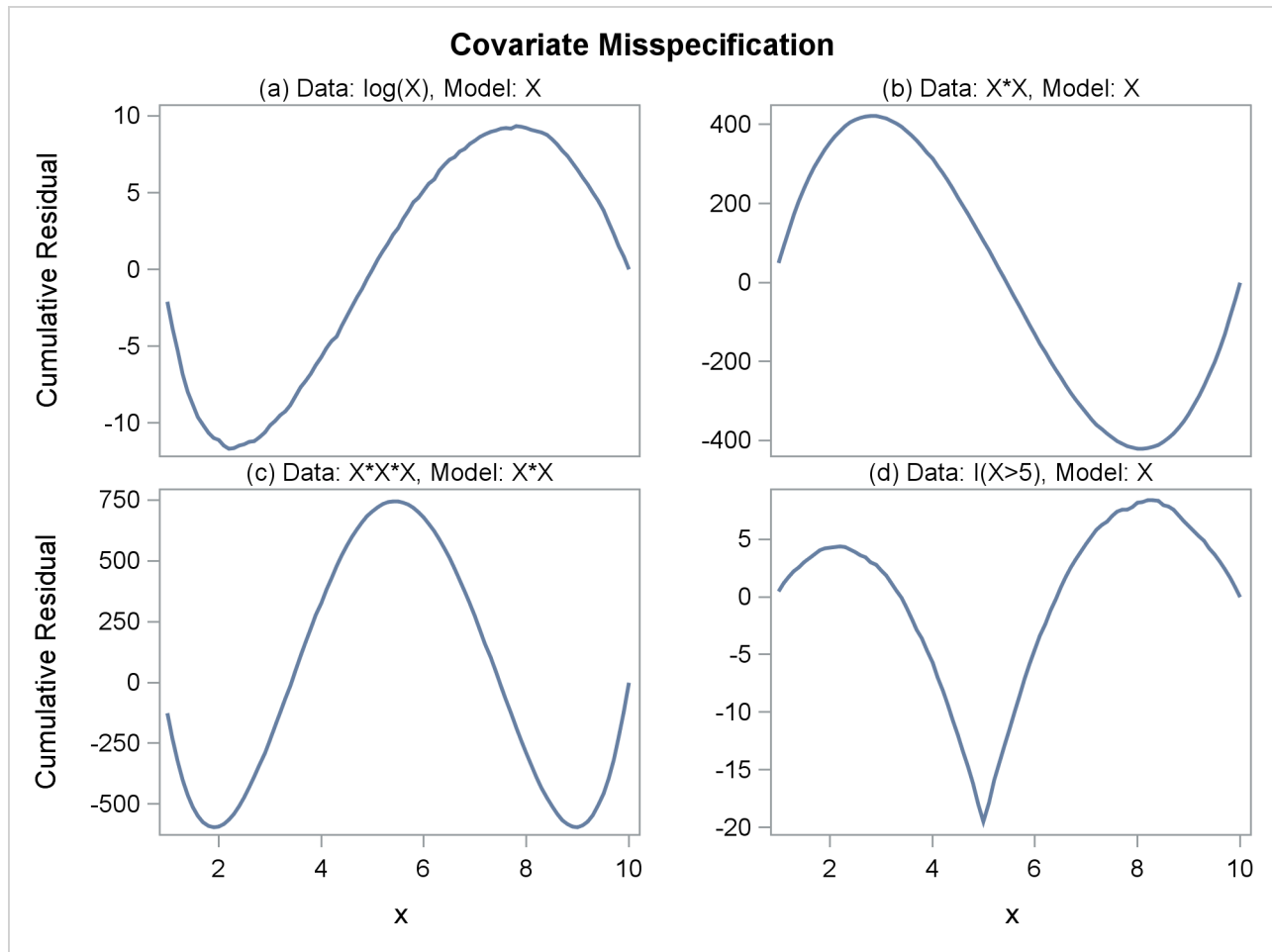


Table 40.19 Model Misspecifications

Plot	Data $E(Y)$	Fitted Model $E(Y)$
(a)	$\log(X)$	X
(b)	$X + X^2$	X
(c)	$X + X^2 + X^3$	$X + X^2$
(d)	$I(X > 5)$	X

The observed cumulative residual pattern in [Output 40.8.3](#) and [Output 40.8.4](#) most resembles the behavior of the curve in plot (a) of [Output 40.8.6](#), indicating that $\log(X_1)$ might be a more appropriate term in the model than X_1 .

The following SAS statements fit a model with `LogX1` in place of `X1` and request a model assessment:

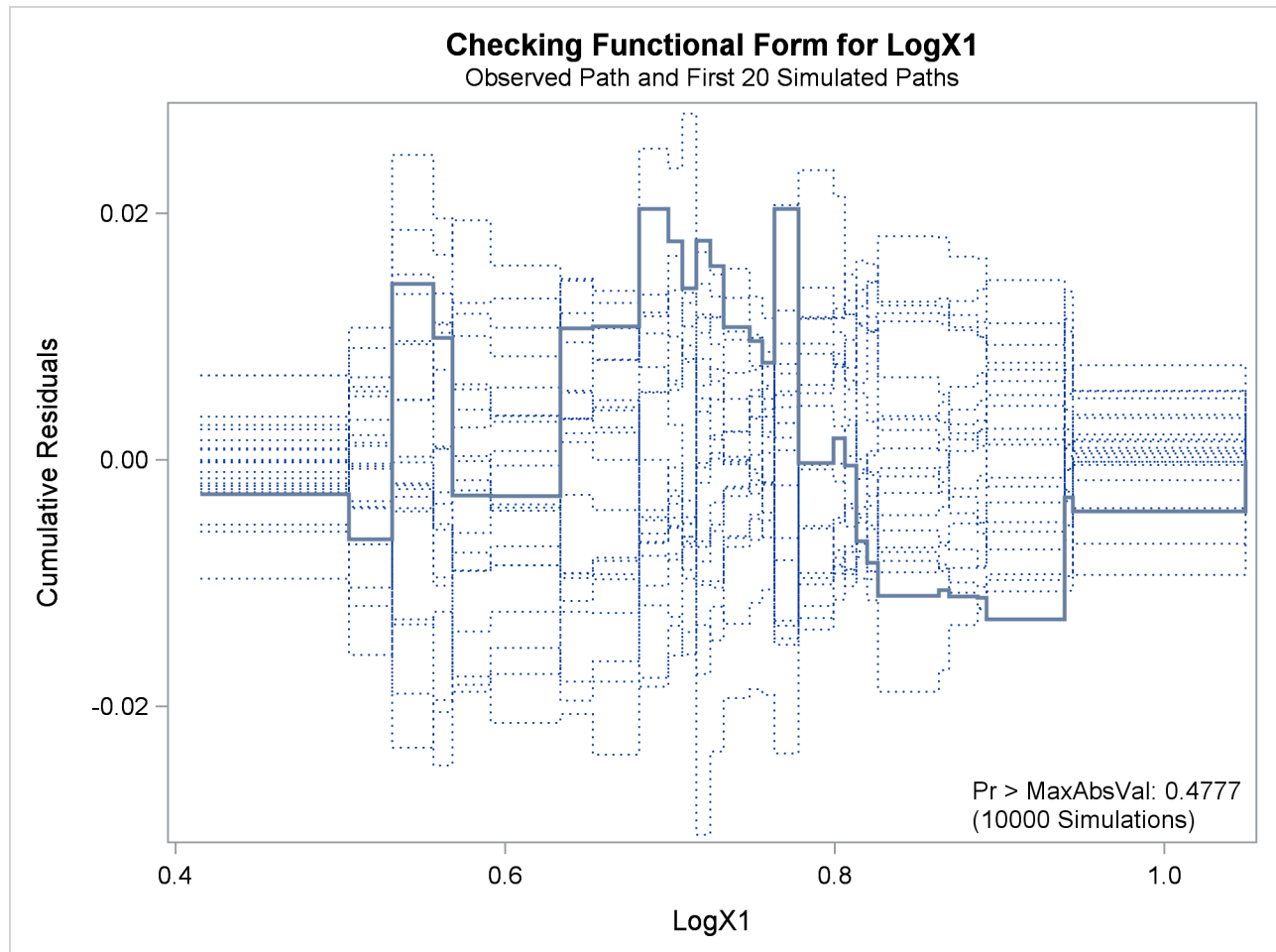
```
proc genmod data=Surg;
  model Y = LogX1 X2 X3 / scale=Pearson;
  assess var=(LogX1) / resample=10000
           seed=603708000;
run;
```


The revised model fit is shown in [Output 40.8.7](#), the p -value from the simulation is 0.4777, and the cumulative residuals plotted in [Output 40.8.8](#) show no systematic trend. The log transformation for X1 is more appropriate. Under the revised model, the p -values for testing the functional forms of X2 and X3 are 0.20 and 0.63, respectively; and the p -value for testing the linearity of the model is 0.65. Thus, the revised model seems reasonable.

Output 40.8.7 Multiple Regression Model with Log(X1)

The GENMOD Procedure							
Analysis Of Maximum Likelihood Parameter Estimates							
Parameter	DF	Estimate	Standard Error	Wald 95% Confidence Limits	Wald Chi-Square	Pr >	ChiSq
Intercept	1	0.1844	0.0504	0.0857 0.2832	13.41		0.0003
LogX1	1	0.9121	0.0491	0.8158 1.0083	345.05		<.0001
X2	1	0.0095	0.0004	0.0088 0.0102	728.62		<.0001
X3	1	0.0096	0.0003	0.0090 0.0101	1139.73		<.0001
Scale	0	0.0434	0.0000	0.0434 0.0434			

NOTE: The scale parameter was estimated by the square root of Pearson's Chi-Square/DOF.

Output 40.8.8 Cumulative Residual Plot with Log(X1)

Example 40.9: Assessment of a Marginal Model for Dependent Data

This example illustrates the use of cumulative residuals to assess the adequacy of a marginal model for dependent data fit by generalized estimating equations (GEEs). The assessment methods are applied to CD4 count data from an AIDS clinical trial reported by Fischl, Richman, and Hansen (1990) and reanalyzed by Lin, Wei, and Ying (2002). The study randomly assigned 360 HIV patients to the drug AZT and 351 patients to placebo. CD4 counts were measured repeatedly over the course of the study. The data used here are the 4328 measurements taken in the first 40 weeks of the study.

The analysis focuses on the time trend of the response. The first model considered is

$$E(y_{ik}) = \beta_0 + \beta_1 T_{ik} + \beta_2 T_{ik}^2 + \beta_3 R_i T_{ik} + \beta_4 R_i T_{ik}^2$$

where T_{ik} is the time (in weeks) of the k th measurement on the i th patient, y_{ik} is the CD4 count at T_{ik} for the i th patient, and R_i is the indicator of AZT for the i th patient. Normal errors and an independent working correlation are assumed.

The following statements create the SAS data set `cd4`:

```

data cd4;
  input Id Y Time Time2 TrtTime TrtTime2;
  Time3 = Time2 * Time;
  TrtTime3 = TrtTime2 * Time;
  datalines;
1      264.00024      -0.28571      0.08163      -0.28571      0.08163
1      175.00070      4.14286      17.16327      4.14286      17.16327
1      306.00150      8.14286      66.30612      8.14286      66.30612
1      331.99835      12.14286     147.44898     12.14286     147.44898
1      309.99929      16.14286     260.59184     16.14286     260.59184
1      185.00077      28.71429     824.51020     28.71429     824.51020
1      175.00070      40.14286     1611.44898     40.14286     1611.44898
2      574.99998      -0.57143      0.32653      0.00000      0.00000

  ... more lines ...

711    363.99859      8.14286      66.30612      8.14286      66.30612
711    488.00224      12.14286     147.44898     12.14286     147.44898
711    240.00026      18.14286     329.16327     18.14286     329.16327
;

```

The following SAS statements fit the preceding model, create the cumulative residual plot in [Output 40.9.1](#), and compute a p -value for the model.

To request these graphs, ODS Graphics must be enabled and you must specify the ASSESS statement. For general information about ODS Graphics, see Chapter 21, “[Statistical Graphics Using ODS.](#)” For specific information about the graphics available in the GENMOD procedure, see the section “[ODS Graphics](#)” on page 2856.

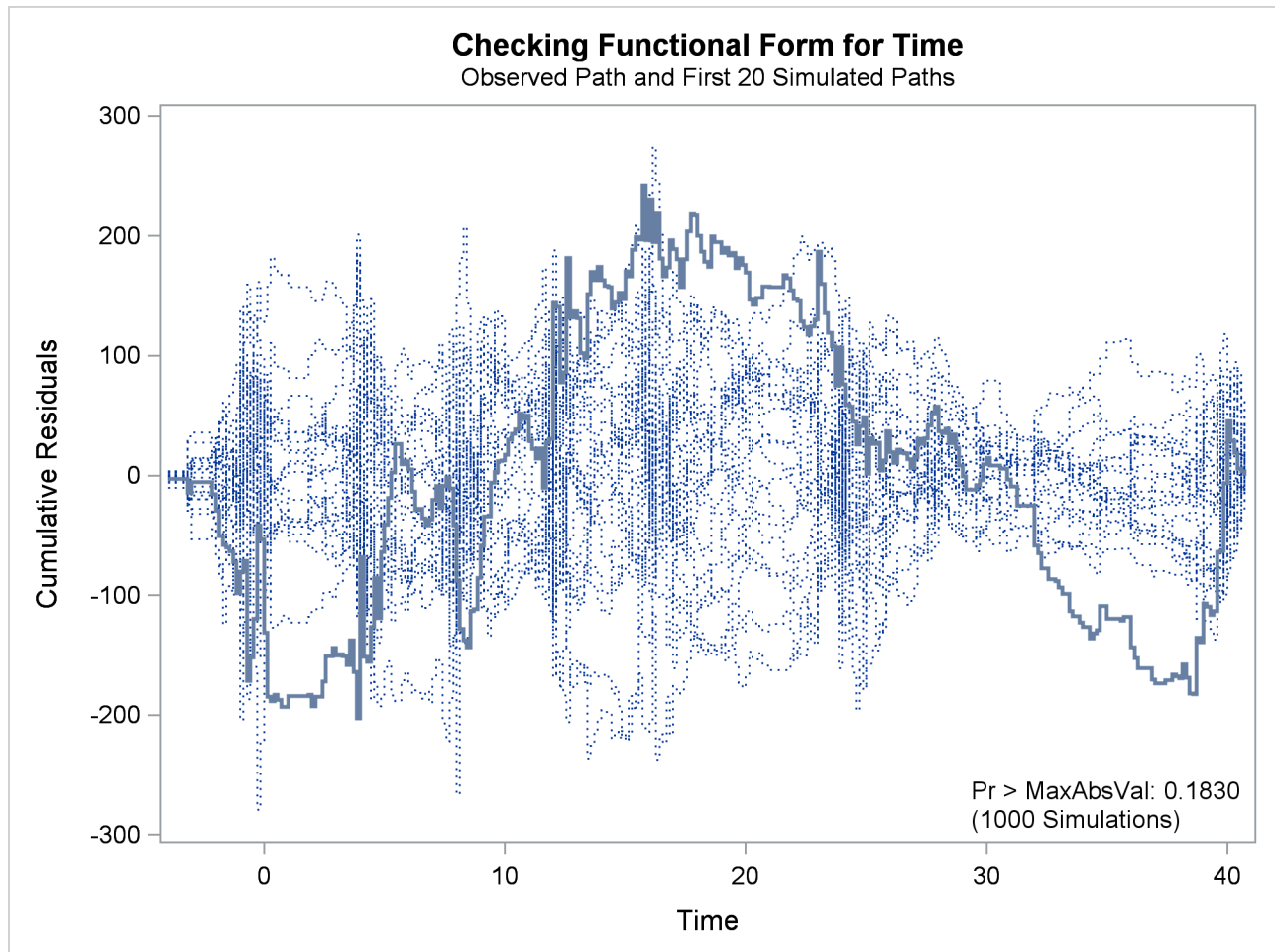
Here, the SAS data set variables Time, Time2, TrtTime, and TrtTime2 correspond to T_{ik} , T_{ik}^2 , $R_i T_{ik}$, and $R_i T_{ik}^2$, respectively. The variable Id identifies individual patients.

```

ods graphics on;

proc genmod data=cd4;
  class Id;
  model Y = Time Time2 TrtTime TrtTime2;
  repeated sub=Id;
  assess var=(Time) / resample
                    seed=603708000;
run;

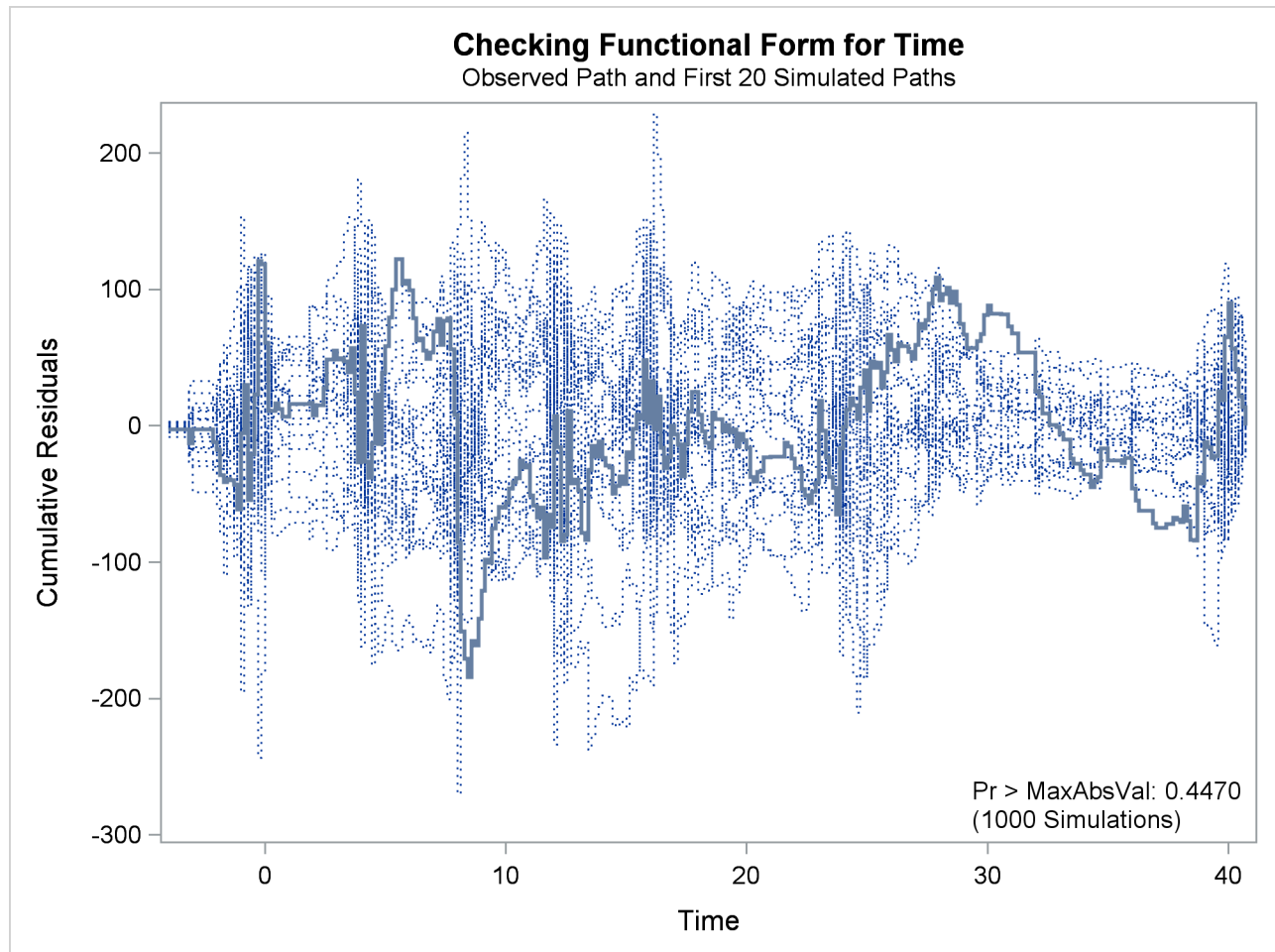
```

Output 40.9.1 Cumulative Residual Plot for Quadratic Time Fit

The cumulative residual plot in [Output 40.9.1](#) displays cumulative residuals versus time for the model and 20 simulated realizations. The associated p -value, also shown in [Output 40.9.1](#), is 0.18. These results indicate that a more satisfactory model might be possible. The observed cumulative residual pattern most resembles plot (c) in [Output 40.8.6](#), suggesting cubic time trends.

The following SAS statements fit the model, create the plot in [Output 40.9.2](#), and compute a p -value for a model with the additional terms T_{ik}^3 and $R_i T_{ik}^3$:

```
proc genmod data=cd4;
  class Id;
  model Y = Time Time2 Time3 TrtTime TrtTime2 TrtTime3;
  repeated sub=Id;
  assess var=(Time) / resample
              seed=603708000;
run;
```

Output 40.9.2 Cumulative Residual Plot for Cubic Time Fit

The observed cumulative residual pattern appears more typical of the simulated realizations, and the p -value is 0.45, indicating that the model with cubic time trends is more appropriate.

Example 40.10: Bayesian Analysis of a Poisson Regression Model

This example illustrates a Bayesian analysis of a log-linear Poisson regression model. Consider the following data on patients from clinical trials. The data set is a subset of the data described in Ibrahim, Chen, and Lipsitz (1999).

```

data Liver;
  input X1-X6 Y;
  datalines;
19.1358    50.0110    51.000    0    0    1    3
23.5970    18.4959    3.429    0    0    1    9
20.0474    56.7699    3.429    1    1    0    6
28.0277    59.7836    4.000    0    0    1    6
28.6851    74.1589    5.714    1    0    1    1
18.8092    31.0630    2.286    0    1    1    61

```

```

28.7201    52.9178    37.286    1    0    1    6
21.3669    61.6603    54.143    0    1    1    6
23.7332    42.2904    0.571    1    0    1    21
20.4783    22.1260    19.000    1    0    1    6

... more lines ...

17.0993    48.8384    3.000    0    0    0    9
19.1327    65.3425    2.571    1    0    0    1
17.3010    51.4493    4.429    1    0    0    6
;
```

The primary interest is in prediction of the number of cancerous liver nodes when a patient enters the trials, by using six other baseline characteristics. The number of nodes is modeled by a Poisson regression model with the six baseline characteristics as covariates. The response and regression variables are as follows:

Y	Number of Cancerous Liver Nodes
X1	Body Mass Index
X2	Age, in Years
X3	Time Since Diagnosis of Disease, in Weeks
X4	Two Biochemical Markers (each classified as normal=1 or abnormal=0)
X5	Anti Hepatitis B Antigen
X6	Associated Jaundice (yes=1, no=0)

Two analyses are performed using PROC GENMOD. The first analysis uses noninformative normal prior distributions, and the second analysis uses an informative normal prior for one of the regression parameters.

In the following BAYES statement, COEFFPRIOR=NORMAL specifies a noninformative independent normal prior distribution with zero mean and variance 10^6 for each parameter.

The initial analysis is performed using PROC GENMOD to obtain Bayesian estimates of the regression coefficients by using the following SAS statements:

```

proc genmod data=Liver;
  model Y = X1-X6 / dist=Poisson link=log;
  bayes seed=1 coeffprior=normal;
run;
```

Maximum likelihood estimates of the model parameters are computed by default. These are shown in the “Analysis of Maximum Likelihood Parameter Estimates” table in [Output 40.10.1](#).

Output 40.10.1 Maximum Likelihood Parameter Estimates

The GENMOD Procedure					
Bayesian Analysis					
Analysis Of Maximum Likelihood Parameter Estimates					
Parameter	DF	Estimate	Standard Error	Wald	95% Confidence Limits
Intercept	1	2.4508	0.2284	2.0032	2.8984
X1	1	-0.0044	0.0080	-0.0201	0.0114
X2	1	-0.0135	0.0024	-0.0181	-0.0088
X3	1	-0.0029	0.0022	-0.0072	0.0014
X4	1	-0.2715	0.0795	-0.4272	-0.1157
X5	1	0.3215	0.0832	0.1585	0.4845
X6	1	0.2077	0.0827	0.0456	0.3698
Scale	0	1.0000	0.0000	1.0000	1.0000

NOTE: The scale parameter was held fixed.

Noninformative independent normal prior distributions with zero means and variances of 10^6 were used in the initial analysis. These are shown in [Output 40.10.2](#).

Output 40.10.2 Regression Coefficient Priors

The GENMOD Procedure		
Bayesian Analysis		
Independent Normal Prior for Regression Coefficients		
Parameter	Mean	Precision
Intercept	0	1E-6
X1	0	1E-6
X2	0	1E-6
X3	0	1E-6
X4	0	1E-6
X5	0	1E-6
X6	0	1E-6

Initial values for the Markov chain are listed in the “Initial Values and Seeds” table in [Output 40.10.3](#). The random number seed is also listed so that you can reproduce the analysis. Since no seed was specified, the seed shown was derived from the time of day.

Output 40.10.3 MCMC Initial Values and Seeds

Initial Values of the Chain						
Chain	Seed	Intercept	X1	X2	X3	X4
1	1	2.450813	-0.00435	-0.01347	-0.00291	-0.27149
Initial Values of the Chain						
		X5	X6			
		0.321507	0.207713			

Summary statistics for the posterior sample are displayed in the “Fit Statistics,” “Descriptive Statistics for the Posterior Sample,” “Interval Statistics for the Posterior Sample,” and “Posterior Correlation Matrix” tables in [Output 40.10.4](#), [Output 40.10.5](#), [Output 40.10.6](#), and [Output 40.10.7](#), respectively. Since noninformative prior distributions for the regression coefficients were used, the mean and standard deviations of the posterior distributions for the model parameters are close to the maximum likelihood estimates and standard errors.

Output 40.10.4 Fit Statistics

Fit Statistics	
DIC (smaller is better)	829.810
pD (effective number of parameters)	7.005

Output 40.10.5 Descriptive Statistics

The GENMOD Procedure						
Bayesian Analysis						
Posterior Summaries						
Parameter	N	Mean	Standard Deviation	Percentiles		
				25%	50%	75%
Intercept	10000	2.4483	0.2320	2.2903	2.4493	2.6093
X1	10000	-0.00475	0.00809	-0.0101	-0.00466	0.000851
X2	10000	-0.0134	0.00237	-0.0150	-0.0134	-0.0118
X3	10000	-0.00303	0.00220	-0.00445	-0.00298	-0.00150
X4	10000	-0.2703	0.0799	-0.3241	-0.2725	-0.2190
X5	10000	0.3202	0.0828	0.2642	0.3209	0.3775
X6	10000	0.2106	0.0838	0.1533	0.2111	0.2663

Output 40.10.6 Interval Statistics

Parameter	Alpha	Posterior Intervals			
		Equal-Tail Interval		HPD Interval	
Intercept	0.050	1.9903	2.9059	2.0289	2.9321
X1	0.050	-0.0209	0.0108	-0.0211	0.0106
X2	0.050	-0.0181	-0.00870	-0.0184	-0.00908
X3	0.050	-0.00761	0.00105	-0.00745	0.00113
X4	0.050	-0.4257	-0.1063	-0.4314	-0.1152
X5	0.050	0.1563	0.4804	0.1574	0.4811
X6	0.050	0.0450	0.3777	0.0468	0.3788

Output 40.10.7 Posterior Sample Correlation Matrix

Parameter	Posterior Correlation Matrix						
	Intercept	X1	X2	X3	X4	X5	X6
Intercept	1.000	-0.708	-0.432	-0.046	-0.261	-0.185	-0.422
X1	-0.708	1.000	-0.202	-0.047	-0.035	0.078	0.129
X2	-0.432	-0.202	1.000	0.035	0.076	0.054	0.117
X3	-0.046	-0.047	0.035	1.000	0.027	-0.042	-0.077
X4	-0.261	-0.035	0.076	0.027	1.000	-0.024	0.127
X5	-0.185	0.078	0.054	-0.042	-0.024	1.000	-0.037
X6	-0.422	0.129	0.117	-0.077	0.127	-0.037	1.000

Posterior sample autocorrelations for each model parameter are shown in [Output 40.10.8](#). The autocorrelation after 10 lags is negligible for all parameters, indicating good mixing in the Markov chain.

Output 40.10.8 Posterior Sample Autocorrelations

The GENMOD Procedure				
Bayesian Analysis				
Posterior Autocorrelations				
Parameter	Lag 1	Lag 5	Lag 10	Lag 50
Intercept	0.3037	0.0152	0.0095	-0.0170
X1	0.3398	0.0025	0.0003	0.0052
X2	0.3036	0.0061	0.0003	-0.0062
X3	0.3489	0.0190	-0.0064	-0.0210
X4	0.2868	0.0213	0.0157	-0.0107
X5	0.2854	0.0108	-0.0288	-0.0012
X6	0.3078	0.0230	0.0073	0.0062

The p -values for the Geweke test statistics shown in [Output 40.10.9](#) all indicate convergence of the MCMC. See the section “Assessing Markov Chain Convergence” on page 139 for more information about convergence diagnostics and their interpretation.

Output 40.10.9 Geweke Diagnostic Statistics

Geweke Diagnostics		
Parameter	z	Pr > z
Intercept	-0.6533	0.5135
X1	0.3418	0.7325
X2	0.3609	0.7182
X3	-0.3345	0.7380
X4	0.2851	0.7755
X5	-0.5266	0.5985
X6	1.1285	0.2591

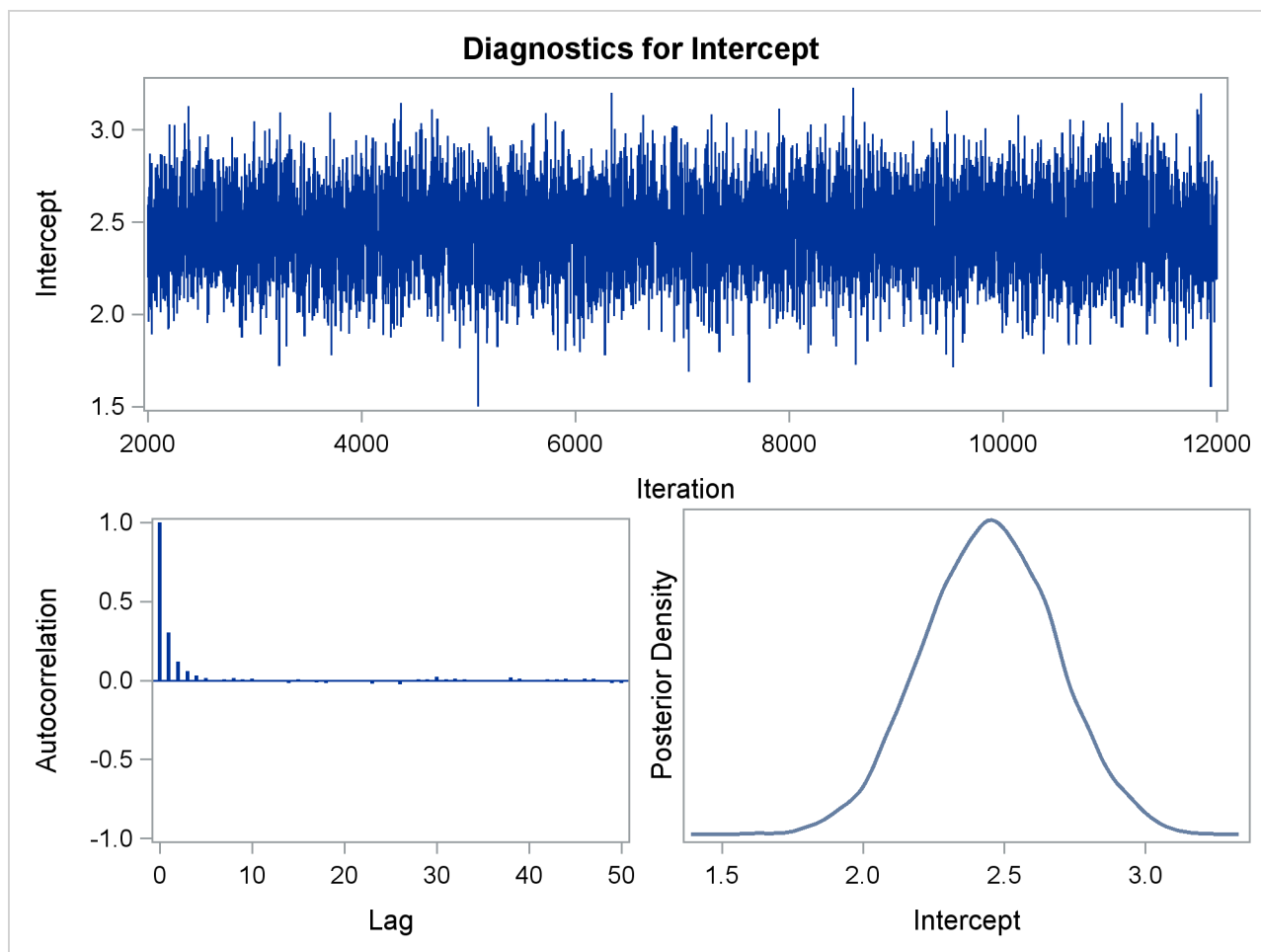
The effective sample sizes for each parameter are shown in [Output 40.10.10](#).

Output 40.10.10 Effective Sample Sizes

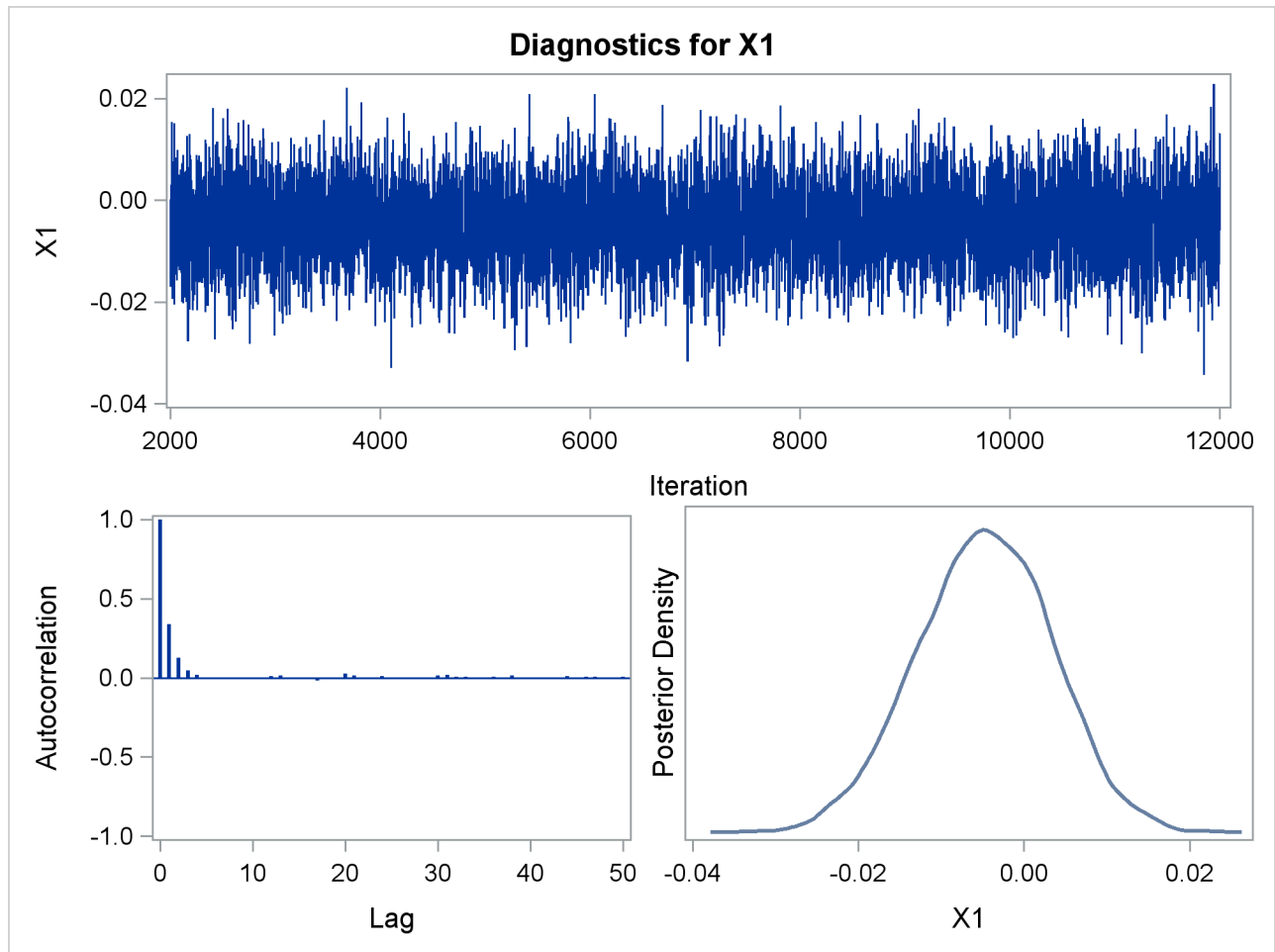
Parameter	ESS	Autocorrelation	
		Time	Efficiency
Intercept	4880.3	2.0491	0.4880
X1	4844.2	2.0643	0.4844
X2	5139.3	1.9458	0.5139
X3	4551.2	2.1972	0.4551
X4	4953.6	2.0187	0.4954
X5	5330.5	1.8760	0.5331
X6	4988.1	2.0048	0.4988

Trace, autocorrelation, and density plots for the seven model parameters are shown in [Output 40.10.11](#) through [Output 40.10.17](#). All indicate satisfactory convergence of the Markov chain.

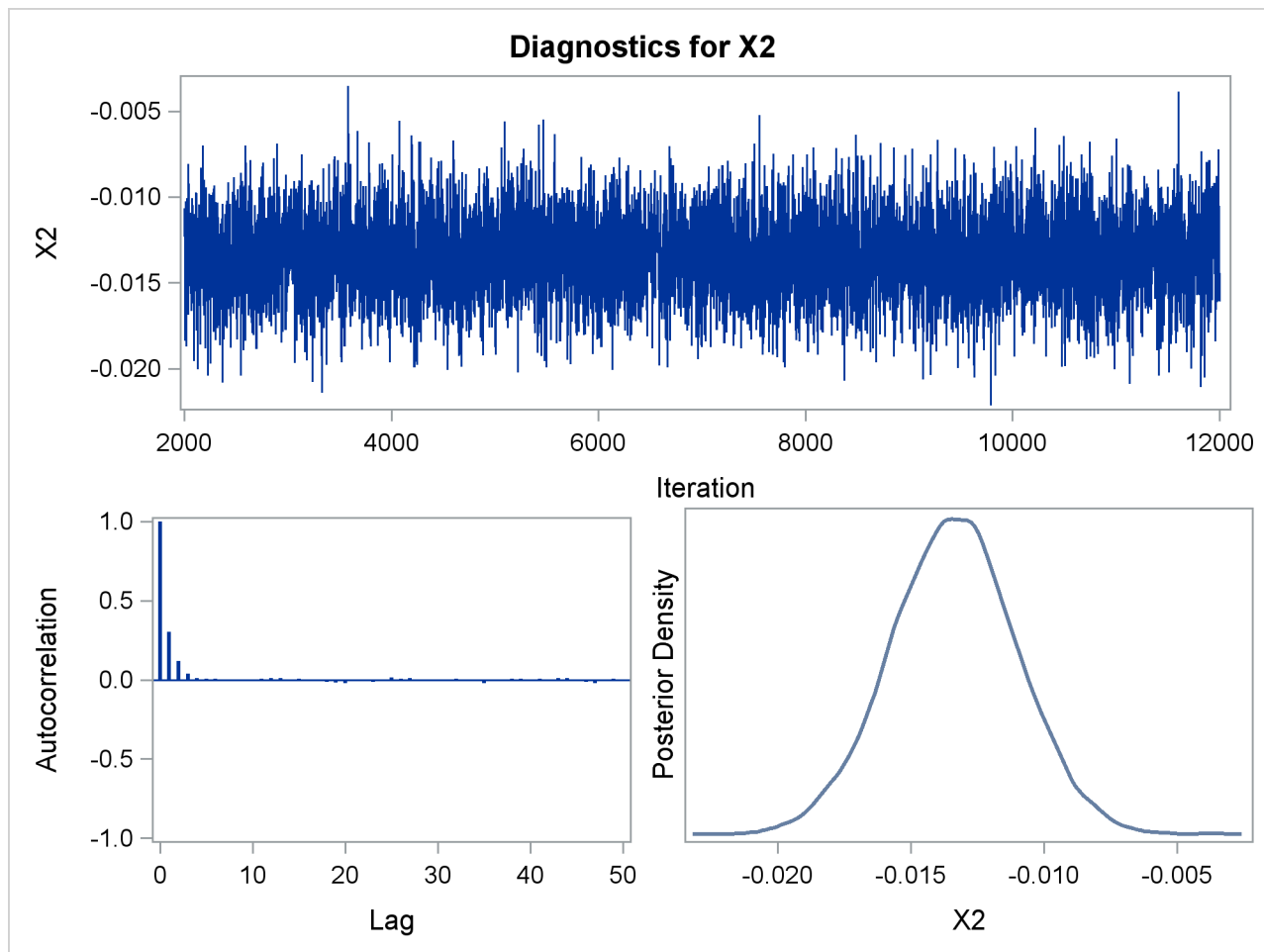
Output 40.10.11 Diagnostic Plots for Intercept



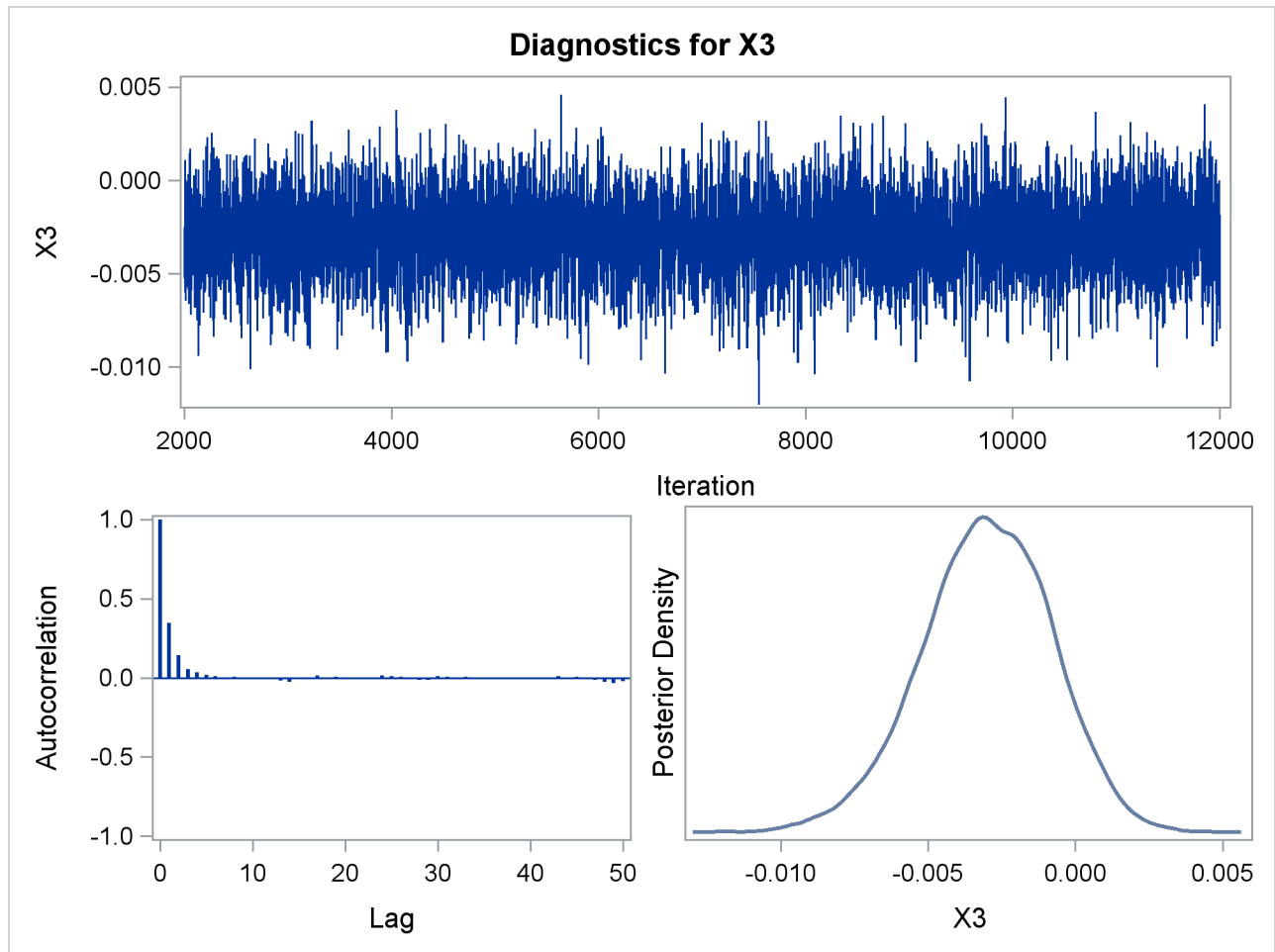
Output 40.10.12 Diagnostic Plots for X1



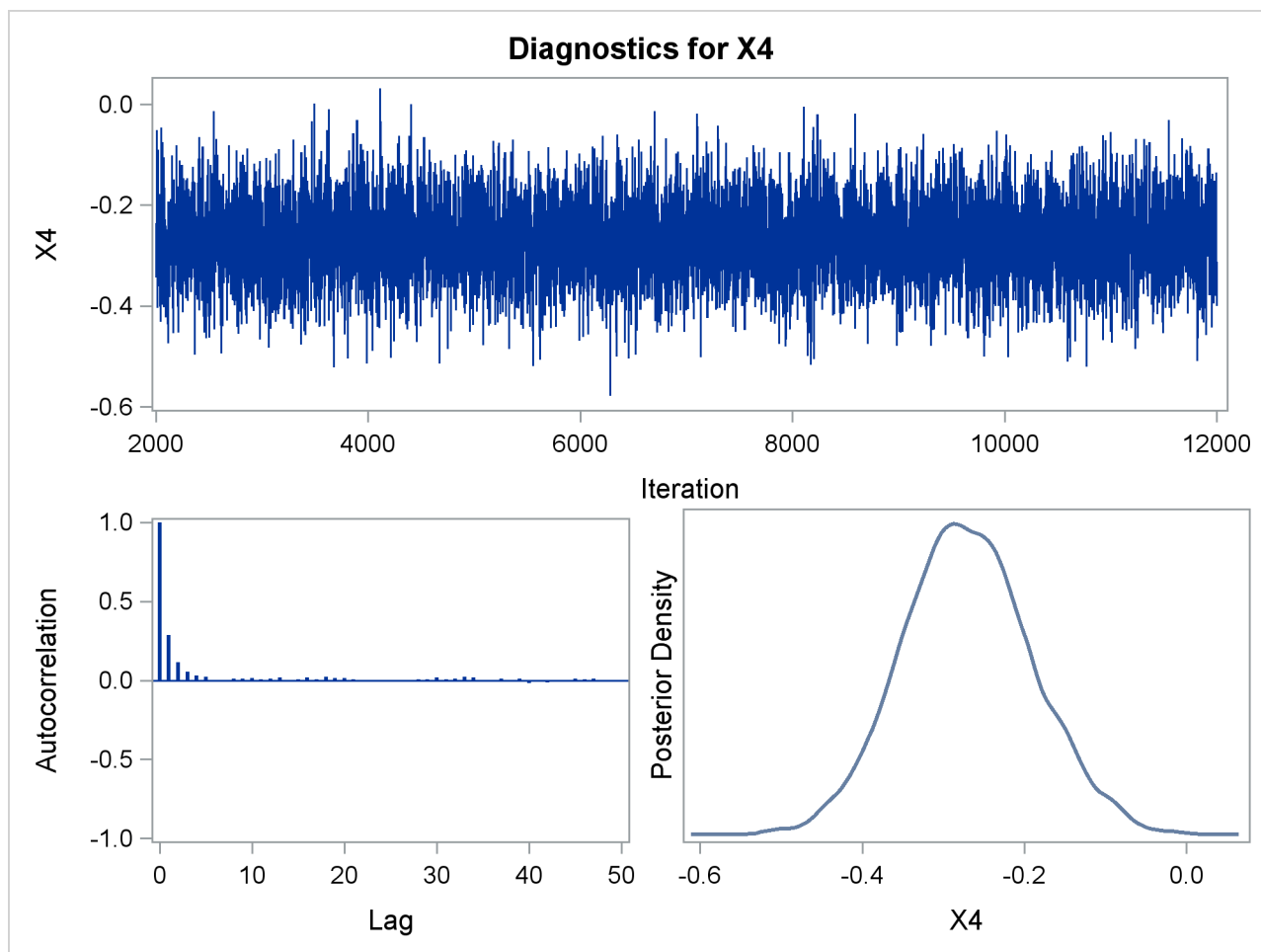
Output 40.10.13 Diagnostic Plots for X2



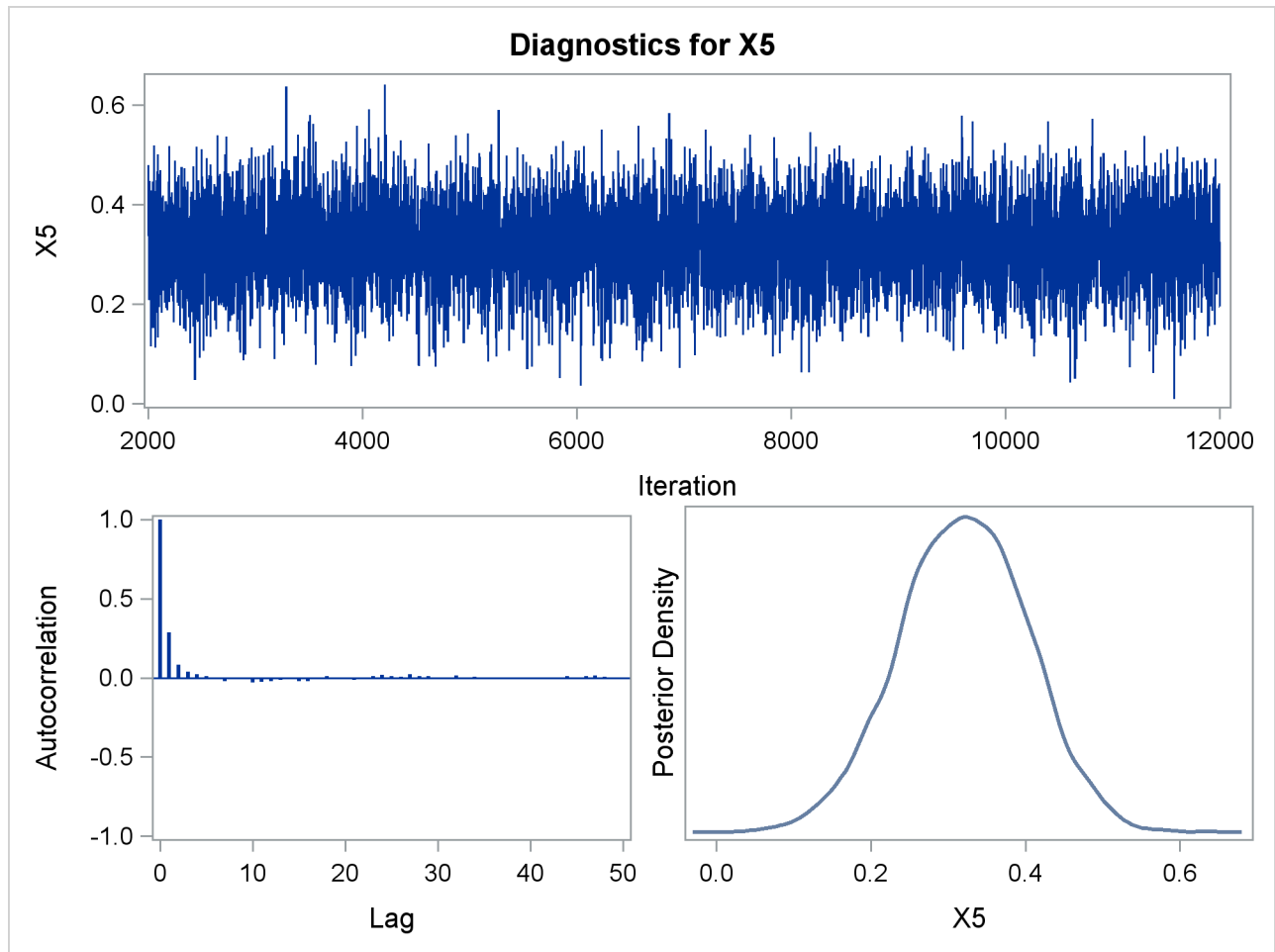
Output 40.10.14 Diagnostic Plots for X3



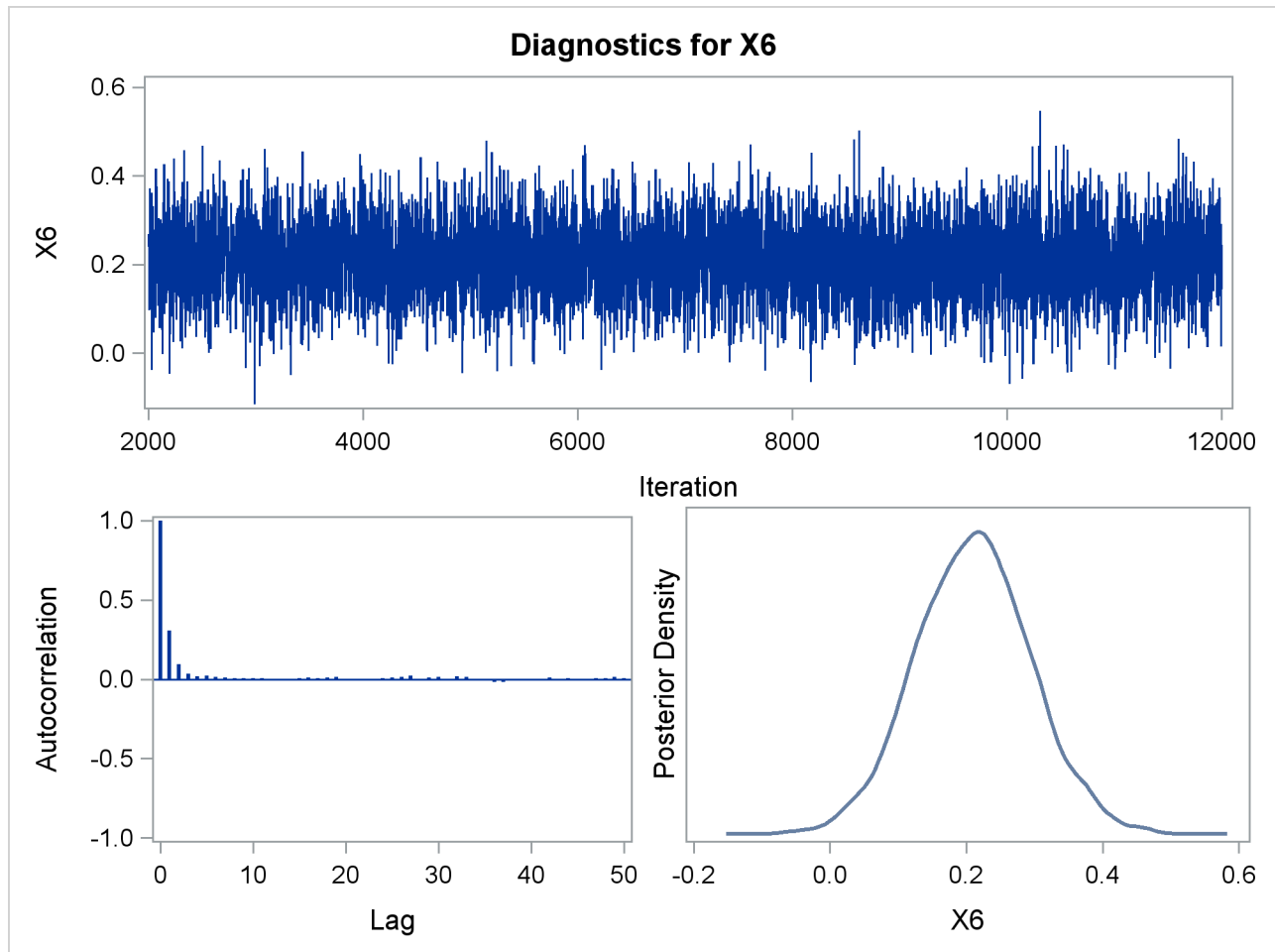
Output 40.10.15 Diagnostic Plots for X4



Output 40.10.16 Diagnostic Plots for X5



Output 40.10.17 Diagnostic Plots for X6



In order to illustrate the use of an informative prior distribution, suppose that researchers expect that a unit increase in body mass index (X_1) will be associated with an increase in the mean number of nodes of between 10% and 20%, and they want to incorporate this prior knowledge in the Bayesian analysis. For log-linear models, the mean and linear predictor are related by $\log(\mu_i) = \mathbf{x}'_i \boldsymbol{\beta}$. If X_{1_1} and X_{1_2} are two values of body mass index, μ_1 and μ_2 are the two mean values, and all other covariates remain equal for the two values of X_1 , then

$$\frac{\mu_1}{\mu_2} = \exp(\beta(X_{1_1} - X_{1_2}))$$

so that for a unit change in X_1 ,

$$\frac{\mu_1}{\mu_2} = \exp(\beta)$$

If $1.1 \leq \frac{\mu_1}{\mu_2} \leq 1.2$, then $1.1 \leq \exp(\beta) \leq 1.2$, or $0.095 \leq \beta \leq 0.182$. This gives you guidance in specifying a prior distribution for the β for body mass index. Taking the mean of the prior normal distribution to be

the midrange of the values of β , and taking $\mu \pm 2\sigma$ to be the extremes of the range, an $N(0.1385, 0.0005)$ is the resulting prior distribution. The second analysis uses this informative normal prior distribution for the coefficient of X1 and uses independent noninformative normal priors with zero means and variances equal to 10^6 for the remaining model regression parameters.

In the following BAYES statement, COEFFPRIOR=NORMAL(INPUT=NormalPrior) specifies the normal prior distribution for the regression coefficients with means and variances contained in the data set NormalPrior.

An analysis is performed using PROC GENMOD to obtain Bayesian estimates of the regression coefficients by using the following SAS statements:

```
data NormalPrior;
  input _type_ $ Intercept X1-X6;
  datalines;
Var 1e6  0.0005      1e6      1e6      1e6      1e6      1e6
Mean 0.0  0.1385      0.0      0.0      0.0      0.0      0.0
;

proc genmod data=Liver;
  model Y = X1-X6 / dist=Poisson link=log;
  bayes seed=1 plots=none coeffprior=normal(input=NormalPrior);
run;
```

The prior distributions for the regression parameters are shown in [Output 40.10.18](#).

Output 40.10.18 Regression Coefficient Priors

The GENMOD Procedure		
Bayesian Analysis		
Independent Normal Prior for Regression Coefficients		
Parameter	Mean	Precision
Intercept	0	1E-6
X1	0.1385	2000
X2	0	1E-6
X3	0	1E-6
X4	0	1E-6
X5	0	1E-6
X6	0	1E-6

Initial values for the MCMC are shown in [Output 40.10.19](#). The initial values of the covariates are joint estimates of their posterior modes. The prior distribution for X1 is informative, so the initial value of X1 is further from the MLE than the rest of the covariates. Initial values for the rest of the covariates are close to their MLEs, since noninformative prior distributions were specified for them.

Output 40.10.19 MCMC Initial Values and Seeds

Initial Values of the Chain						
Chain	Seed	Intercept	X1	X2	X3	X4
1	1	2.14282	0.010595	-0.01434	-0.00301	-0.28062
Initial Values of the Chain						
		X5	X6			
		0.334983	0.231213			

Goodness-of-fit, summary, and interval statistics are shown in [Output 40.10.20](#). Except for X1, the statistics shown in [Output 40.10.20](#) are very similar to the previous statistics for noninformative priors shown in [Output 40.10.4](#) through [Output 40.10.7](#). The point estimate for X1 is now positive. This is expected because the prior distribution on β_1 is quite informative. The distribution reflects the belief that the coefficient is positive. The $N(0.1385, 0.0005)$ distribution places the majority of its probability density on positive values. As a result, the posterior density of β_1 places more likelihood on positive values than in the noninformative case.

Output 40.10.20 Fit Statistics

Fit Statistics						
DIC (smaller is better)		833.074				
pD (effective number of parameters)		6.869				
The GENMOD Procedure						
Bayesian Analysis						
Posterior Summaries						
Parameter	N	Mean	Standard Deviation	Percentiles		
				25%	50%	75%
Intercept	10000	2.1419	0.2157	1.9965	2.1430	2.2894
X1	10000	0.0103	0.00684	0.00573	0.0104	0.0150
X2	10000	-0.0143	0.00233	-0.0159	-0.0142	-0.0127
X3	10000	-0.00318	0.00218	-0.00467	-0.00314	-0.00170
X4	10000	-0.2806	0.0800	-0.3336	-0.2793	-0.2266
X5	10000	0.3341	0.0832	0.2788	0.3341	0.3906
X6	10000	0.2333	0.0826	0.1774	0.2325	0.2880

Output 40.10.20 *continued*

Parameter	Alpha	Posterior Intervals			
		Equal-Tail Interval		HPD Interval	
Intercept	0.050	1.7225	2.5574	1.7293	2.5632
X1	0.050	-0.00344	0.0235	-0.00345	0.0234
X2	0.050	-0.0188	-0.00970	-0.0189	-0.00980
X3	0.050	-0.00757	0.00108	-0.00733	0.00121
X4	0.050	-0.4365	-0.1200	-0.4391	-0.1256
X5	0.050	0.1657	0.4966	0.1682	0.4987
X6	0.050	0.0695	0.3959	0.0725	0.3981

Example 40.11: Exact Poisson Regression

The following data, taken from Cox and Snell (1989, pp. 10–11), consists of the number, Notready, of ingots that are not ready for rolling, out of Total tested, for several combinations of heating time and soaking time:

```
data ingots;
  input Heat Soak Notready Total @@;
  lnTotal= log(Total);
  datalines;
7 1.0 0 10 14 1.0 0 31 27 1.0 1 56 51 1.0 3 13
7 1.7 0 17 14 1.7 0 43 27 1.7 4 44 51 1.7 0 1
7 2.2 0 7 14 2.2 2 33 27 2.2 0 21 51 2.2 0 1
7 2.8 0 12 14 2.8 0 31 27 2.8 1 22 51 4.0 0 1
7 4.0 0 9 14 4.0 0 19 27 4.0 1 16
;
```

The following invocation of PROC GENMOD fits an asymptotic (unconditional) Poisson regression model to the data. The variable Notready is specified as the response variable, and the continuous predictors Heat and Soak are defined in the CLASS statement as categorical predictors that use reference coding. Specifying the offset variable as lnTotal enables you to model the ratio Notready/Total.

```
proc genmod data=ingots;
  class Heat Soak / param=ref;
  model Notready=Heat Soak / offset=lnTotal dist=poisson link=log;
  exact Heat Soak / joint estimate;
  exactoptions statustime=10;
run;
```

The EXACT statement is specified to additionally fit an exact conditional Poisson regression model. Specifying the lnTotal offset variable models the ratio Notready/Total; in this case, the Total variable contains the largest possible response value for each observation. The JOINT option produces a joint test for the significance of the covariates, along with the usual marginal tests. The ESTIMATE option produces exact parameter estimates for the covariates. The STATUSTIME=10 option is specified in the EXACTOPTIONS statement for monitoring the progress of the results; this example can take several minutes to complete due to the JOINT option. If you run out of memory, see the SAS Companion for your system for information about how to increase the available memory.

The “Criteria For Assessing Goodness Of Fit” table is displayed in [Output 40.11.1](#). Comparing the deviance of 10.9363 to an asymptotic chi-square distribution with 11 degrees of freedom, you find that the p -value is 0.449. This indicates that the specified model fits the data reasonably well.

Output 40.11.1 Unconditional Goodness of Fit Criteria

The GENMOD Procedure			
Criteria For Assessing Goodness Of Fit			
Criterion	DF	Value	Value/DF
Deviance	11	10.9363	0.9942
Scaled Deviance	11	10.9363	0.9942
Pearson Chi-Square	11	9.3722	0.8520
Scaled Pearson X2	11	9.3722	0.8520
Log Likelihood		-7.2408	
Full Log Likelihood		-12.9038	
AIC (smaller is better)		41.8076	
AICC (smaller is better)		56.2076	
BIC (smaller is better)		49.3631	

From the “Analysis Of Parameter Estimates” table in [Output 40.11.2](#), you can see that only two of the Heat parameters are deemed significant. Looking at the standard errors, you can see that the unconditional analysis had convergence difficulties with the Heat=7 parameter (Standard Error=264324.6), which means you cannot fit this unconditional Poisson regression model to this data.

Output 40.11.2 Unconditional Maximum Likelihood Parameter Estimates

Analysis Of Maximum Likelihood Parameter Estimates						
Parameter	DF	Estimate	Standard Error	Wald	95% Confidence Limits	Wald Chi-Square
Intercept	1	-1.5700	1.1657	-3.8548	0.7147	1.81
Heat	7	-27.6129	264324.6	-518094	518039.0	0.00
Heat	14	-3.0107	1.0025	-4.9756	-1.0458	9.02
Heat	27	-1.7180	0.7691	-3.2253	-0.2106	4.99
Soak	1	-0.2454	1.1455	-2.4906	1.9998	0.05
Soak	1.7	0.5572	1.1217	-1.6412	2.7557	0.25
Soak	2.2	0.4079	1.2260	-1.9951	2.8109	0.11
Soak	2.8	-0.1301	1.4234	-2.9199	2.6597	0.01
Scale	0	1.0000	0.0000	1.0000	1.0000	

Analysis Of Maximum Likelihood Parameter Estimates		
Parameter		Pr > ChiSq
Intercept		0.1780
Heat	7	0.9999
Heat	14	0.0027
Heat	27	0.0255
Soak	1	0.8304
Soak	1.7	0.6193
Soak	2.2	0.7394
Soak	2.8	0.9272
Scale		

NOTE: The scale parameter was held fixed.

Following the output from the asymptotic analysis, the exact conditional Poisson regression results are displayed, as shown in [Output 40.11.3](#).

Output 40.11.3 Exact Tests

The GENMOD Procedure				
Exact Conditional Analysis				
Exact Conditional Tests				
Effect	Test	Statistic	--- p-Value ---	
			Exact	Mid
Joint	Score	18.3665	0.0137	0.0137
	Probability	1.294E-6	0.0471	0.0471
Heat	Score	15.8259	0.0023	0.0022
	Probability	0.000175	0.0063	0.0062
Soak	Score	1.4612	0.8683	0.8646
	Probability	0.00735	0.8176	0.8139

The Joint test in the “Conditional Exact Tests” table in [Output 40.11.3](#) is produced by specifying the **JOINT** option in the **EXACT** statement. The p -values for this test indicate that the parameters for Heat and Soak are jointly significant as explanatory effects in the model. If the Heat variable is the only explanatory variable in your model, then the rows of this table labeled as “Heat” show the joint significance of all the Heat effect parameters in that reduced model. In this case, a model that contains only the Heat parameters still explains a significant amount of the variability; however, you can see that a model that contains only the Soak parameters would not be significant.

The “Exact Parameter Estimates” table in [Output 40.11.4](#) displays parameter estimates and tests of significance for the levels of the CLASS variables. Again, the Heat=7 parameter has some difficulties; however, in the exact analysis, a *median unbiased estimate* is computed for the parameter instead of a maximum likelihood estimate. The confidence limits show that the Heat variable contains some explanatory power, while the categorical Soak variable is insignificant and can be dropped from the model.

Output 40.11.4 Exact Parameter Estimates

Exact Parameter Estimates						
Parameter		Estimate	Standard Error	95% Confidence Limits		Two-sided p-Value
Heat	7	-2.7552*	.	-Infinity	-0.7864	0.0199
Heat	14	-3.0255	1.0128	-5.7450	-0.6194	0.0113
Heat	27	-1.7846	0.8065	-3.6779	0.2260	0.0844
Soak	1	-0.3231	1.1717	-2.8673	3.6754	1.0000
Soak	1.7	0.5375	1.1284	-1.8056	4.4588	1.0000
Soak	2.2	0.4035	1.2347	-2.5785	4.5054	1.0000
Soak	2.8	-0.1661	1.4214	-4.5490	4.2168	1.0000

NOTE: * indicates a median unbiased estimate.

NOTE: If you want to make predictions from the exact results, you can obtain an estimate for the intercept parameter by specifying the INTERCEPT keyword in the EXACT statement. You should also remove the JOINT option to reduce the amount of time and memory consumed.

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Chapter 41

The GLIMMIX Procedure

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Overview: GLIMMIX Procedure

The GLIMMIX procedure fits statistical models to data with correlations or nonconstant variability and where the response is not necessarily normally distributed. These models are known as generalized linear mixed models (GLMM).

GLMMs, like linear mixed models, assume normal (Gaussian) random effects. Conditional on these random effects, data can have any distribution in the exponential family. The exponential family comprises many of the elementary discrete and continuous distributions. The binary, binomial, Poisson, and negative binomial distributions, for example, are discrete members of this family. The normal, beta, gamma, and chi-square distributions are representatives of the continuous distributions in this family. In the absence of random effects, the GLIMMIX procedure fits generalized linear models (fit by the GENMOD procedure).

GLMMs are useful for the following applications:

- estimating trends in disease rates
- modeling CD4 counts in a clinical trial over time
- modeling the proportion of infected plants on experimental units in a design with randomly selected treatments or randomly selected blocks
- predicting the probability of high ozone levels in counties
- modeling skewed data over time
- analyzing customer preference
- joint modeling of multivariate outcomes

Such data often display correlations among some or all observations as well as nonnormality. The correlations can arise from repeated observation of the same sampling units, shared random effects in an experimental design, spatial (temporal) proximity, multivariate observations, and so on.

The GLIMMIX procedure does not fit hierarchical models with nonnormal random effects. With the GLIMMIX procedure you select the distribution of the response variable conditional on normally distributed random effects.

For more information about the differences between the GLIMMIX procedure and SAS procedures that specialize in certain subsets of the GLMM models, see the section “[PROC GLIMMIX Contrasted with Other SAS Procedures](#)” on page 2920.

Basic Features

The GLIMMIX procedure enables you to specify a generalized linear mixed model and to perform confirmatory inference in such models. The syntax is similar to that of the MIXED procedure and includes **CLASS**, **MODEL**, and **RANDOM** statements. For instructions on how to specify PROC MIXED REPEATED effects with PROC GLIMMIX, see the section “[Comparing the GLIMMIX and MIXED Procedures](#)” on page 3101. The following are some of the basic features of PROC GLIMMIX.

- **SUBJECT=** and **GROUP=** options, which enable blocking of variance matrices and parameter heterogeneity
- choice of linearization approach or integral approximation by quadrature or Laplace method for mixed models with nonlinear random effects or nonnormal distribution
- choice of linearization about expected values or expansion about current solutions of best linear unbiased predictors
- flexible covariance structures for random and residual random effects, including variance components, unstructured, autoregressive, and spatial structures
- **CONTRAST**, **ESTIMATE**, **LSMEANS**, and **LSMESTIMATE** statements, which produce hypothesis tests and estimable linear combinations of effects
- **NLOPTIONS** statement, which enables you to exercise control over the numerical optimization. You can choose techniques, update methods, line search algorithms, convergence criteria, and more. Or, you can choose the default optimization strategies selected for the particular class of model you are fitting.
- computed variables with SAS programming statements inside of PROC GLIMMIX (except for variables listed in the **CLASS** statement). These computed variables can appear in the **MODEL**, **RANDOM**, **WEIGHT**, or **FREQ** statement.
- grouped data analysis
- user-specified link and variance functions
- choice of model-based variance-covariance estimators for the fixed effects or empirical (sandwich) estimators to make analysis robust against misspecification of the covariance structure and to adjust for small-sample bias
- joint modeling for multivariate data. For example, you can model binary and normal responses from a subject jointly and use random effects to relate (fuse) the two outcomes.
- multinomial models for ordinal and nominal outcomes
- univariate and multivariate low-rank mixed model smoothing

Assumptions

The primary assumptions underlying the analyses performed by PROC GLIMMIX are as follows:

- If the model contains random effects, the distribution of the data conditional on the random effects is known. This distribution is either a member of the exponential family of distributions or one of the supplementary distributions provided by the GLIMMIX procedure. In models without random effects, the unconditional (marginal) distribution is assumed to be known for maximum likelihood estimation, or the first two moments are known in the case of quasi-likelihood estimation.

- The conditional expected value of the data takes the form of a linear mixed model after a monotonic transformation is applied.
- The problem of fitting the GLMM can be cast as a singly or doubly iterative optimization problem. The objective function for the optimization is a function of either the actual log likelihood, an approximation to the log likelihood, or the log likelihood of an approximated model.

For a model containing random effects, the GLIMMIX procedure, by default, estimates the parameters by applying pseudo-likelihood techniques as in Wolfinger and O’Connell (1993) and Breslow and Clayton (1993). In a model without random effects (GLM models), PROC GLIMMIX estimates the parameters by maximum likelihood, restricted maximum likelihood, or quasi-likelihood. See the section “[Singly or Doubly Iterative Fitting](#)” on page 3104 about when the GLIMMIX procedure applies noniterative, singly and doubly iterative algorithms, and the section “[Default Estimation Techniques](#)” on page 3106 about the default estimation methods. You can also fit generalized linear mixed models by maximum likelihood where the marginal distribution is numerically approximated by the Laplace method (`METHOD=LAPLACE`) or by adaptive Gaussian quadrature (`METHOD=QUAD`).

Once the parameters have been estimated, you can perform statistical inferences for the fixed effects and covariance parameters of the model. Tests of hypotheses for the fixed effects are based on Wald-type tests and the estimated variance-covariance matrix. The `COVTEST` statement enables you to perform inferences about covariance parameters based on likelihood ratio tests.

PROC GLIMMIX uses the Output Delivery System (ODS) for displaying and controlling the output from SAS procedures. ODS enables you to convert any of the output from PROC GLIMMIX into a SAS data set. See the section “[ODS Table Names](#)” on page 3113 for more information.

The GLIMMIX procedure uses ODS Graphics to create graphs as part of its output. For general information about ODS Graphics, see Chapter 21, “[Statistical Graphics Using ODS](#).” For specific information about the statistical graphics available with the GLIMMIX procedure, see the `PLOTS` options in the `PROC GLIMMIX` and `LSMEANS` statements.

Notation for the Generalized Linear Mixed Model

This section introduces the mathematical notation used throughout the chapter to describe the generalized linear mixed model (GLMM). See the section “[Details: GLIMMIX Procedure](#)” on page 3047 for a description of the fitting algorithms and the mathematical-statistical details.

The Basic Model

Suppose \mathbf{Y} represents the $(n \times 1)$ vector of observed data and $\boldsymbol{\gamma}$ is a $(r \times 1)$ vector of random effects. Models fit by the GLIMMIX procedure assume that

$$E[\mathbf{Y}|\boldsymbol{\gamma}] = g^{-1}(\mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\boldsymbol{\gamma})$$

where $g(\cdot)$ is a differentiable monotonic link function and $g^{-1}(\cdot)$ is its inverse. The matrix \mathbf{X} is an $(n \times p)$ matrix of rank k , and \mathbf{Z} is an $(n \times r)$ design matrix for the random effects. The random effects are assumed to be normally distributed with mean $\mathbf{0}$ and variance matrix \mathbf{G} .

The GLMM contains a linear mixed model inside the inverse link function. This model component is referred to as the linear predictor,

$$\eta = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\boldsymbol{\gamma}$$

The variance of the observations, conditional on the random effects, is

$$\text{Var}[\mathbf{Y}|\boldsymbol{\gamma}] = \mathbf{A}^{1/2}\mathbf{R}\mathbf{A}^{1/2}$$

The matrix \mathbf{A} is a diagonal matrix and contains the variance functions of the model. The variance function expresses the variance of a response as a function of the mean. The GLIMMIX procedure determines the variance function from the `DIST=` option in the `MODEL` statement or from the user-supplied variance function (see the section “[Implied Variance Functions](#)” on page 3043). The matrix \mathbf{R} is a variance matrix specified by the user through the `RANDOM` statement. If the conditional distribution of the data contains an additional scale parameter, it is either part of the variance functions or part of the \mathbf{R} matrix. For example, the gamma distribution with mean μ has the variance function $a(\mu) = \mu^2$ and $\text{Var}[Y|\boldsymbol{\gamma}] = \mu^2\phi$. If your model calls for G-side random effects only (see the next section), the procedure models $\mathbf{R} = \phi\mathbf{I}$, where \mathbf{I} is the identity matrix. [Table 41.19](#) identifies the distributions for which $\phi \equiv 1$.

G-Side and R-Side Random Effects and Covariance Structures

The GLIMMIX procedure distinguishes two types of random effects. Depending on whether the parameters of the covariance structure for random components in your model are contained in \mathbf{G} or in \mathbf{R} , the procedure distinguishes between “G-side” and “R-side” random effects. The associated covariance structures of \mathbf{G} and \mathbf{R} are similarly termed the G-side and R-side covariance structure, respectively. R-side effects are also called “residual” effects. Simply put, if a random effect is an element of $\boldsymbol{\gamma}$, it is a G-side effect and you are modeling the G-side covariance structure; otherwise, you are modeling the R-side covariance structure of the model. Models without G-side effects are also known as marginal (or population-averaged) models. Models fit with the GLIMMIX procedure can have none, one, or more of each type of effect.

Note that an R-side effect in the GLIMMIX procedure is equivalent to a `REPEATED` effect in the `MIXED` procedure. The R-side covariance structure in the GLIMMIX procedure is the covariance structure that you would formulate with the `REPEATED` statement in the `MIXED` procedure. In the GLIMMIX procedure all random effects and their covariance structures are specified through the `RANDOM` statement. See the section “[Comparing the GLIMMIX and MIXED Procedures](#)” on page 3101 for a comparison of the GLIMMIX and MIXED procedures.

The columns of \mathbf{X} are constructed from effects listed on the right side in the `MODEL` statement. Columns of \mathbf{Z} and the variance matrices \mathbf{G} and \mathbf{R} are constructed from the `RANDOM` statement.

The \mathbf{R} matrix is by default the scaled identity matrix, $\mathbf{R} = \phi\mathbf{I}$. The scale parameter ϕ is set to one if the distribution does not have a scale parameter, such as in the case of the binary, binomial, Poisson, and exponential distribution (see [Table 41.19](#)). To specify a different \mathbf{R} matrix, use the `RANDOM` statement with the `_RESIDUAL_` keyword or the `RESIDUAL` option. For example, to specify that the Time effect for each patient is an R-side effect with a first-order autoregressive covariance structure, use the `RESIDUAL` option:

```
random time / type=ar(1) subject=patient residual;
```

To add a multiplicative overdispersion parameter, use the `_RESIDUAL_` keyword:

```
random _residual_;
```

You specify the link function $g(\cdot)$ with the `LINK=` option in the `MODEL` statement or with programming statements. You specify the variance function that controls the matrix \mathbf{A} with the `DIST=` option in the `MODEL` statement or with programming statements.

Unknown quantities subject to estimation are the fixed-effects parameter vector $\boldsymbol{\beta}$ and the covariance parameter vector $\boldsymbol{\theta}$ that comprises all unknowns in \mathbf{G} and \mathbf{R} . The random effects $\boldsymbol{\gamma}$ are not parameters of the model in the sense that they are not estimated. The vector $\boldsymbol{\gamma}$ is a vector of random variables. The solutions for $\boldsymbol{\gamma}$ are predictors of these random variables.

Relationship with Generalized Linear Models

Generalized linear models (Nelder and Wedderburn 1972; McCullagh and Nelder 1989) are a special case of GLMMs. If $\boldsymbol{\gamma} = \mathbf{0}$ and $\mathbf{R} = \phi\mathbf{I}$, the GLMM reduces to either a generalized linear model (GLM) or a GLM with overdispersion. For example, if \mathbf{Y} is a vector of Poisson variables so that \mathbf{A} is a diagonal matrix containing $E[\mathbf{Y}] = \boldsymbol{\mu}$ on the diagonal, then the model is a Poisson regression model for $\phi = 1$ and overdispersed relative to a Poisson distribution for $\phi > 1$. Because the Poisson distribution does not have an extra scale parameter, you can model overdispersion by adding the following statement to your GLIMMIX program:

```
random _residual_;
```

If the only random effect is an overdispersion effect, PROC GLIMMIX fits the model by (restricted) maximum likelihood and not by one of the methods specific to GLMMs.

PROC GLIMMIX Contrasted with Other SAS Procedures

The GLIMMIX procedure generalizes the MIXED and GENMOD procedures in two important ways. First, the response can have a nonnormal distribution. The MIXED procedure assumes that the response is normally (Gaussian) distributed. Second, the GLIMMIX procedure incorporates random effects in the model and so allows for subject-specific (conditional) and population-averaged (marginal) inference. The GENMOD procedure allows only for marginal inference.

The GLIMMIX and MIXED procedure are closely related; see the syntax and feature comparison in the section “Comparing the GLIMMIX and MIXED Procedures” on page 3101. The remainder of this section compares the GLIMMIX procedure with the GENMOD, NLMIXED, LOGISTIC, and CATMOD procedures.

The GENMOD procedure fits generalized linear models for independent data by maximum likelihood. It can also handle correlated data through the marginal GEE approach of Liang and Zeger (1986) and Zeger and Liang (1986). The GEE implementation in the GENMOD procedure is a marginal method that does not incorporate random effects. The GEE estimation in the GENMOD procedure relies on R-side covariances only, and the unknown parameters in \mathbf{R} are estimated by the method of moments. The GLIMMIX procedure allows G-side random effects and R-side covariances. PROC GLIMMIX can fit marginal (GEE-type) models, but the covariance parameters are not estimated by the method of moments. The parameters are estimated by likelihood-based techniques. When the GLIMMIX and GENMOD procedures fit a generalized

linear model where the distribution contains a scale parameter, such as the normal, gamma, inverse Gaussian, or negative binomial distribution, the scale parameter is reported in the “Parameter Estimates” table. For some distributions, the parameterization of this parameter differs. See the section “[Scale and Dispersion Parameters](#)” on page 3050 for details about how the GLIMMIX procedure parameterizes the log-likelihood functions and information about how the reported quantities differ between the two procedures.

Many of the fit statistics and tests in the GENMOD procedure are based on the likelihood. In a GLMM it is not always possible to derive the log likelihood of the data. Even if the log likelihood is tractable, it might be computationally infeasible. In some cases, the objective function must be constructed based on a substitute model. In other cases, only the first two moments of the marginal distribution can be approximated. Consequently, obtaining likelihood-based tests and statistics is difficult for many generalized linear mixed models. The GLIMMIX procedure relies heavily on linearization and Taylor-series techniques to construct Wald-type test statistics and confidence intervals. Likelihood ratio tests and confidence intervals for covariance parameters are available in the GLIMMIX procedure through the [COVTEST](#) statement.

The NLMIXED procedure fits nonlinear mixed models where the conditional mean function is a general nonlinear function. The class of generalized linear mixed models is a special case of the nonlinear mixed models; hence some of the models you can fit with PROC NLMIXED can also be fit with the GLIMMIX procedure. The NLMIXED procedure relies by default on approximating the marginal log likelihood through adaptive Gaussian quadrature. In the GLIMMIX procedure, maximum likelihood estimation by adaptive Gaussian quadrature is available with the [METHOD=QUAD](#) option in the [PROC GLIMMIX](#) statement. The default estimation methods thus differ between the NLMIXED and GLIMMIX procedures, because adaptive quadrature is possible for only a subset of the models available with the GLIMMIX procedure. If you choose [METHOD=LAPLACE](#) or [METHOD=QUAD\(QPOINTS=1\)](#) in the [PROC GLIMMIX](#) statement for a generalized linear mixed model, the GLIMMIX procedure performs maximum likelihood estimation based on a Laplace approximation of the marginal log likelihood. This is equivalent to the [QPOINTS=1](#) option in the NLMIXED procedure.

The LOGISTIC and CATMOD procedures also fit generalized linear models; PROC LOGISTIC accommodates the independence case only. Binary, binomial, multinomial models for ordered data, and generalized logit models that can be fit with PROC LOGISTIC can also be fit with the GLIMMIX procedure. The diagnostic tools and capabilities specific to such data implemented in the LOGISTIC procedure go beyond the capabilities of the GLIMMIX procedure.

Getting Started: GLIMMIX Procedure

Logistic Regressions with Random Intercepts

Researchers investigated the performance of two medical procedures in a multicenter study. They randomly selected 15 centers for inclusion. One of the study goals was to compare the occurrence of side effects for the procedures. In each center n_A patients were randomly selected and assigned to procedure “A,” and n_B patients were randomly assigned to procedure “B.” The following DATA step creates the data set for the analysis:

```

data multicenter;
  input center group$ n sideeffect;
  datalines;
1  A  32  14
1  B  33  18
2  A  30   4
2  B  28   8
3  A  23  14
3  B  24   9
4  A  22   7
4  B  22  10
5  A  20   6
5  B  21  12
6  A  19   1
6  B  20   3
7  A  17   2
7  B  17   6
8  A  16   7
8  B  15   9
9  A  13   1
9  B  14   5
10 A  13   3
10 B  13   1
11 A  11   1
11 B  12   2
12 A  10   1
12 B   9   0
13 A   9   2
13 B   9   6
14 A   8   1
14 B   8   1
15 A   7   1
15 B   8   0
;

```

The variable `group` identifies the two procedures, `n` is the number of patients who received a given procedure in a particular center, and `sideeffect` is the number of patients who reported side effects.

If Y_{iA} and Y_{iB} denote the number of patients in center i who report side effects for procedures A and B , respectively, then—for a given center—these are independent binomial random variables. To model the probability of side effects for the two drugs, π_{iA} and π_{iB} , you need to account for the fixed group effect and the random selection of centers. One possibility is to assume a model that relates group and center effects linearly to the logit of the probabilities:

$$\log \left\{ \frac{\pi_{iA}}{1 - \pi_{iA}} \right\} = \beta_0 + \beta_A + \gamma_i$$

$$\log \left\{ \frac{\pi_{iB}}{1 - \pi_{iB}} \right\} = \beta_0 + \beta_B + \gamma_i$$

In this model, $\beta_A - \beta_B$ measures the difference in the logits of experiencing side effects, and the γ_i are independent random variables due to the random selection of centers. If you think of β_0 as the overall intercept in the model, then the γ_i are random intercept adjustments. Observations from the same center receive the same adjustment, and these vary randomly from center to center with variance $\text{Var}[\gamma_i] = \sigma_c^2$.

Because π_{iA} is the conditional mean of the sample proportion, $E[Y_{iA}/n_{iA}|\gamma_i] = \pi_{iA}$, you can model the sample proportions as binomial ratios in a generalized linear mixed model. The following statements request this analysis under the assumption of normally distributed center effects with equal variance and a logit link function:

```
proc glimmix data=multicenter;
  class center group;
  model sideeffect/n = group / solution;
  random intercept / subject=center;
run;
```

The **PROC GLIMMIX** statement invokes the procedure. The **CLASS** statement instructs the procedure to treat the variables `center` and `group` as classification variables. The **MODEL** statement specifies the response variable as a sample proportion by using the *events/trials* syntax. In terms of the previous formulas, `sideeffect/n` corresponds to Y_{iA}/n_{iA} for observations from group A and to Y_{iB}/n_{iB} for observations from group B. The **SOLUTION** option in the **MODEL** statement requests a listing of the solutions for the fixed-effects parameter estimates. Note that because of the *events/trials* syntax, the GLIMMIX procedure defaults to the binomial distribution, and that distribution’s default link is the logit link. The **RANDOM** statement specifies that the linear predictor contains an intercept term that randomly varies at the level of the center effect. In other words, a random intercept is drawn separately and independently for each center in the study.

The results of this analysis are shown in [Figure 41.1](#)–[Figure 41.9](#).

The “Model Information Table” in [Figure 41.1](#) summarizes important information about the model you fit and about aspects of the estimation technique.

Figure 41.1 Model Information

The GLIMMIX Procedure	
Model Information	
Data Set	WORK.MULTICENTER
Response Variable (Events)	sideeffect
Response Variable (Trials)	n
Response Distribution	Binomial
Link Function	Logit
Variance Function	Default
Variance Matrix Blocked By	center
Estimation Technique	Residual PL
Degrees of Freedom Method	Containment

PROC GLIMMIX recognizes the variables `sideeffect` and `n` as the numerator and denominator in the *events/trials* syntax, respectively. The distribution—conditional on the random center effects—is binomial. The marginal variance matrix is block-diagonal, and observations from the same center form the blocks. The default estimation technique in generalized linear mixed models is residual pseudo-likelihood with a subject-specific expansion (**METHOD=RSPL**).

The “Class Level Information” table lists the levels of the variables specified in the **CLASS** statement and the ordering of the levels. The “Number of Observations” table displays the number of observations read and used in the analysis ([Figure 41.2](#)).

Figure 41.2 Class Level Information and Number of Observations

Class Level Information	
Class	Levels Values
center	15 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15
group	2 A B
Number of Observations Read 30	
Number of Observations Used 30	
Number of Events 155	
Number of Trials 503	

There are two variables listed in the **CLASS** statement. The center variable has fifteen levels, and the group variable has two levels. Because the response is specified through the *events/trial* syntax, the “Number of Observations” table also contains the total number of events and trials used in the analysis.

The “Dimensions” table lists the size of relevant matrices (Figure 41.3).

Figure 41.3 Dimensions

Dimensions	
G-side Cov. Parameters	1
Columns in X	3
Columns in Z per Subject	1
Subjects (Blocks in V)	15
Max Obs per Subject	2

There are three columns in the **X** matrix, corresponding to an intercept and the two levels of the group variable. For each subject (center), the **Z** matrix contains only an intercept column.

The “Optimization Information” table provides information about the methods and size of the optimization problem (Figure 41.4).

Figure 41.4 Optimization Information

Optimization Information	
Optimization Technique	Dual Quasi-Newton
Parameters in Optimization	1
Lower Boundaries	1
Upper Boundaries	0
Fixed Effects	Profiled
Starting From	Data

The default optimization technique for generalized linear mixed models with binomial data is the quasi-Newton method. Because a residual likelihood technique is used to compute the objective function, only the covariance parameters participate in the optimization. A lower boundary constraint is placed on the variance component for the random center effect. The solution for this variance cannot be less than zero.

The “Iteration History” table displays information about the progress of the optimization process. After the initial optimization, the GLIMMIX procedure performed 15 updates before the convergence criterion was met (Figure 41.5). At convergence, the largest absolute value of the gradient was near zero. This indicates that the process stopped at an extremum of the objective function.

Figure 41.5 Iteration History and Convergence Status

Iteration History						
Iteration	Restarts	Subiterations	Objective Function	Change	Max Gradient	
0	0	5	79.688580269	0.11807224	7.851E-7	
1	0	3	81.294622554	0.02558021	8.209E-7	
2	0	2	81.438701534	0.00166079	4.061E-8	
3	0	1	81.444083567	0.00006263	2.311E-8	
4	0	1	81.444265216	0.00000421	0.000025	
5	0	1	81.444277364	0.00000383	0.000023	
6	0	1	81.444266322	0.00000348	0.000021	
7	0	1	81.44427636	0.00000316	0.000019	
8	0	1	81.444267235	0.00000287	0.000017	
9	0	1	81.444275529	0.00000261	0.000016	
10	0	1	81.44426799	0.00000237	0.000014	
11	0	1	81.444274843	0.00000216	0.000013	
12	0	1	81.444268614	0.00000196	0.000012	
13	0	1	81.444274277	0.00000178	0.000011	
14	0	1	81.444269129	0.00000162	9.772E-6	
15	0	0	81.444273808	0.00000000	9.102E-6	

Convergence criterion (PCONV=1.11022E-8) satisfied.

The “Fit Statistics” table lists information about the fitted model (Figure 41.6).

Figure 41.6 Fit Statistics

Fit Statistics	
-2 Res Log Pseudo-Likelihood	81.44
Generalized Chi-Square	30.69
Gener. Chi-Square / DF	1.10

Twice the negative of the residual log likelihood in the final pseudo-model equaled 81.44. The ratio of the generalized chi-square statistic and its degrees of freedom is close to 1. This is a measure of the residual variability in the marginal distribution of the data.

The “Covariance Parameter Estimates” table displays estimates and asymptotic estimated standard errors for all covariance parameters (Figure 41.7).

Figure 41.7 Covariance Parameter Estimates

Covariance Parameter Estimates			
Cov Parm	Subject	Estimate	Standard Error
Intercept	center	0.6176	0.3181

The variance of the random center intercepts on the logit scale is estimated as $\hat{\sigma}_c^2 = 0.6176$.

The “Parameter Estimates” table displays the solutions for the fixed effects in the model (Figure 41.8).

Figure 41.8 Parameter Estimates

Solutions for Fixed Effects						
Effect	group	Estimate	Standard Error	DF	t Value	Pr > t
Intercept		-0.8071	0.2514	14	-3.21	0.0063
group	A	-0.4896	0.2034	14	-2.41	0.0305
group	B	0

Because of the fixed-effects parameterization used in the GLIMMIX procedure, the “Intercept” effect is an estimate of $\beta_0 + \beta_B$, and the “A” group effect is an estimate of $\beta_A - \beta_B$, the log odds ratio. The associated estimated probabilities of side effects in the two groups are

$$\hat{\pi}_A = \frac{1}{1 + \exp\{0.8071 + 0.4896\}} = 0.2147$$

$$\hat{\pi}_B = \frac{1}{1 + \exp\{0.8071\}} = 0.3085$$

There is a significant difference between the two groups ($p = 0.0305$).

The “Type III Tests of Fixed Effect” table displays significance tests for the fixed effects in the model (Figure 41.9).

Figure 41.9 Type III Tests of Fixed Effects

Type III Tests of Fixed Effects				
Effect	Num DF	Den DF	F Value	Pr > F
group	1	14	5.79	0.0305

Because the group effect has only two levels, the p -value for the effect is the same as in the “Parameter Estimates” table, and the “ F Value” is the square of the “ t Value” shown there.

You can produce the estimates of the average logits in the two groups and their predictions on the scale of the data with the `LSMEANS` statement in PROC GLIMMIX:

```
ods select lsmeans;
proc glimmix data=multicenter;
  class center group;
  model sideeffect/n = group / solution;
  random intercept / subject=center;
  lsmeans group / cl ilink;
run;
```

The `LSMEANS` statement requests the least squares means of the group effect on the logit scale. The `CL` option requests their confidence limits. The `ILINK` option adds estimates, standard errors, and confidence limits on the mean (probability) scale (Figure 41.10).

Figure 41.10 Least Squares Means

The GLIMMIX Procedure								
group Least Squares Means								
group	Estimate	Standard Error	DF	t Value	Pr > t	Alpha	Lower	Upper
A	-1.2966	0.2601	14	-4.99	0.0002	0.05	-1.8544	-0.7388
B	-0.8071	0.2514	14	-3.21	0.0063	0.05	-1.3462	-0.2679
group Least Squares Means								
group	Mean	Standard Error Mean	Lower Mean	Upper Mean				
A	0.2147	0.04385	0.1354	0.3233				
B	0.3085	0.05363	0.2065	0.4334				

The “Estimate” column displays the least squares mean estimate on the logit scale, and the “Mean” column represents its mapping onto the probability scale. The “Lower” and “Upper” columns are 95% confidence limits for the logits in the two groups. The “Lower Mean” and “Upper Mean” columns are the corresponding confidence limits for the probabilities of side effects. These limits are obtained by inversely linking the confidence bounds on the linear scale, and thus are not symmetric about the estimate of the probabilities.

Syntax: GLIMMIX Procedure

The following statements are available in the GLIMMIX procedure:

```

PROC GLIMMIX < options > ;
  BY variables ;
  CLASS variable < (REF= option) > ... < variable < (REF= option) > > < / global-options > ;
  CODE < options > ;
  CONTRAST 'label' contrast-specification < , contrast-specification > < , ... > < / options > ;
  COVTEST < 'label' > < test-specification > < / options > ;
  EFFECT effect-specification ;
  ESTIMATE 'label' contrast-specification < (divisor=n) >
    < , 'label' contrast-specification < (divisor=n) > > < , ... > < / options > ;
  FREQ variable ;
  ID variables ;
  LSMEANS fixed-effects < / options > ;
  LSMESTIMATE fixed-effect < 'label' > values < divisor=n >
    < , < 'label' > values < divisor=n > > < , ... > < / options > ;
  MODEL response < (response-options) > = < fixed-effects > < / model-options > ;
  MODEL events/trials = < fixed-effects > < / model-options > ;
  NLOPTIONS < options > ;
  OUTPUT < OUT=SAS-data-set >
    < keyword < (keyword-options) > < =name > > ...
    < keyword < (keyword-options) > < =name > > < / options > ;
  PARMS (value-list) . . < / options > ;
  RANDOM random-effects < / options > ;
  SLICE model-effect < / options > ;
  STORE < OUT= > item-store-name < / LABEL='label' > ;
  WEIGHT variable ;
  Programming statements ;

```

The **CLASS**, **CONTRAST**, **COVTEST**, **EFFECT**, **ESTIMATE**, **LSMEANS**, **LSMESTIMATE**, **RANDOM** and **SLICE** statements and the **programming statements** can appear multiple times. The **PROC GLIMMIX** and **MODEL** statements are required, and the **MODEL** statement must appear after the **CLASS** statement if a **CLASS** statement is included. The **EFFECT** statements must appear before the **MODEL** statement.

The **SLICE** statement is also available in many other procedures. A summary description of functionality and syntax for this statement is given in this chapter. You can find full documentation in the section “**SLICE Statement**” on page 498 of Chapter 19, “**Shared Concepts and Topics**.”

PROC GLIMMIX Statement

```

PROC GLIMMIX < options > ;

```

The **PROC GLIMMIX** statement invokes the **GLIMMIX** procedure. [Table 41.1](#) summarizes the options available in the **PROC GLIMMIX** statement. These and other options in the **PROC GLIMMIX** statement are then described fully in alphabetical order.

Table 41.1 PROC GLIMMIX Statement Options

Option	Description
Basic Options	
DATA=	Specifies the input data set
METHOD=	Determines estimation method
NOFIT	Does not fit the model
NOPROFILE	Includes scale parameter in optimization
NOREML	Determines computation of scale parameters in GLM models
ORDER=	Determines the sort order of CLASS variables
OUTDESIGN	Writes X and/or Z matrices to a SAS data set
PROFILE	Profile scale parameters from the optimization
Displayed Output	
ASYCORR	Displays the asymptotic correlation matrix of the covariance parameter estimates
ASYCOV	Displays the asymptotic covariance matrix of the covariance parameter estimates
GRADIENT	Displays the gradient of the objective function with respect to the parameter estimates
HESSIAN	Displays the Hessian matrix
ITDETAILS	Adds estimates and gradients to the “Iteration History”
NAMELEN=	Specifies the length of long effect names
NOBSDETAIL	Shows data exclusions
NOCLPRINT	Suppresses “Class Level Information” completely or in part
ODDSRATIO	Requests odds ratios
PLOTS	Produces ODS statistical graphics
SUBGRADIENT	Writes subject-specific gradients to a SAS data set
Optimization Options	
MAXOPT=	Specifies the number of optimizations
Computational Options	
CHOLESKY	Constructs and solves mixed model equations using the Cholesky root of the G matrix
EMPIRICAL	Computes empirical (“sandwich”) estimators
EXPHESSIAN	Uses the expected Hessian matrix to compute the covariance matrix of nonprofiled parameters
INFOCRIT	Affects the computation of information criteria
INITGLM	Uses fixed-effects starting values via generalized linear model
INITITER=	Sets the number of initial GLM steps
NOBOUND	Unbounds the covariance parameter estimates
NOINITGLM	Does not use fixed-effects starting values via generalized linear model
SCORING=	Applies Fisher scoring where applicable
SCOREMOD	Bases the Hessian matrix in GLMMs on a modified scoring algorithm

Table 41.1 *continued*

Option	Description
Singularity Tolerances	
ABSPCONV=	Determines the absolute parameter estimate convergence criterion for PL
FDIGITS=	Specifies significant digits in computing objective function
PCONV=	Specifies the relative parameter estimate convergence criterion for PL
SINGCHOL=	Tunes singularity for Cholesky decompositions
SINGRES=	Tunes singularity for the residual variance
SINGULAR=	Tunes general singularity criterion
Debugging Output	
LIST	Lists model program and variables

You can specify the following options in the PROC GLIMMIX statement.

ABSPCONV=*r*

specifies an absolute parameter estimate convergence criterion for doubly iterative estimation methods. For such methods, the GLIMMIX procedure by default examines the *relative* change in parameter estimates between optimizations (see PCONV=). The purpose of the ABSPCONV= criterion is to stop the process when the *absolute* change in parameter estimates is less than the tolerance criterion *r*. The criterion is based on fixed effects and covariance parameters.

Note that this convergence criterion does not affect the convergence criteria applied within any individual optimization. In order to change the convergence behavior within an optimization, you can change the ABSPCONV=, ABSFCONV=, ABSGCONV=, ABSXCONV=, FCONV=, or GCONV= option in the NLOPTIONS statement.

ASYCORR

produces the asymptotic correlation matrix of the covariance parameter estimates. It is computed from the corresponding asymptotic covariance matrix (see the description of the ASYCOV option, which follows).

ASYCOV

requests that the asymptotic covariance matrix of the covariance parameter estimates be displayed. By default, this matrix is the observed inverse Fisher information matrix, which equals $m\mathbf{H}^{-1}$, where \mathbf{H} is the Hessian (second derivative) matrix of the objective function. The factor *m* equals 1 in a GLM and equals 2 in a GLMM.

When you use the SCORING= option and PROC GLIMMIX converges without stopping the scoring algorithm, the procedure uses the expected Hessian matrix to compute the covariance matrix instead of the observed Hessian. Regardless of whether a scoring algorithm is used or the number of scoring iterations has been exceeded, you can request that the asymptotic covariance matrix be based on the expected Hessian with the EXPHESSIAN option in the PROC GLIMMIX statement. If a residual scale parameter is profiled from the likelihood equation, the asymptotic covariance matrix is adjusted for the presence of this parameter; details of this adjustment process are found in Wolfinger, Tobias, and Sall (1994) and in the section “Estimated Precision of Estimates” on page 3056.

CHOLESKY**CHOL**

requests that the mixed model equations be constructed and solved by using the Cholesky root of the \mathbf{G} matrix. This option applies only to estimation methods that involve mixed model equations. The Cholesky root algorithm has greater numerical stability but also requires more computing resources. When the estimated \mathbf{G} matrix is not positive definite during a particular function evaluation, PROC GLIMMIX switches to the Cholesky algorithm for that evaluation and returns to the regular algorithm if $\hat{\mathbf{G}}$ becomes positive definite again. When the CHOLESKY option is in effect, the procedure applies the algorithm all the time.

DATA=SAS-data-set

names the SAS data set to be used by PROC GLIMMIX. The default is the most recently created data set.

EMPIRICAL<=CLASSICAL | HC0>**EMPIRICAL<=DF | HC1>****EMPIRICAL<=MBN<(mbn-options)>>****EMPIRICAL<=ROOT | HC2>****EMPIRICAL<=FIRORES | HC3>****EMPIRICAL<=FIROEEQ<(r)>>**

requests that the covariance matrix of the parameter estimates be computed as one of the asymptotically consistent estimators, known as *sandwich* or *empirical* estimators. The name stems from the layering of the estimator. An empirically based estimate of the inverse variance of the parameter estimates (the “meat”) is wrapped by the model-based variance estimate (the “bread”).

Empirical estimators are useful for obtaining inferences that are not sensitive to the choice of the covariance model. In nonmixed models, they can help, for example, to allay the effects of variance heterogeneity on the tests of fixed effects. Empirical estimators can coarsely be grouped into likelihood-based and residual-based estimators. The distinction arises from the components used to construct the “meat” and “bread” of the estimator. If you specify the EMPIRICAL option without further qualifiers, the GLIMMIX procedure computes the classical sandwich estimator in the appropriate category.

Likelihood-Based Estimator

Let $\mathbf{H}(\boldsymbol{\alpha})$ denote the second derivative matrix of the log likelihood for some parameter vector $\boldsymbol{\alpha}$, and let $\mathbf{g}_i(\boldsymbol{\alpha})$ denote the gradient of the log likelihood with respect to $\boldsymbol{\alpha}$ for the i th of m independent sampling units. The gradient for the entire data is $\sum_{i=1}^m \mathbf{g}_i(\boldsymbol{\alpha})$. A sandwich estimator for the covariance matrix of $\hat{\boldsymbol{\alpha}}$ can then be constructed as (White 1982)

$$\mathbf{H}(\hat{\boldsymbol{\alpha}})^{-1} \left(\sum_{i=1}^m \mathbf{g}_i(\hat{\boldsymbol{\alpha}}) \mathbf{g}_i(\hat{\boldsymbol{\alpha}})' \right) \mathbf{H}(\hat{\boldsymbol{\alpha}})^{-1}$$

If you fit a mixed model by maximum likelihood with Laplace or quadrature approximation (METHOD=LAPLACE, METHOD=QUAD), the GLIMMIX procedure constructs this likelihood-based estimator when you choose EMPIRICAL=CLASSICAL. If you choose EMPIRICAL=MBN, the likelihood-based sandwich estimator is further adjusted (see the section “[Design-Adjusted MBN](#)”).

Estimator” on page 3079 for details). Because Laplace and quadrature estimation in GLIMMIX includes the fixed-effects parameters and the covariance parameters in the optimization, this empirical estimator adjusts the covariance matrix of both types of parameters. The following empirical estimators are not available with `METHOD=LAPLACE` or with `METHOD=QUAD`: `EMPIRICAL=DF`, `EMPIRICAL=ROOT`, `EMPIRICAL=FIRORES`, and `EMPIRICAL=FIROEEQ`.

Residual-Based Estimators

For a general model, let \mathbf{Y} denote the response with mean $\boldsymbol{\mu}$ and variance $\boldsymbol{\Sigma}$, and let \mathbf{D} be the matrix of first derivatives of $\boldsymbol{\mu}$ with respect to the fixed effects $\boldsymbol{\beta}$. The classical sandwich estimator (Huber 1967; White 1980) is

$$\hat{\boldsymbol{\Omega}} \left(\sum_{i=1}^m \hat{\mathbf{D}}_i' \hat{\boldsymbol{\Sigma}}_i^{-1} \mathbf{e}_i \mathbf{e}_i' \hat{\boldsymbol{\Sigma}}_i^{-1} \hat{\mathbf{D}}_i \right) \hat{\boldsymbol{\Omega}}$$

where $\boldsymbol{\Omega} = (\mathbf{D}'\boldsymbol{\Sigma}^{-1}\mathbf{D})^{-1}$, $\mathbf{e}_i = y_i - \hat{\boldsymbol{\mu}}_i$, and m denotes the number of independent sampling units.

Since the expected value of $\mathbf{e}_i \mathbf{e}_i'$ does not equal $\boldsymbol{\Sigma}_i$, the classical sandwich estimator is biased, particularly if m is small. The estimator tends to underestimate the variance of $\hat{\boldsymbol{\beta}}$. The `EMPIRICAL=DF`, `ROOT`, `FIRORES`, `FIROEEQ`, and `MBN` estimators are bias-corrected sandwich estimators. The `DF` estimator applies a simple sample size adjustment. The `ROOT`, `FIRORES`, and `FIROEEQ` estimators are based on Taylor series approximations applied to residuals and estimating equations. For uncorrelated data, the `EMPIRICAL=FIRORES` estimator can be motivated as a jackknife estimator.

In the case of a linear regression model, the various estimators reduce to the *heteroscedasticity-consistent covariance matrix* estimators (HCMM) of White (1980) and MacKinnon and White (1985). The classical estimator, HC0, was found to perform poorly in small samples. Based on simulations in regression models, MacKinnon and White (1985) and Long and Ervin (2000) strongly recommend the HC3 estimator. The sandwich estimators computed by the GLIMMIX procedure can be viewed as an extension of the HC0—HC3 estimators of MacKinnon and White (1985) to accommodate nonnormal data and correlated observations.

The `MBN` estimator, introduced as a residual-based estimator (Morel 1989; Morel, Bokossa, and Neerchal 2003), applies an additive adjustment to the residual crossproduct. It is controlled by three suboptions. The valid *mbn-options* are as follows: a sample size adjustment is applied when the `DF` suboption is in effect. The `NODF` suboption suppresses this component of the adjustment. The lower bound of the design effect parameter $0 \leq r \leq 1$ can be specified with the `R=` option. The magnitude of Morel’s δ parameter is partly determined with the `D=` option ($d \geq 1$).

For details about the general expression for the residual-based estimators and their relationship, see the section “Empirical Covariance (“Sandwich”) Estimators” on page 3078. The `MBN` estimator and its parameters are explained for residual- and likelihood-based estimators in the section “Design-Adjusted MBN Estimator” on page 3079.

The `EMPIRICAL=DF` estimator applies a simple, multiplicative correction factor to the classical estimator (Hinkley 1977). This correction factor is

$$c = \begin{cases} m/(m-k) & m > k \\ 1 & \text{otherwise} \end{cases}$$

where k is the rank of \mathbf{X} , and m equals the sum of all frequencies when PROC GLIMMIX is in GLM mode and equals the number of subjects in GLMM mode. For example, the following statements fit an overdispersed GLM:

```
proc glimmix empirical;
  model y = x;
  random _residual_;
run;
```

PROC GLIMMIX is in GLM mode, and the individual observations are the independent sampling units from which the sandwich estimator is constructed. If you use a **SUBJECT=** effect in the **RANDOM** statement, however, the procedure fits the model in GLMM mode and the subjects represent the sampling units in the construction of the sandwich estimator. In other words, the following statements fit a GEE-type model with independence working covariance structure and subjects (clusters) defined by the levels of ID:

```
proc glimmix empirical;
  class id;
  model y = x;
  random _residual_ / subject=id type=vc;
run;
```

See the section “[GLM Mode or GLMM Mode](#)” on page 3067 for information about how the GLIMMIX procedure determines the estimation mode.

The **EMPIRICAL=ROOT** estimator is based on the residual approximation in Kauermann and Carroll (2001), and the **EMPIRICAL=FIRORES** estimator is based on the approximation in Mancl and DeRouen (2001). The Kauermann and Carroll estimator requires the inverse square root of a nonsymmetric matrix. This square root matrix is obtained from the singular value decomposition in PROC GLIMMIX, and thus this sandwich estimator is computationally more demanding than others. In the linear regression case, the Mancl-DeRouen estimator can be motivated as a jackknife estimator, based on the “leave-one-out” estimates of $\hat{\beta}$; see MacKinnon and White (1985) for details.

The **EMPIRICAL=FIROEEQ** estimator is based on approximating an unbiased estimating equation (Fay and Graubard 2001). It is computationally less demanding than the estimator of Kauermann and Carroll (2001) and, in certain balanced cases, gives identical results. The optional number $0 \leq r < 1$ is chosen to provide an upper bound on the correction factor. The default value for r is 0.75.

When you specify the **EMPIRICAL** option with a residual-based estimator, PROC GLIMMIX adjusts all standard errors and test statistics involving the fixed-effects parameters.

Sampling Units

Computation of an empirical variance estimator requires that the data can be processed by independent sampling units. This is always the case in GLMs. In this case, m , the number of independent units, equals the sum of the frequencies used in the analysis (see “Number of Observations” table). In GLMMs, empirical estimators can be computed only if the data comprise more than one subject as per the “Dimensions” table. See the section “[Processing by Subjects](#)” on page 3082 for information about how the GLIMMIX procedure determines whether the data can be processed by subjects. If a GLMM comprises only a single subject for a particular BY group, the model-based variance estimator is used instead of the empirical estimator, and a message is written to the log.

EXPHESSIAN

requests that the expected Hessian matrix be used in computing the covariance matrix of the nonprofiled parameters. By default, the GLIMMIX procedure uses the observed Hessian matrix in computing the asymptotic covariance matrix of covariance parameters in mixed models and the covariance matrix of fixed effects in models without random effects. The EXPHESSIAN option is ignored if the (conditional) distribution is not a member of the exponential family or is unknown. It is also ignored in models for nominal data.

FDIGITS=*r*

specifies the number of accurate digits in evaluations of the objective function. Fractional values are allowed. The default value is $r = -\log_{10} \epsilon$, where ϵ is the machine precision. The value of r is used to compute the interval size for the computation of finite-difference approximations of the derivatives of the objective function. It is also used in computing the default value of the FCONV= option in the NLOPTIONS statement.

GRADIENT

displays the gradient of the objective function with respect to the parameter estimates in the “Covariance Parameter Estimates” table and/or the “Parameter Estimates” table.

HESSIAN**HESS****H**

displays the Hessian matrix of the optimization.

INFOCRIT=NONE | PQ | Q**IC=NONE | PQ | Q**

determines the computation of information criteria in the “Fit Statistics” table. The GLIMMIX procedure computes various information criteria that typically apply a penalty to the (possibly restricted) log likelihood, log pseudo-likelihood, or log quasi-likelihood that depends on the number of parameters and/or the sample size. If IC=NONE, these criteria are suppressed in the “Fit Statistics” table. This is the default for models based on pseudo-likelihoods.

The AIC, AICC, BIC, CAIC, and HQIC fit statistics are various information criteria. AIC and AICC represent Akaike’s information criteria (Akaike 1974) and a small sample bias corrected version thereof (for AICC, see Hurvich and Tsai 1989; Burnham and Anderson 1998). BIC represents Schwarz’s Bayesian criterion (Schwarz 1978). Table 41.2 gives formulas for the criteria.

Table 41.2 Information Criteria

Criterion	Formula	Reference
AIC	$-2\ell + 2d$	Akaike (1974)
AICC	$-2\ell + 2dn^*/(n^* - d - 1)$	Hurvich and Tsai (1989) Burnham and Anderson (1998)
HQIC	$-2\ell + 2d \log \log n$	Hannan and Quinn (1979)
BIC	$-2\ell + d \log n$	Schwarz (1978)
CAIC	$-2\ell + d(\log n + 1)$	Bozdogan (1987)

Here, ℓ denotes the maximum value of the (possibly restricted) log likelihood, log pseudo-likelihood, or log quasi-likelihood, d is the dimension of the model, and n , n^* reflect the size of the data.

The IC=PQ option requests that the penalties include the number of fixed-effects parameters, when estimation in models with random effects is based on a residual (restricted) likelihood. For **METHOD=MSPL**, **METHOD=MMPL**, **METHOD=LAPLACE**, and **METHOD=QUAD**, IC=Q and IC=PQ produce the same results. IC=Q is the default for linear mixed models with normal errors, and the resulting information criteria are identical to the IC option in the MIXED procedure.

The quantities d , n , and n^* depend on the model and IC= option in the following way:

GLM: IC=Q and IC=PQ options have no effect on the computation.

- d equals the number of parameters in the optimization whose solutions do not fall on the boundary or are otherwise constrained. The scale parameter is included, if it is part of the optimization. If you use the **PARMS** statement to place a hold on a scale parameter, that parameter does not count toward d .
- n equals the sum of the frequencies (f) for maximum likelihood and quasi-likelihood estimation and $f - \text{rank}(\mathbf{X})$ for restricted maximum likelihood estimation.
- n^* equals n , unless $n < d + 2$, in which case $n^* = d + 2$.

GLMM, IC=Q:

- d equals the number of effective covariance parameters—that is, covariance parameters whose solution does not fall on the boundary. For estimation of an unrestricted objective function (**METHOD=MMPL**, **METHOD=MSPL**, **METHOD=LAPLACE**, **METHOD=QUAD**), this value is incremented by $\text{rank}(\mathbf{X})$.
- n equals the effective number of subjects as displayed in the “Dimensions” table, unless this value equals 1, in which case n equals the number of levels of the first G-side **RANDOM** effect specified. If the number of effective subjects equals 1 and there are no G-side random effects, n is determined as

$$n = \begin{cases} f - \text{rank}(\mathbf{X}) & \text{METHOD} = \text{RMPL}, \text{METHOD} = \text{RSPL} \\ f & \text{otherwise} \end{cases}$$

where f is the sum of frequencies used.

- n^* equals f or $f - \text{rank}(\mathbf{X})$ (for **METHOD=RMPL** and **METHOD=RSPL**), unless this value is less than $d + 2$, in which case $n^* = d + 2$.

GLMM, IC=PQ: For **METHOD=MSPL**, **METHOD=MMPL**, **METHOD=LAPLACE**, and **METHOD=QUAD**, the results are the same as for IC=Q. For **METHOD=RSPL** and **METHOD=RMPL**, d equals the number of effective covariance parameters plus $\text{rank}(\mathbf{X})$, and $n = n^*$ equals $f - \text{rank}(\mathbf{X})$. The formulas for the information criteria thus agree with Verbeke and Molenberghs (2000, Table 6.7, p. 74) and Vonesh and Chinchilli (1997, p. 263).

INITGLM

requests that the estimates from a generalized linear model fit (a model without random effects) be used as the starting values for the generalized linear mixed model. This option is the default for **METHOD=LAPLACE** and **METHOD=QUAD**.

INITITER=number

specifies the maximum number of iterations used when a generalized linear model is fit initially to derive starting values for the fixed effects; see the **INITGLM** option. By default, the initial fit involves at most four iteratively reweighted least squares updates. You can change the upper limit of initial iterations with *number*. If the model does not contain random effects, this option has no effect.

ITDETAILS

adds parameter estimates and gradients to the “Iteration History” table.

LIST

requests that the model program and variable lists be displayed. This is a debugging feature and is not normally needed. When you use programming statements to define your statistical model, this option enables you to examine the complete set of statements submitted for processing. See the section “Programming Statements” for more details about how to use SAS statements with the GLIMMIX procedure.

MAXLMMUPDATE=number**MAXOPT=number**

specifies the maximum number of optimizations for doubly iterative estimation methods based on linearizations. After each optimization, a new pseudo-model is constructed through a Taylor series expansion. This step is known as the linear mixed model update. The **MAXLMMUPDATE** option limits the number of updates and thereby limits the number of optimizations. If this option is not specified, *number* is set equal to the value specified in the **MAXITER=** option in the **NLOPTIONS** statement. If no **MAXITER=** value is given, *number* defaults to 20.

METHOD=RSPL**METHOD=MSPL****METHOD=RMPL****METHOD=MMPL****METHOD=LAPLACE****METHOD=QUAD**< (*quad-options*) >

specifies the estimation method in a generalized linear mixed model (GLMM). The default is **METHOD=RSPL**.

Pseudo-Likelihood

Estimation methods ending in “PL” are pseudo-likelihood techniques. The first letter of the **METHOD=** identifier determines whether estimation is based on a residual likelihood (“R”) or a maximum likelihood (“M”). The second letter identifies the expansion locus for the underlying approximation. Pseudo-likelihood methods for generalized linear mixed models can be cast in terms of Taylor series expansions (linearizations) of the GLMM. The expansion locus of the expansion is either the vector of random effects solutions (“S”) or the mean of the random effects (“M”). The expansions are also referred to as the “S”ubject-specific and “M”arginal expansions. The abbreviation “PL” identifies the method as a pseudo-likelihood technique.

Residual methods account for the fixed effects in the construction of the objective function, which reduces the bias in covariance parameter estimates. Estimation methods involving Taylor series create pseudo-data for each optimization. Those data are transformed to have zero mean in a residual

method. While the covariance parameter estimates in a residual method are the maximum likelihood estimates for the transformed problem, the fixed-effects estimates are (estimated) generalized least squares estimates. In a likelihood method that is not residual based, both the covariance parameters and the fixed-effects estimates are maximum likelihood estimates, but the former are known to have greater bias. In some problems, residual likelihood estimates of covariance parameters are unbiased.

For more information about linearization methods for generalized linear mixed models, see the section “[Pseudo-likelihood Estimation Based on Linearization](#)” on page 3054.

Maximum Likelihood with Laplace Approximation

If you choose `METHOD=LAPLACE` with a generalized linear mixed model, PROC GLIMMIX approximates the marginal likelihood by using Laplace’s method. Twice the negative of the resulting log-likelihood approximation is the objective function that the procedure minimizes to determine parameter estimates. Laplace estimates typically exhibit better asymptotic behavior and less small-sample bias than pseudo-likelihood estimators. On the other hand, the class of models for which a Laplace approximation of the marginal log likelihood is available is much smaller compared to the class of models to which PL estimation can be applied.

To determine whether Laplace estimation can be applied in your model, consider the marginal distribution of the data in a mixed model

$$\begin{aligned} p(\mathbf{y}) &= \int p(\mathbf{y}|\boldsymbol{\gamma}) p(\boldsymbol{\gamma}) d\boldsymbol{\gamma} \\ &= \int \exp\{\log\{p(\mathbf{y}|\boldsymbol{\gamma})\} + \log\{p(\boldsymbol{\gamma})\}\} d\boldsymbol{\gamma} \\ &= \int \exp\{nf(\mathbf{y}, \boldsymbol{\gamma})\} d\boldsymbol{\gamma} \end{aligned}$$

The function $f(\mathbf{y}, \boldsymbol{\gamma})$ plays an important role in the Laplace approximation: it is a function of the joint distribution of the data and the random effects (see the section “[Maximum Likelihood Estimation Based on Laplace Approximation](#)” on page 3059). In order to construct a Laplace approximation, PROC GLIMMIX requires a conditional log-likelihood $\log\{p(\mathbf{y}|\boldsymbol{\gamma})\}$ as well as the distribution of the G-side random effects. The random effects are always assumed to be normal with zero mean and covariance structure determined by the `RANDOM` statement. The conditional distribution is determined by the `DIST=` option of the `MODEL` statement or the default associated with a particular response type. Because a valid conditional distribution is required, R-side random effects are not permitted for `METHOD=LAPLACE` in the GLIMMIX procedure. In other words, the GLIMMIX procedure requires for `METHOD=LAPLACE` conditional independence without R-side overdispersion or covariance structure.

Because the marginal likelihood of the data is approximated numerically, certain features of the marginal distribution are not available—for example, you cannot display a marginal variance-covariance matrix. Also, the procedure includes both the fixed-effects parameters and the covariance parameters in the optimization for Laplace estimation. Consequently, this setting imposes some restrictions with respect to available options for Laplace estimation. [Table 41.3](#) lists the options that are assumed for `METHOD=LAPLACE`, and [Table 41.4](#) lists the options that are not compatible with this estimation method.

The section “[Maximum Likelihood Estimation Based on Laplace Approximation](#)” contains details about Laplace estimation in PROC GLIMMIX.

Maximum Likelihood with Adaptive Quadrature

If you choose `METHOD=QUAD` in a generalized linear mixed model, the GLIMMIX procedure approximates the marginal log likelihood with an adaptive Gauss-Hermite quadrature. Compared to `METHOD=LAPLACE`, the models for which parameters can be estimated by quadrature are further restricted. In addition to the conditional independence assumption and the absence of R-side covariance parameters, it is required that models suitable for `METHOD=QUAD` can be processed by subjects. (See the section “[Processing by Subjects](#)” on page 3082 about how the GLIMMIX procedure determines whether the data can be processed by subjects.) This in turn requires that all `RANDOM` statements have `SUBJECT=` effects and in the case of multiple `SUBJECT=` effects that these form a containment hierarchy.

In a containment hierarchy each effect is contained by another effect, and the effect contained by all is considered “the” effect for subject processing. For example, the `SUBJECT=` effects in the following statements form a containment hierarchy:

```
proc glimmix;
  class A B block;
  model y = A B A*B;
  random intercept / subject=block;
  random intercept / subject=A*block;
run;
```

The block effect is contained in the `A*block` interaction and the data are processed by block. The `SUBJECT=` effects in the following statements do not form a containment hierarchy:

```
proc glimmix;
  class A B block;
  model y = A B A*B;
  random intercept / subject=block;
  random block      / subject=A;
run;
```

The section “[Maximum Likelihood Estimation Based on Adaptive Quadrature](#)” on page 3062 contains important details about the computations involved with quadrature approximations. The section “[Aspects Common to Adaptive Quadrature and Laplace Approximation](#)” on page 3064 contains information about issues that apply to Laplace and adaptive quadrature, such as the computation of the prediction variance matrix and the determination of starting values.

You can specify the following *quad-options* for `METHOD=QUAD` in parentheses:

EBDETAILS

reports details about the empirical Bayes suboptimization process should this suboptimization fail.

EBSSFRAC=*r*

specifies the step-shortening fraction to be used while computing empirical Bayes estimates of the random effects. The default value is $r = 0.8$, and it is required that $r > 0$.

EBSSTOL=*r*

specifies the objective function tolerance for determining the cessation of step shortening while computing empirical Bayes estimates of the random effects, $r \geq 0$. The default value is $r=1E-8$.

EBSTEPS=*n*

specifies the maximum number of Newton steps for computing empirical Bayes estimates of random effects, $n \geq 0$. The default value is $n=50$.

EBSUBSTEPS=*n*

specifies the maximum number of step shortenings for computing empirical Bayes estimates of random effects. The default value is $n=20$, and it is required that $n \geq 0$.

EBTOL=*r*

specifies the convergence tolerance for empirical Bayes estimation, $r \geq 0$. The default value is $r = \epsilon \times 1E4$, where ϵ is the machine precision. This default value equals approximately $1E-12$ on most machines.

INITPL=*number*

requests that adaptive quadrature commence after performing up to *number* pseudo-likelihood updates. The initial pseudo-likelihood (PL) steps (METHOD=MSPL) can be useful to provide good starting values for the quadrature algorithm. If you choose *number* large enough so that the initial PL estimation converges, the process is equivalent to starting a quadrature from the PL estimates of the fixed-effects and covariance parameters. Because this also makes available the PL random-effects solutions, the adaptive step of the quadrature that determines the number of quadrature points can take this information into account.

Note that you can combine the INITPL option with the NOINITGLM option in the PROC GLIMMIX statement to define a precise path for starting value construction to the GLIMMIX procedure. For example, the following statement generates starting values in these steps:

```
proc glimmix method=quad(initpl=5);
```

1. A GLM without random effects is fit initially to obtain as starting values for the fixed effects. The INITITER= option in the PROC GLIMMIX statement controls the number of iterations in this step.
2. Starting values for the covariance parameters are then obtained by MIVQUE0 estimation (Goodnight 1978a), using the fixed-effects parameter estimates from step 1.
3. With these values up to five pseudo-likelihood updates are computed.
4. The PL estimates for fixed-effects, covariance parameters, and the solutions for the random effects are then used to determine the number of quadrature points and used as the starting values for the quadrature.

The first step (GLM fixed-effects estimates) is omitted, if you modify the previous statement as follows:

```
proc glimmix method=quad(initpl=5) noinitglm;
```

The NOINITGLM option is the default of the pseudo-likelihood methods you select with the METHOD= option.

QCHECK

performs an adaptive recalculation of the objective function ($-2 \log$ likelihood) at the solution. The increment of the quadrature points, starting from the number of points used in the optimization, follows the same rules as the determination of the quadrature point sequence at the starting values (see the QFAC= and QMAX= suboptions). For example, the following statement estimates the parameters based on a quadrature with seven nodes in each dimension:

```
proc glimmix method=quad(qpoints=7 qcheck);
```

Because the default search sequence is 1, 3, 5, 7, 9, 11, 21, 31, the QCHECK option computes the $-2 \log$ likelihood at the converged solution for 9, 11, 21, and 31 quadrature points and reports relative differences to the converged value and among successive values. The ODS table produced by this option is named “QuadCheck.”

CAUTION: This option is useful to diagnose the sensitivity of the likelihood approximation at the solution. It does **not** diagnose the stability of the solution under changes in the number of quadrature points. For example, if increasing the number of points from 7 to 9 does not alter the objective function, this does not imply that a quadrature with 9 points would arrive at the same parameter estimates as a quadrature with 7 points.

QFAC=*r*

determines the step size for the quadrature point sequence. If the GLIMMIX procedure determines the quadrature nodes adaptively, the log likelihoods are computed for nodes in a pre-determined sequence. If N_{min} and N_{max} denote the values from the QMIN= and QMAX= suboptions, respectively, the sequence for values less than 11 is constructed in increments of 2 starting at N_{min} . Values greater than 11 are incremented in steps of r . The default value is $r=10$. The default sequence, without specifying the QMIN=, QMAX=, or QFAC= option, is thus 1, 3, 5, 7, 9, 11, 21, 31. By contrast, the following statement evaluates the sequence 8, 10, 30, 50:

```
proc glimmix method=quad(qmin=8, qmax=51, qfac=20);
```

QMAX=*n*

specifies an upper bound for the number of quadrature points. The default is $n=31$.

QMIN=*n*

specifies a lower bound for the number of quadrature points. The default is $n=1$ and the value must be less than the QMAX= value.

QPOINTS=*n*

determines the number of quadrature points in each dimension of the integral. Note that if there are r random effects for each subject, the GLIMMIX procedure evaluates n^r conditional log likelihoods for each observation to compute one value of the objective function. Increasing the number of quadrature nodes can substantially increase the computational burden. If you choose QPOINTS=1, the quadrature approximation reduces to the Laplace approximation. If you do not specify the number of quadrature points, it is determined adaptively by increasing the number of nodes at the starting values. See the section “[Aspects Common to Adaptive Quadrature and Laplace Approximation](#)” on page 3064 for details.

QTOL=*r*

specifies a relative tolerance criterion for the successive evaluation of log likelihoods for different numbers of quadrature points. When the GLIMMIX procedure determines the number of quadrature points adaptively, the number of nodes are increased until the QMAX=*n* limit is reached or until two successive evaluations of the log likelihood have a relative change of less than *r*. In the latter case, the lesser number of quadrature nodes is used for the optimization.

The EBSSFRAC, EBSSTOL, EBSTEPS, EBSUBSTEPS, and EBTOL suboptions affect the suboptimization that leads to the empirical Bayes estimates of the random effects. Under normal circumstances, there is no reason to change from the default values. When the sub-optimizations fail, the optimization process can come to a halt. If the EBDDETAILS option is in effect, you might be able to determine why the suboptimization fails and then adjust these values accordingly.

The QMIN, QMAX, QTOL, and QFAC suboptions determine the quadrature point search sequence for the adaptive component of estimation.

As for METHOD=LAPLACE, certain features of the marginal distribution are not available because the marginal likelihood of the data is approximated numerically. For example, you cannot display a marginal variance-covariance matrix. Also, the procedure includes both the fixed-effects and covariance parameters in the optimization for quadrature estimation. Consequently, this setting imposes some restrictions with respect to available options. Table 41.3 lists the options that are assumed for METHOD=QUAD and METHOD=LAPLACE, and Table 41.4 lists the options that are not compatible with these estimation methods.

Table 41.3 Defaults for METHOD=LAPLACE and METHOD=QUAD

Statement	Option
PROC GLIMMIX	NOPROFILE
PROC GLIMMIX	INITGLM
MODEL	NOCENTER

Table 41.4 Options Incompatible with METHOD=LAPLACE and METHOD=QUAD

Statement	Option
PROC GLIMMIX	EXPHESSIAN
PROC GLIMMIX	SCOREMOD
PROC GLIMMIX	SCORING
PROC GLIMMIX	PROFILE
MODEL	DDFM=KENWARDROGER
MODEL	DDFM=SATTERTHWAITE
MODEL	STDcoef
RANDOM	RESIDUAL
RANDOM _RESIDUAL_	All R-side random effects
RANDOM	V
RANDOM	VC
RANDOM	VCI
RANDOM	VCORR
RANDOM	VI

In addition to the options displayed in Table 41.4, the **NOBOUND** option in the **PROC GLIMMIX** and the **NOBOUND** option in the **PARMS** statements are not available with **METHOD=QUAD**. Unbounding the covariance parameter estimates is possible with **METHOD=LAPLACE**, however.

No Random Effects Present

If the model does not contain G-side random effects or contains only a single overdispersion component, then the model belongs to the family of (overdispersed) generalized linear models if the distribution is known or the quasi-likelihood models for independent data if the distribution is not known. The GLIMMIX procedure then estimates model parameters by the following techniques:

- normally distributed data: residual maximum likelihood
- nonnormal data: maximum likelihood
- data with unknown distribution: quasi-likelihood

The **METHOD=** specification then has only an effect with respect to the divisor used in estimating the overdispersion component. With a residual method, the divisor is $f - k$, where f denotes the sum of the frequencies and k is the rank of **X**. Otherwise, the divisor is f .

NAMELEN=number

specifies the length to which long effect names are shortened. The default and minimum value is 20.

NOBOUND

requests the removal of boundary constraints on covariance and scale parameters in mixed models. For example, variance components have a default lower boundary constraint of 0, and the **NOBOUND** option allows their estimates to be negative.

The **NOBOUND** option cannot be used for adaptive quadrature estimation with **METHOD=QUAD**. The scaling of the quadrature abscissas requires an inverse Cholesky root that is possibly not well defined when the **G** matrix of the mixed model is negative definite or indefinite. The Laplace approximation (**METHOD=LAPLACE**) is not subject to this limitation.

NOBSDetail

adds detailed information to the “Number of Observations” table to reflect how many observations were excluded from the analysis and for which reason.

NOCLPRINT<=number>

suppresses the display of the “Class Level Information” table, if you do not specify *number*. If you specify *number*, only levels with totals that are less than *number* are listed in the table.

NOFIT

suppresses fitting of the model. When the **NOFIT** option is in effect, **PROC GLIMMIX** produces the “Model Information,” “Class Level Information,” “Number of Observations,” and “Dimensions” tables. These can be helpful to gauge the computational effort required to fit the model. For example, the “Dimensions” table informs you as to whether the GLIMMIX procedure processes the data by subjects, which is typically more computationally efficient than processing the data as a single subject. See the section “[Processing by Subjects](#)” for more information.

If you request a radial smooth with knot selection by k -d tree methods, **PROC GLIMMIX** also computes the knot locations of the smoother. You can then examine the knots without fitting the model.

This enables you to try out different knot construction methods and bucket sizes. See the [KNOT-METHOD=KDTREE](#) option (and its suboptions) of the [RANDOM](#) statement.

If you combine the [NOFIT](#) option with the [OUTDESIGN](#) option, you can write the **X** and/or **Z** matrix of your model to a SAS data set without fitting the model.

NOINITGLM

requests that the starting values for the fixed effects not be obtained by first fitting a generalized linear model. This option is the default for the pseudo-likelihood estimation methods and for the linear mixed model. For the pseudo-likelihood methods, starting values can be implicitly defined based on an initial pseudo-data set derived from the data and the link function. For linear mixed models, starting values for the fixed effects are not necessary. The [NOINITGLM](#) option is useful in conjunction with the [INITPL=](#) suboption of [METHOD=QUAD](#) in order to perform initial pseudo-likelihood steps prior to an adaptive quadrature.

NOITPRINT

suppresses the display of the “Iteration History” table.

NOPROFILE

includes the scale parameter ϕ into the optimization for models that have such a parameter (see [Table 41.19](#)). By default, the [GLIMMIX](#) procedure profiles scale parameters from the optimization in mixed models. In generalized linear models, scale parameters are not profiled.

NOREML

determines the denominator for the computation of the scale parameter in a GLM for normal data and for overdispersion parameters. By default, the [GLIMMIX](#) procedure computes the scale parameter for the normal distribution as

$$\hat{\phi} = \sum_{i=1}^n \frac{f_i (y_i - \hat{y}_i)^2}{f - k}$$

where k is the rank of **X**, f_i is the frequency associated with the i th observation, and $f = \sum f_i$. Similarly, the overdispersion parameter in an overdispersed GLM is estimated by the ratio of the Pearson statistic and $(f - k)$. If the [NOREML](#) option is in effect, the denominators are replaced by f , the sum of the frequencies. In a GLM for normal data, this yields the maximum likelihood estimate of the error variance. For this case, the [NOREML](#) option is a convenient way to change from [REML](#) to [ML](#) estimation.

In [GLMM](#) models fit by pseudo-likelihood methods, the [NOREML](#) option changes the estimation method to the nonresidual form. See the [METHOD=](#) option for the distinction between residual and nonresidual estimation methods.

ODDSRATIO

OR

requests that odds ratios be added to the output when applicable. Odds ratios and their confidence limits are reported only for models with logit, cumulative logit, or generalized logit link. Specifying the [ODDSRATIO](#) option in the [PROC GLIMMIX](#) statement has the same effect as specifying the [ODDSRATIO](#) option in the [MODEL](#) statement and in all [LSMEANS](#) statements. Note that the [ODDSRATIO](#) option in the [MODEL](#) statement has several suboptions that enable you to construct customized odds ratios. These suboptions are available only through the [MODEL](#) statement. For details about the interpretation and computation of odds and odds ratios with the [GLIMMIX](#) procedure, see the section “Odds and Odds Ratio Estimation” on page 3090.

ORDER=DATA | FORMATTED | FREQ | INTERNAL

specifies the sort order for the levels of the classification variables (which are specified in the **CLASS** statement). This ordering determines which parameters in the model correspond to each level in the data, so the **ORDER=** option can be useful when you use **CONTRAST** or **ESTIMATE** statements. This option applies to the levels for all classification variables, except when you use the (default) **ORDER=FORMATTED** option with numeric classification variables that have no explicit format. With this option, the levels of such variables are ordered by their internal value.

The **ORDER=** option can take the following values:

Value of ORDER=	Levels Sorted By
DATA	Order of appearance in the input data set
FORMATTED	External formatted value, except for numeric variables with no explicit format, which are sorted by their unformatted (internal) value
FREQ	Descending frequency count; levels with the most observations come first in the order
INTERNAL	Unformatted value

By default, **ORDER=FORMATTED**. For **ORDER=FORMATTED** and **ORDER=INTERNAL**, the sort order is machine-dependent.

When the response variable appears in a **CLASS** statement, the **ORDER=** option in the **PROC GLIMMIX** statement applies to its sort order. Specification of a *response-option* in the **MODEL** statement overrides the **ORDER=** option in the **PROC GLIMMIX** statement. For example, in the following statements the sort order of the *wheeze* variable is determined by the formatted value (default):

```
proc glimmix order=data;
  class city;
  model wheeze = city age / dist=binary s;
run;
```

The **ORDER=** option in the **PROC GLIMMIX** statement has no effect on the sort order of the *wheeze* variable because it does not appear in the **CLASS** statement. However, in the following statements the sort order of the *wheeze* variable is determined by the order of appearance in the input data set because the response variable appears in the **CLASS** statement:

```
proc glimmix order=data;
  class city wheeze;
  model wheeze = city age / dist=binary s;
run;
```

For more information about sort order, see the chapter on the **SORT** procedure in the *Base SAS Procedures Guide* and the discussion of **BY**-group processing in *SAS Language Reference: Concepts*.

OUTDESIGN< (*options*) > < =SAS-data-set >

creates a data set that contains the contents of the **X** and **Z** matrix. If the data are processed by subjects as shown in the “Dimensions” table, then the **Z** matrix saved to the data set corresponds to a single subject. By default, the GLIMMIX procedure includes in the OUTDESIGN data set the **X** and **Z** matrix (if present) and the variables in the input data set. You can specify the following *options* in parentheses to control the contents of the OUTDESIGN data set:

NAMES

produces tables associating columns in the OUTDESIGN data set with fixed-effects parameter estimates and random-effects solutions.

NOMISS

excludes from the OUTDESIGN data set observations that were not used in the analysis.

NOVAR

excludes from the OUTDESIGN data set variables from the input data set. Variables listed in the **BY** and **ID** statements and variables needed for identification of **SUBJECT=** effects are always included in the OUTDESIGN data set.

X< =*prefix* >

saves the contents of the **X** matrix. The optional *prefix* is used to name the columns. The default naming prefix is “_X”.

Z< =*prefix* >

saves the contents of the **Z** matrix. The optional *prefix* is used to name the columns. The default naming prefix is “_Z”.

The order of the observations in the OUTDESIGN data set is the same as the order of the input data set. If you do not specify a data set with the OUTDESIGN option, the procedure uses the **DATA=** convention to name the data set.

PCONV=*r*

specifies the parameter estimate convergence criterion for doubly iterative estimation methods. The GLIMMIX procedure applies this criterion to fixed-effects estimates and covariance parameter estimates. Suppose $\hat{\psi}_i^{(u)}$ denotes the estimate of the *i*th parameter at the *u*th optimization. The procedure terminates the doubly iterative process if the largest value

$$2 \times \frac{|\hat{\psi}_i^{(u)} - \hat{\psi}_i^{(u-1)}|}{|\hat{\psi}_i^{(u)}| + |\hat{\psi}_i^{(u-1)}|}$$

is less than *r*. To check an absolute convergence criteria as well, you can set the **ABSPCONV=** option in the PROC GLIMMIX statement. The default value for *r* is 1E8 times the machine epsilon, a product that equals about 1E–8 on most machines.

Note that this convergence criterion does not affect the convergence criteria applied within any individual optimization. In order to change the convergence behavior within an optimization, you can use the **ABSCONV=**, **ABSFCONV=**, **ABSGCONV=**, **ABSXCONV=**, **FCONV=**, or **GCONV=** option in the **NLOPTIONS** statement.

PLOTS <(global-plot-options)> <= plot-request <(options)>>

PLOTS <(global-plot-options)> <= (plot-request <(options)> <... plot-request <(options)>>>
requests that the GLIMMIX procedure produce statistical graphics via ODS Graphics.

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;

proc glimmix data=plants;
  class Block Type;
  model StemLength = Block Type;
  lsmeans type / diff=control plots=controlplot;
run;

ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS](#).”

For examples of the basic statistical graphics produced by the GLIMMIX procedure and aspects of their computation and interpretation, see the section “[ODS Graphics](#)” on page 3115 in this chapter. You can also request statistical graphics for least squares means through the **PLOTS** option in the **LSMEANS** statement, which gives you more control over the display compared to the **PLOTS** option in the **PROC GLIMMIX** statement.

Global Plot Options

The *global-plot-options* apply to all relevant plots generated by the GLIMMIX procedure. The *global-plot-options* supported by the GLIMMIX procedure are as follows:

OBSNO

uses the data set observation number to identify observations in tooltips, provided that the observation number can be determined. Otherwise, the number displayed in tooltips is the index of the observation as it is used in the analysis within the BY group.

UNPACKPANEL

UNPACK

displays each graph separately. (By default, some graphs can appear together in a single panel.)

Specific Plot Options

The following listing describes the specific plots and their options.

ALL

requests that all plots appropriate for the analysis be produced. In models with G-side random effects, residual plots are based on conditional residuals (by using the BLUPs of random effects) on the linear (linked) scale. Plots of least squares means differences are produced for **LSMEANS** statements without options that would contradict such a display.

ANOMPLOT**ANOM**

requests an analysis of means display in which least squares means are compared against an average least squares mean (Ott 1967; Nelson 1982, 1991, 1993). See the **DIFF=** option in the **LSMEANS** statement for the computation of this average. Least squares mean ANOM plots are produced only for those fixed effects that are listed in **LSMEANS** statements that have options that do not contradict the display. For example, if you request ANOM plots with the **PLOTS=** option in the **PROC GLIMMIX** statement, the following **LSMEANS** statements produce analysis of mean plots for effects A and C:

```
lsmeans A / diff=anom;
lsmeans B / diff;
lsmeans C;
```

The **DIFF** option in the second **LSMEANS** statement implies all pairwise differences.

When differences against the average LS-mean are adjusted for multiplicity with the **ADJUST=NELSON** option in the **LSMEANS** statement, the ANOMPLOT display is adjusted accordingly.

BOXPLOT <(boxplot-options)>

requests box plots for the effects in your model that consist of classification effects only. Note that these effects can involve more than one classification variable (interaction and nested effects), but cannot contain any continuous variables. By default, the **BOXPLOT** request produces box plots of (conditional) residuals for the qualifying effects in the **MODEL** and **RANDOM** statements. See the discussion of the *boxplot-options* in a later section for information about how to tune your box plot request.

CONTROLPLOT**CONTROL**

requests a display in which least squares means are visually compared against a reference level. LS-mean control plots are produced only for those fixed effects that are listed in **LSMEANS** statements that have options that do not contradict with the display. For example, the following statements produce control plots for effects A and C if you specify **PLOTS=CONTROL** in the **PROC GLIMMIX** statement:

```
lsmeans A / diff=control('1');
lsmeans B / diff;
lsmeans C;
```

The **DIFF** option in the second **LSMEANS** statement implies all pairwise differences.

When differences against a control level are adjusted for multiplicity with the **ADJUST=** option in the **LSMEANS** statement, the control plot display is adjusted accordingly.

DIFFPLOT< (*diffplot-options*) >

DIFFOGRAM < (*diffplot-options*) >

DIFF< (*diffplot-options*) >

requests a display of all pairwise least squares mean differences and their significance. When constructed from arithmetic means, the display is also known as a “mean-mean scatter plot” (Hsu 1996; Hsu and Peruggia 1994). For each comparison a line segment, centered at the LS-means in the pair, is drawn. The length of the segment corresponds to the projected width of a confidence interval for the least squares mean difference. Segments that fail to cross the 45-degree reference line correspond to significant least squares mean differences.

If you specify the **ADJUST=** option in the **LSMEANS** statement, the lengths of the line segments are adjusted for multiplicity.

LS-mean difference plots are produced only for those fixed effects listed in **LSMEANS** statements that have options that do not conflict with the display. For example, the following statements request differences against a control level for the A effect, all pairwise differences for the B effect, and the least squares means for the C effect:

```
lsmeans A / diff=control('1');
lsmeans B / diff;
lsmeans C;
```

The **DIFF=** type in the first statement contradicts a display of all pairwise differences. Difference plots are produced only for the B and C effects if you specify **PLOTS=DIFF** in the **PROC GLIMMIX** statement.

You can specify the following *diffplot-options*. The **ABS** and **NOABS** options determine the positioning of the line segments in the plot. When the **ABS** option is in effect (this is the default) all line segments are shown on the same side of the reference line. The **NOABS** option separates comparisons according to the sign of the difference. The **CENTER** option marks the center point for each comparison. This point corresponds to the intersection of two least squares means. The **NOLINES** option suppresses the display of the line segments that represent the confidence bounds for the differences of the least squares means. The **NOLINES** option implies the **CENTER** option. The default is to draw line segments in the upper portion of the plot area without marking the center point.

MEANPLOT< (*meanplot-options*) >

requests a display of the least squares means of effects specified in **LSMEANS** statements. The following *meanplot-options* affect the display. Upper and lower confidence limits are plotted when the **CL** option is used. When the **CLBAND** option is in effect, confidence limits are shown as bands and the means are connected. By default, least squares means are not joined by lines. You can achieve that effect with the **JOIN** or **CONNECT** option. Least squares means are displayed in the same order in which they appear in the “Least Squares Means” table. You can change that order for plotting purposes with the **ASCENDING** and **DESCENDING** options. The **ILINK** option requests that results be displayed on the inverse linked (the data) scale.

Note that there is also a **MEANPLOT** suboption of the **PLOTS=** option in the **LSMEANS** statement. In addition to the *meanplot-options* just described, you can also specify classification effects that give you more control over the display of interaction means through the **PLOTBY=** and **SLICEBY=** options. To display interaction means, you typically want to use the **MEANPLOT** option in the **LSMEANS** statement. For example, the next statement requests a plot in

which the levels of A are placed on the horizontal axis and the means that belong to the same level of B are joined by lines:

```
lsmeans A*B / plot=meanplot(sliceby=b join);
```

NONE

requests that no plots be produced.

ODDSRATIO <(oddsratioplot-options)>

requests a display of odds ratios and their confidence limits when the link function permits the computation of odds ratios (see the **ODDSRATIO** option in the **MODEL** statement). Possible suboptions of the **ODDSRATIO** plot request are described below under the heading “Odds Ratio Plot Options.”

RESIDUALPANEL<(residualplot-options)>

requests a paneled display constructed from raw residuals. The panel consists of a plot of the residuals against the linear predictor or predicted mean, a histogram with normal density overlaid, a *Q-Q* plot, and a box plot of the residuals. The *residualplot-options* enable you to specify which type of residual is being graphed. These are further discussed below under the heading “Residual Plot Options.”

STUDENTPANEL<(residualplot-options)>

requests a paneled display constructed from studentized residuals. The same panel organization is applied as for the **RESIDUALPANEL** plot type.

PEARSONPANEL<(residualplot-options)>

requests a paneled display constructed from Pearson residuals. The same panel organization is applied as for the **RESIDUALPANEL** plot type.

Residual Plot Options

The *residualplot-options* apply to the **RESIDUALPANEL**, **STUDENTPANEL**, and **PEARSONPANEL** displays. The primary function of these options is to control which type of a residual to display. The four types correspond to *keyword-options* as for output statistics in the **OUTPUT** statement. The *residualplot-options* take on the following values:

BLUP

CONDITIONAL

uses the predictors of the random effects in computing the residual.

ILINK

NONLINEAR

computes the residual on the inverse linked scale (the data scale).

NOBLUP

MARGINAL

does not use the predictors of the random effects in computing the residual.

NOILINK**LINEAR**

computes the residual on the linked scale.

UNPACK

produces separate plots from the elements of the panel.

You can list a plot request one or more times with different options. For example, the following statements request a panel of marginal raw residuals, individual plots generated from a panel of the conditional raw residuals, and a panel of marginal studentized residuals:

```
ods graphics on;
proc glimmix plots=(ResidualPanel(marginal)
                   ResidualPanel(unpack conditional)
                   StudentPanel(marginal));
```

The default is to compute conditional residuals on the linear scale if the model contains G-side random effects (BLUP NOILINK). Not all combinations of the BLUP/NOBLUP and ILINK/NOILINK suboptions are possible for all residual types and models. For details, see the description of output statistics for the **OUTPUT** statement. Pearson residuals are always displayed against the linear predictor; all other residuals are graphed versus the linear predictor if the NOILINK suboption is in effect (default), and against the corresponding prediction on the mean scale if the ILINK option is in effect. See [Table 41.14](#) for a definition of the residual quantities and exclusions.

Box Plot Options

The *boxplot-options* determine whether box plots are produced for residuals or for residuals and observed values, and for which model effects the box plots are constructed. The available *boxplot-options* are as follows:

BLOCK**BLOCKLEGEND**

displays levels of up to four classification variables of the box plot effect by using block legends instead of axis tick values.

BLUP**CONDITIONAL**

constructs box plots from conditional residuals—that is, residuals that use the estimated BLUPs of random effects.

FIXED

produces box plots for all fixed effects (**MODEL** statement) consisting entirely of classification variables.

GROUP

produces box plots for all **GROUP=** effects in **RANDOM** statements consisting entirely of classification variables.

ILINK**NONLINEAR**

computes the residual on the scale of the data (the inverse linked scale).

NOBLUP**MARGINAL**

constructs box plots from marginal residuals.

NOILINK**LINEAR**

computes the residual on the linked scale.

NPANELPOS=*number*

specifies the number of box positions on the graphic and provides the capability to break a box plot into multiple graphics. If *number* is negative, no balancing of the number of boxes takes place and *number* is the maximum number of boxes per graphic. If *number* is positive, the number of boxes per graphic is balanced. For example, suppose that variable A has 125 levels. The following statements request that the number of boxes per plot results be balanced and result in six plots with 18 boxes each and one plot with 17 boxes:

```
ods graphics on;
proc glimmix plots=boxplot (npanelpos=20);
  class A;
  model y = A;
run;
```

If *number* is zero (this is the default), all levels of the effect are displayed in a single plot.

OBSERVED

adds box plots of the observed data for the selected effects.

PEARSON

constructs box plots from Pearson residuals rather than from the default residuals.

PSEUDO

adds box plots of the pseudo-data for the selected effects. This option is available only for the pseudo-likelihood estimation methods that construct pseudo-data.

RANDOM

produces box plots for all effects in **RANDOM** statements that consist entirely of classification variables. This does not include effects specified in the **GROUP=** or **SUBJECT=** option of the **RANDOM** statements.

RAW

constructs box plots from raw residuals (observed minus predicted).

STUDENT

constructs box plots from studentized residuals rather than from the default residuals.

SUBJECT

produces box plots for all **SUBJECT=** effects in **RANDOM** statements consisting entirely of classification variables.

USEINDEX

uses as the horizontal axis label the index of the effect level, rather than the formatted value(s). For classification variables with many levels or model effects that involve multiple classification variables, the formatted values identifying the effect levels might take up too much space as axis tick values, leading to extensive thinning. The **USEINDEX** option replaces tick values constructed from formatted values with the internal level number.

By default, box plots of residuals are constructed from the raw conditional residuals (on the linked scale) in linear mixed models and from Pearson residuals in all other models. Note that not all combinations of the **BLUP/NOBLUP** and **ILINK/NOILINK** suboptions are possible for all residual types and models. For details, see the description of output statistics for the **OUTPUT** statement.

Odds Ratio Plot Options

The *oddsratioplot-options* determine the display of odds ratios and their confidence limits. The computation of the odds ratios follows the **ODDSRATIO** option in the **MODEL** statement. The available *oddsratioplot-options* are as follows:

LOGBASE= 2 | E | 10

log-scales the odds ratio axis.

NPANELPOS=*n*

provides the capability to break an odds ratio plot into multiple graphics having at most $|n|$ odds ratios per graphic. If n is positive, then the number of odds ratios per graphic is balanced. If n is negative, then no balancing of the number of odds ratios takes place. For example, suppose you want to display 21 odds ratios. Then **NPANELPOS=20** displays two plots, the first with 11 and the second with 10 odds ratios, and **NPANELPOS=-20** displays 20 odds ratios in the first plot and a single odds ratio in the second. If $n=0$ (this is the default), then all odds ratios are displayed in a single plot.

ORDER=ASCENDING | DESCENDING

displays the odds ratios in sorted order. By default the odds ratios are displayed in the order in which they appear in the “Odds Ratio Estimates” table.

RANGE=(*< min >* *<, max >*) | CLIP

specifies the range of odds ratios to display. If you specify **RANGE=CLIP**, then the confidence intervals are clipped and the range contains the minimum and maximum odds ratios. By default the range of view captures the extent of the odds ratio confidence intervals.

STATS

adds the numeric values of the odds ratio and its confidence limits to the graphic.

PROFILE

requests that scale parameters be profiled from the optimization, if possible. This is the default for generalized linear mixed models. In generalized linear models with normally distributed data, you can use the PROFILE option to request profiling of the residual variance.

SCOREMOD

requests that the Hessian matrix in GLMMs be based on a modified scoring algorithm, provided that PROC GLIMMIX is in scoring mode when the Hessian is evaluated. The procedure is in scoring mode during iteration, if the optimization technique requires second derivatives, the SCORING=*n* option is specified, and the iteration count has not exceeded *n*. The procedure also computes the expected (scoring) Hessian matrix when you use the EXPHESSIAN option in the PROC GLIMMIX statement.

The SCOREMOD option has no effect if the SCORING= or EXPHESSIAN option is not specified. The nature of the SCOREMOD modification to the expected Hessian computation is shown in Table 41.21, in the section “Pseudo-likelihood Estimation Based on Linearization” on page 3054. The modification can improve the convergence behavior of the GLMM compared to standard Fisher scoring and can provide a better approximation of the variability of the covariance parameters. For more details, see the section “Estimated Precision of Estimates” on page 3056.

SCORING=*number*

requests that Fisher scoring be used in association with the estimation method up to iteration *number*. By default, no scoring is applied. When you use the SCORING= option and PROC GLIMMIX converges without stopping the scoring algorithm, the procedure uses the expected Hessian matrix to compute approximate standard errors for the covariance parameters instead of the observed Hessian. If necessary, the standard errors of the covariance parameters as well as the output from the ASYCOV and ASYCORR options are adjusted.

If scoring stopped prior to convergence and you want to use the expected Hessian matrix in the computation of standard errors, use the EXPHESSIAN option in the PROC GLIMMIX statement.

Scoring is not possible in models for nominal data. It is also not possible for GLMs with unknown distribution or for those outside the exponential family. If you perform quasi-likelihood estimation, the GLIMMIX procedure is always in scoring mode and the SCORING= option has no effect. See the section “Quasi-likelihood for Independent Data” for a description of the types of models where GLIMMIX applies quasi-likelihood estimation.

The SCORING= option has no effect for optimization methods that do not involve second derivatives. See the TECHNIQUE= option in the NLOPTIONS statement and the section “Choosing an Optimization Algorithm” on page 494 in Chapter 19, “Shared Concepts and Topics,” for details about first- and second-order algorithms.

SINGCHOL=*number*

tunes the singularity criterion in Cholesky decompositions. The default is 1E4 times the machine epsilon; this product is approximately 1E–12 on most computers.

SINGRES=*number*

sets the tolerance for which the residual variance is considered to be zero. The default is 1E4 times the machine epsilon; this product is approximately 1E–12 on most computers.

SINGULAR=number

tunes the general singularity criterion applied by the GLIMMIX procedure in divisions and inversions. The default is 1E4 times the machine epsilon; this product is approximately 1E–12 on most computers.

STARTGLM

is an alias of the [INITGLM](#) option.

SUBGRADIENT< =SAS-data-set >**SUBGRAD< =SAS-data-set >**

creates a data set with information about the gradient of the objective function. The contents and organization of the SUBGRADIENT= data set depend on the type of model. The following paragraphs describe the SUBGRADIENT= data set for the two major estimation modes. See the section “[GLM Mode or GLMM Mode](#)” on page 3067 for details about the estimation modes of the GLIMMIX procedure.

GLMM Mode

If the GLIMMIX procedure operates in GLMM mode, the SUBGRADIENT= data set contains as many observations as there are usable subjects in the analysis. The maximum number of usable subjects is displayed in the “Dimensions” table. Gradient information is not written to the data set for subjects who do not contribute valid observations to the analysis. Note that the objective function in the “Iteration History” table is in terms of the $-2 \log$ (residual, pseudo-) likelihood. The gradients in the SUBGRADIENT= data set are gradients of that objective function.

The gradients are evaluated at the final solution of the estimation problem. If the GLIMMIX procedure fails to converge, then the information in the SUBGRADIENT= data set corresponds to the gradient evaluated at the last iteration or optimization.

The number of gradients saved to the SUBGRADIENT= data set equals the number of parameters in the optimization. For example, with [METHOD=LAPLACE](#) or [METHOD=QUAD](#) the fixed-effects parameters and the covariance parameters take part in the optimization. The order in which the gradients appear in the data set equals the order in which the gradients are displayed when the [ITDETAILS](#) option is in effect: gradients for fixed-effects parameters precede those for covariance parameters, and gradients are not reported for singular columns in the $X'X$ matrix. In models where the residual variance is profiled from the optimization, a subject-specific gradient is not reported for the residual variance. To decompose this gradient by subjects, add the [NOPROFILE](#) option in the [PROC GLIMMIX](#) statement. When the subject-specific gradients in the SUBGRADIENT= data set are summed, the totals equal the values reported by the [GRADIENT](#) option.

GLM Mode

When you fit a generalized linear model (GLM) or a GLM with overdispersion, the SUBGRADIENT= data set contains the observation-wise gradients of the negative log-likelihood function with respect to the parameter estimates. Note that this corresponds to the objective function in GLMs as displayed in the “Iteration History” table. However, the gradients displayed in the “Iteration History” for GLMs—when the [ITDETAILS](#) option is in effect—are possibly those of the centered and scaled coefficients. The gradients reported in the “Parameter Estimates” table and in the SUBGRADIENT= data set are gradients with respect to the uncentered and unscaled coefficients.

The gradients are evaluated at the final estimates. If the model does not converge, the gradients contain missing values. The gradients appear in the SUBGRADIENT= data set in the same order as in the “Parameter Estimates” table, with singular columns removed.

The variables from the input data set are added to the SUBGRADIENT= data set in GLM mode. The data set is organized in the same way as the input data set; observations that do not contribute to the analysis are transferred to the SUBGRADIENT= data set, but gradients are calculated only for observations that take part in the analysis. If you use an ID statement, then only the variables in the ID statement are transferred to the SUBGRADIENT= data set.

BY Statement

BY *variables* ;

You can specify a BY statement with PROC GLIMMIX to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the GLIMMIX procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

Since sorting the data changes the order in which PROC GLMMIX reads observations, the sort order for the levels of the CLASS variables might be affected if you have also specified ORDER=DATA in the PROC GLIMMIX statement. This, in turn, affects specifications in the CONTRAST, ESTIMATE, or LSMESTIMATE statement.

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

CLASS Statement

CLASS *variable* <(REF= *option*)> ... <*variable* <(REF= *option*)>> </ *global-options* > ;

The CLASS statement names the classification variables to be used in the model. Typical classification variables are Treatment, Sex, Race, Group, and Replication. If you use the CLASS statement, it must appear before the MODEL statement.

Classification variables can be either character or numeric. By default, class levels are determined from the entire set of formatted values of the CLASS variables.

NOTE: Prior to SAS 9, class levels were determined by using no more than the first 16 characters of the formatted values. To revert to this previous behavior, you can use the TRUNCATE option in the CLASS statement.

In any case, you can use formats to group values into levels. See the discussion of the FORMAT procedure in the *Base SAS Procedures Guide* and the discussions of the FORMAT statement and SAS formats in *SAS Formats and Informats: Reference*. You can adjust the order of CLASS variable levels with the ORDER= option in the PROC GLIMMIX statement. You can specify the following REF= option to indicate how the levels of an individual classification variable are to be ordered by enclosing it in parentheses after the variable name:

REF= 'level' | FIRST | LAST

specifies a level of the classification variable to be put at the end of the list of levels. This level thus corresponds to the reference level in the usual interpretation of the estimates with PROC GLIMMIX's singular parameterization. You can specify the *level* of the variable to use as the reference level; specify a value that corresponds to the formatted value of the variable if a format is assigned. Alternatively, you can specify REF=FIRST to designate that the first ordered level serve as the reference, or REF=LAST to designate that the last ordered level serve as the reference. To specify that REF=FIRST or REF=LAST be used for all classification variables, use the REF= *global-option* after the slash (/) in the CLASS statement.

You can specify the following *global-options* in the CLASS statement after a slash (/):

REF=FIRST | LAST

specifies a level of all classification variables to be put at the end of the list of levels. This level thus corresponds to the reference level in the usual interpretation of the estimates with PROC GLIMMIX's singular parameterization. Specify REF=FIRST to designate that the first ordered level for each classification variable serve as the reference. Specify REF=LAST to designate that the last ordered level serve as the reference. This option applies to all the variables specified in the CLASS statement. To specify different reference levels for different classification variables, use REF= options for individual variables.

TRUNCATE

specifies that class levels be determined by using only up to the first 16 characters of the formatted values of CLASS variables. When formatted values are longer than 16 characters, you can use this option to revert to the levels as determined in releases prior to SAS 9.

CODE Statement

CODE < options > ;

The CODE statement enables you to write SAS DATA step code for computing predicted values of the fitted model either to a file or to a catalog entry. This code can then be included in a DATA step to score new data.

Table 41.5 summarizes the *options* available in the CODE statement.

Table 41.5 CODE Statement Options

Option	Description
CATALOG=	Names the catalog entry where the generated code is saved
DUMMIES	Retains the dummy variables in the data set
ERROR	Computes the error function
FILE=	Names the file where the generated code is saved
FORMAT=	Specifies the numeric format for the regression coefficients
GROUP=	Specifies the group identifier for array names and statement labels
IMPUTE	Imputes predicted values for observations with missing or invalid covariates
LINESIZE=	Specifies the line size of the generated code
LOOKUP=	Specifies the algorithm for looking up CLASS levels
RESIDUAL	Computes residuals

For details about the syntax of the CODE statement, see the section “CODE Statement” on page 390 in Chapter 19, “Shared Concepts and Topics.”

CONTRAST Statement

```

CONTRAST 'label' contrast-specification
    <, contrast-specification> <, ... >
    </ options> ;

```

The CONTRAST statement provides a mechanism for obtaining custom hypothesis tests. It is patterned after the CONTRAST statement in PROC MIXED and enables you to select an appropriate inference space (McLean, Sanders, and Stroup 1991). The GLIMMIX procedure gives you greater flexibility in entering contrast coefficients for random effects, however, because it permits the usual *value*-oriented positional syntax for entering contrast coefficients, as well as a level-oriented syntax that simplifies entering coefficients for interaction terms and is designed to work with constructed effects that are defined through the experimental EFFECT statement. The differences between the traditional and new-style coefficient syntax are explained in detail in the section “Positional and Nonpositional Syntax for Contrast Coefficients” on page 3097.

You can test the hypothesis $\mathbf{L}'\boldsymbol{\phi} = \mathbf{0}$, where $\mathbf{L}' = [\mathbf{K}' \mathbf{M}']$ and $\boldsymbol{\phi}' = [\boldsymbol{\beta}' \boldsymbol{\gamma}']$, in several inference spaces. The inference space corresponds to the choice of \mathbf{M} . When $\mathbf{M} = \mathbf{0}$, your inferences apply to the entire population from which the random effects are sampled; this is known as the *broad* inference space. When all elements of \mathbf{M} are nonzero, your inferences apply only to the observed levels of the random effects. This is known as the *narrow* inference space, and you can also choose it by specifying all of the random effects as fixed. The GLM procedure uses the narrow inference space. Finally, by zeroing portions of \mathbf{M} corresponding to selected main effects and interactions, you can choose *intermediate* inference spaces. The broad inference space is usually the most appropriate; it is used when you do not specify random effects in the CONTRAST statement.

In the CONTRAST statement,

<i>label</i>	identifies the contrast in the table. A label is required for every contrast specified. Labels can be up to 200 characters and must be enclosed in quotes.
<i>contrast-specification</i>	identifies the fixed effects and random effects and their coefficients from which the L matrix is formed. The syntax representation of a <i>contrast-specification</i> is <code>< fixed-effect values ... > random-effect values ... ></code>
<i>fixed-effect</i>	identifies an effect that appears in the MODEL statement. The keyword INTERCEPT can be used as an effect when an intercept is fitted in the model. You do not need to include all effects that are in the MODEL statement.
<i>random-effect</i>	identifies an effect that appears in the RANDOM statement. The first random effect must follow a vertical bar (); however, random effects do not have to be specified.
<i>values</i>	are constants that are elements of the L matrix associated with the fixed and random effects. There are two basic methods of specifying the entries of the L matrix. The traditional representation—also known as the positional syntax—relies on entering coefficients in the position they assume in the L matrix. For example, in the following statements the elements of L associated with the b main effect receive a 1 in the first position and a -1 in the second position:

```
class a b;
model y = a b a*b;
contrast 'B at A2' b 1 -1 a*b 0 0 1 -1;
```

The elements associated with the interaction receive a 1 in the third position and a -1 in the fourth position. In order to specify coefficients correctly for the interaction term, you need to know how the levels of a and b vary in the interaction, which is governed by the order of the variables in the **CLASS** statement. The nonpositional syntax is designed to make it easier to enter coefficients for interactions and is necessary to enter coefficients for effects constructed with the experimental **EFFECT** statement. In square brackets you enter the coefficient followed by the associated levels of the **CLASS** variables. If B has two and A has three levels, the previous **CONTRAST** statement, by using nonpositional syntax for the interaction term, becomes

```
contrast 'B at A2' b 1 -1 a*b [1, 2 1] [-1, 2 2];
```

It assigns value 1 to the interaction where A is at level 2 and B is at level 1, and it assigns -1 to the interaction where both classification variables are at level 2. The comma separating the entry for the **L** matrix from the level indicators is optional. Further details about the nonpositional contrast syntax and its use with constructed effects can be found in the section “[Positional and Nonpositional Syntax for Contrast Coefficients](#)” on page 3097. Nonpositional syntax is available only for fixed-effects coefficients.

The rows of **L'** are specified in order and are separated by commas. The rows of the **K'** component of **L'** are specified on the left side of the vertical bars (|). These rows test the fixed effects and are, therefore, checked for estimability. The rows of the **M'** component of **L'** are specified on the right side of the vertical bars. They test the random effects, and no estimability checking is necessary.

If PROC GLIMMIX finds the fixed-effects portion of the specified contrast to be nonestimable (see the `SINGULAR=` option), then it displays missing values for the test statistics.

If the elements of **L** are not specified for an effect that contains a specified effect, then the elements of the unspecified effect are automatically “filled in” over the levels of the higher-order effect. This feature is designed to preserve estimability for cases where there are complex higher-order effects. The coefficients for the higher-order effect are determined by equitably distributing the coefficients of the lower-level effect as in the construction of least squares means. In addition, if the intercept is specified, it is distributed over all classification effects that are not contained by any other specified effect. If an effect is not specified and does not contain any specified effects, then all of its coefficients in **L** are set to 0. You can override this behavior by specifying coefficients for the higher-order effect.

If too many values are specified for an effect, the extra ones are ignored; if too few are specified, the remaining ones are set to 0. If no random effects are specified, the vertical bar can be omitted; otherwise, it must be present. If a `SUBJECT` effect is used in the `RANDOM` statement, then the coefficients specified for the effects in the `RANDOM` statement are equitably distributed across the levels of the `SUBJECT` effect. You can use the `E` option to see exactly what **L** matrix is used.

PROC GLIMMIX handles missing level combinations of classification variables similarly to PROC GLM and PROC MIXED. These procedures delete fixed-effects parameters corresponding to missing levels in order to preserve estimability. However, PROC MIXED and PROC GLIMMIX do not delete missing level combinations for random-effects parameters, because linear combinations of the random-effects parameters are always estimable. These conventions can affect the way you specify your `CONTRAST` coefficients.

The `CONTRAST` statement computes the statistic

$$F = \frac{\begin{bmatrix} \hat{\beta} \\ \hat{\gamma} \end{bmatrix}' \mathbf{L}(\mathbf{L}'\mathbf{C}\mathbf{L})^{-1}\mathbf{L}' \begin{bmatrix} \hat{\beta} \\ \hat{\gamma} \end{bmatrix}}{r}$$

where $r = \text{rank}(\mathbf{L}'\mathbf{C}\mathbf{L})$, and approximates its distribution with an F distribution unless `DDFM=NONE`. If you select `DDFM=NONE` as the degrees-of-freedom method in the `MODEL` statement, and if you do not assign degrees of freedom to the contrast with the `DF=` option, then PROC GLIMMIX computes the test statistic $r \times F$ and approximates its distribution with a chi-square distribution. In the expression for F , **C** is an estimate of $\text{Var}[\hat{\beta}, \hat{\gamma} - \boldsymbol{\gamma}]$; see the section “[Estimated Precision of Estimates](#)” on page 3056 and the section “[Aspects Common to Adaptive Quadrature and Laplace Approximation](#)” on page 3064 for details about the computation of **C** in a generalized linear mixed model.

The numerator degrees of freedom in the F approximation and the degrees of freedom in the chi-square approximation are equal to r . The denominator degrees of freedom are taken from the “Tests of Fixed Effects” table and correspond to the final effect you list in the `CONTRAST` statement. You can change the denominator degrees of freedom by using the `DF=` option.

You can specify the following options in the `CONTRAST` statement after a slash (/).

BYCATEGORY

BYCAT

requests that in models for nominal data (generalized logit models) the contrasts not be combined across response categories but reported separately for each category. For example, assume that the response variable `Style` is multinomial with three (unordered) categories. The following GLIMMIX statements fit a generalized logit model relating the preferred style of instruction to school and educational program effects:

```

proc glimmix data=school;
  class School Program;
  model Style(order=data) = School Program / s ddfm=none
                                dist=multinomial link=glogit;

  freq Count;
  contrast 'School 1 vs. 2' school 1 -1;
  contrast 'School 1 vs. 2' school 1 -1 / bycat;
run;

```

The first contrast compares school effects in all categories. This is a two-degrees-of-freedom contrast because there are two nonredundant categories. The second CONTRAST statement produces two single-degree-of-freedom contrasts, one for each nonreference Style category.

The BYCATEGORY option has no effect unless your model is a generalized (mixed) logit model.

CHISQ

requests that chi-square tests be performed for all contrasts in addition to any F tests. A chi-square statistic equals its corresponding F statistic times the numerator degrees of freedom, and these same degrees of freedom are used to compute the p -value for the chi-square test. This p -value will always be less than that for the F test, because it effectively corresponds to an F test with infinite denominator degrees of freedom.

DF=number

specifies the denominator degrees of freedom for the F test. For the degrees of freedom methods [DDFM=BETWITHIN](#), [DDFM=CONTAIN](#), and [DDFM=RESIDUAL](#), the default is the denominator degrees of freedom taken from the “Tests of Fixed Effects” table and corresponds to the final effect you list in the CONTRAST statement. For [DDFM=NONE](#), infinite denominator degrees of freedom are assumed by default, and for [DDFM=SATTERTHWAITE](#) and [DDFM=KENWARDROGER](#), the denominator degrees of freedom are computed separately for each contrast.

E

requests that the **L** matrix coefficients for the contrast be displayed.

GROUP coeffs

sets up random-effect contrasts between different groups when a [GROUP=](#) variable appears in the [RANDOM](#) statement. By default, CONTRAST statement coefficients on random effects are distributed equally across groups. If you enter a multiple row contrast, you can also enter multiple rows for the GROUP coefficients. If the number of GROUP coefficients is less than the number of contrasts in the CONTRAST statement, the GLIMMIX procedure cycles through the GROUP coefficients. For example, the following two statements are equivalent:

```

contrast 'Trt 1 vs 2 @ x=0.4' trt 1 -1 0 | x 0.4,
                                trt 1 0 -1 | x 0.4,
                                trt 1 -1 0 | x 0.5,
                                trt 1 0 -1 | x 0.5 /
                                group 1 -1, 1 0 -1, 1 -1, 1 0 -1;

contrast 'Trt 1 vs 2 @ x=0.4' trt 1 -1 0 | x 0.4,
                                trt 1 0 -1 | x 0.4,
                                trt 1 -1 0 | x 0.5,
                                trt 1 0 -1 | x 0.5 /
                                group 1 -1, 1 0 -1;

```

SINGULAR=number

tunes the estimability checking. If \mathbf{v} is a vector, define $\text{ABS}(\mathbf{v})$ to be the largest absolute value of the elements of \mathbf{v} . If $\text{ABS}(\mathbf{K}' - \mathbf{K}'\mathbf{T})$ is greater than $c*\text{number}$ for any row of \mathbf{K}' in the contrast, then $\mathbf{K}'\boldsymbol{\beta}$ is declared nonestimable. Here, \mathbf{T} is the Hermite form matrix $(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{X}$, and c is $\text{ABS}(\mathbf{K}')$, except when it equals 0, and then c is 1. The value for *number* must be between 0 and 1; the default is 1E-4.

SUBJECT coeffs

sets up random-effect contrasts between different subjects when a **SUBJECT=** variable appears in the **RANDOM** statement. By default, **CONTRAST** statement coefficients on random effects are distributed equally across subjects. Listing subject coefficients for multiple row **CONTRAST** statements follows the same rules as for **GROUP** coefficients.

COVTEST Statement

COVTEST < 'label' > < test-specification > < / options > ;

The **COVTEST** statement provides a mechanism to obtain statistical inferences for the covariance parameters. Significance tests are based on the ratio of (residual) likelihoods or pseudo-likelihoods. Confidence limits and bounds are computed as Wald or likelihood ratio limits. You can specify multiple **COVTEST** statements.

The likelihood ratio test is obtained by fitting the model subject to the constraints imposed by the *test-specification*. The test statistic is formed as twice the difference of the (possibly restricted) log (pseudo-) likelihoods of the full and the reduced models. Note that fitting the null model does not necessarily require fewer computer resources compared to fitting the full model. The optimization settings for refitting the model are the same as for the full model and can be controlled with the **NLOPTIONS** statement.

Common questions in mixed modeling are whether variance components are zero, whether random effects are independent, and whether rows (columns) can be added or removed from an unstructured covariance matrix. When the parameters under the null hypothesis fall on the boundary of the parameter space, the distribution of the likelihood ratio statistic can be a complicated mixture of distributions. In certain situations it is known to be a relatively straightforward mixture of central chi-square distributions. When the **GLIMMIX** procedure recognizes the model and hypothesis as a case for which the mixture is readily available, the *p*-value of the likelihood ratio test is determined accordingly as a linear combination of central chi-square probabilities. The **Note** column in the “Likelihood Ratio Tests for Covariance Parameters” table along with the table’s footnotes informs you about when mixture distributions are used in the calculation of *p*-values. You can find important statistical and computational details about likelihood ratio testing of covariance parameters with the **GLIMMIX** procedure in the section “Statistical Inference for Covariance Parameters” on page 3068.

In generalized linear mixed models that depend on pseudo-data, the **GLIMMIX** procedure fits the null model for a test of covariance parameters to the final pseudo-data of the converged optimization.

Table 41.6 summarizes the options available in the COVTEST statement.

Table 41.6 COVTEST Statement Options

Option	Description
Test specification	
TESTDATA=	Reads in covariance parameter values from a SAS data set
GENERAL	Provides a general facility to test linear combinations of covariance parameters
Covariance Test Options	
CL	Requests confidence limits for the covariance parameter estimates
CLASSICAL	Computes the likelihood ratio test p -value using the classical method
DF=	Specifies the degrees of freedom
ESTIMATES	Displays the estimates of the covariance parameters under the null hypothesis
MAXITER=	Limits the number of iterations
PARMS	Displays the values of the covariance parameters under the null hypothesis
RESTART	Specifies that starting values for the covariance parameters
TOLERANCE=	Sets the tolerance level of the parameter space boundary
WALD	Produces Wald Z tests
WGHT=	Supplies weights for the computation of p -values

Test Specification

The *test-specification* in the COVTEST statement draws on keywords that represent a particular null hypothesis, lists or data sets of parameter values, or general contrast specifications. Valid keywords are as follows:

GLM INDEP	tests the model against a null model of complete independence. All G-side covariance parameters are eliminated and the R-side covariance structure is reduced to a diagonal structure.
DIAGG	tests for a diagonal \mathbf{G} matrix by constraining off-diagonal elements in \mathbf{G} to zero. The R-side structure is not modified.
DIAGR CINDEP	tests for conditional independence by reducing the R-side covariance structure to diagonal form. The G-side structure is not modified.
HOMOGENEITY	tests homogeneity of covariance parameters across groups by imposing equality constraints. For example, the following statements fit a one-way model with heterogeneous variances and test whether the model could be reduced to a one-way analysis with the same variance across groups:

```
proc glimmix;
  class A;
  model y = a;
  random _residual_ / group=A;
  covtest 'common variance' homogeneity;
run;
```

See [Example 41.9](#) for an application with groups and unstructured covariance matrices.

START INITIAL	compares the final estimates to the starting values of the covariance parameter estimates. This option is useful, for example, if you supply starting values in the PARMs statement and want to test whether the optimization produced significantly better values. In GLMMs based on pseudo-data, the likelihoods that use the starting and the final values are based on the final pseudo-data.
ZEROG	tests whether the G matrix can be reduced to a zero matrix. This eliminates all G-side random effects from the model.

Only a single keyword is permitted in the COVTEST statement. To test more complicated hypotheses, you can formulate tests with the following specifications.

TESTDATA=*data-set*

TDATA=*data-set*

reads in covariance parameter values from a SAS data set. The data set should contain the numerical variable Estimate or numerical variables named Covpi. The GLIMMIX procedure associates the values for Covpi with the *i*th covariance parameter.

For data sets containing the numerical variable Estimate, the GLIMMIX procedure fixes the *i*th covariance parameter value at the value of the *i*th observation in the data set. A missing value indicates not to fix the particular parameter. PROC GLIMMIX performs one likelihood ratio test for the TESTDATA= data set.

For data sets containing numerical variables named Covpi, the procedure performs one likelihood ratio test for each observation in the TESTDATA= data set. You do not have to specify a Covpi variable for every covariance parameter. If the value for the variable is not missing, PROC GLIMMIX fixes the associated covariance parameter in the null model. Consider the following statements:

```
data TestDataSet;
  input covp1 covp2 covp3;
  datalines;
. 0 .
0 0 .
. 0 0
0 0 0
;

proc glimmix method=mspl;
  class subject x;
  model y = x age x*age;
  random intercept age / sub=subject type=un;
  covtest testdata=TestDataSet;
run;
```

Because the **G** matrix is a (2 × 2) unstructured matrix, the first observation of the TestDataSet corresponds to zeroing the covariance between the random intercept and the random slope. When the reduced model is fit, the variances of the intercept and slope are reestimated. The second observation reduces the model to one with only a random slope in age. The third reduces the model to a random intercept model. The last observation eliminates the **G** matrix altogether.

Note that the tests associated with the first and last set of covariance parameters in TestDataSet can also be obtained by using keywords:

```

proc glimmix;
  class subject x;
  model y = x age x*age;
  random intercept age / sub=subject type=un;
  covtest DiagG;
  covtest GLM;
run;

```

value-list

supplies a list of values at which to fix the covariance parameters. A missing value in the list indicates that the covariance parameter is not fixed. If the list is shorter than the number of covariance parameters, missing values are assumed for all parameters not specified. The COVTEST statements that test the random intercept and random slope in the previous example are as follows:

```

proc glimmix;
  class subject x;
  model y = x age x*age;
  random intercept age / sub=subject type=un;
  covtest 0 0;
  covtest . 0 0;
run;

```

GENERAL *coefficients* < ,*coefficients* > < ,... >

CONTRAST *coefficients* < ,*coefficients* > < ,... >

provides a general facility to test linear combinations of covariance parameters. You can specify one or more sets of coefficients. The position of a coefficient in the list corresponds to the position of the parameter in the “Covariance Parameter Estimates” table. The linear combination of covariance parameters that is implied by each set of coefficients is tested against zero. If the list of coefficients is shorter than the number of covariance parameters, a zero coefficient is assumed for the remaining parameters.

For example, in a heterogeneous variance model with four groups, the following statements test the simultaneous hypothesis $H: \sigma_1^2 = \sigma_2^2, \sigma_3^2 = \sigma_4^2$:

```

proc glimmix;
  class A;
  model y = a;
  random _residual_ / group=A;
  covtest 'pair-wise homogeneity'
    general 1 -1 0 0,
           0 0 1 -1;
run;

```

In a repeated measures study with four observations per subject, the COVTEST statement in the following example tests whether the four correlation parameters are identical:

```

proc glimmix;
  class subject drug time;
  model y = drug time drug*time;
  random _residual_ / sub=subject type=unr;
  covtest 'Homogeneous correlation'
    general 0 0 0 0 1 -1          ,
            0 0 0 0 1  0 -1      ,
            0 0 0 0 1  0  0 -1   ,
            0 0 0 0 1  0  0  0 -1 ,
            0 0 0 0 1  0  0  0  0 -1;
run;

```

Notice that the variances (the first four covariance parameters) are allowed to vary. The null model for this test is thus a heterogeneous compound symmetry model.

The degrees of freedom associated with these general linear hypotheses are determined as the rank of the matrix \mathbf{LL}' , where \mathbf{L} is the $k \times q$ matrix of coefficients and q is the number of covariance parameters. Notice that the coefficients in a row do not have to sum to zero. The following statement tests $H: \theta_1 = 3\theta_2, \theta_3 = 0$:

```

covtest general 1 -3, 0 0 1;

```

Covariance Test Options

You can specify the following options in the COVTEST statement after a slash (/).

CL<(suboptions)>

requests confidence limits or bounds for the covariance parameter estimates. These limits are displayed as extra columns in the “Covariance Parameter Estimates” table.

The following suboptions determine the computation of confidence bounds and intervals. See the section “[Statistical Inference for Covariance Parameters](#)” on page 3068 for details about constructing likelihood ratio confidence limits for covariance parameters with PROC GLIMMIX.

ALPHA=*number*

determines the confidence level for constructing confidence limits for the covariance parameters. The value of *number* must be between 0 and 1, the default is 0.05, and the confidence level is $1 - \textit{number}$.

LOWERBOUND

LOWER

requests lower confidence bounds.

TYPE=*method*

determines how the GLIMMIX procedure constructs confidence limits for covariance parameters. The valid methods are PLR (or PROFILE), ELR (or ESTIMATED), and WALD.

TYPE=PLR (TYPE=PROFILE) requests confidence bounds by inversion of the profile (restricted) likelihood ratio (PLR). If θ is the parameter of interest, L denotes the likelihood (possibly restricted and possibly a pseudo-likelihood), and θ_2 is the vector of the remaining (nuisance) parameters, then the profile likelihood is defined as

$$L(\theta_2|\tilde{\theta}) = \sup_{\theta_2} L(\tilde{\theta}, \theta_2)$$

for a given value $\tilde{\theta}$ of θ . If $L(\hat{\theta})$ is the overall likelihood evaluated at the estimates $\hat{\theta}$, the $(1 - \alpha) \times 100\%$ confidence region for θ satisfies the inequality

$$2 \left\{ L(\hat{\theta}) - L(\theta_2|\tilde{\theta}) \right\} \leq \chi_{1,(1-\alpha)}^2$$

where $\chi_{1,(1-\alpha)}^2$ is the cutoff from a chi-square distribution with one degree of freedom and α probability to its right. If a residual scale parameter ϕ is profiled from the estimation, and θ is expressed in terms of a ratio with ϕ during estimation, then profile likelihood confidence limits are constructed for the ratio of the parameter with the residual variance. A column showing the ratio estimates is added to the “Covariance Parameter Estimates” table in this case. To obtain profile likelihood ratio limits for the parameters, rather than their ratios, and for the residual variance, use the NOPROFILE option in the PROC GLIMMIX statement. Also note that METHOD=LAPLACE or METHOD=QUAD implies the NOPROFILE option.

The TYPE=ELR (TYPE=ESTIMATED) option constructs bounds from the estimated likelihood (Pawitan 2001), where nuisance parameters are held fixed at the (restricted) maximum (pseudo-) likelihood estimates of the model. Estimated likelihood intervals are computationally less demanding than profile likelihood intervals, but they do not take into account the variability of the nuisance parameters or the dependence among the covariance parameters. See the section “Statistical Inference for Covariance Parameters” on page 3068 for a geometric interpretation and comparison of ELR versus PLR confidence bounds. A $(1 - \alpha) \times 100\%$ confidence region based on the estimated likelihood is defined by the inequality

$$2 \left\{ L(\hat{\theta}) - L(\tilde{\theta}, \hat{\theta}_2) \right\} \leq \chi_{1,(1-\alpha)}^2$$

where $L(\tilde{\theta}, \hat{\theta}_2)$ is the likelihood evaluated at $\tilde{\theta}$ and the component of $\hat{\theta}$ that corresponds to θ_2 . Estimated likelihood ratio intervals tend to perform well when the correlations between the parameter of interest and the nuisance parameters is small. Their coverage probabilities can fall short of the nominal coverage otherwise. You can display the correlation matrix of the covariance parameter estimates with the ASYCORR option in the PROC GLIMMIX statement.

If you choose TYPE=PLR or TYPE=ELR, the GLIMMIX procedure reports the right-tail probability of the associated single-degree-of-freedom likelihood ratio test along with the confidence bounds. This helps you diagnose whether solutions to the inequality could be found. If the reported probability exceeds α , the associated bound does not meet the inequality. This might occur, for example, when the parameter space is bounded and the likelihood at the boundary values has not dropped by a sufficient amount to satisfy the test inequality.

The TYPE=WALD method requests confidence limits based on the Wald-type statistic $Z_\theta = \hat{\theta}/\text{ease}(\hat{\theta})$, where ease is the estimated asymptotic standard error of the covariance parameter. For parameters that have a lower boundary constraint of zero, a Satterthwaite approximation is

used to construct limits of the form

$$\frac{v\hat{\theta}}{\chi_{v,1-\alpha/2}^2} \leq \theta \leq \frac{v\hat{\theta}}{\chi_{v,\alpha/2}^2}$$

where $v = 2Z^2$, and the denominators are quantiles of the χ^2 distribution with v degrees of freedom. See Milliken and Johnson (1992) and Burdick and Graybill (1992) for similar techniques. For all other parameters, Wald Z-scores and normal quantiles are used to construct the limits. Such limits are also provided for variance components if you specify the **NOBOUND** option in the **PROC GLIMMIX** statement or the **PARMS** statement.

UPPERBOUND

UPPER

requests upper confidence bounds.

If you do not specify any suboptions, the default is to compute two-sided Wald confidence intervals with confidence level $1 - \alpha = 0.95$.

CLASSICAL

requests that the p -value of the likelihood ratio test be computed by the classical method. If $\hat{\lambda}$ is the realized value of the test statistic in the likelihood ratio test,

$$p = \Pr(\chi_v^2 \geq \hat{\lambda})$$

where v is the degrees of freedom of the hypothesis.

DF=value-list

enables you to supply degrees of freedom v_1, \dots, v_k for the computation of p -values from chi-square mixtures. The mixture weights w_1, \dots, w_k are supplied with the **WGHT=** option. If no weights are specified, an equal weight distribution is assumed. If $\hat{\lambda}$ is the realized value of the test statistic in the likelihood ratio test, PROC GLIMMIX computes the p -value as (Shapiro 1988)

$$p = \sum_{i=1}^k w_i \Pr(\chi_{v_i}^2 \geq \hat{\lambda})$$

Note that $\chi_0^2 \equiv 0$ and that mixture weights are scaled to sum to one. If you specify more weights than degrees of freedom in *value-list*, the rank of the hypothesis (DF column) is substituted for the missing degrees of freedom.

Specifying a single value v for *value-list* without giving mixture weights is equivalent to computing the p -value as

$$p = \Pr(\chi_v^2 \geq \hat{\lambda})$$

For example, the following statements compute the p -value based on a chi-square distribution with one degree of freedom:

```

proc glimmix noprofile;
  class A sub;
  model score = A;
  random _residual_ / type=ar(1) subject=sub;
  covtest 'ELR low' 30.62555 0.7133361 / df=1;
run;

```

The DF column of the COVTEST output will continue to read 2 regardless of the DF= specification, however, because the DF column reflects the rank of the hypothesis and equals the number of constraints imposed on the full model.

ESTIMATES

EST

displays the estimates of the covariance parameters under the null hypothesis. Specifying the ESTIMATES option in one COVTEST statement has the same effect as specifying the option in every COVTEST statement.

MAXITER=*number*

limits the number of iterations when you are refitting the model under the null hypothesis to *number* iterations. If the null model does not converge before the limit is reached, no *p*-values are produced.

PARMS

displays the values of the covariance parameters under the null hypothesis. This option is useful if you supply multiple sets of parameter values with the TESTDATA= option. Specifying the PARMS option in one COVTEST statement has the same effect as specifying the option in every COVTEST statement.

RESTART

specifies that starting values for the covariance parameters for the null model are obtained by the same mechanism as starting values for the full models. For example, if you do not specify a PARMS statement, the RESTART option computes MIVQUE(0) estimates under the null model (Goodnight 1978a). If you provide starting values with the PARMS statement, the starting values for the null model are obtained by applying restrictions to the starting values for the full model.

By default, PROC GLIMMIX obtains starting values by applying null model restrictions to the converged estimates of the full model. Although this is computationally expedient, the method does not always lead to good starting values for the null model, depending on the nature of the model and hypothesis. In particular, when you receive a warning about parameters not specified under H_0 falling on the boundary, the RESTART option can be useful.

TOLERANCE=*r*

Values within tolerance $r \geq 0$ of the boundary of the parameter space are considered on the boundary when PROC GLIMMIX examines estimates of nuisance parameters under H_0 and determines whether mixture weights and degrees of freedom can be obtained. In certain cases, when parameters not specified under the null hypothesis are on boundaries, the asymptotic distribution of the likelihood ratio statistic is not a mixture of chi-squares (see, for example, case 8 in Self and Liang 1987). The default for *r* is 1E4 times the machine epsilon; this product is approximately 1E-12 on most computers.

WALD

produces Wald Z tests for the covariance parameters based on the estimates and asymptotic standard errors in the “Covariance Parameter Estimates” table.

WGHT=value-list

enables you to supply weights for the computation of p -values from chi-square mixtures. See the **DF=** option for details. Mixture weights are scaled to sum to one.

EFFECT Statement

EFFECT *effect-specification* ;

The experimental EFFECT statement enables you to construct special collections of columns for **X** or **Z** matrices in your model. These collections are referred to as *constructed effects* to distinguish them from the usual model effects formed from continuous or classification variables.

For details about the syntax of the EFFECT statement and how columns of constructed effects are computed, see the section “EFFECT Statement” on page 393 of Chapter 19, “Shared Concepts and Topics.” For specific details concerning the use of the EFFECT statement with the GLIMMIX procedure, see the section “Notes on the EFFECT Statement” on page 3096.

ESTIMATE Statement

ESTIMATE *'label'* *contrast-specification* <(divisor= n)>
<, *'label'* *contrast-specification* <(divisor= n)>> <, ... >
</ *options* > ;

The ESTIMATE statement provides a mechanism for obtaining custom hypothesis tests. As in the **CONTRAST** statement, the basic element of the ESTIMATE statement is the *contrast-specification*, which consists of **MODEL** and G-side random effects and their coefficients. Specifically, a *contrast-specification* takes the form

$$\langle \text{fixed-effect values} \dots \rangle \langle | \text{random-effect values} \dots \rangle$$

Based on the *contrast-specifications* in your ESTIMATE statement, PROC GLIMMIX constructs the matrix $\mathbf{L}' = [\mathbf{K}' \ \mathbf{M}']$, as in the **CONTRAST** statement, where **K** is associated with the fixed effects and **M** is associated with the G-side random effects. The GLIMMIX procedure supports nonpositional syntax for the coefficients of fixed effects in the ESTIMATE statement. For details see the section “Positional and Nonpositional Syntax for Contrast Coefficients” on page 3097.

PROC GLIMMIX then produces for each row l of \mathbf{L}' an approximate t test of the hypothesis $H: \mathbf{l}\phi = 0$, where $\phi = [\beta' \ \gamma']'$. You can also obtain multiplicity-adjusted p -values and confidence limits for multirow estimates with the **ADJUST=** option. The output from multiple ESTIMATE statements is organized as follows. Results from unadjusted estimates are reported first in a single table, followed by separate tables for each of the adjusted estimates. Results from all ESTIMATE statements are combined in the “Estimates” ODS table.

Note that multirow estimates are permitted. Unlike the **CONTRAST** statement, you need to specify a *'label'* for every row of the multirow estimate, because PROC GLIMMIX produces one test per row. PROC

GLIMMIX selects the degrees of freedom to match those displayed in the “Type III Tests of Fixed Effects” table for the final effect you list in the ESTIMATE statement. You can modify the degrees of freedom by using the `DF=` option. If you select `DDFM=NONE` and do not modify the degrees of freedom by using the `DF=` option, PROC GLIMMIX uses infinite degrees of freedom, essentially computing approximate z tests. If PROC GLIMMIX finds the fixed-effects portion of the specified estimate to be nonestimable, then it displays “Non-est” for the estimate entry.

Table 41.7 summarizes the options available in the ESTIMATE statement.

Table 41.7 ESTIMATE Statement Options

Option	Description
Construction and Computation of Estimable Functions	
<code>DIVISOR=</code>	Specifies a list of values to divide the coefficients
<code>GROUP</code>	Sets up random-effect contrasts between different groups
<code>SINGULAR=</code>	Tunes the estimability checking difference
<code>SUBJECT</code>	Sets up random-effect contrasts between different subjects
Degrees of Freedom and p-values	
<code>ADJDFE=</code>	Determines denominator degrees of freedom when p -values and confidence limits are adjusted for multiple comparisons
<code>ADJUST=</code>	Determines the method for multiple comparison adjustment of estimates
<code>ALPHA=α</code>	Determines the confidence level ($1 - \alpha$)
<code>DF=</code>	Assigns a specific value to degrees of freedom for tests and confidence limits
<code>LOWER</code>	Performs one-sided, lower-tailed inference
<code>STEPDOWN</code>	Adjusts multiplicity-corrected p -values further in a step-down fashion
<code>UPPER</code>	Performs one-sided, upper-tailed inference
Statistical Output	
<code>CL</code>	Constructs t -type confidence limits
<code>E</code>	Prints the L matrix
Generalized Linear Modeling	
<code>BYCATEGORY=</code>	Reports estimates separately for each category for models with nominal data
<code>EXP</code>	Displays exponentiated estimates
<code>ILINK</code>	Computes and displays estimates and standard errors on the inverse linked scale

ADJDFE=SOURCE

ADJDFE=ROW

specifies how denominator degrees of freedom are determined when p -values and confidence limits are adjusted for multiple comparisons with the `ADJUST=` option. When you do not specify the `ADJDFE=` option, or when you specify `ADJDFE=SOURCE`, the denominator degrees of freedom for multiplicity-adjusted results are the denominator degrees of freedom for the final effect listed in the ESTIMATE statement from the “Type III Tests of Fixed Effects” table.

The ADJDFE=ROW setting is useful if you want multiplicity adjustments to take into account that denominator degrees of freedom are not constant across estimates. This can be the case, for example, when the DDFM=SATTERTHWAITE or DDFM=KENWARDROGER degrees-of-freedom method is in effect.

ADJUST=BON**ADJUST=SCHEFFE****ADJUST=SIDAK****ADJUST=SIMULATE**< (*simoptions*) >**ADJUST=T**

requests a multiple comparison adjustment for the p -values and confidence limits for the estimates. The adjusted quantities are produced in addition to the unadjusted quantities. Adjusted confidence limits are produced if the CL or ALPHA= option is in effect. For a description of the adjustments, see Chapter 42, “The GLM Procedure,” and Chapter 61, “The MULTTEST Procedure,” and the documentation for the ADJUST= option in the LSMEANS statement. The ADJUST= option is ignored for generalized logit models.

If the STEPDOWN option is in effect, the p -values are further adjusted in a step-down fashion.

ALPHA=number

requests that a t -type confidence interval be constructed with confidence level $1 - \text{number}$. The value of *number* must be between 0 and 1; the default is 0.05. If DDFM=NONE and you do not specify degrees of freedom with the DF= option, PROC GLIMMIX uses infinite degrees of freedom, essentially computing a z interval.

BYCATEGORY**BYCAT**

requests that in models for nominal data (generalized logit models) estimates be reported separately for each category. In contrast to the BYCATEGORY option in the CONTRAST statement, an ESTIMATE statement in a generalized logit model does not distribute coefficients by response category, because ESTIMATE statements always correspond to single rows of the **L** matrix.

For example, assume that the response variable Style is multinomial with three (unordered) categories. The following GLIMMIX statements fit a generalized logit model relating the preferred style of instruction to school and educational program effects:

```
proc glimmix data=school;
  class School Program;
  model Style(order=data) = School Program / s ddfm=none
                                dist=multinomial link=glogit;

  freq Count;
  estimate 'School 1 vs. 2' school 1 -1 / bycat;
  estimate 'School 1 vs. 2' school 1 -1;
run;
```

The first ESTIMATE statement compares school effects separately for each nonredundant category. The second ESTIMATE statement compares the school effects for the first non-reference category.

The BYCATEGORY option has no effect unless your model is a generalized (mixed) logit model.

CL

requests that *t*-type confidence limits be constructed. If **DDFM=NONE** and you do not specify degrees of freedom with the **DF=** option, PROC GLIMMIX uses infinite degrees of freedom, essentially computing a *z* interval. The confidence level is 0.95 by default. These intervals are adjusted for multiplicity when you specify the **ADJUST=** option.

DF=number

specifies the degrees of freedom for the *t* test and confidence limits. The default is the denominator degrees of freedom taken from the “Type III Tests of Fixed Effects” table and corresponds to the final effect you list in the ESTIMATE statement.

DIVISOR=value-list

specifies a list of values by which to divide the coefficients so that fractional coefficients can be entered as integer numerators. If you do not specify *value-list*, a default value of 1.0 is assumed. Missing values in the *value-list* are converted to 1.0.

If the number of elements in *value-list* exceeds the number of rows of the estimate, the extra values are ignored. If the number of elements in *value-list* is less than the number of rows of the estimate, the last value in *value-list* is copied forward.

If you specify a row-specific divisor as part of the specification of the estimate row, this value multiplies the corresponding divisor implied by the *value-list*. For example, the following statement divides the coefficients in the first row by 8, and the coefficients in the third and fourth row by 3:

```
estimate 'One vs. two'   A 2 -2 (divisor=2),
         'One vs. three' A 1  0 -1      ,
         'One vs. four'  A 3  0  0 -3    ,
         'One vs. five'  A 1  0  0  0 -1 / divisor=4,.,3;
```

Coefficients in the second row are not altered.

E

requests that the **L** matrix coefficients be displayed.

EXP

requests exponentiation of the estimate. When you model data with the logit, cumulative logit, or generalized logit link functions, and the estimate represents a log odds ratio or log cumulative odds ratio, the EXP option produces an odds ratio. See “Odds and Odds Ratio Estimation” on page 3090 for important details about the computation and interpretation of odds and odds ratio results with the GLIMMIX procedure. If you specify the **CL** or **ALPHA=** option, the (adjusted) confidence bounds are also exponentiated.

GROUP coeffs

sets up random-effect contrasts between different groups when a **GROUP=** variable appears in the **RANDOM** statement. By default, ESTIMATE statement coefficients on random effects are distributed equally across groups. If you enter a multirow estimate, you can also enter multiple rows for the GROUP coefficients. If the number of GROUP coefficients is less than the number of contrasts in the ESTIMATE statement, the GLIMMIX procedure cycles through the GROUP coefficients. For example, the following two statements are equivalent:

```

estimate 'Trt 1 vs 2 @ x=0.4' trt 1 -1 0 | x 0.4,
         'Trt 1 vs 3 @ x=0.4' trt 1 0 -1 | x 0.4,
         'Trt 1 vs 2 @ x=0.5' trt 1 -1 0 | x 0.5,
         'Trt 1 vs 3 @ x=0.5' trt 1 0 -1 | x 0.5 /
         group 1 -1, 1 0 -1, 1 -1, 1 0 -1;

estimate 'Trt 1 vs 2 @ x=0.4' trt 1 -1 0 | x 0.4,
         'Trt 1 vs 3 @ x=0.4' trt 1 0 -1 | x 0.4,
         'Trt 1 vs 2 @ x=0.5' trt 1 -1 0 | x 0.5,
         'Trt 1 vs 3 @ x=0.5' trt 1 0 -1 | x 0.5 /
         group 1 -1, 1 0 -1;

```

ILINK

requests that the estimate and its standard error are also reported on the scale of the mean (the inverse linked scale). PROC GLIMMIX computes the value on the mean scale by applying the inverse link to the estimate. The interpretation of this quantity depends on the *fixed-effect values* and *random-effect values* specified in your ESTIMATE statement and on the link function. In a model for binary data with logit link, for example, the following statements compute

$$\frac{1}{1 + \exp\{-(\alpha_1 - \alpha_2)\}}$$

where α_1 and α_2 are the fixed-effects solutions associated with the first two levels of the classification effect A:

```

proc glimmix;
  class A;
  model y = A / dist=binary link=logit;
  estimate 'A one vs. two' A 1 -1 / ilink;
run;

```

This quantity is not the difference of the probabilities associated with the two levels,

$$\pi_1 - \pi_2 = \frac{1}{1 + \exp\{-\beta_0 - \alpha_1\}} - \frac{1}{1 + \exp\{-\beta_0 - \alpha_2\}}$$

The standard error of the inversely linked estimate is based on the delta method. If you also specify the **CL** option, the GLIMMIX procedure computes confidence limits for the estimate on the mean scale. In multinomial models for nominal data, the limits are obtained by the delta method. In other models they are obtained from the inverse link transformation of the confidence limits for the estimate. The **ILINK** option is specific to an ESTIMATE statement.

LOWER**LOWERTAILED**

requests that the *p*-value for the *t* test be based only on values less than the test statistic. A two-tailed test is the default. A lower-tailed confidence limit is also produced if you specify the **CL** or **ALPHA=** option.

Note that for **ADJUST=SCHEFFE** the one-sided adjusted confidence intervals and one-sided adjusted *p*-values are the same as the corresponding two-sided statistics, because this adjustment is based on only the right tail of the *F* distribution.

SINGULAR=number

tunes the estimability checking as documented for the **CONTRAST** statement.

STEPDOWN< (*step-down-options*) >

requests that multiplicity adjustments for the p -values of estimates be further adjusted in a step-down fashion. Step-down methods increase the power of multiple testing procedures by taking advantage of the fact that a p -value will never be declared significant unless all smaller p -values are also declared significant. Note that the **STEPDOWN** adjustment combined with **ADJUST=BON** corresponds to the methods of Holm (1979) and “Method 2” of Shaffer (1986); this is the default. Using step-down-adjusted p -values combined with **ADJUST=SIMULATE** corresponds to the method of Westfall (1997).

If the degrees-of-freedom method is **DDFM=KENWARDROGER** or **DDFM=SATTERTHWAITE**, then step-down-adjusted p -values are produced only if the **ADJDFE=ROW** option is in effect.

Also, the **STEPDOWN** option affects only p -values, not confidence limits. For **ADJUST=SIMULATE**, the generalized least squares hybrid approach of Westfall (1997) is employed to increase Monte Carlo accuracy.

You can specify the following *step-down-options* in parentheses after the **STEPDOWN** option.

MAXTIME=n

specifies the time (in seconds) to spend computing the maximal logically consistent sequential subsets of equality hypotheses for **TYPE=LOGICAL**. The default is **MAXTIME=60**. If the **MAXTIME** value is exceeded, the adjusted tests are not computed. When this occurs, you can try increasing the **MAXTIME** value. However, note that there are common multiple comparisons problems for which this computation requires a huge amount of time—for example, all pairwise comparisons between more than 10 groups. In such cases, try to use **TYPE=FREE** (the default) or **TYPE=LOGICAL(n)** for small n .

ORDER=PVALUE**ORDER=ROWS**

specifies the order in which the step-down tests are performed. **ORDER=PVALUE** is the default, with estimates being declared significant only if all estimates with smaller (unadjusted) p -values are significant. If you specify **ORDER=ROWS**, then significances are evaluated in the order in which they are specified in the syntax.

REPORT

specifies that a report on the step-down adjustment be displayed, including a listing of the sequential subsets (Westfall 1997) and, for **ADJUST=SIMULATE**, the step-down simulation results.

TYPE=LOGICAL< (n) >**TYPE=FREE**

If you specify **TYPE=LOGICAL**, the step-down adjustments are computed by using maximal logically consistent sequential subsets of equality hypotheses (Shaffer 1986; Westfall 1997). Alternatively, for **TYPE=FREE**, sequential subsets are computed ignoring logical constraints. The **TYPE=FREE** results are more conservative than those for **TYPE=LOGICAL**, but they can be much more efficient to produce for many estimates. For example, it is not feasible to take logical constraints between all pairwise comparisons of more than about 10 groups. For this reason, **TYPE=FREE** is the default.

However, you can reduce the computational complexity of taking logical constraints into account by limiting the depth of the search tree used to compute them, specifying the optional depth parameter as a number n in parentheses after `TYPE=LOGICAL`. As with `TYPE=FREE`, results for `TYPE=LOGICAL(n)` are conservative relative to the true `TYPE=LOGICAL` results, but even for `TYPE=LOGICAL(0)` they can be appreciably less conservative than `TYPE=FREE` and they are computationally feasible for much larger numbers of estimates. If you do not specify n or if $n = -1$, the full search tree is used.

SUBJECT *coeffs*

sets up random-effect contrasts between different subjects when a `SUBJECT=` variable appears in the `RANDOM` statement. By default, `ESTIMATE` statement coefficients on random effects are distributed equally across subjects. Listing subject coefficients for an `ESTIMATE` statement with multiple rows follows the same rules as for `GROUP` coefficients.

UPPER

UPPERTAILED

requests that the p -value for the t test be based only on values greater than the test statistic. A two-tailed test is the default. An upper-tailed confidence limit is also produced if you specify the `CL` or `ALPHA=` option.

Note that for `ADJUST=SCHEFFE` the one-sided adjusted confidence intervals and one-sided adjusted p -values are the same as the corresponding two-sided statistics, because this adjustment is based on only the right tail of the F distribution.

FREQ Statement

FREQ *variable* ;

The *variable* in the `FREQ` statement identifies a numeric variable in the data set or one computed through `PROC GLIMMIX` programming statements that contains the frequency of occurrence for each observation. `PROC GLIMMIX` treats each observation as if it appears f times, where f is the value of the `FREQ` variable for the observation. If it is not an integer, the frequency value is truncated to an integer. If the frequency value is less than 1 or missing, the observation is not used in the analysis. When the `FREQ` statement is not specified, each observation is assigned a frequency of 1.

The analysis produced by using a `FREQ` statement reflects the expanded number of observations. For an example of a `FREQ` statement in a model with random effects, see [Example 41.11](#) in this chapter.

ID Statement

ID *variables* ;

The `ID` statement specifies which quantities to include in the `OUT=` data set from the `OUTPUT` statement in addition to any statistics requested in the `OUTPUT` statement. If no `ID` statement is given, the `GLIMMIX` procedure includes all variables from the input data set in the `OUT=` data set. Otherwise, only the variables listed in the `ID` statement are included. Automatic variables such as `_LINF_`, `_MU_`, `_VARIANCE_`, etc. are not transferred to the `OUT=` data set unless they are listed in the `ID` statement.

The ID statement can be used to transfer computed quantities that depend on the model to an output data set. In the following example, two sets of Hessian weights are computed in a gamma regression with a noncanonical link. The covariance matrix for the fixed effects can be constructed as the inverse of $\mathbf{X}'\mathbf{W}\mathbf{X}$. \mathbf{W} is a diagonal matrix of the w_{ei} or w_{oi} , depending on whether the expected or observed Hessian matrix is desired, respectively.

```
proc glimmix;
  class group age;
  model cost = group age / s error=gamma link=pow(0.5);
  output out=gmxout pred=pred;
  id _variance_ wei woi;
  vpmu = 2*_mu_;
  if (_mu_ > 1.0e-8) then do;
    gpmu = 0.5 * (_mu_**(-0.5));
    gppmu = -0.25 * (_mu_**(-1.5));
    wei = 1/(_phi_*_variance_*gpmu*gpmu);
    woi = wei + (cost-_mu_) *
          (_variance_*gppmu + vpmu*gpmu) /
          (_variance_*_variance_*gpmu*gpmu*gpmu*_phi_);
  end;
run;
```

The variables `_VARIANCE_` and `_MU_` and other symbols are predefined by PROC GLIMMIX and can be used in programming statements. For rules and restrictions, see the section “Programming Statements” on page 3042.

LSMEANS Statement

LSMEANS *fixed-effects* </ options > ;

The LSMEANS statement computes least squares means (LS-means) of fixed effects. As in the GLM and the MIXED procedures, LS-means are *predicted population margins*—that is, they estimate the marginal means over a balanced population. In a sense, LS-means are to unbalanced designs as class and subclass arithmetic means are to balanced designs. The \mathbf{L} matrix constructed to compute them is the same as the \mathbf{L} matrix formed in PROC GLM; however, the standard errors are adjusted for the covariance parameters in the model. Least squares means computations are not supported for multinomial models.

Each LS-mean is computed as $\mathbf{L}\hat{\boldsymbol{\beta}}$, where \mathbf{L} is the coefficient matrix associated with the least squares mean and $\hat{\boldsymbol{\beta}}$ is the estimate of the fixed-effects parameter vector. The approximate standard error for the LS-mean is computed as the square root of $\mathbf{L}\widehat{\text{Var}}[\hat{\boldsymbol{\beta}}]\mathbf{L}'$. The approximate variance matrix of the fixed-effects estimates depends on the estimation method.

LS-means are constructed on the linked scale—that is, the scale on which the model effects are additive. For example, in a binomial model with logit link, the least squares means are predicted population margins of the logits.

LS-means can be computed for any effect in the MODEL statement that involves only CLASS variables. You can specify multiple effects in one LSMEANS statement or in multiple LSMEANS statements, and all LSMEANS statements must appear after the MODEL statement. As in the ESTIMATE statement, the \mathbf{L} matrix is tested for estimability, and if this test fails, PROC GLIMMIX displays “Non-est” for the LS-means entries.

Assuming the LS-mean is estimable, PROC GLIMMIX constructs an approximate t test to test the null hypothesis that the associated population quantity equals zero. By default, the denominator degrees of freedom for this test are the same as those displayed for the effect in the “Type III Tests of Fixed Effects” table. If the `DDFM=SATTERTHWAITE` or `DDFM=KENWARDROGER` option is specified in the `MODEL` statement, PROC GLIMMIX determines degrees of freedom separately for each test, unless the `DDF=` option overrides it for a particular effect. See the `DDFM=` option for more information. Table 41.8 summarizes options available in the LSMEANS statement. All LSMEANS options are subsequently discussed in alphabetical order.

Table 41.8 LSMEANS Statement Options

Option	Description
Construction and Computation of LS-Means	
<code>AT</code>	Modifies covariate value in computing LS-means
<code>BYLEVEL</code>	Computes separate margins
<code>DIFF</code>	Requests differences of LS-means
<code>OM</code>	Specifies weighting scheme for LS-mean computation as determined by the input data set
<code>SINGULAR=</code>	Tunes estimability checking
<code>SLICE=</code>	Partitions F tests (simple effects)
<code>SLICEDIFF=</code>	Requests simple effects differences
<code>SLICEDIFFTYPE</code>	Determines the type of simple difference
Degrees of Freedom and P-values	
<code>ADJDFE=</code>	Determines whether to compute row-wise denominator degrees of freedom with <code>DDFM=SATTERTHWAITE</code> or <code>DDFM=KENWARDROGER</code>
<code>ADJUST=</code>	Determines the method for multiple comparison adjustment of LS-mean differences
<code>ALPHA=α</code>	Determines the confidence level ($1 - \alpha$)
<code>DF=</code>	Assigns specific value to degrees of freedom for tests and confidence limits
<code>STEPDOWN</code>	Adjusts multiple comparison p -values further in a step-down fashion
Statistical Output	
<code>CL</code>	Constructs confidence limits for means and or mean differences
<code>CORR</code>	Displays correlation matrix of LS-means
<code>COV</code>	Displays covariance matrix of LS-means
<code>E</code>	Prints the L matrix
<code>ILINK</code>	Applies the inverse link transform to the LS-Means (not differences) and produces the standard errors on the inverse linked scale
<code>LINES</code>	Produces “Lines” display for pairwise LS-mean differences
<code>ODDS</code>	Reports odds of levels of fixed effects if permissible by the link function
<code>ODDSRATIO</code>	Reports (simple) differences of least squares means in terms of odds ratios if permissible by the link function
<code>PLOTS=</code>	Requests ODS statistical graphics of means and mean comparisons

You can specify the following options in the LSMEANS statement after a slash (/).

ADJDFE=ROW

ADJDFE=SOURCE

specifies how denominator degrees of freedom are determined when p -values and confidence limits are adjusted for multiple comparisons with the **ADJUST=** option. When you do not specify the **ADJDFE=** option, or when you specify **ADJDFE=SOURCE**, the denominator degrees of freedom for multiplicity-adjusted results are the denominator degrees of freedom for the LS-mean effect in the “Type III Tests of Fixed Effects” table. When you specify **ADJDFE=ROW**, the denominator degrees of freedom for multiplicity-adjusted results correspond to the degrees of freedom displayed in the DF column of the “Differences of Least Squares Means” table.

The **ADJDFE=ROW** setting is particularly useful if you want multiplicity adjustments to take into account that denominator degrees of freedom are not constant across LS-mean differences. This can be the case, for example, when the **DDFM=SATTERTHWAITE** or **DDFM=KENWARDROGER** degrees-of-freedom method is in effect.

In one-way models with heterogeneous variance, combining certain **ADJUST=** options with the **ADJDFE=ROW** option corresponds to particular methods of performing multiplicity adjustments in the presence of heteroscedasticity. For example, the following statements fit a heteroscedastic one-way model and perform Dunnett’s T3 method (Dunnett 1980), which is based on the studentized maximum modulus (**ADJUST=SMM**):

```
proc glimmix;
  class A;
  model y = A / ddfm=satterth;
  random _residual_ / group=A;
  lsmeans A / adjust=smm adjdfe=row;
run;
```

If you combine the **ADJDFE=ROW** option with **ADJUST=SIDAK**, the multiplicity adjustment corresponds to the T2 method of Tamhane (1979), while **ADJUST=TUKEY** corresponds to the method of Games-Howell (Games and Howell 1976). Note that **ADJUST=TUKEY** gives the exact results for the case of fractional degrees of freedom in the one-way model, but it does not take into account that the degrees of freedom are subject to variability. A more conservative method, such as **ADJUST=SMM**, might protect the overall error rate better.

Unless the **ADJUST=** option is specified in the LSMEANS statement, the **ADJDFE=** option has no effect.

ADJUST=BON

ADJUST=DUNNETT

ADJUST=NELSON

ADJUST=SCHEFFE

ADJUST=SIDAK

ADJUST=SIMULATE< (*simoptions*) >

ADJUST=SMM | **GT2**

ADJUST=TUKEY

requests a multiple comparison adjustment for the p -values and confidence limits for the differences of LS-means. The adjusted quantities are produced in addition to the unadjusted quantities. By default, PROC GLIMMIX performs all pairwise differences. If you specify **ADJUST=DUNNETT**, the

procedure analyzes all differences with a control level. If you specify ADJUST=NELSON, ANOM differences are taken. The ADJUST= option implies the DIFF option, unless the SLICEDIFF= option is specified.

The BON (Bonferroni) and SIDAK adjustments involve correction factors described in Chapter 42, “The GLM Procedure,” and Chapter 61, “The MULTTEST Procedure;” also see Westfall and Young (1993) and Westfall et al. (1999). When you specify ADJUST=TUKEY and your data are unbalanced, PROC GLIMMIX uses the approximation described in Kramer (1956) and identifies the adjustment as “Tukey-Kramer” in the results. Similarly, when you specify ADJUST=DUNNETT or ADJUST=NELSON and the LS-means are correlated, the GLIMMIX procedure uses the factor-analytic covariance approximation described in Hsu (1992) and identifies the adjustment in the results as “Dunnett-Hsu” or “Nelson-Hsu,” respectively. The approximation derives an approximate “effective sample sizes” for which exact critical values are computed. Note that computing the exact adjusted p -values and critical values for unbalanced designs can be computationally intensive, in particular for ADJUST=NELSON. A simulation-based approach, as specified by the ADJUST=SIM option, while nondeterministic, can provide inferences that are sufficiently accurate in much less time. The preceding references also describe the SCHEFFE and SMM adjustments.

Nelson’s adjustment applies only to the analysis of means (Ott 1967; Nelson 1982, 1991, 1993), where LS-means are compared against an average LS-mean. It does not apply to all pairwise differences of least squares means, or to slice differences that you specify with the SLICEDIFF= option. See the DIFF=ANOM option for more details regarding the analysis of means with the GLIMMIX procedure.

The SIMULATE adjustment computes adjusted p -values and confidence limits from the simulated distribution of the maximum or maximum absolute value of a multivariate t random vector. All covariance parameters, except the residual scale parameter, are fixed at their estimated values throughout the simulation, potentially resulting in some underdispersion. The simulation estimates q , the true $(1 - \alpha)$ quantile, where $1 - \alpha$ is the confidence coefficient. The default α is 0.05, and you can change this value with the ALPHA= option in the LSMEANS statement.

The number of samples is set so that the tail area for the simulated q is within γ of $1 - \alpha$ with $100(1 - \epsilon)\%$ confidence. In equation form,

$$\Pr(|F(\hat{q}) - (1 - \alpha)| \leq \gamma) = 1 - \epsilon$$

where \hat{q} is the simulated q and F is the true distribution function of the maximum; see Edwards and Berry (1987) for details. By default, $\gamma = 0.005$ and $\epsilon = 0.01$, placing the tail area of \hat{q} within 0.005 of 0.95 with 99% confidence. The ACC= and EPS= *simoptions* reset γ and ϵ , respectively, the NSAMP= *simoption* sets the sample size directly, and the SEED= *simoption* specifies an integer used to start the pseudo-random number generator for the simulation. If you do not specify a seed, or if you specify a value less than or equal to zero, the seed is generated from reading the time of day from the computer clock. For additional descriptions of these and other simulation options, see the section “LSMEANS Statement” on page 3293 in Chapter 42, “The GLM Procedure.”

If the STEPDOWN option is in effect, the p -values are further adjusted in a step-down fashion. For certain options and data, this adjustment is exact under an iid $N(0, \sigma^2)$ model for the dependent variable, in particular for the following:

- for ADJUST=DUNNETT when the means are uncorrelated
- for ADJUST=TUKEY with STEPDOWN(TYPE=LOGICAL) when the means are balanced and uncorrelated.

The first case is a consequence of the nature of the successive step-down hypotheses for comparisons with a control; the second employs an extension of the maximum studentized range distribution appropriate for partition hypotheses (Royen 1989). Finally, for `STEPDOWN(TYPE=FREE)`, `ADJUST=TUKEY` employs the Royen (1989) extension in such a way that the resulting p -values are conservative.

ALPHA=number

requests that a t -type confidence interval be constructed for each of the LS-means with confidence level $1 - \text{number}$. The value of *number* must be between 0 and 1; the default is 0.05.

AT variable=value

AT (variable-list)=(value-list)

AT MEANS

enables you to modify the values of the covariates used in computing LS-means. By default, all covariate effects are set equal to their mean values for computation of standard LS-means. The AT option enables you to assign arbitrary values to the covariates. Additional columns in the output table indicate the values of the covariates.

If there is an effect containing two or more covariates, the AT option sets the effect equal to the product of the individual means rather than the mean of the product (as with standard LS-means calculations). The AT MEANS option sets covariates equal to their mean values (as with standard LS-means) and incorporates this adjustment to crossproducts of covariates.

As an example, consider the following invocation of PROC GLIMMIX:

```
proc glimmix;
  class A;
  model Y = A x1 x2 x1*x2;
  lsmeans A;
  lsmeans A / at means;
  lsmeans A / at x1=1.2;
  lsmeans A / at (x1 x2)=(1.2 0.3);
run;
```

For the first two LSMEANS statements, the LS-means coefficient for x_1 is \bar{x}_1 (the mean of x_1) and for x_2 is \bar{x}_2 (the mean of x_2). However, for the first LSMEANS statement, the coefficient for x_1*x_2 is $\bar{x}_1\bar{x}_2$, but for the second LSMEANS statement, the coefficient is $\bar{x}_1 \times \bar{x}_2$. The third LSMEANS statement sets the coefficient for x_1 equal to 1.2 and leaves it at \bar{x}_2 for x_2 , and the final LSMEANS statement sets these values to 1.2 and 0.3, respectively.

Even if you specify a **WEIGHT** variable, the unweighted covariate means are used for the covariate coefficients if there is no AT specification. If you specify the AT option, **WEIGHT** or **FREQ** variables are taken into account as follows. The weighted covariate means are then used for the covariate coefficients for which no explicit AT values are given, or if you specify AT MEANS. Observations that do not contribute to the analysis because of a missing dependent variable are included in computing the covariate means. You should use the **E** option in conjunction with the AT option to check that the modified LS-means coefficients are the ones you want.

The AT option is disabled if you specify the **BYLEVEL** option.

BYLEVEL

requests that separate margins be computed for each level of the LSMEANS effect.

The standard LS-means have equal coefficients across classification effects. The BYLEVEL option changes these coefficients to be proportional to the observed margins. This adjustment is reasonable when you want your inferences to apply to a population that is not necessarily balanced but has the margins observed in the input data set. In this case, the resulting LS-means are actually equal to raw means for fixed-effects models and certain balanced random-effects models, but their estimated standard errors account for the covariance structure that you have specified. If a **WEIGHT** statement is specified, PROC GLIMMIX uses weighted margins to construct the LS-means coefficients.

If the **AT** option is specified, the BYLEVEL option disables it.

CL

requests that *t*-type confidence limits be constructed for each of the LS-means. If **DDFM=NONE**, then PROC GLIMMIX uses infinite degrees of freedom for this test, essentially computing a *z* interval. The confidence level is 0.95 by default; this can be changed with the **ALPHA=** option. If you specify an **ADJUST=** option, then the confidence limits are adjusted for multiplicity, but if you also specify **STEPDOWN**, then only *p*-values are step-down adjusted, not the confidence limits.

CORR

displays the estimated correlation matrix of the least squares means as part of the “Least Squares Means” table.

COV

displays the estimated covariance matrix of the least squares means as part of the “Least Squares Means” table.

DF=number

specifies the degrees of freedom for the *t* test and confidence limits. The default is the denominator degrees of freedom taken from the “Type III Tests of Fixed Effects” table corresponding to the LS-means effect.

DIFF<=difftype>**PDIFF<=difftype>**

requests that differences of the LS-means be displayed. The optional *difftype* specifies which differences to produce, with possible values ALL, ANOM, CONTROL, CONTROLL, and CONTROLU. The ALL value requests all pairwise differences, and it is the default. The CONTROL *difftype* requests differences with a control, which, by default, is the first level of each of the specified LSMEANS effects.

The ANOM value requests differences between each LS-mean and the average LS-mean, as in the *analysis of means* (Ott 1967). The average is computed as a weighted mean of the LS-means, the weights being inversely proportional to the diagonal entries of the

$$\mathbf{L}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{L}'$$

matrix. If LS-means are nonestimable, this design-based weighted mean is replaced with an equally weighted mean. Note that the ANOM procedure in SAS/QC software implements both tables and graphics for the analysis of means with a variety of response types. For one-way designs and normal data with identity link, the DIFF=ANOM computations are equivalent to the results of PROC ANOM.

If the LS-means being compared are uncorrelated, exact adjusted p -values and critical values for confidence limits can be computed in the analysis of means; see Nelson (1982, 1991, 1993); Guirguis and Tobias (2004) as well as the documentation for the `ADJUST=NELSON` option.

To specify which levels of the effects are the controls, list the quoted formatted values in parentheses after the `CONTROL` keyword. For example, if the effects A, B, and C are classification variables, each having two levels, 1 and 2, the following LSMEANS statement specifies the (1,2) level of A*B and the (2,1) level of B*C as controls:

```
lsmeans A*B B*C / diff=control('1' '2' '2' '1');
```

For multiple effects, the results depend upon the order of the list, and so you should check the output to make sure that the controls are correct.

Two-tailed tests and confidence limits are associated with the `CONTROL difftype`. For one-tailed results, use either the `CONTROLL` or `CONTROLU difftype`. The `CONTROLL difftype` tests whether the noncontrol levels are significantly smaller than the control; the upper confidence limits for the control minus the noncontrol levels are considered to be infinity and are displayed as missing. Conversely, the `CONTROLU difftype` tests whether the noncontrol levels are significantly larger than the control; the upper confidence limits for the noncontrol levels minus the control are considered to be infinity and are displayed as missing.

If you want to perform multiple comparison adjustments on the differences of LS-means, you must specify the `ADJUST=` option.

The differences of the LS-means are displayed in a table titled “Differences of Least Squares Means.”

E

requests that the **L** matrix coefficients for the LSMEANS effects be displayed.

ILINK

requests that estimates and their standard errors in the “Least Squares Means” table also be reported on the scale of the mean (the inverse linked scale). The `ILINK` option is specific to an LSMEANS statement. If you also specify the `CL` option, the GLIMMIX procedure computes confidence intervals for the predicted means by applying the inverse link transform to the confidence limits on the linked (linear) scale. Standard errors on the inverse linked scale are computed by the delta method.

The GLIMMIX procedure applies the inverse link transform to the LS-mean reported in the Estimate column. In a logistic model, for example, this implies that the value reported as the inversely linked estimate corresponds to a predicted probability that is based on an average estimable function (the estimable function that produces the LS-mean on the linear scale). To compute average predicted probabilities, you can average the results from applying the `ILINK` option in the `ESTIMATE` statement for suitably chosen estimable functions.

LINES

presents results of comparisons between all pairs of least squares means by listing the means in descending order and indicating nonsignificant subsets by line segments beside the corresponding LS-means. When all differences have the same variance, these comparison lines are guaranteed to accurately reflect the inferences based on the corresponding tests, made by comparing the respective p -values to the value of the `ALPHA=` option (0.05 by default). However, equal variances might not be the case for differences between LS-means. If the variances are not all the same, then the comparison

lines might be conservative, in the sense that if you base your inferences on the lines alone, you will detect fewer significant differences than the tests indicate. If there are any such differences, PROC GLIMMIX lists the pairs of means that are inferred to be significantly different by the tests but not by the comparison lines. Note, however, that in many cases, even though the variances are unequal, they are similar enough that the comparison lines accurately reflect the test inferences.

ODDS

requests that in models with logit, cumulative logit, and generalized logit link function the odds of the levels of the fixed effects are reported. If you specify the **CL** or **ALPHA=** option, confidence intervals for the odds are also computed. See the section “Odds and Odds Ratio Estimation” on page 3090 for further details about computation and interpretation of odds and odds ratios with the GLIMMIX procedure.

ODDSRATIO

OR

requests that LS-mean differences (**DIFF**, **ADJUST=** options) and simple effect comparisons (**SLICEDIFF** option) are also reported in terms of odds ratios. The **ODDSRATIO** option is ignored unless you use either the logit, cumulative logit, or generalized logit link function. If you specify the **CL** or **ALPHA=** option, confidence intervals for the odds ratios are also computed. These intervals are adjusted for multiplicity when you specify the **ADJUST=** option. See the section “Odds and Odds Ratio Estimation” on page 3090 for further details about computation and interpretation of odds and odds ratios with the GLIMMIX procedure.

OBSMARGINS

OM

specifies a potentially different weighting scheme for the computation of LS-means coefficients. The standard LS-means have equal coefficients across classification effects; however, the **OM** option changes these coefficients to be proportional to those found in the input data set. This adjustment is reasonable when you want your inferences to apply to a population that is not necessarily balanced but has the margins observed in your data.

In computing the observed margins, PROC GLIMMIX uses all observations for which there are no missing or invalid independent variables, including those for which there are missing dependent variables. Also, if you use a **WEIGHT** statement, PROC GLIMMIX computes weighted margins to construct the LS-means coefficients. If your data are balanced, the LS-means are unchanged by the **OM** option.

The **BYLEVEL** option modifies the observed-margins LS-means. Instead of computing the margins across all of the input data set, PROC GLIMMIX computes separate margins for each level of the LSMEANS effect in question. In this case the resulting LS-means are actually equal to raw means for fixed-effects models and certain balanced random-effects models, but their estimated standard errors account for the covariance structure that you have specified.

You can use the **E** option in conjunction with either the **OM** or **BYLEVEL** option to check that the modified LS-means coefficients are the ones you want. It is possible that the modified LS-means are not estimable when the standard ones are estimable, or vice versa.

PDIFF

is the same as the **DIFF** option. See the description of the **DIFF** option on page 2981.

PLOT | PLOTS<=*plot-request*<(*options*)>>**PLOT | PLOTS**<=*(plot-request*<(*options*)> <...*plot-request*<(*options*)> >)>

creates least squares means related graphs when ODS Graphics has been enabled and the plot request does not conflict with other options in the LSMEANS statement. For general information about ODS Graphics, see Chapter 21, “Statistical Graphics Using ODS.” For examples of the basic statistical graphics for least squares means and aspects of their computation and interpretation, see the section “Graphics for LS-Mean Comparisons” on page 3122 in this chapter.

The *options* for a specific plot request (and their suboptions) of the LSMEANS statement include those for the **PLOTS=** option in the **PROC GLIMMIX** statement. You can specify classification effects in the MEANPLOT request of the LSMEANS statement to control the display of interaction means with the **PLOTBY=** and **SLICEBY=** suboptions; these are not available in the **PLOTS=** option in the **PROC GLIMMIX** statement. Options specified in the LSMEANS statement override those in the **PLOTS=** option in the **PROC GLIMMIX** statement.

The available options and suboptions are as follows.

ALL

requests that the default plots corresponding to this LSMEANS statement be produced. The default plot depends on the options in the statement.

ANOMPLOT**ANOM**

requests an analysis of means display in which least squares means are compared to an average least squares mean. Least squares mean ANOM plots are produced only for those model effects listed in LSMEANS statements that have options that do not contradict with the display. For example, the following statements produce analysis of mean plots for effects A and C:

```
lsmeans A / diff=anom plot=anom;
lsmeans B / diff      plot=anom;
lsmeans C /           plot=anom;
```

The **DIFF** option in the second LSMEANS statement implies all pairwise differences.

CONTROLPLOT**CONTROL**

requests a display in which least squares means are visually compared against a reference level. These plots are produced only for statements with options that are compatible with control differences. For example, the following statements produce control plots for effects A and C:

```
lsmeans A / diff=control('1') plot=control;
lsmeans B / diff              plot=control;
lsmeans C                    plot=control;
```

The **DIFF** option in the second LSMEANS statement implies all pairwise differences.

DIFFPLOT<(diffplot-options)>

DIFFOGRAM<(diffplot-options)>

DIFF<(diffplot-options)>

requests a display of all pairwise least squares mean differences and their significance. The display is also known as a “mean-mean scatter plot” when it is based on arithmetic means (Hsu 1996; Hsu and Peruggia 1994). For each comparison a line segment, centered at the LS-means in the pair, is drawn. The length of the segment corresponds to the projected width of a confidence interval for the least squares mean difference. Segments that fail to cross the 45-degree reference line correspond to significant least squares mean differences.

LS-mean difference plots are produced only for statements with options that are compatible with the display. For example, the following statements request differences against a control level for the A effect, all pairwise differences for the B effect, and the least squares means for the C effect:

```
lsmeans A / diff=control('1') plot=diff;
lsmeans B / diff                plot=diff;
lsmeans C                      plot=diff;
```

The **DIFF=** type in the first statement is incompatible with a display of all pairwise differences.

You can specify the following *diffplot-options*. The **ABS** and **NOABS** options determine the positioning of the line segments in the plot. When the **ABS** option is in effect, and this is the default, all line segments are shown on the same side of the reference line. The **NOABS** option separates comparisons according to the sign of the difference. The **CENTER** option marks the center point for each comparison. This point corresponds to the intersection of two least squares means. The **NOLINES** option suppresses the display of the line segments that represent the confidence bounds for the differences of the least squares means. The **NOLINES** option implies the **CENTER** option. The default is to draw line segments in the upper portion of the plot area without marking the center point.

MEANPLOT<(meanplot-options)>

requests displays of the least squares means.

The following *meanplot-options* control the display of the least squares means.

ASCENDING

displays the least squares means in ascending order. This option has no effect if means are sliced or displayed in separate plots.

CL

displays upper and lower confidence limits for the least squares means. By default, 95% limits are drawn. You can change the confidence level with the **ALPHA=** option. Confidence limits are drawn by default if the **CL** option is specified in the LSMEANS statement.

CLBAND

displays confidence limits as bands. This option implies the **JOIN** option.

DESCENDING

displays the least squares means in descending order. This option has no effect if means are sliced or displayed in separate plots.

ILINK

requests that means (and confidence limits) are displayed on the inverse linked scale.

JOIN**CONNECT**

connects the least squares means with lines. This option is implied by the CLBAND option. If the effect contains nested variables, and a SLICEBY= effect contains classification variables that appear as crossed effects, this option is ignored.

SLICEBY=*fixed-effect*

specifies an effect by which to group the means in a single plot. For example, the following statement requests a plot in which the levels of A are placed on the horizontal axis and the means that belong to the same level of B are joined by lines:

```
lsmeans A*B / plot=meanplot(sliceby=b join);
```

Unless the LS-mean effect contains at least two classification variables, the SLICEBY= option has no effect. The *fixed-effect* does not have to be an effect in your MODEL statement, but it must consist entirely of classification variables.

PLOTBY=*fixed-effect*

specifies an effect by which to break interaction plots into separate displays. For example, the following statement requests for each level of C one plot of the A*B cell means that are associated with that level of C:

```
lsmeans A*B*C / plot=meanplot(sliceby=b plotby=c clband);
```

In each plot, levels of A are displayed on the horizontal axis, and confidence bands are drawn around the means that share the same level of B.

The PLOTBY= option has no effect unless the LS-mean effect contains at least three classification variables. The *fixed-effect* does not have to be an effect in the MODEL statement, but it must consist entirely of classification variables.

NONE

requests that no plots be produced.

When LS-mean calculations are adjusted for multiplicity by using the ADJUST= option, the plots are adjusted accordingly.

SINGULAR=*number*

tunes the estimability checking as documented for the CONTRAST statement.

SLICE=*fixed-effect*

SLICE=(fixed-effects)

specifies effects by which to partition interaction LSMEANS effects. This can produce what are known as tests of simple effects (Winer 1971). For example, suppose that $A*B$ is significant, and you want to test the effect of A for each level of B . The appropriate LSMEANS statement is

```
lsmeans A*B / slice=B;
```

This statement tests for the simple main effects of A for B , which are calculated by extracting the appropriate rows from the coefficient matrix for the $A*B$ LS-means and by using them to form an F test.

The SLICE option produces F tests that test the simultaneous equality of cell means at a fixed level of the slice effect (Schabenberger, Gregoire, and Kong 2000). You can request differences of the least squares means while holding one or more factors at a fixed level with the SLICEDIFF= option.

The SLICE option produces a table titled “Tests of Effect Slices.”

SLICEDIFF=fixed-effect**SLICEDIFF=(fixed-effects)****SIMPLEDIFF=fixed-effect****SIMPLEDIFF=(fixed-effects)**

requests that differences of simple effects be constructed and tested against zero. Whereas the SLICE option extracts multiple rows of the coefficient matrix and forms an F test, the SLICEDIFF option tests pairwise differences of these rows. This enables you to perform multiple comparisons among the levels of one factor at a fixed level of the other factor. For example, assume that, in a balanced design, factors A and B have $a = 4$ and $b = 3$ levels, respectively. Consider the following statements:

```
proc glimmix;
  class a b;
  model y = a b a*b;
  lsmeans a*b / slice=a;
  lsmeans a*b / slicediff=a;
run;
```

The first LSMEANS statement produces four F tests, one per level of A . The first of these tests is constructed by extracting the three rows corresponding to the first level of A from the coefficient matrix for the $A*B$ interaction. Call this matrix L_{a1} and its rows $l_{a1}^{(1)}$, $l_{a1}^{(2)}$, and $l_{a1}^{(3)}$. The SLICE tests the two-degrees-of-freedom hypothesis

$$H: \begin{cases} \left(l_{a1}^{(1)} - l_{a1}^{(2)} \right) \boldsymbol{\beta} = 0 \\ \left(l_{a1}^{(1)} - l_{a1}^{(3)} \right) \boldsymbol{\beta} = 0 \end{cases}$$

In a balanced design, where μ_{ij} denotes the mean response if A is at level i and B is at level j , this hypothesis is equivalent to $H: \mu_{11} = \mu_{12} = \mu_{13}$. The SLICEDIFF option considers the three rows of L_{a1} in turn and performs tests of the difference between pairs of rows. How these differences are constructed depends on the SLICEDIFFTYPE= option. By default, all pairwise differences within

the subset of \mathbf{L} are considered; in the example this corresponds to tests of the form

$$H: \left(1_{a1}^{(1)} - 1_{a1}^{(2)}\right) \boldsymbol{\beta} = 0$$

$$H: \left(1_{a1}^{(1)} - 1_{a1}^{(3)}\right) \boldsymbol{\beta} = 0$$

$$H: \left(1_{a1}^{(2)} - 1_{a1}^{(3)}\right) \boldsymbol{\beta} = 0$$

In the example, with $a = 4$ and $b = 3$, the second LSMEANS statement produces four sets of least squares means differences. Within each set, factor A is held fixed at a particular level and each set consists of three comparisons.

When the **ADJUST=** option is specified, the GLIMMIX procedure also adjusts the tests for multiplicity. The adjustment is based on the number of comparisons within each level of the **SLICEDIFF=** effect; see the **SLICEDIFFTYPE=** option. The Nelson adjustment is not available for slice differences.

SLICEDIFFTYPE<=*difftype*>

SIMPLEDIFFTYPE<=*difftype*>

determines the type of simple effect differences produced with the **SLICEDIFF=** option.

The possible values for the *difftype* are ALL, CONTROL, CONTROLL, and CONTROLU. The *difftype* ALL requests all simple effects differences, and it is the default. The *difftype* CONTROL requests the differences with a control, which, by default, is the first level of each of the specified LSMEANS effects.

To specify which levels of the effects are the controls, list the quoted formatted values in parentheses after the keyword CONTROL. For example, if the effects A, B, and C are classification variables, each having three levels (1, 2, and 3), the following LSMEANS statement specifies the (1,3) level of A*B as the control:

```
lsmeans A*B / slicediff=(A B)
                slicedifftype=control('1' '3');
```

This LSMEANS statement first produces simple effects differences holding the levels of A fixed, and then it produces simple effects differences holding the levels of B fixed. In the former case, level '3' of B serves as the control level. In the latter case, level '1' of A serves as the control.

For multiple effects, the results depend upon the order of the list, and so you should check the output to make sure that the controls are correct.

Two-tailed tests and confidence limits are associated with the CONTROL *difftype*. For one-tailed results, use either the CONTROLL or CONTROLU *difftype*. The CONTROLL *difftype* tests whether the noncontrol levels are significantly smaller than the control; the upper confidence limits for the control minus the noncontrol levels are considered to be infinity and are displayed as missing. Conversely, the CONTROLU *difftype* tests whether the noncontrol levels are significantly larger than the control; the upper confidence limits for the noncontrol levels minus the control are considered to be infinity and are displayed as missing.

STEPDOWN< (*step-down options*) >

requests that multiple comparison adjustments for the p -values of LS-mean differences be further adjusted in a step-down fashion. Step-down methods increase the power of multiple comparisons by taking advantage of the fact that a p -value will never be declared significant unless all smaller p -values are also declared significant. Note that the STEPDOWN adjustment combined with **ADJUST=BON** corresponds to the methods of Holm (1979) and “Method 2” of Shaffer (1986); this is the default. Using step-down-adjusted p -values combined with **ADJUST=SIMULATE** corresponds to the method of Westfall (1997).

If the degrees-of-freedom method is **DDFM=KENWARDROGER** or **DDFM=SATTERTHWAITE**, then step-down-adjusted p -values are produced only if the **ADJDFE=ROW** option is in effect.

Also, STEPDOWN affects only p -values, not confidence limits. For **ADJUST=SIMULATE**, the generalized least squares hybrid approach of Westfall (1997) is employed to increase Monte Carlo accuracy.

You can specify the following *step-down options* in parentheses:

MAXTIME= n

specifies the time (in seconds) to spend computing the maximal logically consistent sequential subsets of equality hypotheses for **TYPE=LOGICAL**. The default is **MAXTIME=60**. If the **MAXTIME** value is exceeded, the adjusted tests are not computed. When this occurs, you can try increasing the **MAXTIME** value. However, note that there are common multiple comparisons problems for which this computation requires a huge amount of time—for example, all pairwise comparisons between more than 10 groups. In such cases, try to use **TYPE=FREE** (the default) or **TYPE=LOGICAL(n)** for small n .

REPORT

specifies that a report on the step-down adjustment should be displayed, including a listing of the sequential subsets (Westfall 1997) and, for **ADJUST=SIMULATE**, the step-down simulation results.

TYPE=LOGICAL< (n) >**TYPE=FREE**

If you specify **TYPE=LOGICAL**, the step-down adjustments are computed by using maximal logically consistent sequential subsets of equality hypotheses (Shaffer 1986; Westfall 1997). Alternatively, for **TYPE=FREE**, sequential subsets are computed ignoring logical constraints. The **TYPE=FREE** results are more conservative than those for **TYPE=LOGICAL**, but they can be much more efficient to produce for many comparisons. For example, it is not feasible to take logical constraints between all pairwise comparisons of more than 10 groups. For this reason, **TYPE=FREE** is the default.

However, you can reduce the computational complexity of taking logical constraints into account by limiting the depth of the search tree used to compute them, specifying the optional depth parameter as a number n in parentheses after **TYPE=LOGICAL**. As with **TYPE=FREE**, results for **TYPE=LOGICAL(n)** are conservative relative to the true **TYPE=LOGICAL** results, but even for **TYPE=LOGICAL(0)** they can be appreciably less conservative than **TYPE=FREE** and they are computationally feasible for much larger numbers of comparisons. If you do not specify n or if $n = -1$, the full search tree is used.

LSMESTIMATE Statement

```
LSMESTIMATE fixed-effect <'label'> values <divisor=n>
             <,<'label'> values <divisor=n>> <,&ldots >
             </options>;
```

The LSMESTIMATE statement provides a mechanism for obtaining custom hypothesis tests among the least squares means. In contrast to the hypotheses tested with the ESTIMATE or CONTRAST statements, the LSMESTIMATE statement enables you to form linear combinations of the least squares means, rather than linear combination of fixed-effects parameter estimates and/or random-effects solutions. Multiple-row sets of coefficients are permitted.

The computation of an LSMESTIMATE involves two coefficient matrices. Suppose that the *fixed-effect* has n_l levels. Then the LS-means are formed as $\mathbf{L}_1 \hat{\boldsymbol{\beta}}$, where \mathbf{L}_1 is a $(n_l \times p)$ coefficient matrix. The $(k \times n_l)$ coefficient matrix \mathbf{K} is formed from the *values* that you supply in the k rows of the LSMESTIMATE statement. The least squares means estimates then represent the $(k \times 1)$ vector

$$\mathbf{KL}_1 \boldsymbol{\beta} = \mathbf{L} \boldsymbol{\beta}$$

The GLIMMIX procedure supports nonpositional syntax for the coefficients (*values*) in the LSMESTIMATE statement. For details see the section “Positional and Nonpositional Syntax for Contrast Coefficients” on page 3097.

PROC GLIMMIX produces a t test for each row of coefficients specified in the LSMESTIMATE statement. You can adjust p -values and confidence intervals for multiplicity with the ADJUST= option. You can obtain an F test of single-row or multirow LSMESTIMATEs with the FTEST option.

Note that in contrast to a multirow estimate in the ESTIMATE statement, you specify only a single fixed effect in the LSMESTIMATE statement. The row labels are optional and follow the effects specification. For example, the following statements fit a split-split-plot design and compare the average of the third and fourth LS-mean of the whole-plot factor A to the first LS-mean of the factor:

```
proc glimmix;
  class a b block;
  model y = a b a*b / s;
  random int a / sub=block;
  lsmestimate A 'a1 vs avg(a3,a4)' 2 0 -1 -1 divisor=2;
run;
```

The order in which coefficients are assigned to the least squares means corresponds to the order in which they are displayed in the “Least Squares Means” table. You can use the ELSM option to see how coefficients are matched to levels of the *fixed-effect*.

The optional *divisor=n* specification enables you to assign a separate divisor to each row of the LSMESTIMATE. You can also assign divisor values through the DIVISOR= option. See the documentation that follows for the interaction between the two ways of specifying divisors.

Many options of the LSMESTIMATE statement affect the computation of least squares means—for example, the AT=, BYLEVEL, and OM options. See the documentation for the LSMEANS statement for details.

Table 41.9 summarizes the options available in the LSMESTIMATE statement.

Table 41.9 LSMESTIMATE Statement Options

Option	Description
Construction and Computation of LS-Means	
AT	Modifies covariate values in computing LS-means
BYLEVEL	Computes separate margins
DIVISOR=	Specifies a list of values to divide the coefficients
OM=	Specifies the weighting scheme for LS-means computation as determined by a data set
SINGULAR=	Tunes estimability checking
Degrees of Freedom and p-values	
ADJDFE=	Determines denominator degrees of freedom when p -values and confidence limits are adjusted for multiple comparisons
ADJUST=	Determines the method for multiple comparison adjustment of LS-means differences
ALPHA= α	Determines the confidence level $(1 - \alpha)$
CHISQ	Requests a chi-square test in addition to the F test
DF=	Assigns a specific value to degrees of freedom for tests and confidence limits
FTEST	Produces an F test
LOWER	Performs one-sided, lower-tailed inference
STEPDOWN	Adjusts multiple comparison p -values further in a step-down fashion
UPPER	Performs one-sided, upper-tailed inference
Statistical Output	
CL	Constructs confidence limits for means and mean differences
CORR	Displays the correlation matrix of LS-means
COV	Displays the covariance matrix of LS-means
E	Prints the L matrix
ELSM	Prints the K matrix
JOINT	Produces a joint F or chi-square test for the LS-means and LS-means differences
Generalized Linear Modeling	
EXP	Exponentiates and displays LS-means estimates
ILINK	Computes and displays estimates and standard errors of LS-means (but not differences) on the inverse linked scale

You can specify the following options in the LSMESTIMATE statement after a slash (/).

ADJDFE=SOURCE**ADJDFE=ROW**

specifies how denominator degrees of freedom are determined when p -values and confidence limits are adjusted for multiple comparisons with the **ADJUST=** option. When you do not specify the **ADJDFE=** option, or when you specify **ADJDFE=SOURCE**, the denominator degrees of freedom for

multiplicity-adjusted results are the denominator degrees of freedom for the LS-mean effect in the “Type III Tests of Fixed Effects” table.

The `ADJDFE=ROW` setting is useful if you want multiplicity adjustments to take into account that denominator degrees of freedom are not constant across estimates. This can be the case, for example, when `DDFM=SATTERTHWAITE` or `DDFM=KENWARDROGER` is specified in the `MODEL` statement.

ADJUST=BON

ADJUST=SCHEFFE

ADJUST=SIDAK

ADJUST=SIMULATE< (*simoptions*) >

ADJUST=T

requests a multiple comparison adjustment for the p -values and confidence limits for the LS-mean estimates. The adjusted quantities are produced in addition to the unadjusted p -values and confidence limits. Adjusted confidence limits are produced if the `CL` or `ALPHA=` option is in effect. For a description of the adjustments, see Chapter 42, “The GLM Procedure,” and Chapter 61, “The MULTTEST Procedure,” as well as the documentation for the `ADJUST=` option in the `LSMEANS` statement.

Note that not all adjustment methods of the `LSMEANS` statement are available for the `LSMESTIMATE` statement. Multiplicity adjustments in the `LSMEANS` statement are designed specifically for differences of least squares means.

If you specify the `STEPDOWN` option, the p -values are further adjusted in a step-down fashion.

ALPHA=number

requests that a t -type confidence interval be constructed for each of the LS-means with confidence level $1 - \textit{number}$. The value of *number* must be between 0 and 1; the default is 0.05.

AT variable=value

AT (variable-list)=(value-list)

AT MEANS

enables you to modify the values of the covariates used in computing LS-means. See the `AT` option in the `LSMEANS` statement for details.

BYLEVEL

requests that PROC GLIMMIX compute separate margins for each level of the `LSMEANS` effect.

The standard LS-means have equal coefficients across classification effects. The `BYLEVEL` option changes these coefficients to be proportional to the observed margins. This adjustment is reasonable when you want your inferences to apply to a population that is not necessarily balanced but has the margins observed in the input data set. In this case, the resulting LS-means are actually equal to raw means for fixed-effects models and certain balanced random-effects models, but their estimated standard errors account for the covariance structure that you have specified. If a `WEIGHT` statement is specified, PROC GLIMMIX uses weighted margins to construct the LS-means coefficients.

If the `AT` option is specified, the `BYLEVEL` option disables it.

CHISQ

requests that chi-square tests be performed in addition to F tests, when you request an F test with the **FTEST** option.

CL

requests that t -type confidence limits be constructed for each of the LS-means. If **DDFM=NONE**, then PROC GLIMMIX uses infinite degrees of freedom for this test, essentially computing a z interval. The confidence level is 0.95 by default; this can be changed with the **ALPHA=** option.

CORR

displays the estimated correlation matrix of the linear combination of the least squares means.

COV

displays the estimated covariance matrix of the linear combination of the least squares means.

DF=number

specifies the degrees of freedom for the t test and confidence limits. The default is the denominator degrees of freedom taken from the “Type III Tests of Fixed Effects” table corresponding to the LS-means effect.

DIVISOR=value-list

specifies a list of values by which to divide the coefficients so that fractional coefficients can be entered as integer numerators. If you do not specify *value-list*, a default value of 1.0 is assumed. Missing values in the *value-list* are converted to 1.0.

If the number of elements in *value-list* exceeds the number of rows of the estimate, the extra values are ignored. If the number of elements in *value-list* is less than the number of rows of the estimate, the last value in *value-list* is carried forward.

If you specify a row-specific divisor as part of the specification of the estimate row, this value multiplies the corresponding value in the *value-list*. For example, the following statement divides the coefficients in the first row by 8, and the coefficients in the third and fourth row by 3:

```
lsmestimate A 'One vs. two' 8 -8 divisor=2,
              'One vs. three' 1 0 -1 ,
              'One vs. four' 3 0 0 -3 ,
              'One vs. five' 3 0 0 0 -3 / divisor=4,.,3;
```

Coefficients in the second row are not altered.

E

requests that the **L** coefficients of the estimable function be displayed. These are the coefficients that apply to the fixed-effect parameter estimates. The **E** option displays the coefficients that you would need to enter in an equivalent **ESTIMATE** statement.

ELSM

requests that the **K** matrix coefficients be displayed. These are the coefficients that apply to the LS-means. This option is useful to ensure that you assigned the coefficients correctly to the LS-means.

EXP

requests exponentiation of the least squares means estimate. When you model data with the logit link function and the estimate represents a log odds ratio, the EXP option produces an odds ratio. See the section “[Odds and Odds Ratio Estimation](#)” on page 3090 for important details concerning the computation and interpretation of odds and odds ratio results with the GLIMMIX procedure. If you specify the **CL** or **ALPHA=** option, the (adjusted) confidence limits for the estimate are also exponentiated.

FTEST< (*joint-test-options*) >**JOINT**< (*joint-test-options*) >

produces an F test that jointly tests the rows of the LSMESTIMATE against zero. If the LOWER or UPPER options are in effect or if you specify boundary values with the BOUNDS= suboption, the GLIMMIX procedure computes a simulation-based p -value for the constrained joint test. For more information about these simulation-based p -values, see the section “[Joint Hypothesis Tests with Complex Alternatives, the Chi-Bar-Square Statistic](#)” on page 451 in Chapter 19, “[Shared Concepts and Topics](#).” You can specify the following *joint-test-options* in parentheses:

ACC= γ

specifies the accuracy radius for determining the necessary sample size in the simulation-based approach of Silvapulle and Sen (2004) for tests with order restrictions. The value of γ must be strictly between 0 and 1; the default value is 0.005.

BOUNDS=*value-list*

specifies boundary values for the estimable linear function. The null value of the hypothesis is always zero. If you specify a positive boundary value z , the hypotheses are $H: \theta = 0$ vs. $H_a: \theta > 0$ with the added constraint that $\theta < z$. The same is true for negative boundary values. The alternative hypothesis is then $H_a: \theta < 0$ subject to the constraint $\theta > -|z|$. If you specify a missing value, the hypothesis is assumed to be two-sided. The BOUNDS option enables you to specify sets of one- and two-sided joint hypotheses. If all values in *value-list* are set to missing, the procedure performs a simulation-based p -value calculation for a two-sided test.

EPS= ϵ

specifies the accuracy confidence level for determining the necessary sample size in the simulation-based approach of Silvapulle and Sen (2004) for F tests with order restrictions. The value of ϵ must be strictly between 0 and 1; the default value is 0.01.

LABEL='*label*'

enables you to assign a label to the joint test that identifies the results in the “LSMFtest” table. If you do not specify a label, the first non-default label for the LSMESTIMATE rows is used to label the joint test.

NSAMP= n

specifies the number of samples for the simulation-based method of Silvapulle and Sen (2004). If n is not specified, it is constructed from the values of the ALPHA= α , the ACC= γ , and the EPS= ϵ options. With the default values for γ , ϵ , and α (0.005, 0.01, and 0.05, respectively), NSAMP=12,604 by default.

ILINK

requests that the estimate and its standard error also be reported on the scale of the mean (the inverse linked scale). PROC GLIMMIX computes the value on the mean scale by applying the inverse link to the estimate. The interpretation of this quantity depends on the coefficients that are specified in your LSMESTIMATE statement and the link function. For example, in a model for binary data with a logit link, the following LSMESTIMATE statement computes

$$q = \frac{1}{1 + \exp\{-(\tau_1 - \tau_2)\}}$$

where τ_1 and τ_2 are the least squares means associated with the first two levels of the classification effect A:

```
proc glimmix;
  class A;
  model y = A / dist=binary link=logit;
  lsmestimate A 1 -1 / ilink;
run;
```

The quantity q is not the difference of the probabilities associated with the two levels,

$$\pi_1 - \pi_2 = \frac{1}{1 + \exp\{-\tau_1\}} - \frac{1}{1 + \exp\{-\tau_2\}}$$

The standard error of the inversely linked estimate is based on the delta method. If you also specify the **CL** or **ALPHA=** option, the GLIMMIX procedure computes confidence intervals for the inversely linked estimate. These intervals are obtained by applying the inverse link to the confidence intervals on the linked scale.

JOINT< *joint-test-options* >

is an alias for the **FTEST** option.

LOWER**LOWERTAILED**

requests that the p -value for the t test be based only on values that are less than the test statistic. A two-tailed test is the default. A lower-tailed confidence limit is also produced if you specify the **CL** or **ALPHA=** option.

Note that for **ADJUST=SCHEFFE** the one-sided adjusted confidence intervals and one-sided adjusted p -values are the same as the corresponding two-sided statistics, because this adjustment is based on only the right tail of the F distribution.

If you request an F test with the **FTEST** option, then a one-sided left-tailed order restriction is applied to all estimable functions, and the corresponding chi-bar-square statistic of Silvapulle and Sen (2004) is computed in addition to the two-sided, standard F or chi-square statistic. See the description of the **FTEST** option for information about how to control the computation of the simulation-based chi-bar-square statistic.

OBSMARGINS**OM**

specifies a potentially different weighting scheme for the computation of LS-means coefficients. The standard LS-means have equal coefficients across classification effects; however, the OM option changes these coefficients to be proportional to those found in the input data set. See the **OBSMARGINS** option in the **LSMEANS** statement for further details.

SINGULAR=*number*

tunes the estimability checking as documented for the **CONTRAST** statement.

STEPDOWN< (*step-down-options*) >

requests that multiplicity adjustments for the p -values of LS-mean estimates be further adjusted in a step-down fashion. Step-down methods increase the power of multiple testing procedures by taking advantage of the fact that a p -value will never be declared significant unless all smaller p -values are also declared significant. Note that the STEPDOWN adjustment combined with **ADJUST=BON** corresponds to the Holm (1979) and “Method 2” of Shaffer (1986); this is the default. Using step-down-adjusted p -values combined with **ADJUST=SIMULATE** corresponds to the method of Westfall (1997).

If the degrees-of-freedom method is **DDFM=KENWARDROGER** or **DDFM=SATTERTHWAITE**, then step-down-adjusted p -values are produced only if the **ADJDFE=ROW** option is in effect.

Also, the STEPDOWN option affects only p -values, not confidence limits. For **ADJUST=SIMULATE**, the generalized least squares hybrid approach of Westfall (1997) is employed to increase Monte Carlo accuracy.

You can specify the following *step-down-options* in parentheses:

MAXTIME=*n*

specifies the time (in seconds) to spend computing the maximal logically consistent sequential subsets of equality hypotheses for **TYPE=LOGICAL**. The default is **MAXTIME=60**. If the **MAXTIME** value is exceeded, the adjusted tests are not computed. When this occurs, you can try increasing the **MAXTIME** value. However, note that there are common multiple comparisons problems for which this computation requires a huge amount of time—for example, all pairwise comparisons between more than 10 groups. In such cases, try to use **TYPE=FREE** (the default) or **TYPE=LOGICAL(*n*)** for small n .

ORDER=PVALUE**ORDER=ROWS**

specifies the order in which the step-down tests are performed. **ORDER=PVALUE** is the default, with LS-mean estimates being declared significant only if all LS-mean estimates with smaller (unadjusted) p -values are significant. If you specify **ORDER=ROWS**, then significances are evaluated in the order in which they are specified.

REPORT

specifies that a report on the step-down adjustment be displayed, including a listing of the sequential subsets (Westfall 1997) and, for **ADJUST=SIMULATE**, the step-down simulation results.

TYPE=LOGICAL< (*n*) >**TYPE=FREE**

If you specify **TYPE=LOGICAL**, the step-down adjustments are computed by using maximal logically consistent sequential subsets of equality hypotheses (Shaffer 1986; Westfall 1997). Alternatively, for **TYPE=FREE**, logical constraints are ignored when sequential subsets are computed. The **TYPE=FREE** results are more conservative than those for **TYPE=LOGICAL**, but they can be much more efficient to produce for many estimates. For example, it is not feasible to take logical constraints between all pairwise comparisons of more than about 10 groups. For this reason, **TYPE=FREE** is the default.

However, you can reduce the computational complexity of taking logical constraints into account by limiting the depth of the search tree used to compute them, specifying the optional depth parameter as a number *n* in parentheses after **TYPE=LOGICAL**. As with **TYPE=FREE**, results for **TYPE=LOGICAL**(*n*) are conservative relative to the true **TYPE=LOGICAL** results, but even for **TYPE=LOGICAL**(0), they can be appreciably less conservative than **TYPE=FREE**, and they are computationally feasible for much larger numbers of estimates. If you do not specify *n* or if *n* = -1, the full search tree is used.

UPPER**UPPERTAILED**

requests that the *p*-value for the *t* test be based only on values that are greater than the test statistic. A two-tailed test is the default. An upper-tailed confidence limit is also produced if you specify the **CL** or **ALPHA=** option.

Note that for **ADJUST=SCHEFFE** the one-sided adjusted confidence intervals and one-sided adjusted *p*-values are the same as the corresponding two-sided statistics, because this adjustment is based on only the right tail of the *F* distribution.

If you request a joint test with the **FTEST** option, then a one-sided right-tailed order restriction is applied to all estimable functions, and the corresponding chi-bar-square statistic of Silvapulle and Sen (2004) is computed in addition to the two-sided, standard *F* or chi-square statistic. See the **FTEST** option for information about how to control the computation of the simulation-based chi-bar-square statistic.

MODEL Statement

MODEL *response* < (*response-options*) > = < *fixed-effects* > < / *model-options* > ;

MODEL *events/trials* = < *fixed-effects* > < / *model-options* > ;

The **MODEL** statement is required and names the dependent variable and the fixed effects. The *fixed-effects* determine the **X** matrix of the model (see the section “[Notation for the Generalized Linear Mixed Model](#)” for details). The [specification of effects](#) is the same as in the **GLM** or **MIXED** procedure. In contrast to **PROC GLM**, you do not specify random effects in the **MODEL** statement. However, in contrast to **PROC GLM** and **PROC MIXED**, continuous variables on the left and right side of the **MODEL** statement can be computed through **PROC GLIMMIX programming statements**.

An intercept is included in the fixed-effects model by default. It can be removed with the **NOINT** option.

The dependent variable can be specified by using either the *response* syntax or the *events/trials* syntax. The *events/trials* syntax is specific to models for binomial data. A binomial(n, π) variable is the sum of n independent Bernoulli trials with event probability π . Each Bernoulli trial results in either an event or a nonevent (with probability $1 - \pi$). You use the *events/trials* syntax to indicate to the GLIMMIX procedure that the Bernoulli outcomes are grouped. The value of the second variable, *trials*, gives the number n of Bernoulli trials. The value of the first variable, *events*, is the number of events out of n . The values of both *events* and (*trials*–*events*) must be nonnegative and the value of *trials* must be positive. Observations for which these conditions are not met are excluded from the analysis. If the *events/trials* syntax is used, the GLIMMIX procedure defaults to the binomial distribution. The response is then the *events* variable. The *trials* variable is accounted in model fitting as an additional weight. If you use the *response* syntax, the procedure defaults to the normal distribution.

There are two sets of options in the MODEL statement. The *response-options* determine how the GLIMMIX procedure models probabilities for binary and multinomial data. The *model-options* control other aspects of model formation and inference. Table 41.10 summarizes the options available in the MODEL statement. These are subsequently discussed in detail in alphabetical order by option category.

Table 41.10 MODEL Statement Options

Option	Description
Response Variable Options	
DESCENDING	Reverses the order of response categories
EVENT=	Specifies the event category in binary models
ORDER=	Specifies the sort order for the response variable
REFERENCE=	Specifies the reference category in generalized logit models
Model Building	
DIST=	Specifies the response distribution
LINK=	Specifies the link function
NOINT	Excludes fixed-effect intercept from model
OFFSET=	Specifies the offset variable for linear predictor
Statistical Computations	
ALPHA= α	Determines the confidence level ($1 - \alpha$)
CHISQ	Requests chi-square tests
DDF=	Specifies the denominator degrees of freedom (list)
DDFM=	Specifies the method for computing denominator degrees of freedom
HTYPE=	Selects the type of hypothesis test
LWEIGHT	Determines how weights are used
NOCENTER	Suppresses centering and scaling of X columns during the estimation phase
REFLINP	Specifies a value for the linear predictor
ZETA=	Tunes sensitivity in computing Type III functions
Statistical Output	
CL	Displays confidence limits for fixed-effects parameter estimates
CORRB	Displays the correlation matrix of fixed-effects parameter estimates
COVB	Displays the covariance matrix of fixed-effects parameter estimates
COVBI	Displays the inverse covariance matrix of fixed-effects parameter estimates
E, E1, E2, E3	Displays the L matrix coefficients

Table 41.10 *continued*

Option	Description
INTERCEPT	Adds a row for the intercept to test tables
ODDSRATIO	Displays odds ratios and confidence limits
SOLUTION	Displays fixed-effects parameter estimates (and scale parameter in GLM models)
STDCOEFF	Displays standardized coefficients

Response Variable Options

Response variable options determine how the GLIMMIX procedure models probabilities for binary and multinomial data.

You can specify the following options by enclosing them in parentheses after the response variable. See the section “[Response-Level Ordering and Referencing](#)” on page 3100 for more detail and examples.

DESCENDING

DESC

reverses the order of the response categories. If both the DESCENDING and ORDER= options are specified, PROC GLIMMIX orders the response categories according to the ORDER= option and then reverses that order.

EVENT=*category* | *keyword*

specifies the event category for the binary response model. PROC GLIMMIX models the probability of the event category. The EVENT= option has no effect when there are more than two response categories. You can specify the value (formatted, if a format is applied) of the event category in quotes, or you can specify one of the following keywords:

FIRST

designates the first ordered category as the event. This is the default.

LAST

designates the last ordered category as the event.

ORDER=DATA | FORMATTED | FREQ | INTERNAL

specifies the sort order for the levels of the response variable. When ORDER=FORMATTED (the default) for numeric variables for which you have supplied no explicit format (that is, for which there is no corresponding FORMAT statement in the current PROC GLIMMIX run or in the DATA step that created the data set), the levels are ordered by their internal (numeric) value. If you specify the ORDER= option in the MODEL statement and the ORDER= option in the PROC GLIMMIX statement, the former takes precedence. The following table shows the interpretation of the ORDER= values:

Value of ORDER=	Levels Sorted By
DATA	order of appearance in the input data set
FORMATTED	external formatted value, except for numeric variables with no explicit format, which are sorted by their unformatted (internal) value

Table 41.10 continued

Value of ORDER=	Levels Sorted By
FREQ	descending frequency count; levels with the most observations come first in the order
INTERNAL	unformatted value

By default, ORDER=FORMATTED. For the FORMATTED and INTERNAL values, the sort order is machine dependent.

For more information about sort order, see the chapter on the SORT procedure in the *Base SAS Procedures Guide* and the discussion of BY-group processing in *SAS Language Reference: Concepts*.

REFERENCE='category' | keyword

REF='category' | keyword

specifies the reference category for the generalized logit model and the binary response model. For the generalized logit model, each nonreference category is contrasted with the reference category. For the binary response model, specifying one response category as the reference is the same as specifying the other response category as the event category. You can specify the value (formatted if a format is applied) of the reference category in quotes, or you can specify one of the following keywords:

FIRST

designates the first ordered category as the reference category.

LAST

designates the last ordered category as the reference category. This is the default.

Model Options

ALPHA=number

requests that a *t*-type confidence interval be constructed for each of the fixed-effects parameters with confidence level $1 - \text{number}$. The value of *number* must be between 0 and 1; the default is 0.05.

CHISQ

requests that chi-square tests be performed for all specified effects in addition to the *F* tests. Type III tests are the default; you can produce the Type I and Type II tests by using the **HTYPE=** option.

CL

requests that *t*-type confidence limits be constructed for each of the fixed-effects parameter estimates. The confidence level is 0.95 by default; this can be changed with the **ALPHA=** option.

CORRB

produces the correlation matrix from the approximate covariance matrix of the fixed-effects parameter estimates.

COVB<(DETAILS)>

produces the approximate variance-covariance matrix of the fixed-effects parameter estimates $\hat{\beta}$. In a generalized linear mixed model this matrix typically takes the form $(\mathbf{X}'\hat{\mathbf{V}}^{-1}\mathbf{X})^{-1}$ and can be obtained by sweeping the mixed model equations; see the section “Estimated Precision of Estimates” on

page 3056. In a model without random effects, it is obtained from the inverse of the observed or expected Hessian matrix. Which Hessian is used in the computation depends on whether the procedure is in scoring mode (see the **SCORING=** option in the **PROC GLIMMIX** statement) and whether the **EX-PHESSIAN** option is in effect. Note that if you use **EMPIRICAL=** or **DDFM=KENWARDROGER**, the matrix displayed by the **COVB** option is the empirical (sandwich) estimator or the adjusted estimator, respectively.

The **DETAILS** suboption of the **COVB** option enables you to obtain a table of statistics about the covariance matrix of the fixed effects. If an adjusted estimator is used because of the **EMPIRICAL=** or **DDFM=KENWARDROGER** option, the **GLIMMIX** procedure displays statistics for the adjusted and unadjusted estimators as well as statistics comparing them. This enables you to diagnose, for example, changes in rank (because of an insufficient number of subjects for the empirical estimator) and to assess the extent of the covariance adjustment. In addition, the **GLIMMIX** procedure then displays the unadjusted (=model-based) covariance matrix of the fixed-effects parameter estimates. For more details, see the section “Exploring and Comparing Covariance Matrices” on page 3080.

COVBI

produces the inverse of the approximate covariance matrix of the fixed-effects parameter estimates.

DDF=value-list

DF=value-list

enables you to specify your own denominator degrees of freedom for the fixed effects. The *value-list* specification is a list of numbers or missing values (.) separated by commas. The degrees of freedom should be listed in the order in which the effects appear in the “Type III Tests of Fixed Effects” table. If you want to retain the default degrees of freedom for a particular effect, use a missing value for its location in the list. For example, the statement assigns 3 denominator degrees of freedom to A and 4.7 to A*B, while those for B remain the same:

```
model Y = A B A*B / ddf=3, ., 4.7;
```

If you select a degrees-of-freedom method with the **DDFM=** option, then nonmissing, positive values in *value-list* override the degrees of freedom for the particular effect. For example, the statement assigns 3 and 6 denominator degrees of freedom in the test of the A main effect and the A*B interaction, respectively:

```
model Y = A B A*B / ddf=3, ., 6 ddfm=Satterth;
```

The denominator degrees of freedom for the test for the B effect are determined from a Satterthwaite approximation.

Note that the **DDF=** and **DDFM=** options determine the degrees of freedom in the “Type I Tests of Fixed Effects,” “Type II Tests of Fixed Effects,” and “Type III Tests of Fixed Effects” tables. These degrees of freedom are also used in determining the degrees of freedom in tests and confidence intervals from the **CONTRAST**, **ESTIMATE**, **LSMEANS**, and **LSMESTIMATE** statements. Exceptions from this rule are noted in the documentation for the respective statements.

DDFM=method

specifies the method for computing the denominator degrees of freedom for the tests of fixed effects that result from the **MODEL**, **CONTRAST**, **ESTIMATE**, **LSMEANS**, and **LSMESTIMATE** statements.

You can specify the following *methods*:

BETWITHIN

BW

assigns within-subject degrees of freedom to a fixed effect if the fixed effect changes within a subject, and between-subject degrees of freedom otherwise. This method is the default for models with only R-side random effects and a **SUBJECT=** option. Computational details can be found in the section “[Degrees of Freedom Methods](#)” on page 3075.

CONTAIN

CON

invokes the containment method to compute denominator degrees of freedom. This method is the default when the model contains G-side random effects. Computational details can be found in the section “[Degrees of Freedom Methods](#)” on page 3075.

KENWARDROGER< (FIRSTORDER) >

KENROGER< (FIRSTORDER) >

KR< (FIRSTORDER) >

applies the (prediction) standard error and degrees-of-freedom correction detailed by Kenward and Roger (1997). This approximation involves adjusting the estimated variance-covariance matrix of the fixed and random effects in a manner similar to that of Prasad and Rao (1990); Harville and Jeske (1992); Kackar and Harville (1984). Satterthwaite-type degrees of freedom are then computed based on this adjustment. Computational details can be found in the section “[Degrees of Freedom Methods](#)” on page 3075.

KENWARDROGER2

KENROGER2

KR2

applies the (prediction) standard error and degrees-of-freedom correction that are detailed by Kenward and Roger (2009). This correction further reduces the precision estimator bias for the fixed and random effects under nonlinear covariance structures. Computational details can be found in the section “[Degrees of Freedom Methods](#)” on page 3075.

NONE

specifies that no denominator degrees of freedom be applied. PROC GLIMMIX then essentially assumes that infinite degrees of freedom are available in the calculation of p -values. The p -values for t tests are then identical to p -values that are derived from the standard normal distribution. In the case of F tests, the p -values are equal to those of chi-square tests that are determined as follows: if F_{obs} is the observed value of the F test with l numerator degrees of freedom, then

$$p = \Pr\{F_{l,\infty} > F_{obs}\} = \Pr\{\chi_l^2 > lF_{obs}\}$$

Regardless of the DDFM= method, you can obtain these chi-square p -values with the [CHISQ](#) option in the MODEL statement.

RESIDUAL

RES

performs all tests by using the residual degrees of freedom, $n - \text{rank}(\mathbf{X})$, where n is the sum of the frequencies of observations or the sum of frequencies of *event/trials* pairs. This method is the default degrees of freedom method for GLMs and overdispersed GLMs.

SATTERTHWAITE

SAT

performs a general Satterthwaite approximation for the denominator degrees of freedom in a generalized linear mixed model. This method is a generalization of the techniques that are described in Giesbrecht and Burns (1985); McLean and Sanders (1988); Fai and Cornelius (1996). The method can also include estimated random effects. Computational details can be found in the section “[Degrees of Freedom Methods](#)” on page 3075.

When the asymptotic variance matrix of the covariance parameters is found to be singular, a generalized inverse is used. Covariance parameters with zero variance then do not contribute to the degrees of freedom adjustment for DDFM=SATTERTH and DDFM=KENWARDROGER, and a message is written to the log.

DISTRIBUTION=*keyword*

DIST=*keyword*

D=*keyword*

ERROR=*keyword*

E=*keyword*

specifies the built-in (conditional) probability distribution of the data. If you specify the DIST= option and you do not specify a user-defined link function, a default link function is chosen according to the following table. If you do not specify a distribution, the GLIMMIX procedure defaults to the normal distribution for continuous response variables and to the multinomial distribution for classification or character variables, unless the *events/trial* syntax is used in the MODEL statement. If you choose the *events/trial* syntax, the GLIMMIX procedure defaults to the binomial distribution.

[Table 41.11](#) lists the values of the DIST= option and the corresponding default link functions. For the case of generalized linear models with these distributions, you can find expressions for the log-likelihood functions in the section “[Maximum Likelihood](#)” on page 3047.

Table 41.11 Keyword Values of the DIST= Option

DIST=	Distribution	Default Link Function	Numeric Value
BETA	beta	logit	12
BINARY	binary	logit	4
BINOMIAL BIN B	binomial	logit	3
EXPONENTIAL EXPO	exponential	log	9
GAMMA GAM	gamma	log	5
GAUSSIAN G NORMAL N	normal	identity	1
GEOMETRIC GEOM	geometric	log	8
INVGAUSS IGAUSSIAN IG	inverse Gaussian	inverse squared (power(-2))	6
LOGNORMAL LOGN	lognormal	identity	11
MULTINOMIAL MULTI MULT	multinomial	cumulative logit	NA
NEGBINOMIAL NEGBIN NB	negative binomial	log	7
POISSON POI P	Poisson	log	2
TCENTRAL TDIST T	<i>t</i>	identity	10
BYOBS(<i>variable</i>)	multivariate	varied	NA

Note that the PROC GLIMMIX default link for the gamma or exponential distribution is not the canonical link (the reciprocal link).

The numeric value in the last column of Table 41.11 can be used in combination with DIST=BYOBS. The BYOBS(*variable*) syntax designates a variable whose value identifies the distribution to which an observation belongs. If the variable is numeric, its values must match values in the last column of Table 41.11. If the variable is not numeric, an observation's distribution is identified by the first four characters of the distribution's name in the leftmost column of the table. Distributions whose numeric value is "NA" cannot be used with DIST=BYOBS.

If the variable in BYOBS(*variable*) is a data set variable, it can also be used in the CLASS statement of the GLIMMIX procedure. For example, this provides a convenient method to model multivariate data jointly while varying fixed-effects components across outcomes. Assume that, for example, for each patient, a count and a continuous outcome were observed; the count data are modeled as Poisson data and the continuous data are modeled as gamma variates. The following statements fit a Poisson and a gamma regression model simultaneously:

```
proc sort data=yourdata;
  by patient;
run;
data yourdata;
  set yourdata;
  by patient;
  if first.patient then dist='POIS' else dist='GAMM';
run;
proc glimmix data=yourdata;
  class treatment dist;
  model y = dist treatment*dist / dist=byobs(dist);
run;
```

The two models have separate intercepts and treatment effects. To correlate the outcomes, you can share a random effect between the observations from the same patient:

```
proc glimmix data=yourdata;
  class treatment dist patient;
  model y = dist treatment*dist / dist=byobs(dist);
  random intercept / subject=patient;
run;
```

Or, you could use an R-side correlation structure:

```
proc glimmix data=yourdata;
  class treatment dist patient;
  model y = dist treatment*dist / dist=byobs(dist);
  random _residual_ / subject=patient type=un;
run;
```

Although `DIST=BYOBS(variable)` is used to model multivariate data, you only need a single response variable in PROC GLIMMIX. The responses are in “univariate” form. This allows, for example, different missing value patterns across the responses. It does, however, require that all response variables be numeric.

The default links that are assigned when `DIST=BYOBS` is in effect correspond to the respective default links in [Table 41.11](#).

When you choose `DIST=LOGNORMAL`, the GLIMMIX procedure models the logarithm of the response variable as a normal random variable. That is, the mean and variance are estimated on the logarithmic scale, assuming a normal distribution, $\log\{Y\} \sim N(\mu, \sigma^2)$. This enables you to draw on options that require a distribution in the exponential family—for example, by using a scoring algorithm in a GLM. To convert means and variances for $\log\{Y\}$ into those of Y , use the relationships

$$\begin{aligned} E[Y] &= \exp\{\mu\} \sqrt{\omega} \\ \text{Var}[Y] &= \exp\{2\mu\} \omega(\omega - 1) \\ \omega &= \exp\{\sigma^2\} \end{aligned}$$

The `DIST=T` option models the data as a shifted and scaled central t variable. This enables you to model data with heavy-tailed distributions. If Y denotes the response and X has a t_ν distribution with ν degrees of freedom, then PROC GLIMMIX models

$$Y = \mu + \sqrt{\phi} X$$

In this parameterization, Y has mean μ and variance $\phi\nu/(\nu - 2)$.

By default, $\nu = 3$. You can supply different degrees of freedom for the t variate as in the following statements:

```
proc glimmix;
  class a b;
  model y = b x b*x / dist=tcentral(9.6);
  random a;
run;
```


The GLIMMIX procedure does not accept values for the degrees of freedom parameter less than 3.0. If the t distribution is used with the `DIST=BYOBS(variable)` specification, the degrees of freedom are fixed at $\nu = 3$. For mixed models where parameters are estimated based on linearization, choosing `DIST=T` instead of `DIST=NORMAL` affects only the residual variance, which decreases by the factor $\nu/(\nu - 2)$.

Note that in SAS 9.1, the GLIMMIX procedure modeled $Y = \mu + \phi^* \sqrt{\frac{\nu-2}{\nu}} X$. The scale parameter of the parameterizations are related as $\phi = \phi^* \times \phi^* \times (\nu - 2)/\nu$.

The `DIST=BETA` option implements the parameterization of the beta distribution in Ferrari and Cribari-Neto (2004). If Y has a $\text{beta}(\alpha, \beta)$ density, so that $E[Y] = \mu = \alpha/(\alpha + \beta)$, this parameterization uses the variance function $a(\mu) = \mu(1 - \mu)$ and $\text{Var}[Y] = a(\mu)/(1 + \phi)$.

See the section “[Maximum Likelihood](#)” on page 3047 for the log likelihoods of the distributions fitted by the GLIMMIX procedure.

E

requests that Type I, Type II, and Type III L matrix coefficients be displayed for all specified effects.

E1 | EI

requests that Type I L matrix coefficients be displayed for all specified effects.

E2 | EII

requests that Type II L matrix coefficients be displayed for all specified effects.

E3 | EIII

requests that Type III L matrix coefficients be displayed for all specified effects.

HTYPE=value-list

indicates the type of hypothesis test to perform on the fixed effects. Valid entries for values in the *value-list* are 1, 2, and 3, corresponding to Type I, Type II, and Type III tests. The default value is 3. You can specify several types by separating the values with a comma or a space. The ODS table names are “Tests1,” “Tests2,” and “Tests3” for the Type I, Type II, and Type III tests, respectively.

INTERCEPT

adds a row to the tables for Type I, II, and III tests corresponding to the overall intercept.

LINK=keyword

specifies the link function in the generalized linear mixed model. The keywords and their associated built-in link functions are shown in [Table 41.12](#).

Table 41.12 Built-in Link Functions of the GLIMMIX Procedure

LINK=	Link Function	$g(\mu) = \eta =$	Numeric Value
CUMCLL CCLL	cumulative complementary log-log	$\log(-\log(1 - \pi))$	NA
CUMLOGIT CLOGIT	cumulative logit	$\log(\gamma/(1 - \pi))$	NA
CUMLOGLOG	cumulative log-log	$-\log(-\log(\pi))$	NA
CUMPROBIT CPROBIT	cumulative probit	$\Phi^{-1}(\pi)$	NA
CLOGLOG CLL	complementary log-log	$\log(-\log(1 - \mu))$	5

Table 41.12 continued

LINK=	Link Function	$g(\mu) = \eta =$	Numeric Value
GLOGIT GENLOGIT	generalized logit		NA
IDENTITY ID	identity	μ	1
LOG	log	$\log(\mu)$	4
LOGIT	logit	$\log(\mu/(1 - \mu))$	2
LOGLOG	log-log	$-\log(-\log(\mu))$	6
PROBIT	probit	$\Phi^{-1}(\mu)$	3
POWER(λ) POW(λ)	power with exponent $\lambda = \text{number}$	$\begin{cases} \mu^\lambda & \text{if } \lambda \neq 0 \\ \log(\mu) & \text{if } \lambda = 0 \end{cases}$	NA
POWERMINUS2	power with exponent -2	$1/\mu^2$	8
RECIPROCAL INVERSE	reciprocal	$1/\mu$	7
BYOBS(<i>variable</i>)	varied	varied	NA

For the probit and cumulative probit links, $\Phi^{-1}(\cdot)$ denotes the quantile function of the standard normal distribution. For the other cumulative links, π denotes a cumulative category probability. The cumulative and generalized logit link functions are appropriate only for the multinomial distribution. When you choose a cumulative link function, PROC GLIMMIX assumes that the data are ordinal. When you specify LINK=GLOGIT, the GLIMMIX procedure assumes that the data are nominal (not ordered).

The numeric value in the rightmost column of Table 41.12 can be used in conjunction with LINK=BYOBS(*variable*). This syntax designates a *variable* whose values identify the link function associated with an observation. If the variable is numeric, its values must match those in the last column of Table 41.12. If the variable is not numeric, an observation's link function is determined by the first four characters of the link's name in the first column. Those link functions whose numeric value is "NA" cannot be used with LINK=BYOBS(*variable*).

You can define your own link function through programming statements. See the section "User-Defined Link or Variance Function" on page 3043 for more information about how to specify a link function. If a user-defined link function is in effect, the specification in the LINK= option is ignored. If you specify neither the LINK= option nor a user-defined link function, then the default link function is chosen according to Table 41.11.

LWEIGHT=FIRSTORDER | FIRO

LWEIGHT=NONE

LWEIGHT=VAR

determines how weights are used in constructing the coefficients for Type I through Type III L matrices. The default is LWEIGHT=VAR, and the values of the WEIGHT variable are used in forming crossproduct matrices. If you specify LWEIGHT=FIRO, the weights incorporate the WEIGHT variable as well as the first-order weights of the linearized model. For LWEIGHT=NONE, the L matrix coefficients are based on the raw crossproduct matrix, whether a WEIGHT variable is specified or not.

NOCENTER

requests that the columns of the \mathbf{X} matrix are not centered and scaled. By default, the columns of \mathbf{X} are centered and scaled. Unless the NOCENTER option is in effect, \mathbf{X} is replaced by \mathbf{X}^* during estimation. The columns of \mathbf{X}^* are computed as follows:

- In models with an intercept, the intercept column remains the same and the j th entry in row i of \mathbf{X}^* is

$$x_{ij}^* = \frac{x_{ij} - \bar{x}_j}{\sqrt{\sum_{i=1}^n (x_{ij} - \bar{x}_j)^2}}$$

- In models without intercept, no centering takes place and the j th entry in row i of \mathbf{X}^* is

$$x_{ij}^* = \frac{x_{ij}}{\sqrt{\sum_{i=1}^n (x_{ij} - \bar{x}_j)^2}}$$

The effects of centering and scaling are removed when results are reported. For example, if the covariance matrix of the fixed effects is printed with the COVB option of the MODEL statement, the covariances are reported in terms of the original parameters, not the centered and scaled versions. If you specify the STDCOEf option, fixed-effects parameter estimates and their standard errors are reported in terms of the standardized (scaled and/or centered) coefficients in addition to the usual results in noncentered form.

NOINT

requests that no intercept be included in the fixed-effects model. An intercept is included by default.

ODDSRATIO<(odds-ratio-options)>**OR**<(odds-ratio-options)>

requests estimates of odds ratios and their confidence limits, provided the link function is the logit, cumulative logit, or generalized logit. Odds ratios are produced for the following:

- classification main effects, if they appear in the MODEL statement
- continuous variables in the MODEL statement, unless they appear in an interaction with a classification effect
- continuous variables in the MODEL statement at fixed levels of a classification effect, if the MODEL statement contains an interaction of the two
- continuous variables in the MODEL statement, if they interact with other continuous variables

You can specify the following *odds-ratio-options* to create customized odds ratio results.

AT *var-list=value-list*

specifies the reference values for continuous variables in the model. By default, the average value serves as the reference. Consider, for example, the following statements:

```
proc glimmix;
  class A;
  model y = A x A*x / dist=binary oddsratio;
run;
```

Odds ratios for A are based on differences of least squares means for which x is set to its mean. Odds ratios for x are computed by differencing two sets of least squares mean for the A factor. One set is computed at $x = \bar{x} + 1$, and the second set is computed at $x = \bar{x}$. The following MODEL statement changes the reference value for x to 3:

```
model y = A x A*x / dist=binary
          oddsratio(at x=3);
```

DIFF<=difftype>

controls the type of differences for classification main effects. By default, odds ratios compare the odds of a response for level j of a factor to the odds of the response for the last level of that factor (DIFF=LAST). The DIFF=FIRST option compares the levels against the first level, DIFF=ALL produces odds ratios based on all pairwise differences, and DIFF=NONE suppresses odds ratios for classification main effects.

LABEL

displays a label in the “Odds Ratio Estimates” table. The table describes the comparison associated with the table row.

UNIT var-list=value-list

specifies the units in which the effects of continuous variable in the model are assessed. By default, odds ratios are computed for a change of one unit from the average. Consider a model with a classification factor A with 4 levels. The following statements produce an “Odds Ratio Estimates” table with 10 rows:

```
proc glimmix;
  class A;
  model y = A x A*x / dist=binary
          oddsratio(diff=all unit x=2);
run;
```

The first $4 \times 3/2 = 6$ rows correspond to pairwise differences of levels of A. The underlying log odds ratios are computed as differences of A least squares means. In the least squares mean computation the covariate x is set to \bar{x} . The next four rows compare least squares means for A at $x = \bar{x} + 2$ and at $x = \bar{x}$. You can combine the AT and UNIT options to produce custom odds ratios. For example, the following statements produce an “Odds Ratio Estimates” table with 8 rows:

```
proc glimmix;
  class A;
  model y = A x x*z / dist=binary
          oddsratio(diff=all
                    at x = 3
                    unit x z = 2 4);
run;
```

The first $4 \times 3/2 = 6$ rows correspond to pairwise differences of levels of A. The underlying log odds ratios are computed as differences of A least squares means. In the least squares mean computation, the covariate x is set to 3, and the covariate x*z is set to $3\bar{z}$. The next odds ratio measures the effect of a change in x. It is based on differencing the linear predictor for $x = 3 + 2$

and $x^*z = (3 + 2)\bar{z}$ with the linear predictor for $x = 3$ and $x^*z = 3\bar{z}$. The last odds ratio expresses a change in z by contrasting the linear predictors based on $x = 3$ and $x^*z = 3(\bar{z} + 4)$ with the predictor based on $x = 3$ and $x^*z = 3\bar{z}$.

To compute odds and odds ratios for general estimable functions and least squares means, see the **ODDSRATIO** option in the **LSMEANS** statement and the **EXP** options in the **ESTIMATE** and **LSMESTIMATE** statements.

For important details concerning interpretation and computation of odds ratios with the GLIMMIX procedure, see the section “Odds and Odds Ratio Estimation” on page 3090.

OFFSET=variable

specifies a variable to be used as an offset for the linear predictor. An offset plays the role of a fixed effect whose coefficient is known to be 1. You can use an offset in a Poisson model, for example, when counts have been obtained in time intervals of different lengths. With a log link function, you can model the counts as Poisson variables with the logarithm of the time interval as the offset variable. The offset variable cannot appear in the **CLASS** statement or elsewhere in the **MODEL** or **RANDOM** statement.

REFLINP=r

specifies a value for the linear predictor of the reference level in the generalized logit model for nominal data. By default $r=0$.

SOLUTION

S

requests that a solution for the fixed-effects parameters be produced. Using notation from the section “Notation for the Generalized Linear Mixed Model” on page 2918, the fixed-effects parameter estimates are $\hat{\beta}$, and their (approximate) estimated standard errors are the square roots of the diagonal elements of $\widehat{\text{Var}}[\hat{\beta}]$. This matrix commonly is of the form $(\mathbf{X}'\hat{\mathbf{V}}^{-1}\mathbf{X})^{-1}$ in GLMMs. You can output this approximate variance matrix with the **COVB** option. See the section “Details: GLIMMIX Procedure” on page 3047 on the construction of $\hat{\mathbf{V}}$ in the various models.

Along with the estimates and their approximate standard errors, a t statistic is computed as the estimate divided by its standard error. The degrees of freedom for this t statistic matches the one appearing in the “Type III Tests of Fixed Effects” table under the effect containing the parameter. If **DDFM=KENWARDROGER** or **DDFM=SATTERTHWAITE**, the degrees of freedom are computed separately for each fixed-effect estimate, unless you override the value for any specific effect with the **DDF=value-list** option. The “Pr > |t|” column contains the two-tailed p -value corresponding to the t statistic and associated degrees of freedom. You can use the **CL** option to request confidence intervals for the fixed-effects parameters; they are constructed around the estimate by using a radius of the standard error times a percentage point from the t distribution.

STDCOEF

reports solutions for fixed effects in terms of the standardized (scaled and/or centered) coefficients. This option has no effect when the **NOCENTER** option is specified or in models for multinomial data.

ZETA=number

tunes the sensitivity in forming Type III functions. Any element in the estimable function basis with an absolute value less than *number* is set to 0. The default is 1E–8.

NLOPTIONS Statement

NLOPTIONS < options > ;

Most models fit with the GLIMMIX procedure typically have one or more nonlinear parameters. Estimation requires nonlinear optimization methods. You can control the optimization through options in the NLOPTIONS statement.

Several estimation methods of the GLIMMIX procedure (**METHOD=RSPL**, **MSPL**, **RMPL**, **MMPL**) are doubly iterative in the following sense. The generalized linear mixed model is approximated by a linear mixed model based on current values of the covariance parameter estimates. The resulting linear mixed model is then fit, which is itself an iterative process (with some exceptions). On convergence, new covariance parameters and fixed-effects estimates are obtained and the approximated linear mixed model is updated. Its parameters are again estimated iteratively. It is thus reasonable to refer to *outer* and *inner* iterations. The outer iterations involve the repeated updates of the linear mixed models, and the inner iterations are the iterative steps that lead to parameter estimates in any given linear mixed model. The NLOPTIONS statement controls the inner iterations. The outer iteration behavior can be controlled with options in the **PROC GLIMMIX** statement, such as the **MAXLMMUPDATE=**, **PCONV=**, and **ABSPCONV=** options. If the estimation method involves a singly iterative approach, then there is no need for the outer cycling and the model is fit in a single optimization controlled by the NLOPTIONS statement (see the section “[Singly or Doubly Iterative Fitting](#)” on page 3104).

The syntax and options of the NLOPTIONS statement are described in the section “[NLOPTIONS Statement](#)” on page 482 of Chapter 19, “[Shared Concepts and Topics](#).”

Note that in a GLMM with pseudo-likelihood estimation, specifying **TECHNIQUE=NONE** has the same effect as specifying the **NOITER** option in the **PARMS** statement. If you estimate the parameters by **METHOD=LAPLACE** or **METHOD=QUAD**, **TECHNIQUE=NONE** applies to the optimization after starting values have been determined.

The GLIMMIX procedure applies the default optimization technique shown in [Table 41.13](#), depending on your model.

Table 41.13 Default Techniques

Model Family	Setting	TECHNIQUE=
GLM	DIST=NORMAL LINK=IDENTITY	NONE
GLM	otherwise	NEWRAP
GLMM	PARMS NOITER, PL	NONE
GLMM	binary data, PL	NRRIDG
GLMM	otherwise	QUANEW

OUTPUT Statement

```
OUTPUT < OUT=SAS-data-set >
  < keyword<(keyword-options)> <=name>> ...
  < keyword<(keyword-options)> <=name>> </options> ;
```

The OUTPUT statement creates a data set that contains predicted values and residual diagnostics, computed after fitting the model. By default, all variables in the original data set are included in the output data set.

You can use the ID statement to select a subset of the variables from the input data set as well as computed variables for adding to the output data set. If you reassign a data set variable through programming statements, the value of the variable from the input data set supersedes the recomputed value when observations are written to the output data set. If you list the variable in the ID statement, however, PROC GLIMMIX saves the current value of the variable after the programming statements have been executed.

For example, suppose that data set Scores contains the variables score, machine, and person. The following statements fit a model with fixed machine and random person effects. The variable score divided by 100 is assumed to follow an inverse Gaussian distribution. The (conditional) mean and residuals are saved to the data set igaussout. Because no ID statement is given, the variable score in the output data set contains the values from the input data set.

```
proc glimmix;
  class machine person;
  score = score/100;
  p = 4*_linp_;
  model score = machine / dist=invgauss;
  random int / sub=person;
  output out=igaussout pred=p resid=r;
run;
```

On the contrary, the following statements list explicitly which variables to save to the OUTPUT data set. Because the variable score is listed in the ID statement, and is (re-)assigned through programming statements, the values of score saved to the OUTPUT data set are the input values divided by 100.

```
proc glimmix;
  class machine person;
  score = score / 100;
  model score = machine / dist=invgauss;
  random int / sub=person;
  output out=igaussout pred=p resid=r;
  id machine score _xbeta_ _zgamma_;
run;
```

You can specify the following syntax elements in the OUTPUT statement before the slash (/).

OUT=SAS-data-set

specifies the name of the output data set. If the OUT= option is omitted, the procedure uses the DATA n convention to name the output data set.

keyword<(keyword-options)> <=name>

specifies a statistic to include in the output data set and optionally assigns the variable the name *name*. You can use the *keyword-options* to control which type of a particular statistic to compute. The *keyword-options* can take on the following values:

- BLUP uses the predictors of the random effects in computing the statistic.
- ILINK computes the statistic on the scale of the data.
- NOBLUP does not use the predictors of the random effects in computing the statistic.
- NOILINK computes the statistic on the scale of the link function.

The default is to compute statistics by using BLUPs on the scale of the link function (the linearized scale). For example, the following OUTPUT statements are equivalent:

```
output out=out1 pred=predicted lcl=lower;

output out=out1 pred(blup noilink)=predicted
               lcl (blup noilink)=lower;
```

If a particular combination of keyword and keyword options is not supported, the statistic is not computed and a message is produced in the SAS log.

A **keyword** can appear multiple times in the OUTPUT statement. Table 41.14 lists the keywords and the default names assigned by the GLIMMIX procedure if you do not specify a *name*. In this table, *y* denotes the observed response, and *p* denotes the linearized pseudo-data. See the section “Pseudo-likelihood Estimation Based on Linearization” on page 3054 for details on notation and the section “Notes on Output Statistics” on page 3111 for further details regarding the output statistics.

Table 41.14 Keywords for Output Statistics

Keyword	Options	Description	Expression	Name
PREDICTED	Default	Linear predictor	$\hat{\eta} = \mathbf{x}'\hat{\boldsymbol{\beta}} + \mathbf{z}'\hat{\boldsymbol{\gamma}}$	Pred
	NOBLUP	Marginal linear predictor	$\hat{\eta}_m = \mathbf{x}'\hat{\boldsymbol{\beta}}$	PredPA
	ILINK	Predicted mean	$g^{-1}(\hat{\eta})$	PredMu
	NOBLUP ILINK	Marginal mean	$g^{-1}(\hat{\eta}_m)$	PredMuPA
STDERR	Default	Standard deviation of linear predictor	$\sqrt{\text{Var}[\hat{\eta} - \mathbf{z}'\boldsymbol{\gamma}]}$	StdErr
	NOBLUP	Standard deviation of marginal linear predictor	$\sqrt{\text{Var}[\hat{\eta}_m]}$	StdErrPA
	ILINK	Standard deviation of mean	$\sqrt{\text{Var}[g^{-1}(\hat{\eta} - \mathbf{z}'\boldsymbol{\gamma})]}$	StdErr
	NOBLUP ILINK	Standard deviation of marginal mean	$\sqrt{\text{Var}[g^{-1}(\hat{\eta}_m)]}$	StdErrMuPA
RESIDUAL	Default	Residual	$r = p - \hat{\eta}$	Resid
	NOBLUP	Marginal residual	$r_m = p_m - \hat{\eta}_m$	ResidPA

Table 41.14 continued

Keyword	Options	Description	Expression	Name
	ILINK	Residual on mean scale	$r_y = y - g^{-1}(\hat{\eta})$	ResidMu
	NOBLUP ILINK	Marginal residual on mean scale	$r_{ym} = y - g^{-1}(\hat{\eta}_m)$	ResidMuPA
PEARSON	Default	Pearson-type residual	$r / \sqrt{\widehat{\text{Var}}[p \boldsymbol{y}]}$	Pearson
	NOBLUP	Marginal Pearson-type residual	$r_m / \sqrt{\widehat{\text{Var}}[p_m]}$	PearsonPA
	ILINK	Conditional Pearson-type mean residual	$r_y / \sqrt{\widehat{\text{Var}}[Y \boldsymbol{y}]}$	PearsonMu
STUDENT	Default	Studentized residual	$r / \sqrt{\widehat{\text{Var}}[r]}$	Student
	NOBLUP	Studentized marginal residual	$r_m / \sqrt{\widehat{\text{Var}}[r_m]}$	StudentPA
LCL	Default	Lower prediction limit for linear predictor		LCL
	NOBLUP	Lower confidence limit for marginal linear predictor		LCLPA
	ILINK	Lower prediction limit for mean		LCLMu
	NOBLUP ILINK	Lower confidence limit for marginal mean		LCLMuPA
UCL	Default	Upper prediction limit for linear predictor		UCL
	NOBLUP	Upper confidence limit for marginal linear predictor		UCLPA
	ILINK	Upper prediction limit for mean		UCLMu
	NOBLUP ILINK	Upper confidence limit for marginal mean		UCLMuPA
VARIANCE	Default	Conditional variance of pseudo-data	$\widehat{\text{Var}}[p \boldsymbol{y}]$	Variance
	NOBLUP	Marginal variance of pseudo-data	$\widehat{\text{Var}}[p_m]$	VariancePA
	ILINK	Conditional variance of response	$\widehat{\text{Var}}[Y \boldsymbol{y}]$	Variance_Dep
	NOBLUP ILINK	Marginal variance of response	$\widehat{\text{Var}}[Y]$	Variance_DepPA

Studentized residuals are computed only on the linear scale (scale of the link), unless the link is the identity, in which case the two scales are equal. The keywords RESIDUAL, PEARSON, STUDENT, and VARIANCE are not available with the multinomial distribution. You can use the following short-cuts to request statistics: PRED for PREDICTED, STD for STDERR, RESID for RESIDUAL, and VAR for VARIANCE. Output statistics that depend on the marginal variance $\text{Var}[Y_i]$ are not available with METHOD=LAPLACE or METHOD=QUAD.

Table 41.15 summarizes the options available in the OUTPUT statement.

Table 41.15 OUTPUT Statement Options

Option	Description
ALLSTATS	Computes all statistics
ALPHA= α	Determines the confidence level ($1 - \alpha$)
CPSEUDO	Changes the way in which marginal residuals are computed
DERIVATIVES	Adds derivatives of model quantities to the output data set
NOMISS	Outputs only observations used in the analysis
NOUNIQUE	Requests that names not be made unique
NOVAR	Requests that variables from the input data set not be added to the output data set
OBSCAT	Writes statistics to output data set only for the response level corresponding to the observed level of the observation
SYMBOLS	Adds computed variables to the output data set

You can specify the following options in the OUTPUT statement after a slash (/).

ALLSTATS

requests that all statistics are computed. If you do not use a keyword to assign a name, the GLIMMIX procedure uses the default name.

ALPHA=*number*

determines the coverage probability for two-sided confidence and prediction intervals. The coverage probability is computed as $1 - \textit{number}$. The value of *number* must be between 0 and 1; the default is 0.05.

CPSEUDO

changes the way in which marginal residuals are computed when model parameters are estimated by pseudo-likelihood methods. See the section “Notes on Output Statistics” on page 3111 for details.

DERIVATIVES

DER

adds derivatives of model quantities to the output data set. If, for example, the model fit requires the (conditional) log likelihood of the data, then the DERIVATIVES option writes for each observation the evaluations of the first and second derivatives of the log likelihood with respect to `_LNP_` and `_PHI_` to the output data set. The particular derivatives produced by the GLIMMIX procedure depend on the type of model and the estimation method.

NOMISS

requests that records be written to the output data only for those observations that were used in the analysis. By default, the GLIMMIX procedure produces output statistics for all observations in the input data set.

NOUNIQUE

requests that names not be made unique in the case of naming conflicts. By default, the GLIMMIX procedure avoids naming conflicts by assigning a unique name to each output variable. If you specify the NOUNIQUE option, variables with conflicting names are not renamed. In that case, the first variable added to the output data set takes precedence.

NOVAR

requests that variables from the input data set not be added to the output data set. This option does not apply to variables listed in the **BY** statement or to computed variables listed in the **ID** statement.

OBSCAT

requests that in models for multinomial data statistics be written to the output data set only for the response level that corresponds to the observed level of the observation.

SYMBOLS**SYM**

adds to the output data set computed variables that are defined or referenced in the program.

PARMS Statement

PARMS < (*value-list*) > ... < / *options* > ;

The PARMS statement specifies initial values for the covariance or scale parameters, or it requests a grid search over several values of these parameters in generalized linear mixed models.

The *value-list* specification can take any of several forms:

m	a single value
m_1, m_2, \dots, m_n	several values
m to n	a sequence where m equals the starting value, n equals the ending value, and the increment equals 1
m to n by i	a sequence where m equals the starting value, n equals the ending value, and the increment equals i
m_1, m_2 to m_3	mixed values and sequences

Using the PARMS Statement with a GLM

If you are fitting a GLM or a GLM with overdispersion, the scale parameters are listed at the end of the “Parameter Estimates” table in the same order as *value-list*. If you specify more than one set of initial values, PROC GLIMMIX uses only the first value listed for each parameter. Grid searches by using scale parameters are not possible for these models, because the fixed effects are part of the optimization.

Using the PARS Statement with a GLMM

If you are fitting a GLMM, the *value-list* corresponds to the parameters as listed in the “Covariance Parameter Estimates” table. Note that this order can change depending on whether a residual variance is profiled or not; see the `NOPROFILE` option in the `PROC GLIMMIX` statement.

If you specify more than one set of initial values, `PROC GLIMMIX` performs a grid search of the objective function surface and uses the best point on the grid for subsequent analysis. Specifying a large number of grid points can result in long computing times.

Options in the PARS Statement

You can specify the following options in the `PARMS` statement after a slash (/).

HOLD=*value-list*

specifies which parameter values `PROC GLIMMIX` should hold equal to the specified values. For example, the following statement constrains the first and third covariance parameters to equal 5 and 2, respectively:

```
parms (5) (3) (2) (3) / hold=1,3;
```

Covariance or scale parameters that are held fixed with the `HOLD=` option are treated as constrained parameters in the optimization. This is different from evaluating the objective function, gradient, and Hessian matrix at known values of the covariance parameters. A constrained parameter introduces a singularity in the optimization process. The covariance matrix of the covariance parameters (see the `ASYCOV` option of the `PROC GLIMMIX` statement) is then based on the projected Hessian matrix. As a consequence, the variance of parameters subjected to a `HOLD=` is zero. Such parameters do not contribute to the computation of denominator degrees of freedom with the `DDFM=KENWARDROGER` and `DDFM=SATTERTHWAITE` methods, for example. If you want to treat the covariance parameters as known, without imposing constraints on the optimization, you should use the `NOITER` option.

When you place a hold on all parameters (or when you specify the `NOITER`) option in a GLMM, you might notice that `PROC GLIMMIX` continues to produce an iteration history. Unless your model is a linear mixed model, several recomputations of the pseudo-response might be required in linearization-based methods to achieve agreement between the pseudo-data and the covariance matrix. In other words, the `GLIMMIX` procedure continues to update the fixed-effects estimates (and random-effects solutions) until convergence is achieved.

In certain models, placing a hold on covariance parameters implies that the procedure processes the parameters in the same order as if the `NOPROFILE` were in effect. This can change the order of the covariance parameters when you place a hold on one or more parameters. Models that are subject to this reordering are those with R-side covariance structures whose scale parameter could be profiled. This includes the `TYPE=CS`, `TYPE=SP`, `TYPE=AR(1)`, `TYPE=TOEP`, and `TYPE=ARMA(1,1)` covariance structures.

LOWERB=*value-list*

enables you to specify lower boundary constraints for the covariance or scale parameters. The *value-list* specification is a list of numbers or missing values (.) separated by commas. You must list the numbers in the same order that `PROC GLIMMIX` uses for the *value-list* in the `PARMS` statement, and each number corresponds to the lower boundary constraint. A missing value instructs `PROC`

GLIMMIX to use its default constraint, and if you do not specify numbers for all of the covariance parameters, PROC GLIMMIX assumes that the remaining ones are missing.

This option is useful, for example, when you want to constrain the **G** matrix to be positive definite in order to avoid the more computationally intensive algorithms required when **G** becomes singular. The corresponding statements for a random coefficients model are as follows:

```
proc glimmix;
  class person;
  model y = time;
  random int time / type=chol sub=person;
  parms / lowerb=1e-4, ., 1e-4;
run;
```

Here, the **TYPE=CHOL** structure is used in order to specify a Cholesky root parameterization for the 2×2 unstructured blocks in **G**. This parameterization ensures that the **G** matrix is nonnegative definite, and the **PARMS** statement then ensures that it is positive definite by constraining the two diagonal terms to be greater than or equal to $1E-4$.

NOBOUND

requests the removal of boundary constraints on covariance and scale parameters in mixed models. For example, variance components have a default lower boundary constraint of 0, and the **NOBOUND** option allows their estimates to be negative. See the **NOBOUND** option in the **PROC GLIMMIX** statement for further details.

NOITER

requests that no optimization of the covariance parameters be performed. This option has no effect in generalized linear models.

If you specify the **NOITER** option, PROC GLIMMIX uses the values for the covariance parameters given in the **PARMS** statement to perform statistical inferences. Note that the **NOITER** option is not equivalent to specifying a **HOLD=** value for all covariance parameters. If you use the **NOITER** option, covariance parameters are not constrained in the optimization. This prevents singularities that might otherwise occur in the optimization process.

If a residual variance is profiled, the parameter estimates can change from the initial values you provide as the residual variance is recomputed. To prevent an update of the residual variance, combine the **NOITER** option with the **NOPROFILE** option in the **PROC GLIMMIX** statements, as in the following code:

```
proc glimmix noprofile;
  class A B C rep mp sp;
  model y = A | B | C;
  random rep mp sp;
  parms (180) (200) (170) (1000) / noiter;
run;
```

When you specify the **NOITER** option in a model where parameters are estimated by pseudo-likelihood techniques, you might notice that the GLIMMIX procedure continues to produce an iteration history. Unless your model is a linear mixed model, several recomputations of the pseudo-response might be required in linearization-based methods to achieve agreement between the pseudo-

data and the covariance matrix. In other words, the GLIMMIX procedure continues to update the profiled fixed-effects estimates (and random-effects solutions) until convergence is achieved. To prevent these updates, use the `MAXLMMUPDATE=` option in the `PROC GLIMMIX` statement. Specifying the `NOITER` option in the `PARMS` statement of a GLMM with pseudo-likelihood estimation has the same effect as choosing `TECHNIQUE=NONE` in the `NLOPTIONS` statement.

If you want to base initial fixed-effects estimates on the results of fitting a generalized linear model, then you can combine the `NOITER` option with the `TECHNIQUE=` option. For example, the following statements determine the starting values for the fixed effects by fitting a logistic model (without random effects) with the Newton-Raphson algorithm:

```
proc glimmix startglm inititer=10;
  class clinic A;
  model y/n = A / link=logit dist=binomial;
  random clinic;
  parms (0.4) / noiter;
  nloptions technique=newrap;
run;
```

The initial GLM fit stops at convergence or after at most 10 iterations, whichever comes first. The pseudo-data for the linearized GLMM is computed from the GLM estimates. The variance of the Clinic random effect is held constant at 0.4 during subsequent iterations that update the fixed effects only.

If you also want to combine the GLM fixed-effects estimates with known and fixed covariance parameter values without updating the fixed effects, you can add the `MAXLMMUPDATE=0` option:

```
proc glimmix startglm inititer=10 maxlmmupdate=0;
  class clinic A;
  model y/n = A / link=logit dist=binomial;
  random clinic;
  parms (0.4) / noiter;
  nloptions technique=newrap;
run;
```

In a GLMM with parameter estimation by `METHOD=LAPLACE` or `METHOD=QUAD` the `NOITER` option also leads to an iteration history, since the fixed-effects estimates are part of the optimization and the `PARMS` statement places restrictions on only the covariance parameters.

Finally, the `NOITER` option can be useful if you want to obtain minimum variance quadratic unbiased estimates (with 0 priors), also known as MIVQUE0 estimates (Goodnight 1978a). Because MIVQUE0 estimates are starting values for covariance parameters—unless you provide (*value-list*) in the `PARMS` statement—the following statements produce MIVQUE0 mixed model estimates:

```
proc glimmix noprofile;
  class A B;
  model y = A;
  random int / subject=B;
  parms / noiter;
run;
```

PARMSDATA=SAS-data-set

PDATA=SAS-data-set

reads in covariance parameter values from a SAS data set. The data set should contain the numerical variable ESTIMATE or the numerical variables Covp1–Covp q , where q denotes the number of covariance parameters.

If the PARMSDATA= data set contains multiple sets of covariance parameters, the GLIMMIX procedure evaluates the initial objective function for each set and commences the optimization step by using the set with the lowest function value as the starting values. For example, the following SAS statements request that the objective function be evaluated for three sets of initial values:

```
data data_covp;
  input covp1-covp4;
  datalines;
  180 200 170 1000
  170 190 160 900
  160 180 150 800
;
proc glimmix;
  class A B C rep mainEU smallEU;
  model yield = A|B|C;
  random rep mainEU smallEU;
  parms / pdata=data_covp;
run;
```

Each set comprises four covariance parameters.

The order of the observations in a data set with the numerical variable Estimate corresponds to the order of the covariance parameters in the “Covariance Parameter Estimates” table. In a GLM, the PARMSDATA= option can be used to set the starting value for the exponential family scale parameter. A grid search is not conducted for GLMs if you specify multiple values.

The PARMSDATA= data set must not contain missing values.

If the GLIMMIX procedure is processing the input data set in BY groups, you can add the BY variables to the PARMSDATA= data set. If this data set is sorted by the BY variables, the GLIMMIX procedure matches the covariance parameter values to the current BY group. If the PARMSDATA= data set does not contain all BY variables, the data set is processed in its entirety for every BY group and a message is written to the log. This enables you to provide a single set of starting values across BY groups, as in the following statements:

```
data data_covp;
  input covp1-covp4;
  datalines;
  180 200 170 1000
;
```

```

proc glimmix;
  class A B C rep mainEU smallEU;
  model yield = A|B|C;
  random rep mainEU smallEU;
  parms / pdata=data_covp;
  by year;
run;

```

The same set of starting values is used for each value of the year variable.

UPPERB=*value-list*

enables you to specify upper boundary constraints on the covariance parameters. The *value-list* specification is a list of numbers or missing values (.) separated by commas. You must list the numbers in the same order that PROC GLIMMIX uses for the *value-list* in the PARMs statement, and each number corresponds to the upper boundary constraint. A missing value instructs PROC GLIMMIX to use its default constraint. If you do not specify numbers for all of the covariance parameters, PROC GLIMMIX assumes that the remaining ones are missing.

RANDOM Statement

RANDOM *random-effects* </ options > ;

Using notation from “Notation for the Generalized Linear Mixed Model” on page 2918, the RANDOM statement defines the **Z** matrix of the mixed model, the random effects in the $\boldsymbol{\gamma}$ vector, the structure of **G**, and the structure of **R**.

The **Z** matrix is constructed exactly like the **X** matrix for the fixed effects, and the **G** matrix is constructed to correspond to the effects constituting **Z**. The structures of **G** and **R** are defined by using the **TYPE=** option described on page 3028. The random effects can be classification or continuous effects, and multiple RANDOM statements are possible.

Some reserved keywords have special significance in the *random-effects* list. You can specify INTERCEPT (or INT) as a random effect to indicate the intercept. PROC GLIMMIX does not include the intercept in the RANDOM statement by default as it does in the MODEL statement. You can specify the **_RESIDUAL_** keyword (or RESID, RESIDUAL, **_RESID_**) before the option slash (/) to indicate a residual-type (R-side) random component that defines the **R** matrix. Basically, the **_RESIDUAL_** keyword takes the place of the *random-effect* if you want to specify R-side variances and covariance structures. These keywords take precedence over variables in the data set with the same name. If your data or the covariance structure requires that an effect is specified, you can use the **RESIDUAL** option to instruct the GLIMMIX procedure to model the R-side variances and covariances.

In order to add an overdispersion component to the variance function, simply specify a single residual random component. For example, the following statements fit a polynomial Poisson regression model with overdispersion. The variance function $a(\mu) = \mu$ is replaced by $\phi a(\mu)$:

```

proc glimmix;
  model count = x x*x / dist=poisson;
  random _residual_;
run;

```


Table 41.16 summarizes the options available in the RANDOM statement. All options are subsequently discussed in alphabetical order.

Table 41.16 RANDOM Statement Options

Option	Description
Construction of Covariance Structure	
GCOORD=	Determines coordinate association for G-side spatial structures with repeat levels
GROUP=	Varies covariance parameters by groups
LDATA=	Specifies a data set with coefficient matrices for TYPE= LIN
NOFULLZ	Eliminates columns in \mathbf{Z} corresponding to missing values
RESIDUAL	Designates a covariance structure as R-side
SUBJECT=	Identifies the subjects in the model
TYPE=	Specifies the covariance structure
Mixed Model Smoothing	
KNOTINFO	Displays spline knots
KNOTMAX=	Specifies the upper limit for knot construction
KNOTMETHOD	Specifies the method for constructing knots for radial smoother and penalized B-splines
KNOTMIN=	Specifies the lower limit for knot construction
Statistical Output	
ALPHA= α	Determines the confidence level ($1 - \alpha$)
CL	Requests confidence limits for predictors of random effects
G	Displays the estimated \mathbf{G} matrix
GC	Displays the Cholesky root (lower) of the estimated \mathbf{G} matrix
GCI	Displays the inverse Cholesky root (lower) of the estimated \mathbf{G} matrix
GCORR	Displays the correlation matrix that corresponds to the estimated \mathbf{G} matrix
GI	Displays the inverse of the estimated \mathbf{G} matrix
SOLUTION	Displays solutions $\hat{\boldsymbol{\gamma}}$ of the G-side random effects
V	Displays blocks of the estimated \mathbf{V} matrix
VC	Displays the lower-triangular Cholesky root of blocks of the estimated \mathbf{V} matrix
VCI	Displays the inverse Cholesky root of blocks of the estimated \mathbf{V} matrix
VCORR	Displays the correlation matrix corresponding to blocks of the estimated \mathbf{V} matrix
VI	Displays the inverse of the blocks of the estimated \mathbf{V} matrix

You can specify the following options in the RANDOM statement after a slash (/).

ALPHA=number

requests that a t -type confidence interval with confidence level $1 - \text{number}$ be constructed for the predictors of G-side random effects in this statement. The value of *number* must be between 0 and 1; the default is 0.05. Specifying the ALPHA= option implies the CL option.

CL

requests that t -type confidence limits be constructed for each of the predictors of G-side random effects in this statement. The confidence level is 0.95 by default; this can be changed with the **ALPHA=** option. The CL option implies the **SOLUTION** option.

G

requests that the estimated **G** matrix be displayed for G-side random effects associated with this RANDOM statement. PROC GLIMMIX displays blanks for values that are 0.

GC

displays the lower-triangular Cholesky root of the estimated **G** matrix for G-side random effects.

GCI

displays the inverse Cholesky root of the estimated **G** matrix for G-side random effects.

GCOORD=LAST**GCOORD=FIRST****GCOORD=MEAN**

determines how the GLIMMIX procedure associates coordinates for **TYPE=SP()** covariance structures with effect levels for G-side random effects. In these covariance structures, you specify one or more variables that identify the coordinates of a data point. The levels of classification variables, on the other hand, can occur multiple times for a particular subject. For example, in the following statements the same level of **A** can occur multiple times, and the associated values of **x** might be different:

```
proc glimmix;
  class A B;
  model y = B;
  random A / type=sp(pow) (x);
run;
```

The **GCOORD=LAST** option determines the coordinates for a level of the random effect from the last observation associated with the level. Similarly, the **GCOORD=FIRST** and **GCOORD=MEAN** options determine the coordinate from the first observation and from the average of the observations. Observations not used in the analysis are not considered in determining the first, last, or average coordinate. The default is **GCOORD=LAST**.

GCORR

displays the correlation matrix that corresponds to the estimated **G** matrix for G-side random effects.

GI

displays the inverse of the estimated **G** matrix for G-side random effects.

GROUP=effect**GRP=effect**

identifies groups by which to vary the covariance parameters. Each new level of the grouping effect produces a new set of covariance parameters. Continuous variables and computed variables are permitted as group effects. PROC GLIMMIX does not sort by the values of the continuous variable; rather, it considers the data to be from a new group whenever the value of the continuous variable changes from the previous observation. Using a continuous variable decreases execution time for

models with a large number of groups and also prevents the production of a large “Class Levels Information” table.

Specifying a GROUP effect can greatly increase the number of estimated covariance parameters, which can adversely affect the optimization process.

KNOTINFO

displays the number and coordinates of the knots as determined by the **KNOTMETHOD=** option.

KNOTMAX=number-list

provides upper limits for the values of random effects used in the construction of knots for **TYPE=RSMOOTH**. The items in *number-list* correspond to the random effects of the radial smooth. If the **KNOTMAX=** option is not specified, or if the value associated with a particular random effect is set to missing, the maximum is based on the values in the data set for **KNOTMETHOD=EQUAL** or **KNOTMETHOD=KDTREE**, and is based on the values in the knot data set for **KNOTMETHOD=DATA**.

KNOTMETHOD=KDTREE<(tree-options)>

KNOTMETHOD=EQUAL<(number-list)>

KNOTMETHOD=DATA(SAS-data-set)

determines the method of constructing knots for the radial smoother fit with the **TYPE=RSMOOTH** covariance structure and the **TYPE=PSPLINE** covariance structure.

Unless you select the **TYPE=RSMOOTH** or **TYPE=PSPLINE** covariance structure, the **KNOTMETHOD=** option has no effect. The default for **TYPE=RSMOOTH** is **KNOTMETHOD=KDTREE**. For **TYPE=PSPLINE**, only equally spaced knots are used and you can use the optional *numberlist* argument of **KNOTMETHOD=EQUAL** to determine the number of interior knots for **TYPE=PSPLINE**.

Knot Construction for TYPE=RSMOOTH

PROC GLIMMIX fits a low-rank smoother, meaning that the number of knots is considerably less than the number of observations. By default, PROC GLIMMIX determines the knot locations based on the vertices of a k -d tree (Friedman, Bentley, and Finkel 1977; Cleveland and Grosse 1991). The k -d tree is a tree data structure that is useful for efficiently determining the m nearest neighbors of a point. The k -d tree also can be used to obtain a grid of points that adapts to the configuration of the data. The process starts with a hypercube that encloses the values of the random effects. The space is then partitioned recursively by splitting cells at the median of the data in the cell for the random effect. The procedure is repeated for all cells that contain more than a specified number of points, b . The value b is called the bucket size.

The k -d tree is thus a division of the data into cells such that cells representing leaf nodes contain at most b values. You control the building of the k -d tree through the **BUCKET= tree-option**. You control the construction of knots from the cell coordinates of the tree with the other options as follows.

BUCKET=number

determines the bucket size b . A larger bucket size will result in fewer knots. For k -d trees in more than one dimension, the correspondence between bucket size and number of knots is difficult to determine. It depends on the data configuration and on other suboptions. In the multivariate case, you might need to try out different bucket sizes to obtain the desired number of knots.

The default value of *number* is 4 for univariate trees (a single random effect) and $\lfloor 0.1n \rfloor$ in the multidimensional case.

KNOTTYPE=type

specifies whether the knots are based on vertices of the tree cells or the centroid. The two possible values of *type* are VERTEX and CENTER. The default is KNOTTYPE=VERTEX. For multidimensional smoothing, such as smoothing across irregularly shaped spatial domains, the KNOTTYPE=CENTER option is useful to move knot locations away from the bounding hypercube toward the convex hull.

NEAREST

specifies that knot coordinates are the coordinates of the nearest neighbor of either the centroid or vertex of the cell, as determined by the KNOTTYPE= suboption.

TREEINFO

displays details about the construction of the *k*-d tree, such as the cell splits and the split values.

See the section “[Knot Selection](#)” on page 3085 for a detailed example of how the specification of the bucket size translates into the construction of a *k*-d tree and the spline knots.

The KNOTMETHOD=EQUAL option enables you to define a regular grid of knots. By default, PROC GLIMMIX constructs 10 knots for one-dimensional smooths and 5 knots in each dimension for smoothing in higher dimensions. You can specify a different number of knots with the optional *number-list*. Missing values in the *number-list* are replaced with the default values. A minimum of two knots in each dimension is required. For example, the following statements use a rectangular grid of 35 knots, five knots for *x1* combined with seven knots for *x2*:

```
proc glimmix;
  model y=;
  random x1 x2 / type=rsmooth knotmethod=equal(5 7);
run;
```

When you use the NOFIT option in the PROC GLIMMIX statement, the GLIMMIX procedure computes the knots but does not fit the model. This can be useful if you want to compare knot selections with different suboptions of KNOTMETHOD=KDTREE. Suppose you want to determine the number of knots based on a particular bucket size. The following statements compute and display the knots in a bivariate smooth, constructed from nearest neighbors of the vertices of a *k*-d tree with bucket size 10:

```
proc glimmix nofit;
  model y = Latitude Longitude;
  random Latitude Longitude / type=rsmooth
    knotmethod=kdtree(knottype=vertex
    nearest bucket=10) knotinfo;
run;
```

You can specify a data set that contains variables whose values give the knot coordinates with the KNOTMETHOD=DATA option. The data set must contain numeric variables with the same name as the radial smoothing *random-effects*. PROC GLIMMIX uses only the unique knot coordinates in the knot data set. This option is useful to provide knot coordinates different from those that can be produced from a *k*-d tree. For example, in spatial problems where the domain is irregularly shaped,

you might want to determine knots by a space-filling algorithm. The following SAS statements invoke the OPTEX procedure to compute 45 knots that uniformly cover the convex hull of the data locations (see *SAS/QC User's Guide* for details about the OPTEX procedure).

```
proc optex coding=none;
  model latitude longitude / noint;
  generate n=45 criterion=u method=m_fedorov;
  output out=knotdata;
run;
proc glimmix;
  model y = Latitude Longitude;
  random Latitude Longitude / type=rsmooth
        knotmethod=data (knotdata) ;
run;
```

Knot Construction for TYPE=PSPLINE

Only evenly spaced knots are supported when you fit penalized B-splines with the GLIMMIX procedure. For the **TYPE=PSPLINE** covariance structure, the *numberlist* argument specifies the number m of interior knots, the default is $m = 10$. Suppose that $x_{(1)}$ and $x_{(n)}$ denote the smallest and largest values, respectively. For a B-spline of degree d (de Boor 2001), the interior knots are supplemented with d exterior knots below $x_{(1)}$ and $\max\{1, d\}$ exterior knots above $x_{(n)}$. PROC GLIMMIX computes the location of these $m + d + \max\{1, d\}$ knots as follows. Let $\delta_x = (x_{(n)} - x_{(1)}) / (m + 1)$, then interior knots are placed at

$$x_{(1)} + j\delta_x, \quad j = 1, \dots, m$$

The exterior knots are also evenly spaced with step size δ_x and start at $x_{(1)} \pm 100$ times the machine epsilon. At least one interior knot is required.

KNOTMIN=*number-list*

provides lower limits for the values of random effects used in the construction of knots for **TYPE=RSMOOTH**. The items in *number-list* correspond to the random effects of the radial smooth. If the **KNOTMIN=** option is not specified, or if the value associated with a particular random effect is set to missing, the minimum is based on the values in the data set for **KNOTMETHOD=EQUAL** or **KNOTMETHOD=KDTREE**, and is based on the values in the knot data set for **KNOTMETHOD=DATA**.

LDATA=*SAS-data-set*

reads the coefficient matrices $\mathbf{A}_1, \dots, \mathbf{A}_q$ for the **TYPE=LIN(q)** option. You can specify the **LDATA=** data set in a sparse or dense form. In the sparse form the data set must contain the numeric variables Parm, Row, Col, and Value. The Parm variable contains the indices $i = 1, \dots, q$ of the \mathbf{A}_i matrices. The Row and Col variables identify the position within a matrix and the Value variable contains the matrix element. Values not specified for a particular row and column are set to zero. Missing values are allowed in the Value column of the **LDATA=** data set; these values are also replaced by zeros. The sparse form is particularly useful if the **A** matrices have only a few nonzero elements.

In the dense form the **LDATA=** data set contains the numeric variables Parm and Row (with the same function as above), in addition to the numeric variables Col1–Col q . If you omit one or more of the

Col1–Col q variables from the data set, zeros are assumed for the respective rows and columns of the \mathbf{A} matrix. Missing values for Col1–Col q are ignored in the dense form.

The GLIMMIX procedure assumes that the matrices $\mathbf{A}_1, \dots, \mathbf{A}_q$ are symmetric. In the sparse LDATA= form you do not need to specify off-diagonal elements in position (i, j) and (j, i) . One of them is sufficient. Row-column indices are converted in both storage forms into positions in lower triangular storage. If you specify multiple values in row ($\max\{i, j\}$ and column $\min\{i, j\}$) of a particular matrix, only the last value is used. For example, assume you are specifying elements of a 4×4 matrix. The lower triangular storage of matrix \mathbf{A}_3 defined by

```
data ldata;
  input parm row col value;
  datalines;
3  2  1  2
3  1  2  5
;
```

is

$$\begin{bmatrix} 0 & & & \\ 5 & 0 & & \\ 0 & 0 & 0 & \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

NOFULLZ

eliminates the columns in \mathbf{Z} corresponding to missing levels of random effects involving CLASS variables. By default, these columns are included in \mathbf{Z} . It is sufficient to specify the NOFULLZ option on any G-side RANDOM statement.

RESIDUAL

RSIDE

specifies that the random effects listed in this statement be R-side effects. You use the RESIDUAL option in the RANDOM statement if the nature of the covariance structure requires you to specify an effect. For example, if it is necessary to order the columns of the R-side AR(1) covariance structure by the time variable, you can use the RESIDUAL option as in the following statements:

```
class time id;
random time / subject=id type=ar(1) residual;
```

SOLUTION

S

requests that the solution $\hat{\boldsymbol{\gamma}}$ for the random-effects parameters be produced, if the statement defines G-side random effects.

The numbers displayed in the Std Err Pred column of the “Solution for Random Effects” table are not the standard errors of the $\hat{\boldsymbol{\gamma}}$ displayed in the Estimate column; rather, they are the square roots of the prediction errors $\hat{\boldsymbol{\gamma}}_i - \boldsymbol{\gamma}_i$, where $\hat{\boldsymbol{\gamma}}_i$ is the predictor of the i th random effect and $\boldsymbol{\gamma}_i$ is the i th random effect. In pseudo-likelihood methods that are based on linearization, these EBLUPs are the estimated best linear unbiased predictors in the linear mixed pseudo-model. In models fit by maximum likelihood by using the Laplace approximation or by using adaptive quadrature, the SOLUTION option displays the empirical Bayes estimates (EBE) of $\boldsymbol{\gamma}_i$.

SUBJECT=effect**SUB=effect**

identifies the subjects in your generalized linear mixed model. Complete independence is assumed across subjects. Specifying a subject effect is equivalent to nesting all other effects in the RANDOM statement within the subject effect.

Continuous variables and computed variables are permitted with the SUBJECT= option. PROC GLIMMIX does not sort by the values of the continuous variable but considers the data to be from a new subject whenever the value of the continuous variable changes from the previous observation. Using a continuous variable can decrease execution time for models with a large number of subjects and also prevents the production of a large “Class Levels Information” table.

TYPE=covariance-structure

specifies the covariance structure of **G** for G-side effects and the covariance structure of **R** for R-side effects.

Although a variety of structures are available, many applications call for either simple diagonal (TYPE=VC) or unstructured covariance matrices. The TYPE=VC (variance components) option is the default structure, and it models a different variance component for each random effect. It is recommended to model unstructured covariance matrices in terms of their Cholesky parameterization (TYPE=CHOL) rather than TYPE=UN.

If you want different covariance structures in different parts of **G**, you must use multiple RANDOM statements with different TYPE= options.

Valid values for *covariance-structure* are as follows. Examples are shown in Table 41.18.

The variances and covariances in the formulas that follow in the TYPE= descriptions are expressed in terms of generic random variables ξ_i and ξ_j . They represent the G-side random effects or the residual random variables for which the **G** or **R** matrices are constructed.

ANTE(1)

specifies a first-order ante-dependence structure (Kenward 1987; Patel 1991) parameterized in terms of variances and correlation parameters. If t ordered random variables ξ_1, \dots, ξ_t have a first-order ante-dependence structure, then each ξ_j , $j > 1$, is independent of all other ξ_k , $k < j$, given ξ_{j-1} . This Markovian structure is characterized by its inverse variance matrix, which is tridiagonal. Parameterizing an ANTE(1) structure for a random vector of size t requires $2t - 1$ parameters: variances $\sigma_1^2, \dots, \sigma_t^2$ and $t - 1$ correlation parameters $\rho_1, \dots, \rho_{t-1}$. The covariances among random variables ξ_i and ξ_j are then constructed as

$$\text{Cov} [\xi_i, \xi_j] = \sqrt{\sigma_i^2 \sigma_j^2} \prod_{k=i}^{j-1} \rho_k$$

PROC GLIMMIX constrains the correlation parameters to satisfy $|\rho_k| < 1$, $\forall k$. For variable-order ante-dependence models see Macchiavelli and Arnold (1994).

AR(1)

specifies a first-order autoregressive structure,

$$\text{Cov} [\xi_i, \xi_j] = \sigma^2 \rho^{|i^* - j^*|}$$

The values i^* and j^* are derived for the i th and j th observations, respectively, and are not necessarily the observation numbers. For example, in the following statements the values correspond to the class levels for the time effect of the i th and j th observation within a particular subject:

```

proc glimmix;
  class time patient;
  model y = x x*x;
  random time / sub=patient type=ar(1);
run;

```

PROC GLIMMIX imposes the constraint $|\rho| < 1$ for stationarity.

ARH(1)

specifies a heterogeneous first-order autoregressive structure,

$$\text{Cov}[\xi_i, \xi_j] = \sqrt{\sigma_i^2 \sigma_j^2} \rho^{|i^* - j^*|}$$

with $|\rho| < 1$. This covariance structure has the same correlation pattern as the TYPE=AR(1) structure, but the variances are allowed to differ.

ARMA(1,1)

specifies the first-order autoregressive moving-average structure,

$$\text{Cov}[\xi_i, \xi_j] = \begin{cases} \sigma^2 & i = j \\ \sigma^2 \gamma \rho^{|i^* - j^*| - 1} & i \neq j \end{cases}$$

Here, ρ is the autoregressive parameter, γ models a moving-average component, and σ^2 is a scale parameter. In the notation of Fuller (1976, p. 68), $\rho = \theta_1$ and

$$\gamma = \frac{(1 + b_1 \theta_1)(\theta_1 + b_1)}{1 + b_1^2 + 2b_1 \theta_1}$$

The example in Table 41.18 and $|b_1| < 1$ imply that

$$b_1 = \frac{\beta - \sqrt{\beta^2 - 4\alpha^2}}{2\alpha}$$

where $\alpha = \gamma - \rho$ and $\beta = 1 + \rho^2 - 2\gamma\rho$. PROC GLIMMIX imposes the constraints $|\rho| < 1$ and $|\gamma| < 1$ for stationarity, although for some values of ρ and γ in this region the resulting covariance matrix is not positive definite. When the estimated value of ρ becomes negative, the computed covariance is multiplied by $\cos(\pi d_{ij})$ to account for the negativity.

CHOL<(q)>

specifies an unstructured variance-covariance matrix parameterized through its Cholesky root. This parameterization ensures that the resulting variance-covariance matrix is at least positive semidefinite. If all diagonal values are nonzero, it is positive definite. For example, a 2×2 unstructured covariance matrix can be written as

$$\text{Var}[\boldsymbol{\xi}] = \begin{bmatrix} \theta_1 & \theta_{12} \\ \theta_{12} & \theta_2 \end{bmatrix}$$

Without imposing constraints on the three parameters, there is no guarantee that the estimated variance matrix is positive definite. Even if θ_1 and θ_2 are nonzero, a large value for θ_{12} can lead to a negative eigenvalue of $\text{Var}[\boldsymbol{\xi}]$. The Cholesky root of a positive definite matrix \mathbf{A} is a lower

triangular matrix \mathbf{C} such that $\mathbf{CC}' = \mathbf{A}$. The Cholesky root of the above 2×2 matrix can be written as

$$\mathbf{C} = \begin{bmatrix} \alpha_1 & 0 \\ \alpha_{12} & \alpha_2 \end{bmatrix}$$

The elements of the unstructured variance matrix are then simply $\theta_1 = \alpha_1^2$, $\theta_{12} = \alpha_1\alpha_{12}$, and $\theta_2 = \alpha_{12}^2 + \alpha_2^2$. Similar operations yield the generalization to covariance matrices of higher orders.

For example, the following statements model the covariance matrix of each subject as an unstructured matrix:

```
proc glimmix;
  class sub;
  model y = x;
  random _residual_ / subject=sub type=un;
run;
```

The next set of statements accomplishes the same, but the estimated \mathbf{R} matrix is guaranteed to be nonnegative definite:

```
proc glimmix;
  class sub;
  model y = x;
  random _residual_ / subject=sub type=chol;
run;
```

The GLIMMIX procedure constrains the diagonal elements of the Cholesky root to be positive. This guarantees a unique solution when the matrix is positive definite.

The optional order parameter $q > 0$ determines how many bands below the diagonal are modeled. Elements in the lower triangular portion of \mathbf{C} in bands higher than q are set to zero. If you consider the resulting covariance matrix $\mathbf{A} = \mathbf{CC}'$, then the order parameter has the effect of zeroing all off-diagonal elements that are at least q positions away from the diagonal.

Because of its good computational and statistical properties, the Cholesky root parameterization is generally recommended over a completely unstructured covariance matrix (TYPE=UN). However, it is computationally slightly more involved.

CS

specifies the compound-symmetry structure, which has constant variance and constant covariance

$$\text{Cov}[\xi_i, \xi_j] = \begin{cases} \phi + \sigma & i = j \\ \sigma & i \neq j \end{cases}$$

The compound symmetry structure arises naturally with nested random effects, such as when subsampling error is nested within experimental error. The models constructed with the following two sets of GLIMMIX statements have the same marginal variance matrix, provided σ is positive:

```

proc glimmix;
  class block A;
  model y = block A;
  random block*A / type=vc;
run;

proc glimmix;
  class block A;
  model y = block A;
  random _residual_ / subject=block*A
                    type=cs;
run;

```

In the first case, the `block*A` random effect models the G-side experimental error. Because the distribution defaults to the normal, the \mathbf{R} matrix is of form $\phi\mathbf{I}$ (see Table 41.19), and ϕ is the subsampling error variance. The marginal variance for the data from a particular experimental unit is thus $\sigma_{b*a}^2\mathbf{J} + \phi\mathbf{I}$. This matrix is of compound symmetric form.

Hierarchical random assignments or selections, such as subsampling or split-plot designs, give rise to compound symmetric covariance structures. This implies exchangeability of the observations on the subunit, leading to constant correlations between the observations. Compound symmetric structures are thus usually not appropriate for processes where correlations decline according to some metric, such as spatial and temporal processes.

Note that R-side compound-symmetry structures do not impose any constraint on σ . You can thus use an R-side `TYPE=CS` structure to emulate a variance-component model with unbounded estimate of the variance component.

CSH

specifies the heterogeneous compound-symmetry structure, which is an equi-correlation structure but allows for different variances

$$\text{Cov}[\xi_i, \xi_j] = \begin{cases} \sqrt{\sigma_i^2 \sigma_j^2} & i = j \\ \rho \sqrt{\sigma_i^2 \sigma_j^2} & i \neq j \end{cases}$$

FA(*q*)

specifies the factor-analytic structure with q factors (Jennrich and Schluchter 1986). This structure is of the form $\mathbf{\Lambda}\mathbf{\Lambda}' + \mathbf{D}$, where $\mathbf{\Lambda}$ is a $t \times q$ rectangular matrix and \mathbf{D} is a $t \times t$ diagonal matrix with t different parameters. When $q > 1$, the elements of $\mathbf{\Lambda}$ in its upper-right corner (that is, the elements in the i th row and j th column for $j > i$) are set to zero to fix the rotation of the structure.

FA0(*q*)

specifies a factor-analytic structure with q factors of the form $\text{Var}[\boldsymbol{\xi}] = \mathbf{\Lambda}\mathbf{\Lambda}'$, where $\mathbf{\Lambda}$ is a $t \times q$ rectangular matrix and t is the dimension of \mathbf{Y} . When $q > 1$, $\mathbf{\Lambda}$ is a lower triangular matrix. When $q < t$ —that is, when the number of factors is less than the dimension of the matrix—this structure is nonnegative definite but not of full rank. In this situation, you can use it to approximate an unstructured covariance matrix.

HF

specifies a covariance structure that satisfies the general Huynh-Feldt condition (Huynh and Feldt 1970). For a random vector with t elements, this structure has $t + 1$ positive parameters and covariances

$$\text{Cov}[\xi_i, \xi_j] = \begin{cases} \sigma_i^2 & i = j \\ 0.5(\sigma_i^2 + \sigma_j^2) - \lambda & i \neq j \end{cases}$$

A covariance matrix Σ generally satisfies the Huynh-Feldt condition if it can be written as $\Sigma = \tau \mathbf{1}' + \mathbf{1} \tau' + \lambda \mathbf{I}$. The preceding parameterization chooses $\tau_i = 0.5(\sigma_i^2 - \lambda)$. Several simpler covariance structures give rise to covariance matrices that also satisfy the Huynh-Feldt condition. For example, `TYPE=CS`, `TYPE=VC`, and `TYPE=UN(1)` are nested within `TYPE=HF`. You can use the `COVTEST` statement to test the HF structure against one of these simpler structures. Note also that the HF structure is nested within an unstructured covariance matrix.

The `TYPE=HF` covariance structure can be sensitive to the choice of starting values and the default `MIVQUE(0)` starting values can be poor for this structure; you can supply your own starting values with the `PARMS` statement.

LIN(q)

specifies a general linear covariance structure with q parameters. This structure consists of a linear combination of known matrices that you input with the `LDATA=` option. Suppose that you want to model the covariance of a random vector of length t , and further suppose that $\mathbf{A}_1, \dots, \mathbf{A}_q$ are symmetric ($t \times t$) matrices constructed from the information in the `LDATA=` data set. Then,

$$\text{Cov}[\xi_i, \xi_j] = \sum_{k=1}^q \theta_k [\mathbf{A}_k]_{ij}$$

where $[\mathbf{A}_k]_{ij}$ denotes the element in row i , column j of matrix \mathbf{A}_k .

Linear structures are very flexible and general. You need to exercise caution to ensure that the variance matrix is positive definite. Note that PROC GLIMMIX does not impose boundary constraints on the parameters $\theta_1, \dots, \theta_k$ of a general linear covariance structure. For example, if classification variable `A` has 6 levels, the following statements fit a variance component structure for the random effect without boundary constraints:

```
data ldata;
  retain parm 1 value 1;
  do row=1 to 6; col=row; output; end;
run;

proc glimmix data=MyData;
  class A B;
  model Y = B;
  random A / type=lin(1) ldata=ldata;
run;
```

PSPLINE<(options)>

requests that PROC GLIMMIX form a B-spline basis and fits a penalized B-spline (P-spline, Eilers and Marx 1996) with random spline coefficients. This covariance structure is available only for G-side random effects and only a single continuous random effect can be specified with TYPE=PSPLINE. As for TYPE=RSMOOTH, PROC GLIMMIX forms a modified \mathbf{Z} matrix and fits a mixed model in which the random variables associated with the columns of \mathbf{Z} are independent with a common variance. The \mathbf{Z} matrix is constructed as follows.

Denote as $\tilde{\mathbf{Z}}$ the $(n \times K)$ matrix of B-splines of degree d and denote as \mathbf{D}_r the $(K - r \times K)$ matrix of r th-order differences. For example, for $K = 5$,

$$\mathbf{D}_1 = \begin{bmatrix} 1 & -1 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 1 & -1 \end{bmatrix}$$

$$\mathbf{D}_2 = \begin{bmatrix} 1 & -2 & 1 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & -2 & 1 \end{bmatrix}$$

$$\mathbf{D}_3 = \begin{bmatrix} 1 & -3 & 3 & -1 & 0 \\ 0 & 1 & -3 & 3 & -1 \end{bmatrix}$$

Then, the \mathbf{Z} matrix used in fitting the mixed model is the $(n \times K - r)$ matrix

$$\mathbf{Z} = \tilde{\mathbf{Z}}(\mathbf{D}'_r \mathbf{D}_r)^{-1} \mathbf{D}'_r$$

The construction of the B-spline knots is controlled with the **KNOTMETHOD=** EQUAL(m) option and the **DEGREE=** d suboption of TYPE=PSPLINE. The total number of knots equals the number m of equally spaced interior knots plus d knots at the low end and $\max\{1, d\}$ knots at the high end. The number of columns in the B-spline basis equals $K = m + d + 1$. By default, the interior knots exclude the minimum and maximum of the random-effect values and are based on $m - 1$ equally spaced intervals. Suppose $x_{(1)}$ and $x_{(n)}$ are the smallest and largest random-effect values; then interior knots are placed at

$$x_{(1)} + j(x_{(n)} - x_{(1)})/(m + 1), \quad j = 1, \dots, m$$

In addition, d evenly spaced exterior knots are placed below $x_{(1)}$ and $\max\{d, 1\}$ exterior knots are placed above $x_{(n)}$. The exterior knots are evenly spaced and start at $x_{(1)} \pm 100$ times the machine epsilon. For example, based on the defaults $d = 3$, $r = 3$, the following statements lead to 26 total knots and 21 columns in \mathbf{Z} , $m = 20$, $K = m + d + 1 = 24$, $K - r = 21$:

```
proc glimmix;
  model y = x;
  random x / type=pspline knotmethod=equal(20);
run;
```

Details about the computation and properties of B-splines can be found in de Boor (2001).

You can extend or limit the range of the knots with the `KNOTMIN=` and `KNOTMAX=` options. Table 41.17 lists some of the parameters that control this covariance type and their relationships.

Table 41.17 P-Spline Parameters

Parameter	Description
d	Degree of B-spline, default $d = 3$
r	Order of differencing in construction of \mathbf{D}_r , default $r = 3$
m	Number of interior knots, default $m = 10$
$m + d + \max\{1, d\}$	Total number of knots
$K = m + d + 1$	Number of columns in B-spline basis
$K - r$	Number of columns in \mathbf{Z}

You can specify the following *options* for `TYPE=PSPLINE`:

`DEGREE= d` specifies the degree of the B-spline. The default is $d = 3$.

`DIFFORDER= r` specifies the order of the differencing matrix \mathbf{D}_r . The default and maximum is $r = 3$.

RSMOOTH<(m | **NOLOG**)>

specifies a radial smoother covariance structure for G-side random effects. This results in an approximate low-rank thin-plate spline where the smoothing parameter is obtained by the estimation method selected with the `METHOD=` option of the `PROC GLIMMIX` statement. The smoother is based on the automatic smoother in Ruppert, Wand, and Carroll (2003, Chapter 13.4–13.5), but with a different method of selecting the spline knots. See the section “Radial Smoothing Based on Mixed Models” on page 3084 for further details about the construction of the smoother and the knot selection.

Radial smoothing is possible in one or more dimensions. A univariate smoother is obtained with a single random effect, while multiple random effects in a `RANDOM` statement yield a multivariate smoother. Only continuous random effects are permitted with this covariance structure. If n_r denotes the number of continuous random effects in the `RANDOM` statement, then the covariance structure of the random effects $\boldsymbol{\gamma}$ is determined as follows. Suppose that \mathbf{z}_i denotes the vector of random effects for the i th observation. Let $\boldsymbol{\tau}_k$ denote the $(n_r \times 1)$ vector of knot coordinates, $k = 1, \dots, K$, and K is the total number of knots. The Euclidean distance between the knots is computed as

$$d_{kp} = \|\boldsymbol{\tau}_k - \boldsymbol{\tau}_p\| = \sqrt{\sum_{j=1}^{n_r} (\tau_{jk} - \tau_{jp})^2}$$

and the distance between knots and effects is computed as

$$h_{ik} = \|\mathbf{z}_i - \boldsymbol{\tau}_k\| = \sqrt{\sum_{j=1}^{n_r} (z_{ij} - \tau_{jk})^2}$$

The \mathbf{Z} matrix for the GLMM is constructed as

$$\mathbf{Z} = \tilde{\mathbf{Z}}\boldsymbol{\Omega}^{-1/2}$$

where the $(n \times K)$ matrix $\tilde{\mathbf{Z}}$ has typical element

$$[\tilde{\mathbf{Z}}]_{ik} = \begin{cases} h_{ik}^p & n_r \text{ odd} \\ h_{ik}^p \log\{h_{ik}\} & n_r \text{ even} \end{cases}$$

and the $(K \times K)$ matrix $\mathbf{\Omega}$ has typical element

$$[\mathbf{\Omega}]_{kp} = \begin{cases} d_{kp}^p & n_r \text{ odd} \\ d_{kp}^p \log\{d_{kp}\} & n_r \text{ even} \end{cases}$$

The exponent in these expressions equals $p = 2m - n_r$, where the optional value m corresponds to the derivative penalized in the thin-plate spline. A larger value of m will yield a smoother fit. The GLIMMIX procedure requires $p > 0$ and chooses by default $m = 2$ if $n_r < 3$ and $m = n_r/2 + 1$ otherwise. The NOLOG option removes the $\log\{h_{ik}\}$ and $\log\{d_{kp}\}$ terms from the computation of the $\tilde{\mathbf{Z}}$ and $\mathbf{\Omega}$ matrices when n_r is even; this yields invariance under rescaling of the coordinates.

Finally, the components of $\boldsymbol{\gamma}$ are assumed to have equal variance σ_r^2 . The “smoothing parameter” λ of the low-rank spline is related to the variance components in the model, $\lambda^2 = f(\phi, \sigma_r^2)$. See Ruppert, Wand, and Carroll (2003) for details. If the conditional distribution does not provide a scale parameter ϕ , you can add a single R-side residual parameter.

The knot selection is controlled with the **KNOTMETHOD=** option. The GLIMMIX procedure selects knots automatically based on the vertices of a k -d tree or reads knots from a data set that you supply. See the section “[Radial Smoothing Based on Mixed Models](#)” on page 3084 for further details on radial smoothing in the GLIMMIX procedure and its connection to a mixed model formulation.

SIMPLE

is an alias for TYPE=VC.

SP(EXP)(*c-list*)

models an exponential spatial or temporal covariance structure, where the covariance between two observations depends on a distance metric d_{ij} . The *c-list* contains the names of the numeric variables used as coordinates to determine distance. For a stochastic process in R^k , there are k elements in *c-list*. If the $(k \times 1)$ vectors of coordinates for observations i and j are \mathbf{c}_i and \mathbf{c}_j , then PROC GLIMMIX computes the Euclidean distance

$$d_{ij} = \|\mathbf{c}_i - \mathbf{c}_j\| = \sqrt{\sum_{m=1}^k (c_{mi} - c_{mj})^2}$$

The covariance between two observations is then

$$\text{Cov}[\xi_i, \xi_j] = \sigma^2 \exp\{-d_{ij}/\alpha\}$$

The parameter α is *not* what is commonly referred to as the range parameter in geostatistical applications. The practical range of a (second-order stationary) spatial process is the distance $d^{(p)}$ at which the correlations fall below 0.05. For the SP(EXP) structure, this distance is $d^{(p)} = 3\alpha$. PROC GLIMMIX constrains α to be positive.

SP(GAU)(*c-list*)

models a Gaussian covariance structure,

$$\text{Cov} [\xi_i, \xi_j] = \sigma^2 \exp\{-d_{ij}^2/\alpha^2\}$$

See TYPE=SP(EXP) for the computation of the distance d_{ij} . The parameter α is related to the range of the process as follows. If the practical range $d^{(p)}$ is defined as the distance at which the correlations fall below 0.05, then $d^{(p)} = \sqrt{3}\alpha$. PROC GLIMMIX constrains α to be positive. See TYPE=SP(EXP) for the computation of the distance d_{ij} from the variables specified in *c-list*.

SP(MAT)(*c-list*)

models a covariance structure in the Matérn class of covariance functions (Matérn 1986). The covariance is expressed in the parameterization of Handcock and Stein (1993); Handcock and Wallis (1994); it can be written as

$$\text{Cov} [\xi_i, \xi_j] = \sigma^2 \frac{1}{\Gamma(\nu)} \left(\frac{d_{ij} \sqrt{\nu}}{\rho} \right)^\nu 2K_\nu \left(\frac{2d_{ij} \sqrt{\nu}}{\rho} \right)$$

The function K_ν is the modified Bessel function of the second kind of (real) order $\nu > 0$. The smoothness (continuity) of a stochastic process with covariance function in the Matérn class increases with ν . This class thus enables data-driven estimation of the smoothness properties of the process. The covariance is identical to the exponential model for $\nu = 0.5$ (TYPE=SP(EXP)(*c-list*)), while for $\nu = 1$ the model advocated by Whittle (1954) results. As $\nu \rightarrow \infty$, the model approaches the Gaussian covariance structure (TYPE=SP(GAU)(*c-list*)).

Note that the MIXED procedure offers covariance structures in the Matérn class in two parameterizations, TYPE=SP(MATERN) and TYPE=SP(MATHSW). The TYPE=SP(MAT) in the GLIMMIX procedure is equivalent to TYPE=SP(MATHSW) in the MIXED procedure.

Computation of the function K_ν and its derivatives is numerically demanding; fitting models with Matérn covariance structures can be time-consuming. Good starting values are essential.

SP(POW)(*c-list*)

models a power covariance structure,

$$\text{Cov} [\xi_i, \xi_j] = \sigma^2 \rho^{d_{ij}}$$

where $\rho \geq 0$. This is a reparameterization of the exponential structure, TYPE=SP(EXP). Specifically, $\log\{\rho\} = -1/\alpha$. See TYPE=SP(EXP) for the computation of the distance d_{ij} from the variables specified in *c-list*. When the estimated value of ρ becomes negative, the computed covariance is multiplied by $\cos(\pi d_{ij})$ to account for the negativity.

SP(POWA)(*c-list*)

models an anisotropic power covariance structure in k dimensions, provided that the coordinate list *c-list* has k elements. If c_{im} denotes the coordinate for the i th observation of the m th variable in *c-list*, the covariance between two observations is given by

$$\text{Cov} [\xi_i, \xi_j] = \sigma^2 \rho_1^{|c_{i1}-c_{j1}|} \rho_2^{|c_{i2}-c_{j2}|} \dots \rho_k^{|c_{ik}-c_{jk}|}$$

Note that for $k = 1$, TYPE=SP(POWA) is equivalent to TYPE=SP(POW), which is itself a reparameterization of TYPE=SP(EXP). When the estimated value of ρ_m becomes negative, the computed covariance is multiplied by $\cos(\pi |c_{im} - c_{jm}|)$ to account for the negativity.

SP(SPH)(*c-list*)

models a spherical covariance structure,

$$\text{Cov} [\xi_i, \xi_j] = \begin{cases} \sigma^2 \left\{ 1 - \frac{3d_{ij}}{2\alpha} + \frac{1}{2} \left(\frac{d_{ij}}{\alpha} \right)^3 \right\} & d_{ij} \leq \alpha \\ 0 & d_{ij} > \alpha \end{cases}$$

The spherical covariance structure has a true range parameter. The covariances between observations are exactly zero when their distance exceeds α . See TYPE=SP(EXP) for the computation of the distance d_{ij} from the variables specified in *c-list*.

TOEP

models a Toeplitz covariance structure. This structure can be viewed as an autoregressive structure with order equal to the dimension of the matrix,

$$\text{Cov} [\xi_i, \xi_j] = \begin{cases} \sigma^2 & i = j \\ \sigma_{|i-j|} & i \neq j \end{cases}$$

TOEP(*q*)

specifies a banded Toeplitz structure,

$$\text{Cov} [\xi_i, \xi_j] = \begin{cases} \sigma^2 & i = j \\ \sigma_{|i-j|} & |i - j| < q \end{cases}$$

This can be viewed as a moving-average structure with order equal to $q - 1$. The specification TYPE=TOEP(1) is the same as $\sigma^2 \mathbf{I}$, and it can be useful for specifying the same variance component for several effects.

TOEPH<(q)>

models a Toeplitz covariance structure. The correlations of this structure are banded as the TOEP or TOEP(*q*) structures, but the variances are allowed to vary:

$$\text{Cov} [\xi_i, \xi_j] = \begin{cases} \sigma_i^2 & i = j \\ \rho_{|i-j|} \sqrt{\sigma_i^2 \sigma_j^2} & i \neq j \end{cases}$$

The correlation parameters satisfy $|\rho_{|i-j|}| < 1$. If you specify the optional value q , the correlation parameters with $|i - j| \geq q$ are set to zero, creating a banded correlation structure. The specification TYPE=TOEPH(1) results in a diagonal covariance matrix with heterogeneous variances.

UN<(q)>

specifies a completely general (unstructured) covariance matrix parameterized directly in terms of variances and covariances,

$$\text{Cov} [\xi_i, \xi_j] = \sigma_{ij}$$

The variances are constrained to be nonnegative, and the covariances are unconstrained. This structure is not constrained to be nonnegative definite in order to avoid nonlinear constraints; however, you can use the TYPE=CHOL structure if you want this constraint to be imposed by a Cholesky factorization. If you specify the order parameter q , then PROC GLIMMIX estimates only the first q bands of the matrix, setting elements in all higher bands equal to 0.

UNR<(q)>

specifies a completely general (unstructured) covariance matrix parameterized in terms of variances and correlations,

$$\text{Cov} [\xi_i, \xi_j] = \sigma_i \sigma_j \rho_{ij}$$

where σ_i denotes the standard deviation and the correlation ρ_{ij} is zero when $i = j$ and when $|i - j| \geq q$, provided the order parameter q is given. This structure fits the same model as the TYPE=UN(q) option, but with a different parameterization. The i th variance parameter is σ_i^2 . The parameter ρ_{ij} is the correlation between the i th and j th measurements; it satisfies $|\rho_{ij}| < 1$. If you specify the order parameter q , then PROC GLIMMIX estimates only the first q bands of the matrix, setting all higher bands equal to zero.

VC

specifies standard variance components and is the default structure for both G-side and R-side covariance structures. In a G-side covariance structure, a distinct variance component is assigned to each effect. In an R-side structure TYPE=VC is usually used only to add overdispersion effects or with the GROUP= option to specify a heterogeneous variance model.

Table 41.18 Covariance Structure Examples

Description	Structure	Example
Variance Components	VC (default)	$\begin{bmatrix} \sigma_B^2 & 0 & 0 & 0 \\ 0 & \sigma_B^2 & 0 & 0 \\ 0 & 0 & \sigma_{AB}^2 & 0 \\ 0 & 0 & 0 & \sigma_{AB}^2 \end{bmatrix}$
Compound Symmetry	CS	$\begin{bmatrix} \sigma + \phi & \sigma & \sigma & \sigma \\ \sigma & \sigma + \phi & \sigma & \sigma \\ \sigma & \sigma & \sigma + \phi & \sigma \\ \sigma & \sigma & \sigma & \sigma + \phi \end{bmatrix}$
Heterogeneous CS	CSH	$\begin{bmatrix} \sigma_1^2 & \sigma_1 \sigma_2 \rho & \sigma_1 \sigma_3 \rho & \sigma_1 \sigma_4 \rho \\ \sigma_2 \sigma_1 \rho & \sigma_2^2 & \sigma_2 \sigma_3 \rho & \sigma_2 \sigma_4 \rho \\ \sigma_3 \sigma_1 \rho & \sigma_3 \sigma_2 \rho & \sigma_3^2 & \sigma_3 \sigma_4 \rho \\ \sigma_4 \sigma_1 \rho & \sigma_4 \sigma_2 \rho & \sigma_4 \sigma_3 \rho & \sigma_4^2 \end{bmatrix}$
First-Order Autoregressive	AR(1)	$\sigma^2 \begin{bmatrix} 1 & \rho & \rho^2 & \rho^3 \\ \rho & 1 & \rho & \rho^2 \\ \rho^2 & \rho & 1 & \rho \\ \rho^3 & \rho^2 & \rho & 1 \end{bmatrix}$
Heterogeneous AR(1)	ARH(1)	$\begin{bmatrix} \sigma_1^2 & \sigma_1 \sigma_2 \rho & \sigma_1 \sigma_3 \rho^2 & \sigma_1 \sigma_4 \rho^3 \\ \sigma_2 \sigma_1 \rho & \sigma_2^2 & \sigma_2 \sigma_3 \rho & \sigma_2 \sigma_4 \rho^2 \\ \sigma_3 \sigma_1 \rho^2 & \sigma_3 \sigma_2 \rho & \sigma_3^2 & \sigma_3 \sigma_4 \rho \\ \sigma_4 \sigma_1 \rho^3 & \sigma_4 \sigma_2 \rho & \sigma_4 \sigma_3 \rho & \sigma_4^2 \end{bmatrix}$
Unstructured	UN	$\begin{bmatrix} \sigma_1^2 & \sigma_{21} & \sigma_{31} & \sigma_{41} \\ \sigma_{21} & \sigma_2^2 & \sigma_{32} & \sigma_{42} \\ \sigma_{31} & \sigma_{32} & \sigma_3^2 & \sigma_{43} \\ \sigma_{41} & \sigma_{42} & \sigma_{43} & \sigma_4^2 \end{bmatrix}$

Table 41.18 continued

Description	Structure	Example
Banded Main Diagonal	UN(1)	$\begin{bmatrix} \sigma_1^2 & 0 & 0 & 0 \\ 0 & \sigma_2^2 & 0 & 0 \\ 0 & 0 & \sigma_3^2 & 0 \\ 0 & 0 & 0 & \sigma_4^2 \end{bmatrix}$
Unstructured Correlations	UNR	$\begin{bmatrix} \sigma_1^2 & \sigma_1\sigma_2\rho_{21} & \sigma_1\sigma_3\rho_{31} & \sigma_1\sigma_4\rho_{41} \\ \sigma_2\sigma_1\rho_{21} & \sigma_2^2 & \sigma_2\sigma_3\rho_{32} & \sigma_2\sigma_4\rho_{42} \\ \sigma_3\sigma_1\rho_{31} & \sigma_3\sigma_2\rho_{32} & \sigma_3^2 & \sigma_3\sigma_4\rho_{43} \\ \sigma_4\sigma_1\rho_{41} & \sigma_4\sigma_2\rho_{42} & \sigma_4\sigma_3\rho_{43} & \sigma_4^2 \end{bmatrix}$
Toeplitz	TOEP	$\begin{bmatrix} \sigma^2 & \sigma_1 & \sigma_2 & \sigma_3 \\ \sigma_1 & \sigma^2 & \sigma_1 & \sigma_2 \\ \sigma_2 & \sigma_1 & \sigma^2 & \sigma_1 \\ \sigma_3 & \sigma_2 & \sigma_1 & \sigma^2 \end{bmatrix}$
Toeplitz with Two Bands	TOEP(2)	$\begin{bmatrix} \sigma^2 & \sigma_1 & 0 & 0 \\ \sigma_1 & \sigma^2 & \sigma_1 & 0 \\ 0 & \sigma_1 & \sigma^2 & \sigma_1 \\ 0 & 0 & \sigma_1 & \sigma^2 \end{bmatrix}$
Heterogeneous Toeplitz	TOEPH	$\begin{bmatrix} \sigma_1^2 & \sigma_1\sigma_2\rho_1 & \sigma_1\sigma_3\rho_2 & \sigma_1\sigma_4\rho_3 \\ \sigma_2\sigma_1\rho_1 & \sigma_2^2 & \sigma_2\sigma_3\rho_1 & \sigma_2\sigma_4\rho_2 \\ \sigma_3\sigma_1\rho_2 & \sigma_3\sigma_2\rho_1 & \sigma_3^2 & \sigma_3\sigma_4\rho_1 \\ \sigma_4\sigma_1\rho_3 & \sigma_4\sigma_2\rho_2 & \sigma_4\sigma_3\rho_1 & \sigma_4^2 \end{bmatrix}$
Spatial Power	SP(POW)(c-list)	$\sigma^2 \begin{bmatrix} 1 & \rho^{d_{12}} & \rho^{d_{13}} & \rho^{d_{14}} \\ \rho^{d_{21}} & 1 & \rho^{d_{23}} & \rho^{d_{24}} \\ \rho^{d_{31}} & \rho^{d_{32}} & 1 & \rho^{d_{34}} \\ \rho^{d_{41}} & \rho^{d_{42}} & \rho^{d_{43}} & 1 \end{bmatrix}$
First-Order Autoregressive Moving-Average	ARMA(1,1)	$\sigma^2 \begin{bmatrix} 1 & \gamma & \gamma\rho & \gamma\rho^2 \\ \gamma & 1 & \gamma & \gamma\rho \\ \gamma\rho & \gamma & 1 & \gamma \\ \gamma\rho^2 & \gamma\rho & \gamma & 1 \end{bmatrix}$
First-Order Factor Analytic	FA(1)	$\begin{bmatrix} \lambda_1^2 + d_1 & \lambda_1\lambda_2 & \lambda_1\lambda_3 & \lambda_1\lambda_4 \\ \lambda_2\lambda_1 & \lambda_2^2 + d_2 & \lambda_2\lambda_3 & \lambda_2\lambda_4 \\ \lambda_3\lambda_1 & \lambda_3\lambda_2 & \lambda_3^2 + d_3 & \lambda_3\lambda_4 \\ \lambda_4\lambda_1 & \lambda_4\lambda_2 & \lambda_4\lambda_3 & \lambda_4^2 + d_4 \end{bmatrix}$
Huynh-Feldt	HF	$\begin{bmatrix} \sigma_1^2 & \frac{\sigma_1^2 + \sigma_2^2}{2} - \lambda & \frac{\sigma_1^2 + \sigma_3^2}{2} - \lambda \\ \frac{\sigma_2^2 + \sigma_1^2}{2} - \lambda & \sigma_2^2 & \frac{\sigma_2^2 + \sigma_3^2}{2} - \lambda \\ \frac{\sigma_3^2 + \sigma_1^2}{2} - \lambda & \frac{\sigma_3^2 + \sigma_2^2}{2} - \lambda & \sigma_3^2 \end{bmatrix}$
First-Order Ante-dependence	ANTE(1)	$\begin{bmatrix} \sigma_1^2 & \sigma_1\sigma_2\rho_1 & \sigma_1\sigma_3\rho_1\rho_2 \\ \sigma_2\sigma_1\rho_1 & \sigma_2^2 & \sigma_2\sigma_3\rho_2 \\ \sigma_3\sigma_1\rho_2\rho_1 & \sigma_3\sigma_2\rho_2 & \sigma_3^2 \end{bmatrix}$

V<=*value-list*>

requests that blocks of the estimated marginal variance-covariance matrix $V(\hat{\theta})$ be displayed in generalized linear mixed models. This matrix is based on the last linearization as described in the section “The Pseudo-model” on page 3054. You can use the *value-list* to select the subjects for which the matrix is displayed. If *value-list* is not specified, the **V** matrix for the first subject is chosen.

Note that the *value-list* refers to subjects as the processing units in the “Dimensions” table. For example, the following statements request that the estimated marginal variance matrix for the second subject be displayed:

```
proc glimmix;
  class A B;
  model y = B;
  random int / subject=A;
  random int / subject=A*B v=2;
run;
```

The subject effect for processing in this case is the **A** effect, because it is contained in the **A*B** interaction. If there is only a single subject as per the “Dimensions” table, then the **V** option displays an ($n \times n$) matrix.

See the section “Processing by Subjects” on page 3082 for how the GLIMMIX procedure determines the number of subjects in the “Dimensions” table.

The GLIMMIX procedure displays blanks for values that are 0.

VC<=*value-list*>

displays the lower-triangular Cholesky root of the blocks of the estimated $V(\hat{\theta})$ matrix. See the **V** option for the specification of *value-list*.

VCI<=*value-list*>

displays the inverse Cholesky root of the blocks of the estimated $V(\hat{\theta})$ matrix. See the **V** option for the specification of *value-list*.

VCORR<=*value-list*>

displays the correlation matrix corresponding to the blocks of the estimated $V(\hat{\theta})$ matrix. See the **V** option for the specification of *value-list*.

VI<=*value-list*>

displays the inverse of the blocks of the estimated $V(\hat{\theta})$ matrix. See the **V** option for the specification of *value-list*.

SLICE Statement

SLICE *model-effect* < / options > ;

The SLICE statement provides a general mechanism for performing a partitioned analysis of the LS-means for an interaction. This analysis is also known as an analysis of simple effects (Winer 1971).

The SLICE statement uses most of the options of the LSMEANS statement that are summarized in Table 41.8. The options SLICEDIFF=, SLICEDIFFTYPE=, and ODDS do not apply to the SLICE statement; in the SLICE statement, the relevant options for SLICEDIFF= and SLICEDIFFTYPE= are the SLICEBY= and the DIFF= options, respectively.

For details about the syntax of the SLICE statement, see the section “SLICE Statement” on page 498 of Chapter 19, “Shared Concepts and Topics.”

STORE Statement

STORE < OUT= > *item-store-name* < / LABEL= 'label' > ;

The STORE statement requests that the procedure save the context and results of the statistical analysis. The resulting item store has a binary file format that cannot be modified. The contents of the item store can be processed with the PLM procedure.

For details about the syntax of the STORE statement, see the section “STORE Statement” on page 501 in Chapter 19, “Shared Concepts and Topics.”

WEIGHT Statement

WEIGHT *variable* ;

The WEIGHT statement replaces \mathbf{R} with $\mathbf{W}^{-1/2}\mathbf{R}\mathbf{W}^{-1/2}$, where \mathbf{W} is a diagonal matrix containing the weights. Observations with nonpositive or missing weights are not included in the resulting PROC GLIMMIX analysis. If a WEIGHT statement is not included, all observations used in the analysis are assigned a weight of 1.

Programming Statements

This section lists the programming statements available in PROC GLIMMIX to compute various aspects of the generalized linear mixed model or output quantities. For example, you can compute model effects, weights, frequency, subject, group, and other variables. You can use programming statements to define the mean and variance functions. This section also documents the differences between programming statements in PROC GLIMMIX and programming statements in the SAS DATA step. The syntax of programming statements used in PROC GLIMMIX is identical to that used in the NLMIXED procedure (see Chapter 64, “The NLMIXED Procedure,” and the MODEL procedure (see the *SAS/ETS User’s Guide*). Most of the programming statements that can be used in the DATA step can also be used in the GLIMMIX procedure. See *SAS Statements: Reference* for a description of SAS programming statements. The following are valid statements:

```

ABORT;
ARRAY arrayname < [ dimensions ] > < $ > < variables-and-constants >;
CALL name < (expression < , expression ... >) >;
DELETE;
DO < variable = expression < TO expression > < BY expression > >
    < , expression < TO expression > < BY expression > > ...
    < WHILE expression > < UNTIL expression >;
END;
GOTO statement-label;
IF expression;
IF expression THEN program-statement;
    ELSE program-statement;
variable = expression;
variable + expression;
LINK statement-label;
PUT < variable > < = > ...;
RETURN;
SELECT < (expression) >;
STOP;
SUBSTR(variable, index, length)= expression;
WHEN (expression)program-statement;
    OTHERWISE program-statement;

```

For the most part, the SAS programming statements work the same as they do in the SAS DATA step, as documented in *SAS Language Reference: Concepts*. However, there are several differences:

- The ABORT statement does not allow any arguments.
- The DO statement does not allow a character index variable. Thus

```
do i = 1,2,3;
```

is supported; however, the following statement is not supported:

```
do i = 'A', 'B', 'C';
```

- The LAG function is not supported with PROC GLIMMIX.
- The PUT statement, used mostly for program debugging in PROC GLIMMIX, supports only some of the features of the DATA step PUT statement, and it has some features not available with the DATA step PUT statement:
 - The PROC GLIMMIX PUT statement does not support line pointers, factored lists, iteration factors, overprinting, `_INFILE_`, the colon (:) format modifier, or “\$”.
 - The PROC GLIMMIX PUT statement does support expressions, but the expression must be enclosed in parentheses. For example, the following statement displays the square root of `x`:

```
put (sqrt(x));
```

- The PROC GLIMMIX PUT statement supports the item `_PDV_` to display a formatted listing of all variables in the program. For example:
- ```
put _pdv_;
```
- The WHEN and OTHERWISE statements enable you to specify more than one target statement. That is, DO/END groups are not necessary for multiple statement WHENs. For example, the following syntax is valid:

```
select;
 when (exp1) stmt1;
 stmt2;
 when (exp2) stmt3;
 stmt4;
end;
```

The LINK statement is used in a program to jump immediately to the label `statement_label` and to continue program execution at that point. It is not used to specify a user-defined link function.

When coding your programming statements, you should avoid defining variables that begin with an underscore (`_`), because they might conflict with internal variables created by PROC GLIMMIX.

## User-Defined Link or Variance Function

### Implied Variance Functions

While link functions are not unique for each distribution (see [Table 41.12](#) for the default link functions), the distribution does determine the variance function  $a(\mu)$ . This function expresses the variance of an observation as a function of the mean, apart from weights, frequencies, and additional scale parameters. The implied variance functions  $a(\mu)$  of the GLIMMIX procedure are shown in [Table 41.19](#) for the supported distributions. For the binomial distribution,  $n$  denotes the number of trials in the `events/trials` syntax. For the negative binomial distribution,  $k$  denotes the scale parameter. The multiplicative scale parameter  $\phi$  is not included for the other distributions. The last column of the table indicates whether  $\phi$  has a value equal to 1.0 for the particular distribution.

**Table 41.19** Variance Functions in PROC GLIMMIX

| DIST=                     | Distribution      | Variance function         |                 |
|---------------------------|-------------------|---------------------------|-----------------|
|                           |                   | $a(\mu)$                  | $\phi \equiv 1$ |
| BETA                      | beta              | $\mu(1 - \mu)/(1 + \phi)$ | No              |
| BINARY                    | binary            | $\mu(1 - \mu)$            | Yes             |
| BINOMIAL   BIN   B        | binomial          | $\mu(1 - \mu)/n$          | Yes             |
| EXPONENTIAL   EXPO        | exponential       | $\mu^2$                   | Yes             |
| GAMMA   GAM               | gamma             | $\mu^2$                   | No              |
| GAUSSIAN   G   NORMAL   N | normal            | 1                         | No              |
| GEOMETRIC   GEOM          | geometric         | $\mu + \mu^2$             | Yes             |
| INVGAUSS   IGAUSSIAN   IG | inverse Gaussian  | $\mu^3$                   | No              |
| LOGNORMAL   LOGN          | lognormal         | 1                         | No              |
| NEGBINOMIAL   NEGBIN   NB | negative binomial | $\mu + k\mu^2$            | Yes             |
| POISSON   POI   P         | Poisson           | $\mu$                     | Yes             |
| TCENTRAL   TDIST   T      | $t$               | $v/(v - 2)$               | No              |

To change the variance function, you can use SAS programming statements and the predefined automatic variables, as outlined in the following section. Your definition of a variance function will override the **DIST=** option and its implied variance function. This has the following implication for parameter estimation with the GLIMMIX procedure. When a user-defined link is available, the distribution of the data is determined from the **DIST=** option, or the respective default for the type of response. In a GLM, for example, this enables maximum likelihood estimation. If a user-defined variance function is provided, the **DIST=** option is not honored and the distribution of the data is assumed unknown. In a GLM framework, only quasi-likelihood estimation is then available to estimate the model parameters.

### Automatic Variables

To specify your own link or variance function you can use SAS programming statements and draw on the following automatic variables:

**\_LINP\_** is the current value of the linear predictor. It equals either  $\hat{\eta} = \mathbf{x}'\hat{\boldsymbol{\beta}} + \mathbf{z}'\hat{\boldsymbol{\gamma}} + o$  or  $\hat{\eta} = \mathbf{x}'\hat{\boldsymbol{\beta}} + o$ , where  $o$  is the value of the offset variable, or 0 if no offset is specified. The estimated random effects solutions  $\hat{\boldsymbol{\gamma}}$  are used in the calculation of the linear predictor during the model fitting phase, if a linearization expands about the current values of  $\boldsymbol{\gamma}$ . During the computation of output statistics, the EBLUPs are used if statistics depend on them. For example, the following statements add the variable **p** to the output data set **glimmixout**:

```
proc glimmix;
 model y = x / dist=binary;
 random int / subject=b;
 p = 1/(1+exp(-_linp_));
 output out=glimmixout;
 id p;
run;
```

Because no output statistics are requested in the **OUTPUT** statement that depend on the random-effects solutions (BLUPs, EBEs), the value of `_LINP_` in this example equals  $x'\hat{\beta}$ . On the contrary, the following statements also request conditional residuals on the logistic scale:

```
proc glimmix;
 model y = x / dist=binary;
 random int / subject=b;
 p = 1/(1+exp(-_linp_));
 output out=glimmixout resid(blup)=r;
 id p;
run;
```

The value of `_LINP_` when computing the variable `p` is  $x'\hat{\beta} + z'\hat{\gamma}$ . To ensure that computed statistics are formed from  $x'\hat{\beta}$  and  $z'\hat{\gamma}$  terms as needed, it is recommended that you use the automatic variables `_XBETA_` and `_ZGAMMA_` instead of `_LINP_`.

|                         |                                                                                                                |
|-------------------------|----------------------------------------------------------------------------------------------------------------|
| <code>_MU_</code>       | expresses the mean of an observation as a function of the linear predictor, $\hat{\mu} = g^{-1}(\hat{\eta})$ . |
| <code>_N_</code>        | is the observation number in the sequence of the data read.                                                    |
| <code>_VARIANCE_</code> | is the estimate of the variance function, $a(\hat{\mu})$ .                                                     |
| <code>_XBETA_</code>    | equals $x'\hat{\beta}$ .                                                                                       |
| <code>_ZGAMMA_</code>   | equals $z'\hat{\gamma}$ .                                                                                      |

The automatic variable `_N_` is incremented whenever the procedure reads an observation from the data set. Observations that are not used in the analysis—for example, because of missing values or invalid weights—are counted. The counter is reset to 1 at the start of every new BY group. Only in some circumstances will `_N_` equal the actual observation number. The symbol should thus be used sparingly to avoid unexpected results.

You must observe the following syntax rules when you use the automatic variables. The `_LINP_` symbol cannot appear on the left side of programming statements; you cannot make an assignment to the `_LINP_` variable. The value of the linear predictor is controlled by the **CLASS**, **MODEL**, and **RANDOM** statements as well as the current parameter estimates and solutions. You can, however, use the `_LINP_` variable on the right side of other operations. Suppose, for example, that you want to transform the linear predictor prior to applying the inverse log link. The following statements are not valid because the linear predictor appears in an assignment:

```
proc glimmix;
 linp = sqrt(abs(_linp_));
 mu = exp(_linp_);
 model count = logtstd / dist=poisson;
run;
```

The next statements achieve the desired result:

```
proc glimmix;
 mu = exp(sqrt(abs(_linp_)));
 model count = logtstd / dist=poisson;
run;
```



If the value of the linear predictor is altered in any way through programming statements, you need to ensure that an assignment to `_MU_` follows. The assignment to variable `P` in the next set of GLIMMIX statements is without effect:

```
proc glimmix;
 p = _linp_ + rannor(454);
 model count = logtstd / dist=poisson;
run;
```

A user-defined link function is implied by expressing `_MU_` as a function of `_LNP_`. That is, if  $\mu = g^{-1}(\eta)$ , you are providing an expression for the inverse link function with programming statements. It is neither necessary nor possible to give an expression for the inverse operation,  $\eta = g(\mu)$ . The variance function is determined by expressing `_VARIANCE_` as a function of `_MU_`. If the `_MU_` variable appears in an assignment statement inside PROC GLIMMIX, the `LINK=` option of the `MODEL` statement is ignored. If the `_VARIANCE_` function appears in an assignment statement, the `DIST=` option is ignored. Furthermore, the associated variance function per Table 41.19 is not honored. In short, user-defined expressions take precedence over built-in defaults.

If you specify your own link and variance function, the assignment to `_MU_` must precede an assignment to the variable `_VARIANCE_`.

The following two sets of GLIMMIX statements yield the same parameter estimates, but the models differ statistically:

```
proc glimmix;
 class block entry;
 model y/n = block entry / dist=binomial link=logit;
run;

proc glimmix;
 class block entry;
 prob = 1 / (1+exp(- _linp_));
 mu = n * prob ;
 variance = n * prob *(1-prob);
 model y = block entry;
run;
```

The first GLIMMIX invocation models the proportion  $y/n$  as a binomial proportion with a logit link. The `DIST=` and `LINK=` options are superfluous in this case, because the GLIMMIX procedure defaults to the binomial distribution in light of the *events/trials* syntax. The logit link is that distribution's default link. The second set of GLIMMIX statements models the count variable  $y$  and takes the binomial sample size into account through assignments to the mean and variance function. In contrast to the first set of GLIMMIX statements, the distribution of  $y$  is unknown. Only its mean and variance are known. The model parameters are estimated by maximum likelihood in the first case and by quasi-likelihood in the second case.

---

## Details: GLIMMIX Procedure

---

### Generalized Linear Models Theory

A generalized linear model consists of the following:

- a linear predictor  $\eta = \mathbf{x}'\boldsymbol{\beta}$
- a monotonic mapping between the mean of the data and the linear predictor
- a response distribution in the exponential family of distributions

A density or mass function in this family can be written as

$$f(y) = \exp \left\{ \frac{y\theta - b(\theta)}{\phi} + c(y, f(\phi)) \right\}$$

for some functions  $b(\cdot)$  and  $c(\cdot)$ . The parameter  $\theta$  is called the natural (canonical) parameter. The parameter  $\phi$  is a scale parameter, and it is not present in all exponential family distributions. See [Table 41.19](#) for a list of distributions for which  $\phi \equiv 1$ . In the case where observations are weighted, the scale parameter is replaced with  $\phi/w$  in the preceding density (or mass function), where  $w$  is the weight associated with the observation  $y$ .

The mean and variance of the data are related to the components of the density,  $E[Y] = \mu = b'(\theta)$ ,  $\text{Var}[Y] = \phi b''(\theta)$ , where primes denote first and second derivatives. If you express  $\theta$  as a function of  $\mu$ , the relationship is known as the natural link or the canonical link function. In other words, modeling data with a canonical link assumes that  $\theta = \mathbf{x}'\boldsymbol{\beta}$ ; the effect contributions are additive on the canonical scale. The second derivative of  $b(\cdot)$ , expressed as a function of  $\mu$ , is the variance function of the generalized linear model,  $a(\mu) = b''(\theta(\mu))$ . Note that because of this relationship, the distribution determines the variance function and the canonical link function. You cannot, however, proceed in the opposite direction. If you provide a user-specified variance function, the GLIMMIX procedure assumes that only the first two moments of the response distribution are known. The full distribution of the data is then unknown and maximum likelihood estimation is not possible. Instead, the GLIMMIX procedure then estimates parameters by quasi-likelihood.

### Maximum Likelihood

The GLIMMIX procedure forms the log likelihoods of generalized linear models as

$$L(\boldsymbol{\mu}, \phi; \mathbf{y}) = \sum_{i=1}^n f_i l(\mu_i, \phi; y_i, w_i)$$

where  $l(\mu_i, \phi; y_i, w_i)$  is the log likelihood contribution of the  $i$ th observation with weight  $w_i$  and  $f_i$  is the value of the frequency variable. For the determination of  $w_i$  and  $f_i$ , see the [WEIGHT](#) and [FREQ](#) statements. The individual log likelihood contributions for the various distributions are as follows.

**Beta**

$$l(\mu_i, \phi; y_i, w_i) = \log \left\{ \frac{\Gamma(\phi/w_i)}{\Gamma(\mu\phi/w_i)\Gamma((1-\mu)\phi/w_i)} \right\} \\ + (\mu\phi/w_i - 1) \log\{y_i\} \\ + ((1-\mu)\phi/w_i - 1) \log\{1 - y_i\}$$

$\text{Var}[Y] = \mu(1-\mu)/(1+\phi)$ ,  $\phi > 0$ . See Ferrari and Cribari-Neto (2004).

**Binary**

$$l(\mu_i, \phi; y_i, w_i) = w_i(y_i \log\{\mu_i\} + (1 - y_i) \log\{1 - \mu_i\})$$

$\text{Var}[Y] = \mu(1 - \mu)$ ,  $\phi \equiv 1$ .

**Binomial**

$$l(\mu_i, \phi; y_i, w_i) = w_i(y_i \log\{\mu_i\} + (n_i - y_i) \log\{1 - \mu_i\}) \\ + w_i(\log\{\Gamma(n_i + 1)\} - \log\{\Gamma(y_i + 1)\} - \log\{\Gamma(n_i - y_i + 1)\})$$

where  $y_i$  and  $n_i$  are the *events* and *trials* in the *events/trials* syntax, and  $0 < \mu < 1$ .  
 $\text{Var}[Y/n] = \mu(1 - \mu)/n$ ,  $\phi \equiv 1$ .

**Exponential**

$$l(\mu_i, \phi; y_i, w_i) = \begin{cases} -\log\{\mu_i\} - y_i/\mu_i & w_i = 1 \\ w_i \log\left\{\frac{w_i y_i}{\mu_i}\right\} - \frac{w_i y_i}{\mu_i} - \log\{y_i \Gamma(w_i)\} & w_i \neq 1 \end{cases}$$

$\text{Var}[Y] = \mu^2$ ,  $\phi \equiv 1$ .

**Gamma**

$$l(\mu_i, \phi; y_i, w_i) = w_i \phi \log \left\{ \frac{w_i y_i \phi}{\mu_i} \right\} - \frac{w_i y_i \phi}{\mu_i} - \log\{y_i\} - \log\{\Gamma(w_i \phi)\}$$

$\text{Var}[Y] = \phi \mu^2$ ,  $\phi > 0$ .

**Geometric**

$$l(\mu_i, \phi; y_i, w_i) = y_i \log \left\{ \frac{\mu_i}{w_i} \right\} - (y_i + w_i) \log \left\{ 1 + \frac{\mu_i}{w_i} \right\} \\ + \log \left\{ \frac{\Gamma(y_i + w_i)}{\Gamma(w_i)\Gamma(y_i + 1)} \right\}$$

$\text{Var}[Y] = \mu + \mu^2$ ,  $\phi \equiv 1$ .

**Inverse Gaussian**

$$l(\mu_i, \phi; y_i, w_i) = -\frac{1}{2} \left[ \frac{w_i(y_i - \mu_i)^2}{y_i \phi \mu_i^2} + \log \left\{ \frac{\phi y_i^3}{w_i} \right\} + \log\{2\pi\} \right]$$

$\text{Var}[Y] = \phi \mu^3$ ,  $\phi > 0$ .

**“Lognormal”**

$$l(\mu_i, \phi; \log\{y_i\}, w_i) = -\frac{1}{2} \left[ \frac{w_i (\log\{y_i\} - \mu_i)^2}{\phi} + \log \left\{ \frac{\phi}{w_i} \right\} + \log\{2\pi\} \right]$$

$$\text{Var}[\log\{Y\}] = \phi, \phi > 0.$$

If you specify `DIST=LOGNORMAL` with response variable `Y`, the `GLIMMIX` procedure assumes that  $\log\{Y\} \sim N(\mu, \sigma^2)$ . Note that the preceding density is not the density of `Y`.

**Multinomial**

$$l(\mu_i, \phi; \mathbf{y}_i, w_i) = w_i \sum_{j=1}^J y_{ij} \log\{\mu_{ij}\}$$

$$\phi \equiv 1.$$

**Negative Binomial**

$$l(\mu_i, \phi; y_i, w_i) = y_i \log \left\{ \frac{k\mu_i}{w_i} \right\} - (y_i + w_i/k) \log \left\{ 1 + \frac{k\mu_i}{w_i} \right\} \\ + \log \left\{ \frac{\Gamma(y_i + w_i/k)}{\Gamma(w_i/k)\Gamma(y_i + 1)} \right\}$$

$$\text{Var}[Y] = \mu + k\mu^2, k > 0, \phi \equiv 1.$$

For a given  $k$ , the negative binomial distribution is a member of the exponential family. The parameter  $k$  is related to the scale of the data, because it is part of the variance function. However, it cannot be factored from the variance, as is the case with the  $\phi$  parameter in many other distributions. The parameter  $k$  is designated as “Scale” in the “Parameter Estimates” table of the `GLIMMIX` procedure.

**Normal (Gaussian)**

$$l(\mu_i, \phi; y_i, w_i) = -\frac{1}{2} \left[ \frac{w_i (y_i - \mu_i)^2}{\phi} + \log \left\{ \frac{\phi}{w_i} \right\} + \log\{2\pi\} \right]$$

$$\text{Var}[Y] = \phi, \phi > 0.$$

**Poisson**

$$l(\mu_i, \phi; y_i, w_i) = w_i (y_i \log\{\mu_i\} - \mu_i - \log\{\Gamma(y_i + 1)\})$$

$$\text{Var}[Y] = \mu, \phi \equiv 1.$$

**Shifted T**

$$z_i = -0.5 \log\{\phi/\sqrt{w_i}\} + \log\{\Gamma(0.5(v + 1))\} \\ - \log\{\Gamma(0.5v)\} - 0.5 \times \log\{\pi v\}$$

$$l(\mu_i, \phi; y_i, w_i) = -(v/2 + 0.5) \log \left\{ 1 + \frac{w_i (y_i - \mu_i)^2}{\phi} \right\} + z_i$$

$$\phi > 0, v > 0, \text{Var}[Y] = \phi v / (v - 2).$$

Define the parameter vector for the generalized linear model as  $\boldsymbol{\theta} = \boldsymbol{\beta}$ , if  $\phi \equiv 1$ , and as  $\boldsymbol{\theta} = [\boldsymbol{\beta}', \phi]'$  otherwise.  $\boldsymbol{\beta}$  denotes the fixed-effects parameters in the linear predictor. For the negative binomial distribution, the relevant parameter vector is  $\boldsymbol{\theta} = [\boldsymbol{\beta}', k]'$ . The gradient and Hessian of the negative log likelihood are then

$$\mathbf{g} = -\frac{\partial L(\boldsymbol{\theta}; \mathbf{y})}{\partial \boldsymbol{\theta}} \quad \mathbf{H} = -\frac{\partial^2 L(\boldsymbol{\theta}; \mathbf{y})}{\partial \boldsymbol{\theta} \partial \boldsymbol{\theta}'}$$

The GLIMMIX procedure computes the gradient vector and Hessian matrix analytically, unless your programming statements involve functions whose derivatives are determined by finite differences. If the procedure is in scoring mode,  $\mathbf{H}$  is replaced by its expected value. PROC GLIMMIX is in scoring mode when the number  $n$  of SCORING= $n$  iterations has not been exceeded and the optimization technique uses second derivatives, or when the Hessian is computed at convergence and the EXPHESSIAN option is in effect. Note that the objective function is the negative log likelihood when the GLIMMIX procedure fits a GLM model. The procedure performs a minimization problem in this case.

In models for independent data with known distribution, parameter estimates are obtained by the method of maximum likelihood. No parameters are profiled from the optimization. The default optimization technique for GLMs is the Newton-Raphson algorithm, except for Gaussian models with identity link, which do not require iterative model fitting. In the case of a Gaussian model, the scale parameter is estimated by restricted maximum likelihood, because this estimate is unbiased. The results from the GLIMMIX procedure agree with those from the GLM and REG procedure for such models. You can obtain the maximum likelihood estimate of the scale parameter with the NOREML option in the PROC GLIMMIX statement. To change the optimization algorithm, use the TECHNIQUE= option in the NLOPTIONS statement.

Standard errors of the parameter estimates are obtained from the inverse of the (observed or expected) second derivative matrix  $\mathbf{H}$ .

## Scale and Dispersion Parameters

The parameter  $\phi$  in the log-likelihood functions is a scale parameter. McCullagh and Nelder (1989, p. 29) refer to it as the dispersion parameter. With the exception of the normal distribution,  $\phi$  does not correspond to the variance of an observation, the variance of an observation in a generalized linear model is a function of  $\phi$  and  $\mu$ . In a generalized linear model (GLM mode), the GLIMMIX procedure displays the estimate of  $\phi$  as “Scale” in the “Parameter Estimates” table. Note that for some distributions this scale is different from that reported by the GENMOD procedure in its “Parameter Estimates” table. The scale reported by PROC GENMOD is sometimes a transformation of the dispersion parameter in the log-likelihood function. Table 41.19 displays the relationship between the “Scale” entries reported by the two procedures in terms of the  $\phi$  (or  $k$ ) parameter in the GLIMMIX log-likelihood functions.

**Table 41.19** Scales in Parameter Estimates Table

| Distribution      | GLIMMIX Reports                        | GENMOD Reports      |
|-------------------|----------------------------------------|---------------------|
| Beta              | $\hat{\phi}$                           | N/A                 |
| Gamma             | $\hat{\phi}$                           | $\hat{\phi}$        |
| Inverse Gaussian  | $\hat{\phi}$                           | $\sqrt{\hat{\phi}}$ |
| Negative binomial | $\hat{k}$                              | $\hat{k}$           |
| Normal            | $\hat{\phi} = \widehat{\text{Var}}[Y]$ | $\sqrt{\hat{\phi}}$ |

Note that for normal linear models, PROC GLIMMIX by default estimates the parameters by restricted maximum likelihood, whereas PROC GENMOD estimates the parameters by maximum likelihood. As a consequence, the scale parameter in the “Parameter Estimates” table of the GLIMMIX procedure coincides for these models with the mean-squared error estimate of the GLM or REG procedures. To obtain maximum likelihood estimates in a normal linear model in the GLIMMIX procedure, specify the NOREML option in the PROC GLIMMIX statement.

### Quasi-likelihood for Independent Data

Quasi-likelihood estimation uses only the first and second moment of the response. In the case of independent data, this requires only a specification of the mean and variance of your data. The GLIMMIX procedure estimates parameters by quasi-likelihood, if the following conditions are met:

- The response distribution is unknown, because of a user-specified variance function.
- There are no G-side random effects.
- There are no R-side covariance structures or at most an overdispersion parameter.

Under some mild regularity conditions, the function

$$Q(\mu_i, y_i) = \int_{y_i}^{\mu_i} \frac{y_i - t}{\phi a(t)} dt$$

known as the log quasi-likelihood of the  $i$ th observation, has some properties of a log-likelihood function (McCullagh and Nelder 1989, p. 325). For example, the expected value of its derivative is zero, and the variance of its derivative equals the negative of the expected value of the second derivative. Consequently,

$$QL(\boldsymbol{\mu}, \phi, \mathbf{y}) = \sum_{i=1}^n f_i w_i \frac{Y_i - \mu_i}{\phi a(\mu_i)}$$

can serve as the score function for estimation. Quasi-likelihood estimation takes as the gradient and “Hessian” matrix—with respect to the fixed-effects parameters  $\boldsymbol{\beta}$ —the quantities

$$\mathbf{g}_{ql} = [g_{ql,j}] = \left[ \frac{\partial QL(\boldsymbol{\mu}, \phi, \mathbf{y})}{\partial \beta_j} \right] = \mathbf{D}'\mathbf{V}^{-1}(\mathbf{Y} - \boldsymbol{\mu})/\phi$$

$$\mathbf{H}_{ql} = [h_{ql,jk}] = \left[ \frac{\partial^2 QL(\boldsymbol{\mu}, \phi, \mathbf{y})}{\partial \beta_j \partial \beta_k} \right] = \mathbf{D}'\mathbf{V}^{-1}\mathbf{D}/\phi$$

In this expression,  $\mathbf{D}$  is a matrix of derivatives of  $\boldsymbol{\mu}$  with respect to the elements in  $\boldsymbol{\beta}$ , and  $\mathbf{V}$  is a diagonal matrix containing variance functions,  $\mathbf{V} = [a(\mu_1), \dots, a(\mu_n)]$ . Notice that  $\mathbf{H}_{ql}$  is not the second derivative matrix of  $Q(\boldsymbol{\mu}, \mathbf{y})$ . Rather, it is the negative of the expected value of  $\partial \mathbf{g}_{ql} / \partial \boldsymbol{\beta}$ .  $\mathbf{H}_{ql}$  thus has the form of a “scoring Hessian.”

The GLIMMIX procedure fixes the scale parameter  $\phi$  at 1.0 by default. To estimate the parameter, add the statement

```
random _residual_;
```

The resulting estimator (McCullagh and Nelder 1989, p. 328) is

$$\hat{\phi} = \frac{1}{m} \sum_{i=1}^n f_i w_i \frac{(y_i - \hat{\mu}_i)^2}{a(\hat{\mu}_i)}$$

where  $m = f - \text{rank}\{\mathbf{X}\}$  if the **NOREML** option is in effect,  $m = f$  otherwise, and  $f$  is the sum of the frequencies.

See [Example 41.4](#) for an application of quasi-likelihood estimation with PROC GLIMMIX.

## Effects of Adding Overdispersion

You can add a multiplicative overdispersion parameter to a generalized linear model in the GLIMMIX procedure with the statement

```
random _residual_;
```

For models in which  $\phi \equiv 1$ , this effectively lifts the constraint of the parameter. In models that already contain a  $\phi$  or  $k$  scale parameter—such as the normal, gamma, or negative binomial model—the statement adds a multiplicative scalar (the overdispersion parameter,  $\phi_o$ ) to the variance function.

The overdispersion parameter is estimated from Pearson's statistic after all other parameters have been determined by (restricted) maximum likelihood or quasi-likelihood. This estimate is

$$\hat{\phi}_o = \frac{1}{\phi^p m} \sum_{i=1}^n f_i w_i \frac{(y_i - \mu_i)^2}{a(\mu_i)}$$

where  $m = f - \text{rank}\{\mathbf{X}\}$  if the **NOREML** option is in effect, and  $m = f$  otherwise, and  $f$  is the sum of the frequencies. The power  $p$  is  $-1$  for the gamma distribution and  $1$  otherwise.

Adding an overdispersion parameter does not alter any of the other parameter estimates. It only changes the variance-covariance matrix of the estimates by a certain factor. If overdispersion arises from correlations among the observations, then you should investigate more complex random-effects structures.

## Generalized Linear Mixed Models Theory

### Model or Integral Approximation

In a generalized linear model, the log likelihood is well defined, and an objective function for estimation of the parameters is simple to construct based on the independence of the data. In a GLMM, several problems must be overcome before an objective function can be computed.

- The model might be vacuous in the sense that no valid joint distribution can be constructed either in general or for a particular set of parameter values. For example, if  $\mathbf{Y}$  is an equicorrelated ( $n \times 1$ ) vector of binary responses with the same success probability and a symmetric distribution, then the lower bound on the correlation parameter depends on  $n$  and  $\pi$  (Gilliland and Schabenberger 2001). If further restrictions are placed on the joint distribution, as in Bahadur (1961), the correlation is also restricted from above.

- The dependency between mean and variance for nonnormal data places constraints on the possible correlation models that simultaneously yield valid joint distributions and a desired conditional distributions. Thus, for example, aspiring for conditional Poisson variates that are marginally correlated according to a spherical spatial process might not be possible.
- Even if the joint distribution is feasible mathematically, it still can be out of reach computationally. When data are independent, conditional on the random effects, the marginal log likelihood can in principle be constructed by integrating out the random effects from the joint distribution. However, numerical integration is practical only when the number of random effects is small and when the data have a clustered (subject) structure.

Because of these special features of generalized linear mixed models, many estimation methods have been put forth in the literature. The two basic approaches are (1) to approximate the objective function and (2) to approximate the model. Algorithms in the second category can be expressed in terms of Taylor series (linearizations) and are hence also known as linearization methods. They employ expansions to approximate the model by one based on pseudo-data with fewer nonlinear components. The process of computing the linear approximation must be repeated several times until some criterion indicates lack of further progress. Schabenberger and Gregoire (1996) list numerous algorithms based on Taylor series for the case of clustered data alone. The fitting methods based on linearizations are usually doubly iterative. The generalized linear mixed model is approximated by a linear mixed model based on current values of the covariance parameter estimates. The resulting linear mixed model is then fit, which is itself an iterative process. On convergence, the new parameter estimates are used to update the linearization, which results in a new linear mixed model. The process stops when parameter estimates between successive linear mixed model fits change only within a specified tolerance.

Integral approximation methods approximate the log likelihood of the GLMM and submit the approximated function to numerical optimization. Various techniques are used to compute the approximation: Laplace methods, quadrature methods, Monte Carlo integration, and Markov chain Monte Carlo methods. The advantage of integral approximation methods is to provide an actual objective function for optimization. This enables you to perform likelihood ratio tests among nested models and to compute likelihood-based fit statistics. The estimation process is singly iterative. The disadvantage of integral approximation methods is the difficulty of accommodating crossed random effects and multiple subject effects, and the inability to accommodate R-side covariance structures, even only R-side overdispersion. The number of random effects should be small for integral approximation methods to be practically feasible.

The advantages of linearization-based methods include a relatively simple form of the linearized model that typically can be fit based on only the mean and variance in the linearized form. Models for which the joint distribution is difficult—or impossible—to ascertain can be fit with linearization-based approaches. Models with correlated errors, a large number of random effects, crossed random effects, and multiple types of subjects are thus excellent candidates for linearization methods. The disadvantages of this approach include the absence of a true objective function for the overall optimization process and potentially biased estimates, especially for binary data when the number of observations per subject is small (see the section “[Notes on Bias of Estimators](#)” on page 3066 for further comments and considerations about the bias of estimates in generalized linear mixed models). Because the objective function to be optimized after each linearization update depends on the current pseudo-data, objective functions are not comparable across linearizations. The estimation process can fail at both levels of the double iteration scheme.

By default the GLIMMIX procedure fits generalized linear mixed models based on linearizations. The default estimation method in GLIMMIX for models containing random effects is a technique known as



restricted pseudo-likelihood (RPL) (Wolfinger and O’Connell 1993) estimation with an expansion around the current estimate of the best linear unbiased predictors of the random effects (**METHOD=RSPL**).

Two maximum likelihood estimation methods based on integral approximation are available in the GLIMMIX procedure. If you choose **METHOD=LAPLACE** in a GLMM, the GLIMMIX procedure performs maximum likelihood estimation based on a Laplace approximation of the marginal log likelihood. See the section “[Maximum Likelihood Estimation Based on Laplace Approximation](#)” on page 3059 for details about the Laplace approximation with PROC GLIMMIX. If you choose **METHOD=QUAD** in the PROC GLIMMIX statement in a generalized linear mixed model, the GLIMMIX procedure estimates the model parameters by adaptive Gauss-Hermite quadrature. See the section “[Maximum Likelihood Estimation Based on Adaptive Quadrature](#)” on page 3062 for details about the adaptive Gauss-Hermite quadrature approximation with PROC GLIMMIX.

The following subsections discuss the three estimation methods in turn. Keep in mind that your modeling possibilities are increasingly restricted in the order of these subsections. For example, in the class of generalized linear mixed models, the pseudo-likelihood estimation methods place no restrictions on the covariance structure, and Laplace estimation adds restriction with respect to the R-side covariance structure. Adaptive quadrature estimation further requires a clustered data structure—that is, the data must be processed by subjects.

**Table 41.20** Model Restrictions Depending on Estimation Method

| Method     | Restriction                                                                      |
|------------|----------------------------------------------------------------------------------|
| RSPL, RMPL | None                                                                             |
| MSPL, MMPL | None                                                                             |
| LAPLACE    | No R-side effects                                                                |
| QUAD       | No R-side effects<br>Requires SUBJECT= effect<br>Requires processing by subjects |

## Pseudo-likelihood Estimation Based on Linearization

### The Pseudo-model

Recall from the section “[Notation for the Generalized Linear Mixed Model](#)” on page 2918 that

$$E[\mathbf{Y}|\boldsymbol{\gamma}] = \mathbf{g}^{-1}(\mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\boldsymbol{\gamma}) = \mathbf{g}^{-1}(\boldsymbol{\eta}) = \boldsymbol{\mu}$$

where  $\boldsymbol{\gamma} \sim N(\mathbf{0}, \mathbf{G})$  and  $\text{Var}[\mathbf{Y}|\boldsymbol{\gamma}] = \mathbf{A}^{1/2}\mathbf{R}\mathbf{A}^{1/2}$ . Following Wolfinger and O’Connell (1993), a first-order Taylor series of  $\boldsymbol{\mu}$  about  $\tilde{\boldsymbol{\beta}}$  and  $\tilde{\boldsymbol{\gamma}}$  yields

$$\mathbf{g}^{-1}(\boldsymbol{\eta}) \doteq \mathbf{g}^{-1}(\tilde{\boldsymbol{\eta}}) + \tilde{\boldsymbol{\Delta}}\mathbf{X}(\boldsymbol{\beta} - \tilde{\boldsymbol{\beta}}) + \tilde{\boldsymbol{\Delta}}\mathbf{Z}(\boldsymbol{\gamma} - \tilde{\boldsymbol{\gamma}})$$

where

$$\tilde{\boldsymbol{\Delta}} = \left( \frac{\partial \mathbf{g}^{-1}(\boldsymbol{\eta})}{\partial \boldsymbol{\eta}} \right)_{\tilde{\boldsymbol{\beta}}, \tilde{\boldsymbol{\gamma}}}$$

is a diagonal matrix of derivatives of the conditional mean evaluated at the expansion locus. Rearranging terms yields the expression

$$\tilde{\boldsymbol{\Delta}}^{-1}(\boldsymbol{\mu} - \mathbf{g}^{-1}(\tilde{\boldsymbol{\eta}})) + \mathbf{X}\tilde{\boldsymbol{\beta}} + \mathbf{Z}\tilde{\boldsymbol{\gamma}} \doteq \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\boldsymbol{\gamma}$$

The left side is the expected value, conditional on  $\boldsymbol{\gamma}$ , of

$$\tilde{\mathbf{A}}^{-1}(\mathbf{Y} - g^{-1}(\tilde{\boldsymbol{\eta}})) + \mathbf{X}\tilde{\boldsymbol{\beta}} + \mathbf{Z}\tilde{\boldsymbol{\gamma}} \equiv \mathbf{P}$$

and

$$\text{Var}[\mathbf{P}|\boldsymbol{\gamma}] = \tilde{\mathbf{A}}^{-1}\mathbf{A}^{1/2}\mathbf{R}\mathbf{A}^{1/2}\tilde{\mathbf{A}}^{-1}$$

You can thus consider the model

$$\mathbf{P} = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\boldsymbol{\gamma} + \boldsymbol{\epsilon}$$

which is a linear mixed model with pseudo-response  $\mathbf{P}$ , fixed effects  $\boldsymbol{\beta}$ , random effects  $\boldsymbol{\gamma}$ , and  $\text{Var}[\boldsymbol{\epsilon}] = \text{Var}[\mathbf{P}|\boldsymbol{\gamma}]$ .

### Objective Functions

Now define

$$\mathbf{V}(\boldsymbol{\theta}) = \mathbf{Z}\mathbf{G}\mathbf{Z}' + \tilde{\mathbf{A}}^{-1}\mathbf{A}^{1/2}\mathbf{R}\mathbf{A}^{1/2}\tilde{\mathbf{A}}^{-1}$$

as the marginal variance in the linear mixed pseudo-model, where  $\boldsymbol{\theta}$  is the  $(q \times 1)$  parameter vector containing all unknowns in  $\mathbf{G}$  and  $\mathbf{R}$ . Based on this linearized model, an objective function can be defined, assuming that the distribution of  $\mathbf{P}$  is known. The GLIMMIX procedure assumes that  $\boldsymbol{\epsilon}$  has a normal distribution. The maximum log pseudo-likelihood (MxPL) and restricted log pseudo-likelihood (RxPL) for  $\mathbf{P}$  are then

$$l(\boldsymbol{\theta}, \mathbf{p}) = -\frac{1}{2} \log |\mathbf{V}(\boldsymbol{\theta})| - \frac{1}{2} \mathbf{r}'\mathbf{V}(\boldsymbol{\theta})^{-1}\mathbf{r} - \frac{f}{2} \log\{2\pi\}$$

$$l_R(\boldsymbol{\theta}, \mathbf{p}) = -\frac{1}{2} \log |\mathbf{V}(\boldsymbol{\theta})| - \frac{1}{2} \mathbf{r}'\mathbf{V}(\boldsymbol{\theta})^{-1}\mathbf{r} - \frac{1}{2} \log |\mathbf{X}'\mathbf{V}(\boldsymbol{\theta})^{-1}\mathbf{X}| - \frac{f-k}{2} \log\{2\pi\}$$

with  $\mathbf{r} = \mathbf{p} - \mathbf{X}(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}^{-1}\mathbf{p}$ .  $f$  denotes the sum of the frequencies used in the analysis, and  $k$  denotes the rank of  $\mathbf{X}$ . The fixed-effects parameters  $\boldsymbol{\beta}$  are profiled from these expressions. The parameters in  $\boldsymbol{\theta}$  are estimated by the optimization techniques specified in the **NLOPTIONS** statement. The objective function for minimization is  $-2l(\boldsymbol{\theta}, \mathbf{p})$  or  $-2l_R(\boldsymbol{\theta}, \mathbf{p})$ . At convergence, the profiled parameters are estimated and the random effects are predicted as

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{V}(\hat{\boldsymbol{\theta}})^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}(\hat{\boldsymbol{\theta}})^{-1}\mathbf{p}$$

$$\hat{\boldsymbol{\gamma}} = \hat{\mathbf{G}}\mathbf{Z}'\mathbf{V}(\hat{\boldsymbol{\theta}})^{-1}\hat{\mathbf{r}}$$

With these statistics, the pseudo-response and error weights of the linearized model are recomputed and the objective function is minimized again. The predictors  $\hat{\boldsymbol{\gamma}}$  are the estimated BLUPs in the approximated linear model. This process continues until the relative change between parameter estimates at two successive (outer) iterations is sufficiently small. See the **PCONV=** option in the **PROC GLIMMIX** statement for the computational details about how the GLIMMIX procedure compares parameter estimates across optimizations.

If the conditional distribution contains a scale parameter  $\phi \neq 1$  (Table 41.19), the GLIMMIX procedure profiles this parameter in GLMMs from the log pseudo-likelihoods as well. To this end define

$$\mathbf{V}(\boldsymbol{\theta}^*) = \tilde{\mathbf{A}}^{-1}\mathbf{A}^{1/2}\mathbf{R}^*\mathbf{A}^{1/2}\tilde{\mathbf{A}}^{-1} + \mathbf{Z}\mathbf{G}^*\mathbf{Z}'$$

where  $\boldsymbol{\theta}^*$  is the covariance parameter vector with  $q - 1$  elements. The matrices  $\mathbf{G}^*$  and  $\mathbf{R}^*$  are appropriately reparameterized versions of  $\mathbf{G}$  and  $\mathbf{R}$ . For example, if  $\mathbf{G}$  has a variance component structure and  $\mathbf{R} = \phi\mathbf{I}$ , then  $\boldsymbol{\theta}^*$  contains ratios of the variance components and  $\phi$ , and  $\mathbf{R}^* = \mathbf{I}$ . The solution for  $\hat{\boldsymbol{\phi}}$  is

$$\hat{\boldsymbol{\phi}} = \hat{\mathbf{r}}'\mathbf{V}(\hat{\boldsymbol{\theta}}^*)^{-1}\hat{\mathbf{r}}/m$$

where  $m = f$  for MxPL and  $m = f - k$  for RxPL. Substitution into the previous functions yields the profiled log pseudo-likelihoods,

$$\begin{aligned} l(\boldsymbol{\theta}^*, \mathbf{p}) &= -\frac{1}{2} \log |\mathbf{V}(\boldsymbol{\theta}^*)| - \frac{f}{2} \log \{\mathbf{r}'\mathbf{V}(\boldsymbol{\theta}^*)^{-1}\mathbf{r}\} - \frac{f}{2} (1 + \log\{2\pi/f\}) \\ l_R(\boldsymbol{\theta}^*, \mathbf{p}) &= -\frac{1}{2} \log |\mathbf{V}(\boldsymbol{\theta}^*)| - \frac{f-k}{2} \log \{\mathbf{r}'\mathbf{V}(\boldsymbol{\theta}^*)^{-1}\mathbf{r}\} \\ &\quad - \frac{1}{2} \log |\mathbf{X}'\mathbf{V}(\boldsymbol{\theta}^*)^{-1}\mathbf{X}| - \frac{f-k}{2} (1 + \log\{2\pi/(f-k)\}) \end{aligned}$$

Profiling of  $\phi$  can be suppressed with the **NOPROFILE** option in the **PROC GLIMMIX** statement.

Where possible, the objective function, its gradient, and its Hessian employ the sweep-based W-transformation ( Hemmerle and Hartley 1973; Goodnight 1979; Goodnight and Hemmerle 1979). Further details about the minimization process in the general linear mixed model can be found in Wolfinger, Tobias, and Sall (1994).

### Estimated Precision of Estimates

The GLIMMIX procedure produces estimates of the variability of  $\hat{\boldsymbol{\beta}}$ ,  $\hat{\boldsymbol{\theta}}$ , and estimates of the prediction variability for  $\hat{\boldsymbol{\gamma}}$ ,  $\text{Var}[\hat{\boldsymbol{\gamma}} - \boldsymbol{\gamma}]$ . Denote as  $\mathbf{S}$  the matrix

$$\mathbf{S} \equiv \widehat{\text{Var}}[\mathbf{P}|\boldsymbol{\gamma}] = \widetilde{\boldsymbol{\Delta}}^{-1}\mathbf{A}^{1/2}\mathbf{R}\mathbf{A}^{1/2}\widetilde{\boldsymbol{\Delta}}^{-1}$$

where all components on the right side are evaluated at the converged estimates. The mixed model equations (Henderson 1984) in the linear mixed (pseudo-)model are then

$$\begin{bmatrix} \mathbf{X}'\mathbf{S}^{-1}\mathbf{X} & \mathbf{X}'\mathbf{S}^{-1}\mathbf{Z} \\ \mathbf{Z}'\mathbf{S}^{-1}\mathbf{X} & \mathbf{Z}'\mathbf{S}^{-1}\mathbf{Z} + \mathbf{G}(\hat{\boldsymbol{\theta}})^{-1} \end{bmatrix} \begin{bmatrix} \hat{\boldsymbol{\beta}} \\ \hat{\boldsymbol{\gamma}} \end{bmatrix} = \begin{bmatrix} \mathbf{X}'\mathbf{S}^{-1}\mathbf{p} \\ \mathbf{Z}'\mathbf{S}^{-1}\mathbf{p} \end{bmatrix}$$

and

$$\begin{aligned} \mathbf{C} &= \begin{bmatrix} \mathbf{X}'\mathbf{S}^{-1}\mathbf{X} & \mathbf{X}'\mathbf{S}^{-1}\mathbf{Z} \\ \mathbf{Z}'\mathbf{S}^{-1}\mathbf{X} & \mathbf{Z}'\mathbf{S}^{-1}\mathbf{Z} + \mathbf{G}(\hat{\boldsymbol{\theta}})^{-1} \end{bmatrix}^{-1} \\ &= \begin{bmatrix} \hat{\boldsymbol{\Omega}} & -\hat{\boldsymbol{\Omega}}\mathbf{X}'\mathbf{V}(\hat{\boldsymbol{\theta}})^{-1}\mathbf{Z}\mathbf{G}(\hat{\boldsymbol{\theta}}) \\ -\mathbf{G}(\hat{\boldsymbol{\theta}})\mathbf{Z}'\mathbf{V}(\hat{\boldsymbol{\theta}})^{-1}\mathbf{X}\hat{\boldsymbol{\Omega}} & \mathbf{M} + \mathbf{G}(\hat{\boldsymbol{\theta}})\mathbf{Z}'\mathbf{V}(\hat{\boldsymbol{\theta}})^{-1}\mathbf{X}\hat{\boldsymbol{\Omega}}\mathbf{X}'\mathbf{V}(\hat{\boldsymbol{\theta}})^{-1}\mathbf{Z}\mathbf{G}(\hat{\boldsymbol{\theta}}) \end{bmatrix} \end{aligned}$$

is the approximate estimated variance-covariance matrix of  $[\hat{\boldsymbol{\beta}}', \hat{\boldsymbol{\gamma}}' - \boldsymbol{\gamma}']'$ . Here,  $\hat{\boldsymbol{\Omega}} = (\mathbf{X}'\mathbf{V}(\hat{\boldsymbol{\theta}})^{-1}\mathbf{X})^{-1}$  and  $\mathbf{M} = (\mathbf{Z}'\mathbf{S}^{-1}\mathbf{Z} + \mathbf{G}(\hat{\boldsymbol{\theta}})^{-1})^{-1}$ .

The square roots of the diagonal elements of  $\widehat{\Omega}$  are reported in the Standard Error column of the “Parameter Estimates” table. This table is produced with the **SOLUTION** option in the **MODEL** statement. The prediction standard errors of the random-effects solutions are reported in the Std Err Pred column of the “Solution for Random Effects” table. This table is produced with the **SOLUTION** option in the **RANDOM** statement.

As a cautionary note, **C** tends to underestimate the true sampling variability of  $[\widehat{\beta}', \widehat{\gamma}']'$ , because no account is made for the uncertainty in estimating **G** and **R**. Although inflation factors have been proposed (Kackar and Harville 1984; Kass and Steffey 1989; Prasad and Rao 1990), they tend to be small for data sets that are fairly well balanced. PROC GLIMMIX does not compute any inflation factors by default. The **DDFM=KENWARDROGER** option in the **MODEL** statement prompts PROC GLIMMIX to compute a specific inflation factor (Kenward and Roger 1997), along with Satterthwaite-based degrees of freedom.

If  $\mathbf{G}(\widehat{\theta})$  is singular, or if you use the **CHOL** option of the **PROC GLIMMIX** statement, the mixed model equations are modified as follows. Let **L** denote the lower triangular matrix so that  $\mathbf{L}\mathbf{L}' = \mathbf{G}(\widehat{\theta})$ . PROC GLIMMIX then solves the equations

$$\begin{bmatrix} \mathbf{X}'\mathbf{S}^{-1}\mathbf{X} & \mathbf{X}'\mathbf{S}^{-1}\mathbf{Z}\mathbf{L} \\ \mathbf{L}'\mathbf{Z}'\mathbf{S}^{-1}\mathbf{X} & \mathbf{L}'\mathbf{Z}'\mathbf{S}^{-1}\mathbf{Z}\mathbf{L} + \mathbf{I} \end{bmatrix} \begin{bmatrix} \widehat{\beta} \\ \widehat{\tau} \end{bmatrix} = \begin{bmatrix} \mathbf{X}'\mathbf{S}^{-1}\mathbf{p} \\ \mathbf{L}'\mathbf{Z}'\mathbf{S}^{-1}\mathbf{p} \end{bmatrix}$$

and transforms  $\widehat{\tau}$  and a generalized inverse of the left-side coefficient matrix by using **L**.

The asymptotic covariance matrix of the covariance parameter estimator  $\widehat{\theta}$  is computed based on the observed or expected Hessian matrix of the optimization procedure. Consider first the case where the scale parameter  $\phi$  is not present or not profiled. Because  $\beta$  is profiled from the pseudo-likelihood, the objective function for minimization is  $f(\theta) = -2l(\theta, \mathbf{p})$  for **METHOD=MSPL** and **METHOD=MMPL** and  $f(\theta) = -2l_R(\theta, \mathbf{p})$  for **METHOD=RSPL** and **METHOD=RMPL**. Denote the observed Hessian (second derivative) matrix as

$$\mathbf{H} = \frac{\partial^2 f(\theta)}{\partial \theta \partial \theta'}$$

The GLIMMIX procedure computes the variance of  $\widehat{\theta}$  by default as  $2\mathbf{H}^{-1}$ . If the Hessian is not positive definite, a sweep-based generalized inverse is used instead. When the **EXPHESSIAN** option of the **PROC GLIMMIX** statement is used, or when the procedure is in scoring mode at convergence (see the **SCORING** option in the **PROC GLIMMIX** statement), the observed Hessian is replaced with an approximated expected Hessian matrix in these calculations.

Following Wolfinger, Tobias, and Sall (1994), define the following components of the gradient and Hessian in the optimization:

$$\begin{aligned} \mathbf{g}_1 &= \frac{\partial}{\partial \theta} \mathbf{r}'\mathbf{V}(\theta)^{-1}\mathbf{r} \\ \mathbf{H}_1 &= \frac{\partial^2}{\partial \theta \partial \theta'} \log\{\mathbf{V}(\theta)\} \\ \mathbf{H}_2 &= \frac{\partial^2}{\partial \theta \partial \theta'} \mathbf{r}'\mathbf{V}(\theta)^{-1}\mathbf{r} \\ \mathbf{H}_3 &= \frac{\partial^2}{\partial \theta \partial \theta'} \log\{|\mathbf{X}'\mathbf{V}(\theta)^{-1}\mathbf{X}|\} \end{aligned}$$

Table 41.21 gives expressions for the Hessian matrix  $\mathbf{H}$  depending on estimation method, profiling, and scoring.

**Table 41.21** Hessian Computation in GLIMMIX

| Profiling | Scoring  | MxPL                                                                                                                        | RxPL                                                                                                                                             |
|-----------|----------|-----------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------|
| No        | No       | $\mathbf{H}_1 + \mathbf{H}_2$                                                                                               | $\mathbf{H}_1 + \mathbf{H}_2 + \mathbf{H}_3$                                                                                                     |
| No        | Yes      | $-\mathbf{H}_1$                                                                                                             | $-\mathbf{H}_1 + \mathbf{H}_3$                                                                                                                   |
| No        | Modified | $-\mathbf{H}_1$                                                                                                             | $-\mathbf{H}_1 - \mathbf{H}_3$                                                                                                                   |
| Yes       | No       | $\begin{bmatrix} \mathbf{H}_1 + \mathbf{H}_2/\phi & -\mathbf{g}_2/\phi^2 \\ -\mathbf{g}'_2/\phi^2 & f/\phi^2 \end{bmatrix}$ | $\begin{bmatrix} \mathbf{H}_1 + \mathbf{H}_2/\phi + \mathbf{H}_3 & -\mathbf{g}_2/\phi^2 \\ -\mathbf{g}'_2/\phi^2 & (f - k)/\phi^2 \end{bmatrix}$ |
| Yes       | Yes      | $\begin{bmatrix} -\mathbf{H}_1 & -\mathbf{g}_2/\phi^2 \\ -\mathbf{g}'_2/\phi^2 & f/\phi^2 \end{bmatrix}$                    | $\begin{bmatrix} -\mathbf{H}_1 + \mathbf{H}_3 & -\mathbf{g}_2/\phi^2 \\ -\mathbf{g}'_2/\phi^2 & (f - k)/\phi^2 \end{bmatrix}$                    |
| Yes       | Modified | $\begin{bmatrix} -\mathbf{H}_1 & -\mathbf{g}_2/\phi^2 \\ -\mathbf{g}'_2/\phi^2 & f/\phi^2 \end{bmatrix}$                    | $\begin{bmatrix} -\mathbf{H}_1 - \mathbf{H}_3 & -\mathbf{g}_2/\phi^2 \\ -\mathbf{g}'_2/\phi^2 & (f - k)/\phi^2 \end{bmatrix}$                    |

The “Modified” expressions for the Hessian under scoring in RxPL estimation refer to a modified scoring method. In some cases, the modification leads to faster convergence than the standard scoring algorithm. The modification is requested with the SCOREMOD option in the PROC GLIMMIX statement.

Finally, in the case of a profiled scale parameter  $\phi$ , the Hessian for the  $(\theta^*, \phi)$  parameterization is converted into that for the  $\theta$  parameterization as

$$\mathbf{H}(\theta) = \mathbf{B}\mathbf{H}(\theta^*, \phi)\mathbf{B}'$$

where

$$\mathbf{B} = \begin{bmatrix} 1/\phi & 0 & \dots & 0 & 0 \\ 0 & 1/\phi & \dots & 0 & 0 \\ 0 & \dots & \dots & 1/\phi & 0 \\ -\theta_1^*/\phi & -\theta_2^*/\phi & \dots & -\theta_{q-1}^*/\phi & 1 \end{bmatrix}$$

**Subject-Specific and Population-Averaged (Marginal) Expansions**

There are two basic choices for the expansion locus of the linearization. A subject-specific (SS) expansion uses

$$\tilde{\boldsymbol{\beta}} = \hat{\boldsymbol{\beta}} \quad \tilde{\boldsymbol{\gamma}} = \hat{\boldsymbol{\gamma}}$$

which are the current estimates of the fixed effects and estimated BLUPs. The population-averaged (PA) expansion expands about the same fixed effects and the expected value of the random effects

$$\tilde{\boldsymbol{\beta}} = \hat{\boldsymbol{\beta}} \quad \tilde{\boldsymbol{\gamma}} = \mathbf{0}$$

To recompute the pseudo-response and weights in the SS expansion, the BLUPs must be computed every time the objective function in the linear mixed model is maximized. The PA expansion does not require any BLUPs. The four pseudo-likelihood methods implemented in the GLIMMIX procedure are the  $2 \times 2$  factorial combination between two expansion loci and residual versus maximum pseudo-likelihood estimation. The following table shows the combination and the corresponding values of the `METHOD=` option (PROC GLIMMIX statement); `METHOD=RSPL` is the default.

| Type of<br>PL | Expansion Locus             |                          |
|---------------|-----------------------------|--------------------------|
|               | $\hat{\boldsymbol{\gamma}}$ | $E[\boldsymbol{\gamma}]$ |
| residual      | RSPL                        | RMPL                     |
| maximum       | MSPL                        | MMPL                     |

## Maximum Likelihood Estimation Based on Laplace Approximation

### Objective Function

Let  $\boldsymbol{\beta}$  denote the vector of fixed-effects parameters and  $\boldsymbol{\theta}$  the vector of covariance parameters. For Laplace estimation in the GLIMMIX procedure,  $\boldsymbol{\theta}$  includes the G-side parameters and a possible scale parameter  $\phi$ , provided that the conditional distribution of the data contains such a scale parameter.  $\boldsymbol{\theta}^*$  is the vector of the G-side parameters.

The marginal distribution of the data in a mixed model can be expressed as

$$\begin{aligned} p(\mathbf{y}) &= \int p(\mathbf{y}|\boldsymbol{\gamma}, \boldsymbol{\beta}, \phi) p(\boldsymbol{\gamma}|\boldsymbol{\theta}^*) d\boldsymbol{\gamma} \\ &= \int \exp \{ \log \{ p(\mathbf{y}|\boldsymbol{\gamma}, \boldsymbol{\beta}, \phi) \} + \log \{ p(\boldsymbol{\gamma}|\boldsymbol{\theta}^*) \} \} d\boldsymbol{\gamma} \\ &= \int \exp \{ c_l f(\mathbf{y}, \boldsymbol{\beta}, \boldsymbol{\theta}; \boldsymbol{\gamma}) \} d\boldsymbol{\gamma} \end{aligned}$$

If the constant  $c_l$  is large, the Laplace approximation of this integral is

$$L(\boldsymbol{\beta}, \boldsymbol{\theta}; \hat{\boldsymbol{\gamma}}, \mathbf{y}) = \left( \frac{2\pi}{c_l} \right)^{n_{\boldsymbol{\gamma}}/2} | -f''(\mathbf{y}, \boldsymbol{\beta}, \boldsymbol{\theta}; \hat{\boldsymbol{\gamma}}) |^{-1/2} e^{c_l f(\mathbf{y}, \boldsymbol{\beta}, \boldsymbol{\theta}; \hat{\boldsymbol{\gamma}})}$$

where  $n_{\boldsymbol{\gamma}}$  is the number of elements in  $\boldsymbol{\gamma}$ ,  $f''$  is the second derivative matrix

$$f''(\mathbf{y}, \boldsymbol{\beta}, \boldsymbol{\theta}; \hat{\boldsymbol{\gamma}}) = \left. \frac{\partial^2 f(\mathbf{y}, \boldsymbol{\beta}, \boldsymbol{\theta}; \boldsymbol{\gamma})}{\partial \boldsymbol{\gamma} \partial \boldsymbol{\gamma}'} \right|_{\hat{\boldsymbol{\gamma}}}$$

and  $\hat{\boldsymbol{\gamma}}$  satisfies the first-order condition

$$\frac{\partial f(\mathbf{y}, \boldsymbol{\beta}, \boldsymbol{\theta}; \boldsymbol{\gamma})}{\partial \boldsymbol{\gamma}} = \mathbf{0}$$

The objective function for Laplace parameter estimation in the GLIMMIX procedure is  $-2 \log \{ L(\boldsymbol{\beta}, \boldsymbol{\theta}; \hat{\boldsymbol{\gamma}}, \mathbf{y}) \}$ . The optimization process is singly iterative, but because  $\hat{\boldsymbol{\gamma}}$  depends on  $\hat{\boldsymbol{\beta}}$  and  $\hat{\boldsymbol{\theta}}$ , the GLIMMIX procedure solves a suboptimization problem to determine for given values of  $\hat{\boldsymbol{\beta}}$  and  $\hat{\boldsymbol{\theta}}$  the random-effects solution vector that maximizes  $f(\mathbf{y}, \boldsymbol{\beta}, \boldsymbol{\theta}; \boldsymbol{\gamma})$ .

When you have longitudinal or clustered data with  $m$  independent subjects or clusters, the vector of observations can be written as  $\mathbf{y} = [\mathbf{y}'_1, \dots, \mathbf{y}'_m]'$ , where  $\mathbf{y}_i$  is an  $n_i \times 1$  vector of observations for subject (cluster)  $i$  ( $i = 1, \dots, m$ ). In this case, assuming conditional independence such that

$$p(\mathbf{y}_i | \boldsymbol{\gamma}_i) = \prod_{j=1}^{n_i} p(y_{ij} | \boldsymbol{\gamma}_i)$$

the marginal distribution of the data can be expressed as

$$\begin{aligned} p(\mathbf{y}) &= \prod_{i=1}^m p(\mathbf{y}_i) = \prod_{i=1}^m \int p(\mathbf{y}_i | \boldsymbol{\gamma}_i) p(\boldsymbol{\gamma}_i) d\boldsymbol{\gamma}_i \\ &= \prod_{i=1}^m \int \exp\{n_i f(\mathbf{y}_i, \boldsymbol{\beta}, \boldsymbol{\theta}; \boldsymbol{\gamma}_i)\} d\boldsymbol{\gamma}_i \end{aligned}$$

where

$$\begin{aligned} n_i f(\mathbf{y}_i, \boldsymbol{\beta}, \boldsymbol{\theta}; \boldsymbol{\gamma}_i) &= \log\{p(\mathbf{y}_i | \boldsymbol{\gamma}_i) p(\boldsymbol{\gamma}_i)\} \\ &= \sum_{j=1}^{n_i} \log\{p(y_{ij} | \boldsymbol{\gamma}_i)\} + \log\{p(\boldsymbol{\gamma}_i)\} \end{aligned}$$

When the number of observations within a cluster,  $n_i$ , is large, the Laplace approximation to the  $i$ th individual's marginal probability density function is

$$\begin{aligned} p(\mathbf{y}_i | \boldsymbol{\beta}, \boldsymbol{\theta}) &= \int \exp\{n_i f(\mathbf{y}_i, \boldsymbol{\beta}, \boldsymbol{\theta}; \boldsymbol{\gamma}_i)\} d\boldsymbol{\gamma}_i \\ &= \frac{(2\pi)^{n_\gamma} / 2}{|-n_i f''(\mathbf{y}_i, \boldsymbol{\beta}, \boldsymbol{\theta}; \hat{\boldsymbol{\gamma}}_i)|^{1/2}} \exp\{n_i f(\mathbf{y}_i, \boldsymbol{\beta}, \boldsymbol{\theta}; \hat{\boldsymbol{\gamma}}_i)\} \end{aligned}$$

where  $n_{\boldsymbol{\gamma}_i}$  is the common dimension of the random effects,  $\boldsymbol{\gamma}_i$ . In this case, provided that the constant  $c_l = \min\{n_i\}$  is large, the Laplace approximation to the marginal log likelihood is

$$\begin{aligned} \log\{L(\boldsymbol{\beta}, \boldsymbol{\theta}; \hat{\boldsymbol{\gamma}}, \mathbf{y})\} &= \sum_{i=1}^m \left\{ n_i f(\mathbf{y}_i, \boldsymbol{\beta}, \boldsymbol{\theta}; \hat{\boldsymbol{\gamma}}_i) + \frac{n_{\boldsymbol{\gamma}_i}}{2} \log\{2\pi\} \right. \\ &\quad \left. - \frac{1}{2} \log |-n_i f''(\boldsymbol{\beta}, \boldsymbol{\theta}; \hat{\boldsymbol{\gamma}}_i)| \right\} \end{aligned}$$

which serves as the objective function for the **METHOD=LAPLACE** estimator in PROC GLIMMIX.

The Laplace approximation implemented in the GLIMMIX procedure differs from that in Wolfinger (1993) and Pinheiro and Bates (1995) in important respects. Wolfinger (1993) assumed a flat prior for  $\boldsymbol{\beta}$  and expanded the integrand around  $\boldsymbol{\beta}$  and  $\boldsymbol{\gamma}$ , leaving only the covariance parameters for the overall optimization. The “fixed” effects  $\boldsymbol{\beta}$  and the random effects  $\boldsymbol{\gamma}$  are determined in a suboptimization that takes the form of a linear mixed model step with pseudo-data. The GLIMMIX procedure involves only the random effects vector  $\boldsymbol{\gamma}$  in the suboptimization. Pinheiro and Bates (1995) and Wolfinger (1993) consider a modified Laplace approximation that replaces the second derivative  $f''(\mathbf{y}, \boldsymbol{\beta}, \boldsymbol{\theta}; \hat{\boldsymbol{\gamma}})$  with an (approximate) expected value, akin to scoring. The GLIMMIX procedure does not use an approximation to  $f''(\mathbf{y}, \boldsymbol{\beta}, \boldsymbol{\theta}; \hat{\boldsymbol{\gamma}})$ . The **METHOD=RSPL** estimates in PROC GLIMMIX are equivalent to the estimates obtained with the modified Laplace approximation in Wolfinger (1993). The objective functions of **METHOD=RSPL** and Wolfinger (1993) differ in a constant that depends on the number of parameters.

### Asymptotic Properties and the Importance of Subjects

Suppose that the GLIMMIX procedure processes your data by subjects (see the section “Processing by Subjects” on page 3082) and let  $n_i$  denote the number of observations per subject,  $i = 1, \dots, s$ . Arguments in Vonesh (1996) show that the maximum likelihood estimator based on the Laplace approximation is a consistent estimator to order  $O_p\{\max\{1/\sqrt{s}\}, 1/\min\{n_i\}\}$ . In other words, as the number of subjects and the number of observations per subject grows, the small-sample bias of the Laplace estimator disappears. Note that the term involving the number of subjects in this maximum relates to standard asymptotic theory, and the term involving the number of observations per subject relates to the accuracy of the Laplace approximation (Vonesh 1996). In the case where random effects enter the model linearly, the Laplace approximation is exact and the requirement that  $\min\{n_i\} \rightarrow \infty$  can be dropped.

If your model is not processed by subjects but is equivalent to a subject model, the asymptotics with respect to  $s$  still apply, because the Hessian matrix of the suboptimization for  $\boldsymbol{y}$  breaks into  $s$  separate blocks. For example, the following two models are equivalent with respect to  $s$  and  $n_i$ , although only for the first model does PROC GLIMMIX process the data explicitly by subjects:

```
proc glimmix method=laplace;
 class sub A;
 model y = A;
 random intercept / subject=sub;
run;

proc glimmix method=laplace;
 class sub A;
 model y = A;
 random sub;
run;
```

The same holds, for example, for models with independent nested random effects. The following two models are equivalent, and you can derive asymptotic properties related to  $s$  and  $\min\{n_i\}$  from the model in the first run:

```
proc glimmix method=laplace;
 class A B block;
 model y = A B A*B;
 random intercept A / subject=block;
run;

proc glimmix method=laplace;
 class A B block;
 model y = A B A*B;
 random block a*block;
run;
```

The Laplace approximation requires that the dimension of the integral does not increase with the size of the sample. Otherwise the error of the likelihood approximation does not diminish with  $n_i$ . This is the case, for example, with exchangeable arrays (Shun and McCullagh 1995), crossed random effects (Shun 1997), and correlated random effects of arbitrary dimension (Raudenbush, Yang, and Yosef 2000). Results in Shun (1997), for example, show that even in this case the standard Laplace approximation has smaller bias than pseudo-likelihood estimates.



## Maximum Likelihood Estimation Based on Adaptive Quadrature

Quadrature methods, like the Laplace approximation, approximate integrals. If you choose `METHOD=QUAD` for a generalized linear mixed model, the GLIMMIX procedure approximates the marginal log likelihood with an adaptive Gauss-Hermite quadrature rule. Gaussian quadrature is particularly well suited to numerically evaluate integrals against probability measures (Lange 1999, Ch. 16). And Gauss-Hermite quadrature is appropriate when the density has kernel  $\exp\{-x^2\}$  and integration extends over the real line, as is the case for the normal distribution. Suppose that  $p(x)$  is a probability density function and the function  $f(x)$  is to be integrated against it. Then the quadrature rule is

$$\int_{-\infty}^{\infty} f(x)p(x) dx \approx \sum_{i=1}^N w_i f(x_i)$$

where  $N$  denotes the number of quadrature points, the  $w_i$  are the quadrature weights, and the  $x_i$  are the abscissas. The Gaussian quadrature chooses abscissas in areas of high density, and if  $p(x)$  is continuous, the quadrature rule is exact if  $f(x)$  is a polynomial of up to degree  $2N - 1$ . In the generalized linear mixed model the roles of  $f(x)$  and  $p(x)$  are played by the conditional distribution of the data given the random effects, and the random-effects distribution, respectively. Quadrature abscissas and weights are those of the standard Gauss-Hermite quadrature (Golub and Welsch 1969; see also Table 25.10 of Abramowitz and Stegun 1972; Evans 1993).

A numerical integration rule is called adaptive when it uses a variable step size to control the error of the approximation. For example, an adaptive trapezoidal rule uses serial splitting of intervals at midpoints until a desired tolerance is achieved. The quadrature rule in the GLIMMIX procedure is adaptive in the following sense: if you do not specify the number of quadrature points (nodes) with the `QPOINTS=` suboption of the `METHOD=QUAD` option, then the number of quadrature points is determined by evaluating the log likelihood at the starting values at a successively larger number of nodes until a tolerance is met (for more details see the text under the heading “Starting Values” in the next section). Furthermore, the GLIMMIX procedure centers and scales the quadrature points by using the empirical Bayes estimates (EBEs) of the random effects and the Hessian (second derivative) matrix from the EBE suboptimization. This centering and scaling improves the likelihood approximation by placing the abscissas according to the density function of the random effects. It is not, however, adaptiveness in the previously stated sense.

### Objective Function

Let  $\boldsymbol{\beta}$  denote the vector of fixed-effects parameters and  $\boldsymbol{\theta}$  the vector of covariance parameters. For quadrature estimation in the GLIMMIX procedure,  $\boldsymbol{\theta}$  includes the G-side parameters and a possible scale parameter  $\phi$ , provided that the conditional distribution of the data contains such a scale parameter.  $\boldsymbol{\theta}^*$  is the vector of the G-side parameters. The marginal distribution of the data for subject  $i$  in a mixed model can be expressed as

$$p(\mathbf{y}_i) = \int \cdots \int p(\mathbf{y}_i | \boldsymbol{\gamma}_i, \boldsymbol{\beta}, \phi) p(\boldsymbol{\gamma}_i | \boldsymbol{\theta}^*) d\boldsymbol{\gamma}_i$$

Suppose  $N_q$  denotes the number of quadrature points in each dimension (for each random effect) and  $r$  denotes the number of random effects. For each subject, obtain the empirical Bayes estimates of  $\boldsymbol{\gamma}_i$  as the vector  $\hat{\boldsymbol{\gamma}}_i$  that minimizes

$$-\log \{p(\mathbf{y}_i | \boldsymbol{\gamma}_i, \boldsymbol{\beta}, \phi) p(\boldsymbol{\gamma}_i | \boldsymbol{\theta}^*)\} = f(\mathbf{y}_i, \boldsymbol{\beta}, \boldsymbol{\theta}; \boldsymbol{\gamma}_i)$$

If  $\mathbf{z} = [z_1, \dots, z_{N_q}]$  are the standard abscissas for Gauss-Hermite quadrature, and  $\mathbf{z}_j^* = [z_{j1}, \dots, z_{jr}]$  is a point on the  $r$ -dimensional quadrature grid, then the centered and scaled abscissas are

$$\mathbf{a}_j^* = \hat{\boldsymbol{\gamma}}_i + 2^{1/2} f''(\mathbf{y}_i, \boldsymbol{\beta}, \boldsymbol{\theta}; \hat{\boldsymbol{\gamma}}_i)^{-1/2} \mathbf{z}_j^*$$

As for the Laplace approximation,  $f''$  is the second derivative matrix with respect to the random effects,

$$f''(\mathbf{y}_i, \boldsymbol{\beta}, \boldsymbol{\theta}; \hat{\boldsymbol{\gamma}}_i) = \frac{\partial^2 f(\mathbf{y}_i, \boldsymbol{\beta}, \boldsymbol{\theta}; \boldsymbol{\gamma}_i)}{\partial \boldsymbol{\gamma}_i \partial \boldsymbol{\gamma}_i'} \Big|_{\hat{\boldsymbol{\gamma}}_i}$$

These centered and scaled abscissas, along with the Gauss-Hermite quadrature weights  $\mathbf{w} = [w_1, \dots, w_{N_q}]$ , are used to construct the  $r$ -dimensional integral by a sequence of one-dimensional rules

$$\begin{aligned} p(\mathbf{y}_i) &= \int \cdots \int p(\mathbf{y}_i | \boldsymbol{\gamma}_i, \boldsymbol{\beta}, \phi) p(\boldsymbol{\gamma}_i | \boldsymbol{\theta}^*) d\boldsymbol{\gamma}_i \\ &\approx 2^{r/2} |f''(\mathbf{y}_i, \boldsymbol{\beta}, \boldsymbol{\theta}; \hat{\boldsymbol{\gamma}}_i)|^{-1/2} \\ &\quad \sum_{j_1=1}^{N_q} \cdots \sum_{j_r=1}^{N_q} \left[ p(\mathbf{y}_i | \mathbf{a}_{j^*}, \boldsymbol{\beta}, \phi) p(\mathbf{a}_{j^*} | \boldsymbol{\theta}^*) \prod_{k=1}^r w_{j_k} \exp z_{j_k}^2 \right] \end{aligned}$$

The right-hand side of this expression, properly accumulated across subjects, is the objective function for adaptive quadrature estimation in the GLIMMIX procedure.

### Quadrature or Laplace Approximation

If you select the quadrature rule with a single quadrature point, namely

```
proc glimmix method=quad(qpoints=1);
```

the results will be identical to `METHOD=LAPLACE`. Computationally, the two methods are not identical, however. `METHOD=LAPLACE` can be applied to a considerably larger class of models. For example, crossed random effects, models without subjects, or models with non-nested subjects can be handled with the Laplace approximation but not with quadrature. Furthermore, `METHOD=LAPLACE` draws on a number of computational simplifications that can increase its efficiency compared to a quadrature algorithm with a single node. For example, the Laplace approximation is possible with unbounded covariance parameter estimates (`NOBOUND` option in the `PROC GLIMMIX` statement) and can permit certain types of negative definite or indefinite  $\mathbf{G}$  matrices. The adaptive quadrature approximation with scaled abscissas typically breaks down when  $\mathbf{G}$  is not at least positive semidefinite.

As the number of random effects grows—for example, if you have nested random effects—quadrature quickly becomes computationally infeasible, due to the high dimensionality of the integral. To this end it is worthwhile to clarify the issues of dimensionality and computational effort as related to the number of quadrature nodes. Suppose that the A effect has 4 levels and consider the following statements:

```
proc glimmix method=quad(qpoints=5);
 class A id;
 model y = / dist=negbin;
 random A / subject=id;
run;
```

For each subject, computing the marginal log likelihood requires the numerical evaluation of a four-dimensional integral. As part of this evaluation  $5^4 = 625$  conditional log likelihoods need to be computed for each observation on each pass through the data. As the number of quadrature points or the number of random effects increases, this constitutes a sizable computational effort. Suppose, for example, that an additional random effect with  $b = 2$  levels is added as an interaction. The following statements then require evaluation of  $5^{(4+8)} = 244140625$  conditional log likelihoods for each observation on each pass through the data:

```
proc glimmix method=quad(qpoints=5);
 class A B id;
 model y = / dist=negbin;
 random A A*B / subject=id;
run;
```

As the number of random effects increases, Laplace approximation presents a computationally more expedient alternative.

If you wonder whether `METHOD=LAPLACE` would present a viable alternative to a model that you can fit with `METHOD=QUAD`, the “Optimization Information” table can provide some insights. The table contains as its last entry the number of quadrature points determined by PROC GLIMMIX to yield a sufficiently accurate approximation of the log likelihood (at the starting values). In many cases, a single quadrature node is sufficient, in which case the estimates are identical to those of `METHOD=LAPLACE`.

## Aspects Common to Adaptive Quadrature and Laplace Approximation

### Estimated Precision of Estimates

Denote as  $\mathbf{H}$  the second derivative matrix

$$\mathbf{H} = -\frac{\partial^2 \log\{L(\boldsymbol{\beta}, \boldsymbol{\theta}, \hat{\boldsymbol{\gamma}})\}}{\partial[\boldsymbol{\beta}, \boldsymbol{\theta}] \partial[\boldsymbol{\beta}', \boldsymbol{\theta}']}$$

evaluated at the converged solution of the optimization process. Partition its inverse as

$$\mathbf{H}^{-1} = \begin{bmatrix} \mathbf{C}(\boldsymbol{\beta}, \boldsymbol{\beta}) & \mathbf{C}(\boldsymbol{\beta}, \boldsymbol{\theta}) \\ \mathbf{C}(\boldsymbol{\theta}, \boldsymbol{\beta}) & \mathbf{C}(\boldsymbol{\theta}, \boldsymbol{\theta}) \end{bmatrix}$$

For `METHOD=LAPLACE` and `METHOD=QUAD`, the GLIMMIX procedure computes  $\mathbf{H}$  by finite forward differences based on the analytic gradient of  $\log\{L(\boldsymbol{\beta}, \boldsymbol{\theta}, \hat{\boldsymbol{\gamma}})\}$ . The partition  $\mathbf{C}(\boldsymbol{\theta}, \boldsymbol{\theta})$  serves as the asymptotic covariance matrix of the covariance parameter estimates (`ASYCOV` option in the `PROC GLIMMIX` statement). The standard errors reported in the “Covariance Parameter Estimates” table are based on the diagonal entries of this partition.

If you request an empirical standard error matrix with the `EMPIRICAL` option in the `PROC GLIMMIX` statement, a likelihood-based sandwich estimator is computed based on the subject-specific gradients of the Laplace or quadrature approximation. The sandwich estimator then replaces  $\mathbf{H}^{-1}$  in calculations following convergence.

To compute the standard errors and prediction standard errors of linear combinations of  $\boldsymbol{\beta}$  and  $\boldsymbol{\gamma}$ , PROC GLIMMIX forms an approximate prediction variance matrix for  $[\hat{\boldsymbol{\beta}}, \hat{\boldsymbol{\gamma}}]'$  from

$$\mathbf{P} = \begin{bmatrix} \mathbf{H}^{-1} & \mathbf{H}^{-1} \left( \frac{\partial \hat{\boldsymbol{\gamma}}}{\partial[\boldsymbol{\beta}, \boldsymbol{\theta}]} \right) \\ \left( \frac{\partial \hat{\boldsymbol{\gamma}}}{\partial[\boldsymbol{\beta}', \boldsymbol{\theta}']} \right) \mathbf{H}^{-1} & \boldsymbol{\Gamma}^{-1} + \left( \frac{\partial \hat{\boldsymbol{\gamma}}}{\partial[\boldsymbol{\beta}', \boldsymbol{\theta}']} \right) \mathbf{H}^{-1} \left( \frac{\partial \hat{\boldsymbol{\gamma}}}{\partial[\boldsymbol{\beta}, \boldsymbol{\theta}]} \right) \end{bmatrix}$$

where  $\boldsymbol{\Gamma}$  is the second derivative matrix from the  $\boldsymbol{\gamma}$  suboptimization that maximizes  $f(\mathbf{y}, \boldsymbol{\beta}, \boldsymbol{\theta}; \boldsymbol{\gamma})$  for given values of  $\boldsymbol{\beta}$  and  $\boldsymbol{\theta}$ . The prediction variance submatrix for the random effects is based on approximating the conditional mean squared error of prediction as in Booth and Hobert (1998). Note that even in the normal linear mixed model, the approximate conditional prediction standard errors are not identical to the prediction standard errors you obtain by inversion of the mixed model equations.

### Conditional Fit and Output Statistics

When you estimate the parameters of a mixed model by Laplace approximation or quadrature, the GLIMMIX procedure displays fit statistics related to the marginal distribution as well as the conditional distribution  $p(\mathbf{y}|\hat{\boldsymbol{\gamma}}, \hat{\boldsymbol{\beta}}, \hat{\boldsymbol{\phi}})$ . For ODS purposes, the name of the “Conditional Fit Statistics” table is “CondFitStatistics.” Because the marginal likelihood is approximated numerically for these methods, statistics based on the marginal distribution are not available. Instead of the generalized Pearson chi-square statistic in the “Fit Statistics” table, PROC GLIMMIX reports the Pearson statistic of the conditional distribution in the “Conditional Fit Statistics” table.

The unavailability of the marginal distribution also affects the set of output statistics that can be produced with `METHOD=LAPLACE` and `METHOD=QUAD`. Output statistics and statistical graphics that depend on the marginal variance of the data are not available with these estimation methods.

### User-Defined Variance Function

If you provide your own variance function, PROC GLIMMIX generally assumes that the (conditional) distribution of the data is unknown. Laplace or quadrature estimation would then not be possible. When you specify a variance function with `METHOD=LAPLACE` or `METHOD=QUAD`, the procedure assumes that the conditional distribution is normal. For example, consider the following statements to fit a mixed model to count data:

```
proc glimmix method=laplace;
 class sub;
 variance = _phi_*_mu_;
 model count = x / s link=log;
 random int / sub=sub;
run;
```

The variance function and the link suggest an overdispersed Poisson model. The Poisson distribution cannot accommodate the extra scale parameter `_PHI_`, however. In this situation, the GLIMMIX procedure fits a mixed model with random intercepts, log link function, and variance function  $\phi\mu$ , assuming that the count variable is normally distributed, given the random effects.

### Starting Values

Good starting values for the fixed effects and covariance parameters are important for Laplace and quadrature methods because the process commences with a suboptimization in which the empirical Bayes estimates of the random effects must be obtained before the optimization can get under way. Furthermore, the starting values are important for the adaptive choice of the number of quadrature points.

If you choose `METHOD=LAPLACE` or `METHOD=QUAD` and you do not provide starting values for the covariance parameters through the `PARMS` statement, the GLIMMIX procedure determines starting values in the following steps.

1. A GLM is fit initially to obtain starting values for the fixed-effects parameters. No output is produced from this stage. The number of initial iterations of this GLM fit can be controlled with the `INITITER=` option in the `PROC GLIMMIX` statement. You can suppress this step with the `NOINITGLM` option in the `PROC GLIMMIX` statement.
2. Given the fixed-effects estimates, starting values for the covariance parameters are computed by a MIVQUE0 step (Goodnight 1978a).

3. For **METHOD=QUAD** you can follow these steps with several pseudo-likelihood updates to improve on the estimates and to obtain solutions for the random effects. The number of pseudo-likelihood steps is controlled by the **INITPL=** suboption of **METHOD=QUAD**.
4. For **METHOD=QUAD**, if you do not specify the number of quadrature points with the suboptions of the **METHOD** option, the GLIMMIX procedure attempts to determine a sufficient number of points adaptively as follows. Suppose that  $N_q$  denotes the number of nodes in each dimension. If  $N_{min}$  and  $N_{max}$  denote the values from the **QMIN=** and **QMAX=** suboptions, respectively, the sequence for values less than 11 is constructed in increments of 2 starting at  $N_{min}$ . Values greater than 11 are incremented in steps of  $r$ . The default value is  $r = 10$ . The default sequence, without specifying the **QMIN=**, **QMAX=**, or **QFAC=** option, is thus 1, 3, 5, 7, 9, 11, 21, 31. If the relative difference of the log-likelihood approximation for two values in the sequence is less than the **QTOL= $t$**  value (default  $t = 0.0001$ ), the GLIMMIX procedure uses the lesser value for  $N_q$  in the subsequent optimization. If the relative difference does not fall below the tolerance  $t$  for any two subsequent values in the sequence, no estimation takes place.

### Notes on Bias of Estimators

Generalized linear mixed models are nonlinear models, and the estimation techniques rely on approximations to the log likelihood or approximations of the model. It is thus not surprising that the estimates of the covariance parameters and the fixed effects are usually not unbiased. Whenever estimates are biased, questions arise about the magnitude of the bias, its dependence on other model quantities, and the order of the bias. The order is important because it determines how quickly the bias vanishes while some aspect of the data increases. Typically, studies of asymptotic properties in models for hierarchical data suppose that the number of subjects (clusters) tends to infinity while the size of the clusters is held constant or grows at a particular rate. Note that asymptotic results so established do not extend to designs with fully crossed random effects, for example.

The following paragraphs summarize some important findings from the literature regarding the bias in covariance parameter and fixed-effects estimates with pseudo-likelihood, Laplace, and adaptive quadrature methods. The remarks draw in particular on results in Breslow and Lin (1995); Lin and Breslow (1996); Pinheiro and Chao (2006). Breslow and Lin (1995); Lin and Breslow (1996) study the “worst case” scenario of binary responses in a matched-pairs design. Their models have a variance component structure, comprising either a single variance component (a subject-specific random intercept; Breslow and Lin 1995) or a diagonal  $\mathbf{G}$  matrix (Lin and Breslow 1996). They study the bias in the estimates of the fixed-effects  $\boldsymbol{\beta}$  and the covariance parameters  $\boldsymbol{\theta}$  when the variance components are near the origin and for a canonical link function.

The matched-pairs design gives rise to a generalized linear mixed model with a cluster (subject) size of 2. Recall that the pseudo-likelihood methods rely on a linearization and a probabilistic assumption that the pseudo-data so obtained follow a normal linear mixed model. Obviously, it is difficult to imagine how the subject-specific (conditional) distribution would follow a normal linear mixed models with binary data in a cluster size of 2. The bias in the pseudo-likelihood estimator of  $\boldsymbol{\beta}$  is of order  $\|\boldsymbol{\theta}\|$ . The bias for the Laplace estimator of  $\boldsymbol{\beta}$  is of smaller magnitude; its asymptotic bias has order  $\|\boldsymbol{\theta}\|^2$ .

The Laplace methods and the pseudo-likelihood method produce biased estimators of the variance component  $\theta$  for the model considered in Breslow and Lin (1995). The order of the asymptotic bias for both estimation methods is  $\theta$ , as  $\theta$  approaches zero. Breslow and Lin (1995) comment on the fact that even with matched pairs, the bias vanishes very quickly in the binomial setting. If the conditional mean in the two

groups is equal to 0.5, then the asymptotic bias factor of the pseudo-likelihood estimator is  $1 - 1/(2n)$ , where  $n$  is the binomial denominator. This term goes to 1 quickly as  $n$  increases. This result underlines the importance of grouping binary observations into binomial responses whenever possible.

The results of Breslow and Lin (1995) and Lin and Breslow (1996) are echoed in the simulation study in Pinheiro and Chao (2006). These authors also consider adaptive quadrature in models with nested, hierarchical, random effects and show that adaptive quadrature with a sufficient number of nodes leads to nearly unbiased—or least biased—estimates. Their results also show that results for binary data cannot so easily be ported to other distributions. Even with a cluster size of 2, the pseudo-likelihood estimates of fixed effects and covariance parameters are virtually unbiased in their simulation of a Poisson GLMM. Breslow and Lin (1995) and Lin and Breslow (1996) “eschew” the residual PL version (**METHOD=RSPL**) over the maximum likelihood form (**METHOD=MSPL**). Pinheiro and Chao (2006) consider both forms in their simulation study. As expected, the residual form shows less bias than the MSPL form, for the same reasons REML estimation leads to less biased estimates compared to ML estimation in linear mixed models. The gain is modest, however; see, for example, Table 1 in Pinheiro and Chao (2006). When the variance components are small, there is a sufficient number of observations per cluster, and a reasonable number of clusters, then pseudo-likelihood methods for binary data are very useful—they provide a computational expedient alternative to numerical integration, and they allow the incorporation of R-side covariance structure into the model. Because many group randomized trials involve many observations per group and small random effects variances, Murray, Varnell, and Blitstein (2004) term questioning the use of conditional models for trials with binary outcome an “overreaction.”

---

## GLM Mode or GLMM Mode

The GLIMMIX procedure knows two basic modes of parameter estimation, and it can be important for you to understand the differences between the two modes.

In GLM mode, the data are never correlated and there can be no G-side random effects. Typical examples are logistic regression and normal linear models. When you fit a model in GLM mode, the **METHOD=** option in the PROC GLIMMIX statement has no effect. PROC GLIMMIX estimates the parameters of the model by maximum likelihood, (restricted) maximum likelihood, or quasi-likelihood, depending on the distributional properties of the model (see the section “[Default Estimation Techniques](#)” on page 3106). The “Model Information” table tells you which estimation method was applied. In GLM mode, the individual observations are considered the sampling units. This has bearing, for example, on how sandwich estimators are computed (see the **EMPIRICAL** option and the section “[Empirical Covariance \(“Sandwich”\) Estimators](#)” on page 3078).

In GLMM mode, the procedure assumes that the model contains random effects or possibly correlated errors, or that the data have a clustered structure. The parameters are then estimated by the techniques specified with the **METHOD=** option in the PROC GLIMMIX statement.

In general, adding one overdispersion parameter to a generalized linear model does not trigger the GLMM mode. For example, the model defined by the following statements is fit in GLM mode:

```
proc glimmix;
 model y = x1 x2 / dist=poisson;
 random _residual_;
run;
```



The parameters of the fixed effects are estimated by maximum likelihood, and the covariance matrix of the fixed-effects parameters is adjusted by the overdispersion parameter.

In a model with uncorrelated data you can trigger the GLMM mode by specifying a **SUBJECT=** or **GROUP=** effect in the **RANDOM** statement. For example, the following statements fit the model by using the residual pseudo-likelihood algorithm:

```
proc glimmix;
 class id;
 model y = x1 x2 / dist=poisson;
 random _residual_ / subject=id;
run;
```

If in doubt, you can determine whether a model was fit in GLM mode or GLMM mode. In GLM mode the “Covariance Parameter Estimates” table is not produced. Scale and dispersion parameters in the model appear in the “Parameter Estimates” table.

## Statistical Inference for Covariance Parameters

### The Likelihood Ratio Test

The likelihood ratio test (LRT) compares the likelihoods of two models where parameter estimates are obtained in two parameter spaces, the space  $\Omega$  and the restricted subspace  $\Omega_0$ . In the GLIMMIX procedure, the full model defines  $\Omega$  and the *test-specification* in the **COVTEST** statement determines the null parameter space  $\Omega_0$ . The likelihood ratio procedure consists of the following steps (see, for example, Bickel and Doksum 1977, p. 210):

1. Find the estimate  $\hat{\theta}$  of  $\theta \in \Omega$ . Compute the likelihood  $L(\hat{\theta})$ .
2. Find the estimate  $\hat{\theta}_0$  of  $\theta \in \Omega_0$ . Compute the likelihood  $L(\hat{\theta}_0)$ .
3. Form the likelihood ratio

$$\bar{\lambda} = \frac{L(\hat{\theta})}{L(\hat{\theta}_0)}$$

4. Find a function  $f(\bar{\lambda})$  that has a known distribution.  $f(\cdot)$  serves as the test statistic for the likelihood ratio test.

Please note the following regarding the implementation of these steps in the **COVTEST** statement of the GLIMMIX procedure.

- The function  $f(\cdot)$  in step 4 is always taken to be

$$\lambda = 2 \log \left\{ \bar{\lambda} \right\}$$

which is twice the difference between the log likelihoods for the full model and the model under the **COVTEST** restriction.

- For `METHOD=RSPL` and `METHOD=RMPL`, the test statistic is based on the restricted likelihood.
- For GLMMs involving pseudo-data, the test statistics are based on the pseudo-likelihood or the restricted pseudo-likelihood and are based on the final pseudo-data.
- The parameter space  $\Omega$  for the full model is typically not an unrestricted space. The GLIMMIX procedure imposes boundary constraints for variance components and scale parameters, for example. The specification of the subspace  $\Omega_0$  must be consistent with these full-model constraints; otherwise the test statistic  $\lambda$  does not have the needed distribution. You can remove the boundary restrictions with the `NOBOUND` option in the `PROC GLIMMIX` statement or the `NOBOUND` option in the `PARMS` statement.

### One- and Two-Sided Testing, Mixture Distributions

Consider testing the hypothesis  $H_0: \theta_i = 0$ . If  $\Omega$  is the open interval  $(0, \infty)$ , then only a one-sided alternative hypothesis is meaningful,

$$H_0: \theta_i = 0 \quad H_a: \theta_i > 0$$

This is the appropriate set of hypotheses, for example, when  $\theta_i$  is the variance of a G-side random effect. The positivity constraint on  $\Omega$  is required for valid conditional and marginal distributions of the data. Verbeke and Molenberghs (2003) refer to this situation as the constrained case.

However, if one focuses on the validity of the marginal distribution alone, then negative values for  $\theta_i$  might be permissible, provided that the marginal variance remains positive definite. In the vernacular or Verbeke and Molenberghs (2003), this is the unconstrained case. The appropriate alternative hypothesis is then two-sided,

$$H_0: \theta_i = 0 \quad H_a: \theta_i \neq 0$$

Several important issues are connected to the choice of hypotheses. The GLIMMIX procedure by default imposes constraints on some covariance parameters. For example, variances and scale parameters have a lower bound of 0. This implies a constrained setting with one-sided alternatives. If you specify the `NOBOUND` option in the `PROC GLIMMIX` statement, or the `NOBOUND` option in the `PARMS` statement, the boundary restrictions are lifted from the covariance parameters and the GLIMMIX procedure takes an unconstrained stance in the sense of Verbeke and Molenberghs (2003). The alternative hypotheses for variance components are then two-sided.

When  $H_0: \theta_i = 0$  and  $\Omega = (0, \infty)$ , the value of  $\theta_i$  under the null hypothesis is on the boundary of the parameter space. The distribution of the likelihood ratio test statistic  $\lambda$  is then nonstandard. In general, it is a mixture of distributions, and in certain special cases, it is a mixture of central chi-square distributions. Important contributions to the understanding of the asymptotic behavior of the likelihood ratio and score test statistic in this situation have been made by, for example, Self and Liang (1987); Shapiro (1988); Silvapulle and Silvapulle (1995). Stram and Lee (1994, 1995) applied the results of Self and Liang (1987) to likelihood ratio testing in the mixed model with uncorrelated errors. Verbeke and Molenberghs (2003) compared the score and likelihood ratio tests in random effects models with unstructured **G** matrix and provide further results on mixture distributions.

The GLIMMIX procedure recognizes the following special cases in the computation of  $p$ -values ( $\hat{\lambda}$  denotes the realized value of the test statistic). Notice that the probabilities of general chi-square mixture distributions do not equal linear combination of central chi-square probabilities (Davis 1977; Johnson, Kotz, and Balakrishnan 1994, Section 18.8).



1.  $\nu$  parameters are tested, and neither parameters specified under  $H_0$  nor nuisance parameters are on the boundary of the parameters space (Case 4 in Self and Liang 1987). The  $p$ -value is computed by the classical result:

$$p = \Pr\left(\chi_\nu^2 \geq \widehat{\lambda}\right)$$

2. One parameter is specified under  $H_0$  and it falls on the boundary. No other parameters are on the boundary (Case 5 in Self and Liang 1987).

$$p = \begin{cases} 1 & \widehat{\lambda} = 0 \\ 0.5 \Pr\left(\chi_1^2 \geq \widehat{\lambda}\right) & \widehat{\lambda} > 0 \end{cases}$$

Note that this implies a 50:50 mixture of a  $\chi_0^2$  and a  $\chi_1^2$  distribution. This is also Case 1 in Verbeke and Molenberghs (2000, p. 69).

3. Two parameters are specified under  $H_0$ , and one falls on the boundary. No nuisance parameters are on the boundary (Case 6 in Self and Liang 1987).

$$p = 0.5 \Pr\left(\chi_1^2 \geq \widehat{\lambda}\right) + 0.5 \Pr\left(\chi_2^2 \geq \widehat{\lambda}\right)$$

A special case of this scenario is the addition of a random effect to a model with a single random effect and unstructured covariance matrix (Case 2 in Verbeke and Molenberghs 2000, p. 70).

4. Removing  $j$  random effects from  $j + k$  uncorrelated random effects (Verbeke and Molenberghs 2003).

$$p = 2^{-j} \sum_{i=0}^j \binom{j}{i} \Pr\left(\chi_i^2 \geq \widehat{\lambda}\right)$$

Note that this case includes the case of testing a single random effects variance against zero, which leads to a 50:50 mixture of a  $\chi_0^2$  and a  $\chi_1^2$  as in 2.

5. Removing a random effect from an unstructured  $\mathbf{G}$  matrix (Case 3 in Verbeke and Molenberghs 2000, p. 71).

$$p = 0.5 \Pr\left(\chi_k^2 \geq \widehat{\lambda}\right) + 0.5 \Pr\left(\chi_{k-1}^2 \geq \widehat{\lambda}\right)$$

where  $k$  is the number of random effects (columns of  $\mathbf{G}$ ) in the full model. Case 5 in Self and Liang (1987) describes a special case.

When the GLIMMIX procedure determines that estimates of nuisance parameters (parameters not specified under  $H_0$ ) fall on the boundary, no mixture results are computed.

You can request that the procedure not use mixtures with the **CLASSICAL** option in the **COVTEST** statement. If mixtures are used, the Note column of the “Likelihood Ratio Tests of Covariance Parameters” table contains the “MI” entry. The “DF” entry is used when PROC GLIMMIX determines that the standard computation of  $p$ -values is appropriate. The “-” entry is used when the classical computation was used because the testing and model scenario does not match one of the special cases described previously.

## Handling the Degenerate Distribution

Likelihood ratio testing in mixed models invariably involves the chi-square distribution with zero degrees of freedom. The  $\chi_0^2$  random variable is degenerate at 0, and it occurs in two important circumstances. First, it is a component of mixtures, where typically the value of the test statistic is not zero. In that case, the contribution of the  $\chi_0^2$  component of the mixture to the  $p$ -value is nil. Second, a degenerate distribution of the test statistic occurs when the null model is identical to the full model—for example, if you test a hypothesis that does not impose any (new) constraints on the parameter space. The following statements test whether the **R** matrix in a variance component model is diagonal:

```
proc glimmix;
 class a b;
 model y = a;
 random b a*b;
 covtest diagR;
run;
```

Because no R-side covariance structure is specified (all random effects are G-side effects), the **R** matrix is diagonal in the full model and the **COVTEST** statement does not impose any further restriction on the parameter space. The likelihood ratio test statistic is zero. The **GLIMMIX** procedure computes the  $p$ -value as the probability to observe a value at least as large as the test statistic under the null hypothesis. Hence,

$$p = \Pr(\chi_0^2 \geq 0) = 1$$

## Wald Versus Likelihood Ratio Tests

The Wald test and the likelihood ratio tests are asymptotic tests, meaning that the distribution from which  $p$ -values are calculated for a finite number of samples draws on the distribution of the test statistic as the sample size grows to infinity. The Wald test is a simple test that is easy to compute based only on parameter estimates and their (asymptotic) standard errors. The likelihood ratio test, on the other hand, requires the likelihoods of the full model and the model reduced under  $H_0$ . It is computationally more demanding, but also provides the asymptotically more powerful and reliable test. The likelihood ratio test is almost always preferable to the Wald test, unless computational demands make it impractical to refit the model.

## Confidence Bounds Based on Likelihoods

Families of statistical tests can be inverted to produce confidence limits for parameters. The confidence region for parameter  $\theta$  is the set of values for which the corresponding test fails to reject  $H: \theta = \theta_0$ . When parameters are estimated by maximum likelihood or a likelihood-based technique, it is natural to consider the likelihood ratio test statistic for  $H$  in the test inversion. When there are multiple parameters in the model, however, you need to supply values for these nuisance parameters during the test inversion as well.

In the following, suppose that  $\theta$  is the covariance parameter vector and that one of its elements,  $\theta$ , is the parameter of interest for which you want to construct a confidence interval. The other elements of  $\theta$  are collected in the nuisance parameter vector  $\theta_2$ . Suppose that  $\hat{\theta}$  is the estimate of  $\theta$  from the overall optimization and that  $L(\hat{\theta})$  is the likelihood evaluated at that estimate. If estimation is based on pseudo-data, then  $L(\hat{\theta})$  is the pseudo-likelihood based on the final pseudo-data. If estimation uses a residual (restricted) likelihood, then  $L$  denotes the restricted maximum likelihood and  $\hat{\theta}$  is the REML estimate.

**Profile Likelihood Bounds**

The likelihood ratio test statistic for testing  $H: \theta = \theta_0$  is

$$2 \left\{ \log \left\{ L(\hat{\theta}) \right\} - \log \left\{ L(\theta_0, \hat{\theta}_2) \right\} \right\}$$

where  $\hat{\theta}_2$  is the likelihood estimate of  $\theta_2$  under the restriction that  $\theta = \theta_0$ . To invert this test, a function is defined that returns the maximum likelihood for a fixed value of  $\theta$  by seeking the maximum over the remaining parameters. This function is termed the profile likelihood (Pawitan 2001, Ch. 3.4),

$$\lambda_p = L(\theta_2|\tilde{\theta}) = \sup_{\theta_2} L(\tilde{\theta}, \theta_2)$$

In computing  $\lambda_p$ ,  $\theta$  is fixed at  $\tilde{\theta}$  and  $\theta_2$  is estimated. In mixed models, this step typically requires a separate, iterative optimization to find the estimate of  $\theta_2$  while  $\theta$  is held fixed. The  $(1 - \alpha) \times 100\%$  profile likelihood confidence interval for  $\theta$  is then defined as the set of values for  $\tilde{\theta}$  that satisfy

$$2 \left\{ \log \left\{ L(\hat{\theta}) \right\} - \log \left\{ L(\theta_2|\tilde{\theta}) \right\} \right\} \leq \chi_{1,(1-\alpha)}^2$$

The GLIMMIX procedure seeks the values  $\tilde{\theta}_l$  and  $\tilde{\theta}_u$  that mark the endpoints of the set around  $\hat{\theta}$  that satisfy the inequality. The values  $(\tilde{\theta}_l$  and  $\tilde{\theta}_u)$  are then called the  $(1 - \alpha) \times 100\%$  confidence bounds for  $\theta$ . Note that the GLIMMIX procedure assumes that the confidence region is not disjoint and relies on the convexity of  $L(\hat{\theta})$ .

It is not always possible to find values  $\tilde{\theta}_l$  and  $\tilde{\theta}_u$  that satisfy the inequalities. For example, when the parameter space is  $(0, \infty)$  and

$$2 \left\{ \log \left\{ L(\hat{\theta}) \right\} - \log \left\{ L(\theta_2|0) \right\} \right\} > \chi_{1,(1-\alpha)}^2$$

a lower bound cannot be found at the desired confidence level. The GLIMMIX procedure reports the right-tail probabilities that are achieved by the underlying likelihood ratio statistic separately for lower and upper bounds.

**Effect of Scale Parameter**

When a scale parameter  $\phi$  is eliminated from the optimization by profiling from the likelihood, some parameters might be expressed as ratios with  $\phi$  in the optimization. This is the case, for example, in variance component models. The profile likelihood confidence bounds are reported on the scale of the parameter in the overall optimization. In case parameters are expressed as ratios with  $\phi$  or functions of  $\phi$ , the column RatioEstimate is added to the “Covariance Parameter Estimates” table. If parameters are expressed as ratios with  $\phi$  and you want confidence bounds for the unscaled parameter, you can prevent profiling of  $\phi$  from the optimization with the NOPROFILE option in the PROC GLIMMIX statement, or choose estimated likelihood confidence bounds with the TYPE=ELR suboption of the CL option in the COVTEST statement. Note that the NOPROFILE option is automatically in effect with METHOD=LAPLACE and METHOD=QUAD.

**Estimated Likelihood Bounds**

Computing profile likelihood ratio confidence bounds can be computationally expensive, because of the need to repeatedly estimate  $\theta_2$  in a constrained optimization. A computationally simpler method to construct confidence bounds from likelihood-based quantities is to use the estimated likelihood (Pawitan 2001, Ch. 10.7) instead of the profile likelihood. An estimated likelihood technique replaces the nuisance parameters

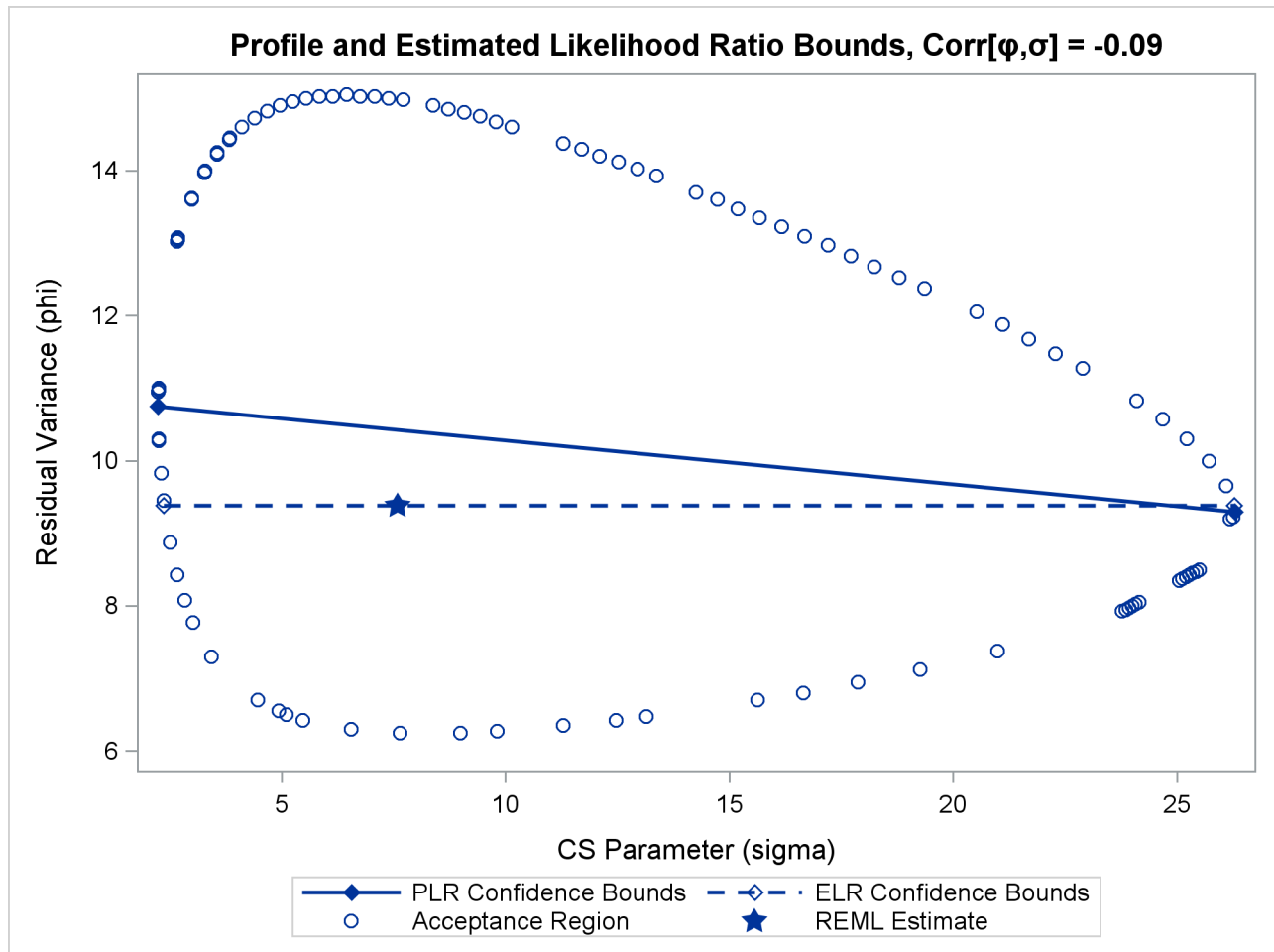
in the test inversion with some other estimate. If you choose the TYPE=ELR suboption of the CL option in the COVTEST statement, the GLIMMIX procedure holds the nuisance parameters fixed at the likelihood estimates. The estimated likelihood statistic for inversion is then

$$\lambda_e = L(\tilde{\theta}, \hat{\theta}_2)$$

where  $\hat{\theta}_2$  are the elements of  $\hat{\theta}$  that correspond to the nuisance parameters. As the values of  $\tilde{\theta}$  are varied, no reestimation of  $\theta_2$  takes place. Although computationally more economical, estimated likelihood intervals do not take into account the variability associated with the nuisance parameters. Their coverage can be satisfactory if the parameter of interest is not (or only weakly) correlated with the nuisance parameters. Estimated likelihood ratio intervals can fall short of the nominal coverage otherwise.

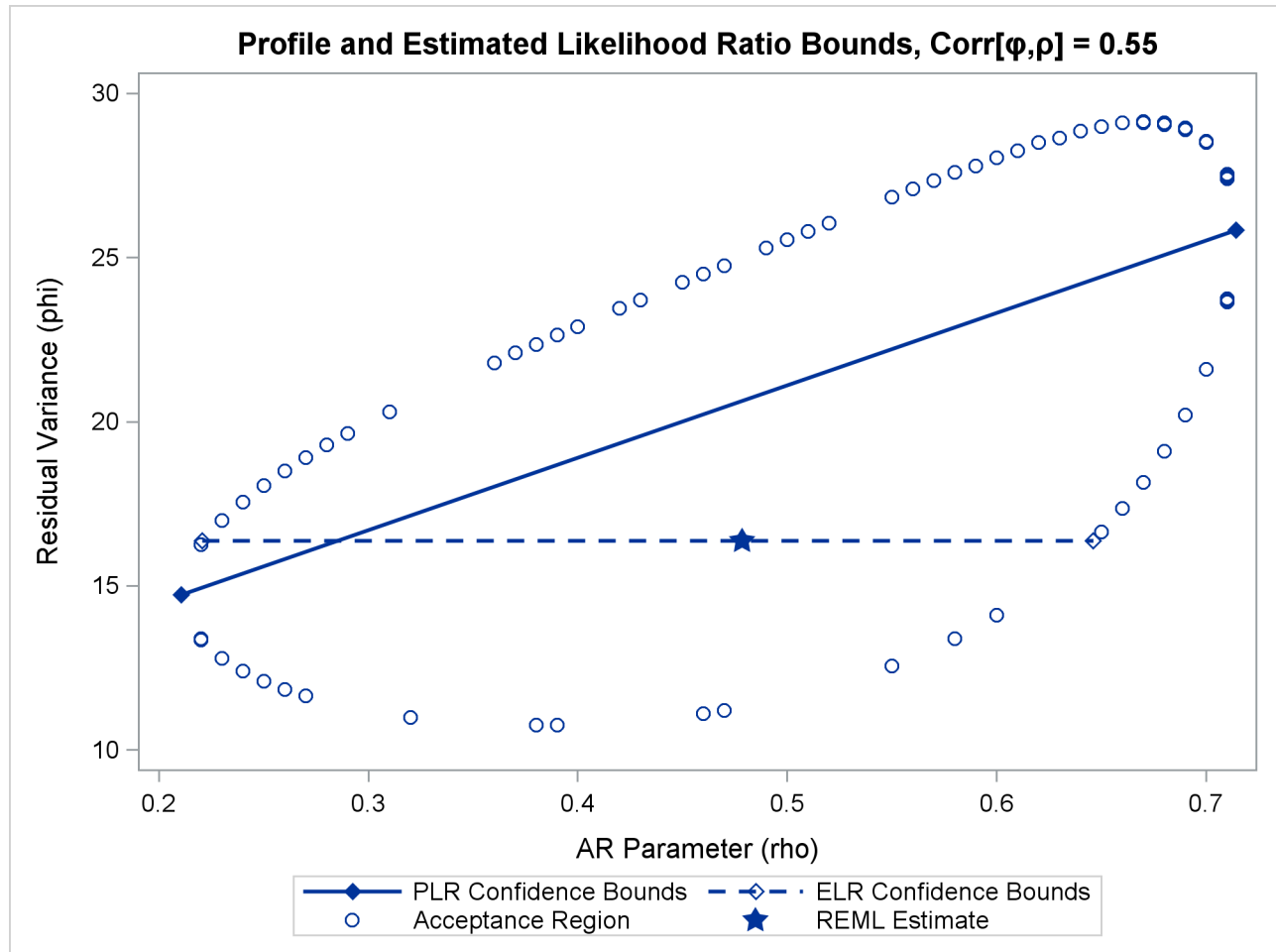
Figure 41.11 depicts profile and estimated likelihood ratio intervals for the parameter  $\sigma$  in a two-parameter compound-symmetric model,  $\theta = [\sigma, \phi]'$ , in which the correlation between the covariance parameters is small. The elliptical shape traces the set of values for which the likelihood ratio test rejects the hypothesis of equality with the solution. The interior of the ellipse is the “acceptance” region of the test. The solid and dashed lines depict the PLR and ELR confidence limits for  $\sigma$ , respectively. Note that both confidence limits intersect the ellipse and that the ELR interval passes through the REML estimate of  $\phi$ . The PLR bounds are found as those points intersecting the ellipse, where  $\phi$  equals the constrained REML estimate.

**Figure 41.11** PLR and ELR Intervals, Small Correlation between Parameters



The major axes of the ellipse in Figure 41.11 are nearly aligned with the major axes of the coordinate system. As a consequence, the line connecting the PLR bounds passes close to the REML estimate in the full model. As a result, ELR bounds will be similar to PLR bounds. Figure 41.12 displays a different scenario, a two-parameter AR(1) covariance structure with a more substantial correlation between the AR(1) parameter ( $\rho$ ) and the residual variance ( $\phi$ ).

**Figure 41.12** PLR and ELR Intervals, Large Correlation between Parameters



The correlation between the parameters yields an acceptance region whose major axes are not aligned with the axes of the coordinate system. The ELR bound for  $\rho$  passes through the REML estimate of  $\phi$  from the full model and is much shorter than the PLR interval. The PLR interval aligns with the major axis of the acceptance region; it is the preferred confidence interval.

## Degrees of Freedom Methods

### Between-Within Degrees of Freedom Approximation

The `DDFM=BETWITHIN` option divides the residual degrees of freedom into between-subject and within-subject portions. PROC GLIMMIX then determines whether a fixed effect changes within any subject. If so, it assigns within-subject degrees of freedom to the effect; otherwise, it assigns the between-subject degrees of freedom to the effect (Schluchter and Elashoff 1990). If the GLIMMIX procedure does not process the data by subjects, the `DDFM=BETWITHIN` option has no effect. See the section “Processing by Subjects” on page 3082 for more information.

If multiple within-subject effects contain classification variables, the within-subject degrees of freedom are partitioned into components that correspond to the subject-by-effect interactions.

One exception to the preceding method is the case where you model only R-side covariation with an unstructured covariance matrix (`TYPE=UN`). In this case, all fixed effects are assigned the between-subject degrees of freedom to provide for better small-sample approximations to the relevant sampling distributions. The `DDFM=BETWITHIN` method is the default for models with only R-side random effects and a `SUBJECT=` option.

### Containment Degrees of Freedom Approximation

The `DDFM=CONTAIN` method is carried out as follows: Denote the fixed effect in question as *A* and search the G-side random effect list for the effects that *syntactically* contain *A*. For example, the effect *B(A)* contains *A*, but the effect *C* does not, even if it has the same levels as *B(A)*.

Among the random effects that contain *A*, compute their rank contributions to the  $[X \ Z]$  matrix (in order). The denominator degrees of freedom that is assigned to *A* is the smallest of these rank contributions. If no effects are found, the denominator degrees of freedom for *A* is set equal to the residual degrees of freedom,  $n - \text{rank}[X \ Z]$ . This choice of degrees of freedom is the same as for the tests performed for balanced split-plot designs and should be adequate for moderately unbalanced designs.

**NOTE:** If you have a *Z* matrix with a large number of columns, the overall memory requirements and the computing time after convergence can be substantial for the containment method. In this case, you might want to use a different degrees-of-freedom method, such as `DDFM=RESIDUAL`, `DDFM=NONE`, or `DDFM=BETWITHIN`.

### Satterthwaite Degrees of Freedom Approximation

The `DDFM=SATTERTHWAITE` option in the `MODEL` statement requests that denominator degrees of freedom in *t* tests and *F* tests be computed according to a general Satterthwaite approximation.

The general Satterthwaite approximation computed in PROC GLIMMIX for the test

$$H: \mathbf{L} \begin{bmatrix} \hat{\boldsymbol{\beta}} \\ \hat{\boldsymbol{\gamma}} \end{bmatrix} = \mathbf{0}$$

is based on the *F* statistic

$$F = \frac{\begin{bmatrix} \hat{\boldsymbol{\beta}} \\ \hat{\boldsymbol{\gamma}} \end{bmatrix}' \mathbf{L}' (\mathbf{LCL}')^{-1} \mathbf{L} \begin{bmatrix} \hat{\boldsymbol{\beta}} \\ \hat{\boldsymbol{\gamma}} \end{bmatrix}}{r}$$

where  $r = \text{rank}(\mathbf{LCL}')$  and  $\mathbf{C}$  is the approximate variance matrix of  $[\hat{\boldsymbol{\beta}}', \hat{\boldsymbol{\gamma}}' - \boldsymbol{\gamma}']'$ . See the section “Estimated Precision of Estimates” on page 3056 and the section “Aspects Common to Adaptive Quadrature and Laplace Approximation” on page 3064.

The approximation proceeds by first performing the spectral decomposition  $\mathbf{LCL}' = \mathbf{U}'\mathbf{D}\mathbf{U}$ , where  $\mathbf{U}$  is an orthogonal matrix of eigenvectors and  $\mathbf{D}$  is a diagonal matrix of eigenvalues, both of dimension  $r \times r$ . Define  $\mathbf{b}_j$  to be the  $j$ th row of  $\mathbf{UL}$ , and let

$$v_j = \frac{2(D_j)^2}{\mathbf{g}'_j \mathbf{A} \mathbf{g}_j}$$

where  $D_j$  is the  $j$ th diagonal element of  $\mathbf{D}$  and  $\mathbf{g}_j$  is the gradient of  $\mathbf{b}_j \mathbf{C} \mathbf{b}'_j$  with respect to  $\boldsymbol{\theta}$ , evaluated at  $\hat{\boldsymbol{\theta}}$ . The matrix  $\mathbf{A}$  is the asymptotic variance-covariance matrix of  $\hat{\boldsymbol{\theta}}$ , which is obtained from the second derivative matrix of the likelihood equations. You can display this matrix with the `ASYCOV` option in the `PROC GLIMMIX` statement.

Finally, let

$$E = \sum_{j=1}^r \frac{v_j}{v_j - 2} I(v_j > 2)$$

where the indicator function eliminates terms for which  $v_j \leq 2$ . The degrees of freedom for  $F$  are then computed as

$$\nu = \frac{2E}{E - \text{rank}(\mathbf{L})}$$

provided  $E > r$ ; otherwise  $\nu$  is set to 0.

In the one-dimensional case, when `PROC GLIMMIX` computes a  $t$  test, the Satterthwaite degrees of freedom for the  $t$  statistic

$$t = \frac{Y' \begin{bmatrix} \hat{\boldsymbol{\beta}} \\ \hat{\boldsymbol{\gamma}} \end{bmatrix}}{Y' \mathbf{C} \mathbf{I}}$$

are computed as

$$\nu = \frac{2(Y' \mathbf{C} \mathbf{I})^2}{\mathbf{g}' \mathbf{A} \mathbf{g}}$$

where  $\mathbf{g}$  is the gradient of  $Y' \mathbf{C} \mathbf{I}$  with respect to  $\boldsymbol{\theta}$ , evaluated at  $\hat{\boldsymbol{\theta}}$ .

The calculation of Satterthwaite degrees of freedom requires extra memory to hold  $q$  matrices that are the size of the mixed model equations, where  $q$  is the number of covariance parameters. Extra computing time is also required to process these matrices. The implemented Satterthwaite method is intended to produce an accurate  $F$  approximation; however, the results can differ from those produced by `PROC GLM`. Also, the small-sample properties of this approximation have not been extensively investigated for the various models available with `PROC GLIMMIX`.

## Kenward-Roger Degrees of Freedom Approximation

The `DDFM=KENWARDROGER` option prompts PROC GLIMMIX to compute the denominator degrees of freedom in  $t$  tests and  $F$  tests by using the approximation described in Kenward and Roger (1997). For inference on the linear combination  $L\beta$  in a Gaussian linear model, they propose a scaled Wald statistic

$$F^* = \lambda F \\ = \frac{\lambda}{l} (\hat{\beta} - \beta)^T L (L^T \hat{\Phi}_A L)^{-1} L^T (\hat{\beta} - \beta),$$

where  $l = \text{rank}(L)$ ,  $\hat{\Phi}_A$  is a bias-adjusted estimator of the precision of  $\hat{\beta}$ , and  $0 < \lambda < 1$ . An appropriate  $F_{l,m}$  approximation to the sampling distribution of  $F^*$  is derived by matching the first two moments of  $F^*$  with those from the approximating  $F$  distribution and solving for the values of  $\lambda$  and  $m$ . The value of  $m$  thus derived is the Kenward-Roger degrees of freedom. The precision estimator  $\hat{\Phi}_A$  is bias-adjusted, in contrast to the conventional precision estimator  $\Phi(\hat{\sigma}) = (X'V(\hat{\sigma})^{-1}X)^{-1}$ , which is obtained by simply replacing  $\sigma$  with  $\hat{\sigma}$  in  $\Phi(\sigma)$ , the asymptotic variance of  $\hat{\beta}$ . This method uses  $\hat{\Phi}_A$  to address the fact that  $\Phi(\hat{\sigma})$  is a biased estimator of  $\Phi(\sigma)$ , and  $\Phi(\sigma)$  itself underestimates  $\text{var}(\hat{\beta})$  when  $\sigma$  is unknown. This bias-adjusted precision estimator is also discussed in Prasad and Rao (1990); Harville and Jeske (1992); Kackar and Harville (1984).

By default, the observed information matrix of the covariance parameter estimates is used in the calculations. For covariance structures that have nonzero second derivatives with respect to the covariance parameters, the Kenward-Roger covariance matrix adjustment includes a second-order term. This term can result in standard error shrinkage. Also, the resulting adjusted covariance matrix can then be indefinite and is not invariant under reparameterization. The `FIRSTORDER` suboption of the `DDFM=KENWARDROGER` option eliminates the second derivatives from the calculation of the covariance matrix adjustment. For scalar estimable functions, the resulting estimator is referred to as the Prasad-Rao estimator  $\tilde{m}^{\text{PR}}$  in Harville and Jeske (1992). You can use the `COVB(DETAILS)` option to diagnose the adjustments that PROC GLIMMIX makes to the covariance matrix of fixed-effects parameter estimates. An application with `DDFM=KENWARDROGER` is presented in Example 41.8. The following are examples of covariance structures that generally lead to nonzero second derivatives: `TYPE=ANTE(1)`, `TYPE=AR(1)`, `TYPE=ARH(1)`, `TYPE=ARMA(1,1)`, `TYPE=CHOL`, `TYPE=CSH`, `TYPE=FA0( $q$ )`, `TYPE=TOEPH`, `TYPE=UNR`, and all `TYPE=SP()` structures.

`DDFM=KENWARDROGER2` specifies an improved F approximation of the `DDFM=KENWARD-ROGER` type that uses a less biased precision estimator, as proposed by Kenward and Roger (2009). An important feature of the KR2 precision estimator is that it is invariant under reparameterization within the classes of intrinsically linear and intrinsically linear inverse covariance structures. For the invariance to hold within these two classes of covariance structures, a modified expected Hessian matrix is used in the computation of the covariance matrix of  $\sigma$ . The two cells classified as “Modified” scoring for RxPL estimation in Table 41.21 give the modified Hessian expressions for the cases where the scale parameter is profiled and not profiled. You can enforce the use of the modified expected Hessian matrix by specifying both the `EXPHESSIAN` and `SCOREMOD` options in the PROC GLIMMIX statement. Kenward and Roger (2009) note that for an intrinsically linear covariance parameterization, `DDFM=KR2` produces the same precision estimator as that obtained using `DDFM=KR(FIRSTORDER)`.



## Empirical Covariance (“Sandwich”) Estimators

### Residual-Based Estimators

The GLIMMIX procedure can compute the classical sandwich estimator of the covariance matrix of the fixed effects, as well as several bias-adjusted estimators. This requires that the model is either an (overdispersed) GLM or a GLMM that can be processed by subjects (see the section “Processing by Subjects” on page 3082).

Consider a statistical model of the form

$$\mathbf{Y} = \boldsymbol{\mu} + \boldsymbol{\epsilon}, \quad \boldsymbol{\epsilon} \sim (\mathbf{0}, \boldsymbol{\Sigma})$$

The general expression of a sandwich covariance estimator is then

$$c \times \widehat{\boldsymbol{\Omega}} \left( \sum_{i=1}^m \mathbf{A}_i \widehat{\mathbf{D}}_i' \widehat{\boldsymbol{\Sigma}}_i^{-1} \mathbf{F}_i' \mathbf{e}_i \mathbf{e}_i' \mathbf{F}_i \widehat{\boldsymbol{\Sigma}}_i^{-1} \widehat{\mathbf{D}}_i \mathbf{A}_i \right) \widehat{\boldsymbol{\Omega}}$$

where  $\mathbf{e}_i = \mathbf{y}_i - \widehat{\boldsymbol{\mu}}_i$ ,  $\boldsymbol{\Omega} = (\mathbf{D}'\boldsymbol{\Sigma}^{-1}\mathbf{D})^{-}$ .

For a GLMM estimated by one of the pseudo-likelihood techniques that involve linearization, you can make the following substitutions:  $\mathbf{Y} \rightarrow \mathbf{P}$ ,  $\boldsymbol{\Sigma} \rightarrow \mathbf{V}(\boldsymbol{\theta})$ ,  $\mathbf{D} \rightarrow \mathbf{X}$ ,  $\widehat{\boldsymbol{\mu}} \rightarrow \mathbf{X}\widehat{\boldsymbol{\beta}}$ . These matrices are defined in the section “Pseudo-likelihood Estimation Based on Linearization” on page 3054.

The various estimators computed by the GLIMMIX procedure differ in the choice of the constant  $c$  and the matrices  $\mathbf{F}_i$  and  $\mathbf{A}_i$ . You obtain the classical estimator, for example, with  $c = 1$ , and  $\mathbf{F}_i = \mathbf{A}_i$  equal to the identity matrix.

The **EMPIRICAL=ROOT** estimator of Kauermann and Carroll (2001) is based on the approximation

$$\text{Var}[\mathbf{e}_i \mathbf{e}_i'] \approx (\mathbf{I} - \mathbf{H}_i) \boldsymbol{\Sigma}_i$$

where  $\mathbf{H}_i = \mathbf{D}_i \boldsymbol{\Omega} \mathbf{D}_i' \boldsymbol{\Sigma}_i^{-1}$ . The **EMPIRICAL=FIRORES** estimator is based on the approximation

$$\text{Var}[\mathbf{e}_i \mathbf{e}_i'] \approx (\mathbf{I} - \mathbf{H}_i) \boldsymbol{\Sigma}_i (\mathbf{I} - \mathbf{H}_i')$$

of Mancl and DeRouen (2001). Finally, the **EMPIRICAL=FIROEEQ** estimator is based on approximating an unbiased estimating equation (Fay and Graubard 2001). For this estimator,  $\mathbf{A}_i$  is a diagonal matrix with entries

$$[\mathbf{A}_i]_{jj} = (1 - \min\{r, [\mathbf{Q}]_{jj}\})^{-1/2}$$

where  $\mathbf{Q} = \mathbf{D}_i' \widehat{\boldsymbol{\Sigma}}_i^{-1} \mathbf{D}_i \widehat{\boldsymbol{\Omega}}$ . The optional number  $0 \leq r < 1$  is chosen to provide an upper bound on the correction factor. For  $r = 0$ , the classical sandwich estimator results. PROC GLIMMIX chooses as default value  $r = 3/4$ . The diagonal entries of  $\mathbf{A}_i$  are then no greater than 2.

Table 41.22 summarizes the components of the computation for the GLMM based on linearization, where  $m$  denotes the number of subjects and  $k$  is the rank of  $\mathbf{X}$ .

**Table 41.22** Empirical Covariance Estimators for a Linearized GLMM

| EMPIRICAL= | $c$                                                                       | $A_i$                                                      | $F_i$                                 |
|------------|---------------------------------------------------------------------------|------------------------------------------------------------|---------------------------------------|
| CLASSICAL  | 1                                                                         | $\mathbf{I}$                                               | $\mathbf{I}$                          |
| DF         | $\begin{cases} \frac{m}{m-k} & m > k \\ 1 & \text{otherwise} \end{cases}$ | $\mathbf{I}$                                               | $\mathbf{I}$                          |
| ROOT       | 1                                                                         | $\mathbf{I}$                                               | $(\mathbf{I} - \mathbf{H}'_i)^{-1/2}$ |
| FIRORES    | 1                                                                         | $\mathbf{I}$                                               | $(\mathbf{I} - \mathbf{H}'_i)^{-1}$   |
| FIROEEQ(r) | 1                                                                         | $\text{Diag}\{(1 - \min\{r, [\mathbf{Q}]_{jj}\})^{-1/2}\}$ | $\mathbf{I}$                          |

Computation of an empirical variance estimator requires that the data can be processed by independent sampling units. This is always the case in GLMs. In this case,  $m$  equals the sum of all frequencies. In GLMMs, the empirical estimators require that the data consist of multiple subjects. In that case,  $m$  equals the number of subjects as per the “Dimensions” table. The following section discusses how the GLIMMIX procedure determines whether the data can be processed by subjects. The section “GLM Mode or GLMM Mode” on page 3067 explains how PROC GLIMMIX determines whether a model is fit in GLM mode or in GLMM mode.

### Design-Adjusted MBN Estimator

Morel (1989) and Morel, Bokossa, and Neerchal (2003) suggested a bias correction of the classical sandwich estimator that rests on an additive correction of the residual crossproducts and a sample size correction. This estimator is available with the EMPIRICAL=MBN option in the PROC GLIMMIX statement. In the notation of the previous section, the residual-based MBN estimator can be written as

$$\widehat{\Omega} \left( \sum_{i=1}^m \widehat{\mathbf{D}}'_i \widehat{\Sigma}_i^{-1} (c \mathbf{e}_i \mathbf{e}'_i + \mathbf{B}_i) \widehat{\Sigma}_i^{-1} \widehat{\mathbf{D}}_i \right) \widehat{\Omega}$$

where

- $c = (f - 1)/(f - k) \times m/(m - 1)$  or  $c = 1$  when you specify the EMPIRICAL=MBN(NODF) option
- $f$  is the sum of the frequencies
- $k$  equals the rank of  $\mathbf{X}$
- $\mathbf{B}_i = \delta_m \phi \widehat{\Sigma}_i$
- $\phi = \max \{r, \text{trace}(\widehat{\Omega} \mathbf{M}) / k^*\}$
- $\mathbf{M} = \sum_{i=1}^m \widehat{\mathbf{D}}'_i \widehat{\Sigma}_i^{-1} \mathbf{e}_i \mathbf{e}'_i \widehat{\Sigma}_i^{-1} \widehat{\mathbf{D}}_i$
- $k^* = k$  if  $m \geq k$ , otherwise  $k^*$  equals the number of nonzero singular values of  $\widehat{\Omega} \mathbf{M}$
- $\delta_m = k/(m - k)$  if  $m > (d + 1)k$  and  $\delta_m = 1/d$  otherwise
- $d \geq 1$  and  $0 \leq r \leq 1$  are parameters supplied with the *mbn-options* of the EMPIRICAL=MBN(*mbn-options*) option. The default values are  $d = 2$  and  $r = 1$ . When the NODF option is in effect, the factor  $c$  is set to 1.

Rearranging terms, the MBN estimator can also be written as an additive adjustment to a sample-size corrected classical sandwich estimator

$$c \times \widehat{\Omega} \left( \sum_{i=1}^m \widehat{D}_i' \widehat{\Sigma}_i^{-1} \mathbf{e}_i \mathbf{e}_i' \widehat{\Sigma}_i^{-1} \widehat{D}_i \right) \widehat{\Omega} + \delta_m \phi \widehat{\Omega}$$

Because  $\delta_m$  is of order  $m^{-1}$ , the additive adjustment to the classical estimator vanishes as the number of independent sampling units (subjects) increases. The parameter  $\phi$  is a measure of the design effect (Morel, Bokossa, and Neerchal 2003). Besides good statistical properties in terms of Type I error rates in small- $m$  situations, the MBN estimator also has the desirable property of recovering rank when the number of sampling units is small. If  $m < k$ , the “meat” piece of the classical sandwich estimator is essentially a sum of rank one matrices. A small number of subjects relative to the rank of  $\mathbf{X}$  can result in a loss of rank and subsequent loss of numerator degrees of freedom in tests. The additive MBN adjustment counters the rank exhaustion. You can examine the rank of an adjusted covariance matrix with the **COVB(Details)** option in the **MODEL** statement.

When the principle of the MBN estimator is applied to the likelihood-based empirical estimator, you obtain

$$\mathbf{H}(\widehat{\alpha})^{-1} \left( \sum_{i=1}^m c \mathbf{g}_i(\widehat{\alpha}) \mathbf{g}_i(\widehat{\alpha})' + \mathbf{B}_i \right) \mathbf{H}(\widehat{\alpha})^{-1}$$

where  $\mathbf{B}_i = -\delta_m \phi \mathbf{H}_i(\widehat{\alpha})$ , and  $\mathbf{H}_i(\widehat{\alpha})$  is the second derivative of the log likelihood for the  $i$ th sampling unit (subject) evaluated at the vector of parameter estimates,  $\widehat{\alpha}$ . Also,  $\mathbf{g}_i(\widehat{\alpha})$  is the first derivative of the log likelihood for the  $i$ th sampling unit. This estimator is computed if you request **EMPIRICAL=MBN** with **METHOD=LAPLACE** or **METHOD=QUAD**.

In terms of adjusting the classical likelihood-based estimator (White 1982), the likelihood MBN estimator can be written as

$$c \times \mathbf{H}(\widehat{\alpha})^{-1} \left( \sum_{i=1}^m \mathbf{g}_i(\widehat{\alpha}) \mathbf{g}_i(\widehat{\alpha})' \right) \mathbf{H}(\widehat{\alpha})^{-1} - \delta_m \phi \mathbf{H}(\widehat{\alpha})^{-1}$$

The parameter  $\phi$  is determined as

- $\phi = \max \{r, \text{trace}(-\mathbf{H}(\widehat{\alpha})^{-1} \mathbf{M}) / k^*\}$
- $\mathbf{M} = \sum_{i=1}^m \mathbf{g}_i(\widehat{\alpha}) \mathbf{g}_i(\widehat{\alpha})'$
- $k^* = k$  if  $m \geq k$ , otherwise  $k^*$  equals the number of nonzero singular values of  $-\mathbf{H}(\widehat{\alpha})^{-1} \mathbf{M}$

---

## Exploring and Comparing Covariance Matrices

If you use an empirical (sandwich) estimator with the **EMPIRICAL=** option in the **PROC GLIMMIX** statement, the procedure replaces the model-based estimator of the covariance of the fixed effects with the sandwich estimator. This affects aspects of inference, such as prediction standard errors, tests of fixed effects, estimates, contrasts, and so forth. Similarly, if you choose the **DDFM=KENWARDROGER** degrees-of-freedom method in the **MODEL** statement, **PROC GLIMMIX** adjusts the model-based covariance matrix

of the fixed effects according to Kenward and Roger (1997) or according to Kackar and Harville (1984) and Harville and Jeske (1992).

In this situation, the `COVB(Details)` option in the `MODEL` statement has two effects. The `GLIMMIX` procedure displays the (adjusted) covariance matrix of the fixed effects and the model-based covariance matrix (the ODS name of the table with the model-based covariance matrix is `CovBModelBased`). The procedure also displays a table of statistics for the unadjusted and adjusted covariance matrix and for their comparison. The ODS name of this table is `CovBDetails`.

If the model-based covariance matrix is not replaced with an adjusted estimator, the `COVB(Details)` option displays the model-based covariance matrix and provides diagnostic measures for it in the “CovB-Details” table.

The table generated by the `COVB(Details)` option consists of several sections. See [Example 41.8](#) for an application.

The trace and log determinant of covariance matrices are general scalar summaries that are sometimes used in direct comparisons, or in formulating other statistics, such as the difference of log determinants. The trace simply represents the sum of the variances of all fixed-effects parameters. If a matrix is indefinite, the determinant is reported instead of the log determinant.

The model-based and adjusted covariance matrices should have the same general makeup of eigenvalues. There should not be any negative eigenvalues, and they should have the same numbers of positive and zero eigenvalues. A reduction in rank due to the adjustment is troublesome for aspects of inference. Negative eigenvalues are listed in the table only if they occur, because a covariance matrix should be at least positive semi-definite. However, the `GLIMMIX` procedure examines the model-based and adjusted covariance matrix for negative eigenvalues. The condition numbers reported by `PROC GLIMMIX` for positive (semi-)definite matrices are computed as the ratio of the largest and smallest nonzero eigenvalue. A large condition number reflects poor conditioning of the matrix.

Matrix norms are extensions of the concept of vector norms to measure the “length” of a matrix. The Frobenius norm of an  $(n \times m)$  matrix  $\mathbf{A}$  is the direct equivalent of the Euclidean vector norm, the square root of the sum of the squared elements,

$$\|\mathbf{A}\|_F = \sqrt{\sum_{i=1}^n \sum_{j=1}^n a_{ij}^2}$$

The  $\infty$ - and 1-norms of matrix  $\mathbf{A}$  are the maximum absolute row and column sums, respectively:

$$\|\mathbf{A}\|_\infty = \max \left\{ \sum_{j=1}^m |a_{ij}| : i = 1, \dots, n \right\}$$

$$\|\mathbf{A}\|_1 = \max \left\{ \sum_{i=1}^n |a_{ij}| : j = 1, \dots, m \right\}$$

These two norms are identical for symmetric matrices.

The “Comparison” section of the “CovBDetails” table provides several statistics that set the matrices in relationship. The concordance correlation reported by the `GLIMMIX` procedure is a standardized measure

of the closeness of the model-based and adjusted covariance matrix. It is a slight modification of the covariance concordance correlation in Vonesh, Chinchilli, and Pu (1996) and Vonesh and Chinchilli (1997, Ch. 8.3). Denote as  $\mathbf{\Omega}$  the  $(p \times p)$  model-based covariance matrix and as  $\mathbf{\Omega}_a$  the adjusted matrix. Suppose that  $\mathbf{K}$  is the matrix obtained from the identity matrix of size  $p$  by replacing diagonal elements corresponding to singular rows in  $\mathbf{\Omega}$  with zeros. The lower triangular portion of  $\mathbf{\Omega}^{-1/2}\mathbf{\Omega}_a\mathbf{\Omega}^{-1/2}$  is stored in vector  $\boldsymbol{\omega}$  and the lower triangular portion of  $\mathbf{K}$  is stored in vector  $\mathbf{k}$ . The matrix  $\mathbf{\Omega}^{-1/2}$  is constructed from an eigenanalysis of  $\mathbf{\Omega}$  and is symmetric. The covariance concordance correlation is then

$$r(\boldsymbol{\omega}) = 1 - \frac{\|\boldsymbol{\omega} - \mathbf{k}\|^2}{\|\boldsymbol{\omega}\|^2 + \|\mathbf{k}\|^2}$$

This measure is 1 if  $\mathbf{\Omega} = \mathbf{\Omega}_a$ . If  $\boldsymbol{\omega}$  is orthogonal to  $\mathbf{k}$ , there is total disagreement between the model-based and the adjusted covariance matrix and  $r(\boldsymbol{\omega})$  is zero.

The discrepancy function reported by PROC GLIMMIX is computed as

$$d = \log\{|\mathbf{\Omega}|\} - \log\{|\mathbf{\Omega}_a|\} + \text{trace}\{\mathbf{\Omega}_a\mathbf{\Omega}^{-}\} - \text{rank}\{\mathbf{\Omega}\}$$

In diagnosing departures between an assumed covariance structure and  $\text{Var}[\mathbf{Y}]$ —using an empirical estimator—Vonesh, Chinchilli, and Pu (1996) find that the concordance correlation is useful in detecting gross departures and propose  $\lambda = n_s d$  to test the correctness of the assumed model, where  $n_s$  denotes the number of subjects.

## Processing by Subjects

Some mixed models can be expressed in different but mathematically equivalent ways with PROC GLIMMIX statements. While equivalent statements lead to equivalent statistical models, the data processing and estimation phase can be quite different, depending on how you write the GLIMMIX statements. For example, the particular use of the **SUBJECT=** option in the **RANDOM** statement affects data processing and estimation. Certain options are available only when the data are processed by subject, such as the **EMPIRICAL** option in the **PROC GLIMMIX** statement.

Consider a GLIMMIX model where variables **A** and **Rep** are classification variables with  $a$  and  $r$  levels, respectively. The following pairs of statements produce the same random-effects structure:

```
class Rep A;
random Rep*A;
```

```
class Rep A;
random intercept / subject=Rep*A;
```

```
class Rep A;
random Rep / subject=A;
```

```
class Rep A;
random A / subject=Rep;
```

In the first case, PROC GLIMMIX does not process the data by subjects because no **SUBJECT=** option was given. The computation of empirical covariance estimators, for example, will not be possible. The marginal variance-covariance matrix has the same block-diagonal structure as for cases 2–4, where each block consists of the observations belonging to a unique combination of **Rep** and **A**. More importantly, the dimension of the **Z** matrix of this model will be  $n \times ra$ , and **Z** will be sparse. In the second case, the **Z<sub>i</sub>** matrix for each of the  $ra$  subjects is a vector of ones.

If the data can be processed by subjects, the procedure typically executes faster and requires less memory. The differences can be substantial, especially if the number of subjects is large. Recall that fitting of generalized linear mixed models might be doubly iterative. Small gains in efficiency for any one optimization can produce large overall savings.

If you interpret the intercept as “1,” then a **RANDOM** statement with **TYPE=VC** (the default) and no **SUBJECT=** option can be converted into a statement with subject by dividing the random effect by the eventual subject effect. However, the presence of the **SUBJECT=** option does not imply processing by subject. If a **RANDOM** statement does not have a **SUBJECT=** effect, processing by subjects is not possible unless the random effect is a pure R-side overdispersion effect. In the following example, the data will not be processed by subjects, because the first **RANDOM** statement specifies a G-side component and does not use a **SUBJECT=** option:

```
proc glimmix;
 class A B;
 model y = B;
 random A;
 random B / subject=A;
run;
```

To allow processing by subjects, you can write the equivalent model with the following statements:

```
proc glimmix;
 class A B;
 model y = B;
 random int / subject=A;
 random B / subject=A;
run;
```

If you denote a variance component effect  $X$  with subject effect  $S$  as  $X-(S)$ , then the “calculus of random effects” applied to the first **RANDOM** statement reads  $A = \text{Int}^*A = \text{Int}-(A) = A-(\text{Int})$ . For the second statement there are even more equivalent formulations:  $A*B = A*B*\text{Int} = A*B-(\text{Int}) = A-(B) = B-(A) = \text{Int}-(A*B)$ .

If there are multiple subject effects, processing by subjects is possible if the effects are equal or contained in each other. Note that in the last example the  $A*B$  interaction is a random effect. The following statements give an equivalent specification to the previous model:

```
proc glimmix;
 class A B;
 model y = B;
 random int / subject=A;
 random A / subject=B;
run;
```

Processing by subjects is not possible in this case, because the two subject effects are not syntactically equal or contained in each other. The following statements depict a case where subject effects are syntactically contained:

```
proc glimmix;
 class A B;
 model y = B;
 random int / subject=A;
 random int / subject=A*B;
run;
```

The A main effect is contained in the A\*B interaction. The GLIMMIX procedure chooses as the subject effect for processing the effect that is contained in all other subject effects. In this case, the subjects are defined by the levels of A.

You can examine the “Model Information” and “Dimensions” tables to see whether the GLIMMIX procedure processes the data by subjects and which effect is used to define subjects. The “Model Information” table displays whether the marginal variance matrix is diagonal (GLM models), blocked, or not blocked. The “Dimensions” table tells you how many subjects (=blocks) there are.

Finally, nesting and crossing of interaction effects in subject effects are equivalent. The following two **RANDOM** statements are equivalent:

```
class Rep A;
random intercept / subject=Rep*A;

class Rep A;
random intercept / subject=Rep(A);
```

---

## Radial Smoothing Based on Mixed Models

The radial smoother implemented with the **TYPE=RSMOOTH** option in the **RANDOM** statement is an approximate low-rank thin-plate spline as described in Ruppert, Wand, and Carroll (2003, Chapter 13.4–13.5). The following sections discuss in more detail the mathematical-statistical connection between mixed models and penalized splines and the determination of the number of spline knots and their location as implemented in the GLIMMIX procedure.

### From Penalized Splines to Mixed Models

The connection between splines and mixed models arises from the similarity of the penalized spline fitting criterion to the minimization problem that yields the mixed model equations and solutions for  $\beta$  and  $\gamma$ . This connection is made explicit in the following paragraphs. An important distinction between classical spline fitting and its mixed model smoothing variant, however, lies in the nature of the spline coefficients. Although they address similar minimization criteria, the solutions for the spline coefficients in the GLIMMIX procedure are the solutions of random effects, not fixed effects. Standard errors of predicted values, for example, account for this source of variation.

Consider the linearized mixed pseudo-model from the section “The Pseudo-model” on page 3054,  $\mathbf{P} = \mathbf{X}\beta + \mathbf{Z}\gamma + \epsilon$ . One derivation of the mixed model equations, whose solutions are  $\hat{\beta}$  and  $\hat{\gamma}$ , is to maximize the joint density of  $f(\gamma, \epsilon)$  with respect to  $\beta$  and  $\gamma$ . This is not a true likelihood problem, because  $\gamma$  is not a parameter, but a random vector.

In the special case with  $\text{Var}[\epsilon] = \phi\mathbf{I}$  and  $\text{Var}[\gamma] = \sigma^2\mathbf{I}$ , the maximization of  $f(\gamma, \epsilon)$  is equivalent to the minimization of

$$Q(\beta, \gamma) = \phi^{-1}(\mathbf{p} - \mathbf{X}\beta - \mathbf{Z}\gamma)'(\mathbf{p} - \mathbf{X}\beta - \mathbf{Z}\gamma) + \sigma^{-2}\gamma'\gamma$$

Now consider a linear spline as in Ruppert, Wand, and Carroll (2003, p. 108),

$$p_i = \beta_0 + \beta_1 x_i + \sum_{j=1}^K \gamma_j (x_i - t_j)_+$$



where the  $\gamma_j$  denote the spline coefficients at knots  $t_1, \dots, t_K$ . The truncated line function is defined as

$$(x - t)_+ = \begin{cases} x - t & x > t \\ 0 & \text{otherwise} \end{cases}$$

If you collect the intercept and regressor  $x$  into the matrix  $\mathbf{X}$ , and if you collect the truncated line functions into the  $(n \times K)$  matrix  $\mathbf{Z}$ , then fitting the linear spline amounts to minimization of the penalized spline criterion

$$Q^*(\boldsymbol{\beta}, \boldsymbol{\gamma}) = (\mathbf{p} - \mathbf{X}\boldsymbol{\beta} - \mathbf{Z}\boldsymbol{\gamma})'(\mathbf{p} - \mathbf{X}\boldsymbol{\beta} - \mathbf{Z}\boldsymbol{\gamma}) + \lambda^2 \boldsymbol{\gamma}'\boldsymbol{\gamma}$$

where  $\lambda$  is the smoothing parameter.

Because minimizing  $Q^*(\boldsymbol{\beta}, \boldsymbol{\gamma})$  with respect to  $\boldsymbol{\beta}$  and  $\boldsymbol{\gamma}$  is equivalent to minimizing  $Q^*(\boldsymbol{\beta}, \boldsymbol{\gamma})/\phi$ , both problems lead to the same solution, and  $\lambda = \phi/\sigma$  is the smoothing parameter. The mixed model formulation of spline smoothing has the advantage that the smoothing parameter is selected “automatically.” It is a function of the covariance parameter estimates, which, in turn, are estimated according to the method you specify with the `METHOD=` option in the `PROC GLIMMIX` statement.

To accommodate nonnormal responses and general link functions, the GLIMMIX procedure uses  $\text{Var}[\boldsymbol{\epsilon}] = \phi \tilde{\boldsymbol{\Delta}}^{-1} \mathbf{A} \tilde{\boldsymbol{\Delta}}^{-1}$ , where  $\mathbf{A}$  is the matrix of variance functions and  $\boldsymbol{\Delta}$  is the diagonal matrix of mean derivatives defined earlier. The correspondence between spline smoothing and mixed modeling is then one between a weighted linear mixed model and a weighted spline. In other words, the minimization criterion that yields the estimates  $\hat{\boldsymbol{\beta}}$  and solutions  $\hat{\boldsymbol{\gamma}}$  is then

$$Q(\boldsymbol{\beta}, \boldsymbol{\gamma}) = \phi^{-1} (\mathbf{p} - \mathbf{X}\boldsymbol{\beta} - \mathbf{Z}\boldsymbol{\gamma})' \tilde{\boldsymbol{\Delta}} \mathbf{A}^{-1} \tilde{\boldsymbol{\Delta}} (\mathbf{p} - \mathbf{X}\boldsymbol{\beta} - \mathbf{Z}\boldsymbol{\gamma})' + \sigma^{-2} \boldsymbol{\gamma}'\boldsymbol{\gamma}$$

If you choose the `TYPE=RSMOOTH` covariance structure, PROC GLIMMIX chooses radial basis functions as the spline basis and transforms them to approximate a thin-plate spline as in Chapter 13.4 of Ruppert, Wand, and Carroll (2003). For computational expediency, the number of knots is chosen to be less than the number of data points. Ruppert, Wand, and Carroll (2003) recommend one knot per every four unique regressor values for one-dimensional smoothers. In the multivariate case, general recommendations are more difficult, because the optimal number and placement of knots depend on the spatial configuration of samples. Their recommendation for a bivariate smoother is one knot per four samples, but at least 20 and no more than 150 knots (Ruppert, Wand, and Carroll 2003, p. 257).

The magnitude of the variance component  $\sigma^2$  depends on the metric of the random effects. For example, if you apply radial smoothing in time, the variance changes if you measure time in days or minutes. If the solution for the variance component is near zero, then a rescaling of the random effect data can help the optimization problem by moving the solution for the variance component away from the boundary of the parameter space.

## Knot Selection

The GLIMMIX procedure computes knots for low-rank smoothing based on the vertices or centroids of a  $k$ -d tree. The default is to use the vertices of the tree as the knot locations, if you use the `TYPE=RSMOOTH` covariance structure. The construction of this tree amounts to a partitioning of the random regressor space until all partitions contain at most  $b$  observations. The number  $b$  is called the *bucket size* of the  $k$ -d tree. You can exercise control over the construction of the tree by changing the bucket size with the `BUCKET=` suboption of the `KNOTMETHOD=KDTREE` option in the `RANDOM` statement. A large bucket size leads to fewer knots, but it is not correct to assume that  $K$ , the number of knots, is simply  $\lfloor n/b \rfloor$ . The number of



vertices depends on the configuration of the values in the regressor space. Also, coordinates of the bounding hypercube are vertices of the tree. In the one-dimensional case, for example, the extreme values of the random effect are vertices.

To demonstrate how the  $k$ -d tree partitions the random-effects space based on observed data and the influence of the bucket size, consider the following example from Chapter 53, “The LOESS Procedure.” The SAS data set Gas contains the results of an engine exhaust emission study (Brinkman 1981). The covariate in this analysis, E, is a measure of the air-fuel mixture richness. The response, NOx, measures the nitric oxide concentration (in micrograms per joule, and normalized).

```
data Gas;
 input NOx E;
 format NOx E f5.3;
 datalines;
4.818 0.831
2.849 1.045
3.275 1.021
4.691 0.97
4.255 0.825
5.064 0.891
2.118 0.71
4.602 0.801
2.286 1.074
0.97 1.148
3.965 1
5.344 0.928
3.834 0.767
1.99 0.701
5.199 0.807
5.283 0.902
3.752 0.997
0.537 1.224
1.64 1.089
5.055 0.973
4.937 0.98
1.561 0.665
;
```

There are 22 observations in the data set, and the values of the covariate are unique. If you want to smooth these data with a low-rank radial smoother, you need to choose the number of knots, as well as their placement within the support of the variable E. The  $k$ -d tree construction depends on the observed values of the variable E; it is independent of the values of nitric oxide in the data. The following statements construct a tree based on a bucket size of  $b = 11$  and display information about the tree and the selected knots:

```
ods select KDtree KnotInfo;
proc glimmix data=gas nofit;
 model NOx = e;
 random e / type=rsmooth
 knotmethod=kdtree(bucket=11 treeinfo knotinfo);
run;
```

The **NOFIT** option prevents the GLIMMIX procedure from fitting the model. This option is useful if you want to investigate the knot construction for various bucket sizes. The **TREEINFO** and **KNOTINFO** suboptions of the **KNOTMETHOD=KDTREE** option request displays of the  $k$ -d tree and the knot coordinates derived from it. Construction of the tree commences by splitting the data in half. For  $b = 11$ ,  $n = 22$ , neither of the two splits contains more than  $b$  observations and the process stops. With a single split value, and the two extreme values, the tree has two terminal nodes and leads to three knots (Figure 41.13). Note that for one-dimensional problems, vertices of the  $k$ -d tree always coincide with data values.

**Figure 41.13**  $K$ -d Tree and Knots for Bucket Size 11

| The GLIMMIX Procedure  |            |             |                 |             |
|------------------------|------------|-------------|-----------------|-------------|
| kd-Tree for RSmooth(E) |            |             |                 |             |
| Node Number            | Left Child | Right Child | Split Direction | Split Value |
| 0                      | 1          | 2           | E               | 0.9280      |
| 1                      |            |             | TERMINAL        |             |
| 2                      |            |             | TERMINAL        |             |
| Radial Smoother        |            |             |                 |             |
| Knots for RSmooth(E)   |            |             |                 |             |
| Knot Number            |            | E           |                 |             |
| 1                      |            | 0.6650      |                 |             |
| 2                      |            | 0.9280      |                 |             |
| 3                      |            | 1.2240      |                 |             |

If the bucket size is reduced to  $b = 8$ , the following statements produce the tree and knots in Figure 41.14:

```
ods select KdTree KnotInfo;
proc glimmix data=gas nofit;
 model NOx = e;
 random e / type=rsmooth
 knotmethod=kdtree(bucket=8 treeinfo knotinfo);
run;
```

The initial split value of 0.9280 leads to two sets of 11 observations. In order to achieve a partition into cells that contain at most eight observations, each initial partition is split at its median one more time. Note that one split value is greater and one split value is less than 0.9280.

**Figure 41.14** K-d Tree and Knots for Bucket Size 8

| The GLIMMIX Procedure  |            |             |                 |             |
|------------------------|------------|-------------|-----------------|-------------|
| kd-Tree for RSmooth(E) |            |             |                 |             |
| Node Number            | Left Child | Right Child | Split Direction | Split Value |
| 0                      | 1          | 2           | E               | 0.9280      |
| 1                      | 3          | 4           | E               | 0.8070      |
| 2                      | 5          | 6           | E               | 1.0210      |
| 3                      |            |             | TERMINAL        |             |
| 4                      |            |             | TERMINAL        |             |
| 5                      |            |             | TERMINAL        |             |
| 6                      |            |             | TERMINAL        |             |

| Radial Smoother      |        |
|----------------------|--------|
| Knots for RSmooth(E) |        |
| Knot Number          | E      |
| 1                    | 0.6650 |
| 2                    | 0.8070 |
| 3                    | 0.9280 |
| 4                    | 1.0210 |
| 5                    | 1.2240 |

A further reduction in bucket size to  $b = 4$  leads to the tree and knot information shown in [Figure 41.15](#).

Figure 41.15 K-d Tree and Knots for Bucket Size 4

| The GLIMMIX Procedure  |            |             |                 |             |
|------------------------|------------|-------------|-----------------|-------------|
| kd-Tree for RSmooth(E) |            |             |                 |             |
| Node Number            | Left Child | Right Child | Split Direction | Split Value |
| 0                      | 1          | 2           | E               | 0.9280      |
| 1                      | 3          | 4           | E               | 0.8070      |
| 2                      | 9          | 10          | E               | 1.0210      |
| 3                      | 5          | 6           | E               | 0.7100      |
| 4                      | 7          | 8           | E               | 0.8910      |
| 5                      |            |             | TERMINAL        |             |
| 6                      |            |             | TERMINAL        |             |
| 7                      |            |             | TERMINAL        |             |
| 8                      |            |             | TERMINAL        |             |
| 9                      | 11         | 12          | E               | 0.9800      |
| 10                     | 13         | 14          | E               | 1.0890      |
| 11                     |            |             | TERMINAL        |             |
| 12                     |            |             | TERMINAL        |             |
| 13                     |            |             | TERMINAL        |             |
| 14                     |            |             | TERMINAL        |             |

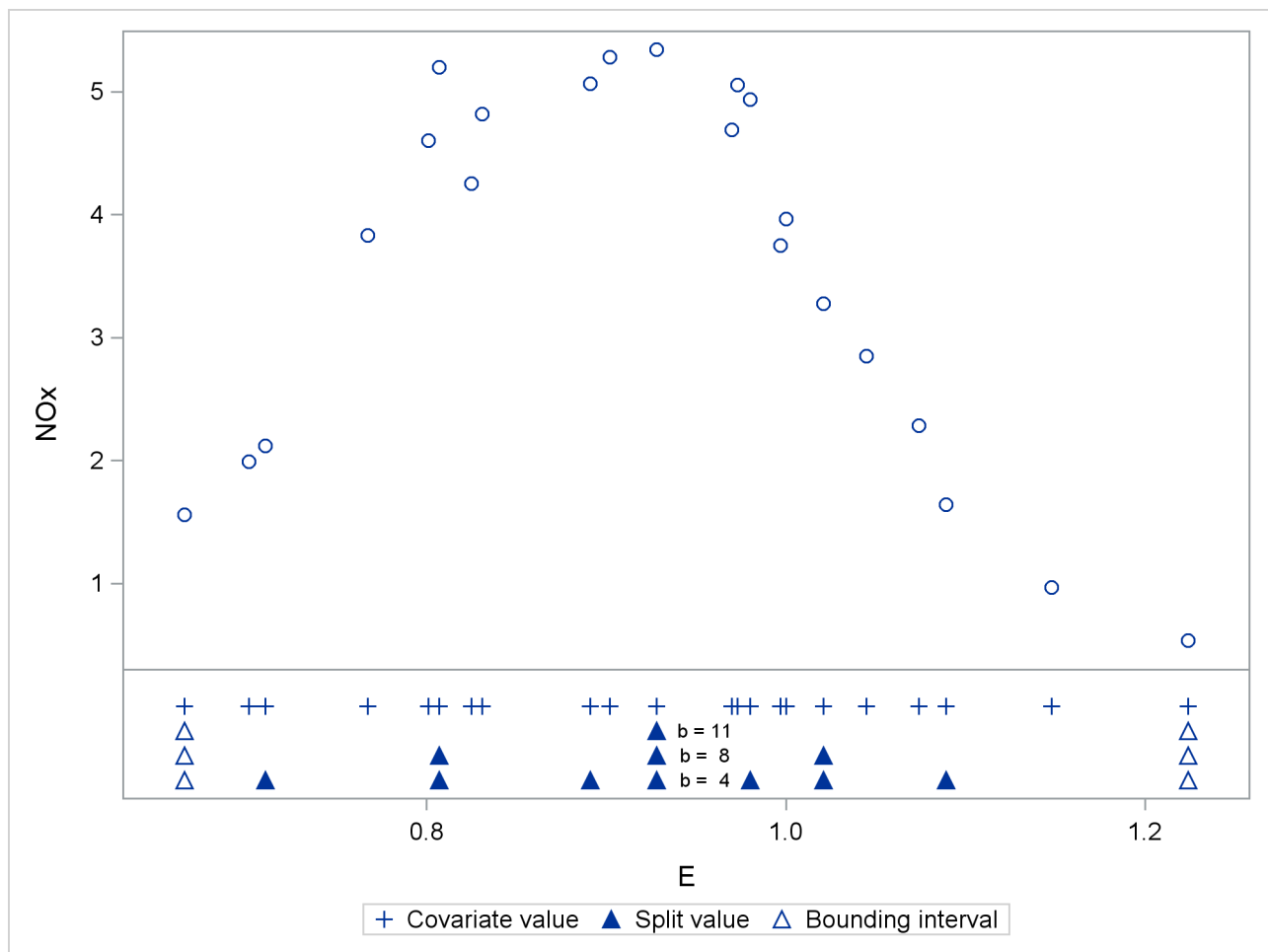
  

| Radial Smoother      |        |
|----------------------|--------|
| Knots for RSmooth(E) |        |
| Knot Number          | E      |
| 1                    | 0.6650 |
| 2                    | 0.7100 |
| 3                    | 0.8070 |
| 4                    | 0.8910 |
| 5                    | 0.9280 |
| 6                    | 0.9800 |
| 7                    | 1.0210 |
| 8                    | 1.0890 |
| 9                    | 1.2240 |

The split value for  $b = 11$  is also a split value for  $b = 8$ , the split values for  $b = 8$  are a subset of those for  $b = 4$ , and so forth. Figure 41.16 displays the data and the location of split values for the three cases. For a one-dimensional problem (a univariate smoother), the vertices comprise the split values and the values on the bounding interval.

You might want to move away from the boundary, in particular for an irregular data configuration or for multivariate smoothing. The `KNOTTYP=`CENTER suboption of the `KNOTMETHOD=` option chooses centroids of the leaf node cells instead of vertices. This tends to move the outer knot locations closer to the convex hull, but not necessarily to data locations. In the emission example, choosing a bucket size of  $b = 11$  and centroids as knot locations yields two knots at  $E=0.7956$  and  $E=1.076$ . If you choose the `NEAREST` suboption, then the nearest neighbor of a vertex or centroid will serve as the knot location. In this case, the knot locations are a subset of the data locations, regardless of the dimension of the smooth.

**Figure 41.16** Vertices of  $k$ -d Trees for Various Bucket Sizes



## Odds and Odds Ratio Estimation

In models with a logit, generalized logit, or cumulative logit link, you can obtain estimates of odds ratios through the `ODDSRATIO` options in the `PROC GLIMMIX`, `LSMEANS`, and `MODEL` statements. This section provides details about the computation and interpretation of the computed quantities. Note that for

these link functions the **EXP** option in the **ESTIMATE** and **LSMESTIMATE** statements also produces odds or odds ratios.

Consider first a model with a dichotomous outcome variable, linear predictor  $\eta = \mathbf{x}'\boldsymbol{\beta} + \mathbf{z}'\boldsymbol{\gamma}$ , and logit link function. Suppose that  $\eta_0$  represents the linear predictor for a condition of interest. For example, in a simple logistic regression model with  $\eta = \alpha + \beta x$ ,  $\eta_0$  might correspond to the linear predictor at a particular value of the covariate—say,  $\eta_0 = \alpha + \beta x_0$ .

The modeled probability is  $\pi = 1/(1 + \exp\{-\eta\})$ , and the odds for  $\eta = \eta_0$  are

$$\frac{\pi_0}{1 - \pi_0} = \frac{1/(1 + \exp\{-\eta_0\})}{\exp\{-\eta_0\}/(1 + \exp\{-\eta_0\})} = \exp\{\eta_0\}$$

Because  $\eta_0$  is a logit, it represents the log odds. The odds ratio  $\psi(\eta_1, \eta_0)$  is defined as the ratio of odds for  $\eta_1$  and  $\eta_0$ ,

$$\psi(\eta_1, \eta_0) = \exp\{\eta_1 - \eta_0\}$$

The odds ratio compares the odds of the outcome under the condition expressed by  $\eta_1$  to the odds under the condition expressed by  $\eta_0$ . In the preceding simple logistic regression example, this ratio equals  $\exp\{\beta(x_1 - x_0)\}$ . The exponentiation of the estimate of  $\beta$  is thus an estimate of the odds ratio comparing conditions for which  $x_1 - x_0 = 1$ . If  $x$  and  $x + 1$  represent standard and experimental conditions, for example,  $\exp\{\beta\}$  compares the odds of the outcome under the experimental condition to the odds under the standard condition. For many other types of models, odds ratios can be expressed as simple functions of parameter estimates. For example, suppose you are fitting a logistic model with a single classification effect with three levels:

```
proc glimmix;
 class A;
 model y = A / dist=binary;
run;
```

The estimated linear predictor for level  $j$  of  $A$  is  $\hat{\eta}_j = \hat{\beta} + \hat{\alpha}_j$ ,  $j = 1, 2, 3$ . Because the  $\mathbf{X}$  matrix is singular in this model due to the presence of an overall intercept, the solution for the intercept estimates  $\beta + \alpha_3$ , and the solution for the  $j$ th treatment effect estimates  $\alpha_j - \alpha_3$ . Exponentiating the solutions for  $\alpha_1$  and  $\alpha_2$  thus produces odds ratios comparing the odds for these levels against the third level of  $A$ .

Results designated as odds or odds ratios in the **GLIMMIX** procedure might reduce to simple exponentiations of solutions in the “Parameter Estimates” table, but they are computed by a different mechanism if the model contains classification variables. The computations rely on general estimable functions; for the **MODEL**, **LSMEANS**, and **LSMESTIMATE** statements, these functions are based on least squares means. This enables you to obtain odds ratio estimates in more complicated models that involve main effects and interactions, including interactions between continuous and classification variables.

In all cases, the results represent the exponentiation of a linear function of the fixed-effects parameters,  $\eta = \mathbf{l}'\boldsymbol{\beta}$ . If  $L_\eta$  and  $U_\eta$  are the confidence limits for  $\eta$  on the logit scale, confidence limits for the odds or the odds ratio are obtained as  $\exp\{L_\eta\}$  and  $\exp\{U_\eta\}$ .

## The Odds Ratio Estimates Table

This table is produced by the **ODDSRATIO** option in the **MODEL** statement. It consists of estimates of odds ratios and their confidence limits. Odds ratios are produced for the following:

- classification main effects, if they appear in the **MODEL** statement
- continuous variables in the **MODEL** statement, unless they appear in an interaction with a classification effect
- continuous variables in the **MODEL** statement at fixed levels of a classification effect, if the **MODEL** statement contains an interaction of the two.
- continuous variables in the **MODEL** statements if they interact with other continuous variables

### The Default Table

Consider the following PROC GLIMMIX statements that fit a logistic model with one classification effect, one continuous variable, and their interaction (the **ODDSRATIO** option in the **MODEL** statement requests the “Odds Ratio Estimates” table).

```
proc glimmix;
 class A;
 model y = A x A*x / dist=binary oddsratio;
run;
```

By default, odds ratios are computed as follows:

- The covariate is set to its average,  $\bar{x}$ , and the least squares means for the A effect are obtained. Suppose  $\mathbf{L}^{(1)}$  denotes the matrix of coefficients defining the estimable functions that produce the  $a$  least squares means  $\mathbf{L}\hat{\boldsymbol{\beta}}$ , and  $\mathbf{l}_j^{(1)}$  denotes the  $j$ th row of  $\mathbf{L}^{(1)}$ . Differences of the least squares means against the last level of the A factor are computed and exponentiated:

$$\begin{aligned} \psi(A_1, A_a) &= \exp \left\{ \left( \mathbf{l}_1^{(1)} - \mathbf{l}_a^{(1)} \right) \hat{\boldsymbol{\beta}} \right\} \\ \psi(A_2, A_a) &= \exp \left\{ \left( \mathbf{l}_2^{(1)} - \mathbf{l}_a^{(1)} \right) \hat{\boldsymbol{\beta}} \right\} \\ &\vdots \\ \psi(A_{a-1}, A_a) &= \exp \left\{ \left( \mathbf{l}_{a-1}^{(1)} - \mathbf{l}_a^{(1)} \right) \hat{\boldsymbol{\beta}} \right\} \end{aligned}$$

The differences are checked for estimability. Notice that this set of odds ratios can also be obtained with the following **LSMESTIMATE** statement (assuming A has five levels):

```
lsmestimate A 1 0 0 0 -1,
 0 1 0 0 -1,
 0 0 1 0 -1,
 0 0 0 1 -1 / exp cl;
```

You can also obtain the odds ratios with this **LSMEANS** statement (assuming the last level of A is coded as 5):

```
lsmeans A / diff=control('5') oddsratio cl;
```

- The odds ratios for the covariate must take into account that  $x$  occurs in an interaction with the  $A$  effect. A second set of least squares means are computed, where  $x$  is set to  $\bar{x} + 1$ . Denote the coefficients of the estimable functions for this set of least squares means as  $L^{(2)}$ . Differences of the least squares means at a given level of factor  $A$  are then computed and exponentiated:

$$\begin{aligned}\psi(A(\bar{x} + 1)_1, A(\bar{x})_1) &= \exp \left\{ \left( l_1^{(2)} - l_1^{(1)} \right) \hat{\beta} \right\} \\ \psi(A(\bar{x} + 1)_2, A(\bar{x})_2) &= \exp \left\{ \left( l_2^{(2)} - l_2^{(1)} \right) \hat{\beta} \right\} \\ &\vdots \\ \psi(A(\bar{x} + 1)_a, A(\bar{x})_a) &= \exp \left\{ \left( l_a^{(2)} - l_a^{(1)} \right) \hat{\beta} \right\}\end{aligned}$$

The differences are checked for estimability. If the continuous covariate does not appear in an interaction with the  $A$  variable, only a single odds ratio estimate related to  $x$  would be produced, relating the odds of a one-unit shift in the regressor from  $\bar{x}$ .

Suppose you fit a model that contains interactions of continuous variables, as with the following statements:

```
proc glimmix;
 class A;
 model y = A x x*z / dist=binary oddsratio;
run;
```

In the computation of the  $A$  least squares means, the continuous effects are set to their means—that is,  $\bar{x}$  and  $\bar{x}\bar{z}$ . In the computation of odds ratios for  $x$ , linear predictors are computed at  $x = \bar{x}$ ,  $x^*z = \bar{x} \times \bar{z}$  and at  $x = \bar{x} + 1$ ,  $x^*z = (\bar{x} + 1)\bar{z}$ .

### **Modifying the Default Table, Customized Odds Ratios**

Several suboptions of the `ODDSRATIO` option in the `MODEL` statement are available to obtain customized odds ratio estimates. For customized odds ratios that cannot be obtained with these suboptions, use the `EXP` option in the `ESTIMATE` or `LSMESTIMATE` statement.

The type of differences constructed when the levels of a classification factor are varied is controlled by the `DIFF=` suboption. By default, differences against the last level are taken. `DIFF=FIRST` computes differences from the first level, and `DIFF=ALL` computes odds ratios based on all pairwise differences.

For continuous variables in the model, you can change both the reference value (with the `AT` suboption) and the units of change (with the `UNIT` suboption). By default, a one-unit change from the mean of the covariate is assessed. For example, the following statements produce all pairwise differences for the  $A$  factor:

```
proc glimmix;
 class A;
 model y = A x A*x / dist=binary
 oddsratio(diff=all
 at x=4
 unit x=3);
run;
```

The covariate  $x$  is set to the reference value  $x = 4$  in the computation of the least squares means for the  $A$  odds ratio estimates. The odds ratios computed for the covariate are based on differencing this set of least squares means with a set of least squares means computed at  $x = 4 + 3$ .



## Odds or Odds Ratio

The odds ratio is the exponentiation of a difference on the logit scale,

$$\psi(\eta_1, \eta_0) = \exp\{(\mathbf{l}_1 - \mathbf{l}_0)\boldsymbol{\beta}\}$$

and  $\exp\{\mathbf{l}_1\boldsymbol{\beta}\}$  and  $\exp\{\mathbf{l}_0\boldsymbol{\beta}\}$  are the corresponding odds. If the ODDSRATIO option is specified in a suitable model in the PROC GLIMMIX statement or the individual statements that support the option, odds ratios are computed in the “Odds Ratio Estimates” table (MODEL statement), the “Differences of Least Squares Means” table (LSMEANS / DIFF), and the “Simple Effect Comparisons of Least Squares Means” table (LSMEANS / SLICEDIFF=). Odds are computed in the “Least Squares Means” table.

## Odds Ratios in Multinomial Models

The GLIMMIX procedure fits two kinds of models to multinomial data. Models with cumulative link functions apply to ordinal data, and generalized logit models are fit to nominal data. If you model a multinomial response with LINK=CUMLOGIT or LINK=GLOGIT, odds ratio results are available for these models.

In the generalized logit model, you model baseline category logits. By default, the GLIMMIX procedure chooses the last category as the reference category. If your nominal response has  $J$  categories, the baseline logit for category  $j$  is

$$\log\{\pi_j/\pi_J\} = \eta_j = \mathbf{x}'\boldsymbol{\beta}_j + \mathbf{z}'\mathbf{u}_j$$

and

$$\pi_j = \frac{\exp\{\eta_j\}}{\sum_{k=1}^J \exp\{\eta_k\}}$$

$$\eta_J = 0$$

As before, suppose that the two conditions to be compared are identified with subscripts 1 and 0. The log odds ratio of outcome  $j$  versus  $J$  for the two conditions is then

$$\log\{\psi(\eta_{j1}, \eta_{j0})\} = \log\left\{\frac{\pi_{j1}/\pi_{J1}}{\pi_{j0}/\pi_{J0}}\right\} = \log\left\{\frac{\exp\{\eta_{j1}\}}{\exp\{\eta_{j0}\}}\right\}$$

$$= \eta_{j1} - \eta_{j0}$$

Note that the log odds ratios are again differences on the scale of the linear predictor, but they depend on the response category. The GLIMMIX procedure determines the estimable functions whose differences represent log odds ratios as discussed previously but produces separate estimates for each nonreference response category.

In models for ordinal data, PROC GLIMMIX models the logits of cumulative probabilities. Thus, the estimates on the linear scale represent log cumulative odds. The cumulative logits are formed as

$$\log\left\{\frac{\Pr(Y \leq j)}{\Pr(Y > j)}\right\} = \eta_j = \alpha_j + \mathbf{x}'\boldsymbol{\beta} + \mathbf{z}'\boldsymbol{\gamma} = \alpha_j + \tilde{\eta}$$

so that the linear predictor depends on the response category only through the intercepts (cutoffs)  $\alpha_1, \dots, \alpha_{J-1}$ . The odds ratio comparing two conditions represented by linear predictors  $\eta_{j1}$  and  $\eta_{j0}$  is then

$$\psi(\eta_{j1}, \eta_{j0}) = \exp\{\eta_{j1} - \eta_{j0}\}$$

$$= \exp\{\tilde{\eta}_1 - \tilde{\eta}_0\}$$

and is independent of category.

---

## Parameterization of Generalized Linear Mixed Models

PROC GLIMMIX constructs a generalized linear mixed model according to the specifications in the **CLASS**, **MODEL**, and **RANDOM** statements. Each effect in the **MODEL** statement generates one or more columns in the matrix **X**, and each G-side effect in the **RANDOM** statement generates one or more columns in the matrix **Z**. R-side effects in the **RANDOM** statement do not generate model matrices; they serve only to index observations within subjects. This section shows how the GLIMMIX procedure builds **X** and **Z**. You can output the **X** and **Z** matrices to a SAS data set with the **OUTDESIGN=** option in the **PROC GLIMMIX** statement.

The general rules and techniques for parameterization of a linear model are given in “GLM Parameterization of Classification Variables and Effects” on page 383 of Chapter 19, “Shared Concepts and Topics.” The following paragraphs discuss how these rules differ in a mixed model, in particular, how parameterization differs between the **X** and the **Z** matrix.

### Intercept

By default, all models automatically include a column of 1s in **X** to estimate a fixed-effect intercept parameter. You can use the **NOINT** option in the **MODEL** statement to suppress this intercept. The **NOINT** option is useful when you are specifying a classification effect in the **MODEL** statement and you want the parameter estimates to be in terms of the (linked) mean response for each level of that effect, rather than in terms of a deviation from an overall mean.

By contrast, the intercept is not included by default in **Z**. To obtain a column of 1s in **Z**, you must specify in the **RANDOM** statement either the **INTERCEPT** effect or some effect that has only one level.

### Interaction Effects

Often a model includes interaction (crossed) effects. With an interaction, PROC GLIMMIX first reorders the terms to correspond to the order of the variables in the **CLASS** statement. Thus, **B\*A** becomes **A\*B** if **A** precedes **B** in the **CLASS** statement. Then, PROC GLIMMIX generates columns for all combinations of levels that occur in the data. The order of the columns is such that the rightmost variables in the cross index faster than the leftmost variables. Empty columns (which would contain all 0s) are not generated for **X**, but they are for **Z**.

See Table 19.5 in the section “GLM Parameterization of Classification Variables and Effects” on page 383 of Chapter 19, “Shared Concepts and Topics,” for an example of an interaction parameterization.

### Nested Effects

Nested effects are generated in the same manner as crossed effects. Hence, the design columns generated by the following two statements are the same (but the ordering of the columns is different):

Note that nested effects are often distinguished from interaction effects by the implied randomization structure of the design. That is, they usually indicate random effects within a fixed-effects framework. The fact that random effects can be modeled directly in the **RANDOM** statement might make the specification of nested effects in the **MODEL** statement unnecessary.

See Table 19.6 in the section “GLM Parameterization of Classification Variables and Effects” on page 383 of Chapter 19, “Shared Concepts and Topics,” for an example of the parameterization of a nested effect.

## Implications of the Non-Full-Rank Parameterization

For models with fixed effects involving classification variables, there are more design columns in  $\mathbf{X}$  constructed than there are degrees of freedom for the effect. Thus, there are linear dependencies among the columns of  $\mathbf{X}$ . In this event, all of the parameters are not estimable; there is an infinite number of solutions to the mixed model equations. The GLIMMIX procedure uses a generalized inverse (a  $g_2$ -inverse, Pringle and Rayner (1971), to obtain values for the estimates (Searle 1971). The solution values are not displayed unless you specify the **SOLUTION** option in the **MODEL** statement. The solution has the characteristic that estimates are 0 whenever the design column for that parameter is a linear combination of previous columns. With this parameterization, hypothesis tests are constructed to test linear functions of the parameters that are estimable.

Some procedures (such as the CATMOD and LOGISTIC procedures) reparameterize models to full rank by using restrictions on the parameters. PROC GLM, PROC MIXED, and PROC GLIMMIX do not reparameterize, making the hypotheses that are commonly tested more understandable. See Goodnight (1978b) for additional reasons for not reparameterizing.

## Missing Level Combinations

PROC GLIMMIX handles missing level combinations of classification variables in the same manner as PROC GLM and PROC MIXED. These procedures delete fixed-effects parameters corresponding to missing levels in order to preserve estimability. However, PROC GLIMMIX does not delete missing level combinations for random-effects parameters because linear combinations of the random-effects parameters are always predictable. These conventions can affect the way you specify your **CONTRAST** and **ESTIMATE** coefficients.

## Notes on the EFFECT Statement

Some restrictions and limitations for models that contain constructed effects are in place with the GLIMMIX procedure. Also, you should be aware of some special defaults and handling that apply only when the model contains constructed fixed and/or random effects.

- Constructed effects can be used in the **MODEL** and **RANDOM** statements but not to specify **SUBJECT=** or **GROUP=** effects.
- Computed variables are not supported in the specification of a constructed effect. All variables needed to form the collection of columns for a constructed effect must be in the data set.
- You cannot use constructed effects that comprise continuous variables or interactions with other constructed effects as the **LSMEANS** or **LSMESTIMATE** effect.
- The calculation of quantities that depend on least squares means, such as odds ratios in the “Odds Ratio Estimates” table, is not possible if the model contains fixed effects that consist of more than one constructed effects, unless all constructed effects are of spline type. For example, least squares means computations are not possible in the following model because the **MM\_AB\*cvars** effect contains two constructed effects:

```
proc glimmix;
 class A B C;
 effect MM_AB = MM(A B);
 effect cvars = COLLECTION(x1 x2 x3);
 model y = C MM_AB*cvars;
run;
```

- If the **MODEL** or **RANDOM** statement contains constructed effects, the default degrees-of-freedom method for mixed models is **DDFM=KENWARDROGER**. The containment degrees-of-freedom method (**DDFM=CONTAIN**) is not available in these models.
- If the model contains fixed spline effects, least squares means are computed at the average spline coefficients across the usable data, possibly further averaged over levels of **CLASS** variables that interact with the spline effects in the model. You can use the **AT** option in the **LSMEANS** and **LSMESTIMATE** statements to construct the splines for particular values of the covariates involved. Consider, for example, the following statements:

```
proc glimmix;
 class A;
 effect spl = spline(x);
 model y = A spl;
 lsmeans A;
 lsmeans A / at means;
 lsmeans A / at x=0.4;
run;
```

Suppose that the **spl** effect contributes seven columns  $[s_1, \dots, s_7]$  to the **X** matrix. The least squares means coefficients for the **spl** effect in the first **LSMEANS** statement are  $[\bar{s}_1, \dots, \bar{s}_7]$  with the averages taken across the observations used in the analysis. The second **LSMEANS** statement computes the spline coefficient at the average value of **x**:  $[s(\bar{x})_1, \dots, s(\bar{x})_7]$ . The final **LSMEANS** statement uses  $[s(0.4)_1, \dots, s(0.4)_7]$ . Using the **AT** option for least squares means calculations with spline effects can resolve inestimability issues.

- Using a spline effect with B-spline basis in the **RANDOM** statement is **not** the same as using a penalized B-spline (P-spline) through the **TYPE=PSPLINE** option in the **RANDOM** statement. The following statement constructs a penalized B-spline by using mixed model methodology:

```
random x / type=pspline;
```

The next set of statements defines a set of B-spline columns in the **Z** matrix with uncorrelated random effects and homogeneous variance:

```
effect bspline = spline(x);
random bspline / type=vc;
```

This does not lead to a properly penalized fit. See the documentation on **TYPE=PSPLINE** about the construction of penalties for B-splines through the covariance matrix of random effects.

## Positional and Nonpositional Syntax for Contrast Coefficients

When you define custom linear hypotheses with the **CONTRAST** or **ESTIMATE** statement, the **GLIMMIX** procedure sets up an **L** vector or matrix that conforms to the fixed-effects solutions or the fixed- and random-effects solutions. With the **LSMESTIMATE** statement, you specify coefficients of the matrix **K** that is then converted into a coefficient matrix that conforms to the fixed-effects solutions.

There are two methods for specifying the entries in a coefficient matrix (hereafter simply referred to as the **L** matrix), termed the positional and nonpositional methods. In the positional form, and this is the traditional method, you provide a list of values that occupy the elements of the **L** matrix associated with the effect in

question in the order in which the values are listed. For traditional model effects comprising continuous and classification variables, the positional syntax is simpler in some cases (main effects) and more cumbersome in others (interactions). When you work with effects constructed through the experimental **EFFECT** statement, the nonpositional syntax is essential.

Consider, for example, the following two-way model with interactions where factors A and B have three and two levels, respectively:

```
proc glimmix;
 class a b block;
 model y = a b a*b / ddfm=kr;
 random block a*block;
run;
```

To test the difference of the B levels at the second level of A with a **CONTRAST** statement (a slice), you need to assign coefficients 1 and -1 to the levels of B and to the levels of the interaction where A is at the second level. Two examples of equivalent **CONTRAST** statements by using positional and nonpositional syntax are as follows:

```
contrast 'B at A2' b 1 -1 a*b 0 0 1 -1 ;
contrast 'B at A2' b 1 -1 a*b [1 2 1] [-1 2 2];
```

Because A precedes B in the **CLASS** statement, the levels of the interaction are formed as  $\alpha_1\beta_1, \alpha_1\beta_2, \alpha_2\beta_1, \alpha_2\beta_2, \dots$ . If B precedes A in the **CLASS** statement, you need to modify the coefficients accordingly:

```
proc glimmix;
 class b a block;
 model y = a b a*b / ddfm=kr;
 random block a*block;
 contrast 'B at A2' b 1 -1 a*b 0 1 0 0 -1 ;
 contrast 'B at A2' b 1 -1 a*b [1 1 2] [-1 2 2];
 contrast 'B at A2' b 1 -1 a*b [1, 1 2] [-1, 2 2];
run;
```

You can optionally separate the **L** value entry from the level indicators with a comma, as in the last **CONTRAST** statement.

The general syntax for defining coefficients with the nonpositional syntax is as follows:

$$\text{effect-name} [\text{multiplier} <, > \text{level-values}] \dots <[\text{multiplier} <, > \text{level-values}] >$$

The first entry in square brackets is the multiplier that is applied to the elements of **L** for the effect after the *level-values* have been resolved and any necessary action forming **L** has been taken.

The *level-values* are organized in a specific form:

- The number of entries should equal the number of terms needed to construct the effect. For effects that do not contain any constructed effects, this number is simply the number of terms in the name of the effect.
- Values of continuous variables needed for the construction of the **L** matrix precede the level indicators of **CLASS** variables.
- If the effect involves constructed effects, then you need to provide as many continuous and classification variables as are needed for the effect formation. For example, if a grouping effect is defined as

```
class c;
effect v = vars(x1 x2 c);
```

then a proper nonpositional syntax would be, for example,

```
v [0.5, 0.2 0.3 3]
```

- If an effect contains both regular terms (old-style effects) and constructed effects, then the order of the coefficients is as follows: continuous values for old-style effects, class levels for **CLASS** variables in old-style effects, continuous values for constructed effects, and finally class levels needed for constructed effects.

Assume that C has four levels so that effect v contributes six elements to the **L** matrix. When PROC GLIMMIX resolves this syntax, the values 0.2 and 0.3 are assigned to the positions for x1 and x2 and a 1 is associated with the third level of C. The resulting vector is then multiplied by 0.5 to produce

```
[0.1 0.15 0 0 0.5 0]
```

Note that you enter the **levels** of the classification variables in the square brackets, not their formatted values. The ordering of the levels of **CLASS** variables can be gleaned from the “Class Level Information” table.

To specify values for continuous variables, simply give their value as one of the terms in the effect. The nonpositional syntax in the following **ESTIMATE** statement is read as “1-time the value 0.4 in the column associated with level 2 of A”

```
proc glimmix;
 class a;
 model y = a a*x / s;
 lsmeans a / e at x=0.4;
 estimate 'A2 at x=0.4' intercept 1 a 0 1 a*x [1,0.4 2] / e;
run;
```

Because the value before the comma serves as a multiplier, the same estimable function could also be constructed with the following statements:

```
estimate 'A2 at x=0.4' intercept 1 a 0 1 a*x [4, 0.1 2];
estimate 'A2 at x=0.4' intercept 1 a 0 1 a*x [2, 0.2 2];
estimate 'A2 at x=0.4' intercept 1 a 0 1 a*x [-1, -0.4 2];
```

Note that continuous variables needed to construct an effect are always listed before any **CLASS** variables.

When you work with constructed effects, the nonpositional syntax works in the same way. For example, the following model contains a classification effect and a B-spline. The first two **ESTIMATE** statements produce predicted values for level one of C when the continuous variable x takes on the values 20 and 10, respectively.

```

proc glimmix;
 class c;
 effect spl = spline(x / knotmethod=equal(5));
 model y = c spl;
 estimate 'C = 1 @ x=20' intercept 1 c 1 spl [1,20],
 'C = 1 @ x=10' intercept 1 c 1 spl [1,10];
 estimate 'Difference' spl [1,20] [-1,10];
run;

```

The GLIMMIX procedure computes the spline coefficients for the first **ESTIMATE** statement based on  $x = 20$ , and similarly in the second statement for  $x = 10$ . The third **ESTIMATE** statement computes the difference of the predicted values. Because the spline effect does not interact with the classification variable, this difference does not depend on the level of C. If such an interaction is present, you can estimate the difference in predicted values for a given level of C by using the nonpositional syntax. Because the effect C\*spl contains both old-style terms (C) and a constructed effect, you specify the values for the old-style terms before assigning values to constructed effects:

```

proc glimmix;
 class c;
 effect spl = spline(x / knotmethod=equal(5));
 model y = spl*c;
 estimate 'C2 = 1, x=20' intercept 1 c*spl [1,1 20];
 estimate 'C2 = 2, x=20' intercept 1 c*spl [1,2 20];
 estimate 'C diff at x=20' c*spl [1,1 20] [-1,2 20];
run;

```

It is recommended to add the E option to the **CONTRAST**, **ESTIMATE**, or **LSMESTIMATE** statement to verify that the L matrix is formed according to your expectations.

In any row of an **ESTIMATE** or **CONTRAST** statement you can choose positional and nonpositional syntax separately for each effect. You cannot mix the two forms of syntax for coefficients of a single effect, however. For example, the following statement is not proper because both forms of syntax are used for the interaction effect:

```

estimate 'A1B1 - A1B2' b 1 -1 a*b 0 1 [-1, 1 2];

```

---

## Response-Level Ordering and Referencing

In models for binary and multinomial data, the response-level ordering is important because it reflects the following:

- which probability is modeled with binary data
- how categories are ordered for ordinal data
- which category serves as the reference category in nominal generalized logit models (models for nominal data)

You should view the “Response Profile” table to ensure that the categories are properly arranged and that the desired outcome is modeled. In this table, response levels are arranged by *Ordered Value*. The lowest



response level is assigned Ordered Value 1, the next lowest is assigned Ordered Value 2, and so forth. In binary models, the probability modeled is the probability of the response level with the lowest Ordered Value.

You can change which probability is modeled and the Ordered Value in the “Response Profile” table with the **DESCENDING**, **EVENT=**, **ORDER=**, and **REF=** response variable options in the **MODEL** statement. See the section “Response Level Ordering” on page 4237 in Chapter 54, “The LOGISTIC Procedure,” for examples about how to use these options to affect the probability being modeled for binary data.

For multinomial models, the response-level ordering affects two important aspects. In cumulative link models the categories are assumed ordered according to their Ordered Value in the “Response Profile” table. If the response variable is a character variable or has a format, you should check this table carefully as to whether the Ordered Values reflect the correct ordinal scale.

In generalized logit models (for multinomial data with unordered categories), one response category is chosen as the reference category in the formulation of the generalized logits. By default, the linear predictor in the reference category is set to 0, and the reference category corresponds to the entry in the “Response Profile” table with the highest Ordered Value. You can affect the assignment of Ordered Values with the **DESCENDING** and **ORDER=** options in the **MODEL** statement. You can choose a different reference category with the **REF=** option. The choice of the reference category for generalized logit models affects the results. It is sometimes recommended that you choose the category with the highest frequency as the reference (see, for example, Brown and Prescott 1999, p. 160). You can achieve this with the GLIMMIX procedure by combining the **ORDER=** and **REF=** options, as in the following statements:

```
proc glimmix;
 class preference;
 model preference(order=freq ref=first) = feature price /
 dist=multinomial
 link=glogit;
 random intercept / subject=store group=preference;
run;
```

The **ORDER=FREQ** option arranges the categories by descending frequency. The **REF=FIRST** option then selects the response category with the lowest Ordered Value—the most frequent category—as the reference.

---

## Comparing the GLIMMIX and MIXED Procedures

The MIXED procedure is subsumed by the GLIMMIX procedure in the following sense:

- Linear mixed models are a special case in the family of generalized linear mixed models; a linear mixed model is a generalized linear mixed model where the conditional distribution is normal and the link function is the identity function.
- Most models that can be fit with the MIXED procedure can also be fit with the GLIMMIX procedure.

Despite this overlap in functionality, there are also some important differences between the two procedures. Awareness of these differences enables you to select the most appropriate tool in situations where you have a choice between procedures and to identify situations where a choice does not exist. Furthermore, the %GLIMMIX macro, which fits generalized linear mixed models by linearization methods, essentially calls



the MIXED procedure repeatedly. If you are aware of the syntax differences between the procedures, you can easily convert your %GLIMMIX macro statements.

Important functional differences between PROC GLIMMIX and PROC MIXED for linear models and linear mixed models include the following:

- The MIXED procedure models R-side effects through the REPEATED statement and G-side effects through the RANDOM statement. The GLIMMIX procedure models all random components of the model through the RANDOM statement. You use the `_RESIDUAL_` keyword or the RESIDUAL option in the RANDOM statement to model R-side covariance structure in the GLIMMIX procedure. For example, the PROC MIXED statement

```
repeated / subject=id type=ar(1);
```

is equivalent to the following RANDOM statement in the GLIMMIX procedure:

```
random _residual_ / subject=id type=ar(1);
```

If you need to specify an effect for levelization—for example, because the construction of the **R** matrix is order-dependent or because you need to account for missing values—the RESIDUAL option in the RANDOM statement of the GLIMMIX procedure is used to indicate that you are modeling an R-side covariance nature. For example, the PROC MIXED statements

```
class time id;
repeated time / subject=id type=ar(1);
```

are equivalent to the following PROC GLIMMIX statements:

```
class time id;
random time / subject=id type=ar(1) residual;
```

- There is generally considerable overlap in the covariance structures available through the TYPE= option in the RANDOM statement in PROC GLIMMIX and through the TYPE= options in the RANDOM and REPEATED statements in PROC MIXED. However, the Kronecker-type structures, the geometrically anisotropic spatial structures, and the GDATA= option in the RANDOM statement of the MIXED procedure are currently not supported in the GLIMMIX procedure. The MIXED procedure, on the other hand, does not support TYPE=RSMOOTH and TYPE=PSPLINE.
- For normal linear mixed models, the (default) METHOD=RSPL in PROC GLIMMIX is identical to the default METHOD=REML in PROC MIXED. Similarly, METHOD=MSPL in PROC GLIMMIX is identical for these models to METHOD=ML in PROC MIXED. The GLIMMIX procedure does not support Type I through Type III (ANOVA) estimation methods for variance component models. Also, the procedure does not have a METHOD=MIVQUE0 option, but you can produce these estimates through the NOITER option in the PARMs statement.
- The MIXED procedure solves the iterative optimization problem by means of a ridge-stabilized Newton-Raphson algorithm. With the GLIMMIX procedure, you can choose from a variety of optimization methods via the NLOPTIONS statement. The default method for most GLMMs is a quasi-Newton algorithm. A ridge-stabilized Newton-Raphson algorithm, akin to the optimization method in

the MIXED procedure, is available in the GLIMMIX procedure through the TECHNIQUE=NRRIDG option in the NLOPTIONS statement. Because of differences in the line-search methods, update methods, and the convergence criteria, you might get slightly different estimates with the two procedures in some instances. The GLIMMIX procedure, for example, monitors several convergence criteria simultaneously.

- You can produce predicted values, residuals, and confidence limits for predicted values with both procedures. The mechanics are slightly different, however. With the MIXED procedure you use the OUTPM= and OUTP= options in the MODEL statement to write statistics to data sets. With the GLIMMIX procedure you use the OUTPUT statement and indicate with keywords which “flavor” of a statistic to compute.
- The following GLIMMIX statements are not available in the MIXED procedure: COVTEST, EFFECT, FREQ, LSMESTIMATE, OUTPUT, and programming statements.
- A sampling-based Bayesian analysis as through the PRIOR statement in the MIXED procedure is not available in the GLIMMIX procedure.
- In the GLIMMIX procedure, several RANDOM statement options apply to the RANDOM statement in which they are specified. For example, the following statements in the GLIMMIX procedure request that the solution vector be printed for the A and A\*B\*C random effects and that the G matrix corresponding to the A\*B interaction random effect be displayed:

```
random a / s;
random a*b / G;
random a*b*c / alpha=0.04;
```

Confidence intervals with a 0.96 coverage probability are produced for the solutions of the A\*B\*C effect. In the MIXED procedure, the S option, for example, when specified in one RANDOM statement, applies to all RANDOM statements.

- If you select nonmissing values in the *value-list* of the DDF= option in the MODEL statement, PROC GLIMMIX uses these values to override degrees of freedom for this effect that might be determined otherwise. For example, the following statements request that the denominator degrees of freedom for tests and confidence intervals involving the A effect be set to 4:

```
proc glimmix;
 class block a b;
 model y = a b a*b / s ddf=4, ., . ddfm=satterthwaite;
 random block a*block / s;
 lsmeans a b a*b / diff;
run;
```

In the example, this applies to the “Type III Tests of Fixed Effects,” “Least Squares Means,” and “Differences of Least Squares Means” tables. In the MIXED procedure, the Satterthwaite approximation overrides the DDF= specification.

- The DDFM=BETWITHIN degrees-of-freedom method in the GLIMMIX procedure requires that the data be processed by subjects; see the section “Processing by Subjects” on page 3082.

- When you add the response variable to the **CLASS** statement, PROC GLIMMIX defaults to the multinomial distribution. Adding the response variable to the **CLASS** statement in PROC MIXED has no effect on the fitted model.
- The ODS name of the table for the solution of fixed effects is SolutionF in the MIXED procedure. In PROC GLIMMIX, the name of the table that contains fixed-effects solutions is “ParameterEstimates.” In generalized linear models, this table also contains scale parameters and overdispersion parameters. The MIXED procedure always produces a “Covariance Parameter Estimates” table. The GLIMMIX procedure produces this table only in mixed models or models with nontrivial R-side covariance structure.
- If you compute predicted values in the GLIMMIX procedure in a model with only R-side random components and missing values for the dependent variable, the predicted values will *not* be kriging predictions as is the case with the MIXED procedure.

---

## Singly or Doubly Iterative Fitting

Depending on the structure of your model, the GLIMMIX procedure determines the appropriate approach for estimating the parameters of the model. The elementary algorithms fall into three categories:

### 1. Noniterative algorithms

A closed form solution exists for all model parameters. Standard linear models with homoscedastic, uncorrelated errors can be fit with noniterative algorithms.

### 2. Singly iterative algorithms

A single optimization, consisting of one or more iterations, is performed to obtain solutions for the parameter estimates by numerical techniques. Linear mixed models for normal data can be fit with singly iterative algorithms. Laplace and quadrature estimation for generalized linear mixed models uses a singly iterative algorithm with a separate suboptimization to compute the random-effects solutions as modes of the log-posterior distribution.

### 3. Doubly iterative algorithms

A model of simpler structure is derived from the target model. The parameters of the simpler model are estimated by noniterative or singly iterative methods. Based on these new estimates, the model of simpler structure is rederived and another estimation step follows. The process continues until changes in the parameter estimates are sufficiently small between two recomputations of the simpler model or until some other criterion is met. The rederivation of the model can often be cast as a change of the response to some pseudo-data along with an update of implicit model weights.

Obviously, noniterative algorithms are preferable to singly iterative ones, which in turn are preferable to doubly iterative algorithms. Two drawbacks of doubly iterative algorithms based on linearization are that likelihood-based measures apply to the pseudo-data, not the original data, and that at the outer level the progress of the algorithm is tied to monitoring the parameter estimates. The advantage of doubly iterative algorithms, however, is to offer—at convergence—the statistical inference tools that apply to the simpler models.

The output and log messages contain information about which algorithm is employed. For a noniterative algorithm, PROC GLIMMIX produces a message that no optimization was performed. Noniterative algorithms are employed automatically for normal data with identity link.

You can determine whether a singly or doubly iterative algorithm was used, based on the “Iteration History” table and the “Convergence Status” table (Figure 41.17).

**Figure 41.17** Iteration History and Convergence Status in Singly Iterative Fit

| The GLIMMIX Procedure |          |             |                       |            |                 |
|-----------------------|----------|-------------|-----------------------|------------|-----------------|
| Iteration History     |          |             |                       |            |                 |
| Iteration             | Restarts | Evaluations | Objective<br>Function | Change     | Max<br>Gradient |
| 0                     | 0        | 4           | 83.039723731          | .          | 13.63536        |
| 1                     | 0        | 3           | 82.189661988          | 0.85006174 | 0.281308        |
| 2                     | 0        | 3           | 82.189255211          | 0.00040678 | 0.000174        |
| 3                     | 0        | 3           | 82.189255211          | 0.00000000 | 1.05E-10        |

Convergence criterion (GCONV=1E-8) satisfied.

The “Iteration History” table contains the Evaluations column that shows how many function evaluations were performed in a particular iteration. The convergence status message informs you which convergence criterion was met when the estimation process concluded. In a singly iterative fit, the criterion is one that applies to the optimization. In other words, it is one of the criteria that can be controlled with the **NLOPTIONS** statement: see the **ABSCONV=**, **ABSFCONV=**, **ABSGCONV=**, **ABSXCONV=**, **FCONV=**, or **GCONV=** option.

In a doubly iterative fit, the “Iteration History” table does not contain an Evaluations column. Instead it displays the number of iterations within an optimization (Subiterations column in Figure 41.18).

**Figure 41.18** Iteration History and Convergence Status in Doubly Iterative Fit

| Iteration History |          |               |                       |            |                 |  |
|-------------------|----------|---------------|-----------------------|------------|-----------------|--|
| Iteration         | Restarts | Subiterations | Objective<br>Function | Change     | Max<br>Gradient |  |
| 0                 | 0        | 5             | 79.688580269          | 0.11807224 | 7.851E-7        |  |
| 1                 | 0        | 3             | 81.294622554          | 0.02558021 | 8.209E-7        |  |
| 2                 | 0        | 2             | 81.438701534          | 0.00166079 | 4.061E-8        |  |
| 3                 | 0        | 1             | 81.444083567          | 0.00006263 | 2.311E-8        |  |
| 4                 | 0        | 1             | 81.444265216          | 0.00000421 | 0.000025        |  |
| 5                 | 0        | 1             | 81.444277364          | 0.00000383 | 0.000023        |  |
| 6                 | 0        | 1             | 81.444266322          | 0.00000348 | 0.000021        |  |
| 7                 | 0        | 1             | 81.44427636           | 0.00000316 | 0.000019        |  |
| 8                 | 0        | 1             | 81.444267235          | 0.00000287 | 0.000017        |  |
| 9                 | 0        | 1             | 81.444275529          | 0.00000261 | 0.000016        |  |
| 10                | 0        | 1             | 81.44426799           | 0.00000237 | 0.000014        |  |
| 11                | 0        | 1             | 81.444274843          | 0.00000216 | 0.000013        |  |
| 12                | 0        | 1             | 81.444268614          | 0.00000196 | 0.000012        |  |
| 13                | 0        | 1             | 81.444274277          | 0.00000178 | 0.000011        |  |
| 14                | 0        | 1             | 81.444269129          | 0.00000162 | 9.772E-6        |  |
| 15                | 0        | 0             | 81.444273808          | 0.00000000 | 9.102E-6        |  |

Convergence criterion (PCONV=1.11022E-8) satisfied.

The Iteration column then counts the number of optimizations. The “Convergence Status” table indicates that the estimation process concludes when a criterion is met that monitors the parameter estimates across optimization, namely the `PCONV=` or `ABSPCONV=` criterion.

You can control the optimization process with the GLIMMIX procedure through the `NLOPTIONS` statement. Its options affect the individual optimizations. In a doubly iterative scheme, these apply to all optimizations.

The default optimization techniques are `TECHNIQUE=NONE` for noniterative estimation, `TECHNIQUE=NEWRAP` for singly iterative methods in GLMs, `TECHNIQUE=NRRIDG` for pseudo-likelihood estimation with binary data, and `TECHNIQUE=QUANEW` for other mixed models.

---

## Default Estimation Techniques

Based on the structure of the model, the GLIMMIX procedure selects the estimation technique for estimating the model parameters. If you fit a generalized linear mixed model, you can change the estimation technique with the `METHOD=` option in the `PROC GLIMMIX` statement. The defaults are determined as follows:

- generalized linear model
  - normal distribution: restricted maximum likelihood
  - all other distributions: maximum likelihood

- generalized linear model with overdispersion  
Parameters ( $\beta$ ;  $\phi$ , if present) are estimated by (restricted) maximum likelihood as for generalized linear models. The overdispersion parameter is estimated from the Pearson statistic after all other parameters have been estimated.
- generalized linear mixed models  
The default technique is `METHOD=RSPL`, corresponding to maximizing the residual log pseudo-likelihood with an expansion about the current solutions of the best linear unbiased predictors of the random effects. In models for normal data with identity link, `METHOD=RSPL` and `METHOD=RMPL` are equivalent to restricted maximum likelihood estimation, and `METHOD=MSPL` and `METHOD=MMPL` are equivalent to maximum likelihood estimation. This is reflected in the labeling of statistics in the “Fit Statistics” table.

---

## Default Output

The following sections describe the output that PROC GLIMMIX produces by default. The output is organized into various tables, which are discussed in the order of appearance. Note that the contents of a table can change with the estimation method or the model being fit.

### Model Information

The “Model Information” table displays basic information about the fitted model, such as the link and variance functions, the distribution of the response, and the data set. If important model quantities—for example, the response, weights, link, or variance function—are user-defined, the “Model Information” table displays the final assignment to the respective variable, as determined from your programming statements. If the table indicates that the variance matrix is blocked by an effect, then PROC GLIMMIX processes the data by subjects. The “Dimensions” table displays the number of subjects. For more information about processing by subjects, see the section “Processing by Subjects” on page 3082. The ODS name of the “Model Information” table is ModelInfo.

### Class Level Information

The “Class Level Information” table lists the levels of every variable specified in the `CLASS` statement. You should check this information to make sure that the data are correct. You can adjust the order of the `CLASS` variable levels with the `ORDER=` option in the `PROC GLIMMIX` statement. The ODS name of the “Class Level Information” table is ClassLevels.

### Number of Observations

The “Number of Observations” table displays the number of observations read from the input data set and the number of observations used in the analysis. If you specify a `FREQ` statement, the table also displays the sum of frequencies read and used. If the *events/trials* syntax is used for the response, the table also displays the number of events and trials used in the analysis. The ODS name of the “Number of Observations” table is NObs.

## Response Profile

For binary and multinomial data, the “Response Profile” table displays the Ordered Value from which the GLIMMIX procedure determines the following:

- the probability being modeled for binary data
- the ordering of categories for ordinal data
- the reference category for generalized logit models

For each response category level, the frequency used in the analysis is reported. The section “Response-Level Ordering and Referencing” on page 3100 explains how you can use the **DESCENDING**, **EVENT=**, **ORDER=**, and **REF=** options to affect the assignment of Ordered Values to the response categories. The ODS name of the “Response Profile” table is ResponseProfile.

## Dimensions

The “Dimensions” table displays information from which you can determine the size of relevant matrices in the model. This table is useful in determining CPU time and memory requirements. For ODS purposes, the name of the “Dimensions” table is “Dimensions.”

## Optimization Information

The “Optimization Information” table displays important details about the optimization process.

The optimization technique that is displayed in the table is the technique that applies to any single optimization. For singly iterative methods that is *the* optimization method.

The number of parameters that are updated in the optimization equals the number of parameters in this table minus the number of equality constraints. The number of constraints is displayed if you fix covariance parameters with the **HOLD=** option in the **PARMS** statement. The GLIMMIX procedure also lists the number of upper and lower boundary constraints. Note that the procedure might impose boundary constraints for certain parameters, such as variance components and correlation parameters. Covariance parameters for which a **HOLD=** was issued have an upper and lower boundary equal to the parameter value.

If a residual scale parameter is profiled from the optimization, it is also shown in the “Optimization Information” table.

In a GLMM for which the parameters are estimated by one of the linearization methods, you need to initiate the process of computing the pseudo-response. This can be done based on existing estimates of the fixed effects, or by using the data themselves—possibly after some suitable adjustment—as an estimate of the initial mean. The default in PROC GLIMMIX is to use the data themselves to derive initial estimates of the mean function and to construct the pseudo-data. The “Optimization Information” table shows how the pseudo-data are determined initially. Note that this issue is separate from the determination of starting values for the covariance parameters. These are computed as minimum variance quadratic unbiased estimates (with 0 priors, MIVQUE0; Goodnight 1978a) or obtained from the *value-list* in the **PARMS** statement.

The ODS name of the table is OptInfo.

## Iteration History

The “Iteration History” table describes the progress of the estimation process. In singly iterative methods, the table displays the following:

- the iteration count, `Iteration`
- the number of restarts, `Restarts`
- the number of function evaluations, `Evaluations`
- the objective function, `Objective`
- the change in the objective function, `Change`
- the absolute value of the largest (projected) gradient, `MaxGradient`

Note that the change in the objective function is not the convergence criterion monitored by the GLIMMIX procedure. PROC GLIMMIX tracks several convergence criteria simultaneously; see the `ABSCONV=`, `ABSFCONV=`, `ABSGCONV=`, `ABSXCONV=`, `FCONV=`, or `GCONV=` option in the `NLOPTIONS` statement.

For doubly iterative estimation methods, the “Iteration History” table does not display the progress of the individual optimizations; instead, it reports on the progress of the outer iterations. Every row of the table then corresponds to an update of the linearization, the computation of a new set of pseudo-data, and a new optimization. In the listing, PROC GLIMMIX displays the following:

- the optimization count, `Iteration`
- the number of restarts, `Restarts`
- the number of iterations per optimization, `Subiterations`
- the change in the parameter estimates, `Change`
- the absolute value of the largest (projected) gradient at the end of the optimization, `MaxGradient`

By default, the change in the parameter estimates is expressed in terms of the relative `PCONV` criterion. If you request an absolute criterion with the `ABSPCONV` option of the `PROC GLIMMIX` statement, the change reflects the largest absolute difference since the last optimization.

If you specify the `ITDETAILS` option in the `PROC GLIMMIX` statement, parameter estimates and their gradients are added to the “Iteration History” table. For ODS purposes, the name of the “Iteration History” table is “IterHistory.”

## Convergence Status

The “Convergence Status” table contains a status message describing the reason for termination of the optimization. The message is also written to the log. The ODS name of the “Convergence Status” table is `ConvergenceStatus`, and you can query the nonprinting numeric variable `Status` to check for a successful optimization. This is useful in batch processing, or when processing `BY` groups, such as in simulations. Successful optimizations are indicated by the value 0 of the `Status` variable.



## Fit Statistics

The “Fit Statistics” table provides statistics about the estimated model. The first entry of the table corresponds to the negative of twice the (possibly restricted) log likelihood, log pseudo-likelihood, or log quasi-likelihood. If the estimation method permits the true log likelihood or residual log likelihood, the description of the first entry reads accordingly. Otherwise, the fit statistics are preceded by the words *Pseudo-* or *Quasi-*, for Pseudo- and Quasi-Likelihood estimation, respectively.

Note that the (residual) log pseudo-likelihood in a GLMM is the (residual) log likelihood of a linearized model. You should not compare these values across different statistical models, even if the models are nested with respect to fixed and/or G-side random effects. It is possible that between two nested models the larger model has a smaller pseudo-likelihood. For this reason, IC=NONE is the default for GLMMs fit by pseudo-likelihood methods.

See the IC= option of the PROC GLIMMIX statement and Table 41.2 for the definition and computation of the information criteria reported in the “Fit Statistics” table.

For generalized linear models, the GLIMMIX procedure reports Pearson’s chi-square statistic

$$X^2 = \sum_i \frac{w_i (y_i - \hat{\mu}_i)^2}{a(\hat{\mu}_i)}$$

where  $a(\hat{\mu}_i)$  is the variance function evaluated at the estimated mean.

For GLMMs, the procedure typically reports a generalized chi-square statistic,

$$X_g^2 = \hat{\mathbf{r}}' \mathbf{V}(\hat{\boldsymbol{\theta}}^*)^{-1} \hat{\mathbf{r}}$$

so that the ratio of  $X^2$  or  $X_g^2$  and the degrees of freedom produces the usual residual dispersion estimate.

If the R-side scale parameter  $\phi$  is not extracted from  $\mathbf{V}$ , the GLIMMIX procedure computes

$$X_g^2 = \hat{\mathbf{r}}' \mathbf{V}(\hat{\boldsymbol{\theta}})^{-1} \hat{\mathbf{r}}$$

as the generalized chi-square statistic. This is the case, for example, if R-side covariance structures are varied by a GROUP= effect or if the scale parameter is not profiled for an R-side TYPE=CS, TYPE=SP, TYPE=AR, TYPE=TOEP, or TYPE=ARMA covariance structure.

For METHOD=LAPLACE, the generalized chi-square statistic is not reported. Instead, the Pearson statistic for the conditional distribution appears in the “Conditional Fit Statistics” table.

If your model contains smooth components (such as TYPE=RSMOOTH), then the “Fit Statistics” table also displays the residual degrees of freedom of the smoother. These degrees of freedom are computed as

$$df_{smooth, res} = f - \text{trace}(\mathbf{S})$$

where  $\mathbf{S}$  is the “smoother” matrix—that is, the matrix that produces the predicted values on the linked scale.

The ODS name of the “Fit Statistics” table is FitStatistics.

## Covariance Parameter Estimates

In a GLMM, the “Covariance Parameter Estimates” table displays the estimates of the covariance parameters and their asymptotic standard errors. This table is produced only for generalized linear *mixed* models. In generalized linear models with scale parameter, or when an overdispersion parameter is present, the estimates of parameters related to the dispersion are displayed in the “Parameter Estimates” table.

The standard error of the covariance parameters is determined from the diagonal entries of the asymptotic variance matrix of the covariance parameter estimates. You can display this matrix with the `ASYCOV` option in the `PROC GLIMMIX` statement.

The ODS name of the “Covariance Parameter Estimates” table is `CovParms`.

## Type III Tests of Fixed Effects

The “Type III Tests of Fixed Effects” table contains hypothesis tests for the significance of each of the fixed effects specified in the `MODEL` statement. By default, `PROC GLIMMIX` computes these tests by first constructing a Type III `L` matrix for each effect; see Chapter 15, “The Four Types of Estimable Functions.” The `L` matrix is then used to construct the test statistic

$$F = \frac{\hat{\boldsymbol{\beta}}' \mathbf{L}' (\mathbf{LQL}')^{-1} \mathbf{L} \hat{\boldsymbol{\beta}}}{\text{rank}(\mathbf{LQL}')}$$

where the matrix `Q` depends on the estimation method and options. For example, in a GLMM, the default is  $\mathbf{Q} = (\mathbf{X}'\mathbf{V}(\hat{\boldsymbol{\theta}})^{-1}\mathbf{X})^{-}$ , where  $\mathbf{V}(\boldsymbol{\theta})$  is the marginal variance of the pseudo-response. If you specify the `DDFM=KENWARDROGER` option, `Q` is the estimated variance matrix of the fixed effects, adjusted by the method of Kenward and Roger (1997). If the `EMPIRICAL=` option is in effect, `Q` corresponds to the selected sandwich estimator.

You can use the `HTYPE=` option in the `MODEL` statement to obtain tables of Type I (sequential) tests and Type II (adjusted) tests in addition to or instead of the table of Type III (partial) tests.

The ODS names of the “Type I Tests of Fixed Effects” through the “Type III Tests of Fixed Effects” tables are `Tests1` through `Tests3`, respectively.

## Notes on Output Statistics

Table 41.14 lists the statistics computed with the `OUTPUT` statement of the `GLIMMIX` procedure and their default names. This section provides further details about these statistics.

The distinction between prediction and confidence limits in Table 41.14 stems from the involvement of the predictors of the random effects. If the random-effect solutions (BLUPs, EBES) are involved, then the associated standard error used in computing the limits are standard errors of prediction rather than standard errors of estimation. The prediction limits are *not* limits for the prediction of a new observation.

The Pearson residuals in Table 41.14 are “Pearson-type” residuals, because the residuals are standardized by the square root of the marginal or conditional variance of an observation. Traditionally, Pearson residuals in generalized linear models are divided by the square root of the variance function. The `GLIMMIX` procedure divides by the square root of the variance so that marginal and conditional residuals have similar expressions. In other words, scale and overdispersion parameters are included.

When residuals or predicted values involve only the fixed effects part of the linear predictor (that is,  $\hat{\eta}_m = \mathbf{x}'\hat{\boldsymbol{\beta}}$ ), then all model quantities are computed based on this predictor. For example, if the variance by which to standardize a marginal residual involves the variance function, then the variance function is also evaluated at the marginal mean,  $g^{-1}(\hat{\eta}_m)$ . Thus the residuals  $p - \hat{\eta}$  and  $p_m - \hat{\eta}_m$  can also be expressed as  $(y - \mu)/\partial\mu$  and  $(y - \mu_m)/\partial\mu_m$ , respectively, where  $\partial\mu$  is the derivative with respect to the linear predictor. To construct the residual  $p - \hat{\eta}_m$  in a GLMM, you can add the value of `_ZGAMMA_` to the conditional residual  $p - \hat{\eta}$ . (The residual  $p - \hat{\eta}_m$  is computed instead of the default marginal residual when you specify the `CPSEUDO` option in the `OUTPUT` statement.) If the predictor involves the BLUPs, then all relevant expressions and evaluations involve the conditional mean  $g^{-1}(\hat{\eta})$ .

The naming convention to add “PA” to quantities not involving the BLUPs is chosen to suggest the concept of a population average. When the link function is nonlinear, these are not truly population-averaged quantities, because  $g^{-1}(\mathbf{x}'\boldsymbol{\beta})$  does not equal  $E[Y]$  in the presence of random effects. For example, if

$$\mu_i = g^{-1}(\mathbf{x}'_i\boldsymbol{\beta} + \mathbf{z}'_i\boldsymbol{\gamma}_i)$$

is the conditional mean for subject  $i$ , then

$$g^{-1}(\mathbf{x}'_i\hat{\boldsymbol{\beta}})$$

does not estimate the average response in the population of subjects but the response of the average subject (the subject for which  $\boldsymbol{\gamma}_i = \mathbf{0}$ ). For models with identity link, the average response and the response of the average subject are identical.

The GLIMMIX procedure obtains standard errors on the scale of the mean by the delta method. If the link is a nonlinear function of the linear predictor, these standard errors are only approximate. For example,

$$\text{Var}[g^{-1}(\hat{\eta}_m)] \doteq \left( \frac{\partial g^{-1}(t)}{\partial t} \Big|_{\hat{\eta}_m} \right)^2 \text{Var}[\hat{\eta}_m]$$

Confidence limits on the scale of the data are usually computed by applying the inverse link function to the confidence limits on the linked scale. The resulting limits on the data scale have the same coverage probability as the limits on the linked scale, but they are possibly asymmetric.

In generalized logit models, confidence limits on the mean scale are based on symmetric limits about the predicted mean in a category. Suppose that the multinomial response in such a model has  $J$  categories. The probability of a response in category  $i$  is computed as

$$\hat{\mu}_i = \frac{\exp\{\hat{\eta}_i\}}{\sum_{j=1}^J \exp\{\hat{\eta}_j\}}$$

The variance of  $\hat{\mu}_i$  is then approximated as

$$\text{Var}[\hat{\mu}_i] \doteq \zeta = \mathbf{v}'_i \text{Var} \begin{bmatrix} \hat{\eta}_1 & \hat{\eta}_2 & \cdots & \hat{\eta}_J \end{bmatrix} \mathbf{v}_i$$

where  $\mathbf{v}_i$  is a  $J \times 1$  vector with  $k$ th element

$$\begin{aligned} \hat{\mu}_i(1 - \hat{\mu}_i) & \quad i = k \\ -\hat{\mu}_i\hat{\mu}_k & \quad i \neq k \end{aligned}$$

The confidence limits in the generalized logit model are then obtained as

$$\hat{\mu}_i \pm t_{\nu, \alpha/2} \sqrt{\zeta}$$

where  $t_{\nu, \alpha/2}$  is the  $100 \times (1 - \alpha/2)$  percentile from a  $t$  distribution with  $\nu$  degrees of freedom. Confidence limits are truncated if they fall outside the  $[0, 1]$  interval.

## ODS Table Names

Each table created by PROC GLIMMIX has a name associated with it, and you must use this name to reference the table when you use ODS statements. These names are listed in Table 41.23.

**Table 41.23** ODS Tables Produced by PROC GLIMMIX

| Table Name        | Description                                                                                                      | Required Statement / Option                                                                                                                      |
|-------------------|------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------|
| AsyCorr           | asymptotic correlation matrix of covariance parameters                                                           | PROC GLIMMIX ASYCORR                                                                                                                             |
| AsyCov            | asymptotic covariance matrix of covariance parameters                                                            | PROC GLIMMIX ASYCOV                                                                                                                              |
| CholG             | Cholesky root of the estimated <b>G</b> matrix                                                                   | RANDOM / GC                                                                                                                                      |
| CholV             | Cholesky root of blocks of the estimated <b>V</b> matrix                                                         | RANDOM / VC                                                                                                                                      |
| ClassLevels       | level information from the <b>CLASS</b> statement                                                                | default output                                                                                                                                   |
| Coef              | <b>L</b> matrix coefficients                                                                                     | E option in <b>MODEL</b> , <b>CONTRAST</b> , <b>ESTIMATE</b> , <b>LSMESTIMATE</b> , or <b>LSMEANS</b> ; <b>ELSM</b> option in <b>LSMESTIMATE</b> |
| ColumnNames       | name association for <b>OUTDESIGN</b> data set                                                                   | PROC GLIMMIX <b>OUTDESIGN(NAMES)</b>                                                                                                             |
| CondFitStatistics | conditional fit statistics                                                                                       | PROC GLIMMIX <b>METHOD=LAPLACE</b>                                                                                                               |
| Contrasts         | results from the <b>CONTRAST</b> statements                                                                      | <b>CONTRAST</b>                                                                                                                                  |
| ConvergenceStatus | status of optimization at conclusion                                                                             | default output                                                                                                                                   |
| CorrB             | approximate correlation matrix of fixed-effects parameter estimates                                              | <b>MODEL / CORRB</b>                                                                                                                             |
| CovB              | approximate covariance matrix of fixed-effects parameter estimates                                               | <b>MODEL / COVB</b>                                                                                                                              |
| CovBDetails       | details about model-based and/or adjusted covariance matrix of fixed effects                                     | <b>MODEL / COVB(DETAILS)</b>                                                                                                                     |
| CovBI             | inverse of approximate covariance matrix of fixed-effects parameter estimates                                    | <b>MODEL / COVBI</b>                                                                                                                             |
| CovBModelBased    | model-based (unadjusted) covariance matrix of fixed effects if <b>DDFM=KR</b> or <b>EMPIRICAL</b> option is used | <b>MODEL / COVB(DETAILS)</b>                                                                                                                     |
| CovParms          | estimated covariance parameters in GLMMs                                                                         | default output (in GLMMs)                                                                                                                        |
| CovTests          | results from <b>COVTEST</b> statements (except for confidence bounds)                                            | <b>COVTEST</b>                                                                                                                                   |

Table 41.23 continued

| Table Name               | Description                                                          | Required Statement / Option                              |
|--------------------------|----------------------------------------------------------------------|----------------------------------------------------------|
| Diffs                    | differences of LS-means                                              | LSMEANS / DIFF (or PDIFF)                                |
| Dimensions               | dimensions of the model                                              | default output                                           |
| Estimates                | results from ESTIMATE statements                                     | ESTIMATE                                                 |
| FitStatistics            | fit statistics                                                       | default                                                  |
| G                        | estimated <b>G</b> matrix                                            | RANDOM / G                                               |
| GCorr                    | correlation matrix from the estimated <b>G</b> matrix                | RANDOM / GCORR                                           |
| Hessian                  | Hessian matrix (observed or expected)                                | PROC GLIMMIX HESSIAN                                     |
| InvCholG                 | inverse Cholesky root of the estimated <b>G</b> matrix               | RANDOM / GCI                                             |
| InvCholV                 | inverse Cholesky root of the blocks of the estimated <b>V</b> matrix | RANDOM / VCI                                             |
| InvG                     | inverse of the estimated <b>G</b> matrix                             | RANDOM / GI                                              |
| InvV                     | inverse of blocks of the estimated <b>V</b> matrix                   | RANDOM / VI                                              |
| IterHistory              | iteration history                                                    | default output                                           |
| kdTree                   | <i>k</i> -d tree information                                         | RANDOM / TYPE=RSMOOTH<br>KNOTMETHOD=<br>KDTREE(TREEINFO) |
| KnotInfo                 | knot coordinates of low-rank spline smoother                         | RANDOM / TYPE=RSMOOTH<br>KNOTINFO                        |
| LSMeans                  | LS-means                                                             | LSMEANS                                                  |
| LSMEstimates             | estimates among LS-means                                             | LSMESTIMATE                                              |
| LSMFtest                 | <i>F</i> test for LSMESTIMATEs                                       | LSMESTIMATE / FTEST                                      |
| LSMLines                 | lines display for LS-means                                           | LSMEANS / LINES                                          |
| ModelInfo                | model information                                                    | default output                                           |
| NObs                     | number of observations read and used, number of trials and events    | default output                                           |
| OddsRatios               | odds ratios of parameter estimates                                   | MODEL / ODDSRATIO                                        |
| OptInfo                  | optimization information                                             | default output                                           |
| ParameterEstimates       | fixed-effects solution; overdispersion and scale parameter in GLMs   | MODEL / S                                                |
| ParmSearch               | parameter search values                                              | PARMS                                                    |
| QuadCheck                | adaptive recalculation of quadrature approximation at solution       | METHOD=QUAD(QCHECK)                                      |
| ResponseProfile          | response categories and category modeled                             | default output in models with binary or nominal response |
| Slices                   | tests of LS-means slices                                             | LSMEANS / SLICE=                                         |
| SliceDiffs               | differences of simple LS-means effects                               | LSMEANS / SLICEDIFF=                                     |
| SolutionR                | random-effects solution vector                                       | RANDOM / S                                               |
| StandardizedCoefficients | fixed-effects solutions from centered and/or scaled model            | MODEL / STDCOEf                                          |
| Tests1                   | Type I tests of fixed effects                                        | MODEL / HTYPE=1                                          |

**Table 41.23** *continued*

| Table Name | Description                                                         | Required Statement / Option |
|------------|---------------------------------------------------------------------|-----------------------------|
| Tests2     | Type II tests of fixed effects                                      | MODEL / HTYPE=2             |
| Tests3     | Type III tests of fixed effects                                     | default output              |
| V          | blocks of the estimated <b>V</b> matrix                             | RANDOM / V                  |
| VCorr      | correlation matrix from the blocks of the estimated <b>V</b> matrix | RANDOM / VCORR              |

The SLICE statement also creates tables, which are not listed in Table 41.23. For information about these tables, see the section “SLICE Statement” on page 498 of Chapter 19, “Shared Concepts and Topics.”

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “Statistical Graphics Using ODS.”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “A Primer on ODS Statistical Graphics” on page 599 in Chapter 21, “Statistical Graphics Using ODS.”

The following subsections provide information about the basic ODS statistical graphics produced by the GLIMMIX procedure. The graphics fall roughly into two categories: diagnostic plots and graphics for least squares means.

### ODS Graph Names

The GLIMMIX procedure does not produce graphs by default. You can reference every graph produced through ODS Graphics with a name. The names of the graphs that PROC GLIMMIX generates are listed in Table 41.24, along with the required statements and options.

**Table 41.24** Graphs Produced by PROC GLIMMIX

| ODS Graph Name | Plot Description                                                | Option                                           |
|----------------|-----------------------------------------------------------------|--------------------------------------------------|
| AnomPlot       | Plot of LS-mean differences against the average LS-mean         | PLOTS=ANOMPLOT<br>LSMEANS / PLOTS=ANOMPLOT       |
| Boxplot        | Box plots of residuals and/or observed values for model effects | PLOTS=BOXPLOT                                    |
| ControlPlot    | Plot of LS-mean differences against a control level             | PLOTS=CONTROLPLOT<br>LSMEANS / PLOTS=CONTROLPLOT |
| DiffPlot       | Plot of LS-mean pairwise differences                            | PLOTS=DIFFPLOT<br>LSMEANS / PLOTS=DIFFPLOT       |

Table 41.24 *continued*

| ODS Graph Name      | Plot Description                                   | Option                                     |
|---------------------|----------------------------------------------------|--------------------------------------------|
| MeanPlot            | Plot of least squares means                        | PLOTS=MEANPLOT<br>LSMEANS / PLOTS=MEANPLOT |
| ORPlot              | Plot of odds ratios                                | PLOTS=ODDSRATIO                            |
| PearsonBoxplot      | Box plot of Pearson residuals                      | PLOTS=PEARSONPANEL(UNPACK)                 |
| PearsonByPredicted  | Pearson residuals vs. mean                         | PLOTS=PEARSONPANEL(UNPACK)                 |
| PearsonHistogram    | Histogram of Pearson residuals                     | PLOTS=PEARSONPANEL(UNPACK)                 |
| PearsonPanel        | Panel of Pearson residuals                         | PLOTS=PEARSONPANEL                         |
| PearsonQQplot       | <i>Q-Q</i> plot of Pearson residuals               | PLOTS=PEARSONPANEL(UNPACK)                 |
| ResidualBoxplot     | Box plot of (raw) residuals                        | PLOTS=RESIDUALPANEL(UNPACK)                |
| ResidualByPredicted | Residuals vs. mean or linear predictor             | PLOTS=RESIDUALPANEL(UNPACK)                |
| ResidualHistogram   | Histogram of (raw) residuals                       | PLOTS=RESIDUALPANEL(UNPACK)                |
| ResidualPanel       | Panel of (raw) residuals                           | PLOTS=RESIDUALPANEL                        |
| ResidualQQplot      | <i>Q-Q</i> plot of (raw) residuals                 | PLOTS=RESIDUALPANEL(UNPACK)                |
| StudentBoxplot      | Box plot of studentized residuals                  | PLOTS=STUDENTPANEL(UNPACK)                 |
| StudentByPredicted  | Studentized residuals vs. mean or linear predictor | PLOTS=STUDENTPANEL(UNPACK)                 |
| StudentHistogram    | Histogram of studentized residuals                 | PLOTS=STUDENTPANEL(UNPACK)                 |
| StudentPanel        | Panel of studentized residuals                     | PLOTS=STUDENTPANEL                         |
| StudentQQplot       | <i>Q-Q</i> plot of studentized residuals           | PLOTS=STUDENTPANEL(UNPACK)                 |

When ODS Graphics is enabled, the SLICE statement can produce plots that are associated with its analysis. For information about these plots, see the section “[SLICE Statement](#)” on page 498 of Chapter 19, “[Shared Concepts and Topics](#).”

## Diagnostic Plots

### Residual Panels

There are three types of residual panels in the GLIMMIX procedure. Their makeup of four component plots is the same; the difference lies in the type of residual from which the panel is computed. Raw residuals are displayed with the `PLOTS=RESIDUALPANEL` option. Studentized residuals are displayed with the `PLOTS=STUDENTPANEL` option, and Pearson residuals with the `PLOTS=PEARSONPANEL` option. By default, conditional residuals are used in the construction of the panels if the model contains G-side random effects. For example, consider the following statements:

```
proc glimmix plots=residualpanel;
 class A;
 model y = x1 x2 / dist=Poisson;
 random int / sub=A;
run;
```

The parameters are estimated by a pseudo-likelihood method, and at the final stage pseudo-data are related to a linear mixed model with random intercepts. The residual panel is constructed from

$$r = p - \mathbf{x}'\hat{\boldsymbol{\beta}} + \mathbf{z}'\hat{\boldsymbol{\gamma}}$$

where  $p$  is the pseudo-data.

The following hypothetical data set contains yields of an industrial process. Material was available from five randomly selected vendors to produce a chemical reaction whose yield depends on two factors (pressure and temperature at 3 and 2 levels, respectively).

```
data Yields;
 input Vendor Pressure Temp Yield @@;
 datalines;
 1 1 1 10.20 1 1 2 9.48 1 2 1 9.74
 1 2 2 8.92 1 3 1 11.79 1 3 2 8.85
 2 1 1 10.43 2 1 2 10.59 2 2 1 10.29
 2 2 2 10.15 2 3 1 11.12 2 3 2 9.30
 3 1 1 6.46 3 1 2 7.34 3 2 1 9.44
 3 2 2 8.11 3 3 1 9.38 3 3 2 8.37
 4 1 1 7.36 4 1 2 9.92 4 2 1 10.99
 4 2 2 10.34 4 3 1 10.24 4 3 2 9.96
 5 1 1 11.72 5 1 2 10.60 5 2 1 11.28
 5 2 2 9.03 5 3 1 14.09 5 3 2 8.92
 ;
```

Consider a linear mixed model with a two-way factorial fixed-effects structure for pressure and temperature effects and independent, homoscedastic random effects for the vendors. The following statements fit this model and request panels of marginal and conditional residuals:



```
ods graphics on;

proc glimmix data=Yields
 plots=residualpanel(conditional marginal);
 class Vendor Pressure Temp;
 model Yield = Pressure Temp Pressure*Temp;
 random vendor;
run;

ods graphics off;
```

The suboptions of the RESIDUALPANEL request produce two panels. The panel of conditional residuals is constructed from  $y - \mathbf{x}'\hat{\boldsymbol{\beta}} - \mathbf{z}'\hat{\boldsymbol{\gamma}}$  (Figure 41.19). The panel of marginal residuals is constructed from  $y - \mathbf{x}'\hat{\boldsymbol{\beta}}$  (Figure 41.20). Note that these residuals are deviations from the observed data, because the model is a normal linear mixed model, and hence it does not involve pseudo-data. Whenever the random-effects solutions  $\hat{\boldsymbol{\gamma}}$  are involved in constructing residuals, the title of the residual graphics identifies them as conditional residuals (Figure 41.19).

**Figure 41.19** Conditional Residuals

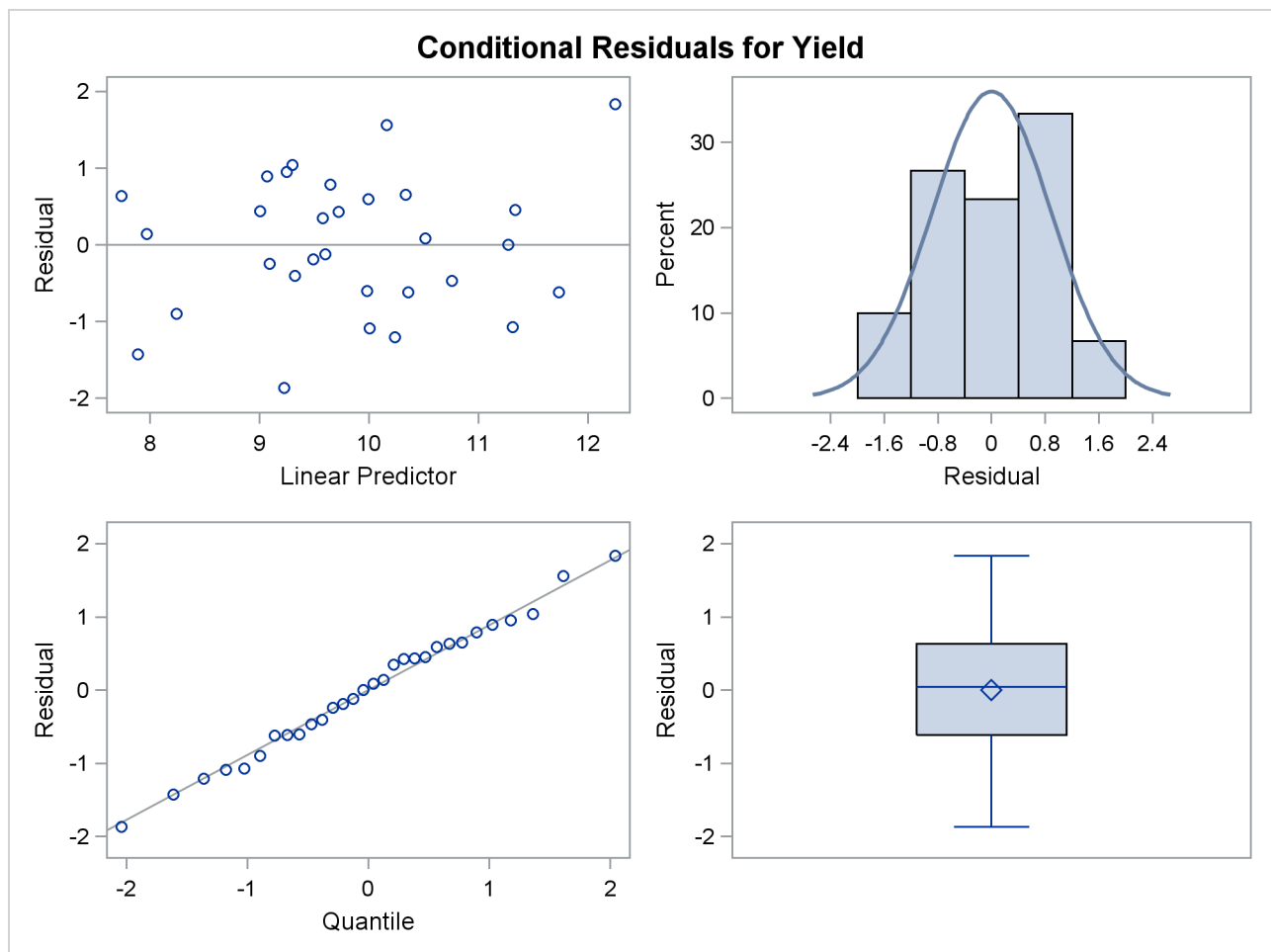
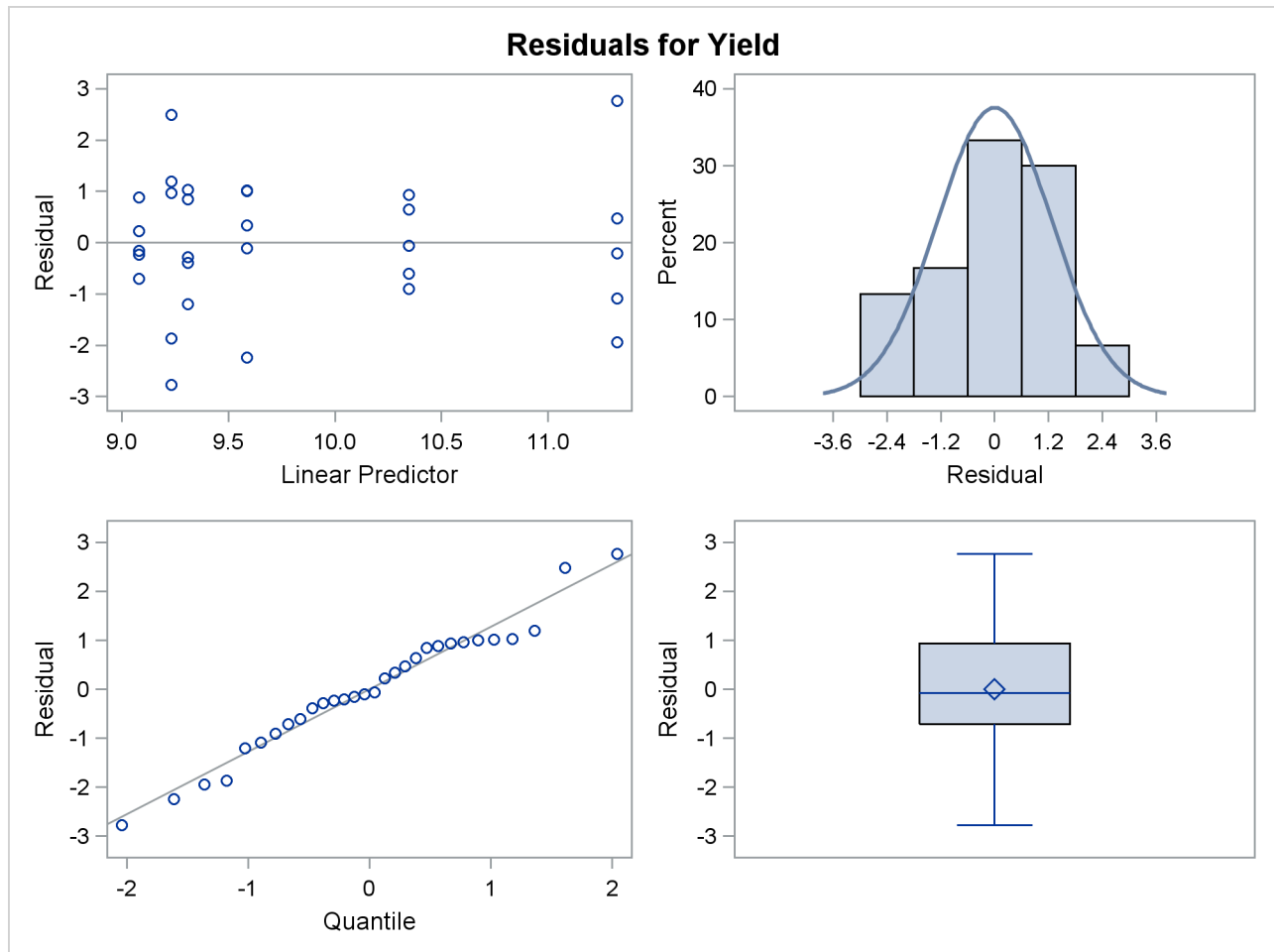


Figure 41.20 Marginal Residuals



The predictor takes on only six values for the marginal residuals, corresponding to the combinations of three temperature and two pressure levels. The assumption of a zero mean for the vendor random effect seems justified; the marginal residuals in the upper-left plot of Figure 41.20 do not exhibit any trend. The conditional residuals in Figure 41.19 are smaller and somewhat closer to normality compared to the marginal residuals.

### Box Plots

You can produce box plots of observed data, pseudo-data, and various residuals for effects in your model that consist of classification variables. Because you might not want to produce box plots for all such effects, you can request subsets with the suboptions of the `BOXPLOT` option in the `PLOTS` option. The `BOXPLOT` request in the following `PROC GLIMMIX` statement produces box plots for the random effects—in this case, the vendor effect. By default, `PROC GLIMMIX` constructs box plots from conditional residuals. The `MARGINAL`, `CONDITIONAL`, and `OBSERVED` suboptions instruct the procedure to construct three box plots for each random effect: box plots of the observed data (Figure 41.21), the marginal residuals (Figure 41.22), and the conditional residuals (Figure 41.23).

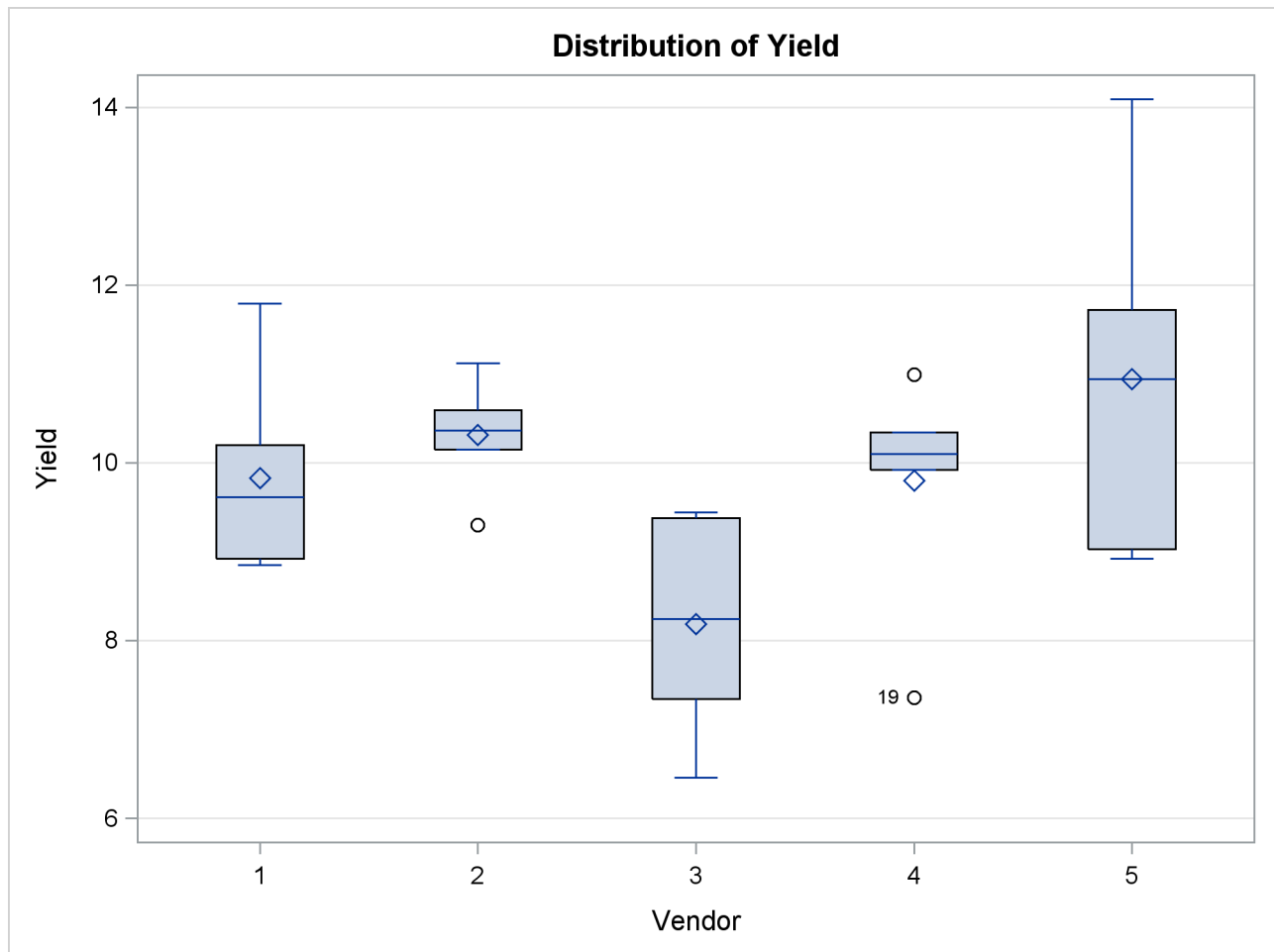
```
ods graphics on;

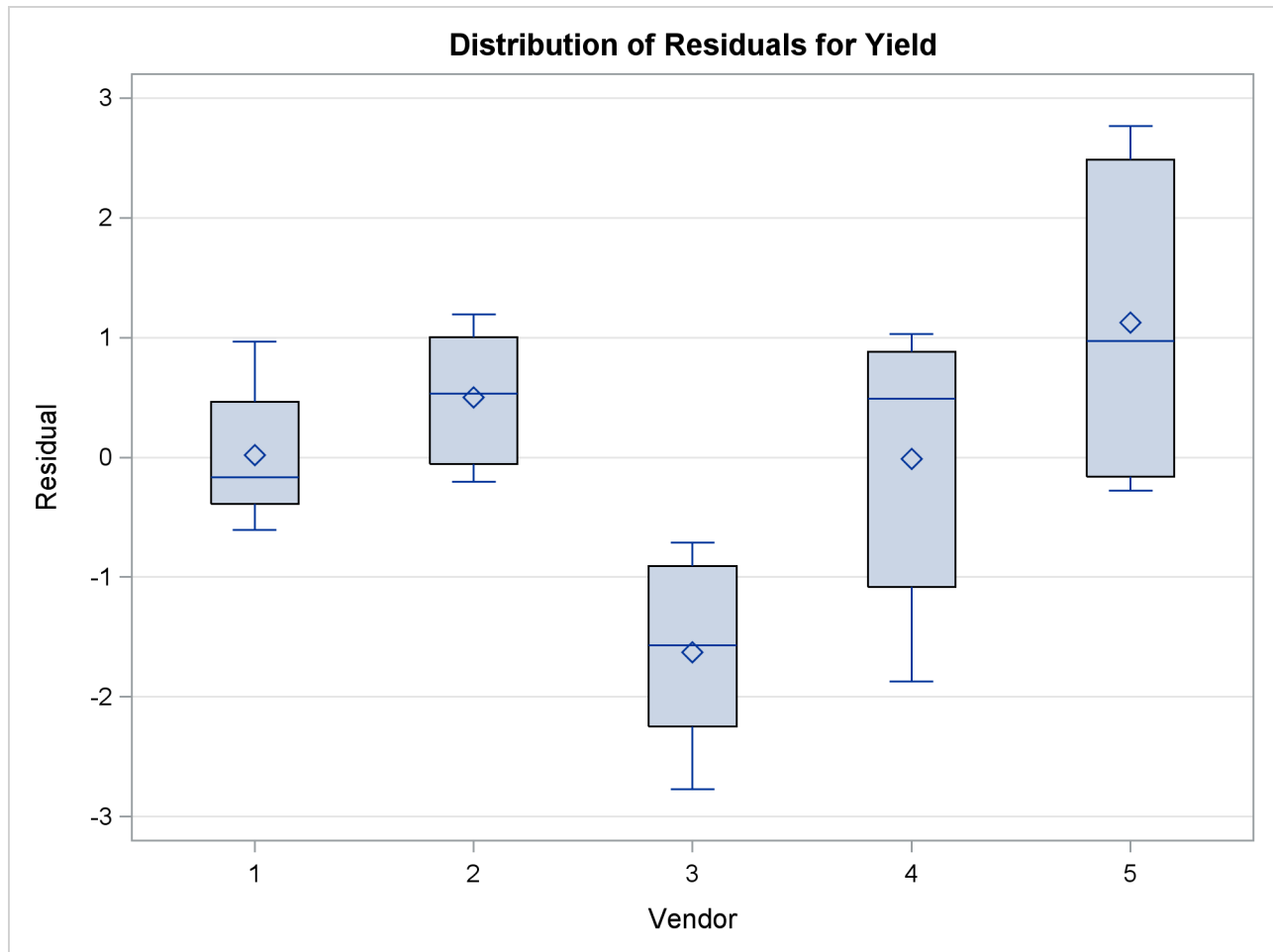
proc glimmix data=Yields
 plots=boxplot(random marginal conditional observed);
 class Vendor Pressure Temp;
 model Yield = Pressure Temp Pressure*Temp;
 random vendor;
run;

ods graphics off;
```

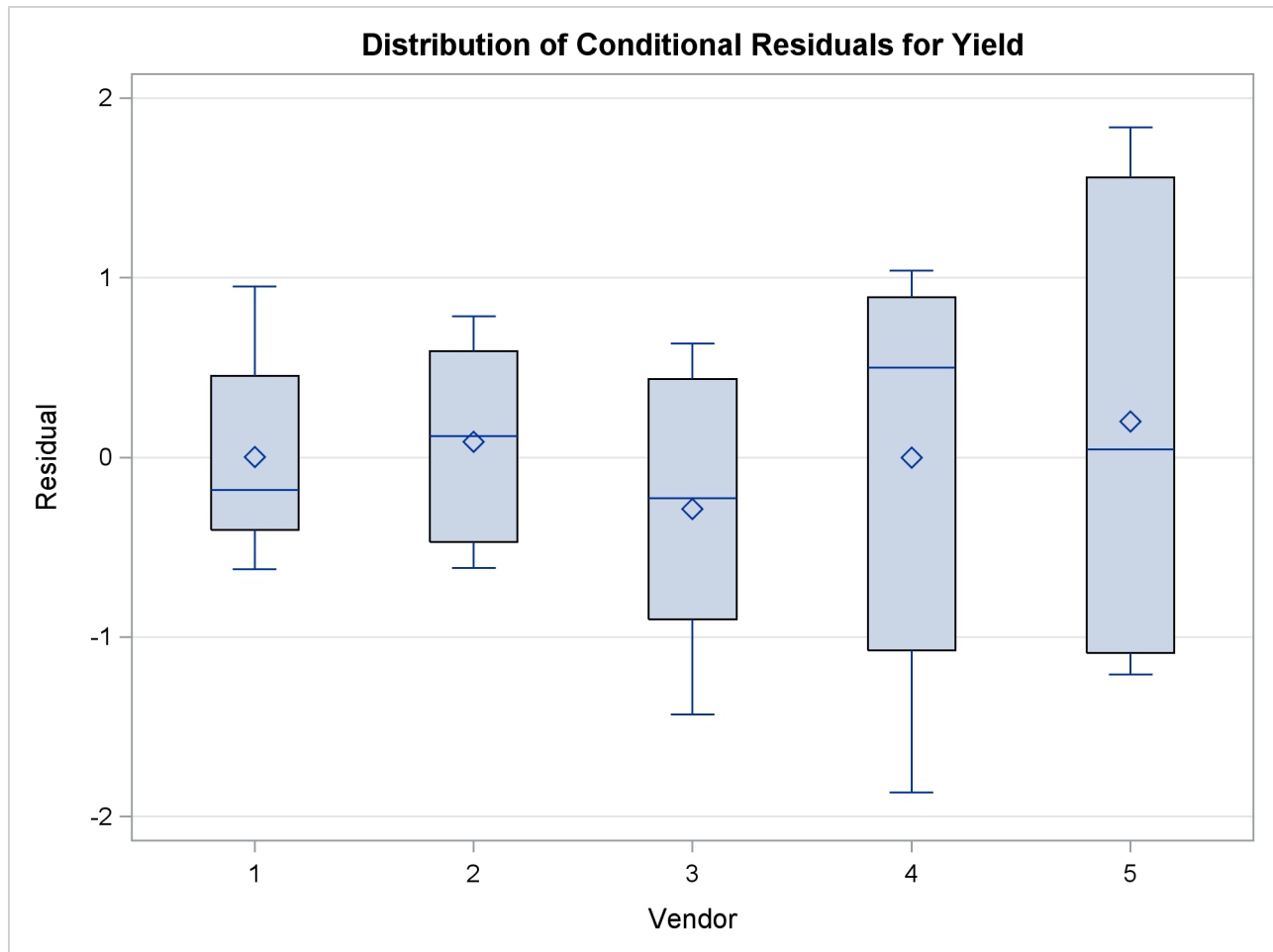
The observed vendor means in Figure 41.21 are different; in particular, vendors 3 and 5 appear to differ from the other vendors and from each other. There is also heterogeneity of variance in the five groups. The marginal residuals in Figure 41.22 continue to show the differences in means by vendor, because vendor enters the model as a random effect. The marginal means are adjusted for vendor effects only in the sense that the vendor variance component affects the marginal variance that is involved in the generalized least squares solution for the pressure and temperature effects.

**Figure 41.21** Box Plots of Observed Values



**Figure 41.22** Box Plots of Marginal Residuals

The conditional residuals account for the vendor effects through the empirical BLUPs. The means and medians have stabilized near zero, but some heterogeneity in these residuals remains (Figure 41.23).

**Figure 41.23** Box Plots of Conditional Residuals

### Graphics for LS-Mean Comparisons

The following subsections provide information about the ODS statistical graphics for least squares means produced by the GLIMMIX procedure. Mean plots display marginal or interaction means. The diffogram, control plot, and ANOM plot display least squares mean comparisons.

#### *Mean Plots*

The following SAS statements request a plot of the Pressure×Temp means in which the pressure trends are plotted for each temperature.

```
ods graphics on;
ods select CovParms Tests3 MeanPlot;
proc glimmix data=Yields;
 class Vendor Pressure Temp;
 model Yield = Pressure Temp Pressure*Temp;
 random Vendor;
 lsmeans Pressure*Temp / plot=mean(sliceby=Temp join);
run;
ods graphics off;
```

There is a significant effect of temperature and an interaction between pressure and temperature (Figure 41.24). Notice that the pressure main effect might be masked by the interaction. Because of the interaction, temperature comparisons depend on the pressure and vice versa. The mean plot option requests a display of the Pressure  $\times$  Temp least squares means with separate trends for each temperature (Figure 41.25).

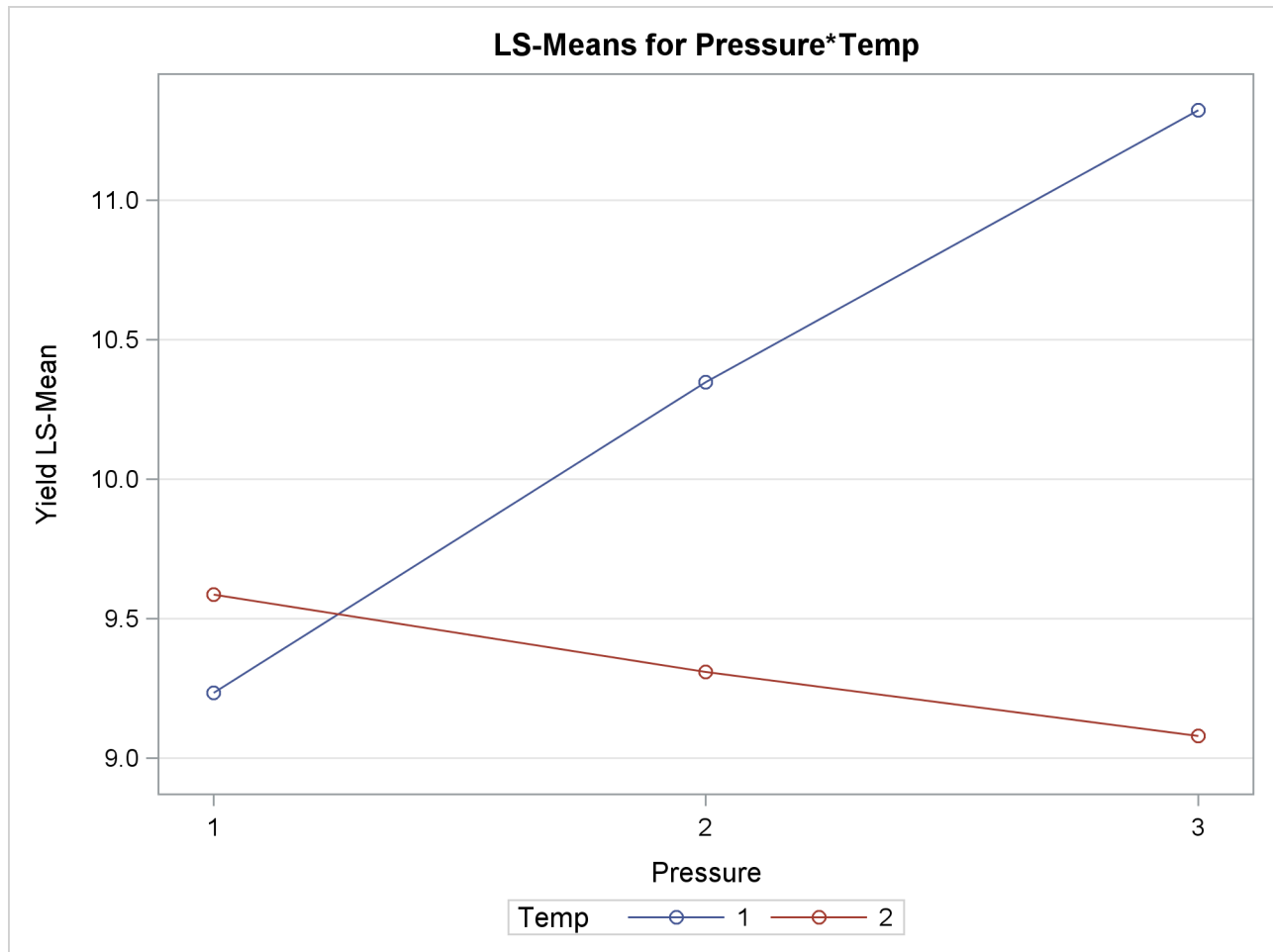
**Figure 41.24** Tests for Fixed Effects

| The GLIMMIX Procedure           |           |           |          |        |
|---------------------------------|-----------|-----------|----------|--------|
| Covariance Parameter Estimates  |           |           |          |        |
| Cov Parm                        | Estimate  |           | Standard |        |
|                                 |           |           | Error    |        |
| Vendor                          | 0.8602    |           | 0.7406   |        |
| Residual                        | 1.1039    |           | 0.3491   |        |
| Type III Tests of Fixed Effects |           |           |          |        |
| Effect                          | Num<br>DF | Den<br>DF | F Value  | Pr > F |
| Pressure                        | 2         | 20        | 1.42     | 0.2646 |
| Temp                            | 1         | 20        | 6.48     | 0.0193 |
| Pressure*Temp                   | 2         | 20        | 3.82     | 0.0393 |

The interaction between the two effects is evident in the lack of parallelism in Figure 41.25. The masking of the pressure main effect can be explained by slopes of different sign for the two trends. Based on these results, inferences about the pressure effects are conducted for a specific temperature. For example, Figure 41.26 is produced by adding the following statement:

```
lsmeans pressure*temp / slicediff=temp slice=temp;
```

**Figure 41.25** Interaction Plot for Pressure x Temperature



**Figure 41.26** Pressure Comparisons at a Given Temperature

| The GLIMMIX Procedure                                                  |          |           |           |                   |        |         |         |
|------------------------------------------------------------------------|----------|-----------|-----------|-------------------|--------|---------|---------|
| Tests of Effect Slices for Pressure*Temp<br>Sliced By Temp             |          |           |           |                   |        |         |         |
|                                                                        | Temp     | Num<br>DF | Den<br>DF | F Value           | Pr > F |         |         |
|                                                                        | 1        | 2         | 20        | 4.95              | 0.0179 |         |         |
|                                                                        | 2        | 2         | 20        | 0.29              | 0.7508 |         |         |
| Simple Effect Comparisons of Pressure*Temp Least Squares Means By Temp |          |           |           |                   |        |         |         |
| Simple<br>Effect<br>Level                                              | Pressure | _Pressure | Estimate  | Standard<br>Error | DF     | t Value | Pr >  t |
| Temp 1                                                                 | 1        | 2         | -1.1140   | 0.6645            | 20     | -1.68   | 0.1092  |
| Temp 1                                                                 | 1        | 3         | -2.0900   | 0.6645            | 20     | -3.15   | 0.0051  |
| Temp 1                                                                 | 2        | 3         | -0.9760   | 0.6645            | 20     | -1.47   | 0.1575  |
| Temp 2                                                                 | 1        | 2         | 0.2760    | 0.6645            | 20     | 0.42    | 0.6823  |
| Temp 2                                                                 | 1        | 3         | 0.5060    | 0.6645            | 20     | 0.76    | 0.4553  |
| Temp 2                                                                 | 2        | 3         | 0.2300    | 0.6645            | 20     | 0.35    | 0.7329  |

The slope differences are evident by the change in sign for comparisons within temperature 1 and within temperature 2. There is a significant effect of pressure at temperature 1 ( $p = 0.0179$ ), but not at temperature 2 ( $p = 0.7508$ ).

### ***Pairwise Difference Plot (Diffogram)***

Graphical displays of LS-means-related analyses consist of plots of all pairwise differences (DiffPlot), plots of differences against a control level (ControlPlot), and plots of differences against an overall average (AnomPlot). The following data set is from an experiment to investigate how snapdragons grow in various soils (Stenstrom 1940). To eliminate the effect of local fertility variations, the experiment is run in blocks, with each soil type sampled in each block. See the “Examples” section of Chapter 42, “The GLM Procedure,” for an in-depth analysis of these data.



```

data plants;
 input Type $ @;
 do Block = 1 to 3;
 input StemLength @;
 output;
 end;
 datalines;
Clarion 32.7 32.3 31.5
Clinton 32.1 29.7 29.1
Knox 35.7 35.9 33.1
ONeill 36.0 34.2 31.2
Compost 31.8 28.0 29.2
Wabash 38.2 37.8 31.9
Webster 32.5 31.1 29.7
;

```

The following statements perform the analysis of the experiment with the GLIMMIX procedure:

```

ods graphics on;
ods select LSMeans DiffPlot;

proc glimmix data=plants order=data plots=Diffogram;
 class Block Type;
 model StemLength = Block Type;
 lsmeans Type;
run;

ods graphics off;

```

The `PLOTS=` option in the `PROC GLIMMIX` statement requests that plots of pairwise least squares means differences are produced for effects that are listed in corresponding `LSMEANS` statements. This is the `Type` effect.

The Type LS-means are shown in Figure 41.27. Note that the order in which the levels appear corresponds to the order in which they were read from the data set. This was accomplished with the `ORDER=DATA` option in the `PROC GLIMMIX` statement.

**Figure 41.27** Least Squares Means for Type Effect

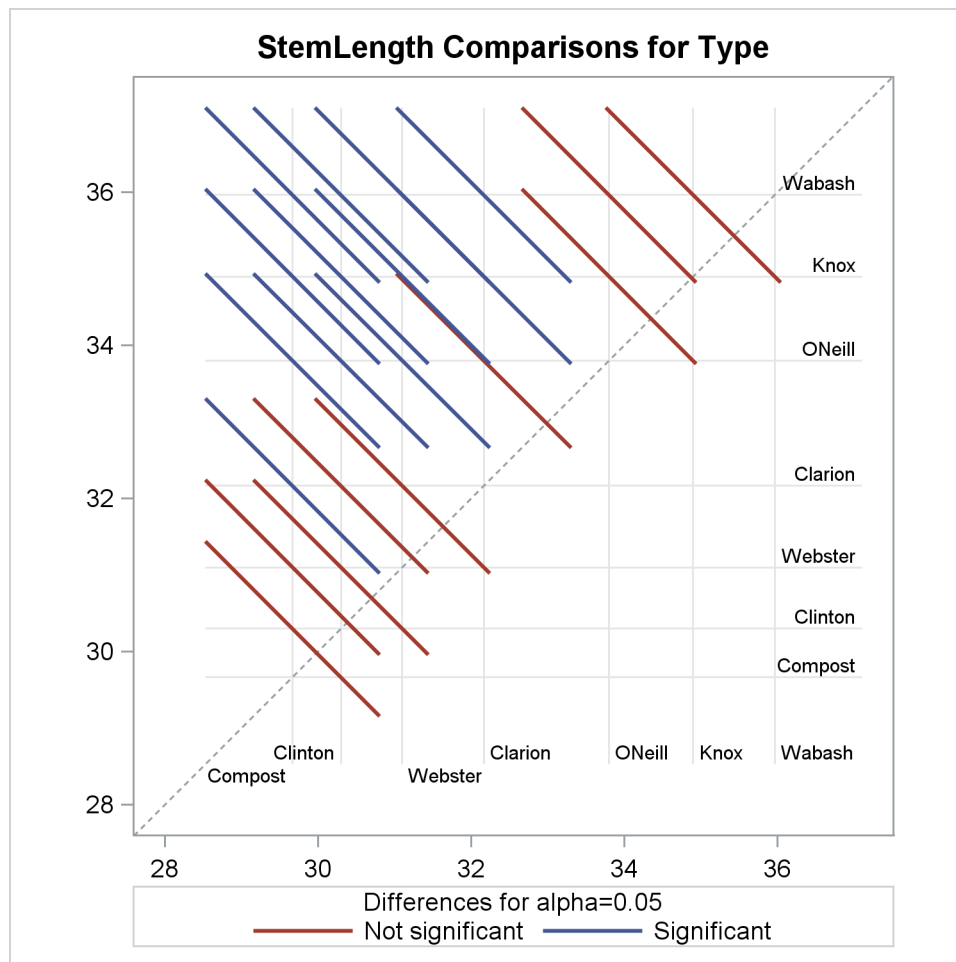
| The GLIMMIX Procedure    |          |                |    |         |         |
|--------------------------|----------|----------------|----|---------|---------|
| Type Least Squares Means |          |                |    |         |         |
| Type                     | Estimate | Standard Error | DF | t Value | Pr >  t |
| Clarion                  | 32.1667  | 0.7405         | 12 | 43.44   | <.0001  |
| Clinton                  | 30.3000  | 0.7405         | 12 | 40.92   | <.0001  |
| Knox                     | 34.9000  | 0.7405         | 12 | 47.13   | <.0001  |
| ONeill                   | 33.8000  | 0.7405         | 12 | 45.64   | <.0001  |
| Compost                  | 29.6667  | 0.7405         | 12 | 40.06   | <.0001  |
| Wabash                   | 35.9667  | 0.7405         | 12 | 48.57   | <.0001  |
| Webster                  | 31.1000  | 0.7405         | 12 | 42.00   | <.0001  |

Because there are seven levels of Type in this analysis, there are  $7(6 - 1)/2 = 21$  pairwise comparisons among the least squares means. The comparisons are performed in the following fashion: the first level of Type is compared against levels 2 through 7; the second level of Type is compared against levels 3 through 7; and so forth.

The default difference plot for these data is shown in Figure 41.28. The display is also known as a “mean-mean scatter plot” (Hsu 1996; Hsu and Peruggia 1994). It contains 21 lines rotated by 45 degrees counterclockwise, and a reference line (dashed 45-degree line). The  $(x, y)$  coordinate for the center of each line corresponds to the two least squares means being compared. Suppose that  $\hat{\eta}_i$  and  $\hat{\eta}_j$  denote the  $i$ th and  $j$ th least squares mean, respectively, for the effect in question, where  $i < j$  according to the ordering of the effect levels. If the ABS option is in effect, which is the default, the line segment is centered at  $(\min\{\hat{\eta}_i, \hat{\eta}_j\}, \max\{\hat{\eta}_i, \hat{\eta}_j\})$ . Take, for example, the comparison of “Clarion” and “Compost” types. The respective estimates of their LS-means are  $\hat{\eta}_{.1} = 32.1667$  and  $\hat{\eta}_{.5} = 29.6667$ . The center of the line segment for  $H_0: \eta_{.1} = \eta_{.5}$  is placed at  $(29.6667, 32.1667)$ .

The length of the line segment for the comparison between means  $i$  and  $j$  corresponds to the width of the confidence interval for the difference  $\eta_i - \eta_j$ . This length is adjusted for the rotation in the plot. As a consequence, comparisons whose confidence interval covers zero cross the 45-degree reference line. These are the nonsignificant comparisons. Lines associated with significant comparisons do not touch or cross the reference line. Because these data are balanced, the estimated standard errors of all pairwise comparisons are identical, and the widths of the line segments are the same.

Figure 41.28 LS-Means Plot of Pairwise Differences



The background grid of the difference plot is drawn at the values of the least squares means for the seven type levels. These grid lines are used to find a particular comparison by intersection. Also, the labels of the grid lines indicate the ordering of the least squares means.

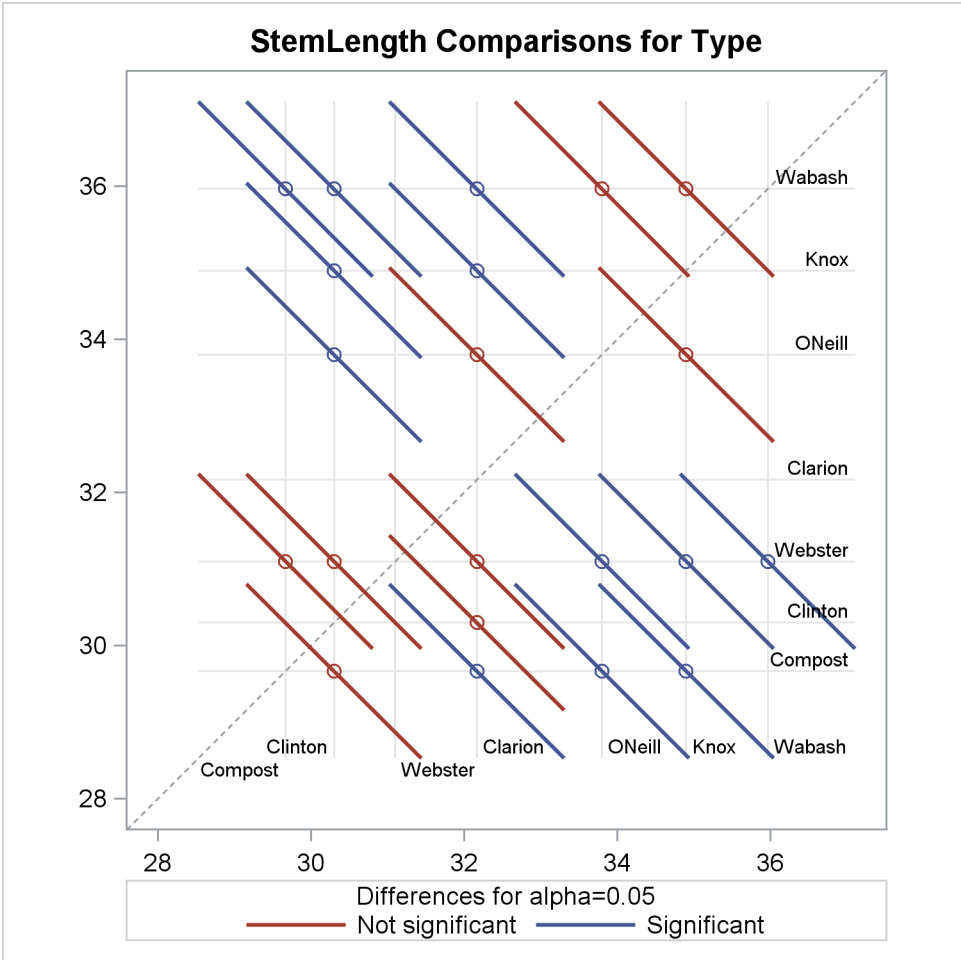
In the next set of statements, the NOABS and CENTER suboptions of the PLOTS=DIFFOGRAM option in the LSMEANS statement modify the appearance of the diffogram:

```
ods graphics on;
proc glimmix data=plants order=data;
 class Block Type;
 model StemLength = Block Type;
 lsmeans Type / plots=diffogram(noabs center);
run;
ods graphics off;
```

The NOABS suboption of the difference plot changes the way in which the GLIMMIX procedure places the line segments (Figure 41.29). If the NOABS suboption is in effect, the line segment is centered at the point  $(\hat{\eta}_{.i}, \hat{\eta}_{.j})$ ,  $i < j$ . For example, the center of the line segment for a comparison of “Clarion” and “Compost” types is centered at  $(\hat{\eta}_{.1}, \hat{\eta}_{.5}) = (32.1667, 29.6667)$ . Whether a line segment appears above or below the reference line depends on the magnitude of the least squares means and the order of their appearance in the “Least Squares Means” table. The CENTER suboption places a marker at the intersection of the least squares means.

Because the ABS option places lines on the same side of the 45-degree reference, it can help to visually discover groups of significant and nonsignificant differences. On the other hand, when the number of levels in the effect is large, the display can get crowded. The NOABS option can then provide a more accessible resolution.

Figure 41.29 Diffogram with NOABS and CENTER Options



**Least Squares Mean Control Plot**

The following SAS statements create the same data set as before, except that one observation for Type="Knox" has been removed for illustrative purposes:

```
data plants;
 input Type $ @;
 do Block = 1 to 3;
 input StemLength @;
 output;
 end;
 datalines;
Clarion 32.7 32.3 31.5
Clinton 32.1 29.7 29.1
Knox 35.7 35.9 .
ONeill 36.0 34.2 31.2
Compost 31.8 28.0 29.2
Wabash 38.2 37.8 31.9
Webster 32.5 31.1 29.7
;
```

The following statements request control plots for effects in **LSMEANS** statements with compatible option:

```
ods graphics on;
ods select Diffs ControlPlot;

proc glimmix data=plants order=data plots=ControlPlot;
 class Block Type;
 model StemLength = Block Type;
 lsmeans Type / diff=control('Clarion') adjust=dunnett;
run;

ods graphics off;
```

The **LSMEANS** statement for the Type effect is compatible; it requests comparisons of Type levels against "Clarion," adjusted for multiplicity with Dunnett's method. Because "Clarion" is the first level of the effect, the **LSMEANS** statement is equivalent to

```
lsmeans type / diff=control adjust=dunnett;
```

The "Differences of Type Least Squares Means" table in [Figure 41.30](#) shows the six comparisons between Type levels and the control level.

**Figure 41.30** Least Squares Means Differences

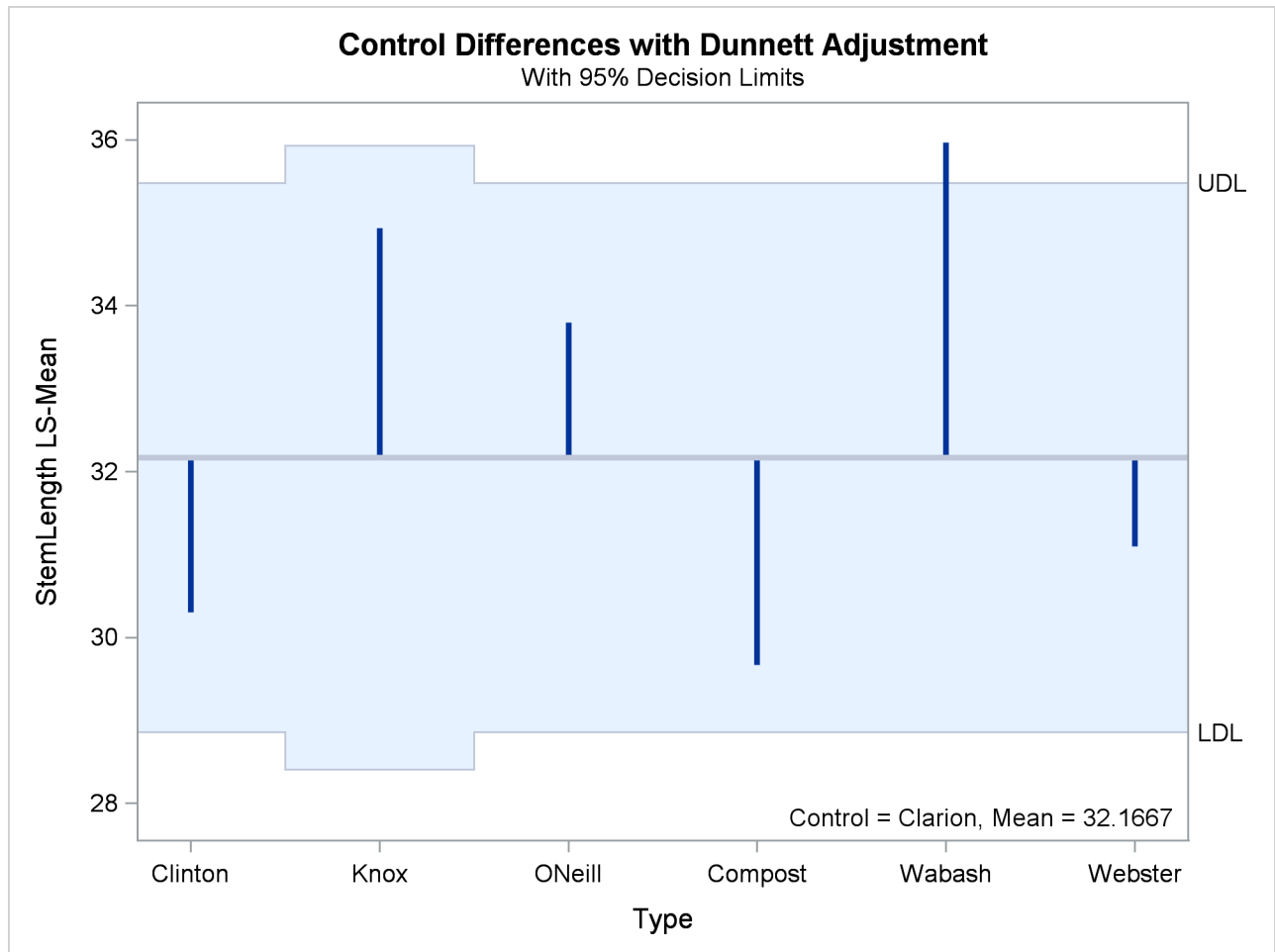
| The GLIMMIX Procedure                        |         |          |                |    |         |         |        |
|----------------------------------------------|---------|----------|----------------|----|---------|---------|--------|
| Differences of Type Least Squares Means      |         |          |                |    |         |         |        |
| Adjustment for Multiple Comparisons: Dunnett |         |          |                |    |         |         |        |
| Type                                         | _Type   | Estimate | Standard Error | DF | t Value | Pr >  t | Adj P  |
| Clinton                                      | Clarion | -1.8667  | 1.0937         | 11 | -1.71   | 0.1159  | 0.3936 |
| Knox                                         | Clarion | 2.7667   | 1.2430         | 11 | 2.23    | 0.0479  | 0.1854 |
| ONeill                                       | Clarion | 1.6333   | 1.0937         | 11 | 1.49    | 0.1635  | 0.5144 |
| Compost                                      | Clarion | -2.5000  | 1.0937         | 11 | -2.29   | 0.0431  | 0.1688 |
| Wabash                                       | Clarion | 3.8000   | 1.0937         | 11 | 3.47    | 0.0052  | 0.0236 |
| Webster                                      | Clarion | -1.0667  | 1.0937         | 11 | -0.98   | 0.3504  | 0.8359 |

The two rightmost columns of the table give the unadjusted and multiplicity-adjusted  $p$ -values. At the 5% significance level, both “Knox” and “Wabash” differ significantly from “Clarion” according to the unadjusted tests. After adjusting for multiplicity, only “Wabash” has a least squares mean significantly different from the control mean. Note that the standard error for the comparison involving “Knox” is larger than that for other comparisons because of the reduced sample size for that soil type.

In the plot of control differences a horizontal line is drawn at the value of the “Clarion” least squares mean. Vertical lines emanating from this reference line terminate in the least squares means for the other levels (Figure 41.31).

The dashed upper and lower horizontal reference lines are the upper and lower decision limits for tests against the control level. If a vertical line crosses the upper or lower decision limit, the corresponding least squares mean is significantly different from the LS-mean in the control group. If the data had been balanced, the UDL and LDL would be straight lines, because all estimates  $\hat{\eta}_i - \hat{\eta}_j$  would have had the same standard error. The limits for the comparison between “Knox” and “Clarion” are wider than for other comparisons, because of the reduced sample size for the “Knox” soil type.

**Figure 41.31** LS-Means Plot of Differences against a Control



The significance level of the decision limits is determined from the `ALPHA=` level in the `LSMEANS` statement. The default are 95% limits. If you choose one-sided comparisons with `DIFF=CONTROL` or `DIFF=CONTROLU` in the `LSMEANS` statement, only one of the decision limits is drawn.

### Analysis of Means (ANOM) Plot

The analysis of means in PROC GLIMMIX compares least squares means not by contrasting them against each other as with all pairwise differences or control differences. Instead, the least squares means are compared against an average value. Consequently, there are  $k$  comparisons for a factor with  $k$  levels. The following statements request ANOM differences for the Type least squares means (Figure 41.32) and plots the differences (Figure 41.33):

```
ods graphics on;
ods select Diffs AnomPlot;
proc glimmix data=plants order=data plots=AnomPlot;
 class Block Type;
 model StemLength = Block Type;
 lsmeans Type / diff=anom;
run;
ods graphics off;
```

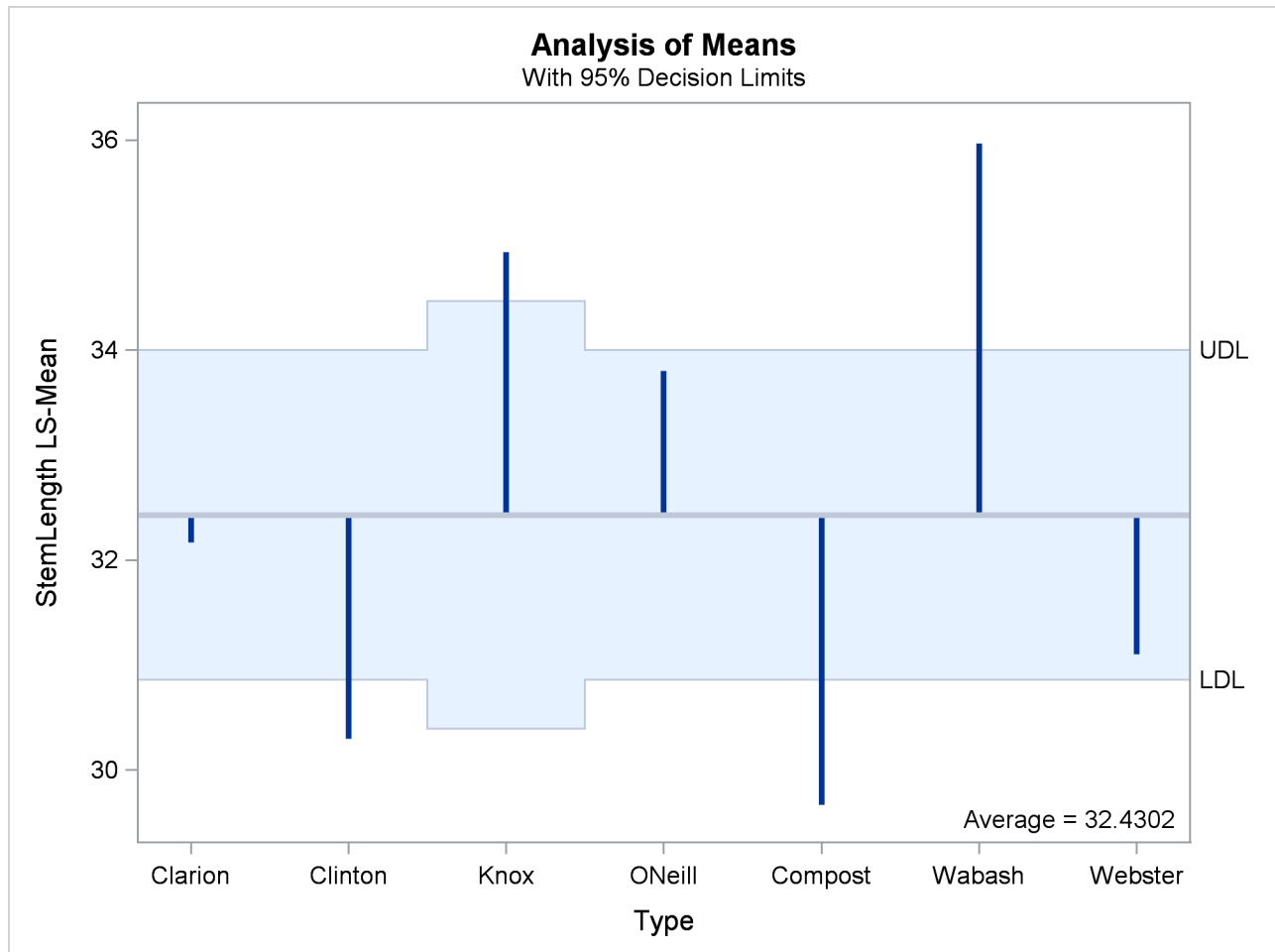
Figure 41.32 ANOM LS-Mean Differences

| The GLIMMIX Procedure                   |       |          |                |    |         |         |
|-----------------------------------------|-------|----------|----------------|----|---------|---------|
| Differences of Type Least Squares Means |       |          |                |    |         |         |
| Type                                    | _Type | Estimate | Standard Error | DF | t Value | Pr >  t |
| Clarion                                 | Avg   | -0.2635  | 0.7127         | 11 | -0.37   | 0.7186  |
| Clinton                                 | Avg   | -2.1302  | 0.7127         | 11 | -2.99   | 0.0123  |
| Knox                                    | Avg   | 2.5032   | 0.9256         | 11 | 2.70    | 0.0205  |
| O'Neill                                 | Avg   | 1.3698   | 0.7127         | 11 | 1.92    | 0.0809  |
| Compost                                 | Avg   | -2.7635  | 0.7127         | 11 | -3.88   | 0.0026  |
| Wabash                                  | Avg   | 3.5365   | 0.7127         | 11 | 4.96    | 0.0004  |
| Webster                                 | Avg   | -1.3302  | 0.7127         | 11 | -1.87   | 0.0888  |

At the 5% level, the “Clarion,” “O’Neill,” and “Webster” soil types are not significantly different from the average. Note that the artificial lack of balance introduced previously reduces the precision of the ANOM comparison for the “Knox” soil type.



Figure 41.33 LS-Means Analysis of Means (ANOM) Plot



The reference line in the ANOM plot is drawn at the average. Vertical lines extend from this reference line upward or downward, depending on the magnitude of the least squares means compared to the reference value. This enables you to quickly see which levels perform above and below the average. The horizontal reference lines are 95% upper and lower decision limits. If a vertical line crosses the limits, you conclude that the least squares mean is significantly different (at the 5% significance level) from the average. You can adjust the comparisons for multiplicity by adding the `ADJUST=NELSON` option in the `LSMEANS` statement.

---

## Examples: GLIMMIX Procedure

---

### Example 41.1: Binomial Counts in Randomized Blocks

In the context of spatial prediction in generalized linear models, Gotway and Stroup (1997) analyze data from an agronomic field trial. Researchers studied 16 varieties (entries) of wheat for their resistance to infestation by the Hessian fly. They arranged the varieties in a randomized complete block design on an  $8 \times 8$  grid. Each  $4 \times 4$  quadrant of that arrangement constitutes a block.

The outcome of interest was the number of damaged plants ( $Y_{ij}$ ) out of the total number of plants growing on the unit ( $n_{ij}$ ). The two subscripts identify the block ( $i = 1, \dots, 4$ ) and the entry ( $j = 1, \dots, 16$ ). The following SAS statements create the data set. The variables `lat` and `lng` denote the coordinate of an experimental unit on the  $8 \times 8$  grid.

```
data HessianFly;
 label Y = 'No. of damaged plants'
 n = 'No. of plants';
 input block entry lat lng n Y @@;
 datalines;
1 14 1 1 8 2 1 16 1 2 9 1
1 7 1 3 13 9 1 6 1 4 9 9
1 13 2 1 9 2 1 15 2 2 14 7
1 8 2 3 8 6 1 5 2 4 11 8
1 11 3 1 12 7 1 12 3 2 11 8
1 2 3 3 10 8 1 3 3 4 12 5
1 10 4 1 9 7 1 9 4 2 15 8
1 4 4 3 19 6 1 1 4 4 8 7
2 15 5 1 15 6 2 3 5 2 11 9
2 10 5 3 12 5 2 2 5 4 9 9
2 11 6 1 20 10 2 7 6 2 10 8
2 14 6 3 12 4 2 6 6 4 10 7
2 5 7 1 8 8 2 13 7 2 6 0
2 12 7 3 9 2 2 16 7 4 9 0
2 9 8 1 14 9 2 1 8 2 13 12
2 8 8 3 12 3 2 4 8 4 14 7
3 7 1 5 7 7 3 13 1 6 7 0
3 8 1 7 13 3 3 14 1 8 9 0
3 4 2 5 15 11 3 10 2 6 9 7
3 3 2 7 15 11 3 9 2 8 13 5
3 6 3 5 16 9 3 1 3 6 8 8
3 15 3 7 7 0 3 12 3 8 12 8
3 11 4 5 8 1 3 16 4 6 15 1
3 5 4 7 12 7 3 2 4 8 16 12
4 9 5 5 15 8 4 4 5 6 10 6
4 12 5 7 13 5 4 1 5 8 15 9
4 15 6 5 17 6 4 6 6 6 8 2
4 14 6 7 12 5 4 7 6 8 15 8
4 13 7 5 13 2 4 8 7 6 13 9
4 3 7 7 9 9 4 10 7 8 6 6
4 2 8 5 12 8 4 11 8 6 9 7
4 5 8 7 11 10 4 16 8 8 15 7
;
```

## Analysis as a GLM

If infestations are independent among experimental units, and all plants within a unit have the same propensity for infestation, then the  $Y_{ij}$  are binomial random variables. The first model considered is a standard generalized linear model for independent binomial counts:

```
proc glimmix data=HessianFly;
 class block entry;
 model y/n = block entry / solution;
run;
```

The **PROC GLIMMIX** statement invokes the procedure. The **CLASS** statement instructs the GLIMMIX procedure to treat both block and entry as classification variables. The **MODEL** statement specifies the response variable and the fixed effects in the model. PROC GLIMMIX constructs the **X** matrix of the model from the terms on the right side of the **MODEL** statement. The GLIMMIX procedure supports two kinds of syntax for the response variable. This example uses the *events/trials* syntax. The variable *y* represents the number of successes (*events*) out of *n* Bernoulli *trials*. When the *events/trials* syntax is used, the GLIMMIX procedure automatically selects the binomial distribution as the response distribution. Once the distribution is determined, the procedure selects the link function for the model. The default link for binomial data is the logit link. The preceding statements are thus equivalent to the following statements:

```
proc glimmix data=HessianFly;
 class block entry;
 model y/n = block entry / dist=binomial link=logit solution;
run;
```

The **SOLUTION** option in the **MODEL** statement requests that solutions for the fixed effects (parameter estimates) be displayed.

The “Model Information” table describes the model and methods used in fitting the statistical model (Output 41.1.1).

The GLIMMIX procedure recognizes that this is a model for uncorrelated data (variance matrix is diagonal) and that parameters can be estimated by maximum likelihood. The default degrees-of-freedom method to denominator degrees of freedom for *F* tests and *t* tests is the RESIDUAL method. This corresponds to choosing  $f - \text{rank}(\mathbf{X})$  as the degrees of freedom, where *f* is the sum of the frequencies used in the analysis. You can change the degrees of freedom method with the **DDFM=** option in the **MODEL** statement.

**Output 41.1.1** Model Information in GLM Analysis

| The GLIMMIX Procedure      |                    |
|----------------------------|--------------------|
| Model Information          |                    |
| Data Set                   | WORK.HESSIANFLY    |
| Response Variable (Events) | Y                  |
| Response Variable (Trials) | n                  |
| Response Distribution      | Binomial           |
| Link Function              | Logit              |
| Variance Function          | Default            |
| Variance Matrix            | Diagonal           |
| Estimation Technique       | Maximum Likelihood |
| Degrees of Freedom Method  | Residual           |

The “Class Level Information” table lists the levels of the variables specified in the **CLASS** statement and the ordering of the levels (Output 41.1.2). The “Number of Observations” table displays the number of observations read and used in the analysis.

**Output 41.1.2** Class Level Information and Number of Observations

| Class Level Information        |                                           |
|--------------------------------|-------------------------------------------|
| Class                          | Levels Values                             |
| block                          | 4 1 2 3 4                                 |
| entry                          | 16 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 |
| Number of Observations Read 64 |                                           |
| Number of Observations Used 64 |                                           |
| Number of Events 396           |                                           |
| Number of Trials 736           |                                           |

The “Dimensions” table lists the size of relevant matrices (Output 41.1.3).

**Output 41.1.3** Model Dimensions Information in GLM Analysis

| Dimensions             |    |
|------------------------|----|
| Columns in X           | 21 |
| Columns in Z           | 0  |
| Subjects (Blocks in V) | 1  |
| Max Obs per Subject    | 64 |

Because of the absence of G-side random effects in this model, there are no columns in the **Z** matrix. The 21 columns in the **X** matrix comprise the intercept, 4 columns for the block effect and 16 columns for the entry effect. Because no **RANDOM** statement with a **SUBJECT=** option was specified, the **GLIMMIX** procedure does not process the data by subjects (see the section “Processing by Subjects” on page 3082 for details about subject processing).

The “Optimization Information” table provides information about the methods and size of the optimization problem (Output 41.1.4).

**Output 41.1.4** Optimization Information in GLM Analysis

| Optimization Information   |                |
|----------------------------|----------------|
| Optimization Technique     | Newton-Raphson |
| Parameters in Optimization | 19             |
| Lower Boundaries           | 0              |
| Upper Boundaries           | 0              |
| Fixed Effects              | Not Profiled   |

With few exceptions, models fit with the GLIMMIX procedure require numerical methods for parameter estimation. The default optimization method for (overdispersed) GLM models is the Newton-Raphson algorithm. In this example, the optimization involves 19 parameters, corresponding to the number of linearly independent columns of the  $X'X$  matrix.

The “Iteration History” table shows that the procedure converged after 3 iterations and 13 function evaluations (Output 41.1.5). The Change column measures the change in the objective function between iterations; however, this is not the monitored convergence criterion. The GLIMMIX procedure monitors several features simultaneously to determine whether to stop an optimization.

**Output 41.1.5** Iteration History in GLM Analysis

| Iteration History |          |             |                    |            |              |
|-------------------|----------|-------------|--------------------|------------|--------------|
| Iteration         | Restarts | Evaluations | Objective Function | Change     | Max Gradient |
| 0                 | 0        | 4           | 134.13393738       | .          | 4.899609     |
| 1                 | 0        | 3           | 132.85058236       | 1.28335502 | 0.206204     |
| 2                 | 0        | 3           | 132.84724263       | 0.00333973 | 0.000698     |
| 3                 | 0        | 3           | 132.84724254       | 0.00000009 | 3.029E-8     |

Convergence criterion (GCONV=1E-8) satisfied.

The “Fit Statistics” table lists information about the fitted model (Output 41.1.6). The  $-2$  Log Likelihood values are useful for comparing nested models, and the information criteria AIC, AICC, BIC, CAIC, and HQIC are useful for comparing nonnested models. On average, the ratio between the Pearson statistic and its degrees of freedom should equal one in GLMs. Values larger than one indicate overdispersion. With a ratio of 2.37, these data appear to exhibit more dispersion than expected under a binomial model with block and varietal effects.

**Output 41.1.6** Fit Statistics in GLM Analysis

| Fit Statistics           |        |
|--------------------------|--------|
| $-2$ Log Likelihood      | 265.69 |
| AIC (smaller is better)  | 303.69 |
| AICC (smaller is better) | 320.97 |
| BIC (smaller is better)  | 344.71 |
| CAIC (smaller is better) | 363.71 |
| HQIC (smaller is better) | 319.85 |
| Pearson Chi-Square       | 106.74 |
| Pearson Chi-Square / DF  | 2.37   |

The “Parameter Estimates” table displays the maximum likelihood estimates (Estimate), standard errors, and  $t$  tests for the hypothesis that the estimate is zero (Output 41.1.7).

**Output 41.1.7** Parameter Estimates in GLM Analysis

| Parameter Estimates |       |       |          |                |    |         |         |
|---------------------|-------|-------|----------|----------------|----|---------|---------|
| Effect              | block | entry | Estimate | Standard Error | DF | t Value | Pr >  t |
| Intercept           |       |       | -1.2936  | 0.3908         | 45 | -3.31   | 0.0018  |
| block               | 1     |       | -0.05776 | 0.2332         | 45 | -0.25   | 0.8055  |
| block               | 2     |       | -0.1838  | 0.2303         | 45 | -0.80   | 0.4289  |
| block               | 3     |       | -0.4420  | 0.2328         | 45 | -1.90   | 0.0640  |
| block               | 4     |       | 0        | .              | .  | .       | .       |
| entry               |       | 1     | 2.9509   | 0.5397         | 45 | 5.47    | <.0001  |
| entry               |       | 2     | 2.8098   | 0.5158         | 45 | 5.45    | <.0001  |
| entry               |       | 3     | 2.4608   | 0.4956         | 45 | 4.97    | <.0001  |
| entry               |       | 4     | 1.5404   | 0.4564         | 45 | 3.38    | 0.0015  |
| entry               |       | 5     | 2.7784   | 0.5293         | 45 | 5.25    | <.0001  |
| entry               |       | 6     | 2.0403   | 0.4889         | 45 | 4.17    | 0.0001  |
| entry               |       | 7     | 2.3253   | 0.4966         | 45 | 4.68    | <.0001  |
| entry               |       | 8     | 1.3006   | 0.4754         | 45 | 2.74    | 0.0089  |
| entry               |       | 9     | 1.5605   | 0.4569         | 45 | 3.42    | 0.0014  |
| entry               |       | 10    | 2.3058   | 0.5203         | 45 | 4.43    | <.0001  |
| entry               |       | 11    | 1.4957   | 0.4710         | 45 | 3.18    | 0.0027  |
| entry               |       | 12    | 1.5068   | 0.4767         | 45 | 3.16    | 0.0028  |
| entry               |       | 13    | -0.6296  | 0.6488         | 45 | -0.97   | 0.3370  |
| entry               |       | 14    | 0.4460   | 0.5126         | 45 | 0.87    | 0.3889  |
| entry               |       | 15    | 0.8342   | 0.4698         | 45 | 1.78    | 0.0826  |
| entry               |       | 16    | 0        | .              | .  | .       | .       |

The “Type III Tests of Fixed Effect” table displays significance tests for the two fixed effects in the model (Output 41.1.8).

**Output 41.1.8** Type III Tests of Block and Entry Effects in GLM Analysis

| Type III Tests of Fixed Effects |        |        |         |        |
|---------------------------------|--------|--------|---------|--------|
| Effect                          | Num DF | Den DF | F Value | Pr > F |
| block                           | 3      | 45     | 1.42    | 0.2503 |
| entry                           | 15     | 45     | 6.96    | <.0001 |

These tests are Wald-type tests, not likelihood ratio tests. The entry effect is clearly significant in this model with a  $p$ -value of <0.0001, indicating that the 16 wheat varieties are not equally susceptible to infestation by the Hessian fly.

**Analysis with Random Block Effects**

There are several possible reasons for the overdispersion noted in Output 41.1.6 (Pearson ratio = 2.37). The data might not follow a binomial distribution, one or more important effects might not have been accounted for in the model, or the data might be positively correlated. If important fixed effects have been omitted,

then you might need to consider adding them to the model. Because this is a designed experiment, it is reasonable not to expect further effects apart from the block and entry effects that represent the treatment and error control design structure. The reasons for the overdispersion must lie elsewhere.

If overdispersion stems from correlations among the observations, then the model should be appropriately adjusted. The correlation can have multiple sources. First, it might not be the case that the plants within an experimental unit responded independently. If the probability of infestation of a particular plant is altered by the infestation of a neighboring plant within the same unit, the infestation counts are not binomial and a different probability model should be used. A second possible source of correlations is the lack of independence of experimental units. Even if treatments were assigned to units at random, they might not respond independently. Shared spatial soil effects, for example, can be the underlying factor. The following analyses take these spatial effects into account.

First, assume that the environmental effects operate at the scale of the blocks. By making the block effects random, the marginal responses will be correlated due to the fact that observations within a block share the same random effects. Observations from different blocks will remain uncorrelated, in the spirit of separate randomizations among the blocks. The next set of statements fits a generalized linear mixed model (GLMM) with random block effects:

```
proc glimmix data=HessianFly;
 class block entry;
 model y/n = entry / solution;
 random block;
run;
```

Because the conditional distribution—conditional on the block effects—is binomial, the marginal distribution will be overdispersed relative to the binomial distribution. In contrast to adding a multiplicative scale parameter to the variance function, treating the block effects as random changes the estimates compared to a model with fixed block effects.

In the presence of random effects and a conditional binomial distribution, PROC GLIMMIX does not use maximum likelihood for estimation. Instead, the GLIMMIX procedure applies a restricted (residual) pseudo-likelihood algorithm (Output 41.1.9). The “restricted” attribute derives from the same rationale by which restricted (residual) maximum likelihood methods for linear mixed models attain their name; the likelihood equations are adjusted for the presence of fixed effects in the model to reduce bias in covariance parameter estimates.

#### Output 41.1.9 Model Information in GLMM Analysis

| The GLIMMIX Procedure      |                 |
|----------------------------|-----------------|
| Model Information          |                 |
| Data Set                   | WORK.HESSIANFLY |
| Response Variable (Events) | Y               |
| Response Variable (Trials) | n               |
| Response Distribution      | Binomial        |
| Link Function              | Logit           |
| Variance Function          | Default         |
| Variance Matrix            | Not blocked     |
| Estimation Technique       | Residual PL     |
| Degrees of Freedom Method  | Containment     |

The “Class Level Information” and “Number of Observations” tables are as before (Output 41.1.10).

**Output 41.1.10** Class Level Information and Number of Observations

| Class                       |  | Levels | Values                                 |
|-----------------------------|--|--------|----------------------------------------|
| block                       |  | 4      | 1 2 3 4                                |
| entry                       |  | 16     | 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 |
| Number of Observations Read |  |        | 64                                     |
| Number of Observations Used |  |        | 64                                     |
| Number of Events            |  |        | 396                                    |
| Number of Trials            |  |        | 736                                    |

The “Dimensions” table indicates that there is a single G-side parameter, the variance of the random block effect (Output 41.1.11). The “Dimensions” table has changed from the previous model (compare Output 41.1.11 to Output 41.1.3). Note that although the block effect has four levels, only a single variance component is estimated. The Z matrix has four columns, however, corresponding to the four levels of the block effect. Because no SUBJECT= option is used in the RANDOM statement, the GLIMMIX procedure treats these data as having arisen from a single subject with 64 observations.

**Output 41.1.11** Model Dimensions Information in GLMM Analysis

| Dimensions             |    |
|------------------------|----|
| G-side Cov. Parameters | 1  |
| Columns in X           | 17 |
| Columns in Z           | 4  |
| Subjects (Blocks in V) | 1  |
| Max Obs per Subject    | 64 |

The “Optimization Information” table indicates that a quasi-Newton method is used to solve the optimization problem. This is the default optimization method for GLMM models (Output 41.1.12).

**Output 41.1.12** Optimization Information in GLMM Analysis

| Optimization Information   |                   |
|----------------------------|-------------------|
| Optimization Technique     | Dual Quasi-Newton |
| Parameters in Optimization | 1                 |
| Lower Boundaries           | 1                 |
| Upper Boundaries           | 0                 |
| Fixed Effects              | Profiled          |
| Starting From              | Data              |



In contrast to the Newton-Raphson method, the quasi-Newton method does not require second derivatives. Because the covariance parameters are not unbounded in this example, the procedure enforces a lower boundary constraint (zero) for the variance of the block effect, and the optimization method is changed to a dual quasi-Newton method. The fixed effects are profiled from the likelihood equations in this model. The resulting optimization problem involves only the covariance parameters.

The “Iteration History” table appears to indicate that the procedure converged after four iterations (Output 41.1.13). Notice, however, that this table has changed slightly from the previous analysis (see Output 41.1.5). The Evaluations column has been replaced by the Subiterations column, because the GLIMMIX procedure applied a doubly iterative fitting algorithm. The entire process consisted of five optimizations, each of which was iterative. The initial optimization required four iterations, the next one required three iterations, and so on.

**Output 41.1.13** Iteration History in GLMM Analysis

| Iteration History                                   |          |               |                       |            |                 |  |
|-----------------------------------------------------|----------|---------------|-----------------------|------------|-----------------|--|
| Iteration                                           | Restarts | Subiterations | Objective<br>Function | Change     | Max<br>Gradient |  |
| 0                                                   | 0        | 4             | 173.28473428          | 0.81019251 | 0.000197        |  |
| 1                                                   | 0        | 3             | 181.66726674          | 0.17550228 | 0.000739        |  |
| 2                                                   | 0        | 2             | 182.20789493          | 0.00614874 | 7.018E-6        |  |
| 3                                                   | 0        | 1             | 182.21315596          | 0.00004386 | 1.213E-8        |  |
| 4                                                   | 0        | 0             | 182.21317662          | 0.00000000 | 3.349E-6        |  |
| Convergence criterion (PCONV=1.11022E-8) satisfied. |          |               |                       |            |                 |  |

The “Fit Statistics” table shows information about the fit of the GLMM (Output 41.1.14). The log likelihood reported in the table is not the residual log likelihood of the data. It is the residual log likelihood for an approximated model. The generalized chi-square statistic measures the residual sum of squares in the final model, and the ratio with its degrees of freedom is a measure of variability of the observation about the mean model.

**Output 41.1.14** Fit Statistics in GLMM Analysis

| Fit Statistics               |        |
|------------------------------|--------|
| -2 Res Log Pseudo-Likelihood | 182.21 |
| Generalized Chi-Square       | 107.96 |
| Gener. Chi-Square / DF       | 2.25   |

The variance of the random block effects is rather small (Output 41.1.15).

**Output 41.1.15** Estimated Covariance Parameters and Approximate Standard Errors

| Covariance Parameter Estimates |          |                |
|--------------------------------|----------|----------------|
| Cov Parm                       | Estimate | Standard Error |
| block                          | 0.01116  | 0.03116        |

If the environmental effects operate on a spatial scale smaller than the block size, the random block model does not provide a suitable adjustment. From the coarse layout of the experimental area, it is not surprising that random block effects alone do not account for the overdispersion in the data. Adding a random component to a generalized linear model is different from adding a multiplicative overdispersion component, for example, via the PSCALE option in PROC GENMOD or a

```
random _residual_;
```

statement in PROC GLIMMIX. Such overdispersion components do not affect the parameter estimates, only their standard errors. A genuine random effect, on the other hand, affects both the parameter estimates and their standard errors (compare Output 41.1.16 to Output 41.1.7).

**Output 41.1.16** Parameter Estimates for Fixed Effects in GLMM Analysis

| Solutions for Fixed Effects |       |          |                |    |         |         |
|-----------------------------|-------|----------|----------------|----|---------|---------|
| Effect                      | entry | Estimate | Standard Error | DF | t Value | Pr >  t |
| Intercept                   |       | -1.4637  | 0.3738         | 3  | -3.92   | 0.0296  |
| entry                       | 1     | 2.9609   | 0.5384         | 45 | 5.50    | <.0001  |
| entry                       | 2     | 2.7807   | 0.5138         | 45 | 5.41    | <.0001  |
| entry                       | 3     | 2.4339   | 0.4934         | 45 | 4.93    | <.0001  |
| entry                       | 4     | 1.5347   | 0.4542         | 45 | 3.38    | 0.0015  |
| entry                       | 5     | 2.7653   | 0.5276         | 45 | 5.24    | <.0001  |
| entry                       | 6     | 2.0014   | 0.4865         | 45 | 4.11    | 0.0002  |
| entry                       | 7     | 2.3518   | 0.4952         | 45 | 4.75    | <.0001  |
| entry                       | 8     | 1.2927   | 0.4739         | 45 | 2.73    | 0.0091  |
| entry                       | 9     | 1.5663   | 0.4554         | 45 | 3.44    | 0.0013  |
| entry                       | 10    | 2.2896   | 0.5179         | 45 | 4.42    | <.0001  |
| entry                       | 11    | 1.5018   | 0.4682         | 45 | 3.21    | 0.0025  |
| entry                       | 12    | 1.5075   | 0.4752         | 45 | 3.17    | 0.0027  |
| entry                       | 13    | -0.5955  | 0.6475         | 45 | -0.92   | 0.3626  |
| entry                       | 14    | 0.4573   | 0.5111         | 45 | 0.89    | 0.3758  |
| entry                       | 15    | 0.8683   | 0.4682         | 45 | 1.85    | 0.0702  |
| entry                       | 16    | 0        | .              | .  | .       | .       |

**Output 41.1.17** Type III Test of Entry in GLMM Analysis

| Type III Tests of Fixed Effects |           |           |         |        |
|---------------------------------|-----------|-----------|---------|--------|
| Effect                          | Num<br>DF | Den<br>DF | F Value | Pr > F |
| entry                           | 15        | 45        | 6.90    | <.0001 |

Because the block variance component is small, the Type III test for the variety effect in [Output 41.1.17](#) is affected only very little compared to the GLM ([Output 41.1.8](#)).

### Analysis with Smooth Spatial Trends

You can also consider these data in an observational sense, where the covariation of the observations is subject to modeling. Rather than deriving model components from the experimental design alone, environmental effects can be modeled by adjusting the mean and/or correlation structure. Gotway and Stroup (1997) and Schabenberger and Pierce (2002) supplant the coarse block effects with smooth-scale spatial components.

The model considered by Gotway and Stroup (1997) is a marginal model in that the correlation structure is modeled through residual-side (R-side) random components. This exponential covariance model is fit with the following statements:

```
proc glimmix data=HessianFly;
 class entry;
 model y/n = entry / solution ddfm=contain;
 random _residual_ / subject=intercept type=sp(exp) (lng lat);
run;
```

Note that the block effects have been removed from the statements. The keyword `_RESIDUAL_` in the `RANDOM` statement instructs the GLIMMIX procedure to model the **R** matrix. Here, **R** is to be modeled as an exponential covariance structure matrix. The `SUBJECT=INTERCEPT` option means that all observations are considered correlated. Because the random effects are residual-type (R-side) effects, there are no columns in the **Z** matrix for this model ([Output 41.1.18](#)).

**Output 41.1.18** Model Dimension Information in Marginal Spatial Analysis

| The GLIMMIX Procedure    |    |
|--------------------------|----|
| Dimensions               |    |
| R-side Cov. Parameters   | 2  |
| Columns in X             | 17 |
| Columns in Z per Subject | 0  |
| Subjects (Blocks in V)   | 1  |
| Max Obs per Subject      | 64 |

In addition to the fixed effects, the GLIMMIX procedure now profiles one of the covariance parameters, the variance of the exponential covariance model (Output 41.1.19). This reduces the size of the optimization problem. Only a single parameter is part of the optimization, the “range” (SP(EXP)) of the spatial process.

**Output 41.1.19** Optimization Information in Spatial Analysis

| Optimization Information   |                   |
|----------------------------|-------------------|
| Optimization Technique     | Dual Quasi-Newton |
| Parameters in Optimization | 1                 |
| Lower Boundaries           | 1                 |
| Upper Boundaries           | 0                 |
| Fixed Effects              | Profiled          |
| Residual Variance          | Profiled          |
| Starting From              | Data              |

The practical range of a spatial process is that distance at which the correlation between data points has decreased to at most 0.05. The parameter reported by the GLIMMIX procedure as SP(EXP) in Output 41.1.20 corresponds to one-third of the practical range. The practical range in this process is  $3 \times 0.9052 = 2.7156$ . Correlations extend beyond a single experimental unit, but they do not appear to exist on the scale of the block size.

**Output 41.1.20** Estimates of Covariance Parameters

| Covariance Parameter Estimates |           |          |                |
|--------------------------------|-----------|----------|----------------|
| Cov Parm                       | Subject   | Estimate | Standard Error |
| SP (EXP)                       | Intercept | 0.9052   | 0.4404         |
| Residual                       |           | 2.5315   | 0.6974         |

The sill of the spatial process, the variance of the underlying residual effect, is estimated as 2.5315.

**Output 41.1.21** Type III Test of Entry Effect in Spatial Analysis

| Type III Tests of Fixed Effects |        |        |         |        |
|---------------------------------|--------|--------|---------|--------|
| Effect                          | Num DF | Den DF | F Value | Pr > F |
| entry                           | 15     | 48     | 3.60    | 0.0004 |

The *F* value for the entry effect has been sharply reduced compared to the previous analyses. The smooth spatial variation accounts for some of the variation among the varieties (Output 41.1.21).

In this example three models were considered for the analysis of a randomized block design with binomial outcomes. If data are correlated, a standard generalized linear model often will indicate overdispersion

relative to the binomial distribution. Two courses of action are considered in this example to address this overdispersion. First, the inclusion of G-side random effects models the correlation indirectly; it is induced through the sharing of random effects among responses from the same block. Second, the R-side spatial covariance structure models covariation directly. In generalized linear (mixed) models these two modeling approaches can lead to different inferences, because the models have different interpretation. The random block effects are modeled on the linked (logit) scale, and the spatial effects were modeled on the mean scale. Only in a linear mixed model are the two scales identical.

---

## Example 41.2: Mating Experiment with Crossed Random Effects

McCullagh and Nelder (1989, Ch. 14.5) describe a mating experiment—conducted by S. Arnold and P. Verell at the University of Chicago, Department of Ecology and Evolution—involving two geographically isolated populations of mountain dusky salamanders. One goal of the experiment was to determine whether barriers to interbreeding have evolved in light of the geographical isolation of the populations. In this case, matings within a population should be more successful than matings between the populations. The experiment conducted in the summer of 1986 involved 40 animals, 20 rough butt (R) and 20 whiteside (W) salamanders, with equal numbers of males and females. The animals were grouped into two sets of R males, two sets of R females, two sets of W males, and two sets of W females, so that each set comprised five salamanders. Each set was mated against one rough butt and one whiteside set, creating eight crossings. Within the pairings of sets, each female was paired to three male animals. The salamander mating data have been used by a number of authors; see, for example, McCullagh and Nelder (1989); Schall (1991); Karim and Zeger (1992); Breslow and Clayton (1993); Wolfinger and O’Connell (1993); Shun (1997).

The following DATA step creates the data set for the analysis.

```
data salamander;
 input day fpop$ fnum mpop$ mnum mating @@;
 datalines;
4 rb 1 rb 1 1 4 rb 2 rb 5 1
4 rb 3 rb 2 1 4 rb 4 rb 4 1
4 rb 5 rb 3 1 4 rb 6 ws 9 1
4 rb 7 ws 8 0 4 rb 8 ws 6 0
4 rb 9 ws 10 0 4 rb 10 ws 7 0
4 ws 1 rb 9 0 4 ws 2 rb 7 0
4 ws 3 rb 8 0 4 ws 4 rb 10 0
4 ws 5 rb 6 0 4 ws 6 ws 5 0
4 ws 7 ws 4 1 4 ws 8 ws 1 1
4 ws 9 ws 3 1 4 ws 10 ws 2 1
8 rb 1 ws 4 1 8 rb 2 ws 5 1
8 rb 3 ws 1 0 8 rb 4 ws 2 1
8 rb 5 ws 3 1 8 rb 6 rb 9 1
8 rb 7 rb 8 0 8 rb 8 rb 6 1
8 rb 9 rb 7 0 8 rb 10 rb 10 0
8 ws 1 ws 9 1 8 ws 2 ws 6 0
8 ws 3 ws 7 0 8 ws 4 ws 10 1
8 ws 5 ws 8 1 8 ws 6 rb 2 0
8 ws 7 rb 1 1 8 ws 8 rb 4 0
8 ws 9 rb 3 1 8 ws 10 rb 5 0
12 rb 1 rb 5 1 12 rb 2 rb 3 1
12 rb 3 rb 1 1 12 rb 4 rb 2 1
```

```

12 rb 5 rb 4 1 12 rb 6 ws 10 1
12 rb 7 ws 9 0 12 rb 8 ws 7 0
12 rb 9 ws 8 1 12 rb 10 ws 6 1
12 ws 1 rb 7 1 12 ws 2 rb 9 0
12 ws 3 rb 6 0 12 ws 4 rb 8 1
12 ws 5 rb 10 0 12 ws 6 ws 3 1
12 ws 7 ws 5 1 12 ws 8 ws 2 1
12 ws 9 ws 1 1 12 ws 10 ws 4 0
16 rb 1 ws 1 0 16 rb 2 ws 3 1
16 rb 3 ws 4 1 16 rb 4 ws 5 0
16 rb 5 ws 2 1 16 rb 6 rb 7 0
16 rb 7 rb 9 1 16 rb 8 rb 10 0
16 rb 9 rb 6 1 16 rb 10 rb 8 0
16 ws 1 ws 10 1 16 ws 2 ws 7 1
16 ws 3 ws 9 0 16 ws 4 ws 8 1
16 ws 5 ws 6 0 16 ws 6 rb 4 0
16 ws 7 rb 2 0 16 ws 8 rb 5 0
16 ws 9 rb 1 1 16 ws 10 rb 3 1
20 rb 1 rb 4 1 20 rb 2 rb 1 1
20 rb 3 rb 3 1 20 rb 4 rb 5 1
20 rb 5 rb 2 1 20 rb 6 ws 6 1
20 rb 7 ws 7 0 20 rb 8 ws 10 1
20 rb 9 ws 9 1 20 rb 10 ws 8 1
20 ws 1 rb 10 0 20 ws 2 rb 6 0
20 ws 3 rb 7 0 20 ws 4 rb 9 0
20 ws 5 rb 8 0 20 ws 6 ws 2 0
20 ws 7 ws 1 1 20 ws 8 ws 5 1
20 ws 9 ws 4 1 20 ws 10 ws 3 1
24 rb 1 ws 5 1 24 rb 2 ws 2 1
24 rb 3 ws 3 1 24 rb 4 ws 4 1
24 rb 5 ws 1 1 24 rb 6 rb 8 1
24 rb 7 rb 6 0 24 rb 8 rb 9 1
24 rb 9 rb 10 1 24 rb 10 rb 7 0
24 ws 1 ws 8 1 24 ws 2 ws 10 0
24 ws 3 ws 6 1 24 ws 4 ws 9 1
24 ws 5 ws 7 0 24 ws 6 rb 1 0
24 ws 7 rb 5 1 24 ws 8 rb 3 0
24 ws 9 rb 4 0 24 ws 10 rb 2 0
i

```

The first observation, for example, indicates that rough butt female 1 was paired in the laboratory on day 4 of the experiment with rough butt male 1, and the pair mated. On the same day rough butt female 7 was paired with whiteside male 8, but the pairing did not result in mating of the animals.

The model adopted by many authors for these data comprises fixed effects for gender and population, their interaction, and male and female random effects. Specifically, let  $\pi_{RR}$ ,  $\pi_{RW}$ ,  $\pi_{WR}$ , and  $\pi_{WW}$  denote the mating probabilities between the populations, where the first subscript identifies the female partner of the pair. Then, you model

$$\log \left\{ \frac{\pi_{kl}}{1 - \pi_{kl}} \right\} = \tau_{kl} + \gamma_f + \gamma_m \quad k, l \in \{R, W\}$$

where  $\gamma_f$  and  $\gamma_m$  are independent random variables representing female and male random effects (20 each), and  $\tau_{kl}$  denotes the average logit of mating between females of population  $k$  and males of population  $l$ .

The following statements fit this model by pseudo-likelihood:

```
proc glimmix data=salamander;
 class fpop fnum mpop mnum;
 model mating(event='1') = fpop|mpop / dist=binary;
 random fpop*fnum mpop*mnum;
 lsmeans fpop*mpop / ilink;
run;
```

The response variable is the two-level variable `mating`. Because it is coded as zeros and ones, and because PROC GLIMMIX models by default the probability of the first level according to the response-level ordering, the `EVENT='1'` option instructs PROC GLIMMIX to model the probability of a successful mating. The distribution of the mating variable, conditional on the random effects, is binary.

The `fpop*fnum` effect in the `RANDOM` statement creates a random intercept for each female animal. Because `fpop` and `fnum` are `CLASS` variables, the effect has 20 levels (10 `rb` and 10 `ws` females). Similarly, the `mpop*mnum` effect creates the random intercepts for the male animals. Because no `TYPE=` is specified in the `RANDOM` statement, the covariance structure defaults to `TYPE=VC`. The random effects and their levels are independent, and each effect has its own variance component. Because the conditional distribution of the data, conditioned on the random effects, is binary, no extra scale parameter ( $\phi$ ) is added.

The `LSMEANS` statement requests least squares means for the four levels of the `fpop*mpop` effect, which are estimates of the cell means in the  $2 \times 2$  classification of female and male populations. The `ILINK` option in the `LSMEANS` statement requests that the estimated means and standard errors are also reported on the scale of the data. This yields estimates of the four mating probabilities,  $\pi_{RR}$ ,  $\pi_{RW}$ ,  $\pi_{WR}$ , and  $\pi_{WW}$ .

The “Model Information” table displays general information about the model being fit (Output 41.2.1).

**Output 41.2.1** Analysis of Mating Experiment with Crossed Random Effects

| The GLIMMIX Procedure     |                 |
|---------------------------|-----------------|
| Model Information         |                 |
| Data Set                  | WORK.SALAMANDER |
| Response Variable         | mating          |
| Response Distribution     | Binary          |
| Link Function             | Logit           |
| Variance Function         | Default         |
| Variance Matrix           | Not blocked     |
| Estimation Technique      | Residual PL     |
| Degrees of Freedom Method | Containment     |

The response variable `mating` follows a binary distribution (conditional on the random effects). Hence, the mean of the data is an event probability,  $\pi$ , and the logit of this probability is linearly related to the linear predictor of the model. The variance function is the default function that is implied by the distribution,  $a(\pi) = \pi(1 - \pi)$ . The variance matrix is not blocked, because the GLIMMIX procedure does not process the data by subjects (see the section “Processing by Subjects” on page 3082 for details). The estimation technique is the default method for GLMMs, residual pseudo-likelihood (`METHOD=RSPL`), and degrees of freedom for tests and confidence intervals are determined by the containment method.

The “Class Level Information” table in Output 41.2.2 lists the levels of the variables listed in the `CLASS` statement, as well as the order of the levels.

**Output 41.2.2** Class Level Information and Number of Observations

| Class Level Information     |        |                      |
|-----------------------------|--------|----------------------|
| Class                       | Levels | Values               |
| fpop                        | 2      | rb ws                |
| fnum                        | 10     | 1 2 3 4 5 6 7 8 9 10 |
| mpop                        | 2      | rb ws                |
| mnum                        | 10     | 1 2 3 4 5 6 7 8 9 10 |
| Number of Observations Read |        | 120                  |
| Number of Observations Used |        | 120                  |

Note that there are two female populations and two male populations; also, the variables fnum and mnum have 10 levels each. As a consequence, the effects fpop\*fnum and mpop\*mnum identify the 20 females and males, respectively. The effect fpop\*mpop identifies the four mating types.

The “Response Profile Table,” which is displayed for binary or multinomial data, lists the levels of the response variable and their order (Output 41.2.3). With binary data, the table also provides information about which level of the response variable defines the event. Because of the EVENT='1' response variable option in the MODEL statement, the probability being modeled is that of the higher-ordered value.

**Output 41.2.3** Response Profiles

| Response Profile |        |                 |
|------------------|--------|-----------------|
| Ordered Value    | mating | Total Frequency |
| 1                | 0      | 50              |
| 2                | 1      | 70              |

The GLIMMIX procedure is modeling the probability that mating='1'.

There are two covariance parameters in this model, the variance of the fpop\*fnum effect and the variance of the mpop\*mnum effect (Output 41.2.4). Both parameters are modeled as G-side parameters. The nine columns in the **X** matrix comprise the intercept, two columns each for the levels of the fpop and mpop effects, and four columns for their interaction. The **Z** matrix has 40 columns, one for each animal. Because the data are not processed by subjects, PROC GLIMMIX assumes the data consist of a single subject (a single block in **V**).

**Output 41.2.4** Model Dimensions Information

| Dimensions             |     |
|------------------------|-----|
| G-side Cov. Parameters | 2   |
| Columns in X           | 9   |
| Columns in Z           | 40  |
| Subjects (Blocks in V) | 1   |
| Max Obs per Subject    | 120 |



The “Optimization Information” table displays basic information about the optimization (Output 41.2.5). The default technique for GLMMs is the quasi-Newton method. There are two parameters in the optimization, which correspond to the two variance components. The 17 fixed effects parameters are not part of the optimization. The initial optimization computes pseudo-data based on the response values in the data set rather than from estimates of a generalized linear model fit.

**Output 41.2.5** Optimization Information

| Optimization Information   |                             |
|----------------------------|-----------------------------|
| Optimization Technique     | Newton-Raphson with Ridging |
| Parameters in Optimization | 2                           |
| Lower Boundaries           | 2                           |
| Upper Boundaries           | 0                           |
| Fixed Effects              | Profiled                    |
| Starting From              | Data                        |

The GLIMMIX procedure performs eight optimizations after the initial optimization (Output 41.2.6). That is, following the initial pseudo-data creation, the pseudo-data were updated eight more times and a total of nine linear mixed models were estimated.

**Output 41.2.6** Iteration History and Convergence Status

| Iteration History |          |               |                       |            |                 |
|-------------------|----------|---------------|-----------------------|------------|-----------------|
| Iteration         | Restarts | Subiterations | Objective<br>Function | Change     | Max<br>Gradient |
| 0                 | 0        | 4             | 537.09173501          | 2.00000000 | 1.719E-8        |
| 1                 | 0        | 3             | 544.12516903          | 0.66319780 | 1.14E-8         |
| 2                 | 0        | 2             | 545.89139118          | 0.13539318 | 1.609E-6        |
| 3                 | 0        | 2             | 546.10489538          | 0.01742065 | 5.89E-10        |
| 4                 | 0        | 1             | 546.13075146          | 0.00212475 | 9.654E-7        |
| 5                 | 0        | 1             | 546.13374731          | 0.00025072 | 1.346E-8        |
| 6                 | 0        | 1             | 546.13409761          | 0.00002931 | 1.84E-10        |
| 7                 | 0        | 0             | 546.13413861          | 0.00000000 | 4.285E-6        |

Convergence criterion (PCONV=1.11022E-8) satisfied.

The “Covariance Parameter Estimates” table lists the estimates for the two variance components and their estimated standard errors (Output 41.2.7). The heterogeneity (in the logit of the mating probabilities) among the females is considerably larger than the heterogeneity among the males.

**Output 41.2.7** Estimated Covariance Parameters and Approximate Standard Errors

| Covariance Parameter Estimates |          |                |
|--------------------------------|----------|----------------|
| Cov Parm                       | Estimate | Standard Error |
| fpop*fnum                      | 1.4099   | 0.8871         |
| mpop*mnum                      | 0.08963  | 0.4102         |

The “Type III Tests of Fixed Effects” table indicates a significant interaction between the male and female populations (Output 41.2.8). A comparison in the logits of mating success in pairs with R females and W females depends on whether the male partner in the pair is the same species. The “fpop\*mpop Least Squares Means” table shows this effect more clearly (Output 41.2.9).

**Output 41.2.8** Tests of Main Effects and Interaction

| Type III Tests of Fixed Effects |        |        |         |        |
|---------------------------------|--------|--------|---------|--------|
| Effect                          | Num DF | Den DF | F Value | Pr > F |
| fpop                            | 1      | 18     | 2.86    | 0.1081 |
| mpop                            | 1      | 17     | 4.71    | 0.0444 |
| fpop*mpop                       | 1      | 81     | 9.61    | 0.0027 |

**Output 41.2.9** Interaction Least Squares Means

| fpop*mpop Least Squares Means |      |          |                |    |         |         |        |                     |
|-------------------------------|------|----------|----------------|----|---------|---------|--------|---------------------|
| fpop                          | mpop | Estimate | Standard Error | DF | t Value | Pr >  t | Mean   | Standard Error Mean |
| rb                            | rb   | 1.1629   | 0.5961         | 81 | 1.95    | 0.0545  | 0.7619 | 0.1081              |
| rb                            | ws   | 0.7839   | 0.5729         | 81 | 1.37    | 0.1750  | 0.6865 | 0.1233              |
| ws                            | rb   | -1.4119  | 0.6143         | 81 | -2.30   | 0.0241  | 0.1959 | 0.09678             |
| ws                            | ws   | 1.0151   | 0.5871         | 81 | 1.73    | 0.0876  | 0.7340 | 0.1146              |

In a pairing with a male rough butt salamander, the logit drops sharply from 1.1629 to  $-1.4119$  when the male is paired with a whiteside female instead of a female from its own population. The corresponding estimated probabilities of mating success are  $\hat{\pi}_{RR} = 0.7619$  and  $\hat{\pi}_{WR} = 0.1959$ . If the same comparisons are made in pairs with whiteside males, then you also notice a drop in the logit if the female comes from a different population, 1.0151 versus 0.7839. The change is considerably less, though, corresponding to mating probabilities of  $\hat{\pi}_{WW} = 0.7340$  and  $\hat{\pi}_{RW} = 0.6865$ . Whiteside females appear to be successful with their own population. Whiteside males appear to succeed equally well with female partners of the two populations.

This insight into the factor-level comparisons can be amplified by graphing the least squares mean comparisons and by subsetting the differences of least squares means. This is accomplished with the following statements:

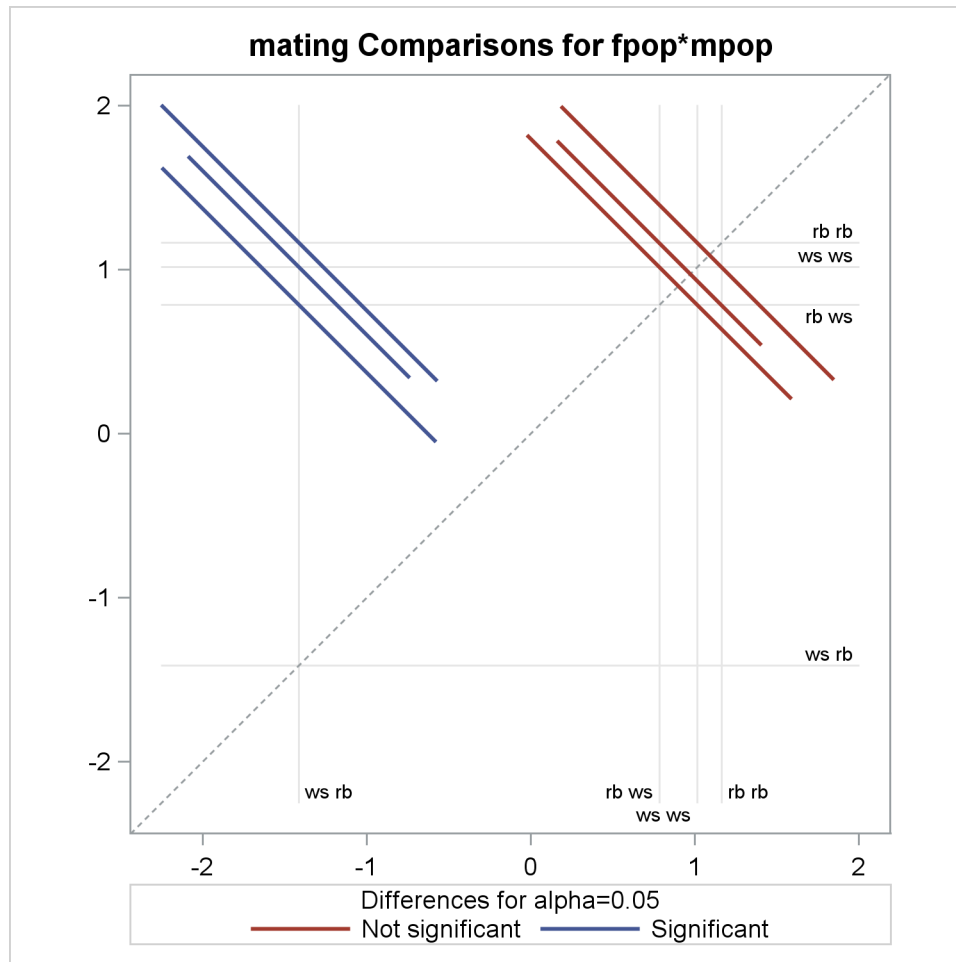
```
ods graphics on;
ods select DiffPlot SliceDiffs;
proc glimmix data=salamander;
 class fpop fnum mpop mnum;
 model mating(event='1') = fpop|mpop / dist=binary;
 random fpop*fnum mpop*mnum;
 lsmeans fpop*mpop / plots=diffplot;
 lsmeans fpop*mpop / slicediff=(mpop fpop);
run;
ods graphics off;
```

The `PLOTS=DIFFPLOT` option in the first `LSMEANS` statement requests a comparison plot that displays the result of all pairwise comparisons (Output 41.2.10). The `SLICEDIFF=(mpop fpop)` option requests differences of simple effects.

The comparison plot in Output 41.2.10 is also known as a mean-mean scatter plot (Hsu 1996). Each solid line in the plot corresponds to one of the possible  $4 \times 3/2 = 6$  unique pairwise comparisons. The line is centered at the intersection of two least squares means, and the length of the line segments corresponds to the width of a 95% confidence interval for the difference between the two least squares means. The length of the segment is adjusted for the rotation. If a line segment crosses the dashed 45-degree line, the comparison between the two factor levels is not significant; otherwise, it is significant. The horizontal and vertical axes of the plot are drawn in least squares means units, and the grid lines are placed at the values of the least squares means.

The six pairs of least squares means comparisons separate into two sets of three pairs. Comparisons in the first set are significant; comparisons in the second set are not significant. For the significant set, the female partner in one of the pairs is a whiteside salamander. For the nonsignificant comparisons, the male partner in one of the pairs is a whiteside salamander.

**Output 41.2.10** LS-Means Diffogram



The “Simple Effect Comparisons” tables show the results of the `SLICEDIFF=` option in the second `LSMEANS` statement (Output 41.2.11).

**Output 41.2.11** Simple Effect Comparisons

| Simple Effect Comparisons of fpop*mpop Least Squares Means By mpop |      |       |          |                |    |         |         |
|--------------------------------------------------------------------|------|-------|----------|----------------|----|---------|---------|
| Simple Effect Level                                                | fpop | _fpop | Estimate | Standard Error | DF | t Value | Pr >  t |
| mpop rb                                                            | rb   | ws    | 2.5748   | 0.8458         | 81 | 3.04    | 0.0031  |
| mpop ws                                                            | rb   | ws    | -0.2312  | 0.8092         | 81 | -0.29   | 0.7758  |

Output 41.2.11 continued

| Simple Effect Comparisons of fpop*mpop Least Squares Means By fpop |      |       |          |                |    |         |         |
|--------------------------------------------------------------------|------|-------|----------|----------------|----|---------|---------|
| Simple Effect Level                                                | mpop | _mpop | Estimate | Standard Error | DF | t Value | Pr >  t |
| fpop rb                                                            | rb   | ws    | 0.3790   | 0.6268         | 81 | 0.60    | 0.5471  |
| fpop ws                                                            | rb   | ws    | -2.4270  | 0.6793         | 81 | -3.57   | 0.0006  |

The first table of simple effect comparisons holds fixed the level of the mpop factor and compares the levels of the fpop factor. Because there is only one possible comparison for each male population, there are two entries in the table. The first entry compares the logits of mating probabilities when the male partner is a rough butt, and the second entry applies when the male partner is from the whiteside population. The second table of simple effects comparisons applies the same logic, but holds fixed the level of the female partner in the pair. Note that these four comparisons are a subset of all six possible comparisons, eliminating those where both factors are varied at the same time. The simple effect comparisons show that there is no difference in mating probabilities if the male partner is a whiteside salamander, or if the female partner is a rough butt. Rough butt females also appear to mate indiscriminately.

### Example 41.3: Smoothing Disease Rates; Standardized Mortality Ratios

Clayton and Kaldor (1987, Table 1) present data on observed and expected cases of lip cancer in the 56 counties of Scotland between 1975 and 1980. The expected number of cases was determined by a separate multiplicative model that accounted for the age distribution in the counties. The goal of the analysis is to estimate the county-specific log-relative risks, also known as standardized mortality ratios (SMR).

If  $Y_i$  is the number of incident cases in county  $i$  and  $E_i$  is the expected number of incident cases, then the ratio of observed to expected counts,  $Y_i/E_i$ , is the standardized mortality ratio. Clayton and Kaldor (1987) assume there exists a relative risk  $\lambda_i$  that is specific to each county and is a random variable. Conditional on  $\lambda_i$ , the observed counts are independent Poisson variables with mean  $E_i \lambda_i$ .

An elementary mixed model for  $\lambda_i$  specifies only a random intercept for each county, in addition to a fixed intercept. Breslow and Clayton (1993), in their analysis of these data, also provide a covariate that measures the percentage of employees in agriculture, fishing, and forestry. The expanded model for the region-specific relative risk in Breslow and Clayton (1993) is

$$\lambda_i = \exp\{\beta_0 + \beta_1 x_i/10 + \gamma_i\}, \quad i = 1, \dots, 56$$

where  $\beta_0$  and  $\beta_1$  are fixed effects, and the  $\gamma_i$  are county random effects.

The following DATA step creates the data set lipcancer. The expected number of cases is based on the observed standardized mortality ratio for counties with lip cancer cases, and based on the expected counts reported by Clayton and Kaldor (1987, Table 1) for the counties without cases. The sum of the expected counts then equals the sum of the observed counts.

```
data lipcancer;
 input county observed expected employment SMR;
 if (observed > 0) then expCount = 100*observed/SMR;
 else expCount = expected;
 datalines;
1 9 1.4 16 652.2
2 39 8.7 16 450.3
3 11 3.0 10 361.8
4 9 2.5 24 355.7
5 15 4.3 10 352.1
6 8 2.4 24 333.3
7 26 8.1 10 320.6
8 7 2.3 7 304.3
9 6 2.0 7 303.0
10 20 6.6 16 301.7
11 13 4.4 7 295.5
12 5 1.8 16 279.3
13 3 1.1 10 277.8
14 8 3.3 24 241.7
15 17 7.8 7 216.8
16 9 4.6 16 197.8
17 2 1.1 10 186.9
18 7 4.2 7 167.5
19 9 5.5 7 162.7
20 7 4.4 10 157.7
21 16 10.5 7 153.0
22 31 22.7 16 136.7
23 11 8.8 10 125.4
24 7 5.6 7 124.6
25 19 15.5 1 122.8
26 15 12.5 1 120.1
27 7 6.0 7 115.9
28 10 9.0 7 111.6
29 16 14.4 10 111.3
30 11 10.2 10 107.8
31 5 4.8 7 105.3
32 3 2.9 24 104.2
33 7 7.0 10 99.6
34 8 8.5 7 93.8
35 11 12.3 7 89.3
36 9 10.1 0 89.1
37 11 12.7 10 86.8
38 8 9.4 1 85.6
39 6 7.2 16 83.3
40 4 5.3 0 75.9
41 10 18.8 1 53.3
42 8 15.8 16 50.7
43 2 4.3 16 46.3
44 6 14.6 0 41.0
45 19 50.7 1 37.5
46 3 8.2 7 36.6
47 2 5.6 1 35.8
48 3 9.3 1 32.1
```

```

49 28 88.7 0 31.6
50 6 19.6 1 30.6
51 1 3.4 1 29.1
52 1 3.6 0 27.6
53 1 5.7 1 17.4
54 1 7.0 1 14.2
55 0 4.2 16 0.0
56 0 1.8 10 0.0
;

```

Because the mean of the Poisson variates, conditional on the random effects, is  $\mu_i = E_i \lambda_i$ , applying a log link yields

$$\log\{\mu_i\} = \log\{E_i\} + \beta_0 + \beta_1 x_i / 10 + \gamma_i$$

The term  $\log\{E_i\}$  is an offset, a regressor variable whose coefficient is known to be one. Note that it is assumed that the  $E_i$  are known; they are not treated as random variables.

The following statements fit this model by residual pseudo-likelihood:

```

proc glimmix data=lipcancer;
 class county;
 x = employment / 10;
 logn = log(expCount);
 model observed = x / dist=poisson offset=logn
 solution ddfm=none;

 random county;
 SMR_pred = 100*exp(_zgamma_ + _xbeta_);
 id employment SMR SMR_pred;
 output out=glimmixout;
run;

```

The offset is created with the assignment statement

```
logn = log(expCount);
```

and is associated with the linear predictor through the **OFFSET=** option in the **MODEL** statement. The statement

```
x = employment / 10;
```

transforms the covariate measuring percentage of employment in agriculture, fisheries, and forestry to agree with the analysis of Breslow and Clayton (1993). The **DDFM=NONE** option in the **MODEL** statement requests chi-square tests and  $z$  tests instead of the default  $F$  tests and  $t$  tests by setting the denominator degrees of freedom in tests of fixed effects to  $\infty$ .

The statement

```
SMR_pred = 100*exp(_zgamma_ + _xbeta_);
```

calculates the fitted standardized mortality rate. Note that the offset variable does not contribute to the exponentiated term.

The **OUTPUT** statement saves results of the calculations to the output data set `glimmixout`. The **ID** statement specifies that only the listed variables are written to the output data set.

**Output 41.3.1** Model Information in Poisson GLMM

```

The GLIMMIX Procedure

Model Information

Data Set WORK.LIPCANCER
Response Variable observed
Response Distribution Poisson
Link Function Log
Variance Function Default
Offset Variable logn = log(expCount);
Variance Matrix Not blocked
Estimation Technique Residual PL
Degrees of Freedom Method None

Class Level Information

Class Levels Values
county 56 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18
 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33
 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48
 49 50 51 52 53 54 55 56

Number of Observations Read 56
Number of Observations Used 56

Dimensions

G-side Cov. Parameters 1
Columns in X 2
Columns in Z 56
Subjects (Blocks in V) 1
Max Obs per Subject 56

```

The GLIMMIX procedure displays in the “Model Information” table that the offset variable was computed with programming statements and the final assignment statement from your GLIMMIX statements (Output 41.3.1). There are two columns in the **X** matrix, corresponding to the intercept and the regressor  $x/10$ . There are 56 columns in the **Z** matrix, however, one for each observation in the data set (Output 41.3.1).



The optimization involves only a single covariance parameter, the variance of the county effect (Output 41.3.2). Because this parameter is a variance, the GLIMMIX procedure imposes a lower boundary constraint; the solution for the variance is bounded by zero from below.

### Output 41.3.2 Optimization Information in Poisson GLMM

| Optimization Information   |                   |
|----------------------------|-------------------|
| Optimization Technique     | Dual Quasi-Newton |
| Parameters in Optimization | 1                 |
| Lower Boundaries           | 1                 |
| Upper Boundaries           | 0                 |
| Fixed Effects              | Profiled          |
| Starting From              | Data              |

Following the initial creation of pseudo-data and the fit of a linear mixed model, the procedure goes through five more updates of the pseudo-data, each associated with a separate optimization (Output 41.3.3). Although the objective function in each optimization is the negative of twice the restricted maximum likelihood for that pseudo-data, there is no guarantee that across the outer iterations the objective function decreases in subsequent optimizations. In this example, minus twice the residual maximum likelihood at convergence takes on its smallest value at the initial optimization and increases in subsequent optimizations.

### Output 41.3.3 Iteration History in Poisson GLMM

| Iteration History                                   |          |               |                       |            |                 |  |
|-----------------------------------------------------|----------|---------------|-----------------------|------------|-----------------|--|
| Iteration                                           | Restarts | Subiterations | Objective<br>Function | Change     | Max<br>Gradient |  |
| 0                                                   | 0        | 4             | 123.64113992          | 0.20997891 | 3.848E-8        |  |
| 1                                                   | 0        | 3             | 127.05866018          | 0.03393332 | 0.000048        |  |
| 2                                                   | 0        | 2             | 127.48839749          | 0.00223427 | 5.753E-6        |  |
| 3                                                   | 0        | 1             | 127.50502469          | 0.00006946 | 1.938E-7        |  |
| 4                                                   | 0        | 1             | 127.50528068          | 0.00000118 | 1.09E-7         |  |
| 5                                                   | 0        | 0             | 127.50528481          | 0.00000000 | 1.299E-6        |  |
| Convergence criterion (PCONV=1.11022E-8) satisfied. |          |               |                       |            |                 |  |

The “Covariance Parameter Estimates” table in Output 41.3.4 shows the estimate of the variance of the region-specific log-relative risks. There is significant county-to-county heterogeneity in risks. If the covariate were removed from the analysis, as in Clayton and Kaldor (1987), the heterogeneity in county-specific risks would increase. (The fitted SMRs in Table 6 of Breslow and Clayton (1993) were obtained without the covariate  $x$  in the model.)

**Output 41.3.4** Estimated Covariance Parameters in Poisson GLMM

| Covariance Parameter Estimates |          |                   |
|--------------------------------|----------|-------------------|
| Cov<br>Parm                    | Estimate | Standard<br>Error |
| county                         | 0.3567   | 0.09869           |

The “Solutions for Fixed Effects” table displays the estimates of  $\beta_0$  and  $\beta_1$  along with their standard errors and test statistics (Output 41.3.5). Because of the DDFM=NONE option in the MODEL statement, PROC GLIMMIX assumes that the degrees of freedom for the  $t$  tests of  $H_0: \beta_j = 0$  are infinite. The  $p$ -values correspond to probabilities under a standard normal distribution. The covariate measuring employment percentages in agriculture, fisheries, and forestry is significant. This covariate might be a surrogate for the exposure to sunlight, an important risk factor for lip cancer.

**Output 41.3.5** Fixed-Effects Parameter Estimates in Poisson GLMM

| Solutions for Fixed Effects |          |                   |       |         |         |
|-----------------------------|----------|-------------------|-------|---------|---------|
| Effect                      | Estimate | Standard<br>Error | DF    | t Value | Pr >  t |
| Intercept                   | -0.4406  | 0.1572            | Infty | -2.80   | 0.0051  |
| x                           | 0.6799   | 0.1409            | Infty | 4.82    | <.0001  |

You can examine the quality of the fit of this model with various residual plots. A panel of studentized residuals is requested with the following statements:

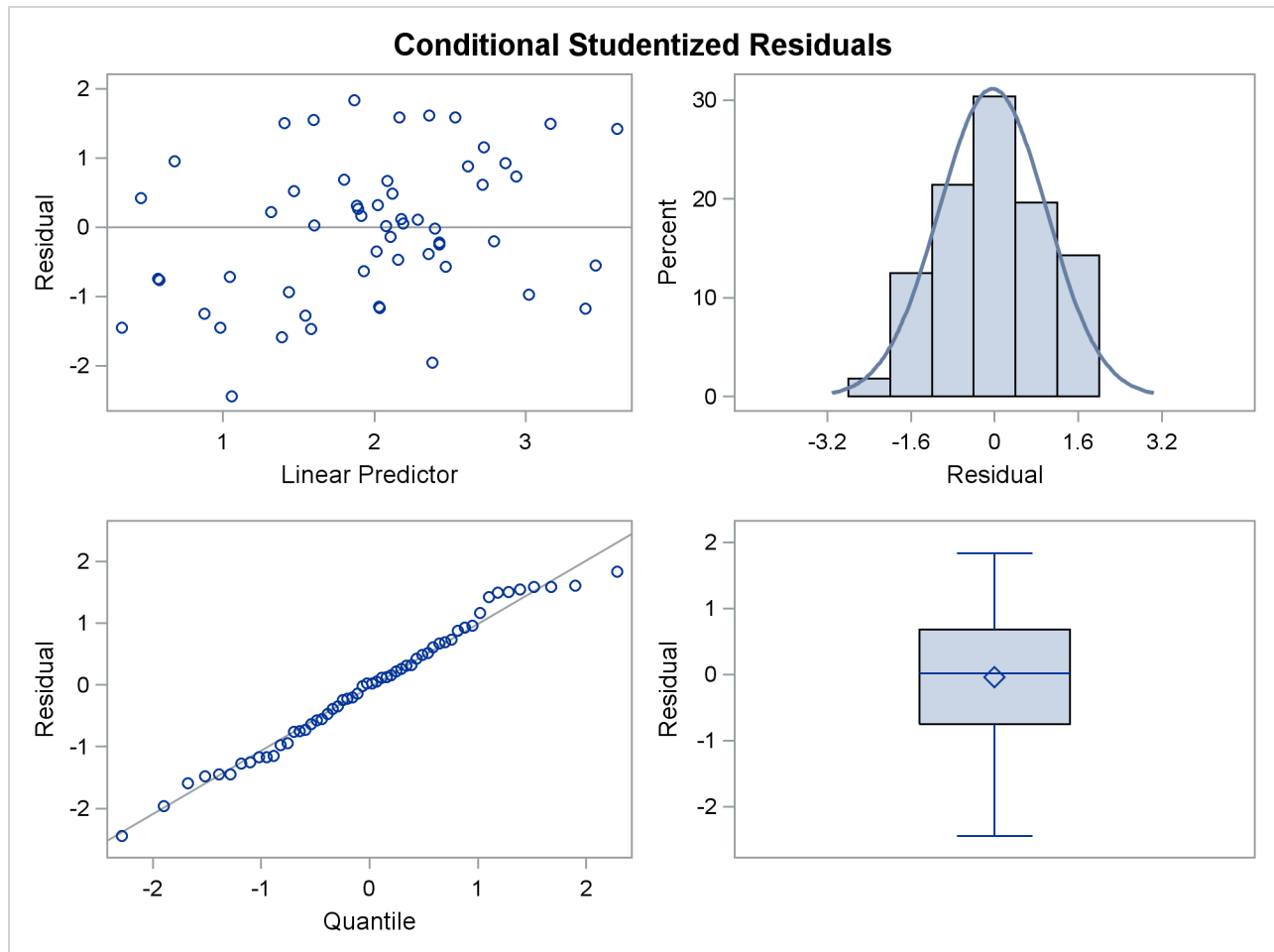
```
ods graphics on;
ods select StudentPanel;

proc glimmix data=lipcancer plots=studentpanel;
 class county;
 x = employment / 10;
 logn = log(expCount);
 model observed = x / dist=poisson offset=logn s ddfm=none;
 random county;
run;

ods graphics off;
```

The graph in the upper-left corner of the panel displays studentized residuals plotted against the linear predictor (Output 41.3.6). The default of the GLIMMIX procedure is to use the estimated BLUPs in the construction of the residuals and to present them on the linear scale, which in this case is the logarithmic scale. You can change the type of the computed residual with the TYPE= suboptions of each paneled display. For example, the option PLOTS=STUDENTPANEL(TYPE=NOBLUP) would request a paneled display of the marginal residuals on the linear scale.

Output 41.3.6 Panel of Studentized Residuals



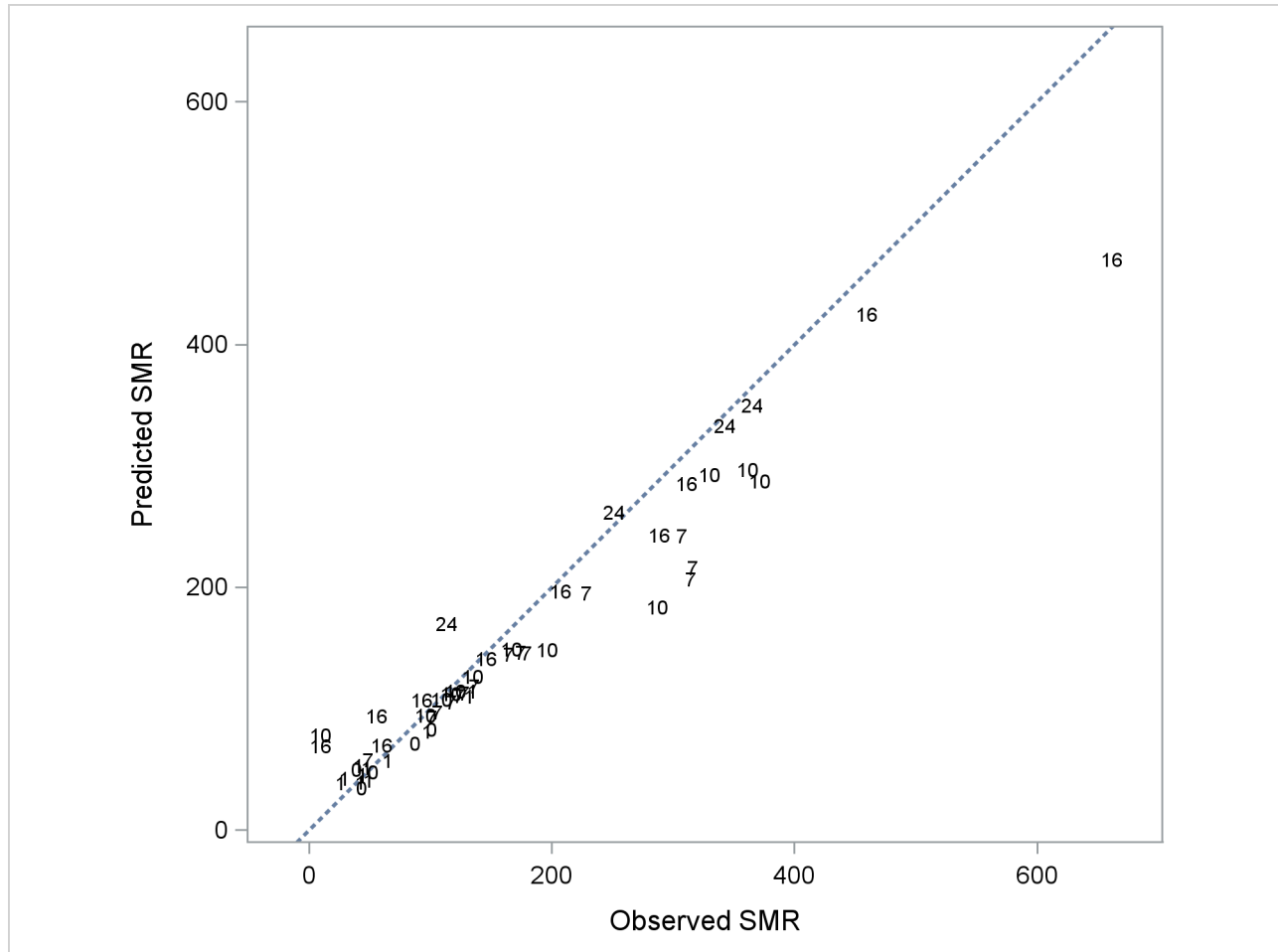
The graph in the upper-right corner of the panel shows a histogram with overlaid normal density. A Q-Q plot and a box plot are shown in the lower cells of the panel.

The following statements produce a graph of the observed and predicted standardized mortality ratios (Output 41.3.7):

```
proc template;
 define statgraph scatter;
 BeginGraph;
 layout overlayequated / yaxisopts=(label='Predicted SMR')
 xaxisopts=(label='Observed SMR')
 equatetype=square;
 lineparm y=0 slope=1 x=0 /
 lineattrs = GraphFit(pattern=dash)
 extend = true;
 scatterplot y=SMR_pred x=SMR /
 markercharacter = employment;
 endlayout;
 EndGraph;
end;
run;
proc sgrender data=glimmixout template=scatter;
run;
```

In **Output 41.3.7**, fitted SMRs tend to be larger than the observed SMRs for counties with small observed SMR and smaller than the observed SMRs for counties with high observed SMR.

**Output 41.3.7** Observed and Predicted SMRs; Data Labels Indicate Covariate Values



To demonstrate the impact of the random effects adjustment to the log-relative risks, the following statements fit a Poisson regression model (a GLM) by maximum likelihood:

```
proc glimmix data=lipcancer;
 x = employment / 10;
 logn = log(expCount);
 model observed = x / dist=poisson offset=logn
 solution ddfm=none;
 SMR_pred = 100*exp(_zgamma_ + _xbeta_);
 id employment SMR SMR_pred;
 output out=glimmixout;
run;
```

The GLIMMIX procedure defaults to maximum likelihood estimation because these statements fit a generalized linear model with nonnormal distribution. As a consequence, the SMRs are county specific only to the extent that the risks vary with the value of the covariate. But risks are no longer adjusted based on county-to-county heterogeneity in the observed incidence count.

Because of the absence of random effects, the GLIMMIX procedure recognizes the model as a generalized linear model and fits it by maximum likelihood (Output 41.3.8). The variance matrix is diagonal because the observations are uncorrelated.

**Output 41.3.8** Model Information in Poisson GLM

| The GLIMMIX Procedure     |                       |
|---------------------------|-----------------------|
| Model Information         |                       |
| Data Set                  | WORK.LIPCANCER        |
| Response Variable         | observed              |
| Response Distribution     | Poisson               |
| Link Function             | Log                   |
| Variance Function         | Default               |
| Offset Variable           | logn = log(expCount); |
| Variance Matrix           | Diagonal              |
| Estimation Technique      | Maximum Likelihood    |
| Degrees of Freedom Method | None                  |

The “Dimensions” table shows that there are no G-side random effects in this model and no R-side scale parameter either (Output 41.3.9).

**Output 41.3.9** Model Dimensions Information in Poisson GLM

| Dimensions             |    |
|------------------------|----|
| Columns in X           | 2  |
| Columns in Z           | 0  |
| Subjects (Blocks in V) | 1  |
| Max Obs per Subject    | 56 |

Because this is a GLM, the GLIMMIX procedure defaults to the Newton-Raphson algorithm, and the fixed effects (intercept and slope) comprise the parameters in the optimization (Output 41.3.10). (The default optimization technique for a GLM is the Newton-Raphson method.)

**Output 41.3.10** Optimization Information in Poisson GLM

| Optimization Information   |                |
|----------------------------|----------------|
| Optimization Technique     | Newton-Raphson |
| Parameters in Optimization | 2              |
| Lower Boundaries           | 0              |
| Upper Boundaries           | 0              |
| Fixed Effects              | Not Profiled   |

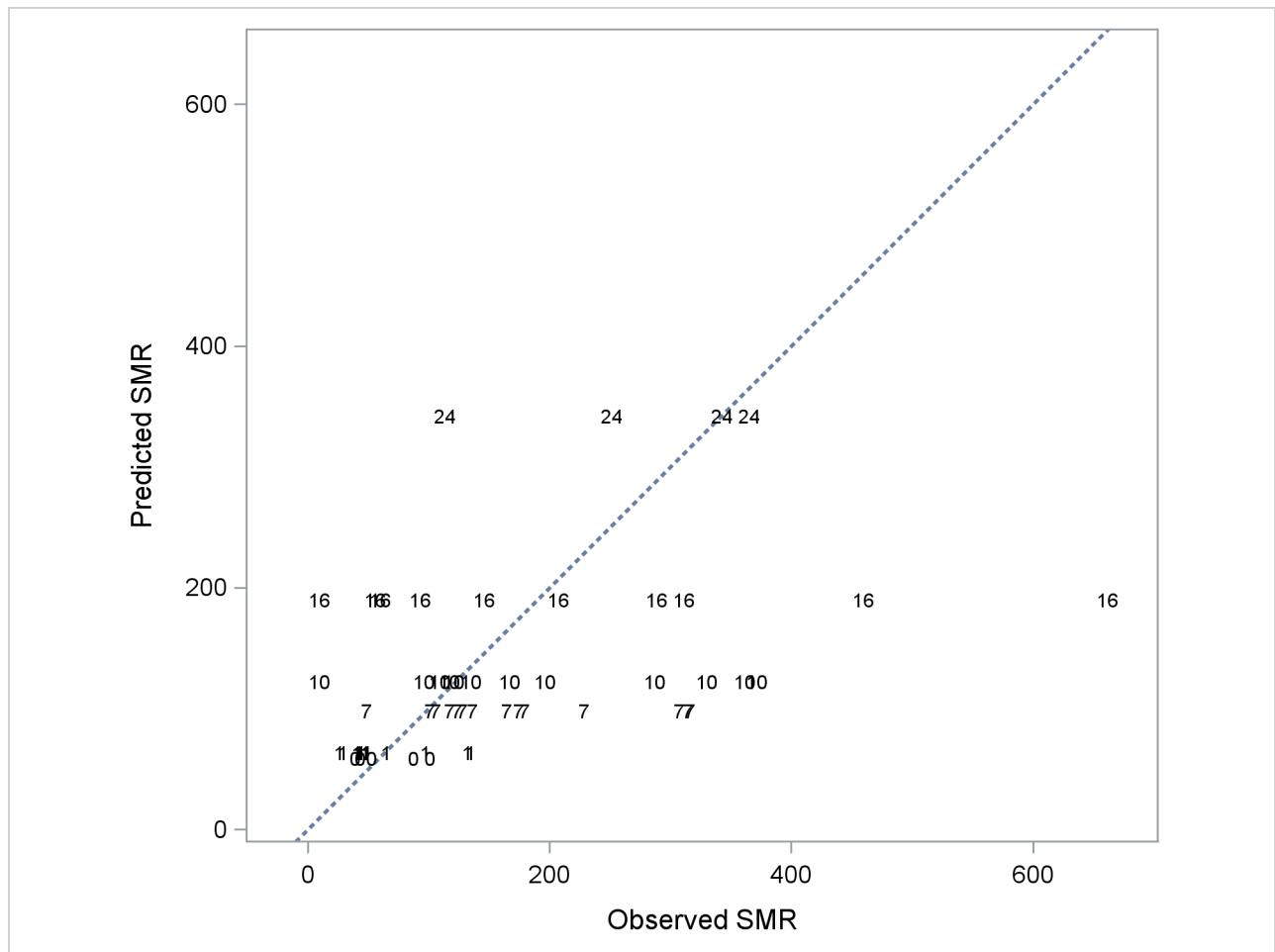
The estimates of  $\beta_0$  and  $\beta_1$  have changed from the previous analysis. In the GLMM, the estimates were  $\hat{\beta}_0 = -0.4406$  and  $\hat{\beta}_1 = 0.6799$  (Output 41.3.11).

**Output 41.3.11** Parameter Estimates in Poisson GLM

| Parameter Estimates |          |                |       |         |         |
|---------------------|----------|----------------|-------|---------|---------|
| Effect              | Estimate | Standard Error | DF    | t Value | Pr >  t |
| Intercept           | -0.5419  | 0.06951        | Infty | -7.80   | <.0001  |
| x                   | 0.7374   | 0.05954        | Infty | 12.38   | <.0001  |

More importantly, without the county-specific adjustments through the best linear unbiased predictors of the random effects, the predicted SMRs are the same for all counties with the same percentage of employees in agriculture, fisheries, and forestry (Output 41.3.12).

**Output 41.3.12** Observed and Predicted SMRs in Poisson GLM



## Example 41.4: Quasi-likelihood Estimation for Proportions with Unknown Distribution

Wedderburn (1974) analyzes data on the incidence of leaf blotch (*Rhynchosporium secalis*) on barley.

The data represent the percentage of leaf area affected in a two-way layout with 10 barley varieties at nine sites. The following DATA step converts these data to proportions, as analyzed in McCullagh and Nelder (1989, Ch. 9.2.4). The purpose of the analysis is to make comparisons among the varieties, adjusted for site effects.

```

data blotch;
 array p{9} pct1-pct9;
 input variety pct1-pct9;
 do site = 1 to 9;
 prop = p{site}/100;
 output;
 end;
 drop pct1-pct9;
 datalines;
1 0.05 0.00 1.25 2.50 5.50 1.00 5.00 5.00 17.50
2 0.00 0.05 1.25 0.50 1.00 5.00 0.10 10.00 25.00
3 0.00 0.05 2.50 0.01 6.00 5.00 5.00 5.00 42.50
4 0.10 0.30 16.60 3.00 1.10 5.00 5.00 5.00 50.00
5 0.25 0.75 2.50 2.50 2.50 5.00 50.00 25.00 37.50
6 0.05 0.30 2.50 0.01 8.00 5.00 10.00 75.00 95.00
7 0.50 3.00 0.00 25.00 16.50 10.00 50.00 50.00 62.50
8 1.30 7.50 20.00 55.00 29.50 5.00 25.00 75.00 95.00
9 1.50 1.00 37.50 5.00 20.00 50.00 50.00 75.00 95.00
10 1.50 12.70 26.25 40.00 43.50 75.00 75.00 75.00 95.00
;

```

Little is known about the distribution of the leaf area proportions. The outcomes are not binomial proportions, because they do not represent the ratio of a count over a total number of Bernoulli trials. However, because the mean proportion  $\mu_{ij}$  for variety  $j$  on site  $i$  must lie in the interval  $[0, 1]$ , you can commence the analysis with a model that treats Prop as a “pseudo-binomial” variable:

$$\begin{aligned}
 E[\text{Prop}_{ij}] &= \mu_{ij} \\
 \mu_{ij} &= 1/(1 + \exp\{-\eta_{ij}\}) \\
 \eta_{ij} &= \beta_0 + \alpha_i + \tau_j \\
 \text{Var}[\text{Prop}_{ij}] &= \phi\mu_{ij}(1 - \mu_{ij})
 \end{aligned}$$

Here,  $\eta_{ij}$  is the linear predictor for variety  $j$  on site  $i$ ,  $\alpha_i$  denotes the  $i$ th site effect, and  $\tau_j$  denotes the  $j$ th barley variety effect. The logit of the expected leaf area proportions is linearly related to these effects. The variance function of the model is that of a binomial( $n, \mu_{ij}$ ) variable, and  $\phi$  is an overdispersion parameter. The moniker “pseudo-binomial” derives not from the pseudo-likelihood methods used to estimate the parameters in the model, but from treating the response variable as if it had first and second moment properties akin to a binomial random variable.

The model is fit in the GLIMMIX procedure with the following statements:

```
proc glimmix data=blotch;
 class site variety;
 model prop = site variety / link=logit dist=binomial;
 random _residual_;
 lsmeans variety / diff=control('1');
run;
```

The **MODEL** statement specifies the distribution as binomial and the logit link. Because the variance function of the binomial distribution is  $a(\mu) = \mu(1 - \mu)$ , you use the statement

```
random _residual_;
```

to specify the scale parameter  $\phi$ . The **LSMEANS** statement requests estimates of the least squares means for the barley variety. The **DIFF=CONTROL('1')** option requests tests of least squares means differences against the first variety.

The “Model Information” table in [Output 41.4.1](#) describes the model and methods used in fitting the statistical model. It is assumed here that the data are binomial proportions.

**Output 41.4.1** Model Information in Pseudo-binomial Analysis

| The GLIMMIX Procedure     |                    |
|---------------------------|--------------------|
| Model Information         |                    |
| Data Set                  | WORK.BLOTCH        |
| Response Variable         | prop               |
| Response Distribution     | Binomial           |
| Link Function             | Logit              |
| Variance Function         | Default            |
| Variance Matrix           | Diagonal           |
| Estimation Technique      | Maximum Likelihood |
| Degrees of Freedom Method | Residual           |

The “Class Level Information” table in [Output 41.4.2](#) lists the number of levels of the Site and Variety effects and their values. All 90 observations read from the data are used in the analysis.

**Output 41.4.2** Class Levels and Number of Observations

| Class Level Information     |        |                      |
|-----------------------------|--------|----------------------|
| Class                       | Levels | Values               |
| site                        | 9      | 1 2 3 4 5 6 7 8 9    |
| variety                     | 10     | 1 2 3 4 5 6 7 8 9 10 |
| Number of Observations Read |        | 90                   |
| Number of Observations Used |        | 90                   |



In [Output 41.4.3](#), the “Dimensions” table shows that the model does not contain G-side random effects. There is a single covariance parameter, which corresponds to  $\phi$ . The “Optimization Information” table shows that the optimization comprises 18 parameters ([Output 41.4.3](#)). These correspond to the 18 nonsingular columns of the  $\mathbf{X}'\mathbf{X}$  matrix.

**Output 41.4.3** Model Fit in Pseudo-binomial Analysis

| Dimensions             |    |
|------------------------|----|
| Covariance Parameters  | 1  |
| Columns in X           | 20 |
| Columns in Z           | 0  |
| Subjects (Blocks in V) | 1  |
| Max Obs per Subject    | 90 |

| Optimization Information   |                |
|----------------------------|----------------|
| Optimization Technique     | Newton-Raphson |
| Parameters in Optimization | 18             |
| Lower Boundaries           | 0              |
| Upper Boundaries           | 0              |
| Fixed Effects              | Not Profiled   |

| Fit Statistics           |        |
|--------------------------|--------|
| -2 Log Likelihood        | 57.15  |
| AIC (smaller is better)  | 93.15  |
| AICC (smaller is better) | 102.79 |
| BIC (smaller is better)  | 138.15 |
| CAIC (smaller is better) | 156.15 |
| HQIC (smaller is better) | 111.30 |
| Pearson Chi-Square       | 6.39   |
| Pearson Chi-Square / DF  | 0.09   |

There are significant site and variety effects in this model based on the approximate Type III  $F$  tests ([Output 41.4.4](#)).

**Output 41.4.4** Tests of Site and Variety Effects in Pseudo-binomial Analysis

| Type III Tests of Fixed Effects |           |           |         |        |
|---------------------------------|-----------|-----------|---------|--------|
| Effect                          | Num<br>DF | Den<br>DF | F Value | Pr > F |
| site                            | 8         | 72        | 18.25   | <.0001 |
| variety                         | 9         | 72        | 13.85   | <.0001 |

[Output 41.4.5](#) displays the Variety least squares means for this analysis. These are obtained by averaging

$$\text{logit}(\hat{\mu}_{ij}) = \hat{\eta}_{ij}$$

across the sites. In other words, LS-means are computed on the linked scale where the model effects are additive. Note that the least squares means are ordered by variety. The estimate of the expected proportion of infected leaf area for the first variety is

$$\hat{\mu}_{.,1} = \frac{1}{1 + \exp\{4.38\}} = 0.0124$$

and that for the last variety is

$$\hat{\mu}_{.,10} = \frac{1}{1 + \exp\{0.127\}} = 0.468$$

**Output 41.4.5** Variety Least Squares Means in Pseudo-binomial Analysis

| variety Least Squares Means |          |                |    |         |         |
|-----------------------------|----------|----------------|----|---------|---------|
| variety                     | Estimate | Standard Error | DF | t Value | Pr >  t |
| 1                           | -4.3800  | 0.5643         | 72 | -7.76   | <.0001  |
| 2                           | -4.2300  | 0.5383         | 72 | -7.86   | <.0001  |
| 3                           | -3.6906  | 0.4623         | 72 | -7.98   | <.0001  |
| 4                           | -3.3319  | 0.4239         | 72 | -7.86   | <.0001  |
| 5                           | -2.7653  | 0.3768         | 72 | -7.34   | <.0001  |
| 6                           | -2.0089  | 0.3320         | 72 | -6.05   | <.0001  |
| 7                           | -1.8095  | 0.3228         | 72 | -5.61   | <.0001  |
| 8                           | -1.0380  | 0.2960         | 72 | -3.51   | 0.0008  |
| 9                           | -0.8800  | 0.2921         | 72 | -3.01   | 0.0036  |
| 10                          | -0.1270  | 0.2808         | 72 | -0.45   | 0.6523  |

Because of the ordering of the least squares means, the differences against the first variety are also ordered from smallest to largest (Output 41.4.6).

**Output 41.4.6** Variety Differences against the First Variety

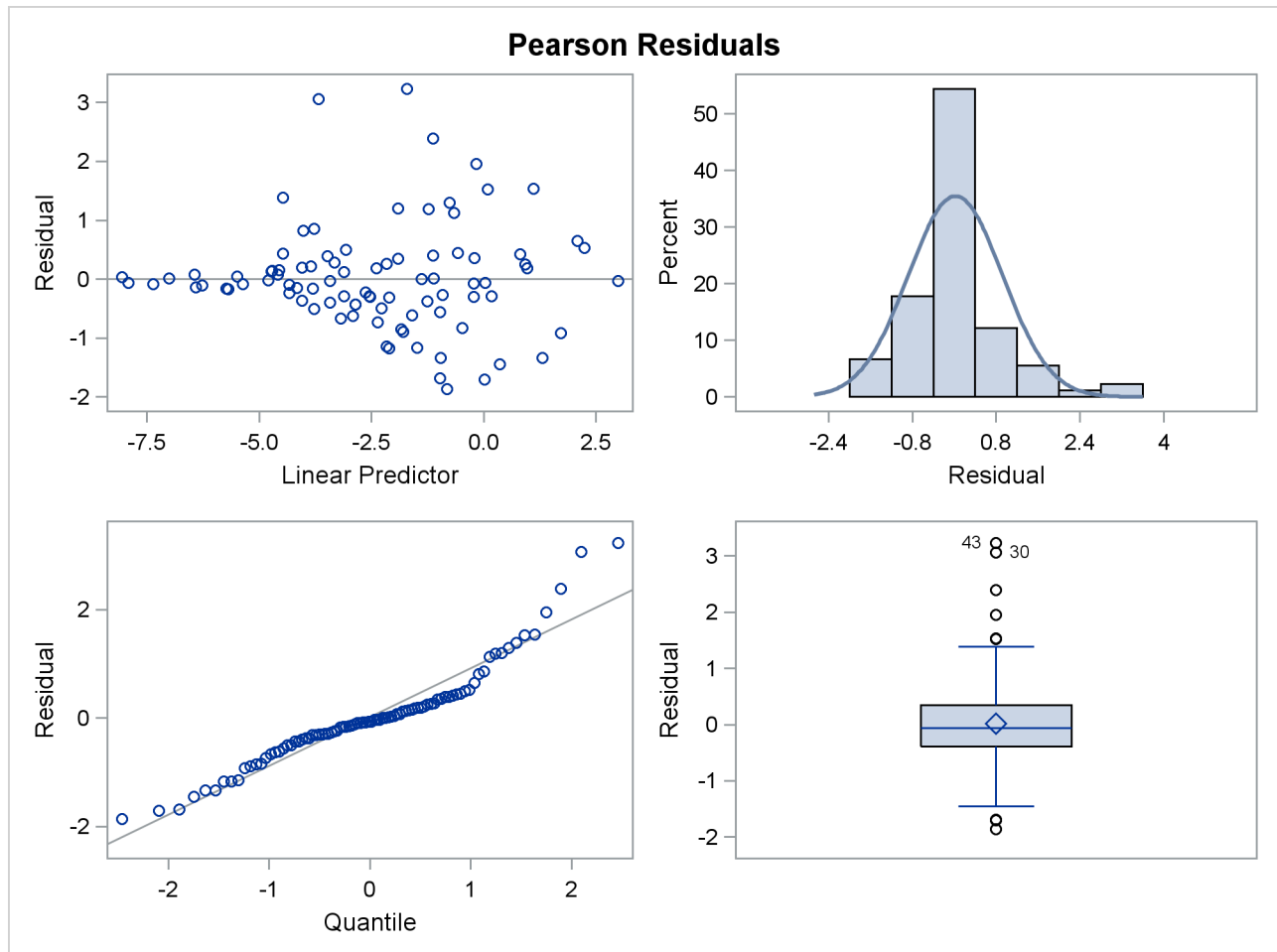
| Differences of variety Least Squares Means |          |          |                |    |         |         |
|--------------------------------------------|----------|----------|----------------|----|---------|---------|
| variety                                    | _variety | Estimate | Standard Error | DF | t Value | Pr >  t |
| 2                                          | 1        | 0.1501   | 0.7237         | 72 | 0.21    | 0.8363  |
| 3                                          | 1        | 0.6895   | 0.6724         | 72 | 1.03    | 0.3086  |
| 4                                          | 1        | 1.0482   | 0.6494         | 72 | 1.61    | 0.1109  |
| 5                                          | 1        | 1.6147   | 0.6257         | 72 | 2.58    | 0.0119  |
| 6                                          | 1        | 2.3712   | 0.6090         | 72 | 3.89    | 0.0002  |
| 7                                          | 1        | 2.5705   | 0.6065         | 72 | 4.24    | <.0001  |
| 8                                          | 1        | 3.3420   | 0.6015         | 72 | 5.56    | <.0001  |
| 9                                          | 1        | 3.5000   | 0.6013         | 72 | 5.82    | <.0001  |
| 10                                         | 1        | 4.2530   | 0.6042         | 72 | 7.04    | <.0001  |

This analysis depends on your choice for the variance function that was implied by the binomial distribution. You can diagnose the distributional assumption by examining various graphical diagnostics measures. The following statements request a panel display of the Pearson-type residuals:

```
ods graphics on;
ods select PearsonPanel;
proc glimmix data=blotch plots=pearsonpanel;
 class site variety;
 model prop = site variety / link=logit dist=binomial;
 random _residual_;
run;
ods graphics off;
```

Output 41.4.7 clearly indicates that the chosen variance function is not appropriate for these data. As  $\mu$  approaches zero or one, the variability in the residuals is less than that implied by the binomial variance function.

**Output 41.4.7** Panel of Pearson-Type Residuals in Pseudo-binomial Analysis



To remedy this situation, McCullagh and Nelder (1989) consider instead the variance function

$$\text{Var}[\text{Prop}_{ij}] = \mu_{ij}^2(1 - \mu_{ij})^2$$

Imagine two varieties with  $\mu_i = 0.1$  and  $\mu_k = 0.5$ . Under the binomial variance function, the variance of the proportion for variety  $k$  is 2.77 times larger than that for variety  $i$ . Under the revised model this ratio increases to  $2.77^2 = 7.67$ .

The analysis of the revised model is obtained with the next set of GLIMMIX statements. Because you need to model a variance function that does not correspond to any of the built-in distributions, you need to supply a function with an assignment to the automatic variable `_VARIANCE_`. The GLIMMIX procedure then considers the distribution of the data as unknown. The corresponding estimation technique is quasi-likelihood. Because this model does not include an extra scale parameter, you can drop the `RANDOM _RESIDUAL_` statement from the analysis.

```
ods graphics on;
ods select ModelInfo FitStatistics LSMeans DiffS PearsonPanel;
proc glimmix data=blotch plots=pearsonpanel;
 class site variety;
 variance = _mu_**2 * (1-_mu_)**2;
 model prop = site variety / link=logit;
 lsmeans variety / diff=control('1');
run;
ods graphics off;
```

The “Model Information” table in [Output 41.4.8](#) now displays the distribution as “Unknown,” because of the assignment made in the GLIMMIX statements to `_VARIANCE_`. The table also shows the expression evaluated as the variance function.

**Output 41.4.8** Model Information in Quasi-likelihood Analysis

| The GLIMMIX Procedure     |                       |
|---------------------------|-----------------------|
| Model Information         |                       |
| Data Set                  | WORK.BLOTCH           |
| Response Variable         | prop                  |
| Response Distribution     | Unknown               |
| Link Function             | Logit                 |
| Variance Function         | _mu_**2 * (1-_mu_)**2 |
| Variance Matrix           | Diagonal              |
| Estimation Technique      | Quasi-Likelihood      |
| Degrees of Freedom Method | Residual              |

The fit statistics of the model are now expressed in terms of the log quasi-likelihood. It is computed as

$$\sum_{i=1}^9 \sum_{j=1}^{10} \int_{y_{ij}}^{\mu_{ij}} \frac{y_{ij} - t}{t^2(1-t)^2} dt$$

Twice the negative of this sum equals  $-85.74$ , which is displayed in the “Fit Statistics” table ([Output 41.4.9](#)).

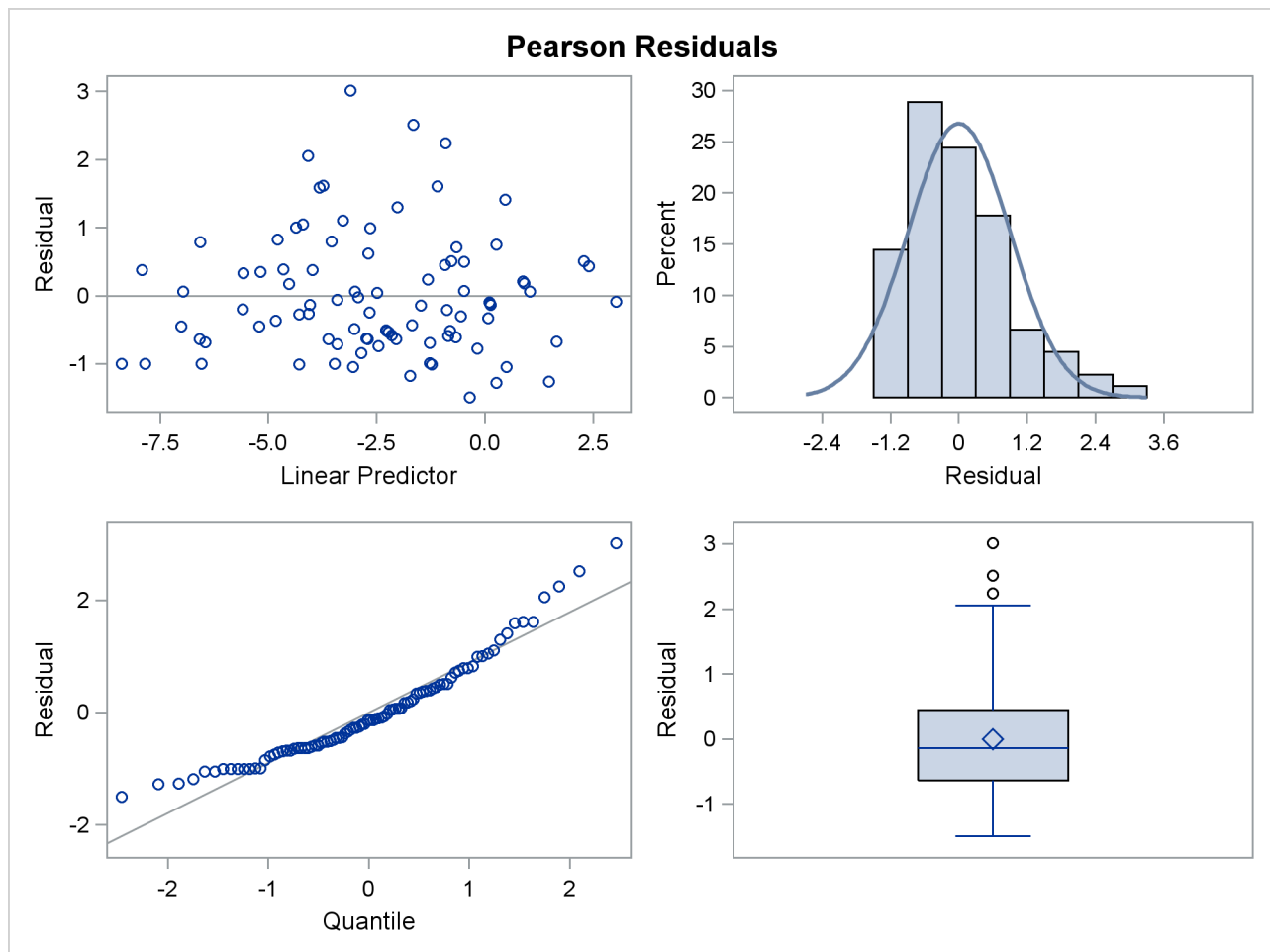
The scaled Pearson statistic is now 0.99. Inclusion of an extra scale parameter  $\phi$  would have little or no effect on the results.

**Output 41.4.9** Fit Statistics in Quasi-likelihood Analysis

| Fit Statistics                 |        |
|--------------------------------|--------|
| -2 Log Quasi-Likelihood        | -85.74 |
| Quasi-AIC (smaller is better)  | -49.74 |
| Quasi-AICC (smaller is better) | -40.11 |
| Quasi-BIC (smaller is better)  | -4.75  |
| Quasi-CAIC (smaller is better) | 13.25  |
| Quasi-HQIC (smaller is better) | -31.60 |
| Pearson Chi-Square             | 71.17  |
| Pearson Chi-Square / DF        | 0.99   |

The panel of Pearson-type residuals now shows a much more adequate distribution for the residuals and a reduction in the number of outlying residuals (Output 41.4.10).

**Output 41.4.10** Panel of Pearson-Type Residuals (Quasi-likelihood)



The least squares means are no longer ordered in size by variety (Output 41.4.11). For example,  $\text{logit}(\hat{\mu}_{.1}) > \text{logit}(\hat{\mu}_{.2})$ . Under the revised model, the second variety has a greater percentage of its leaf area covered by blotch, compared to the first variety. Varieties 5 and 6 and varieties 8 and 9 show similar reversal in ranking.

**Output 41.4.11** Variety Least Squares Means in Quasi-likelihood Analysis

| variety Least Squares Means |          |                |    |         |         |
|-----------------------------|----------|----------------|----|---------|---------|
| variety                     | Estimate | Standard Error | DF | t Value | Pr >  t |
| 1                           | -4.0453  | 0.3333         | 72 | -12.14  | <.0001  |
| 2                           | -4.5126  | 0.3333         | 72 | -13.54  | <.0001  |
| 3                           | -3.9664  | 0.3333         | 72 | -11.90  | <.0001  |
| 4                           | -3.0912  | 0.3333         | 72 | -9.27   | <.0001  |
| 5                           | -2.6927  | 0.3333         | 72 | -8.08   | <.0001  |
| 6                           | -2.7167  | 0.3333         | 72 | -8.15   | <.0001  |
| 7                           | -1.7052  | 0.3333         | 72 | -5.12   | <.0001  |
| 8                           | -0.7827  | 0.3333         | 72 | -2.35   | 0.0216  |
| 9                           | -0.9098  | 0.3333         | 72 | -2.73   | 0.0080  |
| 10                          | -0.1580  | 0.3333         | 72 | -0.47   | 0.6369  |

Interestingly, the standard errors are constant among the LS-means (Output 41.4.11) and among the LS-means differences (Output 41.4.12). This is due to the fact that for the logit link

$$\frac{\partial \mu}{\partial \eta} = \mu(1 - \mu)$$

which cancels with the square root of the variance function in the estimating equations. The analysis is thus orthogonal.

**Output 41.4.12** Variety Differences in Quasi-likelihood Analysis

| Differences of variety Least Squares Means |          |          |                |    |         |         |
|--------------------------------------------|----------|----------|----------------|----|---------|---------|
| variety                                    | _variety | Estimate | Standard Error | DF | t Value | Pr >  t |
| 2                                          | 1        | -0.4673  | 0.4714         | 72 | -0.99   | 0.3249  |
| 3                                          | 1        | 0.07885  | 0.4714         | 72 | 0.17    | 0.8676  |
| 4                                          | 1        | 0.9541   | 0.4714         | 72 | 2.02    | 0.0467  |
| 5                                          | 1        | 1.3526   | 0.4714         | 72 | 2.87    | 0.0054  |
| 6                                          | 1        | 1.3286   | 0.4714         | 72 | 2.82    | 0.0062  |
| 7                                          | 1        | 2.3401   | 0.4714         | 72 | 4.96    | <.0001  |
| 8                                          | 1        | 3.2626   | 0.4714         | 72 | 6.92    | <.0001  |
| 9                                          | 1        | 3.1355   | 0.4714         | 72 | 6.65    | <.0001  |
| 10                                         | 1        | 3.8873   | 0.4714         | 72 | 8.25    | <.0001  |

## Example 41.5: Joint Modeling of Binary and Count Data

Clustered data arise when multiple observations are collected on the same sampling or experimental unit. Often, these multiple observations refer to the same attribute measured at different points in time or space. This leads to repeated measures, longitudinal, and spatial data, which are special forms of multivariate data. A different class of multivariate data arises when the multiple observations refer to different attributes.

The data set `hernio`, created in the following `DATA` step, provides an example of a bivariate outcome variable. It reflects the condition and length of hospital stay for 32 herniorrhaphy patients. These data are based on data given by Mosteller and Tukey (1977) and reproduced in Hand et al. (1994, pp. 390, 391). The data set that follows does not contain all the covariates given in these sources. The response variables are `leave` and `los`; these denote the condition of the patient upon leaving the operating room and the length of hospital stay after the operation (in days). The variable `leave` takes on the value one if a patient experiences a routine recovery, and the value zero if postoperative intensive care was required. The binary variable `OKstatus` distinguishes patients based on their postoperative physical status (“1” implies better status).

```

data hernio;
 input patient age gender$ OKstatus leave los;
 datalines;
 1 78 m 1 0 9
 2 60 m 1 0 4
 3 68 m 1 1 7
 4 62 m 0 1 35
 5 76 m 0 0 9
 6 76 m 1 1 7
 7 64 m 1 1 5
 8 74 f 1 1 16
 9 68 m 0 1 7
 10 79 f 1 0 11
 11 80 f 0 1 4
 12 48 m 1 1 9
 13 35 f 1 1 2
 14 58 m 1 1 4
 15 40 m 1 1 3
 16 19 m 1 1 4
 17 79 m 0 0 3
 18 51 m 1 1 5
 19 57 m 1 1 8
 20 51 m 0 1 8
 21 48 m 1 1 3
 22 48 m 1 1 5
 23 66 m 1 1 8
 24 71 m 1 0 2
 25 75 f 0 0 7
 26 2 f 1 1 0
 27 65 f 1 0 16
 28 42 f 1 0 3
 29 54 m 1 0 2
 30 43 m 1 1 3
 31 4 m 1 1 3
 32 52 m 1 1 8
 ;

```

While the response variable `los` is a Poisson count variable, the response variable `leave` is a binary variable. You can perform separate analysis for the two outcomes, for example, by fitting a logistic model for the operating room exit condition and a Poisson regression model for the length of hospital stay. This, however, would ignore the correlation between the two outcomes. Intuitively, you would expect that the length of postoperative hospital stay is longer for those patients who had more tenuous exit conditions.

The following DATA step converts the data set `hernio` from the multivariate form to the univariate form. In the multivariate form the responses are stored in separate variables. The GLIMMIX procedure requires the univariate data structure.

```
data hernio_uv;
 length dist $7;
 set hernio;
 response = (leave=1);
 dist = "Binary";
 output;
 response = los;
 dist = "Poisson";
 output;
 keep patient age OKstatus response dist;
run;
```

This DATA step expands the 32 observations in the data set `hernio` into 64 observations, stacking two observations per patient. The character variable `dist` identifies the distribution that is assumed for the respective observations within a patient. The first observation for each patient corresponds to the binary response.

The following GLIMMIX statements fit a logistic regression model with two regressors (`age` and `OKStatus`) to the binary observations:

```
proc glimmix data=hernio_uv(where=(dist="Binary"));
 model response(event='1') = age OKStatus / s dist=binary;
run;
```

The `EVENT=('1')` response option requests that PROC GLIMMIX model the probability  $\Pr(\text{leave} = 1)$ —that is, the probability of routine recovery. The fit statistics and parameter estimates for this univariate analysis are shown in [Output 41.5.1](#). The coefficient for the age effect is negative ( $-0.07725$ ) and marginally significant at the 5% level ( $p = 0.0491$ ). The negative sign indicates that the probability of routine recovery decreases with age. The coefficient for the `OKStatus` variable is also negative. Its large standard error and the  $p$ -value of 0.7341 indicate, however, that this regressor is not significant.



**Output 41.5.1** Univariate Logistic Regression

| The GLIMMIX Procedure |                          |                |    |         |         |
|-----------------------|--------------------------|----------------|----|---------|---------|
| Fit Statistics        |                          |                |    |         |         |
|                       | -2 Log Likelihood        |                |    |         | 32.77   |
|                       | AIC (smaller is better)  |                |    |         | 38.77   |
|                       | AICC (smaller is better) |                |    |         | 39.63   |
|                       | BIC (smaller is better)  |                |    |         | 43.17   |
|                       | CAIC (smaller is better) |                |    |         | 46.17   |
|                       | HQIC (smaller is better) |                |    |         | 40.23   |
|                       | Pearson Chi-Square       |                |    |         | 30.37   |
|                       | Pearson Chi-Square / DF  |                |    |         | 1.05    |
| Parameter Estimates   |                          |                |    |         |         |
| Effect                | Estimate                 | Standard Error | DF | t Value | Pr >  t |
| Intercept             | 5.7694                   | 2.8245         | 29 | 2.04    | 0.0503  |
| age                   | -0.07725                 | 0.03761        | 29 | -2.05   | 0.0491  |
| OKstatus              | -0.3516                  | 1.0253         | 29 | -0.34   | 0.7341  |

Based on the univariate logistic regression analysis, you would probably want to revisit the model, examine other regressor variables, test for gender effects and interactions, and so forth. The two-regressor model is sufficient for this example. It is illustrative to trace the relative importance of the two regressors through various types of models.

The next statements fit the same regressors to the count data:

```
proc glimmix data=hernio_uv(where=(dist="Poisson"));
 model response = age OKStatus / s dist=Poisson;
run;
```

For this response, both regressors appear to make significant contributions at the 5% significance level (Output 41.5.2). The sign of the coefficient seems appropriate; the length of hospital stay should increase with patient age and be shorter for patients with better preoperative health. The magnitude of the scaled Pearson statistic (4.48) indicates, however, that there is considerable overdispersion in this model. This could be due to omitted variables or an improper distributional assumption. The importance of preoperative health status, for example, can change with a patient's age, which could call for an interaction term.

**Output 41.5.2** Univariate Poisson Regression

| The GLIMMIX Procedure |                          |                |    |         |         |
|-----------------------|--------------------------|----------------|----|---------|---------|
| Fit Statistics        |                          |                |    |         |         |
|                       | -2 Log Likelihood        |                |    |         | 215.52  |
|                       | AIC (smaller is better)  |                |    |         | 221.52  |
|                       | AICC (smaller is better) |                |    |         | 222.38  |
|                       | BIC (smaller is better)  |                |    |         | 225.92  |
|                       | CAIC (smaller is better) |                |    |         | 228.92  |
|                       | HQIC (smaller is better) |                |    |         | 222.98  |
|                       | Pearson Chi-Square       |                |    |         | 129.98  |
|                       | Pearson Chi-Square / DF  |                |    |         | 4.48    |
| Parameter Estimates   |                          |                |    |         |         |
| Effect                | Estimate                 | Standard Error | DF | t Value | Pr >  t |
| Intercept             | 1.2640                   | 0.3393         | 29 | 3.72    | 0.0008  |
| age                   | 0.01525                  | 0.004454       | 29 | 3.42    | 0.0019  |
| OKstatus              | -0.3301                  | 0.1562         | 29 | -2.11   | 0.0433  |

You can also model both responses jointly. The following statements request a multivariate analysis:

```
proc glimmix data=hernio_uv;
 class dist;
 model response(event='1') = dist dist*age dist*OKstatus /
 noint s dist=byobs(dist);
run;
```

The `DIST=BYOBS` option in the `MODEL` statement instructs the GLIMMIX procedure to examine the variable `dist` in order to identify the distribution of an observation. The variable can be character or numeric. See the `DIST=` option of the `MODEL` statement for a list of the numeric codes for the various distributions that are compatible with the `DIST=BYOBS` formulation. Because no `LINK=` option is specified, the link functions are chosen as the default links that correspond to the respective distributions. In this case, the logit link is applied to the binary observations and the log link is applied to the Poisson outcomes. The `dist` variable is also listed in the `CLASS` statement, which enables you to use interaction terms in the `MODEL` statement to vary the regression coefficients by response distribution. The `NOINT` option is used here so that the parameter estimates of the joint model are directly comparable to those in [Output 41.5.1](#) and [Output 41.5.2](#).

The “Fit Statistics” and “Parameter Estimates” tables of this bivariate estimation process are shown in [Output 41.5.3](#).

## Output 41.5.3 Bivariate Analysis – Independence

| The GLIMMIX Procedure    |         |          |                |    |         |         |
|--------------------------|---------|----------|----------------|----|---------|---------|
| Fit Statistics           |         |          |                |    |         |         |
| Description              |         | Binary   | Poisson        |    | Total   |         |
| -2 Log Likelihood        |         | 32.77    | 215.52         |    | 248.29  |         |
| AIC (smaller is better)  |         | 44.77    | 227.52         |    | 260.29  |         |
| AICC (smaller is better) |         | 48.13    | 230.88         |    | 261.77  |         |
| BIC (smaller is better)  |         | 53.56    | 236.32         |    | 273.25  |         |
| CAIC (smaller is better) |         | 59.56    | 242.32         |    | 279.25  |         |
| HQIC (smaller is better) |         | 47.68    | 230.44         |    | 265.40  |         |
| Pearson Chi-Square       |         | 30.37    | 129.98         |    | 160.35  |         |
| Pearson Chi-Square / DF  |         | 1.05     | 4.48           |    | 2.76    |         |
| Parameter Estimates      |         |          |                |    |         |         |
| Effect                   | dist    | Estimate | Standard Error | DF | t Value | Pr >  t |
| dist                     | Binary  | 5.7694   | 2.8245         | 58 | 2.04    | 0.0456  |
| dist                     | Poisson | 1.2640   | 0.3393         | 58 | 3.72    | 0.0004  |
| age*dist                 | Binary  | -0.07725 | 0.03761        | 58 | -2.05   | 0.0445  |
| age*dist                 | Poisson | 0.01525  | 0.004454       | 58 | 3.42    | 0.0011  |
| OKstatus*dist            | Binary  | -0.3516  | 1.0253         | 58 | -0.34   | 0.7329  |
| OKstatus*dist            | Poisson | -0.3301  | 0.1562         | 58 | -2.11   | 0.0389  |

The “Fit Statistics” table now contains a separate column for each response distribution, as well as an overall contribution. Because the model does not specify any random effects or R-side correlations, the log likelihoods are additive. The parameter estimates and their standard errors in this joint model are identical to those in [Output 41.5.1](#) and [Output 41.5.2](#). The *p*-values reflect the larger “sample size” in the joint analysis. Note that the coefficients would be different from the separate analyses if the *dist* variable had not been used to form interactions with the model effects.

There are two ways in which the correlations between the two responses for the same patient can be incorporated. You can induce them through shared random effects or model the dependency directly. The following statements fit a model that induces correlation:

```
proc glimmix data=hernio_uv;
 class patient dist;
 model response(event='1') = dist dist*age dist*OKstatus /
 noint s dist=byobs(dist);
 random int / subject=patient;
run;
```

Notice that the *patient* variable has been added to the **CLASS** statement and as the **SUBJECT=** effect in the **RANDOM** statement.

The “Fit Statistics” table in [Output 41.5.4](#) no longer has separate columns for each response distribution, because the data are not independent. The log (pseudo-)likelihood does not factor into additive component that correspond to distributions. Instead, it factors into components associated with subjects.

**Output 41.5.4** Bivariate Analysis – Mixed Model

| The GLIMMIX Procedure          |         |          |                |    |         |         |
|--------------------------------|---------|----------|----------------|----|---------|---------|
| Fit Statistics                 |         |          |                |    |         |         |
| -2 Res Log Pseudo-Likelihood   |         |          | 226.71         |    |         |         |
| Generalized Chi-Square         |         |          | 52.25          |    |         |         |
| Gener. Chi-Square / DF         |         |          | 0.90           |    |         |         |
| Covariance Parameter Estimates |         |          |                |    |         |         |
| Cov Parm                       | Subject | Estimate | Standard Error |    |         |         |
| Intercept                      | patient | 0.2990   | 0.1116         |    |         |         |
| Solutions for Fixed Effects    |         |          |                |    |         |         |
| Effect                         | dist    | Estimate | Standard Error | DF | t Value | Pr >  t |
| dist                           | Binary  | 5.7783   | 2.9048         | 29 | 1.99    | 0.0562  |
| dist                           | Poisson | 0.8410   | 0.5696         | 29 | 1.48    | 0.1506  |
| age*dist                       | Binary  | -0.07572 | 0.03791        | 29 | -2.00   | 0.0552  |
| age*dist                       | Poisson | 0.01875  | 0.007383       | 29 | 2.54    | 0.0167  |
| OKstatus*dist                  | Binary  | -0.4697  | 1.1251         | 29 | -0.42   | 0.6794  |
| OKstatus*dist                  | Poisson | -0.1856  | 0.3020         | 29 | -0.61   | 0.5435  |

The estimate of the variance of the random patient intercept is 0.2990, and the estimated standard error of this variance component estimate is 0.1116. There appears to be significant patient-to-patient variation in the intercepts. The estimates of the fixed effects as well as their estimated standard errors have changed from the bivariate-independence analysis (see [Output 41.5.3](#)). When the length of hospital stay and the postoperative condition are modeled jointly, the preoperative health status (variable OKStatus) no longer appears significant. Compare this result to [Output 41.5.3](#); in the separate analyses the initial health status was a significant predictor of the length of hospital stay. A further joint analysis of these data would probably remove this predictor from the model entirely.

A joint model of the second kind, where correlations are modeled directly, is fit with the following GLIMMIX statements:

```
proc glimmix data=hernio_uv;
 class patient dist;
 model response(event='1') = dist dist*age dist*OKstatus /
 noint s dist=byobs(dist);
 random _residual_ / subject=patient type=chol;
run;
```

Instead of a shared G-side random effect, an R-side covariance structure is used to model the correlations. It is important to note that this is a marginal model that models covariation on the scale of the data. The previous model involves the  $Z\mathbf{y}$  random components inside the linear predictor.

The `_RESIDUAL_` keyword instructs PROC GLIMMIX to model the R-side correlations. Because of the `SUBJECT=PATIENT` option, data from different patients are independent, and data from a single patient follow the covariance model specified with the `TYPE=` option. In this case, a generally unstructured  $2 \times 2$  covariance matrix is modeled, but in its Cholesky parameterization. This ensures that the resulting covariance matrix is at least positive semidefinite and stabilizes the numerical optimizations.

#### Output 41.5.5 Bivariate Analysis – Marginal Correlated Error Model

| The GLIMMIX Procedure          |         |          |                |    |         |         |
|--------------------------------|---------|----------|----------------|----|---------|---------|
| Fit Statistics                 |         |          |                |    |         |         |
| -2 Res Log Pseudo-Likelihood   |         |          |                |    |         | 240.98  |
| Generalized Chi-Square         |         |          |                |    |         | 58.00   |
| Gener. Chi-Square / DF         |         |          |                |    |         | 1.00    |
| Covariance Parameter Estimates |         |          |                |    |         |         |
| Cov Parm                       | Subject | Estimate | Standard Error |    |         |         |
| CHOL(1,1)                      | patient | 1.0162   | 0.1334         |    |         |         |
| CHOL(2,1)                      | patient | 0.3942   | 0.3893         |    |         |         |
| CHOL(2,2)                      | patient | 2.0819   | 0.2734         |    |         |         |
| Solutions for Fixed Effects    |         |          |                |    |         |         |
| Effect                         | dist    | Estimate | Standard Error | DF | t Value | Pr >  t |
| dist                           | Binary  | 5.6514   | 2.8283         | 26 | 2.00    | 0.0563  |
| dist                           | Poisson | 1.2463   | 0.7189         | 26 | 1.73    | 0.0948  |
| age*dist                       | Binary  | -0.07568 | 0.03765        | 26 | -2.01   | 0.0549  |
| age*dist                       | Poisson | 0.01548  | 0.009432       | 26 | 1.64    | 0.1128  |
| OKstatus*dist                  | Binary  | -0.3421  | 1.0384         | 26 | -0.33   | 0.7445  |
| OKstatus*dist                  | Poisson | -0.3253  | 0.3310         | 26 | -0.98   | 0.3349  |

The “Covariance Parameter Estimates” table in [Output 41.5.5](#) contains three entries for this model, corresponding to a  $(2 \times 2)$  covariance matrix for each patient. The Cholesky root of the  $\mathbf{R}$  matrix is

$$\mathbf{L} = \begin{bmatrix} 1.0162 & 0 \\ 0.3942 & 2.0819 \end{bmatrix}$$

so that the covariance matrix can be obtained as

$$\mathbf{LL}' = \begin{bmatrix} 1.0162 & 0 \\ 0.3942 & 2.0819 \end{bmatrix} \begin{bmatrix} 1.0162 & 0.3942 \\ 0 & 2.0819 \end{bmatrix} = \begin{bmatrix} 1.0326 & 0.4005 \\ 0.4005 & 4.4897 \end{bmatrix}$$

This is not the covariance matrix of the data, however, because the variance functions need to be accounted for.

The  $p$ -values in the “Solutions for Fixed Effects” table indicate the same pattern of significance and non-significance as in the conditional model with random patient intercepts.

---

## Example 41.6: Radial Smoothing of Repeated Measures Data

This example of a repeated measures study is taken from Diggle, Liang, and Zeger (1994, p. 100). The data consist of body weights of 27 cows, measured at 23 unequally spaced time points over a period of approximately 22 months. Following Diggle, Liang, and Zeger (1994), one animal is removed from the analysis, one observation is removed according to their Figure 5.7, and the time is shifted to start at 0 and is measured in 10-day increments. The design is a  $2 \times 2$  factorial, and the factors are the infection of an animal with *M. paratuberculosis* and whether the animal is receiving iron dosing.

The following DATA steps create the data and arrange them in univariate format.

```

data times;
 input time1-time23;
 datalines;
122 150 166 179 219 247 276 296 324 354 380 445
478 508 536 569 599 627 655 668 723 751 781
;

data cows;
 if _n_ = 1 then merge times;
 array t{23} time1 - time23;
 array w{23} weight1 - weight23;
 input cow iron infection weight1-weight23 @@;
 do i=1 to 23;
 weight = w{i};
 tpoint = (t{i}-t{1})/10;
 output;
 end;
 keep cow iron infection tpoint weight;
 datalines;
1 0 0 4.7 4.905 5.011 5.075 5.136 5.165 5.298 5.323
5.416 5.438 5.541 5.652 5.687 5.737 5.814 5.799
5.784 5.844 5.886 5.914 5.979 5.927 5.94
2 0 0 4.868 5.075 5.193 5.22 5.298 5.416 5.481 5.521
5.617 5.635 5.687 5.768 5.799 5.872 5.886 5.872
5.914 5.966 5.991 6.016 6.087 6.098 6.153
3 0 0 4.868 5.011 5.136 5.193 5.273 5.323 5.416 5.46
5.521 5.58 5.617 5.687 5.72 5.753 5.784 5.784
5.784 5.814 5.829 5.872 5.927 5.9 5.991
4 0 0 4.828 5.011 5.136 5.193 5.273 5.347 5.438 5.561
5.541 5.598 5.67 . 5.737 5.844 5.858 5.872
5.886 5.927 5.94 5.979 6.052 6.028 6.12
5 1 0 4.787 4.977 5.043 5.136 5.106 5.298 5.298 5.371
5.438 5.501 5.561 5.652 5.67 5.737 5.784 5.768
5.784 5.784 5.829 5.858 5.914 5.9 5.94

```

|    |   |   |       |       |       |       |       |       |       |       |
|----|---|---|-------|-------|-------|-------|-------|-------|-------|-------|
| 6  | 1 | 0 | 4.745 | 4.868 | 5.043 | 5.106 | 5.22  | 5.298 | 5.347 | 5.347 |
|    |   |   | 5.416 | 5.501 | 5.561 | 5.58  | 5.687 | 5.72  | 5.737 | 5.72  |
|    |   |   | 5.737 | 5.753 | 5.768 | 5.784 | 5.844 | 5.844 | 5.9   |       |
| 7  | 1 | 0 | 4.745 | 4.905 | 5.011 | 5.106 | 5.165 | 5.273 | 5.371 | 5.416 |
|    |   |   | 5.416 | 5.521 | 5.541 | 5.635 | 5.687 | 5.704 | 5.784 | 5.768 |
|    |   |   | 5.768 | 5.814 | 5.829 | 5.858 | 5.94  | 5.94  | 6.004 |       |
| 8  | 0 | 1 | 4.942 | 5.106 | 5.136 | 5.193 | 5.298 | 5.347 | 5.46  | 5.521 |
|    |   |   | 5.561 | 5.58  | 5.635 | 5.704 | 5.784 | 5.823 | 5.858 | 5.9   |
|    |   |   | 5.94  | 5.991 | 6.016 | 6.064 | 6.052 | 6.016 | 5.979 |       |
| 9  | 0 | 1 | 4.605 | 4.745 | 4.868 | 4.905 | 4.977 | 5.22  | 5.165 | 5.22  |
|    |   |   | 5.22  | 5.247 | 5.298 | 5.416 | 5.501 | 5.521 | 5.58  | 5.58  |
|    |   |   | 5.635 | 5.67  | 5.72  | 5.753 | 5.799 | 5.829 | 5.858 |       |
| 10 | 0 | 1 | 4.7   | 4.868 | 4.905 | 4.977 | 5.011 | 5.106 | 5.165 | 5.22  |
|    |   |   | 5.22  | 5.22  | 5.273 | 5.384 | 5.438 | 5.438 | 5.501 | 5.501 |
|    |   |   | 5.541 | 5.598 | 5.58  | 5.635 | 5.687 | 5.72  | 5.704 |       |
| 11 | 0 | 1 | 4.828 | 5.011 | 5.075 | 5.165 | 5.247 | 5.323 | 5.394 | 5.46  |
|    |   |   | 5.46  | 5.501 | 5.541 | 5.609 | 5.687 | 5.704 | 5.72  | 5.704 |
|    |   |   | 5.704 | 5.72  | 5.737 | 5.768 | 5.858 | 5.9   | 5.94  |       |
| 12 | 0 | 1 | 4.7   | 4.828 | 4.905 | 5.011 | 5.075 | 5.165 | 5.247 | 5.298 |
|    |   |   | 5.298 | 5.323 | 5.416 | 5.505 | 5.561 | 5.58  | 5.561 | 5.635 |
|    |   |   | 5.687 | 5.72  | 5.72  | 5.737 | 5.784 | 5.814 | 5.799 |       |
| 13 | 0 | 1 | 4.828 | 5.011 | 5.075 | 5.136 | 5.22  | 5.273 | 5.347 | 5.416 |
|    |   |   | 5.438 | 5.416 | 5.521 | 5.628 | 5.67  | 5.687 | 5.72  | 5.72  |
|    |   |   | 5.799 | 5.858 | 5.872 | 5.914 | 5.94  | 5.991 | 6.016 |       |
| 14 | 0 | 1 | 4.828 | 4.942 | 5.011 | 5.075 | 5.075 | 5.22  | 5.273 | 5.298 |
|    |   |   | 5.323 | 5.298 | 5.394 | 5.489 | 5.541 | 5.58  | 5.617 | 5.67  |
|    |   |   | 5.704 | 5.753 | 5.768 | 5.814 | 5.872 | 5.927 | 5.927 |       |
| 15 | 0 | 1 | 4.745 | 4.905 | 4.977 | 5.075 | 5.193 | 5.22  | 5.298 | 5.323 |
|    |   |   | 5.394 | 5.394 | 5.438 | 5.583 | 5.617 | 5.652 | 5.687 | 5.72  |
|    |   |   | 5.753 | 5.768 | 5.814 | 5.844 | 5.886 | 5.886 | 5.886 |       |
| 16 | 0 | 1 | 4.7   | 4.868 | 5.011 | 5.043 | 5.106 | 5.165 | 5.247 | 5.298 |
|    |   |   | 5.347 | 5.371 | 5.438 | 5.455 | 5.617 | 5.635 | 5.704 | 5.737 |
|    |   |   | 5.784 | 5.768 | 5.814 | 5.844 | 5.886 | 5.94  | 5.927 |       |
| 17 | 1 | 1 | 4.605 | 4.787 | 4.828 | 4.942 | 5.011 | 5.136 | 5.22  | 5.247 |
|    |   |   | 5.273 | 5.247 | 5.347 | 5.366 | 5.416 | 5.46  | 5.541 | 5.481 |
|    |   |   | 5.501 | 5.635 | 5.652 | 5.598 | 5.635 | 5.635 | 5.598 |       |
| 18 | 1 | 1 | 4.828 | 4.977 | 5.011 | 5.136 | 5.273 | 5.298 | 5.371 | 5.46  |
|    |   |   | 5.416 | 5.416 | 5.438 | 5.557 | 5.617 | 5.67  | 5.72  | 5.72  |
|    |   |   | 5.799 | 5.858 | 5.886 | 5.914 | 5.979 | 6.004 | 6.028 |       |
| 19 | 1 | 1 | 4.7   | 4.905 | 4.942 | 5.011 | 5.043 | 5.136 | 5.193 | 5.193 |
|    |   |   | 5.247 | 5.22  | 5.323 | 5.338 | 5.371 | 5.394 | 5.438 | 5.416 |
|    |   |   | 5.501 | 5.561 | 5.541 | 5.58  | 5.652 | 5.67  | 5.704 |       |
| 20 | 1 | 1 | 4.745 | 4.905 | 4.977 | 5.043 | 5.136 | 5.273 | 5.347 | 5.394 |
|    |   |   | 5.416 | 5.394 | 5.521 | 5.617 | 5.617 | 5.617 | 5.67  | 5.635 |
|    |   |   | 5.652 | 5.687 | 5.652 | 5.617 | 5.687 | 5.768 | 5.814 |       |
| 21 | 1 | 1 | 4.787 | 4.942 | 4.977 | 5.106 | 5.165 | 5.247 | 5.323 | 5.416 |
|    |   |   | 5.394 | 5.371 | 5.438 | 5.521 | 5.521 | 5.561 | 5.635 | 5.617 |
|    |   |   | 5.687 | 5.72  | 5.737 | 5.737 | 5.768 | 5.768 | 5.704 |       |
| 22 | 1 | 1 | 4.605 | 4.828 | 4.828 | 4.977 | 5.043 | 5.165 | 5.22  | 5.273 |
|    |   |   | 5.247 | 5.22  | 5.298 | 5.375 | 5.371 | 5.416 | 5.501 | 5.501 |
|    |   |   | 5.521 | 5.561 | 5.617 | 5.635 | 5.72  | 5.737 | 5.768 |       |
| 23 | 1 | 1 | 4.7   | 4.905 | 5.011 | 5.075 | 5.106 | 5.22  | 5.22  | 5.298 |
|    |   |   | 5.323 | 5.347 | 5.416 | 5.472 | 5.501 | 5.541 | 5.598 | 5.598 |
|    |   |   | 5.598 | 5.652 | 5.67  | 5.704 | 5.737 | 5.768 | 5.784 |       |

```

24 1 1 4.745 4.942 5.011 5.075 5.106 5.247 5.273 5.323
 5.347 5.371 5.416 5.481 5.501 5.541 5.598 5.598
 5.635 5.687 5.704 5.72 5.829 5.844 5.9
25 1 1 4.654 4.828 4.828 4.977 4.977 5.043 5.136 5.165
 5.165 5.165 5.193 5.204 5.22 5.273 5.371 5.347
 5.46 5.58 5.635 5.67 5.753 5.799 5.844
26 1 1 4.828 4.977 5.011 5.106 5.165 5.22 5.273 5.323
 5.371 5.394 5.46 5.576 5.652 5.617 5.687 5.67
 5.72 5.784 5.784 5.784 5.829 5.814 5.844
;

```

The mean response profiles of the cows are not of particular interest; what matters are inferences about the Iron effect, the Infection effect, and their interaction. Nevertheless, the body weight of the cows changes over the 22-month period, and you need to account for these changes in the analysis. A reasonable approach is to apply the approximate low-rank smoother to capture the trends over time. This approach frees you from having to stipulate a parametric model for the response trajectories over time. In addition, you can test hypotheses about the smoothing parameter; for example, whether it should be varied by treatment.

The following statements fit a model with a  $2 \times 2$  factorial treatment structure and smooth trends over time, choosing the Newton-Raphson algorithm with ridging for the optimization:

```

proc glimmix data=cows;
 t2 = tpoint / 100;
 class cow iron infection;
 model weight = iron infection iron*infection tpoint;
 random t2 / type=rsmooth subject=cow
 knotmethod=kdtree(bucket=100 knotinfo);
 output out=gmxout pred(blup)=pred;
 nloptions tech=newrap;
run;

```

The continuous time effect appears in both the **MODEL** statement (tpoint) and the **RANDOM** statement (t2). Because the variance of the radial smoothing component depends on the temporal metric, the time scale was rescaled for the **RANDOM** effect to move the parameter estimate away from the boundary. The knots of the radial smoother are selected as the vertices of a  $k$ -d tree. Specifying **BUCKET=100** sets the bucket size of the tree to  $b = 100$ . Because measurements at each time point are available for 26 (or 25) cows, this groups approximately four time points in a single bucket. The **KNOTINFO** keyword of the **KNOTMETHOD=** option requests a printout of the knot locations for the radial smoother. The **OUTPUT** statement saves the predictions of the mean of each observations to the data set gmxout. Finally, the **TECH=NEWRAP** option in the **NLOPTIONS** statement specifies the Newton-Raphson algorithm for the optimization technique.

The “Class Level Information” table lists the number of levels of the Cow, Iron, and Infection effects (Output 41.6.1).



**Output 41.6.1** Model Information and Class Levels in Repeated Measures Analysis

| The GLIMMIX Procedure      |                               |                                                                         |
|----------------------------|-------------------------------|-------------------------------------------------------------------------|
| Model Information          |                               |                                                                         |
| Data Set                   | WORK.COWS                     |                                                                         |
| Response Variable          | weight                        |                                                                         |
| Response Distribution      | Gaussian                      |                                                                         |
| Link Function              | Identity                      |                                                                         |
| Variance Function          | Default                       |                                                                         |
| Variance Matrix Blocked By | cow                           |                                                                         |
| Estimation Technique       | Restricted Maximum Likelihood |                                                                         |
| Degrees of Freedom Method  | Containment                   |                                                                         |
| Class Level Information    |                               |                                                                         |
| Class                      | Levels                        | Values                                                                  |
| cow                        | 26                            | 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18<br>19 20 21 22 23 24 25 26 |
| iron                       | 2                             | 0 1                                                                     |
| infection                  | 2                             | 0 1                                                                     |

The “Radial Smoother Knots for RSmooth(t2)” table displays the knots computed from the vertices of the t2 *k*-d tree (Output 41.6.2). Notice that knots are spaced unequally and that the extreme time points are among the knot locations. The “Number of Observations” table shows that one observation was not used in the analysis. The 12th observation for cow 4 has a missing value.

**Output 41.6.2** Knot Information and Number of Observations

| Radial Smoother<br>Knots for<br>RSmooth(t2) |         |     |
|---------------------------------------------|---------|-----|
| Knot<br>Number                              | t2      |     |
| 1                                           | 0       |     |
| 2                                           | 0.04400 |     |
| 3                                           | 0.1250  |     |
| 4                                           | 0.2020  |     |
| 5                                           | 0.3230  |     |
| 6                                           | 0.4140  |     |
| 7                                           | 0.5050  |     |
| 8                                           | 0.6010  |     |
| 9                                           | 0.6590  |     |
| Number of Observations Read                 |         | 598 |
| Number of Observations Used                 |         | 597 |

The “Dimensions” table shows that the model contains only two covariance parameters, the G-side variance of the spline coefficients ( $\sigma^2$ ) and the R-side scale parameter ( $\phi$ , [Output 41.6.3](#)). For each subject (cow), there are nine columns in the  $\mathbf{Z}$  matrix, one per knot location. The GLIMMIX procedure processes these data by subjects (cows).

**Output 41.6.3** Dimensions Information in Repeated Measures Analysis

| Dimensions               |    |
|--------------------------|----|
| G-side Cov. Parameters   | 1  |
| R-side Cov. Parameters   | 1  |
| Columns in X             | 10 |
| Columns in Z per Subject | 9  |
| Subjects (Blocks in V)   | 26 |
| Max Obs per Subject      | 23 |

The “Optimization Information” table displays information about the optimization process. Because fixed effects and the residual scale parameter can be profiled from the optimization, the iterative algorithm involves only a single covariance parameter, the variance of the spline coefficients ([Output 41.6.4](#)).

**Output 41.6.4** Optimization Information in Repeated Measures Analysis

| Optimization Information   |                |
|----------------------------|----------------|
| Optimization Technique     | Newton-Raphson |
| Parameters in Optimization | 1              |
| Lower Boundaries           | 1              |
| Upper Boundaries           | 0              |
| Fixed Effects              | Profiled       |
| Residual Variance          | Profiled       |
| Starting From              | Data           |

After 11 iterations, the optimization process terminates ([Output 41.6.5](#)). In this case, the absolute gradient convergence criterion was met.

**Output 41.6.5** Iteration History and Convergence Status

| Iteration History |          |             |                    |              |              |
|-------------------|----------|-------------|--------------------|--------------|--------------|
| Iteration         | Restarts | Evaluations | Objective Function | Change       | Max Gradient |
| 0                 | 0        | 4           | -1302.549272       | .            | 20.33682     |
| 1                 | 0        | 3           | -1451.587367       | 149.03809501 | 9.940495     |
| 2                 | 0        | 3           | -1585.640946       | 134.05357887 | 4.71531      |
| 3                 | 0        | 3           | -1694.516203       | 108.87525722 | 2.176741     |
| 4                 | 0        | 3           | -1775.290458       | 80.77425512  | 0.978577     |
| 5                 | 0        | 3           | -1829.966584       | 54.67612585  | 0.425724     |
| 6                 | 0        | 3           | -1862.878184       | 32.91160012  | 0.175992     |
| 7                 | 0        | 3           | -1879.329133       | 16.45094875  | 0.066061     |
| 8                 | 0        | 3           | -1885.175082       | 5.84594887   | 0.020137     |
| 9                 | 0        | 3           | -1886.238032       | 1.06295071   | 0.00372      |
| 10                | 0        | 3           | -1886.288519       | 0.05048659   | 0.000198     |
| 11                | 0        | 3           | -1886.288673       | 0.00015425   | 6.364E-7     |

Convergence criterion (ABSGCONV=0.00001) satisfied.

The generalized chi-square statistic in the “Fit Statistics” table is small for this model (Output 41.6.6). There is very little residual variation. The radial smoother is associated with 433.55 residual degrees of freedom, computed as 597 minus the trace of the smoother matrix.

**Output 41.6.6** Fit Statistics in Repeated Measures Analysis

| Fit Statistics           |          |
|--------------------------|----------|
| -2 Res Log Likelihood    | -1886.29 |
| AIC (smaller is better)  | -1882.29 |
| AICC (smaller is better) | -1882.27 |
| BIC (smaller is better)  | -1879.77 |
| CAIC (smaller is better) | -1877.77 |
| HQIC (smaller is better) | -1881.56 |
| Generalized Chi-Square   | 0.47     |
| Gener. Chi-Square / DF   | 0.00     |
| Radial Smoother df(res)  | 433.55   |

The “Covariance Parameter Estimates” table in Output 41.6.7 displays the estimates of the covariance parameters. The variance of the random spline coefficients is estimated as  $\hat{\sigma}^2 = 0.5961$ , and the scale parameter (=residual variance) estimate is  $\hat{\phi} = 0.0008$ .

**Output 41.6.7** Estimated Covariance Parameters

| Covariance Parameter Estimates |         |          |                |
|--------------------------------|---------|----------|----------------|
| Cov Parm                       | Subject | Estimate | Standard Error |
| Var[RSmooth(t2)]               | cow     | 0.5961   | 0.08144        |
| Residual                       |         | 0.000800 | 0.000059       |

The “Type III Tests of Fixed Effects” table displays  $F$  tests for the fixed effects in the `MODEL` statement (Output 41.6.8). There is a strong infection effect as well as the absence of an interaction between infection with *M. paratuberculosis* and iron dosing. It is important to note, however, that the interpretation of these tests rests on the assumption that the random effects in the mixed model have zero mean; in this case, the radial smoother coefficients.

**Output 41.6.8** Tests of Fixed Effects

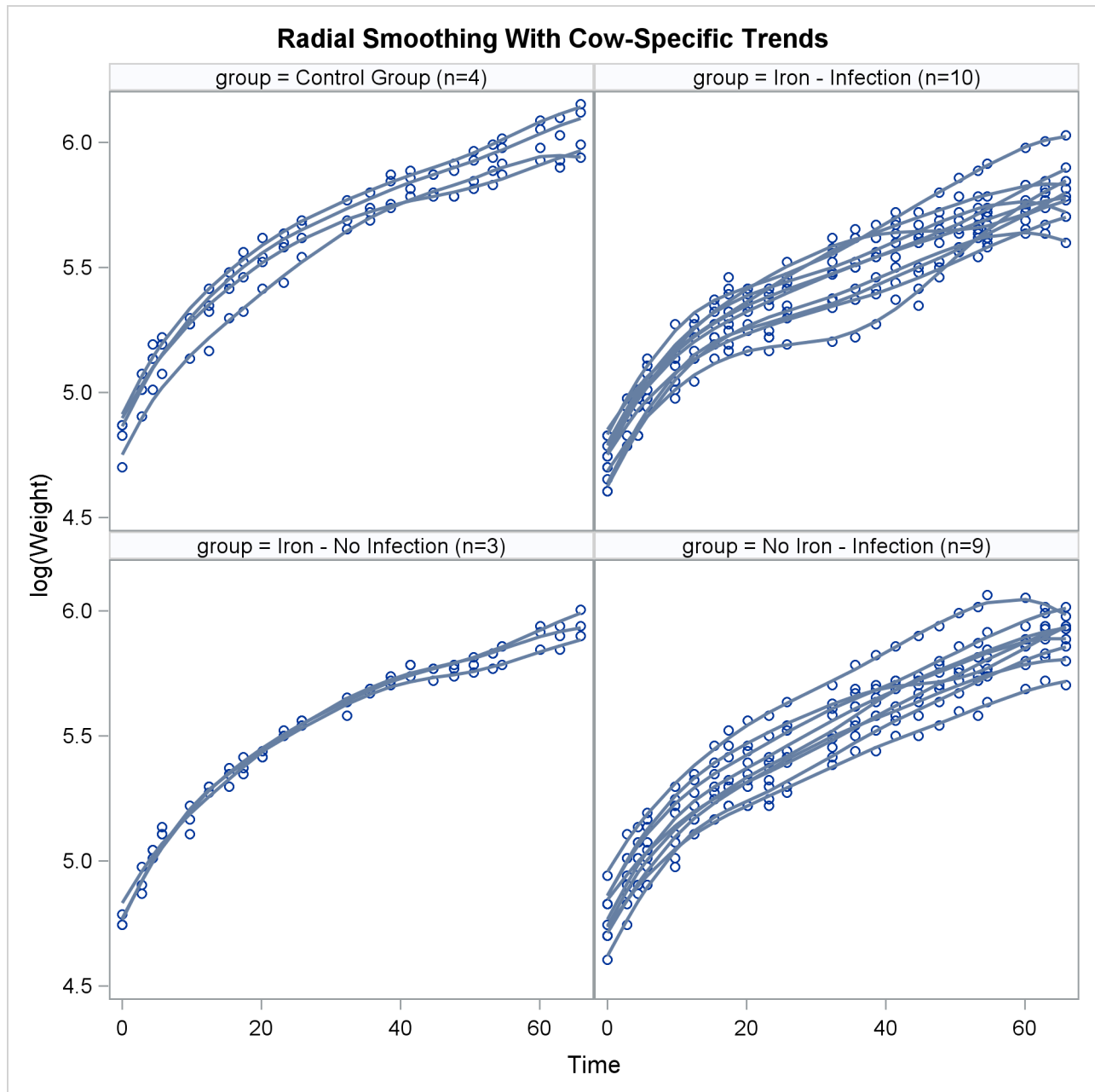
| Type III Tests of Fixed Effects |        |        |         |        |
|---------------------------------|--------|--------|---------|--------|
| Effect                          | Num DF | Den DF | F Value | Pr > F |
| iron                            | 1      | 358    | 3.59    | 0.0588 |
| infection                       | 1      | 358    | 21.16   | <.0001 |
| iron*infection                  | 1      | 358    | 0.09    | 0.7637 |
| tpoint                          | 1      | 358    | 53.88   | <.0001 |

A graph of the observed data and fitted profiles in the four groups is produced with the following statements (Output 41.6.9):

```
data plot;
 set gmxout;
 length group $26;
 if (iron=0) and (infection=0) then group='Control Group (n=4)';
 else if (iron=1) and (infection=0) then group='Iron - No Infection (n=3)';
 else if (iron=0) and (infection=1) then group='No Iron - Infection (n=9)';
 else group = 'Iron - Infection (n=10)';
run;
proc sort data=plot; by group cow;
run;

proc sgpanel data=plot noautolegend;
 title 'Radial Smoothing With Cow-Specific Trends';
 label tpoint='Time' weight='log(Weight)';
 panelby group / columns=2 rows=2;
 scatter x=tpoint y=weight;
 series x=tpoint y=pred / group=cow lineattrs=GraphFit;
run;
```

Output 41.6.9 Observed and Predicted Profiles



The trends are quite smooth, and you can see how the radial smoother adapts to the cow-specific profile. This is the reason for the small scale parameter estimate,  $\hat{\phi} = 0.008$ . Comparing the panels at the top to the panels at the bottom of [Output 41.6.9](#) reveals the effect of Infection. A comparison of the panels on the left to those on the right indicates the weak Iron effect.

The smoothing parameter in this analysis is related to the covariance parameter estimates. Because there is only one radial smoothing variance component, the amount of smoothing is the same in all four treatment groups. To test whether the smoothing parameter should be varied by group, you can refine the analysis of the previous model. The following statements fit the same general model, but they vary the covariance parameters by the levels of the Iron\*Infection interaction. This is accomplished with the **GROUP=** option in the **RANDOM** statement.

```
ods select OptInfo FitStatistics CovParms;
proc glimmix data=cows;
 t2 = tpoint / 100;
 class cow iron infection;
 model weight = iron infection iron*infection tpoint;
 random t2 / type=rsmooth
 subject=cow
 group=iron*infection
 knotmethod=kdtree(bucket=100);
 nloptions tech=newrap;
run;
```

All observations that have the same value combination of the Iron and Infection effects share the same covariance parameter. As a consequence, you obtain different smoothing parameters result in the four groups.

In [Output 41.6.10](#), the “Optimization Information” table shows that there are now four covariance parameters in the optimization, one spline coefficient variance for each group.

#### Output 41.6.10 Analysis with Group-Specific Smoothing Parameter

| The GLIMMIX Procedure      |                |
|----------------------------|----------------|
| Optimization Information   |                |
| Optimization Technique     | Newton-Raphson |
| Parameters in Optimization | 4              |
| Lower Boundaries           | 4              |
| Upper Boundaries           | 0              |
| Fixed Effects              | Profiled       |
| Residual Variance          | Profiled       |
| Starting From              | Data           |
| Fit Statistics             |                |
| -2 Res Log Likelihood      | -1887.95       |
| AIC (smaller is better)    | -1877.95       |
| AICC (smaller is better)   | -1877.85       |
| BIC (smaller is better)    | -1871.66       |
| CAIC (smaller is better)   | -1866.66       |
| HQIC (smaller is better)   | -1876.14       |
| Generalized Chi-Square     | 0.48           |
| Gener. Chi-Square / DF     | 0.00           |
| Radial Smoother df(res)    | 434.72         |

Output 41.6.10 *continued*

| Covariance Parameter Estimates |         |                |     |          |                |
|--------------------------------|---------|----------------|-----|----------|----------------|
| Cov Parm                       | Subject | Group          |     | Estimate | Standard Error |
| Var[RSmooth(t2)]               | cow     | iron*infection | 0 0 | 0.4788   | 0.1922         |
| Var[RSmooth(t2)]               | cow     | iron*infection | 0 1 | 0.5152   | 0.1182         |
| Var[RSmooth(t2)]               | cow     | iron*infection | 1 0 | 0.4904   | 0.2195         |
| Var[RSmooth(t2)]               | cow     | iron*infection | 1 1 | 0.7105   | 0.1409         |
| Residual                       |         |                |     | 0.000807 | 0.000060       |

Varying this variance component by groups has changed the  $-2$  Res Log Likelihood from  $-1886.29$  to  $-1887.95$  (Output 41.6.10). The difference, 1.66, can be viewed (asymptotically) as the realization of a chi-square random variable with three degrees of freedom. The difference is not significant ( $p = 0.64586$ ). The “Covariance Parameter Estimates” table confirms that the estimates of the spline coefficient variance are quite similar in the four groups, ranging from 0.4788 to 0.7105.

Finally, you can apply a different technique for varying the temporal trends among the cows. From Output 41.6.9 it appears that an assumption of parallel trends within groups might be reasonable. In other words, you can fit a model in which the “overall” trend over time in each group is modeled nonparametrically, and this trend is shifted up or down to capture the behavior of the individual cow. You can accomplish this with the following statements:

```
ods select FitStatistics CovParms;
proc glimmix data=cows;
 t2 = tpoint / 100;
 class cow iron infection;
 model weight = iron infection iron*infection tpoint;
 random t2 / type=rsmooth
 subject=iron*infection
 knotmethod=kdtree(bucket=100);
 random intercept / subject=cow;
 output out=gmxout pred(blup)=pred;
 nloptions tech=newrap;
run;
```

There are now two subject effects in this analysis. The first **RANDOM** statement applies the radial smoothing and identifies the experimental conditions as the subject. For each condition, a separate realization of the random spline coefficients is obtained. The second **RANDOM** statement adds a random intercept to the trend for each cow. This random intercept results in the parallel shift of the trends over time.

Results from this analysis are shown in [Output 41.6.11](#).

**Output 41.6.11** Analysis with Parallel Shifts

| The GLIMMIX Procedure          |                |          |                |
|--------------------------------|----------------|----------|----------------|
| Fit Statistics                 |                |          |                |
| -2 Res Log Likelihood          |                | -1788.52 |                |
| AIC (smaller is better)        |                | -1782.52 |                |
| AICC (smaller is better)       |                | -1782.48 |                |
| BIC (smaller is better)        |                | -1788.52 |                |
| CAIC (smaller is better)       |                | -1785.52 |                |
| HQIC (smaller is better)       |                | -1788.52 |                |
| Generalized Chi-Square         |                | 1.17     |                |
| Gener. Chi-Square / DF         |                | 0.00     |                |
| Radial Smoother df(res)        |                | 547.21   |                |
| Covariance Parameter Estimates |                |          |                |
| Cov Parm                       | Subject        | Estimate | Standard Error |
| Var[RSmooth(t2)]               | iron*infection | 0.5398   | 0.1940         |
| Intercept                      | cow            | 0.007122 | 0.002173       |
| Residual                       |                | 0.001976 | 0.000121       |

Because the parallel shift model is not nested within either one of the previous models, the models cannot be compared with a likelihood ratio test. However, you can draw on the other fit statistics.

All statistics indicate that this model does not fit the data as well as the initial model that varies the spline coefficients by cow. The Pearson chi-square statistic is more than twice as large as in the previous model, indicating much more residual variation in the fit. On the other hand, this model generates only four sets of spline coefficients, one for each treatment group, and thus retains more residual degrees of freedom.

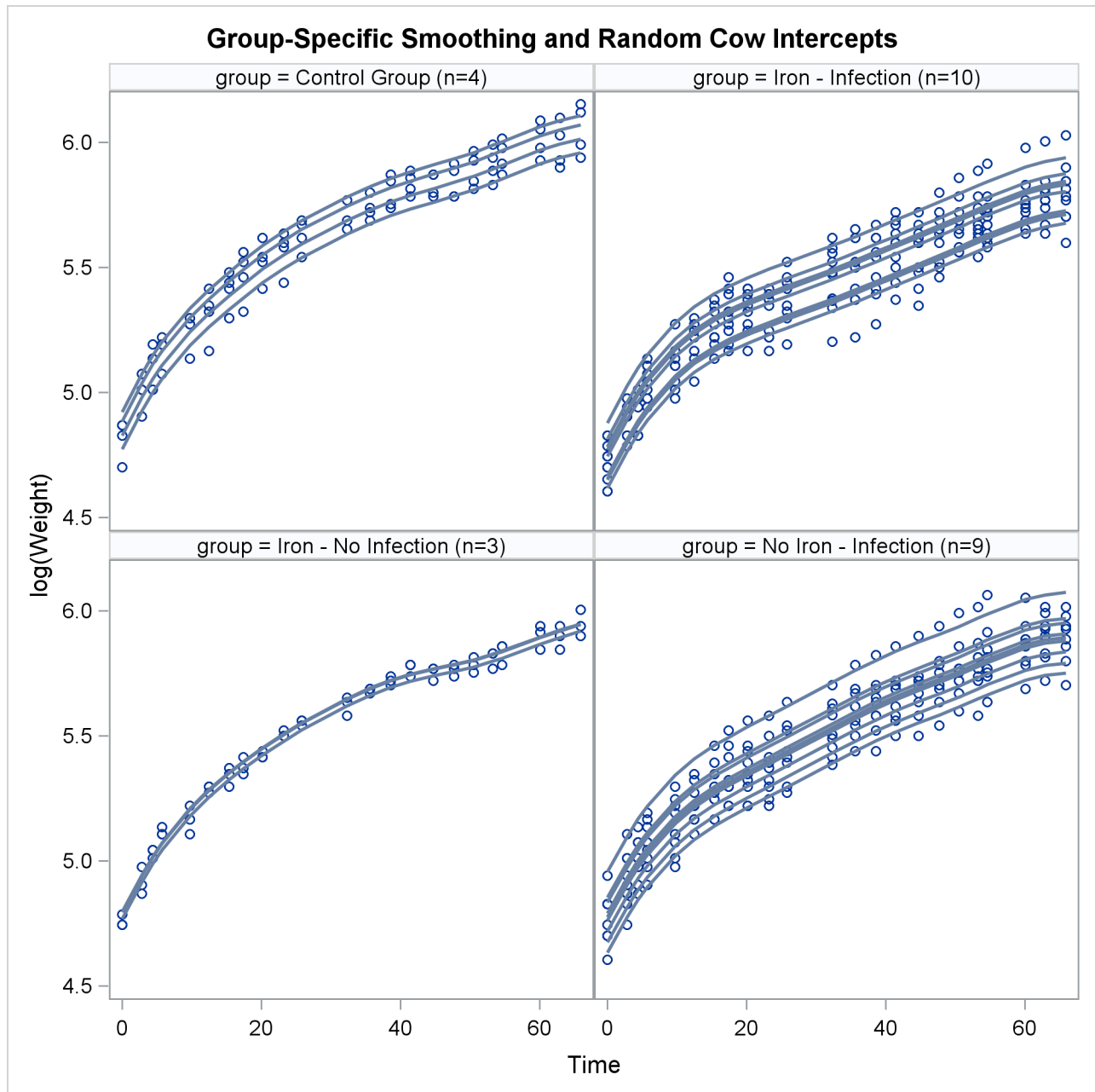
The “Covariance Parameter Estimates” table in [Output 41.6.11](#) displays the solutions for the covariance parameters. The estimate of the variance of the spline coefficients is not that different from the estimate obtained in the first model (0.5961). The residual variance, however, has more than doubled.

Using similar SAS statements as previously, you can produce a plot of the observed and predicted profiles ([Output 41.6.12](#)).

The parallel shifts of the nonparametric smooths are clearly visible in [Output 41.6.12](#). In the groups receiving only iron or only an infection, the parallel lines assumption holds quite well. In the control group and the group receiving iron and the infection, the parallel shift assumption does not hold as well. Two of the profiles in the iron-only group are nearly indistinguishable.



Output 41.6.12 Observed and Predicted Profiles



This example demonstrates that mixed model smoothing techniques can be applied not only to achieve scatter plot smoothing, but also to longitudinal or repeated measures data. You can then use the **SUBJECT=** option in the **RANDOM** statement to obtain independent sets of spline coefficients for different subjects, and the **GROUP=** option in the **RANDOM** statement to vary the degree of smoothing across groups. Also, radial smoothers can be combined with other random effects. For the data considered here, the appropriate model is one with a single smoothing parameter for all treatment group and cow-specific spline coefficients.

## Example 41.7: Isotonic Contrasts for Ordered Alternatives

Dose response studies often focus on testing for monotone increasing or decreasing behavior in the mean values of the dependent variable. Hirotsu and Srivastava (2000) demonstrate one approach by using data that originally appeared in Moriguchi (1976). The data, which follow, consist of ferrite cores subjected to four increasing temperatures. The response variable is the magnetic force of each core.

```
data FerriteCores;
 do Temp = 1 to 4;
 do rep = 1 to 5; drop rep;
 input MagneticForce @@;
 output;
 end;
 end;
 datalines;
10.8 9.9 10.7 10.4 9.7
10.7 10.6 11.0 10.8 10.9
11.9 11.2 11.0 11.1 11.3
11.4 10.7 10.9 11.3 11.7
;
```

It is of interest to test whether the magnetic force of the cores rises monotonically with temperature. The approach of Hirotsu and Srivastava (2000) depends on the lower confidence limits of the *isotonic contrasts* of the force means at each temperature, adjusted for multiplicity. The corresponding isotonic contrast compares the average of a particular group and the preceding groups with the average of the succeeding groups. You can compute adjusted confidence intervals for isotonic contrasts by using the `LSMESTIMATE` statement.

The following statements request an analysis of the `FerriteCores` data as a one-way design and multiplicity-adjusted lower confidence limits for the isotonic contrasts. For the multiplicity adjustment, the `LSMESTIMATE` statement employs simulation, which provides adjusted  $p$ -values and lower confidence limits that are exact up to Monte Carlo error.

```
proc glimmix data=FerriteCores;
 class Temp;
 model MagneticForce = Temp;
 lsestimate Temp
 'avg(1:1)<avg(2:4)' -3 1 1 1 divisor=3,
 'avg(1:2)<avg(3:4)' -1 -1 1 1 divisor=2,
 'avg(1:3)<avg(4:4)' -1 -1 -1 3 divisor=3
 / adjust=simulate(seed=1) cl upper;
 ods select LSMestimates;
run;
```

The results are shown in [Output 41.7.1](#).

**Output 41.7.1** Analysis of LS-Means with Isotonic Contrasts

| The GLIMMIX Procedure                  |                     |          |                |    |         |       |        |
|----------------------------------------|---------------------|----------|----------------|----|---------|-------|--------|
| Least Squares Means Estimates          |                     |          |                |    |         |       |        |
| Adjustment for Multiplicity: Simulated |                     |          |                |    |         |       |        |
| Effect                                 | Label               | Estimate | Standard Error | DF | t Value | Tails | Pr > t |
| Temp                                   | avg(1:1) < avg(2:4) | 0.8000   | 0.1906         | 16 | 4.20    | Upper | 0.0003 |
| Temp                                   | avg(1:2) < avg(3:4) | 0.7000   | 0.1651         | 16 | 4.24    | Upper | 0.0003 |
| Temp                                   | avg(1:3) < avg(4:4) | 0.4000   | 0.1906         | 16 | 2.10    | Upper | 0.0260 |

| Least Squares Means Estimates          |                     |        |       |         |       |
|----------------------------------------|---------------------|--------|-------|---------|-------|
| Adjustment for Multiplicity: Simulated |                     |        |       |         |       |
| Effect                                 | Label               | Adj P  | Alpha | Lower   | Upper |
| Temp                                   | avg(1:1) < avg(2:4) | 0.0010 | 0.05  | 0.4672  | Infty |
| Temp                                   | avg(1:2) < avg(3:4) | 0.0009 | 0.05  | 0.4118  | Infty |
| Temp                                   | avg(1:3) < avg(4:4) | 0.0625 | 0.05  | 0.06721 | Infty |

| Least Squares Means Estimates          |                     |           |           |  |  |
|----------------------------------------|---------------------|-----------|-----------|--|--|
| Adjustment for Multiplicity: Simulated |                     |           |           |  |  |
| Effect                                 | Label               | Adj Lower | Adj Upper |  |  |
| Temp                                   | avg(1:1) < avg(2:4) | 0.3771    | Infty     |  |  |
| Temp                                   | avg(1:2) < avg(3:4) | 0.3337    | Infty     |  |  |
| Temp                                   | avg(1:3) < avg(4:4) | -0.02291  | Infty     |  |  |

With an adjusted  $p$ -value of 0.001, the magnetic force at the first temperature is significantly less than the average of the other temperatures. Likewise, the average of the first two temperatures is significantly less than the average of the last two ( $p = 0.0009$ ). However, the magnetic force at the last temperature is not significantly greater than the average magnetic force of the others ( $p = 0.0625$ ). These results indicate a significant monotone increase over the first three temperatures, but not across all four temperatures.

**Example 41.8: Adjusted Covariance Matrices of Fixed Effects**

The following data are from Pothoff and Roy (1964) and consist of growth measurements for 11 girls and 16 boys at ages 8, 10, 12, and 14. Some of the observations are suspect (for example, the third observation for person 20); however, all of the data are used here for comparison purposes.

```
data pr;
 input child gender$ y1 y2 y3 y4;
 array yy y1-y4;
 do time=1 to 4;
 age = time*2 + 6;
 y = yy{time};
 output;
 end;
 drop y1-y4;
```

```

datalines;
1 F 21.0 20.0 21.5 23.0
2 F 21.0 21.5 24.0 25.5
3 F 20.5 24.0 24.5 26.0
4 F 23.5 24.5 25.0 26.5
5 F 21.5 23.0 22.5 23.5
6 F 20.0 21.0 21.0 22.5
7 F 21.5 22.5 23.0 25.0
8 F 23.0 23.0 23.5 24.0
9 F 20.0 21.0 22.0 21.5
10 F 16.5 19.0 19.0 19.5
11 F 24.5 25.0 28.0 28.0
12 M 26.0 25.0 29.0 31.0
13 M 21.5 22.5 23.0 26.5
14 M 23.0 22.5 24.0 27.5
15 M 25.5 27.5 26.5 27.0
16 M 20.0 23.5 22.5 26.0
17 M 24.5 25.5 27.0 28.5
18 M 22.0 22.0 24.5 26.5
19 M 24.0 21.5 24.5 25.5
20 M 23.0 20.5 31.0 26.0
21 M 27.5 28.0 31.0 31.5
22 M 23.0 23.0 23.5 25.0
23 M 21.5 23.5 24.0 28.0
24 M 17.0 24.5 26.0 29.5
25 M 22.5 25.5 25.5 26.0
26 M 23.0 24.5 26.0 30.0
27 M 22.0 21.5 23.5 25.0
;

```

Jennrich and Schluchter (1986) analyze these data with various models for the fixed effects and the covariance structure. The strategy here is to fit a growth curve model for the boys and girls and to account for subject-to-subject variation through G-side random effects. In addition, serial correlation among the observations within each child is accounted for by a time series process. The data are assumed to be Gaussian, and their  $-2$  restricted log likelihood is minimized to estimate the model parameters.

The following statements fit a mixed model in which a separate growth curve is assumed for each gender:

```

proc glimmix data=pr;
 class child gender time;
 model y = gender age gender*age / covb(details) ddfm=kr;
 random intercept age / type=chol sub=child;
 random time / subject=child type=ar(1) residual;
 ods select ModelInfo CovB CovBModelBased CovBDetails;
run;

```

The growth curve for an individual child differs from the gender-specific trend because of a random intercept and a random slope. The two G-side random effects are assumed to be correlated. Their unstructured covariance matrix is parameterized in terms of the Cholesky root to guarantee a positive (semi-)definite estimate. An AR(1) covariance structure is modeled for the observations over time for each child. Notice the **RESIDUAL** option in the second **RANDOM** statement. It identifies this as an R-side random effect.

The **DDFM=KR** option requests that the covariance matrix of the fixed-effect parameter estimates and denominator degrees of freedom for  $t$  and  $F$  tests are determined according to Kenward and Roger (1997). This is reflected in the “Model Information” table (Output 41.8.1).

**Output 41.8.1** Model Information with DDFM=KR

| The GLIMMIX Procedure       |                               |
|-----------------------------|-------------------------------|
| Model Information           |                               |
| Data Set                    | WORK.PR                       |
| Response Variable           | y                             |
| Response Distribution       | Gaussian                      |
| Link Function               | Identity                      |
| Variance Function           | Default                       |
| Variance Matrix Blocked By  | child                         |
| Estimation Technique        | Restricted Maximum Likelihood |
| Degrees of Freedom Method   | Kenward-Roger                 |
| Fixed Effects SE Adjustment | Kenward-Roger                 |

The **COVB** option in the **MODEL** statement requests that the covariance matrix used for inference about fixed effects in this model is displayed; this is the Kenward-Roger-adjusted covariance matrix. The **DE-TAILS** suboption requests that the unadjusted covariance matrix is also displayed (Output 41.8.2). In addition, a table of diagnostic measures for the covariance matrices is produced.

**Output 41.8.2** Model-Based and Adjusted Covariance Matrix

| Model Based Covariance Matrix for Fixed Effects (Unadjusted) |        |     |          |         |      |          |          |      |
|--------------------------------------------------------------|--------|-----|----------|---------|------|----------|----------|------|
| Effect                                                       | gender | Row | Col1     | Col2    | Col3 | Col4     | Col5     | Col6 |
| Intercept                                                    |        | 1   | 0.9969   | -0.9969 |      | -0.07620 | 0.07620  |      |
| gender                                                       | F      | 2   | -0.9969  | 2.4470  |      | 0.07620  | -0.1870  |      |
| gender                                                       | M      | 3   |          |         |      |          |          |      |
| age                                                          |        | 4   | -0.07620 | 0.07620 |      | 0.007581 | -0.00758 |      |
| age*gender                                                   | F      | 5   | 0.07620  | -0.1870 |      | -0.00758 | 0.01861  |      |
| age*gender                                                   | M      | 6   |          |         |      |          |          |      |
| Covariance Matrix for Fixed Effects                          |        |     |          |         |      |          |          |      |
| Effect                                                       | gender | Row | Col1     | Col2    | Col3 | Col4     | Col5     | Col6 |
| Intercept                                                    |        | 1   | 0.9724   | -0.9724 |      | -0.07412 | 0.07412  |      |
| gender                                                       | F      | 2   | -0.9724  | 2.3868  |      | 0.07412  | -0.1819  |      |
| gender                                                       | M      | 3   |          |         |      |          |          |      |
| age                                                          |        | 4   | -0.07412 | 0.07412 |      | 0.007256 | -0.00726 |      |
| age*gender                                                   | F      | 5   | 0.07412  | -0.1819 |      | -0.00726 | 0.01781  |      |
| age*gender                                                   | M      | 6   |          |         |      |          |          |      |

## Output 41.8.2 continued

## Diagnostics for Covariance Matrices of Fixed Effects

|             |                               | Model-<br>Based | Adjusted |
|-------------|-------------------------------|-----------------|----------|
| Dimensions  | Rows                          | 6               | 6        |
|             | Non-zero entries              | 16              | 16       |
| Summaries   | Trace                         | 3.4701          | 3.3843   |
|             | Log determinant               | -11.95          | -12.17   |
| Eigenvalues | > 0                           | 4               | 4        |
|             | = 0                           | 2               | 2        |
|             | max abs                       | 2.972           | 2.8988   |
|             | min abs non-zero              | 0.0009          | 0.0008   |
|             | Condition number              | 3467.8          | 3698.2   |
| Norms       | Frobenius                     | 3.0124          | 2.9382   |
|             | Infinity                      | 3.7072          | 3.6153   |
| Comparisons | Concordance correlation       |                 | 0.9979   |
|             | Discrepancy function          |                 | 0.0084   |
|             | Frobenius norm of difference  |                 | 0.0742   |
|             | Trace (Adjusted Inv (MBased)) |                 | 3.7801   |

Determinant and inversion results apply to the nonsingular partitions of the covariance matrices.

The “Diagnostics for Covariance Matrices” table in [Output 41.8.2](#) consists of several sections. The trace and log determinant of covariance matrices are general scalar summaries that are sometimes used in direct comparisons, or in formulating further statistics, such as the difference of log determinants. The trace simply represents the sum of the variances of all fixed-effects parameters.

The two matrices have the same number of positive and zero eigenvalues; hence they are of the same rank. There are no negative eigenvalues; hence the matrices are positive semi-definite.

The “Comparisons” section of the table provides several statistics that set the matrices in relationship. The statistics enable you to assess the extent to which the adjustment affected the model-based matrix. If the two matrices are identical, the concordance correlation equals 1, the discrepancy function and the Frobenius norm of the differences equal 0, and the trace of the adjusted and the (generalized) inverse of the model-based matrix equals the rank. See the section “[Exploring and Comparing Covariance Matrices](#)” on page 3080 for computational details regarding these statistics. With increasing discrepancy between the matrices, the difference norm and discrepancy function increase, the concordance correlation falls below 1, and the trace deviates from the rank. In this particular example, there is strong agreement between the two matrices; the adjustment to the covariance matrix associated with  $DDFM=KR$  is only slight. It is noteworthy, however, that the trace of the adjusted covariance matrix falls short of the trace of the unadjusted one. Indeed, from [Output 41.8.2](#) you can see that the diagonal elements of the adjusted covariance matrices are uniformly smaller than those of the model-based covariance matrix.

Standard error “shrinkage” for the Kenward-Roger covariance adjustment is due to the term  $-0.25\mathbf{R}_{ij}$  in equation (3) of Kenward and Roger (1997), which is nonzero for covariance structures with second derivatives, such as the `TYPE=ANTE(1)`, `TYPE=AR(1)`, `TYPE=ARH(1)`, `TYPE=ARMA(1,1)`, `TYPE=CHOL`, `TYPE=CSH`, `TYPE=FA0(q)`, `TYPE=TOEPH`, and `TYPE=UNR` structures and all `TYPE=SP()` structures.

For covariance structures that are linear in the parameters,  $\mathbf{R}_{ij} = \mathbf{0}$ . You can add the `FIRSTORDER` suboption to the `DDFM=KR` option to request that second derivative matrices  $\mathbf{R}_{ij}$  are excluded from computing the covariance matrix adjustment. The resulting covariance adjustment is that of Kackar and Harville (1984) and Harville and Jeske (1992). This estimator is denoted as  $\tilde{m}^{\circledast}$  in Harville and Jeske (1992) and is referred to there as the Prasad-Rao estimator after related work by Prasad and Rao (1990). This standard error adjustment is guaranteed to be positive (semi-)definite. The following statements fit the model with the Kackar-Harville-Jeske estimator and compare model-based and adjusted covariance matrices:

```
proc glimmix data=pr;
 class child gender time;
 model y = gender age gender*age / covb(details)
 ddfm=kr(firstorder);
 random intercept age / type=chol sub=child;
 random time / subject=child type=ar(1) residual;
 ods select ModelInfo CovB CovBDetails;
run;
```

The standard error adjustment is reflected in the “Model Information” table (Output 41.8.3).

**Output 41.8.3** Model Information with DDFM=KR(FIRSTORDER)

| The GLIMMIX Procedure       |                                  |
|-----------------------------|----------------------------------|
| Model Information           |                                  |
| Data Set                    | WORK.PR                          |
| Response Variable           | Y                                |
| Response Distribution       | Gaussian                         |
| Link Function               | Identity                         |
| Variance Function           | Default                          |
| Variance Matrix Blocked By  | child                            |
| Estimation Technique        | Restricted Maximum Likelihood    |
| Degrees of Freedom Method   | Kenward-Roger                    |
| Fixed Effects SE Adjustment | Prasad-Rao-Kackar-Harville-Jeske |

Output 41.8.4 displays the adjusted covariance matrix. Notice that the elements of this matrix, in particular the diagonal elements, are larger in absolute value than those of the model-based estimator (Output 41.8.2).

**Output 41.8.4** Adjusted Covariance Matrix and Comparison to Model-Based Estimator

| Covariance Matrix for Fixed Effects |        |     |          |         |      |          |          |      |
|-------------------------------------|--------|-----|----------|---------|------|----------|----------|------|
| Effect                              | gender | Row | Col1     | Col2    | Col3 | Col4     | Col5     | Col6 |
| Intercept                           |        | 1   | 1.0122   | -1.0122 |      | -0.07758 | 0.07758  |      |
| gender                              | F      | 2   | -1.0122  | 2.4845  |      | 0.07758  | -0.1904  |      |
| gender                              | M      | 3   |          |         |      |          |          |      |
| age                                 |        | 4   | -0.07758 | 0.07758 |      | 0.007706 | -0.00771 |      |
| age*gender                          | F      | 5   | 0.07758  | -0.1904 |      | -0.00771 | 0.01891  |      |
| age*gender                          | M      | 6   |          |         |      |          |          |      |

| Diagnostics for Covariance Matrices of Fixed Effects |                              |                 |          |
|------------------------------------------------------|------------------------------|-----------------|----------|
|                                                      |                              | Model-<br>Based | Adjusted |
| Dimensions                                           | Rows                         | 6               | 6        |
|                                                      | Non-zero entries             | 16              | 16       |
| Summaries                                            | Trace                        | 3.4701          | 3.5234   |
|                                                      | Log determinant              | -11.95          | -11.91   |
| Eigenvalues                                          | > 0                          | 4               | 4        |
|                                                      | = 0                          | 2               | 2        |
|                                                      | max abs                      | 2.972           | 3.0176   |
|                                                      | min abs non-zero             | 0.0009          | 0.0009   |
|                                                      | Condition number             | 3467.8          | 3513.4   |
| Norms                                                | Frobenius                    | 3.0124          | 3.0587   |
|                                                      | Infinity                     | 3.7072          | 3.7647   |
| Comparisons                                          | Concordance correlation      |                 | 0.9999   |
|                                                      | Discrepancy function         |                 | 0.0003   |
|                                                      | Frobenius norm of difference |                 | 0.0463   |
|                                                      | Trace(Adjusted Inv(MBased))  |                 | 4.0352   |

Determinant and inversion results apply to the nonsingular partitions of the covariance matrices.

The “Comparisons” statistics show that the model-based and adjusted covariance matrix of the fixed-effects parameter estimates are very similar. The concordance correlation is near 1, the discrepancy is near zero, and the trace is very close to the number of positive eigenvalues. This is due to the balanced nature of these repeated measures data. Shrinkage of standard errors, however, can not occur with the Kacker-Harville-Jeske estimator.



## Example 41.9: Testing Equality of Covariance and Correlation Matrices

Fisher's iris data are widely used in multivariate statistics. They comprise measurements in millimeters of four flower attributes, the length and width of sepals and petals for 50 specimens from each of three species, *Iris setosa*, *I. versicolor*, and *I. virginica* (Fisher 1936).

When modeling multiple attributes from the same specimen, correlations among measurements from the same flower must be taken into account. Unstructured covariance matrices are common in this multivariate setting. Species comparisons can focus on comparisons of mean response, but comparisons of the variation and covariation are also of interest. In this example, the equivalence of covariance and correlation matrices among the species are examined.

The iris data set is available in the `Sashelp` library. The following step displays the first 10 observations of the iris data in multivariate format—that is, each observation contains multiple response variables. The `DATA` step that follows creates a data set in univariate form, where each observation corresponds to a single response variable. This is the form needed by the `GLIMMIX` procedure.

```
proc print data=Sashelp.iris(obs=10);
run;
```

**Output 41.9.1** Fisher (1936) Iris Data

| Obs | Species | Sepal<br>Length | Sepal<br>Width | Petal<br>Length | Petal<br>Width |
|-----|---------|-----------------|----------------|-----------------|----------------|
| 1   | Setosa  | 50              | 33             | 14              | 2              |
| 2   | Setosa  | 46              | 34             | 14              | 3              |
| 3   | Setosa  | 46              | 36             | 10              | 2              |
| 4   | Setosa  | 51              | 33             | 17              | 5              |
| 5   | Setosa  | 55              | 35             | 13              | 2              |
| 6   | Setosa  | 48              | 31             | 16              | 2              |
| 7   | Setosa  | 52              | 34             | 14              | 2              |
| 8   | Setosa  | 49              | 36             | 14              | 1              |
| 9   | Setosa  | 44              | 32             | 13              | 2              |
| 10  | Setosa  | 50              | 35             | 16              | 6              |

```
data iris_univ;
 set sashelp.iris;
 retain id 0;
 array y (4) SepalLength SepalWidth PetalLength PetalWidth;
 id+1;
 do var=1 to 4;
 response = y{var};
 output;
 end;
 drop SepalLength SepalWidth PetalLength PetalWidth;
run;
```

The following `GLIMMIX` statements fit a model with separate unstructured covariance matrices for each species:

```
ods select FitStatistics CovParms CovTests;
proc glimmix data=iris_univ;
 class species var id;
 model response = species*var;
 random _residual_ / type=un group=species subject=id;
 covtest homogeneity;
run;
```

The mean function is modeled as a cell-means model that allows for different means for each species and outcome variable. The covariances are modeled directly (R-side) rather than through random effects. The ID variable identifies the individual plant, so that responses from different plants are independent. The **GROUP=SPECIES** option varies the parameters of the unstructured covariance matrix by species. Hence, this model has 30 covariance parameters: 10 unique parameters for a  $(4 \times 4)$  covariance matrix for each of three species.

The **COVTEST** statement requests a test of homogeneity—that is, it tests whether varying the covariance parameters by the group effect provides a significantly better fit compared to a model in which different groups share the same parameter.

#### Output 41.9.2 Fit Statistics for Analysis of Fisher’s Iris Data

| The GLIMMIX Procedure    |         |
|--------------------------|---------|
| Fit Statistics           |         |
| -2 Res Log Likelihood    | 2812.89 |
| AIC (smaller is better)  | 2872.89 |
| AICC (smaller is better) | 2876.23 |
| BIC (smaller is better)  | 2963.21 |
| CAIC (smaller is better) | 2993.21 |
| HQIC (smaller is better) | 2909.58 |
| Generalized Chi-Square   | 588.00  |
| Gener. Chi-Square / DF   | 1.00    |

The “Fit Statistics” table shows the  $-2$  restricted (residual) log likelihood in the full model and other fit statistics (Output 41.9.2). The “ $-2$  Res Log Likelihood” sets the benchmark against which a model with homogeneity constraint is compared. Output 41.9.3 displays the 30 covariance parameters in this model.

There appear to be substantial differences among the covariance parameters from different groups. For example, the residual variability of the petal length of the three species is 12.4249, 26.6433, and 40.4343, respectively. The homogeneity hypothesis restricts these variances to be equal and similarly for the other covariance parameters. The results from the **COVTEST** statement are shown in Output 41.9.4.

**Output 41.9.3** Covariance Parameters Varied by Species (TYPE=UN)

| Covariance Parameter Estimates |         |                    |          |                |  |
|--------------------------------|---------|--------------------|----------|----------------|--|
| Cov Parm                       | Subject | Group              | Estimate | Standard Error |  |
| UN(1,1)                        | id      | Species Setosa     | 12.4249  | 2.5102         |  |
| UN(2,1)                        | id      | Species Setosa     | 9.9216   | 2.3775         |  |
| UN(2,2)                        | id      | Species Setosa     | 14.3690  | 2.9030         |  |
| UN(3,1)                        | id      | Species Setosa     | 1.6355   | 0.9052         |  |
| UN(3,2)                        | id      | Species Setosa     | 1.1698   | 0.9552         |  |
| UN(3,3)                        | id      | Species Setosa     | 3.0159   | 0.6093         |  |
| UN(4,1)                        | id      | Species Setosa     | 1.0331   | 0.5508         |  |
| UN(4,2)                        | id      | Species Setosa     | 0.9298   | 0.5859         |  |
| UN(4,3)                        | id      | Species Setosa     | 0.6069   | 0.2755         |  |
| UN(4,4)                        | id      | Species Setosa     | 1.1106   | 0.2244         |  |
| UN(1,1)                        | id      | Species Versicolor | 26.6433  | 5.3828         |  |
| UN(2,1)                        | id      | Species Versicolor | 8.5184   | 2.6144         |  |
| UN(2,2)                        | id      | Species Versicolor | 9.8469   | 1.9894         |  |
| UN(3,1)                        | id      | Species Versicolor | 18.2898  | 4.3398         |  |
| UN(3,2)                        | id      | Species Versicolor | 8.2653   | 2.4149         |  |
| UN(3,3)                        | id      | Species Versicolor | 22.0816  | 4.4612         |  |
| UN(4,1)                        | id      | Species Versicolor | 5.5780   | 1.6617         |  |
| UN(4,2)                        | id      | Species Versicolor | 4.1204   | 1.0641         |  |
| UN(4,3)                        | id      | Species Versicolor | 7.3102   | 1.6891         |  |
| UN(4,4)                        | id      | Species Versicolor | 3.9106   | 0.7901         |  |
| UN(1,1)                        | id      | Species Virginica  | 40.4343  | 8.1690         |  |
| UN(2,1)                        | id      | Species Virginica  | 9.3763   | 3.2213         |  |
| UN(2,2)                        | id      | Species Virginica  | 10.4004  | 2.1012         |  |
| UN(3,1)                        | id      | Species Virginica  | 30.3290  | 6.6262         |  |
| UN(3,2)                        | id      | Species Virginica  | 7.1380   | 2.7395         |  |
| UN(3,3)                        | id      | Species Virginica  | 30.4588  | 6.1536         |  |
| UN(4,1)                        | id      | Species Virginica  | 4.9094   | 2.5916         |  |
| UN(4,2)                        | id      | Species Virginica  | 4.7629   | 1.4367         |  |
| UN(4,3)                        | id      | Species Virginica  | 4.8824   | 2.2750         |  |
| UN(4,4)                        | id      | Species Virginica  | 7.5433   | 1.5240         |  |

**Output 41.9.4** Likelihood Ratio Test of Homogeneity

| Tests of Covariance Parameters<br>Based on the Restricted Likelihood |    |                 |        |            |      |
|----------------------------------------------------------------------|----|-----------------|--------|------------|------|
| Label                                                                | DF | -2 Res Log Like | ChiSq  | Pr > ChiSq | Note |
| Homogeneity                                                          | 20 | 2959.55         | 146.66 | <.0001     | DF   |

DF: P-value based on a chi-square with DF degrees of freedom.

Denote as  $\mathbf{R}_k$  the covariance matrix for species  $k = 1, 2, 3$  with elements  $\sigma_{ijk}$ . In processing the **COVTEST** hypothesis  $H_0: \mathbf{R}_1 = \mathbf{R}_2 = \mathbf{R}_3$ , the GLIMMIX procedure fits a model that satisfies the constraints

$$\begin{aligned}\sigma_{111} &= \sigma_{112} = \sigma_{113} \\ \sigma_{211} &= \sigma_{212} = \sigma_{213} \\ \sigma_{231} &= \sigma_{232} = \sigma_{233} \\ &\vdots \\ \sigma_{441} &= \sigma_{442} = \sigma_{443}\end{aligned}$$

where  $\sigma_{ijk}$  is the covariance between the  $i$ th and  $j$ th variable for the  $k$ th species. The  $-2$  restricted log likelihood of this restricted model is 2959.55 (Output 41.9.4). The change of 146.66 compared to the full model is highly significant. There is sufficient evidence to reject the notion of equal covariance matrices among the three iris species.

Equality of covariance matrices implies equality of correlation matrices, but the reverse is not true. Fewer constraints are needed to equate correlations because the diagonal entries of the covariance matrices are free to vary. In order to test the equality of the correlation matrices among the three species, you can parameterize the unstructured covariance matrix in terms of the correlations and use a **COVTEST** statement with general contrasts, as shown in the following statements:

```
ods select FitStatistics CovParms CovTests;
proc glimmix data=iris_univ;
 class species var id;
 model response = species*var;
 random _residual_ / type=unr group=species subject=id;
 covtest 'Equal Covariance Matrices' homogeneity;
 covtest 'Equal Correlation Matrices' general
 0 0 0 0 1 0 0 0 0 0
 0 0 0 0 -1 0 0 0 0 0,
 0 0 0 0 1 0 0 0 0 0
 0 0 0 0 0 0 0 0 0 0
 0 0 0 0 -1 0 0 0 0 0,
 0 0 0 0 0 1 0 0 0 0
 0 0 0 0 0 -1 0 0 0 0,
 0 0 0 0 0 1 0 0 0 0
 0 0 0 0 0 0 0 0 0 0
 0 0 0 0 0 -1 0 0 0 0,
 0 0 0 0 0 0 1 0 0 0
 0 0 0 0 0 0 -1 0 0 0,
 0 0 0 0 0 0 1 0 0 0
 0 0 0 0 0 0 0 0 0 0
 0 0 0 0 0 0 0 -1 0 0,
 0 0 0 0 0 0 0 0 1 0
 0 0 0 0 0 0 0 0 -1 0,
 0 0 0 0 0 0 0 0 1 0
 0 0 0 0 0 0 0 0 0 0
```

```

0 0 0 0 0 0 0 0 -1 0,
0 0 0 0 0 0 0 0 0 1
0 0 0 0 0 0 0 0 0 -1,
0 0 0 0 0 0 0 0 0 1
0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 -1 / estimates;

```

```
run;
```

The `TYPE=UNR` structure is a reparameterization of `TYPE=UN`. The models provide the same fit, as seen by comparison of the “Fit Statistics” tables in [Output 41.9.2](#) and [Output 41.9.5](#). The covariance parameters are ordered differently, however. In each group, the four variances precede the six correlations ([Output 41.9.5](#)). The first `COVTEST` statement tests the homogeneity hypothesis in terms of the UNR parameterization, and the result is identical to the test in [Output 41.9.4](#). The second `COVTEST` statement restricts the correlations to be equal across groups. If  $\rho_{ijk}$  is the correlation between the  $i$ th and  $j$ th variable for the  $k$ th species, the 12 restrictions are

$$\rho_{211} = \rho_{212} = \rho_{213}$$

$$\rho_{311} = \rho_{312} = \rho_{313}$$

$$\rho_{321} = \rho_{322} = \rho_{323}$$

$$\rho_{411} = \rho_{412} = \rho_{413}$$

$$\rho_{421} = \rho_{422} = \rho_{423}$$

$$\rho_{431} = \rho_{432} = \rho_{433}$$

The `ESTIMATES` option in the `COVTEST` statement requests that the GLIMMIX procedure display the covariance parameter estimates in the restricted model ([Output 41.9.5](#)).

**Output 41.9.5** Fit Statistics, Covariance Parameters (TYPE=UNR), and Likelihood Ratio Tests for Equality of Covariance and Correlation Matrices

| The GLIMMIX Procedure    |         |
|--------------------------|---------|
| Fit Statistics           |         |
| -2 Res Log Likelihood    | 2812.89 |
| AIC (smaller is better)  | 2872.89 |
| AICC (smaller is better) | 2876.23 |
| BIC (smaller is better)  | 2963.21 |
| CAIC (smaller is better) | 2993.21 |
| HQIC (smaller is better) | 2909.58 |
| Generalized Chi-Square   | 588.00  |
| Gener. Chi-Square / DF   | 1.00    |

## Output 41.9.5 continued

| Covariance Parameter Estimates |         |                    |          |                |
|--------------------------------|---------|--------------------|----------|----------------|
| Cov Parm                       | Subject | Group              | Estimate | Standard Error |
| Var (1)                        | id      | Species Setosa     | 12.4249  | 2.5102         |
| Var (2)                        | id      | Species Setosa     | 14.3690  | 2.9030         |
| Var (3)                        | id      | Species Setosa     | 3.0159   | 0.6093         |
| Var (4)                        | id      | Species Setosa     | 1.1106   | 0.2244         |
| Corr (2,1)                     | id      | Species Setosa     | 0.7425   | 0.06409        |
| Corr (3,1)                     | id      | Species Setosa     | 0.2672   | 0.1327         |
| Corr (3,2)                     | id      | Species Setosa     | 0.1777   | 0.1383         |
| Corr (4,1)                     | id      | Species Setosa     | 0.2781   | 0.1318         |
| Corr (4,2)                     | id      | Species Setosa     | 0.2328   | 0.1351         |
| Corr (4,3)                     | id      | Species Setosa     | 0.3316   | 0.1271         |
| Var (1)                        | id      | Species Versicolor | 26.6433  | 5.3828         |
| Var (2)                        | id      | Species Versicolor | 9.8469   | 1.9894         |
| Var (3)                        | id      | Species Versicolor | 22.0816  | 4.4612         |
| Var (4)                        | id      | Species Versicolor | 3.9106   | 0.7901         |
| Corr (2,1)                     | id      | Species Versicolor | 0.5259   | 0.1033         |
| Corr (3,1)                     | id      | Species Versicolor | 0.7540   | 0.06163        |
| Corr (3,2)                     | id      | Species Versicolor | 0.5605   | 0.09797        |
| Corr (4,1)                     | id      | Species Versicolor | 0.5465   | 0.1002         |
| Corr (4,2)                     | id      | Species Versicolor | 0.6640   | 0.07987        |
| Corr (4,3)                     | id      | Species Versicolor | 0.7867   | 0.05445        |
| Var (1)                        | id      | Species Virginica  | 40.4343  | 8.1690         |
| Var (2)                        | id      | Species Virginica  | 10.4004  | 2.1012         |
| Var (3)                        | id      | Species Virginica  | 30.4588  | 6.1536         |
| Var (4)                        | id      | Species Virginica  | 7.5433   | 1.5240         |
| Corr (2,1)                     | id      | Species Virginica  | 0.4572   | 0.1130         |
| Corr (3,1)                     | id      | Species Virginica  | 0.8642   | 0.03616        |
| Corr (3,2)                     | id      | Species Virginica  | 0.4010   | 0.1199         |
| Corr (4,1)                     | id      | Species Virginica  | 0.2811   | 0.1316         |
| Corr (4,2)                     | id      | Species Virginica  | 0.5377   | 0.1015         |
| Corr (4,3)                     | id      | Species Virginica  | 0.3221   | 0.1280         |

Output 41.9.5 continued

| Tests of Covariance Parameters<br>Based on the Restricted Likelihood |    |                 |        |            |                     |      |
|----------------------------------------------------------------------|----|-----------------|--------|------------|---------------------|------|
| Label                                                                | DF | -2 Res Log Like | ChiSq  | Pr > ChiSq | Estimate<br>s H0--- | Est1 |
| Equal Covariance Matrices                                            | 20 | 2959.55         | 146.66 | <.0001     | 26.5004             |      |
| Equal Correlation Matrices                                           | 12 | 2876.38         | 63.49  | <.0001     | 16.4715             |      |

| Tests of Covariance Parameters<br>Based on the Restricted Likelihood |         |         |        |        |        |              |
|----------------------------------------------------------------------|---------|---------|--------|--------|--------|--------------|
| Label                                                                | Est2    | Est3    | Est4   | Est5   | Est6   | Estimates H0 |
| Equal Covariance Matrices                                            | 11.5395 | 18.5179 | 4.1883 | 0.5302 | 0.7562 |              |
| Equal Correlation Matrices                                           | 14.8656 | 4.8427  | 1.4392 | 0.5612 | 0.6827 |              |

| Tests of Covariance Parameters<br>Based on the Restricted Likelihood |        |        |        |        |         |              |
|----------------------------------------------------------------------|--------|--------|--------|--------|---------|--------------|
| Label                                                                | Est7   | Est8   | Est9   | Est10  | Est11   | Estimates H0 |
| Equal Covariance Matrices                                            | 0.3779 | 0.3645 | 0.4705 | 0.4845 | 26.5004 |              |
| Equal Correlation Matrices                                           | 0.4016 | 0.3844 | 0.4976 | 0.5219 | 24.4020 |              |

| Tests of Covariance Parameters<br>Based on the Restricted Likelihood |         |         |        |        |        |              |
|----------------------------------------------------------------------|---------|---------|--------|--------|--------|--------------|
| Label                                                                | Est12   | Est13   | Est14  | Est15  | Est16  | Estimates H0 |
| Equal Covariance Matrices                                            | 11.5395 | 18.5179 | 4.1883 | 0.5302 | 0.7562 |              |
| Equal Correlation Matrices                                           | 9.1566  | 17.4434 | 3.0021 | 0.5612 | 0.6827 |              |

| Tests of Covariance Parameters<br>Based on the Restricted Likelihood |        |        |        |        |         |              |
|----------------------------------------------------------------------|--------|--------|--------|--------|---------|--------------|
| Label                                                                | Est17  | Est18  | Est19  | Est20  | Est21   | Estimates H0 |
| Equal Covariance Matrices                                            | 0.3779 | 0.3645 | 0.4705 | 0.4845 | 26.5004 |              |
| Equal Correlation Matrices                                           | 0.4016 | 0.3844 | 0.4976 | 0.5219 | 35.0544 |              |

**Output 41.9.5** *continued*

| Tests of Covariance Parameters<br>Based on the Restricted Likelihood |                        |         |        |        |        |
|----------------------------------------------------------------------|------------------------|---------|--------|--------|--------|
| Label                                                                | -----Estimates H0----- |         |        |        |        |
|                                                                      | Est22                  | Est23   | Est24  | Est25  | Est26  |
| Equal Covariance Matrices                                            | 11.5395                | 18.5179 | 4.1883 | 0.5302 | 0.7562 |
| Equal Correlation Matrices                                           | 10.8350                | 27.3593 | 8.1395 | 0.5612 | 0.6827 |

| Tests of Covariance Parameters<br>Based on the Restricted Likelihood |                        |        |        |        |      |
|----------------------------------------------------------------------|------------------------|--------|--------|--------|------|
| Label                                                                | -----Estimates H0----- |        |        |        | Note |
|                                                                      | Est27                  | Est28  | Est29  | Est30  |      |
| Equal Covariance Matrices                                            | 0.3779                 | 0.3645 | 0.4705 | 0.4845 | DF   |
| Equal Correlation Matrices                                           | 0.4016                 | 0.3844 | 0.4976 | 0.5219 | DF   |

DF: P-value based on a chi-square with DF degrees of freedom.

The result of the homogeneity test is identical to that in [Output 41.9.4](#). The hypothesis of equality of the correlation matrices is also rejected with a chi-square value of 63.49 and a  $p$ -value of  $< 0.0001$ . Notice, however, that the chi-square statistic is smaller than in the test of homogeneity due to the smaller number of restrictions imposed on the full model. The estimate of the common correlation matrix in the restricted model is

$$\begin{bmatrix} 1 & 0.561 & 0.683 & 0.384 \\ 0.561 & 1 & 0.402 & 0.498 \\ 0.683 & 0.402 & 1 & 0.522 \\ 0.384 & 0.498 & 0.522 & 1 \end{bmatrix}$$

---

### Example 41.10: Multiple Trends Correspond to Multiple Extrema in Profile Likelihoods

Observations for a period of 168 months for the “Southern Oscillation Index,” measurements of monthly averaged atmospheric pressure differences between Easter Island and Darwin, Australia (Kahaner, Moler, and Nash 1989, Ch. 11.9; National Institute of Standards and Technology 1998) is available in the data set ENSO in the Sashelp library. These data are also used as an example in Chapter 53, “The LOESS Procedure.” The following statements print the first 10 observations of this data set in [Output 41.10.1](#).

```
proc print data=Sashelp.enso(obs=10);
run;
```



**Output 41.10.1** El Niño Southern Oscillation Data

| Obs | Month | Year    | Pressure |
|-----|-------|---------|----------|
| 1   | 1     | 0.08333 | 12.9     |
| 2   | 2     | 0.16667 | 11.3     |
| 3   | 3     | 0.25000 | 10.6     |
| 4   | 4     | 0.33333 | 11.2     |
| 5   | 5     | 0.41667 | 10.9     |
| 6   | 6     | 0.50000 | 7.5      |
| 7   | 7     | 0.58333 | 7.7      |
| 8   | 8     | 0.66667 | 11.7     |
| 9   | 9     | 0.75000 | 12.9     |
| 10  | 10    | 0.83333 | 14.3     |

Differences in atmospheric pressure create wind, and the differences recorded in the data set ENSO drive the trade winds in the southern hemisphere. Such time series often do not consist of a single trend or cycle. In this particular case, there are at least two known cycles that reflect the annual weather pattern and a longer cycle that represents the periodic warming of the Pacific Ocean (El Niño).

To estimate the trend in these data by using mixed model technology, you can apply a mixed model smoothing technique such as `TYPE=RSMOOTH` or `TYPE=PSPLINE`. The following statements fit a radial smoother to the ENSO data and obtain profile likelihoods for a series of values for the variance of the random spline coefficients:

```
data tdata;
 do covp1=0,0.0005,0.05,0.1,0.2,0.5,
 1,2,3,4,5,6,8,10,15,20,50,
 75,100,125,140,150,160,175,
 200,225,250,275,300,350;
 output;
 end;
run;

ods select FitStatistics CovParms CovTests;
proc glimmix data=sashelp.enso noprofile;
 model pressure = year;
 random year / type=rsmooth knotmethod=equal(50);
 parms (2) (10);
 covtest tdata=tdata / parms;
 ods output covtests=ct;
run;
```

The `tdata` data set contains value for the variance of the radial smoother variance for which the profile likelihood of the model is to be computed. The profile likelihood is obtained by setting the radial smoother variance at the specified value and estimating all other parameters subject to that constraint.

Because the model contains a residual variance and you need to specify nonzero values for the first covariance parameter, the `NOPROFILE` is added to the `PROC GLIMMIX` statements. If the residual variance is profiled from the estimation, you cannot fix covariance parameters at a given value, because they would be reexpressed during model fitting in terms of ratios with the profiled (and changing) variance.

The `PARMS` statement determines starting values for the covariance parameters for fitting the (full) model. The `PARMS` option in the `COVTEST` statement requests that the input parameters be added to the output and the output data set. This is useful for subsequent plotting of the profile likelihood function.

The “Fit Statistics” table displays the  $-2$  restricted log likelihood of the model (897.76, [Output 41.10.2](#)). The estimate of the variance of the radial smoother coefficients is 3.5719.

The “Test of Covariance Parameters” table displays the  $-2$  restricted log likelihood for each observation in the `tdata` set. Because the `tdata` data set specifies values for only the first covariance parameter, the second covariance parameter is free to vary and the values for  $-2$  Res Log Like are profile likelihoods. Notice that for a number of values of `CovP1` the chi-square statistic is missing in this table. For these values the  $-2$  Res Log Like is *smaller* than that of the full model. The model did not converge to a global minimum of the negative restricted log likelihood.

### Output 41.10.2 REML and Profile Likelihood Analysis

| The GLIMMIX Procedure          |          |                |
|--------------------------------|----------|----------------|
| Fit Statistics                 |          |                |
| -2 Res Log Likelihood          |          | 897.76         |
| AIC (smaller is better)        |          | 901.76         |
| AICC (smaller is better)       |          | 901.83         |
| BIC (smaller is better)        |          | 897.76         |
| CAIC (smaller is better)       |          | 899.76         |
| HQIC (smaller is better)       |          | 897.76         |
| Generalized Chi-Square         |          | 1554.38        |
| Gener. Chi-Square / DF         |          | 9.36           |
| Radial Smoother df(res)        |          | 153.52         |
| Covariance Parameter Estimates |          |                |
| Cov Parm                       | Estimate | Standard Error |
| Var[RSmooth(Year)]             | 3.5719   | 3.7672         |
| Residual                       | 9.3638   | 1.3014         |

Output 41.10.2 continued

| Tests of Covariance Parameters<br>Based on the Restricted Likelihood |    |                 |       |            |                    |        |  |  |
|----------------------------------------------------------------------|----|-----------------|-------|------------|--------------------|--------|--|--|
| Label                                                                | DF | -2 Res Log Like | ChiSq | Pr > ChiSq | -Input Parameters- |        |  |  |
|                                                                      |    |                 |       |            | CovP1              | CovP2  |  |  |
| WORK.TDATA                                                           | 1  | 893.01          | .     | 1.0000     | 0                  | 9.3638 |  |  |
| WORK.TDATA                                                           | 1  | 892.76          | .     | 1.0000     | 0.000500           | 9.3638 |  |  |
| WORK.TDATA                                                           | 1  | 897.34          | .     | 1.0000     | 0.05000            | 9.3638 |  |  |
| WORK.TDATA                                                           | 1  | 898.53          | 0.77  | 0.3816     | 0.1000             | 9.3638 |  |  |
| WORK.TDATA                                                           | 1  | 899.38          | 1.62  | 0.2038     | 0.2000             | 9.3638 |  |  |
| WORK.TDATA                                                           | 1  | 899.49          | 1.73  | 0.1888     | 0.5000             | 9.3638 |  |  |
| WORK.TDATA                                                           | 1  | 898.83          | 1.07  | 0.3016     | 1.0000             | 9.3638 |  |  |
| WORK.TDATA                                                           | 1  | 898.04          | 0.28  | 0.5967     | 2.0000             | 9.3638 |  |  |
| WORK.TDATA                                                           | 1  | 897.79          | 0.03  | 0.8693     | 3.0000             | 9.3638 |  |  |
| WORK.TDATA                                                           | 1  | 897.77          | 0.01  | 0.9145     | 4.0000             | 9.3638 |  |  |
| WORK.TDATA                                                           | 1  | 897.86          | 0.10  | 0.7517     | 5.0000             | 9.3638 |  |  |
| WORK.TDATA                                                           | 1  | 897.99          | 0.23  | 0.6311     | 6.0000             | 9.3638 |  |  |
| WORK.TDATA                                                           | 1  | 898.27          | 0.51  | 0.4761     | 8.0000             | 9.3638 |  |  |
| WORK.TDATA                                                           | 1  | 898.49          | 0.73  | 0.3919     | 10.0000            | 9.3638 |  |  |
| WORK.TDATA                                                           | 1  | 898.70          | 0.94  | 0.3318     | 15.0000            | 9.3638 |  |  |
| WORK.TDATA                                                           | 1  | 898.45          | 0.69  | 0.4068     | 20.0000            | 9.3638 |  |  |
| WORK.TDATA                                                           | 1  | 892.63          | .     | 1.0000     | 50.0000            | 9.3638 |  |  |
| WORK.TDATA                                                           | 1  | 887.44          | .     | 1.0000     | 75.0000            | 9.3638 |  |  |
| WORK.TDATA                                                           | 1  | 883.79          | .     | 1.0000     | 100.00             | 9.3638 |  |  |
| WORK.TDATA                                                           | 1  | 881.55          | .     | 1.0000     | 125.00             | 9.3638 |  |  |
| WORK.TDATA                                                           | 1  | 880.72          | .     | 1.0000     | 140.00             | 9.3638 |  |  |
| WORK.TDATA                                                           | 1  | .               | .     | .          | 150.00             | 9.3638 |  |  |
| WORK.TDATA                                                           | 1  | 880.07          | .     | 1.0000     | 160.00             | 9.3638 |  |  |
| WORK.TDATA                                                           | 1  | 879.85          | .     | 1.0000     | 175.00             | 9.3638 |  |  |
| WORK.TDATA                                                           | 1  | .               | .     | .          | 200.00             | 9.3638 |  |  |
| WORK.TDATA                                                           | 1  | 880.21          | .     | 1.0000     | 225.00             | 9.3638 |  |  |
| WORK.TDATA                                                           | 1  | 880.80          | .     | 1.0000     | 250.00             | 9.3638 |  |  |
| WORK.TDATA                                                           | 1  | 881.56          | .     | 1.0000     | 275.00             | 9.3638 |  |  |
| WORK.TDATA                                                           | 1  | 882.44          | .     | 1.0000     | 300.00             | 9.3638 |  |  |
| WORK.TDATA                                                           | 1  | 884.41          | .     | 1.0000     | 350.00             | 9.3638 |  |  |

| Tests of<br>Covariance<br>Parameters<br>Based on the<br>Restricted<br>Likelihood |      |
|----------------------------------------------------------------------------------|------|
| Label                                                                            | Note |
| WORK.TDATA                                                                       | MI   |
| WORK.TDATA                                                                       | DF   |
| WORK.TDATA                                                                       | DF   |
| WORK.TDATA                                                                       | DF   |
| WORK.TDATA                                                                       | DF   |
| WORK.TDATA                                                                       | DF   |

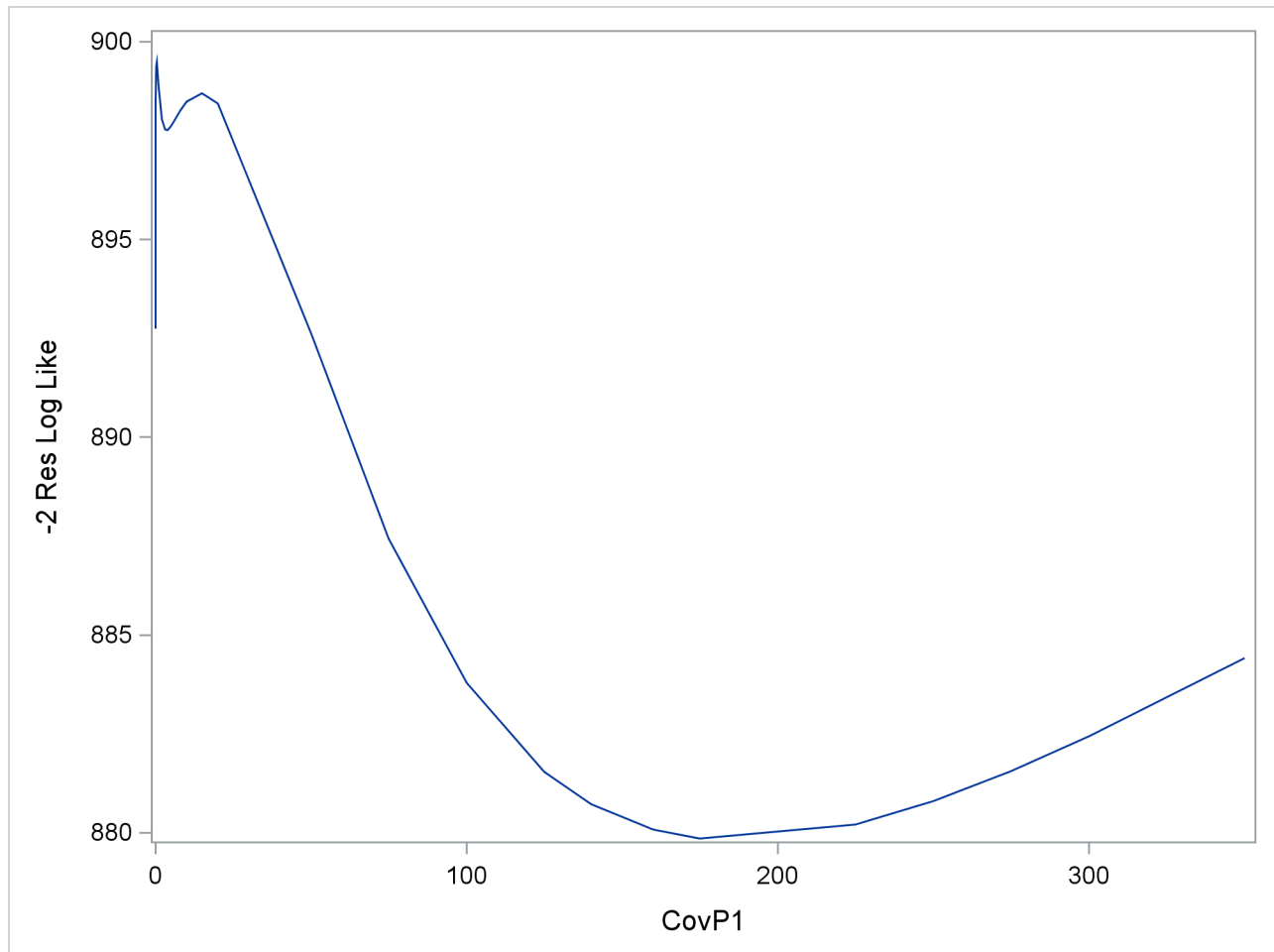
**Output 41.10.2** *continued*

| Tests of<br>Covariance<br>Parameters<br>Based on the<br>Restricted<br>Likelihood |      |
|----------------------------------------------------------------------------------|------|
| Label                                                                            | Note |
| WORK.TDATA                                                                       | DF   |
| WORK.TDATA                                                                       | DF   |
| WORK.TDATA                                                                       | DF   |
| WORK.TDATA                                                                       | DF   |
| WORK.TDATA                                                                       | DF   |
| WORK.TDATA                                                                       | DF   |
| WORK.TDATA                                                                       | DF   |
| WORK.TDATA                                                                       | DF   |
| WORK.TDATA                                                                       | DF   |
| WORK.TDATA                                                                       | DF   |
| WORK.TDATA                                                                       | DF   |
| WORK.TDATA                                                                       | DF   |
| WORK.TDATA                                                                       | DF   |
| WORK.TDATA                                                                       | DF   |
| WORK.TDATA                                                                       | DF   |
| WORK.TDATA                                                                       | DF   |
| WORK.TDATA                                                                       | DF   |
| WORK.TDATA                                                                       | DF   |
| WORK.TDATA                                                                       | DF   |
| WORK.TDATA                                                                       | DF   |
| WORK.TDATA                                                                       | DF   |
| WORK.TDATA                                                                       | DF   |
| WORK.TDATA                                                                       | DF   |
| WORK.TDATA                                                                       | DF   |
| WORK.TDATA                                                                       | DF   |
| WORK.TDATA                                                                       | DF   |
| WORK.TDATA                                                                       | DF   |
| WORK.TDATA                                                                       | DF   |
| WORK.TDATA                                                                       | DF   |
| WORK.TDATA                                                                       | DF   |
| WORK.TDATA                                                                       | DF   |
| WORK.TDATA                                                                       | DF   |

DF: P-value based on a chi-square with DF degrees of freedom.  
MI: P-value based on a mixture of chi-squares.

The following statements plot the  $-2$  restricted profile log likelihood (Output 41.10.3):

```
proc sgplot data=ct;
 series y=objective x=covp1;
run;
```

**Output 41.10.3** –2 Restricted Profile Log Likelihood for Smoothing Variance

The local minimum at which the optimization stopped is clearly visible, as are a second local minimum near zero and the global minimum near 180.

The observed and predicted pressure differences that correspond to the three minima are shown in [Output 41.10.4](#). These results were produced with the following statements:

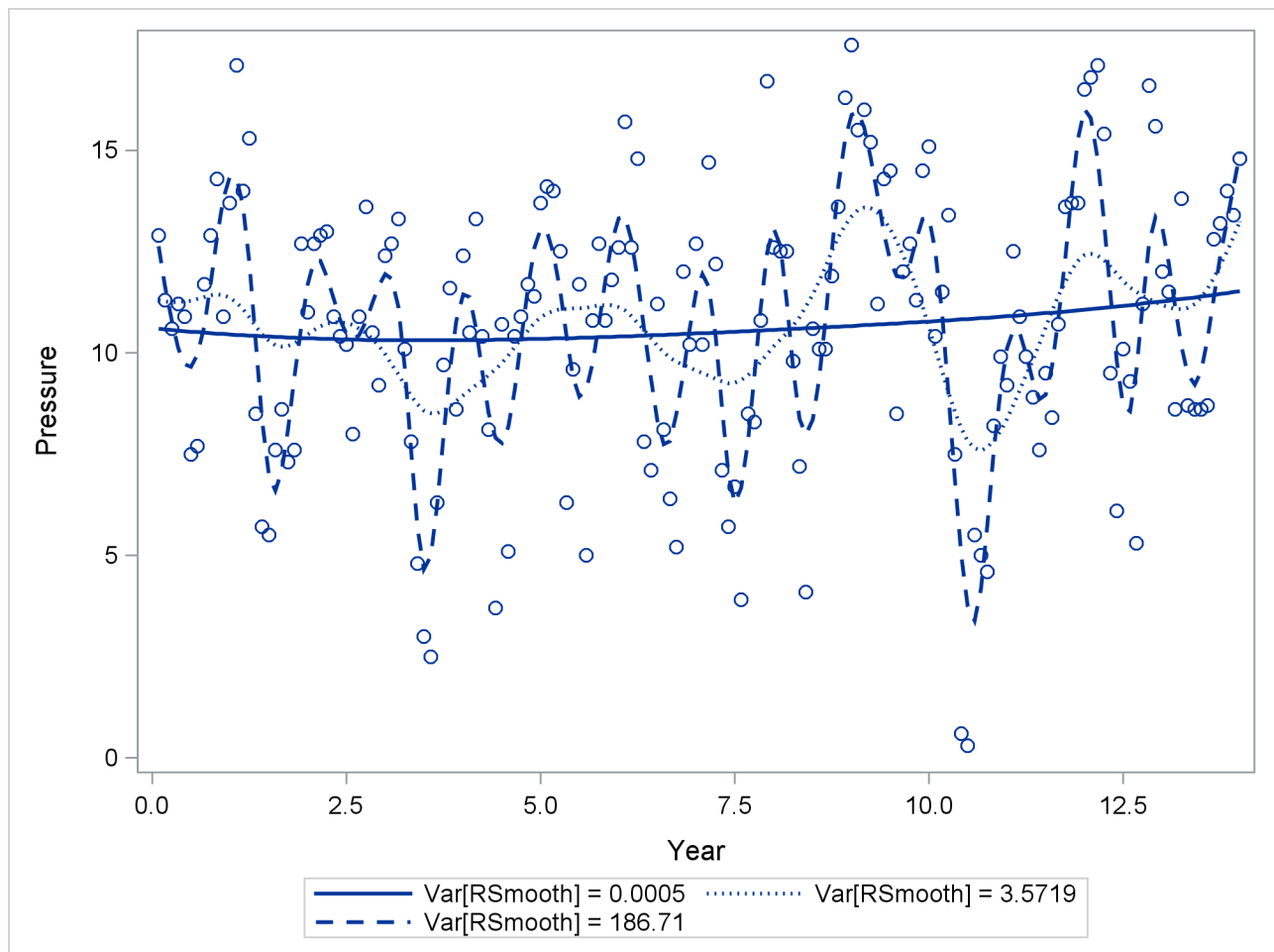
```
proc glimmix data=sashelp.enso;
 model pressure = year;
 random year / type=rsmooth knotmethod=equal(50);
 parms (0) (10);
 output out=gmxout1 pred=pred1;
run;
proc glimmix data=sashelp.enso;
 model pressure = year;
 random year / type=rsmooth knotmethod=equal(50);
 output out=gmxout2 pred=pred2;
 parms (2) (10);
run;
proc glimmix data=sashelp.enso;
 model pressure = year;
 random year / type=rsmooth knotmethod=equal(50);
 output out=gmxout3 pred=pred3;
 parms (200) (10);
run;
```

```

data plotthis; merge gmxout1 gmxout2 gmxout3;
run;
proc sgplot data=plotthis;
 scatter x=year y=Pressure;
 series x=year y=pred1 /
 lineattrs = (pattern=solid thickness=2)
 legendlabel = "Var[RSmooth] = 0.0005"
 name = "pred1";
 series x=year y=pred2 /
 lineattrs = (pattern=dot thickness=2)
 legendlabel = "Var[RSmooth] = 3.5719"
 name = "pred2";
 series x=year y=pred3 /
 lineattrs = (pattern=dash thickness=2)
 legendlabel = "Var[RSmooth] = 186.71"
 name = "pred3";
 keylegend "pred1" "pred2" "pred3" / across=2;
run;

```

Output 41.10.4 Observed and Predicted Pressure Differences



The one-year cycle ( $\hat{\sigma}_r^2 = 186.71$ ) and the El Niño cycle ( $\hat{\sigma}_r^2 = 3.5719$ ) are clearly visible. Notice that a larger smoother variance results in larger BLUPs and hence larger adjustments to the fixed-effects model. A large smoother variance thus results in a more wiggly fit. The third local minimum at  $\hat{\sigma}_r^2 = 0.0005$  applies only very small adjustments to the linear regression between pressure and time, creating slight curvature.

---

### Example 41.11: Maximum Likelihood in Proportional Odds Model with Random Effects

The data for this example are taken from Gilmour, Anderson, and Rae (1987) and concern the foot shape of 2,513 lambs that represent 34 sires. The foot shape of the animals was scored in three ordered categories. The following DATA step lists the data in multivariate form, where each observation corresponds to a sire and contains the outcomes for the three response categories in the variables k1, k2, and k3. For example, for the first sire the first foot shape category was observed for 52 of its offspring, foot shape category 2 was observed for 25 lambs, and none of its offspring was rated in foot shape category 3. The variables yr, b1, b2, and b3 represent contrasts of fixed effects.

```

data foot_mv;
 input yr b1 b2 b3 k1 k2 k3;
 sire = _n_;
 datalines;
1 1 0 0 52 25 0
1 1 0 0 49 17 1
1 1 0 0 50 13 1
1 1 0 0 42 9 0
1 1 0 0 74 15 0
1 1 0 0 54 8 0
1 1 0 0 96 12 0
1 -1 1 0 57 52 9
1 -1 1 0 55 27 5
1 -1 1 0 70 36 4
1 -1 1 0 70 37 3
1 -1 1 0 82 21 1
1 -1 1 0 75 19 0
1 -1 -1 0 17 12 10
1 -1 -1 0 13 23 3
1 -1 -1 0 21 17 3
-1 0 0 1 37 41 23
-1 0 0 1 47 24 12
-1 0 0 1 46 25 9
-1 0 0 1 79 32 11
-1 0 0 1 50 23 5
-1 0 0 1 63 18 8
-1 0 0 -1 30 20 9
-1 0 0 -1 31 33 3
-1 0 0 -1 28 18 4
-1 0 0 -1 42 27 4
-1 0 0 -1 35 22 2
-1 0 0 -1 33 18 3
-1 0 0 -1 35 17 4
-1 0 0 -1 26 13 2

```

```

-1 0 0 -1 37 15 2
-1 0 0 -1 36 14 1
-1 0 0 -1 63 20 3
-1 0 0 -1 41 8 1
;

```

In order to analyze these data as multinomial data with PROC GLIMMIX, the data need to be arranged in univariate form. The following DATA step creates three observations from each record in data set foot\_mv and stores the category counts in the variable count:

```

data footshape; set foot_mv;
 array k{3};
 do Shape = 1 to 3;
 count = k{Shape};
 output;
 end;
 drop k:;
run;

```

Because the sires were selected at random, a model for the three-category response with fixed regression effects for yr, b1–b3, and with random sire effects is considered. Because the response categories are ordered, a proportional odds model is chosen (McCullagh 1980). Gilmour, Anderson, and Rae (1987) consider various analyses for these data. The following GLIMMIX statements fit a model with probit link for the cumulative probabilities by maximum likelihood where the marginal log likelihood is approximated by adaptive quadrature:

```

proc glimmix data=footshape method=quad;
 class sire;
 model Shape = yr b1 b2 b3 / s link=cumprobit dist=multinomial;
 random int / sub=sire s cl;
 ods output Solutionr=solr;
 freq count;
run;

```

The number of observations that share a particular response and covariate pattern (variable count) is used in the FREQ statement. The S and CL options request solutions for the sire effects. These are output to the data set solr for plotting.

The “Model Information” table shows that the parameters are estimated by maximum likelihood and that the marginal likelihood is approximated by Gauss-Hermite quadrature (Output 41.11.1).



**Output 41.11.1** Model and Data Information

| The GLIMMIX Procedure                                                                                                             |       |                          |
|-----------------------------------------------------------------------------------------------------------------------------------|-------|--------------------------|
| Model Information                                                                                                                 |       |                          |
| Data Set                                                                                                                          |       | WORK.FOOTSHAPE           |
| Response Variable                                                                                                                 |       | Shape                    |
| Response Distribution                                                                                                             |       | Multinomial (ordered)    |
| Link Function                                                                                                                     |       | Cumulative Probit        |
| Variance Function                                                                                                                 |       | Default                  |
| Frequency Variable                                                                                                                |       | count                    |
| Variance Matrix Blocked By                                                                                                        |       | sire                     |
| Estimation Technique                                                                                                              |       | Maximum Likelihood       |
| Likelihood Approximation                                                                                                          |       | Gauss-Hermite Quadrature |
| Degrees of Freedom Method                                                                                                         |       | Containment              |
|                                                                                                                                   |       |                          |
| Number of Observations Read                                                                                                       |       | 102                      |
| Number of Observations Used                                                                                                       |       | 96                       |
| Sum of Frequencies Read                                                                                                           |       | 2513                     |
| Sum of Frequencies Used                                                                                                           |       | 2513                     |
|                                                                                                                                   |       |                          |
| Response Profile                                                                                                                  |       |                          |
| Ordered Value                                                                                                                     | Shape | Total Frequency          |
| 1                                                                                                                                 | 1     | 1636                     |
| 2                                                                                                                                 | 2     | 731                      |
| 3                                                                                                                                 | 3     | 146                      |
|                                                                                                                                   |       |                          |
| The GLIMMIX procedure is modeling the probabilities of levels of Shape having lower Ordered Values in the Response Profile table. |       |                          |

The distribution of the data is multinomial with ordered categories. The ordering is implied by the choice of a link function for the cumulative probabilities. Because a frequency variable is specified, the number of observations as well as the number of frequencies is displayed. Observations with zero frequency—that is, foot shape categories that were not observed for a particular sire are not used in the analysis. The “Response Profile Table” shows the ordering of the response variable and gives a breakdown of the frequencies by category.

**Output 41.11.2** Information about the Size of the Optimization Problem

| Dimensions               |    |
|--------------------------|----|
| G-side Cov. Parameters   | 1  |
| Columns in X             | 6  |
| Columns in Z per Subject | 1  |
| Subjects (Blocks in V)   | 34 |
| Max Obs per Subject      | 3  |

**Output 41.11.2** *continued*

| Optimization Information   |                   |
|----------------------------|-------------------|
| Optimization Technique     | Dual Quasi-Newton |
| Parameters in Optimization | 7                 |
| Lower Boundaries           | 1                 |
| Upper Boundaries           | 0                 |
| Fixed Effects              | Not Profiled      |
| Starting From              | GLM estimates     |
| Quadrature Points          | 1                 |

With `METHOD=QUAD`, the “Dimensions” and “Optimization Information” tables are particularly important, because for this estimation methods both fixed effects and covariance parameters participate in the optimization (Output 41.11.2). For GLM models the optimization involves the fixed effects and possibly a single scale parameter. For mixed models the fixed effects are typically profiled from the optimization. Laplace and quadrature estimations are exceptions to these rules. Consequently, there are seven parameters in this optimization, corresponding to six fixed effects and one variance component. The variance component has a lower bound of 0. Also, because the fixed effects are part of the optimizations, PROC GLIMMIX initially performs a few GLM iterations to obtain starting values for the fixed effects. You can control the number of initial iterations with the `INITITER=` option in the PROC GLIMMIX statement.

The last entry in the “Optimization Information” table shows that—at the starting values—PROC GLIMMIX determined that a single quadrature point is sufficient to approximate the marginal log likelihood with the required accuracy. This approximation is thus identical to the Laplace method that is available with `METHOD=LAPLACE`.

For `METHOD=LAPLACE` and `METHOD=QUAD`, the GLIMMIX procedure produces fit statistics based on the conditional and marginal distribution (Output 41.11.3). Within the limits of the numeric likelihood approximation, the information criteria shown in the “Fit Statistics” table can be used to compare models, and the  $-2$  log likelihood can be used to compare among nested models (nested with respect to fixed effects and/or the covariance parameters).

**Output 41.11.3** Marginal and Conditional Fit Statistics

| Fit Statistics                              |         |
|---------------------------------------------|---------|
| -2 Log Likelihood                           | 3870.12 |
| AIC (smaller is better)                     | 3884.12 |
| AICC (smaller is better)                    | 3884.17 |
| BIC (smaller is better)                     | 3894.81 |
| CAIC (smaller is better)                    | 3901.81 |
| HQIC (smaller is better)                    | 3887.76 |
| Fit Statistics for Conditional Distribution |         |
| -2 log L(Shape   r. effects)                | 3807.62 |

The variance of the sire effect is estimated as 0.04849 with estimated asymptotic standard error of 0.01673 (Output 41.11.4). Based on the magnitude of the estimate relative to the standard error, one might conclude that there is significant sire-to-sire variability. Because parameter estimation is based on maximum likelihood, a formal test of the hypothesis of no sire variability is possible. The category cutoffs for the cumulative probabilities are 0.3781 and 1.6435. Except for b3, all fixed effects contrasts are significant.

#### Output 41.11.4 Parameter Estimates

| Covariance Parameter Estimates |           |          |                |      |                |         |
|--------------------------------|-----------|----------|----------------|------|----------------|---------|
|                                | Cov Parm  | Subject  | Estimate       |      | Standard Error |         |
|                                | Intercept | sire     | 0.04849        |      | 0.01673        |         |
| Solutions for Fixed Effects    |           |          |                |      |                |         |
| Effect                         | Shape     | Estimate | Standard Error | DF   | t Value        | Pr >  t |
| Intercept                      | 1         | 0.3781   | 0.04907        | 29   | 7.71           | <.0001  |
| Intercept                      | 2         | 1.6435   | 0.05930        | 29   | 27.72          | <.0001  |
| yr                             |           | 0.1422   | 0.04834        | 2478 | 2.94           | 0.0033  |
| b1                             |           | 0.3781   | 0.07154        | 2478 | 5.28           | <.0001  |
| b2                             |           | 0.3157   | 0.09709        | 2478 | 3.25           | 0.0012  |
| b3                             |           | -0.09887 | 0.06508        | 2478 | -1.52          | 0.1289  |

A likelihood ratio test for the sire variability can be carried out by adding a **COVTEST** statement to the PROC GLIMMIX statements (Output 41.11.5):

```
ods select FitStatistics CovParms Covtests;
proc glimmix data=footshape method=quad;
 class sire;
 model Shape = yr b1 b2 b3 / link=cumprobit dist=multinomial;
 random int / sub=sire;
 covtest GLM;
 freq count;
run;
```

The statement

```
covtest GLM;
```

compares the fitted model to a generalized linear model for independent data by removing the sire variance component from the model. Equivalently, you can specify

```
covtest 0;
```

which compares the fitted model against one where the sire variance is fixed at zero.

**Output 41.11.5** Likelihood Ratio Test for Sire Variance

| The GLIMMIX Procedure                                     |         |             |                |            |         |
|-----------------------------------------------------------|---------|-------------|----------------|------------|---------|
| Fit Statistics                                            |         |             |                |            |         |
| -2 Log Likelihood                                         |         |             |                |            | 3870.12 |
| AIC (smaller is better)                                   |         |             |                |            | 3884.12 |
| AICC (smaller is better)                                  |         |             |                |            | 3884.17 |
| BIC (smaller is better)                                   |         |             |                |            | 3894.81 |
| CAIC (smaller is better)                                  |         |             |                |            | 3901.81 |
| HQIC (smaller is better)                                  |         |             |                |            | 3887.76 |
| Covariance Parameter Estimates                            |         |             |                |            |         |
| Cov Parm                                                  | Subject | Estimate    | Standard Error |            |         |
| Intercept                                                 | sire    | 0.04849     | 0.01673        |            |         |
| Tests of Covariance Parameters<br>Based on the Likelihood |         |             |                |            |         |
| Label                                                     | DF      | -2 Log Like | ChiSq          | Pr > ChiSq | Note    |
| Independence                                              | 1       | 3915.29     | 45.17          | <.0001     | MI      |
| MI: P-value based on a mixture of chi-squares.            |         |             |                |            |         |

The  $-2$  Log Likelihood in the reduced model without the sire effect is 3915.29. Compared to the corresponding marginal fit statistic in the full model (3870.12), this results in a chi-square statistic of 45.17. Because the variance component for the sire effect has a natural lower bound of zero, PROC GLIMMIX performs the likelihood ratio test as a one-sided test. As indicated by the note, the  $p$ -value for this test is computed from a mixture of chi-square distributions, applying the results of Self and Liang (1987). There is significant evidence that the model without sire random effects does not fit the data as well.

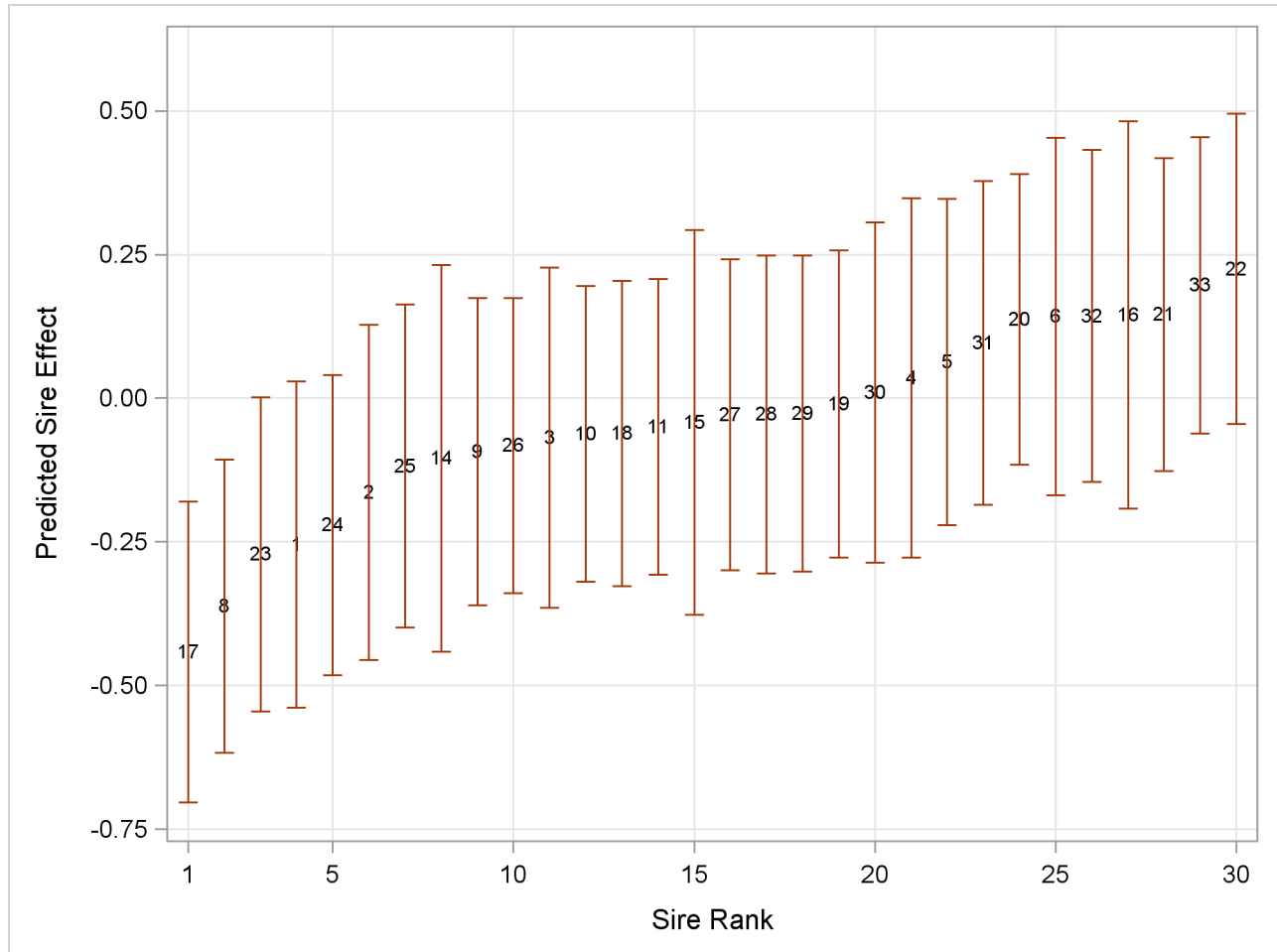
In studies of heritability, one is often interested to rank individuals according to some measure of “breeding value.” The following statements display the empirical Bayes estimates of the sire effects from ML estimation by quadrature along with prediction standard error bars (Output 41.11.6):

```
proc sort data=solr;
 by Estimate;
run;
data solr; set solr;
 length sire $2;
 obs = _n_;
 sire = left(substr(Subject,6,2));
run;
proc sgplot data=solr;
 scatter x=obs y=estimate /
 markerchar = sire
 yerrorupper = upper
 yerrorlower = lower;
```

```

axis grid label='Sire Rank' values=(1 5 10 15 20 25 30);
axis grid label='Predicted Sire Effect';
run;

```

**Output 41.11.6** Ranked Predicted Sire Effects and Prediction Standard Errors

### Example 41.12: Fitting a Marginal (GEE-Type) Model

A marginal GEE-type model for clustered data is a model for correlated data that is specified through a mean function, a variance function, and a “working” covariance structure. Because the assumed covariance structure can be wrong, the covariance matrix of the parameter estimates is not based on the model alone. Rather, one of the empirical (“sandwich”) estimators is used to make inferences robust against the choice of working covariance structure. PROC GLIMMIX can fit marginal models by using R-side random effects and drawing on the distributional specification in the **MODEL** statement to derive the link and variance functions. The **EMPIRICAL=** option in the **PROC GLIMMIX** statement enables you to choose one of a number of empirical covariance estimators.

The data for this example are from Thall and Vail (1990) and reflect the number of seizures of patients suffering from epileptic episodes. After an eight-week period without treatment, patients were observed four times in two-week intervals during which they received a placebo or the drug Progabide in addition to other therapy. These data are also analyzed in [Example 40.7](#) of Chapter 40, “The **GENMOD** Procedure.”

The following DATA step creates the data set seizures. The variable id identifies the subjects in the study, and the variable trt identifies whether a subject received the placebo (trt = 0) or the drug Progabide (trt = 1). The variable x1 takes on value 0 for the baseline measurement and 1 otherwise.

```

data seizures;
 array c{5};
 input id trt c1-c5;
 do i=1 to 5;
 x1 = (i > 1);
 ltime = (i=1)*log(8) + (i ne 1)*log(2);
 cnt = c{i};
 output;
 end;
 keep id cnt x1 trt ltime;
 datalines;
101 1 76 11 14 9 8
102 1 38 8 7 9 4
103 1 19 0 4 3 0
104 0 11 5 3 3 3
106 0 11 3 5 3 3
107 0 6 2 4 0 5
108 1 10 3 6 1 3
110 1 19 2 6 7 4
111 1 24 4 3 1 3
112 1 31 22 17 19 16
113 1 14 5 4 7 4
114 0 8 4 4 1 4
116 0 66 7 18 9 21
117 1 11 2 4 0 4
118 0 27 5 2 8 7
121 1 67 3 7 7 7
122 1 41 4 18 2 5
123 0 12 6 4 0 2
124 1 7 2 1 1 0
126 0 52 40 20 23 12
128 1 22 0 2 4 0
129 1 13 5 4 0 3
130 0 23 5 6 6 5
135 0 10 14 13 6 0
137 1 46 11 14 25 15
139 1 36 10 5 3 8
141 0 52 26 12 6 22
143 1 38 19 7 6 7
145 0 33 12 6 8 4
147 1 7 1 1 2 3
201 0 18 4 4 6 2
202 0 42 7 9 12 14
203 1 36 6 10 8 8
204 1 11 2 1 0 0
205 0 87 16 24 10 9
206 0 50 11 0 0 5
208 1 22 4 3 2 4
209 1 41 8 6 5 7
210 0 18 0 0 3 3

```

```

211 1 32 1 3 1 5
213 0 111 37 29 28 29
214 1 56 18 11 28 13
215 0 18 3 5 2 5
217 0 20 3 0 6 7
218 1 24 6 3 4 0
219 0 12 3 4 3 4
220 0 9 3 4 3 4
221 1 16 3 5 4 3
222 0 17 2 3 3 5
225 1 22 1 23 19 8
226 0 28 8 12 2 8
227 0 55 18 24 76 25
228 1 25 2 3 0 1
230 0 9 2 1 2 1
232 1 13 0 0 0 0
234 0 10 3 1 4 2
236 1 12 1 4 3 2
238 0 47 13 15 13 12
;

```

The model fit initially with the following PROC GLIMMIX statements is a Poisson generalized linear model with effects for an intercept, the baseline measurement, the treatment, and their interaction:

```

proc glimmix data=seizures;
 model cnt = x1 trt x1*trt / dist=poisson offset=ltime
 ddfm=none s;
run;

```

The `DDFM=NONE` option is chosen in the `MODEL` statement to produce chi-square and  $z$  tests instead of  $F$  and  $t$  tests.

Because the initial pretreatment time period is four times as long as the subsequent measurement intervals, an offset variable is used to standardize the counts. If  $Y_{ij}$  denotes the number of seizures of subject  $i$  in time interval  $j$  of length  $t_j$ , then  $Y_{ij}/t_j$  is the number of seizures per time unit. Modeling the average number per time unit with a log link leads to  $\log\{E[Y_{ij}/t_j]\} = \mathbf{x}'\boldsymbol{\beta}$  or  $\log\{E[Y_{ij}]\} = \mathbf{x}'\boldsymbol{\beta} + \log\{t_j\}$ . The logarithm of time (variable `ltime`) thus serves as an offset. Suppose that  $\beta_0$  denotes the intercept,  $\beta_1$  the effect of `x1`, and  $\beta_2$  the effect of `trt`. Then  $\exp\{\beta_0\}$  is the expected number of seizures per week in the placebo group at baseline. The corresponding numbers in the treatment group are  $\exp\{\beta_0 + \beta_2\}$  at baseline and  $\exp\{\beta_0 + \beta_1 + \beta_2\}$  for postbaseline visits.

The “Model Information” table shows that the parameters in this Poisson model are estimated by maximum likelihood (Output 41.12.1). In addition to the default link and variance function, the variable `ltime` is used as an offset.

**Output 41.12.1** Model Information in Poisson GLM

| The GLIMMIX Procedure     |                    |
|---------------------------|--------------------|
| Model Information         |                    |
| Data Set                  | WORK.SEIZURES      |
| Response Variable         | cnt                |
| Response Distribution     | Poisson            |
| Link Function             | Log                |
| Variance Function         | Default            |
| Offset Variable           | ltime              |
| Variance Matrix           | Diagonal           |
| Estimation Technique      | Maximum Likelihood |
| Degrees of Freedom Method | None               |

Fit statistics and parameter estimates are shown in [Output 41.12.2](#).

**Output 41.12.2** Results from Fitting Poisson GLM

| Fit Statistics           |          |                |       |         |         |
|--------------------------|----------|----------------|-------|---------|---------|
| -2 Log Likelihood        |          |                |       |         | 3442.66 |
| AIC (smaller is better)  |          |                |       |         | 3450.66 |
| AICC (smaller is better) |          |                |       |         | 3450.80 |
| BIC (smaller is better)  |          |                |       |         | 3465.34 |
| CAIC (smaller is better) |          |                |       |         | 3469.34 |
| HQIC (smaller is better) |          |                |       |         | 3456.54 |
| Pearson Chi-Square       |          |                |       |         | 3015.16 |
| Pearson Chi-Square / DF  |          |                |       |         | 10.54   |
| Parameter Estimates      |          |                |       |         |         |
| Effect                   | Estimate | Standard Error | DF    | t Value | Pr >  t |
| Intercept                | 1.3476   | 0.03406        | Infty | 39.57   | <.0001  |
| x1                       | 0.1108   | 0.04689        | Infty | 2.36    | 0.0181  |
| trt                      | -0.1080  | 0.04865        | Infty | -2.22   | 0.0264  |
| x1*trt                   | -0.3016  | 0.06975        | Infty | -4.32   | <.0001  |

Because this is a generalized linear model, the large value for the ratio of the Pearson chi-square statistic and its degrees of freedom is indicative of a model shortcoming. The data are considerably more dispersed than is expected under a Poisson model. There could be many reasons for this overdispersion—for example, a misspecified mean model, data that might not be Poisson distributed, an incorrect variance function, and correlations among the observations. Because these data are repeated measurements, the presence of correlations among the observations from the same subject is a likely contributor to the overdispersion.

The following PROC GLIMMIX statements fit a marginal model with correlations. The model is a marginal one, because no G-side random effects are specified on which the distribution could be conditioned. The choice of the id variable as the **SUBJECT** effect indicates that observations from different IDs are uncorre-



lated. Observations from the same ID are assumed to follow a compound symmetry (equicorrelation) model. The **EMPIRICAL** option in the **PROC GLIMMIX** statement requests the classical sandwich estimator as the covariance estimator for the fixed effects:

```
proc glimmix data=seizures empirical;
 class id;
 model cnt = x1 trt x1*trt / dist=poisson offset=ltime
 ddfm=none covb s;
 random _residual_ / subject=id type=cs vcorr;
run;
```

The “Model Information” table shows that the parameters are now estimated by residual pseudo-likelihood (compare [Output 41.12.3](#) and [Output 41.12.1](#)). And in this fact lies the main difference between fitting marginal models with PROC GLIMMIX and with GEE methods as per Liang and Zeger (1986), where parameters of the working correlation matrix are estimated by the method of moments.

**Output 41.12.3** Model Information in Marginal Model

| The GLIMMIX Procedure       |                      |
|-----------------------------|----------------------|
| Model Information           |                      |
| Data Set                    | WORK.SEIZURES        |
| Response Variable           | cnt                  |
| Response Distribution       | Poisson              |
| Link Function               | Log                  |
| Variance Function           | Default              |
| Offset Variable             | ltime                |
| Variance Matrix Blocked By  | id                   |
| Estimation Technique        | Residual PL          |
| Degrees of Freedom Method   | None                 |
| Fixed Effects SE Adjustment | Sandwich - Classical |

According to the compound symmetry model, there is substantial correlation among the observations from the same subject ([Output 41.12.4](#)).

**Output 41.12.4** Covariance Parameter Estimates and Correlation Matrix

| Estimated V Correlation Matrix for id 101 |        |        |        |        |        |
|-------------------------------------------|--------|--------|--------|--------|--------|
| Row                                       | Col1   | Col2   | Col3   | Col4   | Col5   |
| 1                                         | 1.0000 | 0.6055 | 0.6055 | 0.6055 | 0.6055 |
| 2                                         | 0.6055 | 1.0000 | 0.6055 | 0.6055 | 0.6055 |
| 3                                         | 0.6055 | 0.6055 | 1.0000 | 0.6055 | 0.6055 |
| 4                                         | 0.6055 | 0.6055 | 0.6055 | 1.0000 | 0.6055 |
| 5                                         | 0.6055 | 0.6055 | 0.6055 | 0.6055 | 1.0000 |

**Output 41.12.4** *continued*

| Covariance Parameter Estimates |         |          |                |
|--------------------------------|---------|----------|----------------|
| Cov Parm                       | Subject | Estimate | Standard Error |
| CS                             | id      | 6.4653   | 1.3833         |
| Residual                       |         | 4.2128   | 0.3928         |

The parameter estimates in [Output 41.12.5](#) are the same as in the Poisson generalized linear model ([Output 41.12.2](#)), because of the balance in these data. The standard errors have increased substantially, however, by taking into account the correlations among the observations.

**Output 41.12.5** GEE-Type Inference for Fixed Effects

| Solutions for Fixed Effects |          |                |       |         |         |
|-----------------------------|----------|----------------|-------|---------|---------|
| Effect                      | Estimate | Standard Error | DF    | t Value | Pr >  t |
| Intercept                   | 1.3476   | 0.1574         | Infty | 8.56    | <.0001  |
| x1                          | 0.1108   | 0.1161         | Infty | 0.95    | 0.3399  |
| trt                         | -0.1080  | 0.1937         | Infty | -0.56   | 0.5770  |
| x1*trt                      | -0.3016  | 0.1712         | Infty | -1.76   | 0.0781  |

| Empirical Covariance Matrix for Fixed Effects |     |          |          |          |          |
|-----------------------------------------------|-----|----------|----------|----------|----------|
| Effect                                        | Row | Col1     | Col2     | Col3     | Col4     |
| Intercept                                     | 1   | 0.02476  | -0.00115 | -0.02476 | 0.001152 |
| x1                                            | 2   | -0.00115 | 0.01348  | 0.001152 | -0.01348 |
| trt                                           | 3   | -0.02476 | 0.001152 | 0.03751  | -0.00300 |
| x1*trt                                        | 4   | 0.001152 | -0.01348 | -0.00300 | 0.02931  |

## Example 41.13: Response Surface Comparisons with Multiplicity Adjustments

Koch et al. (1990) present data for a multicenter clinical trial testing the efficacy of a respiratory drug in patients with respiratory disease. Within each of two centers, patients were randomly assigned to a placebo (P) or an active (A) treatment. Prior to treatment and at four follow-up visits, patient status was recorded in one of five ordered categories (0=terrible, 1=poor, ..., 4=excellent). The following DATA step creates the SAS data set `clinical` for this study.

```
data Clinical;
 do Center = 1, 2;
 do Gender = 'F', 'M';
 do Drug = 'A', 'P';
```

```

 input nPatient @@;
 do iPatient = 1 to nPatient;
 input ID Age (t0-t4) (1.) @@;
 output;
 end;
 end;
end;
end;
end;
datalines;
2 53 32 12242 18 47 22344
5 5 13 44444 19 31 21022 25 35 10000 28 36 23322
 36 45 22221
25 54 11 44442 12 14 23332 51 15 02333 20 20 33231
 16 22 12223 50 22 21344 3 23 33443 32 23 23444
 56 25 23323 35 26 12232 26 26 22222 21 26 24142
 8 28 12212 30 28 00121 33 30 33442 11 30 34443
 42 31 12311 9 31 33444 37 31 02321 23 32 34433
 6 34 11211 22 46 43434 24 48 23202 38 50 22222
 48 57 33434
24 43 13 34444 41 14 22123 34 15 22332 29 19 23300
 15 20 44444 13 23 33111 27 23 44244 55 24 34443
 17 25 11222 45 26 24243 40 26 12122 44 27 12212
 49 27 33433 39 23 21111 2 28 20000 14 30 10000
 31 37 10000 10 37 32332 7 43 23244 52 43 11132
 4 44 34342 1 46 22222 46 49 22222 47 63 22222
4 30 37 13444 52 39 23444 23 60 44334 54 63 44444
12 28 31 34444 5 32 32234 21 36 33213 50 38 12000
 1 39 12112 48 39 32300 7 44 34444 38 47 23323
 8 48 22100 11 48 22222 4 51 34244 17 58 14220
23 12 13 44444 10 14 14444 27 19 33233 47 20 24443
 16 20 21100 29 21 33444 20 24 44444 25 25 34331
 15 25 34433 2 25 22444 9 26 23444 49 28 23221
 55 31 44444 43 34 24424 26 35 44444 14 37 43224
 36 41 34434 51 43 33442 37 52 12122 19 55 44444
 32 55 22331 3 58 44444 53 68 23334
16 39 11 34444 40 14 21232 24 15 32233 41 15 43334
 33 19 42233 34 20 32444 13 20 14444 45 33 33323
 22 36 24334 18 38 43000 35 42 32222 44 43 21000
 6 45 34212 46 48 44000 31 52 23434 42 66 33344
;

```

Westfall and Tobias (2007) define as the measure of efficacy the average of the ratings at the final two visits and model this average as a function of drug, baseline assessment score, and age. Hence, in their model, the expected efficacy for drug  $d \in A, P$  can be written as

$$E[Y_d] = \beta_{0d} + \beta_{1d}t + \beta_{2d}a$$

where  $t$  is the baseline (pretreatment) assessment score and  $a$  is the patient's age at baseline. The age range for these data extends from 11 to 68 years. Suppose that the scientific question of interest is the comparison of the two response surfaces at a set of values  $S_t \times S_a = \{0, 1, 2, 3, 4\} \times S_a$ . In other words, you want to know for which values of the covariates the average response differs significantly between the treatment group and the placebo group. If the set of ages of interest is  $\{10, 13, 16, \dots, 70\}$ , then this involves  $5 \times 21 = 105$  comparisons, a massive multiple testing problem. The large number of comparisons and the

fact that the set  $S_a$  is chosen somewhat arbitrarily require the application of multiplicity corrections in order to protect the familywise Type I error across the comparisons.

When testing hypotheses that have logical restrictions, the power of multiplicity corrected tests can be increased by taking the restrictions into account. Logical restrictions exist, for example, when not all hypotheses in a set can be simultaneously true. Westfall and Tobias (2007) extend the truncated closed testing procedure (TCTP) of Royen (1989) for pairwise comparisons in ANOVA to general contrasts. Their work is also an extension of the S2 method of Shaffer (1986); see also Westfall (1997). These methods are all *monotonic* in the (unadjusted)  $p$ -values of the individual tests, in the sense that if  $p_j < p_i$  then the multiple test will never retain  $H_j$  while rejecting  $H_i$ . In terms of multiplicity-adjusted  $p$ -values  $\tilde{p}_j$ , monotonicity means that if  $p_j < p_i$ , then  $\tilde{p}_j < \tilde{p}_i$ .

### Analysis as Normal Data with Averaged Endpoints

In order to apply the extended TCTP procedure of Westfall and Tobias (2007) to the problem of comparing response surfaces in the clinical trial, the following convenience macro is helpful to generate the comparisons for the `ESTIMATE` statement in PROC GLIMMIX:

```
%macro Contrast (from,to,byA,byT) ;
 %let nCmp = 0;
 %do age = &from %to %to %by &byA;
 %do t0 = 0 %to 4 %by &byT;
 %let nCmp = %eval(&nCmp+1);
 %end;
 %end;
 %let iCmp = 0;
 %do age = &from %to %to %by &byA;
 %do t0 = 0 %to 4 %by &byT;
 %let iCmp = %eval(&iCmp+1);
 "%trim(%left(&age)) %trim(%left(&t0))"
 drug 1 -1
 drug*age &age -&age
 drug*t0 &t0 -&t0
 %if (&iCmp < &nCmp) %then %do; , %end;
 %end;
 %end;
%mend;
```

The following GLIMMIX statements fit the model to the data and compute the 105 contrasts that compare the placebo to the active response at 105 points in the two-dimensional regressor space:

```
proc glimmix data=clinical;
 t = (t3+t4)/2;
 class drug;
 model t = drug t0 age drug*age drug*t0;
 estimate %contrast (10,70,3,1)
 / adjust=simulate(seed=1)
 stepdown(type=logical);
 ods output Estimates=EstStepDown;
run;
```

Note that only a single `ESTIMATE` statement is used. Each of the 105 comparisons is one comparison in the multirow statement. The `ADJUST` option in the `ESTIMATE` statement requests multiplicity-adjusted

$p$ -values. The extended TCTP method is applied by specifying the `STEPDOWN(TYPE=LOGICAL)` option to compute step-down-adjusted  $p$ -values where logical constraints among the hypotheses are taken into account. The results from the `ESTIMATE` statement are saved to a data set for subsequent processing. Note also that the response, the average of the ratings at the final two visits, is computed with programming statements in PROC GLIMMIX.

The following statements print the 20 most significant estimated differences (Output 41.13.1):

```
proc sort data=EstStepDown;
 by Probt;
run;
proc print data=EstStepDown(obs=20);
 var Label Estimate StdErr Probt AdjP;
run;
```

**Output 41.13.1** The First 20 Observations of the Estimates Data Set

| Obs | Label | Estimate | StdErr | Probt  | AdjP   |
|-----|-------|----------|--------|--------|--------|
| 1   | 37 2  | 0.8310   | 0.2387 | 0.0007 | 0.0071 |
| 2   | 40 2  | 0.8813   | 0.2553 | 0.0008 | 0.0071 |
| 3   | 34 2  | 0.7806   | 0.2312 | 0.0010 | 0.0071 |
| 4   | 43 2  | 0.9316   | 0.2794 | 0.0012 | 0.0071 |
| 5   | 46 2  | 0.9819   | 0.3093 | 0.0020 | 0.0071 |
| 6   | 31 2  | 0.7303   | 0.2338 | 0.0023 | 0.0081 |
| 7   | 49 2  | 1.0322   | 0.3434 | 0.0033 | 0.0107 |
| 8   | 52 2  | 1.0825   | 0.3807 | 0.0054 | 0.0167 |
| 9   | 40 3  | 0.7755   | 0.2756 | 0.0059 | 0.0200 |
| 10  | 37 3  | 0.7252   | 0.2602 | 0.0063 | 0.0201 |
| 11  | 43 3  | 0.8258   | 0.2982 | 0.0066 | 0.0201 |
| 12  | 28 2  | 0.6800   | 0.2461 | 0.0068 | 0.0215 |
| 13  | 55 2  | 1.1329   | 0.4202 | 0.0082 | 0.0239 |
| 14  | 46 3  | 0.8761   | 0.3265 | 0.0085 | 0.0239 |
| 15  | 34 3  | 0.6749   | 0.2532 | 0.0089 | 0.0257 |
| 16  | 43 1  | 1.0374   | 0.3991 | 0.0107 | 0.0329 |
| 17  | 46 1  | 1.0877   | 0.4205 | 0.0111 | 0.0329 |
| 18  | 49 3  | 0.9264   | 0.3591 | 0.0113 | 0.0329 |
| 19  | 40 1  | 0.9871   | 0.3827 | 0.0113 | 0.0329 |
| 20  | 58 2  | 1.1832   | 0.4615 | 0.0118 | 0.0329 |

Notice that the adjusted  $p$ -values (Adj $p$ ) are larger than the unadjusted  $p$ -values, as expected. Also notice that several comparisons share the same adjusted  $p$ -values. This is a result of the monotonicity of the extended TCTP method.

In order to compare the step-down-adjusted  $p$ -values to adjusted  $p$ -values that do not use step-down methods, replace the `ESTIMATE` statement in the previous statements with the following:

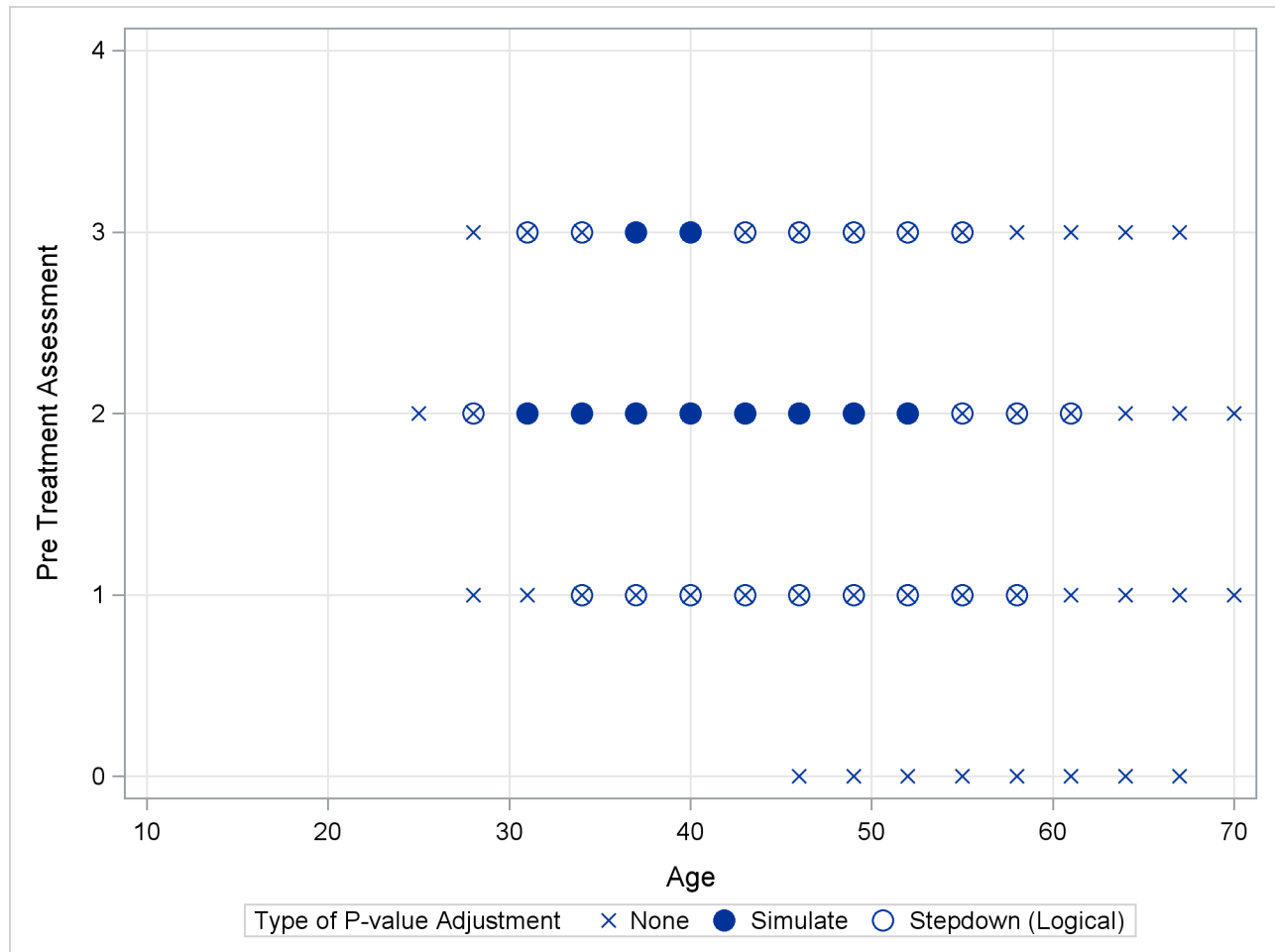
```
estimate %contrast2(10,70,3,1) / adjust=simulate(seed=1);
ods output Estimates=EstAdjust;
```

The following GLIMMIX invocations create output data sets named EstAdjust and EstUnAdjust that contain (non-step-down-) adjusted and unadjusted  $p$ -values:

```
proc glimmix data=clinical;
 t = (t3+t4)/2;
 class drug;
 model t = drug t0 age drug*age drug*t0;
 estimate %contrast(10,70,3,1)
 / adjust=simulate(seed=1);
 ods output Estimates=EstAdjust;
run;
proc glimmix data=clinical;
 t = (t3+t4)/2;
 class drug;
 model t = drug t0 age drug*age drug*t0;
 estimate %contrast(10,70,3,1);
 ods output Estimates=EstUnAdjust;
run;
```

Output 41.13.2 shows a comparison of the significant comparisons ( $p < 0.05$ ) based on unadjusted, adjusted, and step-down (TCTP) adjusted  $p$ -values. Clearly, the unadjusted results indicate the most significant results, but without protecting the Type I error rate for the group of tests. The adjusted  $p$ -values (filled circles) lead to a much smaller region in which the response surfaces between treatment and placebo are significantly different. The increased power of the TCTP procedure (open circles) over the standard multiplicity adjustment—without sacrificing Type I error protection—can be seen in the considerably larger region covered by the open circles.

Output 41.13.2 Comparison of Significance Regions



### Ordinal Repeated Measure Analysis

The outcome variable in this clinical trial is an ordinal rating of patients in categories 0=terrible, 1=poor, 2=fair, 3=good, and 4=excellent. Furthermore, the observations from repeat visits for the same patients are likely correlated. The previous analysis removes the repeated measures aspect by defining efficacy as the average score at the final two visits. These averages are not normally distributed, however. The response surfaces for the two study arms can also be compared based on a model for ordinal data that takes correlation into account through random effects. Keeping with the theme of the previous analysis, the focus here for illustrative purposes is on the final two visits, and the pretreatment assessment score serves as a covariate in the model.

The following DATA step rearranges the data from the third and fourth on-treatment visits in univariate form with separate observations for the visits by patient:

```
data clinical_uv;
 set clinical;
 array time{2} t3-t4;
 do i=1 to 2; rating = time{i}; output; end;
run;
```

The basic model for the analysis is a proportional odds model with cumulative logit link (McCullagh 1980) and  $J = 5$  categories. In this model, separate intercepts (cutoffs) are modeled for the first  $J - 1 = 4$  cumulative categories and the intercepts are monotonically increasing. This guarantees ordering of the cumulative probabilities and nonnegative category probabilities. Using the same covariate structure as in the previous analysis, the probability to observe a rating in at most category  $k \leq 4$  is

$$\Pr(Y_d \leq k) = \frac{1}{1 + \exp\{-\eta_{kd}\}}$$

$$\eta_{kd} = \alpha_k + \beta_{0d} + \beta_{1d}t + \beta_{2d}a$$

Because only the intercepts are dependent on the category, contrasts comparing regression coefficients can be formulated in standard fashion. To accommodate the random and covariance structure of the repeated measures model, a random intercept  $\gamma_i$  is applied to the observations for each patient:

$$\Pr(Y_{id} \leq k) = \frac{1}{1 + \exp\{-\eta_{ikd}\}}$$

$$\eta_{ikd} = \alpha_k + \beta_{0d} + \beta_{1d}t + \beta_{2d}a + \gamma_i$$

$$\gamma_i \sim \text{iid } N(0, \sigma_\gamma^2)$$

The shared random effect of the two observations creates a marginal correlation. Note that the random effects do not depend on category.

The following GLIMMIX statements fit this ordinal repeated measures model by maximum likelihood via the Laplace approximation and compute TCTP-adjusted  $p$ -values for the 105 estimates:

```
proc glimmix data=clinical_uv method=laplace;
 class center id drug;
 model rating = drug t0 age drug*age drug*t0 /
 dist=multinomial link=cumlogit;
 random intercept / subject=id(center);
 covtest 0;
 estimate %contrast(10,70,3,1)
 / adjust=simulate(seed=1)
 stepdown(type=logical);
 ods output Estimates=EstStepDownMulti;
run;
```

The combination of `DIST=MULTINOMIAL` and `LINK=CUMLOGIT` requests the proportional odds model. The `SUBJECT=` effect nests patient IDs within centers, because patient IDs in the data set `clinical` are not unique within centers. (Specifying `SUBJECT=ID*CENTER` would have the same effect.) The `COVTEST` statement requests a likelihood ratio test for the significance of the random patient effect.



The estimate of the variance component for the random patient effect is substantial (Output 41.13.3), but so is its standard error.

### Output 41.13.3 Model and Covariance Parameter Information

| The GLIMMIX Procedure                                     |                       |             |                |            |      |
|-----------------------------------------------------------|-----------------------|-------------|----------------|------------|------|
| Model Information                                         |                       |             |                |            |      |
| Data Set                                                  | WORK.CLINICAL_UV      |             |                |            |      |
| Response Variable                                         | rating                |             |                |            |      |
| Response Distribution                                     | Multinomial (ordered) |             |                |            |      |
| Link Function                                             | Cumulative Logit      |             |                |            |      |
| Variance Function                                         | Default               |             |                |            |      |
| Variance Matrix Blocked By                                | ID(Center)            |             |                |            |      |
| Estimation Technique                                      | Maximum Likelihood    |             |                |            |      |
| Likelihood Approximation                                  | Laplace               |             |                |            |      |
| Degrees of Freedom Method                                 | Containment           |             |                |            |      |
| Covariance Parameter Estimates                            |                       |             |                |            |      |
| Cov Parm                                                  | Subject               | Estimate    | Standard Error |            |      |
| Intercept                                                 | ID(Center)            | 10.3483     | 3.2599         |            |      |
| Tests of Covariance Parameters<br>Based on the Likelihood |                       |             |                |            |      |
| Label                                                     | DF                    | -2 Log Like | ChiSq          | Pr > ChiSq | Note |
| Parameter list                                            | 1                     | 604.70      | 57.64          | <.0001     | MI   |
| MI: P-value based on a mixture of chi-squares.            |                       |             |                |            |      |

The likelihood ratio test provides a better picture of the significance of the variance component. The difference in the  $-2$  log likelihoods is 57.6, highly significant even if one does not apply the Self and Liang (1987) correction that halves the  $p$ -value in this instance.

The results for the 20 most significant estimates are requested with the following statements and shown in Output 41.13.4:

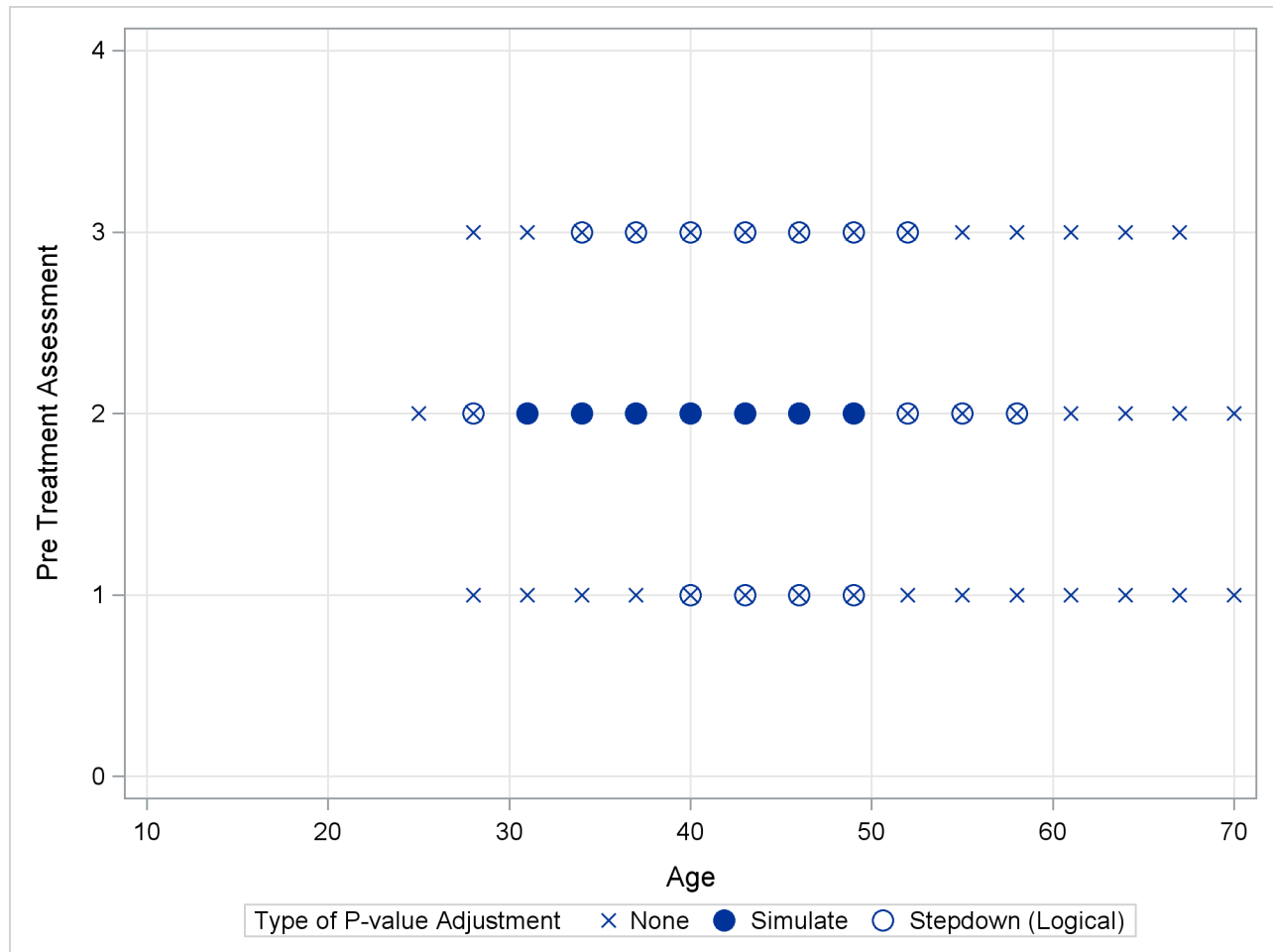
```
proc sort data=EstStepDownMulti;
 by Probt;
run;
proc print data=EstStepDownMulti(obs=20);
 var Label Estimate StdErr Probt AdjP;
run;
```

The  $p$ -values again show the “repeat” pattern corresponding to the monotonicity of the step-down procedure.

**Output 41.13.4** The First 20 Estimates in the Ordinal Analysis

| Obs | Label | Estimate | StdErr | Probt  | AdjP   |
|-----|-------|----------|--------|--------|--------|
| 1   | 37 2  | -2.7224  | 0.8263 | 0.0013 | 0.0133 |
| 2   | 40 2  | -2.8857  | 0.8842 | 0.0015 | 0.0133 |
| 3   | 34 2  | -2.5590  | 0.7976 | 0.0018 | 0.0133 |
| 4   | 43 2  | -3.0491  | 0.9659 | 0.0021 | 0.0133 |
| 5   | 46 2  | -3.2124  | 1.0660 | 0.0032 | 0.0133 |
| 6   | 31 2  | -2.3957  | 0.8010 | 0.0034 | 0.0133 |
| 7   | 49 2  | -3.3758  | 1.1798 | 0.0051 | 0.0164 |
| 8   | 52 2  | -3.5391  | 1.3037 | 0.0077 | 0.0236 |
| 9   | 40 3  | -2.6263  | 0.9718 | 0.0080 | 0.0267 |
| 10  | 37 3  | -2.4630  | 0.9213 | 0.0087 | 0.0267 |
| 11  | 28 2  | -2.2323  | 0.8362 | 0.0088 | 0.0278 |
| 12  | 43 3  | -2.7897  | 1.0451 | 0.0088 | 0.0278 |
| 13  | 46 3  | -2.9530  | 1.1368 | 0.0107 | 0.0291 |
| 14  | 55 2  | -3.7025  | 1.4351 | 0.0112 | 0.0324 |
| 15  | 34 3  | -2.2996  | 0.8974 | 0.0118 | 0.0337 |
| 16  | 49 3  | -3.1164  | 1.2428 | 0.0136 | 0.0344 |
| 17  | 43 1  | -3.3085  | 1.3438 | 0.0154 | 0.0448 |
| 18  | 58 2  | -3.8658  | 1.5722 | 0.0155 | 0.0448 |
| 19  | 40 1  | -3.1451  | 1.2851 | 0.0160 | 0.0448 |
| 20  | 46 1  | -3.4718  | 1.4187 | 0.0160 | 0.0448 |

As previously, the comparisons were also performed with standard  $p$ -value adjustment via simulation. Output 41.13.5 displays the components of the regressor space in which the response surfaces differ significantly ( $p < 0.05$ ) between the two treatment arms. As before, the most significant differences occur with unadjusted  $p$ -values at the cost of protecting only the individual Type I error rate. The standard multiplicity adjustment has considerably less power than the TCTP adjustment.

**Output 41.13.5** Comparison of Significance Regions, Ordinal Analysis

### Example 41.14: Generalized Poisson Mixed Model for Overdispersed Count Data

Overdispersion is the condition by which data appear more dispersed than is expected under a reference model. For count data, the reference models are typically based on the binomial or Poisson distributions. Among the many reasons for overdispersion are an incorrect model, an incorrect distributional specification, incorrect variance functions, positive correlation among the observations, and so forth. In short, correcting an overdispersion problem, if it exists, requires the appropriate remedy. Adding an R-side scale parameter to multiply the variance function is not necessarily the adequate correction. For example, Poisson-distributed data appear overdispersed relative to a Poisson model with regressors when an important regressor is omitted.

If the reference model for count data is Poisson, a number of alternative model formulations are available to increase the dispersion. For example, zero-inflated models add a proportion of zeros (usually from a Bernoulli process) to the zeros of a Poisson process. Hurdle models are two-part models where zeros and nonzeros are generated by different stochastic processes. Zero-inflated and hurdle models are described in detail by Cameron and Trivedi (1998) and cannot be fit with the GLIMMIX procedure. See Section 15.5 in Littell et al. (2006) for examples of using the NLMIXED procedure to fit zero-inflated and hurdle models.

An alternative approach is to derive from the reference distribution a probability distribution that exhibits increased dispersion. By mixing a Poisson process with a gamma distribution for the Poisson parameter, for example, the negative binomial distribution results, which is thus overdispersed relative to the Poisson.

Joe and Zhu (2005) show that the generalized Poisson distribution can also be motivated as a Poisson mixture and hence provides an alternative to the negative binomial (NB) distribution. Like the NB, the generalized Poisson distribution has a scale parameter. It is heavier in the tails than the NB distribution and easily reduces to the standard Poisson. Joe and Zhu (2005) discuss further comparisons between these distributions.

The probability mass function of the generalized Poisson is given by

$$p(y) = \frac{\alpha}{y!} (\alpha + \xi y)^{y-1} \exp \{-\alpha - \xi y\}$$

where  $y = 0, 1, 2, \dots$ ,  $\alpha > 0$ , and  $0 \leq \xi < 1$  (Joe and Zhu 2005). Notice that for  $\xi = 0$  the mass function of the standard Poisson distribution with mean  $\alpha$  results. The mean and variance of  $Y$  in terms of the parameters  $\alpha$  and  $\xi$  are given by

$$E[Y] = \frac{\alpha}{1 - \xi} = \mu$$

$$\text{Var}[Y] = \frac{\alpha}{(1 - \xi)^3} = \frac{\mu}{(1 - \xi)^2}$$

The log likelihood of the generalized Poisson can thus be written in terms of the mean  $\mu$  and scale parameter  $\xi$  as

$$l(\mu, \xi; y) = \log \{\mu(1 - \xi)\} + (y - 1) \log \{\mu - \xi(\mu - y)\} - (\mu - \xi(\mu - y)) - \log \{\Gamma(y + 1)\}$$

The data in the following DATA step are simulated counts. For each of  $i = 1, \dots, 30$  subjects a randomly varying number  $n_i$  of observations were drawn from a count regression model with a single covariate and excess zeros (compared to a Poisson distribution).

```

data counts;
 input ni @@;
 sub = _n_;
 do i=1 to ni;
 input x y @@;
 output;
 end;
datalines;
1 29 0
6 2 0 82 5 33 0 15 2 35 0 79 0
19 81 0 18 0 85 0 99 0 20 0 26 2 29 0 91 2 37 0 39 0 9 1 33 0
3 0 60 0 87 2 80 0 75 0 3 0 63 1
9 18 0 64 0 80 0 0 0 58 0 7 0 81 0 22 3 50 0
15 91 0 2 1 14 0 5 2 27 1 8 1 95 0 76 0 62 0 26 2 9 0 72 1
98 0 94 0 23 1
2 34 0 95 0
18 48 1 5 0 47 0 44 0 27 0 88 0 27 0 68 0 84 0 86 0 44 0 90 0
63 0 27 0 47 0 25 0 72 0 62 1
13 28 1 31 0 63 0 14 0 74 0 44 0 75 0 65 0 74 1 84 0 57 0 29 0

```

```

 41 0
 9 42 0 8 0 91 0 20 0 23 0 22 0 96 0 83 0 56 0
 3 64 0 64 1 15 0
 4 5 0 73 2 50 1 13 0
 2 0 0 41 0
20 21 0 58 0 5 0 61 1 28 0 71 0 75 1 94 16 51 4 51 2 74 0 1 1
 34 0 7 0 11 0 60 3 31 0 75 0 62 0 54 1
 2 66 1 13 0
 5 83 7 98 1 11 1 28 0 18 0
17 29 5 79 0 39 2 47 2 80 1 19 0 37 0 78 1 26 0 72 1 6 0 50 3
 50 4 97 0 37 2 51 0 45 0
17 47 0 57 0 33 0 47 0 2 0 83 0 74 0 93 0 36 0 53 0 26 0 86 0
 6 0 17 0 30 0 70 1 99 0
 7 91 0 25 1 51 4 20 0 61 1 34 0 33 2
14 60 0 87 0 94 0 29 0 41 0 78 0 50 0 37 0 15 0 39 0 22 0 82 0
 93 0 3 0
16 68 0 26 1 19 0 60 1 93 3 65 0 16 0 79 0 14 0 3 1 90 0 28 3
 82 0 34 0 30 0 81 0
19 48 3 48 1 43 2 54 0 45 9 53 0 14 0 92 5 21 1 20 0 73 0 99 0
 66 0 86 2 63 0 10 0 92 14 44 1 74 0
 8 34 1 44 0 62 0 21 0 7 0 17 0 0 2 49 0
13 11 0 27 2 16 1 12 3 52 1 55 0 2 6 89 5 31 5 28 3 51 5 54 13
 64 0
 9 3 0 36 0 57 0 77 0 41 0 39 0 55 0 57 0 88 1
 7 2 0 80 0 41 1 20 0 2 0 27 0 40 0
18 73 1 66 0 10 0 42 0 22 0 59 9 68 0 34 1 96 0 30 0 13 0 35 0
 51 2 47 0 60 1 55 4 83 3 38 0
17 96 0 40 0 34 0 59 0 12 1 47 0 93 0 50 0 39 0 97 0 19 0 54 0
 11 0 29 0 70 2 87 0 47 0
13 59 0 96 0 47 1 64 0 18 0 30 0 37 0 36 1 69 0 78 1 47 1 86 0
 88 0
15 66 0 45 1 96 1 17 0 91 0 4 0 22 0 5 2 47 0 38 0 80 0 7 1
 38 1 33 0 52 0
12 84 6 60 1 33 1 92 0 38 0 6 0 43 3 13 2 18 0 51 0 50 4 68 0
;

```

The following PROC GLIMMIX statements fit a standard Poisson regression model with random intercepts by maximum likelihood. The marginal likelihood of the data is approximated by adaptive quadrature (METHOD=QUAD).

```

proc glimmix data=counts method=quad;
 class sub;
 model y = x / link=log s dist=poisson;
 random int / subject=sub;
run;

```

Output 41.14.1 displays various informational items about the model and the estimation process.

**Output 41.14.1** Poisson: Model and Optimization Information

| The GLIMMIX Procedure      |                          |             |                    |            |              |
|----------------------------|--------------------------|-------------|--------------------|------------|--------------|
| Model Information          |                          |             |                    |            |              |
| Data Set                   | WORK.COUNTS              |             |                    |            |              |
| Response Variable          | y                        |             |                    |            |              |
| Response Distribution      | Poisson                  |             |                    |            |              |
| Link Function              | Log                      |             |                    |            |              |
| Variance Function          | Default                  |             |                    |            |              |
| Variance Matrix Blocked By | sub                      |             |                    |            |              |
| Estimation Technique       | Maximum Likelihood       |             |                    |            |              |
| Likelihood Approximation   | Gauss-Hermite Quadrature |             |                    |            |              |
| Degrees of Freedom Method  | Containment              |             |                    |            |              |
| Optimization Information   |                          |             |                    |            |              |
| Optimization Technique     | Dual Quasi-Newton        |             |                    |            |              |
| Parameters in Optimization | 3                        |             |                    |            |              |
| Lower Boundaries           | 1                        |             |                    |            |              |
| Upper Boundaries           | 0                        |             |                    |            |              |
| Fixed Effects              | Not Profiled             |             |                    |            |              |
| Starting From              | GLM estimates            |             |                    |            |              |
| Quadrature Points          | 5                        |             |                    |            |              |
| Iteration History          |                          |             |                    |            |              |
| Iteration                  | Restarts                 | Evaluations | Objective Function | Change     | Max Gradient |
| 0                          | 0                        | 4           | 862.57645728       | .          | 366.7105     |
| 1                          | 0                        | 5           | 862.43893582       | 0.13752147 | 22.36158     |
| 2                          | 0                        | 6           | 854.49131023       | 7.94762559 | 28.70814     |
| 3                          | 0                        | 2           | 854.47983504       | 0.01147519 | 6.036114     |
| 4                          | 0                        | 4           | 854.47396189       | 0.00587315 | 4.238363     |
| 5                          | 0                        | 4           | 854.47006558       | 0.00389631 | 0.332454     |
| 6                          | 0                        | 3           | 854.47006484       | 0.00000074 | 0.003104     |

The “Model Information” table shows that the parameters are estimated by ML with quadrature. Using the starting values for fixed effects and covariance parameters that the GLIMMIX procedure generates by default, the procedure determined that five quadrature nodes provide a sufficiently accurate approximation of the marginal log likelihood (“Optimization Information” table). The iterative estimation process converges after nine iterations.

The table of conditional fit statistics displays the sum of the independent contributions to the conditional –2 log likelihood (854.47) and the Pearson statistics for the conditional distribution (Output 41.14.2).

## Output 41.14.2 Poisson: Fit Statistics and Estimates

| Fit Statistics                              |          |                |                |         |         |
|---------------------------------------------|----------|----------------|----------------|---------|---------|
| -2 Log Likelihood                           |          |                | 854.47         |         |         |
| AIC (smaller is better)                     |          |                | 860.47         |         |         |
| AICC (smaller is better)                    |          |                | 860.54         |         |         |
| BIC (smaller is better)                     |          |                | 864.67         |         |         |
| CAIC (smaller is better)                    |          |                | 867.67         |         |         |
| HQIC (smaller is better)                    |          |                | 861.81         |         |         |
| Fit Statistics for Conditional Distribution |          |                |                |         |         |
| -2 log L(y   r. effects)                    |          |                | 777.90         |         |         |
| Pearson Chi-Square                          |          |                | 649.58         |         |         |
| Pearson Chi-Square / DF                     |          |                | 1.97           |         |         |
| Covariance Parameter Estimates              |          |                |                |         |         |
| Cov Parm                                    | Subject  | Estimate       | Standard Error |         |         |
| Intercept                                   | sub      | 1.1959         | 0.4334         |         |         |
| Solutions for Fixed Effects                 |          |                |                |         |         |
| Effect                                      | Estimate | Standard Error | DF             | t Value | Pr >  t |
| Intercept                                   | -1.4947  | 0.2745         | 29             | -5.45   | <.0001  |
| x                                           | 0.01207  | 0.002387       | 299            | 5.06    | <.0001  |

The departure of the scaled Pearson statistic from 1.0 is fairly pronounced in this case (1.97). If one deems it to far from 1.0, however, the conclusion has to be that the conditional variation is not properly specified. This could be due to an incorrect variance function, for example. The “Solutions for Fixed Effects” table shows the estimates of the slope and intercept in this model along with their standard errors and tests of significance. Note that the slope in this model is highly significant. The variance of the random subject-specific intercepts is estimated as 1.1959.

To fit the generalized Poisson distribution to these data, you cannot draw on the built-in distributions. Instead, the variance function and the log likelihood are computed directly with PROC GLIMMIX programming statements. The **CLASS**, **MODEL**, and **RANDOM** statements in the following PROC GLIMMIX program are as before, except for the omission of the **DIST=** option in the **MODEL** statement:

```
proc glimmix data=counts method=quad;
 class sub;
 model y = x / link=log s;
 random int / subject=sub;
 xi = (1 - 1/exp(_phi_));
 variance = _mu_ / (1-xi)/(1-xi);
```

```

if (_mu=.) or (_linp_ = .) then _logl_ = .;
else do;
 mustar = _mu_ - xi*(_mu_ - y);
 if (mustar < 1E-12) or (_mu_*(1-xi) < 1e-12) then
 logl = -1E20;
 else do;
 logl = log(_mu_*(1-xi)) + (y-1)*log(mustar) -
 mustar - lgamma(y+1);
 end;
end;
run;

```

The assignments to the variables xi and the reserved symbols `_VARIANCE_` and `_LOGL_` define the variance function and the log likelihood. Because the scale parameter of the generalized Poisson distribution has the range  $0 < \xi < 1$ , and the scale parameter `_PHI_` in the GLIMMIX procedure is bounded only from below (by 0), a reparameterization is applied so that  $\phi = 0 \Leftrightarrow \xi = 0$  and  $\xi$  approaches 1 as  $\phi$  increases. The statements preceding the calculation of the actual log likelihood are intended to prevent floating-point exceptions and to trap missing values.

Output 41.14.3 displays information about the model and estimation process. The “Model Information” table shows that the distribution is not a built-in distribution and echoes the expression for the user-specified variance function. As in the case of the Poisson model, the GLIMMIX procedure determines that five quadrature points are sufficient for accurate estimation of the marginal log likelihood at the starting values. The estimation process converges after 11 iterations.

**Output 41.14.3** Generalized Poisson: Model, Optimization, and Iteration Information

| The GLIMMIX Procedure      |                          |
|----------------------------|--------------------------|
| Model Information          |                          |
| Data Set                   | WORK.COUNTS              |
| Response Variable          | y                        |
| Response Distribution      | User specified           |
| Link Function              | Log                      |
| Variance Function          | $\_mu\_ / (1-xi)/(1-xi)$ |
| Variance Matrix Blocked By | sub                      |
| Estimation Technique       | Maximum Likelihood       |
| Likelihood Approximation   | Gauss-Hermite Quadrature |
| Degrees of Freedom Method  | Containment              |
| Optimization Information   |                          |
| Optimization Technique     | Dual Quasi-Newton        |
| Parameters in Optimization | 4                        |
| Lower Boundaries           | 2                        |
| Upper Boundaries           | 0                        |
| Fixed Effects              | Not Profiled             |
| Starting From              | GLM estimates            |
| Quadrature Points          | 5                        |



Output 41.14.3 *continued*

| Iteration History |          |             |                    |            |              |
|-------------------|----------|-------------|--------------------|------------|--------------|
| Iteration         | Restarts | Evaluations | Objective Function | Change     | Max Gradient |
| 0                 | 0        | 4           | 716.12976769       | .          | 161.1184     |
| 1                 | 0        | 5           | 716.07585953       | 0.05390816 | 11.88788     |
| 2                 | 0        | 4           | 714.27148068       | 1.80437884 | 36.09657     |
| 3                 | 0        | 2           | 711.02643265       | 3.24504804 | 108.4615     |
| 4                 | 0        | 2           | 710.26952196       | 0.75691069 | 216.9822     |
| 5                 | 0        | 2           | 709.96824991       | 0.30127205 | 96.2775      |
| 6                 | 0        | 3           | 709.8419071        | 0.12634280 | 19.07487     |
| 7                 | 0        | 3           | 709.83122731       | 0.01067980 | 0.649164     |
| 8                 | 0        | 3           | 709.83047646       | 0.00075085 | 2.127665     |
| 9                 | 0        | 3           | 709.83046461       | 0.00001185 | 0.383319     |
| 10                | 0        | 3           | 709.83046436       | 0.00000025 | 0.010279     |

The achieved  $-2 \log$  likelihood is lower than in the Poisson model (compare “Fit Statistics” tables in [Output 41.14.4](#) and [Output 41.14.1](#)). The scaled Pearson statistic is now less than 1.0. The fixed slope estimate remains significant at the 5% level, but the test statistics are not as large as in the Poisson model, partly because the generalized Poisson model permits more variation.

## Output 41.14.4 Generalized Poisson: Fit Statistics and Estimates

| Fit Statistics                              |         |          |                |
|---------------------------------------------|---------|----------|----------------|
| -2 Log Likelihood                           |         |          | 709.83         |
| AIC (smaller is better)                     |         |          | 717.83         |
| AICC (smaller is better)                    |         |          | 717.95         |
| BIC (smaller is better)                     |         |          | 723.44         |
| CAIC (smaller is better)                    |         |          | 727.44         |
| HQIC (smaller is better)                    |         |          | 719.62         |
| Fit Statistics for Conditional Distribution |         |          |                |
| -2 log L(y   r. effects)                    |         |          | 665.56         |
| Pearson Chi-Square                          |         |          | 241.42         |
| Pearson Chi-Square / DF                     |         |          | 0.73           |
| Covariance Parameter Estimates              |         |          |                |
| Cov Parm                                    | Subject | Estimate | Standard Error |
| Intercept                                   | sub     | 0.5135   | 0.2400         |
| Scale                                       |         | 0.6401   | 0.09718        |

**Output 41.14.4** continued

| Solutions for Fixed Effects |          |                |     |         |         |
|-----------------------------|----------|----------------|-----|---------|---------|
| Effect                      | Estimate | Standard Error | DF  | t Value | Pr >  t |
| Intercept                   | -0.7264  | 0.2749         | 29  | -2.64   | 0.0131  |
| x                           | 0.003742 | 0.003537       | 299 | 1.06    | 0.2910  |

Based on the large difference in the  $-2 \log$  likelihoods between the Poisson and generalized Poisson models, you conclude that a mixed model based on the latter provides a better fit to these data. From the “Covariance Parameter Estimates” table in [Output 41.14.4](#), you can see that the estimate of the scale parameter is  $\hat{\phi} = 0.6401$  and is considerably larger than 0, taking into account its standard error. The hypothesis  $H: \phi = 0$ , which articulates that a Poisson model fits the data as well as the generalized Poisson model, can be formally tested with a likelihood ratio test. Adding the following statement to the previous PROC GLIMMIX run compares the model to one in which the variance of the random intercepts (the first covariance parameter) is not constrained and the scale parameter is fixed at zero:

```
covtest 'H: phi = 0' . 0 / est;
```

This **COVTEST** statement produces [Output 41.14.5](#).

**Output 41.14.5** Likelihood Ratio Test for Poisson Assumption

| Tests of Covariance Parameters<br>Based on the Likelihood |    |             |        |            |                    |          |      |
|-----------------------------------------------------------|----|-------------|--------|------------|--------------------|----------|------|
| Label                                                     | DF | -2 Log Like | ChiSq  | Pr > ChiSq | ---Estimates H0--- |          | Note |
|                                                           |    |             |        |            | Est1               | Est2     |      |
| H:phi = 0                                                 | 1  | 854.47      | 144.64 | <.0001     | 1.1959             | 1.11E-12 | MI   |

MI: P-value based on a mixture of chi-squares.

Note that the  $-2 \log$  Like reported in [Output 41.14.5](#) agrees with the value reported in the “Fit Statistics” table for the Poisson model ([Output 41.14.2](#)) and that the estimate of the random intercept under the null hypothesis agrees with the “Covariance Parameter Estimates” table in [Output 41.14.2](#). Because the null hypothesis places the parameter  $\phi$  (or  $\xi$ ) on the boundary of the parameter space, a mixture correction is applied in the  $p$ -value calculation. Because of the magnitude of the likelihood ratio statistic (144.64), this correction has no effect on the displayed  $p$ -value.

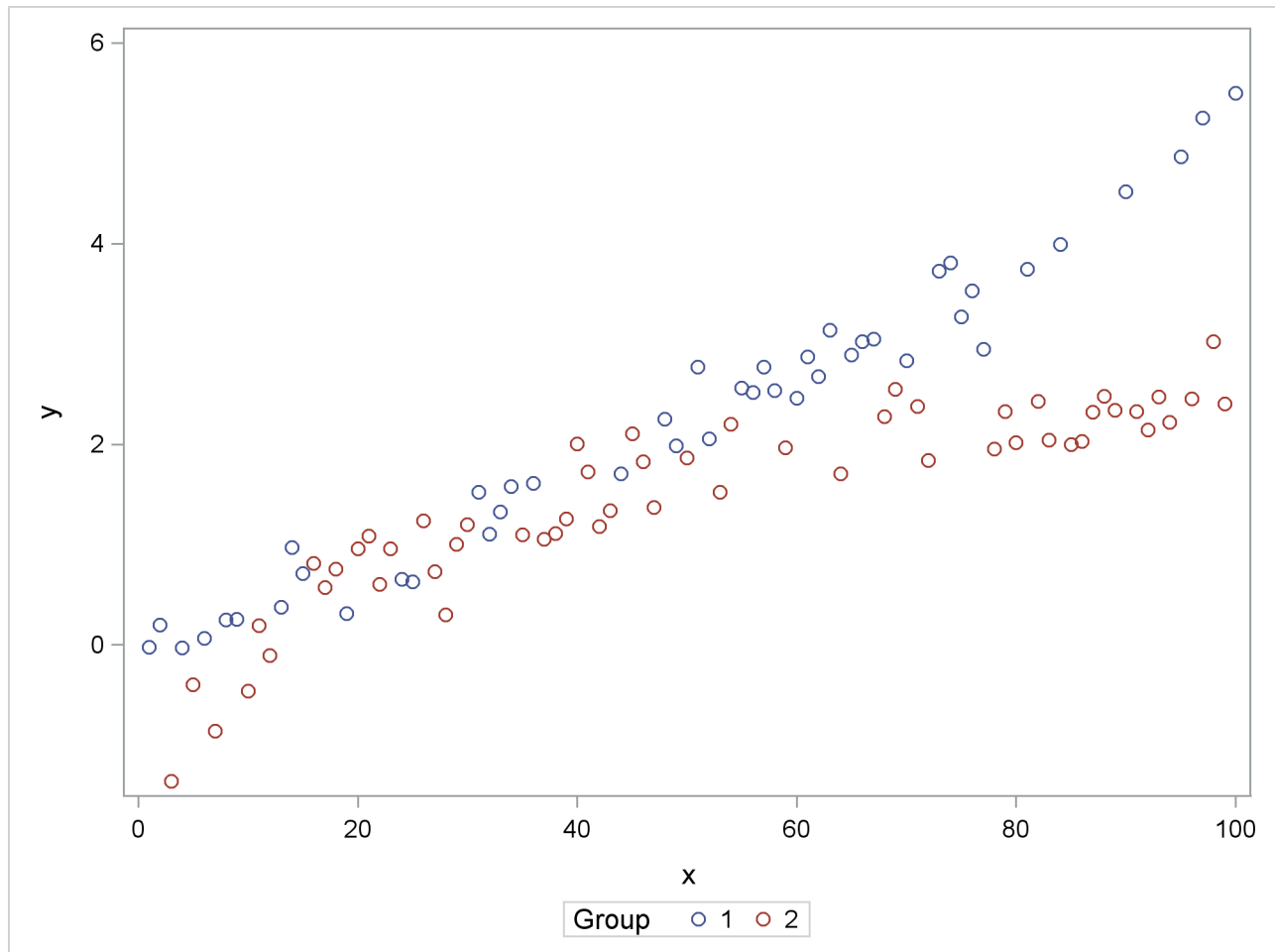
## Example 41.15: Comparing Multiple B-Splines

This example uses simulated data to demonstrate the use of the nonpositional syntax (see the section “[Positional and Nonpositional Syntax for Contrast Coefficients](#)” on page 3097 for details) in combination with the experimental `EFFECT` statement to produce interesting predictions and comparisons in models containing fixed spline effects. Consider the data in the following `DATA` step. Each of the 100 observations for the continuous response variable `y` is associated with one of two groups.

```
data spline;
 input group y @@;
 x = _n_;
 datalines;
1 -.020 1 0.199 2 -1.36 1 -.026
2 -.397 1 0.065 2 -.861 1 0.251
1 0.253 2 -.460 2 0.195 2 -.108
1 0.379 1 0.971 1 0.712 2 0.811
2 0.574 2 0.755 1 0.316 2 0.961
2 1.088 2 0.607 2 0.959 1 0.653
1 0.629 2 1.237 2 0.734 2 0.299
2 1.002 2 1.201 1 1.520 1 1.105
1 1.329 1 1.580 2 1.098 1 1.613
2 1.052 2 1.108 2 1.257 2 2.005
2 1.726 2 1.179 2 1.338 1 1.707
2 2.105 2 1.828 2 1.368 1 2.252
1 1.984 2 1.867 1 2.771 1 2.052
2 1.522 2 2.200 1 2.562 1 2.517
1 2.769 1 2.534 2 1.969 1 2.460
1 2.873 1 2.678 1 3.135 2 1.705
1 2.893 1 3.023 1 3.050 2 2.273
2 2.549 1 2.836 2 2.375 2 1.841
1 3.727 1 3.806 1 3.269 1 3.533
1 2.948 2 1.954 2 2.326 2 2.017
1 3.744 2 2.431 2 2.040 1 3.995
2 1.996 2 2.028 2 2.321 2 2.479
2 2.337 1 4.516 2 2.326 2 2.144
2 2.474 2 2.221 1 4.867 2 2.453
1 5.253 2 3.024 2 2.403 1 5.498
;
```

The following statements produce a scatter plot of the response variable by group ([Output 41.15.1](#)):

```
proc sgplot data=spline;
 scatter y=y x=x / group=group name="data";
 keylegend "data" / title="Group";
run;
```

**Output 41.15.1** Scatter Plot of Observed Data by Group

The trends in the two groups exhibit curvature, but the type of curvature is not the same in the groups. Also, there appear to be ranges of  $x$  values where the groups are similar and areas where the point scatters separate. To model the trends in the two groups separately and with flexibility, you might want to allow for some smooth trends in  $x$  that vary by group. Consider the following PROC GLIMMIX statements:

```
proc glimmix data=spline outdesign=x;
 class group;
 effect spl = spline(x);
 model y = group spl*group / s noint;
 output out=gmxout pred=p;
run;
```

The **EFFECT** statement defines a constructed effect named `spl` by expanding the `x` into a spline with seven columns. The `group` main effect creates separate intercepts for the groups, and the interaction of the `group` variable with the spline effect creates separate trends. The **NOINT** option suppresses the intercept. This is not necessary and is done here only for convenience of interpretation. The **OUTPUT** statement computes predicted values.

The “Parameter Estimates” table contains the estimates of the group-specific “intercepts,” the spline coefficients varied by group, and the residual variance (“Scale,” [Output 41.15.2](#)).

**Output 41.15.2** Parameter Estimates in Two-Group Spline Model

| The GLIMMIX Procedure |     |       |          |                |    |         |         |
|-----------------------|-----|-------|----------|----------------|----|---------|---------|
| Parameter Estimates   |     |       |          |                |    |         |         |
| Effect                | spl | group | Estimate | Standard Error | DF | t Value | Pr >  t |
| group                 |     | 1     | 9.7027   | 3.1342         | 86 | 3.10    | 0.0026  |
| group                 |     | 2     | 6.3062   | 2.6299         | 86 | 2.40    | 0.0187  |
| spl*group             | 1   | 1     | -11.1786 | 3.7008         | 86 | -3.02   | 0.0033  |
| spl*group             | 1   | 2     | -20.1946 | 3.9765         | 86 | -5.08   | <.0001  |
| spl*group             | 2   | 1     | -9.5327  | 3.2576         | 86 | -2.93   | 0.0044  |
| spl*group             | 2   | 2     | -5.8565  | 2.7906         | 86 | -2.10   | 0.0388  |
| spl*group             | 3   | 1     | -8.9612  | 3.0718         | 86 | -2.92   | 0.0045  |
| spl*group             | 3   | 2     | -5.5567  | 2.5717         | 86 | -2.16   | 0.0335  |
| spl*group             | 4   | 1     | -7.2615  | 3.2437         | 86 | -2.24   | 0.0278  |
| spl*group             | 4   | 2     | -4.3678  | 2.7247         | 86 | -1.60   | 0.1126  |
| spl*group             | 5   | 1     | -6.4462  | 2.9617         | 86 | -2.18   | 0.0323  |
| spl*group             | 5   | 2     | -4.0380  | 2.4589         | 86 | -1.64   | 0.1042  |
| spl*group             | 6   | 1     | -4.6382  | 3.7095         | 86 | -1.25   | 0.2146  |
| spl*group             | 6   | 2     | -4.3029  | 3.0479         | 86 | -1.41   | 0.1616  |
| spl*group             | 7   | 1     | 0        | .              | .  | .       | .       |
| spl*group             | 7   | 2     | 0        | .              | .  | .       | .       |
| Scale                 |     |       | 0.07352  | 0.01121        | .  | .       | .       |

Because the B-spline coefficients for an observation sum to 1 and the model contains group-specific constants, the last spline coefficient in each group is zero. In other words, you can achieve exactly the same fit with the `MODEL` statement

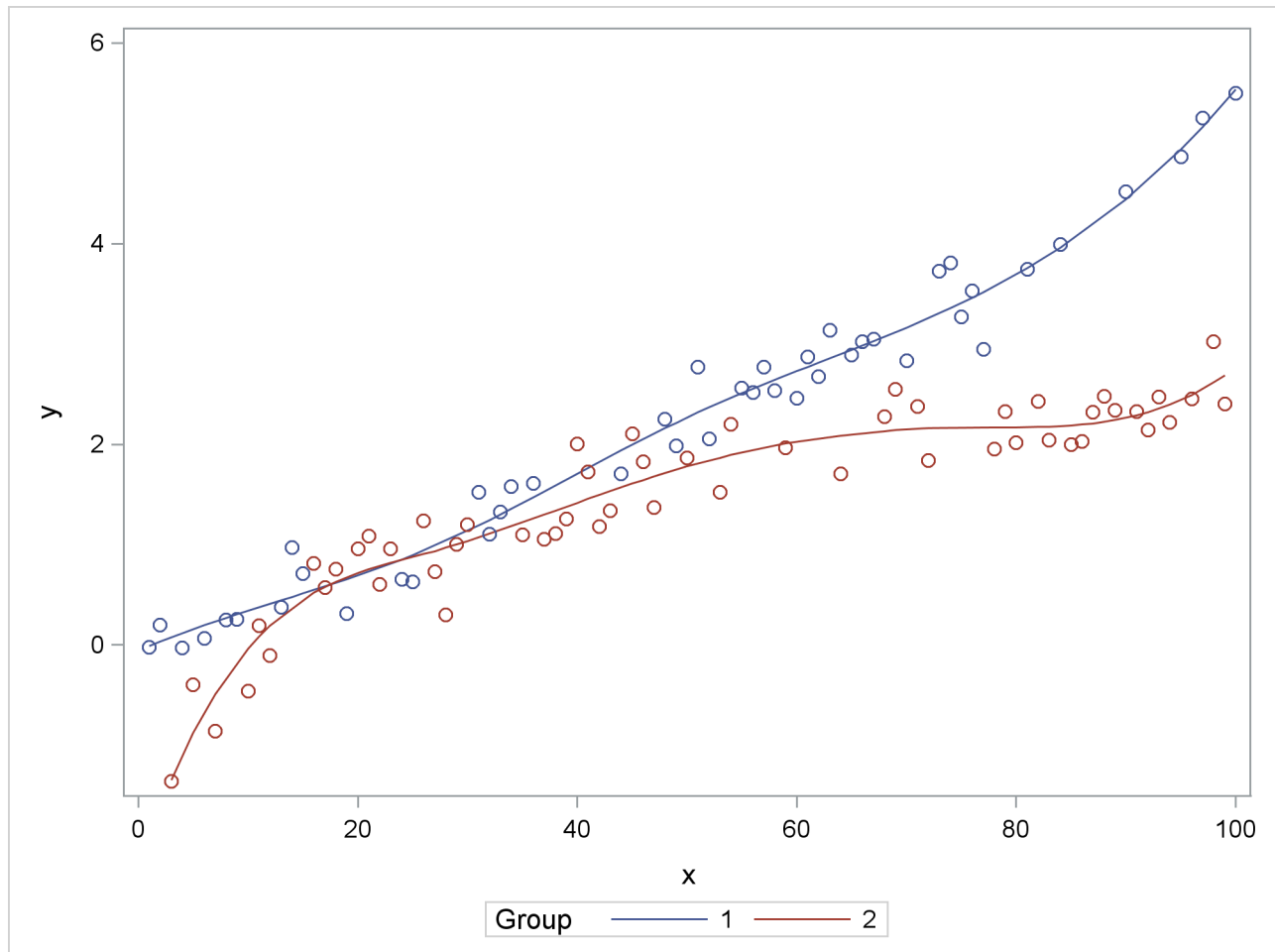
```
model y = spl*group / noint;
```

or

```
model y = spl*group;
```

The following statements graph the observed and fitted values in the two groups (Output 41.15.3):

```
proc sgplot data=gmxout;
 series y=p x=x / group=group name="fit";
 scatter y=y x=x / group=group;
 keylegend "fit" / title="Group";
run;
```

**Output 41.15.3** Observed and Predicted Values by Group

Suppose that you are interested in estimating the mean response at particular values of  $x$  and in performing comparisons of predicted values. The following program uses `ESTIMATE` statements with nonpositional syntax to accomplish this:

```
proc glimmix data=spline;
 class group;
 effect spl = spline(x);
 model y = group spl*group / s noint;
 estimate 'Group 1, x=20' group 1 group*spl [1,1 20] / e;
 estimate 'Group 2, x=20' group 0 1 group*spl [1,2 20];
 estimate 'Diff at x=20 ' group 1 -1 group*spl [1,1 20] [-1,2 20];
run;
```

The first **ESTIMATE** statement predicts the mean response at  $x = 20$  in group 1. The **E** option requests the coefficient vector for this linear combination of the parameter estimates. The coefficient for the group effect is entered with positional (standard) syntax. The coefficients for the **group\*spl** effect are formed based on nonpositional syntax. Because this effect comprises the interaction of a standard effect (**group**) with a constructed effect, the values and levels for the standard effect must precede those for the constructed effect. A similar statement produces the predicted mean at  $x = 20$  in group 2.

The GLIMMIX procedure interprets the syntax

```
group*spl [1,2 20]
```

as follows: construct the spline basis at  $x = 20$  as appropriate for group 2; then multiply the resulting coefficients for these columns of the **L** matrix with 1.

The final **ESTIMATE** statement represents the difference between the predicted values; it is a group comparison at  $x = 20$ .

#### Output 41.15.4 Coefficients from First ESTIMATE Statement

| The GLIMMIX Procedure     |     |       |        |
|---------------------------|-----|-------|--------|
| Coefficients for Estimate |     |       |        |
| Group 1, x=20             |     |       |        |
| Effect                    | spl | group | Row1   |
| group                     |     | 1     | 1      |
| group                     |     | 2     |        |
| spl*group                 | 1   | 1     | 0.0021 |
| spl*group                 | 1   | 2     |        |
| spl*group                 | 2   | 1     | 0.3035 |
| spl*group                 | 2   | 2     |        |
| spl*group                 | 3   | 1     | 0.619  |
| spl*group                 | 3   | 2     |        |
| spl*group                 | 4   | 1     | 0.0754 |
| spl*group                 | 4   | 2     |        |
| spl*group                 | 5   | 1     |        |
| spl*group                 | 5   | 2     |        |
| spl*group                 | 6   | 1     |        |
| spl*group                 | 6   | 2     |        |
| spl*group                 | 7   | 1     |        |
| spl*group                 | 7   | 2     |        |

The “Coefficients” table shows how the value 20 supplied in the **ESTIMATE** statement was expanded into the appropriate spline basis (Output 41.15.4). There is no significant difference between the group means at  $x = 20$  ( $p = 0.8346$ , Output 41.15.5).

## Output 41.15.5 Results from ESTIMATE Statements

| Estimates     |          |                |    |         |         |
|---------------|----------|----------------|----|---------|---------|
| Label         | Estimate | Standard Error | DF | t Value | Pr >  t |
| Group 1, x=20 | 0.6915   | 0.09546        | 86 | 7.24    | <.0001  |
| Group 2, x=20 | 0.7175   | 0.07953        | 86 | 9.02    | <.0001  |
| Diff at x=20  | -0.02602 | 0.1243         | 86 | -0.21   | 0.8346  |

The group comparisons you can achieve in this way are comparable to slices of interaction effects with classification effects. There are, however, no preset number of levels at which to perform the comparisons because  $x$  is continuous. If you add further  $x$  values for the comparisons, a multiplicity correction is in order to control the familywise Type I error. The following statements compare the groups at values  $x = 0, 5, 10, \dots, 80$  and compute simulation-based step-down-adjusted  $p$ -values. The results appear in [Output 41.15.6](#). (The numeric results for simulation-based  $p$ -value adjustments depend slightly on the value of the random number seed.)

```
ods select Estimates;
proc glimmix data=spline;
 class group;
 effect spl = spline(x);
 model y = group spl*group / s;
 estimate 'Diff at x= 0' group 1 -1 group*spl [1,1 0] [-1,2 0],
 'Diff at x= 5' group 1 -1 group*spl [1,1 5] [-1,2 5],
 'Diff at x=10' group 1 -1 group*spl [1,1 10] [-1,2 10],
 'Diff at x=15' group 1 -1 group*spl [1,1 15] [-1,2 15],
 'Diff at x=20' group 1 -1 group*spl [1,1 20] [-1,2 20],
 'Diff at x=25' group 1 -1 group*spl [1,1 25] [-1,2 25],
 'Diff at x=30' group 1 -1 group*spl [1,1 30] [-1,2 30],
 'Diff at x=35' group 1 -1 group*spl [1,1 35] [-1,2 35],
 'Diff at x=40' group 1 -1 group*spl [1,1 40] [-1,2 40],
 'Diff at x=45' group 1 -1 group*spl [1,1 45] [-1,2 45],
 'Diff at x=50' group 1 -1 group*spl [1,1 50] [-1,2 50],
 'Diff at x=55' group 1 -1 group*spl [1,1 55] [-1,2 55],
 'Diff at x=60' group 1 -1 group*spl [1,1 60] [-1,2 60],
 'Diff at x=65' group 1 -1 group*spl [1,1 65] [-1,2 65],
 'Diff at x=70' group 1 -1 group*spl [1,1 70] [-1,2 70],
 'Diff at x=75' group 1 -1 group*spl [1,1 75] [-1,2 75],
 'Diff at x=80' group 1 -1 group*spl [1,1 80] [-1,2 80] /
 adjust=sim(seed=1) stepdown;
run;
```



## Output 41.15.6 Estimates with Multiplicity Adjustments

| The GLIMMIX Procedure                       |          |                |    |         |         |        |
|---------------------------------------------|----------|----------------|----|---------|---------|--------|
| Estimates                                   |          |                |    |         |         |        |
| Adjustment for Multiplicity: Holm-Simulated |          |                |    |         |         |        |
| Label                                       | Estimate | Standard Error | DF | t Value | Pr >  t | Adj P  |
| Diff at x= 0                                | 12.4124  | 4.2130         | 86 | 2.95    | 0.0041  | 0.0210 |
| Diff at x= 5                                | 1.0376   | 0.1759         | 86 | 5.90    | <.0001  | <.0001 |
| Diff at x=10                                | 0.3778   | 0.1540         | 86 | 2.45    | 0.0162  | 0.0554 |
| Diff at x=15                                | 0.05822  | 0.1481         | 86 | 0.39    | 0.6952  | 0.9043 |
| Diff at x=20                                | -0.02602 | 0.1243         | 86 | -0.21   | 0.8346  | 0.9578 |
| Diff at x=25                                | 0.02014  | 0.1312         | 86 | 0.15    | 0.8783  | 0.9578 |
| Diff at x=30                                | 0.1023   | 0.1378         | 86 | 0.74    | 0.4600  | 0.7419 |
| Diff at x=35                                | 0.1924   | 0.1236         | 86 | 1.56    | 0.1231  | 0.2890 |
| Diff at x=40                                | 0.2883   | 0.1114         | 86 | 2.59    | 0.0113  | 0.0465 |
| Diff at x=45                                | 0.3877   | 0.1195         | 86 | 3.24    | 0.0017  | 0.0098 |
| Diff at x=50                                | 0.4885   | 0.1308         | 86 | 3.74    | 0.0003  | 0.0022 |
| Diff at x=55                                | 0.5903   | 0.1231         | 86 | 4.79    | <.0001  | <.0001 |
| Diff at x=60                                | 0.7031   | 0.1125         | 86 | 6.25    | <.0001  | <.0001 |
| Diff at x=65                                | 0.8401   | 0.1203         | 86 | 6.99    | <.0001  | <.0001 |
| Diff at x=70                                | 1.0147   | 0.1348         | 86 | 7.52    | <.0001  | <.0001 |
| Diff at x=75                                | 1.2400   | 0.1326         | 86 | 9.35    | <.0001  | <.0001 |
| Diff at x=80                                | 1.5237   | 0.1281         | 86 | 11.89   | <.0001  | <.0001 |

There are significant differences at the low end and high end of the  $x$  range. Notice that without the multiplicity adjustment you would have concluded at the 0.05 level that the groups are significantly different at  $x = 10$ . At the 0.05 level, the groups separate significantly for  $x < 10$  and  $x > 40$ .

### Example 41.16: Diallel Experiment with Multimember Random Effects

Cockerham and Weir (1977) apply variance component models in the analysis of reciprocal crosses. In these experiments, it is of interest to separate genetically determined variation from variation determined by parentage. This example analyzes the data for the diallel experiment in Cockerham and Weir (1977, Appendix C). A diallel is a mating design that consists of all possible crosses of a set of parental lines. It includes reciprocal crossings, but not self-crossings.

The basic model for a cross is  $Y_{ijk} = \beta + \alpha_{ij} + \epsilon_{ijk}$ , where  $Y_{ijk}$  is the observation for offspring  $k$  from maternal parent  $i$  and paternal parent  $j$ . The various models in Cockerham and Weir (1977) are different decompositions of the term  $\alpha_{ij}$ , the total effect that is due to the parents. Their “bio model” (model (c)) decomposes  $\alpha_{ij}$  into

$$\alpha_{ij} = \eta_i + \eta_j + \mu_i + \phi_j + (\eta\eta)_{ij} + \kappa_{ij}$$

where  $\eta_i$  and  $\eta_j$  are contributions of the female and male parents, respectively. The term  $(\eta\eta)_{ij}$  captures the interaction between maternal and paternal effects. In contrast to usual interaction effects, this term must obey a symmetry because of the reciprocals:  $(\eta\eta)_{ij} = (\eta\eta)_{ji}$ . The terms  $\mu_i$  and  $\phi_j$  in the decomposition are extranuclear maternal and paternal effects, and the remaining interactions are captured by the  $\kappa_{ij}$  term.

The following DATA step creates a SAS data set for the diallel example in Appendix C of Cockerham and Weir (1977):

```

data diallel;
 label time = 'Flowering time in days';
 do p = 1 to 8;
 do m = 1 to 8;
 if (m ne p) then do;
 sym = trim(left(min(m,p))) || ',' || trim(left(max(m,p)));
 do block = 1 to 2;
 input time @@;
 output;
 end;
 end;
 end;
 end;
 datalines;
14.4 16.2 27.2 30.8 17.2 27.0 18.3 20.2 16.2 16.8 18.6 14.4 16.4 16.0
15.4 16.5 14.8 14.6 18.6 18.6 15.2 15.3 17.0 15.2 14.4 14.8 10.8 13.2
31.8 30.4 21.0 23.0 24.6 25.4 19.2 20.0 29.8 28.4 12.8 14.2 13.0 14.4
16.2 17.8 11.4 13.0 16.8 16.3 12.4 14.2 16.8 14.8 12.6 12.2 9.6 11.2
14.6 18.8 12.2 13.6 15.2 15.4 15.2 13.8 18.0 16.0 10.4 12.2 13.4 20.0
20.2 23.4 14.2 14.0 18.6 14.8 22.2 17.0 14.3 17.3 9.0 10.2 11.8 12.8
14.0 16.6 12.2 9.2 13.6 16.2 13.8 14.4 15.6 15.6 15.6 11.0 13.0 9.8
15.2 17.2 10.0 11.6 17.0 18.2 20.8 20.8 20.0 17.4 17.0 12.6 13.0 9.8
;

```

The observations represent mean flowering times of *Nicotiana rustica* (Aztec tobacco) from crosses of inbred varieties grown in two blocks. The variables *p* and *m* identify the eight paternal and maternal lines, respectively. The variable *sym* is used to model the interaction between the parents, subject to the symmetry condition  $(\eta\eta)_{ij} = (\eta\eta)_{ji}$ . For example, the first two observations, 14.4 and 16.2 days, represent the observations from blocks 1 and 2 where paternal line 1 was crossed with maternal line 2.

The following PROC GLIMMIX statements fit the “bio model” in Cockerham and Weir (1977):

```

proc glimmix data=diallel outdesign(z)=zmat;
 class block sym p m;
 effect line = mm(p m);
 model time = block;
 random line sym p m p*m;
run;

```

The **EFFECT** statement defines the nuclear parental contributions as a multimember effect based on the **CLASS** variables *p* and *m*. Each observation has two nonzero entries in the design matrix for the effect that identifies the paternal and maternal lines. The terms in the **RANDOM** statement model the variance components as follows: *line*  $\rightarrow \sigma_n^2$ , *sym*  $\rightarrow \sigma_{(\eta\eta)}^2$ , *p*  $\rightarrow \sigma_\phi^2$ , *m*  $\rightarrow \sigma_\mu^2$ , *p\*m*  $\rightarrow \sigma_\kappa^2$ . The **OUTDESIGN=** option in the **PROC GLIMMIX** statement writes the **Z** matrix to the SAS data set *zmat*. The **EFFECT** statement alleviates the need for complex coding, as in Section 2.3 of Saxton (2004).

**Output 41.16.1** displays the “Class Level Information” table of the diallel model. Because the interaction terms are symmetric, there are only  $8 \times 7/2 = 28$  levels for the 8 lines. The estimates of the variance components and the residual variance in **Output 41.16.1** agree with the results in Table 7 of Cockerham and Weir (1977).

**Output 41.16.1** Class Levels and Covariance Parameter Estimates in Diallel Example

| The GLIMMIX Procedure   |        |                                                                                                                       |
|-------------------------|--------|-----------------------------------------------------------------------------------------------------------------------|
| Class Level Information |        |                                                                                                                       |
| Class                   | Levels | Values                                                                                                                |
| block                   | 2      | 1 2                                                                                                                   |
| sym                     | 28     | 1,2 1,3 1,4 1,5 1,6 1,7 1,8 2,3 2,4 2,5 2,6<br>2,7 2,8 3,4 3,5 3,6 3,7 3,8 4,5 4,6 4,7 4,8<br>5,6 5,7 5,8 6,7 6,8 7,8 |
| p                       | 8      | 1 2 3 4 5 6 7 8                                                                                                       |
| m                       | 8      | 1 2 3 4 5 6 7 8                                                                                                       |

| Covariance Parameter Estimates |          |                |
|--------------------------------|----------|----------------|
| Cov Parm                       | Estimate | Standard Error |
| line                           | 5.1047   | 4.0021         |
| sym                            | 2.3856   | 1.9025         |
| p                              | 3.3080   | 3.4053         |
| m                              | 1.9134   | 2.9891         |
| p*m                            | 4.0196   | 1.8323         |
| Residual                       | 3.6225   | 0.6908         |

The following statements print the **Z** matrix columns that correspond to the multimember line effect for the first 10 observations in block 1 (Output 41.16.2). For each observation there are two nonzero entries, and their column index corresponds to the index of the paternal and maternal line.

```
proc print data=zmat (where=(block=1) obs=10);
 var p m time _z1-_z8;
run;
```

**Output 41.16.2** Z Matrix for Line Effect of the First 10 Observations in Block 1

| Obs | p | m | time | _z1 | _z2 | _z3 | _z4 | _z5 | _z6 | _z7 | _z8 |
|-----|---|---|------|-----|-----|-----|-----|-----|-----|-----|-----|
| 1   | 1 | 2 | 14.4 | 1   | 1   | 0   | 0   | 0   | 0   | 0   | 0   |
| 3   | 1 | 3 | 27.2 | 1   | 0   | 1   | 0   | 0   | 0   | 0   | 0   |
| 5   | 1 | 4 | 17.2 | 1   | 0   | 0   | 1   | 0   | 0   | 0   | 0   |
| 7   | 1 | 5 | 18.3 | 1   | 0   | 0   | 0   | 1   | 0   | 0   | 0   |
| 9   | 1 | 6 | 16.2 | 1   | 0   | 0   | 0   | 0   | 1   | 0   | 0   |
| 11  | 1 | 7 | 18.6 | 1   | 0   | 0   | 0   | 0   | 0   | 1   | 0   |
| 13  | 1 | 8 | 16.4 | 1   | 0   | 0   | 0   | 0   | 0   | 0   | 1   |
| 15  | 2 | 1 | 15.4 | 1   | 1   | 0   | 0   | 0   | 0   | 0   | 0   |
| 17  | 2 | 3 | 14.8 | 0   | 1   | 1   | 0   | 0   | 0   | 0   | 0   |
| 19  | 2 | 4 | 18.6 | 0   | 1   | 0   | 1   | 0   | 0   | 0   | 0   |

## Example 41.17: Linear Inference Based on Summary Data

The GLIMMIX procedure has facilities for multiplicity-adjusted inference through the ADJUST= and STEPDOWN options in the ESTIMATE, LSMEANS, and LSMESTIMATE statements. You can employ these facilities to test linear hypotheses among parameters even in situations where the quantities were obtained outside the GLIMMIX procedure. This example demonstrates the process. The basic idea is to prepare a data set containing the estimates of interest and a data set containing their covariance matrix. These are then passed to the GLIMMIX procedure, preventing updating of the parameters, essentially moving directly into the post-processing stage as if estimates with this covariance matrix had been produced by the GLIMMIX procedure.

The final documentation example in Chapter 63, “The NLIN Procedure,” discusses a nonlinear first-order compartment pharmacokinetic model for theophylline concentration. The data are derived by collapsing and averaging the subject-specific data from Pinheiro and Bates (1995) in a particular—yet unimportant—way that leads to two groups for comparisons. The following DATA step creates these data:

```
data theop;
 input time dose conc @@;
 if (dose = 4) then group=1; else group=2;
 datalines;
0.00 4 0.1633 0.25 4 2.045
0.27 4 4.4 0.30 4 7.37
0.35 4 1.89 0.37 4 2.89
0.50 4 3.96 0.57 4 6.57
0.58 4 6.9 0.60 4 4.6
0.63 4 9.03 0.77 4 5.22
1.00 4 7.82 1.02 4 7.305
1.05 4 7.14 1.07 4 8.6
1.12 4 10.5 2.00 4 9.72
2.02 4 7.93 2.05 4 7.83
2.13 4 8.38 3.50 4 7.54
3.52 4 9.75 3.53 4 5.66
3.55 4 10.21 3.62 4 7.5
3.82 4 8.58 5.02 4 6.275
5.05 4 9.18 5.07 4 8.57
5.08 4 6.2 5.10 4 8.36
7.02 4 5.78 7.03 4 7.47
7.07 4 5.945 7.08 4 8.02
7.17 4 4.24 8.80 4 4.11
9.00 4 4.9 9.02 4 5.33
9.03 4 6.11 9.05 4 6.89
9.38 4 7.14 11.60 4 3.16
11.98 4 4.19 12.05 4 4.57
12.10 4 5.68 12.12 4 5.94
12.15 4 3.7 23.70 4 2.42
24.15 4 1.17 24.17 4 1.05
24.37 4 3.28 24.43 4 1.12
24.65 4 1.15 0.00 5 0.025
0.25 5 2.92 0.27 5 1.505
0.30 5 2.02 0.50 5 4.795
0.52 5 5.53 0.58 5 3.08
0.98 5 7.655 1.00 5 9.855
```

|       |   |        |       |   |       |
|-------|---|--------|-------|---|-------|
| 1.02  | 5 | 5.02   | 1.15  | 5 | 6.44  |
| 1.92  | 5 | 8.33   | 1.98  | 5 | 6.81  |
| 2.02  | 5 | 7.8233 | 2.03  | 5 | 6.32  |
| 3.48  | 5 | 7.09   | 3.50  | 5 | 7.795 |
| 3.53  | 5 | 6.59   | 3.57  | 5 | 5.53  |
| 3.60  | 5 | 5.87   | 5.00  | 5 | 5.8   |
| 5.02  | 5 | 6.2867 | 5.05  | 5 | 5.88  |
| 6.98  | 5 | 5.25   | 7.00  | 5 | 4.02  |
| 7.02  | 5 | 7.09   | 7.03  | 5 | 4.925 |
| 7.15  | 5 | 4.73   | 9.00  | 5 | 4.47  |
| 9.03  | 5 | 3.62   | 9.07  | 5 | 4.57  |
| 9.10  | 5 | 5.9    | 9.22  | 5 | 3.46  |
| 12.00 | 5 | 3.69   | 12.05 | 5 | 3.53  |
| 12.10 | 5 | 2.89   | 12.12 | 5 | 2.69  |
| 23.85 | 5 | 0.92   | 24.08 | 5 | 0.86  |
| 24.12 | 5 | 1.25   | 24.22 | 5 | 1.15  |
| 24.30 | 5 | 0.9    | 24.35 | 5 | 1.57  |

i

In terms of two fixed treatment groups, the nonlinear model for these data can be written as

$$C_{it} = \frac{Dk_{e_i}k_{a_i}}{Cl_i(k_{a_i} - k_{e_i})} [\exp(-k_{e_i}t) - \exp(-k_{a_i}t)] + \epsilon_{it}$$

where  $C_{it}$  is the observed concentration in group  $i$  at time  $t$ ,  $D$  is the dose of theophylline,  $k_{e_i}$  is the elimination rate constant in group  $i$ ,  $k_{a_i}$  is the absorption rate in group  $i$ ,  $Cl_i$  is the clearance in group  $i$ , and  $\epsilon_{it}$  denotes the model error. Because the rates and the clearance must be positive, you can parameterize the model in terms of log rates and the log clearance:

$$\begin{aligned} Cl_i &= \exp\{\beta_{1i}\} \\ k_{a_i} &= \exp\{\beta_{2i}\} \\ k_{e_i} &= \exp\{\beta_{3i}\} \end{aligned}$$

In this parameterization the model contains six parameters, and the rates and clearance vary by group. The following PROC NLIN statements fit the model and obtain the group-specific parameter estimates:

```
proc nlin data=theop outest=cov;
 parms beta1_1=-3.22 beta2_1=0.47 beta3_1=-2.45
 beta1_2=-3.22 beta2_2=0.47 beta3_2=-2.45;
 if (group=1) then do;
 cl = exp(beta1_1);
 ka = exp(beta2_1);
 ke = exp(beta3_1);
 end; else do;
 cl = exp(beta1_2);
 ka = exp(beta2_2);
 ke = exp(beta3_2);
 end;
 mean = dose*ke*ka*(exp(-ke*time)-exp(-ka*time))/cl/(ka-ke);
 model conc = mean;
 ods output ParameterEstimates=ests;
run;
```

The conditional programming statements determine the clearance, elimination, and absorption rates depending on the value of the group variable. The OUTEST= option in the PROC NLIN statement saves estimates and their covariance matrix to the data set cov. The ODS OUTPUT statement saves the “Parameter Estimates” table to the data set ests.

Output 41.17.1 displays the analysis of variance table and the parameter estimates from this NLIN run. Note that the confidence levels in the “Parameter Estimates” table are based on 92 degrees of freedom, corresponding to the residual degrees of freedom in the analysis of variance table.

**Output 41.17.1** Analysis of Variance and Parameter Estimates for Nonlinear Model

| The NLIN Procedure                                   |    |                |             |         |               |
|------------------------------------------------------|----|----------------|-------------|---------|---------------|
| NOTE: An intercept was not specified for this model. |    |                |             |         |               |
| Source                                               | DF | Sum of Squares | Mean Square | F Value | Approx Pr > F |
| Model                                                | 6  | 3247.9         | 541.3       | 358.56  | <.0001        |
| Error                                                | 92 | 138.9          | 1.5097      |         |               |
| Uncorrected Total                                    | 98 | 3386.8         |             |         |               |

| Parameter | Estimate | Approx Std Error | Approximate 95% Confidence Limits |         |
|-----------|----------|------------------|-----------------------------------|---------|
| beta1_1   | -3.5671  | 0.0864           | -3.7387                           | -3.3956 |
| beta2_1   | 0.4421   | 0.1349           | 0.1742                            | 0.7101  |
| beta3_1   | -2.6230  | 0.1265           | -2.8742                           | -2.3718 |
| beta1_2   | -3.0111  | 0.1061           | -3.2219                           | -2.8003 |
| beta2_2   | 0.3977   | 0.1987           | 0.00305                           | 0.7924  |
| beta3_2   | -2.4442  | 0.1618           | -2.7655                           | -2.1229 |

The following DATA step extracts the part of the cov data set that contains the covariance matrix of the parameter estimates in Output 41.17.1 and renames the variables as Col1–Col6. Output 41.17.2 shows the result of the DATA step.

```
data covb;
 set cov(where=(_type_='COVB'));
 rename beta1_1=col1 beta2_1=col2 beta3_1=col3
 beta1_2=col4 beta2_2=col5 beta3_2=col6;
 row = _n_;
 Parm = 1;
 keep parm row beta:;
run;

proc print data=covb;
run;
```

**Output 41.17.2** Covariance Matrix of NLIN Parameter Estimates

| Obs | col1      | col2      | col3      | col4      | col5      | col6      | row | Parm |
|-----|-----------|-----------|-----------|-----------|-----------|-----------|-----|------|
| 1   | 0.007462  | -0.005222 | 0.010234  | 0.000000  | 0.000000  | 0.000000  | 1   | 1    |
| 2   | -0.005222 | 0.018197  | -0.010590 | 0.000000  | 0.000000  | 0.000000  | 2   | 1    |
| 3   | 0.010234  | -0.010590 | 0.015999  | 0.000000  | 0.000000  | 0.000000  | 3   | 1    |
| 4   | 0.000000  | 0.000000  | 0.000000  | 0.011261  | -0.009096 | 0.015785  | 4   | 1    |
| 5   | 0.000000  | 0.000000  | 0.000000  | -0.009096 | 0.039487  | -0.019996 | 5   | 1    |
| 6   | 0.000000  | 0.000000  | 0.000000  | 0.015785  | -0.019996 | 0.026172  | 6   | 1    |

The reason for this transformation of the data is to use the resulting data set to define a covariance structure in PROC GLIMMIX. The following statements reconstitute a model in which the parameter estimates from PROC NLIN are the observations and in which the covariance matrix of the “observations” matches the covariance matrix of the NLIN parameter estimates:

```
proc glimmix data=ests order=data;
 class Parameter;
 model Estimate = Parameter / noint df=92 s;
 random _residual_ / type=lin(1) ldata=covb v;
 parms (1) / noiter;
 lsmeans parameter / cl;
 lsmestimate Parameter
 'beta1 eq. across groups' 1 0 0 -1,
 'beta2 eq. across groups' 0 1 0 0 -1,
 'beta3 eq. across groups' 0 0 1 0 0 -1 /
 adjust=bon stepdown ftest(label='Homogeneity');
run;
```

In other words, you are using PROC GLIMMIX to set up a linear statistical model

$$Y = I\alpha + \epsilon$$

$$\epsilon \sim (0, A)$$

where the covariance matrix  $A$  is given by

$$A = \begin{bmatrix} 0.007 & -0.005 & 0.010 & 0 & 0 & 0 \\ -0.005 & 0.018 & -0.011 & 0 & 0 & 0 \\ 0.010 & -0.011 & 0.016 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.011 & -0.009 & 0.016 \\ 0 & 0 & 0 & -0.009 & 0.039 & -0.019 \\ 0 & 0 & 0 & 0.016 & -0.019 & 0.026 \end{bmatrix}$$

The generalized least squares estimate for  $\alpha$  in this saturated model reproduces the observations:

$$\begin{aligned} \hat{\alpha} &= (I'A^{-1}I)^{-1} I'A^{-1}y \\ &= (A^{-1})^{-1} A^{-1}y \\ &= y \end{aligned}$$

The `ORDER=DATA` option in the `PROC GLIMMIX` statement requests that the sort order of the Parameter variable be identical to the order in which it appeared in the “Parameter Estimates” table of the NLIN procedure (Output 41.17.1). The `MODEL` statement uses the Estimate and Parameter variables from that table to form a model in which the **X** matrix is the identity; hence the `NOINT` option. The `DF=92` option sets the degrees of freedom equal to the value used in the NLIN procedure. The `RANDOM` statement specifies a linear covariance structure with a single component and supplies the values for the structure through the `LDATA=` data set. This structure models the covariance matrix as  $\text{Var}[\mathbf{Y}] = \theta\mathbf{A}$ , where the **A** matrix is given previously. Essentially, the `TYPE=LIN(1)` structure forces an unstructured covariance matrix onto the data. To make this work, the parameter  $\theta$  is held fixed at 1 in the `PARMS` statement.

Output 41.17.3 displays the parameter estimates and least squares means for this model. Note that estimates and least squares means are identical, since the **X** matrix is the identity. Also, the confidence limits agree with the values reported by PROC NLIN (see Output 41.17.1).

**Output 41.17.3** Parameter Estimates and LS-Means from Summary Data

| The GLIMMIX Procedure         |           |                |                |         |         |         |
|-------------------------------|-----------|----------------|----------------|---------|---------|---------|
| Solutions for Fixed Effects   |           |                |                |         |         |         |
| Effect                        | Parameter | Estimate       | Standard Error | DF      | t Value | Pr >  t |
| Parameter                     | beta1_1   | -3.5671        | 0.08638        | 92      | -41.29  | <.0001  |
| Parameter                     | beta2_1   | 0.4421         | 0.1349         | 92      | 3.28    | 0.0015  |
| Parameter                     | beta3_1   | -2.6230        | 0.1265         | 92      | -20.74  | <.0001  |
| Parameter                     | beta1_2   | -3.0111        | 0.1061         | 92      | -28.37  | <.0001  |
| Parameter                     | beta2_2   | 0.3977         | 0.1987         | 92      | 2.00    | 0.0483  |
| Parameter                     | beta3_2   | -2.4442        | 0.1618         | 92      | -15.11  | <.0001  |
| Parameter Least Squares Means |           |                |                |         |         |         |
| Parameter                     | Estimate  | Standard Error | DF             | t Value | Pr >  t | Alpha   |
| beta1_1                       | -3.5671   | 0.08638        | 92             | -41.29  | <.0001  | 0.05    |
| beta2_1                       | 0.4421    | 0.1349         | 92             | 3.28    | 0.0015  | 0.05    |
| beta3_1                       | -2.6230   | 0.1265         | 92             | -20.74  | <.0001  | 0.05    |
| beta1_2                       | -3.0111   | 0.1061         | 92             | -28.37  | <.0001  | 0.05    |
| beta2_2                       | 0.3977    | 0.1987         | 92             | 2.00    | 0.0483  | 0.05    |
| beta3_2                       | -2.4442   | 0.1618         | 92             | -15.11  | <.0001  | 0.05    |
| Parameter Least Squares Means |           |                |                |         |         |         |
| Parameter                     | Lower     | Upper          |                |         |         |         |
| beta1_1                       | -3.7387   | -3.3956        |                |         |         |         |
| beta2_1                       | 0.1742    | 0.7101         |                |         |         |         |
| beta3_1                       | -2.8742   | -2.3718        |                |         |         |         |
| beta1_2                       | -3.2219   | -2.8003        |                |         |         |         |
| beta2_2                       | 0.003050  | 0.7924         |                |         |         |         |
| beta3_2                       | -2.7655   | -2.1229        |                |         |         |         |



The (marginal) covariance matrix of the data is shown in [Output 41.17.4](#) to confirm that it matches the **A** matrix given earlier.

**Output 41.17.4** R-Side Covariance Matrix

| Estimated V Matrix for Subject 1 |          |          |          |          |          |          |
|----------------------------------|----------|----------|----------|----------|----------|----------|
| Row                              | Col1     | Col2     | Col3     | Col4     | Col5     | Col6     |
| 1                                | 0.007462 | -0.00522 | 0.01023  |          |          |          |
| 2                                | -0.00522 | 0.01820  | -0.01059 |          |          |          |
| 3                                | 0.01023  | -0.01059 | 0.01600  |          |          |          |
| 4                                |          |          |          | 0.01126  | -0.00910 | 0.01579  |
| 5                                |          |          |          | -0.00910 | 0.03949  | -0.02000 |
| 6                                |          |          |          | 0.01579  | -0.02000 | 0.02617  |

The **LSMESTIMATE** statement specifies three linear functions. These set equal the  $\beta$  parameters from the groups. The step-down Bonferroni adjustment requests a multiplicity adjustment for the family of three tests. The **FTEST** option requests a joint test of the three estimable functions; it is a global test of parameter homogeneity across groups.

[Output 41.17.5](#) displays the result from the **LSMESTIMATE** statement. The joint test is highly significant ( $F = 30.52$ ,  $p < 0.0001$ ). From the  $p$ -values associated with the individual rows of the estimates, you can see that the lack of homogeneity is due to group differences for  $\beta_1$ , the log clearance.

**Output 41.17.5** Test of Parameter Homogeneity across Groups

| Least Squares Means Estimates            |                         |          |                |        |         |         |  |
|------------------------------------------|-------------------------|----------|----------------|--------|---------|---------|--|
| Adjustment for Multiplicity: Holm        |                         |          |                |        |         |         |  |
| Effect                                   | Label                   | Estimate | Standard Error | DF     | t Value | Pr >  t |  |
| Parameter                                | beta1 eq. across groups | -0.5560  | 0.1368         | 92     | -4.06   | 0.0001  |  |
| Parameter                                | beta2 eq. across groups | 0.04443  | 0.2402         | 92     | 0.18    | 0.8537  |  |
| Parameter                                | beta3 eq. across groups | -0.1788  | 0.2054         | 92     | -0.87   | 0.3862  |  |
| Least Squares Means Estimates            |                         |          |                |        |         |         |  |
| Adjustment for Multiplicity: Holm        |                         |          |                |        |         |         |  |
| Effect                                   | Label                   |          |                |        | Adj P   |         |  |
| Parameter                                | beta1 eq. across groups |          |                |        | 0.0003  |         |  |
| Parameter                                | beta2 eq. across groups |          |                |        | 0.8537  |         |  |
| Parameter                                | beta3 eq. across groups |          |                |        | 0.7725  |         |  |
| F Test for Least Squares Means Estimates |                         |          |                |        |         |         |  |
| Label                                    | Num DF                  | Den DF   | F Value        | Pr > F |         |         |  |
| Homogeneity                              | 3                       | 92       | 30.52          | <.0001 |         |         |  |

An alternative method to set up this model is given by the following statements, where the data set `pdata` contains the covariance parameters:

```
random _residual_ / type=un;
parms / pdata=pdata noiter
```

The following DATA step creates an appropriate `PDATA=` data set from the data set `covb` constructed earlier:

```
data pdata;
 set covb;
 array col{6};
 do i=1 to _n_;
 estimate = col{i};
 output;
 end;
 keep estimate;
run;
```

---

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# Chapter 42

## The GLM Procedure

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## Overview: GLM Procedure

The GLM procedure uses the method of least squares to fit general linear models. Among the statistical methods available in PROC GLM are regression, analysis of variance, analysis of covariance, multivariate analysis of variance, and partial correlation.

PROC GLM analyzes data within the framework of general linear models. PROC GLM handles models relating one or several continuous dependent variables to one or several independent variables. The independent variables can be either *classification* variables, which divide the observations into discrete groups, or *continuous* variables. Thus, the GLM procedure can be used for many different analyses, including the following:

- simple regression

- multiple regression
- analysis of variance (ANOVA), especially for unbalanced data
- analysis of covariance
- response surface models
- weighted regression
- polynomial regression
- partial correlation
- multivariate analysis of variance (MANOVA)
- repeated measures analysis of variance

---

## PROC GLM Features

The following list summarizes the features in PROC GLM:

- PROC GLM enables you to specify any degree of interaction (crossed effects) and nested effects. It also provides for polynomial, continuous-by-class, and continuous-nesting-class effects.
- Through the concept of estimability, the GLM procedure can provide tests of hypotheses for the effects of a linear model regardless of the number of missing cells or the extent of confounding. PROC GLM displays the sum of squares (SS) associated with each hypothesis tested and, upon request, the form of the estimable functions employed in the test. PROC GLM can produce the general form of all estimable functions.
- The **REPEATED** statement enables you to specify effects in the model that represent repeated measurements on the same experimental unit for the same response, providing both univariate and multivariate tests of hypotheses.
- The **RANDOM** statement enables you to specify random effects in the model; expected mean squares are produced for each Type I, Type II, Type III, Type IV, and contrast mean square used in the analysis. Upon request,  $F$  tests that use appropriate mean squares or linear combinations of mean squares as error terms are performed.
- The **ESTIMATE** statement enables you to specify an  $\mathbf{L}$  vector for estimating a linear function of the parameters  $\mathbf{L}\boldsymbol{\beta}$ .
- The **CONTRAST** statement enables you to specify a contrast vector or matrix for testing the hypothesis that  $\mathbf{L}\boldsymbol{\beta} = 0$ . When specified, the contrasts are also incorporated into analyses that use the **MANOVA** and **REPEATED** statements.
- The **MANOVA** statement enables you to specify both the hypothesis effects and the error effect to use for a multivariate analysis of variance.

- PROC GLM can create an output data set containing the input data set in addition to predicted values, residuals, and other diagnostic measures.
- PROC GLM can be used interactively. After you specify and fit a model, you can execute a variety of statements without recomputing the model parameters or sums of squares.
- For analysis involving multiple dependent variables but not the **MANOVA** or **REPEATED** statements, a missing value in one dependent variable does not eliminate the observation from the analysis for other dependent variables. PROC GLM automatically groups together those variables that have the same pattern of missing values within the data set or within a BY group. This ensures that the analysis for each dependent variable brings into use all possible observations.
- The GLM procedure automatically produces graphs as part of its ODS output. For general information about ODS Graphics, see the section “**ODS Graphics**” on page 3388 and Chapter 21, “**Statistical Graphics Using ODS**.”

---

## PROC GLM Contrasted with Other SAS Procedures

As described previously, PROC GLM can be used for many different analyses and has many special features not available in other SAS procedures. However, for some types of analyses, other procedures are available. As discussed in the sections “**PROC GLM for Unbalanced ANOVA**” on page 3269 and “**PROC GLM for Quadratic Least Squares Regression**” on page 3272, sometimes these other procedures are more efficient than PROC GLM. The following procedures perform some of the same analyses as PROC GLM:

|          |                                                                                                                                                                                                                      |
|----------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| ANOVA    | performs analysis of variance for balanced designs. The ANOVA procedure is generally more efficient than PROC GLM for these designs.                                                                                 |
| MIXED    | fits mixed linear models by incorporating covariance structures in the model fitting process. Its <b>RANDOM</b> and <b>REPEATED</b> statements are similar to those in PROC GLM but offer different functionalities. |
| NESTED   | performs analysis of variance and estimates variance components for nested random models. The <b>NESTED</b> procedure is generally more efficient than PROC GLM for these models.                                    |
| NPAR1WAY | performs nonparametric one-way analysis of rank scores. This can also be done using the <b>RANK</b> procedure and PROC GLM.                                                                                          |
| REG      | performs simple linear regression. The <b>REG</b> procedure allows several <b>MODEL</b> statements and gives additional regression diagnostics, especially for detection of collinearity.                            |
| RSREG    | performs quadratic response surface regression, and canonical and ridge analysis. The <b>RSREG</b> procedure is generally recommended for data from a response surface experiment.                                   |

|         |                                                                                                                                                                                                              |
|---------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| TTEST   | compares the means of two groups of observations. Also, tests for equality of variances for the two groups are available. The TTEST procedure is usually more efficient than PROC GLM for this type of data. |
| VARCOMP | estimates variance components for a general linear model.                                                                                                                                                    |

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## Getting Started: GLM Procedure

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### PROC GLM for Unbalanced ANOVA

*Analysis of variance*, or ANOVA, typically refers to partitioning the variation in a variable's values into variation between and within several groups or classes of observations. The GLM procedure can perform simple or complicated ANOVA for balanced or unbalanced data.

This example discusses the analysis of variance for the unbalanced  $2 \times 2$  data shown in [Table 42.1](#). The experimental design is a full factorial, in which each level of one treatment factor occurs at each level of the other treatment factor. Note that there is only one value for the cell with A='A2' and B='B2'. Since one cell contains a different number of values from the other cells in the table, this is an unbalanced design.

**Table 42.1** Unbalanced Two-Way Data

|    | A1     | A2     |
|----|--------|--------|
| B1 | 12, 14 | 20, 18 |
| B2 | 11, 9  | 17     |

The following statements read the data into a SAS data set and then invoke PROC GLM to produce the analysis.

```

title 'Analysis of Unbalanced 2-by-2 Factorial';
data exp;
 input A $ B $ Y @@;
 datalines;
A1 B1 12 A1 B1 14 A1 B2 11 A1 B2 9
A2 B1 20 A2 B1 18 A2 B2 17
;

proc glm data=exp;
 class A B;
 model Y=A B A*B;
run;

```

Both treatments are listed in the **CLASS** statement because they are classification variables. A\*B denotes the interaction of the A effect and the B effect. The results are shown in [Figure 42.1](#) and [Figure 42.2](#).



**Figure 42.1** Class Level Information

| Analysis of Unbalanced 2-by-2 Factorial |        |        |
|-----------------------------------------|--------|--------|
| The GLM Procedure                       |        |        |
| Class Level Information                 |        |        |
| Class                                   | Levels | Values |
| A                                       | 2      | A1 A2  |
| B                                       | 2      | B1 B2  |
| Number of Observations Read             |        | 7      |
| Number of Observations Used             |        | 7      |

Figure 42.1 displays information about the classes as well as the number of observations in the data set. Figure 42.2 shows the ANOVA table, simple statistics, and tests of effects.

**Figure 42.2** ANOVA Table and Tests of Effects

| Analysis of Unbalanced 2-by-2 Factorial |          |                |             |          |        |
|-----------------------------------------|----------|----------------|-------------|----------|--------|
| The GLM Procedure                       |          |                |             |          |        |
| Dependent Variable: Y                   |          |                |             |          |        |
| Source                                  | DF       | Sum of Squares | Mean Square | F Value  | Pr > F |
| Model                                   | 3        | 91.71428571    | 30.57142857 | 15.29    | 0.0253 |
| Error                                   | 3        | 6.00000000     | 2.00000000  |          |        |
| Corrected Total                         | 6        | 97.71428571    |             |          |        |
|                                         | R-Square | Coeff Var      | Root MSE    | Y Mean   |        |
|                                         | 0.938596 | 9.801480       | 1.414214    | 14.42857 |        |
| Source                                  | DF       | Type I SS      | Mean Square | F Value  | Pr > F |
| A                                       | 1        | 80.04761905    | 80.04761905 | 40.02    | 0.0080 |
| B                                       | 1        | 11.26666667    | 11.26666667 | 5.63     | 0.0982 |
| A*B                                     | 1        | 0.40000000     | 0.40000000  | 0.20     | 0.6850 |

Figure 42.2 continued

| Source | DF | Type III SS | Mean Square | F Value | Pr > F |
|--------|----|-------------|-------------|---------|--------|
| A      | 1  | 67.60000000 | 67.60000000 | 33.80   | 0.0101 |
| B      | 1  | 10.00000000 | 10.00000000 | 5.00    | 0.1114 |
| A*B    | 1  | 0.40000000  | 0.40000000  | 0.20    | 0.6850 |

The degrees of freedom can be used to check your data. The Model degrees of freedom for a  $2 \times 2$  factorial design with interaction are  $(ab - 1)$ , where  $a$  is the number of levels of A and  $b$  is the number of levels of B; in this case,  $(2 \times 2 - 1) = 3$ . The Corrected Total degrees of freedom are always one less than the number of observations used in the analysis; in this case,  $7 - 1 = 6$ .

The overall  $F$  test is significant ( $F = 15.29$ ,  $p = 0.0253$ ), indicating strong evidence that the means for the four different A×B cells are different. You can further analyze this difference by examining the individual tests for each effect.

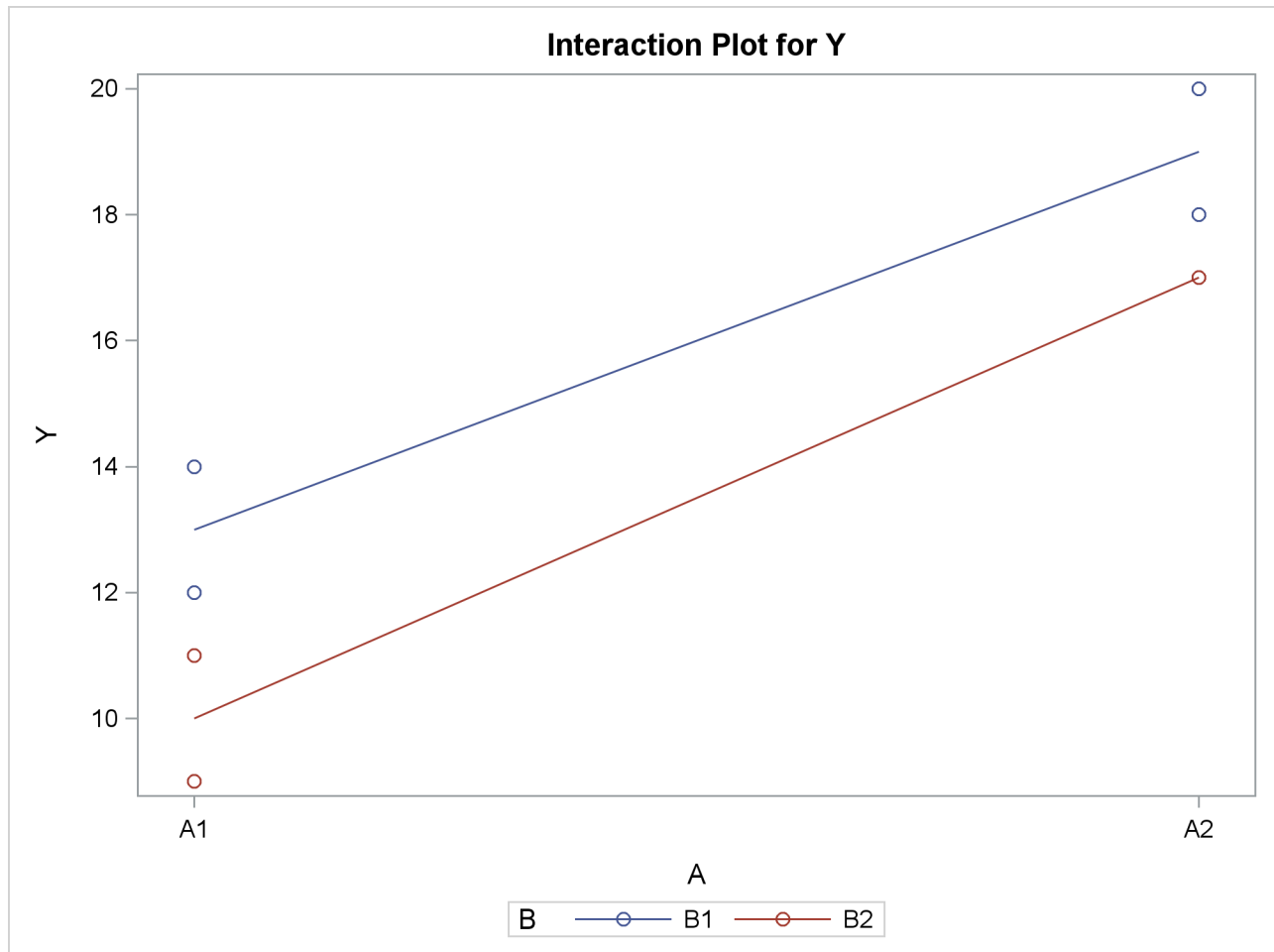
Four types of estimable functions of parameters are available for testing hypotheses in PROC GLM. For data with no missing cells, the Type III and Type IV estimable functions are the same and test the same hypotheses that would be tested if the data were balanced. Type I and Type III sums of squares are typically not equal when the data are unbalanced; Type III sums of squares are preferred in testing effects in unbalanced cases because they test a function of the underlying parameters that is independent of the number of observations per treatment combination.

According to a significance level of 5% ( $\alpha = 0.05$ ), the A\*B interaction is not significant ( $F = 0.20$ ,  $p = 0.6850$ ). This indicates that the effect of A does not depend on the level of B and vice versa. Therefore, the tests for the individual effects are valid, showing a significant A effect ( $F = 33.80$ ,  $p = 0.0101$ ) but no significant B effect ( $F = 5.00$ ,  $p = 0.1114$ ).

If ODS Graphics is enabled, GLM also displays by default an interaction plot for this analysis. The following statements, which are the same as in the previous analysis but with ODS Graphics enabled, additionally produce Figure 42.3.

```
ods graphics on;
proc glm data=exp;
 class A B;
 model Y=A B A*B;
run;
ods graphics off;
```

Figure 42.3 Plot of Y by A and B



The insignificance of the A\*B interaction is reflected in the fact that two lines in Figure 42.3 are nearly parallel. For more information about the graphics that GLM can produce, see the section “ODS Graphics” on page 3388.

## PROC GLM for Quadratic Least Squares Regression

In polynomial regression, the values of a dependent variable (also called a response variable) are described or predicted in terms of polynomial terms involving one or more independent or explanatory variables. An example of quadratic regression in PROC GLM follows. These data are taken from Draper and Smith (1966, p. 57). Thirteen specimens of 90/10 Cu-Ni alloys are tested in a corrosion-wheel setup in order to examine corrosion. Each specimen has a certain iron content. The wheel is rotated in salt sea water at 30 ft/sec for 60 days. Weight loss is used to quantify the corrosion. The `fe` variable represents the iron content, and the `loss` variable denotes the weight loss in milligrams/square decimeter/day in the following DATA step.

```
title 'Regression in PROC GLM';
data iron;
 input fe loss @@;
```

```

datalines;
0.01 127.6 0.48 124.0 0.71 110.8 0.95 103.9
1.19 101.5 0.01 130.1 0.48 122.0 1.44 92.3
0.71 113.1 1.96 83.7 0.01 128.0 1.44 91.4
1.96 86.2
;

```

The SGSCATTER procedure is used in the following statements to request a scatter plot of the response variable versus the independent variable.

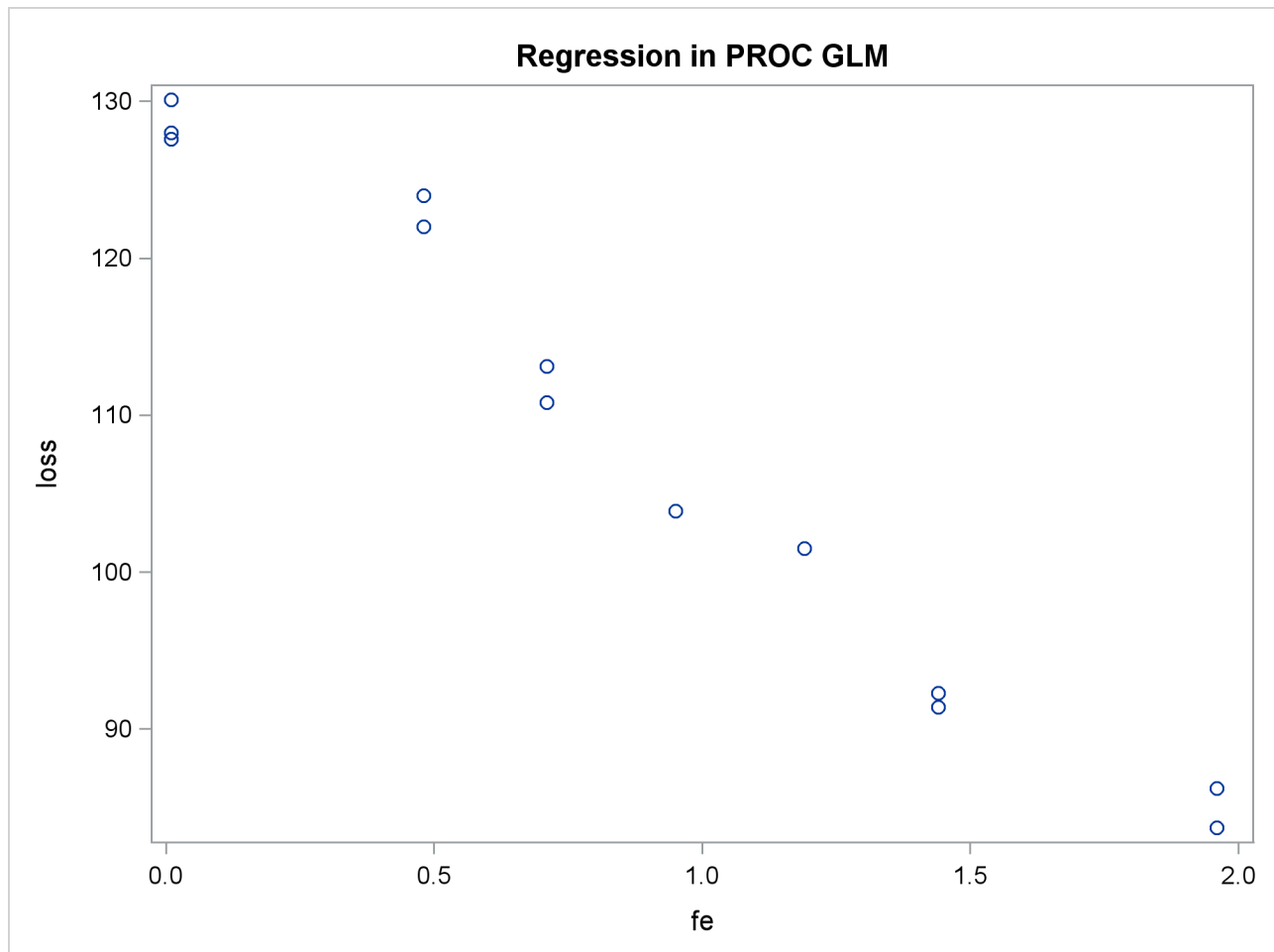
```

ods graphics on;
proc sgscatter data=iron;
 plot loss*fe;
run;
ods graphics off;

```

The plot in Figure 42.4 displays a strong negative relationship between iron content and corrosion resistance, but it is not clear whether there is curvature in this relationship.

**Figure 42.4** Plot of Observed Corrosion Resistance by Iron Content



The following statements fit a quadratic regression model to the data. This enables you to estimate the linear relationship between iron content and corrosion resistance and to test for the presence of a quadratic component. The intercept is automatically fit unless the **NOINT** option is specified.

```
proc glm data=iron;
 model loss=fe fe*fe;
run;
```

The **CLASS** statement is omitted because a regression line is being fitted. Unlike PROC REG, PROC GLM allows polynomial terms in the **MODEL** statement.

PROC GLM first displays preliminary information, shown in Figure 42.5, telling you that the GLM procedure has been invoked and stating the number of observations in the data set. If the model involves classification variables, they are also listed here, along with their levels.

**Figure 42.5** Data Information

| Regression in PROC GLM      |    |
|-----------------------------|----|
| The GLM Procedure           |    |
| Number of Observations Read | 13 |
| Number of Observations Used | 13 |

Figure 42.6 shows the overall ANOVA table and some simple statistics. The degrees of freedom can be used to check that the model is correct and that the data have been read correctly. The Model degrees of freedom for a regression is the number of parameters in the model minus 1. You are fitting a model with three parameters in this case,

$$\text{loss} = \beta_0 + \beta_1 \times (\text{fe}) + \beta_2 \times (\text{fe})^2 + \text{error}$$

so the degrees of freedom are  $3 - 1 = 2$ . The Corrected Total degrees of freedom are always one less than the number of observations used in the analysis.

**Figure 42.6** ANOVA Table

| Regression in PROC GLM   |    |                |             |         |        |
|--------------------------|----|----------------|-------------|---------|--------|
| The GLM Procedure        |    |                |             |         |        |
| Dependent Variable: loss |    |                |             |         |        |
| Source                   | DF | Sum of Squares | Mean Square | F Value | Pr > F |
| Model                    | 2  | 3296.530589    | 1648.265295 | 164.68  | <.0001 |
| Error                    | 10 | 100.086334     | 10.008633   |         |        |
| Corrected Total          | 12 | 3396.616923    |             |         |        |

Figure 42.6 continued

| R-Square | Coeff Var | Root MSE | loss Mean |
|----------|-----------|----------|-----------|
| 0.970534 | 2.907348  | 3.163642 | 108.8154  |

The R square indicates that the model accounts for 97% of the variation in LOSS. The coefficient of variation (Coeff Var), Root MSE (Mean Square for Error), and mean of the dependent variable are also listed.

The overall  $F$  test is significant ( $F = 164.68$ ,  $p < 0.0001$ ), indicating that the model as a whole accounts for a significant amount of the variation in LOSS. Thus, it is appropriate to proceed to testing the effects.

Figure 42.7 contains tests of effects and parameter estimates. The latter are displayed by default when the model contains only continuous variables.

Figure 42.7 Tests of Effects and Parameter Estimates

| Source | DF | Type I SS   | Mean Square | F Value | Pr > F |
|--------|----|-------------|-------------|---------|--------|
| fe     | 1  | 3293.766690 | 3293.766690 | 329.09  | <.0001 |
| fe*fe  | 1  | 2.763899    | 2.763899    | 0.28    | 0.6107 |

| Source | DF | Type III SS | Mean Square | F Value | Pr > F |
|--------|----|-------------|-------------|---------|--------|
| fe     | 1  | 356.7572421 | 356.7572421 | 35.64   | 0.0001 |
| fe*fe  | 1  | 2.7638994   | 2.7638994   | 0.28    | 0.6107 |

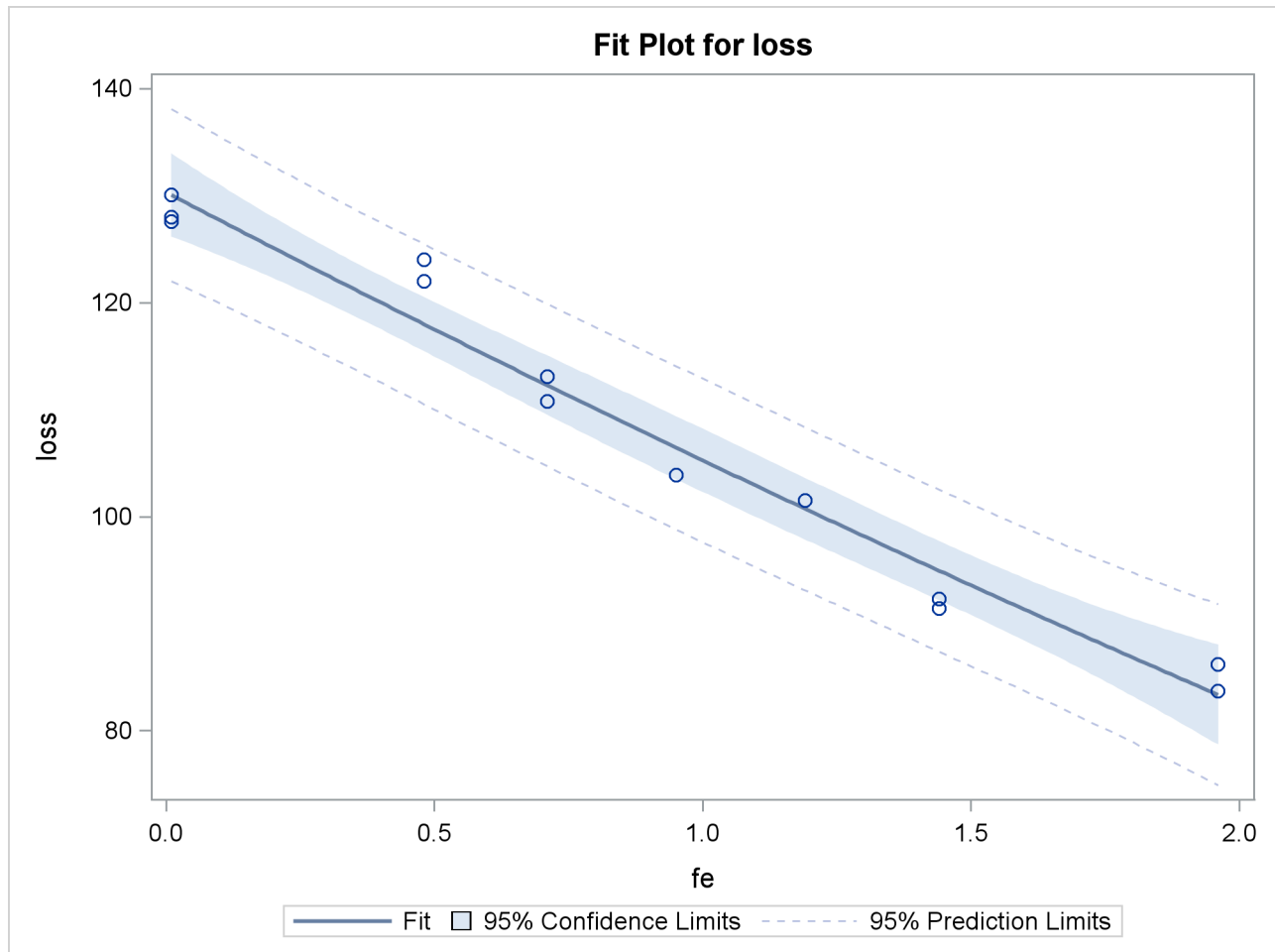
  

| Parameter | Estimate    | Standard Error | t Value | Pr >  t |
|-----------|-------------|----------------|---------|---------|
| Intercept | 130.3199337 | 1.77096213     | 73.59   | <.0001  |
| fe        | -26.2203900 | 4.39177557     | -5.97   | 0.0001  |
| fe*fe     | 1.1552018   | 2.19828568     | 0.53    | 0.6107  |

The  $t$  tests provided are equivalent to the Type III  $F$  tests. The quadratic term is not significant ( $p = 0.6107$ ) and thus can be removed from the model; the linear term is significant ( $p < 0.0001$ ). This suggests that there is indeed a straight-line relationship between loss and fe.

Finally, if ODS Graphics is enabled, PROC GLM also displays by default a scatter plot of the original data, as in Figure 42.4, with the quadratic fit overlaid. The following statements, which are the same as the previous analysis but with ODS Graphics enabled, additionally produce Figure 42.8.

```
ods graphics on;
proc glm data=iron;
 model loss=fe fe*fe;
run;
ods graphics off;
```

**Figure 42.8** Plot of Observed and Fit Corrosion Resistance by Iron Content, Quadratic Model

The insignificance of the quadratic term in the model is reflected in the fact that the fit is nearly linear.

Fitting the model without the quadratic term provides more accurate estimates for  $\beta_0$  and  $\beta_1$ . PROC GLM allows only one **MODEL** statement per invocation of the procedure, so the **PROC GLM** statement must be issued again. The following statements are used to fit the linear model.

```
proc glm data=iron;
 model loss=fe;
run;
```

Figure 42.9 displays the output produced by these statements. The linear term is still significant ( $F = 352.27$ ,  $p < 0.0001$ ). The estimated model is now

$$\text{loss} = 129.79 - 24.02 \times \text{fe}$$

**Figure 42.9** Linear Model Output

| Regression in PROC GLM   |             |                |             |           |        |
|--------------------------|-------------|----------------|-------------|-----------|--------|
| The GLM Procedure        |             |                |             |           |        |
| Dependent Variable: loss |             |                |             |           |        |
| Source                   | DF          | Sum of Squares | Mean Square | F Value   | Pr > F |
| Model                    | 1           | 3293.766690    | 3293.766690 | 352.27    | <.0001 |
| Error                    | 11          | 102.850233     | 9.350021    |           |        |
| Corrected Total          | 12          | 3396.616923    |             |           |        |
|                          | R-Square    | Coeff Var      | Root MSE    | loss Mean |        |
|                          | 0.969720    | 2.810063       | 3.057780    | 108.8154  |        |
| Source                   | DF          | Type I SS      | Mean Square | F Value   | Pr > F |
| fe                       | 1           | 3293.766690    | 3293.766690 | 352.27    | <.0001 |
| Source                   | DF          | Type III SS    | Mean Square | F Value   | Pr > F |
| fe                       | 1           | 3293.766690    | 3293.766690 | 352.27    | <.0001 |
| Parameter                | Estimate    | Standard Error | t Value     | Pr >  t   |        |
| Intercept                | 129.7865993 | 1.40273671     | 92.52       | <.0001    |        |
| fe                       | -24.0198934 | 1.27976715     | -18.77      | <.0001    |        |



## Syntax: GLM Procedure

The following statements are available in the GLM procedure:

```

PROC GLM < options > ;
 CLASS variable < (REF= option) > ... < variable < (REF= option) > > < / global-options > ;
 MODEL dependent-variables = independent-effects < / options > ;
 ABSORB variables ;
 BY variables ;
 CODE < options > ;
 FREQ variable ;
 ID variables ;
 WEIGHT variable ;
 CONTRAST 'label' effect values < ... effect values > < / options > ;
 ESTIMATE 'label' effect values < ... effect values > < / options > ;
 LSMEANS effects < / options > ;
 MANOVA < test-options > < / detail-options > ;
 MEANS effects < / options > ;
 OUTPUT < OUT=SAS-data-set > keyword=names < ... keyword=names > < / option > ;
 RANDOM effects < / options > ;
 REPEATED factor-specification < / options > ;
 STORE < OUT= > item-store-name < / LABEL='label' > ;
 TEST < H=effects > E=effect < / options > ;

```

Although there are numerous statements and options available in PROC GLM, many applications use only a few of them. Often you can find the features you need by looking at an example or by quickly scanning through this section.

To use PROC GLM, the **PROC GLM** and **MODEL** statements are required. You can specify only one **MODEL** statement (in contrast to the REG procedure, for example, which allows several **MODEL** statements in the same PROC REG run). If your model contains classification effects, the classification variables must be listed in a **CLASS** statement, and the **CLASS** statement must appear before the **MODEL** statement. In addition, if you use a **CONTRAST** statement in combination with a **MANOVA**, **RANDOM**, **REPEATED**, or **TEST** statement, the **CONTRAST** statement must be entered first in order for the contrast to be included in the **MANOVA**, **RANDOM**, **REPEATED**, or **TEST** analysis.

Table 42.2 summarizes the positional requirements for the statements in the GLM procedure.

**Table 42.2** Positional Requirements for PROC GLM Statements

| <b>Statement</b> | <b>Must Precede...</b>                                | <b>Must Follow...</b>                 |
|------------------|-------------------------------------------------------|---------------------------------------|
| ABSORB           | First RUN statement                                   |                                       |
| BY               | First RUN statement                                   |                                       |
| CLASS            | MODEL statement                                       |                                       |
| CONTRAST         | MANOVA, REPEATED,<br>or RANDOM statement              | MODEL statement                       |
| ESTIMATE         |                                                       | MODEL statement                       |
| FREQ             | First RUN statement                                   |                                       |
| ID               | First RUN statement                                   |                                       |
| LSMEANS          |                                                       | MODEL statement                       |
| MANOVA           |                                                       | CONTRAST or<br>MODEL statement        |
| MEANS            |                                                       | MODEL statement                       |
| MODEL            | CONTRAST, ESTIMATE,<br>LSMEANS, or MEANS<br>statement | CLASS statement                       |
| OUTPUT           |                                                       | MODEL statement                       |
| RANDOM           |                                                       | CONTRAST or<br>MODEL statement        |
| REPEATED         |                                                       | CONTRAST, MODEL,<br>or TEST statement |
| TEST             | MANOVA or<br>REPEATED statement                       | MODEL statement                       |
| WEIGHT           | First RUN statement                                   |                                       |

Table 42.3 summarizes the function of each statement (other than the PROC statement) in the GLM procedure.

**Table 42.3** Statements in the GLM Procedure

| <b>Statement</b> | <b>Description</b>                                                                                                                           |
|------------------|----------------------------------------------------------------------------------------------------------------------------------------------|
| ABSORB           | Absorbs classification effects in a model                                                                                                    |
| BY               | Specifies variables to define subgroups for the analysis                                                                                     |
| CLASS            | Declares classification variables                                                                                                            |
| CODE             | Requests that the procedure write SAS DATA step code to a file or catalog entry for computing predicted values according to the fitted model |
| CONTRAST         | Constructs and tests linear functions of the parameters                                                                                      |
| ESTIMATE         | Estimates linear functions of the parameters                                                                                                 |
| FREQ             | Specifies a frequency variable                                                                                                               |
| ID               | Identifies observations on output                                                                                                            |
| LSMEANS          | Computes least squares (marginal) means                                                                                                      |
| MANOVA           | Performs a multivariate analysis of variance                                                                                                 |

**Table 42.3** *continued*

| <b>Statement</b> | <b>Description</b>                                                                                      |
|------------------|---------------------------------------------------------------------------------------------------------|
| MEANS            | Computes and optionally compares arithmetic means                                                       |
| MODEL            | Defines the model to be fit                                                                             |
| OUTPUT           | Requests an output data set containing diagnostics for each observation                                 |
| RANDOM           | Declares certain effects to be random and computes expected mean squares                                |
| REPEATED         | Performs multivariate and univariate repeated measures analysis of variance                             |
| STORE            | Requests that the procedure save the context and results of the statistical analysis into an item store |
| TEST             | Constructs tests that use the sums of squares for effects and the error term you specify                |
| WEIGHT           | Specifies a variable for weighting observations                                                         |

The rest of this section provides detailed syntax information for each of these statements, beginning with the `PROC GLM` statement. The remaining statements are covered in alphabetical order.

The `STORE` and `CODE` statements are also used by many other procedures. A summary description of functionality and syntax for these statements is also shown after the `PROC GLM` statement in alphabetical order, but you can find full documentation about them in the section “`STORE Statement`” on page 501 of Chapter 19, “Shared Concepts and Topics.”

---

## PROC GLM Statement

**PROC GLM** *< options >* ;

The `PROC GLM` statement invokes the GLM procedure. [Table 42.4](#) summarizes the options available in the `PROC GLM` statement.

**Table 42.4** PROC GLM Statement Options

| <b>Option</b> | <b>Description</b>                                                                         |
|---------------|--------------------------------------------------------------------------------------------|
| ALPHA=        | Specifies the level of significance for confidence intervals                               |
| DATA=         | Names the SAS data set used by the GLM procedure                                           |
| MANOVA        | Requests the multivariate mode of eliminating observations with missing values             |
| MULTIPASS     | Requests that the input data set be reread when necessary, instead of using a utility file |
| NAMELEN=      | Specifies the length of effect names                                                       |
| NOPRINT       | Suppresses the normal display of results                                                   |
| ORDER=        | Specifies the order in which to sort classification variables                              |
| OUTSTAT=      | Names an output data set for information and statistics on each model effect               |
| PLOTS         | Controls the plots produced through ODS Graphics                                           |

You can specify the following options in the PROC GLM statement.

**ALPHA= $p$**

specifies the level of significance  $p$  for  $100(1 - p)\%$  confidence intervals. The value must be between 0 and 1; the default value of  $p = 0.05$  results in 95% intervals. This value is used as the default confidence level for limits computed by the following options.

| Statement | Options               |
|-----------|-----------------------|
| LSMEANS   | CL                    |
| MEANS     | CLM CLDIFF            |
| MODEL     | CLI CLM CLPARM        |
| OUTPUT    | UCL= LCL= UCLM= LCLM= |

You can override the default in each of these cases by specifying the ALPHA= option for each statement individually.

**DATA=*SAS-data-set***

names the SAS data set used by the GLM procedure. By default, PROC GLM uses the most recently created SAS data set.

**MANOVA**

requests the multivariate mode of eliminating observations with missing values. If any of the dependent variables have missing values, the procedure eliminates that observation from the analysis. The MANOVA option is useful if you use PROC GLM in interactive mode and plan to perform a multivariate analysis.

**MULTIPASS**

requests that PROC GLM reread the input data set when necessary, instead of writing the necessary values of dependent variables to a utility file. This option decreases disk space usage at the expense of increased execution times, and is useful only in rare situations where disk space is at an absolute premium.

**NAMELEN= $n$**

specifies the length of effect names in tables and output data sets to be  $n$  characters long, where  $n$  is a value between 20 and 200 characters. The default length is 20 characters.

**NOPRINT**

suppresses the normal display of results. The NOPRINT option is useful when you want only to create one or more output data sets with the procedure. Note that this option temporarily disables the Output Delivery System (ODS); see Chapter 20, “Using the Output Delivery System,” for more information.

**ORDER=DATA | FORMATTED | FREQ | INTERNAL**

specifies the sort order for the levels of the classification variables (which are specified in the CLASS statement). This ordering determines which parameters in the model correspond to each level in the data, so the ORDER= option can be useful when you specify the CONTRAST or ESTIMATE statement.

This option applies to the levels for all classification variables, except when you use the (default) ORDER=FORMATTED option with numeric classification variables that have no explicit format. With this option, the levels of such variables are ordered by their internal value.

The ORDER= option can take the following values:

| Value of ORDER=  | Levels Sorted By                                                                                                                       |
|------------------|----------------------------------------------------------------------------------------------------------------------------------------|
| <b>DATA</b>      | Order of appearance in the input data set                                                                                              |
| <b>FORMATTED</b> | External formatted value, except for numeric variables with no explicit format, which are sorted by their unformatted (internal) value |
| <b>FREQ</b>      | Descending frequency count; levels with the most observations come first in the order                                                  |
| <b>INTERNAL</b>  | Unformatted value                                                                                                                      |

By default, ORDER=FORMATTED. For ORDER=FORMATTED and ORDER=INTERNAL, the sort order is machine-dependent.

For more information about sort order, see the chapter on the SORT procedure in the *Base SAS Procedures Guide* and the discussion of BY-group processing in *SAS Language Reference: Concepts*.

#### **OUTSTAT=SAS-data-set**

names an output data set that contains sums of squares, degrees of freedom,  $F$  statistics, and probability levels for each effect in the model, as well as for each **CONTRAST** that uses the overall residual or error mean square (MSE) as the denominator in constructing the  $F$  statistic. If you use the **CANONICAL** option in the **MANOVA** statement and do not use an **M=** specification in the **MANOVA** statement, the data set also contains results of the canonical analysis.

See the section “Output Data Sets” on page 3382 for more information.

**PLOTS** <(global-plot-options)> <= plot-request <(options)>>

**PLOTS** <(global-plot-options)> <= (plot-request <(options)> <... plot-request <(options)>>>

controls the plots produced through ODS Graphics. When you specify only one plot request, you can omit the parentheses from around the plot request. For example:

```
PLOTS=NONE
PLOTS=(DIAGNOSTICS RESIDUALS)
PLOTS (UNPACK) =RESIDUALS
PLOT=MEANPLOT (CLBAND)
```

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;
proc glm data=iron;
 model loss=fe fe*fe;
run;
ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS](#).”

If ODS Graphics is enabled but you do not specify the PLOTS= option, then PROC GLM produces a default set of plots, which might be different for different models, as discussed in the following.

- If you specify a one-way analysis of variance model, with just one **CLASS** variable, the GLM procedure produces a grouped box plot of the response values versus the **CLASS** levels. For an example of the box plot, see the section “[One-Way Layout with Means Comparisons](#)” on page 904.
- If you specify a two-way analysis of variance model, with just two **CLASS** variables, the GLM procedure produces an interaction plot of the response values, with horizontal position representing one **CLASS** variable and marker style representing the other; and with predicted response values connected by lines representing the two-way analysis. For an example of the interaction plot, see the section “[PROC GLM for Unbalanced ANOVA](#)” on page 3269.
- If you specify a model with a single continuous predictor, the GLM procedure produces a fit plot of the response values versus the covariate values, with a curve representing the fitted relationship and a band representing the confidence limits for individual mean values. For an example of the fit plot, see the section “[PROC GLM for Quadratic Least Squares Regression](#)” on page 3272.
- If you specify a model with two continuous predictors and no **CLASS** variables, the GLM procedure produces a contour fit plot, overlaying a scatter plot of the data and a contour plot of the predicted surface.
- If you specify an analysis of covariance model, with one or two **CLASS** variables and one continuous variable, the GLM procedure produces an analysis of covariance plot of the response values versus the covariate values, with lines representing the fitted relationship within each classification level. For an example of the analysis of covariance plot, see [Example 42.4](#).
- If you specify an **LSMEANS** statement with the **PDIF** option, the GLM procedure produces a plot appropriate for the type of LS-means comparison. For **PDIF**=ALL (which is the default if you specify only **PDIF**), the procedure produces a diffogram, which displays all pairwise LS-means differences and their significance. The display is also known as a “mean-mean scatter plot” (Hsu 1996). For **PDIF**=CONTROL, the procedure produces a display of each noncontrol LS-mean compared to the control LS-mean, with two-sided confidence intervals for the comparison. For **PDIF**=CONTROL and **PDIF**=CONTROLU a similar display is produced, but with one-sided confidence intervals. Finally, for the **PDIF**=ANOM option, the procedure produces an “analysis of means” plot, comparing each LS-mean to the average LS-mean.
- If you specify a **MEANS** statement, the GLM procedure produces a grouped box plot of the response values versus the effect for which means are being calculated.

The global plot options include the following:

**MAXPOINTS=NONE** | *number*

specifies that plots with elements that require processing of more than *number* points be suppressed. The default is MAXPOINTS=5000. This limit is ignored if you specify MAXPOINTS=NONE.

**ONLY**

suppresses the default plots. Only plots specifically requested are displayed.

**UNPACKPANEL****UNPACK**

suppresses paneling. By default, multiple plots can appear in some output panels. Specify UNPACKPANEL to get each plot in a separate panel. You can specify PLOTS(UNPACKPANEL) to just unpack the default plots. You can also specify UNPACKPANEL as a suboption with DIAGNOSTICS and RESIDUALS.

The following individual plots and plot options are available. If you specify only one *plot*, then you can omit the parentheses.

**ALL**

produces all appropriate plots. You can specify other options with ALL; for example, to request all plots and unpack just the residuals, specify: PLOTS=(ALL RESIDUALS(UNPACK)).

**ANCOVAPLOT<(CLM CLI LIMITS)>**

modifies the analysis of covariance plot produced by default when you have an analysis of covariance model, with one or two CLASS variables and one continuous variable. By default the plot does not show confidence limits around the predicted values. The PLOTS=ANCOVAPLOT(CLM) option adds limits for the expected predicted values, and PLOTS=ANCOVAPLOT(CLI) adds limits for new predictions. Use PLOTS=ANCOVAPLOT(LIMITS) to add both kinds of limits.

**ANOMPLOT**

requests an analysis of means display, in which least squares means are compared against an average least squares mean (Ott 1967; Nelson 1982, 1991, 1993). LS-mean ANOM plots are produced only if you also specify PDIFF=ANOM or ADJUST=NELSON in the LSMEANS statement, and in this case they are produced by default.

**BOXPLOT<(NPANELPOS=*n*)>**

modifies the plot produced by default for the model effect in a one-way analysis of variance model, or for an effect specified in the MEANS statement. Suppose the effect has  $m$  levels. By default, or if you specify PLOTS=BOXPLOT(NPANELPOS=0), all  $m$  levels of the effect are displayed in a single plot. Specifying a nonzero value of  $n$  will result in  $P$  panels, where  $P$  is the integer part of  $m/n + 1$ . If  $n > 0$ , then the levels will be approximately balanced across the  $P$  panels; whereas if  $n < 0$ , precisely  $|n|$  levels will be displayed on each panel except possibly the last.

**CONTOURFIT<(OBS=*obs-options*)>**

modifies the contour fit plot produced by default when you have a model involving only two continuous predictors. The plot displays a contour plot of the predicted surface overlaid with a scatter plot of the observed data. You can use the following *obs-options* to control how the observations are displayed:

**OBS=GRADIENT**

specifies that observations are displayed as circles colored by the observed response. The same color gradient is used to display the fitted surface and the observations. Observations where the predicted response is close to the observed response have similar colors: the

greater the contrast between the color of an observation and the surface, the larger the residual is at that point.

**OBS=NONE**

suppresses the observations.

**OBS=OUTLINE**

specifies that observations are displayed as circles with a border but with a completely transparent fill.

**OBS=OUTLINEGRADIENT**

is the same as OBS=GRADIENT except that a border is shown around each observation. This option is useful to identify the location of observations where the residuals are small, since at these points the color of the observations and the color of the surface are indistinguishable. OBS=OUTLINEGRADIENT is the default if you do not specify any *obs-options*.

**CONTROLPLOT**

requests a display in which least squares means are compared against a reference level. LS-mean control plots are produced only when you specify **PDIFF=CONTROL** or **ADJUST=DUNNETT** in the **LSMEANS** statement, and in this case they are produced by default.

**DIAGNOSTICS<(LABEL UNPACK)>**

requests that a panel of summary diagnostics for the fit be displayed. The panel displays scatter plots of residuals, absolute residuals, studentized residuals, and observed responses by predicted values; studentized residuals by leverage; Cook's *D* by observation; a Q-Q plot of residuals; a residual histogram; and a residual-fit spread plot. The LABEL option displays labels on observations satisfying  $RSTUDENT > 2$ ,  $LEVERAGE > 2p/n$ , and on the Cook's *D* plot,  $COOKSD > 4/n$ , where  $n$  is the number of observations used in fitting the model, and  $p$  is the number of parameters in the model. The label is the first ID variable if the ID statement is specified; otherwise, it is the observation number. The UNPACK option unpanels the diagnostic display and produces the series of individual plots that form the paneled display.

**DIFFPLOT<(ABS NOABS CENTER NOLINES)>**

modifies the plot produced by an **LSMEANS** statement with the **PDIFF=ALL** option (or just **PDIFF**, since ALL is the default argument). The ABS and NOABS options determine the positioning of the line segments in the plot. When the ABS option is in effect, and this is the default, all line segments are shown on the same side of the reference line. The NOABS option separates comparisons according to the sign of the difference. The CENTER option marks the center point for each comparison. This point corresponds to the intersection of two least squares means. The NOLINES option suppresses the display of the line segments that represent the confidence bounds for the differences of the least squares means. The NOLINES option implies the CENTER option. The default is to draw line segments in the upper portion of the plot area without marking the center point.

**FITPLOT<(NOCLM NOCLI NOLIMITS)>**

modifies the fit plot produced by default when you have a model with a single continuous predictor. By default the plot includes confidence limits for both the expected predicted values and individual new predictions. The **PLOTS=FITPLOT(NOCLM)** option removes the limits on the expected values and the **PLOTS=FITPLOT(NOCLI)** option removes the limits on new predictions. The **PLOTS=FITPLOT(NOLIMITS)** option removes both kinds of confidence limits.



**INTPLOT<(CLM CLI LIMITS)>**

modifies the interaction plot produced by default when you have a two-way analysis of variance model, with just two **CLASS** variables. By default the plot does not show confidence limits around the predicted values. The **PLOTS=INTPLOT(CLM)** option adds limits for the expected predicted values and **PLOTS=INTPLOT(CLI)** adds limits for new predictions. Use **PLOTS=INTPLOT(LIMITS)** to add both kinds of limits.

**MEANPLOT<(CL CLBAND CONNECT ASCENDING DESCENDING)>**

modifies the grouped box plot produced by an **MEANS** statement. Upper and lower confidence limits are plotted when the **CL** option is used. When the **CLBAND** option is in effect, confidence limits are shown as bands and the means are connected. By default, means are not joined by lines. You can achieve that effect with the **CONNECT** option. Means are displayed in the same order as they appear in the “Means” table. You can change that order for plotting with the **ASCENDING** and **DESCENDING** options.

**NONE**

specifies that no graphics be displayed.

**RESIDUALS<(SMOOTH UNPACK)>**

requests that scatter plots of the residuals against each continuous covariate be displayed. The **SMOOTH** option overlays a Loess smooth on each residual plot. Note that if a **WEIGHT** variable is specified, then it is not used to weight the smoother. See Chapter 53, “[The LOESS Procedure](#),” for more information. The **UNPACK** option unpanels the residual display and produces a series of individual plots that form the paneled display.

**ABSORB Statement**

**ABSORB** *variables* ;

Absorption is a computational technique that provides a large reduction in time and memory requirements for certain types of models. The *variables* are one or more variables in the input data set.

For a main-effect variable that does not participate in interactions, you can absorb the effect by naming it in an **ABSORB** statement. This means that the effect can be adjusted out before the construction and solution of the rest of the model. This is particularly useful when the effect has a large number of levels.

Several variables can be specified, in which case each one is assumed to be nested in the preceding variable in the **ABSORB** statement.

**NOTE:** When you use the **ABSORB** statement, the data set (or each **BY** group, if a **BY** statement appears) must be sorted by the variables in the **ABSORB** statement. The GLM procedure cannot produce predicted values or least squares means (LS-means) or create an output data set of diagnostic values if an **ABSORB** statement is used. If the **ABSORB** statement is used, it must appear before the first **RUN** statement; otherwise, it is ignored.

When you use an **ABSORB** statement and also use the **INT** option in the **MODEL** statement, the procedure ignores the option but computes the uncorrected total sum of squares (SS) instead of the corrected total sums of squares.

See the section “[Absorption](#)” on page 3343 for more information.

---

## BY Statement

**BY** *variables* ;

You can specify a BY statement with PROC GLM to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the GLM procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

Since sorting the data changes the order in which PROC GLM reads observations, the sort order for the levels of the classification variables might be affected if you also specify **ORDER=DATA** in the **PROC GLM** statement. This, in turn, affects specifications in the **CONTRAST** and **ESTIMATE** statements.

If you specify the BY statement, it must appear before the first RUN statement; otherwise, it is ignored. When you use a BY statement, the interactive features of PROC GLM are disabled.

When both the BY and **ABSORB** statements are used, observations must be sorted first by the variables in the BY statement, and then by the variables in the **ABSORB** statement.

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

---

## CLASS Statement

**CLASS** *variable* < (**REF=** *option*) > . . . < *variable* < (**REF=** *option*) > > < / *global-options* > ;

The CLASS statement names the classification variables to be used in the model. Typical classification variables are Treatment, Sex, Race, Group, and Replication. If you use the CLASS statement, it must appear before the **MODEL** statement.

Classification variables can be either character or numeric. By default, class levels are determined from the entire set of formatted values of the CLASS variables.

**NOTE:** Prior to SAS 9, class levels were determined by using no more than the first 16 characters of the formatted values. To revert to this previous behavior, you can use the TRUNCATE option in the CLASS statement.

In any case, you can use formats to group values into levels. See the discussion of the **FORMAT** procedure in the *Base SAS Procedures Guide* and the discussions of the **FORMAT** statement and SAS formats in *SAS*

*Formats and Informats: Reference.* You can adjust the order of CLASS variable levels with the **ORDER=** option in the **PROC GLM** statement.

The GLM procedure displays a table that summarizes the CLASS variables and their levels. You can use this table to check the ordering of levels and, hence, of the corresponding parameters for main effects. If you need to check the ordering of parameters for interaction effects, use the E option in the **MODEL**, **CONTRAST**, **ESTIMATE**, or **LSMEANS** statement. See the section “Parameterization of PROC GLM Models” on page 3327 for more information.

You can specify the following **REF=** option to indicate how the levels of an individual classification variable are to be ordered by enclosing it in parentheses after the variable name:

**REF= 'level' | FIRST | LAST**

specifies a level of the classification variable to be put at the end of the list of levels. This level thus corresponds to the reference level in the usual interpretation of the estimates with PROC GLM’s singular parameterization. You can specify the *level* of the variable to use as the reference level; specify a value that corresponds to the formatted value of the variable if a format is assigned. Alternatively, you can specify **REF=FIRST** to designate that the first ordered level serve as the reference, or **REF=LAST** to designate that the last ordered level serve as the reference. To specify that **REF=FIRST** or **REF=LAST** be used for all classification variables, use the **REF= global-option** after the slash (/) in the CLASS statement.

You can specify the following *global-options* in the CLASS statement after a slash (/):

**REF=FIRST | LAST**

specifies a level of all classification variables to be put at the end of the list of levels. This level thus corresponds to the reference level in the usual interpretation of the estimates with PROC GLM’s singular parameterization. Specify **REF=FIRST** to designate that the first ordered level for each classification variable serve as the reference. Specify **REF=LAST** to designate that the last ordered level serve as the reference. This option applies to all the variables specified in the CLASS statement. To specify different reference levels for different classification variables, use **REF=** options for individual variables.

**TRUNCATE**

specifies that class levels be determined by using only up to the first 16 characters of the formatted values of CLASS variables. When formatted values are longer than 16 characters, you can use this option to revert to the levels as determined in releases prior to SAS 9.

---

## CODE Statement

**CODE** < options > ;

The CODE statement enables you to write SAS DATA step code for computing predicted values of the fitted model either to a file or to a catalog entry. This code can then be included in a DATA step to score new data.

Table 42.5 summarizes the *options* available in the CODE statement.

**Table 42.5** CODE Statement Options

| Option    | Description                                                                  |
|-----------|------------------------------------------------------------------------------|
| CATALOG=  | Names the catalog entry where the generated code is saved                    |
| DUMMIES   | Retains the dummy variables in the data set                                  |
| ERROR     | Computes the error function                                                  |
| FILE=     | Names the file where the generated code is saved                             |
| FORMAT=   | Specifies the numeric format for the regression coefficients                 |
| GROUP=    | Specifies the group identifier for array names and statement labels          |
| IMPUTE    | Imputes predicted values for observations with missing or invalid covariates |
| LINESIZE= | Specifies the line size of the generated code                                |
| LOOKUP=   | Specifies the algorithm for looking up CLASS levels                          |
| RESIDUAL  | Computes residuals                                                           |

For details about the syntax of the CODE statement, see the section “CODE Statement” on page 390 in Chapter 19, “Shared Concepts and Topics.”

## CONTRAST Statement

**CONTRAST** *'label'* effect values < . . . effect values > < / options > ;

The CONTRAST statement enables you to perform custom hypothesis tests by specifying an **L** vector or matrix for testing the univariate hypothesis  $L\beta = 0$  or the multivariate hypothesis  $LBM = 0$ . Thus, to use this feature you must be familiar with the details of the model parameterization that PROC GLM uses. For more information, see the section “Parameterization of PROC GLM Models” on page 3327. All of the elements of the **L** vector might be given, or if only certain portions of the **L** vector are given, the remaining elements are constructed by PROC GLM from the context (in a manner similar to rule 4 discussed in the section “Construction of Least Squares Means” on page 3363).

There is no limit to the number of CONTRAST statements you can specify, but they must appear after the MODEL statement. In addition, if you use a CONTRAST statement and a MANOVA, REPEATED, or TEST statement, appropriate tests for contrasts are carried out as part of the MANOVA, REPEATED, or TEST analysis. If you use a CONTRAST statement and a RANDOM statement, the expected mean square of the contrast is displayed. As a result of these additional analyses, the CONTRAST statement must appear before the MANOVA, REPEATED, RANDOM, or TEST statement.

In the CONTRAST statement,

|               |                                                                                                                                                                                                                                       |
|---------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <i>label</i>  | identifies the contrast on the output. A label is required for every contrast specified. Labels must be enclosed in quotes.                                                                                                           |
| <i>effect</i> | identifies an effect that appears in the MODEL statement, or the INTERCEPT effect. The INTERCEPT effect can be used when an intercept is fitted in the model. You do not need to include all effects that are in the MODEL statement. |
| <i>values</i> | are constants that are elements of the <b>L</b> vector associated with the effect.                                                                                                                                                    |

You can specify the following options in the CONTRAST statement after a slash (/).

**E**

displays the entire **L** vector. This option is useful in confirming the ordering of parameters for specifying **L**.

**E=effect**

specifies an error term, which must be one of the effects in the model. The procedure uses this effect as the denominator in *F* tests in univariate analysis. In addition, if you use a **MANOVA** or **REPEATED** statement, the procedure uses the effect specified by the **E=** option as the basis of the **E** matrix. By default, the procedure uses the overall residual or error mean square (MSE) as an error term.

**ETYPE=*n***

specifies the type (1, 2, 3, or 4, corresponding to a Type I, II, III, or IV test, respectively) of the **E=** effect. If the **E=** option is specified and the **ETYPE=** option is not, the procedure uses the highest type computed in the analysis.

**SINGULAR=*number***

tunes the estimability checking. If  $\text{ABS}(\mathbf{L} - \mathbf{LH}) > C \times \text{number}$  for any row in the contrast, then **L** is declared nonestimable. **H** is the  $(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{X}$  matrix, and *C* is  $\text{ABS}(\mathbf{L})$  except for rows where **L** is zero, and then it is 1. The default value for the **SINGULAR=** option is  $10^{-4}$ . Values for the **SINGULAR=** option must be between 0 and 1.

As stated previously, the **CONTRAST** statement enables you to perform custom hypothesis tests. If the hypothesis is testable in the univariate case,  $SS(H_0: \mathbf{L}\boldsymbol{\beta} = 0)$  is computed as

$$(\mathbf{Lb})'(\mathbf{L}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{L}')^{-1}(\mathbf{Lb})$$

where  $\mathbf{b} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}$ . This is the sum of squares displayed on the analysis-of-variance table.

For multivariate testable hypotheses, the usual multivariate tests are performed using

$$\mathbf{H} = \mathbf{M}'(\mathbf{LB})'(\mathbf{L}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{L}')^{-1}(\mathbf{LB})\mathbf{M}$$

where  $\mathbf{B} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$  and **Y** is the matrix of multivariate responses or dependent variables. The degrees of freedom associated with the hypothesis are equal to the row rank of **L**. The sum of squares computed in this situation is equivalent to the sum of squares computed using an **L** matrix with any row deleted that is a linear combination of previous rows.

Multiple-degrees-of-freedom hypotheses can be specified by separating the rows of the **L** matrix with commas.

For example, for the model

```
proc glm;
 class A B;
 model Y=A B;
run;
```

with A at 5 levels and B at 2 levels, the parameter vector is

$$(\mu \ \alpha_1 \ \alpha_2 \ \alpha_3 \ \alpha_4 \ \alpha_5 \ \beta_1 \ \beta_2)$$

To test the hypothesis that the pooled A linear and A quadratic effect is zero, you can use the following **L** matrix:

$$\mathbf{L} = \begin{bmatrix} 0 & -2 & -1 & 0 & 1 & 2 & 0 & 0 \\ 0 & 2 & -1 & -2 & -1 & 2 & 0 & 0 \end{bmatrix}$$

The corresponding CONTRAST statement is

```
contrast 'A LINEAR & QUADRATIC'
 a -2 -1 0 1 2,
 a 2 -1 -2 -1 2;
```

If the first level of A is a control level and you want a test of control versus others, you can use this statement:

```
contrast 'CONTROL VS OTHERS' a -1 0.25 0.25 0.25 0.25;
```

See the following discussion of the **ESTIMATE** statement and the section “Specification of **ESTIMATE Expressions**” on page 3345 for rules on specification, construction, distribution, and estimability in the **CONTRAST** statement.

## ESTIMATE Statement

```
ESTIMATE 'label' effect values <... effect values> </ options > ;
```

The **ESTIMATE** statement enables you to estimate linear functions of the parameters by multiplying the vector **L** by the parameter estimate vector **b**, resulting in **Lb**. All of the elements of the **L** vector might be given, or, if only certain portions of the **L** vector are given, the remaining elements are constructed by PROC GLM from the context (in a manner similar to rule 4 discussed in the section “Construction of Least Squares Means” on page 3363).

The linear function is checked for estimability. The estimate **Lb**, where  $\mathbf{b} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}$ , is displayed along with its associated standard error,  $\sqrt{\mathbf{L}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{L}'s^2}$ , and *t* test. If you specify the **CLPARM** option in the **MODEL** statement (see page 3311), confidence limits for the true value are also displayed.

There is no limit to the number of **ESTIMATE** statements that you can specify, but they must appear after the **MODEL** statement. In the **ESTIMATE** statement,

|               |                                                                                                                                                                                                                                                                                |
|---------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <i>label</i>  | identifies the estimate on the output. A label is required for every contrast specified. Labels must be enclosed in quotes.                                                                                                                                                    |
| <i>effect</i> | identifies an effect that appears in the <b>MODEL</b> statement, or the <b>INTERCEPT</b> effect. The <b>INTERCEPT</b> effect can be used as an effect when an intercept is fitted in the model. You do not need to include all effects that are in the <b>MODEL</b> statement. |
| <i>values</i> | are constants that are the elements of the <b>L</b> vector associated with the preceding effect. For example,                                                                                                                                                                  |

```
estimate 'A1 VS A2' A 1 -1;
```

forms an estimate that is the difference between the parameters estimated for the first and second levels of the CLASS variable A.

You can specify the following options in the ESTIMATE statement after a slash (/):

**DIVISOR=***number*

specifies a value by which to divide all coefficients so that fractional coefficients can be entered as integer numerators. For example, you can use

```
estimate '1/3(A1+A2) - 2/3A3' a 1 1 -2 / divisor=3;
```

instead of

```
estimate '1/3(A1+A2) - 2/3A3' a 0.33333 0.33333 -0.66667;
```

**E**

displays the entire **L** vector. This option is useful in confirming the ordering of parameters for specifying **L**.

**SINGULAR=***number*

tunes the estimability checking. If  $ABS(\mathbf{L} - \mathbf{LH}) > C \times \text{number}$ , then the **L** vector is declared nonestimable. **H** is the  $(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{X}$  matrix, and **C** is  $ABS(\mathbf{L})$  except for rows where **L** is zero, and then it is 1. The default value for the SINGULAR= option is  $10^{-4}$ . Values for the SINGULAR= option must be between 0 and 1.

See also the section “Specification of ESTIMATE Expressions” on page 3345.

## FREQ Statement

**FREQ** *variable* ;

The FREQ statement names a variable that provides frequencies for each observation in the DATA= data set. Specifically, if  $n$  is the value of the FREQ variable for a given observation, then that observation is used  $n$  times.

The analysis produced using a FREQ statement reflects the expanded number of observations. For example, means and total degrees of freedom reflect the expanded number of observations. You can produce the same analysis (without the FREQ statement) by first creating a new data set that contains the expanded number of observations. For example, if the value of the FREQ variable is 5 for the first observation, the first 5 observations in the new data set are identical. Each observation in the old data set is replicated  $n_i$  times in the new data set, where  $n_i$  is the value of the FREQ variable for that observation.

If the value of the FREQ variable is missing or is less than 1, the observation is not used in the analysis. If the value is not an integer, only the integer portion is used.

If you specify the FREQ statement, it must appear before the first RUN statement or it is ignored.

---

## ID Statement

**ID** *variables* ;

When predicted values are requested as a **MODEL** statement option, values of the variables given in the ID statement are displayed beside each observed, predicted, and residual value for identification. Although there are no restrictions on the length of ID variables, PROC GLM might truncate the number of values listed in order to display them on one line. The GLM procedure displays a maximum of five ID variables.

If you specify the ID statement, it must appear before the first RUN statement or it is ignored.

---

## LSMEANS Statement

**LSMEANS** *effects* </ *options* > ;

Table 42.6 summarizes the options available in the LSMEANS statement.

**Table 42.6** LSMEANS Statement Options

| Option     | Description                                                                      |
|------------|----------------------------------------------------------------------------------|
| ADJUST=    | Requests a multiple comparison adjustment                                        |
| ALPHA=     | Specifies the level of significance                                              |
| AT         | Enables you to modify the values of the covariates                               |
| BYLEVEL    | Processes the OM data set by each level of the LS-mean effect                    |
| CL         | Requests confidence limits                                                       |
| COV        | Includes variances and covariances of the LS-means                               |
| E          | Displays the coefficients of the linear functions                                |
| E=         | Specifies an effect in the model to use as an error term                         |
| ETYPE=     | Specifies the type of the E= effect                                              |
| LINES      | Uses connecting lines to indicate nonsignificantly different subsets of LS-means |
| NOPRINT    | Suppresses the normal display of results                                         |
| OBSMARGINS | Specifies a potentially different weighting scheme                               |
| OUT=       | Creates an output data set                                                       |
| PDIFF      | Requests that <i>p</i> -values for differences                                   |
| SLICE=     | Specifies effects within which to test for differences                           |
| SINGULAR=  | Tunes the estimability checking                                                  |
| STDERR     | Produces the standard error                                                      |
| TDIFF      | Produces the <i>t</i> values                                                     |

---

Least squares means (LS-means) are computed for each *effect* listed in the LSMEANS statement. You can specify only classification effects in the LSMEANS statement—that is, effects that contain only classification variables. You can also specify options to perform multiple comparisons. In contrast to the **MEANS** statement, the LSMEANS statement performs multiple comparisons on interactions as well as main effects.

LS-means are *predicted population margins*; that is, they estimate the marginal means over a balanced population. In a sense, LS-means are to unbalanced designs as class and subclass arithmetic means are to



balanced designs. Each LS-mean is computed as  $L/b$  for a certain column vector  $L$ , where  $b$  is the vector of parameter estimates—that is, the solution of the normal equations. For further information, see the section “Construction of Least Squares Means” on page 3363.

Multiple effects can be specified in one LSMEANS statement, or multiple LSMEANS statements can be used, but they must all appear after the **MODEL** statement. For example:

```
proc glm;
 class A B;
 model Y=A B A*B;
 lsmeans A B A*B;
run;
```

LS-means are displayed for each level of the A, B, and A\*B effects.

You can specify the following options in the LSMEANS statement after a slash (/):

**ADJUST=BON**

**ADJUST=DUNNETT**

**ADJUST=NELSON**

**ADJUST=SCHEFFE**

**ADJUST=SIDAK**

**ADJUST=SIMULATE** <(simoptions)>

**ADJUST=SMM** | **GT2**

**ADJUST=TUKEY**

**ADJUST=T**

requests a multiple comparison adjustment for the  $p$ -values and confidence limits for the differences of LS-means. The **ADJUST=** option modifies the results of the **TDIFF** and **PDIFF** options; thus, if you omit the **TDIFF** or **PDIFF** option then the **ADJUST=** option implies **PDIFF**. By default, PROC GLM analyzes all pairwise differences. If you specify **ADJUST=DUNNETT**, PROC GLM analyzes all differences with a control level. If you specify the **ADJUST=NELSON** option, PROC GLM analyzes all differences with the average LS-mean. The default is **ADJUST=T**, which really signifies no adjustment for multiple comparisons.

The **BON** (Bonferroni) and **SIDAK** adjustments involve correction factors described in the section “Multiple Comparisons” on page 3349 and in Chapter 61, “The **MULTTEST** Procedure.” When you specify **ADJUST=TUKEY** and your data are unbalanced, PROC GLM uses the approximation described in Kramer (1956) and identifies the adjustment as “Tukey-Kramer” in the results. Similarly, when you specify either **ADJUST=DUNNETT** or the **ADJUST=NELSON** option and the LS-means are correlated, PROC GLM uses the factor-analytic covariance approximation described in Hsu (1992) and identifies the adjustment in the results as “Dunnett-Hsu” or “Nelson-Hsu,” respectively. The preceding references also describe the **SCHEFFE** and **SMM** adjustments.

The **SIMULATE** adjustment computes the adjusted  $p$ -values from the simulated distribution of the maximum or maximum absolute value of a multivariate  $t$  random vector. The simulation estimates  $q$ , the true  $(1 - \alpha)$  quantile, where  $1 - \alpha$  is the confidence coefficient. The default  $\alpha$  is the value of the **ALPHA=** option in the **PROC GLM** statement or 0.05 if that option is not specified. You can change this value with the **ALPHA=** option in the **LSMEANS** statement.

The number of samples for the **SIMULATE** adjustment is set so that the tail area for the simulated  $q$  is within a certain *accuracy radius*  $\gamma$  of  $1 - \alpha$  with an *accuracy confidence* of  $100(1 - \epsilon)\%$ . In equation

form,

$$P(|F(\hat{q}) - (1 - \alpha)| \leq \gamma) = 1 - \epsilon$$

where  $\hat{q}$  is the simulated  $q$  and  $F$  is the true distribution function of the maximum; see Edwards and Berry (1987) for details. By default,  $\gamma = 0.005$  and  $\epsilon = 0.01$ , so that the tail area of  $\hat{q}$  is within 0.005 of 0.95 with 99% confidence.

You can specify the following *simoptions* in parentheses after the ADJUST=SIMULATE option.

**ACC=value**

specifies the target accuracy radius  $\gamma$  of a  $100(1-\epsilon)\%$  confidence interval for the true probability content of the estimated  $(1-\alpha)$  quantile. The default value is ACC=0.005. Note that, if you also specify the CVADJUST *simoption*, then the actual accuracy radius will probably be substantially less than this target.

**CVADJUST**

specifies that the quantile should be estimated by the control variate adjustment method of Hsu and Nelson (1998) instead of simply as the quantile of the simulated sample. Specifying the CVADJUST option typically has the effect of significantly reducing the accuracy radius  $\gamma$  of a  $100 \times (1 - \epsilon)\%$  confidence interval for the true probability content of the estimated  $(1 - \alpha)$  quantile. The control-variate-adjusted quantile estimate takes roughly twice as long to compute, but it is typically much more accurate than the sample quantile.

**EPS=value**

specifies the value  $\epsilon$  for a  $100 \times (1 - \epsilon)\%$  confidence interval for the true probability content of the estimated  $(1 - \alpha)$  quantile. The default value for the accuracy confidence is 99%, corresponding to EPS=0.01.

**NSAMP=n**

specifies the sample size for the simulation. By default,  $n$  is set based on the values of the target accuracy radius  $\gamma$  and accuracy confidence  $100 \times (1 - \epsilon)\%$  for an interval for the true probability content of the estimated  $(1 - \alpha)$  quantile. With the default values for  $\gamma$ ,  $\epsilon$ , and  $\alpha$  (0.005, 0.01, and 0.05, respectively), NSAMP=12604 by default.

**REPORT**

specifies that a report on the simulation should be displayed, including a listing of the parameters, such as  $\gamma$ ,  $\epsilon$ , and  $\alpha$ , as well as an analysis of various methods for estimating or approximating the quantile.

**SEED=number**

specifies an integer used to start the pseudo-random number generator for the simulation. If you do not specify a seed, or specify a value less than or equal to zero, the seed is by default generated from reading the time of day from the computer's clock.

**THREADS**

specifies that the computational work for the simulation be divided into parallel threads, where the number of threads is the value of the SAS system option CPUCOUNT=. For large simulations (as specified directly using the NSAMP= *simoption* or indirectly using the ACC= or EPS= *simoptions*), parallel processing can markedly speed up the computation of adjusted  $p$ -values and confidence intervals. However, because the parallel processing has different pseudo-random number streams, the precise results are different from the default ones, which are

computed in sequence rather than in parallel. This option overrides the SAS system option `THREADS | NOTTHREADS`.

### **NOTTHREADS**

specifies that the computational work for the simulation be performed in sequence rather than in parallel. `NOTTHREADS` is the default. This option overrides the SAS system option `THREADS | NOTTHREADS`.

### **ALPHA=*p***

specifies the level of significance  $p$  for  $100(1 - p)\%$  confidence intervals. This option is useful only if you also specify the `CL` option, and, optionally, the `PDIFF` option. By default,  $p$  is equal to the value of the `ALPHA=` option in the `PROC GLM` statement or 0.05 if that option is not specified. This value is used to set the endpoints for confidence intervals for the individual means as well as for differences between means.

### **AT *variable = value***

### **AT (*variable-list*) = (*value-list*)**

### **AT MEANS**

enables you to modify the values of the covariates used in computing LS-means. By default, all covariate effects are set equal to their mean values for computation of standard LS-means. The `AT` option enables you to set the covariates to whatever values you consider interesting. For more information, see the section “[Setting Covariate Values](#)” on page 3364.

### **BYLEVEL**

requests that `PROC GLM` process the `OM` data set by each level of the LS-mean effect in question. For more details, see the entry for the `OM` option in this section.

### **CL**

requests confidence limits for the individual LS-means. If you specify the `PDIFF` option, confidence limits for differences between means are produced as well. You can control the confidence level with the `ALPHA=` option. Note that, if you specify an `ADJUST=` option, the confidence limits for the differences are adjusted for multiple inference but the confidence intervals for individual means are **not** adjusted.

### **COV**

includes variances and covariances of the LS-means in the output data set specified in the `OUT=` option in the `LSMEANS` statement. Note that this is the covariance matrix for the LS-means themselves, not the covariance matrix for the differences between the LS-means, which is used in the `PDIFF` computations. If you omit the `OUT=` option, the `COV` option has no effect. When you specify the `COV` option, you can specify only one effect in the `LSMEANS` statement.

### **E**

displays the coefficients of the linear functions used to compute the LS-means.

### **E=*effect***

specifies an effect in the model to use as an error term. The procedure uses the mean square for the *effect* as the error mean square when calculating estimated standard errors (requested with the `STDERR` option) and probabilities (requested with the `STDERR`, `PDIFF`, or `TDIFF` option). Unless you specify `STDERR`, `PDIFF` or `TDIFF`, the `E=` option is ignored. By default, if you specify the `STDERR`, `PDIFF`, or `TDIFF` option and do not specify the `E=` option, the procedure uses the error mean square for calculating standard errors and probabilities.

**ETYPE=*n***

specifies the type (1, 2, 3, or 4, corresponding to a Type I, II, III, or IV test, respectively) of the **E=** effect. If you specify the **E=** option but not the **ETYPE=** option, the highest type computed in the analysis is used. If you omit the **E=** option, the **ETYPE=** option has no effect.

**LINES**

presents results of comparisons between all pairs of means (specified by the **PDIFF=ALL** option) by listing the means in descending order and indicating nonsignificant subsets by line segments beside the corresponding means. When all differences have the same variance, these comparison lines are guaranteed to accurately reflect the inferences based on the corresponding tests, made by comparing the respective *p*-values to the value of the **ALPHA=** option (0.05 by default). However, equal variances are rarely the case for differences between LS-means. If the variances are not all the same, then the comparison lines might be conservative, in the sense that if you base your inferences on the lines alone, you will detect fewer significant differences than the tests indicate. If there are any such differences, a note is appended to the table that lists the pairs of means that are inferred to be significantly different by the tests but not by the comparison lines. Note, however, that in many cases, even though the variances are unbalanced, they are near enough that the comparison lines in fact accurately reflect the test inferences.

**NOPRINT**

suppresses the normal display of results from the LSMEANS statement. This option is useful when an output data set is created with the **OUT=** option in the LSMEANS statement.

**OBSMARGINS****OM**

specifies a potentially different weighting scheme for computing LS-means coefficients. The standard LS-means have equal coefficients across classification effects; however, the **OM** option changes these coefficients to be proportional to those found in the input data set. For more information, see the section “[Changing the Weighting Scheme](#)” on page 3365.

The **BYLEVEL** option modifies the observed-margins LS-means. Instead of computing the margins across the entire data set, the procedure computes separate margins for each level of the LS-mean effect in question. The resulting LS-means are actually equal to raw means in this case. If you specify the **BYLEVEL** option, it disables the **AT** option.

**OUT=SAS-data-set**

creates an output data set that contains the values, standard errors, and, optionally, the covariances (see the **COV** option) of the LS-means.

For more information, see the section “[Output Data Sets](#)” on page 3382.

**PDIFF< =difftype >**

requests that *p*-values for differences of the LS-means be produced. The optional *difftype* specifies which differences to display. Possible values for *difftype* are ALL, CONTROL, CONTROLL, CONTROLU, and ANOM. The ALL value requests all pairwise differences, and it is the default. The CONTROL value requests the differences with a control that, by default, is the first level of each of the specified LS-mean effects. The ANOM value requests differences between each LS-mean and the average LS-mean, as in the *analysis of means* (Ott 1967). The average is computed as a weighted mean of the LS-means, the weights being inversely proportional to the variances. Note that the ANOM procedure in SAS/QC software implements both tables and graphics for the analysis of means with a

variety of response types. For one-way designs, the PDIFF=ANOM computations are equivalent to the results of PROC ANOM. See the section “Analysis of Means: Comparing Each Treatments to the Average” on page 3355 for more details.

To specify which levels of the effects are the controls, list the quoted formatted values in parentheses after the keyword CONTROL. For example, if the effects A, B, and C are CLASS variables, each having two levels, '1' and '2', the following LSMEANS statement specifies the '1' '2' level of A\*B and the '2' '1' level of B\*C as controls:

```
lsmeans A*B B*C / pdiff=control('1' '2', '2' '1');
```

For multiple-effect situations such as this one, the ordering of the list is significant, and you should check the output to make sure that the controls are correct.

Two-tailed tests and confidence limits are associated with the CONTROL difftype. For one-tailed results, use either the CONTROLL or CONTROLU difftype.

- PDIFF=CONTROLL tests whether the noncontrol levels are less than the control; you declare a noncontrol level to be significantly less than the control if the associated upper confidence limit for the noncontrol level minus the control is less than zero, and you ignore the associated lower confidence limits (which are set to minus infinity).
- PDIFF=CONTROLU tests whether the noncontrol levels are greater than the control; you declare a noncontrol level to be significantly greater than the control if the associated lower confidence limit for the noncontrol level minus the control is greater than zero, and you ignore the associated upper confidence limits (which are set to infinity).

The default multiple comparisons adjustment for each *difftype* is shown in the following table.

| <i>difftype</i> | Default ADJUST= |
|-----------------|-----------------|
| Not specified   | T               |
| ALL             | TUKEY           |
| CONTROL         |                 |
| CONTROLL        | DUNNETT         |
| CONTROLU        |                 |
| ANOM            | NELSON          |

If no *difftype* is specified, the default for the ADJUST= option is T (that is, no adjustment); for PDIFF=ALL, ADJUST=TUKEY is the default; for PDIFF=CONTROL, PDIFF=CONTROLL, or PDIFF=CONTROLU, the default value for the ADJUST= option is DUNNETT. For PDIFF=ANOM, ADJUST=NELSON is the default. If there is a conflict between the PDIFF= and ADJUST= options, the ADJUST= option takes precedence.

For example, in order to compute one-sided confidence limits for differences with a control, adjusted according to Dunnett's procedure, the following statements are equivalent:

```
lsmeans Treatment / pdiff=controll c1;
lsmeans Treatment / pdiff=controll c1 adjust=dunnett;
```

**SLICE**=*fixed-effect*

**SLICE**=(*fixed-effects*)

specifies effects within which to test for differences between interaction LS-mean effects. This can produce what are known as tests of simple effects (Winer 1971). For example, suppose that A\*B is significant and you want to test for the effect of A within each level of B. The appropriate LSMEANS statement is

```
lsmeans A*B / slice=B;
```

This statement tests for the simple main effects of A for B, which are calculated by extracting the appropriate rows from the coefficient matrix for the A\*B LS-means and using them to form an  $F$  test as performed by the **CONTRAST** statement.

**SINGULAR**=*number*

tunes the estimability checking. If  $ABS(\mathbf{L} - \mathbf{LH}) > C \times \text{number}$  for any row, then  $\mathbf{L}$  is declared nonestimable.  $\mathbf{H}$  is the  $(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{X}$  matrix, and  $C$  is  $ABS(\mathbf{L})$  except for rows where  $\mathbf{L}$  is zero, and then it is 1. The default value for the SINGULAR= option is  $10^{-4}$ . Values for the SINGULAR= option must be between 0 and 1.

**STDERR**

produces the standard error of the LS-means and the probability level for the hypothesis  $H_0: \text{LS-mean} = 0$ .

**TDIFF**

produces the  $t$  values for all hypotheses  $H_0: \text{LS-mean}(i) = \text{LS-mean}(j)$  and the corresponding probabilities.

---

## MANOVA Statement

**MANOVA** < *test-options* > < *detail-options* > ;

If the **MODEL** statement includes more than one dependent variable, you can perform multivariate analysis of variance with the MANOVA statement. The *test-options* define which effects to test, while the *detail-options* specify how to execute the tests and what results to display. [Table 42.7](#) summarizes the options available in the MANOVA statement.

**Table 42.7** MANOVA Statement Options

| Option              | Description                                                   |
|---------------------|---------------------------------------------------------------|
| <b>Test Options</b> |                                                               |
| H=                  | Specifies hypothesis effects                                  |
| E=                  | Specifies the error effect                                    |
| M=                  | Specifies a transformation matrix for the dependent variables |
| MNAMES=             | Provides names for the transformed variables                  |

Table 42.7 continued

| Option                | Description                                                         |
|-----------------------|---------------------------------------------------------------------|
| PREFIX=               | Alternatively identifies the transformed variables                  |
| <b>Detail Options</b> |                                                                     |
| CANONICAL             | Displays a canonical analysis of the <b>H</b> and <b>E</b> matrices |
| ETYPE=                | Specifies the type of the <b>E</b> matrix                           |
| HTYPE=                | Specifies the type of the <b>H</b> matrix                           |
| MSTAT=                | Specifies the method of evaluating the multivariate test statistics |
| ORTH                  | Orthogonalizes the rows of the transformation matrix                |
| PRINTE                | Displays the error SSCP matrix <b>E</b>                             |
| PRINTH                | Displays the hypothesis SSCP matrix <b>H</b>                        |
| SUMMARY               | Produces analysis-of-variance tables for each dependent variable    |

When a MANOVA statement appears before the first RUN statement, PROC GLM enters a multivariate mode with respect to the handling of missing values; in addition to observations with missing independent variables, observations with *any* missing dependent variables are excluded from the analysis. If you want to use this mode of handling missing values and do not need any multivariate analyses, specify the **MANOVA** option in the **PROC GLM** statement.

If you use both the **CONTRAST** and **MANOVA** statements, the **MANOVA** statement must appear after the **CONTRAST** statement.

## Test Options

The following options can be specified in the **MANOVA** statement as *test-options* in order to define which multivariate tests to perform.

### **H=effects** | **INTERCEPT** | **\_ALL\_**

specifies effects in the preceding model to use as hypothesis matrices. For each **H** matrix (the SSCP matrix associated with an effect), the **H=** specification displays the characteristic roots and vectors of  $\mathbf{E}^{-1}\mathbf{H}$  (where **E** is the matrix associated with the error effect), along with the Hotelling-Lawley trace, Pillai's trace, Wilks' lambda, and Roy's greatest root. By default, these statistics are tested with approximations based on the *F* distribution. To test them with exact (but computationally intensive) calculations, use the **MSTAT=EXACT** option.

Use the keyword **INTERCEPT** to produce tests for the intercept. To produce tests for all effects listed in the **MODEL** statement, use the keyword **\_ALL\_** in place of a list of effects.

For background and further details, see the section “**Multivariate Analysis of Variance**” on page 3366.

### **E=effect**

specifies the error effect. If you omit the **E=** specification, the GLM procedure uses the error SSCP (residual) matrix from the analysis.

### **M=equation,...,equation** | (*row-of-matrix,...,row-of-matrix*)

specifies a transformation matrix for the dependent variables listed in the **MODEL** statement. The

equations in the M= specification are of the form

$$c_1 \times \text{dependent-variable} \pm c_2 \times \text{dependent-variable} \\ \dots \pm c_n \times \text{dependent-variable}$$

where the  $c_i$  values are coefficients for the various *dependent-variables*. If the value of a given  $c_i$  is 1, it can be omitted; in other words  $1 \times Y$  is the same as  $Y$ . Equations should involve two or more dependent variables. For sample syntax, see the section “[Examples](#)” on page 3302.

Alternatively, you can input the transformation matrix directly by entering the elements of the matrix with commas separating the rows and parentheses surrounding the matrix. When this alternate form of input is used, the number of elements in each row must equal the number of dependent variables. Although these combinations actually represent the columns of the M matrix, they are displayed by rows.

When you include an M= specification, the analysis requested in the MANOVA statement is carried out for the variables defined by the equations in the specification, not the original dependent variables. If you omit the M= option, the analysis is performed for the original dependent variables in the [MODEL](#) statement.

If an M= specification is included without either the [MNames=](#) or [PREFIX=](#) option, the variables are labeled MVAR1, MVAR2, and so forth, by default. For further information, see the section “[Multivariate Analysis of Variance](#)” on page 3366.

**MNames=names**

provides names for the variables defined by the equations in the M= specification. Names in the list correspond to the M= equations or to the rows of the M matrix (as it is entered).

**PREFIX=name**

is an alternative means of identifying the transformed variables defined by the M= specification. For example, if you specify PREFIX=DIFF, the transformed variables are labeled DIFF1, DIFF2, and so forth.

## Detail Options

You can specify the following options in the MANOVA statement after a slash (/) as *detail-options*.

**CANONICAL**

displays a canonical analysis of the H and E matrices (transformed by the M matrix, if specified) instead of the default display of characteristic roots and vectors.

**ETYPE=n**

specifies the type (1, 2, 3, or 4, corresponding to a Type I, II, III, or IV test, respectively) of the E matrix, the SSCP matrix associated with the E= effect. You need this option if you use the E= specification to specify an error effect other than residual error and you want to specify the type of sums of squares used for the effect. If you specify ETYPE=n, the corresponding test must have been performed in the [MODEL](#) statement, either by options SSn, En, or the default Type I and Type III tests. By default, the procedure uses an ETYPE= value corresponding to the highest type (largest n) used in the analysis.



**HTYPE=*n***

specifies the type (1, 2, 3, or 4, corresponding to a Type I, II, III, or IV test, respectively) of the **H** matrix. See the **ETYPE=** option for more details.

**MSTAT=FAPPROX | EXACT**

specifies the method of evaluating the multivariate test statistics. The default is **MSTAT=FAPPROX**, which specifies that the multivariate tests are evaluated using the usual approximations based on the *F* distribution, as discussed in the section “Multivariate Tests” in Chapter 4, “[Introduction to Regression Procedures](#).” Alternatively, you can specify **MSTAT=EXACT** to compute exact *p*-values for three of the four tests (Wilks’ lambda, the Hotelling-Lawley trace, and Roy’s greatest root) and an improved *F* approximation for the fourth (Pillai’s trace). While **MSTAT=EXACT** provides better control of the significance probability for the tests, especially for Roy’s greatest root, computations for the exact *p*-values can be appreciably more demanding, and are in fact infeasible for large problems (many dependent variables). Thus, although **MSTAT=EXACT** is more accurate for most data, it is not the default method. For more information about the results of **MSTAT=EXACT**, see the section “[Multivariate Analysis of Variance](#)” on page 3366.

**ORTH**

requests that the transformation matrix in the **M=** specification of the MANOVA statement be orthonormalized by rows before the analysis.

**PRINTE**

displays the error SSCP matrix **E**. If the **E** matrix is the error SSCP (residual) matrix from the analysis, the partial correlations of the dependent variables given the independent variables are also produced.

For example, the statement

```
manova / printe;
```

displays the error SSCP matrix and the partial correlation matrix computed from the error SSCP matrix.

**PRINTH**

displays the hypothesis SSCP matrix **H** associated with each effect specified by the **H=** specification.

**SUMMARY**

produces analysis-of-variance tables for each dependent variable. When no **M** matrix is specified, a table is displayed for each original dependent variable from the **MODEL** statement; with an **M** matrix other than the identity, a table is displayed for each transformed variable defined by the **M** matrix.

**Examples**

The following statements provide several examples of using a **MANOVA** statement.

```
proc glm;
 class A B;
 model Y1-Y5=A B(A) / nouni;
 manova h=A e=B(A) / printh printe htype=1 etype=1;
 manova h=B(A) / printe;
 manova h=A e=B(A) m=Y1-Y2, Y2-Y3, Y3-Y4, Y4-Y5
 prefix=diff;
```

```

manova h=A e=B(A) m=(1 -1 0 0 0,
 0 1 -1 0 0,
 0 0 1 -1 0,
 0 0 0 1 -1) prefix=diff;

run;

```

Since this **MODEL** statement requests no options for type of sums of squares, the procedure uses Type I and Type III sums of squares. The first **MANOVA** statement specifies A as the hypothesis effect and B(A) as the error effect. As a result of the **PRINTH** option, the procedure displays the hypothesis SSCP matrix associated with the A effect; and, as a result of the **PRINTE** option, the procedure displays the error SSCP matrix associated with the B(A) effect. The option **HTYPE=1** specifies a Type I H matrix, and the option **ETYPE=1** specifies a Type I E matrix.

The second **MANOVA** statement specifies B(A) as the hypothesis effect. Since no error effect is specified, PROC GLM uses the error SSCP matrix from the analysis as the E matrix. The **PRINTE** option displays this E matrix. Since the E matrix is the error SSCP matrix from the analysis, the partial correlation matrix computed from this matrix is also produced.

The third **MANOVA** statement requests the same analysis as the first **MANOVA** statement, but the analysis is carried out for variables transformed to be successive differences between the original dependent variables. The option **PREFIX=DIFF** labels the transformed variables as DIFF1, DIFF2, DIFF3, and DIFF4.

Finally, the fourth **MANOVA** statement has the identical effect as the third, but it uses an alternative form of the **M=** specification. Instead of specifying a set of equations, the fourth **MANOVA** statement specifies rows of a matrix of coefficients for the five dependent variables.

As a second example of the use of the **M=** specification, consider the following:

```

proc glm;
 class group;
 model dose1-dose4=group / nouni;
 manova h = group
 m = -3*dose1 - dose2 + dose3 + 3*dose4,
 dose1 - dose2 - dose3 + dose4,
 -dose1 + 3*dose2 - 3*dose3 + dose4
 mnames = Linear Quadratic Cubic
 / printe;

run;

```

The **M=** specification gives a transformation of the dependent variables dose1 through dose4 into orthogonal polynomial components, and the **MNAMES=** option labels the transformed variables LINEAR, QUADRATIC, and CUBIC, respectively. Since the **PRINTE** option is specified and the default residual matrix is used as an error term, the partial correlation matrix of the orthogonal polynomial components is also produced.

---

## MEANS Statement

**MEANS** *effects* *</ options >* ;

Within each group corresponding to each effect specified in the **MEANS** statement, PROC GLM computes the arithmetic means and standard deviations of all continuous variables in the model (both dependent and

independent). You can specify only classification effects in the MEANS statement—that is, effects that contain only classification variables.

Note that the arithmetic means are not adjusted for other effects in the model; for adjusted means, see the section “LSMEANS Statement” on page 3293.

If you use a WEIGHT statement, PROC GLM computes weighted means; see the section “Weighted Means” on page 3363.

You can also specify options to perform multiple comparisons. However, the MEANS statement performs multiple comparisons only for main-effect means; for multiple comparisons of interaction means, see the section “LSMEANS Statement” on page 3293.

You can use any number of MEANS statements, provided that they appear after the MODEL statement. For example, suppose A and B each have two levels. Then, if you use the statements

```
proc glm;
 class A B;
 model Y=A B A*B;
 means A B / tukey;
 means A*B;
run;
```

the means, standard deviations, and Tukey’s multiple comparisons tests are displayed for each level of the main effects A and B, and just the means and standard deviations are displayed for each of the four combinations of levels for A\*B. Since multiple comparisons tests apply only to main effects, the single MEANS statement

```
means A B A*B / tukey;
```

produces the same results.

PROC GLM does not compute means for interaction effects containing continuous variables. Thus, if you have the model

```
class A;
model Y=A X A*X;
```

then the effects X and A\*X cannot be used in the MEANS statement. However, if you specify the effect A in the means statement

```
means A;
```

then PROC GLM, by default, displays within-A arithmetic means of both Y and X. You can use the DEONLY option to display means of only the dependent variables.

```
means A / deonly;
```

If you use a WEIGHT statement, PROC GLM computes weighted means and estimates their variance as inversely proportional to the corresponding sum of weights (see the section “Weighted Means” on page 3363). However, note that the statistical interpretation of multiple comparison tests for weighted means is not well understood. See the section “Multiple Comparisons” on page 3349 for formulas. Table 42.8 summarizes the options available in the MEANS statement.

**Table 42.8** MEANS Statement Options

| Option                                                          | Description                                                                                                     |
|-----------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------|
| <b>Modify output</b>                                            |                                                                                                                 |
| DEONLY                                                          | Displays only means for the dependent variables                                                                 |
| <b>Perform multiple comparison tests</b>                        |                                                                                                                 |
| BON                                                             | Performs Bonferroni $t$ tests                                                                                   |
| DUNCAN                                                          | Performs Duncan's multiple range test                                                                           |
| DUNETT                                                          | Performs Dunnett's two-tailed $t$ test                                                                          |
| DUNETTL                                                         | Performs Dunnett's lower one-tailed $t$ test                                                                    |
| DUNETTU                                                         | Performs Dunnett's upper one-tailed $t$ test                                                                    |
| GABRIEL                                                         | Performs Gabriel's multiple-comparison procedure                                                                |
| REGWQ                                                           | Performs the Ryan-Einot-Gabriel-Welsch multiple range test                                                      |
| SCHEFFE                                                         | Performs Scheffé's multiple-comparison procedure                                                                |
| SIDAK                                                           | Performs pairwise $t$ tests on differences between means                                                        |
| SMM or GT2                                                      | Performs pairwise comparisons based on the studentized maximum modulus and Sidak's uncorrelated- $t$ inequality |
| SNK                                                             | Performs the Student-Newman-Keuls multiple range test                                                           |
| T or LSD                                                        | Performs pairwise $t$ tests                                                                                     |
| TUKEY                                                           | Performs Tukey's studentized range test (HSD)                                                                   |
| WALLER                                                          | Performs the Waller-Duncan $k$ -ratio $t$ test                                                                  |
| <b>Specify additional details for multiple comparison tests</b> |                                                                                                                 |
| ALPHA=                                                          | Specifies the level of significance                                                                             |
| CLDIFF                                                          | Presents confidence intervals for all pairwise differences between means                                        |
| CLM                                                             | Presents results as intervals for the mean of each level of the variables                                       |
| E=                                                              | Specifies the error mean square used in the multiple comparisons                                                |
| ETYPE=                                                          | Specifies the type of mean square for the error effect                                                          |
| HTYPE=                                                          | Specifies the MS type for the hypothesis MS                                                                     |
| KRATIO=                                                         | Specifies the Type 1/Type 2 error seriousness ratio                                                             |
| LINES                                                           | Lists the means in descending order and indicating nonsignificant subsets by line segments                      |
| NOSORT                                                          | Prevents the means from being sorted into descending order                                                      |
| <b>Test for homogeneity of variances</b>                        |                                                                                                                 |
| HOVTEST                                                         | Requests a homogeneity of variance test                                                                         |
| <b>Compensate for heterogeneous variances</b>                   |                                                                                                                 |
| WELCH                                                           | Requests the variance-weighted one-way ANOVA of Welch (1951)                                                    |

The options available in the MEANS statement are described in the following list.

**ALPHA=**

ALPHA= $p$  specifies the level of significance for comparisons among the means. By default,  $p$  is equal to the value of the ALPHA= option in the PROC GLM statement or 0.05 if that option is not specified. You can specify any value greater than 0 and less than 1.

**BON**

performs Bonferroni  $t$  tests of differences between means for all main-effect means in the MEANS statement. See the **CLDIFF** and **LINES** options for a discussion of how the procedure displays results.

**CLDIFF**

presents results of the **BON**, **GABRIEL**, **SCHEFFE**, **SIDAK**, **SMM**, **GT2**, **T**, **LSD**, and **TUKEY** options as confidence intervals for all pairwise differences between means, and the results of the **DUNNETT**, **DUNNETTU**, and **DUNNETTL** options as confidence intervals for differences with the control. The **CLDIFF** option is the default for unequal cell sizes unless the **DUNCAN**, **REGWQ**, **SNK**, or **WALLER** option is specified.

**CLM**

presents results of the **BON**, **GABRIEL**, **SCHEFFE**, **SIDAK**, **SMM**, **T**, and **LSD** options as intervals for the mean of each level of the variables specified in the MEANS statement. For all options except **GABRIEL**, the intervals are confidence intervals for the true means. For the **GABRIEL** option, they are *comparison intervals* for comparing means pairwise: in this case, if the intervals corresponding to two means overlap, then the difference between them is insignificant according to Gabriel's method.

**DEPONLY**

displays only means for the dependent variables. By default, PROC GLM produces means for all continuous variables, including continuous independent variables.

**DUNCAN**

performs Duncan's multiple range test on all main-effect means given in the MEANS statement. See the **LINES** option for a discussion of how the procedure displays results.

**DUNNETT** <(formatted-control-values)>

performs Dunnett's two-tailed  $t$  test, testing if any treatments are significantly different from a single control for all main-effect means in the MEANS statement.

To specify which level of the effect is the control, enclose the formatted value in quotes and parentheses after the keyword. If more than one effect is specified in the MEANS statement, you can use a list of control values within the parentheses. By default, the first level of the effect is used as the control. For example:

```
means A / dunnnett('CONTROL');
```

where CONTROL is the formatted control value of A. As another example:

```
means A B C / dunnnett('CNTLA' 'CNTLB' 'CNTLC');
```

where CNTLA, CNTLB, and CNTLC are the formatted control values for A, B, and C, respectively.

**DUNNETTL** <(formatted-control-value)>

performs Dunnett's one-tailed  $t$  test, testing if any treatment is significantly less than the control. Control level information is specified as described for the **DUNNETT** option.

**DUNNETTU** < (*formatted-control-value*) >

performs Dunnett's one-tailed *t* test, testing if any treatment is significantly greater than the control. Control level information is specified as described for the **DUNNETT** option.

**E=effect**

specifies the error mean square used in the multiple comparisons. By default, PROC GLM uses the overall residual or error mean square (MS). The effect specified with the E= option must be a term in the model; otherwise, the procedure uses the residual MS.

**ETYPE=*n***

specifies the type of mean square for the error effect. When you specify E=*effect*, you might need to indicate which type (1, 2, 3, or 4) of MS is to be used. The *n* value must be one of the types specified in or implied by the **MODEL** statement. The default MS type is the highest type used in the analysis.

**GABRIEL**

performs Gabriel's multiple-comparison procedure on all main-effect means in the MEANS statement. See the **CLDIFF** and **LINES** options for discussions of how the procedure displays results.

**GT2**

See the **SMM** option.

**HOVTEST****HOVTEST=BARTLETT****HOVTEST=BF****HOVTEST=LEVENE** < ( **TYPE= ABS | SQUARE** ) >**HOVTEST=OBRIEN** < ( **W=number** ) >

requests a homogeneity of variance test for the groups defined by the MEANS effect. You can optionally specify a particular test; if you do not specify a test, Levene's test (Levene 1960) with TYPE=SQUARE is computed. Note that this option is ignored unless your **MODEL** statement specifies a simple one-way model.

The HOVTEST=BARTLETT option specifies Bartlett's test (Bartlett 1937), a modification of the normal-theory likelihood ratio test.

The HOVTEST=BF option specifies Brown and Forsythe's variation of Levene's test (Brown and Forsythe 1974).

The HOVTEST=LEVENE option specifies Levene's test (Levene 1960), which is widely considered to be the standard homogeneity of variance test. You can use the TYPE= option in parentheses to specify whether to use the absolute residuals (TYPE=ABS) or the squared residuals (TYPE=SQUARE) in Levene's test. TYPE=SQUARE is the default.

The HOVTEST=OBRIEN option specifies O'Brien's test (O'Brien 1979), which is basically a modification of HOVTEST=LEVENE(TYPE=SQUARE). You can use the W= option in parentheses to tune the variable to match the suspected kurtosis of the underlying distribution. By default, W=0.5, as suggested by O'Brien (1979, 1981).

See the section "Homogeneity of Variance in One-Way Models" on page 3362 for more details on these methods. [Example 42.10](#) illustrates the use of the HOVTEST and **WELCH** options in the MEANS statement in testing for equal group variances and adjusting for unequal group variances in a one-way ANOVA.

**HTYPE=*n***

specifies the MS type for the hypothesis MS. The HTYPE= option is needed only when the **WALLER** option is specified. The default HTYPE= value is the highest type used in the model.

**KRATIO=*value***

specifies the Type 1/Type 2 error seriousness ratio for the Waller-Duncan test. Reasonable values for the KRATIO= option are 50, 100, 500, which roughly correspond for the two-level case to **ALPHA** levels of 0.1, 0.05, and 0.01, respectively. By default, the procedure uses the value of 100.

**LINES**

presents results of the **BON**, **DUNCAN**, **GABRIEL**, **REGWQ**, **SCHEFFE**, **SIDAK**, **SMM**, **GT2**, **SNK**, **T**, **LSD**, **TUKEY**, and **WALLER** options by listing the means in descending order and indicating nonsignificant subsets by line segments beside the corresponding means. The **LINES** option is appropriate for equal cell sizes, for which it is the default. The **LINES** option is also the default if the **DUNCAN**, **REGWQ**, **SNK**, or **WALLER** option is specified, or if there are only two cells of unequal size. The **LINES** option cannot be used in combination with the **DUNNETT**, **DUNNETTL**, or **DUNNETTU** option. In addition, the procedure has a restriction that no more than 24 overlapping groups of means can exist. If a mean belongs to more than 24 groups, the procedure issues an error message. You can either reduce the number of levels of the variable or use a multiple comparison test that allows the **CLDIFF** option rather than the **LINES** option.

**NOTE:** If the cell sizes are unequal, the harmonic mean of the cell sizes is used to compute the critical ranges. This approach is reasonable if the cell sizes are not too different, but it can lead to liberal tests if the cell sizes are highly disparate. In this case, you should not use the **LINES** option for displaying multiple comparisons results; use the **TUKEY** and **CLDIFF** options instead.

**LSD**

See the **T** option.

**NOSORT**

prevents the means from being sorted into descending order when the **CLDIFF** or **CLM** option is specified.

**REGWQ**

performs the Ryan-Einot-Gabriel-Welsch multiple range test on all main-effect means in the **MEANS** statement. See the **LINES** option for a discussion of how the procedure displays results.

**SCHEFFE**

performs Scheffé's multiple-comparison procedure on all main-effect means in the **MEANS** statement. See the **CLDIFF** and **LINES** options for discussions of how the procedure displays results.

**SIDAK**

performs pairwise *t* tests on differences between means with levels adjusted according to Sidak's inequality for all main-effect means in the **MEANS** statement. See the **CLDIFF** and **LINES** options for discussions of how the procedure displays results.

**SMM****GT2**

performs pairwise comparisons based on the studentized maximum modulus and Sidak's uncorrelated-*t* inequality, yielding Hochberg's GT2 method when sample sizes are unequal, for all main-effect means in the **MEANS** statement. See the **CLDIFF** and **LINES** options for discussions of how the procedure displays results.



**SNK**

performs the Student-Newman-Keuls multiple range test on all main-effect means in the MEANS statement. See the [LINES](#) option for discussions of how the procedure displays results.

**T****LSD**

performs pairwise *t* tests, equivalent to Fisher's least significant difference test in the case of equal cell sizes, for all main-effect means in the MEANS statement. See the [CLDIFF](#) and [LINES](#) options for discussions of how the procedure displays results.

**TUKEY**

performs Tukey's studentized range test (HSD) on all main-effect means in the MEANS statement. (When the group sizes are different, this is the Tukey-Kramer test.) See the [CLDIFF](#) and [LINES](#) options for discussions of how the procedure displays results.

**WALLER**

performs the Waller-Duncan *k*-ratio *t* test on all main-effect means in the MEANS statement. See the [KRATIO=](#) and [HTYPE=](#) options for information about controlling details of the test, and the [LINES](#) option for a discussion of how the procedure displays results.

**WELCH**

requests the variance-weighted one-way ANOVA of Welch (1951). This alternative to the usual analysis of variance for a one-way model is robust to the assumption of equal within-group variances. This option is ignored unless your [MODEL](#) statement specifies a simple one-way model.

Note that using the [WELCH](#) option merely produces one additional table consisting of Welch's ANOVA. It does not affect all of the other tests displayed by the GLM procedure, which still require the assumption of equal variance for exact validity.

See the section "Homogeneity of Variance in One-Way Models" on page 3362 for more details on Welch's ANOVA. [Example 42.10](#) illustrates the use of the [HOVTEST](#) and [WELCH](#) options in the MEANS statement in testing for equal group variances and adjusting for unequal group variances in a one-way ANOVA.

---

## MODEL Statement

**MODEL** *dependent-variables = independent-effects* </ options > ;

The MODEL statement names the dependent variables and independent effects. The syntax of effects is described in the section "[Specification of Effects](#)" on page 3324. For any model effect involving classification variables (interactions as well as main effects), the number of levels cannot exceed 32,767. If no independent effects are specified, only an intercept term is fit. You can specify only one MODEL statement (in contrast to the REG procedure, for example, which allows several MODEL statements in the same PROC REG run).

[Table 42.9](#) summarizes the options available in the MODEL statement.



**Table 42.9** MODEL Statement Options

| Option                                         | Description                                                                                |
|------------------------------------------------|--------------------------------------------------------------------------------------------|
| <b>Produce effect size information</b>         |                                                                                            |
| EFFECTSIZE                                     | Adds measures of effect size to each analysis of variance table                            |
| <b>Produce tests for the intercept</b>         |                                                                                            |
| INTERCEPT                                      | Produces the hypothesis tests associated with the intercept                                |
| <b>Omit the intercept parameter from model</b> |                                                                                            |
| NOINT                                          | Omits the intercept parameter from the model                                               |
| <b>Produce parameter estimates</b>             |                                                                                            |
| SOLUTION                                       | Produces parameter estimates                                                               |
| <b>Produce tolerance analysis</b>              |                                                                                            |
| TOLERANCE                                      | Displays the tolerances used in the SWEEP routine                                          |
| <b>Suppress univariate tests and output</b>    |                                                                                            |
| NOUNI                                          | Suppresses the display of univariate statistics                                            |
| <b>Display estimable functions</b>             |                                                                                            |
| E                                              | Displays the general form of all estimable functions                                       |
| E1                                             | Displays the Type I estimable functions and computes sums of squares                       |
| E2                                             | Displays the Type II estimable functions and computes sums of squares                      |
| E3                                             | Displays the Type III estimable functions and computes sums of squares                     |
| E4                                             | Displays the Type IV estimable functions computes sums of squares                          |
| ALIASING                                       | Specifies that the estimable functions should be displayed as an <i>aliasing structure</i> |
| <b>Control hypothesis tests performed</b>      |                                                                                            |
| SS1                                            | Displays Type I sum of squares                                                             |
| SS2                                            | Displays Type II sum of squares                                                            |
| SS3                                            | Displays Type III sum of squares                                                           |
| SS4                                            | Displays Type IV sum of squares                                                            |
| <b>Produce confidence intervals</b>            |                                                                                            |
| ALPHA=                                         | Specifies the level of significance                                                        |
| CLI                                            | Produces confidence limits for individual predicted values                                 |
| CLM                                            | Produces confidence limits for a mean predicted value                                      |
| CLPARM                                         | Produces confidence limits for the parameter estimates                                     |
| <b>Display predicted and residual values</b>   |                                                                                            |
| P                                              | Displays observed, predicted, and residual values                                          |
| <b>Display intermediate calculations</b>       |                                                                                            |
| INVERSE                                        | Displays the augmented inverse (or generalized inverse) $X'X$ matrix                       |
| XPX                                            | Displays the augmented $X'X$ crossproducts matrix                                          |
| <b>Tune sensitivity</b>                        |                                                                                            |
| SINGULAR=                                      | Tunes the sensitivity of the regression routine to linear dependencies                     |
| ZETA=                                          | Tunes the sensitivity of the check for estimability for Type III and Type IV functions     |

The options available in the MODEL statement are described in the following list.

**ALIASING**

specifies that the estimable functions should be displayed as an *aliasing structure*, for which each row says which linear combination of the parameters is estimated by each estimable function; also, this option adds a column of the same information to the table of parameter estimates, giving for each parameter the expected value of the estimate associated with that parameter. This option is most useful in fractional factorial experiments that can be analyzed without a **CLASS** statement.

**ALPHA= $p$** 

specifies the level of significance  $p$  for  $100(1 - p)\%$  confidence intervals. By default,  $p$  is equal to the value of the **ALPHA=** option in the **PROC GLM** statement, or 0.05 if that option is not specified. You can use values between 0 and 1.

**CLI**

produces confidence limits for individual predicted values for each observation. The CLI option is ignored if the **CLM** option is also specified.

**CLM**

produces confidence limits for a mean predicted value for each observation.

**CLPARM**

produces confidence limits for the parameter estimates (if the **SOLUTION** option is also specified) and for the results of all **ESTIMATE** statements.

**E**

displays the general form of all estimable functions. This is useful for determining the order of parameters when you are writing **CONTRAST** and **ESTIMATE** statements.

**E1**

displays the Type I estimable functions for each effect in the model and computes the corresponding sums of squares.

**E2**

displays the Type II estimable functions for each effect in the model and computes the corresponding sums of squares.

**E3**

displays the Type III estimable functions for each effect in the model and computes the corresponding sums of squares.

**E4**

displays the Type IV estimable functions for each effect in the model and computes the corresponding sums of squares.

**EFFECTSIZE**

adds measures of effect size to each analysis of variance table displayed by the procedure, except for those displayed by the **TEST** option in the **RANDOM** statement, by **CONTRAST** and **TEST** statements with the **E=** option, and by **MANOVA** and **REPEATED** statements. The effect size measures include the intraclass correlation and both estimates and confidence intervals for the noncentrality for the  $F$  test, as well as for the semipartial and partial correlation ratios. For more information about the computation and interpretation of these measures, see the section “Effect Size Measures for  $F$  Tests in GLM” on page 3338.

**INTERCEPT****INT**

produces the hypothesis tests associated with the intercept as an effect in the model. By default, the procedure includes the intercept in the model but does not display associated tests of hypotheses. Except for producing the uncorrected total sum of squares instead of the corrected total sum of squares, the INT option is ignored when you use an **ABSORB** statement.

**INVERSE****I**

displays the augmented inverse (or generalized inverse)  $X'X$  matrix:

$$\begin{bmatrix} (X'X)^{-} & (X'X)^{-}X'y \\ y'X(X'X)^{-} & y'y - y'X(X'X)^{-}X'y \end{bmatrix}$$

The upper-left corner is the generalized inverse of  $X'X$ , the upper-right corner is the parameter estimates, and the lower-right corner is the error sum of squares.

**NOINT**

omits the intercept parameter from the model. The NOINT option is ignored when you use an **ABSORB** statement.

**NOUNI**

suppresses the display of univariate statistics. You typically use the NOUNI option with a multivariate or repeated measures analysis of variance when you do not need the standard univariate results. The NOUNI option in a MODEL statement does not affect the univariate output produced by the **REPEATED** statement.

**P**

displays observed, predicted, and residual values for each observation that does not contain missing values for independent variables. The Durbin-Watson statistic is also displayed when the P option is specified. The PRESS statistic is also produced if either the **CLM** or **CLI** option is specified.

**SINGULAR=*number***

tunes the sensitivity of the regression routine to linear dependencies in the design. If a diagonal pivot element is less than  $C \times \textit{number}$  as PROC GLM sweeps the  $X'X$  matrix, the associated design column is declared to be linearly dependent with previous columns, and the associated parameter is zeroed.

The  $C$  value adjusts the check to the relative scale of the variable. The  $C$  value is equal to the corrected sum of squares for the variable, unless the corrected sum of squares is 0, in which case  $C$  is 1. If you specify the **NOINT** option but not the **ABSORB** statement, PROC GLM uses the uncorrected sum of squares instead.

The default value of the SINGULAR= option,  $10^{-7}$ , might be too small, but this value is necessary in order to handle the high-degree polynomials used in the literature to compare regression routines.

**SOLUTION**

produces a solution to the normal equations (parameter estimates). PROC GLM displays a solution by default when your model involves no classification variables, so you need this option only if you want to see the solution for models with classification effects.

**SS1**

displays the sum of squares associated with Type I estimable functions for each effect. These are also displayed by default.

**SS2**

displays the sum of squares associated with Type II estimable functions for each effect.

**SS3**

displays the sum of squares associated with Type III estimable functions for each effect. These are also displayed by default.

**SS4**

displays the sum of squares associated with Type IV estimable functions for each effect.

**TOLERANCE**

displays the tolerances used in the SWEEP routine. The tolerances are of the form C/USS or C/CSS, as described in the discussion of the **SINGULAR=** option. The tolerance value for the intercept is not divided by its uncorrected sum of squares.

**XPX**

displays the augmented  $X'X$  crossproducts matrix:

$$\begin{bmatrix} X'X & X'y \\ y'X & y'y \end{bmatrix}$$

**ZETA=value**

tunes the sensitivity of the check for estimability for Type III and Type IV functions. Any element in the estimable function basis with an absolute value less than the ZETA= option is set to zero. The default value for the ZETA= option is  $10^{-8}$ .

Although it is possible to generate data for which this absolute check can be defeated, the check suffices in most practical examples. Additional research is needed in order to make this check relative rather than absolute.

---

## OUTPUT Statement

**OUTPUT** < **OUT=SAS-data-set** > *keyword=names* < . . . *keyword=names* > < *option* > ;

The OUTPUT statement creates a new SAS data set that saves diagnostic measures calculated after fitting the model. At least one specification of the form *keyword=names* is required.

All the variables in the original data set are included in the new data set, along with variables created in the OUTPUT statement. These new variables contain the values of a variety of diagnostic measures that are calculated for each observation in the data set. If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*.

Details on the specifications in the OUTPUT statement follow.

**keyword=names**

specifies the statistics to include in the output data set and provides names to the new variables that contain the statistics. Specify a keyword for each desired statistic (see the following list of keywords), an equal sign, and the variable or variables to contain the statistic.

In the output data set, the first variable listed after a keyword in the OUTPUT statement contains that statistic for the first dependent variable listed in the MODEL statement; the second variable contains the statistic for the second dependent variable in the MODEL statement, and so on. The list of variables following the equal sign can be shorter than the list of dependent variables in the MODEL statement. In this case, the procedure creates the new names in order of the dependent variables in the MODEL statement. See the section “Examples” on page 3315.

The keywords allowed and the statistics they represent are as follows:

**COOKD**

Cook’s  $D$  influence statistic

**COVRATIO**

standard influence of observation on covariance of parameter estimates

**DFFITS**

standard influence of observation on predicted value

**H**

leverage,  $h_i = x_i(\mathbf{X}'\mathbf{X})^{-1}x_i'$

**LCL**

lower bound of a  $100(1 - p)\%$  confidence interval for an individual prediction. The  $p$ -level is equal to the value of the ALPHA= option in the OUTPUT statement or, if this option is not specified, to the ALPHA= option in the PROC GLM statement. If neither of these options is set, then  $p = 0.05$  by default, resulting in the lower bound for a 95% confidence interval. The interval also depends on the variance of the error, as well as the variance of the parameter estimates. For the corresponding upper bound, see the UCL keyword.

**LCLM**

lower bound of a  $100(1 - p)\%$  confidence interval for the expected value (mean) of the predicted value. The  $p$ -level is equal to the value of the ALPHA= option in the OUTPUT statement or, if this option is not specified, to the ALPHA= option in the PROC GLM statement. If neither of these options is set, then  $p = 0.05$  by default, resulting in the lower bound for a 95% confidence interval. For the corresponding upper bound, see the UCLM keyword.

**PREDICTED | P**

predicted values

**PRESS**

residual for the  $i$ th observation that results from dropping it and predicting it on the basis of all other observations. This is the residual divided by  $(1 - h_i)$ , where  $h_i$  is the leverage, defined previously.

**RESIDUAL | R**

residuals, calculated as ACTUAL – PREDICTED

**RSTUDENT**

a studentized residual with the current observation deleted

**STDI**

standard error of the individual predicted value

**STDP**

standard error of the mean predicted value

**STDR**

standard error of the residual

**STUDENT**

studentized residuals, the residual divided by its standard error

**UCL**

upper bound of a  $100(1 - p)\%$  confidence interval for an individual prediction. The  $p$ -level is equal to the value of the **ALPHA=** option in the OUTPUT statement or, if this option is not specified, to the **ALPHA=** option in the PROC GLM statement. If neither of these options is set, then  $p = 0.05$  by default, resulting in the upper bound for a 95% confidence interval. The interval also depends on the variance of the error, as well as the variance of the parameter estimates. For the corresponding lower bound, see the **LCL** keyword.

**UCLM**

upper bound of a  $100(1 - p)\%$  confidence interval for the expected value (mean) of the predicted value. The  $p$ -level is equal to the value of the **ALPHA=** option in the OUTPUT statement or, if this option is not specified, to the **ALPHA=** option in the PROC GLM statement. If neither of these options is set, then  $p = 0.05$  by default, resulting in the upper bound for a 95% confidence interval. For the corresponding lower bound, see the **LCLM** keyword.

**OUT=SAS-data-set**

gives the name of the new data set. By default, the procedure uses the  $DATA_n$  convention to name the new data set.

The following option is available in the OUTPUT statement and is specified after a slash (/):

**ALPHA= $p$** 

specifies the level of significance  $p$  for  $100(1 - p)\%$  confidence intervals. By default,  $p$  is equal to the value of the **ALPHA=** option in the PROC GLM statement or 0.05 if that option is not specified. You can use values between 0 and 1.

See Chapter 4, “Introduction to Regression Procedures,” and the section “Influence Statistics” on page 6717 in Chapter 79, “The REG Procedure,” for details on the calculation of these statistics.

**Examples**

The following statements show the syntax for creating an output data set with a single dependent variable.

```

proc glm;
 class a b;
 model y=a b a*b;
 output out=new p=yhat r=resid stdr=eresid;
run;

```

These statements create an output data set named `new`. In addition to all the variables from the original data set, `new` contains the variable `yhat`, with values that are predicted values of the dependent variable `y`; the variable `resid`, with values that are the residual values of `y`; and the variable `eresid`, with values that are the standard errors of the residuals.

The following statements show a situation with five dependent variables.

```

proc glm;
 by group;
 class a;
 model y1-y5=a x(a);
 output out=pout predicted=py1-py5;
run;

```

The data set `pout` contains five new variables, `py1` through `py5`. The values of `py1` are the predicted values of `y1`; the values of `py2` are the predicted values of `y2`; and so on.

For more information about the data set produced by the `OUTPUT` statement, see the section “[Output Data Sets](#)” on page 3382.

## RANDOM Statement

**RANDOM** *effects* *</ options >* ;

When some model effects are random (that is, assumed to be sampled from a normal population of effects), you can specify these effects in the `RANDOM` statement in order to compute the expected values of mean squares for various model effects and contrasts and, optionally, to perform random effects analysis of variance tests. You can use as many `RANDOM` statements as you want, provided that they appear after the `MODEL` statement. If you use a `CONTRAST` statement with a `RANDOM` statement and you want to obtain the expected mean squares for the contrast hypothesis, you must enter the `CONTRAST` statement before the `RANDOM` statement.

**NOTE:** PROC GLM uses only the information pertaining to expected mean squares when you specify the `TEST` option in the `RANDOM` statement and, even then, only in the extra  $F$  tests produced by the `RANDOM` statement. Other features in the GLM procedure—including the results of the `LSMEANS` and `ESTIMATE` statements—assume that all effects are fixed, so that all tests and estimability checks for these statements are based on a fixed-effects model, even when you use a `RANDOM` statement. Therefore, you should use the `MIXED` procedure to compute tests involving these features that take the random effects into account; see the section “[PROC GLM versus PROC MIXED for Random-Effects Analysis](#)” on page 3375 and Chapter 59, “[The MIXED Procedure](#),” for more information.

When you use the `RANDOM` statement, by default the GLM procedure produces the Type III expected mean squares for model effects and for contrasts specified before the `RANDOM` statement in the program statements. In order to obtain expected values for other types of mean squares, you need to specify which

types of mean squares are of interest in the **MODEL** statement. See the section “[Computing Type I, II, and IV Expected Mean Squares](#)” on page 3378 for more information.

The list of effects in the **RANDOM** statement should contain one or more of the pure classification effects specified in the **MODEL** statement (that is, main effects, crossed effects, or nested effects involving only classification variables). The coefficients corresponding to each effect specified are assumed to be normally and independently distributed with common variance. Levels in different effects are assumed to be independent.

You can specify the following options in the **RANDOM** statement after a slash (/):

#### **Q**

displays all quadratic forms in the fixed effects that appear in the expected mean squares. For some designs, such as large mixed-level factorials, the **Q** option might generate a substantial amount of output.

#### **TEST**

performs hypothesis tests for each effect specified in the model, using appropriate error terms as determined by the expected mean squares.

**CAUTION:** PROC GLM does not automatically declare interactions to be random when the effects in the interaction are declared random. For example,

```
random a b / test;
```

does not produce the same expected mean squares or tests as

```
random a b a*b / test;
```

To ensure correct tests, you need to list all random interactions and random main effects in the **RANDOM** statement.

See the section “[Random-Effects Analysis](#)” on page 3375 for more information about the calculation of expected mean squares and tests and on the similarities and differences between the GLM and MIXED procedures. See Chapter 5, “[Introduction to Analysis of Variance Procedures](#),” and Chapter 59, “[The MIXED Procedure](#),” for more information about random effects.

---

## **REPEATED Statement**

```
REPEATED factor-specification </ options > ;
```

When values of the dependent variables in the **MODEL** statement represent repeated measurements on the same experimental unit, the **REPEATED** statement enables you to test hypotheses about the measurement factors (often called *within-subject factors*) as well as the interactions of within-subject factors with independent variables in the **MODEL** statement (often called *between-subject factors*). The **REPEATED** statement provides multivariate and univariate tests as well as hypothesis tests for a variety of single-degree-of-freedom contrasts. There is no limit to the number of within-subject factors that can be specified.

The **REPEATED** statement is typically used for handling repeated measures designs with one repeated response variable. Usually, the variables on the left-hand side of the equation in the **MODEL** statement



represent one repeated response variable. This does not mean that only one factor can be listed in the REPEATED statement. For example, one repeated response variable (hemoglobin count) might be measured 12 times (implying variables Y1 to Y12 on the left-hand side of the equal sign in the MODEL statement), with the associated within-subject factors treatment and time (implying two factors listed in the REPEATED statement). See the section “Examples” on page 3321 for an example of how PROC GLM handles this case.

Designs with two or more repeated response variables can, however, be handled with the IDENTITY transformation; see the description of this transformation in the following section, and see Example 42.9 for an example of analyzing a doubly multivariate repeated measures design.

When a REPEATED statement appears, the GLM procedure enters a multivariate mode of handling missing values. If any values for variables corresponding to each combination of the within-subject factors are missing, the observation is excluded from the analysis.

If you use a CONTRAST or TEST statement with a REPEATED statement, you must enter the CONTRAST or TEST statement before the REPEATED statement.

The simplest form of the REPEATED statement requires only a *factor-name*. With two repeated factors, you must specify the *factor-name* and number of levels (*levels*) for each factor. Optionally, you can specify the actual values for the levels (*level-values*), a *transformation* that defines single-degree-of-freedom contrasts, and *options* for additional analyses and output. When you specify more than one within-subject factor, the *factor-names* (and associated level and transformation information) must be separated by a comma in the REPEATED statement.

These terms are described in the following section, “Syntax Details.”

## Syntax Details

Table 42.10 summarizes the options available in the REPEATED statement.

**Table 42.10** REPEATED Statement Options

| Option    | Description                                                                                            |
|-----------|--------------------------------------------------------------------------------------------------------|
| CANONICAL | Performs a canonical analysis of the <b>H</b> and <b>E</b> matrices                                    |
| HTYPE=    | Specifies the type of the <b>H</b> matrix used for analysis                                            |
| MEAN      | Generates the overall arithmetic means of the within-subject variables                                 |
| MSTAT=    | Specifies the method of evaluating the test statistics                                                 |
| NOM       | Displays only univariate analyses results                                                              |
| NOU       | Displays only multivariate analyses results                                                            |
| PRINTE    | Displays <b>E</b> and partial correlation matrices for multivariate tests, and prints sphericity tests |
| PRINTH    | Displays the <b>H</b> matrices for multivariate tests                                                  |
| PRINTM    | Displays the transformation matrices that define tested contrasts                                      |
| PRINTRV   | Displays characteristic roots and vectors for multivariate tests                                       |
| SUMMARY   | Produces analysis-of-variance tables for univariate tests                                              |
| UEPSDEF=  | Specifies the <i>F</i> test adjustment for univariate tests                                            |

You can specify the following terms in the REPEATED statement.

*factor-specification*

The *factor-specification* for the REPEATED statement can include any number of individual factor specifications, separated by commas, of the following form:

*factor-name levels* < (*level-values*) > < *transformation* >

where

*factor-name* names a factor to be associated with the dependent variables. The name should not be the same as any variable name that already exists in the data set being analyzed and should conform to the usual conventions of SAS variable names.

When specifying more than one factor, list the dependent variables in the **MODEL** statement so that the within-subject factors defined in the REPEATED statement are nested; that is, the first factor defined in the REPEATED statement should be the one with values that change least frequently.

*levels* gives the number of levels associated with the factor being defined. When there is only one within-subject factor, the number of levels is equal to the number of dependent variables. In this case, *levels* is optional. When more than one within-subject factor is defined, however, *levels* is required, and the product of the number of levels of all the factors must equal the number of dependent variables in the **MODEL** statement.

(*level-values*) gives values that correspond to levels of a repeated-measures factor. These values are used to label output and as spacings for constructing orthogonal polynomial contrasts if you specify a **POLYNOMIAL** transformation. The number of values specified must correspond to the number of levels for that factor in the REPEATED statement. Enclose the *level-values* in parentheses.

The following *transformation* keywords define single-degree-of-freedom contrasts for factors specified in the REPEATED statement. Since the number of contrasts generated is always one less than the number of levels of the factor, you have some control over which contrast is omitted from the analysis by which transformation you select. The only exception is the **IDENTITY** transformation; this transformation is not composed of contrasts and has the same degrees of freedom as the factor has levels. By default, the procedure uses the **CONTRAST** transformation.

**CONTRAST**< (*ordinal-reference-level*) >

generates contrasts between levels of the factor and a reference level. By default, the procedure uses the last level as the reference level; you can optionally specify a reference level in parentheses after the keyword **CONTRAST**. The reference level corresponds to the ordinal value of the level rather than the level value specified. For example, to generate contrasts between the first level of a factor and the other levels, use

**contrast** (1)

**HELMERT**

generates contrasts between each level of the factor and the mean of subsequent levels.

**IDENTITY**

generates an identity transformation corresponding to the associated factor. This transformation is *not* composed of contrasts; it has  $n$  degrees of freedom for an  $n$ -level factor, instead of  $n - 1$ . This can be used for doubly multivariate repeated measures.

**MEAN**

`<(ordinal-reference-level)>` generates contrasts between levels of the factor and the mean of all other levels of the factor. Specifying a reference level eliminates the contrast between that level and the mean. Without a reference level, the contrast involving the last level is omitted. See the CONTRAST transformation for an example.

**POLYNOMIAL**

generates orthogonal polynomial contrasts. Level values, if provided, are used as spacings in the construction of the polynomials; otherwise, equal spacing is assumed.

**PROFILE**

generates contrasts between adjacent levels of the factor.

You can specify the following options in the REPEATED statement after a slash (/).

**CANONICAL**

performs a canonical analysis of the **H** and **E** matrices corresponding to the transformed variables specified in the REPEATED statement.

**HTYPE= $n$** 

specifies the type of the **H** matrix used in the multivariate tests and the type of sums of squares used in the univariate tests. See the **HTYPE=** option in the specifications for the **MANOVA** statement for further details.

**MEAN**

generates the overall arithmetic means of the within-subject variables.

**MSTAT=FAPPROX | EXACT**

specifies the method of evaluating the test statistics for the multivariate analysis. The default is **MSTAT=FAPPROX**, which specifies that the multivariate tests are evaluated using the usual approximations based on the  $F$  distribution, as discussed in the section “Multivariate Tests” in Chapter 4, “Introduction to Regression Procedures.” Alternatively, you can specify **MSTAT=EXACT** to compute exact  $p$ -values for three of the four tests (Wilks’ lambda, the Hotelling-Lawley trace, and Roy’s greatest root) and an improved  $F$  approximation for the fourth (Pillai’s trace). While **MSTAT=EXACT** provides better control of the significance probability for the tests, especially for Roy’s greatest root, computations for the exact  $p$ -values can be appreciably more demanding, and are in fact infeasible for large problems (many dependent variables). Thus, although **MSTAT=EXACT** is more accurate for most data, it is not the default method. For more information about the results of **MSTAT=EXACT**, see the section “Multivariate Analysis of Variance” on page 3366.

**NOM**

displays only the results of the univariate analyses.

**NOU**

displays only the results of the multivariate analyses.

**PRINTE**

displays the **E** matrix for each combination of within-subject factors, as well as partial correlation matrices for both the original dependent variables and the variables defined by the transformations specified in the REPEATED statement. In addition, the PRINTE option provides sphericity tests for each set of transformed variables. If the requested transformations are not orthogonal, the PRINTE option also provides a sphericity test for a set of orthogonal contrasts.

**PRINTH**

displays the **H** (SSCP) matrix associated with each multivariate test.

**PRINTM**

displays the transformation matrices that define the contrasts in the analysis. PROC GLM always displays the **M** matrix so that the transformed variables are defined by the rows, not the columns, of the displayed **M** matrix. In other words, PROC GLM actually displays  $M'$ .

**PRINTRV**

displays the characteristic roots and vectors for each multivariate test.

**SUMMARY**

produces analysis-of-variance tables for each contrast defined by the within-subject factors. Along with tests for the effects of the independent variables specified in the MODEL statement, a term labeled MEAN tests the hypothesis that the overall mean of the contrast is zero.

**UEPSDEF=unbiased-epsilon-definition**

specifies the type of adjustment for the univariate  $F$  test that is displayed in addition to the Greenhouse-Geisser adjustment. The default is UEPSDEF=HFL, corresponding to the corrected form of the Huynh-Feldt adjustment (Huynh and Feldt 1976; Lecoutre 1991). Other alternatives are UEPSDEF=HF, the uncorrected Huynh-Feldt adjustment (the only available method in previous releases of SAS/STAT software), and UEPSDEF=CM, the adjustment of Chi et al. (2012). See the section “[Hypothesis Testing in Repeated Measures Analysis](#)” on page 3370 for details about these adjustments.

**Examples**

When specifying more than one factor, list the dependent variables in the MODEL statement so that the within-subject factors defined in the REPEATED statement are nested; that is, the first factor defined in the REPEATED statement should be the one with values that change least frequently. For example, assume that three treatments are administered at each of four times, for a total of twelve dependent variables on each experimental unit. If the variables are listed in the MODEL statement as Y1 through Y12, then the REPEATED statement in

```
proc glm;
 class group;
 model Y1-Y12=group / nouni;
 repeated trt 3, time 4;
run;
```

implies the following structure:

|               | Dependent Variables |    |    |    |    |    |    |    |    |     |     |     |
|---------------|---------------------|----|----|----|----|----|----|----|----|-----|-----|-----|
|               | Y1                  | Y2 | Y3 | Y4 | Y5 | Y6 | Y7 | Y8 | Y9 | Y10 | Y11 | Y12 |
| Value of trt  | 1                   | 1  | 1  | 1  | 2  | 2  | 2  | 2  | 3  | 3   | 3   | 3   |
| Value of time | 1                   | 2  | 3  | 4  | 1  | 2  | 3  | 4  | 1  | 2   | 3   | 4   |

The REPEATED statement always produces a table like the preceding one. For more information, see the section “[Repeated Measures Analysis of Variance](#)” on page 3367.

---

## STORE Statement

**STORE** <OUT=>*item-store-name* </ LABEL='label'> ;

The STORE statement requests that the procedure save the context and results of the statistical analysis. The resulting item store has a binary file format that cannot be modified. The contents of the item store can be processed with the PLM procedure.

For details about the syntax of the STORE statement, see the section “[STORE Statement](#)” on page 501 in Chapter 19, “[Shared Concepts and Topics](#).”

---

## TEST Statement

**TEST** <H=*effects*> E=*effect* </ options> ;

By default, for each sum of squares in the analysis an  $F$  value is computed that uses the residual MS as an error term. Use a TEST statement to request additional  $F$  tests that use other effects as error terms. You need a TEST statement when a nonstandard error structure (as in a split-plot design) exists. Note, however, that this might not be appropriate if the design is unbalanced, since in most unbalanced designs with nonstandard error structures, mean squares are not necessarily independent with equal expectations under the null hypothesis.

**CAUTION:** The GLM procedure does not check any of the assumptions underlying the  $F$  statistic. When you specify a TEST statement, you assume sole responsibility for the validity of the  $F$  statistic produced. To help validate a test, you can use the [RANDOM](#) statement and inspect the expected mean squares, or you can use the [TEST](#) option of the [RANDOM](#) statement.

You can use as many TEST statements as you want, provided that they appear after the [MODEL](#) statement.

You can specify the following terms in the TEST statement.

### H=*effects*

specifies which effects in the preceding model are to be used as hypothesis (numerator) effects.

### E=*effect*

specifies one, and only one, effect to use as the error (denominator) term. The E= specification is required.

By default, the sum of squares type for all hypothesis sum of squares and error sum of squares is the highest type computed in the model. If the hypothesis type or error type is to be another type that was computed in the model, you should specify one or both of the following options after a slash (/).

**ETYPE=*n***

specifies the type of sum of squares to use for the error term. The type must be a type computed in the model (*n*=1, 2, 3, or 4).

**HTYPE=*n***

specifies the type of sum of squares to use for the hypothesis. The type must be a type computed in the model (*n*=1, 2, 3, or 4).

This example illustrates the TEST statement with a split-plot model:

```
proc glm;
 class a b c;
 model y=a b(a) c a*c b*c(a);
 test h=a e=b(a) / htype=1 etype=1;
 test h=c a*c e=b*c(a) / htype=1 etype=1;
run;
```

---

## WEIGHT Statement

**WEIGHT** *variable* ;

When a WEIGHT statement is used, a weighted residual sum of squares

$$\sum_i w_i (y_i - \hat{y}_i)^2$$

is minimized, where  $w_i$  is the value of the variable specified in the WEIGHT statement,  $y_i$  is the observed value of the response variable, and  $\hat{y}_i$  is the predicted value of the response variable.

If you specify the WEIGHT statement, it must appear before the first RUN statement or it is ignored.

An observation is used in the analysis only if the value of the WEIGHT statement variable is nonmissing and greater than zero.

The WEIGHT statement has no effect on degrees of freedom or number of observations, but it is used by the MEANS statement when calculating means and performing multiple comparison tests (as described in the section “MEANS Statement” on page 3303).

The normal equations used when a WEIGHT statement is present are

$$X'WX\beta = X'WY$$

where **W** is a diagonal matrix consisting of the values of the variable specified in the WEIGHT statement.

If the weights for the observations are proportional to the reciprocals of the error variances, then the weighted least squares estimates are best linear unbiased estimators (BLUE).

---

## Details: GLM Procedure

---

### Statistical Assumptions for Using PROC GLM

The basic statistical assumption underlying the least squares approach to general linear modeling is that the observed values of each dependent variable can be written as the sum of two parts: a fixed component  $x'\beta$ , which is a linear function of the independent coefficients, and a random noise, or error, component  $\epsilon$ :

$$y = x'\beta + \epsilon$$

The independent coefficients  $x$  are constructed from the model effects as described in the section “[Parameterization of PROC GLM Models](#)” on page 3327. Further, the errors for different observations are assumed to be uncorrelated with identical variances. Thus, this model can be written

$$E(Y) = \mathbf{X}\beta, \quad \text{Var}(Y) = \sigma^2 I$$

where  $Y$  is the vector of dependent variable values,  $\mathbf{X}$  is the matrix of independent coefficients,  $I$  is the identity matrix, and  $\sigma^2$  is the common variance for the errors. For multiple dependent variables, the model is similar except that the errors for different dependent variables within the same observation are not assumed to be uncorrelated. This yields a multivariate linear model of the form

$$E(Y) = \mathbf{X}B, \quad \text{Var}(\text{vec}(Y)) = \Sigma \otimes I$$

where  $Y$  and  $B$  are now matrices, with one column for each dependent variable,  $\text{vec}(Y)$  strings  $Y$  out by rows, and  $\otimes$  indicates the Kronecker matrix product.

Under the assumptions thus far discussed, the least squares approach provides estimates of the linear parameters that are unbiased and have minimum variance among linear estimators. Under the further assumption that the errors have a normal (or Gaussian) distribution, the least squares estimates are the maximum likelihood estimates and their distribution is known. All of the significance levels (“ $p$  values”) and confidence limits calculated by the GLM procedure require this assumption of normality in order to be exactly valid, although they are good approximations in many other cases.

---

### Specification of Effects

Each term in a model, called an *effect*, is a variable or combination of variables. Effects are specified with a special notation that uses variable names and operators. There are two kinds of variables: *classification* (or *CLASS*) *variables* and *continuous variables*. There are two primary operators: *crossing* and *nesting*. A third operator, the *bar operator*, is used to simplify effect specification.

In an analysis-of-variance model, independent variables must be variables that identify classification levels. In the SAS System, these are called *classification* (or *class*) *variables* and are declared in the **CLASS** statement. (They can also be called *categorical*, *qualitative*, *discrete*, or *nominal variables*.) Classification variables can be either *numeric* or *character*. The values of a classification variable are called *levels*. For example, the classification variable *Sex* has the levels “male” and “female.”

In a model, an independent variable that is not declared in the **CLASS** statement is assumed to be continuous. Continuous variables, which must be numeric, are used for response variables and covariates. For example, the heights and weights of subjects are continuous variables.

## Types of Effects

There are seven different types of effects used in the GLM procedure. In the following list, assume that A, B, C, D, and E are **CLASS** variables and that X1, X2, and Y are continuous variables:

- Regressor effects are specified by writing continuous variables by themselves: X1 X2.
- Polynomial effects are specified by joining two or more continuous variables with asterisks: X1\*X1 X1\*X2.
- Main effects are specified by writing **CLASS** variables by themselves: A B C.
- Crossed effects (interactions) are specified by joining classification variables with asterisks: A\*B B\*C A\*B\*C.
- Nested effects are specified by following a main effect or crossed effect with a classification variable or list of classification variables enclosed in parentheses. The main effect or crossed effect is nested within the effects listed in parentheses: B(A) C(B\*A) D\*E(C\*B\*A). In this example, B(A) is read “B nested within A.”
- Continuous-by-class effects are written by joining continuous variables and classification variables with asterisks: X1\*A.
- Continuous-nesting-class effects consist of continuous variables followed by a classification variable interaction enclosed in parentheses: X1(A) X1\*X2(A\*B).

One example of the general form of an effect involving several variables is

$$X1*X2*A*B*C(D*E)$$

This example contains crossed continuous terms by crossed classification terms nested within more than one classification variable. The continuous list comes first, followed by the crossed list, followed by the nesting list in parentheses. Note that asterisks can appear within the nested list but not immediately before the left parenthesis. For details on how the design matrix and parameters are defined with respect to the effects specified in this section, see the section “[Parameterization of PROC GLM Models](#)” on page 3327.

The **MODEL** statement and several other statements use these effects. Some examples of **MODEL** statements that use various kinds of effects are shown in the following table; a, b, and c represent classification variables, and y, y1, y2, x, and z represent continuous variables.



| Specification                       | Type of Model                              |
|-------------------------------------|--------------------------------------------|
| <code>model y=x;</code>             | Simple regression                          |
| <code>model y=x z;</code>           | Multiple regression                        |
| <code>model y=x x*x;</code>         | Polynomial regression                      |
| <code>model y1 y2=x z;</code>       | Multivariate regression                    |
| <code>model y=a;</code>             | One-way ANOVA                              |
| <code>model y=a b c;</code>         | Main-effects ANOVA                         |
| <code>model y=a b a*b;</code>       | Factorial ANOVA with interaction           |
| <code>model y=a b(a) c(b a);</code> | Nested ANOVA                               |
| <code>model y1 y2=a b;</code>       | Multivariate analysis of variance (MANOVA) |
| <code>model y=a x;</code>           | Analysis of covariance                     |
| <code>model y=a x(a);</code>        | Separate-slopes regression                 |
| <code>model y=a x x*a;</code>       | Homogeneity-of-slopes regression           |

## The Bar Operator

You can shorten the specification of a large factorial model by using the bar operator. For example, two ways of writing the model for a full three-way factorial model follow:

```
model Y = A B C A*B A*C B*C A*B*C;
```

```
model Y = A|B|C;
```

When the bar (|) is used, the right and left sides become effects, and the cross of them becomes an effect. Multiple bars are permitted. The expressions are expanded from left to right, using rules 2–4 given in Searle (1971, p. 390).

- Multiple bars are evaluated from left to right. For instance, A|B|C is evaluated as follows:

$$\begin{aligned}
 A|B|C &\rightarrow \{A|B\}|C \\
 &\rightarrow \{A B A*B\}|C \\
 &\rightarrow A B A*B C A*C B*C A*B*C
 \end{aligned}$$

- Crossed and nested groups of variables are combined. For example, A(B)|C(D) generates A\*C(B D), among other terms.
- Duplicate variables are removed. For example, A(C)|B(C) generates A\*B(C C), among other terms, and the extra C is removed.
- Effects are discarded if a variable occurs on both the crossed and nested parts of an effect. For instance, A(B)|B(D E) generates A\*B(B D E), but this effect is eliminated immediately.

You can also specify the maximum number of variables involved in any effect that results from bar evaluation by specifying that maximum number, preceded by an @ sign, at the end of the bar effect. For example, the

specification  $A | B | C @ 2$  would result in only those effects that contain 2 or fewer variables: in this case,  $A B A*B C A*C$  and  $B*C$ .

More examples of using the bar and at operators follow:

|                     |                  |                                   |
|---------------------|------------------|-----------------------------------|
| $A   C(B)$          | is equivalent to | $A C(B) A*C(B)$                   |
| $A(B)   C(B)$       | is equivalent to | $A(B) C(B) A*C(B)$                |
| $A(B)   B(D E)$     | is equivalent to | $A(B) B(D E)$                     |
| $A   B(A)   C$      | is equivalent to | $A B(A) C A*C B*C(A)$             |
| $A   B(A)   C @ 2$  | is equivalent to | $A B(A) C A*C$                    |
| $A   B   C   D @ 2$ | is equivalent to | $A B A*B C A*C B*C D A*D B*D C*D$ |
| $A*B(C*D)$          | is equivalent to | $A*B(C D)$                        |

---

## Using PROC GLM Interactively

You can use the GLM procedure interactively. After you specify a model with a **MODEL** statement and run PROC GLM with a **RUN** statement, you can execute a variety of statements without reinvoking PROC GLM.

The section “[Syntax: GLM Procedure](#)” on page 3278 describes which statements can be used interactively. These interactive statements can be executed singly or in groups by following the single statement or group of statements with a **RUN** statement. Note that the **MODEL** statement cannot be repeated; PROC GLM allows only one **MODEL** statement.

If you use PROC GLM interactively, you can end the GLM procedure with a **DATA** step, another PROC step, an **ENDSAS** statement, or a **QUIT** statement.

When you are using PROC GLM interactively, additional **RUN** statements do not end the procedure but tell PROC GLM to execute additional statements.

When you specify a **WHERE** statement with PROC GLM, it should appear before the first **RUN** statement. The **WHERE** statement enables you to select only certain observations for analysis without using a subsetting **DATA** step. For example, **where group ne 5** omits observations with **GROUP=5** from the analysis. See *SAS Statements: Reference* for details on this statement.

When you specify a **BY** statement with PROC GLM, interactive processing is not possible; that is, once the first **RUN** statement is encountered, processing proceeds for each **BY** group in the data set, and no further statements are accepted by the procedure.

Interactivity is also disabled when there are different patterns of missing values among the dependent variables. For details, see the section “[Missing Values](#)” on page 3379.

---

## Parameterization of PROC GLM Models

The GLM procedure constructs a linear model according to the specifications in the **MODEL** statement. Each effect generates one or more columns in a design matrix **X**. This section shows precisely how **X** is built.

## Intercept

All models include a column of 1s by default to estimate an intercept parameter  $\mu$ . You can use the `NOINT` option to suppress the intercept.

## Regression Effects

Regression effects (covariates) have the values of the variables copied into the design matrix directly. Polynomial terms are multiplied out and then installed in **X**.

## Main Effects

If a classification variable has  $m$  levels, PROC GLM generates  $m$  columns in the design matrix for its main effect. Each column is an indicator variable for one of the levels of the classification variable. The default order of the columns is the sort order of the values of their levels; this order can be controlled with the `ORDER=` option in the `PROC GLM` statement, as shown in the following table.

| Data |   | Design Matrix |    |    |    |    |    |
|------|---|---------------|----|----|----|----|----|
| A    | B | $\mu$         | A  |    | B  |    |    |
|      |   |               | A1 | A2 | B1 | B2 | B3 |
| 1    | 1 | 1             | 1  | 0  | 1  | 0  | 0  |
| 1    | 2 | 1             | 1  | 0  | 0  | 1  | 0  |
| 1    | 3 | 1             | 1  | 0  | 0  | 0  | 1  |
| 2    | 1 | 1             | 0  | 1  | 1  | 0  | 0  |
| 2    | 2 | 1             | 0  | 1  | 0  | 1  | 0  |
| 2    | 3 | 1             | 0  | 1  | 0  | 0  | 1  |

There are more columns for these effects than there are degrees of freedom for them; in other words, PROC GLM is using an over-parameterized model.

## Crossed Effects

First, PROC GLM reorders the terms to correspond to the order of the variables in the `CLASS` statement; thus, `B*A` becomes `A*B` if `A` precedes `B` in the `CLASS` statement. Then, PROC GLM generates columns for all combinations of levels that occur in the data. The order of the columns is such that the rightmost variables in the cross index faster than the leftmost variables. No columns are generated corresponding to combinations of levels that do not occur in the data.

| Data |   | Design Matrix |    |    |    |    |    |      |      |      |      |      |      |
|------|---|---------------|----|----|----|----|----|------|------|------|------|------|------|
| A    | B | $\mu$         | A  |    | B  |    |    | A*B  |      |      |      |      |      |
|      |   |               | A1 | A2 | B1 | B2 | B3 | A1B1 | A1B2 | A1B3 | A2B1 | A2B2 | A2B3 |
| 1    | 1 | 1             | 1  | 0  | 1  | 0  | 0  | 1    | 0    | 0    | 0    | 0    | 0    |
| 1    | 2 | 1             | 1  | 0  | 0  | 1  | 0  | 0    | 1    | 0    | 0    | 0    | 0    |
| 1    | 3 | 1             | 1  | 0  | 0  | 0  | 1  | 0    | 0    | 1    | 0    | 0    | 0    |
| 2    | 1 | 1             | 0  | 1  | 1  | 0  | 0  | 0    | 0    | 0    | 1    | 0    | 0    |
| 2    | 2 | 1             | 0  | 1  | 0  | 1  | 0  | 0    | 0    | 0    | 0    | 1    | 0    |
| 2    | 3 | 1             | 0  | 1  | 0  | 0  | 1  | 0    | 0    | 0    | 0    | 0    | 1    |

In this matrix, main-effects columns are not linearly independent of crossed-effect columns; in fact, the column space for the crossed effects contains the space of the main effect.

### Nested Effects

Nested effects are generated in the same manner as crossed effects. Hence, the design columns generated by the following statements are the same (but the ordering of the columns is different):

```

model y=a b(a); (B nested within A)
model y=a a*b; (omitted main effect for B)

```

The nesting operator in PROC GLM is more a notational convenience than an operation distinct from crossing. Nested effects are characterized by the property that the nested variables never appear as main effects. The order of the variables within nesting parentheses is made to correspond to the order of these variables in the CLASS statement. The order of the columns is such that variables outside the parentheses index faster than those inside the parentheses, and the rightmost nested variables index faster than the leftmost variables.

| Data |   | Design Matrix |    |    |      |      |      |      |      |      |
|------|---|---------------|----|----|------|------|------|------|------|------|
| A    | B | $\mu$         | A  |    | B(A) |      |      |      |      |      |
|      |   |               | A1 | A2 | B1A1 | B2A1 | B3A1 | B1A2 | B2A2 | B3A2 |
| 1    | 1 | 1             | 1  | 0  | 1    | 0    | 0    | 0    | 0    | 0    |
| 1    | 2 | 1             | 1  | 0  | 0    | 1    | 0    | 0    | 0    | 0    |
| 1    | 3 | 1             | 1  | 0  | 0    | 0    | 1    | 0    | 0    | 0    |
| 2    | 1 | 1             | 0  | 1  | 0    | 0    | 0    | 1    | 0    | 0    |
| 2    | 2 | 1             | 0  | 1  | 0    | 0    | 0    | 0    | 1    | 0    |
| 2    | 3 | 1             | 0  | 1  | 0    | 0    | 0    | 0    | 0    | 1    |

### Continuous-Nesting-Class Effects

When a continuous variable nests with a classification variable, the design columns are constructed by multiplying the continuous values into the design columns for the class effect.

| Data |   | Design Matrix |    |    |       |       |  |
|------|---|---------------|----|----|-------|-------|--|
| X    | A | $\mu$         | A  |    | X(A)  |       |  |
|      |   |               | A1 | A2 | X(A1) | X(A2) |  |
| 21   | 1 | 1             | 1  | 0  | 21    | 0     |  |
| 24   | 1 | 1             | 1  | 0  | 24    | 0     |  |
| 22   | 1 | 1             | 1  | 0  | 22    | 0     |  |
| 28   | 2 | 1             | 0  | 1  | 0     | 28    |  |
| 19   | 2 | 1             | 0  | 1  | 0     | 19    |  |
| 23   | 2 | 1             | 0  | 1  | 0     | 23    |  |

This model estimates a separate slope for X within each level of A.

## Continuous-by-Class Effects

Continuous-by-class effects generate the same design columns as continuous-nesting-class effects. The two models differ by the presence of the continuous variable as a regressor by itself, in addition to being a contributor to  $X*A$ .

| Data |   | Design Matrix |    |    |    |      |      |
|------|---|---------------|----|----|----|------|------|
| X    | A | $\mu$         | X  | A  |    | X*A  |      |
|      |   |               |    | A1 | A2 | X*A1 | X*A2 |
| 21   | 1 | 1             | 21 | 1  | 0  | 21   | 0    |
| 24   | 1 | 1             | 24 | 1  | 0  | 24   | 0    |
| 22   | 1 | 1             | 22 | 1  | 0  | 22   | 0    |
| 28   | 2 | 1             | 28 | 0  | 1  | 0    | 28   |
| 19   | 2 | 1             | 19 | 0  | 1  | 0    | 19   |
| 23   | 2 | 1             | 23 | 0  | 1  | 0    | 23   |

Continuous-by-class effects are used to test the homogeneity of slopes. If the continuous-by-class effect is nonsignificant, the effect can be removed so that the response with respect to  $X$  is the same for all levels of the classification variables.

## General Effects

An example that combines all the effects is

$$X1*X2*A*B*C(D E)$$

The continuous list comes first, followed by the crossed list, followed by the nested list in parentheses.

The sequencing of parameters is important to learn if you use the **CONTRAST** or **ESTIMATE** statement to compute or test some linear function of the parameter estimates.

Effects might be retitled by PROC GLM to correspond to ordering rules. For example,  $B*A(E D)$  might be retitled  $A*B(D E)$  to satisfy the following:

- Classification variables that occur outside parentheses (crossed effects) are sorted in the order in which they appear in the **CLASS** statement.
- Variables within parentheses (nested effects) are sorted in the order in which they appear in a **CLASS** statement.

The sequencing of the parameters generated by an effect can be described by which variables have their levels indexed faster:

- Variables in the crossed part index faster than variables in the nested list.
- Within a crossed or nested list, variables to the right index faster than variables to the left.

For example, suppose a model includes four effects— $A$ ,  $B$ ,  $C$ , and  $D$ —each having two levels, 1 and 2. If the **CLASS** statement is

```
class A B C D;
```

then the order of the parameters for the effect B\*A(C D), which is retitled A\*B(C D), is as follows.

```
A1B1C1D1
A1B2C1D1
A2B1C1D1
A2B2C1D1
A1B1C1D2
A1B2C1D2
A2B1C1D2
A2B2C1D2
A1B1C2D1
A1B2C2D1
A2B1C2D1
A2B2C2D1
A1B1C2D2
A1B2C2D2
A2B1C2D2
A2B2C2D2
```

Note that first the crossed effects B and A are sorted in the order in which they appear in the CLASS statement so that A precedes B in the parameter list. Then, for each combination of the nested effects in turn, combinations of A and B appear. The B effect changes fastest because it is rightmost in the (renamed) cross list. Then A changes next fastest. The D effect changes next fastest, and C is the slowest since it is leftmost in the nested list.

When numeric classification variables are used, their levels are sorted by their character format, which might not correspond to their numeric sort sequence. Therefore, it is advisable to include a format for numeric classification variables or to use the `ORDER=INTERNAL` option in the `PROC GLM` statement to ensure that levels are sorted by their internal values.

## Degrees of Freedom

For models with classification (categorical) effects, there are more design columns constructed than there are degrees of freedom for the effect. Thus, there are linear dependencies among the columns. In this event, the parameters are not jointly estimable; there is an infinite number of least squares solutions. The GLM procedure uses a generalized  $g_2$ -inverse to obtain values for the estimates; see the section “[Computational Method](#)” on page 3382 for more details. The solution values are not produced unless the `SOLUTION` option is specified in the `MODEL` statement. The solution has the characteristic that estimates are zero whenever the design column for that parameter is a linear combination of previous columns. (Strictly termed, the solution values should not be called estimates, since the parameters might not be formally estimable.) With this full parameterization, hypothesis tests are constructed to test linear functions of the parameters that are estimable.

Other procedures (such as the CATMOD procedure) reparameterize models to full rank by using certain restrictions on the parameters. PROC GLM does not reparameterize, making the hypotheses that are commonly tested more understandable. See Goodnight (1978a) for additional reasons for not reparameterizing.

PROC GLM does not actually construct the entire design matrix  $\mathbf{X}$ ; rather, a row  $x_i$  of  $\mathbf{X}$  is constructed for each observation in the data set and used to accumulate the crossproduct matrix  $\mathbf{X}'\mathbf{X} = \sum_i x_i'x_i$ .

## Hypothesis Testing in PROC GLM

See Chapter 15, “The Four Types of Estimable Functions,” for a complete discussion of the four standard types of hypothesis tests.

### Example

To illustrate the four types of tests and the principles upon which they are based, consider a two-way design with interaction based on the following data:

|   |   | B            |              |
|---|---|--------------|--------------|
|   |   | 1            | 2            |
| A | 1 | 23.5<br>23.7 | 28.7         |
|   | 2 | 8.9          | 5.6<br>8.9   |
|   | 3 | 10.3<br>12.5 | 13.6<br>14.6 |

Invoke PROC GLM and specify all the estimable functions options to examine what the GLM procedure can test. The following statements produce the summary ANOVA table displayed in Figure 42.10.

```
data example;
 input a b y @@;
 datalines;
1 1 23.5 1 1 23.7 1 2 28.7 2 1 8.9 2 2 5.6
2 2 8.9 3 1 10.3 3 1 12.5 3 2 13.6 3 2 14.6
;

proc glm;
 class a b;
 model y=a b a*b / e e1 e2 e3 e4;
run;
```

**Figure 42.10** Summary ANOVA Table from PROC GLM

| The GLM Procedure     |          |                |             |          |        |
|-----------------------|----------|----------------|-------------|----------|--------|
| Dependent Variable: y |          |                |             |          |        |
| Source                | DF       | Sum of Squares | Mean Square | F Value  | Pr > F |
| Model                 | 5        | 520.4760000    | 104.0952000 | 49.66    | 0.0011 |
| Error                 | 4        | 8.3850000      | 2.0962500   |          |        |
| Corrected Total       | 9        | 528.8610000    |             |          |        |
|                       | R-Square | Coeff Var      | Root MSE    | y Mean   |        |
|                       | 0.984145 | 9.633022       | 1.447843    | 15.03000 |        |

The following sections show the general form of estimable functions and discuss the four standard tests, their properties, and abbreviated output for the two-way crossed example.

### Estimability

Figure 42.11 is the general form of estimable functions for the example. In order to be testable, a hypothesis must be able to fit within the framework displayed here.

**Figure 42.11** General Form of Estimable Functions

| The GLM Procedure                   |     |                   |
|-------------------------------------|-----|-------------------|
| General Form of Estimable Functions |     |                   |
| Effect                              |     | Coefficients      |
| Intercept                           |     | L1                |
| a                                   | 1   | L2                |
| a                                   | 2   | L3                |
| a                                   | 3   | L1-L2-L3          |
| b                                   | 1   | L5                |
| b                                   | 2   | L1-L5             |
| a*b                                 | 1 1 | L7                |
| a*b                                 | 1 2 | L2-L7             |
| a*b                                 | 2 1 | L9                |
| a*b                                 | 2 2 | L3-L9             |
| a*b                                 | 3 1 | L5-L7-L9          |
| a*b                                 | 3 2 | L1-L2-L3-L5+L7+L9 |



If a hypothesis is estimable, the **Ls** in the preceding scheme can be set to values that match the hypothesis. All the standard tests in PROC GLM can be shown in the preceding format, with some of the **Ls** zeroed and some set to functions of other **Ls**.

The following sections show how many of the hypotheses can be tested by comparing the model sum-of-squares regression from one model to a submodel. The notation used is

$$SS(B \text{ effects} | A \text{ effects}) = SS(B \text{ effects}, A \text{ effects}) - SS(A \text{ effects})$$

where  $SS(A \text{ effects})$  denotes the regression model sum of squares for the model consisting of  $A \text{ effects}$ . This notation is equivalent to the reduction notation defined by Searle (1971) and summarized in Chapter 15, “The Four Types of Estimable Functions.”

## Type I Tests

Type I sums of squares (SS), also called *sequential sums of squares*, are the incremental improvement in error sums of squares as each effect is added to the model. They can be computed by fitting the model in steps and recording the difference in error sum of squares at each step.

| Source  | Type I SS               |
|---------|-------------------------|
| $A$     | $SS(A   \mu)$           |
| $B$     | $SS(B   \mu, A)$        |
| $A * B$ | $SS(A * B   \mu, A, B)$ |

Type I sums of squares are displayed by default because they are easy to obtain and can be used in various hand calculations to produce sum of squares values for a series of different models. Nelder (1994) and others have argued that Type I and II sums are essentially the only appropriate ones for testing ANOVA effects; however, see also the discussion of Nelder’s article, especially Rodriguez, Tobias, and Wolfinger (1995) and Searle (1995).

The Type I hypotheses have these properties:

- Type I sum of squares for all effects add up to the model sum of squares. None of the other sum of squares types have this property, except in special cases.
- Type I hypotheses can be derived from rows of the Forward-Dolittle transformation of  $\mathbf{X}'\mathbf{X}$  (a transformation that reduces  $\mathbf{X}'\mathbf{X}$  to an upper triangular matrix by row operations).
- Type I sum of squares are statistically independent of each other under the usual **assumption** that the true residual errors are independent and identically normally distributed (see page 3324).
- Type I hypotheses depend on the order in which effects are specified in the **MODEL** statement.
- Type I hypotheses are uncontaminated by parameters corresponding to effects that precede the effect being tested; however, the hypotheses usually involve parameters for effects following the tested effect in the model. For example, in the model

$$Y=A B;$$

the Type I hypothesis for B does not involve A parameters, but the Type I hypothesis for A does involve B parameters.

- Type I hypotheses are functions of the cell counts for unbalanced data; the hypotheses are not usually the same hypotheses that are tested if the data are balanced.
- Type I sums of squares are useful for polynomial models where you want to know the contribution of a term as though it had been made orthogonal to preceding effects. Thus, in polynomial models, Type I sums of squares correspond to tests of the orthogonal polynomial effects.

The Type I estimable functions and associated tests for the example are shown in Figure 42.12.

**Figure 42.12** Type I Estimable Functions and Tests

|           |     | Type I Estimable Functions |             |             |         |        |
|-----------|-----|----------------------------|-------------|-------------|---------|--------|
|           |     | -----Coefficients-----     |             |             |         |        |
| Effect    |     | a                          | b           | a*b         |         |        |
| Intercept |     | 0                          | 0           | 0           |         |        |
| a         | 1   | L2                         | 0           | 0           |         |        |
| a         | 2   | L3                         | 0           | 0           |         |        |
| a         | 3   | -L2-L3                     | 0           | 0           |         |        |
| b         | 1   | 0.1667*L2-0.1667*L3        | L5          | 0           |         |        |
| b         | 2   | -0.1667*L2+0.1667*L3       | -L5         | 0           |         |        |
| a*b       | 1 1 | 0.6667*L2                  | 0.2857*L5   | L7          |         |        |
| a*b       | 1 2 | 0.3333*L2                  | -0.2857*L5  | -L7         |         |        |
| a*b       | 2 1 | 0.3333*L3                  | 0.2857*L5   | L9          |         |        |
| a*b       | 2 2 | 0.6667*L3                  | -0.2857*L5  | -L9         |         |        |
| a*b       | 3 1 | -0.5*L2-0.5*L3             | 0.4286*L5   | -L7-L9      |         |        |
| a*b       | 3 2 | -0.5*L2-0.5*L3             | -0.4286*L5  | L7+L9       |         |        |
| Source    |     | DF                         | Type I SS   | Mean Square | F Value | Pr > F |
| a         |     | 2                          | 494.0310000 | 247.0155000 | 117.84  | 0.0003 |
| b         |     | 1                          | 10.7142857  | 10.7142857  | 5.11    | 0.0866 |
| a*b       |     | 2                          | 15.7307143  | 7.8653571   | 3.75    | 0.1209 |

### Type II Tests

The Type II tests can also be calculated by comparing the error sums of squares (SS) for subset models. The Type II SS are the reduction in error SS due to adding the term after all other terms have been added to the model except terms that contain the effect being tested. An effect is contained in another effect if it can be derived by deleting variables from the latter effect. For example, A and B are both contained in A\*B. For this model, the Type II SS are given by the reduced sums of squares as shown in the following table.

| Source       | Type II SS                 |
|--------------|----------------------------|
| <i>A</i>     | $SS(A \mid \mu, B)$        |
| <i>B</i>     | $SS(B \mid \mu, A)$        |
| <i>A * B</i> | $SS(A * B \mid \mu, A, B)$ |

Type II SS have these properties:

- Type II SS do not necessarily sum to the model SS.
- The hypothesis for an effect does not involve parameters of other effects except for containing effects (which it must involve to be estimable).
- Type II SS are invariant to the ordering of effects in the model.
- For unbalanced designs, Type II hypotheses for effects that are contained in other effects are not usually the same hypotheses that are tested if the data are balanced. The hypotheses are generally functions of the cell counts.

The Type II estimable functions and associated tests for the example are shown in Figure 42.13.

**Figure 42.13** Type II Estimable Functions and Tests

| Type II Estimable Functions |     |                      |             |             |         |        |
|-----------------------------|-----|----------------------|-------------|-------------|---------|--------|
| -----Coefficients-----      |     |                      |             |             |         |        |
| Effect                      |     | a                    | b           | a*b         |         |        |
| Intercept                   |     | 0                    | 0           | 0           |         |        |
| a                           | 1   | L2                   | 0           | 0           |         |        |
| a                           | 2   | L3                   | 0           | 0           |         |        |
| a                           | 3   | -L2-L3               | 0           | 0           |         |        |
| b                           | 1   | 0                    | L5          | 0           |         |        |
| b                           | 2   | 0                    | -L5         | 0           |         |        |
| a*b                         | 1 1 | 0.619*L2+0.0476*L3   | 0.2857*L5   | L7          |         |        |
| a*b                         | 1 2 | 0.381*L2-0.0476*L3   | -0.2857*L5  | -L7         |         |        |
| a*b                         | 2 1 | -0.0476*L2+0.381*L3  | 0.2857*L5   | L9          |         |        |
| a*b                         | 2 2 | 0.0476*L2+0.619*L3   | -0.2857*L5  | -L9         |         |        |
| a*b                         | 3 1 | -0.5714*L2-0.4286*L3 | 0.4286*L5   | -L7-L9      |         |        |
| a*b                         | 3 2 | -0.4286*L2-0.5714*L3 | -0.4286*L5  | L7+L9       |         |        |
| Source                      |     | DF                   | Type II SS  | Mean Square | F Value | Pr > F |
| a                           |     | 2                    | 499.1202857 | 249.5601429 | 119.05  | 0.0003 |
| b                           |     | 1                    | 10.7142857  | 10.7142857  | 5.11    | 0.0866 |
| a*b                         |     | 2                    | 15.7307143  | 7.8653571   | 3.75    | 0.1209 |

## Type III and Type IV Tests

Type III and Type IV sums of squares (SS), sometimes referred to as *partial sums of squares*, are considered by many to be the most desirable; see Searle (1987, Section 4.6). Using PROC GLM's singular parameterization, these SS cannot, in general, be computed by comparing model SS from different models. However, they can sometimes be computed by reduction for methods that reparameterize to full rank, when such a reparameterization effectively imposes Type III linear constraints on the parameters. In PROC GLM, they are computed by constructing a hypothesis matrix  $L$  and then computing the SS associated with the hypothesis  $L\beta = 0$ . As long as there are no missing cells in the design, Type III and Type IV SS are the same.

These are properties of Type III and Type IV SS:

- The hypothesis for an effect does not involve parameters of other effects except for containing effects (which it must involve to be estimable).
- The hypotheses to be tested are invariant to the ordering of effects in the model.
- The hypotheses are the same hypotheses that are tested if there are no missing cells. They are not functions of cell counts.
- The SS do not generally add up to the model SS and, in some cases, can exceed the model SS.

The SS are constructed from the general form of estimable functions. Type III and Type IV tests are different only if the design has missing cells. In this case, the Type III tests have an orthogonality property, while the Type IV tests have a balancing property. These properties are discussed in Chapter 15, “[The Four Types of Estimable Functions](#).” For this example, since the data contain observations for all pairs of levels of A and B, Type IV tests are identical to the Type III tests that are shown in [Figure 42.14](#). (This combines tables from several pages of output.)

**Figure 42.14** Type III Estimable Functions and Tests

| Type III Estimable Functions |     |                        |            |        |
|------------------------------|-----|------------------------|------------|--------|
|                              |     | -----Coefficients----- |            |        |
| Effect                       |     | a                      | b          | a*b    |
| Intercept                    |     | 0                      | 0          | 0      |
| a                            | 1   | L2                     | 0          | 0      |
| a                            | 2   | L3                     | 0          | 0      |
| a                            | 3   | -L2-L3                 | 0          | 0      |
| b                            | 1   | 0                      | L5         | 0      |
| b                            | 2   | 0                      | -L5        | 0      |
| a*b                          | 1 1 | 0.5*L2                 | 0.3333*L5  | L7     |
| a*b                          | 1 2 | 0.5*L2                 | -0.3333*L5 | -L7    |
| a*b                          | 2 1 | 0.5*L3                 | 0.3333*L5  | L9     |
| a*b                          | 2 2 | 0.5*L3                 | -0.3333*L5 | -L9    |
| a*b                          | 3 1 | -0.5*L2-0.5*L3         | 0.3333*L5  | -L7-L9 |
| a*b                          | 3 2 | -0.5*L2-0.5*L3         | -0.3333*L5 | L7+L9  |

Figure 42.14 continued

| Source | DF | Type III SS | Mean Square | F Value | Pr > F |
|--------|----|-------------|-------------|---------|--------|
| a      | 2  | 479.1078571 | 239.5539286 | 114.28  | 0.0003 |
| b      | 1  | 9.4556250   | 9.4556250   | 4.51    | 0.1009 |
| a*b    | 2  | 15.7307143  | 7.8653571   | 3.75    | 0.1209 |

## Effect Size Measures for $F$ Tests in GLM

A significant  $F$  test in a linear model indicates that the effect of the term or contrast being tested might be real. The next thing you want to know is, How big is the effect? Various measures have been devised to give answers to this question that are comparable over different experimental designs. If you specify the experimental `EFFECTSIZE` option in the `MODEL` statement, then GLM adds to each ANOVA table estimates and confidence intervals for three different measures of effect size:

- the noncentrality parameter for the  $F$  test
- the proportion of total variation accounted for (also known as the semipartial correlation ratio or the squared semipartial correlation)
- the proportion of partial variation accounted for (also known as the full partial correlation ratio or the squared full partial correlation)

The adjectives “semipartial” and “full partial” might seem strange. They refer to how other effects are “partialed out” of the dependent variable and the effect being tested. For “semipartial” statistics, all other effects are partialled out of the effect in question, but not the dependent variable. This measures the (adjusted) effect as a proportion of the total variation in the dependent variable. On the other hand, for “full partial” statistics, all other effects are partialled out of *both* the dependent variable and the effect in question. This measures the (adjusted) effect as a proportion of only the dependent variation remaining after partialing, or in other words the partial variation. Details about the computation and interpretation of these estimates and confidence intervals are discussed in the remainder of this section.

The noncentrality parameter is directly related to the true distribution of the  $F$  statistic when the effect being tested has a non-null effect. The uniformly minimum variance unbiased estimate for the noncentrality is

$$NC_{UMVUE} = \frac{DF(DFE - 2)FValue}{DFE} - DF$$

where  $FValue$  is the observed value of the  $F$  statistic for the test and  $DF$  and  $DFE$  are the numerator and denominator degrees of freedom for the test, respectively. An alternative estimate that can be slightly biased but has a somewhat lower expected mean square error is

$$NC_{minMSE} = \frac{DF(DFE - 4)FValue}{DFE} - \frac{DF(DFE - 4)}{DFE - 2}$$

(See Perlman and Rasmussen (1975), cited in Johnson, Kotz, and Balakrishnan (1994).) A  $p \times 100\%$  lower confidence bound for the noncentrality is given by the value of NC for which  $\text{probf}(F\text{Value}, DF, DFE, NC) = p$ , where  $\text{probf}()$  is the cumulative probability function for the non-central  $F$  distribution. This result can be used to form a  $(1 - \alpha) \times 100\%$  confidence interval for the noncentrality.

The partial proportion of variation accounted for by the effect being tested is easiest to define by its natural sample estimate,

$$\hat{\eta}_{\text{partial}}^2 = \frac{SS}{SS + SSE}$$

where SSE is the sample error sum of squares. Note that  $\hat{\eta}_{\text{partial}}^2$  is actually sometimes denoted  $R_{\text{partial}}^2$  or just R square, but in this context the R square notation is reserved for the  $\hat{\eta}^2$  corresponding to the overall model, which is just the familiar R square for the model.  $\hat{\eta}_{\text{partial}}^2$  is actually a biased estimate of the true  $\eta_{\text{partial}}^2$ ; an alternative that is approximately unbiased is given by

$$\omega_{\text{partial}}^2 = \frac{SS - DF \times MSE}{SS + (N - DF)MSE}$$

where  $MSE = SSE/DFE$  is the sample mean square for error and  $N$  is the number of observations. The true  $\eta_{\text{partial}}^2$  is related to the true noncentrality parameter NC by the formula

$$\eta_{\text{partial}}^2 = \frac{NC}{NC + N}$$

This fact can be employed to transform a confidence interval for NC into one for  $\eta_{\text{partial}}^2$ . Note that some authors (Steiger and Fouladi 1997; Fidler and Thompson 2001; Smithson 2003) have published slightly different confidence intervals for  $\eta_{\text{partial}}^2$ , based on a slightly different formula for the relationship between  $\eta_{\text{partial}}^2$  and NC, apparently due to Cohen (1988). Cohen's formula appears to be approximately correct for random predictor values (Maxwell 2000), but the one given previously is correct if the predictor values are assumed fixed, as is standard for the GLM procedure.

Finally, the proportion of total variation accounted for by the effect being tested is again easiest to define by its natural sample estimate, which is known as the (*semipartial*)  $\hat{\eta}^2$  statistic,

$$\hat{\eta}^2 = \frac{SS}{SS_{\text{total}}}$$

where  $SS_{\text{total}}$  is the total sample (corrected) sum of squares, and  $SS$  is the observed sum of squares due to the effect being tested. As with  $\hat{\eta}_{\text{partial}}^2$ ,  $\hat{\eta}^2$  is actually a biased estimate of the true  $\eta^2$ ; an alternative that is approximately unbiased is the (*semipartial*)  $\omega^2$  statistic

$$\omega^2 = \frac{SS - DF \times MSE}{SS_{\text{total}} + MSE}$$

where  $MSE = SSE/DFE$  is the sample mean square for error. Whereas  $\eta_{\text{partial}}^2$  depends only on the noncentrality for its associated  $F$  test, the presence of the total sum of squares in the previous formulas indicates that

$\eta^2$  depends on the noncentralities for all effects in the model. An exact confidence interval is not available, but if you write the formula for  $\hat{\eta}^2$  as

$$\hat{\eta}^2 = \frac{SS}{SS + (SS_{total} - SS)}$$

then a conservative confidence interval can be constructed as for  $\eta_{partial}^2$ , treating  $SS_{total} - SS$  as the SSE and  $N - DF - 1$  as the DFE (Smithson 2004). This confidence interval is conservative in the sense that it implies values of the true  $\eta^2$  that are smaller than they should be.

Estimates and confidence intervals for effect sizes require some care in interpretation. For example, while the true proportions of total and partial variation accounted for are nonnegative quantities, their estimates might be less than zero. Also, confidence intervals for effect sizes are not directly related to the corresponding estimates. In particular, it is possible for the estimate to lie outside the confidence interval.

As for interpreting the actual values of effect size measures, the approximately unbiased  $\omega^2$  estimates are usually preferred for point estimates. Some authors have proposed certain ranges as indicating “small,” “medium,” and “large” effects (Cohen 1988), but general benchmarks like this depend on the nature of the data and the typical signal-to-noise ratio; they should not be expected to apply across various disciplines. For example, while an  $\omega^2$  value of 10% might be viewed as “large” for psychometric data, it can be a relatively small effect for industrial experimentation. Whatever the standard, confidence intervals for true effect sizes typically span more than one category, indicating that in small experiments, it can be difficult to make firm statements about the size of effects.

## Example

The data for this example are similar to data analyzed in Steiger and Fouladi (1997); Fidler and Thompson (2001); Smithson (2003). Consider the following hypothetical design, testing 28 men and 28 women on seven different tasks.

```
data Test;
 do Task = 1 to 7;
 do Gender = 'M', 'F';
 do i = 1 to 4;
 input Response @@;
 output;
 end;
 end;
 end;
 datalines;
7.1 2.8 3.9 3.7 6.5 6.5 6.5 6.6
7.1 5.5 4.8 2.6 3.6 5.4 5.6 4.5
7.2 4.6 4.9 4.6 3.3 5.4 2.8 1.5
5.6 6.2 5.4 6.5 5.6 2.7 3.8 2.3
2.2 5.4 5.6 8.4 1.2 2.0 4.3 4.6
9.1 4.5 7.6 4.9 4.3 7.7 6.5 7.7
4.5 3.8 5.9 6.1 1.7 2.5 4.3 2.7
;
```

This is a balanced two-way design with four replicates per cell. The following statements analyze this data. Since this is a balanced design, you can use the `SS1` option in the `MODEL` statement to display only the Type I sums of squares.

```
proc glm data=Test;
 class Gender Task;
 model Response = Gender|Task / ss1;
run;
```

The analysis of variance results are shown in Figure 42.15.

**Figure 42.15** Two-Way Analysis of Variance

| The GLM Procedure            |    |             |             |         |        |
|------------------------------|----|-------------|-------------|---------|--------|
| Dependent Variable: Response |    |             |             |         |        |
| Source                       | DF | Type I SS   | Mean Square | F Value | Pr > F |
| Gender                       | 1  | 14.40285714 | 14.40285714 | 6.00    | 0.0185 |
| Task                         | 6  | 38.15964286 | 6.35994048  | 2.65    | 0.0285 |
| Gender*Task                  | 6  | 35.99964286 | 5.99994048  | 2.50    | 0.0369 |

You can see that the two main effects as well as their interaction are all significant. Suppose you want to compare the main effect of Gender with the interaction between Gender and Task. The sums of squares for the interaction are more than twice as large, but it's not clear how experimental variability might affect this. The following statements perform the same analysis as before, but add the `EFFECTSIZE` option to the `MODEL` statement; also, with `ALPHA=0.1` option displays 90% confidence intervals, ensuring that inferences based on the  $p$ -values at the 0.05 levels will agree with the lower confidence limit.

```
proc glm data=Test;
 class Gender Task;
 model Response = Gender|Task / ss1 effectsize alpha=0.1;
run;
```

The Type I analysis of variance results with added effect size information are shown in Figure 42.16.



Figure 42.16 Two-Way Analysis of Variance with Effect Sizes

| The GLM Procedure            |    |             |             |         |        |
|------------------------------|----|-------------|-------------|---------|--------|
| Dependent Variable: Response |    |             |             |         |        |
| Source                       | DF | Type I SS   | Mean Square | F Value | Pr > F |
| Gender                       | 1  | 14.40285714 | 14.40285714 | 6.00    | 0.0185 |
| Task                         | 6  | 38.15964286 | 6.35994048  | 2.65    | 0.0285 |
| Gender*Task                  | 6  | 35.99964286 | 5.99994048  | 2.50    | 0.0369 |

| Noncentrality Parameter |                   |                  |                       |      |
|-------------------------|-------------------|------------------|-----------------------|------|
| Source                  | Min Var           |                  | 90% Confidence Limits |      |
|                         | Unbiased Estimate | Low MSE Estimate |                       |      |
| Gender                  | 4.72              | 4.48             | 0.521                 | 17.1 |
| Task                    | 9.14              | 8.69             | 0.870                 | 27.3 |
| Gender*Task             | 8.29              | 7.87             | 0.463                 | 25.9 |

| Total Variation Accounted For |                        |              |                       |        |
|-------------------------------|------------------------|--------------|-----------------------|--------|
| Source                        | Semipartial            |              | 90% Confidence Limits |        |
|                               | Semipartial Eta-Square | Omega-Square | Conservative          |        |
| Gender                        | 0.0761                 | 0.0626       | 0.0019                | 0.2030 |
| Task                          | 0.2015                 | 0.1239       | 0.0000                | 0.2772 |
| Gender*Task                   | 0.1901                 | 0.1126       | 0.0000                | 0.2639 |

| Partial Variation Accounted For |                    |              |                       |        |
|---------------------------------|--------------------|--------------|-----------------------|--------|
| Source                          | Partial            |              | 90% Confidence Limits |        |
|                                 | Partial Eta-Square | Omega-Square |                       |        |
| Gender                          | 0.1250             | 0.0820       | 0.0092                | 0.2342 |
| Task                            | 0.2746             | 0.1502       | 0.0153                | 0.3277 |
| Gender*Task                     | 0.2632             | 0.1385       | 0.0082                | 0.3160 |

The estimated effect sizes for Gender and the interaction all tell pretty much the same story: the effect of the interaction is appreciably greater than the effect of Gender. However, the confidence intervals suggest that this inference should be treated with some caution, since the lower confidence bound for the Gender effect is greater than the lower confidence bound for the interaction in all three cases. Follow-up testing is probably in order, using the estimated effect sizes in this preliminary study to design a large enough sample to distinguish the sizes of the effects.

## Absorption

Absorption is a computational technique used to reduce computing resource needs in certain cases. The classic use of absorption occurs when a blocking factor with a large number of levels is a term in the model.

For example, the statements

```
proc glm;
 absorb herd;
 class a b;
 model y=a b a*b;
run;
```

are equivalent to

```
proc glm;
 class herd a b;
 model y=herd a b a*b;
run;
```

The exception to the previous statements is that the Type II, Type III, or Type IV SS for HERD are not computed when HERD is absorbed.

The algorithm for absorbing variables is similar to the one used by the NESTED procedure for computing a nested analysis of variance. As each new row of  $[X|Y]$  (corresponding to the nonabsorbed independent effects and the dependent variables) is constructed, it is adjusted for the absorbed effects in a Type I fashion. The efficiency of the absorption technique is due to the fact that this adjustment can be done in one pass of the data and without solving any linear equations, assuming that the data have been sorted by the absorbed variables.

Several effects can be absorbed at one time. For example, these statements

```
proc glm;
 absorb herd cow;
 class a b;
 model y=a b a*b;
run;
```

are equivalent to

```
proc glm;
 class herd cow a b;
 model y=herd cow(herd) a b a*b;
run;
```

When you use absorption, the size of the  $X'X$  matrix is a function only of the effects in the **MODEL** statement. The effects being absorbed do not contribute to the size of the  $X'X$  matrix.

For the preceding example, a and b can be absorbed:

```
proc glm;
 absorb a b;
 class herd cow;
 model y=herd cow(herd);
run;
```

Although the sources of variation in the results are listed as

```
a b(a) herd cow(herd)
```

all types of estimable functions for herd and cow(herd) are free of a, b, and a\*b parameters.

To illustrate the savings in computing by using the **ABSORB** statement, PROC GLM is run on generated data with 1147 degrees of freedom in the model with the following statements.

```
data a;
 do herd=1 to 40;
 do cow=1 to 30;
 do treatment=1 to 3;
 do rep=1 to 2;
 y = herd/5 + cow/10 + treatment + rannor(1);
 output;
 end;
 end;
 end;
 end;
run;

proc glm data=a;
 class herd cow treatment;
 model y=herd cow(herd) treatment;
run;
```

This analysis would have required over 6 megabytes of memory for the  $X'X$  matrix had PROC GLM solved it directly. However, in the following statements, the GLM procedure needs only a  $4 \times 4$  matrix for the intercept and treatment because the other effects are absorbed.

```
proc glm data=a;
 absorb herd cow;
 class treatment;
 model y = treatment;
run;
```

These statements produce the results shown in Figure 42.17.

**Figure 42.17** Absorption of Effects

| The GLM Procedure           |        |        |     |
|-----------------------------|--------|--------|-----|
| Class Level Information     |        |        |     |
| Class                       | Levels | Values |     |
| treatment                   | 3      | 1      | 2 3 |
| Number of Observations Read |        | 7200   |     |
| Number of Observations Used |        | 7200   |     |

Figure 42.17 continued

| The GLM Procedure     |          |                |             |          |        |
|-----------------------|----------|----------------|-------------|----------|--------|
| Dependent Variable: y |          |                |             |          |        |
| Source                | DF       | Sum of Squares | Mean Square | F Value  | Pr > F |
| Model                 | 1201     | 49465.40242    | 41.18685    | 41.57    | <.0001 |
| Error                 | 5998     | 5942.23647     | 0.99070     |          |        |
| Corrected Total       | 7199     | 55407.63889    |             |          |        |
|                       | R-Square | Coeff Var      | Root MSE    | y Mean   |        |
|                       | 0.892754 | 13.04236       | 0.995341    | 7.631598 |        |
| Source                | DF       | Type I SS      | Mean Square | F Value  | Pr > F |
| herd                  | 39       | 38549.18655    | 988.44068   | 997.72   | <.0001 |
| cow(herd)             | 1160     | 6320.18141     | 5.44843     | 5.50     | <.0001 |
| treatment             | 2        | 4596.03446     | 2298.01723  | 2319.58  | <.0001 |
| Source                | DF       | Type III SS    | Mean Square | F Value  | Pr > F |
| treatment             | 2        | 4596.034455    | 2298.017228 | 2319.58  | <.0001 |

## Specification of ESTIMATE Expressions

Consider the model

$$E(Y) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3$$

The corresponding `MODEL` statement for PROC GLM is

```
model y=x1 x2 x3;
```

To estimate the difference between the parameters for  $x_1$  and  $x_2$ ,

$$\beta_1 - \beta_2 = (0 \ 1 \ -1 \ 0) \boldsymbol{\beta}, \text{ where } \boldsymbol{\beta} = (\beta_0 \ \beta_1 \ \beta_2 \ \beta_3)'$$

you can use the following `ESTIMATE` statement:

```
estimate 'B1-B2' x1 1 x2 -1;
```

To predict  $y$  at  $x_1 = 1$ ,  $x_2 = 0$ , and  $x_3 = -2$ , you can estimate

$$\beta_0 + \beta_1 - 2\beta_3 = (1 \ 1 \ 0 \ -2) \boldsymbol{\beta}$$

with the following **ESTIMATE** statement:

```
estimate 'B0+B1-2B3' intercept 1 x1 1 x3 -2;
```

Now consider models involving classification variables such as

```
model y=A B A*B;
```

with the associated parameters:

$$(\mu \ \alpha_1 \ \alpha_2 \ \alpha_3 \ \beta_1 \ \beta_2 \ \gamma_{11} \ \gamma_{12} \ \gamma_{21} \ \gamma_{22} \ \gamma_{31} \ \gamma_{32})$$

The LS-mean for the first level of **A** is  $\mathbf{L}\boldsymbol{\beta}$ , where

$$\mathbf{L} = (1 \ | \ 1 \ 0 \ 0 \ | \ 0.5 \ 0.5 \ | \ 0.5 \ 0.5 \ 0 \ 0 \ 0 \ 0)$$

You can estimate this with the following **ESTIMATE** statement:

```
estimate 'LS-mean(A1)' intercept 1 A 1 B 0.5 0.5 A*B 0.5 0.5;
```

Note in this statement that only one element of  $\mathbf{L}$  is specified following the **A** effect, even though **A** has three levels. Whenever the list of constants following an effect name is shorter than the effect's number of levels, zeros are used as the remaining constants. (If the list of constants is longer than the number of levels for the effect, the extra constants are ignored, and a warning message is displayed.)

To estimate the **A** linear effect in the preceding model, assuming equally spaced levels for **A**, you can use the following  $\mathbf{L}$ :

$$\mathbf{L} = (0 \ | \ -1 \ 0 \ 1 \ | \ 0 \ 0 \ | \ -0.5 \ -0.5 \ 0 \ 0 \ 0.5 \ 0.5)$$

The **ESTIMATE** statement for this  $\mathbf{L}$  is written as

```
estimate 'A Linear' A -1 0 1;
```

If you do not specify the elements of  $\mathbf{L}$  for an effect that contains a specified effect, then the elements of the specified effect are equally distributed over the corresponding levels of the higher-order effect. In addition, if you specify the intercept in an **ESTIMATE** or **CONTRAST** statement, it is distributed over all classification effects that are not contained by any other specified effect.

The distribution of lower-order coefficients to higher-order effect coefficients follows the same general rules as in the **LSMEANS** statement, and it is similar to that used to construct Type IV tests. In the previous example, the  $-1$  associated with  $\alpha_1$  is divided by the number  $n_{1j}$  of  $\gamma_{1j}$  parameters; then each  $\gamma_{1j}$  coefficient is set to  $-1/n_{1j}$ . The  $1$  associated with  $\alpha_3$  is distributed among the  $\gamma_{3j}$  parameters in a similar fashion. In the event that an unspecified effect contains several specified effects, only that specified effect with the most factors in common with the unspecified effect is used for distribution of coefficients to the higher-order effect.

Numerous syntactical expressions for the `ESTIMATE` statement were considered, including many that involved specifying the effect and level information associated with each coefficient. For models involving higher-level effects, the requirement of specifying level information can lead to very bulky specifications. Consequently, the simpler form of the `ESTIMATE` statement described earlier was implemented.

The syntax of this `ESTIMATE` statement puts a burden on you to know a priori the order of the parameter list associated with each effect. You can use the `ORDER=` option in the `PROC GLM` statement to ensure that the levels of the classification effects are sorted appropriately.

**NOTE:** If you use the `ESTIMATE` statement with unspecified effects, use the `E` option to make sure that the actual `L` constructed by the preceding rules is the one you intended.

## A Check for Estimability

Each `L` is checked for estimability using the relationship  $\mathbf{L} = \mathbf{LH}$ , where  $\mathbf{H} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{X}$ . The `L` vector is declared nonestimable, if for any  $i$

$$\text{ABS}(\mathbf{L}_i - (\mathbf{LH})_i) > \begin{cases} \epsilon & \text{if } \mathbf{L}_i = 0 \text{ or} \\ \epsilon \times \text{ABS}(\mathbf{L}_i) & \text{otherwise} \end{cases}$$

where  $\epsilon = 10^{-4}$  by default; you can change this with the `SINGULAR=` option. Continued fractions (like  $1/3$ ) should be specified to at least six decimal places, or the `DIVISOR` parameter should be used.

## Comparing Groups

An important task in analyzing data with classification effects is to estimate the typical response for each level of a given effect; often, you also want to compare these estimates to determine which levels are equivalent in terms of the response. You can perform this task in two ways with the `GLM` procedure: with direct, arithmetic group means; and with so-called *least squares means* (LS-means).

### Means versus LS-Means

Computing and comparing arithmetic means—either simple or weighted within-group averages of the input data—is a familiar and well-studied statistical process. This is the right approach to summarizing and comparing groups for one-way and balanced designs. However, in unbalanced designs with more than one effect, the arithmetic mean for a group might not accurately reflect the “typical” response for that group, since it does not take other effects into account.

For example, the following analysis of an unbalanced two-way design produces the ANOVA, means, and LS-means shown in [Figure 42.18](#), [Figure 42.19](#), and [Figure 42.20](#).

```
data twoway;
 input Treatment Block y @@;
 datalines;
1 1 17 1 1 28 1 1 19 1 1 21 1 1 19
1 2 43 1 2 30 1 2 39 1 2 44 1 2 44
1 3 16
2 1 21 2 1 21 2 1 24 2 1 25
2 2 39 2 2 45 2 2 42 2 2 47
2 3 19 2 3 22 2 3 16
```

```

3 1 22 3 1 30 3 1 33 3 1 31
3 2 46
3 3 26 3 3 31 3 3 26 3 3 33 3 3 29 3 3 25
;

title "Unbalanced Two-way Design";
ods select ModelANOVA Means LSMeans;

proc glm data=twoway;
 class Treatment Block;
 model y = Treatment|Block;
 means Treatment;
 lsmeans Treatment;
run;

ods select all;

```

**Figure 42.18** ANOVA Results for Unbalanced Two-Way Design

| Unbalanced Two-way Design |    |             |             |         |        |
|---------------------------|----|-------------|-------------|---------|--------|
| The GLM Procedure         |    |             |             |         |        |
| Dependent Variable: y     |    |             |             |         |        |
| Source                    | DF | Type I SS   | Mean Square | F Value | Pr > F |
| Treatment                 | 2  | 8.060606    | 4.030303    | 0.24    | 0.7888 |
| Block                     | 2  | 2621.864124 | 1310.932062 | 77.95   | <.0001 |
| Treatment*Block           | 4  | 32.684361   | 8.171090    | 0.49    | 0.7460 |
| Source                    | DF | Type III SS | Mean Square | F Value | Pr > F |
| Treatment                 | 2  | 266.130682  | 133.065341  | 7.91    | 0.0023 |
| Block                     | 2  | 1883.729465 | 941.864732  | 56.00   | <.0001 |
| Treatment*Block           | 4  | 32.684361   | 8.171090    | 0.49    | 0.7460 |

**Figure 42.19** Treatment Means for Unbalanced Two-Way Design

| Unbalanced Two-way Design |    |                     |            |
|---------------------------|----|---------------------|------------|
| The GLM Procedure         |    |                     |            |
| Level of Treatment        | N  | -----y-----<br>Mean | Std Dev    |
| 1                         | 11 | 29.0909091          | 11.5104695 |
| 2                         | 11 | 29.1818182          | 11.5569735 |
| 3                         | 11 | 30.1818182          | 6.3058414  |

**Figure 42.20** Treatment LS-means for Unbalanced Two-Way Design

| Unbalanced Two-way Design |            |
|---------------------------|------------|
| The GLM Procedure         |            |
| Least Squares Means       |            |
| Treatment                 | y LSMEAN   |
| 1                         | 25.6000000 |
| 2                         | 28.3333333 |
| 3                         | 34.4444444 |

No matter how you look at them, these data exhibit a strong effect due to the blocks ( $F$  test  $p < 0.0001$ ) and no significant interaction between treatments and blocks ( $F$  test  $p > 0.7$ ). But the lack of balance affects how the treatment effect is interpreted: in a main-effects-only model, there are no significant differences between the treatment means themselves (Type I  $F$  test  $p > 0.7$ ), but there are highly significant differences between the treatment means corrected for the block effects (Type III  $F$  test  $p < 0.01$ ).

LS-means are, in effect, within-group means appropriately adjusted for the other effects in the model. More precisely, they estimate the marginal means for a balanced population (as opposed to the unbalanced design). For this reason, they are also called *estimated population marginal means* by Searle, Speed, and Milliken (1980). In the same way that the Type I  $F$  test assesses differences between the arithmetic treatment means (when the treatment effect comes first in the model), the Type III  $F$  test assesses differences between the LS-means. Accordingly, for the unbalanced two-way design, the discrepancy between the Type I and Type III tests is reflected in the arithmetic treatment means and treatment LS-means, as shown in [Figure 42.19](#) and [Figure 42.20](#). See the section “[Construction of Least Squares Means](#)” on page 3363 for more on LS-means.

Note that, while the arithmetic means are always uncorrelated (under the usual [assumptions](#) for analysis of variance; see page 3324), the LS-means might not be. This fact complicates the problem of multiple comparisons for LS-means; see the following section.

## Multiple Comparisons

When comparing more than two means, an ANOVA  $F$  test tells you whether the means are significantly different from each other, but it does not tell you which means differ from which other means. Multiple-comparison procedures (MCPs), also called *mean separation tests*, give you more detailed information about the differences among the means. The goal in multiple comparisons is to compare the average effects of three or more “treatments” (for example, drugs, groups of subjects) to decide which treatments are better, which ones are worse, and by how much, while controlling the probability of making an incorrect decision. A variety of multiple-comparison methods are available with the [MEANS](#) and [LSMEANS](#) statement in the GLM procedure.

The following classification is due to Hsu (1996). Multiple-comparison procedures can be categorized in two ways: by the comparisons they make and by the strength of inference they provide. With respect to which comparisons are made, the GLM procedure offers two types:

- comparisons between all pairs of means
- comparisons between a control and all other means



The strength of inference says what can be inferred about the structure of the means when a test is significant; it is related to what type of error rate the MCP controls. MCPs available in the GLM procedure provide one of the following types of inference, in order from weakest to strongest:

- Individual: differences between means, unadjusted for multiplicity
- Inhomogeneity: means are different
- Inequalities: which means are different
- Intervals: simultaneous confidence intervals for mean differences

Methods that control only individual error rates are not true MCPs at all. Methods that yield the strongest level of inference, simultaneous confidence intervals, are usually preferred, since they enable you not only to say which means are different but also to put confidence bounds on *how much* they differ, making it easier to assess the practical significance of a difference. They are also less likely to lead nonstatisticians to the invalid conclusion that nonsignificantly different sample means imply equal population means. Interval MCPs are available for both arithmetic means and LS-means via the **MEANS** and **LSMEANS** statements, respectively.<sup>1</sup>

Table 42.12 and Table 42.13 display MCPs available in PROC GLM for all pairwise comparisons and comparisons with a control, respectively, along with associated strength of inference and the syntax (when applicable) for both the **MEANS** and the **LSMEANS** statements.

**Table 42.12** Multiple-Comparison Procedures for All Pairwise Comparisons

| Method               | Strength of Inference | Syntax  |                       |
|----------------------|-----------------------|---------|-----------------------|
|                      |                       | MEANS   | LSMEANS               |
| Student's <i>t</i>   | Individual            | T       | PDIFF ADJUST=T        |
| Duncan               | Individual            | DUNCAN  |                       |
| Student-Newman-Keuls | Inhomogeneity         | SNK     |                       |
| REGWQ                | Inequalities          | REGWQ   |                       |
| Tukey-Kramer         | Intervals             | TUKEY   | PDIFF ADJUST=TUKEY    |
| Bonferroni           | Intervals             | BON     | PDIFF ADJUST=BON      |
| Sidak                | Intervals             | SIDAK   | PDIFF ADJUST=SIDAK    |
| Scheffé              | Intervals             | SCHEFFE | PDIFF ADJUST=SCHEFFE  |
| SMM                  | Intervals             | SMM     | PDIFF ADJUST=SMM      |
| Gabriel              | Intervals             | GABRIEL |                       |
| Simulation           | Intervals             |         | PDIFF ADJUST=SIMULATE |

<sup>1</sup>The Duncan-Waller method does not fit into the preceding scheme, since it is based on the Bayes risk rather than any particular error rate.

**Table 42.13** Multiple-Comparison Procedures for Comparisons with a Control

| Method             | Strength of Inference | Syntax  |                               |
|--------------------|-----------------------|---------|-------------------------------|
|                    |                       | MEANS   | LSMEANS                       |
| Student's <i>t</i> | Individual            |         | PDIFF=CONTROL ADJUST=T        |
| Dunnett            | Intervals             | DUNNETT | PDIFF=CONTROL ADJUST=DUNNETT  |
| Bonferroni         | Intervals             |         | PDIFF=CONTROL ADJUST=BON      |
| Sidak              | Intervals             |         | PDIFF=CONTROL ADJUST=SIDAK    |
| Scheffé            | Intervals             |         | PDIFF=CONTROL ADJUST=SCHEFFE  |
| SMM                | Intervals             |         | PDIFF=CONTROL ADJUST=SMM      |
| Simulation         | Intervals             |         | PDIFF=CONTROL ADJUST=SIMULATE |

**NOTE:** One-sided Dunnett's tests are also available from the **MEANS** statement with the **DUNNETTL** and **DUNNETTU** options and from the **LSMEANS** statement with **PDIFF=CONTROLL** and **PDIFF=CONTROLU**.

A note concerning the ODS tables for the results of the **PDIFF** or **TDIFF** options in the **LSMEANS** statement: The *p/t*-values for differences are displayed in columns of the LSMeans table for **PDIFF/TDIFF=CONTROL** or **PDIFF/TDIFF=ANOM**, and for **PDIFF/TDIFF=ALL** when there are only two LS-means. Otherwise (for **PDIFF/TDIFF=ALL** when there are more than two LS-means), the *p/t*-values for differences are displayed in a separate table called Diff.

Details of these multiple comparison methods are given in the following sections.

### Pairwise Comparisons

All the methods discussed in this section depend on the standardized pairwise differences  $t_{ij} = (\bar{y}_i - \bar{y}_j)/\hat{\sigma}_{ij}$ , where the parts of this expression are defined as follows:

- *i* and *j* are the indices of two groups
- $\bar{y}_i$  and  $\bar{y}_j$  are the means or LS-means for groups *i* and *j*
- $\hat{\sigma}_{ij}$  is the square root of the estimated variance of  $\bar{y}_i - \bar{y}_j$ . For simple arithmetic means,  $\hat{\sigma}_{ij}^2 = s^2(1/n_i + 1/n_j)$ , where  $n_i$  and  $n_j$  are the sizes of groups *i* and *j*, respectively, and  $s^2$  is the mean square for error, with  $\nu$  degrees of freedom. For weighted arithmetic means,  $\hat{\sigma}_{ij}^2 = s^2(1/w_i + 1/w_j)$ , where  $w_i$  and  $w_j$  are the sums of the weights in groups *i* and *j*, respectively. Finally, for LS-means defined by the linear combinations  $\mathbf{l}'_i \mathbf{b}$  and  $\mathbf{l}'_j \mathbf{b}$  of the parameter estimates,  $\hat{\sigma}_{ij}^2 = s^2 \mathbf{l}'_i (\mathbf{X}'\mathbf{X})^{-1} \mathbf{l}_j$ .

Furthermore, all of the methods are discussed in terms of significance tests of the form

$$|t_{ij}| \geq c(\alpha)$$

where  $c(\alpha)$  is some constant depending on the significance level. Such tests can be inverted to form confidence intervals of the form

$$(\bar{y}_i - \bar{y}_j) - \hat{\sigma}_{ij}c(\alpha) \leq \mu_i - \mu_j \leq (\bar{y}_i - \bar{y}_j) + \hat{\sigma}_{ij}c(\alpha)$$

The simplest approach to multiple comparisons is to do a  $t$  test on every pair of means (the **T** option in the **MEANS** statement, **ADJUST=T** in the **LSMEANS** statement). For the  $i$ th and  $j$ th means, you can reject the null hypothesis that the population means are equal if

$$|t_{ij}| \geq t(\alpha; \nu)$$

where  $\alpha$  is the significance level,  $\nu$  is the number of error degrees of freedom, and  $t(\alpha; \nu)$  is the two-tailed critical value from a Student's  $t$  distribution. If the cell sizes are all equal to, say,  $n$ , the preceding formula can be rearranged to give

$$|\bar{y}_i - \bar{y}_j| \geq t(\alpha; \nu)s\sqrt{\frac{2}{n}}$$

the value of the right-hand side being Fisher's least significant difference (LSD).

There is a problem with repeated  $t$  tests, however. Suppose there are 10 means and each  $t$  test is performed at the 0.05 level. There are  $10(10 - 1)/2 = 45$  pairs of means to compare, each with a 0.05 probability of a type 1 error (a false rejection of the null hypothesis). The chance of making at least one type 1 error is much higher than 0.05. It is difficult to calculate the exact probability, but you can derive a pessimistic approximation by assuming that the comparisons are independent, giving an upper bound to the probability of making at least one type 1 error (the experimentwise error rate) of

$$1 - (1 - 0.05)^{45} = 0.90$$

The actual probability is somewhat less than 0.90, but as the number of means increases, the chance of making at least one type 1 error approaches 1.

If you decide to control the individual type 1 error rates for each comparison, you are controlling the individual or comparisonwise error rate. On the other hand, if you want to control the overall type 1 error rate for all the comparisons, you are controlling the experimentwise error rate. It is up to you to decide whether to control the comparisonwise error rate or the experimentwise error rate, but there are many situations in which the experimentwise error rate should be held to a small value. Statistical methods for comparing three or more means while controlling the probability of making at least one type 1 error are called *multiple-comparison procedures*.

It has been suggested that the experimentwise error rate can be held to the  $\alpha$  level by performing the overall ANOVA  $F$  test at the  $\alpha$  level and making further comparisons only if the  $F$  test is significant, as in Fisher's protected LSD. This assertion is false if there are more than three means (Einot and Gabriel 1975). Consider again the situation with 10 means. Suppose that one population mean differs from the others by such a sufficiently large amount that the power (probability of correctly rejecting the null hypothesis) of the  $F$  test is near 1 but that all the other population means are equal to each other. There will be  $9(9 - 1)/2 = 36$   $t$  tests of true null hypotheses, with an upper limit of 0.84 on the probability of at least one type 1 error. Thus, you must distinguish between the experimentwise error rate under the complete null hypothesis, in which all population means are equal, and the experimentwise error rate under a partial null hypothesis, in which some means are equal but others differ. The following abbreviations are used in the discussion:

CER      comparisonwise error rate

EERC     experimentwise error rate under the complete null hypothesis

MEER maximum experimentwise error rate under any complete or partial null hypothesis

These error rates are associated with the different **strengths of inference** discussed on page 3350: individual tests control the CER; tests for inhomogeneity of means control the EERC; tests that yield confidence inequalities or confidence intervals control the MEER. A preliminary  $F$  test controls the EERC but not the MEER.

You can control the MEER at the  $\alpha$  level by setting the CER to a sufficiently small value. The Bonferroni inequality (Miller 1981) has been widely used for this purpose. If

$$\text{CER} = \frac{\alpha}{c}$$

where  $c$  is the total number of comparisons, then the MEER is less than  $\alpha$ . Bonferroni  $t$  tests (the **BON** option in the **MEANS** statement, **ADJUST=BON** in the **LSMEANS** statement) with  $\text{MEER} < \alpha$  declare two means to be significantly different if

$$|t_{ij}| \geq t(\epsilon; \nu)$$

where

$$\epsilon = \frac{2\alpha}{k(k-1)}$$

for comparison of  $k$  means.

Šidák (1967) has provided a tighter bound, showing that

$$\text{CER} = 1 - (1 - \alpha)^{1/c}$$

also ensures that  $\text{MEER} \leq \alpha$  for any set of  $c$  comparisons. A Sidak  $t$  test (Games 1977), provided by the **SIDAK** option, is thus given by

$$|t_{ij}| \geq t(\epsilon; \nu)$$

where

$$\epsilon = 1 - (1 - \alpha)^{\frac{2}{k(k-1)}}$$

for comparison of  $k$  means.

You can use the Bonferroni additive inequality and the Sidak multiplicative inequality to control the MEER for any set of contrasts or other hypothesis tests, not just pairwise comparisons. The Bonferroni inequality can provide simultaneous inferences in any statistical application requiring tests of more than one hypothesis. Other methods discussed in this section for pairwise comparisons can also be adapted for general contrasts (Miller 1981).

Scheffé (1953, 1959) proposes another method to control the MEER for any set of contrasts or other linear hypotheses in the analysis of linear models, including pairwise comparisons, obtained with the SCHEFFE option. Two means are declared significantly different if

$$|t_{ij}| \geq \sqrt{\text{DF} \cdot F(\alpha; \text{DF}, \nu)}$$

where  $F(\alpha; \text{DF}, \nu)$  is the  $\alpha$ -level critical value of an  $F$  distribution with DF numerator degrees of freedom and  $\nu$  denominator degrees of freedom. The value of DF is  $k - 1$  for the MEANS statement, but in other statements the precise definition depends on context. For the LSMEANS statement, DF is the rank of the contrast matrix  $\mathbf{L}$  for LS-means differences. In more general contexts—for example, the ESTIMATE or LSMESTIMATE statements in PROC GLIMMIX—DF is the rank of the contrast covariance matrix  $\mathbf{L}\text{Cov}(\mathbf{b})\mathbf{L}'$ .

Scheffé's test is compatible with the overall ANOVA  $F$  test in that Scheffé's method never declares a contrast significant if the overall  $F$  test is nonsignificant. Most other multiple-comparison methods can find significant contrasts when the overall  $F$  test is nonsignificant and, therefore, suffer a loss of power when used with a preliminary  $F$  test.

Scheffé's method might be more powerful than the Bonferroni or Sidak method if the number of comparisons is large relative to the number of means. For pairwise comparisons, Sidak  $t$  tests are generally more powerful.

Tukey (1952, 1953) proposes a test designed specifically for pairwise comparisons based on the studentized range, sometimes called the "honestly significant difference test," that controls the MEER when the sample sizes are equal. Tukey (1953) and Kramer (1956) independently propose a modification for unequal cell sizes. The Tukey or Tukey-Kramer method is provided by the TUKEY option in the MEANS statement and the ADJUST=TUKEY option in the LSMEANS statement. This method has fared extremely well in Monte Carlo studies (Dunnett 1980). In addition, Hayter (1984) gives a proof that the Tukey-Kramer procedure controls the MEER for means comparisons, and Hayter (1989) describes the extent to which the Tukey-Kramer procedure has been proven to control the MEER for LS-means comparisons. The Tukey-Kramer method is more powerful than the Bonferroni, Sidak, or Scheffé method for pairwise comparisons. Two means are considered significantly different by the Tukey-Kramer criterion if

$$|t_{ij}| \geq q(\alpha; k, \nu)$$

where  $q(\alpha; k, \nu)$  is the  $\alpha$ -level critical value of a studentized range distribution of  $k$  independent normal random variables with  $\nu$  degrees of freedom.

Hochberg (1974) devised a method (the GT2 or SMM option) similar to Tukey's, but it uses the studentized maximum modulus instead of the studentized range and employs the uncorrelated  $t$  inequality of Šidák (1967). It is proven to hold the MEER at a level not exceeding  $\alpha$  with unequal sample sizes. It is generally less powerful than the Tukey-Kramer method and always less powerful than Tukey's test for equal cell sizes. Two means are declared significantly different if

$$|t_{ij}| \geq m(\alpha; c, \nu)$$

where  $m(\alpha; c, \nu)$  is the  $\alpha$ -level critical value of the studentized maximum modulus distribution of  $c$  independent normal random variables with  $\nu$  degrees of freedom and  $c = k(k - 1)/2$ .

Gabriel (1978) proposes another method (the **GABRIEL** option) based on the studentized maximum modulus. This method is applicable only to arithmetic means. It rejects if

$$\frac{|\bar{y}_i - \bar{y}_j|}{s \left( \frac{1}{\sqrt{2n_i}} + \frac{1}{\sqrt{2n_j}} \right)} \geq m(\alpha; k, \nu)$$

For equal cell sizes, Gabriel's test is equivalent to Hochberg's GT2 method. For unequal cell sizes, Gabriel's method is more powerful than GT2 but might become liberal with highly disparate cell sizes (see also Dunnett (1980)). Gabriel's test is the only method for unequal sample sizes that lends itself to a graphical representation as intervals around the means. Assuming  $\bar{y}_i > \bar{y}_j$ , you can rewrite the preceding inequality as

$$\bar{y}_i - m(\alpha; k, \nu) \frac{s}{\sqrt{2n_i}} \geq \bar{y}_j + m(\alpha; k, \nu) \frac{s}{\sqrt{2n_j}}$$

The expression on the left does not depend on  $j$ , nor does the expression on the right depend on  $i$ . Hence, you can form what Gabriel calls an  $(l, u)$ -interval around each sample mean and declare two means to be significantly different if their  $(l, u)$ -intervals do not overlap. See Hsu (1996, section 5.2.1.1) for a discussion of other methods of graphically representing all pairwise comparisons.

### **Comparing All Treatments to a Control**

One special case of means comparison is that in which the only comparisons that need to be tested are between a set of new treatments and a single control. In this case, you can achieve better power by using a method that is restricted to test only comparisons to the single control mean. Dunnett (1955) proposes a test for this situation that declares a mean significantly different from the control if

$$|t_{i0}| \geq d(\alpha; k, \nu, \rho_1, \dots, \rho_{k-1})$$

where  $\bar{y}_0$  is the control mean and  $d(\alpha; k, \nu, \rho_1, \dots, \rho_{k-1})$  is the critical value of the "many-to-one  $t$  statistic" (Miller 1981; Krishnaiah and Armitage 1966) for  $k$  means to be compared to a control, with  $\nu$  error degrees of freedom and correlations  $\rho_1, \dots, \rho_{k-1}$ ,  $\rho_i = n_i / (n_0 + n_i)$ . The correlation terms arise because each of the treatment means is being compared to the same control. Dunnett's test holds the MEER to a level not exceeding the stated  $\alpha$ .

### **Analysis of Means: Comparing Each Treatments to the Average**

*Analysis of means* (ANOM) refers to a technique for comparing group means and displaying the comparisons graphically so that you can easily see which ones are different. Means are judged as different if they are significantly different from the overall average, with significance adjusted for multiplicity. The overall average is computed as a weighted mean of the LS-means, the weights being inversely proportional to the variances. If you use the **PDIF=ANOM** option in the **LSMEANS** statement, the procedure will display the  $p$ -values (adjusted for multiplicity, by default) for tests of the differences between each LS-mean and the average LS-mean. The ANOM procedure in SAS/QC software displays both tables and graphics for the analysis of means with a variety of response types. For one-way designs, confidence intervals for **PDIF=ANOM** comparisons are equivalent to the results of PROC ANOM. The difference is that PROC GLM directly displays the confidence intervals for the differences, while the graphical output of PROC ANOM displays them as decision limits around the overall mean.

If the LS-means being compared are uncorrelated, exact adjusted  $p$ -values and critical values for confidence limits can be computed; see Nelson (1982, 1991, 1993) and Guirguis and Tobias (2004). For correlated LS-means, an approach similar to that of Hsu (1992) is employed, using a factor-analytic approximation of the correlation between the LS-means to derive approximate “effective sample sizes” for which exact critical values are computed. Note that computing the exact adjusted  $p$ -values and critical values for unbalanced designs can be computationally intensive. A simulation-based approach, as specified by the `ADJUST=SIM` option, while nondeterministic, might provide inferences that are accurate enough in much less time. See the section “Approximate and Simulation-Based Methods” on page 3356 for more details.

### Approximate and Simulation-Based Methods

Tukey’s, Dunnett’s, and Nelson’s tests are all based on the same general quantile calculation:

$$q^t(\alpha, \nu, R) = \{q \ni P(\max(|t_1|, \dots, |t_n|) > q) = \alpha\}$$

where the  $t_i$  have a joint multivariate  $t$  distribution with  $\nu$  degrees of freedom and correlation matrix  $R$ . In general, evaluating  $q^t(\alpha, \nu, R)$  requires repeated numerical calculation of an  $(n + 1)$ -fold integral. This is usually intractable, but the problem reduces to a feasible 2-fold integral when  $R$  has a certain symmetry in the case of Tukey’s test, and a *factor analytic structure* (Hsu 1992) in the case of Dunnett’s and Nelson’s tests. The  $R$  matrix has the required symmetry for exact computation of Tukey’s test in the following two cases:

- The  $t_i$ s are studentized differences between  $k(k - 1)/2$  pairs of  $k$  uncorrelated means with equal variances—that is, equal sample sizes.
- The  $t_i$ s are studentized differences between  $k(k - 1)/2$  pairs of  $k$  LS-means from a *variance-balanced* design (for example, a balanced incomplete block design).

See Hsu (1992, 1996) for more information. The  $R$  matrix has the factor analytic structure for exact computation of Dunnett’s and Nelson’s tests in the following two cases:

- if the  $t_i$ s are studentized differences between  $k - 1$  means and a control mean, all uncorrelated. (Dunnett’s one-sided methods depend on a similar probability calculation, without the absolute values.) Note that it is not required that the variances of the means (that is, the sample sizes) be equal.
- if the  $t_i$ s are studentized differences between  $k - 1$  LS-means and a control LS-mean from either a *variance-balanced* design, or a design in which the other factors are *orthogonal* to the treatment factor (for example, a randomized block design with proportional cell frequencies)

However, other important situations that do **not** result in a correlation matrix  $R$  that has the structure for exact computation are the following:

- all pairwise differences with unequal sample sizes
- differences between LS-means in many unbalanced designs

In these situations, exact calculation of  $q^t(\alpha, \nu, R)$  is intractable in general. Most of the preceding methods can be viewed as using various approximations for  $q^t(\alpha, \nu, R)$ . When the sample sizes are unequal, the



Tukey-Kramer test is equivalent to another approximation. For comparisons with a control when the correlation  $R$  does not have a factor analytic structure, Hsu (1992) suggests approximating  $R$  with a matrix  $R^*$  that does have such a structure and correspondingly approximating  $q^t(\alpha, \nu, R)$  with  $q^t(\alpha, \nu, R^*)$ . When you request Dunnett's or Nelson's test for LS-means (the `PDIF=CONTROL` and `ADJUST=DUNNETT` options or the `PDIF=ANOM` and `ADJUST=NELSON` options, respectively), the GLM procedure automatically uses Hsu's approximation when appropriate.

Finally, Edwards and Berry (1987) suggest calculating  $q^t(\alpha, \nu, R)$  by simulation. Multivariate  $t$  vectors are sampled from a distribution with the appropriate  $\nu$  and  $R$  parameters, and Edwards and Berry (1987) suggest estimating  $q^t(\alpha, \nu, R)$  by  $\hat{q}$ , the  $\alpha$  percentile of the observed values of  $\max(|t_1|, \dots, |t_n|)$ . Sufficient samples are generated for the true  $P(\max(|t_1|, \dots, |t_n|) > \hat{q})$  to be within a certain accuracy radius  $\gamma$  of  $\alpha$  with accuracy confidence  $100(1 - \epsilon)$ . You can approximate  $q^t(\alpha, \nu, R)$  by simulation for comparisons between LS-means by specifying `ADJUST=SIM` (with any `PDIF=` type). By default,  $\gamma = 0.005$  and  $\epsilon = 0.01$ , so that the tail area of  $\hat{q}$  is within 0.005 of  $\alpha$  with 99% confidence. You can use the `ACC=` and `EPS=` options with `ADJUST=SIM` to reset  $\gamma$  and  $\epsilon$ , or you can use the `NSAMP=` option to set the sample size directly. You can also control the random number sequence with the `SEED=` option.

Hsu and Nelson (1998) suggest a more accurate simulation method for estimating  $q^t(\alpha, \nu, R)$ , using a control variate adjustment technique. The same independent, standardized normal variates that are used to generate multivariate  $t$  vectors from a distribution with the appropriate  $\nu$  and  $R$  parameters are also used to generate multivariate  $t$  vectors from a distribution for which the exact value of  $q^t(\alpha, \nu, R)$  is known.  $\max(|t_1|, \dots, |t_n|)$  for the second sample is used as a control variate for adjusting the quantile estimate based on the first sample; see Hsu and Nelson (1998) for more details. The control variate adjustment has the drawback that it takes somewhat longer than the crude technique of Edwards and Berry (1987), but it typically yields an estimate that is many times more accurate. In most cases, if you are using `ADJUST=SIM`, then you should specify `ADJUST=SIM(CVADJUST)`. You can also specify `ADJUST=SIM(CVADJUST REPORT)` to display a summary of the simulation that includes, among other things, the actual accuracy radius  $\gamma$ , which should be substantially smaller than the target accuracy radius (0.005 by default).

### Multiple-Stage Tests

You can use all of the methods discussed so far to obtain simultaneous confidence intervals (Miller 1981). By sacrificing the facility for simultaneous estimation, you can obtain simultaneous tests with greater power by using multiple-stage tests (MSTs). MSTs come in both step-up and step-down varieties (Welsch 1977). The step-down methods, which have been more widely used, are available in SAS/STAT software.

Step-down MSTs first test the homogeneity of all the means at a level  $\gamma_k$ . If the test results in a rejection, then each subset of  $k - 1$  means is tested at level  $\gamma_{k-1}$ ; otherwise, the procedure stops. In general, if the hypothesis of homogeneity of a set of  $p$  means is rejected at the  $\gamma_p$  level, then each subset of  $p - 1$  means is tested at the  $\gamma_{p-1}$  level; otherwise, the set of  $p$  means is considered not to differ significantly and none of its subsets are tested. The many varieties of MSTs that have been proposed differ in the levels  $\gamma_p$  and the statistics on which the subset tests are based. Clearly, the EERC of a step-down MST is not greater than  $\gamma_k$ , and the CER is not greater than  $\gamma_2$ , but the MEER is a complicated function of  $\gamma_p$ ,  $p = 2, \dots, k$ .

With unequal cell sizes, PROC GLM uses the harmonic mean of the cell sizes as the common sample size. However, since the resulting operating characteristics can be undesirable, MSTs are recommended only for the balanced case. When the sample sizes are equal, using the range statistic enables you to arrange the means in ascending or descending order and test only contiguous subsets. But if you specify the  $F$  statistic, this shortcut cannot be taken. For this reason, only range-based MSTs are implemented. It is common practice to report the results of an MST by writing the means in such an order and drawing lines parallel



to the list of means spanning the homogeneous subsets. This form of presentation is also convenient for pairwise comparisons with equal cell sizes.

The best-known MSTs are the Duncan (the DUNCAN option) and Student-Newman-Keuls (the SNK option) methods (Miller 1981). Both use the studentized range statistic and, hence, are called *multiple range tests*. Duncan's method is often called the "new" multiple range test despite the fact that it is one of the oldest MSTs in current use.

The Duncan and SNK methods differ in the  $\gamma_p$  values used. For Duncan's method, they are

$$\gamma_p = 1 - (1 - \alpha)^{p-1}$$

whereas the SNK method uses

$$\gamma_p = \alpha$$

Duncan's method controls the CER at the  $\alpha$  level. Its operating characteristics appear similar to those of Fisher's unprotected LSD or repeated  $t$  tests at level  $\alpha$  (Petrinovich and Hardyck 1969). Since repeated  $t$  tests are easier to compute, easier to explain, and applicable to unequal sample sizes, Duncan's method is not recommended. Several published studies (for example, Carmer and Swanson (1973)) have claimed that Duncan's method is superior to Tukey's because of greater power without considering that the greater power of Duncan's method is due to its higher type 1 error rate (Einot and Gabriel 1975).

The SNK method holds the EERC to the  $\alpha$  level but does not control the MEER (Einot and Gabriel 1975). Consider ten population means that occur in five pairs such that means within a pair are equal, but there are large differences between pairs. If you make the usual sampling assumptions and also assume that the sample sizes are very large, all subset homogeneity hypotheses for three or more means are rejected. The SNK method then comes down to five independent tests, one for each pair, each at the  $\alpha$  level. Letting  $\alpha$  be 0.05, the probability of at least one false rejection is

$$1 - (1 - 0.05)^5 = 0.23$$

As the number of means increases, the MEER approaches 1. Therefore, the SNK method cannot be recommended.

A variety of MSTs that control the MEER have been proposed, but these methods are not as well known as those of Duncan and SNK. One approach (Ryan 1959, 1960; Einot and Gabriel 1975; Welsch 1977) sets

$$\gamma_p = \begin{cases} 1 - (1 - \alpha)^{p/k} & \text{for } p < k - 1 \\ \alpha & \text{for } p \geq k - 1 \end{cases}$$

You can use range statistics, leading to what is called the REGWQ method, after the authors' initials. If you assume that the sample means have been arranged in descending order from  $\bar{y}_1$  through  $\bar{y}_k$ , the homogeneity of means  $\bar{y}_i, \dots, \bar{y}_j, i < j$ , is rejected by REGWQ if

$$\bar{y}_i - \bar{y}_j \geq q(\gamma_p; p, \nu) \frac{s}{\sqrt{n}}$$

where  $p = j - i + 1$  and the summations are over  $u = i, \dots, j$  (Einot and Gabriel 1975). To ensure that the MEER is controlled, the current implementation checks whether  $q(\gamma_p; p, \nu)$  is monotonically increasing in  $p$ . If not, then a set of critical values that are increasing in  $p$  is substituted instead.

REGWQ appears to be the most powerful step-down MST in the current literature (for example, Ramsey 1978). Use of a preliminary  $F$  test decreases the power of all the other multiple-comparison methods discussed previously except for Scheffé's test.

### Bayesian Approach

Waller and Duncan (1969) and Duncan (1975) take an approach to multiple comparisons that differs from all the methods previously discussed in minimizing the Bayes risk under additive loss rather than controlling type 1 error rates. For each pair of population means  $\mu_i$  and  $\mu_j$ , null ( $H_0^{ij}$ ) and alternative ( $H_a^{ij}$ ) hypotheses are defined:

$$H_0^{ij}: \quad \mu_i - \mu_j \leq 0$$

$$H_a^{ij}: \quad \mu_i - \mu_j > 0$$

For any  $i, j$  pair, let  $d_0$  indicate a decision in favor of  $H_0^{ij}$  and  $d_a$  indicate a decision in favor of  $H_a^{ij}$ , and let  $\delta = \mu_i - \mu_j$ . The loss function for the decision on the  $i, j$  pair is

$$L(d_0 | \delta) = \begin{cases} 0 & \text{if } \delta \leq 0 \\ \delta & \text{if } \delta > 0 \end{cases}$$

$$L(d_a | \delta) = \begin{cases} -k\delta & \text{if } \delta \leq 0 \\ 0 & \text{if } \delta > 0 \end{cases}$$

where  $k$  represents a constant that you specify rather than the number of means. The loss for the joint decision involving all pairs of means is the sum of the losses for each individual decision. The population means are assumed to have a normal prior distribution with unknown variance, the logarithm of the variance of the means having a uniform prior distribution. For the  $i, j$  pair, the null hypothesis is rejected if

$$\bar{y}_i - \bar{y}_j \geq t_{BS} \sqrt{\frac{2}{n}}$$

where  $t_B$  is the Bayesian  $t$  value (Waller and Kemp 1976) depending on  $k$ , the  $F$  statistic for the one-way ANOVA, and the degrees of freedom for  $F$ . The value of  $t_B$  is a decreasing function of  $F$ , so the Waller-Duncan test (specified by the **WALLER** option) becomes more liberal as  $F$  increases.

### Recommendations

In summary, if you are interested in several individual comparisons and are not concerned about the effects of multiple inferences, you can use repeated  $t$  tests or Fisher's unprotected LSD. If you are interested in all pairwise comparisons or all comparisons with a control, you should use Tukey's or Dunnett's test, respectively, in order to make the strongest possible inferences. If you have weaker inferential requirements and, in particular, if you do not want confidence intervals for the mean differences, you should use the REGWQ method. Finally, if you agree with the Bayesian approach and Waller and Duncan's assumptions, you should use the Waller-Duncan test.

### Interpretation of Multiple Comparisons

When you interpret multiple comparisons, remember that failure to reject the hypothesis that two or more means are equal should not lead you to conclude that the population means are, in fact, equal. Failure to reject the null hypothesis implies only that the difference between population means, if any, is not large enough to be detected with the given sample size. A related point is that nonsignificance is nontransitive: that is, given three sample means, the largest and smallest might be significantly different from each other, while neither is significantly different from the middle one. Nontransitive results of this type occur frequently in multiple comparisons.

Multiple comparisons can also lead to counterintuitive results when the cell sizes are unequal. Consider four cells labeled A, B, C, and D, with sample means in the order  $A > B > C > D$ . If A and D each have two observations, and B and C each have 10,000 observations, then the difference between B and C might be significant, while the difference between A and D is not.

### Simple Effects

Suppose you use the following statements to fit a full factorial model to a two-way design:

```
data twoway;
 input A B Y @@;
 datalines;
 1 1 10.6 1 1 11.0 1 1 10.6 1 1 11.3
 1 2 -0.2 1 2 1.3 1 2 -0.2 1 2 0.2
 1 3 0.1 1 3 0.4 1 3 -0.4 1 3 1.0
 2 1 19.7 2 1 19.3 2 1 18.5 2 1 20.4
 2 2 -0.2 2 2 0.5 2 2 0.8 2 2 -0.4
 2 3 -0.9 2 3 -0.1 2 3 -0.2 2 3 -1.7
 3 1 29.7 3 1 29.6 3 1 29.0 3 1 30.2
 3 2 1.5 3 2 0.2 3 2 -1.5 3 2 1.3
 3 3 0.2 3 3 0.4 3 3 -0.4 3 3 -2.2
 ;

proc glm data=twoway;
 class A B;
 model Y = A B A*B;
run;
```

Partial results for the analysis of variance are shown in [Figure 42.21](#). The Type I and Type III results are the same because this is a balanced design.

**Figure 42.21** Two-Way Design with Significant Interaction

| The GLM Procedure     |    |             |             |         |        |
|-----------------------|----|-------------|-------------|---------|--------|
| Dependent Variable: Y |    |             |             |         |        |
| Source                | DF | Type I SS   | Mean Square | F Value | Pr > F |
| A                     | 2  | 219.905000  | 109.952500  | 165.11  | <.0001 |
| B                     | 2  | 3206.101667 | 1603.050833 | 2407.25 | <.0001 |
| A*B                   | 4  | 487.103333  | 121.775833  | 182.87  | <.0001 |

Figure 42.21 continued

| Source | DF | Type III SS | Mean Square | F Value | Pr > F |
|--------|----|-------------|-------------|---------|--------|
| A      | 2  | 219.905000  | 109.952500  | 165.11  | <.0001 |
| B      | 2  | 3206.101667 | 1603.050833 | 2407.25 | <.0001 |
| A*B    | 4  | 487.103333  | 121.775833  | 182.87  | <.0001 |

The interaction A\*B is significant, indicating that the effect of A depends on the level of B. In some cases, you might be interested in looking at the differences between predicted values across A for different levels of B. Winer (1971) calls this the *simple effects* of A. You can compute simple effects with the **LSMEANS** statement by specifying the **SLICE=** option. In this case, since the GLM procedure is interactive, you can compute the simple effects of A by submitting the following statements after the preceding statements.

```
lsmeans A*B / slice=B;
run;
```

The results are shown Figure 42.22. Note that A has a significant effect for B=1 but not for B=2 and B=3.

Figure 42.22 Interaction LS-Means and Simple Effects

| The GLM Procedure |   |            | Least Squares Means |  |  |
|-------------------|---|------------|---------------------|--|--|
| A                 | B | Y LSMEAN   |                     |  |  |
| 1                 | 1 | 10.8750000 |                     |  |  |
| 1                 | 2 | 0.2750000  |                     |  |  |
| 1                 | 3 | 0.2750000  |                     |  |  |
| 2                 | 1 | 19.4750000 |                     |  |  |
| 2                 | 2 | 0.1750000  |                     |  |  |
| 2                 | 3 | -0.7250000 |                     |  |  |
| 3                 | 1 | 29.6250000 |                     |  |  |
| 3                 | 2 | 0.3750000  |                     |  |  |
| 3                 | 3 | -0.5000000 |                     |  |  |

| The GLM Procedure            |    |                | Least Squares Means |         |        |
|------------------------------|----|----------------|---------------------|---------|--------|
| A*B Effect Sliced by B for Y |    |                |                     |         |        |
| B                            | DF | Sum of Squares | Mean Square         | F Value | Pr > F |
| 1                            | 2  | 704.726667     | 352.363333          | 529.13  | <.0001 |
| 2                            | 2  | 0.080000       | 0.040000            | 0.06    | 0.9418 |
| 3                            | 2  | 2.201667       | 1.100833            | 1.65    | 0.2103 |

## Homogeneity of Variance in One-Way Models

One of the usual *assumptions* in using the GLM procedure is that the underlying errors are all uncorrelated with homogeneous variances (see page 3324). You can test this assumption in PROC GLM by using the **HOVTEST** option in the **MEANS** statement, requesting a *homogeneity of variance* test. This section discusses the computational details behind these tests. Note that the GLM procedure allows homogeneity of variance testing for simple one-way models only. Homogeneity of variance testing for more complex models is a subject of current research.

Bartlett (1937) proposes a test for equal variances that is a modification of the normal-theory likelihood ratio test (the **HOVTEST=BARTLETT** option). While Bartlett's test has accurate Type I error rates and optimal power when the underlying distribution of the data is normal, it can be very inaccurate if that distribution is even slightly nonnormal (Box 1953). Therefore, Bartlett's test is not recommended for routine use.

An approach that leads to tests that are much more robust to the underlying distribution is to transform the original values of the dependent variable to derive a *dispersion variable* and then to perform analysis of variance on this variable. The significance level for the test of homogeneity of variance is the *p*-value for the ANOVA *F* test on the dispersion variable. All of the homogeneity of variance tests available in PROC GLM except Bartlett's use this approach.

Levene's test (Levene 1960) is widely considered to be the standard homogeneity of variance test (the **HOVTEST=LEVENE** option). Levene's test is of the dispersion-variable-ANOVA form discussed previously, where the dispersion variable is either of the following:

$$\begin{aligned} z_{ij}^2 &= (y_{ij} - \bar{y}_i)^2 && \text{(TYPE=SQUARE, the default)} \\ z_{ij} &= |y_{ij} - \bar{y}_i| && \text{(TYPE=ABS)} \end{aligned}$$

O'Brien (1979) proposes a test (**HOVTEST=OBRIEN**) that is basically a modification of Levene's  $z_{ij}^2$ , using the dispersion variable

$$z_{ij}^W = \frac{(W + n_i - 2)n_i(y_{ij} - \bar{y}_i)^2 - W(n_i - 1)\sigma_i^2}{(n_i - 1)(n_i - 2)}$$

where  $n_i$  is the size of the *i*th group and  $\sigma_i^2$  is its sample variance. You can use the **W=** option in parentheses to tune O'Brien's  $z_{ij}^W$  dispersion variable to match the suspected kurtosis of the underlying distribution. The choice of the value of the **W=** option is rarely critical. By default, **W=0.5**, as suggested by O'Brien (1979, 1981).

Finally, Brown and Forsythe (1974) suggest using the absolute deviations from the group *medians*:

$$z_{ij}^{\text{BF}} = |y_{ij} - m_i|$$

where  $m_i$  is the median of the *i*th group. You can use the **HOVTEST=BF** option to specify this test.

Simulation results (Conover, Johnson, and Johnson 1981; Olejnik and Algina 1987) show that, while all of these ANOVA-based tests are reasonably robust to the underlying distribution, the Brown-Forsythe test seems best at providing power to detect variance differences while protecting the Type I error probability. However, since the within-group medians are required for the Brown-Forsythe test, it can be resource intensive if there are very many groups or if some groups are very large.

If one of these tests rejects the assumption of homogeneity of variance, you should use Welch's ANOVA instead of the usual ANOVA to test for differences between group means. However, this conclusion holds only if you use one of the robust homogeneity of variance tests (that is, not for `HOVTEST=BARTLETT`); even then, any homogeneity of variance test has too little power to be relied upon to always detect when Welch's ANOVA is appropriate. Unless the group variances are extremely different or the number of groups is large, the usual ANOVA test is relatively robust when the groups are all about the same size. As Box (1953) notes, "To make the preliminary test on variances is rather like putting to sea in a rowing boat to find out whether conditions are sufficiently calm for an ocean liner to leave port!"

Example 42.10 illustrates the use of the `HOVTEST` and `WELCH` options in the `MEANS` statement in testing for equal group variances and adjusting for unequal group variances in a one-way ANOVA.

### Weighted Means

If you specify a `WEIGHT` statement and one or more of the multiple comparisons options, the variance of the difference between weighted group means for group  $i$  and  $j$  is computed as

$$\text{MSE} \times \left( \frac{1}{w_i} + \frac{1}{w_j} \right)$$

where  $w_i$  is the sum of the weights for the observations in group  $i$ .

### Construction of Least Squares Means

To construct a least squares mean (LS-mean) for a given level of a given effect, construct a row vector  $\mathbf{L}$  according to the following rules and use it in an `ESTIMATE` statement to compute the value of the LS-mean:

1. Set all  $L_i$  corresponding to covariates (continuous variables) to their mean value.
2. Consider effects contained by the given effect. Set the  $L_i$  corresponding to levels associated with the given level equal to 1. Set all other  $L_i$  in these effects equal to 0. (See Chapter 15, "The Four Types of Estimable Functions," for a definition of *containing*.)
3. Consider the given effect. Set the  $L_i$  corresponding to the given level equal to 1. Set the  $L_i$  corresponding to other levels equal to 0.
4. Consider the effects that contain the given effect. If these effects are not nested within the given effect, then set the  $L_i$  corresponding to the given level to  $1/k$ , where  $k$  is the number of such columns. If these effects are nested within the given effect, then set the  $L_i$  corresponding to the given level to  $1/(k_1 k_2)$ , where  $k_1$  is the number of nested levels within this combination of nested effects, and  $k_2$  is the number of such combinations. For  $L_i$  corresponding to other levels, use 0.
5. Consider the other effects not yet considered. If there are no nested factors, then set all  $L_i$  corresponding to this effect to  $1/j$ , where  $j$  is the number of levels in the effect. If there are nested factors, then set all  $L_i$  corresponding to this effect to  $1/(j_1 j_2)$ , where  $j_1$  is the number of nested levels within a given combination of nested effects and  $j_2$  is the number of such combinations.

The consequence of these rules is that the sum of the Xs within any classification effect is 1. This set of Xs forms a linear combination of the parameters that is checked for estimability before it is evaluated.

For example, consider the following model:

```
proc glm;
 class A B C;
 model Y=A B A*B C Z;
 lsmeans A B A*B C;
run;
```

Assume A has 3 levels, B has 2 levels, and C has 2 levels, and assume that every combination of levels of A and B exists in the data. Assume also that Z is a continuous variable with an average of 12.5. Then the least squares means are computed by the following linear combinations of the parameter estimates:

|           | $\mu$ | A   |     |     | B   |     | A*B |     |     |     |     |     | C   |     | Z    |
|-----------|-------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|
|           |       | 1   | 2   | 3   | 1   | 2   | 11  | 12  | 21  | 22  | 31  | 32  | 1   | 2   |      |
| LSM( )    | 1     | 1/3 | 1/3 | 1/3 | 1/2 | 1/2 | 1/6 | 1/6 | 1/6 | 1/6 | 1/6 | 1/6 | 1/2 | 1/2 | 12.5 |
| LSM(A1)   | 1     | 1   | 0   | 0   | 1/2 | 1/2 | 1/2 | 1/2 | 0   | 0   | 0   | 0   | 1/2 | 1/2 | 12.5 |
| LSM(A2)   | 1     | 0   | 1   | 0   | 1/2 | 1/2 | 0   | 0   | 1/2 | 1/2 | 0   | 0   | 1/2 | 1/2 | 12.5 |
| LSM(A3)   | 1     | 0   | 0   | 1   | 1/2 | 1/2 | 0   | 0   | 0   | 0   | 1/2 | 1/2 | 1/2 | 1/2 | 12.5 |
| LSM(B1)   | 1     | 1/3 | 1/3 | 1/3 | 1   | 0   | 1/3 | 0   | 1/3 | 0   | 1/3 | 0   | 1/2 | 1/2 | 12.5 |
| LSM(B2)   | 1     | 1/3 | 1/3 | 1/3 | 0   | 1   | 0   | 1/3 | 0   | 1/3 | 0   | 1/3 | 1/2 | 1/2 | 12.5 |
| LSM(AB11) | 1     | 1   | 0   | 0   | 1   | 0   | 1   | 0   | 0   | 0   | 0   | 0   | 1/2 | 1/2 | 12.5 |
| LSM(AB12) | 1     | 1   | 0   | 0   | 0   | 1   | 0   | 1   | 0   | 0   | 0   | 0   | 1/2 | 1/2 | 12.5 |
| LSM(AB21) | 1     | 0   | 1   | 0   | 1   | 0   | 0   | 0   | 1   | 0   | 0   | 0   | 1/2 | 1/2 | 12.5 |
| LSM(AB22) | 1     | 0   | 1   | 0   | 0   | 1   | 0   | 0   | 0   | 1   | 0   | 0   | 1/2 | 1/2 | 12.5 |
| LSM(AB31) | 1     | 0   | 0   | 1   | 1   | 0   | 0   | 0   | 0   | 0   | 1   | 0   | 1/2 | 1/2 | 12.5 |
| LSM(AB32) | 1     | 0   | 0   | 1   | 0   | 1   | 0   | 0   | 0   | 0   | 0   | 1   | 1/2 | 1/2 | 12.5 |
| LSM(C1)   | 1     | 1/3 | 1/3 | 1/3 | 1/2 | 1/2 | 1/6 | 1/6 | 1/6 | 1/6 | 1/6 | 1/6 | 1   | 0   | 12.5 |
| LSM(C2)   | 1     | 1/3 | 1/3 | 1/3 | 1/2 | 1/2 | 1/6 | 1/6 | 1/6 | 1/6 | 1/6 | 1/6 | 0   | 1   | 12.5 |

### Setting Covariate Values

By default, all covariate effects are set equal to their mean values for computation of standard LS-means. The **AT** option in the **LSMEANS** statement enables you to set the covariates to whatever values you consider interesting.

If there is an effect containing two or more covariates, the **AT** option sets the effect equal to the product of the individual means rather than the mean of the product (as with standard LS-means calculations). The **AT MEANS** option leaves covariates equal to their mean values (as with standard LS-means) and incorporates this adjustment to crossproducts of covariates.

As an example, the following is a model with a classification variable A and two continuous variables, x1 and x2:

```
class A;
model y = A x1 x2 x1*x2;
```

The coefficients for the continuous effects with various **AT** specifications are shown in the following table.

| Syntax                                         | x1          | x2          | x1*x2                       |
|------------------------------------------------|-------------|-------------|-----------------------------|
| <code>lsmeans A;</code>                        | $\bar{x}_1$ | $\bar{x}_2$ | $\bar{x}_1\bar{x}_2$        |
| <code>lsmeans A / at means;</code>             | $\bar{x}_1$ | $\bar{x}_2$ | $\bar{x}_1 \cdot \bar{x}_2$ |
| <code>lsmeans A / at x1=1.2;</code>            | 1.2         | $\bar{x}_2$ | $1.2 \cdot \bar{x}_2$       |
| <code>lsmeans A / at (x1 x2)=(1.2 0.3);</code> | 1.2         | 0.3         | $1.2 \cdot 0.3$             |

For the first two **LSMEANS** statements, the A LS-mean coefficient for x1 is  $\bar{x}_1$  (the mean of x1) and for x2 is  $\bar{x}_2$  (the mean of x2). However, for the first **LSMEANS** statement, the coefficient for x1\*x2 is  $\bar{x}_1\bar{x}_2$ , but for the second **LSMEANS** statement the coefficient is  $\bar{x}_1 \cdot \bar{x}_2$ . The third **LSMEANS** statement sets the coefficient for x1 equal to 1.2 and leaves that for x2 at  $\bar{x}_2$ , and the final **LSMEANS** statement sets these values to 1.2 and 0.3, respectively.

Even if you specify a **WEIGHT** variable, the unweighted covariate means are used for the covariate coefficients if there is no **AT** specification. However, if you also use an **AT** specification, then weighted covariate means are used for the covariate coefficients for which no explicit **AT** values are given, or if you specify **AT MEANS**. Also, observations with missing dependent variables are included in computing the covariate means, unless these observations form a missing cell. You can use the **E** option in conjunction with the **AT** option to check that the modified LS-means coefficients are the ones you want.

The **AT** option is disabled if you specify the **BYLEVEL** option, in which case the coefficients for the covariates are set equal to their means within each level of the LS-mean effect in question.

### Changing the Weighting Scheme

The standard LS-means have equal coefficients across classification effects; however, the **OM** option in the **LSMEANS** statement changes these coefficients to be proportional to those found in the input data set. This adjustment is reasonable when you want your inferences to apply to a population that is not necessarily balanced but has the margins observed in the original data set.

In computing the observed margins, PROC GLM uses all observations for which there are no missing independent variables, including those for which there are missing dependent variables. Also, if there is a **WEIGHT** variable, PROC GLM uses weighted margins to construct the LS-means coefficients. If the analysis data set is balanced or if you specify a simple one-way model, the LS-means will be unchanged by the **OM** option.

The **BYLEVEL** option modifies the observed-margins LS-means. Instead of computing the margins across the entire data set, PROC GLM computes separate margins for each level of the LS-mean effect in question. The resulting LS-means are actually equal to raw means in this case. The **BYLEVEL** option disables the **AT** option if it is specified.

Note that the **MIXED** procedure implements a more versatile form of the **OM** option, enabling you to specifying an alternative data set over which to compute observed margins. If you use the **BYLEVEL** option, too, then this data set is effectively the “population” over which the population marginal means are computed. See Chapter 59, “The **MIXED** Procedure,” for more information.

You might want to use the **E** option in conjunction with either the **OM** or **BYLEVEL** option to check that the modified LS-means coefficients are the ones you want. It is possible that the modified LS-means are not estimable when the standard ones are, or vice versa.



**Estimability of LS-means**

LS-means are defined as certain linear combinations of the parameters. As such, it is possible for them to be inestimable. In fact, it is possible for a pair of LS-means to be both inestimable but their difference estimable. When this happens, only the entries corresponding to the estimable difference are computed and displayed in the Diffis table. If `ADJUST=SIMULATE` is specified when there are inestimable LS-means differences, adjusted results for all differences are displayed as missing.

---

**Multivariate Analysis of Variance**

If you fit several dependent variables to the same effects, you might want to make joint tests involving parameters of several dependent variables. Suppose you have  $p$  dependent variables,  $k$  parameters for each dependent variable, and  $n$  observations. The models can be collected into one equation:

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

where  $\mathbf{Y}$  is  $n \times p$ ,  $\mathbf{X}$  is  $n \times k$ ,  $\boldsymbol{\beta}$  is  $k \times p$ , and  $\boldsymbol{\epsilon}$  is  $n \times p$ . Each of the  $p$  models can be estimated and tested separately. However, you might also want to consider the joint distribution and test the  $p$  models simultaneously.

For multivariate tests, you need to make some assumptions about the errors. With  $p$  dependent variables, there are  $n \times p$  errors that are independent across observations but not across dependent variables. Assume

$$\text{vec}(\boldsymbol{\epsilon}) \sim N(\mathbf{0}, \mathbf{I}_n \otimes \boldsymbol{\Sigma})$$

where  $\text{vec}(\boldsymbol{\epsilon})$  strings  $\boldsymbol{\epsilon}$  out by rows,  $\otimes$  denotes Kronecker product multiplication, and  $\boldsymbol{\Sigma}$  is  $p \times p$ .  $\boldsymbol{\Sigma}$  can be estimated by

$$\mathbf{S} = \frac{\mathbf{e}'\mathbf{e}}{n-r} = \frac{(\mathbf{Y} - \mathbf{X}\mathbf{b})'(\mathbf{Y} - \mathbf{X}\mathbf{b})}{n-r}$$

where  $\mathbf{b} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$ ,  $r$  is the rank of the  $\mathbf{X}$  matrix, and  $\mathbf{e}$  is the matrix of residuals.

If  $\mathbf{S}$  is scaled to unit diagonals, the values in  $\mathbf{S}$  are called *partial correlations of the Ys adjusting for the Xs*. This matrix can be displayed by PROC GLM if `PRINTE` is specified as a `MANOVA` option.

The multivariate general linear hypothesis is written

$$\mathbf{L}\boldsymbol{\beta}\mathbf{M} = \mathbf{0}$$

You can form hypotheses for linear combinations across columns, as well as across rows of  $\boldsymbol{\beta}$ .

The `MANOVA` statement of the GLM procedure tests special cases where  $\mathbf{L}$  corresponds to Type I, Type II, Type III, or Type IV tests, and  $\mathbf{M}$  is the  $p \times p$  identity matrix. These tests are joint tests that the given type of hypothesis holds for all dependent variables in the model, and they are often sufficient to test all hypotheses of interest.

Finally, when these special cases are not appropriate, you can specify your own  $\mathbf{L}$  and  $\mathbf{M}$  matrices by using the `CONTRAST` statement before the `MANOVA` statement and the `M=` specification in the `MANOVA` statement, respectively. Another alternative is to use a `REPEATED` statement, which automatically generates a variety of  $\mathbf{M}$  matrices useful in repeated measures analysis of variance. See the section “`REPEATED Statement`” on page 3317 and the section “`Repeated Measures Analysis of Variance`” on page 3367 for more information.

One useful way to think of a MANOVA analysis with an  $\mathbf{M}$  matrix other than the identity is as an analysis of a set of transformed variables defined by the columns of the  $\mathbf{M}$  matrix. You should note, however, that PROC GLM always displays the  $\mathbf{M}$  matrix in such a way that the transformed variables are defined by the rows, not the columns, of the displayed  $\mathbf{M}$  matrix.

All multivariate tests carried out by the GLM procedure first construct the matrices  $\mathbf{H}$  and  $\mathbf{E}$  corresponding to the numerator and denominator, respectively, of a univariate  $F$  test:

$$\mathbf{H} = \mathbf{M}'(\mathbf{Lb})'(\mathbf{L}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{L}')^{-1}(\mathbf{Lb})\mathbf{M}$$

$$\mathbf{E} = \mathbf{M}'(\mathbf{Y}'\mathbf{Y} - \mathbf{b}'(\mathbf{X}'\mathbf{X})\mathbf{b})\mathbf{M}$$

The diagonal elements of  $\mathbf{H}$  and  $\mathbf{E}$  correspond to the hypothesis and error SS for univariate tests. When the  $\mathbf{M}$  matrix is the identity matrix (the default), these tests are for the original dependent variables on the left side of the MODEL statement. When an  $\mathbf{M}$  matrix other than the identity is specified, the tests are for transformed variables defined by the columns of the  $\mathbf{M}$  matrix. These tests can be studied by requesting the SUMMARY option, which produces univariate analyses for each original or transformed variable.

Four multivariate test statistics, all functions of the eigenvalues of  $\mathbf{E}^{-1}\mathbf{H}$  (or  $(\mathbf{E} + \mathbf{H})^{-1}\mathbf{H}$ ), are constructed:

- Wilks' lambda =  $\det(\mathbf{E})/\det(\mathbf{H} + \mathbf{E})$
- Pillai's trace =  $\text{trace}(\mathbf{H}(\mathbf{H} + \mathbf{E})^{-1})$
- Hotelling-Lawley trace =  $\text{trace}(\mathbf{E}^{-1}\mathbf{H})$
- Roy's greatest root =  $\lambda$ , largest eigenvalue of  $\mathbf{E}^{-1}\mathbf{H}$

By default, all four are reported with  $p$ -values based on  $F$  approximations, as discussed in the "Multivariate Tests" section in Chapter 4, "Introduction to Regression Procedures." Alternatively, if you specify MSTAT=EXACT in the associated MANOVA or REPEATED statement,  $p$ -values for three of the four tests are computed exactly (Wilks' lambda, the Hotelling-Lawley trace, and Roy's greatest root), and the  $p$ -values for the fourth (Pillai's trace) are based on an  $F$  approximation that is more accurate than the default. See the "Multivariate Tests" section in Chapter 4, "Introduction to Regression Procedures," for more details on the exact calculations.

---

## Repeated Measures Analysis of Variance

When several measurements are taken on the same experimental unit (person, plant, machine, and so on), the measurements tend to be correlated with each other. When the measurements represent qualitatively different things, such as weight, length, and width, this correlation is best taken into account by use of multivariate methods, such as multivariate analysis of variance. When the measurements can be thought of as responses to levels of an experimental factor of interest, such as time, treatment, or dose, the correlation can be taken into account by performing a repeated measures analysis of variance.

PROC GLM provides both univariate and multivariate tests for repeated measures for one response. For an overall reference on univariate repeated measures, see Winer (1971). The multivariate approach is covered

in Cole and Grizzle (1966). For a discussion of the relative merits of the two approaches, see LaTour and Miniard (1983).

Another approach to analysis of repeated measures is via general mixed models. This approach can handle balanced as well as unbalanced or missing within-subject data, and it offers more options for modeling the within-subject covariance. The main drawback of the mixed models approach is that it generally requires iteration and, thus, might be less computationally efficient. For further details on this approach, see Chapter 59, “The MIXED Procedure,” and Wolfinger and Chang (1995).

## Organization of Data for Repeated Measure Analysis

In order to deal efficiently with the correlation of repeated measures, the GLM procedure uses the multivariate method of specifying the model, even if only a univariate analysis is desired. In some cases, data might already be entered in the univariate mode, with each repeated measure listed as a separate observation along with a variable that represents the experimental unit (subject) on which measurement is taken. Consider the following data set Old:

```
data Old;
 input Subject Group Time y;
 datalines;
 1 1 1 15
 1 1 2 19
 1 1 3 25
 2 1 1 21
 2 1 2 18
 2 1 3 17
 1 2 1 14
 1 2 2 12
 1 2 3 16
 2 2 1 11
 2 2 2 20
 2 2 3 21
 ... more lines ...
 10 3 1 14
 10 3 2 18
 10 3 3 16
 ;
```

There are three observations for each subject, corresponding to measurements taken at times 1, 2, and 3. These data could be analyzed using the following statements:

```
proc glm data=Old;
 class Group Subject Time;
 model y=Group Subject (Group) Time Group*Time;
 test h=Group e=Subject (Group);
run;
```

However, this analysis assumes subjects' measurements are uncorrelated across time. A repeated measures analysis does not make this assumption. It uses the following data set New:

```

data New;
 input Group y1 y2 y3;
 datalines;
1 15 19 25
1 21 18 17
2 14 12 16
2 11 20 21
2 24 15 12

 ... more lines ...

3 14 18 16
;

```

In the data set `New`, the three measurements for a subject are all in one observation. For example, the measurements for subject 1 for times 1, 2, and 3 are 15, 19, and 25, respectively. For these data, the statements for a repeated measures analysis (assuming default options) are

```

proc glm data=New;
 class Group;
 model y1-y3 = Group / nouni;
 repeated Time;
run;

```

To convert the univariate form of repeated measures data to the multivariate form, you can use a program like the following:

```

proc sort data=Old;
 by Group Subject;
run;

data New(keep=y1-y3 Group);
 array yy(3) y1-y3;
 do Time = 1 to 3;
 set Old;
 by Group Subject;
 yy(Time) = y;
 if last.Subject then return;
 end;
run;

```

Alternatively, you could use PROC TRANSPOSE to achieve the same results with a program like this one:

```

proc sort data=Old;
 by Group Subject;
run;

proc transpose out=New(rename=(_1=y1 _2=y2 _3=y3));
 by Group Subject;
 id Time;
run;

```

See the discussions in *SAS Language Reference: Concepts* for more information about rearrangement of data sets.

## Hypothesis Testing in Repeated Measures Analysis

In repeated measures analysis of variance, the effects of interest are as follows:

- between-subject effects (such as GROUP in the previous example)
- within-subject effects (such as TIME in the previous example)
- interactions between the two types of effects (such as GROUP\*TIME in the previous example)

Repeated measures analyses are distinguished from MANOVA because of interest in testing hypotheses about the within-subject effects and the within-subject-by-between-subject interactions.

For tests that involve only between-subjects effects, both the multivariate and univariate approaches give rise to the same tests. These tests are provided for all effects in the **MODEL** statement, as well as for any **CONTRAST**s specified. The ANOVA table for these tests is labeled “Tests of Hypotheses for Between Subjects Effects” in the PROC GLM results. These tests are constructed by first adding together the dependent variables in the model. Then an analysis of variance is performed on the sum divided by the square root of the number of dependent variables. For example, the statements

```
model y1-y3=group;
repeated time;
```

give a one-way analysis of variance that uses  $(Y1 + Y2 + Y3)/\sqrt{3}$  as the dependent variable for performing tests of hypothesis on the between-subject effect GROUP. Tests for between-subject effects are equivalent to tests of the hypothesis  $L\beta M = 0$ , where **M** is simply a vector of 1s.

For within-subject effects and for within-subject-by-between-subject interaction effects, the univariate and multivariate approaches yield different tests. These tests are provided for the within-subject effects and for the interactions between these effects and the other effects in the **MODEL** statement, as well as for any **CONTRAST**s specified. The univariate tests are displayed in a table labeled “Univariate Tests of Hypotheses for Within Subject Effects.” Results for multivariate tests are displayed in a table labeled “Repeated Measures Analysis of Variance.”

The multivariate tests provided for within-subjects effects and interactions involving these effects are Wilks’ lambda, Pillai’s trace, Hotelling-Lawley trace, and Roy’s greatest root. For further details on these four statistics, see the “Multivariate Tests” section in Chapter 4, “Introduction to Regression Procedures.” As an example, the statements

```
model y1-y3=group;
repeated time;
```

produce multivariate tests for the within-subject effect TIME and the interaction TIME\*GROUP.

The multivariate tests for within-subject effects are produced by testing the hypothesis  $L\beta M = 0$ , where the **L** matrix is the usual matrix corresponding to the Type I, Type II, Type III, or Type IV hypotheses test, and the **M** matrix is one of several matrices depending on the transformation that you specify in the **REPEATED** statement. These multivariate tests require that the column rank of **M** be less than or equal to the number of error degrees of freedom. Besides that, the only assumption required for valid tests is that the dependent variables in the model have a multivariate normal distribution with a common covariance matrix across the between-subject effects.

The univariate tests for within-subject effects and interactions involving these effects require some assumptions for the probabilities provided by the ordinary  $F$  tests to be correct. Specifically, these tests require certain patterns of covariance matrices, known as Type H covariances (Huynh and Feldt 1970). Data with these patterns in the covariance matrices are said to satisfy the Huynh-Feldt condition. You can test this assumption (and the Huynh-Feldt condition) by applying a sphericity test (Anderson 1958) to any set of variables defined by an orthogonal contrast transformation. Such a set of variables is known as a set of orthogonal components. When you use the `PRINTE` option in the `REPEATED` statement, this sphericity test is applied both to the transformed variables defined by the `REPEATED` statement and to a set of orthogonal components if the specified transformation is not orthogonal. It is the test applied to the orthogonal components that is important in determining whether your data have a Type H covariance structure. When there are only two levels of the within-subject effect, there is only one transformed variable, and a sphericity test is not needed. The sphericity test is labeled “Test for Sphericity” in the output.

If your data satisfy the preceding assumptions, use the usual  $F$  tests to test univariate hypotheses for the within-subject effects and associated interactions.

If your data do not satisfy the assumption of Type H covariance, an adjustment to numerator and denominator degrees of freedom can be used. Several such adjustments, based on a degrees-of-freedom adjustment factor known as  $\epsilon$  (epsilon) (Box 1954), are provided in PROC GLM. All these adjustments estimate  $\epsilon$  and then multiply the numerator and denominator degrees of freedom by this estimate before determining significance levels for the  $F$  tests. Significance levels associated with the adjusted tests are labeled “Adj Pr > F” in the output. Two such adjustments are displayed. One is the maximum likelihood estimate of Box’s  $\epsilon$  factor, which is known to be conservative, possibly very much so. The other adjustment is intended to be unbiased although possibly at the cost of being liberal. The first adjustment is labeled as the “Greenhouse-Geisser Epsilon.” It has the form

$$\hat{\epsilon}_{GG} = \frac{\text{trace}^2(\mathbf{E})/b}{\text{trace}(\mathbf{E}^2)}$$

where  $\mathbf{E}$  is the error matrix for the corresponding multivariate test and  $b$  is the degrees of freedom for the hypothesis being tested.  $\hat{\epsilon}_{GG}$  was initially proposed for use in data analysis by Greenhouse and Geisser (1959). Significance levels associated with  $F$  tests thus adjusted are labeled “G-G” in the output.

Huynh and Feldt (1976) showed that  $\hat{\epsilon}_{GG}$  tends to be biased downward (that is, conservative), especially for small samples. Alternative estimates have been proposed to overcome this conservative bias, and there are several options for which estimate to display along with  $\hat{\epsilon}_{GG}$ .

- Huynh and Feldt (1976) proposed an estimate of Box’s epsilon, constructed using estimators of its numerator and denominator that are intended to be unbiased. The Huynh-Feldt epsilon has the form of a modification of the Greenhouse-Geisser epsilon,

$$\hat{\epsilon}_{HF} = \frac{nb\hat{\epsilon}_{GG} - 2}{b(\text{DFE} - b\hat{\epsilon}_{GG})}$$

where  $n$  is the number of subjects and DFE is the degrees of freedom for error. The numerator of this estimate is precisely unbiased only when there are no between-subject effects, but  $\hat{\epsilon}_{HF}$  is still often employed even with nontrivial between-subject models; it was the only unbiased epsilon alternative in SAS/STAT releases before SAS/STAT 9.22. The Huynh-Feldt epsilon is no longer the default, but you can request it and its corresponding  $F$  test by using the `UEPSDEF=HF` option in the

**REPEATED** statement. The estimate is labeled “Huynh-Feldt Epsilon” in the PROC GLM output, and the significance levels associated with adjusted  $F$  tests are labeled “H-F.”

- Lecoutre (1991) gave the unbiased form of the numerator of Box’s epsilon when there is one between-subject effect. The correct form of Huynh and Feldt’s idea in this case is

$$\hat{\epsilon}_{\text{HFL}} = \frac{(\text{DFE} + 1)b\hat{\epsilon}_{\text{GG}} - 2}{b(\text{DFE} - b\hat{\epsilon}_{\text{GG}})}$$

More recently, Gribbin (2007) showed that  $\hat{\epsilon}_{\text{HFL}}$  applies to general between-subject models, and Chi et al. (2012) showed that it extends even to situations where the number of error degrees of freedom is less than the column rank of the within-subject contrast matrix. Thus, the Lecoutre correction of the Huynh-Feldt epsilon is displayed by default along with the Greenhouse-Geisser epsilon; you can also explicitly request it by using the **UEPSDEF=HFL** option in the **REPEATED** statement. The estimate is labeled “Huynh-Feldt-Lecoutre Epsilon” in the PROC GLM output, and the significance levels associated with adjusted  $F$  tests are labeled “H-F-L.”

- Finally, Chi et al. (2012) suggest that Box’s epsilon might be better estimated by replacing the reciprocal of an unbiased form of the denominator with an approximately unbiased form of the reciprocal itself. The resulting estimator can be written as a multiple of the corrected Huynh-Feldt epsilon  $\hat{\epsilon}_{\text{HFL}}$ ,

$$\hat{\epsilon}_{\text{CM}} = \hat{\epsilon}_{\text{HFL}}(v_a - 2)(v_a - 4)/v_a^2$$

where  $v_a = (\text{DFE} - 1) + \text{DFE}(\text{DFE} - 1)/2$ . Simulations indicate that  $\hat{\epsilon}_{\text{CM}}$  does a good job of providing accurate  $p$ -values without being either too conservative or too liberal. Over a wide range of cases, it is never much worse than any other alternative epsilon and often much better. You can request that the Chi-Muller epsilon estimate and its corresponding  $F$  test be displayed by using the **UEPSDEF=CM** option in the **REPEATED** statement. The estimate is labeled “Chi-Muller Epsilon” in the PROC GLM output, and the significance levels associated with adjusted  $F$  tests are labeled “C-M.”

Although  $\epsilon$  must be in the range of 0 to 1, the three approximately unbiased estimators can be outside this range. When any of these estimators is greater than 1, a value of 1 is used in all calculations for probabilities—in other words, the probabilities are not adjusted. Additionally, if  $\hat{\epsilon}_{\text{CM}} < 1/b$ , then the degrees of freedom are adjusted by  $1/b$  instead of  $\hat{\epsilon}_{\text{CM}}$ .

In summary, if your data do not meet the assumptions, use adjusted  $F$  tests. However, when you strongly suspect that your data might not have Type H covariance, all these univariate tests should be interpreted cautiously. In such cases, you should consider using the multivariate tests instead.

The univariate sums of squares for hypotheses involving within-subject effects can be easily calculated from the **H** and **E** matrices corresponding to the multivariate tests described in the section “**Multivariate Analysis of Variance**” on page 3366. If the **M** matrix is orthogonal, the univariate sums of squares is calculated as the trace (sum of diagonal elements) of the appropriate **H** matrix; if it is not orthogonal, PROC GLM calculates the trace of the **H** matrix that results from an orthogonal **M** matrix transformation. The appropriate error term for the univariate  $F$  tests is constructed in a similar way from the error SSCP matrix and is labeled **Error(factorname)**, where *factorname* indicates the **M** matrix that is used in the transformation.

When the design specifies more than one repeated measures factor, PROC GLM computes the **M** matrix for a given effect as the direct (Kronecker) product of the **M** matrices defined by the **REPEATED** statement if

the factor is involved in the effect or as a vector of 1s if the factor is not involved. The test for the main effect of a repeated measures factor is constructed using an **L** matrix that corresponds to a test that the mean of the observation is zero. Thus, the main effect test for repeated measures is a test that the means of the variables defined by the **M** matrix are all equal to zero, while interactions involving repeated measures effects are tests that the between-subjects factors involved in the interaction have no effect on the means of the transformed variables defined by the **M** matrix. In addition, you can specify other **L** matrices to test hypotheses of interest by using the **CONTRAST** statement, since hypotheses defined by **CONTRAST** statements are also tested in the **REPEATED** analysis. To see which combinations of the original variables the transformed variables represent, you can specify the **PRINTM** option in the **REPEATED** statement. This option displays the transpose of **M**, which is labeled as **M** in the PROC GLM results. The tests produced are the same for any choice of transformation (**M**) matrix specified in the **REPEATED** statement; however, depending on the nature of the repeated measurements being studied, a particular choice of transformation matrix, coupled with the **CANONICAL** or **SUMMARY** option, can provide additional insight into the data being studied.

## Transformations Used in Repeated Measures Analysis of Variance

As mentioned in the specifications of the **REPEATED** statement, several different **M** matrices can be generated automatically, based on the transformation that you specify in the **REPEATED** statement. Remember that both the univariate and multivariate tests that PROC GLM performs are unaffected by the choice of transformation; the choice of transformation is important only when you are trying to study the nature of a repeated measures effect, particularly with the **CANONICAL** and **SUMMARY** options. If one of these matrices does not meet your needs for a particular analysis, you might want to use the **M=** option in the **MANOVA** statement to perform the tests of interest.

The following sections describe the transformations available in the **REPEATED** statement, provide an example of the **M** matrix that is produced, and give guidelines for the use of the transformation. As in the PROC GLM output, the displayed matrix is labeled **M**. This is the **M'** matrix.

### **CONTRAST Transformation**

This is the default transformation used by the **REPEATED** statement. It is useful when one level of the repeated measures effect can be thought of as a control level against which the others are compared. For example, if five drugs are administered to each of several animals and the first drug is a control or placebo, the statements

```
proc glm;
 model d1-d5= / nouni;
 repeated drug 5 contrast(1) / summary printm;
run;
```

produce the following **M** matrix:

$$M = \begin{bmatrix} -1 & 1 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 0 & 1 \end{bmatrix}$$

When you examine the analysis of variance tables produced by the **SUMMARY** option, you can tell which of the drugs differed significantly from the placebo.



**POLYNOMIAL Transformation**

This transformation is useful when the levels of the repeated measure represent quantitative values of a treatment, such as dose or time. If the levels are unequally spaced, *level values* can be specified in parentheses after the number of levels in the **REPEATED** statement. For example, if five levels of a drug corresponding to 1, 2, 5, 10, and 20 milligrams are administered to different treatment groups, represented by the variable *group*, the statements

```
proc glm;
 class group;
 model r1-r5=group / noint;
 repeated dose 5 (1 2 5 10 20) polynomial / summary printm;
run;
```

produce the following **M** matrix:

$$M = \begin{bmatrix} -0.4250 & -0.3606 & -0.1674 & 0.1545 & 0.7984 \\ 0.4349 & 0.2073 & -0.3252 & -0.7116 & 0.3946 \\ -0.4331 & 0.1366 & 0.7253 & -0.5108 & 0.0821 \\ 0.4926 & -0.7800 & 0.3743 & -0.0936 & 0.0066 \end{bmatrix}$$

The **SUMMARY** option in this example provides univariate ANOVAs for the variables defined by the rows of this **M** matrix. In this case, they represent the linear, quadratic, cubic, and quartic trends for dose and are labeled *dose\_1*, *dose\_2*, *dose\_3*, and *dose\_4*, respectively.

**HELMERT Transformation**

Since the Helmert transformation compares a level of a repeated measure to the mean of subsequent levels, it is useful when interest lies in the point at which responses cease to change. For example, if four levels of a repeated measures factor represent responses to treatments administered over time to males and females, the statements

```
proc glm;
 class sex;
 model resp1-resp4=sex / noint;
 repeated trtmnt 4 helmert / canon printm;
run;
```

produce the following **M** matrix:

$$M = \begin{bmatrix} 1 & -0.33333 & -0.33333 & -0.33333 \\ 0 & 1 & -0.50000 & -0.50000 \\ 0 & 0 & 1 & -1 \end{bmatrix}$$

**MEAN Transformation**

This transformation can be useful in the same types of situations in which the **CONTRAST** transformation is useful. If you substitute the following statement for the **REPEATED** statement shown in the **CONTRAST Transformation** section,

```
repeated drug 5 mean / printm;
```

the following M matrix is produced:

$$M = \begin{bmatrix} 1 & -0.25 & -0.25 & -0.25 & -0.25 \\ -0.25 & 1 & -0.25 & -0.25 & -0.25 \\ -0.25 & -0.25 & 1 & -0.25 & -0.25 \\ -0.25 & -0.25 & -0.25 & 1 & -0.25 \end{bmatrix}$$

As with the **CONTRAST** transformation, if you want to omit a level other than the last, you can specify it in parentheses after the keyword **MEAN** in the **REPEATED** statement.

### **PROFILE Transformation**

When a repeated measure represents a series of factors administered over time, but a polynomial response is unreasonable, a profile transformation might prove useful. As an example, consider a training program in which four different methods are employed to teach students at several different schools. The repeated measure is the score on tests administered after each of the methods is completed. The statements

```
proc glm;
 class school;
 model t1-t4=school / nouni;
 repeated method 4 profile / summary nom printm;
run;
```

produce the following M matrix:

$$M = \begin{bmatrix} 1 & -1 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 1 & -1 \end{bmatrix}$$

To determine the point at which an improvement in test scores takes place, you can examine the analyses of variance for the transformed variables representing the differences between adjacent tests. These analyses are requested by the **SUMMARY** option in the **REPEATED** statement, and the variables are labeled **METHOD.1**, **METHOD.2**, and **METHOD.3**.

## **Random-Effects Analysis**

When some model effects are random (that is, assumed to be sampled from a normal population of effects), you can specify these effects in the **RANDOM** statement in order to compute the expected values of mean squares for various model effects and contrasts and, optionally, to perform random-effects analysis of variance tests.

### **PROC GLM versus PROC MIXED for Random-Effects Analysis**

Other SAS procedures that can be used to analyze models with random effects include the **MIXED** and **VARCOMP** procedures. Note that, for these procedures, the random-effects specification is an integral part of the model, affecting how both random and fixed effects are fit; for **PROC GLM**, the random effects are treated in a *post hoc* fashion after the complete fixed-effect model is fit. This distinction affects other

features in the GLM procedure, such as the results of the **LSMEANS** and **ESTIMATE** statements. These features assume that all effects are fixed, so that all tests and estimability checks for these statements are based on a fixed-effects model, even when you use a **RANDOM** statement. Standard errors for estimates and LS-means based on the fixed-effects model might be significantly smaller than those based on a true random-effects model; in fact, some functions that are estimable under a true random-effects model might not even be estimable under the fixed-effects model. Therefore, you should use the **MIXED** procedure to compute tests involving these features that take the random effects into account; see Chapter 59, “**The MIXED Procedure**,” for more information.

Note that, for balanced data, the test statistics computed when you specify the **TEST** option in the **RANDOM** statement have an exact  $F$  distribution only when the design is balanced; for unbalanced designs, the  $p$  values for the  $F$  tests are approximate. For balanced data, the values obtained by **PROC GLM** and **PROC MIXED** agree; for unbalanced data, they usually do not.

### Computation of Expected Mean Squares for Random Effects

The **RANDOM** statement in **PROC GLM** declares one or more effects in the model to be random rather than fixed. By default, **PROC GLM** displays the coefficients of the expected mean squares for all terms in the model. In addition, when you specify the **TEST** option in the **RANDOM** statement, the procedure determines what tests are appropriate and provides  $F$  ratios and probabilities for these tests.

The expected mean squares are computed as follows. Consider the model

$$Y = X_0\beta_0 + X_1\beta_1 + \cdots + X_k\beta_k + \epsilon$$

where  $\beta_0$  represents the fixed effects and  $\beta_1, \beta_2, \dots, \epsilon$  represent the random effects. Random effects are assumed to be normally and independently distributed. For any  $L$  in the row space of  $X = (X_0 | X_1 | X_2 | \cdots | X_k)$ , the expected value of the sum of squares for  $L\beta$  is

$$E(SS_L) = \beta_0' C_0' C_0 \beta_0 + SSQ(C_1)\sigma_1^2 + SSQ(C_2)\sigma_2^2 + \cdots + SSQ(C_k)\sigma_k^2 + \text{rank}(L)\sigma_\epsilon^2$$

where  $C$  is of the same dimensions as  $L$  and is partitioned as the  $X$  matrix. In other words,

$$C = (C_0 | C_1 | \cdots | C_k)$$

Furthermore,  $C = ML$ , where  $M$  is the inverse of the lower triangular Cholesky decomposition matrix of  $L(X'X)^{-1}L'$ .  $SSQ(A)$  is defined as  $\text{tr}(A'A)$ .

For the model in the following **MODEL** statement

```
model Y=A B(A) C A*C;
random B(A);
```

with  $B(A)$  declared as random, the expected mean square of each effect is displayed as

$$\text{Var}(\text{Error}) + \text{constant} \times \text{Var}(B(A)) + Q(A, C, A * C)$$

If any fixed effects appear in the expected mean square of an effect, the letter  $Q$  followed by the list of fixed effects in the expected value is displayed. The actual numeric values of the quadratic form ( $Q$  matrix) can be displayed using the **Q** option.

To determine appropriate means squares for testing the effects in the model, the **TEST** option in the **RANDOM** statement performs the following steps:

1. First, it forms a matrix of coefficients of the expected mean squares of those effects that were declared to be random.
2. Next, for each effect in the model, it determines the combination of these expected mean squares that produce an expectation that includes all the terms in the expected mean square of the effect of interest except the one corresponding to the effect of interest. For example, if the expected mean square of an effect A\*B is

$$\text{Var}(\text{Error}) + 3 \times \text{Var}(A) + \text{Var}(A * B)$$

PROC GLM determines the combination of other expected mean squares in the model that has expectation

$$\text{Var}(\text{Error}) + 3 \times \text{Var}(A)$$

3. If the preceding criterion is met by the expected mean square of a single effect in the model (as is often the case in balanced designs), the  $F$  test is formed directly. In this case, the mean square of the effect of interest is used as the numerator, the mean square of the single effect with an expected mean square that satisfies the criterion is used as the denominator, and the degrees of freedom for the test are simply the usual model degrees of freedom.
4. When more than one mean square must be combined to achieve the appropriate expectation, an approximation is employed to determine the appropriate degrees of freedom (Satterthwaite 1946). When effects other than the effect of interest are listed after the Q in the output, tests of hypotheses involving the effect of interest are not valid unless all other fixed effects involved in it are assumed to be zero. When tests such as these are performed by using the **TEST** option in the **RANDOM** statement, a note is displayed reminding you that further assumptions are necessary for the validity of these tests. Remember that although the tests are not valid unless these assumptions are made, this does not provide a basis for these assumptions to be true. The particulars of a given experiment must be examined to determine whether the assumption is reasonable.

For further theoretical discussion, see Goodnight and Speed (1978), Milliken and Johnson (1984, Chapters 22 and 23), and Hocking (1985).

### Sum-to-Zero Assumptions

The formulation and parameterization of the expected mean squares for random effects in mixed models are ongoing items of controversy in the statistical literature. Confusion arises over whether or not to assume that terms involving fixed effects sum to zero. Cornfield and Tukey (1956); Winer (1971), and others assume that they do sum to zero; Searle (1971); Hocking (1973), and others (including PROC GLM) do not.

Different assumptions about these sum-to-zero constraints can lead to different expected mean squares for certain terms, and hence to different  $F$  and  $p$  values.

For arguments in favor of not assuming that terms involving fixed effects sum to zero, see Section 9.7 of Searle (1971) and Sections 1 and 4 of McLean, Sanders, and Stroup (1991). Other references are Hartley and Searle (1969) and Searle, Casella, and McCulloch (1992).

## Computing Type I, II, and IV Expected Mean Squares

When you use the **RANDOM** statement, by default the GLM procedure produces the Type III expected mean squares for model effects and for contrasts specified before the **RANDOM** statement. In order to obtain expected values for other types of mean squares, you need to specify which types of mean squares are of interest in the **MODEL** statement. For example, in order to obtain the Type IV expected mean squares for effects in the **RANDOM** and **CONTRAST** statements, specify the **SS4** option in the **MODEL** statement. If you want both Type III and Type IV expected mean squares, specify both the **SS3** and **SS4** options in the **MODEL** statement. Since the estimable function basis is not automatically calculated for Type I and Type II SS, the **E1** (for Type I) or **E2** (for Type II) option must be specified in the **MODEL** statement in order for the **RANDOM** statement to produce the expected mean squares for the Type I or Type II sums of squares. Note that it is important to list the fixed effects first in the **MODEL** statement when requesting the Type I expected mean squares.

For example, suppose you have a two-way design with factors A and B in which the main effect for B and the interaction are random. In order to compute the Type III expected mean squares (in addition to the fixed-effect analysis), you can use the following statements:

```
proc glm;
 class A B;
 model Y = A B A*B;
 random B A*B;
run;
```

Suppose you use the **SS4** option in the **MODEL** statement, as follows:

```
proc glm;
 class A B;
 model Y = A B A*B / ss4;
 random B A*B;
run;
```

Then only the Type IV expected mean squares are computed (as well as the Type IV fixed-effect tests). For the Type I expected mean squares, you can use the following statements:

```
proc glm;
 class A B;
 model Y = A B A*B / e1;
 random B A*B;
run;
```

For each of these cases, in order to perform random-effect analysis of variance tests for each effect specified in the model, you need to specify the **TEST** option in the **RANDOM** statement, as follows:

```
proc glm;
 class A B;
 model Y = A B A*B;
 random B A*B / test;
run;
```

The GLM procedure automatically determines the appropriate error term for each test, based on the expected mean squares.

---

## Missing Values

For an analysis involving one dependent variable, PROC GLM uses an observation if values are nonmissing for that dependent variable and all the classification variables.

For an analysis involving multiple dependent variables without the [MANOVA](#) or [REPEATED](#) statement, or without the [MANOVA](#) option in the PROC GLM statement, a missing value in one dependent variable does not eliminate the observation from the analysis of other nonmissing dependent variables. On the other hand, for an analysis with the [MANOVA](#) or [REPEATED](#) statement, or with the [MANOVA](#) option in the PROC GLM statement, PROC GLM uses an observation if values are nonmissing for all dependent variables and all the variables used in independent effects.

During processing, the GLM procedure groups the dependent variables by their pattern of missing values across observations so that sums and crossproducts can be collected in the most efficient manner.

If your data have different patterns of missing values among the dependent variables, interactivity is disabled. This can occur when some of the variables in your data set have missing values and either of the following conditions obtain:

- You do not use the [MANOVA](#) option in the PROC GLM statement.
- You do not use a [MANOVA](#) or [REPEATED](#) statement before the first RUN statement.

Note that the REG procedure handles missing values differently in this case; see Chapter 79, “[The REG Procedure](#),” for more information.

---

## Computational Resources

### Memory

For large problems, most of the memory resources are required for holding the  $X'X$  matrix of the sums and crossproducts. The section “[Parameterization of PROC GLM Models](#)” on page 3327 describes how columns of the  $X$  matrix are allocated for various types of effects. For each level that occurs in the data for a combination of classification variables in a given effect, a row and a column for  $X'X$  are needed.

The following example illustrates the calculation. Suppose  $A$  has 20 levels,  $B$  has 4 levels, and  $C$  has 3 levels. Then consider the model

```
proc glm;
 class A B C;
 model Y1 Y2 Y3=A B A*B C A*C B*C A*B*C X1 X2;
run;
```

The  $X'X$  matrix (bordered by  $X'Y$  and  $Y'Y$ ) can have as many as 425 rows and columns:

|    |                        |
|----|------------------------|
| 1  | for the intercept term |
| 20 | for $A$                |
| 4  | for $B$                |

|     |                                          |
|-----|------------------------------------------|
| 80  | for A*B                                  |
| 3   | for C                                    |
| 60  | for A*C                                  |
| 12  | for B*C                                  |
| 240 | for A*B*C                                |
| 2   | for X1 and X2 (continuous variables)     |
| 3   | for Y1, Y2, and Y3 (dependent variables) |

The matrix has 425 rows and columns only if all combinations of levels occur for each effect in the model. For  $m$  rows and columns,  $8m^2$  bytes are needed for crossproducts. In this case,  $8 \cdot 425^2 = 1,445,000$  bytes, or about  $1,445,000/1024 = 1411K$ .

The required memory grows as the square of the number of columns of  $\mathbf{X}$ ; most of the memory is for the A\*B\*C interaction. Without A\*B\*C, you have 185 columns and need 268K for  $\mathbf{X}'\mathbf{X}$ . Without either A\*B\*C or A\*B, you need 86K. If A is recoded to have 10 levels, then the full model has only 220 columns and requires 378K.

The second time that a large amount of memory is needed is when Type III, Type IV, or contrast sums of squares are being calculated. This memory requirement is a function of the number of degrees of freedom of the model being analyzed and the maximum degrees of freedom for any single source. Let Rank equal the sum of the model degrees of freedom, MaxDF be the maximum number of degrees of freedom for any single source, and  $N_y$  be the number of dependent variables in the model. Then the memory requirement in bytes is 8 times

$$\begin{aligned}
 N_y \times \text{Rank} &+ (\text{Rank} \times (\text{Rank} + 1)) / 2 \\
 &+ \text{MaxDF} \times \text{Rank} \\
 &+ (\text{MaxDF} \times (\text{MaxDF} + 1)) / 2 \\
 &+ \text{MaxDF} \times N_y
 \end{aligned}$$

The first two components of this formula are for the estimable model coefficients and their variance; the rest correspond to  $\mathbf{L}$ ,  $\mathbf{L}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{L}'$ , and  $\mathbf{Lb}$  in the computation of  $\text{SS}(\mathbf{L}\boldsymbol{\beta} = 0) = (\mathbf{Lb})'(\mathbf{L}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{L}')^{-1}(\mathbf{Lb})$ . If the operating system enables SAS to run parallel computational threads on multiple CPUs, then GLM will attempt to allocate another  $8 \times \text{Rank} \times \text{Rank}$  bytes in order to perform these calculations in parallel. If this much memory is not available, then the estimability calculations are performed in a single thread.

Unfortunately, these quantities are not available when the  $\mathbf{X}'\mathbf{X}$  matrix is being constructed, so PROC GLM might occasionally request additional memory even after you have increased the memory allocation available to the program.

If you have a large model that exceeds the memory capacity of your computer, these are your options:

- Eliminate terms, especially high-level interactions.
- Reduce the number of levels for variables with many levels.
- Use the [ABSORB](#) statement for parts of the model that are large.

- Use the **REPEATED** statement for repeated measures variables.
- Use PROC ANOVA or PROC REG rather than PROC GLM, if your design allows.

A related limitation is that for any model effect involving classification variables (interactions as well as main effects), the number of levels cannot exceed 32,767. This is because GLM internally indexes effect levels with signed short (16-bit) integers, for which the maximum value is  $2^{15} - 1 = 32,767$ .

## CPU Time

Typically, if the GLM procedure requires a lot of CPU time, it will be for one of several reasons. Suppose that the input data has  $n$  rows (observations) and the model has  $E$  effects that together produce a design matrix  $X$  with  $m$  columns. Then if  $m$  or  $n$  is relatively large, the procedure might spend a lot of time in any of the following areas:

- collecting the sums of squares and crossproducts
- solving the normal equations
- computing the Type III tests

The time required for collecting sums and crossproducts is difficult to calculate because it is a complicated function of the model. The worst case occurs if all columns are continuous variables, involving  $nm^2/2$  multiplications and additions. If the columns are levels of a classification, then only  $m$  sums might be needed, but a significant amount of time might be spent in look-up operations. Solving the normal equations requires time for approximately  $m^3/2$  multiplications and additions, and the number of operations required to compute the Type III tests is also proportional to both  $E$  and  $m^3$ .

Suppose that you know that Type IV sums of squares are appropriate for the model you are analyzing (for example, if your design has no missing cells). You can specify the **SS4** option in your **MODEL** statement, which saves CPU time by requesting the Type IV sums of squares instead of the more computationally burdensome Type III sums of squares. This proves especially useful if you have a factor in your model that has many levels and is involved in several interactions.

If the operating system enables SAS to run parallel computational threads on multiple CPUs, then both the solution of the normal equations and the computation of Type III tests can take advantage of this to reduce the computational time for large models. In solving the normal equations, the fundamental row sweep operations (Goodnight 1979) are performed in parallel. In computing the Type III tests, both the orthogonalization for the estimable functions and the sums of squares calculation have been parallelized (if there is sufficient memory).

The reduction in computational time due to parallel processing depends on the size of the model, the number of processors, and the parallel architecture of the operating system. If the model is large enough that the overwhelming proportion of CPU time for the procedure is accounted for in solving the normal equations and/or computing the Type III tests, then you can expect a reduction in computational time approximately inversely proportional to the number of CPUs. However, as you increase the number of processors, the efficiency of this scaling can be reduced by several effects. One mitigating factor is a purely mathematical one known as “Amdahl’s law,” which is related to the fact that only part of the processing time for the procedure can be parallelized. Even taking Amdahl’s law into account, the parallelization efficiency can be reduced by cache effects related to how fast the multiple processors can access memory. See Cohen (2002)



for a discussion of these issues. For additional information about parallel processing in SAS, see the chapter on “Support for Parallel Processing” in *SAS Language Reference: Concepts*.

---

## Computational Method

Let  $\mathbf{X}$  represent the  $n \times p$  design matrix and  $\mathbf{Y}$  the  $n \times 1$  vector of dependent variables. (See the section “Parameterization of PROC GLM Models” on page 3327 for information about how  $\mathbf{X}$  is formed from your model specification.)

The normal equations  $\mathbf{X}'\mathbf{X}\boldsymbol{\beta} = \mathbf{X}'\mathbf{Y}$  are solved using a modified sweep routine that produces a generalized inverse  $(\mathbf{X}'\mathbf{X})^-$  and a solution  $\mathbf{b} = (\mathbf{X}'\mathbf{X})^- \mathbf{X}'\mathbf{y}$ . The modification is that rows and columns corresponding to diagonal elements that are found during sweeping to be zero (or within the expected level of numerical error of zero) are zeroed out. The  $(\mathbf{X}'\mathbf{X})^-$  produced by this procedure satisfies the following two equations:

$$\begin{aligned} (\mathbf{X}'\mathbf{X}) (\mathbf{X}'\mathbf{X})^- (\mathbf{X}'\mathbf{X}) &= (\mathbf{X}'\mathbf{X}) \\ (\mathbf{X}'\mathbf{X})^- (\mathbf{X}'\mathbf{X}) (\mathbf{X}'\mathbf{X})^- &= (\mathbf{X}'\mathbf{X})^- \end{aligned}$$

Pringle and Rayner (1971) call a generalized inverse with these characteristics a  $g_2$ -inverse, and this is the term usually used in SAS documentation and output. Urqhardt (1968) uses the term *reflexive g-inverse* to emphasize that  $(\mathbf{X}'\mathbf{X})^-$  is a generalized inverse of  $\mathbf{X}'\mathbf{X}$  in the same way that  $\mathbf{X}'\mathbf{X}$  is a generalized inverse of  $(\mathbf{X}'\mathbf{X})^-$ . Note that a  $g_2$ -inverse is not necessarily unique: if  $\mathbf{X}'\mathbf{X}$  is singular, then sweeping the matrix in a different order will result in a different  $g_2$ -inverse that also satisfies the two preceding equations.

For each effect in the model, a matrix  $\mathbf{L}$  is computed such that the rows of  $\mathbf{L}$  are estimable. Tests of the hypothesis  $\mathbf{L}\boldsymbol{\beta} = 0$  are then made by first computing

$$SS(\mathbf{L}\boldsymbol{\beta} = 0) = (\mathbf{L}\mathbf{b})'(\mathbf{L}(\mathbf{X}'\mathbf{X})^- \mathbf{L}')^{-1}(\mathbf{L}\mathbf{b})$$

and then computing the associated  $F$  value by using the mean squared error.

---

## Output Data Sets

### OUT= Data Set Created by the OUTPUT Statement

The `OUTPUT` statement produces an output data set that contains the following:

- all original data from the SAS data set input to PROC GLM
- the new variables corresponding to the diagnostic measures specified with statistics keywords in the `OUTPUT` statement (`PREDICTED=`, `RESIDUAL=`, and so on)

With multiple dependent variables, a name can be specified for any of the diagnostic measures for each of the dependent variables in the order in which they occur in the `MODEL` statement.

For example, suppose that the input data set `A` contains the variables `y1`, `y2`, `y3`, `x1`, and `x2`. Then you can use the following statements:

```
proc glm data=A;
 model y1 y2 y3=x1;
 output out=out p=y1hat y2hat y3hat
 r=y1resid lclm=y1lcl uclm=y1ucl;
run;
```

The output data set out contains y1, y2, y3, x1, x2, y1hat, y2hat, y3hat, y1resid, y1lcl, and y1ucl. The variable x2 is output even though it is not used by PROC GLM. Although predicted values are generated for all three dependent variables, residuals are output for only the first dependent variable.

When any independent variable in the analysis (including all class variables) is missing for an observation, then all new variables that correspond to diagnostic measures are missing for the observation in the output data set.

When a dependent variable in the analysis is missing for an observation, then some new variables that correspond to diagnostic measures are missing for the observation in the output data set, and some are still available. Specifically, in this case, the new variables that correspond to COOKD, COVRATIO, DFFITS, PRESS, R, RSTUDENT, STDR, and STUDENT are missing in the output data set. The variables corresponding to H, LCL, LCLM, P, STDI, STDP, UCL, and UCLM are not missing.

## OUT= Data Set Created by the LSMEANS Statement

The **OUT=** option in the **LSMEANS** statement produces an output data set that contains the following:

- the unformatted values of each classification variable specified in any effect in the **LSMEANS** statement
- a new variable, **LSMEAN**, which contains the LS-mean for the specified levels of the classification variables
- a new variable, **STDERR**, which contains the standard error of the LS-mean

The variances and covariances among the LS-means are also output when the **COV** option is specified along with the **OUT=** option. In this case, only one effect can be specified in the **LSMEANS** statement, and the following variables are included in the output data set:

- new variables, **COV1**, **COV2**, ..., **COV $n$** , where  $n$  is the number of levels of the effect specified in the **LSMEANS** statement. These variables contain the covariances of each LS-mean with every other LS-mean.
- a new variable, **NUMBER**, which provides an index for each observation to identify the covariances that correspond to that observation. The covariances for the observation with **NUMBER** equal to  $n$  can be found in the variable **COV $n$** .

## OUTSTAT= Data Set

The **OUTSTAT=** option in the PROC GLM statement produces an output data set that contains the following:

- the **BY** variables, if any

- `_TYPE_`, a new character variable. `_TYPE_` can take the values ‘SS1’, ‘SS2’, ‘SS3’, ‘SS4’, or ‘CONTRAST’, corresponding to the various types of sums of squares generated, or the values ‘CANCORR’, ‘STRUCTUR’, or ‘SCORE’, if a canonical analysis is performed through the `MANOVA` statement and no `M=` matrix is specified.
- `_SOURCE_`, a new character variable. For each observation in the data set, `_SOURCE_` contains the name of the model effect or contrast label from which the corresponding statistics are generated.
- `_NAME_`, a new character variable. For each observation in the data set, `_NAME_` contains the name of one of the dependent variables in the model or, in the case of canonical statistics, the name of one of the canonical variables (`CAN1`, `CAN2`, and so forth).
- four new numeric variables: `SS`, `DF`, `F`, and `PROB`, containing sums of squares, degrees of freedom,  $F$  values, and probabilities, respectively, for each model or contrast sum of squares generated in the analysis. For observations resulting from canonical analyses, these variables have missing values.
- if there is more than one dependent variable, then variables with the same names as the dependent variables represent the following:
  - for `_TYPE_=SS1`, `SS2`, `SS3`, `SS4`, or `CONTRAST`, the crossproducts of the hypothesis matrices
  - for `_TYPE_=CANCORR`, canonical correlations for each variable
  - for `_TYPE_=STRUCTUR`, coefficients of the total structure matrix
  - for `_TYPE_=SCORE`, raw canonical score coefficients

The output data set can be used to perform special hypothesis tests (for example, with the `IML` procedure in SAS/IML software), to reformat output, to produce canonical variates (through the `SCORE` procedure), or to rotate structure matrices (through the `FACTOR` procedure).

---

## Displayed Output

The GLM procedure produces the following output by default:

- The overall analysis-of-variance table breaks down the Total Sum of Squares for the dependent variable into the portion attributed to the Model and the portion attributed to Error.
- The Mean Square term is the Sum of Squares divided by the degrees of freedom (DF).
- The Mean Square for Error is an estimate of  $\sigma^2$ , the variance of the true errors.
- The  $F$  Value is the ratio produced by dividing the Mean Square for the Model by the Mean Square for Error. It tests how well the model as a whole (adjusted for the mean) accounts for the dependent variable’s behavior. An  $F$  test is a joint test to determine that all parameters except the intercept are zero.
- A small significance probability,  $\text{Pr} > F$ , indicates that some linear function of the parameters is significantly different from zero.

- R-Square,  $R^2$ , measures how much variation in the dependent variable can be accounted for by the model. R square, which can range from 0 to 1, is the ratio of the sum of squares for the model to the corrected total sum of squares. In general, the larger the value of R square, the better the model's fit.
- Coeff Var, the coefficient of variation, which describes the amount of variation in the population, is 100 times the standard deviation estimate of the dependent variable, Root MSE (Mean Square for Error), divided by the Mean. The coefficient of variation is often a preferred measure because it is unitless.
- Root MSE estimates the standard deviation of the dependent variable (or equivalently, the error term) and equals the square root of the Mean Square for Error.
- Mean is the sample mean of the dependent variable.

These tests are used primarily in analysis-of-variance applications:

- The Type I SS (sum of squares) measures incremental sums of squares for the model as each variable is added.
- The Type III SS is the sum of squares for a balanced test of each effect, adjusted for every other effect.

These items are used primarily in regression applications:

- The Estimates for the model Parameters (the intercept and the coefficients)
- t Value is the Student's  $t$  value for testing the null hypothesis that the parameter (if it is estimable) equals zero.
- The significance level,  $\Pr > |t|$ , is the probability of getting a larger value of  $t$  if the parameter is truly equal to zero. A very small value for this probability leads to the conclusion that the independent variable contributes significantly to the model.
- The Standard Error is the square root of the estimated variance of the estimate of the true value of the parameter.

Other portions of output are discussed in the following examples.

---

## ODS Table Names

PROC GLM assigns a name to each table it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in Table 42.14. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

**Table 42.14** ODS Tables Produced by PROC GLM

| ODS Table Name      | Description                                                                      | Statement / Option                                                                            |
|---------------------|----------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------|
| Aliasing            | Type 1,2,3,4 aliasing structure                                                  | MODEL / (E1 E2 E3 or E4) and ALIASING                                                         |
| AltErrContrasts     | ANOVA table for contrasts with alternative error                                 | CONTRAST / E=                                                                                 |
| AltErrTests         | ANOVA table for tests with alternative error                                     | TEST / E=                                                                                     |
| Bartlett            | Bartlett's homogeneity of variance test                                          | MEANS / HOVTEST=BARTLETT                                                                      |
| CLDiffs             | Multiple comparisons of pairwise differences                                     | MEANS / CLDIFF or DUNNETT or (Unequal cells and not LINES)                                    |
| CLDiffsInfo         | Information for multiple comparisons of pairwise differences                     | MEANS / CLDIFF or DUNNETT or (Unequal cells and not LINES)                                    |
| CLMeans             | Multiple comparisons of means with confidence/comparison interval                | MEANS / CLM                                                                                   |
| CLMeansInfo         | Information for multiple comparison of means with confidence/comparison interval | MEANS / CLM                                                                                   |
| CanAnalysis         | Canonical analysis                                                               | (MANOVA or REPEATED) / CANONICAL                                                              |
| CanCoef             | Canonical coefficients                                                           | (MANOVA or REPEATED) / CANONICAL                                                              |
| CanStructure        | Canonical structure                                                              | (MANOVA or REPEATED) / CANONICAL                                                              |
| CharStruct          | Characteristic roots and vectors                                                 | (MANOVA / not CANONICAL) or (REPEATED / PRINTRV)                                              |
| ClassLevels         | Classification variable levels                                                   | CLASS statement                                                                               |
| ContrastCoef        | L matrix for contrast or estimate                                                | CONTRAST / E or ESTIMATE / E                                                                  |
| Contrasts           | ANOVA table for contrasts                                                        | CONTRAST statement                                                                            |
| DependentInfo       | Simultaneously analyzed dependent variables                                      | default when there are multiple dependent variables with different patterns of missing values |
| Diff                | PDiff matrix of least squares means                                              | LSMEANS / PDIFF=ALL and more than two LS-means                                                |
| Epsilons            | Greenhouse-Geisser and Huynh-Feldt epsilons                                      | REPEATED statement                                                                            |
| ErrorSSCP           | Error SSCP matrix                                                                | (MANOVA or REPEATED) / PRINTE                                                                 |
| EstFunc             | Type 1,2,3,4 estimable functions                                                 | MODEL / (E1 E2 E3 or E4)                                                                      |
| Estimates           | Estimate statement results                                                       | ESTIMATE statement                                                                            |
| ExpectedMeanSquares | Expected mean squares                                                            | RANDOM statement                                                                              |
| FitStatistics       | R-Square, Coeff Var, Root MSE, and dependent mean                                | default                                                                                       |
| GAliasing           | General form of aliasing structure                                               | MODEL / E and ALIASING                                                                        |

Table 42.14 continued

| ODS Table Name       | Description                                             | Statement / Option                                                                                               |
|----------------------|---------------------------------------------------------|------------------------------------------------------------------------------------------------------------------|
| GEstFunc             | General form of estimable functions                     | MODEL / E                                                                                                        |
| HOVFTest             | Homogeneity of variance ANOVA                           | MEANS / HOVTEST                                                                                                  |
| HypothesisSSCP       | Hypothesis SSCP matrix                                  | (MANOVA or REPEATED) / PRINTH                                                                                    |
| InvXPX               | inv( $X'X$ ) matrix                                     | MODEL / INVERSE                                                                                                  |
| LSMeanCL             | Confidence interval for LS-means                        | LSMEANS / CL                                                                                                     |
| LSMeanCoef           | Coefficients of least squares means                     | LSMEANS / E                                                                                                      |
| LSMeanDiffCL         | Confidence interval for LS-mean differences             | LSMEANS / PDIFF and CL                                                                                           |
| LSMeans              | Least squares means                                     | LSMEANS statement                                                                                                |
| LSMLines             | Least squares means comparison lines                    | LSMEANS / PDIFF=ALL LINES                                                                                        |
| MANOVATransform      | Multivariate transformation matrix                      | MANOVA / M=                                                                                                      |
| MCLines              | Multiple comparisons <b>LINES</b> output                | MEANS / LINES or ((DUNCAN or WALLER or SNK or REGWQ) and not (CLDIFF or CLM))<br>or (Equal cells and not CLDIFF) |
| MCLinesInfo          | Information for multiple comparison <b>LINES</b> output | MEANS / LINES or ((DUNCAN or WALLER or SNK or REGWQ) and not (CLDIFF or CLM))<br>or (Equal cells and not CLDIFF) |
| MCLinesRange         | Ranges for multiple range MC tests                      | MEANS / LINES or ((DUNCAN or WALLER or SNK or REGWQ) and not (CLDIFF or CLM))<br>or (Equal cells and not CLDIFF) |
| MatrixRepresentation | <b>X</b> matrix element representation                  | as needed for other options                                                                                      |
| Means                | Group means                                             | MEANS statement                                                                                                  |
| ModelANOVA           | ANOVA for model terms                                   | default                                                                                                          |
| MultStat             | Multivariate tests                                      | MANOVA statement                                                                                                 |
| NObs                 | Number of observations                                  | default                                                                                                          |
| OverallANOVA         | Overall ANOVA                                           | default                                                                                                          |
| ParameterEstimates   | Estimated linear model coefficients                     | MODEL / SOLUTION                                                                                                 |
| PartialCorr          | Partial correlation matrix                              | (MANOVA or REPEATED) / PRINTE                                                                                    |
| PredictedInfo        | Predicted values info                                   | MODEL / P or CLM or CLI                                                                                          |
| PredictedValues      | Predicted values                                        | MODEL / P or CLM or CLI                                                                                          |
| QForm                | Quadratic form for expected mean squares                | RANDOM / Q                                                                                                       |

Table 42.14 continued

| ODS Table Name    | Description                                                    | Statement / Option                       |
|-------------------|----------------------------------------------------------------|------------------------------------------|
| RandomModelANOVA  | Random-effect tests                                            | RANDOM / TEST                            |
| RepeatedLevelInfo | Correspondence between dependents and repeated measures levels | REPEATED statement                       |
| RepeatedTransform | Repeated measures transformation matrix                        | REPEATED / PRINTM                        |
| SimDetails        | Details of difference quantile simulation                      | LSMEANS<br>/ ADJUST=SIMULATE(REPORT)     |
| SimResults        | Evaluation of difference quantile simulation                   | LSMEANS<br>/ ADJUST=SIMULATE(REPORT)     |
| SlicedANOVA       | Sliced-effect ANOVA table                                      | LSMEANS / SLICE                          |
| Sphericity Tests  | Sphericity tests<br>Summary ANOVA for specified                | REPEATED / PRINTE<br>MANOVA / H= SUMMARY |
| Tolerances        | $X'X$ tolerances                                               | MODEL / TOLERANCE                        |
| Welch             | Welch's ANOVA                                                  | MEANS / WELCH                            |
| XPX               | $X'X$ matrix                                                   | MODEL / XPX                              |

With the **PDIF** or **TDIF** option in the **LSMEANS** statement, the  $p/t$ -values for differences are displayed in columns of the LSMeans table for **PDIF/TDIF=CONTROL** or **PDIF/TDIF=ANOM**, and for **PDIF/TDIF=ALL** when there are only two LS-means. Otherwise (for **PDIF/TDIF=ALL** when there are more than two LS-means), the  $p/t$ -values for differences are displayed in a separate table called **Diff**.

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “Statistical Graphics Using ODS.”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the **ODS GRAPHICS ON** statement). For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “A Primer on ODS Statistical Graphics” on page 599 in Chapter 21, “Statistical Graphics Using ODS.”

When ODS Graphics is enabled, then for particular models the GLM procedure will produce default graphics.

- If you specify a one-way analysis of variance model, with just one **CLASS** variable, the GLM procedure will produce a grouped box plot of the response values versus the **CLASS** levels. For an example of the box plot, see the section “One-Way Layout with Means Comparisons” on page 904.
- If you specify a two-way analysis of variance model, with just two **CLASS** variables, the GLM procedure will produce an interaction plot of the response values, with horizontal position representing

one **CLASS** variable and marker style representing the other; and with predicted response values connected by lines representing the two-way analysis. For an example of the interaction plot, see the section “[PROC GLM for Unbalanced ANOVA](#)” on page 3269.

- If you specify a model with a single continuous predictor, the GLM procedure will produce a fit plot of the response values versus the covariate values, with a curve representing the fitted relationship. For an example of the fit plot, see the section “[PROC GLM for Quadratic Least Squares Regression](#)” on page 3272.
- If you specify a model with a two continuous predictors and no **CLASS** variables, the GLM procedure will produce a panel of fit plots as in the single predictor case, with a plot of the response values versus one of the covariates at each of several values of the other covariate.
- If you specify an analysis of covariance model, with one or two **CLASS** variables and one continuous variable, the GLM procedure will produce an analysis of covariance plot of the response values versus the covariate values, with lines representing the fitted relationship within each classification level. For an example of the analysis of covariance plot, see [Example 42.4](#).
- If you specify an **LSMEANS** statement with the **PDIF** option, the GLM procedure will produce a plot appropriate for the type of LS-means comparison. For **PDIF=ALL** (which is the default if you specify only **PDIF**), the procedure produces a diffogram, which displays all pairwise LS-means differences and their significance. The display is also known as a “mean-mean scatter plot” (Hsu 1996). For **PDIF=CONTROL**, the procedure produces a display of each noncontrol LS-mean compared to the control LS-mean, with two-sided confidence intervals for the comparison. For **PDIF=CONTROL** and **PDIF=CONTROLU** a similar display is produced, but with one-sided confidence intervals. Finally, for the **PDIF=ANOM** option, the procedure produces an “analysis of means” plot, comparing each LS-mean to the average LS-mean.
- If you specify a **MEANS** statement, the GLM procedure will produce a grouped box plot of the response values versus the effect for which means are being calculated.

In addition to the default graphics mentioned previously, you can request plots that help you diagnose the quality of the fitted model.

- The **PLOTS=DIAGNOSTICS** option in the **PROC GLM** statement requests that a panel of summary diagnostics for the fit be displayed. The panel displays scatter plots of residuals, absolute residuals, studentized residuals, and observed responses by predicted values; studentized residuals by leverage; Cook’s *D* by observation; a Q-Q plot of residuals; a residual histogram; and a residual-fit spread plot.
- The **PLOTS=RESIDUALS** option in the **PROC GLM** statement requests scatter plots of the residuals against each continuous covariate.

## ODS Graph Names

PROC GLM assigns a name to each graph it creates using ODS. You can use these names to reference the graphs when using ODS. The names are listed in [Table 42.15](#).

ODS Graphics must be enabled before requesting plots. For more information about ODS Graphics, see Chapter 21, “[Statistical Graphics Using ODS](#).”



**Table 42.15** Graphs Produced by PROC GLM

| ODS Graph Name      | Plot Description                                         | Option                                 |
|---------------------|----------------------------------------------------------|----------------------------------------|
| ANCOVAPlot          | Analysis of covariance plot                              | Analysis of covariance model           |
| ANOMPlot            | Plot of LS-mean differences against average LS-mean      | LSMEANS / PDIFF=ANOM                   |
| BoxPlot             | Box plot of group means                                  | One-way ANOVA model or MEANS statement |
| ContourFit          | Plot of predicted response surface                       | Two-predictor response surface model   |
| ControlPlot         | Plot of LS-mean differences against a control level      | LSMEANS / PDIFF=CONTROL                |
| DiagnosticsPanel    | Panel of summary diagnostics for the fit                 | PLOTS=DIAGNOSTICS                      |
| CooksDPlot          | Cook's <i>D</i> plot                                     | PLOTS=DIAGNOSTICS(UNPACK)              |
| ObservedByPredicted | Observed by predicted                                    | PLOTS=DIAGNOSTICS(UNPACK)              |
| QQPlot              | Residual Q-Q plot                                        | PLOTS=DIAGNOSTICS(UNPACK)              |
| ResidualByPredicted | Residual by predicted values                             | PLOTS=DIAGNOSTICS(UNPACK)              |
| ResidualHistogram   | Residual histogram                                       | PLOTS=DIAGNOSTICS(UNPACK)              |
| RFPlot              | RF plot                                                  | PLOTS=DIAGNOSTICS(UNPACK)              |
| RStudentByPredicted | Studentized residuals by predicted                       | PLOTS=DIAGNOSTICS(UNPACK)              |
| RStudentByLeverage  | RStudent by hat diagonals                                | PLOTS=DIAGNOSTICS(UNPACK)              |
| DiffPlot            | Plot of LS-mean pairwise differences                     | LSMEANS / PDIFF                        |
| IntPlot             | Interaction plot                                         | Two-way ANOVA model                    |
| FitPlot             | Plot of predicted response by predictor                  | Model with one continuous predictor    |
| ResidualPlots       | Plots of the residuals against each continuous covariate | PLOTS=RESIDUALS                        |

## Examples: GLM Procedure

### Example 42.1: Randomized Complete Blocks with Means Comparisons and Contrasts

This example, reported by Stenstrom (1940), analyzes an experiment to investigate how snapdragons grow in various soils. To eliminate the effect of local fertility variations, the experiment is run in blocks, with each soil type sampled in each block. Since these data are balanced, the Type I and Type III SS are the same and are equal to the traditional ANOVA SS.

First, the standard analysis is shown, followed by an analysis that uses the **SOLUTION** option and includes **MEANS** and **CONTRAST** statements. The **ORDER=DATA** option in the second **PROC GLM** statement is

used so that the ordering of coefficients in the **CONTRAST** statement can correspond to the ordering in the input data. The **SOLUTION** option requests a display of the parameter estimates, which are produced by default only if there are no **CLASS** variables. A **MEANS** statement is used to request a table of the means with two multiple-comparison procedures requested. In experiments with focused treatment questions, **CONTRAST** statements are preferable to general means comparison methods. The following statements produce Output 42.1.1 through Output 42.1.4.

```

title 'Balanced Data from Randomized Complete Block';
data plants;
 input Type $ @;
 do Block = 1 to 3;
 input StemLength @;
 output;
 end;
 datalines;
Clarion 32.7 32.3 31.5
Clinton 32.1 29.7 29.1
Knox 35.7 35.9 33.1
O'Neill 36.0 34.2 31.2
Compost 31.8 28.0 29.2
Wabash 38.2 37.8 31.9
Webster 32.5 31.1 29.7
;

proc glm;
 class Block Type;
 model StemLength = Block Type;
run;

proc glm order=data;
 class Block Type;
 model StemLength = Block Type / solution;

 /*-----clrn-cltn-knox-onel-cpst-wbsh-wstr */
 contrast 'Compost vs. others' Type -1 -1 -1 -1 6 -1 -1;
 contrast 'River soils vs. non' Type -1 -1 -1 -1 0 5 -1,
 Type -1 4 -1 -1 0 0 -1;
 contrast 'Glacial vs. drift' Type -1 0 1 1 0 0 -1;
 contrast 'Clarion vs. Webster' Type -1 0 0 0 0 0 1;
 contrast "Knox vs. O'Neill" Type 0 0 1 -1 0 0 0;
run;

 means Type / waller regwq;
run;

```

**Output 42.1.1** Analysis of Variance for Randomized Complete Blocks

```

Balanced Data from Randomized Complete Block

The GLM Procedure

Class Level Information

Class Levels Values
Block 3 1 2 3
Type 7 Clarion Clinton Compost Knox O'Neill Wabash Webster

Number of Observations Read 21
Number of Observations Used 21

Balanced Data from Randomized Complete Block

The GLM Procedure

Dependent Variable: StemLength

Source DF Sum of Squares Mean Square F Value Pr > F
Model 8 142.1885714 17.7735714 10.80 0.0002
Error 12 19.7428571 1.6452381
Corrected Total 20 161.9314286

R-Square Coeff Var Root MSE StemLength Mean
0.878079 3.939745 1.282668 32.55714

Source DF Type I SS Mean Square F Value Pr > F
Block 2 39.0371429 19.5185714 11.86 0.0014
Type 6 103.1514286 17.1919048 10.45 0.0004

Source DF Type III SS Mean Square F Value Pr > F
Block 2 39.0371429 19.5185714 11.86 0.0014
Type 6 103.1514286 17.1919048 10.45 0.0004

```

This analysis shows that the stem length is significantly different for the different soil types. In addition, there are significant differences in stem length among the three blocks in the experiment.

The GLM procedure is invoked again, this time with the `ORDER=DATA` option. This enables you to write accurate contrast statements more easily because you know the order SAS is using for the levels of the

variable Type. The standard analysis is displayed again, this time including the tests for contrasts that you specified as well as the estimated parameters. These additional results are shown in [Output 42.1.2](#).

**Output 42.1.2** Contrasts and Solutions

| Balanced Data from Randomized Complete Block |    |             |             |         |        |
|----------------------------------------------|----|-------------|-------------|---------|--------|
| The GLM Procedure                            |    |             |             |         |        |
| Dependent Variable: StemLength               |    |             |             |         |        |
| Contrast                                     | DF | Contrast SS | Mean Square | F Value | Pr > F |
| Compost vs. others                           | 1  | 29.24198413 | 29.24198413 | 17.77   | 0.0012 |
| River soils vs. non                          | 2  | 48.24694444 | 24.12347222 | 14.66   | 0.0006 |
| Glacial vs. drift                            | 1  | 22.14083333 | 22.14083333 | 13.46   | 0.0032 |
| Clarion vs. Webster                          | 1  | 1.70666667  | 1.70666667  | 1.04    | 0.3285 |
| Knox vs. O'Neill                             | 1  | 1.81500000  | 1.81500000  | 1.10    | 0.3143 |

| Parameter    | Estimate      | Standard Error | t Value | Pr >  t |
|--------------|---------------|----------------|---------|---------|
| Intercept    | 29.35714286 B | 0.83970354     | 34.96   | <.0001  |
| Block 1      | 3.32857143 B  | 0.68561507     | 4.85    | 0.0004  |
| Block 2      | 1.90000000 B  | 0.68561507     | 2.77    | 0.0169  |
| Block 3      | 0.00000000 B  | .              | .       | .       |
| Type Clarion | 1.06666667 B  | 1.04729432     | 1.02    | 0.3285  |
| Type Clinton | -0.80000000 B | 1.04729432     | -0.76   | 0.4597  |
| Type Knox    | 3.80000000 B  | 1.04729432     | 3.63    | 0.0035  |
| Type O'Neill | 2.70000000 B  | 1.04729432     | 2.58    | 0.0242  |
| Type Compost | -1.43333333 B | 1.04729432     | -1.37   | 0.1962  |
| Type Wabash  | 4.86666667 B  | 1.04729432     | 4.65    | 0.0006  |
| Type Webster | 0.00000000 B  | .              | .       | .       |

NOTE: The X'X matrix has been found to be singular, and a generalized inverse was used to solve the normal equations. Terms whose estimates are followed by the letter 'B' are not uniquely estimable.

The contrast label, degrees of freedom, sum of squares, Mean Square, F Value, and Pr > F are shown for each contrast requested. In this example, the contrast results indicate the following inferences, at the 5% significance level:

- The stem length of plants grown in compost soil is significantly different from the average stem length of plants grown in other soils.
- The stem length of plants grown in river soils is significantly different from the average stem length of those grown in nonriver soils.
- The average stem length of plants grown in glacial soils (Clarion and Webster types) is significantly different from the average stem length of those grown in drift soils (Knox and O'Neill types).

- Stem lengths for Clarion and Webster types are not significantly different.
- Stem lengths for Knox and O'Neill types are not significantly different.

In addition to the estimates for the parameters of the model, the results of  $t$  tests about the parameters are also displayed. The 'B' following the parameter estimates indicates that the estimates are biased and do not represent a unique solution to the normal equations.

### Output 42.1.3 Waller-Duncan tests

| Balanced Data from Randomized Complete Block                                                |        |          |         |
|---------------------------------------------------------------------------------------------|--------|----------|---------|
| The GLM Procedure                                                                           |        |          |         |
| Waller-Duncan K-ratio $t$ Test for StemLength                                               |        |          |         |
| NOTE: This test minimizes the Bayes risk under additive loss and certain other assumptions. |        |          |         |
| Kratio                                                                                      |        |          | 100     |
| Error Degrees of Freedom                                                                    |        |          | 12      |
| Error Mean Square                                                                           |        | 1.645238 |         |
| F Value                                                                                     |        | 10.45    |         |
| Critical Value of $t$                                                                       |        | 2.12034  |         |
| Minimum Significant Difference                                                              |        | 2.2206   |         |
| Means with the same letter are not significantly different.                                 |        |          |         |
| Waller Grouping                                                                             | Mean   | N        | Type    |
| A                                                                                           | 35.967 | 3        | Wabash  |
| A                                                                                           |        |          |         |
| A                                                                                           | 34.900 | 3        | Knox    |
| A                                                                                           |        |          |         |
| B A                                                                                         | 33.800 | 3        | O'Neill |
| B                                                                                           |        |          |         |
| B C                                                                                         | 32.167 | 3        | Clarion |
| C                                                                                           |        |          |         |
| D C                                                                                         | 31.100 | 3        | Webster |
| D                                                                                           |        |          |         |
| D C                                                                                         | 30.300 | 3        | Clinton |
| D                                                                                           |        |          |         |
| D                                                                                           | 29.667 | 3        | Compost |

**Output 42.1.4** Ryan-Einot-Gabriel-Welsch Multiple Range Test

```

Balanced Data from Randomized Complete Block

The GLM Procedure

Ryan-Einot-Gabriel-Welsch Multiple Range Test for StemLength

NOTE: This test controls the Type I experimentwise error rate.

Alpha 0.05
Error Degrees of Freedom 12
Error Mean Square 1.645238

Number of Means 2 3 4 5 6 7
Critical Range 2.9875528 3.2837322 3.4395625 3.5402383 3.5402383 3.6653133

Means with the same letter are not significantly different.

REGWQ Grouping Mean N Type
 A 35.967 3 Wabash
 A
 B A 34.900 3 Knox
 B A
 B A C 33.800 3 O'Neill
 B C
 B D C 32.167 3 Clarion
 D C
 D C 31.100 3 Webster
 D
 D 30.300 3 Clinton
 D
 D 29.667 3 Compost

```

The final two pages of output ([Output 42.1.3](#) and [Output 42.1.4](#)) present results of the Waller-Duncan and REGWQ multiple-comparison procedures. For each test, notes and information pertinent to the test are given in the output. The Type means are arranged from highest to lowest. Means with the same letter are not significantly different. For this example, while some pairs of means are significantly different, there are no clear equivalence classes among the different soils.

For an alternative method of analyzing and displaying mean differences, including high-resolution graphics, see [Example 42.3](#).

---

## Example 42.2: Regression with Mileage Data

A car is tested for gas mileage at various speeds to determine at what speed the car achieves the highest gas mileage. A quadratic model is fit to the experimental data. The following statements produce [Output 42.2.1](#) through [Output 42.2.4](#).

```

title 'Gasoline Mileage Experiment';
data mileage;
 input mph mpg @@;
 datalines;
20 15.4
30 20.2
40 25.7
50 26.2 50 26.6 50 27.4
55 .
60 24.8
;

ods graphics on;
proc glm;
 model mpg=mph mph*mph / p clm;
run;
ods graphics off;

```

**Output 42.2.1** Standard Regression Analysis

| Gasoline Mileage Experiment |          |                |             |          |        |
|-----------------------------|----------|----------------|-------------|----------|--------|
| The GLM Procedure           |          |                |             |          |        |
| Number of Observations Read |          | 8              |             |          |        |
| Number of Observations Used |          | 7              |             |          |        |
| Gasoline Mileage Experiment |          |                |             |          |        |
| The GLM Procedure           |          |                |             |          |        |
| Dependent Variable: mpg     |          |                |             |          |        |
| Source                      | DF       | Sum of Squares | Mean Square | F Value  | Pr > F |
| Model                       | 2        | 111.8086183    | 55.9043091  | 77.96    | 0.0006 |
| Error                       | 4        | 2.8685246      | 0.7171311   |          |        |
| Corrected Total             | 6        | 114.6771429    |             |          |        |
|                             | R-Square | Coeff Var      | Root MSE    | mpg Mean |        |
|                             | 0.974986 | 3.564553       | 0.846836    | 23.75714 |        |
| Source                      | DF       | Type I SS      | Mean Square | F Value  | Pr > F |
| mph                         | 1        | 85.64464286    | 85.64464286 | 119.43   | 0.0004 |
| mph*mph                     | 1        | 26.16397541    | 26.16397541 | 36.48    | 0.0038 |

**Output 42.2.1** *continued*

| Source  | DF | Type III SS | Mean Square | F Value | Pr > F |
|---------|----|-------------|-------------|---------|--------|
| mph     | 1  | 41.01171219 | 41.01171219 | 57.19   | 0.0016 |
| mph*mph | 1  | 26.16397541 | 26.16397541 | 36.48   | 0.0038 |

| Parameter | Estimate     | Standard Error | t Value | Pr >  t |
|-----------|--------------|----------------|---------|---------|
| Intercept | -5.985245902 | 3.18522249     | -1.88   | 0.1334  |
| mph       | 1.305245902  | 0.17259876     | 7.56    | 0.0016  |
| mph*mph   | -0.013098361 | 0.00216852     | -6.04   | 0.0038  |

The overall *F* statistic is significant. The tests of mph and mph\*mph in the Type I sums of squares show that both the linear and quadratic terms in the regression model are significant. The model fits well, with an R square of 0.97. The table of parameter estimates indicates that the estimated regression equation is

$$\text{mpg} = -5.9852 + 1.3052 \times \text{mph} - 0.0131 \times \text{mph}^2$$

**Output 42.2.2** Results of Requesting the P and CLM Options

| Observation | Observed    | Predicted   | Residual    |
|-------------|-------------|-------------|-------------|
| 1           | 15.40000000 | 14.88032787 | 0.51967213  |
| 2           | 20.20000000 | 21.38360656 | -1.18360656 |
| 3           | 25.70000000 | 25.26721311 | 0.43278689  |
| 4           | 26.20000000 | 26.53114754 | -0.33114754 |
| 5           | 26.60000000 | 26.53114754 | 0.06885246  |
| 6           | 27.40000000 | 26.53114754 | 0.86885246  |
| 7 *         | .           | 26.18073770 | .           |
| 8           | 24.80000000 | 25.17540984 | -0.37540984 |

| Observation | 95% Confidence Limits for Mean Predicted Value |             |
|-------------|------------------------------------------------|-------------|
| 1           | 12.69701317                                    | 17.06364257 |
| 2           | 20.01727192                                    | 22.74994119 |
| 3           | 23.87460041                                    | 26.65982582 |
| 4           | 25.44573423                                    | 27.61656085 |
| 5           | 25.44573423                                    | 27.61656085 |
| 6           | 25.44573423                                    | 27.61656085 |
| 7 *         | 24.88679308                                    | 27.47468233 |
| 8           | 23.05954977                                    | 27.29126990 |

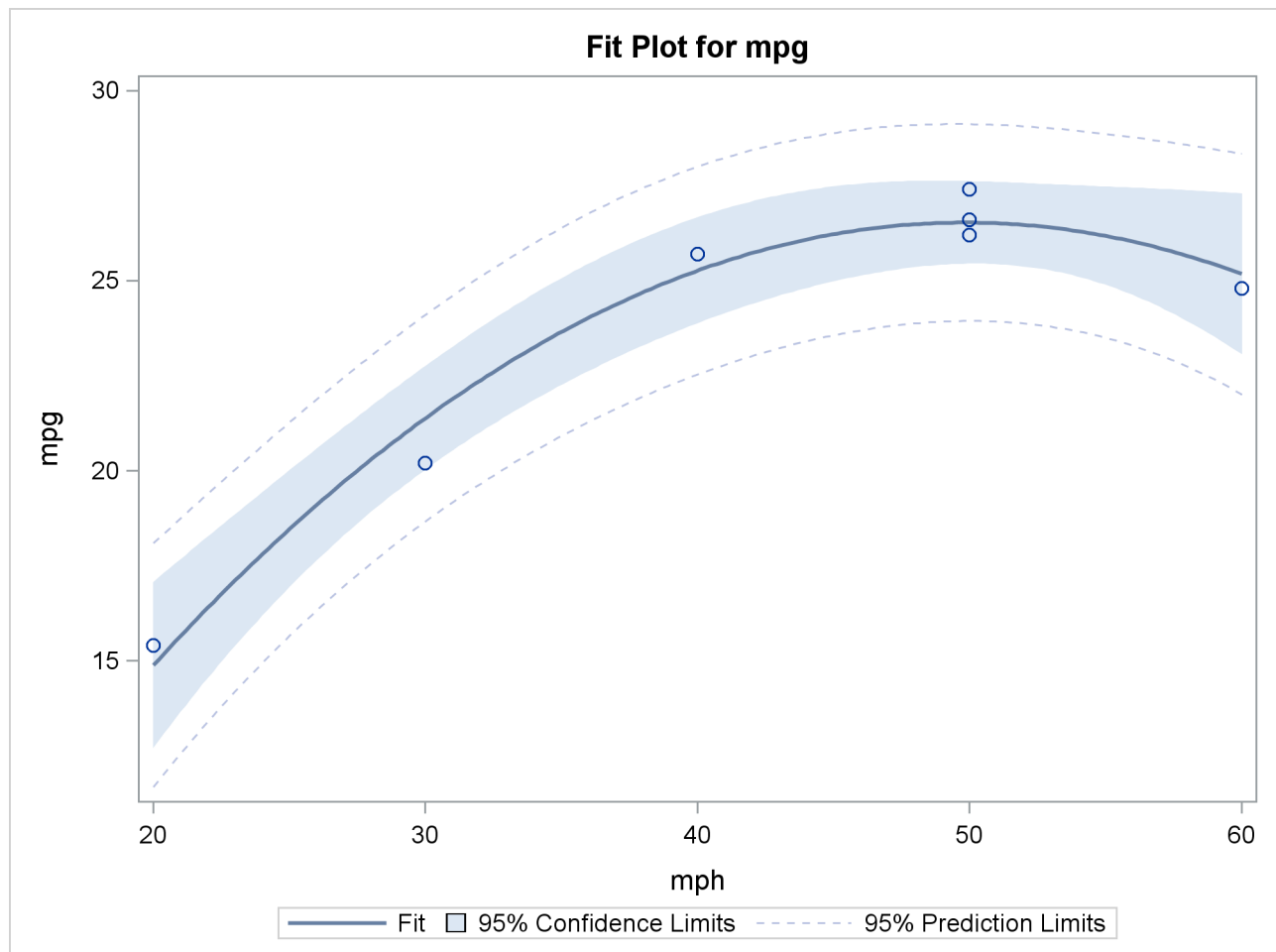
The **P** and **CLM** options in the **MODEL** statement produce the table shown in **Output 42.2.2**. For each observation, the observed, predicted, and residual values are shown. In addition, the 95% confidence limits for a mean predicted value are shown for each observation. Note that the observation with a missing value for mph is not used in the analysis, but predicted and confidence limit values are shown.



**Output 42.2.3** Additional Results of Requesting the P and CLM Options

|                                     |             |
|-------------------------------------|-------------|
| Sum of Residuals                    | -0.00000000 |
| Sum of Squared Residuals            | 2.86852459  |
| Sum of Squared Residuals - Error SS | -0.00000000 |
| PRESS Statistic                     | 23.18107335 |
| First Order Autocorrelation         | -0.54376613 |
| Durbin-Watson D                     | 2.94425592  |

The last portion of the output listing, shown in [Output 42.2.3](#), gives some additional information about the residuals. The Press statistic gives the sum of squares of predicted residual errors, as described in Chapter 4, “[Introduction to Regression Procedures](#).” The First Order Autocorrelation and the Durbin-Watson  $D$  statistic, which measures first-order autocorrelation, are also given.

**Output 42.2.4** Plot of Mileage Data

Finally, the ODS GRAPHICS ON command in the previous statements enables ODS Graphics, which in this case produces the plot shown in [Output 42.2.4](#) of the actual and predicted values for the data, as well as a band representing the confidence limits for individual predictions. The quadratic relationship between mpg and mph is evident.

## Example 42.3: Unbalanced ANOVA for Two-Way Design with Interaction

This example uses data from Kutner (1974, p. 98) to illustrate a two-way analysis of variance. The original data source is Afifi and Azen (1972, p. 166). These statements produce [Output 42.3.1](#) and [Output 42.3.2](#).

```

title 'Unbalanced Two-Way Analysis of Variance';
data a;
 input drug disease @;
 do i=1 to 6;
 input y @;
 output;
 end;
 datalines;
1 1 42 44 36 13 19 22
1 2 33 . 26 . 33 21
1 3 31 -3 . 25 25 24
2 1 28 . 23 34 42 13
2 2 . 34 33 31 . 36
2 3 3 26 28 32 4 16
3 1 . . 1 29 . 19
3 2 . 11 9 7 1 -6
3 3 21 1 . 9 3 .
4 1 24 . 9 22 -2 15
4 2 27 12 12 -5 16 15
4 3 22 7 25 5 12 .
;

proc glm;
 class drug disease;
 model y=drug disease drug*disease / ss1 ss2 ss3 ss4;
run;

```

**Output 42.3.1** Classes and Levels for Unbalanced Two-Way Design

| Unbalanced Two-Way Analysis of Variance |        |         |
|-----------------------------------------|--------|---------|
| The GLM Procedure                       |        |         |
| Class Level Information                 |        |         |
| Class                                   | Levels | Values  |
| drug                                    | 4      | 1 2 3 4 |
| disease                                 | 3      | 1 2 3   |
| Number of Observations Read             |        | 72      |
| Number of Observations Used             |        | 58      |

**Output 42.3.2** Analysis of Variance for Unbalanced Two-Way Design

| Unbalanced Two-Way Analysis of Variance |          |                |             |          |        |
|-----------------------------------------|----------|----------------|-------------|----------|--------|
| The GLM Procedure                       |          |                |             |          |        |
| Dependent Variable: y                   |          |                |             |          |        |
| Source                                  | DF       | Sum of Squares | Mean Square | F Value  | Pr > F |
| Model                                   | 11       | 4259.338506    | 387.212591  | 3.51     | 0.0013 |
| Error                                   | 46       | 5080.816667    | 110.452536  |          |        |
| Corrected Total                         | 57       | 9340.155172    |             |          |        |
|                                         | R-Square | Coeff Var      | Root MSE    | y Mean   |        |
|                                         | 0.456024 | 55.66750       | 10.50964    | 18.87931 |        |
| Source                                  | DF       | Type I SS      | Mean Square | F Value  | Pr > F |
| drug                                    | 3        | 3133.238506    | 1044.412835 | 9.46     | <.0001 |
| disease                                 | 2        | 418.833741     | 209.416870  | 1.90     | 0.1617 |
| drug*disease                            | 6        | 707.266259     | 117.877710  | 1.07     | 0.3958 |
| Source                                  | DF       | Type II SS     | Mean Square | F Value  | Pr > F |
| drug                                    | 3        | 3063.432863    | 1021.144288 | 9.25     | <.0001 |
| disease                                 | 2        | 418.833741     | 209.416870  | 1.90     | 0.1617 |
| drug*disease                            | 6        | 707.266259     | 117.877710  | 1.07     | 0.3958 |
| Source                                  | DF       | Type III SS    | Mean Square | F Value  | Pr > F |
| drug                                    | 3        | 2997.471860    | 999.157287  | 9.05     | <.0001 |
| disease                                 | 2        | 415.873046     | 207.936523  | 1.88     | 0.1637 |
| drug*disease                            | 6        | 707.266259     | 117.877710  | 1.07     | 0.3958 |
| Source                                  | DF       | Type IV SS     | Mean Square | F Value  | Pr > F |
| drug                                    | 3        | 2997.471860    | 999.157287  | 9.05     | <.0001 |
| disease                                 | 2        | 415.873046     | 207.936523  | 1.88     | 0.1637 |
| drug*disease                            | 6        | 707.266259     | 117.877710  | 1.07     | 0.3958 |

Note the differences among the four types of sums of squares. The Type I sum of squares for drug essentially tests for differences between the expected values of the arithmetic mean response for different drugs, unadjusted for the effect of disease. By contrast, the Type II sum of squares for drug measures the differences between arithmetic means for each drug after adjusting for disease. The Type III sum of squares measures the differences between predicted drug means over a balanced drug×disease population—that is, between the LS-means for drug. Finally, the Type IV sum of squares is the same as the Type III sum of squares in this case, since there are data for every drug-by-disease combination.

No matter which sum of squares you prefer to use, this analysis shows a significant difference among the four drugs, while the disease effect and the drug-by-disease interaction are not significant. As the previous discussion indicates, Type III sums of squares correspond to differences between LS-means, so you can follow up the Type III tests with a multiple-comparison analysis of the drug LS-means. Since the GLM procedure is interactive, you can accomplish this by submitting the following statements after the previous ones that performed the ANOVA.

```
lsmeans drug / pdiff=all adjust=tukey;
run;
```

Both the LS-means themselves and a matrix of adjusted *p*-values for pairwise differences between them are displayed; see [Output 42.3.3](#) and [Output 42.3.4](#).

**Output 42.3.3** LS-Means for Unbalanced ANOVA

| Unbalanced Two-Way Analysis of Variance           |            |               |  |
|---------------------------------------------------|------------|---------------|--|
| The GLM Procedure                                 |            |               |  |
| Least Squares Means                               |            |               |  |
| Adjustment for Multiple Comparisons: Tukey-Kramer |            |               |  |
| drug                                              | y LSMEAN   | LSMEAN Number |  |
| 1                                                 | 25.9944444 | 1             |  |
| 2                                                 | 26.5555556 | 2             |  |
| 3                                                 | 9.7444444  | 3             |  |
| 4                                                 | 13.5444444 | 4             |  |

**Output 42.3.4** Adjusted *p*-Values for Pairwise LS-Mean Differences

| Least Squares Means for effect drug  |        |        |        |        |
|--------------------------------------|--------|--------|--------|--------|
| Pr >  t  for H0: LSMean(i)=LSMean(j) |        |        |        |        |
| Dependent Variable: y                |        |        |        |        |
| i/j                                  | 1      | 2      | 3      | 4      |
| 1                                    |        | 0.9989 | 0.0016 | 0.0107 |
| 2                                    | 0.9989 |        | 0.0011 | 0.0071 |
| 3                                    | 0.0016 | 0.0011 |        | 0.7870 |
| 4                                    | 0.0107 | 0.0071 | 0.7870 |        |

The multiple-comparison analysis shows that drugs 1 and 2 have very similar effects, and that drugs 3 and 4 are also insignificantly different from each other. Evidently, the main contribution to the significant drug effect is the difference between the 1/2 pair and the 3/4 pair.

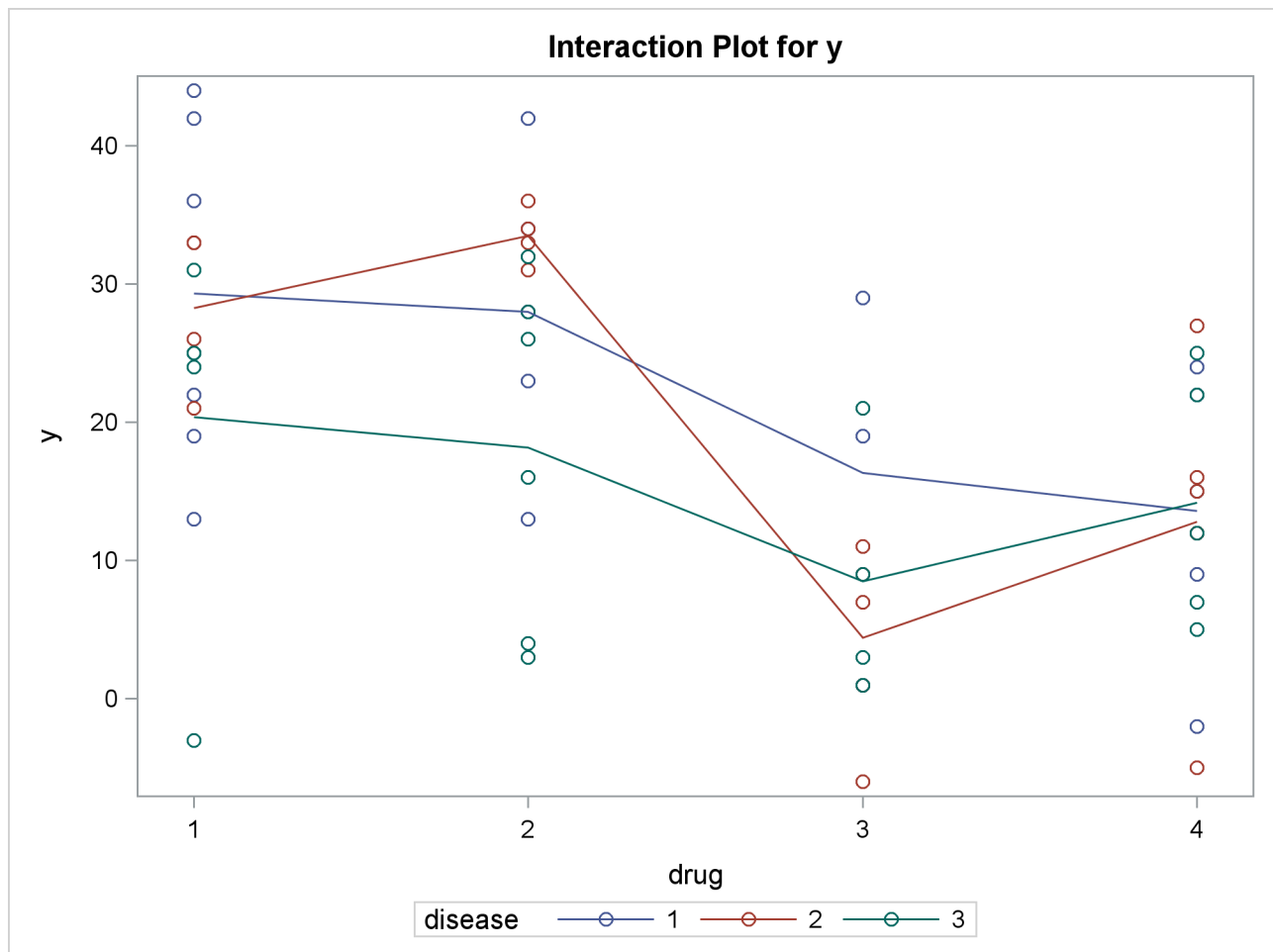
If ODS Graphics is enabled for the previous analysis, GLM also displays three additional plots by default:

- an interaction plot for the effects of disease and drug
- a mean plot of the drug LS-means
- a plot of the adjusted pairwise differences and their significance levels

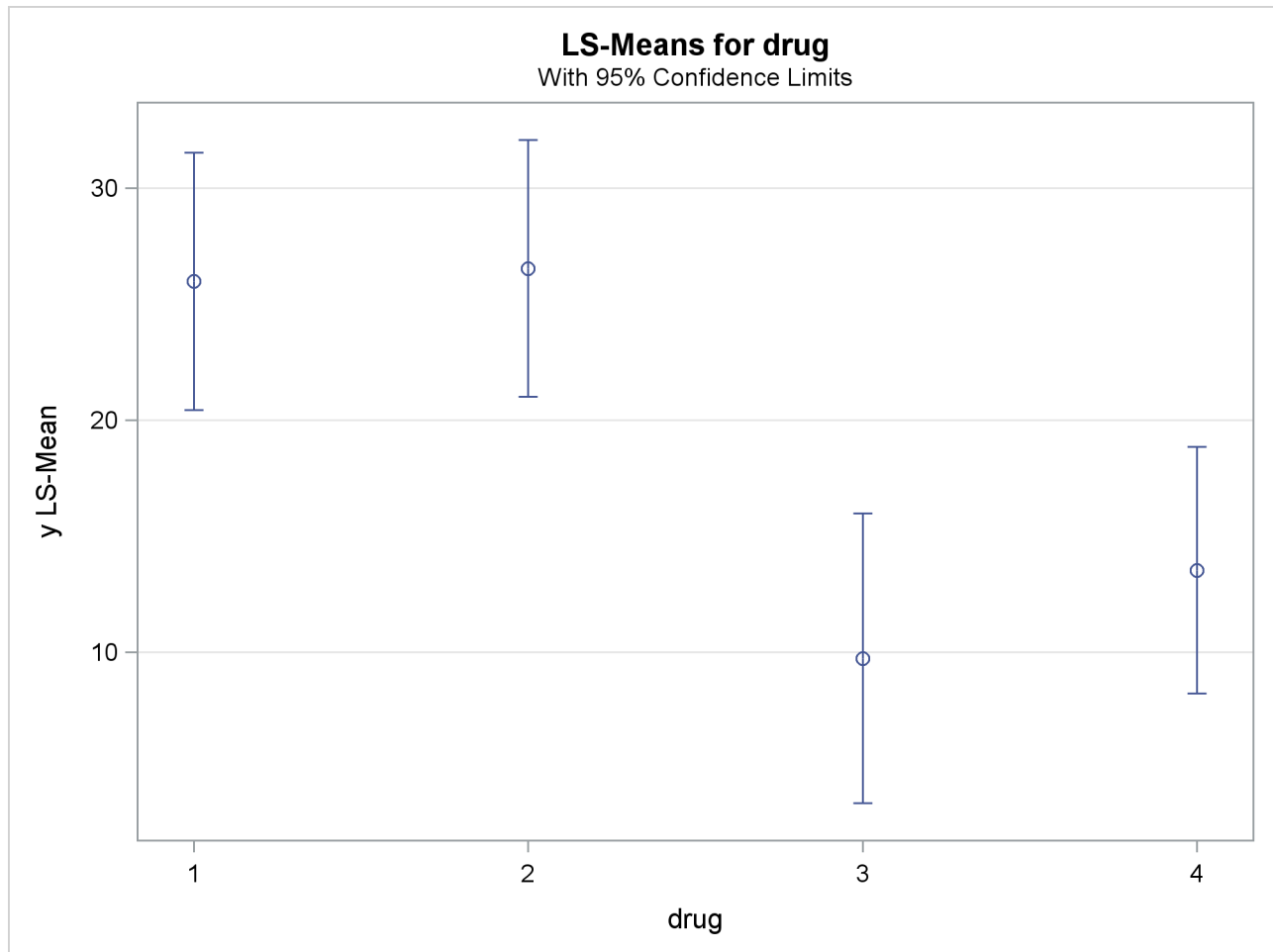
The following statements reproduce the previous analysis with ODS Graphics enabled. Additionally, the `PLOTS=MEANPLOT(CL)` option specifies that confidence limits for the LS-means should also be displayed in the mean plot. The graphical results are shown in [Output 42.3.5](#) through [Output 42.3.7](#).

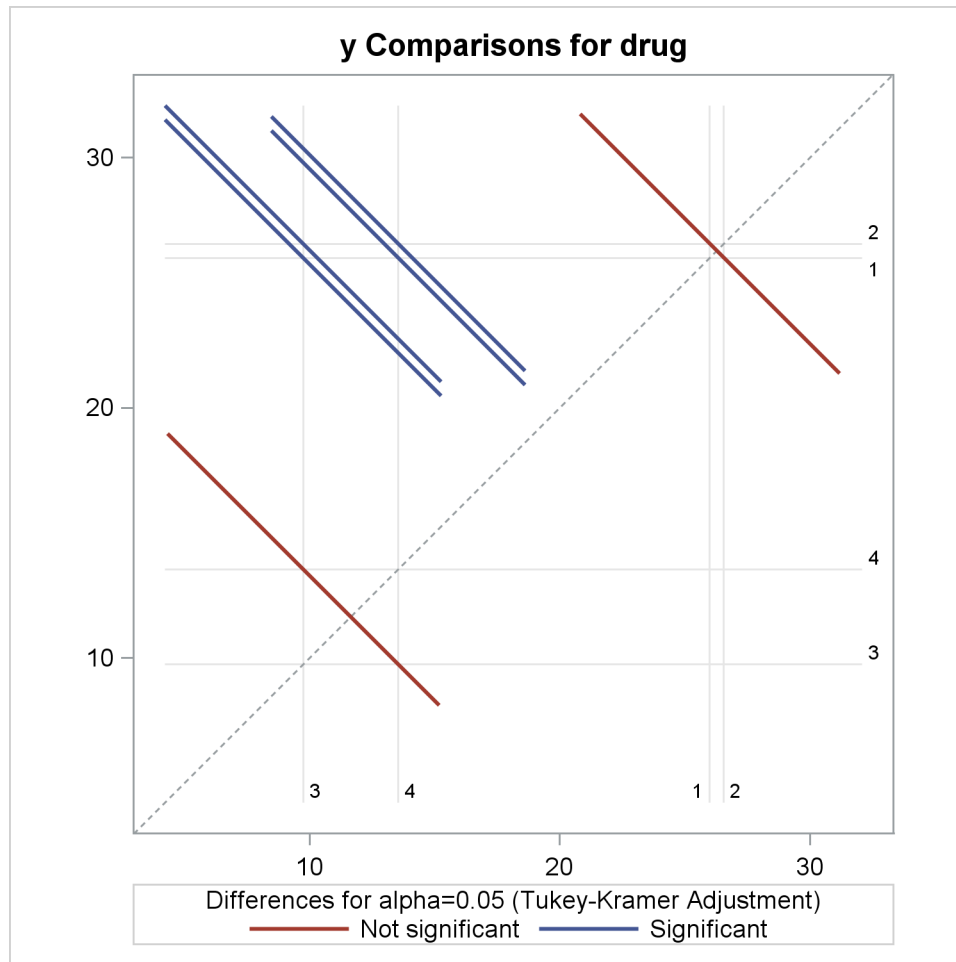
```
ods graphics on;
proc glm plot=meanplot(cl);
 class drug disease;
 model y=drug disease drug*disease;
 lsmeans drug / pdiff=all adjust=tukey;
run;
ods graphics off;
```

**Output 42.3.5** Plot of Response by Drug and Disease



**Output 42.3.6** Plot of Response LS-Means for Drug



**Output 42.3.7** Plot of Response LS-Mean Differences for Drug

The significance of the drug differences is difficult to discern in the original data, as displayed in [Output 42.3.5](#), but the plot of just the LS-means and their individual confidence limits in [Output 42.3.6](#) makes it clearer. Finally, [Output 42.3.7](#) indicates conclusively that the significance of the effect of drug is due to the difference between the two drug pairs (1, 2) and (3, 4).

## Example 42.4: Analysis of Covariance

Analysis of covariance combines some of the features of both regression and analysis of variance. Typically, a continuous variable (the covariate) is introduced into the model of an analysis-of-variance experiment.

Data in the following example are selected from a larger experiment on the use of drugs in the treatment of leprosy (Snedecor and Cochran 1967, p. 422).

Variables in the study are as follows:

|               |                                             |
|---------------|---------------------------------------------|
| Drug          | two antibiotics (A and D) and a control (F) |
| PreTreatment  | a pretreatment score of leprosy bacilli     |
| PostTreatment | a posttreatment score of leprosy bacilli    |

Ten patients are selected for each treatment (Drug), and six sites on each patient are measured for leprosy bacilli.

The covariate (a pretreatment score) is included in the model for increased precision in determining the effect of drug treatments on the posttreatment count of bacilli.

The following statements create the data set, perform a parallel-slopes analysis of covariance with PROC GLM, and compute Drug LS-means. These statements produce [Output 42.4.1](#) and [Output 42.4.2](#).

```

data DrugTest;
 input Drug $ PreTreatment PostTreatment @@;
 datalines;
A 11 6 A 8 0 A 5 2 A 14 8 A 19 11
A 6 4 A 10 13 A 6 1 A 11 8 A 3 0
D 6 0 D 6 2 D 7 3 D 8 1 D 18 18
D 8 4 D 19 14 D 8 9 D 5 1 D 15 9
F 16 13 F 13 10 F 11 18 F 9 5 F 21 23
F 16 12 F 12 5 F 12 16 F 7 1 F 12 20
;

proc glm data=DrugTest;
 class Drug;
 model PostTreatment = Drug PreTreatment / solution;
 lsmeans Drug / stderr pdiff cov out=adjmeans;
run;

proc print data=adjmeans;
run;

```

**Output 42.4.1** Classes and Levels

| The GLM Procedure           |        |        |
|-----------------------------|--------|--------|
| Class Level Information     |        |        |
| Class                       | Levels | Values |
| Drug                        | 3      | A D F  |
| Number of Observations Read |        | 30     |
| Number of Observations Used |        | 30     |



**Output 42.4.2** Overall Analysis of Variance

| The GLM Procedure                 |          |                |             |                    |        |
|-----------------------------------|----------|----------------|-------------|--------------------|--------|
| Dependent Variable: PostTreatment |          |                |             |                    |        |
| Source                            | DF       | Sum of Squares | Mean Square | F Value            | Pr > F |
| Model                             | 3        | 871.497403     | 290.499134  | 18.10              | <.0001 |
| Error                             | 26       | 417.202597     | 16.046254   |                    |        |
| Corrected Total                   | 29       | 1288.700000    |             |                    |        |
|                                   | R-Square | Coeff Var      | Root MSE    | PostTreatment Mean |        |
|                                   | 0.676261 | 50.70604       | 4.005778    | 7.900000           |        |

This model assumes that the slopes relating posttreatment scores to pretreatment scores are parallel for all drugs. You can check this assumption by including the class-by-covariate interaction, Drug\*PreTreatment, in the model and examining the ANOVA test for the significance of this effect. This extra test is omitted in this example, but it is insignificant, justifying the equal-slopes assumption.

In [Output 42.4.3](#), the Type I SS for Drug (293.6) gives the between-drug sums of squares that are obtained for the analysis-of-variance model PostTreatment=Drug. This measures the difference between arithmetic means of posttreatment scores for different drugs, disregarding the covariate. The Type III SS for Drug (68.5537) gives the Drug sum of squares adjusted for the covariate. This measures the differences between Drug LS-means, controlling for the covariate. The Type I test is highly significant ( $p = 0.001$ ), but the Type III test is not. This indicates that, while there is a statistically significant difference between the arithmetic drug means, this difference is reduced to below the level of background noise when you take the pretreatment scores into account. From the table of parameter estimates, you can derive the least squares predictive formula model for estimating posttreatment score based on pretreatment score and drug:

$$\text{post} = \begin{cases} (-0.435 + -3.446) + 0.987 \cdot \text{pre}, & \text{if Drug=A} \\ (-0.435 + -3.337) + 0.987 \cdot \text{pre}, & \text{if Drug=D} \\ -0.435 + 0.987 \cdot \text{pre}, & \text{if Drug=F} \end{cases}$$

**Output 42.4.3** Tests and Parameter Estimates

| Source       | DF | Type I SS   | Mean Square | F Value | Pr > F |
|--------------|----|-------------|-------------|---------|--------|
| Drug         | 2  | 293.6000000 | 146.8000000 | 9.15    | 0.0010 |
| PreTreatment | 1  | 577.8974030 | 577.8974030 | 36.01   | <.0001 |
| Source       | DF | Type III SS | Mean Square | F Value | Pr > F |
| Drug         | 2  | 68.5537106  | 34.2768553  | 2.14    | 0.1384 |
| PreTreatment | 1  | 577.8974030 | 577.8974030 | 36.01   | <.0001 |

**Output 42.4.3** continued

| Parameter    |   | Estimate       | Standard Error | t Value | Pr >  t |
|--------------|---|----------------|----------------|---------|---------|
| Intercept    |   | -0.434671164 B | 2.47135356     | -0.18   | 0.8617  |
| Drug         | A | -3.446138280 B | 1.88678065     | -1.83   | 0.0793  |
| Drug         | D | -3.337166948 B | 1.85386642     | -1.80   | 0.0835  |
| Drug         | F | 0.000000000 B  | .              | .       | .       |
| PreTreatment |   | 0.987183811    | 0.16449757     | 6.00    | <.0001  |

Output 42.4.4 displays the LS-means, which are, in a sense, the means adjusted for the covariate. The **STDERR** option in the **LSMEANS** statement causes the standard error of the LS-means and the probability of getting a larger *t* value under the hypothesis  $H_0: \text{LS-mean} = 0$  to be included in this table as well. Specifying the **PDIF** option causes all probability values for the hypothesis  $H_0: \text{LS-mean}(i) = \text{LS-mean}(j)$  to be displayed, where the indexes *i* and *j* are numbered treatment levels.

**Output 42.4.4** LS-Means

| The GLM Procedure                    |                       |                |         |               |
|--------------------------------------|-----------------------|----------------|---------|---------------|
| Least Squares Means                  |                       |                |         |               |
| Drug                                 | Post Treatment LSMEAN | Standard Error | Pr >  t | LSMEAN Number |
| A                                    | 6.7149635             | 1.2884943      | <.0001  | 1             |
| D                                    | 6.8239348             | 1.2724690      | <.0001  | 2             |
| F                                    | 10.1611017            | 1.3159234      | <.0001  | 3             |
| Least Squares Means for effect Drug  |                       |                |         |               |
| Pr >  t  for H0: LSMean(i)=LSMean(j) |                       |                |         |               |
| Dependent Variable: PostTreatment    |                       |                |         |               |
| i/j                                  | 1                     | 2              | 3       |               |
| 1                                    |                       | 0.9521         | 0.0793  |               |
| 2                                    | 0.9521                |                | 0.0835  |               |
| 3                                    | 0.0793                | 0.0835         |         |               |

The **OUT=** and **COV** options in the **LSMEANS** statement create a data set of the estimates, their standard errors, and the variances and covariances of the LS-means, which is displayed in [Output 42.4.5](#).

**Output 42.4.5** LS-Means Output Data Set

| Obs | _NAME_        | Drug | LSMEAN  | STDERR  | NUMBER | COV1     | COV2     | COV3     |
|-----|---------------|------|---------|---------|--------|----------|----------|----------|
| 1   | PostTreatment | A    | 6.7150  | 1.28849 | 1      | 1.66022  | 0.02844  | -0.08403 |
| 2   | PostTreatment | D    | 6.8239  | 1.27247 | 2      | 0.02844  | 1.61918  | -0.04299 |
| 3   | PostTreatment | F    | 10.1611 | 1.31592 | 3      | -0.08403 | -0.04299 | 1.73165  |

The new graphical features of PROC GLM enable you to visualize the fitted analysis of covariance model. The following statements enable ODS Graphics by specifying the ODS GRAPHICS statement and then fit an analysis-of-covariance model with LS-means for Drug.

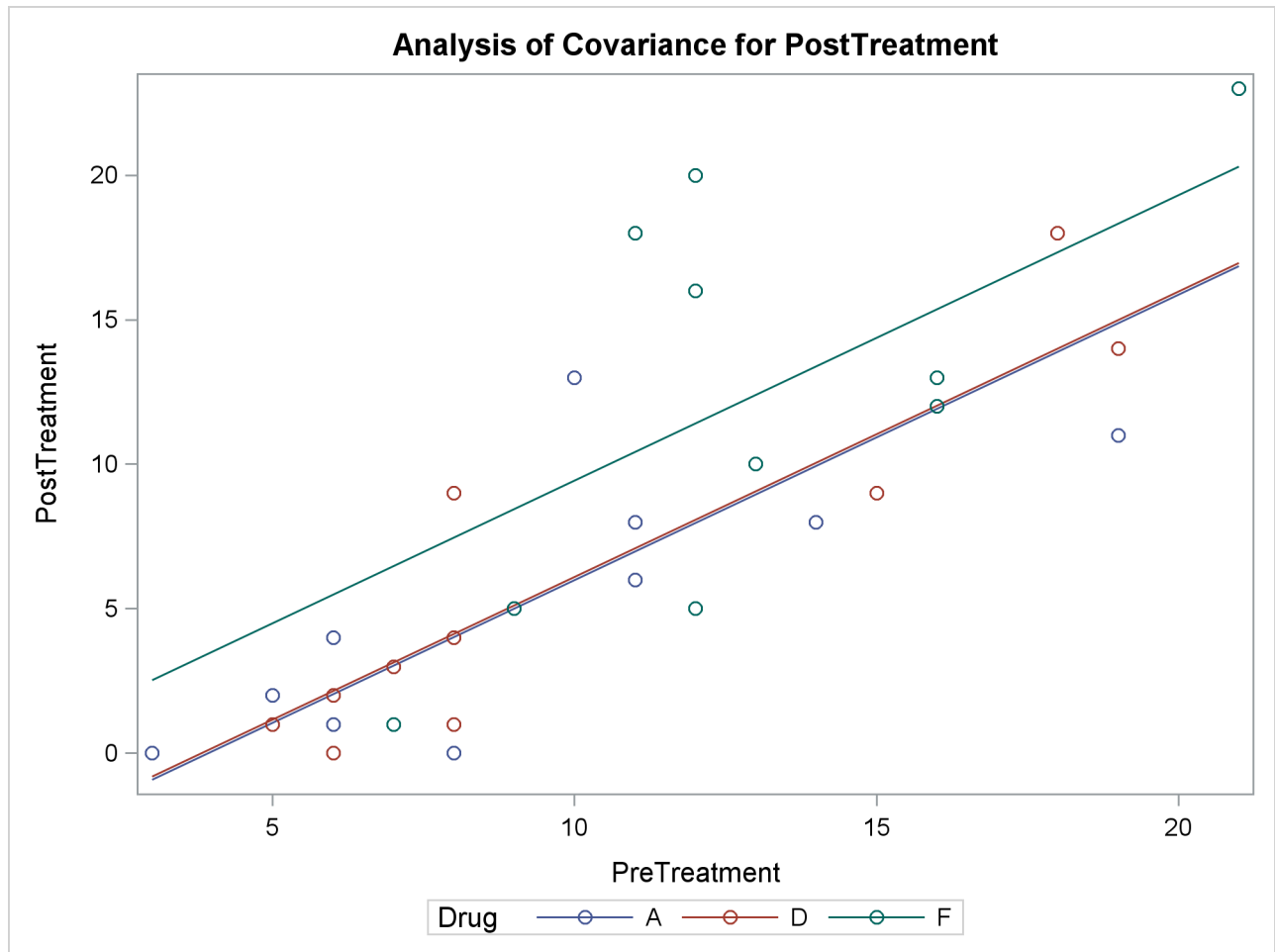
```
ods graphics on;

proc glm data=DrugTest plot=meanplot(cl);
 class Drug;
 model PostTreatment = Drug PreTreatment;
 lsmeans Drug / pdiff;
run;

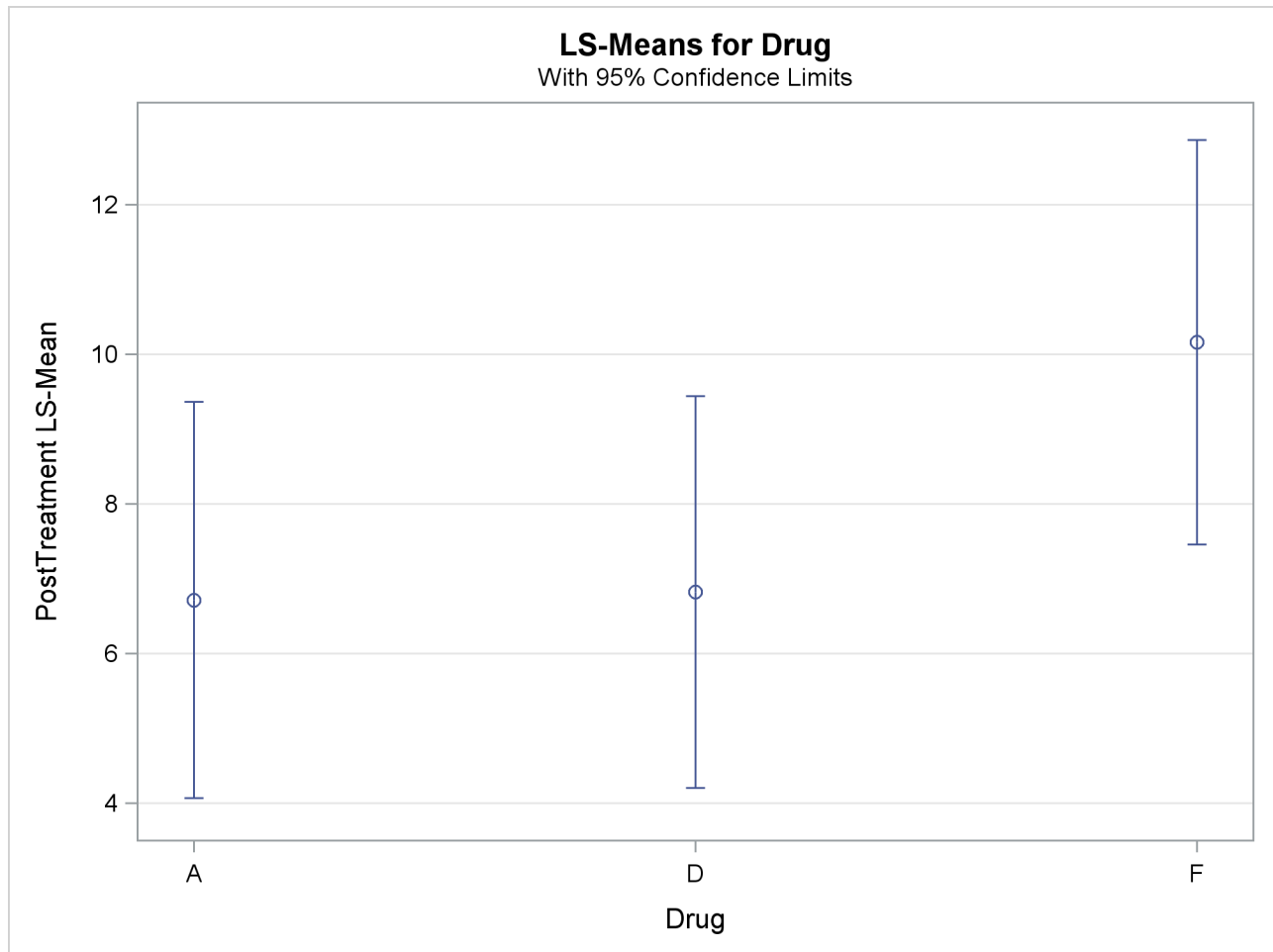
ods graphics off;
```

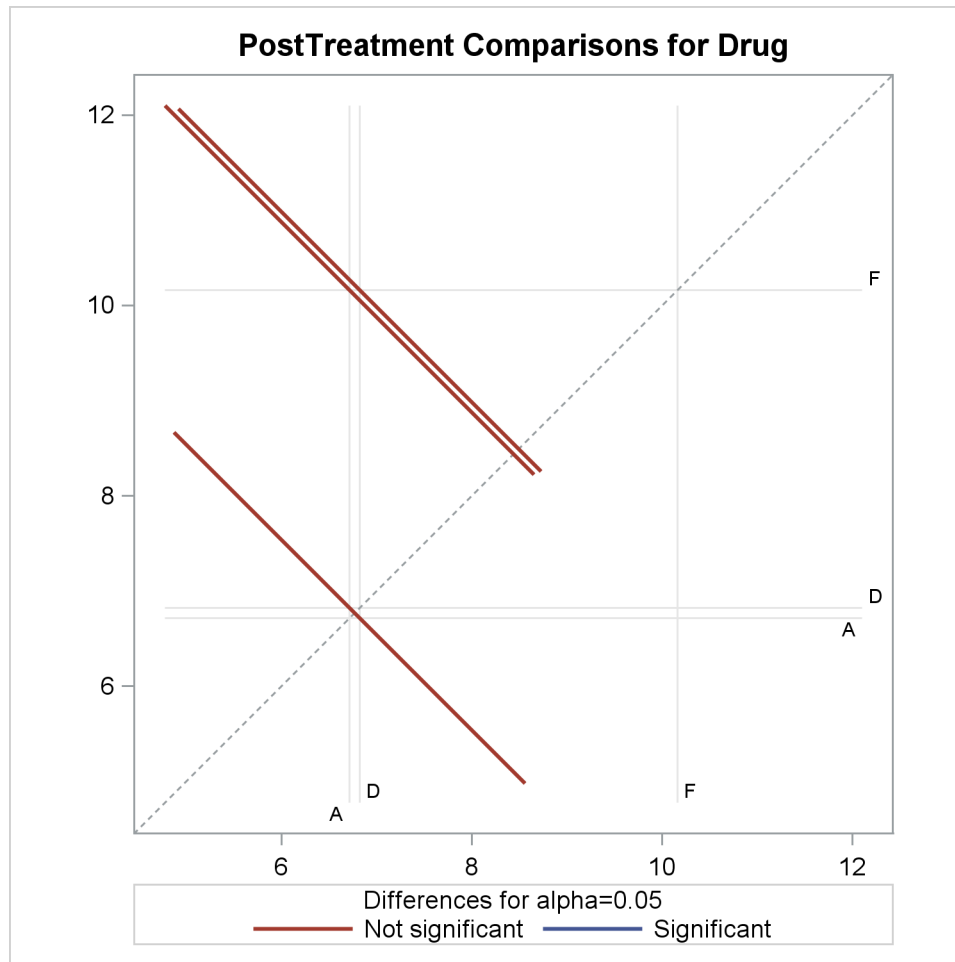
With graphics enabled, the GLM procedure output includes an analysis-of-covariance plot, as in [Output 42.4.6](#). The **LSMEANS** statement produces a plot of the LS-means; the SAS statements previously shown use the **PLOTS=MEANPLOT(CL)** option to add confidence limits for the individual LS-means, shown in [Output 42.4.7](#). If you also specify the **PDIFF** option in the **LSMEANS** statement, the output also includes a plot appropriate for the type of LS-mean differences computed. In this case, the default is to compare all LS-means with each other pairwise, so the plot is a “diffogram” or “mean-mean scatter plot” (Hsu 1996), as in [Output 42.4.8](#). For general information about ODS Graphics, see Chapter 21, “[Statistical Graphics Using ODS](#).” For specific information about the graphics available in the GLM procedure, see the section “[ODS Graphics](#)” on page 3388.

**Output 42.4.6** Analysis of Covariance Plot of PostTreatment Score by Drug and PreTreatment Score



**Output 42.4.7** LS-Means for PostTreatment Score by Drug



**Output 42.4.8** Plot of Differences between Drug LS-Means for PostTreatment Scores

The analysis of covariance plot [Output 42.4.6](#) makes it clear that the control (drug F) has higher posttreatment scores across the range of pretreatment scores, while the fitted models for the two antibiotics (drugs A and D) nearly coincide. Similarly, while the diffogram [Output 42.4.7](#) indicates that none of the LS-mean differences are significant at the 5% level, the difference between the LS-means for the two antibiotics is much closer to zero than the differences between either one and the control.

### Example 42.5: Three-Way Analysis of Variance with Contrasts

This example uses data from Cochran and Cox (1957, p. 176) to illustrate the analysis of a three-way factorial design with replication, including the use of the `CONTRAST` statement with interactions, the `OUTSTAT=` data set, and the `SLICE=` option in the `LSMEANS` statement.

The object of the study is to determine the effects of electric current on denervated muscle. The variables are as follows:

- Rep                    the replicate number, 1 or 2
- Time                  the length of time the current is applied to the muscle, ranging from 1 to 4

Current            the level of electric current applied, ranging from 1 to 4  
 Number            the number of treatments per day, ranging from 1 to 3  
 MuscleWeight      the weight of the denervated muscle

The following statements produce [Output 42.5.1](#) through [Output 42.5.4](#).

```
data muscles;
 do Rep=1 to 2;
 do Time=1 to 4;
 do Current=1 to 4;
 do Number=1 to 3;
 input MuscleWeight @@;
 output;
 end;
 end;
 end;
 end;
 datalines;
72 74 69 61 61 65 62 65 70 85 76 61
67 52 62 60 55 59 64 65 64 67 72 60
57 66 72 72 43 43 63 66 72 56 75 92
57 56 78 60 63 58 61 79 68 73 86 71
46 74 58 60 64 52 71 64 71 53 65 66
44 58 54 57 55 51 62 61 79 60 78 82
53 50 61 56 57 56 56 56 71 56 58 69
46 55 64 56 55 57 64 66 62 59 58 88
;

proc glm outstat=summary;
 class Rep Current Time Number;
 model MuscleWeight = Rep Current|Time|Number;
 contrast 'Time in Current 3'
 Time 1 0 0 -1 Current*Time 0 0 0 0 0 0 0 0 0 1 0 0 -1,
 Time 0 1 0 -1 Current*Time 0 0 0 0 0 0 0 0 0 0 1 0 -1,
 Time 0 0 1 -1 Current*Time 0 0 0 0 0 0 0 0 0 0 0 1 -1;
 contrast 'Current 1 versus 2' Current 1 -1;
 lsmeans Current*Time / slice=Current;
run;

proc print data=summary;
run;
```

The first **CONTRAST** statement examines the effects of Time within level 3 of Current. This is also called the *simple effect* of Time within Current\*Time. Note that, since there are three degrees of freedom, it is necessary to specify three rows in the **CONTRAST** statement, separated by commas. Since the parameterization that PROC GLM uses is determined in part by the ordering of the variables in the **CLASS** statement, Current is specified before Time so that the Time parameters are nested within the Current\*Time parameters; thus, the Current\*Time contrast coefficients in each row are simply the Time coefficients of that row within the appropriate level of Current.

The second **CONTRAST** statement isolates a single-degree-of-freedom effect corresponding to the difference between the first two levels of Current. You can use such a contrast in a large experiment where certain preplanned comparisons are important, but you want to take advantage of the additional error degrees of freedom available when all levels of the factors are considered.

The **LSMEANS** statement with the **SLICE=** option is an alternative way to test for the simple effect of Time within Current\*Time. In addition to listing the LS-means for each current strength and length of time, it gives a table of *F* tests for differences between the LS-means across Time within each Current level. In some cases, this can be a way to disentangle a complex interaction.

**Output 42.5.1 Overall Analysis**

| The GLM Procedure                |          |                |             |                   |        |
|----------------------------------|----------|----------------|-------------|-------------------|--------|
| Class Level Information          |          |                |             |                   |        |
| Class                            | Levels   | Values         |             |                   |        |
| Rep                              | 2        | 1              | 2           |                   |        |
| Current                          | 4        | 1              | 2           | 3                 | 4      |
| Time                             | 4        | 1              | 2           | 3                 | 4      |
| Number                           | 3        | 1              | 2           | 3                 |        |
| Number of Observations Read      |          |                |             |                   | 96     |
| Number of Observations Used      |          |                |             |                   | 96     |
| The GLM Procedure                |          |                |             |                   |        |
| Dependent Variable: MuscleWeight |          |                |             |                   |        |
| Source                           | DF       | Sum of Squares | Mean Square | F Value           | Pr > F |
| Model                            | 48       | 5782.916667    | 120.477431  | 1.77              | 0.0261 |
| Error                            | 47       | 3199.489583    | 68.074246   |                   |        |
| Corrected Total                  | 95       | 8982.406250    |             |                   |        |
|                                  | R-Square | Coeff Var      | Root MSE    | MuscleWeight Mean |        |
|                                  | 0.643805 | 13.05105       | 8.250712    | 63.21875          |        |

The output, shown in [Output 42.5.2](#) and [Output 42.5.3](#), indicates that the main effects for Rep, Current, and Number are significant (with *p*-values of 0.0045, <0.0001, and 0.0461, respectively), but the main effect for Time is not significant, indicating that, in general, it does not matter how long the current is applied. None of the interaction terms are significant, nor are the contrasts significant. Notice that the row in the sliced ANOVA table corresponding to level 3 of current matches the “Time in Current 3” contrast.



Output 42.5.2 Individual Effects and Contrasts

| Source              | DF | Type I SS   | Mean Square | F Value | Pr > F |
|---------------------|----|-------------|-------------|---------|--------|
| Rep                 | 1  | 605.010417  | 605.010417  | 8.89    | 0.0045 |
| Current             | 3  | 2145.447917 | 715.149306  | 10.51   | <.0001 |
| Time                | 3  | 223.114583  | 74.371528   | 1.09    | 0.3616 |
| Current*Time        | 9  | 298.677083  | 33.186343   | 0.49    | 0.8756 |
| Number              | 2  | 447.437500  | 223.718750  | 3.29    | 0.0461 |
| Current*Number      | 6  | 644.395833  | 107.399306  | 1.58    | 0.1747 |
| Time*Number         | 6  | 367.979167  | 61.329861   | 0.90    | 0.5023 |
| Current*Time*Number | 18 | 1050.854167 | 58.380787   | 0.86    | 0.6276 |

| Source              | DF | Type III SS | Mean Square | F Value | Pr > F |
|---------------------|----|-------------|-------------|---------|--------|
| Rep                 | 1  | 605.010417  | 605.010417  | 8.89    | 0.0045 |
| Current             | 3  | 2145.447917 | 715.149306  | 10.51   | <.0001 |
| Time                | 3  | 223.114583  | 74.371528   | 1.09    | 0.3616 |
| Current*Time        | 9  | 298.677083  | 33.186343   | 0.49    | 0.8756 |
| Number              | 2  | 447.437500  | 223.718750  | 3.29    | 0.0461 |
| Current*Number      | 6  | 644.395833  | 107.399306  | 1.58    | 0.1747 |
| Time*Number         | 6  | 367.979167  | 61.329861   | 0.90    | 0.5023 |
| Current*Time*Number | 18 | 1050.854167 | 58.380787   | 0.86    | 0.6276 |

| Contrast           | DF | Contrast SS | Mean Square | F Value | Pr > F |
|--------------------|----|-------------|-------------|---------|--------|
| Time in Current 3  | 3  | 34.83333333 | 11.61111111 | 0.17    | 0.9157 |
| Current 1 versus 2 | 1  | 99.18750000 | 99.18750000 | 1.46    | 0.2334 |

Output 42.5.3 Simple Effects of Time

| The GLM Procedure                                      |    |                |             |         |        |
|--------------------------------------------------------|----|----------------|-------------|---------|--------|
| Least Squares Means                                    |    |                |             |         |        |
| Current*Time Effect Sliced by Current for MuscleWeight |    |                |             |         |        |
| Current                                                | DF | Sum of Squares | Mean Square | F Value | Pr > F |
| 1                                                      | 3  | 271.458333     | 90.486111   | 1.33    | 0.2761 |
| 2                                                      | 3  | 120.666667     | 40.222222   | 0.59    | 0.6241 |
| 3                                                      | 3  | 34.833333      | 11.611111   | 0.17    | 0.9157 |
| 4                                                      | 3  | 94.833333      | 31.611111   | 0.46    | 0.7085 |

The SS,  $F$  statistics, and  $p$ -values can be stored in an `OUTSTAT=` data set, as shown in Output 42.5.4.

## Output 42.5.4 Contents of the OUTSTAT= Data Set

| Obs | _NAME_       | _SOURCE_            | _TYPE_   | DF | SS      | F       | PROB    |
|-----|--------------|---------------------|----------|----|---------|---------|---------|
| 1   | MuscleWeight | ERROR               | ERROR    | 47 | 3199.49 | .       | .       |
| 2   | MuscleWeight | Rep                 | SS1      | 1  | 605.01  | 8.8875  | 0.00454 |
| 3   | MuscleWeight | Current             | SS1      | 3  | 2145.45 | 10.5054 | 0.00002 |
| 4   | MuscleWeight | Time                | SS1      | 3  | 223.11  | 1.0925  | 0.36159 |
| 5   | MuscleWeight | Current*Time        | SS1      | 9  | 298.68  | 0.4875  | 0.87562 |
| 6   | MuscleWeight | Number              | SS1      | 2  | 447.44  | 3.2864  | 0.04614 |
| 7   | MuscleWeight | Current*Number      | SS1      | 6  | 644.40  | 1.5777  | 0.17468 |
| 8   | MuscleWeight | Time*Number         | SS1      | 6  | 367.98  | 0.9009  | 0.50231 |
| 9   | MuscleWeight | Current*Time*Number | SS1      | 18 | 1050.85 | 0.8576  | 0.62757 |
| 10  | MuscleWeight | Rep                 | SS3      | 1  | 605.01  | 8.8875  | 0.00454 |
| 11  | MuscleWeight | Current             | SS3      | 3  | 2145.45 | 10.5054 | 0.00002 |
| 12  | MuscleWeight | Time                | SS3      | 3  | 223.11  | 1.0925  | 0.36159 |
| 13  | MuscleWeight | Current*Time        | SS3      | 9  | 298.68  | 0.4875  | 0.87562 |
| 14  | MuscleWeight | Number              | SS3      | 2  | 447.44  | 3.2864  | 0.04614 |
| 15  | MuscleWeight | Current*Number      | SS3      | 6  | 644.40  | 1.5777  | 0.17468 |
| 16  | MuscleWeight | Time*Number         | SS3      | 6  | 367.98  | 0.9009  | 0.50231 |
| 17  | MuscleWeight | Current*Time*Number | SS3      | 18 | 1050.85 | 0.8576  | 0.62757 |
| 18  | MuscleWeight | Time in Current 3   | CONTRAST | 3  | 34.83   | 0.1706  | 0.91574 |
| 19  | MuscleWeight | Current 1 versus 2  | CONTRAST | 1  | 99.19   | 1.4570  | 0.23344 |

---

## Example 42.6: Multivariate Analysis of Variance

This example employs multivariate analysis of variance (MANOVA) to measure differences in the chemical characteristics of ancient pottery found at four kiln sites in Great Britain. The data are from Tubb, Parker, and Nickless (1980), as reported in Hand et al. (1994).

For each of 26 samples of pottery, the percentages of oxides of five metals are measured. The following statements create the data set and invoke the GLM procedure to perform a one-way MANOVA. Additionally, it is of interest to know whether the pottery from one site in Wales (Llanederyn) differs from the samples from other sites; a **CONTRAST** statement is used to test this hypothesis.

```

title "Romano-British Pottery";
data pottery;
 input Site $12. Al Fe Mg Ca Na;
 datalines;
Llanederyn 14.4 7.00 4.30 0.15 0.51
Llanederyn 13.8 7.08 3.43 0.12 0.17
Llanederyn 14.6 7.09 3.88 0.13 0.20
Llanederyn 11.5 6.37 5.64 0.16 0.14
Llanederyn 13.8 7.06 5.34 0.20 0.20
Llanederyn 10.9 6.26 3.47 0.17 0.22
Llanederyn 10.1 4.26 4.26 0.20 0.18
Llanederyn 11.6 5.78 5.91 0.18 0.16
Llanederyn 11.1 5.49 4.52 0.29 0.30
Llanederyn 13.4 6.92 7.23 0.28 0.20
Llanederyn 12.4 6.13 5.69 0.22 0.54
Llanederyn 13.1 6.64 5.51 0.31 0.24
Llanederyn 12.7 6.69 4.45 0.20 0.22

```

```

Llanederyn 12.5 6.44 3.94 0.22 0.23
Caldicot 11.8 5.44 3.94 0.30 0.04
Caldicot 11.6 5.39 3.77 0.29 0.06
IslandThorns 18.3 1.28 0.67 0.03 0.03
IslandThorns 15.8 2.39 0.63 0.01 0.04
IslandThorns 18.0 1.50 0.67 0.01 0.06
IslandThorns 18.0 1.88 0.68 0.01 0.04
IslandThorns 20.8 1.51 0.72 0.07 0.10
AshleyRails 17.7 1.12 0.56 0.06 0.06
AshleyRails 18.3 1.14 0.67 0.06 0.05
AshleyRails 16.7 0.92 0.53 0.01 0.05
AshleyRails 14.8 2.74 0.67 0.03 0.05
AshleyRails 19.1 1.64 0.60 0.10 0.03
;

proc glm data=pottery;
 class Site;
 model Al Fe Mg Ca Na = Site;
 contrast 'Llanederyn vs. the rest' Site 1 1 1 -3;
 manova h=_all_ / printe printh;
run;

```

After the summary information, displayed in [Output 42.6.1](#), PROC GLM produces the univariate analyses for each of the dependent variables, as shown in [Output 42.6.2](#) through [Output 42.6.6](#). These analyses show that sites are significantly different for all oxides individually. You can suppress these univariate analyses by specifying the `NOUNI` option in the `MODEL` statement.

**Output 42.6.1** Summary Information about Groups

| Romano-British Pottery  |        |                                              |    |
|-------------------------|--------|----------------------------------------------|----|
| The GLM Procedure       |        |                                              |    |
| Class Level Information |        |                                              |    |
| Class                   | Levels | Values                                       |    |
| Site                    | 4      | AshleyRails Caldicot IslandThorns Llanederyn |    |
|                         |        | Number of Observations Read                  | 26 |
|                         |        | Number of Observations Used                  | 26 |

**Output 42.6.2** Univariate Analysis of Variance for Aluminum Oxide

| Romano-British Pottery  |          |                |             |          |        |
|-------------------------|----------|----------------|-------------|----------|--------|
| The GLM Procedure       |          |                |             |          |        |
| Dependent Variable: Al  |          |                |             |          |        |
| Source                  | DF       | Sum of Squares | Mean Square | F Value  | Pr > F |
| Model                   | 3        | 175.6103187    | 58.5367729  | 26.67    | <.0001 |
| Error                   | 22       | 48.2881429     | 2.1949156   |          |        |
| Corrected Total         | 25       | 223.8984615    |             |          |        |
|                         | R-Square | Coeff Var      | Root MSE    | Al Mean  |        |
|                         | 0.784330 | 10.22284       | 1.481525    | 14.49231 |        |
| Source                  | DF       | Type I SS      | Mean Square | F Value  | Pr > F |
| Site                    | 3        | 175.6103187    | 58.5367729  | 26.67    | <.0001 |
| Source                  | DF       | Type III SS    | Mean Square | F Value  | Pr > F |
| Site                    | 3        | 175.6103187    | 58.5367729  | 26.67    | <.0001 |
| Contrast                | DF       | Contrast SS    | Mean Square | F Value  | Pr > F |
| Llanederyn vs. the rest | 1        | 58.58336640    | 58.58336640 | 26.69    | <.0001 |

**Output 42.6.3** Univariate Analysis of Variance for Iron Oxide

| Romano-British Pottery |    |                |             |         |        |
|------------------------|----|----------------|-------------|---------|--------|
| The GLM Procedure      |    |                |             |         |        |
| Dependent Variable: Fe |    |                |             |         |        |
| Source                 | DF | Sum of Squares | Mean Square | F Value | Pr > F |
| Model                  | 3  | 134.2216158    | 44.7405386  | 89.88   | <.0001 |
| Error                  | 22 | 10.9508457     | 0.4977657   |         |        |
| Corrected Total        | 25 | 145.1724615    |             |         |        |

## Output 42.6.3 continued

|                         | R-Square | Coeff Var   | Root MSE    | Fe Mean  |        |  |
|-------------------------|----------|-------------|-------------|----------|--------|--|
|                         | 0.924567 | 15.79171    | 0.705525    | 4.467692 |        |  |
| Source                  | DF       | Type I SS   | Mean Square | F Value  | Pr > F |  |
| Site                    | 3        | 134.2216158 | 44.7405386  | 89.88    | <.0001 |  |
| Source                  | DF       | Type III SS | Mean Square | F Value  | Pr > F |  |
| Site                    | 3        | 134.2216158 | 44.7405386  | 89.88    | <.0001 |  |
| Contrast                | DF       | Contrast SS | Mean Square | F Value  | Pr > F |  |
| Llanederyn vs. the rest | 1        | 71.15144132 | 71.15144132 | 142.94   | <.0001 |  |

## Output 42.6.4 Univariate Analysis of Variance for Calcium Oxide

| Romano-British Pottery  |          |                |             |          |        |  |
|-------------------------|----------|----------------|-------------|----------|--------|--|
| The GLM Procedure       |          |                |             |          |        |  |
| Dependent Variable: Ca  |          |                |             |          |        |  |
| Source                  | DF       | Sum of Squares | Mean Square | F Value  | Pr > F |  |
| Model                   | 3        | 0.20470275     | 0.06823425  | 29.16    | <.0001 |  |
| Error                   | 22       | 0.05148571     | 0.00234026  |          |        |  |
| Corrected Total         | 25       | 0.25618846     |             |          |        |  |
|                         | R-Square | Coeff Var      | Root MSE    | Ca Mean  |        |  |
|                         | 0.799032 | 33.01265       | 0.048376    | 0.146538 |        |  |
| Source                  | DF       | Type I SS      | Mean Square | F Value  | Pr > F |  |
| Site                    | 3        | 0.20470275     | 0.06823425  | 29.16    | <.0001 |  |
| Source                  | DF       | Type III SS    | Mean Square | F Value  | Pr > F |  |
| Site                    | 3        | 0.20470275     | 0.06823425  | 29.16    | <.0001 |  |
| Contrast                | DF       | Contrast SS    | Mean Square | F Value  | Pr > F |  |
| Llanederyn vs. the rest | 1        | 0.03531688     | 0.03531688  | 15.09    | 0.0008 |  |

**Output 42.6.5** Univariate Analysis of Variance for Magnesium Oxide

| Romano-British Pottery  |          |                |             |          |        |
|-------------------------|----------|----------------|-------------|----------|--------|
| The GLM Procedure       |          |                |             |          |        |
| Dependent Variable: Mg  |          |                |             |          |        |
| Source                  | DF       | Sum of Squares | Mean Square | F Value  | Pr > F |
| Model                   | 3        | 103.3505270    | 34.4501757  | 49.12    | <.0001 |
| Error                   | 22       | 15.4296114     | 0.7013460   |          |        |
| Corrected Total         | 25       | 118.7801385    |             |          |        |
|                         | R-Square | Coeff Var      | Root MSE    | Mg Mean  |        |
|                         | 0.870099 | 26.65777       | 0.837464    | 3.141538 |        |
| Source                  | DF       | Type I SS      | Mean Square | F Value  | Pr > F |
| Site                    | 3        | 103.3505270    | 34.4501757  | 49.12    | <.0001 |
| Source                  | DF       | Type III SS    | Mean Square | F Value  | Pr > F |
| Site                    | 3        | 103.3505270    | 34.4501757  | 49.12    | <.0001 |
| Contrast                | DF       | Contrast SS    | Mean Square | F Value  | Pr > F |
| Llanederyn vs. the rest | 1        | 56.59349339    | 56.59349339 | 80.69    | <.0001 |

**Output 42.6.6** Univariate Analysis of Variance for Sodium Oxide

| Romano-British Pottery |    |                |             |         |        |
|------------------------|----|----------------|-------------|---------|--------|
| The GLM Procedure      |    |                |             |         |        |
| Dependent Variable: Na |    |                |             |         |        |
| Source                 | DF | Sum of Squares | Mean Square | F Value | Pr > F |
| Model                  | 3  | 0.25824560     | 0.08608187  | 9.50    | 0.0003 |
| Error                  | 22 | 0.19929286     | 0.00905877  |         |        |
| Corrected Total        | 25 | 0.45753846     |             |         |        |

## Output 42.6.6 continued

|                         | R-Square | Coeff Var   | Root MSE    | Na Mean  |        |  |
|-------------------------|----------|-------------|-------------|----------|--------|--|
|                         | 0.564424 | 60.06350    | 0.095178    | 0.158462 |        |  |
| Source                  | DF       | Type I SS   | Mean Square | F Value  | Pr > F |  |
| Site                    | 3        | 0.25824560  | 0.08608187  | 9.50     | 0.0003 |  |
| Source                  | DF       | Type III SS | Mean Square | F Value  | Pr > F |  |
| Site                    | 3        | 0.25824560  | 0.08608187  | 9.50     | 0.0003 |  |
| Contrast                | DF       | Contrast SS | Mean Square | F Value  | Pr > F |  |
| Llanederyn vs. the rest | 1        | 0.23344446  | 0.23344446  | 25.77    | <.0001 |  |

The **PRINTE** option in the **MANOVA** statement displays the elements of the error matrix, also called the Error Sums of Squares and Crossproducts matrix. (See [Output 42.6.7](#).) The diagonal elements of this matrix are the error sums of squares from the corresponding univariate analyses.

The **PRINTE** option also displays the partial correlation matrix associated with the E matrix. In this example, none of the oxides are very strongly correlated; the strongest correlation ( $r = 0.488$ ) is between magnesium oxide and calcium oxide.

## Output 42.6.7 Error SSCP Matrix and Partial Correlations

| Romano-British Pottery            |              |              |              |              |              |  |
|-----------------------------------|--------------|--------------|--------------|--------------|--------------|--|
| The GLM Procedure                 |              |              |              |              |              |  |
| Multivariate Analysis of Variance |              |              |              |              |              |  |
| E = Error SSCP Matrix             |              |              |              |              |              |  |
|                                   | Al           | Fe           | Mg           | Ca           | Na           |  |
| Al                                | 48.288142857 | 7.0800714286 | 0.6080142857 | 0.1064714286 | 0.5889571429 |  |
| Fe                                | 7.0800714286 | 10.950845714 | 0.5270571429 | -0.155194286 | 0.0667585714 |  |
| Mg                                | 0.6080142857 | 0.5270571429 | 15.429611429 | 0.4353771429 | 0.0276157143 |  |
| Ca                                | 0.1064714286 | -0.155194286 | 0.4353771429 | 0.0514857143 | 0.0100785714 |  |
| Na                                | 0.5889571429 | 0.0667585714 | 0.0276157143 | 0.0100785714 | 0.1992928571 |  |

## Output 42.6.7 continued

| Partial Correlation Coefficients from the Error SSCP Matrix / Prob >  r |                    |                     |                    |                     |                    |
|-------------------------------------------------------------------------|--------------------|---------------------|--------------------|---------------------|--------------------|
| DF = 22                                                                 | Al                 | Fe                  | Mg                 | Ca                  | Na                 |
| Al                                                                      | 1.000000           | 0.307889<br>0.1529  | 0.022275<br>0.9196 | 0.067526<br>0.7595  | 0.189853<br>0.3856 |
| Fe                                                                      | 0.307889<br>0.1529 | 1.000000            | 0.040547<br>0.8543 | -0.206685<br>0.3440 | 0.045189<br>0.8378 |
| Mg                                                                      | 0.022275<br>0.9196 | 0.040547<br>0.8543  | 1.000000           | 0.488478<br>0.0180  | 0.015748<br>0.9431 |
| Ca                                                                      | 0.067526<br>0.7595 | -0.206685<br>0.3440 | 0.488478<br>0.0180 | 1.000000            | 0.099497<br>0.6515 |
| Na                                                                      | 0.189853<br>0.3856 | 0.045189<br>0.8378  | 0.015748<br>0.9431 | 0.099497<br>0.6515  | 1.000000           |

The **PRINTH** option produces the SSCP matrix for the hypotheses being tested (Site and the contrast); see [Output 42.6.8](#) and [Output 42.6.9](#). Since the Type III SS are the highest-level SS produced by PROC GLM by default, and since the **HTYPE=** option is not specified, the SSCP matrix for Site gives the Type III **H** matrix. The diagonal elements of this matrix are the model sums of squares from the corresponding univariate analyses.

Four multivariate tests are computed, all based on the characteristic roots and vectors of  $\mathbf{E}^{-1}\mathbf{H}$ . These roots and vectors are displayed along with the tests. All four tests can be transformed to variates that have  $F$  distributions under the null hypothesis. Note that the four tests all give the same results for the contrast, since it has only one degree of freedom. In this case, the multivariate analysis matches the univariate results: there is an overall difference between the chemical composition of samples from different sites, and the samples from Llanederyn are different from the average of the other sites.

## Output 42.6.8 Hypothesis SSCP Matrix and Multivariate Tests for Overall Site Effect

| Romano-British Pottery            |              |              |              |              |              |
|-----------------------------------|--------------|--------------|--------------|--------------|--------------|
| The GLM Procedure                 |              |              |              |              |              |
| Multivariate Analysis of Variance |              |              |              |              |              |
| H = Type III SSCP Matrix for Site |              |              |              |              |              |
|                                   | Al           | Fe           | Mg           | Ca           | Na           |
| Al                                | 175.61031868 | -149.295533  | -130.8097066 | -5.889163736 | -5.372264835 |
| Fe                                | -149.295533  | 134.22161582 | 117.74503516 | 4.8217865934 | 5.3259491209 |
| Mg                                | -130.8097066 | 117.74503516 | 103.35052703 | 4.2091613187 | 4.7105458242 |
| Ca                                | -5.889163736 | 4.8217865934 | 4.2091613187 | 0.2047027473 | 0.154782967  |
| Na                                | -5.372264835 | 5.3259491209 | 4.7105458242 | 0.154782967  | 0.2582456044 |



## Output 42.6.8 continued

Characteristic Roots and Vectors of: E Inverse \* H, where  
H = Type III SSCP Matrix for Site  
E = Error SSCP Matrix

| Characteristic Root | Percent | Characteristic Vector V'EV=1 |             |             |             |             |
|---------------------|---------|------------------------------|-------------|-------------|-------------|-------------|
|                     |         | Al                           | Fe          | Mg          | Ca          | Na          |
| 34.1611140          | 96.39   | 0.09562211                   | -0.26330469 | -0.05305978 | -1.87982100 | -0.47071123 |
| 1.2500994           | 3.53    | 0.02651891                   | -0.01239715 | 0.17564390  | -4.25929785 | 1.23727668  |
| 0.0275396           | 0.08    | 0.09082220                   | 0.13159869  | 0.03508901  | -0.15701602 | -1.39364544 |
| 0.0000000           | 0.00    | 0.03673984                   | -0.15129712 | 0.20455529  | 0.54624873  | -0.17402107 |
| 0.0000000           | 0.00    | 0.06862324                   | 0.03056912  | -0.10662399 | 2.51151978  | 1.23668841  |

MANOVA Test Criteria and F Approximations for the Hypothesis of No Overall Site Effect  
H = Type III SSCP Matrix for Site  
E = Error SSCP Matrix

S=3    M=0.5    N=8

| Statistic              | Value       | F Value | Num DF | Den DF | Pr > F |
|------------------------|-------------|---------|--------|--------|--------|
| Wilks' Lambda          | 0.01230091  | 13.09   | 15     | 50.091 | <.0001 |
| Pillai's Trace         | 1.55393619  | 4.30    | 15     | 60     | <.0001 |
| Hotelling-Lawley Trace | 35.43875302 | 40.59   | 15     | 29.13  | <.0001 |
| Roy's Greatest Root    | 34.16111399 | 136.64  | 5      | 20     | <.0001 |

NOTE: F Statistic for Roy's Greatest Root is an upper bound.

## Output 42.6.9 Hypothesis SSCP Matrix and Multivariate Tests for Differences between Llanederyn and the Other Sites

H = Contrast SSCP Matrix for Llanederyn vs. the rest

|    | Al           | Fe           | Mg           | Ca           | Na           |
|----|--------------|--------------|--------------|--------------|--------------|
| Al | 58.583366402 | -64.56230291 | -57.57983466 | -1.438395503 | -3.698102513 |
| Fe | -64.56230291 | 71.151441323 | 63.456352116 | 1.5851961376 | 4.0755256878 |
| Mg | -57.57983466 | 63.456352116 | 56.593493386 | 1.4137558201 | 3.6347541005 |
| Ca | -1.438395503 | 1.5851961376 | 1.4137558201 | 0.0353168783 | 0.0907993915 |
| Na | -3.698102513 | 4.0755256878 | 3.6347541005 | 0.0907993915 | 0.2334444577 |

Output 42.6.9 continued

| Characteristic Roots and Vectors of: E Inverse * H, where<br>H = Contrast SSCP Matrix for Llanederyn vs. the rest<br>E = Error SSCP Matrix |         |                       |             |             |             |             |
|--------------------------------------------------------------------------------------------------------------------------------------------|---------|-----------------------|-------------|-------------|-------------|-------------|
| Characteristic Root                                                                                                                        | Percent | Characteristic Vector |             |             |             |             |
|                                                                                                                                            |         | Al                    | Fe          | Mg          | Ca          | Na          |
| 16.1251646                                                                                                                                 | 100.00  | -0.08883488           | 0.25458141  | 0.08723574  | 0.98158668  | 0.71925759  |
| 0.0000000                                                                                                                                  | 0.00    | -0.00503538           | 0.03825743  | -0.17632854 | 5.16256699  | -0.01022754 |
| 0.0000000                                                                                                                                  | 0.00    | 0.00162771            | -0.08885364 | -0.01774069 | -0.83096817 | 2.17644566  |
| 0.0000000                                                                                                                                  | 0.00    | 0.04450136            | -0.15722494 | 0.22156791  | 0.00000000  | 0.00000000  |
| 0.0000000                                                                                                                                  | 0.00    | 0.11939206            | 0.10833549  | 0.00000000  | 0.00000000  | 0.00000000  |

| MANOVA Test Criteria and Exact F Statistics for the Hypothesis<br>of No Overall Llanederyn vs. the rest Effect<br>H = Contrast SSCP Matrix for Llanederyn vs. the rest<br>E = Error SSCP Matrix |             |         |        |        |        |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------|---------|--------|--------|--------|
| S=1    M=1.5    N=8                                                                                                                                                                             |             |         |        |        |        |
| Statistic                                                                                                                                                                                       | Value       | F Value | Num DF | Den DF | Pr > F |
| Wilks' Lambda                                                                                                                                                                                   | 0.05839360  | 58.05   | 5      | 18     | <.0001 |
| Pillai's Trace                                                                                                                                                                                  | 0.94160640  | 58.05   | 5      | 18     | <.0001 |
| Hotelling-Lawley Trace                                                                                                                                                                          | 16.12516462 | 58.05   | 5      | 18     | <.0001 |
| Roy's Greatest Root                                                                                                                                                                             | 16.12516462 | 58.05   | 5      | 18     | <.0001 |

## Example 42.7: Repeated Measures Analysis of Variance

This example uses data from Cole and Grizzle (1966) to illustrate a commonly occurring repeated measures ANOVA design. Sixteen dogs are randomly assigned to four groups. (One animal is removed from the analysis due to a missing value for one dependent variable.) Dogs in each group receive either morphine or trimethaphan (variable Drug) and have either depleted or intact histamine levels (variable Depleted) before receiving the drugs. The dependent variable is the blood concentration of histamine at 0, 1, 3, and 5 minutes after injection of the drug. Logarithms are applied to these concentrations to minimize correlation between the mean and the variance of the data.

The following SAS statements perform both univariate and multivariate repeated measures analyses and produce Output 42.7.1 through Output 42.7.7.

```
data dogs;
 input Drug $12. Depleted $ Histamine0 Histamine1
 Histamine3 Histamine5;
 LogHistamine0=log(Histamine0);
 LogHistamine1=log(Histamine1);
 LogHistamine3=log(Histamine3);
 LogHistamine5=log(Histamine5);
 datalines;
Morphine N .04 .20 .10 .08
```

```

Morphine N .02 .06 .02 .02
Morphine N .07 1.40 .48 .24
Morphine N .17 .57 .35 .24
Morphine Y .10 .09 .13 .14
Morphine Y .12 .11 .10 .
Morphine Y .07 .07 .06 .07
Morphine Y .05 .07 .06 .07
Trimethaphan N .03 .62 .31 .22
Trimethaphan N .03 1.05 .73 .60
Trimethaphan N .07 .83 1.07 .80
Trimethaphan N .09 3.13 2.06 1.23
Trimethaphan Y .10 .09 .09 .08
Trimethaphan Y .08 .09 .09 .10
Trimethaphan Y .13 .10 .12 .12
Trimethaphan Y .06 .05 .05 .05
;

proc glm;
 class Drug Depleted;
 model LogHistamine0--LogHistamine5 =
 Drug Depleted Drug*Depleted / nouni;
 repeated Time 4 (0 1 3 5) polynomial / summary printe;
run;

```

The **NOUNI** option in the **MODEL** statement suppresses the individual ANOVA tables for the original dependent variables. These analyses are usually of no interest in a repeated measures analysis. The **POLYNOMIAL** option in the **REPEATED** statement indicates that the transformation used to implement the repeated measures analysis is an orthogonal polynomial transformation, and the **SUMMARY** option requests that the univariate analyses for the orthogonal polynomial contrast variables be displayed. The parenthetical numbers (0 1 3 5) determine the spacing of the orthogonal polynomials used in the analysis.

#### Output 42.7.1 Summary Information about Groups

| The GLM Procedure              |                         |
|--------------------------------|-------------------------|
| Class Level Information        |                         |
| Class                          | Levels Values           |
| Drug                           | 2 Morphine Trimethaphan |
| Depleted                       | 2 N Y                   |
| Number of Observations Read 16 |                         |
| Number of Observations Used 15 |                         |

The “Repeated Measures Level Information” table gives information about the repeated measures effect; it is displayed in [Output 42.7.2](#). In this example, the within-subject (within-dog) effect is Time, which has the levels 0, 1, 3, and 5.

**Output 42.7.2** Repeated Measures Levels

| The GLM Procedure                      |                   |                   |                   |                   |
|----------------------------------------|-------------------|-------------------|-------------------|-------------------|
| Repeated Measures Analysis of Variance |                   |                   |                   |                   |
| Repeated Measures Level Information    |                   |                   |                   |                   |
| Dependent Variable                     | Log<br>Histamine0 | Log<br>Histamine1 | Log<br>Histamine3 | Log<br>Histamine5 |
| Level of Time                          | 0                 | 1                 | 3                 | 5                 |

The multivariate analyses for within-subject effects and related interactions are displayed in [Output 42.7.3](#). For the example, the first table displayed shows that the TIME effect is significant. In addition, the Time\*Drug\*Depleted interaction is significant, as shown in the fourth table. This means that the effect of Time on the blood concentration of histamine is different for the four Drug\*Depleted combinations studied.

**Output 42.7.3** Multivariate Tests of Within-Subject Effects

| MANOVA Test Criteria and Exact F Statistics for the Hypothesis of no Time Effect      |            |         |        |        |        |
|---------------------------------------------------------------------------------------|------------|---------|--------|--------|--------|
| H = Type III SSCP Matrix for Time                                                     |            |         |        |        |        |
| E = Error SSCP Matrix                                                                 |            |         |        |        |        |
| S=1    M=0.5    N=3.5                                                                 |            |         |        |        |        |
| Statistic                                                                             | Value      | F Value | Num DF | Den DF | Pr > F |
| Wilks' Lambda                                                                         | 0.11097706 | 24.03   | 3      | 9      | 0.0001 |
| Pillai's Trace                                                                        | 0.88902294 | 24.03   | 3      | 9      | 0.0001 |
| Hotelling-Lawley Trace                                                                | 8.01087137 | 24.03   | 3      | 9      | 0.0001 |
| Roy's Greatest Root                                                                   | 8.01087137 | 24.03   | 3      | 9      | 0.0001 |
| MANOVA Test Criteria and Exact F Statistics for the Hypothesis of no Time*Drug Effect |            |         |        |        |        |
| H = Type III SSCP Matrix for Time*Drug                                                |            |         |        |        |        |
| E = Error SSCP Matrix                                                                 |            |         |        |        |        |
| S=1    M=0.5    N=3.5                                                                 |            |         |        |        |        |
| Statistic                                                                             | Value      | F Value | Num DF | Den DF | Pr > F |
| Wilks' Lambda                                                                         | 0.34155984 | 5.78    | 3      | 9      | 0.0175 |
| Pillai's Trace                                                                        | 0.65844016 | 5.78    | 3      | 9      | 0.0175 |
| Hotelling-Lawley Trace                                                                | 1.92774470 | 5.78    | 3      | 9      | 0.0175 |
| Roy's Greatest Root                                                                   | 1.92774470 | 5.78    | 3      | 9      | 0.0175 |

## Output 42.7.3 continued

| MANOVA Test Criteria and Exact F Statistics for<br>the Hypothesis of no Time*Depleted Effect<br>H = Type III SSCP Matrix for Time*Depleted<br>E = Error SSCP Matrix |            |         |        |        |        |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------|---------|--------|--------|--------|
| S=1    M=0.5    N=3.5                                                                                                                                               |            |         |        |        |        |
| Statistic                                                                                                                                                           | Value      | F Value | Num DF | Den DF | Pr > F |
| Wilks' Lambda                                                                                                                                                       | 0.12339988 | 21.31   | 3      | 9      | 0.0002 |
| Pillai's Trace                                                                                                                                                      | 0.87660012 | 21.31   | 3      | 9      | 0.0002 |
| Hotelling-Lawley Trace                                                                                                                                              | 7.10373567 | 21.31   | 3      | 9      | 0.0002 |
| Roy's Greatest Root                                                                                                                                                 | 7.10373567 | 21.31   | 3      | 9      | 0.0002 |

| MANOVA Test Criteria and Exact F Statistics for<br>the Hypothesis of no Time*Drug*Depleted Effect<br>H = Type III SSCP Matrix for Time*Drug*Depleted<br>E = Error SSCP Matrix |            |         |        |        |        |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------|---------|--------|--------|--------|
| S=1    M=0.5    N=3.5                                                                                                                                                         |            |         |        |        |        |
| Statistic                                                                                                                                                                     | Value      | F Value | Num DF | Den DF | Pr > F |
| Wilks' Lambda                                                                                                                                                                 | 0.19383010 | 12.48   | 3      | 9      | 0.0015 |
| Pillai's Trace                                                                                                                                                                | 0.80616990 | 12.48   | 3      | 9      | 0.0015 |
| Hotelling-Lawley Trace                                                                                                                                                        | 4.15915732 | 12.48   | 3      | 9      | 0.0015 |
| Roy's Greatest Root                                                                                                                                                           | 4.15915732 | 12.48   | 3      | 9      | 0.0015 |

Output 42.7.4 displays tests of hypotheses for between-subject (between-dog) effects. This section tests the hypotheses that the different Drugs, Depleteds, and their interactions have no effects on the dependent variables, while ignoring the within-dog effects. From this analysis, there is a significant between-dog effect for Depleted ( $p$ -value=0.0229). The interaction and the main effect for Drug are not significant ( $p$ -values=0.1734 and 0.1281, respectively).

## Output 42.7.4 Tests of Between-Subject Effects

| The GLM Procedure<br>Repeated Measures Analysis of Variance<br>Tests of Hypotheses for Between Subjects Effects |    |             |             |         |        |
|-----------------------------------------------------------------------------------------------------------------|----|-------------|-------------|---------|--------|
| Source                                                                                                          | DF | Type III SS | Mean Square | F Value | Pr > F |
| Drug                                                                                                            | 1  | 5.99336243  | 5.99336243  | 2.71    | 0.1281 |
| Depleted                                                                                                        | 1  | 15.44840703 | 15.44840703 | 6.98    | 0.0229 |
| Drug*Depleted                                                                                                   | 1  | 4.69087508  | 4.69087508  | 2.12    | 0.1734 |
| Error                                                                                                           | 11 | 24.34683348 | 2.21334850  |         |        |

Univariate analyses for within-subject (within-dog) effects and related interactions are displayed in [Output 42.7.6](#). The results for this example are the same as for the multivariate analyses; this is not always the case. In addition, before the univariate analyses are used to make conclusions about the data, the result of the sphericity test (requested with the `PRINTE` option in the `REPEATED` statement and displayed in [Output 42.7.5](#)) should be examined. If the sphericity test is rejected, consider using the adjusted G-G or H-F-L probabilities. See the section “[Repeated Measures Analysis of Variance](#)” on page 3367 for more information.

**Output 42.7.5** Sphericity Test

| Sphericity Tests      |    |                     |            |            |
|-----------------------|----|---------------------|------------|------------|
| Variables             | DF | Mauchly's Criterion | Chi-Square | Pr > ChiSq |
| Transformed Variates  | 5  | 0.1752641           | 16.930873  | 0.0046     |
| Orthogonal Components | 5  | 0.1752641           | 16.930873  | 0.0046     |

**Output 42.7.6** Univariate Tests of Within-Subject Effects

| The GLM Procedure                                         |    |             |             |                              |        |           |              |
|-----------------------------------------------------------|----|-------------|-------------|------------------------------|--------|-----------|--------------|
| Repeated Measures Analysis of Variance                    |    |             |             |                              |        |           |              |
| Univariate Tests of Hypotheses for Within Subject Effects |    |             |             |                              |        |           |              |
| Source                                                    | DF | Type III SS | Mean Square | F Value                      | Pr > F | Adj G - G | Pr > F H-F-L |
| Time                                                      | 3  | 12.05898677 | 4.01966226  | 53.44                        | <.0001 | <.0001    | <.0001       |
| Time*Drug                                                 | 3  | 1.84429514  | 0.61476505  | 8.17                         | 0.0003 | 0.0039    | 0.0023       |
| Time*Depleted                                             | 3  | 12.08978557 | 4.02992852  | 53.57                        | <.0001 | <.0001    | <.0001       |
| Time*Drug*Depleted                                        | 3  | 2.93077939  | 0.97692646  | 12.99                        | <.0001 | 0.0005    | 0.0002       |
| Error (Time)                                              | 33 | 2.48238887  | 0.07522391  |                              |        |           |              |
|                                                           |    |             |             | Greenhouse-Geisser Epsilon   | 0.5694 |           |              |
|                                                           |    |             |             | Huynh-Feldt-Lecoutre Epsilon | 0.6636 |           |              |

[Output 42.7.7](#) is produced by the `SUMMARY` option in the `REPEATED` statement. If the `POLYNOMIAL` option is not used, a similar table is displayed using the default `CONTRAST` transformation. The linear, quadratic, and cubic trends for Time, labeled as ‘Time\_1’, ‘Time\_2’, and ‘Time\_3’, are displayed, and in each case, the Source labeled ‘Mean’ gives a test for the respective trend.

**Output 42.7.7** Tests of Between-Subject Effects for Transformed Variables

| The GLM Procedure                                             |    |             |             |         |        |
|---------------------------------------------------------------|----|-------------|-------------|---------|--------|
| Repeated Measures Analysis of Variance                        |    |             |             |         |        |
| Analysis of Variance of Contrast Variables                    |    |             |             |         |        |
| Time_N represents the nth degree polynomial contrast for Time |    |             |             |         |        |
| Contrast Variable: Time_1                                     |    |             |             |         |        |
| Source                                                        | DF | Type III SS | Mean Square | F Value | Pr > F |
| Mean                                                          | 1  | 2.00963483  | 2.00963483  | 34.99   | 0.0001 |
| Drug                                                          | 1  | 1.18069076  | 1.18069076  | 20.56   | 0.0009 |
| Depleted                                                      | 1  | 1.36172504  | 1.36172504  | 23.71   | 0.0005 |
| Drug*Depleted                                                 | 1  | 2.04346848  | 2.04346848  | 35.58   | <.0001 |
| Error                                                         | 11 | 0.63171161  | 0.05742833  |         |        |
| Contrast Variable: Time_2                                     |    |             |             |         |        |
| Source                                                        | DF | Type III SS | Mean Square | F Value | Pr > F |
| Mean                                                          | 1  | 5.40988418  | 5.40988418  | 57.15   | <.0001 |
| Drug                                                          | 1  | 0.59173192  | 0.59173192  | 6.25    | 0.0295 |
| Depleted                                                      | 1  | 5.94945506  | 5.94945506  | 62.86   | <.0001 |
| Drug*Depleted                                                 | 1  | 0.67031587  | 0.67031587  | 7.08    | 0.0221 |
| Error                                                         | 11 | 1.04118707  | 0.09465337  |         |        |
| Contrast Variable: Time_3                                     |    |             |             |         |        |
| Source                                                        | DF | Type III SS | Mean Square | F Value | Pr > F |
| Mean                                                          | 1  | 4.63946776  | 4.63946776  | 63.04   | <.0001 |
| Drug                                                          | 1  | 0.07187246  | 0.07187246  | 0.98    | 0.3443 |
| Depleted                                                      | 1  | 4.77860547  | 4.77860547  | 64.94   | <.0001 |
| Drug*Depleted                                                 | 1  | 0.21699504  | 0.21699504  | 2.95    | 0.1139 |
| Error                                                         | 11 | 0.80949018  | 0.07359002  |         |        |

**Example 42.8: Mixed Model Analysis of Variance with the RANDOM Statement**

Milliken and Johnson (1984) present an example of an unbalanced mixed model. Three machines, which are considered as a fixed effect, and six employees, which are considered a random effect, are studied. Each employee operates each machine for either one, two, or three different times. The dependent variable is an overall rating, which takes into account the number and quality of components produced.

The following statements form the data set and perform a mixed model analysis of variance by requesting the **TEST** option in the **RANDOM** statement. Note that the machine\*person interaction is declared as a

random effect; in general, when an interaction involves a random effect, it too should be declared as random. The results of the analysis are shown in [Output 42.8.1](#) through [Output 42.8.4](#).

```

data machine;
 input machine person rating @@;
 datalines;
1 1 52.0 1 2 51.8 1 2 52.8 1 3 60.0 1 4 51.1 1 4 52.3 1 5 50.9
1 5 51.8 1 5 51.4 1 6 46.4 1 6 44.8 1 6 49.2 2 1 64.0 2 2 59.7
2 2 60.0 2 2 59.0 2 3 68.6 2 3 65.8 2 4 63.2 2 4 62.8 2 4 62.2
2 5 64.8 2 5 65.0 2 6 43.7 2 6 44.2 2 6 43.0 3 1 67.5 3 1 67.2
3 1 66.9 3 2 61.5 3 2 61.7 3 2 62.3 3 3 70.8 3 3 70.6 3 3 71.0
3 4 64.1 3 4 66.2 3 4 64.0 3 5 72.1 3 5 72.0 3 5 71.1 3 6 62.0
3 6 61.4 3 6 60.5
;

proc glm data=machine;
 class machine person;
 model rating=machine person machine*person;
 random person machine*person / test;
run;

```

The **TEST** option in the **RANDOM** statement requests that PROC GLM determine the appropriate *F* tests based on **person** and **machine\*person** being treated as random effects. As you can see in [Output 42.8.4](#), this requires that a linear combination of mean squares be constructed to test both the machine and person hypotheses; thus, *F* tests that use Satterthwaite approximations are needed.

**Output 42.8.1** Summary Information about Groups

| The GLM Procedure           |        |             |
|-----------------------------|--------|-------------|
| Class Level Information     |        |             |
| Class                       | Levels | Values      |
| machine                     | 3      | 1 2 3       |
| person                      | 6      | 1 2 3 4 5 6 |
| Number of Observations Read |        | 44          |
| Number of Observations Used |        | 44          |



**Output 42.8.2** Fixed-Effect Model Analysis of Variance

| The GLM Procedure          |          |                |             |             |        |
|----------------------------|----------|----------------|-------------|-------------|--------|
| Dependent Variable: rating |          |                |             |             |        |
| Source                     | DF       | Sum of Squares | Mean Square | F Value     | Pr > F |
| Model                      | 17       | 3061.743333    | 180.102549  | 206.41      | <.0001 |
| Error                      | 26       | 22.686667      | 0.872564    |             |        |
| Corrected Total            | 43       | 3084.430000    |             |             |        |
|                            | R-Square | Coeff Var      | Root MSE    | rating Mean |        |
|                            | 0.992645 | 1.560754       | 0.934111    | 59.85000    |        |
| Source                     | DF       | Type I SS      | Mean Square | F Value     | Pr > F |
| machine                    | 2        | 1648.664722    | 824.332361  | 944.72      | <.0001 |
| person                     | 5        | 1008.763583    | 201.752717  | 231.22      | <.0001 |
| machine*person             | 10       | 404.315028     | 40.431503   | 46.34       | <.0001 |
| Source                     | DF       | Type III SS    | Mean Square | F Value     | Pr > F |
| machine                    | 2        | 1238.197626    | 619.098813  | 709.52      | <.0001 |
| person                     | 5        | 1011.053834    | 202.210767  | 231.74      | <.0001 |
| machine*person             | 10       | 404.315028     | 40.431503   | 46.34       | <.0001 |

**Output 42.8.3** Expected Values of Type III Mean Squares

| Source         | Type III Expected Mean Square                                                                            |
|----------------|----------------------------------------------------------------------------------------------------------|
| machine        | $\text{Var}(\text{Error}) + 2.137 \text{Var}(\text{machine*person}) + Q(\text{machine})$                 |
| person         | $\text{Var}(\text{Error}) + 2.2408 \text{Var}(\text{machine*person}) + 6.7224 \text{Var}(\text{person})$ |
| machine*person | $\text{Var}(\text{Error}) + 2.3162 \text{Var}(\text{machine*person})$                                    |

**Output 42.8.4** Mixed Model Analysis of Variance

| The GLM Procedure                                        |        |             |             |         |        |
|----------------------------------------------------------|--------|-------------|-------------|---------|--------|
| Tests of Hypotheses for Mixed Model Analysis of Variance |        |             |             |         |        |
| Dependent Variable: rating                               |        |             |             |         |        |
| Source                                                   | DF     | Type III SS | Mean Square | F Value | Pr > F |
| machine                                                  | 2      | 1238.197626 | 619.098813  | 16.57   | 0.0007 |
| Error                                                    | 10.036 | 375.057436  | 37.370384   |         |        |
| Error: 0.9226*MS(machine*person) + 0.0774*MS(Error)      |        |             |             |         |        |
| Source                                                   | DF     | Type III SS | Mean Square | F Value | Pr > F |
| person                                                   | 5      | 1011.053834 | 202.210767  | 5.17    | 0.0133 |
| Error                                                    | 10.015 | 392.005726  | 39.143708   |         |        |
| Error: 0.9674*MS(machine*person) + 0.0326*MS(Error)      |        |             |             |         |        |
| Source                                                   | DF     | Type III SS | Mean Square | F Value | Pr > F |
| machine*person                                           | 10     | 404.315028  | 40.431503   | 46.34   | <.0001 |
| Error: MS(Error)                                         | 26     | 22.686667   | 0.872564    |         |        |

Note that you can also use the MIXED procedure to analyze mixed models. The following statements use PROC MIXED to reproduce the mixed model analysis of variance; the relevant part of the PROC MIXED results is shown in [Output 42.8.5](#).

```
proc mixed data=machine method=type3;
 class machine person;
 model rating = machine;
 random person machine*person;
run;
```

**Output 42.8.5** PROC MIXED Mixed Model Analysis of Variance (Partial Output)

| The Mixed Procedure         |    |                |             |
|-----------------------------|----|----------------|-------------|
| Type 3 Analysis of Variance |    |                |             |
| Source                      | DF | Sum of Squares | Mean Square |
| machine                     | 2  | 1238.197626    | 619.098813  |
| person                      | 5  | 1011.053834    | 202.210767  |
| machine*person              | 10 | 404.315028     | 40.431503   |
| Residual                    | 26 | 22.686667      | 0.872564    |

| Type 3 Analysis of Variance |                                                                 |
|-----------------------------|-----------------------------------------------------------------|
| Source                      | Expected Mean Square                                            |
| machine                     | Var(Residual) + 2.137 Var(machine*person) + Q(machine)          |
| person                      | Var(Residual) + 2.2408 Var(machine*person) + 6.7224 Var(person) |
| machine*person              | Var(Residual) + 2.3162 Var(machine*person)                      |
| Residual                    | Var(Residual)                                                   |

| Type 3 Analysis of Variance |                                                    |        |         |        |
|-----------------------------|----------------------------------------------------|--------|---------|--------|
| Source                      | Error Term                                         | Error  |         |        |
|                             |                                                    | DF     | F Value | Pr > F |
| machine                     | 0.9226 MS(machine*person)<br>+ 0.0774 MS(Residual) | 10.036 | 16.57   | 0.0007 |
| person                      | 0.9674 MS(machine*person)<br>+ 0.0326 MS(Residual) | 10.015 | 5.17    | 0.0133 |
| machine*person              | MS(Residual)                                       | 26     | 46.34   | <.0001 |
| Residual                    | .                                                  | .      | .       | .      |

The advantage of PROC MIXED is that it offers more versatility for mixed models; the disadvantage is that it can be less computationally efficient for large data sets. See Chapter 59, “The MIXED Procedure,” for more details.

### Example 42.9: Analyzing a Doubly Multivariate Repeated Measures Design

This example shows how to analyze a doubly multivariate repeated measures design by using PROC GLM with an IDENTITY factor in the REPEATED statement. Note that this differs from previous releases of PROC GLM, in which you had to use a MANOVA statement to get a doubly repeated measures analysis.

Two responses, Y1 and Y2, are each measured three times for each subject (pretreatment, posttreatment, and in a later follow-up). Each subject receives one of three treatments; A, B, or the control. In PROC GLM, you use a REPEATED factor of type IDENTITY to identify the different responses and another repeated factor to identify the different measurement times. The repeated measures analysis includes multivariate tests for time and treatment main effects, as well as their interactions, across responses. The following statements produce Output 42.9.1 through Output 42.9.3.

```

options ls=96;
data Trial;
 input Treatment $ Repetition PreY1 PostY1 FollowY1
 PreY2 PostY2 FollowY2;
 datalines;
A 1 3 13 9 0 0 9
A 2 0 14 10 6 6 3
A 3 4 6 17 8 2 6
A 4 7 7 13 7 6 4
A 5 3 12 11 6 12 6
A 6 10 14 8 13 3 8
B 1 9 11 17 8 11 27
B 2 4 16 13 9 3 26
B 3 8 10 9 12 0 18
B 4 5 9 13 3 0 14
B 5 0 15 11 3 0 25
B 6 4 11 14 4 2 9
Control 1 10 12 15 4 3 7
Control 2 2 8 12 8 7 20
Control 3 4 9 10 2 0 10
Control 4 10 8 8 5 8 14
Control 5 11 11 11 1 0 11
Control 6 1 5 15 8 9 10
;

proc glm data=Trial;
 class Treatment;
 model PreY1 PostY1 FollowY1
 PreY2 PostY2 FollowY2 = Treatment / nouni;
 repeated Response 2 identity, Time 3;
run;

```

**Output 42.9.1** A Doubly Multivariate Repeated Measures Design

| The GLM Procedure           |        |             |
|-----------------------------|--------|-------------|
| Class Level Information     |        |             |
| Class                       | Levels | Values      |
| Treatment                   | 3      | A B Control |
| Number of Observations Read |        | 18          |
| Number of Observations Used |        | 18          |

The levels of the repeated factors are displayed in [Output 42.9.2](#). Note that RESPONSE is 1 for all the Y1 measurements and 2 for all the Y2 measurements, while the three levels of Time identify the pretreatment, posttreatment, and follow-up measurements within each response. The multivariate tests for within-subject effects are displayed in [Output 42.9.3](#).

**Output 42.9.2** Repeated Factor Levels

| The GLM Procedure                      |       |        |          |       |        |          |
|----------------------------------------|-------|--------|----------|-------|--------|----------|
| Repeated Measures Analysis of Variance |       |        |          |       |        |          |
| Repeated Measures Level Information    |       |        |          |       |        |          |
| Dependent Variable                     | PreY1 | PostY1 | FollowY1 | PreY2 | PostY2 | FollowY2 |
| Level of Response                      | 1     | 1      | 1        | 2     | 2      | 2        |
| Level of Time                          | 1     | 2      | 3        | 1     | 2      | 3        |

**Output 42.9.3** Within-Subject Tests

| MANOVA Test Criteria and Exact F Statistics for the Hypothesis of no Response Effect         |             |         |        |        |        |  |
|----------------------------------------------------------------------------------------------|-------------|---------|--------|--------|--------|--|
| H = Type III SSCP Matrix for Response                                                        |             |         |        |        |        |  |
| E = Error SSCP Matrix                                                                        |             |         |        |        |        |  |
| S=1      M=0      N=6                                                                        |             |         |        |        |        |  |
| Statistic                                                                                    | Value       | F Value | Num DF | Den DF | Pr > F |  |
| Wilks' Lambda                                                                                | 0.02165587  | 316.24  | 2      | 14     | <.0001 |  |
| Pillai's Trace                                                                               | 0.97834413  | 316.24  | 2      | 14     | <.0001 |  |
| Hotelling-Lawley Trace                                                                       | 45.17686368 | 316.24  | 2      | 14     | <.0001 |  |
| Roy's Greatest Root                                                                          | 45.17686368 | 316.24  | 2      | 14     | <.0001 |  |
| MANOVA Test Criteria and F Approximations for the Hypothesis of no Response*Treatment Effect |             |         |        |        |        |  |
| H = Type III SSCP Matrix for Response*Treatment                                              |             |         |        |        |        |  |
| E = Error SSCP Matrix                                                                        |             |         |        |        |        |  |
| S=2      M=-0.5      N=6                                                                     |             |         |        |        |        |  |
| Statistic                                                                                    | Value       | F Value | Num DF | Den DF | Pr > F |  |
| Wilks' Lambda                                                                                | 0.72215797  | 1.24    | 4      | 28     | 0.3178 |  |
| Pillai's Trace                                                                               | 0.27937444  | 1.22    | 4      | 30     | 0.3240 |  |
| Hotelling-Lawley Trace                                                                       | 0.38261660  | 1.31    | 4      | 15.818 | 0.3074 |  |
| Roy's Greatest Root                                                                          | 0.37698780  | 2.83    | 2      | 15     | 0.0908 |  |
| NOTE: F Statistic for Roy's Greatest Root is an upper bound.                                 |             |         |        |        |        |  |
| NOTE: F Statistic for Wilks' Lambda is exact.                                                |             |         |        |        |        |  |

Output 42.9.3 continued

MANOVA Test Criteria and Exact F Statistics for the Hypothesis of no Response\*Time Effect  
H = Type III SSCP Matrix for Response\*Time  
E = Error SSCP Matrix

|                        | S=1        | M=1     | N=5    |        |        |  |
|------------------------|------------|---------|--------|--------|--------|--|
| Statistic              | Value      | F Value | Num DF | Den DF | Pr > F |  |
| Wilks' Lambda          | 0.14071380 | 18.32   | 4      | 12     | <.0001 |  |
| Pillai's Trace         | 0.85928620 | 18.32   | 4      | 12     | <.0001 |  |
| Hotelling-Lawley Trace | 6.10662362 | 18.32   | 4      | 12     | <.0001 |  |
| Roy's Greatest Root    | 6.10662362 | 18.32   | 4      | 12     | <.0001 |  |

MANOVA Test Criteria and F Approximations for the  
Hypothesis of no Response\*Time\*Treatment Effect  
H = Type III SSCP Matrix for Response\*Time\*Treatment  
E = Error SSCP Matrix

|                        | S=2        | M=0.5   | N=5    |        |        |  |
|------------------------|------------|---------|--------|--------|--------|--|
| Statistic              | Value      | F Value | Num DF | Den DF | Pr > F |  |
| Wilks' Lambda          | 0.22861451 | 3.27    | 8      | 24     | 0.0115 |  |
| Pillai's Trace         | 0.96538785 | 3.03    | 8      | 26     | 0.0151 |  |
| Hotelling-Lawley Trace | 2.52557514 | 3.64    | 8      | 15     | 0.0149 |  |
| Roy's Greatest Root    | 2.12651905 | 6.91    | 4      | 13     | 0.0033 |  |

NOTE: F Statistic for Roy's Greatest Root is an upper bound.  
NOTE: F Statistic for Wilks' Lambda is exact.

The table for Response\*Treatment tests for an overall treatment effect across the two responses; likewise, the tables for Response\*Time and Response\*Treatment\*Time test for time and the treatment-by-time interaction, respectively. In this case, there is a strong main effect for time and possibly for the interaction, but not for treatment.

In previous releases (before the IDENTITY transformation was introduced), in order to perform a doubly repeated measures analysis, you had to use a MANOVA statement with a customized transformation matrix M. You might still want to use this approach to see details of the analysis, such as the univariate ANOVA for each transformed variate. The following statements demonstrate this approach by using the MANOVA statement to test for the overall main effect of time and specifying the SUMMARY option.

```
proc glm data=Trials;
 class Treatment;
 model PreY1 PostY1 FollowY1
 PreY2 PostY2 FollowY2 = Treatment / nouni;
 manova h=intercept m=prey1 - posty1,
 prey1 - followy1,
 prey2 - posty2,
 prey2 - followy2 / summary;
run;
```

The M matrix used to perform the test for time effects is displayed in [Output 42.9.4](#), while the results of the multivariate test are given in [Output 42.9.5](#). Note that the test results are the same as for the Response\*Time effect in [Output 42.9.3](#).

**Output 42.9.4** M Matrix to Test for Time Effect (Repeated Measure)

| The GLM Procedure                         |       |        |          |       |        |          |
|-------------------------------------------|-------|--------|----------|-------|--------|----------|
| Multivariate Analysis of Variance         |       |        |          |       |        |          |
| M Matrix Describing Transformed Variables |       |        |          |       |        |          |
|                                           | PreY1 | PostY1 | FollowY1 | PreY2 | PostY2 | FollowY2 |
| MVAR1                                     | 1     | -1     | 0        | 0     | 0      | 0        |
| MVAR2                                     | 1     | 0      | -1       | 0     | 0      | 0        |
| MVAR3                                     | 0     | 0      | 0        | 1     | -1     | 0        |
| MVAR4                                     | 0     | 0      | 0        | 1     | 0      | -1       |

**Output 42.9.5** Tests for Time Effect (Repeated Measure)

| The GLM Procedure                                                                                                                                     |            |                       |             |             |            |  |
|-------------------------------------------------------------------------------------------------------------------------------------------------------|------------|-----------------------|-------------|-------------|------------|--|
| Multivariate Analysis of Variance                                                                                                                     |            |                       |             |             |            |  |
| Characteristic Roots and Vectors of: E Inverse * H, where                                                                                             |            |                       |             |             |            |  |
| H = Type III SSCP Matrix for Intercept                                                                                                                |            |                       |             |             |            |  |
| E = Error SSCP Matrix                                                                                                                                 |            |                       |             |             |            |  |
| Variables have been transformed by the M Matrix                                                                                                       |            |                       |             |             |            |  |
| Characteristic Root                                                                                                                                   | Percent    | Characteristic Vector |             | V'EV=1      |            |  |
|                                                                                                                                                       |            | MVAR1                 | MVAR2       | MVAR3       | MVAR4      |  |
| 6.10662362                                                                                                                                            | 100.00     | -0.00157729           | 0.04081620  | -0.04210209 | 0.03519437 |  |
| 0.00000000                                                                                                                                            | 0.00       | 0.00796367            | 0.00493217  | 0.05185236  | 0.00377940 |  |
| 0.00000000                                                                                                                                            | 0.00       | -0.03534089           | -0.01502146 | -0.00283074 | 0.04259372 |  |
| 0.00000000                                                                                                                                            | 0.00       | -0.05672137           | 0.04500208  | 0.00000000  | 0.00000000 |  |
| MANOVA Test Criteria and Exact F Statistics for the Hypothesis of No Overall Intercept Effect on the Variables Defined by the M Matrix Transformation |            |                       |             |             |            |  |
| H = Type III SSCP Matrix for Intercept                                                                                                                |            |                       |             |             |            |  |
| E = Error SSCP Matrix                                                                                                                                 |            |                       |             |             |            |  |
|                                                                                                                                                       | S=1        | M=1                   | N=5         |             |            |  |
| Statistic                                                                                                                                             | Value      | F Value               | Num DF      | Den DF      | Pr > F     |  |
| Wilks' Lambda                                                                                                                                         | 0.14071380 | 18.32                 | 4           | 12          | <.0001     |  |
| Pillai's Trace                                                                                                                                        | 0.85928620 | 18.32                 | 4           | 12          | <.0001     |  |
| Hotelling-Lawley Trace                                                                                                                                | 6.10662362 | 18.32                 | 4           | 12          | <.0001     |  |
| Roy's Greatest Root                                                                                                                                   | 6.10662362 | 18.32                 | 4           | 12          | <.0001     |  |

The **SUMMARY** option in the **MANOVA** statement creates an ANOVA table for each transformed variable as defined by the M matrix. MVAR1 and MVAR2 contrast the pretreatment measurement for Y1 with

the posttreatment and follow-up measurements for Y1, respectively; MVAR3 and MVAR4 are the same contrasts for Y2. [Output 42.9.6](#) displays these univariate ANOVA tables and shows that the contrasts are all strongly significant except for the pre-versus-post difference for Y2.

**Output 42.9.6** Summary Output for the Test for Time Effect

| The GLM Procedure                 |    |             |             |         |        |
|-----------------------------------|----|-------------|-------------|---------|--------|
| Multivariate Analysis of Variance |    |             |             |         |        |
| Dependent Variable: MVAR1         |    |             |             |         |        |
| Source                            | DF | Type III SS | Mean Square | F Value | Pr > F |
| Intercept                         | 1  | 512.0000000 | 512.0000000 | 22.65   | 0.0003 |
| Error                             | 15 | 339.0000000 | 22.6000000  |         |        |

| The GLM Procedure                 |    |             |             |         |        |
|-----------------------------------|----|-------------|-------------|---------|--------|
| Multivariate Analysis of Variance |    |             |             |         |        |
| Dependent Variable: MVAR2         |    |             |             |         |        |
| Source                            | DF | Type III SS | Mean Square | F Value | Pr > F |
| Intercept                         | 1  | 813.3888889 | 813.3888889 | 32.87   | <.0001 |
| Error                             | 15 | 371.1666667 | 24.7444444  |         |        |

| The GLM Procedure                 |    |             |             |         |        |
|-----------------------------------|----|-------------|-------------|---------|--------|
| Multivariate Analysis of Variance |    |             |             |         |        |
| Dependent Variable: MVAR3         |    |             |             |         |        |
| Source                            | DF | Type III SS | Mean Square | F Value | Pr > F |
| Intercept                         | 1  | 68.0555556  | 68.0555556  | 3.49    | 0.0814 |
| Error                             | 15 | 292.5000000 | 19.5000000  |         |        |

| The GLM Procedure                 |    |             |             |         |        |
|-----------------------------------|----|-------------|-------------|---------|--------|
| Multivariate Analysis of Variance |    |             |             |         |        |
| Dependent Variable: MVAR4         |    |             |             |         |        |
| Source                            | DF | Type III SS | Mean Square | F Value | Pr > F |
| Intercept                         | 1  | 800.0000000 | 800.0000000 | 26.43   | 0.0001 |
| Error                             | 15 | 454.0000000 | 30.2666667  |         |        |

## Example 42.10: Testing for Equal Group Variances

This example demonstrates how you can test for equal group variances in a one-way design. The data come from the University of Pennsylvania Smell Identification Test (UPSIT), reported in O'Brien and Heft (1995). The study is undertaken to explore how age and gender are related to sense of smell. A total of 180 subjects



20 to 89 years old are exposed to 40 different odors: for each odor, subjects are asked to choose which of four words best describes the odor. The Freeman-Tukey modified arcsine transformation (Bishop, Fienberg, and Holland 1975) is applied to the proportion of correctly identified odors to arrive at an olfactory index. For the following analysis, subjects are divided into five age groups:

$$\text{agegroup} = \begin{cases} 1 & \text{if } \text{age} \leq 25 \\ 2 & \text{if } 25 < \text{age} \leq 40 \\ 3 & \text{if } 40 < \text{age} \leq 55 \\ 4 & \text{if } 55 < \text{age} \leq 70 \\ 5 & \text{if } 70 < \text{age} \end{cases}$$

The following statements create a data set named `upsit`, containing the age group and olfactory index for each subject.

```
data upsit;
 input agegroup smell @@;
 datalines;
1 1.381 1 1.322 1 1.162 1 1.275 1 1.381 1 1.275 1 1.322
1 1.492 1 1.322 1 1.381 1 1.162 1 1.013 1 1.322 1 1.322
1 1.275 1 1.492 1 1.322 1 1.322 1 1.492 1 1.322 1 1.381
1 1.234 1 1.162 1 1.381 1 1.381 1 1.381 1 1.322 1 1.381
1 1.322 1 1.381 1 1.275 1 1.492 1 1.275 1 1.322 1 1.275
1 1.381 1 1.234 1 1.105
2 1.234 2 1.234 2 1.381 2 1.322 2 1.492 2 1.234 2 1.381
2 1.381 2 1.492 2 1.492 2 1.275 2 1.492 2 1.381 2 1.492
2 1.322 2 1.275 2 1.275 2 1.275 2 1.322 2 1.492 2 1.381
2 1.322 2 1.492 2 1.196 2 1.322 2 1.275 2 1.234 2 1.322
2 1.098 2 1.322 2 1.381 2 1.275 2 1.492 2 1.492 2 1.381
2 1.196
3 1.381 3 1.381 3 1.492 3 1.492 3 1.492 3 1.098 3 1.492
3 1.381 3 1.234 3 1.234 3 1.129 3 1.069 3 1.234 3 1.322
3 1.275 3 1.230 3 1.234 3 1.234 3 1.322 3 1.322 3 1.381
4 1.322 4 1.381 4 1.381 4 1.322 4 1.234 4 1.234 4 1.234
4 1.381 4 1.322 4 1.275 4 1.275 4 1.492 4 1.234 4 1.098
4 1.322 4 1.129 4 0.687 4 1.322 4 1.322 4 1.234 4 1.129
4 1.492 4 0.810 4 1.234 4 1.381 4 1.040 4 1.381 4 1.381
4 1.129 4 1.492 4 1.129 4 1.098 4 1.275 4 1.322 4 1.234
4 1.196 4 1.234 4 0.585 4 0.785 4 1.275 4 1.322 4 0.712
4 0.810
5 1.322 5 1.234 5 1.381 5 1.275 5 1.275 5 1.322 5 1.162
5 0.909 5 0.502 5 1.234 5 1.322 5 1.196 5 0.859 5 1.196
5 1.381 5 1.322 5 1.234 5 1.275 5 1.162 5 1.162 5 0.585
5 1.013 5 0.960 5 0.662 5 1.129 5 0.531 5 1.162 5 0.737
5 1.098 5 1.162 5 1.040 5 0.558 5 0.960 5 1.098 5 0.884
5 1.162 5 1.098 5 0.859 5 1.275 5 1.162 5 0.785 5 0.859
;
```

Older people are more at risk for problems with their sense of smell, and this should be reflected in significant differences in the mean of the olfactory index across the different age groups. However, many older people also have an excellent sense of smell, which implies that the older age groups should have greater variability. In order to test this hypothesis and to compute a one-way ANOVA for the olfactory index that is

robust to the possibility of unequal group variances, you can use the **HOVTEST** and **WELCH** options in the **MEANS** statement for the GLM procedure, as shown in the following statements.

```
proc glm data=upsit;
 class agegroup;
 model smell = agegroup;
 means agegroup / hovtest welch;
run;
```

Output 42.10.1, Output 42.10.2, and Output 42.10.3 display the usual ANOVA test for equal age group means, Levene's test for equal age group variances, and Welch's test for equal age group means, respectively. The hypotheses of age effects for mean and variance of the olfactory index are both confirmed.

**Output 42.10.1** Usual ANOVA Test for Age Group Differences in Mean Olfactory Index

| The GLM Procedure         |    |             |             |         |        |
|---------------------------|----|-------------|-------------|---------|--------|
| Dependent Variable: smell |    |             |             |         |        |
| Source                    | DF | Type III SS | Mean Square | F Value | Pr > F |
| agegroup                  | 4  | 2.13878141  | 0.53469535  | 16.65   | <.0001 |

**Output 42.10.2** Levene's Test for Age Group Differences in Olfactory Variability

| The GLM Procedure                               |     |                |             |         |        |
|-------------------------------------------------|-----|----------------|-------------|---------|--------|
| Levene's Test for Homogeneity of smell Variance |     |                |             |         |        |
| ANOVA of Squared Deviations from Group Means    |     |                |             |         |        |
| Source                                          | DF  | Sum of Squares | Mean Square | F Value | Pr > F |
| agegroup                                        | 4   | 0.0799         | 0.0200      | 6.35    | <.0001 |
| Error                                           | 175 | 0.5503         | 0.00314     |         |        |

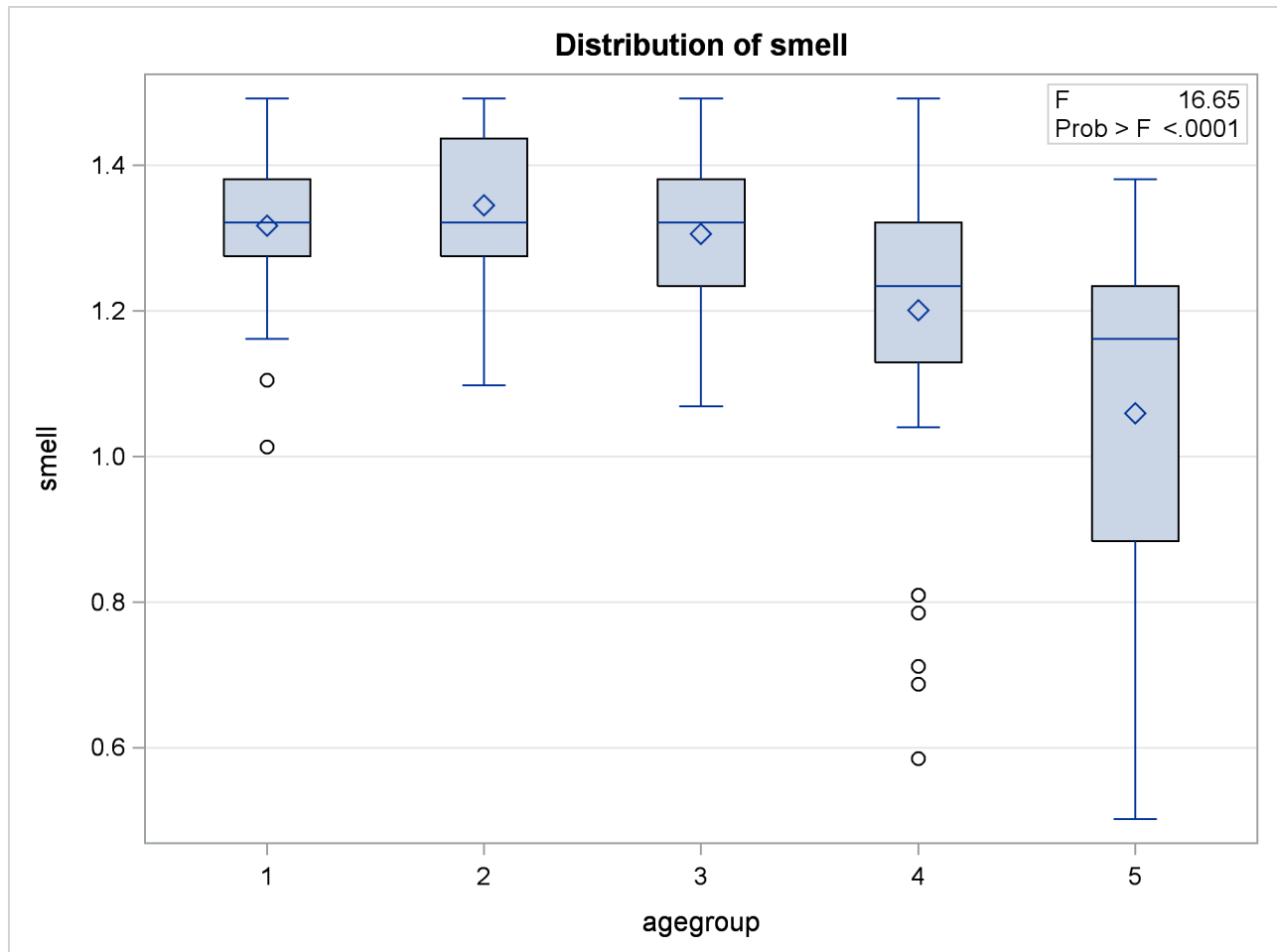
**Output 42.10.3** Welch's Test for Age Group Differences in Mean Olfactory Index

| Welch's ANOVA for smell |         |         |        |
|-------------------------|---------|---------|--------|
| Source                  | DF      | F Value | Pr > F |
| agegroup                | 4.0000  | 13.72   | <.0001 |
| Error                   | 78.7489 |         |        |

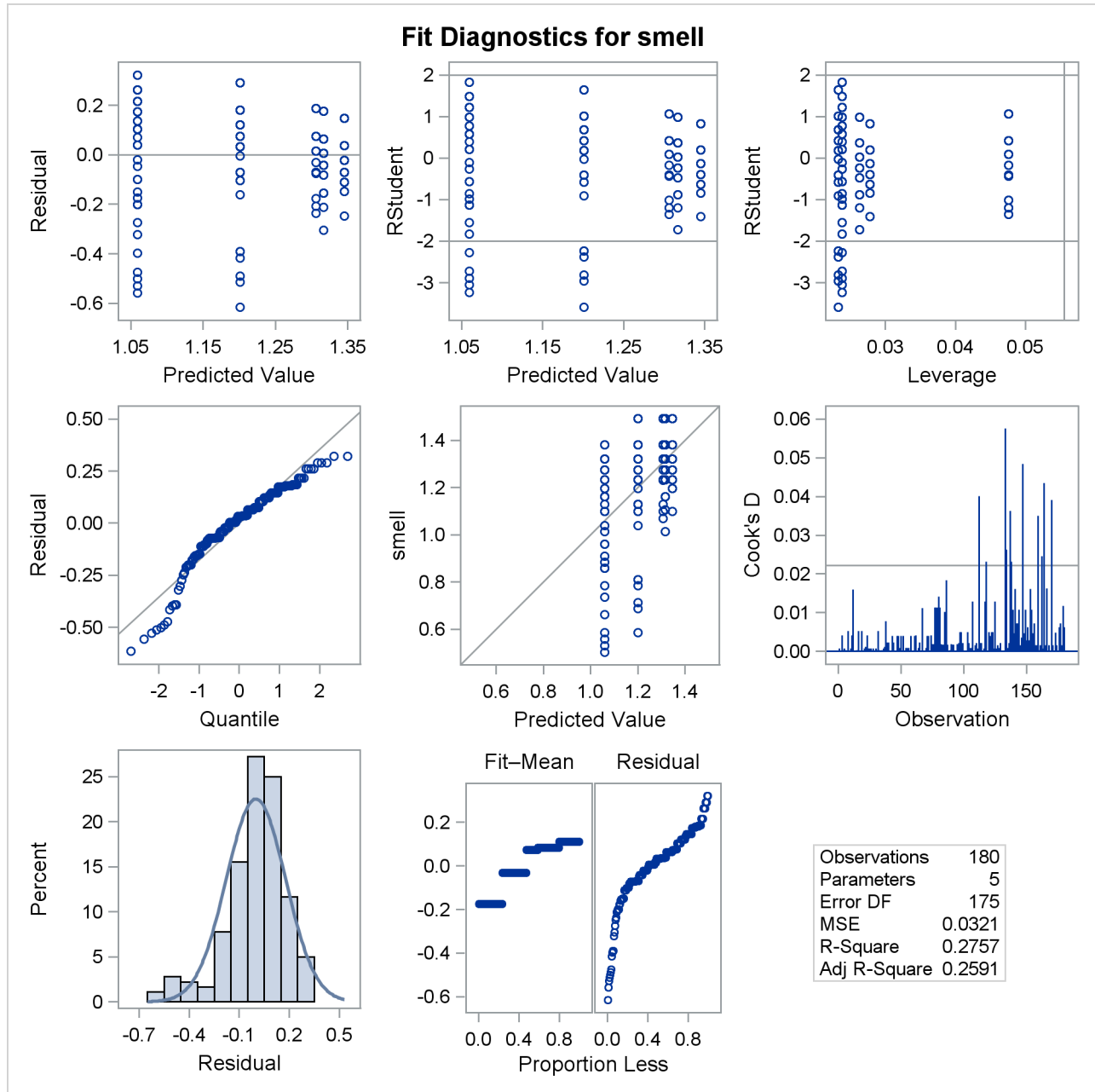
As discussed in “Homogeneity of Variance in One-Way Models” on page 3362, Levene’s test or any other test for homogeneity of variance should not be used as a diagnostic for the assumption of equal group variances that underlies the usual analysis of variance. However, graphical diagnostics can be a useful informal tool for monitoring whether your data meet the assumptions of a GLM analysis. The following statements perform a one-way ANOVA as before, but with ODS Graphics enabled. In addition to the box plot that is produced by default, the `PLOTS=DIAGNOSTICS` option requests a panel of summary diagnostics for the fit. These additional plots are shown in [Output 42.10.4](#) and [Output 42.10.5](#).

```
ods graphics on;
proc glm data=upsit plot=diagnostics;
 class agegroup;
 model smell = agegroup;
run;
ods graphics off;
```

**Output 42.10.4** Box Plot of Olfactory Index by Age Group



**Output 42.10.5** Diagnostics for One-Way ANOVA of Olfactory Index by Age Group



Output 42.10.4 clearly shows different degrees of variability for olfactory index within different age groups, with the variability generally rising with age. Likewise, several of the plots in the diagnostics panel shown in Output 42.10.5 indicate a relationship between olfactory variability and mean olfactory index. Also, note that the plot of Cook's  $D$  statistic indicates that observations in the higher, more variable age groups are overly influential on the analysis of group means. The overall inference from these plots is that an assumption of equal group variances is probably untenable and that the analysis of the group means should thus take this into account.

## Example 42.11: Analysis of a Screening Design

Yin and Jillie (1987) describe an experiment performed on a nitride etch process for a single wafer plasma etcher. The experiment is run using four factors: cathode power (`power`), gas flow (`flow`), reactor chamber pressure (`pressure`), and electrode gap (`gap`). Of interest are the main effects and interaction effects of the factors on the nitride etch rate (`rate`). The following statements create a SAS data set named `HalfFraction`, containing the factor settings and the observed etch rate for each of eight experimental runs.

```
data HalfFraction;
 input power flow pressure gap rate;
 datalines;
0.8 4.5 125 275 550
0.8 4.5 200 325 650
0.8 550.0 125 325 642
0.8 550.0 200 275 601
1.2 4.5 125 325 749
1.2 4.5 200 275 1052
1.2 550.0 125 275 1075
1.2 550.0 200 325 729
;
```

Notice that each of the factors has just two values. This is a common experimental design when the intent is to screen from the many factors that *might* affect the response the few that actually *do*. Since there are  $2^4 = 16$  different possible settings of four two-level factors, this design with only eight runs is called a “half fraction.” The eight runs are chosen specifically to provide unambiguous information on main effects at the cost of confounding interaction effects with each other.

One way to analyze these data is simply to use PROC GLM to compute an analysis of variance, including both main effects and interactions in the model. The following statements demonstrate this approach.

```
proc glm data=HalfFraction;
 class power flow pressure gap;
 model rate=power|flow|pressure|gap@2;
run;
```

The “@2” notation in the `MODEL` statement includes all main effects and two-factor interactions between the factors. The output is shown in [Output 42.11.1](#).

**Output 42.11.1** Analysis of Variance for Nitride Etch Process Half Fraction

| The GLM Procedure       |        |         |
|-------------------------|--------|---------|
| Class Level Information |        |         |
| Class                   | Levels | Values  |
| power                   | 2      | 0.8 1.2 |
| flow                    | 2      | 4.5 550 |
| pressure                | 2      | 125 200 |
| gap                     | 2      | 275 325 |

Output 42.11.1 continued

|                             |          |                |             |           |        |
|-----------------------------|----------|----------------|-------------|-----------|--------|
| Number of Observations Read |          | 8              |             |           |        |
| Number of Observations Used |          | 8              |             |           |        |
| The GLM Procedure           |          |                |             |           |        |
| Dependent Variable: rate    |          |                |             |           |        |
| Source                      | DF       | Sum of Squares | Mean Square | F Value   | Pr > F |
| Model                       | 7        | 280848.0000    | 40121.1429  | .         | .      |
| Error                       | 0        | 0.0000         | .           | .         | .      |
| Corrected Total             | 7        | 280848.0000    |             |           |        |
|                             | R-Square | Coeff Var      | Root MSE    | rate Mean |        |
|                             | 1.000000 | .              | .           | 756.0000  |        |
| Source                      | DF       | Type I SS      | Mean Square | F Value   | Pr > F |
| power                       | 1        | 168780.5000    | 168780.5000 | .         | .      |
| flow                        | 1        | 264.5000       | 264.5000    | .         | .      |
| power*flow                  | 1        | 200.0000       | 200.0000    | .         | .      |
| pressure                    | 1        | 32.0000        | 32.0000     | .         | .      |
| power*pressure              | 1        | 1300.5000      | 1300.5000   | .         | .      |
| flow*pressure               | 1        | 78012.5000     | 78012.5000  | .         | .      |
| gap                         | 1        | 32258.0000     | 32258.0000  | .         | .      |
| power*gap                   | 0        | 0.0000         | .           | .         | .      |
| flow*gap                    | 0        | 0.0000         | .           | .         | .      |
| pressure*gap                | 0        | 0.0000         | .           | .         | .      |
| Source                      | DF       | Type III SS    | Mean Square | F Value   | Pr > F |
| power                       | 1        | 168780.5000    | 168780.5000 | .         | .      |
| flow                        | 1        | 264.5000       | 264.5000    | .         | .      |
| power*flow                  | 0        | 0.0000         | .           | .         | .      |
| pressure                    | 1        | 32.0000        | 32.0000     | .         | .      |
| power*pressure              | 0        | 0.0000         | .           | .         | .      |
| flow*pressure               | 0        | 0.0000         | .           | .         | .      |
| gap                         | 1        | 32258.0000     | 32258.0000  | .         | .      |
| power*gap                   | 0        | 0.0000         | .           | .         | .      |
| flow*gap                    | 0        | 0.0000         | .           | .         | .      |
| pressure*gap                | 0        | 0.0000         | .           | .         | .      |

Notice that there are no error degrees of freedom. This is because there are 10 effects in the model (4 main effects plus 6 interactions) but only 8 observations in the data set. This is another cost of using a fractional design: not only is it impossible to estimate all the main effects and interactions, but there is also no information left to estimate the underlying error rate in order to measure the significance of the effects that are estimable.

Another thing to notice in [Output 42.11.1](#) is the difference between the Type I and Type III ANOVA tables. The rows corresponding to main effects in each are the same, but no Type III interaction tests are estimable, while some Type I interaction tests are estimable. This indicates that there is *aliasing* in the design: some interactions are completely confounded with each other.

In order to analyze this confounding, you should examine the aliasing structure of the design by using the **ALIASING** option in the **MODEL** statement. Before doing so, however, it is advisable to *code* the design, replacing low and high levels of each factor with the values  $-1$  and  $+1$ , respectively. This puts each factor on an equal footing in the model and makes the aliasing structure much more interpretable. The following statements code the data, creating a new data set named Coded.

```
data Coded; set HalfFraction;
 power = -1*(power =0.80) + 1*(power =1.20);
 flow = -1*(flow =4.50) + 1*(flow =550);
 pressure = -1*(pressure=125) + 1*(pressure=200);
 gap = -1*(gap =275) + 1*(gap =325);
run;
```

The following statements use the GLM procedure to reanalyze the coded design, displaying the parameter estimates as well as the functions of the parameters that they each estimate.

```
proc glm data=Coded;
 model rate=power|flow|pressure|gap@2 / solution aliasing;
run;
```

The parameter estimates table is shown in [Output 42.11.2](#).

**Output 42.11.2** Parameter Estimates and Aliases for Nitride Etch Process Half Fraction

| The GLM Procedure        |              |                |         |         |                           |
|--------------------------|--------------|----------------|---------|---------|---------------------------|
| Dependent Variable: rate |              |                |         |         |                           |
| Parameter                | Estimate     | Standard Error | t Value | Pr >  t | Expected Value            |
| Intercept                | 756.000000   | .              | .       | .       | Intercept                 |
| power                    | 145.250000   | .              | .       | .       | power                     |
| flow                     | 5.750000     | .              | .       | .       | flow                      |
| power*flow               | -5.000000 B  | .              | .       | .       | power*flow + pressure*gap |
| pressure                 | 2.000000     | .              | .       | .       | pressure                  |
| power*pressure           | -12.750000 B | .              | .       | .       | power*pressure + flow*gap |
| flow*pressure            | -98.750000 B | .              | .       | .       | flow*pressure + power*gap |
| gap                      | -63.500000   | .              | .       | .       | gap                       |
| power*gap                | 0.000000 B   | .              | .       | .       |                           |
| flow*gap                 | 0.000000 B   | .              | .       | .       |                           |
| pressure*gap             | 0.000000 B   | .              | .       | .       |                           |

In the “Expected Value” column, notice that, while each of the main effects is unambiguously estimated by its associated term in the model, the expected values of the interaction estimates are more complicated. For example, the relatively large effect ( $-98.75$ ) corresponding to `flow*pressure` actually estimates the combined effect of `flow*pressure` and `power*gap`. Without further information, it is impossible to disentangle these

aliased interactions; however, since the main effects of both power and gap are large and those for flow and pressure are small, it is reasonable to suspect that power\*gap is the more “active” of the two interactions.

Fortunately, eight more runs are available for this experiment (the other half fraction). The following statements create a data set containing these extra runs and add it to the previous eight, resulting in a full  $2^4 = 16$  run replicate. Then PROC GLM displays the analysis of variance again.

```
data OtherHalf;
 input power flow pressure gap rate;
 datalines;
0.8 4.5 125 325 669
0.8 4.5 200 275 604
0.8 550.0 125 275 633
0.8 550.0 200 325 635
1.2 4.5 125 275 1037
1.2 4.5 200 325 868
1.2 550.0 125 325 860
1.2 550.0 200 275 1063
;
data FullRep;
 set HalfFraction OtherHalf;
run;

proc glm data=FullRep;
 class power flow pressure gap;
 model rate=power|flow|pressure|gap@2;
run;
```

The results are displayed in [Output 42.11.3](#).

### Output 42.11.3 Analysis of Variance for Nitride Etch Process Full Replicate

| The GLM Procedure           |        |         |
|-----------------------------|--------|---------|
| Class Level Information     |        |         |
| Class                       | Levels | Values  |
| power                       | 2      | 0.8 1.2 |
| flow                        | 2      | 4.5 550 |
| pressure                    | 2      | 125 200 |
| gap                         | 2      | 275 325 |
| Number of Observations Read |        | 16      |
| Number of Observations Used |        | 16      |



Output 42.11.3 *continued*

| The GLM Procedure        |          |                |             |           |        |
|--------------------------|----------|----------------|-------------|-----------|--------|
| Dependent Variable: rate |          |                |             |           |        |
| Source                   | DF       | Sum of Squares | Mean Square | F Value   | Pr > F |
| Model                    | 10       | 521234.1250    | 52123.4125  | 25.58     | 0.0011 |
| Error                    | 5        | 10186.8125     | 2037.3625   |           |        |
| Corrected Total          | 15       | 531420.9375    |             |           |        |
|                          | R-Square | Coeff Var      | Root MSE    | rate Mean |        |
|                          | 0.980831 | 5.816175       | 45.13715    | 776.0625  |        |
| Source                   | DF       | Type I SS      | Mean Square | F Value   | Pr > F |
| power                    | 1        | 374850.0625    | 374850.0625 | 183.99    | <.0001 |
| flow                     | 1        | 217.5625       | 217.5625    | 0.11      | 0.7571 |
| power*flow               | 1        | 18.0625        | 18.0625     | 0.01      | 0.9286 |
| pressure                 | 1        | 10.5625        | 10.5625     | 0.01      | 0.9454 |
| power*pressure           | 1        | 1.5625         | 1.5625      | 0.00      | 0.9790 |
| flow*pressure            | 1        | 7700.0625      | 7700.0625   | 3.78      | 0.1095 |
| gap                      | 1        | 41310.5625     | 41310.5625  | 20.28     | 0.0064 |
| power*gap                | 1        | 94402.5625     | 94402.5625  | 46.34     | 0.0010 |
| flow*gap                 | 1        | 2475.0625      | 2475.0625   | 1.21      | 0.3206 |
| pressure*gap             | 1        | 248.0625       | 248.0625    | 0.12      | 0.7414 |
| Source                   | DF       | Type III SS    | Mean Square | F Value   | Pr > F |
| power                    | 1        | 374850.0625    | 374850.0625 | 183.99    | <.0001 |
| flow                     | 1        | 217.5625       | 217.5625    | 0.11      | 0.7571 |
| power*flow               | 1        | 18.0625        | 18.0625     | 0.01      | 0.9286 |
| pressure                 | 1        | 10.5625        | 10.5625     | 0.01      | 0.9454 |
| power*pressure           | 1        | 1.5625         | 1.5625      | 0.00      | 0.9790 |
| flow*pressure            | 1        | 7700.0625      | 7700.0625   | 3.78      | 0.1095 |
| gap                      | 1        | 41310.5625     | 41310.5625  | 20.28     | 0.0064 |
| power*gap                | 1        | 94402.5625     | 94402.5625  | 46.34     | 0.0010 |
| flow*gap                 | 1        | 2475.0625      | 2475.0625   | 1.21      | 0.3206 |
| pressure*gap             | 1        | 248.0625       | 248.0625    | 0.12      | 0.7414 |

With 16 runs, the analysis of variance tells the whole story: all effects are estimable and there are five degrees of freedom left over to estimate the underlying error. The main effects of **power** and **gap** and their interaction are all significant, and no other effects are. Notice that the Type I and Type III ANOVA tables are the same; this is because the design is orthogonal and all effects are estimable.

This example illustrates the use of the GLM procedure for the model analysis of a screening experiment. Typically, there is much more involved in performing an experiment of this type, from selecting the design points to be studied to graphically assessing significant effects, optimizing the final model, and performing

subsequent experimentation. Specialized tools for this are available in SAS/QC software, in particular the ADX Interface and the FACTEX and OPTEx procedures. See *SAS/QC User's Guide* for more information.

---

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# Chapter 43

## The GLMMOD Procedure

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### Overview: GLMMOD Procedure

The GLMMOD procedure constructs the design matrix for a general linear model; it essentially constitutes the model-building front end for the GLM procedure. You can use the GLMMOD procedure in conjunction with other SAS/STAT software regression procedures or with SAS/IML software to obtain specialized analyses for general linear models that you cannot obtain with the GLM procedure.

While some of the regression procedures in SAS/STAT software provide for general linear effects modeling with classification variables and interaction or polynomial effects, many others do not. For such procedures, you must specify the model directly in terms of distinct variables. For example, if you want to use the REG procedure to fit a polynomial model, you must first create the crossproduct and power terms as new variables, usually in a DATA step. Alternatively, you can use the GLMMOD procedure to create a data set that contains the design matrix for a model as specified using the effects modeling facilities of the GLM procedure.

Note that the TRANSREG procedure provides alternative methods to construct design matrices for full-rank and less-than-full-rank models, polynomials, and splines. See Chapter 97, “The TRANSREG Procedure,” for more information.

---

## Getting Started: GLMMOD Procedure

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### A One-Way Design

A one-way analysis of variance considers one treatment factor with two or more treatment levels. This example employs PROC GLMMOD together with PROC REG to perform a one-way analysis of variance to study the effect of bacteria on the nitrogen content of red clover plants. The treatment factor is bacteria strain, and it has six levels. Red clover plants are inoculated with the treatments, and nitrogen content is later measured in milligrams. The data are derived from an experiment by Erdman (1946) and are analyzed in Chapters 7 and 8 of Steel and Torrie (1980). PROC GLMMOD is used to create the design matrix. The following DATA step creates the SAS data set Clover.

```

title 'Nitrogen Content of Red Clover Plants';
data Clover;
 input Strain $ Nitrogen @@;
 datalines;
3DOK1 19.4 3DOK1 32.6 3DOK1 27.0 3DOK1 32.1 3DOK1 33.0
3DOK5 17.7 3DOK5 24.8 3DOK5 27.9 3DOK5 25.2 3DOK5 24.3
3DOK4 17.0 3DOK4 19.4 3DOK4 9.1 3DOK4 11.9 3DOK4 15.8
3DOK7 20.7 3DOK7 21.0 3DOK7 20.5 3DOK7 18.8 3DOK7 18.6
3DOK13 14.3 3DOK13 14.4 3DOK13 11.8 3DOK13 11.6 3DOK13 14.2
COMPOS 17.3 COMPOS 19.4 COMPOS 19.1 COMPOS 16.9 COMPOS 20.8
;

```

The variable Strain contains the treatment levels, and the variable Nitrogen contains the response. The following statements produce the design matrix:

```

proc glmmod data=Clover;
 class Strain;
 model Nitrogen = Strain;
run;

```

The classification variable, or treatment factor, is specified in the CLASS statement. The MODEL statement defines the response and independent variables. The design matrix produced corresponds to the model

$$Y_{i,j} = \mu + \alpha_i + \epsilon_{i,j}$$

where  $i = 1, \dots, 6$  and  $j = 1, \dots, 5$ .

Figure 43.1 and Figure 43.2 display the output produced by these statements. Figure 43.1 displays information about the data set, which is useful for checking your data.

**Figure 43.1** Class Level Information and Parameter Definitions

| Nitrogen Content of Red Clover Plants |                           |                              |        |       |       |              |
|---------------------------------------|---------------------------|------------------------------|--------|-------|-------|--------------|
| The GLMMOD Procedure                  |                           |                              |        |       |       |              |
| Class Level Information               |                           |                              |        |       |       |              |
| Class                                 | Levels                    | Values                       |        |       |       |              |
| Strain                                | 6                         | 3DOK1                        | 3DOK13 | 3DOK4 | 3DOK5 | 3DOK7 COMPOS |
| Number of Observations Read           |                           |                              |        | 30    |       |              |
| Number of Observations Used           |                           |                              |        | 30    |       |              |
| Parameter Definitions                 |                           |                              |        |       |       |              |
| Column Number                         | Name of Associated Effect | CLASS Variable Values Strain |        |       |       |              |
| 1                                     | Intercept                 |                              |        |       |       |              |
| 2                                     | Strain                    | 3DOK1                        |        |       |       |              |
| 3                                     | Strain                    | 3DOK13                       |        |       |       |              |
| 4                                     | Strain                    | 3DOK4                        |        |       |       |              |
| 5                                     | Strain                    | 3DOK5                        |        |       |       |              |
| 6                                     | Strain                    | 3DOK7                        |        |       |       |              |
| 7                                     | Strain                    | COMPOS                       |        |       |       |              |

The design matrix, shown in Figure 43.2, consists of seven columns: one for the mean and six for the treatment levels. The vector of responses, Nitrogen, is also displayed.

Figure 43.2 Design Matrix

| Observation<br>Number | Nitrogen | Design Points |   |   |   |   |   |   |
|-----------------------|----------|---------------|---|---|---|---|---|---|
|                       |          | 1             | 2 | 3 | 4 | 5 | 6 | 7 |
| 1                     | 19.4     | 1             | 1 | 0 | 0 | 0 | 0 | 0 |
| 2                     | 32.6     | 1             | 1 | 0 | 0 | 0 | 0 | 0 |
| 3                     | 27.0     | 1             | 1 | 0 | 0 | 0 | 0 | 0 |
| 4                     | 32.1     | 1             | 1 | 0 | 0 | 0 | 0 | 0 |
| 5                     | 33.0     | 1             | 1 | 0 | 0 | 0 | 0 | 0 |
| 6                     | 17.7     | 1             | 0 | 0 | 0 | 1 | 0 | 0 |
| 7                     | 24.8     | 1             | 0 | 0 | 0 | 1 | 0 | 0 |
| 8                     | 27.9     | 1             | 0 | 0 | 0 | 1 | 0 | 0 |
| 9                     | 25.2     | 1             | 0 | 0 | 0 | 1 | 0 | 0 |
| 10                    | 24.3     | 1             | 0 | 0 | 0 | 1 | 0 | 0 |
| 11                    | 17.0     | 1             | 0 | 0 | 1 | 0 | 0 | 0 |
| 12                    | 19.4     | 1             | 0 | 0 | 1 | 0 | 0 | 0 |
| 13                    | 9.1      | 1             | 0 | 0 | 1 | 0 | 0 | 0 |
| 14                    | 11.9     | 1             | 0 | 0 | 1 | 0 | 0 | 0 |
| 15                    | 15.8     | 1             | 0 | 0 | 1 | 0 | 0 | 0 |
| 16                    | 20.7     | 1             | 0 | 0 | 0 | 0 | 1 | 0 |
| 17                    | 21.0     | 1             | 0 | 0 | 0 | 0 | 1 | 0 |
| 18                    | 20.5     | 1             | 0 | 0 | 0 | 0 | 1 | 0 |
| 19                    | 18.8     | 1             | 0 | 0 | 0 | 0 | 1 | 0 |
| 20                    | 18.6     | 1             | 0 | 0 | 0 | 0 | 1 | 0 |
| 21                    | 14.3     | 1             | 0 | 1 | 0 | 0 | 0 | 0 |
| 22                    | 14.4     | 1             | 0 | 1 | 0 | 0 | 0 | 0 |
| 23                    | 11.8     | 1             | 0 | 1 | 0 | 0 | 0 | 0 |
| 24                    | 11.6     | 1             | 0 | 1 | 0 | 0 | 0 | 0 |
| 25                    | 14.2     | 1             | 0 | 1 | 0 | 0 | 0 | 0 |
| 26                    | 17.3     | 1             | 0 | 0 | 0 | 0 | 0 | 1 |
| 27                    | 19.4     | 1             | 0 | 0 | 0 | 0 | 0 | 1 |
| 28                    | 19.1     | 1             | 0 | 0 | 0 | 0 | 0 | 1 |
| 29                    | 16.9     | 1             | 0 | 0 | 0 | 0 | 0 | 1 |
| 30                    | 20.8     | 1             | 0 | 0 | 0 | 0 | 0 | 1 |

Usually, you will find PROC GLMMOD most useful for the data sets it can create rather than for its displayed output. For example, the following statements use PROC GLMMOD to save the design matrix for the clover study to the data set CloverDesign instead of displaying it.

```
proc glmmmod data=Clover outdesign=CloverDesign noprint;
 class Strain;
 model Nitrogen = Strain;
run;
```

Now you can use the REG procedure to analyze the data, as the following statements demonstrate:

```
proc reg data=CloverDesign;
 model Nitrogen = Col2-Col7;
run;
```

The results are shown in Figure 43.3.

Figure 43.3 Regression Analysis Using the REG Procedure

| Nitrogen Content of Red Clover Plants                                                                                                                                                   |               |                |                    |                |         |         |
|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------|----------------|--------------------|----------------|---------|---------|
| The REG Procedure                                                                                                                                                                       |               |                |                    |                |         |         |
| Model: MODEL1                                                                                                                                                                           |               |                |                    |                |         |         |
| Dependent Variable: Nitrogen                                                                                                                                                            |               |                |                    |                |         |         |
| Number of Observations Read                                                                                                                                                             |               | 30             |                    |                |         |         |
| Number of Observations Used                                                                                                                                                             |               | 30             |                    |                |         |         |
| Analysis of Variance                                                                                                                                                                    |               |                |                    |                |         |         |
| Source                                                                                                                                                                                  | DF            | Sum of Squares | Mean Square        | F Value        | Pr > F  |         |
| Model                                                                                                                                                                                   | 5             | 847.04667      | 169.40933          | 14.37          | <.0001  |         |
| Error                                                                                                                                                                                   | 24            | 282.92800      | 11.78867           |                |         |         |
| Corrected Total                                                                                                                                                                         | 29            | 1129.97467     |                    |                |         |         |
| Root MSE                                                                                                                                                                                |               | 3.43346        | R-Square           | 0.7496         |         |         |
| Dependent Mean                                                                                                                                                                          |               | 19.88667       | Adj R-Sq           | 0.6975         |         |         |
| Coeff Var                                                                                                                                                                               |               | 17.26515       |                    |                |         |         |
| NOTE: Model is not full rank. Least-squares solutions for the parameters are not unique. Some statistics will be misleading. A reported DF of 0 or B means that the estimate is biased. |               |                |                    |                |         |         |
| NOTE: The following parameters have been set to 0, since the variables are a linear combination of other variables as shown.                                                            |               |                |                    |                |         |         |
| Col7 = Intercept - Col2 - Col3 - Col4 - Col5 - Col6                                                                                                                                     |               |                |                    |                |         |         |
| Parameter Estimates                                                                                                                                                                     |               |                |                    |                |         |         |
| Variable                                                                                                                                                                                | Label         | DF             | Parameter Estimate | Standard Error | t Value | Pr >  t |
| Intercept                                                                                                                                                                               | Intercept     | B              | 18.70000           | 1.53549        | 12.18   | <.0001  |
| Col2                                                                                                                                                                                    | Strain 3DOK1  | B              | 10.12000           | 2.17151        | 4.66    | <.0001  |
| Col3                                                                                                                                                                                    | Strain 3DOK13 | B              | -5.44000           | 2.17151        | -2.51   | 0.0194  |
| Col4                                                                                                                                                                                    | Strain 3DOK4  | B              | -4.06000           | 2.17151        | -1.87   | 0.0738  |
| Col5                                                                                                                                                                                    | Strain 3DOK5  | B              | 5.28000            | 2.17151        | 2.43    | 0.0229  |
| Col6                                                                                                                                                                                    | Strain 3DOK7  | B              | 1.22000            | 2.17151        | 0.56    | 0.5794  |
| Col7                                                                                                                                                                                    | Strain COMPOS | 0              | 0                  | .              | .       | .       |

## Syntax: GLMMOD Procedure

The following statements are available in the GLMMOD procedure.

```

PROC GLMMOD < options > ;
 BY variables ;
 CLASS variables ;
 FREQ variable ;
 MODEL dependents = independents < / options > ;
 WEIGHT variable ;

```

The PROC GLMMOD and MODEL statements are required. If classification effects are used, the classification variables must be declared in a CLASS statement, and the CLASS statement must appear before the MODEL statement.

## PROC GLMMOD Statement

```

PROC GLMMOD < options > ;

```

The PROC GLMMOD statement invokes the GLMMOD procedure. [Table 43.1](#) summarizes the options available in the PROC GLMMOD statement.

**Table 43.1** PROC GLMMOD Statement Options

| Statement  | Description                                                          |
|------------|----------------------------------------------------------------------|
| DATA=      | Specifies the SAS data set to be used                                |
| NAMELEN=   | Specifies the maximum length for an effect name                      |
| NOPRINT    | Suppresses the normal display of results                             |
| OUTPARM=   | Names an output data set describing the design matrix columns        |
| OUTDESIGN= | Names an output data set to contain the columns of the design matrix |
| PREFIX=    | Specifies a prefix to use in naming the columns of the design matrix |
| ZEROBASED  | Modifies the numbering for the columns of the design matrix          |

It has the following options:

### **DATA=SAS-data-set**

specifies the SAS data set to be used by the GLMMOD procedure. If you do not specify the DATA= option, the most recently created SAS data set is used.

### **NAMELEN=*n***

specifies the maximum length for an effect name. Effect names are listed in the table of parameter definitions and stored in the EFFNAME variable in the OUTPARM= data set. By default,  $n = 20$ . You can specify  $20 < n \leq 200$  if 20 characters are not enough to distinguish between effects, which might be the case if the model includes a high-order interaction between variables with relatively long, similar names.

**NOPRINT**

suppresses the normal display of results. This option is generally useful only when one or more output data sets are being produced by the GLMMOD procedure. Note that this option temporarily disables the Output Delivery System (ODS); see Chapter 20, “Using the Output Delivery System,” for more information.

**ORDER=DATA | FORMATTED | FREQ | INTERNAL**

specifies the sort order for the levels of the classification variables (which are specified in the **CLASS** statement). This option applies to the levels for all classification variables, except when you use the (default) **ORDER=FORMATTED** option with numeric classification variables that have no explicit format. With this option, the levels of such variables are ordered by their internal value.

The **ORDER=** option can take the following values:

| Value of <b>ORDER=</b> | Levels Sorted By                                                                                                                       |
|------------------------|----------------------------------------------------------------------------------------------------------------------------------------|
| <b>DATA</b>            | Order of appearance in the input data set                                                                                              |
| <b>FORMATTED</b>       | External formatted value, except for numeric variables with no explicit format, which are sorted by their unformatted (internal) value |
| <b>FREQ</b>            | Descending frequency count; levels with the most observations come first in the order                                                  |
| <b>INTERNAL</b>        | Unformatted value                                                                                                                      |

By default, **ORDER=FORMATTED**. For **ORDER=FORMATTED** and **ORDER=INTERNAL**, the sort order is machine-dependent. For more information about sort order, see the chapter on the **SORT** procedure in the *Base SAS Procedures Guide* and the discussion of **BY**-group processing in *SAS Language Reference: Concepts*.

**OUTPARM=SAS-data-set**

names an output data set to contain the information regarding the association between model effects and design matrix columns.

**OUTDESIGN=SAS-data-set**

names an output data set to contain the columns of the design matrix.

**PREFIX=name**

specifies a prefix to use in naming the columns of the design matrix in the **OUTDESIGN=** data set. The default prefix is **Col** and the column name is formed by appending the column number to the prefix, so that by default the columns are named **Col1**, **Col2**, and so on. If you specify the **ZEROBASED** option, the column numbering starts at zero, so that with the default value of **PREFIX=** the columns of the design matrix in the **OUTDESIGN=** data set are named **Col0**, **Col1**, and so on.

**ZEROBASED**

specifies that the numbering for the columns of the design matrix in the **OUTDESIGN=** data set begin at 0. By default it begins at 1, so that with the default value of **PREFIX=** the columns of the design matrix in the **OUTDESIGN=** data set are named **Col1**, **Col2**, and so on. If you use the **ZEROBASED** option, the column names are instead **Col0**, **Col1**, and so on.



---

## BY Statement

**BY** *variables* ;

You can specify a BY statement with PROC GLMMOD to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the GLMMOD procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

---

## CLASS Statement

**CLASS** *variables* </ TRUNCATE > ;

The CLASS statement names the classification variables to be used in the model. Typical classification variables are Treatment, Sex, Race, Group, and Replication. If you use the CLASS statement, it must appear before the MODEL statement.

Classification variables can be either character or numeric. By default, class levels are determined from the entire set of formatted values of the CLASS variables.

**NOTE:** Prior to SAS 9, class levels were determined by using no more than the first 16 characters of the formatted values. To revert to this previous behavior, you can use the TRUNCATE option in the CLASS statement.

In any case, you can use formats to group values into levels. See the discussion of the FORMAT procedure in the *Base SAS Procedures Guide* and the discussions of the FORMAT statement and SAS formats in *SAS Formats and Informats: Reference*. You can adjust the order of CLASS variable levels with the ORDER= option in the PROC GLMMOD statement. You can specify the following option in the CLASS statement after a slash (/):

### TRUNCATE

specifies that class levels should be determined by using only up to the first 16 characters of the formatted values of CLASS variables. When formatted values are longer than 16 characters, you can use this option to revert to the levels as determined in releases prior to SAS 9.

---

## FREQ and WEIGHT Statements

**FREQ** *variable* ;

**WEIGHT** *variable* ;

FREQ and WEIGHT variables are transferred to the output data sets without change.

---

## MODEL Statement

**MODEL** *dependents = independents </ options >* ;

The MODEL statement names the dependent variables and independent effects. For the syntax of effects, see the section “Specification of Effects” on page 3324 in Chapter 42, “The GLM Procedure.”

You can specify the following option in the MODEL statement after a slash (/):

### **NOINT**

requests that the intercept parameter not be included in the model.

---

## Details: GLMMOD Procedure

---

### Displayed Output

For each pass of the data (that is, for each BY group and for each pass required by the pattern of missing values for the dependent variables), the GLMMOD procedure displays the definitions of the columns of the design matrix along with the following:

- the number of the column
- the name of the associated effect
- the values that the classification variables take for this level of the effect

The design matrix itself is also displayed, along with the following:

- the observation number
- the dependent variable values
- the FREQ and WEIGHT values, if any
- the columns of the design matrix

---

## Missing Values

If some variables have missing values for some observations, then PROC GLMMOD handles missing values in the same way as PROC GLM; see the section “Missing Values” on page 3379 in Chapter 42, “The GLM Procedure,” for further details.

---

## OUTPARM= Data Set

An output data set containing information regarding the association between model effects and design matrix columns is created whenever you specify the OUTPARM= option in the PROC GLMMOD statement. The OUTPARM= data set contains an observation for each column of the design matrix with the following variables:

- a numeric variable, `_COLNUM_`, identifying the number of the column of the design matrix corresponding to this observation
- a character variable, `EFFNAME`, containing the name of the effect that generates the column of the design matrix corresponding to this observation
- the CLASS variables, with the values they have for the column corresponding to this observation, or blanks if they are not involved with the effect associated with this column

If there are BY-group variables or if the pattern of missing values for the dependent variables requires it, the single data set defines several design matrices. In this case, for each of these design matrices, the OUTPARM= data set also contains the following:

- the current values of the BY variables, if you specify a BY statement
- a numeric variable, `_YPASS_`, containing the current pass of the data, if the pattern of missing values for the dependent variables requires multiple passes

---

## OUTDESIGN= Data Set

An output data set containing the design matrix is created whenever you specify the OUTDESIGN= option in the PROC GLMMOD statement. The OUTDESIGN= data set contains an observation for each observation in the DATA= data set, with the following variables:

- the dependent variables
- the FREQ variable, if any
- the WEIGHT variable, if any
- a variable for each column of the design matrix, with names COL1, COL2, and so forth

If there are BY-group variables or if the pattern of missing values for the dependent variables requires it, the single data set contains several design matrices. In this case, for each of these, the OUTDESIGN= data set also contains the following:

- the current values of the BY variables, if you specify a BY statement
- a numeric variable, `_YPASS_`, containing the current pass of the data, if the pattern of missing values for the dependent variables requires multiple passes

---

## ODS Table Names

PROC GLMMOD assigns a name to each table it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in the following table. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

**Table 43.2** ODS Tables Produced by PROC GLMMOD

| ODS Table Name | Description                                 | Statement                                           |
|----------------|---------------------------------------------|-----------------------------------------------------|
| ClassLevels    | Table of class levels                       | CLASS statement                                     |
| DependentInfo  | Simultaneously analyzed dependent variables | default when there are multiple dependent variables |
| DesignPoints   | Design matrix                               | default                                             |
| NObs           | Number of observations                      | default                                             |
| Parameters     | Parameters and associated column numbers    | default                                             |

---

## Examples: GLMMOD Procedure

---

### Example 43.1: A Two-Way Design

The following program uses the GLMMOD procedure to produce the design matrix for a two-way design. The two classification factors have seven and three levels, respectively, so the design matrix contains  $1 + 7 + 3 + 21 = 32$  columns in all. Output 43.1.1, Output 43.1.2, and Output 43.1.3 display the output produced by the following statements.

```
data Plants;
 input Type $ @;
 do Block=1 to 3;
 input StemLength @;
 output;
 end;
 datalines;
Clarion 32.7 32.3 31.5
Clinton 32.1 29.7 29.1
Knox 35.7 35.9 33.1
O'Neill 36.0 34.2 31.2
Compost 31.8 28.0 29.2
Wabash 38.2 37.8 31.9
Webster 32.5 31.1 29.7
;

proc glmmmod data=Plants outparm=Parm outdesign=Design;
 class Type Block;
 model StemLength = Type|Block;
run;

proc print data=Parm;
run;

proc print data=Design;
run;
```

**Output 43.1.1** A Two-Way Design

| The GLMMOD Procedure        |                           |                                                     |        |       |
|-----------------------------|---------------------------|-----------------------------------------------------|--------|-------|
| Class Level Information     |                           |                                                     |        |       |
| Class                       | Levels                    | Values                                              |        |       |
| Type                        | 7                         | Clarion Clinton Compost Knox O'Neill Wabash Webster |        |       |
| Block                       | 3                         | 1 2 3                                               |        |       |
| Number of Observations Read |                           | 21                                                  |        |       |
| Number of Observations Used |                           | 21                                                  |        |       |
| Parameter Definitions       |                           |                                                     |        |       |
| Column Number               | Name of Associated Effect | CLASS Variable Type                                 | Values | Block |
| 1                           | Intercept                 |                                                     |        |       |
| 2                           | Type                      | Clarion                                             |        |       |
| 3                           | Type                      | Clinton                                             |        |       |
| 4                           | Type                      | Compost                                             |        |       |
| 5                           | Type                      | Knox                                                |        |       |
| 6                           | Type                      | O'Neill                                             |        |       |
| 7                           | Type                      | Wabash                                              |        |       |
| 8                           | Type                      | Webster                                             |        |       |
| 9                           | Block                     |                                                     |        | 1     |
| 10                          | Block                     |                                                     |        | 2     |
| 11                          | Block                     |                                                     |        | 3     |
| 12                          | Type*Block                | Clarion                                             |        | 1     |
| 13                          | Type*Block                | Clarion                                             |        | 2     |
| 14                          | Type*Block                | Clarion                                             |        | 3     |
| 15                          | Type*Block                | Clinton                                             |        | 1     |
| 16                          | Type*Block                | Clinton                                             |        | 2     |
| 17                          | Type*Block                | Clinton                                             |        | 3     |
| 18                          | Type*Block                | Compost                                             |        | 1     |
| 19                          | Type*Block                | Compost                                             |        | 2     |
| 20                          | Type*Block                | Compost                                             |        | 3     |
| 21                          | Type*Block                | Knox                                                |        | 1     |
| 22                          | Type*Block                | Knox                                                |        | 2     |
| 23                          | Type*Block                | Knox                                                |        | 3     |
| 24                          | Type*Block                | O'Neill                                             |        | 1     |
| 25                          | Type*Block                | O'Neill                                             |        | 2     |
| 26                          | Type*Block                | O'Neill                                             |        | 3     |
| 27                          | Type*Block                | Wabash                                              |        | 1     |
| 28                          | Type*Block                | Wabash                                              |        | 2     |
| 29                          | Type*Block                | Wabash                                              |        | 3     |
| 30                          | Type*Block                | Webster                                             |        | 1     |
| 31                          | Type*Block                | Webster                                             |        | 2     |
| 32                          | Type*Block                | Webster                                             |        | 3     |



**Output 43.1.2** The OUTPARM= Data Set

| Obs | _COLNUM_ | EFFNAME    | Type    | Block |
|-----|----------|------------|---------|-------|
| 1   | 1        | Intercept  |         |       |
| 2   | 2        | Type       | Clarion |       |
| 3   | 3        | Type       | Clinton |       |
| 4   | 4        | Type       | Compost |       |
| 5   | 5        | Type       | Knox    |       |
| 6   | 6        | Type       | O'Neill |       |
| 7   | 7        | Type       | Wabash  |       |
| 8   | 8        | Type       | Webster |       |
| 9   | 9        | Block      |         | 1     |
| 10  | 10       | Block      |         | 2     |
| 11  | 11       | Block      |         | 3     |
| 12  | 12       | Type*Block | Clarion | 1     |
| 13  | 13       | Type*Block | Clarion | 2     |
| 14  | 14       | Type*Block | Clarion | 3     |
| 15  | 15       | Type*Block | Clinton | 1     |
| 16  | 16       | Type*Block | Clinton | 2     |
| 17  | 17       | Type*Block | Clinton | 3     |
| 18  | 18       | Type*Block | Compost | 1     |
| 19  | 19       | Type*Block | Compost | 2     |
| 20  | 20       | Type*Block | Compost | 3     |
| 21  | 21       | Type*Block | Knox    | 1     |
| 22  | 22       | Type*Block | Knox    | 2     |
| 23  | 23       | Type*Block | Knox    | 3     |
| 24  | 24       | Type*Block | O'Neill | 1     |
| 25  | 25       | Type*Block | O'Neill | 2     |
| 26  | 26       | Type*Block | O'Neill | 3     |
| 27  | 27       | Type*Block | Wabash  | 1     |
| 28  | 28       | Type*Block | Wabash  | 2     |
| 29  | 29       | Type*Block | Wabash  | 3     |
| 30  | 30       | Type*Block | Webster | 1     |
| 31  | 31       | Type*Block | Webster | 2     |
| 32  | 32       | Type*Block | Webster | 3     |





## Example 43.2: Factorial Screening

Screening experiments are undertaken to select from among the many possible factors that might affect a response the few that actually do, either simply (main effects) or in conjunction with other factors (interactions). One method of selecting significant factors is forward model selection, in which the model is built by successively adding the most statistically significant effects. Forward selection is an option in the REG procedure, but the REG procedure does not allow you to specify interactions directly (as the GLM procedure does, for example). You can use the GLMMOD procedure to create the screening model for a design and then use the REG procedure on the results to perform the screening.

The following statements create the SAS data set `Screening`, which contains the results of a screening experiment:

```

title 'PROC GLMMOD and PROC REG for Forward Selection Screening';
data Screening;
 input a b c d e y;
 datalines;
-1 -1 -1 -1 1 -6.688
-1 -1 -1 1 -1 -10.664
-1 -1 1 -1 -1 -1.459
-1 -1 1 1 1 2.042
-1 1 -1 -1 -1 -8.561
-1 1 -1 1 1 -7.095
-1 1 1 -1 1 0.553
-1 1 1 1 -1 -2.352
 1 -1 -1 -1 -1 -4.802
 1 -1 -1 1 1 5.705
 1 -1 1 -1 1 14.639
 1 -1 1 1 -1 2.151
 1 1 -1 -1 1 5.884
 1 1 -1 1 -1 -3.317
 1 1 1 -1 -1 4.048
 1 1 1 1 1 15.248
;

```

The data set contains a single dependent variable (`y`) and five independent factors (`a`, `b`, `c`, `d`, and `e`). The design is a half-fraction of the full  $2^5$  factorial, the precise half-fraction having been chosen to provide uncorrelated estimates of all main effects and two-factor interactions.

The following statements use the GLMMOD procedure to create a design matrix data set containing all the main effects and two-factor interactions for the preceding screening design.

```

ods output DesignPoints = DesignMatrix;
proc glmmod data=Screening;
 model y = a|b|c|d|e@2;
run;

```

Notice that the preceding statements use ODS to create the design matrix data set, instead of the OUTDESIGN= option in the PROC GLMMOD statement. The results are equivalent, but the columns of the data set produced by ODS have names that are directly related to the names of their corresponding effects.

Finally, the following statements use the REG procedure to perform forward model selection for the screening design. Two MODEL statements are used, one without the selection options (which produces the regression analysis for the full model) and one with the selection options. [Output 43.2.1](#) and [Output 43.2.2](#) show the results of the PROC REG analysis.

```
proc reg data=DesignMatrix;
 model y = a--d_e;
 model y = a--d_e / selection = forward
 details = summary
 slentry = 0.05;
run;
```

**Output 43.2.1** PROC REG Full Model Fit

| PROC GLMMOD and PROC REG for Forward Selection Screening |    |                |             |         |        |
|----------------------------------------------------------|----|----------------|-------------|---------|--------|
| The REG Procedure                                        |    |                |             |         |        |
| Model: MODEL1                                            |    |                |             |         |        |
| Dependent Variable: y                                    |    |                |             |         |        |
| Analysis of Variance                                     |    |                |             |         |        |
| Source                                                   | DF | Sum of Squares | Mean Square | F Value | Pr > F |
| Model                                                    | 15 | 861.48436      | 57.43229    | .       | .      |
| Error                                                    | 0  | 0              | .           |         |        |
| Corrected Total                                          | 15 | 861.48436      |             |         |        |
| Root MSE                                                 |    | .              | R-Square    | 1.0000  |        |
| Dependent Mean                                           |    | 0.33325        | Adj R-Sq    | .       |        |
| Coeff Var                                                |    | .              |             |         |        |

Output 43.2.1 continued

| Parameter Estimates |           |    |                    |                |         |         |
|---------------------|-----------|----|--------------------|----------------|---------|---------|
| Variable            | Label     | DF | Parameter Estimate | Standard Error | t Value | Pr >  t |
| Intercept           | Intercept | 1  | 0.33325            | .              | .       | .       |
| a                   |           | 1  | 4.61125            | .              | .       | .       |
| b                   |           | 1  | 0.21775            | .              | .       | .       |
| a_b                 | a*b       | 1  | 0.30350            | .              | .       | .       |
| c                   |           | 1  | 4.02550            | .              | .       | .       |
| a_c                 | a*c       | 1  | 0.05150            | .              | .       | .       |
| b_c                 | b*c       | 1  | -0.20225           | .              | .       | .       |
| d                   |           | 1  | -0.11850           | .              | .       | .       |
| a_d                 | a*d       | 1  | 0.12075            | .              | .       | .       |
| b_d                 | b*d       | 1  | 0.18850            | .              | .       | .       |
| c_d                 | c*d       | 1  | 0.03200            | .              | .       | .       |
| e                   |           | 1  | 3.45275            | .              | .       | .       |
| a_e                 | a*e       | 1  | 1.97175            | .              | .       | .       |
| b_e                 | b*e       | 1  | -0.35625           | .              | .       | .       |
| c_e                 | c*e       | 1  | 0.30900            | .              | .       | .       |
| d_e                 | d*e       | 1  | 0.30750            | .              | .       | .       |

Output 43.2.2 PROC REG Screening Results

| Summary of Forward Selection |                  |       |                |                  |                |      |         |        |
|------------------------------|------------------|-------|----------------|------------------|----------------|------|---------|--------|
| Step                         | Variable Entered | Label | Number Vars In | Partial R-Square | Model R-Square | C(p) | F Value | Pr > F |
| 1                            | a                |       | 1              | 0.3949           | 0.3949         | .    | 9.14    | 0.0091 |
| 2                            | c                |       | 2              | 0.3010           | 0.6959         | .    | 12.87   | 0.0033 |
| 3                            | e                |       | 3              | 0.2214           | 0.9173         | .    | 32.13   | 0.0001 |
| 4                            | a_e              | a*e   | 4              | 0.0722           | 0.9895         | .    | 75.66   | <.0001 |

The full model has 16 parameters (the intercept + 5 main effects + 10 interactions). These are all estimable, but since there are only 16 observations in the design, there are no degrees of freedom left to estimate error; consequently, there is no way to use the full model to test for the statistical significance of effects. However, the forward selection method chooses only four effects for the model: the main effects of factors a, c, and e, and the interaction between a and e. Using this reduced model enables you to estimate the underlying level of noise, although note that the selection method biases this estimate somewhat.

## References

Erdman, L. W. (1946), "Studies to Determine If Antibiosis Occurs among Rhizobia," *Journal of the American Society of Agronomy*, 38, 251–258.

Steel, R. G. D. and Torrie, J. H. (1980), *Principles and Procedures of Statistics*, Second Edition, New York: McGraw-Hill.

# Chapter 44

## The GLMPOWER Procedure

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---

### Overview: GLMPOWER Procedure

Power and sample size analysis optimizes the resource usage and design of a study, improving chances of conclusive results with maximum efficiency. The GLMPOWER procedure performs prospective power and sample size analysis for linear models, with a variety of goals:

- determining the sample size required to get a significant result with adequate probability (power)
- characterizing the power of a study to detect a meaningful effect
- conducting what-if analyses to assess sensitivity of the power or required sample size to other factors

Here *prospective* indicates that the analysis pertains to planning for a future study. This is in contrast to *retrospective* analysis for a past study, which is not supported by this procedure.

The statistical analyses that are covered include Type III tests and contrasts of fixed effects in univariate linear models, optionally with covariates. The covariates can be continuous or categorical. Tests and contrasts involving random effects are not supported. For power and sample size analyses in a variety of other statistical situations, see Chapter 71, “[The POWER Procedure](#).”

Input for PROC GLMPOWER includes the components considered in study planning:

- design (including subject profiles and their allocation weights)
- statistical model
- contrasts of class effects
- significance level (alpha)
- surmised response means for subject profiles (often called “cell means”)
- surmised variability
- power
- sample size

In order to identify power or sample size as the result parameter, you designate it by a missing value in the input. The procedure calculates this result value over one or more scenarios of input values for all other components.

You specify the design and the cell means by using an *exemplary data set*, a data set of artificial values constructed to represent the intended sampling design and the surmised response means in the underlying population. You specify the model and contrasts by using [MODEL](#) and [CONTRAST](#) statements similar to those in the GLM, ANOVA, and MIXED procedures. You specify the remaining parameters with the [POWER](#) statement, which is similar to analysis statements in the POWER procedure.

In addition to tabular results, PROC GLMPOWER produces graphs. You can produce the most common types of plots easily with default settings and use a variety of options for more customized graphics. For example, you can control the choice of axis variables, axis ranges, number of plotted points, mapping of graphical features (such as color, line style, symbol, and panel) to analysis parameters, and legend appearance.

If ODS Graphics is enabled, then PROC GLMPOWER uses ODS Graphics to create graphs; otherwise, traditional graphs are produced.

For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS](#).”

For specific information about the statistical graphics and options available with the GLMPOWER procedure, see the [PLOT](#) statement and the section “[ODS Graphics](#)” on page 3500.

The GLMPOWER procedure is one of several tools available in SAS/STAT software for power and sample size analysis. PROC POWER covers a variety of other analyses such as  $t$  tests, equivalence tests, confidence intervals, binomial proportions, multiple regression, one-way ANOVA, survival analysis, logistic regression, and the Wilcoxon rank-sum test. The Power and Sample Size application provides a user interface and implements many of the analyses supported in the procedures. See Chapter 71, “[The POWER Procedure](#),” and Chapter 72, “[The Power and Sample Size Application](#),” for details.

The following sections of this chapter describe how to use PROC GLMPOWER and discuss the underlying statistical methodology. The section “[Getting Started: GLMPOWER Procedure](#)” on page 3477 introduces PROC GLMPOWER with examples of power computation for a two-way analysis of variance. The section “[Syntax: GLMPOWER Procedure](#)” on page 3483 describes the syntax of the procedure. The section “[Details: GLMPOWER Procedure](#)” on page 3495 summarizes the methods employed by PROC GLMPOWER and provides details on several special topics. The section “[Examples: GLMPOWER Procedure](#)” on page 3501 illustrates the use of the GLMPOWER procedure with several applications.

For an overview of methodology and SAS tools for power and sample size analysis, see Chapter 18, “[Introduction to Power and Sample Size Analysis](#).” For more discussion and examples for linear models, see Castelloe and O’Brien (2001); O’Brien and Shieh (1992); Muller et al. (1992); O’Brien and Muller (1993). For additional discussion of general power and sample size concepts, see O’Brien and Castelloe (2007); Castelloe (2000); Muller and Benignus (1992); Lenth (2001).

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## Getting Started: GLMPOWER Procedure

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### Simple Two-Way ANOVA

This example demonstrates how to use PROC GLMPOWER to compute and plot power for each effect test in a two-way analysis of variance (ANOVA).

Suppose you are planning an experiment to study the effect of light exposure at three levels on the growth of two varieties of flowers. The planned data analysis is a two-way ANOVA with flower height (measured at two weeks) as the response and a model consisting of the effects of light exposure, flower variety, and their interaction. You want to calculate the power of each effect test for a balanced design with a total of 60 specimens (10 for each combination of exposure and variety) with  $\alpha = 0.05$  for each test.

As a first step, create an *exemplary data set* describing your conjectures about the underlying population means. You believe that the mean flower height for each combination of variety and exposure level (that is, for each design profile, or for each *cell* in the design) roughly follows [Table 44.1](#).

**Table 44.1** Mean Flower Height (in cm) by Variety and Exposure

| Variety | Exposure |    |    |
|---------|----------|----|----|
|         | 1        | 2  | 3  |
| 1       | 14       | 16 | 21 |
| 2       | 10       | 15 | 16 |



The following statements create a data set named Exemplary containing these cell means.

```
data Exemplary;
 do Variety = 1 to 2;
 do Exposure = 1 to 3;
 input Height @@;
 output;
 end;
 end;
datalines;
 14 16 21
 10 15 16
;
```

You also conjecture that the error standard deviation is about 5 cm.

Use the `DATA=` option in the `PROC GLMPOWER` statement to specify Exemplary as the exemplary data set. Identify the classification variables (Variety and Exposure) by using the `CLASS` statement. Specify the model by using the `MODEL` statement. Use the `POWER` statement to specify power as the result parameter and provide values for the other analysis parameters, error standard deviation and total sample size. The following SAS statements perform the power analysis:

```
proc glmpower data=Exemplary;
 class Variety Exposure;
 model Height = Variety | Exposure;
 power
 stddev = 5
 ntotal = 60
 power = .;
run;
```

The `MODEL` statement defines the full model including both main effects and the interaction. The `POWER=` option in the `POWER` statement identifies power as the result parameter with a missing value (`POWER=.`). The `STDDEV=` option specifies an error standard deviation of 5, and the `NTOTAL=` option specifies a total sample size of 60. The default value for the `ALPHA=` option sets the significance level to  $\alpha = 0.05$ .

Figure 44.1 shows the output.

**Figure 44.1** Sample Size Analysis for Two-Way ANOVA

| The GLMPOWER Procedure   |        |
|--------------------------|--------|
| Fixed Scenario Elements  |        |
| Dependent Variable       | Height |
| Error Standard Deviation | 5      |
| Total Sample Size        | 60     |
| Alpha                    | 0.05   |
| Error Degrees of Freedom | 54     |

Figure 44.1 *continued*

| Computed Power |                  |            |       |
|----------------|------------------|------------|-------|
| Index          | Source           | Test<br>DF | Power |
| 1              | Variety          | 1          | 0.718 |
| 2              | Exposure         | 2          | 0.957 |
| 3              | Variety*Exposure | 2          | 0.191 |

The power is about 0.72 for the test of the Variety effect. In other words, there is a probability of 0.72 that the test of the Variety effect will produce a significant result (given the assumptions for the means and error standard deviation). The power is 0.96 for the test of the Exposure effect and 0.19 for the interaction test.

Now, suppose you want to account for some of your uncertainty in conjecturing the true error standard deviation by evaluating the power at reasonable low and high values, 4 and 6.5. You also want to plot power for sample sizes between 30 and 90. The following statements perform the analysis:

```
ods listing style=htmlbluecml;
ods graphics on;

proc glmpower data=Exemplary;
 class Variety Exposure;
 model Height = Variety | Exposure;
 power
 stddev = 4 6.5
 ntotal = 60
 power = .;
 plot x=n min=30 max=90;
run;

ods graphics off;
```

The **PLOT** statement with the **X=N** option requests a plot with sample size on the X axis. (The result parameter—in this case, power—is always plotted on the other axis.) The **MIN=** and **MAX=** options in the **PLOT** statement specify the sample size range. The **ODS GRAPHICS ON** statement enables ODS Graphics. The **ODS LISTING STYLE=HTMLBLUECML** statement specifies the HTMLBLUECML style, which is suitable for use with PROC GLMPOWER because it allows both marker symbols and line styles to vary. See the section “ODS Styles Suitable for Use with PROC GLMPOWER” on page 3501 for more information.

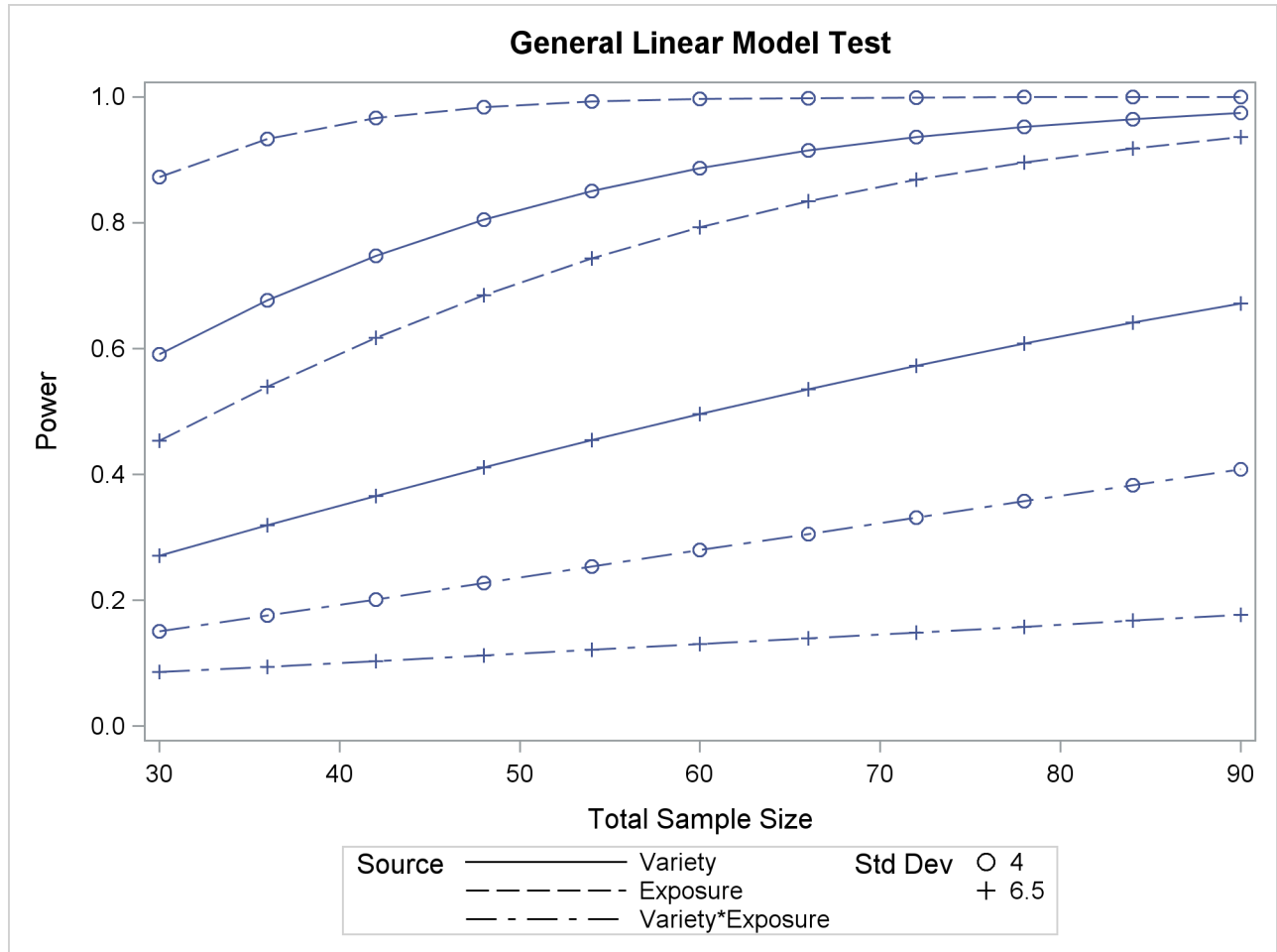
Figure 44.2 shows the output, and Figure 44.3 shows the plot.

**Figure 44.2** Sample Size Analysis for Two-Way ANOVA with Input Ranges

| The GLMPOWER Procedure   |                  |         |         |       |
|--------------------------|------------------|---------|---------|-------|
| Fixed Scenario Elements  |                  |         |         |       |
| Dependent Variable       |                  | Height  |         |       |
| Total Sample Size        |                  | 60      |         |       |
| Alpha                    |                  | 0.05    |         |       |
| Error Degrees of Freedom |                  | 54      |         |       |
| Computed Power           |                  |         |         |       |
| Index                    | Source           | Std Dev | Test DF | Power |
| 1                        | Variety          | 4.0     | 1       | 0.887 |
| 2                        | Variety          | 6.5     | 1       | 0.496 |
| 3                        | Exposure         | 4.0     | 2       | 0.996 |
| 4                        | Exposure         | 6.5     | 2       | 0.793 |
| 5                        | Variety*Exposure | 4.0     | 2       | 0.280 |
| 6                        | Variety*Exposure | 6.5     | 2       | 0.130 |

Figure 44.2 reveals that the power ranges from about 0.130 to 0.996 for the different effect tests and scenarios for standard deviation, with a sample size of 60. In Figure 44.3, the line style identifies the effect test, and the plotting symbol identifies the standard deviation. The locations of the plotting symbols identify actual computed powers; the curves are linear interpolations of these points. Note that the computed points in the plot occur at sample size multiples of 6, because there are 6 cells in the design (and by default, sample sizes are rounded to produce integer cell sizes).

**Figure 44.3** Plot of Power versus Sample Size for Two-Way ANOVA with Input Ranges



## Incorporating Contrasts, Unbalanced Designs, and Multiple Means Scenarios

Suppose you want to compute power for the two-way ANOVA described in the section “Simple Two-Way ANOVA” on page 3477, but you want to additionally perform the following tasks:

- try an unbalanced sample size allocation with respect to Exposure, using twice as many samples for levels 2 and 3 as for level 1
- consider an additional, less optimistic scenario for the cell means, shown in Table 44.2
- test a contrast of Exposure comparing levels 1 and 3

**Table 44.2** Additional Cell Means Scenario

| Variety | Exposure |    |    |
|---------|----------|----|----|
|         | 1        | 2  | 3  |
| 1       | 15       | 16 | 20 |
| 2       | 11       | 14 | 15 |

To specify the unbalanced design and the additional cell means scenario, you can add two new variables to the exemplary data set (Weight for the sample size weights, and HeightNew for the new cell means scenario). Change the name of the original cell means scenario to HeightOrig. The following statements define the exemplary data set:

```
data Exemplary;
 input Variety $ Exposure $ HeightOrig HeightNew Weight;
 datalines;
 1 1 14 15 1
 1 2 16 16 2
 1 3 21 20 2
 2 1 10 11 1
 2 2 15 14 2
 2 3 16 15 2
 ;
```

In PROC GLMPOWER, specify the name of the weight variable by using the **WEIGHT** statement, and specify the name of the cell means variables as dependent variables in the **MODEL** statement. Use the **CONTRAST** statement to specify the contrast as you would in PROC GLM. The following statements perform the sample size analysis.

```
proc glmpower data=Exemplary;
 class Variety Exposure;
 model HeightOrig HeightNew = Variety | Exposure;
 weight Weight;
 contrast 'Exposure=1 vs Exposure=3' Exposure 1 0 -1;
 power
 stddev = 5
 ntotal = 60
 power = .;
run;
```

Figure 44.4 shows the output.

**Figure 44.4** Sample Size Analysis for More Complex Two-Way ANOVA

| The GLMPOWER Procedure  |            |                          |                          |      |        |       |
|-------------------------|------------|--------------------------|--------------------------|------|--------|-------|
| Fixed Scenario Elements |            |                          |                          |      |        |       |
|                         |            | Weight Variable          |                          |      | Weight |       |
|                         |            | Error Standard Deviation |                          |      | 5      |       |
|                         |            | Total Sample Size        |                          |      | 60     |       |
|                         |            | Alpha                    |                          |      | 0.05   |       |
|                         |            | Error Degrees of Freedom |                          |      | 54     |       |
| Computed Power          |            |                          |                          |      |        |       |
| Index                   | Dependent  | Type                     | Source                   | Test | DF     | Power |
| 1                       | HeightOrig | Effect                   | Variety                  |      | 1      | 0.672 |
| 2                       | HeightOrig | Effect                   | Exposure                 |      | 2      | 0.911 |
| 3                       | HeightOrig | Effect                   | Variety*Exposure         |      | 2      | 0.217 |
| 4                       | HeightOrig | Contrast                 | Exposure=1 vs Exposure=3 |      | 1      | 0.951 |
| 5                       | HeightNew  | Effect                   | Variety                  |      | 1      | 0.754 |
| 6                       | HeightNew  | Effect                   | Exposure                 |      | 2      | 0.633 |
| 7                       | HeightNew  | Effect                   | Variety*Exposure         |      | 2      | 0.137 |
| 8                       | HeightNew  | Contrast                 | Exposure=1 vs Exposure=3 |      | 1      | 0.705 |

The power of the contrast of Exposure levels 1 and 3 is about 0.95 for the original cell means scenario (HeightOrig) and only 0.71 for the new one (HeightNew). The power is higher for the test of Variety, but lower for the tests of Exposure and of Variety\*Exposure for the new cell means scenario compared to the original one. Note also for the HeightOrig scenario that the power for the unbalanced design (Figure 44.4) compared to the balanced design (Figure 44.1) is slightly lower for the tests of Variety and Exposure, but slightly higher for the test of Variety\*Exposure.

## Syntax: GLMPOWER Procedure

The following statements are available in the GLMPOWER procedure:

```

PROC GLMPOWER < options > ;
 BY variables ;
 CLASS variables ;
 CONTRAST 'label' effect values < ... effect values > < / options > ;
 MODEL dependents = independents ;
 PLOT < plot-options > < / graph-options > ;
 POWER < options > ;
 WEIGHT variable ;

```

The **PROC GLMPOWER** statement, the **MODEL** statement, and the **POWER** statement are required. If your model contains classification effects, the classification variables must be listed in a **CLASS** statement, and the **CLASS** statement must appear before the **MODEL** statement. In addition, **CONTRAST** and **POWER** statements must appear after the **MODEL** statement. **PLOT** statements must appear after the **POWER** statement that defines the analysis for the plot.

You can use multiple **CONTRAST**, **POWER**, and **PLOT** statements. Each **CONTRAST** statement defines a separate contrast. Each **POWER** statement produces a separate analysis and uses the information contained in the **CLASS**, **MODEL**, **WEIGHT**, and all **CONTRAST** statements. Each **PLOT** statement refers to the previous **POWER** statement and generates a separate graph (or set of graphs).

Table 44.3 summarizes the basic functions of each statement in PROC GLMPOWER. The syntax of each statement in Table 44.3 is described in the following pages.

**Table 44.3** Statements in the GLMPOWER Procedure

| Statement            | Description                                                                                                  |
|----------------------|--------------------------------------------------------------------------------------------------------------|
| <b>PROC GLMPOWER</b> | Invokes procedure and specifies exemplary data set                                                           |
| <b>BY</b>            | Specifies variables to define subgroups for the analysis                                                     |
| <b>CLASS</b>         | Declares classification variables                                                                            |
| <b>CONTRAST</b>      | Defines linear tests of model parameters                                                                     |
| <b>MODEL</b>         | Defines model and specifies dependent variable(s) used for cell means scenarios                              |
| <b>PLOT</b>          | Displays graphs for preceding <b>POWER</b> statement                                                         |
| <b>POWER</b>         | Identifies parameter to solve for and provides one or more scenarios for values of other analysis parameters |
| <b>WEIGHT</b>        | Specifies variable for allocating sample sizes to different subject profiles                                 |

## PROC GLMPOWER Statement

**PROC GLMPOWER** < options > ;

The **PROC GLMPOWER** statement invokes the GLMPOWER procedure. You can specify the following options.

**DATA=SAS-data-set**

names a SAS data set to be used as the exemplary data set, which is an artificial data set constructed to represent the intended sampling design and the conjectured response means for the underlying population.

**ORDER=DATA | FORMATTED | FREQ | INTERNAL**

specifies the sort order for the levels of the classification variables (which are specified in the **CLASS** statement).

This option applies to the levels for all classification variables, except when you use the (default) **ORDER=FORMATTED** option with numeric classification variables that have no explicit format. With this option, the levels of such variables are ordered by their internal value.

The **ORDER=** option can take the following values:

| Value of <b>ORDER=</b> | Levels Sorted By                                                                                                                       |
|------------------------|----------------------------------------------------------------------------------------------------------------------------------------|
| <b>DATA</b>            | Order of appearance in the input data set                                                                                              |
| <b>FORMATTED</b>       | External formatted value, except for numeric variables with no explicit format, which are sorted by their unformatted (internal) value |
| <b>FREQ</b>            | Descending frequency count; levels with the most observations come first in the order                                                  |
| <b>INTERNAL</b>        | Unformatted value                                                                                                                      |

By default, **ORDER=FORMATTED**. For **ORDER=FORMATTED** and **ORDER=INTERNAL**, the sort order is machine-dependent.

For more information about sort order, see the chapter on the **SORT** procedure in the *Base SAS Procedures Guide* and the discussion of **BY**-group processing in *SAS Language Reference: Concepts*.

**PLOTONLY**

specifies that only graphical results from the **PLOT** statement be produced.

---

**BY Statement**

**BY** variables ;

You can specify a **BY** statement with **PROC GLMPOWER** to obtain separate analyses of observations in groups that are defined by the **BY** variables. When a **BY** statement appears, the procedure expects the input data set to be sorted in order of the **BY** variables. If you specify more than one **BY** statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the **SORT** procedure with a similar **BY** statement.
- Specify the **NOTSORTED** or **DESCENDING** option in the **BY** statement for the **GLMPOWER** procedure. The **NOTSORTED** option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the **BY** variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the **BY** variables by using the **DATASETS** procedure (in Base SAS software).



Because sorting the data changes the order in which PROC GLMPOWER reads observations, the sort order for the levels of the classification variables might be affected if you have also specified **ORDER=DATA** in the PROC GLMPOWER statement. This, in turn, affects specifications in **CONTRAST** statements.

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

## CLASS Statement

**CLASS** *variables* ;

The **CLASS** statement names the classification variables to be used in the analysis. If you use the **CLASS** statement, it must appear before the **MODEL** statement.

Classification variables can be either character or numeric. By default, class levels are determined from the entire set of formatted values of the **CLASS** variables.

## CONTRAST Statement

**CONTRAST** *'label'* *effect values* < . . . *effect values* > < / *options* > ;

The **CONTRAST** statement enables you to define custom hypothesis tests by specifying an **L** vector or matrix for testing the hypothesis  $L\beta = 0$ . Thus, to use this feature you must be familiar with the details of the model parameterization used in PROC GLM. For more information, see the section “**Parameterization of PROC GLM Models**” on page 3327 of Chapter 42, “**The GLM Procedure**.” All of the elements of the **L** vector can be given, or if only certain portions of the **L** vector are given, the remaining elements are constructed by PROC GLMPOWER from the context (in a manner similar to rule 4 discussed in the section “**Construction of Least Squares Means**” on page 3363 of Chapter 42, “**The GLM Procedure**”).

There is no limit to the number of **CONTRAST** statements you can specify. Each sample size analysis includes tests for all **CONTRAST** statements.

In the **CONTRAST** statement,

- label* identifies the contrast on the output. A label is required for every contrast specified. Labels must be enclosed in quotes.
- effect* identifies an effect that appears in the **MODEL** statement, or the INTERCEPT effect. You do not need to include all effects that are in the **MODEL** statement.
- values* are constants that are elements of the **L** vector associated with the effect.

You can specify the following option in the **CONTRAST** statement after a slash (/):

**SINGULAR=***number*

tunes the estimability checking. If  $ABS(L - LH) > C \times \text{number}$  for any row in the contrast, then **L** is declared nonestimable. **H** is the  $(X'X)^{-1}X'X$  matrix, and **C** is  $ABS(L)$  except for rows where **L** is zero, and then it is 1. The default value for the **SINGULAR=** option is  $10^{-4}$ . Values for the **SINGULAR=** option must be between 0 and 1.

The **CONTRAST** statement enables you to perform custom hypothesis tests. If the hypothesis is estimable, then the sum of squares due to it,  $SS(H_0: \mathbf{L}\boldsymbol{\beta} = 0)$ , is computed as

$$(\mathbf{Lb})'(\mathbf{L}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{L}')^{-1}(\mathbf{Lb})$$

where  $\mathbf{b} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}$  is the estimated solution vector.

The degrees of freedom associated with the hypothesis are equal to the row rank of  $\mathbf{L}$ . The sum of squares computed in this situation is equivalent to the sum of squares computed using an  $\mathbf{L}$  matrix with any row deleted that is a linear combination of previous rows.

Multiple-degrees-of-freedom hypotheses can be specified by separating the rows of the  $\mathbf{L}$  matrix with commas.

## MODEL Statement

**MODEL** *dependents* = *independents* ;

The **MODEL** statement serves two basic purposes:

- The *dependents* specify scenarios for the cell means.
- The *independents* specify the independent effects.

The *independents* can involve classification variables, continuous variables, or both. You can include main effects and interactions by using the effects notation of PROC GLM; see the section “[Specification of Effects](#)” on page 3324 in Chapter 42, “[The GLM Procedure](#)” for further details. For any model effect involving classification variables (interactions as well as main effects), the number of levels cannot exceed 32,767. If no independent effects are specified, only an intercept term is fit. The **MODEL** statement must appear before the **POWER** statement if the **EFFECTS** option is used in the **POWER** statement.

You can account for covariates in the model by using the **NCOVARIATES=** option and either the **CORRXY=** or **PROPVARREDUCTION=** option in the **POWER** statement.

Each dependent variable refers to a set of surmised cell means in the exemplary data set (named by the **DATA=** option in the **PROC GLMPOWER** statement). These cell means are response means for all of the subject profiles. Multiple dependent variables correspond to multiple scenarios for these cell means. All models are univariate; the GLMPOWER procedure currently does not support multivariate analyses.

The **MODEL** statement is required. You can specify only one **MODEL** statement.

## PLOT Statement

**PLOT** *plot-options* < / *graph-options* > ;

The **PLOT** statement produces a graph or set of graphs for the sample size analysis defined by the previous **POWER** statement. The *plot-options* define the plot characteristics, and the *graph-options* are like those in SAS/GRAPH software. If ODS Graphics is enabled, then the **PLOT** statement uses ODS Graphics to create graphs. For example:

```
ods listing style=htmlbluecml;
ods graphics on;

proc glmpower data=Exemplary;
 class Variety Exposure;
 model Height = Variety | Exposure;
 power
 stddev = 4 6.5
 ntotal = 60
 power = .;
 plot x=n min=30 max=90;
run;

ods graphics off;
```

Otherwise, traditional graphics are produced. For example:

```
ods graphics off;

proc glmpower data=Exemplary;
 class Variety Exposure;
 model Height = Variety | Exposure;
 power
 stddev = 4 6.5
 ntotal = 60
 power = .;
 plot x=n min=30 max=90;
run;
```

For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS](#).”

The ODS LISTING STYLE=HTMLBLUECML statement specifies the HTMLBLUECML style, which is suitable for use with PROC GLMPOWER because it allows both marker symbols and line styles to vary. See the section “[ODS Styles Suitable for Use with PROC GLMPOWER](#)” on page 3501 for more information.

Table 44.4 summarizes the options available in the PLOT statement.

**Table 44.4** PLOT Statement Options

| Option              | Description                                                                 |
|---------------------|-----------------------------------------------------------------------------|
| <b>Plot Options</b> |                                                                             |
| INTERPOL=           | Specifies the type of curve to draw                                         |
| KEY=                | Specifies the style of key for the plot                                     |
| MARKERS=            | Specifies the locations for plotting symbols                                |
| MAX=                | Specifies the maximum of the range of values                                |
| MIN=                | Specifies the minimum of the range of values                                |
| NPOINTS=            | Specifies the number of values                                              |
| STEP=               | Specifies the increment between values                                      |
| VARY                | Specifies how plot features should be linked to varying analysis parameters |
| X=                  | Specifies a plot with the requested type of parameter on the X axis         |
| XOPTS=              | Specifies plot characteristics pertaining to the X axis                     |

Table 44.4 *continued*

| Option               | Description                                                         |
|----------------------|---------------------------------------------------------------------|
| Y=                   | Specifies a plot with the requested type of parameter on the Y axis |
| YOPTS=               | Specifies plot characteristics pertaining to the Y axis             |
| <b>Graph Options</b> |                                                                     |
| DESCRIPTION=         | Specifies a descriptive string                                      |
| NAME=                | Specifies a name for the catalog entry for the plot                 |

## Options

You can specify the following *plot-options* in the **PLOT** statement.

### **INTERPOL=JOIN | NONE**

specifies the type of curve to draw through the computed points. The **INTERPOL=JOIN** option connects computed points with straight lines. The **INTERPOL=NONE** option leaves computed points unconnected.

### **KEY=BYCURVE** < (*bycurve-options*) >

### **KEY=BYFEATURE** < (*byfeature-options*) >

### **KEY=ONCURVES**

specifies the style of key (or “legend”) for the plot. The default is **KEY=BYFEATURE**, which specifies a key with a column of entries for each plot feature (line style, color, and/or symbol). Each entry shows the mapping between a value of the feature and the value(s) of the analysis parameter(s) linked to that feature. The **KEY=BYCURVE** option specifies a key with each row identifying a distinct curve in the plot. The **KEY=ONCURVES** option places a curve-specific label adjacent to each curve.

You can specify the following *byfeature-options* in parentheses after the **KEY=BYCURVE** option.

### **NUMBERS=OFF | ON**

specifies how the key should identify curves. If **NUMBERS=OFF**, then the key includes symbol, color, and line style samples to identify the curves. If **NUMBERS=ON**, then the key includes numbers matching numeric labels placed adjacent to the curves. The default is **NUMBERS=ON**.

### **POS=BOTTOM | INSET**

specifies the position of the key. The **POS=BOTTOM** option places the key below the X axis. The **POS=INSET** option places the key inside the plotting region and attempts to choose the least crowded corner. The default is **POS=BOTTOM**.

You can specify the following *byfeature-options* in parentheses after **KEY=BYFEATURE** option.

### **POS=BOTTOM | INSET**

specifies the position of the key. The **POS=BOTTOM** option places the key below the X axis. The **POS=INSET** option places the key inside the plotting region and attempts to choose the least crowded corner. The default is **POS=BOTTOM**.

**MARKERS=ANALYSIS | COMPUTED | NICE | NONE**

specifies the locations for plotting symbols.

The **MARKERS=ANALYSIS** option places plotting symbols at locations corresponding to the values of the relevant input parameter from the **POWER** statement preceding the **PLOT** statement.

The **MARKERS=COMPUTED** option (the default) places plotting symbols at the locations of actual computed points from the sample size analysis.

The **MARKERS=NICE** option places plotting symbols at tick mark locations (corresponding to the argument axis).

The **MARKERS=NONE** option disables plotting symbols.

**MAX=number | DATAMAX**

specifies the maximum of the range of values for the parameter associated with the “argument” axis (the axis that is *not* representing the parameter being solved for). The default is **DATAMAX**, which specifies the maximum value that occurs for this parameter in the **POWER** statement that precedes the **PLOT** statement.

**MIN=number | DATAMIN**

specifies the minimum of the range of values for the parameter associated with the “argument” axis (the axis that is *not* representing the parameter being solved for). The default is **DATAMIN**, which specifies the minimum value that occurs for this parameter in the **POWER** statement that precedes the **PLOT** statement.

**NPOINTS=number****NPTS=number**

specifies the number of values for the parameter associated with the “argument” axis (the axis that is *not* representing the parameter being solved for). You cannot use the **NPOINTS=** and **STEP=** options simultaneously. The default value for typical situations is 20.

**STEP=number**

specifies the increment between values of the parameter associated with the “argument” axis (the axis that is *not* representing the parameter being solved for). You cannot use the **STEP=** and **NPOINTS=** options simultaneously. By default, the **NPOINTS=** option is used instead of the **STEP=** option.

**VARY ( feature <BY parameter-list> <, ..., feature <BY parameter-list>> )**

specifies how plot features should be linked to varying analysis parameters. Available *features* are **COLOR**, **LINestyle**, **PANEL**, and **SYMBOL**. A “panel” refers to a separate plot with a heading identifying the subset of values represented in the plot.

The *parameter-list* is a list of one or more names separated by spaces. Each name must match the name of an analysis option used in the **POWER** statement preceding the **PLOT** statement, *or* one of the following keywords: **SOURCE** (for the tests) and **DEPENDENT** (for the cell means scenarios). Also, the name must be the *primary* name for the analysis option—that is, the one listed first in the syntax description.

If you omit the < **BY parameter-list** > portion for a feature, then one or more multivalued parameters from the analysis will be automatically selected for you.

**X=N | POWER**

specifies a plot with the requested type of parameter on the X axis and the parameter being solved for on the Y axis. When **X=N**, sample size is assigned to the X axis. When **X=POWER**, power is assigned to the X axis. You cannot use the **X=** and **Y=** options simultaneously. The default is **X=POWER**, unless the result parameter is power, in which case the default is **X=N**.

**XOPTS= ( *x-options* )**

specifies plot characteristics pertaining to the X axis.

You can specify the following *x-options* in parentheses.

**CROSSREF=NO | YES**

specifies whether the reference lines defined by the **REF= *x-option*** should be crossed with a reference line on the Y axis that indicates the solution point on the curve.

**REF=number-list**

specifies locations for reference lines extending from the X axis across the entire plotting region. See the section “[Specifying Value Lists in the POWER Statement](#)” on page 3495 for information about specifying the *number-list*.

**Y=N | POWER**

specifies a plot with the requested type of parameter on the Y axis and the parameter being solved for on the X axis. When **Y=N**, sample size is assigned to the Y axis. When **Y=POWER**, power is assigned to the Y axis. You cannot use the **Y=** and **X=** options simultaneously. By default, the **X=** option is used instead of the **Y=** option.

**YOPTS= ( *y-options* )**

specifies plot characteristics pertaining to the Y axis.

You can specify the following *y-options* in parentheses.

**CROSSREF=NO | YES**

specifies whether the reference lines defined by the **REF= *y-option*** should be crossed with a reference line on the X axis that indicates the solution point on the curve.

**REF=number-list**

specifies locations for reference lines extending from the Y axis across the entire plotting region. See the section “[Specifying Value Lists in the POWER Statement](#)” on page 3495 for information about specifying the *number-list*.

You can specify the following *graph-options* in the **PLOT** statement after a slash (/).

**DESCRIPTION='string'**

specifies a descriptive string of up to 40 characters that appears in the “Description” field of the graphics catalog. The description does not appear on the plots. By default, PROC GLMPOWER assigns a description either of the form “Y versus X” (for a single-panel plot) or of the form “Y versus X (S),” where Y is the parameter on the Y axis, X is the parameter on the X axis, and S is a description of the subset represented on the current panel of a multipanel plot.

**NAME='string'**

specifies a name of up to eight characters for the catalog entry for the plot. The default name is PLOT $n$ , where  $n$  is the number of the plot statement within the current invocation of PROC GLMPOWER. If the name duplicates the name of an existing entry, SAS/GRAPH software adds a number to the duplicate name to create a unique entry—for example, PLOT11 and PLOT12 for the second and third panels of a multipanel plot generated in the first PLOT statement in an invocation of PROC GLMPOWER.

---

## POWER Statement

**POWER** < options > ;

The **POWER** statement performs power and sample size analyses for the Type III test of each effect in the model defined by the **MODEL** statements and for the contrasts defined by all **CONTRAST** statements. The **MODEL** statement must appear before the **POWER** statement if the **EFFECTS** option is used in the **POWER** statement.

### Summary of Options

Table 44.5 summarizes the options available in the **POWER** statement.

**Table 44.5** POWER Statement Options

| Option            | Description                                                               |
|-------------------|---------------------------------------------------------------------------|
| ALPHA=            | Specifies the level of significance of each test                          |
| CORRXY=           | Specifies multiple correlation ( $\rho$ ) between covariates and response |
| DEPENDENT         | Specifies the location of the Dependent column in the output              |
| EFFECTS           | Specifies the model effects                                               |
| NCOVARIATES=      | Specifies additional degrees of freedom due to covariates                 |
| NFRACTIONAL       | Enables fractional input and output for sample sizes                      |
| NTOTAL=           | Specifies the sample size                                                 |
| OUTPUTORDER=      | Controls ordering in output                                               |
| POWER=            | Specifies Power                                                           |
| PROPVARREDUCTION= | Specifies proportional variance reduction ( $r$ ) due to covariates       |
| STDDEV=           | Specifies error standard deviation                                        |

Table 44.6 summarizes the valid result parameters.

**Table 44.6** Summary of Result Parameters in the POWER Statement

| Solve for   | Syntax     |
|-------------|------------|
| Power       | POWER = .  |
| Sample size | NTOTAL = . |



## Dictionary of Options

### **ALPHA=***number-list*

specifies the level of significance of each test. The default is 0.05, corresponding to the usual  $0.05 \times 100\% = 5\%$  level of significance. Note that this is a test-wise significance level with the same value for all tests, not incorporating any corrections for multiple testing. See the section “[Specifying Value Lists in the POWER Statement](#)” on page 3495 for information about specifying the *number-list*.

### **CORRXY=***number-list*

specifies the multiple correlation ( $\rho$ ) between all covariates and the response. The error standard deviation given by the **STDDEV=** option is consequently reduced by multiplying it by a factor of  $(1 - \rho^2)^{\frac{1}{2}}$ , provided that the number of covariates (as determined by the **NCOVARIATES=** option) is greater than zero. You cannot use the **CORRXY=** and the **PROPVARREDUCTION=** options simultaneously. See the section “[Specifying Value Lists in the POWER Statement](#)” on page 3495 for information about specifying the *number-list*.

### **DEPENDENT**

specifies the location of the Dependent column in the output when the **OUTPUTORDER=REVERSE** option or **OUTPUTORDER=SYNTAX** option is used, according to its relative position in the **POWER** statement.

### **EFFECTS** <= <( effect ... effect ) >>

specifies the model effects to include in the power analysis. By default, or if the **EFFECTS** keyword is specified without the equal sign (=), all model effects are included. Specify **EFFECTS=()** to exclude all model effect tests from the power analysis. You can include main effects and interactions by using the effects notation of PROC GLM; see the section “[Specification of Effects](#)” on page 3324 in Chapter 42, “[The GLM Procedure](#)” for further details. The **MODEL** statement must appear before the **POWER** statement if the **EFFECTS** option is used.

### **NCOVARIATES=***number-list*

### **NCOVARIATE=***number-list*

### **NCOVS=***number-list*

### **NCOV=***number-list*

specifies the number of additional degrees of freedom to accommodate covariate effects—both class and continuous—not listed in the **MODEL** statement. The error degrees of freedom are consequently reduced by the value of the **NCOVARIATES=** option, and the error standard deviation (whose unadjusted value is provided with the **STDDEV=** option) is reduced according to the value of the **CORRXY=** or **PROPVARREDUCTION=** option. See the section “[Specifying Value Lists in the POWER Statement](#)” on page 3495 for information about specifying the *number-list*.

### **NFRACTIONAL**

#### **NFRAC**

enables fractional input and output for sample sizes. See the section “[Sample Size Adjustment Options](#)” on page 3495 for information about the ramifications of the presence (and absence) of the **NFRACTIONAL** option.

### **NTOTAL=***number-list*

specifies the sample size or requests a solution for the sample size with a missing value (**NTOTAL=.**). Values for the sample size must be no smaller than the model degrees of freedom (counting the



covariates). See the section “Specifying Value Lists in the POWER Statement” on page 3495 for information about specifying the *number-list*.

### **OUTPUTORDER=INTERNAL | REVERSE | SYNTAX**

controls how the input and default analysis parameters are ordered in the output. **OUTPUTORDER=INTERNAL** (the default) arranges the parameters in the output according to the following order of their corresponding options:

- **DEPENDENT**
- **EFFECTS**
- weight variable (from the **WEIGHT** statement)
- **ALPHA=**
- **NCOVARIATES=**
- **CORRXY=**
- **PROPVARREDUCTION=**
- **STDDEV=**
- **NTOTAL=**
- **POWER=**

The **OUTPUTORDER=SYNTAX** option arranges the parameters in the output in the same order in which their corresponding options are specified in the **POWER** statement. The **OUTPUTORDER=REVERSE** option arranges the parameters in the output in the reverse of the order in which their corresponding options are specified in the **POWER** statement.

### **POWER=number-list**

specifies the desired power of each test or requests a solution for the power with a missing value (**POWER=.**). The power is expressed as a probability (for example, 0.9) rather than a percentage. Note that this is a test-wise power with the same value for all tests, without any correction for multiple testing. See the section “Specifying Value Lists in the POWER Statement” on page 3495 for information about specifying the *number-list*.

### **PROPVARREDUCTION=number-list**

#### **PVRED=number-list**

specifies the proportional reduction ( $r$ ) in total R square incurred by the covariates—in other words, the amount of additional variation explained by the covariates. The error standard deviation given by the **STDDEV=** option is consequently reduced by multiplying it by a factor of  $(1 - r)^{\frac{1}{2}}$ , provided that the number of covariates (as determined by the **NCOVARIATES=** option) is greater than zero. You cannot use the **PROPVARREDUCTION=** and the **CORRXY=** options simultaneously. See the section “Specifying Value Lists in the POWER Statement” on page 3495 for information about specifying the *number-list*.

### **STDDEV=number-list**

specifies the error standard deviation, or root MSE. If covariates are specified using the **NCOVARIATES=** option, then the **STDDEV=** option denotes the error standard deviation before accounting for these covariates. See the section “Specifying Value Lists in the POWER Statement” on page 3495 for information about specifying the *number-list*.

## Restrictions on Option Combinations

For the relationship between covariates and response, specify either the multiple correlation (by using the `CORRXY=` option) or the proportional reduction in total R square (by using the `PROPVARREDUCTION=` option).

---

## WEIGHT Statement

**WEIGHT** *variable* ;

The **WEIGHT** statement names a variable that provides a profile weight (“cell weight”) for each observation in the exemplary data set specified by the `DATA=` option in the **PROC GLMPOWER** statement.

If the **WEIGHT** statement is not used, then a balanced design is assumed with default cell weights of 1.

---

## Details: GLMPOWER Procedure

---

### Specifying Value Lists in the POWER Statement

To specify one or more scenarios for an analysis parameter (or set of parameters) in the **POWER** statement, you provide a list of values for the option that corresponds to the parameter(s). To identify the parameter you want to solve for, you place a missing value in the appropriate list.

Scenarios for scalar-valued parameters, such as power, are represented by a *number-list*.

#### Number-Lists

A *number-list* can be one of two things: a series of one or more numbers expressed in the form of one or more DOLISTS, or a missing value indicator ( . ).

The DOLIST format is the same as in the **DATA** step. For example, you can specify four scenarios (30, 50, 70, and 100) for a total sample size in either of the following ways:

```
NTOTAL = 30 50 70 100
NTOTAL = 30 to 70 by 20 100
```

A missing value identifies a parameter as the result parameter; it is valid only with options representing parameters you can solve for in a given analysis. For example, you can request a solution for **NTOTAL**:

```
NTOTAL = .
```

---

### Sample Size Adjustment Options

By default, **PROC GLMPOWER** rounds sample sizes conservatively (down in the input, up in the output) so that all total sizes *and* sample sizes for individual design profiles are integers. This is generally considered conservative because it selects the closest realistic design providing *at most* the power of the (possibly fractional) input or mathematically optimized design. In addition, all design profile sizes are adjusted to be multiples of their corresponding weights. If a design profile is present more than once in the exemplary

data set, then the weights for that design profile are summed. For example, if a particular design profile is present twice in the exemplary data set with weight values 2 and 6, then all sample sizes for this design profile become multiples of  $2 + 6 = 8$ .

With the `NFRACTIONAL` option, sample size input is not rounded, and sample size output is reported in two versions, a raw “fractional” version and a “ceiling” version rounded up to the nearest integer.

Whenever an input sample size is adjusted, both the original (“nominal”) and adjusted (“actual”) sample sizes are reported. Whenever computed output sample sizes are adjusted, both the original input (“nominal”) power and the achieved (“actual”) power at the adjusted sample size are reported.

---

## Error and Information Output

The Error column in the main output table explains reasons for missing results and flags numerical results that are bounds rather than exact answers.

The Info column provides further information about Error entries, warnings about any boundary conditions detected, and notes about any adjustments to input. Note that the Info column is hidden by default in the main output. You can view it by using the `ODS OUTPUT` statement to save the output as a data set and the `PRINT` procedure. For example, the following SAS statements print both the Error and Info columns for a power computation in a one-way ANOVA:

```
data MyExemp;
 input A $ Y1 Y2;
 datalines;
 1 10 11
 2 12 11
 3 15 11
 ;

proc glmpower data=MyExemp;
 class A;
 model Y1 Y2 = A;
 power
 stddev = 2
 ntotal = 3 10
 power = .;
 ods output output=Power;
run;

proc print noobs data=Power;
 var NominalNTotal NTotal Dependent Power Error Info;
run;
```

The output is shown in [Figure 44.5](#).

**Figure 44.5** Error and Information Columns

| Nominal |        | Dependent | Power | Error         | Info                         |
|---------|--------|-----------|-------|---------------|------------------------------|
| NTotal  | NTotal |           |       |               |                              |
| 3       | 3      | Y1        | .     | Invalid input | Error DF=0                   |
| 10      | 9      | Y1        | 0.557 |               | Input N adjusted             |
| 3       | 3      | Y2        | .     | Invalid input | Error DF=0 / No effect       |
| 10      | 9      | Y2        | 0.050 |               | Input N adjusted / No effect |

The sample size of 3 specified with the `NTOTAL=` option causes an “Invalid input” message in the Error column and an “Error DF=0” message in the Info column, because a sample size of 3 is so small that there are no degrees of freedom left for the error term. The sample size of 10 causes an “Input N adjusted” message in the Info column, because it is rounded down to 9 to produce integer group sizes of 3 per cell. The cell means scenario represented by the dependent variable Y2 causes a “No effect” message to appear in the Info column, because the means in this scenario are all equal.

## Displayed Output

If you use the `PLOTONLY` option in the `PROC GLMPOWER` statement, the procedure displays only graphical output. Otherwise, the displayed output of the `GLMPOWER` procedure includes the following:

- the “Fixed Scenario Elements” table, which shows all applicable single-valued analysis parameters, in the following order: the dependent variable representing the cell means, the source of the test, the weight variable, parameters input explicitly, parameters supplied with defaults, and ancillary results
- an output table showing the following when applicable (in order): the index of the scenario, the dependent variable representing the cell means, the type of the test, the source of the test, all multivalued input, ancillary results, the primary computed result, and error descriptions
- plots (if requested)

The exception to these ordering conventions is that the `DEPENDENT` and `EFFECTS` options may be used along with the `OUTPUTORDER=SYNTAX` or `OUTPUTORDER=REVERSE` option in the `POWER` statement to specify the relative location of the output for dependent variable and type and source of test.

Ancillary results include the following:

- Actual Power, the achieved power, if it differs from the input (Nominal) power value
- fractional sample size, if the `NFRACTIONAL` option is used in the `POWER` statement

If sample size is the result parameter and the `NFRACTIONAL` option is used in the `POWER` statement, then both “Fractional” and “Ceiling” sample size results are displayed. Fractional sample sizes correspond to the “Nominal” values of power. Ceiling sample sizes are simply the fractional sample sizes rounded up to the nearest integer; they correspond to “Actual” values of power.

The noncentrality parameter is computed and stored in a hidden column called Noncentrality in the “Output” table.

## ODS Table Names

PROC GLMPOWER assigns a name to each table that it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in Table 44.7. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

**Table 44.7** ODS Tables Produced by PROC GLMPOWER

| ODS Table Name | Description                                                                                                                                                                        | Statement |
|----------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------|
| FixedElements  | Factoid with single-valued analysis parameters                                                                                                                                     | Default   |
| Output         | All input and computed analysis parameters, error messages, and information messages for each scenario                                                                             | Default   |
| PlotContent    | Data contained in plots, including analysis parameters and indices identifying plot features. (NOTE: This table is saved as a data set and not displayed in PROC GLMPOWER output.) | PLOT      |

## Computational Methods and Formulas

This section describes the approaches used in PROC GLMPOWER to compute power and sample size.

### Contrasts in Fixed-Effect Univariate Models

The univariate linear model has the form

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

where  $\mathbf{y}$  is the  $N \times 1$  vector of responses,  $\mathbf{X}$  is the  $N \times p$  design matrix,  $\boldsymbol{\beta}$  is the  $p \times 1$  vector of model parameters corresponding to the columns of  $\mathbf{X}$ , and  $\boldsymbol{\epsilon}$  is an  $N \times 1$  vector of errors with

$$\epsilon_1, \dots, \epsilon_N \sim N(0, \sigma^2) \quad (\text{i.i.d.})$$

In PROC GLMPOWER, the model parameters  $\boldsymbol{\beta}$  are not specified directly, but rather indirectly as  $\mathbf{y}^*$ , which represents either conjectured response means or typical response values for each design profile. The  $\mathbf{y}^*$  values are manifested as the dependent variable in the MODEL statement. The vector  $\boldsymbol{\beta}$  is obtained from  $\mathbf{y}^*$  according to the least squares equation,

$$\boldsymbol{\beta} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}^*$$

Note that, in general, there is not a 1-to-1 mapping between  $\mathbf{y}^*$  and  $\boldsymbol{\beta}$ . Many different scenarios for  $\mathbf{y}^*$  might lead to the same  $\boldsymbol{\beta}$ . If you specify  $\mathbf{y}^*$  with the intention of representing cell means, keep in mind that PROC GLMPOWER allows scenarios that are *not* valid cell means according to the model specified in the MODEL statement. For example, if  $\mathbf{y}^*$  exhibits an interaction effect but the corresponding interaction term is left out of the model, then the cell means ( $\mathbf{X}\boldsymbol{\beta}$ ) derived from  $\boldsymbol{\beta}$  differ from  $\mathbf{y}^*$ . In particular, the cell means thus derived are the projection of  $\mathbf{y}^*$  onto the model space.

It is convenient in power analysis to parameterize the design matrix  $\mathbf{X}$  in three parts,  $\{\ddot{\mathbf{X}}, \mathbf{w}, N\}$ , defined as follows:

1. The  $q \times p$  essence design matrix  $\ddot{\mathbf{X}}$  is the collection of unique rows of  $\mathbf{X}$ . Its rows are sometimes referred to as “design profiles.” Here,  $q \leq N$  is defined simply as the number of unique rows of  $\mathbf{X}$ .
2. The  $q \times 1$  weight vector  $\mathbf{w}$  reveals the relative proportions of design profiles. Row  $i$  of  $\ddot{\mathbf{X}}$  is to be included in the design  $w_i$  times for every  $w_j$  times row  $j$  is included. The weights are assumed to be standardized (that is, sum up to 1).
3. The total sample size is  $N$ . This is the number of rows in  $\mathbf{X}$ . If you gather  $Nw_i = n_i$  copies of the  $i$ th row of  $\ddot{\mathbf{X}}$ , for  $i = 1, \dots, q$ , then you end up with  $\mathbf{X}$ .

It is useful to express the crossproduct matrix  $\mathbf{X}'\mathbf{X}$  in terms of these three parts,

$$\mathbf{X}'\mathbf{X} = N \ddot{\mathbf{X}}' \text{diag}(\mathbf{w}) \ddot{\mathbf{X}}$$

since this factors out the portion ( $N$ ) depending on sample size and the portion ( $\ddot{\mathbf{X}}' \text{diag}(\mathbf{w}) \ddot{\mathbf{X}}$ ) depending only on the design structure.

A general linear hypothesis for the univariate model has the form

$$H_0: \mathbf{L}\boldsymbol{\beta} = \boldsymbol{\theta}_0$$

$$H_A: \mathbf{L}\boldsymbol{\beta} \neq \boldsymbol{\theta}_0$$

where  $\mathbf{L}$  is an  $r_L \times p$  contrast matrix (assumed to be full rank) and  $\boldsymbol{\theta}_0$  is the null value (usually just a vector of zeros). Note that effect tests are just contrasts that use special forms of  $\mathbf{L}$ . Thus, this scheme covers both effect tests and custom contrasts.

The test statistic is

$$F = \frac{\left(\frac{SS_H}{r_L}\right)}{\hat{\sigma}^2}$$

where

$$SS_H = \frac{1}{N} (\mathbf{L}\hat{\boldsymbol{\beta}} - \boldsymbol{\theta}_0)' (\mathbf{L} (\mathbf{X}'\mathbf{X})^{-1} \mathbf{L}')^{-1} (\mathbf{L}\hat{\boldsymbol{\beta}} - \boldsymbol{\theta}_0)$$

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}'\mathbf{y}$$

$$\hat{\sigma}^2 = \frac{1}{DF_E} (\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}})' (\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}})$$

where  $DF_E = N - \text{rank}(\mathbf{X})$ . Note that  $DF_E = N - p$  if  $\mathbf{X}$  has full rank.

Under  $H_0$ ,  $F \sim F(r_L, DF_E)$ . Under  $H_A$ ,  $F$  is distributed as  $F(r_L, DF_E, \lambda)$  with noncentrality

$$\lambda = N (\mathbf{L}\boldsymbol{\beta} - \boldsymbol{\theta}_0)' \left( \mathbf{L} \left( \ddot{\mathbf{X}}' \text{diag}(\mathbf{w}) \ddot{\mathbf{X}} \right)^{-1} \mathbf{L}' \right)^{-1} (\mathbf{L}\boldsymbol{\beta} - \boldsymbol{\theta}_0) \sigma^{-2}$$

Muller and Peterson (1984) give the exact power of the test as

$$\text{power} = P(F(r_L, DF_E, \lambda) \geq F_{1-\alpha}(r_L, DF_E))$$

Sample size is computed by inverting the power equation.

See Muller et al. (1992) and O'Brien and Shieh (1992) for additional discussion.

## Adjustments for Covariates

If you specify covariates in the model (whether continuous or categorical), then two adjustments are made in order to compute approximate power in the presence of the covariates. Let  $n_v$  denote the number of covariates (counting dummy variables for categorical covariates individually). In other words,  $n_v$  is the total degrees of freedom used by the covariates. The adjustments are as follows:

1. The error degrees of freedom decrease by  $n_v$ .
2. The error standard deviation  $\sigma$  shrinks by a factor of  $(1 - \rho^2)^{\frac{1}{2}}$  (if the **CORRXY=** option to specify the correlation  $\rho$  between covariates and response) or  $(1 - r)^{\frac{1}{2}}$  (if the **PROPVARRREDUCTION=** option is used to specify the proportional reduction in total  $R^2$  incurred by the covariates). Let  $\sigma^*$  represent the updated value of  $\sigma$ .

As a result of these changes, the power is computed as

$$\text{power} = P(F(r_L, DF_E - n_v, \lambda^*) \geq F_{1-\alpha}(r_L, N - r_x - n_v))$$

where  $\lambda^*$  is calculated using  $\sigma^*$  rather than  $\sigma$ :

$$\lambda^* = N (\mathbf{L}\boldsymbol{\beta} - \boldsymbol{\theta}_0)' \left( \mathbf{L} \left( \ddot{\mathbf{X}}' \text{diag}(\mathbf{w}) \ddot{\mathbf{X}} \right)^{-1} \mathbf{L}' \right)^{-1} (\mathbf{L}\boldsymbol{\beta} - \boldsymbol{\theta}_0) (\sigma^*)^{-2}$$

---

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “Statistical Graphics Using ODS.”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “A Primer on ODS Statistical Graphics” on page 599 in Chapter 21, “Statistical Graphics Using ODS.”

If ODS Graphics is not enabled, then PROC GLMPOWER creates traditional graphics.

You can reference every graph produced through ODS Graphics with a name. The names of the graphs that PROC GLMPOWER generates are listed in Table 44.8, along with the required statements and options.

**Table 44.8** Graphs Produced by PROC GLMPOWER

| ODS Graph Name | Plot Description                                                         | Option      |
|----------------|--------------------------------------------------------------------------|-------------|
| PowerPlot      | Plot with power and sample size on the axes                              | <b>PLOT</b> |
| PowerAbort     | Empty plot that shows an error message when a plot could not be produced | <b>PLOT</b> |

---

## ODS Styles Suitable for Use with PROC GLMPOWER

ODS styles control the appearance of graphs produced by PROC GLMPOWER. ODS provides over 50 styles, but most are not suitable for use in PROC GLMPOWER. PROC GLMPOWER requires a style that distinguishes curves based on a combination of color, line style, and symbol marker. Styles that are well-suited for use in PROC GLMPOWER include: STATISTICAL, ANALYSIS, DEFAULT, LISTING, and HTMLBLUECML. The HTMLBLUE and PLATEAU styles are commonly used, but they are not well-suited for use with PROC GLMPOWER because they rely primarily on color to distinguish curves rather than a combination of color, line style, and symbol marker.

In this chapter, a style is explicitly specified at the start of each example that uses ODS Graphics to remind you to use one of the suitable styles. Styles are specified in an ODS destination statement. Destinations include LISTING, HTML, RTF, PDF, and many others. You can set the style and the destination as follows:

```
ods html style=htmlbluecml;
ods graphics on;

proc glmpower data=Exemplary;
 class Variety Exposure;
 model Height = Variety | Exposure;
 power
 stddev = 4 6.5
 ntotal = 60
 power = .;
 plot x=n min=30 max=90;
run;

ods graphics off;
ods html close;
```

For more information about ODS and ODS destinations, see Chapter 20, “Using the Output Delivery System.” For more information ODS styles, see Chapter 21, “Statistical Graphics Using ODS.”

---

## Examples: GLMPOWER Procedure

---

### Example 44.1: One-Way ANOVA

This example deals with the same situation as in [Example 71.1](#) in Chapter 71, “The POWER Procedure.”

Hocking (1985, p. 109) describes a study of the effectiveness of electrolytes in reducing lactic acid buildup for long-distance runners. You are planning a similar study in which you will allocate five different fluids to runners on a 10-mile course and measure lactic acid buildup immediately after the race. The fluids consist of water and two commercial electrolyte drinks, EZDure and LactoZap, each prepared at two concentrations, low (EZD1 and LZ1) and high (EZD2 and LZ2).

You conjecture that the standard deviation of lactic acid measurements given any particular fluid is about 3.75, and that the expected lactic acid values will correspond roughly to [Table 44.9](#). You are least familiar with the LZ1 drink and hence decide to consider a range of reasonable values for that mean.



**Table 44.9** Mean Lactic Acid Buildup by Fluid

| Water | EZD1 | EZD2 | LZ1      | LZ2  |
|-------|------|------|----------|------|
| 35.6  | 33.7 | 30.2 | 29 or 28 | 25.9 |

You are interested in four different comparisons, shown in [Table 44.10](#) with appropriate contrast coefficients.

**Table 44.10** Planned Comparisons

| Comparison                | Contrast Coefficients |      |      |     |     |
|---------------------------|-----------------------|------|------|-----|-----|
|                           | Water                 | EZD1 | EZD2 | LZ1 | LZ2 |
| Water versus electrolytes | 4                     | -1   | -1   | -1  | -1  |
| EZD versus LZ             | 0                     | 1    | 1    | -1  | -1  |
| EZD1 versus EZD2          | 0                     | 1    | -1   | 0   | 0   |
| LZ1 versus LZ2            | 0                     | 0    | 0    | 1   | -1  |

For each of these contrasts you want to determine the sample size required to achieve a power of 0.9 for detecting an effect with magnitude in accord with [Table 44.9](#). You are not yet attempting to choose a single sample size for the study, but rather checking the range of sample sizes needed for individual contrasts. You plan to test each contrast at  $\alpha = 0.025$ . In the interests of reducing costs, you will provide twice as many runners with water as with any of the electrolytes; that is, you will use a sample size weighting scheme of 2:1:1:1:1.

Before calling PROC GLMPOWER, you need to create the *exemplary data set* to specify means and weights for the design profiles:

```
data Fluids;
 input Fluid $ LacticAcid1 LacticAcid2 CellWgt;
 datalines;
 Water 35.6 35.6 2
 EZD1 33.7 33.7 1
 EZD2 30.2 30.2 1
 LZ1 29 28 1
 LZ2 25.9 25.9 1
 ;
```

The variable LacticAcid1 represents the cell means scenario with the larger LZ1 mean (29), and LacticAcid2 represents the scenario with the smaller LZ1 mean (28). The variable CellWgt contains the sample size allocation weights.

Use the `DATA=` option in the PROC GLMPOWER statement to specify Fluids as the exemplary data set. The following statements perform the sample size analysis:

```
proc glmpower data=Fluids;
 class Fluid;
 model LacticAcid1 LacticAcid2 = Fluid;
 weight CellWgt;
 contrast "Water vs. others" Fluid -1 -1 -1 -1 4;
 contrast "EZD vs. LZ" Fluid 1 1 -1 -1 0;
 contrast "EZD1 vs. EZD2" Fluid 1 -1 0 0 0;
```

```

contrast "LZ1 vs. LZ2" Fluid 0 0 1 -1 0;
power
 stddev = 3.75
 alpha = 0.025
 ntotal = .
 power = 0.9;
run;

```

The **CLASS** statement identifies Fluid as a classification variable. The **MODEL** statement specifies the model and the two cell means scenarios LacticAcid1 and LacticAcid2. The **WEIGHT** statement identifies CellWgt as the weight variable. The **CONTRAST** statement specifies the contrasts. Since PROC GLMPOWER by default processes class levels in order of formatted values, the contrast coefficients correspond to the following order: EZD1, EZD2, LZ1, LZ2, Water. (**NOTE:** You could use the **ORDER=DATA** option in the **PROC GLMPOWER** statement to achieve the same ordering as in Table 44.10 instead.) The **POWER** statement specifies total sample size as the result parameter and provides values for the other analysis parameters (error standard deviation, alpha, and power).

Output 44.1.1 displays the results.

**Output 44.1.1** Sample Sizes for One-Way ANOVA Contrasts

| The GLMPOWER Procedure   |             |          |                  |         |          |              |         |
|--------------------------|-------------|----------|------------------|---------|----------|--------------|---------|
| Fixed Scenario Elements  |             |          |                  |         |          |              |         |
| Weight Variable          |             |          |                  | CellWgt |          |              |         |
| Alpha                    |             |          |                  | 0.025   |          |              |         |
| Error Standard Deviation |             |          |                  | 3.75    |          |              |         |
| Nominal Power            |             |          |                  | 0.9     |          |              |         |
| Computed N Total         |             |          |                  |         |          |              |         |
| Index                    | Dependent   | Type     | Source           | Test DF | Error DF | Actual Power | N Total |
| 1                        | LacticAcid1 | Effect   | Fluid            | 4       | 25       | 0.958        | 30      |
| 2                        | LacticAcid1 | Contrast | Water vs. others | 1       | 25       | 0.947        | 30      |
| 3                        | LacticAcid1 | Contrast | EZD vs. LZ       | 1       | 55       | 0.929        | 60      |
| 4                        | LacticAcid1 | Contrast | EZD1 vs. EZD2    | 1       | 169      | 0.901        | 174     |
| 5                        | LacticAcid1 | Contrast | LZ1 vs. LZ2      | 1       | 217      | 0.902        | 222     |
| 6                        | LacticAcid2 | Effect   | Fluid            | 4       | 25       | 0.972        | 30      |
| 7                        | LacticAcid2 | Contrast | Water vs. others | 1       | 19       | 0.901        | 24      |
| 8                        | LacticAcid2 | Contrast | EZD vs. LZ       | 1       | 43       | 0.922        | 48      |
| 9                        | LacticAcid2 | Contrast | EZD1 vs. EZD2    | 1       | 169      | 0.901        | 174     |
| 10                       | LacticAcid2 | Contrast | LZ1 vs. LZ2      | 1       | 475      | 0.902        | 480     |

The sample sizes range from 24 for the comparison of water versus electrolytes to 480 for the comparison of LZ1 versus LZ2, both assuming the smaller LZ1 mean. The sample size for the latter comparison is relatively large because the small mean difference of  $28 - 25.9 = 2.1$  is hard to detect. PROC GLMPOWER also includes the effect test for Fluid. Note that, in this case, it is equivalent to **TEST=OVERALL\_F** in the **ONEWAYANOVA** statement of PROC POWER, since there is only one effect in the model.

The Nominal Power of 0.9 in the “Fixed Scenario Elements” table in [Output 44.1.1](#) represents the input target power, and the Actual Power column in the “Computed N Total” table is the power at the sample size (N Total) adjusted to achieve the specified sample weighting. Note that all of the sample sizes are rounded up to multiples of 6 to preserve integer group sizes (since the group weights add up to 6). You can use the `NFRACTIONAL` option in the `POWER` statement to compute raw fractional sample sizes.

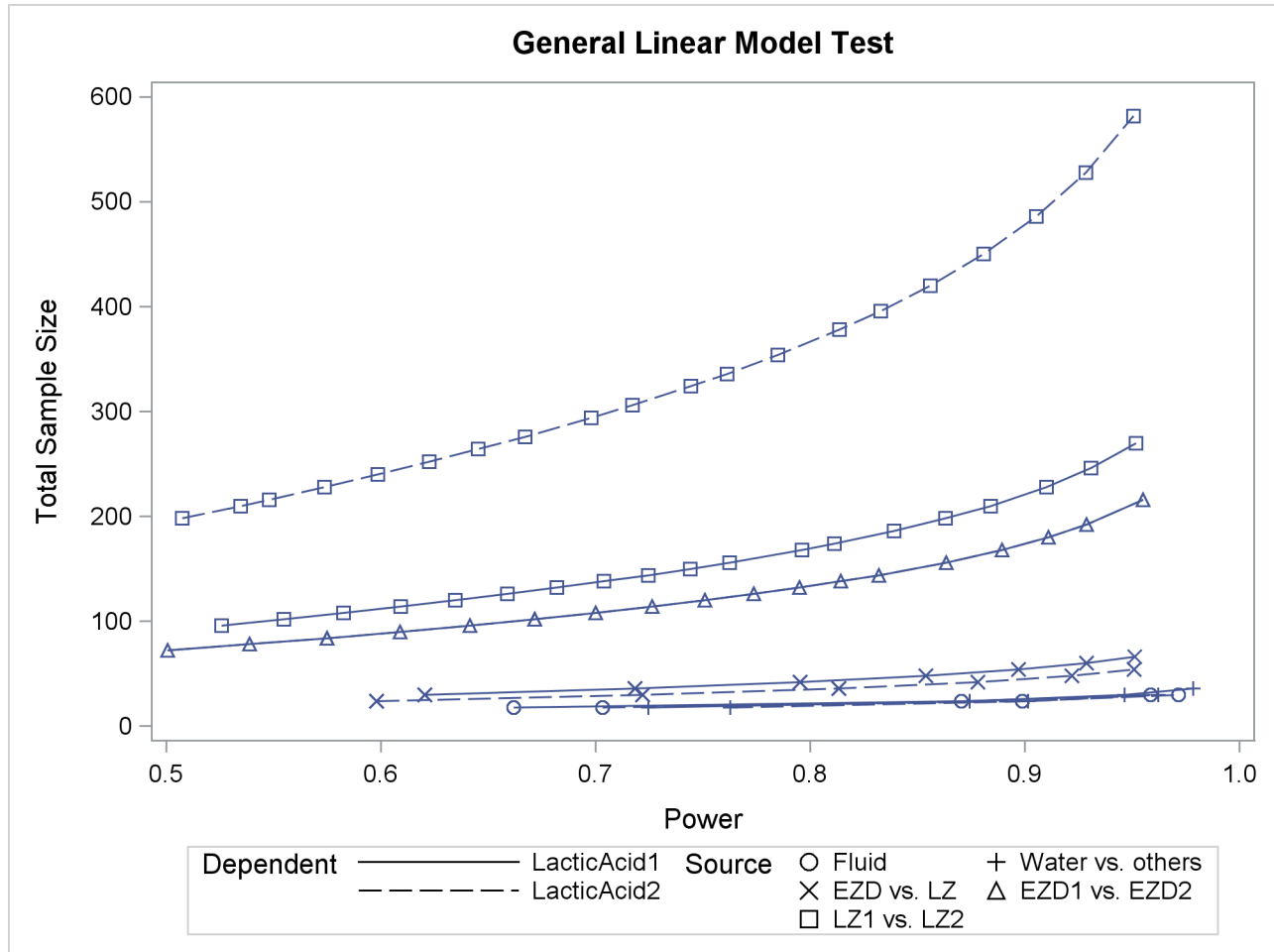
Suppose you want to plot the required sample size for the range of power values from 0.5 to 0.95. First, define the analysis by specifying the same statements as before, but add the `PLOTONLY` option to the `PROC GLMPOWER` statement to disable the nongraphical results. Next, specify the `PLOT` statement with `X=POWER` to request a plot with power on the X axis. (The result parameter—here sample size—is always plotted on the other axis.) Use the `MIN=` and `MAX=` options in the `PLOT` statement to specify the power range. The following statements produce the plot:

```
ods listing style=htmlbluecml;
ods graphics on;

proc glmpower data=Fluids plotonly;
 class Fluid;
 model LacticAcid1 LacticAcid2 = Fluid;
 weight CellWgt;
 contrast "Water vs. others" Fluid -1 -1 -1 -1 4;
 contrast "EZD vs. LZ" Fluid 1 1 -1 -1 0;
 contrast "EZD1 vs. EZD2" Fluid 1 -1 0 0 0;
 contrast "LZ1 vs. LZ2" Fluid 0 0 1 -1 0;
 power
 stddev = 3.75
 alpha = 0.025
 ntotal = .
 power = 0.9;
 plot x=power min=.5 max=.95;
run;
```

The `ODS LISTING STYLE=HTMLBLUECML` statement specifies the `HTMLBLUECML` style, which is suitable for use with `PROC GLMPOWER` because it allows both marker symbols and line styles to vary. See the section “[ODS Styles Suitable for Use with PROC GLMPOWER](#)” on page 3501 for more information. See [Output 44.1.2](#) for the resulting plot.

**Output 44.1.2** Plot of Sample Size versus Power for One-Way ANOVA Contrasts



In Output 44.1.2, the line style identifies the cell means scenario, and the plotting symbol identifies the test. The plotting symbol locations identify actual computed powers; the curves are linear interpolations of these points. The plot shows that the required sample size is highest for the test of LZ1 versus LZ2, which was previously found to require the most resources.

Note that some of the plotted points in [Output 44.1.2](#) are unevenly spaced. This is because the plotted points are the *rounded* sample size results at their corresponding *actual* power levels. The range specified with the `MIN=` and `MAX=` values in the `PLOT` statement corresponds to *nominal* power levels. In some cases, actual power is substantially higher than nominal power. To obtain plots with evenly spaced points (but with *fractional* sample sizes at the computed points), you can use the `NFRACTIONAL` option in the `POWER` statement preceding the `PLOT` statement.

Finally, suppose you want to plot the power for the range of sample sizes you will likely consider for the study (the range of 24 to 480 that achieves 0.9 power for different comparisons). In the `POWER` statement, identify power as the result (`POWER=.`), and specify any total sample size value (say, `NTOTAL=100`). Specify the `PLOT` statement with `X=N` to request a plot with sample size on the X axis.

The following statements produce the plot:

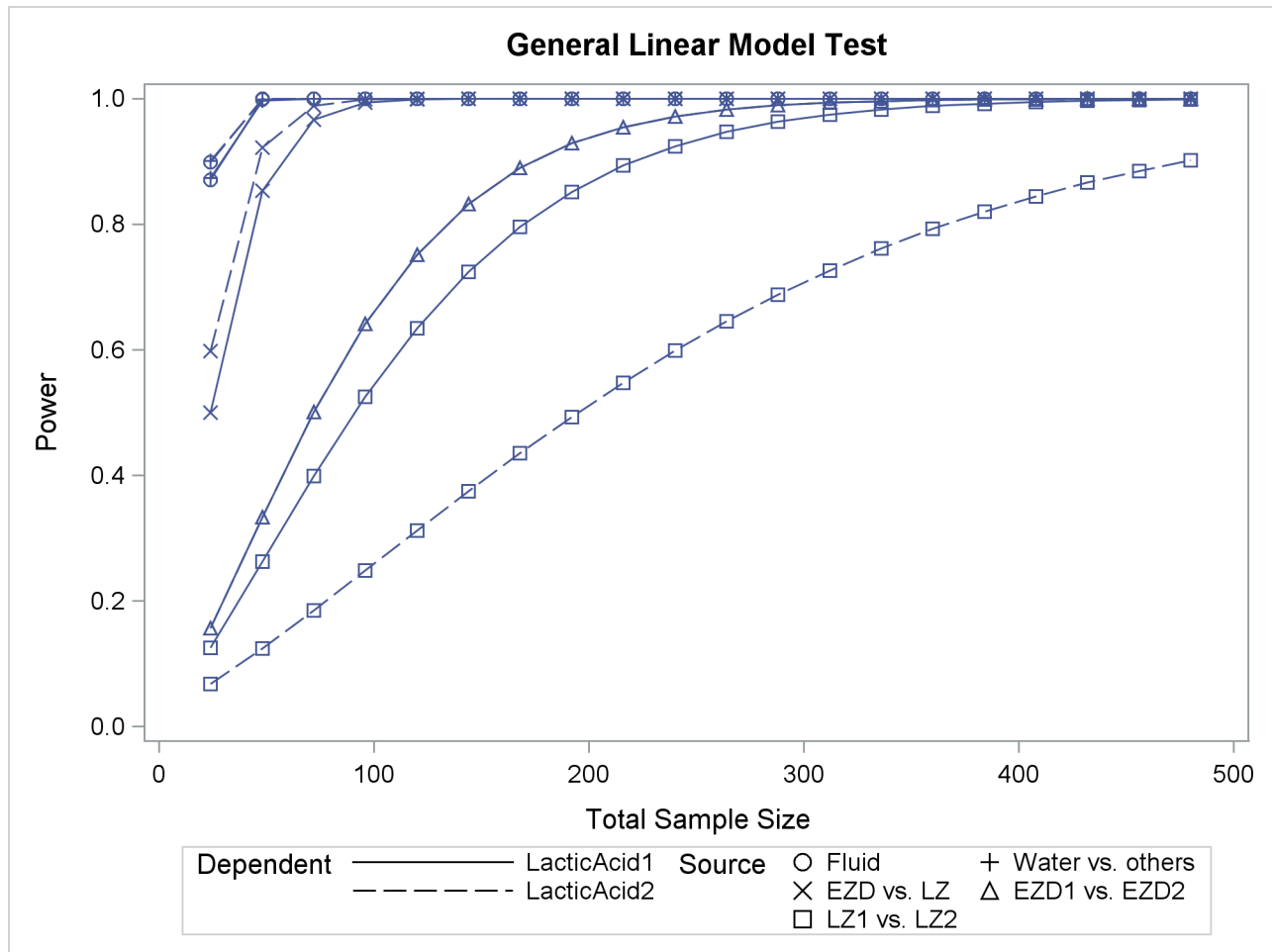
```
proc glmpower data=Fluids plotonly;
 class Fluid;
 model LacticAcid1 LacticAcid2 = Fluid;
 weight CellWgt;
 contrast "Water vs. others" Fluid -1 -1 -1 -1 4;
 contrast "EZD vs. LZ" Fluid 1 1 -1 -1 0;
 contrast "EZD1 vs. EZD2" Fluid 1 -1 0 0 0;
 contrast "LZ1 vs. LZ2" Fluid 0 0 1 -1 0;
 power
 stddev = 3.75
 alpha = 0.025
 ntotal = 24
 power = .;
 plot x=n min=24 max=480;
run;

ods graphics off;
```

Note that the value 100 specified with the `NTOTAL=100` option is not used. It is overridden in the plot by the `MIN=` and `MAX=` options in the `PLOT` statement, and the `PLOTONLY` option in the `PROC GLMPOWER` statement disables nongraphical results. But the `NTOTAL=` option (along with a value) is still needed in the `POWER` statement as a placeholder, to identify the desired parameterization for sample size.

See [Output 44.1.3](#) for the plot.

**Output 44.1.3** Plot of Power versus Sample Size for One-Way ANOVA Contrasts



Although [Output 44.1.2](#) and [Output 44.1.3](#) surface essentially the same computations for practical power ranges, they each provide a different quick visual assessment. [Output 44.1.2](#) reveals the range of required sample sizes for powers of interest, and [Output 44.1.3](#) reveals the range of achieved powers for sample sizes of interest.

## Example 44.2: Two-Way ANOVA with Covariate

Suppose you can enhance the planned study discussed in [Example 44.1](#) in two ways:

- incorporate results from races at two different altitudes (“high” and “low”)
- measure the body mass index of each runner before the race

This is equivalent to adding a second fixed effect and a continuous covariate to your model.

Since lactic acid buildup is more pronounced at higher altitudes, you will include altitude as a factor in the model along with fluid, extending the one-way ANOVA to a two-way ANOVA. In doing so, you expect to lower the residual standard deviation from about 3.75 to 3.5 (in addition to generalizing the study results). You assume there is negligible interaction between fluid and altitude and plan to use a main-effects-only model. You conjecture that the mean lactic acid buildup follows [Table 44.11](#).

**Table 44.11** Mean Lactic Acid Buildup by Fluid and Altitude

| Altitude | Water | Fluid |      |     |      |
|----------|-------|-------|------|-----|------|
|          |       | EZD1  | EZD2 | LZ1 | LZ2  |
| High     | 36.9  | 35.0  | 31.5 | 30  | 27.1 |
| Low      | 34.3  | 32.4  | 28.9 | 27  | 24.7 |

By including a measurement of body mass index as a covariate in the study, you hope to further reduce the error variability. The extent of this reduction in variability is commonly expressed in two alternative ways: (1) the correlation between the covariates and the response or (2) the proportional reduction in total R square incurred by the covariates. You prefer the former and guess that the correlation between body mass index and lactic acid buildup is between 0.2 and 0.3. You specify these estimates with the `NCOVARIATES=` and `CORRXY=` options in the `POWER` statement. The covariate is not included in the `MODEL` statement.

You are interested in the same four fluid comparisons as in [Example 44.1](#), shown in [Table 44.10](#), except this time you want to marginalize over the effect of altitude.

For each of these contrasts, you want to determine the sample size required to achieve a power of 0.9 to detect an effect with magnitude according to [Table 44.11](#). You are not yet attempting to choose a single sample size for the study, but rather checking the range of sample sizes needed by individual contrasts. You plan to test each contrast at  $\alpha = 0.025$ . You will provide twice as many runners with water as with any of the electrolytes, and you predict that you can study approximately two-thirds as many runners at high altitude than at low altitude. The resulting planned sample size weighting scheme is shown in [Table 44.12](#). Since the scheme is only approximate, you use the `NFRACTIONAL` option in the `POWER` statement to disable the rounding of sample sizes up to integers satisfying the weights exactly.

**Table 44.12** Approximate Sample Size Allocation Weights

| Altitude | Fluid |      |      |     |     |
|----------|-------|------|------|-----|-----|
|          | Water | EZD1 | EZD2 | LZ1 | LZ2 |
| High     | 4     | 2    | 2    | 2   | 2   |
| Low      | 6     | 3    | 3    | 3   | 3   |

First, you create the exemplary data set to specify means and weights for the design profiles:

```
data Fluids2;
 input Altitude $ Fluid $ LacticAcid CellWgt;
 datalines;
 High Water 36.9 4
 High EZD1 35.0 2
 High EZD2 31.5 2
 High LZ1 30 2
 High LZ2 27.1 2
 Low Water 34.3 6
 Low EZD1 32.4 3
 Low EZD2 28.9 3
 Low LZ1 27 3
 Low LZ2 24.7 3
 ;
```

The variables `Altitude`, `Fluid`, and `LacticAcid` specify the factors and cell means in [Table 44.11](#). The variable `CellWgt` contains the sample size allocation weights in [Table 44.12](#).



Use the `DATA=` option in the `PROC GLMPOWER` statement to specify `Fluids2` as the exemplary data set. The following statements perform the sample size analysis:

```
proc glmpower data=Fluids2;
 class Altitude Fluid;
 model LacticAcid = Altitude Fluid;
 weight CellWgt;
 contrast "Water vs. others" Fluid -1 -1 -1 -1 4;
 contrast "EZD vs. LZ" Fluid 1 1 -1 -1 0;
 contrast "EZD1 vs. EZD2" Fluid 1 -1 0 0 0;
 contrast "LZ1 vs. LZ2" Fluid 0 0 1 -1 0;
 power
 nfractional
 stddev = 3.5
 ncovariates = 1
 corrxy = 0.2 0.3 0
 alpha = 0.025
 ntotal = .
 power = 0.9;
run;
```

The `CLASS` statement identifies `Altitude` and `Fluid` as classification variables. The `MODEL` statement specifies the model, and the `WEIGHT` statement identifies `CellWgt` as the weight variable. The `CONTRAST` statement specifies the contrasts in [Table 44.10](#). As in [Example 44.1](#), the order of the contrast coefficients corresponds to the formatted class levels (`EZD1`, `EZD2`, `LZ1`, `LZ2`, `Water`). The `POWER` statement specifies total sample size as the result parameter and provides values for the other analysis parameters. The `NCOVARIATES=` option specifies the single covariate (body mass index), and the `CORRXY=` option specifies the two scenarios for its correlation with lactic acid buildup (0.2 and 0.3). [Output 44.2.1](#) displays the results.

#### Output 44.2.1 Sample Sizes for Two-Way ANOVA Contrasts

| The GLMPOWER Procedure               |            |
|--------------------------------------|------------|
| Fixed Scenario Elements              |            |
| Dependent Variable                   | LacticAcid |
| Weight Variable                      | CellWgt    |
| Alpha                                | 0.025      |
| Number of Covariates                 | 1          |
| Std Dev Without Covariate Adjustment | 3.5        |
| Nominal Power                        | 0.9        |

Output 44.2.1 continued

| Computed Ceiling N Total |          |                  |         |             |         |          |                    |
|--------------------------|----------|------------------|---------|-------------|---------|----------|--------------------|
| Index                    | Type     | Source           | Corr XY | Adj Std Dev | Test DF | Error DF | Fractional N Total |
| 1                        | Effect   | Altitude         | 0.2     | 3.43        | 1       | 84       | 90.418451          |
| 2                        | Effect   | Altitude         | 0.3     | 3.34        | 1       | 79       | 85.862649          |
| 3                        | Effect   | Altitude         | 0.0     | 3.50        | 1       | 88       | 94.063984          |
| 4                        | Effect   | Fluid            | 0.2     | 3.43        | 4       | 16       | 22.446173          |
| 5                        | Effect   | Fluid            | 0.3     | 3.34        | 4       | 15       | 21.687544          |
| 6                        | Effect   | Fluid            | 0.0     | 3.50        | 4       | 17       | 23.055716          |
| 7                        | Contrast | Water vs. others | 0.2     | 3.43        | 1       | 15       | 21.720195          |
| 8                        | Contrast | Water vs. others | 0.3     | 3.34        | 1       | 14       | 20.848805          |
| 9                        | Contrast | Water vs. others | 0.0     | 3.50        | 1       | 16       | 22.422381          |
| 10                       | Contrast | EZD vs. LZ       | 0.2     | 3.43        | 1       | 35       | 41.657424          |
| 11                       | Contrast | EZD vs. LZ       | 0.3     | 3.34        | 1       | 33       | 39.674037          |
| 12                       | Contrast | EZD vs. LZ       | 0.0     | 3.50        | 1       | 37       | 43.246415          |
| 13                       | Contrast | EZD1 vs. EZD2    | 0.2     | 3.43        | 1       | 139      | 145.613657         |
| 14                       | Contrast | EZD1 vs. EZD2    | 0.3     | 3.34        | 1       | 132      | 138.173983         |
| 15                       | Contrast | EZD1 vs. EZD2    | 0.0     | 3.50        | 1       | 145      | 151.565917         |
| 16                       | Contrast | LZ1 vs. LZ2      | 0.2     | 3.43        | 1       | 268      | 274.055008         |
| 17                       | Contrast | LZ1 vs. LZ2      | 0.3     | 3.34        | 1       | 253      | 259.919126         |
| 18                       | Contrast | LZ1 vs. LZ2      | 0.0     | 3.50        | 1       | 279      | 285.363976         |

| Computed Ceiling N Total |              |                 |
|--------------------------|--------------|-----------------|
| Index                    | Actual Power | Ceiling N Total |
| 1                        | 0.902        | 91              |
| 2                        | 0.901        | 86              |
| 3                        | 0.903        | 95              |
| 4                        | 0.912        | 23              |
| 5                        | 0.908        | 22              |
| 6                        | 0.919        | 24              |
| 7                        | 0.905        | 22              |
| 8                        | 0.903        | 21              |
| 9                        | 0.910        | 23              |
| 10                       | 0.903        | 42              |
| 11                       | 0.903        | 40              |
| 12                       | 0.906        | 44              |
| 13                       | 0.901        | 146             |
| 14                       | 0.902        | 139             |
| 15                       | 0.901        | 152             |
| 16                       | 0.901        | 275             |
| 17                       | 0.900        | 260             |
| 18                       | 0.901        | 286             |

The sample sizes in [Output 44.2.1](#) range from 21 for the comparison of water versus electrolytes (assuming a correlation of 0.3 between body mass and lactic acid buildup) to 275 for the comparison of LZ1 versus LZ2 (assuming a correlation of 0.2). PROC GLMPower also includes the effect tests for Altitude and Fluid. Note that the required sample sizes for this study are lower than those for the study in [Example 44.1](#).

Note that the error standard deviation has been reduced from 3.5 to 3.43 (when correlation is 0.2) or 3.34 (when correlation is 0.3) in the approximation of the effect of the body mass index covariate. The error degrees of freedom has also been automatically adjusted, lowered by 1 (the number of covariates).

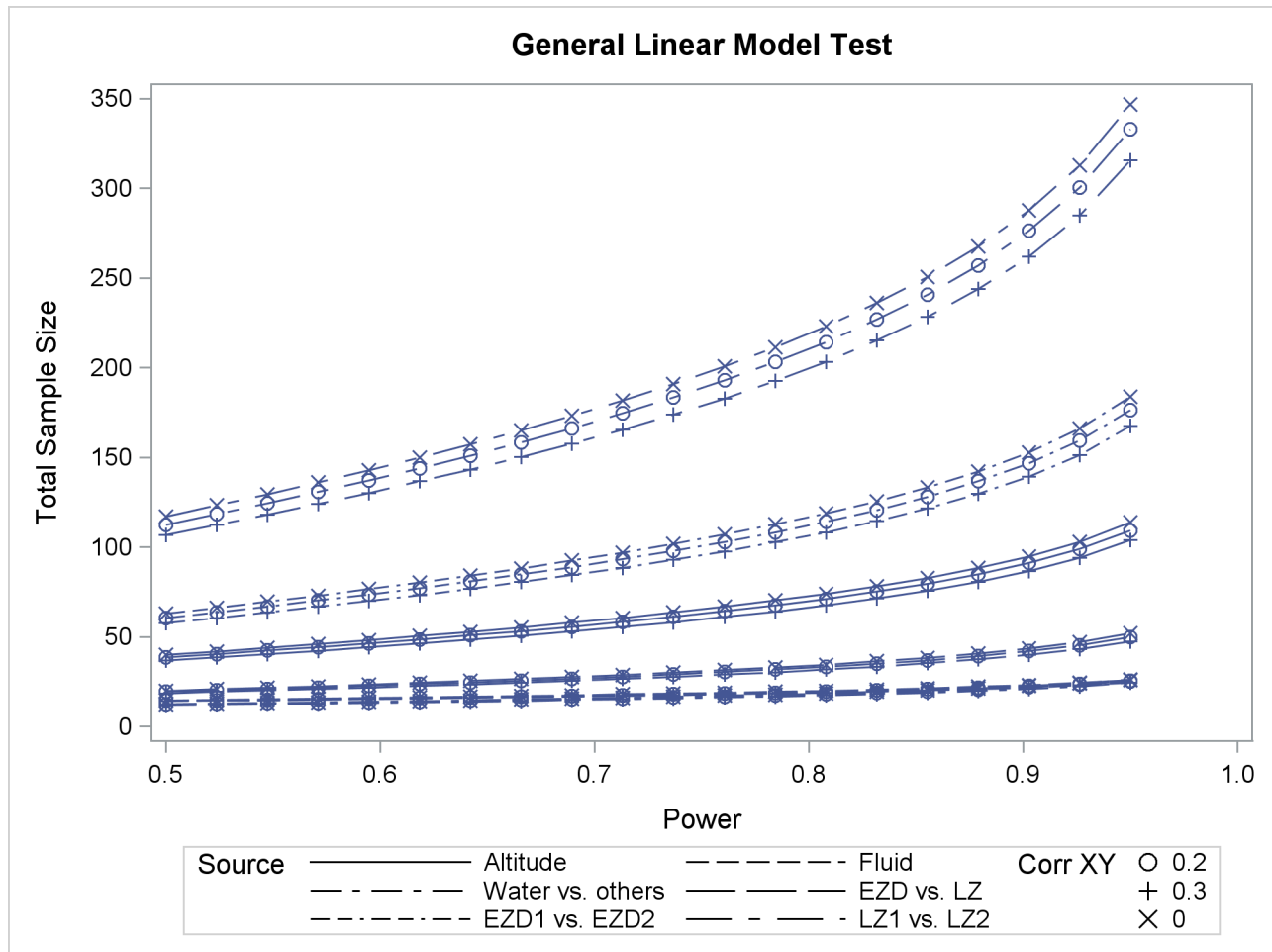
Suppose you want to plot the required sample size for the range of power values from 0.5 to 0.95. First, define the analysis by specifying the same statements as before, but add the **PLOTONLY** option to the **PROC GLMPOWER** statement to disable the nongraphical results. Next, specify the **PLOT** statement with **X=POWER** to request a plot with power on the X axis. Sample size is automatically placed on the Y axis. Use the **MIN=** and **MAX=** options in the **PLOT** statement to specify the power range. The following statements produce the plot:

```
ods listing style=htmlbluecml;
ods graphics on;

proc glmpower data=Fluids2 plotonly;
 class Altitude Fluid;
 model LacticAcid = Altitude Fluid;
 weight CellWgt;
 contrast "Water vs. others" Fluid -1 -1 -1 -1 4;
 contrast "EZD vs. LZ" Fluid 1 1 -1 -1 0;
 contrast "EZD1 vs. EZD2" Fluid 1 -1 0 0 0;
 contrast "LZ1 vs. LZ2" Fluid 0 0 1 -1 0;
 power
 nfractional
 stddev = 3.5
 ncovariates = 1
 corrxxy = 0.2 0.3 0
 alpha = 0.025
 ntotal = .
 power = 0.9;
 plot x=power min=.5 max=.95;
run;
```

The **ODS LISTING STYLE=HTMLBLUECML** statement specifies the **HTMLBLUECML** style, which is suitable for use with **PROC GLMPOWER** because it allows both marker symbols and line styles to vary. See the section “[ODS Styles Suitable for Use with PROC GLMPOWER](#)” on page 3501 for more information. See [Output 44.2.2](#) for the resulting plot.

**Output 44.2.2** Plot of Sample Size versus Power for Two-Way ANOVA Contrasts



In [Output 44.1.2](#), the line style identifies the test, and the plotting symbol identifies the scenario for the correlation between covariate and response. The plotting symbol locations identify actual computed powers; the curves are linear interpolations of these points. As in [Example 44.1](#), the required sample size is highest for the test of LZ1 versus LZ2.

Finally, suppose you want to plot the power for the range of sample sizes you will likely consider for the study (the range of 21 to 275 that achieves 0.9 power for different comparisons). In the **POWER** statement, identify power as the result (**POWER=.**), and specify **NTOTAL=21**. Specify the **PLOT** statement with **X=N** to request a plot with sample size on the X axis.

The following statements produce the plot:

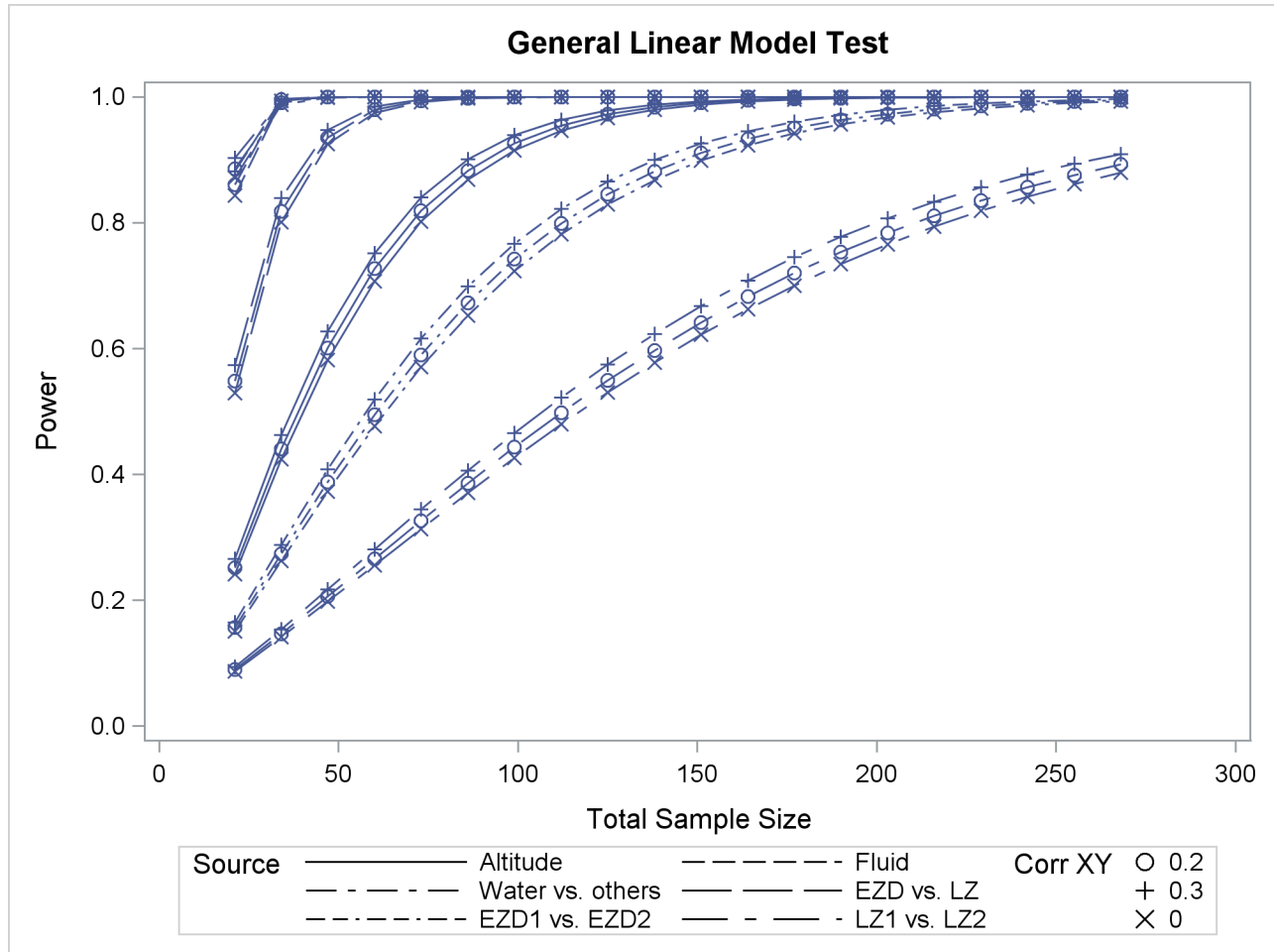
```
proc glmpower data=Fluids2 plotonly;
 class Altitude Fluid;
 model LacticAcid = Altitude Fluid;
 weight CellWgt;
 contrast "Water vs. others" Fluid -1 -1 -1 -1 4;
 contrast "EZD vs. LZ" Fluid 1 1 -1 -1 0;
 contrast "EZD1 vs. EZD2" Fluid 1 -1 0 0 0;
 contrast "LZ1 vs. LZ2" Fluid 0 0 1 -1 0;
 power
 nfractional
 stddev = 3.5
 ncovariates = 1
 corrxxy = 0.2 0.3 0
 alpha = 0.025
 ntotal = 21
 power = .;
 plot x=n min=21 max=275;
run;

ods graphics off;
```

The **MAX=275** option in the **PLOT** statement sets the maximum sample size value. The **MIN=** option automatically defaults to the value of 21 from the **NTOTAL=** option in the **POWER** statement.

See [Output 44.2.3](#) for the plot.

**Output 44.2.3** Plot of Power versus Sample Size for Two-Way ANOVA Contrasts



Although [Output 44.2.2](#) and [Output 44.2.3](#) surface essentially the same computations for practical power ranges, they each provide a different quick visual assessment. [Output 44.2.2](#) reveals the range of required sample sizes for powers of interest, and [Output 44.2.3](#) reveals the range of powers achieved for sample sizes of interest.

---

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# Chapter 45

## The GLMSELECT Procedure

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---

## Overview: GLMSELECT Procedure

The GLMSELECT procedure performs effect selection in the framework of general linear models. A variety of model selection methods are available, including the LASSO method of Tibshirani (1996) and the related LAR method of Efron et al. (2004). The procedure offers extensive capabilities for customizing the selection with a wide variety of selection and stopping criteria, from traditional and computationally efficient significance-level-based criteria to more computationally intensive validation-based criteria. The procedure also provides graphical summaries of the selection search.

The GLMSELECT procedure compares most closely to REG and GLM. The REG procedure supports a variety of model-selection methods but does not support a CLASS statement. The GLM procedure supports a CLASS statement but does not include effect selection methods. The GLMSELECT procedure fills this gap. GLMSELECT focuses on the standard independently and identically distributed general linear model for univariate responses and offers great flexibility for and insight into the model selection algorithm. GLMSELECT provides results (displayed tables, output data sets, and macro variables) that make it easy to take the selected model and explore it in more detail in a subsequent procedure such as REG or GLM.

## Features

The main features of the GLMSELECT procedure are as follows:

- **Model Specification**
  - supports different parameterizations for classification effects
  - supports any degree of interaction (crossed effects) and nested effects
  - supports hierarchy among effects
  - supports partitioning of data into training, validation, and testing roles
  - supports constructed effects including spline and multimember effects

- **Selection Control**

- provides multiple effect selection methods
- enables selection from a very large number of effects (tens of thousands)
- offers selection of individual levels of classification effects
- provides effect selection based on a variety of selection criteria
- provides stopping rules based on a variety of model evaluation criteria
- provides leave-one-out and  $k$ -fold cross validation
- supports data resampling and model averaging

- **Display and Output**

- produces graphical representation of selection process
- produces output data sets containing predicted values and residuals
- produces an output data set containing the design matrix
- produces macro variables containing selected models
- supports parallel processing of BY groups
- supports multiple SCORE statements

The GLMSELECT procedure supports the following effect selection methods. These methods are explained in detail in the section “[Model-Selection Methods](#)” on page 3559.

|          |                                                                                                                                                                                                                                 |
|----------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| FORWARD  | Forward selection. This method starts with no effects in the model and adds effects.                                                                                                                                            |
| BACKWARD | Backward elimination. This method starts with all effects in the model and deletes effects.                                                                                                                                     |
| STEPWISE | Stepwise regression. This is similar to the FORWARD method except that effects already in the model do not necessarily stay there.                                                                                              |
| LAR      | Least angle regression. This method, like forward selection, starts with no effects in the model and adds effects. The parameter estimates at any step are “shrunk” when compared to the corresponding least squares estimates. |
| LASSO    | This method adds and deletes parameters based on a version of ordinary least squares where the sum of the absolute regression coefficients is constrained.                                                                      |

Hybrid versions of LAR and LASSO are also supported. They use LAR or LASSO to select the model, but then estimate the regression coefficients by ordinary weighted least squares.

The GLMSELECT procedure is intended primarily as a model selection procedure and does not include regression diagnostics or other postselection facilities such as hypothesis testing, testing of contrasts, and LS-means analyses. The intention is that you use PROC GLMSELECT to select a model or a set of candidate models. Further investigation of these models can be done by using these models in existing regression procedures.

## Getting Started: GLMSELECT Procedure

The following data set contains salary and performance information for Major League Baseball players who played at least one game in both the 1986 and 1987 seasons, excluding pitchers. The salaries (*Sports Illustrated*, April 20, 1987) are for the 1987 season and the performance measures are from 1986 (Collier Books, *The 1987 Baseball Encyclopedia Update*).

```

data baseball;
 length name $ 18;
 length team $ 12;
 input name $ 1-18 nAtBat nHits nHome nRuns nRBI nBB
 yrMajor crAtBat crHits crHome crRuns crRbi crBB
 league $ division $ team $ position $ nOuts nAssts
 nError salary;
 label name="Player's Name"
 nAtBat="Times at Bat in 1986"
 nHits="Hits in 1986"
 nHome="Home Runs in 1986"
 nRuns="Runs in 1986"
 nRBI="RBIs in 1986"
 nBB="Walks in 1986"
 yrMajor="Years in the Major Leagues"
 crAtBat="Career times at bat"
 crHits="Career Hits"
 crHome="Career Home Runs"
 crRuns="Career Runs"
 crRbi="Career RBIs"
 crBB="Career Walks"
 league="League at the end of 1986"
 division="Division at the end of 1986"
 team="Team at the end of 1986"
 position="Position(s) in 1986"
 nOuts="Put Outs in 1986"
 nAssts="Assists in 1986"
 nError="Errors in 1986"
 salary="1987 Salary in $ Thousands";
 logSalary = log(Salary);
 datalines;
Allanson, Andy 293 66 1 30 29 14
 1 293 66 1 30 29 14
 American East Cleveland C 446 33 20 .
Ashby, Alan 315 81 7 24 38 39
 14 3449 835 69 321 414 375
 National West Houston C 632 43 10 475
Davis, Alan 479 130 18 66 72 76
... more lines ...

Wilson, Willie 631 170 9 77 44 31
 11 4908 1457 30 775 357 249
 American West KansasCity CF 408 4 3 1000
;

```

Suppose you want to investigate whether you can model the players' salaries for the 1987 season based on performance measures for the previous season. The aim is to obtain a parsimonious model that does not overfit this particular data, making it useful for prediction. This example shows how you can use PROC GLMSELECT as a starting point for such an analysis. Since the variation of salaries is much greater for the higher salaries, it is appropriate to apply a log transformation to the salaries before doing the model selection.

The following code selects a model with the default settings:

```
ods graphics on;
proc glmselect data=baseball plots=all;
 class league division;
 model logSalary = nAtBat nHits nHome nRuns nRBI nBB
 yrMajor crAtBat crHits crHome crRuns crRbi
 crBB league division nOuts nAssts nError
 / details=all stats=all;
run;
ods graphics off;
```

PROC GLMSELECT performs effect selection where effects can contain classification variables that you specify in a **CLASS** statement. The “Class Level Information” table shown in [Figure 45.1](#) lists the levels of the classification variables division and league.

**Figure 45.1** Class Level Information

| The GLMSELECT Procedure |        |                   |
|-------------------------|--------|-------------------|
| Class Level Information |        |                   |
| Class                   | Levels | Values            |
| league                  | 2      | American National |
| division                | 2      | East West         |

When you specify effects that contain classification variables, the number of parameters is usually larger than the number of effects. The “Dimensions” table in [Figure 45.2](#) shows the number of effects and the number of parameters considered.

**Figure 45.2** Dimensions

| Dimensions           |    |
|----------------------|----|
| Number of Effects    | 19 |
| Number of Parameters | 21 |

**Figure 45.3** Model Information

| The GLMSELECT Procedure   |               |
|---------------------------|---------------|
| Data Set                  | WORK.BASEBALL |
| Dependent Variable        | logSalary     |
| Selection Method          | Stepwise      |
| Select Criterion          | SBC           |
| Stop Criterion            | SBC           |
| Effect Hierarchy Enforced | None          |

You find details of the default search settings in the “Model Information” table shown in [Figure 45.3](#). The default selection method is a variant of the traditional stepwise selection where the decisions about what effects to add or drop at any step and when to terminate the selection are both based on the Schwarz Bayesian information criterion (SBC). The effect in the current model whose removal yields the maximal decrease in the SBC statistic is dropped provided this lowers the SBC value. Once no decrease in the SBC value can be obtained by dropping an effect in the model, the effect whose addition to the model yields the lowest SBC statistic is added and the whole process is repeated. The method terminates when dropping or adding any effect increases the SBC statistic.

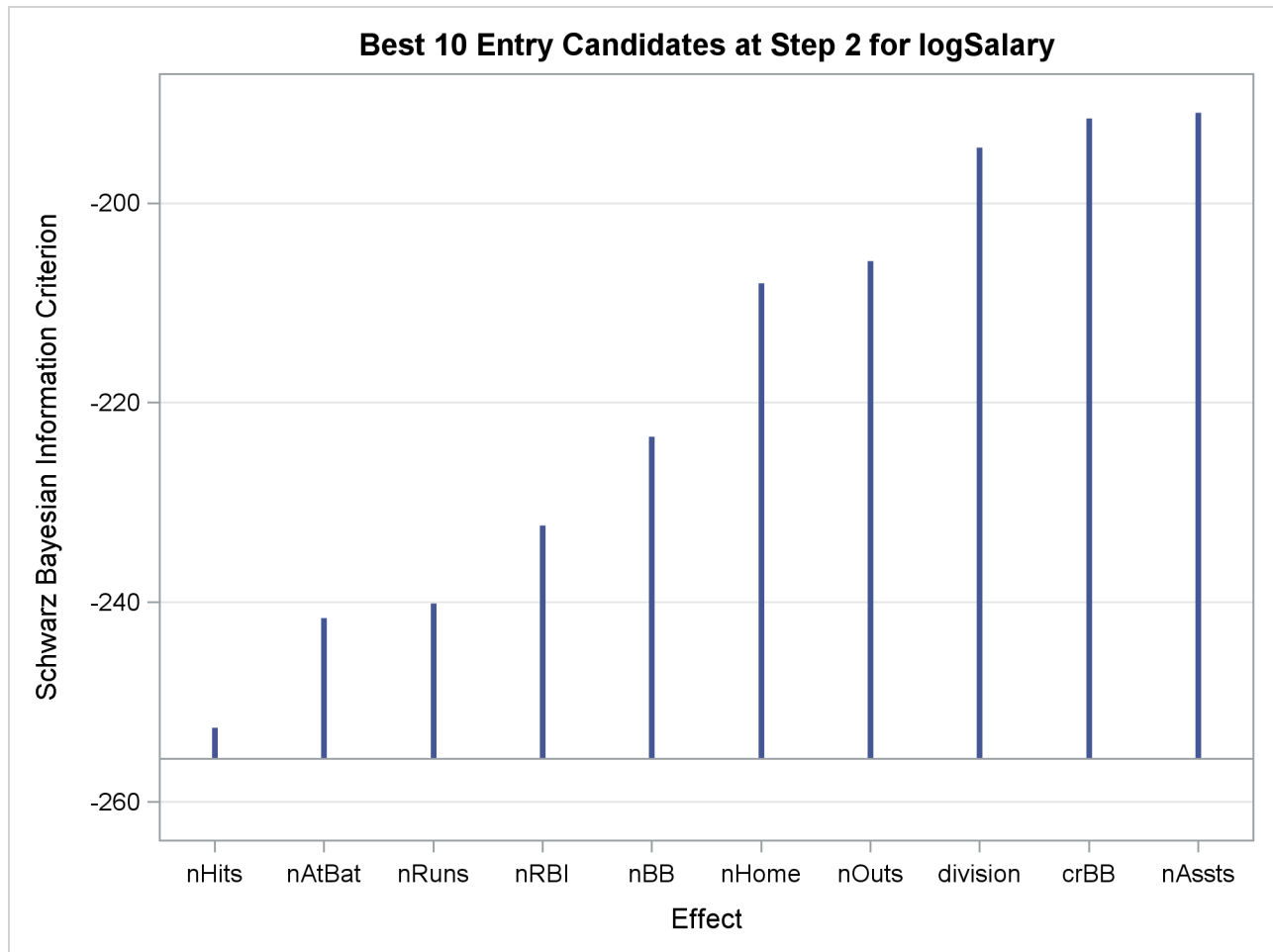
**Figure 45.4** Candidates for Entry at Step Two

| Best 10 Entry Candidates |          |           |
|--------------------------|----------|-----------|
| Rank                     | Effect   | SBC       |
| 1                        | nHits    | -252.5794 |
| 2                        | nAtBat   | -241.5789 |
| 3                        | nRuns    | -240.1010 |
| 4                        | nRBI     | -232.2880 |
| 5                        | nBB      | -223.3741 |
| 6                        | nHome    | -208.0565 |
| 7                        | nOuts    | -205.8107 |
| 8                        | division | -194.4688 |
| 9                        | crBB     | -191.5141 |
| 10                       | nAssts   | -190.9425 |

The `DETAILS=ALL` option requests details of each step of the selection process. The “Best 10 Entry Candidates” table at each step shows the candidates for inclusion or removal at that step ranked from best to worst in terms of the selection criterion, which in this example is the SBC statistic. By default only the 10 best candidates are shown. [Figure 45.4](#) shows the candidate table at step two.

To help in the interpretation of the selection process, you can use graphics supported by PROC GLMSELECT. ODS Graphics must be enabled before requesting plots. For general information about ODS Graphics, see Chapter 21, “[Statistical Graphics Using ODS.](#)” With ODS Graphics enabled, the `PLOTS=ALL` option together with the `DETAILS=STEPS` option in the `MODEL` statement produces a needle plot view of the “Candidates” tables. The plot corresponding to the “Candidates” table at step two is shown in [Figure 45.5](#). You can see that adding the effect 'nHits' yields the smallest SBC value, and so this effect is added at step two.

Figure 45.5 Needle Plot of Entry Candidates at Step Two

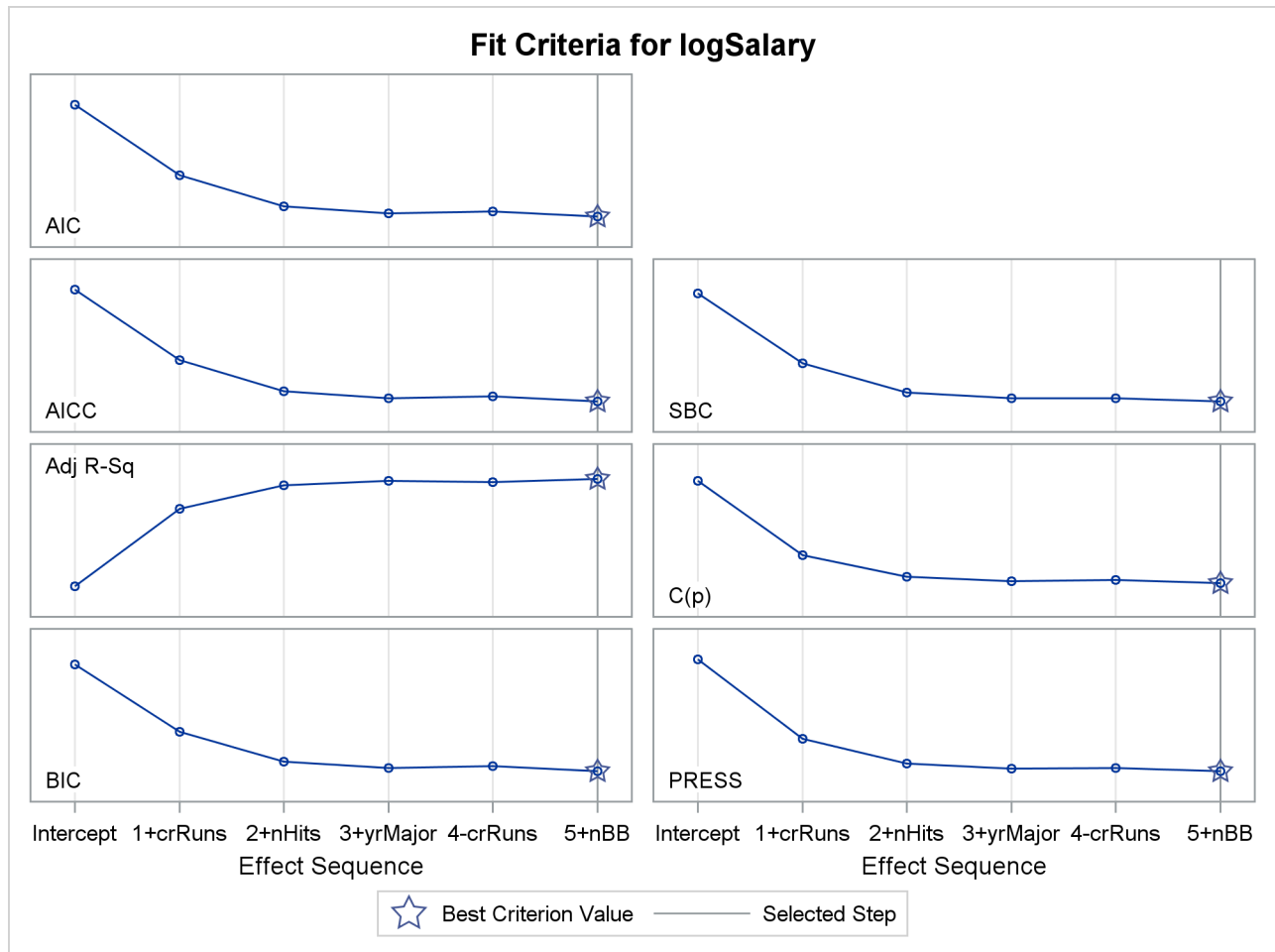


The “Stepwise Selection Summary” table in Figure 45.6 shows the effect that was added or dropped at each step of the selection process together with fit statistics for the model at each step. The `STATS=ALL` option in the `MODEL` statement requests that all the available fit statistics are displayed. See the section “Criteria Used in Model Selection Methods” on page 3568 for descriptions and formulas. The criterion panel in Figure 45.7 provides a graphical view of the progression of these fit criteria as the selection process evolves. Note that none of these criteria has a local optimum before step five.

Figure 45.6 Selection Summary Table

| The GLMSELECT Procedure      |                |                |                   |                 |                |                   |
|------------------------------|----------------|----------------|-------------------|-----------------|----------------|-------------------|
| Stepwise Selection Summary   |                |                |                   |                 |                |                   |
| Step                         | Effect Entered | Effect Removed | Number Effects In | Number Parms In | Model R-Square | Adjusted R-Square |
| 0                            | Intercept      |                | 1                 | 1               | 0.0000         | 0.0000            |
| 1                            | crRuns         |                | 2                 | 2               | 0.4187         | 0.4165            |
| 2                            | nHits          |                | 3                 | 3               | 0.5440         | 0.5405            |
| 3                            | yrMajor        |                | 4                 | 4               | 0.5705         | 0.5655            |
| 4                            |                | crRuns         | 3                 | 3               | 0.5614         | 0.5581            |
| 5                            | nBB            |                | 4                 | 4               | 0.5818         | 0.5770*           |
| * Optimal Value Of Criterion |                |                |                   |                 |                |                   |
| Stepwise Selection Summary   |                |                |                   |                 |                |                   |
| Step                         | Effect Entered | Effect Removed | AIC               | AICC            | BIC            |                   |
| 0                            | Intercept      |                | 204.2238          | 204.2699        | -60.6397       |                   |
| 1                            | crRuns         |                | 63.5391           | 63.6318         | -200.7872      |                   |
| 2                            | nHits          |                | 1.7041            | 1.8592          | -261.8807      |                   |
| 3                            | yrMajor        |                | -12.0208          | -11.7873        | -275.3333      |                   |
| 4                            |                | crRuns         | -8.5517           | -8.3967         | -271.9095      |                   |
| 5                            | nBB            |                | -19.0690*         | -18.8356*       | -282.1700*     |                   |
| * Optimal Value Of Criterion |                |                |                   |                 |                |                   |
| Stepwise Selection Summary   |                |                |                   |                 |                |                   |
| Step                         | Effect Entered | Effect Removed | CP                | SBC             | PRESS          |                   |
| 0                            | Intercept      |                | 375.9275          | -57.2041        | 208.7381       |                   |
| 1                            | crRuns         |                | 111.2315          | -194.3166       | 123.9195       |                   |
| 2                            | nHits          |                | 33.4438           | -252.5794       | 97.6368        |                   |
| 3                            | yrMajor        |                | 18.5870           | -262.7322       | 92.2998        |                   |
| 4                            |                | crRuns         | 22.3357           | -262.8353       | 93.1482        |                   |
| 5                            | nBB            |                | 11.3524*          | -269.7804*      | 89.5434*       |                   |
| * Optimal Value Of Criterion |                |                |                   |                 |                |                   |
| Stepwise Selection Summary   |                |                |                   |                 |                |                   |
| Step                         | Effect Entered | Effect Removed | ASE               | F Value         | Pr > F         |                   |
| 0                            | Intercept      |                | 0.7877            | 0.00            | 1.0000         |                   |
| 1                            | crRuns         |                | 0.4578            | 188.01          | <.0001         |                   |
| 2                            | nHits          |                | 0.3592            | 71.42           | <.0001         |                   |
| 3                            | yrMajor        |                | 0.3383            | 15.96           | <.0001         |                   |
| 4                            |                | crRuns         | 0.3454            | 5.44            | 0.0204         |                   |
| 5                            | nBB            |                | 0.3294            | 12.62           | 0.0005         |                   |
| * Optimal Value Of Criterion |                |                |                   |                 |                |                   |

Figure 45.7 Criterion Panel



The stop reason and stop details tables in Figure 45.8 gives details of why the selection process terminated. This table shows that at step five the best add candidate, 'division', and the best drop candidate, 'nBB', yield models with SBC values of  $-268.6094$  and  $-262.8353$ , respectively. Both of these values are larger than the current SBC value of  $-269.7804$ , and so the selection process stops at the model at step five.

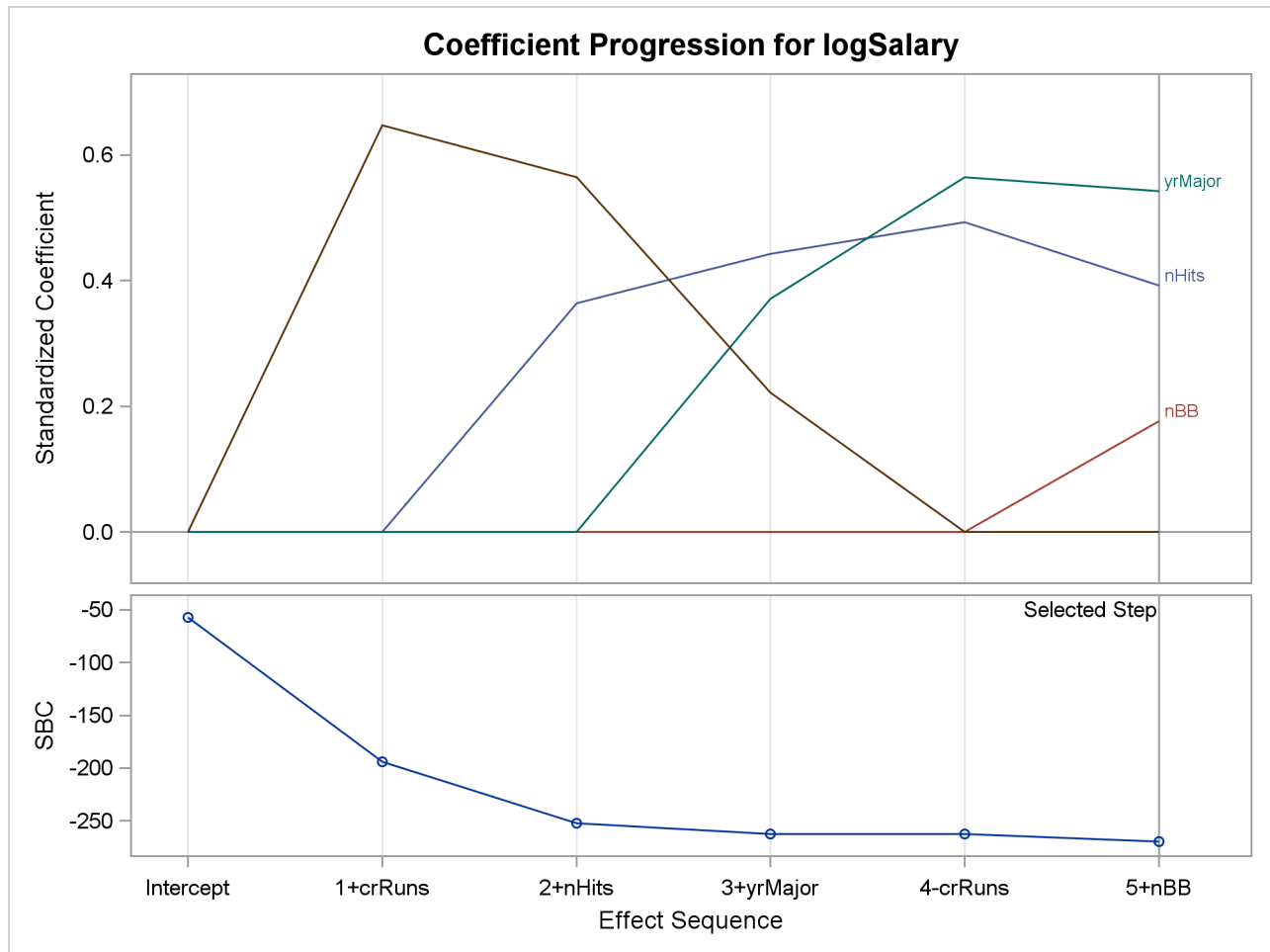
Figure 45.8 Stopping Details

| Selection stopped at a local minimum of the SBC criterion. |          |               |             |
|------------------------------------------------------------|----------|---------------|-------------|
| Stop Details                                               |          |               |             |
| Candidate For                                              | Effect   | Candidate SBC | Compare SBC |
| Entry                                                      | division | -268.6094     | > -269.7804 |
| Removal                                                    | nBB      | -262.8353     | > -269.7804 |



The coefficient panel in [Figure 45.9](#) enables you to visualize the selection process. In this plot, standardized coefficients of all the effects selected at some step of the stepwise method are plotted as a function of the step number. This enables you to assess the relative importance of the effects selected at any step of the selection process as well as providing information as to when effects entered the model. The lower plot in the panel shows how the criterion used to choose the selected model changes as effects enter or leave the model.

**Figure 45.9** Coefficient Progression



The selected effects, analysis of variance, fit statistics, and parameter estimates tables shown in [Figure 45.10](#) give details of the selected model.

Figure 45.10 Details of the Selected Model

| The GLMSELECT Procedure                                    |     |                |                |         |
|------------------------------------------------------------|-----|----------------|----------------|---------|
| Selected Model                                             |     |                |                |         |
| The selected model is the model at the last step (Step 5). |     |                |                |         |
| Effects: Intercept nHits nBB yrMajor                       |     |                |                |         |
| Analysis of Variance                                       |     |                |                |         |
| Source                                                     | DF  | Sum of Squares | Mean Square    | F Value |
| Model                                                      | 3   | 120.52553      | 40.17518       | 120.12  |
| Error                                                      | 259 | 86.62820       | 0.33447        |         |
| Corrected Total                                            | 262 | 207.15373      |                |         |
| Root MSE                                                   |     | 0.57834        |                |         |
| Dependent Mean                                             |     | 5.92722        |                |         |
| R-Square                                                   |     | 0.5818         |                |         |
| Adj R-Sq                                                   |     | 0.5770         |                |         |
| AIC                                                        |     | -19.06903      |                |         |
| AICC                                                       |     | -18.83557      |                |         |
| BIC                                                        |     | -282.17004     |                |         |
| C(p)                                                       |     | 11.35235       |                |         |
| PRESS                                                      |     | 89.54336       |                |         |
| SBC                                                        |     | -269.78041     |                |         |
| ASE                                                        |     | 0.32938        |                |         |
| Parameter Estimates                                        |     |                |                |         |
| Parameter                                                  | DF  | Estimate       | Standard Error | t Value |
| Intercept                                                  | 1   | 4.013911       | 0.111290       | 36.07   |
| nHits                                                      | 1   | 0.007929       | 0.000994       | 7.98    |
| nBB                                                        | 1   | 0.007280       | 0.002049       | 3.55    |
| yrMajor                                                    | 1   | 0.100663       | 0.007551       | 13.33   |

PROC GLMSELECT provides you with the flexibility to use several selection methods and many fit criteria for selecting effects that enter or leave the model. You can also specify criteria to determine when to stop the selection process and to choose among the models at each step of the selection process. You can find continued exploration of the baseball data that uses a variety of these methods in [Example 45.1](#).

---

## Syntax: GLMSELECT Procedure

The following statements are available in the GLMSELECT procedure:

```

PROC GLMSELECT < options > ;
 BY variables ;
 CLASS variable < (v-options) > < variable < (v-options ...) > > < / v-options > < options > ;
 CODE < options > ;
 EFFECT name = effect-type (variables < / options >) ;
 FREQ variable ;
 MODEL variable = < effects > < / options > ;
 MODELAVERAGE < options > ;
 OUTPUT < OUT=SAS-data-set > < keyword< =name > > < ... keyword< =name > > ;
 PARTITION < options > ;
 PERFORMANCE < options > ;
 SCORE < DATA=SAS-data-set > < OUT=SAS-data-set > ;
 STORE < OUT= > item-store-name < / LABEL='label' > ;
 WEIGHT variable ;

```

All statements other than the **MODEL** statement are optional and multiple **SCORE** statements can be used. **CLASS** and **EFFECT** statements, if present, must precede the **MODEL** statement.

The **STORE** and **CODE** statements are also used by many other procedures. A summary description of functionality and syntax for these statements is also shown after the **PROC GLMSELECT** statement in alphabetical order, but you can find full documentation about them in the section “**STORE Statement**” on page 501 of Chapter 19, “Shared Concepts and Topics.”

---

## PROC GLMSELECT Statement

```

PROC GLMSELECT < options > ;

```

The **PROC GLMSELECT** statement invokes the GLMSELECT procedure. Table 45.1 summarizes the options available in the **PROC GLMSELECT** statement.

**Table 45.1** PROC GLMSELECT Statement Options

| Option                  | Description                                         |
|-------------------------|-----------------------------------------------------|
| <b>Data Set Options</b> |                                                     |
| <b>DATA=</b>            | Names a data set to use for the regression          |
| <b>MAXMACRO=</b>        | Sets the maximum number of macro variables produced |
| <b>TESTDATA=</b>        | Names a data set that contains test data            |
| <b>VALDATA=</b>         | Names a data set that contains validation data      |

Table 45.1 *continued*

| Option                      | Description                                                    |
|-----------------------------|----------------------------------------------------------------|
| <b>ODS Graphics Options</b> |                                                                |
| PLOTS=                      | Produces ODS graphical displays                                |
| <b>Other Options</b>        |                                                                |
| OUTDESIGN=                  | Requests a data set that contains the design matrix            |
| NAMELEN=                    | Sets the length of effect names in tables and output data sets |
| NOPRINT                     | Suppresses displayed output including plots                    |
| SEED=                       | Sets the seed used for pseudo-random number generation         |

Following are explanations of the options that you can specify in the PROC GLMSELECT statement (in alphabetical order).

**DATA=SAS-data-set**

names the SAS data set to be used by PROC GLMSELECT. If the DATA= option is not specified, PROC GLMSELECT uses the most recently created SAS data set. If the named data set contains a variable named `_ROLE_`, then this variable is used to assign observations for training, validation, and testing roles. See the section “Using Validation and Test Data” on page 3577 for details on using the `_ROLE_` variable.

**MAXMACRO=*n***

specifies the maximum number of macro variables with selected effects to create. By default, MAXMACRO=100. PROC GLMSELECT saves the list of selected effects in a macro variable, `&_GLSIND`. Say your input effect list consists of `x1-x10`. Then `&_GLSIND` would be set to `x1 x3 x4 x10` if, for example, the first, third, fourth, and tenth effects were selected for the model. This list can be used, for example, in the model statement of a subsequent procedure. If you specify the OUTDESIGN= option in the PROC GLMSELECT statement, then PROC GLMSELECT saves the list of columns in the design matrix in a macro variable named `&_GLSMOD`.

With BY processing, one macro variable is created for each BY group, and the macro variables are indexed by the BY group number. The MAXMACRO= option can be used to either limit or increase the number of these macro variables when you are processing data sets with many BY groups.

With no BY processing, PROC GLMSELECT creates the following:

|                              |                                                                          |
|------------------------------|--------------------------------------------------------------------------|
| <code>_GLSIND</code>         | selected effects                                                         |
| <code>_GLSIND1</code>        | selected effects                                                         |
| <code>_GLSMOD</code>         | design matrix columns                                                    |
| <code>_GLSMOD1</code>        | design matrix columns                                                    |
| <code>_GLSNUMBYS</code>      | number of BY groups                                                      |
| <code>_GLSNUMMACROBYS</code> | number of <code>_GLSIND<sub>i</sub></code> macro variables actually made |

With BY processing, PROC GLMSELECT creates the following:

|                                    |                                                                                                                                                                                                                              |
|------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>_GLSIND</code>               | selected effects for BY group 1                                                                                                                                                                                              |
| <code>_GLSIND1</code>              | selected effects for BY group 1                                                                                                                                                                                              |
| <code>_GLSIND2</code>              | selected effects for BY group 2                                                                                                                                                                                              |
| .                                  |                                                                                                                                                                                                                              |
| .                                  |                                                                                                                                                                                                                              |
| .                                  |                                                                                                                                                                                                                              |
| <code>_GLSIND<math>m</math></code> | selected effects for BY group $m$ , where a number is substituted for $m$                                                                                                                                                    |
| <code>_GLSMOD</code>               | design matrix columns for BY group 1                                                                                                                                                                                         |
| <code>_GLSMOD1</code>              | design matrix columns for BY group 1                                                                                                                                                                                         |
| <code>_GLSMOD2</code>              | design matrix columns for BY group 2                                                                                                                                                                                         |
| .                                  |                                                                                                                                                                                                                              |
| .                                  |                                                                                                                                                                                                                              |
| .                                  |                                                                                                                                                                                                                              |
| <code>_GLSMOD<math>m</math></code> | design matrix columns for BY group $m$ , where a number is substituted for $m$                                                                                                                                               |
| <code>_GLSNUMBYS</code>            | $n$ , the number of BY groups                                                                                                                                                                                                |
| <code>_GLSNUMMACROBYS</code>       | the number $m$ of <code>_GLSIND<math>i</math></code> macro variables actually made. This value can be less than <code>_GLSNUMBYS = <math>n</math></code> , and it is less than or equal to the <code>MAXMACRO=</code> value. |

See the section “[Macro Variables Containing Selected Models](#)” on page 3572 for further details.

#### **NOPRINT**

suppresses all displayed output including plots.

#### **NAMELEN= $n$**

specifies the length of effect names in tables and output data sets to be  $n$  characters long, where  $n$  is a value between 20 and 200 characters. The default length is 20 characters.

#### **OUTDESIGN < (*options*) >< =SAS-data-set >**

creates a data set that contains the design matrix. By default, the GLMSELECT procedure includes in the OUTDESIGN data set the X matrix corresponding to the parameters in the selected model. Two schemes for naming the columns of the design matrix are available. In the first scheme, names of the parameters are constructed from the parameter labels that appear in the ParameterEstimates table. This naming scheme is the default when you do not request BY processing and is not available when you do use BY processing. In the second scheme, the design matrix column names consist of a prefix followed by an index. The default naming prefix is `_X`.

You can specify the following *options* in parentheses to control the contents of the OUTDESIGN data set:

#### **ADDINPUTVARS**

requests that all variables in the input data set be included in the OUTDESIGN= data set.

#### **FULLMODEL**

specifies that parameters corresponding to all the effects specified in the MODEL statement be included in the OUTDESIGN= data set. By default, only parameters corresponding to the selected model are included.

**NAMES**

produces a table associating columns in the OUTDESIGN data set with the labels of the parameters they represent.

**PREFIX=<prefix>**

requests that the design matrix column names consist of a prefix followed by an index. The default naming prefix is `_X`. You can optionally specify a different prefix.

**PARMLABELSTYLE=options**

specifies how parameter names and labels are constructed for nested and crossed effects.

The following *options* are available:

**INTERLACED <(SEPARATOR=quoted string)>**

forms parameter names and labels by positioning levels of classification variables and constructed effects adjacent to the associated variable or constructed effect name and using “ \* ” as the delimiter for both crossed and nested effects. This style of naming parameters and labels is used in the TRANSREG procedure. You can request truncation of the classification variable names used in forming the parameter names and labels by using the CPREFIX= and LPREFIX= options in the CLASS statement. You can use the SEPARATOR= suboption to change the delimiter between the crossed variables in the effect. PARMLABELSTYLE=INTERLACED is not supported if you specify the SPLIT option in an EFFECT statement or a CLASS statement. The following are examples of the parameter labels in this style (Age is a continuous variable, Gender and City are classification variables):

```
Age
Gender male * City Beijing
City London * Age
```

**SEPARATE**

specifies that in forming parameter names and labels, the effect name appears before the levels associated with the classification variables and constructed effects in the effect. You can control the length of the effect name by using the NAMELEN= option in the PROC GLMSELECT statement. In forming parameter labels, the first level that is displayed is positioned so that it starts at the same offset in every parameter label—this enables you to easily distinguish the effect name from the levels when the parameter labels are displayed in a column in the “Parameter Estimates” table. This style of labeling is used in the GLM procedure and is the default if you do not specify the PARMLABELSTYLE option. The following are examples of the parameter labels in this style (Age is a continuous variable, Gender and City are classification variables):

```
Age
Gender*City male Beijing
Age*City London
```

**SEPARATECOMPACT**

requests the same parameter naming and labeling scheme as PARMLABELSTYLE=SEPARATE except that the first level in the parameter label is separated from the effect name by a single blank. This style of labeling is used in the PLS procedure. The following are examples of the parameter labels in this style (Age is a continuous variable, Gender and City are classification variables):

```

Age
Gender*City male Beijing
Age*City London

```

**PLOTS** <(global-plot-options)> <= plot-request <(options)>>

**PLOTS** <(global-plot-options)> <= (plot-request <(options)> <... plot-request <(options)>>>

controls the plots produced through ODS Graphics. When you specify only one plot request, you can omit the parentheses around the plot request. Here are some examples:

```

plots=all
plots=coefficients(unpack)
plots(unpack)=(criteria candidates)

```

ODS Graphics must be enabled before plots can be requested. For example:

```

ods graphics on;

proc glmselect plots=all;
 model y = x1-x100;
run;

ods graphics off;

```

For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

### Global Plot Options

The *global-options* apply to all plots generated by the GLMSELECT procedure, unless it is altered by a *specific-plot-option*.

#### ENDSTEP=*n*

specifies that the step ranges shown on the horizontal axes of plots terminates at specified step. By default, the step range shown terminates at the final step of the selection process. If you specify the ENDSTEP= option as both a global plot option and a specific plot option, then the ENDSTEP= value on the specific plot is used.

#### LOGP | LOGPVALUE

displays the natural logarithm of the entry and removal significance levels when the **SELECT=SL** option is specified.

#### MAXSTEPLABEL=*n*

specifies the maximum number of characters beyond which labels of effects on plots are truncated.

**MAXPARMLABEL= *n***

specifies the maximum number of characters beyond which parameter labels on plots are truncated.

**STARTSTEP=*n***

specifies that the step ranges shown on the horizontal axes of plots start at the specified step. By default, the step range shown starts at the initial step of the selection process. If you specify the STARTSTEP= option both as a global plot option and a specific plot option, then the STARTSTEP= value on the specific plot is used.

**STEPAXIS=EFFECT | NORMB | NUMBER**

specifies the horizontal axis to be used on the plots, where this axis represents the sequence of entering or departing effects.

**STEPAXIS=EFFECT**

requests that each step be labeled by a prefix followed by the name of the effect that enters or leaves at that step. The prefix consists of the step number followed by a “+” sign or a “-” sign depending on whether the effect enters or leaves at that step.

**STEPAXIS=NORMB**

is valid only with LAR and LASSO selection methods and requests that the horizontal axis value at step *i* be the L1 norm of the parameters at step *i*, normalized by the L1 norm of the parameters at the final step.

**STEPAXIS=NUMBER**

requests that each step be labeled by the step number.

**UNPACK**

suppresses paneling. By default, multiple plots can appear in some output panels. Specify UNPACK to get each plot individually. You can also specify UNPACK as a suboption with CRITERIA and COEFFICIENTS.

**Specific Plot Options**

The following listing describes the specific plots and their options.

**ALL**

requests that all default plots be produced. Note that candidate plots are produced only if you specify **DETAILS=STEPS** or **DETAILS=ALL** in the **MODEL** statement.

**ASE | ASEPLOT <(aseplot-option)>**

plots the progression of the average square error on the training data, and the test and validation data whenever these data are provided with the **TESTDATA=** and **VALDATA=** options or are produced by using a **PARTITION** statement. The following *aseplot-option* option is available:

**STEPAXIS=EFFECT | NORMB | NUMBER**

specifies the horizontal axis to be used.



**CANDIDATES | CANDIDATESPLOT** <(candidatesplot-options)>

produces a needle plot of the SELECT= criterion values for the candidates for entry or removal at each step of the selection process, ordered from best to worst. Candidates plots are not available if you specify **SELECTION=NONE**, **SELECTION=LAR**, or **SELECTION=LASSO** in the **MODEL** statement, or if you have not specified **DETAILS=ALL** or **DETAILS=STEPS** in the **MODEL** statement. The following *candidatesplot-options* are available:

**LOGP | LOGPVALUE**

displays the natural logarithm of the entry and removal significance levels when the **SELECT=SL** option is specified.

**SHOW=number**

specifies the maximum number of candidates displayed at each step. The default is **SHOW=10**.

**COEFFICIENTS | COEFFICIENTPANEL** <(coefficientPanel-options)>

plots a panel of two plots. The upper plot shows the progression of the parameter values as the selection process proceeds. The lower plot shows the progression of the **CHOOSE=** criterion. If no **CHOOSE=** criterion is in effect, then the AICC criterion is displayed. The following *coefficientPanel-options* are available:

**LABELGAP=percentage**

specifies the percentage of the vertical axis range that forms the minimum gap between successive parameter labels at the final step of the coefficient progression plot. If the values of more than one parameter at the final step are closer than this gap, then the labels on all but one of these parameters is suppressed. The default value is **LABELGAP=5**. Planned enhancements to the automatic label collision avoidance algorithm will obviate the need for this option in future releases of the GLMSELECT procedure.

**LOGP | LOGPVALUE**

displays the natural logarithm of the entry and removal significance levels when the **SELECT=SL** option is specified.

**STEPAXIS=EFFECT | NORMB | NUMBER**

specifies the horizontal axis to be used.

**UNPACK | UNPACKPANEL**

displays the coefficient progression and the **CHOOSE=** criterion progression in separate plots.

**CRITERIA | CRITERIONPANEL** <(criterionPanel-options)>

plots a panel of model fit criteria. The criteria that are displayed are ADJRSQ, AIC, AICC, and SBC, as well as any other criteria that are named in the **CHOOSE=**, **SELECT=**, **STOP=**, or **STATS=** option in the **MODEL** statement. The following *criterionPanel-options* are available:

**STEPAXIS=EFFECT | NORMB | NUMBER**

specifies the horizontal axis to be used.

**UNPACK | UNPACKPANEL**

displays each criterion progression on a separate plot.

**EFFECTSELECTPCT** <(effectSelectPct-options)>

requests a bar chart whose bars correspond to effects that are selected in at least one sample when you use the **MODEL AVERAGE** statement. The length of a bar corresponds to the percentage of samples where the selected model contains the effect the bar represents. The **EFFECTSELECTPCT** option is ignored if you do not specify a **MODEL AVERAGE** statement. The following *effectSelectPct-options* are available:

**MINPCT=percent**

specifies that effects that appear in fewer than the specified percentage of the sample selected models not be included in the plot. By default, effects that are shown in the EffectSelectPct table are displayed.

**ORDER=ASCENDING | DESCENDING | MODEL**

specifies the ordering of the effects in the bar chart. **ORDER=MODEL** specifies that effects appear in the order in which they appear in the **MODEL** statement. **ORDER=ASCENDING | DESCENDING** specifies that the effects are shown in ascending or descending order of the number of samples in which the effects appear in the selected model. The default is **ORDER=DESCENDING**.

**NONE**

suppresses all plots.

**PARMDIST** <(parmDist-options)>

produces a panel that shows histograms and box plots of the parameter estimate values across samples when you use a **MODEL AVERAGE** statement. There is a histogram and box plot for each parameter that appears in the AvgParmEst table. The **PARMDIST** option is ignored if you do not specify a **MODEL AVERAGE** statement. The following *parmDist-options* are available:

**MINPCT=percent**

specifies that distributions be shown only for parameters whose estimates are nonzero in at least the specified percentage of the selected models. By default, distributions are shown for the all parameters that appear in the AvgParmEst table.

**ORDER=ASCENDING | DESCENDING | MODEL**

specifies the ordering of the parameters in the panels. **ORDER=MODEL** specifies that parameters be shown in the order in which the corresponding effects appear in the **MODEL** statement. **ORDER=ASCENDING | DESCENDING** specifies that the parameters be shown in an ascending or descending order of the number of samples in which the parameter estimate is nonzero. The default is **ORDER=DESCENDING**.

**NOBOXPLOTS**

suppress the box plots.

**PLOTSPERPANEL=number**

specifies the maximum number of parameter distributions that appear in a panel. If the number of relevant parameters is greater than *number*, then multiple panels are produced. Valid values are 1–16 with 9 as the default.

**UNPACK**

specifies that the distribution for each relevant parameter be shown in a separate plot.

**SEED=number**

specifies an integer used to start the pseudo-random number generator for resampling the data, random cross validation, and random partitioning of data for training, testing, and validation. If you do not specify a seed, or if you specify a value less than or equal to zero, the seed is generated from reading the time of day from the computer's clock.

**TESTDATA=SAS-data-set**

names a SAS data set containing test data. This data set must contain all the variables specified in the **MODEL** statement. Furthermore, when a **BY** statement is used and the **TESTDATA=data set** contains any of the **BY** variables, then the **TESTDATA=** data set must also contain all the **BY** variables sorted in the order of the **BY** variables. In this case, only the test data for a specific **BY** group is used with the corresponding **BY** group in the analysis data. If the **TESTDATA=** data set contains none of the **BY** variables, then the entire **TESTDATA =** data set is used with each **BY** group of the analysis data.

If you specify a **TESTDATA=data set**, then you cannot also reserve observations for testing by using a **PARTITION** statement.

**VALDATA=SAS-data-set**

names a SAS data set containing validation data. This data set must contain all the variables specified in the **MODEL** statement. Furthermore, when a **BY** statement is used and the **VALDATA=data set** contains any of the **BY** variables, then the **VALDATA=** data set must also contain all the **BY** variables sorted in the order of the **BY** variables. In this case, only the validation data for a specific **BY** group are used with the corresponding **BY** group in the analysis data. If the **VALDATA=** data set contains none of the **BY** variables, then the entire **VALDATA =** data set is used with each **BY** group of the analysis data.

If you specify a **VALDATA=data set**, then you cannot also reserve observations for validation by using a **PARTITION** statement.

---

## BY Statement

**BY variables ;**

You can specify a **BY** statement with **PROC GLMSELECT** to obtain separate analyses of observations in groups that are defined by the **BY** variables. When a **BY** statement appears, the procedure expects the input data set to be sorted in order of the **BY** variables. If you specify more than one **BY** statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the **SORT** procedure with a similar **BY** statement.
- Specify the **NOTSORTED** or **DESCENDING** option in the **BY** statement for the **GLMSELECT** procedure. The **NOTSORTED** option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the **BY** variables) and that these groups are not necessarily in alphabetical or increasing numeric order.

- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

---

## CLASS Statement

**CLASS** *variable* <(v-options)> . . . <*variable* <(v-options)>> </options> ;

The CLASS statement names the classification variables to be used in the analysis. The CLASS statement must precede the MODEL statement.

Table 45.2 summarizes the options available in the CLASS statement.

**Table 45.2** CLASS Statement Options

| Option     | Description                                                |
|------------|------------------------------------------------------------|
| CPREFIX=   | Specifies maximum number of CLASS variable name characters |
| DELIMITER= | Specifies the delimiter                                    |
| DESCENDING | Reverses the sort order                                    |
| LPREFIX=   | Labels design variables                                    |
| MISSING    | Allows for missing values                                  |
| ORDER=     | Specifies the sort order                                   |
| PARAM=     | Specifies the parameterization method                      |
| REF=       | Specifies the reference level                              |
| SHOW       | Requests a table for each CLASS variable                   |
| SPLIT      | Splits CLASS variables into independent effects            |

The following options can be specified after a slash (/):

### **DELIMITER=***quoted character*

specifies the delimiter that is used between levels of classification variables in building parameter names and lists of class level values. The default if you do not specify DELIMITER= is a space. This option is useful if the levels of a classification variable contain embedded blanks.

### **SHOW | SHOWCODING**

requests a table for each classification variable that shows the coding used for that variable.

You can specify various *v-options* for each variable by enclosing them in parentheses after the variable name. You can also specify global *v-options* for the CLASS statement by placing them after a slash (/). Global *v-options* are applied to all the variables specified in the CLASS statement. If you specify more than one CLASS statement, the global *v-options* specified in any one CLASS statement apply to all CLASS statements. However, individual CLASS variable *v-options* override the global *v-options*.

The following *v-options* are available:

**CPREFIX=*n***

specifies that, at most, the first *n* characters of a CLASS variable name be used in creating names for the corresponding design variables. The default is  $32 - \min(32, \max(2, f))$ , where *f* is the formatted length of the CLASS variable. The CPREFIX= applies only when you specify the PARMLABELSTYLE=INTERLACED option in the PROC GLMSELECT statement.

**DESCENDING****DESC**

reverses the sort order of the classification variable.

**LPREFIX=*n***

specifies that, at most, the first *n* characters of a CLASS variable label be used in creating labels for the corresponding design variables. The default is  $256 - \min(256, \max(2, f))$ , where *f* is the formatted length of the CLASS variable. The LPREFIX= applies only when you specify the PARM-LABELSTYLE=INTERLACED option in the PROC GLMSELECT statement.

**MISSING**

allows missing value (‘.’ for a numeric variable and blanks for a character variables) as a valid value for the CLASS variable.

**ORDER=DATA | FORMATTED | FREQ | INTERNAL**

specifies the sort order for the levels of classification variables. This ordering determines which parameters in the model correspond to each level in the data, so the ORDER= option might be useful when you use the CONTRAST or ESTIMATE statement. If ORDER=FORMATTED for numeric variables for which you have supplied no explicit format, the levels are ordered by their internal values. Note that this represents a change from previous releases for how class levels are ordered. Before SAS 8, numeric class levels with no explicit format were ordered by their BEST12. formatted values, and in order to revert to the previous ordering you can specify this format explicitly for the affected classification variables. The change was implemented because the former default behavior for ORDER=FORMATTED often resulted in levels not being ordered numerically and usually required the user to intervene with an explicit format or ORDER=INTERNAL to get the more natural ordering. The following table shows how PROC GLMSELECT interprets values of the ORDER= option.

| Value of ORDER=  | Levels Sorted By                                                                                                                       |
|------------------|----------------------------------------------------------------------------------------------------------------------------------------|
| <b>DATA</b>      | Order of appearance in the input data set                                                                                              |
| <b>FORMATTED</b> | External formatted value, except for numeric variables with no explicit format, which are sorted by their unformatted (internal) value |
| <b>FREQ</b>      | Descending frequency count; levels with the most observations come first in the order                                                  |
| <b>INTERNAL</b>  | Unformatted value                                                                                                                      |

By default, ORDER=FORMATTED. For FORMATTED and INTERNAL, the sort order is machine dependent.

For more information about sort order, see the chapter on the SORT procedure in the *Base SAS Procedures Guide* and the discussion of BY-group processing in *SAS Language Reference: Concepts*.

**PARAM=keyword**

specifies the parameterization method for the classification variable or variables. Design matrix columns are created from CLASS variables according to the following coding schemes. The default is PARAM=GLM. If PARAM=ORTHOPOLY or PARAM=POLY, and the CLASS levels are numeric, then the ORDER= option in the CLASS statement is ignored, and the internal, unformatted values are used. See the section “CLASS Variable Parameterization and the SPLIT Option” on page 3570 for further details.

|                    |                                                                                                        |
|--------------------|--------------------------------------------------------------------------------------------------------|
| <b>EFFECT</b>      | specifies effect coding.                                                                               |
| <b>GLM</b>         | specifies less-than-full-rank, reference-cell coding; this option can be used only as a global option. |
| <b>ORDINAL</b>     |                                                                                                        |
| <b>THERMOMETER</b> | specifies the cumulative parameterization for an ordinal CLASS variable.                               |
| <b>POLYNOMIAL</b>  |                                                                                                        |
| <b>POLY</b>        | specifies polynomial coding.                                                                           |
| <b>REFERENCE</b>   |                                                                                                        |
| <b>REF</b>         | specifies reference-cell coding.                                                                       |
| <b>ORTHEFFECT</b>  | orthogonalizes PARAM=EFFECT.                                                                           |
| <b>ORTHORDINAL</b> |                                                                                                        |
| <b>ORTHOTHERM</b>  | orthogonalizes PARAM=ORDINAL.                                                                          |
| <b>ORTHOPOLY</b>   | orthogonalizes PARAM=POLYNOMIAL.                                                                       |
| <b>ORTHREF</b>     | orthogonalizes PARAM=REFERENCE.                                                                        |

The EFFECT, POLYNOMIAL, REFERENCE, and ORDINAL schemes and their orthogonal parameterizations are full rank. The REF= option in the CLASS statement determines the reference level for the EFFECT and REFERENCE schemes and their orthogonal parameterizations.

**REF='level' | keyword**

specifies the reference level for PARAM=EFFECT, PARAM=REFERENCE, and their orthogonalizations. For an individual (but not a global) variable REF= option, you can specify the *level* of the variable to use as the reference level. For a global or individual variable REF= option, you can use one of the following keywords. The default is REF=LAST.

|              |                                                  |
|--------------|--------------------------------------------------|
| <b>FIRST</b> | designates the first-ordered level as reference. |
| <b>LAST</b>  | designates the last-ordered level as reference.  |

**SPLIT**

splits the columns of the design matrix that correspond to any effect that contains a split classification variable so that they can enter or leave a model independently of the other design columns for that effect. For example, suppose a variable named `temp` has three levels with values 'hot', 'warm', and 'cold', and a variable named `sex` has two levels with values 'M' and 'F' are used in a PROC GLMSELECT job as follows:

```
proc glmselect;
 class temp sex/split;
 model depVar = sex sex*temp;
run;
```

The two effects named in the **MODEL** statement are split into eight independent effects. The effect 'sex' is split into two effects labeled 'sex\_M' and 'sex\_F'. The effect 'sex\*temp' is split into six effects labeled 'sex\_M\*temp\_hot', 'sex\_F\*temp\_hot', 'sex\_M\*temp\_warm', 'sex\_F\*temp\_warm', 'sex\_M\*temp\_cold', and 'sex\_F\*temp\_cold'. Thus the previous PROC GLMSELECT step is equivalent to the following step:

```
proc glmselect;
 model depVar = sex_M sex_F sex_M*temp_hot sex_F*temp_hot
 sex_M*temp_warm sex_F*temp_warm
 sex_M*temp_cold sex_F*temp_cold;
run;
```

The split option can be used on individual classification variables. For example, consider the following PROC GLMSELECT step:

```
proc glmselect;
 class temp(split) sex;
 model depVar = sex sex*temp;
run;
```

In this case the effect 'sex' is not split and the effect 'sex\*temp' is split into three effects labeled 'sex\*temp\_hot', 'sex\*temp\_warm', and 'sex\*temp\_cold'. Furthermore each of these three split effects now has two parameters that correspond to the two levels of 'sex', and the PROC GLMSELECT step is equivalent to the following:

```
proc glmselect;
 class sex;
 model depVar = sex sex*temp_hot sex*temp_warm sex*temp_cold;
run;
```

---

## CODE Statement

**CODE** < options > ;

The CODE statement enables you to write SAS DATA step code for computing predicted values of the fitted model either to a file or to a catalog entry. This code can then be included in a DATA step to score new data.

Table 45.3 summarizes the *options* available in the CODE statement.

**Table 45.3** CODE Statement Options

| Option    | Description                                                                  |
|-----------|------------------------------------------------------------------------------|
| CATALOG=  | Names the catalog entry where the generated code is saved                    |
| DUMMIES   | Retains the dummy variables in the data set                                  |
| ERROR     | Computes the error function                                                  |
| FILE=     | Names the file where the generated code is saved                             |
| FORMAT=   | Specifies the numeric format for the regression coefficients                 |
| GROUP=    | Specifies the group identifier for array names and statement labels          |
| IMPUTE    | Imputes predicted values for observations with missing or invalid covariates |
| LINESIZE= | Specifies the line size of the generated code                                |
| LOOKUP=   | Specifies the algorithm for looking up CLASS levels                          |
| RESIDUAL  | Computes residuals                                                           |

For details about the syntax of the CODE statement, see the section “CODE Statement” on page 390 in Chapter 19, “Shared Concepts and Topics.”

---

## EFFECT Statement

**EFFECT** *name=effect-type (variables < / options >)* ;

The EFFECT statement enables you to construct special collections of columns for design matrices. These collections are referred to as *constructed effects* to distinguish them from the usual model effects that are formed from continuous or classification variables, as discussed in the section “GLM Parameterization of Classification Variables and Effects” on page 383 in Chapter 19, “Shared Concepts and Topics.”

You can specify the following *effect-types*:

|                          |                                                                                                                                                                                                     |
|--------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>COLLECTION</b>        | is a collection effect that defines one or more variables as a single effect with multiple degrees of freedom. The variables in a collection are considered as a unit for estimation and inference. |
| <b>LAG</b>               | is a classification effect in which the level that is used for a given period corresponds to the level in the preceding period.                                                                     |
| <b>MULTIMEMBER   MM</b>  | is a multimember classification effect whose levels are determined by one or more variables that appear in a CLASS statement.                                                                       |
| <b>POLYNOMIAL   POLY</b> | is a multivariate polynomial effect in the specified numeric variables.                                                                                                                             |



**SPLINE** is a regression spline effect whose columns are univariate spline expansions of one or more variables. A spline expansion replaces the original variable with an expanded or larger set of new variables.

Table 45.4 summarizes the *options* available in the EFFECT statement.

**Table 45.4** EFFECT Statement Options

| Option                             | Description                                                                                                                                           |
|------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Collection Effects Options</b>  |                                                                                                                                                       |
| DETAILS                            | Displays the constituents of the collection effect                                                                                                    |
| <b>Lag Effects Options</b>         |                                                                                                                                                       |
| DESIGNROLE=                        | Names a variable that controls to which lag design an observation is assigned                                                                         |
| DETAILS                            | Displays the lag design of the lag effect                                                                                                             |
| NLAG=                              | Specifies the number of periods in the lag                                                                                                            |
| PERIOD=                            | Names the variable that defines the period                                                                                                            |
| WITHIN=                            | Names the variable or variables that define the group within which each period is defined                                                             |
| <b>Multimember Effects Options</b> |                                                                                                                                                       |
| NOEFFECT                           | Specifies that observations with all missing levels for the multi-member variables should have zero values in the corresponding design matrix columns |
| WEIGHT=                            | Specifies the weight variable for the contributions of each of the classification effects                                                             |
| <b>Polynomial Effects Options</b>  |                                                                                                                                                       |
| DEGREE=                            | Specifies the degree of the polynomial                                                                                                                |
| MDEGREE=                           | Specifies the maximum degree of any variable in a term of the polynomial                                                                              |
| STANDARDIZE=                       | Specifies centering and scaling suboptions for the variables that define the polynomial                                                               |
| <b>Spline Effects Options</b>      |                                                                                                                                                       |
| BASIS=                             | Specifies the type of basis (B-spline basis or truncated power function basis) for the spline expansion                                               |
| DEGREE=                            | Specifies the degree of the spline transformation                                                                                                     |
| KNOTMETHOD=                        | Specifies how to construct the knots for spline effects                                                                                               |

For more information about the syntax of these *effect-types* and how columns of constructed effects are computed, see the section “EFFECT Statement” on page 393 in Chapter 19, “Shared Concepts and Topics.”

---

## FREQ Statement

**FREQ** *variable* ;

The variable specified in the FREQ statement identifies a variable in the input data set containing the frequency of occurrence of each observation. PROC GLMSELECT treats each observation as if it appears  $n$  times, where  $n$  is the value of the FREQ variable for the observation. If it is not an integer, the frequency value is truncated to an integer. If it is less than 1 or if it is missing, the observation is not used.

---

## MODEL Statement

**MODEL** *dependent* = < *effects* > / < *options* > ;

The MODEL statement names the dependent variable and the explanatory effects, including covariates, main effects, constructed effects, interactions, and nested effects; see the section “Specification of Effects” on page 3324 in Chapter 42, “The GLM Procedure,” for more information. If you omit the explanatory effects, the procedure fits an intercept-only model.

After the keyword MODEL, the dependent (response) variable is specified, followed by an equal sign. The explanatory effects follow the equal sign.

Table 45.5 summarizes the options available in the MODEL statement.

**Table 45.5** MODEL Statement Options

| Option      | Description                                                                                                 |
|-------------|-------------------------------------------------------------------------------------------------------------|
| CVDETAILS=  | Requests details when cross validation is used                                                              |
| CVMETHOD=   | Specifies how subsets for cross validation are formed                                                       |
| DETAILS=    | Specifies details to be displayed                                                                           |
| HIERARCHY=  | Specifies the hierarchy of effects to impose                                                                |
| NOINT       | Specifies models without an explicit intercept                                                              |
| ORDERSELECT | Requests that parameter estimates be displayed in the order in which the parameters first entered the model |
| SELECTION=  | Specifies the model selection method                                                                        |
| STATS=      | Specifies additional statistics to be displayed                                                             |
| SHOWPVALUES | Requests $p$ -values in “ANOVA” and “Parameter Estimates” tables                                            |
| STB         | Adds standardized coefficients to “Parameter Estimates” tables                                              |

You can specify the following options in the MODEL statement after a slash (/):

**CVDETAILS=ALL**

**CVDETAILS=COEFFS**

**CVDETAILS=CVPRESS**

specifies the details produced when cross validation is requested as the **CHOOSE=**, **SELECT=**, or **STOP=** criterion in the MODEL statement. If  $n$ -fold cross validation is being used, then the training data are subdivided into  $n$  parts, and at each step of the selection process, models are obtained on

each of the  $n$  subsets of the data obtained by omitting one of these parts. `CVDETAILS=COEFFS` requests that the parameter estimates obtained for each of these  $n$  subsets be included in the parameter estimates table. `CVDETAILS=CVPRESS` requests a table containing the predicted residual sum of squares of each of these models scored on the omitted subset. `CVDETAILS=ALL` requests both `CVDETAILS=COEFFS` and `CVDETAILS=CVPRESS`. If `DETAILS=STEPS` or `DETAILS=ALL` has been specified in the `MODEL` statement, then the requested `CVDETAILS` are produced for every step of the selection process.

**CVMETHOD=BLOCK**  $\langle (n) \rangle$

**CVMETHOD=RANDOM**  $\langle (n) \rangle$

**CVMETHOD=SPLIT**  $\langle (n) \rangle$

**CVMETHOD=INDEX** (*variable*)

specifies how the training data are subdivided into  $n$  parts when you request  $n$ -fold cross validation by using any of the `CHOOSE=CV`, `SELECT=CV`, and `STOP=CV` suboptions of the `SELECTION=` option in the `MODEL` statement.

- `CVMETHOD=BLOCK` requests that parts be formed of  $n$  blocks of consecutive training observations.
- `CVMETHOD=SPLIT` requests that the  $i$ th part consist of training observations  $i, i + n, i + 2n, \dots$
- `CVMETHOD=RANDOM` assigns each training observation randomly to one of the  $n$  parts.
- `CVMETHOD=INDEX(variable)` assigns observations to parts based on the formatted value of the named variable. This input data set variable is treated as a classification variable and the number of parts  $n$  is the number of distinct levels of this variable. By optionally naming this variable in a `CLASS` statement you can use the `CLASS` statement options `ORDER=` and `MISSING` to control how the levelization of this variable is done.

$n$  defaults to 5 with `CVMETHOD=BLOCK`, `CVMETHOD=SPLIT`, or `CVMETHOD=RANDOM`. If you do not specify the `CVMETHOD=` option, then the `CVMETHOD` defaults to `CVMETHOD=RANDOM(5)`.

**DETAILS=level**

**DETAILS=STEPS**  $\langle (step\ options) \rangle$

specifies the level of detail produced, where *level* can be `ALL`, `STEPS`, or `SUMMARY`. The default if the `DETAILS=` option is omitted is `DETAILS=SUMMARY`. The `DETAILS=ALL` option produces the following:

- entry and removal statistics for each variable selected in the model building process
- ANOVA, fit statistics, and parameter estimates
- entry and removal statistics for the top 10 candidates for inclusion or exclusion at each step
- a selection summary table

The `DETAILS=SUMMARY` option produces only the selection summary table.

The option `DETAILS=STEPS`  $\langle (step\ options) \rangle$  provides the step information and the selection summary table. The following options can be specified within parentheses after the `DETAILS=STEPS` option:

**ALL**

requests ANOVA, fit statistics, parameter estimates, and entry or removal statistics for the top 10 candidates for inclusion or exclusion at each selection step.

**ANOVA**

requests ANOVA at each selection step.

**FITSTATISTICS | FITSTATS | FIT**

requests fit statistics at each selection step. The default set of statistics includes all of the statistics named in the **CHOOSE=**, **SELECT=**, and **STOP=** suboptions specified in the **MODEL** statement **SELECTION=** option, but additional statistics can be requested with the **STATS=** option in the **MODEL** statement.

**PARAMETERESTIMATES | PARMEST**

requests parameter estimates at each selection step.

**CANDIDATES <(SHOW= ALL | n)>**

requests entry or removal statistics for the best  $n$  candidate effects for inclusion or exclusion at each step. If you specify **SHOW=ALL**, then all candidates are shown. If **SHOW=** is not specified, then the best 10 candidates are shown. The entry or removal statistic is the statistic named in the **SELECT=** option that is specified in the **MODEL** statement **SELECTION=** option.

**HIERARCHY=keyword****HIER=keyword**

specifies whether and how the model hierarchy requirement is applied. This option also controls whether a single effect or multiple effects are allowed to enter or leave the model in one step. You can specify that only classification effects, or both classification and continuous effects, be subject to the hierarchy requirement. The **HIERARCHY=** option is ignored unless you also specify one of the following options: **SELECTION=FORWARD**, **SELECTION=BACKWARD**, or **SELECTION=STEPWISE**.

Model hierarchy refers to the requirement that for any term to be in the model, all model effects contained in the term must be present in the model. For example, in order for the interaction  $A*B$  to enter the model, the main effects  $A$  and  $B$  must be in the model. Likewise, neither effect  $A$  nor effect  $B$  can leave the model while the interaction  $A*B$  is in the model.

The keywords you can specify in the **HIERARCHY=** option are as follows:

**NONE**

specifies that model hierarchy not be maintained. Any single effect can enter or leave the model at any given step of the selection process.

**SINGLE**

specifies that only one effect enter or leave the model at one time, subject to the model hierarchy requirement. For example, suppose that the model contains the main effects  $A$  and  $B$  and the interaction  $A*B$ . In the first step of the selection process, either  $A$  or  $B$  can enter the model. In the second step, the other main effect can enter the model. The interaction effect can enter the model only when both main effects have already entered. Also, before  $A$  or  $B$  can be removed from the model, the  $A*B$  interaction must first be removed. All effects (**CLASS** and **interval**) are subject to the hierarchy requirement.

**SINGLECLASS**

is the same as HIERARCHY=SINGLE except that only CLASS effects are subject to the hierarchy requirement.

The default value is HIERARCHY=NONE.

**NOINT**

suppresses the intercept term that is otherwise included in the model.

**ORDERSELECT**

specifies that for the selected model, effects be displayed in the order in which they first entered the model. If you do not specify the ORDERSELECT option, then effects in the selected model are displayed in the order in which they appeared in the MODEL statement.

**SELECTION=method <(method options)>**

specifies the method used to select the model, optionally followed by parentheses enclosing options applicable to the specified method. The default if the SELECTION= option is omitted is SELECTION=STEPWISE.

The following methods are available and are explained in detail in the section “[Model-Selection Methods](#)” on page 3559.

|                 |                                                                                                                                                                                                                                                                                                                                                                                                                         |
|-----------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>NONE</b>     | no model selection                                                                                                                                                                                                                                                                                                                                                                                                      |
| <b>FORWARD</b>  | forward selection. This method starts with no effects in the model and adds effects.                                                                                                                                                                                                                                                                                                                                    |
| <b>BACKWARD</b> | backward elimination. This method starts with all effects in the model and deletes effects.                                                                                                                                                                                                                                                                                                                             |
| <b>STEPWISE</b> | stepwise regression. This is similar to the FORWARD method except that effects already in the model do not necessarily stay there.                                                                                                                                                                                                                                                                                      |
| <b>LAR</b>      | least angle regression. This method, like forward selection, starts with no effects in the model and adds effects. The parameter estimates at any step are “shrunk” when compared to the corresponding least squares estimates. If the model contains classification variables, then these classification variables are split. See the <a href="#">SPLIT</a> option in the <a href="#">CLASS</a> statement for details. |
| <b>LASSO</b>    | This method adds and deletes parameters based on a version of ordinary least squares where the sum of the absolute regression coefficients is constrained. If the model contains classification variables, then these classification variables are split. See the <a href="#">SPLIT</a> option in the <a href="#">CLASS</a> statement for details.                                                                      |

[Table 45.6](#) lists the applicable suboptions for each of these methods.

**Table 45.6** Applicable SELECTION= Options by Method

| Option     | FORWARD | BACKWARD | STEPWISE | LAR LASSO |
|------------|---------|----------|----------|-----------|
| STOP =     | x       | x        | x        | x         |
| CHOOSE =   | x       | x        | x        | x         |
| STEPS =    | x       | x        | x        | x         |
| MAXSTEPS = | x       | x        | x        | x         |
| SELECT =   | x       | x        | x        |           |
| INCLUDE =  | x       | x        | x        |           |
| SLENTRY =  | x       |          | x        |           |
| SLSTAY =   |         | x        | x        |           |
| DROP =     |         |          | x        |           |
| ADAPTIVE   |         |          |          | x         |
| LSCOEFFS   |         |          |          | x         |

The syntax of the suboptions that you can specify in parentheses after the SELECTION= option method follows. Note that, as described in Table 45.6, not all selection suboptions are applicable to every SELECTION= method.

**ADAPTIVE** <(< **GAMMA**=*non-negative number* > < **INEST**=*SAS-data-set* > )>

requests that adaptive weights be applied to each of the coefficients in the LAR and LASSO methods. You use the optional INEST= option to name the SAS data set that contains estimates which are used to form the adaptive weights for all the parameters in the model. If you do not specify an INEST= data set, then ordinary least squares estimates of the parameters in the model are used in forming the adaptive weights. You use the GAMMA= option to specify the power transformation that is applied to the parameters in forming the adaptive weights. The default value is GAMMA=1.

**CHOOSE**=*criterion*

specifies the criterion for choosing the model. The specified *criterion* is evaluated at each step of the selection process, and the model that yields the best value of the criterion is chosen. If the optimal value of the criterion occurs for models at more than one step, then the model with the smallest number of parameters is chosen. If you do not specify the CHOOSE= option, then the model at the final step in the selection process is selected.

The criteria that you can specify in the CHOOSE= option are shown in Table 45.7. See the section “Criteria Used in Model Selection Methods” on page 3568 for more detailed descriptions of these criteria.

**Table 45.7** Criteria for the CHOOSE= Option

| <i>Criterion</i> | <b>Criterion</b>                                                      |
|------------------|-----------------------------------------------------------------------|
| <b>ADJRSQ</b>    | Adjusted R-square statistic                                           |
| <b>AIC</b>       | Akaike's information criterion                                        |
| <b>AICC</b>      | Corrected Akaike's information criterion                              |
| <b>BIC</b>       | Sawa Bayesian information criterion                                   |
| <b>CP</b>        | Mallows' C(p) statistic                                               |
| <b>CV</b>        | Predicted residual sum of square with <i>k</i> -fold cross validation |
| <b>PRESS</b>     | Predicted residual sum of squares                                     |
| <b>SBC</b>       | Schwarz Bayesian information criterion                                |
| <b>VALIDATE</b>  | Average square error for the validation data                          |

For ADJRSQ the chosen value is the largest one; for all other criteria, the smallest value is chosen. You can use the CHOOSE=VALIDATE option only if you have specified a VALDATA= data set in the PROC GLMSELECT statement or if you have reserved part of the input data for validation by using either a PARTITION statement or a \_ROLE\_ variable in the input data.

**DROP=*policy***

specifies when effects are eligible to be dropped in the STEPWISE method. Valid values for policy are BEFOREADD and COMPETITIVE.

If you specify DROP=BEFOREADD, then effects currently in the model are examined to see if any meet the requirements to be removed from the model. If so, the effect that gives the best value of the removal criterion is dropped from the model and the stepwise method proceeds to the next step. Only when no effect currently in the model meets the requirement to be removed from the model are any effects added to the model.

DROP=COMPETITIVE can be specified only if the SELECT= criterion is not SL. If you specify DROP=COMPETITIVE, then the SELECT= criterion is evaluated for all models where an effect currently in the model is dropped or an effect not yet in the model is added. The effect whose removal or addition to the model yields the maximum improvement to the SELECT= criterion is dropped or added.

The default if you do not specify DROP= suboption with the STEPWISE method is DROP=BEFOREADD. If SELECT=SL, then this yields the traditional stepwise method as implemented in PROC REG.

**INCLUDE=*n***

forces the first *n* effects listed in the MODEL statement to be included in all models. The selection methods are performed on the other effects in the MODEL statement. The INCLUDE= option is available only with SELECTION=FORWARD, SELECTION=STEPWISE, and SELECTION=BACKWARD.

**LSCOEFFS**

requests a hybrid version of the LAR and LASSO methods, where the sequence of models is determined by the LAR or LASSO algorithm but the coefficients of the parameters for the model at any step are determined by using ordinary least squares.

**MAXSTEP=*n***

specifies the maximum number of selection steps that are done. The default value of *n* is the number of effects in the model statement for the FORWARD, BACKWARD, and LAR methods and is three times the number of effects for the STEPWISE and LASSO methods.

**SELECT=*criterion***

specifies the criterion that PROC GLMSELECT uses to determine the order in which effects enter and/or leave at each step of the specified selection method. The SELECT= option is not valid with the LAR and LASSO methods. The criteria that you can specify with the SELECT= option are ADJRSQ, AIC, AICC, BIC, CP, CV, PRESS, RSQUARE, SBC, SL, and VALIDATE. See the section “Criteria Used in Model Selection Methods” on page 3568 for a description of these criteria. The default value of the SELECT= criterion is SELECT=SBC. You can use SELECT=SL to request the traditional approach where effects enter and leave the model based on the significance level. With other SELECT= criteria, the effect that is selected to enter or leave at a step of the selection process is the effect whose addition to or removal from the current model gives the maximum improvement in the specified criterion.

**SLENTRY=*value*****SLE=*value***

specifies the significance level for entry, used when the STOP=SL or SELECT=SL option is in effect. The defaults are 0.50 for FORWARD and 0.15 for STEPWISE.

**SLSTAY=*value*****SLS=*value***

specifies the significance level for staying in the model, used when the STOP=SL or SELECT=SL option is in effect. The defaults are 0.10 for BACKWARD and 0.15 for STEPWISE.

**STEPS=*n***

specifies the number of selection steps to be done. If the STEPS= option is specified, the STOP= and MAXSTEP= options are ignored.

**STOP=*n*****STOP=*criterion***

specifies when PROC GLMSELECT stops the selection process. If the STEPS= option is specified, then the STOP= option is ignored. If the STOP=option does not cause the selection process to stop before the maximum number of steps for the selection method, then the selection process terminates at the maximum number of steps.

If you do not specify the STOP= option but do specify the SELECT= option, then the criterion named in the SELECT=option is also used as the STOP= criterion. If you do not specify either the STOP= or SELECT= option, then the default is STOP=SBC.

If STOP=*n* is specified, then PROC GLMSELECT stops selection at the first step for which the selected model has *n* effects.

The nonnumeric arguments that you can specify in the STOP= option are shown in Table 45.8. See the section “Criteria Used in Model Selection Methods” on page 3568 for more detailed descriptions of these criteria.



**Table 45.8** Nonnumeric Criteria for the STOP= Option

| Option          | Criteria                                                              |
|-----------------|-----------------------------------------------------------------------|
| <b>NONE</b>     |                                                                       |
| <b>ADJRSQ</b>   | Adjusted R-square statistic                                           |
| <b>AIC</b>      | Akaike's information criterion                                        |
| <b>AICC</b>     | Corrected Akaike's information criterion                              |
| <b>BIC</b>      | Sawa Bayesian information criterion                                   |
| <b>CP</b>       | Mallows' C(p) statistic                                               |
| <b>CV</b>       | Predicted residual sum of square with <i>k</i> -fold cross validation |
| <b>PRESS</b>    | Predicted residual sum of squares                                     |
| <b>SBC</b>      | Schwarz Bayesian information criterion                                |
| <b>SL</b>       | Significance level                                                    |
| <b>VALIDATE</b> | Average square error for the validation data                          |

With the SL criterion, selection stops at the step where the significance level for entry of all the effects not yet in the model is greater than the SLE= value for addition steps in the FORWARDS and STEPWISE methods and where the significance level for removal of any effect in the current model is greater than the SLS= value in the BACKWARD and STEPWISE methods. With the ADJRSQ criterion, selection stops at the step where the next step would yield a model with a smaller value of the Adjusted R-square statistic; for all other criteria, selection stops at the step where the next step would yield a model with a larger value of the criteria. You can use the VALIDATE option only if you have specified a VALDATA= data set in the PROC GLMSELECT statement or if you have reserved part of the input data for validation by using either a PARTITION statement or a \_ROLE\_ variable in the input data.

**STAT|STATS=***name*

**STATS=**(*names*)

specifies which model fit statistics are displayed in the fit summary table and fit statistics tables. If you omit the STATS= option, the default set of statistics that are displayed in these tables includes all the criteria specified in any of the CHOOSE=, SELECT=, and STOP= options specified in the MODEL statement SELECTION= option.

The statistics that you can specify follow:

|               |                                                                                                                                                                                                                                                                                                                                                                                          |
|---------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>ADJRSQ</b> | the adjusted R-square statistic                                                                                                                                                                                                                                                                                                                                                          |
| <b>AIC</b>    | Akaike's information criterion                                                                                                                                                                                                                                                                                                                                                           |
| <b>AICC</b>   | corrected Akaike's information criterion                                                                                                                                                                                                                                                                                                                                                 |
| <b>ASE</b>    | the average square errors for the training, test, and validation data. The ASE statistics for the test and validation data are reported only if you have specified TEST-DATA= and/or VALDATA= in the PROC GLMSELECT statement or if you have reserved part of the input data for testing and/or validation by using either a PARTITION statement or a _ROLE_ variable in the input data. |
| <b>BIC</b>    | the Sawa Bayesian information criterion                                                                                                                                                                                                                                                                                                                                                  |
| <b>CP</b>     | the Mallows' C(p) statistic                                                                                                                                                                                                                                                                                                                                                              |

- FVALUE**            the  $F$  statistic for entering or departing effects
- PRESS**             the predicted residual sum of squares statistic
- RSQUARE**         the R-square statistic
- SBC**                the Schwarz Bayesian information criterion
- SL**                 the significance level of the  $F$  statistic for entering or departing effects

The statistics ADJRSQ, AIC, AICC, FVALUE, RSQUARE, SBC, and SL can be computed with little computation cost. However, computing BIC, CP, CVPRESS, PRESS, and ASE for test and validation data when these are not used in any of the **CHOOSE=**, **SELECT=**, and **STOP=** options specified in the MODEL statement **SELECTION=** option can hurt performance.

**SHOWPVALUES**

**SHOWPVALS**

displays  $p$ -values in the “ANOVA” and “Parameter Estimates” tables. These  $p$ -values are generally liberal because they are not adjusted for the fact that the terms in the model have been selected.

**STB**

produces standardized regression coefficients. A standardized regression coefficient is computed by dividing a parameter estimate by the ratio of the sample standard deviation of the dependent variable to the sample standard deviation of the regressor.

**MODEL AVERAGE Statement (Experimental)**

**MODEL AVERAGE** < options > ;

The experimental MODEL AVERAGE statement requests that model selection be repeated on resampled subsets of the input data. An average model is produced by averaging the parameter estimates of the selected models that are obtained for each resampled subset of the input data.

Table 45.9 summarizes the options available in the MODEL AVERAGE statement.

**Table 45.9** MODEL AVERAGE Statement Options

| <b>Option</b>    | <b>Description</b>                                                     |
|------------------|------------------------------------------------------------------------|
| <b>ALPHA=</b>    | Specifies lower and upper quantiles of the sample parameter            |
| <b>DETAILS</b>   | Displays model selection details                                       |
| <b>NSAMPLES=</b> | Specifies the number of samples used for the refit averaging           |
| <b>REFIT</b>     | Performs a second round of model averaging                             |
| <b>SAMPLING=</b> | Specifies how to generate the samples taken from the training data     |
| <b>SUBSET</b>    | Uses only a subset of the selected models in forming the average model |
| <b>TABLES</b>    | Controls the displayed tables                                          |

The following *options* are available:

**ALPHA= $\alpha$**

controls which lower and upper quantiles of the sample parameter estimates are displayed. The ALPHA= option also controls which quantiles of the predicted values are added to the output data set when the LOWER= and UPPER= options are specified in the OUTPUT statement. The lower and upper quantiles used are  $\alpha/2$  and  $1 - \alpha/2$ , respectively. The value specified must lie in the interval  $[0, 1]$ . The default value is ALPHA=0.5.

**DETAILS**

requests that model selection details be displayed for each sample of the data. The level of detail shown is controlled by the DETAILS= option in the MODEL statement.

**NSAMPLES= $n$**

specifies the number of samples to be used. The default value is NSAMPLES=100.

**REFIT <(refit-options)>**

requests that a second round of model averaging, referred to as the refit averaging, be performed. Usually, the initial round of model averaging produces a model that contains a large number of effects. You can use the refit option to obtain a more parsimonious model. For each data sample in the refit, a least squares model is fit with no effect selection. The effects that are used in the refit depend on the results of the initial round of model averaging. If you do not specify any *refit-options*, then effects that are selected in at least twenty percent of the samples in the initial round of model averaging are used in the refit model average. The following *refit-options* are available:

**BEST= $n$**

specifies that the  $n$  most frequently selected effects in the initial round of model averaging be used in the refit averaging.

**MINPCT=*percent***

specifies that the effects that are selected at least the specified percentage of times in the initial round of model averaging be used in the refit averaging.

**NSAMPLES= $n$**

specifies the number of samples to be used for the refit averaging. The default value is the number of samples used in the initial round of model averaging.

**SAMPLING=SRS | URS <(sampling-options)>**

specifies how the samples of the usable observations in the training data are generated. SAMPLING=SRS specifies simple random sampling in which samples are generated by randomly drawing without replacement. SAMPLING=URS specifies unrestricted random sampling in which samples are generated by randomly drawing with replacement. Model averaging with samples drawn without replacement corresponds to the bootstrap methodology. The default is SAMPLING=URS. If you specify a frequency variable by using a FREQ statement, then the  $i$ th observation is sampled  $f_i$  times, where  $f_i$  is the frequency of the  $i$ th observation.

You can specify one of the following *sampling-options*:

**PERCENT=percent**

specifies the percentage of the training data that is used in each sample. The default value is 75% for SAMPLING=SRS and 100% for SAMPLING=URS.

**SIZE=n**

specifies the sum of frequencies in each sample.

**SUBSET(subset-options)**

specifies that only a subset of the selected models be used in forming the average model and producing predicted values. The following *subset-options* are available:

**BEST=n**

specifies that only the best *n* models be used, where the model ranking criterion used is the frequency score. See the section “Model Selection Frequencies and Frequency Scores” on page 3577 for the definition of the frequency score. If multiple models with the same frequency score correspond to the *n*th best model, then all these tied models are used in forming the average model and producing predicted values.

**MINMODELFREQ=freq**

specifies that only models that are selected at least *freq* times be used in forming the average model and producing predicted values.

**TABLES <(ONLY)> <=table-request <(options)>>**

**TABLES <(ONLY)> <= (table-request <(options)> <... table-request <(options)>>>**

controls the displayed output that is produced in the initial round of model averaging. By default, the following tables are produced:

**EFFECTSELECTPCT** displays the percentage of times that effects appear in the selected models.

**MODELSELECTFREQ** displays the frequency with which models are selected.

**AVGPAREST** displays the mean, standard deviation, and quantiles of the parameter estimates of the parameters that appear in the selected models.

When you specify only one *table-request*, you can omit the outer parentheses. Here are some examples:

```
tables=none
tables=(all parmest (minpct=10))
tables(only)=effectselectpct (order=model minpct=15)
```

The following *table-request* options are available:

**ALL**

requests that all model averaging output tables be produced. You can specify other options with ALL; for example, to request all tables and to require that effects are displayed in decreasing order of selection frequency in the EffectSelectPct table, specify TABLES=(ALL EFFECTSELECTPCT(ORDER=DESCENDING)).

**EFFECTSELECTPCT** < (*effectSelectPct-options*) >

specifies how the effects in the EffectSelectPct table are displayed. The following *effectSelectPct-options* are available:

**ALL**

specifies that effects that appear in the selected model for any sample be displayed.

**MINPCT=percent**

specifies that the effects displayed must appear in the selected model for at least the specified percentage of the samples. By default, this table includes effects that appear in at least twenty percent of the selected models. The MINPCT= option is ignored if you also specify the ALL option as a *effectSelectPct* option.

**ORDER=ASCENDING | DESCENDING | MODEL**

specifies the order in which the effects are displayed. ORDER=MODEL specifies that effects be displayed in the order in which they appear in the **MODEL** statement. ORDER=ASCENDING | DESCENDING specifies that the effects be displayed in ascending or descending order of their selection frequency.

**MODELSELECTFREQ** < (*modelSelectFreq-options*) >

specifies how the models in the ModelSelectFreq table are displayed. The following *modelSelectFreq-options* are available:

**ALL**

specifies that all selected models be displayed in the ModelSelectFreq table.

**BEST=*n***

specifies that only the best *n* models be displayed, where the model ranking criterion used is the frequency score. See the section “[Model Selection Frequencies and Frequency Scores](#)” on page 3577 for the definition of the frequency score. The default value is BEST=20. The BEST= option is ignored if you also specify the ALL option as a *modelSelectFreq-option*.

**ONLY**

suppresses the default output. If you specify the ONLY option within parentheses after the TABLES option, then only the tables specifically requested are produced.

**PARMEST** < (*parmEst-options*) >

specifies how the parameters in the AvgParmEst table are displayed. The following *parmEst-options* are available:

**ALL**

specifies that parameters that are nonzero in the selected model for any sample be displayed.

**MINPCT=percent**

specifies that the parameters displayed must have nonzero estimates in the selected model for at least the specified percentage of the samples. By default, this table includes parameters that appear in at least twenty percent of the selected models. The MINPCT= option is ignored if you also specify the ALL option as a *parmEst* option.

**NONZEROPARMS**

specifies that for each parameter, the sample that is used to compute the estimate mean, standard deviation, and quantiles consist of just the nonzero values of that parameter in the selected models. If you do not specify the NONZEROPARMS option, then parameters that do not appear in a selected model are assigned the value zero in that model and these zero values are retained when computing the estimate means, standard deviations, and quantiles.

**ORDER=ASCENDING | DESCENDING | MODEL**

specifies the order in which the effects are displayed. ORDER=MODEL specifies that effects are displayed in the order in which they appear in the MODEL statement. ORDER=ASCENDING | DESCENDING specifies that the effects are displayed in ascending or descending order of their selection frequency.

---

## OUTPUT Statement

**OUTPUT** < **OUT=SAS-data-set** > < *keyword* < =*name* > > ... < *keyword* < =*name* > > ;

The OUTPUT statement creates a new SAS data set that saves diagnostic measures calculated for the selected model. If you do not specify a *keyword*, then the only diagnostic included is the predicted response.

All the variables in the original data set are included in the new data set, along with variables created in the OUTPUT statement. These new variables contain the values of a variety of statistics and diagnostic measures that are calculated for each observation in the data set. If you specify a BY statement, then a variable `_BY_` that indexes the BY groups is included. For each observation, the value of `_BY_` is the index of the BY group to which this observation belongs. This variable is useful for matching BY groups with macro variables that PROC GLMSELECT creates. See the section “[Macro Variables Containing Selected Models](#)” on page 3572 for details.

If you have requested *n*-fold cross validation by requesting **CHOOSE=CV**, **SELECT=CV**, or **STOP=CV** in the MODEL statement, then a variable `_CVINDEX_` is included in the output data set. For each observation used for model training the value of `_CVINDEX_` is *i* if that observation is omitted in forming the *i*th subset of the training data. See the **CVMETHOD=** for additional details. The value of `_CVINDEX_` is 0 for all observations in the input data set that are not used for model training.

If you have partitioned the input data with a **PARTITION** statement, then a character variable `_ROLE_` is included in the output data set. For each observation the value of `_ROLE_` is as follows:

|                     |                  |
|---------------------|------------------|
| <code>_ROLE_</code> | Observation Role |
| TEST                | testing          |
| TRAIN               | training         |
| VALIDATE            | validation       |

If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*.

Details on the specifications in the OUTPUT statement follow.

*keyword* < =*name* >

specifies the statistics to include in the output data set and optionally names the new variables that contain the statistics. Specify a keyword for each desired statistic (see the following list of keywords), followed optionally by an equal sign, and a variable to contain the statistic.

If you specify *keyword=name*, the new variable that contains the requested statistic has the specified name. If you omit the optional *=name* after a *keyword*, then the new variable name is formed by using a prefix of one or more characters that identify the statistic. For residuals and predicted values, the prefix is followed by an underscore ( ), followed by the dependent variable name.

The keywords allowed and the statistics they represent are as follows:

**PREDICTED | PRED | P** predicted values. The prefix for the default name is *p*.

**RESIDUAL | RESID | R** residual, calculated as ACTUAL – PREDICTED. The prefix for the default name is *r*.

When you also use the **MODEL AVERAGE** statement, the following keywords and the statistics that they represent are also available:

**LOWER**  $\alpha/2$  percentile of the sample predicted values. By default,  $\alpha = 0.5$ , which yields the 25th percentile. You can change the value of  $\alpha$  by using the ALPHA= option in the **MODEL AVERAGE** statement. The default name is *LOWER*.

**MEDIAN** median of the sample predicted values. The default name is *median*.

**SAMPLEFREQ | SF** sample frequencies. For the *i*th sample, a column that contains the frequencies used for that sample is added. The name of this column is formed by appending an index *i* to the name that you specify. If you do not specify a name, then the default prefix is *sf*.

**SAMPLEPRED | SP** sample predictions. For the *i*th sample, a column that contains the predicted values produced by the model selected for that sample is added. The name of this column is formed by appending an index *i* to the name that you specify. If you do not specify a name, then the default prefix is *sp*.

**STANDARDDEVIATION | STDDEV** standard deviation of the sample predicted values. The default name is *stdDev*.

**UPPER**  $1 - \alpha/2$  percentile of the sample predicted values. By default,  $\alpha = 0.5$ , which yields the 75th percentile. You can change the value of  $\alpha$  by using the ALPHA= option in the **MODEL AVERAGE** statement. The default name is *UPPER*.

**OUT=SAS data set**

specifies the name of the new data set. By default, the procedure uses the *DATA*n** convention to name the new data set.

---

## PARTITION Statement

The **PARTITION** statement specifies how observations in the input data set are logically partitioned into disjoint subsets for model training, validation, and testing. Either you can designate a variable in the input data set and a set of formatted values of that variable to determine the role of each observation, or you can specify proportions to use for random assignment of observations for each role.

An alternative to using a **PARTITION** statement is to provide a variable named `_ROLE_` in the input data set to define roles of observations in the input data. If you specify a **PARTITION** statement then the `_ROLE_`



variable if present in the input data set is ignored. If you do not use a PARTITION statement and the input data do not contain a variable named `_ROLE_`, then all observations in the input data set are assigned to model training.

The following mutually exclusive options are available:

**ROLEVAR | ROLE=variable(< TEST='value' > < TRAIN='value' > < VALIDATE='value' >)**

names the variable in the input data set whose values are used to assign roles to each observation. The formatted values of this variable that are used to assign observations roles are specified in the TEST=, TRAIN=, and VALIDATE= suboptions. If you do not specify the TRAIN= suboption, then all observations whose role is not determined by the TEST= or VALIDATE= suboptions are assigned to training. If you specify a TESTDATA= data set in the PROC GLMSELECT statement, then you cannot also specify the TEST= suboption in the PARTITION statement. If you specify a VALDATA= data set in the PROC GLMSELECT statement, then you cannot also specify the VALIDATE= suboption in the PARTITION statement.

**FRACTION(< TEST=fraction > < VALIDATE=fraction >)**

requests that specified proportions of the observations in the input data set be randomly assigned training and validation roles. You specify the proportions for testing and validation by using the TEST= and VALIDATE= suboptions. If you specify both the TEST= and the VALIDATE= suboptions, then the sum of the specified fractions must be less than one and the remaining fraction of the observations are assigned to the training role. If you specify a TESTDATA= data set in the PROC GLMSELECT statement, then you cannot also specify the TEST= suboption in the PARTITION statement. If you specify a VALDATA= data set in the PROC GLMSELECT statement, then you cannot also specify the VALIDATE= suboption in the PARTITION statement.

---

## PERFORMANCE Statement

**PERFORMANCE** < options > ;

The PERFORMANCE statement is used to change default options that affect the performance of PROC GLMSELECT and to request tables that show the performance options in effect and timing details.

The following options are available:

**DETAILS**

requests the PerfSettings table that shows the performance settings in effect and the Timing table that provides a broad timing breakdown of the PROC GLMSELECT step.

**BUILDSSCP=FULL**

**BUILDSSCP=INCREMENTAL**

specifies whether the SSCP matrix is built incrementally as the selection process progresses or whether the SSCP matrix for the full model is built at the outset. Building the SSCP matrix incrementally can significantly reduce the memory required and the time taken to perform model selection in cases where the number of parameters in the selected model is much smaller than the number of parameters in the full model, but it can hurt performance in other cases since it requires at least one pass through the model training data at each step. If you use backward selection or no selection, or if the BIC or CP statistics are required in the selection process, then the BUILDSSCP=INCREMENTAL option is ignored. In other cases, BUILDSSCP=INCREMENTAL is used by default if the number



of effects is greater than 100. See the section “Building the SSCP Matrix” on page 3575 for further details.

---

## SCORE Statement

```
SCORE < DATA=SAS-data-set > < OUT=SAS-data-set > < keyword< =name > > ... < keyword< =name > >
 ;
```

The SCORE statement creates a new SAS data set containing predicted values and optionally residuals for data in a new data set that you name. If you do not specify a DATA= data set, then the input data are scored. If you have multiple data sets to predict, you can specify multiple SCORE statements. If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*.

When a BY statement is used, the score data set must either contain all the BY variables sorted in the order of the BY variables or contain none of the BY variables. If the score data set contains all of the BY variables, then the model selected for a given BY group is used to score just the matching observations in the score data set. If the score data set contains none of the BY variables, then the entire score data set is scored for each BY group.

All observations in the score data set are retained in the output data set. However, only those observations that contain nonmissing values for all the continuous regressors in the selected model and whose levels of the class variables appearing in effects of the selected model are represented in the corresponding class variable in the procedure’s input data set are scored. All the variables in the input data set are included in the output data set, along with variables containing predicted values and optionally residuals.

Details on the specifications in the SCORE statement follow:

### DATA=SAS data set

names the data set to be scored. If you omit this option, then the input data set named in the DATA= option in the PROC GLMSELECT statement is scored.

### keyword< =name >

specifies the statistics to include in the output data set and optionally names the new variables that contain the statistics. Specify a keyword for each desired statistic (see the following list of keywords), followed optionally by an equal sign, and a variable to contain the statistic.

If you specify *keyword=name*, the new variable that contains the requested statistic has the specified name. If you omit the optional *=name* after a *keyword*, then the new variable name is formed by using a prefix of one or more characters that identify the statistic, followed by an underscore (\_), followed by the dependent variable name.

The keywords allowed and the statistics they represent are as follows:

**PREDICTED | PRED | P** predicted values. The prefix for the default name is *p*.

**RESIDUAL | RESID | R** residual, calculated as ACTUAL – PREDICTED. The prefix for the default name is *r*.

**OUT=SAS data set**

gives the name of the new output data set. By default, the procedure uses the *DATA*n** convention to name the new data set.

## STORE Statement

**STORE** < **OUT=** > *item-store-name* < / **LABEL=** 'label' > ;

The STORE statement requests that the procedure save the context and results of the statistical analysis. The resulting item store has a binary file format that cannot be modified. The contents of the item store can be processed with the PLM procedure.

For details about the syntax of the STORE statement, see the section “STORE Statement” on page 501 in Chapter 19, “Shared Concepts and Topics.”

## WEIGHT Statement

**WEIGHT** *variable* ;

A WEIGHT statement names a variable in the input data set with values that are relative weights for a weighted least squares fit. If the weight value is proportional to the reciprocal of the variance for each observation, then the weighted estimates are the best linear unbiased estimates (BLUE).

Values of the weight variable must be nonnegative. If an observation’s weight is zero, the observation is deleted from the analysis. If a weight is negative or missing, it is set to zero, and the observation is excluded from the analysis. A more complete description of the WEIGHT statement can be found in Chapter 42, “The GLM Procedure.”

## Details: GLMSELECT Procedure

### Model-Selection Methods

The model selection methods implemented in PROC GLMSELECT are specified with the **SELECTION=** option in the **MODEL** statement.

#### Full Model Fitted (NONE)

The complete model specified in the **MODEL** statement is used to fit the model and no effect selection is done. You request this by specifying **SELECTION=NONE** in the **MODEL** statement.

#### Forward Selection (FORWARD)

The forward selection technique begins with just the intercept and then sequentially adds the effect that most improves the fit. The process terminates when no significant improvement can be obtained by adding any effect.

In the traditional implementation of forward selection, the statistic used to gauge improvement in fit is an  $F$  statistic that reflects an effect's contribution to the model if it is included. At each step, the effect that yields the most significant  $F$  statistic is added. Note that because effects can contribute different degrees of freedom to the model, it is necessary to compare the  $p$ -values corresponding to these  $F$  statistics.

More precisely, if the current model has  $p$  parameters excluding the intercept, and if you denote its residual sum of squares by  $RSS_p$  and you add an effect with  $k$  degrees of freedom and denote the residual sum of squares of the resulting model by  $RSS_{p+k}$ , then the  $F$  statistic for entry with  $k$  numerator degrees of freedom and  $n - (p + k) - 1$  denominator degrees of freedom is given by

$$F = \frac{(RSS_p - RSS_{p+k})/k}{RSS_{p+k}/(n - (p + k) - 1)}$$

where  $n$  is number of observations used in the analysis.

The process stops when the significance level for adding any effect is greater than some specified entry significance level. A well-known problem with this methodology is that these  $F$  statistics do not follow an  $F$  distribution (Draper, Guttman, and Kanemasu 1971). Hence these  $p$ -values cannot reliably be interpreted as probabilities. Various ways to approximate this distribution are described by Miller (2002). Another issue when you use significance levels of entering effects as a stopping criterion arises because the entry significance level is an a priori specification that does not depend on the data. Thus, the same entry significance level can result in overfitting for some data and underfitting for other data.

One approach to address the critical problem of when to stop the selection process is to assess the quality of the models produced by the forward selection method and choose the model from this sequence that “best” balances goodness of fit against model complexity. PROC GLMSELECT supports several criteria that you can use for this purpose. These criteria fall into two groups—information criteria and criteria based on out-of-sample prediction performance.

You use the **CHOOSE=** option of forward selection to specify the criterion for selecting one model from the sequence of models produced. If you do not specify a **CHOOSE=** criterion, then the model at the final step is the selected model.

For example, if you specify

```
selection=forward(select=SL choose=AIC SLE=0.2)
```

then forward selection terminates at the step where no effect can be added at the 0.2 significance level. However, the selected model is the first one with the minimal value of Akaike's information criterion. Note that in some cases this minimal value might occur at a step much earlier than the final step, while in other cases the AIC criterion might start increasing only if more steps are done (that is, a larger value of SLE is used). If what you are interested in is minimizing AIC, then too many steps are done in the former case and too few in the latter case. To address this issue, PROC GLMSELECT enables you to specify a stopping criterion with the **STOP=** option. With a stopping criterion specified, forward selection continues until a local extremum of the stopping criterion in the sequence of models generated is reached. You can also specify **STOP=** number, which causes forward selection to continue until there are the specified number of effects in the model.

For example, if you specify

```
selection=forward(select=SL stop=AIC)
```

then forward selection terminates at the step where the effect to be added at the next step would produce a model with an AIC statistic larger than the AIC statistic of the current model. Note that in most cases, provided that the entry significance level is large enough that the local extremum of the named criterion occurs before the final step, specifying

```
selection=forward(select=SL choose=CRITERION)
```

or

```
selection=forward(select=SL stop=CRITERION)
```

selects the same model, but more steps are done in the former case. In some cases there might be a better local extremum that cannot be reached if you specify the **STOP=** option but can be found if you use the **CHOOSE=** option. Also, you can use the **CHOOSE=** option in preference to the **STOP=** option if you want examine how the named criterion behaves as you move beyond the step where the first local minimum of this criterion occurs.

Note that you can specify both the **CHOOSE=** and **STOP=** options. You might want to consider models generated by forward selection that have at most some fixed number of effects but select from within this set based on a criterion you specify. For example, specifying

```
selection=forward(stop=20 choose=ADJRSQ)
```

requests that forward selection continue until there are 20 effects in the final model and chooses among the sequence of models the one that has the largest value of the adjusted R-square statistic. You can also combine these options to select a model where one of two conditions is met. For example,

```
selection=forward(stop=AICC choose=PRESS)
```

chooses whatever occurs first between a local minimum of the predicted residual sum of squares (PRESS) and a local minimum of corrected Akaike's information criterion (AICC).

It is important to keep in mind that forward selection bases the decision about what effect to add at any step by considering models that differ by one effect from the current model. This search paradigm cannot guarantee reaching a "best" subset model. Furthermore, the add decision is greedy in the sense that the effect deemed most significant is the effect that is added. However, if your goal is to find a model that is best in terms of some selection criterion other than the significance level of the entering effect, then even this one step choice might not be optimal. For example, the effect you would add to get a model with the smallest value of the PRESS statistic at the next step is not necessarily the same effect that has the most significant entry  $F$  statistic. PROC GLMSELECT enables you to specify the criterion to optimize at each step by using the **SELECT=** option. For example,

```
selection=forward(select=CP)
```

requests that at each step the effect that is added be the one that gives a model with the smallest value of the Mallows'  $C(p)$  statistic. Note that in the case where all effects are variables (that is, effects with one degree of freedom and no hierarchy), using ADJRSQ, AIC, AICC, BIC, CP, RSQUARE, or SBC as the selection criterion for forward selection produces the same sequence of additions. However, if the degrees of freedom contributed by different effects are not constant, or if an out-of-sample prediction-based criterion is used, then different sequences of additions might be obtained.

You can use **SELECT=** together with **CHOOSE=** and **STOP=**. If you specify only the **SELECT=** criterion, then this criterion is also used as the stopping criterion. In the previous example where only the selection criterion is specified, not only do effects enter based on the Mallows'  $C(p)$  statistic, but the selection terminates when the  $C(p)$  statistic first increases.

You can find discussion and references to studies about criteria for variable selection in Burnham and Anderson (2002), along with some cautions and recommendations.

**Examples of Forward Selection Specifications****selection=forward**

adds effects that at each step give the lowest value of the SBC statistic and stops at the step where adding any effect would increase the SBC statistic.

**selection=forward(select=SL)**

adds effects based on significance level and stops when all candidate effects for entry at a step have a significance level greater than the default entry significance level of 0.15.

**selection=forward(select=SL stop=validation)**

adds effects based on significance level and stops at a step where adding any effect increases the error sum of squares computed on the validation data.

**selection=forward(select=AIC)**

adds effects that at each step give the lowest value of the AIC statistic and stops at the step where adding any effect would increase the AIC statistic.

**selection=forward(select=ADJRSQ stop=SL SLE=0.2)**

adds effects that at each step give the largest value of the adjusted R-square statistic and stops at the step where the significance level corresponding to the addition of this effect is greater than 0.2.

**Backward Elimination (BACKWARD)**

The backward elimination technique starts from the full model including all independent effects. Then effects are deleted one by one until a stopping condition is satisfied. At each step, the effect showing the smallest contribution to the model is deleted. In traditional implementations of backward elimination, the contribution of an effect to the model is assessed by using an  $F$  statistic. At any step, the predictor producing the least significant  $F$  statistic is dropped and the process continues until all effects remaining in the model have  $F$  statistics significant at a stay significance level (SLS).

More precisely, if the current model has  $p$  parameters excluding the intercept, and if you denote its residual sum of squares by  $RSS_p$  and you drop an effect with  $k$  degrees of freedom and denote the residual sum of squares of the resulting model by  $RSS_{p-k}$ , then the  $F$  statistic for removal with  $k$  numerator degrees of freedom and  $n - p - k$  denominator degrees of freedom is given by

$$F = \frac{(RSS_{p-k} - RSS_p)/k}{RSS_p/(n - p - k)}$$

where  $n$  is number of observations used in the analysis.

Just as with forward selection, you can change the criterion used to assess effect contributions with the **SELECT=** option. You can also specify a stopping criterion with the **STOP=** option and use a **CHOOSE=** option to provide a criterion used to select among the sequence of models produced. See the discussion in the section “Forward Selection (FORWARD)” on page 3559 for additional details.

### Examples of Backward Selection Specifications

`selection=backward`

removes effects that at each step produce the largest value of the Schwarz Bayesian information criterion (SBC) statistic and stops at the step where removing any effect increases the SBC statistic.

`selection=backward(stop=press)`

removes effects based on the SBC statistic and stops at the step where removing any effect increases the predicted residual sum of squares (PRESS).

`selection=backward(select=SL)`

removes effects based on significance level and stops when all candidate effects for removal at a step have a significance level less than the default stay significance level of 0.15.

`selection=backward(select=SL choose=validate SLS=0.1)`

removes effects based on significance level and stops when all effects in the model are significant at the 0.1 level. Finally, from the sequence of models generated, choose the one that gives the smallest average square error when scored on the validation data.

### Stepwise Selection(STEPWISE)

The stepwise method is a modification of the forward selection technique that differs in that effects already in the model do not necessarily stay there.

In the traditional implementation of stepwise selection method, the same entry and removal  $F$  statistics for the forward selection and backward elimination methods are used to assess contributions of effects as they are added to or removed from a model. If at a step of the stepwise method, any effect in the model is not significant at the `SLSTAY=` level, then the least significant of these effects is removed from the model and the algorithm proceeds to the next step. This ensures that no effect can be added to a model while some effect currently in the model is not deemed significant. Only after all necessary deletions have been accomplished can another effect be added to the model. In this case the effect whose addition yields the most significant  $F$  value is added to the model and the algorithm proceeds to the next step. The stepwise process ends when none of the effects outside the model has an  $F$  statistic significant at the `SLENTRY=` level and every effect in the model is significant at the `SLSTAY=` level. In some cases, neither of these two conditions for stopping is met and the sequence of models cycles. In this case, the stepwise method terminates at the end of the second cycle.

Just as with forward selection and backward elimination, you can change the criterion used to assess effect contributions, with the `SELECT=` option. You can also specify a stopping criterion with the `STOP=` option and use a `CHOOSE=` option to provide a criterion used to select among the sequence of models produced. See the discussion in the section “[Forward Selection \(FORWARD\)](#)” on page 3559 for additional details.

For selection criteria other than significance level, PROC GLMSELECT optionally supports a further modification in the stepwise method. In the standard stepwise method, no effect can enter the model if removing any effect currently in the model would yield an improved value of the selection criterion. In the modification, you can use the `DROP=COMPETITIVE` option to specify that addition and deletion of effects should be treated competitively. The selection criterion is evaluated for all models obtained by deleting an effect from the current model or by adding an effect to this model. The action that most improves the selection criterion is the action taken.

**Examples of Stepwise Selection Specifications**

```
selection=stepwise
```

requests stepwise selection based on the SBC criterion. First, if removing any effect yields a model with a lower SBC statistic than the current model, then the effect producing the smallest SBC statistic is removed. When removing any effect increases the SBC statistic, then provided that adding some effect lowers the SBC statistic, the effect producing the model with the lowest SBC is added.

```
selection=stepwise(select=SL)
```

requests the traditional stepwise method. First, if the removal of any effect yields an  $F$  statistic that is not significant at the default stay level of 0.15, then the effect whose removal produces the least significant  $F$  statistic is removed and the algorithm proceeds to the next step. Otherwise the effect whose addition yields the most significant  $F$  statistic is added, provided that it is significant at the default entry level of 0.15.

```
selection=stepwise(select=SL stop=SBC)
```

is the traditional stepwise method, where effects enter and leave based on significance levels, but with the following extra check: If any effect to be added or removed yields a model whose SBC statistic is greater than the SBC statistic of the current model, then the stepwise method terminates at the current model. Note that in this case, the entry and stay significance levels still play a role as they determine whether an effect is deleted from or added to the model. This might result in the selection terminating before a local minimum of the SBC criterion is found.

```
selection=stepwise(select=SL SLE=0.1 SLS=0.08 choose=AIC)
```

selects effects to enter or drop as in the previous example except that the significance level for entry is now 0.1 and the significance level to stay is 0.08. From the sequence of models produced, the selected model is chosen to yield the minimum AIC statistic.

```
selection=stepwise(select=AICC drop=COMPETITIVE)
```

requests stepwise selection based on the AICC criterion with steps treated competitively. At any step, evaluate the AICC statistics corresponding to the removal of any effect in the current model or the addition of any effect to the current model. Choose the addition or removal that produced this minimum value, provided that this minimum is lower than the AICC statistic of the current model.

```
selection=stepwise(select=SBC drop=COMPETITIVE stop=VALIDATE)
```

requests stepwise selection based on the SBC criterion with steps treated competitively and where stopping is based on the average square error over the validation data. At any step, SBC statistics corresponding to the removal of any effect from the current model or the addition of any effect to the current model are evaluated. The addition or removal that produces the minimum SBC value is made. The average square error on the validation data for the model with this addition or removal is evaluated. If this average square error is greater than the average square error on the validation data prior to this addition or deletion, then the algorithm terminates at this prior model.

**Least Angle Regression (LAR)**

Least angle regression was introduced by Efron et al. (2004). Not only does this algorithm provide a selection method in its own right, but with one additional modification it can be used to efficiently produce LASSO solutions. Just like the forward selection method, the LAR algorithm produces a sequence of



regression models where one parameter is added at each step, terminating at the full least squares solution when all parameters have entered the model.

The algorithm starts by centering the covariates and response, and scaling the covariates so that they all have the same corrected sum of squares. Initially all coefficients are zero, as is the predicted response. The predictor that is most correlated with the current residual is determined and a step is taken in the direction of this predictor. The length of this step determines the coefficient of this predictor and is chosen so that some other predictor and the current predicted response have the same correlation with the current residual. At this point, the predicted response moves in the direction that is equiangular between these two predictors. Moving in this direction ensures that these two predictors continue to have a common correlation with the current residual. The predicted response moves in this direction until a third predictor has the same correlation with the current residual as the two predictors already in the model. A new direction is determined that is equiangular between these three predictors and the predicted response moves in this direction until a fourth predictor joins the set having the same correlation with the current residual. This process continues until all predictors are in the model.

As with other selection methods, the issue of when to stop the selection process is crucial. You can specify a criterion to use to choose among the models at each step with the `CHOOSE=` option. You can also specify a stopping criterion with the `STOP=` option. See the section “Criteria Used in Model Selection Methods” on page 3568 for details and Table 45.10 for the formulas for evaluating these criteria. These formulas use the approximation that at step  $k$  of the LAR algorithm, the model has  $k$  degrees of freedom. See Efron et al. (2004) for a detailed discussion of this so-called simple approximation.

A modification of LAR selection suggested in Efron et al. (2004) uses the LAR algorithm to select the set of covariates in the model at any step, but uses ordinary least squares regression with just these covariates to obtain the regression coefficients. You can request this hybrid method by specifying the `LSCOEFFS` suboption of `SELECTION=LAR`.

## Lasso Selection (LASSO)

LASSO (least absolute shrinkage and selection operator) selection arises from a constrained form of ordinary least squares regression where the sum of the absolute values of the regression coefficients is constrained to be smaller than a specified parameter. More precisely let  $\mathbf{X} = (x_1, x_2, \dots, x_m)$  denote the matrix of covariates and let  $\mathbf{y}$  denote the response, where the  $x_j$ s have been centered and scaled to have unit standard deviation and mean zero, and  $\mathbf{y}$  has mean zero. Then for a given parameter  $t$ , the LASSO regression coefficients  $\boldsymbol{\beta} = (\beta_1, \beta_2, \dots, \beta_m)$  are the solution to the constrained optimization problem

$$\text{minimize } \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|^2 \quad \text{subject to } \sum_{j=1}^m |\beta_j| \leq t$$

Provided that the LASSO parameter  $t$  is small enough, some of the regression coefficients will be exactly zero. Hence, you can view the LASSO as selecting a subset of the regression coefficients for each LASSO parameter. By increasing the LASSO parameter in discrete steps, you obtain a sequence of regression coefficients where the nonzero coefficients at each step correspond to selected parameters.

Early implementations (Tibshirani 1996) of LASSO selection used quadratic programming techniques to solve the constrained least squares problem for each LASSO parameter of interest. Later Osborne, Presnell, and Turlach (2000) developed a “homotopy method” that generates the LASSO solutions for all values of



*t.* Efron et al. (2004) derived a variant of their algorithm for least angle regression that can be used to obtain a sequence of LASSO solutions from which all other LASSO solutions can be obtained by linear interpolation. This algorithm for `SELECTION=LASSO` is used in PROC GLMSELECT. It can be viewed as a stepwise procedure with a single addition to or deletion from the set of nonzero regression coefficients at any step.

As with the other selection methods supported by PROC GLMSELECT, you can specify a criterion to choose among the models at each step of the LASSO algorithm with the `CHOOSE=` option. You can also specify a stopping criterion with the `STOP=` option. See the discussion in the section “**Forward Selection (FORWARD)**” on page 3559 for additional details. The model degrees of freedom PROC GLMSELECT uses at any step of the LASSO are simply the number of nonzero regression coefficients in the model at that step. Efron et al. (2004) cite empirical evidence for doing this but do not give any mathematical justification for this choice.

A modification of LASSO selection suggested in Efron et al. (2004) uses the LASSO algorithm to select the set of covariates in the model at any step, but uses ordinary least squares regression with just these covariates to obtain the regression coefficients. You can request this hybrid method by specifying the `LSCOEFFS` suboption of `SELECTION=LASSO`.

## Adaptive Lasso Selection

Adaptive lasso selection is a modification of lasso selection; in adaptive lasso selection weights are applied to each of the parameters in forming the lasso constraint (Zou 2006). More precisely, suppose that the response  $y$  has mean zero and the regressors  $x$  are scaled to have mean zero and common standard deviation. Furthermore, suppose that you can find a suitable estimator  $\hat{\beta}$  of the parameters in the true model and you define a weight vector by  $w = 1/|\hat{\beta}|^\gamma$ , where  $\gamma \geq 0$ . Then the adaptive lasso regression coefficients  $\beta = (\beta_1, \beta_2, \dots, \beta_m)$  are the solution to the constrained optimization problem

$$\text{minimize } \|y - \mathbf{X}\beta\|^2 \quad \text{subject to } \sum_{j=1}^m |w_j \beta_j| \leq t$$

You can specify  $\hat{\beta}$  by using the `INEST=` suboption of the `SELECTION=LASSO` option in the `MODEL` statement. The `INEST=` data set has the same structure as the `OUTEST=` data set that is produced by several SAS/STAT procedures including the `REG` and `LOGISTIC` procedures. The `INEST=` data set must contain all explanatory variables in the `MODEL` statement. It must also contain an intercept variable named `Intercept` unless the `NOINT` option is specified in the `MODEL` statement. If `BY` processing is used, the `INEST=` data set must also include the `BY` variables, and there must be one observation for each `BY` group. If the `INEST=` data set also contains the `_TYPE_` variable, only observations with `_TYPE_` value 'PARMS' are used.

If you do not specify an `INEST=` data set, then PROC GLMSELECT uses the solution to the unconstrained least squares problem as the estimator  $\hat{\beta}$ . This is appropriate unless collinearity is a concern. If the regressors are collinear or nearly collinear, then Zou (2006) suggests using a ridge regression estimate to form the adaptive weights.

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## Model Selection Issues

Many authors caution against the use of “automatic variable selection” methods and describe pitfalls that plague many such methods. For example, Harrell (2001) states that “stepwise variable selection has been a very popular technique for many years, but if this procedure had just been proposed as a statistical method, it would most likely be rejected because it violates every principle of statistical estimation and hypothesis testing.” He lists and discusses several of these issues and cites a variety of studies that highlight these problems. He also notes that many of these issues are not restricted to stepwise selection, but affect forward selection and backward elimination, as well as methods based on all-subset selection.

In their introductory chapter, Burnham and Anderson (2002) discuss many issues involved in model selection. They also strongly warn against “data dredging,” which they describe as “the process of analyzing data with few or no a priori questions, by subjectively and iteratively searching the data for patterns and ‘significance’.” However, Burnham and Anderson also discuss the desirability of finding parsimonious models. They note that using “full models” that contain many insignificant predictors might avoid some of the inferential problems arising in models with automatically selected variables but will lead to overfitting the particular sample data and produce a model that performs poorly in predicting data not used in training the model.

One problem in the traditional implementations of forward, backward, and stepwise selection methods is that they are based on sequential testing with specified entry (SLE) and stay (SLS) significance levels. However, it is known that the “ $F$ -to-enter” and “ $F$ -to-delete” statistics do not follow an  $F$  distribution (Draper, Guttman, and Kanemasu 1971). Hence the SLE and SLS values cannot reliably be viewed as probabilities. One way to address this difficulty is to replace hypothesis testing as a means of selecting a model with information criteria or out-of-sample prediction criteria. While Harrell (2001) points out that information criteria were developed for comparing only prespecified models, Burnham and Anderson (2002) note that AIC criteria have routinely been used for several decades for performing model selection in time series analysis.

Problems also arise when the selected model is interpreted as if it were prespecified. There is a “selection bias” in the parameter estimates that is discussed in detail in Miller (2002). This bias occurs because a parameter is more likely to be selected if it is above its expected value than if it is below its expected value. Furthermore, because multiple comparisons are made in obtaining the selected model, the  $p$ -values obtained for the selected model are not valid. When a single best model is selected, inference is conditional on that model.

Model averaging approaches provide a way to make more stable inferences based on a set of models. PROC GLMSELECT provides support for model averaging by averaging models that are selected on resampled data. Other approaches for performing model averaging are presented in Burnham and Anderson (2002), and Bayesian approaches are discussed in Raftery, Madigan, and Hoeting (1997).

Despite these difficulties, careful and informed use of variable selection methods still has its place in modern data analysis. For example, Foster and Stine (2004) use a modified version of stepwise selection to build a predictive model for bankruptcy from over 67,000 possible predictors and show that this yields a model whose predictions compare favorably with other recently developed data mining tools. In particular, when the goal is prediction rather than estimation or hypothesis testing, variable selection with careful use of validation to limit both under and over fitting is often a useful starting point of model development.

## Criteria Used in Model Selection Methods

PROC GLMSELECT supports a variety of fit statistics that you can specify as criteria for the **CHOOSE=**, **SELECT=**, and **STOP=** options in the **MODEL** statement. The following statistics are available:

|          |                                                                                                                                        |
|----------|----------------------------------------------------------------------------------------------------------------------------------------|
| ADJRSQ   | adjusted R-square statistic (Darlington 1968; Judge et al. 1985)                                                                       |
| AIC      | Akaike's information criterion (Darlington 1968; Judge et al. 1985)                                                                    |
| AICC     | corrected Akaike's information criterion (Hurvich and Tsai 1989)                                                                       |
| BIC      | Sawa Bayesian information criterion (Sawa 1978; Judge et al. 1985)                                                                     |
| CP       | Mallows' $C_p$ statistic (Mallows 1973; Hocking 1976)                                                                                  |
| PRESS    | predicted residual sum of squares statistic                                                                                            |
| SBC      | Schwarz Bayesian information criterion (Schwarz 1978; Judge et al. 1985)                                                               |
| SL       | significance level of the $F$ statistic used to assess an effect's contribution to the fit when it is added to or removed from a model |
| VALIDATE | average square error over the validation data                                                                                          |

Table 45.10 provides formulas and definitions for the fit statistics.

**Table 45.10** Formulas and Definitions for Model Fit Summary Statistics

| Statistic        | Definition or Formula                                                                         |
|------------------|-----------------------------------------------------------------------------------------------|
| $n$              | Number of observations                                                                        |
| $p$              | Number of parameters including the intercept                                                  |
| $\hat{\sigma}^2$ | Estimate of pure error variance from fitting the full model                                   |
| SST              | Total sum of squares corrected for the mean for the dependent variable                        |
| SSE              | Error sum of squares                                                                          |
| ASE              | $\frac{SSE}{n}$                                                                               |
| MSE              | $\frac{SSE}{n-p}$                                                                             |
| $R^2$            | $1 - \frac{SSE}{SST}$                                                                         |
| ADJRSQ           | $1 - \frac{(n-1)(1-R^2)}{n-p}$                                                                |
| AIC              | $n \ln \left( \frac{SSE}{n} \right) + 2p + n + 2$                                             |
| AICC             | $1 + \ln \left( \frac{SSE}{n} \right) + \frac{2(p+1)}{n-p-2}$                                 |
| BIC              | $n \ln \left( \frac{SSE}{n} \right) + 2(p+2)q - 2q^2$ where $q = \frac{n\hat{\sigma}^2}{SSE}$ |
| CP ( $C_p$ )     | $\frac{SSE}{\hat{\sigma}^2} + 2p - n$                                                         |

Table 45.10 continued

| Statistic | Definition or Formula                                                                                                                                                                  |
|-----------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| PRESS     | $\sum_{i=1}^n \frac{r_i^2}{(1-h_i)^2}$ where<br>$r_i$ = residual at observation $i$ and<br>$h_i$ = leverage of observation $i = \mathbf{x}_i(\mathbf{X}'\mathbf{X})^{-1}\mathbf{x}_i'$ |
| RMSE      | $\sqrt{\text{MSE}}$                                                                                                                                                                    |
| SBC       | $n \ln\left(\frac{\text{SSE}}{n}\right) + p \ln(n)$                                                                                                                                    |

### Formulas for AIC and AICC

There is some inconsistency in the literature on the precise definitions for the AIC and AICC statistics. The definitions used in PROC GLMSELECT changed between the experimental and the production release of the procedure in SAS 9.2. The definitions now used in PROC GLMSELECT yield the same final models as before, but PROC GLMSELECT makes the connection between the AIC statistic and the AICC statistic more transparent.

In the context of linear regression, several different versions of the formulas for AIC and AICC appear in the statistics literature. However, for a fixed number of observations, these different versions differ by additive and positive multiplicative constants. Because the model selected to yield a minimum of a criterion is not affected if the criterion is changed by additive and positive multiplicative constants, these changes in the formula for AIC and AICC do not affect the selection process.

The following section provides details about these changes. Formulas used in the experimental download release are denoted with a superscript of ( $d$ ) and  $n$ ,  $p$  and SSE are defined in Table 45.10.

The experimental download release of PROC GLMSELECT used the following formulas for AIC (Darlington 1968; Judge et al. 1985) and AICC (Hurvich, Simonoff, and Tsai 1998):

$$\text{AIC}^{(d)} = n \log\left(\frac{\text{SSE}}{n}\right) + 2p$$

and

$$\text{AICC}^{(d)} = \log\left(\frac{\text{SSE}}{n}\right) + 1 + \frac{2(p+1)}{n-p-2}$$

PROC GLMSLECT now uses the definitions of AIC and AICC found in Hurvich and Tsai (1989):

$$\text{AIC} = n \log\left(\frac{\text{SSE}}{n}\right) + 2p + n + 2$$

and

$$\text{AICC} = \text{AIC} + \frac{2(p+1)(p+2)}{n-p-2}$$

Hurvich and Tsai (1989) show that the formula for AICC can also be written as

$$\text{AICC} = n \log \left( \frac{\text{SSE}}{n} \right) + \frac{n(n+p)}{n-p-2}$$

The relationships between the alternative forms of the formulas are

$$\text{AIC} = \text{AIC}^{(d)} + n + 2$$

$$\text{AICC} = n \text{AICC}^{(d)}$$

---

## CLASS Variable Parameterization and the SPLIT Option

The GLMSELECT procedure supports nonsingular parameterizations for classification effects. A variety of these nonsingular parameterizations are available. You use the PARAM= option in the CLASS statement to specify the parameterization. See the section “Other Parameterizations” on page 387 in Chapter 19, “Shared Concepts and Topics,” for details.

PROC GLMSELECT also supports the ability to split classification effects. You can use the SPLIT option in the CLASS statement to request that the columns of the design matrix that correspond to any effect that contains a split classification variable can be selected to enter or leave a model independently of the other design columns of that effect. The following statements illustrate the use of SPLIT option together with other features of the CLASS statement:

```
data codingExample;
 drop i;
 do i=1 to 1000;
 c1 = 1 + mod(i,6);
 if i < 50 then c2 = 'very low ';
 else if i < 250 then c2 = 'low';
 else if i < 500 then c2 = 'medium';
 else if i < 800 then c2 = 'high';
 else c2 = 'very high';
 x1 = ranuni(1);
 x2 = ranuni(1);
 y = x1 + 10*(c1=3) +5*(c1=5) +rannor(1);
 output;
 end;
run;
proc glmselect data=codingExample;
 class c1(param=ref split) c2(param=ordinal order=data) /
 delimiter = ',' showcoding;
 model y = c1 c2 x1 x2/orderselect;
run;
```

The “Class Level Information” table shown in Figure 45.11 is produced by default whenever you specify a CLASS statement.

**Figure 45.11** Class Level Information

| The GLMSELECT Procedure |        |                                        |
|-------------------------|--------|----------------------------------------|
| Class Level Information |        |                                        |
| Class                   | Levels | Values                                 |
| c1                      | 6 *    | 1, 2, 3, 4, 5, 6                       |
| c2                      | 5      | very low, low, medium, high, very high |

\* Associated Parameters Split

Note that because the levels of the variable c2 contain embedded blanks, the DELIMITER="," option has been specified. The SHOWCODING option requests the display of the “Class Level Coding” table shown in Figure 45.12. An ordinal parameterization is used for c2 because its levels have a natural order. Furthermore, because these levels appear in their natural order in the data, you can preserve this order by specifying the ORDER=DATA option.

**Figure 45.12** Class Level Coding

| Class Level Coding |                  |   |   |   |   |  |
|--------------------|------------------|---|---|---|---|--|
| c1<br>Level        | Design Variables |   |   |   |   |  |
|                    | 1                | 2 | 3 | 4 | 5 |  |
| 1                  | 1                | 0 | 0 | 0 | 0 |  |
| 2                  | 0                | 1 | 0 | 0 | 0 |  |
| 3                  | 0                | 0 | 1 | 0 | 0 |  |
| 4                  | 0                | 0 | 0 | 1 | 0 |  |
| 5                  | 0                | 0 | 0 | 0 | 1 |  |
| 6                  | 0                | 0 | 0 | 0 | 0 |  |

The SPLIT option has been specified for the classification variable c1. This permits the parameters associated with the effect c1 to enter or leave the model individually. The “Parameter Estimates” table in Figure 45.13 shows that for this example the parameters that correspond to only levels 3 and 5 of c1 are in the selected model. Finally, note that the ORDERSELECT option in the MODEL statement specifies that the parameters are displayed in the order in which they first entered the model.

**Figure 45.13** Parameter Estimates

| Parameter Estimates |    |           |                |         |
|---------------------|----|-----------|----------------|---------|
| Parameter           | DF | Estimate  | Standard Error | t Value |
| Intercept           | 1  | -0.216680 | 0.068650       | -3.16   |
| c1_3                | 1  | 10.160900 | 0.087898       | 115.60  |
| c1_5                | 1  | 5.018015  | 0.087885       | 57.10   |
| x1                  | 1  | 1.315468  | 0.109772       | 11.98   |

## Macro Variables Containing Selected Models

Often you might want to perform postselection analysis by using other SAS procedures. To facilitate this, PROC GLMSELECT saves the list of selected effects in a macro variable. This list does not explicitly include the intercept so that you can use it in the **MODEL** statement of other SAS/STAT regression procedures.

The following table describes the macro variables that PROC GLMSELECT creates. Note that when BY processing is used, one macro variable, indexed by the BY group number, is created for each BY group.

| Macro Variable          | Description                   |
|-------------------------|-------------------------------|
| <b>No BY processing</b> |                               |
| _GLSIND1                | Selected model                |
| <b>BY processing</b>    |                               |
| _GLSNUMBYS              | Number of BY groups           |
| _GLSIND1                | Selected model for BY group 1 |
| _GLSIND2                | Selected model for BY group 2 |
| ...                     |                               |

You can use the macro variable `_GLSIND` as a synonym for `_GLSIND1`. If you do not use BY processing, `_GLSNUMBYS` is still defined and has the value 1.

To aid in associating indexed macro variables with the appropriate observations when BY processing is used, PROC GLMSELECT creates a variable `_BY_` in the output data set specified in an **OUTPUT** statement (see the section “**OUTPUT Statement**” on page 3555) that tags observations with an index that matches the index of the appropriate macro variable.

The following statements create a data set with two BY groups and run PROC GLMSELECT to select a model for each BY group.

```
data one(drop=i j);
 array x{5} x1-x5;
 do i=1 to 1000;
 classVar = mod(i,4)+1;
 do j=1 to 5;
 x{j} = ranuni(1);
 end;
 if i<400 then do;
 byVar = 'group 1';
 y = 3*classVar+7*x2+5*x2*x5+rannor(1);
 end;
 else do;
 byVar = 'group 2';
 y = 2*classVar+x5+rannor(1);
 end;
 output;
 end;
run;
```

```

proc glmselect data=one;
 by byVar;
 class classVar;
 model y = classVar x1|x2|x3|x4|x5 @2 /
 selection=stepwise(stop=aicc);
 output out=glmselectOutput;
run;

```

The preceding PROC GLMSELECT step produces three macro variables:

| Macro Variable | Value             | Description                            |
|----------------|-------------------|----------------------------------------|
| _GLSNUMBYS     | 2                 | Number of BY groups                    |
| _GLSIND1       | classVar x2 x2*x5 | Selected model for the first BY group  |
| _GLSIND2       | classVar x5       | Selected model for the second BY group |

You can now leverage these macro variables and the output data set created by PROC GLMSELECT to perform postselection analyses that match the selected models with the appropriate BY-group observations. For example, the following statements create and run a macro that uses PROC GLM to perform LSMeans analyses.

```

%macro LSMeansAnalysis;
 %do i=1 %to &_GLSNUMBYS;
 title1 "Analysis Using the Selected Model for BY group number &i";
 title2 "Selected Effects: &&_GLSIND&i";

 ods select LSMeans;
 proc glm data=glmselectOutput(where = (_BY_ = &i));
 class classVar;
 model y = &&_GLSIND&i;
 lsmeans classVar;
 run;quit;
 %end;
%mend;
%LSMeansAnalysis;

```

The LSMeans analysis output from PROC GLM is shown in [Output 45.14](#).



**Figure 45.14** LS-Means Analyses for Selected Models

|                                                         |  |            |
|---------------------------------------------------------|--|------------|
| Analysis Using the Selected Model for BY group number 1 |  |            |
| Selected Effects: classVar x2 x2*x5                     |  |            |
| The GLM Procedure                                       |  |            |
| Least Squares Means                                     |  |            |
| class                                                   |  |            |
| Var                                                     |  | y LSMEAN   |
| 1                                                       |  | 7.8832052  |
| 2                                                       |  | 10.9528618 |
| 3                                                       |  | 13.9412216 |
| 4                                                       |  | 16.7929355 |
| Analysis Using the Selected Model for BY group number 2 |  |            |
| Selected Effects: classVar x5                           |  |            |
| The GLM Procedure                                       |  |            |
| Least Squares Means                                     |  |            |
| class                                                   |  |            |
| Var                                                     |  | y LSMEAN   |
| 1                                                       |  | 2.46805014 |
| 2                                                       |  | 4.52102826 |
| 3                                                       |  | 6.53369479 |
| 4                                                       |  | 8.49354763 |

## Using the STORE Statement

The preceding section shows how you can use macro variables to facilitate performing postselection analysis by using other SAS procedures. An alternative approach is to use the STORE statement to save the results of the PROC GLMSELECT step in an *item store*. You can then use the PLM procedure to obtain a rich set of postselection analyses. The following statements show how you can use this approach to obtain the same LSMeans analyses as shown in section “[Macro Variables Containing Selected Models](#)” on page 3572:

```
proc glmselect data=one;
 by byVar;
 class classVar;
 model y = classVar x1|x2|x3|x4|x5 @2 /
 selection=stepwise(stop=aicc);
 store out=glmselectStore;
run;

proc plm source=glmselectStore;
 lsmeans classVar;
run;
```

The LSMeans analysis output for the first BY group is shown in Figure 45.15.

**Figure 45.15** LS-Means Analysis Produced by PROC PLM

| The PLM Procedure            |          |                   |     |         |         |
|------------------------------|----------|-------------------|-----|---------|---------|
| classVar Least Squares Means |          |                   |     |         |         |
| class<br>Var                 | Estimate | Standard<br>Error | DF  | t Value | Pr >  t |
| 1                            | 7.8832   | 0.1050            | 393 | 75.11   | <.0001  |
| 2                            | 10.9529  | 0.1043            | 393 | 104.99  | <.0001  |
| 3                            | 13.9412  | 0.1043            | 393 | 133.70  | <.0001  |
| 4                            | 16.7929  | 0.1042            | 393 | 161.09  | <.0001  |

## Building the SSCP Matrix

Traditional implementations of FORWARD and STEPWISE selection methods start by computing the augmented crossproduct matrix for all the specified effects. This initial crossproduct matrix is updated as effects enter or leave the current model by sweeping the columns corresponding to the parameters of the entering or departing effects. Building the starting crossproduct matrix can be done with a single pass through the data and requires  $O(m^2)$  storage and  $O(nm^2)$  work, where  $n$  is the number of observations and  $m$  is the number of parameters. If  $k$  selection steps are done, then the total work sweeping effects in and out of the model is  $O(km^2)$ . When  $n \gg m$ , the work required is dominated by the time spent forming the crossproduct matrix. However, when  $m$  is large (tens of thousands), just storing the crossproduct matrix becomes intractable even though the number of selected parameters might be small. Note also that when interactions of classification effects are considered, the number of parameters considered can be large, even though the number of effects considered is much smaller.

When the number of selected parameters is smaller than the total number of parameters, it turns out that many of the crossproducts are not needed in the selection process. Let  $y$  denote the dependent variable, and suppose at some step of the selection process that  $\mathbf{X}$  denotes the  $n \times p$  design matrix columns corresponding to the currently selected model. Let  $\mathbf{Z} = \mathbf{z}_1, \mathbf{z}_2, \dots, \mathbf{z}_{m-p}$  denote the design matrix columns corresponding to the  $m - p$  effects not yet in the model. Then in order to compute the reduction in the residual sum of squares when  $\mathbf{z}_j$  is added to the model, the only additional crossproducts needed are  $\mathbf{z}'_j y$ ,  $\mathbf{z}'_j \mathbf{X}$ , and  $\mathbf{z}'_j \mathbf{z}_j$ . Note that it is not necessary to compute any of  $\mathbf{z}'_j \mathbf{z}_i$  with  $i \neq j$  and if  $p \ll m$ , and this yields a substantial saving in both memory required and computational work. Note, however, that this strategy does require a pass through the data at any step where adding an effect to the model is considered.

PROC GLMSELECT supports both of these strategies for building the crossproduct matrix. You can choose which of these strategies to use by specifying the `BUILDSSCP=FULL` or `BUILDSSCP=INCREMENTAL` option in the `PERFORMANCE` statement. If you request BACKWARD selection, then the full SSCP matrix is required. Similarly, if you request the BIC or CP criterion as the `SELECT=`, `CHOOSE=`, or `STOP=` criterion, or if you request the display of one or both of these criteria with the `STATS=BIC`, `STATS=CP`, or `STATS=ALL` option, then the full model needs to be computed. If you do not specify the `BUILDSSCP=` option, then PROC GLMSELECT switches to the incremental strategy if the number of effects is greater than one hundred. This default strategy is designed to give good performance when the number of selected

parameters is less than about 20% of the total number of parameters. Hence if you choose options that you know will cause the selected model to contain a significantly higher percentage of the total number of candidate parameters, then you should consider specifying `BUILDSSCP=FULL`. Conversely, if you specify fewer than 100 effects in the `MODEL` statement but many of these effects have a large number of associated parameters, then specifying `BUILDSSCP=INCREMENTAL` might result in improved performance.

## Model Averaging

As discussed in the section “[Model Selection Issues](#)” on page 3567, some well-known issues arise in performing model selection for inference and prediction. One approach to address these issues is to use resampled data as a proxy for multiple samples that are drawn from some conceptual probability distribution. A model is selected for each resampled set of data, and a predictive model is built by averaging the predictions of these selected models. You can perform this method of model averaging by using the `MODEL AVERAGE` statement. Resampling-based methods, in which samples are obtained by drawing with replacement from your data, fall under the umbrella of the widely studied methodology known as the bootstrap (Efron and Tibshirani 1993). For use of the bootstrap in the context of variable selection, see Breiman (1992).

By default, when the average is formed, models that are selected in multiple samples receive more weight than infrequently selected models. Alternatively, you can start by fitting a prespecified set of models on your data, then use information-theoretic approaches to assign a weight to each model in building a weighted average model. You can find a detailed discussion of this methodology in Burnham and Anderson (2002), in addition to some comparisons of this approach with bootstrap-based methods.

In the linear model context, the average prediction that you obtain from a set of models is the same as the prediction that you obtain with the single model whose parameter estimates are the averages of the corresponding estimates of the set of models. Hence, you can regard model averaging as a selection method that selects this average model. To show this, denote by  $\beta^{(i)}$  the parameter estimates for the sample  $i$  where  $\beta_j^{(i)} = 0$  if parameter  $j$  is not in the selected model for sample  $i$ . Then the predicted values  $\hat{y}^{(i)}$  for average model  $i$  are given by

$$\hat{y}^{(i)} = \mathbf{X}\boldsymbol{\beta}^{(i)}$$

where  $\mathbf{X}$  is the design matrix of the data to be scored. Forming averages gives

$$\hat{y}^{(*)} = \frac{1}{N} \sum_{i=1}^N \hat{y}^{(i)} = \frac{1}{N} \sum_{i=1}^N \mathbf{X}\boldsymbol{\beta}^{(i)} = \mathbf{X} \left( \frac{1}{N} \sum_{i=1}^N \boldsymbol{\beta}^{(i)} \right) = \mathbf{X}\boldsymbol{\beta}^{(*)}$$

where for parameter  $j$ ,  $\beta_j^{(*)} = \frac{1}{N} \sum_{i=1}^N \beta_j^{(i)}$ .

You can see that if a parameter estimate is nonzero for just a few of the sample models, then averaging the estimates for this parameter shrinks this estimate towards zero. It is this shrinkage that ameliorates the bias that a parameter is more likely to be selected if it is above its expected value rather than below it. This reduction in bias often produces improved predictions on new data that you obtain with the average model. However, the average model is not parsimonious since it has nonzero estimates for any parameter that is selected in any sample.

One resampling-based approach for obtaining a parsimonious model is to use the number of times that regressors are selected as an indication of importance and then to fit a new model that uses just the regressors that you deem to be most important. This approach is not without risk. One possible problem is that you

might have several regressors that, for purposes of prediction, can be used as surrogates for one another. In this case it is possible that none of these regressors individually appears in a large enough percentage of the sample models to be deemed important, even though every model contains at least one of them. Despite such potential problems, this strategy is often successful. You can implement this approach by using the REFIT option in the `MODEL AVERAGE` statement. By default, the REFIT option performs a second round of model averaging, where a fixed model that consists of the effects that are selected in a least twenty percent of the samples in the initial round of model averaging is used. The average model is obtained by averaging the ordinary least squares estimates obtained for each sample in the refit. Note that the default selection frequency cutoff of twenty percent is merely a heuristic guideline that often produces reasonable models.

Another approach to obtaining a parsimonious average model is to form the average of just the frequently selected models. You can implement this strategy by using the SUBSET option in the `MODEL AVERAGE` statement. However, in situations where there are many irrelevant regressors, it is often the case that most of the selected models are selected just once. In such situations, having a way to order the models that are selected with the same frequency is desirable. The following section discusses a way to do this.

### Model Selection Frequencies and Frequency Scores

The model frequency score orders models by their selection frequency, but also uses effect selection frequencies to order different models that are selected with the same frequency. Let  $\mathbf{x}_i$  denote the  $i$ th effect and let  $f_i$  denote the selection fraction for this effect.  $f_i$  is computed as the number of samples whose selected model contains effect  $\mathbf{x}_i$  divided by the number of samples. Suppose the  $j$ th model that consists of the  $K$  effects  $\mathbf{x}_{j_1}, \mathbf{x}_{j_2}, \dots, \mathbf{x}_{j_K}$  is selected  $m_j$  times. Then the model *frequency score*,  $s_j$ , for this model is computed as the sum of the model selection frequency and the average selection fraction for this model; that is,

$$s_j = m_j + \frac{\sum_{k=1}^K f_{j_k}}{K}$$

When you use the `BEST= $b$`  suboption of the SUBSET option in the `MODEL AVERAGE` statement, then the average model is formed from the  $b$  models with the largest model frequency scores.

---

## Using Validation and Test Data

When you have sufficient data, you can subdivide your data into three parts called the training, validation, and test data. During the selection process, models are fit on the training data, and the prediction error for the models so obtained is found by using the validation data. This prediction error on the validation data can be used to decide when to terminate the selection process or to decide what effects to include as the selection process proceeds. Finally, once a selected model has been obtained, the test set can be used to assess how the selected model generalizes on data that played no role in selecting the model.

In some cases you might want to use only training and test data. For example, you might decide to use an information criterion to decide what effects to include and when to terminate the selection process. In this case no validation data are required, but test data can still be useful in assessing the predictive performance of the selected model. In other cases you might decide to use validation data during the selection process but forgo assessing the selected model on test data. Hastie, Tibshirani, and Friedman (2001) note that it is difficult to give a general rule on how many observations you should assign to each role. They note that a typical split might be 50% for training and 25% each for validation and testing.

PROC GLMSELECT provides several methods for partitioning data into training, validation, and test data. You can provide data for each role in separate data sets that you specify with the `DATA=`, `TESTDATA=`, and `VALDATA=` options in the PROC GLMSELECT procedure. An alternative method is to use a `PARTITION` statement to logically subdivide the `DATA=` data set into separate roles. You can name the fractions of the data that you want to reserve as test data and validation data. For example, specifying

```
proc glmselect data=inData;
 partition fraction(test=0.25 validate=0.25);
 ...
run;
```

randomly subdivides the `inData` data set, reserving 50% for training and 25% each for validation and testing.

In some cases you might need to exercise more control over the partitioning of the input data set. You can do this by naming a variable in the input data set as well as a formatted value of that variable that correspond to each role. For example, specifying

```
proc glmselect data=inData;
 partition roleVar=group(test='group 1' train='group 2');
 ...
run;
```

assigns all roles observations in the `inData` data set based on the value of the variable named `group` in that data set. Observations where the value of `group` is 'group 1' are assigned for testing, and those with value 'group 2' are assigned to training. All other observations are ignored.

You can also combine the use of the `PARTITION` statement with named data sets for specifying data roles. For example,

```
proc glmselect data=inData testData=inTest;
 partition fraction(validate=0.4);
 ...
run;
```

reserves 40% of the `inData` data set for validation and uses the remaining 60% for training. Data for testing is supplied in the `inTest` data set. Note that in this case, because you have supplied a `TESTDATA=` data set, you cannot reserve additional observations for testing with the `PARTITION` statement.

When you use a `PARTITION` statement, the output data set created with an `OUTPUT` statement contains a character variable `_ROLE_` whose values 'TRAIN', 'TEST', and 'VALIDATE' indicate the role of each observation. `_ROLE_` is blank for observations that were not assigned to any of these three roles. When the input data set specified in the `DATA=` option in the PROC GLMSELECT statement contains an `_ROLE_` variable and no `PARTITION` statement is used, and `TESTDATA=` and `VALDATA=` are not specified, then the `_ROLE_` variable is used to define the roles of each observation. This is useful when you want to rerun PROC GLMSELECT but use the same data partitioning as in a previous PROC GLMSELECT step. For example, the following statements use the same data for testing and training in both PROC GLMSELECT steps:

```
proc glmselect data=inData;
 partition fraction(test=0.5);
 model y=x1-x10/selection=forward;
 output out=outDataForward;
run;
```

```
proc glmselect data=outDataForward;
 model y=x1-x10/selection=backward;
run;
```

When you have reserved observations for training, validation, and testing, a model fit on the training data is scored on the validation and test data, and the average squared error, denoted by ASE, is computed separately for each of these subsets. The ASE for each data role is the error sum of squares for observations in that role divided by the number of observations in that role.

### Using the Validation ASE as the STOP= Criterion

If you have provided observations for validation, then you can specify `STOP=VALIDATE` as a suboption of the `SELECTION=` option in the `MODEL` statement. At step  $k$  of the selection process, the best candidate effect to enter or leave the current model is determined. Note that here “best candidate” means the effect that gives the best value of the `SELECT=` criterion that need not be based on the validation data. The validation ASE for the model with this candidate effect added is computed. If this validation ASE is greater than the validation ASE for the model at step  $k$ , then the selection process terminates at step  $k$ .

### Using the Validation ASE as the CHOOSE= Criterion

When you specify the `CHOOSE=VALIDATE` suboption of the `SELECTION=` option in the `MODEL` statement, the validation ASE is computed for the models at each step of the selection process. The model at the first step yielding the smallest validation ASE is selected.

### Using the Validation ASE as the SELECT= Criterion

You request the validation ASE as the selection criterion by specifying the `SELECT=VALIDATE` suboption of the `SELECTION=` option in the `MODEL` statement. At step  $k$  of the selection process, the validation ASE is computed for each model where a candidate for entry is added or candidate for removal is dropped. The selected candidate for entry or removal is the one that yields a model with the minimal validation ASE.

---

## Cross Validation

Deciding when to stop a selection method is a crucial issue in performing effect selection. Predictive performance of candidate models on data not used in fitting the model is one approach supported by PROC GLMSELECT for addressing this problem (see the section “Using Validation and Test Data” on page 3577). However, in some cases, you might not have sufficient data to create a sizable training set and a validation set that represent the predictive population well. In these cases, cross validation is an attractive alternative for estimating prediction error.

In  $k$ -fold cross validation, the data are split into  $k$  roughly equal-sized parts. One of these parts is held out for validation, and the model is fit on the remaining  $k - 1$  parts. This fitted model is used to compute the predicted residual sum of squares on the omitted part, and this process is repeated for each of  $k$  parts. The sum of the  $k$  predicted residual sum of squares so obtained is the estimate of the prediction error that is denoted by `CVPRESS`. Note that computing the `CVPRESS` statistic for  $k$ -fold cross validation requires fitting  $k$  different models, and so the work and memory requirements increase linearly with the number of cross validation folds.

You can use the `CVMETHOD=` option in the `MODEL` statement to specify the method for splitting the data into  $k$  parts. `CVMETHOD=BLOCK( $k$ )` requests that the  $k$  parts be made of blocks of  $\text{floor}(n/k)$  or  $\text{floor}(n/k) + 1$  successive observations, where  $n$  is the number of observations. `CVMETHOD=SPLIT( $k$ )` requests that parts consist of observations  $\{1, k + 1, 2k + 1, 3k + 1, \dots\}$ ,  $\{2, k + 2, 2k + 2, 3k + 2, \dots\}$ , . . . ,  $\{k, 2k, 3k, \dots\}$ . `CVMETHOD=RANDOM( $k$ )` partitions the data into random subsets each with roughly  $\text{floor}(n/k)$  observations. Finally, you can use the formatted value of an input data set variable to define the parts by specifying `CVMETHOD=variable`. This last partitioning method is useful in cases where you need to exercise extra control over how the data are partitioned by taking into account factors such as important but rare observations that you want to “spread out” across the various parts.

You can request details of the CVPRESS computations by specifying the `CVDETAILS=` option in the `MODEL` statement. When you use cross validation, the output data set created with an `OUTPUT` statement contains an integer-valued variable, `_CVINDEX_`, whose values indicate the subset to which an observation is assigned.

The widely used special case of  $n$ -fold cross validation when you have  $n$  observations is known as *leave-one-out* cross validation. In this case, each omitted part consists of one observation, and CVPRESS statistic can be efficiently obtained without refitting the model  $n$  times. In this case, the CVPRESS statistic is denoted simply by PRESS and is given by

$$\text{PRESS} = \sum_{i=1}^n \left( \frac{r_i}{1 - h_i} \right)^2$$

where  $r_i$  is the residual and  $h_i$  is the leverage of the  $i$ th observation. You can request *leave-one-out* cross validation by specifying PRESS instead of CV with the options `SELECT=`, `CHOOSE=`, and `STOP=` in the `MODEL` statement. For example, if the number of observations in the data set is 100, then the following two PROC GLMSELECT steps are mathematically equivalent, but the second step is computed much more efficiently:

```
proc glmselect;
 model y=x1-x10/selection=forward(stop=CV) cvMethod=split(100);
run;

proc glmselect;
 model y=x1-x10/selection=forward(stop=PRESS);
run;
```

Hastie, Tibshirani, and Friedman (2001) include a discussion about choosing the cross validation fold. They note that as an estimator of true prediction error, cross validation tends to have decreasing bias but increasing variance as the number of folds increases. They recommend five- or tenfold cross validation as a good compromise. By default, PROC GLMSELECT uses `CVMETHOD=RANDOM(5)` for cross validation.

## Using Cross Validation as the STOP= Criterion

You request cross validation as the stopping criterion by specifying the `STOP=CV` suboption of the `SELECTION=` option in the `MODEL` statement. At step  $k$  of the selection process, the best candidate effect to enter or leave the current model is determined. Note that here “best candidate” means the effect that gives the best value of the `SELECT=` criterion that need not be the CV criterion. The CVPRESS score for the model with this candidate effect added or removed is determined. If this CVPRESS score is greater than the CVPRESS score for the model at step  $k$ , then the selection process terminates at step  $k$ .



## Using Cross Validation as the CHOOSE= Criterion

When you specify the `CHOOSE=CV` suboption of the `SELECTION=` option in the `MODEL` statement, the CVPRESS score is computed for the models at each step of the selection process. The model at the first step yielding the smallest CVPRESS score is selected.

## Using Cross Validation as the SELECT= Criterion

You request cross validation as the selection criterion by specifying the `SELECT=CV` suboption of the `SELECTION=` option in the `MODEL` statement. At step  $k$  of the selection process, the CVPRESS score is computed for each model where a candidate for entry is added or a candidate for removal is dropped. The selected candidate for entry or removal is the one that yields a model with the minimal CVPRESS score. Note that at each step of the selection process, this requires forming the CVPRESS statistic for all possible candidate models at the next step. Since forming the CVPRESS statistic for  $k$ -fold requires fitting  $k$  models, using cross validation as the selection criterion is computationally very demanding compared to using other selection criteria.

---

## Displayed Output

The following sections describe the displayed output produced by PROC GLMSELECT. The output is organized into various tables, which are discussed in the order of appearance. Note that the contents of a table might change depending on the options you specify.

### Model Information

The “Model Information” table displays basic information about the data sets and the settings used to control effect selection. These settings include the following:

- the selection method
- the criteria used to select effects, stop the selection, and choose the selected model
- the effect hierarchy enforced

The ODS name of the “Model Information” table is ModelInfo.

### Performance Settings

The “Performance Settings” table displays settings that affect performance. These settings include whether threading is enabled and the number of CPUs available as well as the method used to build the crossproduct matrices. This table is displayed only if you specify the `DETAILS` option in the `PERFORMANCE` statement. The ODS name of the “Performance Settings” table is PerfSettings.

### Number of Observations

The “Number of Observations” table displays the number of observations read from the input data set and the number of observations used in the analysis. If you specify a `FREQ` statement, the table also displays the sum of frequencies read and used. If you use a `PARTITION` statement, the table also displays the number



of observations used for each data role. If you specify `TESTDATA=` or `VALDATA=` data sets in the PROC GLMSELECT statement, then “Number of Observations” tables are also produced for these data sets. The ODS name of the “Number of Observations” table is `NObs`.

### Class Level Information

The “Class Level Information” table lists the levels of every variable specified in the `CLASS` statement. The ODS name of the “Class Level Information” table is `ClassLevelInfo`.

### Class Level Coding

The “Class Level Coding” table shows the coding used for variables specified in the `CLASS` statement. The ODS name of the “Class Level Coding” table is `ClassLevelCoding`.

### Dimensions

The “Dimensions” table displays information about the number of effects and the number of parameters from which the selected model is chosen. If you use split classification variables, then this table also includes the number of effects after splitting is taken into account. The ODS name of the “Dimensions” table is `Dimensions`.

### Candidates

The “Candidates” table displays the effect names and values of the criterion used to select entering or departing effects at each step of the selection process. The effects are displayed in sorted order from best to worst of the selection criterion. You request this table with the `DETAILS=` option in the `MODEL` statement. The ODS name of the “Candidates” table is `Candidates`.

### Selection Summary

The “Selection Summary” table displays details about the sequence of steps of the selection process. For each step, the effect that was entered or dropped is displayed along with the statistics used to select the effect, stop the selection, and choose the selected model. You can request that additional statistics be displayed with the `STATS=` option in the `MODEL` statement. For all criteria that you can use for model selection, the steps at which the optimal values of these criteria occur are also indicated. The ODS name of the “Selection Summary” table is `SelectionSummary`.

### Stop Reason

The “Stop Reason” table displays the reason why the selection stopped. To facilitate programmatic use of this table, an integer code is assigned to each reason and is included if you output this table by using an ODS `OUTPUT` statement. The reasons and their associated codes follow:

## Code Stop Reason

|    |                                                                        |
|----|------------------------------------------------------------------------|
| 1  | maximum number of steps done                                           |
| 2  | specified number of steps done                                         |
| 3  | specified number of effects in model                                   |
| 4  | stopping criterion at local optimum                                    |
| 5  | model is an exact fit                                                  |
| 6  | all entering effects are linearly dependent on those in the model      |
| 7  | all effects are in the model                                           |
| 8  | all effects have been dropped                                          |
| 9  | requested full least squares fit completed                             |
| 10 | stepwise selection is cycling                                          |
| 11 | dropping any effect does not improve the selection criterion           |
| 12 | no effects are significant at the specified SLE or SLS levels          |
| 13 | adding or dropping any effect does not improve the selection criterion |
| 14 | all remaining effects are required                                     |

The ODS name of the “Stop Reason” table is StopReason.

## Stop Details

The “Stop Details” table compares the optimal value of the stopping criterion at the final model with how it would change if the best candidate effect were to enter or leave the model. The ODS name of the “Stop Details” table is StopDetails.

## Selected Effects

The “Selected Effects” table displays a string containing the list of effects in the selected model. The ODS name of the “Selected Effects” table is SelectedEffects.

## ANOVA

The “ANOVA” table displays an analysis of variance for the selected model. This table includes the following:

- the Source of the variation, Model for the fitted regression, Error for the residual error, and C Total for the total variation after correcting for the mean. The Uncorrected Total Variation is produced when the **NOINT** option is used.
- the degrees of freedom (DF) associated with the source
- the Sum of Squares for the term
- the Mean Square, the sum of squares divided by the degrees of freedom
- the *F* Value for testing the hypothesis that all parameters are zero except for the intercept. This is formed by dividing the mean square for Model by the mean square for Error.

- the  $\text{Prob}>F$ , the probability of getting a greater  $F$  statistic than that observed if the hypothesis is true. Note that these  $p$ -values are displayed only if you specify the “SHOWPVALUES” option in the **MODEL** statement. These  $p$ -values are generally liberal because they are not adjusted for the fact that the terms in the model have been selected.

You can request “ANOVA” tables for the models at each step of the selection process with the **DETAILS=** option in the **MODEL** statement. The ODS name of the “ANOVA” table is ANOVA.

## Fit Statistics

The “Fit Statistics” table displays fit statistics for the selected model. The statistics displayed include the following:

- Root MSE, an estimate of the standard deviation of the error term. It is calculated as the square root of the mean square error.
- Dep Mean, the sample mean of the dependent variable
- R-square, a measure between 0 and 1 that indicates the portion of the (corrected) total variation attributed to the fit rather than left to residual error. It is calculated as  $\text{SS}(\text{Model})$  divided by  $\text{SS}(\text{Total})$ . It is also called the *coefficient of determination*. It is the square of the multiple correlation—in other words, the square of the correlation between the dependent variable and the predicted values.
- Adj R-Sq, the adjusted  $R^2$ , a version of  $R^2$  that has been adjusted for degrees of freedom. It is calculated as

$$\bar{R}^2 = 1 - \frac{(n - i)(1 - R^2)}{n - p}$$

where  $i$  is equal to 1 if there is an intercept and 0 otherwise,  $n$  is the number of observations used to fit the model, and  $p$  is the number of parameters in the model.

- fit criteria AIC, AICC, BIC, CP, and PRESS if they are used in the selection process or are requested with the **STATS=** option. See the section “Criteria Used in Model Selection Methods” on page 3568 for details and [Table 45.10](#) for the formulas for evaluating these criteria.
- the CVPRESS statistic when cross validation is used in the selection process. See the section “Cross Validation” on page 3579 for details.
- the average square errors (ASE) on the training, validation, and test data. See the section “Using Validation and Test Data” on page 3577 for details.

You can request “Fit Statistics” tables for the models at each step of the selection process with the **DETAILS=** option in the **MODEL** statement. The ODS name of the “Fit Statistics” table is FitStatistics.

## Cross Validation Details

The “Cross Validation Details” table displays the following:

- the fold number
- the number of observations used for fitting

- the number of observations omitted
- the predicted residual sum of squares on the omitted observations

You can request this table with the `CVDETAILS=` option in the `MODEL` statement whenever cross validation is used in the selection process. This table is displayed for the selected model, but you can request this table at each step of the selection process by using the `DETAILS=` option in the `MODEL` statement. The ODS name of the “Cross Validation Details” table is `CVDetails`.

## Parameter Estimates

The “Parameter Estimates” table displays the parameters in the selected model and their estimates. The information displayed for each parameter in the selected model includes the following:

- the parameter label that includes the effect name and level information for effects containing classification variables
- the degrees of freedom (DF) for the parameter. There is one degree of freedom unless the model is not full rank.
- the parameter estimate
- the standard error, which is the estimate of the standard deviation of the parameter estimate
- T for H0: Parameter=0, the  $t$  test that the parameter is zero. This is computed as the parameter estimate divided by the standard error.
- the Prob > |T|, the probability that a  $t$  statistic would obtain a greater absolute value than that observed given that the true parameter is zero. This is the two-tailed significance probability. Note that these  $p$ -values are displayed only if you specify the `SHOWPVALUES` option in the `MODEL` statement. These  $p$ -values are generally liberal because they are not adjusted for the fact that the terms in the model have been selected.

If cross validation is used in the selection process, then you can request that estimates of the parameters for each cross validation fold be included in the “Parameter Estimates” table by using the `CVDETAILS=` option in the `MODEL` statement. You can request “Parameter Estimates” tables for the models at each step of the selection process with the `DETAILS=` option in the `MODEL` statement. The ODS name of the “Parameter Estimates” table is `ParameterEstimates`.

## Score Information

For each `SCORE` statement, the “Score Information” table displays the names of the score input and output data sets, and the number of observations that were read and successfully scored. The ODS name of the “Score Information” table is `ScoreInfo`.

## Timing Breakdown

The “Timing Breakdown” table displays a broad breakdown of where time was spent in the `PROC GLM-SELECT` step. This table is displayed only if you specify the `DETAILS` option in the `PERFORMANCE` statement. The ODS name of the “Timing Breakdown” table is `Timing`.

## ODS Table Names

PROC GLMSELECT assigns a name to each table it creates. You can use these names to reference the table when you use the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in Table 45.11.

For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

**Table 45.11** ODS Tables Produced by PROC GLMSELECT

| ODS Table Name      | Description                                   | Statement     | Option           |
|---------------------|-----------------------------------------------|---------------|------------------|
| ANOVA               | Selected model ANOVA table                    | MODEL         | Default          |
| AvgParmEst          | Average parameter estimates                   | MODEL AVERAGE | Default          |
| BSplineDetails      | B-spline basis details                        | EFFECT        | DETAILS          |
| Candidates          | Entry/removal effect ranking                  | MODEL         | DETAILS=         |
| ClassLevelCoding    | Classification variable coding                | CLASS         | SHOWCODING       |
| ClassLevelInfo      | Classification variable levels                | CLASS         | Default          |
| CollectionLevelInfo | Levels of collection effects                  | EFFECT        | DETAILS          |
| CVDetails           | Cross validation PRESS by fold                | MODEL         | CVDETAILS=       |
| Dimensions          | Number of effects and parameters              | MODEL         | Default          |
| EffectSelectPct     | Effect selection percentages                  | MODEL AVERAGE | Default          |
| FitStatistics       | Selected model fit statistics                 | MODEL         | Default          |
| MMLevelInfo         | Levels of multimember effects                 | EFFECT        | DETAILS          |
| ModelAvgInfo        | Model averaging information                   | MODEL AVERAGE | Default          |
| ModelInfo           | Model information                             | MODEL         | Default          |
| ModelSelectFreq     | Model selection frequencies                   | MODEL AVERAGE | Default          |
| NObs                | Number of observations                        | MODEL         | Default          |
| ParameterNames      | Labels for column names in the design matrix  | PROC          | OUTDESIGN(names) |
| ParameterEstimates  | Selected model parameter estimates            | MODEL         | Default          |
| PerfSettings        | Performance settings                          | PERFORMANCE   | DETAILS          |
| PolynomialDetails   | Polynomial details                            | EFFECT        | DETAILS          |
| PolynomialScaling   | Polynomial scaling                            | EFFECT        | DETAILS          |
| RefitAvgParmEst     | Refit average parameter estimates             | MODEL AVERAGE | REFIT            |
| ScoreInfo           | Score request information                     | SCORE         | Default          |
| SelectedEffects     | List of selected effects                      | MODEL         | Default          |
| SelectionSummary    | Selection summary                             | MODEL         | Default          |
| StopDetails         | Stopping criterion details                    | MODEL         | Default          |
| StopReason          | Reason why selection stopped                  | MODEL         | Default          |
| Timing              | Timing details                                | PERFORMANCE   | DETAILS          |
| TPFSplineDeatils    | Truncated power function spline basis details | EFFECT        | DETAILS          |

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “Statistical Graphics Using ODS.”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “A Primer on ODS Statistical Graphics” on page 599 in Chapter 21, “Statistical Graphics Using ODS.”

You must also specify the PLOTS= option in the PROC GLMSELECT statement.

The following sections describe the ODS graphical displays produced by PROC GLMSELECT. The examples use the Baseball data set that is described in the section “Getting Started: GLMSELECT Procedure” on page 3520.

## ODS Graph Names

PROC GLMSELECT assigns a name to each graph it creates using ODS. You can use these names to reference the graphs when using ODS. The names are listed in Table 45.12.

**Table 45.12** Graphs Produced by PROC GLMSELECT

| ODS Graph Name      | Plot Description                                 | PLOTS Option         |
|---------------------|--------------------------------------------------|----------------------|
| AdjRSqPlot          | Adjusted R-square by step                        | CRITERIA(UNPACK)     |
| AICCPLOT            | Corrected Akaike’s information criterion by step | CRITERIA(UNPACK)     |
| AICPlot             | Akaike’s information criterion by step           | CRITERIA(UNPACK)     |
| ASEPlot             | Average square errors by step                    | ASE                  |
| BICPlot             | Sawa’s Bayesian information criterion by step    | CRITERIA(UNPACK)     |
| CandidatesPlot      | SELECT= criterion by effect                      | CANDIDATES           |
| ChooseCriterionPlot | CHOOSE= criterion by step                        | COEFFICIENTS(UNPACK) |
| CoefficientPanel    | Coefficients and CHOOSE= criterion by step       | COEFFICIENTS         |
| CoefficientPlot     | Coefficients by step                             | COEFFICIENTS(UNPACK) |
| CPPlot              | Mallows’ $C_p$ by step                           | CRITERIA(UNPACK)     |
| CriterionPanel      | Fit criteria by step                             | CRITERIA             |
| CVPRESSPlot         | Cross validation predicted RSS by step           | CRITERIA(UNPACK)     |
| EffectSelectPctPlot | Resampling effect selection percentages          | EFFECTSELECTPCT      |

Table 45.12 continued

| ODS Graph Name  | Plot Description                                | PLOTS= Option    |
|-----------------|-------------------------------------------------|------------------|
| ParmDistPanel   | Resampling parameter estimate distributions     | PARMDIST         |
| PRESSPlot       | Predicted RSS by step                           | CRITERIA(UNPACK) |
| SBCPlot         | Schwarz Bayesian information criterion by step  | CRITERIA(UNPACK) |
| ValidateASEPlot | Average square error on validation data by step | CRITERIA(UNPACK) |

### Candidates Plot

You request the “Candidates Plot” by specifying the PLOTS=CANDIDATES option in the PROC GLMSELECT statement and the DETAILS=STEPS option in the MODEL statement. This plot shows the values of selection criterion for the candidate effects for entry or removal, sorted from best to worst from left to right across the plot. The leftmost candidate displayed is the effect selected for entry or removal at that step. You can use this plot to see at what steps the decision about which effect to add or drop is clear-cut. See Figure 45.5 for an example.

### Coefficient Panel

When you specify the PLOTS=COEFFICIENTS option in the PROC GLMSELECT statement, PROC GLMSELECT produces a panel of two plots showing how the standardized coefficients and the criterion used to choose the final model evolve as the selection progresses. The following statements provide an example:

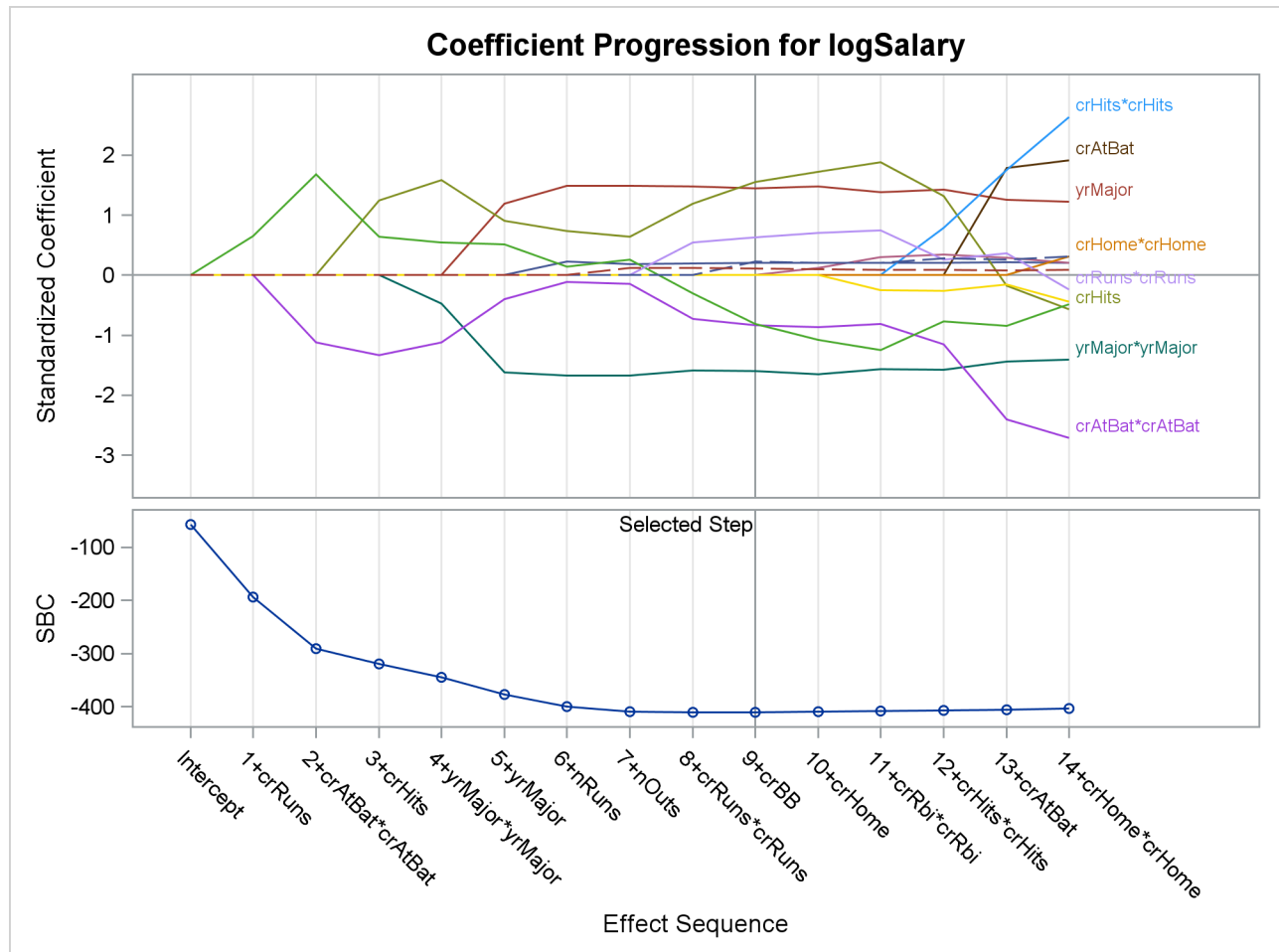
```
ods graphics on;

proc glmselect data=baseball plots=coefficients;
 class league division;
 model logSalary = nAtBat nHits nHome nRuns nRBI nBB
 yrMajor|yrMajor crAtBat|crAtBat crHits|crHits
 crHome|crHome crRuns|crRuns crRbi|crRbi
 crBB|crBB league division nOuts nAssts nError /
 selection=forward(stop=AICC CHOOSE=SBC);
run;
```

Figure 45.16 shows the requested graphic. The upper plot in the panel displays the standardized coefficients as a function of the step number. You can request standardized coefficients in the parameter estimates tables by specifying the STB option in the MODEL statement, but this option is not required to produce this plot. To help in tracing the changes in a parameter, the standardized coefficients for each parameter are connected by lines. Coefficients corresponding to effects that are not in the selected model at a step are zero and hence not observable. For example, consider the parameter crAtBat\*crAtBat in Output 45.16. Because crAtBat\*crAtBat enters the model at step 2, the line that represents this parameter starts rising from zero at step 1 when crRuns enters the model. Parameters that are nonzero at the final step of the selection are labeled if their magnitudes are greater than 1% of the range of the magnitudes of all the nonzero parameters at this step. To avoid collision, labels corresponding to parameters with similar values at the final step might get suppressed. You can control when this label collision avoidance occurs by using the LABELGAP=

suboption of the PLOTS=COEFFICIENTS option. Planned enhancements to the automatic label collision avoidance algorithm will obviate the need for this option in future releases of the GLMSELECT procedure.

**Figure 45.16** Coefficient Panel



The lower plot in the panel shows how the criterion used to choose among the examined models progresses. The selected step occurs at the optimal value of this criterion. In this example, this criterion is the SBC criterion and it achieves its minimal value at step 9 of the forward selection.

In some cases, particularly when the final step contains a large number of parameters, you might be interested in using this plot only to discern if and when the parameters in the model are essential unchanged beyond a certain step. In such cases, you might want to suppress the labeling of the parameters and use a numeric axis on the horizontal axis of the plot. You can do this using the STEPAXIS= and MAXPARMLABEL= suboptions of the PLOTS=CRITERIA option. The following statements provide an example:

```
proc glmselect data=baseball
 plots(unpack maxparmlabel=0 stepaxis=number)=coefficients;

 class league division;
 model logSalary = nAtBat nHits nHome nRuns nRBI nBB
 yrMajor|yrMajor crAtBat|crAtBat crHits|crHits
 crHome|crHome crRuns|crRuns crRbi|crRbi
```



```

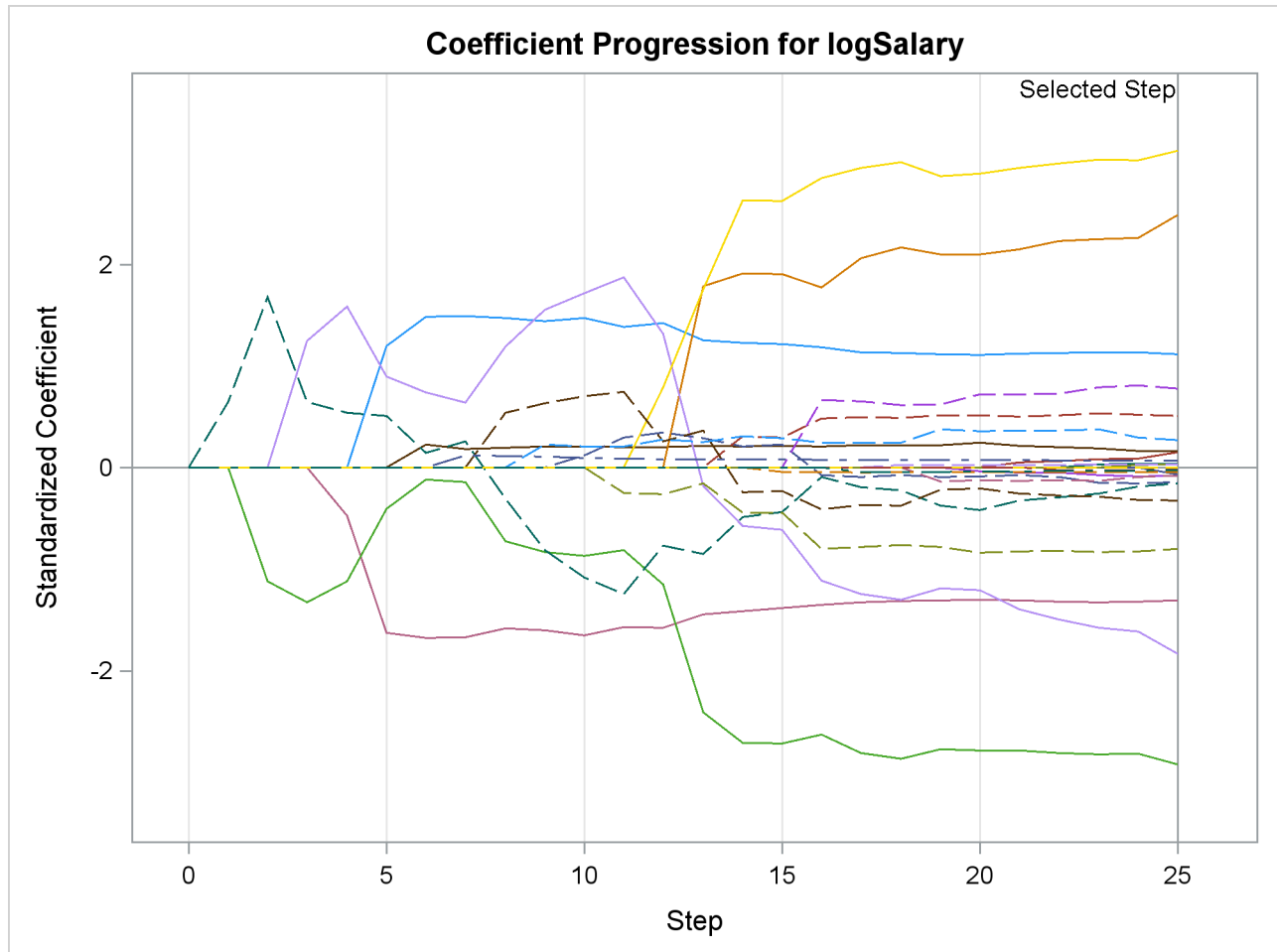
crBB|crBB league division nOuts nAssts nError /
selection=forward(stop=none);

run;

```

The UNPACK = option requests that the plots of the coefficients and CHOOSE= criterion be shown in separate plots. The STEPAXIS=NUMBER option requests a numeric horizontal axis showing step number, and the MAXPAMLABEL=0 option suppresses the labels for the parameters. The “Coefficient Plot” is shown in Figure 45.17. You can see that the standardized coefficients do not vary greatly after step 16.

**Figure 45.17** Coefficient Plot



### Criterion Panel

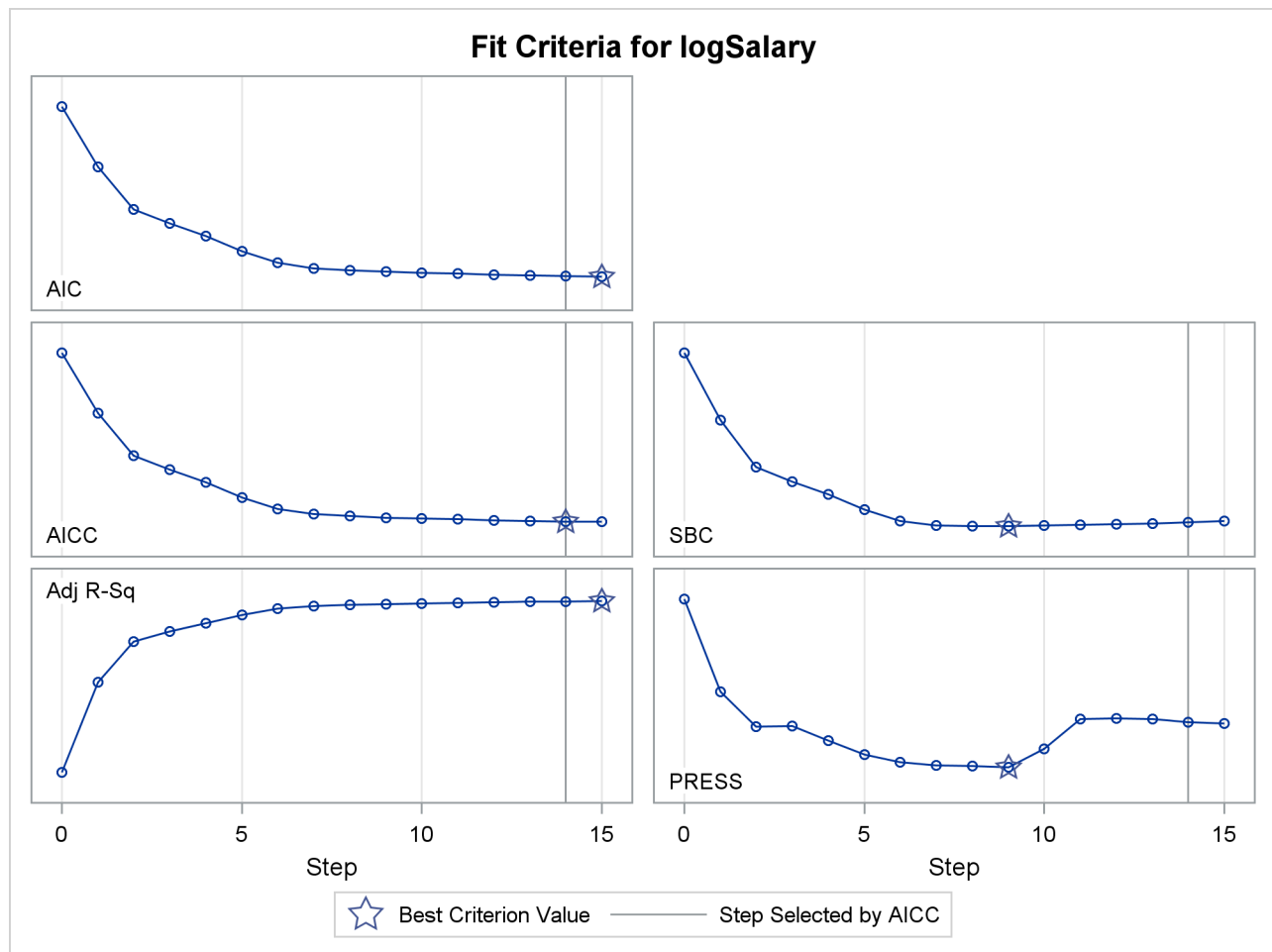
You request the criterion panel by specifying the PLOTS=CRITERIA option in the PROC GLMSELECT statement. This panel displays the progression of the ADJRSQ, AIC, AICC, and SBC criteria, as well as any other criteria that are named in the CHOOSE=, SELECT=, STOP=, or STATS= option in the MODEL statement.

The following statements provide an example:

```
proc glmselect data=baseball plots=criteria;
 class league division;
 model logSalary = nAtBat nHits nHome nRuns nRBI nBB
 yrMajor|yrMajor crAtBat|crAtBat crHits|crHits
 crHome|crHome crRuns|crRuns crRbi|crRbi
 crBB|crBB league division nOuts nAssts nError /
 selection=forward(steps=15 choose=AICC)
 stats=PRESS;
run;
```

Figure 45.18 shows the requested criterion panel. Note that the PRESS criterion is included in the panel because it is named in the `STATS=` option in the `MODEL` statement. The selected step is displayed as a vertical reference line on the plot of each criterion, and the legend indicates which of these criteria is used to make the selection. If the selection terminates for a reason other than optimizing a criterion displayed on this plot, then the legend will not report a reason for the selected step. The optimal value of each criterion is indicated with the “Star” marker. Note that it is possible that a better value of a criterion might have been reached had more steps of the selection process been done.

Figure 45.18 Criterion Panel



## Average Square Error Plot

You request the average square error plot by specifying the `PLOTS=ASE` option in the `PROC GLMSELECT` statement. This plot shows the progression of the average square error (ASE) evaluated separately on the training data, and the test and validation data whenever these data are provided with the `TESTDATA=` and `VALDATA=` options or are produced by using a `PARTITION` statement. You use the plot to detect when overfitting the training data occurs. The ASE decreases monotonically on the training data as parameters are added to a model. However, the average square error on test and validation data typically starts increasing when overfitting occurs. See [Output 45.1.9](#) and [Output 45.2.6](#) for examples.

## Examining Specific Step Ranges

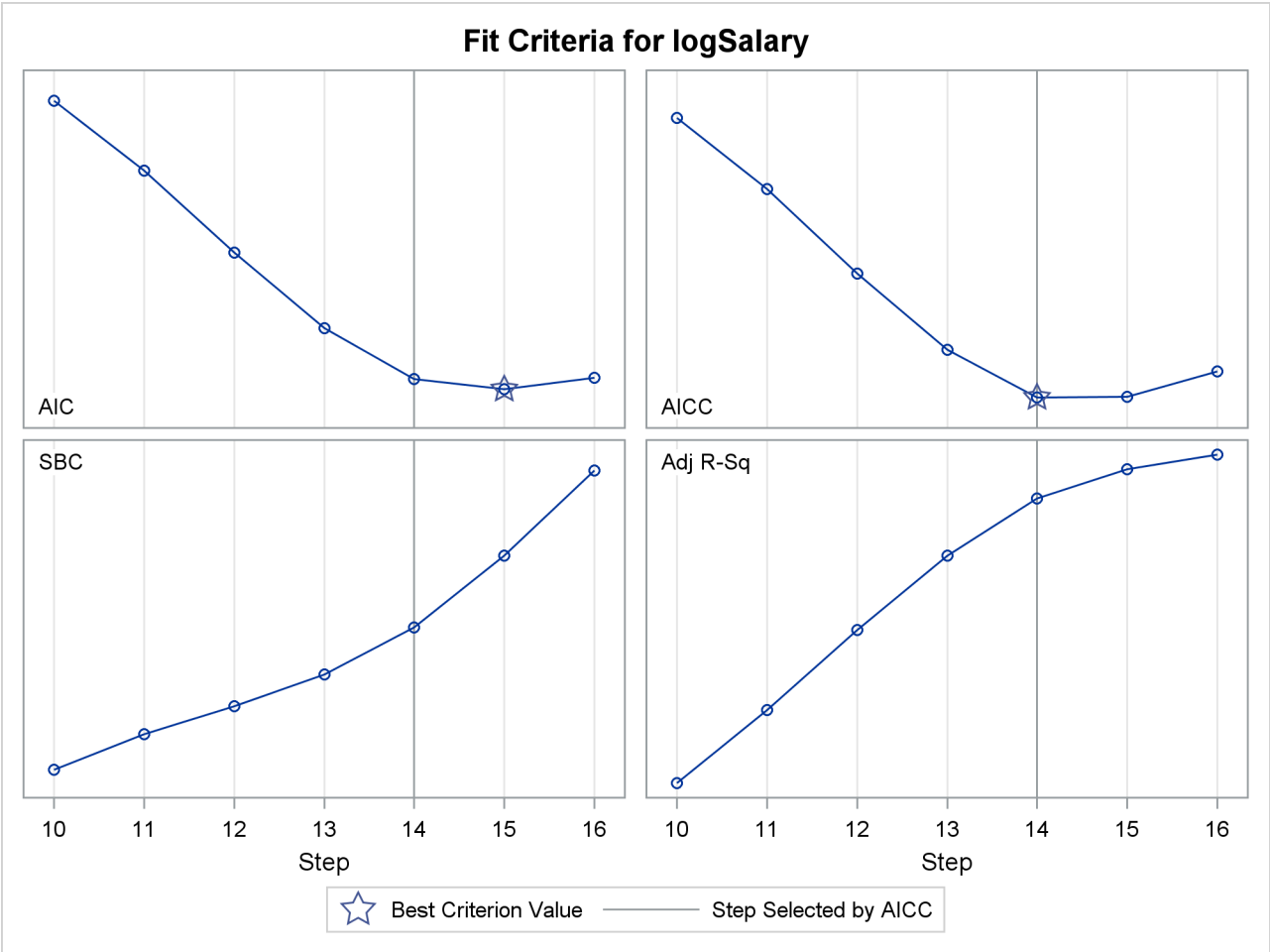
The coefficient panel, criterion panel, and average square error plot display information for all the steps examined in the selection process. In some cases, you might want to focus attention on just a particular step range. For example, it is hard to discern the variation in the criteria displayed in [Figure 45.18](#) near the selected step because the variation in these criteria in the steps close to the selected step is small relative to the variation across all steps. You can request a range of steps to display using the `STARTSTEP=` and `ENDSTEP=` suboptions of the `PLOTS=` option. You can specify these options as both global and specific plot options, with the specific options taking precedence if both are specified. The following statements provide an example:

```
proc glmselect data=baseball plots=criteria(startstep=10 endstep=16);
 class league division;
 model logSalary = nAtBat nHits nHome nRuns nRBI nBB
 yrMajor|yrMajor crAtBat|crAtBat crHits|crHits
 crHome|crHome crRuns|crRuns crRbi|crRbi
 crBB|crBB league division nOuts nAssts nError /
 selection=forward(stop=none choose=AICC);
run;

ods graphics off;
```

[Figure 45.19](#) shows the progression of the fit criteria between steps 10 and 16. Note that if the optimal value of a criterion does not occur in this specified step range, then no optimal marker appears for that criterion. The plot of the SBC criterion in [Figure 45.19](#) is one such case.

Figure 45.19 Criterion Panel for Specified Step Range



---

## Examples: GLMSELECT Procedure

---

### Example 45.1: Modeling Baseball Salaries Using Performance Statistics

This example continues the investigation of the baseball data set introduced in the section “Getting Started: GLMSELECT Procedure” on page 3520. In that example, the default stepwise selection method based on the SBC criterion was used to select a model. In this example, model selection that uses other information criteria and out-of-sample prediction criteria is explored.

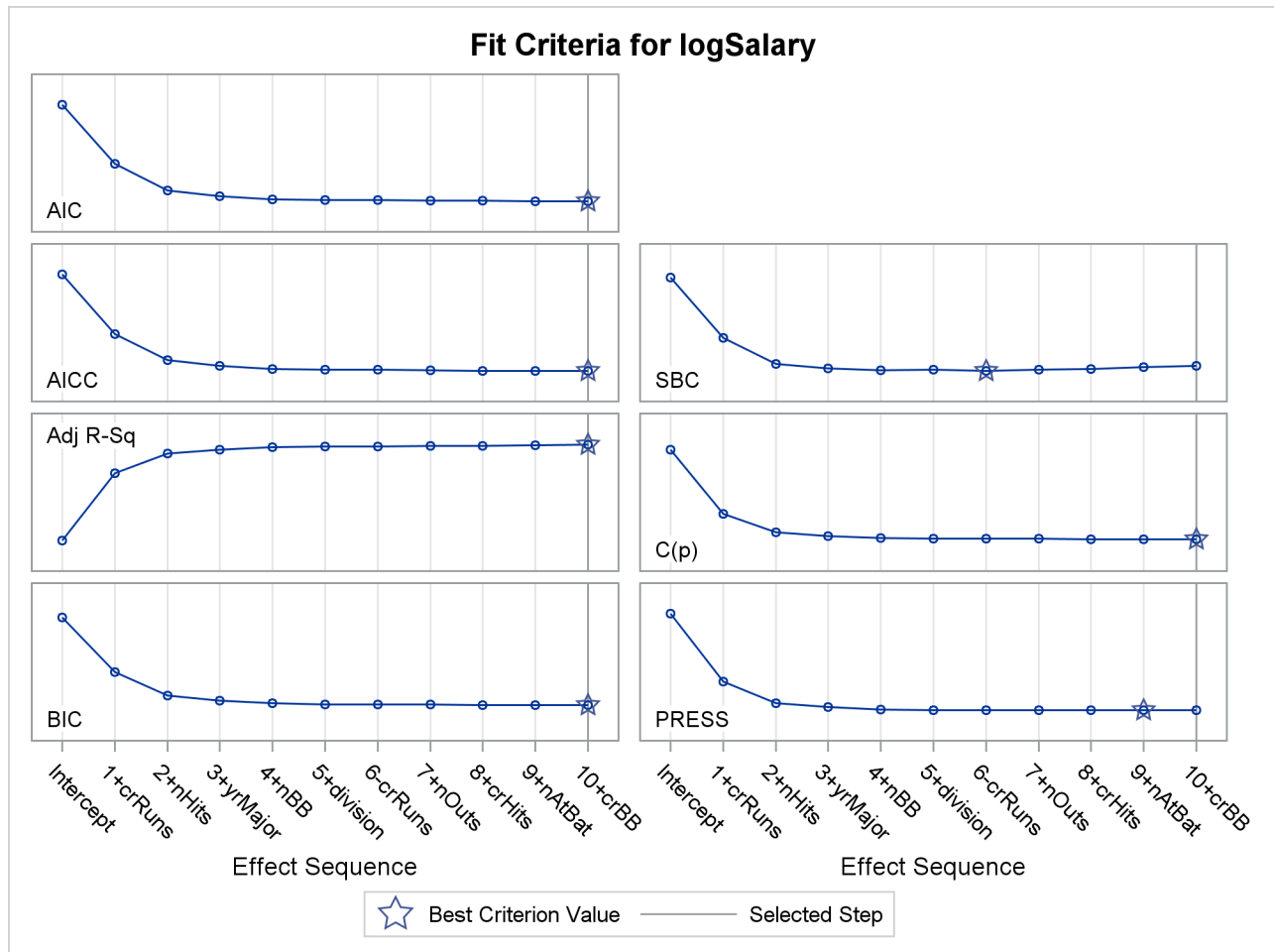
PROC GLMSELECT provides several selection algorithms that you can customize by specifying criteria for selecting effects, stopping the selection process, and choosing a model from the sequence of models at each step. For more details on the criteria available, see the section “Criteria Used in Model Selection Methods” on page 3568. The `SELECT=SL` suboption of the `SELECTION=` option in the `MODEL` statement in the following code requests the traditional hypothesis test-based stepwise selection approach, where effects in the model that are not significant at the stay significance level (SLS) are candidates for removal and effects not yet in the model whose addition is significant at the entry significance level (SLE) are candidates for addition to the model.

```
ods graphics on;

proc glmselect data=baseball plot=CriterionPanel;
 class league division;
 model logSalary = nAtBat nHits nHome nRuns nRBI nBB
 yrMajor crAtBat crHits crHome crRuns crRbi
 crBB league division nOuts nAssts nError
 / selection=stepwise(select=SL) stats=all;
run;
```

The default SLE and SLS values of 0.15 might not be appropriate for these data. One way to investigate alternative ways to stop the selection process is to assess the sequence of models in terms of model fit statistics. The `STATS=ALL` option in the `MODEL` statement requests that all model fit statistics for assessing the sequence of models of the selection process be displayed. To help in the interpretation of the selection process, you can use graphics supported by PROC GLMSELECT. ODS Graphics must be enabled before requesting plots. For general information about ODS Graphics, see Chapter 21, “Statistical Graphics Using ODS.” With ODS Graphics enabled, the `PLOTS=CRITERIONPANEL` option in the PROC GLMSELECT statement produces the criterion panel shown in [Output 45.1.1](#).

Output 45.1.1 Criterion Panel



You can see in [Output 45.1.1](#) that this stepwise selection process would stop at an earlier step if you use the Schwarz Bayesian information criterion (SBC) or predicted residual sum of squares (PRESS) to assess the selected models as stepwise selection progresses. You can use the `CHOOSE=` suboption of the `SELECTION=` option in the `MODEL` statement to specify the criterion you want to use to select among the evaluated models. The following statements use the PRESS statistic to choose among the models evaluated during the stepwise selection.

```
proc glmselect data=baseball;
 class league division;
 model logSalary = nAtBat nHits nHome nRuns nRBI nBB
 yrMajor crAtBat crHits crHome crRuns crRbi
 crBB league division nOuts nAssts nError
 / selection=stepwise(select=SL choose=PRESS);
run;
```

Note that the selected model is the model at step 9. By default, PROC GLMSELECT displays the selected model, ANOVA and fit statistics, and parameter estimates for the selected model. These are shown in [Output 45.1.2](#).

## Output 45.1.2 Details of Selected Model

| The GLMSELECT Procedure                                           |     |                |                |         |
|-------------------------------------------------------------------|-----|----------------|----------------|---------|
| Selected Model                                                    |     |                |                |         |
| The selected model, based on PRESS, is the model at Step 9.       |     |                |                |         |
| Effects: Intercept nAtBat nHits nBB yrMajor crHits division nOuts |     |                |                |         |
| Analysis of Variance                                              |     |                |                |         |
| Source                                                            | DF  | Sum of Squares | Mean Square    | F Value |
| Model                                                             | 7   | 124.67715      | 17.81102       | 55.07   |
| Error                                                             | 255 | 82.47658       | 0.32344        |         |
| Corrected Total                                                   | 262 | 207.15373      |                |         |
| Root MSE                                                          |     | 0.56872        |                |         |
| Dependent Mean                                                    |     | 5.92722        |                |         |
| R-Square                                                          |     | 0.6019         |                |         |
| Adj R-Sq                                                          |     | 0.5909         |                |         |
| AIC                                                               |     | -23.98522      |                |         |
| AICC                                                              |     | -23.27376      |                |         |
| PRESS                                                             |     | 88.55275       |                |         |
| SBC                                                               |     | -260.40799     |                |         |
| Parameter Estimates                                               |     |                |                |         |
| Parameter                                                         | DF  | Estimate       | Standard Error | t Value |
| Intercept                                                         | 1   | 4.176133       | 0.150539       | 27.74   |
| nAtBat                                                            | 1   | -0.001468      | 0.000946       | -1.55   |
| nHits                                                             | 1   | 0.011078       | 0.002983       | 3.71    |
| nBB                                                               | 1   | 0.007226       | 0.002115       | 3.42    |
| yrMajor                                                           | 1   | 0.070056       | 0.018911       | 3.70    |
| crHits                                                            | 1   | 0.000247       | 0.000143       | 1.72    |
| division East                                                     | 1   | 0.143082       | 0.070972       | 2.02    |
| division West                                                     | 0   | 0              | .              | .       |
| nOuts                                                             | 1   | 0.000241       | 0.000134       | 1.81    |

Even though the model that is chosen to give the smallest value of the PRESS statistic is the model at step 9, the stepwise selection process continues to the step where the stopping condition based on entry and stay significance levels is met. If you use the PRESS statistic as the stopping criterion, the stepwise selection process stops at step 9. This ability to stop at the first extremum of the criterion you specify can significantly reduce the amount of computation done, especially in the cases where you are selecting from a large number of effects. The following statements request stopping based on the PRESS statistic. The stop reason and stop details tables are shown in [Output 45.1.3](#).

```
proc glmselect data=baseball plot=Coefficients;
 class league division;
 model logSalary = nAtBat nHits nHome nRuns nRBI nBB
 yrMajor crAtBat crHits crHome crRuns crRbi
 crBB league division nOuts nAssts nError
 / selection=stepwise(select=SL stop=PRESS);
run;
```

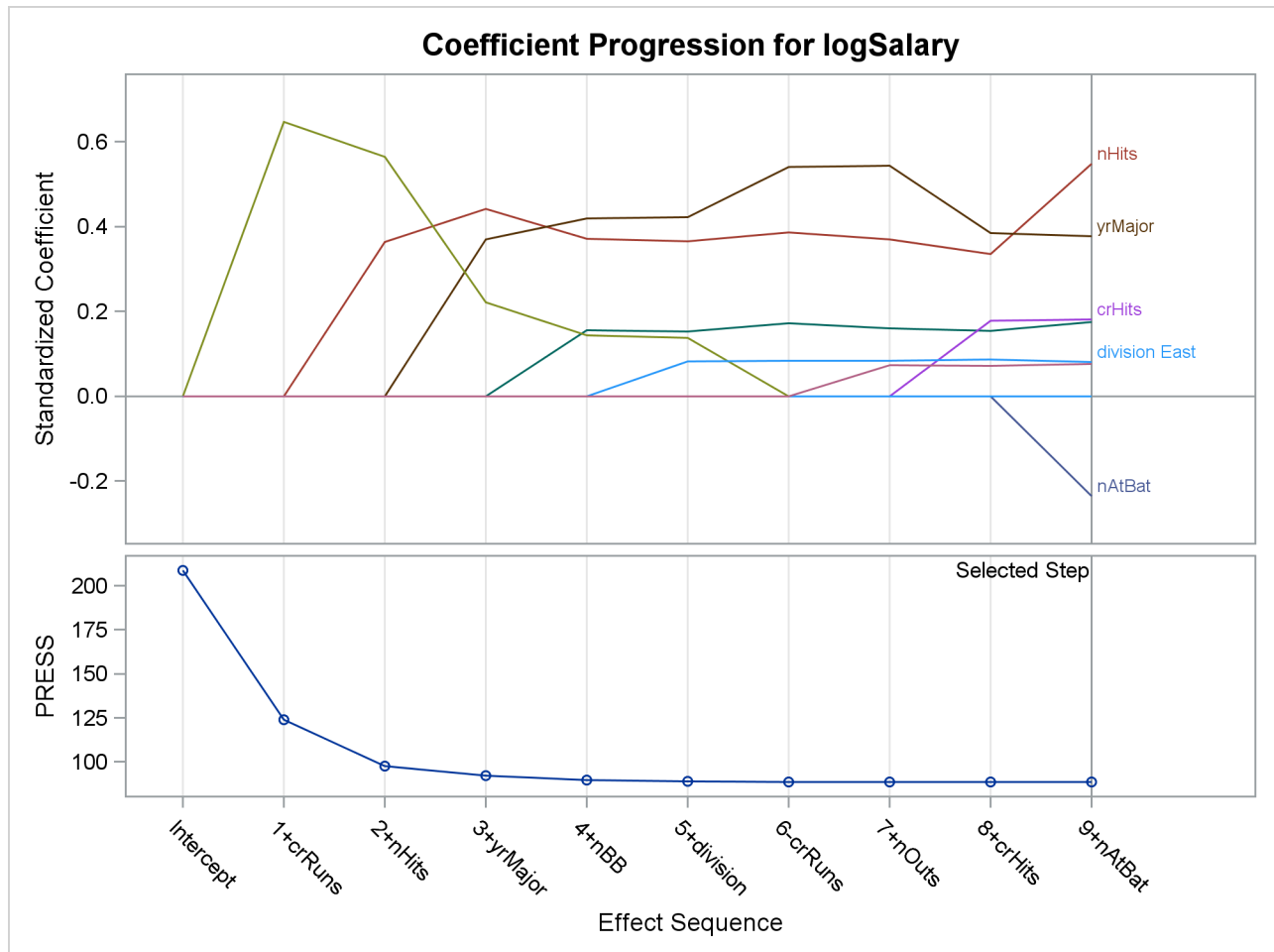
**Output 45.1.3** Stopping Based on PRESS Statistic

| The GLMSELECT Procedure                                      |        |                 |         |         |
|--------------------------------------------------------------|--------|-----------------|---------|---------|
| Selection stopped at a local minimum of the PRESS criterion. |        |                 |         |         |
| Stop Details                                                 |        |                 |         |         |
| Candidate For                                                | Effect | Candidate PRESS | Compare | PRESS   |
| Entry                                                        | crBB   | 88.6321         | >       | 88.5528 |
| Removal                                                      | nAtBat | 88.6866         | >       | 88.5528 |

The `PLOTS=COEFFICIENTS` specification in the PROC GLMSELECT statement requests a plot that enables you to visualize the selection process.



Output 45.1.4 Coefficient Progression Plot



Output 45.1.4 shows the standardized coefficients of all the effects selected at some step of the stepwise method plotted as a function of the step number. This enables you to assess the relative importance of the effects selected at any step of the selection process as well as providing information as to when effects entered the model. The lower plot in the panel shows how the criterion used to choose the selected model changes as effects enter or leave the model.

Model selection is often done in order to obtain a parsimonious model that can be used for prediction on new data. An ever-present danger is that of selecting a model that overfits the “training” data used in the fitting process, yielding a model with poor predictive performance. Using cross validation is one way to assess the predictive performance of the model. Using  $k$ -fold cross validation, the training data are subdivided into  $k$  parts, and at each step of the selection process, models are obtained on each of the  $k$  subsets of the data obtained by omitting one of these parts. The cross validation predicted residual sum of squares, denoted CV PRESS, is obtained by summing the squares of the residuals when each of these submodels is scored on the data omitted in fitting the submodel. Note that the PRESS statistic corresponds to the special case of “leave-one-out” cross validation.

In the preceding example, the PRESS statistic was used to choose among models that were chosen based on entry and stay significance levels. In the following statements, the `SELECT=CVPRESS` suboption of the `SELECTION=` option in the `MODEL` statement requests that the CV PRESS statistic itself be used

as the selection criterion. The `DROP=COMPETITIVE` suboption requests that additions and deletions be considered simultaneously when deciding whether to add or remove an effect. At any step, the CV PRESS statistic for all models obtained by deleting one effect from the model or adding one effect to the model is computed. Among these models, the one yielding the smallest value of the CV PRESS statistic is selected and the process is repeated from this model. The stepwise selection terminates if all additions or deletions increase the CV PRESS statistic. The `CVMETHOD=SPLIT(5)` option requests five-fold cross validation with the five subsets consisting of observations {1, 6, 11, ...}, {2, 7, 12, ...}, and so on.

```
proc glmselect data=baseball plot=Candidates;
 class league division;
 model logSalary = nAtBat nHits nHome nRuns nRBI nBB
 yrMajor crAtBat crHits crHome crRuns crRbi
 crBB league division nOuts nAssts nError
 / selection=stepwise(select=CV drop=competitive)
 cvMethod=split(5);
run;
```

The selection summary table is shown in [Output 45.1.5](#). By comparing [Output 45.1.5](#) and [Output 45.6](#) you can see that the sequence of models produced is different from the sequence when the stepwise selection is based on the SBC statistic.

**Output 45.1.5** Stepwise Selection Based on Cross Validation

| The GLMSELECT Procedure    |                |                |                   |                  |          |
|----------------------------|----------------|----------------|-------------------|------------------|----------|
| Stepwise Selection Summary |                |                |                   |                  |          |
| Step                       | Effect Entered | Effect Removed | Number Effects In | Number Params In | CV PRESS |
| 0                          | Intercept      |                | 1                 | 1                | 208.9638 |
| -----                      |                |                |                   |                  |          |
| 1                          | crRuns         |                | 2                 | 2                | 122.5755 |
| 2                          | nHits          |                | 3                 | 3                | 96.3949  |
| 3                          | yrMajor        |                | 4                 | 4                | 92.2117  |
| 4                          | nBB            |                | 5                 | 5                | 89.5242  |
| 5                          |                | crRuns         | 4                 | 4                | 88.6917  |
| 6                          | league         |                | 5                 | 5                | 88.0417  |
| 7                          | nError         |                | 6                 | 6                | 87.3170  |
| 8                          | division       |                | 7                 | 7                | 87.2147  |
| 9                          | nHome          |                | 8                 | 8                | 87.0960* |

\* Optimal Value Of Criterion

If you have sufficient data, another way you can assess the predictive performance of your model is to reserve part of your data for testing your model. You score the model obtained using the training data on the test data and assess the predictive performance on these data that had no role in the selection process. You can also reserve part of your data to validate the model you obtain in the training process. Note that the validation data are not used in obtaining the coefficients of the model, but they are used to decide when to stop the selection process to limit overfitting.

PROC GLMSELECT enables you to partition your data into disjoint subsets for training validation and testing roles. This partitioning can be done by using random proportions of the data, or you can designate a variable in your data set that defines which observations to use for each role. See the section “[PARTITION Statement](#)” on page 3556 for more details.

The following statements randomly partition the baseball data set, using 50% for training, 30% for validation, and 20% for testing. The model selected at each step is scored on the validation data, and the average residual sums of squares (ASE) is evaluated. The model yielding the lowest ASE on the validation data is selected. The ASE on the test data is also evaluated, but these data play no role in the selection process. Note that a seed for the pseudo-random number generator is specified in the PROC GLMSELECT statement.

```
proc glmselect data=baseball plots=(CriterionPanel ASE) seed=1;
 partition fraction(validate=0.3 test=0.2);
 class league division;
 model logSalary = nAtBat nHits nHome nRuns nRBI nBB
 yrMajor crAtBat crHits crHome crRuns crRbi
 crBB league division nOuts nAssts nError
 / selection=forward(choose=validate stop=10);
run;
```

**Output 45.1.6** Number of Observations Table

| The GLMSELECT Procedure                    |     |
|--------------------------------------------|-----|
| Number of Observations Read                | 322 |
| Number of Observations Used                | 263 |
| Number of Observations Used for Training   | 132 |
| Number of Observations Used for Validation | 80  |
| Number of Observations Used for Testing    | 51  |

Output 45.1.6 shows the number of observation table. You can see that of the 263 observations that were used in the analysis, 132 (50.2%) observations were used for model training, 80 (30.4%) for model validation, and 51 (19.4%) for model testing.

**Output 45.1.7** Selection Summary and Stop Reason

```

The GLMSELECT Procedure

Forward Selection Summary

Step Effect Number Number SBC ASE
Entered Effects In Parm In

0 Intercept 1 1 -30.8531 0.7628

1 crRuns 2 2 -93.9367 0.4558
2 nHits 3 3 -126.2647 0.3439
3 yrMajor 4 4 -128.7570 0.3252
4 nBB 5 5 -132.2409* 0.3052
5 division 6 6 -130.7794 0.2974
6 nOuts 7 7 -128.5897 0.2914
7 nRBI 8 8 -125.7825 0.2868
8 nHome 9 9 -124.7709 0.2786
9 nAtBat 10 10 -121.3767 0.2754

* Optimal Value Of Criterion

Forward Selection Summary

Step Effect Validation Test ASE
Entered ASE

0 Intercept 0.7843 0.8818

1 crRuns 0.4947 0.4210
2 nHits 0.3248 0.4697
3 yrMajor 0.2920* 0.4614
4 nBB 0.3065 0.4297
5 division 0.3050 0.4218
6 nOuts 0.3028 0.4186
7 nRBI 0.3097 0.4489
8 nHome 0.3383 0.4533
9 nAtBat 0.3337 0.4580

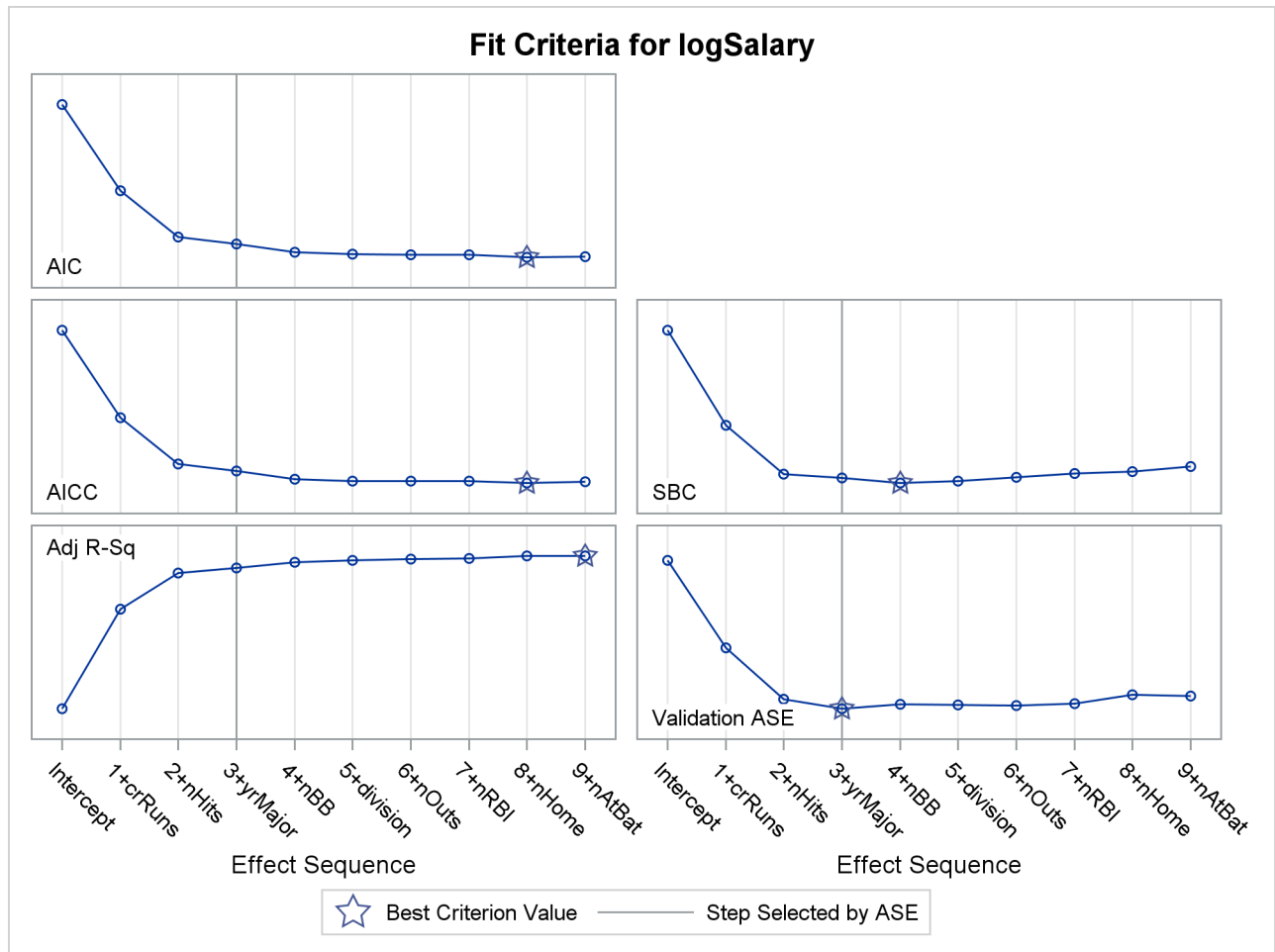
* Optimal Value Of Criterion

Selection stopped at the first model containing the specified number of effects
(10) .

```

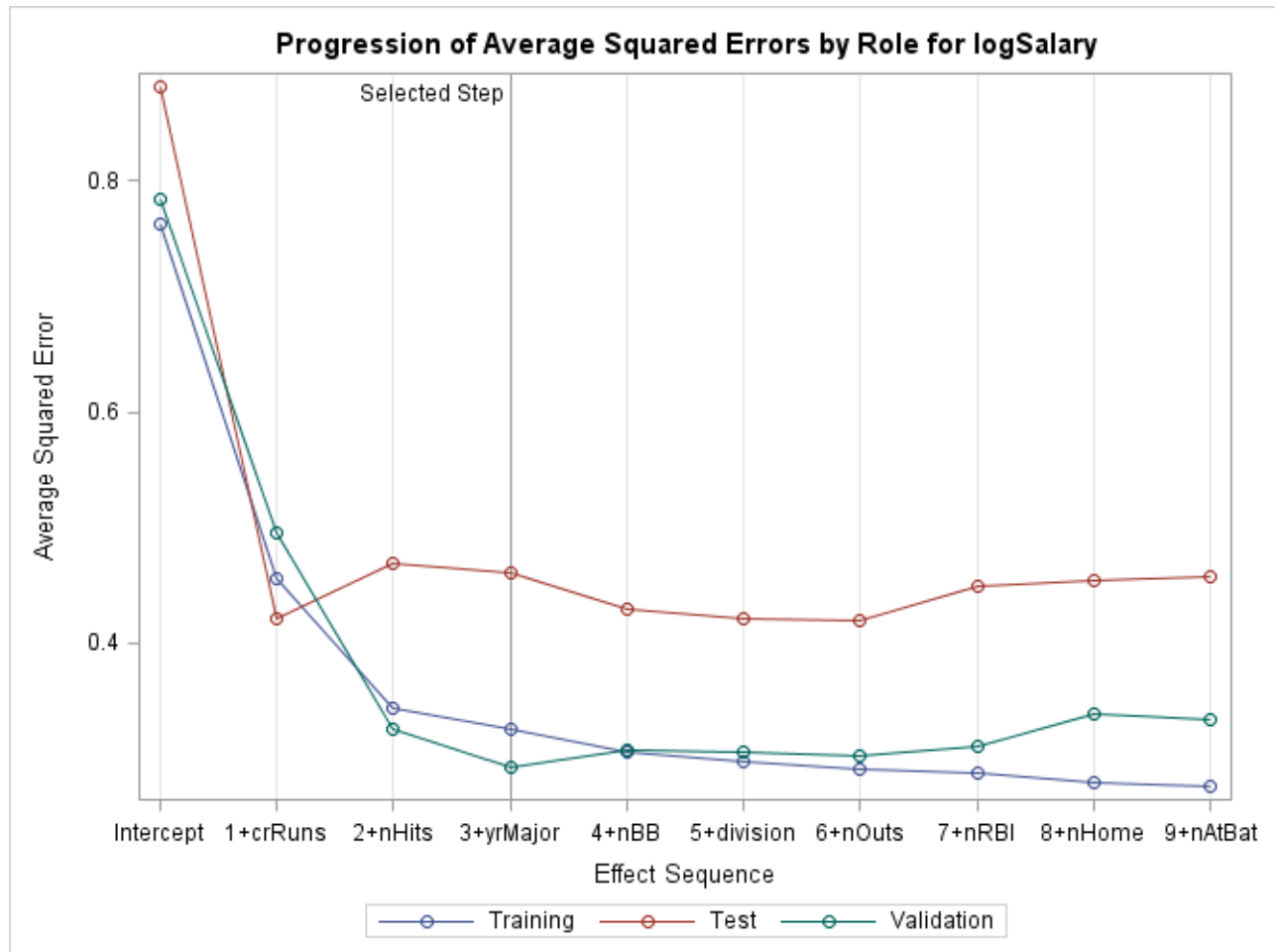
Output 45.1.7 shows the selection summary table and the stop reason. The forward selection stops at step 9 since the model at this step contains 10 effects, and so it satisfies the stopping criterion requested with the STOP=10 suboption. However, the selected model is the model at step 3, where the validation ASE, the CHOOSE= criterion, achieves its minimum.

Output 45.1.8 Criterion Panel



The criterion panel in [Output 45.1.8](#) shows how the various criteria evolved as the stepwise selection method proceeded. Note that other than the ASE evaluated on the validation data, these criteria are evaluated on the training data.

Output 45.1.9 Average Square Errors by Role



Finally, the ASE plot in [Output 45.1.9](#) shows how the average square error evolves on the training, validation, and test data. Note that while the ASE on the training data continued decreasing as the selection steps proceeded, the ASE on the test and validation data behave more erratically.

LASSO selection, pioneered by Tibshirani (1996), is a constrained least squares method that can be viewed as a stepwise-like method where effects enter and leave the model sequentially. You can find additional details about the LASSO method in the section “[Lasso Selection \(LASSO\)](#)” on page 3565. Note that when classification effects are used with LASSO, the design matrix columns for all effects containing classification variables can enter or leave the model individually. The following statements perform LASSO selection for the baseball data. The LASSO selection summary table is shown in [Output 45.1.10](#).

```
proc glmselect data=baseball plot=CriterionPanel ;
 class league division;
 model logSalary = nAtBat nHits nHome nRuns nRBI nBB
 yrMajor crAtBat crHits crHome crRuns crRbi
 crBB league division nOuts nAssts nError
 / selection=lasso(choose=CP steps=20);
run;

ods graphics off;
```

**Output 45.1.10** Selection Summary for LASSO Selection

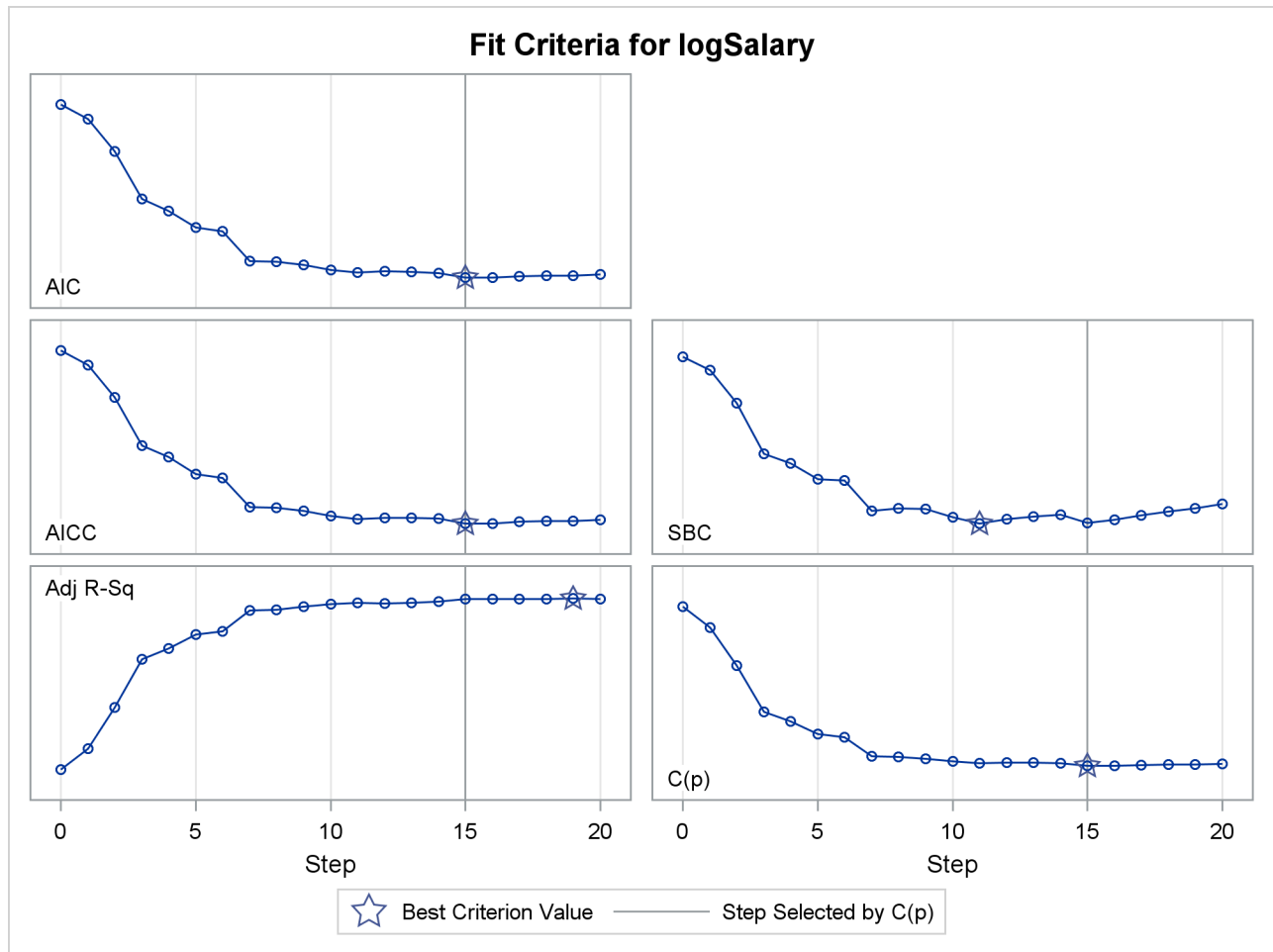
| The GLMSELECT Procedure |                 |                |                   |          |
|-------------------------|-----------------|----------------|-------------------|----------|
| LASSO Selection Summary |                 |                |                   |          |
| Step                    | Effect Entered  | Effect Removed | Number Effects In | CP       |
| 0                       | Intercept       |                | 1                 | 375.9275 |
| -----                   |                 |                |                   |          |
| 1                       | crRuns          |                | 2                 | 328.6492 |
| 2                       | crHits          |                | 3                 | 239.5392 |
| 3                       | nHits           |                | 4                 | 134.0374 |
| 4                       | nBB             |                | 5                 | 111.6638 |
| 5                       | crRbi           |                | 6                 | 81.7296  |
| 6                       | yrMajor         |                | 7                 | 75.0428  |
| 7                       | nRBI            |                | 8                 | 30.4494  |
| 8                       | division_East   |                | 9                 | 29.9913  |
| 9                       | nOuts           |                | 10                | 25.1656  |
| 10                      |                 | crRuns         | 9                 | 18.7295  |
| 11                      |                 | crRbi          | 8                 | 15.1683  |
| 12                      | nError          |                | 9                 | 16.6233  |
| 13                      | nHome           |                | 10                | 16.3741  |
| 14                      | league_National |                | 11                | 14.8794  |
| 15                      |                 | nRBI           | 10                | 8.8477*  |
| 16                      | crBB            |                | 11                | 9.2242   |
| 17                      | crRuns          |                | 12                | 10.7608  |
| 18                      | nAtBat          |                | 13                | 11.6266  |
| 19                      | nAssts          |                | 14                | 11.8572  |
| 20                      | crAtBat         |                | 15                | 13.4020  |

\* Optimal Value Of Criterion

Selection stopped at the specified number of steps (20).

Note that effects enter and leave sequentially. In this example, the STEPS= suboption of the SELECTION= option specifies that 20 steps of LASSO selection be done. You can see how the various model fit statistics evolved in [Output 45.1.11](#).

**Output 45.1.11** Criterion Panel



The **CHOOSE=CP** suboption specifies that the selected model be the model at step 15 that yields the optimal value of Mallows'  $C(p)$  statistic. Details of this selected model are shown in [Output 45.1.12](#).

**Output 45.1.12** Selected Model

```

The GLMSELECT Procedure
Selected Model

The selected model, based on C(p), is the model at Step 15.

Effects: Intercept nHits nHome nBB yrMajor crHits league_National division_East
nOuts nError

```



## Output 45.1.12 continued

| Analysis of Variance |     |                |             |         |
|----------------------|-----|----------------|-------------|---------|
| Source               | DF  | Sum of Squares | Mean Square | F Value |
| Model                | 9   | 125.24302      | 13.91589    | 42.98   |
| Error                | 253 | 81.91071       | 0.32376     |         |
| Corrected Total      | 262 | 207.15373      |             |         |
| Root MSE             |     | 0.56900        |             |         |
| Dependent Mean       |     | 5.92722        |             |         |
| R-Square             |     | 0.6046         |             |         |
| Adj R-Sq             |     | 0.5905         |             |         |
| AIC                  |     | -21.79589      |             |         |
| AICC                 |     | -20.74409      |             |         |
| BIC                  |     | -283.91417     |             |         |
| C(p)                 |     | 8.84767        |             |         |
| SBC                  |     | -251.07435     |             |         |
| Parameter Estimates  |     |                |             |         |
| Parameter            | DF  | Estimate       |             |         |
| Intercept            | 1   | 4.124629       |             |         |
| nHits                | 1   | 0.006942       |             |         |
| nHome                | 1   | 0.002785       |             |         |
| nBB                  | 1   | 0.005727       |             |         |
| yrMajor              | 1   | 0.067054       |             |         |
| crHits               | 1   | 0.000249       |             |         |
| league_National      | 1   | 0.079607       |             |         |
| division_East        | 1   | 0.134723       |             |         |
| nOuts                | 1   | 0.000183       |             |         |
| nError               | 1   | -0.007213      |             |         |

---

**Example 45.2: Using Validation and Cross Validation**

This example shows how you can use both test set and cross validation to monitor and control variable selection. It also demonstrates the use of split classification variables.

The following statements produce analysis and test data sets. Note that the same statements are used to generate the observations that are randomly assigned for analysis and test roles in the ratio of approximately two to one.

```

data analysisData testData;
 drop i j c3Num;
 length c3$ 7;

 array x{20} x1-x20;

 do i=1 to 1500;
 do j=1 to 20;
 x{j} = ranuni(1);
 end;

 c1 = 1 + mod(i,8);
 c2 = ranbin(1,3,.6);

 if i < 50 then do; c3 = 'tiny'; c3Num=1;end;
 else if i < 250 then do; c3 = 'small'; c3Num=1;end;
 else if i < 600 then do; c3 = 'average'; c3Num=2;end;
 else if i < 1200 then do; c3 = 'big'; c3Num=3;end;
 else do; c3 = 'huge'; c3Num=5;end;

 y = 10 + x1 + 2*x5 + 3*x10 + 4*x20 + 3*x1*x7 + 8*x6*x7
 + 5*(c1=3)*c3Num + 8*(c1=7) + 5*rannor(1);

 if ranuni(1) < 2/3 then output analysisData;
 else output testData;
 end;
run;

```

Suppose you suspect that the dependent variable depends on both main effects and two-way interactions. You can use the following statements to select a model:

```

ods graphics on;

proc glmselect data=analysisData testdata=testData
 seed=1 plots(stepAxis=number)=(criterionPanel ASEPlot);
 partition fraction(validate=0.5);
 class c1 c2 c3(order=data);
 model y = c1|c2|c3|x1|x2|x3|x4|x5|x5|x6|x7|x8|x9|x10
 |x11|x12|x13|x14|x15|x16|x17|x18|x19|x20 @2
 / selection=stepwise(choose = validate
 select = s1)
 hierarchy=single stb;
run;

```

Note that a `TESTDATA=` data set is named in the PROC GLMSELECT statement and that a `PARTITION` statement is used to randomly assign half the observations in the analysis data set for model validation and the rest for model training. You find details about the number of observations used for each role in the number of observations tables shown in [Output 45.2.1](#).

**Output 45.2.1** Number of Observations Tables

| The GLMSELECT Procedure                    |      |
|--------------------------------------------|------|
| Observation Profile for Analysis Data      |      |
| Number of Observations Read                | 1010 |
| Number of Observations Used                | 1010 |
| Number of Observations Used for Training   | 510  |
| Number of Observations Used for Validation | 500  |

The “Class Level Information” and “Dimensions” tables are shown in [Output 45.2.2](#). The “Dimensions” table shows that at each step of the selection process, 278 effects are considered as candidates for entry or removal. Since several of these effects have multilevel classification variables as members, there are 661 parameters.

**Output 45.2.2** Class Level Information and Problem Dimensions

| Class Level Information |        |                             |
|-------------------------|--------|-----------------------------|
| Class                   | Levels | Values                      |
| c1                      | 8      | 1 2 3 4 5 6 7 8             |
| c2                      | 4      | 0 1 2 3                     |
| c3                      | 5      | tiny small average big huge |

| Dimensions           |     |
|----------------------|-----|
| Number of Effects    | 278 |
| Number of Parameters | 661 |

The model statement options request stepwise selection with the default entry and stay significance levels used for both selecting entering and departing effects and stopping the selection method. The **CHOOSE=VALIDATE** suboption specifies that the selected model is chosen to minimize the predicted residual sum of squares when the models at each step are scored on the observations reserved for validation. The **HIERARCHY=SINGLE** option specifies that interactions can enter the model only if the corresponding main effects are already in the model, and that main effects cannot be dropped from the model if an interaction with such an effect is in the model. These settings are listed in the model information table shown in [Output 45.2.3](#).

**Output 45.2.3** Model Information

| The GLMSELECT Procedure        |                    |
|--------------------------------|--------------------|
| Data Set                       | WORK.ANALYSISDATA  |
| Test Data Set                  | WORK.TESTDATA      |
| Dependent Variable             | Y                  |
| Selection Method               | Stepwise           |
| Select Criterion               | Significance Level |
| Stop Criterion                 | Significance Level |
| Choose Criterion               | Validation ASE     |
| Entry Significance Level (SLE) | 0.15               |
| Stay Significance Level (SLS)  | 0.15               |
| Effect Hierarchy Enforced      | Single             |
| Random Number Seed             | 1                  |

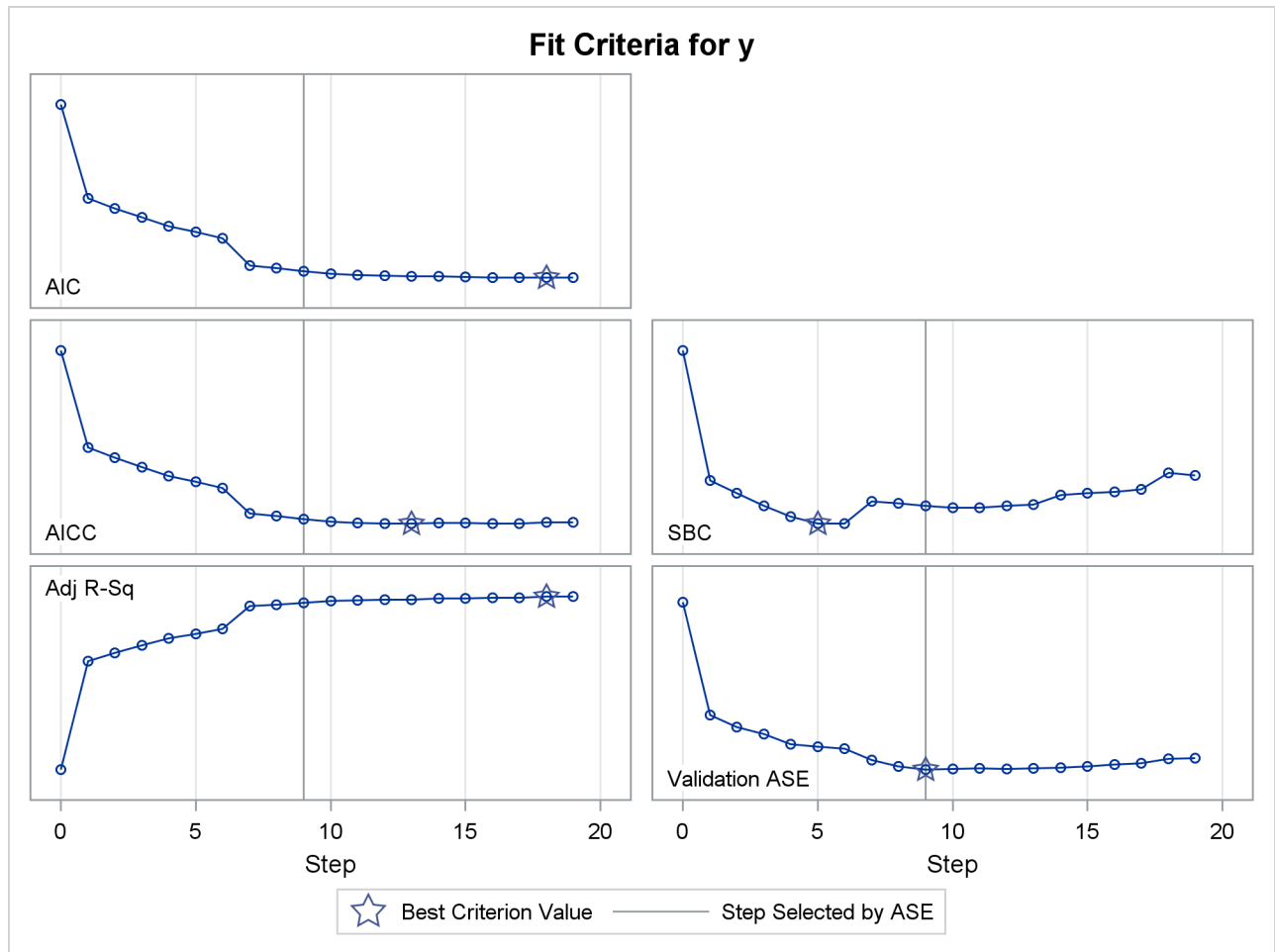
The stop reason and stop details tables are shown in [Output 45.2.4](#). Note that because the `STOP=` suboption of the `SELECTION=` option was not explicitly specified, the stopping criterion used is the selection criterion, namely significance level.

**Output 45.2.4** Stop Details

| Selection stopped because the candidate for entry has SLE > 0.15 and the candidate for removal has SLS < 0.15. |        |                        |         |              |       |
|----------------------------------------------------------------------------------------------------------------|--------|------------------------|---------|--------------|-------|
| Stop Details                                                                                                   |        |                        |         |              |       |
| Candidate For                                                                                                  | Effect | Candidate Significance | Compare | Significance |       |
| Entry                                                                                                          | x2*x5  | 0.1742                 | >       | 0.1500       | (SLE) |
| Removal                                                                                                        | x5*x10 | 0.0534                 | <       | 0.1500       | (SLS) |

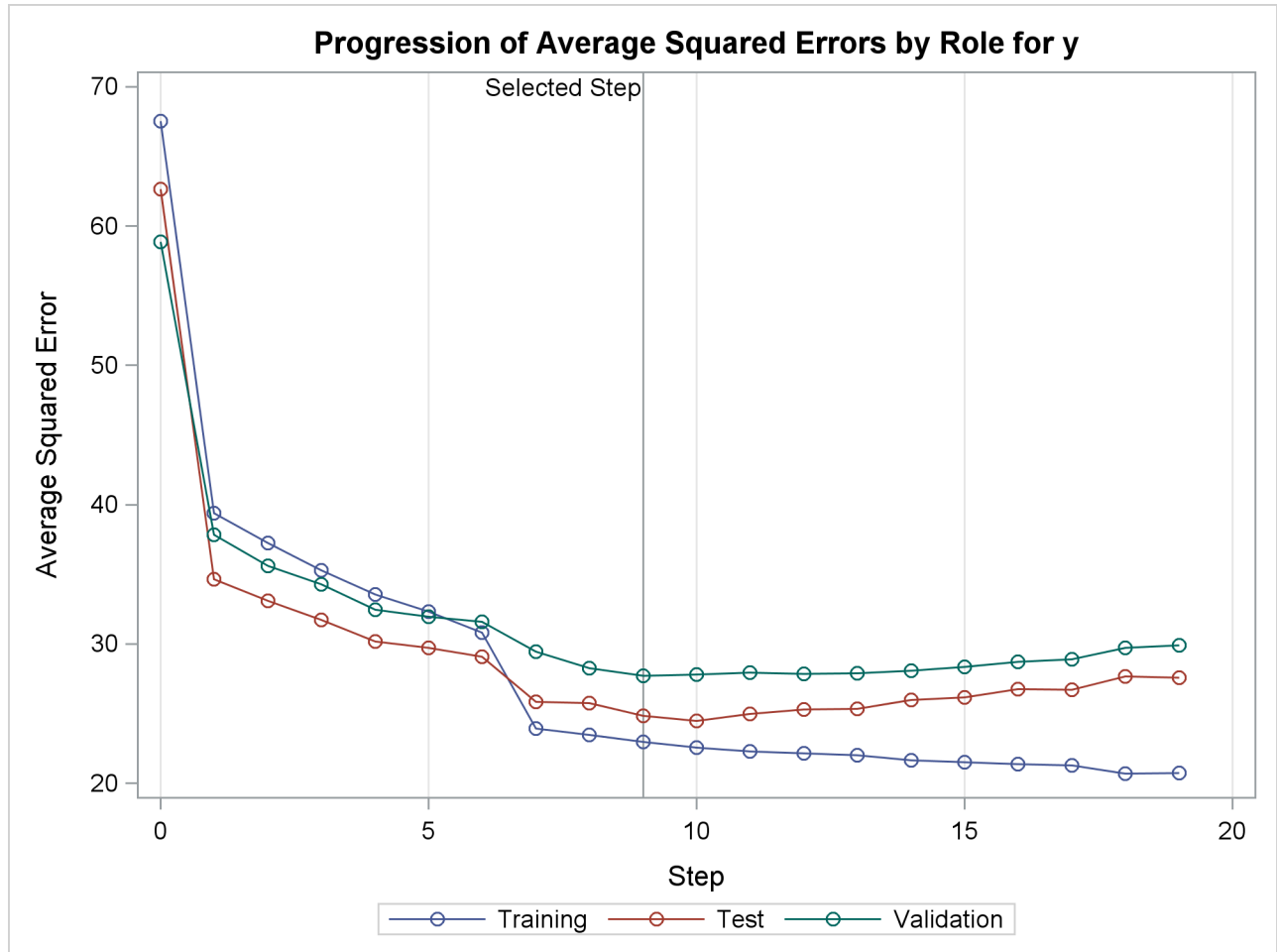
The criterion panel in [Output 45.2.5](#) shows how the various fit criteria evolved as the stepwise selection method proceeded. Note that other than the ASE evaluated on the validation data, these criteria are evaluated on the training data. You see that the minimum of the validation ASE occurs at step 9, and hence the model at this step is selected.

Output 45.2.5 Criterion Panel



Output 45.2.6 shows how the average squared error (ASE) evolved on the training, validation, and test data. Note that while the ASE on the training data decreases monotonically, the errors on both the validation and test data start increasing beyond step 9. This indicates that models after step 9 are beginning to overfit the training data.

**Output 45.2.6** Average Squared Errors



Output 45.2.7 shows the selected effects, analysis of variance, and fit statistics tables for the selected model. Output 45.2.8 shows the parameter estimates table.

**Output 45.2.7** Selected Model Details

| The GLMSELECT Procedure                                              |     |                |             |         |
|----------------------------------------------------------------------|-----|----------------|-------------|---------|
| Selected Model                                                       |     |                |             |         |
| The selected model, based on Validation ASE, is the model at Step 9. |     |                |             |         |
| Effects: Intercept c1 c3 c1+c3 x1 x5 x6 x7 x10 x20                   |     |                |             |         |
| Analysis of Variance                                                 |     |                |             |         |
| Source                                                               | DF  | Sum of Squares | Mean Square | F Value |
| Model                                                                | 44  | 22723          | 516.43621   | 20.49   |
| Error                                                                | 465 | 11722          | 25.20856    |         |
| Corrected Total                                                      | 509 | 34445          |             |         |
| Root MSE                                                             |     | 5.02081        |             |         |
| Dependent Mean                                                       |     | 21.09705       |             |         |
| R-Square                                                             |     | 0.6597         |             |         |
| Adj R-Sq                                                             |     | 0.6275         |             |         |
| AIC                                                                  |     | 2200.75319     |             |         |
| AICC                                                                 |     | 2210.09228     |             |         |
| SBC                                                                  |     | 1879.30167     |             |         |
| ASE (Train)                                                          |     | 22.98427       |             |         |
| ASE (Validate)                                                       |     | 27.71105       |             |         |
| ASE (Test)                                                           |     | 24.82947       |             |         |

**Output 45.2.8** Parameter Estimates

| Parameter Estimates |           |    |            |                       |                |         |
|---------------------|-----------|----|------------|-----------------------|----------------|---------|
| Parameter           |           | DF | Estimate   | Standardized Estimate | Standard Error | t Value |
| Intercept           |           | 1  | 6.867831   | 0                     | 1.524446       | 4.51    |
| c1                  | 1         | 1  | 0.226602   | 0.008272              | 2.022069       | 0.11    |
| c1                  | 2         | 1  | -1.189623  | -0.048587             | 1.687644       | -0.70   |
| c1                  | 3         | 1  | 25.968930  | 1.080808              | 1.693593       | 15.33   |
| c1                  | 4         | 1  | 1.431767   | 0.054892              | 1.903011       | 0.75    |
| c1                  | 5         | 1  | 1.972622   | 0.073854              | 1.664189       | 1.19    |
| c1                  | 6         | 1  | -0.094796  | -0.004063             | 1.898700       | -0.05   |
| c1                  | 7         | 1  | 5.971432   | 0.250037              | 1.846102       | 3.23    |
| c1                  | 8         | 0  | 0          | 0                     | .              | .       |
| c3                  | tiny      | 1  | -2.919282  | -0.072169             | 2.756295       | -1.06   |
| c3                  | small     | 1  | -4.635843  | -0.184338             | 2.218541       | -2.09   |
| c3                  | average   | 1  | 0.736805   | 0.038247              | 1.793059       | 0.41    |
| c3                  | big       | 1  | -1.078463  | -0.063580             | 1.518927       | -0.71   |
| c3                  | huge      | 0  | 0          | 0                     | .              | .       |
| c1*c3               | 1 tiny    | 1  | -2.449964  | -0.018632             | 4.829146       | -0.51   |
| c1*c3               | 1 small   | 1  | 5.265031   | 0.069078              | 3.470382       | 1.52    |
| c1*c3               | 1 average | 1  | -3.489735  | -0.064365             | 2.850381       | -1.22   |
| c1*c3               | 1 big     | 1  | 0.725263   | 0.017929              | 2.516502       | 0.29    |
| c1*c3               | 1 huge    | 0  | 0          | 0                     | .              | .       |
| c1*c3               | 2 tiny    | 1  | 5.455122   | 0.050760              | 4.209507       | 1.30    |
| c1*c3               | 2 small   | 1  | 7.439196   | 0.131499              | 2.982411       | 2.49    |
| c1*c3               | 2 average | 1  | -0.739606  | -0.014705             | 2.568876       | -0.29   |
| c1*c3               | 2 big     | 1  | 3.179351   | 0.078598              | 2.247611       | 1.41    |
| c1*c3               | 2 huge    | 0  | 0          | 0                     | .              | .       |
| c1*c3               | 3 tiny    | 1  | -19.266847 | -0.230989             | 3.784029       | -5.09   |
| c1*c3               | 3 small   | 1  | -15.578909 | -0.204399             | 3.266216       | -4.77   |
| c1*c3               | 3 average | 1  | -18.119398 | -0.395770             | 2.529578       | -7.16   |
| c1*c3               | 3 big     | 1  | -10.650012 | -0.279796             | 2.205331       | -4.83   |
| c1*c3               | 3 huge    | 0  | 0          | 0                     | .              | .       |
| c1*c3               | 4 tiny    | 0  | 0          | 0                     | .              | .       |
| c1*c3               | 4 small   | 1  | 4.432753   | 0.047581              | 3.677008       | 1.21    |
| c1*c3               | 4 average | 1  | -3.976295  | -0.091632             | 2.625564       | -1.51   |
| c1*c3               | 4 big     | 1  | -1.306998  | -0.033003             | 2.401064       | -0.54   |
| c1*c3               | 4 huge    | 0  | 0          | 0                     | .              | .       |
| c1*c3               | 5 tiny    | 1  | 6.714186   | 0.062475              | 4.199457       | 1.60    |
| c1*c3               | 5 small   | 1  | 1.565637   | 0.022165              | 3.182856       | 0.49    |
| c1*c3               | 5 average | 1  | -4.286085  | -0.068668             | 2.749142       | -1.56   |
| c1*c3               | 5 big     | 1  | -2.046468  | -0.045949             | 2.282735       | -0.90   |
| c1*c3               | 5 huge    | 0  | 0          | 0                     | .              | .       |
| c1*c3               | 6 tiny    | 1  | 5.135111   | 0.039052              | 4.754845       | 1.08    |
| c1*c3               | 6 small   | 1  | 4.442898   | 0.081945              | 3.079524       | 1.44    |
| c1*c3               | 6 average | 1  | -2.287870  | -0.056559             | 2.601384       | -0.88   |
| c1*c3               | 6 big     | 1  | 1.598086   | 0.043542              | 2.354326       | 0.68    |
| c1*c3               | 6 huge    | 0  | 0          | 0                     | .              | .       |
| c1*c3               | 7 tiny    | 1  | 1.108451   | 0.010314              | 4.267509       | 0.26    |



Output 45.2.8 continued

| Parameter Estimates |           |    |          |                       |                |         |
|---------------------|-----------|----|----------|-----------------------|----------------|---------|
| Parameter           |           | DF | Estimate | Standardized Estimate | Standard Error | t Value |
| c1*c3               | 7 small   | 1  | 7.441059 | 0.119214              | 3.135404       | 2.37    |
| c1*c3               | 7 average | 1  | 1.796483 | 0.038106              | 2.630570       | 0.68    |
| c1*c3               | 7 big     | 1  | 3.324160 | 0.095173              | 2.303369       | 1.44    |
| c1*c3               | 7 huge    | 0  | 0        | 0                     | .              | .       |
| c1*c3               | 8 tiny    | 0  | 0        | 0                     | .              | .       |
| c1*c3               | 8 small   | 0  | 0        | 0                     | .              | .       |
| c1*c3               | 8 average | 0  | 0        | 0                     | .              | .       |
| c1*c3               | 8 big     | 0  | 0        | 0                     | .              | .       |
| c1*c3               | 8 huge    | 0  | 0        | 0                     | .              | .       |
| x1                  |           | 1  | 2.713527 | 0.091530              | 0.836942       | 3.24    |
| x5                  |           | 1  | 2.810341 | 0.098303              | 0.816290       | 3.44    |
| x6                  |           | 1  | 4.837022 | 0.167394              | 0.810402       | 5.97    |
| x7                  |           | 1  | 5.844394 | 0.207035              | 0.793775       | 7.36    |
| x10                 |           | 1  | 2.463916 | 0.087712              | 0.794599       | 3.10    |
| x20                 |           | 1  | 4.385924 | 0.156155              | 0.787766       | 5.57    |

The magnitudes of the standardized estimates and the  $t$  statistics of the parameters of the effect 'c1' reveal that only levels '3' and '7' of this effect contribute appreciably to the model. This suggests that a more parsimonious model with similar or better predictive power might be obtained if parameters corresponding to the levels of 'c1' are allowed to enter or leave the model independently. You request this with the SPLIT option in the CLASS statement as shown in the following statements:

```
proc glmselect data=analysisData testdata=testData
 seed=1 plots(stepAxis=number)=all;
 partition fraction(validate=0.5);
 class c1(split) c2 c3(order=data);
 model y = c1|c2|c3|x1|x2|x3|x4|x5|x5|x6|x7|x8|x9|x10
 |x11|x12|x13|x14|x15|x16|x17|x18|x19|x20 @2
 / selection=stepwise(stop = validate
 select = s1)
 hierarchy=single;
 output out=outData;
run;
```

The “Class Level Information” and “Dimensions” tables are shown in Output 45.2.9. The “Dimensions” table shows that while the model statement specifies 278 effects, after splitting the parameters corresponding to the levels of c1, there are 439 split effects that are considered for entry or removal at each step of the selection process. Note that the total number of parameters considered is not affected by the split option.

**Output 45.2.9** Class Level Information and Problem Dimensions

```

The GLMSELECT Procedure

Class Level Information

Class Levels Values
c1 8 * 1 2 3 4 5 6 7 8
c2 4 0 1 2 3
c3 5 tiny small average big huge

* Associated Parameters Split

Dimensions

Number of Effects 278
Number of Effects after Splits 439
Number of Parameters 661

```

The stop reason and stop details tables are shown in [Output 45.2.10](#). Since the validation ASE is specified as the stopping criterion, the selection stops at step 11, where the validation ASE achieves a local minimum and the model at this step is the selected model.

**Output 45.2.10** Stop Details

```

Selection stopped at a local minimum of the residual sum of squares of the
validation data.

Stop Details

Candidate Candidate Compare
For Effect Validation ASE Validation ASE
Entry x18 25.9851 > 25.7462
Removal x6*x7 25.7611 > 25.7462

```

You find details of the selected model in [Output 45.2.11](#). The list of selected effects confirms that parameters corresponding to levels '3' and '7' only of c1 are in the selected model. Notice that the selected model with classification variable c1 split contains 18 parameters, whereas the selected model without splitting c1 has 45 parameters. Furthermore, by comparing the fit statistics in [Output 45.2.7](#) and [Output 45.2.11](#), you see that this more parsimonious model has smaller prediction errors on both the validation and test data.

**Output 45.2.11** Details of the Selected Model

| The GLMSELECT Procedure                                           |     |                |             |         |
|-------------------------------------------------------------------|-----|----------------|-------------|---------|
| Selected Model                                                    |     |                |             |         |
| The selected model is the model at the last step (Step 11).       |     |                |             |         |
| Effects: Intercept c1_3 c1_7 c3 c1_3*c3 x1 x5 x6 x7 x6*x7 x10 x20 |     |                |             |         |
| Analysis of Variance                                              |     |                |             |         |
| Source                                                            | DF  | Sum of Squares | Mean Square | F Value |
| Model                                                             | 17  | 22111          | 1300.63200  | 51.88   |
| Error                                                             | 492 | 12334          | 25.06998    |         |
| Corrected Total                                                   | 509 | 34445          |             |         |
| Root MSE                                                          |     | 5.00699        |             |         |
| Dependent Mean                                                    |     | 21.09705       |             |         |
| R-Square                                                          |     | 0.6419         |             |         |
| Adj R-Sq                                                          |     | 0.6295         |             |         |
| AIC                                                               |     | 2172.72685     |             |         |
| AICC                                                              |     | 2174.27787     |             |         |
| SBC                                                               |     | 1736.94624     |             |         |
| ASE (Train)                                                       |     | 24.18515       |             |         |
| ASE (Validate)                                                    |     | 25.74617       |             |         |
| ASE (Test)                                                        |     | 22.57297       |             |         |

When you use a **PARTITION** statement to subdivide the analysis data set, an output data set created with the **OUTPUT** statement contains a variable named `_ROLE_` that shows the role each observation was assigned to. See the section “**OUTPUT Statement**” on page 3555 and the section “**Using Validation and Test Data**” on page 3577 for additional details.

The following statements use **PROC PRINT** to produce **Output 45.2.12**, which shows the first five observations of the `outData` data set.

```
proc print data=outData(obs=5);
run;
```

## Output 45.2.12 Output Data Set with \_ROLE\_ Variable

| Obs | c3   | x1      | x2      | x3      | x4      | x5      | x6      | x7      | x8      |
|-----|------|---------|---------|---------|---------|---------|---------|---------|---------|
| 1   | tiny | 0.18496 | 0.97009 | 0.39982 | 0.25940 | 0.92160 | 0.96928 | 0.54298 | 0.53169 |
| 2   | tiny | 0.47579 | 0.84499 | 0.63452 | 0.59036 | 0.58258 | 0.37701 | 0.72836 | 0.50660 |
| 3   | tiny | 0.51132 | 0.43320 | 0.17611 | 0.66504 | 0.40482 | 0.12455 | 0.45349 | 0.19955 |
| 4   | tiny | 0.42071 | 0.07174 | 0.35849 | 0.71143 | 0.18985 | 0.14797 | 0.56184 | 0.27011 |
| 5   | tiny | 0.42137 | 0.03798 | 0.27081 | 0.42773 | 0.82010 | 0.84345 | 0.87691 | 0.26722 |

| Obs | x9      | x10     | x11     | x12     | x13     | x14     | x15     | x16     | x17     |
|-----|---------|---------|---------|---------|---------|---------|---------|---------|---------|
| 1   | 0.04979 | 0.06657 | 0.81932 | 0.52387 | 0.85339 | 0.06718 | 0.95702 | 0.29719 | 0.27261 |
| 2   | 0.93121 | 0.92912 | 0.58966 | 0.29722 | 0.39104 | 0.47243 | 0.67953 | 0.16809 | 0.16653 |
| 3   | 0.57484 | 0.73847 | 0.43981 | 0.04937 | 0.52238 | 0.34337 | 0.02271 | 0.71289 | 0.93706 |
| 4   | 0.32520 | 0.56918 | 0.04259 | 0.43921 | 0.91744 | 0.52584 | 0.73182 | 0.90522 | 0.57600 |
| 5   | 0.30602 | 0.39705 | 0.34905 | 0.76593 | 0.54340 | 0.61257 | 0.55291 | 0.73591 | 0.37186 |

| Obs | x18     | x19     | x20     | c1 | c2 | y       | _ROLE_   | p_y     |
|-----|---------|---------|---------|----|----|---------|----------|---------|
| 1   | 0.68993 | 0.97676 | 0.22651 | 2  | 1  | 11.4391 | VALIDATE | 18.5069 |
| 2   | 0.87110 | 0.29879 | 0.93464 | 3  | 1  | 31.4596 | TRAIN    | 26.2188 |
| 3   | 0.44599 | 0.94694 | 0.71290 | 4  | 3  | 16.4294 | VALIDATE | 17.0979 |
| 4   | 0.18794 | 0.33133 | 0.69887 | 5  | 3  | 15.4815 | VALIDATE | 16.1567 |
| 5   | 0.64565 | 0.55718 | 0.87504 | 6  | 2  | 26.0023 | TRAIN    | 24.6358 |

Cross validation is often used to assess the predictive performance of a model, especially for when you do not have enough observations for test set validation. See the section “[Cross Validation](#)” on page 3579 for further details. The following statements provide an example where cross validation is used as the `CHOOSE=` criterion.

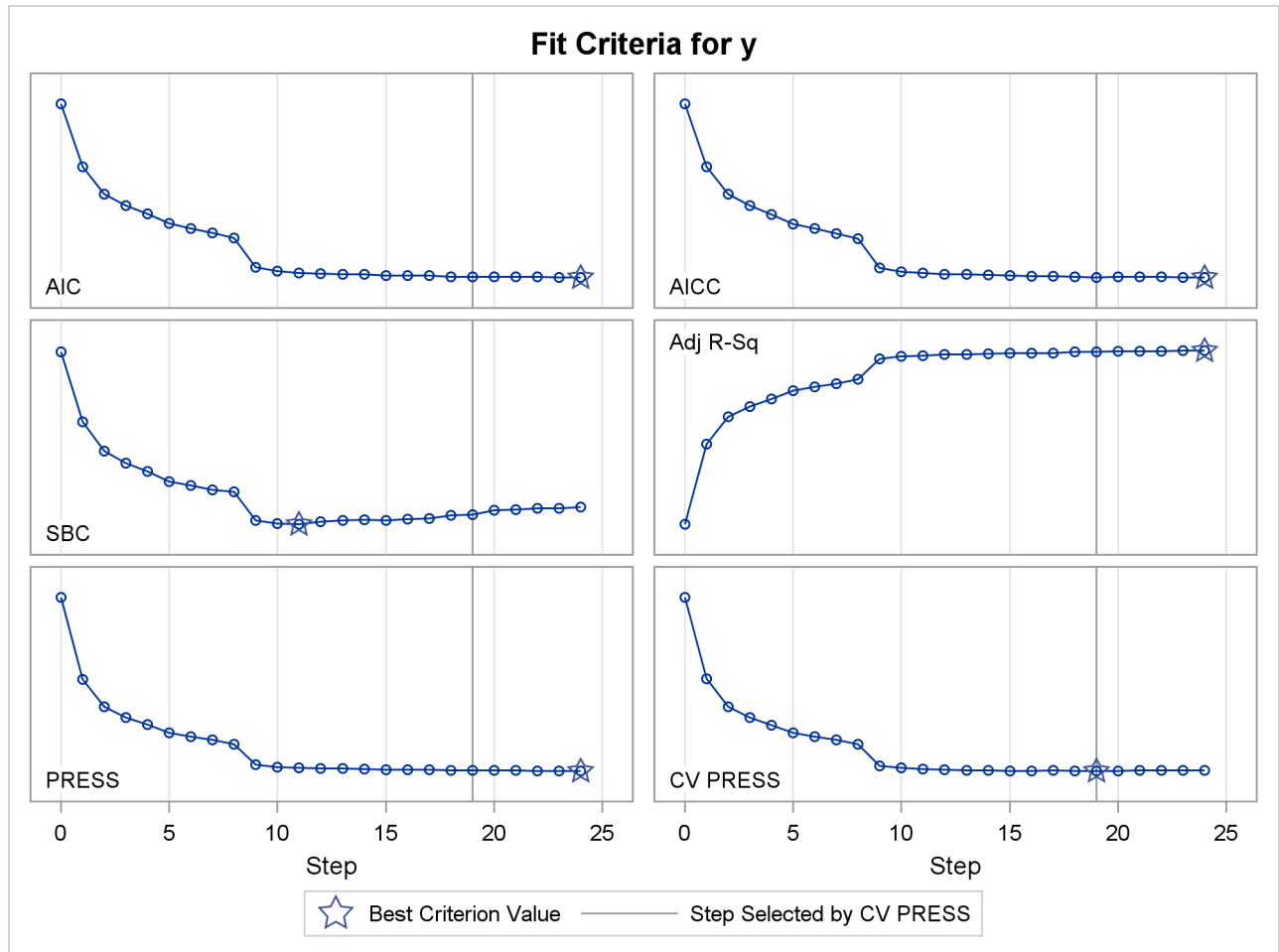
```
proc glmselect data=analysisData testdata=testData
 plots(stepAxis=number)=(criterionPanel ASEPlot);
 class c1(split) c2 c3(order=data);
 model y = c1|c2|c3|x1|x2|x3|x4|x5|x5|x6|x7|x8|x9|x10
 |x11|x12|x13|x14|x15|x16|x17|x18|x19|x20 @2
 / selection = stepwise(choose = cv
 select = s1)

 stats = press
 cvMethod = split(5)
 cvDetails = all
 hierarchy = single;
 output out=outData;
run;
```

The `CVMETHOD=SPLIT(5)` option in the `MODEL` statement requests five-fold cross validation with the five subsets consisting of observations  $\{1, 6, 11, \dots\}$ ,  $\{2, 7, 12, \dots\}$ , and so on. The `STATS=PRESS` option requests that the leave-one-out cross validation predicted residual sum of squares (PRESS) also be computed and displayed at each step, even though this statistic is not used in the selection process.

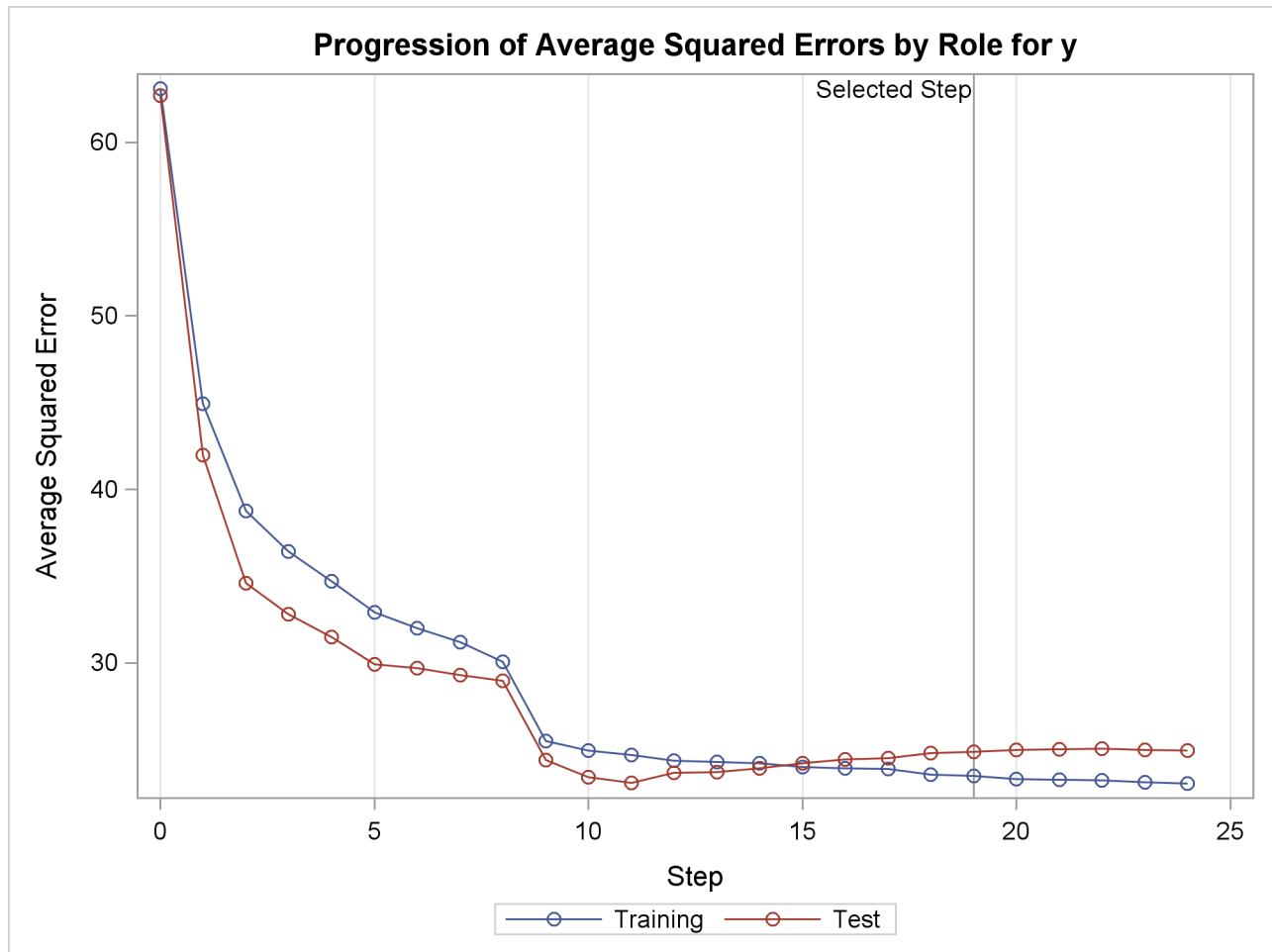
Output 45.2.13 shows how several fit statistics evolved as the selection process progressed. The five-fold CV PRESS statistic achieves its minimum at step 19. Note that this gives a larger model than was selected when the stopping criterion was determined using validation data. Furthermore, you see that the PRESS statistic has not achieved its minimum within 25 steps, so an even larger model would have been selected based on leave-one-out cross validation.

**Output 45.2.13** Criterion Panel



Output 45.2.14 shows how the average squared error compares on the test and training data. Note that the ASE error on the test data achieves a local minimum at step 11 and is already slowly increasing at step 19, which corresponds to the selected model.

Output 45.2.14 Average Squared Error Plot



The `CVDETAILS=ALL` option in the `MODEL` statement requests the “Cross Validation Details” table in [Output 45.2.15](#) and the cross validation parameter estimates that are included in the “Parameter Estimates” table in [Output 45.2.16](#). For each cross validation index, the predicted residual sum of squares on the observations omitted is shown in the “Cross Validation Details” table and the parameter estimates of the corresponding model are included in the “Parameter Estimates” table. By default, these details are shown for the selected model, but you can request this information at every step with the `DETAILS=` option in the `MODEL` statement. You use the `_CVINDEX_` variable in the output data set shown in [Output 45.2.17](#) to find out which observations in the analysis data are omitted for each cross validation fold.

**Output 45.2.15** Breakdown of CV Press Statistic by Fold

| Cross Validation Details |                    |          |            |
|--------------------------|--------------------|----------|------------|
| Index                    | ---Observations--- |          | CV PRESS   |
|                          | Fitted             | Left Out |            |
| 1                        | 808                | 202      | 5059.7375  |
| 2                        | 808                | 202      | 4278.9115  |
| 3                        | 808                | 202      | 5598.0354  |
| 4                        | 808                | 202      | 4950.1750  |
| 5                        | 808                | 202      | 5528.1846  |
| -----                    |                    |          |            |
| Total                    |                    |          | 25293.5024 |

**Output 45.2.16** Cross Validation Parameter Estimates

| Parameter Estimates |                                      |          |          |          |          |
|---------------------|--------------------------------------|----------|----------|----------|----------|
| Parameter           | -----Cross Validation Estimates----- |          |          |          |          |
|                     | 1                                    | 2        | 3        | 4        | 5        |
| Intercept           | 10.7617                              | 10.1200  | 9.0254   | 13.4164  | 12.3352  |
| c1_3                | 28.2715                              | 27.2977  | 27.0696  | 28.6835  | 27.8070  |
| c1_7                | 7.6530                               | 7.6445   | 7.9257   | 7.4217   | 7.6862   |
| c3 tiny             | -3.1103                              | -4.4041  | -5.1793  | -8.4131  | -7.2096  |
| c3 small            | 2.2039                               | 1.5447   | 1.0121   | -0.3998  | 1.4927   |
| c3 average          | 0.3021                               | -1.3939  | -1.2201  | -3.3407  | -2.1467  |
| c3 big              | -0.9621                              | -1.2439  | -1.6092  | -3.7666  | -3.4389  |
| c3 huge             | 0                                    | 0        | 0        | 0        | 0        |
| c1_3*c3 tiny        | -21.9104                             | -21.7840 | -22.0173 | -22.6066 | -21.9791 |
| c1_3*c3 small       | -20.8196                             | -20.2725 | -19.5850 | -20.4515 | -20.7586 |
| c1_3*c3 average     | -16.8500                             | -15.1509 | -15.0134 | -15.3851 | -13.4339 |
| c1_3*c3 big         | -12.7212                             | -12.1554 | -12.0354 | -12.3282 | -13.0174 |
| c1_3*c3 huge        | 0                                    | 0        | 0        | 0        | 0        |
| x1                  | 0.9238                               | 1.7286   | 2.5976   | -0.2488  | 1.2093   |
| x1*c3 tiny          | -1.5819                              | -1.1748  | -3.2523  | -1.7016  | -2.7624  |
| x1*c3 small         | -3.7669                              | -3.2984  | -2.9755  | -1.8738  | -4.0167  |
| x1*c3 average       | 2.2253                               | 2.4489   | 1.5675   | 4.0948   | 2.0159   |
| x1*c3 big           | 0.9222                               | 0.5330   | 0.7960   | 2.6061   | 1.2694   |
| x1*c3 huge          | 0                                    | 0        | 0        | 0        | 0        |
| x5                  | -1.3562                              | 0.5639   | 0.3022   | -0.4700  | -2.5063  |
| x6                  | -0.9165                              | -3.2944  | -1.2163  | -2.2063  | -0.5696  |
| x7                  | 5.2295                               | 5.3015   | 6.2526   | 4.1770   | 5.8364   |
| x6*x7               | 6.4211                               | 7.5644   | 6.1182   | 7.0020   | 5.8730   |
| x10                 | 1.9591                               | 1.4932   | 0.7196   | 0.6504   | -0.3989  |
| x5*x10              | 3.6058                               | 1.7274   | 4.3447   | 2.4388   | 3.8967   |
| x15                 | -0.0079                              | 0.6896   | 1.6811   | 0.0136   | 0.1799   |
| x15*c1_3            | -3.5022                              | -2.7963  | -2.6003  | -4.2355  | -4.7546  |
| x7*x15              | -5.1438                              | -5.8878  | -5.9465  | -3.6155  | -5.3337  |
| x18                 | -2.1347                              | -1.5656  | -2.4226  | -4.0592  | -1.4985  |
| x18*c3 tiny         | 2.2988                               | 1.1931   | 2.6491   | 6.1615   | 5.6204   |
| x18*c3 small        | 4.6033                               | 3.2359   | 4.4183   | 5.5923   | 1.7270   |
| x18*c3 average      | -2.3712                              | -2.5392  | -0.6361  | -1.1729  | -1.6481  |
| x18*c3 big          | 2.3160                               | 1.4654   | 2.7683   | 3.0487   | 2.5768   |
| x18*c3 huge         | 0                                    | 0        | 0        | 0        | 0        |
| x6*x18              | 3.0716                               | 4.2036   | 4.1354   | 4.9196   | 2.7165   |
| x20                 | 4.1229                               | 4.5773   | 4.5774   | 4.6555   | 4.2655   |

The following statements display the first eight observations in the outData data set.

```
proc print data=outData(obs=8);
run;
```



**Output 45.2.17** First Eight Observations in the Output Data Set

| Obs | c3   | x1      | x2      | x3      | x4      | x5      | x6      | x7      | x8      |
|-----|------|---------|---------|---------|---------|---------|---------|---------|---------|
| 1   | tiny | 0.18496 | 0.97009 | 0.39982 | 0.25940 | 0.92160 | 0.96928 | 0.54298 | 0.53169 |
| 2   | tiny | 0.47579 | 0.84499 | 0.63452 | 0.59036 | 0.58258 | 0.37701 | 0.72836 | 0.50660 |
| 3   | tiny | 0.51132 | 0.43320 | 0.17611 | 0.66504 | 0.40482 | 0.12455 | 0.45349 | 0.19955 |
| 4   | tiny | 0.42071 | 0.07174 | 0.35849 | 0.71143 | 0.18985 | 0.14797 | 0.56184 | 0.27011 |
| 5   | tiny | 0.42137 | 0.03798 | 0.27081 | 0.42773 | 0.82010 | 0.84345 | 0.87691 | 0.26722 |
| 6   | tiny | 0.81722 | 0.65822 | 0.02947 | 0.85339 | 0.36285 | 0.37732 | 0.51054 | 0.71194 |
| 7   | tiny | 0.19480 | 0.81673 | 0.08548 | 0.18376 | 0.33264 | 0.70558 | 0.92761 | 0.29642 |
| 8   | tiny | 0.04403 | 0.51697 | 0.68884 | 0.45333 | 0.83565 | 0.29745 | 0.40325 | 0.95684 |

| Obs | x9      | x10     | x11     | x12     | x13     | x14     | x15     | x16     | x17     |
|-----|---------|---------|---------|---------|---------|---------|---------|---------|---------|
| 1   | 0.04979 | 0.06657 | 0.81932 | 0.52387 | 0.85339 | 0.06718 | 0.95702 | 0.29719 | 0.27261 |
| 2   | 0.93121 | 0.92912 | 0.58966 | 0.29722 | 0.39104 | 0.47243 | 0.67953 | 0.16809 | 0.16653 |
| 3   | 0.57484 | 0.73847 | 0.43981 | 0.04937 | 0.52238 | 0.34337 | 0.02271 | 0.71289 | 0.93706 |
| 4   | 0.32520 | 0.56918 | 0.04259 | 0.43921 | 0.91744 | 0.52584 | 0.73182 | 0.90522 | 0.57600 |
| 5   | 0.30602 | 0.39705 | 0.34905 | 0.76593 | 0.54340 | 0.61257 | 0.55291 | 0.73591 | 0.37186 |
| 6   | 0.37533 | 0.22954 | 0.68621 | 0.55243 | 0.58182 | 0.17472 | 0.04610 | 0.64380 | 0.64545 |
| 7   | 0.22404 | 0.14719 | 0.59064 | 0.46326 | 0.41860 | 0.25631 | 0.23045 | 0.08034 | 0.43559 |
| 8   | 0.42194 | 0.78079 | 0.33106 | 0.17210 | 0.91056 | 0.26897 | 0.95602 | 0.13720 | 0.27190 |

| Obs | x18     | x19     | x20     | c1 | c2 | y       | _CVINDEX_ | p_y     |
|-----|---------|---------|---------|----|----|---------|-----------|---------|
| 1   | 0.68993 | 0.97676 | 0.22651 | 2  | 1  | 11.4391 | 1         | 18.1474 |
| 2   | 0.87110 | 0.29879 | 0.93464 | 3  | 1  | 31.4596 | 2         | 24.7930 |
| 3   | 0.44599 | 0.94694 | 0.71290 | 4  | 3  | 16.4294 | 3         | 16.5752 |
| 4   | 0.18794 | 0.33133 | 0.69887 | 5  | 3  | 15.4815 | 4         | 14.7605 |
| 5   | 0.64565 | 0.55718 | 0.87504 | 6  | 2  | 26.0023 | 5         | 24.7479 |
| 6   | 0.09317 | 0.62008 | 0.07845 | 7  | 1  | 16.6503 | 1         | 21.4444 |
| 7   | 0.67020 | 0.42272 | 0.49827 | 1  | 1  | 14.0342 | 2         | 20.9661 |
| 8   | 0.55692 | 0.65825 | 0.68465 | 2  | 3  | 14.9830 | 3         | 17.5644 |

This example demonstrates the usefulness of effect selection when you suspect that interactions of effects are needed to explain the variation in your dependent variable. Ideally, a priori knowledge should be used to decide what interactions to allow, but in some cases this information might not be available. Simply fitting a least squares model allowing all interactions produces a model that overfits your data and generalizes very poorly.

The following statements use forward selection with selection based on the SBC criterion, which is the default selection criterion. At each step, the effect whose addition to the model yields the smallest SBC value is added. The `STOP=NONE` suboption specifies that this process continue even when the SBC statistic grows whenever an effect is added, and so it terminates at a full least squares model. The `BUILDSSCP=FULL` option is specified in a `PERFORMANCE` statement, since building the SSCP matrix incrementally is counterproductive in this case. See the section “`BUILDSSCP=FULL`” on page 3557 for details. Note that if all you are interested in is a full least squares model, then it is much more efficient to simply specify `SELECTION=NONE` in the `MODEL` statement. However, in this example the aim is to add effects in roughly increasing order of explanatory power.

```

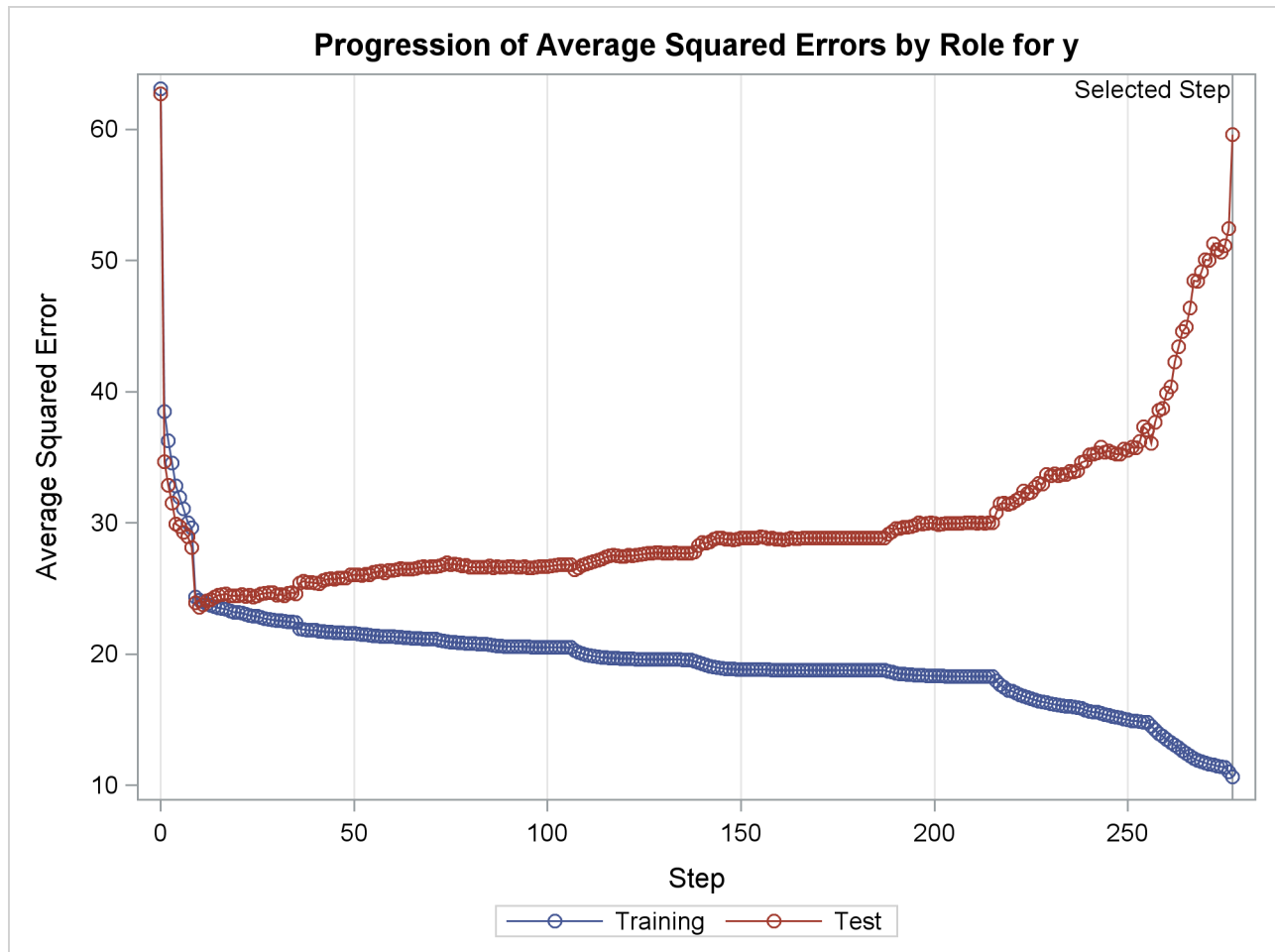
proc glmselect data=analysisData testdata=testData plots=ASEPlot;
 class c1 c2 c3(order=data);
 model y = c1|c2|c3|x1|x2|x3|x4|x5|x5|x6|x7|x8|x9|x10
 |x11|x12|x13|x14|x15|x16|x17|x18|x19|x20 @2
 / selection=forward(stop=none)
 hierarchy=single;
 performance buildSSCP = full;
run;

ods graphics off;

```

The ASE plot shown in [Output 45.2.18](#) clearly demonstrates the danger in overfitting the training data. As more insignificant effects are added to the model, the growth in test set ASE shows how the predictions produced by the resulting models worsen. This decline is particularly rapid in the latter stages of the forward selection, because the use of the SBC criterion results in insignificant effects with lots of parameters being added after insignificant effects with fewer parameters.

**Output 45.2.18** Average Squared Error Plot



### Example 45.3: Scatter Plot Smoothing by Selecting Spline Functions

This example shows how you can use model selection to perform scatter plot smoothing. It illustrates how you can use the experimental EFFECT statement to generate a large collection of B-spline basis functions from which a subset is selected to fit scatter plot data.

The data for this example come from a set of benchmarks developed by Donoho and Johnstone (1994) that have become popular in the statistics literature. The particular benchmark used is the “Bumps” functions to which random noise has been added to create the test data. The following DATA step, extracted from Sarle (2001), creates the data. The constants are chosen so that the noise-free data have a standard deviation of 7. The standard deviation of the noise is  $\sqrt{5}$ , yielding bumpsNoise with a signal-to-noise ratio of 3.13 ( $7/\sqrt{5}$ ).

```
%let random=12345;

data DoJoBumps;
 keep x bumps bumpsWithNoise;

 pi = arcos(-1);

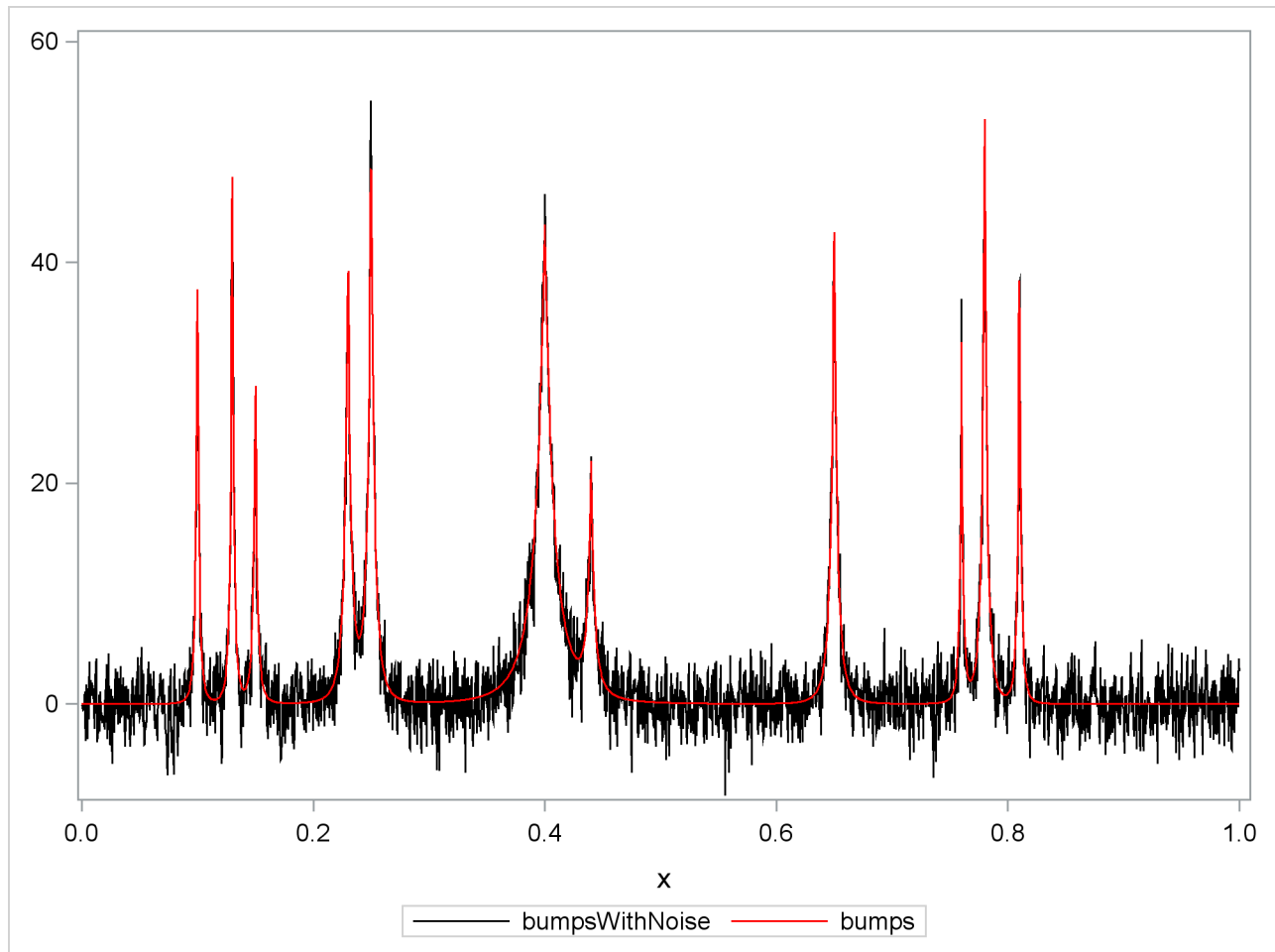
 do n=1 to 2048;
 x=(2*n-1)/4096;
 link compute;
 bumpsWithNoise=bumps+rannor(&random)*sqrt(5);
 output;
 end;
stop;

compute:
 array t(11) _temporary_ (.1 .13 .15 .23 .25 .4 .44 .65 .76 .78 .81);
 array b(11) _temporary_ (4 5 3 4 5 4.2 2.1 4.3 3.1 5.1 4.2);
 array w(11) _temporary_ (.005 .005 .006 .01 .01 .03 .01 .01 .005 .008 .005);

 bumps=0;
 do i=1 to 11;
 bumps=bumps+b[i]*(1+abs((x-t[i])/w[i]))**4;
 end;
 bumps=bumps*10.528514619;
 return;
run;
```

The following statements use the SGPLOT procedure to produce the plot in [Output 45.3.1](#). The plot shows the bumps function superimposed on the function with added noise.

```
proc sgplot data=DoJoBumps;
 yaxis display=(nolabel);
 series x=x y=bumpsWithNoise/lineattrs=(color=black);
 series x=x y=bumps/lineattrs=(color=red);
run;
```

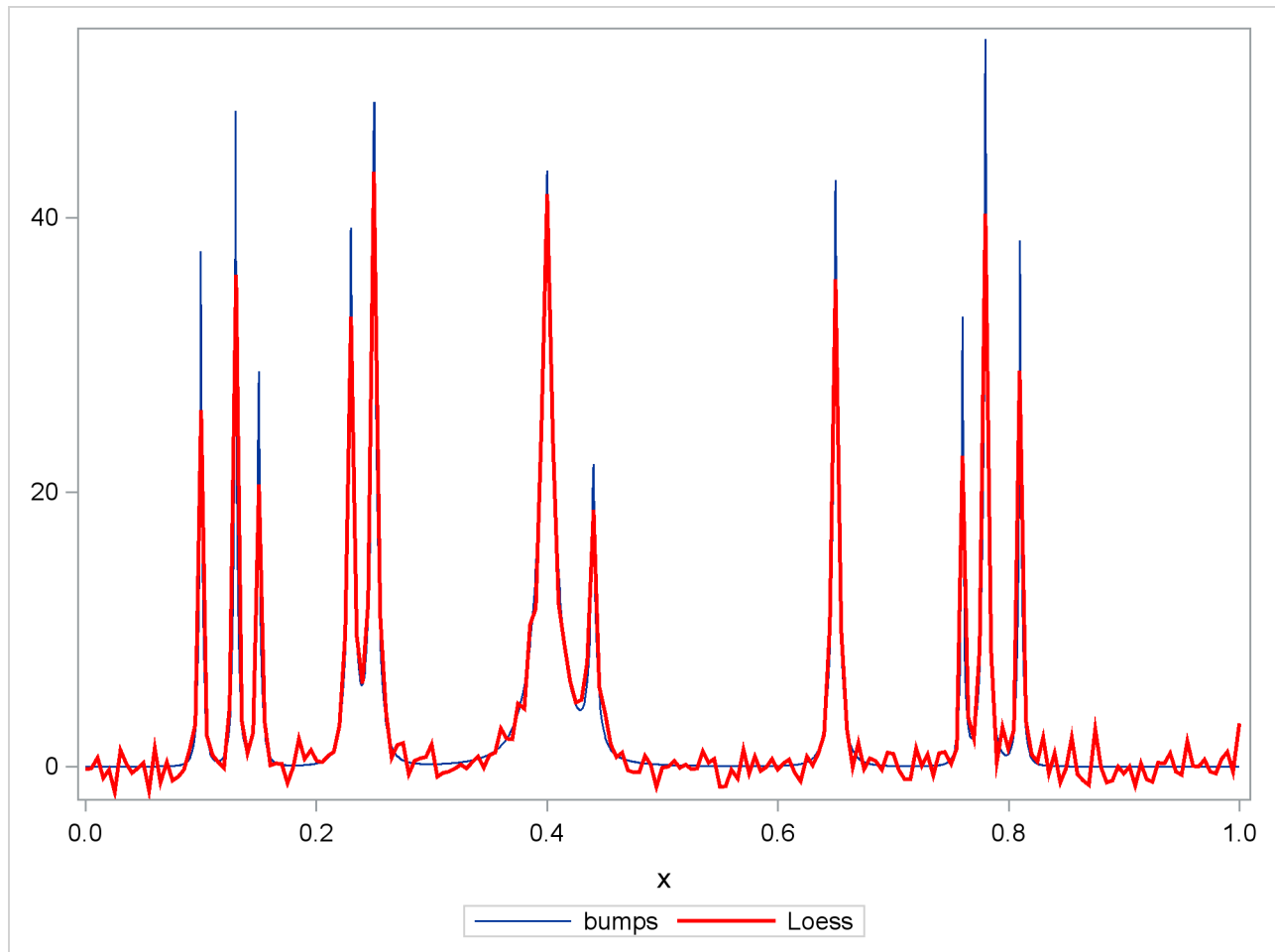
**Output 45.3.1** Donoho-Johnstone Bumps Function

Suppose you want to smooth the noisy data to recover the underlying function. This problem is studied by Sarle (2001), who shows how neural nets can be used to perform the smoothing. The following statements use the LOESS statement in the SGPLOT procedure to show a loess fit superimposed on the noisy data (Output 45.3.2). (See Chapter 53, “The LOESS Procedure,” for information about the loess method.)

```
proc sgplot data=DoJoBumps;
 yaxis display=(nolabel);
 series x=x y=bumps;
 loess x=x y=bumpsWithNoise / lineattrs=(color=red) nomarkers;
run;
```

The algorithm selects a smoothing parameter that is small enough to enable bumps to be resolved. Because there is a single smoothing parameter that controls the number of points for all local fits, the loess method undersmooths the function in the intervals between the bumps.

Output 45.3.2 Loess Fit



Another approach to doing nonparametric fitting is to approximate the unknown underlying function as a linear combination of a set of basis functions. Once you specify the basis functions, then you can use least squares regression to obtain the coefficients of the linear combination. A problem with this approach is that for most data, you do not know a priori what set of basis functions to use. You need to supply a sufficiently rich set to enable the features in the data to be approximated. However, if you use too rich a set of functions, then this approach yields a fit that undersmooths the data and captures spurious features in the noise.

The penalized B-spline method (Eilers and Marx 1996) uses a basis of B-splines (see the section “**EFFECT Statement**” on page 393 of Chapter 19, “**Shared Concepts and Topics**”) corresponding to a large number of equally spaced knots as the set of approximating functions. To control the potential overfitting, their algorithm modifies the least squares objective function to include a penalty term that grows with the complexity of the fit.

The following statements use the PBSPLINE statement in the SGPLOT procedure to show a penalized B-spline fit superimposed on the noisy data (Output 45.3.3). See Chapter 97, “**The TRANSREG Procedure**,” for details about the implementation of the penalized B-spline method.

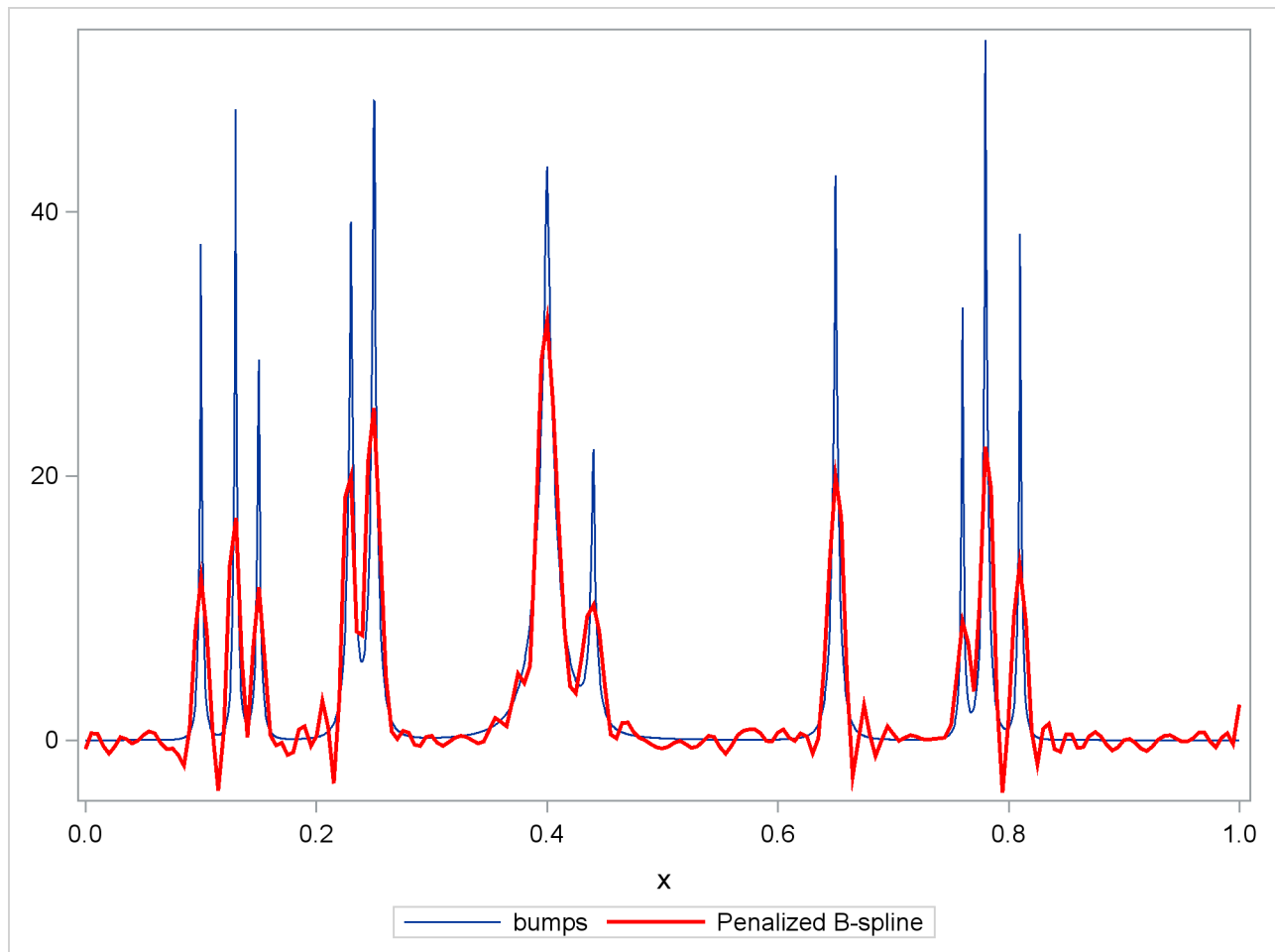
```

proc sgplot data=DoJoBumps;
 yaxis display=(nolabel);
 series x=x y=bumps;
 pbspline x=x y=bumpsWithNoise /
 lineattrs=(color=red) nomarkers;
run;

```

As in the case of loess fitting, you see undersmoothing in the intervals between the bumps because there is only a single smoothing parameter that controls the overall smoothness of the fit.

### Output 45.3.3 Penalized B-spline Fit



An alternative to using a smoothness penalty to control the overfitting is to use variable selection to obtain an appropriate subset of the basis functions. In order to be able to represent features in the data that occur at multiple scales, it is useful to select from B-spline functions defined on just a few knots to capture large scale features of the data as well as B-spline functions defined on many knots to capture fine details of the data. The following statements show how you can use PROC GLMSELECT to implement this strategy:

```

proc glmselect data=dojoBumps;
 effect spl = spline(x / knotmethod=multiscale(endscale=8)
 split details);
 model bumpsWithNoise=spl;
 output out=out1 p=pBumps;
run;

proc sgplot data=out1;
 yaxis display=(nolabel);
 series x=x y=bumps;
 series x=x y=pBumps / lineattrs=(color=red);
run;

```

The `KNOTMETHOD=MULTISCALE` suboption of the `EFFECT spl = SPLINE` statement provides a convenient way to generate B-spline basis functions at multiple scales. The `ENDSCALE=8` option requests that the finest scale use B-splines defined on  $2^8$  equally spaced knots in the interval  $[0, 1]$ . Because the cubic B-splines are nonzero over five adjacent knots, at the finest scale, the support of each B-spline basis function is an interval of length about 0.02 ( $5/256$ ), enabling the bumps in the underlying data to be resolved. The default value is `ENDSCALE=7`. At this scale you will still be able to capture the bumps, but with less sharp resolution. For these data, using a value of `ENDSCALE=` greater than eight provides unneeded resolution, making it more likely that basis functions that fit spurious features in the noise are selected.

[Output 45.3.4](#) shows the model information table. Since no options are specified in the `MODEL` statement, `PROC GLMSELECT` uses the stepwise method with selection and stopping based on the SBC criterion.

#### Output 45.3.4 Model Settings

| The GLMSELECT Procedure   |                |
|---------------------------|----------------|
| Data Set                  | WORK.DOJOBUMPS |
| Dependent Variable        | bumpsWithNoise |
| Selection Method          | Stepwise       |
| Select Criterion          | SBC            |
| Stop Criterion            | SBC            |
| Effect Hierarchy Enforced | None           |

The `DETAILS` suboption in the `EFFECT` statement requests the display of spline knots and spline basis tables. These tables contain information about knots and basis functions at all scales. The results for scale four are shown in [Output 45.3.5](#) and [Output 45.3.6](#).

**Output 45.3.5** Spline Knots

| Knots for Spline Effect spl |       |                         |          |            |
|-----------------------------|-------|-------------------------|----------|------------|
| Knot<br>Number              | Scale | Scale<br>Knot<br>Number | Boundary | x          |
| 40                          | 4     | 1                       | *        | -0.11735   |
| 41                          | 4     | 2                       | *        | -0.05855   |
| 42                          | 4     | 3                       | *        | 0.00024414 |
| 43                          | 4     | 4                       |          | 0.05904    |
| 44                          | 4     | 5                       |          | 0.11783    |
| 45                          | 4     | 6                       |          | 0.17663    |
| 46                          | 4     | 7                       |          | 0.23542    |
| 47                          | 4     | 8                       |          | 0.29422    |
| 48                          | 4     | 9                       |          | 0.35301    |
| 49                          | 4     | 10                      |          | 0.41181    |
| 50                          | 4     | 11                      |          | 0.47060    |
| 51                          | 4     | 12                      |          | 0.52940    |
| 52                          | 4     | 13                      |          | 0.58819    |
| 53                          | 4     | 14                      |          | 0.64699    |
| 54                          | 4     | 15                      |          | 0.70578    |
| 55                          | 4     | 16                      |          | 0.76458    |
| 56                          | 4     | 17                      |          | 0.82337    |
| 57                          | 4     | 18                      |          | 0.88217    |
| 58                          | 4     | 19                      |          | 0.94096    |
| 59                          | 4     | 20                      | *        | 0.99976    |
| 60                          | 4     | 21                      | *        | 1.05855    |
| 61                          | 4     | 22                      | *        | 1.11735    |



**Output 45.3.6** Spline Details

| Basis Details for Spline Effect spl |       |        |                   |         |               |
|-------------------------------------|-------|--------|-------------------|---------|---------------|
| Column                              | Scale | Column | -----Support----- |         | Support Knots |
| 32                                  | 4     | 1      | -0.11735          | 0.05904 | 1-4           |
| 33                                  | 4     | 2      | -0.11735          | 0.11783 | 1-5           |
| 34                                  | 4     | 3      | -0.05855          | 0.17663 | 2-6           |
| 35                                  | 4     | 4      | 0.00024414        | 0.23542 | 3-7           |
| 36                                  | 4     | 5      | 0.05904           | 0.29422 | 4-8           |
| 37                                  | 4     | 6      | 0.11783           | 0.35301 | 5-9           |
| 38                                  | 4     | 7      | 0.17663           | 0.41181 | 6-10          |
| 39                                  | 4     | 8      | 0.23542           | 0.47060 | 7-11          |
| 40                                  | 4     | 9      | 0.29422           | 0.52940 | 8-12          |
| 41                                  | 4     | 10     | 0.35301           | 0.58819 | 9-13          |
| 42                                  | 4     | 11     | 0.41181           | 0.64699 | 10-14         |
| 43                                  | 4     | 12     | 0.47060           | 0.70578 | 11-15         |
| 44                                  | 4     | 13     | 0.52940           | 0.76458 | 12-16         |
| 45                                  | 4     | 14     | 0.58819           | 0.82337 | 13-17         |
| 46                                  | 4     | 15     | 0.64699           | 0.88217 | 14-18         |
| 47                                  | 4     | 16     | 0.70578           | 0.94096 | 15-19         |
| 48                                  | 4     | 17     | 0.76458           | 0.99976 | 16-20         |
| 49                                  | 4     | 18     | 0.82337           | 1.05855 | 17-21         |
| 50                                  | 4     | 19     | 0.88217           | 1.11735 | 18-22         |
| 51                                  | 4     | 20     | 0.94096           | 1.11735 | 19-22         |

The Dimensions table in [Output 45.3.7](#) shows that at each step of the selection process, 548 effects are considered as candidates for entry or removal. Note that although the MODEL statement specifies a single constructed effect spl, the SPLIT suboption causes each of the parameters in this constructed effect to be treated as an individual effect.

**Output 45.3.7** Dimensions

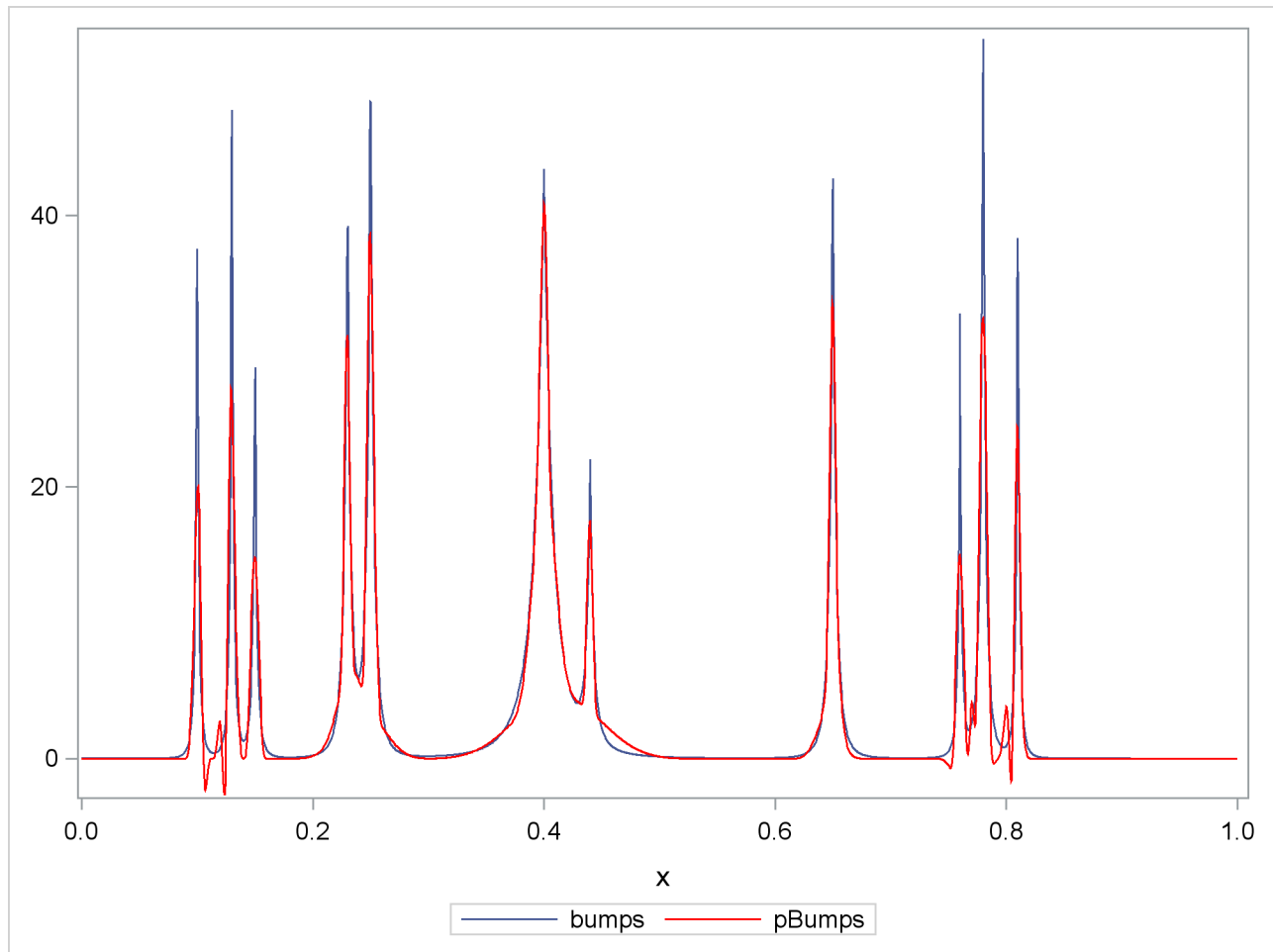
| Dimensions           |     |
|----------------------|-----|
| Number of Effects    | 548 |
| Number of Parameters | 548 |

[Output 45.3.8](#) shows the parameter estimates for the selected model. You can see that the selected model contains 31 B-spline basis functions and that all the selected B-spline basis functions are from scales four through eight. For example, the first basis function listed in the parameter estimates table is spl\_S4:9—the ninth B-spline function at scale 4. You see from [Output 45.3.6](#) that this function is nonzero on the interval (0.29, 0.52).

**Output 45.3.8** Parameter Estimates

| Parameter Estimates |    |            |                |         |
|---------------------|----|------------|----------------|---------|
| Parameter           | DF | Estimate   | Standard Error | t Value |
| Intercept           | 1  | -0.009039  | 0.077412       | -0.12   |
| spl_S4:9            | 1  | 7.070207   | 0.586990       | 12.04   |
| spl_S5:10           | 1  | 5.323121   | 1.199824       | 4.44    |
| spl_S6:17           | 1  | 5.222808   | 1.728910       | 3.02    |
| spl_S6:28           | 1  | 24.562103  | 1.490639       | 16.48   |
| spl_S6:44           | 1  | 4.930829   | 1.243552       | 3.97    |
| spl_S6:52           | 1  | -7.046308  | 2.487700       | -2.83   |
| spl_S7:86           | 1  | 9.592742   | 2.626471       | 3.65    |
| spl_S7:106          | 1  | 16.268550  | 3.334015       | 4.88    |
| spl_S8:27           | 1  | 10.626586  | 1.752152       | 6.06    |
| spl_S8:28           | 1  | 27.882444  | 2.004520       | 13.91   |
| spl_S8:29           | 1  | -6.129939  | 1.752151       | -3.50   |
| spl_S8:33           | 1  | 5.855648   | 1.766912       | 3.31    |
| spl_S8:34           | 1  | -11.782303 | 2.092484       | -5.63   |
| spl_S8:35           | 1  | 38.705178  | 2.092486       | 18.50   |
| spl_S8:36           | 1  | 13.823256  | 1.766916       | 7.82    |
| spl_S8:40           | 1  | 15.975124  | 1.691679       | 9.44    |
| spl_S8:41           | 1  | 14.898716  | 1.691679       | 8.81    |
| spl_S8:61           | 1  | 37.441965  | 2.084375       | 17.96   |
| spl_S8:66           | 1  | 47.484506  | 1.883409       | 25.21   |
| spl_S8:67           | 1  | 16.811502  | 1.910358       | 8.80    |
| spl_S8:104          | 1  | 11.098484  | 1.958676       | 5.67    |
| spl_S8:105          | 1  | 26.704556  | 2.042735       | 13.07   |
| spl_S8:115          | 1  | 21.102920  | 1.576185       | 13.39   |
| spl_S8:169          | 1  | 36.572294  | 2.914521       | 12.55   |
| spl_S8:197          | 1  | 20.869716  | 1.882529       | 11.09   |
| spl_S8:198          | 1  | 16.210987  | 2.693183       | 6.02    |
| spl_S8:200          | 1  | 13.113942  | 3.458187       | 3.79    |
| spl_S8:202          | 1  | 38.463549  | 2.462314       | 15.62   |
| spl_S8:203          | 1  | 34.164644  | 1.757908       | 19.43   |
| spl_S8:209          | 1  | -22.645471 | 3.598587       | -6.29   |
| spl_S8:210          | 1  | 29.024741  | 2.557567       | 11.35   |

The OUTPUT statement captures the predicted values in a data set named out1, and [Output 45.3.9](#) shows a fit plot produced by PROC SGPLOT.

**Output 45.3.9** Fit by Selecting B-splines

### Example 45.4: Multimember Effects and the Design Matrix

This example shows how you can use multimember effects to build predictive models. It also demonstrates several features of the OUTDESIGN= option in the PROC GLMSELECT statement.

The simulated data for this example describe a two-week summer tennis camp. The tennis ability of each camper was assessed and ratings were assigned at the beginning and end of the camp. The camp consisted of supervised group instruction in the mornings with a number of different options in the afternoons. Campers could elect to participate in unsupervised practice and play. Some campers paid for one or more individual lessons from 30 to 90 minutes in length, focusing on forehand and backhand strokes and volleying. The aim of this example is to build a predictive model for the rating improvement of each camper based on the times the camper spent doing each activity and several other variables, including the age, gender, and initial rating of the camper.

The following statements produce the TennisCamp data set:

```

data TennisCamp;
 length forehandCoach $6 backhandCoach $6 volleyCoach $6 gender $1;
 input forehandCoach backhandCoach volleyCoach tLessons tPractice tPlay
 gender inRating nPastCamps age tForehand tBackhand tVolley
 improvement;
 label forehandCoach = "Forehand lesson coach"
 backhandCoach = "Backhand lesson coach"
 volleyCoach = "Volley lesson coach"
 tForehand = "time (1/2 hours) of forehand lesson"
 tBackhand = "time (1/2 hours) of backhand lesson"
 tVolley = "time (1/2 hours) of volley lesson"
 tLessons = "time (1/2 hours) of all lessons"
 tPractice = "total practice time (hours)"
 tPlay = "total play time (hours)"
 nPastCamps = "Number of previous camps attended"
 age = "age (years)"
 inRating = "Rating at camp start"
 improvement = "Rating improvement at end of camp";
 datalines;
. . Tom 1 30 19 f 44 0 13 0 0 1 6
Greg . . 2 12 33 f 48 2 15 2 0 0 14
. . Mike 2 12 24 m 53 0 15 0 0 2 13
. Mike . 1 12 28 f 48 0 13 0 1 0 11
. Bruna . 2 13 34 f 57 0 16 0 2 0 12

... more lines ...

. . . 0 12 38 m 47 1 15 0 0 0 8
Greg Tom Tom 6 3 41 m 48 2 15 2 1 3 19
. Greg Mike 5 30 16 m 52 0 13 0 2 3 18
;

```

A multimember effect (see the section “EFFECT Statement” on page 393 of Chapter 19, “Shared Concepts and Topics”) is appropriate for modeling the effect of coaches on the campers’ improvement, because campers might have worked with multiple coaches. Furthermore, since the time a coach spent with each camper varies, it is appropriate to use these times to weight each coach’s contribution in the multimember effect. It is also important not to exclude campers from the analysis if they did not receive any individual instruction. You can accomplish all these goals by using a multimember effect defined as follows:

```

class forehandCoach backhandCoach volleyCoach;
effect coach = MM(forehandCoach backhandCoach volleyCoach/ noeffect
 weight=(tForehand tBackhand tVolley));

```

Based on similar previous studies, it is known that the time spent practicing should not be included linearly, because there are diminishing returns and perhaps even counterproductive effects beyond about 25 hours. A spline effect with a single knot at 25 provides flexibility in modeling effect of practice time.

The following statements use PROC GLMSELECT to select effects for the model.

```
proc glmselect data=TennisCamp outdesign=designCamp;
 class forehandCoach backhandCoach volleyCoach gender;

 effect coach = mm(forehandCoach backhandCoach volleyCoach / noeffect
 details weight=(tForehand tBackhand tVolley));
 effect practice = spline(tPractice/knotmethod=list(25) details);

 model improvement = coach practice tLessons tPlay age gender
 inRating nPastCamps;

run;
```

Output 45.4.1 shows the class level and MM level information. The levels of the constructed MM effect are the union of the levels of its constituent classification variables. The MM level information is not displayed by default—you request this table by specifying the DETAILS suboption in the relevant **EFFECT** statement.

**Output 45.4.1** Levels of MM EFFECT Coach

| The GLMSELECT Procedure |        |                            |
|-------------------------|--------|----------------------------|
| Class Level Information |        |                            |
| Class                   | Levels | Values                     |
| forehandCoach           | 5      | Bruna Elaine Greg Mike Tom |
| backhandCoach           | 5      | Bruna Elaine Greg Mike Tom |
| volleyCoach             | 5      | Andy Brunna Greg Mike Tom  |
| gender                  | 2      | f m                        |

| The GLMSELECT Procedure           |                                  |
|-----------------------------------|----------------------------------|
| Level Details for MM Effect coach |                                  |
| Levels                            | Values                           |
| 6                                 | Andy Brunna Elaine Greg Mike Tom |

Output 45.4.2 shows the parameter estimates for the selected model. You can see that the constructed multimember effect coach and the spline effect practice are both included in the selected model. All coaches provided benefit (all the parameters of the multimember effect coach are positive), with Greg and Mike being the most effective.

**Output 45.4.2** Parameter Estimates

| Parameter Estimates |        |    |           |                |         |
|---------------------|--------|----|-----------|----------------|---------|
| Parameter           |        | DF | Estimate  | Standard Error | t Value |
| Intercept           |        | 1  | 0.379873  | 0.513431       | 0.74    |
| coach               | Andy   | 1  | 1.444370  | 0.318078       | 4.54    |
| coach               | Bruna  | 1  | 1.446063  | 0.110179       | 13.12   |
| coach               | Elaine | 1  | 1.312290  | 0.281877       | 4.66    |
| coach               | Greg   | 1  | 3.042828  | 0.112256       | 27.11   |
| coach               | Mike   | 1  | 2.840728  | 0.121166       | 23.45   |
| coach               | Tom    | 1  | 1.248946  | 0.115266       | 10.84   |
| practice            | 1      | 1  | 2.538938  | 1.015772       | 2.50    |
| practice            | 2      | 1  | 3.837684  | 1.104557       | 3.47    |
| practice            | 3      | 1  | 2.574775  | 0.930816       | 2.77    |
| practice            | 4      | 1  | -0.034747 | 0.717967       | -0.05   |
| practice            | 5      | 0  | 0         | .              | .       |
| tPlay               |        | 1  | 0.139409  | 0.023043       | 6.05    |

Suppose you want to examine regression diagnostics for the selected model. PROC GLMSELECT does not support such diagnostics, so you might want to use the REG procedure to produce these diagnostics. You can overcome the difficulty that PROC REG does not support CLASS and EFFECT statements by using the OUTDESIGN= option in the PROC GLMSELECT statement to obtain the design matrix that you can use as an input data set for further analysis with other SAS procedures.

The following statements use PROC PRINT to produce Output 45.4.3, which shows the first five observations of the design matrix designCamp.

```
proc print data=designCamp(obs=5);
run;
```

**Output 45.4.3** First Five Observations of the designCamp Data Set

|   | c<br>o<br>a<br>c<br>c                                         |                                           |                                                                    |                                                                         |                                                                         |                                                                         |                                                                         |                                                                         | p<br>r<br>r<br>r<br>r<br>r |         |         |         |         | i<br>m<br>p<br>r<br>o<br>v<br>e<br>m<br>e<br>n<br>t |         |         |         |         |   |
|---|---------------------------------------------------------------|-------------------------------------------|--------------------------------------------------------------------|-------------------------------------------------------------------------|-------------------------------------------------------------------------|-------------------------------------------------------------------------|-------------------------------------------------------------------------|-------------------------------------------------------------------------|----------------------------|---------|---------|---------|---------|-----------------------------------------------------|---------|---------|---------|---------|---|
|   | I<br>n<br>t<br>e<br>r<br>c<br>o<br>m<br>b<br>i<br>n<br>e<br>d | o<br>a<br>c<br>h<br>_<br>B<br>l<br>o<br>g | a<br>c<br>h<br>_<br>E<br>h<br>_<br>A<br>r<br>a<br>n<br>n<br>e<br>g | c<br>c<br>c<br>c<br>c<br>c<br>c<br>c<br>c<br>c<br>c<br>c<br>c<br>c<br>c | c<br>c<br>c<br>c<br>c<br>c<br>c<br>c<br>c<br>c<br>c<br>c<br>c<br>c<br>c | c<br>c<br>c<br>c<br>c<br>c<br>c<br>c<br>c<br>c<br>c<br>c<br>c<br>c<br>c | c<br>c<br>c<br>c<br>c<br>c<br>c<br>c<br>c<br>c<br>c<br>c<br>c<br>c<br>c | c<br>c<br>c<br>c<br>c<br>c<br>c<br>c<br>c<br>c<br>c<br>c<br>c<br>c<br>c | 19                         | 33      | 24      | 28      | 34      | 0.00000                                             | 0.00136 | 0.05077 | 0.58344 | 0.36443 | 6 |
| 1 | 1                                                             | 0                                         | 0                                                                  | 0                                                                       | 0                                                                       | 0                                                                       | 0                                                                       | 1                                                                       | 19                         | 0.00000 | 0.00136 | 0.05077 | 0.58344 | 0.36443                                             | 6       |         |         |         |   |
| 2 | 1                                                             | 0                                         | 0                                                                  | 0                                                                       | 2                                                                       | 0                                                                       | 0                                                                       | 33                                                                      | 0.20633                    | 0.50413 | 0.25014 | 0.03940 | 0.00000 | 14                                                  |         |         |         |         |   |
| 3 | 1                                                             | 0                                         | 0                                                                  | 0                                                                       | 0                                                                       | 2                                                                       | 0                                                                       | 24                                                                      | 0.20633                    | 0.50413 | 0.25014 | 0.03940 | 0.00000 | 13                                                  |         |         |         |         |   |
| 4 | 1                                                             | 0                                         | 0                                                                  | 0                                                                       | 0                                                                       | 1                                                                       | 0                                                                       | 28                                                                      | 0.20633                    | 0.50413 | 0.25014 | 0.03940 | 0.00000 | 11                                                  |         |         |         |         |   |
| 5 | 1                                                             | 0                                         | 2                                                                  | 0                                                                       | 0                                                                       | 0                                                                       | 0                                                                       | 34                                                                      | 0.16228                    | 0.49279 | 0.29088 | 0.05405 | 0.00000 | 12                                                  |         |         |         |         |   |

To facilitate specifying the columns of the design matrix corresponding to the selected model, you can use the macro variable named `_GLSMOD` that PROC GLMSELECT creates whenever you specify the `OUT-DESIGN=` option. The following statements use PROC REG to produce a panel of regression diagnostics corresponding to the model selected by PROC GLMSELECT.

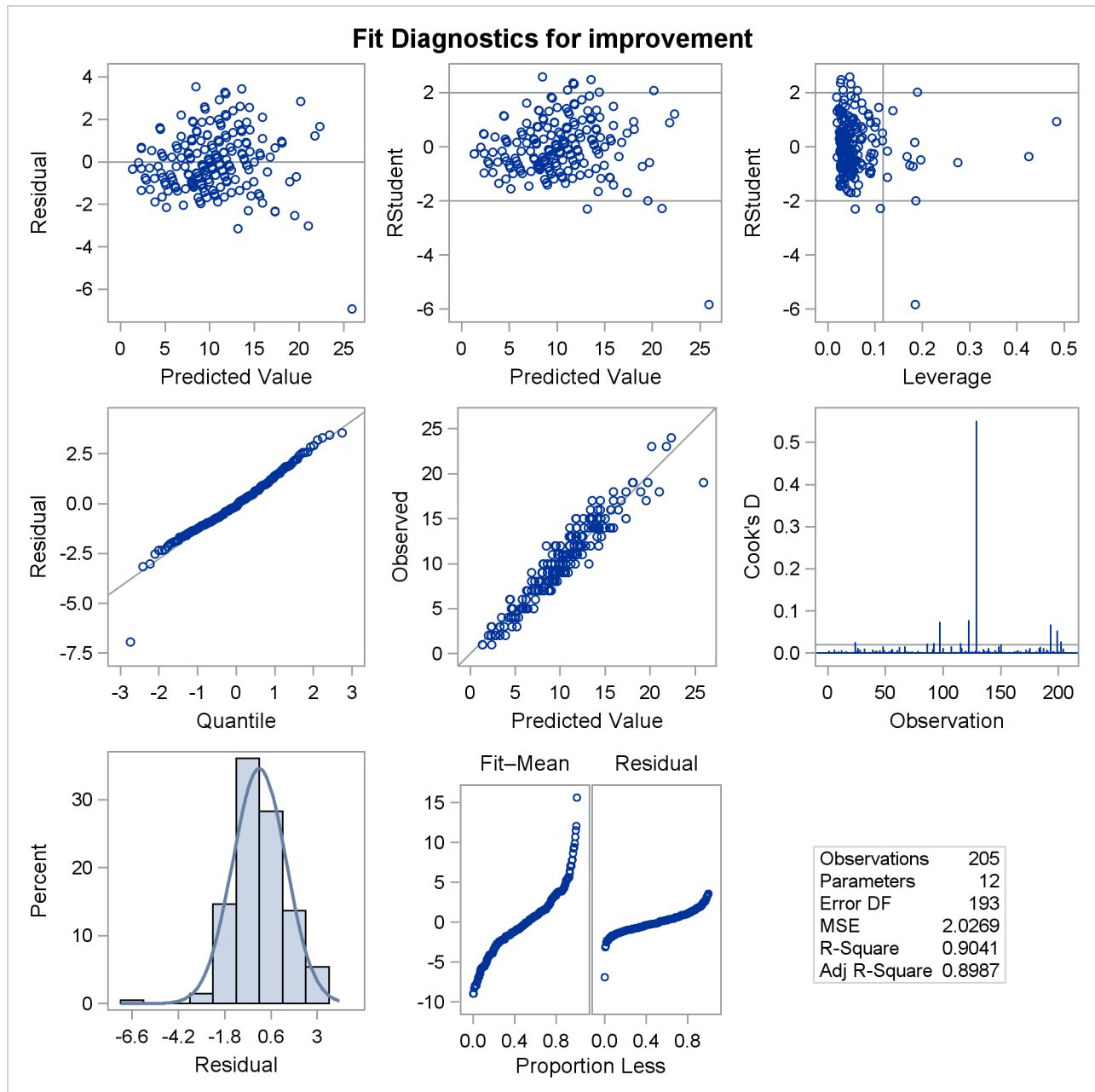
```
ods graphics on;

proc reg data=designCamp;
 model improvement = &_GLSMOD;
quit;

ods graphics off;
```

The regression diagnostics shown in [Output 45.4.4](#) indicate a reasonable model. However, they also reveal the presence of one large outlier and several influential observations that you might want to investigate.

Output 45.4.4 Fit Diagnostics



Sometimes you might want to use subsets of the columns of the design matrix. In such cases, it might be convenient to produce a design matrix with generic names for the columns. You might also want a design matrix containing the columns corresponding to the full model that you specify in the `MODEL` statement. By default, the design matrix includes only the columns that correspond to effects in the selected model. The following statements show how to do this.



```

proc glmselect data=TennisCamp
 outdesign(fullmodel prefix=parm names)=designCampGeneric;
 class forehandCoach backhandCoach volleyCoach gender;

 effect coach = mm(forehandCoach backhandCoach volleyCoach / noeffect
 details weight=(tForehand tBackhand tVolley));
 effect practice = spline(tPractice/knotmethod=list(25) details);

 model improvement = coach practice tLessons tPlay age gender
 inRating nPastCamps;

run;

```

The PREFIX=parm suboption of the OUTDESIGN= option specifies that columns in the design matrix be given the prefix parm with a trailing index. The NAMES suboption requests the table in [Output 45.4.5](#) that associates descriptive labels with the names of columns in the design matrix. Finally, the FULLMODEL suboption specifies that the design matrix include columns corresponding to all effects specified in the MODEL statement.

**Output 45.4.5** Descriptive Names of Design Matrix Columns

| The GLMSELECT Procedure |              |
|-------------------------|--------------|
| Selected Model          |              |
| Parameter Names         |              |
| Name                    | Parameter    |
| parm1                   | Intercept    |
| parm2                   | coach Andy   |
| parm3                   | coach Bruna  |
| parm4                   | coach Elaine |
| parm5                   | coach Greg   |
| parm6                   | coach Mike   |
| parm7                   | coach Tom    |
| parm8                   | practice 1   |
| parm9                   | practice 2   |
| parm10                  | practice 3   |
| parm11                  | practice 4   |
| parm12                  | practice 5   |
| parm13                  | tLessons     |
| parm14                  | tPlay        |
| parm15                  | age          |
| parm16                  | gender f     |
| parm17                  | gender m     |
| parm18                  | inRating     |
| parm19                  | nPastCamps   |

The following statements produce [Output 45.4.6](#), displaying the first five observations of the designCampGeneric data set:

```
proc print data=designCampGeneric (obs=5);
run;
```

**Output 45.4.6** First Five Observations of designCampGeneric Data Set

|   |   |   |   |   |   |   |   |         |         | i<br>m<br>p<br>r<br>o<br>v                     |         |         |   |    |    |   |   |    |   |    |
|---|---|---|---|---|---|---|---|---------|---------|------------------------------------------------|---------|---------|---|----|----|---|---|----|---|----|
|   |   |   |   |   |   |   |   |         |         | a<br>a<br>a<br>a<br>a<br>a<br>a<br>a<br>a<br>a |         |         |   |    |    |   |   |    |   |    |
|   |   |   |   |   |   |   |   |         |         | r<br>r<br>r<br>r<br>r<br>r<br>r<br>r<br>r<br>r |         |         |   |    |    |   |   |    |   |    |
|   |   |   |   |   |   |   |   |         |         | m<br>m<br>m<br>m<br>m<br>m<br>m<br>m<br>m<br>m |         |         |   |    |    |   |   |    |   |    |
|   |   |   |   |   |   |   |   |         |         | 1<br>1<br>1<br>1<br>1<br>1<br>1<br>1<br>1<br>1 |         |         |   |    |    |   |   |    |   |    |
|   |   |   |   |   |   |   |   |         |         | 0<br>1<br>2<br>3<br>4<br>5<br>6<br>7<br>8<br>9 |         |         |   |    |    |   |   |    |   |    |
| 1 | 1 | 0 | 0 | 0 | 0 | 0 | 1 | 0.00000 | 0.00136 | 0.05077                                        | 0.58344 | 0.36443 | 1 | 19 | 13 | 1 | 0 | 44 | 0 | 6  |
| 2 | 1 | 0 | 0 | 0 | 2 | 0 | 0 | 0.20633 | 0.50413 | 0.25014                                        | 0.03940 | 0.00000 | 2 | 33 | 15 | 1 | 0 | 48 | 2 | 14 |
| 3 | 1 | 0 | 0 | 0 | 0 | 2 | 0 | 0.20633 | 0.50413 | 0.25014                                        | 0.03940 | 0.00000 | 2 | 24 | 15 | 0 | 1 | 53 | 0 | 13 |
| 4 | 1 | 0 | 0 | 0 | 0 | 1 | 0 | 0.20633 | 0.50413 | 0.25014                                        | 0.03940 | 0.00000 | 1 | 28 | 13 | 1 | 0 | 48 | 0 | 11 |
| 5 | 1 | 0 | 2 | 0 | 0 | 0 | 0 | 0.16228 | 0.49279 | 0.29088                                        | 0.05405 | 0.00000 | 2 | 34 | 16 | 1 | 0 | 57 | 0 | 12 |

### Example 45.5: Model Averaging

This example shows how you can combine variable selection methods with model averaging to build parsimonious predictive models. This example uses simulated data that consist of observations from the model

$$y = \mathbf{X}\boldsymbol{\beta} + N(0, \sigma^2)$$

where  $\mathbf{X}$  is drawn from a multivariate normal distribution  $N(0, \mathbf{V})$  with  $V_{i,j} = \rho^{|i-j|}$  where  $0 < \rho < 1$ . This setup has been widely studied in investigations of variable selection methods. For examples, see Breiman (1992); Tibshirani (1996); Zou (2006).

The following statements define a macro that uses the SIMNORMAL procedure to generate the regressors. This macro prepares a TYPE=CORR data set that specifies the desired pairwise correlations. This data set is used as the input data for PROC SIMNORMAL which produces the sampled regressors in an output data set named Regressors.

```
%macro makeRegressorData (nObs=100, nVars=8, rho=0.5, seed=1);
data varCorr;
drop i j;
array x{&nVars};
length _NAME_ $8 _TYPE_ $8;
NAME = '';

TYPE = 'MEAN';
do j=1 to &nVars; x{j}=0; end;
output;

TYPE = 'STD';
```

```

do j=1 to &nVars; x{j}=1;end;
output;

__TYPE_ = 'N';
do j=1 to &nVars; x{j}=10000;end;
output;

__TYPE_ = 'CORR';
do i=1 to &nVars;
 __NAME_="x" || trim(left(i));
 do j= 1 to &nVars;
 x{j}=&rho**(abs(i-j));
 end;
 output;
end;
run;

proc simnormal data=varCorr(type=corr) out=Regressors
 numReal=&nObs seed=&seed;
 var x1-x&nVars;
run;
%mend;

```

The following statements use the %makeRegressorData macro to generate a sample of 100 observations with 10 regressors, where  $E(\mathbf{X}_i \mathbf{X}_j) = 0.5^{|i-j|}$ , the true coefficients are  $\boldsymbol{\beta}' = (3, 1.5, 0, 0, 2, 0, 0, 0, 0, 0)$ , and  $\sigma = 3$ .

```

%makeRegressorData (nObs=100, nVars=10, rho=0.5);

data simData;
 set regressors;
 yTrue = 3*x1 + 1.5*x2 + 2*x5;
 y = yTrue + 3*rannor(2);
run;

```

The adaptive lasso algorithm (see “Adaptive Lasso Selection” on page 3566) is a modification of the standard lasso algorithm in which weights are applied to each of the parameters in forming the lasso constraint. Zou (2006) shows that the adaptive lasso has theoretical advantages over the standard lasso. Furthermore, simulation studies show that the adaptive lasso tends to perform better than the standard lasso in selecting the correct regressors, particularly in high signal-to-noise ratio cases. The following statements fit an adaptive lasso model to the simData data:

```

proc glmselect data=simData;
 model y=x1-x10/selection=LASSO(adaptive stop=none choose=svc);
run;

```

The selected model and parameter estimates are shown in [Output 45.5.1](#)

#### Output 45.5.1 Model Selected by Adaptive Lasso

|                                                                                      |
|--------------------------------------------------------------------------------------|
| <p>The GLMSELECT Procedure<br/>Selected Model</p> <p>Effects: Intercept x1 x2 x5</p> |
|--------------------------------------------------------------------------------------|

**Output 45.5.1** *continued*

| Parameter Estimates |    |           |
|---------------------|----|-----------|
| Parameter           | DF | Estimate  |
| Intercept           | 1  | -0.243219 |
| x1                  | 1  | 3.246129  |
| x2                  | 1  | 1.310514  |
| x5                  | 1  | 2.132416  |

You see that the selected model contains only the relevant regressors x1, x2, and x5. You might want to investigate how frequently the adaptive lasso method selects just the relevant regressors and how stable the corresponding parameter estimates are. In a simulation study, you can do this by drawing new samples and repeating this process many times. What can you do when you only have a single sample of the data available? One approach is to repeatedly draw subsamples from the data that you have, and to fit models for each of these samples. You can then form the average model and use this model for prediction. You can also examine how frequently models are selected, and you can use the frequency of effect selection as a measure of effect importance.

The following statements show how you can use the **MODEL AVERAGE** statement to perform such an analysis:

```
ods graphics on;

proc glmselect data=simData seed=3 plots=(EffectSelectPct ParmDistribution);
 model y=x1-x10/selection=LASSO(adaptive stop=none choose=SBC);
 modelAverage tables=(EffectSelectPct(all) ParmEst(all));
run;
```

The ModelAverageInfo table in **Output 45.5.2** shows that the default sampling method is the bootstrap approach of drawing 100 samples with replacement, where the sampling percentage of 100 means that each sample has the same sum of frequencies as the input data. You can use the **SAMPLING=** and **NSAMPLES=** options in the **MODEL AVERAGE** statement to modify the sampling method and the number of samples used.

**Output 45.5.2** Model Averaging Information

| The GLMSELECT Procedure     |                                 |
|-----------------------------|---------------------------------|
| Model Averaging Information |                                 |
| Sampling Method             | Unrestricted (with replacement) |
| Sample Percentage           | 100                             |
| Number of Samples           | 100                             |

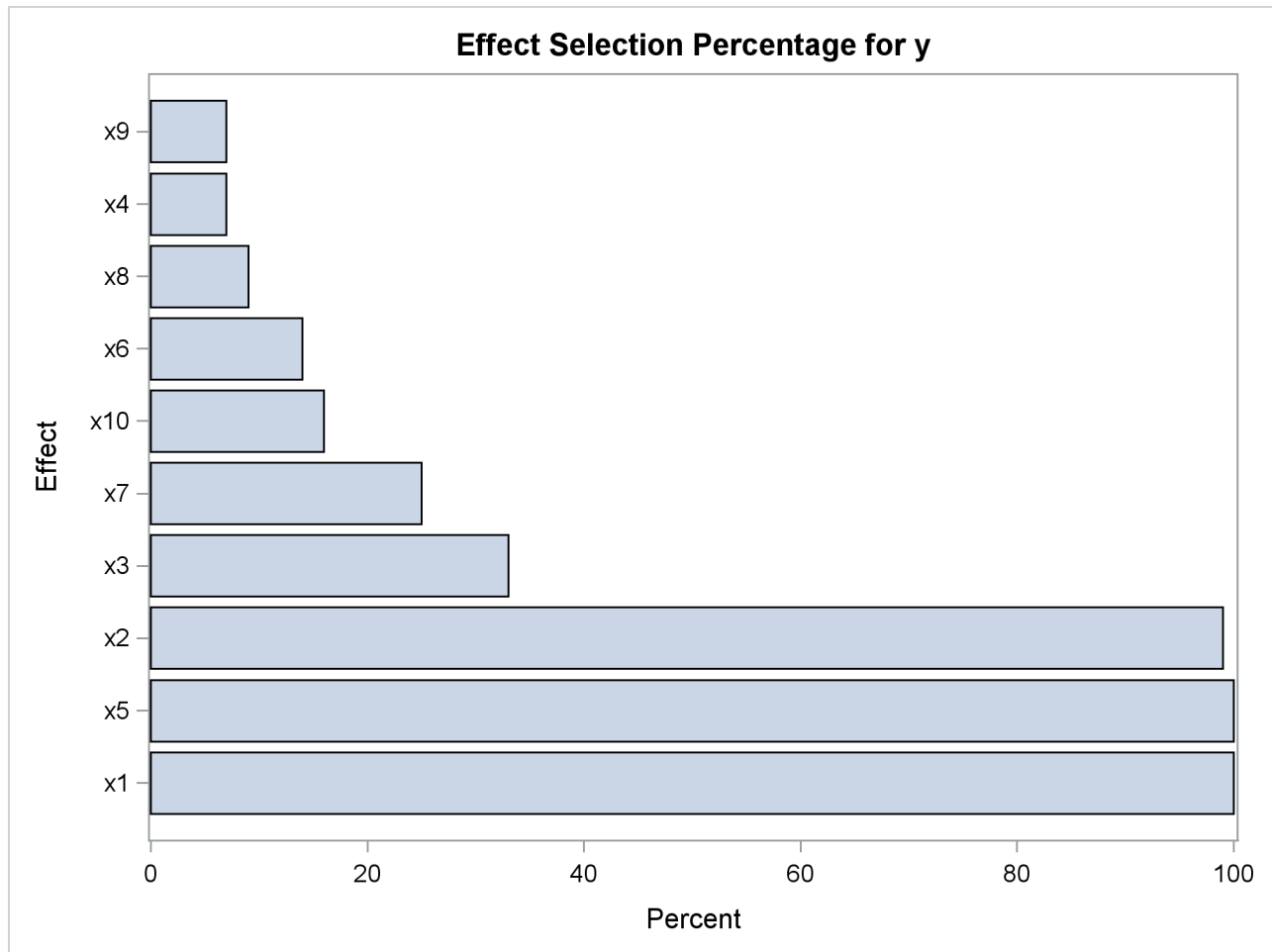
Output 45.5.3 shows the percentage of samples where each effect is in the selected model. The ALL option of the EFFECTSELECTPCT request in the TABLES= option specifies that effects that appear in any selected model are shown. (By default, the “Effect Selection Percentage” table displays only those effects that are selected at least 20 percent of the time.)

**Output 45.5.3** Effect Selection Percentages

| Effect Selection Percentage |                      |
|-----------------------------|----------------------|
| Effect                      | Selection Percentage |
| x1                          | 100.0                |
| x2                          | 99.00                |
| x3                          | 33.00                |
| x4                          | 7.00                 |
| x5                          | 100.0                |
| x6                          | 14.00                |
| x7                          | 25.00                |
| x8                          | 9.00                 |
| x9                          | 7.00                 |
| x10                         | 16.00                |

The EFFECTSELECTPCT request in the PLOTS= option in the PROC GLMSELECT statement produces the bar chart shown in Output 45.5.4, which graphically displays the information in the EffectSelectPct table.

**Output 45.5.4** Effect Selection Percentages



Output 45.5.5 shows the frequencies with which models get selected. By default, only the “best” 20 models are shown. See the section “Model Selection Frequencies and Frequency Scores” on page 3577 for details about how these models are ordered.

**Output 45.5.5** Model Selection Frequency

| Model Selection Frequency |                      |                   |                 |                              |
|---------------------------|----------------------|-------------------|-----------------|------------------------------|
| Times Selected            | Selection Percentage | Number of Effects | Frequency Score | Effects in Model             |
| 44                        | 44.00                | 4                 | 45.00           | Intercept x1 x2 x5           |
| 9                         | 9.00                 | 5                 | 9.86            | Intercept x1 x2 x3 x5        |
| 8                         | 8.00                 | 6                 | 8.76            | Intercept x1 x2 x3 x5 x7     |
| 4                         | 4.00                 | 5                 | 4.82            | Intercept x1 x2 x5 x8        |
| 4                         | 4.00                 | 7                 | 4.67            | Intercept x1 x2 x3 x5 x6 x7  |
| 3                         | 3.00                 | 5                 | 3.85            | Intercept x1 x2 x5 x7        |
| 2                         | 2.00                 | 5                 | 2.83            | Intercept x1 x2 x5 x10       |
| 2                         | 2.00                 | 5                 | 2.81            | Intercept x1 x2 x4 x5        |
| 2                         | 2.00                 | 6                 | 2.74            | Intercept x1 x2 x3 x5 x6     |
| 2                         | 2.00                 | 7                 | 2.66            | Intercept x1 x2 x3 x5 x6 x10 |
| 1                         | 1.00                 | 5                 | 1.83            | Intercept x1 x2 x5 x6        |
| 1                         | 1.00                 | 4                 | 1.81            | Intercept x1 x5 x7           |
| 1                         | 1.00                 | 5                 | 1.81            | Intercept x1 x2 x5 x9        |
| 1                         | 1.00                 | 6                 | 1.75            | Intercept x1 x2 x3 x5 x10    |
| 1                         | 1.00                 | 6                 | 1.74            | Intercept x1 x2 x3 x5 x8     |
| 1                         | 1.00                 | 6                 | 1.73            | Intercept x1 x2 x5 x6 x7     |
| 1                         | 1.00                 | 6                 | 1.72            | Intercept x1 x2 x5 x7 x9     |
| 1                         | 1.00                 | 6                 | 1.71            | Intercept x1 x2 x5 x8 x10    |
| 1                         | 1.00                 | 6                 | 1.70            | Intercept x1 x2 x4 x5 x10    |
| 1                         | 1.00                 | 7                 | 1.68            | Intercept x1 x2 x3 x5 x7 x10 |

You can see that the most frequently selected model is the model that contains just the true underlying regressors. Although this model is selected in 44% of the samples, most of the selected models contain at least one irrelevant regressor. This is not surprising because even though the true model has just a few large effects in this example, the regressors have nontrivial pairwise correlations.

When your goal is simply to obtain a predictive model, then a good strategy is to average the predictions that you get from all the selected models. In the linear model context, this corresponds to using the model whose parameter estimates are the averages of the estimates that you get for each sample, where if a parameter is not in a selected model, the corresponding estimate is defined to be zero. This has the effect of shrinking the estimates of infrequently selected parameters towards zero.

Output 45.5.6 shows the average parameter estimates. The ALL option of the PARMEST request in the TABLES= option specifies that all parameters that are nonzero in any selected model are shown. (By default, the “Average Parameter Estimates” table displays only those parameters that are nonzero in at least 20 percent of the selected models.)

**Output 45.5.6** Average Parameter Estimates

| Average Parameter Estimates |                    |                        |                  |                       |
|-----------------------------|--------------------|------------------------|------------------|-----------------------|
| Parameter                   | Number<br>Non-zero | Non-zero<br>Percentage | Mean<br>Estimate | Standard<br>Deviation |
| Intercept                   | 100                | 100.00                 | -0.271262        | 0.308146              |
| x1                          | 100                | 100.00                 | 3.196392         | 0.377771              |
| x2                          | 99                 | 99.00                  | 1.439966         | 0.416054              |
| x3                          | 33                 | 33.00                  | -0.264831        | 0.412148              |
| x4                          | 7                  | 7.00                   | -0.037810        | 0.142932              |
| x5                          | 100                | 100.00                 | 2.253196         | 0.397032              |
| x6                          | 14                 | 14.00                  | -0.083823        | 0.261641              |
| x7                          | 25                 | 25.00                  | 0.184656         | 0.372813              |
| x8                          | 9                  | 9.00                   | 0.060438         | 0.206621              |
| x9                          | 7                  | 7.00                   | -0.043307        | 0.239940              |
| x10                         | 16                 | 16.00                  | 0.083411         | 0.199573              |

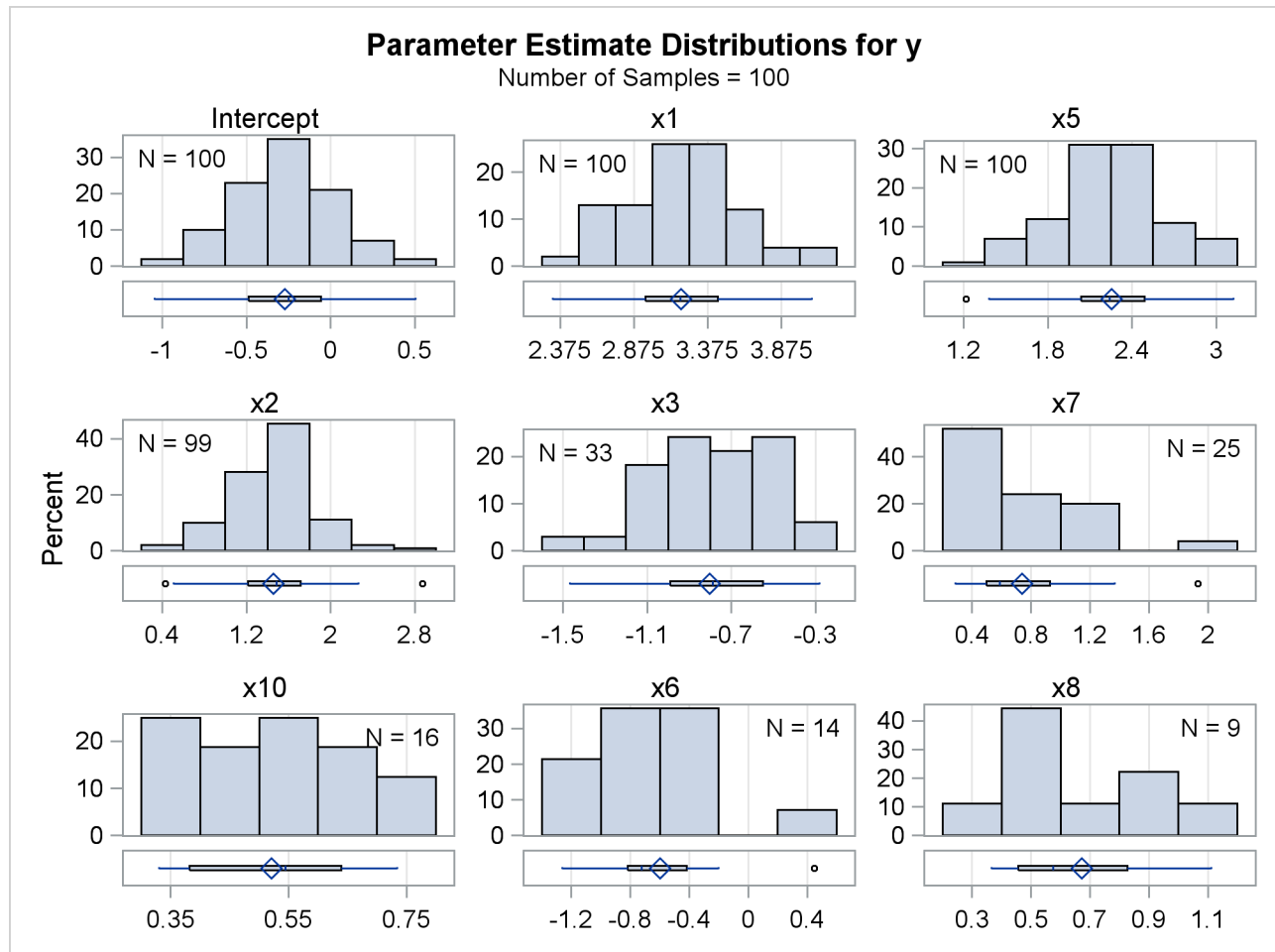
| Average Parameter Estimates |                              |           |           |
|-----------------------------|------------------------------|-----------|-----------|
| Parameter                   | -----Estimate Quantiles----- |           |           |
|                             | 25%                          | Median    | 75%       |
| Intercept                   | -0.489061                    | -0.249163 | -0.058233 |
| x1                          | 2.951551                     | 3.189078  | 3.446055  |
| x2                          | 1.209781                     | 1.484064  | 1.710275  |
| x3                          | -0.536449                    | 0         | 0         |
| x4                          | 0                            | 0         | 0         |
| x5                          | 2.036261                     | 2.242240  | 2.489068  |
| x6                          | 0                            | 0         | 0         |
| x7                          | 0                            | 0         | 0.143317  |
| x8                          | 0                            | 0         | 0         |
| x9                          | 0                            | 0         | 0         |
| x10                         | 0                            | 0         | 0         |

The average estimate for a parameter is computed by dividing the sum of the estimate values for that parameter in each sample by the total number of samples. This corresponds to using zero as the estimate value for the parameter in those samples where the parameter does not appear in the selected model. Similarly, these zero estimates are included in the computation of the estimated standard deviation and quantiles that are displayed in the AvgParmEst table. If you want see the estimates that you get if you do not use zero for nonselected parameters, you can specify the NONZEROPARMS suboption of the PARMEST request in the TABLES=option.

The PARMDISTRIBUTION request in the PLOTS= option in the PROC GLMSELECT statement requests the panel in [Output 45.5.7](#), which shows the distribution of the estimates for each parameter in the average model. For each parameter in the average model, a histogram and box plot of the nonzero values of the estimates are shown. You can use this plot to assess how the selected estimates vary across the samples.



## Output 45.5.7 Effect Selection Percentages



You can obtain details about the model selection for each sample by specifying the **DETAILS** option in the **MODEL AVERAGE** statement. You can use an **OUTPUT** statement to output the mean predicted value and standard deviation, quantiles of the predicted values, as well as the individual sample frequencies and predicted values for each sample. The following statements show how you do this:

```
proc glmselect data=simData seed=3;
 model y=x1-x10/selection=LASSO(adaptive stop=none choose=SBC);
 modelAverage details;
 output out=simOut sampleFreq=sf samplePred=sp
 p=p stddev=stddev lower=q25 upper=q75 median;
run;
```

Output 45.5.8 shows the selection summary and parameter estimates for sample 1 of the model averaging. Note that you can obtain all the model selection output, including graphs, for each sample.

**Output 45.5.8** Selection Details for Sample 1

| The GLMSELECT Procedure      |                |                |                   |           |
|------------------------------|----------------|----------------|-------------------|-----------|
| Sample 1                     |                |                |                   |           |
| LASSO Selection Summary      |                |                |                   |           |
| Step                         | Effect Entered | Effect Removed | Number Effects In | SBC       |
| 0                            | Intercept      |                | 1                 | 374.8287  |
| -----                        |                |                |                   |           |
| 1                            | x1             |                | 2                 | 243.4087  |
| 2                            | x5             |                | 3                 | 227.5991  |
| 3                            | x2             |                | 4                 | 225.7356* |
| 4                            | x7             |                | 5                 | 229.9135  |
| 5                            | x3             |                | 6                 | 233.3660  |
| 6                            | x6             |                | 7                 | 237.7447  |
| 7                            | x10            |                | 8                 | 235.2171  |
| 8                            | x4             |                | 9                 | 238.8085  |
| 9                            | x9             |                | 10                | 239.8353  |
| 10                           | x8             |                | 11                | 244.4236  |
| * Optimal Value Of Criterion |                |                |                   |           |
| Parameter Estimates          |                |                |                   |           |
| Parameter                    | DF             | Estimate       |                   |           |
| Intercept                    | 1              | -0.092885      |                   |           |
| x1                           | 1              | 4.079938       |                   |           |
| x2                           | 1              | 0.505697       |                   |           |
| x5                           | 1              | 1.473929       |                   |           |

The following statements display the subset of the variables in the first five observations of the output data set, as shown in Output 45.5.9.

```
proc print data=simOut (obs=5);
 var p stddev q25 median q75 sf1-sf3 sp1-sp3;
run;
```

Output 45.5.9 Part of the Output Data Set

| O | s       | m       |          |         |         |   |   |   |         |         |         |
|---|---------|---------|----------|---------|---------|---|---|---|---------|---------|---------|
| b | t       | e       |          |         |         |   |   |   |         |         |         |
| s | d       | d       |          |         |         |   |   |   |         |         |         |
|   | q       | i       | q        | s       | s       | s | s | s | s       |         |         |
|   | e       | a       | 7        | f       | f       | f | p | p | p       |         |         |
|   | v       | n       | 5        | 1       | 2       | 3 | 1 | 2 | 3       |         |         |
| 1 | 10.3569 | 0.82219 | 9.95992  | 10.3878 | 10.9194 | 1 | 0 | 1 | 10.1378 | 11.2104 | 11.0124 |
| 2 | -5.5453 | 0.64544 | -6.05563 | -5.6455 | -5.0829 | 1 | 1 | 1 | -4.7517 | -6.7191 | -6.4413 |
| 3 | 6.5066  | 0.75289 | 6.05984  | 6.5077  | 6.9099  | 3 | 2 | 0 | 6.0838  | 7.4880  | 6.3466  |
| 4 | -1.7527 | 0.85168 | -2.26638 | -1.8123 | -1.3312 | 1 | 1 | 2 | -2.1891 | -1.4887 | -1.7083 |
| 5 | -7.5840 | 1.20687 | -8.44679 | -7.5716 | -6.7386 | 3 | 1 | 1 | -6.7051 | -9.0558 | -6.7949 |

By default, the LOWER and UPPER options in the OUTPUT statement produce the lower and upper quartiles of the sample predicted values. You can change the quantiles produced by using the ALPHA= option in the MODEL AVERAGE statement. The variables sf1–sf100 contain the sample frequencies used for each sample, and the variables sp1–sp100 hold the corresponding predicted values. Even if you do not specify the DETAILS option in the MODEL AVERAGE statement, you can use the sample frequencies in the output data set to reproduce the selection results for any particular sample. For example, the following statements recover the selection for sample 1:

```
proc glmselect data=simOut;
 freq sf1;
 model y=x1-x10/selection=LASSO(adaptive stop=none choose=SBC);
run;
```

The average model is not parsimonious—it includes shrunken estimates of infrequently selected parameters which often correspond to irrelevant regressors. It is tempting to ignore the estimates of infrequently selected parameters by setting their estimate values to zero in the average model. However, this can lead to a poorly performing model. Even though a parameter might occur in only one selected model, it might be a very important term in that model. Ignoring its estimate but including some of the estimates of the other parameters in this model leads to biased predictions. One scenario where this might occur is when the data contains two highly correlated regressors which are both strongly correlated with the response.

You can obtain a parsimonious model by using the frequency of effect selection as a measure of effect importance and refitting a model that contains just the effects that you deem important. In this example, Output 45.5.3 shows that the effects x1, x2, and x5 all get selected at least 99 percent of the time, whereas all other effects get selected less than 34 percent of the time. This large gap suggests that using 35% as the selection cutoff for this data will produce a parsimonious model that retains good predictive performance. You can use the REFIT option to implement this strategy. The REFIT option requests a second round of model averaging, where you use the MINPCT= suboption to specify the minimum percentage of times an effect must be selected in the initial set of samples to be included in the second round of model averaging. The average model is obtained by averaging the ordinary least squares estimates obtained for each sample. The following statements show how you do this:

```
proc glmselect data=simData seed=3 plots=(ParmDistribution);
 model y=x1-x10/selection=LASSO(adaptive stop=none choose=SBC);
 modelAverage refit(minpct=35 nsamples=1000) alpha=0.1;
run;
```

```
ods graphics off;
```

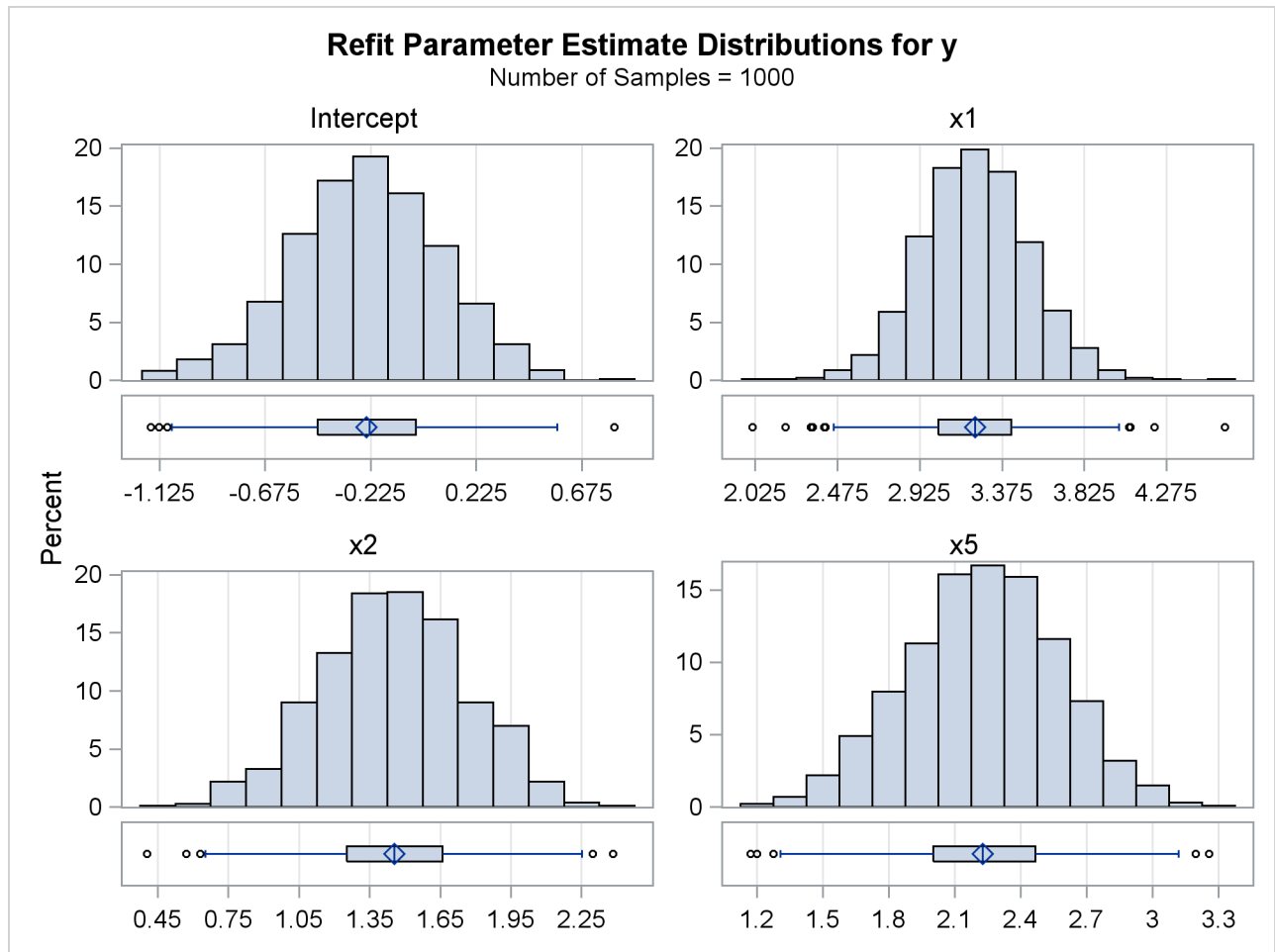
The NSAMPLES=1000 suboption of the REFIT option specifies that 1,000 samples be used in the refit, and the MINPCT=35 suboption specifies the cutoff for inclusion in the refit. The ALPHA=0.1 option specifies that the fifth and 95th percentiles of the estimates be displayed. [Output 45.5.10](#) shows the effects that are used in performing the refit and the resulting average parameter estimates.

**Output 45.5.10** Refit Average Parameter Estimates

| The GLMSELECT Procedure       |           |           |                              |           |          |
|-------------------------------|-----------|-----------|------------------------------|-----------|----------|
| Refit Model Averaging Results |           |           |                              |           |          |
| Effects: Intercept x1 x2 x5   |           |           |                              |           |          |
| Average Parameter Estimates   |           |           |                              |           |          |
| Parameter                     | Mean      | Standard  | -----Estimate Quantiles----- |           |          |
|                               | Estimate  | Deviation | 5%                           | Median    | 95%      |
| Intercept                     | -0.243514 | 0.315207  | -0.762462                    | -0.230630 | 0.271510 |
| x1                            | 3.226252  | 0.299443  | 2.737843                     | 3.226758  | 3.708131 |
| x2                            | 1.453584  | 0.308062  | 0.947059                     | 1.454635  | 1.968231 |
| x5                            | 2.226044  | 0.345185  | 1.627491                     | 2.228189  | 2.780034 |

[Output 45.5.11](#) displays the distributions of the estimates that are obtained for each parameter in the refit model. Because the distributions are approximately normal and a large number of samples are used, it is reasonable to interpret the range between the fifth and 95th percentiles of each estimate as an approximate 90% confidence interval for that estimate.

**Output 45.5.11** Effect Selection Percentages



---

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# Chapter 46

## The HPMIXED Procedure

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## Overview: HPMIXED Procedure

The HPMIXED procedure uses a number of specialized high-performance techniques to fit linear mixed models with variance component structure. The HPMIXED procedure is specifically designed to cope with estimation problems involving a large number of fixed effects, a large number of random effects, or a large number of observations.

The HPMIXED procedure complements the MIXED procedure and other SAS/STAT procedures for mixed modeling. On the one hand, the models supported by the HPMIXED procedure are a subset of the models that you can fit with the MIXED procedure, and the confirmatory inferences available in the HPMIXED procedure are also a subset of the general analyses available with the MIXED procedure. On the other hand, the HPMIXED procedure can have considerably better performance than other SAS/STAT mixed modeling tools, in terms of memory requirements and computational speed.

A mixed model can be large in a number of ways, not all of which are suited for the specialized algorithms and storage techniques implemented in the HPMIXED procedure. The following are examples of linear mixed modeling problems for which the HPMIXED procedure has been specifically designed:

- linear mixed models with thousands of levels for the fixed and/or random effects
- linear mixed models with hierarchically nested fixed and/or random effects, possibly with hundreds or thousands of levels at each level of the hierarchy

---

## Basic Features

The HPMIXED procedure enables you to specify a linear mixed model with variance component structure, to estimate the covariance parameters by restricted maximum likelihood, and to perform confirmatory inference in such models. The HPMIXED procedure fits the specified linear mixed model and produces appropriate statistics.

The following are some of the basic features of the HPMIXED procedure:

- capacity to handle large linear mixed model problems for balanced or unbalanced data
- MIXED-type **MODEL** and **RANDOM** statements for model specification and **CONTRAST**, **ESTIMATE**, **LSMEANS**, and **TEST** statements for inferences
- estimate covariance parameters by restricted maximum likelihood (REML)
- output statistics by using the **OUTPUT** statement

- computation of appropriate standard errors for all specified estimable linear combinations of fixed and random effects, and corresponding  $t$  and  $F$  tests
- subject and group effects that enable blocking and heterogeneity, respectively
- **NLOPTIONS** statement, which enables you to exercise control over the numerical optimization

The HPMIXED procedure uses the Output Delivery System (ODS), a SAS subsystem that provides capabilities for displaying and controlling the output from SAS procedures. ODS enables you to convert any of the output from the HPMIXED procedure into a SAS data set. See the section “ODS Table Names” on page 3699 and Chapter 20, “Using the Output Delivery System,” for further information about using ODS with the HPMIXED procedure.

---

## Assumptions and Notation

The linear mixed models fit by the HPMIXED procedure can be represented as linear statistical models in the following form:

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\boldsymbol{\gamma} + \boldsymbol{\epsilon}$$

$$\boldsymbol{\gamma} \sim N(\mathbf{0}, \mathbf{G})$$

$$\boldsymbol{\epsilon} \sim N(\mathbf{0}, \sigma^2\mathbf{I})$$

$$\text{Cov}[\boldsymbol{\gamma}, \boldsymbol{\epsilon}] = \mathbf{0}$$

The symbols in these expressions denote the following:

- $\mathbf{y}$  the  $(n \times 1)$  vector of responses
- $\mathbf{X}$  the  $(n \times k)$  design matrix for the fixed effects
- $\boldsymbol{\beta}$  the  $(k \times 1)$  vector of fixed-effects parameters
- $\mathbf{Z}$  the  $(n \times q)$  design matrix for the random effects
- $\boldsymbol{\gamma}$  the  $(q \times 1)$  vector of random effects
- $\boldsymbol{\epsilon}$  the  $(n \times 1)$  vector of unobservable residual errors

As is customary for statistical models in the linear mixed model family, the random effects are assumed normally distributed. The same holds for the residual errors and these are furthermore distributed independently of the random effects. As a consequence, these assumptions imply that the response vector  $\mathbf{y}$  has a multivariate normal distribution.

Further assumptions, implicit in the preceding expression, are as follows:

- The conditional mean of the data—given the random effects—is linear in the fixed effects and the random effects.
- The marginal mean of the data is linear in the fixed-effects parameters.

## Computational Approach

The computational methods to efficiently solve large mixed model problems with the HPMIXED procedure rely on a combination of several techniques, including sparse matrix storage, specialized solving of sparse linear systems, and dedicated nonlinear optimization.

### Sparse Storage and Computation

One of the fundamental computational tasks in analyzing a linear mixed model is solving the mixed model equations

$$\begin{bmatrix} \mathbf{X}'\mathbf{X} & \mathbf{X}'\mathbf{Z} \\ \mathbf{Z}'\mathbf{X} & \mathbf{Z}'\mathbf{Z} + \sigma^2\mathbf{G}^{-1} \end{bmatrix} \begin{bmatrix} \boldsymbol{\beta} \\ \boldsymbol{\gamma} \end{bmatrix} = \begin{bmatrix} \mathbf{X}'\mathbf{y} \\ \mathbf{Z}'\mathbf{y} \end{bmatrix}$$

where  $\mathbf{G}$  denotes the variance matrix of the random effects. The mixed model crossproduct matrix

$$\begin{bmatrix} \mathbf{X}'\mathbf{X} & \mathbf{X}'\mathbf{Z} \\ \mathbf{Z}'\mathbf{X} & \mathbf{Z}'\mathbf{Z} + \sigma^2\mathbf{G}^{-1} \end{bmatrix}$$

is a key component of these equations, and it often has many zero values (George and Liu 1981). Sparse storage techniques can result in significant savings in both memory and CPU resources. The HPMIXED procedure draws on sparse matrix representation and storage where appropriate or necessary.

### Conjugate Gradient Algorithm and Iteration-on-Data Technology

Solving the mixed model equations is a critical component of linear mixed model analysis. The two main components of the preconditioned conjugate gradient (PCCG) algorithm are preconditioning and matrix-vector product computing (Shewchuk 1994). The algorithm is guaranteed to converge to the solution within  $n_e$  iterations, where  $n_e$  is equal to the number of distinct eigenvalues of the mixed model equations. This simple yet powerful algorithm can be easily implemented with an iteration-on-data (IOD) technique (Tsuruta, Misztal, and Strandén 2001) that can yield significant savings of memory resources.

The combination of the PCCG algorithm and iteration on data makes it possible to efficiently compute best linear unbiased predictors (BLUPs) for the random effects in mixed models with large mixed model equations.

### Average Information Algorithm

The HPMIXED procedure estimates covariance parameters by restricted maximum likelihood. The default optimization method is a quasi-Newton algorithm. When the Hessian or information matrix is required, the HPMIXED procedure takes advantage of the computational simplifications that are available by *averaging information* (AI). The AI algorithm (Johnson and Thompson 1995; Gilmour, Thompson, and Cullis 1995) replaces the second derivative matrix with the average of the observed and expected information matrices. The computationally intensive trace terms in these information matrices cancel upon averaging. Coarsely, the AI algorithm can be viewed as a hybrid of a Newton-Raphson approach and Fisher scoring.

---

## The HPMIXED Procedure Contrasted with the MIXED Procedure

The HPMIXED procedure is designed to solve large mixed model problems by using sparse matrix techniques. A mixed model can be large in many ways: a large number of observations, a large number of columns in the  $\mathbf{X}$  matrix, a large number of columns in the  $\mathbf{Z}$  matrix, and a large number of covariance parameters. The aim of the HPMIXED procedure is parameter estimation, inference, and prediction in linear mixed models with large  $\mathbf{X}$  and/or  $\mathbf{Z}$  matrices and many observations, but with relatively few covariance parameters.

The models that you can fit with the HPMIXED procedure and the available postprocessing analyses are a subset of the models and analyses available with the MIXED procedure. With the HPMIXED procedure you can model only G-side random effects with variance component structure or an unstructured covariance matrix in a Cholesky parameterization. R-side random effects and direct modeling of their covariance structures are not supported.

The MIXED and HPMIXED procedures offer different balances for computing performance and statistical generality. To some extent the generality of the MIXED procedure means that it cannot serve as a high-performance computing tool for all of the model-data scenarios that it can potentially handle. For example, although efficient sparse algorithms are available to estimate variance components in large linear mixed models, the computational configuration changes profoundly when, for example, Kenward-Roger degree-of-freedom adjustments are requested.

On the other hand, the HPMIXED procedure can handle only a small subset of the models that PROC MIXED can fit. Invariably, some features of high-performance sparse computing methods might be surprising at first. For example, the best computational path depends on the model and the data, so that in models with a singular  $\mathbf{X}'\mathbf{X}$  matrix, the order in which singularities are detected and accounted for can change from one data set to the next.

The following is a list of features available in the MIXED procedure, but *not* available in the HPMIXED procedure:

- a variety of covariance structures by using the TYPE= option in the RANDOM statement
- automatic Type III tests of fixed effects. You request tests of fixed effects in the HPMIXED procedure with the TEST statement.
- ODS statistical graphics
- advanced degree-of-freedom adjustments available by using the DDFM= option
- maximum likelihood or method-of-moments estimation for the covariance parameters
- a PRIOR statement for a sampling-based Bayesian analysis

## Getting Started: HPMIXED Procedure

### Mixed Model with Large Number of Fixed and Random Effects

In animal breeding, it is common to model genetic and environmental effects with a random effect for the animal. When there are many animals being studied, this can lead to very large mixed model equations to be solved. In this example we present an analysis of simulated data with this structure.

Suppose you have 3000 animals from five different genetic species raised on 100 different farms. The following DATA step simulates 40000 observations of milk yield (Yield) from a linear mixed model with variables Species and Farm in the fixed-effect model and Animal as a random effect. The random effect due to Animal is simulated with a variance of 4.0, while the residual error variance is 8.0. These variance component values reflect the fact that variation in milk yield is typically genetically controlled to be no more than 33% ( $4/(4+8)$ ).

```
data Sim;
 keep Species Farm Animal Yield;
 array AnimalEffect{3000};
 array AnimalFarm{3000};
 array AnimalSpecies{3000};
 do i = 1 to dim(AnimalEffect);
 AnimalEffect{i} = sqrt(4.0)*rannor(12345);
 AnimalFarm{i} = 1 + int(100*ranuni(12345));
 AnimalSpecies{i} = 1 + int(5*ranuni(12345));
 end;
 do i = 1 to 40000;
 Animal = 1 + int(3000*ranuni(12345));
 Species = AnimalSpecies{Animal};
 Farm = AnimalFarm{Animal};
 Yield = 1 + Species + Farm/10 + AnimalEffect{Animal}
 + sqrt(8.0)*rannor(12345);
 output;
 end;
run;
```

A simple linear mixed model analysis is performed by using the following SAS statements:

```
proc hpmixed data=Sim;
 class Species Farm Animal;
 model Yield = Species Species*Farm;
 random Animal;
 test Species*Farm;
 contrast 'Species1 = Species2 = Species3'
 Species 1 0 -1,
 Species 0 1 -1;
run;
```

Selected results from the preceding SAS statements are shown in [Figure 46.1](#) through [Figure 46.4](#).

The “Class Level Information” table in [Figure 46.1](#) shows that the three model effects have 5, 100, and 3000 levels, respectively. Only a portion of the levels are displayed by default. The “Dimensions” table shows

that the model contains a single G-side covariance parameter and a single R-side covariance parameter. R-side covariance parameters are those associated with the covariance matrix  $\mathbf{R}$  in the conditional distribution, given the random effects. In the case of the HPMIXED procedure this matrix is simply  $\mathbf{R} = \sigma^2\mathbf{I}$  and the single R-side covariance parameter corresponds to the residual variance. The G-side parameter is the variance of the random Animal effect; the  $\mathbf{G}$  matrix is a diagonal ( $3000 \times 3000$ ) matrix with the common variance on the diagonal.

**Figure 46.1** Class Levels and Dimensions

| The HPMIXED Procedure   |        |                                                           |
|-------------------------|--------|-----------------------------------------------------------|
| Class Level Information |        |                                                           |
| Class                   | Levels | Values                                                    |
| Species                 | 5      | 1 2 3 4 5                                                 |
| Farm                    | 100    | 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18<br>19 20 ... |
| Animal                  | 3000   | 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18<br>19 20 ... |
| Dimensions              |        |                                                           |
| G-side Cov. Parameters  |        | 1                                                         |
| R-side Cov. Parameters  |        | 1                                                         |
| Columns in X            |        | 506                                                       |
| Columns in Z            |        | 3000                                                      |
| Subjects (Blocks in V)  |        | 1                                                         |

Taking into account the intercept as well as the number of levels of the Species and Species\*Farm effects, the  $\mathbf{X}$  matrix for this problem has 506 columns, so that the mixed model equations

$$\begin{bmatrix} \mathbf{X}'\mathbf{X} & \mathbf{X}'\mathbf{Z} \\ \mathbf{Z}'\mathbf{X} & \mathbf{Z}'\mathbf{Z} + \sigma^2\mathbf{G}^{-1} \end{bmatrix} \begin{bmatrix} \boldsymbol{\beta} \\ \boldsymbol{\gamma} \end{bmatrix} = \begin{bmatrix} \mathbf{X}'\mathbf{y} \\ \mathbf{Z}'\mathbf{y} \end{bmatrix}$$

have 3506 rows and columns. This is a substantial computational problem: simply storing a single copy of this matrix in dense format requires nearly 50 megabytes of memory. The sparse matrix techniques of PROC HPMIXED use a small fraction of this amount of memory and a similarly small fraction of the CPU time required to solve the equations with dense techniques. For more information about sparse versus dense techniques, see the section “[Sparse Matrix Techniques](#)” on page 3696.

Figure 46.2 displays the covariance parameter estimates at convergence of the REML algorithm. The variance component estimate for animal effect is  $\hat{\sigma}_a^2 = 3.9889$  and for residual  $\hat{\sigma}^2 = 7.9623$ . These estimates are close to the simulated values (4.0 and 8.0).

**Figure 46.2** Estimates of Variance Components

| Covariance Parameter Estimates |          |
|--------------------------------|----------|
| Cov Parm                       | Estimate |
| Animal                         | 3.9889   |
| Residual                       | 7.9623   |

The **TEST** statement requests a Type III test of the fixed effect in the model. By default, the HPMIXED procedure does not compute Type III tests, because they can be computationally demanding. The tests of the **Species\*Farm** effect is highly significant. That indicates animals of a genetic species perform differently in different environments.

**Figure 46.3** Type III Tests of Fixed Effect

| Type III Tests of Fixed Effects |           |           |         |        |
|---------------------------------|-----------|-----------|---------|--------|
| Effect                          | Num<br>DF | Den<br>DF | F Value | Pr > F |
| Species*Farm                    | 495       | 39500     | 11.72   | <.0001 |

You can use the **CONTRAST** or **ESTIMATE** statement to test custom linear hypotheses involving the fixed and/or random effects. The **CONTRAST** statement in the preceding program tests the null hypothesis that there are no differences among the first three genetic species. Results from this analysis are shown in **Figure 46.4**. The small *p*-value indicates that there are significant differences among the first three genetics species.

**Figure 46.4** Result of CONTRAST Statement

| Contrasts                      |           |           |         |        |
|--------------------------------|-----------|-----------|---------|--------|
| Label                          | Num<br>DF | Den<br>DF | F Value | Pr > F |
| Species1 = Species2 = Species3 | 2         | 39500     | 92.93   | <.0001 |

## Syntax: HPMIXED Procedure

The following statements are available in the HPMIXED procedure:

```

PROC HPMIXED < options > ;
 BY variables ;
 CLASS variable < (REF= option) > ... < variable < (REF= option) > > < / global-options > ;
 EFFECT name=effect-type (variables < / options >) ;
 ID variables ;
 MODEL dependent = < fixed-effects > < / options > ;
 RANDOM random-effects < / options > ;
 REPEATED repeated-effect < / options > ;
 PARMS < (value-list) ... > < / options > ;
 TEST fixed-effects < / options > ;
 CONTRAST 'label' contrast-specification < , contrast-specification > < , ... > < / options > ;
 ESTIMATE 'label' contrast-specification < (divisor=n) >
 < , 'label' contrast-specification < (divisor=n) > > < , ... > < / options > ;
 LSMEANS fixed-effects < / options > ;
 NLOPTIONS < options > ;
 OUTPUT < OUT=SAS-data-set >
 < keyword < (keyword-options) > < =name > > ...
 < keyword < (keyword-options) > < =name > > < / options > ;
 WEIGHT variable ;

```

Items within angle brackets ( < > ) are optional. The CONTRAST, ESTIMATE, LSMEANS, RANDOM, and TEST statements can appear multiple times; all other statements can appear only once.

The PROC HPMIXED and MODEL statements are required, and the MODEL statement must appear after the CLASS statement if these statements are included. The BY, CLASS, MODEL, ID, OUTPUT, TEST, RANDOM, REPEATED and WEIGHT statements are described in full after the PROC HPMIXED statement in alphabetical order. The EFFECT, is shared with many other procedures. Summary descriptions of functionality and syntax for this statement is also given after the PROC HPMIXED statement in alphabetical order, but you can find full documentation on it in Chapter 19, “Shared Concepts and Topics.”

Table 46.1 summarizes the basic functions and important options of each PROC HPMIXED statement.

**Table 46.1** Summary of PROC HPMIXED Statements

| Statement    | Description                                                                       | Options                                                             |
|--------------|-----------------------------------------------------------------------------------|---------------------------------------------------------------------|
| PROC HPMIXED | Invokes the procedure                                                             | DATA= specifies input data set, METHOD= specifies estimation method |
| BY           | Performs multiple PROC HPMIXED analyses in one invocation                         | None                                                                |
| CLASS        | Declares qualitative variables that create indicator variables in design matrices | None                                                                |



Table 46.1 *continued*

| Statement | Description                                                          | Options                                                                                                                                                                                       |
|-----------|----------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| ID        | Lists additional variables to be included in predicted values tables | None                                                                                                                                                                                          |
| MODEL     | Specifies dependent variable and fixed effects, setting up <b>X</b>  | <b>S</b> requests solution for fixed-effects parameters, <b>DDFM=</b> specifies denominator degrees of freedom method                                                                         |
| RANDOM    | Specifies random effects, setting up <b>Z</b> and <b>G</b>           | <b>SUBJECT=</b> creates block-diagonality, <b>TYPE=</b> specifies covariance structure, <b>S</b> requests solution for random-effects parameters                                              |
| REPEATED  | Sets up <b>R</b>                                                     | <b>SUBJECT=</b> creates block-diagonality, <b>TYPE=</b> specifies covariance structure, <b>R=</b> displays estimated blocks of <b>R</b> , <b>GROUP=</b> enables between-subject heterogeneity |
| PARMS     | Specifies a grid of initial values for the covariance parameters     | <b>HOLD=</b> and <b>NOITER</b> hold the covariance parameters or their ratios constant, <b>PARMS-DATA=</b> reads the initial values from a SAS data set                                       |
| CONTRAST  | Constructs custom hypothesis tests                                   | <b>E</b> displays the <b>L</b> matrix coefficients                                                                                                                                            |
| ESTIMATE  | Constructs custom scalar estimates                                   | <b>CL</b> produces confidence limits                                                                                                                                                          |
| LSMEANS   | Computes least squares means for classification fixed effects        | <b>DIFF</b> computes differences of the least squares means, <b>CL</b> produces confidence limits, <b>SLICE=</b> tests simple effects                                                         |
| WEIGHT    | Specifies a variable by which to weight <b>R</b>                     | None                                                                                                                                                                                          |

## PROC HPMIXED Statement

**PROC HPMIXED** < options > ;

The PROC HPMIXED statement invokes the HPMIXED procedure. Table 46.2 summarizes the options available in the PROC HPMIXED statement. These and other options in the PROC HPMIXED statement are then described fully in alphabetical order.

Table 46.2 PROC HPMIXED Statement Options

| Option               | Description                                         |
|----------------------|-----------------------------------------------------|
| <b>Basic Options</b> |                                                     |
| <b>DATA=</b>         | Specifies input data set                            |
| <b>METHOD=</b>       | Specifies the estimation method                     |
| <b>NOPROFILE</b>     | Includes scale parameter in optimization            |
| <b>ORDER=</b>        | Determines the sort order of <b>CLASS</b> variables |

Table 46.2 *continued*

| Option                        | Description                                                   |
|-------------------------------|---------------------------------------------------------------|
| BLUP                          | Computes BLUP/BLUE only                                       |
| <b>Displayed Output</b>       |                                                               |
| IC=                           | Displays a table of information criteria                      |
| ITDETAILS                     | Displays estimates and gradients added to “Iteration History” |
| MAXCLPRINT=                   | Specifies the maximum levels of CLASS variables to print      |
| LOGNOTE                       | Writes periodic status notes to the log                       |
| MMEQ                          | Displays mixed model equations                                |
| NOCLPRINT                     | Suppresses “Class Level Information” completely or in parts   |
| NOITPRINT                     | Suppresses “Iteration History” table                          |
| SIMPLE                        | Displays “Descriptive Statistics” table                       |
| <b>Singularity Tolerances</b> |                                                               |
| SINGCHOL=                     | Tunes singularity for Cholesky decompositions                 |
| SINGRES=                      | Tunes singularity for the residual variance                   |
| SINGULAR=                     | Tunes general singularity criterion                           |

You can specify the following *options*.

**BLUP**< (*suboptions*) >=*SAS-data-set*

creates a data set that contains the BLUE and BLUP solutions. The covariance parameters are assumed to be known and given by PARMs statement. All hypothesis testing is ignored. The statements TEST, ESTIMATE, CONTRAST, LSMEANS, and OUTPUT are all ignored. This option is designed for users who need BLUP solutions for random effects with many levels, up to tens of millions.

You can specify the following suboptions:

ITPRINT=*number* specifies that the iteration history be displayed after every *number* of iterations. This suboption applies only for iterative solving methods (IOC or IOD). The default value is 10, which means the procedure displays the iteration history for every 10 iterations.

MAXITER=*number* specifies the maximum number of iterations allowed. This applies only for iterative solving methods (IOC or IOD). The default value is the number of parameters in the BLUE/BLUP plus two.

METHOD=DIRECT|IOC|IOD specifies the method used to solve for BLUP solutions. METHOD=DIRECT requires storing mixed model equations (MMEQ) in memory and computing the Cholesky decomposition of MMEQ. This method is the most accurate, but it is the most inefficient in terms of speed and memory. METHOD=IOD does not build mixed model equations; instead it iterates on data to solve for the solutions. This method is most efficient in terms of memory. METHOD=IOC requires storing mixed model equations in memory and iterates on MMEQ to solve for the solutions. This method is the most efficient in terms of speed. The default method is IOC.

TOL=*number* specifies the tolerance value. This suboption applies only for iterative solving methods (IOC or IOD). The default value is the square root of machine precision.

**DATA=SAS-data-set**

names the SAS data set to be used by PROC HPMIXED. The default is the most recently created data set.

**INFOCRIT=NONE | PQ | Q****IC=NONE | PQ | Q**

determines the computation of information criteria in the “Fit Statistics” table. The criteria are all in smaller-is-better form, and are described in Table 46.3.

**Table 46.3** Information Criteria

| Criteria | Formula                                                                                       | Reference                                                  |
|----------|-----------------------------------------------------------------------------------------------|------------------------------------------------------------|
| AIC      | $-2\ell + 2d$                                                                                 | Akaike (1974)                                              |
| AICC     | $-2\ell + 2dn^*/(n^* - d - 1)$ for $n^* \geq d + 2$<br>$-2\ell + 2d(d + 2)$ for $n^* < d + 2$ | Hurvich and Tsai (1989) and<br>Burnham and Anderson (1998) |
| HQIC     | $-2\ell + 2d \log(\log(n))$ for $n > 1$                                                       | Hannan and Quinn (1979)                                    |
| BIC      | $-2\ell + d \log(n)$ for $n > 0$                                                              | Schwarz (1978)                                             |
| CAIC     | $-2\ell + d(\log(n) + 1)$ for $n > 0$                                                         | Bozdogan (1987)                                            |

Here  $\ell$  denotes the maximum value of the restricted log likelihood,  $d$  is the dimension of the model, and  $n, n^*$  reflect the size of the data. When  $n \leq 1$ , the value of the HQIC criterion is  $-2\ell$ . When  $n=0$ , the values of the BIC and CAIC criteria are undefined.

The quantities  $d, n$ , and  $n^*$  depend on the model and IC= option.

- models without random effects:
  - The IC=Q and IC=PQ options have no effect on the computation.
  - $d$  equals the number of parameters in the optimization whose solutions do not fall on the boundary or are otherwise constrained.
  - $n$  equals the number of used observations minus  $\text{rank}(\mathbf{X})$ .
  - $n^*$  equals  $n$ , unless  $n < d + 2$ , in which case  $n^* = d + 2$ .
- models with random effects:
  - $d$  equals the number of parameters in the optimization whose solutions do not fall on the boundary or are otherwise constrained. If IC=PQ, this value is incremented by  $\text{rank}(\mathbf{X})$ .
  - $n$  equals the effective number of subjects as displayed in the “Dimensions” table, unless this value equals 1, in which case  $n$  equals the number of levels of the first random effect specified. The IC=Q and IC=PQ options have no effect.
  - $n^*$  equals  $n$ , unless  $n < d + 2$ , in which case  $n^* = d + 2$ . The IC=Q and IC=PQ options have no effect.

The IC=NONE option suppresses the “Fit Statistics” table. IC=Q is the default.

**ITDETAILS**

displays the parameter values at each iteration and enables the writing of notes to the SAS log pertaining to “infinite likelihood” and “singularities” during optimization iterations.

**LOGNOTE**

writes to the log periodic notes that describe the current status of computations. This option is designed for use with analyses that require extensive CPU resources.

**MAXCLPRINT=number**

specifies the maximum levels of CLASS variables to print in the ODS table “ClassLevels.” The default value is 20. MAXCLPRINT=0 enables you to print all levels of each CLASS variable. However, the option **NOCLPRINT** takes precedence over MAXCLPRINT.

**METHOD=**

specifies the estimation method for the covariance parameters. The REML specification performs residual (restricted) maximum likelihood, and it is currently the only available method. This option is therefore currently redundant for PROC HPMIXED, but it is included for consistency with other mixed model procedures in SAS/STAT software.

**MMEQ**

displays coefficients of the mixed model equations. These are

$$\begin{bmatrix} \mathbf{X}'\widehat{\mathbf{R}}^{-1}\mathbf{X} & \mathbf{X}'\widehat{\mathbf{R}}^{-1}\mathbf{Z} \\ \mathbf{Z}'\widehat{\mathbf{R}}^{-1}\mathbf{X} & \mathbf{Z}'\widehat{\mathbf{R}}^{-1}\mathbf{Z} + \widehat{\mathbf{G}}^{-1} \end{bmatrix} \begin{bmatrix} \mathbf{X}'\widehat{\mathbf{R}}^{-1}\mathbf{y} \\ \mathbf{Z}'\widehat{\mathbf{R}}^{-1}\mathbf{y} \end{bmatrix}$$

assuming  $\widehat{\mathbf{G}}$  is nonsingular. If  $\widehat{\mathbf{G}}$  is singular, PROC HPMIXED produces the following coefficients

$$\begin{bmatrix} \mathbf{X}'\widehat{\mathbf{R}}^{-1}\mathbf{X} & \mathbf{X}'\widehat{\mathbf{R}}^{-1}\mathbf{Z}\widehat{\mathbf{G}} \\ \widehat{\mathbf{G}}\mathbf{Z}'\widehat{\mathbf{R}}^{-1}\mathbf{X} & \widehat{\mathbf{G}}\mathbf{Z}'\widehat{\mathbf{R}}^{-1}\mathbf{Z}\widehat{\mathbf{G}} + \widehat{\mathbf{G}} \end{bmatrix} \begin{bmatrix} \mathbf{X}'\widehat{\mathbf{R}}^{-1}\mathbf{y} \\ \widehat{\mathbf{G}}\mathbf{Z}'\widehat{\mathbf{R}}^{-1}\mathbf{y} \end{bmatrix}$$

See the section “Model and Assumptions” on page 3693 for further information about these equations.

**NAMELEN=number**

specifies the length to which long effect names are shortened. The default and minimum value is 20.

**NLPRINT**

requests that optimization-related output options specified in the NLOPTIONS statement override corresponding options in the PROC HPMIXED statement. When you specify NLPRINT, the ITDE-  
TAILS and NOITPRINT options in the PROC HPMIXED statement are ignored and the following six options in the NLOPTIONS statement are enabled: NOPRINT, PHISTORY, PSUMMARY, PALL, PLONG, and PHISTPARMS.

The syntax and options of the NLOPTIONS statement are described in the section “NLOPTIONS Statement” on page 482 in Chapter 19, “Shared Concepts and Topics.”

**NOCLPRINT<=number>**

suppresses the display of the “Class Level Information” table if you do not specify *number*. If you do specify *number*, only levels with totals that are less than *number* are listed in the table.

**NOFIT**

suppresses fitting of the model. When the NOFIT option is in effect, PROC HPMIXED produces the “Model Information,” “Class Level Information,” “Number of Observations,” “Dimensions,” and “Descriptive Statistics” tables. These can be helpful in gauging the computational effort required to fit the model.

**NOINFO**

suppresses the display of the “Model Information,” “Number of Observations,” and “Dimensions” tables.

**NOITPRINT**

suppresses the display of the “Iteration History” table.

**NOPRINT**

suppresses the normal display of results. The NOPRINT option is useful when you want only to create one or more output data sets with the procedure by using the **OUTPUT** statement. Note that this option temporarily disables the Output Delivery System (ODS); see Chapter 20, “Using the Output Delivery System,” for more information.

**NOPROFILE**

includes the residual variance as one of the covariance parameters in the optimization iterations. This option applies only to models that have a residual variance parameter. By default, this parameter is profiled out of the optimization iterations, except when you have specified the **HOLD=** option in the **PARMS** statement.

**ORDER=DATA | FORMATTED | FREQ | INTERNAL**

specifies the sort order for the levels of the classification variables (which are specified in the **CLASS** statement). This option applies to the levels for all classification variables, except when you use the (default) **ORDER=FORMATTED** option with numeric classification variables that have no explicit format. With this option, the levels of such variables are ordered by their internal value.

The **ORDER=** option can take the following values:

| Value of <b>ORDER=</b> | Levels Sorted By                                                                                                                       |
|------------------------|----------------------------------------------------------------------------------------------------------------------------------------|
| <b>DATA</b>            | Order of appearance in the input data set                                                                                              |
| <b>FORMATTED</b>       | External formatted value, except for numeric variables with no explicit format, which are sorted by their unformatted (internal) value |
| <b>FREQ</b>            | Descending frequency count; levels with the most observations come first in the order                                                  |
| <b>INTERNAL</b>        | Unformatted value                                                                                                                      |

By default, **ORDER=FORMATTED**. For **ORDER=FORMATTED** and **ORDER=INTERNAL**, the sort order is machine-dependent. For more information about sort order, see the chapter on the **SORT** procedure in the *Base SAS Procedures Guide* and the discussion of **BY**-group processing in *SAS Language Reference: Concepts*.

**SIMPLE**

displays the mean, standard deviation, coefficient of variation, minimum, and maximum for each variable used in **PROC HPMIXED** that is not a classification variable.

**SINGCHOL=number**

tunes the singularity criterion in Cholesky decompositions. The default is 1E6 times the machine epsilon; this product is approximately 1E–10 on most computers.

**SINGRES=number**

sets the tolerance for which the residual variance is considered to be zero. The default is 1E4 times the machine epsilon; this product is approximately 1E–12 on most computers.

**SINGULAR=number**

tunes the general singularity criterion applied by the HPMIXED procedure in divisions and inversions. The default is 1E4 times the machine epsilon; this product is approximately 1E–12 on most computers.

**UPDATE**

is an alias for the [LOGNOTE](#) option.

## BY Statement

**BY variables ;**

You can specify a BY statement with PROC HPMIXED to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the HPMIXED procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

Since sorting the data changes the order in which PROC HPMIXED reads observations, the sort order for the levels of the [CLASS](#) variable might be affected if you have specified [ORDER=DATA](#) in the [PROC HPMIXED](#) statement. This, in turn, affects specifications in the [CONTRAST](#) and [ESTIMATE](#) statements.

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

## CLASS Statement

**CLASS** *variable* <(REF= option)> ... <*variable* <(REF= option)>> </global-options> ;

The CLASS statement names the classification variables to be used in the model. Typical classification variables are Treatment, Sex, Race, Group, and Replication. If you use the CLASS statement, it must appear before the MODEL statement.

Classification variables can be either character or numeric. By default, class levels are determined from the entire set of formatted values of the CLASS variables.

**NOTE:** Prior to SAS 9, class levels were determined by using no more than the first 16 characters of the formatted values. To revert to this previous behavior, you can use the TRUNCATE option in the CLASS statement.

In any case, you can use formats to group values into levels. See the discussion of the FORMAT procedure in the *Base SAS Procedures Guide* and the discussions of the FORMAT statement and SAS formats in *SAS Formats and Informats: Reference*. You can adjust the order of CLASS variable levels with the ORDER= option in the PROC HPMIXED statement.

You can specify the following REF= option to indicate how the levels of an individual classification variable are to be ordered by enclosing it in parentheses after the variable name:

**REF= 'level' | FIRST | LAST**

specifies a level of the classification variable to be put at the end of the list of levels. (In procedures that solve mixed model equations by sequentially sweeping rows and columns, this level thus corresponds to the reference level in the usual interpretation of the estimates of a singular parameterization. However, since PROC HPMIXED does not necessarily solve mixed model equations in the original order, this interpretation of the specified REF= level does not apply for this procedure.) You can specify the *level* of the variable to use as the reference level; specify a value that corresponds to the formatted value of the variable if a format is assigned. Alternatively, you can specify REF=FIRST to designate that the first ordered level serve as the reference, or REF=LAST to designate that the last ordered level serve as the reference. To specify that REF=FIRST or REF=LAST be used for all classification variables, use the REF= *global-option* after the slash (/) in the CLASS statement.

You can specify the following *global-options* in the CLASS statement after a slash (/):

**REF=FIRST | LAST**

specifies a level of all classification variables to be put at the end of the list of levels. (In procedures that solve mixed model equations by sequentially sweeping rows and columns, this level thus corresponds to the reference level in the usual interpretation of the estimates of a singular parameterization. However, since PROC HPMIXED does not necessarily solve mixed model equations in the original order, this interpretation of the specified REF= level does not apply for this procedure.) Specify REF=FIRST to designate that the first ordered level for each classification variable serve as the reference. Specify REF=LAST to designate that the last ordered level serve as the reference. This option applies to all the variables specified in the CLASS statement. To specify different reference levels for different classification variables, use REF= options for individual variables.

**TRUNCATE**

specifies that class levels be determined by using only up to the first 16 characters of the formatted values of CLASS variables. When formatted values are longer than 16 characters, you can use this option to revert to the levels as determined in releases prior to SAS 9.



## CONTRAST Statement

**CONTRAST** *label* *contrast-specification* < , *contrast-specification* > < , ... > < / *options* > ;

The CONTRAST statement provides a mechanism for obtaining custom hypothesis tests. It is patterned after the CONTRAST statement in PROC MIXED and enables you to select an appropriate inference space (McLean, Sanders, and Stroup 1991).

You can test the hypothesis  $\mathbf{L}'\boldsymbol{\phi} = \mathbf{0}$ , where  $\mathbf{L}' = [\mathbf{K}' \mathbf{M}']$  and  $\boldsymbol{\phi}' = [\boldsymbol{\beta}' \boldsymbol{\gamma}']$ , in several inference spaces. The inference space corresponds to the choice of  $\mathbf{M}$ . When  $\mathbf{M} = \mathbf{0}$ , your inferences apply to the entire population from which the random effects are sampled; this is known as the *broad* inference space. When all elements of  $\mathbf{M}$  are nonzero, your inferences apply only to the observed levels of the random effects. This is known as the *narrow* inference space, and you can also choose it by specifying all of the random effects as fixed. The GLM procedure uses the narrow inference space. Finally, by zeroing portions of  $\mathbf{M}$  corresponding to selected main effects and interactions, you can choose *intermediate* inference spaces. The broad inference space is usually the most appropriate, and it is used when you do not specify any random effects in the CONTRAST statement.

In the CONTRAST statement,

|                               |                                                                                                                                                                                                                                                 |
|-------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <i>label</i>                  | identifies the contrast in the table. A label is required for every contrast specified. Labels can be up to 20 characters and must be enclosed in single quotes.                                                                                |
| <i>contrast-specification</i> | identifies the fixed effects and random effects and their coefficients from which the $\mathbf{L}$ matrix is formed. The syntax representation of a <i>contrast-specification</i> is < fixed-effect values ... > <   random-effect values ... > |
| <i>fixed-effect</i>           | identifies an effect that appears in the <b>MODEL</b> statement. The keyword INTERCEPT can be used as an effect when an intercept is fitted in the model. You do not need to include all effects that are in the <b>MODEL</b> statement.        |
| <i>random-effect</i>          | identifies an effect that appears in the <b>RANDOM</b> statement. The first random effect must follow a vertical bar ( ); however, random effects do not have to be specified.                                                                  |
| <i>values</i>                 | are constants that are elements of the $\mathbf{L}$ matrix associated with the fixed and random effects.                                                                                                                                        |

The rows of  $\mathbf{L}'$  are specified in order and are separated by commas. The rows of the  $\mathbf{K}'$  component of  $\mathbf{L}'$  are specified on the left side of the vertical bars (|). These rows test the fixed effects and are, therefore, checked for estimability. The rows of the  $\mathbf{M}'$  component of  $\mathbf{L}'$  are specified on the right side of the vertical bars. They test the random effects, and no estimability checking is necessary.

If PROC HP MIXED finds the fixed-effects portion of the specified contrast to be nonestimable (see the **SINGULAR=** option on page 3671), then it displays missing values for the test statistics and a note in the log.

If the elements of  $\mathbf{L}$  are not specified for an effect that contains a specified effect, then the elements of the specified effect are automatically “filled in” over the levels of the higher-order effect. This feature is designed to preserve estimability for cases where there are complex higher-order effects. The coefficients for the higher-order effect are determined by equitably distributing the coefficients of the lower-level effect as in the construction of least squares means. In addition, if the intercept is specified, it is distributed over all classification effects that are not contained by any other specified effect. If an effect is not specified and



does not contain any specified effects, then all of its coefficients in **L** are set to 0. You can override this behavior by specifying coefficients for the higher-order effect.

If too many values are specified for an effect, the extra ones are ignored; if too few are specified, the remaining ones are set to 0. If no random effects are specified, the vertical bar can be omitted; otherwise, it must be present. If a SUBJECT effect is used in the **RANDOM** statement, then the coefficients specified for the effects in the **RANDOM** statement are equitably distributed across the levels of the SUBJECT effect. You can use the **E** option to see exactly what **L** matrix is used.

The **SUBJECT** and **GROUP** options in the **CONTRAST** statement are useful for the case where a **SUBJECT=** or **GROUP=** variable appears in the **RANDOM** statement, and you want to contrast different subjects or groups. By default, **CONTRAST** statement coefficients about random effects are distributed equally across subjects and groups.

PROC HPMIXED handles missing level combinations of CLASS variables similarly to the way PROC GLM does. Both procedures delete fixed-effects parameters corresponding to missing levels in order to preserve estimability. However, PROC HPMIXED does not delete missing level combinations for random-effects parameters because linear combinations of the random-effects parameters are always estimable. These conventions can affect the way you specify your **CONTRAST** coefficients.

The **CONTRAST** statement computes the statistic

$$F = \frac{\begin{bmatrix} \hat{\beta} \\ \hat{\gamma} \end{bmatrix}' \mathbf{L}(\mathbf{L}'\hat{\mathbf{C}}\mathbf{L})^{-1}\mathbf{L}' \begin{bmatrix} \hat{\beta} \\ \hat{\gamma} \end{bmatrix}}{r}$$

where  $r = \text{rank}(\mathbf{L}'\hat{\mathbf{C}}\mathbf{L})$  and approximates its distribution with an  $F$  distribution. In this expression,  $\hat{\mathbf{C}}$  is an estimate of the generalized inverse of the coefficient matrix in the mixed model equations.

The numerator degree of freedom in the  $F$  approximation is  $r = \text{rank}(\mathbf{L}'\hat{\mathbf{C}}\mathbf{L})$ , and the denominator degree of freedom is taken from the “Type III Tests of Fixed Effects” table and corresponds to the final effect you list in the **CONTRAST** statement. You can change the denominator degrees of freedom by using the **DF=** option.

You can specify the following *options* in the **CONTRAST** statement after a slash (/).

#### **CHISQ**

requests that  $\chi^2$  tests be performed in addition to any  $F$  tests. A  $\chi^2$  statistic equals its corresponding  $F$  statistic times the associate numerator degree of freedom, and this same degree of freedom is used to compute the  $p$ -value for the  $\chi^2$  test. This  $p$ -value will always be less than that for the  $F$  test, as it effectively corresponds to an  $F$  test with infinite denominator degrees of freedom.

#### **DF=number**

specifies the denominator degrees of freedom for the  $F$  test. The default is the denominator degrees of freedom taken from the “Type III Tests of Fixed Effects” table and corresponds to the final effect you list in the **CONTRAST** statement.

#### **E**

requests that the **L** matrix coefficients for the contrast be displayed. The name of this “L Matrix Coefficients” table is “Coef.”

**GROUP** *coeffs*

sets up random-effect contrasts between different groups when a **GROUP=** variable appears in the **RANDOM** statement. By default, **CONTRAST** statement coefficients about random effects are distributed equally across groups. If you enter a multi-row contrast, you can also enter multiple rows for the **GROUP** coefficients. If the number of **GROUP** coefficients is less than the number of contrasts in the **CONTRAST** statement, the **HPMIXED** procedure cycles through the **GROUP** coefficients. For example, the following two statements are equivalent:

```
contrast 'Trt @ x=0.4 and 0.5' trt 1 -1 0 | x 0.4,
 trt 1 0 -1 | x 0.4,
 trt 1 -1 0 | x 0.5,
 trt 1 0 -1 | x 0.5 /
 group 1 -1, 1 0 -1, 1 -1, 1 0 -1;

contrast 'Trt @ x=0.4 and 0.5' trt 1 -1 0 | x 0.4,
 trt 1 0 -1 | x 0.4,
 trt 1 -1 0 | x 0.5,
 trt 1 0 -1 | x 0.5 /
 group 1 -1, 1 0 -1;
```

**SINGULAR=***number*

tunes the estimability checking. If  $\mathbf{v}$  is a vector, define  $\text{ABS}(\mathbf{v})$  to be the largest absolute value of the element of  $\mathbf{v}$  with the largest absolute value. If  $\text{ABS}(\mathbf{K}' - \mathbf{K}'\mathbf{T})$  is greater than  $c \cdot \text{number}$  for any row of  $\mathbf{K}'$  in the contrast, then  $\mathbf{K}$  is declared nonestimable. Here  $\mathbf{T}$  is the Hermite form matrix  $(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{X}$ , and  $c$  is  $\text{ABS}(\mathbf{K}')$  except when it equals 0, and then  $c$  is 1. The value for *number* must be between 0 and 1; the default is 1E-4.

**SUBJECT** *coeffs*

sets up random-effect contrasts between different subjects when a **SUBJECT=** variable appears in the **RANDOM** statement. By default, **CONTRAST** statement coefficients about random effects are distributed equally across subjects. Listing subject coefficients for multiple row **CONTRASTS** follows the same rules as for **GROUP** coefficients.

---

**EFFECT Statement**

**EFFECT** *name=effect-type (variables </ options>);*

The **EFFECT** statement enables you to construct special collections of columns for design matrices. These collections are referred to as *constructed effects* to distinguish them from the usual model effects that are formed from continuous or classification variables, as discussed in the section “[GLM Parameterization of Classification Variables and Effects](#)” on page 383 in Chapter 19, “[Shared Concepts and Topics](#).”

You can specify the following *effect-types*:

- COLLECTION** is a collection effect that defines one or more variables as a single effect with multiple degrees of freedom. The variables in a collection are considered as a unit for estimation and inference.
- LAG** is a classification effect in which the level that is used for a given period corresponds to the level in the preceding period.

|                          |                                                                                                                                                                                                           |
|--------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>MULTIMEMBER   MM</b>  | is a multimember classification effect whose levels are determined by one or more variables that appear in a CLASS statement.                                                                             |
| <b>POLYNOMIAL   POLY</b> | is a multivariate polynomial effect in the specified numeric variables.                                                                                                                                   |
| <b>SPLINE</b>            | is a regression spline effect whose columns are univariate spline expansions of one or more variables. A spline expansion replaces the original variable with an expanded or larger set of new variables. |

Table 46.4 summarizes the *options* available in the EFFECT statement.

**Table 46.4** EFFECT Statement Options

| Option                             | Description                                                                                                                                          |
|------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Collection Effects Options</b>  |                                                                                                                                                      |
| DETAILS                            | Displays the constituents of the collection effect                                                                                                   |
| <b>Lag Effects Options</b>         |                                                                                                                                                      |
| DESIGNROLE=                        | Names a variable that controls to which lag design an observation is assigned                                                                        |
| DETAILS                            | Displays the lag design of the lag effect                                                                                                            |
| NLAG=                              | Specifies the number of periods in the lag                                                                                                           |
| PERIOD=                            | Names the variable that defines the period                                                                                                           |
| WITHIN=                            | Names the variable or variables that define the group within which each period is defined                                                            |
| <b>Multimember Effects Options</b> |                                                                                                                                                      |
| NOEFFECT                           | Specifies that observations with all missing levels for the multimember variables should have zero values in the corresponding design matrix columns |
| WEIGHT=                            | Specifies the weight variable for the contributions of each of the classification effects                                                            |
| <b>Polynomial Effects Options</b>  |                                                                                                                                                      |
| DEGREE=                            | Specifies the degree of the polynomial                                                                                                               |
| MDEGREE=                           | Specifies the maximum degree of any variable in a term of the polynomial                                                                             |
| STANDARDIZE=                       | Specifies centering and scaling suboptions for the variables that define the polynomial                                                              |
| <b>Spline Effects Options</b>      |                                                                                                                                                      |
| BASIS=                             | Specifies the type of basis (B-spline basis or truncated power function basis) for the spline expansion                                              |
| DEGREE=                            | Specifies the degree of the spline transformation                                                                                                    |
| KNOTMETHOD=                        | Specifies how to construct the knots for spline effects                                                                                              |

For more information about the syntax of these *effect-types* and how columns of constructed effects are computed, see the section “EFFECT Statement” on page 393 in Chapter 19, “Shared Concepts and Topics.”

The HPMIXED procedure does not support the SPLIT or SEPARATED option in spline effects and poly effects.

## ESTIMATE Statement

```
ESTIMATE 'label' contrast-specification <(divisor=n)>
 <, 'label' contrast-specification <(divisor=n)>> <, ... > </ options > ;
```

The ESTIMATE statement provides a mechanism for obtaining custom hypothesis tests. As in the **CONTRAST** statement, the basic element of the ESTIMATE statement is the *contrast-specification*, which consists of **MODEL** and **RANDOM** effects and their coefficients. Specifically, a *contrast-specification* takes the form

```
< fixed-effect values ... > < | random-effect values ... >
```

Based on the *contrast-specifications* in your ESTIMATE statement, PROC HPMIXED constructs the matrix  $L' = [K' M']$ , as in the **CONTRAST** statement, where **K** is associated with the fixed effects and **M** is associated with the G-side random effects.

PROC HPMIXED then produces for each row *l* of  $L'$  an approximate *t* test of the hypothesis  $H: l\phi = 0$ , where  $\phi = [\beta' \gamma']'$ . Results from all ESTIMATE statement are combined in the “Estimates” ODS table.

Note that multi-row estimates are permitted. Unlike the **CONTRAST** statement, you need to specify a *'label'* for every row of the multi-row estimate, since PROC HPMIXED produces one test per row.

PROC HPMIXED selects the degrees of freedom to match those displayed in the “Type III Tests of Fixed Effects” table for the final effect you list in the ESTIMATE statement. You can modify the degrees of freedom by using the **DF=** option. If you select **DDFM=NONE** and do not modify the degrees of freedom by using the **DF=** option, PROC HPMIXED uses infinite degrees of freedom, essentially computing approximate *z* tests.

If PROC HPMIXED finds the fixed-effects portion of the specified estimate to be nonestimable, then it displays “Non-est” for the estimate entry.

The construction of the **L** matrix for an ESTIMATE statement follows the same rules as listed under the **CONTRAST** statement.

Table 46.5 summarizes the options available in the ESTIMATE statement.

**Table 46.5** ESTIMATE Statement Options

| Option    | Description                                      |
|-----------|--------------------------------------------------|
| ALPHA=    | Specifies the confidence level                   |
| CL        | Constructs <i>t</i> -type confidence limits      |
| DF=       | Specifies the degrees of freedom                 |
| DIVISOR=  | Specifies values to divide the coefficients      |
| E         | Displays the matrix coefficients                 |
| GROUP     | Sets up random-effect contrasts between groups   |
| SINGULAR= | Tunes the estimability checking                  |
| SUBJECT   | Sets up random-effect estimates between subjects |

You can specify the following *options* in the ESTIMATE statement after a slash (/).

**ALPHA=number**

requests that a *t*-type confidence interval be constructed with confidence level  $1 - \text{number}$ . The value of *number* must be between 0 and 1 exclusively; the default is 0.05. If **DDFM=NONE** and you do not specify degrees of freedom with the **DF=** option, PROC HPMIXED uses infinite degrees of freedom, essentially computing a *z* interval.

**CL**

requests that *t*-type confidence limits be constructed. If **DDFM=NONE** and you do not specify degrees of freedom with the **DF=** option, PROC HPMIXED uses infinite degrees of freedom, essentially computing a *z* interval. The confidence level is 0.95 by default.

**DF=number**

specifies the degrees of freedom for the *t*-test. The default is the denominator degrees of freedom taken from the “Type III Tests of Fixed Effects” table and corresponds to the final effect you list in the ESTIMATE statement.

**DIVISOR=value-list**

specifies a list of values by which to divide the coefficients so that fractional coefficients can be entered as integer numerators. If you do not specify *value-list*, a default value of 1.0 is assumed. Missing values in the *value-list* are converted to 1.0.

If the number of elements in *value-list* exceeds the number of rows of the estimate, the extra values are ignored. If the number of elements in *value-list* is less than the number of rows of the estimate, the last value in *value-list* is copied forward.

If you specify a row-specific divisor as part of the specification of the estimate row, this value multiplies the corresponding divisor implied by the *value-list*. For example, the following statement divides the coefficients in the first row by 8, and the coefficients in the third and fourth row by 3:

```
estimate 'One vs. two' A 2 -2 (divisor=2),
 'One vs. three' A 1 0 -1 ,
 'One vs. four' A 3 0 0 -3 ,
 'One vs. five' A 1 0 0 0 -1 / divisor=4,.,3;
```

**E**

requests that the matrix coefficients be displayed. For ODS purposes, the name of this “L Matrix Coefficients” table is “Coef.”

**GROUP coeffs**

sets up random-effect contrasts between different groups when a **GROUP=** variable appears in the **RANDOM** statement. By default, ESTIMATE statement coefficients about random effects are distributed equally across groups. If you enter a multi-row estimate, you can also enter multiple rows for the GROUP coefficients. If the number of GROUP coefficients is less than the number of contrasts in the ESTIMATE statement, the HPMIXED procedure cycles through the GROUP coefficients. For example, the following two statements are equivalent:

```

estimate 'Trt 1 vs 2 @ x=0.4' trt 1 -1 0 | x 0.4,
 'Trt 1 vs 3 @ x=0.4' trt 1 0 -1 | x 0.4,
 'Trt 1 vs 2 @ x=0.5' trt 1 -1 0 | x 0.5,
 'Trt 1 vs 3 @ x=0.5' trt 1 0 -1 | x 0.5 /
 group 1 -1, 1 0 -1, 1 -1, 1 0 -1;

estimate 'Trt 1 vs 2 @ x=0.4' trt 1 -1 0 | x 0.4,
 'Trt 1 vs 3 @ x=0.4' trt 1 0 -1 | x 0.4,
 'Trt 1 vs 2 @ x=0.5' trt 1 -1 0 | x 0.5,
 'Trt 1 vs 3 @ x=0.5' trt 1 0 -1 | x 0.5 /
 group 1 -1, 1 0 -1;

```

**SINGULAR=number**

tunes the estimability checking as documented for the **SINGULAR=** in the **CONTRAST** statement.

**SUBJECT coeffs**

sets up random-effect estimates between different subjects when a **SUBJECT=** variable appears in the **RANDOM** statement. By default, **ESTIMATE** statement coefficients about random effects are distributed equally across subjects. Listing subject coefficients for an **ESTIMATE** statement with multiple rows follows the same rules as for **GROUP** coefficients.

## ID Statement

**ID variables ;**

The **ID** statement specifies which variables from the input data set are to be included in the **OUT=** data sets from the **OUTPUT** statement. If you do not specify an **ID** statement, then all variables are included in these data sets. Otherwise, only the variables you list in the **ID** statement are included. Specifying an **ID** statement with no variables prevents any variables from being included in these data sets.

## LSMEANS Statement

**LSMEANS fixed-effects </ options > ;**

The **LSMEANS** statement computes least squares means (LS-means) of fixed effects. As in the **GLM** procedure, LS-means are *predicted population margins*—that is, they estimate the marginal means over a balanced population. In a sense, LS-means are to unbalanced designs as classification and subclassification arithmetic means are to balanced designs. The **L** matrix constructed to compute them is the same as the **L** matrix formed in **PROC GLM**; however, the standard errors are adjusted for the covariance parameters in the model.

Each LS-mean is computed as  $L'\hat{\beta}$ , where **L** is the coefficient matrix associated with the least squares mean and  $\hat{\beta}$  is the estimate of the fixed-effects parameter vector. The approximate standard errors for the LS-mean is computed as the square root of  $L'(X'\hat{V}^{-1}X)^{-1}L$ .

LS-means can be computed for any effect in the **MODEL** statement that involves **CLASS** variables. You can specify multiple effects in one **LSMEANS** statement or in multiple **LSMEANS** statements, and all **LSMEANS** statements must appear after the **MODEL** statement. As in the **ESTIMATE** statement, the **L**

matrix is tested for estimability, and if this test fails, PROC HPMIXED displays “Non-est” for the LS-means entries.

Assuming the LS-mean is estimable, PROC HPMIXED constructs an approximate  $t$  test to test the null hypothesis that the associated population quantity equals zero. By default, the denominator degrees of freedom for this test are the same as those displayed for the effect in the “Type III Tests of Fixed Effects” table (see the section “TEST Statement” on page 3692).

Table 46.6 summarizes the options available in the LSMEANS statement.

**Table 46.6** LSMEANS Statement Options

| Option        | Description                                          |
|---------------|------------------------------------------------------|
| ALPHA=        | Specifies the confidence level                       |
| CL            | Constructs $t$ -type confidence limits               |
| CORR          | Displays the estimated correlation matrix            |
| COV           | Displays the estimated covariance matrix             |
| DF=           | Specifies the degrees of freedom                     |
| DIFF or PDIFF | Displays the differences of the LS-means             |
| E             | Displays the matrix coefficients for LSMEANS effects |
| SINGULAR=     | Tunes the estimability checking                      |
| SLICE=        | Partitions interaction LSMEANS effects               |

You can specify the following *options* in the LSMEANS statement after a slash (/).

**ALPHA=number**

requests that a  $t$ -type confidence interval be constructed for each of the LS-means with confidence level  $1 - \text{number}$ . The value of *number* must be between 0 and 1; the default is 0.05.

**CL**

requests that  $t$ -type confidence limits be constructed for each of the LS-means. If **DDFM=NONE**, then PROC HPMIXED uses infinite degrees of freedom for this test, essentially computing a  $z$  interval. The confidence level is 0.95 by default; this can be changed with the **ALPHA=** option.

**CORR**

displays the estimated correlation matrix of the least squares means as part of the “Least Squares Means” table.

**COV**

displays the estimated covariance matrix of the least squares means as part of the “Least Squares Means” table.

**DF=number**

specifies the degrees of freedom for the  $t$  test and confidence limits. The default is the denominator degrees of freedom taken from the “Type III Tests of Fixed Effects” table corresponding to the LS-means effect. For these **DDFM=** methods, degrees of freedom are determined separately for each test; see the **DDFM=** option on page 3679 for more information.

**DIFF**<=*difftype*>

**PDIFF**<=*difftype*>

requests that differences of the LS-means be displayed. You can specify the following values for the optional *difftype*.

**DIFF=ALL** requests all pairwise differences; it is the default.

**DIFF=ANOM** requests differences between each LS-mean and the average LS-mean, as in the analysis of means (Ott 1967). The average is computed as a weighted mean of the LS-means, with the weights being inversely proportional to the diagonal entries of the  $L(X'X)^{-1}L'$  matrix. When a **WEIGHT** statement is specified, then the preceding matrix is replaced with  $L(X'WX)^{-1}L'$  where **W** is the diagonal matrix that contains the weights. If LS-means are nonestimable, this design-based weighted mean is replaced with an equally weighted mean. Note that the ANOM procedure in SAS/QC software implements both tables and graphics for the analysis of means with a variety of response types. For one-way designs and normally distributed data, the **DIFF=ANOM** computations are equivalent to the results of **PROC ANOM**.

**DIFF=CONTROL** requests differences with a control; by default, the control is the first level of each of the specified LSMEANS effects. To specify which levels of the effects are the controls, list the quoted formatted values in parentheses after the **CONTROL** keyword. For example, if the effects A, B, and C are classification variables, each having two levels, 1 and 2, the following LSMEANS statement specifies the (1,2) level of A\*B and the (2,1) level of B\*C as controls:

```
lsmeans A*B B*C / diff=control('1' '2' '2' '1');
```

For multiple effects, the results depend upon the order of the list, and so you should check the output to make sure that the controls are correct.

**CONTROL** produces two-tailed tests and confidence limits.

**DIFF=CONTROLL** requests one-tailed results and tests whether the noncontrol levels are significantly smaller than the control. The upper confidence limits for the control minus the noncontrol levels are considered to be infinity and are displayed as missing.

**DIFF=CONTROLU** requests one-tailed results and tests whether the noncontrol levels are significantly larger than the control. The upper confidence limits for the noncontrol levels minus the control are considered to be infinity and are displayed as missing.

The differences of the LS-means are displayed in a table titled “Differences of Least Squares Means.” The table name is “Diffs.”

**E**

requests that the matrix coefficients for all LSMEANS effects be displayed. The name of this “Matrix Coefficients” table is “Coef.”

**PDIFF**

is the same as the **DIFF** option. See the description of the **DIFF** option on page 3677.



**SINGULAR=number**

tunes the estimability checking as documented for the **SINGULAR=** in the **CONTRAST** statement.

**SLICE=fixed-effect****SLICE=(fixed-effects)**

specifies effects by which to partition interaction LSMEANS effects. This can produce what are known as tests of simple effects (Winer 1971). For example, suppose that **A\*B** is significant, and you want to test the effect of **A** for each level of **B**. The appropriate LSMEANS statement is

```
lsmeans A*B / slice=B;
```

This statement tests for the simple main effects of **A** for **B**, which are calculated by extracting the appropriate rows from the coefficient matrix for the **A\*B** LS-means and by using them to form an *F* test.

The **SLICE=** option produces *F* tests that test the simultaneous equality of cell means at a fixed level of the slice effect (Schabenberger, Gregoire, and Kong 2000).

The **SLICE=** option produces a table titled “Tests of Effect Slices.” The table name is “Slices.”

## MODEL Statement

**MODEL** *dependent* = < *fixed-effects* > < / *options* > ;

The **MODEL** statement names a single dependent variable and the fixed effects, which determine the **X** matrix of the mixed model. The specification of effects is the same as in the GLM procedure; however, unlike PROC GLM, you do not specify random effects in the **MODEL** statement. The **MODEL** statement is required.

An intercept is included in the fixed-effects model by default. If no fixed effects are specified, only this intercept term is fit. The intercept can be removed by using the **NOINT** option.

You can specify the following *options* in the **MODEL** statement after a slash (/).

**ALPHA=number**

requests that a *t*-type confidence interval be constructed for each of the fixed-effects parameters with confidence level  $1 - \textit{number}$ . The value of *number* must be between 0 and 1; the default is 0.05.

**CL**

requests that *t*-type confidence limits be constructed for each of the fixed-effects parameter estimates. The confidence level is 0.95 by default; this can be changed with the **ALPHA=** option.

**DDF=value-list**

enables you to specify your own denominator degrees of freedom for the fixed effects. The *value-list* specification is a list of numbers or missing values (.) separated by commas. The degrees of freedom should be listed in the order in which the effects appear in the “Type III Tests of Fixed Effects” table. If you want to retain the default degrees of freedom for a particular effect, use a missing value for its location in the list. For example, the following statement assigns 3 denominator degrees of freedom to **A** and 4.7 to **A\*B**, while those for **B** remain the same:

```
model Y = A B A*B / ddf=3, ., 4.7;
```

**DDFM=RESIDUAL | NONE**

specifies the method for computing the denominator degrees of freedom for the tests of fixed effects resulting from the MODEL, CONTRAST, ESTIMATE, LSMEANS, and TEST statements.

The DDFM=RESIDUAL option performs all tests by using the residual degrees of freedom,  $n - \text{rank}(\mathbf{X})$ , where  $n$  is the number of observations used. It is the default degrees of freedom method.

DDFM=NONE specifies that no denominator degrees of freedom be applied. PROC HPMIXED then essentially assumes that infinite degrees of freedom are available in the calculation of  $p$ -values. The  $p$ -values for  $t$  tests are then identical to  $p$ -values derived from the standard normal distribution. In the case of  $F$  tests, the  $p$ -values equal those of chi-square tests determined as follows: if  $F_{obs}$  is the observed value of the  $F$  test with  $l$  numerator degrees of freedom, then

$$p = \Pr\{F_{l,\infty} > F_{obs}\} = \Pr\{\chi_l^2 > lF_{obs}\}$$

**NOINT**

requests that no intercept be included in the model. An intercept is included by default.

**SOLUTION | S**

requests that a solution for the fixed-effects parameters be produced. Using notation from the section “Model Assumptions” on page 3693, the fixed-effects parameter estimates are  $\hat{\beta}$  and their approximate standard errors are the square roots of the diagonal elements of  $(\mathbf{X}'\hat{\mathbf{V}}^{-1}\mathbf{X})^{-}$ .

Along with the estimates and their approximate standard errors, a  $t$  statistic is computed as the estimate divided by its standard error. The degree of freedom for this  $t$  statistic matches the one appearing in the “Type III Tests of Fixed Effects” table under the effect containing the parameter. The “Pr > |t|” column contains the two-tailed  $p$ -value corresponding to the  $t$  statistic and associated degrees of freedom.

**ZETA=number**

tunes the sensitivity in forming Type III functions. Any element in the estimable function basis with an absolute value less than *number* is set to 0. The default is 1E–8.

**NLOPTIONS Statement**

```
NLOPTIONS < options >;
```

For more information about the NLOPTIONS, see the section “NLOPTIONS Statement” on page 482 in Chapter 19, “Shared Concepts and Topics.”

If you choose TECH=NEWRAP, then the default value of LSPRECISION is 0.4 in the HPMIXED procedure.

**OUTPUT Statement**

```
OUTPUT < OUT=SAS-data-set >
 < keyword< (keyword-options) > < =name >> ...
 < keyword< (keyword-options) > < =name >> < / options >;
```

The OUTPUT statement creates a data set that contains predicted values and residual diagnostics, computed after fitting the model. By default, all variables in the original data set are included in the output data set.

You can use the ID statement to select a subset of the variables from the input data set to be added to the output data set.

For example, suppose that the data set Scores contains the variables score, machine, and person. The following statements fit a model with fixed machine and random person effects and save the predicted and residual values to the data set igaussout:

```
proc hpmixed data = Scores;
 class machine person score;
 model score = machine;
 random person;
 output out=igaussout pred=p resid=r;
run;
```

You can specify the following *options* in the OUTPUT statement before the slash (/).

#### OUT=SAS data set

specifies the name of the output data set. If the OUT= option is omitted, the procedure uses the DATA*n* convention to name the output data set.

#### keyword <(keyword-options)> <=name>

specifies a statistic to include in the output data set and optionally assigns the variable the name name. You can use the *keyword-options* to control which type of a particular statistic to compute. The *keyword-options* can take on the following values:

- BLUP                uses the predictors of the random effects in computing the statistic.
- NOBLUP            does not use the predictors of the random effects in computing the statistic.

The default is to compute statistics by using BLUPs. For example, the following two OUTPUT statements are equivalent:

```
output out=out1 pred=predicted lcl=lower;
output out=out1 pred(blup)=predicted lcl(blup)=lower;
```

If a particular combination of keyword and keyword options is not supported, the statistic is not computed and a message is produced in the SAS log.

A *keyword* can appear multiple times in the OUTPUT statement. Table 46.7 lists the keywords and the default names assigned by the HPMIXED procedure if you do not specify a *name*. In this table, *y* denotes the response variable.

**Table 46.7** Keywords for Output Statistics

| Keyword   | Options | Description                            | Expression                                                                                | Name   |
|-----------|---------|----------------------------------------|-------------------------------------------------------------------------------------------|--------|
| PREDICTED | BLUP    | Linear predictor                       | $\hat{\eta} = \mathbf{x}'\hat{\boldsymbol{\beta}} + \mathbf{z}'\hat{\boldsymbol{\gamma}}$ | Pred   |
|           | NOBLUP  | Marginal linear predictor              | $\hat{\eta}_m = \mathbf{x}'\hat{\boldsymbol{\beta}}$                                      | PredPA |
| STDERR    | BLUP    | Standard deviation of linear predictor | $\sqrt{\text{Var}[\hat{\eta} - \mathbf{z}'\boldsymbol{\gamma}]}$                          | StdErr |

Table 46.7 (continued)

| Keyword  | Options | Description                                          | Expression                                               | Name       |
|----------|---------|------------------------------------------------------|----------------------------------------------------------|------------|
|          | NOBLUP  | Standard deviation of marginal linear predictor      | $\sqrt{\widehat{\text{Var}}[\widehat{\eta}_m]}$          | StdErrPA   |
| RESIDUAL | BLUP    | Residual                                             | $r = y - \widehat{\eta}$                                 | Resid      |
|          | NOBLUP  | Marginal residual                                    | $r_m = y - \widehat{\eta}_m$                             | ResidPA    |
| PEARSON  | BLUP    | Pearson-type residual                                | $r / \sqrt{\widehat{\text{Var}}[y \boldsymbol{\gamma}]}$ | Pearson    |
|          | NOBLUP  | Marginal Pearson-type residual                       | $r_m / \sqrt{\widehat{\text{Var}}[y]}$                   | PearsonPA  |
| STUDENT  | BLUP    | Studentized residual                                 | $r / \sqrt{\widehat{\text{Var}}[r]}$                     | Student    |
|          | NOBLUP  | Studentized marginal residual                        | $r_m / \sqrt{\widehat{\text{Var}}[r_m]}$                 | StudentPA  |
| LCL      | BLUP    | Lower prediction limit for linear predictor          |                                                          | LCL        |
|          | NOBLUP  | Lower confidence limit for marginal linear predictor |                                                          | LCLPA      |
| UCL      | BLUP    | Upper prediction limit for linear predictor          |                                                          | UCL        |
|          | NOBLUP  | Upper confidence limit for marginal linear predictor |                                                          | UCLPA      |
| VARIANCE | BLUP    | Conditional variance of response variable            | $\widehat{\text{Var}}[y \boldsymbol{\gamma}]$            | Variance   |
|          | NOBLUP  | Marginal variance of response variable               | $\widehat{\text{Var}}[y]$                                | VariancePA |

You can use the following shortcuts to request statistics: PRED for PREDICTED, STD for STDERR, RESID for RESIDUAL, VAR for VARIANCE.

You can specify the following options of the OUTPUT statement after the slash (/).

### ALLSTATS

requests that all statistics are computed. If you do not use a keyword to assign a name, the HPMIXED procedure uses the default name.

### ALPHA=*number*

determines the coverage probability for two-sided confidence and prediction intervals. The coverage probability is computed as  $1 - \textit{number}$ . The value of *number* must be between 0 and 1 inclusively; the default is 0.05.

### NOMISS

requests that records from the input data set be written to the output data only for those observations that were used in the analysis. By default, the HPMIXED procedure produces output statistics for all observations in the input data set.

**NOUNIQUE**

requests that names not be made unique in the case of naming conflicts. By default, the HPMIXED procedure avoids naming conflicts by assigning a unique name to each output variable. If you specify the NOUNIQUE option, variables with conflicting names are not renamed. In that case, the first variable added to the output data set takes precedence.

**NOVAR**

requests that variables from the input data set not be added to the output data set. This option ignores ID statement but does not apply to variables listed in a BY statement.

---

**PARMS Statement**

**PARMS** <(value-list)... > </options> ;

The PARMS statement specifies initial values for the covariance parameters, or it requests a grid search over several values of these parameters. You must specify the values in the order in which they appear in the “Covariance Parameter Estimates” table.

The *value-list* specification can take any of several forms:

|                        |                                                                                                           |
|------------------------|-----------------------------------------------------------------------------------------------------------|
| $m$                    | a single value                                                                                            |
| $m_1, m_2, \dots, m_n$ | several values                                                                                            |
| $m$ to $n$             | a sequence where $m$ equals the starting value, $n$ equals the ending value, and the increment equals 1   |
| $m$ to $n$ by $i$      | a sequence where $m$ equals the starting value, $n$ equals the ending value, and the increment equals $i$ |
| $m_1, m_2$ to $m_3$    | mixed values and sequences                                                                                |

You can use the PARMS statement to input known parameters. Suppose the three variance components are known to be 2, 1, and 3. The SAS statements to fix the variance components at these values are as follows:

```
proc hpmixed noprofile;
 class Family Gender;
 model Height = Gender;
 random Family Family*Gender;
 parms (2) (1) (3) / noiter;
run;
```

The NOPROFILE option in the PROC HPMIXED statement suppresses profiling the residual variance parameter during its calculations, thereby enabling its value to be held at 3 as specified in the PARMS statement.

If you specify more than one set of initial values, PROC HPMIXED performs a grid search of the likelihood surface and uses the best point on the grid for subsequent analysis. Specifying a large number of grid points can result in long computing times. The grid search feature is also useful for exploring the likelihood surface.

The results from the PARMS statement are the values of the parameters on the specified grid (denoted by CovP1–CovPn), the residual variance (possibly estimated) for models with a residual variance parameter, and various functions of the likelihood.

The name of the “Parameter Search” table is “ParmSearch.”

You can specify the following *options* in the PARMs statement after a slash (/).

**HOLD=***value-list*

#### **HOLD**

specifies which parameter values **PROC HPMIXED** should hold to equal the specified values. To hold all parameters, you can use the second form without giving the *value-list*. For example, the following statement constrains the first and third covariance parameters to equal 5 and 2, respectively.

Specifying the HOLD= option implies the **NOPROFILE** option in the **PROC HPMIXED** statement:

```
parms (5) (3) (2) (3) / hold=1,3;
```

**LOWERB=***value-list*

enables you to specify lower boundary constraints on the covariance parameters. The *value-list* specification is a list of numbers or missing values (.) separated by commas. You must list the numbers in the order that **PROC HPMIXED** uses for the covariance parameters, and each number corresponds to the lower boundary constraint. A missing value instructs **PROC HPMIXED** to use its default constraint, and if you do not specify numbers for all of the covariance parameters, **PROC MIXED** assumes the remaining ones are missing.

#### **NOITER**

requests that no optimization iterations be performed and that **PROC HPMIXED** use the best value from the grid search to perform inferences. By default, iterations begin at the best value from the PARMs grid search. This option is ignored when you specify the **HOLD=** option.

If a residual variance is profiled, the parameter estimates can change from the initial values you provide as the residual variance is recomputed. To prevent an update of the residual variance, combine the **NOITER** option with the **NOPROFILE** option in the **PROC HPMIXED** statements, as in the following program:

```
proc hpmixed noprofile;
 class A B C rep mp sp;
 model y = A | B | C;
 random rep mp sp;
 parms (180) (200) (170) (1000) / noiter;
run;
```

Specifying the **NOITER** option in the PARMs statement has the same effect as specifying **TECHNIQUE=NONE** in the **NLOPTIONS** statement.

Notice that the **NOITER** option can be useful if you want to obtain the starting values **HPMIXED** computes. The following statements produce the starting values:

```
proc hpmixed noprofile;
 class A B;
 model y = A;
 random int / subject=B;
 parms / noiter;
run;
```

**PARMSDATA=SAS-data-set**

**PDATA=SAS data set**

reads in covariance parameter values from a SAS data set. The data set should contain the numerical variable ESTIMATE or the numerical variables Covp1–Covp $q$ , where  $q$  denotes the number of covariance parameters.

If the PARMSDATA= data set contains multiple sets of covariance parameters, the HPMIXED procedure evaluates the initial objective function for each set and commences the optimization step by using the set with the lowest function value as the starting values. For example, the following SAS statements request that the objective function be evaluated for three sets of initial values:

```
data data_covp;
 input covp1-covp4;
 datalines;
180 200 170 1000
170 190 160 900
160 180 150 800
;
proc hpmixed;
 class A B C rep;
 model yield = A;
 random rep B C;
 parms / pdata=data_covp;
run;
```

Each set comprises four covariance parameters.

The order of the observations in a data set with the numerical variable Estimate corresponds to the order of the covariance parameters in the “Covariance Parameter Estimates” table.

The PARMSDATA= data set must contain at least one set of covariance parameters with no missing values.

If the HPMIXED procedure is processing the input data set in BY groups, you can add the BY variables to the PARMSDATA= data set. If this data set is sorted by the BY variables, the HPMIXED procedure matches the covariance parameter values to the current BY group. If the PARMSDATA= data set does not contain all BY variables, the data set is processed in its entirety for every BY group and a message is written to the log. This enables you to provide a single set of starting values across BY groups, as in the following statements:

```
data data_covp;
 input covp1-covp4;
 datalines;
180 200 170 1000
;
proc hpmixed;
 class A B C rep;
 model yield = A;
 random rep B C;
 parms / pdata=data_covp;
 by year;
run;
```

The same set of starting values is used for each value of the year variable.

**UPPERB=value-list**

enables you to specify upper boundary constraints on the covariance parameters. The *value-list* specification is a list of numbers or missing values (.) separated by commas. You must list the numbers in the order that PROC HP MIXED uses for the covariance parameters, and each number corresponds to the upper boundary constraint. A missing value instructs PROC HP MIXED to use its default constraint, and if you do not specify numbers for all of the covariance parameters, PROC HP MIXED assumes that the remaining ones are missing.

---

## RANDOM Statement

**RANDOM** *random-effects* </ options > ;

The RANDOM statement defines the random effects in the mixed model. It can be used to specify traditional variance component models (as in the VARCOMP procedure) and to specify random coefficients. The random effects can be classification or continuous. Multiple RANDOM statements are possible. Random effects specified in a RANDOM statement could be correlated with each other for certain types of covariance structures (see the TYPE= option on page 3686). It is, however, assumed that random effects specified using different RANDOM statements are not correlated.

Using notation from the section “Model Assumptions” on page 3693, the purpose of the RANDOM statement is to define the  $\mathbf{Z}$  matrix of the mixed model, the random effects in the  $\boldsymbol{\gamma}$  vector, and the structure of  $\mathbf{G}$ . The  $\mathbf{Z}$  matrix is constructed exactly like the  $\mathbf{X}$  matrix for the fixed effects, and the  $\mathbf{G}$  matrix is constructed to correspond to the effects constituting  $\mathbf{Z}$ . The structure of  $\mathbf{G}$  is defined by using the TYPE= option described on page 3686.

You can specify INTERCEPT (or INT) as a random effect. PROC HP MIXED does not include the intercept in the RANDOM statement by default, as it does in the MODEL statement.

You can specify the following *options* in the RANDOM statement after a slash (/).

**ALPHA=number**

requests that a  $t$ -type confidence interval with confidence level  $1 - \text{number}$  be constructed for the predictors of random effects in this statement. The value of *number* must be between 0 and 1 exclusively; the default is 0.05. Specifying the ALPHA= option implies the CL option.

**CL**

requests that  $t$ -type confidence limits be constructed for each of the predictors of random effects in this statement. The confidence level is 0.95 by default; this can be changed with the ALPHA= option. The CL option implies the SOLUTION option.

**GROUP=effect**

defines an effect specifying heterogeneity in the covariance structure of  $\mathbf{G}$ . All observations having the same level of the group effect have the same covariance parameters. Each new level of the group effect produces a new set of covariance parameters with the same structure as the original group. You should exercise caution in defining the group effect, because strange covariance patterns can result from its misuse. Also, the group effect can greatly increase the number of estimated covariance parameters, which can adversely affect the optimization process.



Continuous variables are permitted as arguments to the GROUP= option. PROC HPMIXED does not sort by the values of the continuous variable; rather, it considers the data to be from a new group whenever the value of the continuous variable changes from the previous observation. Using a continuous variable decreases execution time for models with a large number of groups and also prevents the production of a large “Class Levels Information” table.

### NOFULLZ

eliminates the columns in  $\mathbf{Z}$  corresponding to missing levels of random effects involving CLASS variables. By default, these columns are included in  $\mathbf{Z}$ . It is sufficient to specify the NOFULLZ option in any RANDOM statement.

### SOLUTION

requests that the solution for the random-effects parameters be produced. Using notation from the section “Model Assumptions” on page 3693, these estimates are the empirical best linear unbiased predictors (BLUPs)  $\hat{\boldsymbol{\gamma}} = \hat{\mathbf{G}}\mathbf{Z}'\hat{\mathbf{V}}^{-1}(\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}})$ . They can be useful for comparing the random effects from different experimental units and can also be treated as residuals in performing diagnostics for your mixed model.

The numbers displayed in the SE Pred column of the “Solution for Random Effects” table are not the standard errors of the  $\hat{\boldsymbol{\gamma}}$  displayed in the Estimate column; rather, they are the standard errors of predictions  $\hat{\boldsymbol{\gamma}}_i - \boldsymbol{\gamma}_i$ , where  $\hat{\boldsymbol{\gamma}}_i$  is the  $i$ th BLUP and  $\boldsymbol{\gamma}_i$  is the  $i$ th random-effect parameter.

### SUBJECT=effect

identifies the subjects in your mixed model. Complete independence is assumed across subjects; thus, for the RANDOM statement, the SUBJECT= option produces a block-diagonal structure in  $\mathbf{G}$  with identical blocks. The  $\mathbf{Z}$  matrix is modified to accommodate this block-diagonality. In fact, specifying a subject effect is equivalent to nesting all other effects in the RANDOM statement within the subject effect.

Continuous variables are permitted as arguments to the SUBJECT= option. PROC HPMIXED does not sort by the values of the continuous variable; rather, it considers the data to be from a new subject whenever the value of the continuous variable changes from the previous observation. Using a continuous variable decreases execution time for models with a large number of subjects and also prevents the production of a large “Class Levels Information” table.

### TYPE=covariance-structure

specifies the structure of the covariance matrix  $\mathbf{G}$  for random effects. The default structure is VC.

If you want different covariance structures in different parts of  $\mathbf{G}$ , you must use multiple RANDOM statements with different TYPE= options.

Valid values for *covariance-structure* are listed in Table 46.8. Examples are shown in Table 46.9.

**Table 46.8** Covariance Structures

| Structure | Description            | Parameters | $(i, j)$ element                              |
|-----------|------------------------|------------|-----------------------------------------------|
| AR(1)     | Autoregressive(1)      | 2          | $\sigma^2\rho^{ i-j }$                        |
| CHOL      | Cholesky root          | $t(t+1)/2$ | $l_{ij}$                                      |
| CS        | Compound symmetry (CS) | 2          | $\sigma_1 + \sigma^2 1(i=j)$                  |
| CSH       | Heterogeneous CS       | $t+1$      | $\sigma_i\sigma_j[\rho 1(i \neq j) + 1(i=j)]$ |

**Table 46.8** *continued*

| Structure | Description              | Parms        | (i, j) element                                                  |
|-----------|--------------------------|--------------|-----------------------------------------------------------------|
| UC        | Uniform correlation (UC) | 2            | $\sigma^2[\rho 1(i \neq j) + 1(i = j)]$                         |
| UCH       | Heterogeneous UC         | $t + 1$      | $\sigma_i \sigma_j [\rho 1(i \neq j) + 1(i = j)]$               |
| UN        | Unstructured             | $t(t + 1)/2$ | $\sigma_{ij}$                                                   |
| VC        | Variance components      | $q$          | $\sigma_k^2 1(i = j)$<br>and $i, j$ correspond to $k$ th effect |

In Table 46.8,  $t$  is the overall dimension of the covariance matrix, and  $1(A)$  equals 1 when  $A$  is true and 0 otherwise. For example,  $1(i = j)$  equals 1 when  $i = j$  and equals 0 otherwise. TYPE=UCH is the same as TYPE=CSH.

Table 46.9 lists some examples of the structures in Table 46.8.

**Table 46.9** Covariance Structure Examples

| Description                | Structure | Example                                                                                                                                                                                                                                                                                                                                                                                            |
|----------------------------|-----------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| First-order autoregressive | AR(1)     | $\sigma^2 \begin{bmatrix} 1 & \rho & \rho^2 & \rho^3 \\ \rho & 1 & \rho & \rho^2 \\ \rho^2 & \rho & 1 & \rho \\ \rho^3 & \rho^2 & \rho & 1 \end{bmatrix}$                                                                                                                                                                                                                                          |
| Cholesky root              | CHOL      | $\begin{bmatrix} l_{11} & 0 & 0 & 0 \\ l_{21} & l_{22} & 0 & 0 \\ l_{31} & l_{32} & l_{33} & 0 \\ l_{41} & l_{42} & l_{43} & l_{44} \end{bmatrix} \begin{bmatrix} l_{11} & l_{21} & l_{31} & l_{41} \\ 0 & l_{22} & l_{32} & l_{42} \\ 0 & 0 & l_{33} & l_{43} \\ 0 & 0 & 0 & l_{44} \end{bmatrix}$                                                                                                |
| Compound symmetry          | CS        | $\begin{bmatrix} \sigma^2 + \sigma_1 & \sigma_1 & \sigma_1 & \sigma_1 \\ \sigma_1 & \sigma^2 + \sigma_1 & \sigma_1 & \sigma_1 \\ \sigma_1 & \sigma_1 & \sigma^2 + \sigma_1 & \sigma_1 \\ \sigma_1 & \sigma_1 & \sigma_1 & \sigma^2 + \sigma_1 \end{bmatrix}$                                                                                                                                       |
| Uniform correlation        | UC        | $\sigma^2 \begin{bmatrix} 1 & \rho & \rho & \rho \\ \rho & 1 & \rho & \rho \\ \rho & \rho & 1 & \rho \\ \rho & \rho & \rho & 1 \end{bmatrix}$                                                                                                                                                                                                                                                      |
| Heterogeneous UC           | UCH       | $\begin{bmatrix} \sigma_1^2 & \sigma_1 \sigma_2 \rho & \sigma_1 \sigma_3 \rho & \sigma_1 \sigma_4 \rho \\ \sigma_2 \sigma_1 \rho & \sigma_2^2 & \sigma_2 \sigma_3 \rho & \sigma_2 \sigma_4 \rho \\ \sigma_3 \sigma_1 \rho & \sigma_3 \sigma_2 \rho & \sigma_3^2 & \sigma_3 \sigma_4 \rho \\ \sigma_4 \sigma_1 \rho & \sigma_4 \sigma_2 \rho^2 & \sigma_4 \sigma_3 \rho & \sigma_4^2 \end{bmatrix}$ |
| Unstructured               | UN        | $\begin{bmatrix} \sigma_1^2 & \sigma_{21} & \sigma_{31} & \sigma_{41} \\ \sigma_{21} & \sigma_2^2 & \sigma_{32} & \sigma_{42} \\ \sigma_{31} & \sigma_{32} & \sigma_3^2 & \sigma_{34} \\ \sigma_{41} & \sigma_{42} & \sigma_{43} & \sigma_4^2 \end{bmatrix}$                                                                                                                                       |

Table 46.9 continued

| Description         | Structure    | Example                                                                                                                              |
|---------------------|--------------|--------------------------------------------------------------------------------------------------------------------------------------|
| Variance components | VC (default) | $\begin{bmatrix} \sigma_A^2 & 0 & 0 & 0 \\ 0 & \sigma_A^2 & 0 & 0 \\ 0 & 0 & \sigma_B^2 & 0 \\ 0 & 0 & 0 & \sigma_B^2 \end{bmatrix}$ |

The variances and covariances in the formulas that follow in the TYPE= descriptions are expressed in terms of generic random variables  $\xi_i$  and  $\xi_j$ . They represent random effects for which the  $\mathbf{G}$  matrices are constructed.

The following list provides some further information about these covariance structures:

TYPE=AR(1) specifies a first-order autoregressive structure,

$$\text{Cov}[\xi_i, \xi_j] = \sigma^2 \rho^{|i-j|}$$

The values  $i$  and  $j$  are derived for the  $i$ th and  $j$ th observations, respectively. For example, in the following statements the values correspond to the class levels for the time effect of the  $i$ th and  $j$ th observation within a particular subject:

```
proc hpmixed;
 class time patient;
 model y = x x*x;
 random time / sub=patient type=ar(1);
run;
```

PROC HPMIXED imposes the constraint  $|\rho| < 1$  for stationarity.

TYPE=CHOL specifies an unstructured variance-covariance matrix parameterized through its Cholesky root. All diagonal values are constrained to be positive. This parameterization guarantees a positive definite covariance matrix. For example, a  $2 \times 2$  unstructured covariance matrix can be written as

$$\text{Var}[\boldsymbol{\xi}] = \begin{bmatrix} \sigma_1^2 & \sigma_{21} \\ \sigma_{21} & \sigma_2^2 \end{bmatrix}$$

Without imposing constraints on the three parameters, there is no guarantee that the estimated variance matrix is positive definite. Even if  $\sigma_1^2$  and  $\sigma_2^2$  are nonzero, a large value for  $\sigma_{21}$  can lead to a negative eigenvalue of  $\text{Var}[\boldsymbol{\xi}]$ . The Cholesky root of a positive definite matrix  $\mathbf{A}$  is a lower triangular matrix  $\mathbf{L}$  such that  $\mathbf{LL}' = \mathbf{A}$ . The Cholesky root of the above  $2 \times 2$  matrix can be written as

$$\mathbf{L} = \begin{bmatrix} l_{11} & 0 \\ l_{21} & l_{22} \end{bmatrix}$$

The elements of the unstructured variance matrix are then simply  $\sigma_1^2 = l_{11}^2$ ,  $\sigma_{21} = l_{21}l_{11}$ , and  $\sigma_2^2 = l_{21}^2 + l_{22}^2$ . Similar operations yield the generalization to covariance matrices of higher orders.

For example, the following statements model the covariance matrix of each subject as an unstructured matrix:

```

proc hpmixed;
 class sub;
 model y = x;
 random time / sub=patient type=chol;
run;

```

The HPMIXED procedure constrains the diagonal elements of the Cholesky root to be positive. This guarantees that the structure is positive definite.

TYPE=CS specifies the compound-symmetry structure, which has constant variance and constant covariance

$$\text{Cov}[\xi_i, \xi_j] = \begin{cases} \sigma^2 + \sigma_1 & i = j \\ \sigma_1 & i \neq j \end{cases}$$

Under compound-symmetry, the  $\mathbf{G}$  matrix is of form  $\sigma^2\mathbf{I} + \sigma_1\mathbf{J}$ . The variance parameter  $\sigma^2$  is constrained to be positive, and the covariance parameter  $\sigma_1$  is constrained to be greater than  $-\sigma^2/t$  where  $t$  is the dimension of the structure. This guarantees the structure is positive definite. The compound-symmetry structure arises naturally with nested random effects, such as when a subsampling error is nested within an experimental error.

TYPE=CSH specifies the heterogeneous compound-symmetry structure. This structure has a different variance parameter for each diagonal element, and it uses the square roots of these parameters in the off-diagonal entries. In Table 46.8,  $\sigma_i^2$  is the  $i$ th variance parameter that satisfies  $\sigma_i^2 > 0$ , and  $\rho$  is the correlation parameter that satisfies  $\rho > -1/(t-1)$ , where  $t$  is the dimension of the structure. This guarantees that the structure is positive definite.

TYPE=UC specifies the uniform correlation structure, which has constant variance and constant correlation

$$\text{Cov}[\xi_i, \xi_j] = \begin{cases} \sigma^2 & i = j \\ \sigma^2\rho & i \neq j \end{cases}$$

Under uniform correlation, the  $\mathbf{G}$  matrix is of form  $\sigma^2[(1-\rho)\mathbf{I} + \rho\mathbf{J}]$ . The variance  $\sigma^2$  is constrained to be positive, and the correlation  $\rho$  is constrained to be greater than  $-1/(t-1)$ , where  $t$  is the dimension of the structure. This guarantees the structure is positive definite. This structure is equivalent to the compound-symmetry structure with a better numerical property in terms of optimization.

The uniform correlation structure arises frequently in agriculture and animal sciences.

TYPE=UCH specifies the heterogeneous uniform correlation structure. This structure has a different variance parameter for each diagonal element, and it uses the square roots of these parameters in the off-diagonal entries. In Table 46.8,  $\sigma_i^2$  is the  $i$ th variance parameter that satisfies  $\sigma_i^2 > 0$ , and  $\rho$  is the correlation parameter that satisfies  $\rho > -1/(t-1)$ , where  $t$  is the dimension of the structure. This guarantees that the structure is positive definite.

TYPE=UN specifies a completely general (unstructured) covariance matrix parameterized directly in terms of variances and covariances. The variances are constrained to be

positive, and the covariances are unconstrained. In addition, this structure is internally constrained to be positive definite.

**TYPE=VC** specifies standard variance components and is the default structure for the **RANDOM** and **REPEATED** statements. In the **RANDOM** statement, a distinct variance component is assigned to each effect. In the **REPEATED** statement, this structure is usually used only with the **GROUP=** option to specify a heterogeneous variance model.

## REPEATED Statement

**REPEATED** *repeated-effect* </ options > ;

The **REPEATED** statement defines the repeated effect and the residual covariance structure in the mixed model. The residual variance-covariance matrix is denoted as **R**. The *repeated-effect* is required and consists entirely of classification variables. The levels of the *repeated-effect* must be different for each observation within a subject in order to avoid the singular **R** matrix. The **SUBJECT=** option is required. The data set must be grouped by subject effect.

Table 46.10 summarizes the options available in the **REPEATED** statement.

**Table 46.10** Summary of **REPEATED** Statement Options

| Option                                      | Description                                                                                 |
|---------------------------------------------|---------------------------------------------------------------------------------------------|
| <b>Construction of Covariance Structure</b> |                                                                                             |
| <b>GROUP=</b>                               | Defines an effect that specifies heterogeneity in the residual covariance structure         |
| <b>SUBJECT=</b>                             | Identifies the subjects in the residual covariance structure                                |
| <b>TYPE=</b>                                | Specifies the residual covariance structure (the default is VC)                             |
| <b>Statistical Output</b>                   |                                                                                             |
| <b>R=</b>                                   | Displays blocks of the estimated <b>R</b> matrix                                            |
| <b>RC=</b>                                  | Display the Cholesky root (lower) of blocks of the estimated <b>R</b> matrix                |
| <b>RCI=</b>                                 | Displays the inverse Cholesky root (lower) of blocks of the estimated <b>R</b> matrix       |
| <b>RCORR=</b>                               | Displays the correlation matrix that corresponds to blocks of the estimated <b>R</b> matrix |
| <b>RI=</b>                                  | Displays the inverse of blocks of the estimated <b>R</b> matrix                             |

You can specify the following *options* in the **REPEATED** statement after a slash (/).

**GROUP=effect**

**GRP=effect**

defines an effect that specifies heterogeneity in the residual covariance structure. All observations that have the same level of the **GROUP** effect have the same covariance parameters. Each new level of the **GROUP** effect produces a new set of covariance parameters with the same structure as the original

group. You should exercise caution in defining the GROUP effect, because strange covariance patterns can result with its misuse. Also, the GROUP effect can greatly increase the number of estimated covariance parameters, which can adversely affect the optimization process.

Continuous variables are permitted as arguments to the GROUP= option. PROC HPMIXED does not sort by the values of the continuous variable; rather, it considers the data to be from a new subject or group whenever the value of the continuous variable changes from the previous observation. Using a continuous variable decreases execution time for models with a large number of subjects or groups and also prevents the production of a large “Class Level Information” table.

**R<=value-list>**

requests that blocks of the estimated **R** matrix be displayed. The first block determined by the **SUBJECT=** effect is the default displayed block.

The *value-list* indicates the subjects for which blocks of **R** are to be displayed. For example, the following statement displays block matrices for the first, third, and fifth persons:

```
repeated time / type=un subject=person r=1,3,5;
```

See the **PARMS** statement for the possible forms of *value-list*.

**RC<=value-list>**

displays the Cholesky root of blocks of the estimated **R** matrix. The *value-list* specification is the same as for the **R=** option.

**RCI<=value-list>**

displays the inverse Cholesky root of blocks of the estimated **R** matrix. The *value-list* specification is the same as for the **R=** option.

**RCORR<=value-list>**

displays the correlation matrix that corresponds to blocks of the estimated **R** matrix. The *value-list* specification is the same as for the **R=** option.

**RI<=value-list>**

produces the inverse of blocks of the estimated **R** matrix. The *value-list* specification is the same as for the **R=** option.

**SUBJECT=effect**

**SUB=effect**

identifies the subjects in your mixed model. Complete independence is assumed across subjects; therefore, the **SUBJECT=** option produces a block-diagonal structure in **R** with identical blocks. The **SUBJECT=** option is required. The data set must be grouped by **SUBJECT=** effect. When the **SUBJECT=** effect consists entirely of classification variables, the blocks of **R** correspond to observations that share the same level of that effect. These blocks are sorted according to this effect as well.

Continuous variables are permitted as arguments to the **SUBJECT=** option. PROC HPMIXED does not sort by the values of the continuous variable; rather, it considers the data to be from a new subject or group whenever the value of the continuous variable changes from the previous observation. Using a continuous variable decreases execution time for models with a large number of subjects or groups and also prevents the production of a large “Class Level Information” table.

If you want to model nonzero covariance among all of the observations in your data, specify `SUBJECT=INTERCEPT` to treat the data as if they are all from one subject. However, be aware that in this case PROC HPMIXED manipulates an **R** matrix with dimensions equal to the number of observations.

**TYPE=covariance-structure**

specifies the structure of the residual variance-covariance matrix **R**. The `SUBJECT=` option defines the blocks of **R**, and the `TYPE=` option specifies the structure of these blocks. PROC HPMIXED supports the following structures: `TYPE=AR(1)`, `TYPE=CHOL`, `TYPE=UN`, and `TYPE=VC`. The default structure is `VC`. See the description in the section “[RANDOM Statement](#)” on page 3685 for more information about these covariance structure types.

## TEST Statement

**TEST** *fixed-effects* *</ options >* ;

The TEST statement performs a hypothesis test on the fixed effects. You can specify multiple effects in one TEST statement or in multiple TEST statements, and all TEST statements must appear after the `MODEL` statement.

You can specify the following *options* in the TEST statement after a slash (/).

**HTYPE=value-list**

indicates the type of hypothesis test to perform on the specified effects. Valid entries for values in the *value-list* are 3, corresponding to a Type III test. The default value is 3. The ODS table name is “Tests3” for the Type III test.

**E**

requests that matrix coefficients associated with test types be displayed for specified effects.

**E3 | EIII**

requests that Type III matrix coefficients be displayed if a Type III test is performed.

**CHISQ**

requests that  $\chi^2$  tests be performed in addition to any *F* tests. A  $\chi^2$  statistic equals its corresponding *F* statistic times the associate numerator degree of freedom, and this same degree of freedom is used to compute the *p*-value for the  $\chi^2$  test. This *p*-value will always be less than that for the *F* test, because it effectively corresponds to an *F* test with infinite denominator degrees of freedom.

## WEIGHT Statement

**WEIGHT** *variable* ;

The WEIGHT statement replaces **R** with  $\mathbf{W}^{-1/2}\mathbf{R}\mathbf{W}^{-1/2}$ , where **W** is a diagonal matrix containing the weights. Observations with nonpositive or missing weights are not included in the resulting PROC HPMIXED analysis. If a WEIGHT statement is not included, all observations used in the analysis are assigned a weight of 1.

If a computation in PROC MIXED involves  $\mathbf{R}$ , then the WEIGHT statement replaces  $\mathbf{R}$  with  $\mathbf{W}^{-1/2}\mathbf{R}\mathbf{W}^{-1/2}$ . For example, the covariance matrix  $\mathbf{V}$  for the observations usually have the form  $\mathbf{V} = \mathbf{Z}\mathbf{G}\mathbf{Z}' + \mathbf{R}$ ; therefore, with the WEIGHT statement, this becomes  $\mathbf{V} = \mathbf{Z}\mathbf{G}\mathbf{Z}' + \mathbf{W}^{-1/2}\mathbf{R}\mathbf{W}^{-1/2}$ .

## Details: HPMIXED Procedure

### Model Assumptions

The following sections provide an overview of the approach used by the HPMIXED procedure for likelihood-based analysis of linear mixed models with sparse matrix technique. Additional theory and examples are provided in Littell et al. (1996); Verbeke and Molenberghs (1997, 2000); Brown and Prescott (1999).

The HPMIXED procedure fits models generally of the form

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\boldsymbol{\gamma} + \boldsymbol{\epsilon}$$

Models of this form contain both fixed-effects parameters,  $\boldsymbol{\beta}$ , and random-effects parameters,  $\boldsymbol{\gamma}$ ; hence, they are called *mixed models*. See Henderson (1990) and Searle, Casella, and McCulloch (1992) for historical developments of the mixed model. Note that the matrix  $\mathbf{Z}$  can contain either continuous or dummy variables, just like  $\mathbf{X}$ .

So far this is the same general form of model fit by the MIXED procedure. The difference between the models handled by the two procedures lies in the assumptions about the distributions of  $\boldsymbol{\gamma}$  and  $\boldsymbol{\epsilon}$ . For both procedures a key assumption is that  $\boldsymbol{\gamma}$  and  $\boldsymbol{\epsilon}$  are normally distributed with

$$\begin{aligned} E \begin{bmatrix} \boldsymbol{\gamma} \\ \boldsymbol{\epsilon} \end{bmatrix} &= \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix} \\ \text{Var} \begin{bmatrix} \boldsymbol{\gamma} \\ \boldsymbol{\epsilon} \end{bmatrix} &= \begin{bmatrix} \mathbf{G} & \mathbf{0} \\ \mathbf{0} & \mathbf{R} \end{bmatrix} \end{aligned}$$

The two procedures differ in their assumptions about the variance matrices  $\mathbf{G}$  and  $\mathbf{R}$  for  $\boldsymbol{\gamma}$  and  $\boldsymbol{\epsilon}$ , respectively. The MIXED procedure allows a variety of different structures for both  $\mathbf{G}$  and  $\mathbf{R}$ ; while in HPMIXED procedure,  $\mathbf{R}$  is always assumed to be of the form  $\mathbf{R} = \mathbf{I}\sigma^2$ , and the structures available for modeling  $\mathbf{G}$  are only a small subset of the structures offered by the MIXED procedure.

Estimates of fixed effects and predictions for random effects are obtained by solving the so-called *mixed model equations*:

$$\begin{bmatrix} \mathbf{X}'\mathbf{X}/\sigma^2 & \mathbf{X}'\mathbf{Z}/\sigma^2 \\ \mathbf{Z}'\mathbf{X}/\sigma^2 & \mathbf{Z}'\mathbf{Z}/\sigma^2 + \mathbf{G}^{-1} \end{bmatrix} \begin{bmatrix} \hat{\boldsymbol{\beta}} \\ \hat{\boldsymbol{\gamma}} \end{bmatrix} = \begin{bmatrix} \mathbf{X}'\mathbf{y}/\sigma^2 \\ \mathbf{Z}'\mathbf{y}/\sigma^2 \end{bmatrix}$$

Let  $\mathbf{C}$  denote the coefficient matrix of the mixed model equations:

$$\mathbf{C} = \begin{bmatrix} \mathbf{X}'\mathbf{X}/\sigma^2 & \mathbf{X}'\mathbf{Z}/\sigma^2 \\ \mathbf{Z}'\mathbf{X}/\sigma^2 & \mathbf{Z}'\mathbf{Z}/\sigma^2 + \mathbf{G}^{-1} \end{bmatrix}$$



Under the assumptions given previously for the moments of  $\boldsymbol{\gamma}$  and  $\boldsymbol{\epsilon}$ , the variance of  $\mathbf{y}$  is  $\mathbf{V} = \mathbf{ZGZ}' + \mathbf{I}\sigma^2$ . You can model  $\mathbf{V}$  by setting up the random-effects design matrix  $\mathbf{Z}$  and by specifying covariance structures for  $\mathbf{G}$ . Let  $\boldsymbol{\theta}$  be a vector of all unknown parameters in  $\mathbf{G}$ . Then the general form of the restricted likelihood function for the mixed models that the HPMIXED procedure can fit is

$$L(\boldsymbol{\theta}, \sigma^2) = -2 \log l = (n - p) \log(2\pi) + \log |\mathbf{C}| + \log |\mathbf{G}| + n \log(\sigma^2) + \mathbf{y}'\mathbf{P}\mathbf{y}$$

where

$$\mathbf{P} = \mathbf{V}^{-1} - \mathbf{V}^{-1}\mathbf{X}(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}^{-1}$$

and  $p$  is the rank of  $\mathbf{X}$ . The HPMIXED procedure minimizes  $L(\boldsymbol{\theta}, \sigma^2)$  over all unknown parameters in  $\boldsymbol{\theta}$  and  $\sigma^2$  by using nonlinear optimization algorithms.

## Computing and Maximizing the Likelihood

In computing the restricted likelihood function given previously, the determinants of the matrices  $\mathbf{C}$  and  $\mathbf{G}$  can be obtained effectively by using Cholesky decomposition. The quadratic term  $\mathbf{y}'\mathbf{P}\mathbf{y}$  can be expressed in terms of solutions of mixed model equations as follows:

$$\mathbf{y}'\mathbf{P}\mathbf{y} = \frac{1}{\sigma^2} \left( \mathbf{y}'\mathbf{y} - \begin{bmatrix} \hat{\boldsymbol{\beta}}' & \hat{\boldsymbol{\gamma}}' \end{bmatrix} \begin{bmatrix} \mathbf{X}'\mathbf{y} \\ \mathbf{Z}'\mathbf{y} \end{bmatrix} \right)$$

By default, the HPMIXED procedure profiles out the residual variance  $\sigma^2$  from the parameter vector  $\boldsymbol{\theta}$ . Let  $\boldsymbol{\theta}^*$  be the new parameter vector such that  $\theta_i^* = \theta_i/\sigma^2$ . The profiled objective function becomes

$$L(\boldsymbol{\theta}^*, \sigma^2) = (n - p) \log(2\pi) + \log |\mathbf{C}^*| + \log |\mathbf{G}^*| - (r_C - r_G - n) \log(\sigma^2) + (n - p)$$

where  $\mathbf{C}^* = \mathbf{C}\sigma^2$  and  $\mathbf{G}^* = \mathbf{G}\sigma^2$  are the profiled versions of  $\mathbf{C}$  and  $\mathbf{G}$ ,  $r_C$  and  $r_G$  are the ranks of  $\mathbf{C}$  and  $\mathbf{G}$ . Minimizing analytically for  $\sigma^2$  yields

$$\hat{\sigma}^2 = \frac{1}{n - p} \left( \mathbf{y}'\mathbf{y} - \begin{bmatrix} \hat{\boldsymbol{\beta}}' & \hat{\boldsymbol{\gamma}}' \end{bmatrix} \begin{bmatrix} \mathbf{X}'\mathbf{y} \\ \mathbf{Z}'\mathbf{y} \end{bmatrix} \right)$$

Optimizing the likelihood calls for derivatives with respect to the parameters. The first and second derivatives of the log-likelihood function  $L$  with respect to scalar variance components  $\theta_i$  and  $\theta_j$  are

$$\frac{\partial L}{\partial \theta_i} = \text{tr} \left( \frac{\partial \mathbf{V}}{\partial \theta_i} \mathbf{P} \right) - \mathbf{y}'\mathbf{P} \frac{\partial \mathbf{V}}{\partial \theta_i} \mathbf{P}\mathbf{y}$$

and

$$\frac{\partial^2 L}{\partial \theta_i \partial \theta_j} = -\text{tr} \left( \frac{\partial \mathbf{V}}{\partial \theta_i} \mathbf{P} \frac{\partial \mathbf{V}}{\partial \theta_j} \mathbf{P} \right) + 2\mathbf{y}'\mathbf{P} \frac{\partial \mathbf{V}}{\partial \theta_i} \mathbf{P} \frac{\partial \mathbf{V}}{\partial \theta_j} \mathbf{P}\mathbf{y}$$

The default quasi-Newton method of optimization for the HPMIXED procedure requires only first derivatives of the log likelihood, and these are readily derived by solving the mixed model equations. For example, when  $\mathbf{G} = \mathbf{I}\sigma_a^2$ , the first derivative of the log likelihood with respect to the parameter  $\sigma_a^2$  can be computed as follows:

$$\frac{\partial L}{\partial \sigma_a^2} = \frac{q}{\sigma_a^2} - \frac{\text{tr}(\mathbf{C}^{aa})}{\sigma_a^4} - \frac{\hat{\boldsymbol{\gamma}}'\hat{\boldsymbol{\gamma}}}{\sigma_a^4}$$

where  $q$  is the size of  $\boldsymbol{\gamma}$  vector and  $\mathbf{C}^{aa}$  is the part of the  $g$ -inverse of the mixed model equation coefficient matrix  $\mathbf{C}$  corresponding to the random effect  $\boldsymbol{\gamma}$ .

The second derivative of the log likelihood needs to be computed only if you specify certain nondefault optimization techniques in the NLOPTIONS statement, namely TECH=NEWRAP, TECH=NRRIDG, or TECH=TRUREG; see “NLOPTIONS Statement” on page 482 in Chapter 19, “Shared Concepts and Topics,” for more information about optimization techniques. For these second-derivative-based optimization techniques, the HPMIXED procedure does not actually use the true second derivative matrix, or *observed information matrix*, as defined earlier. Instead, it uses an alternative matrix that is more efficient to compute for large problems and that can be more stable. This alternative is called the *average information matrix*, and it is defined as follows. The expected value of the second derivative is

$$\mathbf{E}\left(\frac{\partial^2 L}{\partial \theta_i \partial \theta_j}\right) = \text{tr}\left(\frac{\partial \mathbf{V}}{\partial \theta_i} \mathbf{P} \frac{\partial \mathbf{V}}{\partial \theta_j} \mathbf{P}\right)$$

It is this trace that is computationally inefficient to evaluate. But if you average the expected information matrix defined by this formula with the observed information matrix defined by the preceding formula for the true second derivative, then the trace term cancels, leaving just a quadratic expression in  $\mathbf{y}$ . This quadratic expression defines the average information (Johnson and Thompson 1995) with respect to  $\theta_i$  and  $\theta_j$ :

$$\text{AI}(\theta_i, \theta_j) = \mathbf{y}' \mathbf{P} \frac{\partial \mathbf{V}}{\partial \theta_i} \mathbf{P} \frac{\partial \mathbf{V}}{\partial \theta_j} \mathbf{P} \mathbf{y}$$

---

## Computing Starting Values by EM-REML

The EM-REML algorithm (Dempster, Laird, and Rubin 1977) iteratively alternates between an expectation step and a maximization step to maximize the restricted log likelihood. The algorithm is based on augmenting the observed data  $\mathbf{y}$  with the unobservable random effects  $\boldsymbol{\gamma}$ , leading to a simplified form for the log likelihood. For example, if  $\mathbf{G} = \mathbf{I}\sigma_a^2$  then given the realized values  $\tilde{\boldsymbol{\gamma}}$  of the unobservable random effects  $\boldsymbol{\gamma}$ , the REML estimate of  $\sigma_a^2$  satisfies

$$\hat{\sigma}_a^2 = \frac{\tilde{\boldsymbol{\gamma}}' \tilde{\boldsymbol{\gamma}}}{q - \sigma^2 / \sigma_a^2 \text{tr}(\mathbf{C}^{aa})}$$

This corresponds to the maximization step of EM-REML. However, the true realized values  $\tilde{\boldsymbol{\gamma}}$  are unknown in practice. The expectation step of EM-REML replaces them with the conditional expected values  $\hat{\boldsymbol{\gamma}}$  of the random effects, given the observed data  $\mathbf{y}$  and initial values for the parameters. The new estimate of  $\sigma_a^2$  is used in turn to recalculate the conditional expected values, and the iteration is repeated until convergence.

It is well known that EM-REML is generally more robust against a poor choice of starting values than general nonlinear optimization methods such as Newton-Raphson, though it tends to converge slowly as it approaches the optimum. The Newton-Raphson method, on the other hand, converges much faster when it has a good set of starting values. The HPMIXED procedure, thus, employs a scheme that uses EM-REML initially in order to get good starting values, and after a few iterations, when the decrease in log likelihood has significantly slowed down, switching to a more general nonlinear optimization technique (by default, quasi-Newton).

## Sparse Matrix Techniques

A key component of the HPMIXED procedure is the use of sparse matrix techniques for computing and optimizing the likelihood expression given in the section “Model Assumptions” on page 3693. There are two aspects to sparse matrix techniques, namely, sparse matrix storage and sparse matrix computations. Typically, computer programs represent an  $N \times M$  matrix in a dense form as an array of size  $NM$ , making row-wise and column-wise arithmetic operations particularly efficient to compute. However, if many of these  $NM$  numbers are zeros, then correspondingly many of these operations are unnecessary or trivial. Sparse matrix techniques exploit this fact by representing a matrix not as a complete array, but as a set of nonzero elements and their location (row and column) within the matrix. Sparse matrix techniques are more efficient if there are enough zero-element operations in the dense form to make the extra time required to find and operate on matrix elements in the sparse form worthwhile.

The following discussion illustrates sparse techniques. Let the symmetric matrix  $\mathbf{C}$  be the matrix of mixed model equations of size  $5 \times 5$ .

$$\mathbf{C} = \begin{bmatrix} 8.0 & 0 & 0 & 2.0 & 0 \\ 0 & 4.0 & 3.0 & 0 & 0 \\ 0 & 3.0 & 5.0 & 0 & 0 \\ 2.0 & 0 & 0 & 7.0 & 0 \\ 0 & 0 & 0 & 0 & 9.0 \end{bmatrix}$$

There are 15 elements in the upper triangle of  $\mathbf{C}$ , though eight of them are zeros. The row and column indices and the values of seven nonzero elements are listed as follows:

$$\begin{array}{c|cccccc} i & 1 & 1 & 2 & 2 & 3 & 4 & 5 \\ j & 1 & 4 & 2 & 3 & 3 & 4 & 5 \\ C_{ij} & 8.0 & 2.0 & 4.0 & 3.0 & 5.0 & 7.0 & 9.0 \end{array}$$

The most elegant scheme to store these seven elements is to store them in a hash table with row and column indices as a hash key. However, this scheme is not efficient as the number of non-zero elements gets very large. The classical and widely used scheme, and the one the HPMIXED procedure employs, is the  $(\mathbf{i}_c, \mathbf{j}_c, c)$  format, in which the nonzero elements are stored contiguously row by row in the vector  $c$ . To identify the individual nonzero elements in each row, you need to know the column index of an element. These column indices are stored in the vector  $\mathbf{j}_c$ ; that is, if  $c(k) = C_{ij}$ , then  $\mathbf{j}_c(k) = j$ . To identify the individual rows, you need to know where each row starts and ends. These row starting positions are stored in the vector  $\mathbf{i}_c$ . For instance, if  $C_{ij}$  is the first nonzero element in the row  $i$  and  $c(k) = C_{ij}$ , then  $\mathbf{i}_c(i) = k$ . The row  $i$  ending position is one less than  $\mathbf{i}_c(i + 1)$ . Thus, the number of nonzero elements in the row  $i$  is  $\mathbf{i}_c(i + 1) - \mathbf{i}_c(i)$ , these elements in the row  $i$  are stored consecutively starting from the position  $k_i = \mathbf{i}_c(i)$

$$c(k_i), c(k_i + 1), c(k_i + 2), \dots, c(k_{i+1} - 1)$$

and the corresponding columns indices are stored consecutively in

$$\mathbf{j}_c(k_i), \mathbf{j}_c(k_i + 1), \mathbf{j}_c(k_i + 2), \dots, \mathbf{j}_c(k_{i+1} - 1)$$

For example, the seven nonzero elements in matrix  $\mathbf{C}$  are stored in  $(\mathbf{i}_c, \mathbf{j}_c, c)$  format as

|       |     |     |     |     |     |     |     |
|-------|-----|-----|-----|-----|-----|-----|-----|
| $i_c$ | 1   | 3   | 5   | 6   | 7   | 8   |     |
| $j_c$ | 1   | 4   | 2   | 3   | 3   | 4   | 5   |
| $c$   | 8.0 | 2.0 | 4.0 | 3.0 | 5.0 | 7.0 | 9.0 |

Note that since matrices are stored row by row in the  $(i_c, j_c, c)$  format, row-wise operations can be performed efficiently but it is inefficient to retrieve elements column-wise. Thus, this representation will be inefficient for matrix computations requiring column-wise operations. Fortunately, the likelihood calculations for mixed models can usually avoid column-wise operations.

In mixed models, sparse matrices typically arise from a large number of levels for fixed effects and/or random effects. If a linear model contains one or more large CLASS effects, then the mixed model equations are usually very sparse. Storing zeros in mixed model equations not only requires significantly more memory but also results in longer execution time and larger rounding error. As an illustration, the example in the “Getting Started: HPMIXED Procedure” on page 3658 has 3506 mixed model equations. Storing just the upper triangle of these equations in a dense form requires  $(1 + 3506) \times 3506/2 = 6,147,771$  elements. However, there are only 60,944 nonzero elements—less than 1% of what dense storage requires.

Note that as the density of the mixed model equations increases, the advantage of sparse matrix techniques decreases. For instance, a classical regression model typically has a dense coefficient matrix, though the dimension of the matrix is relatively small.

The HPMIXED procedure employs sparse matrix techniques to store the nonzero elements in the mixed model equations and to compute a sparse Cholesky decomposition of these equations. A reordering of the mixed model equations is required in order to keep the minimum memory consumption during the factorization. This reordering process results in a different  $g$ -inverse from what is produced by most other SAS/STAT procedures, for which the  $g$ -inverse is defined by sequential sweeping in the order defined by the model. If mixed model equations are singular, this different  $g$ -inverse produces a different solution of mixed model equations. However, estimable functions and tests based on them are invariant to the choice of  $g$ -inverse, and are thus the same for the HPMIXED procedure as for other procedures.

---

## Hypothesis Tests for Fixed Effects

Unlike most other SAS/STAT procedures for analyzing general linear models, the HPMIXED procedure does not by default provide  $F$  tests for the fixed effects. This is because, for the large mixed model problems that the HPMIXED procedure is designed to address, such tests are often computationally prohibitive to compute. The computation of Type III tests first constructs the Hermite matrix of the mixed model coefficient matrix  $\mathbf{C}$  and then forms the  $\mathbf{L}$  coefficient matrix to obtain the  $F$  value as follows:

$$F = \frac{\begin{bmatrix} \hat{\beta} \\ \hat{\gamma} \end{bmatrix}' \mathbf{L}' (\mathbf{L}\hat{\mathbf{C}}^{-1}\mathbf{L}')^{-1} \mathbf{L} \begin{bmatrix} \hat{\beta} \\ \hat{\gamma} \end{bmatrix}}{r}$$

where  $r = \text{rank}(\mathbf{L}\hat{\mathbf{C}}^{-1}\mathbf{L}')$ . The coefficient matrix  $\mathbf{L}$  corresponding to fixed effects with many levels can be very large and dense, making them very difficult to work with. At the same time, Type III tests for effects with many levels are relatively unlikely to be statistically useful.

For this reason, you must use the TEST statement in PROC HPMIXED to specifically ask for Type III tests for any effects for which you want to compute them. An example of this is given in the section “Getting Started: HPMIXED Procedure” on page 3658.

---

## Default Output

The following sections describe the output PROC HPMIXED produces by default. This output is organized into various tables, and they are discussed in order of appearance.

### Model Information

The “Model Information” table describes the model, some of the variables it involves, and the method used in fitting it. It also lists the method for computing the degrees of freedom.

The name of the “Model Information” table is “ModelInfo.”

### Class Level Information

The “Class Level Information” table lists the first 20 levels of every variable specified in the CLASS statement. You should check this information to make sure the data are correct. You can adjust the order of the CLASS variable levels with the ORDER= option in the PROC HPMIXED statement. The name of the “Class Level Information” table is “ClassLevels.”

### Dimensions

The “Dimensions” table lists the sizes of relevant matrices. This table can be useful in determining CPU time and memory requirements. The name of the “Dimensions” table is “Dimensions.”

### Number of Observations

The “Number of Observations” table shows the number of observations read from the data set and the number of observations used in fitting the model.

### Descriptive Statistics

The “Descriptive Statistics” table lists simple statistics such as means and standard deviations for the dependent variable, for each covariate in the MODEL statement, and for the weight variable in the WEIGHT statement.

### Iteration History

The “Iteration History” table describes the optimization of the residual log likelihood. The function to be minimized (the *objective function*) is  $-2l$ .

The name of the “Iteration History” table is “IterHistory.”

### Covariance Parameter Estimates

The “Covariance Parameter Estimates” table contains the estimates of the parameters in **G** and **R**. Their values are labeled in the “Cov Parm” table along with Subject and Group information if applicable. The estimates are displayed in the Estimate column.

The name of the “Covariance Parameter Estimates” table is “CovParms.”

## Convergence Status

The “Convergence Status” table contains a status message that describes the reason the optimization terminated. The message is also written to the log. The name of the “Convergence Status” table is “ConvergenceStatus.” You can query the nonprinting numeric variable `Status` to check for a successful optimization. This is useful in batch processing, or when processing BY groups, such as in simulations. Successful optimizations are indicated by the value 0 for the `Status` variable.

## Fit Statistics

The “Fit Statistics” table provides some statistics about the estimated mixed model.

In addition, the “Fit Statistics” table lists three information criteria: AIC, AICC, and BIC, all in smaller-is-better form. Expressions for these criteria are described under the `IC=` option on page 3664.

The name of the “Model Fitting Information” table is “FitStatistics.”

---

## ODS Table Names

Each table created by PROC HP MIXED has a name associated with it, and you must use this name to reference the table when using ODS statements. These names are listed in Table 46.11.

**Table 46.11** ODS Tables Produced by PROC HP MIXED

| Table Name        | Description                                                      | Required Statement / Option                      |
|-------------------|------------------------------------------------------------------|--------------------------------------------------|
| CholR             | Cholesky root of blocks of the estimated <b>R</b> matrix         | REPEATED / RC                                    |
| ClassLevels       | Level information from the CLASS statement                       | Default output                                   |
| Coef              | <b>L</b> matrix coefficients                                     | E option in TEST, CONTRAST, ESTIMATE, or LSMEANS |
| Contrasts         | Results from the CONTRAST statements                             | CONTRAST                                         |
| ConvergenceStatus | Convergence status                                               | Default                                          |
| CovParms          | Estimated covariance parameters                                  | Default output                                   |
| DiffS             | Differences of LS-means                                          | LSMEANS / DIFF (or PDIFF)                        |
| Dimensions        | Dimensions of the model                                          | Default output                                   |
| Estimates         | Results from ESTIMATE statements                                 | ESTIMATE                                         |
| FitStatistics     | Fit statistics                                                   | Default                                          |
| InvCholR          | Inverse Cholesky root of blocks of the estimated <b>R</b> matrix | REPEATED / RCI=                                  |
| InvR              | Inverse of blocks of the estimated <b>R</b> matrix               | REPEATED / RI=                                   |
| IterHistory       | Iteration history                                                | Default output                                   |
| LSMeans           | LS-means                                                         | LSMEANS                                          |
| MMEq              | Mixed model equations                                            | PROC HP MIXED MMEQ                               |
| ModelInfo         | Model information                                                | Default output                                   |

Table 46.11 (continued)

| Table Name         | Description                                                           | Required Statement / Option     |
|--------------------|-----------------------------------------------------------------------|---------------------------------|
| NObs               | Number of observations read and used                                  | Default output                  |
| OptInfo            | Optimization information                                              | Default output                  |
| OverallANOVA       | ANOVA table for model without random effect                           | Default output for fixed models |
| ParameterEstimates | Fixed-effects solution                                                | MODEL / SOLUTION                |
| ParmSearch         | Parameter search values                                               | PARMS                           |
| R                  | Blocks of the estimated <b>R</b> matrix                               | REPEATED / R=                   |
| RCorr              | Correlation matrix from blocks of the estimated <b>R</b> matrix       | REPEATED / RCORR=               |
| SimpleStatistics   | Descriptive statistics for dependent variable and covariate variables | PROC HPMIXED SIMPLE             |
| Slices             | Tests of LS-means slices                                              | LSMEANS / SLICE=                |
| SolutionR          | Random-effect solution vector                                         | RANDOM / SOLUTION               |
| Tests3             | Type III tests of fixed effects                                       | TEST                            |

## Examples: HPMIXED Procedure

### Example 46.1: Ranking Many Random-Effect Coefficients

In analyzing models with random effects that have many levels, a frequent goal is to estimate and rank the predicted values of the coefficients corresponding to these levels. For example, in mixed models for animal breeding, the predicted coefficient of the random effect for each animal is referred to as the *estimated breeding value* (EBV) and animals with relatively high EBVs are chosen for breeding. This example demonstrates the use of the HPMIXED procedure for computing EBVs and their precision. Although other mixed modeling tools in SAS/STAT can potentially compute EBVs, PROC HPMIXED is particularly suited for the large, sparse matrix calculations involved. The typical performance of the HPMIXED procedure and other tools for this problem is also discussed.

The data for this problem are generated by simulation. Suppose you are considering analyzing EBVs for animals on 15 farms, with about 100 animals of 5 different species on each farm. The following DATA step simulates data with this structure, where about 40 observations of the response variable Yield are made per animal:

```
%let NFarm = 15;
%let NAnimal = %eval(&NFarm*100);
data Sim;
 keep Species Farm Animal Yield;
 array BV{&NAnimal};
 array AnimalSpecies{&NAnimal};
 array AnimalFarm{&NAnimal};
 do i = 1 to &NAnimal;
```

```

BV {i} = sqrt(4.0)*rannor(12345);
AnimalSpecies{i} = 1 + int(5 *ranuni(12345));
AnimalFarm {i} = 1 + int(&NFarm*ranuni(12345));
end;
do i = 1 to 40*&NAnimal;
 Animal = 1 + int(&NAnimal*ranuni(12345));
 Species = AnimalSpecies{Animal};
 Farm = AnimalFarm {Animal};
 Yield = 1 + Species
 + Farm
 + BV{Animal}
 + sqrt(8.0)*rannor(12345);
 output;
end;
run;

```

In this simulation, the true breeding value for each animal (BV1–BV1500) has a variance component of 4.0, while the level of background variance is 8.0.

In this type of experiment, the effect of Species and the interaction between Species and Farm are typically modeled as fixed effects, while the effect of Animal is modeled as a random effect. The following statements use the HPMIXED procedure to compute predictions for the Animal random effect and save them to the data set EBV. This data set is then sorted and the 10 animals with the highest EBVs are displayed.

```

ods listing close;
proc hpmixed data=Sim;
 class Species Farm Animal;
 model Yield = Species Farm*Species;
 random Animal/cl;
 ods output SolutionR=EBV;
run;
ods listing;

proc sort data=EBV;
 by descending estimate;
run;
proc print data=EBV(obs=10) noobs;
 var Animal Estimate StdErrPred Lower Upper;
run;

```

The preceding statements close the ODS listing destination for the duration of the PROC HPMIXED run. This avoids displaying the long random-effects solution table, since only the top few EBVs are of interest. [Output 46.1.1](#) displays the EBVs of the top 10 animals, along with their precision and confidence bounds.



**Output 46.1.1** Estimated Breeding Values: Top 10 Animals

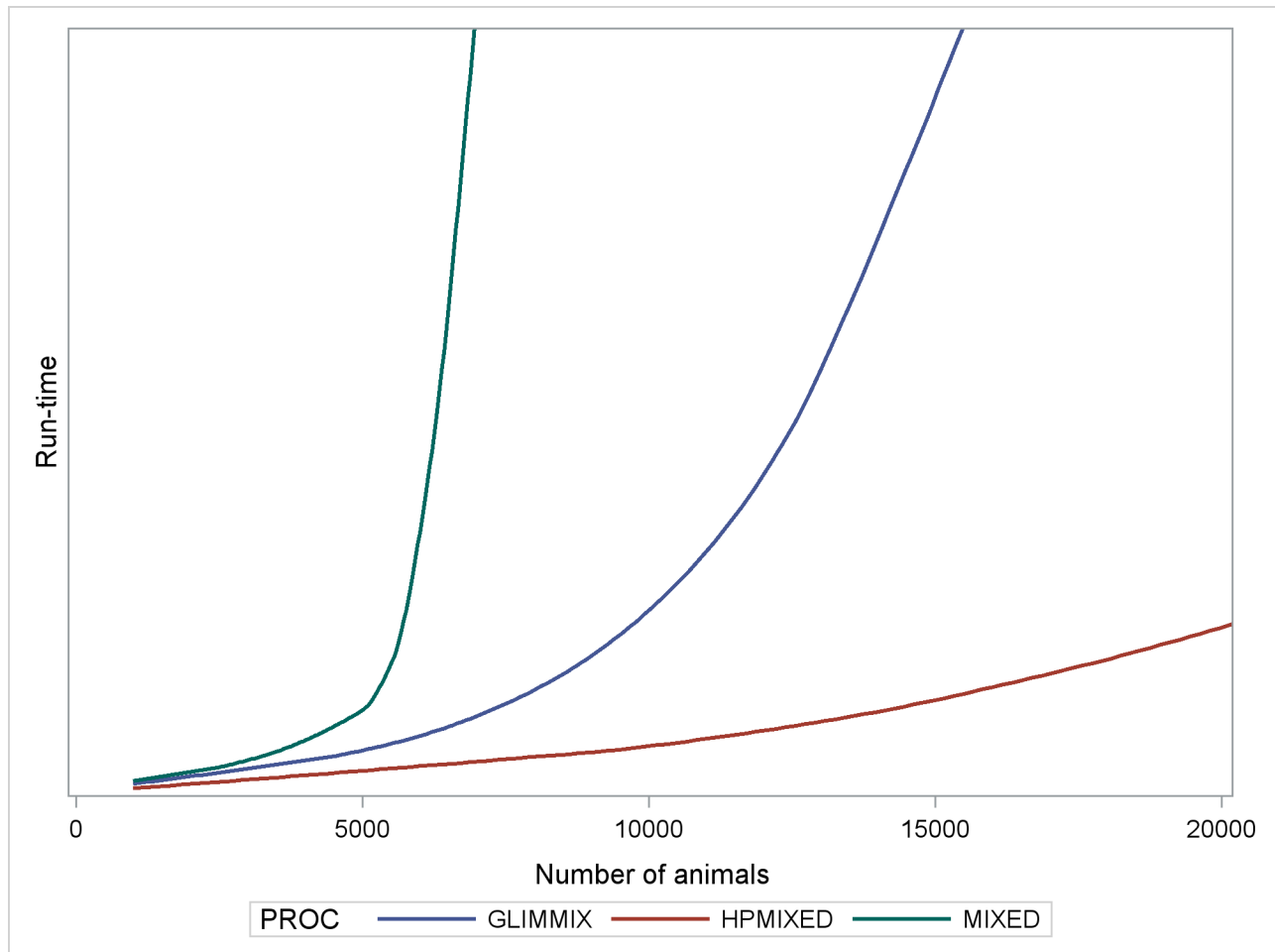
| Animal | Estimate | StdErr<br>Pred | Lower  | Upper  |
|--------|----------|----------------|--------|--------|
| 1294   | 5.9703   | 0.6317         | 4.7321 | 7.2085 |
| 1219   | 5.0081   | 0.6396         | 3.7544 | 6.2618 |
| 1054   | 4.9452   | 0.5874         | 3.7939 | 6.0966 |
| 758    | 4.9340   | 0.6196         | 3.7195 | 6.1485 |
| 986    | 4.9329   | 0.5767         | 3.8025 | 6.0633 |
| 1150   | 4.7444   | 0.5806         | 3.6064 | 5.8824 |
| 962    | 4.6651   | 0.5794         | 3.5294 | 5.8008 |
| 225    | 4.5294   | 0.6137         | 3.3266 | 5.7322 |
| 1252   | 4.5012   | 0.5686         | 3.3868 | 5.6157 |
| 1033   | 4.4971   | 0.6080         | 3.3054 | 5.6889 |

Notice that animal 1294 is ranked as the top animal based on its EBV, but the precision of this estimate, as measured by the standard error of prediction, is lower than that of other animals.

You can also use PROC MIXED and PROC GLIMMIX to compute EBVs, but the performance of these general mixed modeling procedures for this specialized kind of data and model is quite different from that of PROC HPMIXED. The MIXED and GLIMMIX procedures are engineered to have good performance properties across a broad class of models and analyses, a class much broader than what PROC HPMIXED can handle. The HPMIXED procedure, on the other hand, can have better performance, in terms of both memory and run time, for certain specialized models and analyses, of which the current example is one.

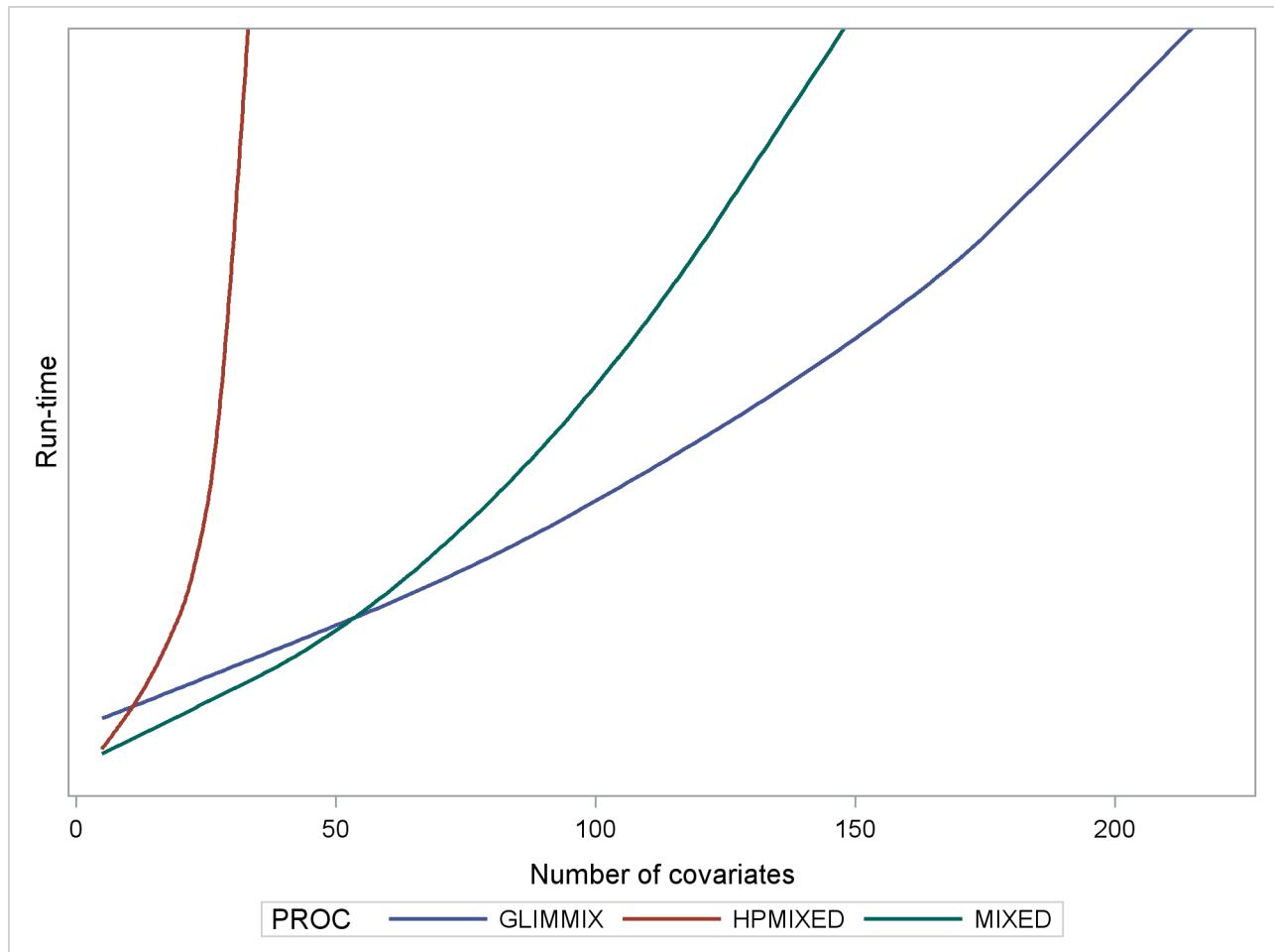
For this example, an equivalent PROC GLIMMIX approach can take twice as long to complete, and PROC MIXED three times as long. Precise relative timings are not feasible, since those of the MIXED and GLIMMIX procedures are sensitive to the speed of disk access for writing to and reading from the utility file that holds the underlying matrices. But the results on any system would be similar: for the limited class of models to which it applies, the sparse matrix representation that the HPMIXED procedure employs should provide better computational performance than a dense representation, in terms of both run time and memory use.

Moreover, for a given analysis, if the size of the problem is increased in such a way that the underlying matrices become sparser, the relative performance of PROC HPMIXED gets even better. As an illustration of this, [Output 46.1.2](#) shows relative performance of the three procedures for simulated data as the number of farms increases. For this plot, each additional farm adds 500 levels of the Animal random effect to the model—a substantial number.

**Output 46.1.2** Comparing Mixed Model Tools for Increasingly Sparse Problems

The vertical axis in [Output 46.1.2](#) measures run time, but the units are omitted: relative performance is what counts, and that is expected to be fairly invariant to machine architecture. The output shows that while the performance of the MIXED and GLIMMIX procedures is relatively competitive with PROC HPMIXED for up to 3000 or 4000 animals, both procedures' relative performance decreases as the number of animals increases into the tens of thousands.

As a caveat, note that PROC HPMIXED can be *inefficient* relative to PROC MIXED and PROC GLIMMIX for models and data that are not sparse, because it can take many times longer to invert a large, dense matrix by sparse techniques. For example, [Output 46.1.3](#) shows relative performance of the three procedures for simulated data like the preceding, but where the fixed part of the model consists of an increasing number of continuous covariates and is thus dense.

**Output 46.1.3** Comparing Mixed Model Tools for Increasingly Dense Problems

As before, the HPMIXED procedure is more efficient than the MIXED and GLIMMIX procedures for few covariates, but when the fixed-effect calculations dominate the run time, PROC HPMIXED rapidly becomes relatively inefficient as the size of the dense fixed-effect matrix increases. Also note that while PROC MIXED is more efficient than PROC GLIMMIX for small to moderate numbers of covariates, PROC GLIMMIX has the best performance as the number of covariates get very large.

### Example 46.2: Comparing Results from PROC HPMIXED and PROC MIXED

This example revisits the mixed model problem from the section “Getting Started: MIXED Procedure” on page 4884, in Chapter 59, “The MIXED Procedure,” with the data set shown in the following statements:

```
data heights;
 input Family Gender$ Height @@;
 datalines;
1 F 67 1 F 66 1 F 64 1 M 71 1 M 72 2 F 63
2 F 63 2 F 67 2 M 69 2 M 68 2 M 70 3 F 63
3 M 64 4 F 67 4 F 66 4 M 67 4 M 67 4 M 69
;
```

The response variable Height measures the heights (in inches) of 18 individuals. The individuals are classified according to Family and Gender. The following statements fit a mixed model with random effects for Family and the Family\*Gender interaction with the MIXED procedure:

```
proc mixed;
 class Family Gender;
 model Height = Gender / s;
 random Family Family*Gender / s;
run;
```

The “Iteration History” and “Fit Statistics” tables for the optimization in PROC MIXED are shown in Output 46.2.1. The MIXED procedure converges after six iterations and achieves a -2 restricted log likelihood of 71.02246.

**Output 46.2.1** Iteration History and Fit Statistics: MIXED Procedure

| The Mixed Procedure |             |                          |            |  |
|---------------------|-------------|--------------------------|------------|--|
| Iteration History   |             |                          |            |  |
| Iteration           | Evaluations | -2 Res Log Like          | Criterion  |  |
| 0                   | 1           | 74.11074833              |            |  |
| 1                   | 2           | 71.51614003              | 0.01441208 |  |
| 2                   | 1           | 71.13845990              | 0.00412226 |  |
| 3                   | 1           | 71.03613556              | 0.00058188 |  |
| 4                   | 1           | 71.02281757              | 0.00001689 |  |
| 5                   | 1           | 71.02245904              | 0.00000002 |  |
| 6                   | 1           | 71.02245869              | 0.00000000 |  |
| Fit Statistics      |             |                          |            |  |
|                     |             | -2 Res Log Likelihood    | 71.0       |  |
|                     |             | AIC (smaller is better)  | 77.0       |  |
|                     |             | AICC (smaller is better) | 79.0       |  |
|                     |             | BIC (smaller is better)  | 75.2       |  |

Output 46.2.2 displays the covariance parameter estimates and the solutions for the fixed and random effects. Because the fixed-effect model contains a classification effect (Gender) and an intercept, the  $X'X$  matrix is singular. Only two fixed-effect parameters can be estimated in this model. The MIXED procedure, relying on a sweep operation in the order in which effects enter the model, determines that the last column of the  $X'X$  matrix is a linear function of previous columns. Consequently, the coefficient for the second level of the Gender variable is zero.

**Output 46.2.2** Parameter Estimates and Solutions: MIXED Procedure

| Covariance Parameter Estimates |        |          |                |              |         |         |         |
|--------------------------------|--------|----------|----------------|--------------|---------|---------|---------|
| Cov Parm                       |        | Estimate |                |              |         |         |         |
| Family                         |        | 2.4010   |                |              |         |         |         |
| Family*Gender                  |        | 1.7657   |                |              |         |         |         |
| Residual                       |        | 2.1668   |                |              |         |         |         |
| Solution for Fixed Effects     |        |          |                |              |         |         |         |
| Effect                         | Gender | Estimate | Standard Error | DF           | t Value | Pr >  t |         |
| Intercept                      |        | 68.2114  | 1.1477         | 3            | 59.43   | <.0001  |         |
| Gender                         | F      | -3.3621  | 1.1923         | 3            | -2.82   | 0.0667  |         |
| Gender                         | M      | 0        | .              | .            | .       | .       |         |
| Solution for Random Effects    |        |          |                |              |         |         |         |
| Effect                         | Gender | Family   | Estimate       | Std Err Pred | DF      | t Value | Pr >  t |
| Family                         |        | 1        | 1.2680         | 1.1201       | 10      | 1.13    | 0.2840  |
| Family                         |        | 2        | 0.08980        | 1.1121       | 10      | 0.08    | 0.9372  |
| Family                         |        | 3        | -1.6660        | 1.1712       | 10      | -1.42   | 0.1853  |
| Family                         |        | 4        | 0.3082         | 1.1201       | 10      | 0.28    | 0.7888  |
| Family*Gender                  | F      | 1        | -0.3198        | 1.0810       | 10      | -0.30   | 0.7734  |
| Family*Gender                  | M      | 1        | 1.2523         | 1.0933       | 10      | 1.15    | 0.2787  |
| Family*Gender                  | F      | 2        | -0.4299        | 1.0774       | 10      | -0.40   | 0.6983  |
| Family*Gender                  | M      | 2        | 0.4959         | 1.0774       | 10      | 0.46    | 0.6551  |
| Family*Gender                  | F      | 3        | -0.08229       | 1.1409       | 10      | -0.07   | 0.9439  |
| Family*Gender                  | M      | 3        | -1.1429        | 1.1409       | 10      | -1.00   | 0.3401  |
| Family*Gender                  | F      | 4        | 0.8320         | 1.0933       | 10      | 0.76    | 0.4642  |
| Family*Gender                  | M      | 4        | -0.6053        | 1.0810       | 10      | -0.56   | 0.5878  |

The “Type 3 Tests of Fixed Effects” table in [Output 46.2.3](#) is produced by the MIXED procedure by default.

**Output 46.2.3** Test of Gender Effect

| Type 3 Tests of Fixed Effects |        |        |         |        |
|-------------------------------|--------|--------|---------|--------|
| Effect                        | Num DF | Den DF | F Value | Pr > F |
| Gender                        | 1      | 3      | 7.95    | 0.0667 |

The same linear mixed model is fit with the HPMIXED procedure with the following statements:

```
proc hpmixed;
 class Family Gender;
 model Height = Gender / s;
 random Family Family*Gender / s;
 test gender;
run;
```

Output 46.2.4 displays the “Iteration History” and “Fit Statistics” tables. The HPMIXED procedure, with its default quasi-Newton algorithm, achieves the same  $-2$  restricted log likelihood as the MIXED procedure (71.02246; see Output 46.2.1).

**Output 46.2.4** Iteration History and Fit Statistics: HPMIXED Procedure

| The HPMIXED Procedure    |             |                    |            |              |  |
|--------------------------|-------------|--------------------|------------|--------------|--|
| Iteration History        |             |                    |            |              |  |
| Iteration                | Evaluations | Objective Function | Change     | Max Gradient |  |
| 0                        | 4           | 71.023177956       | .          | 0.034074     |  |
| 1                        | 3           | 71.022519936       | 0.00065802 | 0.007839     |  |
| 2                        | 3           | 71.022477283       | 0.00004265 | 0.004674     |  |
| 3                        | 2           | 71.0224587         | 0.00001858 | 0.000168     |  |
| 4                        | 2           | 71.022458689       | 0.00000001 | 3.28E-6      |  |
| Fit Statistics           |             |                    |            |              |  |
| -2 Res Log Likelihood    |             |                    | 71.02246   |              |  |
| AIC (smaller is better)  |             |                    | 77.02246   |              |  |
| AICC (smaller is better) |             |                    | 79.02246   |              |  |
| BIC (smaller is better)  |             |                    | 75.18134   |              |  |
| CAIC (smaller is better) |             |                    | 78.18134   |              |  |
| HQIC (smaller is better) |             |                    | 72.98226   |              |  |

Output 46.2.5 displays the results that correspond to those in Output 46.2.2 in the MIXED procedure.

**Output 46.2.5** Parameter Estimates and Solutions: HPMIXED Procedure

| Covariance Parameter Estimates |          |
|--------------------------------|----------|
| Cov Parm                       | Estimate |
| Family                         | 2.4010   |
| Family*Gender                  | 1.7657   |
| Residual                       | 2.1668   |

## Output 46.2.5 continued

| Solution for Fixed Effects |        |          |                |    |         |         |   |
|----------------------------|--------|----------|----------------|----|---------|---------|---|
| Effect                     | Gender | Estimate | Standard Error | DF | t Value | Pr >  t |   |
| Intercept                  |        | 0        | .              | .  | .       | .       | . |
| Gender                     | F      | 64.8493  | 1.1477         | 16 | 56.50   | <.0001  |   |
| Gender                     | M      | 68.2114  | 1.1477         | 16 | 59.43   | <.0001  |   |

| Solution for Random Effects |        |        |          |              |    |         |         |
|-----------------------------|--------|--------|----------|--------------|----|---------|---------|
| Effect                      | Gender | Family | Estimate | Std Err Pred | DF | t Value | Pr >  t |
| Family                      |        | 1      | 1.2680   | 1.1201       | 16 | 1.13    | 0.2743  |
| Family                      |        | 2      | 0.08980  | 1.1121       | 16 | 0.08    | 0.9366  |
| Family                      |        | 3      | -1.6660  | 1.1712       | 16 | -1.42   | 0.1741  |
| Family                      |        | 4      | 0.3082   | 1.1201       | 16 | 0.28    | 0.7867  |
| Family*Gender               | F      | 1      | -0.3198  | 1.0810       | 16 | -0.30   | 0.7712  |
| Family*Gender               | M      | 1      | 1.2523   | 1.0933       | 16 | 1.15    | 0.2689  |
| Family*Gender               | F      | 2      | -0.4299  | 1.0774       | 16 | -0.40   | 0.6951  |
| Family*Gender               | M      | 2      | 0.4959   | 1.0774       | 16 | 0.46    | 0.6515  |
| Family*Gender               | F      | 3      | -0.08229 | 1.1409       | 16 | -0.07   | 0.9434  |
| Family*Gender               | M      | 3      | -1.1429  | 1.1409       | 16 | -1.00   | 0.3314  |
| Family*Gender               | F      | 4      | 0.8320   | 1.0933       | 16 | 0.76    | 0.4577  |
| Family*Gender               | M      | 4      | -0.6053  | 1.0810       | 16 | -0.56   | 0.5832  |

A number of points are noteworthy in comparing the results from the procedures. The covariance parameter estimates are the same, yet the solutions for the fixed effects differ. In fact, both solutions are correct. Solving a sparse system of linear equations requires reordering of the mixed model equations to minimize memory consumption in the factorization process. As a consequence, the order in which singularities are detected can differ from the order in which effects enter the model. Mathematically, the two sets of solutions simply correspond to different choices for the generalized inverse in solving a singular linear system. See the sections “Generalized Inverse Matrices” on page 46 and “Linear Model Theory” on page 55, in Chapter 3, “Introduction to Statistical Modeling with SAS/STAT Software,” for more information about the role and importance of generalized inverses in linear model analysis.

Although the two sets of solutions for the fixed effects correspond to different choices of generalized inverses, many important results are invariant to the choice of the  $g$ -inverse. For example, the solutions for the random effects in Output 46.2.5 and Output 46.2.2 are identical. Also, the test for the Gender effect yields the same  $F$  value in both analyses (compare Output 46.2.6 and Output 46.2.3). However, note that the  $p$ -values associated with both  $F$  tests and  $t$  tests differ between the two procedures. This is due to their different default methods for computing the degrees of freedom. For this model, the HPMIXED procedure use the residual method to determine the denominator degrees of freedom for tests of fixed effects, whereas the MIXED procedure uses the containment method. The containment method is order-dependent, and thus not available in the HPMIXED procedure.

**Output 46.2.6** Parameter Estimates and Solutions: HPMIXED Procedure

| Type III Tests of Fixed Effects |           |           |         |        |
|---------------------------------|-----------|-----------|---------|--------|
| Effect                          | Num<br>DF | Den<br>DF | F Value | Pr > F |
| Gender                          | 1         | 16        | 7.95    | 0.0123 |

## Example 46.3: Using PROC GLIMMIX for Further Analysis of PROC HPMIXED Fit

The HPMIXED procedure handles only a subset of the analyses of the GLIMMIX procedure. However, you can use the HPMIXED procedure to accelerate your GLIMMIX procedure analyses for large problems. The idea is to use PROC HPMIXED to maximize the likelihood and produce parameter estimates more quickly than PROC GLIMMIX, and then to pass these parameter estimates to PROC GLIMMIX for some further analysis that is not available within PROC HPMIXED.

This example revisits the mixed model problem from the section “Getting Started: HPMIXED Procedure” on page 3658 to illustrate how to obtain the covariance estimates from the HPMIXED procedure and, in turn, how to use these estimates in PROC GLIMMIX’s PARMs statement. The following statements again simulate data from animals of different species on different farms:

```

data Sim;
 keep Species Farm Animal Yield;
 array AnimalEffect{3000};
 array AnimalSpecies{3000};
 array AnimalFarm{3000};
 do i = 1 to 3000;
 AnimalEffect{i} = sqrt(4.0)*rannor(12345);
 AnimalSpecies{i} = 1 + int(5*ranuni(12345));
 AnimalFarm{i} = 1 + int(10*ranuni(12345));
 end;
 do i = 1 to 40000;
 Animal = 1 + int(3000*ranuni(12345));
 Species = AnimalSpecies{Animal};
 Farm = AnimalFarm{Animal};
 Yield = 1 + Species + int(Farm/2) + AnimalEffect{Animal}
 + sqrt(8.0)*rannor(12345);
 output;
 end;
run;

```

Note that in the preceding DATA step program, certain pairs of farms are simulated to have the same effect on yield. Suppose that your goal is to determine which farms are significantly different. While the HPMIXED procedure has an LSMEANS statement, it has no options for multiple comparisons. The following statements first use the HPMIXED procedure to obtain the covariance estimates, saving them in the SAS data set HPMEstimate. Then the GLIMMIX procedure is executed with the PARMs statement to initialize the parameter values from the data set HPMEstimate and with the HOLD= and NOITER options to prevent



further optimization iterations. The LSMEANS statement is used in PROC GLIMMIX to perform multiple comparisons of the LS-means for farms, and the results are displayed as a so-called diffogram.

```
proc hpmixed data=Sim;
 class Species Farm Animal;
 model Yield = Farm|Species;
 random Animal;
 test Species Species*Farm;
 ods output CovParms=HPMEstimate;
run;

ods graphics on;
proc glimmix data=Sim;
 class Species Farm Animal;
 model Yield = Farm|Species;
 random int/sub=Animal;
 parms /pdata=HPMEstimate hold=1,2 noiter;
 lsmeans Farm / pdiff=all plot=diffplot;
run;
```

The iteration histories for the two procedures are shown in [Output 46.3.1](#) and [Output 46.3.2](#). Whereas PROC HPMIXED requires several iterations in order to converge, PROC GLIMMIX “converges” to the same value in one step, with no iteration since the options `HOLD=` and `NOITER` are used.

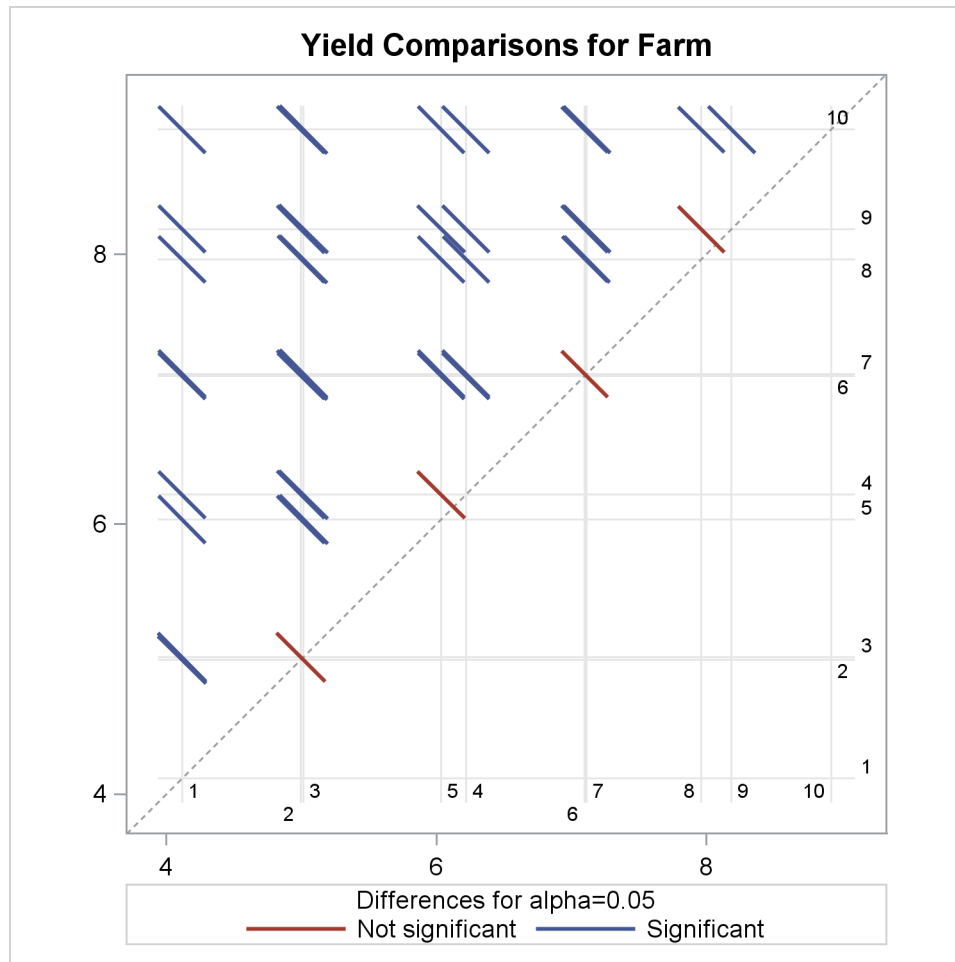
**Output 46.3.1** Iteration History for the HPMIXED Procedure

| The HPMIXED Procedure |             |                    |             |              |  |
|-----------------------|-------------|--------------------|-------------|--------------|--|
| Iteration History     |             |                    |             |              |  |
| Iteration             | Evaluations | Objective Function | Change      | Max Gradient |  |
| 0                     | 4           | 202516.66891       | .           | 0.841954     |  |
| 1                     | 6           | 202516.66887       | 0.00004385  | 0.000641     |  |
| 2                     | 1           | 202516.66887       | -0.00000000 | 0.000641     |  |

**Output 46.3.2** Iteration History for the GLIMMIX Procedure

| The GLIMMIX Procedure |          |             |                    |        |              |
|-----------------------|----------|-------------|--------------------|--------|--------------|
| Iteration History     |          |             |                    |        |              |
| Iteration             | Restarts | Evaluations | Objective Function | Change | Max Gradient |
| 0                     | 0        | 4           | 202516.66887       | .      | 0            |

The graphical multiple-comparisons analysis for the LS-means of farms is shown in [Output 46.3.3](#). It confirms the pairwise equalities between farm effects with which the data were simulated.

**Output 46.3.3** LS-Means Plot of Pairwise Farm Differences

For more information about the interpretation of the LS-means difference plot, see the section “ODS Graphics” on page 3115, in Chapter 41, “The GLIMMIX Procedure.”

## Example 46.4: Mixed Model Analysis of Microarray Data

Microarray experiments are an advanced genomic technique used in the discovery of new treatments for diseases. Microarray analysis allows for the detection of tens of thousands of genes in a single DNA sample. A microarray is a glass slide or membrane that has been spotted or “arrayed” with DNA fragments or oligonucleotides representing specific genes. The response of the gene detected by a spot is proportional to the intensity of fluorescence associated with that spot. These gene responses can indicate associations with disease conditions, but they can also be affected by systematic biases and different treatments such as sex and genotypes. Statistical models for microarray data attempt to assess the significance and magnitude of gene effects across treatments while adjusting for these systematic biases and to evaluate the significance of differences between treatments.

There are two statistical approaches frequently used in mixed model analysis for microarray data. The first approach is to fit multiple gene-specific models to data normalized for systematic biases (Wolfinger et al. 2001; Gibson and Wolfinger 2004). This approach is based on assuming that

the biases are independent from the gene effects. If this assumption is untenable, then a second approach fits a single model that combines both the systematic biases and the gene effects (Kerr, Martin, and Churchill 2000; Churchill 2002; Littell et al. 2006). When the number of genes is very large, several hundreds to tens of thousands, this is an analysis for which the sparse matrix approach implemented in the HPMIXED procedure is well suited.

The following SAS statements simulate a microarray experiment with a so-called loop design structure, which is commonly used in such studies. There are 500 genes, each gene occurs in 6 arrays, and each array has 2 dyes.

```

%let narray = 6;
%let ndye = 2;
%let nrow = 4;
%let ngene = 500;
%let ntrt = 6;
%let npin = 4;
%let ndip = 4;
%let no = %eval(&ndye*&nrow*&ngene);
%let tno = %eval(&narray*&no);

data microarray;
 keep Gene MArray Dye Trt Pin Dip log2i;
 array PinDist{&tno};
 array DipDist{&tno};
 array GeneDist{&tno};

 array ArrayEffect{&narray};
 array ArrayGeneEffect{%eval(&narray*&ngene)};
 array ArrayDipEffect{%eval(&narray*&ndip)};
 array ArrayPinEffect{%eval(&narray*&npin)};

 do i = 1 to &tno;
 PinDist{i} = 1 + int(&npin*ranuni(12345));
 DipDist{i} = 1 + int(&ndip*ranuni(12345));
 GeneDist{i} = 1 + int(&ngene*ranuni(12345));
 end;

 igene = 0;
 idip = 0;
 ipin = 0;
 do i = 1 to &narray;
 ArrayEffect{i} = sqrt(0.014)*rannor(12345);
 do j = 1 to &ngene;
 igene = igene+1;
 ArrayGeneEffect{igene} = sqrt(0.0017)*rannor(12345);
 end;
 do j = 1 to &ndip;
 idip = idip + 1;
 ArrayDipEffect{idip} = sqrt(0.0033)*rannor(12345);
 end;
 do j = 1 to &npin;
 ipin = ipin + 1;
 ArrayPinEffect{ipin} = sqrt(0.037)*rannor(12345);
 end;
 end;

```

```

 end;
end;

i = 0;
do MArray = 1 to &narray;
 do Dye = 1 to &ndye;
 do Row = 1 to &nrow;
 do k = 1 to &ngene;
 if MArray=1 and Dye = 1 then do;
 Trt = 0;
 trtc = 0;
 end;
 else do;
 if trtc >= &no then trtc = 0;
 if trtc = 0 then do;
 Trt = Trt + 1;
 if Trt >= &ntrt then do;
 Trt = 0;
 trtc = 0;
 end;
 end;
 trtc = trtc + 1;
 end;
 i = i + 1;
 Pin = PinDist{i};
 Dip = DipDist{i};
 Gene = GeneDist{i};
 a = ArrayEffect{MArray};
 ag = ArrayGeneEffect{(MArray-1)*&ngene+Gene};
 ad = ArrayDipEffect{(MArray-1)*&ndip+Dip};
 ap = ArrayPinEffect{(MArray-1)*&npin+Pin};
 log2i = 1 +
 + Dye
 + Trt
 + Gene/1000.0
 + Dye*Gene/1000.0
 + Trt*Gene/1000.0
 + Pin
 + a
 + ag
 + ad
 + ap
 + sqrt(0.02)*rannor(12345);
 output;
 end;
 end;
 end;
end;
run;

```

A linear mixed model for fitting the log intensity data  $Y_{ijkmnr}$  from such a design is described by Littell et al. (2006) as follows:

$$Y_{ijkmnr} =$$

|                       |                        | <b>Fixed Effects</b>  |
|-----------------------|------------------------|-----------------------|
|                       | $\mu$                  | Overall mean          |
| +                     | $\lambda_i$            | Gene                  |
| +                     | $\tau_j$               | Treatment             |
| +                     | $\delta_k$             | Dye                   |
| +                     | $(\tau\lambda)_{ij}$   | Treatment-by-gene     |
| +                     | $(\delta\lambda)_{ik}$ | Dye-by-gene           |
| +                     | $p_r$                  | Pin                   |
| <b>Random Effects</b> |                        |                       |
| +                     | $a_m$                  | Microarray            |
| +                     | $(a\lambda)_{im}$      | Microarray-by-gene    |
| +                     | $d(a)_{mn}$            | Dip-within-microarray |
| +                     | $(ap)_{mr}$            | Microarray-by-pin     |
| +                     | $e_{ijkmnr}$           | Residual noise        |

You can use the HPMIXED procedure with the following statements to fit this model:

```
proc hpmixed data=microarray;
 class marray dye trt gene pin dip;
 model log2i = dye trt gene dye*gene trt*gene pin;
 random marray marray*gene dip(marray) pin*marray;
 test trt;
run;
```

The “Dimensions” table shown in [Output 46.4.1](#) indicates that this is a very large model, with 4512 columns in  $\mathbf{X}$  matrix and 3054 columns in  $\mathbf{Z}$  matrix. It will be computationally very inefficient to fit this model by using dense matrix methods; the sparse matrix approach of the HPMIXED procedure is of critical importance.

**Output 46.4.1** Mixed Model Dimensions

| <b>The HPMIXED Procedure</b> |      |
|------------------------------|------|
| <b>Dimensions</b>            |      |
| G-side Cov. Parameters       | 4    |
| R-side Cov. Parameters       | 1    |
| Columns in X                 | 4513 |
| Columns in Z                 | 3054 |
| Subjects (Blocks in V)       | 1    |

The  $p$ -value in [Output 46.4.2](#) indicates that there are significant differences between treatments.

**Output 46.4.2** Type III Tests of Fixed Effects

| Type III Tests of Fixed Effects |           |           |         |        |
|---------------------------------|-----------|-----------|---------|--------|
| Effect                          | Num<br>DF | Den<br>DF | F Value | Pr > F |
| Trt                             | 5         | 20497     | 370005  | <.0001 |

**Example 46.5: Repeated Measures**

The following data are from Pothoff and Roy (1964) and consist of growth measurements for 11 girls and 16 boys at ages 8, 10, 12, and 14. Some of the observations are suspect (for example, the third observation for person 20); however, all of the data are used here for comparison purposes.

The analysis strategy employs a linear growth curve model for the boys and girls in addition to a variance-covariance model that incorporates correlations for all of the observations that arise from the same person. The PROC HPMIXED statements to fit an unstructured variance matrix are as follows:

```
data pr;
 input Person Gender $ y1 y2 y3 y4;
 y=y1; Time=1; Age=8; output;
 y=y2; Time=2; Age=10; output;
 y=y3; Time=3; Age=12; output;
 y=y4; Time=4; Age=14; output;
 drop y1-y4;
 datalines;
1 F 21.0 20.0 21.5 23.0
2 F 21.0 21.5 24.0 25.5
3 F 20.5 24.0 24.5 26.0
4 F 23.5 24.5 25.0 26.5
5 F 21.5 23.0 22.5 23.5
6 F 20.0 21.0 21.0 22.5
7 F 21.5 22.5 23.0 25.0
8 F 23.0 23.0 23.5 24.0
9 F 20.0 21.0 22.0 21.5
10 F 16.5 19.0 19.0 19.5
11 F 24.5 25.0 28.0 28.0
12 M 26.0 25.0 29.0 31.0
13 M 21.5 22.5 23.0 26.5
14 M 23.0 22.5 24.0 27.5
15 M 25.5 27.5 26.5 27.0
16 M 20.0 23.5 22.5 26.0
17 M 24.5 25.5 27.0 28.5
18 M 22.0 22.0 24.5 26.5
19 M 24.0 21.5 24.5 25.5
20 M 23.0 20.5 31.0 26.0
21 M 27.5 28.0 31.0 31.5
22 M 23.0 23.0 23.5 25.0
23 M 21.5 23.5 24.0 28.0
24 M 17.0 24.5 26.0 29.5
```

```

25 M 22.5 25.5 25.5 26.0
26 M 23.0 24.5 26.0 30.0
27 M 22.0 21.5 23.5 25.0
;

proc hpmixed data=pr;
 class Person Gender Time;
 model y = Gender Age Gender*Age;
 test Gender Age Gender*Age;
 repeated Time / type=un subject=Person r;
run;

```

The **MODEL** statement first lists the dependent variable *Y*. The fixed effects are then listed after the equal sign. The variable *Gender* requests a different intercept for the girls and boys, *Age* models an overall linear growth trend, and *Gender\*Age* makes the slopes different over time. It is actually not necessary to specify *Age* separately, but doing so enables PROC HPMIXED to carry out a test for heterogeneous slopes.

The **REPEATED** statement contains a *repeated-effect* *Time*. The **TYPE=UN** option models the covariance as an unstructured block for each **SUBJECT=Person**. Each of the 27 subjects has a maximum of four observations. Therefore, the **R** matrix is block diagonal with 27 blocks, each block consisting of identical 4×4 unstructured matrices. The 10 parameters of these unstructured blocks make up the covariance parameters estimated by restricted maximum likelihood. The **R=** option requests that the first block of **R** be displayed.

The results from this analysis are shown in [Output 46.5.1](#) through [Output 46.5.5](#).

#### Output 46.5.1 Repeated Measures Analysis

| The HPMIXED Procedure    |    |
|--------------------------|----|
| Dimensions               |    |
| G-side Cov. Parameters   | 0  |
| R-side Cov. Parameters   | 10 |
| Columns in X             | 6  |
| Columns in Z per Subject | 0  |
| Subjects (Blocks in V)   | 27 |

In [Output 46.5.1](#), the 10 covariance parameters result from the 4 × 4 unstructured blocks of **R**. There is no **Z** matrix for this model.

#### Output 46.5.2 Repeated Measures Analysis (continued)

|                             |     |
|-----------------------------|-----|
| Number of Observations Read | 108 |
| Number of Observations Used | 108 |

**Output 46.5.2** *continued*

| Iteration History |             |                    |             |              |
|-------------------|-------------|--------------------|-------------|--------------|
| Iteration         | Evaluations | Objective Function | Change      | Max Gradient |
| 0                 | 4           | 483.55903028       | .           | 18.65974     |
| 1                 | 4           | 446.6618154        | 36.89721488 | 14.63195     |
| 2                 | 5           | 430.2967104        | 16.36510500 | 10.93182     |
| 3                 | 5           | 427.86149052       | 2.43521988  | 12.34361     |
| 4                 | 2           | 426.16528163       | 1.69620890  | 8.094057     |
| 5                 | 3           | 425.56874743       | 0.59653420  | 3.517822     |
| 6                 | 2           | 424.91919206       | 0.64955537  | 2.492626     |
| 7                 | 3           | 424.731766         | 0.18742606  | 2.110784     |
| 8                 | 3           | 424.66856966       | 0.06319634  | 1.417574     |
| 9                 | 2           | 424.63858357       | 0.02998609  | 1.468348     |
| 10                | 2           | 424.60787324       | 0.03071033  | 1.174872     |
| 11                | 2           | 424.5593949        | 0.04847834  | 0.601039     |
| 12                | 3           | 424.55305379       | 0.00634111  | 0.316659     |
| 13                | 2           | 424.54886941       | 0.00418438  | 0.170275     |
| 14                | 3           | 424.54696194       | 0.00190747  | 0.072622     |
| 15                | 3           | 424.5468178        | 0.00014413  | 0.019582     |
| 16                | 3           | 424.54680027       | 0.00001753  | 0.001888     |
| 17                | 3           | 424.5468002        | 0.00000007  | 0.000235     |

Convergence criterion (GCONV=1E-8) satisfied.

The 17 quasi-Newton iterations are used to find the maximum likelihood estimates ([Output 46.5.2](#)).

**Output 46.5.3** Repeated Measures Analysis (*continued*)

| Estimated R Matrix for Person 1 |        |        |        |        |
|---------------------------------|--------|--------|--------|--------|
| Row                             | Col1   | Col2   | Col3   | Col4   |
| 1                               | 5.4252 | 2.7092 | 3.8411 | 2.7151 |
| 2                               | 2.7092 | 4.1906 | 2.9745 | 3.3137 |
| 3                               | 3.8411 | 2.9745 | 6.2632 | 4.1332 |
| 4                               | 2.7151 | 3.3137 | 4.1332 | 4.9862 |

The 4×4 matrix in [Output 46.5.3](#) is the estimated unstructured covariance matrix. It is the estimate of the first block of  $\mathbf{R}$ , and the other 26 blocks all have the same estimate.



**Output 46.5.4** Repeated Measures Analysis (*continued*)

| Covariance Parameter Estimates |         |          |
|--------------------------------|---------|----------|
| Cov Parm                       | Subject | Estimate |
| UN(1,1)                        | Person  | 5.4252   |
| UN(2,1)                        | Person  | 2.7092   |
| UN(2,2)                        | Person  | 4.1906   |
| UN(3,1)                        | Person  | 3.8411   |
| UN(3,2)                        | Person  | 2.9745   |
| UN(3,3)                        | Person  | 6.2632   |
| UN(4,1)                        | Person  | 2.7151   |
| UN(4,2)                        | Person  | 3.3137   |
| UN(4,3)                        | Person  | 4.1332   |
| UN(4,4)                        | Person  | 4.9862   |

The “Covariance Parameter Estimates” table in [Output 46.5.4](#) lists the 10 estimated covariance parameters in order; note their correspondence to the first block of **R** displayed in [Output 46.5.3](#). The parameter estimates are labeled according to their location in the block in the Cov Parm column, and all of these estimates are associated with Person as the subject effect.

**Output 46.5.5** Repeated Measures Analysis (*continued*)

| Type III Tests of Fixed Effects |           |           |         |        |
|---------------------------------|-----------|-----------|---------|--------|
| Effect                          | Num<br>DF | Den<br>DF | F Value | Pr > F |
| Gender                          | 1         | 104       | 1.08    | 0.3011 |
| Age                             | 1         | 104       | 102.35  | <.0001 |
| Age*Gender                      | 1         | 104       | 7.40    | 0.0076 |

The “Type III Tests of Fixed Effects” table in [Output 46.5.5](#) displays Type III tests for all of the fixed effects. These tests are partial in the sense that they account for all of the other fixed effects in the model.

Since the different levels of the repeated effect represent different years, it is natural to try fitting a time series model to the data within each subject. To obtain time series structures in **R**, you can replace **TYPE=UN** with **TYPE=AR(1)** to obtain the first-order autoregressive covariance matrices. For example, the statements to fit an AR(1) structure are as follows:

```
proc hpmixed data=pr;
 class Person Gender Time;
 model y = Gender Age Gender*Age;
 repeated Time / type=ar(1) sub=Person r;
run;
```

The estimated AR(1) structure covariance matrix of the first block of **R** is shown in [Output 46.5.6](#)

**Output 46.5.6** Repeated Measures Analysis

| The HPMIXED Procedure           |        |        |        |        |
|---------------------------------|--------|--------|--------|--------|
| Estimated R Matrix for Person 1 |        |        |        |        |
| Row                             | Col1   | Col2   | Col3   | Col4   |
| 1                               | 5.2144 | 3.2563 | 2.0335 | 1.2699 |
| 2                               | 3.2563 | 5.2144 | 3.2563 | 2.0335 |
| 3                               | 2.0335 | 3.2563 | 5.2144 | 3.2563 |
| 4                               | 1.2699 | 2.0335 | 3.2563 | 5.2144 |

---

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# Chapter 47

## The INBREED Procedure

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---

### Overview: INBREED Procedure

The INBREED procedure calculates the covariance or inbreeding coefficients for a pedigree. PROC INBREED is unique in that it handles very large populations.

The INBREED procedure has two modes of operation. One mode carries out analysis on the assumption that all the individuals belong to the same generation. The other mode divides the population into nonoverlapping generations and analyzes each generation separately, assuming that the parents of individuals in the current generation are defined in the previous generation.

PROC INBREED also computes averages of the covariance or inbreeding coefficients within sex categories if the sex of individuals is known.

## Getting Started: INBREED Procedure

This section demonstrates how you can use the INBREED procedure to calculate the inbreeding or covariance coefficients for a pedigree, how you can control the analysis mode if the population consists of nonoverlapping generations, and how you can obtain averages within sex categories.

For you to use PROC INBREED effectively, your input data set must have a definite format. The following sections first introduce this format for a fictitious population and then demonstrate how you can analyze this population by using the INBREED procedure.

### The Format of the Input Data Set

The SAS data set used as input to the INBREED procedure must contain an observation for each individual. Each observation must include one variable identifying the individual and two variables identifying the individual's parents. Optionally, an observation can contain a known covariance coefficient and a character variable defining the gender of the individual.

For example, consider the following data:

```
data Population;
 input Individual $ Parent1 $ Parent2 $
 Covariance Sex $ Generation;
 datalines;
Mark George Lisa . M 1
Kelly Scott Lisa . F 1
Mike George Amy . M 1
. Mark Kelly 0.50 . 1
David Mark Kelly . M 2
Merle Mike Jane . F 2
Jim Mark Kelly 0.50 M 2
Mark Mike Kelly . M 2
;
```

It is important to order the pedigree observations so that individuals are defined before they are used as parents of other individuals. The family relationships between individuals cannot be ascertained correctly unless you observe this ordering. Also, older individuals must precede younger ones. For example, 'Mark' appears as the first parent of 'David' at observation 5; therefore, his observation needs to be defined prior to observation 5. Indeed, this is the case (see observation 1). Also, 'David' is older than 'Jim', whose observation appears after the observation for 'David', as is appropriate.

In populations with distinct, nonoverlapping generations, the older generation (parents) must precede the younger generation. For example, the individuals defined in Generation=1 appear as parents of individuals defined in Generation=2.

PROC INBREED produces warning messages when a parent cannot be found. For example, 'Jane' appears as the second parent of the individual 'Merle' even though there are no previous observations defining her own parents. If the population is treated as an overlapping population, that is, if the generation grouping is ignored, then the procedure inserts an observation for 'Jane' with missing parents just before the sixth observation, which defines 'Merle' as follows:

```
Jane . . . F 2
Merle Mike Jane . F 2
```

However, if generation grouping is taken into consideration, then ‘Jane’ is defined as the last observation in Generation=1, as follows:

```
Mike George Amy . M 1
Jane . . . F 1
```

In this latter case, however, the observation for ‘Jane’ is inserted after the computations are reported for the first generation. Therefore, she does not appear in the covariance/inbreeding matrix, even though her observation is used in computations for the second generation (see [Figure 47.2](#)).

If the data for an individual are duplicated, only the first occurrence of the data is used by the procedure, and a warning message is displayed to note the duplication. For example, individual ‘Mark’ is defined twice, at observations 1 and 8. If generation grouping is ignored, then this is an error and observation 8 is skipped. However, if the population is processed with respect to two distinct generations, then ‘Mark’ refers to two different individuals, one in Generation=1 and the other in Generation=2.

If a covariance is to be assigned between two individuals, then those individuals must be defined prior to the assignment observation. For example, a covariance of 0.50 can be assigned between ‘Mark’ and ‘Kelly’ since they are previously defined. Note that assignment statements must have different formats depending on whether the population is processed with respect to generations (see the section “[DATA= Data Set](#)” on page 3731 for further information). For example, while observation 4 is valid for nonoverlapping generations, it is invalid for a processing mode that ignores generation grouping. In this latter case, observation 7 indicates a valid assignment, and observation 4 is skipped.

The latest covariance specification between any given two individuals overrides the previous one between the same individuals.

---

## Performing the Analysis

To compute the covariance coefficients for the overlapping generation mode, use the following statements:

```
proc inbreed data=Population covar matrix init=0.25;
run;
```

Here, the DATA= option names the SAS data set to be analyzed, and the COVAR and MATRIX options tell the procedure to output the covariance coefficients matrix. If you omit the COVAR option, the inbreeding coefficients are output instead of the covariance coefficients.

Note that the PROC INBREED statement also contains the INIT= option. This option gives an initial covariance between any individual and unknown individuals. For example, the covariance between any individual and ‘Jane’ would be 0.25, since ‘Jane’ is unknown, except when ‘Jane’ appears as a parent (see [Figure 47.4](#)).

**Figure 47.1** Analysis for an Overlapping Population

| The INBREED Procedure   |         |         |        |        |        |        |        |
|-------------------------|---------|---------|--------|--------|--------|--------|--------|
| Covariance Coefficients |         |         |        |        |        |        |        |
| Individual              | Parent1 | Parent2 | George | Lisa   | Mark   | Scott  | Kelly  |
| George                  |         |         | 1.1250 | 0.2500 | 0.6875 | 0.2500 | 0.2500 |
| Lisa                    |         |         | 0.2500 | 1.1250 | 0.6875 | 0.2500 | 0.6875 |
| Mark                    | George  | Lisa    | 0.6875 | 0.6875 | 1.1250 | 0.2500 | 0.5000 |
| Scott                   |         |         | 0.2500 | 0.2500 | 0.2500 | 1.1250 | 0.6875 |
| Kelly                   | Scott   | Lisa    | 0.2500 | 0.6875 | 0.5000 | 0.6875 | 1.1250 |
| Amy                     |         |         | 0.2500 | 0.2500 | 0.2500 | 0.2500 | 0.2500 |
| Mike                    | George  | Amy     | 0.6875 | 0.2500 | 0.4688 | 0.2500 | 0.2500 |
| David                   | Mark    | Kelly   | 0.4688 | 0.6875 | 0.8125 | 0.4688 | 0.8125 |
| Jane                    |         |         | 0.2500 | 0.2500 | 0.2500 | 0.2500 | 0.2500 |
| Merle                   | Mike    | Jane    | 0.4688 | 0.2500 | 0.3594 | 0.2500 | 0.2500 |
| Jim                     | Mark    | Kelly   | 0.4688 | 0.6875 | 0.8125 | 0.4688 | 0.8125 |
| Covariance Coefficients |         |         |        |        |        |        |        |
| Individual              | Parent1 | Parent2 | Amy    | Mike   | David  | Jane   | Merle  |
| George                  |         |         | 0.2500 | 0.6875 | 0.4688 | 0.2500 | 0.4688 |
| Lisa                    |         |         | 0.2500 | 0.2500 | 0.6875 | 0.2500 | 0.2500 |
| Mark                    | George  | Lisa    | 0.2500 | 0.4688 | 0.8125 | 0.2500 | 0.3594 |
| Scott                   |         |         | 0.2500 | 0.2500 | 0.4688 | 0.2500 | 0.2500 |
| Kelly                   | Scott   | Lisa    | 0.2500 | 0.2500 | 0.8125 | 0.2500 | 0.2500 |
| Amy                     |         |         | 1.1250 | 0.6875 | 0.2500 | 0.2500 | 0.4688 |
| Mike                    | George  | Amy     | 0.6875 | 1.1250 | 0.3594 | 0.2500 | 0.6875 |
| David                   | Mark    | Kelly   | 0.2500 | 0.3594 | 1.2500 | 0.2500 | 0.3047 |
| Jane                    |         |         | 0.2500 | 0.2500 | 0.2500 | 1.1250 | 0.6875 |
| Merle                   | Mike    | Jane    | 0.4688 | 0.6875 | 0.3047 | 0.6875 | 1.1250 |
| Jim                     | Mark    | Kelly   | 0.2500 | 0.3594 | 0.8125 | 0.2500 | 0.3047 |
| Covariance Coefficients |         |         |        |        |        |        |        |
| Individual              | Parent1 | Parent2 | Jim    |        |        |        |        |
| George                  |         |         | 0.4688 |        |        |        |        |
| Lisa                    |         |         | 0.6875 |        |        |        |        |
| Mark                    | George  | Lisa    | 0.8125 |        |        |        |        |
| Scott                   |         |         | 0.4688 |        |        |        |        |
| Kelly                   | Scott   | Lisa    | 0.8125 |        |        |        |        |
| Amy                     |         |         | 0.2500 |        |        |        |        |
| Mike                    | George  | Amy     | 0.3594 |        |        |        |        |
| David                   | Mark    | Kelly   | 0.8125 |        |        |        |        |
| Jane                    |         |         | 0.2500 |        |        |        |        |
| Merle                   | Mike    | Jane    | 0.3047 |        |        |        |        |
| Jim                     | Mark    | Kelly   | 1.2500 |        |        |        |        |
| Number of Individuals   |         |         |        | 11     |        |        |        |

In the previous example, PROC INBREED treats the population as a single generation. However, you might want to process the population with respect to distinct, nonoverlapping generations. To accomplish this, you need to identify the generation variable in a CLASS statement, as shown by the following statements:

```
proc inbred data=Population covar matrix init=0.25;
 class Generation;
run;
```

Note that, in this case, the covariance matrix is displayed separately for each generation (see Figure 47.5).

**Figure 47.2** Analysis for a Nonoverlapping Population

|                                |                |                |                              |              |             |             |
|--------------------------------|----------------|----------------|------------------------------|--------------|-------------|-------------|
| <b>The INBREED Procedure</b>   |                |                |                              |              |             |             |
| <b>Generation = 1</b>          |                |                |                              |              |             |             |
| <b>Covariance Coefficients</b> |                |                |                              |              |             |             |
| <b>Individual</b>              | <b>Parent1</b> | <b>Parent2</b> | <b>Mark</b>                  | <b>Kelly</b> | <b>Mike</b> |             |
| <b>Mark</b>                    | <b>George</b>  | <b>Lisa</b>    | 1.1250                       | 0.5000       | 0.4688      |             |
| <b>Kelly</b>                   | <b>Scott</b>   | <b>Lisa</b>    | 0.5000                       | 1.1250       | 0.2500      |             |
| <b>Mike</b>                    | <b>George</b>  | <b>Amy</b>     | 0.4688                       | 0.2500       | 1.1250      |             |
|                                |                |                | <b>Number of Individuals</b> | <b>3</b>     |             |             |
| <b>The INBREED Procedure</b>   |                |                |                              |              |             |             |
| <b>Generation = 2</b>          |                |                |                              |              |             |             |
| <b>Covariance Coefficients</b> |                |                |                              |              |             |             |
| <b>Individual</b>              | <b>Parent1</b> | <b>Parent2</b> | <b>David</b>                 | <b>Merle</b> | <b>Jim</b>  | <b>Mark</b> |
| <b>David</b>                   | <b>Mark</b>    | <b>Kelly</b>   | 1.2500                       | 0.3047       | 0.8125      | 0.5859      |
| <b>Merle</b>                   | <b>Mike</b>    | <b>Jane</b>    | 0.3047                       | 1.1250       | 0.3047      | 0.4688      |
| <b>Jim</b>                     | <b>Mark</b>    | <b>Kelly</b>   | 0.8125                       | 0.3047       | 1.2500      | 0.5859      |
| <b>Mark</b>                    | <b>Mike</b>    | <b>Kelly</b>   | 0.5859                       | 0.4688       | 0.5859      | 1.1250      |
|                                |                |                | <b>Number of Individuals</b> | <b>4</b>     |             |             |

You might also want to see covariance coefficient averages within sex categories. This is accomplished by indicating the variable defining the gender of individuals in a GENDER statement and by adding the AVERAGE option to the PROC INBREED statement. For example, the following statements produce the covariance coefficient averages shown in Figure 47.3:



```

proc inbreed data=Population covar average init=0.25;
 class Generation;
 gender Sex;
run;

```

**Figure 47.3** Averages within Sex Categories for a Nonoverlapping Generation

| The INBREED Procedure                                     |             |                |
|-----------------------------------------------------------|-------------|----------------|
| Generation = 1                                            |             |                |
| Averages of Covariance Coefficient Matrix in Generation 1 |             |                |
|                                                           | On Diagonal | Below Diagonal |
| Male X Male                                               | 1.1250      | 0.4688         |
| Male X Female                                             | .           | 0.3750         |
| Female X Female                                           | 1.1250      | 0.0000         |
| Over Sex                                                  | 1.1250      | 0.4063         |
| Number of Males                                           | 2           |                |
| Number of Females                                         | 1           |                |
| Number of Individuals                                     | 3           |                |
| The INBREED Procedure                                     |             |                |
| Generation = 2                                            |             |                |
| Averages of Covariance Coefficient Matrix in Generation 2 |             |                |
|                                                           | On Diagonal | Below Diagonal |
| Male X Male                                               | 1.2083      | 0.6615         |
| Male X Female                                             | .           | 0.3594         |
| Female X Female                                           | 1.1250      | 0.0000         |
| Over Sex                                                  | 1.1875      | 0.5104         |
| Number of Males                                           | 3           |                |
| Number of Females                                         | 1           |                |
| Number of Individuals                                     | 4           |                |

---

## Syntax: INBREED Procedure

The following statements are available in the INBREED procedure:

```

PROC INBREED < options > ;
 BY variables ;
 CLASS variable ;
 GENDER variable ;
 MATINGS individual-list1 / mate-list1 < , ... , individual-listn / mate-listn > ;
 VAR variables ;

```

The PROC INBREED statement is required. Items within angle brackets (< >) are optional. The syntax of each statement is described in the following sections.

---

## PROC INBREED Statement

```

PROC INBREED < options > ;

```

The PROC INBREED statement invokes the INBREED procedure. [Table 47.1](#) summarizes the options available in the PROC INBREED statement.

**Table 47.1** PROC INBREED Statement Options

| Option                                  | Description                                                               |
|-----------------------------------------|---------------------------------------------------------------------------|
| <b>Specify Data Sets</b>                |                                                                           |
| DATA=                                   | Names the SAS data set                                                    |
| OUTCOV=                                 | Names an output data set to contain the inbreeding coefficients           |
| <b>Control Type of Coefficient</b>      |                                                                           |
| COVAR                                   | Specifies that all coefficients output consist of covariance coefficients |
| SELFDIAG                                | Includes an individual's self-mating kinship coefficient                  |
| <b>Control Displayed Tables</b>         |                                                                           |
| AVERAGE                                 | Produces a table of averages of coefficients                              |
| IND                                     | Displays the individuals' inbreeding coefficients                         |
| MATRIX                                  | Displays the inbreeding coefficient matrix                                |
| <b>Specify Default Covariance Value</b> |                                                                           |
| INIT=                                   | Specifies the covariance value                                            |
| <b>Suppress Output</b>                  |                                                                           |
| INDL                                    | Displays individuals' coefficients for only the last generation           |
| MATRIXL                                 | Displays coefficients for only the last generation                        |
| NOPRINT                                 | Suppresses the display of all output                                      |

---

**AVERAGE****A**

produces a table of averages of coefficients for each pedigree of offspring. The AVERAGE option is used together with the **GENDER** statement to average the inbreeding/covariance coefficients within sex categories.

**COVAR****C**

specifies that all coefficients output consist of covariance coefficients rather than inbreeding coefficients.

**DATA=SAS-data-set**

names the SAS data set to be used by **PROC INBREED**. If you omit the DATA= option, the most recently created SAS data set is used.

**IND****I**

displays the individuals' inbreeding coefficients (diagonal of the inbreeding coefficients matrix) for each pedigree of offspring.

If you also specify the **COVAR** option, the individuals' covariance coefficients (diagonal of the covariance coefficients matrix) are displayed.

**INDL**

displays individuals' coefficients for only the last generation of a multiparous population.

**INIT=COV**

specifies the covariance value *cov* if any of the parents are unknown; a value of 0 is assumed if you do not specify the INIT= option.

**MATRIX****M**

displays the inbreeding coefficient matrix for each pedigree of offspring.

If you also specify the **COVAR** option, the covariance matrices are displayed instead of inbreeding coefficients matrices.

**MATRIXL**

displays coefficients for only the last generation of a multiparous population.

**NOPRINT**

suppresses the display of all output. Note that this option temporarily disables the Output Delivery System (ODS). For more information on ODS, see Chapter 20, "Using the Output Delivery System."

**OUTCOV=SAS-data-set**

names an output data set to contain the inbreeding coefficients. When the **COVAR** option is also specified, covariance estimates are output to the OUTCOV= data set instead of inbreeding coefficients.

**SELFDIAG**

includes an individual's self-mating kinship coefficient instead of the individual's inbreeding coefficient on the diagonal of the matrix in the OUTCOV= data set when the COVAR option is not specified.

**BY Statement**

**BY** *variables* ;

You can specify a BY statement with PROC INBREED to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the INBREED procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

**CLASS Statement**

**CLASS** *variable* ;

To analyze the population within nonoverlapping generations, you must specify the variable that identifies generations in a CLASS statement. Values of the generation variable, called *generation numbers*, must be integers, but generations are assumed to occur in the order of their input in the input data set rather than in numerical order of the generation numbers. The name of an individual needs to be unique only within its generation.

When the **MATRIXL** option or the **INDL** option is specified, each generation requires a unique generation number in order for the specified option to work correctly. If generation numbers are not unique, all the generations with a generation number that is the same as the last generation's are output.

**GENDER Statement**

**GENDER** *variable* ;

The GENDER statement specifies a variable that indicates the sex of the individuals. Values of the sex variable must be character beginning with ‘M’ or ‘F’, for male or female. The GENDER statement is needed only when you specify the AVERAGE option to average the inbreeding/covariance coefficients within sex categories or when you want to include a gender variable in the OUTCOV= data set.

PROC INBREED makes the following assumptions regarding the gender of individuals:

- The first parent is always assumed to be the male. See the section “VAR Statement” on page 3730.
- The second parent is always assumed to be the female. See the section “VAR Statement” on page 3730.
- If the gender of an individual is missing or invalid, this individual is assumed to be a female unless the population is overlapping and this individual appears as the first parent in a later observation.

Any contradictions to these rules are reported in the SAS log.

---

## MATINGS Statement

**MATINGS** *individual-list1 / mate-list1 <, ..., individual-listn / mate-listn>* ;

You can specify the MATINGS statement with PROC INBREED to specify selected matings of individuals. Each individual given in *individual-list* is mated with each individual given in *mate-list*. You can write multiple mating specifications if you separate them by commas or asterisks. The procedure reports the inbreeding coefficients or covariances for each pair of mates. For example, you can use the following statement to specify the mating of an individual named ‘David’ with an individual named ‘Jane’:

```
matings david / jane;
```

---

## VAR Statement

**VAR** *individual parent1 parent2 <covariance>* ;

The VAR statement specifies three or four variables: the first variable contains an individual’s name, the second variable contains the name of the individual’s first parent, and the third variable contains the name of the individual’s second parent. An optional fourth variable assigns a known value to the covariance of the individual’s first and second parents in the current generation.

The first three variables in the VAR statement can be either numeric or character; however, only the first 12 characters of a character variable are recognized by the procedure. The fourth variable, if specified, must be numeric.

If you omit the VAR statement, then the procedure uses the first three unaddressed variables as the names of the individual and its parents. (Unaddressed variables are those that are not referenced in any other PROC INBREED statement.) If the input data set contains an unaddressed fourth variable, then it becomes the covariance variable.

---

## Details: INBREED Procedure

---

### Missing Values

A missing value for a parent implies that the parent is unknown. Unknown parents are assumed to be unrelated and not inbred unless you specify the `INIT=` option.

When the value of the variable identifying the individual is missing, the observation is not added to the list of individuals. However, for a multiparous population, an observation with a missing individual is valid and is used for assigning covariances.

Missing covariance values are determined from the `INIT=cov` option, if specified. Observations with missing generation variables are excluded.

If the gender of an individual is missing, it is determined from the order in which it is listed on the first observation defining its progeny for an overlapping population. If it appears as the first parent, it is set to 'M'; otherwise, it is set to 'F'. When the gender of an individual cannot be determined, it is assigned a default value of 'F'.

---

### DATA= Data Set

Each observation in the input data set should contain necessary information such as the identification of an individual and the first and second parents of an individual. In addition, if a `CLASS` statement is specified, each observation should contain the generation identification; and, if a `GENDER` statement is specified, each observation should contain the gender of an individual. Optionally, each observation might also contain the covariance between the first and the second parents. Depending on how many statements are specified with the procedure, there should be enough variables in the input data set containing this information.

If you omit the `VAR` statement, then the procedure uses the first three *unaddressed variables* in the input data set as the names of the individual and his or her parents. Unaddressed variables in the input data set are those variables that are not referenced by the procedure in any other statements, such as `CLASS`, `GENDER`, or `BY` statements. If the input data set contains an unaddressed fourth variable, then the procedure uses it as the covariance variable.

If the individuals given by the variables associated with the first and second parents are not in the population, they are added to the population. However, if they are in the population, they must be defined prior to the observation that gives their progeny.

When there is a `CLASS` statement, the functions of defining new individuals and assigning covariances must be separated. This is necessary because the parents of any given individual are defined in the previous generation, while covariances are assigned between individuals in the current generation.

Therefore, there could be two types of observations for a multiparous population:

- one to define new individuals in the current generation whose parents have been defined in the previous generation, as in the following, where the missing value is for the covariance variable:

```
Mark George Lisa . M 1
Kelly Scott Lisa . F 1
```

- one to assign covariances between two individuals in the current generation, as in the following, where the individual's name is missing, 'Mark' and 'Kelly' are in the current generation, and the covariance coefficient between these two individuals is 0.50:

```
. Mark Kelly 0.50 . 1
```

Note that the observations defining individuals must precede the observation assigning a covariance value between them. For example, if a covariance is to be assigned between 'Mark' and 'Kelly', then both of them should be defined prior to the assignment observation.

## Computational Details

This section describes the rules that the INBREED procedure uses to compute the covariance and inbreeding coefficients. Each computational rule is explained by an example referring to the fictitious population introduced in the section "Getting Started: INBREED Procedure" on page 3722.

### Coancestry (or Kinship Coefficient)

To calculate the inbreeding coefficient and the covariance coefficients, use the degree of relationship by descent between the two parents, which is called *coancestry* or *kinship coefficient* (Falconer and Mackay 1996, p.85), or *coefficient of parentage* (Kempthorne 1957, p.73). Denote the coancestry between individuals X and Y by  $f_{XY}$ . For information on how to calculate the coancestries among a population, see the section "Calculation of Coancestry" on page 3733.

### Covariance Coefficient (or Coefficient of Relationship)

The covariance coefficient between individuals X and Y is defined by

$$\text{Cov}(X, Y) = 2f_{XY}$$

where  $f_{XY}$  is the coancestry between X and Y. The covariance coefficient is sometimes called the *coefficient of relationship* or the *theoretical correlation* (Falconer and Mackay (1996, p.153); Crow and Kimura (1970, p.134)). If a covariance coefficient cannot be calculated from the individuals in the population, it is assigned to an initial value. The initial value is set to 0 if the INIT= option is not specified or to *cov* if INIT=*cov*. Therefore, the corresponding initial coancestry is set to 0 if the INIT= option is not specified or to  $\frac{1}{2}\text{cov}$  if INIT=*cov*.

## Inbreeding Coefficients

The inbreeding coefficient of an individual is the probability that the pair of alleles carried by the gametes that produced it are identical by descent (Falconer and Mackay (1996, Chapter 5), Kempthorne (1957, Chapter 5)). For individual X, denote its inbreeding coefficient by  $F_X$ . The inbreeding coefficient of an individual is equal to the coancestry between its parents. For example, if X has parents A and B, then the inbreeding coefficient of X is

$$F_X = f_{AB}$$

## Calculation of Coancestry

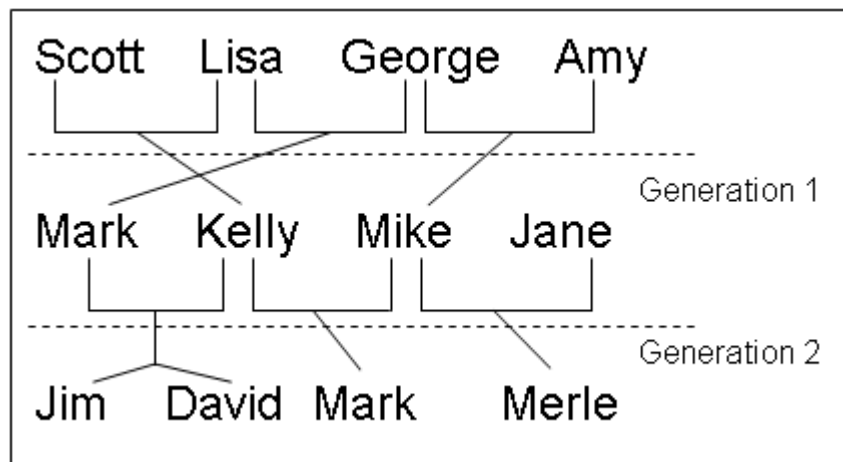
Given individuals X and Y, assume that X has parents A and B and that Y has parents C and D. For nonoverlapping generations, the basic rule to calculate the coancestry between X and Y is given by the following formula (Falconer and Mackay 1996, p.86):

$$f_{XY} = \frac{1}{4}(f_{AC} + f_{AD} + f_{BC} + f_{BD})$$

And the inbreeding coefficient for an offspring of X and Y, called Z, is the coancestry between X and Y:

$$F_Z = f_{XY}$$

**Figure 47.4** Inbreeding Relationship for Nonoverlapping Population



For example, in Figure 47.4, ‘Jim’ and ‘Mark’ from Generation 2 are progenies of ‘Mark’ and ‘Kelly’ and of ‘Mike’ and ‘Kelly’ from Generation 1, respectively. The coancestry between ‘Jim’ and ‘Mark’ is



$$f_{\text{Jim,Mark}} = \frac{1}{(f_{\text{Mark,Mike}} + f_{\text{Mark,Kelly}} + f_{\text{Kelly,Mike}} + f_{\text{Kelly,Kelly}})}$$

From the covariance matrix for Generation=1 in [Figure 47.4](#) and the relationship that coancestry is half of the covariance coefficient,

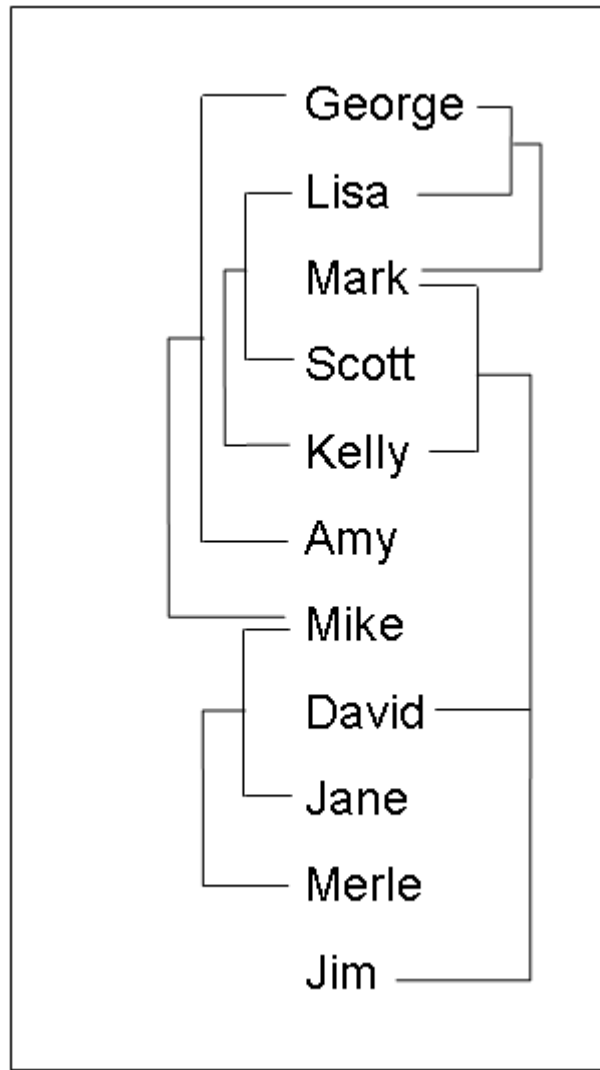
$$f_{\text{Jim,Mark}} = \frac{1}{4} \left( \frac{0.4688}{2} + \frac{0.5}{2} + \frac{0.25}{2} + \frac{1.125}{2} \right) = 0.29298$$

For overlapping generations, if X is older than Y, then the [basic rule](#) can be simplified to

$$F_Z = f_{XY} = \frac{1}{2} (f_{XC} + f_{XD})$$

That is, the coancestry between X and Y is the average of coancestries between older X with younger Y's parents. For example, in [Figure 47.5](#), the coancestry between 'Kelly' and 'David' is

$$f_{\text{Kelly,David}} = \frac{1}{2} (f_{\text{Kelly,Mark}} + f_{\text{Kelly,Kelly}})$$

**Figure 47.5** Inbreeding Relationship for Overlapping Population

This is so because ‘Kelly’ is defined before ‘David’; therefore, ‘Kelly’ is not younger than ‘David’, and the parents of ‘David’ are ‘Mark’ and ‘Kelly’. The covariance coefficient values  $\text{Cov}(\text{Kelly}, \text{Mark})$  and  $\text{Cov}(\text{Kelly}, \text{Kelly})$  from the matrix in Figure 47.5 yield that the coancestry between ‘Kelly’ and ‘David’ is

$$f_{\text{Kelly}, \text{David}} = \frac{1}{2} \left( \frac{0.5}{2} + \frac{1.125}{2} \right) = 0.40625$$

The numerical values for some initial coancestries must be known in order to use these rule. Either the parents of the first generation have to be unrelated, with  $f = 0$  if the `INIT=` option is not specified in the `PROC INBREED` statement, or their coancestries must have an initial value of  $\frac{1}{2} \text{cov}$ , where `cov` is set by the `INIT=` option. Then the subsequent coancestries among their progenies and the inbreeding coefficients of their progenies in the rest of the generations are calculated by using these initial values.

Special rules need to be considered in the calculations of coancestries for the following cases.

**Self-Mating**

The coancestry for an individual X with itself,  $f_{XX}$ , is the inbreeding coefficient of a progeny that is produced by self-mating. The relationship between the inbreeding coefficient and the coancestry for self-mating is

$$f_{XX} = \frac{1}{2}(1 + F_X)$$

The inbreeding coefficient  $F_X$  can be replaced by the coancestry between X's parents A and B,  $f_{AB}$ , if A and B are in the population:

$$f_{XX} = \frac{1}{2}(1 + f_{AB})$$

If X's parents are not in the population, then  $F_X$  is replaced by the initial value  $\frac{1}{2}cov$  if  $cov$  is set by the INIT= option, or  $F_X$  is replaced by 0 if the INIT= option is not specified. For example, the coancestry of 'Jim' with himself is

$$f_{\text{Jim},\text{Jim}} = \frac{1}{2}(1 + f_{\text{Mark},\text{Kelly}})$$

where 'Mark' and 'Kelly' are the parents of 'Jim'. Since the covariance coefficient  $\text{Cov}(\text{Mark},\text{Kelly})$  is 0.5 in Figure 47.5 and also in the covariance matrix for GENDER=1 in Figure 47.4, the coancestry of 'Jim' with himself is

$$f_{\text{Jim},\text{Jim}} = \frac{1}{2}\left(1 + \frac{0.5}{2}\right) = 0.625$$

When INIT=0.25, then the coancestry of 'Jane' with herself is

$$f_{\text{Jane},\text{Jane}} = \frac{1}{2}\left(1 + \frac{0.25}{2}\right) = 0.5625$$

because 'Jane' is not an offspring in the population.

**Offspring and Parent Mating**

Assuming that X's parents are A and B, the coancestry between X and A is

$$f_{XA} = \frac{1}{2}(f_{AB} + f_{AA})$$

The inbreeding coefficient for an offspring of X and A, denoted by Z, is

$$F_Z = f_{XA} = \frac{1}{2}(f_{AB} + f_{AA})$$

For example, ‘Mark’ is an offspring of ‘George’ and ‘Lisa’, so the coancestry between ‘Mark’ and ‘Lisa’ is

$$f_{\text{Mark,Lisa}} = \frac{1}{2}(f_{\text{Lisa,George}} + f_{\text{Lisa,Lisa}})$$

From the covariance coefficient matrix in [Figure 47.5](#),  $f_{\text{Lisa,George}} = 0.25/2 = 0.125$ ,  $f_{\text{Lisa,Lisa}} = 1.125/2 = 0.5625$ , so that

$$f_{\text{Mark,Lisa}} = \frac{1}{2}(0.125 + 0.5625) = 0.34375$$

Thus, the inbreeding coefficient for an offspring of ‘Mark’ and ‘Lisa’ is 0.34375.

### **Full Sibs Mating**

This is a special case for the basic rule given at the beginning of the section “[Calculation of Coancestry](#)” on page 3733. If X and Y are full sibs with same parents A and B, then the coancestry between X and Y is

$$f_{XY} = \frac{1}{4}(2f_{AB} + f_{AA} + f_{BB})$$

and the inbreeding coefficient for an offspring of A and B, denoted by Z, is

$$F_Z = f_{XY} = \frac{1}{4}(2f_{AB} + f_{AA} + f_{BB})$$

For example, ‘David’ and ‘Jim’ are full sibs with parents ‘Mark’ and ‘Kelly’, so the coancestry between ‘David’ and ‘Jim’ is

$$f_{\text{David,Jim}} = \frac{1}{4}(2f_{\text{Mark,Kelly}} + f_{\text{Mark,Mark}} + f_{\text{Kelly,Kelly}})$$

Since the coancestry is half of the covariance coefficient, from the covariance matrix in [Figure 47.5](#),

$$f_{\text{David,Jim}} = \frac{1}{4}\left(2 \times \frac{0.5}{2} + \frac{1.125}{2} + \frac{1.125}{2}\right) = 0.40625$$

**Unknown or Missing Parents**

When individuals or their parents are unknown in the population, their coancestries are assigned by the value  $\frac{1}{2}cov$  if *cov* is set by the INIT= option or by the value 0 if the INIT= option is not specified. That is, if either A or B is unknown, then

$$f_{AB} = \frac{1}{2}cov$$

For example, ‘Jane’ is not in the population, and since ‘Jane’ is assumed to be defined just before the observation at which ‘Jane’ appears as a parent (that is, between observations 4 and 5), then ‘Jane’ is not older than ‘Scott’. The coancestry between ‘Jane’ and ‘Scott’ is then obtained by using the [simplified basic rule](#) (see the section “[Calculation of Coancestry](#)” on page 3733):

$$f_{\text{Scott},\text{Jane}} = \frac{1}{2} (f_{\text{Scott},\cdot} + f_{\text{Scott},\cdot})$$

Here, dots (·) indicate Jane’s unknown parents. Therefore,  $f_{\text{Scott},\cdot}$  is replaced by  $\frac{1}{2}cov$ , where *cov* is set by the INIT= option. If INIT=0.25, then

$$f_{\text{Scott},\text{Jane}} = \frac{1}{2} \left( \frac{0.25}{2} + \frac{0.25}{2} \right) = 0.125$$

For a more detailed discussion on the calculation of coancestries, inbreeding coefficients, and covariance coefficients, see Falconer and Mackay (1996); Kempthorne (1957); Crow and Kimura (1970).

**OUTCOV= Data Set**

The OUTCOV= data set has the following variables:

- a list of BY variables, if there is a **BY** statement
- the generation variable, if there is a **CLASS** statement
- the gender variable, if there is a **GENDER** statement
- `_Type_`, a variable indicating the type of observation. The valid values of the `_Type_` variable are ‘COV’ for covariance estimates and ‘INBREED’ for inbreeding coefficients.
- `_Panel_`, a variable indicating the panel number used when populations delimited by BY groups contain different numbers of individuals. If there are  $n$  individuals in the first BY group and if any subsequent BY group contains a larger population, then its covariance/inbreeding matrix is divided into panels, with each panel containing  $n$  columns of data. If you put these panels side by side in increasing `_Panel_` number order, then you can reconstruct the covariance or inbreeding matrix.

- `_Col_`, a variable used to name columns of the inbreeding or covariance matrix. The values of this variable start with 'COL', followed by a number indicating the column number. The names of the individuals corresponding to any given column  $i$  can be found by reading the individual's name across the row that has a `_Col_` value of 'COL $i$ '. When the inbreeding or covariance matrix is divided into panels, all the rows repeat for the first  $n$  columns, all the rows repeat for the next  $n$  columns, and so on.
- the variable containing the names of the individuals, that is, the first variable listed in the `VAR` statement
- the variable containing the names of the first parents, that is, the second variable listed in the `VAR` statement
- the variable containing the names of the second parents, that is, the third variable listed in the `VAR` statement
- a list of covariance variables `Col1–Col $n$` , where  $n$  is the maximum number of individuals in the first population

The functions of the variables `_Panel_` and `_Col_` can best be demonstrated by an example. Assume that there are three individuals in the first BY group and that, in the current BY group (`Byvar=2`), there are five individuals with the following covariance matrix.

| COV                 | 1        | 2        | 3                   | 4        | 5        |
|---------------------|----------|----------|---------------------|----------|----------|
| 1                   | Cov(1,1) | Cov(1,2) | Cov(1,3)            | Cov(1,4) | Cov(1,5) |
| 2                   | Cov(2,1) | Cov(2,2) | Cov(2,3)            | Cov(2,4) | Cov(2,5) |
| 3                   | Cov(3,1) | Cov(3,2) | Cov(3,3)            | Cov(3,4) | Cov(3,5) |
| 4                   | Cov(4,1) | Cov(4,2) | Cov(4,3)            | Cov(4,4) | Cov(4,5) |
| 5                   | Cov(5,1) | Cov(5,2) | Cov(5,3)            | Cov(5,4) | Cov(5,5) |
| _____ Panel 1 _____ |          |          | _____ Panel 2 _____ |          |          |

Then the `OUTCOV=` data set appears as follows.

| Byvar | _Panel_ | _Col_ | Individual | Parent | Parent2 | Col1     | Col2     | Col3     |
|-------|---------|-------|------------|--------|---------|----------|----------|----------|
| 2     | 1       | COL1  | 1          |        |         | Cov(1,1) | Cov(1,2) | Cov(1,3) |
| 2     | 1       | COL2  | 2          |        |         | Cov(2,1) | Cov(2,2) | Cov(2,3) |
| 2     | 1       | COL3  | 3          |        |         | Cov(3,1) | Cov(3,2) | Cov(3,3) |
| 2     | 1       |       | 4          |        |         | Cov(4,1) | Cov(4,2) | Cov(4,3) |
| 2     | 1       |       | 5          |        |         | Cov(5,1) | Cov(5,2) | Cov(5,3) |
| 2     | 2       |       | 1          |        |         | Cov(1,4) | Cov(1,5) | .        |
| 2     | 2       |       | 2          |        |         | Cov(2,4) | Cov(2,5) | .        |
| 2     | 2       |       | 3          |        |         | Cov(3,4) | Cov(3,5) | .        |
| 2     | 2       | COL1  | 4          |        |         | Cov(4,4) | Cov(4,5) | .        |
| 2     | 2       | COL2  | 5          |        |         | Cov(5,4) | Cov(5,5) | .        |

Notice that the first three columns go to the first panel (`_Panel_=1`), and the remaining two go to the second panel (`_Panel_=2`). Therefore, in the first panel, 'COL1', 'COL2', and 'COL3' correspond to individuals 1, 2, and 3, respectively, while in the second panel, 'COL1' and 'COL2' correspond to individuals 4 and 5, respectively.

---

## Displayed Output

The INBREED procedure can output either covariance coefficients or inbreeding coefficients. Note that the following items can be produced for each generation if generations do not overlap.

The output produced by PROC INBREED can be any or all of the following items:

- a matrix of coefficients
- coefficients of the individuals
- coefficients for selected matings

---

## ODS Table Names

PROC INBREED assigns a name to each table it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in Table 47.2. For more information on ODS, see Chapter 20, "Using the Output Delivery System."

**Table 47.2** ODS Tables Produced by PROC INBREED

| ODS Table Name           | Description                               | Statement | Option            |
|--------------------------|-------------------------------------------|-----------|-------------------|
| AvgCovCoef               | Averages of covariance coefficient matrix | GENDER    | COVAR and AVERAGE |
| AvgInbreedingCoef        | Averages of inbreeding coefficient matrix | GENDER    | AVERAGE           |
| CovarianceCoefficient    | Covariance coefficient table              | PROC      | COVAR and MATRIX  |
| InbreedingCoefficient    | Inbreeding coefficient table              | PROC      | MATRIX            |
| IndividualCovCoef        | Covariance coefficients of individuals    | PROC      | IND and COVAR     |
| IndividualInbreedingCoef | Inbreeding coefficients of individuals    | PROC      | IND               |
| MatingCovCoef            | Covariance coefficients of matings        | MATINGS   | COVAR             |
| MatingInbreedingCoef     | Inbreeding coefficients of matings        | MATINGS   |                   |
| NumberOfObservations     | Number of observations                    | PROC      |                   |

## Examples: INBREED Procedure

### Example 47.1: Monoecious Population Analysis

The following example shows a covariance analysis within nonoverlapping generations for a monoecious population. Parents of generation 1 are unknown and therefore assumed to be unrelated. The following statements produce [Output 47.1.1](#) through [Output 47.1.3](#):

```
data Monoecious;
 input Generation Individual Parent1 Parent2 Covariance @@;
 datalines;
1 1 . . . 1 2 . . . 1 3 . . .
2 1 1 1 . 2 2 1 2 . 2 3 2 3 .
3 1 1 2 . 3 2 1 3 . 3 3 2 1 .
3 4 1 3 . 3 . 2 3 0.50 3 . 4 3 1.135
;

title 'Inbreeding within Nonoverlapping Generations';
proc inbreed ind covar matrix data=Monoecious;
 class Generation;
run;
```

**Output 47.1.1** Monoecious Population Analysis, Generation 1

| Inbreeding within Nonoverlapping Generations |         |         |             |        |        |
|----------------------------------------------|---------|---------|-------------|--------|--------|
| The INBREED Procedure                        |         |         |             |        |        |
| Generation = 1                               |         |         |             |        |        |
| Covariance Coefficients                      |         |         |             |        |        |
| Individual                                   | Parent1 | Parent2 | 1           | 2      | 3      |
| 1                                            |         |         | 1.0000      | .      | .      |
| 2                                            |         |         | .           | 1.0000 | .      |
| 3                                            |         |         | .           | .      | 1.0000 |
| Covariance Coefficients of Individuals       |         |         |             |        |        |
| Individual                                   | Parent1 | Parent2 | Coefficient |        |        |
| 1                                            |         |         | 1.0000      |        |        |
| 2                                            |         |         | 1.0000      |        |        |
| 3                                            |         |         | 1.0000      |        |        |
| Number of Individuals                        |         |         | 3           |        |        |



**Output 47.1.2** Monoecious Population Analysis, Generation 2

| Inbreeding within Nonoverlapping Generations |         |         |             |        |        |
|----------------------------------------------|---------|---------|-------------|--------|--------|
| The INBREED Procedure                        |         |         |             |        |        |
| Generation = 2                               |         |         |             |        |        |
| Covariance Coefficients                      |         |         |             |        |        |
| Individual                                   | Parent1 | Parent2 | 1           | 2      | 3      |
| 1                                            | 1       | 1       | 1.5000      | 0.5000 | .      |
| 2                                            | 1       | 2       | 0.5000      | 1.0000 | 0.2500 |
| 3                                            | 2       | 3       | .           | 0.2500 | 1.0000 |
| Covariance Coefficients of Individuals       |         |         |             |        |        |
| Individual                                   | Parent1 | Parent2 | Coefficient |        |        |
| 1                                            | 1       | 1       | 1.5000      |        |        |
| 2                                            | 1       | 2       | 1.0000      |        |        |
| 3                                            | 2       | 3       | 1.0000      |        |        |
| Number of Individuals                        |         |         | 3           |        |        |

**Output 47.1.3** Monoecious Population Analysis, Generation 3

| Inbreeding within Nonoverlapping Generations |         |         |             |        |        |        |
|----------------------------------------------|---------|---------|-------------|--------|--------|--------|
| The INBREED Procedure                        |         |         |             |        |        |        |
| Generation = 3                               |         |         |             |        |        |        |
| Covariance Coefficients                      |         |         |             |        |        |        |
| Individual                                   | Parent1 | Parent2 | 1           | 2      | 3      | 4      |
| 1                                            | 1       | 2       | 1.2500      | 0.5625 | 0.8750 | 0.5625 |
| 2                                            | 1       | 3       | 0.5625      | 1.0000 | 1.1349 | 0.6250 |
| 3                                            | 2       | 1       | 0.8750      | 1.1349 | 1.2500 | 1.1349 |
| 4                                            | 1       | 3       | 0.5625      | 0.6250 | 1.1349 | 1.0000 |
| Covariance Coefficients of Individuals       |         |         |             |        |        |        |
| Individual                                   | Parent1 | Parent2 | Coefficient |        |        |        |
| 1                                            | 1       | 2       | 1.2500      |        |        |        |
| 2                                            | 1       | 3       | 1.0000      |        |        |        |
| 3                                            | 2       | 1       | 1.2500      |        |        |        |
| 4                                            | 1       | 3       | 1.0000      |        |        |        |

**Output 47.1.3** *continued*

|                       |   |
|-----------------------|---|
| Number of Individuals | 4 |
|-----------------------|---|

Note that, since the parents of the first generation are unknown, off-diagonal elements of the covariance matrix are all 0s and on-diagonal elements are all 1s. If there is an `INIT=cov` value, then the off-diagonal elements would be equal to `cov`, while on-diagonal elements would be equal to  $1 + cov/2$ .

In the third generation, individuals 2 and 4 are full siblings, so they belong to the same family. Since PROC INBREED computes covariance coefficients between families, the second and fourth columns of inbreeding coefficients are the same, except that their intersections with the second and fourth rows are reordered. Notice that, even though there is an observation to assign a covariance of 0.50 between individuals 2 and 3 in the third generation, the covariance between 2 and 3 is set to 1.135, the same value assigned between 4 and 3. This is because families get the same covariances, and later specifications override previous ones.

---

## Example 47.2: Pedigree Analysis

In the following example, an inbreeding analysis is performed for a complicated pedigree. This analysis includes computing selective matings of some individuals and inbreeding coefficients of all individuals. Also, inbreeding coefficients are averaged within sex categories. The following statements produce [Output 47.2.1](#):

```
data Swine;
 input Swine_Number $ Sire $ Dam $ Sex $;
 datalines;
3504 2200 2501 M
3514 2521 3112 F
3519 2521 2501 F
2501 2200 3112 M
2789 3504 3514 F
3501 2521 3514 M
3712 3504 3514 F
3121 2200 3501 F
;

title 'Least Related Matings';
proc inbreed data=Swine ind average;
 var Swine_Number Sire Dam;
 matings 2501 / 3501 3504 ,
 3712 / 3121;
 gender Sex;
run;
```

Note the following from [Output 47.2.1](#):

- Observation 4, which defines `Swine_Number=2501`, should precede the first and third observations where the progeny for 2501 are given. PROC INBREED ignores observation 4 since it is given out of order. As a result, the parents of 2501 are missing or unknown.

- The first column in the “Inbreeding Averages” table corresponds to the averages taken over the on-diagonal elements of the inbreeding coefficients matrix, and the second column gives averages over the off-diagonal elements.

### Output 47.2.1 Pedigree Analysis

| Least Related Matings                  |      |      |             |
|----------------------------------------|------|------|-------------|
| The INBREED Procedure                  |      |      |             |
| Inbreeding Coefficients of Individuals |      |      |             |
| Swine_<br>Number                       | Sire | Dam  | Coefficient |
| 2200                                   |      |      | .           |
| 2501                                   |      |      | .           |
| 3504                                   | 2200 | 2501 | .           |
| 2521                                   |      |      | .           |
| 3112                                   |      |      | .           |
| 3514                                   | 2521 | 3112 | .           |
| 3519                                   | 2521 | 2501 | .           |
| 2789                                   | 3504 | 3514 | .           |
| 3501                                   | 2521 | 3514 | 0.2500      |
| 3712                                   | 3504 | 3514 | .           |
| 3121                                   | 2200 | 3501 | .           |

| Inbreeding Coefficients of Matings |      |             |
|------------------------------------|------|-------------|
| Sire                               | Dam  | Coefficient |
| 2501                               | 3501 | .           |
| 2501                               | 3504 | 0.2500      |
| 3712                               | 3121 | 0.1563      |

| Averages of Inbreeding Coefficient Matrix |            |            |
|-------------------------------------------|------------|------------|
|                                           | Inbreeding | Coancestry |
| Male X Male                               | 0.0625     | 0.1042     |
| Male X Female                             | .          | 0.1362     |
| Female X Female                           | 0.0000     | 0.1324     |
| Over Sex                                  | 0.0227     | 0.1313     |

|                       |    |
|-----------------------|----|
| Number of Males       | 4  |
| Number of Females     | 7  |
| Number of Individuals | 11 |

## Example 47.3: Pedigree Analysis with BY Groups

This example demonstrates the structure of the OUTCOV= data set created by PROC INBREED. Note that the first BY group has three individuals, while the second has five. Therefore, the covariance matrix for the second BY group is broken up into two panels. The following statements produce [Output 47.3.1](#).

```
data Swine;
 input Group Swine_Number $ Sire $ Dam $ Sex $;
 datalines;
1 2789 3504 3514 F
2 2501 2200 3112 .
2 3504 2501 3782 M
;

proc inbreed data=Swine covar noprint outcov=Covariance
 init=0.4;
 var Swine_Number Sire Dam;
 gender Sex;
 by Group;
run;

title 'Printout of OUTCOV= data set';
proc print data=Covariance;
 format Col1-Col3 4.2;
run;
```

**Output 47.3.1** Pedigree Analysis with BY Groups

| Printout of OUTCOV= data set |       |     |        |         |       |                  |      |      |      |      |      |
|------------------------------|-------|-----|--------|---------|-------|------------------|------|------|------|------|------|
| Obs                          | Group | Sex | _TYPE_ | _PANEL_ | _COL_ | Swine_<br>Number | Sire | Dam  | COL1 | COL2 | COL3 |
| 1                            | 1     | M   | COV    | 1       | COL1  | 3504             |      |      | 1.20 | 0.40 | 0.80 |
| 2                            | 1     | F   | COV    | 1       | COL2  | 3514             |      |      | 0.40 | 1.20 | 0.80 |
| 3                            | 1     | F   | COV    | 1       | COL3  | 2789             | 3504 | 3514 | 0.80 | 0.80 | 1.20 |
| 4                            | 2     | M   | COV    | 1       | COL1  | 2200             |      |      | 1.20 | 0.40 | 0.80 |
| 5                            | 2     | F   | COV    | 1       | COL2  | 3112             |      |      | 0.40 | 1.20 | 0.80 |
| 6                            | 2     | M   | COV    | 1       | COL3  | 2501             | 2200 | 3112 | 0.80 | 0.80 | 1.20 |
| 7                            | 2     | F   | COV    | 1       |       | 3782             |      |      | 0.40 | 0.40 | 0.40 |
| 8                            | 2     | M   | COV    | 1       |       | 3504             | 2501 | 3782 | 0.60 | 0.60 | 0.80 |
| 9                            | 2     | M   | COV    | 2       |       | 2200             |      |      | 0.40 | 0.60 | .    |
| 10                           | 2     | F   | COV    | 2       |       | 3112             |      |      | 0.40 | 0.60 | .    |
| 11                           | 2     | M   | COV    | 2       |       | 2501             | 2200 | 3112 | 0.40 | 0.80 | .    |
| 12                           | 2     | F   | COV    | 2       | COL1  | 3782             |      |      | 1.20 | 0.80 | .    |
| 13                           | 2     | M   | COV    | 2       | COL2  | 3504             | 2501 | 3782 | 0.80 | 1.20 | .    |

## References

- Crow, J. F. and Kimura, M. (1970), *An Introduction to Population Genetics Theory*, New York: Harper & Row.
- Falconer, D. S. and Mackay, T. F. C. (1996), *Introduction to Quantitative Genetics*, Fourth Edition, London: Longman.
- Kempthorne, O. (1957), *An Introduction to Genetic Statistics*, New York: John Wiley & Sons.

# Chapter 48

## The KDE Procedure

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## Overview: KDE Procedure

The KDE procedure performs univariate and bivariate kernel density estimation. Statistical *density estimation* involves approximating a hypothesized probability density function from observed data. *Kernel density estimation* is a nonparametric technique for density estimation in which a known density function (the *kernel*) is averaged across the observed data points to create a smooth approximation. PROC KDE uses a Gaussian density as the kernel, and its assumed variance determines the smoothness of the resulting estimate. See Silverman (1986) for a thorough review and discussion.

You can use PROC KDE to compute a variety of common statistics, including estimates of the percentiles of the hypothesized probability density function. You can produce a variety of plots, including univariate and bivariate histograms, plots of the kernel density estimates, and contour plots. You can also save kernel density estimates into SAS data sets.

---

## Getting Started: KDE Procedure

The following example illustrates the basic features of PROC KDE. Assume that 1000 observations are simulated from a bivariate normal density with means (0, 0), variances (10, 10), and covariance 9. The SAS DATA step to accomplish this is as follows:

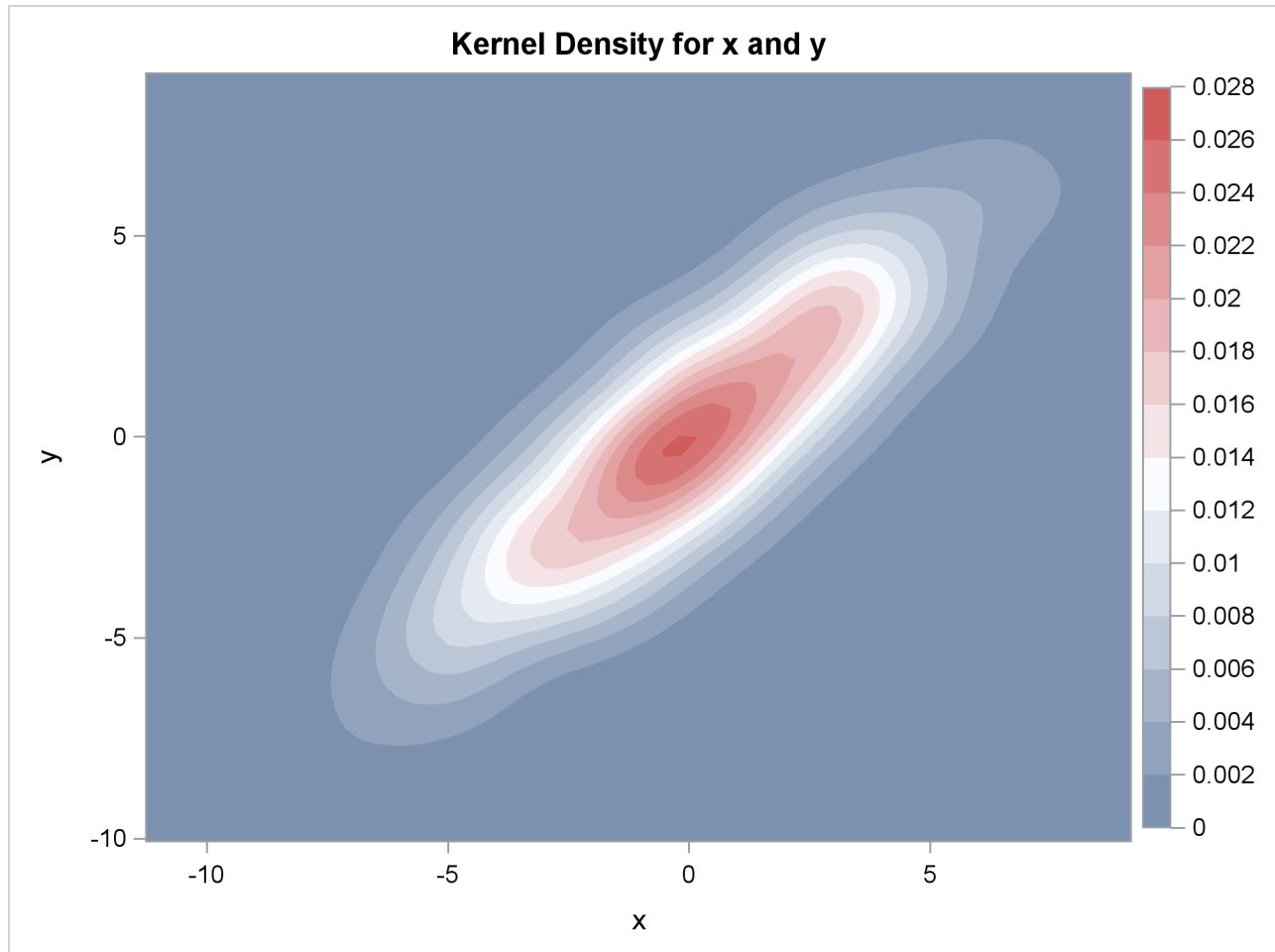
```
data bivnormal;
 seed = 1283470;
 do i = 1 to 1000;
 z1 = rannor(seed);
 z2 = rannor(seed);
 z3 = rannor(seed);
 x = 3*z1+z2;
 y = 3*z1+z3;
 output;
 end;
 drop seed;
run;
```

The following statements request a bivariate kernel density estimate for the variables x and y, with contour and surface plots:

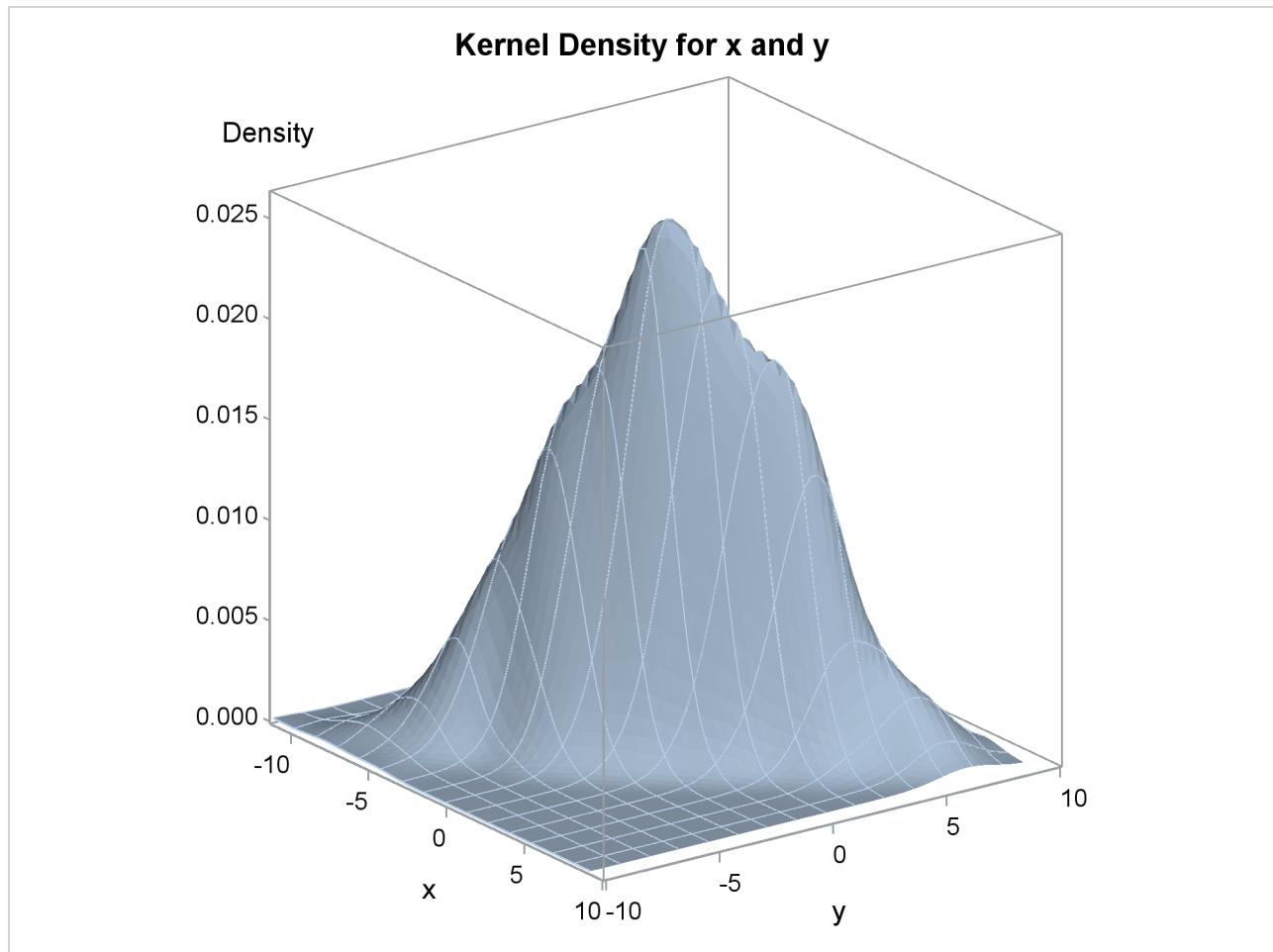
```
ods graphics on;
proc kde data=bivnormal;
 bivar x y / plots=(contour surface);
run;
ods graphics off;
```

The contour plot and the surface plot of the estimate are displayed in [Figure 48.1](#) and [Figure 48.2](#), respectively. Note that the correlation of 0.9 in the original data results in oval-shaped contours. These graphs are produced by specifying the `PLOTS=` option in the `BIVAR` statement with ODS Graphics enabled. For general information about ODS Graphics, see Chapter 21, “[Statistical Graphics Using ODS](#).” For specific information about the graphics available in the KDE procedure, see the section “[ODS Graphics](#)” on page 3767.

**Figure 48.1** Contour Plot of Estimated Density





**Figure 48.2** Surface Plot of Estimated Density

The default output tables for this analysis are shown in Figure 48.3.

**Figure 48.3** Default Bivariate Tables

| The KDE Procedure           |                |
|-----------------------------|----------------|
| Inputs                      |                |
| Data Set                    | WORK.BIVNORMAL |
| Number of Observations Used | 1000           |
| Variable 1                  | x              |
| Variable 2                  | y              |
| Bandwidth Method            | Simple Normal  |
|                             | Reference      |

Figure 48.3 continued

| Controls             |        |        |
|----------------------|--------|--------|
|                      | x      | y      |
| Grid Points          | 60     | 60     |
| Lower Grid Limit     | -11.25 | -10.05 |
| Upper Grid Limit     | 9.1436 | 9.0341 |
| Bandwidth Multiplier | 1      | 1      |

The “Inputs” table lists basic information about the density fit, including the input data set, the number of observations, and the variables. The bandwidth method is the technique used to select the amount of smoothing in the estimate. A simple normal reference rule is used for bivariate smoothing.

The “Controls” table lists the primary numbers controlling the kernel density fit. Here a  $60 \times 60$  grid is fit to the entire range of the data, and no adjustment is made to the default bandwidth.

---

## Syntax: KDE Procedure

The following statements are available in the KDE procedure:

```

PROC KDE < options > ;
 BIVAR variable-list < / options > ;
 UNIVAR variable-list < / options > ;
 BY variables ;
 FREQ variable ;
 WEIGHT variable ;

```

The PROC KDE statement invokes the procedure. The BIVAR statement requests that one or more bivariate kernel density estimates be computed. The UNIVAR statement requests one or more univariate kernel density estimates. You can specify any number of BIVAR and UNIVAR statements.

---

## PROC KDE Statement

```

PROC KDE < options > ;

```

The PROC KDE statement invokes the procedure. It also specifies the input data set.

```

DATA=SAS-data-set

```

specifies the input SAS data set to be used by PROC KDE. The default is the most recently created data set.

## BIVAR Statement

The BIVAR statement computes bivariate kernel density estimates. Table 48.1 summarizes the options available in the BIVAR statement.

**Table 48.1** BIVAR Statement Options

| Option      | Description                                                                                             |
|-------------|---------------------------------------------------------------------------------------------------------|
| BIVSTATS    | Produces a table for each density estimate                                                              |
| BWM=        | Specifies the bandwidth multiplier                                                                      |
| GRIDL=      | Specifies the lower grid limit                                                                          |
| GRIDU=      | Specifies the upper grid limit                                                                          |
| LEVELS      | Requests a table of levels for contours of the bivariate density                                        |
| NGRID=      | Specifies the number of grid points associated with each variable                                       |
| NOPRINT     | Suppresses output tables                                                                                |
| OUT=        | Specifies the name of the output data set                                                               |
| PERCENTILES | Requests that a table of percentiles be computed                                                        |
| PLOTS=      | Requests one or more plots                                                                              |
| UNISTATS    | Produces a table for each density estimate containing standard univariate statistics and the bandwidths |

The basic syntax for the BIVAR statement specifies two variables:

```
BIVAR v1 <(v-options)> v2 <(v-options)> </ options> ;
```

This statement requests a bivariate kernel density estimate for the variables v1 and v2. The *v-options* optionally specified in parentheses after a variable name apply only to that variable, and override corresponding global *options* specified following a slash (/).

You can specify a list of more than two variables:

```
BIVAR v1 <(v-options)> v2 <(v-options)> ... vN <(v-options)> </ options> ;
```

This statement requests a bivariate kernel density estimate for each distinct pair of variables in the list. For example, if you specify

```
bivar x y z;
```

then a bivariate kernel density estimate is computed for each of the variable pairs (x, y), (x, z), and (y, z).

Alternatively, you can specify an explicit list of variable pairs, with each pair enclosed in parentheses:

```
BIVAR (v1 v2)(v3 v4)...(vN-1 vN)</ options> ;
```

(You can also specify *v-options* following a variable name appearing in an explicit pair, but they are omitted here for clarity.) This statement requests a bivariate kernel density estimate for each pair of variables. For example, if you specify

```
bivar (x y) (y z);
```

then bivariate kernel density estimates are computed for (x, y) and (y, z).

**NOTE:** The VAR statement supported by PROC KDE in SAS 8 and earlier releases is now obsolete. The VAR statement has been replaced by the UNIVAR and the BIVAR statements, which enable you to produce multiple kernel density estimates with a single invocation of the procedure.

You can specify the following options in the BIVAR statement. As noted, some options can be used as *v-options*.

### **BIVSTATS**

produces a table for each density estimate containing the covariance and correlation between the two variables.

### **BWM=number**

specifies the bandwidth multiplier applied to each variable in each kernel density estimate. The default value is 1. Larger multipliers produce a smoother estimate, and smaller ones produce a rougher estimate. To specify different bandwidth multipliers for different variables, specify BWM= as a *v-option*.

### **GRIDL=number**

specifies the lower grid limit applied to each variable in each kernel density estimate. The default value for a given variable is the minimum observed value of that variable. To specify different lower grid limits for different variables, specify GRIDL= as a *v-option*.

### **GRIDU=number**

specifies the upper grid limit applied to each variable in each kernel density estimate. The default value for a given variable is the maximum observed value of that variable. To specify different upper grid limits for different variables, specify GRIDU= as a *v-option*.

### **LEVELS**

#### **LEVELS=numlist**

requests a table of levels for contours of the bivariate density. The contours are defined in such a way that the density has a constant level along each contour, and the volume enclosed by each contour corresponds to a specified percent. In other words, the contours correspond to slices or levels of the density surface taken along the density axis. You can specify the percents used to define the contours. The default values are 1, 5, 10, 50, 90, 95, 99, and 100. The “Levels” table also provides the minimum and maximum values for each contour along the directions of the two data variables.

### **NGRID=number**

#### **NG=number**

specifies the number of grid points associated with each variable in each kernel density estimate. The default value is 60. To specify different numbers of grid points for different variables, specify NGRID= as a *v-option*.

### **NOPRINT**

suppresses output tables produced by the BIVAR statement. You can use the NOPRINT option when you want to produce graphical output only.

### **OUT=SAS-data-set**

specifies the name of the output data set in which kernel density estimates are saved. This output data set contains the following variables:

- `var1`, whose value is the name of the first variable in a bivariate kernel density estimate
- `var2`, whose value is the name of the second variable in a bivariate kernel density estimate
- `value1`, with values corresponding to grid coordinates for the first variable
- `value2`, with values corresponding to grid coordinates for the second variable
- `density`, with values equal to kernel density estimates at the associated grid point
- `count`, containing the number of original observations contained in the bin corresponding to a grid point

## PERCENTILES

**PERCENTILES**=*numlist*

requests that a table of percentiles be computed for each BIVAR variable. You can specify a list of percentiles to be computed. The default percentiles are 0.5, 1, 2.5, 5, 10, 25, 50, 75, 90, 95, 97.5, 99, and 99.5.

**PLOTS**=*plot-request*< (*options*)> | **ALL** | **NONE**

**PLOTS**=(*plot-request*< (*options*)> < . . . *plot-request*< (*options*)> >)

requests one or more plots of the bivariate data and kernel density estimate. When you specify only one plot request, you can omit the parentheses around the plot request.

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;

proc kde data=octane;
 bivar Rater Customer / plots=all;
run;

ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

By default, if ODS Graphics is enabled and you do not specify the PLOTS= option, then the BIVAR statement creates a contour plot. If you specify the PLOTS= option, you get only the requested plots.

The following *plot-requests* are available.

### ALL

produces all bivariate plots.

### CONTOUR

produces a contour plot of the bivariate density estimate.

### CONTOURSCATTER

produces a contour plot of the bivariate density estimate overlaid with a scatter plot of the data.

**HISTOGRAM** < (*view-options*)>

produces a bivariate histogram of the data. The following *view-options* can be specified:

**ROTATE=angle**

rotates the histogram *angle* degrees, where  $-180 < angle < 180$ . By default, *angle* = 54.

**TILT=angle**

tilts the histogram *angle* degrees, where  $-180 < angle < 180$ . By default, *angle* = 20.

**HISTSURFACE <(view-options)>**

produces a bivariate histogram of the data overlaid with a surface plot of the bivariate kernel density estimate. The following *view-options* can be specified:

**ROTATE=angle**

rotates the histogram and kernel density surface *angle* degrees, where  $-180 < angle < 180$ . By default, *angle* = 54.

**TILT=angle**

tilts the histogram and kernel density surface *angle* degrees, where  $-180 < angle < 180$ . By default, *angle* = 20.

**NONE**

suppresses all plots, including the contour plot that is produced by default when ODS Graphics is enabled and the PLOTS= option is not specified.

**SCATTER**

produces a scatter plot of the data.

**SURFACE <(view-options)>**

produces a surface plot of the bivariate kernel density estimate. The following *view-options* can be specified:

**ROTATE=angle**

rotates the kernel density surface *angle* degrees, where  $-180 < angle < 180$ . By default, *angle* = 54.

**TILT=angle**

tilts the kernel density surface *angle* degrees, where  $-180 < angle < 180$ . By default, *angle* = 20.

**UNISTATS**

produces a table for each density estimate containing standard univariate statistics for each of the two variables and the bandwidths used to compute the kernel density estimate. The statistics listed are the mean, variance, standard deviation, range, and interquartile range.

---

## UNIVAR Statement

**UNIVAR** *variable* <(v-options)> <... variable <(v-options)>> </ options> ;

The UNIVAR statement computes univariate kernel density estimates. You can specify various *v-options* for each variable by enclosing them in parentheses after the variable name. You can also specify global *options* among the UNIVAR statement options following a slash (/). Global *options* apply to all the variables specified in the UNIVAR statement. However, individual variable *v-options* override the global *options*.

**NOTE:** The VAR statement supported by PROC KDE in SAS 8 and earlier releases is now obsolete. The VAR statement has been replaced by the UNIVAR and BIVAR statements, which enable you to produce multiple kernel density estimates with a single invocation of the procedure.

Table 48.2 summarizes the options available in the UNIVAR statement.

**Table 48.2** UNIVAR Statement Options

| Option      | Description                                                                                    |
|-------------|------------------------------------------------------------------------------------------------|
| BWM=        | Specifies a bandwidth multiplier                                                               |
| GRIDL=      | Specifies a lower grid limit                                                                   |
| GRIDU=      | Specifies an upper grid limit                                                                  |
| METHOD=     | Specifies the method used to compute the bandwidth                                             |
| NGRID=      | Specifies a number of grid points                                                              |
| NOPRINT     | Suppresses output tables produced                                                              |
| OUT=        | Specifies the output SAS data set containing the kernel density estimate                       |
| PERCENTILES | Requests that a table of percentiles                                                           |
| PLOTS=      | Requests plots of the univariate kernel density estimate                                       |
| SJPIMAX=    | Specifies the maximum grid value in determining the Sheather-Jones plug-in bandwidth           |
| SJPIMIN=    | Specifies the minimum grid value in determining the Sheather-Jones plug-in bandwidth           |
| SJPINUM=    | Specifies the number of grid values used in determining the Sheather-Jones plug-in bandwidth   |
| SJPITOL=    | Specifies the tolerance for termination of the bisection algorithm                             |
| UNISTATS    | Produces a table for each variable containing standard univariate statistics and the bandwidth |

You can specify the following options in the UNIVAR statement. As noted, some options can be used as *v-options*.

**BWM=number**

specifies a bandwidth multiplier used for each kernel density estimate. The default value is 1. Larger multipliers produce a smoother estimate, and smaller ones produce a rougher estimate. To specify different bandwidth multipliers for different variables, specify BWM= as a *v-option*.

**GRIDL=number**

specifies a lower grid limit used for each kernel density estimate. The default value for a given variable is the minimum observed value of that variable. To specify different lower grid limits for different variables, specify GRIDL= as a *v-option*.

**GRIDU=number**

specifies an upper grid limit used for each kernel density estimate. The default value for a given variable is the maximum observed value of that variable. To specify different upper grid limits for different variables, specify GRIDU= as a *v-option*.

**METHOD=SJPI | SNR | SNRQ | SROT | OS**

specifies the method used to compute the bandwidth. Available methods are Sheather-Jones plugin (SJPI), simple normal reference (SNR), simple normal reference that uses the interquartile range (SNRQ), Silverman's rule of thumb (SROT), and oversmoothed (OS). See the section “[Bandwidth Selection](#)” on page 3765 and see Jones, Marron, and Sheather (1996) for a description of these methods. SJPI is the default method.

**NGRID=number****NG=number**

specifies a number of grid points used for each kernel density estimate. The default value is 401. To specify different numbers of grid points for different variables, specify NGRID= as a *v-option*.

**NOPRINT**

suppresses output tables produced by the UNIVAR statement. You can use the NOPRINT option when you want to produce graphical output only.

**OUT=SAS-data-set**

specifies the output SAS data set containing the kernel density estimate. This output data set contains the following variables:

- var, whose value is the name of the variable in the kernel density estimate
- value, with values corresponding to grid coordinates for the variable
- density, with values equal to kernel density estimates at the associated grid point
- count, containing the number of original observations contained in the bin corresponding to a grid point

**PERCENTILES****PERCENTILES=numlist**

requests that a table of percentiles be computed for each UNIVAR variable. You can specify a list of percentiles to be computed. The default percentiles are 0.5, 1, 2.5, 5, 10, 25, 50, 75, 90, 95, 97.5, 99, and 99.5.

**PLOTS=plot-request | ALL | NONE****PLOTS=(plot-request < . . . plot-request >)**

requests plots of the univariate kernel density estimate. When you specify only one plot request, you can omit the parentheses around the plot request.

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;

proc kde data=channel;
 univar length / plots=histdensity;
run;

ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS](#).”



The following table shows the available *plot-requests*.

| Keyword        | Description                                                              |
|----------------|--------------------------------------------------------------------------|
| ALL            | produces all plots                                                       |
| DENSITY        | univariate kernel density estimate curve                                 |
| DENSITYOVERLAY | overlaid univariate kernel density estimate curves                       |
| HISTDENSITY    | univariate histogram of data overlaid with kernel density estimate curve |
| HISTOGRAM      | univariate histogram of data                                             |
| NONE           | suppresses all plots                                                     |

By default, if you ODS Graphics is enabled and you do not specify the PLOTS= option, then the UNIVAR statement creates a histogram overlaid with a kernel density estimate. If you specify the PLOTS= option, you get only the requested plots.

If you specify more than one variable in the UNIVAR statement, the DENSITYOVERLAY keyword overlays the density curves for all the variables on a single plot. The other keywords each produce a separate plot for every variable listed in the UNIVAR statement.

**SJPIMAX=number**

specifies the maximum grid value in determining the Sheather-Jones plug-in bandwidth. The default value is two times the oversmoothed estimate.

**SJPIMIN=number**

specifies the minimum grid value in determining the Sheather-Jones plug-in bandwidth. The default value is the maximum value divided by 18.

**SJPINUM=number**

specifies the number of grid values used in determining the Sheather-Jones plug-in bandwidth. The default is 21.

**SJPITOL=number**

specifies the tolerance for termination of the bisection algorithm used in computing the Sheather-Jones plug-in bandwidth. The default value is 0.001.

**UNISTATS**

produces a table for each variable containing standard univariate statistics and the bandwidth used to compute its kernel density estimate. The statistics listed are the mean, variance, standard deviation, range, and interquartile range.

## Examples

Suppose you have the variables x1, x2, x3, and x4 in the SAS data set MyData. You can request a univariate kernel density estimate for each of these variables with the following statements:

```
proc kde data=MyData;
 univar x1 x2 x3 x4;
run;
```

You can also specify different bandwidths and other options for each variable. For example, the following statements request kernel density estimates that use Silverman's rule of thumb (SROT) method for all variables:

```
proc kde data=MyData;
 univar x1 (bwm=2)
 x2 (bwm=0.5 ngrid=100)
 x3 x4 / ngrid=200 method=srot;
run;
```

The option NGRID=200 applies to the variables x1, x3, and x4, but the *v-option* NGRID=100 is applied to x2. Bandwidth multipliers of 2 and 0.5 are specified for the variables x1 and x2, respectively.

---

## BY Statement

**BY** *variables* ;

You can specify a BY statement with PROC KDE to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the KDE procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

---

## FREQ Statement

**FREQ** *variable* ;

The FREQ statement specifies a variable that provides frequencies for each observation in the DATA= data set. Specifically, if  $n$  is the value of the FREQ variable for a given observation, then that observation is used  $n$  times. If the value of the FREQ variable is missing or is less than 1, the observation is not used in the analysis. If the value is not an integer, only the integer portion is used.

---

## WEIGHT Statement

**WEIGHT** *variable* ;

The WEIGHT statement specifies a variable that weights the observations in computing the kernel density estimate. Observations with higher weights have more influence in the computations. If an observation has a nonpositive or missing weight, then the entire observation is omitted from the analysis. You should be cautious in using data sets with extreme weights, because they can produce unreliable results.

---

## Details: KDE Procedure

---

### Computational Overview

The two main computational tasks of PROC KDE are automatic bandwidth selection and the construction of a kernel density estimate once a bandwidth has been selected. The primary computational tools used to accomplish these tasks are binning, convolutions, and the fast Fourier transform. The following sections provide analytical details on these topics, beginning with the density estimates themselves.

---

### Kernel Density Estimates

A weighted univariate kernel density estimate involves a variable  $X$  and a weight variable  $W$ . Let  $(X_i, W_i)$ ,  $i = 1, 2, \dots, n$ , denote a sample of  $X$  and  $W$  of size  $n$ . The weighted kernel density estimate of  $f(x)$ , the density of  $X$ , is as follows:

$$\hat{f}(x) = \frac{1}{\sum_{i=1}^n W_i} \sum_{i=1}^n W_i \varphi_h(x - X_i)$$

where  $h$  is the bandwidth and

$$\varphi_h(x) = \frac{1}{\sqrt{2\pi}h} \exp\left(-\frac{x^2}{2h^2}\right)$$

is the standard normal density rescaled by the bandwidth. If  $h \rightarrow 0$  and  $nh \rightarrow \infty$ , then the optimal bandwidth is

$$h_{\text{AMISE}} = \left[ \frac{1}{2\sqrt{\pi}n \int (f'')^2} \right]^{1/5}$$

This optimal value is unknown, and so approximations methods are required. For a derivation and discussion of these results, see Silverman (1986, Chapter 3) and Jones, Marron, and Sheather (1996).

For the bivariate case, let  $\mathbf{X} = (X, Y)$  be a bivariate random element taking values in  $R^2$  with joint density function

$$f(x, y), (x, y) \in R^2$$

and let  $\mathbf{X}_i = (X_i, Y_i)$ ,  $i = 1, 2, \dots, n$ , be a sample of size  $n$  drawn from this distribution. The kernel density estimate of  $f(x, y)$  based on this sample is

$$\begin{aligned} \hat{f}(x, y) &= \frac{1}{n} \sum_{i=1}^n \varphi_{\mathbf{h}}(x - X_i, y - Y_i) \\ &= \frac{1}{nh_X h_Y} \sum_{i=1}^n \varphi\left(\frac{x - X_i}{h_X}, \frac{y - Y_i}{h_Y}\right) \end{aligned}$$

where  $(x, y) \in R^2$ ,  $h_X > 0$  and  $h_Y > 0$  are the bandwidths, and  $\varphi_h(x, y)$  is the rescaled normal density

$$\varphi_h(x, y) = \frac{1}{h_X h_Y} \varphi\left(\frac{x}{h_X}, \frac{y}{h_Y}\right)$$

where  $\varphi(x, y)$  is the standard normal density function

$$\varphi(x, y) = \frac{1}{2\pi} \exp\left(-\frac{x^2 + y^2}{2}\right)$$

Under mild regularity assumptions about  $f(x, y)$ , the mean integrated squared error (MISE) of  $\hat{f}(x, y)$  is

$$\begin{aligned} \text{MISE}(h_X, h_Y) &= E \int (\hat{f} - f)^2 \\ &= \frac{1}{4\pi n h_X h_Y} + \frac{h_X^4}{4} \int \left(\frac{\partial^2 f}{\partial X^2}\right)^2 dx dy \\ &\quad + \frac{h_Y^4}{4} \int \left(\frac{\partial^2 f}{\partial Y^2}\right)^2 dx dy + O\left(h_X^4 + h_Y^4 + \frac{1}{n h_X h_Y}\right) \end{aligned}$$

as  $h_X \rightarrow 0$ ,  $h_Y \rightarrow 0$  and  $n h_X h_Y \rightarrow \infty$ .

Now set

$$\begin{aligned} \text{AMISE}(h_X, h_Y) &= \frac{1}{4\pi n h_X h_Y} + \frac{h_X^4}{4} \int \left(\frac{\partial^2 f}{\partial X^2}\right)^2 dx dy \\ &\quad + \frac{h_Y^4}{4} \int \left(\frac{\partial^2 f}{\partial Y^2}\right)^2 dx dy \end{aligned}$$

which is the asymptotic mean integrated squared error (AMISE). For fixed  $n$ , this has a minimum at  $(h_{\text{AMISE}_X}, h_{\text{AMISE}_Y})$  defined as

$$h_{\text{AMISE}_X} = \left[ \frac{\int \left(\frac{\partial^2 f}{\partial X^2}\right)^2}{4n\pi} \right]^{1/6} \left[ \frac{\int \left(\frac{\partial^2 f}{\partial X^2}\right)^2}{\int \left(\frac{\partial^2 f}{\partial Y^2}\right)^2} \right]^{2/3}$$

and

$$h_{\text{AMISE}_Y} = \left[ \frac{\int \left(\frac{\partial^2 f}{\partial Y^2}\right)^2}{4n\pi} \right]^{1/6} \left[ \frac{\int \left(\frac{\partial^2 f}{\partial Y^2}\right)^2}{\int \left(\frac{\partial^2 f}{\partial X^2}\right)^2} \right]^{2/3}$$

These are the optimal asymptotic bandwidths in the sense that they minimize MISE. However, as in the univariate case, these expressions contain the second derivatives of the unknown density  $f$  being estimated, and so approximations are required. See Wand and Jones (1993) for further details.

## Binning

Binning, or assigning data to discrete categories, is an effective and fast method for large data sets (Fan and Marron 1994). When the sample size  $n$  is large, direct evaluation of the kernel estimate  $\hat{f}$  at any point would involve  $n$  kernel evaluations, as shown in the preceding formulas. To evaluate the estimate at each point of a grid of size  $g$  would thus require  $ng$  kernel evaluations. When you use  $g = 401$  in the univariate case or  $g = 60 \times 60 = 3600$  in the bivariate case and  $n \geq 1000$ , the amount of computation can be prohibitively large. With binning, however, the computational order is reduced to  $g$ , resulting in a much quicker algorithm that is nearly as accurate as direct evaluation.

To bin a set of weighted univariate data  $X_1, X_2, \dots, X_n$  to a grid  $x_1, x_2, \dots, x_g$ , simply assign each sample  $X_i$ , together with its weight  $W_i$ , to the nearest grid point  $x_j$  (also called the bin center). When binning is completed, each grid point  $x_i$  has an associated number  $c_i$ , which is the sum total of all the weights that correspond to sample points that have been assigned to  $x_i$ . These  $c_i$ s are known as the *bin counts*.

This procedure replaces the data  $(X_i, W_i)$ ,  $i = 1, 2, \dots, n$ , with the smaller set  $(x_i, c_i)$ ,  $i = 1, 2, \dots, g$ , and the estimation is carried out with these new data. This is so-called *simple binning*, versus the finer *linear binning* described in Wand (1994). PROC KDE uses simple binning for the sake of faster and easier implementation. Also, it is assumed that the bin centers  $x_1, x_2, \dots, x_g$  are equally spaced and in increasing order. In addition, assume for notational convenience that  $\sum_{i=1}^n W_i = n$  and, therefore,  $\sum_{i=1}^g c_i = n$ .

If you replace the data  $(X_i, W_i)$ ,  $i = 1, 2, \dots, n$ , with  $(x_i, c_i)$ ,  $i = 1, 2, \dots, g$ , the weighted estimator  $\hat{f}$  then becomes

$$\hat{f}(x) = \frac{1}{n} \sum_{i=1}^g c_i \varphi_h(x - x_i)$$

with the same notation as used previously. To evaluate this estimator at the  $g$  points of the same grid vector  $grid = (x_1, x_2, \dots, x_g)'$  is to calculate

$$\hat{f}(x_i) = \frac{1}{n} \sum_{j=1}^g c_j \varphi_h(x_i - x_j)$$

for  $i = 1, 2, \dots, g$ . This can be rewritten as

$$\hat{f}(x_i) = \frac{1}{n} \sum_{j=1}^g c_j \varphi_h(|i - j|\delta)$$

where  $\delta = x_2 - x_1$  is the increment of the grid.

The same idea of binning works similarly with bivariate data, where you estimate  $\hat{f}$  over the grid matrix  $grid = grid_X \times grid_Y$  as follows:

$$grid = \begin{bmatrix} \mathbf{x}_{1,1} & \mathbf{x}_{1,2} & \dots & \mathbf{x}_{1,g_Y} \\ \mathbf{x}_{2,1} & \mathbf{x}_{2,2} & \dots & \mathbf{x}_{2,g_Y} \\ \vdots & & & \\ \mathbf{x}_{g_X,1} & \mathbf{x}_{g_X,2} & \dots & \mathbf{x}_{g_X,g_Y} \end{bmatrix}$$

where  $\mathbf{x}_{i,j} = (x_i, y_j)$ ,  $i = 1, 2, \dots, g_X$ ,  $j = 1, 2, \dots, g_Y$ , and the estimates are

$$\hat{f}(\mathbf{x}_{i,j}) = \frac{1}{n} \sum_{k=1}^{g_X} \sum_{l=1}^{g_Y} c_{k,l} \varphi_h(|i - k|\delta_X, |j - l|\delta_Y)$$

where  $\delta_X = x_2 - x_1$  and  $\delta_Y = y_2 - y_1$  are the increments of the grid.

## Convolutions

The formulas for the binned estimator  $\hat{f}$  in the previous subsection are in the form of a convolution product between two matrices, one of which contains the bin counts, the other of which contains the rescaled kernels evaluated at multiples of grid increments. This section defines these two matrices explicitly, and shows that  $\hat{f}$  is their convolution.

Beginning with the weighted univariate case, define the following matrices:

$$\begin{aligned}\mathbf{K} &= \frac{1}{n}(\varphi_h(0), \varphi_h(\delta), \dots, \varphi_h((g-1)\delta))' \\ \mathbf{C} &= (c_1, c_2, \dots, c_g)'\end{aligned}$$

The first thing to note is that many terms in  $\mathbf{K}$  are negligible. The term  $\varphi_h(i\delta)$  is taken to be 0 when  $|i\delta/h| \geq 5$ , so you can define

$$l = \min(g-1, \text{floor}(5h/\delta))$$

as the maximum integer multiple of the grid increment to get nonzero evaluations of the rescaled kernel. Here  $\text{floor}(x)$  denotes the largest integer less than or equal to  $x$ .

Next, let  $p$  be the smallest power of 2 that is greater than  $g + l + 1$ ,

$$p = 2^{\text{ceil}(\log_2(g+l+1))}$$

where  $\text{ceil}(x)$  denotes the smallest integer greater than or equal to  $x$ .

Modify  $\mathbf{K}$  as follows:

$$\mathbf{K} = \frac{1}{n}(\varphi_h(0), \varphi_h(\delta), \dots, \varphi_h(l\delta), \underbrace{0, \dots, 0}_{p-2l-1}, \varphi_h(l\delta), \dots, \varphi_h(\delta))'$$

Essentially, the negligible terms of  $\mathbf{K}$  are omitted, and the rest are *symmetrized* (except for one term). The whole matrix is then padded to size  $p \times 1$  with zeros in the middle. The dimension  $p$  is a highly composite number—that is, one that decomposes into many factors—leading to the most efficient fast Fourier transform operation (see Wand 1994).

The third operation is to pad the bin count matrix  $\mathbf{C}$  with zeros to the same size as  $\mathbf{K}$ :

$$\mathbf{C} = (c_1, c_2, \dots, c_g, \underbrace{0, \dots, 0}_{p-g})'$$

The convolution  $\mathbf{K} * \mathbf{C}$  is then a  $p \times 1$  matrix, and the preceding formulas show that its first  $g$  entries are exactly the estimates  $\hat{f}(x_i)$ ,  $i = 1, 2, \dots, g$ .

For bivariate smoothing, the matrix  $\mathbf{K}$  is defined similarly as

$$\mathbf{K} = \begin{bmatrix} \kappa_{0,0} & \kappa_{0,1} & \dots & \kappa_{0,l_Y} & \mathbf{0} & \kappa_{0,l_Y} & \dots & \kappa_{0,1} \\ \kappa_{1,0} & \kappa_{1,1} & \dots & \kappa_{1,l_Y} & \mathbf{0} & \kappa_{1,l_Y} & \dots & \kappa_{1,1} \\ \vdots & & & & & & & \\ \kappa_{l_X,0} & \kappa_{l_X,1} & \dots & \kappa_{l_X,l_Y} & \mathbf{0} & \kappa_{l_X,l_Y} & \dots & \kappa_{l_X,1} \\ \mathbf{0} & \mathbf{0} & \dots & \mathbf{0} & \mathbf{0} & \mathbf{0} & \dots & \mathbf{0} \\ \kappa_{l_X,0} & \kappa_{l_X,1} & \dots & \kappa_{l_X,l_Y} & \mathbf{0} & \kappa_{l_X,l_Y} & \dots & \kappa_{l_X,1} \\ \vdots & & & & & & & \\ \kappa_{1,0} & \kappa_{1,1} & \dots & \kappa_{1,l_Y} & \mathbf{0} & \kappa_{1,l_Y} & \dots & \kappa_{1,1} \end{bmatrix}_{p_X \times p_Y}$$

where  $l_X = \min(g_X - 1, \text{floor}(5h_X/\delta_X))$ ,  $p_X = 2^{\text{ceil}(\log_2(g_X + l_X + 1))}$ , and so forth, and  $\kappa_{i,j} = \frac{1}{n} \varphi_h(i\delta_X, j\delta_Y)$   $i = 0, 1, \dots, l_X$ ,  $j = 0, 1, \dots, l_Y$ .

The bin count matrix  $\mathbf{C}$  is defined as

$$\mathbf{C} = \begin{bmatrix} c_{1,1} & c_{1,2} & \dots & c_{1,g_Y} & 0 & \dots & 0 \\ c_{2,1} & c_{2,2} & \dots & c_{2,g_Y} & 0 & \dots & 0 \\ \vdots & & & & & & \\ c_{g_X,1} & c_{g_X,2} & \dots & c_{g_X,g_Y} & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 & 0 & \dots & 0 \\ \vdots & & & & & & \\ 0 & 0 & \dots & 0 & 0 & \dots & 0 \end{bmatrix}_{p_X \times p_Y}$$

As with the univariate case, the  $g_X \times g_Y$  upper-left corner of the convolution  $\mathbf{K} * \mathbf{C}$  is the matrix of the estimates  $\hat{f}(\text{grid})$ .

Most of the results in this subsection are found in Wand (1994).

## Fast Fourier Transform

As shown in the last subsection, kernel density estimates can be expressed as a submatrix of a certain convolution. The fast Fourier transform (FFT) is a computationally effective method for computing such convolutions. For a reference on this material, see Press et al. (1988).

The *discrete Fourier transform* of a complex vector  $\mathbf{z} = (z_0, \dots, z_{N-1})$  is the vector  $\mathbf{Z} = (Z_0, \dots, Z_{N-1})$ , where

$$Z_j = \sum_{l=0}^{N-1} z_l e^{2\pi i l j / N}, \quad j = 0, \dots, N-1$$

and  $i$  is the square root of  $-1$ . The vector  $\mathbf{z}$  can be recovered from  $\mathbf{Z}$  by applying the *inverse discrete Fourier transform* formula

$$z_l = N^{-1} \sum_{j=0}^{N-1} Z_j e^{-2\pi i l j / N}, \quad l = 0, \dots, N-1$$

Discrete Fourier transforms and their inverses can be computed quickly using the FFT algorithm, especially when  $N$  is *highly composite*; that is, it can be decomposed into many factors, such as a power of 2. By the *discrete convolution theorem*, the convolution of two vectors is the inverse Fourier transform of the element-by-element product of their Fourier transforms. This, however, requires certain periodicity assumptions, which explains why the vectors  $\mathbf{K}$  and  $\mathbf{C}$  require zero-padding. This is to avoid *wrap-around* effects (see Press et al. 1988, pp. 410–411). The vector  $\mathbf{K}$  is actually mirror-imaged so that the convolution of  $\mathbf{C}$  and  $\mathbf{K}$  will be the vector of binned estimates. Thus, if  $S$  denotes the inverse Fourier transform of the element-by-element product of the Fourier transforms of  $\mathbf{K}$  and  $\mathbf{C}$ , then the first  $g$  elements of  $S$  are the estimates.

The bivariate Fourier transform of an  $N_1 \times N_2$  complex matrix having  $(l_1 + 1, l_2 + 1)$  entry equal to  $z_{l_1 l_2}$  is the  $N_1 \times N_2$  matrix with  $(j_1 + 1, j_2 + 1)$  entry given by

$$Z_{j_1 j_2} = \sum_{l_1=0}^{N_1-1} \sum_{l_2=0}^{N_2-1} z_{l_1 l_2} e^{2\pi i(l_1 j_1 / N_1 + l_2 j_2 / N_2)}$$

and the formula of the inverse is

$$z_{l_1 l_2} = (N_1 N_2)^{-1} \sum_{j_1=0}^{N_1-1} \sum_{j_2=0}^{N_2-1} Z_{j_1 j_2} e^{-2\pi i(l_1 j_1 / N_1 + l_2 j_2 / N_2)}$$

The same discrete convolution theorem applies, and zero-padding is needed for matrices  $\mathbf{C}$  and  $\mathbf{K}$ . In the case of  $\mathbf{K}$ , the matrix is mirror-imaged twice. Thus, if  $S$  denotes the inverse Fourier transform of the element-by-element product of the Fourier transforms of  $\mathbf{K}$  and  $\mathbf{C}$ , then the upper-left  $g_X \times g_Y$  corner of  $S$  contains the estimates.

---

## Bandwidth Selection

Several different bandwidth selection methods are available in PROC KDE in the univariate case. Following the recommendations of Jones, Marron, and Sheather (1996), the default method follows a plug-in formula of Sheather and Jones.

This method solves the fixed-point equation

$$h = \left[ \frac{R(\varphi)}{nR(\hat{f}_g''(h)) \left( \int x^2 \varphi(x) dx \right)^2} \right]^{1/5}$$

where  $R(\varphi) = \int \varphi^2(x) dx$ .

PROC KDE solves this equation by first evaluating it on a grid of values spaced equally on a log scale. The largest two values from this grid that bound a solution are then used as starting values for a bisection algorithm.

The simple normal reference rule works by assuming  $\hat{f}$  is Gaussian in the preceding fixed-point equation. This results in

$$\begin{aligned} h &= \hat{\sigma} [4/(3n)]^{1/5} \\ &= 1.06 \hat{\sigma} n^{-1/5} \end{aligned}$$

where  $\hat{\sigma}$  is the sample standard deviation.



Alternatively, the bandwidth can be computed using the interquartile range,  $Q$ :

$$\begin{aligned} h &= 1.06 \hat{\sigma} n^{-1/5} \\ &\approx 1.06 (Q/1.34) n^{-1/5} \\ &\approx 0.785 Q n^{-1/5} \end{aligned}$$

Silverman's rule of thumb (Silverman 1986, Section 3.4.2) is computed as

$$h = 0.9 \min[\hat{\sigma}, Q/1.34] n^{-1/5}$$

The oversmoothed bandwidth is computed as

$$h = 3\hat{\sigma} [1/(70\sqrt{\pi n})]^{1/5}$$

When you specify a WEIGHT variable, PROC KDE uses weighted versions of  $Q_3$ ,  $Q_1$ , and  $\hat{\sigma}$  in the preceding expressions. The weighted quartiles are computed as weighted order statistics, and the weighted variance takes the form

$$\hat{\sigma}^2 = \frac{\sum_{i=1}^n W_i (X_i - \bar{X})^2}{\sum_{i=1}^n W_i}$$

where  $\bar{X} = (\sum_{i=1}^n W_i X_i) / (\sum_{i=1}^n W_i)$  is the weighted sample mean.

For the bivariate case, Wand and Jones (1993) note that automatic bandwidth selection is both difficult and computationally expensive. Their study of various ways of specifying a bandwidth matrix also shows that using two bandwidths, one in each coordinate's direction, is often adequate. PROC KDE enables you to adjust the two bandwidths by specifying a multiplier for the default bandwidths recommended by Bowman and Foster (1993):

$$\begin{aligned} h_X &= \hat{\sigma}_X n^{-1/6} \\ h_Y &= \hat{\sigma}_Y n^{-1/6} \end{aligned}$$

Here  $\hat{\sigma}_X$  and  $\hat{\sigma}_Y$  are the sample standard deviations of  $X$  and  $Y$ , respectively. These are the optimal bandwidths for two independent normal variables that have the same variances as  $X$  and  $Y$ . They are, therefore, conservative in the sense that they tend to oversmooth the surface.

You can specify the BWM= option to adjust the aforementioned bandwidths to provide the appropriate amount of smoothing for your application.

## ODS Table Names

PROC KDE assigns a name to each table it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in Table 48.3. For more information about ODS, see Chapter 20, "Using the Output Delivery System."

**Table 48.3** ODS Tables Produced in PROC KDE

| ODS Table Name       | Description                | Statement      | Option      |
|----------------------|----------------------------|----------------|-------------|
| BivariateStatistics  | Bivariate statistics       | BIVAR          | BIVSTATS    |
| Controls             | Control variables          | default        |             |
| Inputs               | Input information          | default        |             |
| Levels               | Levels of density estimate | BIVAR          | LEVELS      |
| Percentiles          | Percentiles of data        | BIVAR / UNIVAR | PERCENTILES |
| UnivariateStatistics | Basic statistics           | BIVAR / UNIVAR | UNISTATS    |

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “Statistical Graphics Using ODS.”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “A Primer on ODS Statistical Graphics” on page 599 in Chapter 21, “Statistical Graphics Using ODS.”

## ODS Graph Names

PROC KDE assigns a name to each graph it creates using the Output Delivery System (ODS). You can use these names to reference the graphs when using ODS. The names are listed in Table 48.4.

**Table 48.4** Graphs Produced by PROC KDE

| ODS Graph Name     | Plot Description                                                                    | Statement | PLOTS= Option  |
|--------------------|-------------------------------------------------------------------------------------|-----------|----------------|
| BivariateHistogram | Bivariate histogram of data                                                         | BIVAR     | HISTOGRAM      |
| ContourPlot        | Contour plot of bivariate kernel density estimate                                   | BIVAR     | CONTOUR        |
| ContourScatterPlot | Contour plot of bivariate kernel density estimate overlaid with scatter plot        | BIVAR     | CONTOURSCATTER |
| DensityPlot        | Univariate kernel density estimate curve                                            | UNIVAR    | DENSITY        |
| DensityOverlayPlot | Overlaid univariate kernel density estimate curves                                  | UNIVAR    | DENSITYOVERLAY |
| HistogramDensity   | Univariate histogram overlaid with kernel density estimate curve                    | UNIVAR    | HISTDENSITY    |
| Histogram          | Univariate histogram of data                                                        | UNIVAR    | HISTOGRAM      |
| HistogramSurface   | Bivariate histogram overlaid with surface plot of bivariate kernel density estimate | BIVAR     | HISTSURFACE    |

Table 48.4 (continued)

| ODS Graph Name | Plot Description                                  | Statement | PLOTS= Option |
|----------------|---------------------------------------------------|-----------|---------------|
| ScatterPlot    | Scatter plot of data                              | BIVAR     | SCATTER       |
| SurfacePlot    | Surface plot of bivariate kernel density estimate | BIVAR     | SURFACE       |

## Bivariate Plots

You can specify the PLOTS= option in the BIVAR statement to request graphical displays of bivariate kernel density estimates.

**PLOTS=** *option1* < *option2* . . . >

requests one or more plots of the bivariate kernel density estimate. The following table shows the available plot *options*.

| Option         | Description                                                                   |
|----------------|-------------------------------------------------------------------------------|
| ALL            | all available displays                                                        |
| CONTOUR        | contour plot of bivariate density estimate                                    |
| CONTOURSCATTER | contour plot of bivariate density estimate overlaid with scatter plot of data |
| HISTOGRAM      | bivariate histogram of data                                                   |
| HISTSURFACE    | bivariate histogram overlaid with bivariate kernel density estimate           |
| NONE           | suppresses all plots                                                          |
| SCATTER        | scatter plot of data                                                          |
| SURFACE        | surface plot of bivariate kernel density estimate                             |

By default, if ODS Graphics is enabled and you do not specify the PLOTS= option, then the BIVAR statement creates a contour plot. If you specify the PLOTS= option, you get only the requested plots.

## Univariate Plots

You can specify the PLOTS= option in the UNIVAR statement to request graphical displays of univariate kernel density estimates.

**PLOTS=** *option1* < *option2* . . . >

requests one or more plots of the univariate kernel density estimate. The following table shows the available plot *options*.

| Option         | Description                                                              |
|----------------|--------------------------------------------------------------------------|
| ALL            | all available displays                                                   |
| DENSITY        | univariate kernel density estimate curve                                 |
| DENSITYOVERLAY | overlaid univariate kernel density estimate curves                       |
| HISTDENSITY    | univariate histogram of data overlaid with kernel density estimate curve |
| HISTOGRAM      | univariate histogram of data                                             |
| NONE           | suppresses all plots                                                     |

By default, if ODS Graphics is enabled and you do not specify the PLOTS= option, then the UNIVAR statement creates a histogram overlaid with a kernel density estimate. If you specify the PLOTS= option, you get only the requested plots.

### Binning of Bivariate Histogram

Let  $(X_i, Y_i)$ ,  $i = 1, 2, \dots, n$ , be a sample of size  $n$  drawn from a bivariate distribution. For the marginal distribution of  $X_i$ ,  $i = 1, 2, \dots, n$ , the number of bins ( $\text{Nbins}_X$ ) in the bivariate histogram is calculated according to the formula

$$\text{Nbins}_X = \text{ceil}(\text{range}_X / \text{width}_X)$$

where  $\text{ceil}(x)$  denotes the smallest integer greater than or equal to  $x$ ,

$$\text{range}_X = \max_{1 \leq i \leq n} (X_i) - \min_{1 \leq i \leq n} (X_i)$$

and the optimal bin width is obtained, following Scott (1992, p. 84), as

$$\text{width}_X = 3.504 \hat{\sigma}_X (1 - \hat{\rho}^2)^{3/8} n^{-1/4}$$

Here,  $\hat{\sigma}_X$  and  $\hat{\rho}$  are the sample variance and the sample correlation coefficient, respectively. When you specify a WEIGHT variable, PROC KDE uses weighted versions of  $\hat{\sigma}_X$  and  $\hat{\rho}$  in the preceding expressions.

Similar formulas are used to compute the number of bins for the marginal distribution of  $Y_i$ ,  $i = 1, 2, \dots, n$ . Further details can be found in Scott (1992).

Notice that if  $|\hat{\rho}| > 0.99$ , then  $\text{Nbins}_X$  is calculated as in the univariate case (see Terrell and Scott 1985). In this case  $\text{Nbins}_Y = \text{Nbins}_X$ .

---

## Examples: KDE Procedure

---

### Example 48.1: Computing a Basic Kernel Density Estimate

This example illustrates the basic functionality of the UNIVAR statement. The effective channel length (in microns) is measured for 1225 field effect transistors. The channel lengths are saved as values of the variable length in a SAS data set named channel; see the file *kdex1.sas* in the SAS Sample Library. These statements create the channel data set:

```
data channel;
 input length @@;
 datalines;
0.91 1.01 0.95 1.13 1.12 0.86 0.96 1.17 1.36 1.10
0.98 1.27 1.13 0.92 1.15 1.26 1.14 0.88 1.03 1.00
0.98 0.94 1.09 0.92 1.10 0.95 1.05 1.05 1.11 1.15
1.11 0.98 0.78 1.09 0.94 1.05 0.89 1.16 0.88 1.19

... more lines ...

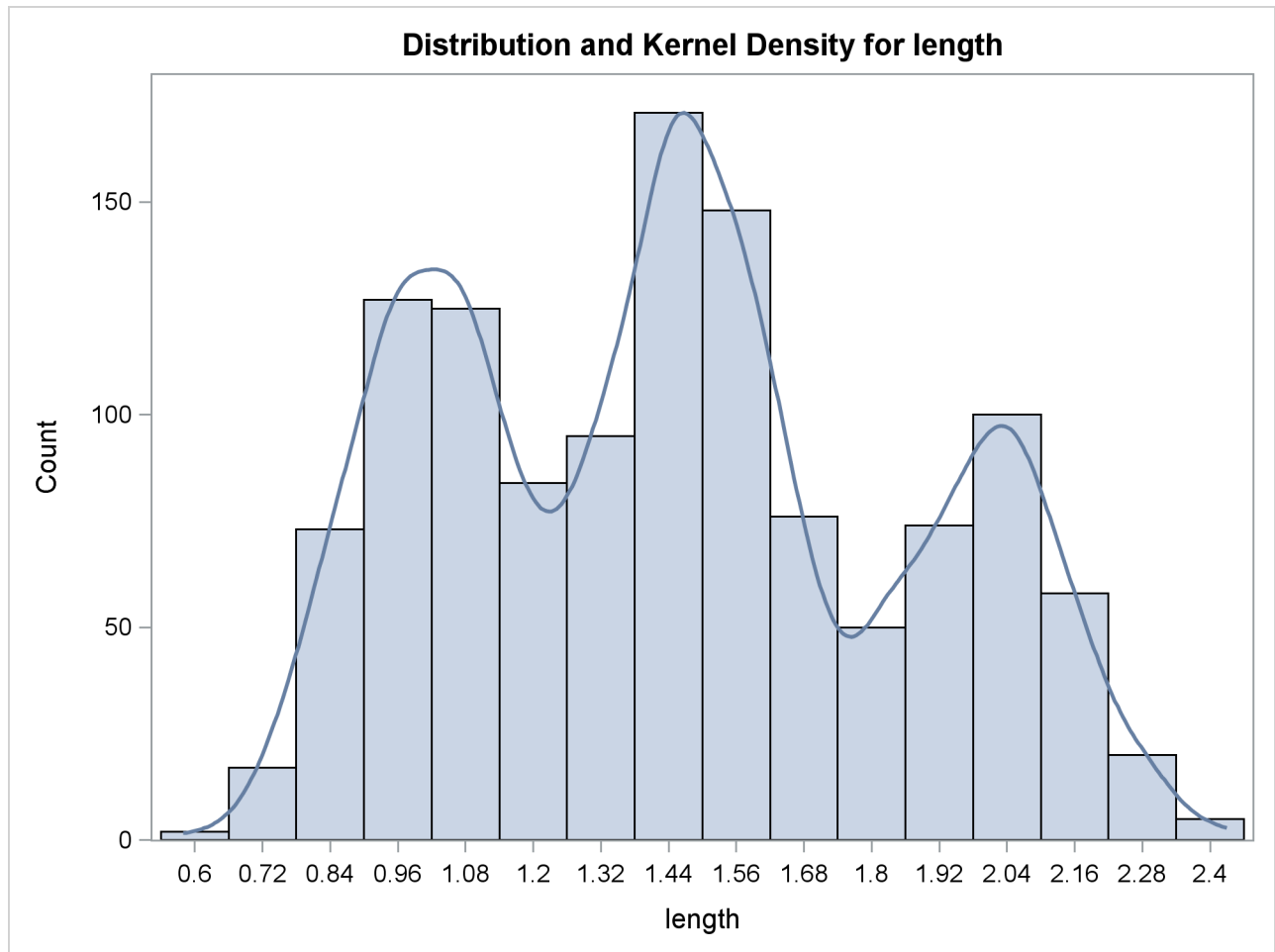
2.13 2.05 1.90 2.07 2.15 1.96 2.15 1.89 2.15 2.04
1.95 1.93 2.22 1.74 1.91
;
```

The following statements request a kernel density estimate of the variable length:

```
ods graphics on;
proc kde data=channel;
 univar length;
run;
```

Because ODS Graphics is enabled, PROC KDE produces a histogram with an overlaid kernel density estimate by default, although the PLOTS= option is not specified. The resulting graph is shown in [Output 48.1.1](#). For general information about ODS Graphics, see Chapter 21, “[Statistical Graphics Using ODS](#).” For specific information about the graphics available in the KDE procedure, see the section “[ODS Graphics](#)” on page 3767.

**Output 48.1.1** Histogram with Overlaid Kernel Density Estimate



The default output tables for this analysis are the “Inputs” and “Controls” tables, shown in [Output 48.1.2](#).

**Output 48.1.2** Univariate Inputs Table

| The KDE Procedure           |                |
|-----------------------------|----------------|
| Inputs                      |                |
| Data Set                    | WORK.CHANNEL   |
| Number of Observations Used | 1225           |
| Variable                    | length         |
| Bandwidth Method            | Sheather-Jones |
|                             | Plug In        |

**Output 48.1.2** *continued*

| Controls             |        |
|----------------------|--------|
|                      | length |
| Grid Points          | 401    |
| Lower Grid Limit     | 0.58   |
| Upper Grid Limit     | 2.43   |
| Bandwidth Multiplier | 1      |

The “Inputs” table lists basic information about the density fit, including the input data set, the number of observations, the variable used, and the bandwidth method. The default bandwidth method is the Sheather-Jones plug-in.

The “Controls” table lists the primary numbers controlling the kernel density fit. Here the default number of grid points is used and no adjustment is made to the default bandwidth.

---

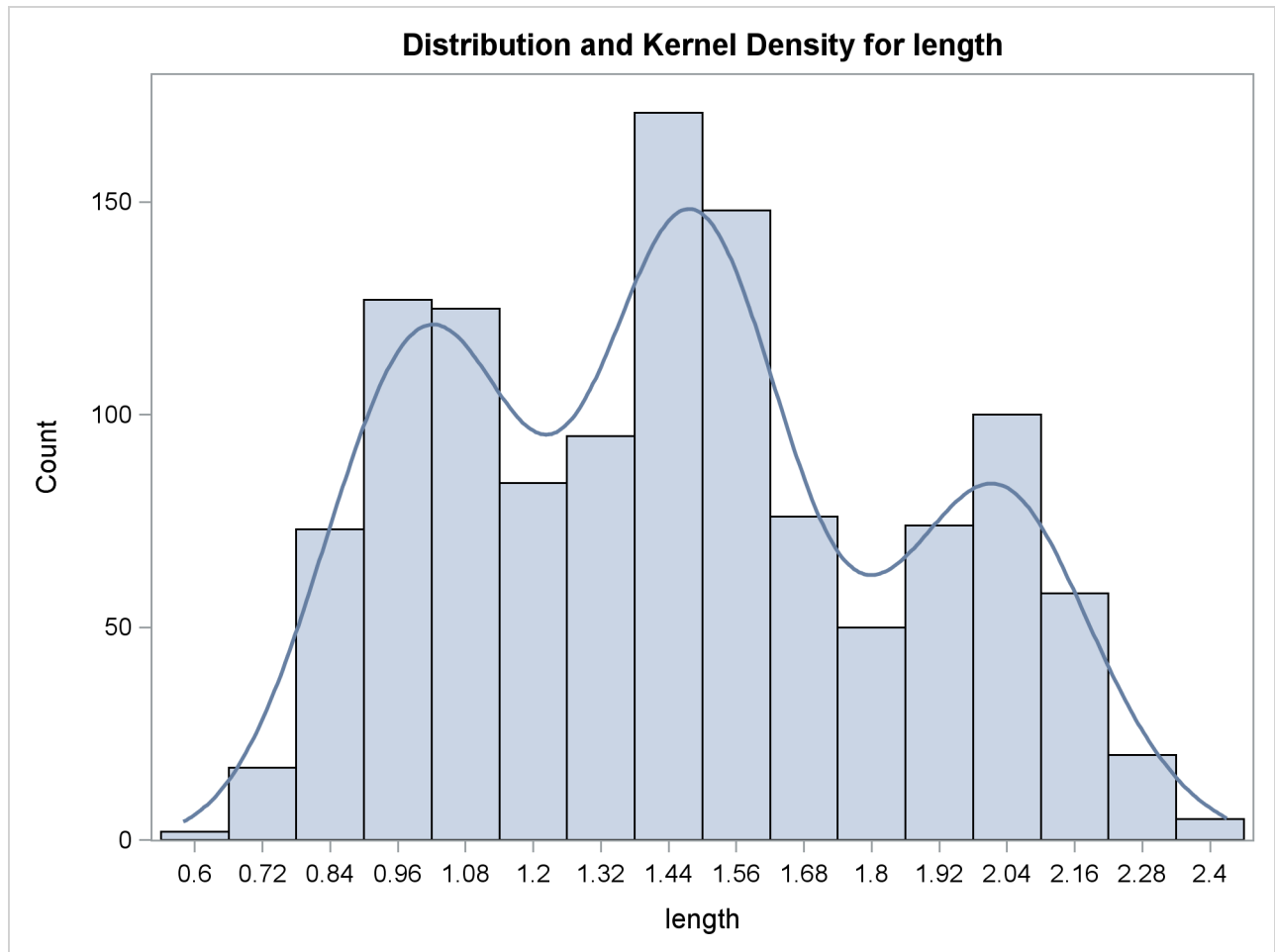
## Example 48.2: Changing the Bandwidth

Continuing with [Example 48.1](#), you can specify different bandwidth multipliers that determine the smoothness of the kernel density estimate. The following statements show kernel density estimates for the variable `length` by specifying two different bandwidth multipliers with the `BWM=` option:

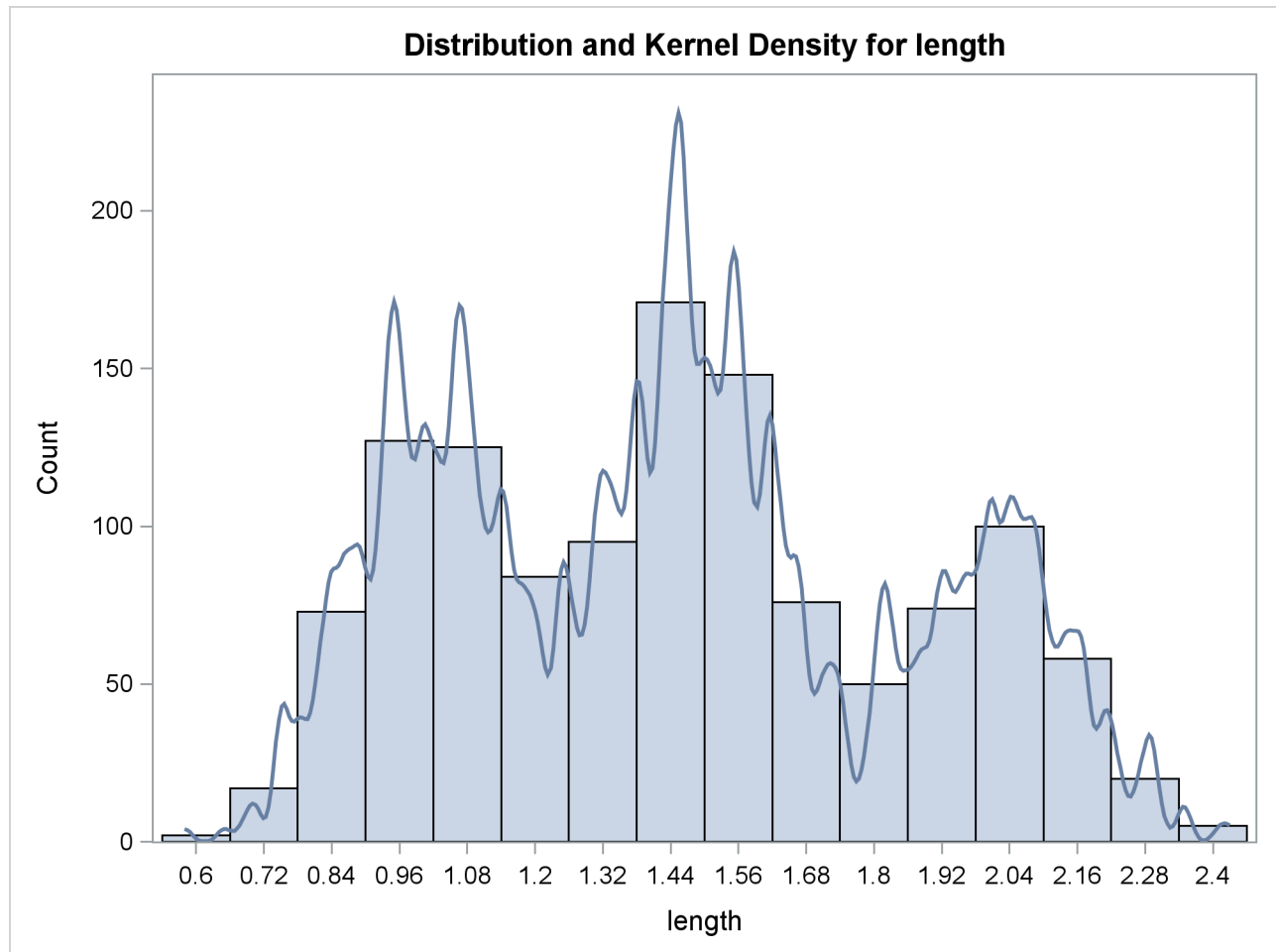
```
proc kde data=channel;
 univar length (bwm=2) length (bwm=0.25);
run;
ods graphics off;
```

[Output 48.2.1](#) shows an oversmoothed estimate because the bandwidth multiplier is 2. [Output 48.2.2](#) is created by specifying `BWM=0.25`, so it is an undersmoothed estimate.

**Output 48.2.1** Histogram with Oversmoothed Kernel Density Estimate





**Output 48.2.2** Histogram with Undersmoothed Kernel Density Estimate

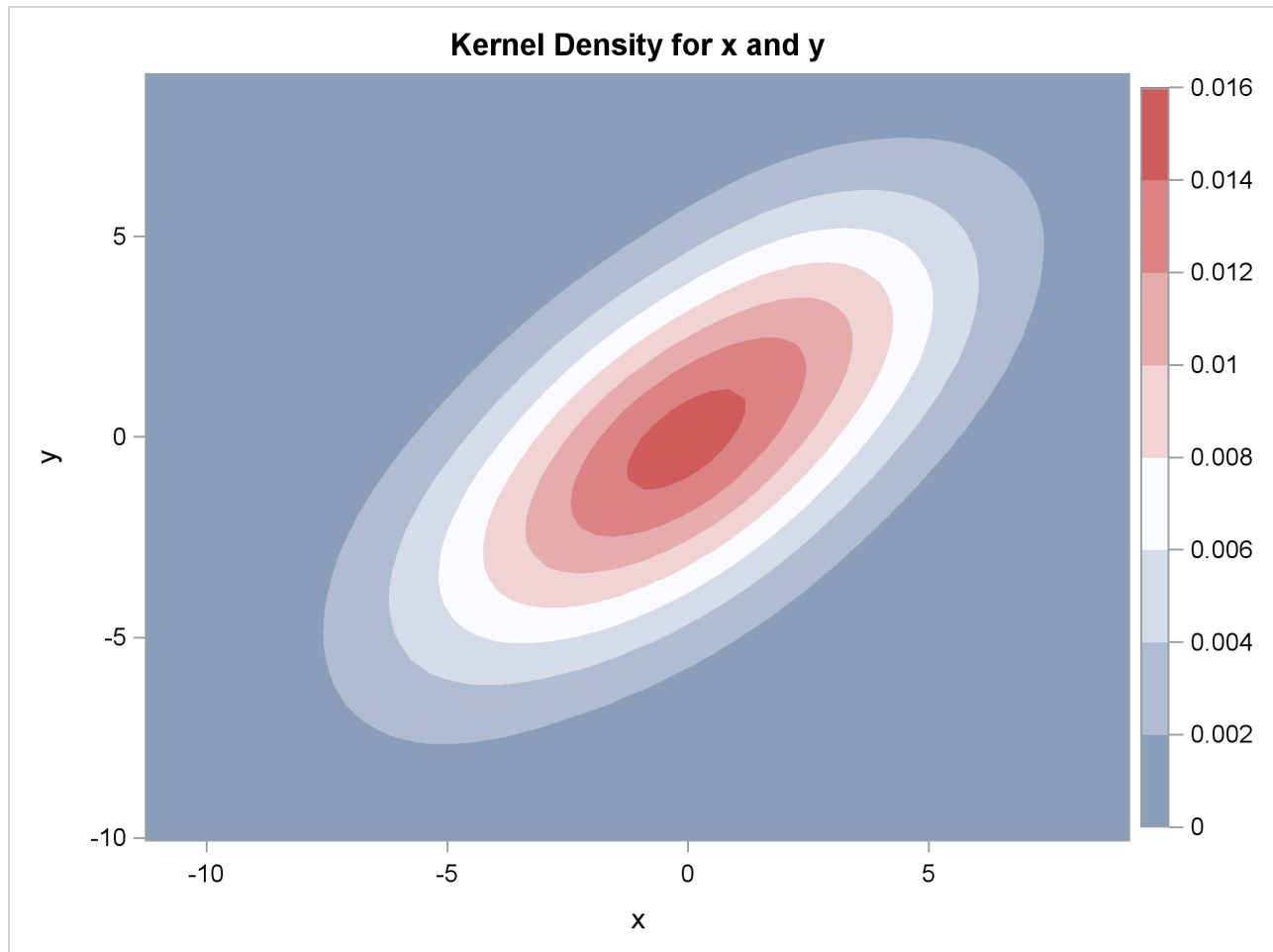

---

### Example 48.3: Changing the Bandwidth (Bivariate)

Recall the analysis from the section “Getting Started: KDE Procedure” on page 3748. Suppose you would like a slightly smoother estimate. You could then rerun the analysis with a larger bandwidth:

```
ods graphics on;
proc kde data=bivnormal;
 bivar x y / bwm=2;
run;
```

The BWM= option requests bandwidth multipliers of 2 for both x and y. With ODS Graphics enabled, the BIVAR statement produces a contour plot, as shown in [Output 48.3.1](#).

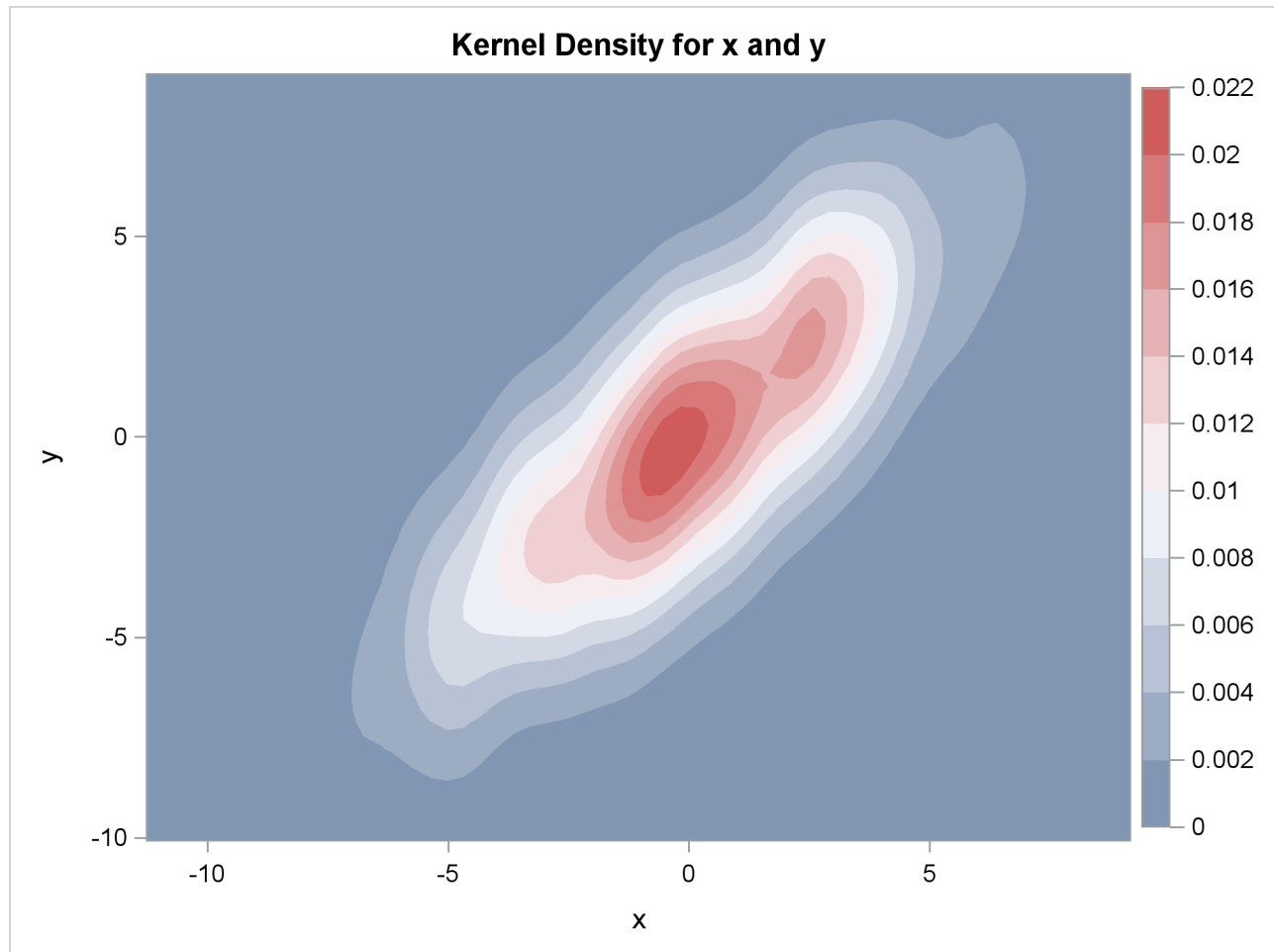
**Output 48.3.1** Contour Plot of Estimated Density with Additional Smoothing

### Multiple Bandwidths

You can also specify multiple bandwidths with only one run of the KDE procedure. Notice that by specifying pairs of variables inside parentheses, a kernel density estimate is computed for each pair. In the following statements the first kernel density is computed with the default bandwidth, but the second kernel density specifies a bandwidth multiplier of 0.5 for the variable *x* and a multiplier of 2 for the variable *y*:

```
proc kde data=bivnormal;
 bivar (x y) (x (bwm=0.5) y (bwm=2));
run;
ods graphics off;
```

The contour plot of the second kernel density estimate is shown in [Output 48.3.2](#).

**Output 48.3.2** Contour Plot of Estimated Density with Different Smoothing for x and y


---

### Example 48.4: Requesting Additional Output Tables

This example illustrates how to request output tables with summary statistics in addition to the default output tables. Using the same data as in the section “Getting Started: KDE Procedure” on page 3748, the following statements request univariate and bivariate summary statistics, percentiles, and levels of the kernel density estimate:

```
proc kde data=bivnormal;
 bivar x y / bivstats levels percentiles unistats;
run;
```

The resulting output is shown in [Output 48.4.1](#).

**Output 48.4.1** Bivariate Kernel Density Estimate Tables

| The KDE Procedure           |                            |        |
|-----------------------------|----------------------------|--------|
| Inputs                      |                            |        |
| Data Set                    | WORK.BIVNORMAL             |        |
| Number of Observations Used | 1000                       |        |
| Variable 1                  | x                          |        |
| Variable 2                  | y                          |        |
| Bandwidth Method            | Simple Normal<br>Reference |        |
| Controls                    |                            |        |
|                             | x                          | y      |
| Grid Points                 | 60                         | 60     |
| Lower Grid Limit            | -11.25                     | -10.05 |
| Upper Grid Limit            | 9.1436                     | 9.0341 |
| Bandwidth Multiplier        | 1                          | 1      |
| Univariate Statistics       |                            |        |
|                             | x                          | y      |
| Mean                        | -0.075                     | -0.070 |
| Variance                    | 9.73                       | 9.93   |
| Standard Deviation          | 3.12                       | 3.15   |
| Range                       | 20.39                      | 19.09  |
| Interquartile Range         | 4.46                       | 4.51   |
| Bandwidth                   | 0.99                       | 1.00   |
| Bivariate Statistics        |                            |        |
| Covariance                  | 8.88                       |        |
| Correlation                 | 0.90                       |        |

## Output 48.4.1 continued

| Percentiles |       |        |
|-------------|-------|--------|
|             | x     | y      |
| 0.5         | -7.71 | -8.44  |
| 1.0         | -7.08 | -7.46  |
| 2.5         | -6.17 | -6.31  |
| 5.0         | -5.28 | -5.23  |
| 10.0        | -4.18 | -4.11  |
| 25.0        | -2.24 | -2.30  |
| 50.0        | -0.11 | -0.058 |
| 75.0        | 2.22  | 2.21   |
| 90.0        | 3.81  | 3.94   |
| 95.0        | 4.88  | 5.22   |
| 97.5        | 6.03  | 5.94   |
| 99.0        | 6.90  | 6.77   |
| 99.5        | 7.71  | 7.07   |

| Levels  |          |             |             |             |             |
|---------|----------|-------------|-------------|-------------|-------------|
| Percent | Density  | Lower for x | Upper for x | Lower for y | Upper for y |
| 1       | 0.001181 | -8.14       | 8.45        | -8.76       | 8.39        |
| 5       | 0.003031 | -7.10       | 7.07        | -7.14       | 6.77        |
| 10      | 0.004989 | -6.41       | 5.69        | -6.49       | 6.12        |
| 50      | 0.01591  | -3.64       | 3.96        | -3.58       | 3.86        |
| 90      | 0.02388  | -1.22       | 1.19        | -1.32       | 0.95        |
| 95      | 0.02525  | -0.88       | 0.50        | -0.99       | 0.62        |
| 99      | 0.02608  | -0.53       | 0.16        | -0.67       | 0.30        |
| 100     | 0.02629  | -0.19       | -0.19       | -0.35       | -0.35       |

The “Univariate Statistics” table contains standard univariate statistics for each variable, as well as statistics associated with the density estimate. Note that the estimated variances for both  $x$  and  $y$  are fairly close to the true values of 10.

The “Bivariate Statistics” table lists the covariance and correlation between the two variables. Note that the estimated correlation is equal to its true value to two decimal places.

The “Percentiles” table lists percentiles for each variable.

The “Levels” table lists contours of the density corresponding to percentiles of the bivariate data, and the minimum and maximum values of each variable on those contours. For example, 5% of the observed data have a density value less than 0.0030. The minimum  $x$  and  $y$  values on this contour are  $-7.10$  and  $-7.14$ , respectively (the Lower for  $x$  and Lower for  $y$  columns), and the maximum values are  $7.07$  and  $6.77$ , respectively (the Upper for  $x$  and Upper for  $y$  columns).

You can also request “Percentiles” or “Levels” tables with specific percentiles:

```
proc kde data=bivnormal;
 bivar x y / levels=2.5, 50, 97.5
 percentiles=2.5, 25, 50, 75, 97.5;
run;
```

The resulting “Percentiles” and “Levels” tables are shown in [Output 48.4.2](#).

**Output 48.4.2** Customized Percentiles and Levels Tables

| The KDE Procedure |         |          |                |                |                |                |
|-------------------|---------|----------|----------------|----------------|----------------|----------------|
| Percentiles       |         |          |                |                |                |                |
|                   |         | x        |                | y              |                |                |
|                   | 2.5     | -6.17    |                | -6.31          |                |                |
|                   | 25.0    | -2.24    |                | -2.30          |                |                |
|                   | 50.0    | -0.11    |                | -0.058         |                |                |
|                   | 75.0    | 2.22     |                | 2.21           |                |                |
|                   | 97.5    | 6.03     |                | 5.94           |                |                |
| Levels            |         |          |                |                |                |                |
|                   | Percent | Density  | Lower<br>for x | Upper<br>for x | Lower<br>for y | Upper<br>for y |
|                   | 2.5     | 0.001914 | -7.79          | 8.11           | -7.79          | 7.74           |
|                   | 50.0    | 0.01591  | -3.64          | 3.96           | -3.58          | 3.86           |
|                   | 97.5    | 0.02573  | -0.88          | 0.50           | -0.99          | 0.30           |

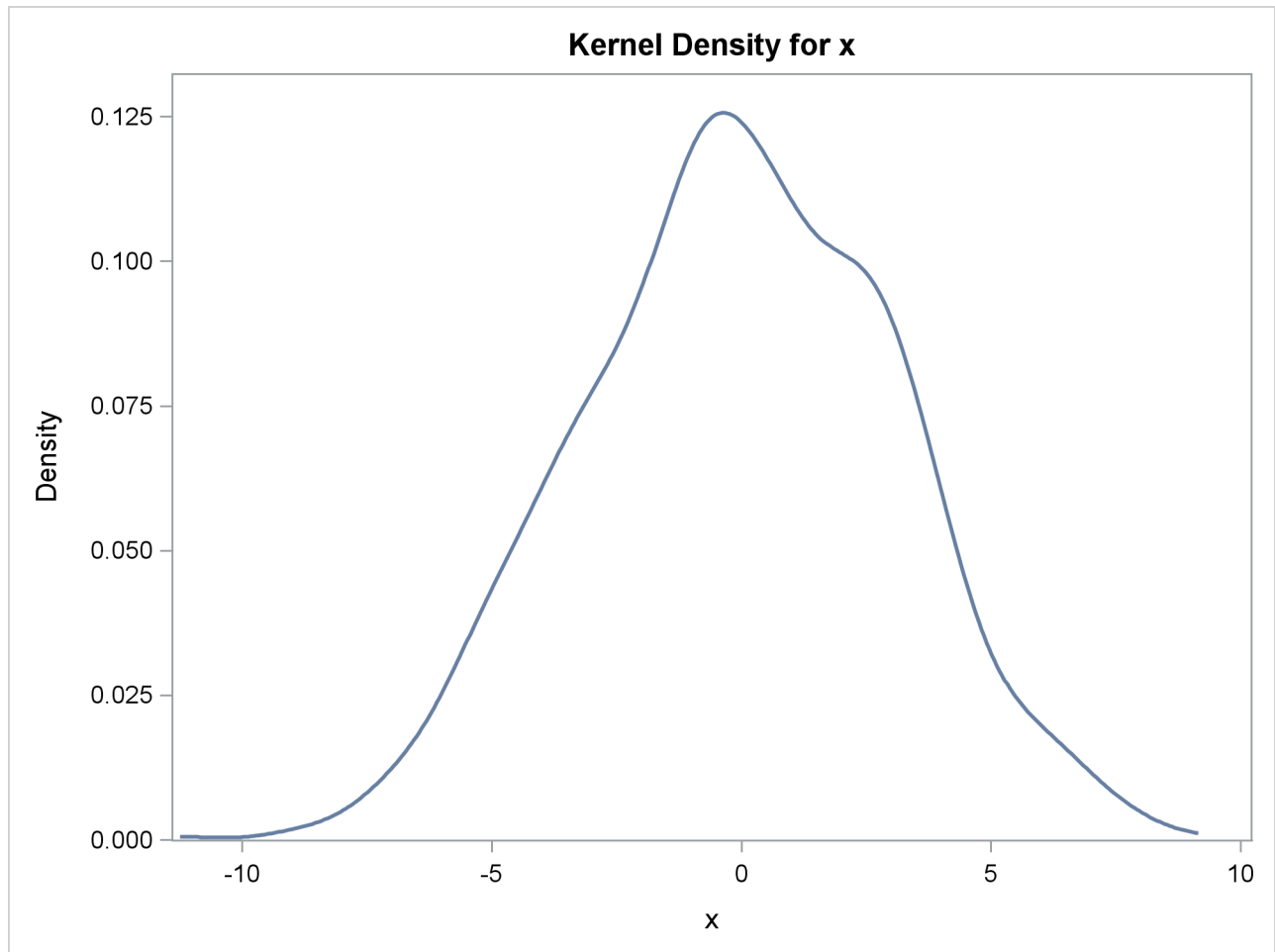
## Example 48.5: Univariate KDE Graphics

This example uses data from the section “[Getting Started: KDE Procedure](#)” to illustrate the use of ODS Graphics. The following statements request the available univariate plots in PROC KDE:

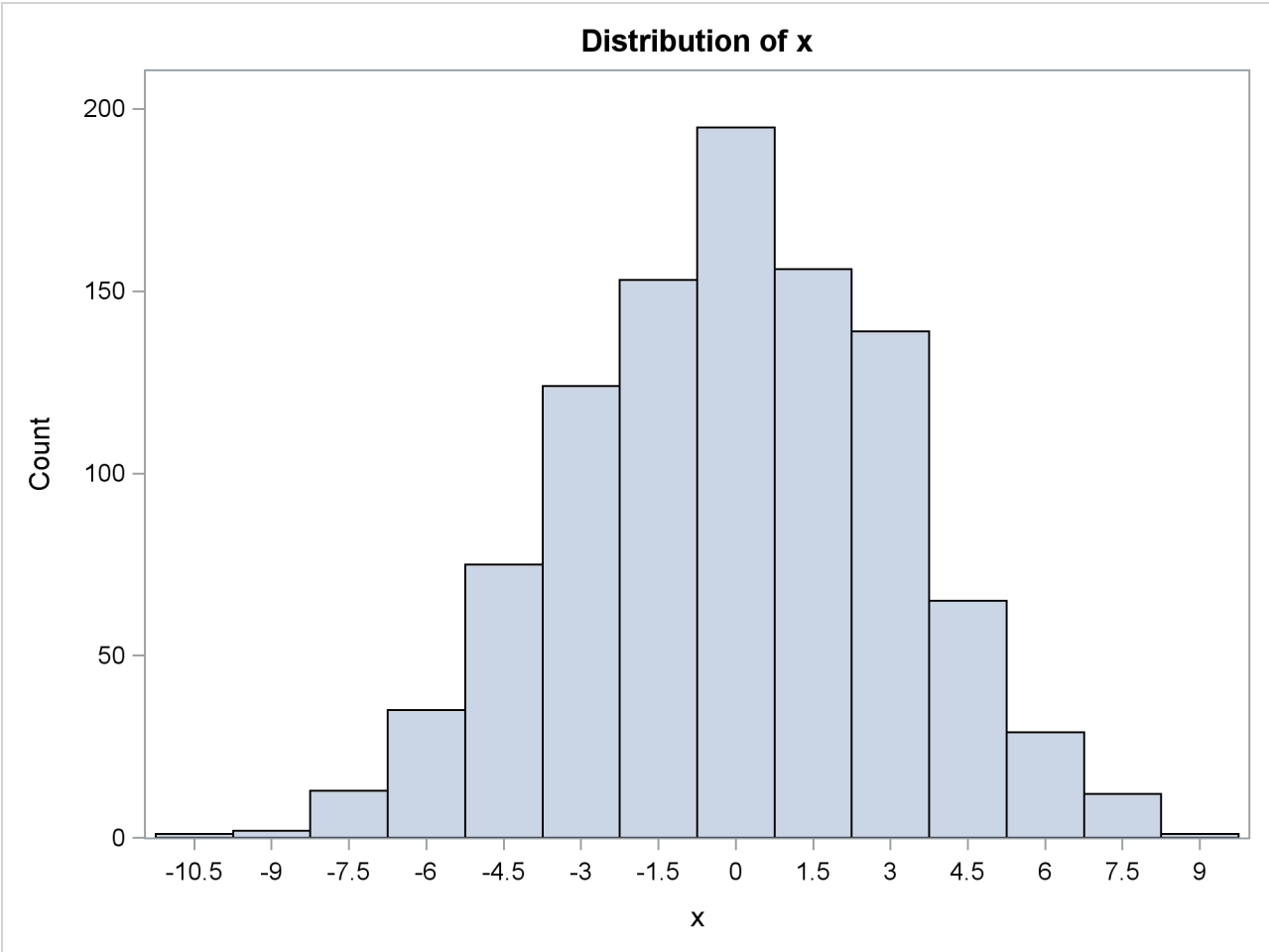
```
ods graphics on;
proc kde data=bivnormal;
 univar x / plots=(density histogram histdensity);
 univar x y / plots=densityoverlay;
run;
ods graphics off;
```

Graphs are requested by specifying the `PLOTS=` option in the `UNIVAR` statement with ODS Graphics enabled. [Output 48.5.1](#), [Output 48.5.2](#), and [Output 48.5.3](#) show the kernel density estimate, histogram, and histogram with kernel density estimate overlaid, respectively, produced by the first `UNIVAR` statement.

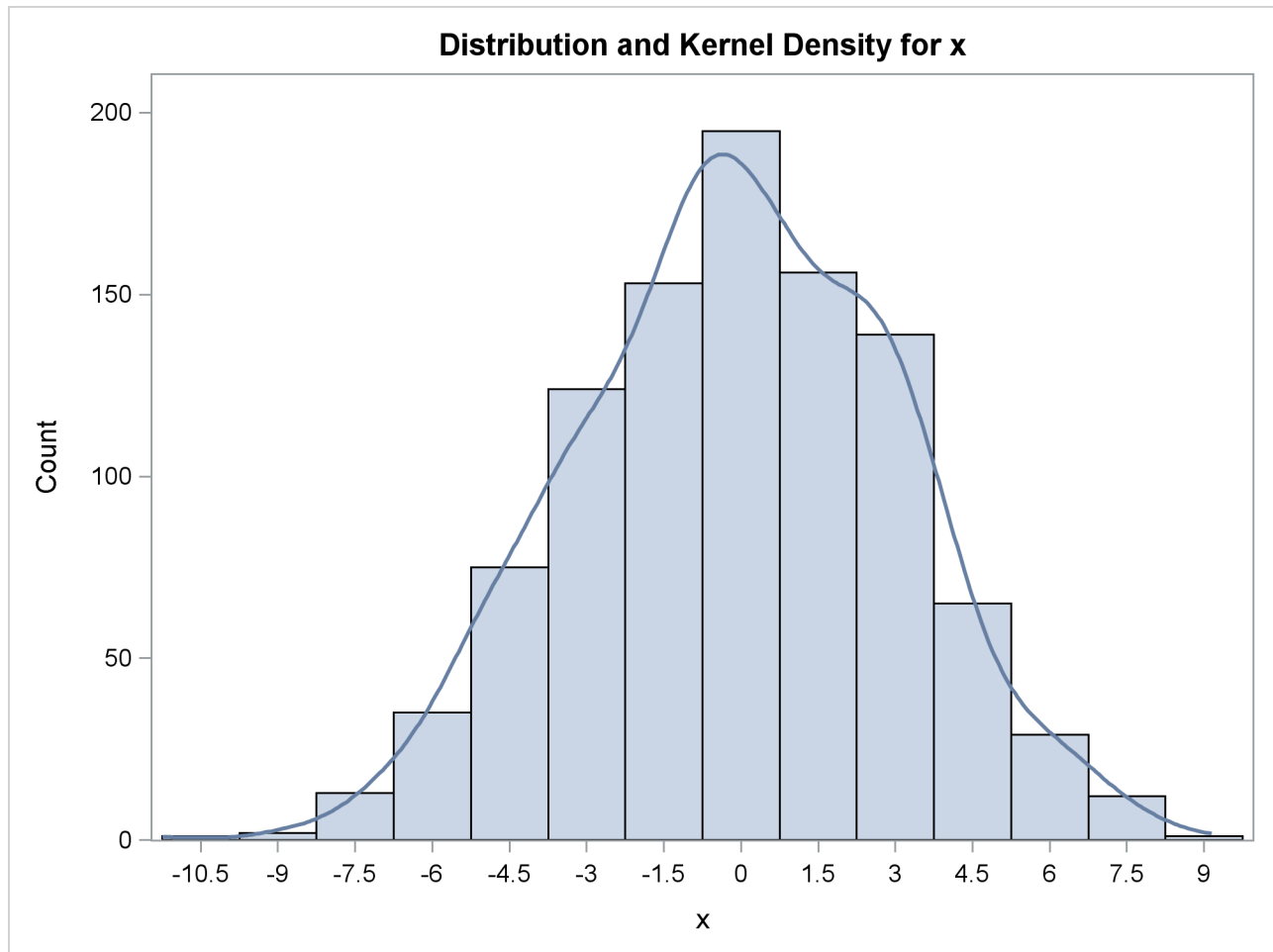
**Output 48.5.1** Kernel Density Estimate



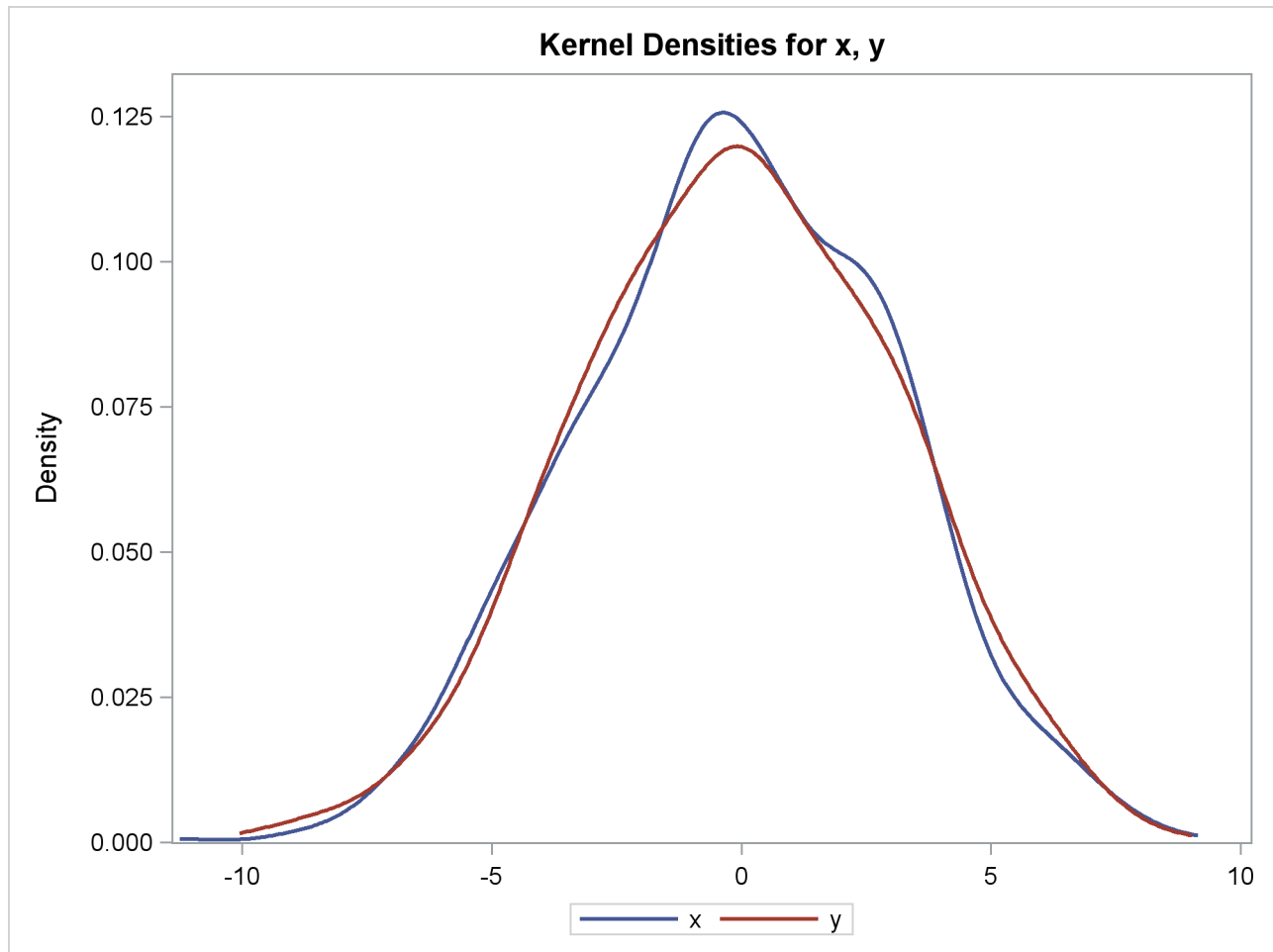
Output 48.5.2 Histogram





**Output 48.5.3** Histogram with Overlaid Kernel Density Estimate

Output 48.5.4 shows the plot produced by the second UNIVAR statement, in which the kernel density estimates for x and y are overlaid.

**Output 48.5.4** Overlaid Kernel Density Estimates

For general information about ODS Graphics, see Chapter 21, “Statistical Graphics Using ODS.” For specific information about the graphics available in the KDE procedure, see the section “ODS Graphics” on page 3767.

---

## Example 48.6: Bivariate KDE Graphics

This example illustrates the available bivariate graphics in PROC KDE. The octane data set comes from Rodriguez and Taniguchi (1980), where it is used for predicting customer octane satisfaction by using trained-rater observations. The variables in this data set are Rater and Customer. Either variable might have missing values. See the file *kdex3.sas* in the SAS Sample Library. The following statements create the octane data set:

```
data octane;
 input Rater Customer;
 label Rater = 'Rater'
 Customer = 'Customer';
 datalines;
94.5 92.0
94.0 88.0
94.0 90.0
93.0 93.0

... more lines ...

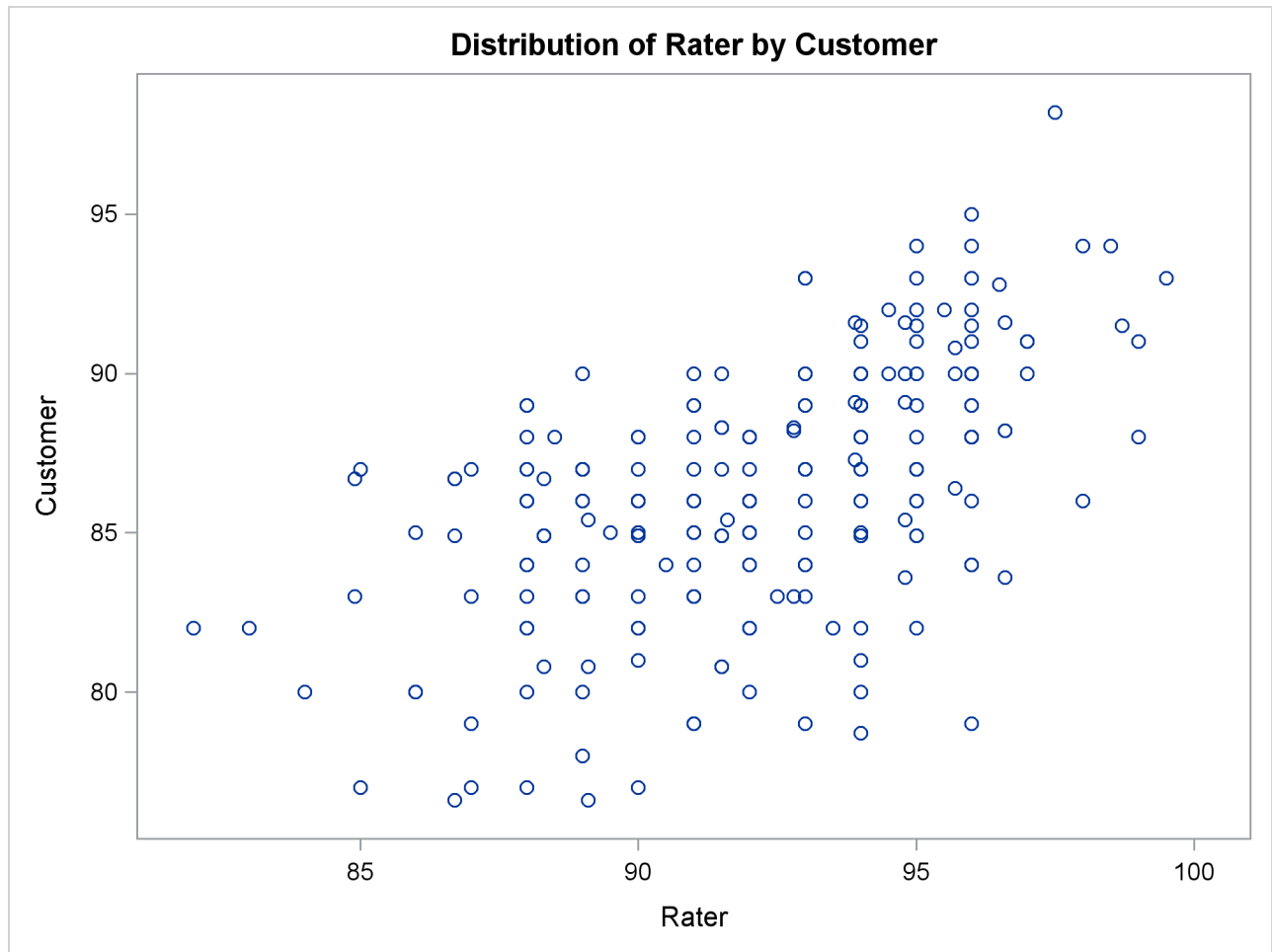
88.0 84.0
.H 90.0
;
```

The following statements request all the available bivariate plots in PROC KDE:

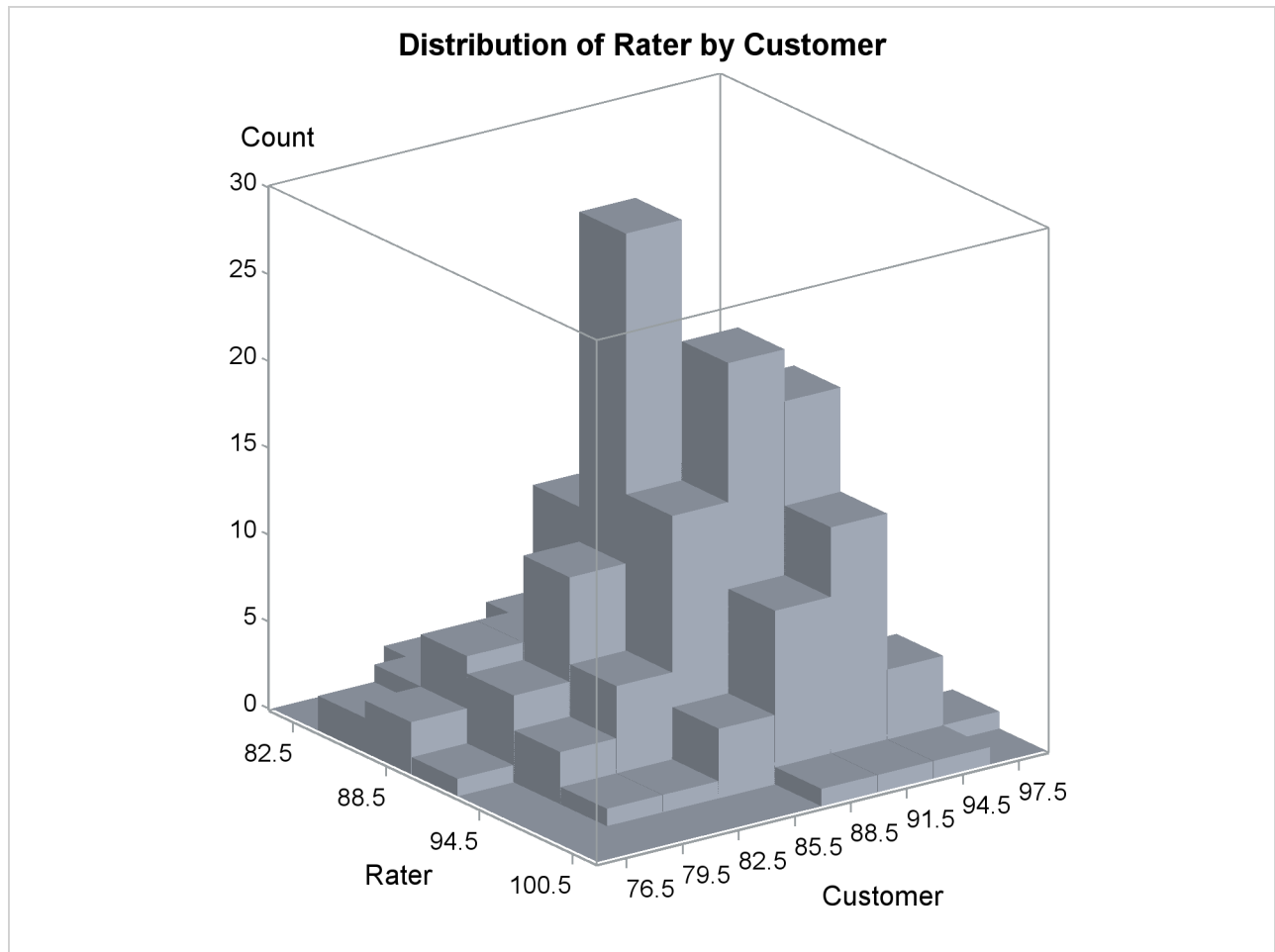
```
ods graphics on;
proc kde data=octane;
 bivar Rater Customer / plots=all;
run;
ods graphics off;
```

Output 48.6.1 shows a scatter plot of the data, Output 48.6.2 shows a bivariate histogram of the data, Output 48.6.3 shows a contour plot of bivariate density estimate, Output 48.6.4 shows a contour plot of bivariate density estimate overlaid with a scatter plot of data, Output 48.6.5 shows a surface plot of bivariate kernel density estimate, and Output 48.6.6 shows a bivariate histogram overlaid with a bivariate kernel density estimate. These graphical displays are requested by specifying the **PLOTS=** option in the **BIVAR** statement with ODS Graphics enabled. For general information about ODS Graphics, see Chapter 21, “Statistical Graphics Using ODS.” For specific information about the graphics available in the KDE procedure, see the section “ODS Graphics” on page 3767.

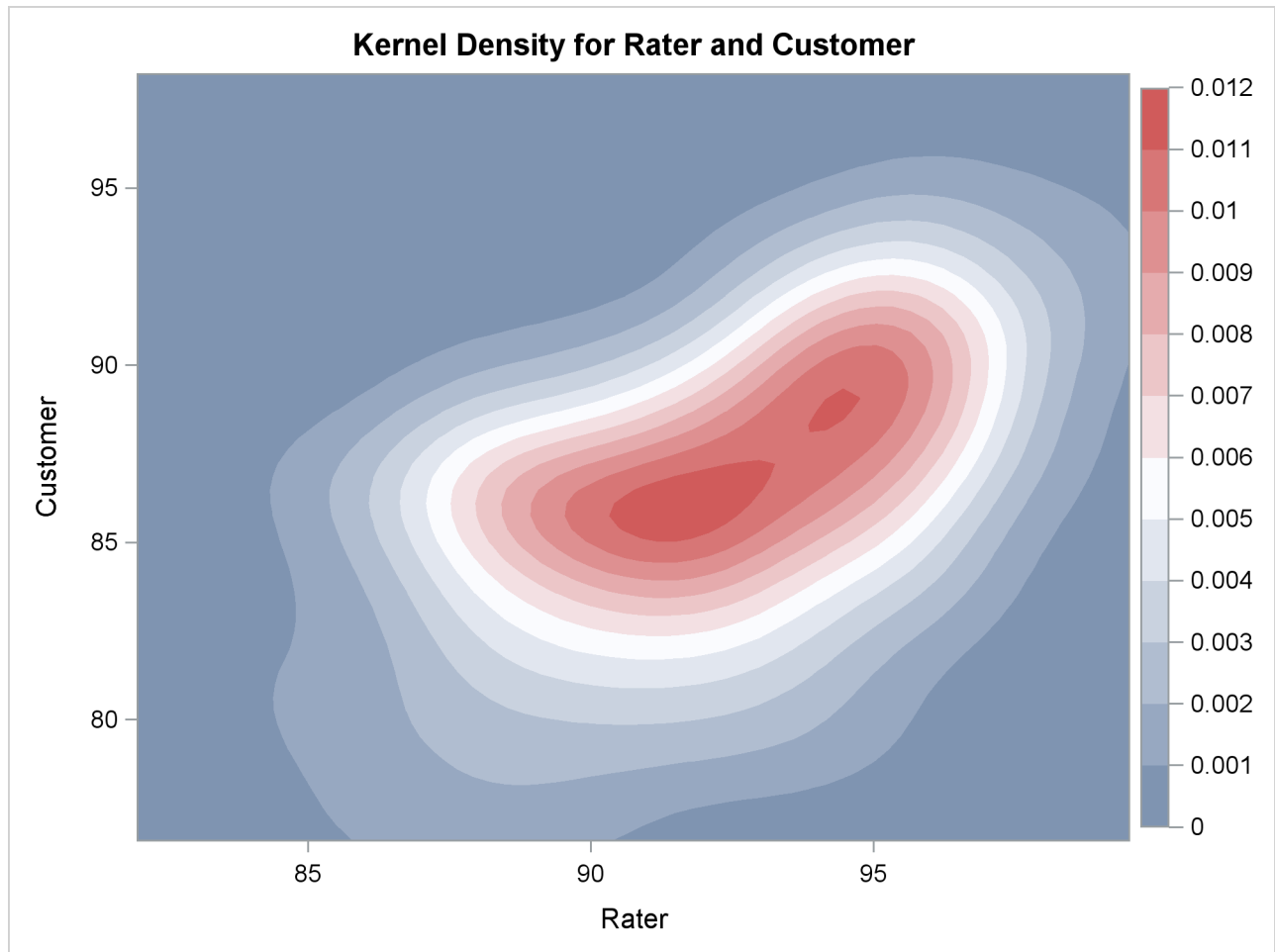
Output 48.6.1 Scatter Plot



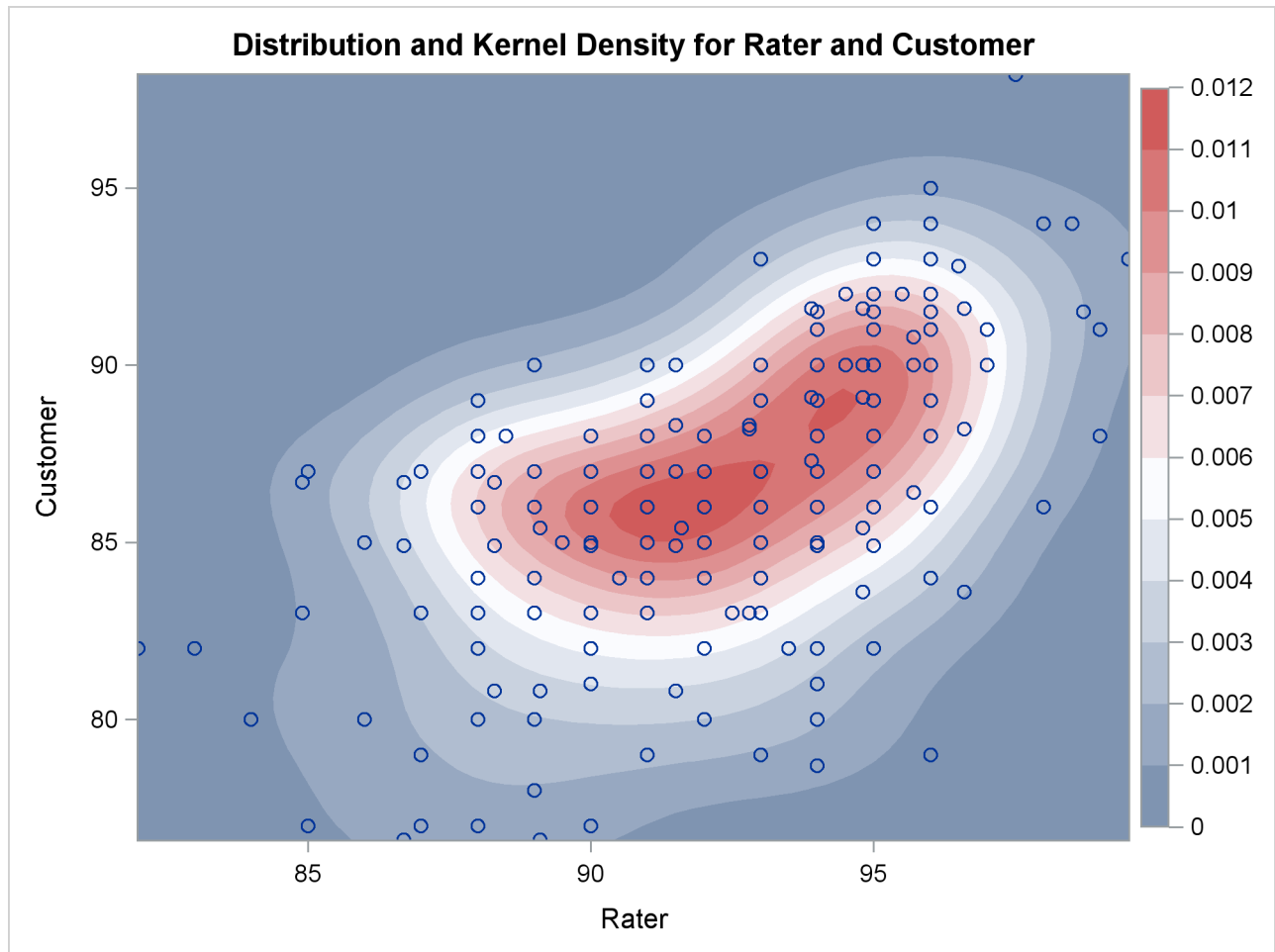
**Output 48.6.2** Bivariate Histogram



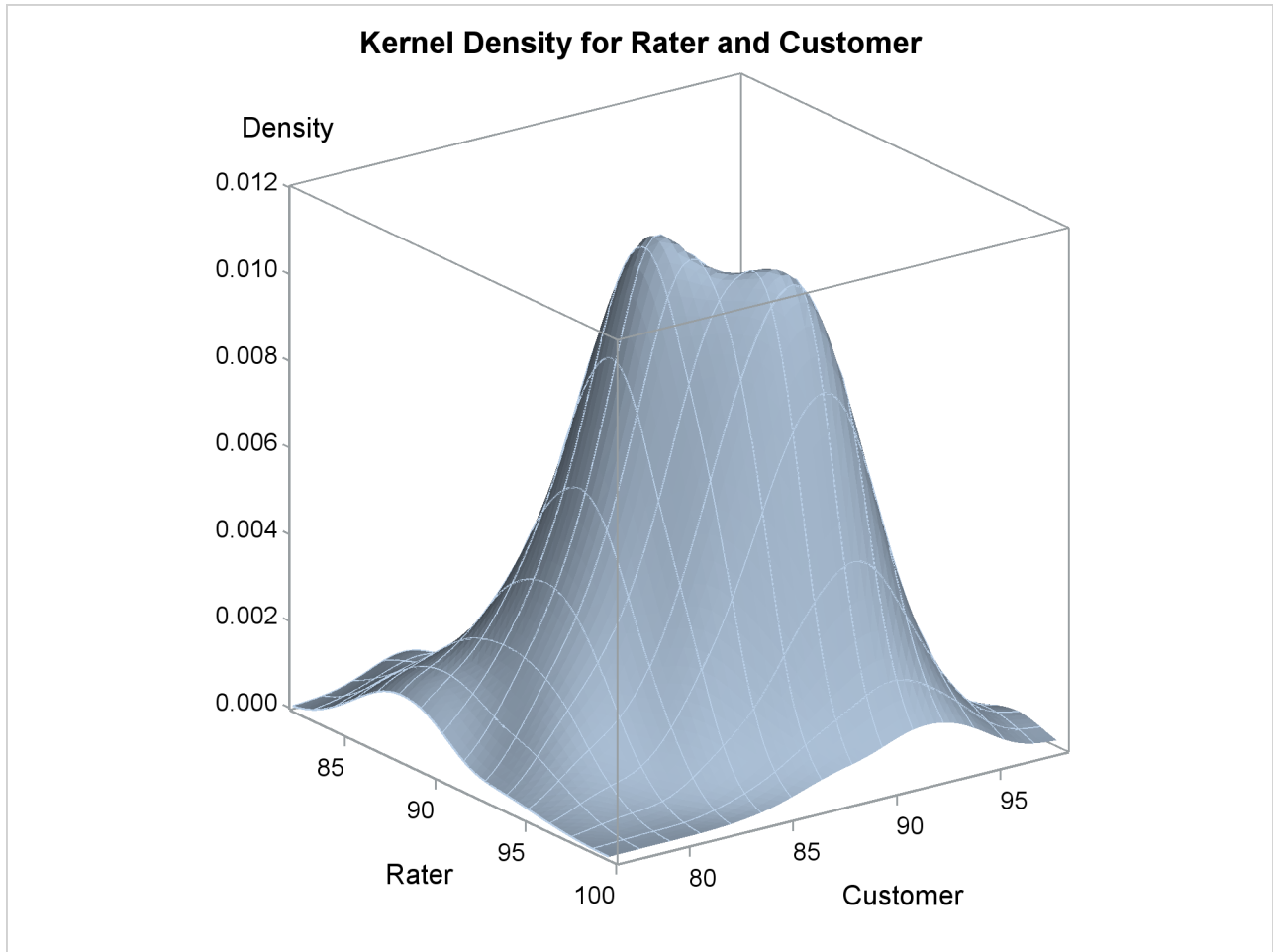
Output 48.6.3 Contour Plot



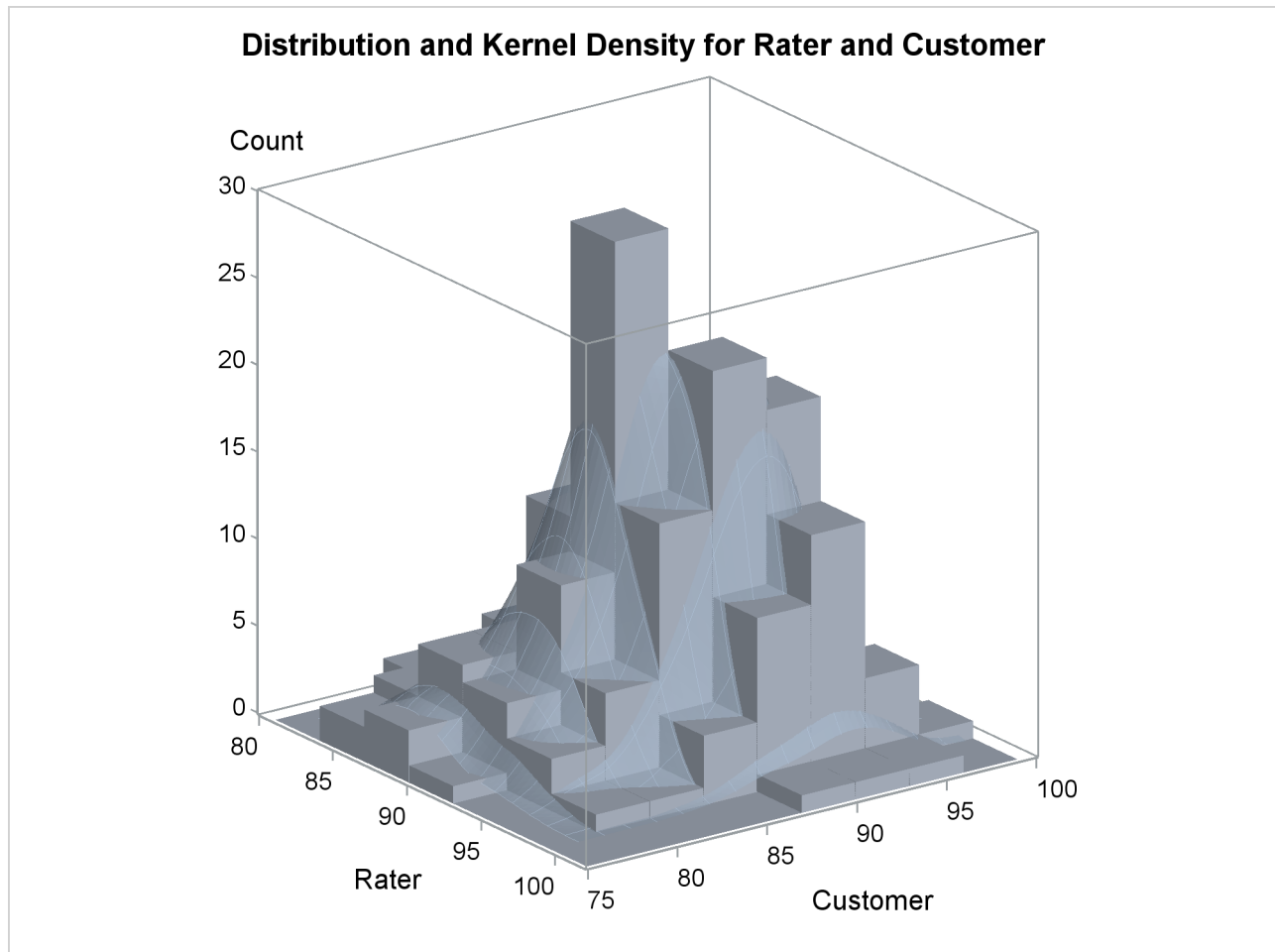
**Output 48.6.4** Contour Plot with Overlaid Scatter Plot



Output 48.6.5 Surface Plot





**Output 48.6.6** Bivariate Histogram with Overlaid Surface Plot


---

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# Chapter 49

## The KRIGE2D Procedure

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## Overview: KRIGE2D Procedure

The KRIGE2D procedure performs ordinary kriging in two dimensions. PROC KRIGE2D can handle anisotropic and nested semivariogram models. Eight semivariogram models are supported: the Gaussian, exponential, spherical, power, cubic, pentaspherical, sine hole effect, and Matérn models. A single nugget effect is also supported. You can specify the correlation model by naming the form and supplying the associated parameters, or by using the contents of an item store file that was previously created by PROC VARIOGRAM.

You can specify the locations of kriging predictions in a **GRID** statement, or they can be read from a SAS data set. The grid specification is most suitable for a regular grid; the data set specification can handle any irregular pattern of points.

Local kriging is supported through the specification of a radius around a grid point or the specification of the number of nearest neighbors to use in the kriging system. When you perform local kriging, a separate kriging system is solved at each grid point by using a neighborhood of the data point established by the radius or number specification.

The KRIGE2D procedure writes the kriging predictions and associated standard errors for each grid to an output data set. When you perform local kriging, PROC KRIGE2D writes the neighborhood information for each grid point to an additional, optional data set. The KRIGE2D procedure does not produce any displayed output.

The KRIGE2D procedure uses ODS Graphics to create graphs as part of its output. For general information about ODS Graphics, see Chapter 21, “Statistical Graphics Using ODS.” For more information about the graphics available in PROC KRIGE2D, see the section “ODS Graphics” on page 3845.

---

## Introduction to Spatial Prediction

Many activities in science and technology involve measurements of one or more quantities at given spatial locations, with the goal of predicting the measured quantities at unsampled locations. Application areas include reservoir prediction in mining and petroleum exploration, in addition to modeling in a broad spectrum of fields (for example, environmental health, environmental pollution, natural resources and energy, hydrology, and risk analysis). Often, the unsampled locations are on a regular grid, and the predictions are used to produce surface plots or contour maps.

The preceding tasks fall within the scope of *spatial prediction*, which, in general, is any prediction method that incorporates spatial dependence. The study of these tasks involves naturally occurring uncertainties that cannot be ignored. Stochastic analysis frameworks and methods are often used to account for these uncertainties. Hence, the terms *stochastic spatial prediction* and *stochastic modeling* are also used to characterize this type of analysis.

A popular method of spatial prediction is *ordinary kriging*, which produces both predicted values and associated standard errors. Ordinary kriging requires the complete specification (the form and parameter values) of the spatial dependence that characterizes the spatial process. For this purpose, models for the spatial dependence are expressed in terms of the distance between any two locations in the spatial domain of interest. These models take the form of a covariance or semivariance function.

Spatial prediction, then, involves two steps. First, you model the covariance or semivariance of the spatial process. These measures are typically not known in advance. This step involves computing an empirical estimate, in addition to determining both the mathematical form and the values of any parameters for a theoretical form of the dependence model. Second, you use this dependence model to solve the kriging system at a specified set of spatial points, resulting in predicted values and associated standard errors.

The KRIGE2D procedure performs the second of these steps by using ordinary kriging of two-dimensional data.

This introduction concludes with a note on terminology. You might commonly encounter the terms *estimation* and *prediction* used interchangeably by experts in different fields; this could be a source of confusion. A precise statistical vernacular uses the term *estimation* to refer to inferences about the value of fixed but unknown parameters, whereas *prediction* concerns inferences about the value of random variables—see, for example, Cressie (1993, p. 106). In light of these definitions, kriging methods are clearly predictive techniques, since they are concerned with making inferences about the value of a spatial random field at observed or unobserved locations. The SAS/STAT suite of procedures for spatial analysis and prediction (VARIOGRAM, KRIGE2D, and SIM2D) follows the statistical vernacular in the use of the terms *estimation* and *prediction*.

## Getting Started: KRIGE2D Procedure

### Spatial Prediction Using Kriging, Contour Plots

After an appropriate semivariogram model is chosen, a number of choices are involved in producing the kriging surface. In order to illustrate these choices, you use the theoretical semivariogram model that was fitted to the coal seam thickness data empirical semivariogram in “Theoretical Semivariogram Model Fitting” on page 8571 in the VARIOGRAM procedure. This model is Gaussian,

$$\gamma_z(h) = c_0 \left[ 1 - \exp\left(-\frac{h^2}{a_0^2}\right) \right]$$

with a scale of  $c_0 = 7.4599$  (that is, the model sill) and a range of  $a_0 = 30.1111$ , based on the weighted least squares fitting results in the PROC VARIOGRAM example.

The first choice is whether to use local or global kriging. Local kriging uses only data points in the neighborhood of a grid point, and you choose this type of analysis by specifying a data search radius around the grid point. Global kriging uses all data points.

The most important consideration in this decision is the spatial covariance structure. Global kriging is appropriate when the correlation range  $\epsilon$  is approximately equal to the length of the spatial domain. The correlation range  $\epsilon$  is the distance  $r_\epsilon$  (also known as *effective* or *practical* range) at which the covariance is 5% of its value at zero. That is,

$$C_Z(r_\epsilon) = 0.05C_Z(0)$$

For a Gaussian model,  $r_\epsilon$  is  $\sqrt{3}a_0 \approx 52,000$  feet. The data points are scattered uniformly throughout a  $100 \times 100$  ( $10^6$  ft<sup>2</sup>) area. Hence, the linear dimension of the data is nearly double the  $r_\epsilon$  range. This indicates that local kriging rather than global kriging is appropriate because data that are farther away than  $r_\epsilon$  essentially add to the computational burden without significant contribution to the prediction. The following DATA step inputs the thickness data set `thick`, which is available from the `Sashelp` library. In the `thick` data set, thickness is represented by the `Thick` variable.

```

title 'Spatial Prediction With Kriging';

data thick;
 input East North Thick @@;
 label Thick='Coal Seam Thickness';
 datalines;
 0.7 59.6 34.1 2.1 82.7 42.2 4.7 75.1 39.5
 4.8 52.8 34.3 5.9 67.1 37.0 6.0 35.7 35.9
 6.4 33.7 36.4 7.0 46.7 34.6 8.2 40.1 35.4
 13.3 0.6 44.7 13.3 68.2 37.8 13.4 31.3 37.8
 17.8 6.9 43.9 20.1 66.3 37.7 22.7 87.6 42.8
 23.0 93.9 43.6 24.3 73.0 39.3 24.8 15.1 42.3
 24.8 26.3 39.7 26.4 58.0 36.9 26.9 65.0 37.8
 27.7 83.3 41.8 27.9 90.8 43.3 29.1 47.9 36.7
 29.5 89.4 43.0 30.1 6.1 43.6 30.8 12.1 42.8
 32.7 40.2 37.5 34.8 8.1 43.3 35.3 32.0 38.8
 37.0 70.3 39.2 38.2 77.9 40.7 38.9 23.3 40.5
 39.4 82.5 41.4 43.0 4.7 43.3 43.7 7.6 43.1
 46.4 84.1 41.5 46.7 10.6 42.6 49.9 22.1 40.7
 51.0 88.8 42.0 52.8 68.9 39.3 52.9 32.7 39.2
 55.5 92.9 42.2 56.0 1.6 42.7 60.6 75.2 40.1
 62.1 26.6 40.1 63.0 12.7 41.8 69.0 75.6 40.1
 70.5 83.7 40.9 70.9 11.0 41.7 71.5 29.5 39.8
 78.1 45.5 38.7 78.2 9.1 41.7 78.4 20.0 40.8
 80.5 55.9 38.7 81.1 51.0 38.6 83.8 7.9 41.6
 84.5 11.0 41.5 85.2 67.3 39.4 85.5 73.0 39.8
 86.7 70.4 39.6 87.2 55.7 38.8 88.1 0.0 41.6
 88.4 12.1 41.3 88.4 99.6 41.2 88.8 82.9 40.5
 88.9 6.2 41.5 90.6 7.0 41.5 90.7 49.6 38.9
 91.5 55.4 39.0 92.9 46.8 39.1 93.4 70.9 39.7
 55.8 50.5 38.1 96.2 84.3 40.3 98.2 58.2 39.5
 ;

```

Local kriging is performed by using only data points within a specified radius of each grid point. In this example, a radius of 60,000 feet is used. Other choices involved in local kriging are the minimum and maximum number of data points in each neighborhood (around a grid point). The minimum number is left at the default value of 20; the maximum number defaults to all observations in the data set within the specified radius.

The last step in contouring the data is to define the prediction grid point (node) locations. The prediction grid is typically rectangular, and you decide on the grid points population and spacing based on your available data in addition to your application needs. A convenient area that encompasses all the data points is a square of side length 100,000 feet. In the present analysis, a distance of 2,500 feet between nodes in the prediction grid is selected to obtain a smooth contour plot. Based on this choice, you obtain predictions on a square grid with 41 nodes on each side, which yields a total of 1681 grid points.

You can visualize the outcome of your analysis by using the **PLOTS** option in the **PROC KRIGE2D** statement. By default, **PROC KRIGE2D** produces one plot that displays the kriging prediction and its corresponding standard error at each output grid point. The locations of the Thick observations are displayed too, as outlines in the default plot. You can also ask for a plot of the thick data set observations and their values by specifying the **OBSERV** option in the **PLOTS** option.

The kriging analysis with the **KRIGE2D** procedure requires that you provide the prediction parameters in the **PREDICT** statement. You use the **VAR=** option to specify that you want to use the Thick variable in the kriging system, and the **RADIUS=** option to specify the radius of the local kriging regression. In this scenario you want to consider for your predictions all the neighboring data within a radius of 60,000 feet from each prediction location. You can specify more than one **PREDICT** statements; for example, you can do this when you want predictions for different variables in your **DATA=** data set.

The coordinates of your variable are specified in the **COORDINATES** statement. The **MODEL** statement contains the parameters that describe your data spatial correlation. Namely, the **FORM=** option specifies the model type, based on its mathematical form. The **SCALE=** and **RANGE=** options specify the model sill and range, respectively. You can specify more than one **MODEL** statement for the same **PREDICT** statement in order to obtain predictions based on different correlation models.

When you use the **RADIUS=** option to perform local kriging, as in the present example, it is suggested that the radius parameter be at least as large as your model range, so that you include data points that can contribute to your prediction.

Eventually, you specify the region of predictions with the **GRID** statement. The following SAS statements compute the kriged surface by using the preceding options and grid choice:

```
ods graphics on;

proc krige2d data=thick;
 coordinates xc=East yc=North;
 predict var=Thick radius=60;
 model scale=7.4599 range=30.1111 form=gauss;
 grid x=0 to 100 by 2.5 y=0 to 100 by 2.5;
run;

ods graphics off;
```



The table in Figure 49.1 shows the number of observations read and used in the kriging prediction. This table provides you with useful information in case you have missing values in the input data.

**Figure 49.1** Number of Observations for the thick Data Set

| Spatial Prediction With Kriging |    |
|---------------------------------|----|
| The KRIGE2D Procedure           |    |
| Dependent Variable: Thick       |    |
| Number of Observations Read     | 75 |
| Number of Observations Used     | 75 |

Figure 49.2 shows some general information about the kriging analysis. This includes the count of the output grid points. You have specified the `RADIUS=` option; therefore you also see that local kriging is requested. Because this is a local analysis, the table also displays the parameters related to the neighborhood search around the grid points.

**Figure 49.2** Kriging Analysis Information

| Kriging Information        |                   |
|----------------------------|-------------------|
| Prediction Grid Points     | 1681              |
| Type of Analysis           | Local             |
| Neighborhood Search Radius | 60                |
| Minimum Neighbors          | 20                |
| Maximum Neighbors          | All Within Radius |

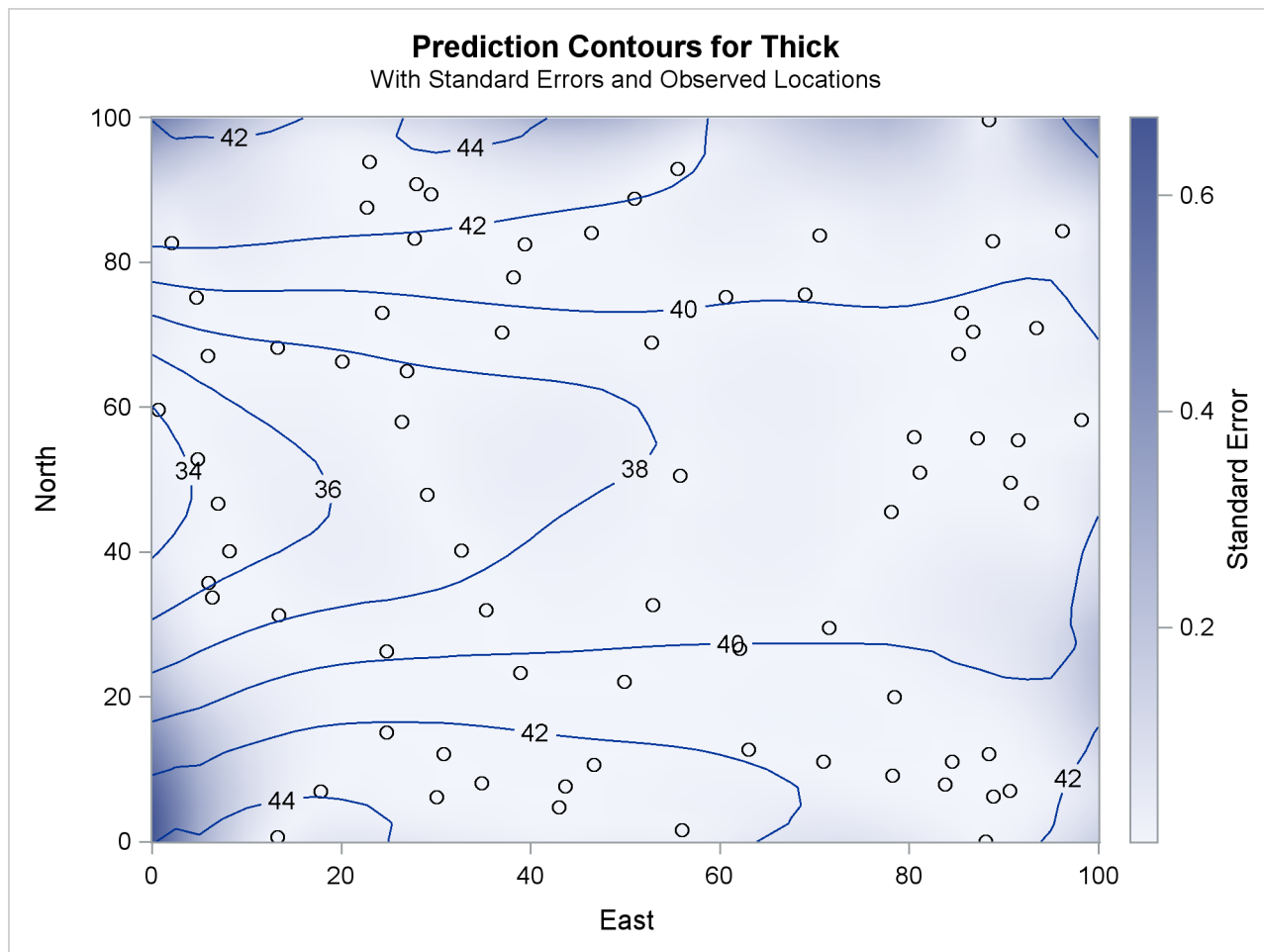
The covariance model parameters, including the effective range of the Gaussian model you specified, are shown in Figure 49.3.

**Figure 49.3** Kriging Covariance Model Information

| Spatial Prediction With Kriging  |           |
|----------------------------------|-----------|
| The KRIGE2D Procedure            |           |
| Dependent Variable: Thick        |           |
| Prediction: Pred1, Model: Model1 |           |
| Covariance Model Information     |           |
| Type                             | Gaussian  |
| Sill                             | 7.4599    |
| Range                            | 30.1111   |
| Effective Range                  | 52.153955 |
| Nugget Effect                    | 0         |

Figure 49.4 shows a map of the kriging prediction contours based on the Thick observations in the specified spatial domain. The prediction error is displayed as a surface in the background.

**Figure 49.4** Contour Plot of Kriged Coal Seam Thickness



Note the locations of the observed data in Figure 49.4. The figure suggests that the Thick sampling locations are not ideally spread around the prediction area; however, there are no extended areas lacking measurements.

Based on the spatial distribution of the Thick data and the range  $r_\epsilon$  of your covariance model, you can roughly see that for each prediction location there are at least several neighboring data points that contribute to the prediction value. Except perhaps for the nodes close to the boundaries of the prediction grid, you can then expect the prediction errors to be reasonably low compared to the predicted Thick values.

The kriging outcome in Figure 49.4 indicates that the standard errors are smaller in the neighborhoods where data are available. The size of these neighborhoods depends on the range of the specified covariance model that characterizes the spatial continuity of the domain, and on the prediction radius, if one is specified as in this example. The standard errors tend to increase toward the borders of the prediction area, beyond which no observations are available.

## Syntax: KRIGE2D Procedure

The following statements are available in the KRIGE2D procedure:

```

PROC KRIGE2D options ;
 BY variables ;
 COORDINATES | COORD coordinate-variables ;
 GRID grid-options ;
 ID variable ;
 PREDICT | PRED | P predict-options ;
 MODEL model-options ;
 RESTORE restore-options ;

```

The **PREDICT** and **MODEL** statements are hierarchical; the **PREDICT** statement is followed by a **MODEL** statement. If more than one **MODEL** statement is given, only the last one is used for the analysis. The **MODEL** statement following a **PREDICT** statement uses the variable and neighborhood specifications in that **PREDICT** statement.

You must specify at least one **PREDICT** statement and one **MODEL** statement. You must supply a single **COORDINATES** statement to identify the  $x$  and  $y$  coordinate variables in the input data set. You must also specify a single **GRID** statement to include the grid information.

Table 49.1 outlines the options available in PROC KRIGE2D classified by function.

**Table 49.1** Options Available in the KRIGE2D Procedure

| Task                                                                  | Statement    | Option   |
|-----------------------------------------------------------------------|--------------|----------|
| <b>Data Set Options</b>                                               |              |          |
| Specifies input data set                                              | PROC KRIGE2D | DATA=    |
| Specifies grid data set                                               | GRID         | GDATA=   |
| Specifies labels for individual grid points or in 1-D                 | GRID         | LABEL    |
| Specifies model data set                                              | MODEL        | MDATA=   |
| Writes kriging predictions and standard errors                        | PROC KRIGE2D | OUTEST=  |
| Writes neighborhood information for each grid point                   | PROC KRIGE2D | OUTNBHD= |
| Specifies plot display and options                                    | PROC KRIGE2D | PLOTS    |
| <b>Declaring the Role of Variables</b>                                |              |          |
| Specifies variables to define analysis subgroups                      | BY           |          |
| Specifies variable with observation labels                            | ID           |          |
| Specifies the variables to be predicted (kriged)                      | PREDICT      | VAR=     |
| Specifies the $x$ and $y$ coordinate variables in the DATA= data set  | COORDINATES  | XC= YC=  |
| Specifies the $x$ and $y$ coordinate variables in the GDATA= data set | GRID         | XC= YC=  |
| <b>Controlling the Prediction</b>                                     |              |          |
| Specifies the number of grid points in one-dimensional cases          | GRID         | NPTS=    |

Table 49.1 *continued*

| Task                                                        | Statement | Option      |
|-------------------------------------------------------------|-----------|-------------|
| <b>Controlling Kriging Neighborhoods</b>                    |           |             |
| Specifies the radius of a neighborhood for all grid points  | PREDICT   | RADIUS=     |
| Specifies the number of neighbors for all grid points       | PREDICT   | NUMPOINTS=  |
| Specifies the maximum of neighbors for all grid points      | PREDICT   | MAXPOINTS=  |
| Specifies the minimum of neighbors for all grid points      | PREDICT   | MINPOINTS=  |
| Specifies the action when maximum not met                   | PREDICT   | NODECREMENT |
| Specifies the action when minimum not met                   | PREDICT   | NOINCREMENT |
| <b>Controlling the Semivariogram Model</b>                  |           |             |
| Specifies an angle for an anisotropic model                 | MODEL     | ANGLE=      |
| Specifies a type with a functional form                     | MODEL     | FORM=       |
| Specifies an item store with correlation information        | RESTORE   | IN=         |
| Specifies a nugget effect                                   | MODEL     | NUGGET=     |
| Allows power exponent values outside [0,2)                  | MODEL     | POWNOBOUND  |
| Specifies a range parameter                                 | MODEL     | RANGE=      |
| Specifies a minor-major axis ratio for an anisotropic model | MODEL     | RATIO=      |
| Specifies a scale parameter                                 | MODEL     | SCALE=      |
| Specifies model and parameters from an item store           | MODEL     | STORESELECT |

## PROC KRIGE2D Statement

**PROC KRIGE2D** *options* ;

The PROC KRIGE2D statement invokes the KRIGE2D procedure. Table 49.2 summarizes the options available in the PROC KRIGE2D statement.

Table 49.2 PROC KRIGE2D Statement Options

| Option        | Description                                                               |
|---------------|---------------------------------------------------------------------------|
| DATA=         | Specifies input data set                                                  |
| IDGLOBAL      | Uses ascending observation numbers as observation labels across BY groups |
| IDNUM         | Uses observation number as observation labels                             |
| NOPRINT       | Suppresses the normal display of results                                  |
| OUTEST=       | Writes kriging predictions and standard errors                            |
| OUTNBHD=      | Writes neighborhood information for each grid point                       |
| PLOTS         | Specifies plot display and options                                        |
| PREDICTION    | Produces the kriging prediction plot                                      |
| SEMIVARIOGRAM | Produces the semivariogram used for the kriging prediction                |
| SINGULARMSG=  | Controls the number of warning messages displayed for a singular matrix   |

You can specify the following options in the PROC KRIGE2D statement.

**DATA=SAS-data-set**

specifies a SAS data set that contains the  $x$  and  $y$  coordinate variables and the **VAR=** variables in the **PREDICT** statement.

**IDGLOBAL**

specifies that ascending observation numbers be used across **BY** groups for the observation labels in the appropriate output data sets and the **OBSERVATIONS** plot, instead of resetting the observation number in the beginning of each **BY** group. The **IDGLOBAL** option is ignored if no **BY** variables are specified. Also, if you specify the **ID** statement, then the **IDGLOBAL** option is ignored unless you also specify the **IDNUM** option in the **PROC KRIGE2D** statement.

**IDNUM**

specifies that the observation number be used for the observation labels in the appropriate output data sets and the **OBSERVATIONS** plot. The **IDNUM** option takes effect when you specify the **ID** statement; otherwise, it is ignored.

**NOPRINT**

suppresses the normal display of results. The **NOPRINT** option is useful when you want only to create one or more output data sets with the procedure. **NOTE:** This option temporarily disables the Output Delivery System (ODS); see the section “**ODS Graphics**” on page 3845 for more information.

**OUTEST=SAS-data-set**

**OUTE=SAS-data-set**

specifies a SAS data set in which to store the kriging predictions, standard errors, and grid location. For details, see the section “**OUTEST=SAS-data-set**” on page 3843.

**OUTNBHD=SAS-data-set**

**OUTN=SAS-data-set**

specifies a SAS data set in which to store the neighborhood information for each grid point. Information is written to this data set only if one or more **PREDICT** statements have options that specify local kriging. For details, see the section “**OUTNBHD=SAS-data-set**” on page 3844.

**PLOTS** < (*global-plot-option*) > < = *plot-request* < (*options*) > >

**PLOTS** < (*global-plot-option*) > < = (*plot-request* < (*options*) > < ... *plot-request* < (*options*) > > >

controls the plots produced through ODS Graphics. When you specify only one plot request, you can omit the parentheses around the plot request. Here are some examples:

```
plots=none
plots=observ
plots=(observ(out1) prediction)
plots=(prediction(fill=pred line=se obs=grad) prediction(fill=se))
```

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;

proc krige2d data=thick;
 coordinates xc=East yc=North;
 predict var=thick r=60;
 model scale=7.4599 range=30.1111 form=gauss;
 grid x=0 to 100 by 10 y=0 to 100 by 10;
run;

ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

If ODS Graphics is enabled but you omitted the PLOTS option or have specified PLOTS=ALL, then PROC KRIGE2D produces a default plot for each MODEL statement of every PREDICT statement that you specify. The default PROC KRIGE2D plot displays a contour plot of the kriging prediction and the gradient of the kriging prediction standard error at every location of the prediction grid, in addition to empty circles that indicate the observation locations. See Figure 49.4 for an example of the default KRIGE2D plot.

The following *global-plot-option* is available:

#### ONLY

suppresses the default plot. Only plots that are specifically requested are displayed.

The following individual *plot-requests* and *plot options* are available:

#### ALL

produces all appropriate plots. You can specify other *options* with ALL. For example, to request the default plot and an additional plot of the predictions, specify PLOTS=(ALL PREDICTION).

#### EQUATE

specifies that all appropriate plots be produced in a way that the axes coordinates have equal size units.

#### NONE

suppresses all plots.

**OBSERVATIONS** <(observations-plot-options)>

**OBSERV** <(observations-plot-options)>

**OBS** <(observations-plot-options)>

produces the observed data plot. Only one observations plot is created if you specify the OBSERVATIONS option more than once within a PLOTS option.

The OBSERVATIONS option has the following suboptions:

**GRADIENT**

specifies that observations be displayed as circles colored by the observed measurement.

**LABEL** < (*label-option*) >

labels the observations. The label is the ID variable if the ID statement is specified; otherwise, it is the observation number. The *label-option* can be one of the following:

**EQ=number**

specifies that labels show for any observation whose value is equal to the specified *number*.

**MAX=number**

specifies that labels show for observations with values smaller than or equal to the specified *number*.

**MIN=number**

specifies that labels show for observations with values equal to or greater than the specified *number*.

If you specify multiple instances of the OBSERVATIONS option and you specify the LABEL suboption in any of those, then the resulting observations plot displays the observations labels. If more than one *label-option* is specified in multiple LABEL suboptions, then the prevailing *label-option* in the resulting OBSERVATIONS plot emerges by adhering to the choosing order: MIN, MAX, EQ.

**OUTLINE**

specifies that observations be displayed as circles with a border but with a completely transparent fill.

**OUTLINEGRADIENT**

is the same as OBSERVATIONS(GRADIENT) except that a border is shown around each observation.

**SHOWMISSING**

specifies that observations with missing values be displayed in addition to the observations with nonmissing values. By default, missing values locations are not shown on the plot. If you specify multiple instances of the OBSERVATIONS option and you specify the SHOWMISSING suboption in any of those, then the resulting observations plot displays the observations with missing values.

If you omit any of the GRADIENT, OUTLINE, and OUTLINEGRADIENT suboptions, the OUTLINEGRADIENT is the default suboption. If you specify multiple instances of the OBSERVATIONS option or multiple suboptions for OBSERVATIONS, then the resulting observations plot honors the last specified GRADIENT, OUTLINE, or OUTLINEGRADIENT suboption.

**PREDICTION** < (*prediction-plot-options*) >**PRED** < (*prediction-plot-options*) >

specifies that the kriging prediction plot be produced. You can specify the PREDICTION option multiple times in the same PLOTS option to request instances of plots with the following *prediction-plot-options*:

**ALPHA=number**

specifies a parameter to obtain the confidence level for constructing confidence limits based on the prediction standard error. The value of *number* must be between 0 and 1, and the confidence level is  $1 - \text{number}$ . The default is ALPHA=0.05; this corresponds to the confidence level of 95%, or about 1.96 times the prediction standard error. The ALPHA= suboption is used only for prediction plots in one dimension, and it is incompatible with the FILL and LINE suboptions.

**CLONLY**

specifies that only the confidence limits be shown in a prediction plot without the predicted values. This suboption can be useful for identifying confidence limits when the prediction standard error is small at the prediction locations. CLONLY is used only for prediction plots in one dimension, and it is incompatible with the FILL and LINE suboptions.

**CONNP**

specifies that grid points that you provide as individual prediction locations be connected with a line on the area map. This suboption is ignored when you have a single grid point, a prediction grid in two dimensions, or when you also specify the NOMAP suboption. The CONNP suboption is incompatible with the FILL and LINE suboptions.

**FILL=NONE | PRED | SE**

produces a surface plot for either the predicted values or the standard errors. FILL=SE is the default. However, if you omit the FILL suboption, the behavior depends on the LINE suboption as follows: If you specify LINE=NONE or entirely omit the LINE suboption, then the FILL suboption is set to its default value. If LINE=PRED or LINE=SE, then the FILL suboption is set to the same value as the LINE suboption.

**LINE=NONE | PRED | SE**

produces a contour line plot for either the predicted values or the standard errors. LINE=PRED is the default. However, if you omit the LINE suboption the behavior depends on the FILL suboption as follows: If you specify FILL=NONE or entirely omit the FILL suboption, then the LINE suboption is set to its default value. If FILL=PRED or FILL=SE, then the LINE suboption is set to the same value as the FILL suboption.

**NOMAP**

specifies that the prediction plot be produced without a map of the domain where you have observations. The NOMAP suboption is used in the case of prediction in one dimension or at individual points. It is incompatible with the FILL and LINE suboptions.

**OBS=obs-options**

produces an overlaid scatter plot of the observations in addition to the specified contour plots. The following *obs-options* are available:



**GRAD**

specifies that observations be displayed as circles colored by the observed measurement. The same color gradient displays the prediction surface and the observations. Observations where the prediction is close to the observed values have similar colors—the greater the contrast between the color of an observation and the surface, the larger the prediction standard error is at that point.

**LINEGRAD**

is the same as OBS=GRAD except that a border is shown around each observation. This option is useful for identifying the location of observations where the standard errors are small, because at these points the color of the observations and the color of the surface are indistinguishable.

**NONE**

specifies that no observations be displayed.

**OUTL**

specifies that observations be displayed as circles with a border but with a completely transparent fill.

OBS=NONE is the default when you specify a grid in two dimensions, and OBS=LINEGRAD is the default used in the area map when you have a grid in one dimension. However, the default PROC KRIGE2D plot for a surface grid displays the observations locations as outlines.

**SHOWD**

specifies that the horizontal axis in scatter plots of linear prediction grids show the distance between grid points instead of the grid points' coordinates. When the area map is displayed, the prediction locations are also connected with a line. In all other grid configurations the SHOWD suboption is ignored, and it is incompatible with the FILL and LINE suboptions.

**SHOWP**

specifies that the grid points in band plots of linear prediction grids be shown as marks on the band plot. In all other grid configurations the SHOWP suboption is ignored, and it is incompatible with the FILL and LINE suboptions.

**TYPE=BAND | SCAT**

requests a particular type of plot when you have a linear grid, regardless of the default PREDICTION plot behavior in this case. The TYPE suboption is incompatible with the FILL and LINE suboptions.

If you specify multiple instances of the ALPHA, FILL, LINE, OBS, or TYPE suboptions in the same PREDICTION option, then the resulting predictions plot honors the last value specified for any of the suboptions. Any combination where you specify FILL=NONE and LINE=NONE is not available. When the prediction grid is in two dimensions, only the FILL, LINE, and OBS suboptions apply. If you specify incompatible suboptions in the same PREDICTION plot, then the plot instance is skipped.

The PREDICTION option produces a surface or contour line plot for grids in two dimensions and a band plot or scatter plot with error bars for grids in one dimension or individual points. In two dimensions the plot illustrates the predicted values and prediction error at each grid point.

By default, when you specify a linear grid with fewer than 10 points, PROC KRIGE2D produces a PREDICTION scatter plot for each one of the prediction grid points. For 10 or more points in a linear grid, the PREDICTION plot is a band plot of the predicted means and the confidence limits at the 95% confidence level. You can override the default behavior in linear grids with the TYPE suboption. Prediction at individual locations always produces a PREDICTION scatter plot.

In cases of prediction in one dimension or at individual points, an area map is produced that shows the observations and the grid points. Band plots of linear grids display the grid points as a line on the map. When you specify individual prediction locations, the grid points are indicated with marks on the area map. The area map appears on the side of the prediction band plot or scatter plot, unless you specify the NOMAP suboption. You can also label the individual grid points or the ends of linear grid segments with the LABEL option of the GRID statement.

**SEMIVARIOGRAM** < (*semivar-plot-option*) >

**SEMIVAR** < (*semivar-plot-option*) >

specifies that the semivariogram used for the kriging prediction be produced. You can use the following *semivar-plot-option*:

**MAXD=number**

specifies a positive value for the upper limit of the semivariogram horizontal axis of distance. The SEMIVARIOGRAM plot extends by default to a distance that depends on the correlation model range. You can use the MAXD= option to adjust the default maximum distance value for the plot.

The SEMIVARIOGRAM option produces a plot for each correlation model that you specify for your prediction tasks. In an anisotropic case, the plot is not produced if you assign different anisotropy angles for different model components. The only exception is when you specify zonal components at right angles with the nonzonal model components. Also, the SEMIVARIOGRAM option is ignored for models that consist of purely zonal components.

**SINGULARMSG=number**

**SMSG=number**

controls the number of warning messages displayed for a singular matrix. When local kriging is performed, a separate kriging system is solved for each grid point. Anytime a singular matrix is encountered, a warning message is displayed up to a total of *number* times. The default is SINGULARMSG=10.

---

## BY Statement

**BY** *variables* ;

You can specify a BY statement with PROC KRIGE2D to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the KRIGE2D procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

---

## COORDINATES Statement

**COORDINATES** | **COORD** *coordinate-variables* ;

The following two options specify the names of the variables in the **DATA=** data set that contains the values of the  $x$  and  $y$  coordinates of the data.

Only one COORDINATES statement is allowed, and it is applied to all **PREDICT** statements. In other words, it is assumed that all the **VAR=** variables in all **PREDICT** statements have the same  $x$  and  $y$  coordinates.

This is not a limitation. Since each **VAR=** variable is processed separately, observations for which the current **VAR=** variable is missing are excluded. With the next **VAR=** variable, the entire data are read again, this time excluding missing values in this next variable. Hence, a single run of PROC KRIGE2D can be used for variables measured at different locations without overlap.

**XCOORD=** (*variable-name*)

**XC=** (*variable-name*)

specifies the name of the variable that contains the  $x$  coordinate of the data locations in the **DATA=** data set.

**YCOORD=** (*variable-name*)

**YC=** (*variable-name*)

specifies the name of the variable that contains the  $y$  coordinate of the data locations in the **DATA=** data set.

---

## GRID Statement

**GRID** *grid-options* </ option > ;

The GRID statement specifies the grid of spatial locations for kriging predictions. The grid specification is applied to all **PREDICT** and **MODEL** statements. Specify the grid in one of the following three ways:

- Specify the  $x$  and  $y$  coordinates explicitly for a grid in two dimensions.
- Specify the NPTS= option in addition to the  $x$  and  $y$  coordinates to define a grid of individual points or in one dimension.
- Specify the coordinates by using a SAS data set for a grid of individual points or in one dimension.

The GRID statement has the following *grid-options*:

**NPTS=number**

**NPTS=ALL**

controls specification of a grid in one dimension or a grid of individual prediction locations.

When you specify the NPTS=*number* option and the coordinates of two points in the GRIDDATA= data set or in both the X= and Y= options, you request a linear prediction grid. Its direction is across the line defined by the specified points. The grid size is equal to the *number* of points that you specify in the NPTS= option, where  $number \geq 2$ .

When you specify the NPTS=ALL option and the coordinates for any number of points in the GRIDDATA= data set or in each of the X= and Y= options, the KRIGE2D procedure performs prediction only at the specified individual locations. Use the NPTS=ALL option to examine a set of individual points anywhere on the XY plane or to specify a custom grid in one dimension.

If the number of  $x$  coordinates and the number of  $y$  coordinates in the X= and Y= options, respectively, are different, then the NPTS= option is ignored; in that case, a two-dimensional grid is used according to the specified X= and Y= options.

If you specify a prediction grid with any number of points other than two in the GRIDDATA= data set, then the option NPTS=ALL has the same effect as omitting the NPTS= option.

**X=number**

**X= $x_1, \dots, x_m$**

**X= $x_1$  to  $x_m$**

**X= $x_1$  to  $x_m$  by  $\delta x$**

specifies the  $x$  coordinate of the grid locations.

**Y=number**

**Y= $y_1, \dots, y_m$**

**Y= $y_1$  to  $y_m$**

**Y= $y_1$  to  $y_m$  by  $\delta y$**

specifies the  $y$  coordinate of the grid locations.

Use the X= and Y= options of the GRID statement to specify a grid in one or two dimensions, or a grid of individual prediction locations.

For example, the following two GRID statements are equivalent.

```
grid x=1,2,3,4,5 y=0,2,4,6,8,10;
```

```
grid x=1 to 5 y=0 to 10 by 2;
```

In the following example, the first GRID statement produces a grid in two dimensions. The second statement produces predictions only for the four individual points at the locations (1,0), (2,5), (3,7), and (4,10) on the XY plane.

```
grid x=1 to 4 y=0,5,7,10;
```

```
grid x=1 to 4 y=0,5,7,10 npts=all;
```

In the next example, the first GRID statement specifies a 2-by-2 grid in two dimensions. The second GRID statement specifies a linear grid of eight points. The grid is in the direction of the line defined by the specified points (2,8) and (3,5) on the XY plane and it extends between these two points.

```
grid x=2,3 y=8,5;
```

```
grid x=2,3 y=8,5 npts=8;
```

The last example shows a GRID statement that specifies a linear grid made of seven points across the Y axis. In this case, the syntax is sufficient to fully define a linear grid without the NPTS= option.

```
grid x=5 y=3 to 9;
```

To specify grid locations from a SAS data set, you must provide the name of the data set and the variables that contain the values of the  $x$  and  $y$  coordinates.

**GRIDDATA=***SAS-data-set*

**GDATA=***SAS-data-set*

specifies a SAS data set that contains the  $x$  and  $y$  grid coordinates. Use the GRIDDATA= option of the GRID statement to specify a grid in one dimension or a grid of individual prediction locations.

**XCOORD=** (*variable-name*)

**XC=** (*variable-name*)

specifies the name of the variable that contains the  $x$  coordinate of the grid locations in the **GRID-DATA=** data set.

**YCOORD=** (*variable-name*)

**YC=** (*variable-name*)

specifies the name of the variable that contains the  $y$  coordinate of the grid locations in the **GRID-DATA=** data set.

You can specify the following option in the GRID statement after a slash (/):

**LABEL** < (*suboption*) > = (*character-list*)

specifies labels to tag grid points in prediction plots when you use grids in one dimension. You can specify one or more such labels as quoted strings in the *character-list*.

When the number of labels in the *character-list* exceeds the number of points in your grid, the labels in the list are used sequentially and any labels in excess are ignored. When the number of labels in the *character-list* is smaller than the number of points in your grid, the behavior is as follows:

- If an area map is included in the prediction plot, then blank labels are assigned to the remaining nonlabeled grid points on the map.
- For the prediction band and scatter plots, the coordinates of nonlabeled grid points are automatically assigned as their labels.

If the grid points are collinear and the horizontal axis displays distance, then two labels appear by default in the prediction plot. These are assigned to the first and the last points of the grid to help identify the ends of the linear grid segment on the plot map. This label pair is shown only when the plot includes an area map. Specifically, the two labels appear when you request prediction band plots, or prediction scatter plots for which you specify the **PREDICTION(SHOWD)** suboption, if applicable. The two labels do not appear if you specify explicitly the **NOMAP** suboption in the **PLOTS=PRED** option.

The two labels have default values, unless you choose to specify your own labels with the **LABEL=** option. If you specify more than two labels in the *character-list* under these conditions, then only the first and last labels in the list are used; any additional labels in between are ignored.

The **LABEL=** option has the following *suboption*:

#### **ALL**

specifies that all individual points in the grid be assigned sequentially the labels you specify in the **LABEL(ALL)=** option when the **PREDICTION(SHOWD)** suboption is applicable and specified in a prediction scatter plot. In all other cases, the **ALL** suboption is ignored.

The **ALL** suboption enables you to override the default behavior when the **PREDICTION(SHOWD)** suboption is specified (the default behavior is to display labels only for the first and last grid points). As a result, you can use the **ALL** suboption to label grid points regardless of whether you specify the **NOMAP** suboption in the **PLOTS=PRED** option.

The **LABEL=** option is ignored when you produce prediction plots of grids in two dimensions.

---

## **ID Statement**

**ID** *variable* ;

The **ID** statement specifies which variable to include for identification of the observations in the **OUTNBHD=** output data set. The **ID** statement variable is also used for the labels and tool tips in the **OBSERVATIONS** plot and the tool tips in the **PREDICTION** plot.

In the **KRIGE2D** procedure you can specify only one **ID** variable in the **ID** statement. If no **ID** statement is given, then **PROC KRIGE2D** uses the observation number in the data sets and the plots.

## PREDICT Statement

**PREDICT** | **PRED** | **P** *predict-options* ;

You can specify the following options in a PREDICT statement.

**MAXPOINTS=number**

**MAXP=number**

**MAX=number**

specifies the maximum number of data points in a neighborhood. You specify this option in conjunction with the **RADIUS=** option. When the number of data points in the neighborhood formed at a given grid point by the **RADIUS=** option is greater than the **MAXPOINTS=** value, the **RADIUS=** value is decreased just enough to honor the **MAXPOINTS=** value unless you specify the **NODECREMENT** option. The default is to include all data points within the specified **RADIUS=** value. Neighborhoods with very large numbers of data points might lead to unnecessarily slow execution times and potential lack of memory issues, depending on the problem setup and your computational resources. In that case, you could use the **MAXPOINTS=** option to set a cap for your neighborhood size. For details about numerical considerations, see the section “[Computational Resources](#)” on page 3843. Unless the **RADIUS=** option is also specified, when the **MAXPOINTS=** and **NUMPOINTS=** options are specified in the same **PREDICT** statement the **MAXPOINTS=** option is ignored.

**MINPOINTS=number**

**MINP=number**

**MIN=number**

specifies the minimum number of data points in a neighborhood. You specify this option in conjunction with the **RADIUS=** option. When the number of data points in the neighborhood formed at a given grid point by the **RADIUS=** option is less than the **MINPOINTS=** value, the **RADIUS=** value is increased just enough to honor the **MINPOINTS=** value unless you specify the **NOINCREMENT** option. The default is **MINPOINTS=20**. When enough data are available, you might improve prediction if you increase this value. When the **MINPOINTS=** and **NUMPOINTS=** options are specified in the same **PREDICT** statement, the **MINPOINTS=** option is set to the value of **NUMPOINTS=**.

**NODECREMENT** | **NODECR**

requests that the **RADIUS=** value not be decremented when the **MAXPOINTS=** value is exceeded at a grid point. This option is relevant only when you specify both a **RADIUS=** value and a **MAXPOINTS=** value. In this case, when the number of points in the neighborhood constructed from the **RADIUS=** specification is greater than the **MAXPOINTS=** value, the **RADIUS=** value is decremented enough to honor the **MAXPOINTS=** value, and the kriging system is solved for this grid point. If you specify the **NODECREMENT** option, no decrementing is done, prediction is skipped at this grid point, and a message is written to the log.

**NOINCREMENT** | **NOINCR**

requests that the **RADIUS=** value not be incremented when the **MINPOINTS=** value is not met at a grid point. This option is relevant only when you specify both a **RADIUS=** value and a **MINPOINTS=** number. In this case, when the number of points in the neighborhood constructed from the **RADIUS=** specification is less than the **MINPOINTS=** value, the **RADIUS=** value is incremented enough to honor the **MINPOINTS=** value, and the kriging system is solved for this grid point. If you specify the **NOINCREMENT** option, no incrementing is done, prediction is skipped at this grid point, and a message is written to the log.

**NUMPOINTS=***number*

**NPOINTS=***number*

**NPTS=***number*

**NP=***number*

specifies the exact size of a neighborhood. This option is incompatible with all other **PREDICT** statement options that control the neighborhood; it must appear by itself. In particular, if you specify both **NUMPOINTS=** and the **RADIUS=** option in the same **PREDICT** statement, then **RADIUS=** is honored, instead. In this event the value of the **MINPOINTS=** option is set to **NUMPOINTS=**, and the value of the **MAXPOINTS=** option is set to default, regardless of whether these options have been specified or not. If you specify any of the **MINPOINTS=** or **MAXPOINTS=** option without the **RADIUS=** option in the same **PREDICT** statement as **NUMPOINTS=**, then the **NUMPOINTS=** option is honored.

**RADIUS=***number*

**R=***number*

specifies the radius to use in a local kriging regression. When you specify this option, a separate kriging system is solved at each grid point by finding the neighborhood of this grid point that consists of all data points within the distance specified by the **RADIUS=** value. Thus, you can avoid unnecessary computational burden in your analysis by specifying the **RADIUS=** value to include data points situated within the extent of your problem's spatial correlation. For additional control on the neighborhood, see the **MAXPOINTS=** and **MINPOINTS=** options. When you specify the **RADIUS=** and **NUMPOINTS=** options in the same **PREDICT** statement, then **RADIUS=** is honored.

**VAR=** *variable-name*

specifies the single numeric variable used in the kriging system.

---

## MODEL Statement

**MODEL** *model-options* ;

The **MODEL** statement specifies details about the correlation model that you use in the kriging system for prediction. The specified model is used in the kriging system defined by the most previous **PREDICT** statement. You can specify a semivariogram or covariance model in three ways:

- You specify the required parameters **SCALE**, **RANGE**, **FORM**, and **SMOOTH** (if you specify the **MATERN** form), and possibly the optional parameters **NUGGET**, **ANGLE**, and **RATIO**, explicitly in the **MODEL** statement.
- You specify an **MDATA=** data set. This data set contains variables that correspond to the required parameters **SCALE**, **RANGE**, **FORM** and **SMOOTH** (if you specify the **MATERN** form), and optionally variables for the **NUGGET**, **ANGLE**, and **RATIO** parameters.
- You can specify an input item store in the **RESTORE** statement. The item store contains one or more correlation models for one or more direction angles. You can specify these models in the **STORESELECT** option of the **MODEL** statement to perform a prediction task.



The three methods are mutually exclusive: you specify all parameters explicitly, they are all read from the `MDATA=` data set, or you select a model and its parameters from an input item store.

Table 49.3 summarizes the options available in the MODEL statement.

**Table 49.3** MODEL Statement Options

| Option      | Description                                                                      |
|-------------|----------------------------------------------------------------------------------|
| ANGLE=      | Specifies the angle of the major axis                                            |
| FORM=       | Specifies the functional form (type)                                             |
| MDATA=      | Specifies the input data set containing parameter values                         |
| NUGGET=     | Specifies the nugget effect for the model                                        |
| POWNOBOUND  | Allows values for the power model exponent parameter outside the range of [0, 2) |
| RANGE=      | Specifies the range parameter                                                    |
| RATIO=      | Specifies the ratio of the length of the minor axis                              |
| SCALE=      | Specifies the scale parameter                                                    |
| SINGULAR=   | Gives the singularity criterion for solving kriging systems                      |
| SMOOTH=     | Specifies the smoothness parameter                                               |
| STORESELECT | Uses the information from an input item store                                    |

You can use the following *model-options* with the MODEL statement:

**ANGLE=***angle*

**ANGLE=**(*angle1*, ..., *anglek*)

specifies the angle of the major axis for anisotropic models, measured in degrees clockwise from the N-S axis. The default is ANGLE=0.

In the case of a nested semivariogram model with  $k$  nestings, you have the following two ways to specify the anisotropy major axis: you can specify only one *angle* which is then applied to all nested forms, or you can specify one angle for each of the  $k$  nestings.

**NOTE:** The syntax makes it possible to specify different angles for different forms of the nested model, but this practice is rarely used.

**FORM=***form*

**FORM=**(*form1*, ..., *formk*)

specifies the functional form (type) of the semivariogram model. Use the syntax with the single *form* to specify a non-nested model. Use the syntax with forms *form<sub>i</sub>*,  $i = 1, \dots, k$ , to specify a nested model with  $k$  structures. Each of the forms can be any of the following:

**CUBIC | EXPONENTIAL | GAUSSIAN | MATERN |  
PENTASPHERICAL | POWER | SINEHOLEEFFECT | SPHERICAL**

**CUB | EXP | GAU | MAT | PEN | POW | SHE | SPH**

Usage examples follow.

For example, the syntax

```
FORM=GAU
```

specifies a model with a single Gaussian structure. Also, the syntax

```
FORM= (EXP , SHE , MAT)
```

specifies a nested model with an exponential, a sine hole effect, and a Matérn structure. Finally

```
FORM= (EXP , EXP)
```

specifies a nested model with two structures both of which are exponential.

**NOTE:** In the documentation, models are named either by using their full names or by using the first three letters of their structures. Also, the names of different structures in a nested model are separated by a hyphen (-). According to this convention, the previous examples illustrate how to specify a GAU, an EXP-SHE-MAT, and an EXP-EXP model, respectively, with the FORM= option.

All the supported model forms have two parameters specified by the SCALE= and RANGE= options, except for the MATERN model which has a third parameter specified by the SMOOTH= option. A FORM= value is required, unless you specify the MDATA= option or the STORESELECT option.

Computation of the MATERN covariance is numerically demanding. As a result, predictions that use Matérn covariance structures can be time-consuming.

See the section “Theoretical Semivariogram Models” on page 3823 for details about how the FORM= forms are determined.

#### **MDATA=SAS-data-set**

specifies the input data set that contains parameter values for the covariance or semivariogram model. The MDATA= option cannot be combined with any of the FORM= or STORESELECT options.

The MDATA= data set must contain variables named SCALE, RANGE, and FORM, and it can optionally contain variables NUGGET, ANGLE, and RATIO. If you specify the MATERN form, then you must also include a variable named SMOOTH in the MDATA= data set.

The FORM variable must be a character variable, and it can assume only the values allowed in the explicit FORM= syntax described previously. The RANGE, SCALE and SMOOTH variables must be numeric. The optional variables ANGLE, RATIO, and NUGGET must also be numeric if present.

The number of observations present in the MDATA= data set corresponds to the level of nesting of the covariance or semivariogram model. For example, to specify a non-nested model that uses a spherical covariance, an MDATA= data set might be given by the following statement:

```
data mdl;
 input scale range form $;
 datalines;
 25 10 SPH
run;
```

The PROC KRIGE2D statement to use the `MDATA=` specification is of the form shown in the following:

```
proc krige2d data=...;
 predict var=...;
 model mdata=mdl;
run;
```

This is equivalent to the following explicit specification of the covariance model parameters:

```
proc krige2d data=...;
 predict var=...;
 model scale=25 range=10 form=sph;
run;
```

The following `MDATA=` data set is an example of an anisotropic nested model:

```
data mdl;
 input scale range form $ nugget angle ratio;
 datalines;
 20 8 SPH 5 35 0.7 .
 12 3 MAT 5 0 0.8 2.8
 4 1 GAU 5 45 0.5 .
 ;
```

This is equivalent to the following explicit specification of the covariance model parameters:

```
proc krige2d data=...;
 predict var=...;
 model scale=(20,12,4) range=(8,3,1) form=(SPH,MAT,GAU)
 angle=(35,0,45) ratio=(0.7,0.8,0.5) nugget=5 smooth=2.8;
run;
```

This example is somewhat artificial in that it is usually hard to detect different anisotropy directions and ratios for different nestings by using an empirical semivariogram. **NOTE:** The NUGGET variable value is the same for all nestings. This is always the case; the nugget effect is a single additive term for all models. For further details, see the section “[The Nugget Effect](#)” on page 3830.

The example also shows that if you specify a MATERN form in the nested model, then the SMOOTH variable must be specified for all nestings in the `MDATA=` data set. You simply specify the SMOOTH value as missing for nestings other than MATERN.

#### **NUGGET=***number*

specifies the nugget effect for the model. The nugget effect is due to a discontinuity in the semivariogram as determined by plotting the sample semivariogram. For details, see the section “[The Nugget Effect](#)” on page 3830 and Chapter 102, “[The VARIOGRAM Procedure.](#)” For models without any nugget effect, this option is left out; the default is `NUGGET=0`.

**POWNOBOUND**

specifies that values for the power model exponent parameter outside the range of  $[0, 2)$  be allowed. The POWNOBOUND option applies only when you specify a power form in the MODEL statement.

Power models yield permissible covariance models only when the exponent parameter is nonnegative and less than 2. By default, PROC KRIGE2D produces an error if you specify a negative power exponent or one that is equal to or larger than 2 in the RANGE= option of the MODEL statement.

See the section “[The Power Semivariogram Model](#)” on page 3828 for more details about the power model form and its exponent parameter.

**RANGE=range****RANGE=(range1, ..., rangek)**

specifies the range parameter in semivariogram models. If you have anisotropy, you must specify the range of the major anisotropy axis, or the range of the minor anisotropy axis for any zonal components. In the case of a nested semivariogram model with  $k$  nestings, you must specify a range for each nested structure.

The range parameter has units of distance, and it is related to the correlation scale for the underlying spatial process.

**NOTE:** If you specify this parameter for a power model, then it does not correspond to a range. For power models, the parameter you specify in the RANGE option is a dimensionless power exponent whose value must range within  $[0, 2)$  so that the power model is a valid semivariance function. See also the POWNOBOUND option of the MODEL statement.

See the section “[Theoretical Semivariogram Models](#)” on page 3823 for details about how the RANGE= values are determined.

**RATIO=ratio****RATIO=(ratio1, ..., ratiok)**

specifies the ratio of the length of the minor axis to the length of the major axis for anisotropic models. The value of the RATIO= option must be between 0 and 1. An exception is the case of zonal anisotropy, where the ratio of zonal components must be designated by a very large number for the RATIO= option. For further details, see the section “[Zonal Anisotropy](#)” on page 3835.

In the case of a nested semivariogram model with  $k$  nestings, you can specify a ratio for each nesting. The default is RATIO=1.

**SCALE=scale****SCALE=(scale1, ..., scalek)**

specifies the scale parameter in semivariogram models. In the case of a nested semivariogram model with  $k$  nestings, you must specify a scale for each nesting.

The scale parameter is the multiplicative factor in all supported models; it has the same units as the variance of the VAR= variable in the preceding PREDICT statement.

In power models the SCALE= parameter does not correspond to a sill because the power model has no sill. Instead, PROC KRIGE2D uses the SCALE= option to designate the slope (or scaling factor) in power model forms. The power model slope has the same variance units as the VAR= variable.

See the section “[Theoretical Semivariogram Models](#)” on page 3823 for details about how the SCALE= values are determined.

**SINGULAR=number**

gives the singularity criterion for solving kriging systems. The larger the value of the SINGULAR= option, the easier it is for a kriging system to be declared singular. The default is SINGULAR=1E-7. See the section “[Ordinary Kriging](#)” on page 3840 for more detailed information.

**SMOOTH=smooth****SMOOTH=(smooth1, ..., smoothm)**

specifies the smoothness parameter  $\nu > 0$  in the Matérn type of semivariance structures. The special case  $\nu = 0.5$  is equivalent to the exponential model, whereas  $\nu \rightarrow \infty$  gives the Gaussian model.

When you specify  $m$  different MATERN forms in the **FORM=** option, you must also provide  $m$  smoothness values in the SMOOTH option. If you must specify more than one smoothness value, the values are assigned sequentially to the MATERN nestings in the order the nestings are specified. If you specify more smoothness values than necessary, then values in excess are ignored.

**STORESELECT(ssel-options)****SSEL(ssel-options)**

specifies that information from an input item store be used for the prediction. You cannot combine the STORESELECT option with any of the **FORM=** or **MDATA=** options. The STORESELECT option has the following *ssel-options*:

**TYPE=field-type**

specifies whether to perform isotropic or anisotropic prediction. You can choose the *field-type* from one of the following:

**ISO**

specifies an isotropic field for the prediction.

**ANIGEO | GEO**

specifies a field with geometric anisotropy for the prediction.

**ANIZON(zonal-form1, ..., zonal-formn)****ZON(zonal-form1, ..., zonal-formn)**

specifies a field with zonal anisotropy for the prediction. Each *zonal-formi*,  $i = 1, \dots, n$ , can be any of the following:

**CUB | EXP | GAU | MAT | PEN | POW | SHE | SPH**

Each *zonal-formi*,  $i = 1, \dots, n$ , is a structure in the purely zonal component of the correlation model in the direction angle of the minor anisotropy axis. For this reason, when you specify the TYPE=ANIZON suboption you must also specify the nonzonal component of the correlation model in the **MODEL=** suboption of the STORESELECT option.

Assume the nonzonal component has  $k$  structures; these are common across all directions and each one has the same scale in all directions. In that sense, you use the TYPE=ANIZON suboption to specify only the  $n$  zonal anisotropy structures of an input store ( $k + n$ )-structure nested model in the direction angle of the minor anisotropy axis.

Given this specification,  $k + n$  must be up to the maximum number of nested model structures that is supported by the item store. See also the **MODEL=** suboption of the STORESELECT option.

In conclusion, you can use an input item store for prediction with zonal anisotropy if you know that every structure in the nonzonal model component has the same scale across all directions. When this condition does not apply for the item store models, specify the model parameters explicitly in the **MODEL** statement. For more details, see the examples in the section “[Zonal Anisotropy](#)” on page 3835.

Computation of the MATERN covariance is numerically demanding. As a result, predictions that use Matérn covariance structures can be time-consuming.

If you omit the **TYPE=** option, the default behavior is **TYPE=ISO** when the input item store contains information for only one angle or for the omnidirectional case. If you specify an item store with information for more than one direction, then the default behavior is **TYPE=ANIGEO**.

When you specify **TYPE=ISO** to request isotropic analysis in the presence of an item store with information for multiple directions, you must specify the **ANGLEID=** suboption of the **STORESELECT** option with one argument. This argument specifies which of the direction angles information to use for the isotropic analysis.

When you indicate the presence of anisotropy with the **TYPE=ANIGEO** or **TYPE=ANIZON** suboptions of the **STORESELECT** option, the following conditions apply:

- You must specify the **ANGLEID=** suboption of the **STORESELECT** option to designate the major and minor anisotropy axes. See the **ANGLEID=** suboption of the **STORESELECT** option for details.
- – For **TYPE=ANIGEO**, ensure that you have the same scale in all anisotropy directions.
- – For **TYPE=ANIZON**, ensure that the nonzonal component scale is the same in all anisotropy directions.

If you import a nested model, these rules also apply to each one of the nested structures.

- Model ranges in the major anisotropy axis must be longer than ranges in the minor anisotropy axis.
- Any Matérn covariance structure must maintain its smoothness parameter value in all anisotropy directions.

**ANGLEID=***angleid1*

**ANGLEID=**(*angleid1*, *angleid2*)

specifies which direction angles in the input item store be used for prediction. The angles are identified by the corresponding number in the **AngleID** column of the “Store Models Information” table, or by the **AngleID** parameter in the table title when you specify the **INFO(DETAILS)** option in the **RESTORE** statement.

If you request isotropic prediction in the **TYPE=** suboption of the **STORESELECT** option and the item store has omnidirectional contents or information about only one angle, then the **ANGLEID=** option is ignored. The prediction input comes from the omnidirectional information. In the case of a single angle, you still perform isotropic prediction and the model parameters are provided by the model in the single direction angle in the item store. However, if the item store contains information for more than one angle, then you must specify one angle ID in *angleid1*. The model information from the corresponding angle is then used in your isotropic prediction.

When you specify an anisotropic prediction in the **TYPE=** option of the **STORESELECT** option, you need to have information about two perpendicular direction angles. One of them is the

major and the other is the minor anisotropy axis. You must always specify the major anisotropy axis angle ID in *angleid1* and the minor anisotropy axis angle ID in *angleid2*. This means that the range parameters of the model forms in the angle designated by the *angleid1* need to be larger than the corresponding ranges of the forms in the angle designated by the *angleid2*. Conveniently, if the item store has only two angles, then you only need to specify the ID *angleid1* of the major anisotropy axis angle. If the item store has only one angle, then you cannot perform anisotropic prediction with input from the item store.

**NOTE:** You can perform geometric anisotropic analysis even if the item store does not contain information about a direction that is perpendicular to the one specified by *angleid1*. This is possible due to the geometry of the ellipse. In particular, when you specify the major axis with *angleid1* and an angle ID for a second direction with a corresponding smaller range, then PROC KRIGE2D automatically computes the minor anisotropy axis range and the necessary range ratio parameter.

Anisotropic analysis is not possible when you specify instances of the same angle in the input item store. It is possible that PROC VARIOGRAM produces an item store in which two or more directions can be the same if their corresponding correlation models were obtained for different angle tolerances or bandwidths in the VARIOGRAM procedure. Consequently, you cannot specify anisotropic prediction if the input store contains only two angles that are the same or if you specify *angleid1* and *angleid2* that correspond to equal angles.

**MODEL=***form*

**MODEL=**(*form1*, . . . , *formk*)

specifies the theoretical semivariogram model selection to use for the prediction. Use any combination of one, two, or three forms to describe a model in the input item store because up to three nested structures are supported. Each *form<sub>i</sub>*,  $i = 1, \dots, k$ , can be any of the following:

**CUB | EXP | GAU | MAT | PEN | POW | SHE | SPH**

Computation of the MATERN covariance is numerically demanding. As a result, predictions that use Matérn covariance structures can be time-consuming.

All fitted models that are stored in the input item store contain information about their component parameters and also about the nugget effect if any. The KRIGE2D procedure retrieves this information when you make a model selection in the MODEL= option, and you do not need to individually specify a nugget effect or any other parameter of the model.

By default, the model that is ranked first among the models for a given angle in the item store is used for the prediction task. If more than one model is available in the item store, then you can specify the MODEL= option to use a different model for the prediction.

In an anisotropic prediction, the default selection is the model that is ranked first in the direction angle of the major anisotropy axis. If you specify the TYPE=ANIGEO option, then a model that consists of identical structures needs to be present in the selected minor anisotropy axis angle in the item store. If you specify the TYPE=ANIZON option, then a model with the exact same first  $k$  structures must be present in the selected minor anisotropy axis angle, and it must feature at least one more structure as a zonal component. The zonal component is specified separately in the TYPE=ANIZON suboption of the STORESELECT option. Consequently, remember that in zonal anisotropy the MODEL= suboption designates only the nonzonal component of the correlation model in the minor anisotropy axis direction. In all, if there are  $k$  common structures



and  $n$  structures in the purely zonal component, then  $k + n$  must be up to the maximum number of nested model structures that is supported by the item store.

In comparison to the other two ways of specifying a correlation model in PROC KRIGE2D, the STORESELECT option is quite different because you can avoid explicit specification of all parameter values of a model. When you specify the STORESELECT option, then the corresponding scale, range, nugget effect, and smoothness (if appropriate) parameter values are invoked as saved attributes of the model that you select from the item store.

In the case of anisotropy, you specify the angles indirectly with the ANGLEID= option of the STORESELECT option, and the ratios are computed implicitly by using the selected model ranges. Explore how to specify valid anisotropical models imported from an input item store with the two examples that follow.

In the first example, assume the input item store InStoreGeo contains exponential models in the angles  $\theta_1 = 0^\circ$ ,  $\theta_2 = 45^\circ$ , and  $\theta_3 = 90^\circ$ . You know in advance that all models have the same scale  $c_1 = c_2 = c_3$  across these directions and that the respective ranges are  $a_1 = 15$ ,  $a_2 = 20$ , and  $a_3 = 25$  in distance units. Hence, you have a case of geometric anisotropy where the major anisotropy axis is in the direction of angle  $\theta_3$  and the minor anisotropy axis is in the direction of angle  $\theta_1$ . The following statements in PROC KRIGE2D use the information in the item store InStoreGeo to perform simulation under the assumption of geometric anisotropy:

```
proc krig2d data=...;
 restore in=InStoreGeo;
 predict var=...;
 model storeselect(model=exp type=anigeo angleid=(3,1));
run;
```

For the second example, assume a case of zonal anisotropy. Consider the input item store InStoreZon, which contains models in the two angles,  $\theta_1 = 30^\circ$  and  $\theta_2 = 120^\circ$ . Specifically, in  $\theta_1$  you have an exponential-spherical model: the exponential structure has scale  $c_{1E} = 3$  and range  $a_{1E} = 10$ ; the spherical structure has scale  $c_{1S} = 1$  and range  $a_{1S} = 6$ . In direction  $\theta_2$  you have an exponential model with scale  $c_{1E} = 3$  and range  $a_{1E} = 12$ . Hence, the zonal anisotropy major axis is in the direction of the lowest total variance, which is in angle  $\theta_2$ ; then, the minor axis is in the direction of angle  $\theta_1$ . The following statements in PROC KRIGE2D use the information in the store InStoreZon to perform prediction under the assumption of zonal anisotropy:

```
proc krig2d data=...;
 restore in=InStoreZon;
 predict var=...;
 model storeselect(model=exp type=anizon(sph) angleid=(2,1));
run;
```

---

## RESTORE Statement

**RESTORE IN=store-name** </option> ;

The RESTORE statement specifies an item store that provides spatial correlation model input for the PROC KRIGE2D prediction tasks. An item store is a binary file defined by the SAS System. You cannot mod-



ify the contents of an item store. The KRIGE2D procedure can use only item stores created by PROC VARIOGRAM.

Item stores enable you to use saved correlation models without having to repeat specification of these models in the **MODEL** statement. In principle, an item store contains the chosen model from a model fitting process in PROC VARIOGRAM. If more than one model form is fitted, then all successful fits are included in the item store. In this case, you can choose any of the available models to use for prediction with the **STORESELECT(MODEL=)** option in the **MODEL** statement. Successfully fitted models might include questionable fits, which are so flagged when you specify the **INFO** option to display model names.

The *store-name* is a usual one- or two-level SAS name, as for SAS data sets. If you specify a one-level name, then the item store resides in the WORK library and is deleted at the end of the SAS session. Since item stores are often used for postprocessing tasks, typical usage specifies a two-level name of the form *libname.membername*.

When you specify the **RESTORE** statement, the default output contains some general information about the input item store. This information includes the store name, label (if assigned), the data set that was used to create the store, **BY** group information, the procedure that created the store, and the creation date.

You can specify the following option in the **RESTORE** statement after a slash (/):

**INFO** < ( *info-options* ) >

specifies that additional information about the input item store be printed. This information is provided in two ODS tables. One table displays the variables in the item store, in addition to the mean and standard deviation for each of them. These statistics are based on the observations that were used to produce the store results. The second table shows the model on top of the list of all fitted models for each direction angle in the item store. The **INFO** option has the following *info-options*:

**DETAILS**

**DET**

specifies that more detailed information be displayed about the input item store. This option produces the full list of models for each direction angle in the item store, in addition to the model equivalence class. For more information about classes of equivalence, see the section “Classes of Equivalence” on page 8634 in the VARIOGRAM procedure. The **DETAILS** option is ignored if the input item store contains information about a single fitted model.

**ONLY**

specifies that only information about the input item store without any prediction tasks be displayed.

When you specify an input item store with the **RESTORE** statement in PROC KRIGE2D, all the **DATA=** input data set variables must match input item store variables. If there are **BY** groups in the input **DATA=** set or in the input **RESTORE** variables, then PROC KRIGE2D handles the different cases as follows:

- If both PROC KRIGE2D has **BY** groups and the **RESTORE** statement has **BY** groups, then the analysis variables must match. This matching assumes implicitly that in each **BY** group of PROC KRIGE2D and the item store, the corresponding set of observations and correlation model comes from the same random field. This assumption is valid if you use the same data set, first in PROC VARIOGRAM to fit a model and save it in the item store, and then in PROC KRIGE2D to perform predictions with the resulting correlation models.

- If PROC KRIGE2D has BY groups but the item store does not, then the item store is accepted only if the procedure and the item store analysis variables match. In this case, the same item store model choice iterates across the BY groups of the input data. You are advised to proceed with caution: each BY group in the input DATA= set corresponds to a different realization of a random field. Hence, by using the same correlation model for prediction purposes, you implicitly assume that all these different realizations are instances of the same random field.
- If PROC KRIGE2D has no BY groups but the item store does, then the item store is rejected.

---

## Details: KRIGE2D Procedure

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### Theoretical Semivariogram Models

Consider a stochastic spatial process represented by the stationary spatial random field (SRF)  $\{Z(s), s \in D \subset \mathcal{R}^2\}$  (Christakos 1992). The VARIOGRAM procedure computes the empirical (also known as sample or experimental) semivariance of  $Z(s)$ . Prediction of the spatial process  $Z(s)$  at unsampled locations by techniques such as ordinary kriging requires a theoretical semivariogram or covariance.

When you use PROC VARIOGRAM and PROC KRIGE2D to perform spatial prediction, you must determine a suitable theoretical semivariogram based on the sample semivariogram. Various methods exist to fit semivariogram models, such as least squares, maximum likelihood, and robust methods (Cressie 1993, section 2.6). You can use PROC VARIOGRAM to perform automated fitting of a semivariogram model with weighted or ordinary least squares. A different approach is manual fitting, in which a theoretical semivariogram is chosen based on visual inspection of the empirical estimate; see, for example, Hohn (1988, p. 25).

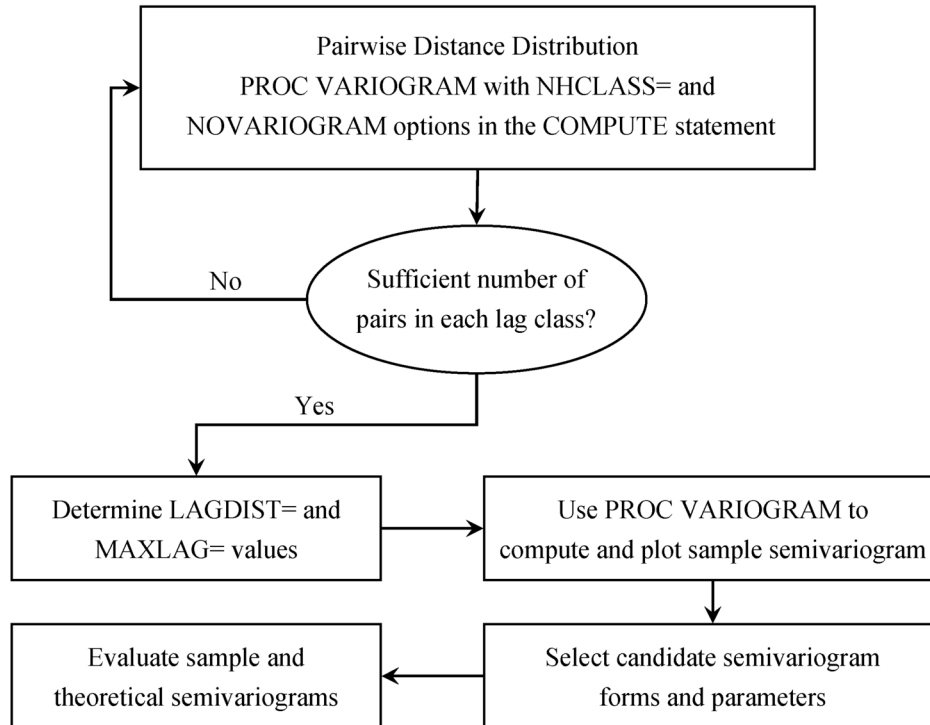
In some cases, a plot of the experimental semivariogram suggests that a single theoretical model is inadequate. Nested models, anisotropic models, and the nugget effect increase the scope of theoretical models available. All of these concepts are discussed in this section. The specification of the final theoretical model is provided by the syntax of PROC KRIGE2D.

Figure 49.5 shows the general flow of investigation. The empirical semivariogram is computed after a suitable choice is made for the LAGDISTANCE= and MAXLAGS= options in PROC VARIOGRAM, and possibly the NDIR= option or the DIRECTIONS statement for computations in more than one directions. Potential theoretical models (which can also incorporate nesting, anisotropy, and the nugget effect) are then plotted against the empirical semivariogram and evaluated. A suitable theoretical model is found by using the methodology presented in the section “[Examples: VARIOGRAM Procedure](#)” on page 8648 in the VARIOGRAM procedure.

Eight theoretical models are supported by PROC KRIGE2D: the Gaussian, exponential, Matérn, spherical, cubic, pentaspherical, sine hole effect and power models. See also the section “[Theoretical Semivariogram Models](#)” on page 8608 in the VARIOGRAM procedure. These eight model forms are now examined in more detail: the Gaussian, exponential, and Matérn forms are examined as one group; the spherical, cubic, and pentaspherical as a second group; and the remaining power and sine hole effect models are examined individually. For comparison purposes, the axes in the forms’ illustrations are kept the same across the plots, and the corresponding parameters of the different forms have the same values.

In PROC KRIGE2D the parameters  $a_0$  and  $c_0$  for all forms correspond to the **RANGE=** and **SCALE=** options, respectively, in the **MODEL** statement. For all model forms, the dimension of  $c_0$  is the same as the dimension of the variance of the spatial process  $Z(s)$ . For all forms but the power model, the dimension of  $a_0$  is length with same units as the distance  $h$  in the semivariance  $\gamma_z(h)$ . See the section “The Power Semivariogram Model” on page 3828 for more details about interpretation of the power model  $a_0$  parameter.

**Figure 49.5** Flowchart for Semivariogram Selection



### The Gaussian Semivariogram Model

The form of the Gaussian model is

$$\gamma_z(h) = c_0 \left[ 1 - \exp\left(-\frac{h^2}{a_0^2}\right) \right]$$

The shape is displayed in Figure 49.6, using range  $a_0 = 1$  and scale  $c_0 = 4$ .

The vertical line at  $h = r_\epsilon = \sqrt{3}a_0$  shows the *effective* (or *practical*) range as defined by Deutsch and Journel (1992) or the *range*  $\epsilon$  defined by Christakos (1992). The effective range is the  $h$ -value where the covariance is approximately 5% of its value at zero. Alternatively, the stationarity assumption implies that the effective range is the  $h$  value where the semivariance is approximately 5% of the sill value, as shown in Figure 49.6.

In the Gaussian model the semivariance  $\gamma_z(h)$  approaches the sill asymptotically at  $c_0$ .

### The Exponential Semivariogram Model

The form of the exponential model is

$$\gamma_z(h) = c_0 \left[ 1 - \exp\left(-\frac{h}{a_0}\right) \right]$$

The shape is displayed in Figure 49.6, using range  $a_0 = 1$  and scale  $c_0 = 4$ .

The vertical line at  $h = r_\epsilon = 3a_0$  is the *effective* (or *practical*) *range* or the *range*  $\epsilon$  (that is, the  $h$ -value where the covariance is approximately 5% of its value at zero).

As in the Gaussian model, the sill in this example is at 4.0 variance units (corresponding to  $c_0 = 4$ ) and is approached asymptotically.

The major distinguishing feature of the Gaussian and exponential forms is the shape in the neighborhood of the origin  $h = 0$ , as Figure 49.6 illustrates. In general, small lags are important in determining an appropriate theoretical form based on an empirical semivariogram.

### The Matérn Semivariogram Model

The form of the Matérn model is

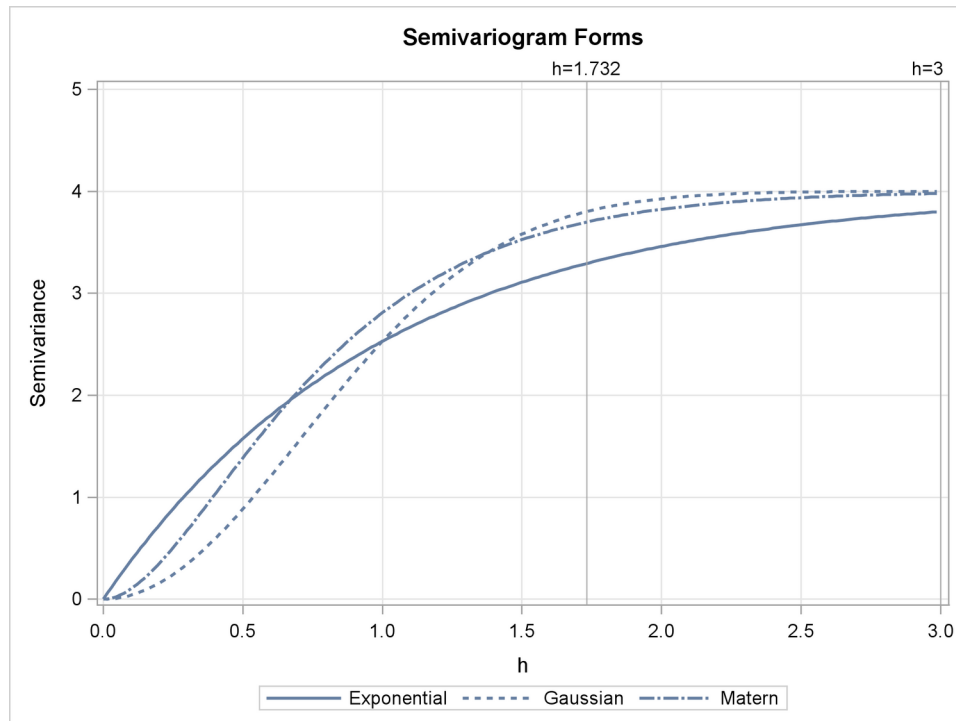
$$\gamma_z(h) = c_0 \left[ 1 - \frac{2}{\Gamma(\nu)} \left( \frac{h\sqrt{\nu}}{a_0} \right)^\nu K_\nu \left( 2 \frac{h\sqrt{\nu}}{a_0} \right) \right]$$

where  $\nu > 0$  is the smoothness factor parameter. Figure 49.6 shows an example of the Matérn form, where range  $a_0 = 1$ , scale  $c_0 = 4$ , and  $\nu = 1.5$ .

The Matérn semivariance  $\gamma_z(h)$  is a class of semivariance models that emerge for different values of the smoothing parameter  $\nu$ . The Matérn form reaches its sill value  $c_0$  asymptotically.

The Gaussian and exponential semivariances are two frequently used members of the Matérn class of semivariances. In particular, the exponential semivariance model is derived from the Matérn class of models for  $\nu = 0.5$ . Also, when  $\nu \rightarrow \infty$  then the Matérn semivariance gives the Gaussian model. In Figure 49.6 the selected value of  $\nu = 1.5$  places the Matérn form in between the Gaussian and the exponential. The Matérn semivariance typically begins to look and behave as the Gaussian for values of  $\nu > 10$ .

**Figure 49.6** Gaussian, Exponential, and Matérn Semivariograms with Parameters  $a_0 = 1$ ,  $c_0 = 4$ , and  $\nu = 1.5$



### The Spherical Semivariogram Model

The form of the spherical model is

$$\gamma_z(h) = \begin{cases} c_0 \left[ \frac{3}{2} \frac{h}{a_0} - \frac{1}{2} \left( \frac{h}{a_0} \right)^3 \right] & \text{for } h \leq a_0 \\ c_0 & \text{for } h > a_0 \end{cases}$$

The shape is displayed in Figure 49.7, using range  $a_0 = 1$  and scale  $c_0 = 4$ .

The vertical line at  $h = 1$  shows the range  $a_0$  of the model.

In the case of the spherical model,  $\gamma_z(h)$  actually reaches the sill value at  $c_0$ , unlike the Gaussian and exponential types where the sill is a horizontal asymptote.

### The Cubic Semivariogram Model

The form of the cubic model is

$$\gamma_z(h) = \begin{cases} c_0 \left[ 7 \left( \frac{h}{a_0} \right)^2 - \frac{35}{4} \left( \frac{h}{a_0} \right)^3 + \frac{7}{2} \left( \frac{h}{a_0} \right)^5 - \frac{3}{4} \left( \frac{h}{a_0} \right)^7 \right] & \text{for } h \leq a_0 \\ c_0 & \text{for } h > a_0 \end{cases}$$

The cubic form shape is displayed in Figure 49.7, using range  $a_0 = 1$  and scale  $c_0 = 4$ .

The vertical line at  $h = 1$  shows the range  $a_0$  of the model.

Similarly to the spherical model, the cubic model,  $\gamma_z(h)$  reaches the sill value at  $c_0$  and maintains this value after a distance  $h$  equal to the model range.

## The Pentaspherical Semivariogram Model

The form of the pentaspherical model is

$$\gamma_z(h) = \begin{cases} c_0 \left[ \frac{15}{8} \frac{h}{a_0} - \frac{5}{4} \left( \frac{h}{a_0} \right)^3 + \frac{3}{8} \left( \frac{h}{a_0} \right)^5 \right] & \text{for } h \leq a_0 \\ c_0 & \text{for } h > a_0 \end{cases}$$

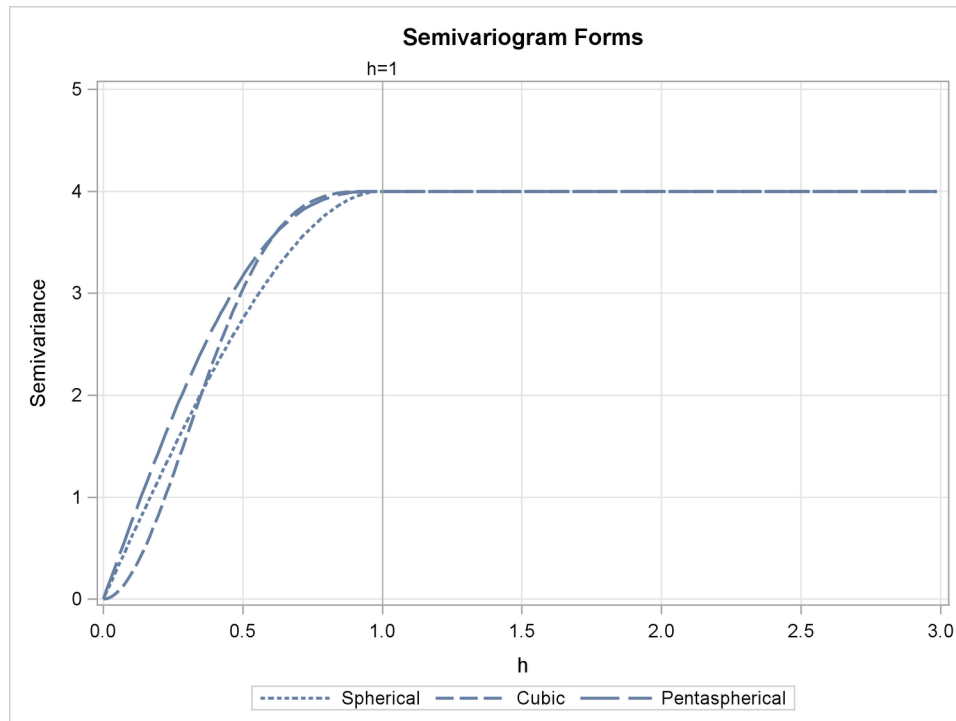
The pentaspherical form shape is displayed in [Figure 49.7](#), using range  $a_0 = 1$  and scale  $c_0 = 4$ .

The vertical line at  $h = 1$  shows the range  $a_0$  of the model.

The pentaspherical semivariance behaves like the spherical and cubic semivariances, in that  $\gamma_z(h)$  increases with distance until it reaches the sill value  $c_0$  at the distance  $h$  equal to the model range  $a_0$ .

[Figure 49.7](#) accents the differences in the behavior of the featured semivariances. Specifically, the cubic and pentaspherical forms reach the sill value faster than the spherical form. Also, the spherical and pentaspherical forms exhibit a more linear behavior at distances close to the origin  $h = 0$ .

**Figure 49.7** Spherical, Cubic, and Pentaspherical Semivariograms with Parameters  $a_0 = 1$  and  $c_0 = 4$



## The Sine Hole Effect Semivariogram Model

The form of the sine hole effect model is

$$\gamma_z(h) = c_0 \left[ 1 - \frac{\sin(\pi h/a_0)}{\pi h/a_0} \right]$$

[Figure 49.8](#) shows an example of the sine hole effect form, where range  $a_0 = 1$  and scale  $c_0 = 4$ .

The vertical line at  $h = 1$  shows the range  $a_0$  of the model.

The sine hole effect semivariance  $\gamma_z(h)$  increases with distance. It has the distinct characteristic that it reaches the sill at a distance  $h = a_0$  equal to the model range and then it oscillates around the sill value with a decreasing amplitude as it moves to higher values of  $h$ .

### The Power Semivariogram Model

The form of the power model is

$$\gamma_z(h) = c_0 h^{a_0}$$

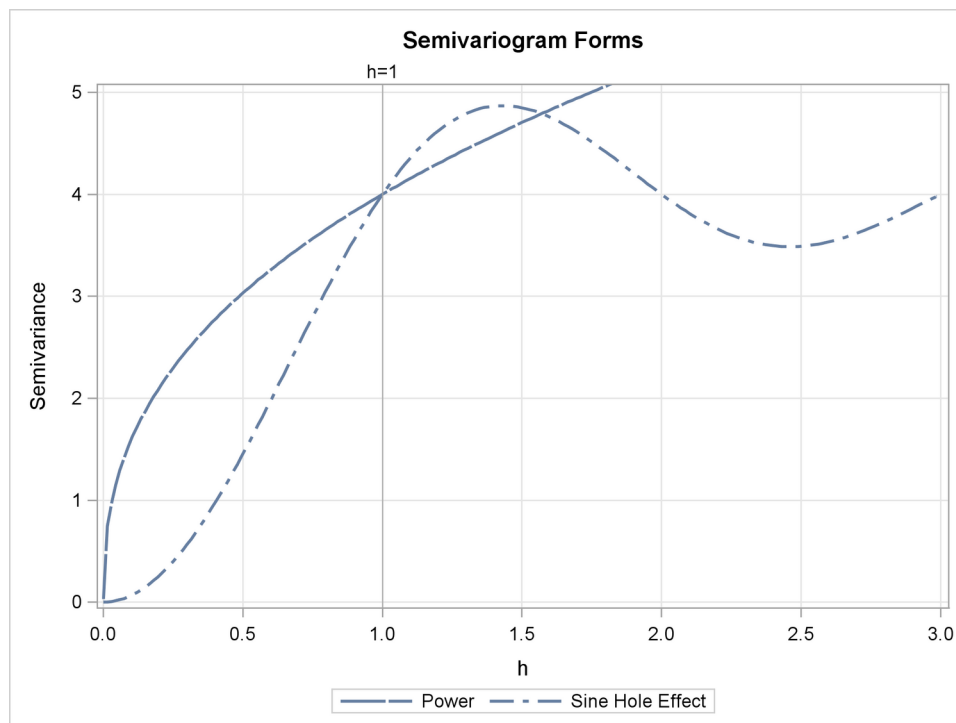
For this model, the parameter  $a_0$  is known as the power exponent. This is a dimensionless quantity which must range within  $0 \leq a_0 < 2$  so that the power model is a permissible semivariance model.

The KRIGE2D procedure enables you to specify power exponent values that are outside this range when you also explicitly specify the **POWNOBOUND** option in the **MODEL** statement. However, parameter values equal to or greater than 2 can result in singular covariance matrices or negative prediction errors.

For the special case of  $a_0 = 1$  the form yields a straight line. In this case the power model reduces to the linear model. The parameter  $c_0$  designates the slope of the power form and has dimensions of the variance as in the other models.

The power model has no sill; this differentiates it from the rest of the models presented earlier. Spatial correlation that is described by a power model indicates that the stochastic process variance increases constantly with distance. The shape of the power model with  $a_0 = 0.4$  and  $c_0 = 4$  is displayed in [Figure 49.8](#).

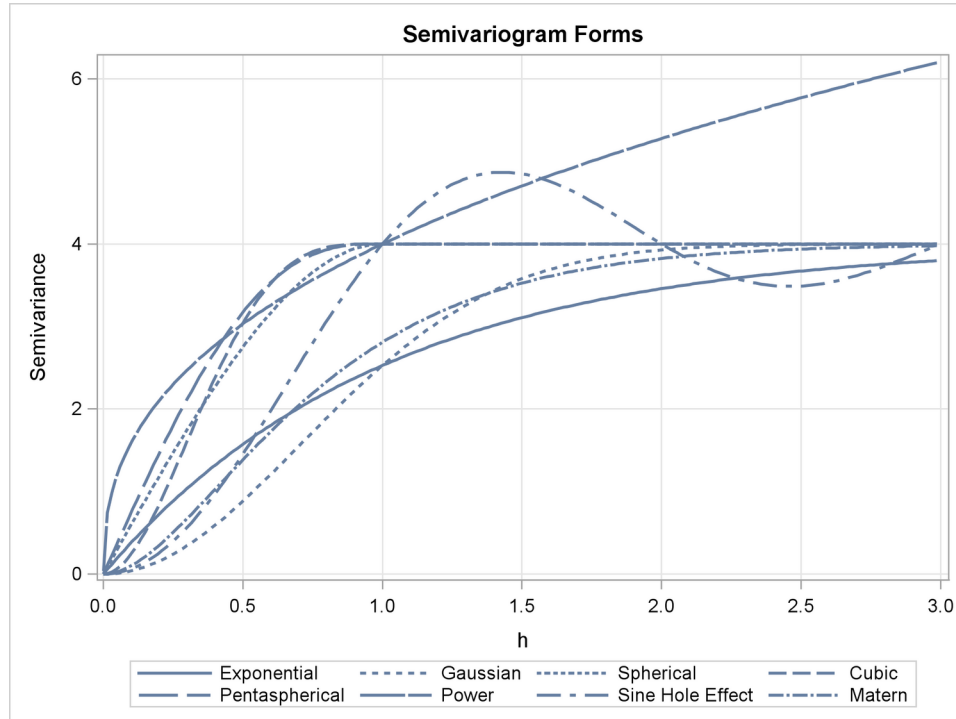
**Figure 49.8** Sine Hole Effect Semivariogram with Range  $a_0 = 1$  and Scale  $c_0 = 4$ , and Power Semivariogram with Exponent  $a_0 = 0.4$  and Slope  $c_0 = 4$



For comparison purposes, [Figure 49.9](#) displays all eight semivariance forms that you can use with PROC

KRIGE2D. The figure displays a composition of the different forms with the parameter values selected earlier throughout this section. Depending on the empirical semivariogram, these models provide you with flexibility to select an appropriate theoretical semivariance model for prediction.

**Figure 49.9** Semivariogram Forms Used in PROC KRIGE2D



### Nested Models

For a given set of spatial data, a plot of an experimental semivariogram might not seem to fit any of the individual theoretical models. In such a case, you might obtain a more accurate fit if you consider your covariance model to be the sum of two or more covariance structures. Such covariance models are called *nested* models. Nesting is common in geologic applications where correlations can exist at different length scales. At small lag distances  $h$ , the smaller scale correlations dominate, while the large scale correlations dominate at larger lag distances.

Nested models are permissible covariances if they are the sum of permissible models. Therefore, you can include in a sum any combination of the models presented in the preceding subsections and produce permissible covariance models. As an illustration, consider two semivariogram models: an exponential and a spherical,

$$\gamma_{z,1}(h) = c_{0,1} \exp\left(-\frac{h}{a_{0,1}}\right)$$

and

$$\gamma_{z,2}(h) = \begin{cases} c_{0,2} \left[ \frac{3}{2} \frac{h}{a_{0,2}} - \frac{1}{2} \left( \frac{h}{a_{0,2}} \right)^3 \right], & \text{for } h \leq a_{0,2} \\ c_{0,2}, & \text{for } h > a_{0,2} \end{cases}$$



with  $c_{0,1} = 1$ ,  $a_{0,1} = 2.5$ ,  $c_{0,2} = 2$ , and  $a_{0,2} = 1$ . If both of these correlation structures are present in a spatial process  $\{Z(s), s \in D\}$ , then the semivariance  $\gamma_z(h)$  of this process can be expressed as

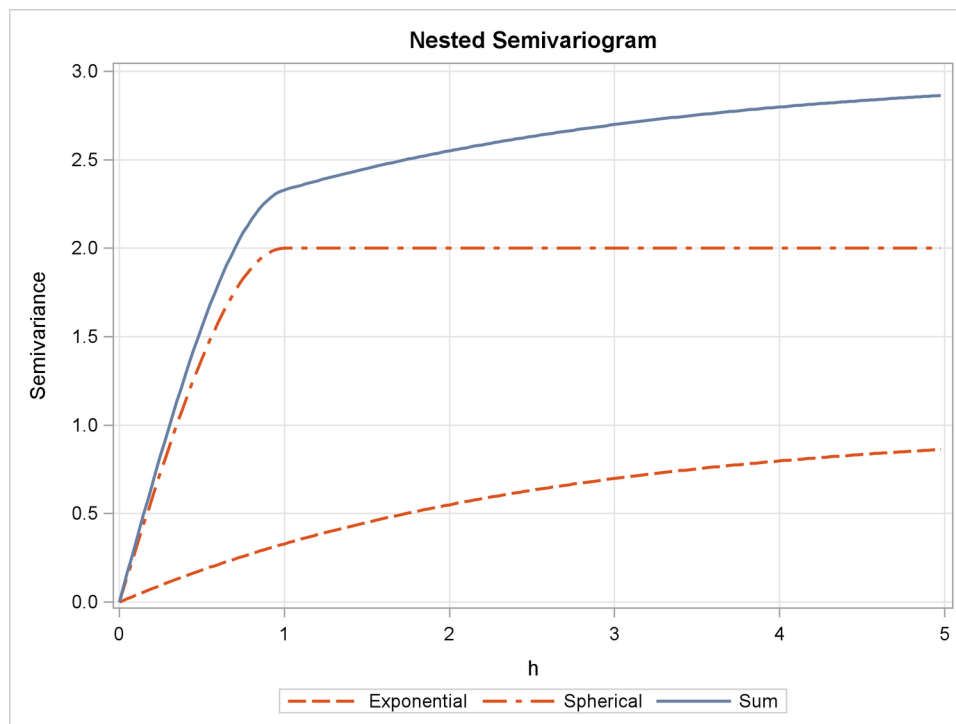
$$\gamma_z(h) = \gamma_{z,1}(h) + \gamma_{z,2}(h)$$

In this case, the experimental semivariogram  $\gamma_z(h)$  for the process  $Z(s)$  resembles the semivariogram of the sum of  $\gamma_{z,1}(h)$  and  $\gamma_{z,2}(h)$ . This is illustrated in Figure 49.10.

The sum of  $\gamma_{z,1}(h)$  and  $\gamma_{z,2}(h)$  in Figure 49.10 does not resemble any *single* theoretical semivariogram; however, its shape at  $h = 1$  is similar to a spherical form. The asymptotic approach to a sill at three variance units, along with the shape around  $h = 0$ , indicates an exponential structure. The sill value  $c_0$  of the sum is the sum of the individual sills  $c_{0,1} = 1$  and  $c_{0,2} = 2$ . In general, a nested model has a sill equal to the sum of the sills of its nested structures plus the nugget effect, if present.

See Hohn (1988, p. 38ff) for further examples of nested correlation structures.

**Figure 49.10** Sum of Exponential and Spherical Structures at Different Scales



## The Nugget Effect

For all the semivariogram models considered previously, the following property holds:

$$\gamma_z(0) = \lim_{h \downarrow 0} \gamma_z(h) = 0$$

However, a plot of the experimental semivariogram might indicate a discontinuity at  $h = 0$ ; that is,  $\gamma_z(h) \rightarrow c_n > 0$  as  $h \rightarrow 0$ , while  $\gamma_z(0) = 0$ . The quantity  $c_n$  is called the *nugget effect*; this term is from mining

geostatistics where nuggets literally exist, and it represents variations at a much smaller scale than any of the measured pairwise distances—that is, at distances  $h \ll h_{min}$ , where

$$h_{min} = \min_{i,j} h_{ij} = \min_{i,j} |s_i - s_j|$$

Nonzero nugget effects have been associated with conceptual and theoretical difficulties; see Cressie (1993, section 2.3.1) and Christakos (1992, section 7.4.3) for details. There is no *practical* difficulty, however; you simply visually extrapolate the experimental semivariogram as  $h \rightarrow 0$ . The importance of availability of data at small lag distances is again illustrated.

As an example, an exponential semivariogram with a nugget effect  $c_n$  has the form

$$\gamma_z(h) = c_n + \sigma_0^2 \left[ 1 - \exp\left(-\frac{h}{a_0}\right) \right], h > 0$$

and

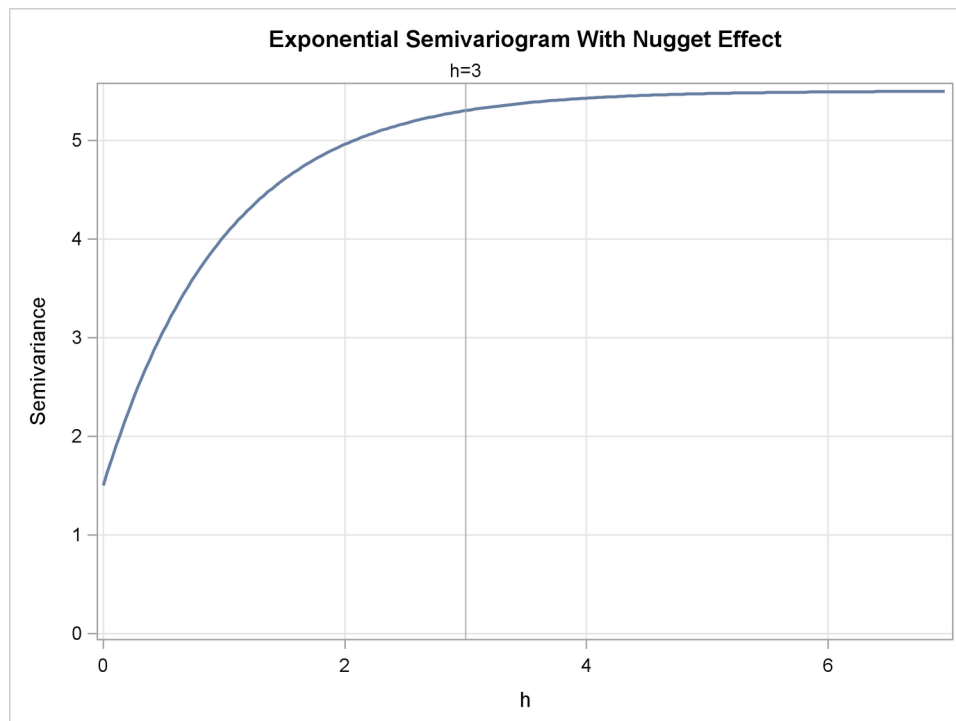
$$\gamma_z(0) = 0$$

where the factor  $\sigma_0^2$  is called the *partial sill* and the sill  $c_0 = c_n + \sigma_0^2$ .

This is illustrated in Figure 49.11 for the parameters  $a_0 = 1$ ,  $\sigma_0^2 = 4$ , and nugget effect  $c_n = 1.5$ .

You can specify the nugget effect in PROC KRIGE2D with the **NUGGET=** option in the **MODEL** statement. It is a separate, additive term independent of direction; that is, it is isotropic. The way to approximate an anisotropic nugget effect is described in the following section.

**Figure 49.11** Exponential Semivariogram Model with a Nugget Effect  $c_n = 1.5$



## Anisotropic Models

In all of the theoretical models considered previously, the lag distance  $h$  is entered as a scalar value. This implies that the correlation between the spatial process at two point pairs  $P_1, P_2$  is dependent *only* on the separation distance  $h = |P_1 P_2|$ , not on the orientation of the vector  $\mathbf{h}$ . A spatial process described by an SRF  $\{Z(\mathbf{s}), \mathbf{s} \in D \subset \mathcal{R}^2\}$  with this property is called isotropic, as is the associated covariance or semivariogram.

However, real spatial phenomena often show directional effects. Particularly in geologic applications, measurements along a particular direction might be highly correlated, while typically the perpendicular direction shows little or no correlation. Such processes are called anisotropic; see, for example, Journel and Huijbregts (1978, section III.B.4).

When the correlation structure varies across different directions, you need different models for each direction so that you can account correctly for the continuity within the SRF. The following subsections describe how techniques are applied to override the anisotropy effects for computational purposes. First, characteristics of anisotropy are examined.

The semivariogram sill is a measure of the process variability; hence the direction of the highest continuity is perpendicular to the direction where the highest sill occurs. If the sill is the same in all directions, then the direction with the highest range indicates highest continuity. The directions in which the spatial process  $\{Z(\mathbf{s}), \mathbf{s} \in D\}$  is most and least correlated are called the *major* and *minor* axis of anisotropy, respectively.

In some cases, these directions are known a priori. This can occur in mining applications where the geology of a region is known in advance. In most cases however, nothing is known about possible anisotropy. Depending on the amount of data available, using several directions is usually sufficient to determine the presence of anisotropy and to find the approximate major and minor axis directions; see the discussion in the section “Anisotropy” on page 8616 in the VARIOGRAM procedure documentation. You can find a detailed example of anisotropy investigation in the section “[Example 102.2: An Anisotropic Case Study with Surface Trend in the Data](#)” on page 8658 in the VARIOGRAM procedure documentation.

After you explore an anisotropic process and you identify the minor and major axis directions, you can compute the *anisotropy factor* parameter  $R$  which is defined as

$$R = \frac{a_0^{min}}{a_0^{max}}$$

where  $a_0^{min}$  is the semivariogram range in the direction of the minor axis and  $a_0^{max}$  is the semivariogram range in the direction of the major axis.

There are two types of anisotropy, depending on which semivariogram characteristics change in different directions. These types are the *geometric* and the *zonal* anisotropy, and either or both can be present. Both are examined in detail in the following subsections.

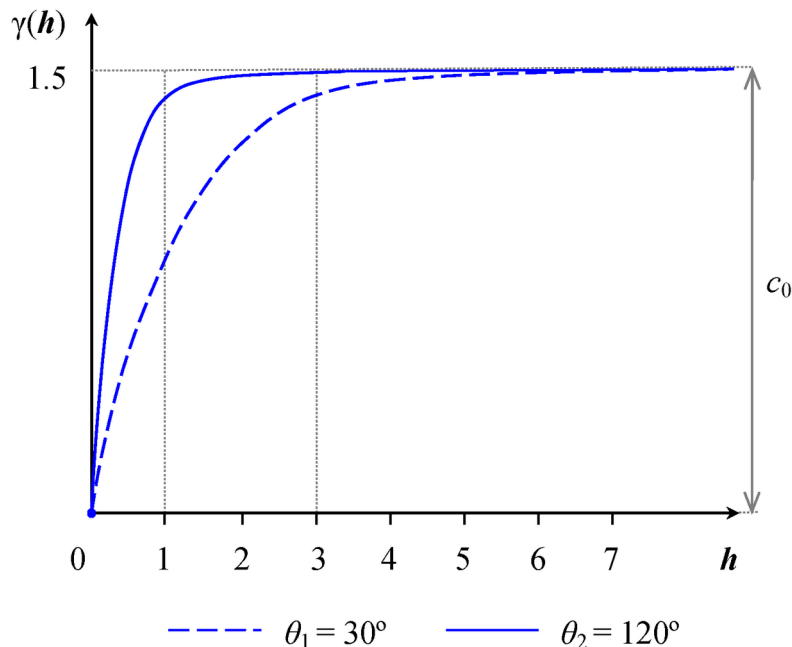
## Geometric Anisotropy

Geometric anisotropy is the simplest type of anisotropy. It occurs when the same sill (or scale) parameter  $c_0$  is present in all directions but the range  $a_0$  changes with direction. In geometric anisotropy the covariance model uses the same forms in all directions.

Therefore, geometric anisotropy features one single sill value, and depending on the direction the semivariogram reaches the sill within a different distance. This is illustrated in Figure 49.12, where an anisotropic exponential semivariogram is plotted. Assume that the two curves displayed in this figure have the same sill  $c_0 = 1.5$  and are generated using the ranges  $a_{0,1} = 3$  in the direction  $\theta_1 = 30^\circ$  (effective range is  $r_{\epsilon,1} = 9$ ) and  $a_{0,2} = 1$  in the direction  $\theta_2 = 120^\circ$  (effective range is  $r_{\epsilon,2} = 3$ ).

As you can see from the figure, the ratio of the shorter to longer range is  $R = 1/3$ . The anisotropy factor  $R$  is the value to use in the `RATIO=` parameter in the `MODEL` statement in PROC KRIGE2D. When you model geometric anisotropy  $R \leq 1$ . In fact, isotropy is a partial case of geometric anisotropy for which  $a_0^{min} = a_0^{max}$  and  $R = 1$ .

**Figure 49.12** Geometric Anisotropy with Major Axis in the Direction  $\theta_1 = 30^\circ$



The values of the `RANGE=` and `ANGLE=` parameters in the `MODEL` statement in PROC KRIGE2D are set based on the major anisotropy axis characteristics. Specifically, the `RANGE=` parameter is the value of the major axis range  $a_0^{max} = a_{0,1}$ , and the `ANGLE=` parameter is the angle  $\theta_1$  of the major axis measured clockwise from north (angles measured in this way are also known as *azimuths*). You can then specify the following `MODEL` statement in PROC KRIGE2D to approximate the covariance structure:

```
model form=exp range=3 scale=1.5 angle=30 ratio=0.3333;
```

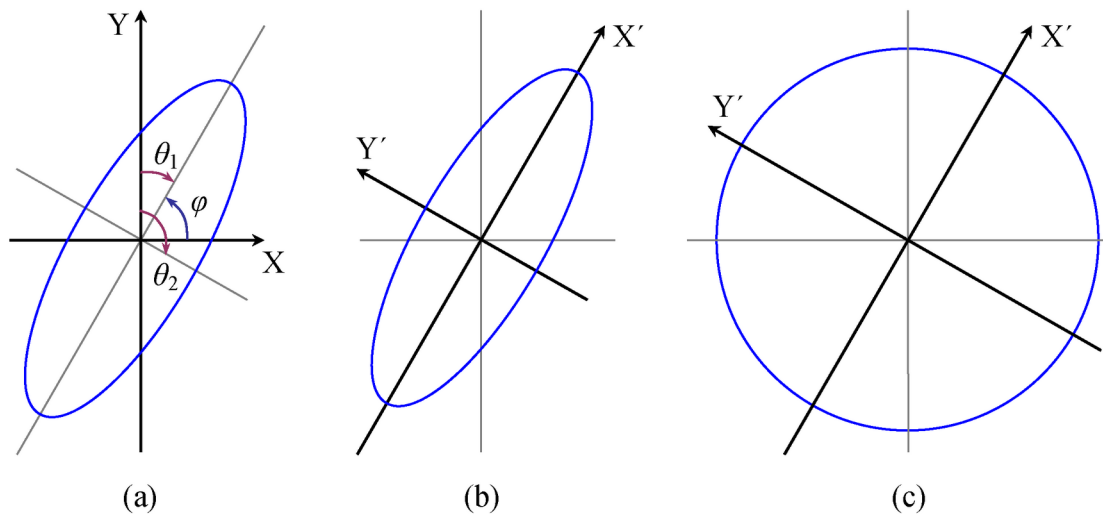
If you use a nested model, provide the type for each one of the nested structures with the `FORM=` option, and assign the individual `SCALE=` parameters so that they add up to the total sill (include in the sum the nugget effect, if present). In the typical case, all of your nested structures have the same anisotropy axes. This means that you specify the same `ANGLE=` parameter value for all structures. Each structure likely has its own values for the `RANGE=` and `RATIO=` parameters depending on the degree of its contribution to the nested model.

The terminology associated with geometric anisotropy is that of ellipses. To see how this comes about, consider the following hypothetical set of calculations. Let  $\{Z(s), s \in D \subset \mathcal{R}^2\}$  be a geometrically anisotropic process, and assume sufficient data points are present to calculate an experimental semivariogram at a large number of angle classes  $\theta \in \{0, \delta\theta, 2\delta\theta, \dots, 180^\circ\}$ . At each of these angles  $\theta$ , the experimental semivariogram is plotted and the range  $a_0$  is recorded. A diagram in polar coordinates  $(a_0, \theta)$  yields an ellipse with the major axis  $a_0^{max}$  in the direction of the largest  $a_0$  and the minor axis  $a_0^{min}$  perpendicular to it. For the example in Figure 49.12, the ellipse is shown in Figure 49.13(a). Its major axis has size  $a_0^{max}$  situated at angle  $\theta_1$  clockwise from north, and the minor axis has size  $a_0^{min}$  oriented at angle  $\theta_2$  clockwise from north.

The KRIGE2D procedure handles geometric anisotropy by applying a reversible transformation in two steps that converts geometric anisotropy into isotropic conditions.

The first step is to align your coordinates axes with the anisotropy ellipse axes. Specifically, you choose to rotate by an angle  $\varphi$  the standard Cartesian orientation of the  $(x, y)$  coordinates system shown in Figure 49.13(a) so that the Y axis coincides with the ellipse minor axis. The rotation result is illustrated in Figure 49.13(b). The second step is to elongate the minor axis so its length equals that of the major axis of the ellipse. You can see the result in Figure 49.13(c). The computational details are shown in the following.

**Figure 49.13** Transformation Applied to Geometric Anisotropy



The transformation angle  $\varphi$  is measured in standard Cartesian orientation counterclockwise from the X axis (east). If the major axis azimuth is  $\theta_1$ , then the Cartesian system of  $(x, y)$  needs to be rotated by  $\varphi = 90^\circ - \theta_1$  so that the Y axis can coincide with the ellipse minor axis; see Figure 49.13(a).

Let us call the ellipse major axis  $X'$  and the minor axis  $Y'$ . The transformation that converts any coordinates in the  $(x, y)$  system into  $(x', y')$  coordinates in terms of  $\varphi$  is given by the matrix:

$$\mathbf{H} = \begin{pmatrix} \cos(\varphi) & \sin(\varphi) \\ -\sin(\varphi) & \cos(\varphi) \end{pmatrix}$$

The elongation of the minor axis in the second step is performed with the matrix:

$$\mathbf{D}_R = \begin{pmatrix} 1 & 0 \\ 0 & 1/R \end{pmatrix}$$

**NOTE:** These two steps are sequential and their order cannot be reversed. For any point pair  $P_1$  and  $P_2$  with respective coordinates  $\mathbf{s}_1 = (x_1, y_1)$  and  $\mathbf{s}_2 = (x_2, y_2)$  in the  $(x, y)$  axes, their distance is given by

$$|P_i P_j|_{(x,y)} = h = \sqrt{(\delta x)^2 + (\delta y)^2}$$

where the distance components  $\delta x = x_2 - x_1$  and  $\delta y = y_2 - y_1$ . Based on the previous, the corresponding distances  $\delta x'$  and  $\delta y'$  in the  $(x', y')$  coordinates system are given by the vector:

$$\begin{pmatrix} \delta x' \\ \delta y' \end{pmatrix} = \mathbf{D}_R \mathbf{H} \begin{pmatrix} \delta x \\ \delta y \end{pmatrix} = \begin{pmatrix} \cos(\varphi) & \sin(\varphi) \\ -\sin(\varphi)/R & \cos(\varphi)/R \end{pmatrix} \begin{pmatrix} \delta x \\ \delta y \end{pmatrix}$$

The transformed interpair distance is then:

$$|P_i P_j|_{(x',y')} = h' = \sqrt{(\delta x')^2 + (\delta y')^2}$$

As a result, the original anisotropic semivariogram in Figure 49.12 that was a function  $\gamma(\mathbf{h}) = \gamma(h, \theta)$  of both  $h$  and  $\theta$  is then transformed to an equivalent function  $\hat{\gamma}(h')$  only of  $h'$ :

$$\hat{\gamma}(h') = \gamma(\mathbf{h})$$

This single isotropic semivariogram  $\hat{\gamma}(h')$  is then used for kriging purposes.

The two steps used by PROC KRIGE2D in the previous analysis can also be performed in a different manner. For instance, you might equivalently choose to rotate the  $(x, y)$  Cartesian coordinates so that the  $Y$  axis coincides with the ellipse major axis, rather than with the minor axis as was shown earlier. Also, you might prefer to compress the major axis rather than elongating the short one. In any case, you need to perform the appropriate computations for the transformation of your choice.

## Zonal Anisotropy

In zonal anisotropy, the sill (or scale) parameter  $c_0$  is different for different directions. It is not possible to transform such a structure into an isotropic semivariogram. Instead, nesting and geometric anisotropy are used together to approximate zonal anisotropy.

When the scale varies with direction, the lowest scale (that is, the lowest variance) naturally corresponds to the maximum continuity direction. The same direction has the longest range, as also discussed in the section “Geometric Anisotropy” on page 3833.

A varying scale with direction can be interpreted as having one or more model components whose individual contributions to the total variance differ with direction. For each such component, its contribution (scale) ranges between zero and a maximum value. This makes it unlikely that you can describe a natural process with a pure zonal model, because doing so would imply zero continuity in the direction of zero contribution; see also Chilès and Delfiner (1999, p. 96).

In a simple case of zonal anisotropy, a model includes one zonal component. The zonal component makes its highest contribution in a direction perpendicular to the maximum continuity direction, and it contributes zero to the maximum continuity direction. This is necessary; otherwise, there would be a direction with a total scale less than the scale in the maximum continuity direction. Following a similar reasoning, the zonal component's direction of maximum contribution cannot coincide with the one of maximum continuity. In the general case, there can be multiple zonal components, each making its highest contribution in a different direction.

The following describes how to deal with zonal anisotropy in your analysis; see also Goovaerts (1997, p. 96) and Deutsch and Journel (1992, pp. 27–32). If you start with an empirical semivariogram, you can investigate zonal anisotropy by identifying whether a maximum and a minimum scale exist in two specific directions. If they exist, typically these two directions might be perpendicular. Then proceed to identify the zonal component that causes the difference in scale by fitting the empirical semivariogram. You represent zonal component as an additional nested structure in the direction of maximum total scale.

If the minimum and maximum sills are not in perpendicular directions, then you might be seeing the combined effects of multiple zonal components in different directions. In that case you might be able to approximate the continuity behavior by assuming a single zonal component in the direction that is perpendicular to the one of maximum continuity. Alternatively, you might decide to investigate a more elaborate configuration for the model components. In this case, you need to maintain a geometrical anisotropy part across all directions and add zonal components in an appropriate way to match your empirical semivariance in different directions.

After you have a theoretical semivariance model with zonal anisotropy, the next step is to include zonal components in your prediction or simulation analysis. In PROC KRIGE2D you can specify zonal components either explicitly or with the use of results previously saved in item stores produced by the VARIOGRAM procedure.

Specifying a zonal component explicitly in the **MODEL** statement has the following implications:

- The **RANGE=** parameter for the zonal component refers to the range value in the direction of maximum zonal contribution, unlike the case of ranges specified for nonzonal components that refer to the direction of maximum continuity.
- The anisotropy factor  $R$  in the **RATIO=** parameter for the zonal component should be specified as a large positive value to designate zero contribution in the perpendicular direction.

To explain the previous point, remember that  $R$  is defined as  $R = a_0^{min}/a_0^{max}$ . Its value specifies how much to elongate the minor anisotropy axis to make it equal to the major anisotropy axis, in order to transform geometric anisotropy into isotropy. Intuitively, an infinite  $R$  value makes it impossible for the minor axis to become as large as the major axis. This is equivalent to having a very large major anisotropy axis; hence, it indicates a very large range across the major axis direction. Indeed, you can consider a zero zonal contribution in the major anisotropy axis as a very large range of the zonal component along this direction. The particular range is so large that the zonal component practically never reaches its scale along this direction, and this is interpreted as zero contribution.

In the case where you specify zonal anisotropy by using the contents of an item store, you only need to specify the geometric anisotropy components in the `SSEL(MODEL=)` option, and the zonal components as suboptions of the `SSEL(TYPE=ANIZON)` option. Then, the KRIGE2D or SIM2D procedure checks whether the item store contains models that are suitable to use, based on your specifications.

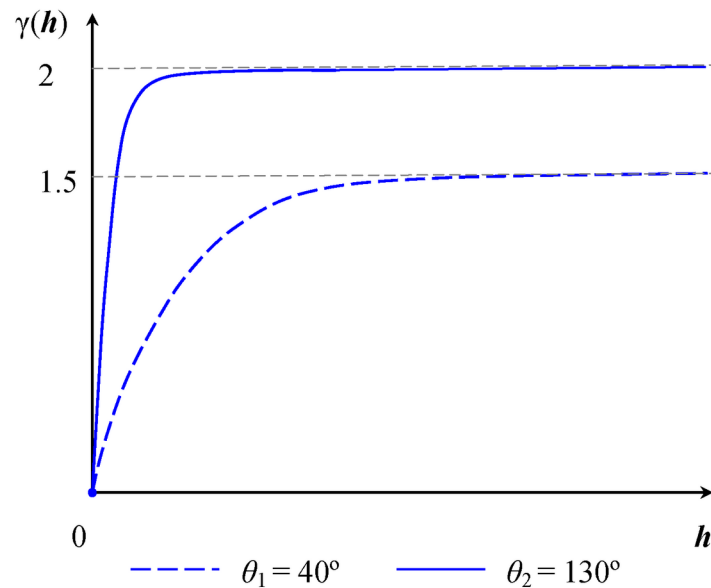
The following two examples illustrate different instances of zonal anisotropy and how to specify the corresponding covariance model parameters in PROC KRIGE2D.

### Example 1

The first example shows that if you can model the direction with the highest sill as a nested model, then you can treat the case as a composition of geometric anisotropy and an additional structure that acts only in the direction of the increased sill.

Consider a spatial process in which the fitting of theoretical models in your experimental semivariogram produces a correlation structure like the one shown in Figure 49.14. In the direction  $\theta_1 = 40^\circ$ , the covariance model has a single exponential structure  $\gamma_1(\mathbf{h}) = \text{Exp}(a_{0,1E}, c_{0,1E})$  with range  $a_{0,1E} = 2$  and sill  $c_{0,1E} = 1.5$ . In the direction  $\theta_2 = 130^\circ$ , the covariance model  $\gamma_2(\mathbf{h}) = \text{Exp}(a_{0,2E}, c_{0,2E}) + \text{Sph}(a_{0,2S}, c_{0,2S})$  has two nested structures: an exponential structure with range  $a_{0,2E} = 0.5$  and sill  $c_{0,2E} = 1.5$  and a spherical structure with range  $a_{0,2S} = 1$  and sill  $c_{0,2S} = 0.5$ .

Figure 49.14 Zonal Anisotropy in Two Directions



The total sill in the direction  $\theta_2$  of highest variance is the sum of the nested structures' sills  $c_{0,2E} + c_{0,2S} = 2$ . You can consider that your process is characterized by a geometrically anisotropic exponential structure with common sill  $c_{0,E} = 1.5$  across all directions and major axis range  $a_{0,1E} = 2$ , and by a spherical structure which is a zonal anisotropy component that contributes only in the  $\theta_2$  direction. Based on the remarks in this section, the `RATIO=` parameter for the exponential structure is  $R_E = 0.5/2 = 0.25$ , whereas for the spherical structure you choose a large value, such as  $R_S = 10^8$ .

Then, you can approximate this structure in PROC KRIGE2D by specifying the two structures with the following `MODEL` statement:



```

model form=(exp,sph) range=(2,1) scale=(1.5,0.5)
 angle=(40,130) ratio=(0.25,1e8);

```

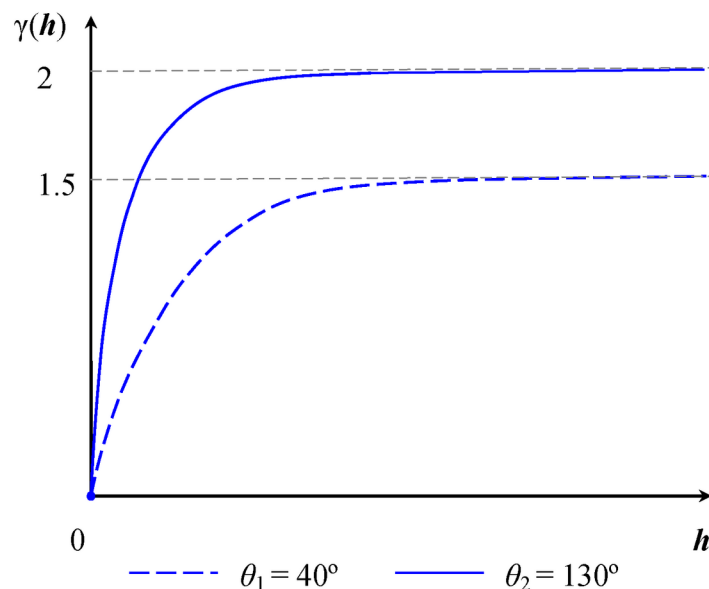
You can handle more elaborate cases in a similar way, where the covariance models in different directions might all be nested models. Your goal is to model the continuity by starting with a sum of isotropic or geometrically anisotropic structures whose total sill is the lowest sill in all directions. Then, in each of the directions with higher sills you add a zonal anisotropy component to the corresponding sum to compensate for the increased variability in that direction.

### Example 2

The second example provides important perspective about the physics of zonal anisotropy analysis. It is an extreme case of the general guidelines for zonal anisotropy. You examine what happens when each of the directions is modeled with a single-form, non-nested model, and the sills for these models are clearly different.

Consider a spatial process with a continuity description almost identical to the one in the previous example. In the direction  $\theta_1 = 40^\circ$ , the covariance model has again a single exponential structure  $\gamma_1(\mathbf{h}) = \text{Exp}(a_{0,1E}, c_{0,1E})$  with range  $a_{0,1E} = 2$  and sill  $c_{0,1E} = 1.5$ . However, this time in the direction  $\theta_2 = 130^\circ$  you have fit the experimental semivariogram by using a single exponential structure  $\gamma_2(\mathbf{h}) = \text{Exp}(a_{0,2E}, c_{0,2E})$  with range  $a_{0,2E} = 1$  and sill  $c_{0,2E} = 2$ . These models are shown in Figure 49.15.

Figure 49.15 Zonal Anisotropy in Two Directions



In this case you have a simplified situation with a single covariance structure in each direction, and the two structures have different scale parameter values. This is a case of zonal anisotropy in which all directions have no shared component. Hence, you have a case with two pure zonal components, where both structures can be practically approximated by specifying two models with large **RATIO=** values. You could then use the following **MODEL** statement in PROC KRIGE2D to describe the covariance in this example:

```
model form=(exp,exp) range=(2,1) scale=(1.5,2)
 angle=(40,130) ratio=(1e8,1e8);
```

The semivariogram of the specified model is accurately shown in Figure 49.15, because the angles  $\theta_1$  and  $\theta_2$  are perpendicular and each component has a contribution to all directions except for the one that is perpendicular to its angle. In the general case,  $\theta_1$  and  $\theta_2$  might not be perpendicular; hence the maximum and minimum scale values can be different from those displayed in Figure 49.15.

In general, avoid configurations with pure zonal components. Correlation models with pure zonal components might imply zero continuity along some direction, which is a very unlikely occurrence in natural processes. For that reason, in similar cases try to use the analysis illustrated in the previous example. In particular, try to model the highest sill direction as a nested structure (such that it contains a geometrical anisotropy component whose cumulative sill is equal to the lower sill) and a zonal anisotropy component that accounts for the sill difference.

### Anisotropic Nugget Effect

Isotropic nugget effects can be approximated with nested models, where one of the nested structures has a very small range. Applying a geometric anisotropy specification to this nested structure results in an anisotropic nugget effect.

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## Details of Ordinary Kriging

### Introduction

Three common characteristics are often observed with spatial data (that is, data indexed by their spatial locations):

- (i) slowly varying, large-scale variations in the measured values
- (ii) irregular, small-scale variations
- (iii) similarity of measurements at locations close together

As an illustration, consider a hypothetical example in which an organic solvent leaks from an industrial site and spreads over a large area. Assume the solvent is absorbed and immobilized into the subsoil above any groundwater level, so you can ignore any time dependence.

To find the areal extent and the concentration values of the solvent, you need measurements. Although the problem is inherently three-dimensional, if you measure total concentration in a column of soil or take a depth-averaged concentration, it can be handled reasonably well with two-dimensional techniques.

You usually assume that measured concentrations are higher closer to the source and decrease at larger distances from the source. On top of this smooth variation, measured concentrations typically have small-scale variations, due perhaps to the inherent variability of soil properties.

You also tend to suspect that measurements made close together yield similar concentration values, while measurements made far apart can have very different values.

These physically reasonable qualitative statements have no explicit probabilistic content. A number of numerical smoothing techniques, such as inverse distance weighting and splines, make use of large-scale variations and “close distance-close value” characteristics of spatial data to interpolate the measured concentrations for contouring purposes.

While characteristics (i) and (iii) are handled by such smoothing methods, characteristic (ii), the small-scale residual variation in the concentration field, is not accounted for.

There can be situations, due to the use of the prediction map or the relative magnitude of the irregular fluctuations, where you cannot ignore these small-scale irregular fluctuations. In other words, the smoothed or predicted values of the concentration field alone are not a sufficient characterization; you also need the possible spread around these contoured values.

## Spatial Random Fields

One method of incorporating characteristic (ii) into the construction of a contour map is to model the concentration field as a spatial random field (SRF). The mathematical details of SRF models are given in a number of texts, such as Cressie (1993) and Christakos (1992). The mathematics of SRFs is formidable. However, under certain simplifying assumptions, it produces classical linear predictors with very simple properties, enabling easy implementation for prediction purposes. These predictors, primarily ordinary kriging (OK), give both a prediction and a standard error of prediction at unsampled locations. This allows the construction of a map of both predicted values and level of uncertainty about the predicted values.

The key assumption in applying the SRF formalism is that the measurements come from a single realization of the SRF. However, in most geostatistical applications, the focus is on a single, unique realization. This is unlike most other situations in stochastic modeling in which there will be future experiments or observational activities (at least conceptually) under similar circumstances. This renders many traditional ideas of statistical inference ambiguous and somewhat counterintuitive.

Additional logical and methodological problems could stand in the way of applying a stochastic model to a unique but partly unknown natural process; see the introduction in Matheron (1971) and Cressie (1993, section 2.3). These difficulties have resulted in attempts to frame the prediction problem in a completely deterministic way (Isaaks and Srivastava 1988; Journel 1985). Also, some issues with kriging, and with spatial prediction methods in general, are related to the necessary assumption of ergodicity of the spatial process. This assumption is required to estimate the covariance or semivariogram from sample data. Details are provided in Cressie (1993, pp. 52–58).

Despite these difficulties, ordinary kriging remains a popular and widely used tool in modeling spatial data, especially in generating surface plots and contour maps. An abbreviated derivation of the OK predictor for point prediction and the associated standard error is discussed in the following section. Full details are given in Journel and Huijbregts (1978); Christakos (1992); Cressie (1993).

## Ordinary Kriging

Denote the SRF by  $Z(\mathbf{s})$ ,  $\mathbf{s} \in D \subset \mathcal{R}^2$ . Following the notation in Cressie (1993), the following model for  $Z(\mathbf{s})$  is assumed:

$$Z(\mathbf{s}) = \mu + \varepsilon(\mathbf{s})$$

Here,  $\mu$  is the fixed, unknown mean of the process, and  $\varepsilon(\mathbf{s})$  is a zero mean SRF, which represents the variation around the mean.

In most practical applications, an additional assumption is required in order to estimate the covariance  $C_z$  of the  $Z(\mathbf{s})$  process. This assumption is second-order stationarity:

$$C_z(\mathbf{s}_1, \mathbf{s}_2) = E[\varepsilon(\mathbf{s}_1)\varepsilon(\mathbf{s}_2)] = C_z(\mathbf{s}_1 - \mathbf{s}_2) = C_z(\mathbf{h})$$

This requirement can be relaxed slightly when you are using the semivariogram instead of the covariance. In this case, second-order stationarity is required of the differences  $\varepsilon(\mathbf{s}_1) - \varepsilon(\mathbf{s}_2)$  rather than  $\varepsilon(\mathbf{s})$ :

$$\gamma_z(\mathbf{s}_1, \mathbf{s}_2) = \frac{1}{2}E[(\varepsilon(\mathbf{s}_1) - \varepsilon(\mathbf{s}_2))^2] = \gamma_z(\mathbf{s}_1 - \mathbf{s}_2) = \gamma_z(\mathbf{h})$$

By performing local kriging, the spatial processes represented by the previous equation for  $Z(\mathbf{s})$  are more general than they appear. In local kriging, at an unsampled location  $\mathbf{s}_0$ , a separate model is fit using only data in a neighborhood of  $\mathbf{s}_0$ . This has the effect of fitting a separate mean  $\mu$  at each point, and it is similar to the *kriging with trend* (KT) method discussed in Journel and Rossi (1989).

Given the  $N$  measurements  $Z(\mathbf{s}_1), \dots, Z(\mathbf{s}_N)$  at known locations  $\mathbf{s}_1, \dots, \mathbf{s}_N$ , you want to obtain a prediction of  $Z$  at an unsampled location  $\mathbf{s}_0$ . When the following three requirements are imposed on the predictor  $\hat{Z}$ , the OK predictor is obtained:

- (i)  $\hat{Z}$  is linear in  $Z(\mathbf{s}_1), \dots, Z(\mathbf{s}_N)$
- (ii)  $\hat{Z}$  is unbiased
- (iii)  $\hat{Z}$  minimizes the mean square prediction error  $E[(Z(\mathbf{s}_0) - \hat{Z}(\mathbf{s}_0))^2]$

Linearity requires the following form for  $\hat{Z}(\mathbf{s}_0)$ :

$$\hat{Z}(\mathbf{s}_0) = \sum_{i=1}^N \lambda_i Z(\mathbf{s}_i)$$

Applying the unbiasedness condition to the preceding equation yields

$$E[\hat{Z}(\mathbf{s}_0)] = \mu \Rightarrow \sum_{i=1}^N \lambda_i E[Z(\mathbf{s}_i)] = \mu \Rightarrow \sum_{i=1}^N \lambda_i \mu = \mu \Rightarrow \sum_{i=1}^N \lambda_i = 1$$

Finally, the third condition requires a constrained linear optimization that involves  $\lambda_1, \dots, \lambda_N$  and a Lagrange parameter  $2m$ . This constrained linear optimization can be expressed in terms of the function  $L(\lambda_1, \dots, \lambda_N, m)$  given by

$$L = E \left[ \left( Z(\mathbf{s}_0) - \sum_{i=1}^N \lambda_i Z(\mathbf{s}_i) \right)^2 \right] - 2m \left( \sum_{i=1}^N \lambda_i - 1 \right)$$

Define the  $N \times 1$  column vector  $\boldsymbol{\lambda}$  by

$$\boldsymbol{\lambda} = (\lambda_1, \dots, \lambda_N)'$$

and the  $(N + 1) \times 1$  column vector  $\lambda_0$  by

$$\lambda_0 = (\lambda_1, \dots, \lambda_N, m)' = \begin{pmatrix} \lambda \\ m \end{pmatrix}$$

The optimization is performed by solving

$$\frac{\partial L}{\partial \lambda_0} = \mathbf{0}$$

in terms of  $\lambda_1, \dots, \lambda_N$  and  $m$ .

The resulting matrix equation can be expressed in terms of either the covariance  $C_z(\mathbf{h})$  or semivariogram  $\gamma_z(\mathbf{h})$ . In terms of the covariance, the preceding equation results in the matrix equation

$$\mathbf{C}\lambda_0 = \mathbf{C}_0$$

where

$$\mathbf{C} = \begin{pmatrix} C_z(\mathbf{0}) & C_z(s_1 - s_2) & \cdots & C_z(s_1 - s_N) & 1 \\ C_z(s_2 - s_1) & C_z(\mathbf{0}) & \cdots & C_z(s_2 - s_N) & 1 \\ & & \ddots & & \\ C_z(s_N - s_1) & C_z(s_N - s_2) & \cdots & C_z(\mathbf{0}) & 1 \\ 1 & 1 & \cdots & 1 & 0 \end{pmatrix}$$

and

$$\mathbf{C}_0 = \begin{pmatrix} C_z(s_0 - s_1) \\ C_z(s_0 - s_2) \\ \vdots \\ C_z(s_0 - s_N) \\ 1 \end{pmatrix}$$

The solution to the previous matrix equation is

$$\hat{\lambda}_0 = \mathbf{C}^{-1}\mathbf{C}_0$$

Using this solution for  $\lambda$  and  $m$ , the ordinary kriging prediction at  $r_0$  is

$$\hat{Z}(s_0) = \lambda_1 Z(s_1) + \cdots + \lambda_N Z(s_N)$$

with associated prediction error the square root of the variance

$$\sigma_z^2(s_0) = C_z(\mathbf{0}) - \lambda' \mathbf{c}_0 + m$$

where  $\mathbf{c}_0$  is  $\mathbf{C}_0$  with the 1 in the last row removed, making it an  $N \times 1$  vector.

These formulas are used in the best linear unbiased prediction (BLUP) of random variables (Robinson 1991). Further details are provided in Cressie (1993, pp. 119–123).

Because of possible numeric problems when solving the previous matrix equation, Deutsch and Journel (1992) suggest replacing the last row and column of 1s in the preceding matrix  $\mathbf{C}$  by  $C_z(0)$ , keeping the 0 in the  $(N + 1, N + 1)$  position and similarly replacing the last element in the preceding right-hand vector  $\mathbf{C}_0$  with  $C_z(0)$ . This results in an equivalent system but avoids numeric problems when  $C_z(0)$  is large or small relative to 1.

---

## Computational Resources

To generate a predicted value at a single grid point by using  $N$  data points, PROC KRIGE2D must solve the kriging system

$$C\lambda_0 = C_0$$

where the dimensions of  $C$  are  $(N + 1) \times (N + 1)$  and the right-hand-side  $C_0$  has one column.

Holding the matrix and vector associated with this system in core requires approximately  $8N^2/2$  bytes. The CPU time used in solving the system is proportional to  $N^3$ . For large  $N$ , this time dominates the  $O(N^2)$  time to compute the elements of the covariance matrix  $C$  from the specified covariance or semivariogram model.

For local kriging, the kriging system is set up and solved for each grid point. Part of the setup process involves determining the neighborhood of each grid point. A fast K-D tree algorithm determines neighborhoods. For  $G$  grid points, the dominant CPU time factor is setting up and solving the  $G$  kriging systems. The  $N$  in the algorithm of the section “[Ordinary Kriging](#)” on page 3840 is the number of data points in a given neighborhood, and it can differ for each grid point.

In global kriging, the entire input data set and all grid points set up and solve the single system

$$C\lambda_0 = C_0$$

Again  $C$  has dimensions  $(N + 1) \times (N + 1)$ , but  $\lambda_0$  and  $C_0$  now have  $G$  columns, where  $G$  is the number of grid points. Memory requirements are approximately  $8[(N^2/2) + GN]$  bytes. The CPU time used in solving the system is still dominated by the  $N^3$  factorization of the left-hand side.

---

## Output Data Sets

The KRIGE2D procedure produces two data sets: the `OUTEST=SAS-data-set` and the `OUTNBHD=SAS-data-set`. These data sets are described as follows.

### **OUTEST=SAS-data-set**

The `OUTEST=` data set contains the kriging predictions and the associated standard errors. The `OUTEST=` data set contains the following variables:

- ESTIMATE, which is the kriging prediction for the current variable.
- GXC, which is the  $x$  coordinate of the grid point at which the kriging prediction is made.
- GYC, which is the  $y$  coordinate of the grid point at which the kriging prediction is made.
- LABEL, which is the label for the current `PREDICT/MODEL` combination that produces the kriging prediction. If you do not specify a label, default labels of the form `Predj.Modelk` are used.
- NPOINTS, which is the number of points used in the prediction. This number varies for each grid point if local kriging is performed.

- STDERR, which is the standard error of the kriging predict.
- VARNAME, which is the variable name.

### OUTNBHD=SAS-data-set

When you specify the **RADIUS=** option or the **NUMPOINTS=** option in the **PREDICT** statement, local kriging is performed. Local kriging is simply ordinary kriging at a given grid location, using only those data points in a neighborhood defined by the **RADIUS=** value or the **NUMPOINTS=** value.

The **OUTNBHD=** data set contains one observation for each data point in each neighborhood. Hence, this data set can be large. For example, if the grid specification results in 1,000 grid points and each grid point has a neighborhood of 100 points, the resulting **OUTNBHD=** data set contains 100,000 points.

The **OUTNBHD=** data set contains the following variables:

- **GXC**, which is the  $x$  coordinate of the grid point.
- **GYC**, which is the  $y$  coordinate of the grid point.
- **ID**, which is the ID variable value or observation. number of the current data point
- **LABEL**, which is the label for the current **PREDICT/MODEL** combination. If you do not specify a label, default labels of the form *Predj.Modelk* are used.
- **NPOINTS**, which is the number of points used in the prediction.
- **RADIUS**, which is the radius used for each neighborhood.
- **VALUE**, which is the value of the variable at the current data point.
- **VARNAME**, which is the variable name of the current variable.
- **XC**, which is the  $x$  coordinate of the current data point.
- **YC**, which is the  $y$  coordinate of the current data point.

If no **ID** statement is specified, then the corresponding observation number is assigned to the variable **ID**, instead.

---

## Displayed Output

In addition to the output data sets, the **KRIGE2D** procedure produces output objects as well. The **KRIGE2D** procedure output objects are the following:

- a default “Number of Observations” table that displays the number of observations read from the input data set and the number of observations used in the analysis.
- a map that shows the spatial distribution of the observations of the current **VAR=** variable in the **PREDICT** statement. The observations are displayed by default with circled markers whose color indicates the **VAR=** value at the corresponding location.

- a default table for each **PREDICT** statement that sums up basic information about the kriging analysis.
- a default table for each **MODEL** statement that shows the covariance model parameters for the corresponding **PREDICT** statement.
- plots of the kriging prediction and the prediction standard error at each point of the specified output grid or at specified individual locations. The **KRIGE2D** procedure produces by default a plot of the kriging prediction and the corresponding prediction error for each **MODEL** statement of every **PREDICT** statement that you specify. You can produce more of these plots with styles that you can specify by using the available suboptions of the **PLOTS=PREDICTION** option.
- a “Store Info” table with basic information about the input item store. This table is produced by default when you specify the **RESTORE** statement.
- a “Store Variables Information” table that describes the analysis variables of an input item store. The table is produced by default when you specify an item store with the **RESTORE** statement.
- a “Store Models Information” table with detailed information about the models and direction angles that are contained in an input item store. The table is produced by default when you specify an item store with the **RESTORE** statement.

---

## ODS Table Names

Each table created by PROC KRIGE2D has a name associated with it, and you must use this name to reference the table when using ODS Graphics. These names are listed in [Table 49.4](#).

**Table 49.4** ODS Tables Produced by PROC KRIGE2D

| ODS Table Name                 | Description                                                         | Statement | Option         |
|--------------------------------|---------------------------------------------------------------------|-----------|----------------|
| <a href="#">KrigInfo</a>       | Kriging analysis general information                                | PROC      | Default output |
| <a href="#">ModelInfo</a>      | Parameters of the covariance model used in current kriging analysis | PROC      | Default output |
| <a href="#">NObs</a>           | Number of observations read and used                                | PROC      | Default output |
| <a href="#">StoreInfo</a>      | Input item store identity information                               | RESTORE   | Default output |
| <a href="#">StoreModelInfo</a> | Input item direction angles and models information                  | RESTORE   | INFO           |
| <a href="#">StoreVarInfo</a>   | Input item store variables and their statistics                     | RESTORE   | INFO           |

---

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “[Statistical Graphics Using ODS](#).”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the **ODS GRAPHICS ON** statement). For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS](#).”



The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “A Primer on ODS Statistical Graphics” on page 599 in Chapter 21, “Statistical Graphics Using ODS.”

For additional control of the graphics that are displayed, see the PLOTS option in the section “PROC KRIGE2D Statement” on page 3801.

## ODS Graph Names

PROC KRIGE2D assigns a name to each graph it creates by using ODS Graphics. You can use these names to reference the graphs when using ODS Graphics. You must also specify the PLOTS= option indicated in Table 49.5.

**Table 49.5** Graphs Produced by PROC KRIGE2D

| ODS Graph Name   | Plot Description                                                                                                    | Statement | Option           |
|------------------|---------------------------------------------------------------------------------------------------------------------|-----------|------------------|
| ObservationsPlot | Scatter plot of observed data and colored markers indicating observed values                                        | PROC      | PLOTS=OBSERV     |
| PredictionPlot   | Contour plots of the kriging prediction, surface of the prediction error, and outlines of the observation locations | PROC      | PLOTS=PREDICTION |
| Semivariogram    | Plots of the semivariogram models used for all prediction tasks                                                     | PROC      | PLOTS=SEMIVAR    |

## Examples: KRIGE2D Procedure

### Example 49.1: Spatial Prediction of Pollutant Concentration

The example in the section “Example 102.1: Aspects of Semivariogram Model Fitting” on page 8648 in the VARIOGRAM procedure investigates fitting of a theoretical model to describe spatial correlation in a study of 138 simulated arsenic logarithm concentration ( $\log As$ ) observations. These observations form the `logAsData` data set, which is treated as actual data for illustration in the examples.

In this example, you use the `logAsData` data set and the semivariogram analysis results to predict the `logAs` variable values across space in a specified square region of size 500 km  $\times$  500 km. Your goal is to answer scientific questions in your analysis by means of your prediction results. This application highlights the impact of the correlation model choice on predictions. The example in section “Example 49.2: Investigating the Effect of Model Specification on Spatial Prediction” on page 3856 examines additional aspects of this impact.

The World Health Organization (WHO) standard for maximum arsenic concentration in drinking water is 10  $\mu\text{g}/\text{lt}$ . Assume that you want to answer the following question: In what percentage of the study area does the Arsenic concentration exceed the WHO regulatory standard?

First, you read the `logAsData` data set with the following DATA step:

```

title 'Spatial Prediction of Log-Arsenic Concentration';

data logAsData;
 input East North logAs @@;
 label logAs='log(As) Concentration';
 datalines;
193.0 296.6 -0.68153 232.6 479.1 0.96279 268.7 312.5 -1.02908
 43.6 4.9 0.65010 152.6 54.9 1.87076 449.1 395.8 0.95932
310.9 493.6 -1.66208 287.8 164.9 -0.01779 330.0 8.0 2.06837
225.7 241.7 0.15899 452.3 83.4 -1.21217 156.5 462.5 -0.89031
 11.5 84.4 -0.24496 144.4 335.7 0.11950 149.0 431.8 -0.57251
234.3 123.2 -1.33642 37.8 197.8 -0.27624 183.1 173.9 -2.14558
149.3 426.7 -1.06506 434.4 67.5 -1.04657 439.6 237.0 -0.09074
 36.4 175.2 -1.21211 370.6 244.0 3.28091 452.0 96.5 -0.77081
247.0 86.8 0.04720 413.6 373.2 1.78235 253.5 291.7 0.56132
129.7 111.9 1.34000 352.7 42.1 0.23621 279.3 82.7 2.12350
382.6 290.7 0.86756 188.2 222.8 -1.23308 382.8 154.5 -0.94094
304.4 309.2 -1.95158 337.5 387.2 -1.31294 490.7 189.8 0.40206
159.0 100.1 -0.22272 245.5 329.2 -0.26082 372.1 379.5 -1.89078
417.8 84.1 -1.25176 173.9 407.6 -0.24240 121.5 107.7 1.54509
453.5 313.6 0.65895 143.5 346.7 -0.87196 157.4 125.5 -1.96165
371.8 353.2 -0.59464 358.9 338.2 -1.07133 8.6 437.8 1.44203
395.9 394.2 -0.24144 149.5 58.9 1.17459 453.5 420.6 -0.63951
182.3 85.0 1.00005 21.0 290.1 0.31016 11.1 352.2 -0.88418
131.2 238.4 -0.57184 104.9 6.3 1.12054 247.3 256.0 0.14019
428.4 383.7 0.92448 327.8 481.1 -2.72543 199.2 92.8 -0.05717
453.9 230.1 0.16571 205.0 250.6 0.07581 459.5 271.6 0.93700
229.5 262.8 1.83590 370.4 228.6 2.96611 330.2 281.9 1.79723
354.8 388.3 -3.18262 406.2 222.7 2.41594 254.4 393.1 2.03221
 96.7 85.2 -0.47156 407.2 256.8 0.66747 498.5 273.8 1.03041
417.2 471.4 -1.42766 368.8 424.3 -0.70506 303.0 59.1 1.43070
403.1 264.1 1.64554 21.2 360.8 0.67094 148.2 78.1 2.15323
305.5 310.7 -1.47985 228.5 180.3 -0.68386 161.1 143.3 1.07901
 70.5 155.1 0.54652 363.1 282.6 -0.43051 86.0 472.5 -1.18855
175.9 105.3 -2.08112 96.8 426.3 1.56592 475.1 453.1 -1.53776
125.7 485.4 1.40054 277.9 201.6 -0.54565 406.2 125.0 -1.38657
 60.0 275.5 -0.59966 431.3 494.6 -0.36860 399.9 399.0 -0.77265
 28.8 311.1 0.91693 166.1 348.2 -0.49056 266.6 83.5 0.67277
 54.7 356.3 0.49596 433.5 460.3 -1.61309 201.7 167.6 -1.40678
158.1 203.6 -1.32499 67.6 230.4 1.14672 81.9 250.0 0.63378
372.0 50.7 0.72445 26.4 264.6 1.00862 300.1 91.7 -0.74089
303.0 447.4 1.74589 108.4 386.2 1.12847 55.6 191.7 0.95175
 36.3 273.2 1.78880 94.5 298.3 -2.43320 366.1 187.3 -0.80526
130.7 389.2 -0.31513 37.2 324.2 0.24489 295.5 211.8 0.41899
 58.6 206.2 0.18495 346.3 142.8 -0.92038 484.2 215.9 0.08012
451.4 415.7 0.02773 58.9 86.5 0.17652 212.6 363.9 0.17215
378.7 407.6 0.51516 265.9 305.0 -0.30718 123.2 314.8 -0.90591
 26.9 471.7 1.70285 16.5 7.1 0.51736 255.1 472.6 2.02381
111.5 148.4 -0.09658 440.4 375.0 1.23285 406.4 19.5 1.01181
321.2 65.8 -0.02095 466.4 357.1 -0.49272 2.0 484.6 0.50994
200.9 205.1 0.43543 30.3 337.0 1.60882 297.0 12.7 1.79824
158.2 450.7 0.05295 122.8 105.3 1.53936 417.8 329.7 -2.08124
;

```

For prediction of the logAs values in the specified area, assume a rectangular grid of nodes with an equal spacing of 5 km between neighboring nodes in the north and east directions. This produces a total of  $101 \times 101 = 10201$  prediction locations.

In the section “[Example 102.1: Aspects of Semivariogram Model Fitting](#)” on page 8648 in the VARIOGRAM procedure, you saved the selected fitted model that resulted from the correlation analysis into the SemivAsStore item store as shown in the following statements:

```
ods graphics on;

proc variogram data=logAsData plots=none;
 store out=SemivAsStore / label='LogAs Concentration Models';
 compute lagd=5 maxlag=40;
 coord xc=East yc=North;
 model form=auto (mlist=(exp,gau,mat) nest=1 to 2);
 var logAs;
run;
```

In the KRIGE2D procedure you specify the name of the item store you want to use for prediction input in the **IN=** option of the **RESTORE** statement. You request use of the selected model for prediction by specifying the **STORESELECT** option in the **MODEL** statement.

The **INFO** option of the **RESTORE** statement produces a table with information about the selected fitted model in the item store. To review all models in the input item store, specify the two **INFO** option suboptions. In particular, specify the **DET** suboption to request details about all additional fitted models that are included in the item store and the **ONLY** suboption to suppress prediction and produce only the tables about the item store, as shown in the following statements:

```
proc krige2d data=logAsData outest=pred plots=none;
 restore in=SemivAsStore / info(det only);
 coordinates xc=East yc=North;
 predict var=logAs;
 model storeselect;
 grid x=0 to 500 by 5 y=0 to 500 by 5;
run;
```

PROC KRIGE2D produces a table with general information about the input item store identity, as shown in [Output 49.1.1](#).

**Output 49.1.1** PROC KRIGE2D and Input Item Store General Information

| Spatial Prediction of Log-Arsenic Concentration |                            |
|-------------------------------------------------|----------------------------|
| The KRIGE2D Procedure                           |                            |
| Correlation Model Item Store Information        |                            |
| Input Item Store                                | WORK.SEMIVASSTORE          |
| Item Store Label                                | LogAs Concentration Models |
| Data Set Created From                           | WORK.LOGASDATA             |
| By-group Information                            | No By-groups Present       |
| Created By                                      | PROC VARIOGRAM             |
| Date Created                                    | 07JUN12:11:31:33           |

The second table in [Output 49.1.2](#) itemizes the variables in the item store and displays the sample mean and standard deviation of their data set of origin. Hence, the values shown in [Output 49.1.2](#) refer to the observations in the logAsData data set.

**Output 49.1.2** Variables in the Input Item Store

| Item Store Variables |          |               |
|----------------------|----------|---------------|
| Variable             | Mean     | Std Deviation |
| logAs                | 0.084309 | 1.527707      |

The table in [Output 49.1.3](#) presents all the correlation models fitted to the arsenic logarithm logAs empirical semivariance that are saved in the SemivAsStore item store.

**Output 49.1.3** Angle and Models Information in the Input Item Store

| Item Store Models For logAs |         |
|-----------------------------|---------|
| Class                       | Model   |
| 1                           | Gau-Gau |
|                             | Gau-Mat |
| 2                           | Exp-Gau |
| 3                           | Exp-Mat |
| 4                           | Mat     |
| 5                           | Gau     |
| 6                           | Exp     |
|                             | Exp-Exp |
|                             | Mat-Exp |
|                             | Gau-Exp |

According to [Output 49.1.3](#), the Gaussian-Gaussian model is the selected model for the empirical semivariance fit based on the specific weighted least squares fit and ranking criteria. In the section “[Example 102.1: Aspects of Semivariogram Model Fitting](#)” on page 8648 in the VARIOGRAM procedure, it is noted that all fitted models in the first five equivalence classes produce very similar semivariograms, and this is likely to lead to similar results in prediction analysis. For comparison purposes, you choose to examine the selected model, in addition to the exponential model in the SemivAsStore item store. As shown in [Output 49.1.3](#), the exponential model is one of the least well-fit models based on the criteria used for the specific fit. You are interested in comparing the predictions from each one of these two models, and you examine their impact on your analysis.

The default item store model selection is the model on top of the list in [Output 49.1.3](#). Hence, you specify the `STORESELECT` option in the `MODEL` statement without any suboptions, and it invokes the Gaussian-Gaussian model from the SemivAsStore item store. You assign the label `SELMODEL` to the corresponding `MODEL` statement.

You also specify a second **MODEL** statement with the label **EXPMODEL** to request prediction based on the exponential correlation form. In this case you specify the **STORESELECT(MODEL=)** option in the **MODEL** statement to request the desired form.

You omit the **INFO** option from the **RESTORE** statement. You specify the **PRED** and the **SEMIVAR** options in the **PLOTS** option of the **PROC KRIGE2D** statement to produce plots of the predicted values and the semivariance model, respectively, for each **MODEL** statement. You request that the prediction output be saved in the **Pred** output data set.

You satisfy the preceding requests by specifying the following statements:

```
proc krige2d data=logAsData outest=Pred plots(only)=(pred semivar);
 restore in=SemivAsStore;
 coordinates xc=East yc=North;
 predict var=logAs;
 SelModel: model storeselect;
 ExpModel: model storeselect(model=exp);
 grid x=0 to 500 by 5 y=0 to 500 by 5;
run;
```

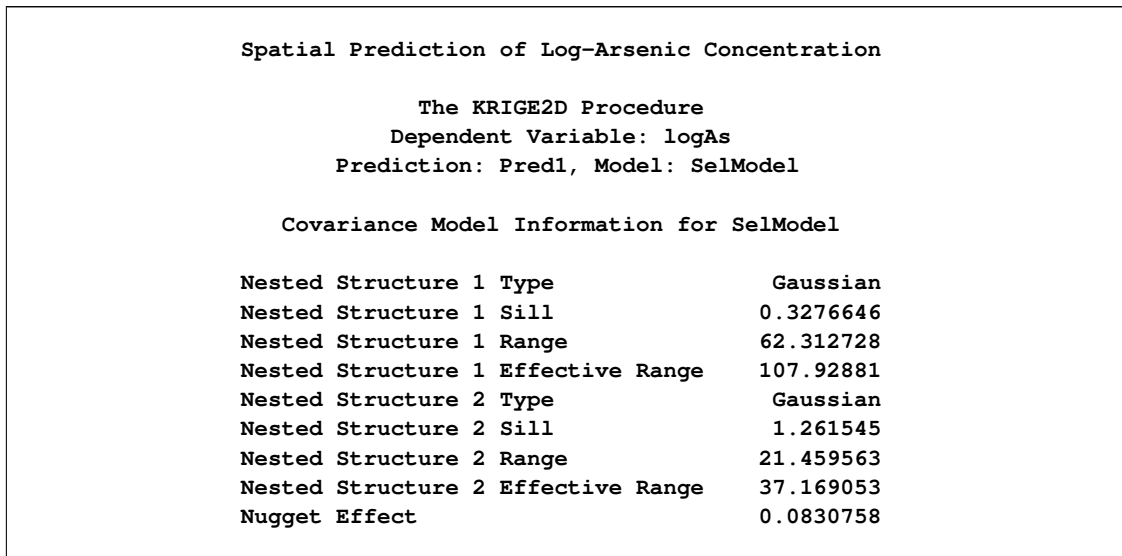
When you run these statements, in addition to the input item store information table, **PROC KRIGE2D** also produces the number of observations table and general kriging process information, as shown in [Output 49.1.4](#).

**Output 49.1.4** Number of Observations and Kriging Information Tables

|                                                 |        |
|-------------------------------------------------|--------|
| Spatial Prediction of Log-Arsenic Concentration |        |
| The KRIGE2D Procedure                           |        |
| Dependent Variable: logAs                       |        |
| Number of Observations Read                     | 138    |
| Number of Observations Used                     | 138    |
| Kriging Information                             |        |
| Prediction Grid Points                          | 10201  |
| Type of Analysis                                | Global |

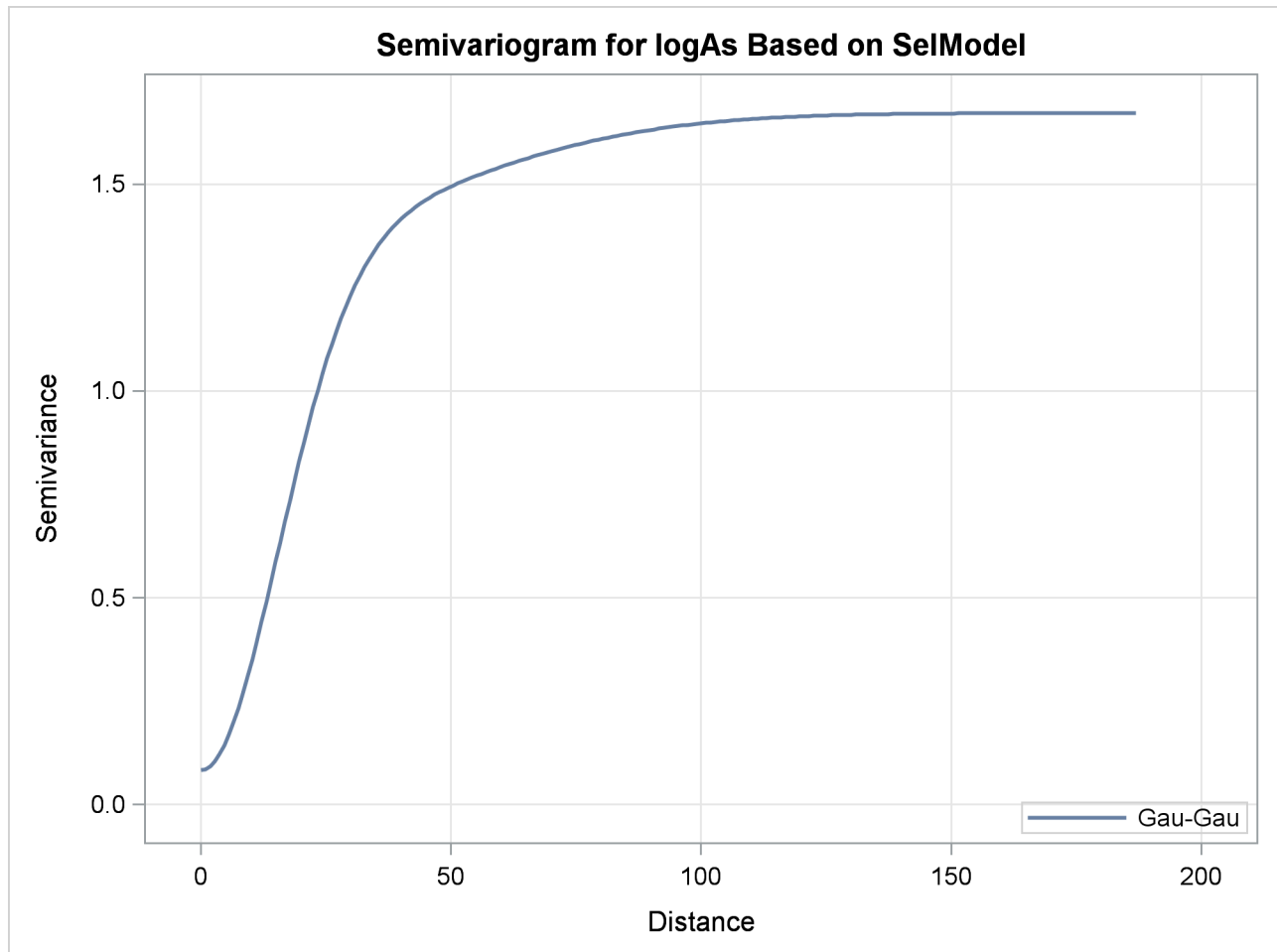
**PROC KRIGE2D** first uses the Gaussian-Gaussian model. The table in [Output 49.1.5](#) shows the saved parameter values of the fitted Gaussian-Gaussian model in the **SemivAsStore** item store. **PROC KRIGE2D** uses these parameters for the prediction based on the selected model.

**Output 49.1.5** Information about the Gaussian-Gaussian Model



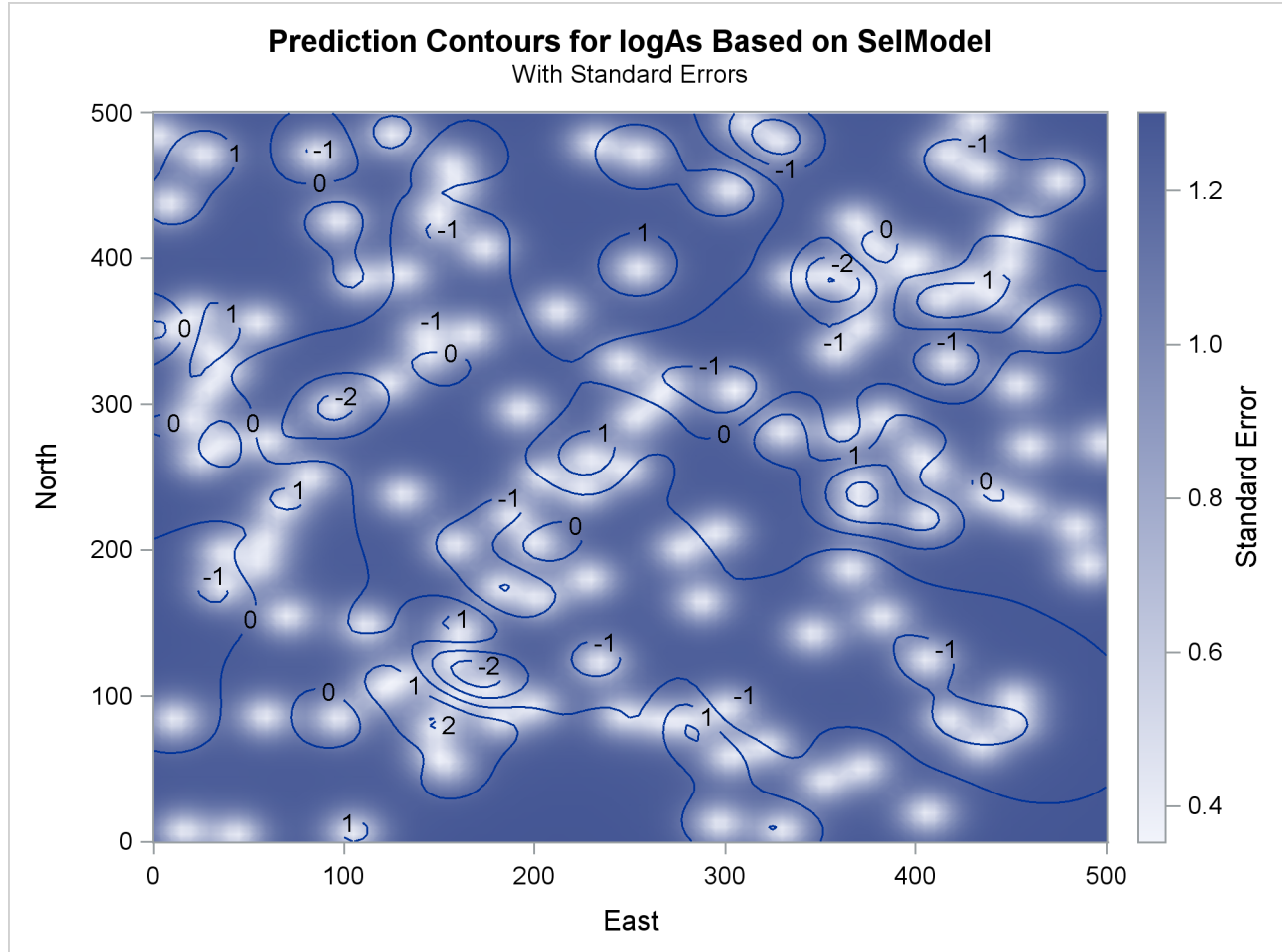
The semivariogram of the Gaussian-Gaussian model with the parameters shown in [Output 49.1.5](#) is depicted in [Output 49.1.6](#).

**Output 49.1.6** Gaussian-Gaussian Semivariogram Model Used in Kriging Predictions



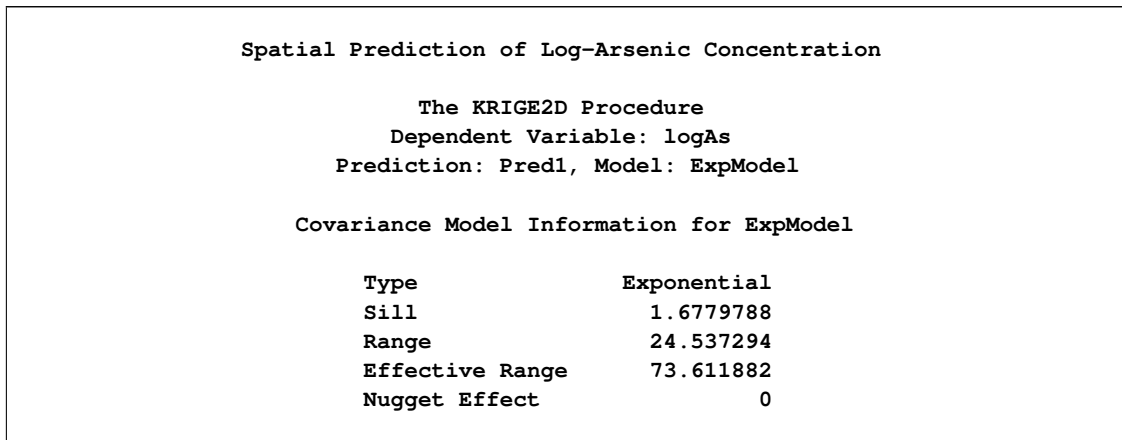
Output 49.1.7 is a map of the kriging prediction of the arsenic concentration values  $\log As$  in the specified domain. The prediction error surface shows a naturally increasing error as you move farther away from the observation locations. Interestingly, kriging predicts a small area of increased arsenic concentration values located in the central-eastern part of the domain. The WHO threshold of  $10 \mu\text{g}/\text{lt}$  for the maximum allowed arsenic concentration in water translates into about 2.3 in the log scale, and the particular area exhibits values in excess of 3. Due to the suggested violation of the WHO standard, this particular area is very likely to be the focus of further environmental risk analysis.

**Output 49.1.7** Predicted Arsenic Logarithm Values with Gaussian-Gaussian Covariance



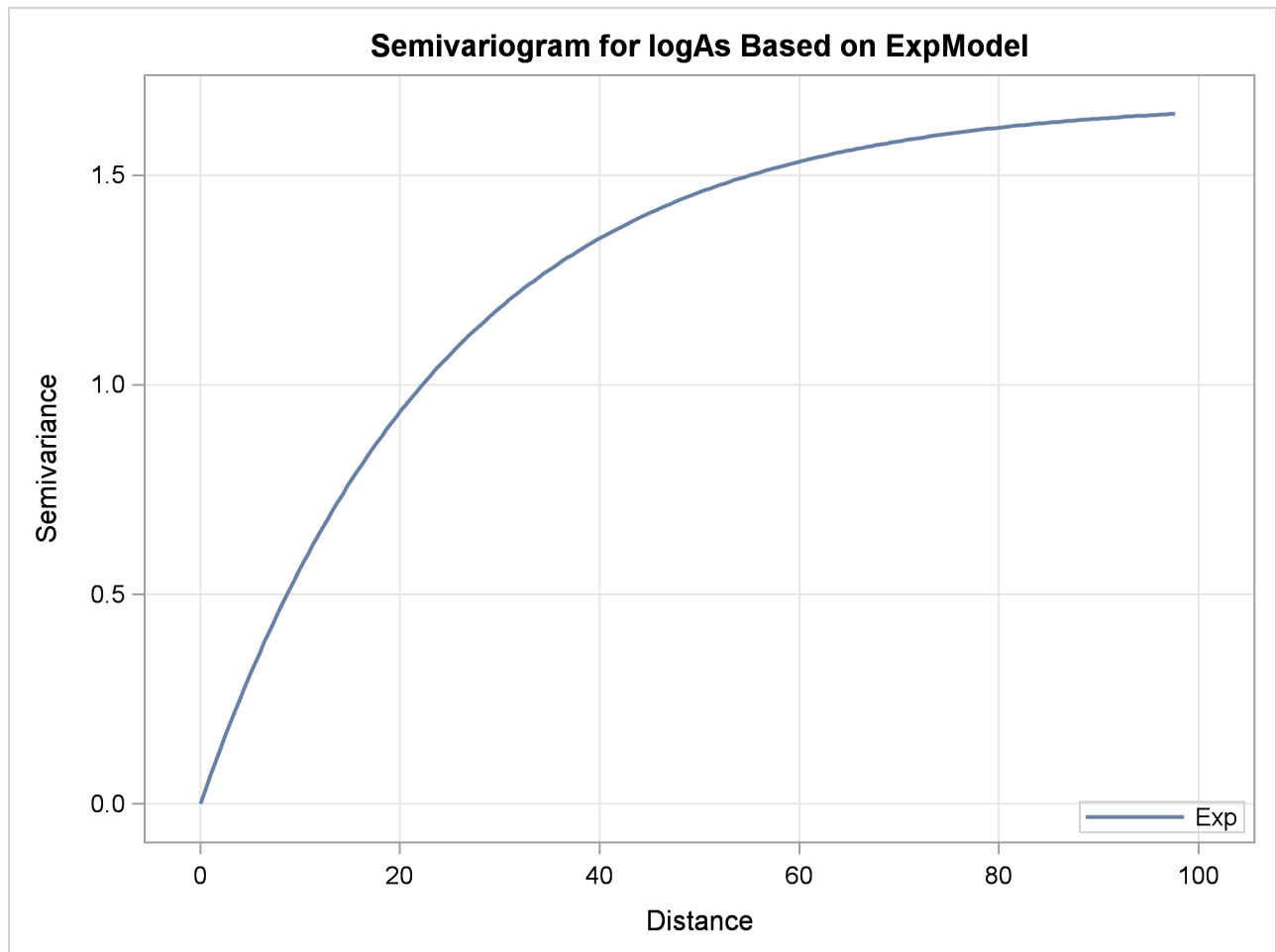
Next, PROC KRIGE2D performs prediction with the exponential model. The model parameters are also read from the SemivAsStore item store and are shown in Output 49.1.8.

**Output 49.1.8** Information about the Exponential Model



Output 49.1.9 illustrates the semivariogram of the nested exponential model where its parameter values are those shown in Output 49.1.8.

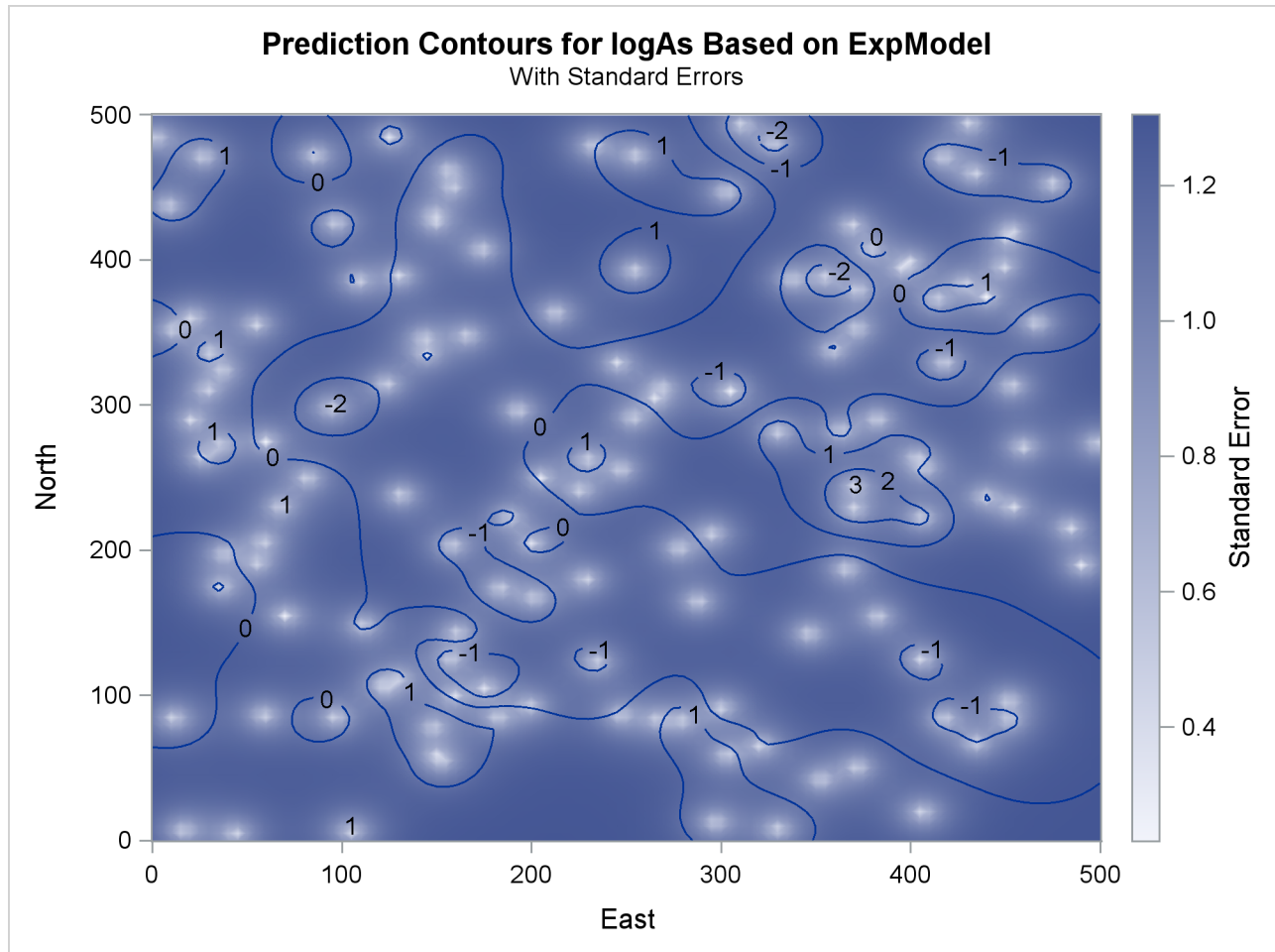
**Output 49.1.9** Exponential Semivariogram Model Used in Kriging Predictions





The prediction plot for the exponential model is shown in [Output 49.1.10](#). Prediction values and spatial patterns are similar overall to those of the Gaussian-Gaussian case. Clearly, although both models predict the same basic characteristics for the arsenic logarithm concentration distribution, the exponential model suggests a more limited spatial variability in closely neighboring locations. The lack of a nugget effect in the exponential model justifies this behavior. Also, the exponential model predictions seem less inclined to deviate farther away from the near-zero mean than the Gaussian-Gaussian model predictions. The prediction error reaches about the same upper values for both models, though its low values are slightly smaller in the exponential model.

**Output 49.1.10** Predicted Arsenic Logarithm Values with Exponential Covariance



In the following two-step computation, you proceed to compute the percentage of the study area where the arsenic concentration exceeds the WHO regulatory standard according to your predictions. First, a DATA step marks the arsenic predicted values in excess of the WHO concentration threshold of  $10 \mu\text{g}/\text{lt}$  and saves the outcome into an indicator variable `OverLimit`. The DATA step input is the prediction `Pred` output data set, where the logarithm arsenic prediction is stored in the estimate variable. The DATA step also transforms the arsenic logarithm values back into arsenic concentration values to compare them to the threshold value. You use the following statements:

```

data AsOverLimit;
 set Pred;
 OverLimit = (exp(estimate) > 10) * 100;
run;

```

The second step uses the MEANS procedure to express the selected nodes population, where the WHO arsenic concentration limit violation occurs, as a percentage of the entire domain area. You study the results of each correlation model separately by specifying the BY statement in the PROC MEANS. The BY variable is the Label variable in the AsOverLimit and Pred data sets. You need to sort the AsOverLimit data prior to using PROC MEANS. You run the following statements:

```

proc sort data=AsOverLimit;
 by Label;
run;
proc means data=AsOverLimit mean;
 var OverLimit;
 by label;
 label Overlimit="Percent above WHO threshold";
run;

ods graphics off;

```

The Gaussian-Gaussian model prediction produces the result in [Output 49.1.11](#). The analysis suggests a minimal occurrence of excessive arsenic concentration in drinking water in about 0.43% of the study region.

#### **Output 49.1.11** Violation of Arsenic Concentration Threshold Using Gaussian-Gaussian Model

```

 Spatial Prediction of Log-Arsenic Concentration
----- Label for the PREDICT/MODEL combination=Pred1.SelModel -----

 The MEANS Procedure

Analysis Variable : OverLimit Percent above WHO threshold

 Mean

 0.4313303

```

The exponential model predicts that the WHO arsenic concentration threshold is exceeded in about 0.27% of the domain, as shown in [Output 49.1.12](#). Although this is still a minimal occurrence of the threshold violation across the region, the exponential model estimates the impact to be at about two thirds of the Gaussian-Gaussian model percentage.

**Output 49.1.12** Violation of Arsenic Concentration Threshold Using Exponential Model

```

 Spatial Prediction of Log-Arsenic Concentration
----- Label for the PREDICT/MODEL combination=Pred1.ExpModel -----
 The MEANS Procedure
 Analysis Variable : OverLimit Percent above WHO threshold

 Mean

 0.2744829

```

The results in [Output 49.1.11](#) and [Output 49.1.12](#) suggest that it might not be possible to provide a unique answer about the area percentage that is affected by increased arsenic concentration. You chose to examine two different correlation models whose performance is relatively similar, and they provide impact estimates that differ by about 37%.

You might conclude that the answer to the initial question about the percentage value lies in the neighborhood of the results given by the two correlation models. Further analysis with more models is necessary to validate this assumption. It is important to note that apart from the continuity model choice, additional factors contribute to this investigation. Such factors could be the use of local instead of global kriging, or even going back to the empirical semivariogram computation stage and repeating the analysis for different possible spatial continuity empirical estimates. A sensible approach to tackle this analysis would be to investigate the range of the impact suggested by all candidate correlation models and to proceed by defining the best and worst case scenarios for the size of the affected area.

Eventually, when it comes to using your findings, it is important to account for the subjective nature of stochastic analysis and multiple possible answers to your questions. In that sense, some scientific questions might be more sensible than others to interpret your results correctly. For instance, you might want to investigate only whether the adversely affected domain percentage is below 1%, rather than attempting to provide a specific value for it. Then, you might consider the preceding findings sufficient, despite any fluctuations in the estimated percentage. In a different scenario, the areas with high pollutant concentration could be populated. Hence, any local health standard violation is probably unacceptable, and it can be crucial that you provide solid and more detailed assessment in that case.

The section “[Example 85.3: Risk Analysis with Simulation](#)” on page 7423 in the SIM2D procedure investigates a different aspect of this study and offers additional perspective about spatial analysis.

---

## **Example 49.2: Investigating the Effect of Model Specification on Spatial Prediction**

It is generally believed that spatial prediction is robust against model specification, while the standard error computation is not so robust. This example investigates the effect of using these different models on the prediction and associated standard errors.

In the section “[Theoretical Semivariogram Model Fitting](#)” on page 8571 in the VARIOGRAM procedure, a particular theoretical semivariogram is fitted to the coal seam thickness data empirical semivariogram. The chosen semivariogram is Gaussian with a scale (sill) of  $c_0 = 7.2881$  and a range of  $a_0 = 30.6239$ .

Another possible model choice could be the spherical semivariogram. First, use a DATA step to input the thickness data:

```

title 'Effect of Model Specification on Prediction';

data thick;
 input East North Thick @@;
 label Thick='Coal Seam Thickness';
 datalines;
 0.7 59.6 34.1 2.1 82.7 42.2 4.7 75.1 39.5
 4.8 52.8 34.3 5.9 67.1 37.0 6.0 35.7 35.9
 6.4 33.7 36.4 7.0 46.7 34.6 8.2 40.1 35.4
 13.3 0.6 44.7 13.3 68.2 37.8 13.4 31.3 37.8
 17.8 6.9 43.9 20.1 66.3 37.7 22.7 87.6 42.8
 23.0 93.9 43.6 24.3 73.0 39.3 24.8 15.1 42.3
 24.8 26.3 39.7 26.4 58.0 36.9 26.9 65.0 37.8
 27.7 83.3 41.8 27.9 90.8 43.3 29.1 47.9 36.7
 29.5 89.4 43.0 30.1 6.1 43.6 30.8 12.1 42.8
 32.7 40.2 37.5 34.8 8.1 43.3 35.3 32.0 38.8
 37.0 70.3 39.2 38.2 77.9 40.7 38.9 23.3 40.5
 39.4 82.5 41.4 43.0 4.7 43.3 43.7 7.6 43.1
 46.4 84.1 41.5 46.7 10.6 42.6 49.9 22.1 40.7
 51.0 88.8 42.0 52.8 68.9 39.3 52.9 32.7 39.2
 55.5 92.9 42.2 56.0 1.6 42.7 60.6 75.2 40.1
 62.1 26.6 40.1 63.0 12.7 41.8 69.0 75.6 40.1
 70.5 83.7 40.9 70.9 11.0 41.7 71.5 29.5 39.8
 78.1 45.5 38.7 78.2 9.1 41.7 78.4 20.0 40.8
 80.5 55.9 38.7 81.1 51.0 38.6 83.8 7.9 41.6
 84.5 11.0 41.5 85.2 67.3 39.4 85.5 73.0 39.8
 86.7 70.4 39.6 87.2 55.7 38.8 88.1 0.0 41.6
 88.4 12.1 41.3 88.4 99.6 41.2 88.8 82.9 40.5
 88.9 6.2 41.5 90.6 7.0 41.5 90.7 49.6 38.9
 91.5 55.4 39.0 92.9 46.8 39.1 93.4 70.9 39.7
 55.8 50.5 38.1 96.2 84.3 40.3 98.2 58.2 39.5
 ;

```

Fitting of the Gaussian model is performed in the section “[Theoretical Semivariogram Model Fitting](#)” on page 8571 in the VARIOGRAM procedure, and the fitting parameters are saved in the SemivStoreGau item store with the following statements:

```

ods graphics on;

proc variogram data=thick noprint;
 store out=SemivStoreGau / label='Thickness Gaussian Model';
 compute lagd=7 maxlag=10;
 coord xc=East yc=North;
 model form=gau;
 var Thick;
run;

```

For prediction with the saved Gaussian model, you use the following statements to run the KRIGE2D procedure with input from the SemivStoreGau item store. You invoke the item store with the **RESTORE** statement. The **STORESELECT** option in the **MODEL** statement that specifies that you want to use the selected model in the item store as input for your prediction.

```
proc krige2d data=thick outest=pred1 noprint;
 restore in=SemivStoreGau;
 coordinates xc=East yc=North;
 predict var=Thick r=60;
 model storeselect;
 grid x=0 to 100 by 10 y=0 to 100 by 10;
run;
```

Then, you run the KRIGE2D procedure by using a spherical model. Start by using the VARIOGRAM procedure to fit a spherical model to the thick data set empirical semivariogram. You specify the **STORE** statement again in PROC VARIOGRAM to save the spherical model estimated parameters in an item store with the name SemivStoreSph. You use the following statements:

```
proc variogram data=thick plots(only)=fit;
 store out=SemivStoreSph / label='Thickness Sph Model';
 compute lagd=7 maxlag=10;
 coord xc=East yc=North;
 model form=sph;
 var Thick;
run;
```

The VARIOGRAM procedure fits the spherical model successfully, and the estimated parameters for this fit are shown in [Output 49.2.1](#).

**Output 49.2.1** Spherical Model Fitting Parameter Estimates

| Effect of Model Specification on Prediction |          |                     |    |         |                   |
|---------------------------------------------|----------|---------------------|----|---------|-------------------|
| The VARIOGRAM Procedure                     |          |                     |    |         |                   |
| Dependent Variable: Thick                   |          |                     |    |         |                   |
| Angle: Omnidirectional                      |          |                     |    |         |                   |
| Current Model: Spherical                    |          |                     |    |         |                   |
| Parameter Estimates                         |          |                     |    |         |                   |
| Parameter                                   | Estimate | Approx<br>Std Error | DF | t Value | Approx<br>Pr >  t |
| Nugget                                      | 0        | 0                   | 8  | .       | .                 |
| Scale                                       | 7.1914   | 0.2827              | 8  | 25.44   | <.0001            |
| Range                                       | 63.2351  | 4.1050              | 8  | 15.40   | <.0001            |

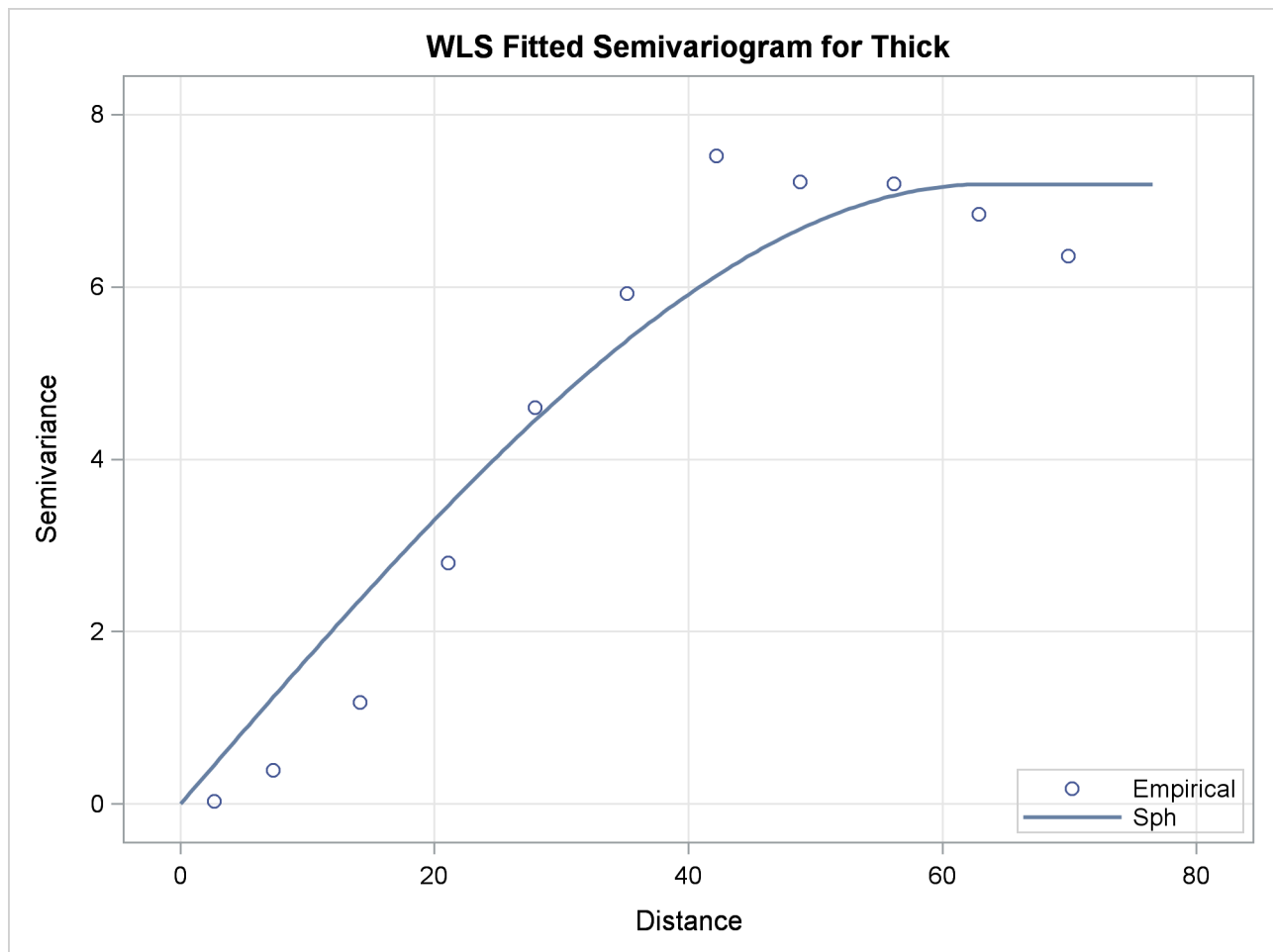
The fit summary is displayed in [Output 49.2.2](#). When compared to the corresponding result in the section “[Theoretical Semivariogram Model Fitting](#)” on page 8571 in the VARIOGRAM procedure, the goodness-of-fit criteria indicate a worse statistical fit for the spherical model compared to the Gaussian.

**Output 49.2.2** Spherical Model Fit Summary

| Fit Summary |              |          |
|-------------|--------------|----------|
| Model       | Weighted SSE | AIC      |
| Sph         | 52.26791     | 23.14336 |

Output 49.2.3 suggests an acceptable fit of the spherical model to the thick data set. Obviously, the fit of the spherical model in the sensitive area near the semivariogram origin is less faithful to the empirical semivariance than the Gaussian model. The following analysis explores the consequence in the kriging prediction of this discrepancy.

**Output 49.2.3** Fitted Spherical and Empirical Thick Semivariogram



For the next step, you run the KRIGE2D procedure by using the spherical model parameters stored in the SemivStoreSph item store. You use the following statements:

```

proc krige2d data=thick outest=pred2 noprint;
 restore in=SemivStoreSph;
 coordinates xc=East yc=North;
 predict var=Thick r=60;
 model storeselect;
 grid x=0 to 100 by 10 y=0 to 100 by 10;
run;

```

Eventually, you compare the prediction results and errors of the two models. You use a DATA step to compute the relative difference of the predicted values and the prediction error for each one of the Gaussian and the spherical models. You store the prediction relative difference in the `prdRelDif` variable and the prediction relative error in the `stdRelDif` variable. You save the output in the `compare` data set with the following statements:

```

data compare;
 merge pred1(rename=(estimate=g_prd stderr=g_std))
 pred2(rename=(estimate=s_prd stderr=s_std));
 prdRelDif = ((g_prd-s_prd) / s_prd) * 100;
 stdRelDif = ((g_std-s_std) / s_std) * 100;
run;

```

The MEANS procedure uses the `compare` data set to produce statistics about the prediction relative difference and error for each one of the `prdRelDif` and `stdRelDif` variables with the following statements:

```

proc means data=compare;
 var prdRelDif stdRelDif;
run;

ods graphics off;

```

Output 49.2.4 shows that on average the predicted values are very close for the two semivariogram models. The mean relative difference in the prediction values is close to zero with a low standard deviation, whereas the relative difference values fluctuate with an absolute maximum of about 5%.

However, note that the mean relative standard error is about -96%. According to the definition of the `stdRelDif` variable, the high negative value indicates that the prediction error difference between the two models is very close to the spherical model prediction error. Hence, the prediction standard error of the spherical model is substantially larger than that of the Gaussian model. In fact, the prediction relative error never gets smaller than about 66% for the two models, where the negative sign in the Minimum and Maximum columns in Output 49.2.4 means that the prediction error is always greater for the spherical model.

**Output 49.2.4** Comparison of Gaussian and Spherical Models

| Effect of Model Specification on Prediction |     |             |           |             |             |
|---------------------------------------------|-----|-------------|-----------|-------------|-------------|
| The MEANS Procedure                         |     |             |           |             |             |
| Variable                                    | N   | Mean        | Std Dev   | Minimum     | Maximum     |
| prdRelDif                                   | 121 | -0.0544593  | 1.3384023 | -5.0751449  | 5.1926236   |
| stdRelDif                                   | 121 | -96.2515099 | 5.9400029 | -99.8974418 | -65.9275907 |

## Example 49.3: Data Quality and Prediction with Missing Values

Kriging methods depend primarily on your data. The quantity and quality of your observations are important factors in minimizing prediction errors and increasing accuracy in your prediction analysis.

A typical aspect of data quality is measurement accuracy. In principle, the accuracy level of your data is not a parameter in kriging prediction; kriging assumes by definition that your data are perfectly accurate (hard) measurements. Whether you accept this assumption depends on your application. For example, an instrumentation error of  $\pm 1\%$  in the data values might be regarded as considerable in one case, whereas the same level of uncertainty might be trivial within a different framework. Your experience and judgment are crucial when you consider whether observations in a data set might be too noisy for kriging predictions to be useful.

A second aspect of data quality involves the spatial arrangement of your observations. You need to have a sufficient number of observations in order to perform spatial prediction. Also, a key element in minimizing prediction errors is an adequate sampling density. Interpretation of the expressions “sufficient number” and “adequate sampling” is again case-specific. In any event, you want enough measurements so that you can deduce the underlying spatial correlation in the working domain; see also the discussion in the section “Choosing the Size of Classes” on page 8623 in the VARIOGRAM procedure.

This example focuses on the effects of different sampling densities on the prediction analysis. The demonstration is a slight variation of the example in the section “Getting Started: KRIGE2D Procedure” on page 3795. Specifically, you use the same correlation structure and prediction grid. However, the thick data set, is modified as follows: three values in the central area of the grid are assumed missing, namely the observation values at locations  $s_1 = (x_1, y_1) = (55.8, 50.5)$ ,  $s_2 = (x_2, y_2) = (52.8, 68.9)$ , and  $s_3 = (x_3, y_3) = (52.9, 32.7)$ . These locations have been selected so that an extended area without observations is created in the domain. The following DATA step is the input for the modified thick data set:

```

title 'Kriging Prediction in the Presence of Missing Values';

data thick;
 input East North Thick @@;
 label Thick='Coal Seam Thickness';
 datalines;
 0.7 59.6 34.1 2.1 82.7 42.2 4.7 75.1 39.5
 4.8 52.8 34.3 5.9 67.1 37.0 6.0 35.7 35.9
 6.4 33.7 36.4 7.0 46.7 34.6 8.2 40.1 35.4
 13.3 0.6 44.7 13.3 68.2 37.8 13.4 31.3 37.8
 17.8 6.9 43.9 20.1 66.3 37.7 22.7 87.6 42.8
 23.0 93.9 43.6 24.3 73.0 39.3 24.8 15.1 42.3
 24.8 26.3 39.7 26.4 58.0 36.9 26.9 65.0 37.8
 27.7 83.3 41.8 27.9 90.8 43.3 29.1 47.9 36.7
 29.5 89.4 43.0 30.1 6.1 43.6 30.8 12.1 42.8
 32.7 40.2 37.5 34.8 8.1 43.3 35.3 32.0 38.8
 37.0 70.3 39.2 38.2 77.9 40.7 38.9 23.3 40.5
 39.4 82.5 41.4 43.0 4.7 43.3 43.7 7.6 43.1
 46.4 84.1 41.5 46.7 10.6 42.6 49.9 22.1 40.7
 51.0 88.8 42.0 52.8 68.9 . 52.9 32.7 .
 55.5 92.9 42.2 56.0 1.6 42.7 60.6 75.2 40.1
 62.1 26.6 40.1 63.0 12.7 41.8 69.0 75.6 40.1
 70.5 83.7 40.9 70.9 11.0 41.7 71.5 29.5 39.8
 ;

```



```

78.1 45.5 38.7 78.2 9.1 41.7 78.4 20.0 40.8
80.5 55.9 38.7 81.1 51.0 38.6 83.8 7.9 41.6
84.5 11.0 41.5 85.2 67.3 39.4 85.5 73.0 39.8
86.7 70.4 39.6 87.2 55.7 38.8 88.1 0.0 41.6
88.4 12.1 41.3 88.4 99.6 41.2 88.8 82.9 40.5
88.9 6.2 41.5 90.6 7.0 41.5 90.7 49.6 38.9
91.5 55.4 39.0 92.9 46.8 39.1 93.4 70.9 39.7
55.8 50.5 . 96.2 84.3 40.3 98.2 58.2 39.5
;

```

```
ods graphics on;
```

**NOTE:** Here you assume prior knowledge of the correlation structure model, because its parameters are based on the complete thick data set. A covariance model extracted from the incomplete set with the missing values would be a covariance model coming from a different data set; hence, it is likely to have different parameters.

After you define the modified data set, you run PROC KRIGE2D and request the **OBSERVATIONS** plot with the **SHOWMISSING** suboption. You also request two instances of the **PREDICTION** plot: one that displays the prediction surface and contours, and another that plots the kriging standard error surface and contours. In both of these **PREDICTION** plots you specify that the observations be shown as gradient markers with outlines. The following statements compute the kriged predictions and produce the requested graphics:

```

proc krige2d data=thick outest=predictions
 plots(only)=(observ(showmissing)
 pred(fill=pred line=pred obs=linegrad)
 pred(fill=se line=se obs=linegrad));
 coordinates xc=East yc=North;
 predict var=Thick r=60;
 model scale=7.4599 range=30.1111 form=gauss;
 grid x=0 to 100 by 2.5 y=0 to 100 by 2.5;
run;

ods graphics off;

```

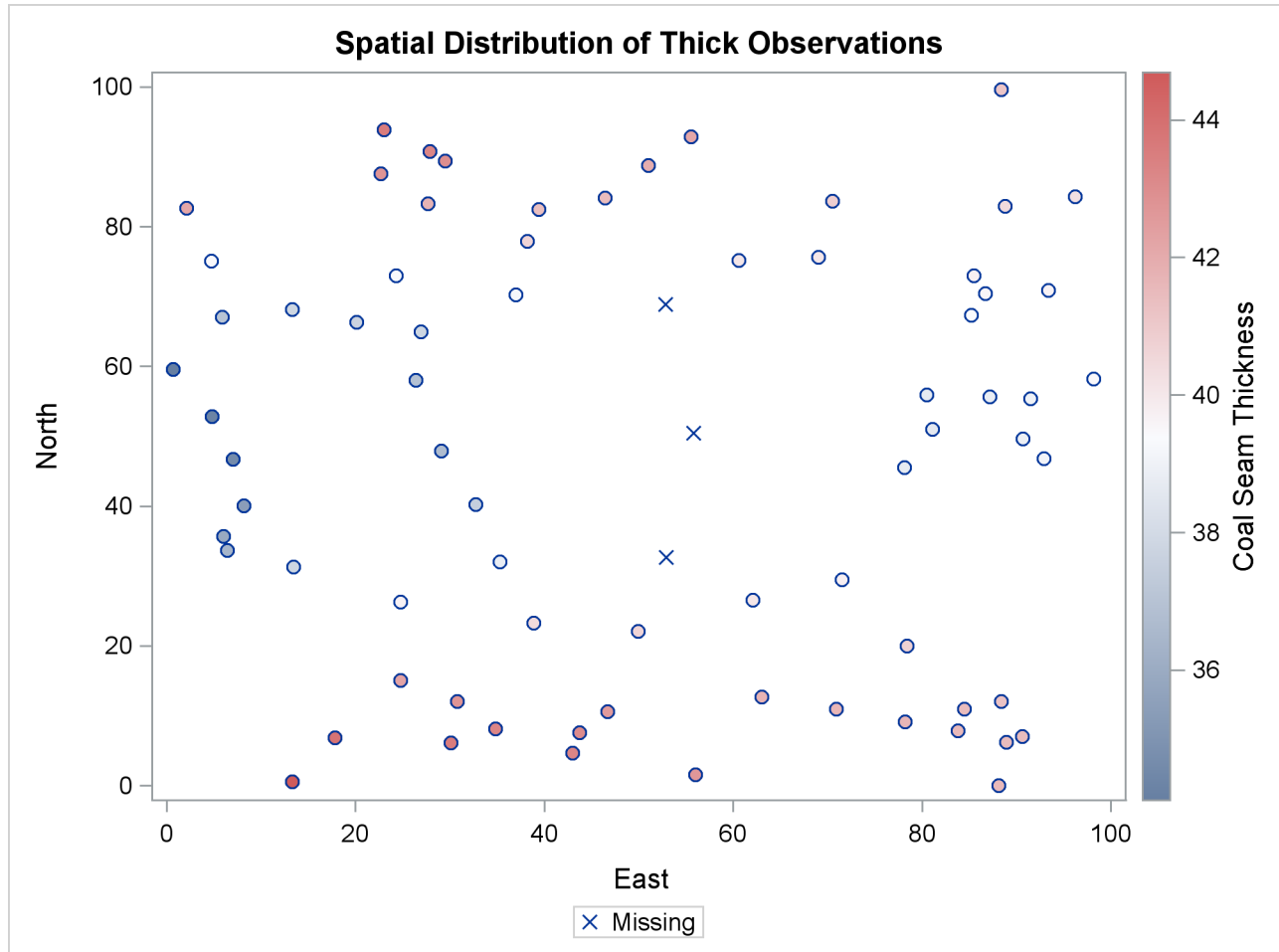
The number of observations table indicates the three missing values in [Output 49.3.1](#).

#### Output 49.3.1 Number of Observations for the Modified thick Data Set

| Kriging Prediction in the Presence of Missing Values |    |
|------------------------------------------------------|----|
| The KRIGE2D Procedure                                |    |
| Dependent Variable: Thick                            |    |
| Number of Observations Read                          | 75 |
| Number of Observations Used                          | 72 |

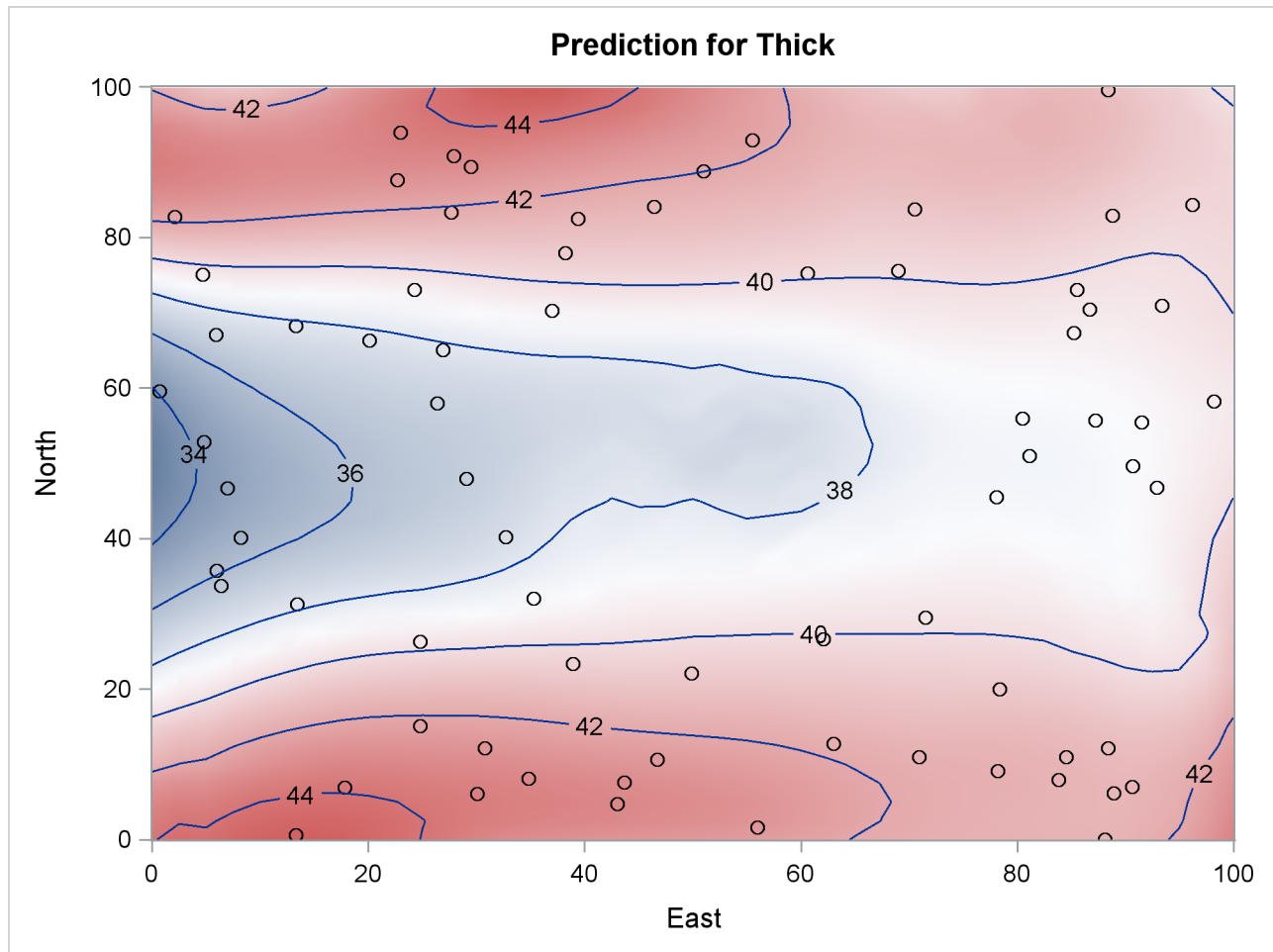
Output 49.3.2 is a scatter plot of the modified observed data. The `SHOWMISSING` suboption produces marks in the observations plot that conveniently indicate the locations  $s_1$ ,  $s_2$ , and  $s_3$  of the missing values. Consequently, Output 49.3.2 displays an extended area with no observed Thick values in the central part of the domain.

**Output 49.3.2** Scatter Plot of the Observations Spatial Distribution



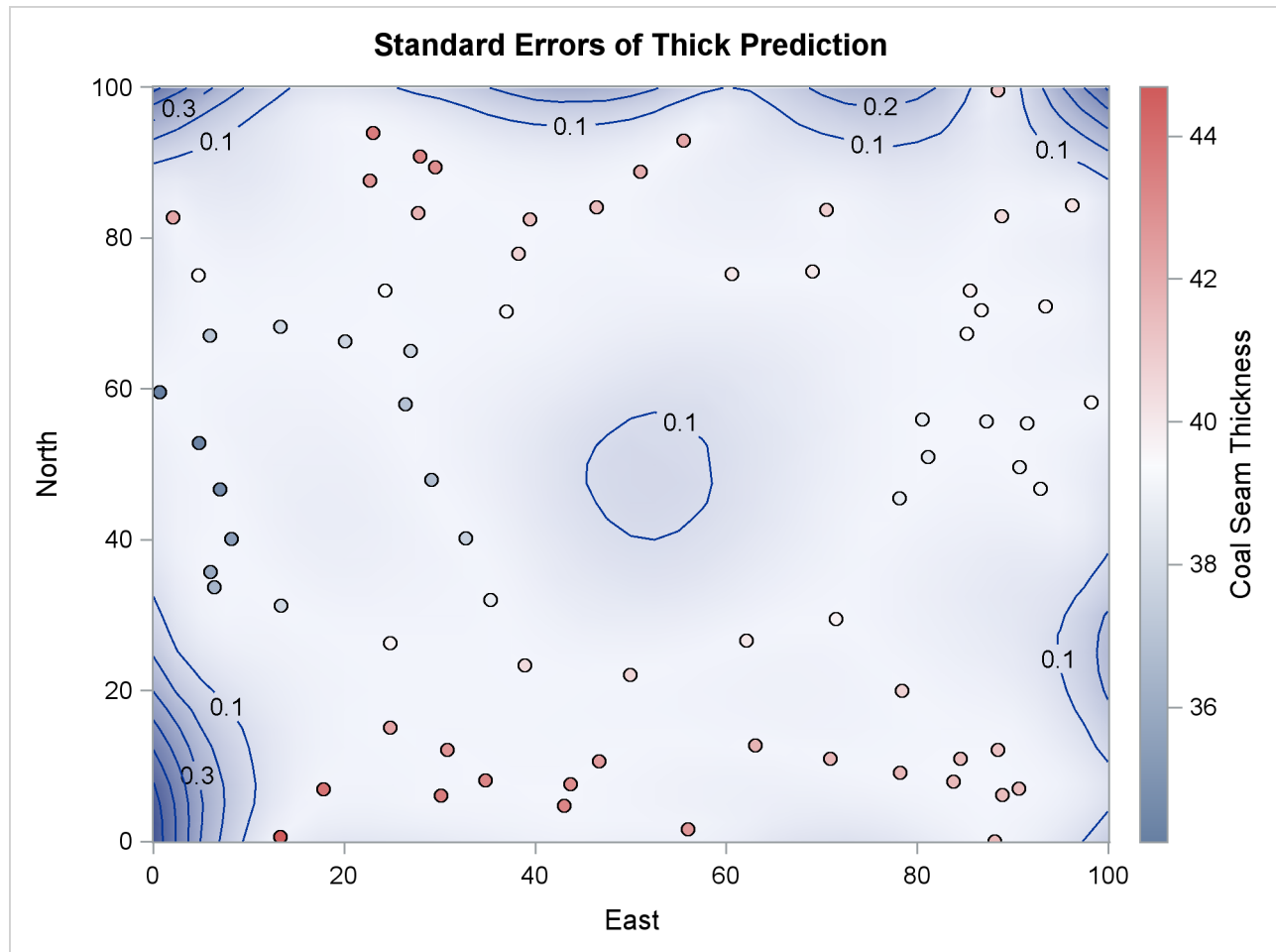
Predictions at grid points with few neighboring data points rely heavily on the underlying covariance structure. The covariance model has a range of about 30,000 feet, which suggests that within this range a grid point might have no data neighbors at all and still obtain a prediction value on the basis of the correlation structure alone. This type of behavior is demonstrated in the Output 49.3.3, which shows a circular region in the center of the plot that has no data points. Predictions at the nodes in this area are mostly influenced by the covariance structure.

You can see the impact of this effect on the predictions if you compare the prediction contours in the Output 49.3.3 to the ones in Figure 49.4. Despite the contribution of the neighboring Thick data values to the predictions within the area of no observations, the outcome is clearly altered by the absence of observations at the locations  $s_1$ ,  $s_2$ , and  $s_3$ .

**Output 49.3.3** Surface Plot and Contours of Kriged Coal Seam Thickness

A noticeable difference is also apparent in the plot of the prediction standard errors. [Output 49.3.4](#) displays these errors, and you can compare it to the standard error surface in [Figure 49.4](#). The comparison shows a slight difference in the color gradient within the area of the missing data values. [Output 49.3.4](#) uses standard error contours to enhance the effect of this difference.

The lack of information from the removed data results in an increase of the prediction uncertainty at the grid nodes that are most remotely situated from any observation in the central part of the domain. According to [Output 49.3.4](#), the standard error at these nodes is almost comparable to the error observed near the borders of the domain, where the nodes of the prediction grid have relatively fewer data neighbors than other nodes in the domain.

**Output 49.3.4** Surface Plot and Contours of Prediction Standard Errors

On a side note, **PREDICTION** plots display only observations with nonmissing values, as the plots in Output 49.3.3 and Output 49.3.4 demonstrate.

---

## References

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# Chapter 50

## The LATTICE Procedure

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## Overview: LATTICE Procedure

The LATTICE procedure computes the analysis of variance and analysis of simple covariance for data from an experiment with a lattice design. PROC LATTICE analyzes balanced square lattices, partially balanced square lattices, and some rectangular lattices.

In balanced square lattices, the number of treatments is equal to the square of the number of units per block. Incomplete blocks are grouped to form mutually orthogonal replications. The number of replicates in the basic plan is always 1 plus the number of units per block.

Partially balanced square lattices are similar to balanced lattices, although the number of replicates can vary. Partially balanced designs are constructed of the replicates in the basic plan, but not all replicates are included the same number of times, and some might not be included at all.

In rectangular lattices, there are  $k$  units per block and  $k(k+1)$  treatments. As in square lattices, blocks are grouped to form mutually orthogonal replicates in the basic plan. PROC LATTICE can analyze simple rectangular lattices (two orthogonal replications) and triple rectangular lattices (three orthogonal replications). The experiment can include several repetitions of the basic plan.

The LATTICE procedure determines from the data set which type of design has been used. It also checks to see whether the design is valid and displays an appropriate message if it is not.

## Getting Started: LATTICE Procedure

An example of a balanced square design is an experiment to investigate the effects of nine diets on the growth rate of pigs.

In some breeds of pigs, past experience has shown that a large part of the total variation in growth rates between animals can be attributed to the litter. Therefore, this experiment is planned so that litter differences do not contribute to the intrablock error.

First, the pigs are separated into sets of three litter-mates. Each block is assigned two sets of the three litter-mates. In a given block, one pig from each set receives a diet. Therefore, the experimental unit is a pair of pigs feeding in a particular pen on one of the nine diets. The response variable, growth rate, is the sum of the growth rates for the two pigs in a particular pen. To get the adjusted diet mean per pig, the adjusted treatment mean for the pen must be divided by 2.

The special numeric SAS variables named Group, Block, Treatment, and Rep must be used to define the design. In this example, the Treatment variable ranges from 1 to 9 and indicates the particular diet. The Block variable is 1, 2, or 3 and indicates the pen containing the two pigs. The Group variable ranges from 1 to 4 and specifies which replication within the basic plan includes the experimental unit. In this example, you would not use the Rep variable since the entire basic plan is not replicated.

You can use the following DATA step and PROC LATTICE statement to analyze this experiment. The response variable is Weight.

```

title 'Examining the Growth Rate of Pigs';

data Pigs;
 input Group Block Treatment Weight @@;
 datalines;
1 1 1 2.20 1 1 2 1.84 1 1 3 2.18 1 2 4 2.05 1 2 5 0.85
1 2 6 1.86 1 3 7 0.73 1 3 8 1.60 1 3 9 1.76
2 1 1 1.19 2 1 4 1.20 2 1 7 1.15 2 2 2 2.26 2 2 5 1.07
2 2 8 1.45 2 3 3 2.12 2 3 6 2.03 2 3 9 1.63
3 1 1 1.81 3 1 5 1.16 3 1 9 1.11 3 2 2 1.76 3 2 6 2.16
3 2 7 1.80 3 3 3 1.71 3 3 4 1.57 3 3 8 1.13
4 1 1 1.77 4 1 6 1.57 4 1 8 1.43 4 2 2 1.50 4 2 4 1.60
4 2 9 1.42 4 3 3 2.04 4 3 5 0.93 4 3 7 1.78
;

proc lattice data=Pigs;
 var Weight;
run;

```

The SAS code produces the output shown in [Figure 50.1](#).

**Figure 50.1** Output from Example LATTICE Procedure

| Examining the Growth Rate of Pigs |    |                |             |
|-----------------------------------|----|----------------|-------------|
| The Lattice Procedure             |    |                |             |
| Analysis of Variance for Weight   |    |                |             |
| Source                            | DF | Sum of Squares | Mean Square |
| Replications                      | 3  | 0.07739        | 0.02580     |
| Blocks within Replications (Adj.) | 8  | 1.4206         | 0.1776      |
| Component B                       | 8  | 1.4206         | 0.1776      |
| Treatments (Unadj.)               | 8  | 3.2261         | 0.4033      |
| Intra Block Error                 | 16 | 1.2368         | 0.07730     |
| Randomized Complete Block Error   | 24 | 2.6574         | 0.1107      |
| Total                             | 35 | 5.9609         | 0.1703      |

| Additional Statistics for Weight |         |
|----------------------------------|---------|
| Variance of Means in Same Block  | 0.04593 |
| LSD at .01 Level                 | 0.6259  |
| LSD at .05 Level                 | 0.4543  |
| Efficiency Relative to RCBD      | 120.55  |

| Adjusted Treatment Means for Weight |        |
|-------------------------------------|--------|
| Treatment                           | Mean   |
| 1                                   | 1.8035 |
| 2                                   | 1.7544 |
| 3                                   | 1.9643 |
| 4                                   | 1.7267 |
| 5                                   | 0.9393 |
| 6                                   | 1.8448 |
| 7                                   | 1.3870 |
| 8                                   | 1.4347 |
| 9                                   | 1.5004 |

Diet 3 yields the highest mean growth rate at 1.9643 pounds for the two pigs (0.9822 per pig), while diet 5 has the lowest rate at 0.9393 (0.4696 per pig). The efficiency of the experiment relative to a randomized complete block design is 120.55 percent, so using the lattice design increased precision, producing more accurate estimates of the treatment effects. The different elements of the LATTICE procedure's output are discussed in the "Displayed Output" on page 3872 section.



---

## Syntax: LATTICE Procedure

The following statements are available in the LATTICE procedure:

```
PROC LATTICE < options > ;
 BY variables ;
 VAR variables ;
```

Three specific numeric SAS variables, Group, Block, and Treatment, *must* be present in the data set to which PROC LATTICE is applied. For compatibility with previous releases, the variable Treatment can alternatively be named Treatmnt. A fourth numeric variable named Rep must be present when the design involves repetition of the entire basic plan. (See the “[Input Data Set](#)” on page 3871 section for more information.)

Every numeric variable other than Group, Block, Treatment, or Rep in the input SAS data set may be considered a response variable. A VAR statement tells PROC LATTICE that only the variables listed in the VAR statement are to be considered response variables. If the VAR statement is omitted, then all numeric variables, excluding Group, Block, Treatment, and Rep, are considered response variables. PROC LATTICE performs an analysis for each response variable.

---

## PROC LATTICE Statement

```
PROC LATTICE < options > ;
```

The PROC LATTICE statement invokes the LATTICE procedure.

### **DATA=SAS-data-set**

names the SAS data set to be used by PROC LATTICE. If you omit the DATA= option, the most recently created SAS data set is used.

### **COVARIANCE**

#### **COV**

calculates sums of products for every possible pair of response variables. A sum of products is given for each source of variation in the analysis of variance table. For each pair of response variables, the one appearing later in the data set (or in the VAR statement) is the covariable.

---

## BY Statement

```
BY variables ;
```

You can specify a BY statement with PROC LATTICE to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.

- Specify the NOTSORTED or DESCENDING option in the BY statement for the LATTICE procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

---

## VAR Statement

**VAR** *variables* ;

The VAR statement specifies the response variables. If you do not include a VAR statement, all numeric variables in the data set are considered response variables (except Group, Block, Treatment, and Rep).

---

## Details: LATTICE Procedure

---

### Input Data Set

Four numeric SAS variables, Group, Block, Treatment, and Rep, are used in the input data set to define the lattice design. The Group, Block, and Treatment variables are required in the data set to which PROC LATTICE is applied. For compatibility with previous releases, the third variable can alternatively be named Treatmnt. The Rep variable must be present when the design involves repetition of the entire basic plan.

|           |                                                                                                                                                                                                                                              |
|-----------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Group     | specifies which orthogonal replication in the basic plan includes the experimental unit. Values of Group must be $1, 2, \dots, n$ , where $n$ is the number of replicates in the basic plan.                                                 |
| Block     | specifies the block in which the experimental unit is present. Values of Block must be $1, 2, \dots, m$ , where $m$ is the number of blocks in a replication.                                                                                |
| Treatment | specifies which treatment was applied to the experimental unit. Values of Treatment must be $1, 2, \dots, i$ , where $i$ is the number of treatments in a replication.                                                                       |
| Rep       | specifies which repetition of the basic plan includes the experimental unit. Values of Rep must be $1, 2, \dots, p$ , where $p$ is the number of replications of the entire basic plan. Thus, the experiment has a total of $np$ replicates. |

---

### Missing Values

If a value of Group, Block, Treatment, or Rep is missing, the analysis is not performed and an appropriate error message is displayed.

If a value of a response variable is missing, this entire variable is dropped from the analysis. If other response variables exist that do not have missing values, they are analyzed.

---

## Displayed Output

For each response variable, PROC LATTICE displays the following

- an “Analysis of Variance” table and related statistics, including the following as separate sources of variations:
  - Replications
  - Blocks within Replications (adjusted for treatments)
  - Treatments (unadjusted)
  - Intra-block Error
  - Randomized Complete Block Error

The Blocks within Replications sum of squares is further broken down into “Component A” and “Component B.” If there is no repetition of the basic plan, the Component B sum of squares is the same as the Blocks within Replications sum of squares. If there is repetition of the basic plan, the Component A sum of squares reflects the variation among blocks that contain the same treatments.

The source of variation called Randomized Complete Block Error is the sum of the Blocks within Replications sum of squares and the Intra-block Error sum of squares. It is the appropriate error term if the experimental design is a randomized complete block design, with the replications filling the roles of complete blocks.

- two values for the Variance of Means. For some lattice designs, these are only approximations. The first value is applicable when the two treatments appear in the same block; the other (when it appears) applies when the two treatments never appear in the same block (a possibility in partially balanced and rectangular designs).
- an Average of Variance. Except with small designs, it is sufficient to use this average variance of means for tests between treatments (whether the two treatments appear in the same block or not); see Cochran and Cox (1957).
- the Least Significant Differences (LSDs) at the 0.01 and 0.05 levels of significance, based on the Average of Variance
- Efficiency Relative to RCBD, the efficiency of the lattice design relative to a randomized complete block design. The efficiency is the ratio of the randomized complete block mean squared error to the effective error variance; see Cochran and Cox (1957).
- the Adjusted Treatment Means. These are adjusted for blocks if the relative precision is greater than 105%.

When you specify the COVARIANCE option, PROC LATTICE produces sums of products and the mean product for each source of variation in the analysis of variance table.

## ODS Table Names

PROC LATTICE assigns a name to each table it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in Table 50.1. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

**Table 50.1** ODS Tables Produced by PROC LATTICE

| ODS Table Name    | Description              | PROC LATTICE Option |
|-------------------|--------------------------|---------------------|
| ANOVA             | Analysis of variance     | default             |
| AdjTreatmentMeans | Adjusted treatment means | default             |
| Statistics        | Additional statistics    | default             |

## Example: LATTICE Procedure

### Example 50.1: Analysis of Variance through PROC LATTICE

In the following example, from Cochran and Cox (1957, p. 406), the data are yields (Yield) in bushels per acre of 25 varieties (Treatment) of soybeans. The data are collected in two replications (Group) of 25 varieties in five blocks (Block) containing five varieties each. This is an example of a partially balanced square lattice design.

```
data Soy(drop=plot);
 do Group = 1 to 2;
 do Block = 1 to 5;
 do Plot = 1 to 5;
 input Treatment Yield @@;
 output;
 end;
 end;
 end;
 datalines;
 1 6 2 7 3 5 4 8 5 6 6 16 7 12 8 12 9 13 10 8
 11 17 12 7 13 7 14 9 15 14 16 18 17 16 18 13 19 13 20 14
 21 14 22 15 23 11 24 14 25 14 1 24 6 13 11 24 16 11 21 8
 2 21 7 11 12 14 17 11 22 23 3 16 8 4 13 12 18 12 23 12
 4 17 9 10 14 30 19 9 24 23 5 15 10 15 15 22 20 16 25 19
;

proc print data=Soy;
 id Treatment;
run;

proc lattice data=Soy;
run;
```

The results from these statements are shown in [Output 50.1.1](#) and [Output 50.1.2](#).

**Output 50.1.1** Displayed Output from PROC PRINT

| Treatment | Group | Block | Yield |
|-----------|-------|-------|-------|
| 1         | 1     | 1     | 6     |
| 2         | 1     | 1     | 7     |
| 3         | 1     | 1     | 5     |
| 4         | 1     | 1     | 8     |
| 5         | 1     | 1     | 6     |
| 6         | 1     | 2     | 16    |
| 7         | 1     | 2     | 12    |
| 8         | 1     | 2     | 12    |
| 9         | 1     | 2     | 13    |
| 10        | 1     | 2     | 8     |
| 11        | 1     | 3     | 17    |
| 12        | 1     | 3     | 7     |
| 13        | 1     | 3     | 7     |
| 14        | 1     | 3     | 9     |
| 15        | 1     | 3     | 14    |
| 16        | 1     | 4     | 18    |
| 17        | 1     | 4     | 16    |
| 18        | 1     | 4     | 13    |
| 19        | 1     | 4     | 13    |
| 20        | 1     | 4     | 14    |
| 21        | 1     | 5     | 14    |
| 22        | 1     | 5     | 15    |
| 23        | 1     | 5     | 11    |
| 24        | 1     | 5     | 14    |
| 25        | 1     | 5     | 14    |
| 1         | 2     | 1     | 24    |
| 6         | 2     | 1     | 13    |
| 11        | 2     | 1     | 24    |
| 16        | 2     | 1     | 11    |
| 21        | 2     | 1     | 8     |
| 2         | 2     | 2     | 21    |
| 7         | 2     | 2     | 11    |
| 12        | 2     | 2     | 14    |
| 17        | 2     | 2     | 11    |
| 22        | 2     | 2     | 23    |
| 3         | 2     | 3     | 16    |
| 8         | 2     | 3     | 4     |
| 13        | 2     | 3     | 12    |
| 18        | 2     | 3     | 12    |
| 23        | 2     | 3     | 12    |
| 4         | 2     | 4     | 17    |
| 9         | 2     | 4     | 10    |
| 14        | 2     | 4     | 30    |
| 19        | 2     | 4     | 9     |
| 24        | 2     | 4     | 23    |
| 5         | 2     | 5     | 15    |
| 10        | 2     | 5     | 15    |
| 15        | 2     | 5     | 22    |
| 20        | 2     | 5     | 16    |
| 25        | 2     | 5     | 19    |

**Output 50.1.2** Displayed Output from PROC LATTICE

| The Lattice Procedure               |    |                |             |
|-------------------------------------|----|----------------|-------------|
| Analysis of Variance for Yield      |    |                |             |
| Source                              | DF | Sum of Squares | Mean Square |
| Replications                        | 1  | 212.18         | 212.18      |
| Blocks within Replications (Adj.)   | 8  | 501.84         | 62.7300     |
| Component B                         | 8  | 501.84         | 62.7300     |
| Treatments (Unadj.)                 | 24 | 559.28         | 23.3033     |
| Intra Block Error                   | 16 | 218.48         | 13.6550     |
| Randomized Complete Block Error     | 24 | 720.32         | 30.0133     |
| Total                               | 49 | 1491.78        | 30.4445     |
| Additional Statistics for Yield     |    |                |             |
| Variance of Means in Same Block     |    | 15.7915        |             |
| Variance of Means in Different Bloc |    | 17.9280        |             |
| Average of Variance                 |    | 17.2159        |             |
| LSD at .01 Level                    |    | 12.1189        |             |
| LSD at .05 Level                    |    | 8.7959         |             |
| Efficiency Relative to RCBD         |    | 174.34         |             |

**Output 50.1.2** *continued*

| Adjusted Treatment<br>Means for Yield |         |
|---------------------------------------|---------|
| Treatment                             | Mean    |
| 1                                     | 19.0681 |
| 2                                     | 16.9728 |
| 3                                     | 14.6463 |
| 4                                     | 14.7687 |
| 5                                     | 12.8470 |
| 6                                     | 13.1701 |
| 7                                     | 9.0748  |
| 8                                     | 6.7483  |
| 9                                     | 8.3707  |
| 10                                    | 8.4489  |
| 11                                    | 23.5511 |
| 12                                    | 12.4558 |
| 13                                    | 12.6293 |
| 14                                    | 20.7517 |
| 15                                    | 19.3299 |
| 16                                    | 12.6224 |
| 17                                    | 10.5272 |
| 18                                    | 10.7007 |
| 19                                    | 7.3231  |
| 20                                    | 11.4013 |
| 21                                    | 11.6259 |
| 22                                    | 18.5306 |
| 23                                    | 12.2041 |
| 24                                    | 17.3265 |
| 25                                    | 15.4048 |

The efficiency of the experiment relative to a randomized complete block design is 174.34%. Precision is gained using the lattice design via the recovery of intra-block error information, enabling more accurate estimates of the treatment effects. Variety 8 of soybean had the lowest adjusted treatment mean (6.7483 bushels per acre), while variety 11 of soybean had the highest adjusted treatment mean (23.5511 bushels per acre).

---

## References

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- Comstock, R. E., Peterson, W. J., and Stewart, H. A. (1948), "An Application of the Balanced Lattice Design in a Feeding Trial with Swine," *Journal of Animal Science*, 7, 320–331.
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- Robinson, H. F. and Watson, G. S. (1949), *Analysis of Simple and Triple Rectangular Designs*, Technical Report 88, North Carolina Agricultural Experiment Station.

# Chapter 51

## The LIFEREG Procedure

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---

## Overview: LIFEREG Procedure

The LIFEREG procedure fits parametric models to failure time data that can be uncensored, right censored, left censored, or interval censored. The models for the response variable consist of a linear effect composed of the covariates and a random disturbance term. The distribution of the random disturbance can be taken from a class of distributions that includes the extreme value, normal, logistic, and, by using a log transformation, the exponential, Weibull, lognormal, log-logistic, and three-parameter gamma distributions.

The model assumed for the response  $y$  is

$$y = \mathbf{X}\boldsymbol{\beta} + \sigma\epsilon$$

where  $y$  is a vector of response values, often the log of the failure times,  $\mathbf{X}$  is a matrix of covariates or independent variables (usually including an intercept term),  $\boldsymbol{\beta}$  is a vector of unknown regression parameters,  $\sigma$  is an unknown scale parameter, and  $\epsilon$  is a vector of errors assumed to come from a known distribution (such as the standard normal distribution). If an offset variable  $O$  is specified, the form of the model is  $y = \mathbf{X}\boldsymbol{\beta} + O + \sigma\epsilon$ , where  $O$  is a vector of values of the offset variable  $O$ . The distribution might also depend on additional shape parameters. These models are equivalent to accelerated failure time models when the log of the response is the quantity being modeled. The effect of the covariates in an accelerated failure time model is to change the scale, and not the location, of a baseline distribution of failure times.

The LIFEREG procedure estimates the parameters by maximum likelihood with a Newton-Raphson algorithm. PROC LIFEREG estimates the standard errors of the parameter estimates from the inverse of the observed information matrix.

The accelerated failure time model assumes that the effect of independent variables on an event time distribution is multiplicative on the event time. Usually, the scale function is  $\exp(\mathbf{x}'_c\boldsymbol{\beta}_c)$ , where  $\mathbf{x}'_c$  is the vector of covariate values (not including the intercept term) and  $\boldsymbol{\beta}_c$  is a vector of unknown parameters. Thus, if  $T_0$  is an event time sampled from the baseline distribution corresponding to values of zero for the covariates,

then the accelerated failure time model specifies that, if the vector of covariates is  $\mathbf{x}_c$ , the event time is  $T = \exp(\mathbf{x}'_c \boldsymbol{\beta}_c) T_0$ . If  $y = \log(T)$  and  $y_0 = \log(T_0)$ , then

$$y = \mathbf{x}'_c \boldsymbol{\beta}_c + y_0$$

This is a linear model with  $y_0$  as the error term.

In terms of survival or exceedance probabilities, this model is

$$\Pr(T > t \mid \mathbf{x}_c) = \Pr(T_0 > \exp(-\mathbf{x}'_c \boldsymbol{\beta}_c) t)$$

The probability on the left-hand side of the equal sign is evaluated given the value  $\mathbf{x}_c$  for the covariates, and the right-hand side is computed using the baseline probability distribution but at a scaled value of the argument. The right-hand side of the equation represents the value of the baseline survival function evaluated at  $\exp(-\mathbf{x}'_c \boldsymbol{\beta}_c) t$ .

Models usually have an intercept parameter and a scale parameter. In terms of the original untransformed event times, the effects of the intercept term and the scale term are to scale the event time and to raise the event time to a power, respectively. That is, if

$$\log(T_0) = \mu + \sigma \log(T_\epsilon)$$

then

$$T_0 = \exp(\mu) T_\epsilon^\sigma$$

Although it is possible to fit these models to the original response variable by using the NOLOG option, it is more common to model the log of the response variable. Because of this log transformation, zero values for the observed failure times are not allowed unless the NOLOG option is specified. Similarly, small values for the observed failure times lead to large negative values for the transformed response. The NOLOG option should be used only if you want to fit a distribution appropriate for the untransformed response, such as the extreme value instead of the Weibull. If you specify the normal or logistic distributions, the responses are not log transformed; that is, the NOLOG option is implicitly assumed.

Parameter estimates for the normal distribution are sensitive to large negative values, and care must be taken that the fitted model is not unduly influenced by them. Large negative values for the normal distribution can occur when fitting the lognormal distribution by log transforming the response, and some response values are near zero. Likewise, values that are extremely large after the log transformation have a strong influence in fitting the Weibull distribution (that is, the extreme value distribution for log responses). You should examine the residuals and check the effects of removing observations with large residuals or extreme values of covariates on the model parameters. The logistic distribution gives robust parameter estimates in the sense that the estimates have a bounded influence function.

The standard errors of the parameter estimates are computed from large sample normal approximations by using the observed information matrix. In small samples, these approximations might be poor. See Lawless (2003) for additional discussion and references. You can sometimes construct better confidence intervals by transforming the parameters. For example, large sample theory is often more accurate for  $\log(\sigma)$  than  $\sigma$ . Therefore, it might be more accurate to construct confidence intervals for  $\log(\sigma)$  and transform these into confidence intervals for  $\sigma$ . The parameter estimates and their estimated covariance matrix are available in an output SAS data set and can be used to construct additional tests or confidence intervals for the parameters. Alternatively, tests of parameters can be based on log-likelihood ratios. See Cox and Oakes (1984) for a

discussion of the merits of some possible test methods including score, Wald, and likelihood ratio tests. Likelihood ratio tests are generally more reliable for small samples than tests based on the information matrix.

The log-likelihood function is computed using the log of the failure time as a response. This log likelihood differs from the log likelihood obtained using the failure time as the response by an additive term of  $\sum \log(t_i)$ , where the sum is over the uncensored failure times. This term does not depend on the unknown parameters and does not affect parameter or standard error estimates. However, many published values of log likelihoods use the failure time as the basic response variable and, hence, differ by the additive term from the value computed by the LIFEREG procedure.

The classic Tobit model also fits into this class of models but with data usually censored on the left. The data considered by Tobin (1958) in his original paper came from a survey of consumers where the response variable is the ratio of expenditures on durable goods to the total disposable income. The two explanatory variables are the age of the head of household and the ratio of liquid assets to total disposable income. Because many observations in this data set have a value of zero for the response variable, the model fit by Tobin is

$$y = \max(\mathbf{x}'\boldsymbol{\beta} + \epsilon, 0)$$

which is a regression model with left censoring, where  $\mathbf{x}' = (1, \mathbf{x}'_c)$ .

Bayesian analysis of parametric survival models can be requested by using the BAYES statement in the LIFEREG procedure. In Bayesian analysis, the model parameters are treated as random variables, and inference about parameters is based on the posterior distribution of the parameters, given the data. The posterior distribution is obtained using Bayes' theorem as the likelihood function of the data weighted with a prior distribution. The prior distribution enables you to incorporate knowledge or experience of the likely range of values of the parameters of interest into the analysis. If you have no prior knowledge of the parameter values, you can use a noninformative prior distribution, and the results of the Bayesian analysis will be very similar to a classical analysis based on maximum likelihood. A closed form of the posterior distribution is often not feasible, and a Markov chain Monte Carlo method by Gibbs sampling is used to simulate samples from the posterior distribution. See Chapter 7, "[Introduction to Bayesian Analysis Procedures](#)," for an introduction to the basic concepts of Bayesian statistics. Also see the section "[Bayesian Analysis: Advantages and Disadvantages](#)" on page 132 for a discussion of the advantages and disadvantages of Bayesian analysis. See Ibrahim, Chen, and Sinha (2001) and Gilks, Richardson, and Spiegelhalter (1996) for more information about Bayesian analysis, including guidance in choosing prior distributions.

For Bayesian analysis, PROC LIFEREG generates a Gibbs chain for the posterior distribution of the model parameters. Summary statistics (mean, standard deviation, quartiles, HPD and credible intervals, correlation matrix) and convergence diagnostics (autocorrelations; Gelman-Rubin, Geweke, Raftery-Lewis, and Heidelberger and Welch tests; and the effective sample size) are computed for each parameter, as well as the correlation matrix of the posterior sample. Trace plots, posterior density plots, and autocorrelation function plots that are created using ODS Graphics are also provided for each parameter.

The LIFEREG procedure uses ODS Graphics to create graphs as part of its output. For general information about ODS Graphics, see Chapter 21, "[Statistical Graphics Using ODS](#)."

---

## Getting Started: LIFEREG Procedure

The following examples demonstrate how you can use the LIFEREG procedure to fit a parametric model to failure time data.

Suppose you have a response variable  $y$  that represents failure time; a binary variable, `ensor`, with `ensor=0` indicating censored values; and two linearly independent variables,  $x_1$  and  $x_2$ . The following statements perform a typical accelerated failure time model analysis. Higher-order effects such as interactions and nested effects are allowed in the independent variables list, but they are not shown in this example.

```
proc lifereg;
 model y*censor(0) = x1 x2;
run;
```

PROC LIFEREG can fit models to interval-censored data. The syntax for specifying interval-censored data is as follows:

```
proc lifereg;
 model (begin, end) = x1 x2;
run;
```

You can also model binomial data by using the *events/trials* syntax for the response, as illustrated in the following statements:

```
proc lifereg;
 model r/n=x1 x2;
run;
```

The variable  $n$  represents the number of trials, and the variable  $r$  represents the number of events.

---

## Modeling Right-Censored Failure Time Data

The following example demonstrates how you can use the LIFEREG procedure to fit a model to right-censored failure time data.

Suppose you conduct a study of two headache pain relievers. You divide patients into two groups, with each group receiving a different type of pain reliever. You record the time taken (in minutes) for each patient to report headache relief. Because some of the patients never report relief for the entire study, some of the observations are censored.

The following DATA step creates the SAS data set `headache`:

```
data Headache;
 input Minutes Group Censor @@;
 datalines;
11 1 0 12 1 0 19 1 0 19 1 0
19 1 0 19 1 0 21 1 0 20 1 0
21 1 0 21 1 0 20 1 0 21 1 0
20 1 0 21 1 0 25 1 0 27 1 0
30 1 0 21 1 1 24 1 1 14 2 0
16 2 0 16 2 0 21 2 0 21 2 0
23 2 0 23 2 0 23 2 0 23 2 0
```

```

25 2 1 23 2 0 24 2 0 24 2 0
26 2 1 32 2 1 30 2 1 30 2 0
32 2 1 20 2 1
;

```

The data set `Headache` contains the variable `Minutes`, which represents the reported time to headache relief; the variable `Group`, the group to which the patient is assigned; and the variable `Censor`, a binary variable indicating whether the observation is censored. Valid values of the variable `Censor` are 0 (no) and 1 (yes). Figure 51.1 shows the first five records of the data set `Headache`.

**Figure 51.1** Headache Data

|  | Obs | Minutes | Group | Censor |
|--|-----|---------|-------|--------|
|  | 1   | 11      | 1     | 0      |
|  | 2   | 12      | 1     | 0      |
|  | 3   | 19      | 1     | 0      |
|  | 4   | 19      | 1     | 0      |
|  | 5   | 19      | 1     | 0      |

The following statements invoke the LIFEREG procedure:

```

proc lifereg data=Headache;
 class Group;
 model Minutes*Censor(1)=Group;
 output out=New cdf=Prob;
run;

```

The CLASS statement specifies the variable `Group` as the classification variable. The MODEL statement syntax indicates that the response variable `Minutes` is right censored when the variable `Censor` takes the value 1. The MODEL statement specifies the variable `Group` as the single explanatory variable. Because the MODEL statement does not specify the DISTRIBUION= option, the LIFEREG procedure fits the default type 1 extreme-value distribution by using  $\log(\text{Minutes})$  as the response. This is equivalent to fitting the Weibull distribution.

The OUTPUT statement creates the output data set `New`. In addition to containing the variables in the original data set `Headache`, the SAS data set `New` also contains the variable `Prob`. This new variable is created by the CDF= option to contain the estimates of the cumulative distribution function evaluated at the observed response.

The results of this analysis are displayed in the following figures.

**Figure 51.2** Model Fitting Information from the LIFEREG Procedure

| The LIFEREG Procedure    |               |        |
|--------------------------|---------------|--------|
| Model Information        |               |        |
| Data Set                 | WORK.HEADACHE |        |
| Dependent Variable       | Log(Minutes)  |        |
| Censoring Variable       | Censor        |        |
| Censoring Value(s)       | 1             |        |
| Number of Observations   | 38            |        |
| Noncensored Values       | 30            |        |
| Right Censored Values    | 8             |        |
| Left Censored Values     | 0             |        |
| Interval Censored Values | 0             |        |
| Number of Parameters     | 3             |        |
| Name of Distribution     | Weibull       |        |
| Log Likelihood           | -9.37930239   |        |
| Class Level Information  |               |        |
| Name                     | Levels        | Values |
| Group                    | 2             | 1 2    |

Figure 51.2 displays the class level information and model fitting information. There are 30 uncensored observations and 8 right-censored observations. The log likelihood for the Weibull distribution is  $-9.3793$ . The log-likelihood value can be used to compare the goodness of fit for nested models with different covariates, but with the same distribution.

**Figure 51.3** Model Fit Statistics from the LIFEREG Procedure

| Fit Statistics                     |         |
|------------------------------------|---------|
| -2 Log Likelihood                  | 18.759  |
| AIC (smaller is better)            | 24.759  |
| AICC (smaller is better)           | 25.464  |
| BIC (smaller is better)            | 29.671  |
| Fit Statistics (Unlogged Response) |         |
| -2 Log Likelihood                  | 199.747 |
| Weibull AIC (smaller is better)    | 205.747 |
| Weibull AICC (smaller is better)   | 206.453 |
| Weibull BIC (smaller is better)    | 210.660 |

Figure 51.3 displays fit statistics for the model. The “Fit Statistics” table displays statistics based on the maximum extreme-value log likelihood fit by using  $\log(\text{Minutes})$  as the response. These statistics are useful

in comparing the fit of a different model when the fit criteria from the model that you compare is also based on the log likelihood using  $\log(\text{Minutes})$  as the response. The “Fit Statistics (Unlogged Response)” table is based on the maximum Weibull log likelihood using Minutes as the response. The AIC, BIC, and AICC statistics in this table can be used to compare models with different covariates, in addition to models with different distributions, as long as the fit statistics for the models that you compare use Minutes as the response.

**Figure 51.4** Model Parameter Estimates from the LIFEREG Procedure

| Analysis of Maximum Likelihood Parameter Estimates |     |          |                |                       |         |            |            |
|----------------------------------------------------|-----|----------|----------------|-----------------------|---------|------------|------------|
| Parameter                                          | DF  | Estimate | Standard Error | 95% Confidence Limits |         | Chi-Square | Pr > ChiSq |
| Intercept                                          | 1   | 3.3091   | 0.0589         | 3.1938                | 3.4245  | 3161.70    | <.0001     |
| Group                                              | 1 1 | -0.1933  | 0.0786         | -0.3473               | -0.0393 | 6.05       | 0.0139     |
| Group                                              | 2 0 | 0.0000   | .              | .                     | .       | .          | .          |
| Scale                                              | 1   | 0.2122   | 0.0304         | 0.1603                | 0.2809  |            |            |
| Weibull Shape                                      | 1   | 4.7128   | 0.6742         | 3.5604                | 6.2381  |            |            |

The table of parameter estimates is displayed in Figure 51.4. Both the intercept and the slope parameter for the variable group are significantly different from 0 at the 0.05 level. Because the variable group has only one degree of freedom, parameter estimates are given for only one level of the variable group (group=1). However, the estimate for the intercept parameter provides a baseline for group=2.

The resulting model is as follows:

$$\log(\text{minutes}) = \begin{cases} 3.30911843 - 0.1933025 & \text{for group} = 1 \\ 3.30911843 & \text{for group} = 2 \end{cases}$$

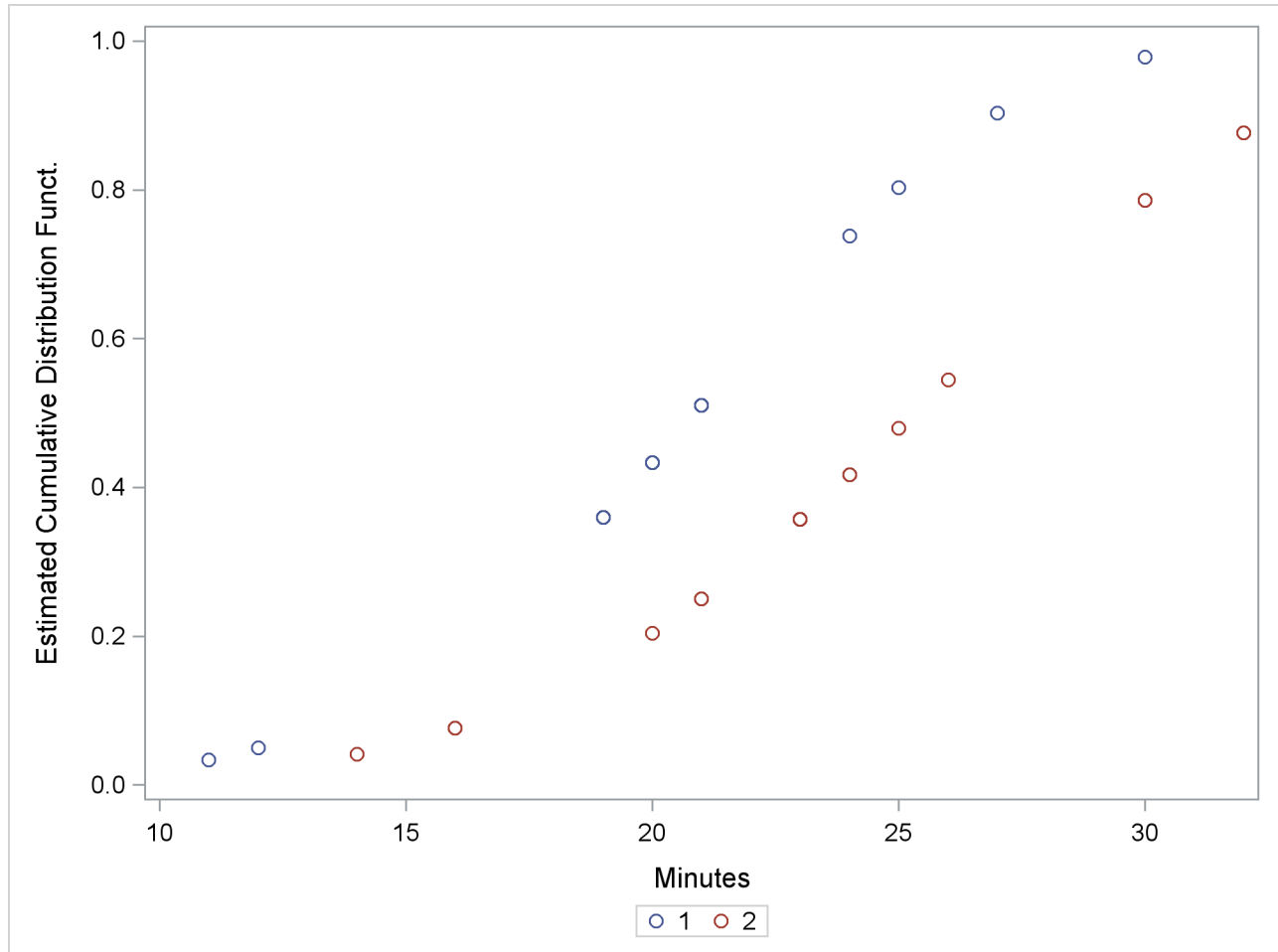
Note that the Weibull shape parameter for this model is the reciprocal of the extreme-value scale parameter estimate shown in Figure 51.4 ( $1/0.21219 = 4.7128$ ).

The following statements produce a graph of the cumulative distribution values versus the variable Minutes.

```
proc sgplot data=New;
 scatter x=Minutes y=Prob / group=Group;
 discretelegend;
run;
```

Figure 51.5 displays the estimated cumulative distribution function values contained in the output data set New for each group.

**Figure 51.5** Plot of the Estimated Cumulative Distribution Function



## Bayesian Analysis of Right-Censored Data

Nelson (1982) describes a study of the lifetimes of locomotive engine fans. This example shows how to use PROC LIFEREG to carry out a Bayesian analysis of the engine fan data. In this example, a lognormal distribution is used to model the engine lifetimes, but other survival time distributions, such as the Weibull, can also be used.



The following SAS statements create the SAS data set `Fan`. This data set contains a censoring indicator variable and right-censored survival times for the 70 locomotive engine fans in the study.

```
data Fan;
 input Lifetime Censor@@;
 datalines;
 450 0 460 1 1150 0 1150 0 1560 1
 1600 0 1660 1 1850 1 1850 1 1850 1
 1850 1 1850 1 2030 1 2030 1 2030 1
 2070 0 2070 0 2080 0 2200 1 3000 1
 3000 1 3000 1 3000 1 3100 0 3200 1
 3450 0 3750 1 3750 1 4150 1 4150 1
 4150 1 4150 1 4300 1 4300 1 4300 1
 4300 1 4600 0 4850 1 4850 1 4850 1
 4850 1 5000 1 5000 1 5000 1 6100 1
 6100 0 6100 1 6100 1 6300 1 6450 1
 6450 1 6700 1 7450 1 7800 1 7800 1
 8100 1 8100 1 8200 1 8500 1 8500 1
 8500 1 8750 1 8750 0 8750 1 9400 1
 9900 1 10100 1 10100 1 10100 1 11500 1
 ;
```

Some of the fans had not failed at the time the data were collected, and the unfailed units have right-censored lifetimes. The variable `Lifetime` represents either a failure time or a censoring time. The variable `Censor` is equal to 0 if the value of `Lifetime` is a failure time, and it is equal to 1 if the value is a censoring time.

The following SAS statements specify a Bayesian analysis that uses a lognormal model for the engine lifetimes. There are no covariates, so the model is an intercept-only model. The `OUTPOST=` option saves the samples from the posterior distribution in the SAS data set `Post` for further processing.

```
ods graphics on;
proc lifereg data=Fan;
 model Lifetime*Censor(1)= / dist=lognormal;
 bayes seed=1 outpost=Post;
run;
ods graphics off;
```

The `SEED=` option is specified to maintain reproducibility; no other options are specified in the `BAYES` statement. By default, a uniform prior distribution is assumed for the intercept coefficient. The uniform prior is a flat prior on the real line with a distribution that reflects ignorance of the location of the parameter, placing equal probability on all possible values the regression coefficient can take. Using the uniform prior in the following example, you would expect the Bayesian estimates to resemble the classical results of maximizing the likelihood. If you can elicit an informative prior on the regression coefficients, you should use the `COEFFPRIOR=` option to specify it. A default noninformative gamma prior is used for the lognormal scale parameter  $\sigma$ .

You should make sure that the posterior distribution samples have achieved convergence before using them for Bayesian inference. If you do not specify additional options, `PROC LIFEREG` produces by default three convergence diagnostics: autocorrelations of the posterior sample, effective sample size, and the Geweke statistic. See the section “[Assessing Markov Chain Convergence](#)” on page 139 for information about assessing the convergence of the chain of posterior samples. Trace plots, posterior density plots, and autocorrelation function plots that are created using `ODS Graphics` are also provided for each parameter. See the section “[Visual Analysis via Trace Plots](#)” on page 139 for help in interpreting these plots.

The “Analysis of Maximum Likelihood Parameter Estimates” table in Figure 51.6 summarizes maximum likelihood estimates of the lognormal intercept and scale parameters.

**Figure 51.6** Maximum Likelihood Estimates from the LIFEREG Procedure

| The LIFEREG Procedure                              |    |          |                |                       |         |
|----------------------------------------------------|----|----------|----------------|-----------------------|---------|
| Bayesian Analysis                                  |    |          |                |                       |         |
| Analysis of Maximum Likelihood Parameter Estimates |    |          |                |                       |         |
| Parameter                                          | DF | Estimate | Standard Error | 95% Confidence Limits |         |
| Intercept                                          | 1  | 10.1432  | 0.5211         | 9.1219                | 11.1646 |
| Scale                                              | 1  | 1.6796   | 0.3893         | 1.0664                | 2.6453  |

Since no prior distribution for the intercept was specified, the default uniform improper distribution shown in the “Uniform Prior for Regression Coefficients” table in Figure 51.7 is used.

Noninformative prior distributions are appropriate if you have no prior knowledge of the likely range of values of the parameters, and if you want to make probability statements about the parameters or functions of the parameters. Refer, for example, to Ibrahim, Chen, and Sinha (2001) for more information about choosing prior distributions.

The default noninformative gamma prior distribution for the lognormal scale parameter is shown in the “Independent Prior Distributions for Model Parameters” table in Figure 51.7.

**Figure 51.7** Noninformative Prior Distributions

| The LIFEREG Procedure                                |                    |                 |       |               |       |
|------------------------------------------------------|--------------------|-----------------|-------|---------------|-------|
| Bayesian Analysis                                    |                    |                 |       |               |       |
| Uniform Prior for Regression Coefficients            |                    |                 |       |               |       |
| Parameter                                            | Prior              |                 |       |               |       |
| Intercept                                            | Constant           |                 |       |               |       |
| Independent Prior Distributions for Model Parameters |                    |                 |       |               |       |
| Parameter                                            | Prior Distribution | Hyperparameters |       |               |       |
| Scale                                                | Gamma              | Shape           | 0.001 | Inverse Scale | 0.001 |

By default, posterior mode estimates of the model parameters are used as the starting value for the simulation. These are listed in the “Initial Values of the Chain” table in Figure 51.8.

**Figure 51.8** Markov Chain Initial Values

| Initial Values of the Chain |      |           |         |
|-----------------------------|------|-----------|---------|
| Chain                       | Seed | Intercept | Scale   |
| 1                           | 1    | 10.0501   | 1.59544 |

Summary statistics for the posterior sample are displayed in the “Fit Statistics,” “Descriptive Statistics for the Posterior Sample,” “Interval Statistics for the Posterior Sample,” and “Posterior Correlation Matrix” tables in Figure 51.9. Since noninformative prior distributions were used, these results are consistent with the maximum likelihood estimates shown in Figure 51.6.

**Figure 51.9** Posterior Sample Summary Statistics

| Fit Statistics                      |           |                     |                       |              |         |         |
|-------------------------------------|-----------|---------------------|-----------------------|--------------|---------|---------|
| DIC (smaller is better)             |           | 87.245              |                       |              |         |         |
| pD (effective number of parameters) |           | 1.823               |                       |              |         |         |
| The LIFEREG Procedure               |           |                     |                       |              |         |         |
| Bayesian Analysis                   |           |                     |                       |              |         |         |
| Posterior Summaries                 |           |                     |                       |              |         |         |
| Parameter                           | N         | Mean                | Standard<br>Deviation | Percentiles  |         |         |
|                                     |           |                     |                       | 25%          | 50%     | 75%     |
| Intercept                           | 10000     | 10.4196             | 0.6172                | 9.9670       | 10.3259 | 10.7959 |
| Scale                               | 10000     | 1.9196              | 0.4809                | 1.5675       | 1.8476  | 2.1931  |
| Posterior Intervals                 |           |                     |                       |              |         |         |
| Parameter                           | Alpha     | Equal-Tail Interval |                       | HPD Interval |         |         |
| Intercept                           | 0.050     | 9.4477              | 11.8994               | 9.3216       | 11.6752 |         |
| Scale                               | 0.050     | 1.1906              | 3.0570                | 1.1104       | 2.8834  |         |
| Posterior Correlation Matrix        |           |                     |                       |              |         |         |
| Parameter                           | Intercept |                     | Scale                 |              |         |         |
| Intercept                           | 1.0000    |                     | 0.8297                |              |         |         |
| Scale                               | 0.8297    |                     | 1.0000                |              |         |         |

By default, PROC LIFEREG computes three convergence diagnostics: the lag1, lag5, lag10, and lag50 autocorrelations; the Geweke diagnostic; and the effective sample size. These are displayed in [Figure 51.10](#). There is no indication that the Markov chain has not converged. See the section “[Assessing Markov Chain Convergence](#)” on page 139 for more information about convergence diagnostics and their interpretation.

**Figure 51.10** Posterior Sample Summary Statistics

| The LIFEREG Procedure      |         |                      |            |         |
|----------------------------|---------|----------------------|------------|---------|
| Bayesian Analysis          |         |                      |            |         |
| Posterior Autocorrelations |         |                      |            |         |
| Parameter                  | Lag 1   | Lag 5                | Lag 10     | Lag 50  |
| Intercept                  | 0.6973  | 0.1765               | 0.0190     | -0.0017 |
| Scale                      | 0.6955  | 0.1713               | 0.0172     | -0.0002 |
| Geweke Diagnostics         |         |                      |            |         |
| Parameter                  | z       | Pr >  z              |            |         |
| Intercept                  | -0.9183 | 0.3585               |            |         |
| Scale                      | -0.9233 | 0.3559               |            |         |
| Effective Sample Sizes     |         |                      |            |         |
| Parameter                  | ESS     | Autocorrelation Time | Efficiency |         |
| Intercept                  | 1772.8  | 5.6408               | 0.1773     |         |
| Scale                      | 1805.0  | 5.5400               | 0.1805     |         |

Summary statistics of the posterior distribution samples are produced by default. However, these statistics might not be sufficient for carrying out your Bayesian inference. The samples from the posterior distribution saved in the SAS data set Post created with the OUTPOST= option can be used for further analysis.

Trace, autocorrelation, and density plots for the three model parameters shown in Figure 51.11 and Figure 51.12 are useful in diagnosing whether the Markov chain of posterior samples has converged. These plots show no evidence that the chain has not converged. See the section “Visual Analysis via Trace Plots” on page 139 for more information about interpreting these types of diagnostic plots.

**Figure 51.11** Diagnostic Plots

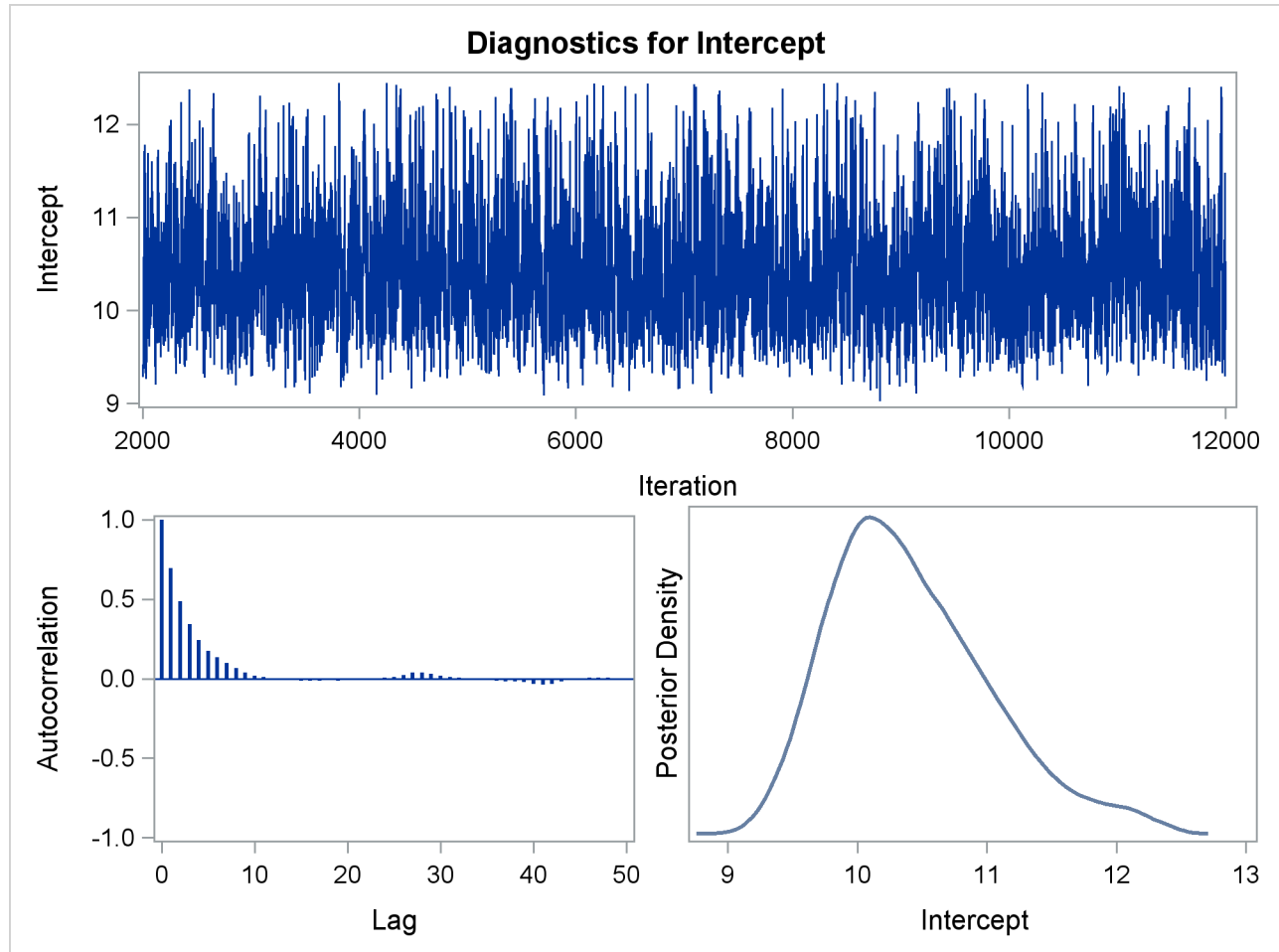
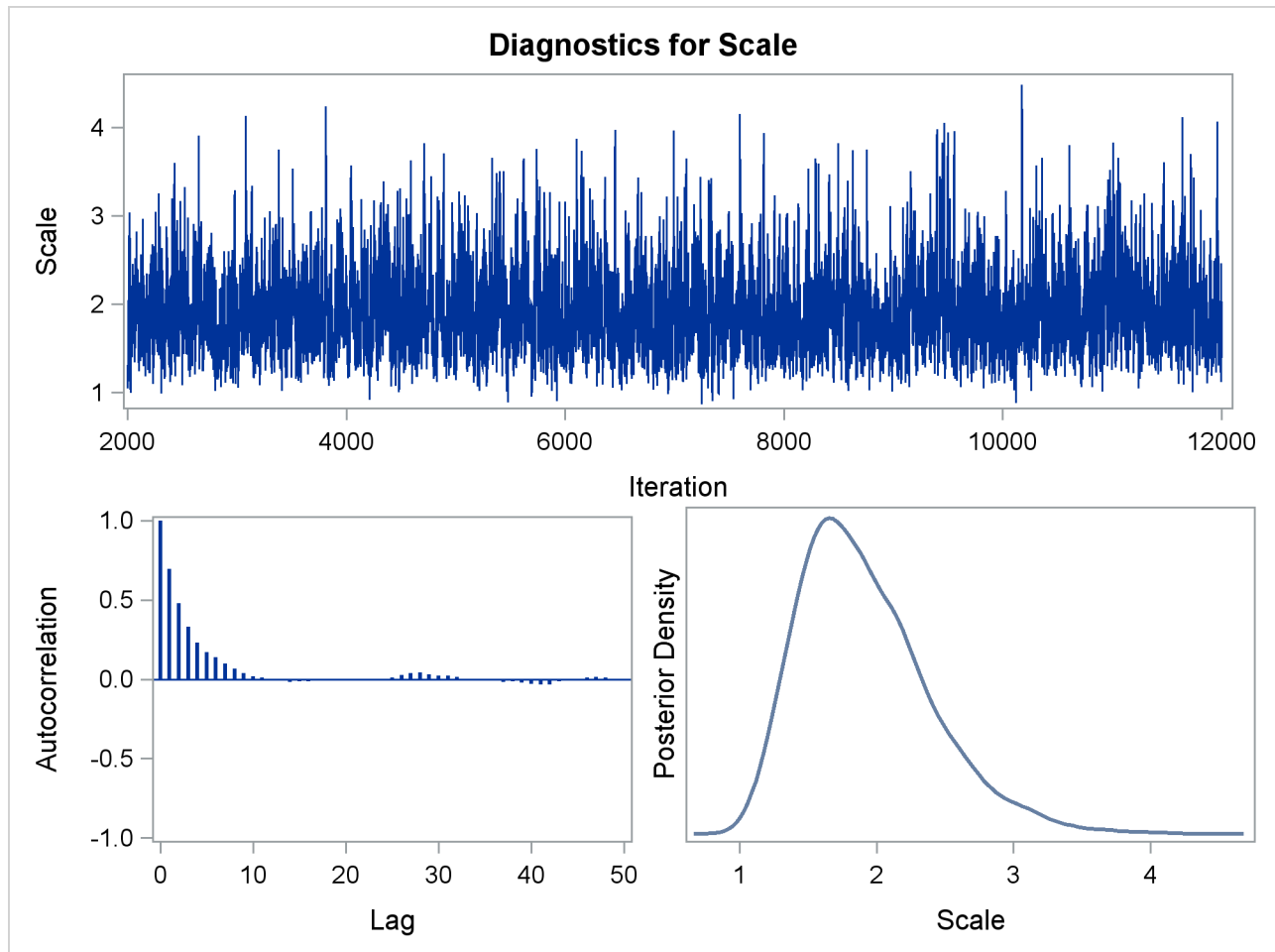


Figure 51.12 Diagnostic Plots



The fraction failing in the first 8000 hours of operation might be a quantity of interest. This kind of information could be useful, for example, in determining whether to improve the reliability of the engine components due to warranty considerations. The following SAS statements compute the mean and percentiles of the distribution of the fraction failing in the first 8000 hours from the posterior sample data set Post:

```
data Prob;
 set Post;
 Frac = ProbNorm((log(8000) - Intercept) / Scale);
 label Frac= 'Fraction Failing in 8000 Hours';
run;

proc means data = Prob(keep=Frac) n mean p10 p25 p50 p75 p90;
run;
```

The mean fraction of failures in the first 8000 hours, shown in Figure 51.13, is about 0.24, which could be used in further analysis of warranty costs. The 10th percentile is about 0.16 and the 90th percentile is about 0.32, which gives an assessment of the probable range of the fraction failing in the first 8000 hours.

**Figure 51.13** Fraction Failing in 8000 Hours

| The MEANS Procedure                                     |           |           |           |           |           |
|---------------------------------------------------------|-----------|-----------|-----------|-----------|-----------|
| Analysis Variable : Frac Fraction Failing in 8000 Hours |           |           |           |           |           |
| N                                                       | Mean      | 10th Pctl | 25th Pctl | 50th Pctl | 75th Pctl |
| 10000                                                   | 0.2381467 | 0.1628591 | 0.1953691 | 0.2336756 | 0.2766051 |
| Analysis Variable : Frac Fraction Failing in 8000 Hours |           |           |           |           |           |
|                                                         |           |           | 90th Pctl |           |           |
|                                                         |           |           | 0.3190883 |           |           |

## Syntax: LIFEREG Procedure

The following statements are available in the LIFEREG procedure:

```

PROC LIFEREG < options > ;
 BAYES < options > ;
 BY variables ;
 CLASS variables ;
 ESTIMATE < 'label' > estimate-specification < (divisor=n) >
 < , ... < 'label' > estimate-specification < (divisor=n) > > < / options > ;
 EFFECTPLOT < plot-type < (plot-definition-options) > > < / options > ;
 INSET < keyword-list > < / options > ;
 LSMEANS < model-effects > < / options > ;
 LSMESTIMATE model-effect < 'label' > values < (divisor=n) >
 < , ... < 'label' > values < (divisor=n) > > < / options > ;
 MODEL response = < effects > < / options > ;
 OUTPUT < OUT=SAS-data-set > < keyword=name ... keyword=name > < options > ;
 PROBPLOT < / options > ;
 SLICE model-effect < / options > ;
 STORE < OUT= > item-store-name < / LABEL='label' > ;
 TEST < model-effects > < / options > ;
 WEIGHT variable ;

```

The MODEL statement is required; it specifies both the variables that are used in the regression part of the model and the distribution that is used for the error (random) component of the model. Each invocation of the LIFEREG procedure can use only one MODEL statement. If multiple MODEL statements are present, only

the last is used. You can specify main effects and interaction terms in the MODEL statement, as in the GLM procedure. You can specify initial values in the MODEL statement or in an INEST= data set. If no initial values are specified, the starting estimates are obtained by ordinary least squares. The CLASS statement determines which explanatory variables are treated as categorical. The WEIGHT statement identifies a *variable* with values that are used to weight the observations. Observations with zero or negative weights are not used to fit the model, although predicted values can be computed for them. The OUTPUT statement creates an output data set that contains predicted values and residuals.

The ESTIMATE, EFFECTPLOT, LSMEANS, LSMESTIMATE, SLICE, STORE, and TEST statements are common to many procedures. Summary descriptions of functionality and syntax for these statements are also given after the PROC LIFEREG statement in alphabetical order, and full documentation about them is available in Chapter 19, “Shared Concepts and Topics.”

---

## PROC LIFEREG Statement

**PROC LIFEREG** < options > ;

The PROC LIFEREG statement invokes the LIFEREG procedure. Table 51.1 summarizes the options available in the PROC LIFEREG statement.

**Table 51.1** PROC LIFEREG Statement Options

| Option   | Description                                                                |
|----------|----------------------------------------------------------------------------|
| COVOUT   | Writes the estimated covariance matrix to the OUTEST= data set             |
| DATA=    | Specifies the input SAS data set                                           |
| GOUT=    | Specifies a graphics catalog                                               |
| INEST=   | Specifies an input SAS data set that contains initial estimates            |
| NAMELEN= | Specifies the length of effect names                                       |
| NOPRINT  | Suppresses the display of the output                                       |
| ORDER=   | Specifies the sort order for the levels of the classification variables    |
| OUTEST=  | Specifies an output SAS data set                                           |
| PLOTS=   | Controls graphics created by ODS Graphics                                  |
| XDATA=   | Specifies a SAS input data containing values for the independent variables |

You can specify the following *options* in the PROC LIFEREG statement.

### COVOUT

writes the estimated covariance matrix to the OUTEST= data set if convergence is attained.

### DATA=*SAS-data-set*

specifies the input SAS data set used by PROC LIFEREG. By default, the most recently created SAS data set is used.

### GOUT=*graphics-catalog*

specifies a graphics catalog in which to save graphics output.



**INEST=SAS-data-set**

specifies an input SAS data set that contains initial estimates for all the parameters in the model. See the section “[INEST= Data Set](#)” on page 3945 for a detailed description of the contents of the INEST= data set.

**NAMELEN=*n***

specifies the length of effect names in tables and output data sets to be *n* characters, where *n* is a value between 20 and 200. The default length is 20 characters.

**NOPRINT**

suppresses the display of the output. Note that this option temporarily disables the Output Delivery System (ODS). For more information, see Chapter 20, “[Using the Output Delivery System.](#)”

**ORDER=DATA | FORMATTED | FREQ | INTERNAL**

specifies the sort order for the levels of the classification variables (which are specified in the **CLASS** statement). This option applies to the levels for all classification variables, except when you use the (default) ORDER=FORMATTED option with numeric classification variables that have no explicit format. With this option, the levels of such variables are ordered by their internal value.

The ORDER= option can take the following values:

| Value of ORDER=  | Levels Sorted By                                                                                                                       |
|------------------|----------------------------------------------------------------------------------------------------------------------------------------|
| <b>DATA</b>      | Order of appearance in the input data set                                                                                              |
| <b>FORMATTED</b> | External formatted value, except for numeric variables with no explicit format, which are sorted by their unformatted (internal) value |
| <b>FREQ</b>      | Descending frequency count; levels with the most observations come first in the order                                                  |
| <b>INTERNAL</b>  | Unformatted value                                                                                                                      |

By default, ORDER=FORMATTED. For ORDER=FORMATTED and ORDER=INTERNAL, the sort order is machine-dependent. For more information about sort order, see the chapter on the SORT procedure in the *Base SAS Procedures Guide* and the discussion of BY-group processing in *SAS Language Reference: Concepts*.

**OUTEST=SAS-data-set**

specifies an output SAS data set containing the parameter estimates, the maximized log likelihood, and, if the COVOUT option is specified, the estimated covariance matrix. See the section “[OUTEST= Data Set](#)” on page 3946 for a detailed description of the contents of the OUTEST= data set.

**PLOTS=NONE | PROBLOT**

specifies options that control graphics created by ODS Graphics.

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;

proc lifereg plots=probplot;
 model y = x;
run;

ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The following plot requests are available.

- NONE suppresses any plots created by ODS Graphics specified in other LIFEREG statements, such as the BAYES or PROBPLOT statement.
- PROBPLOT creates a default probability plot based on information in the MODEL statement. If a PROBPLOT option is also specified, the probability plot specified in the PROBPLOT statement is created, and this option is ignored.

#### **XDATA=SAS-data-set**

specifies an input SAS data set that contains values for all the independent variables in the MODEL statement and variables in the CLASS statement for probability plotting. If there are covariates specified in a MODEL statement and a probability plot is requested with a PROBPLOT statement, you specify fixed values for the effects in the MODEL statement with the XDATA= data set. See the section “XDATA= Data Set” on page 3947 for a detailed description of the contents of the XDATA= data set.

---

## **BAYES Statement**

**BAYES** < options > ;

The BAYES statement requests a Bayesian analysis of the regression model by using Gibbs sampling. The Bayesian posterior samples (also known as the chain) for the regression parameters are not tabulated. The Bayesian posterior samples (also known as the chain) for the model parameters can be output to a SAS data set.

Table 51.2 summarizes the options available in the BAYES statement.

**Table 51.2** BAYES Statement Options

| <b>Option</b>              | <b>Description</b>                                                                 |
|----------------------------|------------------------------------------------------------------------------------|
| <b>Monte Carlo Options</b> |                                                                                    |
| <b>INITIAL=</b>            | Specifies initial values of the chain                                              |
| <b>INITIALMLE</b>          | Specifies that maximum likelihood estimates be used as initial values of the chain |

Table 51.2 (continued)

| Option                                                | Description                                                      |
|-------------------------------------------------------|------------------------------------------------------------------|
| METROPOLIS=                                           | Specifies the use of a Metropolis step                           |
| NBI=                                                  | Specifies the number of burn-in iterations                       |
| NMC=                                                  | Specifies the number of iterations after burn-in                 |
| SEED=                                                 | Specifies the random number generator seed                       |
| THINNING=                                             | Controls the thinning of the Markov chain                        |
| <b>Model and Prior Options</b>                        |                                                                  |
| COEFFPRIOR=                                           | Specifies the prior of the regression coefficients               |
| EXPONENTIALSCALEPRIOR=                                | Specifies the prior of the exponential scale parameter           |
| GAMMASHAPEPRIOR=                                      | Specifies the prior of the three-parameter gamma shape parameter |
| SCALEPRIOR=                                           | Specifies the prior of the scale parameter                       |
| WEIBULLSCALEPRIOR=                                    | Specifies the prior of the Weibull scale parameter               |
| WEIBULLSHAPEPRIOR=                                    | Specifies the prior of the Weibull shape parameter               |
| <b>Summary Statistics and Convergence Diagnostics</b> |                                                                  |
| DIAGNOSTICS=                                          | Displays convergence diagnostics                                 |
| PLOTS=                                                | Displays diagnostic plots                                        |
| STATISTICS=                                           | Displays summary statistics of the posterior samples             |
| <b>Posterior Samples</b>                              |                                                                  |
| OUTPOST=                                              | Names a SAS data set for the posterior samples                   |

The following list describes these options and their suboptions.

**COEFFPRIOR=UNIFORM | NORMAL** <(normal-options)>

**CPRIOR=UNIFORM | NORMAL** <(option)>

**COEFF=UNIFORM | NORMAL** <(option)>

specifies the prior distribution for the regression coefficients. The default is COEFFPRIOR=UNIFORM. The available prior distributions are as follows:

**NORMAL**<(normal-option)>

specifies a normal distribution. The *normal-options* include the following:

**CONDITIONAL**

specifies that the normal prior, conditional on the current Markov chain value of the location-scale model precision parameter  $\tau = \frac{1}{\sigma^2}$ , is  $N(\boldsymbol{\mu}, \tau^{-1}\boldsymbol{\Sigma})$ , where  $\boldsymbol{\mu}$  and  $\boldsymbol{\Sigma}$  are the mean and covariance of the normal prior specified by other normal options.

**INPUT= SAS-data-set**

specifies a SAS data set that contains the mean and covariance information of the normal prior. The data set must have a `_TYPE_` variable to represent the type of each observation and a variable for each regression coefficient. If the data set also contains a `_NAME_` variable, the values of this variable are used to identify the covariances for the `_TYPE_='COV'` observations; otherwise, the `_TYPE_='COV'` observations are assumed to be in the same order as the explanatory variables in the MODEL statement. PROC LIFEREG reads the

mean vector from the observation with `_TYPE_='MEAN'` and reads the covariance matrix from observations with `_TYPE_='COV'`. For an independent normal prior, the variances can be specified with `_TYPE_='VAR'`; alternatively, the precisions (inverse of the variances) can be specified with `_TYPE_='PRECISION'`.

**RELVAR<=c>**

specifies the normal prior  $N(\mathbf{0}, c\mathbf{J})$ , where  $\mathbf{J}$  is a diagonal matrix with diagonal elements equal to the variances of the corresponding ML estimator. By default,  $c = 10^6$ .

**VAR<=c>**

specifies the normal prior  $N(\mathbf{0}, c\mathbf{I})$ , where  $\mathbf{I}$  is the identity matrix.

If you do not specify an option, the normal prior  $N(\mathbf{0}, 10^6\mathbf{I})$ , where  $\mathbf{I}$  is the identity matrix, is used. See the section “[Normal Prior](#)” on page 3949 for more details.

**UNIFORM**

specifies a flat prior—that is, the prior that is proportional to a constant ( $p(\beta_1, \dots, \beta_k) \propto 1$  for all  $-\infty < \beta_i < \infty$ ).

**DIAGNOSTICS=ALL | NONE | (keyword-list)**

**DIAG=ALL | NONE | (keyword-list)**

controls the number of diagnostics produced. You can request all the following diagnostics by specifying `DIAGNOSTICS=ALL`. If you do not want any of these diagnostics, specify `DIAGNOSTICS=NONE`. If you want some but not all of the diagnostics, or if you want to change certain settings of these diagnostics, specify a subset of the following keywords. The default is `DIAGNOSTICS=(AUTOCORR ESS GEWEKE)`.

**AUTOCORR <(LAGS= numeric-list)>**

computes the autocorrelations of lags given by `LAGS= list` for each parameter. Elements in the list are truncated to integers and repeated values are removed. If the `LAGS=` option is not specified, autocorrelations of lags 1, 5, 10, and 50 are computed for each variable. See the section “[Autocorrelations](#)” on page 152 for details.

**ESS**

computes Carlin’s estimate of the effective sample size, the correlation time, and the efficiency of the chain for each parameter. See the section “[Effective Sample Size](#)” on page 152 for details.

**GELMAN <(gelman-options)>**

computes the Gelman and Rubin convergence diagnostics. You can specify one or more of the following *gelman-options*:

**NCHAIN=number**

**N=number**

specifies the number of parallel chains used to compute the diagnostic, and must be 2 or larger. The default is `NCHAIN=3`. If an `INITIAL=` data set is used, `NCHAIN` defaults to the number of rows in the `INITIAL=` data set. If any number other than this is specified with the `NCHAIN=` option, the `NCHAIN=` value is ignored.

**ALPHA=***value*

specifies the significance level for the upper bound. The default is ALPHA=0.05, resulting in a 97.5% bound.

See the section “[Gelman and Rubin Diagnostics](#)” on page 145 for details.

**GEWEKE** <(geweke-options)>

computes the Geweke spectral density diagnostics, which are essentially a two-sample  $t$  test between the first  $f_1$  portion and the last  $f_2$  portion of the chain. The default is  $f_1 = 0.1$  and  $f_2 = 0.5$ , but you can choose other fractions by using the following *geweke-options*:

**FRAC1=***value*

specifies the fraction  $f_1$  for the first window.

**FRAC2=***value*

specifies the fraction  $f_2$  for the second window.

See the section “[Geweke Diagnostics](#)” on page 146 for details.

**HEIDELBERGER** <(heidel-options)>

computes the Heidelberg and Welch diagnostic for each variable, which consists of a stationarity test of the null hypothesis that the sample values form a stationary process. If the stationarity test is not rejected, a halfwidth test is then carried out. Optionally, you can specify one or more of the following *heidel-options*:

**SALPHA=***value*

specifies the  $\alpha$  level ( $0 < \alpha < 1$ ) for the stationarity test.

**HALPHA=***value*

specifies the  $\alpha$  level ( $0 < \alpha < 1$ ) for the halfwidth test.

**EPS=***value*

specifies a positive number  $\epsilon$  such that if the halfwidth is less than  $\epsilon$  times the sample mean of the retained iterates, the halfwidth test is passed.

See the section “[Heidelberg and Welch Diagnostics](#)” on page 148 for details.

**MCSE****MCERROR**

computes the Monte Carlo standard error for each parameter. The Monte Carlo standard error, which measures the simulation accuracy, is the standard error of the posterior mean estimate and is calculated as the posterior standard deviation divided by the square root of the effective sample size. See the section “[Standard Error of the Mean Estimate](#)” on page 153 for details.

**RAFTERY**<(raftery-options)>

computes the Raftery and Lewis diagnostics that evaluate the accuracy of the estimated quantile ( $\hat{\theta}_Q$  for a given  $Q \in (0, 1)$ ) of a chain.  $\hat{\theta}_Q$  can achieve any degree of accuracy when the chain is allowed to run for a long time. A stopping criterion is when the estimated probability  $\hat{P}_Q = \Pr(\theta \leq \hat{\theta}_Q)$  reaches within  $\pm R$  of the value  $Q$  with probability  $S$ ; that is,  $\Pr(Q - R \leq \hat{P}_Q \leq Q + R) = S$ . The following *raftery-options* enable you to specify  $Q$ ,  $R$ ,  $S$ , and a precision level  $\epsilon$  for the test:

**QUANTILE | Q=value**

specifies the order (a value between 0 and 1) of the quantile of interest. The default is 0.025.

**ACCURACY | R=value**

specifies a small positive number as the margin of error for measuring the accuracy of estimation of the quantile. The default is 0.005.

**PROBABILITY | S=value**

specifies the probability of attaining the accuracy of the estimation of the quantile. The default is 0.95.

**EPSILON | EPS=value**

specifies the tolerance level (a small positive number) for the stationary test. The default is 0.001.

See the section “[Raftery and Lewis Diagnostics](#)” on page 149 for details.

**EXPSCALEPRIOR=GAMMA<(options)> | IMPROPER****ESCALEPRIOR=GAMMA<(options)> | IMPROPER****ESCPRIOR=GAMMA<(options)> | IMPROPER**

specifies that Gibbs sampling be performed on the exponential distribution scale parameter and the prior distribution for the scale parameter. This prior distribution applies only when the exponential distribution and no covariates are specified.

A gamma prior  $G(a, b)$  with density  $f(t) = \frac{b(bt)^{a-1}e^{-bt}}{\Gamma(a)}$  is specified by EXPSCALEPRIOR=GAMMA, which can be followed by one of the following *gamma-options* enclosed in parentheses. The hyperparameters  $a$  and  $b$  are the shape and inverse-scale parameters of the gamma distribution, respectively. See the section “[Gamma Prior](#)” on page 3949 for more details. The default is  $G(10^{-4}, 10^{-4})$ .

**RELSHAPE<=c>**

specifies independent  $G(c\hat{\alpha}, c)$  distribution, where  $\hat{\alpha}$  is the MLE of the exponential scale parameter. With this choice of hyperparameters, the mean of the prior distribution is  $\hat{\alpha}$  and the variance is  $\frac{\hat{\alpha}}{c^2}$ . By default,  $c=10^{-4}$ .

**SHAPE=a****ISCALE=b**

when both specified, results in a  $G(a, b)$  prior.

**SHAPE=c**

when specified alone, results in a  $G(c, c)$  prior.

**ISCALE=c**

when specified alone, results in a  $G(c, c)$  prior.

An improper prior with density  $f(t)$  proportional to  $t^{-1}$  is specified with EXPSCALEPRIOR=IMPROPER.

**GAMMASHAPEPRIOR=NORMAL<(options)>****GAMASHAPEPRIOR=NORMAL<(options)>****SHAPE1PRIOR=NORMAL<(options)>**

specifies the prior distribution for the gamma distribution shape parameter. If you do not specify any options in a gamma model, the  $N(0, 10^6)$  prior for the shape is used. You can specify MEAN= and VAR= or RELVAR= options, either alone or together, to specify the mean and variance of the normal prior for the gamma shape parameter.

**MEAN=*a***

specifies a normal prior  $N(a, 10^6)$ . By default,  $a=0$ .

**RELVAR=<=*b*>**

specifies the normal prior  $N(0, bJ)$ , where  $J$  is the variance of the MLE of the shape parameter. By default,  $b=10^6$ .

**VAR=*c***

specifies the normal prior  $N(0, c)$ . By default,  $c=10^6$ .

**INITIAL=*SAS-data-set***

specifies the SAS data set that contains the initial values of the Markov chains. The INITIAL= data set must contain all the variables of the model. You can specify multiple rows as the initial values of the parallel chains for the Gelman-Rubin statistics, but posterior summaries, diagnostics, and plots are computed only for the first chain. If the data set also contains the variable `_SEED_`, the value of the `_SEED_` variable is used as the seed of the random number generator for the corresponding chain.

**INITIALMLE**

specifies that maximum likelihood estimates of the model parameters be used as initial values of the Markov chain. If this option is not specified, estimates of the mode of the posterior distribution obtained by optimization are used as initial values.

**METROPOLIS=YES****METROPOLIS=NO**

specifies the use of a Metropolis step to generate Gibbs samples for posterior distributions that are not log concave. The default value is METROPOLIS=YES.

**NBI=*number***

specifies the number of burn-in iterations before the chains are saved. The default is 2000.

**NMC=*number***

specifies the number of iterations after the burn-in. The default is 10000.

**OUTPOST=*SAS-data-set*****OUT=*SAS-data-set***

names the SAS data set that contains the posterior samples. See the section “[OUTPOST= Output Data Set](#)” on page 3951 for more information. Alternatively, you can create the output data set by specifying an ODS OUTPUT statement as follows:

```
ODS OUTPUT POSTERIORSAMPLE=SAS-data-set
```

**PLOTS<(global-plot-options)>=*plot-request*****PLOTS<(global-plot-options)>=*(plot-request < ...plot-request>)***

controls the display of diagnostic plots. Three types of plots can be requested: trace plots, autocorrelation function plots, and kernel density plots. By default, the plots are displayed in panels unless the global plot option UNPACK is specified. Also, when specifying more than one type of plots, the plots are displayed by parameters unless the global plot option GROUPBY is specified. When you specify only one plot request, you can omit the parentheses around the plot request. For example:

```
plots=none
plots(unpack)=trace
plots=(trace autocorr)
```

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;
proc lifereg;
 model y=x;
 bayes plots=trace;
run;
ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS](#).”

The global plot options are as follows:

#### **FRINGE**

creates a fringe plot on the X axis of the density plot.

#### **GROUPBY=PARAMETER**

#### **GROUPBY=TYPE**

specifies how the plots are grouped when there is more than one type of plot.

#### **GROUPBY=TYPE**

specifies that the plots be grouped by type.

#### **GROUPBY=PARAMETER**

specifies that the plots be grouped by parameter.

GROUPBY=PARAMETER is the default.

#### **LAGS=*n***

specifies that autocorrelations be plotted up to lag *n*. If this option is not specified, autocorrelations are plotted up to lag 50.

#### **SMOOTH**

displays a fitted penalized B-spline curve for each trace plot.

#### **UNPACKPANEL**

#### **UNPACK**

specifies that all paneled plots be unpacked, meaning that each plot in a panel is displayed separately.



The plot requests include the following:

**ALL**

specifies all types of plots. PLOTS=ALL is equivalent to specifying PLOTS=(TRACE AUTO-CORR DENSITY).

**AUTOCORR**

displays the autocorrelation function plots for the parameters.

**DENSITY**

displays the kernel density plots for the parameters.

**NONE**

suppresses all diagnostic plots.

**TRACE**

displays the trace plots for the parameters. See the section “[Visual Analysis via Trace Plots](#)” on page 139 for details.

**SCALEPRIOR=GAMMA**< (*options*) >

specifies that Gibbs sampling be performed on the location-scale model scale parameter and the prior distribution for the scale parameter.

A gamma prior  $G(a, b)$  with density  $f(t) = \frac{b(bt)^{a-1}e^{-bt}}{\Gamma(a)}$  is specified by SCALEPRIOR=GAMMA, which can be followed by one of the following *gamma-options* enclosed in parentheses. The hyperparameters  $a$  and  $b$  are the shape and inverse-scale parameters of the gamma distribution, respectively. See the section “[Gamma Prior](#)” on page 3949 for details. The default is  $G(10^{-4}, 10^{-4})$ .

**RELSHAPE**<=*c*>

specifies independent  $G(c\hat{\sigma}, c)$  distribution, where  $\hat{\sigma}$  is the MLE of the scale parameter. With this choice of hyperparameters, the mean of the prior distribution is  $\hat{\sigma}$  and the variance is  $\frac{\hat{\sigma}}{c}$ . By default,  $c=10^{-4}$ .

**SHAPE**=*a***ISCALE**=*b*

when both specified, results in a  $G(a, b)$  prior.

**SHAPE**=*c*

when specified alone, results in a  $G(c, c)$  prior.

**ISCALE**=*c*

when specified alone, results in a  $G(c, c)$  prior.

**SEED**=*number*

specifies an integer seed in the range 1 to  $2^{31} - 1$  for the random number generator in the simulation. Specifying a seed enables you to reproduce identical Markov chains for the same specification. If the SEED= option is not specified, or if you specify a nonpositive seed, a random seed is derived from the time of day.

**STATISTICS** <(global-options)> = **ALL** | **NONE** | *keyword* | (*keyword-list*)

**STATS** <(global-statoptions)> = **ALL** | **NONE** | *keyword* | (*keyword-list*)

controls the number of posterior statistics produced. Specifying STATISTICS=ALL is equivalent to specifying STATISTICS= (SUMMARY INTERVAL COV CORR). If you do not want any posterior statistics, you specify STATISTICS=NONE. The default is STATISTICS=(SUMMARY INTERVAL). See the section “[Summary Statistics](#)” on page 153 for details. The *global-options* include the following:

**ALPHA**=*numeric-list*

controls the probabilities of the credible intervals. The ALPHA= values must be between 0 and 1. Each ALPHA= value produces a pair of 100(1-ALPHA)% equal-tail and HPD intervals for each parameters. The default is ALPHA=0.05, which yields the 95% credible intervals for each parameter.

**PERCENT**=*numeric-list*

requests the percentile points of the posterior samples. The PERCENT= values must be between 0 and 100. The default is PERCENT=25, 50, 75, which yields the 25th, 50th, and 75th percentile points, respectively, for each parameter.

The list of *keywords* includes the following:

**CORR**

produces the posterior correlation matrix.

**COV**

produces the posterior covariance matrix.

**SUMMARY**

produces the means, standard deviations, and percentile points for the posterior samples. The default is to produce the 25th, 50th, and 75th percentile points, but you can use the global PERCENT= option to request specific percentile points.

**INTERVAL**

produces equal-tail credible intervals and HPD intervals. The default is to produce the 95% equal-tail credible intervals and 95% HPD intervals, but you can use the global ALPHA= option to request intervals of any probabilities.

**NONE**

suppresses printing all summary statistics.

**THINNING**=*number*

**THIN**=*number*

controls the thinning of the Markov chain. Only one in every  $k$  samples is used when THINNING= $k$ , and if  $NBI=n_0$  and  $NMC=n$ , the number of samples kept is

$$\left[ \frac{n_0 + n}{k} \right] - \left[ \frac{n_0}{k} \right]$$

where  $[a]$  represents the integer part of the number  $a$ . The default is THINNING=1.

**WEIBULLSCALEPRIOR=GAMMA**< *options* >

**WSCALEPRIOR=GAMMA**< *options* >

**WSCPRIOR=GAMMA**< *options* >

specifies that Gibbs sampling be performed on the Weibull model scale parameter and the prior distribution for the scale parameter. This option applies only when a Weibull distribution and no covariates are specified. When this option is specified, PROC LIFEREG performs Gibbs sampling on the Weibull scale parameter, which is defined as  $\exp(\mu)$ , where  $\mu$  is the intercept term.

A gamma prior  $G(a, b)$  is specified by WEIBULLSCALEPRIOR=GAMMA, which can be followed by one of the following *gamma-options* enclosed in parentheses. The gamma probability density is given by  $g(t) = \frac{b(bt)^{a-1}e^{-bt}}{\Gamma(a)}$ . The hyperparameters  $a$  and  $b$  are the shape and inverse-scale parameters of the gamma distribution, respectively. See the section “Gamma Prior” on page 3949 for details about the gamma prior. The default is  $G(10^{-4}, 10^{-4})$ .

**RELSHAPE**<=*c*>

specifies independent  $G(c\hat{\alpha}, c)$  distribution, where  $\hat{\alpha}$  is the MLE of the Weibull scale parameter. With this choice of hyperparameters, the mean of the prior distribution is  $\hat{\alpha}$  and the variance is  $\frac{\hat{\alpha}}{c}$ . By default,  $c=10^{-4}$ .

**SHAPE**=*a*

**ISCALE**=*b*

when both specified, results in a  $G(a, b)$  prior.

**SHAPE**=*c*

when specified alone, results in a  $G(c, c)$  prior.

**ISCALE**=*c*

when specified alone, results in a  $G(c, c)$  prior.

**WEIBULLSHAPEPRIOR=GAMMA**< *options* >

**WSHAPEPRIOR=GAMMA**< *options* >

**WSPRIOR=GAMMA**< *options* >

specifies that Gibbs sampling be performed on the Weibull model shape parameter and the prior distribution for the shape parameter. When this option is specified, PROC LIFEREG performs Gibbs sampling on the Weibull shape parameter, which is defined as  $\sigma^{-1}$ , where  $\sigma$  is the location-scale model scale parameter.

A gamma prior  $G(a, b)$  with density  $f(t) = \frac{b(bt)^{a-1}e^{-bt}}{\Gamma(a)}$  is specified by WEIBULLSHAPEPRIOR=GAMMA, which can be followed by one of the following *gamma-options* enclosed in parentheses. The hyperparameters  $a$  and  $b$  are the shape and inverse-scale parameters of the gamma distribution, respectively. See the section “Gamma Prior” on page 3949 for details about the gamma prior. The default is  $G(10^{-4}, 10^{-4})$ .

**RELSHAPE**<=*c*>

specifies independent  $G(c\hat{\beta}, c)$  distribution, where  $\hat{\beta}$  is the MLE of the Weibull shape parameter. With this choice of hyperparameters, the mean of the prior distribution is  $\hat{\beta}$  and the variance is  $\frac{\hat{\beta}}{c}$ . By default,  $c=10^{-4}$ .

**SHAPE**< =*a* >

**ISCALE**=*b*

when both specified, results in a  $G(a, b)$  prior.

**SHAPE**=*c*

when specified alone, results in a  $G(c, c)$  prior.

**ISCALE**=*c*

when specified alone, results in a  $G(c, c)$  prior.

## BY Statement

**BY** *variables* ;

You can specify a BY statement with PROC LIFEREG to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the LIFEREG procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

## CLASS Statement

**CLASS** *variables* < / **TRUNCATE** > ;

The CLASS statement names the classification variables to be used in the model. Typical classification variables are Treatment, Sex, Race, Group, and Replication. If you use the CLASS statement, it must appear before the MODEL statement.

Classification variables can be either character or numeric. By default, class levels are determined from the entire set of formatted values of the CLASS variables.

**NOTE:** Prior to SAS 9, class levels were determined by using no more than the first 16 characters of the formatted values. To revert to this previous behavior, you can use the TRUNCATE option in the CLASS statement.

In any case, you can use formats to group values into levels. See the discussion of the FORMAT procedure in the *Base SAS Procedures Guide* and the discussions of the FORMAT statement and SAS formats in *SAS*

*Formats and Informats: Reference.* You can adjust the order of CLASS variable levels with the **ORDER=** option in the **PROC LIFEREG** statement. You can specify the following option in the CLASS statement after a slash (/):

### TRUNCATE

specifies that class levels should be determined by using only up to the first 16 characters of the formatted values of CLASS variables. When formatted values are longer than 16 characters, you can use this option to revert to the levels as determined in releases prior to SAS 9.

## EFFECTPLOT Statement

**EFFECTPLOT** < *plot-type* < (*plot-definition-options*) >> < / *options* > ;

The EFFECTPLOT statement produces a display of the fitted model and provides options for changing and enhancing the displays. Table 51.3 describes the available *plot-types* and their *plot-definition-options*.

**Table 51.3** *Plot-Types and Plot-Definition-Options*

| Plot-Type and Description                                                                                                                                                                                                                 | Plot-Definition-Options                                                                                                            |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------|
| <p><b>BOX</b><br/>Displays a box plot of continuous response data at each level of a CLASS effect, with predicted values superimposed and connected by a line. This is an alternative to the <b>INTERACTION</b> <i>plot-type</i>.</p>     | <p><b>PLOTBY=</b> variable or CLASS effect<br/><b>X=</b> CLASS variable or effect</p>                                              |
| <p><b>CONTOUR</b><br/>Displays a contour plot of predicted values against two continuous covariates.</p>                                                                                                                                  | <p><b>PLOTBY=</b> variable or CLASS effect<br/><b>X=</b> continuous variable<br/><b>Y=</b> continuous variable</p>                 |
| <p><b>FIT</b><br/>Displays a curve of predicted values versus a continuous variable.</p>                                                                                                                                                  | <p><b>PLOTBY=</b> variable or CLASS effect<br/><b>X=</b> continuous variable</p>                                                   |
| <p><b>INTERACTION</b><br/>Displays a plot of predicted values (possibly with error bars) versus the levels of a CLASS effect. The predicted values are connected with lines and can be grouped by the levels of another CLASS effect.</p> | <p><b>PLOTBY=</b> variable or CLASS effect<br/><b>SLICEBY=</b> variable or CLASS effect<br/><b>X=</b> CLASS variable or effect</p> |
| <p><b>SLICEFIT</b><br/>Displays a curve of predicted values versus a continuous variable grouped by the levels of a CLASS effect.</p>                                                                                                     | <p><b>PLOTBY=</b> variable or CLASS effect<br/><b>SLICEBY=</b> variable or CLASS effect<br/><b>X=</b> continuous variable</p>      |

For full details about the syntax and options of the EFFECTPLOT statement, see the section “**EFFECTPLOT Statement**” on page 411 in Chapter 19, “**Shared Concepts and Topics**.”

## ESTIMATE Statement

```
ESTIMATE <'label'> estimate-specification <(divisor=n)>
 <, ... <'label'> estimate-specification <(divisor=n)>>
 </options>;
```

The ESTIMATE statement provides a mechanism for obtaining custom hypothesis tests. Estimates are formed as linear estimable functions of the form  $\mathbf{L}\boldsymbol{\beta}$ . You can perform hypothesis tests for the estimable functions, construct confidence limits, and obtain specific nonlinear transformations.

Table 51.4 summarizes the options available in the ESTIMATE statement.

**Table 51.4** ESTIMATE Statement Options

| Option                                                     | Description                                                               |
|------------------------------------------------------------|---------------------------------------------------------------------------|
| <b>Construction and Computation of Estimable Functions</b> |                                                                           |
| DIVISOR=                                                   | Specifies a list of values to divide the coefficients                     |
| NOFILL                                                     | Suppresses the automatic fill-in of coefficients for higher-order effects |
| SINGULAR=                                                  | Tunes the estimability checking difference                                |
| <b>Degrees of Freedom and <math>p</math>-values</b>        |                                                                           |
| ADJUST=                                                    | Determines the method for multiple comparison adjustment of estimates     |
| ALPHA= $\alpha$                                            | Determines the confidence level ( $1 - \alpha$ )                          |
| LOWER                                                      | Performs one-sided, lower-tailed inference                                |
| STEPDOWN                                                   | Adjusts multiplicity-corrected $p$ -values further in a step-down fashion |
| TESTVALUE=                                                 | Specifies values under the null hypothesis for tests                      |
| UPPER                                                      | Performs one-sided, upper-tailed inference                                |
| <b>Statistical Output</b>                                  |                                                                           |
| CL                                                         | Constructs confidence limits                                              |
| CORR                                                       | Displays the correlation matrix of estimates                              |
| COV                                                        | Displays the covariance matrix of estimates                               |
| E                                                          | Prints the $\mathbf{L}$ matrix                                            |
| JOINT                                                      | Produces a joint $F$ or chi-square test for the estimable functions       |
| PLOTS=                                                     | Requests ODS statistical graphics if the analysis is sampling-based       |
| SEED=                                                      | Specifies the seed for computations that depend on random numbers         |

For details about the syntax of the ESTIMATE statement, see the section “ESTIMATE Statement” on page 437 in Chapter 19, “Shared Concepts and Topics.”

## INSET Statement

**INSET** < keyword-list > < / options > ;

The box or table of summary information produced on plots made with the **PROBPLOT** statement is called an *inset*. You can use the **INSET** statement to customize the information that is displayed in the inset box as well as to customize the appearance of the inset box. To supply the information that is displayed in the inset box, you specify *keywords* corresponding to the information that you want shown. For example, the following statements produce a probability plot with the number of observations, the number of right-censored observations, the name of the distribution, and the estimated Weibull shape parameter in the inset:

```
proc lifereg data=epidemic;
 model life = dose / dist = Weibull;
 probplot;
 inset nobs right dist shape;
run;
```

By default, inset entries are identified with appropriate labels. However, you can provide a customized label by specifying the *keyword* for that entry followed by the equal sign (=) and the label in quotes. For example, the following **INSET** statement produces an inset containing the number of observations and the name of the distribution, labeled “Sample Size” and “Distribution” in the inset:

```
inset nobs='Sample Size' dist='Distribution';
```

If you specify a keyword that does not apply to the plot you are creating, then the keyword is ignored.

If you specify more than one **INSET** statement, only the first one is used.

Table 51.5 lists keywords available in the **INSET** statement to display summary statistics, distribution parameters, and distribution fitting information.

**Table 51.5** INSET Statement Keywords

| Keyword           | Description                                         |
|-------------------|-----------------------------------------------------|
| <b>CONFIDENCE</b> | Confidence coefficient for all confidence intervals |
| <b>DIST</b>       | Name of the distribution                            |
| <b>INTERVAL</b>   | Number of interval-censored observations            |
| <b>LEFT</b>       | Number of left-censored observations                |
| <b>NOBS</b>       | Number of observations                              |
| <b>NMISS</b>      | Number of observations with missing values          |
| <b>RIGHT</b>      | Number of right-censored observations               |
| <b>SCALE</b>      | Value of the scale parameter                        |
| <b>SHAPE</b>      | Value of the shape parameter                        |
| <b>UNCENSORED</b> | Number of uncensored observations                   |

The following *options* control the appearance of the box when you use traditional graphics. These options are not available if ODS Graphics is enabled. Table 51.6 summarizes the options available in the **INSET** statement.

**Table 51.6** INSET Statement Options

| Option           | Description                                    |
|------------------|------------------------------------------------|
| <b>CFILL=</b>    | Specifies the color for the filling box        |
| <b>CFILLH=</b>   | Specifies the color for the filling box header |
| <b>CFRAME=</b>   | Specifies the color for the frame              |
| <b>CHEADER=</b>  | Specifies the color for text in the header     |
| <b>CTEXT=</b>    | Specifies the color for the text               |
| <b>FONT=</b>     | Specifies the software font for the text       |
| <b>HEIGHT=</b>   | Specifies the height of the text               |
| <b>HEADER=</b>   | Specifies the text for the header or box title |
| <b>NOFRAME</b>   | Omits the frame around the box                 |
| <b>POS=</b>      | Determines the position of the inset           |
| <b>REFPOINT=</b> | Specifies the reference point for an inset     |

All *options* are specified after the slash (/) in the INSET statement.

**CFILL=***color*

specifies the color for the filling box.

**CFILLH=***color*

specifies the color for the filling box header.

**CFRAME=***color*

specifies the color for the frame.

**CHEADER=***color*

specifies the color for text in the header.

**CTEXT=***color*

specifies the color for the text.

**FONT=***font*

specifies the software font for the text.

**HEIGHT=***value*

specifies the height of the text.

**HEADER=**'*quoted string*'

specifies the text for the header or box title.

**NOFRAME**

omits the frame around the box.

**POS=***value* < **DATA** | **PERCENT** >

determines the position of the inset. The *value* can be a compass point (N, NE, E, SE, S, SW, W, NW) or a pair of coordinates (x, y) enclosed in parentheses. The coordinates can be specified in screen percentage units or axis data units. The default is screen percentage units.



**REFPOINT=*name***

specifies the reference point for an inset that is positioned by a pair of coordinates with the POS= option. You use the REFPOINT= option in conjunction with the POS= coordinates. The REFPOINT= option specifies which corner of the inset frame you have specified with coordinates (x, y), and it can take the value of BR (bottom right), BL (bottom left), TR (top right), or TL (top left). The default is REFPOINT=BL. If the inset position is specified as a compass point, then the REFPOINT= option is ignored.

---

## LSMEANS Statement

**LSMEANS** < *model-effects* > < / *options* > ;

The LSMEANS statement computes and compares least squares means (LS-means) of fixed effects. LS-means are *predicted population margins*—that is, they estimate the marginal means over a balanced population. In a sense, LS-means are to unbalanced designs as class and subclass arithmetic means are to balanced designs.

Table 51.7 summarizes the options available in the LSMEANS statement.

**Table 51.7** LSMEANS Statement Options

| Option                                          | Description                                                                                 |
|-------------------------------------------------|---------------------------------------------------------------------------------------------|
| <b>Construction and Computation of LS-Means</b> |                                                                                             |
| AT                                              | Modifies the covariate value in computing LS-means                                          |
| BYLEVEL                                         | Computes separate margins                                                                   |
| DIFF                                            | Requests differences of LS-means                                                            |
| OM=                                             | Specifies the weighting scheme for LS-means computation as determined by the input data set |
| SINGULAR=                                       | Tunes estimability checking                                                                 |
| <b>Degrees of Freedom and <i>p</i>-values</b>   |                                                                                             |
| ADJUST=                                         | Determines the method for multiple-comparison adjustment of LS-means differences            |
| ALPHA= $\alpha$                                 | Determines the confidence level ( $1 - \alpha$ )                                            |
| STEPDOWN                                        | Adjusts multiple-comparison <i>p</i> -values further in a step-down fashion                 |
| <b>Statistical Output</b>                       |                                                                                             |
| CL                                              | Constructs confidence limits for means and mean differences                                 |
| CORR                                            | Displays the correlation matrix of LS-means                                                 |
| COV                                             | Displays the covariance matrix of LS-means                                                  |
| E                                               | Prints the <b>L</b> matrix                                                                  |
| LINES                                           | Produces a “Lines” display for pairwise LS-means differences                                |
| MEANS                                           | Prints the LS-means                                                                         |
| PLOTS=                                          | Requests graphs of means and mean comparisons                                               |
| SEED=                                           | Specifies the seed for computations that depend on random numbers                           |

---

For details about the syntax of the LSMEANS statement, see the section “LSMEANS Statement” on page 453 in Chapter 19, “Shared Concepts and Topics.”

---

## LSMESTIMATE Statement

```
LSMESTIMATE model-effect <'label'> values <divisor=n>
 < , ... <'label'> values <divisor=n> >
 </options> ;
```

The LSMESTIMATE statement provides a mechanism for obtaining custom hypothesis tests among least squares means.

Table 51.8 summarizes the options available in the LSMESTIMATE statement.

**Table 51.8** LSMESTIMATE Statement Options

| Option                                              | Description                                                                         |
|-----------------------------------------------------|-------------------------------------------------------------------------------------|
| <b>Construction and Computation of LS-Means</b>     |                                                                                     |
| AT                                                  | Modifies covariate values in computing LS-means                                     |
| BYLEVEL                                             | Computes separate margins                                                           |
| DIVISOR=                                            | Specifies a list of values to divide the coefficients                               |
| OM=                                                 | Specifies the weighting scheme for LS-means computation as determined by a data set |
| SINGULAR=                                           | Tunes estimability checking                                                         |
| <b>Degrees of Freedom and <math>p</math>-values</b> |                                                                                     |
| ADJUST=                                             | Determines the method for multiple-comparison adjustment of LS-means differences    |
| ALPHA= $\alpha$                                     | Determines the confidence level $(1 - \alpha)$                                      |
| LOWER                                               | Performs one-sided, lower-tailed inference                                          |
| STEPDOWN                                            | Adjusts multiple-comparison $p$ -values further in a step-down fashion              |
| TESTVALUE=                                          | Specifies values under the null hypothesis for tests                                |
| UPPER                                               | Performs one-sided, upper-tailed inference                                          |
| <b>Statistical Output</b>                           |                                                                                     |
| CL                                                  | Constructs confidence limits for means and mean differences                         |
| CORR                                                | Displays the correlation matrix of LS-means                                         |
| COV                                                 | Displays the covariance matrix of LS-means                                          |
| E                                                   | Prints the <b>L</b> matrix                                                          |
| ELSM                                                | Prints the <b>K</b> matrix                                                          |
| JOINT                                               | Produces a joint $F$ or chi-square test for the LS-means and LS-means differences   |
| PLOTS=                                              | Requests graphs of means and mean comparisons                                       |
| SEED=                                               | Specifies the seed for computations that depend on random numbers                   |

---

For details about the syntax of the LSMESTIMATE statement, see the section “LSMESTIMATE Statement” on page 470 in Chapter 19, “Shared Concepts and Topics.”

## MODEL Statement

```
<label:> MODEL response< *censor(list)> = effects </ options> ;
```

```
<label:> MODEL (lower,upper)= effects </ options> ;
```

```
<label:> MODEL events/trials = effects </ options> ;
```

Only a single MODEL statement can be used with one invocation of the LIFEREG procedure. If multiple MODEL statements are present, only the last is used. The optional *label* is used to label the model estimates in the output SAS data set and OUTEST= data set.

The first MODEL syntax is appropriate for right censoring. The variable *response* is possibly right censored. If the *response* variable can be right censored, then a second variable, denoted *censor*, must appear after the *response* variable with a list of parenthesized values, separated by commas or blanks, to indicate censoring. That is, if the *censor* variable takes on a value given in the list, the *response* is a right-censored value; otherwise, it is an observed value.

The second MODEL syntax specifies two variables, *lower* and *upper*, that contain values of the endpoints of the censoring interval. If the two values are the same (and not missing), it is assumed that there is no censoring and the actual response value is observed. If the lower value is missing, then the upper value is used as a left-censored value. If the upper value is missing, then the lower value is taken as a right-censored value. If both values are present and the lower value is less than the upper value, it is assumed that the values specify a censoring interval. If the lower value is greater than the upper value or both values are missing, then the observation is not used in the analysis, although predicted values can still be obtained if none of the covariates are missing.

The following table summarizes the ways of specifying censoring.

| <i>lower</i> | <i>upper</i> | Comparison    | Interpretation                      |
|--------------|--------------|---------------|-------------------------------------|
| Not missing  | Not missing  | Equal         | No censoring                        |
| Not missing  | Not missing  | Lower < upper | Censoring interval                  |
| Missing      | Not missing  |               | Upper used as left-censoring value  |
| Not missing  | Missing      |               | Lower used as right-censoring value |
| Not missing  | Not missing  | Lower > upper | Observation not used                |
| Missing      | Missing      |               | Observation not used                |

The third MODEL syntax specifies two variables that contain count data for a binary response. The value of the first variable, *events*, is the number of successes. The value of the second variable, *trials*, is the number of tries. The values of both *events* and (*trials-events*) must be nonnegative, and *trials* must be positive for the response to be valid. The values of the two variables do not need to be integers and are not modified to be integers.

The *effects* following the equal sign are the covariates in the model. Higher-order effects, such as interactions and nested terms, are allowed in the list, similar to the GLM procedure. Variable names and combinations of variable names representing higher-order terms are allowed to appear in this list. Classification, or CLASS, variables can be used as effects, and indicator variables are generated for the class levels. If you do not specify any covariates following the equal sign, an intercept-only model is fit.

Examples of three valid MODEL statements follow:

```
a: model time*flag(1,3)=temp;
```

```
b: model (start, finish)=;
```

```
c: model r/n=dose;
```

MODEL statement a indicates that the response is contained in a variable named time and that, if the variable flag takes on the values 1 or 3, the observation is right censored. The explanatory variable is temp, which could be a CLASS variable. MODEL statement b indicates that the response is known to be in the interval between the values of the variables start and finish and that there are no covariates except for a default intercept term. MODEL statement c indicates a binary response, with the variable r containing the number of responses and the variable n containing the number of trials.

Table 51.9 summarizes the options available in the MODEL statement.

**Table 51.9** MODEL Statement Options

| Option                     | Description                                                                  |
|----------------------------|------------------------------------------------------------------------------|
| <b>Model specification</b> |                                                                              |
| ALPHA=                     | Sets the significance level                                                  |
| DISTRIBUTION=              | Specifies the distribution type for failure time                             |
| NOLOG                      | Requests no log transformation of response                                   |
| INTERCEPT=                 | Specifies initial estimate for intercept term                                |
| NOINT                      | Holds the intercept term fixed                                               |
| INITIAL=                   | Specifies initial estimates for regression parameters                        |
| OFFSET=                    | Specifies an offset variable                                                 |
| SCALE=                     | Initializes the scale parameter                                              |
| NOSCALE                    | Holds the scale parameter fixed                                              |
| SHAPE1=                    | Initializes the first shape parameter                                        |
| NOSHAPE1                   | Holds the first shape parameter fixed                                        |
| <b>Model fitting</b>       |                                                                              |
| CONVERGE=                  | Sets the convergence criterion                                               |
| MAXITER=                   | Sets the maximum number of iterations                                        |
| SINGULAR=                  | Sets the tolerance for testing singularity                                   |
| <b>Output</b>              |                                                                              |
| CORRB                      | Displays the estimated correlation matrix                                    |
| COVB                       | Displays the estimated covariance matrix                                     |
| ITPRINT                    | Displays the iteration history, final gradient, and second derivative matrix |

The following options can appear in the MODEL statement.

**ALPHA=value**

sets the significance level for the confidence intervals for regression parameters and estimated survival probabilities. The value must be between 0 and 1. By default, ALPHA=0.05.

**CONVERGE=value**

sets the convergence criterion. Convergence is declared when the maximum change in the parameter estimates between Newton-Raphson steps is less than the value specified. The change is a relative change if the parameter is greater than 0.01 in absolute value; otherwise, it is an absolute change. By default, CONVERGE=1E-8.

**CONVG=value**

sets the relative Hessian convergence criterion; *value* must be between 0 and 1. After convergence is determined with the change in parameter criterion specified with the CONVERGE= option, the quantity  $tc = \frac{\mathbf{g}'\mathbf{H}^{-1}\mathbf{g}}{|f|}$  is computed and compared to *value*, where  $\mathbf{g}$  is the gradient vector,  $\mathbf{H}$  is the Hessian matrix for the model parameters, and  $f$  is the log-likelihood function. If  $tc$  is greater than *value*, a warning that the relative Hessian convergence criterion has been exceeded is displayed. This criterion detects the occasional case where the change in parameter convergence criterion is satisfied, but a maximum in the log-likelihood function has not been attained. By default, CONVG=1E-4.

**CORRB**

produces the estimated correlation matrix of the parameter estimates.

**COVB**

produces the estimated covariance matrix of the parameter estimates.

**DISTRIBUTION=distribution-type****DIST=distribution-type****D=distribution-type**

specifies the distribution type assumed for the failure time. By default, PROC LIFEREG fits a type 1 extreme-value distribution to the log of the response. This is equivalent to fitting the Weibull distribution, since the scale parameter for the extreme-value distribution is related to a Weibull shape parameter and the intercept is related to the Weibull scale parameter in this case. When the NOLOG option is specified, PROC LIFEREG models the untransformed response with a type 1 extreme-value distribution as the default. See the section “Supported Distributions” on page 3933 for descriptions of the distributions. The following are valid values for *distribution-type*:

|                    |                                                                                                                                          |
|--------------------|------------------------------------------------------------------------------------------------------------------------------------------|
| <b>EXPONENTIAL</b> | the exponential distribution, which is treated as a restricted Weibull distribution                                                      |
| <b>GAMMA</b>       | a generalized gamma distribution (Lawless 2003, p. 240). The standard two-parameter gamma distribution is not available in PROC LIFEREG. |
| <b>LLOGISTIC</b>   | a log-logistic distribution                                                                                                              |
| <b>LNORMAL</b>     | a lognormal distribution                                                                                                                 |
| <b>LOGISTIC</b>    | a logistic distribution (equivalent to LLOGISTIC when the NOLOG option is specified)                                                     |
| <b>NORMAL</b>      | a normal distribution (equivalent to LNORMAL when the NOLOG option is specified)                                                         |

**WEIBULL** a Weibull distribution. If NOLOG is specified, it fits a type 1 extreme-value distribution to the raw, untransformed data.

By default, PROC LIFEREG transforms the response with the natural logarithm before fitting the specified model when you specify the GAMMA, LLOGISTIC, LNORMAL, or WEIBULL option. You can suppress the log transformation with the NOLOG option. The following table summarizes the resulting distributions when the preceding distribution options are used in combination with the NOLOG option.

|                      | <b>NOLOG</b>      |                                                                                                                                               |
|----------------------|-------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| <b>DISTRIBUTION=</b> | <b>Specified?</b> | <b>Resulting Distribution</b>                                                                                                                 |
| <b>EXPONENTIAL</b>   | No                | Exponential                                                                                                                                   |
| <b>EXPONENTIAL</b>   | Yes               | One-parameter extreme value                                                                                                                   |
| <b>GAMMA</b>         | No                | Generalized log-gamma using the log of the response.<br>(This is the same as fitting the generalized gamma using the untransformed response.) |
| <b>GAMMA</b>         | Yes               | Generalized log-gamma with untransformed responses                                                                                            |
| <b>LOGISTIC</b>      | No                | Logistic                                                                                                                                      |
| <b>LOGISTIC</b>      | Yes               | Logistic (NOLOG has no effect)                                                                                                                |
| <b>LLOGISTIC</b>     | No                | Log-logistic                                                                                                                                  |
| <b>LLOGISTIC</b>     | Yes               | Logistic                                                                                                                                      |
| <b>LNORMAL</b>       | No                | Lognormal                                                                                                                                     |
| <b>LNORMAL</b>       | Yes               | Normal                                                                                                                                        |
| <b>NORMAL</b>        | No                | Normal                                                                                                                                        |
| <b>NORMAL</b>        | Yes               | Normal (NOLOG has no effect)                                                                                                                  |
| <b>WEIBULL</b>       | No                | Weibull                                                                                                                                       |
| <b>WEIBULL</b>       | Yes               | Extreme value                                                                                                                                 |

**INITIAL=values**

sets initial values for the regression parameters. This option can be helpful in the case of convergence difficulty. Specified values are used to initialize the regression coefficients for the covariates specified in the MODEL statement. The intercept parameter is initialized with the INTERCEPT= option and is not included here. The values are assigned to the variables in the MODEL statement in the same order in which they are listed in the MODEL statement. Note that a CLASS variable requires  $k - 1$  values when the CLASS variable takes on  $k$  different levels. The order of the CLASS levels is determined by the ORDER= option. If there is no intercept term, the first CLASS variable requires  $k$  initial values. If a BY statement is used, all CLASS variables must take on the same number of levels in each BY group or no meaningful initial values can be specified. The INITIAL= option can be specified as follows.

| <b>Type of List</b>      | <b>Specification</b>       |
|--------------------------|----------------------------|
| List separated by blanks | <b>initial=3 4 5</b>       |
| List separated by commas | <b>initial=3,4,5</b>       |
| x to y                   | <b>initial=3 to 5</b>      |
| x to y by z              | <b>initial=3 to 5 by 1</b> |
| Combination of methods   | <b>initial=1,3 to 5,9</b>  |

By default, PROC LIFEREG computes initial estimates with ordinary least squares. See the section “Computational Method” on page 3931 for details.

**NOTE:** The INITIAL= option is overwritten by the INEST= option. See the section “INEST= Data Set” on page 3945 for details.

**INTERCEPT=***value*

initializes the intercept term to *value*. By default, the intercept is initialized by an ordinary least squares estimate.

**ITPRINT**

displays the iteration history for computing maximum likelihood estimates, the final evaluation of the gradient, and the final evaluation of the negative of the second derivative matrix—that is, the negative of the Hessian. If you perform a Bayesian analysis by specifying the BAYES statement, the iteration history for computing the mode of the posterior distribution is also displayed.

**MAXITER=***n*

sets the maximum allowable number of iterations during the model estimation. By default, MAXITER=50.

**NOINT**

holds the intercept term fixed. Because of the usual log transformation of the response, the intercept parameter is usually a scale parameter for the untransformed response, or a location parameter for a transformed response.

**NOLOG**

requests that no log transformation of the response variable be performed. By default, PROC LIFEREG models the log of the response variable for the GAMMA, LLOGISTIC, LOGNORMAL, and WEIBULL distribution options. NOLOG is implicitly assumed for the NORMAL and LOGISTIC distribution options.

**NOSCALE**

holds the scale parameter fixed. Note that if the log transformation has been applied to the response, the effect of the scale parameter is a power transformation of the original response. If no SCALE= value is specified, the scale parameter is fixed at the value 1.

**NOSHAPE1**

holds the first shape parameter, SHAPE1, fixed. If no SHAPE1= value is specified, SHAPE1 is fixed at a value that depends on the DISTRIBUTION type.

**OFFSET=***variable*

specifies a variable in the input data set to be used as an offset variable. This variable cannot be a CLASS variable, and it cannot be the response variable or one of the explanatory variables.

**SCALE=***value*

initializes the scale parameter to *value*. If the Weibull distribution is specified, this scale parameter is the scale parameter of the type 1 extreme-value distribution, not the Weibull scale parameter. Note that, with a log transformation, the exponential model is the same as a Weibull model with the scale parameter fixed at the value 1.

**SHAPE1=value**

initializes the first shape parameter to *value*. If the specified distribution does not depend on this parameter, then this option has no effect. The only distribution that depends on this shape parameter is the generalized gamma distribution. See the section “Supported Distributions” on page 3933 for descriptions of the parameterizations of the distributions.

**SINGULAR=value**

sets the tolerance for testing singularity of the information matrix and the crossproducts matrix for the initial least squares estimates. Roughly, the test requires that a pivot be at least this value times the original diagonal value. By default, SINGULAR=1E-12.

---

## OUTPUT Statement

**OUTPUT** < **OUT=SAS-data-set** > < *keyword=name* > ... < *keyword=name* > ;

The OUTPUT statement creates a new SAS data set containing statistics calculated after fitting the model. At least one specification of the form *keyword=name* is required.

All variables in the original data set are included in the new data set, along with the variables created as options for the OUTPUT statement. These new variables contain fitted values and estimated quantiles. If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*. Each OUTPUT statement applies to the preceding MODEL statement. See [Example 51.1](#) for illustrations of the OUTPUT statement.

The following specifications can appear in the OUTPUT statement:

**OUT=SAS-data-set**

specifies the new data set. By default, the procedure uses the *DATA**n* convention to name the new data set.

*keyword=name*

specifies the statistics to include in the output data set and gives names to the new variables. Specify a keyword for each desired statistic (see the following list of keywords), an equal sign, and the variable to contain the statistic.

The keywords allowed and the statistics they represent are as follows:

**CENSORED=variable**

specifies a *variable* to signal whether an observation is censored, and the type of censoring. The variable takes on values according to [Table 51.10](#).

**Table 51.10** Censoring Variable Values

| Type of Response  | CENSORED Variable Value |
|-------------------|-------------------------|
| Uncensored        | 0                       |
| Right-censored    | 1                       |
| Left-censored     | 2                       |
| Interval-censored | 3                       |



**CDF=variable**

specifies a *variable* to contain the estimates of the cumulative distribution function evaluated at the observed response. If the data are interval censored, then the cumulative distribution function is evaluated at the response lower interval endpoint. See the section “[Predicted Values](#)” on page 3937 for more information.

**CONTROL=variable**

specifies a *variable* in the input data set to control the estimation of quantiles. See [Example 51.1](#) for an illustration. If the specified variable has the value 1, estimates for all the values listed in the QUANTILE= list are computed for that observation in the input data set; otherwise, no estimates are computed. If no CONTROL= variable is specified, all quantiles are estimated for all observations. If the response variable in the MODEL statement is binomial, then this option has no effect.

**CRESIDUAL | CRES=variable**

specifies a *variable* to contain the Cox-Snell residuals

$$-\log(S(u_i))$$

where  $S$  is the standard survival function and

$$u_i = \frac{y_i - \mathbf{x}'_i \mathbf{b}}{\sigma}$$

If the data are interval censored, residuals are computed for  $y_i$  values corresponding to lower interval endpoints. If the response variable in the corresponding model statement is binomial, then the residuals are not computed, and this variable contains missing values.

**SRESIDUAL | SRES=variable**

specifies a *variable* to contain the standardized residuals

$$\frac{y_i - \mathbf{x}'_i \mathbf{b}}{\sigma}$$

If the data are interval censored, residuals are computed for  $y_i$  values corresponding to lower interval endpoints. If the response variable in the corresponding model statement is binomial, then the residuals are not computed, and this variable contains missing values.

**PREDICTED | P=variable**

specifies a *variable* to contain the quantile estimates. If the response variable in the corresponding model statement is binomial, then this variable contains the estimated probabilities,  $1 - F(-\mathbf{x}'\mathbf{b})$ .

**QUANTILES | QUANTILE | Q=value-list**

gives a list of *values* for which quantiles are calculated. The values must be between 0 and 1, noninclusive. For each value, a corresponding quantile is estimated. This option is not used if the response variable in the corresponding MODEL statement is binomial.

By default, QUANTILES=0.5. When the response is not binomial, a numeric variable, `_PROB_`, is added to the OUTPUT data set whenever the QUANTILES= option is specified. The variable `_PROB_` gives the probability value for the quantile estimates. These are the values taken from the QUANTILES= list and are given as values between 0 and 1, not as values between 0 and 100. The list of QUANTILES values can be specified as in [Table 51.11](#).

**Table 51.11** Types of Value Lists

| Type of List             | Specification      |
|--------------------------|--------------------|
| List separated by blanks | .2 .4 .6 .8        |
| List separated by commas | .2, .4, .6, .8     |
| x to y                   | .2 to .8           |
| x to y by z              | .2 to .8 by .1     |
| Combination of methods   | .1, .2 to .8 by .2 |

**STD\_ERR | STD=variable**

specifies a *variable* to contain the estimates of the standard errors of the estimated quantiles or  $x'b$ . If the response used in the MODEL statement is a binomial response, then these are the standard errors of  $x'b$ . Otherwise, they are the standard errors of the quantile estimates. These estimates can be used to compute confidence intervals for the quantiles. However, if the model is fit to the log of the event time, better confidence intervals can usually be computed by transforming the confidence intervals for the log response. See [Example 51.1](#) for such a transformation.

**XBETA=variable**

specifies a *variable* to contain the computed value of  $x'b$ , where  $x$  is the covariate vector and  $b$  is the vector of parameter estimates.

---

## PROBPLOT Statement

**PROBPLOT | PLOT** </options> ;

You can use the PROBPLOT statement to create a probability plot from lifetime data. The data can be uncensored, right censored, or arbitrarily censored. You can specify any number of PROBPLOT statements after a MODEL statement. The syntax used for the response in the MODEL statement determines the type of censoring assumed in creating the probability plot. The model fit with the MODEL statement is plotted along with the data. If there are covariates in the model, they are set to constant values specified in the XDATA= data set when creating the probability plot. If no XDATA= data set is specified, continuous variables are set to their overall mean values and categorical variables specified in the CLASS statement are set to their highest levels.

Table 51.12 summarizes the options available in the PROBPLOT statement.

**Table 51.12** PROBPLOT Statement Options

| Option                      | Description                                          |
|-----------------------------|------------------------------------------------------|
| <b>Traditional Graphics</b> |                                                      |
| ANNOTATE=                   | Specifies an Annotate data set                       |
| CAXIS=                      | Specifies the color used for the axes and tick marks |
| CCENSOR=                    | Specifies the color for filling the censor plot area |
| CENBIN                      | Plots censored data as frequency counts              |
| CENCOLOR=                   | Specifies the color for the censor symbol            |
| CENSYMBOL=                  | Specifies symbols for censored values                |

Table 51.12 continued

| Option       | Description                                                                      |
|--------------|----------------------------------------------------------------------------------|
| CFIT=        | Specifies the color for the fitted probability line and confidence curves        |
| CFRAME=      | Specifies the color for the area enclosed by the axes and frame                  |
| CGRID=       | Specifies the color for grid lines                                               |
| CHREF=       | Specifies the color for lines requested by the HREF= option                      |
| CTEXT=       | Specifies the color for tick mark values and axis labels                         |
| CVREF=       | Specifies the color for lines requested by the VREF= option                      |
| DESCRIPTION= | Specifies a description that appears in the PROC GREPLAY master menu             |
| FONT=        | Specifies a software font for reference line and axis labels                     |
| HCL          | Computes and draws confidence limits                                             |
| HEIGHT=      | Specifies the height of text used outside framed areas                           |
| HLOWER=      | Specifies the lower limit on the lifetime axis scale                             |
| HOFFSET=     | Specifies the offset for the horizontal axis                                     |
| HUPPER=      | Specifies <i>value</i> as the upper lifetime axis tick mark                      |
| HREF         | Draws reference lines perpendicular to the horizontal axis                       |
| HREFLABELS=  | Specifies labels for the lines requested by the HREF= option                     |
| HREFLABPOS=  | Specifies the vertical position of labels for HREF= lines                        |
| INBORDER     | Requests a border around probability plots                                       |
| INTERTILE=   | Specifies the distance between tiles                                             |
| ITPRINTEM    | Displays the iteration history for the Turnbull algorithm                        |
| JITTER=      | Specifies the amount to jitter overlaying plot symbols, in units of symbol width |
| LFIT=        | Specifies a line style for fitted curves and confidence limits                   |
| LGRID=       | Specifies a line style for all grid lines                                        |
| LHREF=       | Specifies the line type for lines requested by the HREF= option                  |
| LVREF=       | Specifies the line type for lines requested by the VREF= option                  |
| MAXITEM=     | Specifies the maximum number of iterations for the Turnbull algorithm            |
| NAME=        | Specifies a name for the plot                                                    |
| NOCENPLOT    | Suppresses the plotting of censored data points                                  |
| NOCONF       | Suppresses the default confidence bands                                          |
| NODATA       | Suppresses plotting of the estimated empirical probability plot                  |
| NOFIT        | Suppresses the fitted probability (percentile) line and confidence bands         |
| NOFRAME      | Suppresses the frame around plotting areas                                       |
| NOGRID       | Suppresses grid lines                                                            |
| NOHLABEL     | Suppresses horizontal label                                                      |
| NOHTICK      | Suppresses horizontal tick marks                                                 |
| NOPOLISH     | Suppresses setting small interval probabilities to zero                          |
| NOVLABEL     | Suppresses vertical labels                                                       |
| NOVTICK      | Suppresses vertical tick marks                                                   |
| NPINTERVALS= | Displays one of the two kinds of confidence limit                                |
| PCTLIST=     | Specifies the list of percentages for which to compute percentile estimates      |
| FLOWER=      | Specifies the lower limit on the probability axis scale                          |
| PRINTPROBS   | Displays intervals and associated probabilities for the Turnbull algorithm       |
| PUPPER=      | Specifies the upper limit on the probability axis scale                          |
| PPOS=        | Specifies the plotting position type                                             |
| PPOUT        | Displays a table of the cumulative probabilities                                 |

Table 51.12 continued

| Option              | Description                                                                                    |
|---------------------|------------------------------------------------------------------------------------------------|
| PROBLIST=           | Specifies the list of initial values for the Turnbull algorithm                                |
| ROTATE              | Requests probability plots with probability scale on the horizontal axis                       |
| SQUARE              | Makes the layout of the probability plots square                                               |
| TOLLIKE=            | Specifies the criterion for convergence in the Turnbull algorithm                              |
| TOLPROB=            | Specifies the criterion for setting the interval probability to zero in the Turnbull algorithm |
| VAXISLABEL=         | Specifies a label for the vertical axis                                                        |
| VREF                | Draws reference lines perpendicular to the vertical axis                                       |
| VREFLABELS=         | Specifies labels for the lines requested by the VREF= option                                   |
| VREFLABPOS=         | Specifies the horizontal position of labels for VREF= lines                                    |
| WAXIS=              | Specifies line thickness for axes and frame                                                    |
| WFIT=               | Specifies line thickness for fitted curves                                                     |
| WGRID=              | Specifies line thickness for grids                                                             |
| WREFL=              | Specifies line thickness for reference lines                                                   |
| <b>ODS Graphics</b> |                                                                                                |
| HCL                 | Computes and draws confidence limits for the predicted probabilities                           |
| HLOWER=             | Specifies <i>value</i> as the lower lifetime axis tick mark                                    |
| HUPPER=             | Specifies <i>value</i> as the upper lifetime axis tick mark                                    |
| HREF                | Draws reference lines perpendicular to the horizontal axis                                     |
| HREFLABELS=         | Specifies labels for the lines requested by the HREF= option                                   |
| ITPRINTEM           | Displays the iteration history for the Turnbull algorithm                                      |
| MAXITEM=            | Specifies the maximum number of iterations for the Turnbull algorithm                          |
| NOCENPLOT           | Suppresses the plotting of censored data points                                                |
| NOCONF              | Suppresses the default confidence bands                                                        |
| NODATA              | Suppresses plotting of the estimated empirical probability plot                                |
| NOFIT               | Suppresses the fitted probability (percentile) line and confidence bands                       |
| NOFRAME             | Suppresses the frame around plotting areas                                                     |
| NOGRID              | Suppresses grid lines                                                                          |
| NOPOLISH            | Suppresses setting small interval probabilities to zero in the Turnbull algorithm              |
| NPINTERVALS=        | Displays one of the two kinds of confidence limits                                             |
| PCTLIST=            | Specifies the list of percentages for which to compute percentile estimates                    |
| PLOWER=             | Specifies the lower limit on the probability axis scale                                        |
| PRINTPROBS          | Displays intervals and associated probabilities for the Turnbull algorithm                     |
| PUPPER=             | Specifies the upper limit on the probability axis scale                                        |
| PPOS=               | Specifies the plotting position type                                                           |
| PPOUT               | Displays a table of the cumulative probabilities                                               |
| PROBLIST=           | Specifies the list of initial values for the Turnbull algorithm                                |
| ROTATE              | Requests probability plots with probability scale on the horizontal axis                       |
| SQUARE              | Makes the layout of the probability plots square                                               |
| TOLLIKE=            | Specifies the criterion for convergence in the Turnbull algorithm                              |
| TOLPROB=            | Specifies the criterion for setting the interval probability to zero in the Turnbull algorithm |
| VREF                | Draws reference lines perpendicular to the vertical axis                                       |

You can specify the following options to control the content, layout, and appearance of a probability plot.

## Traditional Graphics

The following options are available if you use traditional graphics—that is, if ODS Graphics is not enabled.

**ANNOTATE=***SAS-data-set*

**ANNO=***SAS-data-set*

specifies an Annotate data set, as described in *SAS/GRAPH: Reference*, that enables you to add features to the probability plot. The data set you specify with the ANNOTATE= option in the PROBLOT statement provides the Annotate data set for all plots created by the statement.

**CAXIS=***color*

**CAXES=***color*

specifies the color used for the axes and tick marks. This option overrides any COLOR= specifications in an AXIS statement. The default is the first color in the device color list.

**CCENSOR=***color*

specifies the color for filling the censor plot area. The default is the first color in the device color list.

**CENBIN**

plots censored data as frequency counts (rounding for noninteger frequency) rather than as individual points.

**CENCOLOR=***color*

specifies the color for the censor symbol. The default is the first color in the device color list.

**CENSYMBOL=***symbol* | (*symbol list*)

specifies symbols for censored values. The *symbol* is one of the symbol names (plus, star, square, diamond, triangle, hash, paw, point, dot, and circle) or a letter (A–Z). If you do not specify the CENSYMBOL= option, the symbol used for censored values is the same as for failures.

**CFIT=***color*

specifies the color for the fitted probability line and confidence curves. The default is the first color in the device color list.

**CFRAME=***color*

**CFR=***color*

specifies the color for the area enclosed by the axes and frame. This area is not shaded by default.

**CGRID=***color*

specifies the color for grid lines. The default is the first color in the device color list.

**CHREF=***color*

**CH=***color*

specifies the color for lines requested by the HREF= option. The default is the first color in the device color list.

**CTEXT=***color*

specifies the color for tick mark values and axis labels. The default is the color specified for the CTEXT= option in the most recent GOPTIONS statement.

**CVREF=***color*

**CV=***color*

specifies the color for lines requested by the VREF= option. The default is the first color in the device color list.

**DESCRIPTION=**'*string*'

**DES=**'*string*'

specifies a description, up to 40 characters, that appears in the PROC GREPLAY master menu. The default is the variable name.

**FONT=***font*

specifies a software font for reference line and axis labels. You can also specify fonts for axis labels in an AXIS statement. The FONT= font takes precedence over the FTEXT= font specified in the most recent GOPTIONS statement. Hardware characters are used by default.

**HCL**

computes and draws confidence limits for the predicted probabilities based on distribution percentiles instead of the default CDF limits. See the section “[Confidence Limits for Percentiles](#)” on page 3945 for details of the computation.

**HEIGHT=***value*

specifies the height of text used outside framed areas. The default value is 3.846 (in percentage).

**HLOWER=***value*

specifies the lower limit on the lifetime axis scale. The HLOWER= option specifies *value* as the lower lifetime axis tick mark. The tick mark interval and the upper axis limit are determined automatically.

**HOFFSET=***value*

specifies the offset for the horizontal axis. The default value is 1.

**HUPPER=***value*

specifies *value* as the upper lifetime axis tick mark. The tick mark interval and the lower axis limit are determined automatically.

**HREF < (INTERSECT) > =***value-list*

requests reference lines perpendicular to the horizontal axis be drawn at horizontal axis values in the *value-list*. If (INTERSECT) is specified, a second reference line perpendicular to the vertical axis is drawn that intersects the fit line at the same point as the horizontal axis reference line. If a horizontal axis reference line label is specified with the HREFLABELS= option, the intersecting vertical axis reference line is labeled with the vertical axis value. See also the CHREF=, HREFLABELS=, and LHREF= options.

**HREFLABELS=**'*label1*' ... '*labeln*'

**HREFLABEL=**'*label1*' ... '*labeln*'

**HREFLAB=**'*label1*' ... '*labeln*'

specifies labels for the lines requested by the HREF= option. The number of labels must equal the number of lines. Enclose each label in quotes. Labels can be up to 16 characters.

**HREFLABPOS=*n***

specifies the vertical position of labels for HREF= lines. The following table shows the valid values for *n* and the corresponding label placements.

| <i>n</i> | Label Placement         |
|----------|-------------------------|
| 1        | Top                     |
| 2        | Staggered from top      |
| 3        | Bottom                  |
| 4        | Staggered from bottom   |
| 5        | Alternating from top    |
| 6        | Alternating from bottom |

**INBORDER**

requests a border around probability plots.

**INTERTILE=*value***

specifies the distance between tiles.

**ITPRINTEM**

displays the iteration history for the Turnbull algorithm.

**JITTER=*value***

specifies the amount to jitter overlaying plot symbols, in units of symbol width.

**LFIT=*linetype***

specifies a line style for fitted curves and confidence limits. By default, fitted curves are drawn by connecting solid lines (*linetype* = 1), and confidence limits are drawn by connecting dashed lines (*linetype* = 3).

**LGRID=*linetype***

specifies a line style for all grid lines; *linetype* is between 1 and 46. The default is 35.

**LHREF=*linetype*****LH=*linetype***

specifies the line type for lines requested by the HREF= option. The default is 2, which produces a dashed line.

**LVREF=*linetype*****LV=*linetype***

specifies the line type for lines requested by the VREF= option. The default is 2, which produces a dashed line.

**MAXITEM=*n1* <, *n2*>**

specifies the maximum number of iterations for the Turnbull algorithm. Iteration history will be displayed in increments of *n2* if requested with the ITPRINTEM option. See the section “[Arbitrarily Censored Data](#)” on page 3942 for details.

**NAME=*'string'***

specifies a name for the plot, up to eight characters, that appears in the PROC GREPLAY master menu. The default is 'LIFEREG'.

**NOCENPLOT**

suppresses the plotting of censored data points.

**NOCONF**

suppresses the default confidence bands on the probability plot.

**NODATA**

suppresses plotting of the estimated empirical probability plot.

**NOFIT**

suppresses the fitted probability (percentile) line and confidence bands.

**NOFRAME**

suppresses the frame around plotting areas.

**NOGRID**

suppresses grid lines.

**NOHLABEL**

suppresses horizontal labels.

**NOHTICK**

suppresses horizontal tick marks.

**NOPOLISH**

suppresses setting small interval probabilities to zero in the Turnbull algorithm.

**NOVLABEL**

suppresses vertical labels.

**NOVTICK**

suppresses vertical tick marks.

**NPINTERVALS=*interval type***

specifies one of the two kinds of confidence limits for the estimated cumulative probabilities, pointwise (NPINTERVALS=POINT) or simultaneous (NPINTERVALS=SIMUL), requested by the PPOUT option to be displayed in the tabular output.

**PCTLIST=*value-list***

specifies the list of percentages for which to compute percentile estimates; *value-list* must be a list of values separated by blanks or commas. Each value in the list must be between 0 and 100.

**PLOWER=*value***

specifies the lower limit on the probability axis scale. The PLOWER= option specifies *value* as the lower probability axis tick mark. The tick mark interval and the upper axis limit are determined automatically.

**PRINTPROBS**

displays intervals and associated probabilities for the Turnbull algorithm.



**PUPPER=***value*

specifies the upper limit on the probability axis scale. The PUPPER= option specifies *value* as the upper probability axis tick mark. The tick mark interval and the lower axis limit are determined automatically.

**PPOS=***character-list*

specifies the plotting position type. See the section “Probability Plotting” on page 3940 for details.

| <b>PPOS=</b>    | <b>Method</b>                   |
|-----------------|---------------------------------|
| <b>EXPRANK</b>  | Expected ranks                  |
| <b>MEDRANK</b>  | Median ranks                    |
| <b>MEDRANK1</b> | Median ranks (exact formula)    |
| <b>KM</b>       | Kaplan-Meier                    |
| <b>MKM</b>      | Modified Kaplan-Meier (default) |

**PPOUT**

specifies that a table of the cumulative probabilities plotted on the probability plot be displayed. Kaplan-Meier estimates of the cumulative probabilities are also displayed, along with standard errors and confidence limits. The confidence limits can be pointwise or simultaneous, as specified by the NPINTERVALS= option.

**PROBLIST=***value-list*

specifies the list of initial values for the Turnbull algorithm.

**ROTATE**

requests probability plots with probability scale on the horizontal axis.

**SQUARE**

makes the layout of the probability plots square.

**TOLLIKE=***value*

specifies the criterion for convergence in the Turnbull algorithm.

**TOLPROB=***value*

specifies the criterion for setting the interval probability to zero in the Turnbull algorithm.

**VAXISLABEL=***'string'*

specifies a label for the vertical axis.

**VREF**<(INTERSECT)>=*value-list*

requests reference lines perpendicular to the vertical axis be drawn at vertical axis values in the *value-list*. If (INTERSECT) is specified, a second reference line perpendicular to the horizontal axis is drawn that intersects the fit line at the same point as the vertical axis reference line. If a vertical axis reference line label is specified with the VREFLABELS= option, the intersecting horizontal axis reference line is labeled with the horizontal axis value. See also the CVREF=, LVREF=, and VREFLABELS= options.

**VREFLABELS=**'label1' ... 'labeln'

**VREFLABEL=**'label1' ... 'labeln'

**VREFLAB=**'label1' ... 'labeln'

specifies labels for the lines requested by the VREF= option. The number of labels must equal the number of lines. Enclose each label in quotes. Labels can be up to 16 characters.

**VREFLABPOS=***n*

specifies the horizontal position of labels for VREF= lines. The valid values for *n* and the corresponding label placements are shown in the following table.

| <i>n</i> | Label Placement |
|----------|-----------------|
| 1        | Left            |
| 2        | Right           |

**WAXIS=***n*

specifies line thickness for axes and frame. The default value is 1.

**WFIT=***n*

specifies line thickness for fitted curves. The default value is 1.

**WGRID=***n*

specifies line thickness for grids. The default value is 1.

**WREFL=***n*

specifies line thickness for reference lines. The default value is 1.

## ODS Graphics

The following options are available if ODS Graphics is enabled.

**HCL**

computes and draws confidence limits for the predicted probabilities in the horizontal direction.

**HLOWER=***value*

specifies the lower limit on the lifetime axis scale. The HLOWER= option specifies *value* as the lower lifetime axis tick mark. The tick mark interval and the upper axis limit are determined automatically.

**HUPPER=***value*

specifies *value* as the upper lifetime axis tick mark. The tick mark interval and the lower axis limit are determined automatically.

**HREF < (INTERSECT) > =***value-list*

requests reference lines perpendicular to the horizontal axis be drawn at horizontal axis values in the *value-list*. If (INTERSECT) is specified, a second reference line perpendicular to the vertical axis is drawn that intersects the fit line at the same point as the horizontal axis reference line. If a horizontal axis reference line label is specified with the HREFLABELS= option, the intersecting vertical axis reference line is labeled with the vertical axis value. See also the CHREF=, HREFLABELS=, and LHREF= options.

**HREFLABELS=***'label1' ... 'labeln'*

**HREFLABEL=***'label1' ... 'labeln'*

**HREFLAB=***'label1' ... 'labeln'*

specifies labels for the lines requested by the HREF= option. The number of labels must equal the number of lines. Enclose each label in quotes. Labels can be up to 16 characters.

**ITPRINTEM**

displays the iteration history for the Turnbull algorithm.

**MAXITEM=***n1 <,n2>*

specifies the maximum number of iterations for the Turnbull algorithm. Iteration history will be displayed in increments of *n2* if requested with the ITPRINTEM option. See the section “[Arbitrarily Censored Data](#)” on page 3942 for details.

**NOCENPLOT**

suppresses the plotting of censored data points.

**NOCONF**

suppresses the default confidence bands on the probability plot.

**NODATA**

suppresses plotting of the estimated empirical probability plot.

**NOFIT**

suppresses the fitted probability (percentile) line and confidence bands.

**NOFRAME**

suppresses the frame around plotting areas.

**NOGRID**

suppresses grid lines.

**NOPOLISH**

suppresses setting small interval probabilities to zero in the Turnbull algorithm.

**NPINTERVALS=***interval type*

specifies one of the two kinds of confidence limits for the estimated cumulative probabilities, pointwise (NPINTERVALS=POINT) or simultaneous (NPINTERVALS=SIMUL), requested by the PPOUT option to be displayed in the tabular output.

**PCTLIST=***value-list*

specifies the list of percentages for which to compute percentile estimates; *value-list* must be a list of values separated by blanks or commas. Each value in the list must be between 0 and 100.

**PLOWER=***value*

specifies the lower limit on the probability axis scale. The PLOWER= option specifies *value* as the lower probability axis tick mark. The tick mark interval and the upper axis limit are determined automatically.

**PRINTPROBS**

displays intervals and associated probabilities for the Turnbull algorithm.

**PUPPER=*value***

specifies the upper limit on the probability axis scale. The PUPPER= option specifies *value* as the upper probability axis tick mark. The tick mark interval and the lower axis limit are determined automatically.

**PPOS=*plotting-position-type***

specifies the plotting position type. See the section “Probability Plotting” on page 3940 for details.

| <b>PPOS=</b>    | <b>Method</b>                   |
|-----------------|---------------------------------|
| <b>EXPRANK</b>  | Expected ranks                  |
| <b>MEDRANK</b>  | Median ranks                    |
| <b>MEDRANK1</b> | Median ranks (exact formula)    |
| <b>KM</b>       | Kaplan-Meier                    |
| <b>MKM</b>      | Modified Kaplan-Meier (default) |

**PPOUT**

specifies that a table of the cumulative probabilities plotted on the probability plot be displayed. Kaplan-Meier estimates of the cumulative probabilities are also displayed, along with standard errors and confidence limits. The confidence limits can be pointwise or simultaneous, as specified by the NPINTERVALS= option.

**PROBLIST=*value-list***

specifies the list of initial values for the Turnbull algorithm.

**ROTATE**

requests probability plots with probability scale on the horizontal axis.

**SQUARE**

makes the layout of the probability plots square.

**TOLLIKE=*value***

specifies the criterion for convergence in the Turnbull algorithm.

**TOLPROB=*value***

specifies the criterion for setting the interval probability to zero in the Turnbull algorithm.

**VREF<(INTERSECT)>=*value-list***

requests reference lines perpendicular to the vertical axis be drawn at vertical axis values in the *value-list*. If (INTERSECT) is specified, a second reference line perpendicular to the horizontal axis is drawn that intersects the fit line at the same point as the vertical axis reference line. If a vertical axis reference line label is specified with the VREFLABELS= option, the intersecting horizontal axis reference line is labeled with the horizontal axis value. See also the CVREF=, LVREF=, and VREFLABELS= options.

**VREFLABELS=*'label1' ... 'labeln'*****VREFLABEL=*'label1' ... 'labeln'*****VREFLAB=*'label1' ... 'labeln'***

specifies labels for the lines requested by the VREF= option. The number of labels must equal the number of lines. Enclose each label in quotes. Labels can be up to 16 characters.

---

## SLICE Statement

**SLICE** *model-effect* </ options > ;

The SLICE statement provides a general mechanism for performing a partitioned analysis of the LS-means for an interaction. This analysis is also known as an analysis of simple effects.

The SLICE statement uses the same options as the LSMEANS statement, which are summarized in Table 19.21. For details about the syntax of the SLICE statement, see the section “SLICE Statement” on page 498 in Chapter 19, “Shared Concepts and Topics.”

---

## STORE Statement

**STORE** < **OUT=** > *item-store-name* </ **LABEL=** 'label' > ;

The STORE statement requests that the procedure save the context and results of the statistical analysis. The resulting item store has a binary file format that cannot be modified. The contents of the item store can be processed with the PLM procedure.

For details about the syntax of the STORE statement, see the section “STORE Statement” on page 501 in Chapter 19, “Shared Concepts and Topics.”

---

## TEST Statement

**TEST** < *model-effects* > </ options > ;

The TEST statement enables you to perform chi-square tests for model effects that test Type I, Type II, or Type III hypotheses. By default, the Type III tests are performed. For more information, see Chapter 19, “Shared Concepts and Topics.”

---

## WEIGHT Statement

**WEIGHT** *variable* ;

If you want to use weights for each observation in the input data set, place the weights in a variable in the data set and specify the name in a WEIGHT statement. The values of the WEIGHT variable can be nonintegral and are not truncated. Observations with nonpositive or missing values for the weight variable do not contribute to the fit of the model. The WEIGHT variable multiplies the contribution to the log likelihood for each observation.

---

## Details: LIFEREG Procedure

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### Missing Values

Any observation with missing values for the dependent variable is not used in the model estimation unless it is one and only one of the values in an interval specification. Also, if one of the explanatory variables or the censoring variable is missing, the observation is not used. For any observation to be used in the estimation of a model, only the variables needed in that model have to be nonmissing. Predicted values are computed for all observations with no missing explanatory variable values. If the censoring variable is missing, the CENSORED= variable in the OUT= SAS data set is also missing.

---

### Model Specification

Main effects as well as interaction terms are allowed in the model specification, similar to the GLM procedure. For numeric variables, a main effect is a linear term equal to the value of the variable unless the variable appears in the CLASS statement. For variables listed in the CLASS statement, PROC LIFEREG creates indicator variables (variables taking the values zero or one) for every level of the variable except the last level. If there is no intercept term, the first CLASS variable has indicator variables created for all levels including the last level. The levels are ordered according to the ORDER= option. Estimates of a main effect depend upon other effects in the model and, therefore, are adjusted for the presence of other effects in the model.

---

### Computational Method

By default, the LIFEREG procedure computes initial values for the parameters by using ordinary least squares (OLS) and ignoring censoring. This might not be the best set of starting values for a given set of data. For example, if there are extreme values in your data, the OLS fit might be excessively influenced by the extreme observations, causing an overflow or convergence problems. See [Example 51.3](#) for one way to deal with convergence problems.

You can specify the INITIAL= option in the MODEL statement to override these starting values. You can also specify the INTERCEPT=, SCALE=, and SHAPE= options to set initial values of the intercept, scale, and shape parameters. For models with multilevel interaction effects, it is a little difficult to use the INITIAL= option to provide starting values for all parameters. In this case, you can use the INEST= data set. See the section “[INEST= Data Set](#)” on page 3945 for details. The INEST= data set overrides all previous specifications for starting values of parameters.

The rank of the design matrix  $\mathbf{X}$  is estimated before the model is fit. Columns of  $\mathbf{X}$  that are judged linearly dependent on other columns have the corresponding parameters set to zero. The test for linear dependence is controlled by the SINGULAR= option in the MODEL statement. Variables are included in the model in the order in which they are listed in the MODEL statement with the continuous variables included in the model before any classification variables.

The log-likelihood function is maximized by means of a ridge-stabilized Newton-Raphson algorithm. The maximized value of the log likelihood can take positive or negative values, depending on the specified model and the values of the maximum likelihood estimates of the model parameters.

If convergence of the maximum likelihood estimates is attained, a Type III chi-square test statistic is computed for each effect, testing whether there is any contribution from any of the levels of the effect. This statistic is computed as a quadratic form in the appropriate parameter estimates by using the corresponding submatrix of the asymptotic covariance matrix estimate. See Chapter 42, “The GLM Procedure,” and Chapter 15, “The Four Types of Estimable Functions,” for more information about Type III estimable functions. The asymptotic covariance matrix is computed as the inverse of the observed information matrix. Note that if the NOINT option is specified and CLASS variables are used, the first CLASS variable contains a contribution from an intercept term. The results are displayed in an ODS table named “Type3Analysis.” Chi-square tests for individual parameters are Wald tests based on the observed information matrix and the parameter estimates. If an effect has a single degree of freedom in the parameter estimates table, the chi-square test for this parameter is equivalent to the Type III test for this effect.

Before SAS 8.2, a multiple-degree-of-freedom statistic was computed for each effect to test for contribution from any level of the effect. In general, the Type III test statistic in a main-effect-only model (no interaction terms) will be equal to the previously computed effect statistic, unless there are collinearities among the effects. If there are collinearities, the Type III statistic will adjust for them, and the value of the Type III statistic and the number of degrees of freedom might not be equal to those of the previous effect statistic.

Suppose there are  $n$  observations from the model  $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \sigma\boldsymbol{\epsilon}$  (or  $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{O} + \sigma\boldsymbol{\epsilon}$  if there is an offset variable), where  $\mathbf{X}$  is an  $n \times k$  matrix of covariate values (including the intercept),  $\mathbf{y}$  is a vector of responses,  $\mathbf{O}$  is a vector of offset variable values, and  $\boldsymbol{\epsilon}$  is a vector of errors with survival function  $S$ , cumulative distribution function  $F$ , and probability density function  $f$ . That is,  $S(t) = \Pr(\epsilon_i > t)$ ,  $F(t) = \Pr(\epsilon_i \leq t)$ , and  $f(t) = dF(t)/dt$ , where  $\epsilon_i$  is a component of the error vector. Then, if all the responses are observed, the log likelihood,  $L$ , can be written as

$$L = \sum \log \left( \frac{f(u_i)}{\sigma} \right)$$

where  $u_i = \frac{1}{\sigma}(y_i - \mathbf{x}'_i\boldsymbol{\beta})$ .

If some of the responses are left, right, or interval censored, the log likelihood can be written as

$$L = \sum \log \left( \frac{f(u_i)}{\sigma} \right) + \sum \log (S(u_i)) + \sum \log (F(u_i)) + \sum \log (F(u_i) - F(v_i))$$

with the first sum over uncensored observations, the second sum over right-censored observations, the third sum over left-censored observations, the last sum over interval-censored observations, and

$$v_i = \frac{1}{\sigma}(z_i - \mathbf{x}'_i\boldsymbol{\beta})$$

where  $z_i$  is the lower end of a censoring interval.

If the response is specified in the binomial format, *events/trials*, then the log-likelihood function is

$$L = \sum r_i \log(P_i) + (n_i - r_i) \log(1 - P_i)$$

where  $r_i$  is the number of events and  $n_i$  is the number of trials for the  $i$ th observation. In this case,  $P_i = 1 - F(-\mathbf{x}'_i\boldsymbol{\beta})$ . For the symmetric distributions, logistic and normal, this is the same as  $F(\mathbf{x}'_i\boldsymbol{\beta})$ . Additional

information about censored and limited dependent variable models can be found in Kalbfleisch and Prentice (1980) and Maddala (1983).

The estimated covariance matrix of the parameter estimates is computed as the negative inverse of  $\mathbf{I}$ , which is the information matrix of second derivatives of  $L$  with respect to the parameters evaluated at the final parameter estimates. If  $\mathbf{I}$  is not positive definite, a positive-definite submatrix of  $\mathbf{I}$  is inverted, and the remaining rows and columns of the inverse are set to zero. If some of the parameters, such as the scale and intercept, are restricted, the corresponding elements of the estimated covariance matrix are set to zero. The standard error estimates for the parameter estimates are taken as the square roots of the corresponding diagonal elements.

For restrictions placed on the intercept, scale, and shape parameters, one-degree-of-freedom Lagrange multiplier test statistics are computed. These statistics are computed as

$$\chi^2 = \frac{g^2}{V}$$

where  $g$  is the derivative of the log likelihood with respect to the restricted parameter at the restricted maximum and

$$V = \mathbf{I}_{11} - \mathbf{I}_{12}\mathbf{I}_{22}^{-1}\mathbf{I}_{21}$$

where the 1 subscripts refer to the restricted parameter and the 2 subscripts refer to the unrestricted parameters. The information matrix is evaluated at the restricted maximum. These statistics are asymptotically distributed as chi-squares with one degree of freedom under the null hypothesis that the restrictions are valid, provided that some regularity conditions are satisfied. See Rao (1973, p. 418) for a more complete discussion. It is possible for these statistics to be missing if the observed information matrix is not positive definite. Higher-degree-of-freedom tests for multiple restrictions are not currently computed.

A Lagrange multiplier test statistic is computed to test this constraint. Notice that this test statistic is comparable to the Wald test statistic for testing that the scale is one. The Wald statistic is the result of squaring the difference of the estimate of the scale parameter from one and dividing this by the square of its estimated standard error.

---

## Supported Distributions

For most distributions, the baseline survival function ( $S$ ) and the probability density function ( $f$ ) are listed for the additive random disturbance ( $y_0$  or  $\log(T_0)$ ) with location parameter  $\mu$  and scale parameter  $\sigma$ . See the section “[Overview: LIFEREG Procedure](#)” on page 3878 for more information. These distributions apply when the log of the response is modeled (this is the default analysis). The corresponding survival function ( $G$ ) and its density function ( $g$ ) are given for the untransformed baseline distribution ( $T_0$ ).

For the normal and logistic distributions, the response is not log transformed by PROC LIFEREG, and the survival functions and probability density functions listed apply to the untransformed response.

For example, for the WEIBULL distribution,  $S(w)$  and  $f(w)$  are the survival function and the probability density function for the extreme-value distribution (distribution of the log of the response), while  $G(t)$  and  $g(t)$  are the survival function and the probability density function of a Weibull distribution (using the untransformed response).

The chosen baseline functions define the meaning of the intercept, scale, and shape parameters. Only the gamma distribution has a free shape parameter in the following parameterizations. Notice that some of the



distributions do not have mean zero and that  $\sigma$  is not, in general, the standard deviation of the baseline distribution.

For the Weibull distribution, the accelerated failure time model is also a proportional-hazards model. However, the parameterization for the covariates differs by a multiple of the scale parameter from the parameterization commonly used for the proportional hazards model.

The distributions supported in the LIFEREG procedure follow. If there are no covariates in the model,  $\mu =$  Intercept in the output; otherwise,  $\mu = \mathbf{x}'\boldsymbol{\beta}$ .  $\sigma =$  Scale in the output.

## Exponential

$$\begin{aligned} S(w) &= \exp(-\exp(w - \mu)) \\ f(w) &= \exp(w - \mu) \exp(-\exp(w - \mu)) \\ G(t) &= \exp(-\alpha t) \\ g(t) &= \alpha \exp(-\alpha t) \end{aligned}$$

where  $\exp(-\mu) = \alpha$ .

## Generalized Gamma

$S(w) = S'(u)$ ,  $f(w) = \sigma^{-1} f'(u)$ ,  $G(t) = G'(v)$ ,  $g(t) = \frac{v}{t\sigma} g'(v)$ ,  $u = \frac{w-\mu}{\sigma}$ ,  $v = \exp(\frac{\log(t)-\mu}{\sigma})$ , and

$$\begin{aligned} S'(u) &= \begin{cases} 1 - \frac{\Gamma(\delta^{-2}, \delta^{-2} \exp(\delta u))}{\Gamma(\delta^{-2})} & \text{if } \delta > 0 \\ \frac{\Gamma(\delta^{-2}, \delta^{-2} \exp(\delta u))}{\Gamma(\delta^{-2})} & \text{if } \delta < 0 \end{cases} \\ f'(u) &= \frac{|\delta|}{\Gamma(\delta^{-2})} (\delta^{-2} \exp(\delta u))^{\delta^{-2}} \exp(-\exp(\delta u) \delta^{-2}) \\ G'(v) &= \begin{cases} 1 - \frac{\Gamma(\delta^{-2}, \delta^{-2} v^\delta)}{\Gamma(\delta^{-2})} & \text{if } \delta > 0 \\ \frac{\Gamma(\delta^{-2}, \delta^{-2} v^\delta)}{\Gamma(\delta^{-2})} & \text{if } \delta < 0 \end{cases} \\ g'(v) &= \frac{|\delta|}{v\Gamma(\delta^{-2})} (\delta^{-2} v^\delta)^{\delta^{-2}} \exp(-v^\delta \delta^{-2}) \end{aligned}$$

where  $\Gamma(a)$  denotes the complete gamma function,  $\Gamma(a, z)$  denotes the incomplete gamma function, and  $\delta$  is a free shape parameter. The  $\delta$  parameter is called Shape by PROC LIFEREG. See Lawless (2003, p. 240), and Klein and Moeschberger (1997, p. 386) for a description of the generalized gamma distribution.

**Logistic**

$$S(w) = \left(1 + \exp\left(\frac{w - \mu}{\sigma}\right)\right)^{-1}$$

$$f(w) = \frac{\exp\left(\frac{w - \mu}{\sigma}\right)}{\sigma \left(1 + \exp\left(\frac{w - \mu}{\sigma}\right)\right)^2}$$

**Log-Logistic**

$$S(w) = \left(1 + \exp\left(\frac{w - \mu}{\sigma}\right)\right)^{-1}$$

$$f(w) = \frac{\exp\left(\frac{w - \mu}{\sigma}\right)}{\sigma \left(1 + \exp\left(\frac{w - \mu}{\sigma}\right)\right)^2}$$

$$G(t) = \frac{1}{1 + \alpha t^\gamma}$$

$$g(t) = \frac{\alpha \gamma t^{\gamma-1}}{(1 + \alpha t^\gamma)^2}$$

where  $\gamma = 1/\sigma$  and  $\alpha = \exp(-\mu/\sigma)$ .

**Lognormal**

$$S(w) = 1 - \Phi\left(\frac{w - \mu}{\sigma}\right)$$

$$f(w) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2}\left(\frac{w - \mu}{\sigma}\right)^2\right)$$

$$G(t) = 1 - \Phi\left(\frac{\log(t) - \mu}{\sigma}\right)$$

$$g(t) = \frac{1}{\sqrt{2\pi}\sigma t} \exp\left(-\frac{1}{2}\left(\frac{\log(t) - \mu}{\sigma}\right)^2\right)$$

where  $\Phi$  is the cumulative distribution function for the normal distribution.

**Normal**

$$S(w) = 1 - \Phi\left(\frac{w - \mu}{\sigma}\right)$$

$$f(w) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2}\left(\frac{w - \mu}{\sigma}\right)^2\right)$$

where  $\Phi$  is the cumulative distribution function for the normal distribution.

**Weibull**

$$S(w) = \exp\left(-\exp\left(\frac{w - \mu}{\sigma}\right)\right)$$

$$f(w) = \frac{1}{\sigma} \exp\left(\frac{w - \mu}{\sigma}\right) \exp\left(-\exp\left(\frac{w - \mu}{\sigma}\right)\right)$$

$$G(t) = \exp(-\alpha t^\gamma)$$

$$g(t) = \gamma \alpha t^{\gamma-1} \exp(-\alpha t^\gamma)$$

where  $\sigma = 1/\gamma$  and  $\alpha = \exp(-\mu/\sigma)$ .

If your parameterization is different from the ones shown here, you can still use the procedure to fit your model. For example, a common parameterization for the Weibull distribution is

$$g(t; \lambda, \beta) = \left(\frac{\beta}{\lambda}\right) \left(\frac{t}{\lambda}\right)^{\beta-1} \exp\left(-\left(\frac{t}{\lambda}\right)^\beta\right)$$

$$G(t; \lambda, \beta) = \exp\left(-\left(\frac{t}{\lambda}\right)^\beta\right)$$

so that  $\lambda = \exp(\mu)$  and  $\beta = 1/\sigma$ .

Again note that the expected value of the baseline log response is, in general, not zero and that the distributions are not symmetric in all cases. Thus, for a given set of covariates,  $\mathbf{x}$ , the expected value of the log response is not always  $\mathbf{x}'\boldsymbol{\beta}$ .

Some relations among the distributions are as follows:

- The gamma with Shape=1 is a Weibull distribution.
- The gamma with Shape=0 is a lognormal distribution.
- The Weibull with Scale=1 is an exponential distribution.

## Predicted Values

For a given set of covariates,  $\mathbf{x}$  (including the intercept term), the  $p$ th quantile of the log response,  $y_p$ , is given by

$$y_p = \mathbf{x}'\boldsymbol{\beta} + \sigma u_p$$

if no offset variable has been specified, or

$$y_p = \mathbf{x}'\boldsymbol{\beta} + o + \sigma u_p$$

for a given value  $o$  of an offset variable, where  $u_p$  is the  $p$ th quantile of the baseline distribution. The estimated quantile is computed by replacing the unknown parameters with their estimates, including any shape parameters on which the baseline distribution might depend. The estimated quantile of the original response is obtained by taking the exponential of the estimated log quantile unless the NOLOG option is specified in the preceding MODEL statement.

The following table shows how  $u_p$  is computed from the baseline distribution  $F(u)$ :

**Table 51.13** Baseline Probability Functions and  $u_p$

| Distribution      | $F(u)$                                                                                                                                                                                                                                     | $u_p$                |
|-------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------|
| Exponential       | $1 - \exp(-\exp(u))$                                                                                                                                                                                                                       | $\log(-\log(1 - p))$ |
| Generalized Gamma | $\begin{cases} \frac{\Gamma(\delta^{-2}, \delta^{-2} \exp(\delta u))}{\Gamma(\delta^{-2})} & \text{if } \delta > 0 \\ 1 - \frac{\Gamma(\delta^{-2}, \delta^{-2} \exp(\delta u))}{\Gamma(\delta^{-2})} & \text{if } \delta < 0 \end{cases}$ | $F^{-1}(p)$          |
| Logistic          | $1 - (1 + \exp(u))^{-1}$                                                                                                                                                                                                                   | $\log(p/(1 - p))$    |
| Log-logistic      | $1 - (1 + \exp(u))^{-1}$                                                                                                                                                                                                                   | $\log(p/(1 - p))$    |
| Lognormal         | $\Phi(u)$                                                                                                                                                                                                                                  | $\Phi^{-1}(p)$       |
| Normal            | $\Phi(u)$                                                                                                                                                                                                                                  | $\Phi^{-1}(p)$       |
| Weibull           | $1 - \exp(-\exp(u))$                                                                                                                                                                                                                       | $\log(-\log(1 - p))$ |

For the generalized gamma distribution,  $u_p$  is computed numerically.

The standard errors of the quantile estimates are computed using the estimated covariance matrix of the parameter estimates and a Taylor series expansion of the quantile estimate. The standard error is computed as

$$\text{STD} = \sqrt{\mathbf{z}'\mathbf{V}\mathbf{z}}$$

where  $\mathbf{V}$  is the estimated covariance matrix of the parameter vector  $(\boldsymbol{\beta}', \sigma, \delta)'$ , and  $\mathbf{z}$  is the vector

$$\mathbf{z} = \begin{bmatrix} \mathbf{x} \\ \hat{u}_p \\ \hat{\sigma} \frac{\partial u_p}{\partial \delta} \end{bmatrix}$$

where  $\delta$  is the vector of the shape parameters. Unless the NOLOG option is specified, this standard error estimate is converted into a standard error estimate for  $\exp(y_p)$  as  $\exp(\hat{y}_p)\text{STD}$ . It might be more desirable

to compute confidence limits for the log response and convert them back to the original response variable than to use the standard error estimates for  $\exp(y_p)$  directly. See [Example 51.1](#) for a 90% confidence interval of the response constructed by exponentiating a confidence interval for the log response.

The variable CDF is computed as

$$\text{CDF}_i = F(u_i)$$

where the residual is defined by

$$u_i = \left( \frac{y_i - \mathbf{x}'_i \mathbf{b}}{\hat{\sigma}} \right)$$

and  $F$  is the baseline cumulative distribution function. If the data are interval-censored, then the cumulative distribution function,  $\text{CDF}_i = F(u_i)$ , is evaluated at the lower interval endpoint.

## Confidence Intervals

Confidence intervals are computed for all model parameters and are reported in the “Analysis of Parameter Estimates” table. The confidence coefficient can be specified with the ALPHA= $\alpha$  MODEL statement option, resulting in a  $(1 - \alpha) \times 100\%$  two-sided confidence coefficient. The default confidence coefficient is 95%, corresponding to  $\alpha = 0.05$ .

## Regression Parameters

A two-sided  $(1 - \alpha) \times 100\%$  confidence interval  $[\beta_{iL}, \beta_{iU}]$  for the regression parameter  $\beta_i$  is based on the asymptotic normality of the maximum likelihood estimator  $\hat{\beta}_i$  and is computed by

$$\beta_{iL} = \hat{\beta}_i - z_{1-\alpha/2}(\text{SE}_{\hat{\beta}_i})$$

$$\beta_{iU} = \hat{\beta}_i + z_{1-\alpha/2}(\text{SE}_{\hat{\beta}_i})$$

where  $\text{SE}_{\hat{\beta}_i}$  is the estimated standard error of  $\hat{\beta}_i$ , and  $z_p$  is the  $p \times 100\%$  percentile of the standard normal distribution.

## Scale Parameter

A two-sided  $(1 - \alpha) \times 100\%$  confidence interval  $[\sigma_L, \sigma_U]$  for the scale parameter  $\sigma$  in the location-scale model is based on the asymptotic normality of the logarithm of the maximum likelihood estimator  $\log(\hat{\sigma})$ , and is computed by

$$\sigma_L = \hat{\sigma} / \exp[z_{1-\alpha/2}(\text{SE}_{\hat{\sigma}})/\hat{\sigma}]$$

$$\sigma_U = \hat{\sigma} \exp[z_{1-\alpha/2}(\text{SE}_{\hat{\sigma}})/\hat{\sigma}]$$

See Meeker and Escobar (1998) for more information.

## Weibull Scale and Shape Parameters

The Weibull distribution scale parameter  $\eta$  and shape parameter  $\beta$  are obtained by transforming the extreme-value location parameter  $\mu$  and scale parameter  $\sigma$ :

$$\eta = \exp(\mu)$$

$$\beta = 1/\sigma$$

Consequently, two-sided  $(1 - \alpha) \times 100\%$  confidence intervals for the Weibull scale and shape parameters are computed as

$$[\eta_L, \eta_U] = [\exp(\mu_L), \exp(\mu_U)]$$

$$[\beta_L, \beta_U] = [1/\sigma_U, 1/\sigma_L]$$

## Gamma Shape Parameter

A two-sided  $(1 - \alpha) \times 100\%$  confidence interval for the three-parameter gamma shape parameter  $\delta$  is computed by

$$[\delta_L, \delta_U] = [\hat{\delta} - z_{1-\alpha/2}(\text{SE}_{\hat{\delta}}), \hat{\delta} + z_{1-\alpha/2}(\text{SE}_{\hat{\delta}})]$$

---

## Fit Statistics

Suppose that the model contains  $p$  parameters and that  $n$  observations are used in model fitting. The fit criteria displayed by the LIFEREG procedure are calculated as follows:

- $-2 \log$  likelihood:

$$-2\log(L)$$

where  $L$  is the maximized likelihood for the model.

- Akaike's information criterion:

$$\text{AIC} = -2\log(L) + 2p$$

- corrected Akaike's information criterion:

$$\text{AICC} = \text{AIC} + \frac{2p(p+1)}{n-p-1}$$

- Bayesian information criterion:

$$\text{BIC} = -2\log(L) + p \log(n)$$

If you specify the Weibull, exponential, lognormal, log-logistic, or gamma distribution, then maximum likelihood estimates of model parameters are computed by maximizing the log likelihood of the distribution of the logarithm of the response. This is equivalent to computing maximum likelihood parameter estimates based on the response on the original, rather than log, scale. If you specify the Weibull, exponential, lognormal, log-logistic, or gamma distribution, then fit statistics based on the maximized log likelihood  $\log(L)$  of the log of the response are reported in the “Fit Statistics” table. Fit criteria computed in this way cannot be meaningfully compared with fit criteria that are based on the log likelihood of the unlogged response. If you specify the normal or logistic distribution, or if you specify the NOLOG option in the MODEL statement, then the fit criteria reported in the “Fit Statistics” table are based on the response on the original, rather than log, scale.

In addition to the “Fit Statistics” table described previously, if you specify the Weibull, exponential, lognormal, log-logistic, or gamma distribution, fit criteria that are based on the distribution of the response on the original scale, rather than the log of the response, are reported in the “Fit Statistics (Unlogged Response)” table.

When comparing models, you should compare fit criteria based on the log likelihood that is computed by using the response on the same scale, either always based on the log of the response or always based on the response on the original scale.

See Akaike (1981, 1979) for details of AIC and BIC. See Simonoff (2003) for a discussion of using AIC, AICC, and BIC in statistical modeling.

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## Probability Plotting

Probability plots are useful tools for the display and analysis of lifetime data. Probability plots use an inverse distribution scale so that a cumulative distribution function (CDF) plots as a straight line. A nonparametric estimate of the CDF of the lifetime data will plot approximately as a straight line, thus providing a visual assessment of goodness of fit.

You can use the PROBLOT statement in PROC LIFEREG to create probability plots of data that are complete, right censored, interval censored, or a combination of censoring types (arbitrarily censored). A line representing the maximum likelihood fit from the MODEL statement and pointwise parametric confidence bands for the cumulative probabilities are also included in the plot.

A random variable  $Y$  belongs to a *location-scale* family of distributions if its CDF  $F$  is of the form

$$\Pr\{Y \leq y\} = F(y) = G\left(\frac{y - \mu}{\sigma}\right)$$

where  $\mu$  is the location parameter and  $\sigma$  is the scale parameter. Here,  $G$  is a CDF that cannot depend on any unknown parameters, and  $G$  is the CDF of  $Y$  if  $\mu = 0$  and  $\sigma = 1$ . For example, if  $Y$  is a normal random variable with mean  $\mu$  and standard deviation  $\sigma$ ,

$$G(u) = \Phi(u) = \int_{-\infty}^u \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{u^2}{2}\right) du$$

and

$$F(y) = \Phi\left(\frac{y - \mu}{\sigma}\right)$$

The normal, extreme-value, and logistic distributions are location-scale models. The three-parameter gamma distribution is a location-scale model if the shape parameter  $\delta$  is fixed. If  $T$  has a lognormal, Weibull, or log-logistic distribution, then  $\log(T)$  has a distribution that is a location-scale model. These distributions are said to be of type log-location-scale. Probability plots are constructed for lognormal, Weibull, and log-logistic distributions by using  $\log(T)$  instead of  $T$  in the plots.

Let  $y_{(1)} \leq y_{(2)} \leq \dots \leq y_{(n)}$  be ordered observations of a random sample with distribution function  $F(y)$ . A probability plot is a plot of the points  $y_{(i)}$  against  $m_i = G^{-1}(a_i)$ , where  $a_i = \hat{F}(y_i)$  is an estimate of the CDF  $F(y_{(i)}) = G\left(\frac{y_{(i)} - \mu}{\sigma}\right)$ . The nonparametric CDF estimates  $a_i$  are sometimes called *plotting positions*. The axis on which the points  $m_i$  are plotted is usually labeled with a probability scale (the scale of  $a_i$ ).

If  $F$  is one of the location-scale distributions, then  $y$  is the lifetime; otherwise, the log of the lifetime is used to transform the distribution to a location-scale model.

If the data actually have the stated distribution, then  $\hat{F} \approx F$ ,

$$m_i = G^{-1}(\hat{F}(y_i)) \approx G^{-1}\left(G\left(\frac{y_{(i)} - \mu}{\sigma}\right)\right) = \frac{y_{(i)} - \mu}{\sigma}$$

and points  $(y_{(i)}, m_i)$  should fall approximately in a straight line.

There are several ways to compute the nonparametric CDF estimates used in probability plots from lifetime data. These are discussed in the next two sections.

## Complete and Right-Censored Data

The censoring times must be taken into account when you compute plotting positions for right-censored data. The modified Kaplan-Meier method described in the following section is the default method for computing nonparametric CDF estimates for display on probability plots. See Abernethy (1996), Meeker and Escobar (1998), and Nelson (1982) for discussions of the methods described in the following sections.

### Expected Ranks, Kaplan-Meier, and Modified Kaplan-Meier Methods

Let  $y_{(1)} \leq y_{(2)} \leq \dots \leq y_{(n)}$  be ordered observations of a random sample including failure times and censor times. Order the data in increasing order. Label all the data with reverse ranks  $r_i$ , with  $r_1 = n, \dots, r_n = 1$ . For the lifetime (not censoring time) corresponding to reverse rank  $r_i$ , compute the survival function estimate

$$S_i = \left[ \frac{r_i}{r_i + 1} \right] S_{i-1}$$

with  $S_0 = 1$ . The expected rank plotting position is computed as  $a_i = 1 - S_i$ . The option PPOS=EXPRANK specifies the expected rank plotting position.

For the Kaplan-Meier method,

$$S_i = \left[ \frac{r_i - 1}{r_i} \right] S_{i-1}$$

The Kaplan-Meier plotting position is then computed as  $a'_i = 1 - S_i$ . The option PPOS=KM specifies the Kaplan-Meier plotting position.

For the modified Kaplan-Meier method, use

$$S'_i = \frac{S_i + S_{i-1}}{2}$$



where  $S_i$  is computed from the Kaplan-Meier formula with  $S_0 = 1$ . The plotting position is then computed as  $a_i'' = 1 - S_i'$ . The option PPOS=MKM specifies the modified Kaplan-Meier plotting position. If the PPOS option is not specified, the modified Kaplan-Meier plotting position is used as the default method.

For complete samples,  $a_i = i/(n + 1)$  for the expected rank method,  $a_i' = i/n$  for the Kaplan-Meier method, and  $a_i'' = (i - 0.5)/n$  for the modified Kaplan-Meier method. If the largest observation is a failure for the Kaplan-Meier estimator, then  $F_n = 1$  and the point is not plotted.

### Median Ranks

Let  $y_{(1)} \leq y_{(2)} \leq \dots \leq y_{(n)}$  be ordered observations of a random sample including failure times and censor times. A failure order number  $j_i$  is assigned to the  $i$ th failure:  $j_i = j_{i-1} + \Delta$ , where  $j_0 = 0$ . The increment  $\Delta$  is initially 1 and is modified when a censoring time is encountered in the ordered sample. The new increment is computed as

$$\Delta = \frac{(n + 1) - \text{previous failure order number}}{1 + \text{number of items beyond previous censored item}}$$

The plotting position is computed for the  $i$ th failure time as

$$a_i = \frac{j_i - 0.3}{n + 0.4}$$

For complete samples, the failure order number  $j_i$  is equal to  $i$ , the order of the failure in the sample. In this case, the preceding equation for  $a_i$  is an approximation of the median plotting position computed as the median of the  $i$ th-order statistic from the uniform distribution on  $(0, 1)$ . In the censored case,  $j_i$  is not necessarily an integer, but the preceding equation still provides an approximation to the median plotting position. The PPOS=MEDRANK option specifies the median rank plotting position.

### Arbitrarily Censored Data

The LIFEREG procedure can create probability plots for data that consist of combinations of exact, left-censored, right-censored, and interval-censored lifetimes—that is, arbitrarily censored data. The LIFEREG procedure uses an iterative algorithm developed by Turnbull (1976) to compute a nonparametric maximum likelihood estimate of the cumulative distribution function for the data. Since the technique is maximum likelihood, standard errors of the cumulative probability estimates are computed from the inverse of the associated Fisher information matrix. This algorithm is an example of the expectation-maximization (EM) algorithm. The default initial estimate assigns equal probabilities to each interval. You can specify different initial values with the PROBLIST= option. Convergence is determined if the change in the log likelihood between two successive iterations is less than delta, where the default value of delta is  $10^{-8}$ . You can specify a different value for delta with the TOLLIKE= option. Iterations will be terminated if the algorithm does not converge after a fixed number of iterations. The default maximum number of iterations is 1000. Some data might require more iterations for convergence. You can specify the maximum allowed number of iterations with the MAXITEM= option in the PROBLOT statement. The iteration history of the log likelihood is displayed if you specify the ITPRINTEM option. The iteration history of the estimated interval probabilities are also displayed if you specify both options ITPRINTEM and PRINTPROBS.

If an interval probability is smaller than a tolerance ( $10^{-6}$  by default) after convergence, the probability is set to zero, the interval probabilities are renormalized so that they add to one, and iterations are restarted. Usually the algorithm converges in just a few more iterations. You can change the default value of the tolerance with the TOLPROB= option. You can specify the NOPOLISH option to avoid setting small probabilities to zero and restarting the algorithm.

If you specify the ITPRINTEM option, a table summarizing the Turnbull estimate of the interval probabilities is displayed. The columns labeled “Reduced Gradient” and “Lagrange Multiplier” are used in checking final convergence of the maximum likelihood estimate. The Lagrange multipliers must all be greater than or equal to zero, or the solution is not maximum likelihood. See Gentleman and Geyer (1994) for more details of the convergence checking. Also see Meeker and Escobar (1998, Chapter 3) for more information.

See Example 51.6 for an illustration.

## Nonparametric Confidence Intervals

You can use the PPOUT option in the PROB PLOT statement to create a table containing the nonparametric CDF estimates computed by the selected method, Kaplan-Meier CDF estimates, standard errors of the Kaplan-Meier estimator, and nonparametric confidence limits for the CDF. The confidence limits are either pointwise or simultaneous, depending on the value of the NPINTERVALS= option in the PROB PLOT statement. The method used in the LIFEREG procedure for computation of approximate pointwise and simultaneous confidence intervals for cumulative failure probabilities relies on the Kaplan-Meier estimator of the cumulative distribution function of failure time and approximate standard deviation of the Kaplan-Meier estimator. For the case of arbitrarily censored data, the Turnbull algorithm, discussed previously, provides an extension of the Kaplan-Meier estimator. Both the Kaplan-Meier and the Turnbull estimators provide an estimate of the standard error of the CDF estimator,  $se_{\hat{F}}$ , that is used in computing confidence intervals.

### Pointwise Confidence Intervals

Approximate  $(1 - \alpha)100\%$  pointwise confidence intervals are computed as in Meeker and Escobar (1998, Section 3.6) as

$$[F_L, F_U] = \left[ \frac{\hat{F}}{\hat{F} + (1 - \hat{F})w}, \frac{\hat{F}}{\hat{F} + (1 - \hat{F})/w} \right]$$

where

$$w = \exp \left[ \frac{z_{1-\alpha/2} se_{\hat{F}}}{(\hat{F}(1 - \hat{F}))} \right]$$

where  $z_p$  is the  $p$ th quantile of the standard normal distribution.

### Simultaneous Confidence Intervals

Approximate  $(1 - \alpha)100\%$  simultaneous confidence bands valid over the lifetime interval  $(t_a, t_b)$  are computed as the “Equal Precision” case of Nair (1984) and Meeker and Escobar (1998, Section 3.8) as

$$[F_L, F_U] = \left[ \frac{\hat{F}}{\hat{F} + (1 - \hat{F})w}, \frac{\hat{F}}{\hat{F} + (1 - \hat{F})/w} \right]$$

where

$$w = \exp \left[ \frac{e_{a,b,1-\alpha/2} \text{SE}_{\hat{F}}}{(\hat{F}(1 - \hat{F}))} \right]$$

where the factor  $x = e_{a,b,1-\alpha/2}$  is the solution of

$$x \exp(-x^2/2) \log \left[ \frac{(1-a)b}{(1-b)a} \right] / \sqrt{8\pi} = \alpha/2$$

The time interval  $(t_a, t_b)$  over which the bands are valid depends in a complicated way on the constants  $a$  and  $b$  defined in Nair (1984),  $0 < a < b < 1$ . The constants  $a$  and  $b$  are chosen by default so that the confidence bands are valid between the lowest and highest times corresponding to failures in the case of multiply censored data, or to the lowest and highest intervals for which probabilities are computed for arbitrarily censored data. You can optionally specify  $a$  and  $b$  directly with the NPINTERVALS=SIMULTANEOUS( $a$ ,  $b$ ) option in the PROBLOT statement.

## Parametric Confidence Intervals

Pointwise parametric confidence bands are displayed in a probability plot, unless you specify the NOCONF option in the PROBLOT statement. Two kinds of confidence intervals are available for display in a probability plot: confidence limits for the estimated cumulative distribution function (CDF) and confidence limits for estimated distribution percentiles.

### Confidence Limits for the Estimated CDF

If the distribution is of type log-location-scale, let  $y = \log(t)$  where  $t$  is the value of time at which the confidence limits are to be computed. If the distribution is of type location-scale, let  $y$  be the value at which you want to evaluate confidence limits for the estimated CDF  $\hat{F}(y)$ . Let

$$\hat{u} = \frac{y - \mathbf{x}'\hat{\boldsymbol{\beta}}}{\hat{\sigma}}$$

where the column vector  $\mathbf{x}$  of covariate values is determined by the rules summarized in the section “XDATA= Data Set” on page 3947. If an offset variable is specified, the mean of the offset variable values is included in  $\mathbf{x}'\hat{\boldsymbol{\beta}}$ .

The CDF estimate is given by

$$\hat{F}(y) = G(\hat{u})$$

where  $G$  is the baseline distribution. The approximate standard error of  $\hat{F}(y)$  is computed as in Meeker and Escobar (1998, Section 8.4.3) as

$$\text{SE}_{\hat{F}} = \frac{g(\hat{u})}{\hat{\sigma}} \left[ \text{Var}(\mathbf{x}'\hat{\boldsymbol{\beta}}) + 2\hat{u}\text{Cov}(\mathbf{x}'\hat{\boldsymbol{\beta}}, \hat{\sigma}) + \hat{u}^2 \text{Var}(\hat{\sigma}) \right]^{\frac{1}{2}}$$

where  $g$  is the probability density function corresponding to  $G$ . Two-sided  $(1 - \alpha) \times 100\%$  confidence limits are given by

$$[F_L, F_U] = \left[ \frac{\hat{F}}{\hat{F} + (1 - \hat{F}) \times w}, \frac{\hat{F}}{\hat{F} + (1 - \hat{F})/w} \right]$$

where

$$w = \exp \left[ \frac{z_{1-\alpha/2} \text{SE}_{\hat{F}}}{\hat{F}(1 - \hat{F})} \right]$$

and  $z_p$  is the  $p \times 100\%$  percentile of the standard normal distribution. The quantities  $\text{Var}(\mathbf{x}'\hat{\boldsymbol{\beta}})$ ,  $\text{Cov}(\mathbf{x}'\hat{\boldsymbol{\beta}}, \hat{\sigma})$ , and  $\text{Var}(\hat{\sigma})$  are computed based on the covariance matrix of the estimated parameter vector  $(\hat{\boldsymbol{\beta}}, \hat{\sigma})$ .

### Confidence Limits for Percentiles

If the **HCL** option is specified in the **PROBPLOT** statement, confidence limits based on estimated distribution percentiles instead of the default CDF limits are displayed in the probability plot.

For location-scale distributions, the estimated  $p \times 100\%$  percentile of the distribution  $F$  is given by

$$y_p = \mathbf{x}'\hat{\boldsymbol{\beta}} + G^{-1}(p)\hat{\sigma}$$

where  $G$  is the baseline distribution and the column vector  $\mathbf{x}$  of covariate values is determined by the rules summarized in the section “**XDATA= Data Set**” on page 3947. The standard error of  $y_p$  is estimated by  $\text{SE}_y = \mathbf{z}'\Sigma\mathbf{z}$  where  $\mathbf{z} = (\mathbf{x}', G^{-1}(p))'$  and  $\Sigma$  is the covariance matrix of the parameter estimates  $(\hat{\boldsymbol{\beta}}, \hat{\sigma})'$ . Two-sided  $(1 - \alpha) \times 100\%$  confidence limits for  $y_p$  are given by

$$[y_L, y_U] = [y_p - z_{1-\alpha/2}\text{SE}_y, y_p + z_{1-\alpha/2}\text{SE}_y]$$

For distributions of type log-location-scale, the confidence limits are computed as

$$[t_L = \exp(y_L), t_U = \exp(y_U)]$$

For example, if  $T$  has the Weibull distribution,  $G$  is the standardized extreme value distribution,  $[y_L, y_U]$  are confidence limits for the  $p \times 100\%$  percentile of the extreme value distribution for  $\log(T)$ , and  $[t_L = \exp(y_L), t_U = \exp(y_U)]$  are confidence limits for the  $p \times 100\%$  percentile of the Weibull distribution for  $T$ .

---

## INEST= Data Set

If specified, the **INEST=** data set specifies initial estimates for all the parameters in the model. The **INEST=** data set must contain the intercept variable (named **Intercept**) and all independent variables in the **MODEL** statement.

If **BY** processing is used, the **INEST=** data set should also include the **BY** variables, and there must be at least one observation for each **BY** group. If there is more than one observation in one **BY** group, the first observation read is used for that **BY** group.

If the **INEST=** data set also contains the **\_TYPE\_** variable, only observations with **\_TYPE\_** value 'PARMS' are used as starting values. Combining the **INEST=** data set and the **MAXITER=** option in the **MODEL**

statement, partial scoring can be done, such as predicting on a validation data set by using the model built from a training data set.

You can specify starting values for the iterative algorithm in the INEST= data set. This data set overwrites the INITIAL= option in the MODEL statement, which is a little difficult to use for models including multilevel interaction effects. The INEST= data set has the same structure as the OUTEST= data set but is not required to have all the variables or observations that appear in the OUTEST= data set. One simple use of the INEST= option is passing the previous OUTEST= data set directly to the next model as an INEST= data set, assuming that the two models have the same parameterization. See [Example 51.3](#) for an illustration.

---

## OUTEST= Data Set

The OUTEST= data set contains parameter estimates and the log likelihood for the model. You can specify a label in the MODEL statement to distinguish between the estimates for different models fit with the LIFEREG procedure. If the COVOUT option is specified, the OUTEST= data set also contains the estimated covariance matrix of the parameter estimates. Note that, if the LIFEREG procedure does not converge, the parameter estimates are set to missing in the OUTEST data set.

The OUTEST= data set contains all variables specified in the MODEL statement and the BY statement. One observation consists of parameter values for the model with the dependent variable having the value  $-1$ . If the COVOUT option is specified, there are additional observations containing the rows of the estimated covariance matrix. For these observations, the dependent variable contains the parameter estimate for the corresponding row variable. The following variables are also added to the data set:

|                        |                                                                                                                                                                        |
|------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>_MODEL_</code>   | a character variable containing the label of the MODEL statement, if present. Otherwise, the variable's value is blank.                                                |
| <code>_NAME_</code>    | a character variable containing the name of the dependent variable for the parameter estimates observations or the name of the row for the covariance matrix estimates |
| <code>_TYPE_</code>    | a character variable containing the type of the observation, either PARMS for parameter estimates or COV for covariance estimates                                      |
| <code>_DIST_</code>    | a character variable containing the name of the distribution modeled                                                                                                   |
| <code>_LNLIKE_</code>  | a numeric variable containing the last computed value of the log likelihood                                                                                            |
| <code>INTERCEPT</code> | a numeric variable containing the intercept parameter estimates and covariances                                                                                        |
| <code>_SCALE_</code>   | a numeric variable containing the scale parameter estimates and covariances                                                                                            |
| <code>_SHAPE1_</code>  | a numeric variable containing the first shape parameter estimates and covariances if the specified distribution has additional shape parameters                        |

Any BY variables specified are also added to the OUTEST= data set.

---

## XDATA= Data Set

The XDATA= data set is used for plotting the predicted probability when there are covariates specified in a MODEL statement and a probability plot is specified with a PROBPLOT statement. See [Example 51.4](#) for an illustration.

The XDATA= data set is an input SAS data set that contains values for all the independent variables in the MODEL statement and variables in the CLASS statement. The XDATA= data set has the same structure as the DATA= data set but is not required to have all the variables or observations that appear in the DATA= data set.

The XDATA= data set must contain all the independent variables in the MODEL statement and variables in the CLASS statement. Even though variables in the CLASS statement might not be used, valid values are required for these variables in the XDATA= data set. Missing values are not allowed. Missing values are not allowed in the XDATA= data set for any of the independent variables, either. Missing values are allowed for the dependent variables and other variables if they are included in the XDATA= data set.

If BY processing is used, the XDATA= data set should also include the BY variables, and there must be at least one valid observation for each BY group. If there is more than one valid observation in a BY group, the last one read is used for that BY group.

If there is no XDATA= data set in the PROC LIFEREG statement, by default, the LIFEREG procedure will use the overall mean for effects containing a continuous variable (or variables) and the highest level of a single classification variable as reference level. The rules are summarized as follows:

- If the effect contains a continuous variable (or variables), the overall mean of this effect (not the variables) is used.
- If the effect is a single classification variable, the highest level of the variable is used.

---

## Computational Resources

Let  $p$  be the number of parameters estimated in the model. The minimum working space (in bytes) needed is

$$16p^2 + 100p$$

However, if sufficient space is available, the input data set is also kept in memory; otherwise, the input data set is reread for each evaluation of the likelihood function and its derivatives, with the resulting execution time of the procedure substantially increased.

Let  $n$  be the number of observations used in the model estimation. Each evaluation of the likelihood function and its first and second derivatives requires  $O(np^2)$  multiplications and additions,  $n$  individual function evaluations for the log density or log distribution function, and  $n$  evaluations of the first and second derivatives of the function. The calculation of each updating step from the gradient and Hessian requires  $O(p^3)$  multiplications and additions. The  $O(v)$  notation means that, for large values of the argument,  $v$ ,  $O(v)$  is approximately a constant times  $v$ .

## Bayesian Analysis

### Gibbs Sampling

This section provides details about Bayesian analysis by Gibbs sampling in the location-scale models for survival data available in PROC LIFEREG. See the section “Gibbs Sampler” on page 135 for a general discussion of Gibbs sampling. PROC LIFEREG fits parametric location-scale survival models. That is, the probability density of the response  $Y$  can be expressed in the general form

$$f(y) = g\left(\frac{y - \mu}{\sigma}\right)$$

where  $Y = \log(T)$  for lifetimes  $T$ . The function  $g$  determines the specific distribution. The location parameter  $\mu_i$  is modeled through regression parameters as  $\mu_i = \mathbf{x}_i' \boldsymbol{\beta}$ . The LIFEREG procedure can provide Bayesian estimates of the regression parameters and  $\sigma$ . The OUTPUT and PROBPLOT statements, if specified, are ignored. The PLOTS=PROBPLOT option in the PROC LIFEREG statement and the CORRB and COVB options in the MODEL statement are also ignored.

For the Weibull distribution, you can specify that Gibbs sampling be performed on the Weibull shape parameter  $\beta = \sigma^{-1}$  instead of the scale parameter  $\sigma$  by specifying a prior distribution for the shape parameter with the WEIBULLSHAPEPRIOR= option. In addition, if there are no covariates in the model, you can specify Gibbs sampling on the Weibull scale parameter  $\alpha = \exp(\mu)$ , where  $\mu$  is the intercept term, with the WEIBULLSCALEPRIOR= option.

In the case of the exponential distribution with no covariates, you can specify Gibbs sampling on the exponential scale parameter  $\alpha = \exp(\mu)$ , where  $\mu$  is the intercept term, with the EXPSCALEPRIOR= option.

Let  $\boldsymbol{\theta} = (\theta_1, \dots, \theta_k)'$  be the parameter vector. For location-scale models, the  $\theta_i$ 's are the regression coefficients  $\beta_i$ 's and the scale parameter  $\sigma$ . In the case of the three-parameter gamma distribution, there is an additional gamma shape parameter  $\tau$ . Let  $L(D|\boldsymbol{\theta})$  be the likelihood function, where  $D$  is the observed data. Let  $\pi(\boldsymbol{\theta})$  be the prior distribution. The full conditional distribution of  $[\theta_i|\theta_j, i \neq j]$  is proportional to the joint distribution; that is,

$$\pi(\theta_i|\theta_j, i \neq j, D) \propto L(D|\boldsymbol{\theta})p(\boldsymbol{\theta})$$

For instance, the one-dimensional conditional distribution of  $\theta_1$  given  $\theta_j = \theta_j^*, 2 \leq j \leq k$ , is computed as

$$\pi(\theta_1|\theta_j = \theta_j^*, 2 \leq j \leq k, D) = L(D|(\boldsymbol{\theta} = (\theta_1, \theta_2^*, \dots, \theta_k^*)'))p(\boldsymbol{\theta} = (\theta_1, \theta_2^*, \dots, \theta_k^*)')$$

Suppose you have a set of arbitrary starting values  $\{\theta_1^{(0)}, \dots, \theta_k^{(0)}\}$ . Using the ARMS (adaptive rejection Metropolis sampling) algorithm of Gilks and Wild (1992) and Gilks, Best, and Tan (1995), you can do the following:

draw  $\theta_1^{(1)}$  from  $[\theta_1|\theta_2^{(0)}, \dots, \theta_k^{(0)}]$   
 draw  $\theta_2^{(1)}$  from  $[\theta_2|\theta_1^{(1)}, \theta_3^{(0)}, \dots, \theta_k^{(0)}]$   
 ...  
 draw  $\theta_k^{(1)}$  from  $[\theta_k|\theta_1^{(1)}, \dots, \theta_{k-1}^{(1)}]$

This completes one iteration of the Gibbs sampler. After one iteration, you have  $\{\theta_1^{(1)}, \dots, \theta_k^{(1)}\}$ . After  $n$  iterations, you have  $\{\theta_1^{(n)}, \dots, \theta_k^{(n)}\}$ . PROC LIFEREG implements the ARMS algorithm based on a program provided by Gilks (2003) to draw a sample from a full conditional distribution. See the section “Assessing Markov Chain Convergence” on page 139 for information about assessing the convergence of the chain of posterior samples.

You can output these posterior samples into a SAS data set. The following option in the BAYES statement outputs the posterior samples into the SAS data set Post: `OUTPOST=Post`. The data set also includes the variables LogPost and LogLike, which represent the log of the posterior distribution and the log of the likelihood, respectively.

## Priors for Model Parameters

The model parameters are the regression coefficients and the dispersion parameter (or the precision or scale), if the model has one. The priors for the dispersion parameter and the priors for the regression coefficients are assumed to be independent, while you can have a joint multivariate normal prior for the regression coefficients.

### Scale and Shape Parameters

**Gamma Prior** The gamma distribution  $G(a, b)$  has a PDF

$$f_{a,b}(u) = \frac{b(bu)^{a-1}e^{-bu}}{\Gamma(a)}, \quad u > 0$$

where  $a$  is the shape parameter and  $b$  is the inverse-scale parameter. The mean is  $\frac{a}{b}$  and the variance is  $\frac{a}{b^2}$ .

**Improper Prior** The joint prior density is given by

$$p(u) \propto u^{-1}, \quad u > 0$$

### Regression Coefficients

Let  $\boldsymbol{\beta}$  be the regression coefficients.

**Normal Prior** Assume  $\boldsymbol{\beta}$  has a multivariate normal prior with mean vector  $\boldsymbol{\beta}_0$  and covariance matrix  $\boldsymbol{\Sigma}_0$ . The joint prior density is given by

$$p(\boldsymbol{\beta}) \propto e^{-\frac{1}{2}(\boldsymbol{\beta}-\boldsymbol{\beta}_0)'\boldsymbol{\Sigma}_0^{-1}(\boldsymbol{\beta}-\boldsymbol{\beta}_0)}$$

**Uniform Prior** The joint prior density is given by

$$p(\boldsymbol{\beta}) \propto 1$$

## Posterior Distribution

Denote the observed data by  $D$ .

The posterior distribution is

$$\pi(\boldsymbol{\theta}|D) \propto L_P(D|\boldsymbol{\theta})p(\boldsymbol{\theta})$$

where  $L_P(D|\boldsymbol{\theta})$  is the likelihood function with regression coefficients and any additional parameters, such as scale or shape,  $\boldsymbol{\theta}$  as parameters; and  $p(\boldsymbol{\theta})$  is the joint prior distribution of the parameters.



## Deviance Information Criterion

Let  $\theta_i$  be the model parameters at iteration  $i$  of the Gibbs sampler, and let  $LL(\theta_i)$  be the corresponding model log likelihood. PROC LIFEREG computes the following fit statistics defined by Spiegelhalter et al. (2002):

- effective number of parameters:

$$p_D = \overline{LL(\theta)} - LL(\bar{\theta})$$

- deviance information criterion (DIC):

$$DIC = \overline{LL(\theta)} + p_D$$

where

$$\overline{LL(\theta)} = \frac{1}{n} \sum_{i=1}^n LL(\theta_i)$$

$$\bar{\theta} = \frac{1}{n} \sum_{i=1}^n \theta_i$$

and  $n$  is the number of Gibbs samples.

## Starting Values of the Markov Chains

When the BAYES statement is specified, PROC LIFEREG generates one Markov chain containing the approximate posterior samples of the model parameters. Additional chains are produced when the Gelman-Rubin diagnostics are requested. Starting values (or initial values) can be specified in the INITIAL= data set in the BAYES statement. If INITIAL= option is not specified, PROC LIFEREG picks its own initial values for the chains.

Denote  $[x]$  as the integral value of  $x$ . Denote  $\hat{s}(X)$  as the estimated standard error of the estimator  $X$ .

### Regression Coefficients and Gamma Shape Parameter

For the first chain that the summary statistics and regression diagnostics are based on, the default initial values are estimates of the mode of the posterior distribution. If the INITIALMLE option is specified, the initial values are the maximum likelihood estimates; that is,

$$\beta_i^{(0)} = \hat{\beta}_i$$

Initial values for the  $r$ th chain ( $r \geq 2$ ) are given by

$$\beta_i^{(0)} = \hat{\beta}_i \pm \left( 2 + \left\lceil \frac{r}{2} \right\rceil \right) \hat{s}(\hat{\beta}_i)$$

with the plus sign for odd  $r$  and minus sign for even  $r$ .

**Scale, Exponential Scale, Weibull Scale, or Weibull Shape Parameter  $\lambda$** 

Let  $\lambda$  be the parameter sampled.

For the first chain that the summary statistics and diagnostics are based on, the initial values are estimates of the mode of the posterior distribution; or the maximum likelihood estimates if the INITIALMLE option is specified; that is,

$$\lambda^{(0)} = \hat{\lambda}$$

The initial values of the  $r$ th chain ( $r \geq 2$ ) are given by

$$\lambda^{(0)} = \hat{\lambda} e^{\pm \left( \left[ \frac{r}{2} \right] + 2 \right) \hat{s}(\hat{\lambda})}$$

with the plus sign for odd  $r$  and minus sign for even  $r$ .

**OUTPOST= Output Data Set**

The OUTPOST= data set contains the generated posterior samples. There are  $2+n$  variables, where  $n$  is the number of model parameters. The variable Iteration represents the iteration number and the variable LogPost contains the log posterior likelihood values. The other  $n$  variables represent the draws of the Markov chain for the model parameters.

**Displayed Output for Classical Analysis**

For each model, PROC LIFEREG displays the following.

**Model Information**

The “Model Information” table displays the two-level name of the input data set, the distribution name, and the name and label of the dependent variable; the name and label of the censor indicator variable, for right-censored data; if you specify the WEIGHT statement, the name and label of the weight variable; and the maximum value of the log likelihood.

**Number of Observations**

The “Number of Observations” table displays the number of observations read from the input data set, and the number of observations used in the analysis.

**Class Level Information**

The “Class Level Information” table displays the levels of classification variables if you specify a CLASS statement.

**Fit Statistics**

The “Fit Statistics” table displays the negative of twice the log likelihood, Akaike’s information criterion (AIC), the corrected Akaike’s information criterion (AICC), and the Bayesian information criterion (BIC). If the specified distribution is Weibull, lognormal, log-logistic, or gamma, the fit criteria are based on the log likelihood for the log of the response, rather than for the response on the original scale.

### Fit Statistics (Unlogged Response)

If the specified distribution is Weibull, lognormal, log-logistic, or gamma, the “Fit Statistics (Unlogged Response)” table displays fit criteria that are based on the log likelihood for the response on the original, rather than log, scale. The negative of twice the log likelihood, Akaike’s information criterion (AIC), the corrected Akaike’s information criterion (AICC), and the Bayesian information criterion (BIC) are displayed.

### Type III Analysis of Effects

The “Type III Analysis of Effects” table displays, for each effect in the model, the effect name, the degrees of freedom associated with the type III contrast for the effect, the chi-square statistic for the contrast, and the  $p$ -value for the statistic.

### Analysis of Maximum Likelihood Parameter Estimates

The “Analysis of Maximum Likelihood Parameter Estimates” table displays the parameter name, the degrees of freedom for each parameter, the maximum likelihood estimate of each parameter, the estimated standard error of the parameter estimator, confidence limits for each parameter, a chi-square statistic for testing whether the parameter is zero, and the associated  $p$ -value for the statistic.

### Lagrange Multiplier Statistics

If there are constrained parameters in the model, such as the scale or intercept, then the “Lagrange Multiplier Statistics” table displays a Lagrange multiplier test for the constraint.

---

## Displayed Output for Bayesian Analysis

If a Bayesian analysis is requested with a BAYES statement, the displayed output includes the following.

### Model Information

The “Model Information” table displays the two-level name of the input data set, the number of burn-in iterations, the number of iterations after the burn-in, the number of thinning iterations, the distribution name, and the name and label of the dependent variable; the name and label of the censor indicator variable, for right-censored data; if you specify the WEIGHT statement, the name and label of the weight variable; and the maximum value of the log likelihood.

### Class Level Information

The “Class Level Information” table displays the levels of classification variables if you specify a CLASS statement.

### Maximum Likelihood Estimates

The “Analysis of Maximum Likelihood Parameter Estimates” table displays the maximum likelihood estimate of each parameter, the estimated standard error of the parameter estimator, and confidence limits for each parameter.

## Coefficient Prior

The “Coefficient Prior” table displays the prior distribution of the regression coefficients.

## Independent Prior Distributions for Model Parameters

The “Independent Prior Distributions for Model Parameters” table displays the prior distributions of additional model parameters (scale, exponential scale, Weibull scale, Weibull shape, gamma shape).

## Initial Values and Seeds

The “Initial Values and Seeds” table displays the initial values and random number generator seeds for the Gibbs chains.

## Fit Statistics

The “Fit Statistics” table displays the deviance information criterion (DIC) and the effective number of parameters.

## Posterior Summaries

The “Posterior Summaries” table contains the size of the sample, the mean, the standard deviation, and the quartiles for each model parameter.

## Posterior Intervals

The “Posterior Intervals” table contains the HPD intervals and the credible intervals for each model parameter.

## Correlation Matrix of the Posterior Samples

The “Correlation Matrix of the Posterior Samples” table is produced if you include the CORR suboption in the SUMMARY= option in the BAYES statement. This table displays the sample correlation of the posterior samples.

## Covariance Matrix of the Posterior Samples

The “Covariance Matrix of the Posterior Samples” table is produced if you include the COV suboption in the SUMMARY= option in the BAYES statement. This table displays the sample covariance of the posterior samples.

## Autocorrelations of the Posterior Samples

The “Autocorrelations of the Posterior Samples” table displays the lag1, lag5, lag10, and lag50 autocorrelations for each parameter.

## Gelman and Rubin Diagnostics

The “Gelman and Rubin Diagnostics” table is produced if you include the GELMAN suboption in the DIAGNOSTIC= option in the BAYES statement. This table displays the estimate of the potential scale reduction factor and its 97.5% upper confidence limit for each parameter.

## Geweke Diagnostics

The “Geweke Diagnostics” table displays the Geweke statistic and its  $p$ -value for each parameter.

## Raftery and Lewis Diagnostics

The “Raftery Diagnostics” tables is produced if you include the RAFTERY suboption in the DIAGNOSTIC= option in the BAYES statement. This table displays the Raftery and Lewis diagnostics for each variable.

## Heidelberger and Welch Diagnostics

The “Heidelberger and Welch Diagnostics” table is displayed if you include the HEIDELBERGER suboption in the DIAGNOSTIC= option in the BAYES statement. This table shows the results of a stationary test and a halfwidth test for each parameter.

## Effective Sample Size

The “Effective Sample Size” table displays, for each parameter, the effective sample size, the correlation time, and the efficiency.

## Monte Carlo Standard Errors

The “Monte Carlo Standard Errors” table displays, for each parameter, the Monte Carlo standard error, the posterior sample standard deviation, and the ratio of the two.

---

## ODS Table Names

PROC LIFEREG assigns a name to each table it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed separately in Table 51.14 for a maximum likelihood analysis and in Table 51.15 for a Bayesian analysis. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

**Table 51.14** ODS Tables Produced in PROC LIFEREG for a Classical Analysis

| ODS Table Name     | Description                              | Statement | Option                                                       |
|--------------------|------------------------------------------|-----------|--------------------------------------------------------------|
| ClassLevels        | Classification variable levels           | CLASS     | Default*                                                     |
| ConvergenceStatus  | Convergence status                       | MODEL     | Default                                                      |
| CorrB              | Parameter estimate correlation matrix    | MODEL     | CORRB                                                        |
| CovB               | Parameter estimate covariance matrix     | MODEL     | COVB                                                         |
| IterEM             | Iteration history for Turnbull algorithm | PROBPLOT  | ITPRINTM                                                     |
| FitStatistics      | Fit statistics                           | MODEL     | Default                                                      |
| FitStatisticsUL    | Fit statistics for unlogged response     | MODEL     | DISTRIBUTION=WEIBULL,<br>LOGNORMAL, LLO-<br>GISTIC, or GAMMA |
| IterHistory        | Iteration history                        | MODEL     | ITPRINT                                                      |
| LagrangeStatistics | Lagrange statistics                      | MODEL     | NOINT   NOSCALE                                              |
| LastGrad           | Last evaluation of the gradient          | MODEL     | ITPRINT                                                      |

Table 51.14 *continued*

| ODS Table Name       | Description                                   | Statement | Option    |
|----------------------|-----------------------------------------------|-----------|-----------|
| LastHess             | Last evaluation of the Hessian                | MODEL     | ITPRINT   |
| ModelInfo            | Model information                             | MODEL     | Default   |
| NObs                 | Number of observations                        | MODEL     | Default   |
| ParameterEstimates   | Parameter estimates                           | MODEL     | Default   |
| ParmInfo             | Parameter indices                             | MODEL     | Default   |
| ProbabilityEstimates | Nonparametric CDF estimates                   | PROBPLOT  | PPOUT     |
| TConvergenceStatus   | Convergence status for Turnbull algorithm     | PROBPLOT  | Default   |
| Turnbull             | Probability estimates from Turnbull algorithm | PROBPLOT  | ITPRINTEM |
| Type3Analysis        | Type 3 tests                                  | MODEL     | Default*  |

\* Depending on the data.

Table 51.15 ODS Tables Produced in PROC LIFEREG for a Bayesian Analysis

| ODS Table Name     | Description                                           | Statement | Option            |
|--------------------|-------------------------------------------------------|-----------|-------------------|
| AutoCorr           | Autocorrelations of the posterior samples             | BAYES     | Default           |
| ClassLevels        | Classification variable levels                        | CLASS     | Default*          |
| CoeffPrior         | Prior distribution of the regression coefficients     | BAYES     | Default           |
| ConvergenceStatus  | Convergence status of maximum likelihood estimation   | MODEL     | Default           |
| Corr               | Correlation matrix of the posterior samples           | BAYES     | SUMMARY=CORR      |
| ESS                | Effective sample size                                 | BAYES     | Default           |
| FitStatistics      | Fit statistics                                        | BAYES     | Default           |
| Gelman             | Gelman and Rubin convergence diagnostics              | BAYES     | DIAG=GELMAN       |
| Geweke             | Geweke convergence diagnostics                        | BAYES     | Default           |
| Heidelberger       | Heidelberger and Welch convergence diagnostics        | BAYES     | DIAG=HEIDELBERGER |
| InitialValues      | Initial values of the Markov chains                   | BAYES     | Default           |
| MCErr              | Monte Carlo standard errors                           | BAYES     | DIAG=MCSE         |
| ModelInfo          | Model information                                     | MODEL     | Default           |
| NObs               | Number of observations                                | MODEL     | Default           |
| ParameterEstimates | Maximum likelihood estimates of model parameters      | MODEL     | Default           |
| ParmPrior          | Prior distribution for scale and shape                | BAYES     | Default           |
| PostIntervals      | HPD and equal-tail intervals of the posterior samples | BAYES     | Default           |
| PosteriorSample    | Posterior samples (for output data set only)          | BAYES     |                   |

Table 51.15 continued

| ODS Table Name | Description                                 | Statement | Option       |
|----------------|---------------------------------------------|-----------|--------------|
| PostSummaries  | Summary statistics of the posterior samples | BAYES     | Default      |
| Raftery        | Raftery and Lewis convergence diagnostics   | BAYES     | DIAG=RAFTERY |

\* Depending on the data.

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “[Statistical Graphics Using ODS.](#)”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS.](#)”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “[A Primer on ODS Statistical Graphics](#)” on page 599 in Chapter 21, “[Statistical Graphics Using ODS.](#)”

Some graphs are produced by default; other graphs are produced by using statements and options.

## ODS Graph Names

PROC LIFEREG assigns a name to each graph it creates using ODS. You can use these names to reference the graphs when using ODS. The names of the graphs that PROC LIFEREG generates are listed in [Table 51.16](#), along with the required statements and options.

Table 51.16 Graphs Produced by PROC LIFEREG

| ODS Graph Name | Description                                        | Statement             | Option                                |
|----------------|----------------------------------------------------|-----------------------|---------------------------------------|
| ADPanel        | Autocorrelation function and density panel         | BAYES                 | <code>PLOTS=(AUTOCORR DENSITY)</code> |
| AutocorrPanel  | Autocorrelation function panel                     | BAYES                 | <code>PLOTS= AUTOCORR</code>          |
| AutocorrPlot   | Autocorrelation function plot                      | BAYES                 | <code>PLOTS(UNPACK)=AUTOCORR</code>   |
| ProbPlot       | Probability plot                                   | <code>PROBPLOT</code> | Default                               |
| TAPanel        | Trace and autocorrelation function panel           | BAYES                 | <code>PLOTS=(TRACE AUTOCORR)</code>   |
| TADPanel       | Trace, autocorrelation, and density function panel | BAYES                 | Default                               |
| TDPanel        | Trace and density panel                            | BAYES                 | <code>PLOTS=(TRACE DENSITY)</code>    |
| TracePanel     | Trace panel                                        | BAYES                 | <code>PLOTS=TRACE</code>              |
| TracePlot      | Trace plot                                         | BAYES                 | <code>PLOTS(UNPACK)=TRACE</code>      |

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## Examples: LIFEREG Procedure

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### Example 51.1: Motorette Failure

This example fits a Weibull model and a lognormal model to the example given in Kalbfleisch and Prentice (1980, p. 5). An output data set called `models` is specified to contain the parameter estimates. By default, the natural log of the variable `time` is used by the procedure as the response. After this log transformation, the Weibull model is fit using the extreme-value baseline distribution, and the lognormal is fit using the normal baseline distribution.

Since the extreme-value and normal distributions do not contain any shape parameters, the variable `SHAPE1` is missing in the `models` data set. An additional output data set, `out`, is created that contains the predicted quantiles and their standard errors for values of the covariate corresponding to `temp=130` and `temp=150`. This is done with the control variable, which is set to 1 for only two observations.

Using the standard error estimates obtained from the output data set, approximate 90% confidence limits for the predicted quantities are then created in a subsequent `DATA` step for the log response. The logs of the predicted values are obtained because the values of the `P=` variable in the `OUT=` data set are in the same units as the original response variable, `time`. The standard errors of the quantiles of  $\log(\text{time})$  are approximated (using a Taylor series approximation) by the standard deviation of `time` divided by the mean value of `time`. These confidence limits are then converted back to the original scale by the exponential function.

The following statements produce [Output 51.1.1](#):

```

title 'Motorette Failures With Operating Temperature as a Covariate';
data motors;
 input time censor temp @@;
 if _N_=1 then
 do;
 temp=130;
 time=.;
 control=1;
 z=1000/(273.2+temp);
 output;
 temp=150;
 time=.;
 control=1;
 z=1000/(273.2+temp);
 output;
 end;
 if temp>150;
 control=0;
 z=1000/(273.2+temp);
 output;
datalines;
8064 0 150 8064 0 150 8064 0 150 8064 0 150 8064 0 150
8064 0 150 8064 0 150 8064 0 150 8064 0 150 8064 0 150
1764 1 170 2772 1 170 3444 1 170 3542 1 170 3780 1 170
4860 1 170 5196 1 170 5448 0 170 5448 0 170 5448 0 170
 408 1 190 408 1 190 1344 1 190 1344 1 190 1440 1 190

```



```

1680 0 190 1680 0 190 1680 0 190 1680 0 190 1680 0 190
 408 1 220 408 1 220 504 1 220 504 1 220 504 1 220
 528 0 220 528 0 220 528 0 220 528 0 220 528 0 220
;
proc print data=motors;
run;

```

### Output 51.1.1 Motorette Failure Data

| Motorette Failures With Operating Temperature as a Covariate |      |       |      |         |         |
|--------------------------------------------------------------|------|-------|------|---------|---------|
| Obs                                                          | time | ensor | temp | control | z       |
| 1                                                            | .    | 0     | 130  | 1       | 2.48016 |
| 2                                                            | .    | 0     | 150  | 1       | 2.36295 |
| 3                                                            | 1764 | 1     | 170  | 0       | 2.25632 |
| 4                                                            | 2772 | 1     | 170  | 0       | 2.25632 |
| 5                                                            | 3444 | 1     | 170  | 0       | 2.25632 |
| 6                                                            | 3542 | 1     | 170  | 0       | 2.25632 |
| 7                                                            | 3780 | 1     | 170  | 0       | 2.25632 |
| 8                                                            | 4860 | 1     | 170  | 0       | 2.25632 |
| 9                                                            | 5196 | 1     | 170  | 0       | 2.25632 |
| 10                                                           | 5448 | 0     | 170  | 0       | 2.25632 |
| 11                                                           | 5448 | 0     | 170  | 0       | 2.25632 |
| 12                                                           | 5448 | 0     | 170  | 0       | 2.25632 |
| 13                                                           | 408  | 1     | 190  | 0       | 2.15889 |
| 14                                                           | 408  | 1     | 190  | 0       | 2.15889 |
| 15                                                           | 1344 | 1     | 190  | 0       | 2.15889 |
| 16                                                           | 1344 | 1     | 190  | 0       | 2.15889 |
| 17                                                           | 1440 | 1     | 190  | 0       | 2.15889 |
| 18                                                           | 1680 | 0     | 190  | 0       | 2.15889 |
| 19                                                           | 1680 | 0     | 190  | 0       | 2.15889 |
| 20                                                           | 1680 | 0     | 190  | 0       | 2.15889 |
| 21                                                           | 1680 | 0     | 190  | 0       | 2.15889 |
| 22                                                           | 1680 | 0     | 190  | 0       | 2.15889 |
| 23                                                           | 408  | 1     | 220  | 0       | 2.02758 |
| 24                                                           | 408  | 1     | 220  | 0       | 2.02758 |
| 25                                                           | 504  | 1     | 220  | 0       | 2.02758 |
| 26                                                           | 504  | 1     | 220  | 0       | 2.02758 |
| 27                                                           | 504  | 1     | 220  | 0       | 2.02758 |
| 28                                                           | 528  | 0     | 220  | 0       | 2.02758 |
| 29                                                           | 528  | 0     | 220  | 0       | 2.02758 |
| 30                                                           | 528  | 0     | 220  | 0       | 2.02758 |
| 31                                                           | 528  | 0     | 220  | 0       | 2.02758 |
| 32                                                           | 528  | 0     | 220  | 0       | 2.02758 |

The following statements produce [Output 51.1.2](#) and [Output 51.1.3](#):

```
proc lifereg data=motors outest=modela covout;
 a: model time*censor(0)=z;
 output out=outa quantiles=.1 .5 .9 std=std p=predtime
 control=control;
run;

proc lifereg data=motors outest=modelb covout;
 b: model time*censor(0)=z / dist=lnormal;
 output out=outb quantiles=.1 .5 .9 std=std p=predtime
 control=control;
run;
```

**Output 51.1.2** Motorette Failure: Model A

| Motorette Failures With Operating Temperature as a Covariate |              |            |                |                       |         |            |            |
|--------------------------------------------------------------|--------------|------------|----------------|-----------------------|---------|------------|------------|
| The LIFEREG Procedure                                        |              |            |                |                       |         |            |            |
| Model Information                                            |              |            |                |                       |         |            |            |
| Data Set                                                     | WORK.MOTORS  |            |                |                       |         |            |            |
| Dependent Variable                                           | Log(time)    |            |                |                       |         |            |            |
| Censoring Variable                                           | censor       |            |                |                       |         |            |            |
| Censoring Value(s)                                           | 0            |            |                |                       |         |            |            |
| Number of Observations                                       | 30           |            |                |                       |         |            |            |
| Noncensored Values                                           | 17           |            |                |                       |         |            |            |
| Right Censored Values                                        | 13           |            |                |                       |         |            |            |
| Left Censored Values                                         | 0            |            |                |                       |         |            |            |
| Interval Censored Values                                     | 0            |            |                |                       |         |            |            |
| Number of Parameters                                         | 3            |            |                |                       |         |            |            |
| Name of Distribution                                         | Weibull      |            |                |                       |         |            |            |
| Log Likelihood                                               | -22.95148315 |            |                |                       |         |            |            |
| Type III Analysis of Effects                                 |              |            |                |                       |         |            |            |
| Effect                                                       | DF           | Wald       |                | Pr > ChiSq            |         |            |            |
|                                                              |              | Chi-Square |                |                       |         |            |            |
| z                                                            | 1            | 99.5239    |                | <.0001                |         |            |            |
| Analysis of Maximum Likelihood Parameter Estimates           |              |            |                |                       |         |            |            |
| Parameter                                                    | DF           | Estimate   | Standard Error | 95% Confidence Limits |         | Chi-Square | Pr > ChiSq |
| Intercept                                                    | 1            | -11.8912   | 1.9655         | -15.7435              | -8.0389 | 36.60      | <.0001     |
| z                                                            | 1            | 9.0383     | 0.9060         | 7.2626                | 10.8141 | 99.52      | <.0001     |
| Scale                                                        | 1            | 0.3613     | 0.0795         | 0.2347                | 0.5561  |            |            |
| Weibull Shape                                                | 1            | 2.7679     | 0.6091         | 1.7982                | 4.2605  |            |            |

## Output 51.1.3 Motorette Failure: Model B

| Motorette Failures With Operating Temperature as a Covariate |              |            |                |                       |         |            |            |
|--------------------------------------------------------------|--------------|------------|----------------|-----------------------|---------|------------|------------|
| The LIFEREG Procedure                                        |              |            |                |                       |         |            |            |
| Model Information                                            |              |            |                |                       |         |            |            |
| Data Set                                                     | WORK.MOTORS  |            |                |                       |         |            |            |
| Dependent Variable                                           | Log(time)    |            |                |                       |         |            |            |
| Censoring Variable                                           | censor       |            |                |                       |         |            |            |
| Censoring Value(s)                                           | 0            |            |                |                       |         |            |            |
| Number of Observations                                       | 30           |            |                |                       |         |            |            |
| Noncensored Values                                           | 17           |            |                |                       |         |            |            |
| Right Censored Values                                        | 13           |            |                |                       |         |            |            |
| Left Censored Values                                         | 0            |            |                |                       |         |            |            |
| Interval Censored Values                                     | 0            |            |                |                       |         |            |            |
| Number of Parameters                                         | 3            |            |                |                       |         |            |            |
| Name of Distribution                                         | Lognormal    |            |                |                       |         |            |            |
| Log Likelihood                                               | -24.47381031 |            |                |                       |         |            |            |
| Type III Analysis of Effects                                 |              |            |                |                       |         |            |            |
| Effect                                                       | DF           | Wald       |                |                       |         |            |            |
|                                                              |              | Chi-Square | Pr >           | ChiSq                 |         |            |            |
| z                                                            | 1            | 42.0001    | <.0001         |                       |         |            |            |
| Analysis of Maximum Likelihood Parameter Estimates           |              |            |                |                       |         |            |            |
| Parameter                                                    | DF           | Estimate   | Standard Error | 95% Confidence Limits |         | Chi-Square | Pr > ChiSq |
| Intercept                                                    | 1            | -10.4706   | 2.7719         | -15.9034              | -5.0377 | 14.27      | 0.0002     |
| z                                                            | 1            | 8.3221     | 1.2841         | 5.8052                | 10.8389 | 42.00      | <.0001     |
| Scale                                                        | 1            | 0.6040     | 0.1107         | 0.4217                | 0.8652  |            |            |

The following statements produce [Output 51.1.4](#):

```
data models;
 set modela modelb;
run;

proc print data=models;
 id _model_;
 title 'Fitted Models';
run;
```

## Output 51.1.4 Motorette Failure: Fitted Models

| Fitted Models |             |             |             |               |               |
|---------------|-------------|-------------|-------------|---------------|---------------|
| <u>MODEL</u>  | <u>NAME</u> | <u>TYPE</u> | <u>DIST</u> | <u>STATUS</u> | <u>LNLIKE</u> |
| a             | time        | PARMS       | Weibull     | 0 Converged   | -22.9515      |
| a             | Intercept   | COV         | Weibull     | 0 Converged   | -22.9515      |
| a             | z           | COV         | Weibull     | 0 Converged   | -22.9515      |
| a             | Scale       | COV         | Weibull     | 0 Converged   | -22.9515      |
| b             | time        | PARMS       | Lognormal   | 0 Converged   | -24.4738      |
| b             | Intercept   | COV         | Lognormal   | 0 Converged   | -24.4738      |
| b             | z           | COV         | Lognormal   | 0 Converged   | -24.4738      |
| b             | Scale       | COV         | Lognormal   | 0 Converged   | -24.4738      |
| <u>MODEL</u>  | time        | Intercept   | z           | <u>SCALE</u>  |               |
| a             | -1.0000     | -11.8912    | 9.03834     | 0.36128       |               |
| a             | -11.8912    | 3.8632      | -1.77878    | 0.03448       |               |
| a             | 9.0383      | -1.7788     | 0.82082     | -0.01488      |               |
| a             | 0.3613      | 0.0345      | -0.01488    | 0.00632       |               |
| b             | -1.0000     | -10.4706    | 8.32208     | 0.60403       |               |
| b             | -10.4706    | 7.6835      | -3.55566    | 0.03267       |               |
| b             | 8.3221      | -3.5557     | 1.64897     | -0.01285      |               |
| b             | 0.6040      | 0.0327      | -0.01285    | 0.01226       |               |

The following statements produce [Output 51.1.5](#):

```

data out;
 set outa outb;
run;

data out1;
 set out;
 ltime=log(predtime);
 stde=std/predtime;
 upper=exp(ltime+1.64*stde);
 lower=exp(ltime-1.64*stde);
run;

title 'Quantile Estimates and Confidence Limits';
proc print data=out1;
 id temp;
run;
title;

```

**Output 51.1.5** Motorette Failure: Quantile Estimates and Confidence Limits

| Quantile Estimates and Confidence Limits |   |     |         |     |          |          |         |         |           |          |
|------------------------------------------|---|-----|---------|-----|----------|----------|---------|---------|-----------|----------|
|                                          |   |     | P       |     |          |          |         |         |           |          |
| c                                        |   |     | r       |     |          |          |         |         |           |          |
| c o                                      |   |     | e       |     |          |          |         |         |           |          |
| e n                                      |   |     | P       |     |          |          |         |         |           |          |
| t t n t                                  |   |     | R       |     |          |          |         |         |           |          |
| e i s r                                  |   |     | O       |     |          |          |         |         |           |          |
| m m o o                                  |   |     | B       |     |          |          |         |         |           |          |
| p e r l z                                |   |     | e       |     |          |          |         |         |           |          |
|                                          |   |     | —       |     |          |          |         |         |           |          |
| 130                                      | . | 0 1 | 2.48016 | 0.1 | 16519.27 | 5999.85  | 9.7123  | 0.36320 | 29969.51  | 9105.47  |
| 130                                      | . | 0 1 | 2.48016 | 0.5 | 32626.65 | 9874.33  | 10.3929 | 0.30265 | 53595.71  | 19861.63 |
| 130                                      | . | 0 1 | 2.48016 | 0.9 | 50343.22 | 15044.35 | 10.8266 | 0.29884 | 82183.49  | 30838.80 |
| 150                                      | . | 0 1 | 2.36295 | 0.1 | 5726.74  | 1569.34  | 8.6529  | 0.27404 | 8976.12   | 3653.64  |
| 150                                      | . | 0 1 | 2.36295 | 0.5 | 11310.68 | 2299.92  | 9.3335  | 0.20334 | 15787.62  | 8103.28  |
| 150                                      | . | 0 1 | 2.36295 | 0.9 | 17452.49 | 3629.28  | 9.7672  | 0.20795 | 24545.37  | 12409.24 |
| 130                                      | . | 0 1 | 2.48016 | 0.1 | 12033.19 | 5482.34  | 9.3954  | 0.45560 | 25402.68  | 5700.09  |
| 130                                      | . | 0 1 | 2.48016 | 0.5 | 26095.68 | 11359.45 | 10.1695 | 0.43530 | 53285.36  | 12779.95 |
| 130                                      | . | 0 1 | 2.48016 | 0.9 | 56592.19 | 26036.90 | 10.9436 | 0.46008 | 120349.65 | 26611.42 |
| 150                                      | . | 0 1 | 2.36295 | 0.1 | 4536.88  | 1443.07  | 8.4200  | 0.31808 | 7643.71   | 2692.83  |
| 150                                      | . | 0 1 | 2.36295 | 0.5 | 9838.86  | 2901.15  | 9.1941  | 0.29487 | 15957.38  | 6066.36  |
| 150                                      | . | 0 1 | 2.36295 | 0.9 | 21336.97 | 7172.34  | 9.9682  | 0.33615 | 37029.72  | 12294.62 |

**Example 51.2: Computing Predicted Values for a Tobit Model**

The LIFEREG procedure can be used to perform a Tobit analysis. The Tobit model, described by Tobin (1958), is a regression model for left-censored data assuming a normally distributed error term. The model parameters are estimated by maximum likelihood. PROC LIFEREG provides estimates of the parameters of the distribution of the *uncensored* data. See Greene (1993) and Maddala (1983) for a more complete discussion of censored normal data and related distributions. This example shows how you can use PROC LIFEREG and the DATA step to compute two of the three types of predicted values discussed there.

Consider a continuous random variable  $Y$  and a constant  $C$ . If you were to sample from the distribution of  $Y$  but discard values less than (greater than)  $C$ , the distribution of the remaining observations would be *truncated* on the left (right). If you were to sample from the distribution of  $Y$  and report values less than (greater than)  $C$  as  $C$ , the distribution of the sample would be left (right) *censored*.

The probability density function of the truncated random variable  $Y'$  is given by

$$f_{Y'}(y) = \frac{f_Y(y)}{\Pr(Y > C)} \text{ for } y > C$$

where  $f_Y(y)$  is the probability density function of  $Y$ . PROC LIFEREG cannot compute the proper likelihood function to estimate parameters or predicted values for a truncated distribution. Suppose the model being fit is specified as follows:

$$Y_i^* = \mathbf{x}_i' \boldsymbol{\beta} + \epsilon_i$$

where  $\epsilon_i$  is a normal error term with zero mean and standard deviation  $\sigma$ .

Define the censored random variable  $Y_i$  as

$$\begin{aligned} Y_i &= 0 \text{ if } Y_i^* \leq 0 \\ Y_i &= Y_i^* \text{ if } Y_i^* > 0 \end{aligned}$$

This is the Tobit model for left-censored normal data.  $Y_i^*$  is sometimes called the *latent variable*. PROC LIFEREG estimates parameters of the distribution of  $Y_i^*$  by maximum likelihood.

You can use the LIFEREG procedure to compute predicted values based on the mean functions of the latent and observed variables. The mean of the latent variable  $Y_i^*$  is  $\mathbf{x}'_i\boldsymbol{\beta}$ , and you can compute values of the mean for different settings of  $\mathbf{x}_i$  by specifying `XBETA=variable-name` in an OUTPUT statement. Estimates of  $\mathbf{x}'_i\boldsymbol{\beta}$  for each observation will be written to the OUT= data set. Predicted values of the observed variable  $Y_i$  can be computed based on the mean

$$E(Y_i) = \Phi\left(\frac{\mathbf{x}'_i\boldsymbol{\beta}}{\sigma}\right)(\mathbf{x}'_i\boldsymbol{\beta} + \sigma\lambda_i)$$

where

$$\lambda_i = \frac{\phi(\mathbf{x}'_i\boldsymbol{\beta}/\sigma)}{\Phi(\mathbf{x}'_i\boldsymbol{\beta}/\sigma)}$$

$\phi$  and  $\Phi$  represent the normal probability density and cumulative distribution functions.

Although the distribution of  $\epsilon_i$  in the Tobit model is often assumed normal, you can use other distributions for the Tobit model in the LIFEREG procedure by specifying a distribution with the `DISTRIBUTION=` option in the MODEL statement. One distribution that should be mentioned is the logistic distribution. For this distribution, the MLE has bounded influence function with respect to the response variable, but not the design variables. If you believe your data have outliers in the response direction, you might try this distribution for some robust estimation of the Tobit model.

With the logistic distribution, the predicted values of the observed variable  $Y_i$  can be computed based on the mean of  $Y_i^*$ ,

$$E(Y_i) = \sigma \ln(1 + \exp(\mathbf{x}'_i\boldsymbol{\beta}/\sigma))$$

The following table shows a subset of the Mroz (1987) data set. In these data, Hours is the number of hours the wife worked outside the household in a given year, Yrs\_Ed is the years of education, and Yrs\_Exp is the years of work experience. A Tobit model will be fit to the hours worked with years of education and experience as covariates.

| Hours | Yrs_Ed | Yrs_Exp |
|-------|--------|---------|
| 0     | 8      | 9       |
| 0     | 8      | 12      |
| 0     | 9      | 10      |
| 0     | 10     | 15      |
| 0     | 11     | 4       |
| 0     | 11     | 6       |
| 1000  | 12     | 1       |
| 1960  | 12     | 29      |
| 0     | 13     | 3       |
| 2100  | 13     | 36      |
| 3686  | 14     | 11      |
| 1920  | 14     | 38      |
| 0     | 15     | 14      |
| 1728  | 16     | 3       |
| 1568  | 16     | 19      |
| 1316  | 17     | 7       |
| 0     | 17     | 15      |

If the wife was not employed (worked 0 hours), her hours worked will be left censored at zero. In order to accommodate left censoring in PROC LIFEREG, you need two variables to indicate censoring status of observations. You can think of these variables as lower and upper endpoints of interval censoring. If there is no censoring, set both variables to the observed value of Hours. To indicate left censoring, set the lower endpoint to missing and the upper endpoint to the censored value, zero in this case.

The following statements create a SAS data set with the variables Hours, Yrs\_Ed, and Yrs\_Exp from the preceding data. A new variable, Lower, is created such that Lower=. if Hours=0 and Lower=Hours if Hours>0.

```

data subset;
 input Hours Yrs_Ed Yrs_Exp @@;
 if Hours eq 0
 then Lower=.;
 else Lower=Hours;
 datalines;
0 8 9 0 8 12 0 9 10 0 10 15 0 11 4 0 11 6
1000 12 1 1960 12 29 0 13 3 2100 13 36
3686 14 11 1920 14 38 0 15 14 1728 16 3
1568 16 19 1316 17 7 0 17 15
;

```

The following statements fit a normal regression model to the left-censored Hours data with Yrs\_Ed and Yrs\_Exp as covariates. You need the estimated standard deviation of the normal distribution to compute the predicted values of the censored distribution from the preceding formulas. The data set OUTEST contains the standard deviation estimate in a variable named `_SCALE_`. You also need estimates of  $x'_i\beta$ . These are contained in the data set OUT as the variable Xbeta.

```
proc lifereg data=subset outest=OUTEST(keep=_scale_);
 model (lower, hours) = yrs_ed yrs_exp / d=normal;
 output out=OUT xbeta=xbeta;
run;
```

Output 51.2.1 shows the results of the model fit. These tables show parameter estimates for the uncensored, or latent variable, distribution.

**Output 51.2.1** Parameter Estimates from PROC LIFEREG

| The LIFEREG Procedure                              |             |          |                |                       |          |            |            |
|----------------------------------------------------|-------------|----------|----------------|-----------------------|----------|------------|------------|
| Model Information                                  |             |          |                |                       |          |            |            |
| Data Set                                           | WORK.SUBSET |          |                |                       |          |            |            |
| Dependent Variable                                 | Lower       |          |                |                       |          |            |            |
| Dependent Variable                                 | Hours       |          |                |                       |          |            |            |
| Number of Observations                             | 17          |          |                |                       |          |            |            |
| Noncensored Values                                 | 8           |          |                |                       |          |            |            |
| Right Censored Values                              | 0           |          |                |                       |          |            |            |
| Left Censored Values                               | 9           |          |                |                       |          |            |            |
| Interval Censored Values                           | 0           |          |                |                       |          |            |            |
| Number of Parameters                               | 4           |          |                |                       |          |            |            |
| Name of Distribution                               | Normal      |          |                |                       |          |            |            |
| Log Likelihood                                     | -74.9369977 |          |                |                       |          |            |            |
| Analysis of Maximum Likelihood Parameter Estimates |             |          |                |                       |          |            |            |
| Parameter                                          | DF          | Estimate | Standard Error | 95% Confidence Limits |          | Chi-Square | Pr > ChiSq |
| Intercept                                          | 1           | -5598.64 | 2850.248       | -11185.0              | -12.2553 | 3.86       | 0.0495     |
| Yrs_Ed                                             | 1           | 373.1477 | 191.8872       | -2.9442               | 749.2397 | 3.78       | 0.0518     |
| Yrs_Exp                                            | 1           | 63.3371  | 38.3632        | -11.8533              | 138.5276 | 2.73       | 0.0987     |
| Scale                                              | 1           | 1582.870 | 442.6732       | 914.9433              | 2738.397 |            |            |

The following statements combine the two data sets created by PROC LIFEREG to compute predicted values for the censored distribution. The OUTEST= data set contains the estimate of the standard deviation from the uncensored distribution, and the OUT= data set contains estimates of  $x_i'\beta$ .

```
data predict;
 drop lambda _scale_ _prob_;
 set out;
 if _n_ eq 1 then set outest;
 lambda = pdf('NORMAL', Xbeta/_scale_)
 / cdf('NORMAL', Xbeta/_scale_);
 Predict = cdf('NORMAL', Xbeta/_scale_)
 * (Xbeta + _scale_*lambda);
 label Xbeta='MEAN OF UNCENSORED VARIABLE'
 Predict = 'MEAN OF CENSORED VARIABLE';
run;
```



Output 51.2.2 shows the original variables, the predicted means of the uncensored distribution, and the predicted means of the censored distribution.

**Output 51.2.2** Predicted Means from PROC LIFEREG

| Hours | Lower | Yrs_Ed | Yrs_Exp | MEAN OF<br>UNCENSORED<br>VARIABLE | MEAN OF<br>CENSORED<br>VARIABLE |
|-------|-------|--------|---------|-----------------------------------|---------------------------------|
| 0     | .     | 8      | 9       | -2043.42                          | 73.46                           |
| 0     | .     | 8      | 12      | -1853.41                          | 94.23                           |
| 0     | .     | 9      | 10      | -1606.94                          | 128.10                          |
| 0     | .     | 10     | 15      | -917.10                           | 276.04                          |
| 0     | .     | 11     | 4       | -1240.67                          | 195.76                          |
| 0     | .     | 11     | 6       | -1113.99                          | 224.72                          |
| 1000  | 1000  | 12     | 1       | -1057.53                          | 238.63                          |
| 1960  | 1960  | 12     | 29      | 715.91                            | 1052.94                         |
| 0     | .     | 13     | 3       | -557.71                           | 391.42                          |
| 2100  | 2100  | 13     | 36      | 1532.42                           | 1672.50                         |
| 3686  | 3686  | 14     | 11      | 322.14                            | 805.58                          |
| 1920  | 1920  | 14     | 38      | 2032.24                           | 2106.81                         |
| 0     | .     | 15     | 14      | 885.30                            | 1170.39                         |
| 1728  | 1728  | 16     | 3       | 561.74                            | 951.69                          |
| 1568  | 1568  | 16     | 19      | 1575.13                           | 1708.24                         |
| 1316  | 1316  | 17     | 7       | 1188.23                           | 1395.61                         |
| 0     | .     | 17     | 15      | 1694.93                           | 1809.97                         |

---

### Example 51.3: Overcoming Convergence Problems by Specifying Initial Values

This example illustrates the use of parameter initial value specification to help overcome convergence difficulties.

The following statements create a SAS data set.

```
data raw;
 input censor x c1 @@;
 datalines;
0 16 0.00 0 17 0.00 0 18 0.00
0 17 0.04 0 18 0.04 0 18 0.04
0 23 0.40 0 22 0.40 0 22 0.40
0 33 4.00 0 34 4.00 0 35 4.00
1 54 40.00 1 54 40.00 1 54 40.00
1 54 400.00 1 54 400.00 1 54 400.00
;
```

Output 51.3.1 shows the contents of the data set raw.

**Output 51.3.1** Contents of the Data Set

| Obs | sensor | x  | c1     |
|-----|--------|----|--------|
| 1   | 0      | 16 | 0.00   |
| 2   | 0      | 17 | 0.00   |
| 3   | 0      | 18 | 0.00   |
| 4   | 0      | 17 | 0.04   |
| 5   | 0      | 18 | 0.04   |
| 6   | 0      | 18 | 0.04   |
| 7   | 0      | 23 | 0.40   |
| 8   | 0      | 22 | 0.40   |
| 9   | 0      | 22 | 0.40   |
| 10  | 0      | 33 | 4.00   |
| 11  | 0      | 34 | 4.00   |
| 12  | 0      | 35 | 4.00   |
| 13  | 1      | 54 | 40.00  |
| 14  | 1      | 54 | 40.00  |
| 15  | 1      | 54 | 40.00  |
| 16  | 1      | 54 | 400.00 |
| 17  | 1      | 54 | 400.00 |
| 18  | 1      | 54 | 400.00 |

The following SAS statements request that a Weibull regression model be fit to the data:

```

title 'OLS (Default) Initial Values';
proc lifereg data=raw;
 model x*censor(1) = c1 / distribution = Weibull itprint;
run;

```

Convergence was not attained in 50 iterations for this model, as the following messages to the log indicate:

```

WARNING: Convergence was not attained in 50 iterations. You might want to
increase the maximum number of iterations (MAXITER= option) or
change the convergence criteria (CONVERGE = value) in the MODEL
statement.

```

```

WARNING: The procedure is continuing in spite of the above warning. Results
shown are based on the last maximum likelihood iteration. Validity
of the model fit is questionable.

```

The first line (iter=0) of the iteration history table, shown in [Output 51.3.2](#), shows the default initial ordinary least squares (OLS) estimates of the parameters.

## Output 51.3.2 Initial Least Squares

| OLS (Default) Initial Values              |       |               |              |              |              |
|-------------------------------------------|-------|---------------|--------------|--------------|--------------|
| The LIFEREG Procedure                     |       |               |              |              |              |
| Iteration History for Parameter Estimates |       |               |              |              |              |
| Iter                                      | Ridge | Loglikelihood | Intercept    | c1           | Scale        |
| 0                                         | 0     | -22.891088    | 3.2324769714 | 0.0020664542 | 0.3995754195 |
| 1                                         | 0     | -16.427074    | 3.5337141598 | 0.0028713635 | 0.3283544365 |
| 2                                         | 0     | -13.216768    | 3.4480787541 | 0.0052801225 | 0.3816964358 |
| 3                                         | 0     | -5.0786635    | 3.1966395335 | 0.0191439929 | 0.2325418958 |
| 4                                         | 0     | -2.0018885    | 3.1848047525 | 0.0275425402 | 0.1963590539 |
| 5                                         | 0     | -0.1814984    | 3.1478989655 | 0.0374731819 | 0.2103607621 |
| 6                                         | 0     | 2.90712131    | 3.0858183316 | 0.0659946149 | 0.1818245261 |
| 7                                         | 0.063 | 2.9991781     | 3.1014479187 | 0.0661096622 | 0.1648677081 |
| 8                                         | 0.063 | 3.01557837    | 3.0995493638 | 0.0662333056 | 0.1670552505 |
| 9                                         | 0.063 | 3.0301815     | 3.0992317977 | 0.0663580659 | 0.1669529486 |
| 10                                        | 0.063 | 3.0448013     | 3.0989901232 | 0.0664827053 | 0.1667371524 |
| 11                                        | 0.063 | 3.05941254    | 3.0987507448 | 0.0666071514 | 0.1665197313 |
| 12                                        | 0.063 | 3.07401474    | 3.0985118143 | 0.0667314052 | 0.1663026517 |
| 13                                        | 0.063 | 3.08860788    | 3.0982732928 | 0.066855467  | 0.1660859472 |
| 14                                        | 0.063 | 3.10319193    | 3.0980351787 | 0.0669793371 | 0.1658696184 |
| 15                                        | 0.063 | 3.11776689    | 3.0977974713 | 0.0671030156 | 0.1656536651 |
| 16                                        | 0.063 | 3.13233272    | 3.0975601698 | 0.0672265029 | 0.1654380873 |
| 17                                        | 0.063 | 3.1468894     | 3.0973232737 | 0.0673497993 | 0.165222885  |
| 18                                        | 0.063 | 3.16143692    | 3.0970867821 | 0.0674729049 | 0.1650080579 |
| 19                                        | 0.063 | 3.17597526    | 3.0968506943 | 0.06759582   | 0.1647936061 |
| 20                                        | 0.063 | 3.19050439    | 3.0966150098 | 0.0677185449 | 0.1645795293 |
| 21                                        | 0.063 | 3.2050243     | 3.0963797277 | 0.0678410799 | 0.1643658275 |
| 22                                        | 0.063 | 3.21953496    | 3.0961448474 | 0.0679634252 | 0.1641525006 |
| 23                                        | 0.063 | 3.23403635    | 3.0959103682 | 0.068085581  | 0.1639395483 |
| 24                                        | 0.063 | 3.24852845    | 3.0956762896 | 0.0682075476 | 0.1637269705 |
| 25                                        | 0.063 | 3.26301123    | 3.0954426107 | 0.0683293253 | 0.1635147672 |
| 26                                        | 0.063 | 3.27748468    | 3.095209331  | 0.0684509143 | 0.163302938  |
| 27                                        | 0.063 | 3.29194878    | 3.0949764498 | 0.0685723149 | 0.1630914829 |
| 28                                        | 0.063 | 3.3064035     | 3.0947439665 | 0.0686935273 | 0.1628804017 |
| 29                                        | 0.063 | 3.32084881    | 3.0945118805 | 0.0688145517 | 0.1626696942 |
| 30                                        | 0.063 | 3.3352847     | 3.0942801911 | 0.0689353885 | 0.1624593601 |
| 31                                        | 0.063 | 3.34971114    | 3.0940488977 | 0.0690560378 | 0.1622493994 |
| 32                                        | 0.063 | 3.36412812    | 3.0938179997 | 0.0691765    | 0.1620398118 |
| 33                                        | 0.063 | 3.3785356     | 3.0935874965 | 0.0692967752 | 0.1618305971 |
| 34                                        | 0.063 | 3.39293356    | 3.0933573875 | 0.0694168637 | 0.161621755  |
| 35                                        | 0.063 | 3.40732199    | 3.093127672  | 0.0695367658 | 0.1614132855 |
| 36                                        | 0.063 | 3.42170085    | 3.0928983495 | 0.0696564816 | 0.1612051882 |
| 37                                        | 0.063 | 3.43607013    | 3.0926694194 | 0.0697760116 | 0.1609974629 |
| 38                                        | 0.063 | 3.45042979    | 3.0924408811 | 0.0698953558 | 0.1607901095 |
| 39                                        | 0.063 | 3.46477983    | 3.092212734  | 0.0700145146 | 0.1605831276 |
| 40                                        | 0.063 | 3.4791202     | 3.0919849776 | 0.0701334882 | 0.160376517  |
| 41                                        | 0.063 | 3.4934509     | 3.0917576112 | 0.0702522768 | 0.1601702775 |
| 42                                        | 0.063 | 3.50777188    | 3.0915306343 | 0.0703708808 | 0.1599644088 |
| 43                                        | 0.063 | 3.52208314    | 3.0913040464 | 0.0704893002 | 0.1597589108 |
| 44                                        | 0.063 | 3.53638465    | 3.0910778468 | 0.0706075354 | 0.159553783  |
| 45                                        | 0.063 | 3.55067637    | 3.0908520349 | 0.0707255867 | 0.1593490254 |
| 46                                        | 0.063 | 3.5649583     | 3.0906266104 | 0.0708434542 | 0.1591446376 |
| 47                                        | 0.063 | 3.57923039    | 3.0904015725 | 0.0709611382 | 0.1589406193 |
| 48                                        | 0.063 | 3.59349263    | 3.0901769207 | 0.0710786389 | 0.1587369703 |
| 49                                        | 0.063 | 3.607745      | 3.0899526546 | 0.0711959567 | 0.1585336903 |
| 50                                        | 0.063 | 3.62198746    | 3.0897287734 | 0.0713130916 | 0.1583307791 |

The log-logistic distribution is more robust to large values of the response than the Weibull distribution, so one approach to improving the convergence performance is to fit a log-logistic distribution, and if this converges, use the resulting parameter estimates as initial values in a subsequent fit of a model with the Weibull distribution.

The following statements fit a log-logistic distribution to the data:

```
proc lifereg data=raw;
 model x*censor(1) = c1 / distribution = llogistic;
run;
```

The algorithm converges, and the maximum likelihood estimates for the log-logistic distribution are shown in [Output 51.3.3](#)

**Output 51.3.3** Estimates from the Log-Logistic Distribution

| OLS (Default) Initial Values                       |    |          |                |                       |        |            |            |
|----------------------------------------------------|----|----------|----------------|-----------------------|--------|------------|------------|
| The LIFEREG Procedure                              |    |          |                |                       |        |            |            |
| Analysis of Maximum Likelihood Parameter Estimates |    |          |                |                       |        |            |            |
| Parameter                                          | DF | Estimate | Standard Error | 95% Confidence Limits |        | Chi-Square | Pr > ChiSq |
| Intercept                                          | 1  | 2.8983   | 0.0318         | 2.8360                | 2.9606 | 8309.43    | <.0001     |
| c1                                                 | 1  | 0.1592   | 0.0133         | 0.1332                | 0.1852 | 143.85     | <.0001     |
| Scale                                              | 1  | 0.0498   | 0.0122         | 0.0308                | 0.0804 |            |            |

The following statements refit the Weibull model by using the maximum likelihood estimates from the log-logistic fit as initial values:

```
proc lifereg data=raw outest=outest;
 model x*censor(1) = c1 / itprint distribution = weibull
 intercept=2.898 initial=0.16 scale=0.05;
 output out=out xbeta=xbeta;
run;
```

Examination of the resulting output in [Output 51.3.4](#) shows that the convergence problem has been solved by specifying different initial values.

**Output 51.3.4** Final Estimates from the Weibull Distribution

```

 OLS (Default) Initial Values

 The LIFEREG Procedure

 Model Information

 Data Set WORK.RAW
 Dependent Variable Log(x)
 Censoring Variable censor
 Censoring Value(s) 1
 Number of Observations 18
 Noncensored Values 12
 Right Censored Values 6
 Left Censored Values 0
 Interval Censored Values 0
 Number of Parameters 3
 Name of Distribution Weibull
 Log Likelihood 11.232023272

 Algorithm converged.

 Analysis of Maximum Likelihood Parameter Estimates

 Parameter DF Estimate Standard 95% Confidence Chi-
 Error Limits Square Pr > ChiSq

 Intercept 1 2.9699 0.0326 2.9059 3.0338 8278.86 <.0001
 c1 1 0.1435 0.0165 0.1111 0.1758 75.43 <.0001
 Scale 1 0.0844 0.0189 0.0544 0.1308
 Weibull Shape 1 11.8526 2.6514 7.6455 18.3749

```

As an example of an alternative way of specifying initial values, the following invocation of PROC LIFEREG, using the INEST= data set to provide starting values for the three parameters, is equivalent to the previous invocation:

```

data in;
 input intercept c1 scale;
 datalines;
2.898 0.16 0.05
;

proc lifereg data=raw inest=in outest=outest;
 model x*censor(1) = c1 / itprint distribution = weibull;
 output out=out xbeta=xbeta;
run;

```

## Example 51.4: Analysis of Arbitrarily Censored Data with Interaction Effects

The artificial data in this example are from a study of the natural recovery time of mice after injection of a certain toxin. Twenty mice were grouped by sex (sex: 1 = Male, 2 = Female) with equal sizes. Their ages (in days) were recorded at the injection. Their recovery times (in minutes) were also recorded. Toxin density in blood was used to decide whether a mouse recovered. Mice were checked at two times for recovery. If a mouse had recovered at the first time, the observation is left censored, and no further measurement is made. The variable `time1` is set to missing and `time2` is set to the measurement time to indicate left censoring. If a mouse had not recovered at the first time, it was checked later at a second time. If it had recovered by the second measurement time, the observation is interval censored, and the variable `time1` is set to the first measurement time and `time2` is set to the second measurement time. If there was no recovery at the second measurement, the observation is right censored, and `time1` is set to the second measurement time and `time2` is set to missing to indicate right censoring.

The following statements create a SAS data set containing the data from the experiment:

```

title 'Natural Recovery Time';
data mice;
 input sex age time1 time2;
 datalines;
1 57 631 631
1 45 . 170
1 54 227 227
1 43 143 143
1 64 916 .
1 67 691 705
1 44 100 100
1 59 730 .
1 47 365 365
1 74 1916 1916
2 79 1326 .
2 75 837 837
2 84 1200 1235
2 54 . 365
2 74 1255 1255
2 71 1823 .
2 65 537 637
2 33 583 683
2 77 955 .
2 46 577 577
;

```

The following SAS statements create the SAS data sets xrow1 and xrow2:

```
data xrow1;
 input sex age time1 time2;
 datalines;
1 50 . .
;

data xrow2;
 input sex age time1 time2;
 datalines;
2 60.6 . .
;
```

The following SAS statements fit a Weibull model with age, sex, and an age-by-sex interaction term as covariates, and create a plot of predicted probabilities against recovery time for the fixed values of age and sex specified in the SAS data set xrow1:

```
ods graphics on;
proc lifereg data=mice xdata=xrow1;
 class sex;
 model (time1, time2) = age sex age*sex / dist=Weibull;

 probplot / nodata
 plower=.5
 vref(intersect) = 75
 vreflab = '75 Percent';
 inset;
run;
```

Standard output is shown in [Output 51.4.1](#). Tables containing general model information, Type III tests for the main effects and interaction terms, and parameter estimates are created.

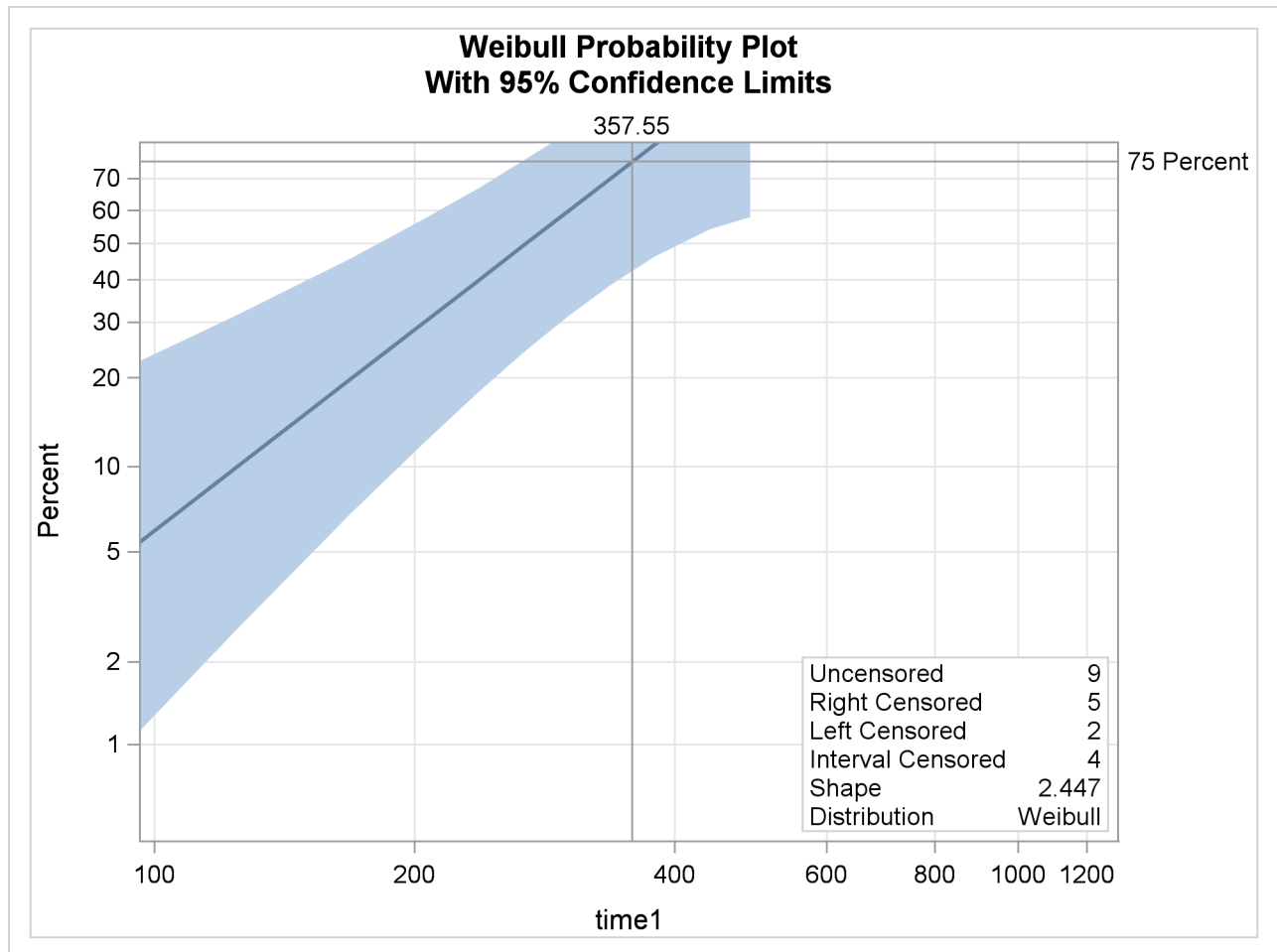
**Output 51.4.1** Parameter Estimates for the Interaction Model

| Natural Recovery Time                              |              |            |                |                       |         |            |            |
|----------------------------------------------------|--------------|------------|----------------|-----------------------|---------|------------|------------|
| The LIFEREG Procedure                              |              |            |                |                       |         |            |            |
| Model Information                                  |              |            |                |                       |         |            |            |
| Data Set                                           | WORK.MICE    |            |                |                       |         |            |            |
| Dependent Variable                                 | Log(time1)   |            |                |                       |         |            |            |
| Dependent Variable                                 | Log(time2)   |            |                |                       |         |            |            |
| Number of Observations                             | 20           |            |                |                       |         |            |            |
| Noncensored Values                                 | 9            |            |                |                       |         |            |            |
| Right Censored Values                              | 5            |            |                |                       |         |            |            |
| Left Censored Values                               | 2            |            |                |                       |         |            |            |
| Interval Censored Values                           | 4            |            |                |                       |         |            |            |
| Number of Parameters                               | 5            |            |                |                       |         |            |            |
| Name of Distribution                               | Weibull      |            |                |                       |         |            |            |
| Log Likelihood                                     | -25.91033295 |            |                |                       |         |            |            |
| Type III Analysis of Effects                       |              |            |                |                       |         |            |            |
| Effect                                             | DF           | Wald       |                | Pr > ChiSq            |         |            |            |
|                                                    |              | Chi-Square |                |                       |         |            |            |
| age                                                | 1            | 33.8496    |                | <.0001                |         |            |            |
| sex                                                | 1            | 14.0245    |                | 0.0002                |         |            |            |
| age*sex                                            | 1            | 10.7196    |                | 0.0011                |         |            |            |
| Analysis of Maximum Likelihood Parameter Estimates |              |            |                |                       |         |            |            |
| Parameter                                          | DF           | Estimate   | Standard Error | 95% Confidence Limits |         | Chi-Square | Pr > ChiSq |
| Intercept                                          | 1            | 5.4110     | 0.5549         | 4.3234                | 6.4986  | 95.08      | <.0001     |
| age                                                | 1            | 0.0250     | 0.0086         | 0.0081                | 0.0419  | 8.42       | 0.0037     |
| sex                                                | 1            | -3.9808    | 1.0630         | -6.0643               | -1.8974 | 14.02      | 0.0002     |
| sex                                                | 2            | 0.0000     | .              | .                     | .       | .          | .          |
| age*sex                                            | 1            | 0.0613     | 0.0187         | 0.0246                | 0.0980  | 10.72      | 0.0011     |
| age*sex                                            | 2            | 0.0000     | .              | .                     | .       | .          | .          |
| Scale                                              | 1            | 0.4087     | 0.0900         | 0.2654                | 0.6294  |            |            |
| Weibull Shape                                      | 1            | 2.4468     | 0.5391         | 1.5887                | 3.7682  |            |            |



The following two plots display the predicted probability against the recovery time for two different populations. **Output 51.4.2** is created with the `PROBPLOT` statement with the option `XDATA= xrow1`, which specifies the population with `sex = 1`, `age = 50`. **Output 51.4.3** is created with the `PROBPLOT` statement with the option `XDATA= xrow2`, which specifies the population with `sex = 2`, `age = 60.6`. These are the default values that the `LIFEREG` procedure would use for the probability plot if the `XDATA=` option had not been specified. Reference lines are used to display specified predicted probability points and their relative locations in the plot.

**Output 51.4.2** Probability Plot for Recovery Time with `sex = 1`, `age = 50`

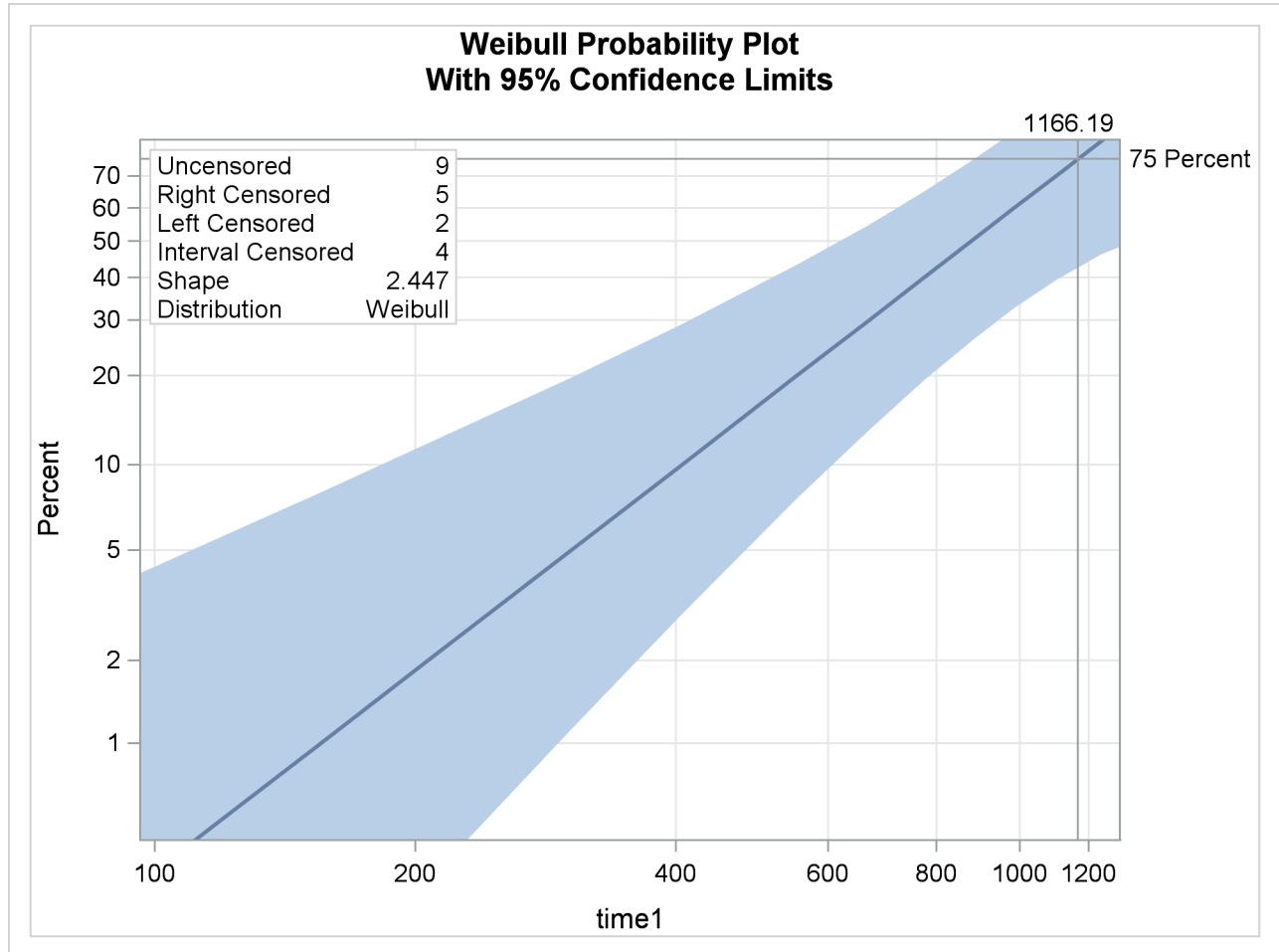


The following SAS statements fit a Weibull model with age, sex, and an age-by-sex interaction term as covariates, and create the plot of predicted probabilities against recovery time shown in [Output 51.4.3](#), for the fixed values of age and sex specified in the SAS data set xrow2:

```
proc lifereg data=mice xdata=xrow2;
 class sex;
 model (time1, time2) = age sex age*sex / dist=Weibull;

 probplot / nodata
 plower=.5
 vref(intersect) = 75
 vreflab = '75 Percent';
 inset;
run;
title;
ods graphics off;
```

**Output 51.4.3** Probability Plot for Recovery Time with sex = 2, age = 60.6



## Example 51.5: Probability Plotting—Right Censoring

The following statements create a SAS data set containing observed and right-censored lifetimes of 70 diesel engine fans (Nelson 1982):

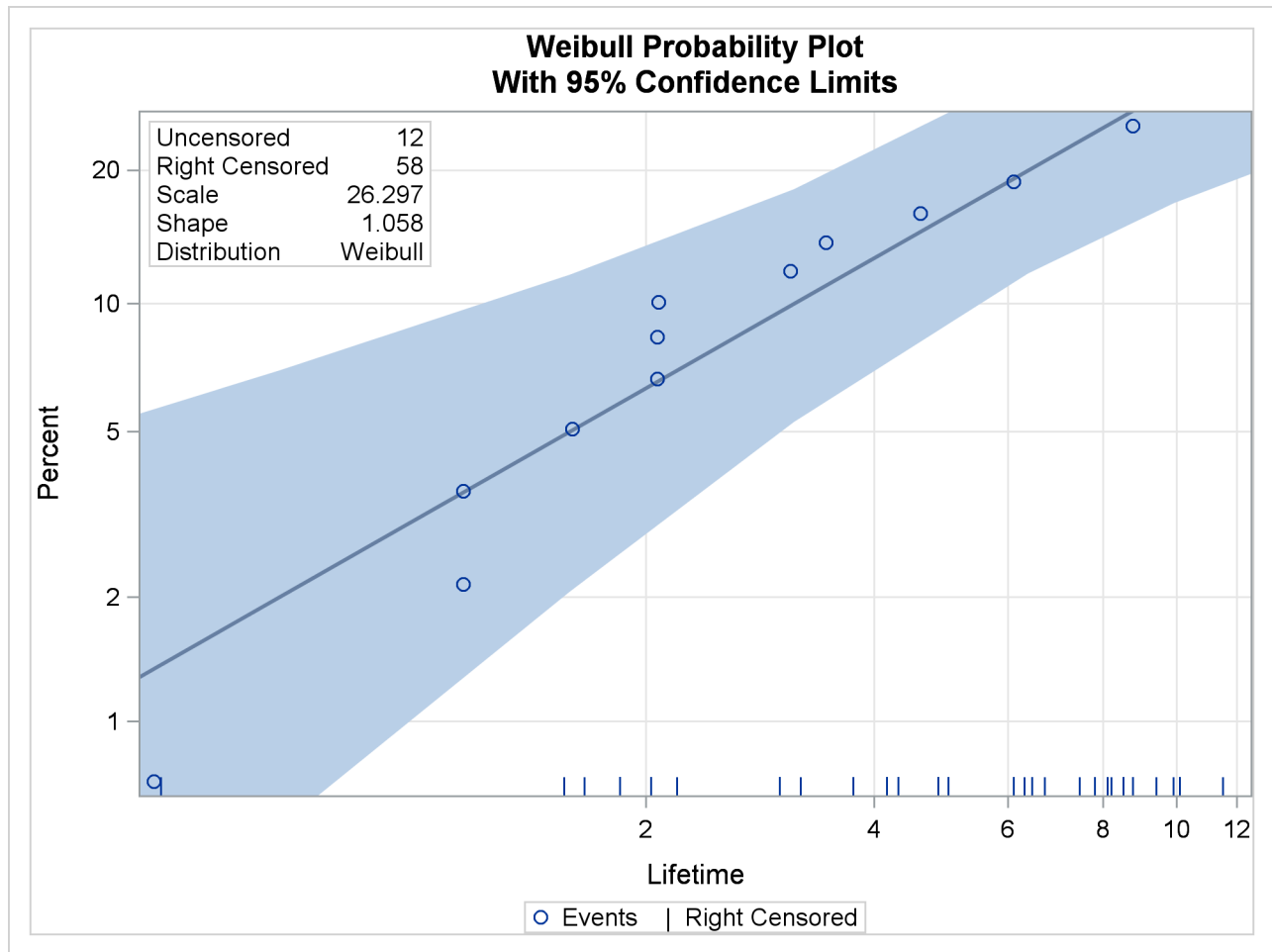
```
data Fan;
 input Lifetime Censor@@;
 Lifetime = Lifetime / 1000;
 datalines;
 450 0 460 1 1150 0 1150 0 1560 1
 1600 0 1660 1 1850 1 1850 1 1850 1
 1850 1 1850 1 2030 1 2030 1 2030 1
 2070 0 2070 0 2080 0 2200 1 3000 1
 3000 1 3000 1 3000 1 3100 0 3200 1
 3450 0 3750 1 3750 1 4150 1 4150 1
 4150 1 4150 1 4300 1 4300 1 4300 1
 4300 1 4600 0 4850 1 4850 1 4850 1
 4850 1 5000 1 5000 1 5000 1 6100 1
 6100 0 6100 1 6100 1 6300 1 6450 1
 6450 1 6700 1 7450 1 7800 1 7800 1
 8100 1 8100 1 8200 1 8500 1 8500 1
 8500 1 8750 1 8750 0 8750 1 9400 1
 9900 1 10100 1 10100 1 10100 1 11500 1
;
```

Some of the fans had not failed at the time the data were collected, and the unfailed units have right-censored lifetimes. The variable LIFETIME represents either a failure time or a censoring time, in thousands of hours. The variable CENSOR is equal to 0 if the value of LIFETIME is a failure time, and it is equal to 1 if the value is a censoring time. The following statements use the LIFEREG procedure to produce the probability plot with an inset for the engine lifetimes:

```
ods graphics on;
proc lifereg data=Fan;
 model Lifetime*Censor(1) = / d = Weibull;
 probplot
 ppout
 npintervals=simul;
 inset;
run;
ods graphics off;
```

The resulting graphical output is shown in [Output 51.5.1](#). The estimated CDF, a line representing the maximum likelihood fit, and pointwise parametric confidence bands are plotted in the body of [Output 51.5.1](#). The values of right-censored observations are plotted along the bottom of the graph. The “Cumulative Probability Estimates” table is also created in [Output 51.5.2](#).

**Output 51.5.1** Probability Plot for the Fan Data



**Output 51.5.2** CDF Estimates

| Lifetime | Cumulative Probability Estimates |                                    |        | Kaplan-Meier Estimate | Kaplan-Meier Standard Error |
|----------|----------------------------------|------------------------------------|--------|-----------------------|-----------------------------|
|          | Cumulative Probability           | Simultaneous 95% Confidence Limits |        |                       |                             |
|          |                                  | Lower                              | Upper  |                       |                             |
| 0.45     | 0.0071                           | 0.0007                             | 0.2114 | 0.0143                | 0.0142                      |
| 1.15     | 0.0215                           | 0.0033                             | 0.2114 | 0.0288                | 0.0201                      |
| 1.15     | 0.0360                           | 0.0073                             | 0.2168 | 0.0433                | 0.0244                      |
| 1.6      | 0.0506                           | 0.0125                             | 0.2304 | 0.0580                | 0.0282                      |
| 2.07     | 0.0666                           | 0.0190                             | 0.2539 | 0.0751                | 0.0324                      |
| 2.07     | 0.0837                           | 0.0264                             | 0.2760 | 0.0923                | 0.0361                      |
| 2.08     | 0.1008                           | 0.0344                             | 0.2972 | 0.1094                | 0.0392                      |
| 3.1      | 0.1189                           | 0.0436                             | 0.3223 | 0.1283                | 0.0427                      |
| 3.45     | 0.1380                           | 0.0535                             | 0.3471 | 0.1477                | 0.0460                      |
| 4.6      | 0.1602                           | 0.0653                             | 0.3844 | 0.1728                | 0.0510                      |
| 6.1      | 0.1887                           | 0.0791                             | 0.4349 | 0.2046                | 0.0581                      |
| 8.75     | 0.2488                           | 0.0884                             | 0.6391 | 0.2930                | 0.0980                      |

### Example 51.6: Probability Plotting—Arbitrary Censoring

Table 51.17 contains microprocessor failure data (Nelson 1990). Units were inspected at predetermined time intervals. The data consist of inspection interval endpoints (in hours) and the number of units failing in each interval. A missing (.) lower endpoint indicates left censoring, and a missing upper endpoint indicates right censoring. These can be thought of as semi-infinite intervals with a lower (upper) endpoint of negative (positive) infinity for left (right) censoring.

**Table 51.17** Interval-Censored Data

| Lower Endpoint | Upper Endpoint | Number Failed |
|----------------|----------------|---------------|
| .              | 6              | 6             |
| 6              | 12             | 2             |
| 24             | 48             | 2             |
| 24             | .              | 1             |
| 48             | 168            | 1             |
| 48             | .              | 839           |
| 168            | 500            | 1             |
| 168            | .              | 150           |
| 500            | 1000           | 2             |
| 500            | .              | 149           |
| 1000           | 2000           | 1             |
| 1000           | .              | 147           |
| 2000           | .              | 122           |

The following SAS statements create the SAS data set Micro:

```
data Micro;
 input t1 t2 f;
 datalines;
. 6 6
6 12 2
12 24 0
24 48 2
24 . 1
48 168 1
48 . 839
168 500 1
168 . 150
500 1000 2
500 . 149
1000 2000 1
1000 . 147
2000 . 122
;
```

The following SAS statements compute the nonparametric Turnbull estimate of the cumulative distribution function and create a lognormal probability plot:

```
ods graphics on;
proc lifereg data=Micro;
 model (t1 t2) = / d=lognormal intercept=25 scale=5;
 weight f;
 probplot
 pupper = 10
 itprintem
 printprobs
 maxitem = (1000,25)
 ppout;
 inset;
run;
ods graphics off;
```

The two initial values INTERCEPT=25 and SCALE=5 in the MODEL statement are used to aid convergence in the model-fitting algorithm.

The following tables are created by the PROBLOT statement in addition to the standard tabular output from the MODEL statement. Output 51.6.1 shows the iteration history for the Turnbull estimate of the CDF for the microprocessor data. With both options ITPRINTEM and PRINTPROBS specified in the PROBLOT statement, this table contains the log likelihoods and interval probabilities for every 25th iteration and the last iteration. It would contain only the log likelihoods if the option PRINTPROBS were not specified.

**Output 51.6.1** Iteration History for the Turnbull Estimate

| The LIFEREG Procedure |               |                                                        |             |              |            |
|-----------------------|---------------|--------------------------------------------------------|-------------|--------------|------------|
| Iteration             | Loglikelihood | Iteration History for the Turnbull Estimate of the CDF |             |              |            |
|                       |               | (., 6)                                                 | (6, 12)     | (24, 48)     | (48, 168)  |
|                       |               | (168, 500)                                             | (500, 1000) | (1000, 2000) | (2000, .)  |
| 0                     | -1133.4051    | 0.125                                                  | 0.125       | 0.125        | 0.125      |
|                       |               | 0.125                                                  | 0.125       | 0.125        | 0.125      |
| 25                    | -104.16622    | 0.00421644                                             | 0.00140548  | 0.00140648   | 0.00173338 |
|                       |               | 0.00237846                                             | 0.00846094  | 0.04565407   | 0.93474475 |
| 50                    | -101.15151    | 0.00421644                                             | 0.00140548  | 0.00140648   | 0.00173293 |
|                       |               | 0.00234891                                             | 0.00727679  | 0.01174486   | 0.96986811 |
| 75                    | -101.06641    | 0.00421644                                             | 0.00140548  | 0.00140648   | 0.00173293 |
|                       |               | 0.00234891                                             | 0.00727127  | 0.00835638   | 0.9732621  |
| 100                   | -101.06534    | 0.00421644                                             | 0.00140548  | 0.00140648   | 0.00173293 |
|                       |               | 0.00234891                                             | 0.00727125  | 0.00801814   | 0.97360037 |
| 125                   | -101.06533    | 0.00421644                                             | 0.00140548  | 0.00140648   | 0.00173293 |
|                       |               | 0.00234891                                             | 0.00727125  | 0.00798438   | 0.97363413 |
| 130                   | -101.06533    | 0.00421644                                             | 0.00140548  | 0.00140648   | 0.00173293 |
|                       |               | 0.00234891                                             | 0.00727125  | 0.007983     | 0.97363551 |

The table in [Output 51.6.2](#) summarizes the Turnbull estimates of the interval probabilities, the reduced gradients, and Lagrange multipliers as described in the section “[Arbitrarily Censored Data](#)” on page 3942.

**Output 51.6.2** Summary for the Turnbull Algorithm

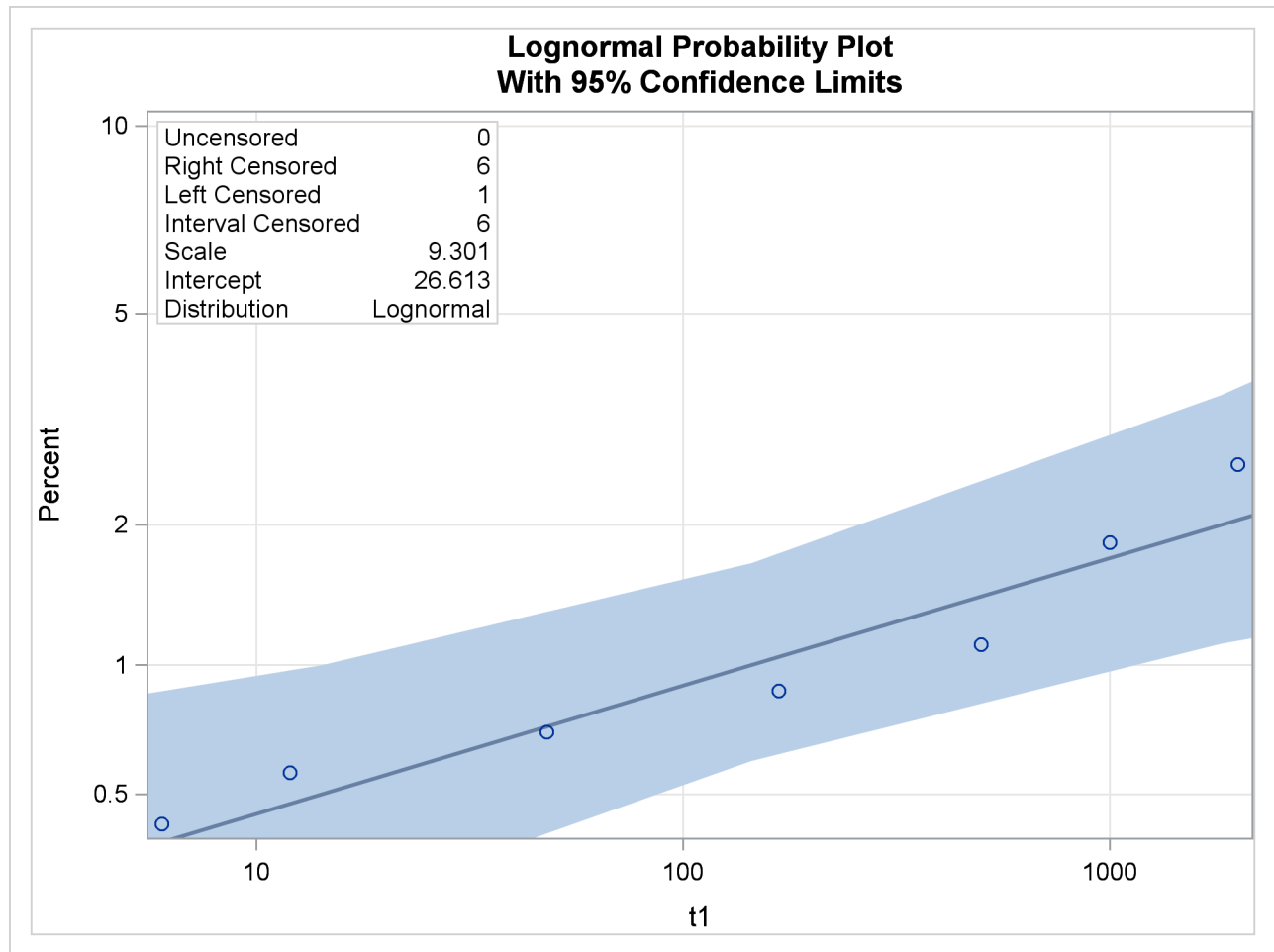
| Lower Lifetime | Upper Lifetime | Probability | Reduced Gradient | Lagrange Multiplier |
|----------------|----------------|-------------|------------------|---------------------|
| .              | 6              | 0.0042      | 0                | 0                   |
| 6              | 12             | 0.0014      | 0                | 0                   |
| 24             | 48             | 0.0014      | 0                | 0                   |
| 48             | 168            | 0.0017      | 0                | 0                   |
| 168            | 500            | 0.0023      | 0                | 0                   |
| 500            | 1000           | 0.0073      | -7.219342E-9     | 0                   |
| 1000           | 2000           | 0.0080      | -0.037063236     | 0                   |
| 2000           | .              | 0.9736      | 0.0003038877     | 0                   |

[Output 51.6.3](#) shows the final estimate of the CDF, along with standard errors and nonparametric confidence limits. Two kinds of nonparametric confidence limits, pointwise or simultaneous, are available. The default is the pointwise nonparametric confidence limits. You can specify the simultaneous nonparametric confidence limits by using the NPINTERVALS=SIMUL option.

**Output 51.6.3** Final CDF Estimates for Turnbull Algorithm

| Cumulative Probability Estimates |                |                        |                                 |        |                |
|----------------------------------|----------------|------------------------|---------------------------------|--------|----------------|
| Lower Lifetime                   | Upper Lifetime | Cumulative Probability | Pointwise 95% Confidence Limits |        | Standard Error |
|                                  |                |                        | Lower                           | Upper  |                |
| 6                                | 6              | 0.0042                 | 0.0019                          | 0.0094 | 0.0017         |
| 12                               | 24             | 0.0056                 | 0.0028                          | 0.0112 | 0.0020         |
| 48                               | 48             | 0.0070                 | 0.0038                          | 0.0130 | 0.0022         |
| 168                              | 168            | 0.0088                 | 0.0047                          | 0.0164 | 0.0028         |
| 500                              | 500            | 0.0111                 | 0.0058                          | 0.0211 | 0.0037         |
| 1000                             | 1000           | 0.0184                 | 0.0094                          | 0.0357 | 0.0063         |
| 2000                             | 2000           | 0.0264                 | 0.0124                          | 0.0553 | 0.0101         |

[Output 51.6.4](#) shows the CDF estimates, maximum likelihood fit, and pointwise parametric confidence limits plotted on a lognormal probability plot.

**Output 51.6.4** Lognormal Probability Plot for the Microprocessor Data

## Example 51.7: Bayesian Analysis of Clinical Trial Data

Consider the data on melanoma patients from a clinical trial described in Ibrahim, Chen, and Sinha (2001). A partial listing of the data is shown in [Output 51.7.1](#).

The survival time is modeled by a Weibull regression model with three covariates. An analysis of the right-censored survival data is performed with PROC LIFEREG to obtain Bayesian estimates of the regression coefficients by using the following SAS statements:

```
ods graphics on;
proc lifereg data=e1684;
 class Sex;
 model Survtime*Surv cens(1)=Age Sex Perform / dist=Weibull;
 bayes WeibullShapePrior=gamma seed=9999;
run;
ods graphics off;
```



**Output 51.7.1** Clinical Trial Data

| Obs | survtime | survcens | age     | sex | perform |
|-----|----------|----------|---------|-----|---------|
| 1   | 1.57808  | 2        | 35.9945 | 1   | 0       |
| 2   | 1.48219  | 2        | 41.9014 | 1   | 0       |
| 3   | 7.33425  | 1        | 70.2164 | 2   | 0       |
| 4   | 0.65479  | 2        | 58.1753 | 2   | 1       |
| 5   | 2.23288  | 2        | 33.7096 | 1   | 0       |
| 6   | 9.38356  | 1        | 47.9726 | 1   | 0       |
| 7   | 3.27671  | 2        | 31.8219 | 2   | 0       |
| 8   | 0.00000  | 1        | 72.3644 | 2   | 0       |
| 9   | 0.80274  | 2        | 40.7151 | 2   | 0       |
| 10  | 9.64384  | 1        | 32.9479 | 1   | 0       |
| 11  | 1.66575  | 2        | 35.9205 | 1   | 0       |
| 12  | 0.94247  | 2        | 40.5068 | 2   | 0       |
| 13  | 1.68767  | 2        | 57.0384 | 1   | 0       |
| 14  | 5.94247  | 2        | 63.1452 | 1   | 0       |
| 15  | 2.34247  | 2        | 62.0630 | 1   | 0       |
| 16  | 0.89863  | 2        | 56.5342 | 1   | 1       |
| 17  | 9.03288  | 1        | 22.9945 | 2   | 0       |
| 18  | 9.63014  | 1        | 18.4712 | 1   | 0       |
| 19  | 0.52603  | 2        | 41.2521 | 1   | 0       |
| 20  | 1.82192  | 2        | 29.5178 | 1   | 0       |

Maximum likelihood estimates of the model parameters shown in [Output 51.7.2](#) are displayed by default.

**Output 51.7.2** Maximum Likelihood Parameter Estimates

| The LIFEREG Procedure                              |    |          |                |                       |        |
|----------------------------------------------------|----|----------|----------------|-----------------------|--------|
| Bayesian Analysis                                  |    |          |                |                       |        |
| Analysis of Maximum Likelihood Parameter Estimates |    |          |                |                       |        |
| Parameter                                          | DF | Estimate | Standard Error | 95% Confidence Limits |        |
| Intercept                                          | 1  | 2.4402   | 0.3716         | 1.7119                | 3.1685 |
| age                                                | 1  | -0.0115  | 0.0070         | -0.0253               | 0.0023 |
| sex                                                | 1  | -0.1170  | 0.1978         | -0.5046               | 0.2707 |
| sex                                                | 2  | 0        | .              | .                     | .      |
| perform                                            | 1  | 0.2905   | 0.3222         | -0.3411               | 0.9220 |
| Scale                                              | 1  | 1.2537   | 0.0824         | 1.1021                | 1.4260 |
| Weibull Shape                                      | 1  | 0.7977   | 0.0524         | 0.7012                | 0.9073 |

Since no prior distributions for the regression coefficients were specified, the default uniform improper distributions shown in the “Uniform Prior for Regression Coefficients” table in [Output 51.7.3](#) are used. The specified gamma prior for the Weibull shape parameter is also shown in [Output 51.7.3](#).

**Output 51.7.3** Model Parameter Priors

```

The LIFEREG Procedure

Bayesian Analysis

Uniform Prior for Regression Coefficients

Parameter Prior
Intercept Constant
age Constant
sex1 Constant
perform Constant

Independent Prior Distributions for Model Parameters

Parameter Prior Distribution Hyperparameters
Weibull Shape Gamma Shape 0.001 Inverse Scale 0.001

```

Fit statistics, descriptive statistics, interval statistics, and the sample parameter correlation matrix for the posterior sample are displayed in the tables in **Output 51.7.4**. Since noninformative prior distributions for the regression coefficients were used, the mean and standard deviations of the posterior distributions for the model parameters are close to the maximum likelihood estimates and standard errors.

**Output 51.7.4** Posterior Sample Statistics

```

Fit Statistics

DIC (smaller is better) 875.251
pD (effective number of parameters) 4.984

The LIFEREG Procedure

Bayesian Analysis

Posterior Summaries

Parameter N Mean Standard Percentiles
 N Mean Deviation 25% 50% 75%
Intercept 10000 2.4668 0.3862 2.1989 2.4621 2.7256
age 10000 -0.0115 0.00733 -0.0163 -0.0115 -0.00652
sex1 10000 -0.1255 0.2004 -0.2584 -0.1247 0.00817
perform 10000 0.3304 0.3317 0.1071 0.3188 0.5470
WeibShape 10000 0.7834 0.0518 0.7481 0.7815 0.8178

```

**Output 51.7.4** *continued*

| Posterior Intervals |       |                     |         |              |         |
|---------------------|-------|---------------------|---------|--------------|---------|
| Parameter           | Alpha | Equal-Tail Interval |         | HPD Interval |         |
| Intercept           | 0.050 | 1.7279              | 3.2368  | 1.7234       | 3.2264  |
| age                 | 0.050 | -0.0260             | 0.00263 | -0.0261      | 0.00244 |
| sex1                | 0.050 | -0.5197             | 0.2676  | -0.5260      | 0.2583  |
| perform             | 0.050 | -0.2898             | 1.0072  | -0.3200      | 0.9726  |
| WeibShape           | 0.050 | 0.6846              | 0.8905  | 0.6805       | 0.8849  |

| Posterior Correlation Matrix |           |        |        |         |            |
|------------------------------|-----------|--------|--------|---------|------------|
| Parameter                    | Intercept | age    | sex1   | perform | Weib Shape |
| Intercept                    | 1.0000    | -.9018 | -.3099 | -.0888  | -.1140     |
| age                          | -.9018    | 1.0000 | -.0259 | -.0363  | 0.0493     |
| sex1                         | -.3099    | -.0259 | 1.0000 | 0.1248  | 0.0371     |
| perform                      | -.0888    | -.0363 | 0.1248 | 1.0000  | -.0355     |
| WeibShape                    | -.1140    | 0.0493 | 0.0371 | -.0355  | 1.0000     |

The default diagnostic statistics are displayed in [Output 51.7.5](#). See the section “[Assessing Markov Chain Convergence](#)” on page 139 for more details on Bayesian convergence diagnostics.

**Output 51.7.5** Convergence Diagnostics

| The LIFEREG Procedure      |         |         |         |         |
|----------------------------|---------|---------|---------|---------|
| Bayesian Analysis          |         |         |         |         |
| Posterior Autocorrelations |         |         |         |         |
| Parameter                  | Lag 1   | Lag 5   | Lag 10  | Lag 50  |
| Intercept                  | 0.0564  | 0.0030  | 0.0082  | 0.0234  |
| age                        | -0.0079 | -0.0184 | -0.0015 | 0.0239  |
| sex1                       | 0.6293  | 0.0700  | 0.0055  | -0.0199 |
| perform                    | 0.6514  | 0.0773  | 0.0397  | -0.0123 |
| WeibShape                  | 0.0719  | -0.0083 | -0.0062 | 0.0112  |

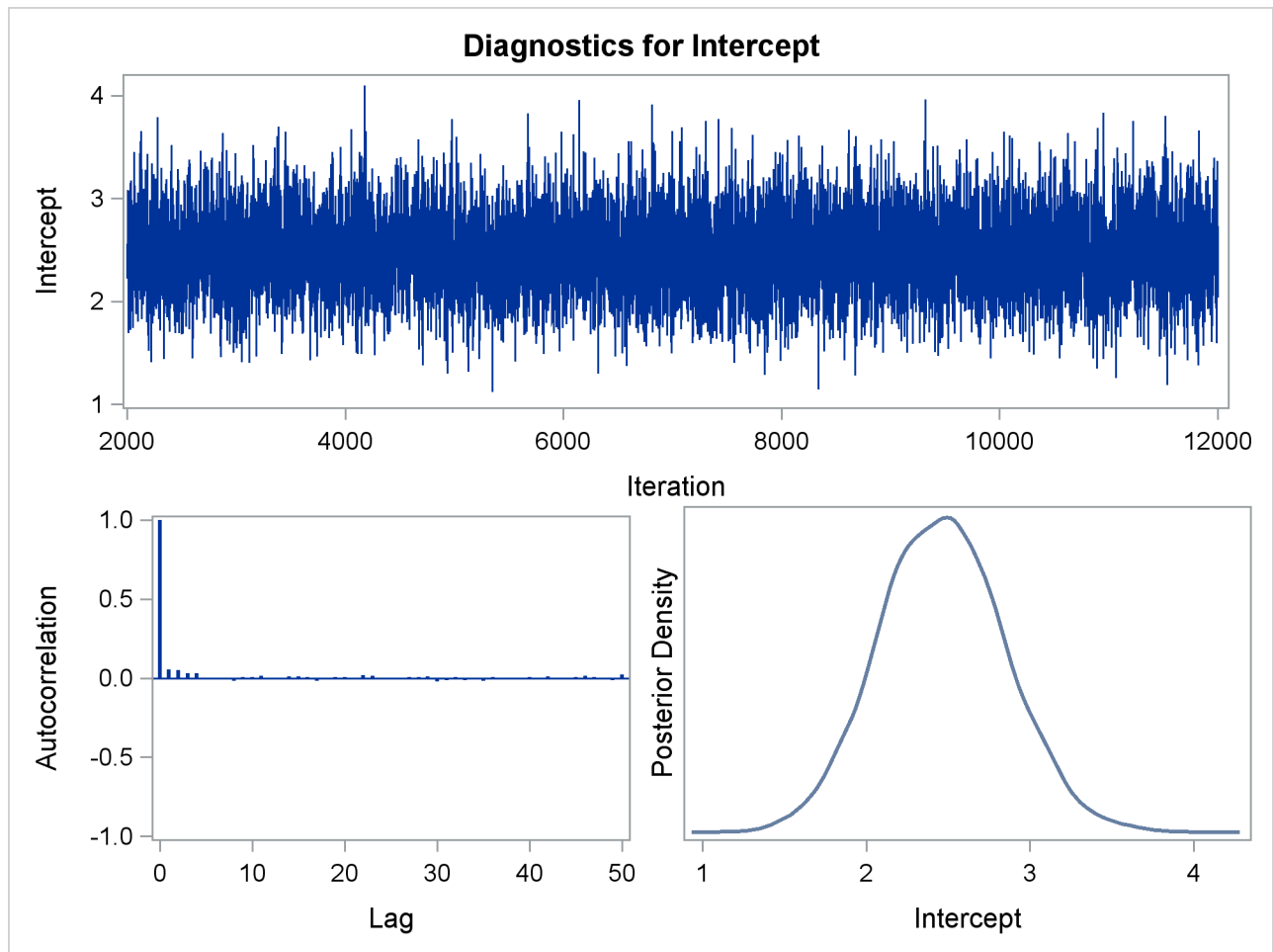
| Geweke Diagnostics |         |         |
|--------------------|---------|---------|
| Parameter          | z       | Pr >  z |
| Intercept          | 0.4962  | 0.6198  |
| age                | -0.4119 | 0.6804  |
| sex1               | -0.2519 | 0.8011  |
| perform            | -0.1049 | 0.9165  |
| WeibShape          | -0.6573 | 0.5110  |

**Output 51.7.5** *continued*

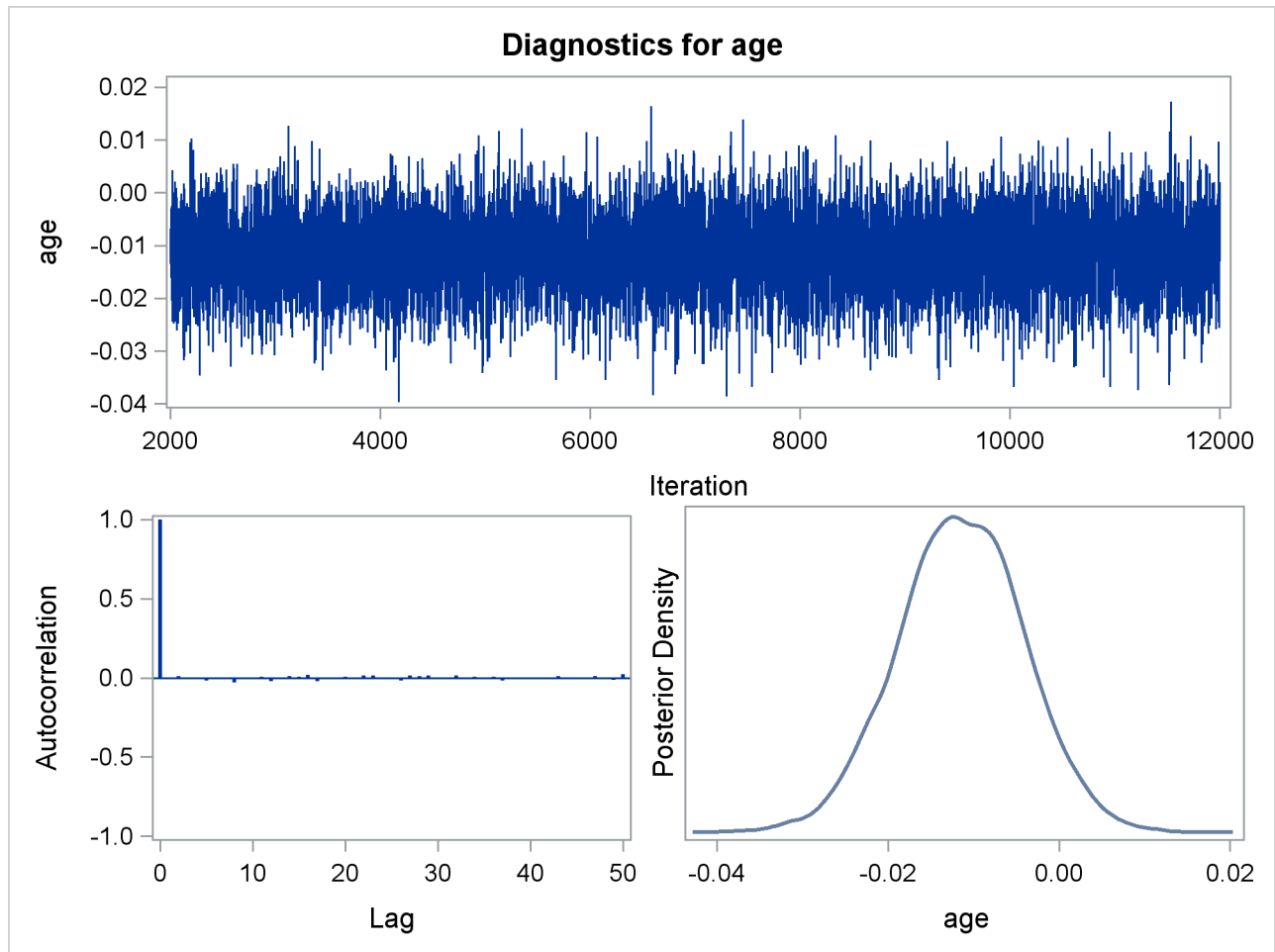
| Effective Sample Sizes |         |                 |            |
|------------------------|---------|-----------------|------------|
| Parameter              | ESS     | Autocorrelation |            |
|                        |         | Time            | Efficiency |
| Intercept              | 7476.1  | 1.3376          | 0.7476     |
| age                    | 10000.0 | 1.0000          | 1.0000     |
| sex1                   | 2482.1  | 4.0288          | 0.2482     |
| perform                | 2174.0  | 4.5998          | 0.2174     |
| WeibShape              | 8538.8  | 1.1711          | 0.8539     |

Trace, autocorrelation, and density plots for the seven model parameters are shown in [Output 51.7.6](#) through [Output 51.7.10](#). These plots show no indication that the Markov chains have not converged. See the sections “Assessing Markov Chain Convergence” on page 139 and “Visual Analysis via Trace Plots” on page 139 for more information about assessing the convergence of the chain of posterior samples.

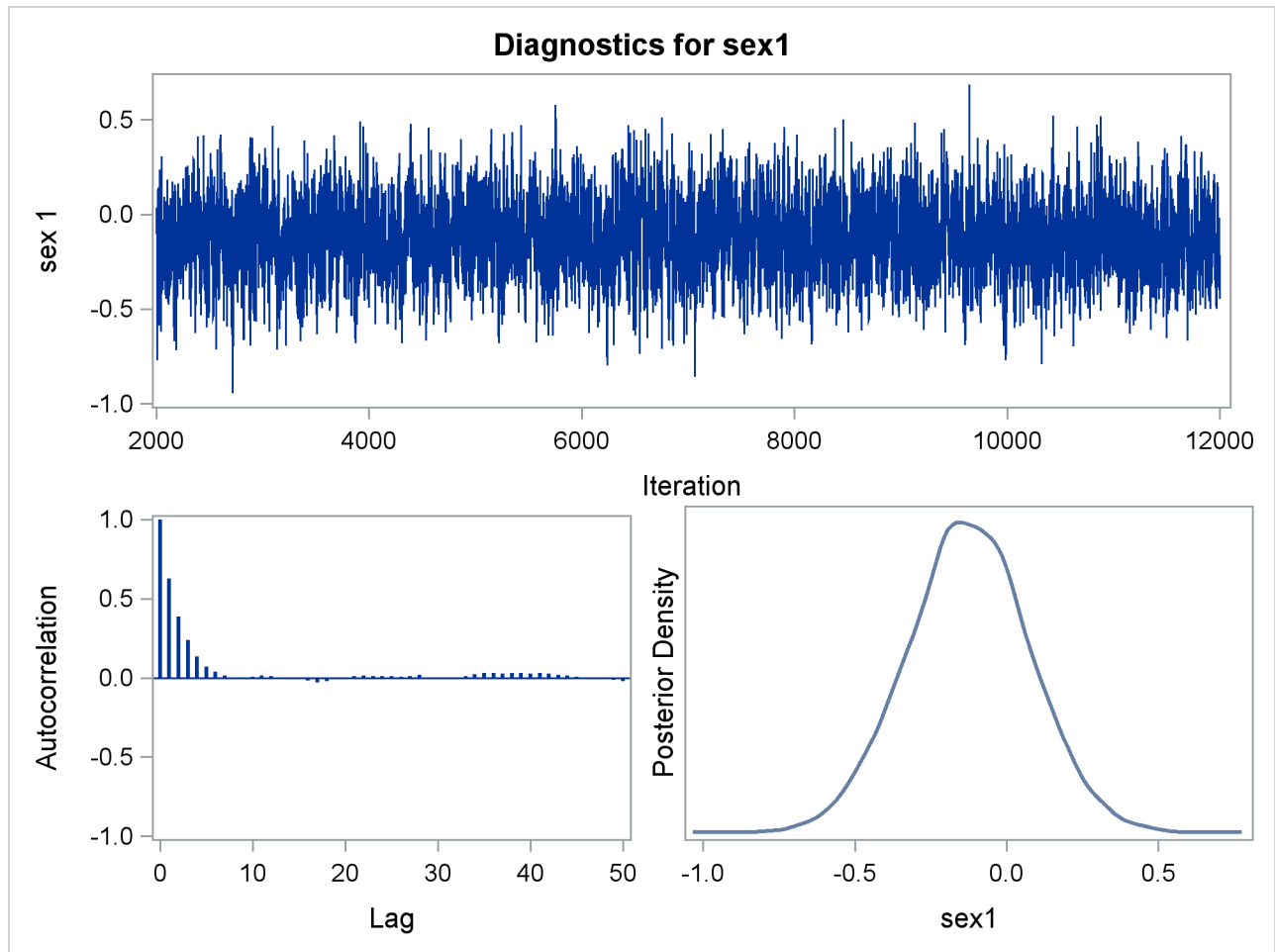
**Output 51.7.6** Diagnostic Plots



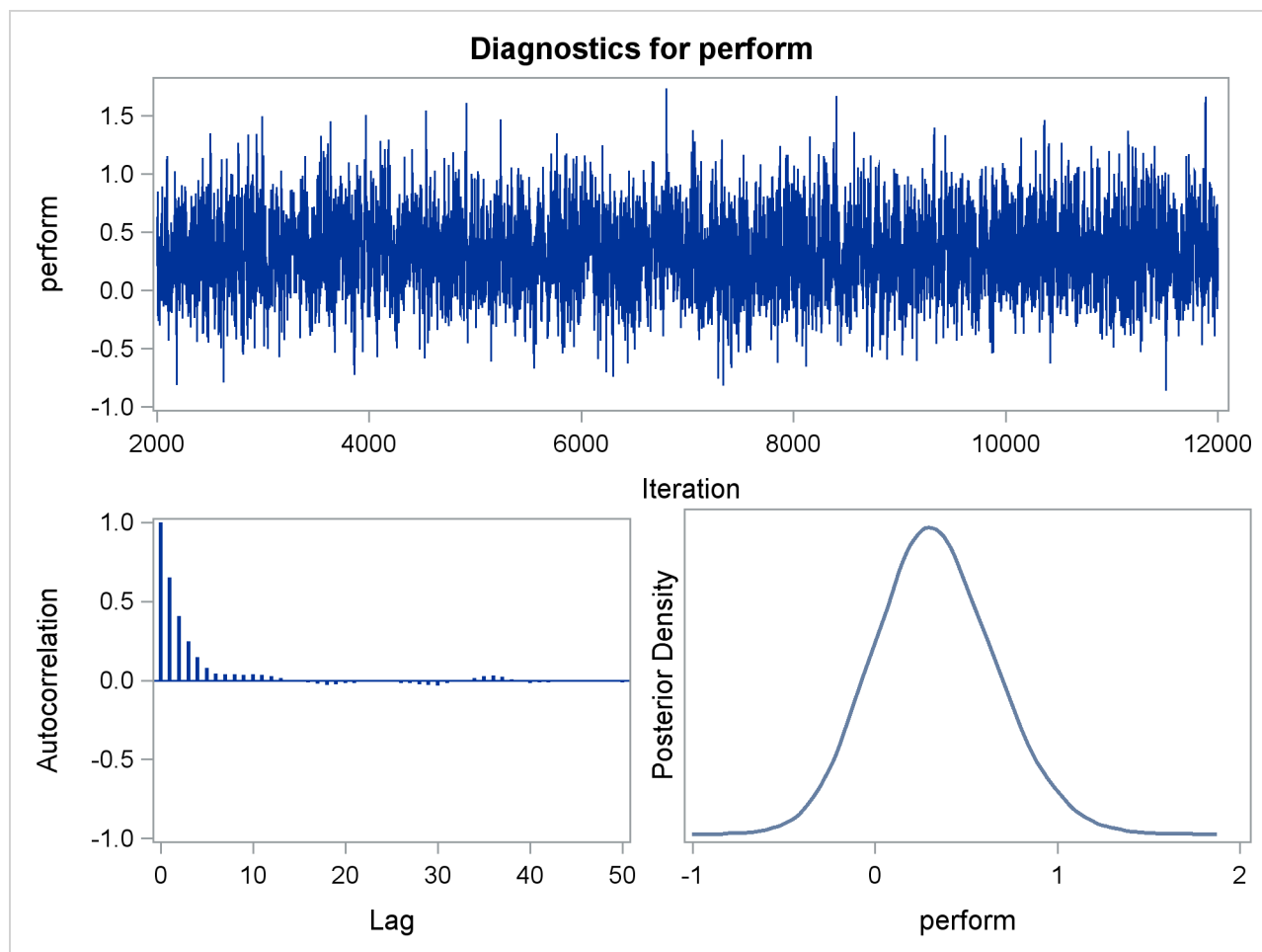
Output 51.7.7 Diagnostic Plots



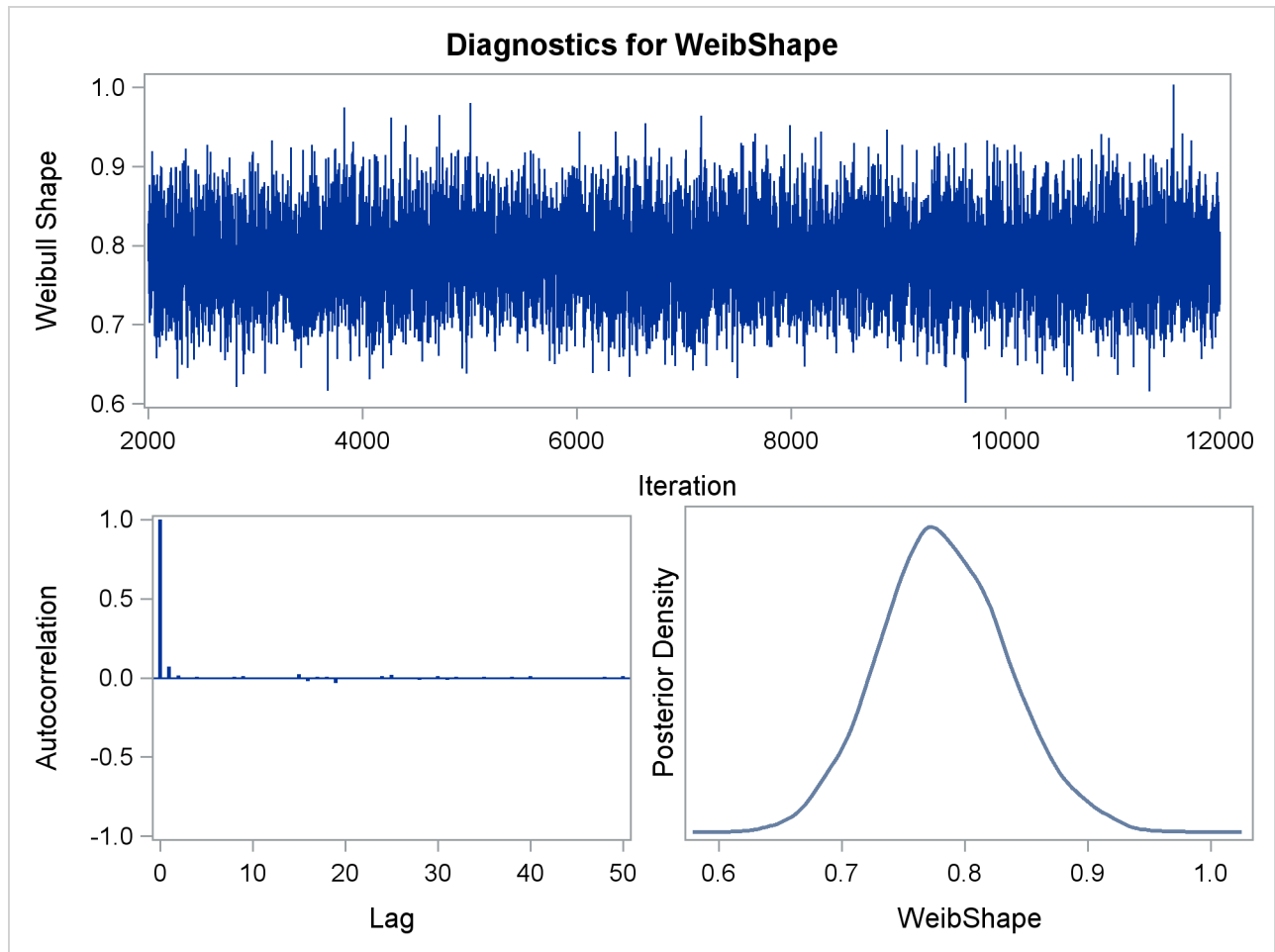
Output 51.7.8 Diagnostic Plots



Output 51.7.9 Diagnostic Plots



Output 51.7.10 Diagnostic Plots





## Example 51.8: Model Postfitting Analysis

PROC LIFEREG enables you to make model-based inferences. This example uses the larynx cancer data (Klein and Moeschberger 1997) to illustrate usage of the LSMEANS, LSMESTIMATE, and EFFECTPLOT statements for model postfitting analysis.

The survival time is modeled by a proportional odds model with two covariates: patient age and cancer stage (1, 2, 3, 4). The following statements use PROC LIFEREG to fit this model:

```
ods graphics on;

proc sort data=Larynx;
 by DESCENDING Stage;
run;

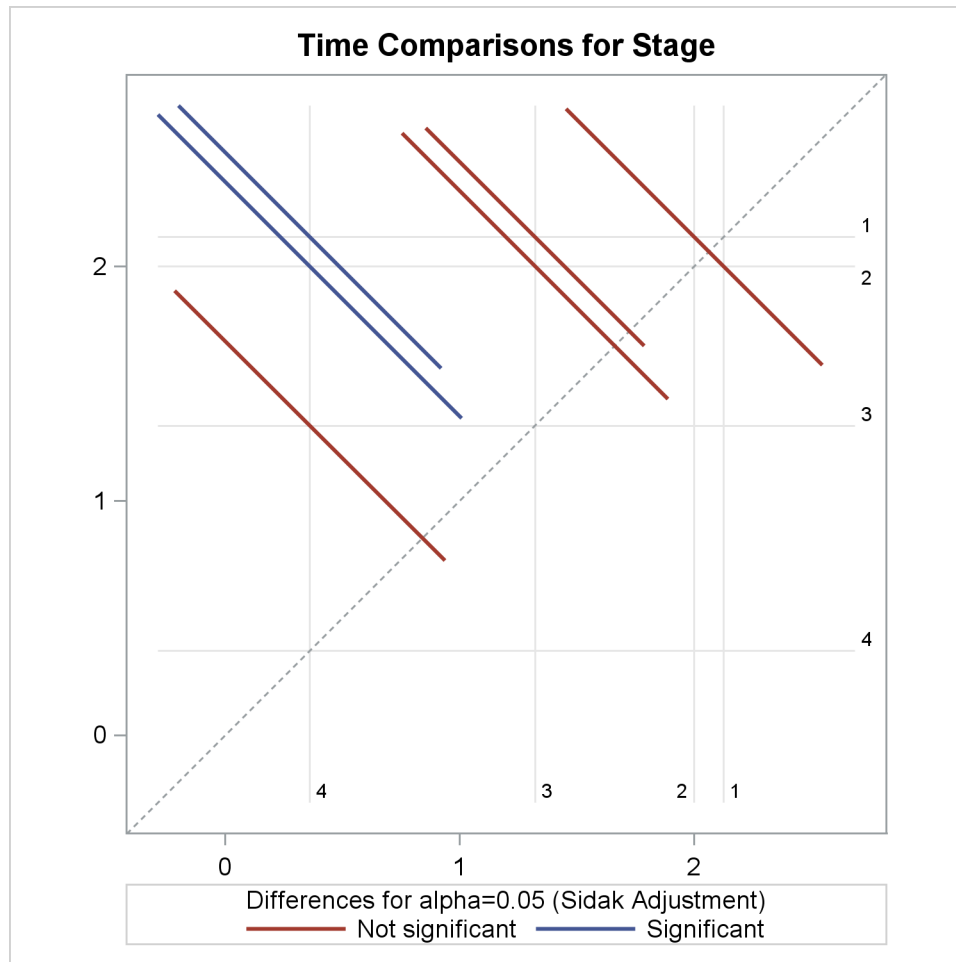
proc lifereg data=Larynx order=data;
 class Stage;
 model Time*Death(0) = Age Stage / dist = llogistic;
 lsmeans Stage / diff adjust=Sidak;
 effectplot / noobs;
run;
```

The LSMEANS statement compares pairwise differences in survival times among the four different cancer stages, while adjusting for age. The ADJUST=SIDAK option uses the Sidak method to control the overall Type I error rate of these comparisons. Results are displayed in [Output 51.8.1](#).

**Output 51.8.1** LS-Means Differences between Disease Stages

| The LIFEREG Procedure                      |        |          |                |         |         |        |
|--------------------------------------------|--------|----------|----------------|---------|---------|--------|
| Differences of Stage Least Squares Means   |        |          |                |         |         |        |
| Adjustment for Multiple Comparisons: Sidak |        |          |                |         |         |        |
| Stage                                      | _Stage | Estimate | Standard Error | z Value | Pr >  z | Adj P  |
| 4                                          | 3      | -0.9604  | 0.4379         | -2.19   | 0.0283  | 0.1581 |
| 4                                          | 2      | -1.6404  | 0.4931         | -3.33   | 0.0009  | 0.0053 |
| 4                                          | 1      | -1.7661  | 0.4257         | -4.15   | <.0001  | 0.0002 |
| 3                                          | 2      | -0.6800  | 0.4316         | -1.58   | 0.1151  | 0.5199 |
| 3                                          | 1      | -0.8057  | 0.3539         | -2.28   | 0.0228  | 0.1292 |
| 2                                          | 1      | -0.1257  | 0.4152         | -0.30   | 0.7621  | 0.9998 |

All the LS-means differences and their significance are displayed by the mean-mean scatter plot in [Output 51.8.2](#).

**Output 51.8.2** Plot of Pairwise LS-Means Differences

Suppose you want to jointly test whether the effects of stages 2, 3, and 4 are different from stage 1. The following LSMESTIMATE statement contrasts the LS-means of stages 2, 3, and 4 against the LS-means of stage 1:

```
proc lifereg data=Larynx order=data;
 class Stage year;
 model Time*Death(0) = Age Stage / dist = llogistic;
 lsmestimate Stage 'Stage 4 vs 1' 1 0 0 -1,
 'Stage 3 vs 1' 0 1 0 -1,
 'Stage 2 vs 1' 0 0 1 -1 / cl adjust=Sidak;
run;
```

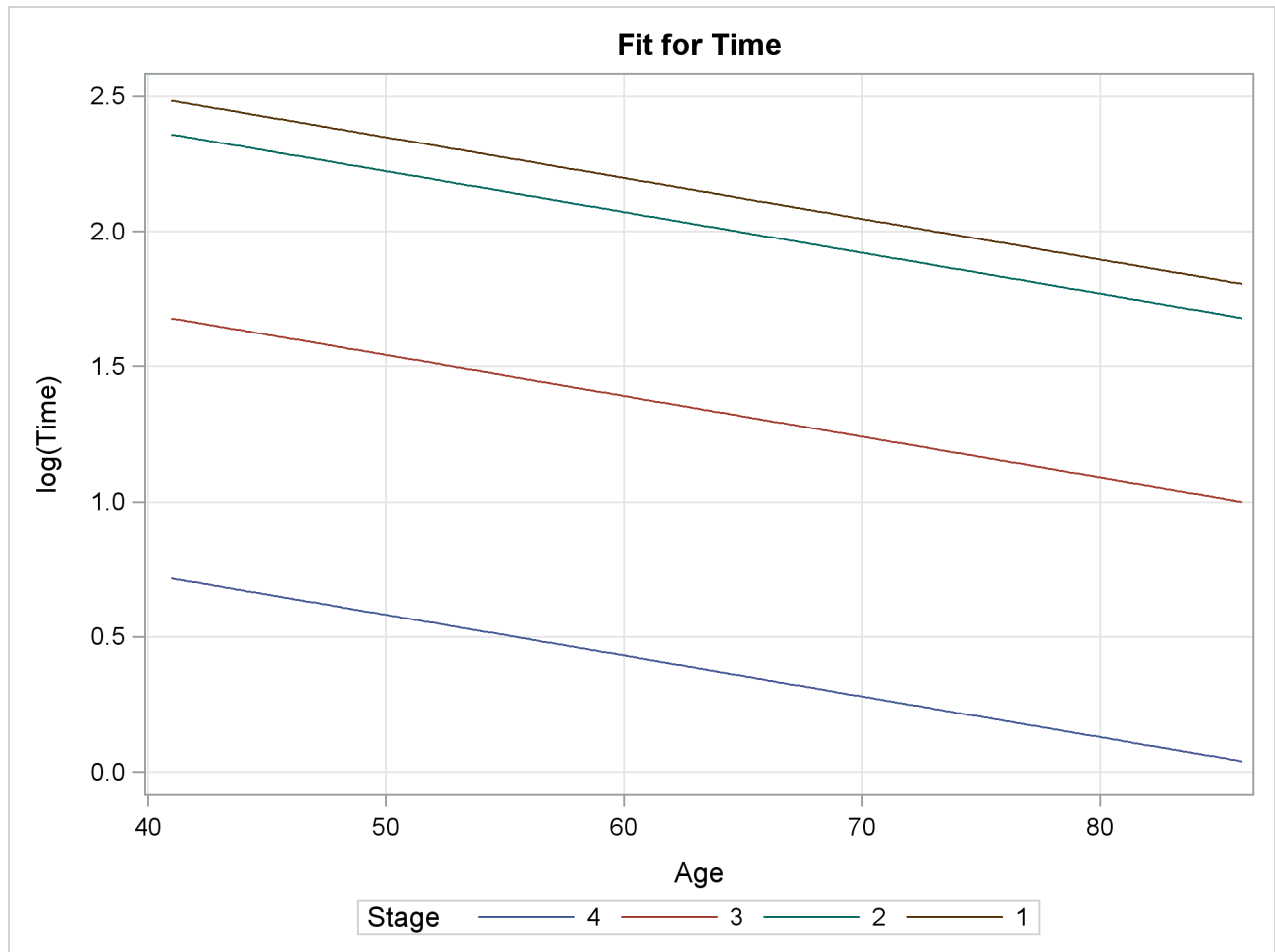
The CL option produces 95% confidence limits, including both unadjusted ones and those adjusted for multiple comparisons according to the ADJUST= option. Results are displayed in [Output 51.8.3](#).

**Output 51.8.3** Custom LS-Means Tests and Relative Odds

| The LIFEREG Procedure              |              |          |                |         |         |        |       |
|------------------------------------|--------------|----------|----------------|---------|---------|--------|-------|
| Least Squares Means Estimates      |              |          |                |         |         |        |       |
| Adjustment for Multiplicity: Sidak |              |          |                |         |         |        |       |
| Effect                             | Label        | Estimate | Standard Error | z Value | Pr >  z | Adj P  | Alpha |
|                                    |              |          |                |         |         |        |       |
| Stage                              | Stage 4 vs 1 | -1.7661  | 0.4257         | -4.15   | <.0001  | 0.0001 | 0.05  |
| Stage                              | Stage 3 vs 1 | -0.8057  | 0.3539         | -2.28   | 0.0228  | 0.0668 | 0.05  |
| Stage                              | Stage 2 vs 1 | -0.1257  | 0.4152         | -0.30   | 0.7621  | 0.9865 | 0.05  |
| Least Squares Means Estimates      |              |          |                |         |         |        |       |
| Adjustment for Multiplicity: Sidak |              |          |                |         |         |        |       |
| Effect                             | Label        | Lower    | Upper          | Adj     |         |        |       |
|                                    |              |          |                | Lower   | Upper   |        |       |
| Stage                              | Stage 4 vs 1 | -2.6004  | -0.9319        | -2.7825 | -0.7498 |        |       |
| Stage                              | Stage 3 vs 1 | -1.4993  | -0.1122        | -1.6507 | 0.03921 |        |       |
| Stage                              | Stage 2 vs 1 | -0.9395  | 0.6881         | -1.1171 | 0.8657  |        |       |

As displayed in [Output 51.8.4](#), the EFFECTPLOT statement generates a plot of age effects on survival time on a natural logarithm scale by four disease stages.

Output 51.8.4 Age Effects by Disease Stages



You can also perform the preceding analysis for a Bayesian model. The following statements generate posterior samples from a Bayesian model and request an LS-means analysis to compare the stage effects:

```
proc lifereg data=Larynx order=data;
 class Stage;
 model Time*Death(0) = Age Stage / dist = llogistic;
 bayes seed=100 nmc=500 nbi=500 diagnostic=none outpost=000;
 lsmeans Stage / diff exp;
 lsmestimate Stage 'Stage 4 vs 1' 1 0 0 -1,
 'Stage 3 vs 1' 0 1 0 -1,
 'Stage 2 vs 1' 0 0 1 -1
 / cl plots=boxplot(orient=horizontal);
run;
```

Because no prior distributions for the regression coefficients were specified, the default uniform improper distributions shown in the “Uniform Prior for Regression Coefficients” table in [Output 51.8.5](#) are used. The specified gamma prior for the scale parameter is also shown in [Output 51.8.5](#).

**Output 51.8.5** Model Parameter Priors

| The LIFEREG Procedure                                |                    |                 |       |               |       |
|------------------------------------------------------|--------------------|-----------------|-------|---------------|-------|
| Bayesian Analysis                                    |                    |                 |       |               |       |
| Uniform Prior for Regression Coefficients            |                    |                 |       |               |       |
| Parameter                                            |                    | Prior           |       |               |       |
| Intercept                                            |                    | Constant        |       |               |       |
| Age                                                  |                    | Constant        |       |               |       |
| Stage4                                               |                    | Constant        |       |               |       |
| Stage3                                               |                    | Constant        |       |               |       |
| Stage2                                               |                    | Constant        |       |               |       |
| Independent Prior Distributions for Model Parameters |                    |                 |       |               |       |
| Parameter                                            | Prior Distribution | Hyperparameters |       |               |       |
| Scale                                                | Gamma              | Shape           | 0.001 | Inverse Scale | 0.001 |

Under the Bayesian framework, the LS-means differences are treated as random variables for which posterior samples are readily available according to the linear relationship of LS-means and the regression coefficients. [Output 51.8.6](#) lists the sample mean, standard deviation, and percentiles for each LS-means difference.

**Output 51.8.6** LS-Means Differences between Disease Stages

| Sample Differences of Stage Least Squares Means |        |     |          |                    |                       |         |         |
|-------------------------------------------------|--------|-----|----------|--------------------|-----------------------|---------|---------|
| Stage                                           | _Stage | N   | Estimate | Standard Deviation | -----Percentiles----- |         |         |
|                                                 |        |     |          |                    | 25th                  | 50th    | 75th    |
| 4                                               | 3      | 500 | -0.9307  | 0.4752             | -1.2743               | -0.9446 | -0.6086 |
| 4                                               | 2      | 500 | -1.6591  | 0.5327             | -2.0161               | -1.6573 | -1.2861 |
| 4                                               | 1      | 500 | -1.8001  | 0.4321             | -2.0951               | -1.7943 | -1.5491 |
| 3                                               | 2      | 500 | -0.7284  | 0.4828             | -1.0488               | -0.7219 | -0.3975 |
| 3                                               | 1      | 500 | -0.8694  | 0.3727             | -1.1199               | -0.8541 | -0.6149 |
| 2                                               | 1      | 500 | -0.1410  | 0.4413             | -0.4126               | -0.1417 | 0.1363  |

| Sample Differences of Stage Least Squares Means |        |               |                                 |                                         |        |        |  |
|-------------------------------------------------|--------|---------------|---------------------------------|-----------------------------------------|--------|--------|--|
| Stage                                           | _Stage | Exponentiated | Standard Error of Exponentiated | -----Percentiles for Exponentiated----- |        |        |  |
|                                                 |        |               |                                 | 25th                                    | 50th   | 75th   |  |
| 4                                               | 3      | 0.4426        | 0.232690                        | 0.2796                                  | 0.3888 | 0.5441 |  |
| 4                                               | 2      | 0.2181        | 0.115808                        | 0.1332                                  | 0.1907 | 0.2763 |  |
| 4                                               | 1      | 0.1815        | 0.082975                        | 0.1231                                  | 0.1663 | 0.2124 |  |
| 3                                               | 2      | 0.5410        | 0.268735                        | 0.3504                                  | 0.4858 | 0.6720 |  |
| 3                                               | 1      | 0.4488        | 0.168055                        | 0.3263                                  | 0.4257 | 0.5407 |  |
| 2                                               | 1      | 0.9585        | 0.462376                        | 0.6619                                  | 0.8679 | 1.1461 |  |

The LSMESTIMATE statement produces summary statistics of the posterior samples for the specified LS-means contrasts. Results are presented in [Output 51.8.7](#); they are very similar to the results based on maximum likelihood in [Output 51.8.3](#).

**Output 51.8.7** Summary Statistics of Custom LS-Means Differences

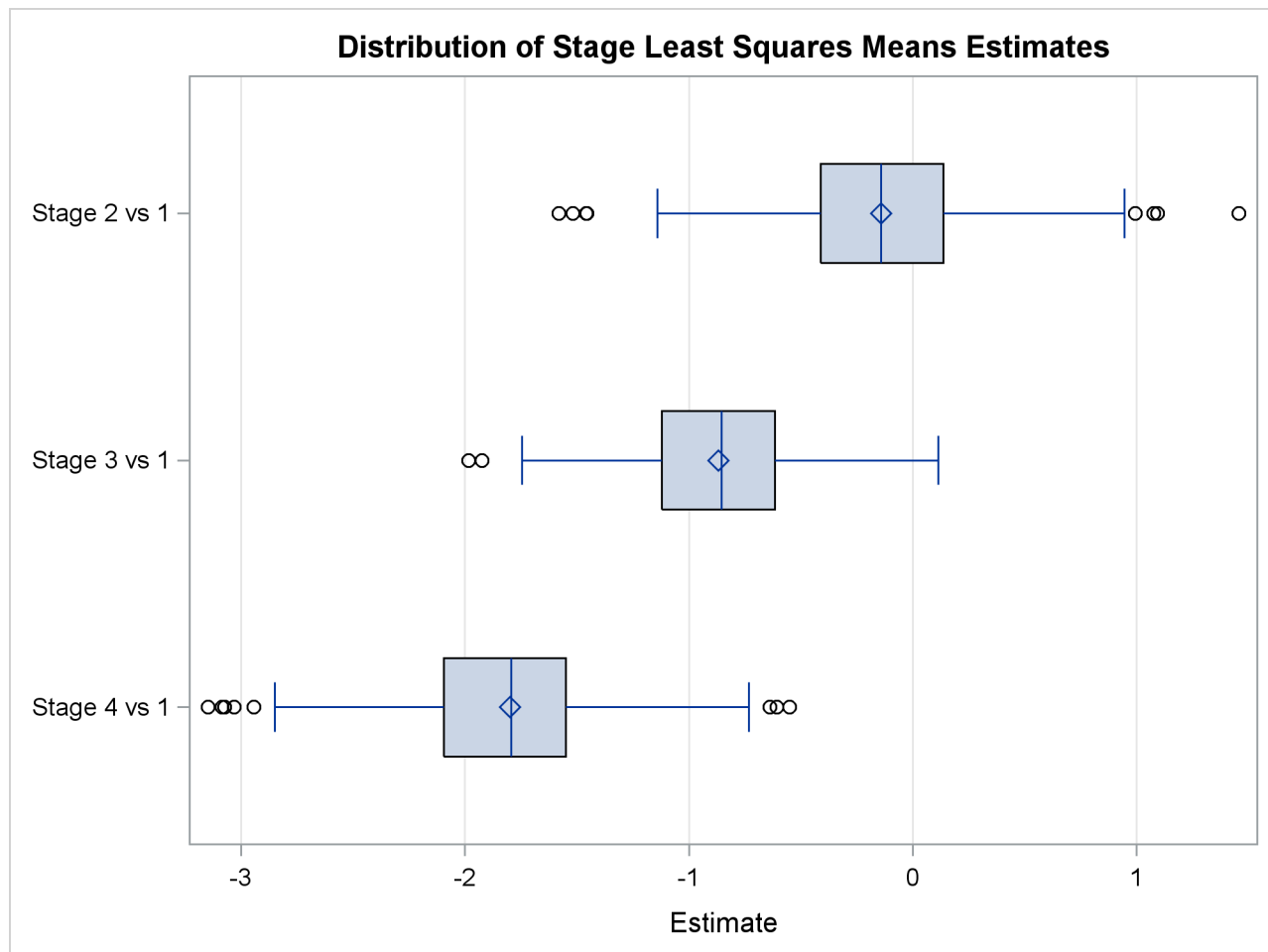
| Sample Least Squares Means Estimates |              |     |          |                    |                       |         |         |
|--------------------------------------|--------------|-----|----------|--------------------|-----------------------|---------|---------|
| Effect                               | Label        | N   | Estimate | Standard Deviation | -----Percentiles----- |         |         |
|                                      |              |     |          |                    | 25th                  | 50th    | 75th    |
| Stage                                | Stage 4 vs 1 | 500 | -1.8001  | 0.4321             | -2.0951               | -1.7943 | -1.5491 |
| Stage                                | Stage 3 vs 1 | 500 | -0.8694  | 0.3727             | -1.1199               | -0.8541 | -0.6149 |
| Stage                                | Stage 2 vs 1 | 500 | -0.1410  | 0.4413             | -0.4126               | -0.1417 | 0.1363  |

| Sample Least Squares Means Estimates |              |       |           |           |
|--------------------------------------|--------------|-------|-----------|-----------|
| Effect                               | Label        | Alpha | Lower HPD | Upper HPD |
| Stage                                | Stage 4 vs 1 | 0.05  | -2.6279   | -0.8897   |
| Stage                                | Stage 3 vs 1 | 0.05  | -1.6033   | -0.2031   |
| Stage                                | Stage 2 vs 1 | 0.05  | -1.1401   | 0.6252    |

The PLOTS= option uses ODS Graphics to display the Bayesian samples. A box plot is presented in Output 51.8.8.

**Output 51.8.8** Box Plot of Sampled LS-Means Differences



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# Chapter 52

## The LIFETEST Procedure

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## Overview: LIFETEST Procedure

A common feature of lifetime or survival data is the presence of right-censored observations due either to withdrawal of experimental units or to termination of the experiment. For such observations, you know only that the lifetime exceeded a given value; the exact lifetime remains unknown. Such data cannot be analyzed by ignoring the censored observations because, among other considerations, the longer-lived units are generally more likely to be censored. The analysis methodology must correctly use the censored observations in addition to the uncensored observations.

Texts that discuss the survival analysis methodology include Collett (1994), Cox and Oakes (1984); Kalbfleisch and Prentice (1980); Klein and Moeschberger (1997); Lawless (1982); Lee (1992). Users interested in the theory should consult Fleming and Harrington (1991); Andersen et al. (1992).

Usually, a first step in the analysis of survival data is the estimation of the distribution of the survival times. Survival times are often called *failure* times, and *event* times are uncensored survival times. The survival distribution function (SDF), also known as the survivor function, is used to describe the lifetimes of the population of interest. The SDF evaluated at  $t$  is the probability that an experimental unit from the population will have a lifetime that exceeds  $t$ —that is,

$$S(t) = \Pr(T > t)$$

where  $S(t)$  denotes the survivor function and  $T$  is the lifetime of a randomly selected experimental unit. The LIFETEST procedure can be used to compute nonparametric estimates of the survivor function either by the product-limit method (also called the Kaplan-Meier method) or by the life-table method (also called the actuarial method). The life-table estimator is a grouped-data analog of the Kaplan-Meier estimator. The procedure can also compute the Breslow estimator or the Fleming-Harrington estimator, which are asymptotic equivalent alternatives to the Kaplan-Meier estimator.

Some functions closely related to the SDF are the cumulative distribution function (CDF), the probability density function (PDF), and the hazard function. The CDF, denoted  $F(t)$ , is defined as  $1 - S(t)$  and is the probability that a lifetime does not exceed  $t$ . The PDF, denoted  $f(t)$ , is defined as the derivative of  $F(t)$ , and the hazard function, denoted  $h(t)$ , is defined as  $f(t)/S(t)$ . If the life-table method is chosen, the estimates of the probability density function can also be computed. Plots of these estimates can be produced by a graphical or line printer device, or based on the output delivery system (ODS).

An important task in the analysis of survival data is the comparison of survival curves. It is of interest to determine whether the underlying populations of  $k$  ( $k \geq 2$ ) samples have identical survivor functions. PROC LIFETEST provides nonparametric  $k$ -sample tests based on weighted comparisons of the estimated hazard rate of the individual population under the null and alternative hypotheses. Corresponding to various weight functions, a variety of tests can be specified, which include the log-rank test, Wilcoxon test, Tarone-Ware test, Peto-Peto test, modified Peto-Peto test, and Fleming-Harrington  $G_\rho$  family of tests. PROC LIFETEST also provides corresponding trend tests to detect ordered alternatives. Stratified tests can be specified to adjust for prognostic factors that affect the events rates in the various populations. A likelihood ratio test, based on an underlying exponential model, is also included to compare the survival curves of the samples.

There are other prognostic variables, called covariates, that are thought to be related to the failure time. These covariates can also be used to construct statistics to test for association between the covariates and the lifetime variable. PROC LIFETEST can compute two such test statistics: censored data linear rank statistics based on the exponential scores and the Wilcoxon scores. The corresponding tests are known as the log-rank test and the Wilcoxon test, respectively. These tests are computed by pooling over any defined strata, thus adjusting for the stratum variables.

One change in SAS 9.2 and later is that the calculation of confidence limits for the quartiles of survival time is based on the transformation specified by the `CONFTYPE=` option. Another change is that the SURVIVAL statement in SAS 9.1 is folded into the PROC LIFETEST statement; that is, options that were in the SURVIVAL statement can now be specified in the PROC LIFETEST statement. The SURVIVAL statement is no longer needed and it is not documented.

---

## Getting Started: LIFETEST Procedure

You can use the LIFETEST procedure to compute nonparametric estimates of the survivor functions, to compare survival curves, and to compute rank tests for association of the failure time variable with covariates.

For simple analyses, only the PROC LIFETEST and TIME statements are required. Consider a sample of survival data. Suppose that the time variable is T and the censoring variable is C with value 1 indicating censored observations. The following statements compute the product-limit estimate for the sample:

```
proc lifetest;
 time t*c(1);
run;
```

You can use the STRATA statement to divide the data into various strata. A separate survivor function is then estimated for each stratum, and tests of the homogeneity of strata are performed. However, if the GROUP= option is also specified in the STRATA statement, the GROUP= variable is used to identify the samples whose survivor functions are to be compared, and the STRATA variables are used to define the strata for the stratified tests. You can specify covariates (prognostic variables) in the TEST statement, and PROC LIFETEST computes linear rank statistics to test the effects of these covariates on survival.

For example, consider the results of a small randomized trial on rats. Suppose you randomize 40 rats that have been exposed to a carcinogen into two treatment groups (Drug X and Placebo). The event of interest is death from cancer induced by the carcinogen. The response is the time from randomization to death. Four rats died of other causes; their survival times are regarded as censored observations. Interest lies in whether the survival distributions differ between the two treatments.

The following DATA step creates the data set Exposed, which contains four variables: Days (survival time in days from treatment to death), Status (censoring indicator variable: 0 if censored and 1 if not censored), Treatment (treatment indicator), and Sex (gender: F if female and M if male).

```

proc format;
 value Rx 1='Drug X' 0='Placebo';
run;
data exposed;
 input Days Status Treatment Sex $ @@;
 format Treatment Rx.;
 datalines;
179 1 1 F 378 0 1 M
256 1 1 F 355 1 1 M
262 1 1 M 319 1 1 M
256 1 1 F 256 1 1 M
255 1 1 M 171 1 1 F
224 0 1 F 325 1 1 M
225 1 1 F 325 1 1 M
287 1 1 M 217 1 1 F
319 1 1 M 255 1 1 F
264 1 1 M 256 1 1 F
237 0 0 F 291 1 0 M
156 1 0 F 323 1 0 M
270 1 0 M 253 1 0 M
257 1 0 M 206 1 0 F
242 1 0 M 206 1 0 F
157 1 0 F 237 1 0 M
249 1 0 M 211 1 0 F
180 1 0 F 229 1 0 F
226 1 0 F 234 1 0 F
268 0 0 M 209 1 0 F
;

```

PROC LIFETEST is invoked as follows to compute the product-limit estimate of the survivor function for each treatment and to compare the survivor functions between the two treatments:

```

ods graphics on;
proc lifetest data=Exposed plots=(survival(atrisk) logsurv);
 time Days*Status(0);
 strata Treatment;
run;
ods graphics off;

```

In the TIME statement, the survival time variable, Days, is crossed with the censoring variable, Status, with the value 0 indicating censoring. That is, the values of Days are considered censored if the corresponding values of Status are 0; otherwise, they are considered as event times. In the STRATA statement, the variable Treatment is specified, which indicates that the data are to be divided into strata based on the values of Treatment. ODS Graphics must be enabled before producing graphs. Two plots are requested through the PLOTS= option—a plot of the survival curves with at risk numbers and a plot of the negative log of the survival curves.

The results of the analysis are displayed in the following figures.

Figure 52.1 displays the product-limit survival estimate for the Drug X group (Treatment=1). The figure lists, for each observed time, the survival estimate, failure rate, standard error of the estimate, cumulative number of failures, and number of subjects remaining in the study.

**Figure 52.1** Survivor Function Estimate for the Drug X-Treated Rats

| The LIFETEST Procedure           |          |         |                               |                  |                |
|----------------------------------|----------|---------|-------------------------------|------------------|----------------|
| Stratum 1: Treatment = Drug X    |          |         |                               |                  |                |
| Product-Limit Survival Estimates |          |         |                               |                  |                |
| Days                             | Survival | Failure | Survival<br>Standard<br>Error | Number<br>Failed | Number<br>Left |
| 0.000                            | 1.0000   | 0       | 0                             | 0                | 20             |
| 171.000                          | 0.9500   | 0.0500  | 0.0487                        | 1                | 19             |
| 179.000                          | 0.9000   | 0.1000  | 0.0671                        | 2                | 18             |
| 217.000                          | 0.8500   | 0.1500  | 0.0798                        | 3                | 17             |
| 224.000*                         | .        | .       | .                             | 3                | 16             |
| 225.000                          | 0.7969   | 0.2031  | 0.0908                        | 4                | 15             |
| 255.000                          | .        | .       | .                             | 5                | 14             |
| 255.000                          | 0.6906   | 0.3094  | 0.1053                        | 6                | 13             |
| 256.000                          | .        | .       | .                             | 7                | 12             |
| 256.000                          | .        | .       | .                             | 8                | 11             |
| 256.000                          | .        | .       | .                             | 9                | 10             |
| 256.000                          | 0.4781   | 0.5219  | 0.1146                        | 10               | 9              |
| 262.000                          | 0.4250   | 0.5750  | 0.1135                        | 11               | 8              |
| 264.000                          | 0.3719   | 0.6281  | 0.1111                        | 12               | 7              |
| 287.000                          | 0.3187   | 0.6813  | 0.1071                        | 13               | 6              |
| 319.000                          | .        | .       | .                             | 14               | 5              |
| 319.000                          | 0.2125   | 0.7875  | 0.0942                        | 15               | 4              |
| 325.000                          | .        | .       | .                             | 16               | 3              |
| 325.000                          | 0.1062   | 0.8938  | 0.0710                        | 17               | 2              |
| 355.000                          | 0.0531   | 0.9469  | 0.0517                        | 18               | 1              |
| 378.000*                         | 0.0531   | .       | .                             | 18               | 0              |

NOTE: The marked survival times are censored observations.

Figure 52.2 displays summary statistics of survival times for the Drug X group. It contains estimates of the 25th, 50th, and 75th percentiles and the corresponding 95% confidence limits. The median survival time for rats in this treatment is 256 days. The mean and standard error are also displayed; however, these values are underestimated because the largest observed time is censored and the estimation is restricted to the largest event time.

**Figure 52.2** Summary Statistics of Survival Times for Drug X-Treated Rats

| Quartile Estimates |                   |                         |         |         |
|--------------------|-------------------|-------------------------|---------|---------|
| Percent            | Point<br>Estimate | 95% Confidence Interval |         |         |
|                    |                   | Transform               | [Lower  | Upper)  |
| 75                 | 319.000           | LOGLOG                  | 256.000 | 355.000 |
| 50                 | 256.000           | LOGLOG                  | 255.000 | 319.000 |
| 25                 | 255.000           | LOGLOG                  | 171.000 | 256.000 |

**Figure 52.2** *continued*

| Mean    | Standard Error |
|---------|----------------|
| 271.131 | 11.877         |

NOTE: The mean survival time and its standard error were underestimated because the largest observation was censored and the estimation was restricted to the largest event time.

Figure 52.3 and Figure 52.4 display the survival estimates and the summary statistics of the survival times for Placebo (Treatment=0). The median survival time for rats in this treatment is 235 days.

**Figure 52.3** Survivor Function Estimate for Placebo-Treated Rats

The LIFETEST Procedure

Stratum 2: Treatment = Placebo

Product-Limit Survival Estimates

| Days     | Survival | Failure | Survival Standard Error | Number Failed | Number Left |
|----------|----------|---------|-------------------------|---------------|-------------|
| 0.000    | 1.0000   | 0       | 0                       | 0             | 20          |
| 156.000  | 0.9500   | 0.0500  | 0.0487                  | 1             | 19          |
| 157.000  | 0.9000   | 0.1000  | 0.0671                  | 2             | 18          |
| 180.000  | 0.8500   | 0.1500  | 0.0798                  | 3             | 17          |
| 206.000  | .        | .       | .                       | 4             | 16          |
| 206.000  | 0.7500   | 0.2500  | 0.0968                  | 5             | 15          |
| 209.000  | 0.7000   | 0.3000  | 0.1025                  | 6             | 14          |
| 211.000  | 0.6500   | 0.3500  | 0.1067                  | 7             | 13          |
| 226.000  | 0.6000   | 0.4000  | 0.1095                  | 8             | 12          |
| 229.000  | 0.5500   | 0.4500  | 0.1112                  | 9             | 11          |
| 234.000  | 0.5000   | 0.5000  | 0.1118                  | 10            | 10          |
| 237.000  | 0.4500   | 0.5500  | 0.1112                  | 11            | 9           |
| 237.000* | .        | .       | .                       | 11            | 8           |
| 242.000  | 0.3938   | 0.6063  | 0.1106                  | 12            | 7           |
| 249.000  | 0.3375   | 0.6625  | 0.1082                  | 13            | 6           |
| 253.000  | 0.2813   | 0.7188  | 0.1038                  | 14            | 5           |
| 257.000  | 0.2250   | 0.7750  | 0.0971                  | 15            | 4           |
| 268.000* | .        | .       | .                       | 15            | 3           |
| 270.000  | 0.1500   | 0.8500  | 0.0891                  | 16            | 2           |
| 291.000  | 0.0750   | 0.9250  | 0.0693                  | 17            | 1           |
| 323.000  | 0        | 1.0000  | .                       | 18            | 0           |

NOTE: The marked survival times are censored observations.

**Figure 52.4** Summary Statistics of Survival Times for Placebo-Treated Rats

| Quartile Estimates |                |                                   |         |         |
|--------------------|----------------|-----------------------------------|---------|---------|
| Percent            | Point Estimate | 95% Confidence Interval Transform | [Lower  | Upper)  |
| 75                 | 257.000        | LOGLOG                            | 237.000 | 323.000 |
| 50                 | 235.500        | LOGLOG                            | 206.000 | 253.000 |
| 25                 | 207.500        | LOGLOG                            | 156.000 | 229.000 |
| Mean               |                | Standard Error                    |         |         |
| 235.156            |                | 10.211                            |         |         |

A summary of the number of censored and event observations is shown in [Figure 52.5](#). The figure lists, for each stratum, the number of event and censored observations, and the percentage of censored observations.

**Figure 52.5** Number of Event and Censored Observations

| Summary of the Number of Censored and Uncensored Values |           |       |        |          |                  |
|---------------------------------------------------------|-----------|-------|--------|----------|------------------|
| Stratum                                                 | Treatment | Total | Failed | Censored | Percent Censored |
| 1                                                       | Drug X    | 20    | 18     | 2        | 10.00            |
| 2                                                       | Placebo   | 20    | 18     | 2        | 10.00            |
| -----                                                   |           |       |        |          |                  |
| Total                                                   |           | 40    | 36     | 4        | 10.00            |

[Figure 52.6](#) displays the graph of the product-limit survivor function estimates versus survival time. The two treatments differ primarily at larger survival times. Note the number of subjects at risk in the plot. You can display the number of subjects at risk at specific time points by using the `ATRISK=` option.



**Figure 52.6** Plot of Estimated Survivor Functions

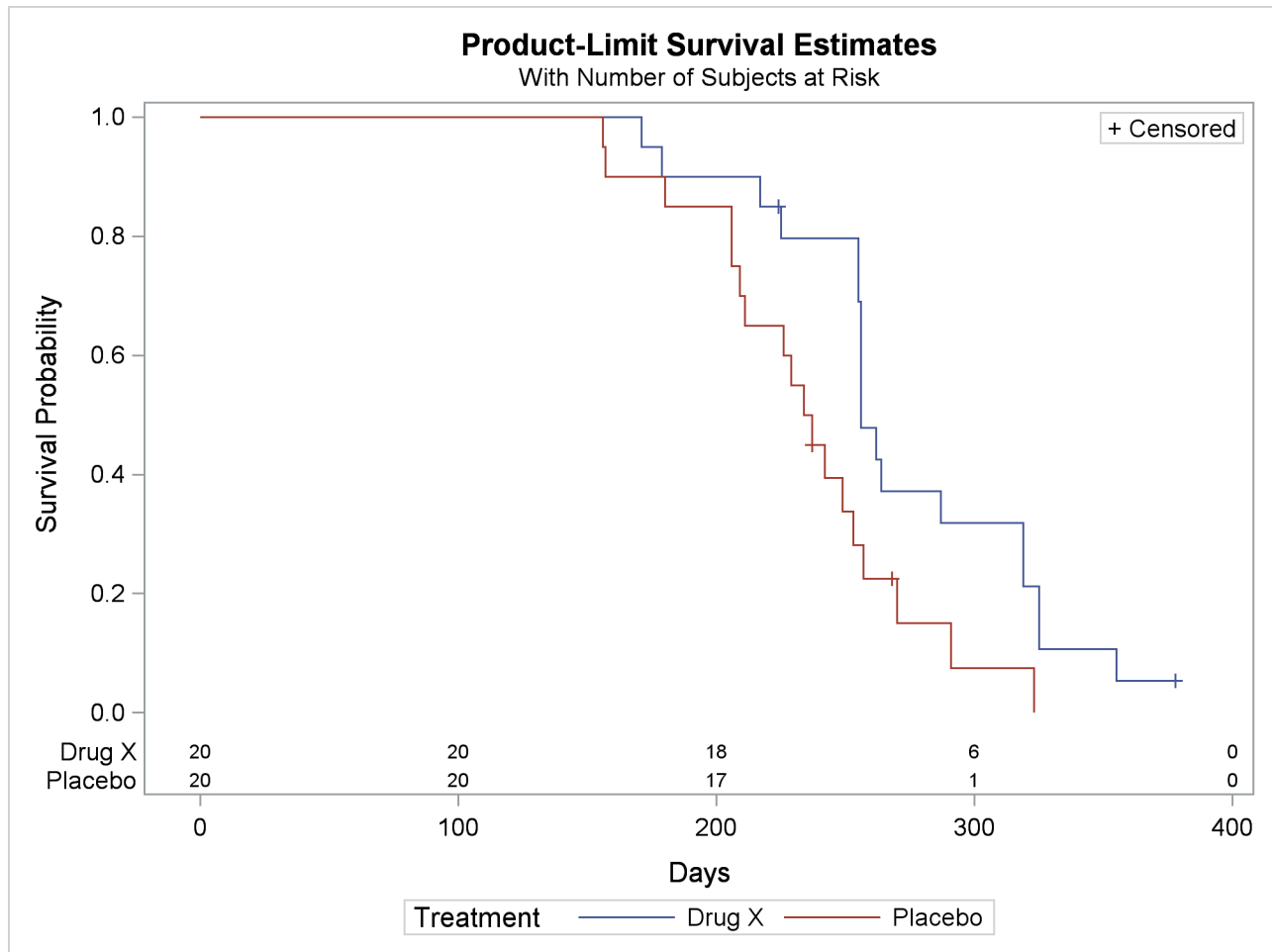
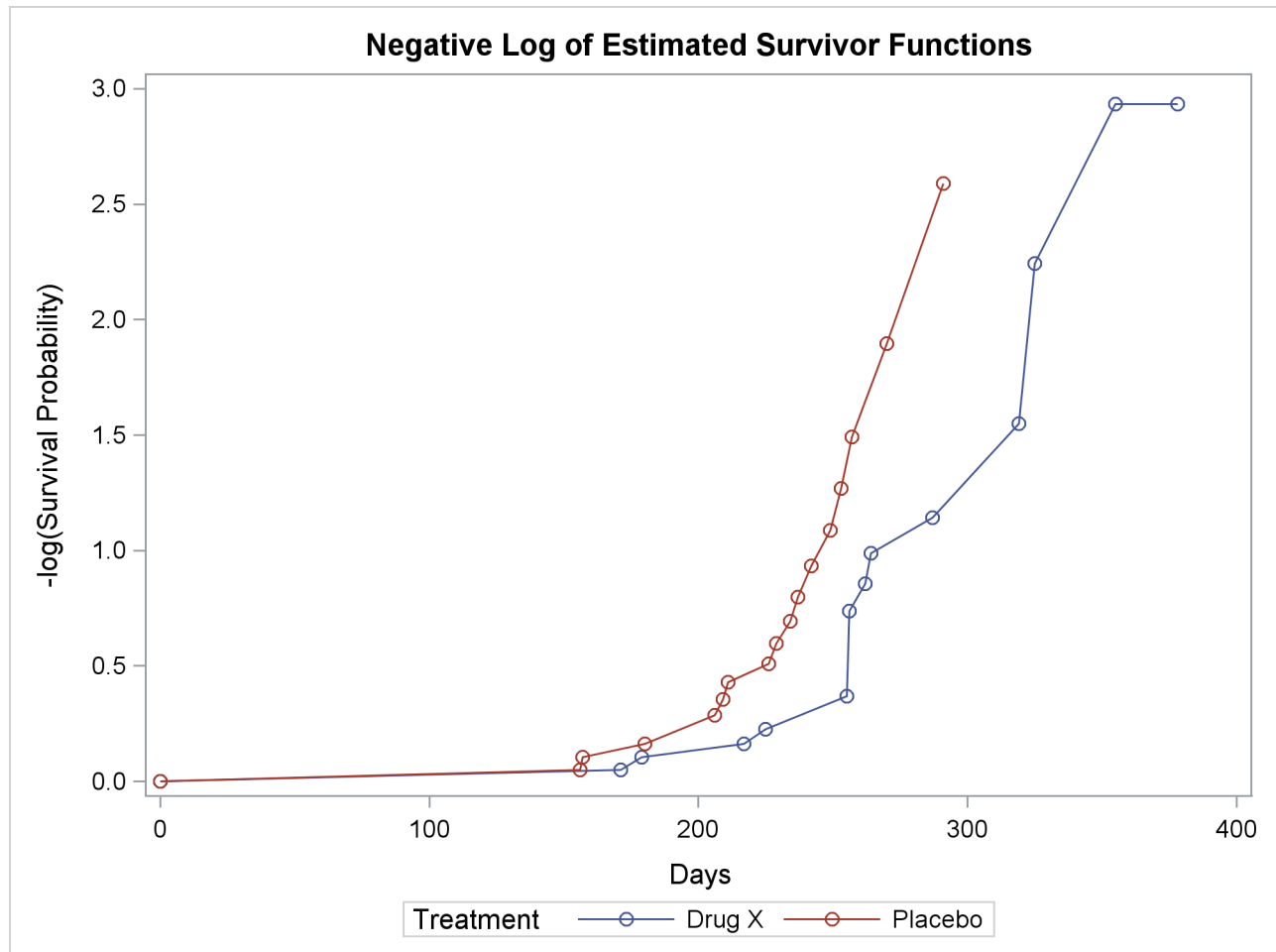


Figure 52.7 displays the graph of the log survivor function estimates versus survival time. Neither curve approximates a straight line through the origin—the exponential model is not appropriate for the survival data.

Note that these graphical displays are generated through ODS. For general information about ODS Graphics, see Chapter 21, “Statistical Graphics Using ODS.”

**Figure 52.7** Plot of Estimated Negative Log Survivor Functions

Results of the comparison of survival curves between the two treatments are shown in Figure 52.8. The rank tests for homogeneity indicate a significant difference between the treatments ( $p = 0.0175$  for the log-rank test and  $p = 0.0249$  for the Wilcoxon test). Rats treated with Drug X live significantly longer than those treated with Placebo. Since the survival curves for the two treatments differ primarily at longer survival times, the Wilcoxon test, which places more weight on shorter survival times, becomes less significant than the log-rank test. As noted earlier, the exponential model is not appropriate for the given survival data; consequently, the result of the likelihood ratio test should be ignored.

**Figure 52.8** Results of the Two-Sample Tests

| Test of Equality over Strata |            |    |                 |
|------------------------------|------------|----|-----------------|
| Test                         | Chi-Square | DF | Pr > Chi-Square |
| Log-Rank                     | 5.6485     | 1  | 0.0175          |
| Wilcoxon                     | 5.0312     | 1  | 0.0249          |
| -2Log(LR)                    | 0.1983     | 1  | 0.6561          |

Next, suppose male rats and female rats are thought to have different survival rates, and you want to assess the treatment effect while adjusting for the gender differences. By specifying the variable `Sex` in the `STRATA` statement as a stratifying variable and by specifying the variable `Treatment` in the `GROUP=` option, you can carry out a stratified test to test `Treatment` while adjusting for `Sex`. The test statistics are computed by pooling over the strata defined by the values of `Sex`, thus controlling for the effect of `Sex`. The `NOTABLE` option is added to the `PROC LIFETEST` statement as follows to avoid estimating a survival curve for each gender:

```
proc lifetest data=Exposed notable;
 time Days*Status(0);
 strata Sex / group=Treatment;
run;
```

Results of the stratified tests are shown in [Figure 52.9](#). The treatment effect is statistically significant for both the log-rank test ( $p = 0.0071$ ) and the Wilcoxon test ( $p = 0.0150$ ). As compared to the results of the unstratified tests in [Figure 52.8](#), the significance of the treatment effect has been sharpened by controlling for the effect of the gender of the subjects.

**Figure 52.9** Results of the Stratified Two-Sample Tests

| The LIFETEST Procedure                 |            |    |                    |
|----------------------------------------|------------|----|--------------------|
| Stratified Test of Equality over Group |            |    |                    |
| Test                                   | Chi-Square | DF | Pr ><br>Chi-Square |
| Log-Rank                               | 7.2466     | 1  | 0.0071             |
| Wilcoxon                               | 5.9179     | 1  | 0.0150             |

Since `Treatment` is a binary variable, another way to study the effect of `Treatment` is to carry out a censored linear rank test with `Treatment` as an independent variable. This test is less popular than the two-sample test; nevertheless, in situations where the independent variables are continuous and are difficult to discretize, it might be infeasible to perform a  $k$ -sample test. To compute the censored linear rank statistics to test the `Treatment` effect, `Treatment` is specified in the `TEST` statement as follows:

```
proc lifetest data=Exposed notable;
 time Days*Status(0);
 test Treatment;
run;
```

Results of the linear rank tests are shown [Figure 52.10](#). The  $p$ -values are very similar to those of the two-sample tests in [Figure 52.8](#).

**Figure 52.10** Results of Linear Rank Tests of Treatment

| The LIFETEST Procedure                       |                   |                   |            |                    |
|----------------------------------------------|-------------------|-------------------|------------|--------------------|
| Univariate Chi-Squares for the Wilcoxon Test |                   |                   |            |                    |
| Variable                                     | Test<br>Statistic | Standard<br>Error | Chi-Square | Pr ><br>Chi-Square |
| Treatment                                    | 3.9525            | 1.7524            | 5.0875     | 0.0241             |
| Univariate Chi-Squares for the Log-Rank Test |                   |                   |            |                    |
| Variable                                     | Test<br>Statistic | Standard<br>Error | Chi-Square | Pr ><br>Chi-Square |
| Treatment                                    | 6.2708            | 2.6793            | 5.4779     | 0.0193             |

With Sex as a prognostic factor that you want to control, you can compute a stratified linear rank statistic to test the effect of Treatment by specifying Sex in the STRATA statement and Treatment in the TEST statement as in the following program. The TEST=NONE option is specified in the STRATA statement to suppress the two-sample tests for Sex.

```
proc lifetest data=Exposed notable;
 time Days*Status(0);
 strata Sex / test=none;
 test Treatment;
run;
```

Results of the stratified linear rank tests are shown in Figure 52.11. The  $p$ -values are very similar to those of the stratified tests in Figure 52.9.

**Figure 52.11** Results of Stratified Linear Rank Tests of Treatment

| The LIFETEST Procedure                       |                   |                   |            |                    |
|----------------------------------------------|-------------------|-------------------|------------|--------------------|
| Univariate Chi-Squares for the Wilcoxon Test |                   |                   |            |                    |
| Variable                                     | Test<br>Statistic | Standard<br>Error | Chi-Square | Pr ><br>Chi-Square |
| Treatment                                    | 4.2372            | 1.7371            | 5.9503     | 0.0147             |
| Univariate Chi-Squares for the Log-Rank Test |                   |                   |            |                    |
| Variable                                     | Test<br>Statistic | Standard<br>Error | Chi-Square | Pr ><br>Chi-Square |
| Treatment                                    | 6.8021            | 2.5419            | 7.1609     | 0.0075             |

---

## Syntax: LIFETEST Procedure

The following statements are available in the LIFETEST procedure:

```

PROC LIFETEST < options > ;
 BY variables ;
 FREQ variable ;
 ID variables ;
 STRATA variable < (list) > < . . . variable < (list) > > < / options > ;
 TEST variables ;
 TIME variable < * censor(list) > ;
 WEIGHT variable ;

```

The simplest use of PROC LIFETEST is to request the nonparametric estimates of the survivor function for a sample of survival times. In such a case, only the PROC LIFETEST statement and the TIME statement are required. You can use the STRATA statement to divide the data into various strata. A separate survivor function is then estimated for each stratum, and tests of the homogeneity of strata are performed. However, if the GROUP= option is also specified in the STRATA statement, stratified tests are carried out to test the  $k$  samples defined by the GROUP= variable while controlling for the effect of the STRATA variables. You can specify covariates in the TEST statement. PROC LIFETEST computes linear rank statistics to test the effects of these covariates on survival.

The PROC LIFETEST statement invokes the procedure. All statements except the TIME statement are optional, and there is no required order for the statements that follow the PROC LIFETEST statement. The TIME statement is used to specify the variables that define the survival time and censoring indicator. The STRATA statement specifies a variable or set of variables that define the strata for the analysis. The TEST statement specifies a list of numeric covariates to be tested for their association with the response survival time. Each variable is tested individually, and a joint test statistic is also computed. The ID statement provides a list of variables whose values are used to identify observations in the product-limit, Breslow, or Fleming-Harrington estimates. When only the TIME statement appears, no strata are defined and no tests of homogeneity are performed.

---

## PROC LIFETEST Statement

```

PROC LIFETEST < options > ;

```

The PROC LIFETEST statement invokes the LIFETEST procedure. Optionally, this statement identifies an input and an OUTSURV= data set, and specifies the computation details of the survivor function estimation. Table 52.1 summarizes the options available in the PROC LIFETEST statement. These options are described in alphabetic order. If no options are requested, PROC LIFETEST computes and displays the product-limit estimate of the survivor function; and if ODS Graphics is enabled, a plot of the estimated survivor function is also displayed.

**Table 52.1** Options Available in the PROC LIFETEST Statement

| Option                                    | Description                                                                                               |
|-------------------------------------------|-----------------------------------------------------------------------------------------------------------|
| <b>Input and Output Data Sets</b>         |                                                                                                           |
| DATA=                                     | Specifies the input SAS data set                                                                          |
| OUTSURV=                                  | Names an output data set to contain survival estimates and confidence limits                              |
| OUTTEST=                                  | Names an output data set to contain rank test statistics for association of survival time with covariates |
| <b>Nonparametric Estimation</b>           |                                                                                                           |
| INTERVALS=                                | Specifies interval endpoints for life-table estimates                                                     |
| NELSON                                    | Adds the Nelson-Aalen estimates                                                                           |
| METHOD=                                   | Specifies the method to compute survivor function                                                         |
| NINTERVAL=                                | Specifies the number of intervals for life-table estimates                                                |
| WIDTH=                                    | Specifies the width of intervals for life-table estimates                                                 |
| <b>Confidence Limits for Survivorship</b> |                                                                                                           |
| ALPHA=                                    | Sets the confidence level for interval estimation estimates                                               |
| BANDMAXTIME=                              | Specifies the maximum time for confidence band                                                            |
| BANDMINTIME=                              | Specifies the minimum time for confidence band                                                            |
| CONFBAND=                                 | Specifies the type of confidence band in the OUTSURV= data set                                            |
| CONFTYPE=                                 | Specifies the transformation applied to the survivor function to obtain confidence limits                 |
| <b>Line Printer Plots</b>                 |                                                                                                           |
| FORMCHAR(1,2,7,9)=                        | Defines the characters used for line printer plot axes                                                    |
| LINEPRINTER                               | Specifies that plots be produced by a line printer                                                        |
| MAXTIME=                                  | Specifies the maximum time value for plotting                                                             |
| NOCENSLOT                                 | Suppresses the plot of censored observations                                                              |
| PLOTS=                                    | Specifies the plots to display                                                                            |
| <b>ODS Graphics</b>                       |                                                                                                           |
| MAXTIME=                                  | Specifies the maximum time value for plotting                                                             |
| PLOTS=                                    | Specifies plots to display                                                                                |
| <b>Traditional Graphics</b>               |                                                                                                           |
| ANNOTATE=                                 | Specifies an Annotate data set that adds features to plots                                                |
| CENSORED SYMBOL=                          | Defines the symbol used for censored observations in plots                                                |
| DESCRIPTION=                              | Specifies the string that appears in the description field of the PROC GREPLAY master menu for the plots  |
| EVENTSYMBOL=                              | Specifies the symbol used for event observations in plots                                                 |
| GOUT=                                     | Specifies the graphics catalog name for saving graphics output                                            |
| LANNOTATE=                                | Specifies an input data set that contains variables for local annotation                                  |
| MAXTIME=                                  | Specifies the maximum time value for plotting                                                             |
| PLOTS=                                    | Specifies the plots to display                                                                            |
| <b>Control Output</b>                     |                                                                                                           |
| ATRISK                                    | Adds the number of subjects at risk to the survival estimate table                                        |

Table 52.1 *continued*

| Option               | Description                                                                                |
|----------------------|--------------------------------------------------------------------------------------------|
| NOPRINT              | Suppresses the display of printed output                                                   |
| NOTABLE              | Suppresses the display of survival function estimates                                      |
| INTERVALS=           | Displays only the estimate for the smallest time in each interval                          |
| NOLEFT               | Suppresses the Number Left column in the survival estimate table                           |
| TIMELIST=            | Specifies a list of time points to display the survival estimate                           |
| REDUCEOUT            | Specifies that only INTERVAL= or TIMELIST= observations be listed in the OUTSURV= data set |
| <b>Miscellaneous</b> |                                                                                            |
| ALPHAQT=             | Sets the confidence level for survival time quartiles                                      |
| MISSING              | Allows missing values to be a stratum level                                                |
| SINGULAR=            | Sets the tolerance for testing singularity of covariance matrix of rank statistics         |
| STDERR               | Outputs the standard error for the survival estimators to the OUTSURV= data set            |
| TIMELIM=             | Specifies the time limit used to estimate the mean survival time and its standard error    |

The PLOTS= option in the PROC LIFETEST statement specifies the plots to display. You can select one of the following three types of graphics in PROC LIFETEST: line printer, traditional, and ODS. If you specify the LINEPRINTER option, line printer plots are produced; otherwise traditional graphics are produced if ODS Graphics is not enabled, or ODS Graphics plots are produced if the ODS Graphics is enabled.

For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

Table 52.2 shows whether graphics are produced, and the type of graphics, for all possible combinations:

Table 52.2 Ways of Displaying Graphics

| ODS Graphics | PLOTS= Option | LINEPRINTER Option | Graphics Results           |
|--------------|---------------|--------------------|----------------------------|
| Disabled     | No            | No                 | No graphics                |
| Disabled     | No            | Yes                | No graphics                |
| Disabled     | Yes           | No                 | Traditional graphics       |
| Disabled     | Yes           | Yes                | Line printer plot          |
| Enabled      | No            | No                 | ODS Graphics survival plot |
| Enabled      | No            | Yes                | No graphics                |
| Enabled      | Yes           | No                 | ODS Graphics               |
| Enabled      | Yes           | Yes                | Line printer plot          |

ODS Graphics is the preferred method of creating graphs. Many new features have been added to the ODS Graphics plots in PROC LIFETEST. For example, you can display the number of subjects at risk in a survival plot through ODS Graphics, but such a feature is not available in traditional graphics or line printer plots. The PLOTS= option syntax is documented separately for each type of graphics and is preceded by a heading that indicates the graphics type.

**ALPHA= $\alpha$** 

specifies the level of significance  $\alpha$  for the  $100(1 - \alpha)\%$  confidence intervals for the survivor, hazard, and density functions. For example, the option ALPHA=0.05 requests the 95% confidence limits for the survivor function. The default value is 0.05.

**ALPHAQT= $\alpha$** 

specifies the significance level  $\alpha$  for the  $100(1 - \alpha)\%$  confidence intervals for the quartiles of the survival time. For example, the option ALPHAQT=0.05 requests a 95% confidence interval for the quartiles of the survival time. The default value is 0.05.

**ANNOTATE=SAS-data-set****ANNO=SAS-data-set**

specifies an input data set that contains appropriate variables for annotation of the traditional graphics. The ANNOTATE= option enables you to add features (for example, labels that explain extreme observations) to plots produced on graphics devices. The ANNOTATE= option cannot be used if the [LINEPRINTER](#) option is specified or if ODS Graphics is enabled. The data set specified must be an ANNOTATE= type data set, as described in *SAS/GRAPH: Reference*.

The data set specified with the ANNOTATE= option in the PROC LIFETEST statement is “global” in the sense that the information in this data set is displayed in every plot produced by a single invocation of PROC LIFETEST.

**ATRISK**

adds a column that represents the number of subjects at risk to the survival estimate table. Also added is a column that represents the number of events at each observed time. This option has no effect for the life-table method.

**BANDMAXTIME=value****BANDMAX=value**

specifies the maximum time for the confidence bands. The default is the largest observed event time. If the specified BANDMAX= time exceeds the largest observed event time, it is truncated to the largest observed event time.

**BANDMINTIME=value****BANDMIN=value**

specifies the minimum time for the confidence bands. The default is the smallest observed event time. For the equal-precision band, if the BANDMIN= value is less than the smallest observed event time, it is defaulted to the smallest observed event time.

**CENSORED SYMBOL=name | 'string'****CS=name | 'string'**

specifies the symbol value for the censored observations in traditional graphics. The value, *name* or *'string'*, is the symbol value specification allowed in SAS/GRAPH software. The default is CS=CIRCLE. If you want to omit plotting the censored observations, specify CS=NONE. The CENSORED SYMBOL= option cannot be used if the [LINEPRINTER](#) option is specified or if ODS Graphics is enabled.



**CONF BAND=keyword**

specifies the confidence bands to be output to the OUTSURV= data set. Confidence bands are available for METHOD=KM, METHOD=BRESLOW, or METHOD=FH. You can use the following *keywords*:

|     |                                                                         |
|-----|-------------------------------------------------------------------------|
| ALL | outputs both the Hall-Wellner and the equal-precision confidence bands. |
| EP  | outputs the equal-precision confidence bands.                           |
| HW  | outputs the Hall-Wellner confidence bands.                              |

**CONFTYPE=keyword**

specifies the transformation applied to  $S(t)$  to obtain the pointwise confidence intervals and the confidence bands for the survivor function in addition to the confidence intervals for the quartiles of the survival times. The following *keywords* can be used; the default is CONFTYPE=LOGLOG.

ASINSQRT      the arcsine-square root transformation,

$$g(x) = \sin^{-1}(\sqrt{x})$$

LOGLOG      the log-log transformation,

$$g(x) = \log(-\log(x))$$

This is also referred to as the log cumulative hazard transformation since it applies the logarithmic function to the cumulative hazard function. Collett (1994) and Lachin (2000) refer to it as the complementary log-log transformation.

LINEAR      the identity transformation,

$$g(x) = x$$

LOG      the logarithmic transformation,

$$g(x) = \log(x)$$

LOGIT      the logit transformation,

$$g(x) = \log\left(\frac{x}{1-x}\right)$$

**DATA=SAS-data-set**

names the SAS data set used by PROC LIFETEST. By default, the most recently created SAS data set is used.

**DESCRIPTION='string'****DES='string'**

specifies a descriptive string of up to 256 characters that appears in the “Description” field of the traditional graphics catalog. The description does not appear in the plots. By default, PROC LIFETEST assigns a description of the form PLOT OF *vname* versus *hname*, where *vname* and *hname* are the names of the y variable and the x variable, respectively. The DESCRIPTION= option cannot be used if the **LINEPRINTER** option is specified or if ODS Graphics is enabled.

**EVENTSYMBOL**=*name* | '*string*'

**ES**=*name* | '*string*'

specifies the symbol value for the event observations in traditional graphics. The value, *name* or '*string*', is the symbol value specification allowed in SAS/GRAPH software. The default is ES=NONE. The EVENTSYMBOL= option cannot be used if the [LINEPRINTER](#) option is specified or if ODS Graphics is enabled.

**FORMCHAR(1,2,7,9)**= '*string*'

defines the characters used for constructing the vertical and horizontal axes of the line printer plots. The string should be four characters. The first and second characters define the vertical and horizontal bars, respectively, which are also used in drawing the steps of the Kaplan-Meier, Breslow, or Fleming-Harrington survival curve. The third character defines the tick mark for the axes, and the fourth character defines the lower left corner of the plot. The default is FORMCHAR(1,2,7,9)='|+-'. Any character or hexadecimal string can be used to customize the plot appearance. If you use hexadecimal, you must put an x after the closing quote. For example, to send the plot output to a printer with the IBM graphics character set (1 or 2), specify the following:

```
formchar (1, 2, 7, 9) = 'B3C4C5C0' x
```

See the chapter titled “The PLOT Procedure” in the *Base SAS Procedures Guide* for further information.

**GOUT**=*graphics-catalog*

specifies the graphics catalog for saving traditional graphics output from PROC LIFETEST. The default is Work.Gseg. The GOUT= option cannot be used if the [LINEPRINTER](#) option is specified or if ODS Graphics is enabled. For more information, see the chapter titled “The GREPLAY Procedure” in *SAS/GRAPH: Reference*.

**INTERVALS**=*values*

specifies a list of interval endpoints for the life-table method. These endpoints must all be nonnegative numbers. The initial interval is assumed to start at zero whether or not zero is specified in the list. Each interval contains its lower endpoint but does not contain its upper endpoint. When this option is used with METHOD=KM, METHOD=BRESLOW, or METHOD=FH, it reduces the number of survival estimates displayed by showing only the estimates for the smallest time within each specified interval. The INTERVALS= option can be specified in any of the following ways:

- A list separated by blanks      **INTERVALS=1 3 5 7**
- A list separated by commas      **INTERVALS=1, 3, 5, 7**
- *x* to *y*      **INTERVALS=1 to 7**
- *x* to *y* BY *z*      **INTERVALS=1 to 7 by 1**
- A combination of the above      **INTERVALS=1, 3 to 5, 7**

For example, the specification

```
intervals=5,10 to 30 by 10
```

produces the set of intervals

```
{[0, 5), [5, 10), [10, 20), [20, 30), [30, ∞)}
```

**LANNOTATE=SAS-data-set**

**LANN=SAS-data-set**

specifies an input data set that contains variables for local annotation of traditional graphics. You can use the LANNOTATE= option to specify a different annotation for each BY group, in which case the BY variables must be included in the LANNOTATE= data set. The LANNOTATE= option cannot be used if the **LINEPRINTER** option is specified or if ODS Graphics is enabled. The data set specified must be an **ANNOTATE=** type data set, as described in *SAS/GRAPH: Reference*.

If there is no BY-group processing, the **ANNOTATE=** and **LANNOTATE=** options have the same effects.

**LINEPRINTER**

**LS**

specifies that plots are produced by a line printer instead of by a graphical device.

**MAXTIME=value**

specifies the maximum value of the time variable allowed on the plots so that outlying points do not determine the scale of the time axis of the plots. This option affects only the displayed plots and has no effect on any calculations.

**METHOD=type**

specifies the method to be used to compute the survival function estimates. Valid values for *type* are as follows:

**BRESLOW**

specifies that the Breslow estimates be computed. The Breslow estimator is the exponentiation of the negative Nelson-Aalen estimator of the cumulative hazard function.

**FH**

specifies that the Fleming-Harrington (FH) estimates be computed. The FH estimator is a tie-breaking modification of the Breslow estimator. If there are no tied event times, this estimator is the same as the Breslow estimator.

**KM**

**PL**

specifies that Kaplan-Meier estimates (also known as the product-limit estimates) be computed.

**ACT**

**LIFE**

**LT**

specifies that life-table estimates (also known as actuarial estimates) be computed.

By default, **METHOD=KM**.

**MISSING**

allows missing values for numeric variables and blank values for character variables as valid stratum levels. See the section “**Missing Values**” on page 4031 for details.

By default, PROC LIFETEST does not use observations with missing values for any stratum variables.

**NELSON****AALEN**

produces the Nelson-Aalen estimates of the cumulative hazards and the corresponding standard errors. This option is ignored if METHOD=LT is specified.

**NINTERVAL=***value*

specifies the number of intervals used to compute the life-table estimates of the survivor function. This parameter is overridden by the WIDTH= option or the INTERVALS= option. When you specify the NINTERVAL= option, PROC LIFETEST tries to find an interval that results in round numbers for the endpoints. Consequently, the number of intervals can be different from the number requested. Use the INTERVALS= option to control the interval endpoints. The default is NINTERVAL=10.

**NOCENS PLOT****NOCENS**

requests that the plot of censored observations be suppressed when the LINEPRINTER and PLOTS= options are specified. This option is not needed when the life-table method is used to compute the survival estimates, because the plot of censored observations is not produced.

**NOLEFT**

suppresses the Number Left and Number Event columns in the survival estimate table. This option has no effect for the life-table estimate.

**NOPRINT**

suppresses the display of output. This option is useful when only an output data set is needed. It temporarily disables the Output Delivery System (ODS); see Chapter 20, “Using the Output Delivery System” for more information.

**NOTABLE**

suppresses the display of survival function estimates. Only the number of censored and event times, plots, and test results is displayed.

**OUTSURV=***SAS-data-set***OUTS=***SAS-data-set*

creates an output SAS data set to contain the estimates of the survival function and corresponding confidence limits for all strata. See the section “OUTSURV= Data Set” on page 4049 for more information about the contents of the OUTSURV= data set.

**OUTTEST=***SAS-data-set***OUTT=***SAS-data-set*

creates an output SAS data set to contain the overall chi-square test statistic for association with failure time for the variables in the TEST statement, the values of the univariate rank test statistics for each variable in the TEST statement, and the estimated covariance matrix of the univariate rank test statistics. See the section “OUTTEST= Data Set” on page 4051 for more information about the contents of the OUTTEST= data set.

**Line Printer PLOTS= Option****PLOTS=***plot-request***PLOTS=**(*plot-requests*)

controls the line printer plots produced. You must also specify the **LINEPRINTER** option to obtain line printer plots. When you specify only one *plot-request*, you can omit the parentheses around the *plot-request*. Here are some examples:

```
plots=s
plots=(s ls lls)
```

The *plot-requests* include the following:

**CENSORED****C**

specifies a plot of censored observations. This option is available for **METHOD=KM**, **METHOD=BRESLOW**, or **METHOD=FH** only.

**SURVIVAL****S**

specifies a plot of the estimated SDF versus time.

**LOGSURV****LS**

specifies a plot of the negative log of the estimated SDF versus time.

**LOGLOGS****LLS**

specifies a plot of the log of the negative log of the estimated SDF versus the log of time.

**HAZARD****H**

specifies a plot of the estimated hazard function versus time (life-table method only).

**PDF****P**

specifies a plot of the estimated probability density function versus time (life-table method only).

**ODS Graphics PLOTS= Option****PLOTS**< (*global-plot-option*) > = *plot-request* < (*options*) >**PLOTS**< (*global-plot-option*) > = (*plot-request* < (*options*) > < ... *plot-request* < (*options*) > >

controls the plots produced using ODS Graphics. When you specify only one *plot-request*, you can omit the parentheses around the *plot-request*. Here are some examples:

```
plots=none
plots=(survival(atrisk=100 to 350 by 50) logsurv)
plots(only)=hazard
```

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;

proc lifetest plots=survival(atrisk);
 time T*Status(0);
run;

ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

If ODS Graphics is enabled but you do not specify the PLOTS= option, then PROC LIFETEST produces a plot of the estimated survivor functions by default.

The only *global-plot-option* follows:

#### ONLY

specifies that only the specified plots in the list be produced; otherwise, the default survivor function plot is also displayed.

The *plot-requests* and *plot-request options* include the following.

#### ALL

produces all appropriate plots. For METHOD=KM, METHOD=BRESLOW, or METHOD=FH, specifying PLOTS=ALL is equivalent to specifying PLOTS=(SURVIVAL LOGSURV LOGLOGLS HAZARD); for the life-table method, PLOTS=ALL is equivalent to specifying PLOTS=(SURVIVAL LOGSURV LOGLOGS DENSITY HAZARD).

#### HAZARD <(hazard-options)>

##### H <hazard-options>

plots the estimated hazard functions. Kernel-smoothed estimates are produced for METHOD=KM, METHOD=BRESLOW, or METHOD=FH. You can specify the following *hazard-options*, but only the CL option can be used for the life-table method:

##### BANDWIDTH=*bandwidth-option*

##### BW=*bandwidth-option*

specifies what bandwidth is chosen for the kernel-smoothing and how it is chosen. You can specify one of the following *bandwidth-options*.

##### *value*

sets the bandwidth to the given *value*.

##### *numeric-list*

selects the bandwidth from the given *numeric-list* that minimizes the mean integrated squared error.

##### RANGE(*lower,upper*)

selects the bandwidth from the interval (*lower, upper*) that minimizes the mean integrated squared error. PROC LIFETEST uses the golden section search algorithm to find the minimum. If there is more than one local minimum in the interval, there is no guarantee that the local minimum found is also the global minimum.

See the section “Optimal Bandwidth” on page 4042 for details about the mean integrated squared error. If the BANDWIDTH= option is not specified, the default is BANDWIDTH=RANGE(0.2b,20b), where  $b = \frac{g_u - g_l}{8n^{.2}}$ ,  $g_l$  and  $g_u$  are the values of the GRIDL= and GRIDU= options, respectively, and  $n$  is the total number of noncensored observations.

**GRIDL=number**

specifies the lower grid limit for the kernel-smoothed estimate. The default value is the time origin.

**GRIDU=number**

specifies the upper grid limit for the kernel-smoothed estimate. The default value equals the maximum event time.

**KERNEL=kernel-option**

specifies the kernel used. The choices are as follows:

**BIWEIGHT****BW**

$$K_{BW}(x) = \frac{15}{16}(1 - x^2)^2, \quad -1 \leq x \leq 1$$

**EPANECHNIKOV****E**

$$K_E(x) = \frac{3}{4}(1 - x^2), \quad -1 \leq x \leq 1$$

**UNIFORM****U**

$$K_U(x) = \frac{1}{2}, \quad -1 \leq x \leq 1$$

The default is KERNEL=EPANECHNIKOV.

**NMINGRID=number**

specifies the number of grid points in determining the mean integrated square error (MISE). The default value is 51.

**NGRID=number**

specifies the number of grid points. The default is 101.

**CL**

displays the pointwise confidence limits for the smoothed hazard.

**LOGLOGS****LLS**

plots the log of negative log of estimated survivor functions versus the log of time.

**LOGSURV****LS**

plots the negative log of estimated survivor functions versus time.

**NONE**

suppresses all plots.

**PDF <(CL)>****P <(CL)>**

plots the estimated probability density functions (life-table method only). Pointwise confidence limits are displayed optionally by specifying the CL option.

**SURVIVAL <(survival-options)>****S <(survival-options)>**

plots the estimated survivor functions. Censored times are plotted as a plus sign on the Kaplan-Meier, Breslow, or Fleming-Harrington survival curves unless the NOCENSOR option is specified. You can customize the display by using the following *survival-options*. If these options are not sufficient for your purposes, you can customize the survival plot by modifying its graphical template (see the section “[Modifying the ODS Template for Survival Plots](#)” on page 4061 for more information).

**ATRISK <(options)> <=number-list >**

displays the numbers of subjects at risk at the given times. The following *options* can be specified:

**ATRISKTICK****ATRISKLABEL**

shows the time values at which the numbers of subjects at risk are displayed.

**MAXLEN=*n***

specifies the number of characters *n* that are allowed for displaying the stratum labels. If *n* is greater than or equal to the maximum length of the stratum labels, the stratum labels are used in the at-risk display; otherwise, the stratum numbers are used. The default is MAXLEN=12.

**OUTSIDE<(ρ)>**

specifies that the at-risk table be drawn outside the plot area. PROC LIFETEST uses an ODS graphical template with a two-row lattice layout. The upper cell displays the survival plot, and the bottom cell displays the at-risk table. You can specify an optional number *ρ* that represents the fractional proportion of the at-risk table height relative to the overall grid height. By default, *ρ* is set to 0.035 times the number of strata, with a maximum value of 0.5.

The *number-list* identifies the times at which the numbers at risk are displayed. If the *number-list* is not specified, PROC LIFETEST uses the default list  $\{0, a, 2a, \dots, n \times a\}$ , where *a* and *n* are computed by the following algorithm. Let *m* be the MAXTIME= value or the largest observed time if the MAXTIME= option is not specified; let *b* =



$10^{\text{ceil}(\log_{10}(m)-1)}$ , where  $\text{ceil}()$  is the ceiling function.

$$a = \begin{cases} \frac{b}{2} & \text{if } m < 0.25b \\ 2b & \text{if } m > 0.75b \\ b & \text{otherwise} \end{cases}$$

$$n = \text{integral value of } m/a$$

**CB** <=*keyword*>

displays the confidence bands (that is, simultaneous confidence intervals) for the survivor functions. You can specify one of the following *keywords*. The default is CB=HW.

**ALL**

displays both the equal-precision and the Hall-Wellner bands.

**EP**

displays the equal-precision band.

**HW**

displays the Hall-Wellner confidence band.

**CL**

displays the pointwise confidence limits for the survivor functions.

**FAILURE**

**F**

changes all the displays for survivor functions to those for the failure functions. For example, if both the FAILURE and CL options are specified, the plot displays the failure curves in addition to the pointwise confidence limits for the failure functions.

**NOCENSOR**

suppresses the plotting of the censored times on a Kaplan-Meier, Breslow, or Fleming-Harrington survival curve.

**STRATA**=*strata-option*

specifies how to display the survival/failure curves for multiple strata. This option has no effect if there is only one stratum. You can choose one of the following *strata options*:

**INDIVIDUAL**

**UNPACK**

specifies that a separate plot be displayed for each stratum.

**OVERLAY**

specifies that the survival/failure curves for the strata be overlaid in one plot.

**PANEL**

specifies that separate plots for the strata be organized into panels of two or four plots, depending on the number of strata.

The default is STRATA=OVERLAY.

**TEST**

displays the  $p$ -value of a homogeneity test specified in the STRATA statement. If more than one test is produced, the test is chosen in the following order: LOGRANK, WILCOXON, TARONE, PETO, MODPETO, FLEMING, and LR.

**Traditional Graphics PLOTS= Option**

**PLOTS=***plot-request* <(NAME=*name* | '*string*')>

**PLOTS=**(*plot-request* <(NAME=*name* | '*string*')> <, ..., *plot-request* <(NAME=*name* | '*string*')> >)

controls plots produced in traditional graphics. To obtain traditional graphics, you must neither enable ODS Graphics nor specify the **LINEPRINTER** option. For each *plot-request*, you can use the NAME= option to specify a name to identify the plot. The name can be specified as a SAS name or as a quoted string of up to 256 characters. Only the first eight characters are used as the entry name in the **GOUT=** catalog. The *plot-requests* include the following:

**SURVIVAL****S**

plots the estimated survivor functions versus time.

**LOGSURV****LS**

plots the negative log of estimated survivor functions versus time.

**LOGLOGS****LLS**

plots the log of negative log of estimated survivor functions versus the log of time.

**HAZARD****H**

plots estimated hazard function versus time (life-table method only).

**PDF****P**

plots the estimated probability density function versus time (life-table method only).

When you specify only one *plot-request*, you can omit the parentheses around the *plot-request*. Here are some examples:

```
plots=s
plots=(s(name=Surv2), h(name=Haz2))
```

The latter requests a plot of the estimated survivor function versus time and a plot of the estimated hazard function versus time, with Surv2 and Haz2 as their names in the **GOUT=** catalog, respectively.

**REDUCEOUT**

specifies that the **OUTSURV=** data set contain only those observations that are included in the **INTERVALS=** or **TIMELIST=** option. This option has no effect if the **OUTSURV=** option is not specified. It also has no effect if neither the **INTERVALS=** option nor the **TIMELIST=** option is specified.

**SINGULAR=value**

specifies the tolerance for testing singularity of the covariance matrix for the rank test statistics. The test requires that a pivot for sweeping a covariance matrix be at least this number times a norm of the matrix. The default value is 1E-12.

**STDERR**

specifies that the standard error of the survivor function (SDF\_STDERR) be output to the OUT-SURV= data set. If the life-table method is used, the standard error of the density function (PDF\_STDERR) and the standard error of the hazard function (HAZ\_STDERR) are also output.

**TIMELIM=time-limit**

specifies the time limit used in the estimation of the mean survival time and its standard error. The mean survival time can be shown to be the area under the Kaplan-Meier survival curve. However, if the largest observed time in the data is censored, the area under the survival curve is not a closed area. In such a situation, you can choose a time limit  $L$  and estimate the mean survival curve limited to a time  $L$  (Lee 1992, pp. 72–76). This option is ignored if the largest observed time is an event time. Valid *time-limit* values are as follows:

**EVENT****LET**

specifies that the time limit  $L$  be the largest event time in the data. TIMELIM=EVENT is the default.

**OBSERVED****LOT**

specifies that the time limit  $L$  be the largest observed time in the data.

*number*

specifies that the time limit  $L$  be the given *number*. The *number* must be positive and at least as large as the largest event time in the data.

**TIMELIST=number-list**

specifies a list of time points at which the Kaplan-Meier estimates are displayed. The time points are listed in the column labeled Timelist. Since the Kaplan-Meier survival curve is a decreasing step function, each given time point falls in an interval that has a constant survival estimate. The event time that corresponds to the beginning of the time interval is displayed along with its survival estimate.

**WIDTH=value**

sets the width of the intervals used in the life-table calculation of the survival function. This parameter is overridden by the INTERVALS= option.

**BY Statement****BY variables ;**

You can specify a BY statement with PROC LIFETEST to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the LIFETEST procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

The BY statement is more efficient than the STRATA statement for defining strata in large data sets. However, if you use the BY statement to define strata, PROC LIFETEST does not pool over strata for testing the association of survival time with covariates, nor does it test for homogeneity across the BY groups.

When the life-table method is used to estimate survivor functions, each BY group might have a different set of intervals. To make intervals the same across BY groups, use the INTERVALS= or WIDTH= option in the PROC LIFETEST statement.

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

## FREQ Statement

**FREQ** *variable* </ *option* > ;

The FREQ statement identifies a *variable* that contains the frequency of occurrence of each observation. PROC LIFETEST treats each observation as if it appeared  $n$  times, where  $n$  is the value of the FREQ variable for the observation. The FREQ statement is useful for producing life tables when the data are already in the form of a summary data set. If it is not an integer, it is truncated to an integer unless the NOTRUNCATE option is specified. If it is missing or less than or equal zero, the observation is not used.

The following *option* can be specified in the FREQ statement after a slash (/):

### NOTRUNCATE

#### NOTRUNC

specifies that the frequency values are not truncated to integers. This option does not apply to the Fleming-Harrington estimator (METHOD=FH).

## ID Statement

**ID** *variables* ;

The ID statement identifies *variables* whose values are used to label the observations of the Kaplan-Meier, Breslow, or Fleming-Harrington survivor function estimates. SAS format statements can be used to format the values of the ID variables.

## STRATA Statement

**STRATA** *variable* <(list)> <... *variable* <(list)>> </ options > ;

The STRATA statement identifies the variables that determine the strata levels. Strata are formed according to the nonmissing values of these variables. The MISSING option can be used to allow missing values as a valid stratum level. Other options enable you to specify various  $k$ -sample tests, stratified tests, or trend tests and to make multiple-comparison adjustments for paired differences.

In the preceding syntax, *variable* is a variable whose values determine the stratum levels, and *list* is a list of endpoints for a numeric variable. The values for *variable* can be formatted or unformatted. If *variable* is a character variable, or if *variable* is numeric and no list appears, then the strata are defined by the unique values of the STRATA *variable*. More than one *variable* can be specified in the STRATA statement, and each numeric variable can be followed by a list. Each interval contains its lower endpoint but not its upper endpoint. The corresponding strata are formed by the combination of levels. If a variable is numeric and is followed by a list, then the levels for that variable correspond to the intervals defined by the list. The initial interval is assumed to start at  $-\infty$ , and the final interval is assumed to end at  $\infty$ .

The specification of a STRATA *variable* can have any of the following forms:

- A list separated by blanks      **Age (5 10 20 30)**
- A list separated by commas      **Age (5, 10, 20, 30)**
- $x$  to  $y$       **Age (5 to 10)**
- $x$  to  $y$  by  $z$       **Age (5 to 30 by 10)**
- A combination of the above      **Age (5, 10 to 50 by 10)**

For example, the specification

```
strata Age(5,20 to 50 by 10) Sex;
```

indicates the following levels for the Age variable:

$\{(-\infty, 5), [5, 20), [20, 30), [30, 40), [40, 50), [50, \infty)\}$

This statement also specifies that the Age strata be further subdivided by values of the variable Sex. In this example, there are six age groups by two sex groups, forming a total of 12 strata.

The specification of several STRATA *variables*, such as

```
strata A B C;
```

is equivalent to the A\*B\*C syntax of the TABLES statement in the FREQ procedure. The number of strata levels usually grows very rapidly with the number of STRATA variables, so you must be cautious when specifying the list of STRATA variables.

When comparing more than two survival curves, a  $k$ -sample test tells you whether the curves are significantly different from each other, but it does not identify which pairs of curves are different. A multiple-comparison adjustment of the  $p$ -values for the paired comparisons retains the same overall false positives as the  $k$ -sample test. Two types of paired comparisons can be made: comparisons between all pairs of curves and comparisons between a control curve and all other curves. You use the DIFF= option to specify the comparison type, and you use the ADJUST= option to select a method of multiple-comparison adjustments.

Table 52.3 summarizes the options available in the STRATA statement.

**Table 52.3** Options Available in the STRATA Statement

| Option                      | Description                                                  |
|-----------------------------|--------------------------------------------------------------|
| <b>Homogeneity Tests</b>    |                                                              |
| GROUP=                      | Specifies the group variable for stratified tests            |
| NODETAIL                    | Suppresses printing the test statistic and covariance matrix |
| NOTEST                      | Suppresses any tests                                         |
| TEST=                       | Specifies tests corresponding to various weight functions    |
| TREND                       | Requests a trend test                                        |
| <b>Multiple Comparisons</b> |                                                              |
| ADJUST=                     | Requests a multiple-comparison adjustment                    |
| DIFF=                       | Specifies the type of differences to consider                |
| <b>Missing Strata Value</b> |                                                              |
| MISSING                     | Allows missing values as valid stratum values                |
| <b>Display Option</b>       |                                                              |
| NOLABEL                     | Uses the names of the STRATA variables in the display        |

You can specify the following *options* in the STRATA statement after a slash (“/”).

**ADJUST=method**

specifies the multiple-comparison method for adjusting the  $p$ -values of the paired tests. See the section “Multiple-Comparison Adjustments” on page 4045 for mathematical details; also see Westfall et al. (1999). The adjustment methods include the following:

**BONFERRONI****BON**

applies the Bonferroni correction to the raw  $p$ -values.

**DUNNETT**

performs Dunnett’s two-tailed comparisons of the control group with all other groups. PROC LIFETEST uses the factor-analytic covariance approximation described in Hsu (1992) and identifies the adjustment in the results as “Dunnett-Hsu.” Note that ADJUST=DUNNETT is incompatible with DIFF=ALL.

**SCHEFFE**

performs Scheffé’s multiple-comparison adjustment.

**SIDAK**

applies the Šidák correction to the raw  $p$ -values.

**SMM****GTE**

performs the paired comparisons based on the studentized maximum modulus test.

**TUKEY**

performs the paired comparisons based on Tukey’s studentized range test. PROC LIFETEST uses the approximation described in Kramer (1956) and identifies the adjustment as “Tukey-Kramer” in the results. Note that ADJUST=TUKEY is incompatible with DIFF=CONTROL.

**SIMULATE** <(simulate-options)>

computes the adjusted  $p$ -values from the simulated distribution of the maximum or maximum absolute value of a multivariate normal random vector. The simulation estimates  $q$ , the true  $(1 - \alpha)$  quantile, where  $\alpha$  is the value of the ALPHA= *simulate-option*.

The number of samples for the SIMULATE adjustment is set so that the tail area for the simulated  $q$  is within a certain accuracy radius  $\gamma$  of  $1 - \alpha$  with an accuracy confidence of  $100(1 - \epsilon)\%$ . In equation form,

$$\Pr(|F(\hat{q}) - (1 - \alpha)| \leq \gamma) = 1 - \epsilon$$

where  $\hat{q}$  is the simulated  $q$  and  $F$  is the true distribution function of the maximum; see Edwards and Berry (1987) for details. By default,  $\gamma = 0.005$  and  $\epsilon = 0.01$  so that the tail area of  $\hat{q}$  is within 0.005 of 0.95 with 99% confidence.

The *simulate-options* include the following:

**ACC=***value*

specifies the target accuracy radius  $\gamma$  of a  $100(1 - \epsilon)\%$  confidence interval for the true probability content of the estimated  $(1 - \alpha)$  quantile. The default value is ACC=0.005.

**ALPHA=***value*

specifies the value  $\alpha$  for estimating the  $(1 - \alpha)$  quantile. The default value is the ALPHA= value in the PROC LIFETEST statement, or 0.05 if that option is not specified.

**EPS=***value*

specifies the value  $\epsilon$  for a  $100(1 - \epsilon)\%$  confidence interval for the true probability content of the estimated  $(1 - \alpha)$  quantile. The default value for the accuracy confidence is 99%, corresponding to EPS=0.01.

**NSAMP=***n*

specifies the sample size for the simulation. By default,  $n$  is set based on the values of the target accuracy radius  $\gamma$  and accuracy confidence  $100(1 - \epsilon)\%$  for an interval for the true probability content of the estimated  $(1 - \alpha)$  quantile. With the default values for  $\gamma$ ,  $\epsilon$ , and  $\alpha$  (0.005, 0.01, and 0.05, respectively), NSAMP=12604 by default.

**REPORT**

specifies that a report on the simulation should be displayed, including a listing of the parameters, such as  $\gamma$ ,  $\epsilon$ , and  $\alpha$ , in addition to an analysis of various methods for estimating or approximating the quantile.

**SEED=***number*

specifies an integer used to start the pseudorandom number generator for the simulation. If you do not specify a seed, or if you specify a value less than or equal to zero, the seed is generated by default from reading the time of day from the computer's clock.

**DIFF=ALL | CONTROL**<('string' <... , 'string')>

specifies which pairs of survival curves are considered for the multiple comparisons.

**DIFF=ALL**

requests all paired comparisons

**DIFF=CONTROL** <('string' <... 'string'>)>

requests comparisons of the control curve with all other curves. To specify the control curve, you specify the quotes strings of formatted values that represent the curve in parentheses. For example, if Cell='large' identifies the control group, you specify

```
DIFF=CONTROL (' large ')
```

If more than one variable is used to identify the curves (for example, if Cell='large' and Sex='F' represent the control), you specify

```
DIFF=CONTROL (' large ' ' F ')
```

The order of the quoted strings should correspond to the order of the stratum variables. If no specific curve is specified as the control, the first stratum or group value is used.

By default, DIFF=ALL unless you specify **ADJUST= DUNNETT**, in which case DIFF=CONTROL.

**GROUP=variable**

specifies the variable whose formatted values identify the various samples whose underlying survival curves are to be compared. The tests are stratified on the levels of the STRATA variables. For example, in a multicenter trial in which two forms of therapy are to be compared, you specify the variable that identifies therapies as the **GROUP= variable** and the variable that identifies centers as the STRATA variable, in order to perform a stratified test to compare the therapies while controlling the effect of the centers.

**MISSING**

allows missing values to be a stratum level or a valid value of the **GROUP= variable**.

**NODETAIL**

suppresses the display of the rank statistics and the corresponding covariance matrices for various strata. If you specified the **TREND** option, the display of the scores for computing the trend tests is suppressed.

**NOLABEL**

specifies that the names instead of the labels of the STRATA variables be used in the display of the survival estimate table and in the legend of the survival plot.

**NOTEST**

suppresses the *k*-sample tests, stratified tests, and trend tests.

**ORDER=FORMATTED | INTERNAL**

specifies the sorting order of the values of the STRATA variables. The strata are presented in the specified order in the analysis results. You can use this option, for example, to display the curve labels in your preferred order in the survival plot legend (see [Example 52.2](#) for an illustration). The default is **ORDER=FORMATTED**, which sorts the strata according to their external formatted values, except for numeric variable with no explicit format, which are sorted by the unformatted (internal) values. **ORDER=INTERNAL** sorts the strata by their internal values. The **ORDER=** option has no effect on a stratum variable with cutpoints specified.



**TREND**

computes the trend tests for testing the null hypothesis that the  $k$  population hazards rate are the same versus an ordered alternatives. If there is only one STRATA variable and the variable is numeric, the unformatted values of the variable are used as the scores; otherwise, the scores are 1, 2, . . . , in the given order of the strata.

**TEST**=*test-request*

**TEST**=(*test-request* < . . . *test-request* > )

controls the tests produced. Each test corresponds to a different weight function (see the section “Nonparametric Tests” on page 4043 for the weight functions). The *test-requests* include the following:

|                             |                                                                                                                                                                                                                                                                                                                                                                                                                                             |
|-----------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| ALL                         | specifies all the nonparametric tests with $\rho_1=1$ and $\rho_2=0$ for the Fleming and Harrington test—FLEMING(1,0).                                                                                                                                                                                                                                                                                                                      |
| FLEMING( $\rho_1, \rho_2$ ) | specifies the family of tests in Harrington and Fleming (1982), where $\rho_1$ and $\rho_2$ are nonnegative numbers. FLEMING( $\rho_1, \rho_2$ ) reduces to the Fleming-Harrington $G^{\rho}$ family (Fleming and Harrington 1981) when $\rho_2=0$ , which you can specify as FLEMING( $\rho$ ) with one argument. When $\rho=0$ , the test becomes the log-rank test. When $\rho=1$ , the test should be very close to the Peto-Peto test. |
| LOGRANK                     | specifies the log-rank test.                                                                                                                                                                                                                                                                                                                                                                                                                |
| NONE                        | suppresses all comparison tests. Specifying TEST=NONE is equivalent to specify NOTEST.                                                                                                                                                                                                                                                                                                                                                      |
| LR                          | specifies the likelihood ratio test based on the exponential model.                                                                                                                                                                                                                                                                                                                                                                         |
| MODPETO                     | specifies the modified Peto-Peto test.                                                                                                                                                                                                                                                                                                                                                                                                      |
| PETO                        | specifies the Peto-Peto test. The test is also referred to as the Peto-Peto-Prentice test.                                                                                                                                                                                                                                                                                                                                                  |
| WILCOXON                    | specifies the Wilcoxon test. The test is also referred to as the Gehan test or the Breslow test.                                                                                                                                                                                                                                                                                                                                            |
| TARONE                      | specifies the Tarone-Ware test.                                                                                                                                                                                                                                                                                                                                                                                                             |

By default, TEST=(LOGRANK WILCOXON LR) for the  $k$ -sample tests, and TEST=(LOGRANK WILCOXON) for stratified and trend tests.

---

## TEST Statement

**TEST** *variables* ;

The TEST statement specifies a list of numeric covariates (prognostic variables) that you want tested for association with the failure time.

Two sets of rank statistics are computed. These rank statistics and their variances are pooled over all strata. Univariate (marginal) test statistics are displayed for each of the covariates.

Additionally, a sequence of test statistics for joint effects of covariates is displayed. The first element of the sequence is the largest univariate test statistic. Other variables are then added on the basis of the largest

increase in the joint test statistic. The process continues until all the variables have been added or until the remaining variables are linearly dependent on the previously added variables.

See the section “Rank Tests for the Association of Survival Time with Covariates” on page 4047 for more information.

## TIME Statement

**TIME** *variable* < \*  *censor(list)* > ;

The TIME statement is required. It is used to indicate the failure time variable, where *variable* is the name of the failure time variable that can be optionally followed by an asterisk, the name of the censoring variable, and a parenthetical list of values that correspond to right censoring. The censoring values should be numeric, nonmissing values. For example, the statement

```
time T*Flag(1,2);
```

identifies the variable T as containing the observed failure times (event or censored). If the variable Flag has the value 1 or 2, the corresponding value of T is a right-censored value.

## WEIGHT Statement

**WEIGHT** *variable* ;

The *variable* in the WEIGHT statement identifies the variable in the input data set that contains the weights of the subjects. Values of the WEIGHT *variable* can be nonintegral and are not truncated. Observations with negative, zero, or missing values for the WEIGHT *variable* are not used in the computation.

The implementation of weights in PROC LIFETEST is based on Xie and Liu (2005, 2011), who use inverse probability of treatment weights to reduce confounding effects. A weight is assigned to each subject as the inverse probability of being in a certain group. If a subject has a higher probability of being in a group, it is considered as overrepresented and is therefore assigned a lower weight; on the other hand, if the subject has a smaller probability of being in a group, it is considered as underrepresented and is assigned a higher weight.

## Details: LIFETEST Procedure

### Missing Values

Observations with a missing value for either the failure time or the censoring variable are not used in the analysis. If a stratum variable value is missing, the observation is not used; however, the MISSING option can be used to request that missing values be treated as valid stratum values. If any variable specified in the TEST statement has a missing value, that observation is not used in the calculation of the rank statistics.

## Computational Formulas

### Breslow, Fleming-Harrington, and Kaplan-Meier Methods

Let  $t_1 < t_2 < \dots < t_D$  represent the distinct event times. For each  $i = 1, \dots, D$ , let  $Y_i$  be the number of surviving units (the size of the risk set) just prior to  $t_i$  and let  $d_i$  be the number of units that fail at  $t_i$ . If the NOTRUNCATE option is specified in the FREQ statement,  $Y_i$  and  $d_i$  can be nonintegers.

The Breslow estimate of the survivor function is

$$\hat{S}(t_i) = \exp\left(-\sum_{j=1}^i \frac{d_j}{Y_j}\right)$$

Note that the Breslow estimate is the exponentiation of the negative Nelson-Aalen estimate of the cumulative hazard function.

The Fleming-Harrington estimate (Fleming and Harrington 1984) of the survivor function is

$$\hat{S}(t_i) = \exp\left(-\sum_{k=1}^i \sum_{j=0}^{d_k-1} \frac{1}{Y_k - j}\right)$$

If the frequency values are not integers, the Fleming-Harrington estimate cannot be computed.

The Kaplan-Meier (product-limit) estimate of the survivor function at  $t_i$  is the cumulative product

$$\hat{S}(t_i) = \prod_{j=1}^i \left(1 - \frac{d_j}{Y_j}\right)$$

Notice that all the estimators are defined to be right continuous; that is, the events at  $t_i$  are included in the estimate of  $S(t_i)$ . The corresponding estimate of the standard error is computed using Greenwood's formula (Kalbfleisch and Prentice 1980) as

$$\hat{\sigma}\left(\hat{S}(t_i)\right) = \hat{S}(t_i) \sqrt{\sum_{j=1}^i \frac{d_j}{Y_j(Y_j - d_j)}}$$

The first quartile (or the 25th percentile) of the survival time is the time beyond which 75% of the subjects in the population under study are expected to survive. It is estimated by

$$q_{.25} = \min\{t_j | \hat{S}(t_j) < 0.75\}$$

If  $\hat{S}(t)$  is exactly equal to 0.75 from  $t_j$  to  $t_{j+1}$ , the first quartile is taken to be  $(t_j + t_{j+1})/2$ . If it happens that  $\hat{S}(t)$  is greater than 0.75 for all values of  $t$ , the first quartile cannot be estimated and is represented by a missing value in the printed output.

The general formula for estimating the 100 $p$  percentile point is

$$q_p = \min\{t_j | \hat{S}(t_j) < 1 - p\}$$

The second quartile (the median) and the third quartile of survival times correspond to  $p = 0.5$  and  $p = 0.75$ , respectively.

Brookmeyer and Crowley (1982) have constructed the confidence interval for the median survival time based on the confidence interval for the  $S(t)$ . The methodology is generalized to construct the confidence interval for the  $100p$  percentile based on a  $g$ -transformed confidence interval for  $S(t)$  (Klein and Moeschberger 1997). You can use the CONFTYPE= option to specify the  $g$ -transformation. The  $100(1 - \alpha)\%$  confidence interval for the first quantile survival time is the set of all points  $t$  that satisfy

$$\left| \frac{g(\hat{S}(t)) - g(1 - 0.25)}{g'(\hat{S}(t))\hat{\sigma}(\hat{S}(t))} \right| \leq z_{1-\frac{\alpha}{2}}$$

where  $g'(x)$  is the first derivative of  $g(x)$  and  $z_{1-\frac{\alpha}{2}}$  is the  $100(1 - \frac{\alpha}{2})$  percentile of the standard normal distribution.

Consider the bone marrow transplant data described in Example 52.2. The following table illustrates the construction of the confidence limits for the first quartile in the ALL group. Values of  $\frac{g(\hat{S}(t)) - g(1 - 0.25)}{g'(\hat{S}(t))\hat{\sigma}(\hat{S}(t))}$  that lie between  $\pm z_{1-\frac{0.05}{2}} = \pm 1.965$  are highlighted.

| Constructing 95% Confidence Limits for the 25th Percentile |              |                            |                                                                              |                 |                |                 |                 |
|------------------------------------------------------------|--------------|----------------------------|------------------------------------------------------------------------------|-----------------|----------------|-----------------|-----------------|
| t                                                          | $\hat{S}(t)$ | $\hat{\sigma}(\hat{S}(t))$ | $\frac{g(\hat{S}(t)) - g(1 - 0.25)}{g'(\hat{S}(t))\hat{\sigma}(\hat{S}(t))}$ |                 |                |                 |                 |
|                                                            |              |                            | LINEAR                                                                       | LOGLOG          | LOG            | ASINSQRT        | LOGIT           |
| 1                                                          | 0.97368      | 0.025967                   | 8.6141                                                                       | 2.37831         | 9.7871         | 4.44648         | 2.47903         |
| 55                                                         | 0.94737      | 0.036224                   | 5.4486                                                                       | 2.36375         | 6.1098         | 3.60151         | 2.46635         |
| 74                                                         | 0.92105      | 0.043744                   | 3.9103                                                                       | 2.16833         | 4.3257         | 2.94398         | 2.25757         |
| 86                                                         | 0.89474      | 0.049784                   | 2.9073                                                                       | <b>1.89961</b>  | 3.1713         | 2.38164         | 1.97023         |
| 104                                                        | 0.86842      | 0.054836                   | 2.1595                                                                       | <b>1.59196</b>  | 2.3217         | <b>1.87884</b>  | <b>1.64297</b>  |
| 107                                                        | 0.84211      | 0.059153                   | <b>1.5571</b>                                                                | <b>1.26050</b>  | <b>1.6490</b>  | <b>1.41733</b>  | <b>1.29331</b>  |
| 109                                                        | 0.81579      | 0.062886                   | <b>1.0462</b>                                                                | <b>0.91307</b>  | <b>1.0908</b>  | <b>0.98624</b>  | <b>0.93069</b>  |
| 110                                                        | 0.78947      | 0.066135                   | <b>0.5969</b>                                                                | <b>0.55415</b>  | <b>0.6123</b>  | <b>0.57846</b>  | <b>0.56079</b>  |
| 122                                                        | 0.73684      | 0.071434                   | <b>-0.1842</b>                                                               | <b>-0.18808</b> | <b>-0.1826</b> | <b>-0.18573</b> | <b>-0.18728</b> |
| 129                                                        | 0.71053      | 0.073570                   | <b>-0.5365</b>                                                               | <b>-0.56842</b> | <b>-0.5222</b> | <b>-0.54859</b> | <b>-0.56101</b> |
| 172                                                        | 0.68421      | 0.075405                   | <b>-0.8725</b>                                                               | <b>-0.95372</b> | <b>-0.8330</b> | <b>-0.90178</b> | <b>-0.93247</b> |
| 192                                                        | 0.65789      | 0.076960                   | <b>-1.1968</b>                                                               | <b>-1.34341</b> | <b>-1.1201</b> | <b>-1.24712</b> | <b>-1.30048</b> |
| 194                                                        | 0.63158      | 0.078252                   | <b>-1.5133</b>                                                               | <b>-1.73709</b> | <b>-1.3870</b> | <b>-1.58613</b> | <b>-1.66406</b> |
| 230                                                        | 0.60412      | 0.079522                   | <b>-1.8345</b>                                                               | -2.14672        | <b>-1.6432</b> | <b>-1.92995</b> | -2.03291        |
| 276                                                        | 0.57666      | 0.080509                   | -2.1531                                                                      | -2.55898        | <b>-1.8825</b> | -2.26871        | -2.39408        |
| 332                                                        | 0.54920      | 0.081223                   | -2.4722                                                                      | -2.97389        | -2.1070        | -2.60380        | -2.74691        |
| 383                                                        | 0.52174      | 0.081672                   | -2.7948                                                                      | -3.39146        | -2.3183        | -2.93646        | -3.09068        |
| 418                                                        | 0.49428      | 0.081860                   | -3.1239                                                                      | -3.81166        | -2.5177        | -3.26782        | -3.42460        |
| 466                                                        | 0.46682      | 0.081788                   | -3.4624                                                                      | -4.23445        | -2.7062        | -3.59898        | -3.74781        |
| 487                                                        | 0.43936      | 0.081457                   | -3.8136                                                                      | -4.65971        | -2.8844        | -3.93103        | -4.05931        |
| 526                                                        | 0.41190      | 0.080862                   | -4.1812                                                                      | -5.08726        | -3.0527        | -4.26507        | -4.35795        |
| 609                                                        | 0.38248      | 0.080260                   | -4.5791                                                                      | -5.52446        | -3.2091        | -4.60719        | -4.64271        |
| 662                                                        | 0.35306      | 0.079296                   | -5.0059                                                                      | -5.96222        | -3.3546        | -4.95358        | -4.90900        |

Consider the LINEAR transformation where  $g(x) = x$ . The event times that satisfy  $\left| \frac{g(\hat{S}(t)) - g(1 - p)}{g'(\hat{S}(t))\sqrt{\hat{V}(\hat{S}(t))}} \right| \leq 1.9599$  include 107, 109, 110, 122, 129, 172, 192, 194, and 230. The confidence of the interval [107, 230] is less than 95%. Brookmeyer and Crowley (1982) suggest extending the confidence interval to but not

including the next event time. As such the 95% confidence interval for the first quartile based on the linear transform is [107, 276). The following table lists the confidence intervals for the various transforms.

| 95% CI's for the 25th Percentile |        |        |
|----------------------------------|--------|--------|
| CONFTYPE                         | [Lower | Upper) |
| LINEAR                           | 107    | 276    |
| LOGLOG                           | 86     | 230    |
| LOG                              | 107    | 332    |
| ASINSQRT                         | 104    | 276    |
| LOGIT                            | 104    | 230    |

Sometimes, the confidence limits for the quartiles cannot be estimated. For convenience of explanation, consider the linear transform  $g(x) = x$ . If the curve that represents the upper confidence limits for the survivor function lies above 0.75, the upper confidence limit for first quartile cannot be estimated. On the other hand, if the curve that represents the lower confidence limits for the survivor function lies above 0.75, the lower confidence limit for the quartile cannot be estimated.

The estimated mean survival time is

$$\hat{\mu} = \sum_{i=1}^D \hat{S}(t_{i-1})(t_i - t_{i-1})$$

where  $t_0$  is defined to be zero. When the largest observed time is censored, this sum underestimates the mean. The standard error of  $\hat{\mu}$  is estimated as

$$\hat{\sigma}(\hat{\mu}) = \sqrt{\frac{m}{m-1} \sum_{i=1}^{D-1} \frac{A_i^2}{Y_i(Y_i - d_i)}}$$

where

$$A_i = \sum_{j=i}^{D-1} \hat{S}(t_j)(t_{j+1} - t_j)$$

$$m = \sum_{j=1}^D d_j$$

If the largest observed time is not an event, you can use the TIMELIM= option to specify a time limit  $L$  and estimate the mean survival time limited to the time  $L$  and its standard error by replacing  $k$  by  $k + 1$  with  $t_{k+1} = L$ .

### **Nelson-Aalen Estimate of the Cumulative Hazard Function**

The Nelson-Aalen cumulative hazard estimator, defined up to the largest observed time on study, is

$$\tilde{H}(t) = \sum_{t_i \leq t} \frac{d_i}{Y_i}$$

and its estimated variance is

$$\hat{\sigma}^2(\tilde{H}(t)) = \sum_{t_i \leq t} \frac{d_i}{Y_i^2}$$

### Adjusted Kaplan-Meier Estimate

PROC LIFETEST computes the adjusted Kaplan-Meier estimate (AKME) of the survivor function if you specify both METHOD=KM and the WEIGHT statement. Let  $(T_i, \delta_i, w_i), i = 1, \dots, n$ , denote an independent sample of right-censored survival data, where  $T_i$  is the possibly right-censored time,  $\delta_i$  is the censoring indicator ( $\delta_i = 0$  if  $T_i$  is censored and  $\delta_i = 1$  if  $T_i$  is an event time), and  $w_i$  is the weight (from the WEIGHT statement). Let  $t_1 < t_2, \dots < t_D$  be the  $D$  distinct event times in the sample. At time  $t_j, j = 1, \dots, D$ , there are  $d_j = \sum_i \delta_i I(T_i = t_j)$  events out of  $Y_j = \sum_i I(T_i \geq t_j)$  subjects. The weighted number of events and the weighted number at risk are  $d_j^w = \sum_i w_i \delta_i I(T_i = t_j)$  and  $Y_j^w = \sum_i w_i I(T_i \geq t_j)$ , respectively. The AKME (Xie and Liu 2005) is

$$\hat{S}(t) = \begin{cases} 1 & \text{if } t < t_1 \\ \prod_{t_j \leq t} \left[ 1 - \frac{d_j^w}{Y_j^w} \right] & \text{if } t \geq t_1 \end{cases}$$

The estimated variance of  $\hat{S}(t)$  is

$$\hat{\sigma}^2(\hat{S}(t)) = (\hat{S}(t))^2 \sum_{j:t_j \leq t} \frac{d_j^w / Y_j^w}{M_j (1 - d_j^w / Y_j^w)}$$

where

$$M_j = \frac{\left( \sum_{i:T_i \geq t_j} w_i \right)^2}{\sum_{i:T_i \geq t_j} w_i^2}$$

### Life-Table Method

The life-table estimates are computed by counting the numbers of censored and uncensored observations that fall into each of the time intervals  $[t_{i-1}, t_i), i = 1, 2, \dots, k + 1$ , where  $t_0 = 0$  and  $t_{k+1} = \infty$ . Let  $n_i$  be the number of units that enter the interval  $[t_{i-1}, t_i)$ , and let  $d_i$  be the number of events that occur in the interval. Let  $b_i = t_i - t_{i-1}$ , and let  $n'_i = n_i - w_i/2$ , where  $w_i$  is the number of units censored in the interval. The effective sample size of the interval  $[t_{i-1}, t_i)$  is denoted by  $n'_i$ . Let  $t_{mi}$  denote the midpoint of  $[t_{i-1}, t_i)$ .

The conditional probability of an event in  $[t_{i-1}, t_i)$  is estimated by

$$\hat{q}_i = \frac{d_i}{n'_i}$$

and its estimated standard error is

$$\hat{\sigma}(\hat{q}_i) = \sqrt{\frac{\hat{q}_i \hat{p}_i}{n'_i}}$$

where  $\hat{p}_i = 1 - \hat{q}_i$ .

The estimate of the survival function at  $t_i$  is

$$\hat{S}(t_i) = \begin{cases} 1 & i = 0 \\ \hat{S}(t_{i-1})p_{i-1} & i > 0 \end{cases}$$

and its estimated standard error is

$$\hat{\sigma}(\hat{S}(t_i)) = \hat{S}(t_i) \sqrt{\sum_{j=1}^{i-1} \frac{\hat{q}_j}{n'_j \hat{p}_j}}$$

The density function at  $t_{mi}$  is estimated by

$$\hat{f}(t_{mi}) = \frac{\hat{S}(t_i)\hat{q}_i}{b_i}$$

and its estimated standard error is

$$\hat{\sigma}(\hat{f}(t_{mi})) = \hat{f}(t_{mi}) \sqrt{\sum_{j=1}^{i-1} \frac{\hat{q}_j}{n'_j \hat{p}_j} + \frac{\hat{p}_i}{n'_i \hat{q}_i}}$$

The estimated hazard function at  $t_{mi}$  is

$$\hat{h}(t_{mi}) = \frac{2\hat{q}_i}{b_i(1 + \hat{p}_i)}$$

and its estimated standard error is

$$\hat{\sigma}(\hat{h}(t_{mi})) = \hat{h}(t_{mi}) \sqrt{\frac{1 - (b_i \hat{h}(t_{mi})/2)^2}{n'_i \hat{q}_i}}$$

Let  $[t_{j-1}, t_j]$  be the interval in which  $\hat{S}(t_{j-1}) \geq \hat{S}(t_i)/2 > \hat{S}(t_j)$ . The median residual lifetime at  $t_i$  is estimated by

$$\hat{M}_i = t_{j-1} - t_i + b_j \frac{\hat{S}(t_{j-1}) - \hat{S}(t_i)/2}{\hat{S}(t_{j-1}) - \hat{S}(t_j)}$$

and the corresponding standard error is estimated by

$$\hat{\sigma}(\hat{M}_i) = \frac{\hat{S}(t_i)}{2\hat{f}(t_{mj})\sqrt{n'_i}}$$

### Interval Determination

If you want to determine the intervals exactly, use the INTERVALS= option in the PROC LIFETEST statement to specify the interval endpoints. Use the WIDTH= option to specify the width of the intervals, thus indirectly determining the number of intervals. If neither the INTERVALS= option nor the WIDTH= option is specified in the life-table estimation, the number of intervals is determined by the NINTERVAL= option. The width of the time intervals is 2, 5, or 10 times an integer (possibly a negative integer) power of 10. Let

$c = \log_{10}(\text{maximum observed time/number of intervals})$ , and let  $b$  be the largest integer not exceeding  $c$ . Let  $d = 10^{c-b}$  and let

$$a = 2 \times I(d \leq 2) + 5 \times I(2 < d \leq 5) + 10 \times I(d > 5)$$

with  $I$  being the indicator function. The width is then given by

$$\text{width} = a \times 10^b$$

By default, NINTERVAL=10.

### Pointwise Confidence Limits in the OUTSURV= Data Set

Pointwise confidence limits are computed for the survivor function, and for the density function and hazard function when the life-table method is used. Let  $\alpha$  be specified by the ALPHA= option. Let  $z_{\alpha/2}$  be the critical value for the standard normal distribution. That is,  $\Phi(-z_{\alpha/2}) = \alpha/2$ , where  $\Phi$  is the cumulative distribution function of the standard normal random variable.

#### Survivor Function

When the computation of confidence limits for the survivor function  $S(t)$  is based on the asymptotic normality of the survival estimator  $\hat{S}(t)$ , the approximate confidence interval might include impossible values outside the range  $[0,1]$  at extreme values of  $t$ . This problem can be avoided by applying the asymptotic normality to a transformation of  $S(t)$  for which the range is unrestricted. In addition, certain transformed confidence intervals for  $S(t)$  perform better than the usual linear confidence intervals (Borgan and Liestøl 1990). The CONFTYPE= option enables you to pick one of the following transformations: the log-log function (Kalbfleisch and Prentice 1980), the arcsine-square root function (Nair 1984), the logit function (Meeker and Escobar 1998), the log function, and the linear function.

Let  $g$  be the transformation that is being applied to the survivor function  $S(t)$ . By the delta method, the standard error of  $g(\hat{S}(t))$  is estimated by

$$\tau(t) = \hat{\sigma} \left[ g(\hat{S}(t)) \right] = g'(\hat{S}(t)) \hat{\sigma}[\hat{S}(t)]$$

where  $g'$  is the first derivative of the function  $g$ . The  $100(1-\alpha)\%$  confidence interval for  $S(t)$  is given by

$$g^{-1} \left\{ g[\hat{S}(t)] \pm z_{\alpha/2} g'[\hat{S}(t)] \hat{\sigma}[\hat{S}(t)] \right\}$$

where  $g^{-1}$  is the inverse function of  $g$ . That choices of the transformation  $g$  are as follows:

- arcsine-square root transformation: The estimated variance of  $\sin^{-1}(\sqrt{\hat{S}(t)})$  is  $\hat{\tau}^2(t) = \frac{\hat{\sigma}^2[\hat{S}(t)]}{4\hat{S}(t)[1-\hat{S}(t)]}$ . The  $100(1-\alpha)\%$  confidence interval for  $S(t)$  is given by

$$\sin^2 \left\{ \max \left[ 0, \sin^{-1}(\sqrt{\hat{S}(t)}) - z_{\alpha/2} \hat{\tau}(t) \right] \right\} \leq S(t) \leq \sin^2 \left\{ \min \left[ \frac{\pi}{2}, \sin^{-1}(\sqrt{\hat{S}(t)}) + z_{\alpha/2} \hat{\tau}(t) \right] \right\}$$

- linear transformation: This is the same as having no transformation in which  $g$  is the identity. The  $100(1-\alpha)\%$  confidence interval for  $S(t)$  is given by

$$\hat{S}(t) - z_{\alpha/2} \hat{\sigma}[\hat{S}(t)] \leq S(t) \leq \hat{S}(t) + z_{\alpha/2} \hat{\sigma}[\hat{S}(t)]$$



- log transformation: The estimated variance of  $\log(\hat{S}(t))$  is  $\hat{\tau}^2(t) = \frac{\hat{\sigma}^2(\hat{S}(t))}{\hat{S}^2(t)}$ . The  $100(1-\alpha)\%$  confidence interval for  $S(t)$  is given by

$$\hat{S}(t) \exp\left(-z_{\frac{\alpha}{2}} \hat{\tau}(t)\right) \leq S(t) \leq \hat{S}(t) \exp\left(z_{\frac{\alpha}{2}} \hat{\tau}(t)\right)$$

- log-log transformation: The estimated variance of  $\log(-\log(\hat{S}(t)))$  is  $\hat{\tau}^2(t) = \frac{\hat{\sigma}^2[\hat{S}(t)]}{[\hat{S}(t) \log(\hat{S}(t))]^2}$ . The  $100(1-\alpha)\%$  confidence interval for  $S(t)$  is given by

$$\left[\hat{S}(t)\right]^{\exp\left(z_{\frac{\alpha}{2}} \hat{\tau}(t)\right)} \leq S(t) \leq \left[\hat{S}(t)\right]^{\exp\left(-z_{\frac{\alpha}{2}} \hat{\tau}(t)\right)}$$

- logit transformation: The estimated variance of  $\log\left(\frac{\hat{S}(t)}{1-\hat{S}(t)}\right)$  is

$$\hat{\tau}^2(t) = \frac{\hat{\sigma}^2(\hat{S}(t))}{\hat{S}^2(t)[1-\hat{S}(t)]^2}$$

The  $100(1-\alpha)\%$  confidence limits for  $S(t)$  are given by

$$\frac{\hat{S}(t)}{\hat{S}(t) + \left[1 - \hat{S}(t)\right] \exp\left(z_{\frac{\alpha}{2}} \hat{\tau}(t)\right)} \leq S(t) \leq \frac{\hat{S}(t)}{\hat{S}(t) + \left[1 - \hat{S}(t)\right] \exp\left(-z_{\frac{\alpha}{2}} \hat{\tau}(t)\right)}$$

### Density and Hazard Functions

For the life-table method, a  $100(1-\alpha)\%$  confidence interval for hazard function or density function at time  $t$  is computed as

$$\hat{g}(t) \pm z_{\alpha/2} \hat{\sigma}[\hat{g}(t)]$$

where  $\hat{g}(t)$  is the estimate of either the hazard function or the density function at time  $t$ , and  $\hat{\sigma}[\hat{g}(t)]$  is the corresponding standard error estimate.

### Simultaneous Confidence Intervals for Kaplan-Meier Curves

The pointwise confidence interval for the survivor function  $S(t)$  is valid for a single fixed time at which the inference is to be made. In some applications, it is of interest to find the upper and lower confidence bands that guarantee, with a given confidence level, that the survivor function falls within the band for all  $t$  in some interval. Hall and Wellner (1980) and Nair (1984) provide two different approaches for deriving the confidence bands. An excellent review can be found in Klein and Moeschberger (1997). You can use the CONF BAND= option in the SURVIVAL statement to select the confidence bands. The EP confidence band provides confidence bounds that are proportional to the pointwise confidence interval, while those of the HW band are not proportional to the pointwise confidence bounds. The maximum time,  $t_U$ , for the bands can be specified by the BANDMAX= option; the minimum time,  $t_L$ , can be specified by the BANDMIN= option. Transformations that are used to improve the pointwise confidence intervals can be applied to improve the confidence bands. It might turn out that the upper and lower bounds of the confidence bands are not decreasing in  $t_L < t < t_U$ , which is contrary to the nonincreasing characteristic of survivor function. Meeker and Escobar (1998) suggest making an adjustment so that the bounds do not increase: if the upper bound is increasing on the right, it is made flat from the minimum to  $t_U$ ; if the lower bound is

increasing from the right, it is made flat from  $t_L$  to the maximum. PROC LIFETEST does not make any adjustment for the nondecreasing behavior of the confidence bands in the OUTSURV= data set. However, the adjustment was made in the display of the confidence bands by using ODS Graphics.

For Kaplan-Meier estimation, let  $t_1 < t_2 < \dots < t_D$  be the  $D$  distinct events times, and at time  $t_i$ , there are  $d_i$  events. Let  $Y_i$  be the number of individuals who are at risk at time  $t_i$ . The variance of  $\hat{S}(t)$ , given by the Greenwood formula, is  $\hat{\sigma}^2[\hat{S}(t)] = \sigma_S^2(t)\hat{S}^2(t)$ , where

$$\sigma_S^2(t) = \sum_{t_i \leq t} \frac{d_i}{Y_i(Y_i - d_i)}$$

Let  $t_L < t_U$  be the time range for the confidence band so that  $t_U$  is less than or equal to the largest event time. For the Hall-Wellner band,  $t_L$  can be zero, but for the equal-precision band,  $t_L$  is greater than or equal to the smallest event time. Let

$$a_L = \frac{n\sigma_S^2(t_L)}{1 + n\sigma_S^2(t_L)} \quad \text{and} \quad a_U = \frac{n\sigma_S^2(t_U)}{1 + n\sigma_S^2(t_U)}$$

Let  $\{W^0(u), 0 \leq u \leq 1\}$  be a Brownian bridge.

### Hall-Wellner Band

The 100(1- $\alpha$ )% HW band of Hall and Wellner (1980) is

$$\hat{S}(t) - h_\alpha(a_L, a_U)n^{-\frac{1}{2}}[1 + n\sigma_S^2(t)]\hat{S}(t) \leq S(t) \leq \hat{S}(t) + h_\alpha(a_L, a_U)n^{-\frac{1}{2}}[1 + n\sigma_S^2(t)]\hat{S}(t)$$

for all  $t_L \leq t \leq t_U$ , where the critical value  $h_\alpha(a_L, a_U)$  is given by

$$\alpha = \Pr\left\{ \sup_{a_L \leq u \leq a_U} |W^0(u)| > h_\alpha(a_L, a_U) \right\}$$

The critical values are computed from the results in Chung (1986).

Note that the given confidence band has a formula similar to that of the (linear) pointwise confidence interval, where  $h_\alpha(a_L, a_U)$  and  $n^{-\frac{1}{2}}[1 + n\sigma_S^2(t)]\hat{S}(t)$  in the former correspond to  $z_{\frac{\alpha}{2}}$  and  $\hat{\sigma}(\hat{S}(t))$  in the latter, respectively. You can obtain the other transformations (arcsine-square root, log-log, log, and logit) for the confidence bands by replacing  $z_{\frac{\alpha}{2}}$  and  $\hat{\tau}(t)$  in the corresponding pointwise confidence interval formula by  $h_\alpha(a_L, a_U)$  and the following  $\hat{\tau}(t)$ , respectively:

- arcsine-square root transformation:

$$\hat{\tau}(t) = \frac{1 + n\sigma_S^2(t)}{2} \sqrt{\frac{S(t)}{n[1 - S(t)]}}$$

- log transformation:

$$\hat{\tau}(t) = \frac{1 + n\sigma_S^2(t)}{\sqrt{n}}$$

- log-log transformation:

$$\hat{t}(t) = \frac{1 + n\sigma_S^2(t)}{\sqrt{n}|\log[\hat{S}(t)]|}$$

- logit transformation:

$$\hat{t}(t) = \frac{1 + n\sigma_S^2(t)}{\sqrt{n}[1 - \hat{S}(t)]}$$

### Equal-Precision Band

The  $100(1-\alpha)\%$  EP band of Nair (1984) is

$$\hat{S}(t) - e_\alpha(a_L, a_U)\hat{S}(t)\sigma_S(t) \leq S(t) \leq \hat{S}(t) + e_\alpha(a_L, a_U)\hat{S}(t)\sigma_S(t)$$

for all  $t_L \leq t \leq t_U$ , where  $e_\alpha(a_L, a_U)$  is given by

$$\alpha = \Pr\left\{ \sup_{a_L \leq u \leq a_U} \frac{|W^0(u)|}{[u(1-u)]^{\frac{1}{2}}} > e_\alpha(a_L, a_U) \right\}$$

PROC LIFETEST uses the approximation of Miller and Siegmund (1982, Equation 8) to approximate the tail probability in which  $e_\alpha(a_L, a_U)$  is obtained by solving  $x$  in

$$\frac{4x\phi(x)}{x} + \phi(x) \left( x - \frac{1}{x} \right) \log \left[ \frac{a_U(1-a_L)}{a_L(1-a_U)} \right] = \alpha$$

where  $\phi(x)$  is the standard normal density function evaluated at  $x$ . Note that the confidence bounds given are proportional to the pointwise confidence intervals. As a matter of fact, this confidence band and the (linear) pointwise confidence interval have the same formula except for the critical values ( $z_{\frac{\alpha}{2}}$  for the pointwise confidence interval and  $e_\alpha(a_L, a_U)$  for the band). You can obtain the other transformations (arcsine-square root, log-log, log, and logit) for the confidence bands by replacing  $z_{\frac{\alpha}{2}}$  by  $e_\alpha(a_L, a_U)$  in the formula of the pointwise confidence intervals.

### Kernel-Smoothed Hazard Estimate

Kernel-smoothed estimators of the hazard function  $h(t)$  are based on the Nelson-Aalen estimator  $\tilde{H}(t)$  and its variance  $\hat{V}(\tilde{H}(t))$ . Consider the jumps of  $\tilde{H}(t)$  and  $\hat{V}(\tilde{H}(t))$  at the event times  $t_1 < t_2 < \dots < t_D$  as follows:

$$\begin{aligned} \Delta\tilde{H}(t_i) &= \tilde{H}(t_i) - \tilde{H}(t_{i-1}) \\ \hat{V}(\tilde{H}(t_i)) &= \hat{V}(\tilde{H}(t_i)) - \hat{V}(\tilde{H}(t_{i-1})) \end{aligned}$$

where  $t_0=0$ .

The kernel-smoothed estimator of  $h(t)$  is a weighted average of  $\Delta\tilde{H}(t)$  over event times that are within a bandwidth distance  $b$  of  $t$ . The weights are controlled by the choice of kernel function,  $K()$ , defined on the interval  $[-1,1]$ . The choices are as follows:

- uniform kernel:

$$K_U(x) = \frac{1}{2}, \quad -1 \leq x \leq 1$$

- Epanechnikov kernel:

$$K_E(x) = \frac{3}{4}(1 - x^2), \quad -1 \leq x \leq 1$$

- biweight kernel:

$$K_{BW}(x) = \frac{15}{16}(1 - x^2)^2, \quad -1 \leq x \leq 1$$

The kernel-smoothed hazard rate estimator is defined for all time points on  $(0, t_D)$ . For time points  $t$  for which  $b \leq t \leq t_D - b$ , the kernel-smoothed estimated of  $h(t)$  based on the kernel  $K()$  is given by

$$\hat{h}(t) = \frac{1}{b} \sum_{i=1}^D K\left(\frac{t - t_i}{b}\right) \Delta \tilde{H}(t_i)$$

The variance of  $\hat{h}(t)$  is estimated by

$$\hat{\sigma}^2(\hat{h}(t)) = \frac{1}{b^2} \sum_{i=1}^D K\left(\frac{t - t_i}{b}\right)^2 \Delta \hat{V}(\tilde{H}(t_i))$$

For  $t < b$ , the symmetric kernels  $K()$  are replaced by the corresponding asymmetric kernels of Gasser and Müller (1979). Let  $q = \frac{t}{b}$ . The modified kernels are as follows:

- uniform kernel:

$$K_{U,q}(x) = \frac{4(1 + q^3)}{(1 + q)^4} + \frac{6(1 - q)}{(1 + q)^3}x, \quad -1 \leq x \leq q$$

- Epanechnikov kernel:

$$K_{E,q}(x) = K_E(x) \frac{64(2 - 4q + 6q^2 - 3q^3) + 240(1 - q)^2x}{(1 + q)^4(19 - 18q + 3q^2)}, \quad -1 \leq x \leq q$$

- biweight kernel:

$$K_{BW,q}(x) = K_{BW}(x) \frac{64(8 - 24q + 48q^2 - 45q^3 + 15q^4) + 1120(1 - q)^3x}{(1 + q)^5(81 - 168q + 126q^2 - 40q^3 + 5q^4)}, \quad -1 \leq x \leq q$$

For  $t_D - b \leq t \leq t_D$ , let  $q = \frac{t_D - t}{b}$ . The asymmetric kernels for  $t < b$  are used with  $x$  replaced by  $-x$ .

Using the log transform on the smoothed hazard rate, the  $100(1 - \alpha)\%$  pointwise confidence interval for the smoothed hazard rate  $h(t)$  is given by

$$\hat{h}(t) = \hat{h}(t) \exp\left[\pm \frac{z_{1-\alpha/2} \hat{\sigma}(\hat{h}(t))}{\hat{h}(t)}\right]$$

where  $z_{1-\frac{\alpha}{2}}$  is the  $100(1 - \frac{\alpha}{2})$ th percentile of the standard normal distribution.

### Optimal Bandwidth

The following mean integrated squared error (MISE) over the range  $\tau_L$  and  $\tau_U$  is used as a measure of the global performance of the kernel function estimator:

$$\begin{aligned} \text{MISE}(b) &= E \int_{\tau_L}^{\tau_U} (\hat{h}(i) - h(u))^2 du \\ &= E \int_{\tau_L}^{\tau_U} \hat{h}^2(u) du - 2E \int_{\tau_L}^{\tau_U} \hat{h}(u)h(u) du + E \int_{\tau_L}^{\tau_U} h^2(u) du \end{aligned}$$

The last term is independent of the choice of the kernel and bandwidth and can be ignored when you are looking for the best value of  $b$ . The first integral can be approximated by using the trapezoid rule by evaluating  $\hat{h}(t)$  at a grid of points  $\tau_L = u_1 < \dots < u_M = \tau_U$ . You can specify  $\tau_L$ ,  $\tau_R$ , and  $M$  by using the options GRIDL=, GRIDU=, and NMINGRID=, respectively, of the HAZARD plot. The second integral can be estimated by the Ramlau-Hansen (1983a, b) cross-validation estimate:

$$\frac{1}{b} \sum_{i \neq j} K\left(\frac{t_i - t_j}{b}\right) \Delta \hat{H}(t_i) \Delta \hat{H}(t_j)$$

Therefore, for a fixed kernel, the optimal bandwidth is the quantity  $b$  that minimizes

$$g(b) = \sum_{i=1}^{M-1} \left[ \frac{u_{i+1} - u_i}{2} \left( \hat{h}^2(u_i) + \hat{h}^2(u_{i+1}) \right) \right] - \frac{2}{b} \sum_{i \neq j} K\left(\frac{t_i - t_j}{b}\right) \Delta \hat{H}(t_i) \Delta \hat{H}(t_j)$$

The minimization is carried out by the golden section search algorithm.

### Comparison of Two or More Groups of Survival Data

Let  $K$  be the number of groups. Let  $S_k(t)$  be the underlying survivor function of the  $k$ th group,  $k = 1, \dots, K$ . The null and alternative hypotheses to be tested are

$$H_0 : S_1(t) = S_2(t) = \dots = S_K(t) \text{ for all } t \leq \tau$$

versus

$$H_1 : \text{at least one of the } S_k(t)\text{'s is different for some } t \leq \tau$$

respectively, where  $\tau$  is the largest observed time.

### Likelihood Ratio Test

The likelihood ratio test statistic (Lawless 1982) for test  $H_0$  versus  $H_1$  assumes that the data in the various samples are exponentially distributed and tests that the scale parameters are equal. The test statistic is computed as

$$\chi^2 = 2N \log\left(\frac{T}{N}\right) - 2 \sum_{k=1}^K N_k \log\left(\frac{T_k}{N_k}\right)$$

where  $N_k$  is the total number of events in the  $k$ th group,  $N = \sum_{k=1}^K N_k$ ,  $T_k$  is the total time on test in the  $k$ th stratum, and  $T = \sum_{k=1}^K T_k$ . The approximate probability value is computed by treating  $\chi^2$  as having a chi-square distribution with  $K - 1$  degrees of freedom.

**Nonparametric Tests**

Let  $(T_i, \delta_i, X_i), i = 1, \dots, n$ , denote an independent sample of right-censored survival data, where  $T_i$  is the possibly right-censored time,  $\delta_i$  is the censoring indicator ( $\delta_i=0$  if  $T_i$  is censored and  $\delta_i=1$  if  $T_i$  is an event time), and  $X_i = 1, \dots, K$  for  $K$  different groups. Let  $t_1 < t_2 < \dots < t_D$  be the distinct event times in the sample. At time  $t_j, j = 1, \dots, D$ , let  $W(t_j)$  be a positive weight function, and let  $Y_{jk} = \sum_{i:T_i \geq t_j} I(X_i = k)$  and  $d_{jk} = \sum_{i:T_i = t_j} \delta_i I(X_i = k)$  be the size of the risk set and the number of events in the  $k$ th group, respectively. Let  $Y_j = \sum_{k=1}^K Y_{jk}, d_j = \sum_{k=1}^K d_{jk}$ .

The choices of the weight function  $W(t_j)$  are given in Table 52.4.

**Table 52.4** Weight Functions for Various Tests

| Test                       | $W(t_i)$                                                    |
|----------------------------|-------------------------------------------------------------|
| Log-rank                   | 1.0                                                         |
| Wilcoxon                   | $Y_j$                                                       |
| Tarone-Ware                | $\sqrt{Y_j}$                                                |
| Peto-Peto                  | $\hat{S}(t_j)$                                              |
| Modified Peto-Peto         | $\tilde{S}(t_j) \frac{Y_j}{Y_j+1}$                          |
| Harrington-Fleming $(p,q)$ | $[\hat{S}(t_j)]^p [1 - \hat{S}(t_j)]^q, p \geq 0, q \geq 0$ |

In Table 52.4,  $\hat{S}(t)$  is the product-limit estimate at  $t$  for the pooled sample, and  $\tilde{S}(t)$  is a survivor function estimate close to  $\hat{S}(t)$  given by

$$\tilde{S}(t) = \prod_{t_j \leq t} \left( 1 - \frac{d_j}{Y_j + 1} \right)$$

**Unstratified Tests** The rank statistics (Klein and Moeschberger 1997, Section 7.3) for testing  $H_0$  versus  $H_1$  have the form of a  $K$ -vector  $\mathbf{v} = (v_1, v_2, \dots, v_K)'$  with

$$v_k = \sum_{j=1}^D \left[ W(t_j) \left( d_{jk} - Y_{jk} \frac{d_j}{Y_j} \right) \right]$$

and the variance of  $v_k$  and the covariance of  $v_k$  and  $v_h$  are, respectively,

$$V_{kk} = \sum_{j=1}^D \left[ W^2(t_j) \frac{d_j(Y_j - d_j)Y_{jk}(Y_j - Y_{jk})}{Y_j^2(Y_j - 1)} \right], \quad 1 \leq k \leq K$$

$$V_{kh} = - \sum_{j=1}^D \left[ W^2(t_j) \frac{d_j(Y_j - d_j)Y_{jk}Y_{jh}}{Y_j^2(Y_j - 1)} \right], \quad 1 \leq k \neq h \leq K$$

The statistic  $v_k$  can be interpreted as a weighted sum of observed minus expected numbers of failure for the  $k$ th group under the null hypothesis of identical survival curves. Let  $\mathbf{V} = (V_{kh})$ . The overall test statistic for homogeneity is  $\mathbf{v}'\mathbf{V}^-\mathbf{v}$ , where  $\mathbf{V}^-$  denotes a generalized inverse of  $\mathbf{V}$ . This statistic is treated as having a chi-square distribution with degrees of freedom equal to the rank of  $\mathbf{V}$  for the purposes of computing an approximate probability level.

**Adjusted Log-Rank Test** PROC LIFETEST computes the weighted log-rank test (Xie and Liu 2005, 2011) if you specify the WEIGHT statement. Let  $(T_i, \delta_i, X_i, w_i), i = 1, \dots, n$ , denote an independent sample of right-censored survival data, where  $T_i$  is the possibly right-censored time,  $\delta_i$  is the censoring indicator ( $\delta_i=0$  if  $T_i$  is censored and  $\delta_i=1$  if  $T_i$  is an event time),  $X_i = 1, \dots, K$  for  $K$  different groups, and  $w_i$  is the weight from the WEIGHT statement. Let  $t_1 < t_2 < \dots < t_D$  be the distinct event times in the sample. At each  $t_j, j = 1, \dots, D$ , and for each  $1 \leq k \leq K$ , let

$$d_{jk} = \sum_{i:T_i=t_j} I(X_i = k) \quad d_{jk}^w = \sum_{i:T_i=t_j} w_i I(X_i = k)$$

$$Y_{jk} = \sum_{i:T_i \geq t_j} I(X_i = k) \quad Y_{jk}^w = \sum_{i:T_i \geq t_j} w_i I(X_i = k)$$

Let  $d_j = \sum_{k=1}^K d_{jk}$  and  $Y_j = \sum_{k=1}^K Y_{jk}$  denote the number of events and the number at risk, respectively, in the combined sample at time  $t_j$ . Similarly, let  $d_j^w = \sum_{k=1}^K d_{jk}^w$  and  $Y_j^w = \sum_{k=1}^K Y_{jk}^w$  denote the weighted number of events and the weighted number at risk, respectively, in the combined sample at time  $t_j$ . The test statistic is

$$v_k = \sum_{j=1}^D \left( d_{jk}^w - Y_{jk}^w \frac{d_j^w}{Y_j^w} \right) \quad k = 1, \dots, K$$

and the variance of  $v_k$  and the covariance of  $v_k$  and  $v_h$  are, respectively,

$$V_{kk} = \sum_{j=1}^D \left\{ \frac{d_j(Y_j - d_j)}{Y_j(Y_j - 1)} \sum_{i=1}^{Y_j} \left[ \left( \frac{Y_{jk}^w}{Y_j^w} \right)^2 w_i^2 I\{X_i \neq k\} + \left( \frac{Y_j^w - Y_{jk}^w}{Y_j^w} \right)^2 w_i^2 I\{X_i = k\} \right] \right\}, \quad 1 \leq k \leq K$$

$$V_{kh} = \sum_{j=1}^D \left\{ \frac{d_j(Y_j - d_j)}{Y_j(Y_j - 1)} \sum_{i=1}^{Y_j} \left[ \frac{Y_{jk}^w Y_{jh}^w}{(Y_j^w)^2} w_i^2 I\{X_i \neq k, h\} - \frac{(Y_j^w - Y_{jk}^w) Y_{jh}^w}{(Y_j^w)^2} w_i^2 I\{X_i = k\} \right. \right. \\ \left. \left. - \frac{(Y_j^w - Y_{jh}^w) Y_{jk}^w}{(Y_j^w)^2} w_i^2 I\{X_i = h\} \right] \right\}, \quad 1 \leq k \neq h \leq K$$

Let  $V = (V_{kh})$ . Under  $H_0$ , the weighted  $K$ -sample test has a  $\chi^2$  statistic given by

$$\chi^2 = (v_1, \dots, v_K) \mathbf{V}^{-1} (v_1, \dots, v_K)'$$

with  $K - 1$  degrees of freedom.

**Stratified Tests** Suppose the test is to be stratified on  $M$  levels of a set of STRATA variables. Based only on the data of the  $s$ th stratum ( $s = 1 \dots M$ ), let  $\mathbf{v}_s$  be the test statistic (Klein and Moeschberger 1997, Section 7.5) for the  $s$ th stratum, and let  $\mathbf{V}_s$  be its covariance matrix. Let

$$\mathbf{v} = \sum_{s=1}^M \mathbf{v}_s$$

$$\mathbf{V} = \sum_{s=1}^M \mathbf{V}_s$$

A global test statistic is constructed as

$$\chi^2 = \mathbf{v}'\mathbf{V}^{-1}\mathbf{v}$$

Under the null hypothesis, the test statistic has a  $\chi^2$  distribution with the same degrees of freedom as the individual test for each stratum.

**Multiple-Comparison Adjustments** Let  $\chi_r^2$  denote a chi-square random variable with  $r$  degrees of freedom. Denote  $\phi$  and  $\Phi$  as the density function and the cumulative distribution function of a standard normal distribution, respectively. Let  $m$  be the number of comparisons; that is,

$$m = \begin{cases} \frac{k(k-1)}{2} & \text{DIFF} = \text{ALL} \\ k-1 & \text{DIFF} = \text{CONTROL} \end{cases}$$

For a two-sided test that compares the survival of the  $j$ th group with that of  $l$ th group,  $1 \leq j \neq l \leq r$ , the test statistic is

$$z_{jl}^2 = \frac{(v_j - v_l)^2}{V_{jj} + V_{ll} - 2V_{jl}}$$

and the raw  $p$ -value is

$$p = \Pr(\chi_1^2 > z_{jl}^2)$$

Adjusted  $p$ -values for various multiple-comparison adjustments are computed as follows:

- Bonferroni adjustment:

$$p = \min\{1, m\Pr(\chi_1^2 > z_{jl}^2)\}$$

- Dunnett-Hsu adjustment: With the first group being the control, let  $\mathbf{C} = (c_{ij})$  be the  $(r-1) \times r$  matrix of contrasts; that is,

$$c_{ij} = \begin{cases} 1 & i = 1, \dots, r-1, j = 2, \dots, r \\ -1 & j = i+1, i = 2, \dots, r \\ 0 & \text{otherwise} \end{cases}$$

Let  $\mathbf{\Sigma} \equiv (\sigma_{ij})$  and  $\mathbf{R} \equiv (r_{ij})$  be covariance and correlation matrices of  $\mathbf{C}\mathbf{v}$ , respectively; that is,

$$\mathbf{\Sigma} = \mathbf{C}\mathbf{V}\mathbf{C}'$$

and

$$r_{ij} = \frac{\sigma_{ij}}{\sqrt{\sigma_{ii}\sigma_{jj}}}$$

The factor-analytic covariance approximation of Hsu (1992) is to find  $\lambda_1, \dots, \lambda_{r-1}$  such that

$$\mathbf{R} = \mathbf{D} + \boldsymbol{\lambda}\boldsymbol{\lambda}'$$



where  $\mathbf{D}$  is a diagonal matrix with the  $j$ th diagonal element being  $1 - \lambda_j$  and  $\boldsymbol{\lambda} = (\lambda_1, \dots, \lambda_{r-1})'$ . The adjusted  $p$ -value is

$$p = 1 - \int_{-\infty}^{\infty} \phi(y) \prod_{i=1}^{r-1} \left[ \Phi\left(\frac{\lambda_i y + z_{jl}}{\sqrt{1 - \lambda_i^2}}\right) - \Phi\left(\frac{\lambda_i y - z_{jl}}{\sqrt{1 - \lambda_i^2}}\right) \right] dy$$

which can be obtained in a DATA step as

$$p = \text{PROBMC}(\text{"DUNNETT2"}, z_{ij}, \dots, r - 1, \lambda_1, \dots, \lambda_{r-1}).$$

- Scheffé adjustment:

$$p = \Pr(\chi_{r-1}^2 > z_{jl}^2)$$

- Šidák adjustment:

$$p = 1 - \{1 - \Pr(\chi_1^2 > z_{jl}^2)\}^m$$

- SMM adjustment:

$$p = 1 - [2\Phi(z_{jl}) - 1]^m$$

which can also be evaluated in a DATA step as

$$p = 1 - \text{PROBMC}(\text{"MAXMOD"}, z_{jl}, \dots, m).$$

- Tukey adjustment:

$$p = 1 - \int_{-\infty}^{\infty} r\phi(y)[\Phi(y) - \Phi(y - \sqrt{2}z_{jl})]^{r-1} dy$$

which can also be evaluated in a DATA step as

$$p = 1 - \text{PROBMC}(\text{"RANGE"}, \sqrt{2}z_{jl}, \dots, r).$$

**Trend Tests** Trend tests (Klein and Moeschberger 1997, Section 7.4) have more power to detect ordered alternatives as

$$H_2 : S_1(t) \geq S_2(t) \geq \dots \geq S_k(t), t \leq \tau, \text{ with at least one inequality}$$

or

$$H_2 : S_1(t) \leq S_2(t) \leq \dots \leq S_k(t), t \leq \tau, \text{ with at least one inequality}$$

Let  $a_1 < a_2 < \dots < a_k$  be a sequence of scores associated with the  $k$  samples. The test statistic and its standard error are given by  $\sum_{j=1}^k a_j v_j$  and  $\sum_{j=1}^k \sum_{l=1}^k a_j a_l V_{jl}$ , respectively. Under  $H_0$ , the  $z$ -score

$$Z = \frac{\sum_{j=1}^k a_j v_j}{\sqrt{\sum_{j=1}^k \sum_{l=1}^k a_j a_l V_{jl}}}$$

has, asymptotically, a standard normal distribution. PROC LIFETEST provides both one-tail and two-tail  $p$ -values for the test.

## Rank Tests for the Association of Survival Time with Covariates

The rank tests for the association of covariates (Kalbfleisch and Prentice 1980, Chapter 6) are more general cases of the rank tests for homogeneity. In this section, the index  $\alpha$  is used to label all observations,  $\alpha = 1, 2, \dots, n$ , and the indices  $i, j$  range only over the observations that correspond to events,  $i, j = 1, 2, \dots, k$ . The ordered event times are denoted as  $t_{(i)}$ , the corresponding vectors of covariates are denoted as  $\mathbf{z}_{(i)}$ , and the ordered times, both censored and event times, are denoted as  $t_\alpha$ .

The rank test statistics have the form

$$\mathbf{v} = \sum_{\alpha=1}^n c_{\alpha, \delta_\alpha} \mathbf{z}_\alpha$$

where  $n$  is the total number of observations,  $c_{\alpha, \delta_\alpha}$  are rank scores, which can be either log-rank or Wilcoxon rank scores,  $\delta_\alpha$  is 1 if the observation is an event and 0 if the observation is censored, and  $\mathbf{z}_\alpha$  is the vector of covariates in the TEST statement for the  $\alpha$ th observation. Notice that the scores,  $c_{\alpha, \delta_\alpha}$ , depend on the censoring pattern and that the terms are summed up over all observations.

The log-rank scores are

$$c_{\alpha, \delta_\alpha} = \sum_{(j:t_{(j)} \leq t_\alpha)} \left( \frac{1}{n_j} - \delta_\alpha \right)$$

and the Wilcoxon scores are

$$c_{\alpha, \delta_\alpha} = 1 - (1 + \delta_\alpha) \prod_{(j:t_{(j)} \leq t_\alpha)} \frac{n_j}{n_j + 1}$$

where  $n_j$  is the number at risk just prior to  $t_{(j)}$ .

The estimates used for the covariance matrix of the log-rank statistics are

$$\mathbf{V} = \sum_{i=1}^k \frac{\mathbf{V}_i}{n_i}$$

where  $\mathbf{V}_i$  is the corrected sum of squares and crossproducts matrix for the risk set at time  $t_{(i)}$ ; that is,

$$\mathbf{V}_i = \sum_{(\alpha:t_\alpha \geq t_{(i)})} (\mathbf{z}_\alpha - \bar{\mathbf{z}}_i)' (\mathbf{z}_\alpha - \bar{\mathbf{z}}_i)$$

where

$$\bar{\mathbf{z}}_i = \sum_{(\alpha:t_\alpha \geq t_{(i)})} \frac{\mathbf{z}_\alpha}{n_i}$$

The estimate used for the covariance matrix of the Wilcoxon statistics is

$$\mathbf{V} = \sum_{i=1}^k \left[ a_i (1 - a_i^*) (2\mathbf{z}_{(i)} \mathbf{z}'_{(i)} + \mathbf{S}_i) - (a_i^* - a_i) \left( a_i \mathbf{x}_i \mathbf{x}'_i + \sum_{j=i+1}^k a_j (\mathbf{x}_i \mathbf{x}'_j + \mathbf{x}_j \mathbf{x}'_i) \right) \right]$$

where

$$a_i = \prod_{j=1}^i \frac{n_j}{n_j + 1}$$

$$a_i^* = \prod_{j=1}^i \frac{n_j + 1}{n_j + 2}$$

$$S_i = \sum_{(\alpha: t_{(i+1)} > t_\alpha > t_{(i)})} \mathbf{z}_\alpha \mathbf{z}'_\alpha$$

$$\mathbf{x}_i = 2\mathbf{z}_{(i)} + \sum_{(\alpha: t_{(i+1)} > t_\alpha > t_{(i)})} \mathbf{z}_\alpha$$

In the case of tied failure times, the statistics  $\mathbf{v}$  are averaged over the possible orderings of the tied failure times. The covariance matrices are also averaged over the tied failure times. Averaging the covariance matrices over the tied orderings produces functions with appropriate symmetries for the tied observations; however, the actual variances of the  $\mathbf{v}$  statistics would be smaller than the preceding estimates. Unless the proportion of ties is large, it is unlikely that this will be a problem.

The univariate tests for each covariate are formed from each component of  $\mathbf{v}$  and the corresponding diagonal element of  $\mathbf{V}$  as  $v_i^2 / V_{ii}$ . These statistics are treated as coming from a chi-square distribution for calculation of probability values.

The statistic  $\mathbf{v}'\mathbf{V}^{-1}\mathbf{v}$  is computed by sweeping each pivot of the  $\mathbf{V}$  matrix in the order of greatest increase to the statistic. The corresponding sequence of partial statistics is tabulated. Sequential increments for including a given covariate and the corresponding probabilities are also included in the same table. These probabilities are calculated as the tail probabilities of a chi-square distribution with one degree of freedom. Because of the selection process, these probabilities should not be interpreted as  $p$ -values.

If desired for data screening purposes, the output data set requested by the OUTTEST= option can be treated as a sum of squares and crossproducts matrix and processed by the REG procedure by using the option METHOD=RSQUARE. Then the sets of variables of a given size can be found that give the largest test statistics. [Output 52.1](#) illustrates this process.

---

## Computer Resources

The data are first read and sorted into strata. If the data are originally sorted by failure time and censoring state, with smaller failure times coming first and event values preceding censored values in cases of ties, the data can be processed by strata without additional sorting. Otherwise, the data are read into memory by strata and sorted.

## Memory Requirements

For a given BY group, define the following:

|      |                                                       |
|------|-------------------------------------------------------|
| $N$  | the total number of observations                      |
| $V$  | the number of STRATA variables                        |
| $C$  | the number of covariates listed in the TEST statement |
| $L$  | total length of the ID variables in bytes             |
| $S$  | number of strata                                      |
| $n$  | maximum number of observations within strata          |
| $b$  | $12 + 8C + L$                                         |
| $m1$ | $(112 + 16V) \times S$                                |
| $m2$ | $50 \times b \times S$                                |
| $m3$ | $(50 + n) \times (b + 4)$                             |
| $m4$ | $8(C + 4)^2$                                          |
| $m5$ | $20N + 8S \times (S + 4)$                             |

The memory, in bytes, required to process the BY group is at least

$$m1 + \max(m2, m3) + m4$$

The test of equality of survival functions across strata requires additional memory ( $m5$  bytes). However, if this additional memory is not available, PROC LIFETEST skips the test for equality of survival functions and finishes the other computations. Additional memory is required for the PLOTS= option. Temporary storage of  $16n$  bytes is required to store the product-limit estimates for plotting.

---

## Output Data Sets

### OUTSURV= Data Set

You can specify the OUTSURV= option in the PROC LIFETEST statement to create an output data set that contains the following columns:

- any specified BY variables
- any specified STRATA variables, their values coming from either their original values or the midpoints of the stratum intervals if endpoints are used to define strata (semi-infinite intervals are labeled by their finite endpoint)
- STRATUM, a numeric variable that numbers the strata

- the time variable as given in the TIME statement. For METHOD=KM, METHOD=BRESLOW, or METHOD=FM, it contains the observed failure or censored times. For the life-table estimates, it contains the lower endpoints of the time intervals.
- SURVIVAL, a variable that contains the survivor function estimates
- CONFTYPE, a variable that contains the name of the transformation applied to the survival time in the computation of confidence intervals (if the OUT= option is specified in the SURVIVAL statement)
- SDF\_LCL, a variable that contains the lower limits of the pointwise confidence intervals for the survivor function
- SDF\_UCL, a variable that contains the upper limits of the pointwise confidence intervals for the survivor function

If the estimation uses the product-limit, Breslow, or Fleming-Harrington method, then the data set also contains the following:

- \_CENSOR\_, an indicator variable that has a value 1 for a censored observation and a value 0 for an event observation
- SDF\_STDERR, a variable that contains the standard error of the survivor function estimator (if the STDERR option is specified in the PROC LIFETEST statement)
- HW\_LCL, a variable that contains the lower limits of the Hall-Wellner confidence bands (if the CONFBAND=HW option or the CONFBAND=ALL option is specified in the PROC LIFETEST statement)
- HW\_UCL, a variable that contains the upper limits of the Hall-Wellner confidence bands (if the CONFBAND=HW option or the CONFBAND=ALL option is specified in the PROC LIFETEST statement)
- EP\_LCL, a variable that contains the lower limits of the equal-precision confidence bands (if the CONFBAND=EP option or the CONFBAND=ALL option is specified in the PROC LIFETEST statement)
- EP\_UCL, a variable that contains the upper limits of the equal-precision confidence bands (if the CONFBAND=EP option or the CONFBAND=ALL option is specified in the PROC LIFETEST statement)

If the estimation uses the life-table method, then the data set also contains the following:

- MIDPOINT, a variable that contains the value of the midpoint of the time interval
- PDF, a variable that contains the density function estimates
- PDF\_LCL, a variable that contains the lower endpoints of the PDF confidence intervals
- PDF\_UCL, a variable that contains the upper endpoints of the PDF confidence intervals
- HAZARD, a variable that contains the hazard estimates
- HAZ\_LCL, a variable that contains the lower endpoints of the hazard confidence intervals

- HAZ\_UCL, a variable that contains the upper endpoints of the hazard confidence intervals

Each survival function contains an initial observation with the value 1 for the SDF and the value 0 for the time. The output data set contains an observation for each distinct failure time if the product-limit, Breslow, or Fleming-Harrington method is used, or it contains an observation for each time interval if the life-table method is used. The product-limit, Breslow, or Fleming-Harrington survival estimates are defined to be right continuous; that is, the estimates at a given time include the factor for the failure events that occur at that time.

Labels are assigned to all the variables in the output data set except the BY variable and the STRATA variable.

### OUTTEST= Data Set

The OUTTEST= option in the LIFETEST statement creates an output data set that contains the rank statistics for testing the association of failure time with covariates. It contains the following:

- any specified BY variables
- \_TYPE\_, a character variable of length 8 that labels the type of rank test, either “LOG-RANK” or “WILCOXON”
- \_NAME\_, a character variable of length 8 that labels the rows of the covariance matrix and the test statistics
- the TIME variable, containing the overall test statistic in the observation that has \_NAME\_ equal to the name of the time variable and the univariate test statistics under their respective covariates.
- all variables listed in the TEST statement

The output is in the form of a symmetric matrix formed by the covariance matrix of the rank statistics bordered by the rank statistics and the overall chi-square statistic. If the value of \_NAME\_ is the name of a variable in the TEST statement, the observation contains a row of the covariance matrix and the value of the rank statistic in the time variable. If the value of \_NAME\_ is the name of the TIME variable, the observation contains the values of the rank statistics in the variables from the TEST list and the value of the overall chi-square test statistic in the TIME variable.

Two complete sets of statistics labeled by the \_TYPE\_ variable are produced, one for the log-rank test and one for the Wilcoxon test.

---

## Displayed Output

If you use the NOPRINT option in the PROC LIFETEST statement, the procedure does not display any output.

## Product-Limit Survival Estimates

The “Product-Limit Survival Estimates” table is displayed if you request the product-limit method of estimation. The table displays the following:

- the observed (event or censored) time
- the number of units at risk (if you specify the ATRISK option in the PROC LIFETEST statement)
- the number of events (if you specify the ATRISK option in the PROC LIFETEST statement)
- the product-limit estimate of the survivor function
- the corresponding estimate of the cumulative distribution function of the failure time
- the standard error estimate of the survivor function estimator
- the Nelson-Aalen cumulative hazard function estimate (if the NELSON option is specified in the PROC LIFETEST statement)
- the standard error of the Nelson-Aalen estimator (if the NELSON option is specified in the PROC LIFETEST statement)
- the number of event times that have been observed
- the number of event or censored times that remain to be observed
- the frequency of the observed times (if you specify the FREQ statement)
- values of the ID variables (if you specify the ID statement)

The ODS name of this table is ProductLimitEstimates.

## Breslow Survival Estimates

The “Breslow Survival Estimates” table is displayed if you request the Breslow method of estimation. The table displays the following:

- the observed (event or censored) time
- the number of units at risk (if you specify the ATRISK option in the PROC LIFETEST statement)
- the number of events (if you specify the ATRISK option in the PROC LIFETEST statement)
- the Breslow estimate of the survivor function
- the corresponding estimate of the cumulative distribution function of the failure time
- the standard error estimate of the survivor function estimator
- the Nelson-Aalen cumulative hazard function estimate (if the NELSON option is specified in the PROC LIFETEST statement)
- the standard error of the Nelson-Aalen estimator (if the NELSON option is specified in the PROC LIFETEST statement)

- the number of event times that have been observed
- the number of event or censored times that remain to be observed
- the frequency of the observed times (if you specify the `FREQ` statement)
- values of the ID variables (if you specify the `ID` statement)

The ODS name of this table is `BreslowEstimates`.

### Fleming-Harrington Survival Estimates

The “Fleming-Harrington Survival Estimates” table is displayed if you request the Fleming-Harrington method of estimation. The table displays the following:

- the observed (event or censored) time
- the number of units at risk (if you specify the `ATRISK` option in the `PROC LIFETEST` statement)
- the number of events (if you specify the `ATRISK` option in the `PROC LIFETEST` statement)
- the Fleming-Harrington estimate of the survivor function
- the corresponding estimate of the cumulative distribution function of the failure time
- the standard error estimate of the survivor function estimator
- the Nelson-Aalen cumulative hazard function estimate (if the `NELSON` option is specified in the `PROC LIFETEST` statement)
- the standard error of the Nelson-Aalen estimator (if the `NELSON` option is specified in the `PROC LIFETEST` statement)
- the number of event times that have been observed
- the number of event or censored times that remain to be observed
- the frequency of the observed times (if you specify the `FREQ` statement)
- values of the ID variables (if you specify the `ID` statement)

The ODS name of this table is `FlemingEstimates`.

### Quartile Estimates

The “Quartiles Estimates” table is displayed if you request the product-limit, Breslow, or Fleming-Harrington method of estimation. The table displays the following:

- point estimates of the quartiles of the survival times
- the lower and upper confidence limits for the quartiles

For ODS purposes, the name of this table is “Quartiles.”



## Mean Estimate

The “Mean Estimate” table is displayed if you request the product-limit, Breslow, or Fleming-Harrington method of estimation. The table displays the following:

- the estimated mean survival time
- the estimated standard error of the mean estimator

The ODS name of this table is Means.

## Life-Table Survival Estimates

The “Life-Table Survival Estimates” table is displayed if you request the life-table method of estimation. The table displays the following:

- the time intervals into which the failure and censored times are distributed. Each interval is from the lower limit, up to but not including the upper limit; if the upper limit is infinity, the missing value is printed.
- the number of events that occur in the interval
- the number of censored observations that fall into the interval
- the effective sample size for the interval
- the estimate of conditional probability of events (failures) in the interval
- the standard error of the conditional probability estimator
- the estimate of the survival function at the beginning of the interval
- the estimate of the cumulative distribution function of the failure time at the beginning of the interval
- the standard error estimate of the survivor function estimator
- the estimate of the median residual lifetime, which is the amount of time elapsed before reducing the number of at-risk units to one-half. This is also known as the *median future lifetime* in Elandt-Johnson and Johnson (1980).
- the estimated standard error of the median residual lifetime estimator
- the density function estimated at the midpoint of the interval
- the standard error estimate of the density estimator
- the hazard rate estimated at the midpoint of the interval
- the standard error estimate of the hazard estimator

The ODS name of this table is LifetableEstimates.

## Summary of the Number of Censored and Uncensored Values

The “Summary of the Number of Censored and Uncensored Values” table displays following:

- the stratum identification (if the STRATA statement is specified)
- the total number of observations
- the number of event observations
- the number of censored observations
- the percentage of censored observations

The ODS name of this table is CensoredSummary.

## Rank Statistics

The “Rank Statistics” table contains the test statistics of the nonparametric  $k$ -sample tests. The ODS name of this table is HomStats.

## Covariance Matrix for the Log-Rank Statistics

The “Covariance Matrix for the Log-Rank Statistics” table is displayed if the log-rank  $k$ -sample test is requested. The ODS name of this table is LogrankHomCov.

## Covariance Matrix for the Wilcoxon Statistics

The “Covariance Matrix for the Wilcoxon Statistics” table is displayed if the Wilcoxon  $k$ -sample test is requested. The ODS name of this table is WilHomCov.

## Covariance Matrix for the Tarone Statistics

The “Covariance Matrix for the Tarone Statistics” table is displayed if the Tarone-Ware  $k$ -sample test is requested. The ODS name of this table is TaroneHomCov.

## Covariance Matrix for the Peto Statistics

The “Covariance Matrix for the Peto Statistics” table is displayed if the Peto-Peto  $k$ -sample test is requested. The ODS name of this table is PetoHomCov.

## Covariance Matrix for the ModPeto Statistics

The “Covariance Matrix for the ModPeto Statistics” table is displayed if the modified Peto-Peto  $k$ -sample test is requested. The ODS name of this table is ModPetoHomCov.

## Covariance Matrix for the Fleming Statistics

The “Covariance Matrix for the Fleming Statistics” table is displayed if the Fleming-Harrington  $k$ -sample test is requested. The ODS name of this table is FlemingHomCov.

### Test of Equality over Strata

The “Test of Equality over Strata” table is displayed if an unstratified  $k$ -sample test is carried out. The table contains the chi-square statistics, degrees of freedom, and  $p$ -values of the nonparametric tests and the likelihood ratio test (which is based on the exponential distribution). The ODS name of this table is HomTests.

### Stratified Test of Equality over Group

The “Stratified Test of Equality over Group” table is displayed if a stratified test is carried out. The table contains the chi-square statistics, degrees of freedom, and  $p$ -values of the stratified tests. The ODS name of this table is HomTests.

### Scores for Trend Test

The “Scores for Trend Test” table is displayed if the TREND option is specified in the STRATA statement. The table contains the set of scores used to construct the trend tests. For ODS purposes, the name of this table is “TrendScores.”

### Trend Tests

The “Trend Tests” table is displayed if the TREND option is specified in the STRATA statement. The table contains the results of the trend tests. The ODS name of this table is TrendTests.

### Adjustment for Multiple Comparisons for the Log-Rank Test

The “Adjustment for Multiple Comparisons for the Log-Rank Test” table is displayed if the log-rank test and a multiple-comparison adjustment method are specified. The table contains the chi-square statistics and the raw and adjusted  $p$ -values of the paired comparisons. The ODS name of this table is SurvDiff.

### Adjustment for Multiple Comparisons for the Wilcoxon Test

The “Adjustment for Multiple Comparisons for the Wilcoxon Test” table is displayed if the Wilcoxon test and a multiple-comparison method are specified. The table contains the chi-square statistics and the raw and adjusted  $p$ -values of the paired comparisons. The ODS name of this table is SurvDiff.

### Adjustment for Multiple Comparisons for the Tarone Test

The “Adjustment for Multiple Comparisons for the Tarone Test” table is displayed if the Tarone-Ware test and a multiple-comparison method are specified. The table contains the chi-square statistics and the raw and adjusted  $p$ -values of the paired comparisons. The ODS name of this table is SurvDiff.

### Adjustment for Multiple Comparisons for the Peto Test

The “Adjustment for Multiple Comparisons for the Peto Test” table is displayed if the Peto-Peto test and a multiple-comparison method are specified. The table contains the chi-square statistics and the raw and adjusted  $p$ -values of the paired comparisons. The ODS name of this table is SurvDiff.

### Adjustment for Multiple Comparisons for the ModPeto Test

The “Adjustment for Multiple Comparisons for the ModPeto Test” table is displayed if the modified Peto-Peto test and a multiple-comparison method are specified. The table contains the chi-square statistics and the raw and adjusted  $p$ -values of the paired comparisons. The ODS name of this table is SurvDiff.

### Adjustment for Multiple Comparisons for the Fleming Test

The “Adjustment for Multiple Comparisons for the Fleming Test” table is displayed if the Fleming-Harrington test and a multiple-comparison method are specified. The table contains the chi-square statistics and the raw and adjusted  $p$ -values of the paired comparisons. The ODS name of this table is SurvDiff.

### Univariate Chi-Squares for the Log-Rank Test

The “Univariate Chi-Squares for the Log-Rank Test” table is displayed if the TEST statement is specified. The table displays the log-rank test results for individual variables in the TEST statement. The ODS name of this table is LogUniChiSq.

### Covariance Matrix of the Log-Rank Statistics

The “Covariance Matrix of the Log-Rank Statistics” table is displayed if the TEST statement is specified. The table displays the estimated covariance matrix of the log-rank statistics for association. The ODS name of this table is LogTestCov.

### Forward Stepwise Sequence of Chi-Squares for the Log-Rank Test

The “Forward Stepwise Sequence of Chi-Squares for the Log-Rank Test” table is displayed if the TEST statement is specified. The table contains the sequence of partial chi-square statistics for the log-rank test in the order of the greatest increase to the overall test statistic, the degrees of freedom of the partial chi-square statistics, the approximate probability values of the partial chi-square statistics, the chi-square increments for including the given variables, and the probability values of the chi-square increments. The ODS name of this table is LogForStepSeq.

### Univariate Chi-Squares for the Wilcoxon Test

The “Univariate Chi-Squares for the Wilcoxon Test” table displays the Wilcoxon test results for individual variables in the TEST statement. The ODS name of this table is WilUniChiSq.

### Covariance Matrix of the Wilcoxon Statistics

The “Covariance Matrix of the Wilcoxon Statistics” table is displayed if the TEST statement is specified. The table displays the estimated covariance matrix of the Wilcoxon statistics for association. The ODS name of this table is WilTestCov.

### Forward Stepwise Sequence of Chi-Squares for the Wilcoxon Test

The “Forward Stepwise Sequence of Chi-Squares for the Wilcoxon Test” table is displayed if the TEST statement is specified. The table contains the sequence of partial chi-square statistics for the Wilcoxon test in the order of the greatest increase to the overall test statistic, the degrees of freedom of the partial chi-square statistics, the approximate probability values of the partial chi-square statistics, the chi-square

increments for including the given variables, and the probability values of the chi-square increments. The ODS name of this table is WilForStepSeq.

## ODS Table Names

PROC LIFETEST assigns a name to each table it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in Table 52.5. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

**Table 52.5** ODS Tables Produced by PROC LIFETEST

| ODS Table Name        | Description                                                           | Statement / Option                  |
|-----------------------|-----------------------------------------------------------------------|-------------------------------------|
| BreslowEstimates      | Breslow estimates                                                     | PROC LIFETEST METHOD=B              |
| CensoredSummary       | Number of event and censored observations                             | PROC LIFETEST<br>METHOD=PL   B   FH |
| FlemingEstimates      | Fleming-Harrington estimates                                          | PROC LIFETEST<br>METHOD=FH          |
| FlemingHomCov         | Covariance matrix for $k$ -sample FLEMING statistics                  | STRATA / TEST=FLEMING               |
| HomStats              | Test statistics for $k$ -sample tests                                 | STRATA / TEST=                      |
| HomTests              | Results of $k$ -sample tests                                          | STRATA / TEST=                      |
| LifetableEstimates    | Life-table survival estimates                                         | PROC LIFETEST<br>METHOD=LT          |
| LogForStepSeq         | Forward stepwise sequence for the log-rank statistics for association | TEST                                |
| LogrankHomCov         | Covariance matrix for $k$ -sample LOGRANK statistics                  | STRATA / TEST=LOGRANK               |
| LogTestCov            | Covariance matrix for log-rank statistics for association             | TEST                                |
| LogUniChisq           | Univariate chi-squares for log-rank statistics for association        | TEST                                |
| Means                 | Mean and standard error of survival times                             | PROC LIFETEST<br>METHOD=PL          |
| ModPetoHomCov         | Covariance matrix for $k$ -sample MODPETO statistics                  | STRATA / TEST=MODPETO               |
| PetoHomCov            | Covariance matrix for $k$ -sample PETO statistics                     | STRATA / TEST=PETO                  |
| ProductLimitEstimates | Product-limit survival estimates                                      | PROC LIFETEST<br>METHOD=PL          |
| Quartiles             | Quartiles of the survival times                                       | PROC LIFETEST<br>METHOD=PL   B   FH |
| SurvDiff              | Adjustments for multiple comparisons                                  | STRATA / ADJUST= and DIFF=          |
| TaroneHomCov          | Covariance matrix for $k$ -sample TARONE statistics                   | STRATA / TEST=TARONE                |

**Table 52.5** *continued*

| ODS Table Name | Description                                                           | Statement / Option     |
|----------------|-----------------------------------------------------------------------|------------------------|
| TrendScores    | Scores used to construct trend tests                                  | STRATA / TREND         |
| TrendTests     | Results of trend tests                                                | STRATA / TREND         |
| WilForStepSeq  | Forward stepwise sequence for the log-rank statistics for association | TEST                   |
| WilcoxonHomCov | Covariance matrix for $k$ -sample WILCOXON statistics                 | STRATA / TEST=WILCOXON |
| WilTestCov     | Covariance matrix for log-rank statistics for association             | TEST                   |
| WilUniChiSq    | Univariate chi-squares for Wilcoxon statistics for association        | TEST                   |

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “[Statistical Graphics Using ODS.](#)”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS.](#)”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “[A Primer on ODS Statistical Graphics](#)” on page 599 in Chapter 21, “[Statistical Graphics Using ODS.](#)”

The survival plot is produced by default; other graphs are produced by using the PLOTS= option in the PROC LIFETEST statement. You can reference every graph produced through ODS Graphics with a name. The names of the graphs that PROC LIFETEST generates are listed in [Table 52.6](#), along with the required keywords for the PLOTS= option.

**Table 52.6** Graphs Produced by PROC LIFETEST

| ODS Graph Name        | Plot Description                                                                                                            | PLOTS=Option      |
|-----------------------|-----------------------------------------------------------------------------------------------------------------------------|-------------------|
| DensityPlot           | Estimated density for life-table method                                                                                     | PDF               |
| FailurePlot           | Estimated failure function                                                                                                  | SURVIVAL(FAILURE) |
| HazardPlot            | Estimated hazard function for life-table method or smoothed hazard for product-limit, Breslow, or Fleming-Harrington method | HAZARD            |
| LogNegLogSurvivalPlot | Log of negative log of the estimated survivor function                                                                      | LOGLOGS           |

Table 52.6 *continued*

| ODS Graph Name     | Plot Description                                              | PLOTS=Option      |
|--------------------|---------------------------------------------------------------|-------------------|
| NegLogSurvivalPlot | Negative log of the estimated survivor function               | LOGSURV           |
| SurvivalPlot       | Estimated survivor function                                   | SURVIVAL          |
| SurvivalPlot       | Estimated survivor function with number of subjects at risk   | SURVIVAL(ATRISK=) |
| SurvivalPlot       | Estimated survivor function with point-wise confidence limits | SURVIVAL(CL)      |
| SurvivalPlot       | Estimated survivor function with equal-precision band         | SURVIVAL(CB=EP)   |
| SurvivalPlot       | Estimated survivor function with Hall-Wellner band            | SURVIVAL(CB=HW)   |
| SurvivalPlot       | Estimated survivor function with homogeneity test $p$ -value  | SURVIVAL(TEST)    |

### Additional Dynamic Variables for Survival Plots Using ODS Graphics

PROC LIFETEST passes a number of summary statistics as dynamic variables to the ODS Graphics for survival plots. Table 52.7 and Table 52.8 list these additional dynamic variables for the Kaplan-Meier curves and the life-table curves, respectively. These dynamic variables are not declared in the templates for the survival curves, but you can declare them and use them to enhance the default plots. The names of the dynamic variables depend on the STRATA= suboption of the PLOTS=SURVIVAL option: STRATA=INDIVIDUAL produces a separate plot for each stratum, and STRATA=OVERALL produces one plot with overlaid curves.

Table 52.7 Additional Dynamic Variables for `Stat.Graphics.ProductLimitSurvival`

| STRATA=    | Dynamic         | Description                                      |
|------------|-----------------|--------------------------------------------------|
| OVERLAY    | StrVal $j$      | Label for the $j$ th stratum                     |
|            | NObs $j$        | Number of observations in the $j$ th stratum     |
|            | NEvent $j$      | Number of events in the $j$ th stratum           |
|            | Median $j$      | Median survival time of the $j$ th stratum       |
|            | LowerMedian $j$ | Lower median survival time of the $j$ th stratum |
|            | UpperMedian $j$ | Upper median survival time of the $j$ th stratum |
| INDIVIDUAL | PctMedianConfid | Confidence of the median intervals in percent    |
|            | NObs            | Number of observations                           |
|            | NEvent          | Number of events                                 |
|            | Median          | Median survival time                             |
|            | LowerMedian     | Lower median survival time                       |
|            | UpperMedian     | Upper median survival time                       |
|            | PctMedianConfid | Confidence of the median interval in percent     |

**Table 52.8** Additional Dynamic Variables for `Stat.Graphics.LifetableSurvival`

| STRATA=    | Dynamic | Description                                       |
|------------|---------|---------------------------------------------------|
| OVERLAY    | StrValj | Label for the <i>j</i> th stratum                 |
|            | NObsj   | Number of observations in the <i>j</i> th stratum |
|            | NEventj | Number of events in the <i>j</i> th stratum       |
| INDIVIDUAL | NObs    | Number of observations                            |
|            | NEvent  | Number of events                                  |

See the section “The Graph Template Language” on page 707 in Chapter 22, “ODS Graphics Template Modification,” for the general use of dynamic variables. For the use of the particular dynamic variables shown in this section, see the sections “Modifying the Layout and Adding a New Inset Table” on page 766 and “Displaying Survival Summary Statistics” on page 784 in Chapter 22, “ODS Graphics Template Modification.”

## Modifying the ODS Template for Survival Plots

PROC LIFETEST, like other statistical procedures, provides a PLOTS= option and other options for modifying its output without requiring template changes. Those options are sufficient for most purposes. When those options are not sufficient, you can change a graph by changing the graph template. “Example 22.3: Customizing Survival Plots” on page 748 in Chapter 22, “ODS Graphics Template Modification,” shows how to find the name of the template, display the template by using PROC TEMPLATE and the SOURCE statement, and make a series of template changes.

The example consists of the following parts:

- **Modifying the plot title:** This part identifies the template, displays it, explains its overall structure, and modifies the titles. See the section “Modifying the Plot Title” on page 749 in Chapter 22, “ODS Graphics Template Modification.”
- **Modifying the axes:** This part explains the options that control the X and Y axes, and shows how to modify the ticks and axis labels. See the section “Modifying the Axes” on page 753 in Chapter 22, “ODS Graphics Template Modification.”
- **Creating a template that is easy to modify:** This part shows how you can reorganize and modularize the entire template to make it easy to customize in various ways. See the section “Creating a Template That Is Easy to Modify” on page 756 in Chapter 22, “ODS Graphics Template Modification.”
- **Modifying the plot title in the revised template:** This part shows how to change the title by using the revised template. See the section “Modifying the Plot Title in the Revised Template” on page 762 in Chapter 22, “ODS Graphics Template Modification.”
- **Modifying the legend and inset table:** This part removes the small inset table and moves the legend inside the graph. The censoring information above the X axis is moved outside the graph. See the section “Modifying the Legend and Inset Table” on page 763 in Chapter 22, “ODS Graphics Template Modification.”



- **Modifying the layout and adding a new inset table:** This part moves the event and total information out of the graph and the legend in. It also moves the small inset table. See the section “[Modifying the Layout and Adding a New Inset Table](#)” on page 766 in Chapter 22, “[ODS Graphics Template Modification](#).”
- **Changing line styles:** This part shows how to modify a style template to change line colors and styles. See the section “[Changing Line Styles](#)” on page 773 in Chapter 22, “[ODS Graphics Template Modification](#).”
- **Changing fonts:** This part shows how to change the graph template and the style template to change some of the fonts that are used in the graph. See the section “[Changing Fonts](#)” on page 776 in Chapter 22, “[ODS Graphics Template Modification](#).”
- **Changing how censored data are displayed:** This part shows how to change or remove the plus marks that are used to display censored observations. See the section “[Changing How Censored Data Are Displayed](#)” on page 781 in Chapter 22, “[ODS Graphics Template Modification](#).”
- **Displaying survival summary statistics:** This part adds to the graph a table with event, censoring, and survival information. See the section “[Displaying Survival Summary Statistics](#)” on page 784 in Chapter 22, “[ODS Graphics Template Modification](#).”

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## Examples: LIFETEST Procedure

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### Example 52.1: Product-Limit Estimates and Tests of Association

The data presented in Appendix I of Kalbfleisch and Prentice (1980) are coded in the following DATA step. The response variable, `SurvTime`, is the survival time in days of a lung cancer patient. Negative values of `SurvTime` are censored values. The covariates are `Cell` (type of cancer cell), `Therapy` (type of therapy: standard or test), `Prior` (prior therapy: 0=no, 1=yes), `Age` (age in years), `DiagTime` (time in months from diagnosis to entry into the trial), and `Kps` (performance status). A censoring indicator variable `Censor` is created from the data, with the value 1 indicating a censored time and the value 0 indicating an event time. Since there are only two types of therapy, an indicator variable, `Treatment`, is constructed for therapy type, with value 0 for standard therapy and value 1 for test therapy.

```
data VALung;
 drop check m;
 retain Therapy Cell;
 infile cards column=column;
 length Check $ 1;
 label SurvTime='Failure or Censoring Time'
 Kps='Karnofsky Index'
 DiagTime='Months till Randomization'
 Age='Age in Years'
 Prior='Prior Treatment?'
 Cell='Cell Type'
 Therapy='Type of Treatment'
```

```

Treatment='Treatment Indicator';
M=Column;
input Check $ @@;
if M>Column then M=1;
if Check='s'|Check='t' then input @M Therapy $ Cell $;
else input @M SurvTime Kps DiagTime Age Prior @@;
if SurvTime > .;
 censor=(SurvTime<0);
 SurvTime=abs(SurvTime);
 Treatment=(Therapy='test');
datalines;
standard squamous
 72 60 7 69 0 411 70 5 64 10 228 60 3 38 0 126 60 9 63 10
118 70 11 65 10 10 20 5 49 0 82 40 10 69 10 110 80 29 68 0
314 50 18 43 0 -100 70 6 70 0 42 60 4 81 0 8 40 58 63 10
144 30 4 63 0 -25 80 9 52 10 11 70 11 48 10
standard small
 30 60 3 61 0 384 60 9 42 0 4 40 2 35 0 54 80 4 63 10
 13 60 4 56 0 -123 40 3 55 0 -97 60 5 67 0 153 60 14 63 10
 59 30 2 65 0 117 80 3 46 0 16 30 4 53 10 151 50 12 69 0
 22 60 4 68 0 56 80 12 43 10 21 40 2 55 10 18 20 15 42 0
139 80 2 64 0 20 30 5 65 0 31 75 3 65 0 52 70 2 55 0
287 60 25 66 10 18 30 4 60 0 51 60 1 67 0 122 80 28 53 0
 27 60 8 62 0 54 70 1 67 0 7 50 7 72 0 63 50 11 48 0
392 40 4 68 0 10 40 23 67 10
standard adeno
 8 20 19 61 10 92 70 10 60 0 35 40 6 62 0 117 80 2 38 0
132 80 5 50 0 12 50 4 63 10 162 80 5 64 0 3 30 3 43 0
 95 80 4 34 0
standard large
177 50 16 66 10 162 80 5 62 0 216 50 15 52 0 553 70 2 47 0
278 60 12 63 0 12 40 12 68 10 260 80 5 45 0 200 80 12 41 10
156 70 2 66 0 -182 90 2 62 0 143 90 8 60 0 105 80 11 66 0
103 80 5 38 0 250 70 8 53 10 100 60 13 37 10
test squamous
999 90 12 54 10 112 80 6 60 0 -87 80 3 48 0 -231 50 8 52 10
242 50 1 70 0 991 70 7 50 10 111 70 3 62 0 1 20 21 65 10
587 60 3 58 0 389 90 2 62 0 33 30 6 64 0 25 20 36 63 0
357 70 13 58 0 467 90 2 64 0 201 80 28 52 10 1 50 7 35 0
 30 70 11 63 0 44 60 13 70 10 283 90 2 51 0 15 50 13 40 10
test small
 25 30 2 69 0 -103 70 22 36 10 21 20 4 71 0 13 30 2 62 0
 87 60 2 60 0 2 40 36 44 10 20 30 9 54 10 7 20 11 66 0
 24 60 8 49 0 99 70 3 72 0 8 80 2 68 0 99 85 4 62 0
 61 70 2 71 0 25 70 2 70 0 95 70 1 61 0 80 50 17 71 0
 51 30 87 59 10 29 40 8 67 0
test adeno
 24 40 2 60 0 18 40 5 69 10 -83 99 3 57 0 31 80 3 39 0
 51 60 5 62 0 90 60 22 50 10 52 60 3 43 0 73 60 3 70 0
 8 50 5 66 0 36 70 8 61 0 48 10 4 81 0 7 40 4 58 0
140 70 3 63 0 186 90 3 60 0 84 80 4 62 10 19 50 10 42 0
 45 40 3 69 0 80 40 4 63 0
test large
 52 60 4 45 0 164 70 15 68 10 19 30 4 39 10 53 60 12 66 0

```

```

 15 30 5 63 0 43 60 11 49 10 340 80 10 64 10 133 75 1 65 0
 111 60 5 64 0 231 70 18 67 10 378 80 4 65 0 49 30 3 37 0
;

```

In the following statements, PROC LIFETEST is invoked to compute the product-limit estimate of the survivor function for each type of cancer cell and to analyze the effects of the variables Age, Prior, DiagTime, Kps, and Treatment on the survival of the patients. These prognostic factors are specified in the TEST statement, and the variable Cell is specified in the STRATA statement. ODS Graphics must be enabled before producing graphs. Graphical displays of the product-limit estimates (S), the negative log estimates (LS), and the log of negative log estimates (LLS) are requested through the PLOTS= option in the PROC LIFETEST statement. Because of a few large survival times, a MAXTIME of 600 is used to set the scale of the time axis; that is, the time scale extends from 0 to a maximum of 600 days in the plots. The variable Therapy is specified in the ID statement to identify the type of therapy for each observation in the product-limit estimates. The OUTTEST option specifies the creation of an output data set named Test to contain the rank test matrices for the covariates.

```

ods graphics on;
proc lifetest data=VALung plots=(s,ls,lls) outtest=Test maxtime=600;
 time SurvTime*Censor(1);
 id Therapy;
 strata Cell;
 test Age Prior DiagTime Kps Treatment;
run;
ods graphics off;

```

Output 52.1.1 through Output 52.1.4 display the product-limit estimates of the survivor functions for the four cell types. Summary statistics of the survival times are also shown. The median survival times are 51 days, 156 days, 51 days, and 118 days for patients with adeno cells, large cells, small cells, and squamous cells, respectively.

**Output 52.1.1** Estimation Results for Adeno Cells

| The LIFETEST Procedure           |          |         |                               |                  |                |          |
|----------------------------------|----------|---------|-------------------------------|------------------|----------------|----------|
| Stratum 1: Cell Type = adeno     |          |         |                               |                  |                |          |
| Product-Limit Survival Estimates |          |         |                               |                  |                |          |
| SurvTime                         | Survival | Failure | Survival<br>Standard<br>Error | Number<br>Failed | Number<br>Left | Therapy  |
| 0.000                            | 1.0000   | 0       | 0                             | 0                | 27             |          |
| 3.000                            | 0.9630   | 0.0370  | 0.0363                        | 1                | 26             | standard |
| 7.000                            | 0.9259   | 0.0741  | 0.0504                        | 2                | 25             | test     |
| 8.000                            | .        | .       | .                             | 3                | 24             | standard |
| 8.000                            | 0.8519   | 0.1481  | 0.0684                        | 4                | 23             | test     |
| 12.000                           | 0.8148   | 0.1852  | 0.0748                        | 5                | 22             | standard |
| 18.000                           | 0.7778   | 0.2222  | 0.0800                        | 6                | 21             | test     |
| 19.000                           | 0.7407   | 0.2593  | 0.0843                        | 7                | 20             | test     |
| 24.000                           | 0.7037   | 0.2963  | 0.0879                        | 8                | 19             | test     |
| 31.000                           | 0.6667   | 0.3333  | 0.0907                        | 9                | 18             | test     |
| 35.000                           | 0.6296   | 0.3704  | 0.0929                        | 10               | 17             | standard |
| 36.000                           | 0.5926   | 0.4074  | 0.0946                        | 11               | 16             | test     |
| 45.000                           | 0.5556   | 0.4444  | 0.0956                        | 12               | 15             | test     |
| 48.000                           | 0.5185   | 0.4815  | 0.0962                        | 13               | 14             | test     |
| 51.000                           | 0.4815   | 0.5185  | 0.0962                        | 14               | 13             | test     |
| 52.000                           | 0.4444   | 0.5556  | 0.0956                        | 15               | 12             | test     |
| 73.000                           | 0.4074   | 0.5926  | 0.0946                        | 16               | 11             | test     |
| 80.000                           | 0.3704   | 0.6296  | 0.0929                        | 17               | 10             | test     |
| 83.000*                          | .        | .       | .                             | 17               | 9              | test     |
| 84.000                           | 0.3292   | 0.6708  | 0.0913                        | 18               | 8              | test     |
| 90.000                           | 0.2881   | 0.7119  | 0.0887                        | 19               | 7              | test     |
| 92.000                           | 0.2469   | 0.7531  | 0.0850                        | 20               | 6              | standard |
| 95.000                           | 0.2058   | 0.7942  | 0.0802                        | 21               | 5              | standard |
| 117.000                          | 0.1646   | 0.8354  | 0.0740                        | 22               | 4              | standard |
| 132.000                          | 0.1235   | 0.8765  | 0.0659                        | 23               | 3              | standard |
| 140.000                          | 0.0823   | 0.9177  | 0.0553                        | 24               | 2              | test     |
| 162.000                          | 0.0412   | 0.9588  | 0.0401                        | 25               | 1              | standard |
| 186.000                          | 0        | 1.0000  | .                             | 26               | 0              | test     |

NOTE: The marked survival times are censored observations.

## Output 52.1.2 Estimation Results for Large Cells

| The LIFETEST Procedure           |          |         |                               |                  |                |          |
|----------------------------------|----------|---------|-------------------------------|------------------|----------------|----------|
| Stratum 2: Cell Type = large     |          |         |                               |                  |                |          |
| Product-Limit Survival Estimates |          |         |                               |                  |                |          |
| SurvTime                         | Survival | Failure | Survival<br>Standard<br>Error | Number<br>Failed | Number<br>Left | Therapy  |
| 0.000                            | 1.0000   | 0       | 0                             | 0                | 27             |          |
| 12.000                           | 0.9630   | 0.0370  | 0.0363                        | 1                | 26             | standard |
| 15.000                           | 0.9259   | 0.0741  | 0.0504                        | 2                | 25             | test     |
| 19.000                           | 0.8889   | 0.1111  | 0.0605                        | 3                | 24             | test     |
| 43.000                           | 0.8519   | 0.1481  | 0.0684                        | 4                | 23             | test     |
| 49.000                           | 0.8148   | 0.1852  | 0.0748                        | 5                | 22             | test     |
| 52.000                           | 0.7778   | 0.2222  | 0.0800                        | 6                | 21             | test     |
| 53.000                           | 0.7407   | 0.2593  | 0.0843                        | 7                | 20             | test     |
| 100.000                          | 0.7037   | 0.2963  | 0.0879                        | 8                | 19             | standard |
| 103.000                          | 0.6667   | 0.3333  | 0.0907                        | 9                | 18             | standard |
| 105.000                          | 0.6296   | 0.3704  | 0.0929                        | 10               | 17             | standard |
| 111.000                          | 0.5926   | 0.4074  | 0.0946                        | 11               | 16             | test     |
| 133.000                          | 0.5556   | 0.4444  | 0.0956                        | 12               | 15             | test     |
| 143.000                          | 0.5185   | 0.4815  | 0.0962                        | 13               | 14             | standard |
| 156.000                          | 0.4815   | 0.5185  | 0.0962                        | 14               | 13             | standard |
| 162.000                          | 0.4444   | 0.5556  | 0.0956                        | 15               | 12             | standard |
| 164.000                          | 0.4074   | 0.5926  | 0.0946                        | 16               | 11             | test     |
| 177.000                          | 0.3704   | 0.6296  | 0.0929                        | 17               | 10             | standard |
| 182.000*                         | .        | .       | .                             | 17               | 9              | standard |
| 200.000                          | 0.3292   | 0.6708  | 0.0913                        | 18               | 8              | standard |
| 216.000                          | 0.2881   | 0.7119  | 0.0887                        | 19               | 7              | standard |
| 231.000                          | 0.2469   | 0.7531  | 0.0850                        | 20               | 6              | test     |
| 250.000                          | 0.2058   | 0.7942  | 0.0802                        | 21               | 5              | standard |
| 260.000                          | 0.1646   | 0.8354  | 0.0740                        | 22               | 4              | standard |
| 278.000                          | 0.1235   | 0.8765  | 0.0659                        | 23               | 3              | standard |
| 340.000                          | 0.0823   | 0.9177  | 0.0553                        | 24               | 2              | test     |
| 378.000                          | 0.0412   | 0.9588  | 0.0401                        | 25               | 1              | test     |
| 553.000                          | 0        | 1.0000  | .                             | 26               | 0              | standard |

NOTE: The marked survival times are censored observations.

**Output 52.1.3** Estimation Results for Small Cells

| The LIFETEST Procedure           |          |         |                               |                  |                |          |
|----------------------------------|----------|---------|-------------------------------|------------------|----------------|----------|
| Stratum 3: Cell Type = small     |          |         |                               |                  |                |          |
| Product-Limit Survival Estimates |          |         |                               |                  |                |          |
| SurvTime                         | Survival | Failure | Survival<br>Standard<br>Error | Number<br>Failed | Number<br>Left | Therapy  |
| 0.000                            | 1.0000   | 0       | 0                             | 0                | 48             |          |
| 2.000                            | 0.9792   | 0.0208  | 0.0206                        | 1                | 47             | test     |
| 4.000                            | 0.9583   | 0.0417  | 0.0288                        | 2                | 46             | standard |
| 7.000                            | .        | .       | .                             | 3                | 45             | standard |
| 7.000                            | 0.9167   | 0.0833  | 0.0399                        | 4                | 44             | test     |
| 8.000                            | 0.8958   | 0.1042  | 0.0441                        | 5                | 43             | test     |
| 10.000                           | 0.8750   | 0.1250  | 0.0477                        | 6                | 42             | standard |
| 13.000                           | .        | .       | .                             | 7                | 41             | standard |
| 13.000                           | 0.8333   | 0.1667  | 0.0538                        | 8                | 40             | test     |
| 16.000                           | 0.8125   | 0.1875  | 0.0563                        | 9                | 39             | standard |
| 18.000                           | .        | .       | .                             | 10               | 38             | standard |
| 18.000                           | 0.7708   | 0.2292  | 0.0607                        | 11               | 37             | standard |
| 20.000                           | .        | .       | .                             | 12               | 36             | standard |
| 20.000                           | 0.7292   | 0.2708  | 0.0641                        | 13               | 35             | test     |
| 21.000                           | .        | .       | .                             | 14               | 34             | standard |
| 21.000                           | 0.6875   | 0.3125  | 0.0669                        | 15               | 33             | test     |
| 22.000                           | 0.6667   | 0.3333  | 0.0680                        | 16               | 32             | standard |
| 24.000                           | 0.6458   | 0.3542  | 0.0690                        | 17               | 31             | test     |
| 25.000                           | .        | .       | .                             | 18               | 30             | test     |
| 25.000                           | 0.6042   | 0.3958  | 0.0706                        | 19               | 29             | test     |
| 27.000                           | 0.5833   | 0.4167  | 0.0712                        | 20               | 28             | standard |
| 29.000                           | 0.5625   | 0.4375  | 0.0716                        | 21               | 27             | test     |
| 30.000                           | 0.5417   | 0.4583  | 0.0719                        | 22               | 26             | standard |
| 31.000                           | 0.5208   | 0.4792  | 0.0721                        | 23               | 25             | standard |
| 51.000                           | .        | .       | .                             | 24               | 24             | standard |
| 51.000                           | 0.4792   | 0.5208  | 0.0721                        | 25               | 23             | test     |
| 52.000                           | 0.4583   | 0.5417  | 0.0719                        | 26               | 22             | standard |
| 54.000                           | .        | .       | .                             | 27               | 21             | standard |
| 54.000                           | 0.4167   | 0.5833  | 0.0712                        | 28               | 20             | standard |
| 56.000                           | 0.3958   | 0.6042  | 0.0706                        | 29               | 19             | standard |
| 59.000                           | 0.3750   | 0.6250  | 0.0699                        | 30               | 18             | standard |
| 61.000                           | 0.3542   | 0.6458  | 0.0690                        | 31               | 17             | test     |
| 63.000                           | 0.3333   | 0.6667  | 0.0680                        | 32               | 16             | standard |
| 80.000                           | 0.3125   | 0.6875  | 0.0669                        | 33               | 15             | test     |
| 87.000                           | 0.2917   | 0.7083  | 0.0656                        | 34               | 14             | test     |
| 95.000                           | 0.2708   | 0.7292  | 0.0641                        | 35               | 13             | test     |
| 97.000*                          | .        | .       | .                             | 35               | 12             | standard |
| 99.000                           | .        | .       | .                             | 36               | 11             | test     |
| 99.000                           | 0.2257   | 0.7743  | 0.0609                        | 37               | 10             | test     |
| 103.000*                         | .        | .       | .                             | 37               | 9              | test     |
| 117.000                          | 0.2006   | 0.7994  | 0.0591                        | 38               | 8              | standard |
| 122.000                          | 0.1755   | 0.8245  | 0.0567                        | 39               | 7              | standard |
| 123.000*                         | .        | .       | .                             | 39               | 6              | standard |
| 139.000                          | 0.1463   | 0.8537  | 0.0543                        | 40               | 5              | standard |
| 151.000                          | 0.1170   | 0.8830  | 0.0507                        | 41               | 4              | standard |
| 153.000                          | 0.0878   | 0.9122  | 0.0457                        | 42               | 3              | standard |
| 287.000                          | 0.0585   | 0.9415  | 0.0387                        | 43               | 2              | standard |
| 384.000                          | 0.0293   | 0.9707  | 0.0283                        | 44               | 1              | standard |
| 392.000                          | 0        | 1.0000  | .                             | 45               | 0              | standard |

NOTE: The marked survival times are censored observations.

## Output 52.1.4 Estimation Results for Squamous Cells

| The LIFETEST Procedure           |          |         |                               |                  |                |          |
|----------------------------------|----------|---------|-------------------------------|------------------|----------------|----------|
| Stratum 4: Cell Type = squamous  |          |         |                               |                  |                |          |
| Product-Limit Survival Estimates |          |         |                               |                  |                |          |
| SurvTime                         | Survival | Failure | Survival<br>Standard<br>Error | Number<br>Failed | Number<br>Left | Therapy  |
| 0.000                            | 1.0000   | 0       | 0                             | 0                | 35             |          |
| 1.000                            | .        | .       | .                             | 1                | 34             | test     |
| 1.000                            | 0.9429   | 0.0571  | 0.0392                        | 2                | 33             | test     |
| 8.000                            | 0.9143   | 0.0857  | 0.0473                        | 3                | 32             | standard |
| 10.000                           | 0.8857   | 0.1143  | 0.0538                        | 4                | 31             | standard |
| 11.000                           | 0.8571   | 0.1429  | 0.0591                        | 5                | 30             | standard |
| 15.000                           | 0.8286   | 0.1714  | 0.0637                        | 6                | 29             | test     |
| 25.000                           | 0.8000   | 0.2000  | 0.0676                        | 7                | 28             | test     |
| 25.000*                          | .        | .       | .                             | 7                | 27             | standard |
| 30.000                           | 0.7704   | 0.2296  | 0.0713                        | 8                | 26             | test     |
| 33.000                           | 0.7407   | 0.2593  | 0.0745                        | 9                | 25             | test     |
| 42.000                           | 0.7111   | 0.2889  | 0.0772                        | 10               | 24             | standard |
| 44.000                           | 0.6815   | 0.3185  | 0.0794                        | 11               | 23             | test     |
| 72.000                           | 0.6519   | 0.3481  | 0.0813                        | 12               | 22             | standard |
| 82.000                           | 0.6222   | 0.3778  | 0.0828                        | 13               | 21             | standard |
| 87.000*                          | .        | .       | .                             | 13               | 20             | test     |
| 100.000*                         | .        | .       | .                             | 13               | 19             | standard |
| 110.000                          | 0.5895   | 0.4105  | 0.0847                        | 14               | 18             | standard |
| 111.000                          | 0.5567   | 0.4433  | 0.0861                        | 15               | 17             | test     |
| 112.000                          | 0.5240   | 0.4760  | 0.0870                        | 16               | 16             | test     |
| 118.000                          | 0.4912   | 0.5088  | 0.0875                        | 17               | 15             | standard |
| 126.000                          | 0.4585   | 0.5415  | 0.0876                        | 18               | 14             | standard |
| 144.000                          | 0.4257   | 0.5743  | 0.0873                        | 19               | 13             | standard |
| 201.000                          | 0.3930   | 0.6070  | 0.0865                        | 20               | 12             | test     |
| 228.000                          | 0.3602   | 0.6398  | 0.0852                        | 21               | 11             | standard |
| 231.000*                         | .        | .       | .                             | 21               | 10             | test     |
| 242.000                          | 0.3242   | 0.6758  | 0.0840                        | 22               | 9              | test     |
| 283.000                          | 0.2882   | 0.7118  | 0.0820                        | 23               | 8              | test     |
| 314.000                          | 0.2522   | 0.7478  | 0.0793                        | 24               | 7              | standard |
| 357.000                          | 0.2161   | 0.7839  | 0.0757                        | 25               | 6              | test     |
| 389.000                          | 0.1801   | 0.8199  | 0.0711                        | 26               | 5              | test     |
| 411.000                          | 0.1441   | 0.8559  | 0.0654                        | 27               | 4              | standard |
| 467.000                          | 0.1081   | 0.8919  | 0.0581                        | 28               | 3              | test     |
| 587.000                          | 0.0720   | 0.9280  | 0.0487                        | 29               | 2              | test     |
| 991.000                          | 0.0360   | 0.9640  | 0.0352                        | 30               | 1              | test     |
| 999.000                          | 0        | 1.0000  | .                             | 31               | 0              | test     |

NOTE: The marked survival times are censored observations.

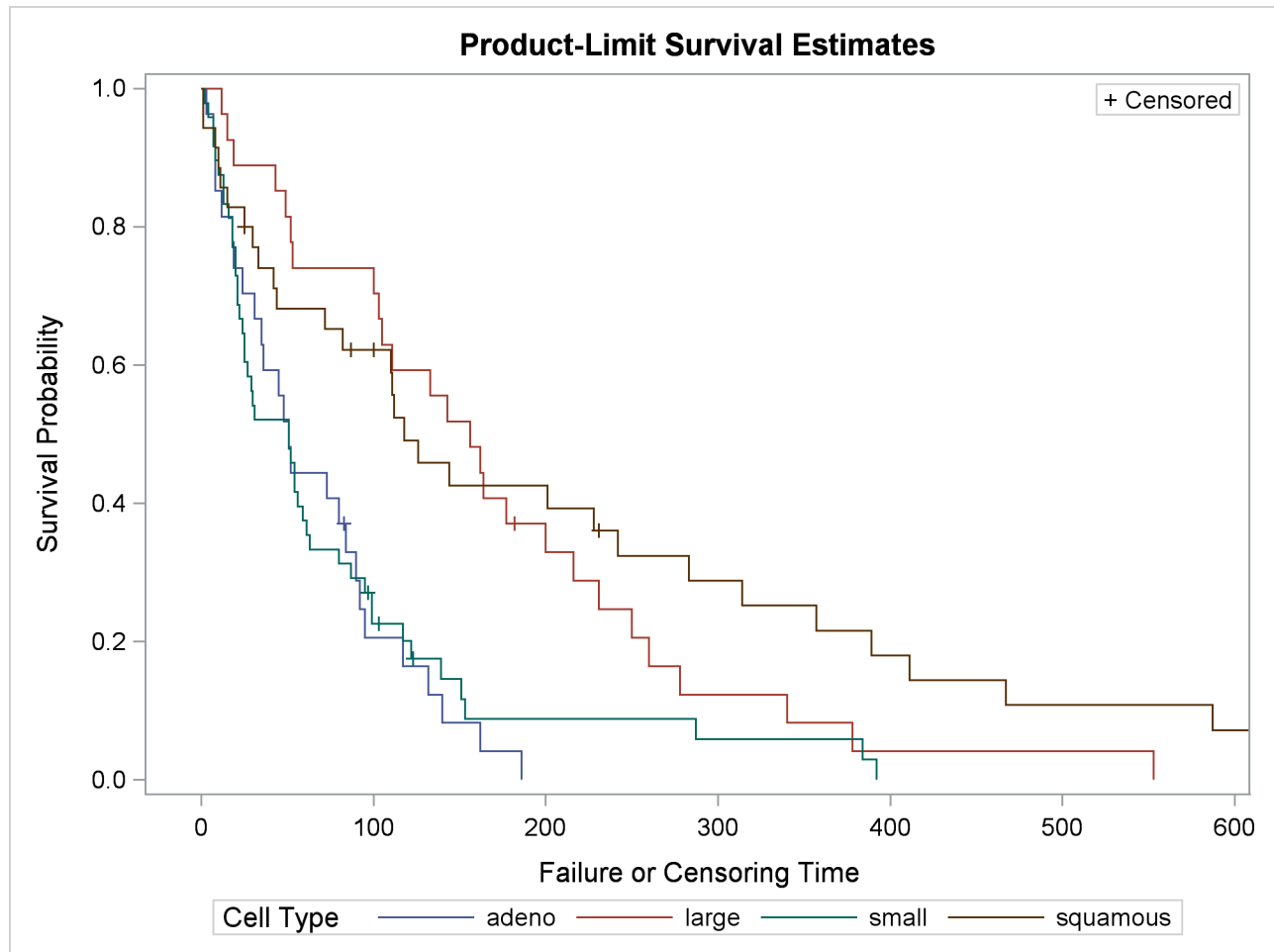
The distribution of event and censored observations among the four cell types is summarized in [Output 52.1.5](#).

**Output 52.1.5** Summary of Censored and Uncensored Values

| Summary of the Number of Censored and Uncensored Values |          |       |        |          |                  |
|---------------------------------------------------------|----------|-------|--------|----------|------------------|
| Stratum                                                 | Cell     | Total | Failed | Censored | Percent Censored |
| 1                                                       | adeno    | 27    | 26     | 1        | 3.70             |
| 2                                                       | large    | 27    | 26     | 1        | 3.70             |
| 3                                                       | small    | 48    | 45     | 3        | 6.25             |
| 4                                                       | squamous | 35    | 31     | 4        | 11.43            |
| -----                                                   |          |       |        |          |                  |
| Total                                                   |          | 137   | 128    | 9        | 6.57             |

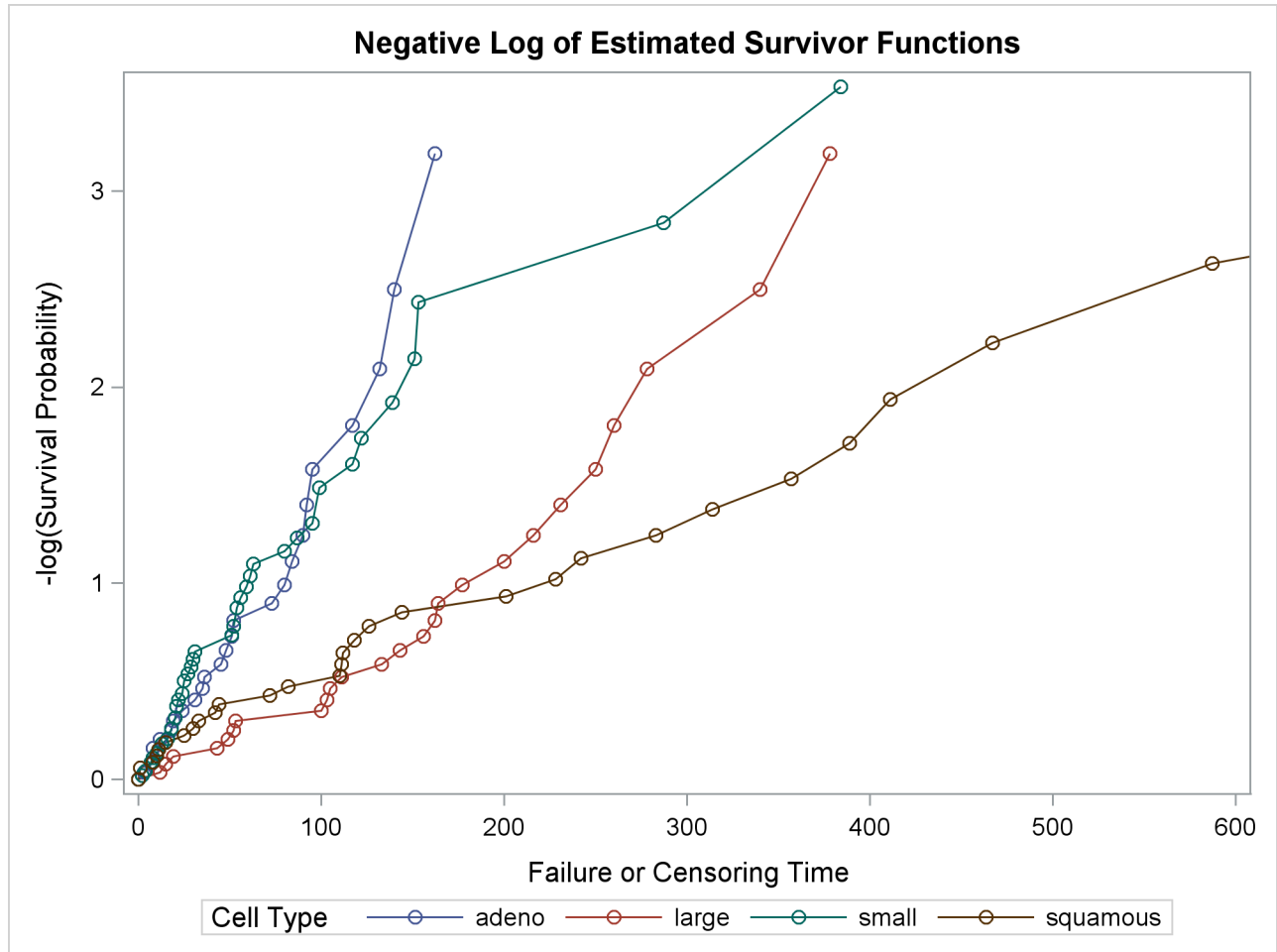
The graph of the estimated survivor functions is shown in [Output 52.1.6](#). The adeno cell curve and the small cell curve are much closer to each other than they are to the large cell curve or the squamous cell curve. The survival rates of the adeno cell patients and the small cell patients decrease rapidly to approximately 29% in 90 days. Shapes of the large cell curve and the squamous cell curve are quite different, although both decrease less rapidly than those of the adeno and small cells. The squamous cell curve decreases more rapidly initially than the large cell curve, but the role is reversed in the later period.



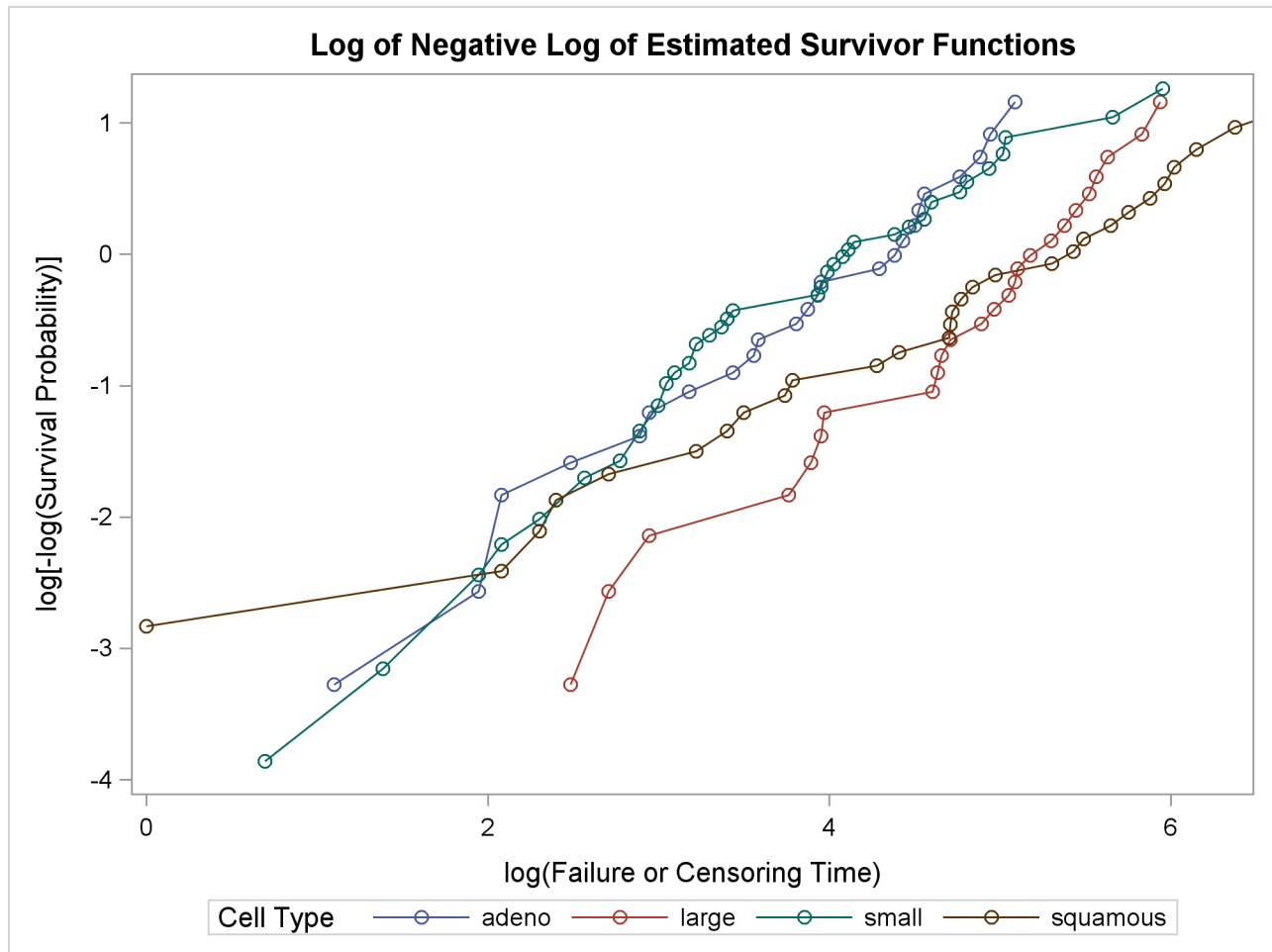
**Output 52.1.6** Graph of the Estimated Survivor Functions

The graph of the negative log of the estimated survivor functions is displayed in [Output 52.1.7](#). [Output 52.1.8](#) displays the log of the negative log of the estimated survivor functions against the log of time.

Output 52.1.7 Graph of Negative Log of the Estimated Survivor Functions



**Output 52.1.8** Graph of Log of the Negative Log of the Estimated Survivor Functions



Results of the homogeneity tests across cell types are given in [Output 52.1.9](#). The log-rank and Wilcoxon statistics and their corresponding covariance matrices are displayed. Also given is a table that consists of the approximate chi-square statistics, degrees of freedom, and  $p$ -values for the log-rank, Wilcoxon, and likelihood ratio tests. All three tests indicate strong evidence of a significant difference among the survival curves for the four types of cancer cells ( $p < 0.0001$ ).

**Output 52.1.9** Homogeneity Tests across Cell Types

| Rank Statistics |          |          |
|-----------------|----------|----------|
| Cell            | Log-Rank | Wilcoxon |
| adeno           | 10.306   | 697.0    |
| large           | -8.549   | -1085.0  |
| small           | 14.898   | 1278.0   |
| squamous        | -16.655  | -890.0   |

**Output 52.1.9** *continued*

| Covariance Matrix for the Log-Rank Statistics |         |          |         |          |
|-----------------------------------------------|---------|----------|---------|----------|
| Cell                                          | adeno   | large    | small   | squamous |
| adeno                                         | 12.9662 | -4.0701  | -4.4087 | -4.4873  |
| large                                         | -4.0701 | 24.1990  | -7.8117 | -12.3172 |
| small                                         | -4.4087 | -7.8117  | 21.7543 | -9.5339  |
| squamous                                      | -4.4873 | -12.3172 | -9.5339 | 26.3384  |

| Covariance Matrix for the Wilcoxon Statistics |        |        |        |          |
|-----------------------------------------------|--------|--------|--------|----------|
| Cell                                          | adeno  | large  | small  | squamous |
| adeno                                         | 121188 | -34718 | -46639 | -39831   |
| large                                         | -34718 | 151241 | -59948 | -56576   |
| small                                         | -46639 | -59948 | 175590 | -69002   |
| squamous                                      | -39831 | -56576 | -69002 | 165410   |

| Test of Equality over Strata |            |    |                 |
|------------------------------|------------|----|-----------------|
| Test                         | Chi-Square | DF | Pr > Chi-Square |
| Log-Rank                     | 25.4037    | 3  | <.0001          |
| Wilcoxon                     | 19.4331    | 3  | 0.0002          |
| -2Log(LR)                    | 33.9343    | 3  | <.0001          |

Results of the log-rank test of the prognostic variables are shown in [Output 52.1.10](#). The univariate test results correspond to testing each prognostic factor marginally. The joint covariance matrix of these univariate test statistics is also displayed. In computing the overall chi-square statistic, the partial chi-square statistics following a forward stepwise entry approach are tabulated.

Consider the log-rank test in [Output 52.1.10](#). Since the univariate test for Kps has the largest chi-square (43.4747) among all the covariates, Kps is entered first. At this stage, the partial chi-square and the chi-square increment for Kps are the same as the univariate chi-square. Among all the covariates not in the model (Age, Prior, DiagTime, Treatment), Treatment has the largest approximate chi-square increment (1.7261) and is entered next. The approximate chi-square for the model that contains Kps and Treatment is  $43.4747 + 1.7261 = 45.2008$  with 2 degrees of freedom. The third covariate entered is Age. The fourth is Prior, and the fifth is DiagTime. The overall chi-square statistic in the last line of the output is the partial chi-square for including all the covariates. It has a value of 46.4200 with 5 degrees of freedom, which is highly significant ( $p < 0.0001$ ).

**Output 52.1.10** Log-Rank Test of the Prognostic Factors

| Univariate Chi-Squares for the Log-Rank Test |                |                |            |                 |                           |
|----------------------------------------------|----------------|----------------|------------|-----------------|---------------------------|
| Variable                                     | Test Statistic | Standard Error | Chi-Square | Pr > Chi-Square | Label                     |
| Age                                          | -40.7383       | 105.7          | 0.1485     | 0.7000          | Age in Years              |
| Prior                                        | -19.9435       | 46.9836        | 0.1802     | 0.6712          | Prior Treatment?          |
| DiagTime                                     | -115.9         | 97.8708        | 1.4013     | 0.2365          | Months till Randomization |
| Kps                                          | 1123.1         | 170.3          | 43.4747    | <.0001          | Karnofsky Index           |
| Treatment                                    | -4.2076        | 5.0407         | 0.6967     | 0.4039          | Treatment Indicator       |

| Covariance Matrix for the Log-Rank Statistics |         |        |          |         |           |
|-----------------------------------------------|---------|--------|----------|---------|-----------|
| Variable                                      | Age     | Prior  | DiagTime | Kps     | Treatment |
| Age                                           | 11175.4 | -301.2 | -892.2   | -2948.4 | 119.3     |
| Prior                                         | -301.2  | 2207.5 | 2010.9   | 78.6    | 13.9      |
| DiagTime                                      | -892.2  | 2010.9 | 9578.7   | -2295.3 | 21.9      |
| Kps                                           | -2948.4 | 78.6   | -2295.3  | 29015.6 | 61.9      |
| Treatment                                     | 119.3   | 13.9   | 21.9     | 61.9    | 25.4      |

| Forward Stepwise Sequence of Chi-Squares for the Log-Rank Test |    |            |                 |                      |                |
|----------------------------------------------------------------|----|------------|-----------------|----------------------|----------------|
| Variable                                                       | DF | Chi-Square | Pr > Chi-Square | Chi-Square Increment | Pr > Increment |
| Kps                                                            | 1  | 43.4747    | <.0001          | 43.4747              | <.0001         |
| Treatment                                                      | 2  | 45.2008    | <.0001          | 1.7261               | 0.1889         |
| Age                                                            | 3  | 46.3012    | <.0001          | 1.1004               | 0.2942         |
| Prior                                                          | 4  | 46.4134    | <.0001          | 0.1122               | 0.7377         |
| DiagTime                                                       | 5  | 46.4200    | <.0001          | 0.0065               | 0.9350         |

| Variable  | Label                     |
|-----------|---------------------------|
| Kps       | Karnofsky Index           |
| Treatment | Treatment Indicator       |
| Age       | Age in Years              |
| Prior     | Prior Treatment?          |
| DiagTime  | Months till Randomization |

You can establish this forward stepwise entry of prognostic factors by passing the matrix corresponding to the log-rank test to the RSQUARE method in the REG procedure, as follows. PROC REG finds the sets of variables that yield the largest chi-square statistics.

```

data RSq;
 set Test;
 if _type_='LOG RANK';
 type='cov';
run;
proc print data=RSq;
run;
proc reg data=RSq(type=COV);
 model SurvTime=Age Prior DiagTime Kps Treatment
 / selection=rsquare;
 title 'All Possible Subsets of Covariates for the log-rank Test';
run;

```

Output 52.1.11 displays the univariate statistics and their covariance matrix for the log-rank test.

**Output 52.1.11** Log-Rank Statistics and Covariance Matrix

| Obs | _TYPE_ | _NAME_    | SurvTime | Age      | Prior   | DiagTime | Kps      | Treatment |
|-----|--------|-----------|----------|----------|---------|----------|----------|-----------|
| 1   | cov    | SurvTime  | 46.42    | -40.74   | -19.94  | -115.86  | 1123.14  | -4.208    |
| 2   | cov    | Age       | -40.74   | 11175.44 | -301.23 | -892.24  | -2948.45 | 119.297   |
| 3   | cov    | Prior     | -19.94   | -301.23  | 2207.46 | 2010.85  | 78.64    | 13.875    |
| 4   | cov    | DiagTime  | -115.86  | -892.24  | 2010.85 | 9578.69  | -2295.32 | 21.859    |
| 5   | cov    | Kps       | 1123.14  | -2948.45 | 78.64   | -2295.32 | 29015.62 | 61.945    |
| 6   | cov    | Treatment | -4.21    | 119.30   | 13.87   | 21.86    | 61.95    | 25.409    |

Results of the best subset regression are shown in [Output 52.1.12](#). The variable Kps generates the largest univariate test statistic among all the covariates, the pair Kps and Age generate the largest test statistic among any other pairs of covariates, and so on. The entry order of covariates is identical to that of PROC LIFETEST.

**Output 52.1.12** Best Subset Regression from the REG Procedure

```

All Possible Subsets of Covariates for the log-rank Test

The REG Procedure
Model: MODEL1
Dependent Variable: SurvTime

R-Square Selection Method

Number in
Model R-Square Variables in Model

1 0.9366 Kps
1 0.0302 DiagTime
1 0.0150 Treatment
1 0.0039 Prior
1 0.0032 Age

2 0.9737 Kps Treatment
2 0.9472 Age Kps
2 0.9417 Prior Kps
2 0.9382 DiagTime Kps
2 0.0434 DiagTime Treatment
2 0.0353 Age DiagTime
2 0.0304 Prior DiagTime
2 0.0181 Prior Treatment
2 0.0159 Age Treatment
2 0.0075 Age Prior

3 0.9974 Age Kps Treatment
3 0.9774 Prior Kps Treatment
3 0.9747 DiagTime Kps Treatment
3 0.9515 Age Prior Kps
3 0.9481 Age DiagTime Kps
3 0.9418 Prior DiagTime Kps
3 0.0456 Age DiagTime Treatment
3 0.0438 Prior DiagTime Treatment
3 0.0355 Age Prior DiagTime
3 0.0192 Age Prior Treatment

4 0.9999 Age Prior Kps Treatment
4 0.9976 Age DiagTime Kps Treatment
4 0.9774 Prior DiagTime Kps Treatment
4 0.9515 Age Prior DiagTime Kps
4 0.0459 Age Prior DiagTime Treatment

5 1.0000 Age Prior DiagTime Kps Treatment

```

## Example 52.2: Enhanced Survival Plot and Multiple-Comparison Adjustments

This example highlights a number of features in the survival plot that uses ODS Graphics. Also shown in this example are comparisons of survival curves based on multiple comparison adjustments. Data of 137 bone marrow transplant patients extracted from Klein and Moeschberger (1997) have been saved in the data set BMT in the Sashelp library. At the time of transplant, each patient is classified into one of three risk categories: ALL (acute lymphoblastic leukemia), AML (acute myelocytic leukemia)-Low Risk, and AML-High Risk. The endpoint of interest is the disease-free survival time, which is the time to death or relapse or to the end of the study in days. In this data set, the variable Group represents the patient's risk category, the variable T represents the disease-free survival time, and the variable Status is the censoring indicator, with the value 1 indicating an event time and the value 0 a censored time.

The following step displays the first 10 observations of the BMT data set in [Output 52.2.1](#). The data set is available in the Sashelp library.

```
proc print data=Sashelp.BMT(obs=10);
run;
```

**Output 52.2.1** A Subset of the Bone Marrow Transplant Data

| Obs | Group | T    | Status |
|-----|-------|------|--------|
| 1   | ALL   | 2081 | 0      |
| 2   | ALL   | 1602 | 0      |
| 3   | ALL   | 1496 | 0      |
| 4   | ALL   | 1462 | 0      |
| 5   | ALL   | 1433 | 0      |
| 6   | ALL   | 1377 | 0      |
| 7   | ALL   | 1330 | 0      |
| 8   | ALL   | 996  | 0      |
| 9   | ALL   | 226  | 0      |
| 10  | ALL   | 1199 | 0      |

In the following statements, PROC LIFETEST is invoked to compute the product-limit estimate of the survivor function for each risk category. Using ODS Graphics, you can display the number of subjects at risk in the survival plot. The **PLOTS=** option requests that the survival curves be plotted, and the **ATRISK=** suboption specifies the time points at which the at-risk numbers are displayed. In the STRATA statement, the **ADJUST=SIDAK** option requests the Šidák multiple-comparison adjustment, and by default, all paired comparisons are carried out.

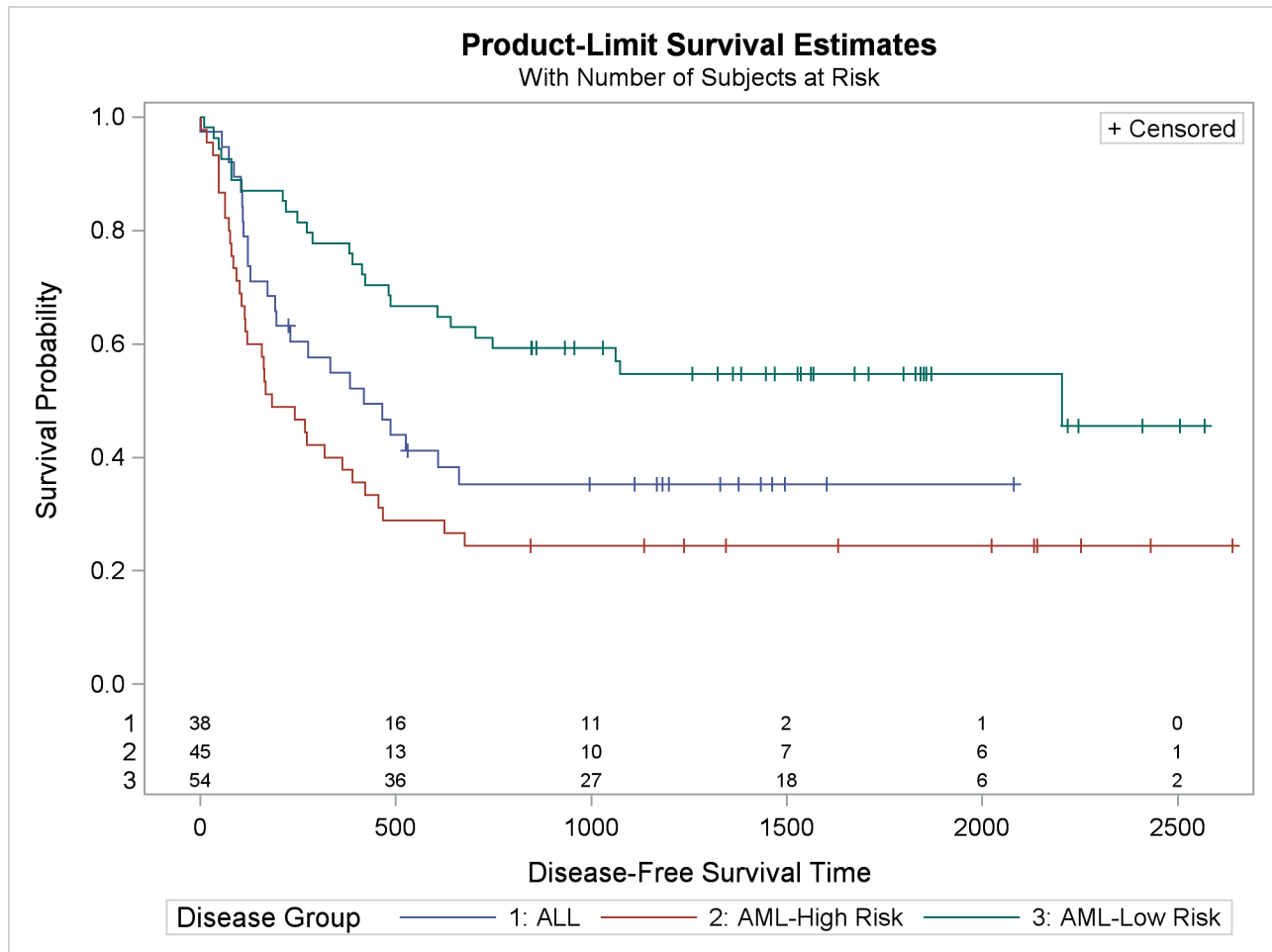
```
ods graphics on;

proc lifetest data=sashelp.BMT plots=survival(atrisk=0 to 2500 by 500);
 time T * Status(0);
 strata Group / test=logrank adjust=sidak;
run;
```

[Output 52.2.2](#) displays the estimated disease-free survival for the three leukemia groups with the number of subjects at risk at 0, 500, 1,000, 1,500, 2,000, and 2,500 days. Patients in the AML-Low Risk group experience a longer disease-free survival than those in the ALL group, who in turn fare better than those in the AML-High Risk group.



**Output 52.2.2** Estimated Disease-Free Survival for 137 Bone Marrow Transplant Patients



The log-rank test (Output 52.2.3) shows that the disease-free survival times for these three risk groups are significantly different ( $p = 0.001$ ).

**Output 52.2.3** Log-Rank Test of Disease Group Homogeneity

| Test of Equality over Strata |            |    |                 |
|------------------------------|------------|----|-----------------|
| Test                         | Chi-Square | DF | Pr > Chi-Square |
| Log-Rank                     | 13.8037    | 2  | 0.0010          |

The Šidák multiple-comparison results are shown in [Output 52.2.4](#). There is no significant difference in disease-free survivor functions between the ALL and AML-High Risk groups ( $p = 0.2779$ ). The difference between the ALL and AML-Low Risk groups is marginal ( $p = 0.0685$ ), but the AML-Low Risk and AML-High Risk groups have significantly different disease-free survivor functions ( $p = 0.0006$ ).

**Output 52.2.4** All Paired Comparisons

| Adjustment for Multiple Comparisons for the Logrank Test |               |            |          |        |
|----------------------------------------------------------|---------------|------------|----------|--------|
| Strata Comparison                                        |               |            | p-Values |        |
| Group                                                    | Group         | Chi-Square | Raw      | Sidak  |
| ALL                                                      | AML-High Risk | 2.6610     | 0.1028   | 0.2779 |
| ALL                                                      | AML-Low Risk  | 5.1400     | 0.0234   | 0.0685 |
| AML-High Risk                                            | AML-Low Risk  | 13.8011    | 0.0002   | 0.0006 |

Suppose you consider the AML-Low Risk group as the reference group. You can use the `DIFF=` option in the `STRATA` statement to designate this risk group as the control and apply a multiple-comparison adjustment to the  $p$ -values for the paired comparison between the AML-Low Risk group with each of the other groups. Consider the Šidák correction again. You specify the `ADJUST=` and `DIFF=` options as in the following statements:

```
proc lifetest data=sashelp.BMT notable plots=none;
 time T * Status(0);
 strata Group / test=logrank adjust=sidak diff=control('AML-Low Risk');
run;
```

[Output 52.2.5](#) shows that although both the ALL and AML-High Risk groups differ from the AML-Low Risk group at the 0.05 level, the difference between the AML-High Risk and the AML-Low Risk group is highly significant ( $p = 0.0004$ ).

**Output 52.2.5** Comparisons with the Reference Group

| The LIFETEST Procedure                                   |              |            |          |        |
|----------------------------------------------------------|--------------|------------|----------|--------|
| Adjustment for Multiple Comparisons for the Logrank Test |              |            | p-Values |        |
| Strata Comparison                                        |              |            | p-Values |        |
| Group                                                    | Group        | Chi-Square | Raw      | Sidak  |
| ALL                                                      | AML-Low Risk | 5.1400     | 0.0234   | 0.0462 |
| AML-High Risk                                            | AML-Low Risk | 13.8011    | 0.0002   | 0.0004 |

The survival plot that is displayed in [Output 52.2.2](#) might be sufficient for many purposes, but you might have other preferences. Typical alternatives include displaying the number of subjects at risk outside the plot area, reordering the stratum labels in the survival plot legend, and displaying the strata in the at-risk table by using their full labels. PROC LIFETEST provides options that you can use to make these changes without requiring template changes. In the `sashelp.BMT` data set, the variable `Group` that represents the strata is a character variable with three values, namely (in alphabetical order), ALL, AML-High Risk, and AML-Low Risk. It might be desirable to present the strata in the order ALL, AML-Low Risk, and AML-High Risk. The `ORDER=INTERNAL` option in the `STRATA` statement enables you to order the strata by their internal values. In the following statements, the new dataset `Bmt2` is a copy of `sashelp.BMT` with the variable `Group` changed to a numeric variable with values 1, 2, and 3 representing ALL, AML-Low Risk, and AML-High Risk, respectively. The original character values of `Group` are kept as the formatted values, which are used to label the strata in the printed output.

```
proc format;
 invalue $bmtifmt 'ALL' = 1 'AML-Low Risk' = 2 'AML-High Risk' = 3;
 value bmtfmt 1 = 'ALL' 2 = 'AML-Low Risk' 3 = 'AML-High Risk';
run;

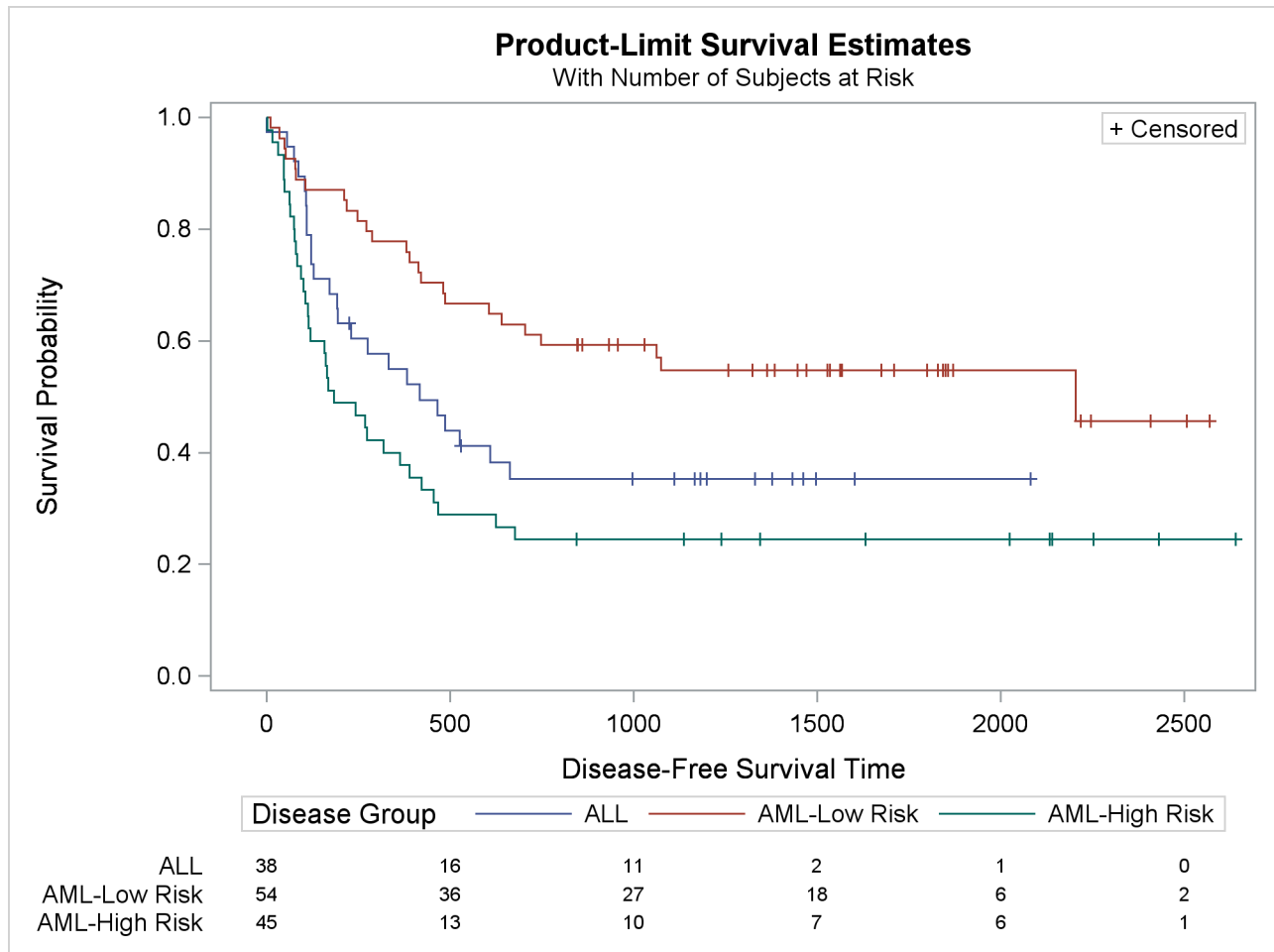
data Bmt2;
 set sashelp.BMT(rename=(Group=G));
 Group = input(input(G, $bmtifmt.), 1.);
 label Group = 'Disease Group';
 format Group bmtfmt.;
run;
```

The following statements produce a survival plot that has all the aforementioned modifications. The new data set `Bmt2` is used as the input data. The `OUTSIDE` and `MAXLEN=` options are specified in the `PLOTS=` option. The `OUTSIDE` option draws the at-risk table outside the plot area. Because the longest label of the strata has 13 characters, specifying `MAXLEN=13` is sufficient to display all the stratum labels in the at-risk table. The `ORDER=INTERNAL` option in the `STRATA` statement orders the strata by their numerical values 1, 2, and 3, which represent the order ALL, AML-Low Risk, and AML-High Risk, respectively.

```
proc LIFETEST data=Bmt2 plots=s(atrisk(outside maxlen=13)=0 to 2500 by 500);
 time T*Status(0);
 strata Group / order=internal;
run;
```

The modified survival plot is displayed in [Output 52.2.6](#). The most noticeable change from [Output 52.2.2](#) is that the number of subjects at risk is displayed below the time axis. Other changes include displaying the full labels of the strata in the at-risk table and presenting the strata in the order ALL, AML-Low Risk, and AML-High Risk.

**Output 52.2.6** Modified Disease-Free Survival for Bone Marrow Transplant Patients



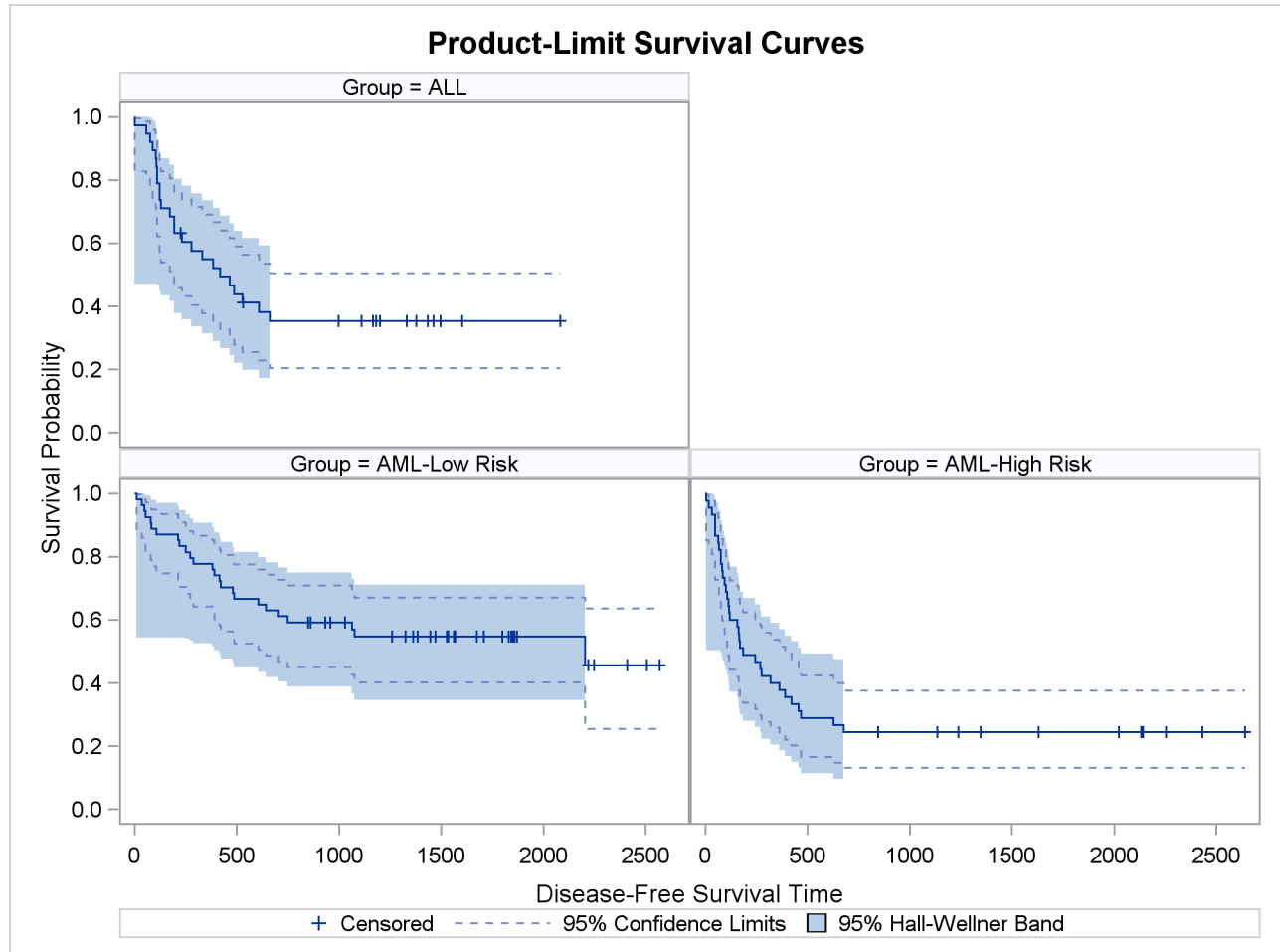
Klein and Moeschberger (1997, Section 4.4) describe in detail how to compute the Hall-Wellner (HW) and equal-precision (EP) confidence bands for the survivor function. You can output these simultaneous confidence intervals to a SAS data set by using the `CONFBAND=` and `OUTSURV=` options in the `PROC LIFETEST` statement. You can display survival curves with pointwise and simultaneous confidence limits through ODS Graphics. When the survival data are stratified, displaying all the survival curves and their confidence limits in the same plot can make the plot appear cluttered. In the following statements, the `PLOTS=` specification requests that the survivor functions be displayed along with their pointwise confidence limits (CL) and Hall-Wellner confidence bands (`CB=HW`). The `STRATA=``PANEL` specification requests that the survival curves be displayed in a panel of three plots, one for each risk group.

```
proc lifetest data=Bmt2 plots=survival(cl cb=hw strata=panel);
 time T * Status(0);
 strata Group/order=internal;
run;
```

```
ods graphics off;
```

The panel plot is shown in [Output 52.2.7](#).

**Output 52.2.7** Estimated Disease-Free Survivor Functions with Confidence Limits



## Example 52.3: Life-Table Estimates for Males with Angina Pectoris

The data in this example come from Lee (1992, p. 91) and represent the survival rates of males with angina pectoris. Survival time is measured as years from the time of diagnosis. In the following DATA step, the data are read as number of events and number of withdrawals in each one-year time interval for 16 intervals. Three variables are constructed from the data: Years (an artificial time variable with values that are the midpoints of the time intervals), Censored (a censoring indicator variable with the value 1 indicating censored observations and the value 0 indicating event observations), and Freq (the frequency variable). Two observations are created for each interval, one representing the event observations and the other representing the censored observations.

```

title 'Survival of Males with Angina Pectoris';
data Males;
 keep Freq Years Censored;
 retain Years -.5;
 input fail withdraw @@;
 Years + 1;
 Censored=0;
 Freq=fail;
 output;
 Censored=1;
 Freq=withdraw;
 output;
 datalines;
456 0 226 39 152 22 171 23 135 24 125 107
 83 133 74 102 51 68 42 64 43 45 34 53
 18 33 9 27 6 23 0 30
;

```

In the following statements, the ODS GRAPHICS ON specification enables ODS Graphics. PROC LIFETEST is invoked to compute the various life-table survival estimates, the median residual time, and their standard errors. The life-table method of computing estimates is requested by specifying METHOD=LT. The intervals are specified by the INTERVAL= option. Graphical displays of the life-table survivor function estimate, negative log of the estimate, log of negative log of the estimate, estimated density function, and estimated hazard function are requested by the PLOTS= option. No tests for homogeneity are carried out because the data are not stratified.

```

ods graphics on;
proc lifetest data=Males method=lt intervals=(0 to 15 by 1)
 plots=(s,ls,lls,h,p);
 time Years*Censored(1);
 freq Freq;
run;
ods graphics off;

```

Results of the life-table estimation are shown in [Output 52.3.1](#). The five-year survival rate is 0.5193 with a standard error of 0.0103. The estimated median residual lifetime, which is 5.33 years initially, reaches a maximum of 6.34 years at the beginning of the second year and decreases gradually to a value lower than the initial 5.33 years at the beginning of the seventh year.

**Output 52.3.1** Life-Table Survivor Function Estimate

| Survival of Males with Angina Pectoris |                  |                    |                             |                                          |                                                 |         |
|----------------------------------------|------------------|--------------------|-----------------------------|------------------------------------------|-------------------------------------------------|---------|
| The LIFETEST Procedure                 |                  |                    |                             |                                          |                                                 |         |
| Life Table Survival Estimates          |                  |                    |                             |                                          |                                                 |         |
| Interval<br>[Lower, Upper)             | Number<br>Failed | Number<br>Censored | Effective<br>Sample<br>Size | Conditional<br>Probability<br>of Failure | Conditional<br>Probability<br>Standard<br>Error |         |
| 0                                      | 1                | 456                | 0                           | 2418.0                                   | 0.1886                                          | 0.00796 |
| 1                                      | 2                | 226                | 39                          | 1942.5                                   | 0.1163                                          | 0.00728 |
| 2                                      | 3                | 152                | 22                          | 1686.0                                   | 0.0902                                          | 0.00698 |
| 3                                      | 4                | 171                | 23                          | 1511.5                                   | 0.1131                                          | 0.00815 |
| 4                                      | 5                | 135                | 24                          | 1317.0                                   | 0.1025                                          | 0.00836 |
| 5                                      | 6                | 125                | 107                         | 1116.5                                   | 0.1120                                          | 0.00944 |
| 6                                      | 7                | 83                 | 133                         | 871.5                                    | 0.0952                                          | 0.00994 |
| 7                                      | 8                | 74                 | 102                         | 671.0                                    | 0.1103                                          | 0.0121  |
| 8                                      | 9                | 51                 | 68                          | 512.0                                    | 0.0996                                          | 0.0132  |
| 9                                      | 10               | 42                 | 64                          | 395.0                                    | 0.1063                                          | 0.0155  |
| 10                                     | 11               | 43                 | 45                          | 298.5                                    | 0.1441                                          | 0.0203  |
| 11                                     | 12               | 34                 | 53                          | 206.5                                    | 0.1646                                          | 0.0258  |
| 12                                     | 13               | 18                 | 33                          | 129.5                                    | 0.1390                                          | 0.0304  |
| 13                                     | 14               | 9                  | 27                          | 81.5                                     | 0.1104                                          | 0.0347  |
| 14                                     | 15               | 6                  | 23                          | 47.5                                     | 0.1263                                          | 0.0482  |
| 15                                     | .                | 0                  | 30                          | 15.0                                     | 0                                               | 0       |

| Interval<br>[Lower, Upper) | Survival | Failure | Survival<br>Standard<br>Error | Median<br>Residual<br>Lifetime | Median<br>Standard<br>Error |
|----------------------------|----------|---------|-------------------------------|--------------------------------|-----------------------------|
| 0                          | 1        | 1.0000  | 0                             | 5.3313                         | 0.1749                      |
| 1                          | 2        | 0.8114  | 0.1886                        | 6.2499                         | 0.2001                      |
| 2                          | 3        | 0.7170  | 0.2830                        | 6.3432                         | 0.2361                      |
| 3                          | 4        | 0.6524  | 0.3476                        | 6.2262                         | 0.2361                      |
| 4                          | 5        | 0.5786  | 0.4214                        | 6.2185                         | 0.1853                      |
| 5                          | 6        | 0.5193  | 0.4807                        | 5.9077                         | 0.1806                      |
| 6                          | 7        | 0.4611  | 0.5389                        | 5.5962                         | 0.1855                      |
| 7                          | 8        | 0.4172  | 0.5828                        | 5.1671                         | 0.2713                      |
| 8                          | 9        | 0.3712  | 0.6288                        | 4.9421                         | 0.2763                      |
| 9                          | 10       | 0.3342  | 0.6658                        | 4.8258                         | 0.4141                      |
| 10                         | 11       | 0.2987  | 0.7013                        | 4.6888                         | 0.4183                      |
| 11                         | 12       | 0.2557  | 0.7443                        | .                              | .                           |
| 12                         | 13       | 0.2136  | 0.7864                        | .                              | .                           |
| 13                         | 14       | 0.1839  | 0.8161                        | .                              | .                           |
| 14                         | 15       | 0.1636  | 0.8364                        | .                              | .                           |

**Output 52.3.1** *continued*

| Survival of Males with Angina Pectoris    |        |          |          |          |          |          |
|-------------------------------------------|--------|----------|----------|----------|----------|----------|
| The LIFETEST Procedure                    |        |          |          |          |          |          |
| Interval                                  |        | Survival | Failure  | Survival | Median   | Median   |
| [Lower,                                   | Upper) |          |          | Standard | Residual | Standard |
|                                           |        |          |          | Error    | Lifetime | Error    |
| 15                                        | .      | 0.1429   | 0.8571   | 0.0133   | .        | .        |
| Evaluated at the Midpoint of the Interval |        |          |          |          |          |          |
| Interval                                  |        | PDF      | PDF      | Hazard   | Hazard   |          |
| [Lower,                                   | Upper) |          | Standard | Standard | Standard | Error    |
|                                           |        |          | Error    | Error    | Error    |          |
| 0                                         | 1      | 0.1886   | 0.00796  | 0.208219 | 0.009698 |          |
| 1                                         | 2      | 0.0944   | 0.00598  | 0.123531 | 0.008201 |          |
| 2                                         | 3      | 0.0646   | 0.00507  | 0.09441  | 0.007649 |          |
| 3                                         | 4      | 0.0738   | 0.00543  | 0.119916 | 0.009154 |          |
| 4                                         | 5      | 0.0593   | 0.00495  | 0.108043 | 0.009285 |          |
| 5                                         | 6      | 0.0581   | 0.00503  | 0.118596 | 0.010589 |          |
| 6                                         | 7      | 0.0439   | 0.00469  | 0.1      | 0.010963 |          |
| 7                                         | 8      | 0.0460   | 0.00518  | 0.116719 | 0.013545 |          |
| 8                                         | 9      | 0.0370   | 0.00502  | 0.10483  | 0.014659 |          |
| 9                                         | 10     | 0.0355   | 0.00531  | 0.112299 | 0.017301 |          |
| 10                                        | 11     | 0.0430   | 0.00627  | 0.155235 | 0.023602 |          |
| 11                                        | 12     | 0.0421   | 0.00685  | 0.17942  | 0.030646 |          |
| 12                                        | 13     | 0.0297   | 0.00668  | 0.149378 | 0.03511  |          |
| 13                                        | 14     | 0.0203   | 0.00651  | 0.116883 | 0.038894 |          |
| 14                                        | 15     | 0.0207   | 0.00804  | 0.134831 | 0.054919 |          |
| 15                                        | .      | .        | .        | .        | .        | .        |

The breakdown of event and censored observations in the data is shown in [Output 52.3.2](#). Note that 32.8% of the patients have withdrawn from the study.

**Output 52.3.2** Summary of Censored and Event Observations

| Summary of the Number of Censored and Uncensored Values                              |        |          |                  |  |
|--------------------------------------------------------------------------------------|--------|----------|------------------|--|
| Total                                                                                | Failed | Censored | Percent Censored |  |
| 2418                                                                                 | 1625   | 793      | 32.80            |  |
| NOTE: 2 observations with invalid time, censoring, or frequency values were deleted. |        |          |                  |  |



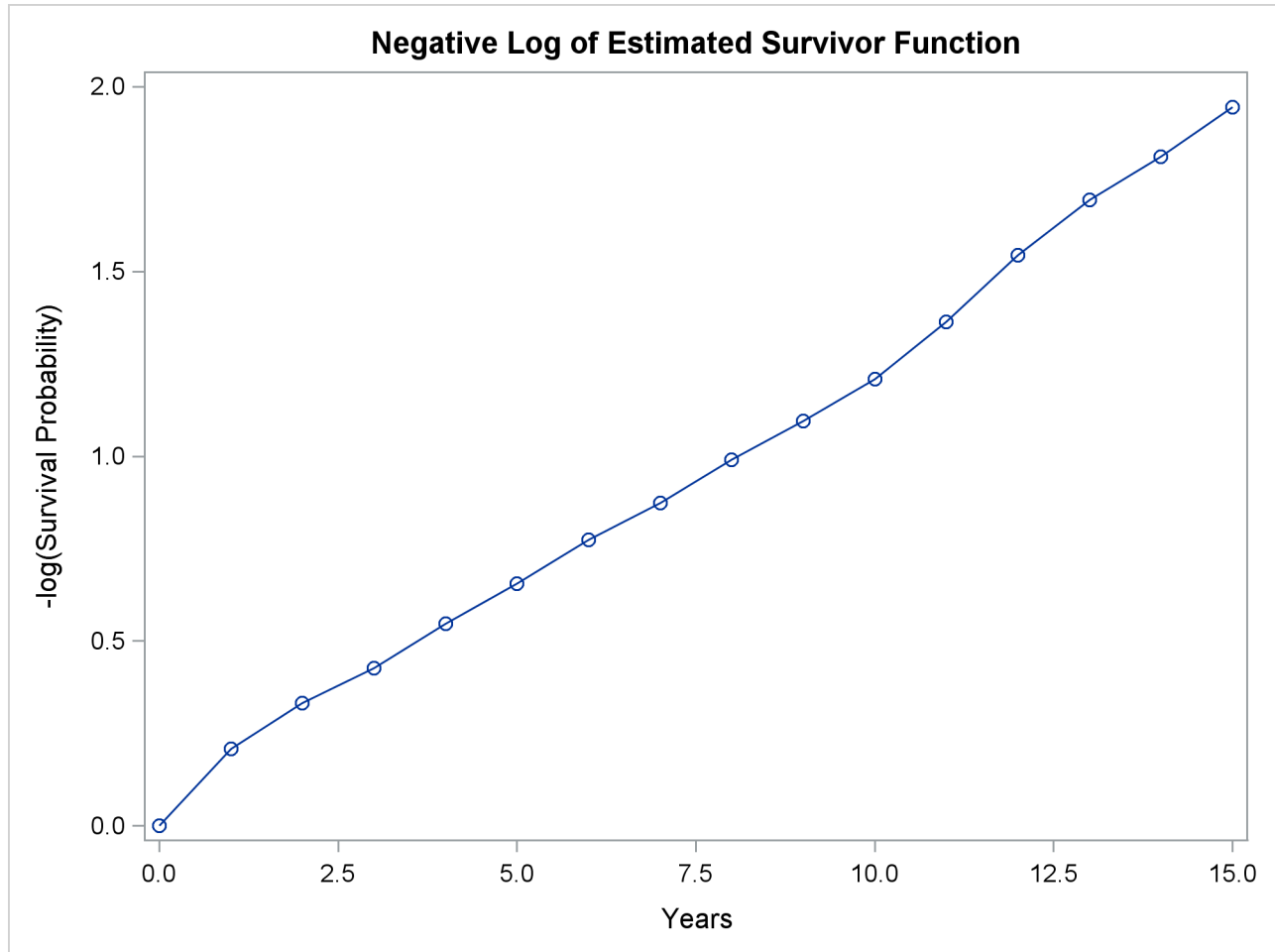
Output 52.3.3 displays the graph of the life-table survivor function estimate. The median survival time, read from the survivor function curve, is 5.33 years, and the 25th and 75th percentiles are 1.04 and 11.13 years, respectively.

**Output 52.3.3** Life-Table Survivor Function Estimate



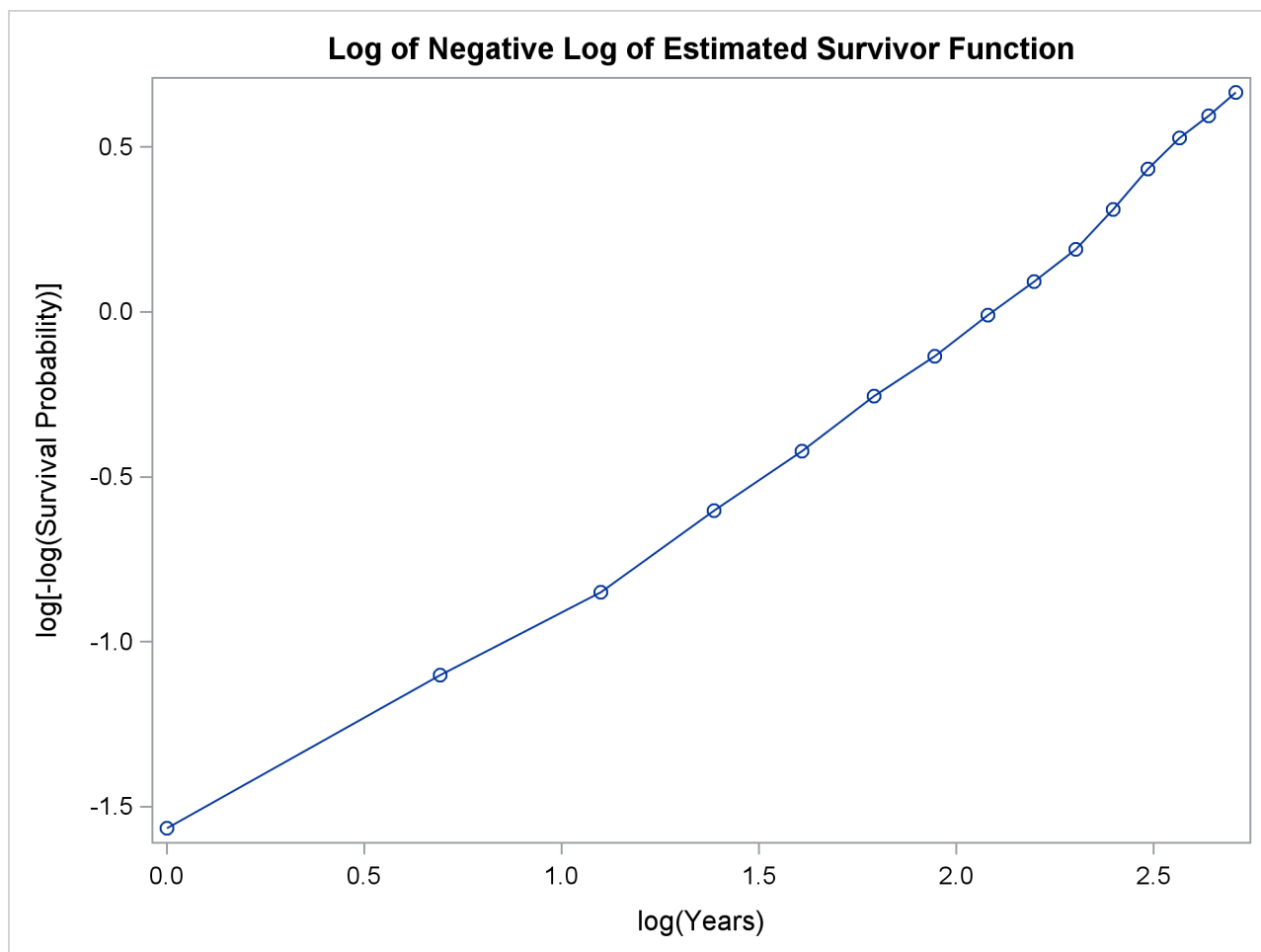
An exponential model might be appropriate for the survival of these male patients with angina pectoris since the curve of the negative log of the survivor function estimate versus the survival time (Output 52.3.4) approximates a straight line through the origin. Note that the graph of the log of the negative log of the survivor function estimate versus the log of time (Output 52.3.5) is practically a straight line.

**Output 52.3.4** Negative Log of Survivor Function Estimate

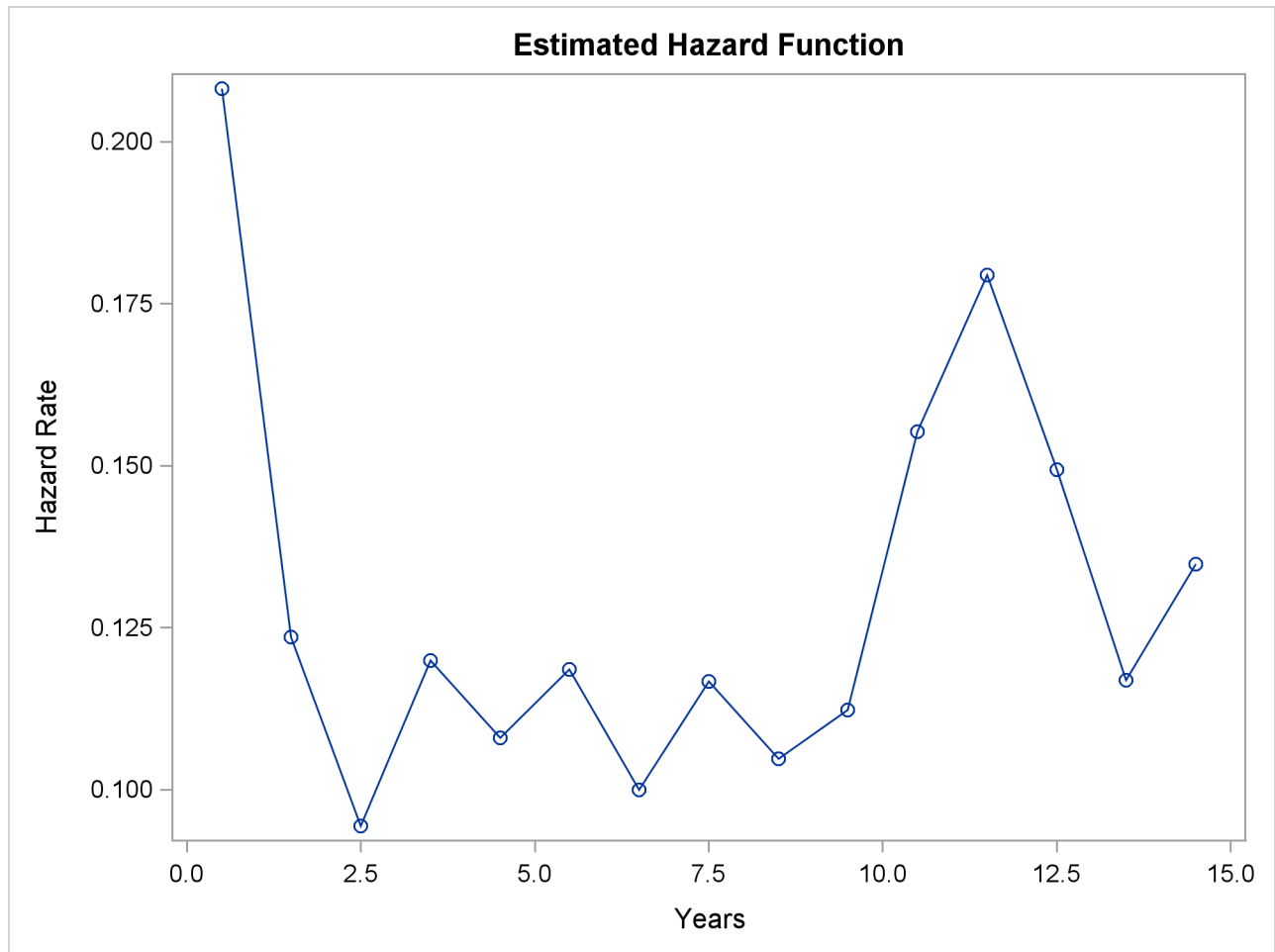


As discussed in Lee (1992), the graph of the estimated hazard function ([Output 52.3.6](#)) shows that the death rate is highest in the first year of diagnosis. From the end of the first year to the end of the tenth year, the death rate remains relatively constant, fluctuating between 0.09 and 0.12. The death rate is generally higher after the tenth year. This could indicate that a patient who has survived the first year has a better chance than a patient who has just been diagnosed. The profile of the median residual lifetimes also supports this interpretation.

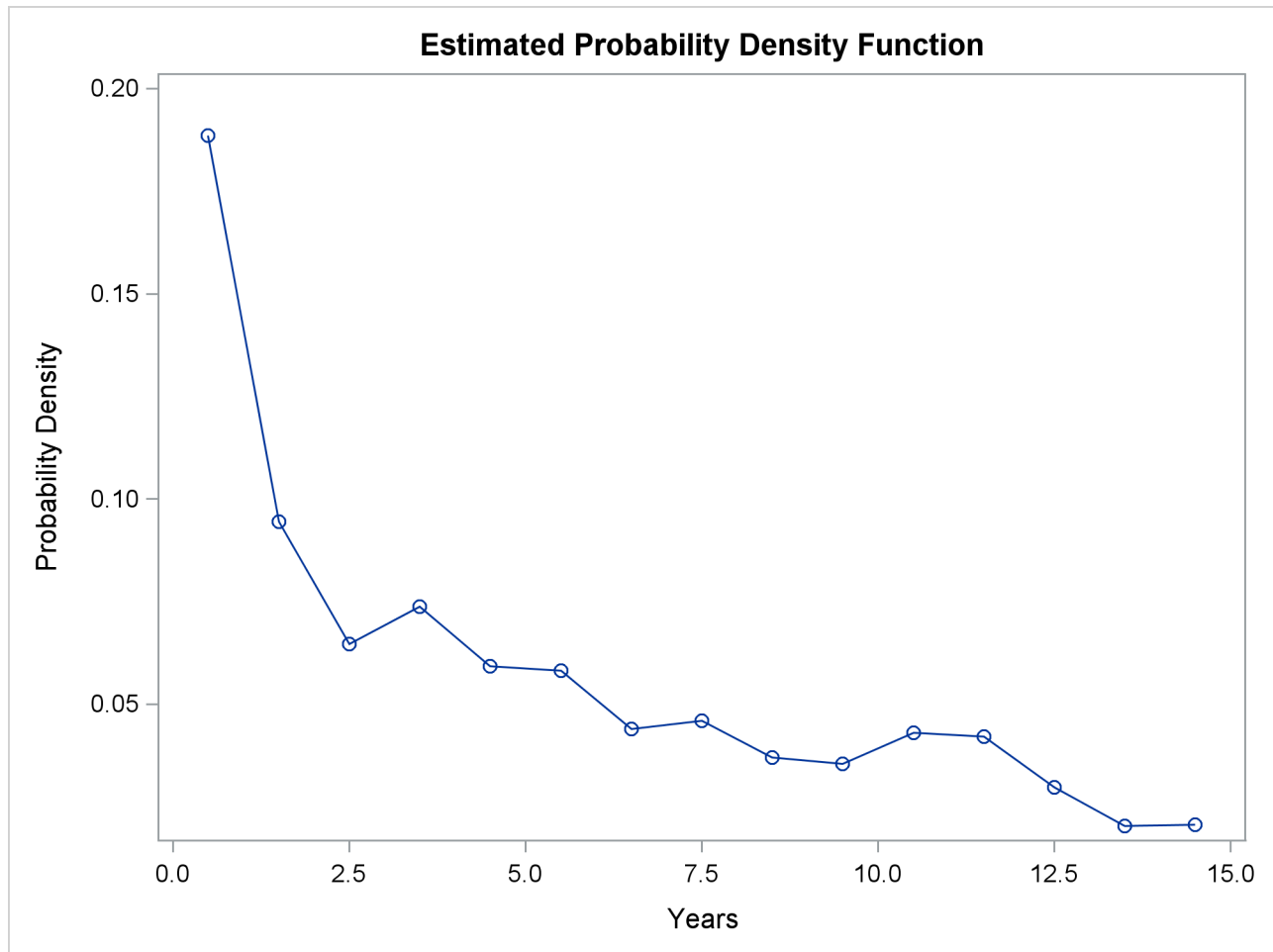
**Output 52.3.5** Log of Negative Log of Survivor Function Estimate



Output 52.3.6 Hazard Function Estimate



The density estimate is shown in (Output 52.3.7). Visually, it resembles the density function of an exponential distribution.

**Output 52.3.7** Density Function Estimate

---

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# Chapter 53

## The LOESS Procedure

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## Overview: LOESS Procedure

The LOESS procedure implements a nonparametric method for estimating regression surfaces pioneered by Cleveland, Devlin, and Grosse (1988); Cleveland and Grosse (1991); Cleveland, Grosse, and Shyu (1992). The LOESS procedure allows great flexibility because no assumptions about the parametric form of the regression surface are needed.

The SAS System provides many regression procedures such as the GLM, REG, and NLIN procedures for situations in which you can specify a reasonable parametric model for the regression surface. You can use the LOESS procedure for situations in which you do not know a suitable parametric form of the regression surface. Furthermore, the LOESS procedure is suitable when there are outliers in the data and a robust fitting method is necessary.

The main features of the LOESS procedure are as follows:

- fits nonparametric models
- supports the use of multidimensional data
- supports multiple dependent variables
- supports both direct and interpolated fitting that uses  $k$ -d trees
- performs statistical inference
- performs automatic smoothing parameter selection
- performs iterative reweighting to provide robust fitting when there are outliers in the data
- produces graphs with ODS Graphics

---

## Local Regression and the Loess Method

Assume that for  $i = 1$  to  $n$ , the  $i$ th measurement  $y_i$  of the response  $y$  and the corresponding measurement  $x_i$  of the vector  $\mathbf{x}$  of  $p$  predictors are related by

$$y_i = g(x_i) + \epsilon_i$$

where  $g$  is the regression function and  $\epsilon_i$  is a random error. The idea of local regression is that at a predictor  $\mathbf{x}$ , the regression function  $g(\mathbf{x})$  can be locally approximated by the value of a function in some specified parametric class. Such a local approximation is obtained by fitting a regression surface to the data points within a chosen neighborhood of the point  $x_i$ .

In the loess method, weighted least squares is used to fit linear or quadratic functions of the predictors at the centers of neighborhoods. The radius of each neighborhood is chosen so that the neighborhood contains a specified percentage of the data points. The fraction of the data, called the *smoothing parameter*, in each local neighborhood controls the smoothness of the estimated surface. Data points in a given local neighborhood are weighted by a smooth decreasing function of their distance from the center of the neighborhood.

In a direct implementation, such fitting is done at each point at which the regression surface is to be estimated. A much faster computational procedure is to perform such local fitting at a selected sample of points in predictor space and then to blend these local polynomials to obtain a regression surface.

You can use the LOESS procedure to perform statistical inference provided that the error distribution satisfies some basic assumptions. In particular, such analysis is appropriate when the  $\epsilon_i$  are iid normal random variables with mean 0. By using the iterative reweighting, the LOESS procedure can also provide statistical inference when the error distribution is symmetric but not necessarily normal. Furthermore, by doing iterative reweighting, you can use the LOESS procedure to perform robust fitting in the presence of outliers in the data.

While all output of the LOESS procedure can be optionally displayed, most often the LOESS procedure is used to produce output data sets that will be viewed and manipulated by other SAS procedures. PROC LOESS uses the Output Delivery System (ODS) to place results in output data sets. Alternatively, PROC LOESS also provides an OUTPUT statement to create SAS data sets from analysis results.

---

## Getting Started: LOESS Procedure

---

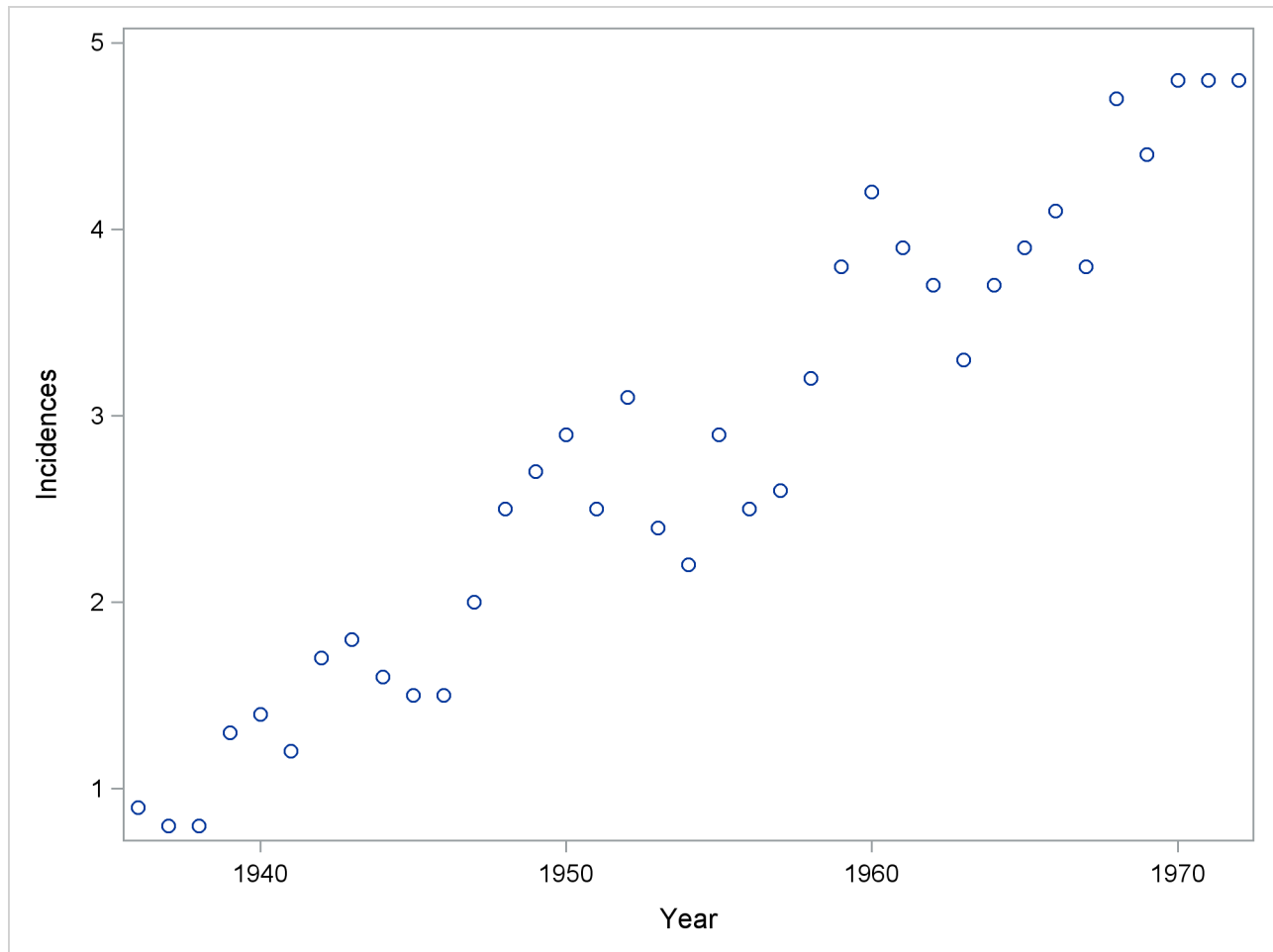
### Scatter Plot Smoothing

The following data from the Connecticut Tumor Registry presents age-adjusted numbers of melanoma incidences per 100,000 people for the 37 years from 1936 to 1972 (Houghton, Flannery, and Viola 1980).

```
data Melanoma;
 input Year Incidences @@;
 format Year d4.0;
 datalines;
1936 0.9 1937 0.8 1938 0.8 1939 1.3
1940 1.4 1941 1.2 1942 1.7 1943 1.8
1944 1.6 1945 1.5 1946 1.5 1947 2.0
1948 2.5 1949 2.7 1950 2.9 1951 2.5
1952 3.1 1953 2.4 1954 2.2 1955 2.9
1956 2.5 1957 2.6 1958 3.2 1959 3.8
1960 4.2 1961 3.9 1962 3.7 1963 3.3
1964 3.7 1965 3.9 1966 4.1 1967 3.8
1968 4.7 1969 4.4 1970 4.8 1971 4.8
1972 4.8
;
```

The following PROC SGPLOT statements produce the simple scatter plot of these data displayed in [Figure 53.1](#).

```
proc sgplot data=Melanoma;
 scatter y=Incidence x=Year;
run;
```

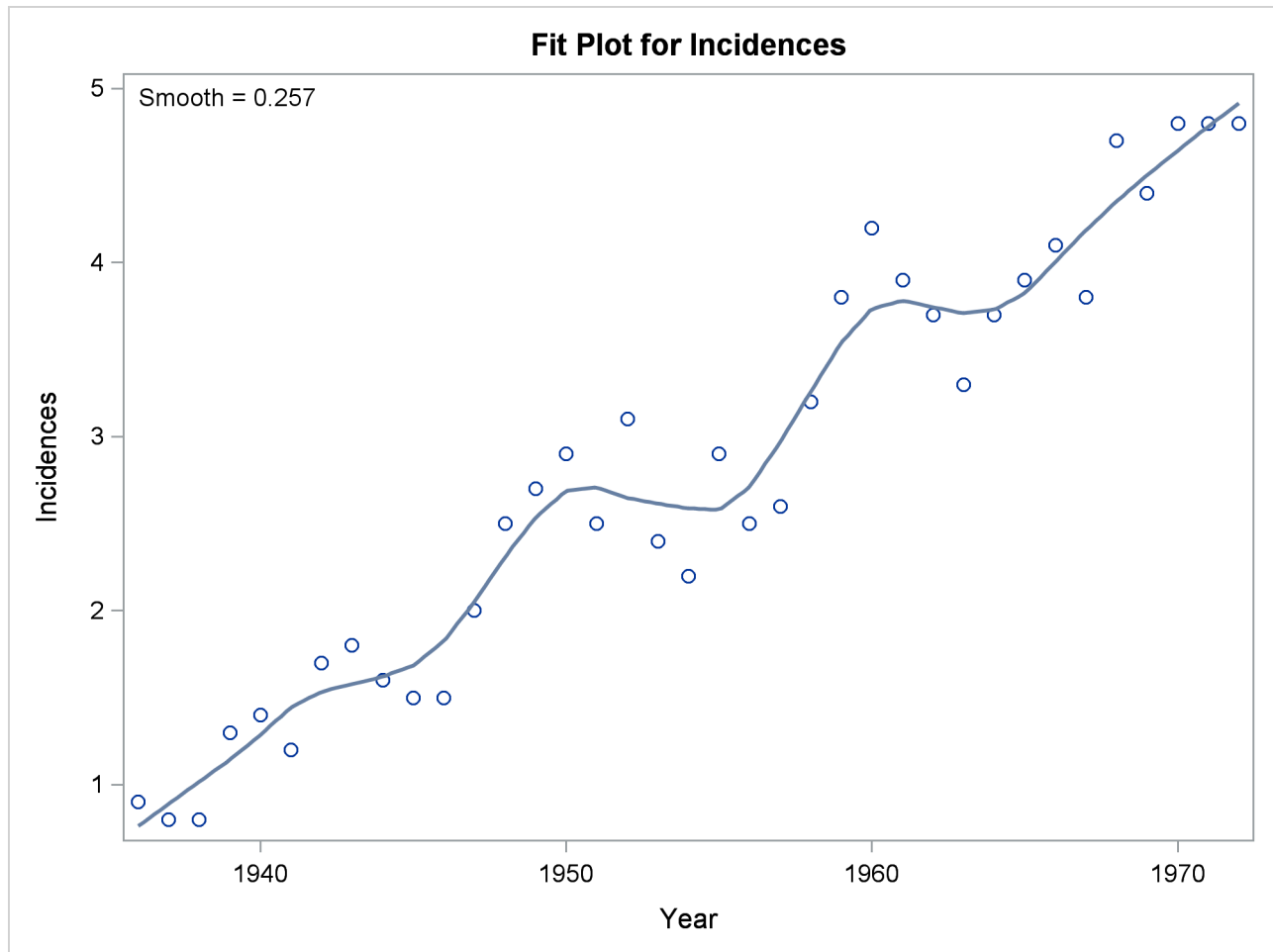
**Figure 53.1** Scatter Plot of the Melanoma Data

Suppose that you want to smooth the response variable `Incidence` as a function of the variable `Year`. The following PROC LOESS statements request this analysis with the default settings:

```
ods graphics on;

proc loess data=Melanoma;
 model Incidence=Year;
run;
```

You use the PROC LOESS statement to invoke the procedure and specify the data set. The MODEL statement names the dependent and independent variables.

**Figure 53.2** Default Loess Fit for the Melanoma Data

When ODS Graphics is enabled, PROC LOESS produces several default plots. [Figure 53.2](#) shows the “Fit Plot” that overlays the loess fit on a scatter plot of the data. You can see that the loess fit captures the increasing trend in the data as well as the periodic pattern in the data, which is related to an 11-year sunspot activity cycle.

**Figure 53.3** Fit Summary

| The LOESS Procedure                 |          |
|-------------------------------------|----------|
| Selected Smoothing Parameter: 0.257 |          |
| Dependent Variable: Incidences      |          |
| Fit Summary                         |          |
| Fit Method                          | kd Tree  |
| Blending                            | Linear   |
| Number of Observations              | 37       |
| Number of Fitting Points            | 37       |
| kd Tree Bucket Size                 | 1        |
| Degree of Local Polynomials         | 1        |
| Smoothing Parameter                 | 0.25676  |
| Points in Local Neighborhood        | 9        |
| Residual Sum of Squares             | 2.03105  |
| Trace[L]                            | 8.62243  |
| GCV                                 | 0.00252  |
| AICC                                | -1.17277 |

Figure 53.3 shows the “Fit Summary” table. This table details the settings used and provides statistics about the fit that is produced. You can see that smoothing parameter value for this loess fit is 0.257. This smoothing parameter determines the fraction of the data in each local neighborhood. In this example, there are 37 data points and so the smoothing parameter value of 0.257 yields local neighborhoods containing 9 observations.

**Figure 53.4** Smoothing Parameter Selection

| Optimal Smoothing<br>Criterion |                        |
|--------------------------------|------------------------|
| AICC                           | Smoothing<br>Parameter |
| -1.17277                       | 0.25676                |

The “Smoothing Criterion” table provides information about how this smoothing parameter value is selected. The default method implemented in PROC LOESS chooses the smoothing parameter that minimizes the AICC criterion (Hurvich, Simonoff, and Tsai 1998) that strikes a balance between the residual sum of squares and the complexity of the fit.

You use options in the MODEL statement to change the default settings and request optionally displayed tables. For example, the following statements request that the “Model Summary” and “Output Statistics” tables be included in the displayed output. By default, these tables are not displayed.

```
proc loess data=Melanoma;
 model Incidences=Year / details(ModelSummary OutputStatistics);
run;
```

**Figure 53.5** Model Summary Table

| The LOESS Procedure            |                 |             |         |          |
|--------------------------------|-----------------|-------------|---------|----------|
| Dependent Variable: Incidences |                 |             |         |          |
| Model Summary                  |                 |             |         |          |
| Smoothing<br>Parameter         | Local<br>Points | Residual SS | GCV     | AICC     |
| 0.41892                        | 15              | 3.42229     | 0.00339 | -0.96252 |
| 0.68919                        | 25              | 4.05838     | 0.00359 | -0.93459 |
| 0.31081                        | 11              | 2.51054     | 0.00279 | -1.12034 |
| 0.20270                        | 7               | 1.58513     | 0.00239 | -1.12221 |
| 0.17568                        | 6               | 1.56896     | 0.00241 | -1.09706 |
| 0.28378                        | 10              | 2.50487     | 0.00282 | -1.10402 |
| 0.20270                        | 7               | 1.58513     | 0.00239 | -1.12221 |
| 0.25676                        | 9               | 2.03105     | 0.00252 | -1.17277 |
| 0.22973                        | 8               | 2.02965     | 0.00256 | -1.15145 |
| 0.25676                        | 9               | 2.03105     | 0.00252 | -1.17277 |

The “Model Summary” table shown in [Figure 53.5](#) provides information about all the models that PROC LOESS evaluated in choosing the smoothing parameter value.

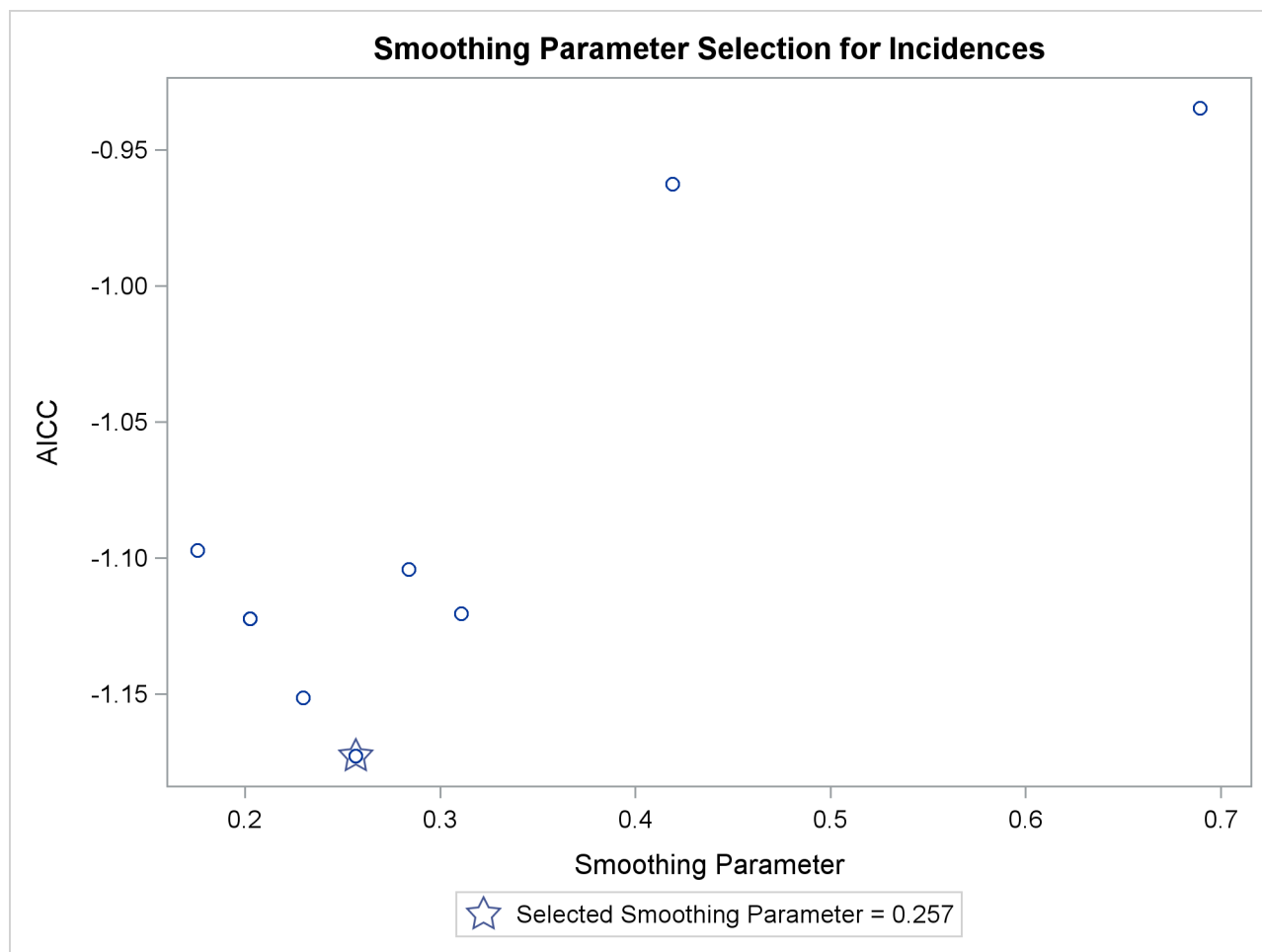
**Figure 53.6** AICC Criterion by Smoothing Parameter

Figure 53.6 shows the “Criterion Plot” that provides a graphical display of the smoothing parameter selection process.

Figure 53.7 Output Statistics

| The LOESS Procedure                 |      |            |                      |          |
|-------------------------------------|------|------------|----------------------|----------|
| Selected Smoothing Parameter: 0.257 |      |            |                      |          |
| Dependent Variable: Incidences      |      |            |                      |          |
| Output Statistics                   |      |            |                      |          |
| Obs                                 | Year | Incidences | Predicted Incidences | Residual |
| 1                                   | 1936 | 0.90000    | 0.76235              | 0.13765  |
| 2                                   | 1937 | 0.80000    | 0.88992              | -0.08992 |
| 3                                   | 1938 | 0.80000    | 1.01764              | -0.21764 |
| 4                                   | 1939 | 1.30000    | 1.14303              | 0.15697  |
| 5                                   | 1940 | 1.40000    | 1.28654              | 0.11346  |
| 6                                   | 1941 | 1.20000    | 1.44528              | -0.24528 |
| 7                                   | 1942 | 1.70000    | 1.53482              | 0.16518  |
| 8                                   | 1943 | 1.80000    | 1.57895              | 0.22105  |
| 9                                   | 1944 | 1.60000    | 1.62058              | -0.02058 |
| 10                                  | 1945 | 1.50000    | 1.68627              | -0.18627 |
| 11                                  | 1946 | 1.50000    | 1.82449              | -0.32449 |
| 12                                  | 1947 | 2.00000    | 2.04976              | -0.04976 |
| 13                                  | 1948 | 2.50000    | 2.30981              | 0.19019  |
| 14                                  | 1949 | 2.70000    | 2.53653              | 0.16347  |
| 15                                  | 1950 | 2.90000    | 2.68921              | 0.21079  |
| 16                                  | 1951 | 2.50000    | 2.70779              | -0.20779 |
| 17                                  | 1952 | 3.10000    | 2.64837              | 0.45163  |
| 18                                  | 1953 | 2.40000    | 2.61468              | -0.21468 |
| 19                                  | 1954 | 2.20000    | 2.58792              | -0.38792 |
| 20                                  | 1955 | 2.90000    | 2.57877              | 0.32123  |
| 21                                  | 1956 | 2.50000    | 2.71078              | -0.21078 |
| 22                                  | 1957 | 2.60000    | 2.96981              | -0.36981 |
| 23                                  | 1958 | 3.20000    | 3.26005              | -0.06005 |
| 24                                  | 1959 | 3.80000    | 3.54143              | 0.25857  |
| 25                                  | 1960 | 4.20000    | 3.73482              | 0.46518  |
| 26                                  | 1961 | 3.90000    | 3.78186              | 0.11814  |
| 27                                  | 1962 | 3.70000    | 3.74362              | -0.04362 |
| 28                                  | 1963 | 3.30000    | 3.70904              | -0.40904 |
| 29                                  | 1964 | 3.70000    | 3.72917              | -0.02917 |
| 30                                  | 1965 | 3.90000    | 3.82382              | 0.07618  |
| 31                                  | 1966 | 4.10000    | 4.00515              | 0.09485  |
| 32                                  | 1967 | 3.80000    | 4.18573              | -0.38573 |
| 33                                  | 1968 | 4.70000    | 4.35152              | 0.34848  |
| 34                                  | 1969 | 4.40000    | 4.50284              | -0.10284 |
| 35                                  | 1970 | 4.80000    | 4.64413              | 0.15587  |
| 36                                  | 1971 | 4.80000    | 4.78291              | 0.01709  |
| 37                                  | 1972 | 4.80000    | 4.91602              | -0.11602 |

Figure 53.7 show the “Output Statistics” table that contains the predicted loess fit value at each observation in the input data set.

Although the default method for selecting the smoothing parameter value is often satisfactory, it is often a good practice to examine how the loess fit varies with the smoothing parameter. In some cases, fits with different smoothing parameters might reveal important features of the data that cannot be discerned by looking at a fit with just a single “best” smoothing parameter. Example 53.4 provides such an example.



You can produce the loess fits for a range of smoothing parameters by using the `SMOOTH=` option in the `MODEL` statement as follows:

```
proc loess data=Melanoma;
 model Incidences=Year/smooth=0.1 0.25 0.4 0.6 residual;
 ods output OutputStatistics=Results;
run;
```

The `RESIDUAL` option causes the residuals to be added to the “Output Statistics” table. Note that, even if you do not specify the `DETAILS` option in the `MODEL` statement to request the display of the “Output Statistics” table, you can use an `ODS OUTPUT` statement to output this and other optionally displayed tables as data sets.

`PROC PRINT` displays the first five observations of the Results data set:

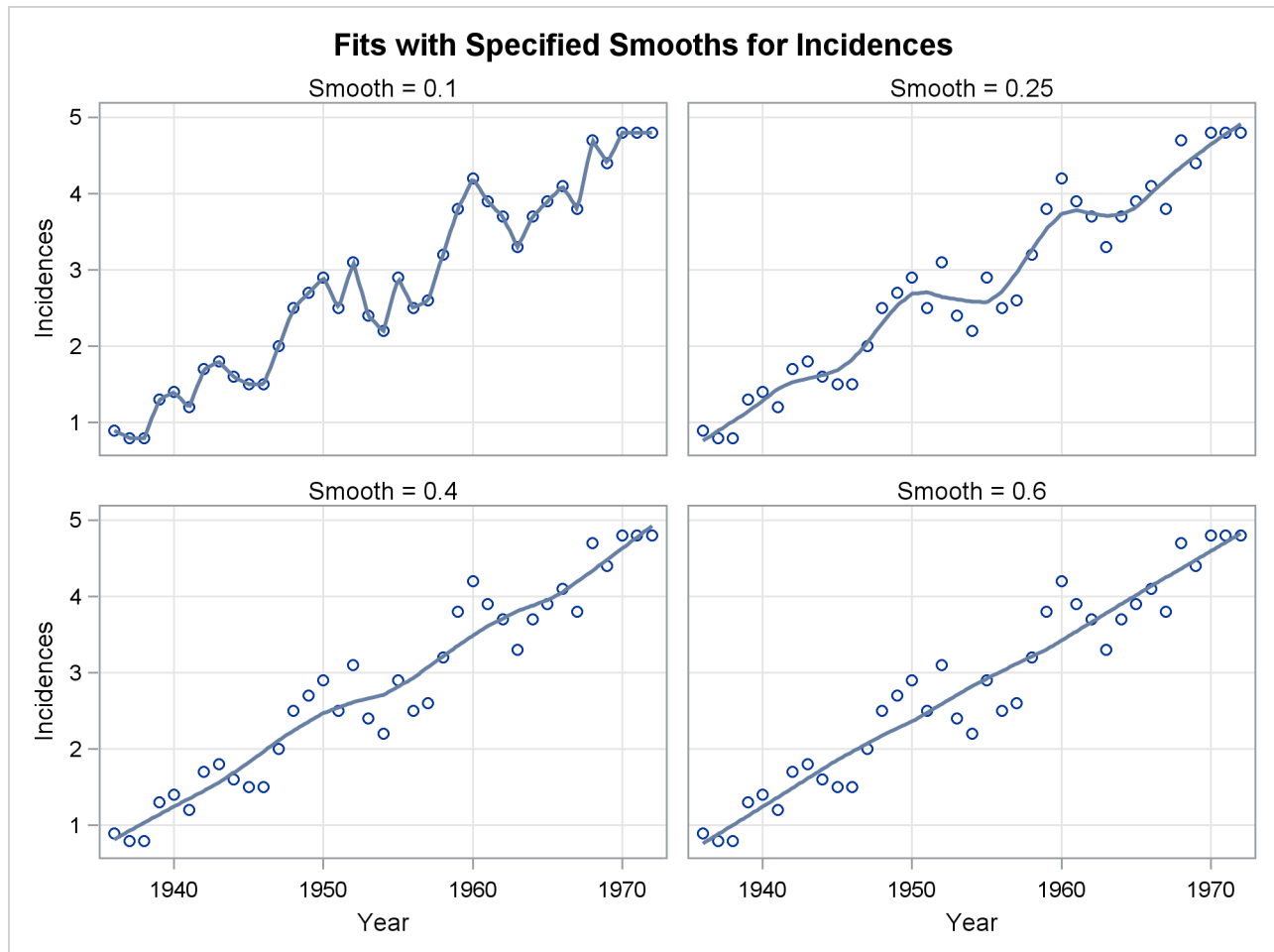
```
proc print data=Results(obs=5);
 id obs;
run;
```

**Figure 53.8** PROC PRINT Output of the Results Data Set

| Obs | Smoothing<br>Parameter | Year | Dep<br>Var | Pred    | Residual |
|-----|------------------------|------|------------|---------|----------|
| 1   | 0.1                    | 1936 | 0.9        | 0.90000 | 0        |
| 2   | 0.1                    | 1937 | 0.8        | 0.80000 | 0        |
| 3   | 0.1                    | 1938 | 0.8        | 0.80000 | 0        |
| 4   | 0.1                    | 1939 | 1.3        | 1.30000 | 0        |
| 5   | 0.1                    | 1940 | 1.4        | 1.40000 | 0        |

Note that the fits for all the smoothing parameters are placed in single data set. A variable named `SmoothingParameter` that you use to distinguish each fit is included in this data set.

When you specify a list of smoothing parameters for a model and `ODS Graphics` is enabled, `PROC LOESS` produces a panel containing up to six plots that show the fit obtained for each value of the smoothing parameter that you specify. If you specify more than six smoothing values, then multiple panels are produced. For each regressor, `PROC LOESS` also produces panels of the residuals versus each regressor by the smoothing parameters that you specify.

**Figure 53.9** Loess Fits for a Range of Smoothing Parameters

If you examine the plots in [Figure 53.9](#), you see that a visually reasonable fit is obtained with smoothing parameter values of 0.25. With smoothing parameter value 0.1, there is gross overfitting in the sense that the original data are exactly interpolated. When the smoothing parameter value is 0.4, you obtain an overly smooth fit where the contribution of the sunspot cycle has been mostly averaged away. At smoothing parameter value 0.6 the fit shows just the increasing trend in the data.

It is also instructive to look at scatter plots of the residuals for each of the fits. These are also produced by default by PROC LOESS when ODS Graphics is enabled.

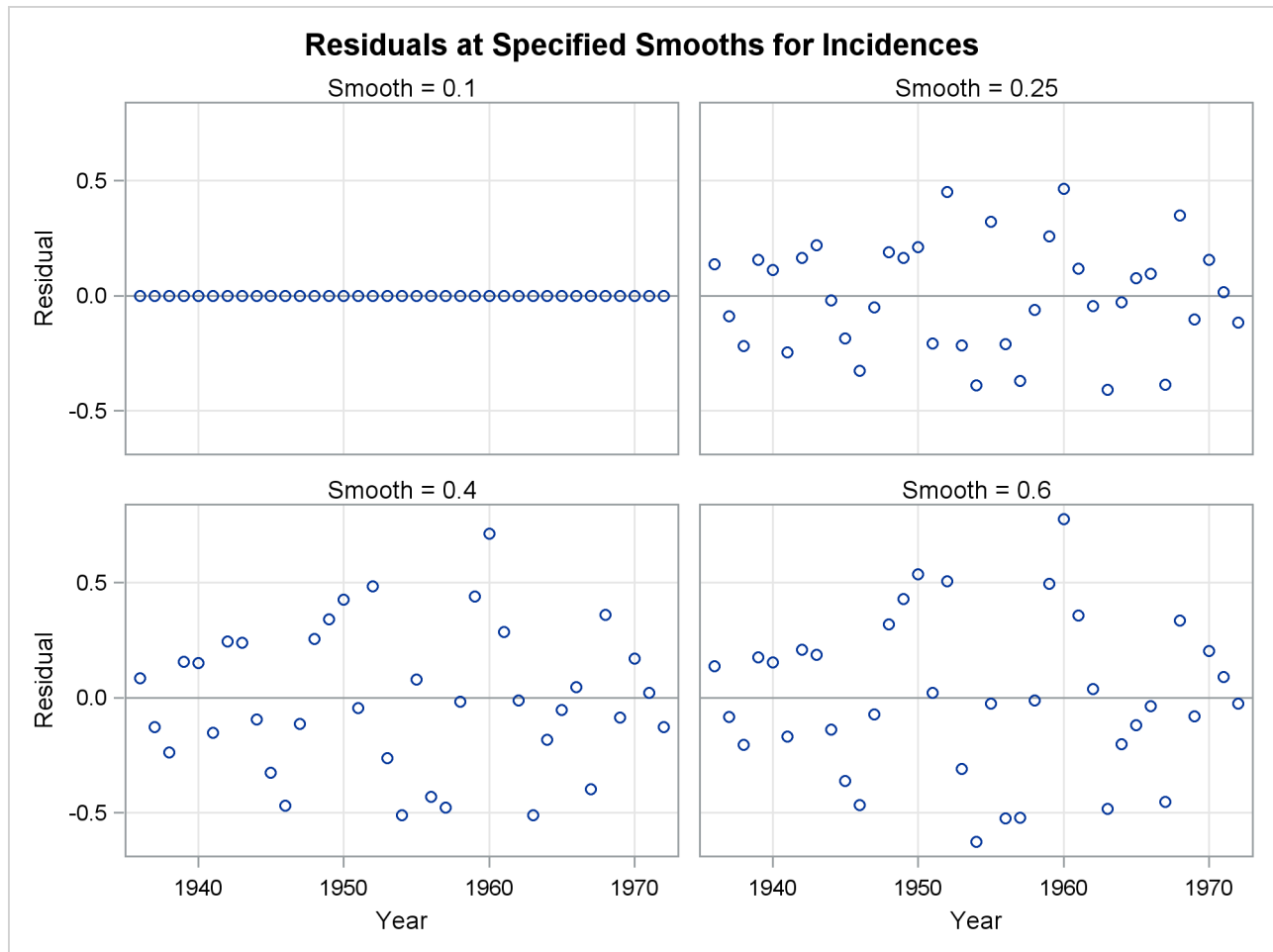
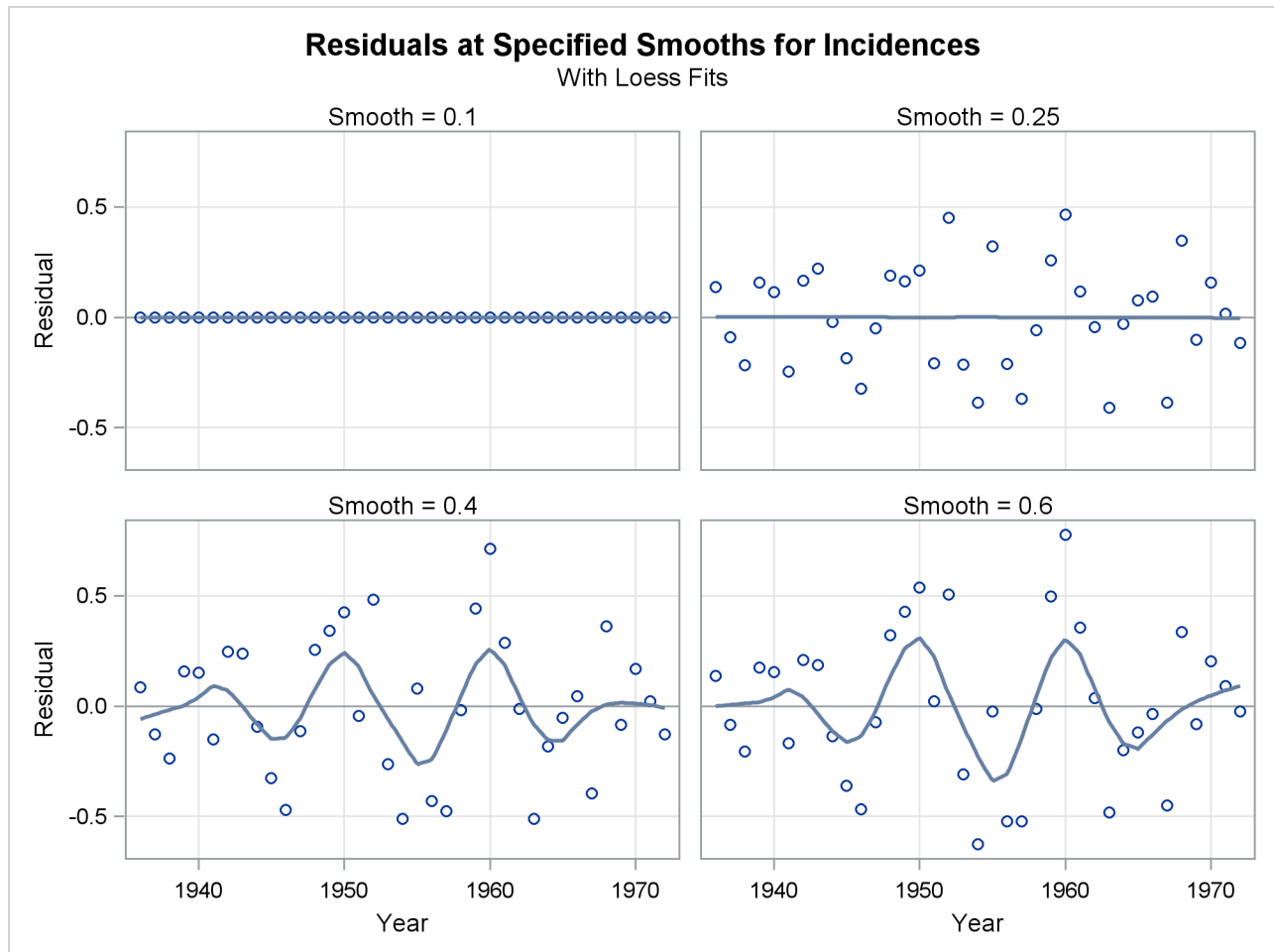
**Figure 53.10** Residuals of Loess Fits for a Range of Smoothing Parameters

Figure 53.10 shows a scatter plot of the residuals by year for each smoothing parameter value. One way to discern patterns in these residuals is to superimpose a loess fit on each plot in the panel. You request loess fits on the residual plots in this panel by specifying the `SMOOTH=` suboption of the `PLOTS=RESIDUALSBYSMOOTH` option in the `PROC LOESS` statement. Note that the loess fits that are displayed on each of the residual plots are obtained independently of the loess fit that produces these residuals. The following statements show how you do this for the Melanoma data.

```
proc loess data=Melanoma plots=ResidualsBySmooth(smooth);
 model Incidences=Year/smooth=0.1 0.25 0.4 0.6;
run;
```

**Figure 53.11** Residuals with Superimposed Loess Fits

The loess fits shown on the plots in [Figure 53.11](#) help confirm the conclusions obtained when you look at [Figure 53.9](#). Note that residuals for smoothing parameter value 0.25 do not exhibit any pattern, confirming that at this value the loess fit of the melanoma data has successfully modeled the variation in this data. By contrast, the residuals for the fit with smoothing parameter 0.6 retain the variation caused by the sunspot cycle.

The examination of the fits and residuals obtained with a range of smoothing parameter values confirms that the value of 0.257 that PROC LOESS selects automatically is appropriate for these data. The next step in this analysis is to examine fit diagnostics and produce confidence limit for the fit. If ODS Graphics is enabled, then a panel of fit diagnostics is produced. Furthermore, you can request prediction confidence limits by adding the CLM option in the MODEL statement. By default 95% limits are produced, but you can use the ALPHA= option in the MODEL statement to change the significance level. The following statements request 90% confidence limits.

```
proc loess data=Melanoma;
 model Incidences=Year/clm alpha=0.1;
run;

ods graphics off;
```

Figure 53.12 Fit Diagnostics

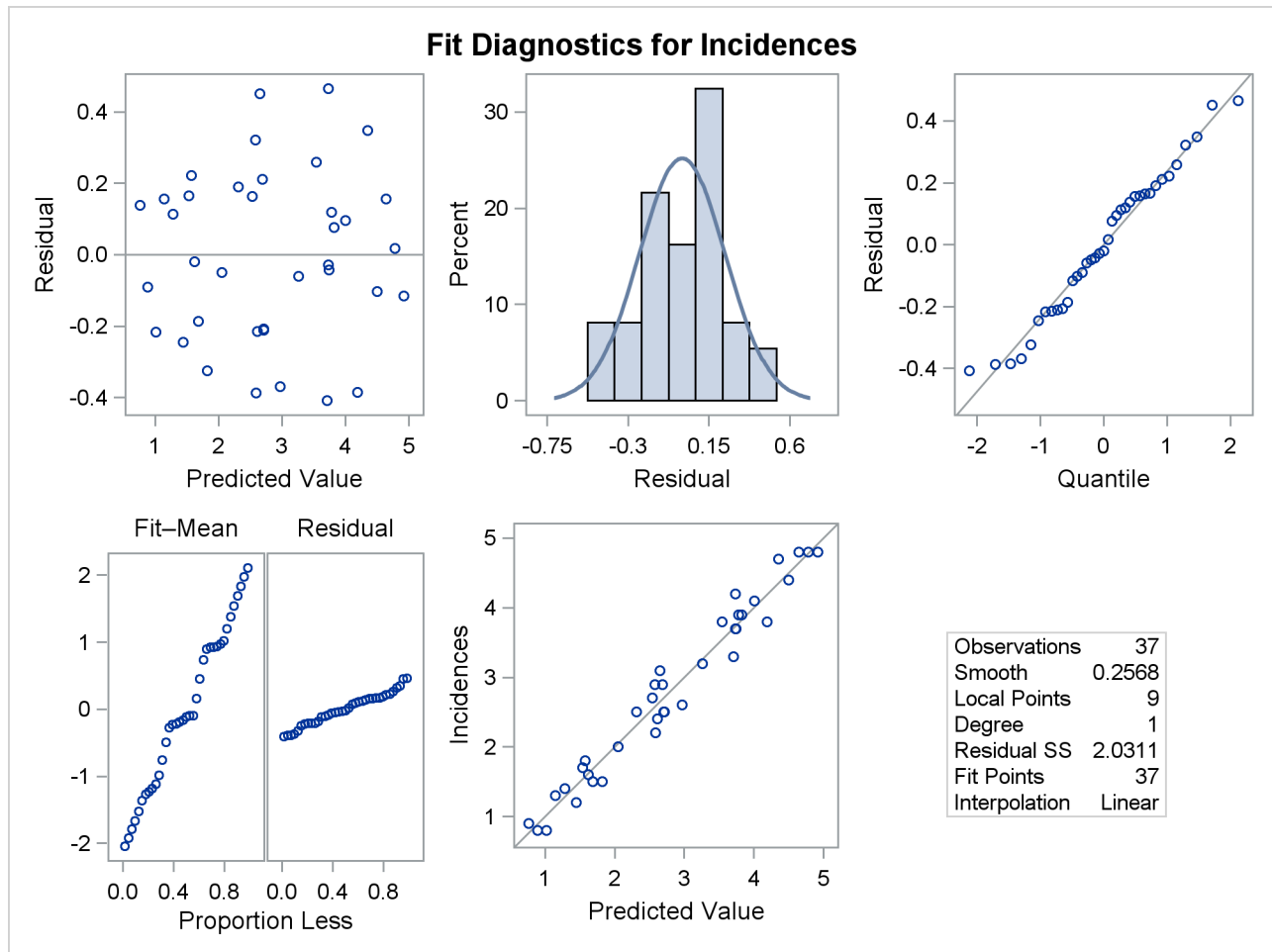
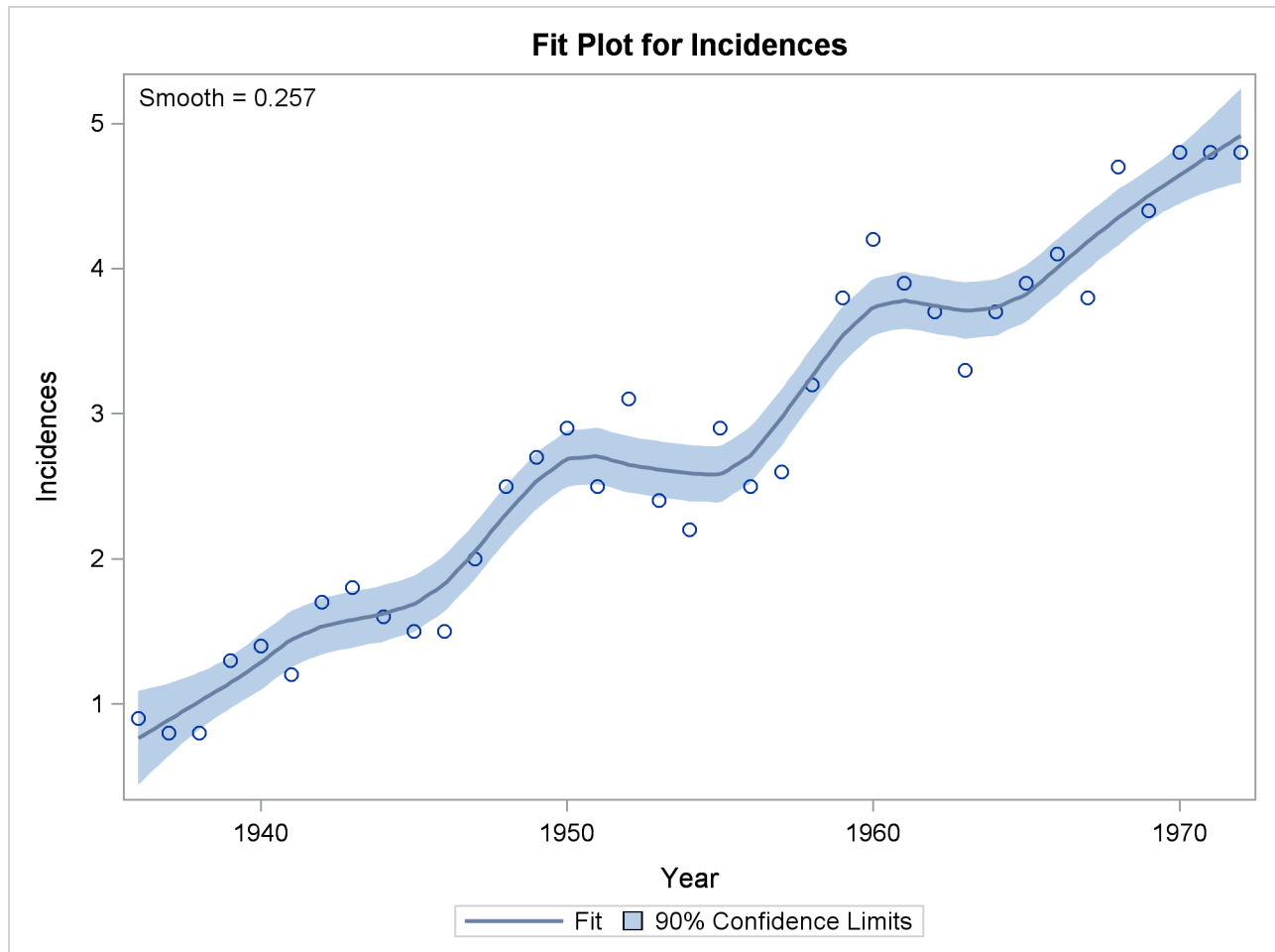


Figure 53.12 shows the fit diagnostics panel. The histogram of the residuals with overlaid normal density estimator and the normal quantile plot show that the residuals do exhibit some small departure from normality. The “Residual-Fit” spread plot shows that the spread in the centered fit is much wider than the spread in the residuals. This indicates that the fit has accounted for most of the variation in the incidences of melanoma in this data. This conclusion is supported by the absence of any clear pattern in the scatter plot of residuals by predicted values and the closeness of the points to the 45-degree reference line in the plot of observed by predicted values.

**Figure 53.13** Loess Fit of Melanoma Data with 90% Confidence Limits

Finally, Figure 53.13 shows the selected loess fit with 90% confidence limits.

## Syntax: LOESS Procedure

The following statements are available in the LOESS procedure:

```

PROC LOESS < DATA=SAS-data-set > ;
 MODEL dependents = regressors < / options > ;
 OUTPUT < OUT=SAS-data-set > < keyword < =name > > < ... keyword < =name > > < / options > ;
 ID variables ;
 BY variables ;
 WEIGHT variable ;
 SCORE DATA=SAS-data-set < ID=(variable-list) > < / options > ;

```

The PROC LOESS and MODEL statements are required. The OUTPUT, BY, WEIGHT, and ID statements are optional. The SCORE statement is optional, and more than one SCORE statement can be used.

The statements used with the LOESS procedure, in addition to the PROC LOESS statement, are as follows.

|               |                                                                                                                                                        |
|---------------|--------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>BY</b>     | specifies variables to define subgroups for the analysis.                                                                                              |
| <b>ID</b>     | names variables to identify observations in the displayed output.                                                                                      |
| <b>MODEL</b>  | specifies the dependent and independent variables in the loess model, details and parameters for the computational algorithm, and the required output. |
| <b>OUTPUT</b> | creates an output data set containing predicted values, residuals, and results of statistical inference.                                               |
| <b>SCORE</b>  | specifies a data set containing observations to be scored.                                                                                             |
| <b>WEIGHT</b> | declares a variable to weight observations.                                                                                                            |

---

## PROC LOESS Statement

**PROC LOESS** < options > ;

The PROC LOESS statement invokes the LOESS procedure. The PROC LOESS statement is required. You can specify the following options in the PROC LOESS statement:

**DATA=SAS-data-set**

names the SAS data set to be used by PROC LOESS. If the DATA= option is not specified, PROC LOESS uses the most recently created SAS data set.

**PLOTS** < (global-plot-options) > < = plot-request < (options) > >

**PLOTS** < (global-plot-options) > < = (plot-request < (options) > < ... plot-request < (options) > > >

controls the plots produced through ODS Graphics. When you specify only one plot request, you can omit the parentheses around the plot request. Here are some examples:

```
plots=none
plots=residuals(smooth)
plots(unpack)=diagnostics
plots(only)=(fit residualHistogram)
```

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;

proc loess;
 model y = x;
run;

ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS](#).”

If ODS Graphics is enabled but you do not specify the PLOTS= option, then PROC LOESS produces a default set of plots. The following table lists the default set of plots produced.

**Table 53.1** Default Graphs Produced

| Plot              | Conditional On                                                     |
|-------------------|--------------------------------------------------------------------|
| ContourFitPanel   | SMOOTH= option specified in the <b>MODEL</b> statement             |
| ContourFit        | Model with two regressors                                          |
| CriterionPlot     | Smoothing parameter selection performed                            |
| DiagnosticsPanel  | Unconditional                                                      |
| ResidualsBySmooth | SMOOTH= option specified in the <b>MODEL</b> statement             |
| ResidualPanel     | Unconditional                                                      |
| FitPanel          | SMOOTH= option specified in the <b>MODEL</b> statement             |
| FitPlot           | Model with one regressor                                           |
| ScorePlot         | One or more <b>SCORE</b> statements and a model with one regressor |

For models with multiple dependent variables, separate plots are produced for each dependent variable. For models where multiple smoothing parameters are requested with the SMOOTH= option in the **MODEL** statement and smoothing parameter value selection is not requested, separate plots are produced for each smoothing parameter. If smoothing parameter value selection is requested with the SELECT= option in the **MODEL** statement, then the plots are produced for the selected model only. However, if you specify the STEPS suboption of the SELECT= option, then plots are produced for all smoothing parameters examined in the selection process.

The *global-plot-options* apply to all relevant plots generated by the LOESS procedure, unless they are overridden with a *specific-plot-option*. The *global-plot-options* supported by the LOESS procedure follow.

## Global Plot Options

### **MAXPOINTS=NONE** | *number*

specifies that plots with elements that require processing more than *number* points are suppressed. The default is MAXPOINTS=5000. This cutoff is ignored if you specify MAXPOINTS=NONE.

### **ONLY**

suppresses the default plots. Only the plots specifically requested are produced.

### **UNPACK**

suppresses paneling. By default, multiple plots can appear in some output panels. Specify UNPACK to get each plot individually. You can specify PLOTS(UNPACK) to unpack the default plots. You can also specify UNPACK as a suboption with CONTOURFITPANEL, DIAGNOSTICS, FITPANEL, RESIDUALS and RESIDUALSBYSMOOTH.

## Specific Plot Options

The following listing describes the specific plots and their options.

### **ALL**

requests that all plots appropriate for the particular analysis be produced. You can specify other options with ALL; for example, to request all plots and unpack only the residuals, specify PLOTS=(ALL RESIDUALS(UNPACK)).



**CONTOURFIT** <(contour-options)>

produces a contour plot of the fitted surface overlaid with a scatter plot of the data for models with two regressors. Contour plots are not produced if you specify the **DIRECT** option in the **MODEL** statement. You can use the following *contour-options* to control how the observations are displayed:

**OBS=GRADIENT**

specifies that observations be displayed as circles colored by the observed response. The same color gradient is used to display the fitted surface and the observations. Observations where the predicted response is close to the observed response have similar colors—the greater the contrast between the color of an observation and the surface, the larger the residual is at that point. **OBS=GRADIENT** is the default if you do not specify any *contour-options*.

**OBS=NONE**

suppresses the observations.

**OBS=OUTLINE**

specifies that observations be displayed as circles with a border but with a completely transparent fill.

**OBS=OUTLINEGRADIENT**

is the same as **OBS=GRADIENT** except that a border is shown around each observation. This option is useful to identify the location of observations where the residuals are small, because at these points the color of the observations and the color of the surface are indistinguishable.

**CONTOURFITPANEL** <(UNPACK < contour-options > )>

produces panels of contour plots overlaid with a scatter plot of the data for each smoothing parameter specified in the **SMOOTH=** option in the **MODEL** statement, for models with two regressors. This plot is not produced if you specify the **DIRECT** option in the **MODEL** statement. If you do not specify the **SMOOTH=** option or if the model does not have two regressors, then this plot is not produced. If you specify the **SELECT=** option in addition to the **SMOOTH=** option in the **MODEL** statement, then you need to additionally specify the **STEPS** suboption of the **SELECT=** option to obtain this plot. Note that each panel contains at most six plots, and multiple panels are used in the case that there are more than six smoothing parameters in the **SMOOTH=** option in the **MODEL** statement. See the **CONTOURFIT** option for a description of the individual plots in this panel. The **UNPACK** option suppresses paneling, and the *contour-options* are the same as for the **CONTOURFIT** option.

**CRITERIONPLOT** | **CRITERION**

displays a scatter plot of the value of the **SELECTION=** criterion versus the smoothing parameter value for all smoothing parameter values examined in the selection process. This plot is not produced if smoothing parameter selection is not done.

**DIAGNOSTICSPANEL** | **DIAGNOSTICS** <(UNPACK)>

produces a summary panel of fit diagnostics consisting of the following:

- residuals versus the predicted values
- histogram of the residuals
- normal quantile plot of the residuals
- a “Residual-Fit” (or RF) plot consisting of side-by-side quantile plots of the centered fit and the residuals.

- dependent variable values versus the predicted values

You can request the five plots in this panel as individual plots by specifying the UNPACK option. You can also request individual plots in the panel by name without having to unpack the panel. Note that the fit diagnostics panel is produced by default whenever ODS Graphics is enabled.

#### **FITPANEL <(UNPACK)>**

produces panels of plots showing the fitted LOESS curve overlaid on a scatter plot of the input data for each smoothing parameter specified in the SMOOTH= option in the **MODEL** statement. If you do not specify the SMOOTH= option or the model has more than one regressor, then this plot is not produced. If you specify the SELECT= option in addition to the SMOOTH= option in the **MODEL** statement, then you need to additionally specify the STEPS suboption of the SELECT= option to obtain this plot. Note that each panel contains at most six plots, and multiple panels are used in the case that there are more than six smoothing parameters in the SMOOTH= option in the **MODEL** statement. If the CLM option is specified in the **MODEL** statement, then a confidence band at the significance level specified in the ALPHA= option is included in each plot in the panels. If you specify the UNPACK option, then all fit panels are unpacked.

#### **FITPLOT | FIT**

produces a scatter plot of the input data with the fitted LOESS curve overlaid for models with a single regressor. If the CLM option is specified in the **MODEL** statement, then a confidence band at the significance level specified in the ALPHA= option is included in the plot.

#### **NONE**

suppresses all plots.

#### **OBSERVEDBYPREDICTED**

produces a scatter plot of the dependent variable values by the predicted values.

#### **QQPLOT | QQ**

produces a normal quantile plot of the residuals.

#### **RESIDUALSBYSMOOTH <(< UNPACK > < SMOOTH > )>**

produces for each regressor panels of plots showing the residuals of the LOESS fit versus the regressor for each smoothing parameter specified in the SMOOTH= option in the **MODEL** statement. If you do not specify the SMOOTH= option, then this plot is not produced. If you specify the SELECT= option in addition to the SMOOTH= option in the **MODEL** statement, then you need to additionally specify the STEPS suboption of the SELECT= option to obtain this plot. Note that each panel contains at most six plots, and multiple panels are used in the case that there are more than six smoothing parameters in the SMOOTH= option in the **MODEL** statement. If you specify the UNPACK option, then all RESIDUALSBYSMOOTH panels are unpacked.

The SMOOTH option requests that a nonparametric fit line be shown in each plot in the panel. The type of nonparametric fit and the options used are controlled by the template that underlies this plot. In the standard template that is provided, the nonparametric smooth is specified to be a loess fit corresponding to the default options of PROC LOESS, except that the PRESEARCH suboption is always used. It is important to note that the loess fit that is shown in each of the residual plots is computed independently of the loess fit that is used to obtain the residuals.

**RESIDUALBYPREDICTED**

produces a scatter plot of the residuals by the predicted values.

**RESIDUALHISTOGRAM**

produces a histogram of the residuals.

**RESIDUALPANEL | RESIDUALS** <(residual-options)>

produces panels of the residuals versus the regressors in the model. Note that each panel contains at most six plots, and multiple panels are used when there are more than six regressors in the model.

The following *residual-options* are available:

**SMOOTH**

requests that a nonparametric fit line be shown in each plot in the panel. The type of nonparametric fit and the options used are controlled by the template that underlies this plot. In the standard template that is provided, the nonparametric smooth is specified to be a loess fit corresponding to the default options of PROC LOESS, except that the PRESEARCH suboption is always used. It is important to note that the loess fit that is shown in each of the residual plots is computed independently of the loess fit that is used to obtain the residuals.

**UNPACK**

suppresses paneling.

**RFPLOT | RF**

produces a “Residual-Fit” (or RF) plot consisting of side-by-side quantile plots of the centered fit and the residuals. This plot “shows how much variation in the data is explained by the fit and how much remains in the residuals” (Cleveland 1993).

**SCOREPLOT | SCORE**

produces a scatter plot of the scored values at the score points for each **SCORE** statement. **SCORE** plots are not produced for models with more than one regressor. If the **CLM** option is specified in the **MODEL** statement, then confidence bars at the significance level specified in the **ALPHA=** option are shown at score data points.

**BY Statement**

**BY** *variables* ;

You can specify a **BY** statement with PROC LOESS to obtain separate analyses of observations in groups that are defined by the **BY** variables. When a **BY** statement appears, the procedure expects the input data set to be sorted in order of the **BY** variables. If you specify more than one **BY** statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar **BY** statement.
- Specify the **NOTSORTED** or **DESCENDING** option in the **BY** statement for the LOESS procedure. The **NOTSORTED** option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the **BY** variables) and that these groups are not necessarily in alphabetical or increasing numeric order.

- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

---

## ID Statement

**ID** *variables* ;

The ID statement is optional, and more than one ID statement can be used. The variables listed in any of the ID statements are displayed in the “Output Statistics” table beside each observation. Any variables specified as a regressor or dependent variable in the **MODEL** statement already appear in the “Output Statistics” table and are not treated as ID variables, even if they appear in the variable list of an ID statement.

---

## MODEL Statement

**MODEL** *dependents = regressors </ options >* ;

The MODEL statement names the dependent variables and the independent variables. Variables specified in the MODEL statement must be numeric variables in the data set being analyzed.

Table 53.2 summarizes the options available in the MODEL statement.

**Table 53.2** Summary of MODEL Statement Options

| Option                                 | Description                                                                                    |
|----------------------------------------|------------------------------------------------------------------------------------------------|
| <b>Fit Options</b>                     |                                                                                                |
| BUCKET=                                | specifies the number of points in <i>k</i> -d tree buckets                                     |
| DEGREE=                                | specifies the degree of local polynomials (1 or 2)                                             |
| DFMETHOD=                              | specifies the method of computing lookup degrees of freedom                                    |
| DIRECT                                 | specifies direct fitting at every data point                                                   |
| DROPSQUARE=                            | specifies the variables whose squares are to be dropped from local quadratic polynomials       |
| INTERP=                                | specifies the interpolating polynomials (linear or cubic)                                      |
| ITERATIONS=                            | specifies the number of reweighting iterations                                                 |
| SCALE=                                 | specifies the method used to scale the regressor variables                                     |
| SELECT=                                | specifies that automatic smoothing parameter selection be done                                 |
| SMOOTH=                                | specifies the list of smoothing values                                                         |
| <b>Output Statistics Table Options</b> |                                                                                                |
| ALL                                    | requests <b>CLM</b> , <b>RESIDUAL</b> , <b>SCALEDINDEP</b> , <b>STD</b> , and <b>T</b> options |
| CLM                                    | displays confidence limits for mean predictions                                                |
| RESIDUAL                               | displays residuals                                                                             |
| SCALEDINDEP                            | displays scaled independent variable coordinates                                               |
| STD                                    | displays standard errors of the mean predicted values                                          |

Table 53.2 continued

| Option               | Description                                      |
|----------------------|--------------------------------------------------|
| T                    | displays $t$ statistics                          |
| <b>Other options</b> |                                                  |
| ALPHA=               | sets significance level for confidence intervals |
| DETAILS=             | specifies which tables are to be displayed       |
| TRACEL               | displays the trace of the smoothing matrix       |

The following options are available in the MODEL statement after a slash (/).

**ALL**

requests all these options: CLM, RESIDUAL, SCALEDINDEP, STD, and T.

**ALPHA=number**

sets the significance level used for the construction of confidence intervals for the current MODEL statement. The value must be between 0 and 1; the default value of 0.05 results in 95% intervals.

**BUCKET=number**

specifies the maximum number of points in the leaf nodes of the  $k$ -d tree. The default value used is  $s * n/5$ , where  $s$  is a smoothing parameter value specified using the SMOOTH= option and  $n$  is the number of observations being used in the current BY group. The BUCKET= option is ignored if the DIRECT option is specified.

**CLM**

requests that  $100(1 - \alpha)\%$  confidence limits on the mean predicted value be added to the “Output Statistics” table. By default, 95% limits are computed; the ALPHA= option in the MODEL statement can be used to change the significance level. The use of this option implicitly selects the model option DFMETHOD=EXACT if the DFMETHOD= option has not been explicitly used.

**DEGREE=1 | 2**

sets the degree of the local polynomials to use for each local regression. The valid values are 1 for local linear fitting and 2 for local quadratic fitting, with 1 being the default.

**DETAILS < ( tables ) >**

selects which tables to display, where *tables* is one or more of the specifications KDTREE, MODEL-SUMMARY, OUTPUTSTATISTICS, and PREDATVERTICES:

- KDTREE displays the  $k$ -d tree structure.
- MODELSUMMARY displays the fit criteria for all smoothing parameter values that are specified in the SMOOTH= option in the MODEL statement, or that are fit with automatic smoothing parameter selection.
- OUTPUTSTATISTICS displays the predicted values and other requested statistics at the points in the input data set.
- PREDATVERTICES displays fitted values and coordinates of the  $k$ -d tree vertices where the local least squares fitting is done.

The KDTREE and PREDATVERTICES specifications are ignored if the DIRECT option is specified in the MODEL statement. Specifying the option DETAILS with no qualifying list outputs all tables.

**DFMETHOD=NONE | EXACT | APPROX <(approx-options)>**

specifies the method used to calculate the lookup degrees of freedom used in performing statistical inference. The default is DFMETHOD=NONE, unless you specify any of the MODEL statement options ALL, CLM, STD, and T, or any SCORE statement CLM option, in which case the default is DFMETHOD=EXACT.

You can specify the following *approx-options* in parentheses after the DFMETHOD=APPROX option:

**QUANTILE=number**

specifies that the smallest 100(*number*)% of the nonzero coefficients in the smoothing matrix be set to zero in computing the approximate lookup degrees of freedom. The default value is QUANTILE=0.9.

**CUTOFF=number**

specifies that coefficients in the smoothing matrix whose magnitude is less than the specified value be set to zero in computing the approximate lookup degrees of freedom. Using the CUTOFF= option overrides the QUANTILE= option.

See the section “Sparse and Approximate Degrees of Freedom Computation” on page 4130 for a description of the method used when the DFMETHOD=APPROX option is specified.

**DIRECT**

specifies that local least squares fits are to be done at every point in the input data set. When the direct option is not specified, a computationally faster method is used. This faster method performs local fitting at vertices of a *k*-d tree decomposition of the predictor space followed by blending of the local polynomials to obtain a regression surface.

**DROPSQUARE=(variables)**

specifies the quadratic monomials to exclude from the local quadratic fits. This option is ignored unless the DEGREE=2 option has been specified.

For example,

```
model z=x y / degree=2 dropsquare=(y)
```

uses the monomials 1, *x*, *y*,  $x^2$ , and *xy* in performing the local fitting.

**INTERP=LINEAR | CUBIC**

specifies the degree of the interpolating polynomials used for blending local polynomial fits at the *k*-d tree vertices. This option is ignored if the DIRECT option is specified in the model statement. INTERP=CUBIC is not supported for models with more than two regressors. The default is INTERP=LINEAR.

**ITERATIONS=number**

specifies the total number of iterations to be done. The first iteration performs an initial LOESS fit. Subsequent iterations perform iterative reweighting. Such iterations are appropriate when there are outliers in the data or when the error distribution is a symmetric long-tailed distribution. The default number of iterations is 1.

**RESIDUAL | R**

specifies that residuals be included in the “Output Statistics” table.

**SCALE=NONE | SD < (number) >**

specifies the scaling method to be applied to scale the regressors. The default is NONE, in which case no scaling is applied. A specification of SD(*number*) indicates that a trimmed standard deviation is to be used as a measure of scale, where *number* is the trimming fraction. A specification of SD with no qualification defaults to 10% trimmed standard deviation.

**SCALEDINDEP**

specifies that scaled regressor coordinates be included in the output tables. This option is ignored if the SCALE= model option is not used or if SCALE=NONE is specified.

**SELECT=criterion** < ( < GLOBAL > < PRESEARCH > < STEPS > < RANGE(*lower,upper*) > ) >

**SELECT=DFCriterion** < ( *target* < GLOBAL > < PRESEARCH > < STEPS > < RANGE(*lower,upper*) > ) >

specifies that automatic smoothing parameter selection be done using the named *criterion* or *DFCriterion*. Valid values for the *criterion* are as follows:

- AICC specifies the  $AIC_C$  criterion (Hurvich, Simonoff, and Tsai 1998).
- AICC1 specifies the  $AIC_{C_1}$  criterion (Hurvich, Simonoff, and Tsai 1998).
- GCV specifies the generalized cross validation criterion (Craven and Wahba 1979).

The *DFCriterion* specifies the measure used to estimate the model degrees of freedom. The measures implemented in PROC LOESS all depend on prediction matrix **L** relating the observed and predicted values of the dependent variable. Valid values for the *DFCriterion* are as follows:

- DF1 specifies Trace(**L**).
- DF2 specifies Trace(**L'L**).
- DF3 specifies  $2\text{Trace}(\mathbf{L}) - \text{Trace}(\mathbf{L}'\mathbf{L})$ .

For both types of selection, the smoothing parameter value is selected to yield a minimum of an optimization criterion. If you specify *criterion* as one of AICC, AICC1, or GCV, the optimization criterion is the specified *criterion*. If you specify *DFCriterion* as one of DF1, DF2, or DF3, the optimization criterion is  $|DFCriterion - target|$ , where *target* is a specified target degree of freedom value. Note that if you specify a *DFCriterion*, then you must also specify a target value. See the section “[Automatic Smoothing Parameter Selection](#)” on page 4127 for definitions and properties of the selection criteria.

The selection is done as follows:

- If you specify the SMOOTH=*value-list* option, then PROC LOESS selects the largest value in this list that yields the global minimum of the specified optimization criterion.
- If you do not specify the SMOOTH= option, then PROC LOESS finds a local minimum of the specified optimization criterion by using a golden section search of values less than or equal to one.

You can specify the following suboptions in parentheses after the specified criterion to alter the behavior of the SELECT= option:



**GLOBAL**

specifies that a global minimum be found within the range of smoothing parameter values examined. This suboption has no effect if you also specify the SMOOTH= option in the MODEL statement.

**PRESEARCH**

requests an initial grid search to find a smoothing parameter range within which the subsequent golden section search is done. The initial point in this grid is the smoothing parameter value corresponding to the smallest number of points,  $n$ , in the local neighborhoods that yields a fit that does not interpolate all the data points. Subsequent fits with number of local points  $n + 1$ ,  $n + 2$ ,  $n + 4$ ,  $n + 8$ , ... are evaluated until either the number of local points exceeds the number of fitting points or the SELECT=criterion starts increasing. This suboption is ignored if you additionally specify the GLOBAL suboption of the SELECT= option or if you specify the SMOOTH= option in the MODEL statement. If you additionally specify the RANGE= suboption, then the golden section search is done on the intersection of the range found by this grid search and the range that you specify in the RANGE= suboption. This option is useful for data exhibiting features at multiple scales, because in such cases the SELECT= criterion often has multiple local minima. Using the PRESEARCH option increases the likelihood that the golden section search will find the global minimum of the SELECT= criterion. See [Example 53.4](#) for such an example.

**RANGE(lower,upper)**

specifies that only smoothing parameter values greater than or equal to *lower* and less than or equal to *upper* be examined.

**STEPS**

specifies that all models evaluated in the selection process be displayed.

For models with one dependent variable, if you specify neither the SELECT= nor the SMOOTH= options in the MODEL statement, then PROC LOESS uses SELECT=AICC.

The following table summarizes how the smoothing parameter values are chosen for various combinations of the SMOOTH= option, the SELECT= option, and the SELECT= option modifiers.

**Table 53.3** Smoothing Parameter Value(s) Used for Combinations of SMOOTH= and SELECT= OPTIONS for Models with One Dependent Variable

| Syntax                                                                        | Search Method             | Search Domain                                        |
|-------------------------------------------------------------------------------|---------------------------|------------------------------------------------------|
| <i>default</i>                                                                | golden section using AICC | (0, 1]                                               |
| SMOOTH= <i>list</i>                                                           | no selection              | values in <i>list</i>                                |
| SMOOTH= <i>list</i> SELECT= <i>criterion</i>                                  | global                    | values in <i>list</i>                                |
| SMOOTH= <i>list</i> SELECT= <i>criterion</i> ( RANGE( <i>l</i> , <i>u</i> ) ) | global                    | values in <i>list</i> within [ <i>l</i> , <i>u</i> ] |
| SELECT= <i>criterion</i>                                                      | golden section            | (0, 1]                                               |
| SELECT= <i>criterion</i> ( RANGE( <i>l</i> , <i>u</i> ) )                     | golden section            | [ <i>l</i> , <i>u</i> ]                              |
| SELECT= <i>criterion</i> ( GLOBAL )                                           | global                    | (0, 1]                                               |
| SELECT= <i>criterion</i> ( GLOBAL RANGE( <i>l</i> , <i>u</i> ) )              | global                    | [ <i>l</i> , <i>u</i> ]                              |



Some examples of using the SELECT= option follow:

|                      |                                                                                                                                                               |
|----------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------|
| SELECT=GCV           | specifies selection that uses the GCV <i>criterion</i> .                                                                                                      |
| SELECT=DF1(6.3)      | specifies selection that uses the DF1 <i>DFCriterion</i> with target value 6.3.                                                                               |
| SELECT=AICC(STEPS)   | specifies selection that uses the AICC <i>criterion</i> , showing all step details.                                                                           |
| SELECT=DF2(7 GLOBAL) | specifies selection that uses a global search algorithm to find the smoothing parameter that yields the DF2 <i>DFCriterion</i> closest to the target value 7. |

**NOTE:** The SELECT= option cannot be used for models with more than one dependent variable.

**SMOOTH=***value-list*

specifies a list of positive smoothing parameter values. If you do not specify the SELECT= option in the MODEL statement, then a separate fit is obtained for each SMOOTH= value specified. If you do specify the SELECT= option, then models with all values specified in the SMOOTH= list are examined, and PROC LOESS selects the value that minimizes the criterion specified in the SELECT= option.

For models with two or more dependent variables, if the SMOOTH= option is not specified in the MODEL statement, then SMOOTH=0.5 is used as a default.

**STD**

specifies that standard errors of the mean predicted values be included in the “Output Statistics” table. The use of this option implicitly selects the model option DFMETHOD=EXACT if the DFMETHOD= option has not been explicitly used.

**T**

specifies that *t* statistics are to be included in the “Output Statistics” table. The use of this option implicitly selects the model option DFMETHOD=EXACT if the DFMETHOD= option has not been explicitly used.

**TRACEL**

specifies that the trace of the prediction matrix as well as the GCV and AICC statistics be included in the “Fit Summary” table. The use of any of the MODEL statement options ALL, CLM, DFMETHOD=EXACT, DIRECT, SELECT=, STD, and T implicitly selects the TRACEL option.

## OUTPUT Statement

**OUTPUT** <OUT= SAS-data-set> <keyword <= name>> <... keyword <=name>> </options>;

The OUTPUT statement creates a new SAS data set that saves the predicted values and other requested statistics that are calculated after models for all smoothing parameter values that are specified in the SMOOTH= option in the MODEL statement have been fit. If you do not specify a *keyword*, then only the predicted response is included.

All the variables in the original data set are included in the new data set, along with variables created by the OUTPUT statement. These new variables contain the predicted values and a variety of other statistics that are calculated for each observation in the data set.

If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*.

You can specify the following *options* in the OUTPUT statement:

**OUT=SAS data set**

specifies the name of the new data set. By default, the procedure uses the *DATA*n** convention to name the new data set.

*keyword* <=*name*>

specifies the statistics to include in the output data set as new variables and optionally names the new variables. Specify a keyword for each desired statistic (see the following list of keywords), followed optionally by an equal sign and a variable to contain the statistic.

The new variables are named as follows: If you specify *keyword=**name*, the new variable has the specified *name*. If you omit the optional *=name* after a *keyword*, then the new variable name is formed by using a default character string that identifies the statistic. In either case, if you also specify the ROWWISE option after a slash and you specify more than one dependent variable or smoothing value in the MODEL statement, the variable name is appended with an order number. For details, see the ROWWISE option.

The keywords allowed and the statistics they represent are as follows:

- |                      |                                                                                                                                                                                                                                                                                                                                                                                                                                           |
|----------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>PREDICTED   P</b> | creates a new variable that contains predicted values. The default <i>name</i> is Predicted.                                                                                                                                                                                                                                                                                                                                              |
| <b>RESIDUAL   R</b>  | creates a new variable that contains residual values, which are calculated as ACTUAL – PREDICTED. The default <i>name</i> is Residual.                                                                                                                                                                                                                                                                                                    |
| <b>STD</b>           | creates a new variable that contains standard errors of the mean predicted values. The use of this option implicitly selects the model option DFMETHOD=EXACT even if the DFMETHOD= option has not been explicitly used. The default <i>name</i> is StdErr.                                                                                                                                                                                |
| <b>T</b>             | creates a new variable that contains <i>t</i> statistics. The use of this option implicitly selects the model option DFMETHOD=EXACT even if the DFMETHOD= option has not been explicitly used. The default <i>name</i> is tValue.                                                                                                                                                                                                         |
| <b>LCLM</b>          | creates a new variable that contains the lower part of 100(1 – $\alpha$ )% confidence limits on the mean predicted value. By default, the 95% limits are computed; the ALPHA= option in the <b>MODEL</b> statement can be used to change the significance level. The use of this option implicitly selects the model option DFMETHOD=EXACT even if the DFMETHOD= option has not been explicitly used. The default <i>name</i> is LowerCL. |
| <b>UCLM</b>          | creates a new variable that contains the upper part of 100(1 – $\alpha$ )% confidence limits on the mean predicted value. By default, the 95% limits are computed; the ALPHA= option in the <b>MODEL</b> statement can be used to change the significance level. The use of this option implicitly selects the model option DFMETHOD=EXACT even if the DFMETHOD= option has not been explicitly used. The default <i>name</i> is UpperCL. |

You can specify the following *options* in the OUTPUT statement after a slash (/).

**ALL**

requests all these keywords: PREDICTED, RESIDUAL, STD, T, LCLM, and UCLM.

**ROWWISE | ROW**

arranges the created OUTPUT data set in rowwise format. For each dependent variable and each smoothing value specified in the SMOOTH= option in the MODEL statement, one variable is generated for each specified keyword and the variable name is appended with an order number if there are multiple occurrences of the requested statistic. Those variables appear in an order that corresponds to the specified order of the dependent variables and the smoothing values in the MODEL statement. For each variable generated, a label is also created automatically; the label contains the default name of the represented statistic, the name of the dependent variable selected to be modeled, and the smoothing value used for calculating the represented statistic.

By default, the OUTPUT data set is created in columnwise format, where the input data is repeated for each dependent variable and for each smoothing value. Three extra columns, named SmoothingParameter for smoothing parameter values, DepVar for dependent variable names, and Obs for observation numbers, are also added to the OUTPUT data set to distinguish each model.

---

## SCORE Statement

**SCORE DATA=SAS-data-set < ID=(variable-list) > < / options > ;**

The fitted loess model is used to score the data in the specified SAS data set. This data set must contain all the regressor variables specified in the MODEL statement. Furthermore, when a BY statement is used, the score data set must also contain all the BY variables sorted in the order of the BY variables. A SCORE statement is optional, and more than one SCORE statement can be used. SCORE statements cannot be used if the DIRECT option is specified in the MODEL statement. The optional ID= (variable-list) specifies ID variables to be included in the “Score Results” table.

You find the results of the SCORE statement in the “Score Results” table. This table contains all the data in the data set named in the SCORE statement, including observations with missing values. However, only those observations with nonmissing regressor variables are scored. If no data set is named in the SCORE statement, the data set named in the PROC LOESS statement is scored. You use the PRINT option in the SCORE statement to request that the “Score Results” table be displayed. You can place the “Score Results” table in an output data set by using an ODS OUTPUT statement even if this table is not displayed.

You can specify the following options in the SCORE statement after a slash (/).

**CLM**

requests that  $100(1 - \alpha)\%$  confidence limits on the mean predicted value be added to the “Score Results” table. By default the 95% limits are computed; the ALPHA= option in the MODEL statement can be used to change the significance level. The use of this option implicitly selects the model option DFMETHOD=EXACT if the DFMETHOD= option has not been explicitly used.

**PRINT < (VAR=variables) >**

specifies that the “Score Results” table be displayed. By default only the variables named in the MODEL statement, the variables listed in the ID list in the SCORE statement, and the scored dependent variables are displayed. You can use the VAR= option to specify additional variables in the score data set that are to be included in the displayed output. Note, however, that all columns in the SCORE

data set are placed in the SCORE results table, even if you do not request that they be included in the displayed output.

#### **RESIDUAL | R**

requests that residuals be added to the “Score Results” table. If the data set you specify in DATA= option in the SCORE statement does not contain one or more of the model dependent variables, then the corresponding residual values in the “Score Results” table are set to missing.

#### **SCALEDINDEP**

specifies that scaled regressor coordinates be included in the “Score Results” table. This option is ignored if the SCALE= option is not specified in the MODEL statement.

#### **STEPS**

requests that all models evaluated during smoothing parameter value selection be scored, provided that the SELECT= option together with the STEPS modifier is specified in the MODEL statement. By default only the selected model is scored.

## **WEIGHT Statement**

**WEIGHT** *variable* ;

The WEIGHT statement specifies a variable in the input data set that contains values to be used as a priori weights for a loess fit.

The values of the weight variable must be nonnegative. If an observation’s weight is zero, negative, or missing, the observation is deleted from the analysis.

## **Details: LOESS Procedure**

### **Missing Values**

PROC LOESS deletes any observation with missing values for any variable specified in the MODEL statement. This enables the procedure to reuse the  $k$ -d tree for all the dependent variables that appear in the MODEL statement. If you have multiple dependent variables with different missing value structures for the same set of independent variables, you might want to use separate PROC LOESS steps for each dependent variable.

### **Output Data Sets**

PROC LOESS assigns a name to each table it creates. You can use the ODS OUTPUT statement to place one or more of these tables in output data sets. See the section “ODS Table Names” on page 4131 for a list of the table names created by PROC LOESS. For detailed information about ODS, see Chapter 20, “Using the Output Delivery System.”

For example, the following statements create an output data set named MyOutStats containing the “Output Statistics” table and an output data set named MySummary containing the “Fit Summary” table.

```
proc loess data=Melanoma;
 model Incidences=Year;
 ods output OutputStatistics = MyOutStats
 FitSummary = MySummary;
run;
```

Often, a single MODEL statement describes more than one model. For example, the following statements fit eight different models (four smoothing parameter values for each dependent variable).

```
proc loess;
 model y1 y2 = x1 x2 x3/smooth =0.1 to 0.7 by 0.2;
 ods output OutputStatistics = MyOutStats;
run;
```

The eight “Output Statistics” tables for these models are stacked in a single data set called MyOutStats. The data set contains a column named DepVarName and a column named SmoothingParameter that distinguish each model (see [Figure 53.8](#) for an example). If you want the “Output Statistics” table for each model to be in its own data set, you can use the MATCH\_ALL option in the ODS OUTPUT statement. The following statements create eight data sets named MyOutStats, MyOutStats1, . . . , MyOutStats7.

```
proc loess;
 model y1 y2 = x1 x2 x3/smooth =0.1 to 0.7 by 0.2;
 ods output OutputStatistics(match_all) = MyOutStats;
run;
```

For further options available in the ODS OUTPUT statement, see Chapter 20, “Using the Output Delivery System.”

Only the “Scale Details” and “Fit Summary” tables are displayed by default. The other tables are optionally displayed by using the DETAILS option in the MODEL statement and the PRINT option in the SCORE statement. Note that it is not necessary to display a table in order for that table to be used in an ODS OUTPUT statement. For example, the following statements display the “Output Statistics” and “*k*-d Tree” tables but place the “Output Statistics” and “Prediction at Vertices” tables in output data sets.

```
proc loess data=Melanoma;
 model Incidences=Year/details(OutputStatistics kdTree);
 ods output OutputStatistics = MyOutStats
 PredAtVertices = MyVerticesOut;
run;
```

Using the DETAILS option alone causes all tables to be displayed.

The MODEL statement options CLM, RESIDUAL, STD, SCALEDINDEP, and T control which optional columns are added to the OutputStatistics table. For example, to obtain an OutputStatistics output data set containing residuals and confidence limits in addition to the model variables and predicted value, you need to specify the RESIDUAL and CLM options in the MODEL statement as in the following example:

```
proc loess data=Melanoma;
 model Incidences=Year/residual clm;
 ods output OutputStatistics = MyOutStats;
run;
```

Finally, note that using the ALL option in the MODEL statement causes all optional columns to be included in the output. Also, ID columns can be added to the OutputStatistics table by using the ID statement.

---

## Data Scaling

The loess algorithm to obtain a predicted value at a given point in the predictor space proceeds by doing a least squares fit that uses all data points close to the given point. Thus the algorithm depends critically on the metric used to define closeness. This has the consequence that if you have more than one predictor variable and these predictor variables have significantly different scales, then closeness depends almost entirely on the variable with the largest scaling. It also means that merely changing the units of one of your predictors can significantly change the loess model fit.

To circumvent this problem, it is necessary to standardize the scale of the independent variables in the loess model. The SCALE= option in the MODEL statement is provided for this purpose. PROC LOESS uses a symmetrically trimmed standard deviation as the scale estimate for each independent variable of the loess model. This is a robust scale estimator in that extreme values of a variable are discarded before estimating the data scaling. For example, to compute a 10% trimmed standard deviation of a sample, you discard the smallest and largest 5% of the data and compute the standard deviation of the remaining 90% of the data points. In this case, the trimming fraction is 0.1.

For example, the following statement specifies that the variables Temperature and Catalyst are scaled before performing the loess fitting. In this case, because the trimming fraction is 0.1, the scale estimate used for each of these variables is a 10% trimmed standard deviation.

```
model Yield=Temperature Catalyst / scale = SD(0.1);
```

The default trimming fraction used by PROC LOESS is 0.1 and need not be specified by the SCALE= option. Thus the following MODEL statement is equivalent to the previous MODEL statement.

```
model Yield=Temperature Catalyst / scale = SD;
```

If the SCALE= option is not specified, no scaling of the independent variables is done. This is appropriate when there is only a single independent variable or when all the independent variables are a priori scaled similarly.

When the SCALE= option is specified, the scaling details for each independent variable are added to the ScaleDetails table (see [Output 53.3.2](#) for an example). By default, this table contains only the minimum and maximum values of each independent variable in the model. Finally, note that when the SCALE= option is used, specifying the SCALEDINDEP option in the MODEL statement adds the scaled values of the independent variables to the OutputStatistics and PredAtVertices tables. If the SCALEDINDEP option is specified in the SCORE statement, then scaled values of the independent variables are included in the ScoreResults table. By default, only the unscaled values are placed in these tables.

---

## Direct versus Interpolated Fitting

Local regression to obtain a predicted value at a given point in the predictor space is done by doing a least squares fit that uses all data points in a local neighborhood of the given point. This method is computationally expensive because a local neighborhood must be determined and a least squares problem must be solved for each point at which a fitted value is required. A faster method is to obtain such fits at a representative sample of points in the predictor space and to obtain fitted values at all other points by interpolation.

PROC LOESS can fit models by using either of these two methods. By default, PROC LOESS uses fitting at a sample of points and interpolation. The method fitting a local model at every data point is selected by specifying the `DIRECT` option in the `MODEL` statement.

---

## *k*-d Trees and Blending

PROC LOESS uses a *k*-d tree to divide the box (also called the *initial cell* or *bucket*) enclosing all the predictor data points into rectangular cells. The vertices of these cells are the points at which local least squares fitting is done.

Starting from the initial cell, the direction of the longest cell edge is selected as the split direction. The median of this coordinate of the data in the cell is the split value. The data in the starting cell are partitioned into two child cells. The left child consists of all data from the parent cell whose coordinate in the split direction is less than the split value. This procedure is repeated for each child cell that has more than a prespecified number of points, called the *bucket size* of the *k*-d tree.

You can specify the bucket size with the `BUCKET=` option in the `MODEL` statement. If you do not specify the `BUCKET=` option, the default value used is the largest integer less than or equal to  $ns/5$ , where  $n$  is the number of observations and  $s$  is the value of the smoothing parameter. Note that if fitting is being done for a range of smoothing parameter values, the bucket size can change for each value.

The set of vertices of all the cells of the *k*-d tree are the points at which PROC LOESS performs its local fitting. The fitted value at an original data point (or at any other point within the original data cell) is obtained by blending the fitted values at the vertices of the *k*-d tree cell that contains that data point.

The univariate blending methods available in PROC LOESS are linear and cubic polynomial interpolation, with linear interpolation being the default. You can request cubic interpolation by specifying the `INTERP=CUBIC` option in the `MODEL` statement. In this case, PROC LOESS uses the unique cubic polynomial whose values and first derivatives match those of the fitted local polynomials evaluated at the two endpoints of the *k*-d tree cell edge.

In the multivariate case, such univariate interpolating polynomials are computed on each edge of the *k*-d tree cells and are combined using blending functions (Gordon 1971). In the case of two regressors, if you specify `INTERP=CUBIC` in the `MODEL` statement, PROC LOESS uses Hermite cubic polynomials as blending functions. If you do not specify `INTERP=CUBIC`, or if you specify a model with more than two regressors, then PROC LOESS uses linear polynomials as blending functions. In these cases, the blending method reduces to tensor product interpolation from the  $2^p$  vertices of each *k*-d tree cell, where  $p$  is the number of regressors.

While the details of the *k*-d tree and the fitted values at the vertices of the *k*-d tree are implementation details that seldom need to be examined, PROC LOESS does provide options for their display. Each *k*-d tree subdivision of the data used by PROC LOESS is placed in the “kdTree” table. The predicted values at



the vertices of each  $k$ -d tree are placed in the “PredAtVertices” table. You can request these tables by using the DETAILS option in the MODEL statement.

---

## Local Weighting

The size of the local neighborhoods that PROC LOESS uses in performing local fitting is determined by the smoothing parameter value  $s$ . When  $s < 1$ , the local neighborhood used at a point  $x_i$  contains the  $s$  fraction of the data points closest to the point  $x_i$ . When  $s \geq 1$ , all data points are used.

Suppose  $q$  denotes the number of points in the local neighborhoods and  $d_1, d_2, \dots, d_q$  denote the distances in increasing order of the  $q$  points closest to  $x_i$ . The point at distance  $d_i$  from  $x_i$  is given a weight  $w_i$  in the local regression that decreases as the distance from  $x_i$  increases. PROC LOESS uses a tricube weight function to define

$$w_i = \frac{32}{5} \left( 1 - \left( \frac{d_i}{d_q} \right)^3 \right)^3$$

If  $s > 1$ , then  $d_q$  is replaced by  $d_q s^{1/p}$  in the previous formula, where  $p$  is the number of predictors in the model.

Finally, note that if a weight variable has been specified using a WEIGHT statement, then  $w_i$  is multiplied by the corresponding value of the specified weight variable.

---

## Iterative Reweighting

PROC LOESS can do iterative reweighting to improve the robustness of the fit in the presence of outliers in the data. Iterative reweighting is also appropriate when statistical inference is requested and the error distribution is symmetric but not Gaussian.

The number of iterations is specified by the ITERATIONS= option in the MODEL statement. The default is ITERATIONS=1, which corresponds to no reweighting.

At iterations beyond the first iteration, the local weights  $w_i$  of the previous section are replaced by  $r_i w_i$ , where  $r_i$  is a weight that decreases as the residual of the fitted value at the previous iteration at the point corresponding to  $d_i$  increases. See Cleveland and Grosse (1991) and Cleveland, Grosse, and Shyu (1992) for details.

---

## Specifying the Local Polynomials

PROC LOESS uses linear or quadratic polynomials in doing the local least squares fitting. The option DEGREE = in the MODEL statement is used to specify the degree of the local polynomials used by PROC LOESS, with DEGREE = 1 being the default. In addition, when DEGREE = 2 is specified, the MODEL statement DROPSQUARE= option can be used to exclude specific monomials during the least squares fitting.

For example, the following statements use the monomials 1, x1, x2, x1\*x2, and x2\*x2 for the local least squares fitting.



```
proc loess;
 model y= x1 x2/ degree=2 dropsquare=(x1);
run;
```

---

## Smoothing Matrix

When no iterative reweighting is done, the “Smoothing Matrix” denoted by  $\mathbf{L}$  defines the linear relationship between the fitted and observed dependent variable values of a loess model. You can obtain the predicted values of a loess fit from the observed values via

$$\hat{\mathbf{y}} = \mathbf{L}\mathbf{y}$$

where  $\mathbf{y}$  is the vector of observed values and  $\hat{\mathbf{y}}$  is the corresponding vector of predicted values of the dependent variable. Note that  $\mathbf{L}$  is an  $n$  by  $n$  matrix, where  $n$  is the number of observations in the analysis. PROC LOESS does not explicitly form  $\mathbf{L}$  if the DFMETHOD=EXACT option is not explicitly or implicitly selected.

---

## Model Degrees of Freedom

The approximate model degrees of freedom in a nonparametric fit is a number that is analogous to the number of free parameters in a parametric model. There are three commonly used measures of model degrees of freedom in nonparametric models. These criteria are as follows:

$$\begin{aligned} \text{DF1} &\equiv \text{Trace}(\mathbf{L}) \\ \text{DF2} &\equiv \text{Trace}(\mathbf{L}'\mathbf{L}) \\ \text{DF3} &\equiv 2\text{Trace}\mathbf{L} - \text{Trace}(\mathbf{L}'\mathbf{L}) \end{aligned}$$

A discussion of their properties can be found in Hastie and Tibshirani (1990). DF2 is also referred to as the “Equivalent Number of Parameters,” and this is the name that PROC LOESS uses for DF2 when it appears in the “Fit Summary” table.

---

## Statistical Inference and Lookup Degrees of Freedom

If you denote the  $i$ th measurement of the response by  $y_i$  and the corresponding measurement of predictors by  $x_i$ , then

$$y_i = g(x_i) + \epsilon_i$$

where  $g$  is the regression function and  $\epsilon_i$  are independent random errors with mean zero. If the errors are normally distributed with constant variance, then you can obtain confidence intervals for the predictions

from PROC LOESS. You can also obtain confidence limits in the case where  $\epsilon_i$  is heteroscedastic but  $a_i\epsilon_i$  has constant variance and  $a_i$  are a priori weights that are specified using the **WEIGHT** statement of PROC LOESS. You can do inference in the case in which the error distribution is symmetric by using iterative reweighting. Formulas for doing statistical inference under the preceding conditions can be found in Cleveland and Grosse (1991) and Cleveland, Grosse, and Shyu (1992). Cleveland and Grosse (1991) show that standardized residuals for a loess model follow a  $t$  distribution with  $\rho$  degrees of freedom where

$$\begin{aligned}\delta_1 &\equiv \text{Trace}(\mathbf{I} - \mathbf{L})'(\mathbf{I} - \mathbf{L}) \\ \delta_2 &\equiv \text{Trace}((\mathbf{I} - \mathbf{L})'(\mathbf{I} - \mathbf{L}))^2 \\ \rho &\equiv \text{Lookup Degrees of Freedom} \\ &\equiv \delta_1^2/\delta_2\end{aligned}$$

The residual standard error that you find in the “Fit Summary” table is defined by

$$\text{Residual Standard Error} \equiv \sqrt{\text{Residual SS}/\delta_1}$$

The determination of  $\rho$  is computationally expensive and is not done by default. It is computed if you specify the **DFMETHOD=EXACT** or **DFMETHOD=APPROX** option in the **MODEL** statement. It is also computed if you specify any of the options **CLM**, **STD**, and **T** in the **MODEL** statement. Note that the values of  $\delta_1$ ,  $\delta_2$ , and  $\rho$  are reported in the “Fit Summary” table.

If you specify the **CLM** option in the **MODEL** statement, confidence limits are added to the **OutputStatistics** table. By default, 95% limits are computed, but you can change this by using the **ALPHA=** option in the **MODEL** statement.

---

## Automatic Smoothing Parameter Selection

There are several methodologies for automatic smoothing parameter selection. One class of methods chooses the smoothing parameter value to minimize a criterion that incorporates both the tightness of the fit and model complexity. Such a criterion can usually be written as a function of the error mean square,  $\hat{\sigma}^2$ , and a penalty function designed to decrease with increasing smoothness of the fit. This penalty function is usually defined in terms of the smoothing matrix **L** (see the section “Smoothing Matrix” on page 4126).

Examples of specific criteria are generalized cross validation (Craven and Wahba 1979) and the Akaike information criterion (Akaike 1973). These classical selectors have two undesirable properties when used with local polynomial and kernel estimators: they tend to undersmooth small data sets and tend to be nonrobust in the sense that small variations of the input data can change the choice of smoothing parameter value significantly. Hurvich, Simonoff, and Tsai (1998) obtained several corrected AIC criteria that address the small-sample bias and perform comparably with the *plug-in selectors* (Ruppert, Sheather, and Wand 1995). PROC LOESS provides automatic smoothing parameter selection that uses two of these corrected AIC criteria, named  $\text{AIC}_{C_1}$  and  $\text{AIC}_C$  in Hurvich, Simonoff, and Tsai (1998), and generalized cross validation, denoted by GCV.

The relevant formulas are

$$\begin{aligned} \text{AIC}_{C_1} &= n \log(\hat{\sigma}^2) + n \frac{\delta_1/\delta_2(n + \nu_1)}{\delta_1^2/\delta_2 - 2} \\ \text{AIC}_C &= \log(\hat{\sigma}^2) + 1 + \frac{2(\text{Trace}(\mathbf{L}) + 1)}{n - \text{Trace}(\mathbf{L}) - 2} \\ \text{GCV} &= \frac{n\hat{\sigma}^2}{(n - \text{Trace}(\mathbf{L}))^2} \end{aligned}$$

where  $n$  is the number of observations and

$$\begin{aligned} \delta_1 &\equiv \text{Trace}(\mathbf{I} - \mathbf{L})'(\mathbf{I} - \mathbf{L}) \\ \delta_2 &\equiv \text{Trace}((\mathbf{I} - \mathbf{L})'(\mathbf{I} - \mathbf{L}))^2 \\ \nu_1 &\equiv \text{Equivalent Number of Parameters} \\ &\equiv \text{Trace}(\mathbf{L}'\mathbf{L}) \end{aligned}$$

You invoke these methods for automatic smoothing parameter selection by specifying the `SELECT=criterion` option in the `MODEL` statement, where *criterion* is AICC1, AICC, or GCV. The LOESS procedure evaluates the specified criterion for a sequence of smoothing parameter values and selects the value in this sequence that minimizes the specified criterion. If multiple values yield the optimum, then the largest of these values is selected.

A second class of methods seeks to set an approximate measure of model degrees of freedom to a specified target value. These methods are useful for making meaningful comparisons between loess fits and other nonparametric and parametric fits. Three approximate model degrees of freedom for a loess model are defined in the section “[Model Degrees of Freedom](#)” on page 4126. You invoke these methods by specifying the `SELECT=DFcriterion(target)` option in the `MODEL` statement, where *DFcriterion* is DF1, DF2, or DF3. The criterion that is minimized is given in the following table.

**Table 53.4** Minimization Criteria

| Syntax                          | Minimization Criterion                                                              |
|---------------------------------|-------------------------------------------------------------------------------------|
| <code>SELECT=DF1(target)</code> | $ \text{Trace}(\mathbf{L}) - \text{target} $                                        |
| <code>SELECT=DF2(target)</code> | $ \text{Trace}(\mathbf{L}'\mathbf{L}) - \text{target} $                             |
| <code>SELECT=DF3(target)</code> | $ 2\text{Trace}(\mathbf{L}) - \text{Trace}(\mathbf{L}'\mathbf{L}) - \text{target} $ |

The results are summarized in the “Smoothing Criterion” table. This table is displayed whenever automatic smoothing parameter selection is performed. You can obtain details of the sequence of models examined by specifying the `DETAILS(MODELSUMMARY)` option in the `MODEL` statement to display the “Model Summary” table.

There are several ways in which you can control the sequence of models examined by PROC LOESS. If you specify the `SMOOTH=value-list` option in the `MODEL` statement, then only the values in this list are examined in performing the selection. For example, the following statements select the model that

minimizes the AICC1 criterion among the three models with smoothing parameter values 0.1, 0.3, and 0.4:

```
proc loess;
 model y= x1/ smooth=0.1 0.3 0.4 select=AICC1;
run;
```

If you do not specify the SMOOTH= option in the MODEL statement, then by default PROC LOESS uses a golden section search method to find a local minimum of the specified criterion in the range (0, 1]. You can use the RANGE(*lower,upper*) modifier in the SELECT= option to change the interval in which the golden section search is performed. For example, the following statements request a golden section search to find a local minimizer of the GCV criterion for smoothing parameter values in the interval [0.1,0.5]:

```
proc loess;
 model y= x1/select=GCV(range(0.1,0.5));
run;
```

If you want to be sure of obtaining a global minimum in the range of smoothing parameter values examined, you can specify the GLOBAL modifier in the SELECT= option. For example, the following statements request that a global minimizer of the AICC criterion be obtained for smoothing parameter values in the interval [0.2, 0.8]:

```
proc loess;
 model y= x1/select=AICC(global range(0.2,0.8));
run;
```

Note that even though the smoothing parameter is a continuous variable, a given range of smoothing parameter values corresponds to a finite set of local models. For example, for a data set with 100 observations, the range [0.2, 0.4] corresponds to models with 20, 21, 22, . . . , 40 points in the local neighborhoods. If the GLOBAL modifier is specified, all possible models in the range are evaluated sequentially.

Note that by default PROC LOESS displays a “Fit Summary” and other optionally requested tables only for the selected model. You can request that these tables be displayed for all models in the selection process by adding the STEPS modifier in the SELECT= option. Also note that by default scoring requested with SCORE statements is done only for the selected model. However, if you specify the STEPS in both the MODEL and SCORE statements, then all models evaluated in the selection process are scored.

In terms of computation,  $AIC_C$ , GCV, and DF1 depend on the smoothing matrix  $\mathbf{L}$  only through its trace. In the direct method, this trace can be computed efficiently. In the interpolated method that uses  $k$ -d trees, there is some additional computational cost but the overall work is not significant compared to the rest of the computation. In contrast, the quantities  $\delta_1$ ,  $\delta_2$ , and  $\nu_1$  that appear in the  $AIC_{C_1}$  criterion, and the DF2 and DF3 criteria, depend on the entire  $\mathbf{L}$  matrix and for this reason, the time needed to compute these quantities dominates the time required for the model fitting. Hence SELECT=AICC1, SELECT=DF2, and SELECT=DF3 are much more computationally expensive than SELECT=AICC, SELECT=GCV, and SELECT=DF1, especially when combined with the GLOBAL modifier. Hurvich, Simonoff, and Tsai (1998) note that  $AIC_C$  can be regarded as an approximation of  $AIC_{C_1}$  and that “the  $AIC_C$  selector generally performs well in all circumstances.”

For models with one dependent variable, PROC LOESS uses SELECT=AICC as its default, if you specify neither the SMOOTH= nor the SELECT= option in the MODEL statement. With two or more dependent variables, automatic smoothing parameter selection needs to be done separately for each dependent variable. For this reason automatic smoothing parameter selection is not available for models with multiple dependent

variables. In such cases you should use a separate PROC LOESS step for each dependent variable, if you want to use automatic smoothing parameter selection.

---

## Sparse and Approximate Degrees of Freedom Computation

As noted in the section “Statistical Inference and Lookup Degrees of Freedom” on page 4126, obtaining confidence limits in loess models requires the computation of the lookup degrees of freedom. This in turn requires the computation of

$$\delta_2 \equiv \text{Trace}((\mathbf{I} - \mathbf{L})'(\mathbf{I} - \mathbf{L}))^2$$

where  $\mathbf{L}$  is the loess smoothing matrix (see the section “Smoothing Matrix” on page 4126).

The work in a direct implementation of this formula grows as  $n^3$ , where  $n$  is the number of observations in analysis. For large  $n$ , this work dominates the time needed to fit the loess model itself. To alleviate this computational bottleneck, Cleveland and Grosse (1991) and Cleveland, Grosse, and Shyu (1992) developed approximate methods for estimating this quantity in terms of more readily computable statistics. A different approach to obtaining a computationally cheap estimate of  $\delta_2$  has been implemented in PROC LOESS.

For large data sets with significant local structure, the loess model is often used with small values of the smoothing parameter. Recalling that the smoothing parameter defines the fraction of the data used in each local regression, this means that the loess fit at any point in regressor space depends on only a small fraction of the data. This is reflected in the smoothing matrix  $\mathbf{L}$  whose  $(i, j)$  entry is nonzero only if the  $i$ th and  $j$ th observations lie in at least one common local neighborhood. Hence the smoothing matrix is a sparse matrix (has mostly zero entries) in such cases. By exploiting this sparsity, PROC LOESS now computes  $\delta_2$  orders of magnitude faster than in previous implementations.

When each local neighborhood contains a large subset of the data—i.e., when the smoothing parameter is large—then it is no longer true that the smoothing matrix is sparse. However, since a point in a local neighborhood is given a local weight that decreases with its distance from the center of the neighborhood, many of the coefficients in the smoothing matrix turn out to be nonzero but with orders of magnitude smaller than that of the larger coefficients in the matrix. The approximate method for computing  $\delta_2$  that has been implemented in PROC LOESS exploits these disparities in magnitudes of the elements in the smoothing matrix by setting the small elements to zero. This creates a sparse approximation of the smoothing matrix to which the fast sparse methods can be applied.

In order to decide the threshold at which elements in the smoothing matrix are set to zero, PROC LOESS samples the elements in the smoothing matrix to obtain the value of the element in a specified lower quantile in this sample. The magnitude of the element at this quantile is used as a cutoff value, and all elements in the smoothing matrix whose magnitude is less than this cutoff are set to zero for the approximate computation. By default all elements in the lower ninetieth percentile are set to zero. You can use the `DFMETHOD=APPROX(QUANTILE= )` option in the `MODEL` statement to change this value. As you increase the value for the quantile to be zeroed, you speed up the degrees of freedom computation at the expense of increasing approximation errors. You can also use the `DFMETHOD=APPROX(CUTOFF= )` option in the `MODEL` statement to specify the cutoff value directly.

For small data sets, the approximate computation is not needed and would be rougher than for larger data sets. Hence PROC LOESS performs the exact computation for analyses with fewer than 500 points, even if `DFMETHOD=APPROX` is specified in the model statement. Also, for small values of the smoothing

parameter, elements in the lower specified quantile might already all be zero. In such cases the approximate method is the same as the exact method. PROC LOESS labels as approximate any statistics that depend on the approximate computation of  $\delta_2$  only in the cases where the approximate computation was used and is different from the exact computation.

---

## Scoring Data Sets

One or more **SCORE** statements can be used with PROC LOESS. A data set that includes all the variables specified in the **MODEL** and **BY** statements must be specified in each **SCORE** statement. Score results are placed in the ScoreResults table. This table is not displayed by default, but specifying the **PRINT** option in the **SCORE** statement produces the table. If you specify the **CLM** option in the **SCORE** statement, confidence intervals are included in the ScoreResults table.

Note that scoring is not supported when the **DIRECT** option is specified in the **MODEL** statement. Scoring at a point specified in a score data set is done by first finding the cell in the  $k$ -d tree containing this point and then interpolating the scored value from the predicted values at the vertices of this cell. This methodology precludes scoring any points that are not contained in the box that surrounds the data used in fitting the loess model.

---

## ODS Table Names

PROC LOESS assigns a name to each table it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in the following table. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

**Table 53.5** ODS Tables Produced by PROC LOESS

| ODS Table Name     | Description                                           | Statement | Option                    |
|--------------------|-------------------------------------------------------|-----------|---------------------------|
| FitSummary         | Specified fit parameters and fit summary              |           | default                   |
| kdTree             | Structure of $k$ -d tree used                         | MODEL     | DETAILS(kdTree)           |
| ModelSummary       | Summary of all models evaluated                       | MODEL     | DETAILS(ModelSummary)     |
| OutputStatistics   | Coordinates and fit results at input data points      | MODEL     | DETAILS(OutputStatistics) |
| PredAtVertices     | Coordinates and fitted values at $k$ -d tree vertices | MODEL     | DETAILS(PredAtVertices)   |
| ScaleDetails       | Extent and scaling of the independent variables       |           | default                   |
| ScoreResults       | Coordinates and fit results at scoring points         | SCORE     | PRINT                     |
| SmoothingCriterion | Criterion value and selected smoothing parameter      | MODEL     | SELECT                    |

---

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “Statistical Graphics Using ODS.”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “A Primer on ODS Statistical Graphics” on page 599 in Chapter 21, “Statistical Graphics Using ODS.”

You can reference every graph produced through ODS Graphics with a name. The names of the graphs that PROC LOESS generates are listed in Table 53.6, along with the relevant PLOTS= options.

**Table 53.6** Graphs Produced by PROC LOESS

| ODS Graph Name      | Plot Description                                                         | PLOTS Option        |
|---------------------|--------------------------------------------------------------------------|---------------------|
| ContourFitPanel     | Panel of loess contour surfaces overlaid on scatter plots of data        | CONTOURFITPANEL     |
| ContourFit          | Loess contour surface overlaid on scatter plot of data                   | CONTOURFITPANEL     |
| DiagnosticsPanel    | Panel of fit diagnostics                                                 | DIAGNOSTICS         |
| FitPanel            | Panel of loess curves overlaid on scatter plots of data                  | FITPANEL            |
| FitPlot             | Loess curve overlaid on scatter plot of data                             | FIT                 |
| ObservedByPredicted | Dependent variable versus loess fit                                      | OBSERVEDBYPREDICTED |
| QQPlot              | Normal quantile plot of residuals                                        | QQPLOT              |
| ResidualsBySmooth   | Panel of residuals versus regressor by smoothing parameter values        | RESIDUALSBYSMOOTH   |
| ResidualByPredicted | Residuals versus loess fit                                               | RESIDUALBYPREDICTED |
| ResidualHistogram   | Histogram of fit residuals                                               | RESIDUALHISTOGRAM   |
| ResidualPanel       | Panel of residuals versus regressors for fixed smoothing parameter value | RESIDUALS           |
| ResidualPlot        | Plot of residuals versus regressor                                       | RESIDUALS           |
| RFPlot              | Side-by-side plots of quantiles of centered fit and residuals            | RFPLOT              |
| ScorePlot           | Loess fit evaluated at scoring points                                    | SCOREPLOT           |
| CriterionPlot       | Selection criterion versus smoothing parameter                           | CRITERION           |

---

## Examples: LOESS Procedure

---

### Example 53.1: Engine Exhaust Emissions

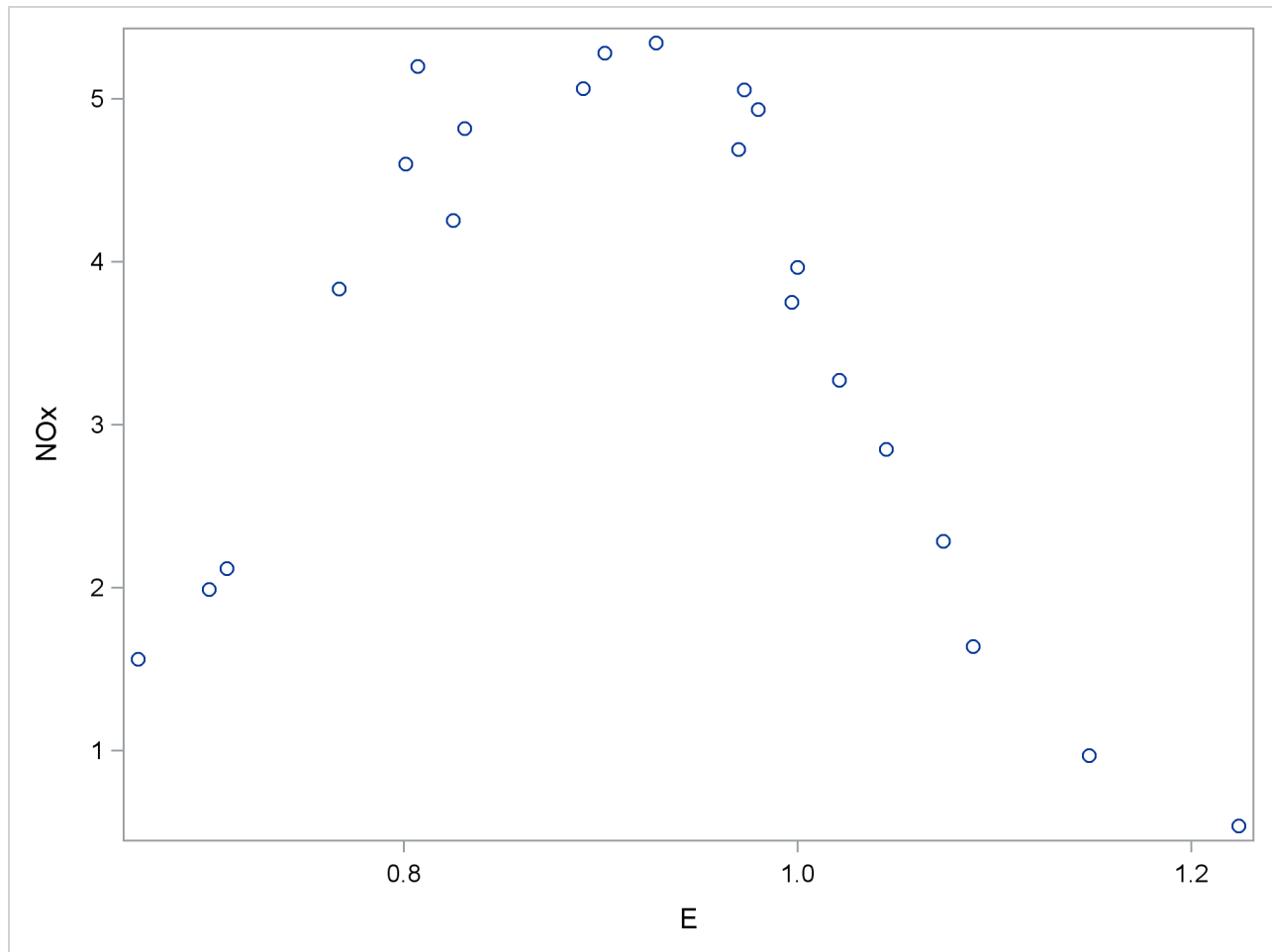
Investigators studied the exhaust emissions of a one-cylinder engine (Brinkman 1981). The SAS data set Gas contains the results data. The dependent variable, NO<sub>x</sub>, measures the concentration, in micrograms per joule, of nitric oxide and nitrogen dioxide normalized by the amount of work of the engine. The independent variable, E, is a measure of the richness of the air and fuel mixture.

```
data Gas;
 input NOx E @@;
 format NOx f3.1;
 format E f3.1;
 datalines;
4.818 0.831 2.849 1.045
3.275 1.021 4.691 0.97
4.255 0.825 5.064 0.891
2.118 0.71 4.602 0.801
2.286 1.074 0.97 1.148
3.965 1 5.344 0.928
3.834 0.767 1.99 0.701
5.199 0.807 5.283 0.902
3.752 0.997 0.537 1.224
1.64 1.089 5.055 0.973
4.937 0.98 1.561 0.665
;
```

The following PROC SGPLOT statements produce the simple scatter plot of these data displayed in [Output 53.1.1](#).

```
proc sgplot data=Gas;
 scatter x=E y=NOx;
run;
```



**Output 53.1.1** Scatter Plot of the Gas Data

The following statements fit two loess models for these data. Because this is a small data set, it is reasonable to do direct fitting at every data point. As there is substantial curvature in the data, quadratic local polynomials are used. An ODS OUTPUT statement creates two output data sets containing the “Output Statistics” and “Fit Summary” tables.

```
ods graphics on;

proc loess data=Gas;
 ods output OutputStatistics = GasFit
 FitSummary=Summary;
 model NOx = E / degree=2 select=AICC(steps) smooth = 0.6 1.0
 direct alpha=.01 all details;
run;

ods graphics off;
```

**Output 53.1.2** Fit Summary Table

| The LOESS Procedure               |          |
|-----------------------------------|----------|
| Selected Smoothing Parameter: 0.6 |          |
| Dependent Variable: NOx           |          |
| Fit Summary                       |          |
| Fit Method                        | Direct   |
| Number of Observations            | 22       |
| Degree of Local Polynomials       | 2        |
| Smoothing Parameter               | 0.60000  |
| Points in Local Neighborhood      | 13       |
| Residual Sum of Squares           | 1.71852  |
| Trace[L]                          | 6.42184  |
| GCV                               | 0.00708  |
| AICC                              | -0.45637 |
| AICC1                             | -9.39715 |
| Delta1                            | 15.12582 |
| Delta2                            | 14.73089 |
| Equivalent Number of Parameters   | 5.96950  |
| Lookup Degrees of Freedom         | 15.53133 |
| Residual Standard Error           | 0.33707  |

The “Fit Summary” table for smoothing parameter value 0.6, shown in [Output 53.1.2](#), records the fitting parameters specified and some overall fit statistics. See the section “[Smoothing Matrix](#)” on page 4126 for a definition of the smoothing matrix  $L$ , and the sections “[Model Degrees of Freedom](#)” on page 4126 and “[Statistical Inference and Lookup Degrees of Freedom](#)” on page 4126 for definitions of the statistics that appear in this table.

The “Output Statistics” table for smoothing parameter value 0.6 is shown in [Output 53.1.3](#). Note that, because the ALL option is specified in the `MODEL` statement, this table includes all the relevant optional columns. Furthermore, because the ALPHA=0.01 option is specified in the `MODEL` statement, the confidence limits in this table are 99% limits.

## Output 53.1.3 Output Statistics Table

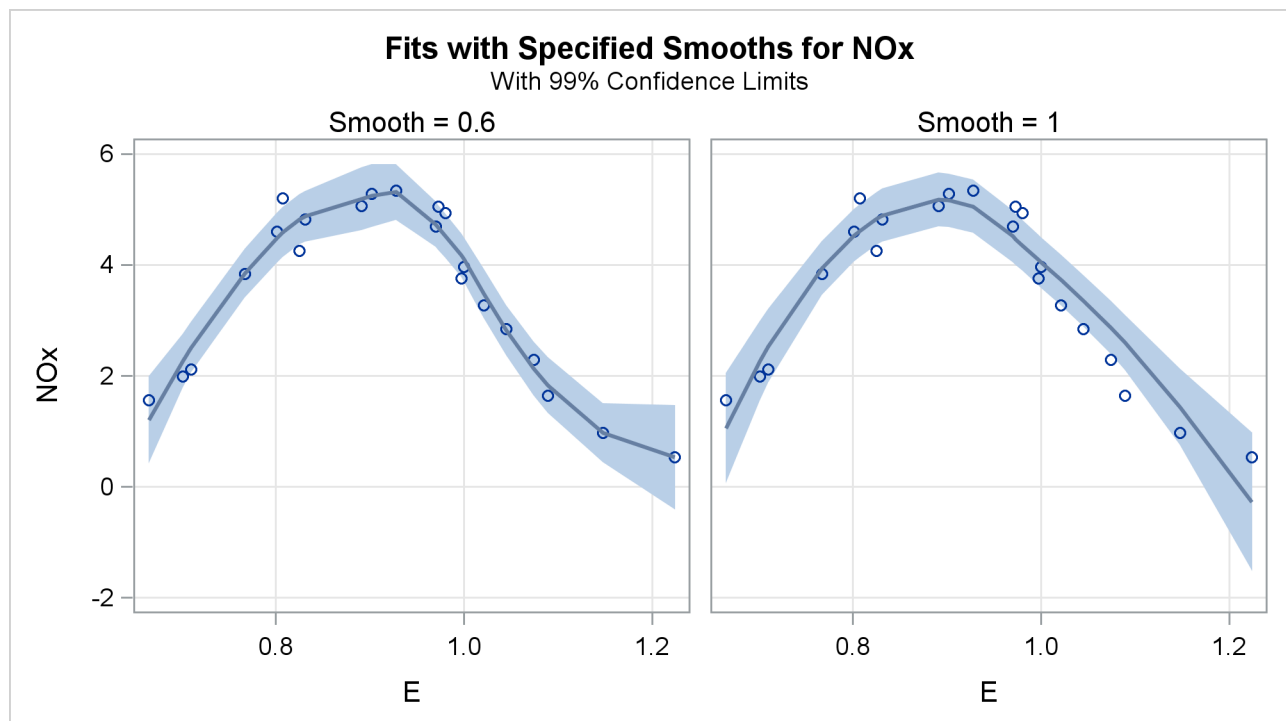
| The LOESS Procedure               |                       |         |                  |                                          |          |         |  |
|-----------------------------------|-----------------------|---------|------------------|------------------------------------------|----------|---------|--|
| Selected Smoothing Parameter: 0.6 |                       |         |                  |                                          |          |         |  |
| Dependent Variable: NOx           |                       |         |                  |                                          |          |         |  |
| Output Statistics                 |                       |         |                  |                                          |          |         |  |
| Obs                               | E                     | NOx     | Predicted<br>NOx | Estimated<br>Prediction<br>Std Deviation | Residual | t Value |  |
| 1                                 | 0.8                   | 4.8     | 4.87377          | 0.15528                                  | -0.05577 | -0.36   |  |
| 2                                 | 1.0                   | 2.8     | 2.81984          | 0.15380                                  | 0.02916  | 0.19    |  |
| 3                                 | 1.0                   | 3.3     | 3.48153          | 0.15187                                  | -0.20653 | -1.36   |  |
| 4                                 | 1.0                   | 4.7     | 4.73249          | 0.13923                                  | -0.04149 | -0.30   |  |
| 5                                 | 0.8                   | 4.3     | 4.82305          | 0.15278                                  | -0.56805 | -3.72   |  |
| 6                                 | 0.9                   | 5.1     | 5.18561          | 0.19337                                  | -0.12161 | -0.63   |  |
| 7                                 | 0.7                   | 2.1     | 2.51120          | 0.15528                                  | -0.39320 | -2.53   |  |
| 8                                 | 0.8                   | 4.6     | 4.48267          | 0.15285                                  | 0.11933  | 0.78    |  |
| 9                                 | 1.1                   | 2.3     | 2.12619          | 0.16683                                  | 0.15981  | 0.96    |  |
| 10                                | 1.1                   | 1.0     | 0.97120          | 0.18134                                  | -0.00120 | -0.01   |  |
| 11                                | 1.0                   | 4.0     | 4.09987          | 0.13477                                  | -0.13487 | -1.00   |  |
| 12                                | 0.9                   | 5.3     | 5.31258          | 0.17283                                  | 0.03142  | 0.18    |  |
| 13                                | 0.8                   | 3.8     | 3.84572          | 0.14929                                  | -0.01172 | -0.08   |  |
| 14                                | 0.7                   | 2.0     | 2.26578          | 0.16712                                  | -0.27578 | -1.65   |  |
| 15                                | 0.8                   | 5.2     | 4.58394          | 0.15363                                  | 0.61506  | 4.00    |  |
| 16                                | 0.9                   | 5.3     | 5.24741          | 0.19319                                  | 0.03559  | 0.18    |  |
| 17                                | 1.0                   | 3.8     | 4.16979          | 0.13478                                  | -0.41779 | -3.10   |  |
| 18                                | 1.2                   | 0.5     | 0.53059          | 0.32170                                  | 0.00641  | 0.02    |  |
| 19                                | 1.1                   | 1.6     | 1.83157          | 0.17127                                  | -0.19157 | -1.12   |  |
| 20                                | 1.0                   | 5.1     | 4.66733          | 0.13735                                  | 0.38767  | 2.82    |  |
| 21                                | 1.0                   | 4.9     | 4.52385          | 0.13556                                  | 0.41315  | 3.05    |  |
| 22                                | 0.7                   | 1.6     | 1.19888          | 0.26774                                  | 0.36212  | 1.35    |  |
| Output Statistics                 |                       |         |                  |                                          |          |         |  |
| Obs                               | 99% Confidence Limits |         |                  |                                          |          |         |  |
| 1                                 | 4.41841               | 5.32912 |                  |                                          |          |         |  |
| 2                                 | 2.36883               | 3.27085 |                  |                                          |          |         |  |
| 3                                 | 3.03617               | 3.92689 |                  |                                          |          |         |  |
| 4                                 | 4.32419               | 5.14079 |                  |                                          |          |         |  |
| 5                                 | 4.37503               | 5.27107 |                  |                                          |          |         |  |
| 6                                 | 4.61855               | 5.75266 |                  |                                          |          |         |  |
| 7                                 | 2.05585               | 2.96655 |                  |                                          |          |         |  |
| 8                                 | 4.03444               | 4.93089 |                  |                                          |          |         |  |
| 9                                 | 1.63697               | 2.61541 |                  |                                          |          |         |  |
| 10                                | 0.43942               | 1.50298 |                  |                                          |          |         |  |
| 11                                | 3.70467               | 4.49507 |                  |                                          |          |         |  |
| 12                                | 4.80576               | 5.81940 |                  |                                          |          |         |  |
| 13                                | 3.40794               | 4.28350 |                  |                                          |          |         |  |
| 14                                | 1.77571               | 2.75584 |                  |                                          |          |         |  |
| 15                                | 4.13342               | 5.03445 |                  |                                          |          |         |  |
| 16                                | 4.68089               | 5.81393 |                  |                                          |          |         |  |
| 17                                | 3.77457               | 4.56502 |                  |                                          |          |         |  |
| 18                                | -0.41278              | 1.47397 |                  |                                          |          |         |  |
| 19                                | 1.32933               | 2.33380 |                  |                                          |          |         |  |
| 20                                | 4.26456               | 5.07010 |                  |                                          |          |         |  |
| 21                                | 4.12632               | 4.92139 |                  |                                          |          |         |  |
| 22                                | 0.41375               | 1.98401 |                  |                                          |          |         |  |

**Output 53.1.4** Output Statistics Table

| Optimal Smoothing Criterion |                     |
|-----------------------------|---------------------|
| AICC                        | Smoothing Parameter |
| -0.45637                    | 0.60000             |

The combination of the options `SELECT=AICC` and `SMOOTH=0.6 1` in the `MODEL` statement specifies that PROC LOESS fit models with smoothing parameters of 0.6 and 1 and select the model that yields the smaller value of the AICC statistic. The “Smoothing Criterion” shown in [Output 53.1.4](#) shows that PROC LOESS selects the model with smoothing parameter value 0.6 as it yields the smaller value of the AICC statistic.

With ODS Graphics enabled, PROC LOESS produces a panel of fit plots whenever you specify the `SMOOTH=` option in the `MODEL` statement. These fit plots include confidence limits if you additionally specify the `CLM` option in the `MODEL` statement.

**Output 53.1.5** Loess Fits with 99% Confidence Limits for the Gas Data

[Output 53.1.5](#) shows the “Fit Panel” that displays the fitted models with 99% confidence limits overlaid on scatter plots of the data.

Based on the AICC criterion, the model with smoothing parameter 0.6 is preferred. You can address the question of whether the differences between these models are significant using analysis of variance. You do this by using the model with smoothing parameter value 1 as the null model.

The statistic

$$F = \frac{(\text{rss}^{(n)} - \text{rss}) / (\delta_1^{(n)} - \delta_1)}{\text{rss} / \delta_1}$$

has a distribution that is well approximated by an  $F$  distribution with

$$\nu = \frac{(\delta_1^{(n)} - \delta_1)^2}{\delta_2^{(n)} - \delta_2}$$

numerator degrees of freedom and  $\rho$  denominator degrees of freedom (Cleveland and Grosse 1991). Here quantities with superscript  $n$  refer to the null model,  $\text{rss}$  is the residual sum of squares, and  $\delta_1$ ,  $\delta_2$ , and  $\rho$  are defined in the section “[Statistical Inference and Lookup Degrees of Freedom](#)” on page 4126.

The “Fit Summary” tables contain the information needed to carry out such an analysis. These tables have been captured in the output data set named `Summary` by using an `ODS OUTPUT` statement. The following statements extract the relevant information from this data set and carry out the analysis of variance:

```

data h0 h1;
 set Summary(keep=SmoothingParameter Label1 nValue1
 where=(Label1 in ('Residual Sum of Squares', 'Delta1',
 'Delta2', 'Lookup Degrees of Freedom')));
 if SmoothingParameter = 1 then output h0;
 else output h1;
run;

proc transpose data=h0(drop=SmoothingParameter Label1) out=h0;
run;

data h0(drop=_NAME_);
 set h0;
 rename Col1 = RSSNull
 Col2 = delta1Null
 Col3 = delta2Null;
run;

proc transpose data=h1(drop=SmoothingParameter Label1) out=h1;
run;

data h1(drop=_NAME_);
 set h1;
 rename Col1 = RSS Col2 = delta1
 Col3 = delta2 Col4 = rho;
run;

data ftest;
 merge h0 h1;
 nu = (delta1Null - delta1)**2 / (delta2Null - delta2);
 Numerator = (RSSNull - RSS)/(delta1Null - delta1);
 Denominator = RSS/delta1;
 FValue = Numerator / Denominator;
 PValue = 1 - ProbF(FValue, nu, rho);
 label nu = 'Num DF' rho = 'Den DF'
 FValue = 'F Value' PValue = 'Pr > F';

```

```
run;

proc print data=ftest label;
 var nu rho Numerator Denominator FValue PValue;
 format nu rho FValue 7.2 PValue 6.4;
run;
```

The results are shown in [Output 53.1.6](#).

**Output 53.1.6** Test ANOVA for Loess Models of Gas Data

| Obs | Num DF | Den DF | Numerator | Denominator | F Value | Pr > F |
|-----|--------|--------|-----------|-------------|---------|--------|
| 1   | 2.67   | 15.53  | 1.05946   | 0.11362     | 9.32    | 0.0012 |

The small  $p$ -value confirms that the fit with smoothing parameter value 0.6 is significantly different from the loess model with smoothing parameter value 1.

Alternatively, you can use the OUTPUT statement to generate the statistics you want to include in the output data set. The following statements produce essentially the same results as the ODS OUTPUT statement does, except all the statistics for each of the two smoothing parameter values are included because the SELECT= option is not specified in the MODEL statement. In addition, with the ROW option specified, the output data set is arranged in rowwise format which enables you to compare statistics side-by-side for a sequence of smoothing values. The ALL option after the slash produces all the statistics (predicted values, residual values, standard errors of the mean predicted values,  $t$  statistics, and the lower and upper parts of  $100(1 - \alpha)\%$  confidence limits on the mean predicted value). All these requested statistics are given their respective default names in the output data set except the predicted value. The P=PREDVAL option causes the name for the predicted value to start with predval.

```
proc loess data=Gas;
 model NOx = E / degree=2 smooth = 0.6 1.0
 direct alpha=.01;
 output out=GasFit p=predval /all row;
run;
```

---

## Example 53.2: Sulfate Deposits in the U.S. for 1990

The following data set contains measurements in grams per square meter of sulfate ( $\text{SO}_4$ ) deposits during 1990 at 179 sites throughout the 48 contiguous states.

```
data SO4;
 input Latitude Longitude SO4 @@;
 format Latitude f4.0;
 format Longitude f4.0;
 format SO4 f4.1;
 datalines;
32.45833 87.24222 1.403 34.28778 85.96889 2.103
33.07139 109.86472 0.299 36.07167 112.15500 0.304
31.95056 112.80000 0.263 33.60500 92.09722 1.950
```

```

34.17944 93.09861 2.168 36.08389 92.58694 1.578

... more lines ...

43.87333 104.19222 0.306 44.91722 110.42028 0.210
45.07611 72.67556 2.646
;

```

As longitudes decrease from west to east in the western hemisphere, the roles of east and west get interchanged if you use these longitudes on the horizontal axis of a plot. You can address this by using negative values to represent longitudes in the western hemisphere. The following statements change the sign of longitude in the SO4 data set and define a format to display these negative values with a suffix of “W”.

```

proc format;
 picture latitude -90 - 0 = '000S'
 0 - 90 = '000N';
 picture longitude -180 - 0 = '000W'
 0 - 180 = '000E';
run;
data SO4;
 set SO4;
 format longitude longitude. latitude latitude.;
 longitude = -longitude;
run;

```

The following statements use ODS Graphics to plot the locations of the sulfate measurements. The circles indicating the locations are colored using a gradient that denotes the value of SO4.

```

proc template;
 define statgraph gradientScatter;
 beginGraph;
 layout overlay;
 scatterPlot x=longitude y=latitude /
 markercolorgradient = SO4
 markerattrs = (symbol=circleFilled)
 colormodel = ThreeColorRamp
 name = "Scatter";
 scatterPlot x=longitude y=latitude /
 markerattrs = (symbol=circle);
 continuousLegend "Scatter"/title= "SO4";
 endlayout;
 endgraph;
 end;
run;

proc sgrender data=SO4 template=gradientScatter;
run;

```

Output 53.2.1 Sulfate Measurements

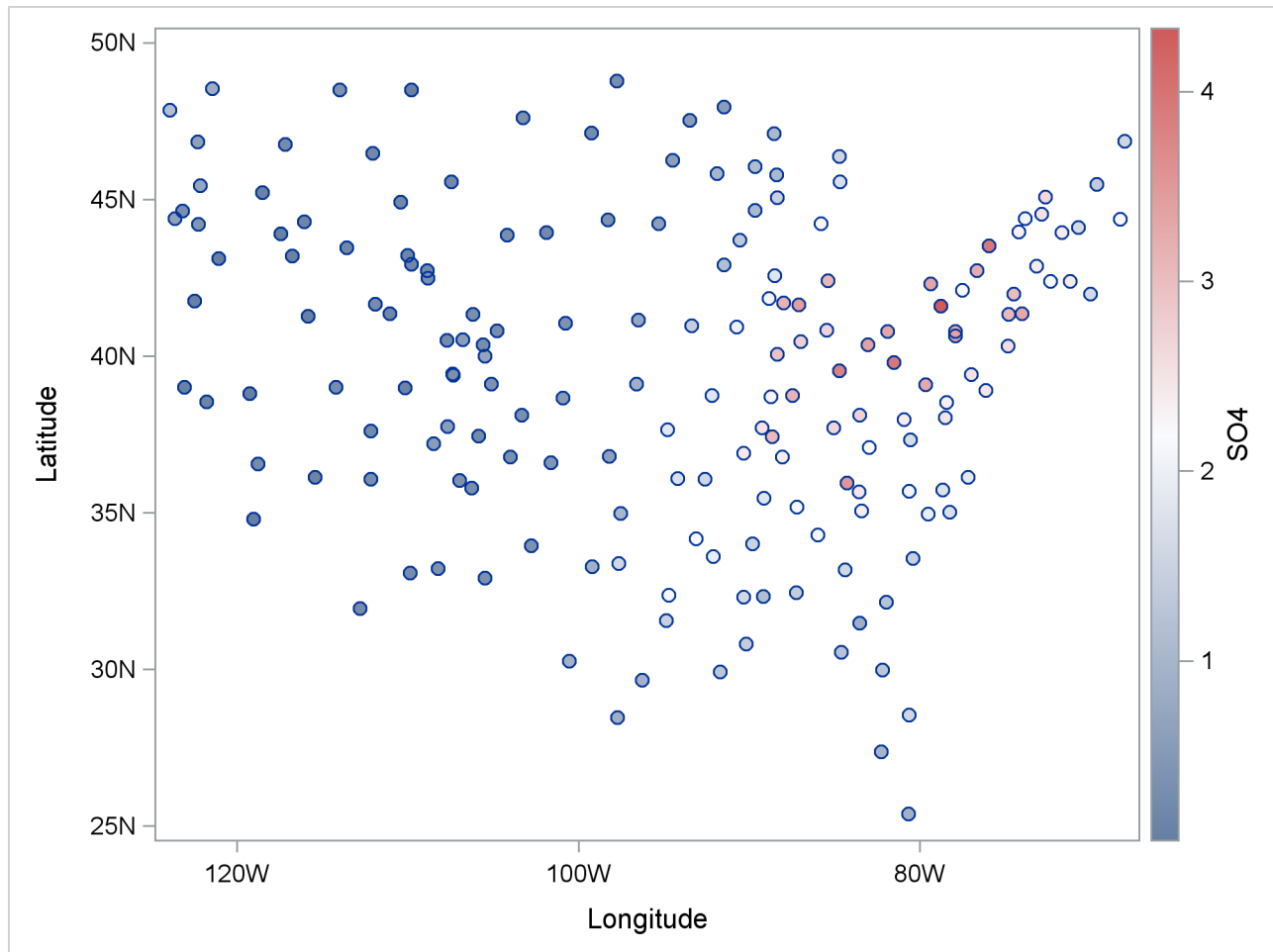


Figure 53.2.1 shows that the largest concentrations of sulfate deposits occur in the northeastern United States.

The following statements fit a loess model.

```
ods graphics on;

proc loess data=SO4;
 model SO4=Longitude Latitude / degree=2 interp=cubic;
run;

ods graphics off;
```



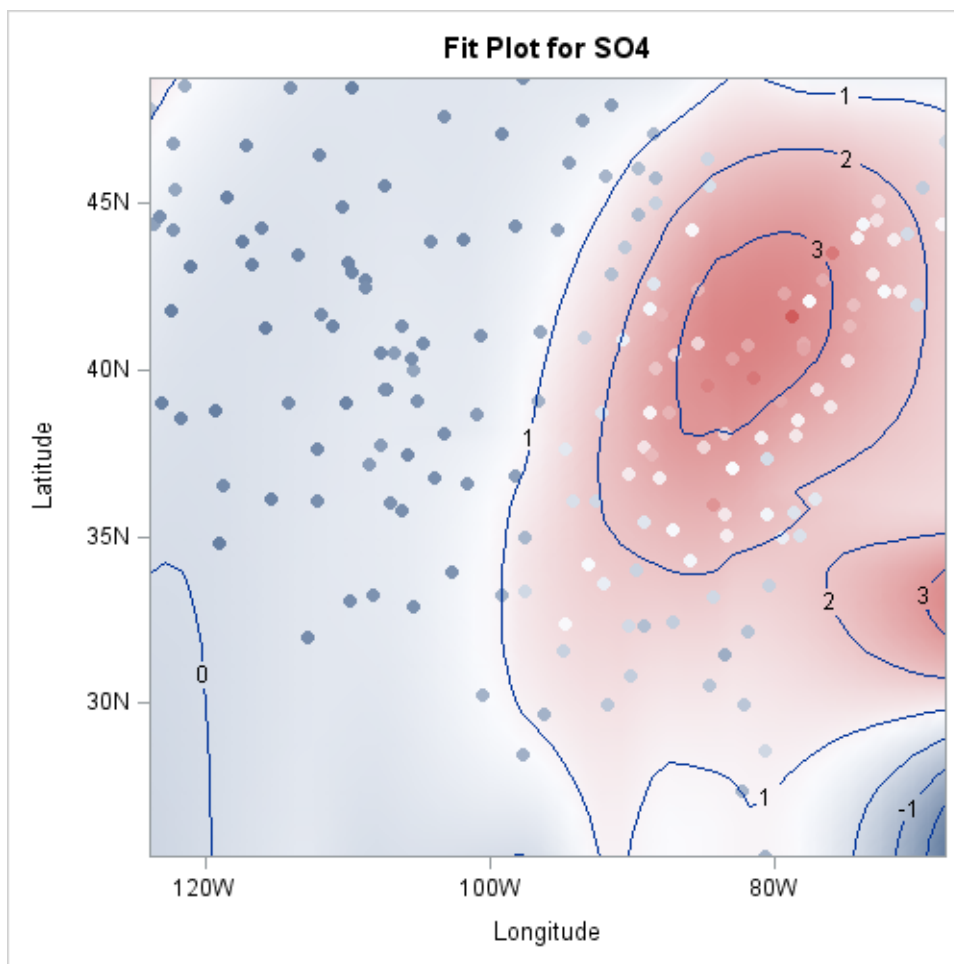
**Output 53.2.2** Fit Plot for the SO4 Data

Figure 53.2.2 shows a contour plot of the fitted loess surface overlaid with a scatter plot of the data. The data are colored by the observed sulfate concentrations, using the same color gradient as the gradient-filled contour plot of the fitted surface. Note that for observations where the residual is small, the observations blend in with the contour plot. The greater the size of the residual, the greater the contrast between the observation color and the surface color.

The sulfate measurements are irregularly spaced. To facilitate producing a plot of the fitted loess surface, you can create a data set containing a regular grid of longitudes and latitudes and then use the **SCORE** statement to evaluate the loess surface at these points. The following statements show how you do this:

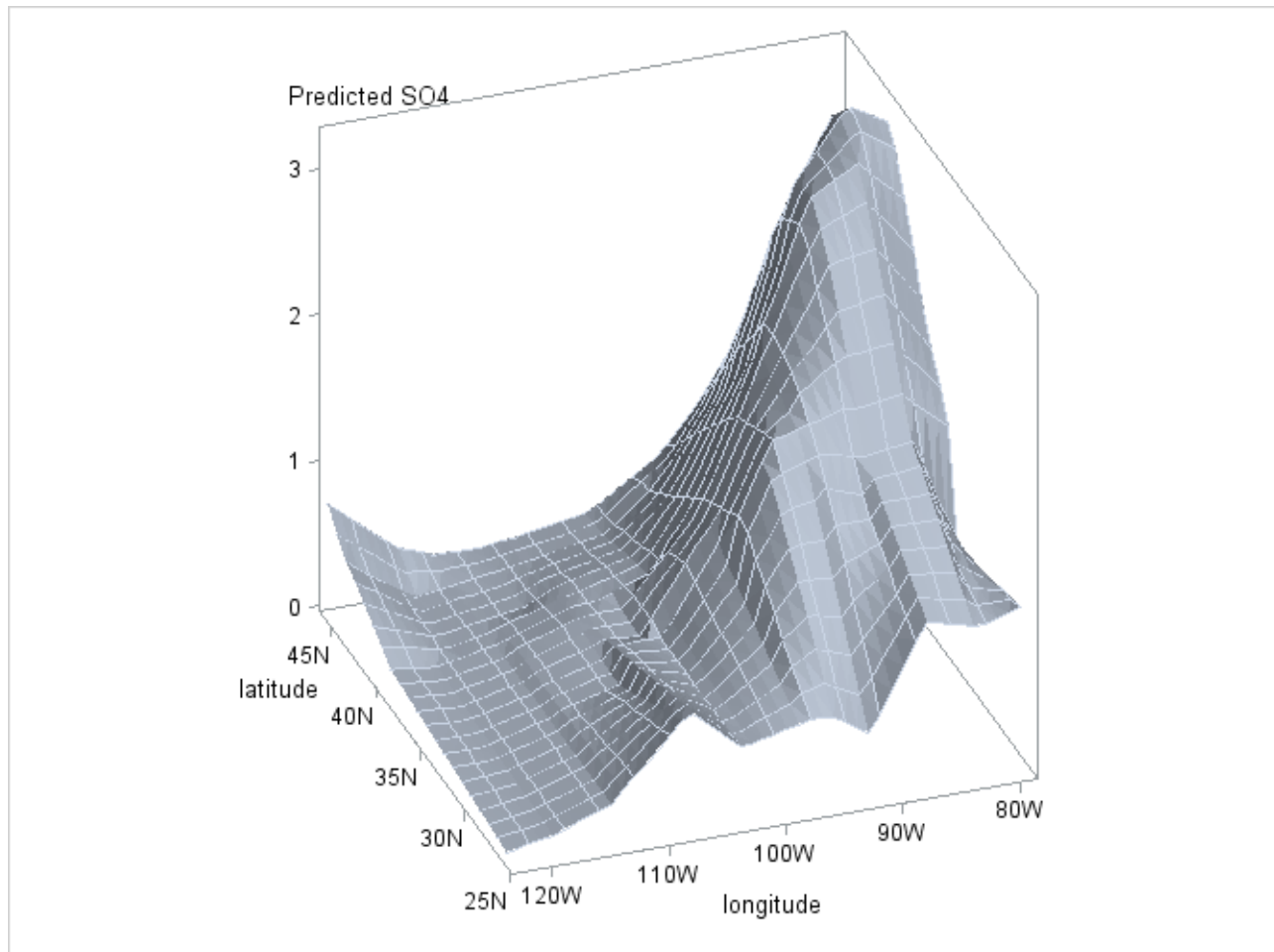
```
data PredPoints;
 format longitude longitude.
 latitude latitude.;
 do Latitude = 26 to 46 by 1;
 do Longitude = -79 to -123 by -1;
 output;
 end;
 end;
run;

proc loess data=S04;
 model S04=Longitude Latitude;
 score data=PredPoints / print;
 ods Output ScoreResults=ScoreOut;
run;
```

The **PRINT** option in the **SCORE** statement requests that the “Score Results” table be displayed as part of the PROC LOESS output. The ODS OUTPUT statement outputs this table to a data set named ScoreOut. If you do not want to display the score results but you do want the score results in an output data set, then you can omit the **PRINT** option from the **SCORE** statement. To plot the surface shown in Figure 53.2.3 by using ODS Graphics, use the following statements:

```
proc template;
 define statgraph surface;
 begingraph;
 layout overlay3d / rotate=340 tilt=30 cube=false;
 surfaceplotparm x=Longitude y=Latitude z=p_S04;
 endlayout;
 endgraph;
end;
run;

proc sgrender data=ScoreOut template=surface;
run;
```

**Output 53.2.3** Loess Fit of SO4 Surface


---

### Example 53.3: Catalyst Experiment

The following data set records the results of an experiment to determine how the yield of a chemical reaction varies with temperature and amount of a catalyst used.

```

data Experiment;
 input Temperature Catalyst MeasuredYield;
 if ranuni(1) < 0.1
 then CorruptedYield = MeasuredYield + 10 * ranuni(1);
 else CorruptedYield = MeasuredYield;
 datalines;
80 0.000 6.85601
80 0.002 7.26355
80 0.004 7.41448
80 0.006 7.82640

... more lines ...

140 0.078 5.20562
140 0.080 5.49371
;

```

The aim of this example is to show how you can use PROC LOESS for robust fitting in the presence of outliers. To simulate an intermittent equipment malfunction, the variable `CorruptedYield` is the same as the variable `MeasuredYield` except for about 10% of the observations where an offset has been added. This example shows how you can use PROC LOESS obtain a fit for `CorruptedYield` that is close to the fit you obtain for `MeasuredYield`.

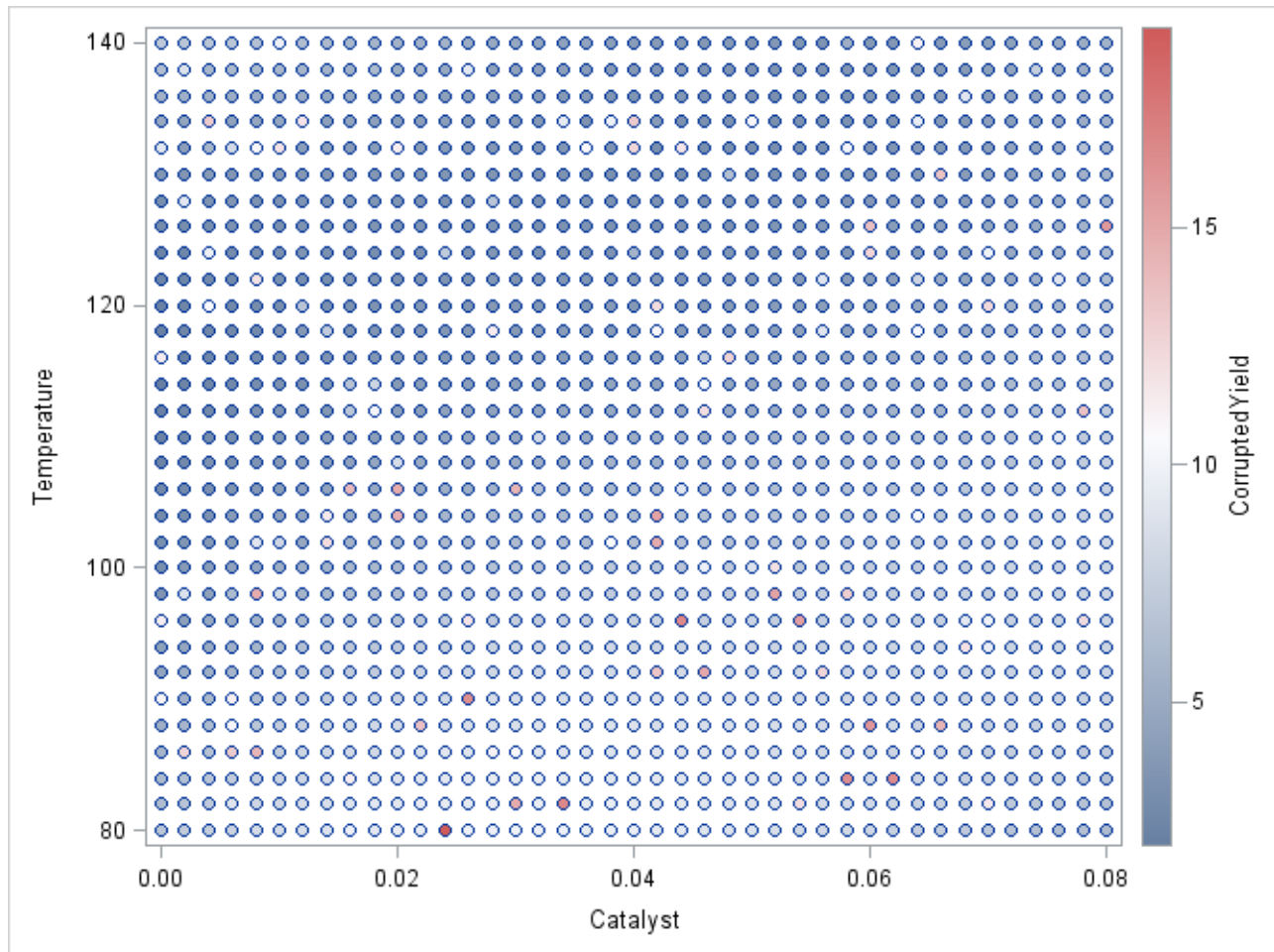
The following statements produce a scatter plot of Temperature by Catalyst where the observations are colored by `CorruptedYield`:

```
proc template;
 define statgraph gradientScatter;
 beginGraph;
 layout overlay;
 scatterPlot x=Catalyst y=Temperature /
 markercolorgradient = CorruptedYield
 markerattrs = (symbol=circleFilled)
 colormodel = ThreeColorRamp
 name = "Yield";

 scatterPlot x=Catalyst y=Temperature /
 markerattrs = (symbol=circle);

 continuousLegend "Yield" / title= "CorruptedYield";
 endlayout;
 endgraph;
 end;
run;

proc sgrender data=Experiment template=gradientScatter;
run;
```

**Output 53.3.1** Scatter Plot of Experiment Data Colored by CorruptedYield

Output 53.3.1 shows a scatter plot of the data where the observations are shaded by the value of `CorruptedYield`. The darkly shaded points that are surrounded by lightly shaded points are points where the simulated incorrect measurements occur.

The following code fits a loess model to the measured data:

```
ods graphics on;

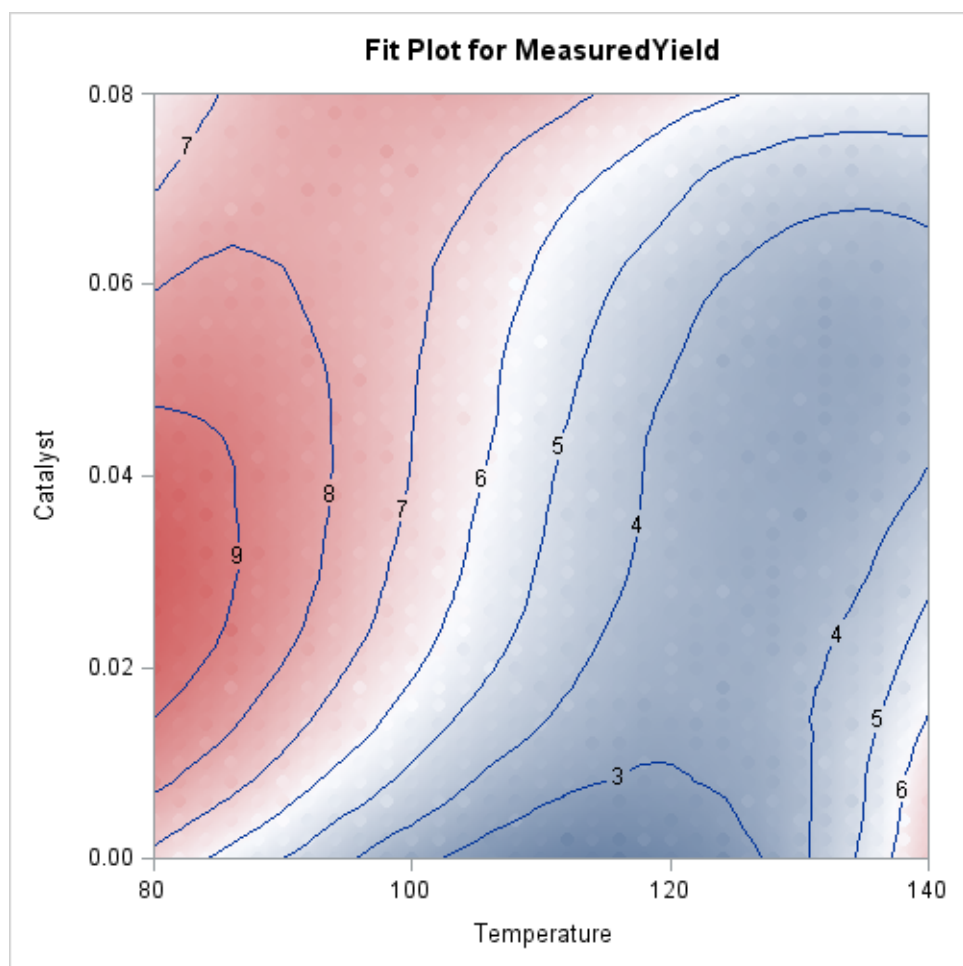
proc loess data=Experiment;
 model MeasuredYield = Temperature Catalyst / scale=sd(0.1);
run;
```

**Output 53.3.2** Scale Details for the Experiment Data

| The LOESS Procedure                             |             |          |
|-------------------------------------------------|-------------|----------|
| Independent Variable Scaling                    |             |          |
| Scaling applied: 10% trimmed standard deviation |             |          |
| Statistic                                       | Temperature | Catalyst |
| Minimum Value                                   | 80.00000    | 0        |
| Maximum Value                                   | 140.00000   | 0.08000  |
| Trimmed Mean                                    | 110.00000   | 0.04000  |
| Trimmed Standard Deviation                      | 14.32149    | 0.01894  |

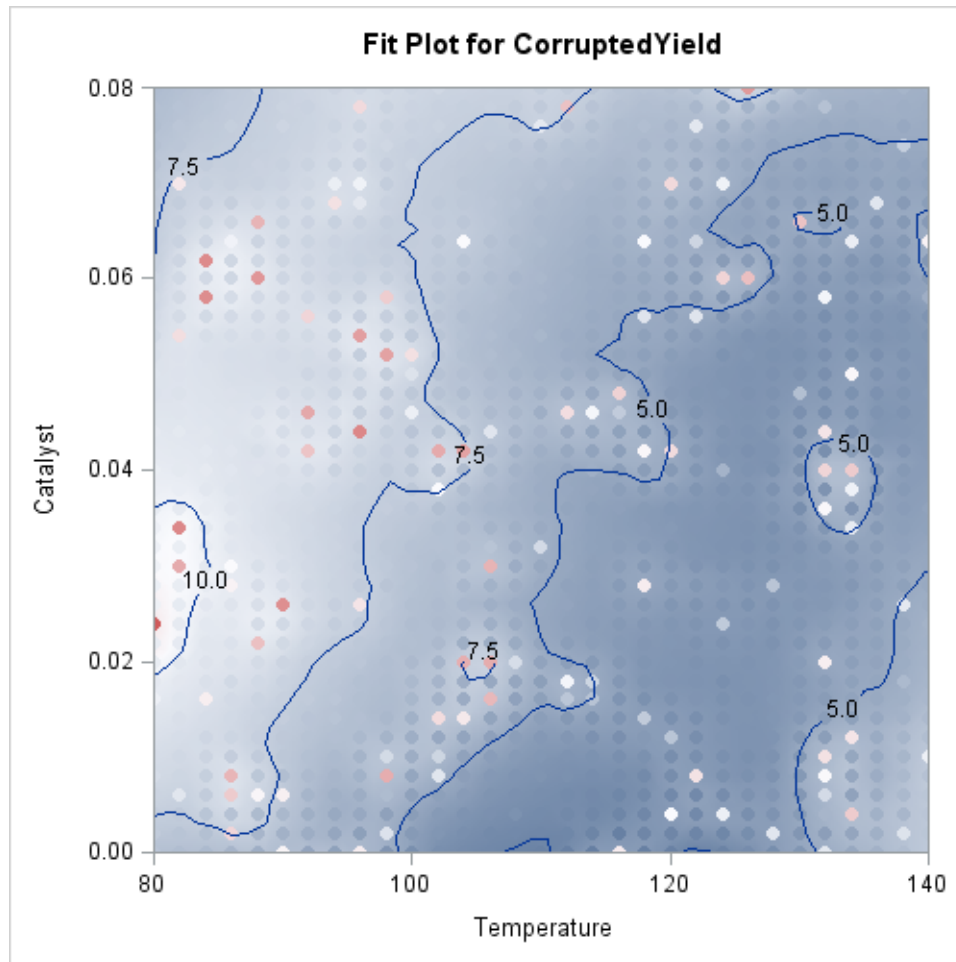
The `SCALE=SD(0.1)` option in the `MODEL` statement specifies that the independent variables in the model are to be divided by their respective 10% trimmed standard deviations before the fitted model is computed. This is appropriate because the independent variables `Temperature` and `Catalyst` are not similarly scaled. The “Scale Details” table in [Output 53.3.2](#) displays the details of ranges of the regressors and the scale factors applied to each regressor.

[Output 53.3.3](#) displays the loess fit. Because the fitted surface is a good fit of the observed data, the observations on this plot are not clearly distinguishable from the fitted surface. The results are dramatically different when the outliers are included. The following statements fit a loess model to the corrupted response, using the same smoothing parameter that was selected for the measured response.

**Output 53.3.3** Fit for MeasuredYield

```
proc loess data=Experiment;
 model CorruptedYield = Temperature Catalyst /
 scale=sd(0.1) smooth=0.018;
run;
```

Output 53.3.4 Fit for CorruptedYield

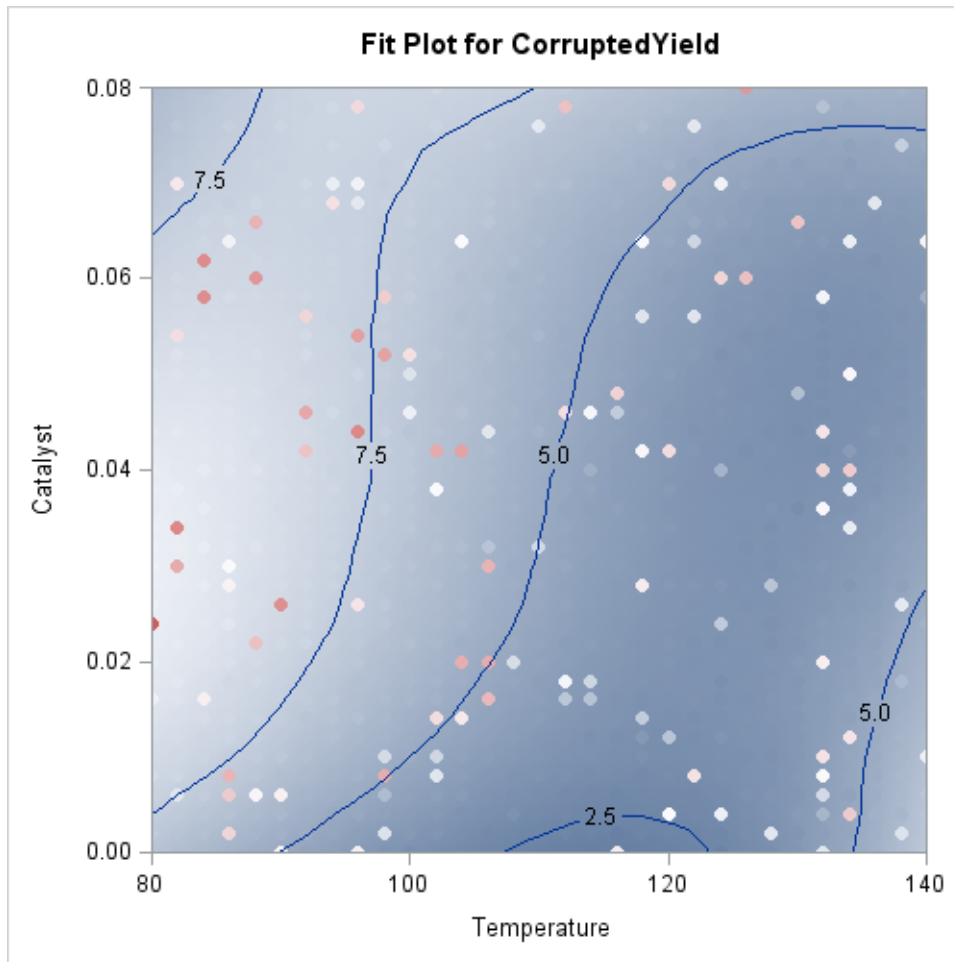


Output 53.3.4 displays the loess fit. The fit is pulled upward in the neighborhoods of these outliers. If you use a larger smoothing parameter value, then these local perturbations in the fit get smoothed out, but at the expense of smoothing away the information in the underlying measured response. In such cases a robust fitting method is indicated. The following statements show how you do this:

```
proc loess data=Experiment;
 model CorruptedYield = Temperature Catalyst /
 scale = sd(0.1)
 smooth = 0.018
 iterations=4;
run;
```

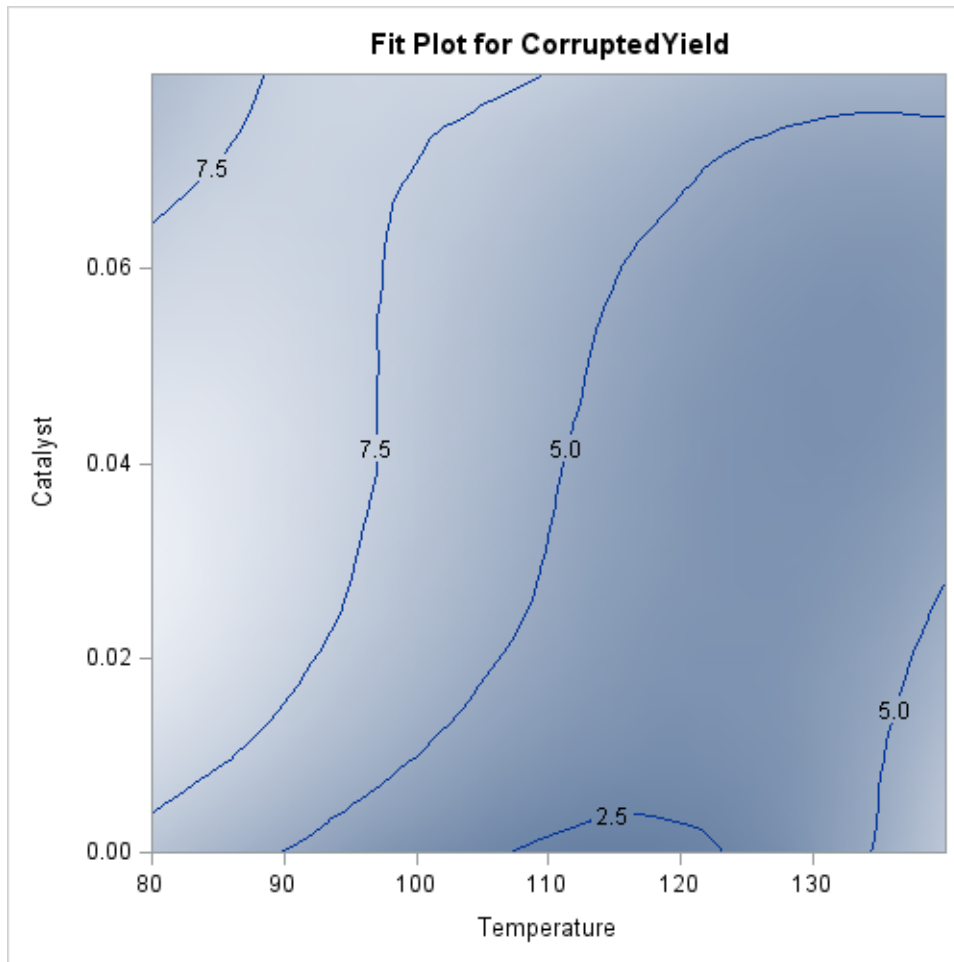
The ITERATIONS=4 option in the MODEL statement requests the initial loess fit followed by three iteratively reweighted iterations.



**Output 53.3.5** Robust Fit for CorruptedYield

You can see the impact of the robust fitting by comparing the robust fit shown in [Output 53.3.5](#) with the nonrobust fit in [Output 53.3.4](#). In the robust fit you see that the local perturbations caused by the outliers have been eliminated as these the outlying observations get down-weighted during the robustness iterations. By comparing the labeled contours on the fit plot for the uncorrupted response shown in [Output 53.3.3](#) with the labeled contours for the corrupted response shown in [Output 53.3.4](#), you can see that the robust fit has produced a reasonable fit for the underlying measured data. The color gradient in [Output 53.3.5](#) is chosen to accommodate the outliers that are present in the observed data, and so you cannot easily compare the color gradient in this plot with that in [Output 53.3.3](#). The following statements repeat the robust analysis with an option added to suppress the display of the observations on the fit plot:

```
proc loess data=Experiment plots=contourFit(obs=None);
 model CorruptedYield = Temperature Catalyst /
 scale = sd(0.1)
 smooth = 0.018
 iterations=4;
run;
ods graphics off;
```

**Output 53.3.6** Robust Fit for CorruptedYield with Observations Suppressed

Output 53.3.6 shows the robust fit with the observations suppressed. The range of the fitted surface values in this plot is similar to the range in Output 53.3.3. By comparing this contour plot with the contour plot in Output 53.3.3, you clearly see that the robust loess fit has successfully modeled the underlying surface despite the presence of the outliers.

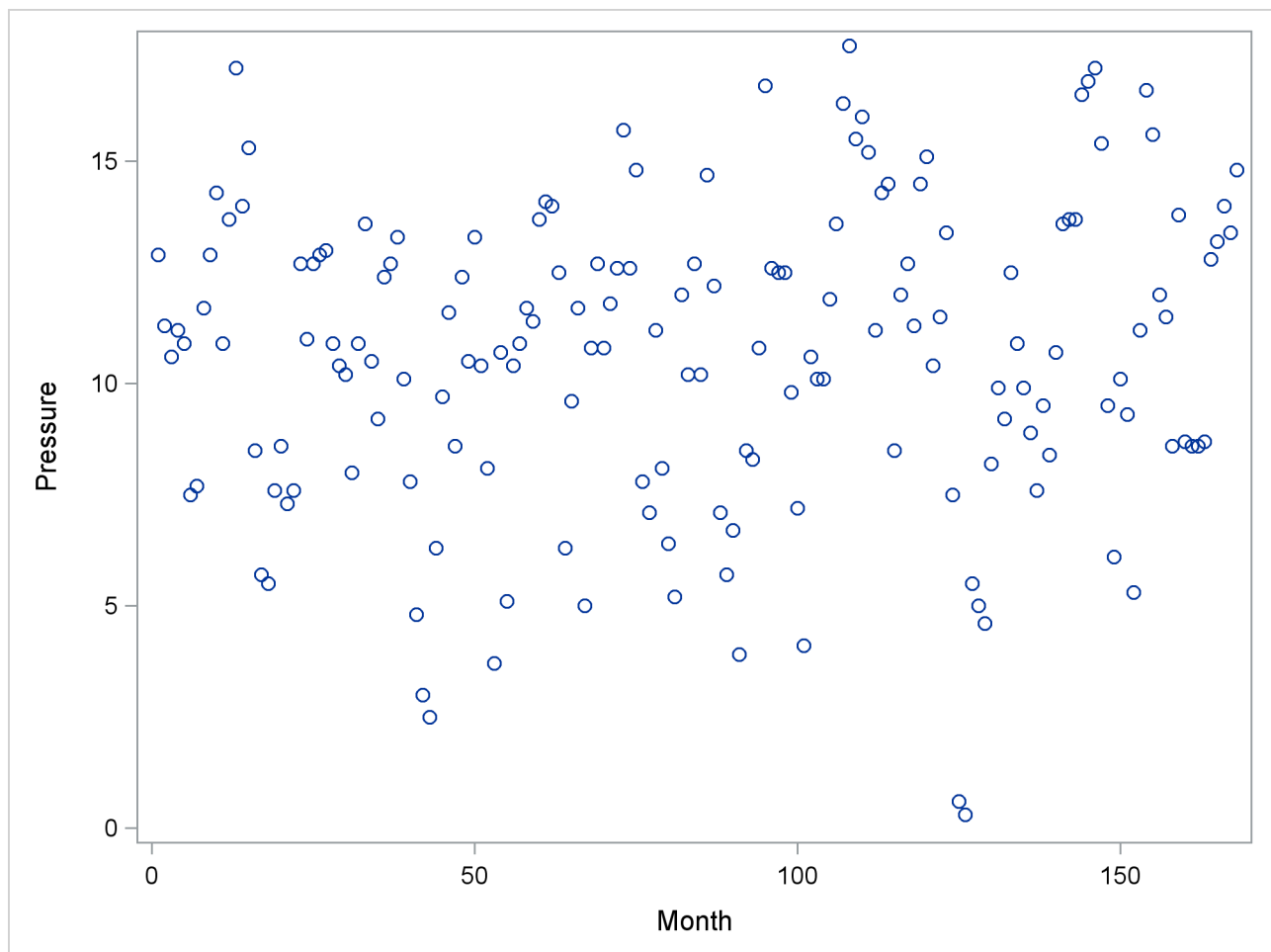
### Example 53.4: El Niño Southern Oscillation

The data set `sashelp. ENSO`, which is available in the `Sashelp` library, contains measurements of monthly averaged atmospheric pressure differences between Easter Island and Darwin, Australia, for a period of 168 months (National Institute of Standards and Technology 1998).

The following PROC SGPLOT statements produce the simple scatter plot of the ENSO data, displayed in Output 53.4.1.

```
proc sgplot data=sashelp. ENSO;
 scatter y=Pressure x=Month;
run;
```

Output 53.4.1 Scatter Plot of ENSO Data



You can compute a loess fit and obtain graphical results for these data by using the following statements:

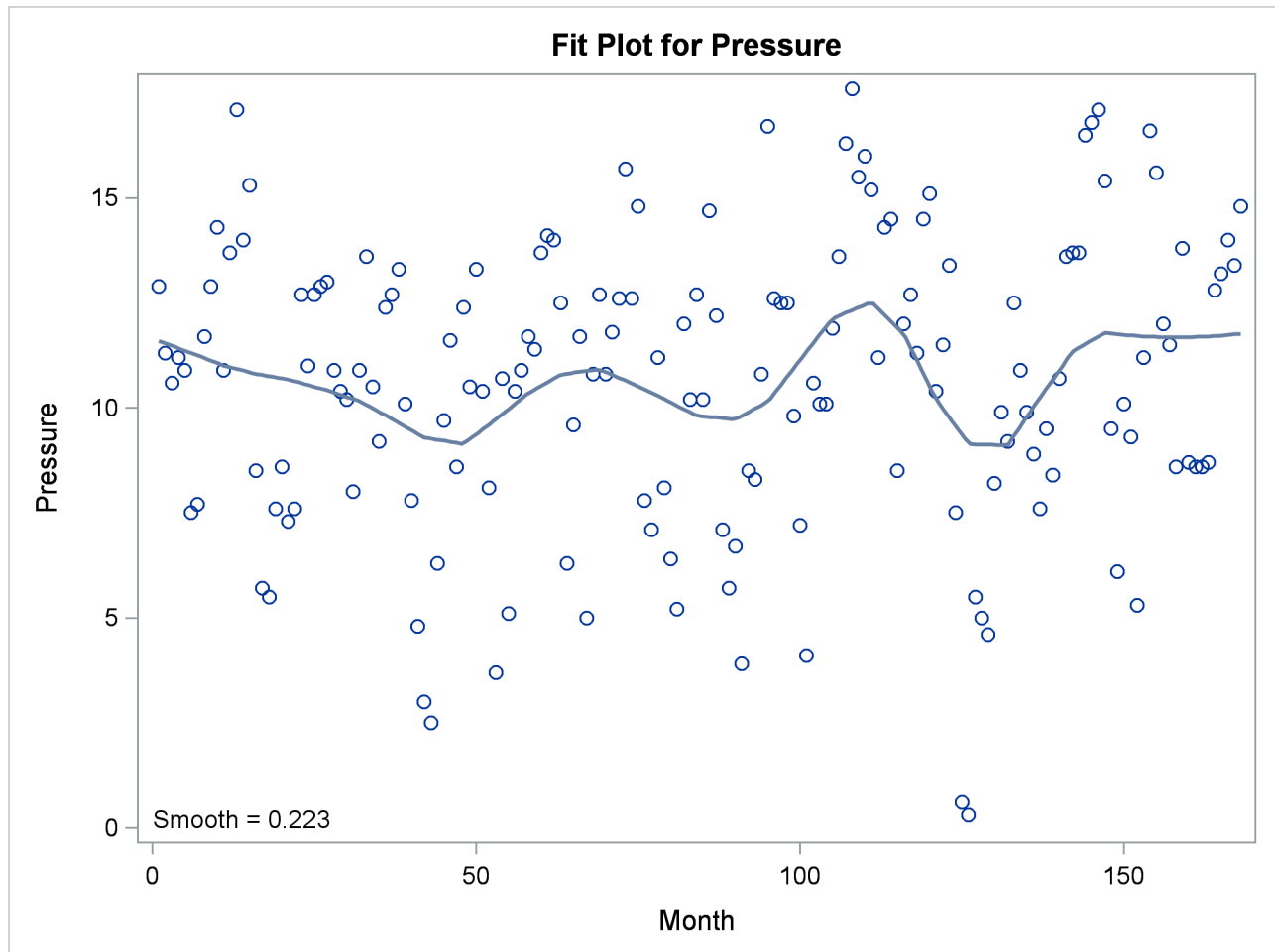
```
ods graphics on;

proc loess data=sashelp.ENS0 plots=residuals(smooth);
 model Pressure=Month;
run;
```

The “Smoothing Criterion” and “Fit Summary” tables are shown in [Output 53.4.2](#), and the fit plot is shown in [Output 53.4.3](#).

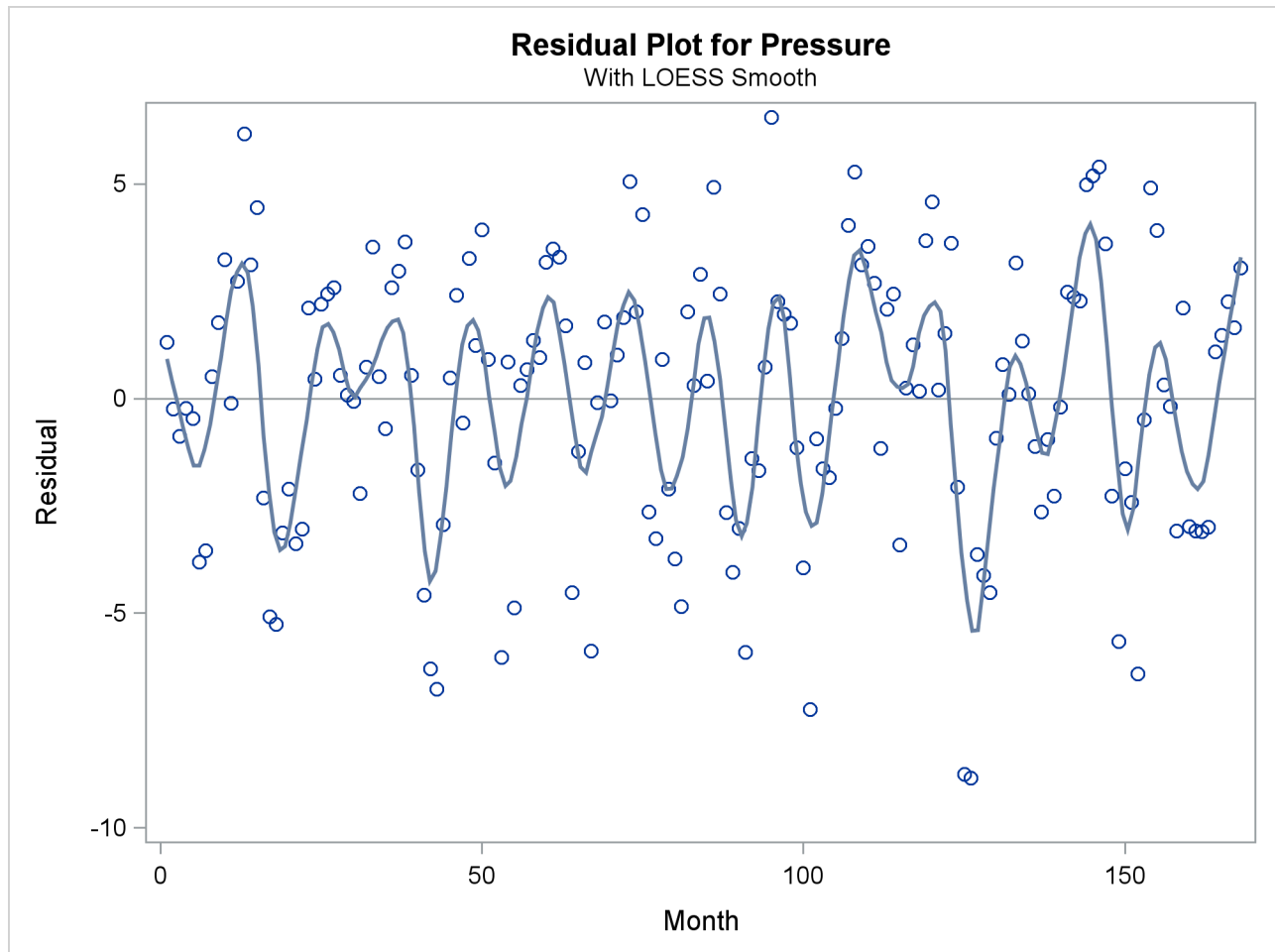
### Output 53.4.2 Output from PROC LOESS

|                                     |                        |
|-------------------------------------|------------------------|
| The LOESS Procedure                 |                        |
| Dependent Variable: Pressure        |                        |
| Optimal Smoothing<br>Criterion      |                        |
| AICC                                | Smoothing<br>Parameter |
| 3.41105                             | 0.22321                |
| The LOESS Procedure                 |                        |
| Selected Smoothing Parameter: 0.223 |                        |
| Dependent Variable: Pressure        |                        |
| Fit Summary                         |                        |
| Fit Method                          | kd Tree                |
| Blending                            | Linear                 |
| Number of Observations              | 168                    |
| Number of Fitting Points            | 33                     |
| kd Tree Bucket Size                 | 7                      |
| Degree of Local Polynomials         | 1                      |
| Smoothing Parameter                 | 0.22321                |
| Points in Local Neighborhood        | 37                     |
| Residual Sum of Squares             | 1654.27725             |
| Trace[L]                            | 8.74180                |
| GCV                                 | 0.06522                |
| AICC                                | 3.41105                |

**Output 53.4.3** Oversmoothed Loess Fit for the ENSO Data

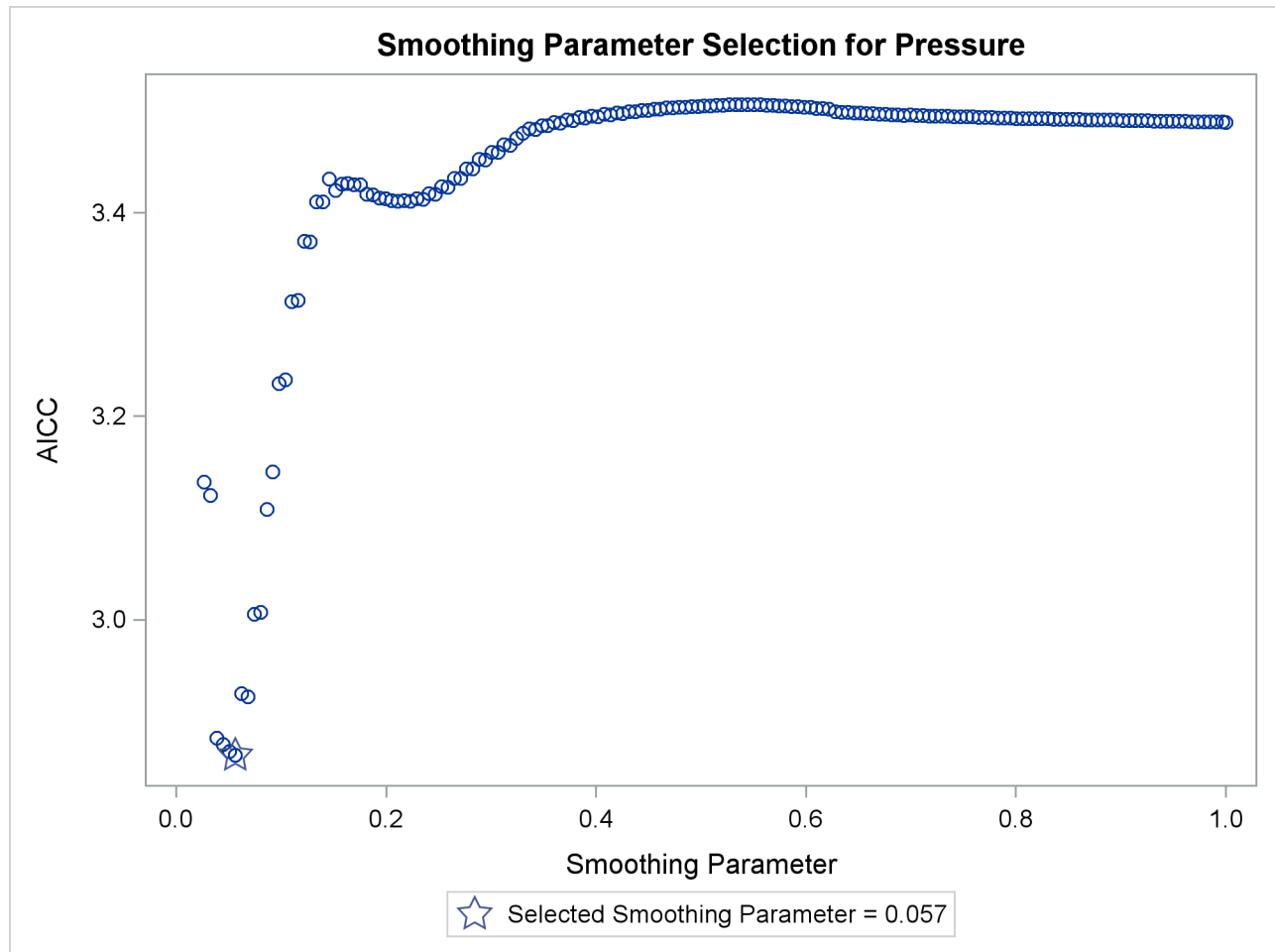
This weather-related data should exhibit an annual cycle. However, the loess fit in [Output 53.4.3](#) indicates a longer cycle but no annual cycle. This suggests that the loess fit is oversmoothed. One way to detect oversmoothing is to look for patterns in the fit residuals. With ODS Graphics enabled, PROC LOESS produces a scatter plot of the residuals versus each regressor in the model. To aid in visually detecting patterns in these scatter plots, it is useful to superimpose a nonparametric fit on these scatter plots. You can request this by specifying the SMOOTH suboption of the PLOTS=RESIDUALS option in the PROC LOESS statement. The nonparametric fit that is produced is again a loess fit that is produced independently of the loess fit used to obtain these residuals.

With the superimposed loess fit shown in [Output 53.4.4](#), you can clearly identify an annual cycle in the residuals, which confirms that the loess fit for the ENSO is oversmoothed. What accounts for this poor fit?

**Output 53.4.4** Residuals for the Loess Fit for the ENSO Data

The smoothing parameter value used for the loess fit shown in [Output 53.4.3](#) was chosen using the default method of PROC LOESS, namely a golden section minimization of the AICC criterion over the interval (0, 1]. One possibility is that the golden section search has found a local rather than a global minimum of the AICC criterion. You can test this by redoing the fit requesting a global minimum. You do this with the following statements:

```
proc loess data=sashelp.ENS0;
 model Pressure=Month/select=AICC(global);
run;
```

**Output 53.4.5** AICC versus Smoothing Parameter Showing Local Minima

The explanation for the oversmoothed fit in [Output 53.4.3](#) is now apparent. [Output 53.4.5](#) shows that the golden section search algorithm found the local minimum that occurs near the value 0.22 of the smoothing parameter rather than the global minimum that occurs near 0.06. Note that if you restrict the range of smoothing parameter values examined to lie below 0.2, then the golden section search finds the global minimum, as the following statements demonstrate:

```
proc loess data=sashelp.ENS0;
 model Pressure=Month/select=AICC(range(0.03,0.2));
run;
```

**Output 53.4.6** Selected Smoothing Parameter Value

| The LOESS Procedure          |                     |
|------------------------------|---------------------|
| Dependent Variable: Pressure |                     |
| Optimal Smoothing Criterion  |                     |
| AICC                         | Smoothing Parameter |
| 2.86660                      | 0.05655             |

Output 53.4.6 shows that with the restricted range of smoothing parameter values examined, PROC LOESS finds the global minimum of the AICC criterion. Often you might not know an appropriate range of smoothing parameter values to examine. In such cases, you can use the PRESEARCH suboption of the SELECT= option in the MODEL statement. When you specify this option, PROC LOESS does a preliminary search to try to locate a smoothing parameter value range that contains just the first local minimum of the criterion being used for the selection. The following statements provide an example.

```
proc loess data=sashelp. ENSO plots=residuals(smooth);
 model Pressure=Month/select=AICC(presearch);
run;

ods graphics off;
```

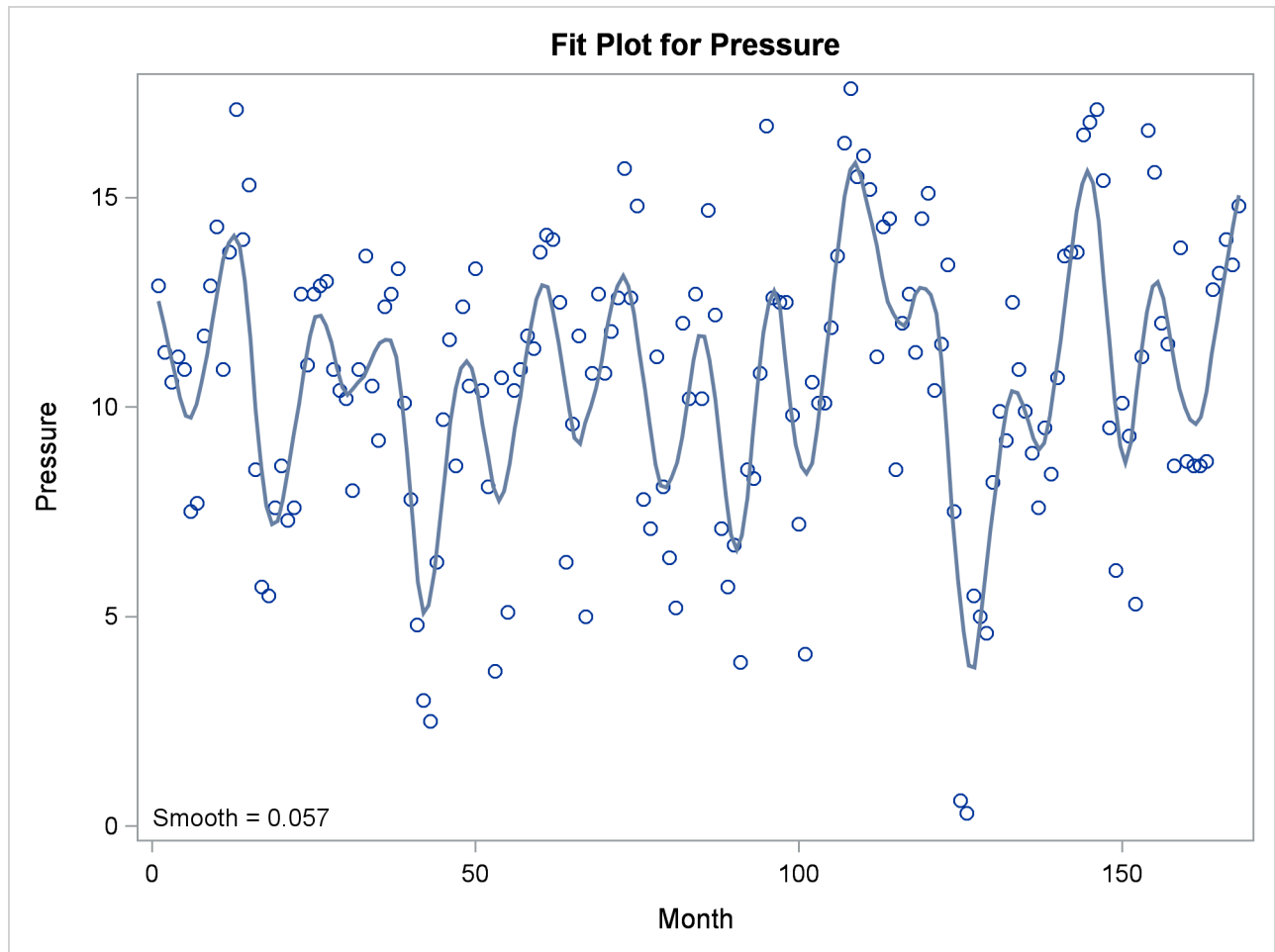
**Output 53.4.7** Selected Smoothing Parameter Value When Presearch Is Specified

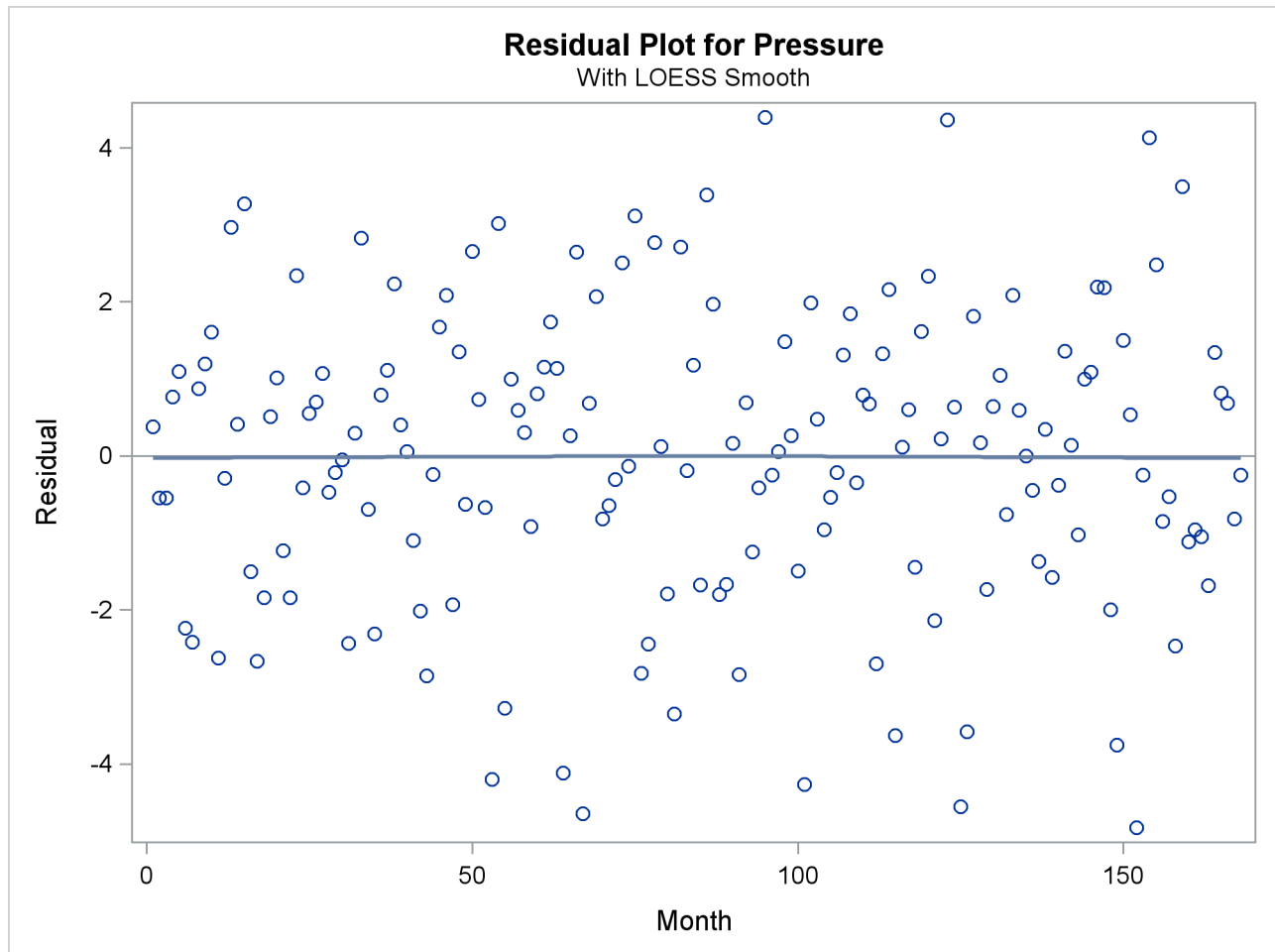
| The LOESS Procedure          |                     |
|------------------------------|---------------------|
| Dependent Variable: Pressure |                     |
| Optimal Smoothing Criterion  |                     |
| AICC                         | Smoothing Parameter |
| 2.86660                      | 0.05655             |

Output 53.4.7 shows that with the PRESEARCH suboption specified, PROC LOESS selects the smoothing parameter value that yields the global minimum of the AICC criterion. The fit obtained is shown in Output 53.4.8, and a plot of the residuals with a superimposed loess fit is shown in Output 53.4.9.



**Output 53.4.8** Loess Fit Showing an Annual Cycle



**Output 53.4.9** Residuals of the Selected Model

In contrast to the residual plot shown in [Output 53.4.4](#), the residuals plotted in [Output 53.4.9](#) do not exhibit any pattern, indicating that the corresponding loess fit has captured all the systematic variation in the data.

An interesting question is whether there is some phenomenon captured in the data that would explain the presence of the local minimum near 0.22 in the AICC curve. Note that there is some evidence of a cycle of about 42 months in the oversmoothed fit in [Output 53.4.3](#). You can see this cycle because the strong annual cycle in [Output 53.4.8](#) has been smoothed out. The physical phenomenon that accounts for the existence of this cycle has been identified as the periodic warming of the Pacific Ocean known as “El Niño.”

---

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# Chapter 54

## The LOGISTIC Procedure

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## Overview: LOGISTIC Procedure

Binary responses (for example, success and failure), ordinal responses (for example, normal, mild, and severe), and nominal responses (for example, major TV networks viewed at a certain hour) arise in many fields of study. Logistic regression analysis is often used to investigate the relationship between these discrete responses and a set of explanatory variables. Texts that discuss logistic regression include Agresti (2002); Allison (1999); Collett (2003); Cox and Snell (1989); Hosmer and Lemeshow (2000); Stokes, Davis, and Koch (2012).

For binary response models, the response,  $Y$ , of an individual or an experimental unit can take on one of two possible values, denoted for convenience by 1 and 2 (for example,  $Y = 1$  if a disease is present, otherwise  $Y = 2$ ). Suppose  $\mathbf{x}$  is a vector of explanatory variables and  $\pi = \Pr(Y = 1 \mid \mathbf{x})$  is the response probability to be modeled. The linear logistic model has the form

$$\text{logit}(\pi) \equiv \log\left(\frac{\pi}{1 - \pi}\right) = \alpha + \boldsymbol{\beta}'\mathbf{x}$$

where  $\alpha$  is the intercept parameter and  $\boldsymbol{\beta} = (\beta_1, \dots, \beta_s)'$  is the vector of  $s$  slope parameters. Notice that the LOGISTIC procedure, by default, models the probability of the *lower* response levels.

The logistic model shares a common feature with a more general class of linear models: a function  $g = g(\mu)$  of the mean of the response variable is assumed to be linearly related to the explanatory variables. Since the mean  $\mu$  implicitly depends on the stochastic behavior of the response, and the explanatory variables are assumed to be fixed, the function  $g$  provides the link between the random (stochastic) component and the systematic (deterministic) component of the response variable  $Y$ . For this reason, Nelder and Wedderburn (1972) refer to  $g(\mu)$  as a link function. One advantage of the logit function over other link functions is that differences on the logistic scale are interpretable regardless of whether the data are sampled prospectively or retrospectively (McCullagh and Nelder 1989, Chapter 4). Other link functions that are widely used in practice are the probit function and the complementary log-log function. The LOGISTIC procedure enables you to choose one of these link functions, resulting in fitting a broader class of binary response models of the form

$$g(\pi) = \alpha + \boldsymbol{\beta}'\mathbf{x}$$

For ordinal response models, the response,  $Y$ , of an individual or an experimental unit might be restricted to one of a (usually small) number of ordinal values, denoted for convenience by  $1, \dots, k, k + 1$ . For example, the severity of coronary disease can be classified into three response categories as 1=no disease, 2=angina pectoris, and 3=myocardial infarction. The LOGISTIC procedure fits a common slopes cumulative model, which is a parallel lines regression model based on the cumulative probabilities of the response categories rather than on their individual probabilities. The cumulative model has the form

$$g(\Pr(Y \leq i \mid \mathbf{x})) = \alpha_i + \boldsymbol{\beta}'\mathbf{x}, \quad i = 1, \dots, k$$

where  $\alpha_1, \dots, \alpha_k$  are  $k$  intercept parameters, and  $\boldsymbol{\beta}$  is the vector of slope parameters. This model has been considered by many researchers. Aitchison and Silvey (1957) and Ashford (1959) employ a probit scale and provide a maximum likelihood analysis; Walker and Duncan (1967) and Cox and Snell (1989) discuss the use of the log odds scale. For the log odds scale, the cumulative logit model is often referred to as the *proportional odds* model.

For nominal response logistic models, where the  $k + 1$  possible responses have no natural ordering, the logit model can also be extended to a *multinomial* model known as a *generalized* or *baseline-category* logit model, which has the form

$$\log \left( \frac{\Pr(Y = i | \mathbf{x})}{\Pr(Y = k + 1 | \mathbf{x})} \right) = \alpha_i + \boldsymbol{\beta}'_i \mathbf{x}, \quad i = 1, \dots, k$$

where the  $\alpha_1, \dots, \alpha_k$  are  $k$  intercept parameters, and the  $\boldsymbol{\beta}_1, \dots, \boldsymbol{\beta}_k$  are  $k$  vectors of slope parameters. These models are a special case of the *discrete choice* or *conditional logit* models introduced by McFadden (1974).

The LOGISTIC procedure fits linear logistic regression models for discrete response data by the method of maximum likelihood. It can also perform conditional logistic regression for binary response data and exact logistic regression for binary and nominal response data. The maximum likelihood estimation is carried out with either the Fisher scoring algorithm or the Newton-Raphson algorithm, and you can perform the bias-reducing penalized likelihood optimization as discussed by Firth (1993) and Heinze and Schemper (2002). You can specify starting values for the parameter estimates. The logit link function in the logistic regression models can be replaced by the probit function, the complementary log-log function, or the generalized logit function.

Any term specified in the model is referred to as an *effect*. The LOGISTIC procedure enables you to specify categorical variables (also known as *classification* or *CLASS variables*) and continuous variables as explanatory effects. You can also specify more complex model terms such as interactions and nested terms in the same way as in the GLM procedure. You can create complex *constructed effects* with the EFFECT statement. An effect in the model that is not an interaction or a nested term or a constructed effect is referred to as a *main effect*.

The LOGISTIC procedure allows either a full-rank parameterization or a less-than-full-rank parameterization of the CLASS variables. The full-rank parameterization offers eight coding methods: effect, reference, ordinal, polynomial, and orthogonalizations of these. The effect coding is the same method that is used in the CATMOD procedure. The less-than-full-rank parameterization, often called *dummy coding*, is the same coding as that used in the GLM procedure.

The LOGISTIC procedure provides four effect selection methods: forward selection, backward elimination, stepwise selection, and best subset selection. The best subset selection is based on the likelihood score statistic. This method identifies a specified number of best models containing one, two, three effects, and so on, up to a single model containing effects for all the explanatory variables.

The LOGISTIC procedure has some additional options to control how to move effects in and out of a model with the forward selection, backward elimination, or stepwise selection model-building strategies. When there are no interaction terms, a main effect can enter or leave a model in a single step based on the  $p$ -value of the score or Wald statistic. When there are interaction terms, the selection process also depends on whether you want to preserve model hierarchy. These additional options enable you to specify whether model hierarchy is to be preserved, how model hierarchy is applied, and whether a single effect or multiple effects can be moved in a single step.

Odds ratio estimates are displayed along with parameter estimates. You can also specify the change in the continuous explanatory main effects for which odds ratio estimates are desired. Confidence intervals for the regression parameters and odds ratios can be computed based either on the profile-likelihood function or on the asymptotic normality of the parameter estimators. You can also produce odds ratios for effects that are involved in interactions or nestings, and for any type of parameterization of the CLASS variables.

Various methods to correct for overdispersion are provided, including Williams' method for grouped binary response data. The adequacy of the fitted model can be evaluated by various goodness-of-fit tests, including the Hosmer-Lemeshow test for binary response data.

Like many procedures in SAS/STAT software that enable the specification of CLASS variables, the LOGISTIC procedure provides a **CONTRAST** statement for specifying customized hypothesis tests concerning the model parameters. The **CONTRAST** statement also provides estimation of individual rows of contrasts, which is particularly useful for obtaining odds ratio estimates for various levels of the CLASS variables. The LOGISTIC procedure also provides testing capability through the **ESTIMATE** and **TEST** statements. Analyses of LS-means are enabled with the **LSMEANS**, **LSMESTIMATE**, and **SLICE** statements.

You can perform a conditional logistic regression on binary response data by specifying the **STRATA** statement. This enables you to perform matched-set and case-control analyses. The number of events and nonevents can vary across the strata. Many of the features available with the unconditional analysis are also available with a conditional analysis.

The LOGISTIC procedure enables you to perform exact logistic regression, also known as exact conditional logistic regression, by specifying one or more **EXACT** statements. You can test individual parameters or conduct a joint test for several parameters. The procedure computes two exact tests: the exact conditional score test and the exact conditional probability test. You can request exact estimation of specific parameters and corresponding odds ratios where appropriate. Point estimates, standard errors, and confidence intervals are provided. You can perform stratified exact logistic regression by specifying the **STRATA** statement.

Further features of the LOGISTIC procedure enable you to do the following:

- control the ordering of the response categories
- compute a generalized R Square measure for the fitted model
- reclassify binary response observations according to their predicted response probabilities
- test linear hypotheses about the regression parameters
- create a data set for producing a receiver operating characteristic curve for each fitted model
- specify contrasts to compare several receiver operating characteristic curves
- create a data set containing the estimated response probabilities, residuals, and influence diagnostics
- score a data set by using a previously fitted model

The LOGISTIC procedure uses ODS Graphics to create graphs as part of its output. For general information about ODS Graphics, see Chapter 21, “[Statistical Graphics Using ODS](#).” For more information about the plots implemented in PROC LOGISTIC, see the section “[ODS Graphics](#)” on page 4294.

The remaining sections of this chapter describe how to use PROC LOGISTIC and discuss the underlying statistical methodology. The section “[Getting Started: LOGISTIC Procedure](#)” on page 4166 introduces PROC LOGISTIC with an example for binary response data. The section “[Syntax: LOGISTIC Procedure](#)” on page 4174 describes the syntax of the procedure. The section “[Details: LOGISTIC Procedure](#)” on page 4237 summarizes the statistical technique employed by PROC LOGISTIC. The section “[Examples: LOGISTIC Procedure](#)” on page 4295 illustrates the use of the LOGISTIC procedure.

For more examples and discussion on the use of PROC LOGISTIC, see Stokes, Davis, and Koch (2012); Allison (1999); SAS Institute Inc. (1995).



## Getting Started: LOGISTIC Procedure

The LOGISTIC procedure is similar in use to the other regression procedures in the SAS System. To demonstrate the similarity, suppose the response variable  $y$  is binary or ordinal, and  $x_1$  and  $x_2$  are two explanatory variables of interest. To fit a logistic regression model, you can specify a MODEL statement similar to that used in the REG procedure. For example:

```
proc logistic;
 model y=x1 x2;
run;
```

The response variable  $y$  can be either character or numeric. PROC LOGISTIC enumerates the total number of response categories and orders the response levels according to the response variable option ORDER= in the MODEL statement.

You can also input binary response data that are grouped. In the following statements,  $n$  represents the number of trials and  $r$  represents the number of events:

```
proc logistic;
 model r/n=x1 x2;
run;
```

The following example illustrates the use of PROC LOGISTIC. The data, taken from Cox and Snell (1989, pp. 10–11), consist of the number,  $r$ , of ingots not ready for rolling, out of  $n$  tested, for a number of combinations of heating time and soaking time.

```
data ingots;
 input Heat Soak r n @@;
 datalines;
7 1.0 0 10 14 1.0 0 31 27 1.0 1 56 51 1.0 3 13
7 1.7 0 17 14 1.7 0 43 27 1.7 4 44 51 1.7 0 1
7 2.2 0 7 14 2.2 2 33 27 2.2 0 21 51 2.2 0 1
7 2.8 0 12 14 2.8 0 31 27 2.8 1 22 51 4.0 0 1
7 4.0 0 9 14 4.0 0 19 27 4.0 1 16
;
```

The following invocation of PROC LOGISTIC fits the binary logit model to the grouped data. The continuous covariates Heat and Soak are specified as predictors, and the bar notation (“|”) includes their interaction, Heat\*Soak. The ODDSRATIO statement produces odds ratios in the presence of interactions, and a graphical display of the requested odds ratios is produced when ODS Graphics is enabled.

```
ods graphics on;
proc logistic data=ingots;
 model r/n = Heat | Soak;
 oddsratio Heat / at (Soak=1 2 3 4);
run;
ods graphics off;
```

The results of this analysis are shown in the following figures. PROC LOGISTIC first lists background information in Figure 54.1 about the fitting of the model. Included are the name of the input data set, the response variable(s) used, the number of observations used, and the link function used.

**Figure 54.1** Binary Logit Model

| The LOGISTIC Procedure      |                  |
|-----------------------------|------------------|
| Model Information           |                  |
| Data Set                    | WORK.INGOTS      |
| Response Variable (Events)  | r                |
| Response Variable (Trials)  | n                |
| Model                       | binary logit     |
| Optimization Technique      | Fisher's scoring |
|                             |                  |
| Number of Observations Read | 19               |
| Number of Observations Used | 19               |
| Sum of Frequencies Read     | 387              |
| Sum of Frequencies Used     | 387              |

The “Response Profile” table (Figure 54.2) lists the response categories (which are Event and Nonevent when grouped data are input), their ordered values, and their total frequencies for the given data.

**Figure 54.2** Response Profile with Events/Trials Syntax

| Response Profile                              |                |                 |
|-----------------------------------------------|----------------|-----------------|
| Ordered Value                                 | Binary Outcome | Total Frequency |
| 1                                             | Event          | 12              |
| 2                                             | Nonevent       | 375             |
|                                               |                |                 |
| Model Convergence Status                      |                |                 |
| Convergence criterion (GCONV=1E-8) satisfied. |                |                 |

The “Model Fit Statistics” table (Figure 54.3) contains Akaike’s information criterion (AIC), the Schwarz criterion (SC), and the negative of twice the log likelihood ( $-2 \text{ Log L}$ ) for the intercept-only model and the fitted model. AIC and SC can be used to compare different models, and the ones with smaller values are preferred. Results of the likelihood ratio test and the efficient score test for testing the joint significance of the explanatory variables (Soak, Heat, and their interaction) are included in the “Testing Global Null Hypothesis: BETA=0” table (Figure 54.3); the small  $p$ -values reject the hypothesis that all slope parameters are equal to zero.

**Figure 54.3** Fit Statistics and Hypothesis Tests

| Model Fit Statistics |           |                          |                     |
|----------------------|-----------|--------------------------|---------------------|
| Criterion            | Intercept | Intercept and Covariates |                     |
|                      | Only      | Log Likelihood           | Full Log Likelihood |
| AIC                  | 108.988   | 103.222                  | 35.957              |
| SC                   | 112.947   | 119.056                  | 51.791              |
| -2 Log L             | 106.988   | 95.222                   | 27.957              |

| Testing Global Null Hypothesis: BETA=0 |            |    |            |
|----------------------------------------|------------|----|------------|
| Test                                   | Chi-Square | DF | Pr > ChiSq |
| Likelihood Ratio                       | 11.7663    | 3  | 0.0082     |
| Score                                  | 16.5417    | 3  | 0.0009     |
| Wald                                   | 13.4588    | 3  | 0.0037     |

The “Analysis of Maximum Likelihood Estimates” table in [Figure 54.4](#) lists the parameter estimates, their standard errors, and the results of the Wald test for individual parameters. Note that the Heat\*Soak parameter is not significantly different from zero ( $p=0.727$ ), nor is the Soak variable ( $p=0.6916$ ).

**Figure 54.4** Parameter Estimates

| Analysis of Maximum Likelihood Estimates |    |          |                |                 |            |
|------------------------------------------|----|----------|----------------|-----------------|------------|
| Parameter                                | DF | Estimate | Standard Error | Wald Chi-Square | Pr > ChiSq |
| Intercept                                | 1  | -5.9901  | 1.6666         | 12.9182         | 0.0003     |
| Heat                                     | 1  | 0.0963   | 0.0471         | 4.1895          | 0.0407     |
| Soak                                     | 1  | 0.2996   | 0.7551         | 0.1574          | 0.6916     |
| Heat*Soak                                | 1  | -0.00884 | 0.0253         | 0.1219          | 0.7270     |

The “Association of Predicted Probabilities and Observed Responses” table ([Figure 54.5](#)) contains four measures of association for assessing the predictive ability of a model. They are based on the number of pairs of observations with different response values, the number of concordant pairs, and the number of discordant pairs, which are also displayed. Formulas for these statistics are given in the section “Rank Correlation of Observed Responses and Predicted Probabilities” on page 4253.

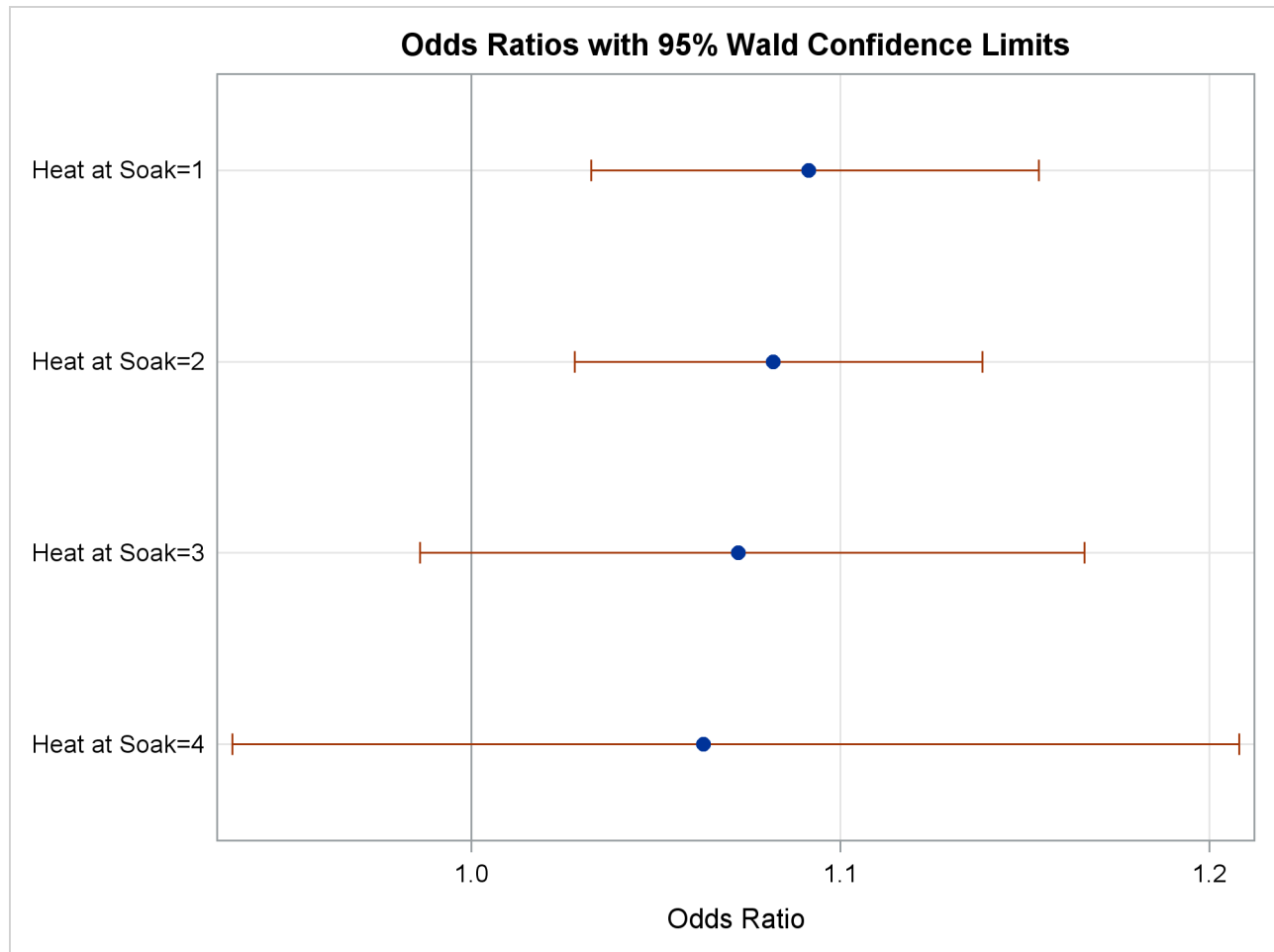
**Figure 54.5** Association Table

| Association of Predicted Probabilities and Observed Responses |      |           |       |
|---------------------------------------------------------------|------|-----------|-------|
| Percent Concordant                                            | 70.9 | Somers' D | 0.537 |
| Percent Discordant                                            | 17.3 | Gamma     | 0.608 |
| Percent Tied                                                  | 11.8 | Tau-a     | 0.032 |
| Pairs                                                         | 4500 | c         | 0.768 |

The **ODDSRATIO** statement produces the “Odds Ratio Estimates and Wald Confidence Intervals” table (Figure 54.6), and a graphical display of these estimates is shown in Figure 54.7. The differences between the odds ratios are small compared to the variability shown by their confidence intervals, which confirms the previous conclusion that the Heat\*Soak parameter is not significantly different from zero.

**Figure 54.6** Odds Ratios of Heat at Several Values of Soak

| Odds Ratio Estimates and Wald Confidence Intervals |          |                       |       |
|----------------------------------------------------|----------|-----------------------|-------|
| Label                                              | Estimate | 95% Confidence Limits |       |
| Heat at Soak=1                                     | 1.091    | 1.032                 | 1.154 |
| Heat at Soak=2                                     | 1.082    | 1.028                 | 1.139 |
| Heat at Soak=3                                     | 1.072    | 0.986                 | 1.166 |
| Heat at Soak=4                                     | 1.063    | 0.935                 | 1.208 |

**Figure 54.7** Plot of Odds Ratios of Heat at Several Values of Soak

Since the Heat\*Soak interaction is nonsignificant, the following statements fit a main-effects model:

```
proc logistic data=ingots;
 model r/n = Heat Soak;
run;
```

The results of this analysis are shown in the following figures. The model information and response profiles are the same as those in Figure 54.1 and Figure 54.2 for the saturated model. The “Model Fit Statistics” table in Figure 54.8 shows that the AIC and SC for the main-effects model are smaller than for the saturated model, indicating that the main-effects model might be the preferred model. As in the preceding model, the “Testing Global Null Hypothesis: BETA=0” table indicates that the parameters are significantly different from zero.

**Figure 54.8** Fit Statistics and Hypothesis Tests

| The LOGISTIC Procedure |           |                          |                     |
|------------------------|-----------|--------------------------|---------------------|
| Model Fit Statistics   |           |                          |                     |
| Criterion              | Intercept | Intercept and Covariates |                     |
|                        | Only      | Log Likelihood           | Full Log Likelihood |
| AIC                    | 108.988   | 101.346                  | 34.080              |
| SC                     | 112.947   | 113.221                  | 45.956              |
| -2 Log L               | 106.988   | 95.346                   | 28.080              |

| Testing Global Null Hypothesis: BETA=0 |            |    |            |
|----------------------------------------|------------|----|------------|
| Test                                   | Chi-Square | DF | Pr > ChiSq |
| Likelihood Ratio                       | 11.6428    | 2  | 0.0030     |
| Score                                  | 15.1091    | 2  | 0.0005     |
| Wald                                   | 13.0315    | 2  | 0.0015     |

The “Analysis of Maximum Likelihood Estimates” table in [Figure 54.9](#) again shows that the Soak parameter is not significantly different from zero ( $p=0.8639$ ). The odds ratio for each effect parameter, estimated by exponentiating the corresponding parameter estimate, is shown in the “Odds Ratios Estimates” table ([Figure 54.9](#)), along with 95% Wald confidence intervals. The confidence interval for the Soak parameter contains the value 1, which also indicates that this effect is not significant.

**Figure 54.9** Parameter Estimates and Odds Ratios

| Analysis of Maximum Likelihood Estimates |    |          |                |                 |            |
|------------------------------------------|----|----------|----------------|-----------------|------------|
| Parameter                                | DF | Estimate | Standard Error | Wald Chi-Square | Pr > ChiSq |
| Intercept                                | 1  | -5.5592  | 1.1197         | 24.6503         | <.0001     |
| Heat                                     | 1  | 0.0820   | 0.0237         | 11.9454         | 0.0005     |
| Soak                                     | 1  | 0.0568   | 0.3312         | 0.0294          | 0.8639     |

| Odds Ratio Estimates |                |                            |       |
|----------------------|----------------|----------------------------|-------|
| Effect               | Point Estimate | 95% Wald Confidence Limits |       |
| Heat                 | 1.085          | 1.036                      | 1.137 |
| Soak                 | 1.058          | 0.553                      | 2.026 |

Figure 54.9 continued

| Association of Predicted Probabilities and Observed Responses |      |           |       |
|---------------------------------------------------------------|------|-----------|-------|
| Percent Concordant                                            | 64.4 | Somers' D | 0.460 |
| Percent Discordant                                            | 18.4 | Gamma     | 0.555 |
| Percent Tied                                                  | 17.2 | Tau-a     | 0.028 |
| Pairs                                                         | 4500 | c         | 0.730 |

Using these parameter estimates, you can calculate the estimated logit of  $\pi$  as

$$-5.5592 + 0.082 \times \text{Heat} + 0.0568 \times \text{Soak}$$

For example, if Heat=7 and Soak=1, then  $\text{logit}(\hat{\pi}) = -4.9284$ . Using this logit estimate, you can calculate  $\hat{\pi}$  as follows:

$$\hat{\pi} = 1/(1 + e^{4.9284}) = 0.0072$$

This gives the predicted probability of the event (ingot not ready for rolling) for Heat=7 and Soak=1. Note that PROC LOGISTIC can calculate these statistics for you; use the **OUTPUT** statement with the **PREDICTED=** option, or use the **SCORE** statement.

To illustrate the use of an alternative form of input data, the following program creates the ingots data set with the new variables NotReady and Freq instead of n and r. The variable NotReady represents the response of individual units; it has a value of 1 for units not ready for rolling (event) and a value of 0 for units ready for rolling (nonevent). The variable Freq represents the frequency of occurrence of each combination of Heat, Soak, and NotReady. Note that, compared to the previous data set, NotReady=1 implies Freq=r, and NotReady=0 implies Freq=n-r.

```
data ingots;
 input Heat Soak NotReady Freq @@;
 datalines;
7 1.0 0 10 14 1.0 0 31 14 4.0 0 19 27 2.2 0 21 51 1.0 1 3
7 1.7 0 17 14 1.7 0 43 27 1.0 1 1 27 2.8 1 1 51 1.0 0 10
7 2.2 0 7 14 2.2 1 2 27 1.0 0 55 27 2.8 0 21 51 1.7 0 1
7 2.8 0 12 14 2.2 0 31 27 1.7 1 4 27 4.0 1 1 51 2.2 0 1
7 4.0 0 9 14 2.8 0 31 27 1.7 0 40 27 4.0 0 15 51 4.0 0 1
;
```

The following statements invoke PROC LOGISTIC to fit the main-effects model by using the alternative form of the input data set:

```
proc logistic data=ingots;
 model NotReady(event='1') = Heat Soak;
 freq Freq;
run;
```

Results of this analysis are the same as the preceding single-trial main-effects analysis. The displayed output for the two runs are identical except for the background information of the model fit and the “Response Profile” table shown in Figure 54.10.

**Figure 54.10** Response Profile with Single-Trial Syntax

| The LOGISTIC Procedure |          |                 |
|------------------------|----------|-----------------|
| Response Profile       |          |                 |
| Ordered Value          | NotReady | Total Frequency |
| 1                      | 0        | 375             |
| 2                      | 1        | 12              |

Probability modeled is NotReady=1.

By default, Ordered Values are assigned to the sorted response values in ascending order, and PROC LOGISTIC models the probability of the response level that corresponds to the Ordered Value 1. There are several methods to change these defaults; the preceding statements specify the response variable option `EVENT=` to model the probability of `NotReady=1` as displayed in Figure 54.10. See the section “Response Level Ordering” on page 4237 for more details.



## Syntax: LOGISTIC Procedure

The following statements are available in the LOGISTIC procedure:

```

PROC LOGISTIC < options > ;
 BY variables ;
 CLASS variable < (options) > < variable < (options) > ... > < / options > ;
 CODE < options > ;
 CONTRAST 'label' effect values< , effect values, ... > < / options > ;
 EFFECT name=effect-type(variables < / options >) ;
 EFFECTPLOT < plot-type < (plot-definition-options) > > < / options > ;
 ESTIMATE < 'label' > estimate-specification < / options > ;
 EXACT < 'label' > < INTERCEPT > < effects > < / options > ;
 EXACTOPTIONS options ;
 FREQ variable ;
 ID variables ;
 LSMEANS < model-effects > < / options > ;
 LSMESTIMATE model-effect lsmestimate-specification < / options > ;
 < label: > MODEL variable < (variable_options) > = < effects > < / options > ;
 < label: > MODEL events/trials = < effects > < / options > ;
 NLOPTIONS options ;
 ODDSRATIO < 'label' > variable < / options > ;
 OUTPUT < OUT=SAS-data-set > < keyword=name < keyword=name ... > > < / option > ;
 ROC < 'label' > < specification > < / options > ;
 ROCCONTRAST < 'label' > < contrast > < / options > ;
 SCORE < options > ;
 SLICE model-effect < / options > ;
 STORE < OUT= > item-store-name < / LABEL='label' > ;
 STRATA effects < / options > ;
 < label: > TEST equation1 < ,equation2, ... > < / option > ;
 UNITS < independent1=list1 < independent2=list2 ... > > < / option > ;
 WEIGHT variable < / option > ;

```

The PROC LOGISTIC and MODEL statements are required. The CLASS and EFFECT statements (if specified) must precede the MODEL statement, and the CONTRAST, EXACT, and ROC statements (if specified) must follow the MODEL statement.

The PROC LOGISTIC, MODEL, and ROCCONTRAST statements can be specified at most once. If a FREQ or WEIGHT statement is specified more than once, the variable specified in the first instance is used. If a BY, OUTPUT, or UNITS statement is specified more than once, the last instance is used.

The rest of this section provides detailed syntax information for each of the preceding statements, beginning with the PROC LOGISTIC statement. The remaining statements are covered in alphabetical order. The CODE, EFFECT, EFFECTPLOT, ESTIMATE, LSMEANS, LSMESTIMATE, SLICE, and STORE statements are also available in many other procedures. Summary descriptions of functionality and syntax for these statements are provided, but you can find full documentation on them in the corresponding sections of Chapter 19, “Shared Concepts and Topics.”

## PROC LOGISTIC Statement

**PROC LOGISTIC** < options > ;

The PROC LOGISTIC statement invokes the LOGISTIC procedure. Optionally, it identifies input and output data sets, suppresses the display of results, and controls the ordering of the response levels. Table 54.1 summarizes the options available in the PROC LOGISTIC statement.

**Table 54.1** PROC LOGISTIC Statement Options

| Option                                     | Description                                                      |
|--------------------------------------------|------------------------------------------------------------------|
| <b>Input/Output Data Set Options</b>       |                                                                  |
| COVOUT                                     | Displays the estimated covariance matrix in the OUTEST= data set |
| DATA=                                      | Names the input SAS data set                                     |
| INEST=                                     | Specifies the initial estimates SAS data set                     |
| INMODEL=                                   | Specifies the model information SAS data set                     |
| NOCOVAR                                    | Does not save covariance matrix in the OUTMODEL= data set        |
| OUTDESIGN=                                 | Specifies the design matrix output SAS data set                  |
| OUTDESIGNONLY                              | Outputs the design matrix only                                   |
| OUTEST=                                    | Specifies the parameter estimates output SAS data set            |
| OUTMODEL=                                  | Specifies the model output data set for scoring                  |
| <b>Response and CLASS Variable Options</b> |                                                                  |
| DESCENDING                                 | Reverses the sort order of the response variable                 |
| NAMELEN=                                   | Specifies the maximum length of effect names                     |
| ORDER=                                     | Specifies the sort order of the response variable                |
| TRUNCATE                                   | Truncates class level names                                      |
| <b>Displayed Output Options</b>            |                                                                  |
| ALPHA=                                     | Specifies the significance level for confidence intervals        |
| NOPRINT                                    | Suppresses all displayed output                                  |
| PLOTS                                      | Specifies options for plots                                      |
| SIMPLE                                     | Displays descriptive statistics                                  |
| <b>Large Data Set Option</b>               |                                                                  |
| MULTIPASS                                  | Does not copy the input SAS data set for internal computations   |
| <b>Control of Other Statement Options</b>  |                                                                  |
| EXACTONLY                                  | Performs exact analysis only                                     |
| EXACTOPTIONS                               | Specifies global options for EXACT statements                    |
| ROCOPTIONS                                 | Specifies global options for ROC statements                      |

### **ALPHA=number**

specifies the level of significance  $\alpha$  for  $100(1 - \alpha)\%$  confidence intervals. The value *number* must be between 0 and 1; the default value is 0.05, which results in 95% intervals. This value is used as the default confidence level for limits computed by the following options:

| Statement     | Options                    |
|---------------|----------------------------|
| CONTRAST      | ESTIMATE=                  |
| EXACT         | ESTIMATE=                  |
| MODEL         | CLODDS= CLPARM=            |
| ODDSRATIO     | CL=                        |
| OUTPUT        | LOWER= UPPER=              |
| PROC LOGISTIC | PLOTS=EFFECT(CLBAR CLBAND) |
| ROCONTRAST    | ESTIMATE=                  |
| SCORE         | CLM                        |

You can override the default in most of these cases by specifying the ALPHA= option in the separate statements.

### COVOUT

adds the estimated covariance matrix to the OUTEST= data set. For the COVOUT option to have an effect, the OUTEST= option must be specified. See the section “OUTEST= Output Data Set” on page 4279 for more information.

### DATA=SAS-data-set

names the SAS data set containing the data to be analyzed. If you omit the DATA= option, the procedure uses the most recently created SAS data set. The INMODEL= option cannot be specified with this option.

### DESCENDING

#### DESC

reverses the sort order for the levels of the response variable. If both the DESCENDING and ORDER= options are specified, PROC LOGISTIC orders the levels according to the ORDER= option and then reverses that order. This option has the same effect as the response variable option DESCENDING in the MODEL statement. See the section “Response Level Ordering” on page 4237 for more detail.

### EXACTONLY

requests only the exact analyses. The asymptotic analysis that PROC LOGISTIC usually performs is suppressed.

### EXACTOPTIONS (options)

specifies options that apply to every EXACT statement in the program. The available options are summarized here, and full descriptions are available in the EXACTOPTIONS statement.

| Option       | Description                                                              |
|--------------|--------------------------------------------------------------------------|
| ADDTOBS      | Adds the observed sufficient statistic to the sampled exact distribution |
| BUILDSUBSETS | Builds every distribution for sampling                                   |
| EPSILON=     | Specifies the comparison fuzz for partial sums of sufficient statistics  |
| MAXTIME=     | Specifies the maximum time allowed in seconds                            |
| METHOD=      | Specifies the DIRECT, NETWORK, or NETWORKMC algorithm                    |
| N=           | Specifies the number of Monte Carlo samples                              |
| ONDISK       | Uses disk space                                                          |
| SEED=        | Specifies the initial seed for sampling                                  |
| STATUSN=     | Specifies the sampling interval for printing a status line               |
| STATUSTIME=  | Specifies the time interval for printing a status line                   |

**INEST=SAS-data-set**

names the SAS data set that contains initial estimates for all the parameters in the model. If BY-group processing is used, it must be accommodated in setting up the INEST= data set. See the section “INEST= Input Data Set” on page 4280 for more information.

**INMODEL=SAS-data-set**

specifies the name of the SAS data set that contains the model information needed for scoring new data. This INMODEL= data set is the OUTMODEL= data set saved in a previous PROC LOGISTIC call. The OUTMODEL= data set should not be modified before its use as an INMODEL= data set.

The DATA= option cannot be specified with this option; instead, specify the data sets to be scored in the SCORE statements. FORMAT statements are not allowed when the INMODEL= data set is specified; variables in the DATA= and PRIOR= data sets in the SCORE statement should be formatted within the data sets.

You can specify the BY statement provided that the INMODEL= data set is created under the same BY-group processing.

The CLASS, EFFECT, EFFECTPLOT, ESTIMATE, EXACT, LSMEANS, LSMESTIMATE, MODEL, OUTPUT, ROC, ROCONTRAST, SLICE, STORE, TEST, and UNIT statements are not available with the INMODEL= option.

**MULTIPASS**

forces the procedure to reread the DATA= data set as needed rather than require its storage in memory or in a temporary file on disk. By default, the data set is cleaned up and stored in memory or in a temporary file. This option can be useful for large data sets. All exact analyses are ignored in the presence of the MULTIPASS option. If a STRATA statement is specified, then the data set must first be grouped or sorted by the strata variables.

**NAMELEN=n**

specifies the maximum length of effect names in tables and output data sets to be *n* characters, where *n* is a value between 20 and 200. The default length is 20 characters.

**NOCOV**

specifies that the covariance matrix not be saved in the OUTMODEL= data set. The covariance matrix is needed for computing the confidence intervals for the posterior probabilities in the OUT= data set in the SCORE statement. Specifying this option will reduce the size of the OUTMODEL= data set.

**NOPRINT**

suppresses all displayed output. Note that this option temporarily disables the Output Delivery System (ODS); see Chapter 20, “Using the Output Delivery System,” for more information.

**ORDER=DATA | FORMATTED | FREQ | INTERNAL****RORDER=DATA | FORMATTED | INTERNAL**

specifies the sort order for the levels of the response variable. See the response variable option ORDER= in the MODEL statement for more information. For ordering of CLASS variable levels, see the ORDER= option in the CLASS statement.

**OUTDESIGN=SAS-data-set**

specifies the name of the data set that contains the design matrix for the model. The data set contains the same number of observations as the corresponding DATA= data set and includes the response

variable (with the same format as in the DATA= data set), the **FREQ** variable, the **WEIGHT** variable, the **OFFSET=** variable, and the design variables for the covariates, including the Intercept variable of constant value 1 unless the **NOINT** option in the **MODEL** statement is specified.

#### **OUTDESIGNONLY**

suppresses the model fitting and creates only the **OUTDESIGN=** data set. This option is ignored if the **OUTDESIGN=** option is not specified.

#### **OUTEST=SAS-data-set**

creates an output SAS data set that contains the final parameter estimates and, optionally, their estimated covariances (see the preceding **COVOUT** option). The output data set also includes a variable named **\_LNLIKE\_**, which contains the log likelihood. See the section “**OUTEST= Output Data Set**” on page 4279 for more information.

#### **OUTMODEL=SAS-data-set**

specifies the name of the SAS data set that contains the information about the fitted model. This data set contains sufficient information to score new data without having to refit the model. It is solely used as the input to the **INMODEL=** option in a subsequent PROC LOGISTIC call. The **OUTMODEL=** option is not available with the **STRATA** statement. Information in this data set is stored in a very compact form, so you should not modify it manually.

**NOTE:** The **STORE** statement can also be used to save your model. See the section “**STORE Statement**” on page 4233 for more information.

**PLOTS** < (*global-plot-options*) > < =*plot-request*< (*options*) > >

**PLOTS** < (*global-plot-options*) > =(*plot-request*< (*options*)>< ... *plot-request*< (*options*)>>

controls the plots produced through ODS Graphics. When you specify only one *plot-request*, you can omit the parentheses from around the *plot-request*. For example:

```
PLOTS = ALL
PLOTS = (ROC EFFECT INFLUENCE (UNPACK))
PLOTS (ONLY) = EFFECT (CLBAR SHOWOBS)
```

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;
proc logistic plots=all;
 model y=x;
run;
ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “**Enabling and Disabling ODS Graphics**” on page 600 in Chapter 21, “**Statistical Graphics Using ODS**.”

If the **PLOTS** option is not specified or is specified with no *plot-requests*, then graphics are produced by default in the following situations:

- If the **INFLUENCE** or **IPLOTS** option is specified in the **MODEL** statement, then the line-printer plots are suppressed, and the **INFLUENCE** plots are produced unless the **MAXPOINTS=** cutoff is exceeded.

- If you specify the **OUTROC=** option in the **MODEL** statement, then ROC curves are produced. If you also specify a **SELECTION=** method, then an overlaid plot of all the ROC curves for each step of the selection process is displayed.
- If the **OUTROC=** option is specified in a **SCORE** statement, then the ROC curve for the scored data set is displayed.
- If you specify **ROC** statements, then an overlaid plot of the ROC curves for the model (or the selected model if a **SELECTION=** method is specified) and for all the ROC statement models is displayed.
- If an odds ratio table is produced, then a plot of the odds ratios and their confidence limits is displayed. These plots correspond to the default odds ratio table and the tables produced by the **CLODDS=** option in the **MODEL** statement and the tables produced by the **ODDSRATIO** statement.

For general information about ODS Graphics, see Chapter 21, “Statistical Graphics Using ODS.”

The following *global-plot-options* are available:

#### **LABEL**

displays a label on diagnostic plots to aid in identifying the outlying observations. This option enhances the plots produced by the **DFBETAS**, **DPC**, **INFLUENCE**, **LEVERAGE**, and **PHAT** options. If an **ID** statement is specified, then the plots are labeled with the ID variables. Otherwise, the observation number is displayed.

#### **MAXPOINTS=NONE** | *number*

suppresses the plots produced by the **DFBETAS**, **DPC**, **INFLUENCE**, **LEVERAGE**, and **PHAT** options if there are more than *number* observations. Also, observations are not displayed on the **EFFECT** plots when the cutoff is exceeded. The default is **MAXPOINTS=5000**. The cutoff is ignored if you specify **MAXPOINTS=NONE**.

#### **ONLY**

specifically requested *plot-requests* are displayed.

#### **UNPACKPANELS** | **UNPACK**

suppresses paneling. By default, multiple plots can appear in some output *panels*. Specify **UNPACKPANEL** to display each plot separately.

The following *plot-requests* are available:

#### **ALL**

produces all appropriate plots. You can specify other options with **ALL**. For example, to display all plots and unpack the **DFBETAS** plots you can specify **plots=(all dfbetas(unpack))**.

#### **DFBETAS <(UNPACK)>**

displays plots of **DFBETAS** versus the case (observation) number. This displays the statistics generated by the **DFBETAS=\_ALL\_** option in the **OUTPUT** statement. The **UNPACK** option displays the plots separately. See [Output 54.6.5](#) for an example of this plot.

**DPC<(UNPACK)>**

displays plots of **DIFCHISQ** and **DIFDEV** versus the predicted event probability, and colors the markers according to the value of the confidence interval displacement **C**. The **UNPACK** option displays the plots separately. See [Output 54.6.8](#) for an example of this plot.

**EFFECT<(effect-options)>**

displays and enhances the effect plots for the model. For more information about effect plots and the available *effect-options*, see the section “**PLOTS=EFFECT Plots**” on page 4182.

**NOTE:** The **EFFECTPLOT** statement provides you with much of the same functionality and more options for creating effect plots. See [Outputs 54.2.11, 54.3.5, 54.4.8, 54.7.4, and 54.15.4](#) for examples of effect plots.

**INFLUENCE<(UNPACK | STDRES)>**

displays index plots of **RESCHI**, **RESDEV**, leverage, confidence interval displacements **C** and **CBar**, **DIFCHISQ**, and **DIFDEV**. These plots are produced by default when any *plot-request* is specified and the **MAXPOINTS=** cutoff is not exceeded. The **UNPACK** option displays the plots separately. The **STDRES** option also displays index plots of **STDRESCHI**, **STDRESDEV**, and **RESLIK**. See [Outputs 54.6.3 and 54.6.4](#) for examples of these plots.

**LEVERAGE<(UNPACK)>**

displays plots of **DIFCHISQ**, **DIFDEV**, confidence interval displacement **C**, and the predicted probability versus the leverage. The **UNPACK** option displays the plots separately. See [Output 54.6.7](#) for an example of this plot.

**NONE**

suppresses all plots.

**ODDSRATIO <(oddsratio-options)>**

displays and enhances the odds ratio plots for the model. For more information about odds ratio plots and the available *oddsratio-options*, see the section “**Odds Ratio Plots**” on page 4185. See [Outputs 54.7, 54.2.9, 54.3.3, and 54.4.5](#) for examples of this plot.

**PHAT<(UNPACK)>**

displays plots of **DIFCHISQ**, **DIFDEV**, confidence interval displacement **C**, and leverage versus the predicted event probability. The **UNPACK** option displays the plots separately. See [Output 54.6.6](#) for an example of this plot.

**ROC<(ID<=keyword>)>**

displays the ROC curve. If you also specify a **SELECTION=** method, then an overlaid plot of all the ROC curves for each step of the selection process is displayed. If you specify **ROC** statements, then an overlaid plot of the model (or the selected model if a **SELECTION=** method is specified) and the ROC statement models is displayed. If the **OUTROC=** option is specified in a **SCORE** statement, then the ROC curve for the scored data set is displayed.

The **ID=** option labels certain points on the ROC curve. Typically, the labeled points are closest to the upper-left corner of the plot, and points directly below or to the right of a labeled point are suppressed. This option is identical to, and has the same *keywords* as, the **ID=** suboption of the **ROCOPTIONS** option.

See [Output 54.7.3](#) and [Example 54.8](#) for examples of these ROC plots.



**ROCOPTIONS** (*options*)

specifies options that apply to every model specified in a **ROC** statement. Some of these options also apply to the **SCORE** statement. The following *options* are available:

**ALPHA=number**

sets the significance level for creating confidence limits of the areas and the pairwise differences. The **ALPHA=** value specified in the PROC LOGISTIC statement is the default. If neither **ALPHA=** value is specified, then **ALPHA=0.05** by default.

**EPS=value**

is an alias for the **ROCEPS=** option in the MODEL statement. This value is used to determine which predicted probabilities are equal. The default value is the square root of the machine epsilon, which is about  $1E-8$ .

**ID<=keyword>**

displays labels on certain points on the individual ROC curves and also on the **SCORE** statement's ROC curve. This option overrides the **ID=** suboption of the **PLOTS=ROC** option. If several observations lie at the same place on the ROC curve, the value for the last observation is displayed. If you specify the **ID** option with no *keyword*, any variables that are listed in the **ID** statement are used. If no **ID** statement is specified, the observation number is displayed. The following *keywords* are available:

|                 |                                                                  |
|-----------------|------------------------------------------------------------------|
| <b>PROB</b>     | displays the model predicted probability.                        |
| <b>OBS</b>      | displays the (last) observation number.                          |
| <b>SENSIT</b>   | displays the true positive fraction (sensitivity).               |
| <b>1MSPEC</b>   | displays the false positive fraction (1–specificity).            |
| <b>FALPOS</b>   | displays the fraction of nonevents that are predicted as events. |
| <b>FALNEG</b>   | displays the fraction of events that are predicted as nonevents. |
| <b>POSPRED</b>  | displays the positive predictive value (1–FALPOS).               |
| <b>NEGPRED</b>  | displays the negative predictive value (1–FALNEG).               |
| <b>MISCLASS</b> | displays the misclassification rate.                             |
| <b>ID</b>       | displays the ID variables.                                       |

The **SENSIT**, **1MSPEC**, **FALPOS**, and **FALNEG** statistics are defined in the section “**Receiver Operating Characteristic Curves**” on page 4260. The misclassification rate is the number of events that are predicted as nonevents and the number of nonevents that are predicted as events as calculated by using the given cutpoint (predicted probability) divided by the number of observations. If the **PEVENT=** option is also specified, then **FALPOS** and **FALNEG** are computed using the first **PEVENT=** value and Bayes' theorem, as discussed in the section “**Predicted Probability of an Event for Classification**” on page 4255.

**NODETAILS**

suppresses the display of the model fitting information for the models specified in the **ROC** statements.



**OUT=SAS-data-set-name**

is an alias for the **OUTROC=** option in the **MODEL** statement.

**WEIGHTED**

uses frequency×weight in the ROC computations (Izrael et al. 2002) instead of just frequency. Typically, weights are considered in the fit of the model only, and hence are accounted for in the parameter estimates. The “Association of Predicted Probabilities and Observed Responses” table uses frequency (unless the **BINWIDTH=0** option is also specified on the **MODEL** statement), and is suppressed when ROC comparisons are performed. This option also affects **SCORE** statement ROC and AUC computations.

**SIMPLE**

displays simple descriptive statistics (mean, standard deviation, minimum and maximum) for each continuous explanatory variable. For each **CLASS** variable involved in the modeling, the frequency counts of the classification levels are displayed. The **SIMPLE** option generates a breakdown of the simple descriptive statistics or frequency counts for the entire data set and also for individual response categories.

**TRUNCATE**

determines class levels by using no more than the first 16 characters of the formatted values of **CLASS**, response, and strata variables. When formatted values are longer than 16 characters, you can use this option to revert to the levels as determined in releases previous to SAS 9.0. This option invokes the same option in the **CLASS** statement.

**PLOTS=EFFECT Plots**

Only one **PLOTS=EFFECT** plot is produced by default; you must specify other *effect-options* to produce multiple plots. For binary response models, the following plots are produced when an **EFFECT** option is specified with no *effect-options*:

- If you only have continuous covariates in the model, then a plot of the predicted probability versus the first continuous covariate fixing all other continuous covariates at their means is displayed. See [Output 54.7.4](#) for an example with one continuous covariate.
- If you only have classification covariates in the model, then a plot of the predicted probability versus the first **CLASS** covariate at each level of the second **CLASS** covariate, if any, holding all other **CLASS** covariates at their reference levels is displayed.
- If you have **CLASS** and continuous covariates, then a plot of the predicted probability versus the first continuous covariate at up to 10 cross-classifications of the **CLASS** covariate levels, while fixing all other continuous covariates at their means and all other **CLASS** covariates at their reference levels, is displayed. For example, if your model has four binary covariates, there are 16 cross-classifications of the **CLASS** covariate levels. The plot displays the 8 cross-classifications of the levels of the first three covariates while the fourth covariate is fixed at its reference level.

For polytomous response models, similar plots are produced by default, except that the response levels are used in place of the **CLASS** covariate levels. Plots for polytomous response models involving **OFFSET=** variables with multiple values are not available.

The following *effect-options* specify the type of graphic to produce:

**AT**(*variable=value-list* | **ALL**<...*variable=value-list* | **ALL**>)

specifies fixed values for a covariate. For continuous covariates, you can specify one or more numbers in the *value-list*. For classification covariates, you can specify one or more formatted levels of the covariate enclosed in single quotes (for example, **A='cat' 'dog'**), or you can specify the keyword **ALL** to select all levels of the classification variable. You can specify a variable at most once in the **AT** option. By default, continuous covariates are set to their means when they are not used on an axis, while classification covariates are set to their reference level when they are not used as an **X=**, **SLICEBY=**, or **PLOTBY=** effect. For example, for a model that includes a classification variable **A={cat,dog}** and a continuous covariate **X**, specifying **AT (A='cat' X=7 9)** will set **A** to 'cat' when **A** does not appear in the plot. When **X** does not define an axis it first produces plots setting **X = 7** and then produces plots setting **X = 9**. Note in this example that specifying **AT ( A=ALL )** is the same as specifying the **PLOTBY=A** option.

**FITOBSONLY**

computes the predicted values only at the observed data. If the **FITOBSONLY** option is omitted and the **X**-axis variable is continuous, the predicted values are computed at a grid of points extending slightly beyond the range of the data (see the **EXTEND=** option for more information). If the **FITOBSONLY** option is omitted and the **X**-axis effect is categorical, the predicted values are computed at all possible categories.

**INDIVIDUAL**

displays the individual probabilities instead of the cumulative probabilities. This option is available only with cumulative models, and it is not available with the **LINK** option.

**LINK**

displays the linear predictors instead of the probabilities on the **Y** axis. For example, for a binary logistic regression, the **Y** axis will be displayed on the logit scale. The **INDIVIDUAL** and **POLYBAR** options are not available with the **LINK** option.

**PLOTBY=effect**

displays an effect plot at each unique level of the **PLOTBY=** effect. You can specify *effect* as one **CLASS** variable or as an interaction of classification covariates. For polytomous-response models, you can also specify the response variable as the lone **PLOTBY=** effect. For nonsingular parameterizations, the complete cross-classification of the **CLASS** variables specified in the effect define the different **PLOTBY=** levels. When the **GLM** parameterization is used, the **PLOTBY=** levels can depend on the model and the data.

**SLICEBY=effect**

displays predicted probabilities at each unique level of the **SLICEBY=** effect. You can specify *effect* as one **CLASS** variable or as an interaction of classification covariates. For polytomous-response models, you can also specify the response variable as the lone **SLICEBY=** effect. For nonsingular parameterizations, the complete cross-classification of the **CLASS** variables specified in the effect define the different **SLICEBY=** levels. When the **GLM** parameterization is used, the **SLICEBY=** levels can depend on the model and the data.

**X=effect****X=(effect...effect)**

specifies effects to be used on the **X** axis of the effect plots. You can specify several different **X** axes: continuous variables must be specified as main effects, while **CLASS** variables can be crossed. For nonsingular parameterizations, the complete cross-classification of the **CLASS** variables specified in

the effect define the axes. When the **GLM** parameterization is used, the **X=** levels can depend on the model and the data. The response variable is not allowed as an *effect*.

**NOTE:** Any variable not specified in a **SLICEBY=** or **PLOTBY=** option is available to be displayed on the X axis. A variable can be specified in at most one of the **SLICEBY=**, **PLOTBY=**, and **X=** options.

The following *effect-options* enhance the graphical output:

**ALPHA=number**

specifies the size of the confidence limits. The **ALPHA=** value specified in the PROC LOGISTIC statement is the default. If neither **ALPHA=** value is specified, then **ALPHA=0.05** by default.

**CLBAND<=YES | NO>**

displays confidence limits on the plots. This option is not available with the **INDIVIDUAL** option. If you have **CLASS** covariates on the X axis, then error bars are displayed (see the **CLBAR** option) unless you also specify the **CONNECT** option.

**CLBAR**

displays the error bars on the plots when you have **CLASS** covariates on the X axis; if the X axis is continuous, then this invokes the **CLBAND** option. For polytomous-response models with **CLASS** covariates only and with the **POLYBAR** option specified, the stacked bar charts are replaced by side-by-side bar charts with error bars.

**CLUSTER<=percent>**

displays the levels of the **SLICEBY=** effect in a side-by-side fashion instead of stacking them. This option is available when you have **CLASS** covariates on the X axis. You can specify *percent* as a percentage of half the distance between X levels. The *percent* value must be between 0.1 and 1; the default *percent* depends on the number of X levels and the number of **SLICEBY=** levels. Default clustering can be removed by specifying the **NOCLUSTER** option.

**CONNECT<=YES | NO>**

**JOIN<=YES | NO>**

connects the predicted values with a line. This option is available when you have **CLASS** covariates on the X axis. Default connecting lines can be suppressed by specifying the **NOCONNECT** option.

**EXTEND=value**

extends continuous X axes by a factor of *value/2* in each direction. By default, **EXTEND=0.2**.

**MAXATLEN=length**

specifies the maximum number of characters used to display the levels of all the fixed variables. If the text is too long, it is truncated and ellipses (“...”) are appended. By default, *length* is equal to its maximum allowed value, 256.

**NOCLUSTER**

prevents clustering of the levels of the **SLICEBY=** effect. This option is available when you have **CLASS** covariates on the X axis.

**NOCONNECT**

removes the line that connects the predicted values. This option is available when you have **CLASS** covariates on the X axis.

**POLYBAR**

replaces scatter plots of polytomous response models with bar charts. This option has no effect on binary-response models, and it is overridden by the **CONNECT** option. By default, the X axis is chosen to be a crossing of available classification variables so that there are no more than 16 levels; if no such crossing is possible then the first available classification variable is used. You can override this default by specifying the **X=** option.

**SHOWOBS<=YES | NO>**

displays observations on the plot when the **MAXPOINTS=** cutoff is not exceeded. For events/trials notation, the observed proportions are displayed; for single-trial binary-response models, the observed events are displayed at  $\hat{p} = 1$  and the observed nonevents are displayed at  $\hat{p} = 0$ . For polytomous response models the predicted probabilities at the observed values of the covariate are computed and displayed.

**YRANGE=(*< min >*,*< max >*)**

displays the Y axis as [*min*,*max*]. Note that the axis might extend beyond your specified values. By default, the entire Y axis, [0,1], is displayed for the predicted probabilities. This option is useful if your predicted probabilities are all contained in some subset of this range.

**Odds Ratio Plots**

The odds ratios and confidence limits from the default Odds Ratio Estimates table and from the tables produced by the **CLODDS=** option or the **ODDSRATIO** statement can be displayed in a graphic. If you have many odds ratios, you can produce multiple graphics, or *panels*, by displaying subsets of the odds ratios. Odds ratios with duplicate labels are not displayed. See Outputs 54.2.9 and 54.3.3 for examples of odds ratio plots.

The following *oddsratio-options* modify the default odds ratio plot:

**CLDISPLAY=**SERIF** | **LINE** | **BAR**< *width* >**

controls the look of the confidence limit error bars. The default **CLDISPLAY=SERIF** displays the confidence limits as lines with serifs, **CLDISPLAY=LINE** removes the serifs from the error bars, and **CLDISPLAY=BAR** < *width* > displays the limits with a bar of width equal to the size of the marker. You can control the width of the bars and the size of the marker by specifying the *width* value as a percentage of the distance between the bars,  $0 < \textit{width} \leq 1$ .

**NOTE:** Your bar might disappear with small values of *width*.

**DOTPLOT**

displays dotted gridlines on the plot.

**GROUP**

displays the odds ratios in panels defined by the **ODDSRATIO** statements. The **NPANELPOS=** option is ignored when this option is specified.

**LOGBASE=2 | E | 10**

displays the odds ratio axis on the specified log scale.

**NPANELPOS=*n***

breaks the plot into multiple graphics having at most  $|n|$  odds ratios per graphic. If  $n$  is positive, then the number of odds ratios per graphic is balanced; but if  $n$  is negative, then no balancing of the number of odds ratios takes place. By default,  $n = 0$  and all odds ratios are displayed in a single plot. For example, suppose you want to display 21 odds ratios. Then specifying **NPANELPOS=20** displays two plots, the first with 11 odds ratios and the second with 10; but specifying **NPANELPOS=-20** displays 20 odds ratios in the first plot and only 1 odds ratio in the second.

**ORDER=ASCENDING | DESCENDING**

displays the odds ratios in sorted order. By default the odds ratios are displayed in the order in which they appear in the corresponding table.

**RANGE=(*< min >* , *< max >*) | CLIP**

specifies the range of the displayed odds ratio axis. The RANGE=CLIP option has the same effect as specifying the minimum odds ratio as *min* and the maximum odds ratio as *max*. By default, all odds ratio confidence intervals are displayed.

**TYPE=HORIZONTAL | HORIZONTALSTAT | VERTICAL | VERTICALBLOCK**

controls the look of the graphic. The default TYPE=HORIZONTAL option places the odds ratio values on the X axis, while the TYPE=HORIZONTALSTAT option also displays the values of the odds ratios and their confidence limits on the right side of the graphic. The TYPE=VERTICAL option places the odds ratio values on the Y axis, while the TYPE=VERTICALBLOCK option (available only with the CLODDS= option) places the odds ratio values on the Y axis and puts boxes around the labels.

**BY Statement**

**BY variables ;**

You can specify a BY statement with PROC LOGISTIC to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the LOGISTIC procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

If a SCORE statement is specified, then define the *training data set* to be the DATA= data set or the IN-MODEL= data set in the PROC LOGISTIC statement, and define the *scoring data set* to be the DATA= data set and PRIOR= data set in the SCORE statement. The training data set contains all of the BY variables, and

the scoring data set must contain either all of them or none of them. If the scoring data set contains all the BY variables, matching is carried out between the training and scoring data sets. If the scoring data set does not contain any of the BY variables, the entire scoring data set is used for every BY group in the training data set and the BY variables are added to the output data sets that are specified in the **SCORE** statement.

**CAUTION:** The order of the levels in the response and classification variables is determined from all the data regardless of BY groups. However, different sets of levels might appear in different BY groups. This might affect the value of the reference level for these variables, and hence your interpretation of the model and the parameters.

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

---

## CLASS Statement

```
CLASS variable <(options)> ... <variable <(options)>> </global-options>;
```

The CLASS statement names the classification variables to be used as explanatory variables in the analysis. Response variables do not need to be specified in the CLASS statement.

The CLASS statement must precede the **MODEL** statement. Most options can be specified either as individual variable *options* or as *global-options*. You can specify *options* for each variable by enclosing the options in parentheses after the variable name. You can also specify *global-options* for the CLASS statement by placing them after a slash (/). *Global-options* are applied to all the variables specified in the CLASS statement. If you specify more than one CLASS statement, the *global-options* specified in any one CLASS statement apply to all CLASS statements. However, individual CLASS variable *options* override the *global-options*. You can specify the following values for either an *option* or a *global-option*:

### **CPREFIX=*n***

specifies that, at most, the first *n* characters of a CLASS variable name be used in creating names for the corresponding design variables. The default is  $32 - \min(32, \max(2, f))$ , where *f* is the formatted length of the CLASS variable.

### **DESCENDING**

#### **DESC**

reverses the sort order of the classification variable. If both the DESCENDING and **ORDER=** options are specified, PROC LOGISTIC orders the categories according to the ORDER= option and then reverses that order.

### **LPREFIX=*n***

specifies that, at most, the first *n* characters of a CLASS variable label be used in creating labels for the corresponding design variables. The default is  $256 - \min(256, \max(2, f))$ , where *f* is the formatted length of the CLASS variable.

### **MISSING**

treats missing values ('.', '.\_', '.A', ..., '.Z' for numeric variables and blanks for character variables) as valid values for the CLASS variable.

**ORDER=DATA | FORMATTED | FREQ | INTERNAL**

specifies the sort order for the levels of classification variables. This ordering determines which parameters in the model correspond to each level in the data, so the ORDER= option can be useful when you use the CONTRAST statement. By default, ORDER=FORMATTED. For ORDER=FORMATTED and ORDER=INTERNAL, the sort order is machine-dependent. When ORDER=FORMATTED is in effect for numeric variables for which you have supplied no explicit format, the levels are ordered by their internal values.

The following table shows how PROC LOGISTIC interprets values of the ORDER= option.

| Value of ORDER= | Levels Sorted By                                                                                                                         |
|-----------------|------------------------------------------------------------------------------------------------------------------------------------------|
| DATA            | Order of appearance in the input data set                                                                                                |
| FORMATTED       | External formatted values, except for numeric variables with no explicit format, which are sorted by their unformatted (internal) values |
| FREQ            | Descending frequency count; levels with more observations come earlier in the order                                                      |
| INTERNAL        | Unformatted value                                                                                                                        |

For more information about sort order, see the chapter on the SORT procedure in the *Base SAS Procedures Guide* and the discussion of BY-group processing in *SAS Language Reference: Concepts*.

**PARAM=keyword**

specifies the parameterization method for the classification variable or variables. You can specify any of the *keywords* shown in the following table; the default is PARAM=EFFEFFECT. Design matrix columns are created from CLASS variables according to the corresponding coding schemes:

| Value of PARAM=           | Coding                                                                                              |
|---------------------------|-----------------------------------------------------------------------------------------------------|
| EFFEFFECT                 | Effect coding                                                                                       |
| GLM                       | Less-than-full-rank reference cell coding (this <i>keyword</i> can be used only in a global option) |
| ORDINAL<br>THERMOMETER    | Cumulative parameterization for an ordinal CLASS variable                                           |
| POLYNOMIAL<br>POLY        | Polynomial coding                                                                                   |
| REFERENCE<br>REF          | Reference cell coding                                                                               |
| ORTHEFFECT                | Orthogonalizes PARAM=EFFEFFECT coding                                                               |
| ORTHORDINAL<br>ORTHOTHERM | Orthogonalizes PARAM=ORDINAL coding                                                                 |
| ORTHPOLY                  | Orthogonalizes PARAM=POLYNOMIAL coding                                                              |
| ORTHREF                   | Orthogonalizes PARAM=REFERENCE coding                                                               |

All parameterizations are full rank, except for the GLM parameterization. The REF= option in the



CLASS statement determines the reference level for EFFECT and REFERENCE coding and for their orthogonal parameterizations. It also indirectly determines the reference level for a singular GLM parameterization through the order of levels.

If PARAM=ORTHPOLY or PARAM=POLY and the classification variable is numeric, then the ORDER= option in the CLASS statement is ignored, and the internal unformatted values are used. See the section “Other Parameterizations” on page 387 of Chapter 19, “Shared Concepts and Topics,” for further details.

**REF=** *'level' | keyword*

specifies the reference level for PARAM=EFFECT, PARAM=REFERENCE, and their orthogonalizations. For PARAM=GLM, the REF= option specifies a level of the classification variable to be put at the end of the list of levels. This level thus corresponds to the reference level in the usual interpretation of the linear estimates with a singular parameterization.

For an individual variable REF= option (but not for a global REF= option), you can specify the *level* of the variable to use as the reference level. Specify the formatted value of the variable if a format is assigned. For a global or individual variable REF= option, you can use one of the following *keywords*. The default is REF=LAST.

**FIRST**     designates the first ordered level as reference.

**LAST**       designates the last ordered level as reference.

**TRUNCATE**< =*n*>

specifies the length *n* of CLASS variable values to use in determining CLASS variable levels. The default is to use the full formatted length of the CLASS variable. If you specify TRUNCATE without the length *n*, the first 16 characters of the formatted values are used. When formatted values are longer than 16 characters, you can use this option to revert to the levels as determined in releases before SAS 9. The TRUNCATE option is available only as a global option.

## Class Variable Naming Convention

Parameter names for a CLASS predictor variable are constructed by concatenating the CLASS variable name with the CLASS levels. However, for the POLYNOMIAL and orthogonal parameterizations, parameter names are formed by concatenating the CLASS variable name and keywords that reflect the parameterization. See the section “Other Parameterizations” on page 387 in Chapter 19, “Shared Concepts and Topics,” for examples and further details.

## Class Variable Parameterization with Unbalanced Designs

PROC LOGISTIC initially parameterizes the CLASS variables by looking at the levels of the variables across the complete data set. If you have an *unbalanced* replication of levels across variables or BY groups, then the design matrix and the parameter interpretation might be different from what you expect. For instance, suppose you have a model with one CLASS variable A with three levels (1, 2, and 3), and another CLASS variable B with two levels (1 and 2). If the third level of A occurs only with the first level of B, if you use the EFFECT parameterization, and if your model contains the effect A(B) and an intercept, then the design for A within the second level of B is not a differential effect. In particular, the design looks like the following:



|   |   | Design Matrix |    |        |    |
|---|---|---------------|----|--------|----|
|   |   | A(B=1)        |    | A(B=2) |    |
| B | A | A1            | A2 | A1     | A2 |
| 1 | 1 | 1             | 0  | 0      | 0  |
| 1 | 2 | 0             | 1  | 0      | 0  |
| 1 | 3 | -1            | -1 | 0      | 0  |
| 2 | 1 | 0             | 0  | 1      | 0  |
| 2 | 2 | 0             | 0  | 0      | 1  |

PROC LOGISTIC detects linear dependency among the last two design variables and sets the parameter for A2(B=2) to zero, resulting in an interpretation of these parameters as if they were reference- or dummy-coded. The REFERENCE or GLM parameterization might be more appropriate for such problems.

## CODE Statement

**CODE** < options > ;

The CODE statement enables you to write SAS DATA step code for computing predicted values of the fitted model either to a file or to a catalog entry. This code can then be included in a DATA step to score new data.

Table 54.2 summarizes the *options* available in the CODE statement.

**Table 54.2** CODE Statement Options

| Option    | Description                                                                  |
|-----------|------------------------------------------------------------------------------|
| CATALOG=  | Names the catalog entry where the generated code is saved                    |
| DUMMIES   | Retains the dummy variables in the data set                                  |
| ERROR     | Computes the error function                                                  |
| FILE=     | Names the file where the generated code is saved                             |
| FORMAT=   | Specifies the numeric format for the regression coefficients                 |
| GROUP=    | Specifies the group identifier for array names and statement labels          |
| IMPUTE    | Imputes predicted values for observations with missing or invalid covariates |
| LINESIZE= | Specifies the line size of the generated code                                |
| LOOKUP=   | Specifies the algorithm for looking up CLASS levels                          |
| RESIDUAL  | Computes residuals                                                           |

For details about the syntax of the CODE statement, see the section “CODE Statement” on page 390 in Chapter 19, “Shared Concepts and Topics.”

## CONTRAST Statement

**CONTRAST** 'label' row-description<, . . . , row-description > < / options > ;

where a *row-description* is defined as follows:

*effect values*<, . . . , *effect values*>

The CONTRAST statement provides a mechanism for obtaining customized hypothesis tests. It is similar to the CONTRAST and ESTIMATE statements in other modeling procedures.

The CONTRAST statement enables you to specify a matrix,  $\mathbf{L}$ , for testing the hypothesis  $\mathbf{L}\boldsymbol{\beta} = \mathbf{0}$ , where  $\boldsymbol{\beta}$  is the vector of intercept and slope parameters. You must be familiar with the details of the model parameterization that PROC LOGISTIC uses (for more information, see the [PARAM=](#) option in the section “[CLASS Statement](#)” on page 4187). Optionally, the CONTRAST statement enables you to estimate each row,  $\mathbf{l}'_i\boldsymbol{\beta}$ , of  $\mathbf{L}\boldsymbol{\beta}$  and test the hypothesis  $\mathbf{l}'_i\boldsymbol{\beta} = 0$ . Computed statistics are based on the asymptotic chi-square distribution of the Wald statistic.

There is no limit to the number of CONTRAST statements that you can specify, but they must appear after the [MODEL](#) statement.

The following parameters are specified in the CONTRAST statement:

- label* identifies the contrast in the displayed output. A label is required for every contrast specified, and it must be enclosed in quotes.
- effect* identifies an effect that appears in the [MODEL](#) statement. The name INTERCEPT can be used as an effect when one or more intercepts are included in the model. You do not need to include all effects that are included in the [MODEL](#) statement.
- values* are constants that are elements of the  $\mathbf{L}$  matrix associated with the effect. To correctly specify your contrast, it is crucial to know the ordering of parameters within each effect and the variable levels associated with any parameter. The “Class Level Information” table shows the ordering of levels within variables. The [E](#) option, described later in this section, enables you to verify the proper correspondence of *values* to parameters. If too many values are specified for an effect, the extra ones are ignored. If too few values are specified, the remaining ones are set to 0.

Multiple degree-of-freedom hypotheses can be tested by specifying multiple *row-descriptions*; the rows of  $\mathbf{L}$  are specified in order and are separated by commas. The degrees of freedom is the number of linearly independent constraints implied by the CONTRAST statement—that is, the rank of  $\mathbf{L}$ .

More details for specifying contrasts involving effects with full-rank parameterizations are given in the section “[Full-Rank Parameterized Effects](#)” on page 4192, while details for less-than-full-rank parameterized effects are given in the section “[Less-Than-Full-Rank Parameterized Effects](#)” on page 4193.

You can specify the following options after a slash (/):

**ALPHA=***number*

specifies the level of significance  $\alpha$  for the  $100(1-\alpha)\%$  confidence interval for each contrast when the ESTIMATE option is specified. The value of *number* must be between 0 and 1. By default, *number* is equal to the value of the [ALPHA=](#) option in the PROC LOGISTIC statement, or 0.05 if that option is not specified.

**E**

displays the  $\mathbf{L}$  matrix.

**ESTIMATE=keyword**

estimates and tests each individual contrast (that is, each row,  $l'_i\beta$ , of  $L\beta$ ), exponentiated contrast ( $e^{l'_i\beta}$ ), or predicted probability for the contrast ( $g^{-1}(l'_i\beta)$ ). PROC LOGISTIC displays the point estimate, its standard error, a Wald confidence interval, and a Wald chi-square test. The significance level of the confidence interval is controlled by the **ALPHA=** option. You can estimate the individual contrast, the exponentiated contrast, or the predicted probability for the contrast by specifying one of the following *keywords*:

**PARM**

estimates the individual contrast.

**EXP**

estimates the exponentiated contrast.

**BOTH**

estimates both the individual contrast and the exponentiated contrast.

**PROB**

estimates the predicted probability of the contrast.

**ALL**

estimates the individual contrast, the exponentiated contrast, and the predicted probability of the contrast.

For details about the computations of the standard errors and confidence limits, see the section “[Linear Predictor, Predicted Probability, and Confidence Limits](#)” on page 4253.

**SINGULAR=number**

tunes the estimability check. This option is ignored when a full-rank parameterization is specified. If  $\mathbf{v}$  is a vector, define  $\text{ABS}(\mathbf{v})$  to be the largest absolute value of the elements of  $\mathbf{v}$ . For a row vector  $l'$  of the contrast matrix  $L$ , define  $c = \text{ABS}(l')$  if  $\text{ABS}(l')$  is greater than 0; otherwise,  $c = 1$ . If  $\text{ABS}(l' - l'\mathbf{T})$  is greater than  $c * \text{number}$ , then  $l$  is declared nonestimable. The  $\mathbf{T}$  matrix is the Hermite form matrix  $\mathbf{I}_0^{-1}\mathbf{I}_0$ , where  $\mathbf{I}_0^{-1}$  represents a generalized inverse of the (observed or expected) information matrix  $\mathbf{I}_0$  of the null model. The value for *number* must be between 0 and 1; the default value is 1E-4.

**Full-Rank Parameterized Effects**

If an effect involving a CLASS variable with a full-rank parameterization does not appear in the CONTRAST statement, then all of its coefficients in the  $L$  matrix are set to 0.

If you use effect coding by default or by specifying **PARAM=EFFECT** in the **CLASS** statement, then all parameters are directly estimable and involve no other parameters. For example, suppose an effect-coded CLASS variable  $A$  has four levels. Then there are three parameters ( $\beta_1, \beta_2, \beta_3$ ) representing the first three levels, and the fourth parameter is represented by

$$-\beta_1 - \beta_2 - \beta_3$$

To test the first versus the fourth level of  $A$ , you would test

$$\beta_1 = -\beta_1 - \beta_2 - \beta_3$$

or, equivalently,

$$2\beta_1 + \beta_2 + \beta_3 = 0$$

which, in the form  $\mathbf{L}\boldsymbol{\beta} = 0$ , is

$$\begin{bmatrix} 2 & 1 & 1 \end{bmatrix} \begin{bmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \end{bmatrix} = 0$$

Therefore, you would use the following CONTRAST statement:

```
contrast '1 vs. 4' A 2 1 1;
```

To contrast the third level with the average of the first two levels, you would test

$$\frac{\beta_1 + \beta_2}{2} = \beta_3$$

or, equivalently,

$$\beta_1 + \beta_2 - 2\beta_3 = 0$$

Therefore, you would use the following CONTRAST statement:

```
contrast '1&2 vs. 3' A 1 1 -2;
```

Other CONTRAST statements are constructed similarly. For example:

```
contrast '1 vs. 2' A 1 -1 0;
contrast '1&2 vs. 4' A 3 3 2;
contrast '1&2 vs. 3&4' A 2 2 0;
contrast 'Main Effect' A 1 0 0,
A 0 1 0,
A 0 0 1;
```

## Less-Than-Full-Rank Parameterized Effects

When you use the less-than-full-rank parameterization (by specifying `PARAM=GLM` in the `CLASS` statement), each row is checked for estimability; see the section “[Estimable Functions](#)” on page 59 in Chapter 3, “[Introduction to Statistical Modeling with SAS/STAT Software](#),” for more information. If PROC LOGISTIC finds a contrast to be nonestimable, it displays missing values in corresponding rows in the results. PROC LOGISTIC handles missing level combinations of classification variables in the same manner as PROC GLM: parameters corresponding to missing level combinations are not included in the model. This convention can affect the way in which you specify the  $\mathbf{L}$  matrix in your CONTRAST statement. If the elements of  $\mathbf{L}$  are not specified for an effect that contains a specified effect, then the elements of the specified effect are distributed over the levels of the higher-order effect just as the GLM procedure does for its CONTRAST and ESTIMATE statements. For example, suppose that the model contains effects A and B and their interaction A\*B. If you specify a CONTRAST statement involving A alone, the  $\mathbf{L}$  matrix contains nonzero terms for both A and A\*B, since A\*B contains A. See rule 4 in the section “[Construction of Least Squares Means](#)” on page 3363 in Chapter 42, “[The GLM Procedure](#),” for more details.

## EFFECT Statement

**EFFECT** *name=effect-type (variables < / options>)* ;

The EFFECT statement enables you to construct special collections of columns for design matrices. These collections are referred to as *constructed effects* to distinguish them from the usual model effects that are formed from continuous or classification variables, as discussed in the section “GLM Parameterization of Classification Variables and Effects” on page 383 in Chapter 19, “Shared Concepts and Topics.”

You can specify the following *effect-types*:

|                          |                                                                                                                                                                                                           |
|--------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>COLLECTION</b>        | is a collection effect that defines one or more variables as a single effect with multiple degrees of freedom. The variables in a collection are considered as a unit for estimation and inference.       |
| <b>LAG</b>               | is a classification effect in which the level that is used for a given period corresponds to the level in the preceding period.                                                                           |
| <b>MULTIMEMBER   MM</b>  | is a multimember classification effect whose levels are determined by one or more variables that appear in a CLASS statement.                                                                             |
| <b>POLYNOMIAL   POLY</b> | is a multivariate polynomial effect in the specified numeric variables.                                                                                                                                   |
| <b>SPLINE</b>            | is a regression spline effect whose columns are univariate spline expansions of one or more variables. A spline expansion replaces the original variable with an expanded or larger set of new variables. |

Table 54.3 summarizes the *options* available in the EFFECT statement.

**Table 54.3** EFFECT Statement Options

| Option                             | Description                                                                                                                                          |
|------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Collection Effects Options</b>  |                                                                                                                                                      |
| DETAILS                            | Displays the constituents of the collection effect                                                                                                   |
| <b>Lag Effects Options</b>         |                                                                                                                                                      |
| DESIGNROLE=                        | Names a variable that controls to which lag design an observation is assigned                                                                        |
| DETAILS                            | Displays the lag design of the lag effect                                                                                                            |
| NLAG=                              | Specifies the number of periods in the lag                                                                                                           |
| PERIOD=                            | Names the variable that defines the period                                                                                                           |
| WITHIN=                            | Names the variable or variables that define the group within which each period is defined                                                            |
| <b>Multimember Effects Options</b> |                                                                                                                                                      |
| NOEFFECT                           | Specifies that observations with all missing levels for the multimember variables should have zero values in the corresponding design matrix columns |
| WEIGHT=                            | Specifies the weight variable for the contributions of each of the classification effects                                                            |

Table 54.3 *continued*

| Option                            | Description                                                                                             |
|-----------------------------------|---------------------------------------------------------------------------------------------------------|
| <b>Polynomial Effects Options</b> |                                                                                                         |
| DEGREE=                           | Specifies the degree of the polynomial                                                                  |
| MDEGREE=                          | Specifies the maximum degree of any variable in a term of the polynomial                                |
| STANDARDIZE=                      | Specifies centering and scaling suboptions for the variables that define the polynomial                 |
| <b>Spline Effects Options</b>     |                                                                                                         |
| BASIS=                            | Specifies the type of basis (B-spline basis or truncated power function basis) for the spline expansion |
| DEGREE=                           | Specifies the degree of the spline transformation                                                       |
| KNOTMETHOD=                       | Specifies how to construct the knots for spline effects                                                 |

For more information about the syntax of these *effect-types* and how columns of constructed effects are computed, see the section “EFFECT Statement” on page 393 in Chapter 19, “Shared Concepts and Topics.”

## EFFECTPLOT Statement

**EFFECTPLOT** < *plot-type* < (*plot-definition-options*) > > < / *options* > ;

The EFFECTPLOT statement produces a display of the fitted model and provides options for changing and enhancing the displays. Table 54.4 describes the available *plot-types* and their *plot-definition-options*.

Table 54.4 *Plot-Types and Plot-Definition-Options*

| Plot-Type and Description                                                                                                                                                                                                      | Plot-Definition-Options                                                                                   |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------|
| <b>BOX</b><br>Displays a box plot of continuous response data at each level of a CLASS effect, with predicted values superimposed and connected by a line. This is an alternative to the <b>INTERACTION</b> <i>plot-type</i> . | <b>PLOTBY=</b> variable or CLASS effect<br><b>X=</b> CLASS variable or effect                             |
| <b>CONTOUR</b><br>Displays a contour plot of predicted values against two continuous covariates.                                                                                                                               | <b>PLOTBY=</b> variable or CLASS effect<br><b>X=</b> continuous variable<br><b>Y=</b> continuous variable |
| <b>FIT</b><br>Displays a curve of predicted values versus a continuous variable.                                                                                                                                               | <b>PLOTBY=</b> variable or CLASS effect<br><b>X=</b> continuous variable                                  |

Table 54.4 continued

| Plot-Type and Description                                                                                                                                                                                                                    | Plot-Definition-Options                                                                                             |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------|
| <p><b>INTERACTION</b></p> <p>Displays a plot of predicted values (possibly with error bars) versus the levels of a CLASS effect. The predicted values are connected with lines and can be grouped by the levels of another CLASS effect.</p> | <p>PLOTBY= variable or CLASS effect</p> <p>SLICEBY= variable or CLASS effect</p> <p>X= CLASS variable or effect</p> |
| <p><b>SLICEFIT</b></p> <p>Displays a curve of predicted values versus a continuous variable grouped by the levels of a CLASS effect.</p>                                                                                                     | <p>PLOTBY= variable or CLASS effect</p> <p>SLICEBY= variable or CLASS effect</p> <p>X= continuous variable</p>      |

For full details about the syntax and options of the EFFECTPLOT statement, see the section “EFFECTPLOT Statement” on page 411 in Chapter 19, “Shared Concepts and Topics.”

See Outputs 54.2.11, 54.2.12, 54.3.5, 54.4.8, 54.7.4, and 54.15.4 for examples of plots produced by this statement.

## ESTIMATE Statement

```
ESTIMATE <'label'> estimate-specification <(divisor=n)>
 < , ... <'label'> estimate-specification <(divisor=n)> >
 </ options > ;
```

The ESTIMATE statement provides a mechanism for obtaining custom hypothesis tests. Estimates are formed as linear estimable functions of the form  $L\beta$ . You can perform hypothesis tests for the estimable functions, construct confidence limits, and obtain specific nonlinear transformations.

Table 54.5 summarizes the options available in the ESTIMATE statement.

Table 54.5 ESTIMATE Statement Options

| Option                                                     | Description                                                               |
|------------------------------------------------------------|---------------------------------------------------------------------------|
| <b>Construction and Computation of Estimable Functions</b> |                                                                           |
| DIVISOR=                                                   | Specifies a list of values to divide the coefficients                     |
| NOFILL                                                     | Suppresses the automatic fill-in of coefficients for higher-order effects |
| SINGULAR=                                                  | Tunes the estimability checking difference                                |

Table 54.5 *continued*

| Option                                              | Description                                                                     |
|-----------------------------------------------------|---------------------------------------------------------------------------------|
| <b>Degrees of Freedom and <math>p</math>-values</b> |                                                                                 |
| ADJUST=                                             | Determines the method for multiple comparison adjustment of estimates           |
| ALPHA= $\alpha$                                     | Determines the confidence level ( $1 - \alpha$ )                                |
| LOWER                                               | Performs one-sided, lower-tailed inference                                      |
| STEPDOWN                                            | Adjusts multiplicity-corrected $p$ -values further in a step-down fashion       |
| TESTVALUE=                                          | Specifies values under the null hypothesis for tests                            |
| UPPER                                               | Performs one-sided, upper-tailed inference                                      |
| <b>Statistical Output</b>                           |                                                                                 |
| CL                                                  | Constructs confidence limits                                                    |
| CORR                                                | Displays the correlation matrix of estimates                                    |
| COV                                                 | Displays the covariance matrix of estimates                                     |
| E                                                   | Prints the $L$ matrix                                                           |
| JOINT                                               | Produces a joint $F$ or chi-square test for the estimable functions             |
| SEED=                                               | Specifies the seed for computations that depend on random numbers               |
| <b>Generalized Linear Modeling</b>                  |                                                                                 |
| CATEGORY=                                           | Specifies how to construct estimable functions with multinomial data            |
| EXP                                                 | Exponentiates and displays estimates                                            |
| ILINK                                               | Computes and displays estimates and standard errors on the inverse linked scale |

For details about the syntax of the ESTIMATE statement, see the section “ESTIMATE Statement” on page 437 in Chapter 19, “Shared Concepts and Topics.”

## EXACT Statement

**EXACT** < *label* > < INTERCEPT > < *effects* > < / *options* > ;

The EXACT statement performs exact tests of the parameters for the specified *effects* and optionally estimates the parameters and outputs the exact conditional distributions. You can specify the keyword INTERCEPT and any effects in the MODEL statement. Inference on the parameters of the specified effects is performed by conditioning on the sufficient statistics of all the other model parameters (possibly including the intercept).

You can specify several EXACT statements, but they must follow the MODEL statement. Each statement can optionally include an identifying *label*. If several EXACT statements are specified, any statement without a label is assigned a label of the form “Exact $n$ ,” where  $n$  indicates the  $n$ th EXACT statement. The label is included in the headers of the displayed exact analysis tables.



If a **STRATA** statement is also specified, then a stratified exact logistic regression is performed. The model contains a different intercept for each stratum, and these intercepts are conditioned out of the model along with any other nuisance parameters (parameters for effects specified in the **MODEL** statement that are not in the **EXACT** statement).

If the **LINK=GLOGIT** option is specified in the **MODEL** statement, then the **METHOD=DIRECT** option is invoked in the **EXACTOPTIONS** statement by default and a generalized logit model is fit. Since each effect specified in the **MODEL** statement adds  $k$  parameters to the model (where  $k + 1$  is the number of response levels), exact analysis of the generalized logit model by using this method is limited to rather small problems.

The **CONTRAST**, **ESTIMATE**, **LSMEANS**, **LSMESTIMATE**, **ODDSRATIO**, **OUTPUT**, **ROC**, **ROCCONTRAST**, **SCORE**, **SLICE**, **STORE**, **TEST**, and **UNITS** statements are not available with an exact analysis; results from these statements are based on the asymptotic results. Exact analyses are not performed when you specify a **WEIGHT** statement, a link other than **LINK=LOGIT** or **LINK=GLOGIT**, an offset variable, the **NOFIT** option, or a model selection method. Exact estimation is not available for ordinal response models.

For classification variables, use of the reference parameterization is recommended.

The following options can be specified in each **EXACT** statement after a slash (/):

**ALPHA=number**

specifies the level of significance  $\alpha$  for  $100(1 - \alpha)\%$  confidence limits for the parameters or odds ratios. The value of *number* must be between 0 and 1. By default, *number* is equal to the value of the **ALPHA=** option in the **PROC LOGISTIC** statement, or 0.05 if that option is not specified.

**CLTYPE=EXACT | MIDP**

requests either the exact or mid- $p$  confidence intervals for the parameter estimates. By default, the exact intervals are produced. The confidence coefficient can be specified with the **ALPHA=** option. The mid- $p$  interval can be modified with the **MIDPFACTOR=** option. See the section “Exact Conditional Logistic Regression” on page 4274 for details.

**ESTIMATE <=keyword>**

estimates the individual parameters (conditioned on all other parameters) for the effects specified in the **EXACT** statement. For each parameter, a point estimate, a standard error, a confidence interval, and a  $p$ -value for a two-sided test that the parameter is zero are displayed. Note that the two-sided  $p$ -value is twice the one-sided  $p$ -value. You can optionally specify one of the following keywords:

**PARAM** specifies that the parameters be estimated. This is the default.

**ODDS** specifies that the odds ratios be estimated. If you have classification variables, then you must also specify the **PARAM=REF** option in the **CLASS** statement.

**BOTH** specifies that both the parameters and odds ratios be estimated.

**JOINT**

performs the joint test that all of the parameters are simultaneously equal to zero, performs individual hypothesis tests for the parameter of each continuous variable, and performs joint tests for the parameters of each classification variable. The joint test is indicated in the “Conditional Exact Tests” table by the label “Joint.”

**JOINTONLY**

performs only the joint test of the parameters. The test is indicated in the “Conditional Exact Tests” table by the label “Joint.” When this option is specified, individual tests for the parameters of each continuous variable and joint tests for the parameters of the classification variables are not performed.

**MIDPFACTOR= $\delta_1$  | ( $\delta_1, \delta_2$ )**

sets the tie factors used to produce the mid- $p$  hypothesis statistics and the mid- $p$  confidence intervals.  $\delta_1$  modifies both the hypothesis tests and confidence intervals, while  $\delta_2$  affects only the hypothesis tests. By default,  $\delta_1 = 0.5$  and  $\delta_2 = 1.0$ . See the section “[Exact Conditional Logistic Regression](#)” on page 4274 for details.

**ONESIDED**

requests one-sided confidence intervals and  $p$ -values for the individual parameter estimates and odds ratios. The one-sided  $p$ -value is the smaller of the left- and right-tail probabilities for the observed sufficient statistic of the parameter under the null hypothesis that the parameter is zero. The two-sided  $p$ -values (default) are twice the one-sided  $p$ -values. See the section “[Exact Conditional Logistic Regression](#)” on page 4274 for more details.

**OUTDIST=*SAS-data-set***

names the SAS data set that contains the exact conditional distributions. This data set contains all of the exact conditional distributions that are required to process the corresponding EXACT statement. This data set contains the possible sufficient statistics for the parameters of the effects specified in the EXACT statement, the counts, and, when hypothesis tests are performed on the parameters, the probability of occurrence and the score value for each sufficient statistic. When you request an OUTDIST= data set, the observed sufficient statistics are displayed in the “Sufficient Statistics” table. See the section “[OUTDIST= Output Data Set](#)” on page 4281 for more information.

**EXACT Statement Examples**

In the following example, two exact tests are computed: one for  $x_1$  and the other for  $x_2$ . The test for  $x_1$  is based on the exact conditional distribution of the sufficient statistic for the  $x_1$  parameter given the observed values of the sufficient statistics for the intercept,  $x_2$ , and  $x_3$  parameters; likewise, the test for  $x_2$  is conditional on the observed sufficient statistics for the intercept,  $x_1$ , and  $x_3$ .

```
proc logistic;
 model y= x1 x2 x3;
 exact x1 x2;
run;
```

PROC LOGISTIC determines, from all the specified EXACT statements, the distinct conditional distributions that need to be evaluated. For example, there is only one exact conditional distribution for the following two EXACT statements:

```
exact 'One' x1 / estimate=parm;
exact 'Two' x1 / estimate=parm onesided;
```

For each EXACT statement, individual tests for the parameters of the specified effects are computed unless the **JOINTONLY** option is specified. Consider the following EXACT statements:

```

exact 'E12' x1 x2 / estimate;
exact 'E1' x1 / estimate;
exact 'E2' x2 / estimate;
exact 'J12' x1 x2 / joint;

```

In the E12 statement, the parameters for x1 and x2 are estimated and tested separately. Specifying the E12 statement is equivalent to specifying both the E1 and E2 statements. In the J12 statement, the joint test for the parameters of x1 and x2 is computed in addition to the individual tests for x1 and x2.

---

## EXACTOPTIONS Statement

**EXACTOPTIONS** *options* ;

The EXACTOPTIONS statement specifies options that apply to every **EXACT** statement in the program. The following *options* are available:

### ABSFCNV=*value*

specifies the absolute function convergence criterion. Convergence requires a small change in the log-likelihood function in subsequent iterations,

$$|l_i - l_{i-1}| < \textit{value}$$

where  $l_i$  is the value of the log-likelihood function at iteration  $i$ .

By default, ABSFCNV=1E-12. You can also specify the **FCNV=** and **XCONV=** criteria; optimizations are terminated as soon as one criterion is satisfied.

### ADDTOBS

adds the observed sufficient statistic to the sampled exact distribution if the statistic was not sampled. This option has no effect unless the **METHOD=NETWORKMC** option is specified and the **ESTIMATE** option is specified in the **EXACT** statement. If the observed statistic has not been sampled, then the parameter estimate does not exist; by specifying this option, you can produce (biased) estimates.

### BUILDSUBSETS

builds every distribution for sampling. By default, some exact distributions are created by taking a subset of a previously generated exact distribution. When the **METHOD=NETWORKMC** option is invoked, this subsetting behavior has the effect of using fewer than the desired  $n$  samples; see the **N=** option for more details. Use the **BUILDSUBSETS** option to suppress this subsetting.

### EPSILON=*value*

controls how the partial sums  $\sum_{i=1}^j y_i x_i$  are compared. *value* must be between 0 and 1; by default, *value*=1E-8.

### FCNV=*value*

specifies the relative function convergence criterion. Convergence requires a small relative change in the log-likelihood function in subsequent iterations,

$$\frac{|l_i - l_{i-1}|}{|l_{i-1}| + 1\text{E-}6} < \textit{value}$$

where  $l_i$  is the value of the log likelihood at iteration  $i$ .

By default, FCONV=1E-8. You can also specify the ABSFCONV= and XCONV= criteria; if more than one criterion is specified, then optimizations are terminated as soon as one criterion is satisfied.

**MAXTIME=seconds**

specifies the maximum clock time (in seconds) that PROC LOGISTIC can use to calculate the exact distributions. If the limit is exceeded, the procedure halts all computations and prints a note to the LOG. The default maximum clock time is seven days.

**METHOD=keyword**

specifies which exact conditional algorithm to use for every EXACT statement specified. You can specify one of the following keywords:

**DIRECT** invokes the multivariate shift algorithm of Hirji, Mehta, and Patel (1987). This method directly builds the exact distribution, but it can require an excessive amount of memory in its intermediate stages. METHOD=DIRECT is invoked by default when you are conditioning out at most the intercept, or when the LINK=GLOGIT option is specified in the MODEL statement.

**NETWORK** invokes an algorithm described in Mehta, Patel, and Senchaudhuri (1992). This method builds a network for each parameter that you are conditioning out, combines the networks, then uses the multivariate shift algorithm to create the exact distribution. The NETWORK method can be faster and require less memory than the DIRECT method. The NETWORK method is invoked by default for most analyses.

**NETWORKMC** invokes the hybrid network and Monte Carlo algorithm of Mehta, Patel, and Senchaudhuri (1992). This method creates a network, then samples from that network; this method does not reject any of the samples at the cost of using a large amount of memory to create the network. METHOD=NETWORKMC is most useful for producing parameter estimates for problems that are too large for the DIRECT and NETWORK methods to handle and for which asymptotic methods are invalid—for example, for sparse data on a large grid.

**N=n**

specifies the number of Monte Carlo samples to take when the METHOD=NETWORKMC option is specified. By default,  $n = 10,000$ . If the procedure cannot obtain  $n$  samples due to a lack of memory, then a note is printed in the SAS log (the number of valid samples is also reported in the listing) and the analysis continues.

The number of samples used to produce any particular statistic might be smaller than  $n$ . For example, let  $X1$  and  $X2$  be continuous variables, denote their joint distribution by  $f(X1, X2)$ , and let  $f(X1 | X2 = x2)$  denote the marginal distribution of  $X1$  conditioned on the observed value of  $X2$ . If you request the JOINT test of  $X1$  and  $X2$ , then  $n$  samples are used to generate the estimate  $\hat{f}(X1, X2)$  of  $f(X1, X2)$ , from which the test is computed. However, the parameter estimate for  $X1$  is computed from the subset of  $\hat{f}(X1, X2)$  that has  $X2 = x2$ , and this subset need not contain  $n$  samples. Similarly, the distribution for each level of a classification variable is created by extracting the appropriate subset from the joint distribution for the CLASS variable.

In some cases, the marginal sample size can be too small to admit accurate estimation of a particular statistic; a note is printed in the SAS log when a marginal sample size is less than 100. Increasing  $n$

increases the number of samples used in a marginal distribution; however, if you want to control the sample size exactly, you can either specify the **BUILDSUBSETS** option or do both of the following:

- Remove the **JOINT** option from the **EXACT** statement.
- Create dummy variables in a **DATA** step to represent the levels of a **CLASS** variable, and specify them as independent variables in the **MODEL** statement.

### **NOLOGSCALE**

specifies that computations for the exact conditional models be computed by using normal scaling. Log scaling can handle numerically larger problems than normal scaling; however, computations in the log scale are slower than computations in normal scale.

### **ONDISK**

uses disk space instead of random access memory to build the exact conditional distribution. Use this option to handle larger problems at the cost of slower processing.

### **SEED=seed**

specifies the initial seed for the random number generator used to take the Monte Carlo samples when the **METHOD=NETWORKMC** option is specified. The value of the **SEED=** option must be an integer. If you do not specify a seed, or if you specify a value less than or equal to zero, then PROC LOGISTIC uses the time of day from the computer's clock to generate an initial seed.

### **STATUSN=number**

prints a status line in the SAS log after every *number* of Monte Carlo samples when the **METHOD=NETWORKMC** option is specified. The number of samples taken and the current exact *p*-value for testing the significance of the model are displayed. You can use this status line to track the progress of the computation of the exact conditional distributions.

### **STATUSTIME=seconds**

specifies the time interval (in seconds) for printing a status line in the LOG. You can use this status line to track the progress of the computation of the exact conditional distributions. The time interval you specify is approximate; the actual time interval varies. By default, no status reports are produced.

### **XCONV=value**

specifies the relative parameter convergence criterion. Convergence requires a small relative parameter change in subsequent iterations,

$$\max_j |\delta_j^{(i)}| < value$$

where

$$\delta_j^{(i)} = \begin{cases} \beta_j^{(i)} - \beta_j^{(i-1)} & |\beta_j^{(i-1)}| < 0.01 \\ \frac{\beta_j^{(i)} - \beta_j^{(i-1)}}{\beta_j^{(i-1)}} & \text{otherwise} \end{cases}$$

and  $\beta_j^{(i)}$  is the estimate of the *j*th parameter at iteration *i*.

By default, **XCONV=1E-4**. You can also specify the **ABSFCNV=** and **FCONV=** criteria; if more than one criterion is specified, then optimizations are terminated as soon as one criterion is satisfied.

---

## FREQ Statement

**FREQ** *variable* ;

The FREQ statement identifies a *variable* that contains the frequency of occurrence of each observation. PROC LOGISTIC treats each observation as if it appears  $n$  times, where  $n$  is the value of the FREQ variable for the observation. If it is not an integer, the frequency value is truncated to an integer. If the frequency value is less than 1 or missing, the observation is not used in the model fitting. When the FREQ statement is not specified, each observation is assigned a frequency of 1. If you specify more than one FREQ statement, then the first statement is used.

If a SCORE statement is specified, then the FREQ variable is used for computing fit statistics and the ROC curve, but they are not required for scoring. If the DATA= data set in the SCORE statement does not contain the FREQ variable, the frequency values are assumed to be 1 and a warning message is issued in the LOG. If you fit a model and perform the scoring in the same run, the same FREQ variable is used for fitting and scoring. If you fit a model in a previous run and input it with the INMODEL= option in the current run, then the FREQ variable can be different from the one used in the previous run. However, if a FREQ variable was not specified in the previous run, you can still specify a FREQ variable in the current run.

---

## ID Statement

**ID** *variable*< *variable*,... > ;

The ID statement specifies variables in the DATA= data set that are used for labeling ROC curves and influence diagnostic plots. If more than one ID variable is specified, then the plots are labeled by concatenating the ID variable values together. See the PLOTS(LABEL) and ROCOPTIONS(ID) options in the PROC LOGISTIC statement for more details.

---

## LSMEANS Statement

**LSMEANS** < *model-effects* > < / *options* > ;

The LSMEANS statement computes and compares least squares means (LS-means) of fixed effects. LS-means are *predicted population margins*—that is, they estimate the marginal means over a balanced population. In a sense, LS-means are to unbalanced designs as class and subclass arithmetic means are to balanced designs.

Table 54.6 summarizes the options available in the LSMEANS statement.

**Table 54.6** LSMEANS Statement Options

| Option                                              | Description                                                                                                       |
|-----------------------------------------------------|-------------------------------------------------------------------------------------------------------------------|
| <b>Construction and Computation of LS-Means</b>     |                                                                                                                   |
| AT                                                  | Modifies the covariate value in computing LS-means                                                                |
| BYLEVEL                                             | Computes separate margins                                                                                         |
| DIFF                                                | Requests differences of LS-means                                                                                  |
| OM=                                                 | Specifies the weighting scheme for LS-means computation as determined by the input data set                       |
| SINGULAR=                                           | Tunes estimability checking                                                                                       |
| <b>Degrees of Freedom and <math>p</math>-values</b> |                                                                                                                   |
| ADJUST=                                             | Determines the method for multiple-comparison adjustment of LS-means differences                                  |
| ALPHA= $\alpha$                                     | Determines the confidence level ( $1 - \alpha$ )                                                                  |
| STEPDOWN                                            | Adjusts multiple-comparison $p$ -values further in a step-down fashion                                            |
| <b>Statistical Output</b>                           |                                                                                                                   |
| CL                                                  | Constructs confidence limits for means and mean differences                                                       |
| CORR                                                | Displays the correlation matrix of LS-means                                                                       |
| COV                                                 | Displays the covariance matrix of LS-means                                                                        |
| E                                                   | Prints the L matrix                                                                                               |
| LINES                                               | Produces a “Lines” display for pairwise LS-means differences                                                      |
| MEANS                                               | Prints the LS-means                                                                                               |
| PLOTS=                                              | Requests graphs of means and mean comparisons                                                                     |
| SEED=                                               | Specifies the seed for computations that depend on random numbers                                                 |
| <b>Generalized Linear Modeling</b>                  |                                                                                                                   |
| EXP                                                 | Exponentiates and displays estimates of LS-means or LS-means differences                                          |
| ILINK                                               | Computes and displays estimates and standard errors of LS-means (but not differences) on the inverse linked scale |
| ODDSRATIO                                           | Reports (simple) differences of least squares means in terms of odds ratios if permitted by the link function     |

For details about the syntax of the LSMEANS statement, see the section “LSMEANS Statement” on page 453 in Chapter 19, “Shared Concepts and Topics.”

**NOTE:** If you have classification variables in your model, then the LSMEANS statement is allowed only if you also specify the `PARAM=GLM` option.

---

## LSMESTIMATE Statement

```
LSMESTIMATE model-effect <'label'> values <divisor=n>
 < , ... <'label'> values <divisor=n> >
 </ options > ;
```

The LSMESTIMATE statement provides a mechanism for obtaining custom hypothesis tests among least squares means.

Table 54.7 summarizes the options available in the LSMESTIMATE statement.

**Table 54.7** LSMESTIMATE Statement Options

| Option                                              | Description                                                                         |
|-----------------------------------------------------|-------------------------------------------------------------------------------------|
| <b>Construction and Computation of LS-Means</b>     |                                                                                     |
| AT                                                  | Modifies covariate values in computing LS-means                                     |
| BYLEVEL                                             | Computes separate margins                                                           |
| DIVISOR=                                            | Specifies a list of values to divide the coefficients                               |
| OM=                                                 | Specifies the weighting scheme for LS-means computation as determined by a data set |
| SINGULAR=                                           | Tunes estimability checking                                                         |
| <b>Degrees of Freedom and <math>p</math>-values</b> |                                                                                     |
| ADJUST=                                             | Determines the method for multiple-comparison adjustment of LS-means differences    |
| ALPHA= $\alpha$                                     | Determines the confidence level ( $1 - \alpha$ )                                    |
| LOWER                                               | Performs one-sided, lower-tailed inference                                          |
| STEPDOWN                                            | Adjusts multiple-comparison $p$ -values further in a step-down fashion              |
| TESTVALUE=                                          | Specifies values under the null hypothesis for tests                                |
| UPPER                                               | Performs one-sided, upper-tailed inference                                          |
| <b>Statistical Output</b>                           |                                                                                     |
| CL                                                  | Constructs confidence limits for means and mean differences                         |
| CORR                                                | Displays the correlation matrix of LS-means                                         |
| COV                                                 | Displays the covariance matrix of LS-means                                          |
| E                                                   | Prints the <b>L</b> matrix                                                          |
| ELSM                                                | Prints the <b>K</b> matrix                                                          |
| JOINT                                               | Produces a joint $F$ or chi-square test for the LS-means and LS-means differences   |
| SEED=                                               | Specifies the seed for computations that depend on random numbers                   |

---



Table 54.7 continued

| Option                             | Description                                                                                                       |
|------------------------------------|-------------------------------------------------------------------------------------------------------------------|
| <b>Generalized Linear Modeling</b> |                                                                                                                   |
| CATEGORY=                          | Specifies how to construct estimable functions with multinomial data                                              |
| EXP                                | Exponentiates and displays LS-means estimates                                                                     |
| ILINK                              | Computes and displays estimates and standard errors of LS-means (but not differences) on the inverse linked scale |

For details about the syntax of the LSMESTIMATE statement, see the section “[LSMESTIMATE Statement](#)” on page 470 in Chapter 19, “[Shared Concepts and Topics](#).”

**NOTE:** If you have classification variables in your model, then the LSMESTIMATE statement is allowed only if you also specify the [PARAM=GLM](#) option.

## MODEL Statement

```
< label: > MODEL variable< (variable_options) > = < effects > < / options > ;
```

```
< label: > MODEL events/trials = < effects > < / options > ;
```

The MODEL statement names the response variable and the explanatory effects, including covariates, main effects, interactions, and nested effects; see the section “[Specification of Effects](#)” on page 3324 of Chapter 42, “[The GLM Procedure](#),” for more information. If you omit the explanatory effects, the procedure fits an intercept-only model. You must specify exactly one MODEL statement.

Two forms of the MODEL statement can be specified. The first form, referred to as *single-trial* syntax, is applicable to binary, ordinal, and nominal response data. The second form, referred to as *events/trials* syntax, is restricted to the case of binary response data. The single-trial syntax is used when each observation in the DATA= data set contains information about only a single trial, such as a single subject in an experiment. When each observation contains information about multiple binary-response trials, such as the counts of the number of subjects observed and the number responding, then events/trials syntax can be used.

In the events/trials syntax, you specify two variables that contain count data for a binomial experiment. These two variables are separated by a slash. The value of the first variable, *events*, is the number of positive responses (or events). The value of the second variable, *trials*, is the number of trials. The values of both *events* and (*trials*–*events*) must be nonnegative and the value of *trials* must be positive for the response to be valid.

In the single-trial syntax, you specify one variable (on the left side of the equal sign) as the response variable. This variable can be character or numeric. [Variable\\_options](#) specific to the response variable can be specified immediately after the response variable with parentheses around them.

For both forms of the MODEL statement, explanatory *effects* follow the equal sign. Variables can be either continuous or classification variables. Classification variables can be character or numeric, and they must be declared in the [CLASS](#) statement. When an effect is a classification variable, the procedure inserts a set of coded columns into the design matrix instead of directly entering a single column containing the values of the variable.

## Response Variable Options

### DESCENDING | DESC

reverses the order of the response categories. If both the DESCENDING and ORDER= options are specified, PROC LOGISTIC orders the response categories according to the ORDER= option and then reverses that order. See the section “Response Level Ordering” on page 4237 for more detail.

### EVENT='category' | keyword

specifies the event category for the binary response model. PROC LOGISTIC models the probability of the event category. The EVENT= option has no effect when there are more than two response categories. You can specify the value (formatted if a format is applied) of the event category in quotes, or you can specify one of the following keywords. The default is EVENT=FIRST.

#### FIRST

designates the first ordered category as the event.

#### LAST

designates the last ordered category as the event.

One of the most common sets of response levels is {0,1}, with 1 representing the event for which the probability is to be modeled. Consider the example where Y takes the values 1 and 0 for event and nonevent, respectively, and Exposure is the explanatory variable. To specify the value 1 as the event category, use the following MODEL statement:

```
model Y(event='1') = Exposure;
```

### ORDER= DATA | FORMATTED | FREQ | INTERNAL

specifies the sort order for the levels of the response variable. The following table displays the available ORDER= options:

| ORDER=    | Levels Sorted By                                                                                                                       |
|-----------|----------------------------------------------------------------------------------------------------------------------------------------|
| DATA      | order of appearance in the input data set                                                                                              |
| FORMATTED | external formatted value, except for numeric variables with no explicit format, which are sorted by their unformatted (internal) value |
| FREQ      | descending frequency count; levels with the most observations come first in the order                                                  |
| INTERNAL  | unformatted value                                                                                                                      |

By default, ORDER=FORMATTED. For ORDER=FORMATTED and ORDER=INTERNAL, the sort order is machine dependent. When ORDER=FORMATTED is in effect for numeric variables for which you have supplied no explicit format, the levels are ordered by their internal values.

For more information about sort order, see the chapter on the SORT procedure in the *Base SAS Procedures Guide* and the discussion of BY-group processing in *SAS Language Reference: Concepts*.

**REFERENCE=**'category' | keyword

**REF=**'category' | keyword

specifies the reference category for the generalized logit model and the binary response model. For the generalized logit model, each logit contrasts a nonreference category with the reference category. For the binary response model, specifying one response category as the reference is the same as specifying the other response category as the event category. You can specify the value (formatted if a format is applied) of the reference category in quotes, or you can specify one of the following keywords:

**FIRST** designates the first ordered category as the reference.

**LAST** designates the last ordered category as the reference. This is the default.

## Model Options

Table 54.8 summarizes the options available in the MODEL statement. These options can be specified after a slash (/).

**Table 54.8** Model Statement Options

| Option                                     | Description                                                                                                                                        |
|--------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Model Specification Options</b>         |                                                                                                                                                    |
| <b>LINK=</b>                               | Specifies the link function                                                                                                                        |
| <b>NOFIT</b>                               | Suppresses model fitting                                                                                                                           |
| <b>NOINT</b>                               | Suppresses the intercept                                                                                                                           |
| <b>OFFSET=</b>                             | Specifies the offset variable                                                                                                                      |
| <b>SELECTION=</b>                          | Specifies the effect selection method                                                                                                              |
| <b>UNEQUALSLOPES</b>                       | Specifies cumulative partial proportional odds models                                                                                              |
| <b>Effect Selection Options</b>            |                                                                                                                                                    |
| <b>BEST=</b>                               | Controls the number of models displayed for <b>SCORE</b> selection                                                                                 |
| <b>DETAILS</b>                             | Requests detailed results at each step                                                                                                             |
| <b>FAST</b>                                | Uses the fast elimination method                                                                                                                   |
| <b>HIERARCHY=</b>                          | Specifies whether and how hierarchy is maintained and whether a single effect or multiple effects are allowed to enter or leave the model per step |
| <b>INCLUDE=</b>                            | Specifies the number of effects included in every model                                                                                            |
| <b>MAXSTEP=</b>                            | Specifies the maximum number of steps for <b>STEPWISE</b> selection                                                                                |
| <b>SEQUENTIAL</b>                          | Adds or deletes effects in sequential order                                                                                                        |
| <b>SLENTRY=</b>                            | Specifies the significance level for entering effects                                                                                              |
| <b>SLSTAY=</b>                             | Specifies the significance level for removing effects                                                                                              |
| <b>START=</b>                              | Specifies the number of variables in the first model                                                                                               |
| <b>STOP=</b>                               | Specifies the number of variables in the final model                                                                                               |
| <b>STOPRES</b>                             | Adds or deletes variables by the residual chi-square criterion                                                                                     |
| <b>Model-Fitting Specification Options</b> |                                                                                                                                                    |
| <b>ABSFCNV=</b>                            | Specifies the absolute function convergence criterion                                                                                              |
| <b>FCONV=</b>                              | Specifies the relative function convergence criterion                                                                                              |

Table 54.8 *continued*

| Option                                                 | Description                                                                                                                |
|--------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------|
| FIRTH                                                  | Specifies Firth's penalized likelihood method                                                                              |
| GCONV=                                                 | Specifies the relative gradient convergence criterion                                                                      |
| MAXFUNCTION=                                           | Specifies the maximum number of function calls for the conditional analysis                                                |
| MAXITER=                                               | Specifies the maximum number of iterations                                                                                 |
| NOCHECK                                                | Suppresses checking for infinite parameters                                                                                |
| RIDGING=                                               | Specifies the technique used to improve the log-likelihood function when its value is worse than that of the previous step |
| SINGULAR=                                              | Specifies the tolerance for testing singularity                                                                            |
| TECHNIQUE=                                             | Specifies the iterative algorithm for maximization                                                                         |
| XCONV=                                                 | Specifies the relative parameter convergence criterion                                                                     |
| <b>Confidence Interval Options</b>                     |                                                                                                                            |
| ALPHA=                                                 | Specifies $\alpha$ for the $100(1 - \alpha)\%$ confidence intervals                                                        |
| CLODDS=                                                | Computes confidence intervals for odds ratios                                                                              |
| CLPARAM=                                               | Computes confidence intervals for parameters                                                                               |
| PLCONV=                                                | Specifies the profile-likelihood convergence criterion                                                                     |
| <b>Classification Options</b>                          |                                                                                                                            |
| CTABLE                                                 | Displays the classification table                                                                                          |
| PEVENT=                                                | Specifies prior event probabilities                                                                                        |
| PPROB=                                                 | Specifies probability cutpoints for classification                                                                         |
| <b>Overdispersion and Goodness-of-Fit Test Options</b> |                                                                                                                            |
| AGGREGATE=                                             | Determines subpopulations for Pearson chi-square and deviance                                                              |
| LACKFIT                                                | Requests the Hosmer and Lemeshow goodness-of-fit test                                                                      |
| SCALE=                                                 | Specifies the method to correct overdispersion                                                                             |
| <b>ROC Curve Options</b>                               |                                                                                                                            |
| OUTROC=                                                | Names the output ROC data set                                                                                              |
| ROCEPS=                                                | Specifies the probability grouping criterion                                                                               |
| <b>Regression Diagnostics Options</b>                  |                                                                                                                            |
| INFLUENCE                                              | Displays influence statistics                                                                                              |
| ILOTS                                                  | Requests index plots                                                                                                       |
| <b>Display Options</b>                                 |                                                                                                                            |
| CORRB                                                  | Displays the correlation matrix                                                                                            |
| COVB                                                   | Displays the covariance matrix                                                                                             |
| EXPB                                                   | Displays exponentiated values of the estimates                                                                             |
| ITPRINT                                                | Displays the iteration history                                                                                             |
| NODUMMYPRINT                                           | Suppresses the "Class Level Information" table                                                                             |
| PARMLABEL                                              | Displays parameter labels                                                                                                  |
| PCORR                                                  | Displays the partial correlation statistic                                                                                 |
| RSQUARE                                                | Displays the generalized R Square                                                                                          |
| STB                                                    | Displays standardized estimates                                                                                            |

Table 54.8 continued

| Option                       | Description                                                  |
|------------------------------|--------------------------------------------------------------|
| <b>Computational Options</b> |                                                              |
| <b>BINWIDTH=</b>             | Specifies the bin size for estimating association statistics |
| <b>NOLOGSCALE</b>            | Performs calculations by using normal scaling                |

The following list describes these options.

**ABSFCNV=*value***

specifies the absolute function convergence criterion. Convergence requires a small change in the log-likelihood function in subsequent iterations,

$$|l_i - l_{i-1}| < \textit{value}$$

where  $l_i$  is the value of the log-likelihood function at iteration  $i$ . See the section “[Convergence Criteria](#)” on page 4242 for more information.

**AGGREGATE<=(*variable-list*)>**

specifies the subpopulations on which the Pearson chi-square test statistic and the likelihood ratio chi-square test statistic (deviance) are calculated. Observations with common values in the given list of variables are regarded as coming from the same subpopulation. Variables in the list can be any variables in the input data set. Specifying the AGGREGATE option is equivalent to specifying the AGGREGATE= option with a variable list that includes all explanatory variables in the MODEL statement. The deviance and Pearson goodness-of-fit statistics are calculated only when the SCALE= option is specified. Thus, the AGGREGATE (or AGGREGATE=) option has no effect if the SCALE= option is not specified.

See the section “[Rescaling the Covariance Matrix](#)” on page 4257 for more information.

**ALPHA=*number***

sets the level of significance  $\alpha$  for  $100(1 - \alpha)\%$  confidence intervals for regression parameters or odds ratios. The value of *number* must be between 0 and 1. By default, *number* is equal to the value of the ALPHA= option in the PROC LOGISTIC statement, or 0.05 if the option is not specified. This option has no effect unless confidence limits for the parameters (CLPARM= option) or odds ratios (CLODDS= option or ODDSRATIO statement) are requested.

**BEST=*n***

specifies that  $n$  models with the highest score chi-square statistics are to be displayed for each model size. It is used exclusively with the SCORE model selection method. If the BEST= option is omitted and there are no more than 10 explanatory variables, then all possible models are listed for each model size. If the option is omitted and there are more than 10 explanatory variables, then the number of models selected for each model size is, at most, equal to the number of explanatory variables listed in the MODEL statement.

**BINWIDTH=*width***

specifies the size of the bins used for estimating the association statistics. See the section “[Rank Correlation of Observed Responses and Predicted Probabilities](#)” on page 4253 for details. Valid values are  $0 \leq \textit{width} < 1$  (for polytomous response models,  $0 < \textit{width} < 1$ ). The default *width* is 0.002. If the *width* does not evenly divide the unit interval, it is reduced to a valid value and a message

is displayed in the SAS log. The width is also constrained by the amount of memory available on your machine; if you specify a *width* that is too small, it is adjusted to a value for which memory can be allocated and a note is displayed in the SAS log.

If you have a binary response and specify **BINWIDTH=0**, then no binning is performed and the exact values of the statistics are computed; this method is a bit slower and might require more memory than the binning approach.

The **BINWIDTH=** option is ignored and no binning is performed when a **ROC** statement is specified, when ROC graphics are produced, or when the **SCORE** statement computes an ROC area.

#### **CLODDS=PL | WALD | BOTH**

produces confidence intervals for odds ratios of main effects not involved in interactions or nestings. Computation of these confidence intervals is based on the profile likelihood (**CLODDS=PL**) or based on individual Wald tests (**CLODDS=WALD**). By specifying **CLODDS=BOTH**, the procedure computes two sets of confidence intervals for the odds ratios, one based on the profile likelihood and the other based on the Wald tests. The confidence coefficient can be specified with the **ALPHA=** option. The **CLODDS=PL** option is not available with the **STRATA** statement. Classification main effects that use parameterizations other than **REF**, **EFFECT**, or **GLM** are ignored. If you need to compute odds ratios for an effect involved in interactions or nestings, or using some other parameterization, then you should specify an **ODDSRATIO** statement for that effect.

#### **CLPARM=PL | WALD | BOTH**

requests confidence intervals for the parameters. Computation of these confidence intervals is based on the profile likelihood (**CLPARM=PL**) or individual Wald tests (**CLPARM=WALD**). If you specify **CLPARM=BOTH**, the procedure computes two sets of confidence intervals for the parameters, one based on the profile likelihood and the other based on individual Wald tests. The confidence coefficient can be specified with the **ALPHA=** option. The **CLPARM=PL** option is not available with the **STRATA** statement.

See the section “[Confidence Intervals for Parameters](#)” on page 4248 for more information.

#### **CORRB**

displays the correlation matrix of the parameter estimates.

#### **COVB**

displays the covariance matrix of the parameter estimates.

#### **CTABLE**

classifies the input binary response observations according to whether the predicted event probabilities are above or below some cutpoint value  $z$  in the range (0, 1). An observation is predicted as an event if the predicted event probability exceeds or equals  $z$ . You can supply a list of cutpoints other than the default list by specifying the **PPROB=** option (page 4217). Also, false positive and negative rates can be computed as posterior probabilities by using Bayes’ theorem. You can use the **PEVENT=** option to specify prior probabilities for computing these rates. The **CTABLE** option is ignored if the data have more than two response levels. The **CTABLE** option is not available with the **STRATA** statement.

For more information, see the section “[Classification Table](#)” on page 4255.

**DETAILS**

produces a summary of computational details for each step of the effect selection process. It produces the “Analysis of Effects Eligible for Entry” table before displaying the effect selected for entry for forward or stepwise selection. For each model fitted, it produces the “Type 3 Analysis of Effects” table if the fitted model involves CLASS variables, the “Analysis of Maximum Likelihood Estimates” table, and measures of association between predicted probabilities and observed responses. For the statistics included in these tables, see the section “[Displayed Output](#)” on page 4286. The DETAILS option has no effect when SELECTION=NONE.

**EXPB****EXPEST**

displays the exponentiated values ( $e^{\hat{\beta}_i}$ ) of the parameter estimates  $\hat{\beta}_i$  in the “Analysis of Maximum Likelihood Estimates” table for the logit model. These exponentiated values are the estimated odds ratios for parameters corresponding to the continuous explanatory variables, and for CLASS effects that use reference or GLM parameterizations.

**FAST**

uses a computational algorithm of Lawless and Singhal (1978) to compute a first-order approximation to the remaining slope estimates for each subsequent elimination of a variable from the model. Variables are removed from the model based on these approximate estimates. The FAST option is extremely efficient because the model is not refitted for every variable removed. The FAST option is used when SELECTION=BACKWARD and in the backward elimination steps when SELECTION=STEPWISE. The FAST option is ignored when SELECTION=FORWARD or SELECTION=NONE.

**FCONV=value**

specifies the relative function convergence criterion. Convergence requires a small relative change in the log-likelihood function in subsequent iterations,

$$\frac{|l_i - l_{i-1}|}{|l_{i-1}| + 1\text{E-}6} < \text{value}$$

where  $l_i$  is the value of the log likelihood at iteration  $i$ . See the section “[Convergence Criteria](#)” on page 4242 for more information.

**FIRTH**

performs Firth’s penalized maximum likelihood estimation to reduce bias in the parameter estimates (Heinze and Schemper 2002; Firth 1993). This method is useful in cases of separability, as often occurs when the event is rare, and is an alternative to performing an exact logistic regression. See the section “[Firth’s Bias-Reducing Penalized Likelihood](#)” on page 4242 for more information.

**NOTE:** The intercept-only log likelihood is modified by using the full-model Hessian, computed with the slope parameters equal to zero. Therefore, in order to use the likelihood ratio test to compare models, you should use the log likelihoods from the “Model Fit Statistics” tables instead of the Likelihood Ratio statistic that is reported in the “Testing Global Null Hypothesis: BETA=0” table. When fitting a model and scoring a data set in the same PROC LOGISTIC step, the model is fit using Firth’s penalty for parameter estimation purposes, but the penalty is not applied to the scored log likelihood.



**GCONV=value**

specifies the relative gradient convergence criterion. Convergence requires that the normalized prediction function reduction is small,

$$\frac{\mathbf{g}'_i \mathbf{I}_i^{-1} \mathbf{g}_i}{|l_i| + 1\text{E-}6} < \text{value}$$

where  $l_i$  is the value of the log-likelihood function,  $\mathbf{g}_i$  is the gradient vector, and  $\mathbf{I}_i$  is the negative (expected) Hessian matrix, all at iteration  $i$ . This is the default convergence criterion, and the default value is 1E-8. See the section “[Convergence Criteria](#)” on page 4242 for more information.

**HIERARCHY=keyword****HIER=keyword**

specifies whether and how the model hierarchy requirement is applied and whether a single effect or multiple effects are allowed to enter or leave the model in one step. You can specify that only CLASS effects, or both CLASS and interval effects, be subject to the hierarchy requirement. The HIERARCHY= option is ignored unless you also specify one of the following options: [SELECTION=FORWARD](#), [SELECTION=BACKWARD](#), or [SELECTION=STEPWISE](#).

Model hierarchy refers to the requirement that, for any term to be in the model, all effects contained in the term must be present in the model. For example, in order for the interaction A\*B to enter the model, the main effects A and B must be in the model. Likewise, neither effect A nor B can leave the model while the interaction A\*B is in the model.

The keywords you can specify in the HIERARCHY= option are as follows:

**NONE** indicates that the model hierarchy is not maintained. Any single effect can enter or leave the model at any given step of the selection process.

**SINGLE** indicates that only one effect can enter or leave the model at one time, subject to the model hierarchy requirement. For example, suppose that you specify the main effects A and B and the interaction A\*B in the model. In the first step of the selection process, either A or B can enter the model. In the second step, the other main effect can enter the model. The interaction effect can enter the model only when both main effects have already been entered. Also, before A or B can be removed from the model, the A\*B interaction must first be removed. All effects (CLASS and interval) are subject to the hierarchy requirement.

**SINGLECLASS** is the same as HIERARCHY=SINGLE except that only CLASS effects are subject to the hierarchy requirement.

**MULTIPLE** indicates that more than one effect can enter or leave the model at one time, subject to the model hierarchy requirement. In a forward selection step, a single main effect can enter the model, or an interaction can enter the model together with all the effects that are contained in the interaction. In a backward elimination step, an interaction itself, or the interaction together with all the effects that the interaction contains, can be removed. All effects (CLASS and continuous) are subject to the hierarchy requirement.

**MULTIPLECLASS** is the same as HIERARCHY=MULTIPLE except that only CLASS effects are subject to the hierarchy requirement.

The default value is HIERARCHY=SINGLE, which means that model hierarchy is to be maintained for all effects (that is, both CLASS and continuous effects) and that only a single effect can enter or leave the model at each step.



**INCLUDE=*n***

includes the first *n* effects in the MODEL statement in every model. By default, INCLUDE=0. The INCLUDE= option has no effect when SELECTION=NONE.

Note that the INCLUDE= and START= options perform different tasks: the INCLUDE= option includes the first *n* effects variables in every model, whereas the START= option requires only that the first *n* effects appear in the first model.

**INFLUENCE<(STDRES)>**

displays diagnostic measures for identifying influential observations in the case of a binary response model. For each observation, the INFLUENCE option displays the case number (which is the sequence number of the observation), the values of the explanatory variables included in the final model, and the regression diagnostic measures developed by Pregibon (1981). The STDRES option includes standardized and likelihood residuals in the display.

For a discussion of these diagnostic measures, see the section “Regression Diagnostics” on page 4263. When a STRATA statement is specified, the diagnostics are computed following Storer and Crowley (1985); see the section “Regression Diagnostic Details” on page 4272 for details.

**IPLOTS**

produces an index plot for the regression diagnostic statistics developed by Pregibon (1981). An index plot is a scatter plot with the regression diagnostic statistic represented on the Y axis and the case number on the X axis. See Example 54.6 for an illustration.

**ITPRINT**

displays the iteration history of the maximum-likelihood model fitting. The ITPRINT option also displays the last evaluation of the gradient vector and the final change in the  $-2$  Log Likelihood.

**LACKFIT<(n)>**

performs the Hosmer and Lemeshow goodness-of-fit test (Hosmer and Lemeshow 2000) for the case of a binary response model. The subjects are divided into approximately 10 groups of roughly the same size based on the percentiles of the estimated probabilities. The discrepancies between the observed and expected number of observations in these groups are summarized by the Pearson chi-square statistic, which is then compared to a chi-square distribution with *t* degrees of freedom, where *t* is the number of groups minus *n*. By default, *n* = 2. A small *p*-value suggests that the fitted model is not an adequate model. The LACKFIT option is not available with the STRATA statement. See the section “The Hosmer-Lemeshow Goodness-of-Fit Test” on page 4259 for more information.

**LINK=keyword****L=keyword**

specifies the link function linking the response probabilities to the linear predictors. You can specify one of the following keywords. The default is LINK=LOGIT.

**CLOGLOG** is the complementary log-log function. PROC LOGISTIC fits the binary complementary log-log model when there are two response categories and fits the cumulative complementary log-log model when there are more than two response categories. The aliases are CCLOGLOG, CCLL, and CUMCLOGLOG.

- GLOGIT** is the generalized logit function. PROC LOGISTIC fits the generalized logit model where each nonreference category is contrasted with the reference category. You can use the response variable option **REF=** to specify the reference category.
- LOGIT** is the log odds function. PROC LOGISTIC fits the binary logit model when there are two response categories and fits the cumulative logit model when there are more than two response categories. The aliases are CLOGIT and CUMLOGIT.
- PROBIT** is the inverse standard normal distribution function. PROC LOGISTIC fits the binary probit model when there are two response categories and fits the cumulative probit model when there are more than two response categories. The aliases are NORMIT, CPROBIT, and CUMPROBIT.

The **LINK=** option is not available with the **STRATA** statement.

See the section “[Link Functions and the Corresponding Distributions](#)” on page 4238 for more details.

**MAXFUNCTION=number**

specifies the maximum number of function calls to perform when maximizing the conditional likelihood. This option is valid only when a **STRATA** statement or the **UNEQUALSLOPES** option is specified. The default values are as follows:

- 125 when the number of parameters  $p < 40$
- 500 when  $40 \leq p < 400$
- 1000 when  $p \geq 400$

Since the optimization is terminated only after completing a full iteration, the number of function calls that are actually performed can exceed *number*. If convergence is not attained, the displayed output and all output data sets created by the procedure contain results based on the last maximum likelihood iteration.

**MAXITER=number**

specifies the maximum number of iterations to perform. By default, **MAXITER=25**. If convergence is not attained in *number* iterations, the displayed output and all output data sets created by the procedure contain results that are based on the last maximum likelihood iteration.

**MAXSTEP=n**

specifies the maximum number of times any explanatory variable is added to or removed from the model when **SELECTION=STEPWISE**. The default number is twice the number of explanatory variables in the MODEL statement. When the **MAXSTEP=** limit is reached, the stepwise selection process is terminated. All statistics displayed by the procedure (and included in output data sets) are based on the last model fitted. The **MAXSTEP=** option has no effect when **SELECTION=NONE**, **FORWARD**, or **BACKWARD**.

**NOCHECK**

disables the checking process to determine whether maximum likelihood estimates of the regression parameters exist. If you are sure that the estimates are finite, this option can reduce the execution time if the estimation takes more than eight iterations. For more information, see the section “[Existence of Maximum Likelihood Estimates](#)” on page 4242.

**NODUMMYPRINT****NODESIGNPRINT****NODP**

suppresses the “Class Level Information” table, which shows how the design matrix columns for the CLASS variables are coded.

**NOINT**

suppresses the intercept for the binary response model, the first intercept for the ordinal response model (which forces all intercepts to be nonnegative), or all intercepts for the generalized logit model. This can be particularly useful in conditional logistic analysis; see [Example 54.11](#).

**NOFIT**

performs the global score test without fitting the model. The global score test evaluates the joint significance of the effects in the MODEL statement. No further analyses are performed. If the NOFIT option is specified along with other MODEL statement options, NOFIT takes effect and all other options except FIRTH, LINK=, NOINT, OFFSET=, ROC, and TECHNIQUE= are ignored. The NOFIT option is not available with the STRATA statement.

**NOLOGSCALE**

specifies that computations for the conditional and exact logistic regression models should be computed by using normal scaling. Log scaling can handle numerically larger problems than normal scaling; however, computations in the log scale are slower than computations in normal scale.

**OFFSET=*name***

names the offset variable. The regression coefficient for this variable will be fixed at 1. For an example that uses this option, see [Example 54.13](#). You can also use the OFFSET= option to restrict parameters to a fixed value. For example, if you want to restrict the parameter for variable X1 to 1 and the parameter for X2 to 2, compute Restrict=  $X1 + 2 * X2$  in a DATA step, specify the option `offset=Restrict`, and leave X1 and X2 out of the model.

**OUTROC=*SAS-data-set*****OUTR=*SAS-data-set***

creates, for binary response models, an output SAS data set that contains the data necessary to produce the receiver operating characteristic (ROC) curve. The OUTROC= option is not available with the STRATA statement. See the section “[OUTROC= Output Data Set](#)” on page 4283 for the list of variables in this data set.

**PARMLABEL**

displays the labels of the parameters in the “Analysis of Maximum Likelihood Estimates” table.

**PCORR**

computes the partial correlation statistic  $sign(\beta_i) \sqrt{\frac{\chi_i^2 - 2}{-2 \log L_0}}$  for each parameter  $i$ , where  $\chi_i^2$  is the Wald chi-square statistic for the parameter and  $\log L_0$  is the log-likelihood of the intercept-only model (Hilbe 2009, p. 101). If  $\chi_i^2 < 2$  then the partial correlation is set to 0. The partial correlation for the intercept terms is set to missing.

**PEVENT=*value***

**PEVENT=(*list*)**

specifies one prior probability or a list of prior probabilities for the event of interest. The false positive and false negative rates are then computed as posterior probabilities by Bayes' theorem. The prior probability is also used in computing the rate of correct prediction. For each prior probability in the given list, a classification table of all observations is computed. By default, the prior probability is the total sample proportion of events. The PEVENT= option is useful for stratified samples. It has no effect if the CTABLE option is not specified. For more information, see the section “False Positive, False Negative, and Correct Classification Rates Using Bayes' Theorem” on page 4256. Also see the PPROB= option for information about how the *list* is specified.

**PLCL**

is the same as specifying **CLPARAM=PL**.

**PLCONV=*value***

controls the convergence criterion for confidence intervals based on the profile-likelihood function. The quantity *value* must be a positive number, with a default value of 1E-4. The PLCONV= option has no effect if profile-likelihood confidence intervals (**CLPARAM=PL**) are not requested.

**PLRL**

is the same as specifying **CLODDS=PL**.

**PPROB=*value***

**PPROB=(*list*)**

specifies one critical probability value (or cutpoint) or a list of critical probability values for classifying observations with the **CTABLE** option. Each *value* must be between 0 and 1. A response that has a cross validated predicted probability greater than or equal to the current PPROB= value is classified as an event response. The PPROB= option is ignored if the **CTABLE** option is not specified.

A classification table for each of several cutpoints can be requested by specifying a list. For example, the following statement requests a classification of the observations for each of the cutpoints 0.3, 0.5, 0.6, 0.7, and 0.8:

```
pprob= (0.3, 0.5 to 0.8 by 0.1)
```

If the PPROB= option is not specified, the default is to display the classification for a range of probabilities from the smallest estimated probability (rounded down to the nearest 0.02) to the highest estimated probability (rounded up to the nearest 0.02) with 0.02 increments.

**RIDGING=ABSOLUTE | RELATIVE | NONE**

specifies the technique used to improve the log-likelihood function when its value in the current iteration is less than that in the previous iteration. If you specify the **RIDGING=ABSOLUTE** option, the diagonal elements of the negative (expected) Hessian are inflated by adding the ridge value. If you specify the **RIDGING=RELATIVE** option, the diagonal elements are inflated by a factor of 1 plus the ridge value. If you specify the **RIDGING=NONE** option, the crude line search method of taking half a step is used instead of ridging. By default, **RIDGING=RELATIVE**.

**RISKLIMITS****RL****WALDRL**

is the same as specifying `CLODDS=WALD`.

**ROCEPS=*number***

specifies a criterion for the ROC curve used for grouping estimated event probabilities that are close to each other. In each group, the difference between the largest and the smallest estimated event probabilities does not exceed the given value. The value for *number* must be between 0 and 1; the default value is the square root of the machine epsilon, which is about 1E-8 (in releases prior to 9.2, the default was 1E-4). The smallest estimated probability in each group serves as a cutpoint for predicting an event response. The `ROCEPS=` option has no effect unless the `OUTROC=` option, the `BINWIDTH=0` option, or a `ROC` statement is specified.

**RSQUARE****RSQ**

requests a generalized R Square measure for the fitted model. For more information, see the section “Generalized Coefficient of Determination” on page 4246.

**SCALE=*scale***

enables you to supply the value of the dispersion parameter or to specify the method for estimating the dispersion parameter. It also enables you to display the “Deviance and Pearson Goodness-of-Fit Statistics” table. To correct for overdispersion or underdispersion, the covariance matrix is multiplied by the estimate of the dispersion parameter. Valid values for *scale* are as follows:

**D | DEVIANCE** specifies that the dispersion parameter be estimated by the deviance divided by its degrees of freedom.

**P | PEARSON** specifies that the dispersion parameter be estimated by the Pearson chi-square statistic divided by its degrees of freedom.

**WILLIAMS** *<(constant)>* specifies that Williams’ method be used to model overdispersion. This option can be used only with the events/trials syntax. An optional *constant* can be specified as the scale parameter; otherwise, a scale parameter is estimated under the full model. A set of weights is created based on this scale parameter estimate. These weights can then be used in fitting subsequent models of fewer terms than the full model. When fitting these submodels, specify the computed scale parameter as *constant*. See [Example 54.10](#) for an illustration.

**N | NONE** specifies that no correction is needed for the dispersion parameter; that is, the dispersion parameter remains as 1. This specification is used for requesting the deviance and the Pearson chi-square statistic without adjusting for overdispersion.

*constant* sets the estimate of the dispersion parameter to be the square of the given *constant*. For example, `SCALE=2` sets the dispersion parameter to 4. The value *constant* must be a positive number.

You can use the `AGGREGATE` (or `AGGREGATE=`) option to define the subpopulations for calculating the Pearson chi-square statistic and the deviance. In the absence of the `AGGREGATE` (or `AGGREGATE=`) option, each observation is regarded as coming from a different subpopulation. For the events/trials syntax, each observation consists of *n* Bernoulli trials, where *n* is the value of the

*trials* variable. For single-trial syntax, each observation consists of a single response, and for this setting it is not appropriate to carry out the Pearson or deviance goodness-of-fit analysis. Thus, PROC LOGISTIC ignores specifications SCALE=P, SCALE=D, and SCALE=N when single-trial syntax is specified without the **AGGREGATE** (or **AGGREGATE=**) option.

The “Deviance and Pearson Goodness-of-Fit Statistics” table includes the Pearson chi-square statistic, the deviance, the degrees of freedom, the ratio of each statistic divided by its degrees of freedom, and the corresponding *p*-value. The SCALE= option is not available with the **STRATA** statement. For more information, see the section “**Overdispersion**” on page 4257.

**SELECTION=BACKWARD | B**

| **FORWARD | F**

| **NONE | N**

| **STEPWISE | S**

| **SCORE**

specifies the method used to select the variables in the model. **BACKWARD** requests backward elimination, **FORWARD** requests forward selection, **NONE** fits the complete model specified in the MODEL statement, and **STEPWISE** requests stepwise selection. **SCORE** requests best subset selection. By default, SELECTION=NONE.

For more information, see the section “**Effect-Selection Methods**” on page 4244.

**SEQUENTIAL**

**SEQ**

forces effects to be added to the model in the order specified in the MODEL statement or eliminated from the model in the reverse order of that specified in the MODEL statement. The model-building process continues until the next effect to be added has an insignificant adjusted chi-square statistic or until the next effect to be deleted has a significant Wald chi-square statistic. The SEQUENTIAL option has no effect when **SELECTION=NONE**.

**SINGULAR=value**

specifies the tolerance for testing the singularity of the Hessian matrix (Newton-Raphson algorithm) or the expected value of the Hessian matrix (Fisher scoring algorithm). The Hessian matrix is the matrix of second partial derivatives of the log-likelihood function. The test requires that a pivot for sweeping this matrix be at least this number times a norm of the matrix. Values of the SINGULAR= option must be numeric. By default, *value* is the machine epsilon times 1E7, which is approximately 1E-9.

**SLENTY=value**

**SLE=value**

specifies the significance level of the score chi-square for entering an effect into the model in the FORWARD or STEPWISE method. Values of the SLENTY= option should be between 0 and 1, inclusive. By default, SLENTY=0.05. The SLENTY= option has no effect when **SELECTION=NONE**, **SELECTION=BACKWARD**, or **SELECTION=SCORE**.

**SLSTAY=value****SLS=value**

specifies the significance level of the Wald chi-square for an effect to stay in the model in a backward elimination step. Values of the SLSTAY= option should be between 0 and 1, inclusive. By default, SLSTAY=0.05. The SLSTAY= option has no effect when **SELECTION=NONE**, **SELECTION=FORWARD**, or **SELECTION=SCORE**.

**START=n**

begins the FORWARD, BACKWARD, or STEPWISE effect selection process with the first  $n$  effects listed in the MODEL statement. The value of  $n$  ranges from 0 to  $s$ , where  $s$  is the total number of effects in the MODEL statement. The default value of  $n$  is  $s$  for the BACKWARD method and 0 for the FORWARD and STEPWISE methods. Note that START= $n$  specifies only that the first  $n$  effects appear in the first model, while **INCLUDE= $n$**  requires that the first  $n$  effects be included in every model. For the SCORE method, START= $n$  specifies that the smallest models contain  $n$  effects, where  $n$  ranges from 1 to  $s$ ; the default value is 1. The START= option has no effect when **SELECTION=NONE**.

**STB**

displays the standardized estimates for the parameters in the “Analysis of Maximum Likelihood Estimates” table. The standardized estimate of  $\beta_i$  is given by  $\hat{\beta}_i / (s/s_i)$ , where  $s_i$  is the total sample standard deviation for the  $i$ th explanatory variable and

$$s = \begin{cases} \pi/\sqrt{3} & \text{Logistic} \\ 1 & \text{Normal} \\ \pi/\sqrt{6} & \text{Extreme-value} \end{cases}$$

The sample standard deviations for parameters associated with **CLASS** and **EFFECT** variables are computed using their codings. For the intercept parameters, the standardized estimates are set to missing.

**STOP=n**

specifies the maximum (**SELECTION=FORWARD**) or minimum (**SELECTION=BACKWARD**) number of effects to be included in the final model. The effect selection process is stopped when  $n$  effects are found. The value of  $n$  ranges from 0 to  $s$ , where  $s$  is the total number of effects in the MODEL statement. The default value of  $n$  is  $s$  for the FORWARD method and 0 for the BACKWARD method. For the SCORE method, STOP= $n$  specifies that the largest models contain  $n$  effects, where  $n$  ranges from 1 to  $s$ ; the default value of  $n$  is  $s$ . The STOP= option has no effect when **SELECTION=NONE** or **STEPWISE**.

**STOPRES****SR**

specifies that the removal or entry of effects be based on the value of the residual chi-square. If **SELECTION=FORWARD**, then the STOPRES option adds the effects into the model one at a time until the residual chi-square becomes insignificant (until the  $p$ -value of the residual chi-square exceeds the **SLENTY= value**). If **SELECTION=BACKWARD**, then the STOPRES option removes effects from the model one at a time until the residual chi-square becomes significant (until the  $p$ -value of the residual chi-square becomes less than the **SLSTAY= value**). The STOPRES option has no effect when **SELECTION=NONE** or **SELECTION=STEPWISE**.



**TECHNIQUE=FISHER | NEWTON****TECH=FISHER | NEWTON**

specifies the optimization technique for estimating the regression parameters. NEWTON (or NR) is the Newton-Raphson algorithm and FISHER (or FS) is the Fisher scoring algorithm. Both techniques yield the same estimates, but the estimated covariance matrices are slightly different except for the case when the LOGIT link is specified for binary response data. The default is TECHNIQUE=FISHER. If the LINK=GLOGIT option is specified, then Newton-Raphson is the default and only available method. The TECHNIQUE= option is not applied to conditional and exact conditional analyses. This option is not available when the UNEQUALSLOPES option is specified. See the section “Iterative Algorithms for Model Fitting” on page 4240 for more details.

**UNEQUALSLOPES< =effect | (effect-list)>**

specifies one or more effects in a cumulative response model that have a different set of parameters for each response function. If you specify more than one effect, enclose the effects in parentheses. The effects must be explanatory effects that are specified in the MODEL statement.

If you do not specify this option, the cumulative response models make the parallel lines assumption,  $F(\Pr(Y < i)) = \alpha_i + \mathbf{x}'\boldsymbol{\beta}$ , where each response function has the same slope parameters  $\boldsymbol{\beta}$ . If you specify this option without an *effect* or *effect-list*, all slope parameters vary across the response functions, resulting in the model  $F(\Pr(Y < i)) = \alpha_i + \mathbf{x}'\boldsymbol{\beta}_i$ . Specifying an *effect* or *effect-list* enables you to choose which effects have different parameters across the response functions. If you select the first  $\mathbf{x}_1$  parameters to have equal slopes and the remaining  $\mathbf{x}_2$  parameters to have unequal slopes, the model can be written as  $F(\Pr(Y < i)) = \alpha_i + \mathbf{x}'_1\boldsymbol{\beta}_1 + \mathbf{x}'_2\boldsymbol{\beta}_{2i}$ . A model that uses the CLOGIT link is called a *partial proportional odds model* (Peterson and Harrell 1990).

For more information, see Example 54.17. The following statements are not available with this option: EFFECTPLOT, ESTIMATE, EXACT, LSMEANS, LSMESTIMATE, ROC, ROCCONTRAST, SLICE, STORE, and STRATA. The following options are not available with this option: FIRTH, RIDGING=, TECHNIQUE=, CTABLE, PEVENT=, PPROB=, OUTROC=, and ROCEPS=.

**WALDCL****CL**

is the same as specifying CLPARM=WALD.

**XCONV=value**

specifies the relative parameter convergence criterion. Convergence requires a small relative parameter change in subsequent iterations,

$$\max_j |\delta_j^{(i)}| < value$$

where

$$\delta_j^{(i)} = \begin{cases} \frac{\beta_j^{(i)} - \beta_j^{(i-1)}}{\beta_j^{(i-1)}} & |\beta_j^{(i-1)}| < 0.01 \\ \beta_j^{(i)} - \beta_j^{(i-1)} & \text{otherwise} \end{cases}$$

and  $\beta_j^{(i)}$  is the estimate of the  $j$ th parameter at iteration  $i$ . See the section “Convergence Criteria” on page 4242 for more information.



---

## NLOPTIONS Statement

**NLOPTIONS** < options > ;

The NLOPTIONS statement controls the optimization process for conditional analyses (which result from specifying a **STRATA** statement) and for partial parallel slope models (which result from specifying the **UNEQUALSLOPES** option in the **MODEL** statement). An *option* specified in the NLOPTIONS statement takes precedence over the same option specified in the **MODEL** statement.

The default optimization techniques are chosen according to the number of parameters,  $p$ , as follows:

- Newton-Raphson with ridging when  $p < 40$
- quasi-Newton when  $40 \leq p < 400$
- conjugate gradient when  $p \geq 400$

The available *options* are described in the section “NLOPTIONS Statement” on page 482 of Chapter 19, “Shared Concepts and Topics.”

---

## ODDSRATIO Statement

**ODDSRATIO** < 'label' > variable < / options > ;

The ODDSRATIO statement produces odds ratios for *variable* even when the variable is involved in interactions with other covariates, and for classification variables that use any parameterization. You can also specify variables on which **constructed effects** are based, in addition to the names of **COLLECTION** or **MULTIMEMBER** effects. You can specify several ODDSRATIO statements.

If *variable* is continuous, then the odds ratios honor any values specified in the **UNITS** statement. If *variable* is a classification variable, then odds ratios comparing each pairwise difference between the levels of *variable* are produced. If *variable* interacts with a continuous variable, then the odds ratios are produced at the mean of the interacting covariate by default. If *variable* interacts with a classification variable, then the odds ratios are produced at each level of the interacting covariate by default. The computed odds ratios are independent of the parameterization of any classification variable.

The odds ratios are uniquely labeled by concatenating the following terms to *variable*:

1. If this is a polytomous response model, then prefix the response variable and the level describing the logit followed by a colon; for example, “Y 0:”.
2. If *variable* is continuous and the **UNITS** statement provides a value that is not equal to 1, then append “Units=value”; otherwise, if *variable* is a classification variable, then append the levels being contrasted; for example, “cat vs dog”.
3. Append all interacting covariates preceded by “At”; for example, “At X=1.2 A=cat”.

If you are also creating odds ratio plots, then this label is displayed on the plots (see the **PLOTS** option for more information). If you specify a ‘label’ in the ODDSRATIO statement, then the odds ratios produced by this statement are also labeled: ‘label’, ‘label 2’, ‘label 3’, . . . , and these are the labels used in the plots. If

there are any duplicated labels across all ODDSRATIO statements, then the corresponding odds ratios are not displayed on the plots.

The following *options* are available:

**AT**(*covariate=value-list* | **REF** | **ALL**< ...*covariate=value-list* | **REF** | **ALL**>)

specifies fixed levels of the interacting covariates. If a specified *covariate* does not interact with the *variable*, then its AT list is ignored.

For continuous interacting covariates, you can specify one or more numbers in the *value-list*. For classification covariates, you can specify one or more formatted levels of the covariate enclosed in single quotes (for example, **A=' cat' ' dog'**), you can specify the keyword **REF** to select the reference-level, or you can specify the keyword **ALL** to select all levels of the classification variable. By default, continuous covariates are set to their means, while **CLASS** covariates are set to **ALL**. For a model that includes a classification variable  $A=\{\text{cat,dog}\}$  and a continuous covariate  $X$ , specifying **AT (A=' cat' x=7 9)** will set  $A$  to 'cat', and  $X$  to 7 and then 9.

**CL=WALD** | **PL** | **BOTH**

specifies whether to create Wald or profile-likelihood confidence limits, or both. By default, Wald confidence limits are produced.

**DIFF=REF** | **ALL**

specifies whether the odds ratios for a classification variable are computed against the reference level, or all pairs of variable are compared. By default, **DIFF=ALL**. The **DIFF=** option is ignored when variable is continuous.

**PLCONV=value**

controls the convergence criterion for confidence intervals based on the profile-likelihood function. The quantity *value* must be a positive number, with a default value of  $1E-4$ . The **PLCONV=** option has no effect if profile-likelihood confidence intervals (**CL=PL**) are not requested.

**PLMAXITER=n**

specifies the maximum number of iterations to perform. By default, **PLMAXITER=25**. If convergence is not attained in  $n$  iterations, the odds ratio or the confidence limits are set to missing. The **PLMAXITER=** option has no effect if profile-likelihood confidence intervals (**CL=PL**) are not requested.

**PLSINGULAR=value**

specifies the tolerance for testing the singularity of the Hessian matrix (Newton-Raphson algorithm) or the expected value of the Hessian matrix (Fisher scoring algorithm). The test requires that a pivot for sweeping this matrix be at least this number times a norm of the matrix. Values of the **PLSINGULAR=** option must be numeric. By default, *value* is the machine epsilon times  $1E7$ , which is approximately  $1E-9$ . The **PLSINGULAR=** option has no effect if profile-likelihood confidence intervals (**CL=PL**) are not requested.

---

## OUTPUT Statement

**OUTPUT** < **OUT=SAS-data-set** > < *options* > ;

The OUTPUT statement creates a new SAS data set that contains all the variables in the input data set and, optionally, the estimated linear predictors and their standard error estimates, the estimates of the cumulative or individual response probabilities, and the confidence limits for the cumulative probabilities. Regression diagnostic statistics and estimates of cross validated response probabilities are also available for binary response models. If you specify more than one OUTPUT statement, only the last one is used. Formulas for the statistics are given in the sections “[Linear Predictor, Predicted Probability, and Confidence Limits](#)” on page 4253 and “[Regression Diagnostics](#)” on page 4263, and, for conditional logistic regression, in the section “[Conditional Logistic Regression](#)” on page 4271.

If you use the single-trial syntax, the data set also contains a variable named `_LEVEL_`, which indicates the level of the response that the given row of output is referring to. For instance, the value of the cumulative probability variable is the probability that the response variable is as large as the corresponding value of `_LEVEL_`. For details, see the section “[OUT= Output Data Set in the OUTPUT Statement](#)” on page 4280.

The estimated linear predictor, its standard error estimate, all predicted probabilities, and the confidence limits for the cumulative probabilities are computed for all observations in which the explanatory variables have no missing values, even if the response is missing. By adding observations with missing response values to the input data set, you can compute these statistics for new observations or for settings of the explanatory variables not present in the data without affecting the model fit. Alternatively, the SCORE statement can be used to compute predicted probabilities and confidence intervals for new observations.

Table 54.9 summarizes the options available in the OUTPUT statement. These options can be specified after a slash (/). The statistic and diagnostic options specify the statistics to be included in the output data set and name the new variables that contain the statistics. If a STRATA statement is specified, only the PREDICTED=, DFBETAS=, and H= options are available; see the section “[Regression Diagnostic Details](#)” on page 4272 for details.

**Table 54.9** OUTPUT Statement Options

| Option                                        | Description                                                                     |
|-----------------------------------------------|---------------------------------------------------------------------------------|
| ALPHA=                                        | Specifies $\alpha$ for the $100(1 - \alpha)\%$ confidence intervals             |
| OUT=                                          | Names the output data set                                                       |
| <b>Statistic Options</b>                      |                                                                                 |
| LOWER=                                        | Names the lower confidence limit                                                |
| PREDICTED=                                    | Names the predicted probabilities                                               |
| PREDPROBS=                                    | Requests the individual, cumulative, or cross validated predicted probabilities |
| STDXBETA=                                     | Names the standard error estimate of the linear predictor                       |
| UPPER=                                        | Names the upper confidence limit                                                |
| XBETA=                                        | Names the linear predictor                                                      |
| <b>Diagnostic Options for Binary Response</b> |                                                                                 |
| C=                                            | Names the confidence interval displacement                                      |
| CBAR=                                         | Names the confidence interval displacement                                      |
| DFBETAS=                                      | Names the standardized deletion parameter differences                           |
| DIFCHISQ=                                     | Names the deletion chi-square goodness-of-fit change                            |
| DIFDEV=                                       | Names the deletion deviance change                                              |
| H=                                            | Names the leverage                                                              |
| RESCHI=                                       | Names the Pearson chi-square residual                                           |
| RESDEV=                                       | Names the deviance residual                                                     |

Table 54.9 *continued*

| Option     | Description                                        |
|------------|----------------------------------------------------|
| RESLIK=    | Names the likelihood residual                      |
| STDRESCHI= | Names the standardized Pearson chi-square residual |
| STDRESDEV= | Names the standardized deviance residual           |

The following list describes these options.

**ALPHA=number**

sets the level of significance  $\alpha$  for  $100(1 - \alpha)\%$  confidence limits for the appropriate response probabilities. The value of *number* must be between 0 and 1. By default, *number* is equal to the value of the ALPHA= option in the PROC LOGISTIC statement, or 0.05 if that option is not specified.

**C=name**

specifies the confidence interval displacement diagnostic that measures the influence of individual observations on the regression estimates.

**CBAR=name**

specifies the confidence interval displacement diagnostic that measures the overall change in the global regression estimates due to deleting an individual observation.

**DFBETAS= \_ALL\_****DFBETAS=var-list**

specifies the standardized differences in the regression estimates for assessing the effects of individual observations on the estimated regression parameters in the fitted model. You can specify a list of up to  $s + 1$  variable names, where  $s$  is the number of explanatory variables in the MODEL statement, or you can specify just the keyword `_ALL_`. In the former specification, the first variable contains the standardized differences in the intercept estimate, the second variable contains the standardized differences in the parameter estimate for the first explanatory variable in the MODEL statement, and so on. In the latter specification, the DFBETAS statistics are named DFBETA\_XXX, where XXX is the name of the regression parameter. For example, if the model contains two variables X1 and X2, the specification DFBETAS=\_ALL\_ produces three DFBETAS statistics: DFBETA\_Intercept, DFBETA\_X1, and DFBETA\_X2. If an explanatory variable is not included in the final model, the corresponding output variable named in DFBETAS=var-list contains missing values.

**DIFCHISQ=name**

specifies the change in the chi-square goodness-of-fit statistic attributable to deleting the individual observation.

**DIFDEV=name**

specifies the change in the deviance attributable to deleting the individual observation.

**H=name**

specifies the diagonal element of the hat matrix for detecting extreme points in the design space.

**LOWER=name****L=name**

names the variable containing the lower confidence limits for  $\pi$ , where  $\pi$  is the probability of the event response if events/trials syntax or single-trial syntax with binary response is specified; for a cumulative model,  $\pi$  is cumulative probability (that is, the probability that the response is less than

or equal to the value of `_LEVEL_`); for the generalized logit model, it is the individual probability (that is, the probability that the response category is represented by the value of `_LEVEL_`). See the [ALPHA=](#) option to set the confidence level.

**OUT=SAS-data-set**

names the output data set. If you omit the `OUT=` option, the output data set is created and given a default name by using the `DATAn` convention.

**PREDICTED=name****PRED=name****PROB=name****P=name**

names the variable containing the predicted probabilities. For the events/trials syntax or single-trial syntax with binary response, it is the predicted event probability. For a cumulative model, it is the predicted cumulative probability (that is, the probability that the response variable is less than or equal to the value of `_LEVEL_`); and for the generalized logit model, it is the predicted individual probability (that is, the probability of the response category represented by the value of `_LEVEL_`).

**PREDPROBS=(keywords)**

requests individual, cumulative, or cross validated predicted probabilities. Descriptions of the *keywords* are as follows.

**INDIVIDUAL | I** requests the predicted probability of each response level. For a response variable `Y` with three levels, 1, 2, and 3, the individual probabilities are  $\Pr(Y=1)$ ,  $\Pr(Y=2)$ , and  $\Pr(Y=3)$ .

**CUMULATIVE | C** requests the cumulative predicted probability of each response level. For a response variable `Y` with three levels, 1, 2, and 3, the cumulative probabilities are  $\Pr(Y \leq 1)$ ,  $\Pr(Y \leq 2)$ , and  $\Pr(Y \leq 3)$ . The cumulative probability for the last response level always has the constant value of 1. For generalized logit models, the cumulative predicted probabilities are not computed and are set to missing.

**CROSSVALIDATE | XVALIDATE | X** requests the cross validated individual predicted probability of each response level. These probabilities are derived from the leave-one-out principle—that is, dropping the data of one subject and reestimating the parameter estimates. PROC LOGISTIC uses a less expensive one-step approximation to compute the parameter estimates. This option is valid only for binary response models; for nominal and ordinal models, the cross validated probabilities are not computed and are set to missing.

See the section “[Details of the PREDPROBS= Option](#)” on page 4227 at the end of this section for further details.

**RESCHI=name**

specifies the Pearson (chi-square) residual for identifying observations that are poorly accounted for by the model.

**RESDEV=name**

specifies the deviance residual for identifying poorly fitted observations.

**RESLIK=*name***

specifies the likelihood residual for identifying poorly fitted observations.

**STDRESCHI=*name***

specifies the standardized Pearson (chi-square) residual for identifying observations that are poorly accounted for by the model.

**STDRESDEV=*name***

specifies the standardized deviance residual for identifying poorly fitted observations.

**STDXBETA=*name***

names the variable containing the standard error estimates of **XBETA**. See the section “[Linear Predictor, Predicted Probability, and Confidence Limits](#)” on page 4253 for details.

**UPPER=*name*****U=*name***

names the variable containing the upper confidence limits for  $\pi$ , where  $\pi$  is the probability of the event response if events/trials syntax or single-trial syntax with binary response is specified; for a cumulative model,  $\pi$  is cumulative probability (that is, the probability that the response is less than or equal to the value of `_LEVEL_`); for the generalized logit model, it is the individual probability (that is, the probability that the response category is represented by the value of `_LEVEL_`). See the [ALPHA=](#) option to set the confidence level.

**XBETA=*name***

names the variable containing the estimates of the linear predictor  $\alpha_i + \beta'x$ , where  $i$  is the corresponding ordered value of `_LEVEL_`.

## Details of the PREDPROBS= Option

You can request any of the three types of predicted probabilities. For example, you can request both the individual predicted probabilities and the cross validated probabilities by specifying `PREDPROBS=(I X)`.

When you specify the `PREDPROBS=` option, two automatic variables, `_FROM_` and `_INTO_`, are included for the single-trial syntax and only one variable, `_INTO_`, is included for the events/trials syntax. The variable `_FROM_` contains the formatted value of the observed response. The variable `_INTO_` contains the formatted value of the response level with the largest individual predicted probability.

If you specify `PREDPROBS=INDIVIDUAL`, the `OUT=` data set contains  $k$  additional variables representing the individual probabilities, one for each response level, where  $k$  is the maximum number of response levels across all `BY` groups. The names of these variables have the form `IP_xxx`, where `xxx` represents the particular level. The representation depends on the following situations:

- If you specify events/trials syntax, `xxx` is either ‘Event’ or ‘Nonevent’. Thus, the variable containing the event probabilities is named `IP_Event` and the variable containing the nonevent probabilities is named `IP_Nonevent`.
- If you specify the single-trial syntax with more than one `BY` group, `xxx` is 1 for the first ordered level of the response, 2 for the second ordered level of the response, and so forth, as given in the “Response Profile” table. The variable containing the predicted probabilities  $\Pr(Y=1)$  is named `IP_1`, where `Y` is the response variable. Similarly, `IP_2` is the name of the variable containing the predicted probabilities  $\Pr(Y=2)$ , and so on.

- If you specify the single-trial syntax with no BY-group processing, *xxx* is the left-justified formatted value of the response level (the value might be truncated so that *IP\_**xxx* does not exceed 32 characters). For example, if *Y* is the response variable with response levels ‘None’, ‘Mild’, and ‘Severe’, the variables representing individual probabilities  $\Pr(Y='None')$ ,  $\Pr(Y='Mild')$ , and  $\Pr(Y='Severe')$  are named *IP\_None*, *IP\_Mild*, and *IP\_Severe*, respectively.

If you specify `PREDPROBS=CUMULATIVE`, the `OUT=` data set contains *k* additional variables representing the cumulative probabilities, one for each response level, where *k* is the maximum number of response levels across all BY groups. The names of these variables have the form *CP\_**xxx*, where *xxx* represents the particular response level. The naming convention is similar to that given by `PREDPROBS=INDIVIDUAL`. The `PREDPROBS=CUMULATIVE` values are the same as those output by the `PREDICT=` option, but are arranged in variables on each output observation rather than in multiple output observations.

If you specify `PREDPROBS=CROSSVALIDATE`, the `OUT=` data set contains *k* additional variables representing the cross validated predicted probabilities of the *k* response levels, where *k* is the maximum number of response levels across all BY groups. The names of these variables have the form *XP\_**xxx*, where *xxx* represents the particular level. The representation is the same as that given by `PREDPROBS=INDIVIDUAL` except that for the events/trials syntax there are four variables for the cross validated predicted probabilities instead of two:

*XP\_EVENT\_R1E* is the cross validated predicted probability of an event when a single event is removed from the current observation.

*XP\_NONEVENT\_R1E* is the cross validated predicted probability of a nonevent when a single event is removed from the current observation.

*XP\_EVENT\_R1N* is the cross validated predicted probability of an event when a single nonevent is removed from the current observation.

*XP\_NONEVENT\_R1N* is the cross validated predicted probability of a nonevent when a single nonevent is removed from the current observation.

The cross validated predicted probabilities are precisely those used in the `CTABLE` option. See the section “[Predicted Probability of an Event for Classification](#)” on page 4255 for details of the computation.

---

## ROC Statement

```
ROC < 'label' > < specification > < / options > ;
```

The ROC statements specify models to be used in the ROC comparisons. You can specify more than one ROC statement. ROC statements are identified by their *label*—if you do not specify a *label*, the *i*th ROC statement is labeled “ROC*i*”. Additionally, the specified or selected model is labeled with the `MODEL` statement label or “Model” if the `MODEL` label is not present. The *specification* can be either a list of effects that have previously been specified in the `MODEL` statement, or `PRED=variable`, where the *variable* does not have to be specified in the `MODEL` statement. The `PRED=` option enables you to input a criterion produced outside PROC LOGISTIC; for example, you can fit a random-intercept model by using PROC GLIMMIX or use survey weights in PROC SURVEYLOGISTIC, then use the predicted values from those models to produce an ROC curve for the comparisons. If you do not make a *specification*, then an intercept-only model is fit to the data, resulting in a noninformative ROC curve that can be used for comparing the area under another ROC curve to 0.5.



You can specify a **ROCCONTRAST** statement and a **ROCOPTIONS** option in the PROC LOGISTIC statement to control how the models are compared, while the **PLOTS=ROC** option controls the ODS Graphics displays. See [Example 54.8](#) for an example that uses the ROC statement.

If you specify any *options*, then a “ROC Model Information” table summarizing the new ROC model is displayed. The *options* are ignored for the PRED= specification. The following *options* are available:

#### **NOOFFSET**

does not include an offset variable if the OFFSET= option is specified in the **MODEL** statement. A constant offset has no effect on the ROC curve, although the cutpoints might be different, but a nonconstant offset can affect the parameter estimates and hence the ROC curve.

#### **LINK=keyword**

specifies the link function to be used in the model. The available keywords are LOGIT, NORMIT, and CLOGLOG. The logit link is the default. Note that the **LINK=** option in the MODEL statement is ignored.

---

## **ROCCONTRAST Statement**

**ROCCONTRAST** < 'label' > < contrast > < / options > ;

The ROCCONTRAST statement compares the different ROC models. You can specify only one ROCCONTRAST statement. The **ROCOPTIONS** options in the PROC LOGISTIC statement control how the models are compared. You can specify one of the following *contrast* specifications:

#### **REFERENCE**< (MODEL | 'roc-label') >

produces a contrast matrix of differences between each ROC curve and a reference curve. The MODEL keyword specifies that the reference curve is that produced from the MODEL statement; the *roc-label* specifies the *label* of the ROC curve that is to be used as the reference curve. If neither the MODEL keyword nor the *roc-label* label is specified, then the reference ROC curve is either the curve produced from the MODEL statement, the selected model if a selection method is specified, or the model from the first ROC statement if the **NOFIT** option is specified.

#### **ADJACENTPAIRS**

produces a contrast matrix of each ROC curve minus the succeeding curve.

#### *matrix*

specifies the contrast in the form **row1, row2, . . .**, where each *row* contains the coefficients used to compare the ROC curves. Each *row* must contain the same number of entries as there are ROC curves being compared. The elements of each *row* refer to the ROC statements in the order in which they are specified. However, the first element of each *row* refers either to the fitted model, the selected model if a **SELECTION=** method is specified, or the first specified ROC statement if the **NOFIT** option is specified.

If no *contrast* is specified, then the REFERENCE contrast with the default reference curve is used. See the section “[Comparing ROC Curves](#)” on page 4261 for more information about comparing ROC curves, and see [Example 54.8](#) for an example.

The following *options* are available:



**E**

displays the contrast.

**ESTIMATE <= ROWS | ALLPAIRS >**

produces estimates of each row of the contrast when ESTIMATE or ESTIMATE=ROWS is specified. If the ESTIMATE=ALLPAIRS option is specified, then estimates of every pairwise difference of ROC curves are produced.

The row contrasts are labeled “ModelLabel1 – ModelLabel2”, where the model labels are as described in the ROC statement; in particular, for the REFERENCE contrast, ModelLabel2 is the reference model label. If you specify your own contrast matrix, then the *i*th contrast row estimate is labeled “Row*i*”.

**COV**

displays covariance matrices used in the computations.

---

## SCORE Statement

**SCORE** < options > ;

The SCORE statement creates a data set that contains all the data in the DATA= data set together with posterior probabilities and, optionally, prediction confidence intervals. Fit statistics are displayed on request. If you have binary response data, the SCORE statement can be used to create a data set containing data for the ROC curve. You can specify several SCORE statements. **FREQ**, **WEIGHT**, and **BY** statements can be used with the SCORE statements. The SCORE statement is not available with the STRATA statement.

If a SCORE statement is specified in the same run as fitting the model, FORMAT statements should be specified after the SCORE statement in order for the formats to apply to all the DATA= and PRIOR= data sets in the SCORE statement.

See the section “Scoring Data Sets” on page 4266 for more information, and see Example 54.15 for an illustration of how to use this statement.

Table 54.10 summarizes the options available in the SCORE statement.

**Table 54.10** SCORE Statement Options

| Option      | Description                                                                |
|-------------|----------------------------------------------------------------------------|
| ALPHA=      | Specifies the significance level                                           |
| CLM         | Outputs the Wald-test-based confidence limits                              |
| CUMULATIVE  | Outputs the cumulative predicted probabilities                             |
| DATA=       | Names the SAS data that you want to score                                  |
| FITSTAT     | Displays fit statistics                                                    |
| OUT=        | Names the SAS data set that contains the predicted information             |
| OUTROC=     | Names the SAS data set that contains the ROC curve                         |
| PRIOR=      | Names the SAS data set that contains the priors of the response categories |
| PRIOREVENT= | Specifies the prior event probability                                      |
| ROCEPS=     | Specifies the criterion for grouping estimated event probabilities         |

You can specify the following options:

**ALPHA=number**

specifies the significance level  $\alpha$  for  $100(1 - \alpha)\%$  confidence intervals. By default, the value of *number* is equal to the **ALPHA=** option in the PROC LOGISTIC statement, or 0.05 if that option is not specified. This option has no effect unless the **CLM** option in the SCORE statement is requested.

**CLM**

outputs the Wald-test-based confidence limits for the predicted probabilities. This option is not available when the **INMODEL=** data set is created with the **NOCOV** option.

**CUMULATIVE**

outputs the cumulative predicted probabilities  $\Pr(Y \leq i), i = 1, \dots, k + 1$ , to the **OUT=** data set. This option is valid only when you have more than two response levels; otherwise, the option is ignored and a note is printed in the SAS log. These probabilities are named *CP\_level\_i*, where *level\_i* is the *i*th response level.

If the **CLM** option is also specified in the SCORE statement, then the Wald-based confidence limits for the cumulative predicted probabilities are also output. The confidence limits are named *CLCL\_level\_i* and *CUCL\_level\_i*. In particular, for the lowest response level, the cumulative values (CP, CLCL, CUCL) should be identical to the individual values (P, LCL, UCL), and for the highest response level  $CP=CLCL=CUCL=1$ .

**DATA=SAS-data-set**

names the SAS data set that you want to score. If you omit the **DATA=** option in the SCORE statement, then scoring is performed on the **DATA=** input data set in the PROC LOGISTIC statement, if specified; otherwise, the **DATA=\_LAST\_** data set is used.

It is not necessary for the **DATA=** data set in the SCORE statement to contain the response variable unless you are specifying the **FITSTAT** or **OUTROC=** option.

Only those variables involved in the fitted model effects are required in the **DATA=** data set in the SCORE statement. For example, the following statements use forward selection to select effects:

```
proc logistic data=Neuralgia outmodel=sasuser.Model;
 class Treatment Sex;
 model Pain(event='Yes') = Treatment|Sex Age
 / selection=forward sle=.01;
run;
```

Suppose Treatment and Age are the effects selected for the final model. You can score a data set that does not contain the variable Sex since the effect Sex is not in the model that the scoring is based on. For example, the following statements score the Neuralgia data set after dropping the Sex variable:

```
proc logistic inmodel=sasuser.Model;
 score data=Neuralgia(drop=Sex);
run;
```

**FITSTAT**

displays fit statistics for the data set you are scoring. The data set must contain the response variable. See the section “[Fit Statistics for Scored Data Sets](#)” on page 4266 for details.

**OUT=SAS-data-set**

names the SAS data set that contains the predicted information. If you omit the OUT= option, the output data set is created and given a default name by using the DATA*n* convention.

**OUTROC=SAS-data-set**

names the SAS data set that contains the ROC curve for the DATA= data set. The ROC curve is computed only for binary response data. See the section “[OUTROC= Output Data Set](#)” on page 4283 for the list of variables in this data set.

**PRIOR=SAS-data-set**

names the SAS data set that contains the priors of the response categories. The priors can be values proportional to the prior probabilities; thus, they do not necessarily sum to one. This data set should include a variable named `_PRIOR_` that contains the prior probabilities. For events/trials MODEL statement syntax, this data set should also include an `_OUTCOME_` variable that contains the values EVENT and NONEVENT; for single-trial syntax, this data set should include the response variable that contains the unformatted response categories. See [Example 54.15](#) for an example.

**PRIOREVENT=value**

specifies the prior event probability for a binary response model. If both PRIOR= and PRIOREVENT= options are specified, the PRIOR= option takes precedence.

**ROCEPS=value**

specifies the criterion for grouping estimated event probabilities that are close to each other for the ROC curve. In each group, the difference between the largest and the smallest estimated event probability does not exceed the given value. The *value* must be between 0 and 1; the default value is the square root of the machine epsilon, which is about 1E–8 (in releases prior to 9.2, the default was 1E–4). The smallest estimated probability in each group serves as a cutpoint for predicting an event response. The ROCEPS= option has no effect if the OUTROC= option is not specified in the SCORE statement.

**SLICE Statement**

```
SLICE model-effect </ options > ;
```

The SLICE statement provides a general mechanism for performing a partitioned analysis of the LS-means for an interaction. This analysis is also known as an analysis of simple effects.

The SLICE statement uses the same options as the LSMEANS statement, which are summarized in [Table 19.21](#). For details about the syntax of the SLICE statement, see the section “[SLICE Statement](#)” on page 498 in Chapter 19, “[Shared Concepts and Topics](#).”

**NOTE:** If you have classification variables in your model, then the SLICE statement is allowed only if you also specify the PARAM=GLM option.

---

## STORE Statement

**STORE** <OUT=>*item-store-name* </ LABEL='label'> ;

The STORE statement requests that the procedure save the context and results of the statistical analysis. The resulting item store has a binary file format that cannot be modified. The contents of the item store can be processed with the PLM procedure.

For details about the syntax of the STORE statement, see the section “STORE Statement” on page 501 in Chapter 19, “Shared Concepts and Topics.”

---

## STRATA Statement

**STRATA** *variable* <(option)> ... <*variable* <(option)>> </ options> ;

The STRATA statement names the *variables* that define *strata* or *matched sets* to use in *stratified logistic regression* of binary response data.

Observations that have the same *variable* values are in the same matched set. For a stratified logistic model, you can analyze 1: 1, 1:  $n$ ,  $m$ :  $n$ , and general  $m_i$ :  $n_i$  matched sets where the number of cases and controls varies across strata. At least one variable must be specified to invoke the stratified analysis, and the usual unconditional asymptotic analysis is not performed. The stratified logistic model has the form

$$\text{logit}(\pi_{hi}) = \alpha_h + \mathbf{x}'_{hi} \boldsymbol{\beta}$$

where  $\pi_{hi}$  is the event probability for the  $i$ th observation in stratum  $h$  with covariates  $\mathbf{x}_{hi}$  and where the stratum-specific intercepts  $\alpha_h$  are the nuisance parameters that are to be conditioned out.

STRATA variables can also be specified in the MODEL statement as classification or continuous covariates; however, the effects are nondegenerate only when crossed with a nonstratification variable. Specifying several STRATA statements is the same as specifying one STRATA statement that contains all the strata variables. The STRATA variables can be either character or numeric, and the formatted values of the STRATA variables determine the levels. Thus, you can also use formats to group values into levels; see the discussion of the FORMAT procedure in the *Base SAS Procedures Guide*.

The “Strata Summary” table is displayed by default. For an exact logistic regression, it displays the number of strata that have a specific number of events and non-events. For example, if you are analyzing a 1: 5 matched study, this table enables you to verify that every stratum in the analysis has exactly one event and five non-events. Strata that contain only events or only non-events are reported in this table, but such strata are uninformative and are not used in the analysis.

If an EXACT statement is also specified, then a stratified *exact* logistic regression is performed.

The EFFECTPLOT, SCORE, and WEIGHT statements are not available with a STRATA statement. The following MODEL options are also not supported with a STRATA statement: CLPARM=PL, CLODDS=PL, CTABLE, FIRTH, LACKFIT, LINK=, NOFIT, OUTMODEL=, OUTROC=, ROC, and SCALE=.

The following *option* can be specified for a stratification variable by enclosing the option in parentheses after the variable name, or it can be specified globally for all STRATA variables after a slash (/).

**MISSING**

treats missing values ('.', '\_', 'A', ..., 'Z' for numeric variables and blanks for character variables) as valid STRATA variable values.

The following strata *options* are also available after the slash:

**CHECKDEPENDENCY | CHECK=keyword**

specifies which variables are to be tested for dependency before the analysis is performed. The available *keywords* are as follows:

**NONE** performs no dependence checking. Typically, a message about a singular information matrix is displayed if you have dependent variables. Dependent variables can be identified after the analysis by noting any missing parameter estimates.

**COVARIATES** checks dependence between covariates and an added intercept. Dependent covariates are removed from the analysis. However, covariates that are linear functions of the strata variable might not be removed, which results in a singular information matrix message being displayed in the SAS log. This is the default.

**ALL** checks dependence between all the strata and covariates. This option can adversely affect performance if you have a large number of strata.

**NOSUMMARY**

suppresses the display of the “Strata Summary” table.

**INFO**

displays the “Strata Information” table, which includes the stratum number, levels of the STRATA variables that define the stratum, the number of events, the number of non-events, and the total frequency for each stratum. Since the number of strata can be very large, this table is displayed only by request.

**TEST Statement**

```
<label> TEST equation1 <, equation2, ... > </option>;
```

The TEST statement tests linear hypotheses about the regression coefficients. The Wald test is used to perform a joint test of the null hypotheses  $H_0: \mathbf{L}\boldsymbol{\beta} = \mathbf{c}$  specified in a single TEST statement, where  $\boldsymbol{\beta}$  is the vector of intercept and slope parameters. When  $\mathbf{c} = \mathbf{0}$  you should specify a CONTRAST statement instead.

Each *equation* specifies a linear hypothesis (a row of the **L** matrix and the corresponding element of the **c** vector). Multiple *equations* are separated by commas. The *label*, which must be a valid SAS name, is used to identify the resulting output and should always be included. You can submit multiple TEST statements.

The form of an *equation* is as follows:

```
term< ± term ... > <= ± term < ± term ... >>
```

where *term* is a parameter of the model, or a constant, or a constant times a parameter. Intercept and CLASS variable parameter names should be specified as described in the section “Parameter Names in the OUTEST= Data Set” on page 4279. Note for generalized logit models that this enables you to construct tests of parameters from specific logits. When no equal sign appears, the expression is set to 0. The following statements illustrate possible uses of the TEST statement:

```

proc logistic;
 model y= a1 a2 a3 a4;
 test1: test intercept + .5 * a2 = 0;
 test2: test intercept + .5 * a2;
 test3: test a1=a2=a3;
 test4: test a1=a2, a2=a3;
run;

```

Note that the first and second TEST statements are equivalent, as are the third and fourth TEST statements.

You can specify the following option in the TEST statement after a slash(/):

### PRINT

displays intermediate calculations in the testing of the null hypothesis  $H_0: \mathbf{L}\boldsymbol{\beta} = \mathbf{c}$ . This includes  $\mathbf{L}\widehat{\mathbf{V}}(\widehat{\boldsymbol{\beta}})\mathbf{L}'$  bordered by  $(\mathbf{L}\widehat{\boldsymbol{\beta}} - \mathbf{c})$  and  $[\mathbf{L}\widehat{\mathbf{V}}(\widehat{\boldsymbol{\beta}})\mathbf{L}']^{-1}$  bordered by  $[\mathbf{L}\widehat{\mathbf{V}}(\widehat{\boldsymbol{\beta}})\mathbf{L}']^{-1}(\mathbf{L}\widehat{\boldsymbol{\beta}} - \mathbf{c})$ , where  $\widehat{\boldsymbol{\beta}}$  is the maximum likelihood estimator of  $\boldsymbol{\beta}$  and  $\widehat{\mathbf{V}}(\widehat{\boldsymbol{\beta}})$  is the estimated covariance matrix of  $\widehat{\boldsymbol{\beta}}$ .

For more information, see the section “Testing Linear Hypotheses about the Regression Coefficients” on page 4262.

## UNITS Statement

**UNITS** < *independent1=list1* < *independent2=list2* . . . > < / *option* > ;

The UNITS statement enables you to specify units of change for the continuous explanatory variables so that customized odds ratios can be estimated. If you specify more than one UNITS statement, only the last one is used. An estimate of the corresponding odds ratio is produced for each unit of change specified for an explanatory variable. The UNITS statement is ignored for CLASS variables. Odds ratios are computed only for main effects that are not involved in interactions or nestings, unless an **ODDSRATIO** statement is also specified. If the **CLODDS=** option is specified in the MODEL statement, the corresponding confidence limits for the odds ratios are also displayed, as are odds ratios and confidence limits for any CLASS main effects that are not involved in interactions or nestings. The CLASS effects must use the GLM, reference, or effect coding.

The UNITS statement also enables you to customize the odds ratios for effects specified in **ODDSRATIO** statements, in which case interactions and nestings are allowed, and CLASS variables can be specified with any parameterization.

The term *independent* is the name of an explanatory variable and *list* represents a list of units of change, separated by spaces, that are of interest for that variable. Each unit of change in a list has one of the following forms:

- *number*
- SD or –SD
- *number* \* SD

where *number* is any nonzero number, and SD is the sample standard deviation of the corresponding independent variable. For example,  $X = -2$  requests an odds ratio that represents the change in the odds when

the variable  $X$  is decreased by two units.  $X = 2*SD$  requests an estimate of the change in the odds when  $X$  is increased by two sample standard deviations.

You can specify the following option in the UNITS statement after a slash(/):

**DEFAULT=*list***

gives a list of units of change for all explanatory variables that are not specified in the UNITS statement. Each unit of change can be in any of the forms described previously. If the DEFAULT= option is not specified, PROC LOGISTIC does not produce customized odds ratio estimates for any continuous explanatory variable that is not listed in the UNITS statement.

For more information, see the section “Odds Ratio Estimation” on page 4250.

## WEIGHT Statement

**WEIGHT** *variable* </ option > ;

When a WEIGHT statement appears, each observation in the input data set is weighted by the value of the WEIGHT variable. Unlike a FREQ variable, the values of the WEIGHT variable can be nonintegral and are not truncated. Observations with negative, zero, or missing values for the WEIGHT variable are not used in the model fitting. When the WEIGHT statement is not specified, each observation is assigned a weight of 1. The WEIGHT statement is not available with the STRATA statement. If you specify more than one WEIGHT statement, then the first WEIGHT variable is used.

If a SCORE statement is specified, then the WEIGHT variable is used for computing fit statistics and the ROC curve, but it is not required for scoring. If the DATA= data set in the SCORE statement does not contain the WEIGHT variable, the weights are assumed to be 1 and a warning message is issued in the SAS log. If you fit a model and perform the scoring in the same run, the same WEIGHT variable is used for fitting and scoring. If you fit a model in a previous run and input it with the INMODEL= option in the current run, then the WEIGHT variable can be different from the one used in the previous run; however, if a WEIGHT variable was not specified in the previous run, you can still specify a WEIGHT variable in the current run.

**CAUTION:** PROC LOGISTIC does not compute the proper variance estimators if you are analyzing survey data and specifying the sampling weights through the WEIGHT statement. The SURVEYLOGISTIC procedure is designed to perform the necessary, and correct, computations.

The following option can be added to the WEIGHT statement after a slash (/):

**NORMALIZE**

**NORM**

causes the weights specified by the WEIGHT variable to be normalized so that they add up to the actual sample size. Weights  $w_i$  are normalized by multiplying them by  $\frac{n}{\sum_{i=1}^n w_i}$ , where  $n$  is the sample size. With this option, the estimated covariance matrix of the parameter estimators is invariant to the scale of the WEIGHT variable.



---

## Details: LOGISTIC Procedure

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### Missing Values

Any observation with missing values for the response, offset, strata, or explanatory variables is excluded from the analysis; however, missing values are valid for variables specified with the `MISSING` option in the `CLASS` or `STRATA` statement. Observations with a nonpositive or missing weight or with a frequency less than 1 are also excluded. The estimated linear predictor and its standard error estimate, the fitted probabilities and confidence limits, and the regression diagnostic statistics are not computed for any observation with missing offset or explanatory variable values. However, if only the response value is missing, the linear predictor, its standard error, the fitted individual and cumulative probabilities, and confidence limits for the cumulative probabilities can be computed and output to a data set by using the `OUTPUT` statement.

---

### Response Level Ordering

Response level ordering is important because, by default, PROC LOGISTIC models the probability of response levels with *lower Ordered Value*. Ordered Values are assigned to response levels in ascending sorted order (that is, the lowest response level is assigned Ordered Value 1, the next lowest is assigned Ordered Value 2, and so on) and are displayed in the “Response Profiles” table. If your response variable  $Y$  takes values in  $\{1, \dots, k + 1\}$ , then, by default, the functions modeled with the binary or cumulative model are

$$\text{logit}(\Pr(Y \leq i | \mathbf{x})), \quad i = 1, \dots, k$$

and for the generalized logit model the functions modeled are

$$\log \left( \frac{\Pr(Y = i | \mathbf{x})}{\Pr(Y = k + 1 | \mathbf{x})} \right), \quad i = 1, \dots, k$$

where the highest Ordered Value  $Y = k + 1$  is the reference level. You can change which probabilities are modeled by specifying the `EVENT=`, `REF=`, `DESCENDING`, or `ORDER=` response variable options in the `MODEL` statement.

For binary response data with event and nonevent categories, if your event category has a higher Ordered Value, then by default the nonevent is modeled. Since the default response function modeled is

$$\text{logit}(\pi) = \log \left( \frac{\pi}{1 - \pi} \right)$$

where  $\pi$  is the probability of the response level assigned Ordered Value 1, and since

$$\text{logit}(\pi) = -\text{logit}(1 - \pi)$$

the effect of modeling the nonevent is to change the signs of  $\alpha$  and  $\beta$  in the model for the event,  $\text{logit}(\pi) = \alpha + \beta' \mathbf{x}$ .

For example, suppose the binary response variable  $Y$  takes the values 1 and 0 for event and nonevent, respectively, and `Exposure` is the explanatory variable. By default, PROC LOGISTIC assigns Ordered



Value 1 to response level  $Y=0$ , and Ordered Value 2 to response level  $Y=1$ . As a result, PROC LOGISTIC models the probability of the nonevent (Ordered Value=1) category, and your parameter estimates have the opposite sign from those in the model for the event. To model the event without using a DATA step to change the values of the variable  $Y$ , you can control the ordering of the response levels or select the event or reference level, as shown in the following list:

- Explicitly state which response level is to be modeled by using the response variable option `EVENT=` in the `MODEL` statement:

```
model Y(event='1') = Exposure;
```

- Specify the nonevent category for the response variable in the response variable option `REF=` in the `MODEL` statement. This option is most useful for generalized logit models where the `EVENT=` option cannot be used.

```
model Y(ref='0') = Exposure;
```

- Specify the response variable option `DESCENDING` in the `MODEL` statement to assign the lowest Ordered Value to  $Y=1$ :

```
model Y(descending)=Exposure;
```

- Assign a format to  $Y$  such that the first formatted value (when the formatted values are put in sorted order) corresponds to the event. In the following example,  $Y=1$  is assigned the formatted value 'event' and  $Y=0$  is assigned the formatted value 'nonevent'. Since `ORDER=FORMATTED` by default, Ordered Value 1 is assigned to response level  $Y=1$ , so the procedure models the event.

```
proc format;
 value Disease 1='event' 0='nonevent';
run;
proc logistic;
 format Y Disease.;
 model Y=Exposure;
run;
```

---

## Link Functions and the Corresponding Distributions

Four link functions are available in the LOGISTIC procedure. The logit function is the default. To specify a different link function, use the `LINK=` option in the `MODEL` statement. The link functions and the corresponding distributions are as follows:

- The logit function

$$g(p) = \log(p/(1 - p))$$

is the inverse of the cumulative logistic distribution function, which is

$$F(x) = 1/(1 + \exp(-x)) = \exp(x)/(1 + \exp(x))$$

- The probit (or normit) function

$$g(p) = \Phi^{-1}(p)$$

is the inverse of the cumulative standard normal distribution function, which is

$$F(x) = \Phi(x) = (2\pi)^{-1/2} \int_{-\infty}^x \exp(-z^2/2) dz$$

Traditionally, the probit function contains the additive constant 5, but throughout PROC LOGISTIC, the terms probit and normit are used interchangeably.

- The complementary log-log function

$$g(p) = \log(-\log(1 - p))$$

is the inverse of the cumulative extreme-value function (also called the Gompertz distribution), which is

$$F(x) = 1 - \exp(-\exp(x))$$

- The generalized logit function extends the binary logit link to a vector of levels  $(p_1, \dots, p_{k+1})$  by contrasting each level with a fixed level

$$g(p_i) = \log(p_i/p_{k+1}) \quad i = 1, \dots, k$$

The variances of the normal, logistic, and extreme-value distributions are not the same. Their respective means and variances are shown in the following table:

| Distribution  | Mean      | Variance  |
|---------------|-----------|-----------|
| Normal        | 0         | 1         |
| Logistic      | 0         | $\pi^2/3$ |
| Extreme-value | $-\gamma$ | $\pi^2/6$ |

Here  $\gamma$  is the Euler constant. In comparing parameter estimates from different link functions, you need to take into account the different scalings of the corresponding distributions and, for the complementary log-log function, a possible shift in location. For example, if the fitted probabilities are in the neighborhood of 0.1 to 0.9, then the parameter estimates from the logit link function should be about  $\pi/\sqrt{3}$  larger than the estimates from the probit link function.

---

## Determining Observations for Likelihood Contributions

If you use events/trials MODEL statement syntax, split each observation into two observations. One has response value 1 with a frequency equal to the frequency of the original observation (which is 1 if the FREQ statement is not used) times the value of the *events* variable. The other observation has response value 2 and a frequency equal to the frequency of the original observation times the value of (*trials-events*). These two observations will have the same explanatory variable values and the same FREQ and WEIGHT values as the original observation.

For either single-trial or events/trials syntax, let  $j$  index all observations. In other words, for single-trial syntax,  $j$  indexes the actual observations. And, for events/trials syntax,  $j$  indexes the observations after splitting (as described in the preceding paragraph). If your data set has 30 observations and you use single-trial syntax,  $j$  has values from 1 to 30; if you use events/trials syntax,  $j$  has values from 1 to 60.

Suppose the response variable in a cumulative response model can take on the ordered values  $1, \dots, k, k+1$ , where  $k$  is an integer  $\geq 1$ . The likelihood for the  $j$ th observation with ordered response value  $y_j$  and explanatory variables vector  $\mathbf{x}_j$  is given by

$$L_j = \begin{cases} F(\alpha_1 + \boldsymbol{\beta}'\mathbf{x}_j) & y_j = 1 \\ F(\alpha_i + \boldsymbol{\beta}'\mathbf{x}_j) - F(\alpha_{i-1} + \boldsymbol{\beta}'\mathbf{x}_j) & 1 < y_j = i \leq k \\ 1 - F(\alpha_k + \boldsymbol{\beta}'\mathbf{x}_j) & y_j = k + 1 \end{cases}$$

where  $F(\cdot)$  is the logistic, normal, or extreme-value distribution function,  $\alpha_1, \dots, \alpha_k$  are ordered intercept parameters, and  $\boldsymbol{\beta}$  is the common slope parameter vector.

For the generalized logit model, letting the  $k+1$ st level be the reference level, the intercepts  $\alpha_1, \dots, \alpha_k$  are unordered and the slope vector  $\boldsymbol{\beta}_i$  varies with each logit. The likelihood for the  $j$ th observation with response value  $y_j$  and explanatory variables vector  $\mathbf{x}_j$  is given by

$$L_j = \Pr(Y = y_j | \mathbf{x}_j) = \begin{cases} \frac{e^{\alpha_i + \mathbf{x}'_j \boldsymbol{\beta}_i}}{1 + \sum_{m=1}^k e^{\alpha_m + \mathbf{x}'_j \boldsymbol{\beta}_m}} & 1 \leq y_j = i \leq k \\ \frac{1}{1 + \sum_{m=1}^k e^{\alpha_m + \mathbf{x}'_j \boldsymbol{\beta}_m}} & y_j = k + 1 \end{cases}$$

---

## Iterative Algorithms for Model Fitting

Two iterative maximum likelihood algorithms are available in PROC LOGISTIC for fitting an unconditional logistic regression, and these two methods are discussed in this section. For conditional logistic regression and models with the `UNEQUALSLOPES` specification, see the section “`NLOPTIONS` Statement” on page 4222 for details about available optimization techniques. Exact logistic regression uses a special algorithm described in the section “`Exact Conditional Logistic Regression`” on page 4274.

The default maximum likelihood algorithm is the Fisher scoring method, which is equivalent to fitting by iteratively reweighted least squares. The alternative algorithm is the Newton-Raphson method. Both algorithms give the same parameter estimates; however, the estimated covariance matrix of the parameter estimators can differ slightly. This is due to the fact that Fisher scoring is based on the expected information matrix while the Newton-Raphson method is based on the observed information matrix. In the case of a binary logit model, the observed and expected information matrices are identical, resulting in identical estimated covariance matrices for both algorithms. You can specify the `TECHNIQUE=` option to select a fitting algorithm, and specify the `FIRTH` option to perform a bias-reducing penalized maximum likelihood fit. Note for generalized logit models that only the Newton-Raphson technique is available.

### Iteratively Reweighted Least Squares Algorithm (Fisher Scoring)

Consider the multinomial variable  $\mathbf{Z}_j = (Z_{1j}, \dots, Z_{k+1,j})'$  such that

$$Z_{ij} = \begin{cases} 1 & \text{if } Y_j = i \\ 0 & \text{otherwise} \end{cases}$$

With  $\pi_{ij}$  denoting the probability that the  $j$ th observation has response value  $i$ , the expected value of  $\mathbf{Z}_j$  is  $\boldsymbol{\pi}_j = (\pi_{1j}, \dots, \pi_{k+1,j})'$  where  $\pi_{k+1,j} = 1 - \sum_{i=1}^k \pi_{ij}$ . The covariance matrix of  $\mathbf{Z}_j$  is  $\mathbf{V}_j$ , which is the covariance matrix of a multinomial random variable for one trial with parameter vector  $\boldsymbol{\pi}_j$ . Let  $\boldsymbol{\beta}$  be the vector of regression parameters; in other words,  $\boldsymbol{\beta} = (\alpha_1, \dots, \alpha_k, \beta_1, \dots, \beta_s)'$ . Let  $\mathbf{D}_j$  be the matrix of partial derivatives of  $\boldsymbol{\pi}_j$  with respect to  $\boldsymbol{\beta}$ . The estimating equation for the regression parameters is

$$\sum_j \mathbf{D}'_j \mathbf{W}_j (\mathbf{Z}_j - \boldsymbol{\pi}_j) = \mathbf{0}$$

where  $\mathbf{W}_j = w_j f_j \mathbf{V}_j^-$ ,  $w_j$  and  $f_j$  are the weight and frequency of the  $j$ th observation, and  $\mathbf{V}_j^-$  is a generalized inverse of  $\mathbf{V}_j$ . PROC LOGISTIC chooses  $\mathbf{V}_j^-$  as the inverse of the diagonal matrix with  $\boldsymbol{\pi}_j$  as the diagonal.

With a starting value of  $\boldsymbol{\beta}^{(0)}$ , the maximum likelihood estimate of  $\boldsymbol{\beta}$  is obtained iteratively as

$$\boldsymbol{\beta}^{(m+1)} = \boldsymbol{\beta}^{(m)} + \left( \sum_j \mathbf{D}'_j \mathbf{W}_j \mathbf{D}_j \right)^{-1} \sum_j \mathbf{D}'_j \mathbf{W}_j (\mathbf{Z}_j - \boldsymbol{\pi}_j)$$

where  $\mathbf{D}_j$ ,  $\mathbf{W}_j$ , and  $\boldsymbol{\pi}_j$  are evaluated at  $\boldsymbol{\beta}^{(m)}$ . The expression after the plus sign is the step size. If the likelihood evaluated at  $\boldsymbol{\beta}^{(m+1)}$  is less than that evaluated at  $\boldsymbol{\beta}^{(m)}$ , then  $\boldsymbol{\beta}^{(m+1)}$  is recomputed by step-halving or ridging as determined by the value of the RIDGING= option. The iterative scheme continues until convergence is obtained—that is, until  $\boldsymbol{\beta}^{(m+1)}$  is sufficiently close to  $\boldsymbol{\beta}^{(m)}$ . Then the maximum likelihood estimate of  $\boldsymbol{\beta}$  is  $\hat{\boldsymbol{\beta}} = \boldsymbol{\beta}^{(m+1)}$ .

The covariance matrix of  $\hat{\boldsymbol{\beta}}$  is estimated by

$$\widehat{\text{Cov}}(\hat{\boldsymbol{\beta}}) = \left( \sum_j \widehat{\mathbf{D}}'_j \widehat{\mathbf{W}}_j \widehat{\mathbf{D}}_j \right)^{-1} = \widehat{\mathbf{I}}^{-1}$$

where  $\widehat{\mathbf{D}}_j$  and  $\widehat{\mathbf{W}}_j$  are, respectively,  $\mathbf{D}_j$  and  $\mathbf{W}_j$  evaluated at  $\hat{\boldsymbol{\beta}}$ .  $\widehat{\mathbf{I}}$  is the information matrix, or the negative expected Hessian matrix, evaluated at  $\hat{\boldsymbol{\beta}}$ .

By default, starting values are zero for the slope parameters, and for the intercept parameters, starting values are the observed cumulative logits (that is, logits of the observed cumulative proportions of response). Alternatively, the starting values can be specified with the INEST= option.

## Newton-Raphson Algorithm

For cumulative models, let the parameter vector be  $\boldsymbol{\beta} = (\alpha_1, \dots, \alpha_k, \beta_1, \dots, \beta_s)'$ , and for the generalized logit model let  $\boldsymbol{\beta} = (\alpha_1, \dots, \alpha_k, \beta'_1, \dots, \beta'_k)'$ . The gradient vector and the Hessian matrix are given, respectively, by

$$\mathbf{g} = \sum_j w_j f_j \frac{\partial l_j}{\partial \boldsymbol{\beta}}$$

$$\mathbf{H} = \sum_j w_j f_j \frac{\partial^2 l_j}{\partial \boldsymbol{\beta}^2}$$

where  $l_j = \log L_j$  is the log likelihood for the  $j$ th observation. With a starting value of  $\boldsymbol{\beta}^{(0)}$ , the maximum likelihood estimate  $\hat{\boldsymbol{\beta}}$  of  $\boldsymbol{\beta}$  is obtained iteratively until convergence is obtained:

$$\boldsymbol{\beta}^{(m+1)} = \boldsymbol{\beta}^{(m)} - \mathbf{H}^{-1} \mathbf{g}$$

where  $\mathbf{H}$  and  $\mathbf{g}$  are evaluated at  $\boldsymbol{\beta}^{(m)}$ . If the likelihood evaluated at  $\boldsymbol{\beta}^{(m+1)}$  is less than that evaluated at  $\boldsymbol{\beta}^{(m)}$ , then  $\boldsymbol{\beta}^{(m+1)}$  is recomputed by step-halving or ridging.

The covariance matrix of  $\hat{\boldsymbol{\beta}}$  is estimated by

$$\widehat{\text{Cov}}(\hat{\boldsymbol{\beta}}) = \hat{\mathbf{I}}^{-1}$$

where the observed information matrix  $\hat{\mathbf{I}} = -\hat{\mathbf{H}}$  is computed by evaluating  $\mathbf{H}$  at  $\hat{\boldsymbol{\beta}}$ .

### Firth's Bias-Reducing Penalized Likelihood

Firth's method is currently available only for binary logistic models. It replaces the usual score (gradient) equation

$$g(\beta_j) = \sum_{i=1}^n (y_i - \pi_i) x_{ij} = 0 \quad (j = 1, \dots, p)$$

where  $p$  is the number of parameters in the model, with the modified score equation

$$g(\beta_j)^* = \sum_{i=1}^n \{y_i - \pi_i + h_i(0.5 - \pi_i)\} x_{ij} = 0 \quad (j = 1, \dots, p)$$

where the  $h_i$ s are the  $i$ th diagonal elements of the hat matrix  $\mathbf{W}^{1/2} \mathbf{X}(\mathbf{X}'\mathbf{W}\mathbf{X})^{-1} \mathbf{X}'\mathbf{W}^{1/2}$  and  $\mathbf{W} = \text{diag}\{\pi_i(1 - \pi_i)\}$ . The Hessian matrix is not modified by this penalty, and the optimization method is performed in the usual manner.

## Convergence Criteria

Four convergence criteria are available: `ABSFCONV=`, `FCONV=`, `GCONV=`, and `XCONV=`. If you specify more than one convergence criterion, the optimization is terminated as soon as one of the criteria is satisfied. If none of the criteria is specified, the default is `GCONV=1E-8`.

If you specify a `STRATA` statement or the `UNEQUALSLOPES` option in the `MODEL` statement, all unspecified (or nondefault) criteria are also compared to zero. For example, specifying only the criterion `XCONV=1E-8` but attaining `FCONV=0` terminates the optimization even if the `XCONV=` criterion is not satisfied, because the log likelihood has reached its maximum. More convergence criteria are also available; see the section “`NLOPTIONS` Statement” on page 4222 for details.

## Existence of Maximum Likelihood Estimates

The likelihood equation for a logistic regression model does not always have a finite solution. Sometimes there is a nonunique maximum on the boundary of the parameter space, at infinity. The existence, finiteness, and uniqueness of maximum likelihood estimates for the logistic regression model depend on the patterns of data points in the observation space (Albert and Anderson 1984; Santner and Duffy 1986). Existence checks are not performed for conditional logistic regression.

Consider a binary response model. Let  $Y_j$  be the response of the  $j$ th subject, and let  $\mathbf{x}_j$  be the vector of explanatory variables (including the constant 1 associated with the intercept). There are three mutually exclusive and exhaustive types of data configurations: complete separation, quasi-complete separation, and overlap.

**Complete Separation** There is a complete separation of data points if there exists a vector  $\mathbf{b}$  that correctly allocates all observations to their response groups; that is,

$$\begin{cases} \mathbf{b}'\mathbf{x}_j > 0 & Y_j = 1 \\ \mathbf{b}'\mathbf{x}_j < 0 & Y_j = 2 \end{cases}$$

This configuration gives nonunique infinite estimates. If the iterative process of maximizing the likelihood function is allowed to continue, the log likelihood diminishes to zero, and the dispersion matrix becomes unbounded.

**Quasi-complete Separation** The data are not completely separable, but there is a vector  $\mathbf{b}$  such that

$$\begin{cases} \mathbf{b}'\mathbf{x}_j \geq 0 & Y_j = 1 \\ \mathbf{b}'\mathbf{x}_j \leq 0 & Y_j = 2 \end{cases}$$

and equality holds for at least one subject in each response group. This configuration also yields nonunique infinite estimates. If the iterative process of maximizing the likelihood function is allowed to continue, the dispersion matrix becomes unbounded and the log likelihood diminishes to a nonzero constant.

**Overlap** If neither complete nor quasi-complete separation exists in the sample points, there is an overlap of sample points. In this configuration, the maximum likelihood estimates exist and are unique.

Complete separation and quasi-complete separation are problems typically encountered with small data sets. Although complete separation can occur with any type of data, quasi-complete separation is not likely with truly continuous explanatory variables.

The LOGISTIC procedure uses a simple empirical approach to recognize the data configurations that lead to infinite parameter estimates. The basis of this approach is that any convergence method of maximizing the log likelihood must yield a solution giving complete separation, if such a solution exists. In maximizing the log likelihood, there is no checking for complete or quasi-complete separation if convergence is attained in eight or fewer iterations. Subsequent to the eighth iteration, the probability of the observed response is computed for each observation. If the predicted response equals the observed response for every observation, there is a complete separation of data points and the iteration process is stopped. If the complete separation of data has not been determined and an observation is identified to have an extremely large probability ( $\geq 0.95$ ) of predicting the observed response, there are two possible situations. First, there is overlap in the data set, and the observation is an atypical observation of its own group. The iterative process, if allowed to continue, will stop when a maximum is reached. Second, there is quasi-complete separation in the data set, and the asymptotic dispersion matrix is unbounded. If any of the diagonal elements of the dispersion matrix for the standardized observations vectors (all explanatory variables standardized to zero mean and unit variance) exceeds 5000, quasi-complete separation is declared and the iterative process is stopped. If either complete separation or quasi-complete separation is detected, a warning message is displayed in the procedure output.

Checking for quasi-complete separation is less foolproof than checking for complete separation. The **NOCHECK** option in the **MODEL** statement turns off the process of checking for infinite parameter estimates. In cases of complete or quasi-complete separation, turning off the checking process typically results

in the procedure failing to converge. The presence of a **WEIGHT** statement also turns off the checking process.

To address the separation issue, you can change your model, specify the **FIRTH** option to use Firth's penalized likelihood method, or for small data sets specify an **EXACT** statement to perform an exact logistic regression.

---

## Effect-Selection Methods

Five effect-selection methods are available by specifying the **SELECTION=** option in the **MODEL** statement. The simplest method (and the default) is **SELECTION=NONE**, for which PROC LOGISTIC fits the complete model as specified in the **MODEL** statement. The other four methods are **FORWARD** for forward selection, **BACKWARD** for backward elimination, **STEPWISE** for stepwise selection, and **SCORE** for best subsets selection. Intercept parameters are forced to stay in the model unless the **NOINT** option is specified.

When **SELECTION=FORWARD**, PROC LOGISTIC first estimates parameters for effects forced into the model. These effects are the intercepts and the first  $n$  explanatory effects in the **MODEL** statement, where  $n$  is the number specified by the **START=** or **INCLUDE=** option in the **MODEL** statement ( $n$  is zero by default). Next, the procedure computes the score chi-square statistic for each effect not in the model and examines the largest of these statistics. If it is significant at the **SLENTRY=** level, the corresponding effect is added to the model. Once an effect is entered in the model, it is never removed from the model. The process is repeated until none of the remaining effects meet the specified level for entry or until the **STOP=** value is reached.

When **SELECTION=BACKWARD**, parameters for the complete model as specified in the **MODEL** statement are estimated unless the **START=** option is specified. In that case, only the parameters for the intercepts and the first  $n$  explanatory effects in the **MODEL** statement are estimated, where  $n$  is the number specified by the **START=** option. Results of the Wald test for individual parameters are examined. The least significant effect that does not meet the **SLSTAY=** level for staying in the model is removed. Once an effect is removed from the model, it remains excluded. The process is repeated until no other effect in the model meets the specified level for removal or until the **STOP=** value is reached. Backward selection is often less successful than forward or stepwise selection because the full model fit in the first step is the model most likely to result in a complete or quasi-complete separation of response values as described in the section “Existence of Maximum Likelihood Estimates” on page 4242.

The **SELECTION=STEPWISE** option is similar to the **SELECTION=FORWARD** option except that effects already in the model do not necessarily remain. Effects are entered into and removed from the model in such a way that each forward selection step can be followed by one or more backward elimination steps. The stepwise selection process terminates if no further effect can be added to the model or if the current model is identical to a previously visited model.

For **SELECTION=SCORE**, PROC LOGISTIC uses the branch-and-bound algorithm of Furnival and Wilson (1974) to find a specified number of models with the highest likelihood score (chi-square) statistic for all possible model sizes, from 1, 2, 3 effect models, and so on, up to the single model containing all of the explanatory effects. The number of models displayed for each model size is controlled by the **BEST=** option. You can use the **START=** option to impose a minimum model size, and you can use the **STOP=** option to impose a maximum model size. For instance, with **BEST=3**, **START=2**, and **STOP=5**, the **SCORE** selection method displays the best three models (that is, the three models with the highest score chi-squares)

containing 2, 3, 4, and 5 effects. The **SELECTION=SCORE** option is not available for models with CLASS variables.

The options **FAST**, **SEQUENTIAL**, and **STOPRES** can alter the default criteria for entering or removing effects from the model when they are used with the **FORWARD**, **BACKWARD**, or **STEPWISE** selection method.

---

## Model Fitting Information

For the  $j$ th observation, let  $\hat{\pi}_j$  be the estimated probability of the observed response. The three criteria displayed by the LOGISTIC procedure are calculated as follows:

- $-2 \log$  likelihood:

$$-2 \text{ Log L} = -2 \sum_j \frac{w_j}{\sigma^2} f_j \log(\hat{\pi}_j)$$

where  $w_j$  and  $f_j$  are the weight and frequency values of the  $j$ th observation, and  $\sigma^2$  is the dispersion parameter, which equals 1 unless the **SCALE=** option is specified. For binary response models that use events/trials MODEL statement syntax, this is

$$-2 \text{ Log L} = -2 \sum_j \frac{w_j}{\sigma^2} f_j \left[ \log \binom{n_j}{r_j} + r_j \log(\hat{\pi}_j) + (n_j - r_j) \log(1 - \hat{\pi}_j) \right]$$

where  $r_j$  is the number of events,  $n_j$  is the number of trials,  $\hat{\pi}_j$  is the estimated event probability, and the statistic is reported both with and without the constant term.

- Akaike's information criterion:

$$\text{AIC} = -2 \text{ Log L} + 2p$$

where  $p$  is the number of parameters in the model. For cumulative response models,  $p = k + s$ , where  $k$  is the total number of response levels minus one and  $s$  is the number of explanatory effects. For the generalized logit model,  $p = k(s + 1)$ .

- Schwarz (Bayesian information) criterion:

$$\text{SC} = -2 \text{ Log L} + p \log \left( \sum_j f_j n_j \right)$$

where  $p$  is the number of parameters in the model,  $n_j$  is the number of trials when events/trials syntax is specified, and  $n_j = 1$  with single-trial syntax.

The AIC and SC statistics give two different ways of adjusting the  $-2 \text{ Log L}$  statistic for the number of terms in the model and the number of observations used. These statistics can be used when comparing different models for the same data (for example, when you use the **SELECTION=STEPWISE** option in the MODEL statement). The models being compared do not have to be nested; lower values of the statistics indicate a more desirable model.



The difference in the  $-2 \text{ Log L}$  statistics between the intercepts-only model and the specified model has a  $p - k$  degree-of-freedom chi-square distribution under the null hypothesis that all the explanatory effects in the model are zero, where  $p$  is the number of parameters in the specified model and  $k$  is the number of intercepts. The likelihood ratio test in the “Testing Global Null Hypothesis: BETA=0” table displays this difference and the associated  $p$ -value for this statistic. The score and Wald tests in that table test the same hypothesis and are asymptotically equivalent; see the sections “Residual Chi-Square” on page 4247 and “Testing Linear Hypotheses about the Regression Coefficients” on page 4262 for details.

---

## Generalized Coefficient of Determination

Cox and Snell (1989, pp. 208–209) propose the following generalization of the coefficient of determination to a more general linear model:

$$R^2 = 1 - \left\{ \frac{L(\mathbf{0})}{L(\hat{\boldsymbol{\beta}})} \right\}^{\frac{2}{n}}$$

where  $L(\mathbf{0})$  is the likelihood of the intercept-only model,  $L(\hat{\boldsymbol{\beta}})$  is the likelihood of the specified model,  $n = \sum_j f_j n_j$  is the sample size,  $f_j$  is the frequency of the  $j$ th observation, and  $n_j$  is the number of trials when events/trials syntax is specified or  $n_j = 1$  with single-trial syntax.

The quantity  $R^2$  achieves a maximum of less than one for discrete models, where the maximum is given by

$$R_{\max}^2 = 1 - \{L(\mathbf{0})\}^{\frac{2}{n}}$$

Nagelkerke (1991) proposes the following adjusted coefficient, which can achieve a maximum value of one:

$$\tilde{R}^2 = \frac{R^2}{R_{\max}^2}$$

Specifying the **NORMALIZE** option in the **WEIGHT** statement makes these coefficients invariant to the scale of the weights.

Like the AIC and SC statistics described in the section “Model Fitting Information” on page 4245,  $R^2$  and  $\tilde{R}^2$  are most useful for comparing competing models that are not necessarily nested—larger values indicate better models. More properties and interpretation of  $R^2$  and  $\tilde{R}^2$  are provided in Nagelkerke (1991). In the “Testing Global Null Hypothesis: BETA=0” table,  $R^2$  is labeled as “RSquare” and  $\tilde{R}^2$  is labeled as “Max-rescaled RSquare.” Use the **RSQUARE** option to request  $R^2$  and  $\tilde{R}^2$ .

---

## Score Statistics and Tests

To understand the general form of the score statistics, let  $\mathbf{g}(\boldsymbol{\beta})$  be the vector of first partial derivatives of the log likelihood with respect to the parameter vector  $\boldsymbol{\beta}$ , and let  $\mathbf{H}(\boldsymbol{\beta})$  be the matrix of second partial derivatives of the log likelihood with respect to  $\boldsymbol{\beta}$ . That is,  $\mathbf{g}(\boldsymbol{\beta})$  is the gradient vector, and  $\mathbf{H}(\boldsymbol{\beta})$  is the Hessian matrix. Let  $\mathbf{I}(\boldsymbol{\beta})$  be either  $-\mathbf{H}(\boldsymbol{\beta})$  or the expected value of  $-\mathbf{H}(\boldsymbol{\beta})$ . Consider a null hypothesis  $H_0$ . Let  $\hat{\boldsymbol{\beta}}_{H_0}$  be the MLE of  $\boldsymbol{\beta}$  under  $H_0$ . The chi-square score statistic for testing  $H_0$  is defined by

$$\mathbf{g}'(\hat{\boldsymbol{\beta}}_{H_0}) \mathbf{I}^{-1}(\hat{\boldsymbol{\beta}}_{H_0}) \mathbf{g}(\hat{\boldsymbol{\beta}}_{H_0})$$

and it has an asymptotic  $\chi^2$  distribution with  $r$  degrees of freedom under  $H_0$ , where  $r$  is the number of restrictions imposed on  $\boldsymbol{\beta}$  by  $H_0$ .

## Residual Chi-Square

When you use **SELECTION=FORWARD**, **BACKWARD**, or **STEPWISE**, the procedure calculates a residual chi-square score statistic and reports the statistic, its degrees of freedom, and the  $p$ -value. This section describes how the statistic is calculated.

Suppose there are  $s$  explanatory effects of interest. The full cumulative response model has a parameter vector

$$\boldsymbol{\beta} = (\alpha_1, \dots, \alpha_k, \beta_1, \dots, \beta_s)'$$

where  $\alpha_1, \dots, \alpha_k$  are intercept parameters, and  $\beta_1, \dots, \beta_s$  are the common slope parameters for the  $s$  explanatory effects. The full generalized logit model has a parameter vector

$$\begin{aligned} \boldsymbol{\beta} &= (\alpha_1, \dots, \alpha_k, \boldsymbol{\beta}'_1, \dots, \boldsymbol{\beta}'_k)' \quad \text{with} \\ \boldsymbol{\beta}'_i &= (\beta_{i1}, \dots, \beta_{is}), \quad i = 1, \dots, k \end{aligned}$$

where  $\beta_{ij}$  is the slope parameter for the  $j$ th effect in the  $i$ th logit.

Consider the null hypothesis  $H_0: \beta_{t+1} = \dots = \beta_s = 0$ , where  $t < s$  for the cumulative response model, and  $H_0: \beta_{i,t+1} = \dots = \beta_{is} = 0, t < s, i = 1, \dots, k$ , for the generalized logit model. For the reduced model with  $t$  explanatory effects, let  $\hat{\alpha}_1, \dots, \hat{\alpha}_k$  be the MLEs of the unknown intercept parameters, let  $\hat{\beta}_1, \dots, \hat{\beta}_t$  be the MLEs of the unknown slope parameters, and let  $\hat{\boldsymbol{\beta}}'_{i(t)} = (\hat{\beta}_{i1}, \dots, \hat{\beta}_{it}), i = 1, \dots, k$ , be those for the generalized logit model. The residual chi-square is the chi-square score statistic testing the null hypothesis  $H_0$ ; that is, the residual chi-square is

$$\mathbf{g}'(\hat{\boldsymbol{\beta}}_{H_0}) \mathbf{I}^{-1}(\hat{\boldsymbol{\beta}}_{H_0}) \mathbf{g}(\hat{\boldsymbol{\beta}}_{H_0})$$

where for the cumulative response model  $\hat{\boldsymbol{\beta}}_{H_0} = (\hat{\alpha}_1, \dots, \hat{\alpha}_k, \hat{\beta}_1, \dots, \hat{\beta}_t, 0, \dots, 0)'$ , and for the generalized logit model  $\hat{\boldsymbol{\beta}}_{H_0} = (\hat{\alpha}_1, \dots, \hat{\alpha}_k, \hat{\boldsymbol{\beta}}'_{1(t)}, \mathbf{0}'_{(s-t)}, \dots, \hat{\boldsymbol{\beta}}'_{k(t)}, \mathbf{0}'_{(s-t)})'$ , where  $\mathbf{0}_{(s-t)}$  denotes a vector of  $s - t$  zeros.

The residual chi-square has an asymptotic chi-square distribution with  $s - t$  degrees of freedom ( $k(s - t)$  for the generalized logit model). A special case is the global score chi-square, where the reduced model consists of the  $k$  intercepts and no explanatory effects. The global score statistic is displayed in the “Testing Global Null Hypothesis: BETA=0” table. The table is not produced when the **NOFIT** option is used, but the global score statistic is displayed.

## Testing Individual Effects Not in the Model

These tests are performed when you specify **SELECTION=FORWARD** or **STEPWISE**, and are displayed when the **DETAILS** option is specified. In the displayed output, the tests are labeled “Score Chi-Square” in the “Analysis of Effects Not in the Model” table and in the “Summary of Stepwise (Forward) Selection” table. This section describes how the tests are calculated.

Suppose that  $k$  intercepts and  $t$  explanatory variables (say  $v_1, \dots, v_t$ ) have been fit to a model and that  $v_{t+1}$  is another explanatory variable of interest. Consider a full model with the  $k$  intercepts and  $t + 1$  explanatory variables ( $v_1, \dots, v_t, v_{t+1}$ ) and a reduced model with  $v_{t+1}$  excluded. The significance of  $v_{t+1}$  adjusted for  $v_1, \dots, v_t$  can be determined by comparing the corresponding residual chi-square with a chi-square distribution with one degree of freedom ( $k$  degrees of freedom for the generalized logit model).

## Testing the Parallel Lines Assumption

For an ordinal response, PROC LOGISTIC performs a test of the parallel lines assumption. In the displayed output, this test is labeled “Score Test for the Equal Slopes Assumption” when the LINK= option is NORMIT or CLOGLOG. When LINK=LOGIT, the test is labeled as “Score Test for the Proportional Odds Assumption” in the output. For small sample sizes, this test might be too liberal (Stokes, Davis, and Koch 2000, p. 249). This section describes the methods used to calculate the test.

For this test the number of response levels,  $k + 1$ , is assumed to be strictly greater than 2. Let  $Y$  be the response variable taking values  $1, \dots, k, k + 1$ . Suppose there are  $s$  explanatory variables. Consider the general cumulative model without making the parallel lines assumption

$$g(\Pr(Y \leq i | \mathbf{x})) = (1, \mathbf{x}')\boldsymbol{\beta}_i, \quad 1 \leq i \leq k$$

where  $g(\cdot)$  is the link function, and  $\boldsymbol{\beta}_i = (\alpha_i, \beta_{i1}, \dots, \beta_{is})'$  is a vector of unknown parameters consisting of an intercept  $\alpha_i$  and  $s$  slope parameters  $\beta_{i1}, \dots, \beta_{is}$ . The parameter vector for this general cumulative model is

$$\boldsymbol{\beta} = (\boldsymbol{\beta}'_1, \dots, \boldsymbol{\beta}'_k)'$$

Under the null hypothesis of parallelism  $H_0: \beta_{1m} = \beta_{2m} = \dots = \beta_{km}, 1 \leq m \leq s$ , there is a single common slope parameter for each of the  $s$  explanatory variables. Let  $\beta_1, \dots, \beta_s$  be the common slope parameters. Let  $\hat{\alpha}_1, \dots, \hat{\alpha}_k$  and  $\hat{\beta}_1, \dots, \hat{\beta}_s$  be the MLEs of the intercept parameters and the common slope parameters. Then, under  $H_0$ , the MLE of  $\boldsymbol{\beta}$  is

$$\hat{\boldsymbol{\beta}}_{H_0} = (\hat{\boldsymbol{\beta}}'_1, \dots, \hat{\boldsymbol{\beta}}'_k)' \quad \text{with} \quad \hat{\boldsymbol{\beta}}_i = (\hat{\alpha}_i, \hat{\beta}_1, \dots, \hat{\beta}_s)' \quad 1 \leq i \leq k$$

and the chi-square score statistic  $\mathbf{g}'(\hat{\boldsymbol{\beta}}_{H_0})\mathbf{I}^{-1}(\hat{\boldsymbol{\beta}}_{H_0})\mathbf{g}(\hat{\boldsymbol{\beta}}_{H_0})$  has an asymptotic chi-square distribution with  $s(k - 1)$  degrees of freedom. This tests the parallel lines assumption by testing the equality of separate slope parameters simultaneously for all explanatory variables.

---

## Confidence Intervals for Parameters

There are two methods of computing confidence intervals for the regression parameters. One is based on the profile-likelihood function, and the other is based on the asymptotic normality of the parameter estimators. The latter is not as time-consuming as the former, since it does not involve an iterative scheme; however, it is not thought to be as accurate as the former, especially with small sample size. You use the CLPARM= option to request confidence intervals for the parameters.

## Likelihood Ratio-Based Confidence Intervals

The likelihood ratio-based confidence interval is also known as the profile-likelihood confidence interval. The construction of this interval is derived from the asymptotic  $\chi^2$  distribution of the generalized likelihood ratio test (Venzon and Moolgavkar 1988). Suppose that the parameter vector is  $\boldsymbol{\beta} = (\beta_0, \beta_1, \dots, \beta_s)'$  and you want to compute a confidence interval for  $\beta_j$ . The profile-likelihood function for  $\beta_j = \gamma$  is defined as

$$l_j^*(\gamma) = \max_{\boldsymbol{\beta} \in \mathcal{B}_j(\gamma)} l(\boldsymbol{\beta})$$

where  $\mathcal{B}_j(\gamma)$  is the set of all  $\boldsymbol{\beta}$  with the  $j$ th element fixed at  $\gamma$ , and  $l(\boldsymbol{\beta})$  is the log-likelihood function for  $\boldsymbol{\beta}$ . If  $l_{\max} = l(\hat{\boldsymbol{\beta}})$  is the log likelihood evaluated at the maximum likelihood estimate  $\hat{\boldsymbol{\beta}}$ , then  $2(l_{\max} - l_j^*(\beta_j))$  has a limiting chi-square distribution with one degree of freedom if  $\beta_j$  is the true parameter value. Let  $l_0 = l_{\max} - 0.5\chi_1^2(1 - \alpha)$ , where  $\chi_1^2(1 - \alpha)$  is the  $100(1 - \alpha)$  percentile of the chi-square distribution with one degree of freedom. A  $100(1 - \alpha)\%$  confidence interval for  $\beta_j$  is

$$\{\gamma : l_j^*(\gamma) \geq l_0\}$$

The endpoints of the confidence interval are found by solving numerically for values of  $\beta_j$  that satisfy equality in the preceding relation. To obtain an iterative algorithm for computing the confidence limits, the log-likelihood function in a neighborhood of  $\boldsymbol{\beta}$  is approximated by the quadratic function

$$\tilde{l}(\boldsymbol{\beta} + \boldsymbol{\delta}) = l(\boldsymbol{\beta}) + \boldsymbol{\delta}'\mathbf{g} + \frac{1}{2}\boldsymbol{\delta}'\mathbf{V}\boldsymbol{\delta}$$

where  $\mathbf{g} = \mathbf{g}(\boldsymbol{\beta})$  is the gradient vector and  $\mathbf{V} = \mathbf{V}(\boldsymbol{\beta})$  is the Hessian matrix. The increment  $\boldsymbol{\delta}$  for the next iteration is obtained by solving the likelihood equations

$$\frac{d}{d\boldsymbol{\delta}} \{\tilde{l}(\boldsymbol{\beta} + \boldsymbol{\delta}) + \lambda(\mathbf{e}_j'\boldsymbol{\delta} - \gamma)\} = \mathbf{0}$$

where  $\lambda$  is the Lagrange multiplier,  $\mathbf{e}_j$  is the  $j$ th unit vector, and  $\gamma$  is an unknown constant. The solution is

$$\boldsymbol{\delta} = -\mathbf{V}^{-1}(\mathbf{g} + \lambda\mathbf{e}_j)$$

By substituting this  $\boldsymbol{\delta}$  into the equation  $\tilde{l}(\boldsymbol{\beta} + \boldsymbol{\delta}) = l_0$ , you can estimate  $\lambda$  as

$$\lambda = \pm \left( \frac{2(l_0 - l(\boldsymbol{\beta}) + \frac{1}{2}\mathbf{g}'\mathbf{V}^{-1}\mathbf{g})}{\mathbf{e}_j'\mathbf{V}^{-1}\mathbf{e}_j} \right)^{\frac{1}{2}}$$

The upper confidence limit for  $\beta_j$  is computed by starting at the maximum likelihood estimate of  $\boldsymbol{\beta}$  and iterating with positive values of  $\lambda$  until convergence is attained. The process is repeated for the lower confidence limit by using negative values of  $\lambda$ .

Convergence is controlled by the value  $\epsilon$  specified with the `PLCONV=` option in the `MODEL` statement (the default value of  $\epsilon$  is  $1\text{E-}4$ ). Convergence is declared on the current iteration if the following two conditions are satisfied:

$$|l(\boldsymbol{\beta}) - l_0| \leq \epsilon$$

and

$$(\mathbf{g} + \lambda\mathbf{e}_j)'\mathbf{V}^{-1}(\mathbf{g} + \lambda\mathbf{e}_j) \leq \epsilon$$

## Wald Confidence Intervals

Wald confidence intervals are sometimes called the normal confidence intervals. They are based on the asymptotic normality of the parameter estimators. The  $100(1 - \alpha)\%$  Wald confidence interval for  $\beta_j$  is given by

$$\widehat{\beta}_j \pm z_{1-\alpha/2} \widehat{\sigma}_j$$

where  $z_p$  is the  $100p$  percentile of the standard normal distribution,  $\widehat{\beta}_j$  is the maximum likelihood estimate of  $\beta_j$ , and  $\widehat{\sigma}_j$  is the standard error estimate of  $\widehat{\beta}_j$ .

---

## Odds Ratio Estimation

Consider a dichotomous response variable with outcomes *event* and *nonevent*. Consider a dichotomous risk factor variable  $X$  that takes the value 1 if the risk factor is present and 0 if the risk factor is absent. According to the logistic model, the log odds function,  $\text{logit}(X)$ , is given by

$$\text{logit}(X) \equiv \log\left(\frac{\Pr(\text{event} | X)}{\Pr(\text{nonevent} | X)}\right) = \alpha + X\beta$$

The odds ratio  $\psi$  is defined as the ratio of the odds for those with the risk factor ( $X = 1$ ) to the odds for those without the risk factor ( $X = 0$ ). The log of the odds ratio is given by

$$\log(\psi) \equiv \log(\psi(X = 1, X = 0)) = \text{logit}(X = 1) - \text{logit}(X = 0) = (\alpha + 1 \times \beta) - (\alpha + 0 \times \beta) = \beta$$

In general, the odds ratio can be computed by exponentiating the difference of the logits between any two population profiles. This is the approach taken by the **ODDSRATIO** statement, so the computations are available regardless of parameterization, interactions, and nestings. However, as shown in the preceding equation for  $\log(\psi)$ , odds ratios of main effects can be computed as functions of the parameter estimates, and the remainder of this section is concerned with this methodology.

The parameter,  $\beta$ , associated with  $X$  represents the change in the log odds from  $X = 0$  to  $X = 1$ . So the odds ratio is obtained by simply exponentiating the value of the parameter associated with the risk factor. The odds ratio indicates how the odds of the event change as you change  $X$  from 0 to 1. For instance,  $\psi = 2$  means that the odds of an event when  $X = 1$  are twice the odds of an event when  $X = 0$ . You can also express this as follows: the percent change in the odds of an event from  $X = 0$  to  $X = 1$  is  $(\psi - 1)100\% = 100\%$ .

Suppose the values of the dichotomous risk factor are coded as constants  $a$  and  $b$  instead of 0 and 1. The odds when  $X = a$  become  $\exp(\alpha + a\beta)$ , and the odds when  $X = b$  become  $\exp(\alpha + b\beta)$ . The odds ratio corresponding to an increase in  $X$  from  $a$  to  $b$  is

$$\psi = \exp[(b - a)\beta] = [\exp(\beta)]^{b-a} \equiv [\exp(\beta)]^c$$

Note that for any  $a$  and  $b$  such that  $c = b - a = 1$ ,  $\psi = \exp(\beta)$ . So the odds ratio can be interpreted as the change in the odds for any increase of one unit in the corresponding risk factor. However, the change in odds for some amount other than one unit is often of greater interest. For example, a change of one pound in body weight might be too small to be considered important, while a change of 10 pounds might be more meaningful. The odds ratio for a change in  $X$  from  $a$  to  $b$  is estimated by raising the odds ratio estimate for a unit change in  $X$  to the power of  $c = b - a$  as shown previously.

For a polytomous risk factor, the computation of odds ratios depends on how the risk factor is parameterized. For illustration, suppose that Race is a risk factor with four categories: White, Black, Hispanic, and Other.

For the effect parameterization scheme (**PARAM=EFFECT**) with White as the reference group (**REF='White'**), the design variables for Race are as follows:

| Race     | Design Variables |       |       |
|----------|------------------|-------|-------|
|          | $X_1$            | $X_2$ | $X_3$ |
| Black    | 1                | 0     | 0     |
| Hispanic | 0                | 1     | 0     |
| Other    | 0                | 0     | 1     |
| White    | -1               | -1    | -1    |

The log odds for Black is

$$\begin{aligned}\text{logit(Black)} &= \alpha + (X_1 = 1)\beta_1 + (X_2 = 0)\beta_2 + (X_3 = 0)\beta_3 \\ &= \alpha + \beta_1\end{aligned}$$

The log odds for White is

$$\begin{aligned}\text{logit(White)} &= \alpha + (X_1 = -1)\beta_1 + (X_2 = -1)\beta_2 + (X_3 = -1)\beta_3 \\ &= \alpha - \beta_1 - \beta_2 - \beta_3\end{aligned}$$

Therefore, the log odds ratio of Black versus White becomes

$$\begin{aligned}\log(\psi(\text{Black, White})) &= \text{logit(Black)} - \text{logit(White)} \\ &= 2\beta_1 + \beta_2 + \beta_3\end{aligned}$$

For the reference cell parameterization scheme (**PARAM=REF**) with White as the reference cell, the design variables for race are as follows:

| Race     | Design Variables |       |       |
|----------|------------------|-------|-------|
|          | $X_1$            | $X_2$ | $X_3$ |
| Black    | 1                | 0     | 0     |
| Hispanic | 0                | 1     | 0     |
| Other    | 0                | 0     | 1     |
| White    | 0                | 0     | 0     |

The log odds ratio of Black versus White is given by

$$\begin{aligned}\log(\psi(\text{Black, White})) &= \text{logit(Black)} - \text{logit(White)} \\ &= (\alpha + (X_1 = 1)\beta_1 + (X_2 = 0)\beta_2 + (X_3 = 0)\beta_3) - \\ &\quad (\alpha + (X_1 = 0)\beta_1 + (X_2 = 0)\beta_2 + (X_3 = 0)\beta_3) \\ &= \beta_1\end{aligned}$$

For the GLM parameterization scheme (**PARAM=GLM**), the design variables are as follows:

| Race     | Design Variables |       |       |       |
|----------|------------------|-------|-------|-------|
|          | $X_1$            | $X_2$ | $X_3$ | $X_4$ |
| Black    | 1                | 0     | 0     | 0     |
| Hispanic | 0                | 1     | 0     | 0     |
| Other    | 0                | 0     | 1     | 0     |
| White    | 0                | 0     | 0     | 1     |

The log odds ratio of Black versus White is

$$\begin{aligned}
 \log(\psi(\text{Black}, \text{White})) &= \text{logit}(\text{Black}) - \text{logit}(\text{White}) \\
 &= (\alpha + (X_1 = 1)\beta_1 + (X_2 = 0)\beta_2 + (X_3 = 0)\beta_3 + (X_4 = 0)\beta_4) - \\
 &\quad (\alpha + (X_1 = 0)\beta_1 + (X_2 = 0)\beta_2 + (X_3 = 0)\beta_3 + (X_4 = 1)\beta_4) \\
 &= \beta_1 - \beta_4
 \end{aligned}$$

Consider the hypothetical example of heart disease among race in Hosmer and Lemeshow (2000, p. 56). The entries in the following contingency table represent counts:

| Disease Status | Race  |       |          |       |
|----------------|-------|-------|----------|-------|
|                | White | Black | Hispanic | Other |
| Present        | 5     | 20    | 15       | 10    |
| Absent         | 20    | 10    | 10       | 10    |

The computation of odds ratio of Black versus White for various parameterization schemes is tabulated in Table 54.11.

**Table 54.11** Odds Ratio of Heart Disease Comparing Black to White

| PARAM= | Parameter Estimates |                 |                 |                 | Odds Ratio Estimates                          |
|--------|---------------------|-----------------|-----------------|-----------------|-----------------------------------------------|
|        | $\hat{\beta}_1$     | $\hat{\beta}_2$ | $\hat{\beta}_3$ | $\hat{\beta}_4$ |                                               |
| EFFECT | 0.7651              | 0.4774          | 0.0719          |                 | $\exp(2 \times 0.7651 + 0.4774 + 0.0719) = 8$ |
| REF    | 2.0794              | 1.7917          | 1.3863          |                 | $\exp(2.0794) = 8$                            |
| GLM    | 2.0794              | 1.7917          | 1.3863          | 0.0000          | $\exp(2.0794) = 8$                            |

Since the log odds ratio ( $\log(\psi)$ ) is a linear function of the parameters, the Wald confidence interval for  $\log(\psi)$  can be derived from the parameter estimates and the estimated covariance matrix. Confidence intervals for the odds ratios are obtained by exponentiating the corresponding confidence limits for the log odds ratios. In the displayed output of PROC LOGISTIC, the “Odds Ratio Estimates” table contains the odds ratio estimates and the corresponding 95% Wald confidence intervals. For continuous explanatory variables, these odds ratios correspond to a unit increase in the risk factors.

To customize odds ratios for specific units of change for a continuous risk factor, you can use the **UNITS** statement to specify a list of relevant units for each explanatory variable in the model. Estimates of these customized odds ratios are given in a separate table. Let  $(L_j, U_j)$  be a confidence interval for  $\log(\psi)$ . The corresponding lower and upper confidence limits for the customized odds ratio  $\exp(c\beta_j)$  are  $\exp(cL_j)$  and  $\exp(cU_j)$ , respectively (for  $c > 0$ ), or  $\exp(cU_j)$  and  $\exp(cL_j)$ , respectively (for  $c < 0$ ). You use the **CLODDS=** option or **ODDSRATIO** statement to request the confidence intervals for the odds ratios.

For a generalized logit model, odds ratios are computed similarly, except  $k$  odds ratios are computed for each effect, corresponding to the  $k$  logits in the model.

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## Rank Correlation of Observed Responses and Predicted Probabilities

The predicted mean score of an observation is the sum of the Ordered Values (shown in the “Response Profile” table) minus one, weighted by the corresponding predicted probabilities for that observation; that is, the predicted means score =  $\sum_{i=1}^{k+1} (i-1)\hat{\pi}_i$ , where  $k+1$  is the number of response levels and  $\hat{\pi}_i$  is the predicted probability of the  $i$ th (ordered) response.

A pair of observations with different observed responses is said to be *concordant* if the observation with the lower ordered response value has a lower predicted mean score than the observation with the higher ordered response value. If the observation with the lower ordered response value has a higher predicted mean score than the observation with the higher ordered response value, then the pair is *discordant*. If the pair is neither concordant nor discordant, it is a *tie*. Enumeration of the total numbers of concordant and discordant pairs is carried out by categorizing the predicted mean score into intervals of length  $k/500$  and accumulating the corresponding frequencies of observations. Note that the length of these intervals can be modified by specification of the `BINWIDTH=` option in the `MODEL` statement.

Let  $N$  be the sum of observation frequencies in the data. Suppose there are a total of  $t$  pairs with different responses:  $n_c$  of them are concordant,  $n_d$  of them are discordant, and  $t - n_c - n_d$  of them are tied. PROC LOGISTIC computes the following four indices of rank correlation for assessing the predictive ability of a model:

$$\begin{aligned} c &= (n_c + 0.5(t - n_c - n_d))/t \\ \text{Somers' } D \text{ (Gini coefficient)} &= (n_c - n_d)/t \\ \text{Goodman-Kruskal Gamma} &= (n_c - n_d)/(n_c + n_d) \\ \text{Kendall's Tau-}a &= (n_c - n_d)/(0.5N(N - 1)) \end{aligned}$$

If there are no ties, then Somers'  $D$  (Gini's coefficient) =  $2c - 1$ . Note that the concordance index,  $c$ , also gives an estimate of the area under the receiver operating characteristic (ROC) curve when the response is binary (Hanley and McNeil 1982). See the section “ROC Computations” on page 4261 for more information about this area.

For binary responses, the predicted mean score is equal to the predicted probability for Ordered Value 2. As such, the preceding definition of concordance is consistent with the definition used in previous releases for the binary response model.

These statistics are not available when the `STRATA` statement is specified.

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## Linear Predictor, Predicted Probability, and Confidence Limits

This section describes how predicted probabilities and confidence limits are calculated by using the maximum likelihood estimates (MLEs) obtained from PROC LOGISTIC. For a specific example, see the section “Getting Started: LOGISTIC Procedure” on page 4166. Predicted probabilities and confidence limits can be output to a data set with the `OUTPUT` statement.



## Binary and Cumulative Response Models

For a vector of explanatory variables  $\mathbf{x}$ , the linear predictor

$$\eta_i = g(\Pr(Y \leq i | \mathbf{x})) = \alpha_i + \mathbf{x}'\boldsymbol{\beta} \quad 1 \leq i \leq k$$

is estimated by

$$\hat{\eta}_i = \hat{\alpha}_i + \mathbf{x}'\hat{\boldsymbol{\beta}}$$

where  $\hat{\alpha}_i$  and  $\hat{\boldsymbol{\beta}}$  are the MLEs of  $\alpha_i$  and  $\boldsymbol{\beta}$ . The estimated standard error of  $\eta_i$  is  $\hat{\sigma}(\hat{\eta}_i)$ , which can be computed as the square root of the quadratic form  $(1, \mathbf{x}')\hat{\mathbf{V}}_{\mathbf{b}}(1, \mathbf{x})'$ , where  $\hat{\mathbf{V}}_{\mathbf{b}}$  is the estimated covariance matrix of the parameter estimates. The asymptotic  $100(1 - \alpha)\%$  confidence interval for  $\eta_i$  is given by

$$\hat{\eta}_i \pm z_{\alpha/2}\hat{\sigma}(\hat{\eta}_i)$$

where  $z_{\alpha/2}$  is the  $100(1 - \alpha/2)$  percentile point of a standard normal distribution.

The predicted probability and the  $100(1 - \alpha)\%$  confidence limits for  $\pi_i = \Pr(Y \leq i | \mathbf{x})$  are obtained by back-transforming the corresponding measures for the linear predictor, as shown in the following table:

| Link    | Predicted Probability           | 100(1- $\alpha$ )% Confidence Limits                                       |
|---------|---------------------------------|----------------------------------------------------------------------------|
| LOGIT   | $1/(1 + \exp(-\hat{\eta}_i))$   | $1/(1 + \exp(-\hat{\eta}_i \pm z_{\alpha/2}\hat{\sigma}(\hat{\eta}_i)))$   |
| PROBIT  | $\Phi(\hat{\eta}_i)$            | $\Phi(\hat{\eta}_i \pm z_{\alpha/2}\hat{\sigma}(\hat{\eta}_i))$            |
| CLOGLOG | $1 - \exp(-\exp(\hat{\eta}_i))$ | $1 - \exp(-\exp(\hat{\eta}_i \pm z_{\alpha/2}\hat{\sigma}(\hat{\eta}_i)))$ |

The **CONTRAST** statement also enables you to estimate the exponentiated contrast,  $e^{\hat{\eta}_i}$ . The corresponding standard error is  $e^{\hat{\eta}_i}\hat{\sigma}(\hat{\eta}_i)$ , and the confidence limits are computed by exponentiating those for the linear predictor:  $\exp\{\hat{\eta}_i \pm z_{\alpha/2}\hat{\sigma}(\hat{\eta}_i)\}$ .

## Generalized Logit Model

For a vector of explanatory variables  $\mathbf{x}$ , define the linear predictors  $\eta_i = \alpha_i + \mathbf{x}'\boldsymbol{\beta}_i$ , and let  $\pi_i$  denote the probability of obtaining the response value  $i$ :

$$\pi_i = \begin{cases} \pi_{k+1}e^{\eta_i} & 1 \leq i \leq k \\ \frac{1}{1 + \sum_{j=1}^k e^{\eta_j}} & i = k + 1 \end{cases}$$

By the *delta method*,

$$\sigma^2(\pi_i) = \left(\frac{\partial \pi_i}{\partial \boldsymbol{\beta}}\right)' \mathbf{V}(\boldsymbol{\beta}) \frac{\partial \pi_i}{\partial \boldsymbol{\beta}}$$

A  $100(1 - \alpha)\%$  confidence level for  $\pi_i$  is given by

$$\hat{\pi}_i \pm z_{\alpha/2}\hat{\sigma}(\hat{\pi}_i)$$

where  $\hat{\pi}_i$  is the estimated expected probability of response  $i$ , and  $\hat{\sigma}(\hat{\pi}_i)$  is obtained by evaluating  $\sigma(\pi_i)$  at  $\boldsymbol{\beta} = \hat{\boldsymbol{\beta}}$ .

Note that the contrast  $\hat{\eta}_i$  and exponentiated contrast  $e^{\hat{\eta}_i}$ , their standard errors, and their confidence intervals are computed in the same fashion as for the cumulative response models, replacing  $\boldsymbol{\beta}$  with  $\boldsymbol{\beta}_i$ .

## Classification Table

For binary response data, the response is either an *event* or a *nonevent*. In PROC LOGISTIC, the response with Ordered Value 1 is regarded as the event, and the response with Ordered Value 2 is the nonevent. PROC LOGISTIC models the probability of the event. From the fitted model, a predicted event probability can be computed for each observation. A method to compute a reduced-bias estimate of the predicted probability is given in the section “[Predicted Probability of an Event for Classification](#)” on page 4255. If the predicted event probability exceeds or equals some cutpoint value  $z \in [0, 1]$ , the observation is predicted to be an event observation; otherwise, it is predicted as a nonevent. A  $2 \times 2$  frequency table can be obtained by cross-classifying the observed and predicted responses. The `CTABLE` option produces this table, and the `PPROB=` option selects one or more cutpoints. Each cutpoint generates a classification table. If the `PEVENT=` option is also specified, a classification table is produced for each combination of `PEVENT=` and `PPROB=` values.

The accuracy of the classification is measured by its *sensitivity* (the ability to predict an event correctly) and *specificity* (the ability to predict a nonevent correctly). *Sensitivity* is the proportion of event responses that were predicted to be events. *Specificity* is the proportion of nonevent responses that were predicted to be nonevents. PROC LOGISTIC also computes three other conditional probabilities: *false positive rate*, *false negative rate*, and *rate of correct classification*. The *false positive rate* is the proportion of predicted event responses that were observed as nonevents. The *false negative rate* is the proportion of predicted nonevent responses that were observed as events. Given prior probabilities specified with the `PEVENT=` option, these conditional probabilities can be computed as posterior probabilities by using Bayes’ theorem.

### Predicted Probability of an Event for Classification

When you classify a set of binary data, if the same observations used to fit the model are also used to estimate the classification error, the resulting error-count estimate is biased. One way of reducing the bias is to remove the binary observation to be classified from the data, reestimate the parameters of the model, and then classify the observation based on the new parameter estimates. However, it would be costly to fit the model by leaving out each observation one at a time. The LOGISTIC procedure provides a less expensive one-step approximation to the preceding parameter estimates. Let  $\hat{\boldsymbol{\beta}}$  be the MLE of the parameter vector  $(\alpha, \beta_1, \dots, \beta_s)'$  based on all observations. Let  $\hat{\boldsymbol{\beta}}_{(j)}$  denote the MLE computed without the  $j$ th observation. The one-step estimate of  $\hat{\boldsymbol{\beta}}_{(j)}$  is given by

$$\hat{\boldsymbol{\beta}}_{(j)}^1 = \hat{\boldsymbol{\beta}} - \frac{w_j(y_j - \hat{\pi}_j)}{1 - h_j} \hat{\mathbf{V}}(\hat{\boldsymbol{\beta}}) \begin{pmatrix} 1 \\ \mathbf{x}_j \end{pmatrix}$$

where

- $y_j$  is 1 for an observed event response and 0 otherwise
- $w_j$  is the weight of the observation
- $\hat{\pi}_j$  is the predicted event probability based on  $\hat{\boldsymbol{\beta}}$
- $h_j$  is the **hat diagonal element** (defined on page 4263) with  $n_j = 1$  and  $r_j = y_j$
- $\hat{\mathbf{V}}(\hat{\boldsymbol{\beta}})$  is the estimated covariance matrix of  $\hat{\boldsymbol{\beta}}$

### False Positive, False Negative, and Correct Classification Rates Using Bayes' Theorem

Suppose  $n_1$  of  $n$  individuals experience an event, such as a disease. Let this group be denoted by  $\mathcal{C}_1$ , and let the group of the remaining  $n_2 = n - n_1$  individuals who do not have the disease be denoted by  $\mathcal{C}_2$ . The  $j$ th individual is classified as giving a positive response if the predicted probability of disease ( $\hat{\pi}_{(j)}^*$ ) is large. The probability  $\hat{\pi}_{(j)}^*$  is the reduced-bias estimate based on the one-step approximation given in the preceding section. For a given cutpoint  $z$ , the  $j$ th individual is predicted to give a positive response if  $\hat{\pi}_{(j)}^* \geq z$ .

Let  $B$  denote the event that a subject has the disease, and let  $\bar{B}$  denote the event of not having the disease. Let  $A$  denote the event that the subject responds positively, and let  $\bar{A}$  denote the event of responding negatively. Results of the classification are represented by two conditional probabilities,  $\Pr(A|B)$  and  $\Pr(A|\bar{B})$ , where  $\Pr(A|B)$  is the sensitivity and  $\Pr(A|\bar{B})$  is one minus the specificity.

These probabilities are given by

$$\Pr(A|B) = \frac{\sum_{j \in \mathcal{C}_1} I(\hat{\pi}_{(j)}^* \geq z)}{n_1}$$

$$\Pr(A|\bar{B}) = \frac{\sum_{j \in \mathcal{C}_2} I(\hat{\pi}_{(j)}^* \geq z)}{n_2}$$

where  $I(\cdot)$  is the indicator function.

Bayes' theorem is used to compute several rates of the classification. For a given prior probability  $\Pr(B)$  of the disease, the false positive rate  $P_{F+}$ , the false negative rate  $P_{F-}$ , and the correct classification rate  $P_C$  are given by Fleiss (1981, pp. 4–5) as follows:

$$P_{F+} = \Pr(\bar{B}|A) = \frac{\Pr(A|\bar{B})[1 - \Pr(B)]}{\Pr(A|\bar{B}) + \Pr(B)[\Pr(A|B) - \Pr(A|\bar{B})]}$$

$$P_{F-} = \Pr(B|\bar{A}) = \frac{[1 - \Pr(A|B)]\Pr(B)}{1 - \Pr(A|\bar{B}) - \Pr(B)[\Pr(A|B) - \Pr(A|\bar{B})]}$$

$$P_C = \Pr(B|A) + \Pr(\bar{B}|\bar{A}) = \Pr(A|B)\Pr(B) + \Pr(\bar{A}|\bar{B})[1 - \Pr(B)]$$

The prior probability  $\Pr(B)$  can be specified by the `PEVENT=` option. If the `PEVENT=` option is not specified, the sample proportion of diseased individuals is used; that is,  $\Pr(B) = n_1/n$ . In such a case, the false positive rate and the false negative rate reduce to

$$P_{F+} = \frac{\sum_{j \in \mathcal{C}_2} I(\hat{\pi}_{(j)}^* \geq z)}{\sum_{j \in \mathcal{C}_1} I(\hat{\pi}_{(j)}^* \geq z) + \sum_{j \in \mathcal{C}_2} I(\hat{\pi}_{(j)}^* \geq z)}$$

$$P_{F-} = \frac{\sum_{j \in \mathcal{C}_1} I(\hat{\pi}_{(j)}^* < z)}{\sum_{j \in \mathcal{C}_1} I(\hat{\pi}_{(j)}^* < z) + \sum_{j \in \mathcal{C}_2} I(\hat{\pi}_{(j)}^* < z)}$$

$$P_C = \frac{\sum_{j \in \mathcal{C}_1} I(\hat{\pi}_{(j)}^* \geq z) + \sum_{j \in \mathcal{C}_2} I(\hat{\pi}_{(j)}^* < z)}{n}$$

Note that for a stratified sampling situation in which  $n_1$  and  $n_2$  are chosen a priori,  $n_1/n$  is not a desirable estimate of  $\Pr(B)$ . For such situations, the `PEVENT=` option should be specified.

## Overdispersion

For a correctly specified model, the Pearson chi-square statistic and the deviance, divided by their degrees of freedom, should be approximately equal to one. When their values are much larger than one, the assumption of binomial variability might not be valid and the data are said to exhibit overdispersion. Underdispersion, which results in the ratios being less than one, occurs less often in practice.

When fitting a model, there are several problems that can cause the goodness-of-fit statistics to exceed their degrees of freedom. Among these are such problems as outliers in the data, using the wrong link function, omitting important terms from the model, and needing to transform some predictors. These problems should be eliminated before proceeding to use the following methods to correct for overdispersion.

### Rescaling the Covariance Matrix

One way of correcting overdispersion is to multiply the covariance matrix by a dispersion parameter. This method assumes that the sample sizes in each subpopulation are approximately equal. You can supply the value of the dispersion parameter directly, or you can estimate the dispersion parameter based on either the Pearson chi-square statistic or the deviance for the fitted model.

The Pearson chi-square statistic  $\chi_P^2$  and the deviance  $\chi_D^2$  are given by

$$\chi_P^2 = \sum_{i=1}^m \sum_{j=1}^{k+1} \frac{(r_{ij} - n_i \hat{\pi}_{ij})^2}{n_i \hat{\pi}_{ij}}$$

$$\chi_D^2 = 2 \sum_{i=1}^m \sum_{j=1}^{k+1} r_{ij} \log \left( \frac{r_{ij}}{n_i \hat{\pi}_{ij}} \right)$$

where  $m$  is the number of subpopulation profiles,  $k + 1$  is the number of response levels,  $r_{ij}$  is the total weight (sum of the product of the frequencies and the weights) associated with  $j$ th level responses in the  $i$ th profile,  $n_i = \sum_{j=1}^{k+1} r_{ij}$ , and  $\hat{\pi}_{ij}$  is the fitted probability for the  $j$ th level at the  $i$ th profile. Each of these chi-square statistics has  $mk - p$  degrees of freedom, where  $p$  is the number of parameters estimated. The dispersion parameter is estimated by

$$\widehat{\sigma}^2 = \begin{cases} \chi_P^2 / (mk - p) & \text{SCALE=PEARSON} \\ \chi_D^2 / (mk - p) & \text{SCALE=DEVIANC} \\ (\text{constant})^2 & \text{SCALE=constant} \end{cases}$$

In order for the Pearson statistic and the deviance to be distributed as chi-square, there must be sufficient replication within the subpopulations. When this is not true, the data are sparse, and the  $p$ -values for these statistics are not valid and should be ignored. Similarly, these statistics, divided by their degrees of freedom, cannot serve as indicators of overdispersion. A large difference between the Pearson statistic and the deviance provides some evidence that the data are too sparse to use either statistic.

You can use the **AGGREGATE** (or **AGGREGATE=**) option to define the subpopulation profiles. If you do not specify this option, each observation is regarded as coming from a separate subpopulation. For events/trials syntax, each observation represents  $n$  Bernoulli trials, where  $n$  is the value of the *trials* variable; for single-trial syntax, each observation represents a single trial. Without the **AGGREGATE**

(or AGGREGATE=) option, the Pearson chi-square statistic and the deviance are calculated only for events/trials syntax.

Note that the parameter estimates are not changed by this method. However, their standard errors are adjusted for overdispersion, affecting their significance tests.

### Williams' Method

Suppose that the data consist of  $n$  binomial observations. For the  $i$ th observation, let  $r_i/n_i$  be the observed proportion and let  $\mathbf{x}_i$  be the associated vector of explanatory variables. Suppose that the response probability for the  $i$ th observation is a random variable  $P_i$  with mean and variance

$$E(P_i) = \pi_i \quad \text{and} \quad V(P_i) = \phi\pi_i(1 - \pi_i)$$

where  $\pi_i$  is the probability of the event, and  $\phi$  is a nonnegative but otherwise unknown scale parameter. Then the mean and variance of  $r_i$  are

$$E(r_i) = n_i\pi_i \quad \text{and} \quad V(r_i) = n_i\pi_i(1 - \pi_i)[1 + (n_i - 1)\phi]$$

Williams (1982) estimates the unknown parameter  $\phi$  by equating the value of Pearson's chi-square statistic for the full model to its approximate expected value. Suppose  $w_i^*$  is the weight associated with the  $i$ th observation. The Pearson chi-square statistic is given by

$$\chi^2 = \sum_{i=1}^n \frac{w_i^*(r_i - n_i\hat{\pi}_i)^2}{n_i\hat{\pi}_i(1 - \hat{\pi}_i)}$$

Let  $g'(\cdot)$  be the first derivative of the link function  $g(\cdot)$ . The approximate expected value of  $\chi^2$  is

$$E_{\chi^2} = \sum_{i=1}^n w_i^*(1 - w_i^*v_i d_i)[1 + \phi(n_i - 1)]$$

where  $v_i = n_i/(\pi_i(1 - \pi_i)[g'(\pi_i)]^2)$  and  $d_i$  is the variance of the linear predictor  $\hat{\alpha}_i + \mathbf{x}_i'\hat{\boldsymbol{\beta}}$ . The scale parameter  $\phi$  is estimated by the following iterative procedure.

At the start, let  $w_i^* = 1$  and let  $\pi_i$  be approximated by  $r_i/n_i$ ,  $i = 1, 2, \dots, n$ . If you apply these weights and approximated probabilities to  $\chi^2$  and  $E_{\chi^2}$  and then equate them, an initial estimate of  $\phi$  is

$$\hat{\phi}_0 = \frac{\chi^2 - (n - p)}{\sum_i (n_i - 1)(1 - v_i d_i)}$$

where  $p$  is the total number of parameters. The initial estimates of the weights become  $\hat{w}_{i0}^* = [1 + (n_i - 1)\hat{\phi}_0]^{-1}$ . After a weighted fit of the model, the  $\hat{\alpha}_i$  and  $\hat{\boldsymbol{\beta}}$  are recalculated, and so is  $\chi^2$ . Then a revised estimate of  $\phi$  is given by

$$\hat{\phi}_1 = \frac{\chi^2 - \sum_i w_i^*(1 - w_i^*v_i d_i)}{w_i^*(n_i - 1)(1 - w_i^*v_i d_i)}$$

The iterative procedure is repeated until  $\chi^2$  is very close to its degrees of freedom.

Once  $\phi$  has been estimated by  $\hat{\phi}$  under the full model, weights of  $(1 + (n_i - 1)\hat{\phi})^{-1}$  can be used to fit models that have fewer terms than the full model. See [Example 54.10](#) for an illustration.

**NOTE:** If the **WEIGHT** statement is specified with the **NORMALIZE** option, then the initial  $w_i^*$  values are set to the normalized weights, and the weights resulting from Williams' method will not add up to the actual sample size. However, the estimated covariance matrix of the parameter estimates remains invariant to the scale of the **WEIGHT** variable.

## The Hosmer-Lemeshow Goodness-of-Fit Test

Sufficient replication within subpopulations is required to make the Pearson and deviance goodness-of-fit tests valid. When there are one or more continuous predictors in the model, the data are often too sparse to use these statistics. Hosmer and Lemeshow (2000) proposed a statistic that they show, through simulation, is distributed as chi-square when there is no replication in any of the subpopulations. This test is available only for binary response models.

First, the observations are sorted in increasing order of their estimated event probability. The event is the response level specified in the response variable option `EVENT=`, or the response level that is not specified in the `REF=` option, or, if neither of these options was specified, then the event is the response level identified in the “Response Profiles” table as “Ordered Value 1”. The observations are then divided into approximately 10 groups according to the following scheme. Let  $N$  be the total number of subjects. Let  $M$  be the target number of subjects for each group given by

$$M = [0.1 \times N + 0.5]$$

where  $[x]$  represents the integral value of  $x$ . If the single-trial syntax is used, blocks of subjects are formed of observations with identical values of the explanatory variables. Blocks of subjects are not divided when being placed into groups.

Suppose there are  $n_1$  subjects in the first block and  $n_2$  subjects in the second block. The first block of subjects is placed in the first group. Subjects in the second block are added to the first group if

$$n_1 < M \quad \text{and} \quad n_1 + [0.5 \times n_2] \leq M$$

Otherwise, they are placed in the second group. In general, suppose subjects of the  $(j - 1)$  block have been placed in the  $k$ th group. Let  $c$  be the total number of subjects currently in the  $k$ th group. Subjects for the  $j$ th block (containing  $n_j$  subjects) are also placed in the  $k$ th group if

$$c < M \quad \text{and} \quad c + [0.5 \times n_j] \leq M$$

Otherwise, the  $n_j$  subjects are put into the next group. In addition, if the number of subjects in the last group does not exceed  $[0.05 \times N]$  (half the target group size), the last two groups are collapsed to form only one group.

Note that the number of groups,  $g$ , can be smaller than 10 if there are fewer than 10 patterns of explanatory variables. There must be at least three groups in order for the Hosmer-Lemeshow statistic to be computed.

The Hosmer-Lemeshow goodness-of-fit statistic is obtained by calculating the Pearson chi-square statistic from the  $2 \times g$  table of observed and expected frequencies, where  $g$  is the number of groups. The statistic is written

$$\chi_{HL}^2 = \sum_{i=1}^g \frac{(O_i - N_i \bar{\pi}_i)^2}{N_i \bar{\pi}_i (1 - \bar{\pi}_i)}$$

where  $N_i$  is the total frequency of subjects in the  $i$ th group,  $O_i$  is the total frequency of event outcomes in the  $i$ th group, and  $\bar{\pi}_i$  is the average estimated predicted probability of an event outcome for the  $i$ th group. (Note that the predicted probabilities are computed as shown in the section “[Linear Predictor, Predicted Probability, and Confidence Limits](#)” on page 4253 and are not the cross validated estimates discussed in the section “[Classification Table](#)” on page 4255.) The Hosmer-Lemeshow statistic is then compared to a chi-square distribution with  $(g - n)$  degrees of freedom, where the value of  $n$  can be specified in the `LACKFIT` option in the `MODEL` statement. The default is  $n = 2$ . Large values of  $\chi_{HL}^2$  (and small  $p$ -values) indicate a lack of fit of the model.

## Receiver Operating Characteristic Curves

ROC curves are used to evaluate and compare the performance of diagnostic tests; they can also be used to evaluate model fit. An ROC curve is just a plot of the proportion of true positives (events predicted to be events) versus the proportion of false positives (nonevents predicted to be events).

In a sample of  $n$  individuals, suppose  $n_1$  individuals are observed to have a certain condition or event. Let this group be denoted by  $C_1$ , and let the group of the remaining  $n_2 = n - n_1$  individuals who do not have the condition be denoted by  $C_2$ . Risk factors are identified for the sample, and a logistic regression model is fitted to the data. For the  $j$ th individual, an estimated probability  $\hat{\pi}_j$  of the event of interest is calculated. Note that the  $\hat{\pi}_j$  are computed as shown in the section “[Linear Predictor, Predicted Probability, and Confidence Limits](#)” on page 4253 and are not the cross validated estimates discussed in the section “[Classification Table](#)” on page 4255.

Suppose the  $n$  individuals undergo a test for predicting the event and the test is based on the estimated probability of the event. Higher values of this estimated probability are assumed to be associated with the event. A receiver operating characteristic (ROC) curve can be constructed by varying the cutpoint that determines which estimated event probabilities are considered to predict the event. For each cutpoint  $z$ , the following measures can be output to a data set by specifying the `OUTROC=` option in the `MODEL` statement or the `OUTROC=` option in the `SCORE` statement:

$$\begin{aligned} \_POS\_ (z) &= \sum_{i \in C_1} I(\hat{\pi}_i \geq z) \\ \_NEG\_ (z) &= \sum_{i \in C_2} I(\hat{\pi}_i < z) \\ \_FALPOS\_ (z) &= \sum_{i \in C_2} I(\hat{\pi}_i \geq z) \\ \_FALNEG\_ (z) &= \sum_{i \in C_1} I(\hat{\pi}_i < z) \\ \_SENSIT\_ (z) &= \frac{\_POS\_ (z)}{n_1} \\ \_1MSPEC\_ (z) &= \frac{\_FALPOS\_ (z)}{n_2} \end{aligned}$$

where  $I(\cdot)$  is the indicator function.

Note that  $\_POS\_ (z)$  is the number of correctly predicted event responses,  $\_NEG\_ (z)$  is the number of correctly predicted nonevent responses,  $\_FALPOS\_ (z)$  is the number of falsely predicted event responses,  $\_FALNEG\_ (z)$  is the number of falsely predicted nonevent responses,  $\_SENSIT\_ (z)$  is the sensitivity of the test, and  $\_1MSPEC\_ (z)$  is one minus the specificity of the test.

The ROC curve is a plot of sensitivity ( $\_SENSIT\_$ ) against 1–specificity ( $\_1MSPEC\_$ ). The plot can be produced by using the `PLOTS` option or by using the `GPLOT` or `SGPLOT` procedure with the `OUTROC=` data set. See [Example 54.7](#) for an illustration. The area under the ROC curve, as determined by the trapezoidal rule, is estimated by the concordance index,  $c$ , in the “Association of Predicted Probabilities and Observed Responses” table.



## Comparing ROC Curves

ROC curves can be created from each model fit in a selection routine, from the specified model in the **MODEL** statement, from specified models in ROC statements, or from input variables which act as  $\hat{\pi}$  in the preceding discussion. Association statistics are computed for these models, and the models are compared when the **ROCCONTRAST** statement is specified. The ROC comparisons are performed by using a contrast matrix to take differences of the areas under the empirical ROC curves (DeLong, DeLong, and Clarke-Pearson 1988). For example, if you have three curves and the second curve is the reference, the contrast used for the overall test is

$$\mathbf{L}_1 = \begin{pmatrix} I'_1 \\ I'_2 \end{pmatrix} = \begin{bmatrix} 1 & -1 & 0 \\ 0 & -1 & 1 \end{bmatrix}$$

and you can optionally estimate and test each row of this contrast, in order to test the difference between the reference curve and each of the other curves. If you do not want to use a reference curve, the global test optionally uses the following contrast:

$$\mathbf{L}_2 = \begin{pmatrix} I'_1 \\ I'_2 \end{pmatrix} = \begin{bmatrix} 1 & -1 & 0 \\ 0 & 1 & -1 \end{bmatrix}$$

You can also specify your own contrast matrix. Instead of estimating the rows of these contrasts, you can request that the difference between every pair of ROC curves be estimated and tested.

By default for the reference contrast, the specified or selected model is used as the reference unless the **NOFIT** option is specified in the **MODEL** statement, in which case the first ROC model is the reference.

In order to label the contrasts, a name is attached to every model. The name for the specified or selected model is the **MODEL** statement label, or “Model” if the **MODEL** label is not present. The ROC statement models are named with their labels, or as “ROC*i*” for the *i*th ROC statement if a label is not specified. The contrast  $\mathbf{L}_1$  is labeled as “Reference = ModelName”, where ModelName is the reference model name, while  $\mathbf{L}_2$  is labeled “Adjacent Pairwise Differences”. The estimated rows of the contrast matrix are labeled “ModelName1 – ModelName2”. In particular, for the rows of  $\mathbf{L}_1$ , ModelName2 is the reference model name. If you specify your own contrast matrix, then the contrast is labeled “Specified” and the *i*th contrast row estimates are labeled “Row*i*”.

If ODS Graphics is enabled, then all ROC curves are displayed individually and are also overlaid in a final display. If a selection method is specified, then the curves produced in each step of the model selection process are overlaid onto a single plot and are labeled “Step*i*”, and the selected model is displayed on a separate plot and on a plot with curves from specified ROC statements. See [Example 54.8](#) for an example.

## ROC Computations

The trapezoidal area under an empirical ROC curve is equal to the Mann-Whitney two-sample rank measure of association statistic (a generalized *U*-statistic) applied to two samples,  $\{X_i\}, i = 1, \dots, n_1$ , in  $\mathcal{C}_1$  and  $\{Y_i\}, i = 1, \dots, n_2$ , in  $\mathcal{C}_2$ . PROC LOGISTIC uses the predicted probabilities in place of **X** and **Y**; however, in general any criterion could be used. Denote the frequency of observation *i* in  $\mathcal{C}_k$  as  $f_{ki}$ , and denote the total frequency in  $\mathcal{C}_k$  as  $F_k$ . The **WEIGHTED** option replaces  $f_{ki}$  with  $f_{ki}w_{ki}$ , where  $w_{ki}$  is the weight of



observation  $i$  in group  $C_k$ . The trapezoidal area under the curve is computed as

$$\hat{c} = \frac{1}{F_1 F_2} \sum_{i=1}^{n_1} \sum_{j=1}^{n_2} \psi(X_i, Y_j) f_{1i} f_{2j}$$

$$\psi(X, Y) = \begin{cases} 1 & Y < X \\ \frac{1}{2} & Y = X \\ 0 & Y > X \end{cases}$$

so that  $E(\hat{c}) = \Pr(Y < X) + \frac{1}{2} \Pr(Y = X)$ . Note that the concordance index,  $c$ , in the “Association of Predicted Probabilities and Observed Responses” table does not use weights unless both the **WEIGHTED** and **BINWIDTH=0** options are specified. Also, in this table,  $c$  is computed by creating 500 bins and binning the  $X_i$  and  $Y_j$ ; this results in more ties than the preceding method (unless the **BINWIDTH=0** or **ROCEPS=0** option is specified), so  $c$  is not necessarily equal to  $E(\hat{c})$ .

To compare  $K$  empirical ROC curves, first compute the trapezoidal areas. Asymptotic normality of the estimated area follows from  $U$ -statistic theory, and a covariance matrix  $\mathbf{S}$  can be computed; see DeLong, DeLong, and Clarke-Pearson (1988) for details. A Wald confidence interval for the  $r$ th area,  $1 \leq r \leq K$ , can be constructed as

$$\hat{c}_r \pm z_{1-\frac{\alpha}{2}} s_{r,r}$$

where  $s_{r,r}$  is the  $r$ th diagonal of  $\mathbf{S}$ .

For a contrast of ROC curve areas,  $\mathbf{Lc}$ , the statistic

$$(\hat{\mathbf{c}} - \mathbf{c})' \mathbf{L}' [\mathbf{LSL}']^{-1} \mathbf{L}(\hat{\mathbf{c}} - \mathbf{c})$$

has a chi-square distribution with  $\text{df} = \text{rank}(\mathbf{LSL}')$ . For a row of the contrast,  $\mathbf{l}'\mathbf{c}$ ,

$$\frac{\mathbf{l}'\hat{\mathbf{c}} - \mathbf{l}'\mathbf{c}}{[\mathbf{l}'\mathbf{S}\mathbf{l}]^{1/2}}$$

has a standard normal distribution. The corresponding confidence interval is

$$\mathbf{l}'\hat{\mathbf{c}} \pm z_{1-\frac{\alpha}{2}} [\mathbf{l}'\mathbf{S}\mathbf{l}]^{1/2}$$

## Testing Linear Hypotheses about the Regression Coefficients

Linear hypotheses for  $\boldsymbol{\beta}$  are expressed in matrix form as

$$H_0: \mathbf{L}\boldsymbol{\beta} = \mathbf{c}$$

where  $\mathbf{L}$  is a matrix of coefficients for the linear hypotheses, and  $\mathbf{c}$  is a vector of constants. The vector of regression coefficients  $\boldsymbol{\beta}$  includes slope parameters as well as intercept parameters. The Wald chi-square statistic for testing  $H_0$  is computed as

$$\chi_W^2 = (\mathbf{L}\hat{\boldsymbol{\beta}} - \mathbf{c})' [\mathbf{L}\hat{\mathbf{V}}(\hat{\boldsymbol{\beta}})\mathbf{L}']^{-1} (\mathbf{L}\hat{\boldsymbol{\beta}} - \mathbf{c})$$

where  $\hat{\mathbf{V}}(\hat{\boldsymbol{\beta}})$  is the estimated covariance matrix. Under  $H_0$ ,  $\chi_W^2$  has an asymptotic chi-square distribution with  $r$  degrees of freedom, where  $r$  is the rank of  $\mathbf{L}$ .

## Regression Diagnostics

For binary response data, regression diagnostics developed by Pregibon (1981) can be requested by specifying the **INFLUENCE** option. For diagnostics available with conditional logistic regression, see the section “Regression Diagnostic Details” on page 4272. These diagnostics can also be obtained from the **OUTPUT** statement.

This section uses the following notation:

- $r_j, n_j$      $r_j$  is the number of event responses out of  $n_j$  trials for the  $j$ th observation. If events/trials syntax is used,  $r_j$  is the value of *events* and  $n_j$  is the value of *trials*. For single-trial syntax,  $n_j = 1$ , and  $r_j = 1$  if the ordered response is 1, and  $r_j = 0$  if the ordered response is 2.
- $w_j$         is the weight of the  $j$ th observation.
- $\pi_j$         is the probability of an event response for the  $j$ th observation given by  $\pi_j = F(\alpha + \beta'x_j)$ , where  $F(\cdot)$  is the **inverse link function** defined on page 4238.
- $\hat{\beta}$         is the maximum likelihood estimate (MLE) of  $(\alpha, \beta_1, \dots, \beta_s)'$ .
- $\hat{V}(\hat{\beta})$     is the estimated covariance matrix of  $\hat{\beta}$ .
- $\hat{p}_j, \hat{q}_j$      $\hat{p}_j$  is the estimate of  $\pi_j$  evaluated at  $\hat{\beta}$ , and  $\hat{q}_j = 1 - \hat{p}_j$ .

Pregibon (1981) suggests using the index plots of several diagnostic statistics to identify influential observations and to quantify the effects on various aspects of the maximum likelihood fit. In an index plot, the diagnostic statistic is plotted against the observation number. In general, the distributions of these diagnostic statistics are not known, so cutoff values cannot be given for determining when the values are large. However, the **IPLOTS** and **INFLUENCE** options in the **MODEL** statement and the **PLOTS** option in the **PROC LOGISTIC** statement provide displays of the diagnostic values, allowing visual inspection and comparison of the values across observations. In these plots, if the model is correctly specified and fits all observations well, then no extreme points should appear.

The next five sections give formulas for these diagnostic statistics.

### Hat Matrix Diagonal (Leverage)

The diagonal elements of the hat matrix are useful in detecting extreme points in the design space where they tend to have larger values. The  $j$ th diagonal element is

$$h_j = \begin{cases} \tilde{w}_j(1, \mathbf{x}'_j)\hat{V}(\hat{\beta})(1, \mathbf{x}'_j)' & \text{Fisher scoring} \\ \hat{w}_j(1, \mathbf{x}'_j)\hat{V}(\hat{\beta})(1, \mathbf{x}'_j)' & \text{Newton-Raphson} \end{cases}$$

where

$$\tilde{w}_j = \frac{w_j n_j}{\hat{p}_j \hat{q}_j [g'(\hat{p}_j)]^2}$$

$$\hat{w}_j = \tilde{w}_j + \frac{w_j (r_j - n_j \hat{p}_j) [\hat{p}_j \hat{q}_j g''(\hat{p}_j) + (\hat{q}_j - \hat{p}_j) g'(\hat{p}_j)]}{(\hat{p}_j \hat{q}_j)^2 [g'(\hat{p}_j)]^3}$$

and  $g'(\cdot)$  and  $g''(\cdot)$  are the first and second derivatives of the link function  $g(\cdot)$ , respectively.

For a binary response logit model, the hat matrix diagonal elements are

$$h_j = w_j n_j \hat{p}_j \hat{q}_j (1, \mathbf{x}'_j) \widehat{\mathbf{V}}(\widehat{\boldsymbol{\beta}}) \begin{pmatrix} 1 \\ \mathbf{x}_j \end{pmatrix}$$

If the estimated probability is extreme (less than 0.1 and greater than 0.9, approximately), then the hat diagonal might be greatly reduced in value. Consequently, when an observation has a very large or very small estimated probability, its hat diagonal value is not a good indicator of the observation's distance from the design space (Hosmer and Lemeshow 2000, p. 171).

## Residuals

Residuals are useful in identifying observations that are not explained well by the model. Pearson residuals are components of the Pearson chi-square statistic and deviance residuals are components of the deviance. The Pearson residual for the  $j$ th observation is

$$\chi_j = \frac{\sqrt{w_j}(r_j - n_j \hat{p}_j)}{\sqrt{n_j \hat{p}_j \hat{q}_j}}$$

The Pearson chi-square statistic is the sum of squares of the Pearson residuals.

The deviance residual for the  $j$ th observation is

$$d_j = \begin{cases} -\sqrt{-2w_j n_j \log(\hat{q}_j)} & \text{if } r_j = 0 \\ \pm \sqrt{2w_j [r_j \log(\frac{r_j}{n_j \hat{p}_j}) + (n_j - r_j) \log(\frac{n_j - r_j}{n_j \hat{q}_j})]} & \text{if } 0 < r_j < n_j \\ \sqrt{-2w_j n_j \log(\hat{p}_j)} & \text{if } r_j = n_j \end{cases}$$

where the plus (minus) in  $\pm$  is used if  $r_j/n_j$  is greater (less) than  $\hat{p}_j$ . The deviance is the sum of squares of the deviance residuals.

The STDRES option in the **INFLUENCE** and **PLOTS=INFLUENCE** options computes three more residuals (Collett 2003). The Pearson and deviance residuals are standardized to have approximately unit variance:

$$e_{pj} = \frac{\chi_j}{\sqrt{1 - h_j}}$$

$$e_{dj} = \frac{d_j}{\sqrt{1 - h_j}}$$

The likelihood residuals, which estimate components of a likelihood ratio test of deleting an individual observation, are a weighted combination of the standardized Pearson and deviance residuals

$$e_{lj} = \text{sign}(r_j - n_j \hat{p}_j) \sqrt{h_j e_{pj}^2 + (1 - h_j) e_{dj}^2}$$

## DFBETAS

For each parameter estimate, the procedure calculates a DFBETAS diagnostic for each observation. The DFBETAS diagnostic for an observation is the standardized difference in the parameter estimate due to deleting the observation, and it can be used to assess the effect of an individual observation on each estimated parameter of the fitted model. Instead of reestimating the parameter every time an observation is deleted, PROC LOGISTIC uses the one-step estimate. See the section “[Predicted Probability of an Event for Classification](#)” on page 4255. For the  $j$ th observation, the DFBETAS are given by

$$\text{DFBETAS}_{ij} = \Delta_i \hat{\beta}_j^1 / \hat{\sigma}_i$$

where  $i = 0, 1, \dots, s$ ,  $\hat{\sigma}_i$  is the standard error of the  $i$ th component of  $\hat{\beta}$ , and  $\Delta_i \hat{\beta}_j^1$  is the  $i$ th component of the one-step difference

$$\Delta \hat{\beta}_j^1 = \frac{w_j(r_j - n_j \hat{p}_j)}{1 - h_j} \hat{\mathbf{V}}(\hat{\beta}) \begin{pmatrix} 1 \\ \mathbf{x}_j \end{pmatrix}$$

$\Delta \hat{\beta}_j^1$  is the approximate change ( $\hat{\beta} - \hat{\beta}_j^1$ ) in the vector of parameter estimates due to the omission of the  $j$ th observation. The DFBETAS are useful in detecting observations that are causing instability in the selected coefficients.

## C and CBAR

C and CBAR are confidence interval displacement diagnostics that provide scalar measures of the influence of individual observations on  $\hat{\beta}$ . These diagnostics are based on the same idea as the Cook distance in linear regression theory (Cook and Weisberg 1982), but use the one-step estimate. C and CBAR for the  $j$ th observation are computed as

$$C_j = \chi_j^2 h_j / (1 - h_j)^2$$

and

$$\bar{C}_j = \chi_j^2 h_j / (1 - h_j)$$

respectively.

Typically, to use these statistics, you plot them against an index and look for outliers.

## DIFDEV and DIFCHISQ

DIFDEV and DIFCHISQ are diagnostics for detecting ill-fitted observations; in other words, observations that contribute heavily to the disagreement between the data and the predicted values of the fitted model. DIFDEV is the change in the deviance due to deleting an individual observation while DIFCHISQ is the change in the Pearson chi-square statistic for the same deletion. By using the one-step estimate, DIFDEV and DIFCHISQ for the  $j$ th observation are computed as

$$\text{DIFDEV} = d_j^2 + \bar{C}_j$$

and

$$\text{DIFCHISQ} = \bar{C}_j / h_j$$

---

## Scoring Data Sets

*Scoring a data set*, which is especially important for predictive modeling, means applying a previously fitted model to a new data set in order to compute the conditional, or *posterior*, probabilities of each response category given the values of the explanatory variables in each observation.

The **SCORE** statement enables you to score new data sets and output the scored values and, optionally, the corresponding confidence limits into a SAS data set. If the response variable is included in the new data set, then you can request **fit statistics** for the data, which is especially useful for test or validation data. If the response is binary, you can also create a SAS data set containing the *receiver operating characteristic* (ROC) curve. You can specify multiple **SCORE** statements in the same invocation of PROC LOGISTIC.

By default, the posterior probabilities are based on implicit prior probabilities that are proportional to the frequencies of the response categories in the *training data* (the data used to fit the model). Explicit prior probabilities should be specified with the **PRIOR=** or **PRIOREVENT=** option when the sample proportions of the response categories in the training data differ substantially from the operational data to be scored. For example, to detect a rare category, it is common practice to use a training set in which the rare categories are overrepresented; without prior probabilities that reflect the true incidence rate, the predicted posterior probabilities for the rare category will be too high. By specifying the correct priors, the posterior probabilities are adjusted appropriately.

The model fit to the **DATA=** data set in the PROC LOGISTIC statement is the default model used for the scoring. Alternatively, you can save a model fit in one run of PROC LOGISTIC and use it to score new data in a subsequent run. The **OUTMODEL=** option in the PROC LOGISTIC statement saves the model information in a SAS data set. Specifying this data set in the **INMODEL=** option of a new PROC LOGISTIC run will score the **DATA=** data set in the **SCORE** statement without refitting the model.

The **STORE** statement can also be used to save your model. The PLM procedure can use this model to score new data sets; see Chapter 69, “The PLM Procedure,” for more information. You cannot specify priors in PROC PLM.

### Fit Statistics for Scored Data Sets

Specifying the **FITSTAT** option displays the following fit statistics when the data set being scored includes the response variable:

| Statistic                                | Description                                                                        |
|------------------------------------------|------------------------------------------------------------------------------------|
| Total frequency                          | $F = \sum_i f_i n_i$                                                               |
| Total weight                             | $W = \sum_i f_i w_i n_i$                                                           |
| Log likelihood                           | $\log L = \sum_i f_i w_i \log(\hat{\pi}_i)$                                        |
| Full log likelihood                      | $\log L_f = \text{constant} + \log L$                                              |
| Misclassification (error) rate           | $\frac{\sum_i 1\{F\_Y_i \neq L\_Y_i\} f_i n_i}{F}$                                 |
| AIC                                      | $-2 \log L_f + 2p$                                                                 |
| AICC                                     | $-2 \log L_f + \frac{2pn}{n-p-1}$                                                  |
| BIC                                      | $-2 \log L_f + p \log(n)$                                                          |
| SC                                       | $-2 \log L_f + p \log(F)$                                                          |
| R-square                                 | $R^2 = 1 - \left(\frac{L_0}{L}\right)^{2/F}$                                       |
| Maximum-rescaled R-square                | $\frac{R^2}{1 - L_0^{2/F}}$                                                        |
| AUC                                      | Area under the ROC curve                                                           |
| Brier score (polytomous response)        | $\frac{1}{W} \sum_i f_i w_i \sum_j (y_{ij} - \hat{\pi}_{ij})^2$                    |
| Brier score (binary response)            | $\frac{1}{W} \sum_i f_i w_i (r_i (1 - \hat{\pi}_i)^2 + (n_i - r_i) \hat{\pi}_i^2)$ |
| Brier reliability (events/trials syntax) | $\frac{1}{W} \sum_i f_i w_i (r_i / n_i - \hat{\pi}_i)^2$                           |

In the preceding table,  $f_i$  is the frequency of the  $i$ th observation in the data set being scored,  $w_i$  is the weight of the observation, and  $n = \sum_i f_i$ . The number of trials when events/trials syntax is specified is  $n_i$ , and with single-trial syntax  $n_i = 1$ . The values  $F\_Y_i$  and  $L\_Y_i$  are described in the section “[OUT= Output Data Set in a SCORE Statement](#)” on page 4281. The indicator function  $1\{A\}$  is 1 if  $A$  is true and 0 otherwise. The likelihood of the model is  $L$ , and  $L_0$  denotes the likelihood of the intercept-only model. For polytomous response models,  $y_i$  is the observed polytomous response level,  $\hat{\pi}_{ij}$  is the predicted probability of the  $j$ th response level for observation  $i$ , and  $y_{ij} = 1\{y_i = j\}$ . For binary response models,  $\hat{\pi}_i$  is the predicted probability of the observation,  $r_i$  is the number of events when you specify events/trials syntax, and  $r_i = y_i$  when you specify single-trial syntax.

The log likelihood, Akaike’s information criterion (AIC), and Schwarz criterion (SC) are described in the section “[Model Fitting Information](#)” on page 4245. The full log likelihood is displayed for models specified with events/trials syntax, and the constant term is described in the section “[Model Fitting Information](#)” on page 4245. The AICC is a small-sample bias-corrected version of the AIC (Hurvich and Tsai 1993; Burnham and Anderson 1998). The Bayesian information criterion (BIC) is the same as the SC except when events/trials syntax is specified. The area under the ROC curve for binary response models is defined in the section “[ROC Computations](#)” on page 4261. The R-square and maximum-rescaled R-square statistics, defined in “[Generalized Coefficient of Determination](#)” on page 4246, are not computed when you specify both an `OFFSET=` variable and the `INMODEL=` data set. The Brier score (Brier 1950) is the weighted squared difference between the predicted probabilities and their observed response levels. For events/trials syntax, the Brier reliability is the weighted squared difference between the predicted probabilities and the observed proportions (Murphy 1973).

## Posterior Probabilities and Confidence Limits

Let  $F$  be the inverse link function. That is,

$$F(t) = \begin{cases} \frac{1}{1+\exp(-t)} & \text{logistic} \\ \Phi(t) & \text{normal} \\ 1 - \exp(-\exp(t)) & \text{complementary log-log} \end{cases}$$

The first derivative of  $F$  is given by

$$F'(t) = \begin{cases} \frac{\exp(-t)}{(1+\exp(-t))^2} & \text{logistic} \\ \phi(t) & \text{normal} \\ \exp(t) \exp(-\exp(t)) & \text{complementary log-log} \end{cases}$$

Suppose there are  $k + 1$  response categories. Let  $Y$  be the response variable with levels  $1, \dots, k + 1$ . Let  $\mathbf{x} = (x_0, x_1, \dots, x_s)'$  be a  $(s + 1)$ -vector of covariates, with  $x_0 \equiv 1$ . Let  $\boldsymbol{\beta}$  be the vector of intercept and slope regression parameters.

Posterior probabilities are given by

$$p(Y = i | \mathbf{x}) = \frac{p_o(Y = i | \mathbf{x}) \frac{\tilde{p}(Y=i)}{p_o(Y=i)}}{\sum_j p_o(Y = j | \mathbf{x}) \frac{\tilde{p}(Y=j)}{p_o(Y=j)}} \quad i = 1, \dots, k + 1$$

where the old posterior probabilities ( $p_o(Y = i | \mathbf{x}), i = 1, \dots, k + 1$ ) are the conditional probabilities of the response categories given  $\mathbf{x}$ , the old priors ( $p_o(Y = i), i = 1, \dots, k + 1$ ) are the sample proportions of response categories of the training data, and the new priors ( $\tilde{p}(Y = i), i = 1, \dots, k + 1$ ) are specified in the **PRIOR=** or **PRIOREVENT=** option. To simplify notation, absorb the old priors into the new priors; that is

$$p(Y = i) = \frac{\tilde{p}(Y = i)}{p_o(Y = i)} \quad i = 1, \dots, k + 1$$

Note if the **PRIOR=** and **PRIOREVENT=** options are not specified, then  $p(Y = i) = 1$ .

The posterior probabilities are functions of  $\boldsymbol{\beta}$  and their estimates are obtained by substituting  $\boldsymbol{\beta}$  by its MLE  $\hat{\boldsymbol{\beta}}$ . The variances of the estimated posterior probabilities are given by the *delta method* as follows:

$$\text{Var}(\hat{p}(Y = i | \mathbf{x})) = \left[ \frac{\partial p(Y = i | \mathbf{x})}{\partial \boldsymbol{\beta}} \right]' \text{Var}(\hat{\boldsymbol{\beta}}) \left[ \frac{\partial p(Y = i | \mathbf{x})}{\partial \boldsymbol{\beta}} \right]$$

where

$$\frac{\partial p(Y = i | \mathbf{x})}{\partial \boldsymbol{\beta}} = \frac{\frac{\partial p_o(Y=i|\mathbf{x})}{\partial \boldsymbol{\beta}} p(Y = i)}{\sum_j p_o(Y = j | \mathbf{x}) p(Y = j)} - \frac{p_o(Y = i | \mathbf{x}) p(Y = i) \sum_j \frac{\partial p_o(Y=j|\mathbf{x})}{\partial \boldsymbol{\beta}} p(Y = j)}{[\sum_j p_o(Y = j | \mathbf{x}) p(Y = j)]^2}$$

and the old posterior probabilities  $p_o(Y = i | \mathbf{x})$  are described in the following sections.

A  $100(1 - \alpha)\%$  confidence interval for  $p(Y = i | \mathbf{x})$  is

$$\hat{p}(Y = i | \mathbf{x}) \pm z_{1-\alpha/2} \sqrt{\widehat{\text{Var}}(\hat{p}(Y = i | \mathbf{x}))}$$

where  $z_\tau$  is the upper  $100\tau$  percentile of the standard normal distribution.

**Binary and Cumulative Response Models**

Let  $\alpha_1, \dots, \alpha_k$  be the intercept parameters and let  $\boldsymbol{\beta}_s$  be the vector of slope parameters. Denote  $\boldsymbol{\beta} = (\alpha_1, \dots, \alpha_k, \boldsymbol{\beta}_s)'$ . Let

$$\eta_i = \eta_i(\boldsymbol{\beta}) = \alpha_i + \mathbf{x}'\boldsymbol{\beta}_s, i = 1, \dots, k$$

Estimates of  $\eta_1, \dots, \eta_k$  are obtained by substituting the maximum likelihood estimate  $\widehat{\boldsymbol{\beta}}$  for  $\boldsymbol{\beta}$ .

The predicted probabilities of the responses are

$$\widehat{p}_o(Y = i|\mathbf{x}) = \widehat{\Pr}(Y = i) = \begin{cases} F(\widehat{\eta}_1) & i = 1 \\ F(\widehat{\eta}_i) - F(\widehat{\eta}_{i-1}) & i = 2, \dots, k \\ 1 - F(\widehat{\eta}_k) & i = k + 1 \end{cases}$$

For  $i = 1, \dots, k$ , let  $\boldsymbol{\delta}_i(\mathbf{x})$  be a  $(k + 1)$  column vector with  $i$ th entry equal to 1,  $k + 1$  entry equal to  $\mathbf{x}$ , and all other entries 0. The derivative of  $p_o(Y = i|\mathbf{x})$  with respect to  $\boldsymbol{\beta}$  are

$$\frac{\partial p_o(Y = i|\mathbf{x})}{\partial \boldsymbol{\beta}} = \begin{cases} F'(\alpha_1 + \mathbf{x}'\boldsymbol{\beta}_s)\boldsymbol{\delta}_1(\mathbf{x}) & i = 1 \\ F'(\alpha_i + \mathbf{x}'\boldsymbol{\beta}_s)\boldsymbol{\delta}_i(\mathbf{x}) - F'(\alpha_{i-1} + \mathbf{x}'\boldsymbol{\beta}_s)\boldsymbol{\delta}_{i-1}(\mathbf{x}) & i = 2, \dots, k \\ -F'(\alpha_k + \mathbf{x}'\boldsymbol{\beta}_s)\boldsymbol{\delta}_k(\mathbf{x}) & i = k + 1 \end{cases}$$

The cumulative posterior probabilities are

$$p(Y \leq i|\mathbf{x}) = \frac{\sum_{j=1}^i p_o(Y = j|\mathbf{x})p(Y = j)}{\sum_{j=1}^{k+1} p_o(Y = j|\mathbf{x})p(Y = j)} = \sum_{j=1}^i p(Y = j|\mathbf{x}) \quad i = 1, \dots, k + 1$$

Their derivatives are

$$\frac{\partial p(Y \leq i|\mathbf{x})}{\partial \boldsymbol{\beta}} = \sum_{j=1}^i \frac{\partial p(Y = j|\mathbf{x})}{\partial \boldsymbol{\beta}} \quad i = 1, \dots, k + 1$$

In the delta-method equation for the variance, replace  $p(Y = \cdot|\mathbf{x})$  with  $p(Y \leq \cdot|\mathbf{x})$ .

Finally, for the cumulative response model, use

$$\begin{aligned} \widehat{p}_o(Y \leq i|\mathbf{x}) &= F(\widehat{\eta}_i) \quad i = 1, \dots, k \\ \widehat{p}_o(Y \leq k + 1|\mathbf{x}) &= 1 \\ \frac{\partial p_o(Y \leq i|\mathbf{x})}{\partial \boldsymbol{\beta}} &= F'(\alpha_i + \mathbf{x}'\boldsymbol{\beta}_s)\boldsymbol{\delta}_i(\mathbf{x}) \quad i = 1, \dots, k \\ \frac{\partial p_o(Y \leq k + 1|\mathbf{x})}{\partial \boldsymbol{\beta}} &= 0 \end{aligned}$$



**Generalized Logit Model**

Consider the last response level ( $Y=k+1$ ) as the reference. Let  $\beta_1, \dots, \beta_k$  be the (intercept and slope) parameter vectors for the first  $k$  logits, respectively. Denote  $\beta = (\beta'_1, \dots, \beta'_k)'$ . Let  $\eta = (\eta_1, \dots, \eta_k)'$  with

$$\eta_i = \eta_i(\beta) = \mathbf{x}'\beta_i \quad i = 1, \dots, k$$

Estimates of  $\eta_1, \dots, \eta_k$  are obtained by substituting the maximum likelihood estimate  $\hat{\beta}$  for  $\beta$ .

The predicted probabilities are

$$\begin{aligned} \widehat{p}_o(Y = k + 1|\mathbf{x}) &\equiv \Pr(Y = k + 1|\mathbf{x}) = \frac{1}{1 + \sum_{l=1}^k \exp(\hat{\eta}_l)} \\ \widehat{p}_o(Y = i|\mathbf{x}) &\equiv \Pr(Y = i|\mathbf{x}) = \widehat{p}_o(Y = k + 1|\mathbf{x}) \exp(\eta_i), i = 1, \dots, k \end{aligned}$$

The derivative of  $p_o(Y = i|\mathbf{x})$  with respect to  $\beta$  are

$$\begin{aligned} \frac{\partial p_o(Y = i|\mathbf{x})}{\partial \beta} &= \frac{\partial \eta}{\partial \beta} \frac{\partial p_o(Y = i|\mathbf{x})}{\partial \eta} \\ &= (I_k \otimes \mathbf{x}) \left( \frac{\partial p_o(Y = i|\mathbf{x})}{\partial \eta_1}, \dots, \frac{\partial p_o(Y = i|\mathbf{x})}{\partial \eta_k} \right)' \end{aligned}$$

where

$$\frac{\partial p_o(Y = i|\mathbf{x})}{\partial \eta_j} = \begin{cases} p_o(Y = i|\mathbf{x})(1 - p_o(Y = i|\mathbf{x})) & j = i \\ -p_o(Y = i|\mathbf{x})p_o(Y = j|\mathbf{x}) & \text{otherwise} \end{cases}$$

**Special Case of Binary Response Model with No Priors**

Let  $\beta$  be the vector of regression parameters. Let

$$\eta = \eta(\beta) = \mathbf{x}'\beta$$

The variance of  $\hat{\eta}$  is given by

$$\text{Var}(\hat{\eta}) = \mathbf{x}'\text{Var}(\hat{\beta})\mathbf{x}$$

A  $100(1 - \alpha)$  percent confidence interval for  $\eta$  is

$$\hat{\eta} \pm z_{1-\alpha/2} \sqrt{\widehat{\text{Var}}(\hat{\eta})}$$

Estimates of  $p_o(Y = 1|\mathbf{x})$  and confidence intervals for the  $p_o(Y = 1|\mathbf{x})$  are obtained by back-transforming  $\hat{\eta}$  and the confidence intervals for  $\eta$ , respectively. That is,

$$\widehat{p}_o(Y = 1|\mathbf{x}) = F(\hat{\eta})$$

and the confidence intervals are

$$F \left( \hat{\eta} \pm z_{1-\alpha/2} \sqrt{\widehat{\text{Var}}(\hat{\eta})} \right)$$

## Conditional Logistic Regression

The method of maximum likelihood described in the preceding sections relies on large-sample asymptotic normality for the validity of estimates and especially of their standard errors. When you do not have a large sample size compared to the number of parameters, this approach might be inappropriate and might result in biased inferences. This situation typically arises when your data are stratified and you fit intercepts to each stratum so that the number of parameters is of the same order as the sample size. For example, in a 1:1 matched pairs study with  $n$  pairs and  $p$  covariates, you would estimate  $n - 1$  intercept parameters and  $p$  slope parameters. Taking the stratification into account by “conditioning out” (and not estimating) the stratum-specific intercepts gives consistent and asymptotically normal MLEs for the slope coefficients. See Breslow and Day (1980) and Stokes, Davis, and Koch (2012) for more information. If your nuisance parameters are not just stratum-specific intercepts, you can perform an [exact conditional logistic regression](#).

### Computational Details

For each stratum  $h$ ,  $h = 1, \dots, H$ , number the observations as  $i = 1, \dots, n_h$  so that  $hi$  indexes the  $i$ th observation in stratum  $h$ . Denote the  $p$  covariates for the  $hi$ th observation as  $\mathbf{x}_{hi}$  and its binary response as  $y_{hi}$ , and let  $\mathbf{y} = (y_{11}, \dots, y_{1n_1}, \dots, y_{H1}, \dots, y_{Hn_H})'$ ,  $\mathbf{X}_h = (\mathbf{x}_{h1} \dots \mathbf{x}_{hn_h})'$ , and  $\mathbf{X} = (\mathbf{X}'_1 \dots \mathbf{X}'_H)'$ . Let the dummy variables  $z_h$ ,  $h = 1, \dots, H$ , be indicator functions for the strata ( $z_h = 1$  if the observation is in stratum  $h$ ), and denote  $\mathbf{z}_{hi} = (z_1, \dots, z_H)$  for the  $hi$ th observation,  $\mathbf{Z}_h = (\mathbf{z}_{h1} \dots \mathbf{z}_{hn_h})'$ , and  $\mathbf{Z} = (\mathbf{Z}'_1 \dots \mathbf{Z}'_H)'$ . Denote  $\mathbf{X}^* = (\mathbf{Z}|\mathbf{X})$  and  $\mathbf{x}^*_{hi} = (\mathbf{z}'_{hi}|\mathbf{x}'_{hi})'$ . Arrange the observations in each stratum  $h$  so that  $y_{hi} = 1$  for  $i = 1, \dots, m_h$ , and  $y_{hi} = 0$  for  $i = m_h + 1, \dots, n_h$ . Suppose all observations have unit frequency.

Consider the binary logistic regression model on page 4163 written as

$$\text{logit}(\boldsymbol{\pi}) = \mathbf{X}^* \boldsymbol{\theta}$$

where the parameter vector  $\boldsymbol{\theta} = (\boldsymbol{\alpha}', \boldsymbol{\beta}')'$  consists of  $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_H)'$ ,  $\alpha_h$  is the intercept for stratum  $h$ ,  $h = 1, \dots, H$ , and  $\boldsymbol{\beta}$  is the parameter vector for the  $p$  covariates.

From the section “Determining Observations for Likelihood Contributions” on page 4239, you can write the likelihood contribution of observation  $hi$ ,  $i = 1, \dots, n_h$ ,  $h = 1, \dots, H$ , as

$$L_{hi}(\boldsymbol{\theta}) = \frac{e^{y_{hi}\mathbf{x}^*_{hi}'\boldsymbol{\theta}}}{1 + e^{\mathbf{x}^*_{hi}'\boldsymbol{\theta}}}$$

where  $y_{hi} = 1$  when the response takes Ordered Value 1, and  $y_{hi} = 0$  otherwise.

The full likelihood is

$$L(\boldsymbol{\theta}) = \prod_{h=1}^H \prod_{i=1}^{n_h} L_{hi}(\boldsymbol{\theta}) = \frac{e^{\mathbf{y}'\mathbf{X}^*\boldsymbol{\theta}}}{\prod_{h=1}^H \prod_{i=1}^{n_h} (1 + e^{\mathbf{x}^*_{hi}'\boldsymbol{\theta}})}$$

Unconditional likelihood inference is based on maximizing this likelihood function.

When your nuisance parameters are the stratum-specific intercepts  $(\alpha_1, \dots, \alpha_H)'$ , and the slopes  $\boldsymbol{\beta}$  are your parameters of interest, “conditioning out” the nuisance parameters produces the conditional likelihood (Lachin 2000)

$$L(\boldsymbol{\beta}) = \prod_{h=1}^H L_h(\boldsymbol{\beta}) = \prod_{h=1}^H \frac{\prod_{i=1}^{m_h} \exp(\mathbf{x}'_{hi}\boldsymbol{\beta})}{\sum \prod_{j=j_1}^{j_{m_h}} \exp(\mathbf{x}'_{hj}\boldsymbol{\beta})}$$

where the summation is over all  $\binom{n_h}{m_h}$  subsets  $\{j_1, \dots, j_{m_h}\}$  of  $m_h$  observations chosen from the  $n_h$  observations in stratum  $h$ . Note that the nuisance parameters have been factored out of this equation.

For conditional asymptotic inference, maximum likelihood estimates  $\hat{\beta}$  of the regression parameters are obtained by maximizing the conditional likelihood, and asymptotic results are applied to the conditional likelihood function and the maximum likelihood estimators. A relatively fast method of computing this conditional likelihood and its derivatives is given by Gail, Lubin, and Rubinstein (1981) and Howard (1972). The optimization techniques can be controlled by specifying the **NLOPTIONS** statement.

Sometimes the log likelihood converges but the estimates diverge. This condition is flagged by having inordinately large standard errors for some of your parameter estimates, and can be monitored by specifying the **ITPRINT** option. Unfortunately, broad existence criteria such as those discussed in the section “**Existence of Maximum Likelihood Estimates**” on page 4242 do not exist for this model. It might be possible to circumvent such a problem by standardizing your independent variables before fitting the model.

### Regression Diagnostic Details

Diagnostics are used to indicate observations that might have undue influence on the model fit or that might be outliers. Further investigation should be performed before removing such an observation from the data set.

The derivations in this section use an augmentation method described by Storer and Crowley (1985), which provides an estimate of the “one-step” **DFBETAS** estimates advocated by Pregibon (1984). The method also provides estimates of conditional stratum-specific predicted values, residuals, and leverage for each observation. The augmentation method can take a lot of time and memory.

Following Storer and Crowley (1985), the log-likelihood contribution can be written as

$$l_h = \log(L_h) = \mathbf{y}'_h \boldsymbol{\gamma}_h - a(\boldsymbol{\gamma}_h) \quad \text{where}$$

$$a(\boldsymbol{\gamma}_h) = \log \left[ \sum_{j=j_1}^{j_{m_h}} \prod_{j=j_1}^{j_{m_h}} \exp(\boldsymbol{\gamma}_{hj}) \right]$$

and the  $h$  subscript on matrices indicates the submatrix for the stratum,  $\boldsymbol{\gamma}_h = (\gamma_{h1}, \dots, \gamma_{hn_h})'$ , and  $\gamma_{hi} = \mathbf{x}'_{hi} \boldsymbol{\beta}$ . Then the gradient and information matrix are

$$\mathbf{g}(\boldsymbol{\beta}) = \left\{ \frac{\partial l_h}{\partial \boldsymbol{\beta}} \right\}_{h=1}^H = \mathbf{X}'(\mathbf{y} - \boldsymbol{\pi})$$

$$\boldsymbol{\Lambda}(\boldsymbol{\beta}) = \left\{ \frac{\partial^2 l_h}{\partial \boldsymbol{\beta}^2} \right\}_{h=1}^H = \mathbf{X}' \text{diag}(\mathbf{U}_1, \dots, \mathbf{U}_H) \mathbf{X}$$

where

$$\begin{aligned}\pi_{hi} &= \frac{\partial a(\boldsymbol{\gamma}_h)}{\partial \gamma_{hi}} = \frac{\sum_{j(i)} \prod_{j=j_1}^{j_{m_h}} \exp(\gamma_{hj})}{\sum \prod_{j=j_1}^{j_{m_h}} \exp(\gamma_{hj})} \\ \boldsymbol{\pi}_h &= (\pi_{h1}, \dots, \pi_{hn_h}) \\ \mathbf{U}_h &= \frac{\partial^2 a(\boldsymbol{\gamma}_h)}{\partial \boldsymbol{\gamma}_h^2} = \left\{ \frac{\partial^2 a(\boldsymbol{\gamma}_h)}{\partial \gamma_{hi} \partial \gamma_{hj}} \right\} = \{a_{ij}\} \\ a_{ij} &= \frac{\sum_{k(i,j)} \prod_{k=k_1}^{k_{m_h}} \exp(\gamma_{hk})}{\sum \prod_{k=k_1}^{k_{m_h}} \exp(\gamma_{hk})} - \frac{\partial a(\boldsymbol{\gamma}_h)}{\partial \gamma_{hi}} \frac{\partial a(\boldsymbol{\gamma}_h)}{\partial \gamma_{hj}} = \pi_{hij} - \pi_{hi} \pi_{hj}\end{aligned}$$

and where  $\pi_{hi}$  is the conditional stratum-specific probability that subject  $i$  in stratum  $h$  is a case, the summation on  $j(i)$  is over all subsets from  $\{1, \dots, n_h\}$  of size  $m_h$  that contain the index  $i$ , and the summation on  $k(i, j)$  is over all subsets from  $\{1, \dots, n_h\}$  of size  $m_h$  that contain the indices  $i$  and  $j$ .

To produce the true one-step estimate  $\boldsymbol{\beta}_{hi}^1$ , start at the MLE  $\widehat{\boldsymbol{\beta}}$ , delete the  $h$ th observation, and use this reduced data set to compute the next Newton-Raphson step. Note that if there is only one event or one nonevent in a stratum, deletion of that single observation is equivalent to deletion of the entire stratum. The augmentation method does not take this into account.

The augmented model is

$$\text{logit}(\Pr(y_{hi} = 1 | \mathbf{x}_{hi})) = \mathbf{x}'_{hi} \boldsymbol{\beta} + \mathbf{z}'_{hi} \gamma$$

where  $\mathbf{z}_{hi} = (0, \dots, 0, 1, 0, \dots, 0)'$  has a 1 in the  $h$ th coordinate, and use  $\boldsymbol{\beta}^0 = (\widehat{\boldsymbol{\beta}}', 0)'$  as the initial estimate for  $(\boldsymbol{\beta}', \gamma)'$ . The gradient and information matrix before the step are

$$\begin{aligned}\mathbf{g}(\boldsymbol{\beta}^0) &= \begin{bmatrix} \mathbf{X}' \\ \mathbf{z}'_{hi} \end{bmatrix} (\mathbf{y} - \boldsymbol{\pi}) = \begin{bmatrix} \mathbf{0} \\ y_{hi} - \pi_{hi} \end{bmatrix} \\ \boldsymbol{\Lambda}(\boldsymbol{\beta}^0) &= \begin{bmatrix} \mathbf{X}' \\ \mathbf{z}'_{hi} \end{bmatrix} \mathbf{U} [\mathbf{X} \quad \mathbf{z}_{hi}] = \begin{bmatrix} \boldsymbol{\Lambda}(\boldsymbol{\beta}) & \mathbf{X}' \mathbf{U} \mathbf{z}_{hi} \\ \mathbf{z}'_{hi} \mathbf{U} \mathbf{X} & \mathbf{z}'_{hi} \mathbf{U} \mathbf{z}_{hi} \end{bmatrix}\end{aligned}$$

Inserting the  $\boldsymbol{\beta}^0$  and  $(\mathbf{X}', \mathbf{z}'_{hi})'$  into the Gail, Lubin, and Rubinstein (1981) algorithm provides the appropriate estimates of  $\mathbf{g}(\boldsymbol{\beta}^0)$  and  $\boldsymbol{\Lambda}(\boldsymbol{\beta}^0)$ . Indicate these estimates with  $\widehat{\boldsymbol{\pi}} = \boldsymbol{\pi}(\widehat{\boldsymbol{\beta}})$ ,  $\widehat{\mathbf{U}} = \mathbf{U}(\widehat{\boldsymbol{\beta}})$ ,  $\widehat{\mathbf{g}}$ , and  $\widehat{\boldsymbol{\Lambda}}$ .

DFBETA is computed from the information matrix as

$$\begin{aligned}\Delta_{hi} \boldsymbol{\beta} &= \boldsymbol{\beta}^0 - \boldsymbol{\beta}_{hi}^1 \\ &= -\widehat{\boldsymbol{\Lambda}}^{-1}(\boldsymbol{\beta}^0) \widehat{\mathbf{g}}(\boldsymbol{\beta}^0) \\ &= -\widehat{\boldsymbol{\Lambda}}^{-1}(\widehat{\boldsymbol{\beta}}) (\mathbf{X}' \widehat{\mathbf{U}} \mathbf{z}_{hi}) \mathbf{M}^{-1} \mathbf{z}'_{hi} (\mathbf{y} - \widehat{\boldsymbol{\pi}})\end{aligned}$$

where

$$\mathbf{M} = (\mathbf{z}'_{hi} \widehat{\mathbf{U}} \mathbf{z}_{hi}) - (\mathbf{z}'_{hi} \widehat{\mathbf{U}} \mathbf{X}) \widehat{\boldsymbol{\Lambda}}^{-1}(\widehat{\boldsymbol{\beta}}) (\mathbf{X}' \widehat{\mathbf{U}} \mathbf{z}_{hi})$$

For each observation in the data set, a DFBETA statistic is computed for each parameter  $\beta_j$ ,  $1 \leq j \leq p$ , and standardized by the standard error of  $\beta_j$  from the full data set to produce the estimate of DFBETAS.

The estimated leverage is defined as

$$h_{hi} = \frac{\text{trace}\{(\mathbf{z}'_{hi} \widehat{\mathbf{U}} \mathbf{X}) \widehat{\mathbf{\Lambda}}^{-1}(\widehat{\boldsymbol{\beta}}) (\mathbf{X}' \widehat{\mathbf{U}} \mathbf{z}_{hi})\}}{\text{trace}\{\mathbf{z}'_{hi} \widehat{\mathbf{U}} \mathbf{z}_{hi}\}}$$

This definition of leverage produces different values from those defined by Pregibon (1984); Moolgavkar, Lustbader, and Venzon (1985); Hosmer and Lemeshow (2000); however, it has the advantage that no extra computations beyond those for the DFBETAS are required.

The estimated residuals  $e_{hi} = y_{hi} - \widehat{\pi}_{hi}$  are obtained from  $\widehat{\mathbf{g}}(\boldsymbol{\beta}^0)$ , and the weights, or predicted probabilities, are then  $\widehat{\pi}_{hi} = y_{hi} - e_{hi}$ . The residuals are standardized and reported as (estimated) Pearson residuals:

$$\frac{r_{hi} - n_{hi} \widehat{\pi}_{hi}}{\sqrt{n_{hi} \widehat{\pi}_{hi} (1 - \widehat{\pi}_{hi})}}$$

where  $r_{hi}$  is the number of events in the observation and  $n_{hi}$  is the number of trials.

The STDRES option in the INFLUENCE and PLOTS=INFLUENCE options computes the standardized Pearson residual:

$$e_{s,hi} = \frac{e_{hi}}{\sqrt{1 - h_{hi}}}$$

For events/trials MODEL statement syntax, treat each observation as two observations (the first for the nonevents and the second for the events) with frequencies  $f_{h,2i-1} = n_{hi} - r_{hi}$  and  $f_{h,2i} = r_{hi}$ , and augment the model with a matrix  $\mathbf{Z}_{hi} = [\mathbf{z}_{h,2i-1} \mathbf{z}_{h,2i}]$  instead of a single  $\mathbf{z}_{hi}$  vector. Writing  $\gamma_{hi} = \mathbf{x}'_{hi} \boldsymbol{\beta}$  in the preceding section results in the following gradient and information matrix:

$$\mathbf{g}(\boldsymbol{\beta}^0) = \begin{bmatrix} \mathbf{0} \\ f_{h,2i-1}(y_{h,2i-1} - \pi_{h,2i-1}) \\ f_{h,2i}(y_{h,2i} - \pi_{h,2i}) \end{bmatrix}$$

$$\mathbf{\Lambda}(\boldsymbol{\beta}^0) = \begin{bmatrix} \mathbf{\Lambda}(\boldsymbol{\beta}) & \mathbf{X}' \text{diag}(\mathbf{f}) \text{Udiag}(\mathbf{f}) \mathbf{Z}_{hi} \\ \mathbf{Z}'_{hi} \text{diag}(\mathbf{f}) \text{Udiag}(\mathbf{f}) \mathbf{X} & \mathbf{Z}'_{hi} \text{diag}(\mathbf{f}) \text{Udiag}(\mathbf{f}) \mathbf{Z}_{hi} \end{bmatrix}$$

The predicted probabilities are then  $\widehat{\pi}_{hi} = y_{h,2i} - e_{h,2i} / r_{h,2i}$ , while the leverage and the DFBETAS are produced from  $\mathbf{\Lambda}(\boldsymbol{\beta}^0)$  in a fashion similar to that for the preceding single-trial equations.

---

## Exact Conditional Logistic Regression

The theory of exact logistic regression, also known as exact conditional logistic regression, was originally laid out by Cox (1970), and the computational methods employed in PROC LOGISTIC are described in Hirji, Mehta, and Patel (1987); Hirji (1992); Mehta, Patel, and Senchaudhuri (1992). Other useful references for the derivations include Cox and Snell (1989); Agresti (1990); Mehta and Patel (1995).

Exact conditional inference is based on generating the conditional distribution for the sufficient statistics of the parameters of interest. This distribution is called the *permutation* or *exact conditional* distribution. Using the notation in the section “Computational Details” on page 4271, follow Mehta and Patel (1995) and

first note that the sufficient statistics  $\mathbf{T} = (T_1, \dots, T_p)$  for the parameter vector of intercepts and slopes,  $\boldsymbol{\beta}$ , are

$$T_j = \sum_{i=1}^n y_i x_{ij}, \quad j = 1, \dots, p$$

Denote a vector of observable sufficient statistics as  $\mathbf{t} = (t_1, \dots, t_p)'$ .

The probability density function (PDF) for  $\mathbf{T}$  can be created by summing over all binary sequences  $\mathbf{y}$  that generate an observable  $\mathbf{t}$  and letting  $C(\mathbf{t}) = |\{\mathbf{y} : \mathbf{y}'\mathbf{X} = \mathbf{t}\}|$  denote the number of sequences  $\mathbf{y}$  that generate  $\mathbf{t}$

$$\Pr(\mathbf{T} = \mathbf{t}) = \frac{C(\mathbf{t}) \exp(\mathbf{t}'\boldsymbol{\beta})}{\prod_{i=1}^n [1 + \exp(\mathbf{x}_i'\boldsymbol{\beta})]}$$

In order to condition out the nuisance parameters, partition the parameter vector  $\boldsymbol{\beta} = (\boldsymbol{\beta}'_N, \boldsymbol{\beta}'_I)'$ , where  $\boldsymbol{\beta}_N$  is a  $p_N \times 1$  vector of the nuisance parameters, and  $\boldsymbol{\beta}_I$  is the parameter vector for the remaining  $p_I = p - p_N$  parameters of interest. Likewise, partition  $\mathbf{X}$  into  $\mathbf{X}_N$  and  $\mathbf{X}_I$ ,  $\mathbf{T}$  into  $\mathbf{T}_N$  and  $\mathbf{T}_I$ , and  $\mathbf{t}$  into  $\mathbf{t}_N$  and  $\mathbf{t}_I$ . The nuisance parameters can be removed from the analysis by conditioning on their sufficient statistics to create the conditional likelihood of  $\mathbf{T}_I$  given  $\mathbf{T}_N = \mathbf{t}_N$ ,

$$\begin{aligned} \Pr(\mathbf{T}_I = \mathbf{t}_I | \mathbf{T}_N = \mathbf{t}_N) &= \frac{\Pr(\mathbf{T} = \mathbf{t})}{\Pr(\mathbf{T}_N = \mathbf{t}_N)} \\ &= f_{\boldsymbol{\beta}_I}(\mathbf{t}_I | \mathbf{t}_N) = \frac{C(\mathbf{t}_N, \mathbf{t}_I) \exp(\mathbf{t}'_I \boldsymbol{\beta}_I)}{\sum_{\mathbf{u}} C(\mathbf{t}_N, \mathbf{u}) \exp(\mathbf{u}' \boldsymbol{\beta}_I)} \end{aligned}$$

where  $C(\mathbf{t}_N, \mathbf{u})$  is the number of vectors  $\mathbf{y}$  such that  $\mathbf{y}'\mathbf{X}_N = \mathbf{t}_N$  and  $\mathbf{y}'\mathbf{X}_I = \mathbf{u}$ . Note that the nuisance parameters have factored out of this equation, and that  $C(\mathbf{t}_N, \mathbf{t}_I)$  is a constant.

The goal of the exact conditional analysis is to determine how likely the observed response  $\mathbf{y}_0$  is with respect to all  $2^n$  possible responses  $\mathbf{y} = (y_1, \dots, y_n)'$ . One way to proceed is to generate every  $\mathbf{y}$  vector for which  $\mathbf{y}'\mathbf{X}_N = \mathbf{t}_N$ , and count the number of vectors  $\mathbf{y}$  for which  $\mathbf{y}'\mathbf{X}_I$  is equal to each unique  $\mathbf{t}_I$ . Generating the conditional distribution from complete enumeration of the joint distribution is conceptually simple; however, this method becomes computationally infeasible very quickly. For example, if you had only 30 observations, you would have to scan through  $2^{30}$  different  $\mathbf{y}$  vectors.

Several algorithms are available in PROC LOGISTIC to generate the exact distribution. All of the algorithms are based on the following observation. Given any  $\mathbf{y} = (y_1, \dots, y_n)'$  and a design  $\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_n)'$ , let  $\mathbf{y}_{(i)} = (y_1, \dots, y_i)'$  and  $\mathbf{X}_{(i)} = (\mathbf{x}_1, \dots, \mathbf{x}_i)'$  be the first  $i$  rows of each matrix. Write the sufficient statistic based on these  $i$  rows as  $\mathbf{t}_{(i)} = \mathbf{y}_{(i)}'\mathbf{X}_{(i)}$ . A recursion relation results:  $\mathbf{t}_{(i+1)} = \mathbf{t}_{(i)} + y_{i+1}\mathbf{x}_{i+1}$ .

The following methods are available:

- The *multivariate shift algorithm* developed by Hirji, Mehta, and Patel (1987), which steps through the recursion relation by adding one observation at a time and building an intermediate distribution at each step. If it determines that  $\mathbf{t}_{(i)}$  for the nuisance parameters could eventually equal  $\mathbf{t}$ , then  $\mathbf{t}_{(i)}$  is added to the intermediate distribution.
- An extension of the multivariate shift algorithm to generalized logit models by Hirji (1992). Since the generalized logit model fits a new set of parameters to each logit, the number of parameters in the

model can easily get too large for this algorithm to handle. Note for these models that the hypothesis tests for each effect are computed across the logit functions, while individual parameters are estimated for each logit function.

- A network algorithm described in Mehta, Patel, and Senchaudhuri (1992), which builds a network for each parameter that you are conditioning out in order to identify feasible  $y_i$  for the  $\mathbf{y}$  vector. These networks are combined and the set of feasible  $y_i$  is further reduced, and then the multivariate shift algorithm uses this knowledge to build the exact distribution without adding as many intermediate  $t_{(i+1)}$  as the multivariate shift algorithm does.
- A hybrid Monte Carlo and network algorithm described by Mehta, Patel, and Senchaudhuri (2000), which extends their 1992 algorithm by sampling from the combined network to build the exact distribution.

The bulk of the computation time and memory for these algorithms is consumed by the creation of the networks and the exact joint distribution. After the joint distribution for a set of effects is created, the computational effort required to produce hypothesis tests and parameter estimates for any subset of the effects is (relatively) trivial. See the section “Computational Resources for Exact Logistic Regression” on page 4284 for more computational notes about exact analyses.

**NOTE:** An alternative to using these exact conditional methods is to perform Firth’s bias-reducing penalized likelihood method (see the **FIRTH** option in the **MODEL** statement); this method has the advantage of being much faster and less memory intensive than exact algorithms, but it might not converge to a solution.

## Hypothesis Tests

Consider testing the null hypothesis  $H_0: \boldsymbol{\beta}_I = \mathbf{0}$  against the alternative  $H_A: \boldsymbol{\beta}_I \neq \mathbf{0}$ , conditional on  $\mathbf{T}_N = \mathbf{t}_N$ . Under the null hypothesis, the test statistic for the *exact probability test* is just  $f_{\boldsymbol{\beta}_I=\mathbf{0}}(\mathbf{t}_I|\mathbf{t}_N)$ , while the corresponding  $p$ -value is the probability of getting a less likely (more extreme) statistic,

$$p(\mathbf{t}_I|\mathbf{t}_N) = \sum_{\mathbf{u} \in \Omega_p} f_0(\mathbf{u}|\mathbf{t}_N)$$

where  $\Omega_p = \{\mathbf{u}: \text{there exist } \mathbf{y} \text{ with } \mathbf{y}'\mathbf{X}_I = \mathbf{u}, \mathbf{y}'\mathbf{X}_N = \mathbf{t}_N, \text{ and } f_0(\mathbf{u}|\mathbf{t}_N) \leq f_0(\mathbf{t}_I|\mathbf{t}_N)\}$ .

For the *exact conditional scores test*, the conditional mean  $\boldsymbol{\mu}_I$  and variance matrix  $\boldsymbol{\Sigma}_I$  of the  $\mathbf{T}_I$  (conditional on  $\mathbf{T}_N = \mathbf{t}_N$ ) are calculated, and the score statistic for the observed value,

$$s = (\mathbf{t}_I - \boldsymbol{\mu}_I)' \boldsymbol{\Sigma}_I^{-1} (\mathbf{t}_I - \boldsymbol{\mu}_I)$$

is compared to the score for each member of the distribution

$$S(\mathbf{T}_I) = (\mathbf{T}_I - \boldsymbol{\mu}_I)' \boldsymbol{\Sigma}_I^{-1} (\mathbf{T}_I - \boldsymbol{\mu}_I)$$

The resulting  $p$ -value is

$$p(\mathbf{t}_I|\mathbf{t}_N) = \Pr(S \geq s) = \sum_{\mathbf{u} \in \Omega_s} f_0(\mathbf{u}|\mathbf{t}_N)$$

where  $\Omega_s = \{\mathbf{u}: \text{there exist } \mathbf{y} \text{ with } \mathbf{y}'\mathbf{X}_I = \mathbf{u}, \mathbf{y}'\mathbf{X}_N = \mathbf{t}_N, \text{ and } S(\mathbf{u}) \geq s\}$ .

The mid- $p$  statistic, defined as

$$p(\mathbf{t}_I|\mathbf{t}_N) - \frac{1}{2}f_0(\mathbf{t}_I|\mathbf{t}_N)$$

was proposed by Lancaster (1961) to compensate for the discreteness of a distribution. See Agresti (1992) for more information. However, to allow for more flexibility in handling ties, you can write the mid- $p$  statistic as (based on a suggestion by Lamotte (2002) and generalizing Vollset, Hirji, and Afifi (1991))

$$\sum_{u \in \Omega_{<}} f_0(\mathbf{u}|\mathbf{t}_N) + \delta_1 f_0(\mathbf{t}_I|\mathbf{t}_N) + \delta_2 \sum_{u \in \Omega_{=}} f_0(\mathbf{u}|\mathbf{t}_N)$$

where, for  $i \in \{p, s\}$ ,  $\Omega_{<}$  is  $\Omega_i$  using strict inequalities, and  $\Omega_{=}$  is  $\Omega_i$  using equalities with the added restriction that  $\mathbf{u} \neq \mathbf{t}_I$ . Letting  $(\delta_1, \delta_2) = (0.5, 1.0)$  yields Lancaster's mid- $p$ .

**CAUTION:** When the exact distribution has ties and `METHOD=NETWORKMCMC` is specified, the Monte Carlo algorithm estimates  $p(\mathbf{t}|\mathbf{t}_N)$  with error, and hence it cannot determine precisely which values contribute to the reported  $p$ -values. For example, if the exact distribution has densities  $\{0.2, 0.2, 0.2, 0.4\}$  and if the observed statistic has probability 0.2, then the exact probability  $p$ -value is exactly 0.6. Under Monte Carlo sampling, if the densities after  $N$  samples are  $\{0.18, 0.21, 0.23, 0.38\}$  and the observed probability is 0.21, then the resulting  $p$ -value is 0.39. Therefore, the exact probability test  $p$ -value for this example fluctuates between 0.2, 0.4, and 0.6, and the reported  $p$ -values are actually lower bounds for the true  $p$ -values. If you need more precise values, you can specify the `OUTDIST=` option, determine appropriate cutoff values for the observed probability and score, and then construct the true  $p$ -value estimates from the `OUTDIST=` data set and display them in the SAS log by using the following statements:

```
data _null_;
 set outdist end=end;
 retain pvalueProb 0 pvalueScore 0;
 if prob < ProbCutOff then pvalueProb+prob;
 if score > ScoreCutOff then pvalueScore+prob;
 if end then put pvalueProb= pvalueScore=;
run;
```

## Inference for a Single Parameter

Exact parameter estimates are derived for a single parameter  $\beta_i$  by regarding all the other parameters  $\boldsymbol{\beta}_N = (\beta_1, \dots, \beta_{i-1}, \beta_{i+1}, \dots, \beta_{p_N+p_I})'$  as nuisance parameters. The appropriate sufficient statistics are  $\mathbf{T}_I = T_i$  and  $\mathbf{T}_N = (T_1, \dots, T_{i-1}, T_{i+1}, \dots, T_{p_N+p_I})'$ , with their observed values denoted by the lowercase  $t$ . Hence, the conditional PDF used to create the parameter estimate for  $\beta_i$  is

$$f_{\beta_i}(t_i|\mathbf{t}_N) = \frac{C(\mathbf{t}_N, t_i) \exp(t_i \beta_i)}{\sum_{u \in \Omega} C(\mathbf{t}_N, u) \exp(u \beta_i)}$$

for  $\Omega = \{u: \text{there exist } y \text{ with } T_i = u \text{ and } \mathbf{T}_N = \mathbf{t}_N\}$ .

The maximum exact conditional likelihood estimate is the quantity  $\hat{\beta}_i$ , which maximizes the conditional PDF. A Newton-Raphson algorithm is used to perform this search. However, if the observed  $t_i$  attains either its maximum or minimum value in the exact distribution (that is, either  $t_i = \min\{u : u \in \Omega\}$  or  $t_i = \max\{u : u \in \Omega\}$ ), then the conditional PDF is monotonically increasing in  $\beta_i$  and cannot be maximized. In this case, a median unbiased estimate (Hirji, Tsiatis, and Mehta 1989)  $\hat{\beta}_i$  is produced that satisfies  $f_{\hat{\beta}_i}(t_i|\mathbf{t}_N) = 0.5$ , and a Newton-Raphson algorithm is used to perform the search.



The standard error of the exact conditional likelihood estimate is just the negative of the inverse of the second derivative of the exact conditional log likelihood (Agresti 2002).

Likelihood ratio tests based on the conditional PDF are used to test the null  $H_0: \beta_i = 0$  against the alternative  $H_A: \beta_i > 0$ . The critical region for this UMP test consists of the upper tail of values for  $T_i$  in the exact distribution. Thus, the one-sided significance level  $p_+(t_i; 0)$  is

$$p_+(t_i; 0) = \sum_{u \geq t_i} f_0(u | \mathbf{t}_N)$$

Similarly, the one-sided significance level  $p_-(t_i; 0)$  against  $H_A: \beta_i < 0$  is

$$p_-(t_i; 0) = \sum_{u \leq t_i} f_0(u | \mathbf{t}_N)$$

The two-sided significance level  $p(t_i; 0)$  against  $H_A: \beta_i \neq 0$  is calculated as

$$p(t_i; 0) = 2 \min[p_-(t_i; 0), p_+(t_i; 0)]$$

An upper  $100(1 - 2\epsilon)\%$  exact confidence limit for  $\hat{\beta}_i$  corresponding to the observed  $t_i$  is the solution  $\beta_U(t_i)$  of  $\epsilon = p_-(t_i, \beta_U(t_i))$ , while the lower exact confidence limit is the solution  $\beta_L(t_i)$  of  $\epsilon = p_+(t_i, \beta_L(t_i))$ . Again, a Newton-Raphson procedure is used to search for the solutions. Note that one of the confidence limits for a median unbiased estimate is set to infinity, but the other is still computed at  $\epsilon$ . This results in the display of a one-sided  $100(1 - \epsilon)\%$  confidence interval; if you want the  $2\epsilon$  limit instead, you can specify the **ONESIDED** option.

Specifying the **ONESIDED** option displays only one  $p$ -value and one confidence interval, because small values of  $p_+(t_i; 0)$  and  $p_-(t_i; 0)$  support different alternative hypotheses and only one of these  $p$ -values can be less than 0.50.

The mid- $p$  confidence limits are the solutions to  $\min\{p_-(t_i, \beta(t_i)), p_+(t_i, \beta(t_i))\} - (1 - \delta_1) f_{\beta(t_i)}(t_i | \mathbf{t}_N) = \epsilon$  for  $\epsilon = \alpha/2, 1 - \alpha/2$  (Vollset, Hirji, and Afifi 1991).  $\delta_1 = 1$  produces the usual exact (or *max-p*) confidence interval,  $\delta_1 = 0.5$  yields the mid- $p$  interval, and  $\delta_1 = 0$  gives the *min-p* interval. The mean of the endpoints of the *max-p* and *min-p* intervals provides the *mean-p* interval as defined by Hirji, Mehta, and Patel (1988).

Estimates and confidence intervals for the odds ratios are produced by exponentiating the estimates and interval endpoints for the parameters.

### Notes about Exact $p$ -Values

In the “Conditional Exact Tests” table, the exact probability test is not necessarily a sum of tail areas and can be inflated if the distribution is skewed. The more robust exact conditional scores test is a sum of tail areas and is generally preferred over the exact probability test.

The  $p$ -value reported for a single parameter in the “Exact Parameter Estimates” table is twice the one-sided tail area of a likelihood ratio test against the null hypothesis of the parameter equaling zero.

## Input and Output Data Sets

### OUTEST= Output Data Set

The OUTEST= data set contains one observation for each BY group containing the maximum likelihood estimates of the regression coefficients. If you also use the COVOUT option in the PROC LOGISTIC statement, there are additional observations containing the rows of the estimated covariance matrix. If you specify SELECTION=FORWARD, BACKWARD, or STEPWISE, only the estimates of the parameters and covariance matrix for the final model are output to the OUTEST= data set.

#### *Variables in the OUTEST= Data Set*

The OUTEST= data set contains the following variables:

- any BY variables specified
- `_LINK_`, a character variable of length 8 with four possible values: CLOGLOG for the complementary log-log function, LOGIT for the logit function, NORMIT for the probit (alias normit) function, and GLOGIT for the generalized logit function
- `_TYPE_`, a character variable of length 8 with two possible values: PARMS for parameter estimates or COV for covariance estimates. If an EXACT statement is also specified, then two other values are possible: EPARMMLE for the exact maximum likelihood estimates and EPARMMUE for the exact median unbiased estimates.
- `_NAME_`, a character variable containing the name of the response variable when `_TYPE_=PARMS`, EPARMMLE, and EPARMMUE, or the name of a model parameter when `_TYPE_=COV`
- `_STATUS_`, a character variable that indicates whether the estimates have converged
- one variable for each intercept parameter
- one variable for each slope parameter and one variable for the offset variable if the OFFSET= option is specified. If an effect is not included in the final model in a model building process, the corresponding parameter estimates and covariances are set to missing values.
- `_LNLIKE_`, the log likelihood

#### *Parameter Names in the OUTEST= Data Set*

If there are only two response categories in the entire data set, the intercept parameter is named Intercept. If there are more than two response categories in the entire data set, the intercept parameters are named Intercept\_xxx, where xxx is the value (formatted if a format is applied) of the corresponding response category.

For continuous explanatory variables, the names of the parameters are the same as the corresponding variables. For CLASS variables, the parameter names are obtained by concatenating the corresponding CLASS variable name with the CLASS category; see the section “[Class Variable Naming Convention](#)” on page 4189 for more details. For interaction and nested effects, the parameter names are created by concatenating the names of each effect.

For the generalized logit model, names of parameters corresponding to each nonreference category contain `_xxx` as the suffix, where xxx is the value (formatted if a format is applied) of the corresponding nonreference

category. For example, suppose the variable Net3 represents the television network (ABC, CBS, and NBC) viewed at a certain time. The following statements fit a generalized logit model with Age and Gender (a CLASS variable with values Female and Male) as explanatory variables:

```
proc logistic;
 class Gender;
 model Net3 = Age Gender / link=glogit;
run;
```

There are two logit functions, one contrasting ABC with NBC and the other contrasting CBS with NBC. For each logit, there are three parameters: an intercept parameter, a slope parameter for Age, and a slope parameter for Gender (since there are only two gender levels and the EFFECT parameterization is used by default). The names of the parameters and their descriptions are as follows:

|                  |                                                                      |
|------------------|----------------------------------------------------------------------|
| Intercept_ABC    | intercept parameter for the logit contrasting ABC with NBC           |
| Intercept_CBS    | intercept parameter for the logit contrasting CBS with NBC           |
| Age_ABC          | Age slope parameter for the logit contrasting ABC with NBC           |
| Age_CBS          | Age slope parameter for the logit contrasting CBS with NBC           |
| GenderFemale_ABC | Gender=Female slope parameter for the logit contrasting ABC with NBC |
| GenderFemale_CBS | Gender=Female slope parameter for the logit contrasting CBS with NBC |

### INEST= Input Data Set

You can specify starting values for the iterative algorithm in the INEST= data set. The INEST= data set has the same structure as the OUTEST= data set but is not required to have all the variables or observations that appear in the OUTEST= data set. A previous OUTEST= data set can be used as, or modified for use as, an INEST= data set.

The INEST= data set must contain the intercept variables (named Intercept for binary response models and Intercept, Intercept\_2, Intercept\_3, and so forth, for ordinal and nominal response models) and all explanatory variables in the MODEL statement. If BY processing is used, the INEST= data set should also include the BY variables, and there must be one observation for each BY group. If the INEST= data set also contains the \_TYPE\_ variable, only observations with \_TYPE\_ value 'PARMS' are used as starting values.

### OUT= Output Data Set in the OUTPUT Statement

The OUT= data set in the OUTPUT statement contains all the variables in the input data set along with statistics you request by specifying *keyword=name* options or the PREDPROBS= option in the OUTPUT statement. In addition, if you use the single-trial syntax and you request any of the XBETA=, STDXBETA=, PREDICTED=, LCL=, and UCL= options, the OUT= data set contains the automatic variable \_LEVEL\_. The value of \_LEVEL\_ identifies the response category upon which the computed values of XBETA=, STDXBETA=, PREDICTED=, LCL=, and UCL= are based.

When there are more than two response levels, only variables named by the XBETA=, STDXBETA=, PREDICTED=, LOWER=, and UPPER= options and the variables given by PREDPROBS=(INDIVIDUAL CUMULATIVE) have their values computed; the other variables have missing values. If you fit a generalized logit model, the cumulative predicted probabilities are not computed.

When there are only two response categories, each input observation produces one observation in the OUT= data set.

If there are more than two response categories and you specify only the PREDPROBS= option, then each input observation produces one observation in the OUT= data set. However, if you fit an ordinal (cumulative) model and specify options other than the PREDPROBS= options, each input observation generates as many output observations as one fewer than the number of response levels, and the predicted probabilities and their confidence limits correspond to the cumulative predicted probabilities. If you fit a generalized logit model and specify options other than the PREDPROBS= options, each input observation generates as many output observations as the number of response categories; the predicted probabilities and their confidence limits correspond to the probabilities of individual response categories.

For observations in which only the response variable is missing, values of the XBETA=, STDXBETA=, PREDICTED=, UPPER=, LOWER=, and the PREDPROBS= options are computed even though these observations do not affect the model fit. This enables, for instance, predicted probabilities to be computed for new observations.

### OUT= Output Data Set in a SCORE Statement

The OUT= data set in a SCORE statement contains all the variables in the data set being scored. The data set being scored can be either the input DATA= data set in the PROC LOGISTIC statement or the DATA= data set in the SCORE statement. The DATA= data set in the SCORE statement does not need to contain the response variable.

If the data set being scored contains the response variable, then denote the *normalized* levels (left-justified, formatted values of 16 characters or less) of your response variable Y by  $Y_1, \dots, Y_{k+1}$ . For each response level, the OUT= data set also contains the following:

- F\_Y, the normalized levels of the response variable Y in the data set being scored. If the events/trials syntax is used, the F\_Y variable is not created.
- I\_Y, the normalized levels that the observations are classified into. Note that an observation is classified into the level with the largest probability. If the events/trials syntax is used, the \_INTO\_ variable is created instead, and it contains the values EVENT and NONEVENT.
- P\_Y<sub>i</sub>, the posterior probabilities of the normalized response level Y<sub>i</sub>
- If the CLM option is specified in the SCORE statement, the OUT= data set also includes the following:
  - LCL\_Y<sub>i</sub>, the lower 100(1 – α)% confidence limits for P\_Y<sub>i</sub>
  - UCL\_Y<sub>i</sub>, the upper 100(1 – α)% confidence limits for P\_Y<sub>i</sub>

### OUTDIST= Output Data Set

The OUTDIST= data set contains every exact conditional distribution necessary to process the corresponding EXACT statement. For example, the following statements create one distribution for the x1 parameter and another for the x2 parameters, and produce the data set dist shown in Table 54.12:

```

data test;
 input y x1 x2 count;
 datalines;
0 0 0 1
1 0 0 1
0 1 1 2
1 1 1 1
1 0 2 3
1 1 2 1
1 2 0 3
1 2 1 2
1 2 2 1
;

proc logistic data=test exactonly;
 class x2 / param=ref;
 model y=x1 x2;
 exact x1 x2/ outdist=dist;
run;
proc print data=dist;
run;

```

Table 54.12 OUTDIST= Data Set

| Obs | x1 | x20 | x21 | Count | Score   | Prob    |
|-----|----|-----|-----|-------|---------|---------|
| 1   | .  | 0   | 0   | 3     | 5.81151 | 0.03333 |
| 2   | .  | 0   | 1   | 15    | 1.66031 | 0.16667 |
| 3   | .  | 0   | 2   | 9     | 3.12728 | 0.10000 |
| 4   | .  | 1   | 0   | 15    | 1.46523 | 0.16667 |
| 5   | .  | 1   | 1   | 18    | 0.21675 | 0.20000 |
| 6   | .  | 1   | 2   | 6     | 4.58644 | 0.06667 |
| 7   | .  | 2   | 0   | 19    | 1.61869 | 0.21111 |
| 8   | .  | 2   | 1   | 2     | 3.27293 | 0.02222 |
| 9   | .  | 3   | 0   | 3     | 6.27189 | 0.03333 |
| 10  | 2  | .   | .   | 6     | 3.03030 | 0.12000 |
| 11  | 3  | .   | .   | 12    | 0.75758 | 0.24000 |
| 12  | 4  | .   | .   | 11    | 0.00000 | 0.22000 |
| 13  | 5  | .   | .   | 18    | 0.75758 | 0.36000 |
| 14  | 6  | .   | .   | 3     | 3.03030 | 0.06000 |

The first nine observations in the `dist` data set contain an exact distribution for the parameters of the `x2` effect (hence the values for the `x1` parameter are missing), and the remaining five observations are for the `x1` parameter. If a joint distribution was created, there would be observations with values for both the `x1` and `x2` parameters. For **CLASS** variables, the corresponding parameters in the `dist` data set are identified by concatenating the variable name with the appropriate classification level.

The data set contains the possible sufficient statistics of the parameters for the effects specified in the **EXACT** statement, and the `Count` variable contains the number of different responses that yield these statistics. In particular, there are six possible response vectors  $y$  for which the dot product  $y'x1$  was equal to 2, and

for which  $y/x20$ ,  $y/x21$ , and  $y/1$  were equal to their actual observed values (displayed in the “Sufficient Statistics” table).

When hypothesis tests are performed on the parameters, the **Prob** variable contains the probability of obtaining that statistic (which is just the count divided by the total count), and the **Score** variable contains the score for that statistic.

The **OUTDIST=** data set can contain a different exact conditional distribution for each specified **EXACT** statement. For example, consider the following **EXACT** statements:

```
exact 'O1' x1 / outdist=o1;
exact 'OJ12' x1 x2 / jointonly outdist=oj12;
exact 'OA12' x1 x2 / joint outdist=oa12;
exact 'OE12' x1 x2 / estimate outdist=oe12;
```

The **O1** statement outputs a single exact conditional distribution. The **OJ12** statement outputs only the joint distribution for  $x1$  and  $x2$ . The **OA12** statement outputs three conditional distributions: one for  $x1$ , one for  $x2$ , and one jointly for  $x1$  and  $x2$ . The **OE12** statement outputs two conditional distributions: one for  $x1$  and the other for  $x2$ . Data set **oe12** contains both the  $x1$  and  $x2$  variables; the distribution for  $x1$  has missing values in the  $x2$  column while the distribution for  $x2$  has missing values in the  $x1$  column.

## OUTROC= Output Data Set

The **OUTROC=** data set contains data necessary for producing the ROC curve, and can be created by specifying the **OUTROC=** option in the **MODEL** statement or the **OUTROC=** option in the **SCORE** statement: It has the following variables:

- any **BY** variables specified
- **\_STEP\_**, the model step number. This variable is not included if model selection is not requested.
- **\_PROB\_**, the estimated probability of an event. These estimated probabilities serve as cutpoints for predicting the response. Any observation with an estimated event probability that exceeds or equals **\_PROB\_** is predicted to be an event; otherwise, it is predicted to be a nonevent. Predicted probabilities that are close to each other are grouped together, with the maximum allowable difference between the largest and smallest values less than a constant that is specified by the **ROCEPS=** option. The smallest estimated probability is used to represent the group.
- **\_POS\_**, the number of correctly predicted event responses
- **\_NEG\_**, the number of correctly predicted nonevent responses
- **\_FALPOS\_**, the number of falsely predicted event responses
- **\_FALNEG\_**, the number of falsely predicted nonevent responses
- **\_SENSIT\_**, the sensitivity, which is the proportion of event observations that were predicted to have an event response
- **\_1MSPEC\_**, one minus specificity, which is the proportion of nonevent observations that were predicted to have an event response

Note that none of these statistics are affected by the bias-correction method discussed in the section “Classification Table” on page 4255. An ROC curve is obtained by plotting `_SENSIT_` against `_1MSPEC_`.

For more information, see the section “Receiver Operating Characteristic Curves” on page 4260.

---

## Computational Resources

The memory needed to fit an unconditional model is approximately  $8n(p + 2) + 24(p + 2)^2$  bytes, where  $p$  is the number of parameters estimated and  $n$  is the number of observations in the data set. For cumulative response models with more than two response levels, a test of the parallel lines assumption requires an additional memory of approximately  $4k^2(m + 1)^2 + 24(m + 2)^2$  bytes, where  $k$  is the number of response levels and  $m$  is the number of slope parameters. However, if this additional memory is not available, the procedure skips the test and finishes the other computations. You might need more memory if you use the `SELECTION=` option for model building.

The data that consist of relevant variables (including the design variables for model effects) and observations for fitting the model are stored in a temporary utility file. If sufficient memory is available, such data will also be kept in memory; otherwise, the data are reread from the utility file for each evaluation of the likelihood function and its derivatives, with the resulting execution time of the procedure substantially increased. Specifying the `MULTIPASS` option in the `MODEL` statement avoids creating this utility file and also does not store the data in memory; instead, the `DATA=` data set is reread when needed. This saves approximately  $8n(p + 2)$  bytes of memory but increases the execution time.

If a conditional logistic regression is performed, then approximately  $4(m^2 + m + 4) \max_h(m_h) + (8s_H + 36)H + 12s_H$  additional bytes of memory are needed, where  $m_h$  is the number of events in stratum  $h$ ,  $H$  is the total number of strata, and  $s_H$  is the number of variables used to define the strata. If the `CHECK-DEPENDENCY=ALL` option is specified in the `STRATA` statement, then an extra  $4(m + H)(m + H + 1)$  bytes are required, and the resulting execution time of the procedure might be substantially increased.

## Computational Resources for Exact Logistic Regression

Many problems require a prohibitive amount of time and memory for exact computations, depending on the speed and memory available on your computer. For such problems, consider whether exact methods are really necessary. Stokes, Davis, and Koch (2012) suggest looking at exact  $p$ -values when the sample size is small and the approximate  $p$ -values from the unconditional analysis are less than 0.10, and they provide *rules of thumb* for determining when various models are valid.

A formula does not exist that can predict the amount of time and memory necessary to generate the exact conditional distributions for a particular problem. The time and memory required depends on several factors, including the total sample size, the number of parameters of interest, the number of nuisance parameters, and the order in which the parameters are processed. To provide a feel for how these factors affect performance, 19 data sets containing  $\text{Nobs} \in \{10, \dots, 500\}$  observations consisting of up to 10 independent uniform binary covariates ( $X_1, \dots, X_N$ ) and a binary response variable ( $Y$ ), are generated, and the following statements create exact conditional distributions for  $X_1$  conditional on the other covariates by using the default `METHOD=NETWORK`. Figure 54.11 displays results obtained on a 400Mhz PC with 768MB RAM running Microsoft Windows NT.

```
data one;
 do obs=1 to HalfNobs;
```

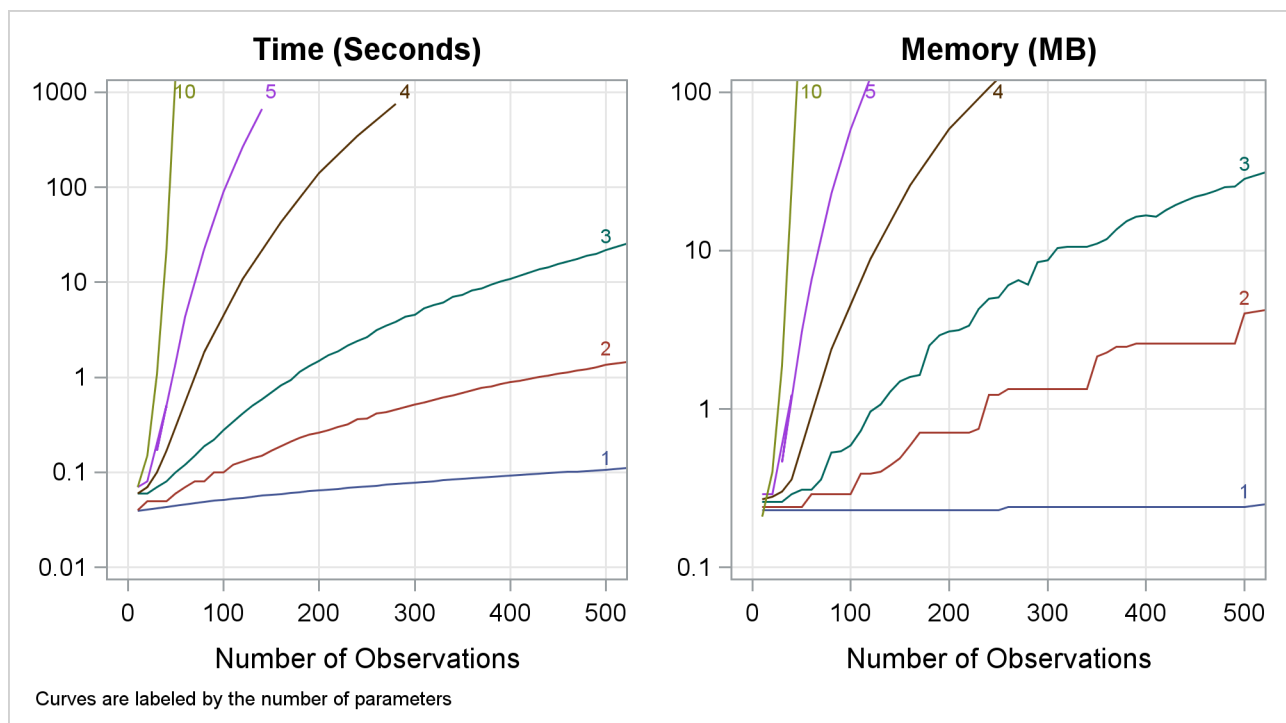


```

do Y=0 to 1;
 X1=round(ranuni(0));
 ...
 XN=round(ranuni(0));
 output;
end;
end;
options fullstimer;
proc logistic exactonly;
 exactoptions method=network maxtime=1200;
 class X1...XN / param=ref;
 model Y=X1...XN;
 exact X1 / outdist=dist;
run;

```

Figure 54.11 Mean Time and Memory Required



At any time while PROC LOGISTIC is deriving the distributions, you can terminate the computations by pressing the system interrupt key sequence (see the SAS Companion for your system) and choosing to stop computations. If you run out of memory, see the SAS Companion for your system to see how to allocate more.

You can use the **EXACTOPTIONS** option **MAXTIME=** to limit the total amount of time PROC LOGISTIC uses to derive all of the exact distributions. If PROC LOGISTIC does not finish within that time, the procedure terminates.

Calculation of frequencies are performed in the log scale by default. This reduces the need to check for excessively large frequencies but can be slower than not scaling. You can turn off the log scaling by specifying the **NOLOGSCALE** option in the **EXACTOPTIONS** statement. If a frequency in the exact distribution is larger than the largest integer that can be held in double precision, a warning is printed to the SAS log. But



since inaccuracies due to adding small numbers to these large frequencies might have little or no effect on the statistics, the exact computations continue.

You can monitor the progress of the procedure by submitting your program with the `EXACTOPTIONS` option `STATUSTIME=`. If the procedure is too slow, you can try another method by specifying the `EXACTOPTIONS` option `METHOD=`, you can try reordering the variables in the `MODEL` statement (note that `CLASS` variables are always processed before continuous covariates), or you can try reparameterizing your classification variables as in the following statement:

```
class class-variables / param=ref ref=first order=freq;
```

---

## Displayed Output

If you use the `NOPRINT` option in the `PROC LOGISTIC` statement, the procedure does not display any output. Otherwise, the tables displayed by the LOGISTIC procedure are discussed in the following section in the order in which they appear in the output. Some of the tables appear only in conjunction with certain options or statements; see the section “[ODS Table Names](#)” on page 4291 for details.

**NOTE:** The `EFFECT`, `ESTIMATE`, `LSMEANS`, `LSMESTIMATE`, and `SLICE` statements also create tables, which are not listed in this section. For information about these tables, see the corresponding sections of Chapter 19, “[Shared Concepts and Topics](#).”

## Table Summary

### ***Model Information and the Number of Observations***

See the section “[Missing Values](#)” on page 4237 for information about missing-value handling, and the sections “[FREQ Statement](#)” on page 4203 and “[WEIGHT Statement](#)” on page 4236 for information about valid frequencies and weights.

### ***Response Profile***

Displays the Ordered Value assigned to each response level. See the section “[Response Level Ordering](#)” on page 4237 for details.

### ***Class Level Information***

Displays the design values for each `CLASS` explanatory variable. See the section “[Other Parameterizations](#)” on page 387 in Chapter 19, “[Shared Concepts and Topics](#),” for details.

### ***Simple Statistics Tables***

The following tables are displayed if you specify the `SIMPLE` option in the `PROC LOGISTIC` statement:

- **Descriptive Statistics for Continuous Explanatory Variables**
- **Frequency Distribution of Class Variables**
- **Weight Distribution of Class Variables**  
Displays if you also specify a `WEIGHT` statement.

### **Strata Tables for (Exact) Conditional Logistic Regression**

The following tables are displayed if you specify a `STRATA` statement:

- **Strata Summary**  
Shows the pattern of the number of events and the number of nonevents in a stratum. See the section “[STRATA Statement](#)” on page 4233 for more information.
- **Strata Information**  
Displays if you specify the `INFO` option in a `STRATA` statement.

### **Maximum Likelihood Iteration History**

Displays if you specify the `ITPRINT` option in the `MODEL` statement. See the sections “[Iterative Algorithms for Model Fitting](#)” on page 4240, “[Convergence Criteria](#)” on page 4242, and “[Existence of Maximum Likelihood Estimates](#)” on page 4242 for details.

### **Deviance and Pearson Goodness-of-Fit Statistics**

Displays if you specify the `SCALE=` option in the `MODEL` statement. Small  $p$ -values reject the null hypothesis that the fitted model is adequate. See the section “[Overdispersion](#)” on page 4257 for details.

### **Score Test for the Equal Slopes (Proportional Odds) Assumption**

Tests the parallel lines assumption if you fit an ordinal response model with the `LINK=CLOGLOG` or `LINK=PROBIT` options. If you specify `LINK=LOGIT`, this is called the “Proportional Odds” assumption. The table is not displayed if you specify the `UNEQUALSLOPES` option in the `MODEL` statement. Small  $p$ -values reject the null hypothesis that the slope parameters for each explanatory variable are constant across all the response functions. See the section “[Testing the Parallel Lines Assumption](#)” on page 4248 for details.

### **Model Fit Statistics**

Computes various fit criteria based on a model with intercepts only and a model with intercepts and explanatory variables. If you specify the `NOINT` option in the `MODEL` statement, these statistics are calculated without considering the intercept parameters. See the section “[Model Fitting Information](#)” on page 4245 for details.

### **Testing Global Null Hypothesis: BETA=0**

Tests the joint effect of the explanatory variables included in the model. Small  $p$ -values reject the null hypothesis that all slope parameters are equal to zero,  $H_0: \beta = \mathbf{0}$ . See the sections “[Model Fitting Information](#)” on page 4245, “[Residual Chi-Square](#)” on page 4247, and “[Testing Linear Hypotheses about the Regression Coefficients](#)” on page 4262 for details. If you also specify the `RSQUARE` option in the `MODEL` statement, two generalized R Square measures are included; see the section “[Generalized Coefficient of Determination](#)” on page 4246 for details.

### **Score Test for Global Null Hypothesis**

Displays instead of the “Testing Global Null Hypothesis: BETA=0” table if the `NOFIT` option is specified in the `MODEL` statement. The global score test evaluates the joint significance of the effects in the `MODEL` statement. Small  $p$ -values reject the null hypothesis that all slope parameters are equal to zero,  $H_0: \beta = \mathbf{0}$ . See the section “[Residual Chi-Square](#)” on page 4247 for details.

### Model Selection Tables

The tables in this section are produced when the `SELECTION=` option is specified in the `MODEL` statement. See the section “Effect-Selection Methods” on page 4244 for more information.

- **Residual Chi-Square Test**

Displays if you specify `SELECTION=FORWARD`, `BACKWARD`, or `STEPWISE` in the `MODEL` statement. Small  $p$ -values reject the null hypothesis that the reduced model is adequate. See the section “Residual Chi-Square” on page 4247 for details.

- **Analysis of Effects Eligible for Entry**

Displays if you specify the `DETAILS` option and the `SELECTION=FORWARD` or `STEPWISE` option in the `MODEL` statement. Small  $p$ -values reject  $H_0: \beta_i \neq 0$ . The score chi-square is used to determine entry; see the section “Testing Individual Effects Not in the Model” on page 4247 for details.

- **Analysis of Effects Eligible for Removal**

Displays if you specify the `SELECTION=BACKWARD` or `STEPWISE` option in the `MODEL` statement. Small  $p$ -values reject  $H_0: \beta_i = 0$ . The Wald chi-square is used to determine removal; see the section “Testing Linear Hypotheses about the Regression Coefficients” on page 4262 for details.

- **Analysis of Effects Removed by Fast Backward Elimination**

Displays if you specify the `FAST` option and the `SELECTION=BACKWARD` or `STEPWISE` option in the `MODEL` statement. This table gives the approximate chi-square statistic for the variable removed, the corresponding  $p$ -value with respect to a chi-square distribution with one degree of freedom, the residual chi-square statistic for testing the joint significance of the variable and the preceding ones, the degrees of freedom, and the  $p$ -value of the residual chi-square with respect to a chi-square distribution with the corresponding degrees of freedom.

- **Summary of Forward, Backward, and Stepwise Selection**

Displays if you specify `SELECTION=FORWARD`, `BACKWARD`, or `STEPWISE` in the `MODEL` statement. The score chi-square is used to determine entry; see the section “Testing Individual Effects Not in the Model” on page 4247 for details. The Wald chi-square is used to determine removal; see the section “Testing Linear Hypotheses about the Regression Coefficients” on page 4262 for details.

- **Regression Models Selected by Score Criterion**

Displays the score chi-square for all models if you specify the `SELECTION=SCORE` option in the `MODEL` statement. Small  $p$ -values reject the null hypothesis that the fitted model is adequate. See the section “Effect-Selection Methods” on page 4244 for details.

### Type 3 Analysis of Effect

Displays if the model contains a `CLASS` variable. Performs Wald chi-square tests of the joint effect of the parameters for each `CLASS` variable in the model. Small  $p$ -values reject  $H_0: \beta_i = 0$ . See the section “Testing Linear Hypotheses about the Regression Coefficients” on page 4262 for details.

### Analysis of Maximum Likelihood Estimates

`CLASS` effects are identified by their (nonreference) level. For generalized logit models, a response variable column displays the nonreference level of the logit. The table includes the following:

- the estimated standard error of the parameter estimate, computed as the square root of the corresponding diagonal element of the estimated covariance matrix
- the Wald chi-square statistic, computed by squaring the ratio of the parameter estimate divided by its standard error estimate. See the section “Testing Linear Hypotheses about the Regression Coefficients” on page 4262 for details.
- the  $p$ -value tests the null hypothesis  $H_0: \beta_i = 0$ ; small values reject the null.
- the standardized estimate for the slope parameter, if you specify the **STB** option in the **MODEL** statement. See the **STB** option on page 4220 for details.
- exponentiated values of the estimates of the slope parameters, if you specify the **EXPB** option in the **MODEL** statement. See the **EXPB** option on page 4212 for details.
- the label of the variable, if you specify the **PARMLABEL** option in the **MODEL** statement and if space permits. Due to constraints on the line size, the variable label might be suppressed in order to display the table in one panel. Use the SAS system option **LINESIZE=** to specify a larger line size to accommodate variable labels. A shorter line size can break the table into two panels allowing labels to be displayed.

### ***Odds Ratio Estimates***

Displays the odds ratio estimates and the corresponding 95% Wald confidence intervals for variables that are not involved in nestings or interactions. For continuous explanatory variables, these odds ratios correspond to a unit increase in the risk factors. See the section “Odds Ratio Estimation” on page 4250 for details.

### ***Association of Predicted Probabilities and Observed Responses***

See the section “Rank Correlation of Observed Responses and Predicted Probabilities” on page 4253 for details.

### ***Parameter Estimates and Profile-Likelihood or Wald Confidence Intervals***

Displays if you specify the **CLPARAM=** option in the **MODEL** statement. See the section “Confidence Intervals for Parameters” on page 4248 for details.

### ***Odds Ratio Estimates and Profile-Likelihood or Wald Confidence Intervals***

Displays if you specify the **ODDSRATIO** statement for any effects with any class parameterizations. Also displays if you specify the **CLODDS=** option in the **MODEL** statement, except odds ratios are computed only for main effects not involved in interactions or nestings, and if the main effect is a **CLASS** variable, the parameterization must be **EFFECT**, **REFERENCE**, or **GLM**. See the section “Odds Ratio Estimation” on page 4250 for details.

### ***Estimated Covariance or Correlation Matrix***

Displays if you specify the **COVB** or **CORRB** option in the **MODEL** statement. See the section “Iterative Algorithms for Model Fitting” on page 4240 for details.

**Contrast Test Results**

Displays the Wald test for each specified **CONTRAST** statement. Small  $p$ -values reject  $H_0: \mathbf{L}\boldsymbol{\beta} = \mathbf{0}$ . The “Coefficients of Contrast” table displays the contrast matrix if you specify the **E** option, and the “Contrast Estimation and Testing Results by Row” table displays estimates and Wald tests for each row of the contrast matrix if you specify the **ESTIMATE=** option. See the sections “**CONTRAST Statement**” on page 4190, “**Testing Linear Hypotheses about the Regression Coefficients**” on page 4262, and “**Linear Predictor, Predicted Probability, and Confidence Limits**” on page 4253 for details.

**Linear Hypotheses Testing Results**

Displays the Wald test for each specified **TEST** statement. See the sections “**Testing Linear Hypotheses about the Regression Coefficients**” on page 4262 and “**TEST Statement**” on page 4234 for details.

**Hosmer and Lemeshow Goodness-of-Fit Test**

Displays if you specify the **LACKFIT** option in the **MODEL** statement. Small  $p$ -values reject the null hypothesis that the fitted model is adequate. The “Partition for the Hosmer and Lemeshow Test” table displays the grouping used in the test. See the section “**The Hosmer-Lemeshow Goodness-of-Fit Test**” on page 4259 for details.

**Classification Table**

Displays if you use the **CTABLE** option in the **MODEL** statement. If you specify a list of cutpoints with the **PPROB=** option, then the cutpoints are displayed in the Prob Level column. If you specify the prior event probabilities with the **PEVENT=** option, then the probabilities are displayed in the Prob Event column. The Correct column displays the number of correctly classified events and nonevents, the Incorrect Event column displays the number of nonevents incorrectly classified as events, and the Incorrect Nonevent column gives the number of nonevents incorrectly classified as events. See the section “**Classification Table**” on page 4255 for more details.

**Regression Diagnostics**

Displays if you specify the **INFLUENCE** option in the **MODEL** statement. See the section “**Regression Diagnostics**” on page 4263 for more information about diagnostics from an unconditional analysis, and the section “**Regression Diagnostic Details**” on page 4272 for information about diagnostics from a conditional analysis.

**Fit Statistics for SCORE Data**

Displays if you specify the **FITSTAT** option in the **SCORE** statement. See the section “**Scoring Data Sets**” on page 4266 for details.

**ROC Association Statistic and Contrast Tables**

Displayed if a **ROC** statement or a **ROCCONTRAST** statement is specified. See the section “**ROC Computations**” on page 4261 for details about the Mann-Whitney statistics and the test and estimation computations, and see the section “**Rank Correlation of Observed Responses and Predicted Probabilities**” on page 4253 for details about the other statistics.

**Exact Conditional Logistic Regression Tables**

The tables in this section are produced when the **EXACT** statement is specified. If the **METHOD=NETWORKMC** option is specified, the test and estimate tables are renamed “Monte Carlo” tables and a Monte Carlo standard error column ( $\sqrt{p(1-p)/n}$ ) is displayed.

- **Sufficient Statistics**

Displays if you request an `OUTDIST=` data set in an `EXACT` statement. The table lists the parameters and their observed sufficient statistics.

- **(Monte Carlo) Conditional Exact Tests**

See the section “[Hypothesis Tests](#)” on page 4276 for details.

- **(Monte Carlo) Exact Parameter Estimates**

Displays if you specify the `ESTIMATE` option in the `EXACT` statement. This table gives individual parameter estimates for each variable (conditional on the values of all the other parameters in the model), confidence limits, and a two-sided  $p$ -value (twice the one-sided  $p$ -value) for testing that the parameter is zero. See the section “[Inference for a Single Parameter](#)” on page 4277 for details.

- **(Monte Carlo) Exact Odds Ratios**

Displays if you specify the `ESTIMATE=ODDS` or `ESTIMATE=BOTH` option in the `EXACT` statement. See the section “[Inference for a Single Parameter](#)” on page 4277 for details.

---

## ODS Table Names

PROC LOGISTIC assigns a name to each table it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in [Table 54.13](#). For more information about ODS, see Chapter 20, “[Using the Output Delivery System](#).”

The `EFFECT`, `ESTIMATE`, `LSMEANS`, `LSMESTIMATE`, and `SLICE` statements also create tables, which are not listed in [Table 54.13](#). For information about these tables, see the corresponding sections of Chapter 19, “[Shared Concepts and Topics](#).”

**Table 54.13** ODS Tables Produced by PROC LOGISTIC

| ODS Table Name | Description                                                      | Statement                 | Option                       |
|----------------|------------------------------------------------------------------|---------------------------|------------------------------|
| Association    | Association of predicted probabilities and observed responses    | MODEL<br>(without STRATA) | Default                      |
| BestSubsets    | Best subset selection                                            | MODEL                     | SELECTION=SCORE              |
| ClassFreq      | Frequency breakdown of CLASS variables                           | PROC                      | Simple<br>(with CLASS vars)  |
| ClassLevelInfo | CLASS variable levels and design variables                       | MODEL                     | Default<br>(with CLASS vars) |
| Classification | Classification table                                             | MODEL                     | CTABLE                       |
| ClassWgt       | Weight breakdown of CLASS variables                              | PROC, WEIGHT              | Simple<br>(with CLASS vars)  |
| CLOddsPL       | Odds ratio estimates and profile-likelihood confidence intervals | MODEL                     | CLODDS=PL                    |
| CLOddsWald     | Odds ratio estimates and Wald confidence intervals               | MODEL                     | CLODDS=WALD                  |

Table 54.13 continued

| ODS Table Name       | Description                                                     | Statement | Option                                        |
|----------------------|-----------------------------------------------------------------|-----------|-----------------------------------------------|
| CLParmPL             | Parameter estimates and profile-likelihood confidence intervals | MODEL     | CLPARM=PL                                     |
| CLParmWald           | Parameter estimates and Wald confidence intervals               | MODEL     | CLPARM=WALD                                   |
| ContrastCoeff        | L matrix from CONTRAST                                          | CONTRAST  | E                                             |
| ContrastEstimate     | Estimates from CONTRAST                                         | CONTRAST  | ESTIMATE=                                     |
| ContrastTest         | Wald test for CONTRAST                                          | CONTRAST  | Default                                       |
| ConvergenceStatus    | Convergence status                                              | MODEL     | Default                                       |
| CorrB                | Estimated correlation matrix of parameter estimators            | MODEL     | CORRB                                         |
| CovB                 | Estimated covariance matrix of parameter estimators             | MODEL     | COVB                                          |
| CumulativeModelTest  | Test of the cumulative model assumption                         | MODEL     | (Ordinal response)                            |
| EffectNotInModel     | Test for effects not in model                                   | MODEL     | SELECTION=SIF                                 |
| ExactOddsRatio       | Exact odds ratios                                               | EXACT     | ESTIMATE=ODDS,<br>ESTIMATE=BOTH               |
| ExactParmEst         | Parameter estimates                                             | EXACT     | ESTIMATE,<br>ESTIMATE=PARAM,<br>ESTIMATE=BOTH |
| ExactTests           | Conditional exact tests                                         | EXACT     | Default                                       |
| FastElimination      | Fast backward elimination                                       | MODEL     | SELECTION=B,FAST                              |
| FitStatistics        | Model fit statistics                                            | MODEL     | Default                                       |
| GlobalScore          | Global score test                                               | MODEL     | NOFIT                                         |
| GlobalTests          | Test for global null hypothesis                                 | MODEL     | Default                                       |
| GoodnessOfFit        | Pearson and deviance goodness-of-fit tests                      | MODEL     | SCALE                                         |
| IndexPlots           | Batch capture of the index plots                                | MODEL     | IPLOTS                                        |
| Influence            | Regression diagnostics                                          | MODEL     | INFLUENCE                                     |
| IterHistory          | Iteration history                                               | MODEL     | ITPRINT                                       |
| LackFitChiSq         | Hosmer-Lemeshow chi-square test results                         | MODEL     | LACKFIT                                       |
| LackFitPartition     | Partition for the Hosmer-Lemeshow test                          | MODEL     | LACKFIT                                       |
| LastGradient         | Last evaluation of gradient                                     | MODEL     | ITPRINT                                       |
| Linear               | Linear combination                                              | PROC      | Default                                       |
| LogLikeChange        | Final change in the log likelihood                              | MODEL     | ITPRINT                                       |
| ModelBuildingSummary | Summary of model building                                       | MODEL     | SELECTION=BIFIS                               |
| ModelInfo            | Model information                                               | PROC      | Default                                       |
| NObs                 | Number of observations                                          | PROC      | Default                                       |



Table 54.13 *continued*

| ODS Table Name      | Description                                                                                                                                      | Statement   | Option                            |
|---------------------|--------------------------------------------------------------------------------------------------------------------------------------------------|-------------|-----------------------------------|
| OddsEst             | Adjusted odds ratios                                                                                                                             | UNITS       | Default                           |
| OddsRatios          | Odds ratio estimates                                                                                                                             | MODEL       | Default                           |
| OddsRatiosWald      | Odds ratio estimates and Wald confidence intervals                                                                                               | ODDSRATIOS  | CL=WALD                           |
| OddsRatiosPL        | Odds ratio estimates and PL confidence intervals                                                                                                 | ODDSRATIOS  | CL=PL                             |
| ParameterEstimates  | Maximum likelihood estimates of model parameters                                                                                                 | MODEL       | Default                           |
| RSquare             | R-square                                                                                                                                         | MODEL       | RSQUARE                           |
| ResidualChiSq       | Residual chi-square                                                                                                                              | MODEL       | SELECTION=FIB                     |
| ResponseProfile     | Response profile                                                                                                                                 | PROC        | Default                           |
| ROCAssociation      | Association table for ROC models                                                                                                                 | ROC         | Default                           |
| ROCContrastCoeff    | L matrix from ROCCONTRAST                                                                                                                        | ROCCONTRAST | E                                 |
| ROCContrastCov      | Covariance of ROCCONTRAST rows                                                                                                                   | ROCCONTRAST | COV                               |
| ROCContrastEstimate | Estimates from ROCCONTRAST                                                                                                                       | ROCCONTRAST | ESTIMATE=                         |
| ROCContrastTest     | Wald test from ROCCONTRAST                                                                                                                       | ROCCONTRAST | Default                           |
| ROCCov              | Covariance between ROC curves                                                                                                                    | ROCCONTRAST | COV                               |
| ScoreFitStat        | Fit statistics for Scored data                                                                                                                   | SCORE       | FITSTAT                           |
| SimpleStatistics    | Summary statistics for explanatory variables                                                                                                     | PROC        | SIMPLE                            |
| StrataSummary       | Number of strata with specific response frequencies                                                                                              | STRATA      | Default                           |
| StrataInfo          | Event and nonevent frequencies for each stratum                                                                                                  | STRATA      | INFO                              |
| SuffStats           | Sufficient statistics                                                                                                                            | EXACT       | OUTDIST=                          |
| TestPrint1          | $\mathbf{L}[\text{Cov}(\mathbf{b})]\mathbf{L}'$ and $\mathbf{Lb-c}$                                                                              | TEST        | PRINT                             |
| TestPrint2          | $\mathbf{Ginv}(\mathbf{L}[\text{Cov}(\mathbf{b})]\mathbf{L}')$ and $\mathbf{Ginv}(\mathbf{L}[\text{Cov}(\mathbf{b})]\mathbf{L}')(\mathbf{Lb-c})$ | TEST        | PRINT                             |
| TestStmts           | Linear hypotheses testing results                                                                                                                | TEST        | Default                           |
| Type3               | Type 3 tests of effects                                                                                                                          | MODEL       | Default<br>(with CLASS variables) |



## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “[Statistical Graphics Using ODS](#).”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS](#).”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “[A Primer on ODS Statistical Graphics](#)” on page 599 in Chapter 21, “[Statistical Graphics Using ODS](#).”

You must also specify the options in the PROC LOGISTIC statement that are indicated in [Table 54.14](#).

When ODS Graphics is enabled, then the EFFECT, EFFECTPLOT, ESTIMATE, LSMEANS, LSMESTIMATE, and SLICE statements can produce plots that are associated with their analyses. For information about these plots, see the corresponding sections of Chapter 19, “[Shared Concepts and Topics](#).”

PROC LOGISTIC assigns a name to each graph it creates using ODS. You can use these names to reference the graphs when using ODS. The names are listed in [Table 54.14](#).

**Table 54.14** Graphs Produced by PROC LOGISTIC

| ODS Graph Name          | Plot Description                                                                                      | Statement or Option                               |
|-------------------------|-------------------------------------------------------------------------------------------------------|---------------------------------------------------|
| DfBetasPlot             | Panel of dfbetas by case number                                                                       | PLOTS=DFBETAS<br>or MODEL / INFLUENCE or IPLOTS   |
| DPCPlot                 | Effect dfbetas by case number<br>Difchisq and/or difdev by predicted probability by CI displacement C | PLOTS=DFBETAS(UNPACK)<br>PLOTS=DPC                |
| EffectPlot              | Predicted probability                                                                                 | PLOTS=EFFECT                                      |
| InfluencePlots          | Panel of influence statistics by case number                                                          | PLOTS=INFLUENCE<br>or MODEL / INFLUENCE or IPLOTS |
| CBarPlot                | CI displacement Cbar by case number                                                                   | PLOTS=INFLUENCE(UNPACK)                           |
| CPlot                   | CI displacement C by case number                                                                      | PLOTS=INFLUENCE(UNPACK)                           |
| DevianceResidualPlot    | Deviance residual by case number                                                                      | PLOTS=INFLUENCE(UNPACK)                           |
| DifChisqPlot            | Difchisq by case number                                                                               | PLOTS=INFLUENCE(UNPACK)                           |
| DifDeviancePlot         | Difdev by case number                                                                                 | PLOTS=INFLUENCE(UNPACK)                           |
| LeveragePlot            | Hat diagonal by case number                                                                           | PLOTS=INFLUENCE(UNPACK)                           |
| LikelihoodResidualPlot  | Likelihood residual by case number                                                                    | PLOTS=INFLUENCE(UNPACK<br>STDRES)                 |
| PearsonResidualPlot     | Pearson chi-square residual by case number                                                            | PLOTS=INFLUENCE(UNPACK)                           |
| StdDevianceResidualPlot | Standardized deviance residual by case number                                                         | PLOTS=INFLUENCE(UNPACK<br>STDRES)                 |
| StdPearsonResidualPlot  | Standardized Pearson chi-square residual by case number                                               | PLOTS=INFLUENCE(UNPACK<br>STDRES)                 |

Table 54.14 *continued*

| ODS Graph Name       | Plot Description                            | Statement or Option                                                  |
|----------------------|---------------------------------------------|----------------------------------------------------------------------|
| LeveragePlots        | Panel of influence statistics by leverage   | PLOTS=LEVERAGE                                                       |
| LeverageCPlot        | CI displacement C by leverage               | PLOTS=LEVERAGE(UNPACK)                                               |
| LeverageDifChisqPlot | Difchisq by leverage                        | PLOTS=LEVERAGE(UNPACK)                                               |
| LeverageDifDevPlot   | Difdev by leverage                          | PLOTS=LEVERAGE(UNPACK)                                               |
| LeveragePhatPlot     | Predicted probability by leverage           | PLOTS=LEVERAGE(UNPACK)                                               |
| ORPlot               | Odds ratios                                 | Default or<br>PLOTS=ODDSRATIO and<br>MODEL / CLODDS=<br>or ODDSRATIO |
| PhatPlots            | Panel of influence by predicted probability | PLOTS=PHAT                                                           |
| PhatCPlot            | CI displacement C by predicted probability  | PLOTS=PHAT(UNPACK)                                                   |
| PhatDifChisqPlot     | Difchisq by predicted probability           | PLOTS=PHAT(UNPACK)                                                   |
| PhatDifDevPlot       | Difdev by predicted probability             | PLOTS=PHAT(UNPACK)                                                   |
| PhatLeveragePlot     | Leverage by predicted probability           | PLOTS=PHAT(UNPACK)                                                   |
| ROCCurve             | Receiver operating characteristics curve    | PLOTS=ROC<br>or MODEL / OUTROC=<br>or SCORE OUTROC=<br>or ROC        |
| ROCOverlay           | ROC curves for comparisons                  | PLOTS=ROC and<br>MODEL / SELECTION=<br>or ROC                        |

## Examples: LOGISTIC Procedure

### Example 54.1: Stepwise Logistic Regression and Predicted Values

Consider a study on cancer remission (Lee 1974). The data consist of patient characteristics and whether or not cancer remission occurred. The following DATA step creates the data set Remission containing seven variables. The variable remiss is the cancer remission indicator variable with a value of 1 for remission and a value of 0 for nonremission. The other six variables are the risk factors thought to be related to cancer remission.

```
data Remission;
 input remiss cell smear infil li blast temp;
 label remiss='Complete Remission';
 datalines;
1 .8 .83 .66 1.9 1.1 .996
1 .9 .36 .32 1.4 .74 .992
```

```

0 .8 .88 .7 .8 .176 .982
0 1 .87 .87 .7 1.053 .986
1 .9 .75 .68 1.3 .519 .98
0 1 .65 .65 .6 .519 .982
1 .95 .97 .92 1 1.23 .992
0 .95 .87 .83 1.9 1.354 1.02
0 1 .45 .45 .8 .322 .999
0 .95 .36 .34 .5 0 1.038
0 .85 .39 .33 .7 .279 .988
0 .7 .76 .53 1.2 .146 .982
0 .8 .46 .37 .4 .38 1.006
0 .2 .39 .08 .8 .114 .99
0 1 .9 .9 1.1 1.037 .99
1 1 .84 .84 1.9 2.064 1.02
0 .65 .42 .27 .5 .114 1.014
0 1 .75 .75 1 1.322 1.004
0 .5 .44 .22 .6 .114 .99
1 1 .63 .63 1.1 1.072 .986
0 1 .33 .33 .4 .176 1.01
0 .9 .93 .84 .6 1.591 1.02
1 1 .58 .58 1 .531 1.002
0 .95 .32 .3 1.6 .886 .988
1 1 .6 .6 1.7 .964 .99
1 1 .69 .69 .9 .398 .986
0 1 .73 .73 .7 .398 .986
;

```

The following invocation of PROC LOGISTIC illustrates the use of [stepwise selection](#) to identify the prognostic factors for cancer remission. A significance level of 0.3 is required to allow a variable into the model (`SLENTRY=0.3`), and a significance level of 0.35 is required for a variable to stay in the model (`SLSTAY=0.35`). A detailed account of the variable selection process is requested by specifying the `DETAILS` option. The Hosmer and Lemeshow goodness-of-fit test for the final selected model is requested by specifying the `LACKFIT` option. The `OUTEST=` and `COVOUT` options in the PROC LOGISTIC statement create a data set that contains parameter estimates and their covariances for the final selected model. The response variable option `EVENT=` chooses `remiss=1` (remission) as the event so that the probability of remission is modeled. The `OUTPUT` statement creates a data set that contains the cumulative predicted probabilities and the corresponding confidence limits, and the individual and cross validated predicted probabilities for each observation.

```

title 'Stepwise Regression on Cancer Remission Data';
proc logistic data=Remission outest=betas covout;
 model remiss(event='1')=cell smear infil li blast temp
 / selection=stepwise
 slentry=0.3
 slstay=0.35
 details
 lackfit;
 output out=pred p=phat lower=lcl upper=ucl
 predprob=(individual crossvalidate);
run;

```

```
proc print data=betas;
 title2 'Parameter Estimates and Covariance Matrix';
run;

proc print data=pred;
 title2 'Predicted Probabilities and 95% Confidence Limits';
run;
```

In stepwise selection, an attempt is made to remove any insignificant variables from the model before adding a significant variable to the model. Each addition or deletion of a variable to or from a model is listed as a separate step in the displayed output, and at each step a new model is fitted. Details of the model selection steps are shown in Outputs 54.1.1 through 54.1.5.

Prior to the first step, the intercept-only model is fit and individual score statistics for the potential variables are evaluated (Output 54.1.1).

**Output 54.1.1** Startup Model

| Stepwise Regression on Cancer Remission Data  |            |          |                |                 |            |
|-----------------------------------------------|------------|----------|----------------|-----------------|------------|
| The LOGISTIC Procedure                        |            |          |                |                 |            |
| Step 0. Intercept entered:                    |            |          |                |                 |            |
| Model Convergence Status                      |            |          |                |                 |            |
| Convergence criterion (GCONV=1E-8) satisfied. |            |          |                |                 |            |
| -2 Log L = 34.372                             |            |          |                |                 |            |
| Analysis of Maximum Likelihood Estimates      |            |          |                |                 |            |
| Parameter                                     | DF         | Estimate | Standard Error | Wald Chi-Square | Pr > ChiSq |
| Intercept                                     | 1          | -0.6931  | 0.4082         | 2.8827          | 0.0895     |
| Residual Chi-Square Test                      |            |          |                |                 |            |
|                                               | Chi-Square | DF       | Pr > ChiSq     |                 |            |
|                                               | 9.4609     | 6        | 0.1493         |                 |            |

## Output 54.1.1 continued

| Analysis of Effects Eligible for Entry |    |            |            |
|----------------------------------------|----|------------|------------|
| Effect                                 | DF | Score      |            |
|                                        |    | Chi-Square | Pr > ChiSq |
| cell                                   | 1  | 1.8893     | 0.1693     |
| smear                                  | 1  | 1.0745     | 0.2999     |
| infil                                  | 1  | 1.8817     | 0.1701     |
| li                                     | 1  | 7.9311     | 0.0049     |
| blast                                  | 1  | 3.5258     | 0.0604     |
| temp                                   | 1  | 0.6591     | 0.4169     |

In Step 1 (Output 54.1.2), the variable li is selected into the model since it is the most significant variable among those to be chosen ( $p = 0.0049 < 0.3$ ). The intermediate model that contains an intercept and li is then fitted. li remains significant ( $p = 0.0146 < 0.35$ ) and is not removed.

## Output 54.1.2 Step 1 of the Stepwise Analysis

|                                               |                  |                |                          |                |                 |            |
|-----------------------------------------------|------------------|----------------|--------------------------|----------------|-----------------|------------|
| Step 1. Effect li entered:                    |                  |                |                          |                |                 |            |
| Model Convergence Status                      |                  |                |                          |                |                 |            |
| Convergence criterion (GCONV=1E-8) satisfied. |                  |                |                          |                |                 |            |
| Model Fit Statistics                          |                  |                |                          |                |                 |            |
|                                               | Criterion        | Intercept Only | Intercept and Covariates |                |                 |            |
|                                               | AIC              | 36.372         | 30.073                   |                |                 |            |
|                                               | SC               | 37.668         | 32.665                   |                |                 |            |
|                                               | -2 Log L         | 34.372         | 26.073                   |                |                 |            |
| Testing Global Null Hypothesis: BETA=0        |                  |                |                          |                |                 |            |
|                                               | Test             | Chi-Square     | DF                       | Pr > ChiSq     |                 |            |
|                                               | Likelihood Ratio | 8.2988         | 1                        | 0.0040         |                 |            |
|                                               | Score            | 7.9311         | 1                        | 0.0049         |                 |            |
|                                               | Wald             | 5.9594         | 1                        | 0.0146         |                 |            |
| Analysis of Maximum Likelihood Estimates      |                  |                |                          |                |                 |            |
|                                               | Parameter        | DF             | Estimate                 | Standard Error | Wald Chi-Square | Pr > ChiSq |
|                                               | Intercept        | 1              | -3.7771                  | 1.3786         | 7.5064          | 0.0061     |
|                                               | li               | 1              | 2.8973                   | 1.1868         | 5.9594          | 0.0146     |

**Output 54.1.2** *continued*

| Odds Ratio Estimates |                |                            |         |
|----------------------|----------------|----------------------------|---------|
| Effect               | Point Estimate | 95% Wald Confidence Limits |         |
| li                   | 18.124         | 1.770                      | 185.563 |

| Association of Predicted Probabilities and Observed Responses |      |           |       |
|---------------------------------------------------------------|------|-----------|-------|
| Percent Concordant                                            | 84.0 | Somers' D | 0.710 |
| Percent Discordant                                            | 13.0 | Gamma     | 0.732 |
| Percent Tied                                                  | 3.1  | Tau-a     | 0.328 |
| Pairs                                                         | 162  | c         | 0.855 |

| Residual Chi-Square Test |    |            |  |
|--------------------------|----|------------|--|
| Chi-Square               | DF | Pr > ChiSq |  |
| 3.1174                   | 5  | 0.6819     |  |

| Analysis of Effects Eligible for Removal |    |                 |            |
|------------------------------------------|----|-----------------|------------|
| Effect                                   | DF | Wald Chi-Square | Pr > ChiSq |
| li                                       | 1  | 5.9594          | 0.0146     |

NOTE: No effects for the model in Step 1 are removed.

| Analysis of Effects Eligible for Entry |    |                  |            |
|----------------------------------------|----|------------------|------------|
| Effect                                 | DF | Score Chi-Square | Pr > ChiSq |
| cell                                   | 1  | 1.1183           | 0.2903     |
| smear                                  | 1  | 0.1369           | 0.7114     |
| infil                                  | 1  | 0.5715           | 0.4497     |
| blast                                  | 1  | 0.0932           | 0.7601     |
| temp                                   | 1  | 1.2591           | 0.2618     |

In Step 2 (Output 54.1.3), the variable temp is added to the model. The model then contains an intercept and the variables li and temp. Both li and temp remain significant at 0.35 level; therefore, neither li nor temp is removed from the model.

## Output 54.1.3 Step 2 of the Stepwise Analysis

Step 2. Effect temp entered:

## Model Convergence Status

Convergence criterion (GCONV=1E-8) satisfied.

## Model Fit Statistics

| Criterion | Intercept<br>Only | Intercept<br>and<br>Covariates |
|-----------|-------------------|--------------------------------|
| AIC       | 36.372            | 30.648                         |
| SC        | 37.668            | 34.535                         |
| -2 Log L  | 34.372            | 24.648                         |

## Testing Global Null Hypothesis: BETA=0

| Test             | Chi-Square | DF | Pr > ChiSq |
|------------------|------------|----|------------|
| Likelihood Ratio | 9.7239     | 2  | 0.0077     |
| Score            | 8.3648     | 2  | 0.0153     |
| Wald             | 5.9052     | 2  | 0.0522     |

## Analysis of Maximum Likelihood Estimates

| Parameter | DF | Estimate | Standard<br>Error | Wald<br>Chi-Square | Pr > ChiSq |
|-----------|----|----------|-------------------|--------------------|------------|
| Intercept | 1  | 47.8448  | 46.4381           | 1.0615             | 0.3029     |
| li        | 1  | 3.3017   | 1.3593            | 5.9002             | 0.0151     |
| temp      | 1  | -52.4214 | 47.4897           | 1.2185             | 0.2697     |

## Odds Ratio Estimates

| Effect | Point<br>Estimate | 95% Wald<br>Confidence Limits |          |
|--------|-------------------|-------------------------------|----------|
| li     | 27.158            | 1.892                         | 389.856  |
| temp   | <0.001            | <0.001                        | >999.999 |

## Association of Predicted Probabilities and Observed Responses

|                    |      |           |       |
|--------------------|------|-----------|-------|
| Percent Concordant | 87.0 | Somers' D | 0.747 |
| Percent Discordant | 12.3 | Gamma     | 0.752 |
| Percent Tied       | 0.6  | Tau-a     | 0.345 |
| Pairs              | 162  | c         | 0.873 |

**Output 54.1.3** *continued*

| Residual Chi-Square Test |    |            |  |
|--------------------------|----|------------|--|
| Chi-Square               | DF | Pr > ChiSq |  |
| 2.1429                   | 4  | 0.7095     |  |

| Analysis of Effects Eligible for Removal |    |            |            |
|------------------------------------------|----|------------|------------|
| Effect                                   | DF | Wald       | Pr > ChiSq |
|                                          |    | Chi-Square |            |
| li                                       | 1  | 5.9002     | 0.0151     |
| temp                                     | 1  | 1.2185     | 0.2697     |

NOTE: No effects for the model in Step 2 are removed.

| Analysis of Effects Eligible for Entry |    |            |            |
|----------------------------------------|----|------------|------------|
| Effect                                 | DF | Score      | Pr > ChiSq |
|                                        |    | Chi-Square |            |
| cell                                   | 1  | 1.4700     | 0.2254     |
| smear                                  | 1  | 0.1730     | 0.6775     |
| infil                                  | 1  | 0.8274     | 0.3630     |
| blast                                  | 1  | 1.1013     | 0.2940     |

In Step 3 (Output 54.1.4), the variable cell is added to the model. The model then contains an intercept and the variables li, temp, and cell. None of these variables are removed from the model since all are significant at the 0.35 level.

**Output 54.1.4** Step 3 of the Stepwise Analysis

Step 3. Effect cell entered:

| Model Convergence Status                      |  |  |
|-----------------------------------------------|--|--|
| Convergence criterion (GCONV=1E-8) satisfied. |  |  |

| Model Fit Statistics |           |            |
|----------------------|-----------|------------|
| Criterion            | Intercept | Intercept  |
|                      | Only      | and        |
|                      |           | Covariates |
| AIC                  | 36.372    | 29.953     |
| SC                   | 37.668    | 35.137     |
| -2 Log L             | 34.372    | 21.953     |



## Output 54.1.4 continued

## Testing Global Null Hypothesis: BETA=0

| Test             | Chi-Square | DF | Pr > ChiSq |
|------------------|------------|----|------------|
| Likelihood Ratio | 12.4184    | 3  | 0.0061     |
| Score            | 9.2502     | 3  | 0.0261     |
| Wald             | 4.8281     | 3  | 0.1848     |

## Analysis of Maximum Likelihood Estimates

| Parameter | DF | Estimate | Standard Error | Wald Chi-Square | Pr > ChiSq |
|-----------|----|----------|----------------|-----------------|------------|
| Intercept | 1  | 67.6339  | 56.8875        | 1.4135          | 0.2345     |
| cell      | 1  | 9.6521   | 7.7511         | 1.5507          | 0.2130     |
| li        | 1  | 3.8671   | 1.7783         | 4.7290          | 0.0297     |
| temp      | 1  | -82.0737 | 61.7124        | 1.7687          | 0.1835     |

## Odds Ratio Estimates

| Effect | Point Estimate | 95% Wald Confidence Limits |
|--------|----------------|----------------------------|
| cell   | >999.999       | 0.004 >999.999             |
| li     | 47.804         | 1.465 >999.999             |
| temp   | <0.001         | <0.001 >999.999            |

## Association of Predicted Probabilities and Observed Responses

|                    |      |           |       |
|--------------------|------|-----------|-------|
| Percent Concordant | 88.9 | Somers' D | 0.778 |
| Percent Discordant | 11.1 | Gamma     | 0.778 |
| Percent Tied       | 0.0  | Tau-a     | 0.359 |
| Pairs              | 162  | c         | 0.889 |

## Residual Chi-Square Test

| Chi-Square | DF | Pr > ChiSq |
|------------|----|------------|
| 0.1831     | 3  | 0.9803     |

## Analysis of Effects Eligible for Removal

| Effect | DF | Wald Chi-Square | Pr > ChiSq |
|--------|----|-----------------|------------|
| cell   | 1  | 1.5507          | 0.2130     |
| li     | 1  | 4.7290          | 0.0297     |
| temp   | 1  | 1.7687          | 0.1835     |

**Output 54.1.4** *continued*

NOTE: No effects for the model in Step 3 are removed.

Analysis of Effects Eligible for Entry

| Effect | DF | Score      |            |
|--------|----|------------|------------|
|        |    | Chi-Square | Pr > ChiSq |
| smear  | 1  | 0.0956     | 0.7572     |
| infil  | 1  | 0.0844     | 0.7714     |
| blast  | 1  | 0.0208     | 0.8852     |

Finally, none of the remaining variables outside the model meet the entry criterion, and the stepwise selection is terminated. A summary of the stepwise selection is displayed in [Output 54.1.5](#).

**Output 54.1.5** Summary of the Stepwise Selection

Summary of Stepwise Selection

| Step | Effect  |         | DF | Number In | Score      | Wald       |            |
|------|---------|---------|----|-----------|------------|------------|------------|
|      | Entered | Removed |    |           | Chi-Square | Chi-Square | Pr > ChiSq |
| 1    | li      |         | 1  | 1         | 7.9311     |            | 0.0049     |
| 2    | temp    |         | 1  | 2         | 1.2591     |            | 0.2618     |
| 3    | cell    |         | 1  | 3         | 1.4700     |            | 0.2254     |

Results of the Hosmer and Lemeshow test are shown in [Output 54.1.6](#). There is no evidence of a lack of fit in the selected model ( $p = 0.5054$ ).

**Output 54.1.6** Display of the LACKFIT Option

Partition for the Hosmer and Lemeshow Test

| Group | Total | remiss = 1 |          | remiss = 0 |          |
|-------|-------|------------|----------|------------|----------|
|       |       | Observed   | Expected | Observed   | Expected |
| 1     | 3     | 0          | 0.00     | 3          | 3.00     |
| 2     | 3     | 0          | 0.01     | 3          | 2.99     |
| 3     | 3     | 0          | 0.19     | 3          | 2.81     |
| 4     | 3     | 0          | 0.56     | 3          | 2.44     |
| 5     | 4     | 1          | 1.09     | 3          | 2.91     |
| 6     | 3     | 2          | 1.35     | 1          | 1.65     |
| 7     | 3     | 2          | 1.84     | 1          | 1.16     |
| 8     | 3     | 3          | 2.15     | 0          | 0.85     |
| 9     | 2     | 1          | 1.80     | 1          | 0.20     |

**Output 54.1.6** *continued*

| Hosmer and Lemeshow Goodness-of-Fit Test |    |            |
|------------------------------------------|----|------------|
| Chi-Square                               | DF | Pr > ChiSq |
| 6.2983                                   | 7  | 0.5054     |

The data set betas created by the `OUTEST=` and `COVOUT` options is displayed in [Output 54.1.7](#). The data set contains parameter estimates and the covariance matrix for the final selected model. Note that all explanatory variables listed in the `MODEL` statement are included in this data set; however, variables that are not included in the final model have all missing values.

**Output 54.1.7** Data Set of Estimates and Covariances

| Stepwise Regression on Cancer Remission Data<br>Parameter Estimates and Covariance Matrix |             |             |               |             |           |               |                |
|-------------------------------------------------------------------------------------------|-------------|-------------|---------------|-------------|-----------|---------------|----------------|
| Obs                                                                                       | <u>LINK</u> | <u>TYPE</u> | <u>STATUS</u> | <u>NAME</u> | Intercept | cell          |                |
| 1                                                                                         | LOGIT       | PARMS       | 0 Converged   | remiss      | 67.63     | 9.652         |                |
| 2                                                                                         | LOGIT       | COV         | 0 Converged   | Intercept   | 3236.19   | 157.097       |                |
| 3                                                                                         | LOGIT       | COV         | 0 Converged   | cell        | 157.10    | 60.079        |                |
| 4                                                                                         | LOGIT       | COV         | 0 Converged   | smear       | .         | .             |                |
| 5                                                                                         | LOGIT       | COV         | 0 Converged   | infil       | .         | .             |                |
| 6                                                                                         | LOGIT       | COV         | 0 Converged   | li          | 64.57     | 6.945         |                |
| 7                                                                                         | LOGIT       | COV         | 0 Converged   | blast       | .         | .             |                |
| 8                                                                                         | LOGIT       | COV         | 0 Converged   | temp        | -3483.23  | -223.669      |                |
| Obs                                                                                       | smear       | infil       | li            | blast       | temp      | <u>LNLIKE</u> | <u>ESTTYPE</u> |
| 1                                                                                         | .           | .           | 3.8671        | .           | -82.07    | -10.9767      | MLE            |
| 2                                                                                         | .           | .           | 64.5726       | .           | -3483.23  | -10.9767      | MLE            |
| 3                                                                                         | .           | .           | 6.9454        | .           | -223.67   | -10.9767      | MLE            |
| 4                                                                                         | .           | .           | .             | .           | .         | -10.9767      | MLE            |
| 5                                                                                         | .           | .           | .             | .           | .         | -10.9767      | MLE            |
| 6                                                                                         | .           | .           | 3.1623        | .           | -75.35    | -10.9767      | MLE            |
| 7                                                                                         | .           | .           | .             | .           | .         | -10.9767      | MLE            |
| 8                                                                                         | .           | .           | -75.3513      | .           | 3808.42   | -10.9767      | MLE            |

The data set `pred` created by the `OUTPUT` statement is displayed in [Output 54.1.8](#). It contains all the variables in the input data set, the variable `phat` for the (cumulative) predicted probability, the variables `lcl` and `ucl` for the lower and upper confidence limits for the probability, and four other variables (`IP_1`, `IP_0`, `XP_1`, and `XP_0`) for the `PREDPROBS=` option. The data set also contains the variable `_LEVEL_`, indicating the response value to which `phat`, `lcl`, and `ucl` refer. For instance, for the first row of the `OUTPUT` data set, the values of `_LEVEL_` and `phat`, `lcl`, and `ucl` are 1, 0.72265, 0.16892, and 0.97093, respectively; this means that the estimated probability that `remiss=1` is 0.723 for the given explanatory variable values, and the corresponding 95% confidence interval is (0.16892, 0.97093). The variables `IP_1` and `IP_0` contain the predicted probabilities that `remiss=1` and `remiss=0`, respectively. Note that values of `phat` and `IP_1` are identical since they both contain the probabilities that `remiss=1`. The variables `XP_1` and `XP_0` contain the cross validated predicted probabilities that `remiss=1` and `remiss=0`, respectively.

**Output 54.1.8** Predicted Probabilities and Confidence Intervals

| Stepwise Regression on Cancer Remission Data      |         |         |         |         |         |         |         |        |        |         |  |
|---------------------------------------------------|---------|---------|---------|---------|---------|---------|---------|--------|--------|---------|--|
| Predicted Probabilities and 95% Confidence Limits |         |         |         |         |         |         |         |        |        |         |  |
| Obs                                               | remiss  | cell    | smear   | infil   | li      | blast   | temp    | _FROM_ | _INTO_ | IP_0    |  |
| 1                                                 | 1       | 0.80    | 0.83    | 0.66    | 1.9     | 1.100   | 0.996   | 1      | 1      | 0.27735 |  |
| 2                                                 | 1       | 0.90    | 0.36    | 0.32    | 1.4     | 0.740   | 0.992   | 1      | 1      | 0.42126 |  |
| 3                                                 | 0       | 0.80    | 0.88    | 0.70    | 0.8     | 0.176   | 0.982   | 0      | 0      | 0.89540 |  |
| 4                                                 | 0       | 1.00    | 0.87    | 0.87    | 0.7     | 1.053   | 0.986   | 0      | 0      | 0.71742 |  |
| 5                                                 | 1       | 0.90    | 0.75    | 0.68    | 1.3     | 0.519   | 0.980   | 1      | 1      | 0.28582 |  |
| 6                                                 | 0       | 1.00    | 0.65    | 0.65    | 0.6     | 0.519   | 0.982   | 0      | 0      | 0.72911 |  |
| 7                                                 | 1       | 0.95    | 0.97    | 0.92    | 1.0     | 1.230   | 0.992   | 1      | 0      | 0.67844 |  |
| 8                                                 | 0       | 0.95    | 0.87    | 0.83    | 1.9     | 1.354   | 1.020   | 0      | 1      | 0.39277 |  |
| 9                                                 | 0       | 1.00    | 0.45    | 0.45    | 0.8     | 0.322   | 0.999   | 0      | 0      | 0.83368 |  |
| 10                                                | 0       | 0.95    | 0.36    | 0.34    | 0.5     | 0.000   | 1.038   | 0      | 0      | 0.99843 |  |
| 11                                                | 0       | 0.85    | 0.39    | 0.33    | 0.7     | 0.279   | 0.988   | 0      | 0      | 0.92715 |  |
| 12                                                | 0       | 0.70    | 0.76    | 0.53    | 1.2     | 0.146   | 0.982   | 0      | 0      | 0.82714 |  |
| Obs                                               | IP_1    | XP_0    | XP_1    | _LEVEL_ | phat    | lcl     | ucl     |        |        |         |  |
| 1                                                 | 0.72265 | 0.43873 | 0.56127 | 1       | 0.72265 | 0.16892 | 0.97093 |        |        |         |  |
| 2                                                 | 0.57874 | 0.47461 | 0.52539 | 1       | 0.57874 | 0.26788 | 0.83762 |        |        |         |  |
| 3                                                 | 0.10460 | 0.87060 | 0.12940 | 1       | 0.10460 | 0.00781 | 0.63419 |        |        |         |  |
| 4                                                 | 0.28258 | 0.67259 | 0.32741 | 1       | 0.28258 | 0.07498 | 0.65683 |        |        |         |  |
| 5                                                 | 0.71418 | 0.36901 | 0.63099 | 1       | 0.71418 | 0.25218 | 0.94876 |        |        |         |  |
| 6                                                 | 0.27089 | 0.67269 | 0.32731 | 1       | 0.27089 | 0.05852 | 0.68951 |        |        |         |  |
| 7                                                 | 0.32156 | 0.72923 | 0.27077 | 1       | 0.32156 | 0.13255 | 0.59516 |        |        |         |  |
| 8                                                 | 0.60723 | 0.09906 | 0.90094 | 1       | 0.60723 | 0.10572 | 0.95287 |        |        |         |  |
| 9                                                 | 0.16632 | 0.80864 | 0.19136 | 1       | 0.16632 | 0.03018 | 0.56123 |        |        |         |  |
| 10                                                | 0.00157 | 0.99840 | 0.00160 | 1       | 0.00157 | 0.00000 | 0.68962 |        |        |         |  |
| 11                                                | 0.07285 | 0.91723 | 0.08277 | 1       | 0.07285 | 0.00614 | 0.49982 |        |        |         |  |
| 12                                                | 0.17286 | 0.63838 | 0.36162 | 1       | 0.17286 | 0.00637 | 0.87206 |        |        |         |  |

## Output 54.1.8 continued

| Stepwise Regression on Cancer Remission Data      |        |      |       |       |     |       |       |        |        |         |
|---------------------------------------------------|--------|------|-------|-------|-----|-------|-------|--------|--------|---------|
| Predicted Probabilities and 95% Confidence Limits |        |      |       |       |     |       |       |        |        |         |
| Obs                                               | remiss | cell | smear | infil | li  | blast | temp  | _FROM_ | _INTO_ | IP_0    |
| 13                                                | 0      | 0.80 | 0.46  | 0.37  | 0.4 | 0.380 | 1.006 | 0      | 0      | 0.99654 |
| 14                                                | 0      | 0.20 | 0.39  | 0.08  | 0.8 | 0.114 | 0.990 | 0      | 0      | 0.99982 |
| 15                                                | 0      | 1.00 | 0.90  | 0.90  | 1.1 | 1.037 | 0.990 | 0      | 1      | 0.42878 |
| 16                                                | 1      | 1.00 | 0.84  | 0.84  | 1.9 | 2.064 | 1.020 | 1      | 1      | 0.28530 |
| 17                                                | 0      | 0.65 | 0.42  | 0.27  | 0.5 | 0.114 | 1.014 | 0      | 0      | 0.99938 |
| 18                                                | 0      | 1.00 | 0.75  | 0.75  | 1.0 | 1.322 | 1.004 | 0      | 0      | 0.77711 |
| 19                                                | 0      | 0.50 | 0.44  | 0.22  | 0.6 | 0.114 | 0.990 | 0      | 0      | 0.99846 |
| 20                                                | 1      | 1.00 | 0.63  | 0.63  | 1.1 | 1.072 | 0.986 | 1      | 1      | 0.35089 |
| 21                                                | 0      | 1.00 | 0.33  | 0.33  | 0.4 | 0.176 | 1.010 | 0      | 0      | 0.98307 |
| 22                                                | 0      | 0.90 | 0.93  | 0.84  | 0.6 | 1.591 | 1.020 | 0      | 0      | 0.99378 |
| 23                                                | 1      | 1.00 | 0.58  | 0.58  | 1.0 | 0.531 | 1.002 | 1      | 0      | 0.74739 |
| 24                                                | 0      | 0.95 | 0.32  | 0.30  | 1.6 | 0.886 | 0.988 | 0      | 1      | 0.12989 |

| Obs | IP_1    | XP_0    | XP_1    | _LEVEL_ | phat    | lcl     | ucl     |
|-----|---------|---------|---------|---------|---------|---------|---------|
| 13  | 0.00346 | 0.99644 | 0.00356 | 1       | 0.00346 | 0.00001 | 0.46530 |
| 14  | 0.00018 | 0.99981 | 0.00019 | 1       | 0.00018 | 0.00000 | 0.96482 |
| 15  | 0.57122 | 0.35354 | 0.64646 | 1       | 0.57122 | 0.25303 | 0.83973 |
| 16  | 0.71470 | 0.47213 | 0.52787 | 1       | 0.71470 | 0.15362 | 0.97189 |
| 17  | 0.00062 | 0.99937 | 0.00063 | 1       | 0.00062 | 0.00000 | 0.62665 |
| 18  | 0.22289 | 0.73612 | 0.26388 | 1       | 0.22289 | 0.04483 | 0.63670 |
| 19  | 0.00154 | 0.99842 | 0.00158 | 1       | 0.00154 | 0.00000 | 0.79644 |
| 20  | 0.64911 | 0.42053 | 0.57947 | 1       | 0.64911 | 0.26305 | 0.90555 |
| 21  | 0.01693 | 0.98170 | 0.01830 | 1       | 0.01693 | 0.00029 | 0.50475 |
| 22  | 0.00622 | 0.99348 | 0.00652 | 1       | 0.00622 | 0.00003 | 0.56062 |
| 23  | 0.25261 | 0.84423 | 0.15577 | 1       | 0.25261 | 0.06137 | 0.63597 |
| 24  | 0.87011 | 0.03637 | 0.96363 | 1       | 0.87011 | 0.40910 | 0.98481 |

| Stepwise Regression on Cancer Remission Data      |        |      |       |       |     |       |       |        |        |         |
|---------------------------------------------------|--------|------|-------|-------|-----|-------|-------|--------|--------|---------|
| Predicted Probabilities and 95% Confidence Limits |        |      |       |       |     |       |       |        |        |         |
| Obs                                               | remiss | cell | smear | infil | li  | blast | temp  | _FROM_ | _INTO_ | IP_0    |
| 25                                                | 1      | 1.00 | 0.60  | 0.60  | 1.7 | 0.964 | 0.990 | 1      | 1      | 0.06868 |
| 26                                                | 1      | 1.00 | 0.69  | 0.69  | 0.9 | 0.398 | 0.986 | 1      | 0      | 0.53949 |
| 27                                                | 0      | 1.00 | 0.73  | 0.73  | 0.7 | 0.398 | 0.986 | 0      | 0      | 0.71742 |

| Obs | IP_1    | XP_0    | XP_1    | _LEVEL_ | phat    | lcl     | ucl     |
|-----|---------|---------|---------|---------|---------|---------|---------|
| 25  | 0.93132 | 0.08017 | 0.91983 | 1       | 0.93132 | 0.44114 | 0.99573 |
| 26  | 0.46051 | 0.62312 | 0.37688 | 1       | 0.46051 | 0.16612 | 0.78529 |
| 27  | 0.28258 | 0.67259 | 0.32741 | 1       | 0.28258 | 0.07498 | 0.65683 |

Next, a different variable selection method is used to select prognostic factors for cancer remission, and an efficient algorithm is employed to eliminate insignificant variables from a model. The following statements invoke PROC LOGISTIC to perform the backward elimination analysis:

```

title 'Backward Elimination on Cancer Remission Data';
proc logistic data=Remission;
 model remiss(event='1')=temp cell li smear blast
 / selection=backward fast slstay=0.2 ctable;
run;

```

The backward elimination analysis (**SELECTION=BACKWARD**) starts with a model that contains all explanatory variables given in the **MODEL** statement. By specifying the **FAST** option, PROC LOGISTIC eliminates insignificant variables without refitting the model repeatedly. This analysis uses a significance level of 0.2 to retain variables in the model (**SLSTAY=0.2**), which is different from the previous stepwise analysis where **SLSTAY=.35**. The **CTABLE** option is specified to produce classifications of input observations based on the final selected model.

Results of the fast elimination analysis are shown in [Output 54.1.9](#) and [Output 54.1.10](#). Initially, a full model containing all six risk factors is fit to the data ([Output 54.1.9](#)). In the next step ([Output 54.1.10](#)), PROC LOGISTIC removes blast, smear, cell, and temp from the model all at once. This leaves li and the intercept as the only variables in the final model. Note that in this analysis, only parameter estimates for the final model are displayed because the **DETAILS** option has not been specified.

**Output 54.1.9** Initial Step in Backward Elimination

| Backward Elimination on Cancer Remission Data |                  |                    |
|-----------------------------------------------|------------------|--------------------|
| The LOGISTIC Procedure                        |                  |                    |
| Model Information                             |                  |                    |
| Data Set                                      | WORK.REMISSION   |                    |
| Response Variable                             | remiss           | Complete Remission |
| Number of Response Levels                     | 2                |                    |
| Model                                         | binary logit     |                    |
| Optimization Technique                        | Fisher's scoring |                    |
| Number of Observations Read                   |                  | 27                 |
| Number of Observations Used                   |                  | 27                 |
| Response Profile                              |                  |                    |
| Ordered Value                                 | remiss           | Total Frequency    |
| 1                                             | 0                | 18                 |
| 2                                             | 1                | 9                  |
| Probability modeled is remiss=1.              |                  |                    |

Output 54.1.9 *continued*

| Backward Elimination Procedure                |                   |                                |            |
|-----------------------------------------------|-------------------|--------------------------------|------------|
| Step 0. The following effects were entered:   |                   |                                |            |
| Intercept temp cell li smear blast            |                   |                                |            |
| Model Convergence Status                      |                   |                                |            |
| Convergence criterion (GCONV=1E-8) satisfied. |                   |                                |            |
| Model Fit Statistics                          |                   |                                |            |
| Criterion                                     | Intercept<br>Only | Intercept<br>and<br>Covariates |            |
| AIC                                           | 36.372            | 33.857                         |            |
| SC                                            | 37.668            | 41.632                         |            |
| -2 Log L                                      | 34.372            | 21.857                         |            |
| Testing Global Null Hypothesis: BETA=0        |                   |                                |            |
| Test                                          | Chi-Square        | DF                             | Pr > ChiSq |
| Likelihood Ratio                              | 12.5146           | 5                              | 0.0284     |
| Score                                         | 9.3295            | 5                              | 0.0966     |
| Wald                                          | 4.7284            | 5                              | 0.4499     |

## Output 54.1.10 Fast Elimination Step

| Step 1. Fast Backward Elimination:                       |            |    |            |                        |    |                           |
|----------------------------------------------------------|------------|----|------------|------------------------|----|---------------------------|
| Analysis of Effects Removed by Fast Backward Elimination |            |    |            |                        |    |                           |
| Effect<br>Removed                                        | Chi-Square | DF | Pr > ChiSq | Residual<br>Chi-Square | DF | Pr ><br>Residual<br>ChiSq |
| blast                                                    | 0.0008     | 1  | 0.9768     | 0.0008                 | 1  | 0.9768                    |
| smear                                                    | 0.0951     | 1  | 0.7578     | 0.0959                 | 2  | 0.9532                    |
| cell                                                     | 1.5134     | 1  | 0.2186     | 1.6094                 | 3  | 0.6573                    |
| temp                                                     | 0.6535     | 1  | 0.4189     | 2.2628                 | 4  | 0.6875                    |
| Model Convergence Status                                 |            |    |            |                        |    |                           |
| Convergence criterion (GCONV=1E-8) satisfied.            |            |    |            |                        |    |                           |

**Output 54.1.10** *continued*

| Model Fit Statistics                     |                |                            |                |                 |            |
|------------------------------------------|----------------|----------------------------|----------------|-----------------|------------|
| Criterion                                | Intercept Only | Intercept and Covariates   |                |                 |            |
| AIC                                      | 36.372         | 30.073                     |                |                 |            |
| SC                                       | 37.668         | 32.665                     |                |                 |            |
| -2 Log L                                 | 34.372         | 26.073                     |                |                 |            |
| Testing Global Null Hypothesis: BETA=0   |                |                            |                |                 |            |
| Test                                     | Chi-Square     | DF                         | Pr > ChiSq     |                 |            |
| Likelihood Ratio                         | 8.2988         | 1                          | 0.0040         |                 |            |
| Score                                    | 7.9311         | 1                          | 0.0049         |                 |            |
| Wald                                     | 5.9594         | 1                          | 0.0146         |                 |            |
| Residual Chi-Square Test                 |                |                            |                |                 |            |
| Chi-Square                               | DF             | Pr > ChiSq                 |                |                 |            |
| 2.8530                                   | 4              | 0.5827                     |                |                 |            |
| Summary of Backward Elimination          |                |                            |                |                 |            |
| Step                                     | Effect Removed | DF                         | Number In      | Wald Chi-Square | Pr > ChiSq |
| 1                                        | blast          | 1                          | 4              | 0.0008          | 0.9768     |
| 1                                        | smear          | 1                          | 3              | 0.0951          | 0.7578     |
| 1                                        | cell           | 1                          | 2              | 1.5134          | 0.2186     |
| 1                                        | temp           | 1                          | 1              | 0.6535          | 0.4189     |
| Analysis of Maximum Likelihood Estimates |                |                            |                |                 |            |
| Parameter                                | DF             | Estimate                   | Standard Error | Wald Chi-Square | Pr > ChiSq |
| Intercept                                | 1              | -3.7771                    | 1.3786         | 7.5064          | 0.0061     |
| li                                       | 1              | 2.8973                     | 1.1868         | 5.9594          | 0.0146     |
| Odds Ratio Estimates                     |                |                            |                |                 |            |
| Effect                                   | Point Estimate | 95% Wald Confidence Limits |                |                 |            |
| li                                       | 18.124         | 1.770                      | 185.563        |                 |            |



**Output 54.1.10** *continued*

| Association of Predicted Probabilities and Observed Responses |      |           |       |
|---------------------------------------------------------------|------|-----------|-------|
| Percent Concordant                                            | 84.0 | Somers' D | 0.710 |
| Percent Discordant                                            | 13.0 | Gamma     | 0.732 |
| Percent Tied                                                  | 3.1  | Tau-a     | 0.328 |
| Pairs                                                         | 162  | c         | 0.855 |

Note that you can also use the FAST option when `SELECTION=STEPWISE`. However, the FAST option operates only on backward elimination steps. In this example, the stepwise process only adds variables, so the FAST option would not be useful.

Results of the `CTABLE` option are shown in [Output 54.1.11](#).

**Output 54.1.11** Classifying Input Observations

| Classification Table |         |           |           |           |             |             |             |           |           |
|----------------------|---------|-----------|-----------|-----------|-------------|-------------|-------------|-----------|-----------|
| Prob Level           | Correct |           | Incorrect |           | Percentages |             |             |           |           |
|                      | Event   | Non-Event | Event     | Non-Event | Correct     | Sensitivity | Specificity | False POS | False NEG |
| 0.060                | 9       | 0         | 18        | 0         | 33.3        | 100.0       | 0.0         | 66.7      | .         |
| 0.080                | 9       | 2         | 16        | 0         | 40.7        | 100.0       | 11.1        | 64.0      | 0.0       |
| 0.100                | 9       | 4         | 14        | 0         | 48.1        | 100.0       | 22.2        | 60.9      | 0.0       |
| 0.120                | 9       | 4         | 14        | 0         | 48.1        | 100.0       | 22.2        | 60.9      | 0.0       |
| 0.140                | 9       | 7         | 11        | 0         | 59.3        | 100.0       | 38.9        | 55.0      | 0.0       |
| 0.160                | 9       | 10        | 8         | 0         | 70.4        | 100.0       | 55.6        | 47.1      | 0.0       |
| 0.180                | 9       | 10        | 8         | 0         | 70.4        | 100.0       | 55.6        | 47.1      | 0.0       |
| 0.200                | 8       | 13        | 5         | 1         | 77.8        | 88.9        | 72.2        | 38.5      | 7.1       |
| 0.220                | 8       | 13        | 5         | 1         | 77.8        | 88.9        | 72.2        | 38.5      | 7.1       |
| 0.240                | 8       | 13        | 5         | 1         | 77.8        | 88.9        | 72.2        | 38.5      | 7.1       |
| 0.260                | 6       | 13        | 5         | 3         | 70.4        | 66.7        | 72.2        | 45.5      | 18.8      |
| 0.280                | 6       | 13        | 5         | 3         | 70.4        | 66.7        | 72.2        | 45.5      | 18.8      |
| 0.300                | 6       | 13        | 5         | 3         | 70.4        | 66.7        | 72.2        | 45.5      | 18.8      |
| 0.320                | 6       | 14        | 4         | 3         | 74.1        | 66.7        | 77.8        | 40.0      | 17.6      |
| 0.340                | 5       | 14        | 4         | 4         | 70.4        | 55.6        | 77.8        | 44.4      | 22.2      |
| 0.360                | 5       | 14        | 4         | 4         | 70.4        | 55.6        | 77.8        | 44.4      | 22.2      |
| 0.380                | 5       | 15        | 3         | 4         | 74.1        | 55.6        | 83.3        | 37.5      | 21.1      |
| 0.400                | 5       | 15        | 3         | 4         | 74.1        | 55.6        | 83.3        | 37.5      | 21.1      |
| 0.420                | 5       | 15        | 3         | 4         | 74.1        | 55.6        | 83.3        | 37.5      | 21.1      |
| 0.440                | 5       | 15        | 3         | 4         | 74.1        | 55.6        | 83.3        | 37.5      | 21.1      |
| 0.460                | 4       | 16        | 2         | 5         | 74.1        | 44.4        | 88.9        | 33.3      | 23.8      |
| 0.480                | 4       | 16        | 2         | 5         | 74.1        | 44.4        | 88.9        | 33.3      | 23.8      |
| 0.500                | 4       | 16        | 2         | 5         | 74.1        | 44.4        | 88.9        | 33.3      | 23.8      |
| 0.520                | 4       | 16        | 2         | 5         | 74.1        | 44.4        | 88.9        | 33.3      | 23.8      |
| 0.540                | 3       | 16        | 2         | 6         | 70.4        | 33.3        | 88.9        | 40.0      | 27.3      |
| 0.560                | 3       | 16        | 2         | 6         | 70.4        | 33.3        | 88.9        | 40.0      | 27.3      |
| 0.580                | 3       | 16        | 2         | 6         | 70.4        | 33.3        | 88.9        | 40.0      | 27.3      |
| 0.600                | 3       | 16        | 2         | 6         | 70.4        | 33.3        | 88.9        | 40.0      | 27.3      |
| 0.620                | 3       | 16        | 2         | 6         | 70.4        | 33.3        | 88.9        | 40.0      | 27.3      |
| 0.640                | 3       | 16        | 2         | 6         | 70.4        | 33.3        | 88.9        | 40.0      | 27.3      |
| 0.660                | 3       | 16        | 2         | 6         | 70.4        | 33.3        | 88.9        | 40.0      | 27.3      |
| 0.680                | 3       | 16        | 2         | 6         | 70.4        | 33.3        | 88.9        | 40.0      | 27.3      |
| 0.700                | 3       | 16        | 2         | 6         | 70.4        | 33.3        | 88.9        | 40.0      | 27.3      |
| 0.720                | 2       | 16        | 2         | 7         | 66.7        | 22.2        | 88.9        | 50.0      | 30.4      |
| 0.740                | 2       | 16        | 2         | 7         | 66.7        | 22.2        | 88.9        | 50.0      | 30.4      |
| 0.760                | 2       | 16        | 2         | 7         | 66.7        | 22.2        | 88.9        | 50.0      | 30.4      |
| 0.780                | 2       | 16        | 2         | 7         | 66.7        | 22.2        | 88.9        | 50.0      | 30.4      |
| 0.800                | 2       | 17        | 1         | 7         | 70.4        | 22.2        | 94.4        | 33.3      | 29.2      |
| 0.820                | 2       | 17        | 1         | 7         | 70.4        | 22.2        | 94.4        | 33.3      | 29.2      |
| 0.840                | 0       | 17        | 1         | 9         | 63.0        | 0.0         | 94.4        | 100.0     | 34.6      |
| 0.860                | 0       | 17        | 1         | 9         | 63.0        | 0.0         | 94.4        | 100.0     | 34.6      |
| 0.880                | 0       | 17        | 1         | 9         | 63.0        | 0.0         | 94.4        | 100.0     | 34.6      |
| 0.900                | 0       | 17        | 1         | 9         | 63.0        | 0.0         | 94.4        | 100.0     | 34.6      |
| 0.920                | 0       | 17        | 1         | 9         | 63.0        | 0.0         | 94.4        | 100.0     | 34.6      |
| 0.940                | 0       | 17        | 1         | 9         | 63.0        | 0.0         | 94.4        | 100.0     | 34.6      |
| 0.960                | 0       | 18        | 0         | 9         | 66.7        | 0.0         | 100.0       | .         | 33.3      |

Each row of the “Classification Table” corresponds to a cutpoint applied to the predicted probabilities, which is given in the Prob Level column. The  $2 \times 2$  frequency tables of observed and predicted responses are given by the next four columns. For example, with a cutpoint of 0.5, 4 events and 16 nonevents were classified correctly. On the other hand, 2 nonevents were incorrectly classified as events and 5 events were incorrectly classified as nonevents. For this cutpoint, the correct classification rate is  $20/27$  ( $=74.1\%$ ), which is given in the sixth column. Accuracy of the classification is summarized by the sensitivity, specificity, and false positive and negative rates, which are displayed in the last four columns. You can control the number of cutpoints used, and their values, by using the `PPROB=` option.

## Example 54.2: Logistic Modeling with Categorical Predictors

Consider a study of the analgesic effects of treatments on elderly patients with neuralgia. Two test treatments and a placebo are compared. The response variable is whether the patient reported pain or not. Researchers recorded the age and gender of 60 patients and the duration of complaint before the treatment began. The following DATA step creates the data set Neuralgia:

```
data Neuralgia;
 input Treatment $ Sex $ Age Duration Pain $ @@;
 datalines;
P F 68 1 No B M 74 16 No P F 67 30 No
P M 66 26 Yes B F 67 28 No B F 77 16 No
A F 71 12 No B F 72 50 No B F 76 9 Yes
A M 71 17 Yes A F 63 27 No A F 69 18 Yes
B F 66 12 No A M 62 42 No P F 64 1 Yes
A F 64 17 No P M 74 4 No A F 72 25 No
P M 70 1 Yes B M 66 19 No B M 59 29 No
A F 64 30 No A M 70 28 No A M 69 1 No
B F 78 1 No P M 83 1 Yes B F 69 42 No
B M 75 30 Yes P M 77 29 Yes P F 79 20 Yes
A M 70 12 No A F 69 12 No B F 65 14 No
B M 70 1 No B M 67 23 No A M 76 25 Yes
P M 78 12 Yes B M 77 1 Yes B F 69 24 No
P M 66 4 Yes P F 65 29 No P M 60 26 Yes
A M 78 15 Yes B M 75 21 Yes A F 67 11 No
P F 72 27 No P F 70 13 Yes A M 75 6 Yes
B F 65 7 No P F 68 27 Yes P M 68 11 Yes
P M 67 17 Yes B M 70 22 No A M 65 15 No
P F 67 1 Yes A M 67 10 No P F 72 11 Yes
A F 74 1 No B M 80 21 Yes A F 69 3 No
;
```

The data set Neuralgia contains five variables: Treatment, Sex, Age, Duration, and Pain. The last variable, Pain, is the response variable. A specification of Pain=Yes indicates there was pain, and Pain=No indicates no pain. The variable Treatment is a categorical variable with three levels: A and B represent the two test treatments, and P represents the placebo treatment. The gender of the patients is given by the categorical variable Sex. The variable Age is the age of the patients, in years, when treatment began. The duration of complaint, in months, before the treatment began is given by the variable Duration.

The following statements use the LOGISTIC procedure to fit a two-way logit with interaction model for the effect of Treatment and Sex, with Age and Duration as covariates. The categorical variables Treatment and

Sex are declared in the `CLASS` statement.

```
proc logistic data=Neuralgia;
 class Treatment Sex;
 model Pain= Treatment Sex Treatment*Sex Age Duration / expb;
run;
```

In this analysis, PROC LOGISTIC models the probability of no pain (Pain=No). By default, effect coding is used to represent the CLASS variables. Two design variables are created for Treatment and one for Sex, as shown in [Output 54.2.1](#).

**Output 54.2.1** Effect Coding of CLASS Variables

| The LOGISTIC Procedure  |       |                  |    |
|-------------------------|-------|------------------|----|
| Class Level Information |       |                  |    |
| Class                   | Value | Design Variables |    |
| Treatment               | A     | 1                | 0  |
|                         | B     | 0                | 1  |
|                         | P     | -1               | -1 |
| Sex                     | F     | 1                |    |
|                         | M     | -1               |    |

PROC LOGISTIC displays a table of the Type 3 analysis of effects based on the Wald test ([Output 54.2.2](#)). Note that the Treatment\*Sex interaction and the duration of complaint are not statistically significant ( $p = 0.9318$  and  $p = 0.8752$ , respectively). This indicates that there is no evidence that the treatments affect pain differently in men and women, and no evidence that the pain outcome is related to the duration of pain.

**Output 54.2.2** Wald Tests of Individual Effects

| Type 3 Analysis of Effects |    |                 |            |
|----------------------------|----|-----------------|------------|
| Effect                     | DF | Wald Chi-Square | Pr > ChiSq |
| Treatment                  | 2  | 11.9886         | 0.0025     |
| Sex                        | 1  | 5.3104          | 0.0212     |
| Treatment*Sex              | 2  | 0.1412          | 0.9318     |
| Age                        | 1  | 7.2744          | 0.0070     |
| Duration                   | 1  | 0.0247          | 0.8752     |

Parameter estimates are displayed in [Output 54.2.3](#). The Exp(Est) column contains the exponentiated parameter estimates requested with the `EXPB` option. These values can, but do not necessarily, represent odds ratios for the corresponding variables. For continuous explanatory variables, the Exp(Est) value corresponds to the odds ratio for a unit increase of the corresponding variable. For CLASS variables that use effect coding, the Exp(Est) values have no direct interpretation as a comparison of levels. However, when

the reference coding is used, the Exp(Est) values represent the odds ratio between the corresponding level and the reference level. Following the parameter estimates table, PROC LOGISTIC displays the odds ratio estimates for those variables that are not involved in any interaction terms. If the variable is a CLASS variable, the odds ratio estimate comparing each level with the reference level is computed regardless of the coding scheme. In this analysis, since the model contains the Treatment\*Sex interaction term, the odds ratios for Treatment and Sex were not computed. The odds ratio estimates for Age and Duration are precisely the values given in the Exp(Est) column in the parameter estimates table.

### Output 54.2.3 Parameter Estimates with Effect Coding

| Analysis of Maximum Likelihood Estimates |    |          |                |                 |            |          |
|------------------------------------------|----|----------|----------------|-----------------|------------|----------|
| Parameter                                | DF | Estimate | Standard Error | Wald Chi-Square | Pr > ChiSq | Exp(Est) |
| Intercept                                | 1  | 19.2236  | 7.1315         | 7.2661          | 0.0070     | 2.232E8  |
| Treatment A                              | 1  | 0.8483   | 0.5502         | 2.3773          | 0.1231     | 2.336    |
| Treatment B                              | 1  | 1.4949   | 0.6622         | 5.0956          | 0.0240     | 4.459    |
| Sex F                                    | 1  | 0.9173   | 0.3981         | 5.3104          | 0.0212     | 2.503    |
| Treatment*Sex A F                        | 1  | -0.2010  | 0.5568         | 0.1304          | 0.7180     | 0.818    |
| Treatment*Sex B F                        | 1  | 0.0487   | 0.5563         | 0.0077          | 0.9302     | 1.050    |
| Age                                      | 1  | -0.2688  | 0.0996         | 7.2744          | 0.0070     | 0.764    |
| Duration                                 | 1  | 0.00523  | 0.0333         | 0.0247          | 0.8752     | 1.005    |

| Odds Ratio Estimates |                |                            |       |
|----------------------|----------------|----------------------------|-------|
| Effect               | Point Estimate | 95% Wald Confidence Limits |       |
| Age                  | 0.764          | 0.629                      | 0.929 |
| Duration             | 1.005          | 0.942                      | 1.073 |

The following PROC LOGISTIC statements illustrate the use of forward selection on the data set Neuralgia to identify the effects that differentiate the two Pain responses. The option **SELECTION=FORWARD** is specified to carry out the forward selection. The term Treatment|Sex@2 illustrates another way to specify main effects and two-way interactions. (Note that, in this case, the “@2” is unnecessary because no interactions besides the two-way interaction are possible).

```
proc logistic data=Neuralgia;
 class Treatment Sex;
 model Pain=Treatment|Sex@2 Age Duration
 /selection=forward expb;
run;
```

Results of the forward selection process are summarized in [Output 54.2.4](#). The variable Treatment is selected first, followed by Age and then Sex. The results are consistent with the previous analysis ([Output 54.2.2](#)) in which the Treatment\*Sex interaction and Duration are not statistically significant.

**Output 54.2.4** Effects Selected into the Model

| The LOGISTIC Procedure       |                |    |           |                  |            |
|------------------------------|----------------|----|-----------|------------------|------------|
| Summary of Forward Selection |                |    |           |                  |            |
| Step                         | Effect Entered | DF | Number In | Score Chi-Square | Pr > ChiSq |
| 1                            | Treatment      | 2  | 1         | 13.7143          | 0.0011     |
| 2                            | Age            | 1  | 2         | 10.6038          | 0.0011     |
| 3                            | Sex            | 1  | 3         | 5.9959           | 0.0143     |

Output 54.2.5 shows the Type 3 analysis of effects, the parameter estimates, and the odds ratio estimates for the selected model. All three variables, Treatment, Age, and Sex, are statistically significant at the 0.05 level ( $p=0.0018$ ,  $p=0.0213$ , and  $p=0.0057$ , respectively). Since the selected model does not contain the Treatment\*Sex interaction, odds ratios for Treatment and Sex are computed. The estimated odds ratio is 24.022 for treatment A versus placebo, 41.528 for Treatment B versus placebo, and 6.194 for female patients versus male patients. Note that these odds ratio estimates are not the same as the corresponding values in the Exp(Est) column in the parameter estimates table because effect coding was used. From Output 54.2.5, it is evident that both Treatment A and Treatment B are better than the placebo in reducing pain; females tend to have better improvement than males; and younger patients are faring better than older patients.

**Output 54.2.5** Type 3 Effects and Parameter Estimates with Effect Coding

| Type 3 Analysis of Effects |    |                 |            |  |  |  |
|----------------------------|----|-----------------|------------|--|--|--|
| Effect                     | DF | Wald Chi-Square | Pr > ChiSq |  |  |  |
| Treatment                  | 2  | 12.6928         | 0.0018     |  |  |  |
| Sex                        | 1  | 5.3013          | 0.0213     |  |  |  |
| Age                        | 1  | 7.6314          | 0.0057     |  |  |  |

| Analysis of Maximum Likelihood Estimates |    |          |                |                 |            |          |
|------------------------------------------|----|----------|----------------|-----------------|------------|----------|
| Parameter                                | DF | Estimate | Standard Error | Wald Chi-Square | Pr > ChiSq | Exp(Est) |
| Intercept                                | 1  | 19.0804  | 6.7882         | 7.9007          | 0.0049     | 1.9343E8 |
| Treatment A                              | 1  | 0.8772   | 0.5274         | 2.7662          | 0.0963     | 2.404    |
| Treatment B                              | 1  | 1.4246   | 0.6036         | 5.5711          | 0.0183     | 4.156    |
| Sex F                                    | 1  | 0.9118   | 0.3960         | 5.3013          | 0.0213     | 2.489    |
| Age                                      | 1  | -0.2650  | 0.0959         | 7.6314          | 0.0057     | 0.767    |

Output 54.2.5 continued

| Odds Ratio Estimates |                |                            |         |
|----------------------|----------------|----------------------------|---------|
| Effect               | Point Estimate | 95% Wald Confidence Limits |         |
| Treatment A vs P     | 24.022         | 3.295                      | 175.121 |
| Treatment B vs P     | 41.528         | 4.500                      | 383.262 |
| Sex F vs M           | 6.194          | 1.312                      | 29.248  |
| Age                  | 0.767          | 0.636                      | 0.926   |

Finally, the following statements refit the previously selected model, except that reference coding is used for the CLASS variables instead of effect coding:

```
ods graphics on;
proc logistic data=Neuralgia plots (only)=(oddsratio(range=clip));
 class Treatment Sex /param=ref;
 model Pain= Treatment Sex Age;
 oddsratio Treatment;
 oddsratio Sex;
 oddsratio Age;
 contrast 'Pairwise A vs P' Treatment 1 0 / estimate=exp;
 contrast 'Pairwise B vs P' Treatment 0 1 / estimate=exp;
 contrast 'Pairwise A vs B' Treatment 1 -1 / estimate=exp;
 contrast 'Female vs Male' Sex 1 / estimate=exp;
 effectplot / at(Sex=all) noobs;
 effectplot slicefit(sliceby=Sex plotby=Treatment) / noobs;
run;
ods graphics off;
```

The **ODDSRATIO** statements compute the odds ratios for the covariates. Four **CONTRAST** statements are specified; they provide another method of producing the odds ratios. The three contrasts labeled ‘Pairwise’ specify a contrast vector,  $L$ , for each of the pairwise comparisons between the three levels of Treatment. The contrast labeled ‘Female vs Male’ compares female to male patients. The option **ESTIMATE=EXP** is specified in all **CONTRAST** statements to exponentiate the estimates of  $L'\beta$ . With the given specification of contrast coefficients, the first of the ‘Pairwise’ **CONTRAST** statements corresponds to the odds ratio of A versus P, the second corresponds to B versus P, and the third corresponds to A versus B. You can also specify the ‘Pairwise’ contrasts in a single contrast statement with three rows. The ‘Female vs Male’ **CONTRAST** statement corresponds to the odds ratio that compares female to male patients.

The **PLOTS(ONLY)=** option displays only the requested odds ratio plot when ODS Graphics is enabled. The **EFFECTPLOT** statements do not honor the **ONLY** option, and display the fitted model. The first **EFFECTPLOT** statement by default produces a plot of the predicted values against the continuous Age variable, grouped by the Treatment levels. The **AT** option produces one plot for males and another for females; the **NOOBS** option suppresses the display of the observations. In the second **EFFECTPLOT** statement, a **SLICEFIT** plot is specified to display the Age variable on the X axis, the fits are grouped by the Sex levels, and the **PLOTBY=** option produces a panel of plots that displays each level of the Treatment variable.

The reference coding is shown in [Output 54.2.6](#). The Type 3 analysis of effects, the parameter estimates for the reference coding, and the odds ratio estimates are displayed in [Output 54.2.7](#). Although the parameter

estimates are different because of the different parameterizations, the “Type 3 Analysis of Effects” table and the “Odds Ratio” table remain the same as in [Output 54.2.5](#). With effect coding, the treatment A parameter estimate (0.8772) estimates the effect of treatment A compared to the average effect of treatments A, B, and placebo. The treatment A estimate (3.1790) under the reference coding estimates the difference in effect of treatment A and the placebo treatment.

**Output 54.2.6** Reference Coding of CLASS Variables

| The LOGISTIC Procedure  |       |                  |   |
|-------------------------|-------|------------------|---|
| Class Level Information |       |                  |   |
| Class                   | Value | Design Variables |   |
| Treatment               | A     | 1                | 0 |
|                         | B     | 0                | 1 |
|                         | P     | 0                | 0 |
| Sex                     | F     | 1                |   |
|                         | M     | 0                |   |

**Output 54.2.7** Type 3 Effects and Parameter Estimates with Reference Coding

| Type 3 Analysis of Effects |    |                 |            |
|----------------------------|----|-----------------|------------|
| Effect                     | DF | Wald Chi-Square | Pr > ChiSq |
| Treatment                  | 2  | 12.6928         | 0.0018     |
| Sex                        | 1  | 5.3013          | 0.0213     |
| Age                        | 1  | 7.6314          | 0.0057     |

| Analysis of Maximum Likelihood Estimates |    |          |                |                 |            |
|------------------------------------------|----|----------|----------------|-----------------|------------|
| Parameter                                | DF | Estimate | Standard Error | Wald Chi-Square | Pr > ChiSq |
| Intercept                                | 1  | 15.8669  | 6.4056         | 6.1357          | 0.0132     |
| Treatment A                              | 1  | 3.1790   | 1.0135         | 9.8375          | 0.0017     |
| Treatment B                              | 1  | 3.7264   | 1.1339         | 10.8006         | 0.0010     |
| Sex F                                    | 1  | 1.8235   | 0.7920         | 5.3013          | 0.0213     |
| Age                                      | 1  | -0.2650  | 0.0959         | 7.6314          | 0.0057     |

The **ODDSRATIO** statement results are shown in [Output 54.2.8](#), and the resulting plot is displayed in [Output 54.2.9](#). Note in [Output 54.2.9](#) that the odds ratio confidence limits are truncated due to specifying the **RANGE=CLIP** option; this enables you to see which intervals contain “1” more clearly. The odds ratios are identical to those shown in the “Odds Ratio Estimates” table in [Output 54.2.7](#) with the addition of the odds ratio for “Treatment A vs B”. Both treatments A and B are highly effective over placebo in reducing pain, as can be seen from the odds ratios comparing treatment A against P and treatment B against P (the second

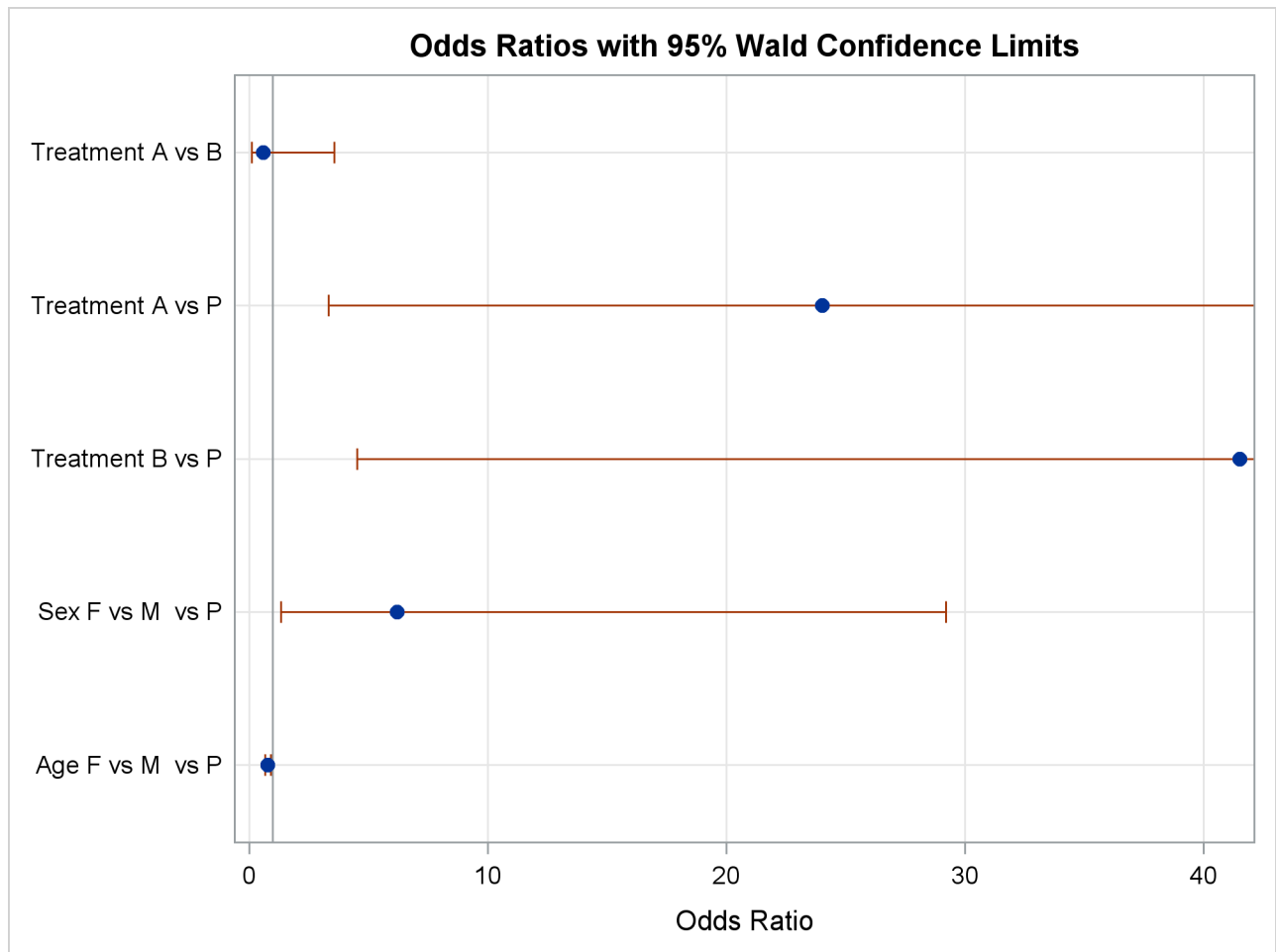


and third rows in the table). However, the 95% confidence interval for the odds ratio comparing treatment A to B is (0.0932, 3.5889), indicating that the pain reduction effects of these two test treatments are not very different. Again, the 'Sex F vs M' odds ratio shows that female patients fared better in obtaining relief from pain than male patients. The odds ratio for Age shows that a patient one year older is 0.77 times as likely to show no pain; that is, younger patients have more improvement than older patients.

**Output 54.2.8** Results from the ODDS RATIO Statements

| Odds Ratio Estimates and Wald Confidence Intervals |          |                       |         |
|----------------------------------------------------|----------|-----------------------|---------|
| Label                                              | Estimate | 95% Confidence Limits |         |
| Treatment A vs B                                   | 0.578    | 0.093                 | 3.589   |
| Treatment A vs P                                   | 24.022   | 3.295                 | 175.121 |
| Treatment B vs P                                   | 41.528   | 4.500                 | 383.262 |
| Sex F vs M                                         | 6.194    | 1.312                 | 29.248  |
| Age                                                | 0.767    | 0.636                 | 0.926   |

**Output 54.2.9** Plot of the ODDS RATIO Statement Results



Output 54.2.10 contains two tables: the “Contrast Test Results” table and the “Contrast Estimation and Testing Results by Row” table. The former contains the overall Wald test for each CONTRAST statement. The latter table contains estimates and tests of individual contrast rows. The estimates for the first two rows of the ‘Pairwise’ CONTRAST statements are the same as those given in the two preceding odds ratio tables (Output 54.2.7 and Output 54.2.8). The third row estimates the odds ratio comparing A to B, agreeing with Output 54.2.8, and the last row computes the odds ratio comparing pain relief for females to that for males.

**Output 54.2.10** Results of CONTRAST Statements

| Contrast Test Results |    |                    |            |  |  |  |
|-----------------------|----|--------------------|------------|--|--|--|
| Contrast              | DF | Wald<br>Chi-Square | Pr > ChiSq |  |  |  |
| Pairwise A vs P       | 1  | 9.8375             | 0.0017     |  |  |  |
| Pairwise B vs P       | 1  | 10.8006            | 0.0010     |  |  |  |
| Pairwise A vs B       | 1  | 0.3455             | 0.5567     |  |  |  |
| Female vs Male        | 1  | 5.3013             | 0.0213     |  |  |  |

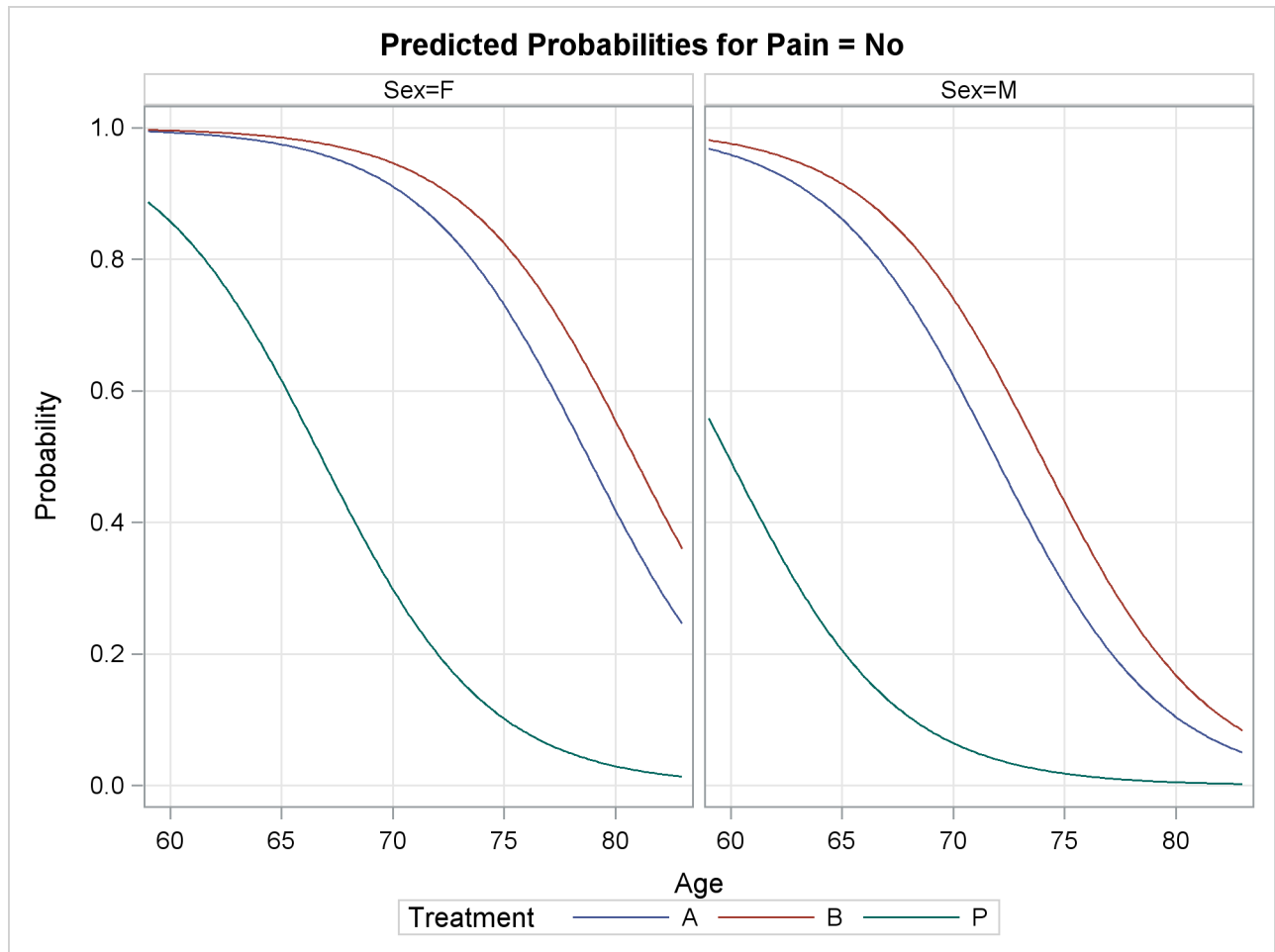
| Contrast Estimation and Testing Results by Row |      |     |          |                   |       |                   |         |
|------------------------------------------------|------|-----|----------|-------------------|-------|-------------------|---------|
| Contrast                                       | Type | Row | Estimate | Standard<br>Error | Alpha | Confidence Limits |         |
| Pairwise A vs P                                | EXP  | 1   | 24.0218  | 24.3473           | 0.05  | 3.2951            | 175.1   |
| Pairwise B vs P                                | EXP  | 1   | 41.5284  | 47.0877           | 0.05  | 4.4998            | 383.3   |
| Pairwise A vs B                                | EXP  | 1   | 0.5784   | 0.5387            | 0.05  | 0.0932            | 3.5889  |
| Female vs Male                                 | EXP  | 1   | 6.1937   | 4.9053            | 0.05  | 1.3116            | 29.2476 |

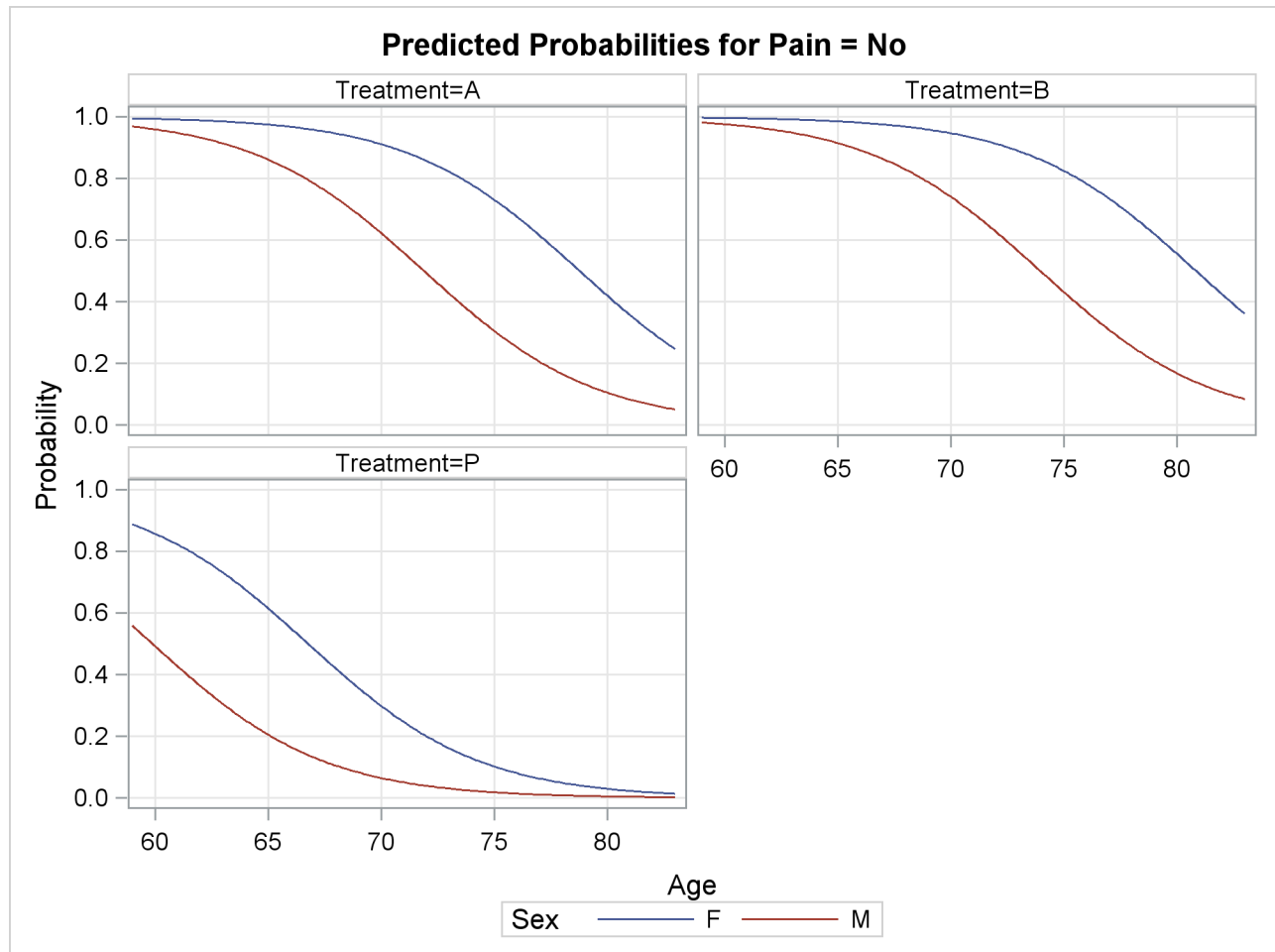
  

| Contrast Estimation and Testing Results by Row |      |     |                    |            |  |  |
|------------------------------------------------|------|-----|--------------------|------------|--|--|
| Contrast                                       | Type | Row | Wald<br>Chi-Square | Pr > ChiSq |  |  |
| Pairwise A vs P                                | EXP  | 1   | 9.8375             | 0.0017     |  |  |
| Pairwise B vs P                                | EXP  | 1   | 10.8006            | 0.0010     |  |  |
| Pairwise A vs B                                | EXP  | 1   | 0.3455             | 0.5567     |  |  |
| Female vs Male                                 | EXP  | 1   | 5.3013             | 0.0213     |  |  |

ANCOVA-style plots of the model-predicted probabilities against the Age variable for each combination of Treatment and Sex are displayed in Output 54.2.11 and Output 54.2.12. These plots confirm that females always have a higher probability of pain reduction in each treatment group, the placebo treatment has a lower probability of success than the other treatments, and younger patients respond to treatment better than older patients.

**Output 54.2.11** Model-Predicted Probabilities by Sex



**Output 54.2.12** Model-Predicted Probabilities by Treatment

### Example 54.3: Ordinal Logistic Regression

Consider a study of the effects on taste of various cheese additives. Researchers tested four cheese additives and obtained 52 response ratings for each additive. Each response was measured on a scale of nine categories ranging from strong dislike (1) to excellent taste (9). The data, given in McCullagh and Nelder (1989, p. 175) in the form of a two-way frequency table of additive by rating, are saved in the data set `Cheese` by using the following program. The variable `y` contains the response rating. The variable `Additive` specifies the cheese additive (1, 2, 3, or 4). The variable `freq` gives the frequency with which each additive received each rating.

```
data Cheese;
 do Additive = 1 to 4;
 do y = 1 to 9;
 input freq @@;
 output;
 end;
 end;
 label y='Taste Rating';
 datalines;
```

```

0 0 1 7 8 8 19 8 1
6 9 12 11 7 6 1 0 0
1 1 6 8 23 7 5 1 0
0 0 0 1 3 7 14 16 11
;

```

The response variable  $y$  is ordinally scaled. A cumulative logit model is used to investigate the effects of the cheese additives on taste. The following statements invoke PROC LOGISTIC to fit this model with  $y$  as the response variable and three indicator variables as explanatory variables, with the fourth additive as the reference level. With this parameterization, each Additive parameter compares an additive to the fourth additive. The COVB option displays the estimated covariance matrix. The ODDSRATIO statement computes odds ratios for all combinations of the Additive levels. The PLOTS option produces a graphical display of the odds ratios, and the EFFECTPLOT statement displays the predicted probabilities.

```

ods graphics on;
proc logistic data=Cheese plots(only)=oddsratio(range=clip);
 freq freq;
 class Additive (param=ref ref='4');
 model y=Additive / covb;
 oddsratio Additive;
 effectplot / polybar;
 title 'Multiple Response Cheese Tasting Experiment';
run;
ods graphics off;

```

The “Response Profile” table in [Output 54.3.1](#) shows that the strong dislike ( $y=1$ ) end of the rating scale is associated with lower Ordered Values in the “Response Profile” table; hence the probability of disliking the additives is modeled.

The score chi-square for testing the proportional odds assumption is 17.287, which is not significant with respect to a chi-square distribution with 21 degrees of freedom ( $p = 0.694$ ). This indicates that the proportional odds assumption is reasonable. The positive value (1.6128) for the parameter estimate for Additive1 indicates a tendency toward the lower-numbered categories of the first cheese additive relative to the fourth. In other words, the fourth additive tastes better than the first additive. The second and third additives are both less favorable than the fourth additive. The relative magnitudes of these slope estimates imply the preference ordering: fourth, first, third, second.

### Output 54.3.1 Proportional Odds Model Regression Analysis

| Multiple Response Cheese Tasting Experiment |                  |              |
|---------------------------------------------|------------------|--------------|
| The LOGISTIC Procedure                      |                  |              |
| Model Information                           |                  |              |
| Data Set                                    | WORK.CHEESE      |              |
| Response Variable                           | y                | Taste Rating |
| Number of Response Levels                   | 9                |              |
| Frequency Variable                          | freq             |              |
| Model                                       | cumulative logit |              |
| Optimization Technique                      | Fisher's scoring |              |

**Output 54.3.1** *continued*

|                             |     |
|-----------------------------|-----|
| Number of Observations Read | 36  |
| Number of Observations Used | 28  |
| Sum of Frequencies Read     | 208 |
| Sum of Frequencies Used     | 208 |

Response Profile

| Ordered Value | y | Total Frequency |
|---------------|---|-----------------|
| 1             | 1 | 7               |
| 2             | 2 | 10              |
| 3             | 3 | 19              |
| 4             | 4 | 27              |
| 5             | 5 | 41              |
| 6             | 6 | 28              |
| 7             | 7 | 39              |
| 8             | 8 | 25              |
| 9             | 9 | 12              |

Probabilities modeled are cumulated over the lower Ordered Values.

NOTE: 8 observations having nonpositive frequencies or weights were excluded since they do not contribute to the analysis.

Class Level Information

| Class    | Value | Design Variables |   |   |
|----------|-------|------------------|---|---|
| Additive | 1     | 1                | 0 | 0 |
|          | 2     | 0                | 1 | 0 |
|          | 3     | 0                | 0 | 1 |
|          | 4     | 0                | 0 | 0 |

Model Convergence Status

Convergence criterion (GCONV=1E-8) satisfied.

Score Test for the Proportional Odds Assumption

| Chi-Square | DF | Pr > ChiSq |
|------------|----|------------|
| 17.2866    | 21 | 0.6936     |

## Output 54.3.1 continued

| Model Fit Statistics                                          |                |                          |                |                 |            |
|---------------------------------------------------------------|----------------|--------------------------|----------------|-----------------|------------|
| Criterion                                                     | Intercept Only | Intercept and Covariates |                |                 |            |
| AIC                                                           | 875.802        | 733.348                  |                |                 |            |
| SC                                                            | 902.502        | 770.061                  |                |                 |            |
| -2 Log L                                                      | 859.802        | 711.348                  |                |                 |            |
| Testing Global Null Hypothesis: BETA=0                        |                |                          |                |                 |            |
| Test                                                          | Chi-Square     | DF                       | Pr > ChiSq     |                 |            |
| Likelihood Ratio                                              | 148.4539       | 3                        | <.0001         |                 |            |
| Score                                                         | 111.2670       | 3                        | <.0001         |                 |            |
| Wald                                                          | 115.1504       | 3                        | <.0001         |                 |            |
| Type 3 Analysis of Effects                                    |                |                          |                |                 |            |
| Effect                                                        | DF             | Wald Chi-Square          | Pr > ChiSq     |                 |            |
| Additive                                                      | 3              | 115.1504                 | <.0001         |                 |            |
| Analysis of Maximum Likelihood Estimates                      |                |                          |                |                 |            |
| Parameter                                                     | DF             | Estimate                 | Standard Error | Wald Chi-Square | Pr > ChiSq |
| Intercept 1                                                   | 1              | -7.0801                  | 0.5624         | 158.4851        | <.0001     |
| Intercept 2                                                   | 1              | -6.0249                  | 0.4755         | 160.5500        | <.0001     |
| Intercept 3                                                   | 1              | -4.9254                  | 0.4272         | 132.9484        | <.0001     |
| Intercept 4                                                   | 1              | -3.8568                  | 0.3902         | 97.7087         | <.0001     |
| Intercept 5                                                   | 1              | -2.5205                  | 0.3431         | 53.9704         | <.0001     |
| Intercept 6                                                   | 1              | -1.5685                  | 0.3086         | 25.8374         | <.0001     |
| Intercept 7                                                   | 1              | -0.0669                  | 0.2658         | 0.0633          | 0.8013     |
| Intercept 8                                                   | 1              | 1.4930                   | 0.3310         | 20.3439         | <.0001     |
| Additive 1                                                    | 1              | 1.6128                   | 0.3778         | 18.2265         | <.0001     |
| Additive 2                                                    | 1              | 4.9645                   | 0.4741         | 109.6427        | <.0001     |
| Additive 3                                                    | 1              | 3.3227                   | 0.4251         | 61.0931         | <.0001     |
| Association of Predicted Probabilities and Observed Responses |                |                          |                |                 |            |
| Percent Concordant                                            | 67.6           | Somers' D                | 0.578          |                 |            |
| Percent Discordant                                            | 9.8            | Gamma                    | 0.746          |                 |            |
| Percent Tied                                                  | 22.6           | Tau-a                    | 0.500          |                 |            |
| Pairs                                                         | 18635          | c                        | 0.789          |                 |            |

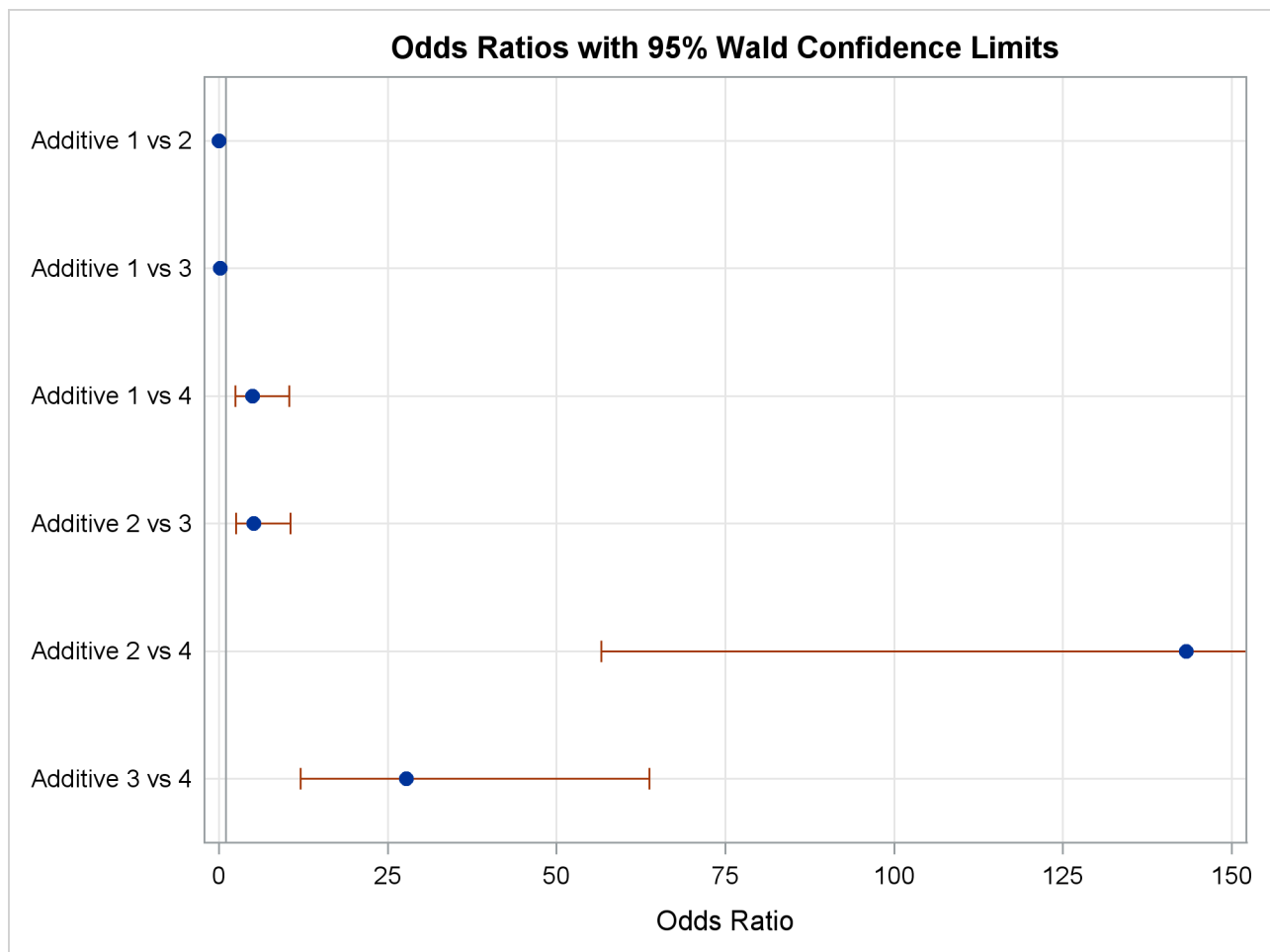
The odds ratio results in [Output 54.3.2](#) show the preferences more clearly. For example, the “Additive 1 vs 4” odds ratio says that the first additive has 5.017 times the odds of receiving a lower score than the fourth

additive; that is, the first additive is 5.017 times more likely than the fourth additive to receive a lower score. [Output 54.3.3](#) displays the odds ratios graphically; the range of the confidence limits is truncated by the `RANGE=CLIP` option, so you can see that “1” is not contained in any of the intervals.

**Output 54.3.2** Odds Ratios of All Pairs of Additive Levels

| Odds Ratio Estimates and Wald Confidence Intervals |          |                       |         |
|----------------------------------------------------|----------|-----------------------|---------|
| Label                                              | Estimate | 95% Confidence Limits |         |
| Additive 1 vs 2                                    | 0.035    | 0.015                 | 0.080   |
| Additive 1 vs 3                                    | 0.181    | 0.087                 | 0.376   |
| Additive 1 vs 4                                    | 5.017    | 2.393                 | 10.520  |
| Additive 2 vs 3                                    | 5.165    | 2.482                 | 10.746  |
| Additive 2 vs 4                                    | 143.241  | 56.558                | 362.777 |
| Additive 3 vs 4                                    | 27.734   | 12.055                | 63.805  |

**Output 54.3.3** Plot of Odds Ratios for Additive



The estimated covariance matrix of the parameters is displayed in [Output 54.3.4](#).



**Output 54.3.4** Estimated Covariance Matrix

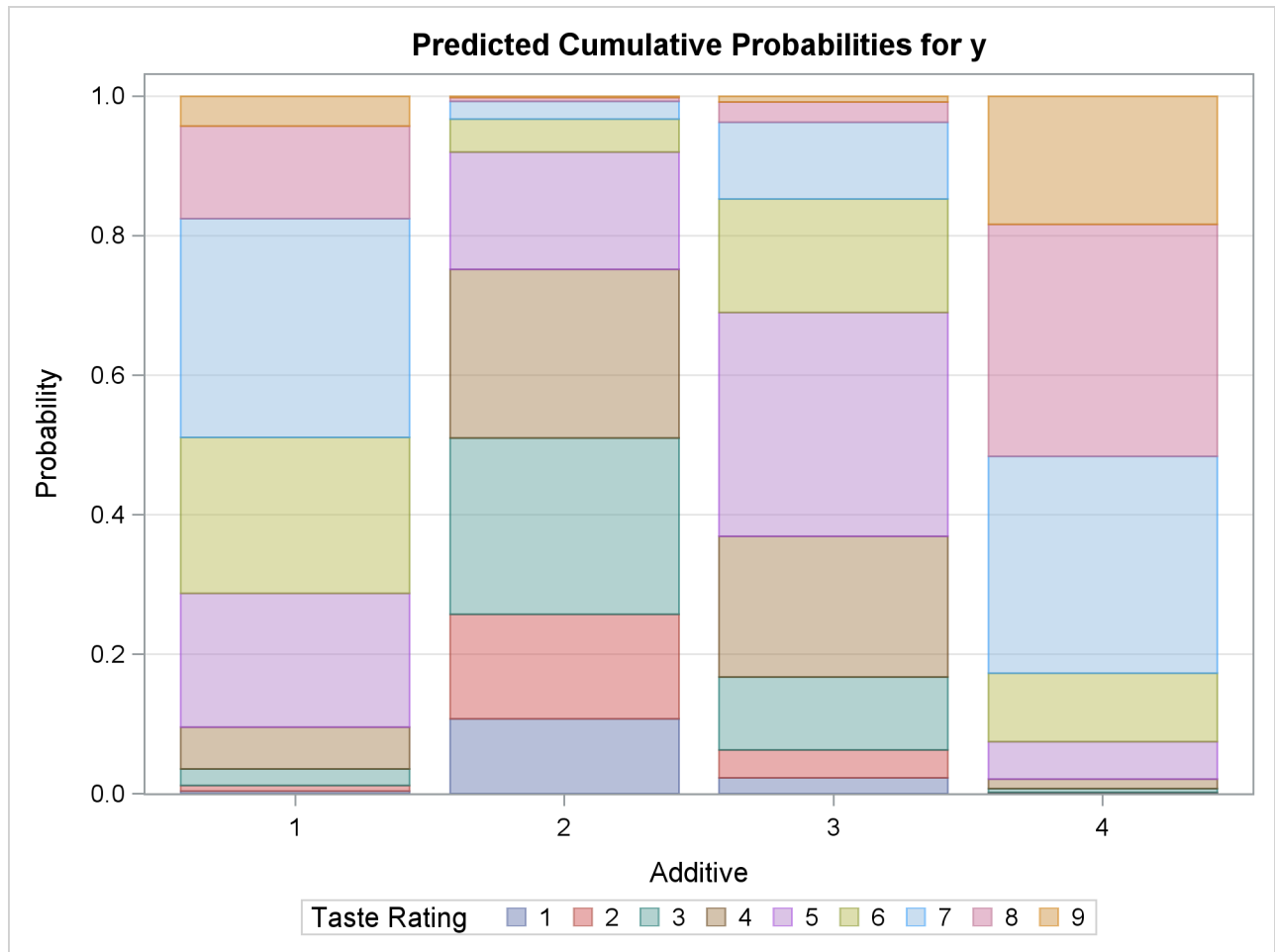
| Estimated Covariance Matrix |                 |                 |                 |                 |                 |
|-----------------------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| Parameter                   | Intercept_<br>1 | Intercept_<br>2 | Intercept_<br>3 | Intercept_<br>4 | Intercept_<br>5 |
| Intercept_1                 | 0.316291        | 0.219581        | 0.176278        | 0.147694        | 0.114024        |
| Intercept_2                 | 0.219581        | 0.226095        | 0.177806        | 0.147933        | 0.11403         |
| Intercept_3                 | 0.176278        | 0.177806        | 0.182473        | 0.148844        | 0.114092        |
| Intercept_4                 | 0.147694        | 0.147933        | 0.148844        | 0.152235        | 0.114512        |
| Intercept_5                 | 0.114024        | 0.11403         | 0.114092        | 0.114512        | 0.117713        |
| Intercept_6                 | 0.091085        | 0.091081        | 0.091074        | 0.091109        | 0.091821        |
| Intercept_7                 | 0.057814        | 0.057813        | 0.057807        | 0.05778         | 0.057721        |
| Intercept_8                 | 0.041304        | 0.041304        | 0.0413          | 0.041277        | 0.041162        |
| Additive1                   | -0.09419        | -0.09421        | -0.09427        | -0.09428        | -0.09246        |
| Additive2                   | -0.18686        | -0.18161        | -0.1687         | -0.14717        | -0.11415        |
| Additive3                   | -0.13565        | -0.13569        | -0.1352         | -0.13118        | -0.11207        |

| Estimated Covariance Matrix |                 |                 |                 |           |           |           |
|-----------------------------|-----------------|-----------------|-----------------|-----------|-----------|-----------|
| Parameter                   | Intercept_<br>6 | Intercept_<br>7 | Intercept_<br>8 | Additive1 | Additive2 | Additive3 |
| Intercept_1                 | 0.091085        | 0.057814        | 0.041304        | -0.09419  | -0.18686  | -0.13565  |
| Intercept_2                 | 0.091081        | 0.057813        | 0.041304        | -0.09421  | -0.18161  | -0.13569  |
| Intercept_3                 | 0.091074        | 0.057807        | 0.0413          | -0.09427  | -0.1687   | -0.1352   |
| Intercept_4                 | 0.091109        | 0.05778         | 0.041277        | -0.09428  | -0.14717  | -0.13118  |
| Intercept_5                 | 0.091821        | 0.057721        | 0.041162        | -0.09246  | -0.11415  | -0.11207  |
| Intercept_6                 | 0.09522         | 0.058312        | 0.041324        | -0.08521  | -0.09113  | -0.09122  |
| Intercept_7                 | 0.058312        | 0.07064         | 0.04878         | -0.06041  | -0.05781  | -0.05802  |
| Intercept_8                 | 0.041324        | 0.04878         | 0.109562        | -0.04436  | -0.0413   | -0.04143  |
| Additive1                   | -0.08521        | -0.06041        | -0.04436        | 0.142715  | 0.094072  | 0.092128  |
| Additive2                   | -0.09113        | -0.05781        | -0.0413         | 0.094072  | 0.22479   | 0.132877  |
| Additive3                   | -0.09122        | -0.05802        | -0.04143        | 0.092128  | 0.132877  | 0.180709  |

Output 54.3.5 displays the probability of each taste rating  $y$  within each additive. You can see that Additive=1 mostly receives ratings of 5 to 7, Additive=2 mostly receives ratings of 2 to 5, Additive=3 mostly receives ratings of 4 to 6, and Additive=4 mostly receives ratings of 7 to 9, which also confirms the previously discussed preference orderings.

**Output 54.3.5** Model-Predicted Probabilities



### Example 54.4: Nominal Response Data: Generalized Logits Model

Over the course of one school year, third graders from three different schools are exposed to three different styles of mathematics instruction: a self-paced computer-learning style, a team approach, and a traditional class approach. The students are asked which style they prefer and their responses, classified by the type of program they are in (a regular school day versus a regular day supplemented with an afternoon school program), are displayed in Table 54.15. The data set is from Stokes, Davis, and Koch (2012), and is also analyzed in the section “Generalized Logits Model” on page 1784 of Chapter 30, “The CATMOD Procedure.”

**Table 54.15** School Program Data

| School | Program   | Learning Style Preference |      |       |
|--------|-----------|---------------------------|------|-------|
|        |           | Self                      | Team | Class |
| 1      | Regular   | 10                        | 17   | 26    |
| 1      | Afternoon | 5                         | 12   | 50    |
| 2      | Regular   | 21                        | 17   | 26    |
| 2      | Afternoon | 16                        | 12   | 36    |
| 3      | Regular   | 15                        | 15   | 16    |
| 3      | Afternoon | 12                        | 12   | 20    |

The levels of the response variable (self, team, and class) have no essential ordering, so a logistic regression is performed on the generalized logits. The model to be fit is

$$\log\left(\frac{\pi_{hij}}{\pi_{hir}}\right) = \alpha_j + \mathbf{x}'_{hi}\boldsymbol{\beta}_j$$

where  $\pi_{hij}$  is the probability that a student in school  $h$  and program  $i$  prefers teaching style  $j$ ,  $j \neq r$ , and style  $r$  is the baseline style (in this case, class). There are separate sets of intercept parameters  $\alpha_j$  and regression parameters  $\boldsymbol{\beta}_j$  for each logit, and the vector  $\mathbf{x}_{hi}$  is the set of explanatory variables for the  $h$ th population. Thus, two logits are modeled for each school and program combination: the logit comparing self to class and the logit comparing team to class.

The following statements create the data set `school` and request the analysis. The `LINK=GLOGIT` option forms the generalized logits. The response variable option `ORDER=DATA` means that the response variable levels are ordered as they exist in the data set: self, team, and class; thus, the logits are formed by comparing self to class and by comparing team to class. The `ODDSRATIO` statement produces odds ratios in the presence of interactions, and a graphical display of the requested odds ratios is produced when ODS Graphics is enabled.

```
data school;
 length Program $ 9;
 input School Program $ Style $ Count @@;
 datalines;
1 regular self 10 1 regular team 17 1 regular class 26
1 afternoon self 5 1 afternoon team 12 1 afternoon class 50
2 regular self 21 2 regular team 17 2 regular class 26
2 afternoon self 16 2 afternoon team 12 2 afternoon class 36
3 regular self 15 3 regular team 15 3 regular class 16
3 afternoon self 12 3 afternoon team 12 3 afternoon class 20
;

ods graphics on;
proc logistic data=school;
 freq Count;
 class School Program(ref=first);
 model Style(order=data)=School Program School*Program / link=glogit;
 oddsratio program;
run;
ods graphics off;
```

Summary information about the model, the response variable, and the classification variables are displayed in [Output 54.4.1](#).

**Output 54.4.1** Analysis of Saturated Model

```

The LOGISTIC Procedure

Model Information

Data Set WORK.SCHOOL
Response Variable Style
Number of Response Levels 3
Frequency Variable Count
Model generalized logit
Optimization Technique Newton-Raphson

Number of Observations Read 18
Number of Observations Used 18
Sum of Frequencies Read 338
Sum of Frequencies Used 338

Response Profile

Ordered Value Style Total Frequency
1 self 79
2 team 85
3 class 174

Logits modeled use Style='class' as the reference category.

Class Level Information

Class Value Design Variables
School 1 1 0
 2 0 1
 3 -1 -1

Program afternoon -1
 regular 1

Model Convergence Status

Convergence criterion (GCONV=1E-8) satisfied.

```

The “Testing Global Null Hypothesis: BETA=0” table in [Output 54.4.2](#) shows that the parameters are significantly different from zero.

**Output 54.4.2** Analysis of Saturated Model

| Model Fit Statistics |                   |                                |
|----------------------|-------------------|--------------------------------|
| Criterion            | Intercept<br>Only | Intercept<br>and<br>Covariates |
| AIC                  | 699.404           | 689.156                        |
| SC                   | 707.050           | 735.033                        |
| -2 Log L             | 695.404           | 665.156                        |

| Testing Global Null Hypothesis: BETA=0 |            |    |            |
|----------------------------------------|------------|----|------------|
| Test                                   | Chi-Square | DF | Pr > ChiSq |
| Likelihood Ratio                       | 30.2480    | 10 | 0.0008     |
| Score                                  | 28.3738    | 10 | 0.0016     |
| Wald                                   | 25.6828    | 10 | 0.0042     |

However, the “Type 3 Analysis of Effects” table in [Output 54.4.3](#) shows that the interaction effect is clearly nonsignificant.

**Output 54.4.3** Analysis of Saturated Model

| Type 3 Analysis of Effects |    |                    |            |
|----------------------------|----|--------------------|------------|
| Effect                     | DF | Wald<br>Chi-Square | Pr > ChiSq |
| School                     | 4  | 14.5522            | 0.0057     |
| Program                    | 2  | 10.4815            | 0.0053     |
| School*Program             | 4  | 1.7439             | 0.7827     |

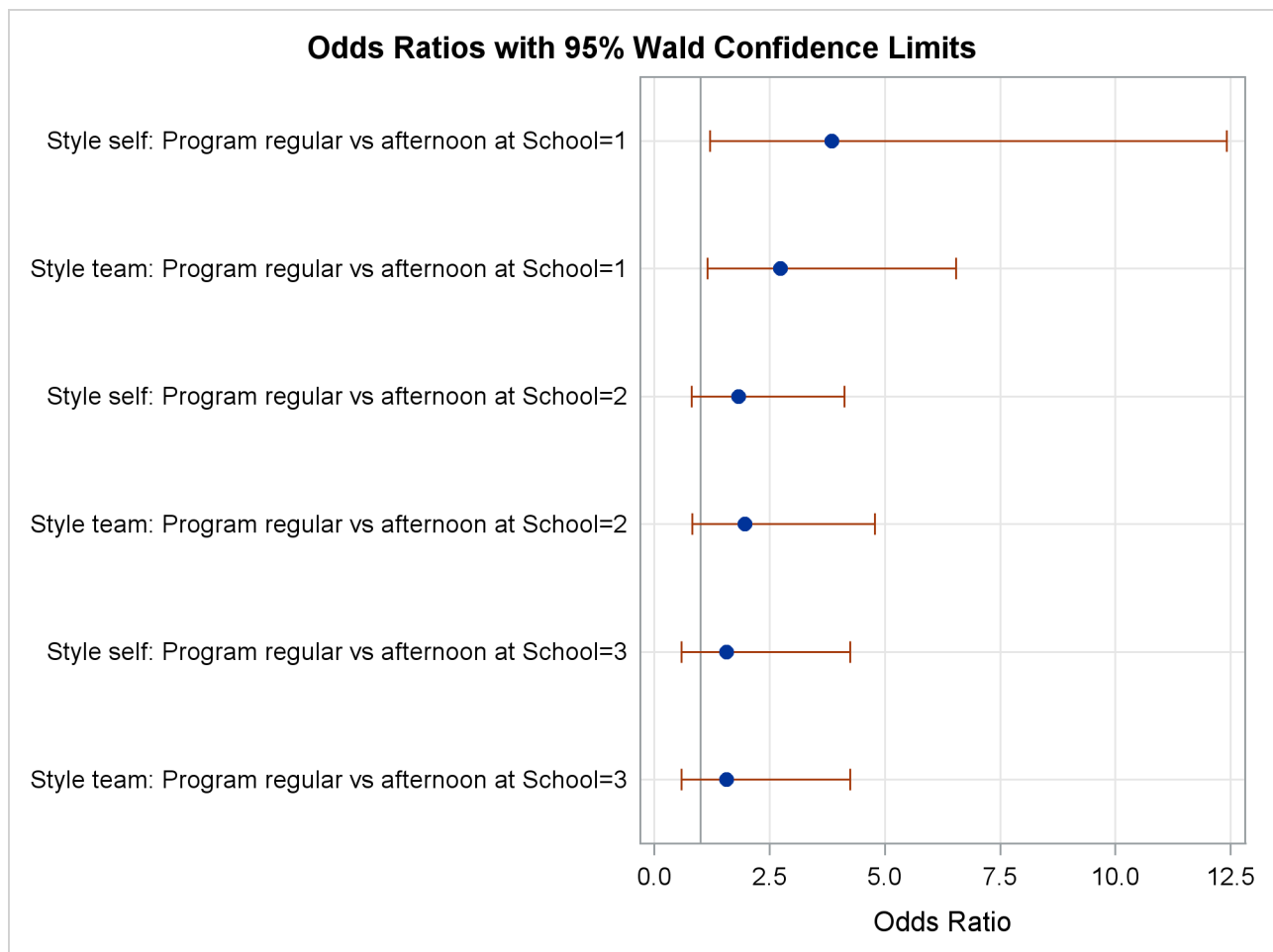
| Analysis of Maximum Likelihood Estimates |       |    |          |                   |                    |            |  |
|------------------------------------------|-------|----|----------|-------------------|--------------------|------------|--|
| Parameter                                | Style | DF | Estimate | Standard<br>Error | Wald<br>Chi-Square | Pr > ChiSq |  |
| Intercept                                | self  | 1  | -0.8097  | 0.1488            | 29.5989            | <.0001     |  |
| Intercept                                | team  | 1  | -0.6585  | 0.1366            | 23.2449            | <.0001     |  |
| School 1                                 | self  | 1  | -0.8194  | 0.2281            | 12.9066            | 0.0003     |  |
| School 1                                 | team  | 1  | -0.2675  | 0.1881            | 2.0233             | 0.1549     |  |
| School 2                                 | self  | 1  | 0.2974   | 0.1919            | 2.4007             | 0.1213     |  |
| School 2                                 | team  | 1  | -0.1033  | 0.1898            | 0.2961             | 0.5863     |  |
| Program regular                          | self  | 1  | 0.3985   | 0.1488            | 7.1684             | 0.0074     |  |
| Program regular                          | team  | 1  | 0.3537   | 0.1366            | 6.7071             | 0.0096     |  |
| School*Program 1 regular                 | self  | 1  | 0.2751   | 0.2281            | 1.4547             | 0.2278     |  |
| School*Program 1 regular                 | team  | 1  | 0.1474   | 0.1881            | 0.6143             | 0.4332     |  |
| School*Program 2 regular                 | self  | 1  | -0.0998  | 0.1919            | 0.2702             | 0.6032     |  |
| School*Program 2 regular                 | team  | 1  | -0.0168  | 0.1898            | 0.0079             | 0.9293     |  |

The table produced by the `ODDSRATIO` statement is displayed in [Output 54.4.4](#). The differences between the program preferences are small across all the styles (logits) compared to their variability as displayed by the confidence limits in [Output 54.4.5](#), confirming that the interaction effect is nonsignificant.

**Output 54.4.4** Odds Ratios for Style

| Odds Ratio Estimates and Wald Confidence Intervals   |          |                       |        |
|------------------------------------------------------|----------|-----------------------|--------|
| Label                                                | Estimate | 95% Confidence Limits |        |
| Style self: Program regular vs afternoon at School=1 | 3.846    | 1.190                 | 12.435 |
| Style team: Program regular vs afternoon at School=1 | 2.724    | 1.132                 | 6.554  |
| Style self: Program regular vs afternoon at School=2 | 1.817    | 0.798                 | 4.139  |
| Style team: Program regular vs afternoon at School=2 | 1.962    | 0.802                 | 4.799  |
| Style self: Program regular vs afternoon at School=3 | 1.562    | 0.572                 | 4.265  |
| Style team: Program regular vs afternoon at School=3 | 1.562    | 0.572                 | 4.265  |

**Output 54.4.5** Plot of Odds Ratios for Style



Since the interaction effect is clearly nonsignificant, a main-effects model is fit with the following statements. The `EFFECTPLOT` statement creates a plot of the predicted values versus the levels of the School

variable at each level of the Program variables. The **CLM** option adds confidence bars, and the **NOOBS** option suppresses the display of the observations.

```
ods graphics on;
proc logistic data=school;
 freq Count;
 class School Program(ref=first);
 model Style(order=data)=School Program / link=glogit;
 effectplot interaction(plotby=Program) / clm noobs;
run;
ods graphics off;
```

All of the global fit tests in [Output 54.4.6](#) suggest the model is significant, and the Type 3 tests show that the school and program effects are also significant.

**Output 54.4.6** Analysis of Main-Effects Model

| The LOGISTIC Procedure                        |                   |                                |            |
|-----------------------------------------------|-------------------|--------------------------------|------------|
| Model Convergence Status                      |                   |                                |            |
| Convergence criterion (GCONV=1E-8) satisfied. |                   |                                |            |
| Model Fit Statistics                          |                   |                                |            |
| Criterion                                     | Intercept<br>Only | Intercept<br>and<br>Covariates |            |
| AIC                                           | 699.404           | 682.934                        |            |
| SC                                            | 707.050           | 713.518                        |            |
| -2 Log L                                      | 695.404           | 666.934                        |            |
| Testing Global Null Hypothesis: BETA=0        |                   |                                |            |
| Test                                          | Chi-Square        | DF                             | Pr > ChiSq |
| Likelihood Ratio                              | 28.4704           | 6                              | <.0001     |
| Score                                         | 27.1190           | 6                              | 0.0001     |
| Wald                                          | 25.5881           | 6                              | 0.0003     |
| Type 3 Analysis of Effects                    |                   |                                |            |
| Effect                                        | DF                | Wald<br>Chi-Square             | Pr > ChiSq |
| School                                        | 4                 | 14.8424                        | 0.0050     |
| Program                                       | 2                 | 10.9160                        | 0.0043     |

The parameter estimates, tests for individual parameters, and odds ratios are displayed in [Output 54.4.7](#). The Program variable has nearly the same effect on both logits, while School=1 has the largest effect of the schools.

**Output 54.4.7** Estimates

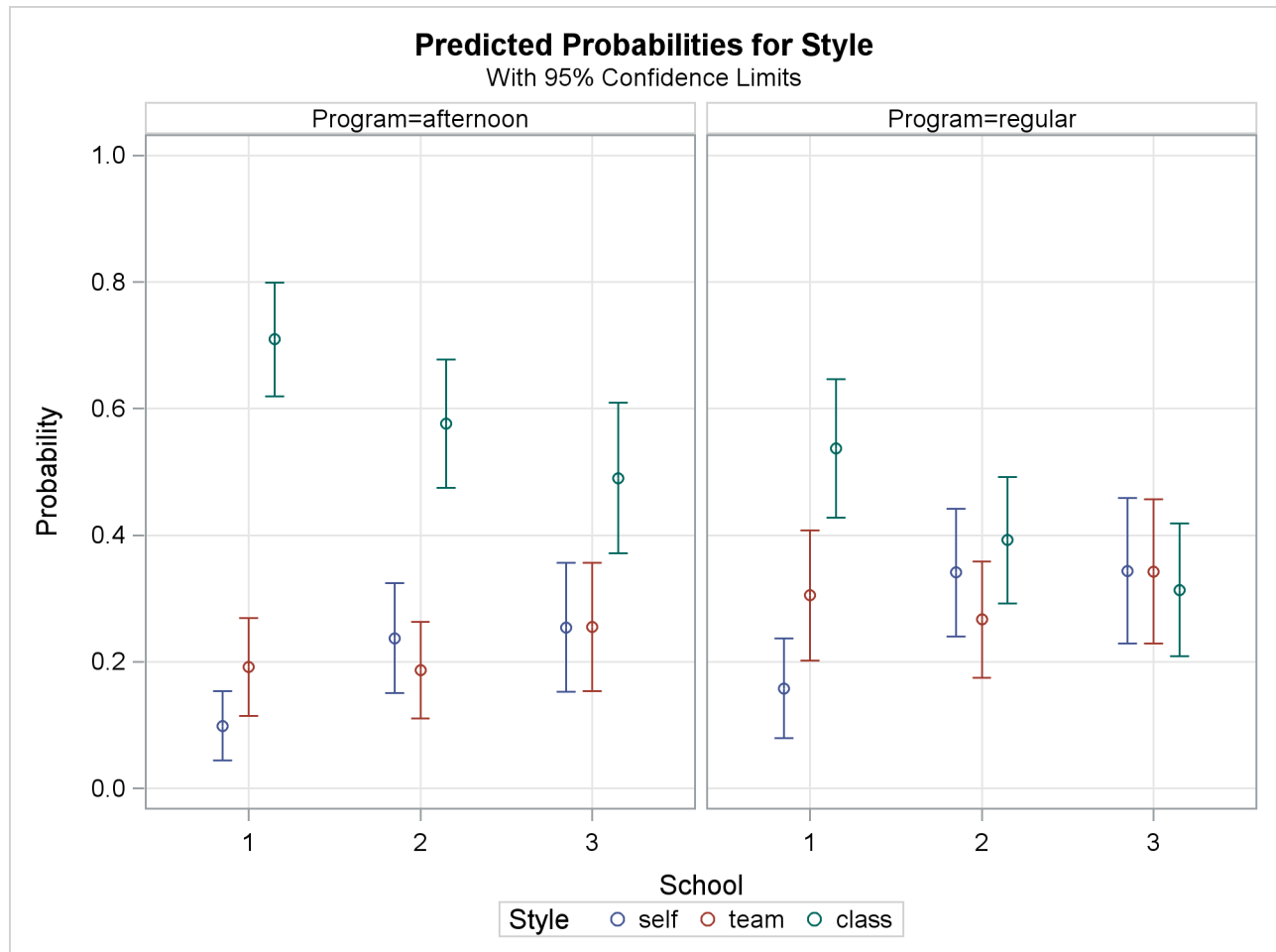
| Analysis of Maximum Likelihood Estimates |       |    |          |                |                 |            |
|------------------------------------------|-------|----|----------|----------------|-----------------|------------|
| Parameter                                | Style | DF | Estimate | Standard Error | Wald Chi-Square | Pr > ChiSq |
| Intercept                                | self  | 1  | -0.7978  | 0.1465         | 29.6502         | <.0001     |
| Intercept                                | team  | 1  | -0.6589  | 0.1367         | 23.2300         | <.0001     |
| School 1                                 | self  | 1  | -0.7992  | 0.2198         | 13.2241         | 0.0003     |
| School 1                                 | team  | 1  | -0.2786  | 0.1867         | 2.2269          | 0.1356     |
| School 2                                 | self  | 1  | 0.2836   | 0.1899         | 2.2316          | 0.1352     |
| School 2                                 | team  | 1  | -0.0985  | 0.1892         | 0.2708          | 0.6028     |
| Program regular                          | self  | 1  | 0.3737   | 0.1410         | 7.0272          | 0.0080     |
| Program regular                          | team  | 1  | 0.3713   | 0.1353         | 7.5332          | 0.0061     |

| Odds Ratio Estimates         |       |                |                            |       |
|------------------------------|-------|----------------|----------------------------|-------|
| Effect                       | Style | Point Estimate | 95% Wald Confidence Limits |       |
| School 1 vs 3                | self  | 0.269          | 0.127                      | 0.570 |
| School 1 vs 3                | team  | 0.519          | 0.267                      | 1.010 |
| School 2 vs 3                | self  | 0.793          | 0.413                      | 1.522 |
| School 2 vs 3                | team  | 0.622          | 0.317                      | 1.219 |
| Program regular vs afternoon | self  | 2.112          | 1.215                      | 3.670 |
| Program regular vs afternoon | team  | 2.101          | 1.237                      | 3.571 |

The interaction plots in [Output 54.4.8](#) show that School=1 and Program=afternoon have a preference for the traditional classroom style. Of course, since these are not simultaneous confidence intervals, the nonoverlapping 95% confidence limits do not take the place of an actual test.



**Output 54.4.8** Model-Predicted Probabilities

### Example 54.5: Stratified Sampling

Consider the hypothetical example in Fleiss (1981, pp. 6–7), in which a test is applied to a sample of 1,000 people known to have a disease and to another sample of 1,000 people known not to have the same disease. In the diseased sample, 950 test positive; in the nondiseased sample, only 10 test positive. If the true disease rate in the population is 1 in 100, specifying `PEVENT=0.01` results in the correct false positive and negative rates for the stratified sampling scheme. Omitting the `PEVENT=` option is equivalent to using the overall sample disease rate ( $1000/2000 = 0.5$ ) as the value of the `PEVENT=` option, which would ignore the stratified sampling.

The statements to create the data set and perform the analysis are as follows:

```
data Screen;
 do Disease='Present', 'Absent';
 do Test=1,0;
 input Count @@;
 output;
 end;
 end;
end;
```

```

 datalines;
950 50
10 990
;

proc logistic data=Screen;
 freq Count;
 model Disease(event='Present')=Test
 / pevent=.5 .01 ctable pprob=.5;
run;

```

The response variable option `EVENT=` indicates that `Disease='Present'` is the event. The `CTABLE` option is specified to produce a classification table. Specifying `PPROB=0.5` indicates a cutoff probability of 0.5. A list of two probabilities, 0.5 and 0.01, is specified for the `PEVENT=` option; 0.5 corresponds to the overall sample disease rate, and 0.01 corresponds to a true disease rate of 1 in 100.

The classification table is shown in [Output 54.5.1](#).

**Output 54.5.1** False Positive and False Negative Rates

| The LOGISTIC Procedure |               |         |               |           |               |             |                  |                  |              |              |
|------------------------|---------------|---------|---------------|-----------|---------------|-------------|------------------|------------------|--------------|--------------|
| Classification Table   |               |         |               |           |               |             |                  |                  |              |              |
| Prob<br>Event          | Prob<br>Level | Correct |               | Incorrect |               | Percentages |                  |                  |              |              |
|                        |               | Event   | Non-<br>Event | Event     | Non-<br>Event | Correct     | Sensi-<br>tivity | Speci-<br>ficity | False<br>POS | False<br>NEG |
| 0.500                  | 0.500         | 950     | 990           | 10        | 50            | 97.0        | 95.0             | 99.0             | 1.0          | 4.8          |
| 0.010                  | 0.500         | 950     | 990           | 10        | 50            | 99.0        | 95.0             | 99.0             | 51.0         | 0.1          |

In the classification table, the column “Prob Level” represents the cutoff values (the settings of the `PPROB=` option) for predicting whether an observation is an event. The “Correct” columns list the numbers of subjects that are correctly predicted as events and nonevents, respectively, and the “Incorrect” columns list the number of nonevents incorrectly predicted as events and the number of events incorrectly predicted as nonevents, respectively. For `PEVENT=0.5`, the false positive rate is 1% and the false negative rate is 4.8%. These results ignore the fact that the samples were stratified and incorrectly assume that the overall sample proportion of disease (which is 0.5) estimates the true disease rate. For a true disease rate of 0.01, the false positive rate and the false negative rate are 51% and 0.1%, respectively, as shown in the second line of the classification table.

## Example 54.6: Logistic Regression Diagnostics

In a controlled experiment to study the effect of the rate and volume of air intake on a transient reflex vasoconstriction in the skin of the digits, 39 tests under various combinations of rate and volume of air intake were obtained (Finney 1947). The endpoint of each test is whether or not vasoconstriction occurred. Pregibon (1981) uses this set of data to illustrate the diagnostic measures he proposes for detecting influential observations and to quantify their effects on various aspects of the maximum likelihood fit.

The vasoconstriction data are saved in the data set vaso:

```

data vaso;
 length Response $12;
 input Volume Rate Response @@;
 LogVolume=log(Volume);
 LogRate=log(Rate);
 datalines;
3.70 0.825 constrict 3.50 1.09 constrict
1.25 2.50 constrict 0.75 1.50 constrict
0.80 3.20 constrict 0.70 3.50 constrict
0.60 0.75 no_constrict 1.10 1.70 no_constrict
0.90 0.75 no_constrict 0.90 0.45 no_constrict
0.80 0.57 no_constrict 0.55 2.75 no_constrict
0.60 3.00 no_constrict 1.40 2.33 constrict
0.75 3.75 constrict 2.30 1.64 constrict
3.20 1.60 constrict 0.85 1.415 constrict
1.70 1.06 no_constrict 1.80 1.80 constrict
0.40 2.00 no_constrict 0.95 1.36 no_constrict
1.35 1.35 no_constrict 1.50 1.36 no_constrict
1.60 1.78 constrict 0.60 1.50 no_constrict
1.80 1.50 constrict 0.95 1.90 no_constrict
1.90 0.95 constrict 1.60 0.40 no_constrict
2.70 0.75 constrict 2.35 0.03 no_constrict
1.10 1.83 no_constrict 1.10 2.20 constrict
1.20 2.00 constrict 0.80 3.33 constrict
0.95 1.90 no_constrict 0.75 1.90 no_constrict
1.30 1.625 constrict
;

```

In the data set vaso, the variable Response represents the outcome of a test. The variable LogVolume represents the log of the volume of air intake, and the variable LogRate represents the log of the rate of air intake.

The following statements invoke PROC LOGISTIC to fit a logistic regression model to the vasoconstriction data, where Response is the response variable, and LogRate and LogVolume are the explanatory variables. Regression diagnostics are displayed when ODS Graphics is enabled, and the INFLUENCE option is specified to display a table of the regression diagnostics.

```

ods graphics on;
title 'Occurrence of Vasoconstriction';
proc logistic data=vaso;
 model Response=LogRate LogVolume/influence iplots;
run;
ods graphics off;

```

Results of the model fit are shown in [Output 54.6.1](#). Both LogRate and LogVolume are statistically significant to the occurrence of vasoconstriction ( $p = 0.0131$  and  $p = 0.0055$ , respectively). Their positive parameter estimates indicate that a higher inspiration rate or a larger volume of air intake is likely to increase the probability of vasoconstriction.

**Output 54.6.1** Logistic Regression Analysis for Vasoconstriction Data

```

Occurrence of Vasoconstriction

The LOGISTIC Procedure

Model Information

Data Set WORK.VASO
Response Variable Response
Number of Response Levels 2
Model binary logit
Optimization Technique Fisher's scoring

Number of Observations Read 39
Number of Observations Used 39

Response Profile

Ordered Value Response Total
 Response Frequency
1 constrict 20
2 no_constrict 19

Probability modeled is Response='constrict'.

Model Convergence Status

Convergence criterion (GCONV=1E-8) satisfied.

Model Fit Statistics

Criterion Intercept
 Intercept
 Only and
 Only Covariates
AIC 56.040 35.227
SC 57.703 40.218
-2 Log L 54.040 29.227

Testing Global Null Hypothesis: BETA=0

Test Chi-Square DF Pr > ChiSq
Likelihood Ratio 24.8125 2 <.0001
Score 16.6324 2 0.0002
Wald 7.8876 2 0.0194

```

Output 54.6.1 *continued*

| Analysis of Maximum Likelihood Estimates |    |          |                |                 |            |
|------------------------------------------|----|----------|----------------|-----------------|------------|
| Parameter                                | DF | Estimate | Standard Error | Wald Chi-Square | Pr > ChiSq |
| Intercept                                | 1  | -2.8754  | 1.3208         | 4.7395          | 0.0295     |
| LogRate                                  | 1  | 4.5617   | 1.8380         | 6.1597          | 0.0131     |
| LogVolume                                | 1  | 5.1793   | 1.8648         | 7.7136          | 0.0055     |

| Odds Ratio Estimates |                |                            |          |
|----------------------|----------------|----------------------------|----------|
| Effect               | Point Estimate | 95% Wald Confidence Limits |          |
| LogRate              | 95.744         | 2.610                      | >999.999 |
| LogVolume            | 177.562        | 4.592                      | >999.999 |

| Association of Predicted Probabilities and Observed Responses |      |           |       |
|---------------------------------------------------------------|------|-----------|-------|
| Percent Concordant                                            | 93.7 | Somers' D | 0.874 |
| Percent Discordant                                            | 6.3  | Gamma     | 0.874 |
| Percent Tied                                                  | 0.0  | Tau-a     | 0.448 |
| Pairs                                                         | 380  | c         | 0.937 |

The INFLUENCE option displays the values of the explanatory variables (LogRate and LogVolume) for each observation, a column for each diagnostic produced, and the *case number* that represents the sequence number of the observation (Output 54.6.2).

**Output 54.6.2** Regression Diagnostics from the INFLUENCE Option

| Regression Diagnostics |            |            |                  |                   |                     |                  |                |
|------------------------|------------|------------|------------------|-------------------|---------------------|------------------|----------------|
| Case Number            | Covariates |            |                  | Deviance Residual | Hat Matrix Diagonal | Intercept DfBeta | LogRate DfBeta |
|                        | LogRate    | Log Volume | Pearson Residual |                   |                     |                  |                |
| 1                      | -0.1924    | 1.3083     | 0.2205           | 0.3082            | 0.0927              | -0.0165          | 0.0193         |
| 2                      | 0.0862     | 1.2528     | 0.1349           | 0.1899            | 0.0429              | -0.0134          | 0.0151         |
| 3                      | 0.9163     | 0.2231     | 0.2923           | 0.4049            | 0.0612              | -0.0492          | 0.0660         |
| 4                      | 0.4055     | -0.2877    | 3.5181           | 2.2775            | 0.0867              | 1.0734           | -0.9302        |
| 5                      | 1.1632     | -0.2231    | 0.5287           | 0.7021            | 0.1158              | -0.0832          | 0.1411         |
| 6                      | 1.2528     | -0.3567    | 0.6090           | 0.7943            | 0.1524              | -0.0922          | 0.1710         |
| 7                      | -0.2877    | -0.5108    | -0.0328          | -0.0464           | 0.00761             | -0.00280         | 0.00274        |
| 8                      | 0.5306     | 0.0953     | -1.0196          | -1.1939           | 0.0559              | -0.1444          | 0.0613         |
| 9                      | -0.2877    | -0.1054    | -0.0938          | -0.1323           | 0.0342              | -0.0178          | 0.0173         |
| 10                     | -0.7985    | -0.1054    | -0.0293          | -0.0414           | 0.00721             | -0.00245         | 0.00246        |
| 11                     | -0.5621    | -0.2231    | -0.0370          | -0.0523           | 0.00969             | -0.00361         | 0.00358        |
| 12                     | 1.0116     | -0.5978    | -0.5073          | -0.6768           | 0.1481              | -0.1173          | 0.0647         |
| 13                     | 1.0986     | -0.5108    | -0.7751          | -0.9700           | 0.1628              | -0.0931          | -0.00946       |
| 14                     | 0.8459     | 0.3365     | 0.2559           | 0.3562            | 0.0551              | -0.0414          | 0.0538         |
| 15                     | 1.3218     | -0.2877    | 0.4352           | 0.5890            | 0.1336              | -0.0940          | 0.1408         |
| 16                     | 0.4947     | 0.8329     | 0.1576           | 0.2215            | 0.0402              | -0.0198          | 0.0234         |
| 17                     | 0.4700     | 1.1632     | 0.0709           | 0.1001            | 0.0172              | -0.00630         | 0.00701        |
| 18                     | 0.3471     | -0.1625    | 2.9062           | 2.1192            | 0.0954              | 0.9595           | -0.8279        |
| 19                     | 0.0583     | 0.5306     | -1.0718          | -1.2368           | 0.1315              | -0.2591          | 0.2024         |
| 20                     | 0.5878     | 0.5878     | 0.2405           | 0.3353            | 0.0525              | -0.0331          | 0.0421         |
| 21                     | 0.6931     | -0.9163    | -0.1076          | -0.1517           | 0.0373              | -0.0180          | 0.0158         |
| 22                     | 0.3075     | -0.0513    | -0.4193          | -0.5691           | 0.1015              | -0.1449          | 0.1237         |
| 23                     | 0.3001     | 0.3001     | -1.0242          | -1.1978           | 0.0761              | -0.1961          | 0.1275         |
| 24                     | 0.3075     | 0.4055     | -1.3684          | -1.4527           | 0.0717              | -0.1281          | 0.0410         |
| 25                     | 0.5766     | 0.4700     | 0.3347           | 0.4608            | 0.0587              | -0.0403          | 0.0570         |
| 26                     | 0.4055     | -0.5108    | -0.1595          | -0.2241           | 0.0548              | -0.0366          | 0.0329         |
| 27                     | 0.4055     | 0.5878     | 0.3645           | 0.4995            | 0.0661              | -0.0327          | 0.0496         |
| 28                     | 0.6419     | -0.0513    | -0.8989          | -1.0883           | 0.0647              | -0.1423          | 0.0617         |
| 29                     | -0.0513    | 0.6419     | 0.8981           | 1.0876            | 0.1682              | 0.2367           | -0.1950        |
| 30                     | -0.9163    | 0.4700     | -0.0992          | -0.1400           | 0.0507              | -0.0224          | 0.0227         |
| 31                     | -0.2877    | 0.9933     | 0.6198           | 0.8064            | 0.2459              | 0.1165           | -0.0996        |
| 32                     | -3.5066    | 0.8544     | -0.00073         | -0.00103          | 0.000022            | -3.22E-6         | 3.405E-6       |
| 33                     | 0.6043     | 0.0953     | -1.2062          | -1.3402           | 0.0510              | -0.0882          | -0.0137        |
| 34                     | 0.7885     | 0.0953     | 0.5447           | 0.7209            | 0.0601              | -0.0425          | 0.0877         |
| 35                     | 0.6931     | 0.1823     | 0.5404           | 0.7159            | 0.0552              | -0.0340          | 0.0755         |
| 36                     | 1.2030     | -0.2231    | 0.4828           | 0.6473            | 0.1177              | -0.0867          | 0.1381         |
| 37                     | 0.6419     | -0.0513    | -0.8989          | -1.0883           | 0.0647              | -0.1423          | 0.0617         |
| 38                     | 0.6419     | -0.2877    | -0.4874          | -0.6529           | 0.1000              | -0.1395          | 0.1032         |
| 39                     | 0.4855     | 0.2624     | 0.7053           | 0.8987            | 0.0531              | 0.0326           | 0.0190         |

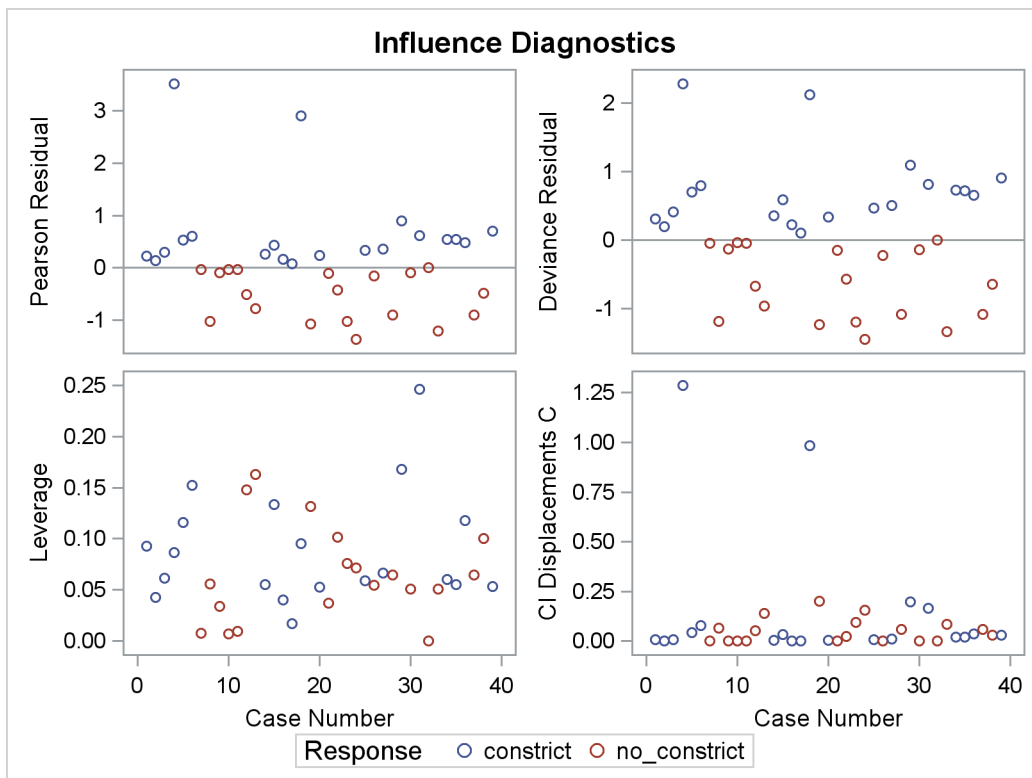
## Output 54.6.2 continued

| Regression Diagnostics |                   |                                    |                                       |                |                  |
|------------------------|-------------------|------------------------------------|---------------------------------------|----------------|------------------|
| Case Number            | Log Volume DfBeta | Confidence Interval Displacement C | Confidence Interval Displacement CBar | Delta Deviance | Delta Chi-Square |
| 1                      | 0.0556            | 0.00548                            | 0.00497                               | 0.1000         | 0.0536           |
| 2                      | 0.0261            | 0.000853                           | 0.000816                              | 0.0369         | 0.0190           |
| 3                      | 0.0589            | 0.00593                            | 0.00557                               | 0.1695         | 0.0910           |
| 4                      | -1.0180           | 1.2873                             | 1.1756                                | 6.3626         | 13.5523          |
| 5                      | 0.0583            | 0.0414                             | 0.0366                                | 0.5296         | 0.3161           |
| 6                      | 0.0381            | 0.0787                             | 0.0667                                | 0.6976         | 0.4376           |
| 7                      | 0.00265           | 8.321E-6                           | 8.258E-6                              | 0.00216        | 0.00109          |
| 8                      | 0.0570            | 0.0652                             | 0.0616                                | 1.4870         | 1.1011           |
| 9                      | 0.0153            | 0.000322                           | 0.000311                              | 0.0178         | 0.00911          |
| 10                     | 0.00211           | 6.256E-6                           | 6.211E-6                              | 0.00172        | 0.000862         |
| 11                     | 0.00319           | 0.000014                           | 0.000013                              | 0.00274        | 0.00138          |
| 12                     | 0.1651            | 0.0525                             | 0.0447                                | 0.5028         | 0.3021           |
| 13                     | 0.1775            | 0.1395                             | 0.1168                                | 1.0577         | 0.7175           |
| 14                     | 0.0527            | 0.00404                            | 0.00382                               | 0.1307         | 0.0693           |
| 15                     | 0.0643            | 0.0337                             | 0.0292                                | 0.3761         | 0.2186           |
| 16                     | 0.0307            | 0.00108                            | 0.00104                               | 0.0501         | 0.0259           |
| 17                     | 0.00914           | 0.000089                           | 0.000088                              | 0.0101         | 0.00511          |
| 18                     | -0.8477           | 0.9845                             | 0.8906                                | 5.3817         | 9.3363           |
| 19                     | -0.00488          | 0.2003                             | 0.1740                                | 1.7037         | 1.3227           |
| 20                     | 0.0518            | 0.00338                            | 0.00320                               | 0.1156         | 0.0610           |
| 21                     | 0.0208            | 0.000465                           | 0.000448                              | 0.0235         | 0.0120           |
| 22                     | 0.1179            | 0.0221                             | 0.0199                                | 0.3437         | 0.1956           |
| 23                     | 0.0357            | 0.0935                             | 0.0864                                | 1.5212         | 1.1355           |
| 24                     | -0.1004           | 0.1558                             | 0.1447                                | 2.2550         | 2.0171           |
| 25                     | 0.0708            | 0.00741                            | 0.00698                               | 0.2193         | 0.1190           |
| 26                     | 0.0373            | 0.00156                            | 0.00147                               | 0.0517         | 0.0269           |
| 27                     | 0.0788            | 0.0101                             | 0.00941                               | 0.2589         | 0.1423           |
| 28                     | 0.1025            | 0.0597                             | 0.0559                                | 1.2404         | 0.8639           |
| 29                     | 0.0286            | 0.1961                             | 0.1631                                | 1.3460         | 0.9697           |
| 30                     | 0.0159            | 0.000554                           | 0.000526                              | 0.0201         | 0.0104           |
| 31                     | 0.1322            | 0.1661                             | 0.1253                                | 0.7755         | 0.5095           |
| 32                     | 2.48E-6           | 1.18E-11                           | 1.18E-11                              | 1.065E-6       | 5.324E-7         |
| 33                     | -0.00216          | 0.0824                             | 0.0782                                | 1.8744         | 1.5331           |
| 34                     | 0.0671            | 0.0202                             | 0.0190                                | 0.5387         | 0.3157           |
| 35                     | 0.0711            | 0.0180                             | 0.0170                                | 0.5295         | 0.3091           |
| 36                     | 0.0631            | 0.0352                             | 0.0311                                | 0.4501         | 0.2641           |
| 37                     | 0.1025            | 0.0597                             | 0.0559                                | 1.2404         | 0.8639           |
| 38                     | 0.1397            | 0.0293                             | 0.0264                                | 0.4526         | 0.2639           |
| 39                     | 0.0489            | 0.0295                             | 0.0279                                | 0.8355         | 0.5254           |

The index plots produced by the IPLOTS option are essentially the same line-printer plots as those produced by the INFLUENCE option, but with a 90-degree rotation and perhaps on a more refined scale. Since ODS Graphics is enabled, the line-printer plots from the INFLUENCE and IPLOTS options are suppressed and ODS Graphics versions of the plots are displayed in Outputs 54.6.3 through 54.6.5. For general information about ODS Graphics, see Chapter 21, “Statistical Graphics Using ODS.” For specific information about the graphics available in the LOGISTIC procedure, see the section “ODS Graphics” on page 4294. The vertical axis of an index plot represents the value of the diagnostic, and the horizontal axis represents the sequence (case number) of the observation. The index plots are useful for identification of extreme values.

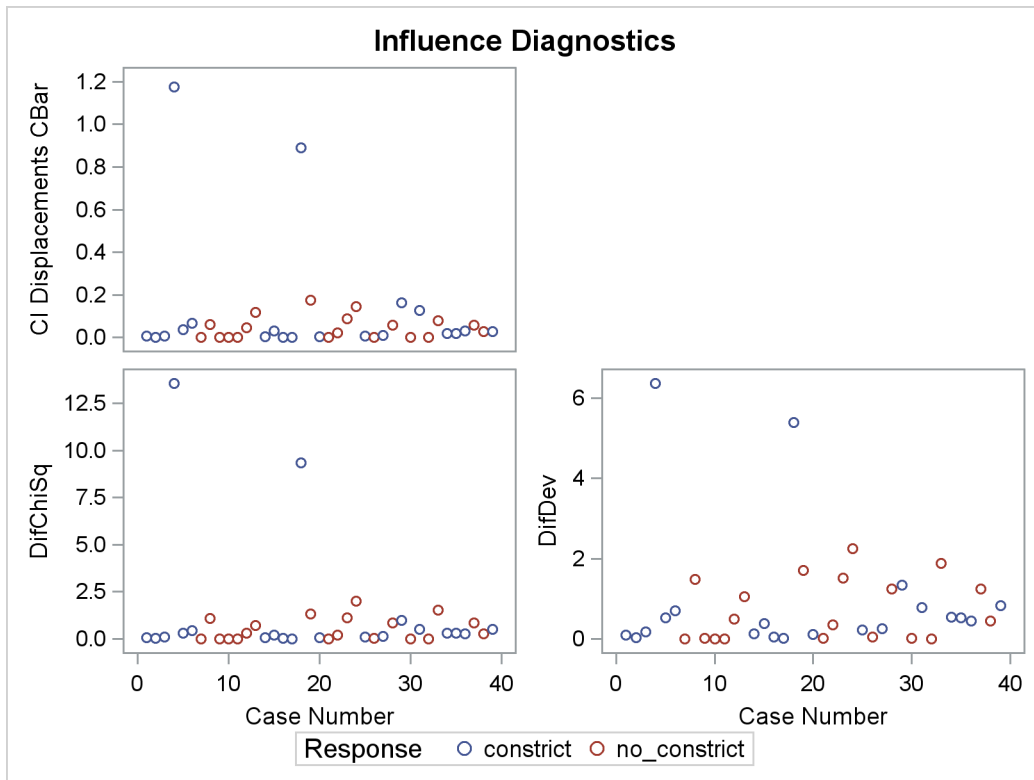
The index plots of the Pearson residuals and the deviance residuals (Output 54.6.3) indicate that case 4 and case 18 are poorly accounted for by the model. The index plot of the diagonal elements of the hat matrix (Output 54.6.3) suggests that case 31 is an extreme point in the design space. The index plots of DFBETAS (Output 54.6.5) indicate that case 4 and case 18 are causing instability in all three parameter estimates. The other four index plots in Outputs 54.6.3 and 54.6.4 also point to these two cases as having a large impact on the coefficients and goodness of fit.

**Output 54.6.3** Residuals, Hat Matrix, and CI Displacement C

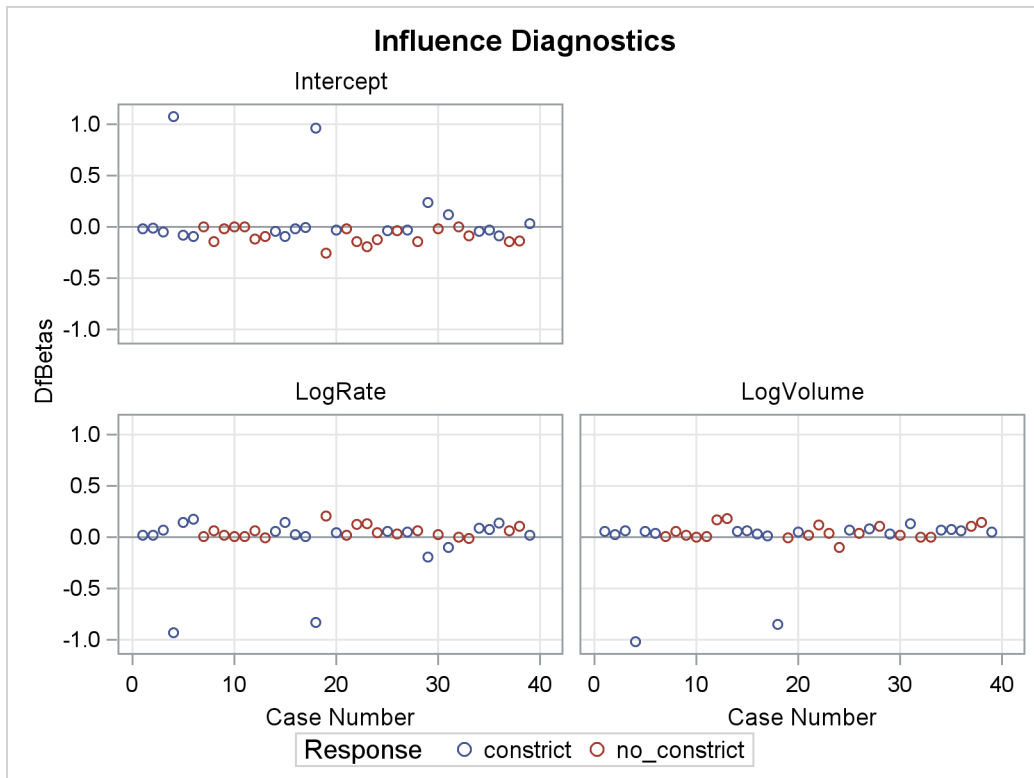




**Output 54.6.4** CI Displacement CBar, Change in Deviance and Pearson Chi-Square



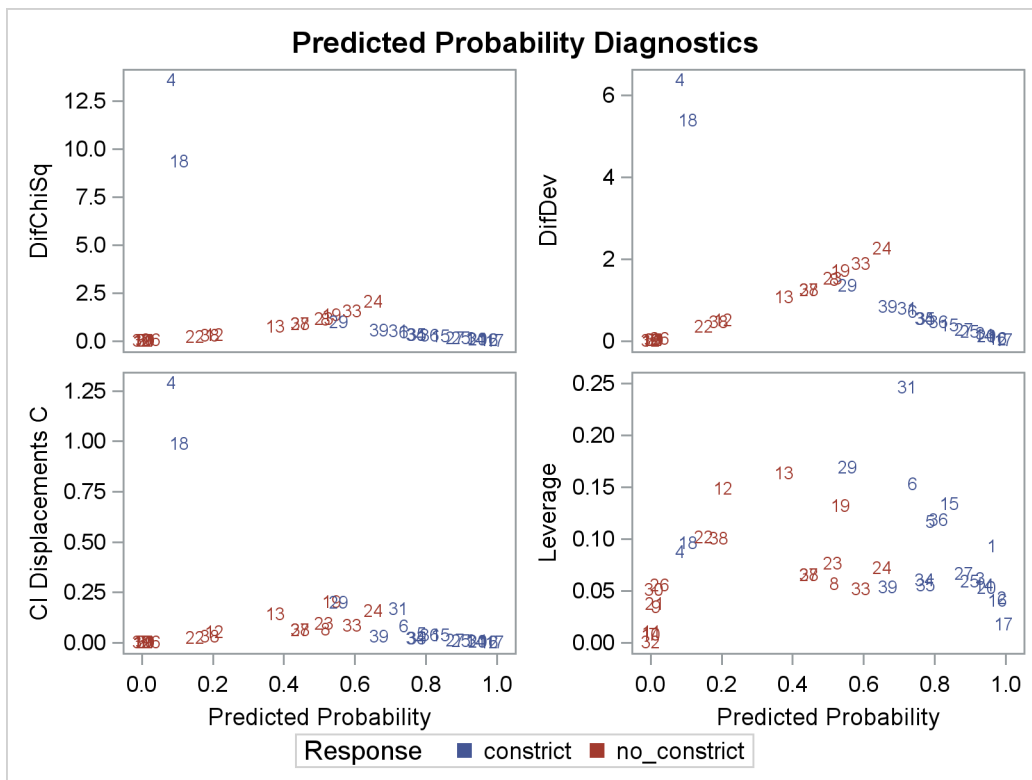
**Output 54.6.5** DFBETAS Plots



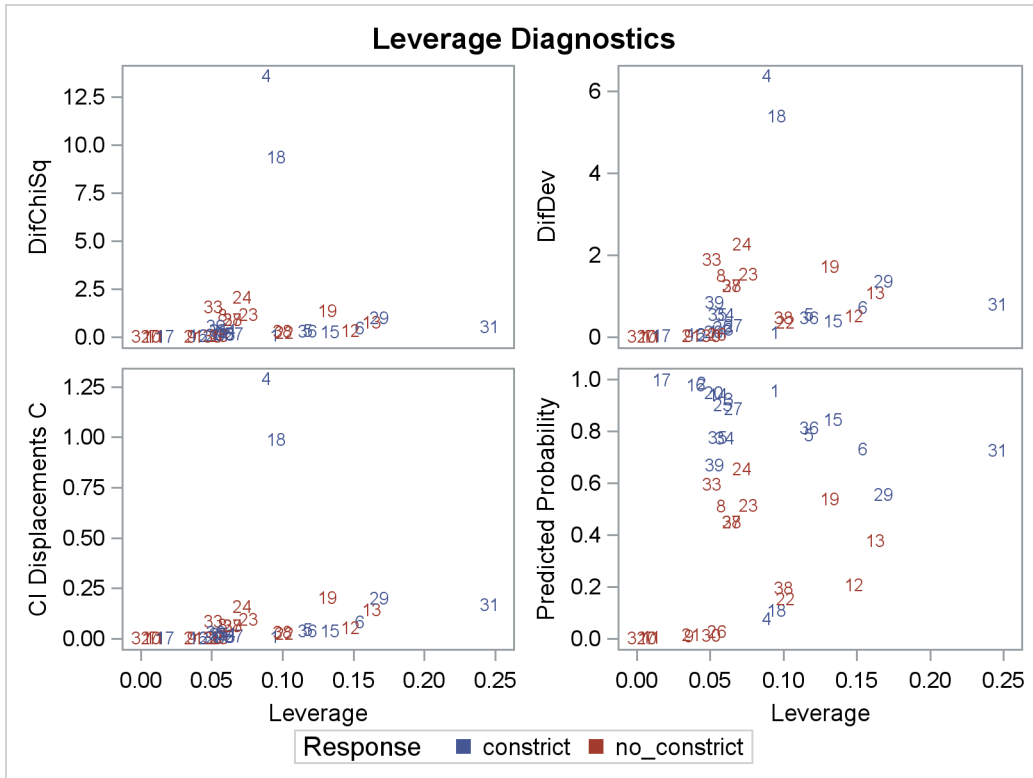
Other versions of diagnostic plots can be requested by specifying the appropriate options in the `PLOTS=` option. For example, the following statements produce three other sets of influence diagnostic plots: the `PHAT` option plots several diagnostics against the predicted probabilities ([Output 54.6.6](#)), the `LEVERAGE` option plots several diagnostics against the leverage ([Output 54.6.7](#)), and the `DPC` option plots the deletion diagnostics against the predicted probabilities and colors the observations according to the confidence interval displacement diagnostic ([Output 54.6.8](#)). The `LABEL` option displays the observation numbers on the plots. In all plots, you are looking for the outlying observations, and again cases 4 and 18 are noted.

```
ods graphics on;
proc logistic data=vaso plots(only label)=(phat leverage dpc);
 model Response=LogRate LogVolume;
run;
ods graphics off;
```

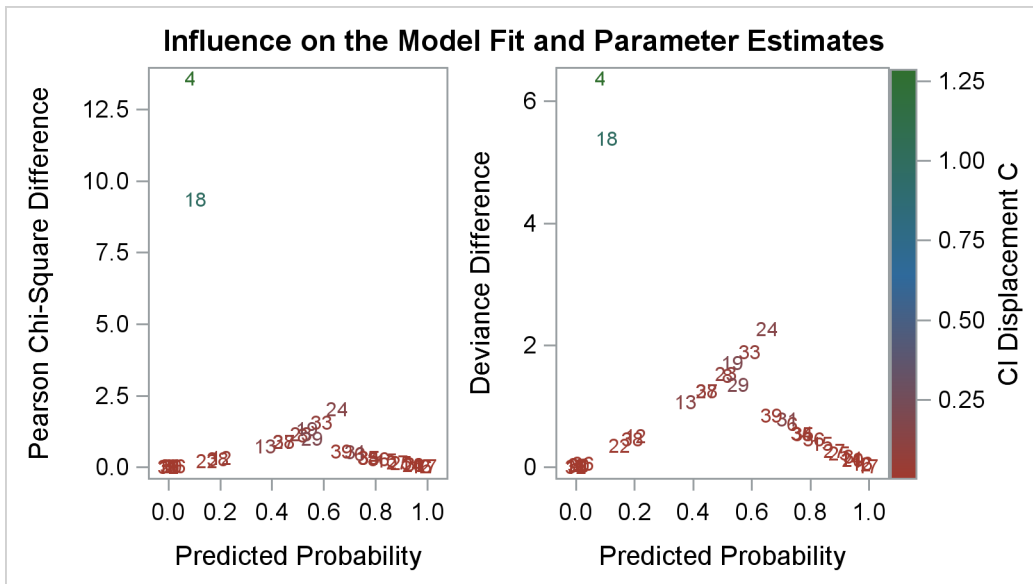
**Output 54.6.6** Diagnostics versus Predicted Probability



**Output 54.6.7** Diagnostics versus Leverage



**Output 54.6.8** Three Diagnostics



## Example 54.7: ROC Curve, Customized Odds Ratios, Goodness-of-Fit Statistics, R-Square, and Confidence Limits

This example plots an ROC curve, estimates a customized odds ratio, produces the traditional goodness-of-fit analysis, displays the generalized R Square measures for the fitted model, calculates the normal confidence intervals for the regression parameters, and produces a display of the probability function and prediction curves for the fitted model. The data consist of three variables: *n* (number of subjects in the sample), *disease* (number of diseased subjects in the sample), and *age* (age for the sample). A linear logistic regression model is used to study the effect of age on the probability of contracting the disease. The statements to produce the data set and perform the analysis are as follows:

```
data Data1;
 input disease n age;
 datalines;
0 14 25
0 20 35
0 19 45
7 18 55
6 12 65
17 17 75
;

ods graphics on;
proc logistic data=Data1 plots(only)=roc(id=obs);
 model disease/n=age / scale=none
 clparm=wald
 clodds=pl
 rsquare;

 units age=10;
 effectplot;
run;
ods graphics off;
```

The option **SCALE=NONE** is specified to produce the deviance and Pearson goodness-of-fit analysis without adjusting for overdispersion. The **RSQUARE** option is specified to produce generalized R Square measures of the fitted model. The **CLPARM=WALD** option is specified to produce the Wald confidence intervals for the regression parameters. The **UNITS** statement is specified to produce customized odds ratio estimates for a change of 10 years in the age variable, and the **CLODDS=PL** option is specified to produce profile-likelihood confidence limits for the odds ratio. The **PLOTS=** option with ODS Graphics enabled produces a graphical display of the ROC curve, and the **EFFECTPLOT** statement displays the model fit.

The results in [Output 54.7.1](#) show that the deviance and Pearson statistics indicate no lack of fit in the model.

**Output 54.7.1** Deviance and Pearson Goodness-of-Fit Analysis

| The LOGISTIC Procedure                          |        |    |          |            |
|-------------------------------------------------|--------|----|----------|------------|
| Deviance and Pearson Goodness-of-Fit Statistics |        |    |          |            |
| Criterion                                       | Value  | DF | Value/DF | Pr > ChiSq |
| Deviance                                        | 7.7756 | 4  | 1.9439   | 0.1002     |
| Pearson                                         | 6.6020 | 4  | 1.6505   | 0.1585     |
| Number of events/trials observations: 6         |        |    |          |            |

Output 54.7.2 shows that the R-square for the model is 0.74. The odds of an event increases by a factor of 7.9 for each 10-year increase in age.

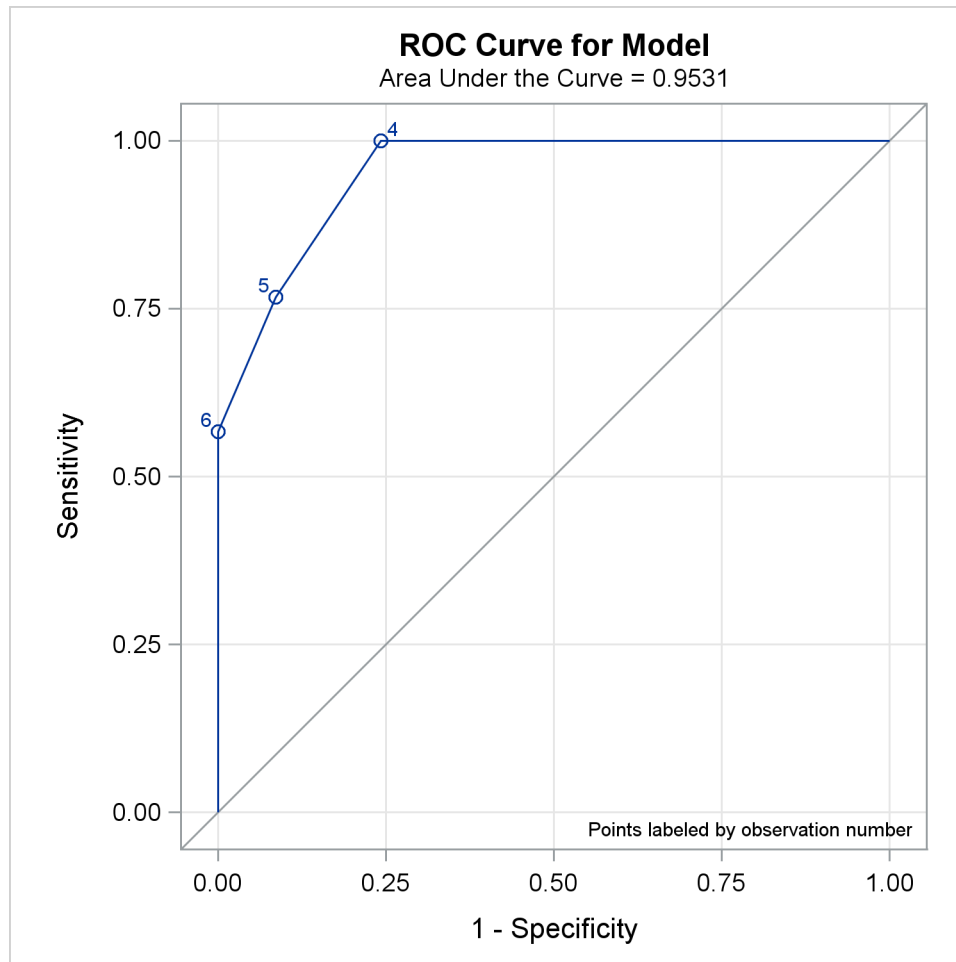
**Output 54.7.2** R-Square, Confidence Intervals, and Customized Odds Ratio

| Model Fit Statistics                     |                |                          |                     |                 |            |
|------------------------------------------|----------------|--------------------------|---------------------|-----------------|------------|
| Criterion                                | Intercept Only | Intercept and Covariates |                     |                 |            |
|                                          |                | Log Likelihood           | Full Log Likelihood |                 |            |
| AIC                                      | 124.173        | 52.468                   | 18.075              |                 |            |
| SC                                       | 126.778        | 57.678                   | 23.285              |                 |            |
| -2 Log L                                 | 122.173        | 48.468                   | 14.075              |                 |            |
| R-Square                                 | 0.5215         | Max-rescaled R-Square    | 0.8925              |                 |            |
| Testing Global Null Hypothesis: BETA=0   |                |                          |                     |                 |            |
| Test                                     | Chi-Square     | DF                       | Pr > ChiSq          |                 |            |
| Likelihood Ratio                         | 73.7048        | 1                        | <.0001              |                 |            |
| Score                                    | 55.3274        | 1                        | <.0001              |                 |            |
| Wald                                     | 23.3475        | 1                        | <.0001              |                 |            |
| Analysis of Maximum Likelihood Estimates |                |                          |                     |                 |            |
| Parameter                                | DF             | Estimate                 | Standard Error      | Wald Chi-Square | Pr > ChiSq |
| Intercept                                | 1              | -12.5016                 | 2.5555              | 23.9317         | <.0001     |
| age                                      | 1              | 0.2066                   | 0.0428              | 23.3475         | <.0001     |

**Output 54.7.2** *continued*

| Association of Predicted Probabilities and Observed Responses    |          |                       |                       |        |
|------------------------------------------------------------------|----------|-----------------------|-----------------------|--------|
| Percent Concordant                                               | 92.6     | Somers' D             | 0.906                 |        |
| Percent Discordant                                               | 2.0      | Gamma                 | 0.958                 |        |
| Percent Tied                                                     | 5.4      | Tau-a                 | 0.384                 |        |
| Pairs                                                            | 2100     | c                     | 0.953                 |        |
| Parameter Estimates and Wald<br>Confidence Intervals             |          |                       |                       |        |
| Parameter                                                        | Estimate | 95% Confidence Limits |                       |        |
| Intercept                                                        | -12.5016 | -17.5104              | -7.4929               |        |
| age                                                              | 0.2066   | 0.1228                | 0.2904                |        |
| Odds Ratio Estimates and Profile-Likelihood Confidence Intervals |          |                       |                       |        |
| Effect                                                           | Unit     | Estimate              | 95% Confidence Limits |        |
| age                                                              | 10.0000  | 7.892                 | 3.881                 | 21.406 |

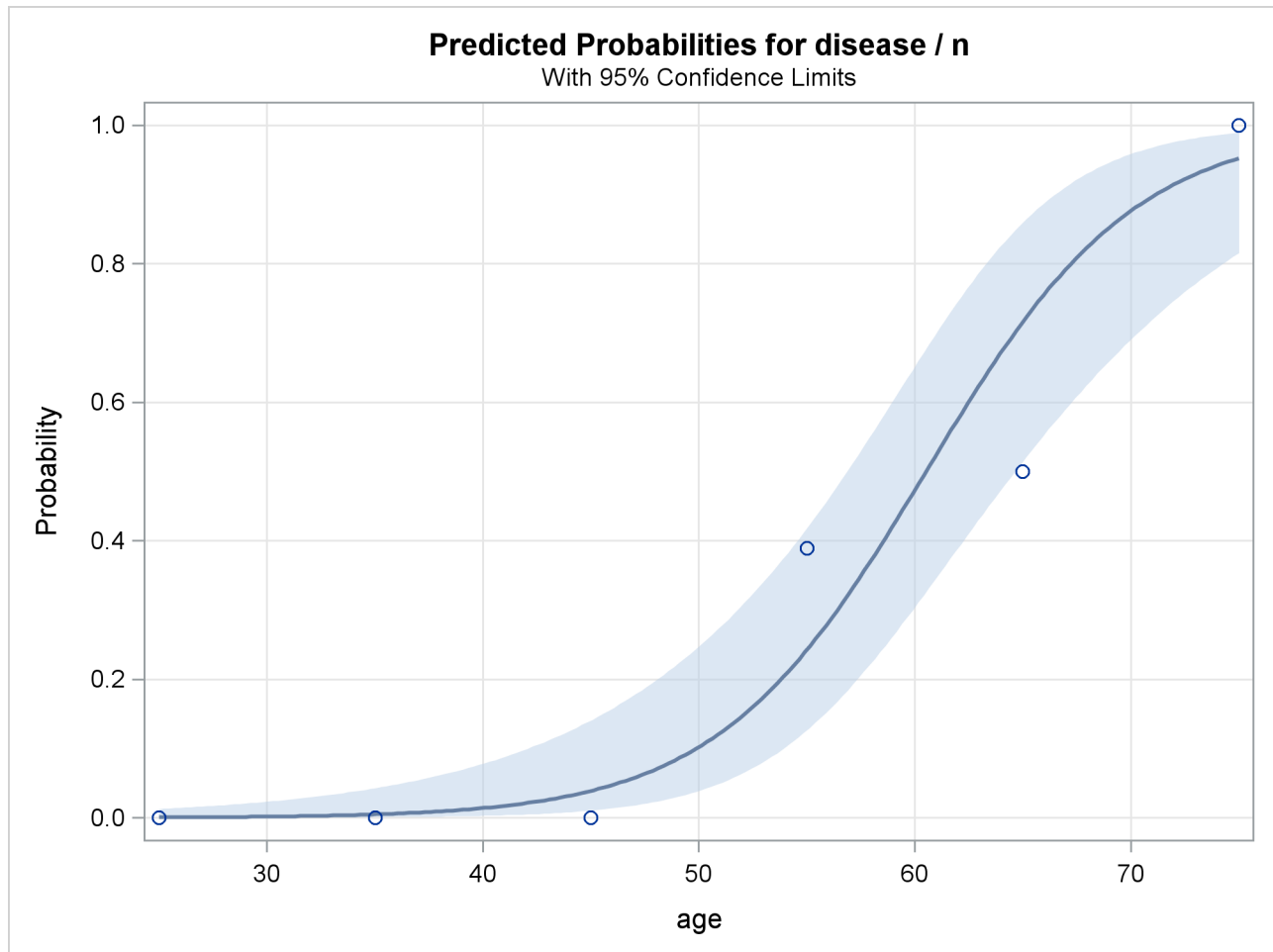
Since ODS Graphics is enabled, a graphical display of the ROC curve is produced as shown in [Output 54.7.3](#).

**Output 54.7.3** Receiver Operating Characteristic Curve

Note that the area under the ROC curve is estimated by the statistic  $c$  in the “Association of Predicted Probabilities and Observed Responses” table. In this example, the area under the ROC curve is 0.953.

Since there is only one continuous covariate and since ODS Graphics is enabled, the `EFFECTPLOT` statement produces a graphical display of the predicted probability curve with bounding 95% confidence limits as shown in [Output 54.7.4](#).

**Output 54.7.4** Predicted Probability and 95% Prediction Limits



### Example 54.8: Comparing Receiver Operating Characteristic Curves

DeLong, DeLong, and Clarke-Pearson (1988) report on 49 patients with ovarian cancer who also suffer from an intestinal obstruction. Three (correlated) screening tests are measured to determine whether a patient will benefit from surgery. The three tests are the K-G score and two measures of nutritional status: total protein and albumin. The data are as follows:

```

data roc;
 input alb tp totscore popind @@;
 totscore = 10 - totscore;
 datalines;
3.0 5.8 10 0 3.2 6.3 5 1 3.9 6.8 3 1 2.8 4.8 6 0
3.2 5.8 3 1 0.9 4.0 5 0 2.5 5.7 8 0 1.6 5.6 5 1
3.8 5.7 5 1 3.7 6.7 6 1 3.2 5.4 4 1 3.8 6.6 6 1
4.1 6.6 5 1 3.6 5.7 5 1 4.3 7.0 4 1 3.6 6.7 4 0
2.3 4.4 6 1 4.2 7.6 4 0 4.0 6.6 6 0 3.5 5.8 6 1
3.8 6.8 7 1 3.0 4.7 8 0 4.5 7.4 5 1 3.7 7.4 5 1
3.1 6.6 6 1 4.1 8.2 6 1 4.3 7.0 5 1 4.3 6.5 4 1
3.2 5.1 5 1 2.6 4.7 6 1 3.3 6.8 6 0 1.7 4.0 7 0

```



```

3.7 6.1 5 1 3.3 6.3 7 1 4.2 7.7 6 1 3.5 6.2 5 1
2.9 5.7 9 0 2.1 4.8 7 1 2.8 6.2 8 0 4.0 7.0 7 1
3.3 5.7 6 1 3.7 6.9 5 1 3.6 6.6 5 1
;

```

In the following statements, the **NOFIT** option is specified in the **MODEL** statement to prevent PROC LOGISTIC from fitting the model with three covariates. Each **ROC** statement lists one of the covariates, and PROC LOGISTIC then fits the model with that single covariate. Note that the original data set contains six more records with missing values for one of the tests, but PROC LOGISTIC ignores all records with missing values; hence there is a common sample size for each of the three models. The **ROCCONTRAST** statement implements the nonparameteric approach of DeLong, DeLong, and Clarke-Pearson (1988) to compare the three ROC curves, the **REFERENCE** option specifies that the K-G Score curve is used as the reference curve in the contrast, the **E** option displays the contrast coefficients, and the **ESTIMATE** option computes and tests each comparison. With ODS Graphics enabled, the **plots=roc(id=prob)** specification in the PROC LOGISTIC statement displays several plots, and the plots of individual ROC curves have certain points labeled with their predicted probabilities.

```

ods graphics on;
proc logistic data=roc plots=roc(id=prob);
 model popind(event='0') = alb tp totscore / nofit;
 roc 'Albumin' alb;
 roc 'K-G Score' totscore;
 roc 'Total Protein' tp;
 roccontrast reference('K-G Score') / estimate e;
run;
ods graphics off;

```

The initial model information is displayed in [Output 54.8.1](#).

**Output 54.8.1** Initial LOGISTIC Output

| The LOGISTIC Procedure           |        |                  |
|----------------------------------|--------|------------------|
| Model Information                |        |                  |
| Data Set                         |        | WORK.ROC         |
| Response Variable                |        | popind           |
| Number of Response Levels        |        | 2                |
| Model                            |        | binary logit     |
| Optimization Technique           |        | Fisher's scoring |
|                                  |        |                  |
| Number of Observations Read      |        | 43               |
| Number of Observations Used      |        | 43               |
| Response Profile                 |        |                  |
| Ordered Value                    | popind | Total Frequency  |
| 1                                | 0      | 12               |
| 2                                | 1      | 31               |
| Probability modeled is popind=0. |        |                  |

**Output 54.8.1** *continued*

| Score Test for Global Null Hypothesis |    |            |
|---------------------------------------|----|------------|
| Chi-Square                            | DF | Pr > ChiSq |
| 10.7939                               | 3  | 0.0129     |

For each ROC model, the model fitting details in Outputs 54.8.2, 54.8.4, and 54.8.6 can be suppressed with the `ROCOPTIONS(NODETAILS)` option; however, the convergence status is always displayed.

The ROC curves for the three models are displayed in Outputs 54.8.3, 54.8.5, and 54.8.7. Note that the labels on the ROC curve are produced by specifying the `ID=PROB` option, and are the predicted probabilities for the cutpoints.

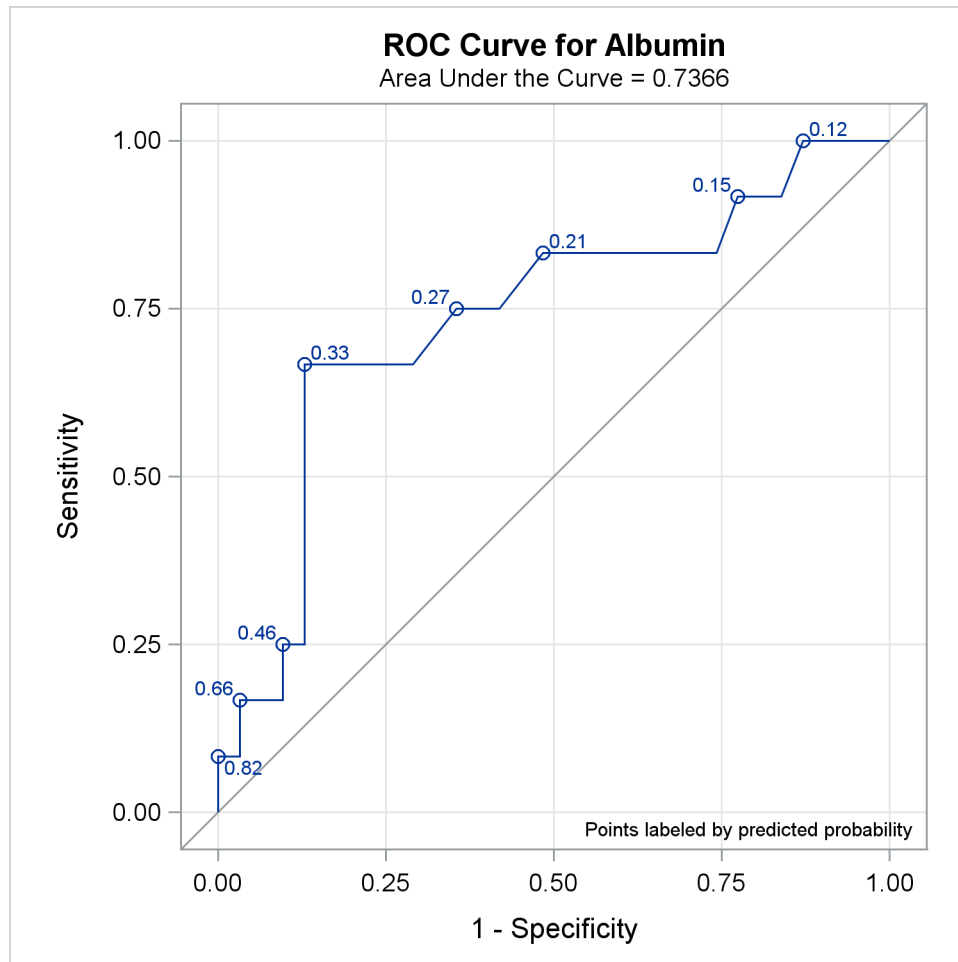
**Output 54.8.2** Fit Tables for Popind=Alb

| Model Convergence Status                      |                |                          |                |                 |            |
|-----------------------------------------------|----------------|--------------------------|----------------|-----------------|------------|
| Convergence criterion (GCONV=1E-8) satisfied. |                |                          |                |                 |            |
| Model Fit Statistics                          |                |                          |                |                 |            |
| Criterion                                     | Intercept Only | Intercept and Covariates |                |                 |            |
| AIC                                           | 52.918         | 49.384                   |                |                 |            |
| SC                                            | 54.679         | 52.907                   |                |                 |            |
| -2 Log L                                      | 50.918         | 45.384                   |                |                 |            |
| Testing Global Null Hypothesis: BETA=0        |                |                          |                |                 |            |
| Test                                          | Chi-Square     | DF                       | Pr > ChiSq     |                 |            |
| Likelihood Ratio                              | 5.5339         | 1                        | 0.0187         |                 |            |
| Score                                         | 5.6893         | 1                        | 0.0171         |                 |            |
| Wald                                          | 4.6869         | 1                        | 0.0304         |                 |            |
| Analysis of Maximum Likelihood Estimates      |                |                          |                |                 |            |
| Parameter                                     | DF             | Estimate                 | Standard Error | Wald Chi-Square | Pr > ChiSq |
| Intercept                                     | 1              | 2.4646                   | 1.5913         | 2.3988          | 0.1214     |
| alb                                           | 1              | -1.0520                  | 0.4859         | 4.6869          | 0.0304     |

**Output 54.8.2** *continued*

| Odds Ratio Estimates |                |                            |       |
|----------------------|----------------|----------------------------|-------|
| Effect               | Point Estimate | 95% Wald Confidence Limits |       |
| alb                  | 0.349          | 0.135                      | 0.905 |

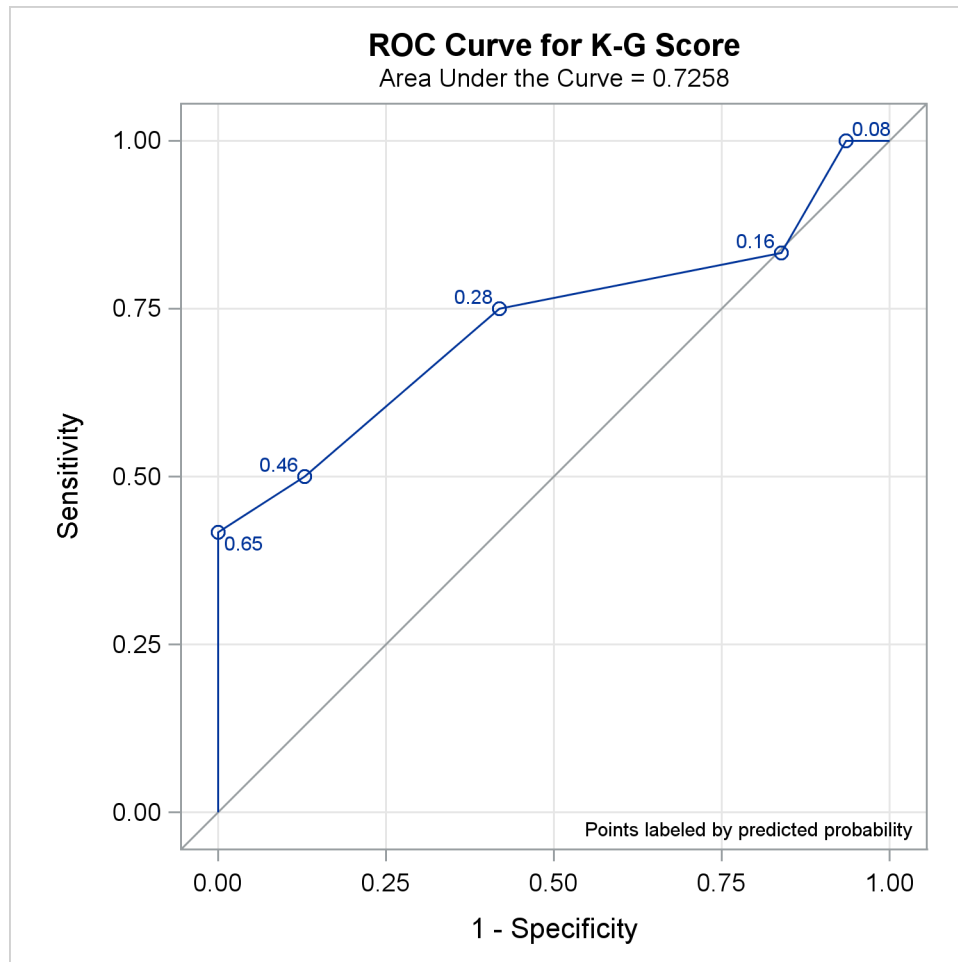
**Output 54.8.3** ROC Curve for Popind=Alb



**Output 54.8.4** Fit Tables for Popind=Totscore

| Model Convergence Status                      |                |                            |                          |                 |            |
|-----------------------------------------------|----------------|----------------------------|--------------------------|-----------------|------------|
| Convergence criterion (GCONV=1E-8) satisfied. |                |                            |                          |                 |            |
| Model Fit Statistics                          |                |                            |                          |                 |            |
| Criterion                                     | Intercept Only |                            | Intercept and Covariates |                 |            |
| AIC                                           | 52.918         |                            | 46.262                   |                 |            |
| SC                                            | 54.679         |                            | 49.784                   |                 |            |
| -2 Log L                                      | 50.918         |                            | 42.262                   |                 |            |
| Testing Global Null Hypothesis: BETA=0        |                |                            |                          |                 |            |
| Test                                          | Chi-Square     | DF                         | Pr > ChiSq               |                 |            |
| Likelihood Ratio                              | 8.6567         | 1                          | 0.0033                   |                 |            |
| Score                                         | 8.3613         | 1                          | 0.0038                   |                 |            |
| Wald                                          | 6.3845         | 1                          | 0.0115                   |                 |            |
| Analysis of Maximum Likelihood Estimates      |                |                            |                          |                 |            |
| Parameter                                     | DF             | Estimate                   | Standard Error           | Wald Chi-Square | Pr > ChiSq |
| Intercept                                     | 1              | 2.1542                     | 1.2477                   | 2.9808          | 0.0843     |
| totscore                                      | 1              | -0.7696                    | 0.3046                   | 6.3845          | 0.0115     |
| Odds Ratio Estimates                          |                |                            |                          |                 |            |
| Effect                                        | Point Estimate | 95% Wald Confidence Limits |                          |                 |            |
| totscore                                      | 0.463          | 0.255                      | 0.841                    |                 |            |

**Output 54.8.5** ROC Curve for Popind=Totscore



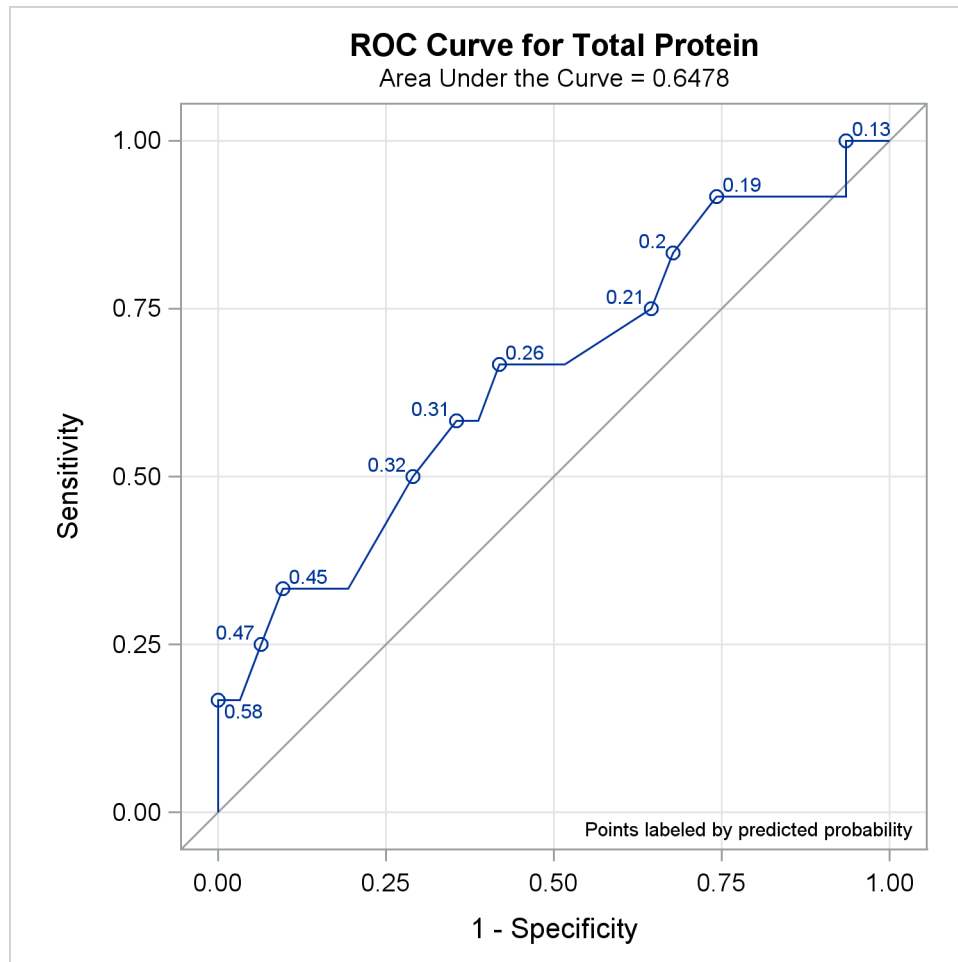
**Output 54.8.6** Fit Tables for Popind=Tp

| Model Convergence Status                      |                |                          |
|-----------------------------------------------|----------------|--------------------------|
| Convergence criterion (GCONV=1E-8) satisfied. |                |                          |
| Model Fit Statistics                          |                |                          |
| Criterion                                     | Intercept Only | Intercept and Covariates |
| AIC                                           | 52.918         | 51.794                   |
| SC                                            | 54.679         | 55.316                   |
| -2 Log L                                      | 50.918         | 47.794                   |

**Output 54.8.6** *continued*

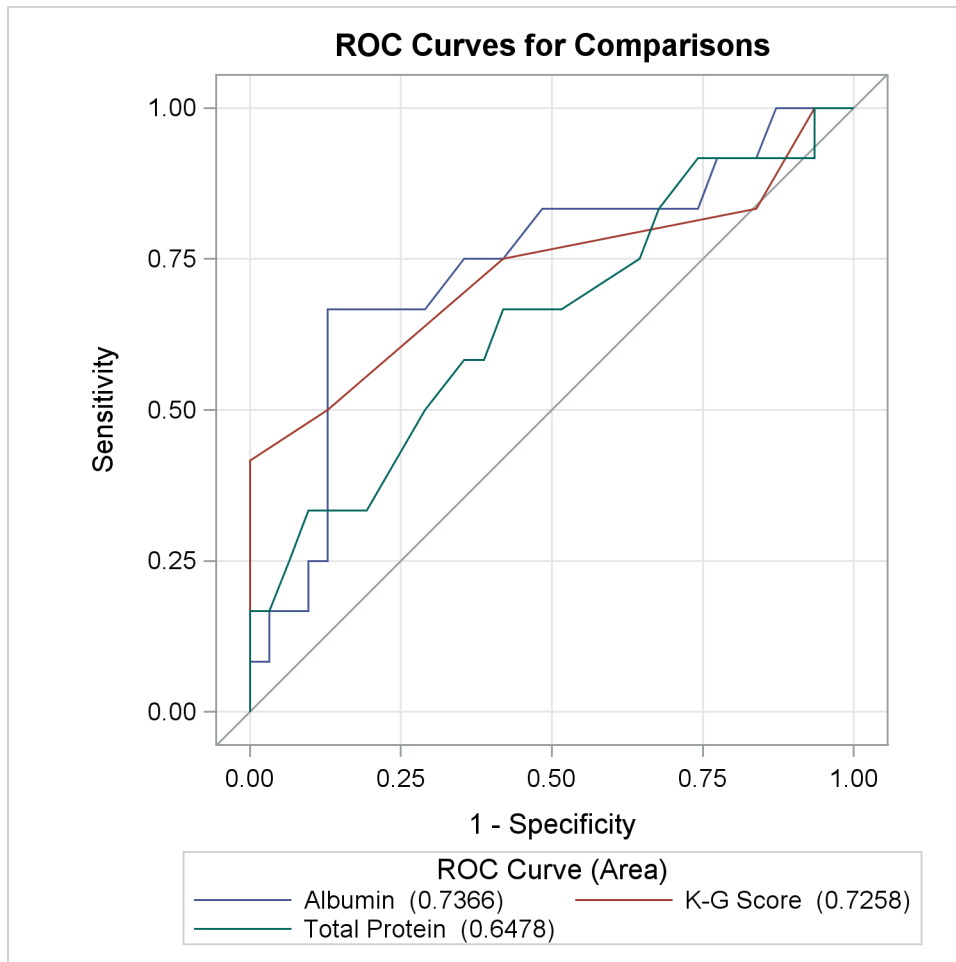
| Testing Global Null Hypothesis: BETA=0   |    |                |                            |                 |            |
|------------------------------------------|----|----------------|----------------------------|-----------------|------------|
| Test                                     |    | Chi-Square     | DF                         | Pr > ChiSq      |            |
| Likelihood Ratio                         |    | 3.1244         | 1                          | 0.0771          |            |
| Score                                    |    | 3.1123         | 1                          | 0.0777          |            |
| Wald                                     |    | 2.9059         | 1                          | 0.0883          |            |
| Analysis of Maximum Likelihood Estimates |    |                |                            |                 |            |
| Parameter                                | DF | Estimate       | Standard Error             | Wald Chi-Square | Pr > ChiSq |
| Intercept                                | 1  | 2.8295         | 2.2065                     | 1.6445          | 0.1997     |
| tp                                       | 1  | -0.6279        | 0.3683                     | 2.9059          | 0.0883     |
| Odds Ratio Estimates                     |    |                |                            |                 |            |
| Effect                                   |    | Point Estimate | 95% Wald Confidence Limits |                 |            |
| tp                                       |    | 0.534          | 0.259                      | 1.099           |            |

**Output 54.8.7** ROC Curve for Popind=Tp



All ROC curves being compared are also overlaid on the same plot, as shown in Output 54.8.8.

**Output 54.8.8** Overlay of All Models Being Compared



Output 54.8.9 displays the association statistics, and displays the area under the ROC curve along with its standard error and a confidence interval for each model in the comparison. The confidence interval for Total Protein contains 0.50; hence it is not significantly different from random guessing, which is represented by the diagonal line in the preceding ROC plots.

**Output 54.8.9** ROC Association Table

| ROC Association Statistics |        |                |                            |                     |        |        |  |
|----------------------------|--------|----------------|----------------------------|---------------------|--------|--------|--|
| ROC Model                  | Area   | Mann-Whitney   |                            | Somers' D<br>(Gini) | Gamma  | Tau-a  |  |
|                            |        | Standard Error | 95% Wald Confidence Limits |                     |        |        |  |
| Albumin                    | 0.7366 | 0.0927         | 0.5549 0.9182              | 0.4731              | 0.4809 | 0.1949 |  |
| K-G Score                  | 0.7258 | 0.1028         | 0.5243 0.9273              | 0.4516              | 0.5217 | 0.1860 |  |
| Total Protein              | 0.6478 | 0.1000         | 0.4518 0.8439              | 0.2957              | 0.3107 | 0.1218 |  |



Output 54.8.10 shows that the contrast used 'K-G Score' as the reference level. This table is produced by specifying the E option in the ROCCONTRAST statement.

**Output 54.8.10** ROC Contrast Coefficients

| ROC Contrast Coefficients |      |      |
|---------------------------|------|------|
| ROC Model                 | Row1 | Row2 |
| Albumin                   | 1    | 0    |
| K-G Score                 | -1   | -1   |
| Total Protein             | 0    | 1    |

Output 54.8.11 shows that the 2-degrees-of-freedom test that the 'K-G Score' is different from at least one other test is not significant at the 0.05 level.

**Output 54.8.11** ROC Test Results (2 Degrees of Freedom)

| ROC Contrast Test Results |    |            |            |
|---------------------------|----|------------|------------|
| Contrast                  | DF | Chi-Square | Pr > ChiSq |
| Reference = K-G Score     | 2  | 2.5340     | 0.2817     |

Output 54.8.12 is produced by specifying the ESTIMATE option in the ROCCONTRAST statement. Each row shows that the curves are not significantly different.

**Output 54.8.12** ROC Contrast Row Estimates (1-Degree-of-Freedom Tests)

| ROC Contrast Estimation and Testing Results by Row |          |                |                            |            |            |  |
|----------------------------------------------------|----------|----------------|----------------------------|------------|------------|--|
| Contrast                                           | Estimate | Standard Error | 95% Wald Confidence Limits | Chi-Square | Pr > ChiSq |  |
| Albumin - K-G Score                                | 0.0108   | 0.0953         | -0.1761 0.1976             | 0.0127     | 0.9102     |  |
| Total Protein - K-G Score                          | -0.0780  | 0.1046         | -0.2830 0.1271             | 0.5554     | 0.4561     |  |

## Example 54.9: Goodness-of-Fit Tests and Subpopulations

A study is done to investigate the effects of two binary factors, A and B, on a binary response, Y. Subjects are randomly selected from subpopulations defined by the four possible combinations of levels of A and B. The number of subjects responding with each level of Y is recorded, and the following DATA step creates the data set One:

```

data One;
 do A=0,1;
 do B=0,1;
 do Y=1,2;
 input F @@;
 output;
 end;
 end;
 end;
 datalines;
23 63 31 70 67 100 70 104
;

```

The following statements fit a full model to examine the main effects of A and B as well as the interaction effect of A and B:

```

proc logistic data=One;
 freq F;
 model Y=A B A*B;
run;

```

Results of the model fit are shown in [Output 54.9.1](#). Notice that neither the A\*B interaction nor the B main effect is significant.

**Output 54.9.1** Full Model Fit

| The LOGISTIC Procedure      |   |                  |
|-----------------------------|---|------------------|
| Model Information           |   |                  |
| Data Set                    |   | WORK.ONE         |
| Response Variable           |   | Y                |
| Number of Response Levels   |   | 2                |
| Frequency Variable          |   | F                |
| Model                       |   | binary logit     |
| Optimization Technique      |   | Fisher's scoring |
|                             |   |                  |
| Number of Observations Read |   | 8                |
| Number of Observations Used |   | 8                |
| Sum of Frequencies Read     |   | 528              |
| Sum of Frequencies Used     |   | 528              |
|                             |   |                  |
| Response Profile            |   |                  |
| Ordered Value               | Y | Total Frequency  |
| 1                           | 1 | 191              |
| 2                           | 2 | 337              |
|                             |   |                  |
| Probability modeled is Y=1. |   |                  |

## Output 54.9.1 continued

| Model Convergence Status                      |                |                          |                |                 |            |
|-----------------------------------------------|----------------|--------------------------|----------------|-----------------|------------|
| Convergence criterion (GCONV=1E-8) satisfied. |                |                          |                |                 |            |
| Model Fit Statistics                          |                |                          |                |                 |            |
| Criterion                                     | Intercept Only | Intercept and Covariates |                |                 |            |
| AIC                                           | 693.061        | 691.914                  |                |                 |            |
| SC                                            | 697.330        | 708.990                  |                |                 |            |
| -2 Log L                                      | 691.061        | 683.914                  |                |                 |            |
| Testing Global Null Hypothesis: BETA=0        |                |                          |                |                 |            |
| Test                                          | Chi-Square     | DF                       | Pr > ChiSq     |                 |            |
| Likelihood Ratio                              | 7.1478         | 3                        | 0.0673         |                 |            |
| Score                                         | 6.9921         | 3                        | 0.0721         |                 |            |
| Wald                                          | 6.9118         | 3                        | 0.0748         |                 |            |
| Analysis of Maximum Likelihood Estimates      |                |                          |                |                 |            |
| Parameter                                     | DF             | Estimate                 | Standard Error | Wald Chi-Square | Pr > ChiSq |
| Intercept                                     | 1              | -1.0074                  | 0.2436         | 17.1015         | <.0001     |
| A                                             | 1              | 0.6069                   | 0.2903         | 4.3714          | 0.0365     |
| B                                             | 1              | 0.1929                   | 0.3254         | 0.3515          | 0.5533     |
| A*B                                           | 1              | -0.1883                  | 0.3933         | 0.2293          | 0.6321     |

Pearson and deviance goodness-of-fit tests cannot be obtained for this model since a full model containing four parameters is fit, leaving no residual degrees of freedom. For a binary response model, the goodness-of-fit tests have  $m - q$  degrees of freedom, where  $m$  is the number of subpopulations and  $q$  is the number of model parameters. In the preceding model,  $m = q = 4$ , resulting in zero degrees of freedom for the tests.

The following statements fit a reduced model containing only the A effect, so two degrees of freedom become available for testing goodness of fit. Specifying the `SCALE=NONE` option requests the Pearson and deviance statistics. With single-trial syntax, the `AGGREGATE=` option is needed to define the subpopulations in the study. Specifying `AGGREGATE=(A B)` creates subpopulations of the four combinations of levels of A and B. Although the B effect is being dropped from the model, it is still needed to define the original subpopulations in the study. If `AGGREGATE=(A)` were specified, only two subpopulations would be created from the levels of A, resulting in  $m = q = 2$  and zero degrees of freedom for the tests.

```
proc logistic data=One;
 freq F;
 model Y=A / scale=none aggregate=(A B);
run;
```

The goodness-of-fit tests in [Output 54.9.2](#) show that dropping the B main effect and the A\*B interaction simultaneously does not result in significant lack of fit of the model. The tests' large  $p$ -values indicate insufficient evidence for rejecting the null hypothesis that the model fits.

**Output 54.9.2** Reduced Model Fit

| The LOGISTIC Procedure                          |        |    |          |            |
|-------------------------------------------------|--------|----|----------|------------|
| Deviance and Pearson Goodness-of-Fit Statistics |        |    |          |            |
| Criterion                                       | Value  | DF | Value/DF | Pr > ChiSq |
| Deviance                                        | 0.3541 | 2  | 0.1770   | 0.8377     |
| Pearson                                         | 0.3531 | 2  | 0.1765   | 0.8382     |
| Number of unique profiles: 4                    |        |    |          |            |

## Example 54.10: Overdispersion

In a seed germination test, seeds of two cultivars were planted in pots of two soil conditions. The following statements create the data set `seeds`, which contains the observed proportion of seeds that germinated for various combinations of cultivar and soil condition. The variable `n` represents the number of seeds planted in a pot, and the variable `r` represents the number germinated. The indicator variables `cult` and `soil` represent the cultivar and soil condition, respectively.

```
data seeds;
 input pot n r cult soil;
 datalines;
 1 16 8 0 0
 2 51 26 0 0
 3 45 23 0 0
 4 39 10 0 0
 5 36 9 0 0
 6 81 23 1 0
 7 30 10 1 0
 8 39 17 1 0
 9 28 8 1 0
 10 62 23 1 0
 11 51 32 0 1
 12 72 55 0 1
 13 41 22 0 1
 14 12 3 0 1
 15 13 10 0 1
 16 79 46 1 1
 17 30 15 1 1
 18 51 32 1 1
 19 74 53 1 1
 20 56 12 1 1
 ;
```

PROC LOGISTIC is used as follows to fit a logit model to the data, with cult, soil, and cult × soil interaction as explanatory variables. The option `SCALE=NONE` is specified to display goodness-of-fit statistics.

```
proc logistic data=seeds;
 model r/n=cult soil cult*soil/scale=none;
 title 'Full Model With SCALE=NONE';
run;
```

Results of fitting the full factorial model are shown in [Output 54.10.1](#). Both Pearson  $\chi^2$  and deviance are highly significant ( $p < 0.0001$ ), suggesting that the model does not fit well.

#### Output 54.10.1 Results of the Model Fit for the Two-Way Layout

| Full Model With SCALE=NONE                      |                          |                              |                                   |                 |            |
|-------------------------------------------------|--------------------------|------------------------------|-----------------------------------|-----------------|------------|
| The LOGISTIC Procedure                          |                          |                              |                                   |                 |            |
| Deviance and Pearson Goodness-of-Fit Statistics |                          |                              |                                   |                 |            |
| Criterion                                       | Value                    | DF                           | Value/DF                          | Pr > ChiSq      |            |
| Deviance                                        | 68.3465                  | 16                           | 4.2717                            | <.0001          |            |
| Pearson                                         | 66.7617                  | 16                           | 4.1726                            | <.0001          |            |
| Number of events/trials observations: 20        |                          |                              |                                   |                 |            |
| Model Fit Statistics                            |                          |                              |                                   |                 |            |
| Criterion                                       | Intercept and Covariates |                              |                                   |                 |            |
|                                                 | Intercept Only           | Intercept and Log Likelihood | Intercept and Full Log Likelihood |                 |            |
| AIC                                             | 1256.852                 | 1213.003                     | 156.533                           |                 |            |
| SC                                              | 1261.661                 | 1232.240                     | 175.769                           |                 |            |
| -2 Log L                                        | 1254.852                 | 1205.003                     | 148.533                           |                 |            |
| Testing Global Null Hypothesis: BETA=0          |                          |                              |                                   |                 |            |
| Test                                            | Chi-Square               | DF                           | Pr > ChiSq                        |                 |            |
| Likelihood Ratio                                | 49.8488                  | 3                            | <.0001                            |                 |            |
| Score                                           | 49.1682                  | 3                            | <.0001                            |                 |            |
| Wald                                            | 47.7623                  | 3                            | <.0001                            |                 |            |
| Analysis of Maximum Likelihood Estimates        |                          |                              |                                   |                 |            |
| Parameter                                       | DF                       | Estimate                     | Standard Error                    | Wald Chi-Square | Pr > ChiSq |
| Intercept                                       | 1                        | -0.3788                      | 0.1489                            | 6.4730          | 0.0110     |
| cult                                            | 1                        | -0.2956                      | 0.2020                            | 2.1412          | 0.1434     |
| soil                                            | 1                        | 0.9781                       | 0.2128                            | 21.1234         | <.0001     |
| cult*soil                                       | 1                        | -0.1239                      | 0.2790                            | 0.1973          | 0.6569     |

If the link function and the model specification are correct and if there are no outliers, then the lack of fit might be due to overdispersion. Without adjusting for the overdispersion, the standard errors are likely to be underestimated, causing the Wald tests to be too sensitive. In PROC LOGISTIC, there are three `SCALE=` options to accommodate overdispersion. With unequal sample sizes for the observations, `SCALE=WILLIAMS` is preferred. The Williams model estimates a scale parameter  $\phi$  by equating the value of Pearson  $\chi^2$  for the full model to its approximate expected value. The full model considered in the following statements is the model with cultivar, soil condition, and their interaction. Using a full model reduces the risk of contaminating  $\phi$  with lack of fit due to incorrect model specification.

```
proc logistic data=seeds;
 model r/n=cult soil cult*soil / scale=williams;
 title 'Full Model With SCALE=WILLIAMS';
run;
```

Results of using Williams' method are shown in [Output 54.10.2](#). The estimate of  $\phi$  is 0.075941 and is given in the formula for the Weight Variable at the beginning of the displayed output.

**Output 54.10.2** Williams' Model for Overdispersion

| Full Model With SCALE=WILLIAMS                |                                |                 |              |
|-----------------------------------------------|--------------------------------|-----------------|--------------|
| The LOGISTIC Procedure                        |                                |                 |              |
| Model Information                             |                                |                 |              |
| Data Set                                      | WORK.SEEDS                     |                 |              |
| Response Variable (Events)                    | r                              |                 |              |
| Response Variable (Trials)                    | n                              |                 |              |
| Weight Variable                               | 1 / ( 1 + 0.075941 * (n - 1) ) |                 |              |
| Model                                         | binary logit                   |                 |              |
| Optimization Technique                        | Fisher's scoring               |                 |              |
|                                               |                                |                 |              |
| Number of Observations Read                   |                                |                 | 20           |
| Number of Observations Used                   |                                |                 | 20           |
| Sum of Frequencies Read                       |                                |                 | 906          |
| Sum of Frequencies Used                       |                                |                 | 906          |
| Sum of Weights Read                           |                                |                 | 198.3216     |
| Sum of Weights Used                           |                                |                 | 198.3216     |
|                                               |                                |                 |              |
| Response Profile                              |                                |                 |              |
| Ordered Value                                 | Binary Outcome                 | Total Frequency | Total Weight |
| 1                                             | Event                          | 437             | 92.95346     |
| 2                                             | Nonevent                       | 469             | 105.36819    |
|                                               |                                |                 |              |
| Model Convergence Status                      |                                |                 |              |
| Convergence criterion (GCONV=1E-8) satisfied. |                                |                 |              |

## Output 54.10.2 continued

| Deviance and Pearson Goodness-of-Fit Statistics                                                                                                                                              |                |                          |                     |                 |            |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------|--------------------------|---------------------|-----------------|------------|
| Criterion                                                                                                                                                                                    | Value          | DF                       | Value/DF            | Pr > ChiSq      |            |
| Deviance                                                                                                                                                                                     | 16.4402        | 16                       | 1.0275              | 0.4227          |            |
| Pearson                                                                                                                                                                                      | 16.0000        | 16                       | 1.0000              | 0.4530          |            |
| Number of events/trials observations: 20                                                                                                                                                     |                |                          |                     |                 |            |
| NOTE: Since the Williams method was used to accommodate overdispersion, the Pearson chi-squared statistic and the deviance can no longer be used to assess the goodness of fit of the model. |                |                          |                     |                 |            |
| Model Fit Statistics                                                                                                                                                                         |                |                          |                     |                 |            |
| Criterion                                                                                                                                                                                    | Intercept Only | Intercept and Covariates |                     |                 |            |
|                                                                                                                                                                                              |                | Log Likelihood           | Full Log Likelihood |                 |            |
| AIC                                                                                                                                                                                          | 276.155        | 273.586                  | 44.579              |                 |            |
| SC                                                                                                                                                                                           | 280.964        | 292.822                  | 63.815              |                 |            |
| -2 Log L                                                                                                                                                                                     | 274.155        | 265.586                  | 36.579              |                 |            |
| Testing Global Null Hypothesis: BETA=0                                                                                                                                                       |                |                          |                     |                 |            |
| Test                                                                                                                                                                                         | Chi-Square     | DF                       | Pr > ChiSq          |                 |            |
| Likelihood Ratio                                                                                                                                                                             | 8.5687         | 3                        | 0.0356              |                 |            |
| Score                                                                                                                                                                                        | 8.4856         | 3                        | 0.0370              |                 |            |
| Wald                                                                                                                                                                                         | 8.3069         | 3                        | 0.0401              |                 |            |
| Analysis of Maximum Likelihood Estimates                                                                                                                                                     |                |                          |                     |                 |            |
| Parameter                                                                                                                                                                                    | DF             | Estimate                 | Standard Error      | Wald Chi-Square | Pr > ChiSq |
| Intercept                                                                                                                                                                                    | 1              | -0.3926                  | 0.2932              | 1.7932          | 0.1805     |
| cult                                                                                                                                                                                         | 1              | -0.2618                  | 0.4160              | 0.3963          | 0.5290     |
| soil                                                                                                                                                                                         | 1              | 0.8309                   | 0.4223              | 3.8704          | 0.0491     |
| cult*soil                                                                                                                                                                                    | 1              | -0.0532                  | 0.5835              | 0.0083          | 0.9274     |

Since neither cult nor cult  $\times$  soil is statistically significant ( $p = 0.5290$  and  $p = 0.9274$ , respectively), a reduced model that contains only the soil condition factor is fitted, with the observations weighted by  $1/(1 + 0.075941(N - 1))$ . This can be done conveniently in PROC LOGISTIC by including the scale estimate in the SCALE=WILLIAMS option as follows:

```
proc logistic data=seeds;
 model r/n=soil / scale=williams(0.075941);
 title 'Reduced Model With SCALE=WILLIAMS(0.075941)';
run;
```

Results of the reduced model fit are shown in [Output 54.10.3](#). Soil condition remains a significant factor ( $p = 0.0064$ ) for the seed germination.

**Output 54.10.3** Reduced Model with Overdispersion Controlled

| Reduced Model With SCALE=WILLIAMS(0.075941) |    |          |                |                 |            |
|---------------------------------------------|----|----------|----------------|-----------------|------------|
| The LOGISTIC Procedure                      |    |          |                |                 |            |
| Analysis of Maximum Likelihood Estimates    |    |          |                |                 |            |
| Parameter                                   | DF | Estimate | Standard Error | Wald Chi-Square | Pr > ChiSq |
| Intercept                                   | 1  | -0.5249  | 0.2076         | 6.3949          | 0.0114     |
| soil                                        | 1  | 0.7910   | 0.2902         | 7.4284          | 0.0064     |

### Example 54.11: Conditional Logistic Regression for Matched Pairs Data

In matched pairs, or *case-control*, studies, conditional logistic regression is used to investigate the relationship between an outcome of being an event (case) or a nonevent (control) and a set of prognostic factors.

The following data are a subset of the data from the Los Angeles Study of the Endometrial Cancer Data in Breslow and Day (1980). There are 63 matched pairs, each consisting of a case of endometrial cancer (Outcome=1) and a control (Outcome=0). The case and corresponding control have the same ID. Two prognostic factors are included: Gall (an indicator variable for gall bladder disease) and Hyper (an indicator variable for hypertension). The goal of the case-control analysis is to determine the relative risk for gall bladder disease, controlling for the effect of hypertension.

```
data Data1;
 do ID=1 to 63;
 do Outcome = 1 to 0 by -1;
 input Gall Hyper @@;
 output;
 end;
 end;
 datalines;
0 0 0 0 0 0 0 0 0 1 0 1 0 0 1 0 1 0 0 1 1 0 0 1
0 1 0 0 1 0 0 0 1 1 0 1 0 0 0 0 0 0 0 0 0 0 0 0
1 0 0 0 0 0 0 1 1 0 0 1 1 0 1 0 1 0 1 0 0 1 1 0 0 1
0 1 0 0 0 0 1 1 0 0 1 1 0 0 0 1 0 1 0 0 0 1 0 0 0
0 0 1 1 0 1 0 1 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 1 1 0 0 1 0 0 1 0 0 0 1 1 0 0 0 0 0 1 0 0 0
0 1 0 0 0 1 0 0 0 1 0 0 0 0 0 0 0 0 0 0 1 1 1 1
0 0 0 1 0 1 0 0 0 1 0 1 0 1 0 1 0 1 0 1 0 1 0 0 0
0 0 0 0 0 1 1 0 0 0 0 1 0 0 0 0 0 0 0 0 1 0 0 0
0 0 0 0 1 1 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 1 0 1
0 0 0 0 0 1 0 1 0 1 0 1 0 0 0 1 0 0 0 1 0 0 0 0
0 0 0 0 1 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 1 1 0 0
1 0 1 0 0 1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
;
```



There are several ways to approach this problem with PROC LOGISTIC:

- Specify the **STRATA** statement to perform a conditional logistic regression.
- Specify **EXACT** and **STRATA** statements to perform an exact logistic regression on the original data set, if you believe the data set is too small or too sparse for the usual asymptotics to hold.
- Transform each matched pair into a single observation, and then specify a PROC LOGISTIC statement on this transformed data without a STRATA statement; this also performs a conditional logistic regression and produces essentially the same results.
- Specify an **EXACT** statement on the transformed data.

SAS statements and selected results for these four approaches are given in the remainder of this example.

### Conditional Analysis Using the STRATA Statement

In the following statements, PROC LOGISTIC is invoked with the ID variable declared in the **STRATA** statement to obtain the conditional logistic model estimates for a model containing Gall as the only predictor variable:

```
proc logistic data=Data1;
 strata ID;
 model outcome(event='1')=Gall;
run;
```

Results from the conditional logistic analysis are shown in [Output 54.11.1](#). Note that there is no intercept term in the “Analysis of Maximum Likelihood Estimates” tables.

The odds ratio estimate for Gall is 2.60, which is marginally significant ( $p = 0.0694$ ) and which is an estimate of the relative risk for gall bladder disease. A 95% confidence interval for this relative risk is (0.927, 7.293).

**Output 54.11.1** Conditional Logistic Regression (Gall as Risk Factor)

| The LOGISTIC Procedure      |                      |
|-----------------------------|----------------------|
| Conditional Analysis        |                      |
| Model Information           |                      |
| Data Set                    | WORK.DATA1           |
| Response Variable           | Outcome              |
| Number of Response Levels   | 2                    |
| Number of Strata            | 63                   |
| Model                       | binary logit         |
| Optimization Technique      | Newton-Raphson ridge |
| Number of Observations Read | 126                  |
| Number of Observations Used | 126                  |

**Output 54.11.1** *continued*

| Response Profile                                     |                    |                 |                  |                 |            |
|------------------------------------------------------|--------------------|-----------------|------------------|-----------------|------------|
| Ordered Value                                        | Outcome            | Total Frequency |                  |                 |            |
| 1                                                    | 0                  | 63              |                  |                 |            |
| 2                                                    | 1                  | 63              |                  |                 |            |
| Probability modeled is Outcome=1.                    |                    |                 |                  |                 |            |
| Strata Summary                                       |                    |                 |                  |                 |            |
| Response Pattern                                     | Outcome            |                 | Number of Strata | Frequency       |            |
|                                                      | 0                  | 1               |                  |                 |            |
| 1                                                    | 1                  | 1               | 63               | 126             |            |
| Newton-Raphson Ridge Optimization                    |                    |                 |                  |                 |            |
| Without Parameter Scaling                            |                    |                 |                  |                 |            |
| Convergence criterion (GCONV=1E-8) satisfied.        |                    |                 |                  |                 |            |
| Model Fit Statistics                                 |                    |                 |                  |                 |            |
| Criterion                                            | Without Covariates |                 | With Covariates  |                 |            |
| AIC                                                  | 87.337             |                 | 85.654           |                 |            |
| SC                                                   | 87.337             |                 | 88.490           |                 |            |
| -2 Log L                                             | 87.337             |                 | 83.654           |                 |            |
| Testing Global Null Hypothesis: BETA=0               |                    |                 |                  |                 |            |
| Test                                                 | Chi-Square         | DF              | Pr > ChiSq       |                 |            |
| Likelihood Ratio                                     | 3.6830             | 1               | 0.0550           |                 |            |
| Score                                                | 3.5556             | 1               | 0.0593           |                 |            |
| Wald                                                 | 3.2970             | 1               | 0.0694           |                 |            |
| Analysis of Conditional Maximum Likelihood Estimates |                    |                 |                  |                 |            |
| Parameter                                            | DF                 | Estimate        | Standard Error   | Wald Chi-Square | Pr > ChiSq |
| Gall                                                 | 1                  | 0.9555          | 0.5262           | 3.2970          | 0.0694     |

**Output 54.11.1** *continued*

| Odds Ratio Estimates |                |                            |       |
|----------------------|----------------|----------------------------|-------|
| Effect               | Point Estimate | 95% Wald Confidence Limits |       |
| Gall                 | 2.600          | 0.927                      | 7.293 |

**Exact Analysis Using the STRATA Statement**

When you believe there are not enough data or that the data are too sparse, you can perform a stratified exact logistic regression. The following statements perform stratified exact logistic regressions on the original data set by specifying both the **STRATA** and **EXACT** statements:

```
proc logistic data=Data1 exactonly;
 strata ID;
 model outcome(event='1')=Gall;
 exact Gall / estimate=both;
run;
```

**Output 54.11.2** Exact Logistic Regression (Gall as Risk Factor)

| The LOGISTIC Procedure     |             |                       |                       |                   |                   |
|----------------------------|-------------|-----------------------|-----------------------|-------------------|-------------------|
| Exact Conditional Analysis |             |                       |                       |                   |                   |
| Exact Conditional Tests    |             |                       |                       |                   |                   |
| Effect                     | Test        | Statistic             | --- p-Value ---       |                   |                   |
|                            |             |                       | Exact                 | Mid               |                   |
| Gall                       | Score       | 3.5556                | 0.0963                | 0.0799            |                   |
|                            | Probability | 0.0327                | 0.0963                | 0.0799            |                   |
| Exact Parameter Estimates  |             |                       |                       |                   |                   |
| Parameter                  | Estimate    | Standard Error        | 95% Confidence Limits |                   | Two-sided p-Value |
| Gall                       | 0.9555      | 0.5262                | -0.1394               | 2.2316            | 0.0963            |
| Exact Odds Ratios          |             |                       |                       |                   |                   |
| Parameter                  | Estimate    | 95% Confidence Limits |                       | Two-sided p-Value |                   |
| Gall                       | 2.600       | 0.870                 | 9.315                 | 0.0963            |                   |

Note that the score statistic in the “Conditional Exact Tests” table in [Output 54.11.2](#) is identical to the score statistic in [Output 54.11.1](#) from the conditional analysis. The exact odds ratio confidence interval is much wider than its conditional analysis counterpart, but the parameter estimates are similar. The exact analysis confirms the marginal significance of Gall as a predictor variable.

### Conditional Analysis Using Transformed Data

When each matched set consists of one event and one nonevent, the conditional likelihood is given by

$$\prod_i (1 + \exp(-\beta'(x_{i1} - x_{i0})))^{-1}$$

where  $x_{i1}$  and  $x_{i0}$  are vectors representing the prognostic factors for the event and nonevent, respectively, of the  $i$ th matched set. This likelihood is identical to the likelihood of fitting a logistic regression model to a set of data with constant response, where the model contains no intercept term and has explanatory variables given by  $d_i = x_{i1} - x_{i0}$  (Breslow 1982).

To apply this method, the following DATA step transforms each matched pair into a single observation, where the variables Gall and Hyper contain the differences between the corresponding values for the case and the control (case-control). The variable Outcome, which will be used as the response variable in the logistic regression model, is given a constant value of 0 (which is the Outcome value for the control, although any constant, numeric or character, will suffice).

```
data Data2;
 set Data1;
 drop id1 gall1 hyper1;
 retain id1 gall1 hyper1 0;
 if (ID = id1) then do;
 Gall=gall1-Gall; Hyper=hyper1-Hyper;
 output;
 end;
 else do;
 id1=ID; gall1=Gall; hyper1=Hyper;
 end;
run;
```

Note that there are 63 observations in the data set, one for each matched pair. Since the number of observations  $n$  is halved, statistics that depend on  $n$  such as R Square (see the “[Generalized Coefficient of Determination](#)” on page 4246 section) will be incorrect. The variable Outcome has a constant value of 0.

In the following statements, PROC LOGISTIC is invoked with the NOINT option to obtain the conditional logistic model estimates. Because the option CLODDS=PL is specified, PROC LOGISTIC computes a 95% profile-likelihood confidence interval for the odds ratio for each predictor variable; note that profile-likelihood confidence intervals are not currently available when a STRATA statement is specified.

```
proc logistic data=Data2;
 model outcome=Gall / noint clodds=PL;
run;
```

The results are not displayed here.

## Exact Analysis Using Transformed Data

Sometimes the original data set in a matched-pairs study is too large for the exact methods to handle. In such cases it might be possible to use the transformed data set. The following statements perform exact logistic regressions on the transformed data set. The results are not displayed here.

```
proc logistic data=Data2 exactonly;
 model outcome=Gall / noint;
 exact Gall / estimate=both;
run;
```

---

## Example 54.12: Firth's Penalized Likelihood Compared with Other Approaches

Firth's penalized likelihood approach is a method of addressing issues of separability, small sample sizes, and bias of the parameter estimates. This example performs some comparisons between results from using the `FIRTH` option to results from the usual unconditional, conditional, and exact logistic regression analyses. When the sample size is large enough, the unconditional estimates and the Firth penalized-likelihood estimates should be nearly the same. These examples show that Firth's penalized likelihood approach compares favorably with unconditional, conditional, and exact logistic regression; however, this is not an exhaustive analysis of Firth's method. For more detailed analyses with separable data sets, see Heinze (2006, 1999) and Heinze and Schemper (2002).

### Comparison on 2x2 Tables with One Zero Cell

A  $2 \times 2$  table with one cell having zero frequency, where the rows of the table are the levels of a covariate while the columns are the levels of the response variable, is an example of a quasi-completely separated data set. The parameter estimate for the covariate under unconditional logistic regression will move off to infinity, although PROC LOGISTIC will stop the iterations at an earlier point in the process. An exact logistic regression is sometimes performed to determine the importance of the covariate in describing the variation in the data, but the median-unbiased parameter estimate, while finite, might not be near the true value, and one confidence limit (for this example, the upper) is always infinite.

The following DATA step produces 1000 different  $2 \times 2$  tables, all following an underlying probability structure, with one cell having a near zero probability of being observed:

```
%let beta0=-15;
%let beta1=16;
data one;
 keep sample X y pry;
 do sample=1 to 1000;
 do i=1 to 100;
 X=rantbl(987987, .4, .6)-1;
 xb= &beta0 + X*&beta1;
 exb=exp(xb);
 pry= exb/(1+exb);
 cut= ranuni(393993);
 if (pry < cut) then y=1; else y=0;
 output;
 end;
 end;
```

```
end;
run;
```

The following statements perform the bias-corrected and exact logistic regression on each of the 1000 different data sets, output the odds ratio tables by using the ODS OUTPUT statement, and compute various statistics across the data sets by using the MEANS procedure:

```
ods exclude all;
proc logistic data=one;
 by sample;
 class X(param=ref);
 model y(event='1')=X / firth clodds=pl;
 ods output cloddspl=firth;
run;
proc logistic data=one exactonly;
 by sample;
 class X(param=ref);
 model y(event='1')=X;
 exact X / estimate=odds;
 ods output exactoddsratio=exact;
run;
ods select all;
proc means data=firth;
 var LowerCL OddsRatioEst UpperCL;
run;
proc means data=exact;
 var LowerCL Estimate UpperCL;
run;
```

The results of the PROC MEANS statements are summarized in [Table 54.16](#). You can see that the odds ratios are all quite large; the confidence limits on every table suggest that the covariate X is a significant factor in explaining the variability in the data.

**Table 54.16** Odds Ratio Results

| Method | Mean Estimate | Standard Error | Minimum Lower CL | Maximum Upper CL |
|--------|---------------|----------------|------------------|------------------|
| Firth  | 231.59        | 83.57          | 10.40            | 111317           |
| Exact  | 152.02        | 52.30          | 11.16            | ∞                |

### Comparison on Case-Control Data

Case-control models contain an intercept term for every case-control pair in the data set. This means that there are a large number of parameters compared to the number of observations. Breslow and Day (1980) note that the estimates from unconditional logistic regression are biased with the corresponding odds ratios off by a power of 2 from the true value; conditional logistic regression was developed to remedy this.

The following DATA step produces 1000 case-control data sets, with pair indicating the strata:

```

%let beta0=1;
%let beta1=2;
data one;
 do sample=1 to 1000;
 do pair=1 to 20;
 ran=ranuni(939393);
 a=3*ranuni(9384984)-1;
 pdf0= pdf('NORMAL', a, .4, 1);
 pdf1= pdf('NORMAL', a, 1, 1);
 pry0= pdf0/(pdf0+pdf1);
 pry1= 1-pry0;
 xb= log(pry0/pry1);
 x= (xb-&beta0*pair/100) / &beta1;
 y=0;
 output;
 x= (-xb-&beta0*pair/100) / &beta1;
 y=1;
 output;
 end;
 end;
run;

```

Unconditional, conditional, exact, and Firth-adjusted analyses are performed on the data sets, and the mean, minimum, and maximum odds ratios and the mean upper and lower limits for the odds ratios are displayed in Table 54.17. **CAUTION:** Due to the exact analyses, this program takes a long time and a lot of resources to run. You might want to reduce the number of samples generated.

```

ods exclude all;
proc logistic data=one;
 by sample;
 class pair / param=ref;
 model y=x pair / clodds=pl;
 ods output cloddspl=oru;
run;
data oru;
 set oru;
 if Effect='x';
 rename lowercl=lclu uppercl=uclu oddsratioest=orestu;
run;
proc logistic data=one;
 by sample;
 strata pair;
 model y=x / clodds=wald;
 ods output cloddswald=orc;
run;
data orc;
 set orc;
 if Effect='x';
 rename lowercl=lclc uppercl=uclc oddsratioest=orestc;
run;
proc logistic data=one exactonly;
 by sample;
 strata pair;

```

```

model y=x;
exact x / estimate=both;
ods output ExactOddsRatio=ore;
run;
proc logistic data=one;
by sample;
class pair / param=ref;
model y=x pair / firth clodds=pl;
ods output cloddspl=orf;
run;
data orf;
set orf;
if Effect='x';
rename lowercl=lclf uppercl=uclf oddsratioest=orestf;
run;
data all;
merge oru orc ore orf;
run;
ods select all;
proc means data=all;
run;

```

You can see from Table 54.17 that the conditional, exact, and Firth-adjusted results are all comparable, while the unconditional results are several orders of magnitude different.

**Table 54.17** Odds Ratio Estimates

| Method        | N    | Minimum | Mean   | Maximum |
|---------------|------|---------|--------|---------|
| Unconditional | 1000 | 0.00045 | 112.09 | 38038   |
| Conditional   | 1000 | 0.021   | 4.20   | 195     |
| Exact         | 1000 | 0.021   | 4.20   | 195     |
| Firth         | 1000 | 0.018   | 4.89   | 71      |

Further examination of the data set all shows that the differences between the square root of the unconditional odds ratio estimates and the conditional estimates have mean  $-0.00019$  and standard deviation  $0.0008$ , verifying that the unconditional odds ratio is about the square of the conditional odds ratio. The conditional and exact conditional odds ratios are also nearly equal, with their differences having mean  $3E-7$  and standard deviation  $6E-6$ . The differences between the Firth and the conditional odds ratios can be large (mean  $0.69$ , standard deviation  $5.40$ ), but their relative differences,  $\frac{\text{Firth} - \text{Conditional}}{\text{Conditional}}$ , have mean  $0.20$  with standard deviation  $0.19$ , so the largest differences occur with the larger estimates.

### Example 54.13: Complementary Log-Log Model for Infection Rates

Antibodies produced in response to an infectious disease like malaria remain in the body after the individual has recovered from the disease. A serological test detects the presence or absence of such antibodies. An individual with such antibodies is called seropositive. In geographic areas where the disease is endemic, the inhabitants are at fairly constant risk of infection. The probability of an individual never having been



infected in  $Y$  years is  $\exp(-\mu Y)$ , where  $\mu$  is the mean number of infections per year (see the appendix of Draper, Voller, and Carpenter 1972). Rather than estimating the unknown  $\mu$ , epidemiologists want to estimate the probability of a person living in the area being infected in one year. This infection rate  $\gamma$  is given by

$$\gamma = 1 - e^{-\mu}$$

The following statements create the data set `sero`, which contains the results of a serological survey of malarial infection. Individuals of nine age groups (Group) were tested. The variable `A` represents the midpoint of the age range for each age group. The variable `N` represents the number of individuals tested in each age group, and the variable `R` represents the number of individuals that are seropositive.

```
data sero;
 input Group A N R;
 X=log(A);
 label X='Log of Midpoint of Age Range';
 datalines;
1 1.5 123 8
2 4.0 132 6
3 7.5 182 18
4 12.5 140 14
5 17.5 138 20
6 25.0 161 39
7 35.0 133 19
8 47.0 92 25
9 60.0 74 44
;
```

For the  $i$ th group with the age midpoint  $A_i$ , the probability of being seropositive is  $p_i = 1 - \exp(-\mu A_i)$ . It follows that

$$\log(-\log(1 - p_i)) = \log(\mu) + \log(A_i)$$

By fitting a binomial model with a complementary log-log link function and by using `X=log(A)` as an offset term, you can estimate  $\alpha = \log(\mu)$  as an intercept parameter. The following statements invoke PROC LOGISTIC to compute the maximum likelihood estimate of  $\alpha$ . The `LINK=CLOGLOG` option is specified to request the complementary log-log link function. Also specified is the `CLPARM=PL` option, which requests the profile-likelihood confidence limits for  $\alpha$ .

```
proc logistic data=sero;
 model R/N= / offset=X
 link=cloglog
 clparm=pl
 scale=none;
 title 'Constant Risk of Infection';
run;
```

Results of fitting this constant risk model are shown in [Output 54.13.1](#).

**Output 54.13.1** Modeling Constant Risk of Infection

| Constant Risk of Infection                      |                  |                              |                 |            |
|-------------------------------------------------|------------------|------------------------------|-----------------|------------|
| The LOGISTIC Procedure                          |                  |                              |                 |            |
| Model Information                               |                  |                              |                 |            |
| Data Set                                        | WORK.SERO        |                              |                 |            |
| Response Variable (Events)                      | R                |                              |                 |            |
| Response Variable (Trials)                      | N                |                              |                 |            |
| Offset Variable                                 | X                | Log of Midpoint of Age Range |                 |            |
| Model                                           | binary cloglog   |                              |                 |            |
| Optimization Technique                          | Fisher's scoring |                              |                 |            |
|                                                 |                  |                              |                 |            |
| Number of Observations Read                     |                  |                              |                 | 9          |
| Number of Observations Used                     |                  |                              |                 | 9          |
| Sum of Frequencies Read                         |                  |                              |                 | 1175       |
| Sum of Frequencies Used                         |                  |                              |                 | 1175       |
|                                                 |                  |                              |                 |            |
| Response Profile                                |                  |                              |                 |            |
|                                                 | Ordered Value    | Binary Outcome               | Total Frequency |            |
|                                                 | 1                | Event                        | 193             |            |
|                                                 | 2                | Nonevent                     | 982             |            |
|                                                 |                  |                              |                 |            |
| Intercept-Only Model Convergence Status         |                  |                              |                 |            |
| Convergence criterion (GCONV=1E-8) satisfied.   |                  |                              |                 |            |
|                                                 |                  |                              |                 |            |
| -2 Log L = 967.1158                             |                  |                              |                 |            |
|                                                 |                  |                              |                 |            |
| Deviance and Pearson Goodness-of-Fit Statistics |                  |                              |                 |            |
| Criterion                                       | Value            | DF                           | Value/DF        | Pr > ChiSq |
| Deviance                                        | 41.5032          | 8                            | 5.1879          | <.0001     |
| Pearson                                         | 50.6883          | 8                            | 6.3360          | <.0001     |
|                                                 |                  |                              |                 |            |
| Number of events/trials observations: 9         |                  |                              |                 |            |

Output 54.13.1 continued

| Analysis of Maximum Likelihood Estimates |    |          |                |                 |            |
|------------------------------------------|----|----------|----------------|-----------------|------------|
| Parameter                                | DF | Estimate | Standard Error | Wald Chi-Square | Pr > ChiSq |
| Intercept                                | 1  | -4.6605  | 0.0725         | 4133.5626       | <.0001     |
| X                                        | 0  | 1.0000   | 0              | .               | .          |

| Parameter Estimates and Profile-Likelihood Confidence Intervals |          |                       |         |
|-----------------------------------------------------------------|----------|-----------------------|---------|
| Parameter                                                       | Estimate | 95% Confidence Limits |         |
| Intercept                                                       | -4.6605  | -4.8057               | -4.5219 |

Output 54.13.1 shows that the maximum likelihood estimate of  $\alpha = \log(\mu)$  and its estimated standard error are  $\hat{\alpha} = -4.6605$  and  $\hat{\sigma}_{\hat{\alpha}} = 0.0725$ , respectively. The infection rate is estimated as

$$\hat{\gamma} = 1 - e^{-\hat{\mu}} = 1 - e^{-e^{\hat{\beta}_0}} = 1 - e^{-e^{-4.6605}} = 0.00942$$

The 95% confidence interval for  $\gamma$ , obtained by back-transforming the 95% confidence interval for  $\alpha$ , is (0.0082, 0.0108); that is, there is a 95% chance that, in repeated sampling, the interval of 8 to 11 infections per thousand individuals contains the true infection rate.

The goodness-of-fit statistics for the constant risk model are statistically significant ( $p < 0.0001$ ), indicating that the assumption of constant risk of infection is not correct. You can fit a more extensive model by allowing a separate risk of infection for each age group. Suppose  $\mu_i$  is the mean number of infections per year for the  $i$ th age group. The probability of seropositive for the  $i$ th group with the age midpoint  $A_i$  is  $p_i = 1 - \exp(-\mu_i A_i)$ , so that

$$\log(-\log(1 - p_i)) = \log(\mu_i) + \log(A_i)$$

In the following statements, a complementary log-log model is fit containing Group as an explanatory classification variable with the GLM coding (so that a dummy variable is created for each age group), no intercept term, and X=log(A) as an offset term. The ODS OUTPUT statement saves the estimates and their 95% profile-likelihood confidence limits to the ClparmPL data set. Note that  $\log(\mu_i)$  is the regression parameter associated with Group=  $i$ .

```
proc logistic data=sero;
 ods output ClparmPL=ClparmPL;
 class Group / param=glm;
 model R/N=Group / noint
 offset=X
 link=cloglog
 clparm=pl;
 title 'Infectious Rates and 95% Confidence Intervals';
run;
```

Results of fitting the model with a separate risk of infection are shown in Output 54.13.2.

**Output 54.13.2** Modeling Separate Risk of Infection

| Infectious Rates and 95% Confidence Intervals |    |          |                |                 |            |  |
|-----------------------------------------------|----|----------|----------------|-----------------|------------|--|
| The LOGISTIC Procedure                        |    |          |                |                 |            |  |
| Analysis of Maximum Likelihood Estimates      |    |          |                |                 |            |  |
| Parameter                                     | DF | Estimate | Standard Error | Wald Chi-Square | Pr > ChiSq |  |
| Group 1                                       | 1  | -3.1048  | 0.3536         | 77.0877         | <.0001     |  |
| Group 2                                       | 1  | -4.4542  | 0.4083         | 119.0164        | <.0001     |  |
| Group 3                                       | 1  | -4.2769  | 0.2358         | 328.9593        | <.0001     |  |
| Group 4                                       | 1  | -4.7761  | 0.2674         | 319.0600        | <.0001     |  |
| Group 5                                       | 1  | -4.7165  | 0.2238         | 443.9920        | <.0001     |  |
| Group 6                                       | 1  | -4.5012  | 0.1606         | 785.1350        | <.0001     |  |
| Group 7                                       | 1  | -5.4252  | 0.2296         | 558.1114        | <.0001     |  |
| Group 8                                       | 1  | -4.9987  | 0.2008         | 619.4666        | <.0001     |  |
| Group 9                                       | 1  | -4.1965  | 0.1559         | 724.3157        | <.0001     |  |
| X                                             | 0  | 1.0000   | 0              | .               | .          |  |

| Parameter Estimates and Profile-Likelihood Confidence Intervals |   |          |                       |         |
|-----------------------------------------------------------------|---|----------|-----------------------|---------|
| Parameter                                                       |   | Estimate | 95% Confidence Limits |         |
| Group 1                                                         | 1 | -3.1048  | -3.8880               | -2.4833 |
| Group 2                                                         | 2 | -4.4542  | -5.3769               | -3.7478 |
| Group 3                                                         | 3 | -4.2769  | -4.7775               | -3.8477 |
| Group 4                                                         | 4 | -4.7761  | -5.3501               | -4.2940 |
| Group 5                                                         | 5 | -4.7165  | -5.1896               | -4.3075 |
| Group 6                                                         | 6 | -4.5012  | -4.8333               | -4.2019 |
| Group 7                                                         | 7 | -5.4252  | -5.9116               | -5.0063 |
| Group 8                                                         | 8 | -4.9987  | -5.4195               | -4.6289 |
| Group 9                                                         | 9 | -4.1965  | -4.5164               | -3.9037 |

For the first age group (Group=1), the point estimate of  $\log(\mu_1)$  is  $-3.1048$ , which transforms into an infection rate of  $1 - \exp(-\exp(-3.1048)) = 0.0438$ . A 95% confidence interval for this infection rate is obtained by transforming the 95% confidence interval for  $\log(\mu_1)$ . For the first age group, the lower and upper confidence limits are  $1 - \exp(-\exp(-3.8880)) = 0.0203$  and  $1 - \exp(-\exp(-2.4833)) = 0.0801$ , respectively; that is, there is a 95% chance that, in repeated sampling, the interval of 20 to 80 infections per thousand individuals contains the true infection rate. The following statements perform this transformation on the estimates and confidence limits saved in the ClparmPL data set; the resulting estimated infection rates in one year's time for each age group are displayed in Table 54.18. Note that the infection rate for the first age group is high compared to that of the other age groups.

```
data ClparmPL;
 set ClparmPL;
 Estimate=round(1000*(1-exp(-exp(Estimate))));
 LowerCL =round(1000*(1-exp(-exp(LowerCL)));
 UpperCL =round(1000*(1-exp(-exp(UpperCL)));
run;
```

**Table 54.18** Infection Rate in One Year

| Age Group | Number Infected per 1,000 People |           |           |
|-----------|----------------------------------|-----------|-----------|
|           | Point Estimate                   | 95% Lower | 95% Upper |
| 1         | 44                               | 20        | 80        |
| 2         | 12                               | 5         | 23        |
| 3         | 14                               | 8         | 21        |
| 4         | 8                                | 5         | 14        |
| 5         | 9                                | 6         | 13        |
| 6         | 11                               | 8         | 15        |
| 7         | 4                                | 3         | 7         |
| 8         | 7                                | 4         | 10        |
| 9         | 15                               | 11        | 20        |

### Example 54.14: Complementary Log-Log Model for Interval-Censored Survival Times

Often survival times are not observed more precisely than the interval (for instance, a day) within which the event occurred. Survival data of this form are known as grouped or interval-censored data. A discrete analog of the continuous proportional hazards model (Prentice and Gloeckler 1978; Allison 1982) is used to investigate the relationship between these survival times and a set of explanatory variables.

Suppose  $T_i$  is the discrete survival time variable of the  $i$ th subject with covariates  $\mathbf{x}_i$ . The discrete-time hazard rate  $\lambda_{it}$  is defined as

$$\lambda_{it} = \Pr(T_i = t \mid T_i \geq t, \mathbf{x}_i), \quad t = 1, 2, \dots$$

Using elementary properties of conditional probabilities, it can be shown that

$$\Pr(T_i = t) = \lambda_{it} \prod_{j=1}^{t-1} (1 - \lambda_{ij}) \quad \text{and} \quad \Pr(T_i > t) = \prod_{j=1}^t (1 - \lambda_{ij})$$

Suppose  $t_i$  is the observed survival time of the  $i$ th subject. Suppose  $\delta_i = 1$  if  $T_i = t_i$  is an event time and 0 otherwise. The likelihood for the grouped survival data is given by

$$\begin{aligned} L &= \prod_i [\Pr(T_i = t_i)]^{\delta_i} [\Pr(T_i > t_i)]^{1-\delta_i} \\ &= \prod_i \left( \frac{\lambda_{it_i}}{1 - \lambda_{it_i}} \right)^{\delta_i} \prod_{j=1}^{t_i} (1 - \lambda_{ij}) \\ &= \prod_i \prod_{j=1}^{t_i} \left( \frac{\lambda_{ij}}{1 - \lambda_{ij}} \right)^{y_{ij}} (1 - \lambda_{ij}) \end{aligned}$$

where  $y_{ij} = 1$  if the  $i$ th subject experienced an event at time  $T_i = j$  and 0 otherwise.

Note that the likelihood  $L$  for the grouped survival data is the same as the likelihood of a binary response model with event probabilities  $\lambda_{ij}$ . If the data are generated by a continuous-time proportional hazards model, Prentice and Gloeckler (1978) have shown that

$$\lambda_{ij} = 1 - \exp(-\exp(\alpha_j + \boldsymbol{\beta}'\mathbf{x}_i))$$

which can be rewritten as

$$\log(-\log(1 - \lambda_{ij})) = \alpha_j + \boldsymbol{\beta}'\mathbf{x}_i$$

where the coefficient vector  $\boldsymbol{\beta}$  is identical to that of the continuous-time proportional hazards model, and  $\alpha_j$  is a constant related to the conditional survival probability in the interval defined by  $T_i = j$  at  $\mathbf{x}_i = \mathbf{0}$ . The grouped data survival model is therefore equivalent to the binary response model with complementary log-log link function. To fit the grouped survival model by using PROC LOGISTIC, you must treat each discrete time unit for each subject as a separate observation. For each of these observations, the response is dichotomous, corresponding to whether or not the subject died in the time unit.

Consider a study of the effect of insecticide on flour beetles. Four different concentrations of an insecticide were sprayed on separate groups of flour beetles. The following DATA step saves the number of male and female flour beetles dying in successive intervals in the data set Beetles:

```
data Beetles(keep=time sex conc freq);
 input time m20 f20 m32 f32 m50 f50 m80 f80;
 conc=.20; freq= m20; sex=1; output;
 freq= f20; sex=2; output;
 conc=.32; freq= m32; sex=1; output;
 freq= f32; sex=2; output;
 conc=.50; freq= m50; sex=1; output;
 freq= f50; sex=2; output;
 conc=.80; freq= m80; sex=1; output;
 freq= f80; sex=2; output;
 datalines;
 1 3 0 7 1 5 0 4 2
 2 11 2 10 5 8 4 10 7
 3 10 4 11 11 11 6 8 15
 4 7 8 16 10 15 6 14 9
 5 4 9 3 5 4 3 8 3
 6 3 3 2 1 2 1 2 4
 7 2 0 1 0 1 1 1 1
 8 1 0 0 1 1 4 0 1
 9 0 0 1 1 0 0 0 0
 10 0 0 0 0 0 0 1 1
 11 0 0 0 0 1 1 0 0
 12 1 0 0 0 0 1 0 0
 13 1 0 0 0 0 1 0 0
 14 101 126 19 47 7 17 2 4
 ;
```

The data set Beetles contains four variables: time, sex, conc, and freq. The variable time represents the interval death time; for example, time=2 is the interval between day 1 and day 2. Insects surviving the duration (13 days) of the experiment are given a time value of 14. The variable sex represents the sex of the insects (1=male, 2=female), conc represents the concentration of the insecticide (mg/cm<sup>2</sup>), and freq represents the frequency of the observations.

To use PROC LOGISTIC with the grouped survival data, you must expand the data so that each beetle has a separate record for each day of survival. A beetle that died in the third day (`time=3`) would contribute three observations to the analysis, one for each day it was alive at the beginning of the day. A beetle that survives the 13-day duration of the experiment (`time=14`) would contribute 13 observations.

The following DATA step creates a new data set named `Days` containing the beetle-day observations from the data set `Beetles`. In addition to the variables `sex`, `conc`, and `freq`, the data set contains an outcome variable `y` and a classification variable `day`. The variable `y` has a value of 1 if the observation corresponds to the day that the beetle died, and it has a value of 0 otherwise. An observation for the first day will have a value of 1 for `day`; an observation for the second day will have a value of 2 for `day`, and so on. For instance, [Output 54.14.1](#) shows an observation in the `Beetles` data set with `time=3`, and [Output 54.14.2](#) shows the corresponding beetle-day observations in the data set `Days`.

```
data Days;
 set Beetles;
 do day=1 to time;
 if (day < 14) then do;
 y= (day=time);
 output;
 end;
 end;
run;
```

**Output 54.14.1** An Observation with Time=3 in Beetles Data Set

| Obs | time | conc | freq | sex |
|-----|------|------|------|-----|
| 17  | 3    | 0.2  | 10   | 1   |

**Output 54.14.2** Corresponding Beetle-Day Observations in Days

| Obs | time | conc | freq | sex | day | y |
|-----|------|------|------|-----|-----|---|
| 25  | 3    | 0.2  | 10   | 1   | 1   | 0 |
| 26  | 3    | 0.2  | 10   | 1   | 2   | 0 |
| 27  | 3    | 0.2  | 10   | 1   | 3   | 1 |

The following statements invoke PROC LOGISTIC to fit a complementary log-log model for binary data with the response variable `Y` and the explanatory variables `day`, `sex`, and `Variableconc`. Specifying the `EVENT=` option ensures that the event (`y=1`) probability is modeled. The GLM coding in the `CLASS` statement creates an indicator column in the design matrix for each level of `day`. The coefficients of the indicator effects for `day` can be used to estimate the baseline survival function. The `NOINT` option is specified to prevent any redundancy in estimating the coefficients of `day`. The Newton-Raphson algorithm is used for the maximum likelihood estimation of the parameters.

```
proc logistic data=Days outest=est1;
 class day / param=glm;
 model y(event='1')= day sex conc
 / noint link=cloglog technique=newton;
 freq freq;
run;
```

Results of the model fit are given in [Output 54.14.3](#). Both sex and conc are statistically significant for the survival of beetles sprayed by the insecticide. Female beetles are more resilient to the chemical than male beetles, and increased concentration of the insecticide increases its effectiveness.

**Output 54.14.3** Parameter Estimates for the Grouped Proportional Hazards Model

| Analysis of Maximum Likelihood Estimates |    |          |                |                 |            |
|------------------------------------------|----|----------|----------------|-----------------|------------|
| Parameter                                | DF | Estimate | Standard Error | Wald Chi-Square | Pr > ChiSq |
| day                                      | 1  | -3.9314  | 0.2934         | 179.5602        | <.0001     |
| day                                      | 2  | -2.8751  | 0.2412         | 142.0596        | <.0001     |
| day                                      | 3  | -2.3985  | 0.2299         | 108.8833        | <.0001     |
| day                                      | 4  | -1.9953  | 0.2239         | 79.3960         | <.0001     |
| day                                      | 5  | -2.4920  | 0.2515         | 98.1470         | <.0001     |
| day                                      | 6  | -3.1060  | 0.3037         | 104.5799        | <.0001     |
| day                                      | 7  | -3.9704  | 0.4230         | 88.1107         | <.0001     |
| day                                      | 8  | -3.7917  | 0.4007         | 89.5233         | <.0001     |
| day                                      | 9  | -5.1540  | 0.7316         | 49.6329         | <.0001     |
| day                                      | 10 | -5.1350  | 0.7315         | 49.2805         | <.0001     |
| day                                      | 11 | -5.1131  | 0.7313         | 48.8834         | <.0001     |
| day                                      | 12 | -5.1029  | 0.7313         | 48.6920         | <.0001     |
| day                                      | 13 | -5.0951  | 0.7313         | 48.5467         | <.0001     |
| sex                                      | 1  | -0.5651  | 0.1141         | 24.5477         | <.0001     |
| conc                                     | 1  | 3.0918   | 0.2288         | 182.5665        | <.0001     |

The coefficients of parameters for the day variable are the maximum likelihood estimates of  $\alpha_1, \dots, \alpha_{13}$ , respectively. The baseline survivor function  $S_0(t)$  is estimated by

$$\hat{S}_0(t) = \widehat{\Pr}(T > t) = \prod_{j \leq t} \exp(-\exp(\hat{\alpha}_j))$$

and the survivor function for a given covariate pattern (sex= $x_1$  and conc= $x_2$ ) is estimated by

$$\hat{S}(t) = [\hat{S}_0(t)]^{\exp(-0.5651x_1 + 3.0918x_2)}$$

The following statements compute the survival curves for male and female flour beetles exposed to the insecticide in concentrations of 0.20 mg/cm<sup>2</sup> and 0.80 mg/cm<sup>2</sup>:



```

data one (keep=day survival element s_m20 s_f20 s_m80 s_f80);
 array dd day1-day13;
 array sc[4] m20 f20 m80 f80;
 array s_sc[4] s_m20 s_f20 s_m80 s_f80 (1 1 1 1);
 set est1;
 m20= exp(sex + .20 * conc);
 f20= exp(2 * sex + .20 * conc);
 m80= exp(sex + .80 * conc);
 f80= exp(2 * sex + .80 * conc);
 survival=1;
 day=0;
 output;
 do over dd;
 element= exp(-exp(dd));
 survival= survival * element;
 do i=1 to 4;
 s_sc[i] = survival ** sc[i];
 end;
 day + 1;
 output;
 end;
run;

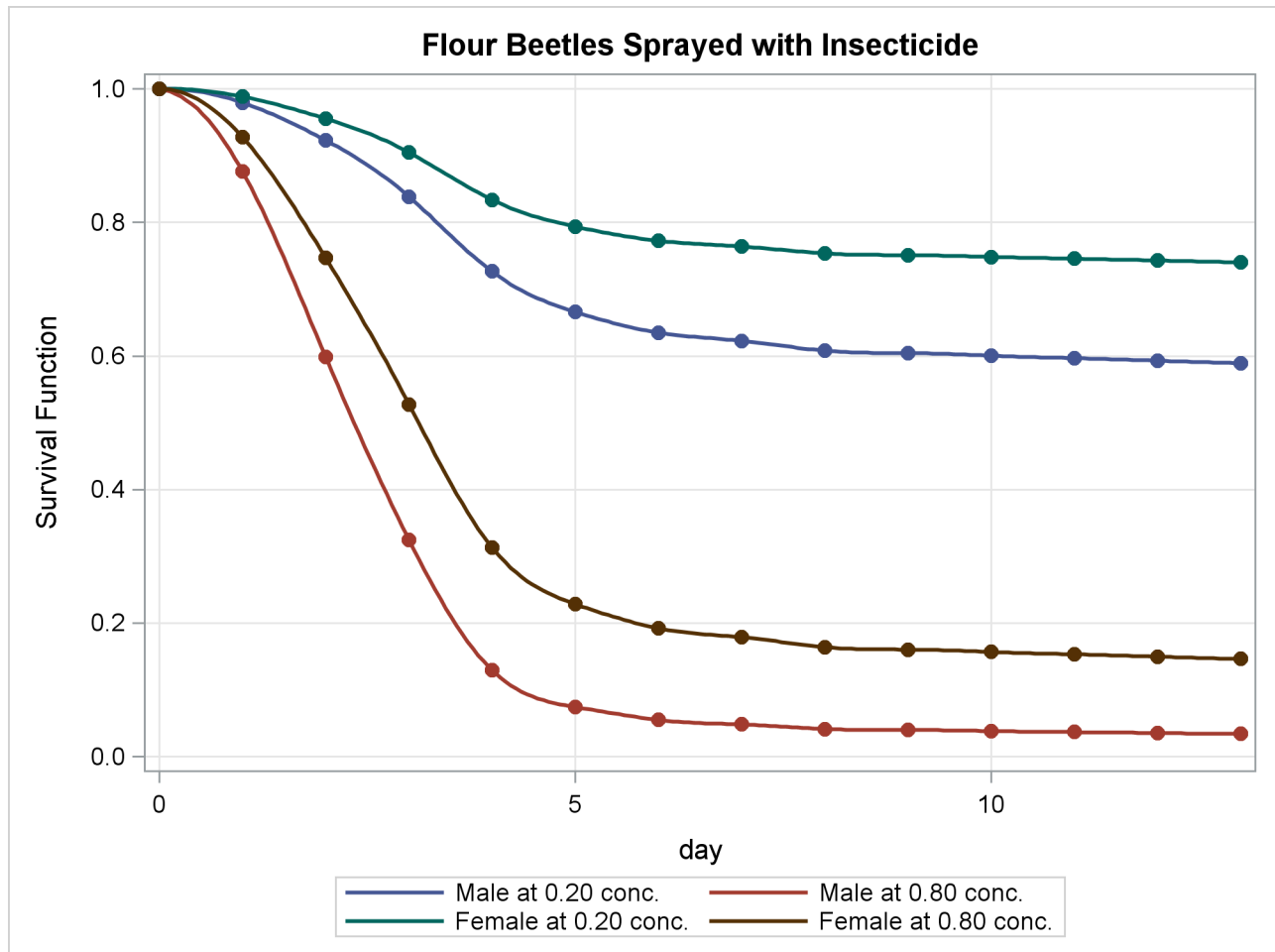
```

Instead of plotting the curves as step functions, the following statements use the PBSPLINE statement in the SGPLOT procedure to smooth the curves with a penalized B-spline. See Chapter 97, “The TRANSREG Procedure,” for details about the implementation of the penalized B-spline method. The SAS autocall macro %MODSTYLE is specified to change the marker symbols for the plot. For more information about the %MODSTYLE macro, see the section “Style Template Modification Macro” on page 667 in Chapter 21, “Statistical Graphics Using ODS.” The smoothed survival curves are displayed in Output 54.14.4.

```

%modstyle(name=LogiStyle,parent=htmlblue,markers=circlefilled);
ods listing style=LogiStyle;
proc sgplot data=one;
 title 'Flour Beetles Sprayed with Insecticide';
 xaxis grid integer;
 yaxis grid label='Survival Function';
 pbspline y=s_m20 x=day /
 legendlabel = "Male at 0.20 conc." name="pred1";
 pbspline y=s_m80 x=day /
 legendlabel = "Male at 0.80 conc." name="pred2";
 pbspline y=s_f20 x=day /
 legendlabel = "Female at 0.20 conc." name="pred3";
 pbspline y=s_f80 x=day /
 legendlabel = "Female at 0.80 conc." name="pred4";
 discretelegend "pred1" "pred2" "pred3" "pred4" / across=2;
run;

```

**Output 54.14.4** Predicted Survival at Insecticide Concentrations of 0.20 and 0.80 mg/cm<sup>2</sup>

The probability of survival is displayed on the vertical axis. Notice that most of the insecticide effect occurs by day 6 for both the high and low concentrations.

## Example 54.15: Scoring Data Sets

This example first illustrates the syntax used for scoring data sets, then uses a previously scored data set to score a new data set. A generalized logit model is fit to the remote-sensing data set used in the section “[Example 33.4: Linear Discriminant Analysis of Remote-Sensing Data on Crops](#)” on page 2146 of Chapter 33, “[The DISCRIM Procedure](#),” to illustrate discrimination and classification methods. In the following DATA step, the response variable is Crop and the prognostic factors are x1 through x4:

```
data Crops;
 length Crop $ 10;
 infile datalines truncover;
 input Crop $ @@;
 do i=1 to 3;
 input x1-x4 @@;
 if (x1 ^= .) then output;
```

```

end;
input;
datalines;
Corn 16 27 31 33 15 23 30 30 16 27 27 26
Corn 18 20 25 23 15 15 31 32 15 32 32 15
Corn 12 15 16 73
Soybeans 20 23 23 25 24 24 25 32 21 25 23 24
Soybeans 27 45 24 12 12 13 15 42 22 32 31 43
Cotton 31 32 33 34 29 24 26 28 34 32 28 45
Cotton 26 25 23 24 53 48 75 26 34 35 25 78
Sugarbeets 22 23 25 42 25 25 24 26 34 25 16 52
Sugarbeets 54 23 21 54 25 43 32 15 26 54 2 54
Clover 12 45 32 54 24 58 25 34 87 54 61 21
Clover 51 31 31 16 96 48 54 62 31 31 11 11
Clover 56 13 13 71 32 13 27 32 36 26 54 32
Clover 53 08 06 54 32 32 62 16
;

```

In the following statements, you specify a **SCORE** statement to use the fitted model to score the Crops data. The data together with the predicted values are saved in the data set Score1. The output from the **EFFECTPLOT** statement is discussed at the end of this section.

```

ods graphics on;
proc logistic data=Crops;
 model Crop=x1-x4 / link=glogit;
 score out=Score1;
 effectplot slicefit (x=x3);
run;
ods graphics off;

```

In the following statements, the model is fit again, and the data and the predicted values are saved into the data set Score2. The **OUTMODEL=** option saves the fitted model information in the permanent SAS data set sasuser.CropModel, and the **STORE** statement saves the fitted model information into the SAS data set CropModel2. Both the **OUTMODEL=** option and the **STORE** statement are specified to illustrate their use; you would usually specify only one of these model-storing methods.

```

proc logistic data=Crops outmodel=sasuser.CropModel;
 model Crop=x1-x4 / link=glogit;
 score data=Crops out=Score2;
 store CropModel2;
run;

```

To score data without refitting the model, specify the **INMODEL=** option to identify a previously saved SAS data set of model information. In the following statements, the model is read from the sasuser.CropModel data set, and the data and the predicted values are saved in the data set Score3. Note that the data set being scored does not have to include the response variable.

```

proc logistic inmodel=sasuser.CropModel;
 score data=Crops out=Score3;
run;

```

Another method available to score the data without refitting the model is to invoke the PLM procedure. In the following statements, the stored model is named in the **SOURCE=** option. The **PREDICTED=** option computes the linear predictors, and the **ILINK** option transforms the linear predictors to the probability

scale. The SCORE statement scores the Crops data set, and the predicted probabilities are saved in the data set ScorePLM. See Chapter 69, “The PLM Procedure,” for more information.

```
proc plm source=CropModel2;
 score data=Crops out=ScorePLM predicted=p / ilink;
run;
```

For each observation in the Crops data set, the ScorePLM data set contains 5 observations—one for each level of the response variable. The following statements transform this data set into a form that is similar to the other scored data sets in this example:

```
proc transpose data=ScorePLM out=Score4 prefix=P_ let;
 id _LEVEL_;
 var p;
 by x1-x4 notsorted;
run;
data Score4(drop=_NAME_ _LABEL_);
 merge Score4 Crops(keep=Crop x1-x4);
 F_Crop=Crop;
run;
proc summary data=ScorePLM nway;
 by x1-x4 notsorted;
 var p;
 output out=into maxid(p(_LEVEL_))=I_Crop;
run;
data Score4;
 merge Score4 into(keep=I_Crop);
run;
```

To set prior probabilities on the responses, specify the **PRIOR=** option to identify a SAS data set containing the response levels and their priors. In the following statements, the Prior data set contains the values of the response variable (because this example uses single-trial MODEL statement syntax) and a **\_PRIOR\_** variable containing values proportional to the default priors. The data and the predicted values are saved in the data set Score5.

```
data Prior;
 length Crop $10.;
 input Crop _PRIOR_;
 datalines;
Clover 11
Corn 7
Cotton 6
Soybeans 6
Sugarbeets 6
;

proc logistic inmodel=sasuser.CropModel;
 score data=Crops prior=prior out=Score5 fitstat;
run;
```

The “Fit Statistics for SCORE Data” table displayed in [Output 54.15.1](#) shows that 47.22% of the observations are misclassified.

**Output 54.15.1** Fit Statistics for Data Set Prior

| Fit Statistics for SCORE Data |                 |                |                       |          |             |          |
|-------------------------------|-----------------|----------------|-----------------------|----------|-------------|----------|
| Data Set                      | Total Frequency | Log Likelihood | Error Rate            | AIC      | AICC        | BIC      |
| WORK.CROPS                    | 36              | -32.2247       | 0.4722                | 104.4493 | 160.4493    | 136.1197 |
| Data Set                      | SC              | R-Square       | Max-Rescaled R-Square | AUC      | Brier Score |          |
| WORK.CROPS                    | 136.1197        | 0.744081       | 0.777285              | .        | 0.492712    |          |

The data sets Score1, Score2, Score3, Score4, and Score5 are identical. The following statements display the scoring results in [Output 54.15.2](#):

```
proc freq data=Score1;
 table F_Crop*I_Crop / nocol nocum nopercent;
run;
```

**Output 54.15.2** Classification of Data Used for Scoring

| Table of F_Crop by I_Crop |                    |             |            |            |            |       |
|---------------------------|--------------------|-------------|------------|------------|------------|-------|
| F_Crop(From: Crop)        | I_Crop(Into: Crop) |             |            |            |            | Total |
| Frequency  <br>Row Pct    | Clover             | Corn        | Cotton     | Soybeans   | Sugarbeets |       |
| Clover                    | 6<br>54.55         | 0<br>0.00   | 2<br>18.18 | 2<br>18.18 | 1<br>9.09  | 11    |
| Corn                      | 0<br>0.00          | 7<br>100.00 | 0<br>0.00  | 0<br>0.00  | 0<br>0.00  | 7     |
| Cotton                    | 4<br>66.67         | 0<br>0.00   | 1<br>16.67 | 1<br>16.67 | 0<br>0.00  | 6     |
| Soybeans                  | 1<br>16.67         | 1<br>16.67  | 1<br>16.67 | 3<br>50.00 | 0<br>0.00  | 6     |
| Sugarbeets                | 2<br>33.33         | 0<br>0.00   | 0<br>0.00  | 2<br>33.33 | 2<br>33.33 | 6     |
| Total                     | 13                 | 8           | 4          | 8          | 3          | 36    |

The following statements use the previously fitted and saved model in the sasuser.CropModel data set to score the observations in a new data set, Test. The results of scoring the test data are saved in the ScoredTest data set and displayed in [Output 54.15.3](#).

```

data Test;
 input Crop $ 1-10 x1-x4;
 datalines;
Corn 16 27 31 33
Soybeans 21 25 23 24
Cotton 29 24 26 28
Sugarbeets 54 23 21 54
Clover 32 32 62 16
;

proc logistic noprint inmodel=sasuser.CropModel;
 score data=Test out=ScoredTest;
run;

proc print data=ScoredTest label noobs;
 var F_Crop I_Crop P_Clover P_Corn P_Cotton P_Soybeans P_Sugarbeets;
run;

```

**Output 54.15.3** Classification of Test Data

| From: Crop | Into: Crop | Predicted Probability: Crop=Clover | Predicted Probability: Crop=Corn |
|------------|------------|------------------------------------|----------------------------------|
| Corn       | Corn       | 0.00342                            | 0.90067                          |
| Soybeans   | Soybeans   | 0.04801                            | 0.03157                          |
| Cotton     | Clover     | 0.43180                            | 0.00015                          |
| Sugarbeets | Clover     | 0.66681                            | 0.00000                          |
| Clover     | Cotton     | 0.41301                            | 0.13386                          |

| Predicted Probability: Crop=Cotton | Predicted Probability: Crop=Soybeans | Predicted Probability: Crop=Sugarbeets |
|------------------------------------|--------------------------------------|----------------------------------------|
| 0.00500                            | 0.08675                              | 0.00416                                |
| 0.02865                            | 0.82933                              | 0.06243                                |
| 0.21267                            | 0.07623                              | 0.27914                                |
| 0.17364                            | 0.00000                              | 0.15955                                |
| 0.43649                            | 0.00033                              | 0.01631                                |

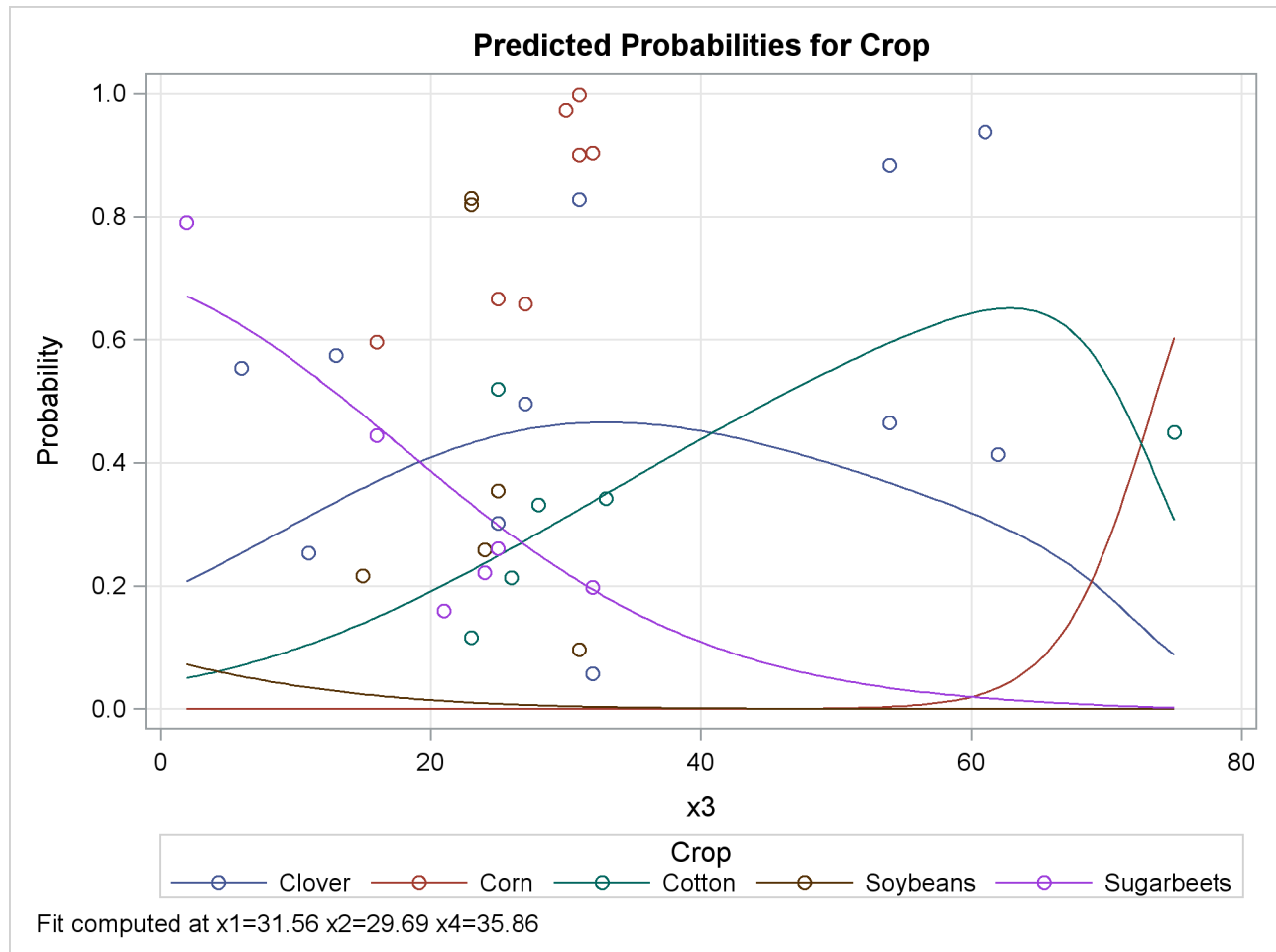
The **EFFECTPLOT** statement that is specified in the first PROC LOGISTIC invocation produces a plot of the model-predicted probabilities versus X3 while holding the other three covariates at their means (Output 54.15.4). This plot shows how the value of X3 affects the probabilities of the various crops when the other prognostic factors are fixed at their means. If you are interested in the effect of X3 when the other covariates are fixed at a certain level—say, 10—specify the following EFFECTPLOT statement.

```

effectplot slicefit(x=x3) / at(x1=10 x2=10 x4=10)

```

Output 54.15.4 Model-Predicted Probabilities



### Example 54.16: Using the LSMEANS Statement

Recall the main-effects model fit to the Neuralgia data set in [Example 54.2](#). The Treatment\*Sex interaction, which was previously shown to be nonsignificant, is added back into the model for this discussion.

In the following statements, the **ODDSRATIO** statement is specified to produce odds ratios of pairwise differences of the Treatment parameters in the presence of the Sex interaction. The **LSMEANS** statement is specified with several options: the **E** option displays the coefficients that are used to compute the LS-means for each Treatment level, the **DIFF** option takes all pairwise differences of the LS-means for the levels of the Treatment variable, the **ODDSRATIO** option computes odds ratios of these differences, the **CL** option produces confidence intervals for the differences and odds ratios, and the **ADJUST=BON** option performs a very conservative adjustment of the *p*-values and confidence intervals.

```
proc logistic data=Neuralgia;
 class Treatment Sex / param=glm;
 model Pain= Treatment|Sex Age;
 oddsratio Treatment;
 lsmeans Treatment / e diff oddsratio cl adjust=bon;
run;
```

The results from the **ODDSRATIO** statement are displayed in [Output 54.16.1](#). All pairwise differences of levels of the Treatment effect are compared. However, because of the interaction between the Treatment and Sex variables, each difference is computed at each of the two levels of the Sex variable. These results show that the difference between Treatment levels A and B is insignificant for both genders.

To compute these odds ratios, you must first construct a linear combination of the parameters,  $l'\beta$ , for each level that is compared with all other levels fixed at some value. For example, to compare Treatment=A with B for Sex=F, you fix the Age variable at its mean, 70.05, and construct the following  $l$  vectors:

|               | Intercept | Treatment |    |   | Sex |   | Treatment*Sex |    |    |    |    |    | Age   |
|---------------|-----------|-----------|----|---|-----|---|---------------|----|----|----|----|----|-------|
|               |           | A         | B  | P | F   | M | AF            | AM | BF | BM | PF | PM |       |
| $l'_A$        | 1         | 1         | 0  | 0 | 1   | 0 | 1             | 0  | 0  | 0  | 0  | 0  | 70.05 |
| $l'_B$        | 1         | 0         | 1  | 0 | 1   | 0 | 0             | 0  | 1  | 0  | 0  | 0  | 70.05 |
| $l'_A - l'_B$ | 0         | 1         | -1 | 0 | 0   | 0 | 1             | 0  | -1 | 0  | 0  | 0  | 0     |

Then the odds ratio for Treatment A versus B at Sex=F is computed as  $\exp((l'_A - l'_B)\beta)$ . Different  $l$  vectors must be similarly constructed when Sex=M because the resulting odds ratio will be different due to the interaction.

**Output 54.16.1** Odds Ratios from the ODDSRATIO Statement

| Odds Ratio Estimates and Wald Confidence Intervals |          |                       |          |
|----------------------------------------------------|----------|-----------------------|----------|
| Label                                              | Estimate | 95% Confidence Limits |          |
| Treatment A vs B at Sex=F                          | 0.398    | 0.016                 | 9.722    |
| Treatment A vs P at Sex=F                          | 16.892   | 1.269                 | 224.838  |
| Treatment B vs P at Sex=F                          | 42.492   | 2.276                 | 793.254  |
| Treatment A vs B at Sex=M                          | 0.663    | 0.078                 | 5.623    |
| Treatment A vs P at Sex=M                          | 34.766   | 1.807                 | 668.724  |
| Treatment B vs P at Sex=M                          | 52.458   | 2.258                 | >999.999 |

The results from the **LSMEANS** statement are displayed in [Output 54.16.2](#) through [Output 54.16.4](#).

The LS-means are computed by constructing each of the  $l$  coefficient vectors shown in [Output 54.16.2](#), and then computing  $l'\beta$ . The LS-means are not estimates of the event probabilities; they are estimates of the linear predictors on the logit scale. In order to obtain event probabilities, you need to apply the inverse-link transformation by specifying the **ILINK** option in the **LSMEANS** statement. Notice in [Output 54.16.2](#) that the Sex rows do not indicate either Sex=F or Sex=M. Instead, the LS-means are computed at an average of these two levels, so only one result needs to be reported. For more information about the construction of LS-means, see the section “[Construction of Least Squares Means](#)” on page 3363 of Chapter 42, “[The GLM Procedure](#).”



**Output 54.16.2** Treatment LS-Means Coefficients

| Coefficients for Treatment Least Squares Means |           |     |       |       |       |
|------------------------------------------------|-----------|-----|-------|-------|-------|
| Parameter                                      | Treatment | Sex | Row1  | Row2  | Row3  |
| Intercept: Pain=No                             |           |     | 1     | 1     | 1     |
| Treatment A                                    | A         |     | 1     |       |       |
| Treatment B                                    | B         |     |       | 1     |       |
| Treatment P                                    | P         |     |       |       | 1     |
| Sex F                                          |           | F   | 0.5   | 0.5   | 0.5   |
| Sex M                                          |           | M   | 0.5   | 0.5   | 0.5   |
| Treatment A * Sex F                            | A         | F   | 0.5   |       |       |
| Treatment A * Sex M                            | A         | M   | 0.5   |       |       |
| Treatment B * Sex F                            | B         | F   |       | 0.5   |       |
| Treatment B * Sex M                            | B         | M   |       | 0.5   |       |
| Treatment P * Sex F                            | P         | F   |       |       | 0.5   |
| Treatment P * Sex M                            | P         | M   |       |       | 0.5   |
| Age                                            |           |     | 70.05 | 70.05 | 70.05 |

The Treatment LS-means shown in [Output 54.16.3](#) are all significantly nonzero at the 0.05 level. These LS-means are *predicted population margins* of the logits; that is, they estimate the marginal means over a balanced population, and they are effectively the within-Treatment means appropriately adjusted for the other effects in the model. The LS-means are not event probabilities; in order to obtain event probabilities, you need to apply the inverse-link transformation by specifying the ILINK option in the LSMEANS statement. For more information about LS-means, see the section “LSMEANS Statement” on page 453 of Chapter 19, “Shared Concepts and Topics.”

**Output 54.16.3** Treatment LS-Means

| Treatment Least Squares Means |          |                |         |         |       |         |         |
|-------------------------------|----------|----------------|---------|---------|-------|---------|---------|
| Treatment                     | Estimate | Standard Error | z Value | Pr >  z | Alpha | Lower   | Upper   |
| A                             | 1.3195   | 0.6664         | 1.98    | 0.0477  | 0.05  | 0.01331 | 2.6257  |
| B                             | 1.9864   | 0.7874         | 2.52    | 0.0116  | 0.05  | 0.4431  | 3.5297  |
| P                             | -1.8682  | 0.7620         | -2.45   | 0.0142  | 0.05  | -3.3618 | -0.3747 |

Pairwise differences between the Treatment LS-means, requested with the DIFF option, are displayed in [Output 54.16.4](#). The LS-mean for the level that is displayed in the \_Treatment column is subtracted from the LS-mean for the level in the Treatment column, so the first row displays the LS-mean for Treatment level A minus the LS-mean for Treatment level B. The Pr > |z| column indicates that the A and B levels are not significantly different; however, both of these levels are different from level P. If the inverse-link transformation is specified with the ILINK option, then these differences do not transform back to differences in probabilities.

There are two odds ratios for Treatment level A versus B in [Output 54.16.1](#); these are constructed at each level of the interacting covariate Sex. In contrast, there is only one LS-means odds ratio for Treatment level A versus B in [Output 54.16.4](#). This odds ratio is computed at an average of the interacting effects by creating the  $l$  vectors shown in [Output 54.16.2](#) (the Row1 column corresponds to  $l_A$  and the Row2 column corresponds to  $l_B$ ) and computing  $\exp(l'_A \beta - l'_B \beta)$ .

Since multiple tests are performed, you can protect yourself from falsely significant results by adjusting your *p*-values for multiplicity. The **ADJUST=BON** option performs the very conservative Bonferroni adjustment, and adds the columns labeled with ‘Adj’ to [Output 54.16.4](#). Comparing the Pr > |z| column to the Adj P column, you can see that the *p*-values are adjusted upwards; in this case, there is no change in your conclusions. The confidence intervals are also adjusted for multiplicity—all adjusted intervals are wider than the unadjusted intervals, but again your conclusions in this example are unchanged.

**Output 54.16.4** Differences and Odds Ratios for the Treatment LS-Means

| Differences of Treatment Least Squares Means<br>Adjustment for Multiple Comparisons: Bonferroni |            |          |                |         |         |        |       |
|-------------------------------------------------------------------------------------------------|------------|----------|----------------|---------|---------|--------|-------|
| Treatment                                                                                       | _Treatment | Estimate | Standard Error | z Value | Pr >  z | Adj P  | Alpha |
| A                                                                                               | B          | -0.6669  | 1.0026         | -0.67   | 0.5059  | 1.0000 | 0.05  |
| A                                                                                               | P          | 3.1877   | 1.0376         | 3.07    | 0.0021  | 0.0064 | 0.05  |
| B                                                                                               | P          | 3.8547   | 1.2126         | 3.18    | 0.0015  | 0.0044 | 0.05  |

| Differences of Treatment Least Squares Means<br>Adjustment for Multiple Comparisons: Bonferroni |            |         |        |           |           |            |
|-------------------------------------------------------------------------------------------------|------------|---------|--------|-----------|-----------|------------|
| Treatment                                                                                       | _Treatment | Lower   | Upper  | Adj Lower | Adj Upper | Odds Ratio |
| A                                                                                               | B          | -2.6321 | 1.2982 | -3.0672   | 1.7334    | 0.513      |
| A                                                                                               | P          | 1.1541  | 5.2214 | 0.7037    | 5.6717    | 24.234     |
| B                                                                                               | P          | 1.4780  | 6.2313 | 0.9517    | 6.7576    | 47.213     |

| Differences of Treatment Least Squares Means<br>Adjustment for Multiple Comparisons: Bonferroni |            |                                       |                                       |                      |                      |
|-------------------------------------------------------------------------------------------------|------------|---------------------------------------|---------------------------------------|----------------------|----------------------|
| Treatment                                                                                       | _Treatment | Lower Confidence Limit for Odds Ratio | Upper Confidence Limit for Odds Ratio | Adj Lower Odds Ratio | Adj Upper Odds Ratio |
| A                                                                                               | B          | 0.072                                 | 3.663                                 | 0.047                | 5.660                |
| A                                                                                               | P          | 3.171                                 | 185.195                               | 2.021                | 290.542              |
| B                                                                                               | P          | 4.384                                 | 508.441                               | 2.590                | 860.612              |

If you want to jointly test whether the active treatments are different from the placebo, you can specify a custom hypothesis test with the **LSMESTIMATE** statement. In the following statements, the LS-means for the two treatments are contrasted against the LS-mean of the placebo, and the **JOINT** option performs a joint test that the two treatments are not different from placebo.

```
proc logistic data=Neuralgia;
 class Treatment Sex / param=glm;
 model Pain= Treatment|Sex Age;
 lsmestimate treatment 1 0 -1, 0 1 -1 / joint;
run;
```

[Output 54.16.5](#) displays the results from the **LSMESTIMATE** statement. The “Least Squares Means Es-

imate” table displays the differences of the two active treatments against the placebo, and the results are identical to the second and third rows of [Output 54.16.3](#). The “Chi-Square Test for Least Squares Means Estimates” table displays the joint test. In all of these tests, you reject the null hypothesis that the treatment has the same effect as the placebo.

**Output 54.16.5** Custom LS-Mean Tests

| Least Squares Means Estimates                     |        |            |                |         |         |
|---------------------------------------------------|--------|------------|----------------|---------|---------|
| Effect                                            | Label  | Estimate   | Standard Error | z Value | Pr >  z |
| Treatment                                         | Row 1  | 3.1877     | 1.0376         | 3.07    | 0.0021  |
| Treatment                                         | Row 2  | 3.8547     | 1.2126         | 3.18    | 0.0015  |
| Chi-Square Test for Least Squares Means Estimates |        |            |                |         |         |
| Effect                                            | Num DF | Chi-Square | Pr > ChiSq     |         |         |
| Treatment                                         | 2      | 12.13      | 0.0023         |         |         |

If you want to work with LS-means but you prefer to compute the Treatment odds ratios within the Sex levels in the same fashion as the [ODDSRATIO](#) statement does, you can specify the [SLICE](#) statement. In the following statements, you specify the same options in the [SLICE](#) statement as you do in the [LSMEANS](#) statement, except that you also specify the [SLICEBY=](#) option to perform an LS-means analysis partitioned into sets that are defined by the Sex variable:

```
proc logistic data=Neuralgia;
 class Treatment Sex / param=glm;
 model Pain= Treatment|Sex Age;
 slice Treatment*Sex / sliceby=Sex diff oddsratio cl adjust=bon;
run;
```

The results for Sex=F are displayed in [Output 54.16.6](#) and [Output 54.16.7](#). The joint test in [Output 54.16.6](#) tests the equality of the LS-means of the levels of Treatment for Sex=F, and rejects equality at level 0.05. In [Output 54.16.7](#), the odds ratios and confidence intervals match those reported for Sex=F in [Output 54.16.1](#), and multiplicity adjustments are performed.

**Output 54.16.6** Joint Test of Treatment Equality for Females

| Chi-Square Test for Treatment*Sex<br>Least Squares Means Slice |        |            |            |
|----------------------------------------------------------------|--------|------------|------------|
| Slice                                                          | Num DF | Chi-Square | Pr > ChiSq |
| Sex F                                                          | 2      | 8.22       | 0.0164     |

**Output 54.16.7** Differences of the Treatment LS-Means for Females

| Simple Differences of Treatment*Sex Least Squares Means<br>Adjustment for Multiple Comparisons: Bonferroni |           |            |          |                |         |         |        |
|------------------------------------------------------------------------------------------------------------|-----------|------------|----------|----------------|---------|---------|--------|
| Slice                                                                                                      | Treatment | _Treatment | Estimate | Standard Error | z Value | Pr >  z | Adj P  |
| Sex F                                                                                                      | A         | B          | -0.9224  | 1.6311         | -0.57   | 0.5717  | 1.0000 |
| Sex F                                                                                                      | A         | P          | 2.8269   | 1.3207         | 2.14    | 0.0323  | 0.0970 |
| Sex F                                                                                                      | B         | P          | 3.7493   | 1.4933         | 2.51    | 0.0120  | 0.0361 |

| Simple Differences of Treatment*Sex Least Squares Means<br>Adjustment for Multiple Comparisons: Bonferroni |           |            |       |         |        |           |           |
|------------------------------------------------------------------------------------------------------------|-----------|------------|-------|---------|--------|-----------|-----------|
| Slice                                                                                                      | Treatment | _Treatment | Alpha | Lower   | Upper  | Adj Lower | Adj Upper |
| Sex F                                                                                                      | A         | B          | 0.05  | -4.1193 | 2.2744 | -4.8272   | 2.9824    |
| Sex F                                                                                                      | A         | P          | 0.05  | 0.2384  | 5.4154 | -0.3348   | 5.9886    |
| Sex F                                                                                                      | B         | P          | 0.05  | 0.8225  | 6.6761 | 0.1744    | 7.3243    |

| Simple Differences of Treatment*Sex Least Squares Means<br>Adjustment for Multiple Comparisons: Bonferroni |           |            |            |                                       |                                       |  |  |
|------------------------------------------------------------------------------------------------------------|-----------|------------|------------|---------------------------------------|---------------------------------------|--|--|
| Slice                                                                                                      | Treatment | _Treatment | Odds Ratio | Lower Confidence Limit for Odds Ratio | Upper Confidence Limit for Odds Ratio |  |  |
| Sex F                                                                                                      | A         | B          | 0.398      | 0.016                                 | 9.722                                 |  |  |
| Sex F                                                                                                      | A         | P          | 16.892     | 1.269                                 | 224.838                               |  |  |
| Sex F                                                                                                      | B         | P          | 42.492     | 2.276                                 | 793.254                               |  |  |

| Simple Differences of Treatment*Sex Least Squares Means<br>Adjustment for Multiple Comparisons: Bonferroni |           |            |                |       |          |  |  |
|------------------------------------------------------------------------------------------------------------|-----------|------------|----------------|-------|----------|--|--|
| Slice                                                                                                      | Treatment | _Treatment | Adj Odds Ratio | Lower | Upper    |  |  |
| Sex F                                                                                                      | A         | B          | 0.008          |       | 19.734   |  |  |
| Sex F                                                                                                      | A         | P          | 0.715          |       | 398.848  |  |  |
| Sex F                                                                                                      | B         | P          | 1.190          |       | >999.999 |  |  |

Similarly, the results for Sex=M are shown in [Output 54.16.8](#) and [Output 54.16.9](#).

**Output 54.16.8** Joint Test of Treatment Equality for Males

| Chi-Square Test for Treatment*Sex<br>Least Squares Means Slice |           |            |            |
|----------------------------------------------------------------|-----------|------------|------------|
| Slice                                                          | Num<br>DF | Chi-Square | Pr > ChiSq |
| Sex M                                                          | 2         | 6.64       | 0.0361     |

**Output 54.16.9** Differences of the Treatment LS-Means for Males

| Simple Differences of Treatment*Sex Least Squares Means<br>Adjustment for Multiple Comparisons: Bonferroni |           |            |          |                   |         |         |        |
|------------------------------------------------------------------------------------------------------------|-----------|------------|----------|-------------------|---------|---------|--------|
| Slice                                                                                                      | Treatment | _Treatment | Estimate | Standard<br>Error | z Value | Pr >  z | Adj P  |
| Sex M                                                                                                      | A         | B          | -0.4114  | 1.0910            | -0.38   | 0.7061  | 1.0000 |
| Sex M                                                                                                      | A         | P          | 3.5486   | 1.5086            | 2.35    | 0.0187  | 0.0560 |
| Sex M                                                                                                      | B         | P          | 3.9600   | 1.6049            | 2.47    | 0.0136  | 0.0408 |

| Simple Differences of Treatment*Sex Least Squares Means<br>Adjustment for Multiple Comparisons: Bonferroni |           |            |       |         |        |              |              |
|------------------------------------------------------------------------------------------------------------|-----------|------------|-------|---------|--------|--------------|--------------|
| Slice                                                                                                      | Treatment | _Treatment | Alpha | Lower   | Upper  | Adj<br>Lower | Adj<br>Upper |
| Sex M                                                                                                      | A         | B          | 0.05  | -2.5496 | 1.7268 | -3.0231      | 2.2003       |
| Sex M                                                                                                      | A         | P          | 0.05  | 0.5919  | 6.5054 | -0.06286     | 7.1601       |
| Sex M                                                                                                      | B         | P          | 0.05  | 0.8145  | 7.1055 | 0.1180       | 7.8021       |

| Simple Differences of Treatment*Sex Least Squares Means<br>Adjustment for Multiple Comparisons: Bonferroni |           |            |               |                                                |                                                |  |
|------------------------------------------------------------------------------------------------------------|-----------|------------|---------------|------------------------------------------------|------------------------------------------------|--|
| Slice                                                                                                      | Treatment | _Treatment | Odds<br>Ratio | Lower<br>Confidence<br>Limit for<br>Odds Ratio | Upper<br>Confidence<br>Limit for<br>Odds Ratio |  |
| Sex M                                                                                                      | A         | B          | 0.663         | 0.078                                          | 5.623                                          |  |
| Sex M                                                                                                      | A         | P          | 34.766        | 1.807                                          | 668.724                                        |  |
| Sex M                                                                                                      | B         | P          | 52.458        | 2.258                                          | >999.999                                       |  |

| Simple Differences of Treatment*Sex<br>Least Squares Means<br>Adjustment for Multiple Comparisons: Bonferroni |           |            |                         |                         |  |
|---------------------------------------------------------------------------------------------------------------|-----------|------------|-------------------------|-------------------------|--|
| Slice                                                                                                         | Treatment | _Treatment | Adj Lower<br>Odds Ratio | Adj Upper<br>Odds Ratio |  |
| Sex M                                                                                                         | A         | B          | 0.049                   | 9.028                   |  |
| Sex M                                                                                                         | A         | P          | 0.939                   | >999.999                |  |
| Sex M                                                                                                         | B         | P          | 1.125                   | >999.999                |  |

## Example 54.17: Partial Proportional Odds Model

Cameron and Trivedi (1998, p. 68) studied the number of doctor visits from the Australian Health Survey 1977–78. The data set contains a dependent variable, `dvisits`, which contains the number of doctor visits in the past two weeks (0, 1, or 2, where 2 represents two or more visits) and the following explanatory variables: `sex`, which indicates whether the patient is female; `age`, which contains the patient’s age in years divided by 100; `income`, which contains the patient’s annual income (in units of \$10,000); `levyplus`, which indicates whether the patient has private health insurance; `freepoor`, which indicates that the patient has free government health insurance due to low income; `freerepa`, which indicates that the patient has free government health insurance for other reasons; `illness`, which contains the number of illnesses in the past two weeks; `actdays`, which contains the number of days the illness caused reduced activity; `hscore`, which is a questionnaire score; `chcond1`, which indicates a chronic condition that does not limit activity; and `chcond2`, which indicates a chronic condition that limits activity.

```
data docvisit;
 input sex age agesq income levyplus freepoor freerepa
 illness actdays hscore chcond1 chcond2 dvisits;
 if (dvisits > 2) then dvisits = 2;
datalines;
1 0.19 0.0361 0.55 1 0 0 1 4 1 0 0 1
1 0.19 0.0361 0.45 1 0 0 1 2 1 0 0 1
0 0.19 0.0361 0.90 0 0 0 3 0 0 0 0 1

... more lines ...

1 0.37 0.1369 0.25 0 0 1 1 0 1 0 0 0
1 0.52 0.2704 0.65 0 0 0 0 0 0 0 0 0
0 0.72 0.5184 0.25 0 0 1 0 0 0 0 0 0
;
```

Because the response variable `dvisits` has three levels, the proportional odds model constructs two response functions. There is an intercept parameter for each of the two response functions,  $\alpha_1 < \alpha_2$ , and common slope parameters  $\beta = (\beta_1, \dots, \beta_{12})$  across the functions. The model can be written as

$$\text{logit}(\Pr(Y \leq i | \mathbf{x})) = \alpha_i + \beta' \mathbf{x}, \quad i = 1, 2$$

The following statements fit a proportional odds model to this data:

```
proc logistic data=docvisit;
 model dvisits = sex age agesq income levyplus
 freepoor freerepa illness actdays hscore
 chcond1 chcond2;
run;
```

Selected results are displayed in [Output 54.17.1](#).

**Output 54.17.1** Test of Proportional Odds Assumption

| Score Test for the Proportional Odds Assumption |            |            |            |
|-------------------------------------------------|------------|------------|------------|
| Chi-Square                                      | DF         | Pr > ChiSq |            |
| 27.4256                                         | 12         | 0.0067     |            |
| Testing Global Null Hypothesis: BETA=0          |            |            |            |
| Test                                            | Chi-Square | DF         | Pr > ChiSq |
| Likelihood Ratio                                | 734.2971   | 12         | <.0001     |
| Score                                           | 811.8964   | 12         | <.0001     |
| Wald                                            | 690.7156   | 12         | <.0001     |

The test of the proportional odds assumption in [Output 54.17.1](#) rejects the null hypothesis that all the slopes are equal across the two response functions. This test is very anticonservative; that is, it tends to reject the null hypothesis even when the proportional odds assumption is reasonable.

The proportional odds assumption for ordinal response models can be relaxed by specifying the `UNEQUALSLOPES` option in the `MODEL` statement. A fully nonproportional odds model has different slope parameters  $\beta_i = (\beta_{1,i}, \dots, \beta_{12,i})$  for every logit  $i$ :

$$\text{logit}(\Pr(Y \leq i | \mathbf{x})) = \alpha_i + \beta'_i \mathbf{x}, \quad i = 1, 2$$

The nonproportional odds model is fit with the following statements. The `TEST` statements test the proportional odds assumption for each of the covariates in the model.

```
proc logistic data=docvisit;
 model dvisits = sex age agesq income levyplus
 freepoor freerepa illness actdays hscore
 chcond1 chcond2 / unequalslopes;
 sex: test sex_0 =sex_1;
 age: test age_0 =age_1;
 agesq: test agesq_0 =agesq_1;
 income: test income_0 =income_1;
 levyplus: test levyplus_0 =levyplus_1;
 freepoor: test freepoor_0 =freepoor_1;
 freerepa: test freerepa_0 =freerepa_1;
 illness: test illness_0 =illness_1;
 actdays: test actdays_0 =actdays_1;
 hscore: test hscore_0 =hscore_1;
 chcond1: test chcond1_0 =chcond1_1;
 chcond2: test chcond2_0 =chcond2_1;
run;
```

Selected results from fitting the nonproportional odds model to the data are displayed in [Output 54.17.2](#).

**Output 54.17.2** Results for Nonproportional Odds Model

| Testing Global Null Hypothesis: BETA=0   |         |            |          |                |                 |            |
|------------------------------------------|---------|------------|----------|----------------|-----------------|------------|
| Test                                     |         | Chi-Square | DF       |                | Pr > ChiSq      |            |
| Likelihood Ratio                         |         | 761.4797   | 24       |                | <.0001          |            |
| Score                                    |         | 957.6793   | 24       |                | <.0001          |            |
| Wald                                     |         | 688.2306   | 24       |                | <.0001          |            |
| Analysis of Maximum Likelihood Estimates |         |            |          |                |                 |            |
| Parameter                                | dvisits | DF         | Estimate | Standard Error | Wald Chi-Square | Pr > ChiSq |
| Intercept                                | 0       | 1          | 2.3238   | 0.2754         | 71.2018         | <.0001     |
| Intercept                                | 1       | 1          | 4.2862   | 0.4890         | 76.8368         | <.0001     |
| sex                                      | 0       | 1          | -0.2637  | 0.0818         | 10.3909         | 0.0013     |
| sex                                      | 1       | 1          | -0.1232  | 0.1451         | 0.7210          | 0.3958     |
| age                                      | 0       | 1          | 1.7489   | 1.5115         | 1.3389          | 0.2472     |
| age                                      | 1       | 1          | -2.0974  | 2.6003         | 0.6506          | 0.4199     |
| agesq                                    | 0       | 1          | -2.4718  | 1.6636         | 2.2076          | 0.1373     |
| agesq                                    | 1       | 1          | 2.6883   | 2.8398         | 0.8961          | 0.3438     |
| income                                   | 0       | 1          | -0.00857 | 0.1266         | 0.0046          | 0.9460     |
| income                                   | 1       | 1          | 0.6464   | 0.2375         | 7.4075          | 0.0065     |
| levyplus                                 | 0       | 1          | -0.2658  | 0.0997         | 7.0999          | 0.0077     |
| levyplus                                 | 1       | 1          | -0.2869  | 0.1820         | 2.4848          | 0.1150     |
| freepoor                                 | 0       | 1          | 0.6773   | 0.2601         | 6.7811          | 0.0092     |
| freepoor                                 | 1       | 1          | 0.9020   | 0.4911         | 3.3730          | 0.0663     |
| freerepa                                 | 0       | 1          | -0.4044  | 0.1382         | 8.5637          | 0.0034     |
| freerepa                                 | 1       | 1          | -0.0958  | 0.2361         | 0.1648          | 0.6848     |
| illness                                  | 0       | 1          | -0.2645  | 0.0287         | 84.6792         | <.0001     |
| illness                                  | 1       | 1          | -0.3083  | 0.0499         | 38.1652         | <.0001     |
| actdays                                  | 0       | 1          | -0.1521  | 0.0116         | 172.2764        | <.0001     |
| actdays                                  | 1       | 1          | -0.1863  | 0.0134         | 193.7700        | <.0001     |
| hscore                                   | 0       | 1          | -0.0620  | 0.0172         | 12.9996         | 0.0003     |
| hscore                                   | 1       | 1          | -0.0568  | 0.0252         | 5.0940          | 0.0240     |
| chcond1                                  | 0       | 1          | -0.1140  | 0.0909         | 1.5721          | 0.2099     |
| chcond1                                  | 1       | 1          | -0.2478  | 0.1743         | 2.0201          | 0.1552     |
| chcond2                                  | 0       | 1          | -0.2660  | 0.1255         | 4.4918          | 0.0341     |
| chcond2                                  | 1       | 1          | -0.3146  | 0.2116         | 2.2106          | 0.1371     |



Output 54.17.2 *continued*

| Linear Hypotheses Testing Results |                    |    |            |
|-----------------------------------|--------------------|----|------------|
| Label                             | Wald<br>Chi-Square | DF | Pr > ChiSq |
| sex                               | 1.0981             | 1  | 0.2947     |
| age                               | 2.5658             | 1  | 0.1092     |
| agesq                             | 3.8309             | 1  | 0.0503     |
| income                            | 8.8006             | 1  | 0.0030     |
| levyplus                          | 0.0162             | 1  | 0.8989     |
| freepoor                          | 0.2569             | 1  | 0.6122     |
| freerepa                          | 2.0099             | 1  | 0.1563     |
| illness                           | 0.8630             | 1  | 0.3529     |
| actdays                           | 6.9407             | 1  | 0.0084     |
| hscore                            | 0.0476             | 1  | 0.8273     |
| chcond1                           | 0.6906             | 1  | 0.4060     |
| chcond2                           | 0.0615             | 1  | 0.8042     |

The preceding nonproportional odds model fits  $12 \times 2 = 24$  slope parameters, and the model seems to overfit the data. You can obtain a more parsimonious model by specifying a subset of the parameters to have nonproportional odds. The following statements allow the parameters for the variables in the “Linear Hypotheses Testing Results” table that have  $p$ -values less than 0.1 (actdays, agesq, and income) to vary across the response functions:

```
proc logistic data=docvisit;
 model dvisits= sex age agesq income levyplus freepoor
 freerepa illness actdays hscore chcond1 chcond2
 / unequalslopes=(actdays agesq income);
run;
```

Selected results from fitting this partial proportional odds model are displayed in [Output 54.17.3](#).

## Output 54.17.3 Results for Partial Proportional Odds Model

| Testing Global Null Hypothesis: BETA=0 |            |    |            |
|----------------------------------------|------------|----|------------|
| Test                                   | Chi-Square | DF | Pr > ChiSq |
| Likelihood Ratio                       | 752.5512   | 15 | <.0001     |
| Score                                  | 947.3269   | 15 | <.0001     |
| Wald                                   | 683.4719   | 15 | <.0001     |

## Output 54.17.3 continued

| Analysis of Maximum Likelihood Estimates |         |    |          |                |                 |            |
|------------------------------------------|---------|----|----------|----------------|-----------------|------------|
| Parameter                                | dvisits | DF | Estimate | Standard Error | Wald Chi-Square | Pr > ChiSq |
| Intercept                                | 0       | 1  | 2.3882   | 0.2716         | 77.2988         | <.0001     |
| Intercept                                | 1       | 1  | 3.7597   | 0.3138         | 143.5386        | <.0001     |
| sex                                      |         | 1  | -0.2485  | 0.0807         | 9.4789          | 0.0021     |
| age                                      |         | 1  | 1.3000   | 1.4864         | 0.7649          | 0.3818     |
| agesq                                    | 0       | 1  | -2.0110  | 1.6345         | 1.5139          | 0.2186     |
| agesq                                    | 1       | 1  | -0.8789  | 1.6512         | 0.2833          | 0.5945     |
| income                                   | 0       | 1  | 0.0209   | 0.1261         | 0.0275          | 0.8683     |
| income                                   | 1       | 1  | 0.4283   | 0.2221         | 3.7190          | 0.0538     |
| levyplus                                 |         | 1  | -0.2703  | 0.0989         | 7.4735          | 0.0063     |
| freepoor                                 |         | 1  | 0.6936   | 0.2589         | 7.1785          | 0.0074     |
| freerepa                                 |         | 1  | -0.3648  | 0.1358         | 7.2155          | 0.0072     |
| illness                                  |         | 1  | -0.2707  | 0.0281         | 92.7123         | <.0001     |
| actdays                                  | 0       | 1  | -0.1522  | 0.0115         | 173.5696        | <.0001     |
| actdays                                  | 1       | 1  | -0.1868  | 0.0129         | 209.7134        | <.0001     |
| hscore                                   |         | 1  | -0.0609  | 0.0166         | 13.5137         | 0.0002     |
| chcond1                                  |         | 1  | -0.1200  | 0.0901         | 1.7756          | 0.1827     |
| chcond2                                  |         | 1  | -0.2628  | 0.1227         | 4.5849          | 0.0323     |

The partial proportional odds model can be written in the same form as the nonproportional odds model by letting  $\mathbf{x} = (x_1, \dots, x_q, x_{q+1}, \dots, x_{12})$  and  $\boldsymbol{\beta}_i = (\beta_1, \dots, \beta_q, \beta_{q+1,i}, \dots, \beta_{12,i})$ , so the first  $q$  parameters have proportional odds and the remaining parameters do not. The last  $12-q$  parameters can be rewritten to have a common slope:  $\beta_{q+j} + \gamma_{q+j,i}$ ,  $j = 1, \dots, 12 - q$ , where the new parameters  $\gamma_i$  contain the increments from the common slopes. The model in this form makes it obvious that the proportional odds model is a submodel of the partial proportional odds models, and both of these are submodels of the nonproportional odds model. This means that you can use likelihood ratio tests to compare models.

You can use the following statements to compute the likelihood ratio tests from the Likelihood Ratio row of the “Testing Global Null hypothesis: BETA=0” tables in the preceding outputs:

```
data a;
 label p='Pr>ChiSq';
 format p 8.6;
 input Test $10. ChiSq1 DF1 ChiSq2 DF2;
 ChiSq= ChiSq1-ChiSq2;
 DF= DF1-DF2;
 p=1-probchi(ChiSq,DF);
 keep Test ChiSq DF p;
 datalines;
Non vs PO 761.4797 24 734.2971 12
PPO vs PO 752.5512 15 734.2971 12
Non vs PPO 761.4797 24 752.5512 15
;

proc print data=a label noobs;
 var Test ChiSq DF p;
run;
```

**Output 54.17.4** Likelihood Ratio Tests

| Test       | ChiSq   | DF | Pr>ChiSq |
|------------|---------|----|----------|
| Non vs PO  | 27.1826 | 12 | 0.007273 |
| PPO vs PO  | 18.2541 | 3  | 0.000390 |
| Non vs PPO | 8.9285  | 9  | 0.443900 |

Therefore, you reject the proportional odds model in favor of both the nonproportional odds model and the partial proportional odds model, and the partial proportional odds model fits as well as the nonproportional odds model. The likelihood ratio test of the nonproportional odds model versus the proportional odds model is very similar to the score test of the proportional odds assumption in [Output 54.17.1](#) because of the large sample size (Stokes, Davis, and Koch 2000, p. 249).

**NOTE:** The proportional odds model has increasing intercepts, which ensures the increasing nature of the cumulative response functions. However, none of the parameters in the partial or nonproportional odds models are constrained. Because of this, sometimes during the optimization process a predicted individual probability can be negative; the optimization continues because it might recover from this situation. Sometimes your final model will predict negative individual probabilities for some of the observations; in this case a message is displayed, and you should check your data for outliers and possibly redefine your model. Other times the model fits your data well, but if you try to score new data you can get negative individual probabilities. This means the model is not appropriate for the data you are trying to score, a message is displayed, and the estimates are set to missing.

---

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# Chapter 55

## The MCMC Procedure

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## Overview: MCMC Procedure

The MCMC procedure is a general purpose Markov chain Monte Carlo (MCMC) simulation procedure that is designed to fit Bayesian models. Bayesian statistics is different from traditional statistical methods such as frequentist or classical methods. For a short introduction to Bayesian analysis and related basic concepts, see Chapter 7, “[Introduction to Bayesian Analysis Procedures](#).” Also see the section “[A Bayesian Reading List](#)” on page 156 for a guide to Bayesian textbooks of varying degrees of difficulty.

In essence, Bayesian statistics treats parameters as unknown random variables, and it makes inferences based on the posterior distributions of the parameters. There are several advantages associated with this approach to statistical inference. Some of the advantages include its ability to use prior information and to directly answer specific scientific questions that can be easily understood. For further discussions of the relative advantages and disadvantages of Bayesian analysis, see the section “[Bayesian Analysis: Advantages and Disadvantages](#)” on page 132.

It follows from Bayes’ theorem that a posterior distribution is the product of the likelihood function and the prior distribution of the parameter. In all but the simplest cases, it is very difficult to obtain the posterior distribution directly and analytically. Often, Bayesian methods rely on simulations to generate sample from the desired posterior distribution and use the simulated draws to approximate the distribution and to make all of the inferences.

PROC MCMC is a flexible, simulation-based procedure that is suitable for fitting a wide range of Bayesian models. To use PROC MCMC, you need to specify a likelihood function for the data and a prior distribution for the parameters. If you are fitting hierarchical models, you can specify a hyperprior distribution or distributions for the random-effects parameters. PROC MCMC then obtains samples from the corresponding posterior distributions, produces summary and diagnostic statistics, and saves the posterior samples in an output data set that can be used for further analysis. Although PROC MCMC supports a suite of standard distributions, you can analyze data that have any likelihood, prior, or hyperprior, as long as these functions are programmable using the SAS DATA step functions. There are no constraints on how the parameters can enter the model, in either linear or any nonlinear functional form.

The **MODEL** statement in PROC MCMC can automatically model missing data, response variables, or covariates. In releases before SAS/STAT 12.1, observations with missing values were discarded prior to the analysis. Now, PROC MCMC treats the missing values as unknown parameters and incorporates the sampling of the missing values as part of the simulation.

PROC MCMC selects a sampling method for each parameter or a block of parameters. For example, when conjugacy is available, samples are drawn directly from the full conditional distribution by using standard random number generators. In other cases, PROC MCMC uses an adaptive blocked random walk Metropolis algorithm that uses a normal proposal distribution. You can also choose alternative sampling algorithms, such as the slice sampler.

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## PROC MCMC Compared with Other SAS Procedures

PROC MCMC is unlike most other SAS/STAT procedures in that the nature of the statistical inference is Bayesian. You specify prior distributions for the parameters with **PRIOR** statements and the likelihood function for the data with **MODEL** statements. PROC MCMC derives inferences from simulation rather than through analytic or numerical methods. You should expect slightly different answers from each run

for the same problem, unless the same random number seed is used. The model specification is similar to PROC NLIN, and PROC MCMC shares some of the syntax of PROC NLMIXED.

You can also carry out a Bayesian analysis with the GENMOD, PHREG, LIFEREG, and FMM procedures for generalized linear models, accelerated life failure models, Cox regression models, piecewise constant baseline hazard models (also known as piecewise exponential models), and finite mixture models. See Chapter 40, “The GENMOD Procedure,” Chapter 67, “The PHREG Procedure,” Chapter 51, “The LIFEREG Procedure,” and Chapter 37, “The FMM Procedure.”

## Getting Started: MCMC Procedure

There are three examples in this “Getting Started” section: a simple linear regression, the Behrens-Fisher estimation problem, and a random-effects model. The regression model is chosen for its simplicity; the Behrens-Fisher problem illustrates some advantages of the Bayesian approach; and the random-effects model is one of the most prevalently used models.

Keep in mind that **PARMS** statements declare the parameters in the model, **PRIOR** statements declare the prior distributions, **MODEL** statements declare the likelihood for the data, and **RANDOM** statements declare the random effects. In most cases, you do not need to supply initial values. PROC MCMC advises you if it is unable to generate starting values for the Markov chain.

### Simple Linear Regression

This section illustrates some basic features of PROC MCMC by using a linear regression model. The model is as follows:

$$Y_i = \beta_0 + \beta_1 X_i + \epsilon_i$$

for the observations  $i = 1, 2, \dots, n$ .

The following statements create a SAS data set with measurements of Height and Weight for a group of children:

```

title 'Simple Linear Regression';

data Class;
 input Name $ Height Weight @@;
 datalines;
Alfred 69.0 112.5 Alice 56.5 84.0 Barbara 65.3 98.0
Carol 62.8 102.5 Henry 63.5 102.5 James 57.3 83.0
Jane 59.8 84.5 Janet 62.5 112.5 Jeffrey 62.5 84.0
John 59.0 99.5 Joyce 51.3 50.5 Judy 64.3 90.0
Louise 56.3 77.0 Mary 66.5 112.0 Philip 72.0 150.0
Robert 64.8 128.0 Ronald 67.0 133.0 Thomas 57.5 85.0
William 66.5 112.0
;

```

The equation of interest is as follows:

$$\text{Weight}_i = \beta_0 + \beta_1 \text{Height}_i + \epsilon_i$$

The observation errors,  $\epsilon_i$ , are assumed to be independent and identically distributed with a normal distribution with mean zero and variance  $\sigma^2$ .

$$\text{Weight}_i \sim \text{normal}(\beta_0 + \beta_1 \text{Height}_i, \sigma^2)$$

The likelihood function for each of the `Weight`, which is specified in the `MODEL` statement, is as follows:

$$p(\text{Weight}|\beta_0, \beta_1, \sigma^2, \text{Height}_i) = \phi(\beta_0 + \beta_1 \text{Height}_i, \sigma^2)$$

where  $p(\cdot|\cdot)$  denotes a conditional probability density and  $\phi$  is the normal density. There are three parameters in the likelihood:  $\beta_0$ ,  $\beta_1$ , and  $\sigma^2$ . You use the `PARMS` statement to indicate that these are the parameters in the model.

Suppose you want to use the following three prior distributions on each of the parameters:

$$\begin{aligned} \pi(\beta_0) &= \phi(0, \text{var} = 1e6) \\ \pi(\beta_1) &= \phi(0, \text{var} = 1e6) \\ \pi(\sigma^2) &= f_{i\Gamma}(\text{shape} = 3/10, \text{scale} = 10/3) \end{aligned}$$

where  $\pi(\cdot)$  indicates a prior distribution and  $f_{i\Gamma}$  is the density function for the inverse-gamma distribution. The normal priors on  $\beta_0$  and  $\beta_1$  have large variances, expressing your lack of knowledge about the regression coefficients. The priors correspond to an equal-tail 95% credible intervals of approximately (-2000, 2000) for  $\beta_0$  and  $\beta_1$ . Priors of this type are often called *vague* or *diffuse* priors. See the section “[Prior Distributions](#)” on page 127 for more information. Typically diffuse prior distributions have little influence on the posterior distribution and are appropriate when stronger prior information about the parameters is not available.

A frequently used prior for the variance parameter  $\sigma^2$  is the inverse-gamma distribution. See [Table 55.22](#) in the section “[Standard Distributions](#)” on page 4476 for the density definition. The inverse-gamma distribution is a conjugate prior (see the section “[Conjugate Sampling](#)” on page 4472) for the variance parameter in a normal distribution. Also see the section “[Gamma and Inverse-Gamma Distributions](#)” on page 4512 for typical usages of the gamma and inverse-gamma prior distributions. With a shape parameter of 3/10 and a scale parameter of 10/3, this prior corresponds to an equal-tail 95% credible interval of (1.7, 1E6), with the mode at 2.5641 for  $\sigma^2$ . Alternatively, you can use any other prior distribution with positive support on this variance component. For example, you can use the gamma prior.

According to Bayes’ theorem, the likelihood function and prior distributions determine the posterior (joint) distribution of  $\beta_0$ ,  $\beta_1$ , and  $\sigma^2$  as follows:

$$\pi(\beta_0, \beta_1, \sigma^2 | \text{Weight}, \text{Height}) \propto \pi(\beta_0)\pi(\beta_1)\pi(\sigma^2)p(\text{Weight}|\beta_0, \beta_1, \sigma^2, \text{Height})$$

You do not need to know the form of the posterior distribution when you use PROC MCMC. PROC MCMC automatically obtains samples from the desired posterior distribution, which is determined by the prior and likelihood you supply.

The following statements fit this linear regression model with diffuse prior information:

```
ods graphics on;
proc mcmc data=class outpost=classout nmc=10000 thin=2 seed=246810;
 parms beta0 0 beta1 0;
 parms sigma2 1;
 prior beta0 beta1 ~ normal(mean = 0, var = 1e6);
 prior sigma2 ~ igamma(shape = 3/10, scale = 10/3);
 mu = beta0 + beta1*height;
 model weight ~ n(mu, var = sigma2);
run;
ods graphics off;
```

When ODS Graphics is enabled, diagnostic plots, such as the trace and autocorrelation function plots of the posterior samples, are displayed. For more information about ODS Graphics, see Chapter 21, “[Statistical Graphics Using ODS](#).”

The PROC MCMC statement invokes the procedure and specifies the input data set `Class`. The output data set `Classout` contains the posterior samples for all of the model parameters. The `NMC=` option specifies the number of posterior simulation iterations. The `THIN=` option controls the thinning of the Markov chain and specifies that one of every 2 samples is kept. Thinning is often used to reduce the correlations among posterior sample draws. In this example, 5,000 simulated values are saved in the `Classout` data set. The `SEED=` option specifies a seed for the random number generator, which guarantees the reproducibility of the random stream. For more information about Markov chain sample size, burn-in, and thinning, see the section “[Burn-in, Thinning, and Markov Chain Samples](#)” on page 138.

The `PARMS` statements identify the three parameters in the model: `beta0`, `beta1`, and `sigma2`. Each statement also forms a block of parameters, where the parameters are updated simultaneously in each iteration. In this example, `beta0` and `beta1` are sampled jointly, conditional on `sigma2`; and `sigma2` is sampled conditional on fixed values of `beta0` and `beta1`. In simple regression models such as this, you expect the parameters `beta0` and `beta1` to have high posterior correlations, and placing them both in the same block improves the mixing of the chain—that is, the efficiency that the posterior parameter space is explored by the Markov chain. For more information, see the section “[Blocking of Parameters](#)” on page 4466. The `PARMS` statements also assign initial values to the parameters (see the section “[Initial Values of the Markov Chains](#)” on page 4474). The regression parameters are given 0 as their initial values, and the scale parameter `sigma2` starts at value 1. If you do not provide initial values, PROC MCMC chooses starting values for every parameter.

The `PRIOR` statements specify prior distributions for the parameters. The parameters `beta0` and `beta1` both share the same prior—a normal prior with mean 0 and variance 1e6. The parameter `sigma2` has an inverse-gamma distribution with a shape parameter of 3/10 and a scale parameter of 10/3. For a list of standard distributions that PROC MCMC supports, see the section “[Standard Distributions](#)” on page 4476.

The `MU` assignment statement calculates the expected value of `Weight` as a linear function of `Height`. The `MODEL` statement uses the shorthand notation, `n`, for the normal distribution to indicate that the response variable, `Weight`, is normally distributed with parameters `mu` and `sigma2`. The functional argument `MEAN=` in the normal distribution is optional, but you have to indicate whether `sigma2` is a variance (`VAR=`), a standard deviation (`SD=`), or a precision (`PRECISION=`) parameter. See [Table 55.2](#) in the section “[MODEL Statement](#)” on page 4443 for distribution specifications.

The distribution parameters can contain expressions. For example, you can write the `MODEL` statement as follows:

```
model weight ~ n(beta0 + beta1*height, var = sigma2);
```

Before you do any posterior inference, it is essential that you examine the convergence of the Markov chain (see the section “[Assessing Markov Chain Convergence](#)” on page 139). You cannot make valid inferences if the Markov chain has not converged. A very effective convergence diagnostic tool is the trace plot. Although PROC MCMC produces graphs at the end of the procedure output (see [Figure 55.5](#)), you should visually examine the convergence graph first.

The first table that PROC MCMC produces is the “Number of Observations” table, as shown in [Figure 55.1](#). This table lists the number of observations read from the `DATA=` data set and the number of observations used in the analysis.

**Figure 55.1** Observation Information

| Simple Linear Regression    |    |
|-----------------------------|----|
| The MCMC Procedure          |    |
| Number of Observations Read | 19 |
| Number of Observations Used | 19 |

The “Parameters” table, shown in [Figure 55.2](#), lists the names of the parameters, the blocking information, the sampling method used, the starting values, and the prior distributions. For more information about blocking information, see the section “[Blocking of Parameters](#)” on page 4466; for more information about starting values, see the section “[Initial Values of the Markov Chains](#)” on page 4474. The first block, which consists of the parameters `beta0` and `beta1`, uses a random walk Metropolis algorithm. The second block, which consists of the parameter `sigma2`, is updated via its full conditional distribution in conjugacy. You should check this table to ensure that you have specified the parameters correctly, especially for complicated models.

**Figure 55.2** Parameter Information

| Parameters |                     |                 |               |                                    |
|------------|---------------------|-----------------|---------------|------------------------------------|
| Block      | Parameter           | Sampling Method | Initial Value | Prior Distribution                 |
| 1          | <code>beta0</code>  | N-Metropolis    | 0             | normal(mean = 0, var = 1e6)        |
|            | <code>beta1</code>  |                 | 0             | normal(mean = 0, var = 1e6)        |
| 2          | <code>sigma2</code> | Conjugate       | 1.0000        | igamma(shape = 3/10, scale = 10/3) |

For each posterior distribution, PROC MCMC also reports summary statistics (posterior means, standard deviations, and quantiles) and interval statistics (95% equal-tail and highest posterior density credible intervals), as shown in [Figure 55.3](#). For more information about posterior statistics, see the section “[Summary Statistics](#)” on page 153.

**Figure 55.3** MCMC Summary and Interval Statistics

| Simple Linear Regression |      |        |                       |             |        |        |
|--------------------------|------|--------|-----------------------|-------------|--------|--------|
| The MCMC Procedure       |      |        |                       |             |        |        |
| Posterior Summaries      |      |        |                       |             |        |        |
| Parameter                | N    | Mean   | Standard<br>Deviation | Percentiles |        |        |
|                          |      |        |                       | 25%         | 50%    | 75%    |
| beta0                    | 5000 | -142.8 | 33.4326               | -164.8      | -142.3 | -120.0 |
| beta1                    | 5000 | 3.8924 | 0.5333                | 3.5361      | 3.8826 | 4.2395 |
| sigma2                   | 5000 | 137.3  | 51.1030               | 101.9       | 127.2  | 161.2  |

| Posterior Intervals |       |                     |        |              |          |
|---------------------|-------|---------------------|--------|--------------|----------|
| Parameter           | Alpha | Equal-Tail Interval |        | HPD Interval |          |
|                     |       | beta0               | 0.050  | -208.9       | -78.7305 |
| beta1               | 0.050 | 2.8790              | 4.9449 | 2.9056       | 4.9545   |
| sigma2              | 0.050 | 69.1351             | 259.8  | 59.2362      | 236.3    |

By default, PROC MCMC also computes a number of convergence diagnostics to help you determine whether the chain has converged. These are the Monte Carlo standard errors, the autocorrelations at selected lags, the Geweke diagnostics, and the effective sample sizes. These statistics are shown in [Figure 55.4](#). For details and interpretations of these diagnostics, see the section “[Assessing Markov Chain Convergence](#)” on page 139.

The “Monte Carlo Standard Errors” table indicates that the standard errors of the mean estimates for each of the parameters are relatively small, with respect to the posterior standard deviations. The values in the “MCSE/SD” column (ratios of the standard errors and the standard deviations) are small, around 0.03. This means that only a fraction of the posterior variability is due to the simulation. The “Autocorrelations of the Posterior Samples” table shows that the autocorrelations among posterior samples reduce quickly and become almost nonexistent after a few lags. The “Geweke Diagnostics” table indicates that no parameter failed the test, and the “Effective Sample Sizes” table reports the number of effective sample sizes of the Markov chain.

**Figure 55.4** MCMC Convergence Diagnostics

| Simple Linear Regression    |        |                       |         |
|-----------------------------|--------|-----------------------|---------|
| The MCMC Procedure          |        |                       |         |
| Monte Carlo Standard Errors |        |                       |         |
| Parameter                   | MCSE   | Standard<br>Deviation | MCSE/SD |
| beta0                       | 1.0070 | 33.4326               | 0.0301  |
| beta1                       | 0.0159 | 0.5333                | 0.0299  |
| sigma2                      | 0.9473 | 51.1030               | 0.0185  |

Figure 55.4 continued

| Posterior Autocorrelations |        |        |        |         |
|----------------------------|--------|--------|--------|---------|
| Parameter                  | Lag 1  | Lag 5  | Lag 10 | Lag 50  |
| beta0                      | 0.6177 | 0.1083 | 0.0250 | -0.0007 |
| beta1                      | 0.6162 | 0.1052 | 0.0217 | 0.0029  |
| sigma2                     | 0.1224 | 0.0216 | 0.0098 | 0.0197  |

| Geweke Diagnostics |         |         |
|--------------------|---------|---------|
| Parameter          | z       | Pr >  z |
| beta0              | 1.0267  | 0.3046  |
| beta1              | -0.9305 | 0.3521  |
| sigma2             | -0.3578 | 0.7205  |

| Effective Sample Sizes |        |                 |            |
|------------------------|--------|-----------------|------------|
| Parameter              | ESS    | Autocorrelation |            |
|                        |        | Time            | Efficiency |
| beta0                  | 1102.2 | 4.5366          | 0.2204     |
| beta1                  | 1119.0 | 4.4684          | 0.2238     |
| sigma2                 | 2910.1 | 1.7182          | 0.5820     |

PROC MCMC produces a number of graphs, shown in Figure 55.5, which also aid convergence diagnostic checks. With the trace plots, there are two important aspects to examine. First, you want to check whether the mean of the Markov chain has stabilized and appears constant over the graph. Second, you want to check whether the chain has good mixing and is “dense,” in the sense that it quickly traverses the support of the distribution to explore both the tails and the mode areas efficiently. The plots show that the chains appear to have reached their stationary distributions.

Next, you should examine the autocorrelation plots, which indicate the degree of autocorrelation for each of the posterior samples. High correlations usually imply slow mixing. Finally, the kernel density plots estimate the posterior marginal distributions for each parameter.



**Figure 55.5** Diagnostic Plots for  $\beta_0$ ,  $\beta_1$  and  $\sigma^2$

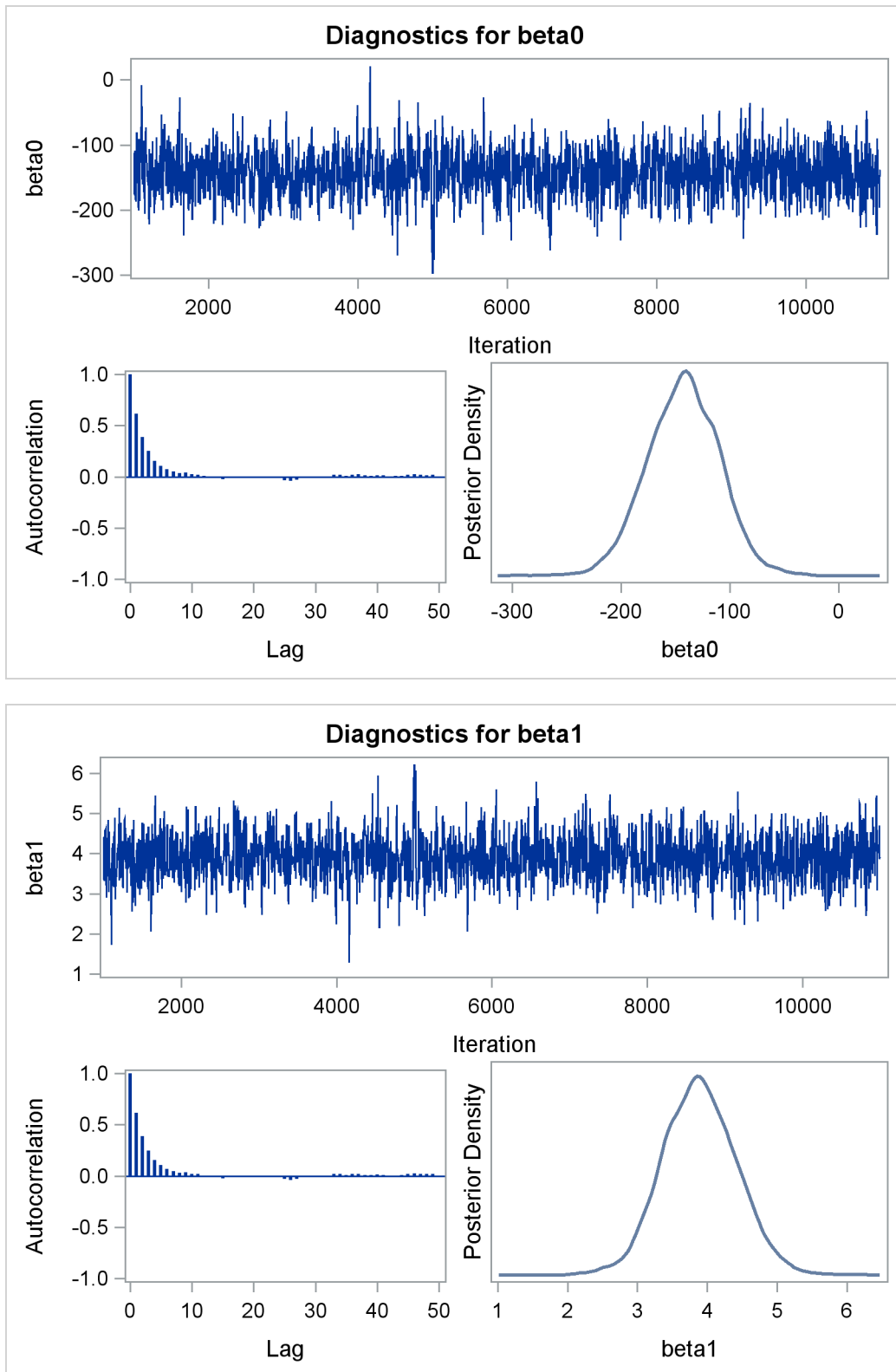
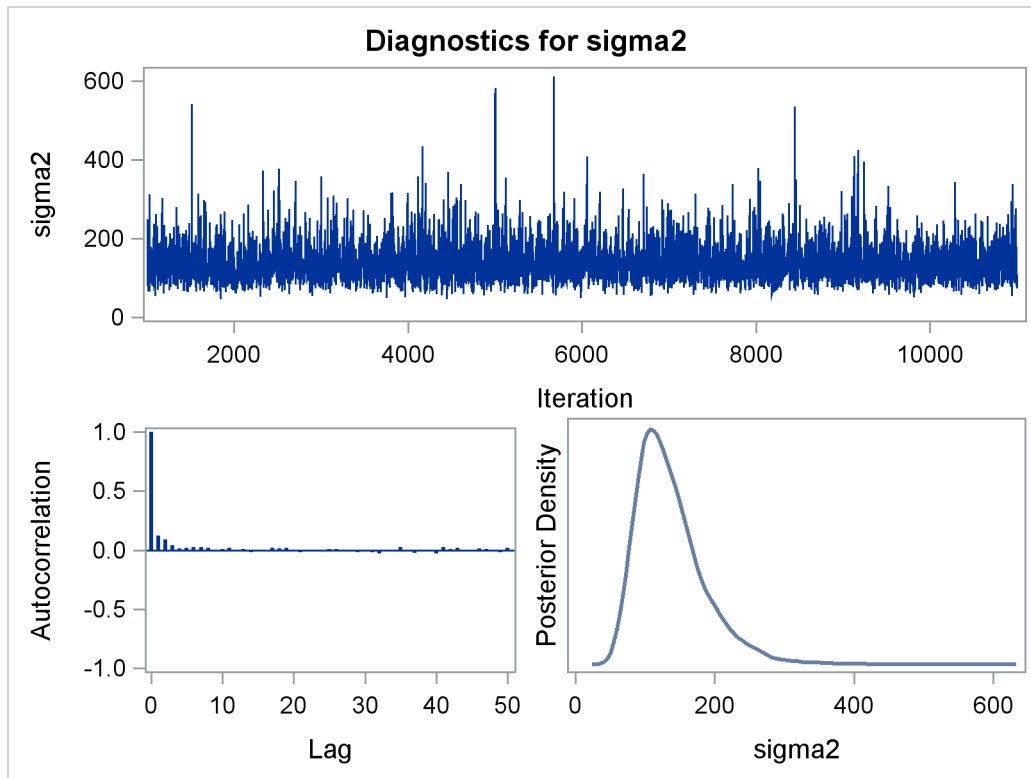


Figure 55.5 continued



In regression models such as this, you expect the posterior estimates to be very similar to the maximum likelihood estimators with noninformative priors on the parameters. The REG procedure produces the following fitted model (code not shown):

$$\text{Weight} = -143.0 + 3.9 \times \text{Height}$$

These are very similar to the means show in Figure 55.3. With PROC MCMC, you can carry out informative analysis that uses specifications to indicate prior knowledge on the parameters. Informative analysis is likely to produce different posterior estimates, which are the result of information from both the likelihood and the prior distributions. Incorporating additional information in the analysis is one major difference between the classical and Bayesian approaches to statistical inference.

---

## The Behrens-Fisher Problem

One of the famous examples in the history of statistics is the Behrens-Fisher problem (Fisher 1935). Consider the situation where there are two independent samples from two different normal distributions:

$$y_{11}, y_{12}, \dots, y_{1n_1} \sim \text{normal}(\mu_1, \sigma_1^2)$$

$$y_{21}, y_{22}, \dots, y_{2n_2} \sim \text{normal}(\mu_2, \sigma_2^2)$$

Note that  $n_1 \neq n_2$ . When you do not want to assume that the variances are equal, testing the hypothesis  $H_0 : \mu_1 = \mu_2$  is a difficult problem in the classical statistics framework, because the distribution under  $H_0$

is not known. Within the Bayesian framework, this problem is straightforward because you can estimate the posterior distribution of  $\mu_1 - \mu_2$  while taking into account the uncertainties in all of parameters by treating them as random variables.

Suppose you have the following set of data:

```

title 'The Behrens-Fisher Problem';

data behrens;
 input y ind @@;
 datalines;
121 1 94 1 119 1 122 1 142 1 168 1 116 1
172 1 155 1 107 1 180 1 119 1 157 1 101 1
145 1 148 1 120 1 147 1 125 1 126 2 125 2
130 2 130 2 122 2 118 2 118 2 111 2 123 2
126 2 127 2 111 2 112 2 121 2
 ;

```

The response variable is  $y$ , and the  $\text{ind}$  variable is the group indicator, which takes two values: 1 and 2. There are 19 observations that belong to group 1 and 14 that belong to group 2.

The likelihood functions for the two samples are as follows:

$$\begin{aligned}
 p(y_{1i} | \mu_1, \sigma_1^2) &= \phi(y_{1i}; \mu_1, \sigma_1^2) \quad \text{for } i = 1, \dots, 19 \\
 p(y_{2j} | \mu_2, \sigma_2^2) &= \phi(y_{2j}; \mu_2, \sigma_2^2) \quad \text{for } j = 1, \dots, 14
 \end{aligned}$$

Berger (1985) showed that a uniform prior on the support of the location parameter is a noninformative prior. The distribution is invariant under location transformations—that is,  $\theta = \mu + c$ . You can use this prior for the mean parameters in the model:

$$\begin{aligned}
 \pi(\mu_1) &\propto 1 \\
 \pi(\mu_2) &\propto 1
 \end{aligned}$$

In addition, Berger (1985) showed that a prior of the form  $1/\sigma^2$  is noninformative for the scale parameter, and it is invariant under scale transformations (that is  $\tau = c\sigma^2$ ). You can use this prior for the variance parameters in the model:

$$\begin{aligned}
 \pi(\sigma_1^2) &\propto 1/\sigma_1^2 \\
 \pi(\sigma_2^2) &\propto 1/\sigma_2^2
 \end{aligned}$$

The log densities of the prior distributions on  $\sigma_1^2$  and  $\sigma_2^2$  are:

$$\begin{aligned}
 \log(\pi(\sigma_1^2)) &= -\log(\sigma_1^2) \\
 \log(\pi(\sigma_2^2)) &= -\log(\sigma_2^2)
 \end{aligned}$$

The following statements generate posterior samples of  $\mu_1, \mu_2, \sigma_1^2, \sigma_2^2$ , and the difference in the means:  $\mu_1 - \mu_2$ :

```

proc mcmc data=behrens outpost=postout seed=123
 nmc=40000 thin=10 monitor=(_parms_ mudif)
 statistics(alpha=0.01)=(summary interval);
ods select PostSummaries PostIntervals;
parm mu1 0 mu2 0;
parm sig21 1;
parm sig22 1;
prior mu: ~ general(0);
prior sig21 ~ general(-log(sig21), lower=0);
prior sig22 ~ general(-log(sig22), lower=0);
mudif = mu1 - mu2;
if ind = 1 then do;
 mu = mu1;
 s2 = sig21;
end;
else do;
 mu = mu2;
 s2 = sig22;
end;
model y ~ normal(mu, var=s2);
run;

```

The PROC MCMC statement specifies an input data set (Behrens), an output data set containing the posterior samples (Postout), a random number seed, the simulation size, and the thinning rate. The **MONITOR=** option specifies a list of symbols, which can be either parameters or functions of the parameters in the model, for which inference is to be done. The symbol `_parms_` is a shorthand for all model parameters—in this case,  $\mu_1$ ,  $\mu_2$ ,  $\text{sig21}$ , and  $\text{sig22}$ . The symbol `mudif` is defined in the program as the difference between  $\mu_1$  and  $\mu_2$ .

The **STATISTICS=** option requests the calculation of summary and interval statistics. The global suboption `ALPHA=0.01` specifies 99% equal-tail and highest posterior density (HPD) credible intervals for all parameters.

The ODS SELECT statement displays the summary statistics and interval statistics tables while excluding all other output. For a complete list of ODS tables that PROC MCMC can produce, see the sections “[Displayed Output](#)” on page 4533 and “[ODS Table Names](#)” on page 4537.

The **PARMS** statements assign the parameters  $\mu_1$  and  $\mu_2$  to the same block, and  $\text{sig21}$  and  $\text{sig22}$  each to their own separate blocks. There are a total of three blocks. The **PARMS** statements also assign an initial value to each parameter.

The **PRIOR** statements specify prior distributions for the parameters. Because the priors are all nonstandard (uniform on the real axis for  $\mu_1$  and  $\mu_2$  and  $1/\sigma^2$  for  $\sigma_1^2$  and  $\sigma_2^2$ ), you must use the **GENERAL** function here. The argument in the **GENERAL** function is an expression for the log of the distribution, up to an additive constant. This distribution can have any functional form, as long as it is programmable using SAS functions and expressions. The function specifies a distribution on the log scale, not on the original scale. The log of the prior on  $\mu_1$  and  $\mu_2$  is 0, and the log of the priors on  $\text{sig21}$  and  $\text{sig22}$  are  $-\log(\text{sig21})$  and  $-\log(\text{sig22})$  respectively. See the section “[Specifying a New Distribution](#)” on page 4490 for more information about how to specify an arbitrary distribution. The **LOWER=** option indicates that both variance terms must be strictly positive.

The MUDIF assignment statement calculates the difference between  $\mu_1$  and  $\mu_2$ . The IF-ELSE statements enable different  $y$ 's to have different mean and variance, depending on their group indicator *ind*. The MODEL statement specifies the normal likelihood function for each observation in the model.

Figure 55.6 displays the posterior summary and interval statistics.

**Figure 55.6** Posterior Summary and Interval Statistics

| The Behrens-Fisher Problem |      |         |                       |             |         |         |
|----------------------------|------|---------|-----------------------|-------------|---------|---------|
| The MCMC Procedure         |      |         |                       |             |         |         |
| Posterior Summaries        |      |         |                       |             |         |         |
| Parameter                  | N    | Mean    | Standard<br>Deviation | Percentiles |         |         |
|                            |      |         |                       | 25%         | 50%     | 75%     |
| mu1                        | 4000 | 134.8   | 6.0065                | 130.9       | 134.7   | 138.7   |
| mu2                        | 4000 | 121.4   | 1.9150                | 120.2       | 121.4   | 122.7   |
| sig21                      | 4000 | 683.2   | 259.9                 | 507.8       | 630.1   | 792.3   |
| sig22                      | 4000 | 51.3975 | 24.2881               | 35.0212     | 45.7449 | 61.2582 |
| mudif                      | 4000 | 13.3596 | 6.3335                | 9.1732      | 13.4078 | 17.6332 |

| Posterior Intervals |       |                     |         |              |         |
|---------------------|-------|---------------------|---------|--------------|---------|
| Parameter           | Alpha | Equal-Tail Interval |         | HPD Interval |         |
| mu1                 | 0.010 | 118.7               | 150.6   | 119.3        | 151.0   |
| mu2                 | 0.010 | 115.9               | 126.6   | 116.2        | 126.7   |
| sig21               | 0.010 | 292.0               | 1821.1  | 272.8        | 1643.7  |
| sig22               | 0.010 | 18.5883             | 158.8   | 16.3730      | 140.5   |
| mudif               | 0.010 | -3.2537             | 29.9987 | -3.1915      | 30.0558 |

The mean difference has a posterior mean value of 13.36, and the lower endpoints of the 99% credible intervals are negative. This suggests that the mean difference is positive with a high probability. However, if you want to estimate the probability that  $\mu_1 - \mu_2 > 0$ , you can do so as follows.

The following statements produce Figure 55.7:

```
proc format;
 value diffmt low=0 = 'mu1 - mu2 <= 0' 0<-high = 'mu1 - mu2 > 0';
run;

proc freq data = postout;
 tables mudif /nocum;
 format mudif diffmt.;
run;
```

The sample estimate of the posterior probability that  $\mu_1 - \mu_2 > 0$  is 0.98. This example illustrates an advantage of Bayesian analysis. You are not limited to making inferences based on model parameters only. You can accurately quantify uncertainties with respect to any function of the parameters, and this allows for flexibility and easy interpretations in answering many scientific questions.

**Figure 55.7** Estimated Probability of  $\mu_1 - \mu_2 > 0$ .

| The Behrens-Fisher Problem |           |         |
|----------------------------|-----------|---------|
| The FREQ Procedure         |           |         |
| mudif                      | Frequency | Percent |
| mu1 - mu2 <= 0             | 77        | 1.93    |
| mu1 - mu2 > 0              | 3923      | 98.08   |

## Random-Effects Model

This example illustrates how you can fit a normal likelihood random-effects model in PROC MCMC. PROC MCMC offers you the ability to model beyond the normal likelihood (see “Example 55.7: Logistic Regression Random-Effects Model” on page 4579, “Example 55.8: Nonlinear Poisson Regression Multilevel Random-Effects Model” on page 4581, and “Example 55.16: Piecewise Exponential Frailty Model” on page 4631).

Consider a scenario in which data are collected in groups and you want to model group-specific effects. You can use a random-effects model (sometimes also known as a variance-components model):

$$y_{ij} = \beta_0 + \beta_1 x_{ij} + \gamma_i + e_{ij}, \quad e_{ij} \sim \text{normal}(0, \sigma^2)$$

where  $i = 1, 2, \dots, I$  is the group index and  $j = 1, 2, \dots, n_i$  indexes the observations in the  $i$ th group. In the regression model, the fixed effects  $\beta_0$  and  $\beta_1$  are the intercept and the coefficient for variable  $x_{ij}$ , respectively. The random effect  $\gamma_i$  is the mean for the  $i$ th group, and  $e_{ij}$  are the error term.

Consider the following SAS data set:

```

title 'Random-Effects Model';

data heights;
 input Family G$ Height @@;
 datalines;
1 F 67 1 F 66 1 F 64 1 M 71 1 M 72 2 F 63
2 F 63 2 F 67 2 M 69 2 M 68 2 M 70 3 F 63
3 M 64 4 F 67 4 F 66 4 M 67 4 M 67 4 M 69
;

```

The response variable Height measures the heights (in inches) of 18 individuals. The covariate  $x$  is the gender (variable G), and the individuals are grouped according to Family (group index). Since the variable G is a character variable and PROC MCMC does not support a CLASS statement, you need to create the corresponding design matrix. In this example, the design matrix for a factor variable of level 2 (M and F) can be constructed using the following statement:

```

data input;
 set heights;
 if g eq 'F' then gf = 1;
 else gf = 0;
 drop g;
run;

```

The data set variable `gf` is a numeric variable and can be used in the regression model in PROC MCMC.

In data sets with factor variables that have more levels, you can consider using PROC TRANSREG to construct the design matrix. See the section “[Create Design Matrix](#)” on page 4502 for more information.

To model the data, you can assume that Height is normally distributed:

$$y_{ij} \sim \text{normal}(\mu_{ij}, \sigma^2), \quad \mu_{ij} = \beta_0 + \beta_1 \text{gf}_{ij} + \gamma_i$$

The priors on the parameters  $\beta_0$ ,  $\beta_1$ ,  $\gamma_i$  are also assumed to be normal:

$$\begin{aligned} \beta_0 &\sim \text{normal}(0, \text{var} = 1e5) \\ \beta_1 &\sim \text{normal}(0, \text{var} = 1e5) \\ \gamma_i &\sim \text{normal}(0, \text{var} = \sigma_\gamma^2) \end{aligned}$$

Priors on the variance terms,  $\sigma^2$  and  $\sigma_\gamma^2$ , are inverse-gamma:

$$\begin{aligned} \sigma^2 &\sim \text{igamma}(\text{shape} = 0.01, \text{scale} = 0.01) \\ \sigma_\gamma^2 &\sim \text{igamma}(\text{shape} = 0.01, \text{scale} = 0.01) \end{aligned}$$

The inverse-gamma distribution is a conjugate prior for the variance in the normal likelihood and the variance in the prior distribution of the random effect.

The following statements fit a linear random-effects model to the data and produce the output shown in [Figure 55.9](#) and [Figure 55.10](#):

```

ods graphics on;
proc mcmc data=input outpost=postout nmc=50000 thin=5 seed=7893 plots=trace;
 ods select Parameters REparameters PostSummaries PostIntervals
 tracepanel;
 parms b0 0 b1 0 s2 1 s2g 1;

 prior b: ~ normal(0, var = 10000);
 prior s: ~ igamma(0.01, scale = 0.01);
 random gamma ~ normal(0, var = s2g) subject=family monitor=(gamma);
 mu = b0 + b1 * gf + gamma;
 model height ~ normal(mu, var = s2);
run;
ods graphics off;

```

Some of the statements are very similar to those shown in the previous two examples. The ODS GRAPHICS ON statement enables ODS Graphics. The PROC MCMC statement specifies the input and output data sets, the simulation size, the thinning rate, and a random number seed. The ODS SELECT statement displays

the model parameter and random-effects parameter information tables, summary statistics table, the interval statistics table, and the trace plots.

The **PARMS** statement lumps all four model parameters in a single block. They are  $b_0$  (overall intercept),  $b_1$  (main effect for *gf*),  $s_2$  (variance of the likelihood function), and  $s_{2g}$  (variance of the random effect). If a random walk Metropolis sampler is the only applicable sampler for all parameters, then these four parameters are updated in a single block. However, because PROC MCMC updates the parameters  $s_2$  and  $s_{2g}$  via conjugacy, these parameters are separated into individual blocks. (See the Block column in “Parameters” table in Figure 55.8.)

The **PRIOR** statements specify priors for all the parameters. The notation  $b:$  is a shorthand for all symbols that start with the letter ‘ $b$ ’. In this example,  $b:$  includes  $b_0$  and  $b_1$ . Similarly,  $s:$  stands for both  $s_2$  and  $s_{2g}$ . This shorthand notation can save you some typing, and it keeps your statements tidy.

The **RANDOM** statement specifies a single random effect to be  $\gamma$ , and specifies that it has a normal prior centered at 0 with variance  $s_{2g}$ . The **SUBJECT=** argument in the **RANDOM** statement defines a group index (family) in the model, where all observations from the same family should have the same group indicator value. The **MONITOR=** option outputs analysis for all the random-effects parameters.

Finally, the **MU** assignment statement calculates the expected value of the height of the model. The calculation includes the random-effects term  $\gamma$ . The **MODEL** statement specifies the likelihood function for height.

The “Parameters” and “Random-Effects Parameters” tables, shown in Figure 55.8, contain information about the model parameters and the four random-effects parameters.

**Figure 55.8** Model and Random-Effects Parameter Information

| Random-Effects Model     |                 |                 |                    |                            |                            |
|--------------------------|-----------------|-----------------|--------------------|----------------------------|----------------------------|
| The MCMC Procedure       |                 |                 |                    |                            |                            |
| Parameters               |                 |                 |                    |                            |                            |
| Block                    | Parameter       | Sampling Method | Initial Value      | Prior Distribution         |                            |
| 1                        | $s_2$           | Conjugate       | 1.0000             | igamma(0.01, scale = 0.01) |                            |
| 2                        | $s_{2g}$        | Conjugate       | 1.0000             | igamma(0.01, scale = 0.01) |                            |
| 3                        | $b_0$           | N-Metropolis    | 0                  | normal(0, var = 10000)     |                            |
|                          | $b_1$           |                 | 0                  | normal(0, var = 10000)     |                            |
| Random Effect Parameters |                 |                 |                    |                            |                            |
| Parameter                | Sampling Method | Subject         | Number of Subjects | Subject Values             | Prior Distribution         |
| $\gamma$                 | N-Metropolis    | Family          | 4                  | 1 2 3 4                    | normal(0, var = $s_{2g}$ ) |

The posterior summary and interval statistics for the model parameters and the random-effects parameters are shown in Figure 55.9.



**Figure 55.9** Posterior Summary and Interval Statistics

| Random-Effects Model |       |         |                       |             |         |         |
|----------------------|-------|---------|-----------------------|-------------|---------|---------|
| The MCMC Procedure   |       |         |                       |             |         |         |
| Posterior Summaries  |       |         |                       |             |         |         |
| Parameter            | N     | Mean    | Standard<br>Deviation | Percentiles |         |         |
|                      |       |         |                       | 25%         | 50%     | 75%     |
| b0                   | 10000 | 68.4717 | 1.2735                | 67.7757     | 68.4495 | 69.1213 |
| b1                   | 10000 | -3.5533 | 0.9740                | -4.1829     | -3.5381 | -2.9375 |
| s2                   | 10000 | 4.1334  | 1.9372                | 2.8024      | 3.7093  | 4.9790  |
| s2g                  | 10000 | 5.1508  | 23.4698               | 0.2312      | 1.3104  | 4.2433  |
| gamma_1              | 10000 | 0.9404  | 1.3219                | 0.0860      | 0.6963  | 1.6322  |
| gamma_2              | 10000 | 0.0131  | 1.1935                | -0.4020     | 0.0214  | 0.4878  |
| gamma_3              | 10000 | -1.3481 | 1.6535                | -2.1852     | -0.9346 | -0.1252 |
| gamma_4              | 10000 | 0.0945  | 1.1931                | -0.3323     | 0.0528  | 0.5643  |

| Posterior Intervals |       |                     |         |              |         |
|---------------------|-------|---------------------|---------|--------------|---------|
| Parameter           | Alpha | Equal-Tail Interval |         | HPD Interval |         |
| b0                  | 0.050 | 65.8646             | 71.1331 | 65.9097      | 71.1712 |
| b1                  | 0.050 | -5.5058             | -1.6127 | -5.4201      | -1.5651 |
| s2                  | 0.050 | 1.7166              | 9.0766  | 1.3678       | 7.8796  |
| s2g                 | 0.050 | 0.00983             | 32.7002 | 0.00105      | 19.0298 |
| gamma_1             | 0.050 | -1.0884             | 4.0560  | -1.0160      | 4.0923  |
| gamma_2             | 0.050 | -2.5942             | 2.5279  | -2.5357      | 2.5636  |
| gamma_3             | 0.050 | -5.4957             | 0.6638  | -4.7168      | 1.0677  |
| gamma_4             | 0.050 | -2.4901             | 2.7349  | -2.5895      | 2.5888  |

Trace plots for all the parameters are shown in [Figure 55.10](#). The mixing looks very reasonable, suggesting convergence.

**Figure 55.10** Plots for  $b_1$  and Log of the Posterior Density

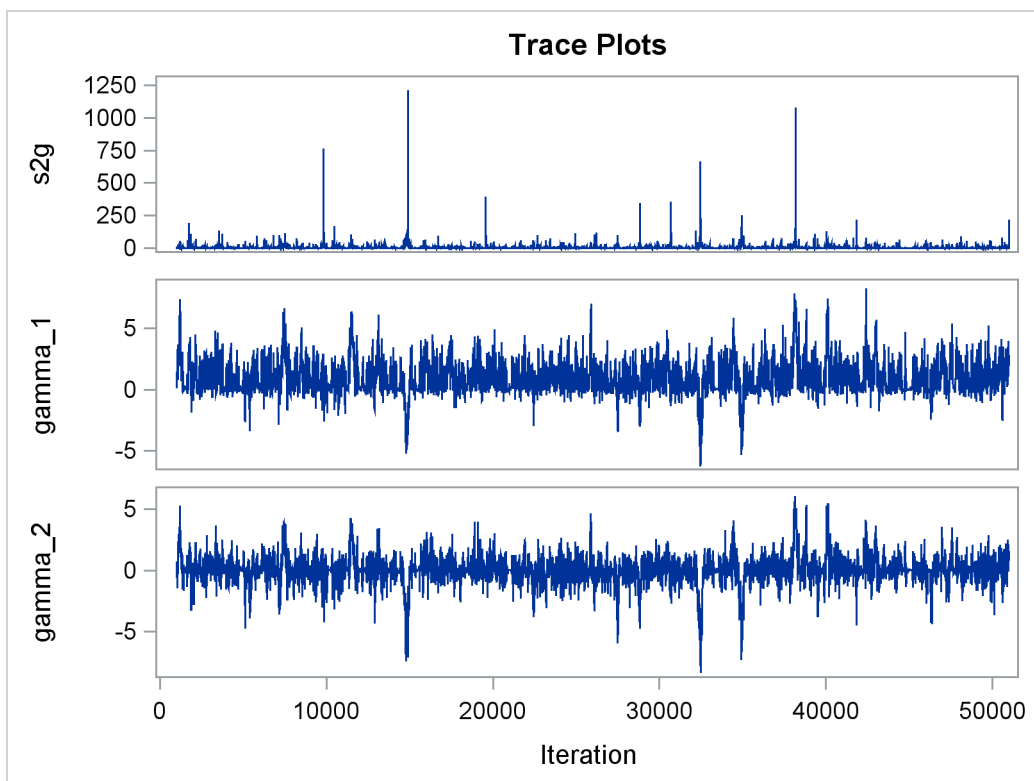
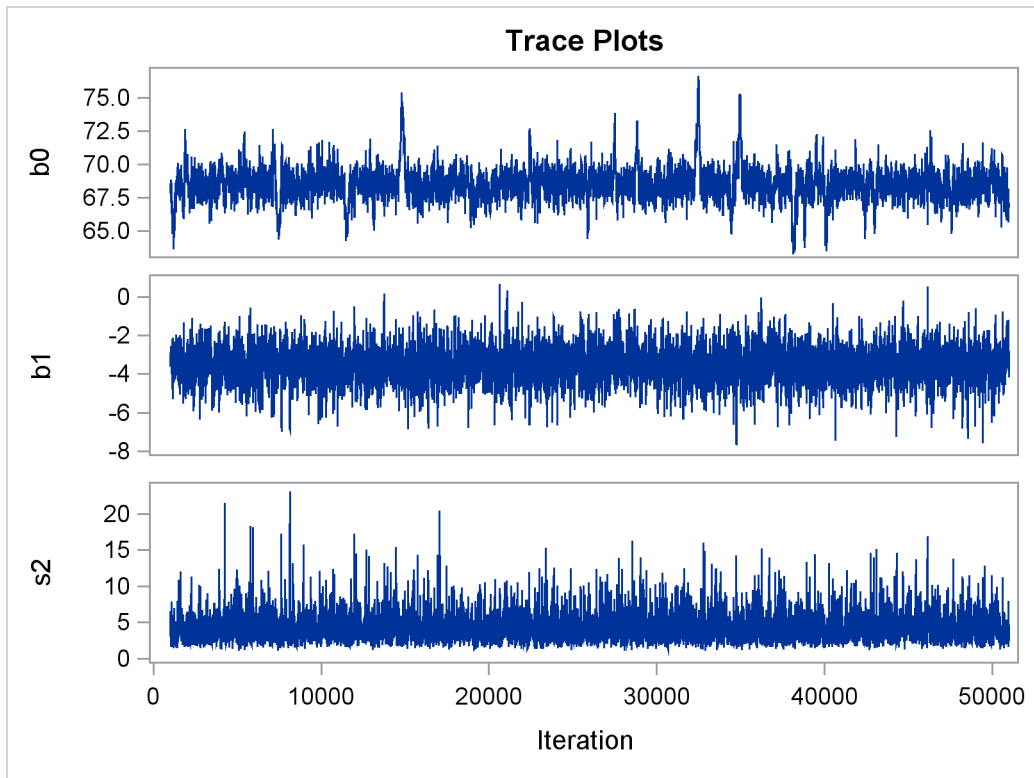
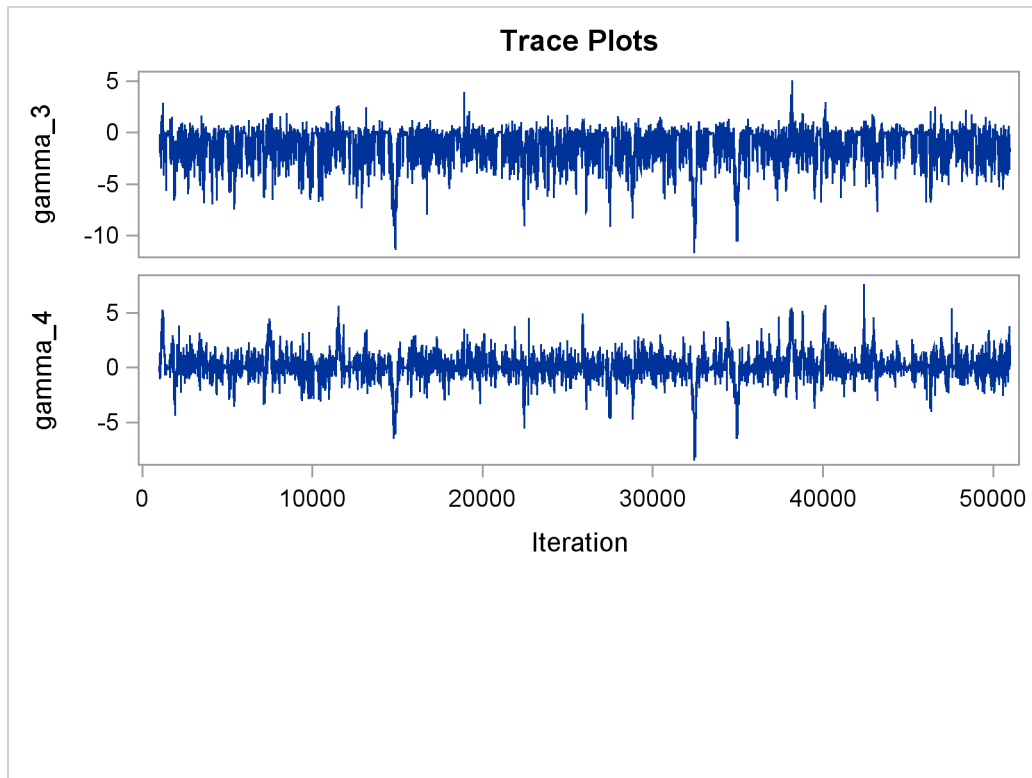


Figure 55.10 continued



From the interval statistics table, you see that both the equal-tail and HPD intervals for  $\beta_0$  are positive, strongly indicating the positive effect of the parameter. On the other hand, both intervals for  $\beta_1$  cover the value zero, indicating that  $gf$  does not have a strong impact on predicting height in this model.

## Syntax: MCMC Procedure

The following statements are available in the MCMC procedure. Items within  $\langle \rangle$  are optional.

```

PROC MCMC $\langle options \rangle$;
 ARRAY arrayname [dimensions] $\langle \$ \rangle$ $\langle variables-and-constants \rangle$;
 BEGINCNST/ENDCNST ;
 BEGINNODATA/ENDNODATA ;
 BY variables ;
 MODEL variable \sim distribution $\langle options \rangle$;
 PARMS parameter $\langle = \rangle$ number $\langle / options \rangle$;
 PREDDIST $\langle 'label' \rangle$ OUTPRED=SAS-data-set $\langle options \rangle$;
 PRIOR/HYPERPRIOR parameter \sim distribution ;
 Programming statements ;
 RANDOM random-effects-specification $\langle / options \rangle$;
 UDS subroutine-name (subroutine-argument-list) ;

```

The **PARMS** statements declare parameters in the model and assign optional starting values for the Markov chain. The **PRIOR/HYPERPRIOR** statements specify the prior distributions of the parameters. The **MODEL** statements specify the log-likelihood functions for the response variables. These statements form the basis of most Bayesian models.

In addition, you can use the **ARRAY** statement to define constant or parameter arrays, the **BEGINCNST/ENDCNST** and **BEGINNODATA/ENDNODATA** statements to omit unnecessary evaluation and reduce simulation time, the **PREDDIST** statement to generate samples from the posterior predictive distribution, the **program statements** to specify more complicated models that you want to fit, the **RANDOM** statement to specify random effects and their prior distributions, and the **UDS** statement to define your own Gibbs samplers to sample parameters in the model.

The following sections provide a description of each of these statements.

---

## PROC MCMC Statement

**PROC MCMC options ;**

The PROC MCMC statement invokes the MCMC procedure. [Table 55.1](#) summarizes the options available in the PROC MCMC statement.

**Table 55.1** PROC MCMC Statement Options

| Option                                   | Description                                                                              |
|------------------------------------------|------------------------------------------------------------------------------------------|
| <b>Basic options</b>                     |                                                                                          |
| <b>DATA=</b>                             | Names the input data set                                                                 |
| <b>OUTPOST=</b>                          | Names the output data set for posterior samples of parameters                            |
| <b>Debugging output</b>                  |                                                                                          |
| <b>LIST</b>                              | Displays model program and variables                                                     |
| <b>LISTCODE</b>                          | Displays compiled model program                                                          |
| <b>TRACE</b>                             | Displays detailed model execution messages                                               |
| <b>Frequently used MCMC options</b>      |                                                                                          |
| <b>MAXTUNE=</b>                          | Specifies the maximum number of tuning loops                                             |
| <b>MINTUNE=</b>                          | Specifies the minimum number of tuning loops                                             |
| <b>NBI=</b>                              | Specifies the number of burn-in iterations                                               |
| <b>NMC=</b>                              | Specifies the number of MCMC iterations, excluding the burn-in iterations                |
| <b>NTU=</b>                              | Specifies the number of tuning iterations                                                |
| <b>PROPCOV=</b>                          | Controls options for constructing the initial proposal covariance matrix                 |
| <b>SEED=</b>                             | Specifies the random seed for simulation                                                 |
| <b>THIN=</b>                             | Specifies the thinning rate                                                              |
| <b>Less frequently used MCMC options</b> |                                                                                          |
| <b>ACCEPTTOL=</b>                        | Specifies the acceptance rate tolerance                                                  |
| <b>DISCRETE=</b>                         | Controls sampling discrete parameters                                                    |
| <b>INIT=</b>                             | Controls generating initial values                                                       |
| <b>MCHISTORY=</b>                        | Displays Markov chain sampling history                                                   |
| <b>MAXINDEXPRINT=</b>                    | Specifies the maximum number of observation indices to print in models with missing data |

---

Table 55.1 (continued)

| Option                                            | Description                                                                                                |
|---------------------------------------------------|------------------------------------------------------------------------------------------------------------|
| MAXSUBVALUEPRINT=                                 | Specifies the maximum number of subject values to print in the “Random Effects Parameters” table           |
| PROPDIST=                                         | Specifies the proposal distribution                                                                        |
| REOBSINFO                                         | Displays more detailed information about each random effect                                                |
| SCALE=                                            | Specifies the initial scale applied to the proposal distribution                                           |
| TARGACCEPT=                                       | Specifies the target acceptance rate for random walk sampler                                               |
| TARGACCEPTI=                                      | Specifies the target acceptance rate for independence sampler                                              |
| TUNEWT=                                           | Specifies the weight used in covariance updating                                                           |
| <b>Summary, diagnostics, and plotting options</b> |                                                                                                            |
| AUTOCORLAG=                                       | Specifies the number of autocorrelation lags used to compute effective sample sizes and Monte Carlo errors |
| DIAGNOSTICS=                                      | Controls the convergence diagnostics                                                                       |
| DIC                                               | Computes deviance information criterion (DIC)                                                              |
| MONITOR=                                          | Outputs analysis for a list of symbols of interest                                                         |
| PLOTS=                                            | Controls plotting                                                                                          |
| STATISTICS=                                       | Controls posterior statistics                                                                              |
| <b>Other Options</b>                              |                                                                                                            |
| INF=                                              | Specifies the machine numerical limit for infinity                                                         |
| JOINTMODEL                                        | Specifies joint log-likelihood function                                                                    |
| MISSING=                                          | Indicates how missing values are handled.                                                                  |
| NOLOGDIST                                         | Omits the calculation of the logarithm of the joint distribution of the parameters                         |
| SIMREPORT=                                        | Controls the frequency of report for expected run time                                                     |
| SINGDEN=                                          | Specifies the singularity tolerance                                                                        |

These options are described in alphabetical order.

**ACCEPTTOL=*n***

specifies a tolerance for acceptance probabilities. By default, ACCEPTTOL=0.075.

**AUTOCORLAG=*n*****ACLAG=*n***

specifies the maximum number of autocorrelation lags used in computing the effective sample size; see the section “Effective Sample Size” on page 152 for more details. The value is used in the calculation of the Monte Carlo standard error; see the section “Standard Error of the Mean Estimate” on page 153. By default, AUTOCORLAG=MIN(500, MCsample/4), where MCsample is the Markov chain sample size kept after thinning—that is,  $MCsample = \left\lceil \frac{NMC}{NTHIN} \right\rceil$ . If AUTOCORLAG= is set too low, you might observe significant lags, and the effective sample size cannot be calculated accurately. A WARNING message appears, and you can either increase AUTOCORLAG= or NMC=, accordingly.

**DISCRETE=***keyword*

specifies the proposal distribution used in sampling discrete parameters. The default is DISCRETE=BINNING.

The *keyword* values are as follows:

**BINNING**

uses continuous proposal distributions for all discrete parameter blocks. The proposed sample is then discretized (binned) before further calculations. This sampling method approximates the correlation structure among the discrete parameters in the block and could improve mixing in some cases.

**GEO**

uses independent symmetric geometric proposal distributions for all discrete parameter blocks. This proposal does not take parameter correlations into account. However, it can work better than the BINNING option in cases where the range of the parameters is relatively small and a normal approximation can perform poorly.

**DIAGNOSTICS=NONE** | (*keyword-list*)**DIAG=NONE** | (*keyword-list*)

specifies options for MCMC convergence diagnostics. By default, PROC MCMC computes the Geweke test, sample autocorrelations, effective sample sizes, and Monte Carlo errors. The Raftery-Lewis and Heidelberger-Welch tests are also available. See the section “[Assessing Markov Chain Convergence](#)” on page 139 for more details on convergence diagnostics. You can request all of the diagnostic tests by specifying DIAGNOSTICS=ALL. You can suppress all the tests by specifying DIAGNOSTICS=NONE.

You can use postprocessing autocall macros to calculate convergence diagnostics of the posterior samples after PROC MCMC has exited. See the section “[Autocall Macros for Postprocessing](#)” on page 4510.

The following *options* are available.

**ALL**

computes all diagnostic tests and statistics. You can combine the option ALL with any other specific tests to modify test options. For example DIAGNOSTICS=(ALL AUTOCORR(LAGS=(1 5 35))) computes all tests with default settings and autocorrelations at lags 1, 5, and 35.

**AUTOCORR** < (*autocorr-options*) >

computes default autocorrelations at lags 1, 5, 10, and 50 for each variable. You can choose other lags by using the following *autocorr-options*:

**LAGS** | **AC=***numeric-list*

specifies autocorrelation lags. The *numeric-list* must take positive integer values.

**ESS**

computes the effective sample sizes (Kass et al. (1998)) of the posterior samples of each parameter. It also computes the correlation time and the efficiency of the chain for each parameter. Small values of ESS might indicate a lack of convergence. See the section “[Effective Sample Size](#)” on page 152 for more details.

**GEWEKE** < (*Geweke-options*) >

computes the Geweke spectral density diagnostics; this is a two-sample  $t$ -test between the first  $f_1$  portion and the last  $f_2$  portion of the chain. See the section “[Geweke Diagnostics](#)” on page 146 for more details. The default is  $\text{FRAC1}=0.1$  and  $\text{FRAC2}=0.5$ , but you can choose other fractions by using the following *Geweke-options*:

**FRAC1** | **F1**=*value*

specifies the beginning  $\text{FRAC1}$  proportion of the Markov chain. By default,  $\text{FRAC1}=0.1$ .

**FRAC2** | **F2**=*value*

specifies the end  $\text{FRAC2}$  proportion of the Markov chain. By default,  $\text{FRAC2}=0.5$ .

**HEIDELBERGER** | **HEIDEL** < (*Heidel-options*) >

computes the Heidelberg and Welch diagnostic (which consists of a stationarity test and a halfwidth test) for each variable. The stationary diagnostic test tests the null hypothesis that the posterior samples are generated from a stationary process. If the stationarity test is passed, a halfwidth test is then carried out. See the section “[Heidelberg and Welch Diagnostics](#)” on page 148 for more details.

These diagnostics are not performed by default. You can specify the `DIAGNOSTICS=HEIDELBERGER` option to request these diagnostics, and you can also specify suboptions, such as `DIAGNOSTICS=HEIDELBERGER(EPS=0.05)`, as follows:

**SALPHA**=*value*

specifies the  $\alpha$  level ( $0 < \alpha < 1$ ) for the stationarity test. By default,  $\text{SALPHA}=0.05$ .

**HALPHA**=*value*

specifies the  $\alpha$  level ( $0 < \alpha < 1$ ) for the halfwidth test. By default,  $\text{HALPHA}=0.05$ .

**EPS**=*value*

specifies a small positive number  $\epsilon$  such that if the halfwidth is less than  $\epsilon$  times the sample mean of the retaining iterates, the halfwidth test is passed. By default,  $\text{EPS}=0.1$ .

**MCSE****MCERROR**

computes the Monte Carlo standard error for the posterior samples of each parameter.

**NONE**

suppresses all of the diagnostic tests and statistics. This is not recommended.

**RAFTERY** | **RL** < (*Raftery-options*) >

computes the Raftery and Lewis diagnostics, which evaluate the accuracy of the estimated quantile ( $\hat{\theta}_Q$  for a given  $Q \in (0, 1)$ ) of a chain.  $\hat{\theta}_Q$  can achieve any degree of accuracy when the chain is allowed to run for a long time. The algorithm stops when the estimated probability  $\hat{P}_Q = \Pr(\theta \leq \hat{\theta}_Q)$  reaches within  $\pm R$  of the value  $Q$  with probability  $S$ ; that is,  $\Pr(Q - R \leq \hat{P}_Q \leq Q + R) = S$ . See the section “[Raftery and Lewis Diagnostics](#)” on page 149

for more details. The *Raftery-options* enable you to specify Q, R, S, and a precision level  $\epsilon$  for a stationary test.

These diagnostics are not performed by default. You can specify the `DIAGNOSTICS=RAFERTY` option to request these diagnostics, and you can also specify suboptions, such as `DIAGNOSTICS=RAFERTY(QUANTILE=0.05)`, as follows:

**QUANTILE | Q=value**

specifies the order (a value between 0 and 1) of the quantile of interest. By default, `QUANTILE=0.025`.

**ACCURACY | R=value**

specifies a small positive number as the margin of error for measuring the accuracy of estimation of the quantile. By default, `ACCURACY=0.005`.

**PROB | S=value**

specifies the probability of attaining the accuracy of the estimation of the quantile. By default, `PROB=0.95`.

**EPS=value**

specifies the tolerance level (a small positive number) for the stationary test. By default, `EPS=0.001`.

**DIC**

computes the Deviance Information Criterion (DIC). DIC is calculated using the posterior mean estimates of the parameters. See the section “[Deviance Information Criterion \(DIC\)](#)” on page 155 for more details.

**DATA=SAS-data-set**

specifies the input data set. Observations in this data set are used to compute the log-likelihood function that you specify with PROC MCMC statements.

**INF=value**

specifies the numerical definition of infinity in PROC MCMC. The default is `INF=1E15`. For example, PROC MCMC considers `1E16` to be outside of the support of the normal distribution and assigns a missing value to the log density evaluation. You can select a larger value with the `INF=` option. The minimum value allowed is `1E10`.

**INIT=(keyword-list)**

specifies options for generating the initial values for the parameters. These options apply only to prior distributions that are recognized by PROC MCMC. See the section “[Standard Distributions](#)” on page 4476 for a list of these distributions. If either of the functions `GENERAL` or `DGENERAL` is used, you must supply explicit initial values for the parameters. By default, `INIT=MODE`. The following keywords are used:



**MODE**

uses the mode of the prior density as the initial value of the parameter, if you did not provide one. If the mode does not exist or if it is on the boundary of the support of the density, the mean value is used. If the mean is outside of the support or on the boundary, which can happen if the prior distribution is truncated, a random number drawn from the prior is used as the initial value.

**PINIT**

tabulates parameter values after the tuning phase. This option also tabulates the tuned proposal parameters used by the Metropolis algorithm. These proposal parameters include covariance matrices for continuous parameters and probability vectors for discrete parameters for each block. By default, PROC MCMC does not display the initial values or the tuned proposal parameters after the tuning phase.

**RANDOM**

generates a random number from the prior density and uses it as the initial value of the parameter, if you did not provide one.

**REINIT**

resets the parameters, after the tuning phase, with the initial values that you provided explicitly or that were assigned by PROC MCMC. By default, PROC MCMC does not reset the parameters because the tuning phase usually moves the Markov chains to a more favorable place in the posterior distribution.

**LIST**

displays the model program and variable lists. The LIST option is a debugging feature and is not normally needed.

**LISTCODE**

displays the compiled program code. The LISTCODE option is a debugging feature and is not normally needed.

**JOINTMODEL****JOINTLLIKE**

specifies how the likelihood function is calculated. By default, PROC MCMC assumes that the observations in the data set are independent so that the joint log-likelihood function is the sum of the individual log-likelihood functions for the observations, where the individual log-likelihood function is specified in the [MODEL](#) statement. When your data are not independent, you can specify the JOINTMODEL option to modify the way that PROC MCMC computes the joint log-likelihood function. In this situation, PROC MCMC no longer steps through the input data set to sum the individual log likelihood.

To use this option correctly, you need to do the following two things:

- create ARRAY symbols to store all data set variables that are used in the program. This can be accomplished with the [BEGINCNST](#) and [ENDCNST](#) statements.
- program the joint log-likelihood function by using these ARRAY symbols only. The [MODEL](#) statement specifies the joint log-likelihood function for the entire data set. Typically, you use the function [GENERAL](#) in the [MODEL](#) statement.

See the sections “[BEGINCNST/ENDCNST Statement](#)” on page 4441 and “[Modeling Joint Likelihood](#)” on page 4504 for details.

**MAXTUNE=*n***

specifies an upper limit for the number of proposal tuning loops. By default, MAXTUNE=24. See the section “[Covariance Tuning](#)” on page 4470 for more details.

**MAXINDEXPRINT=*number* | ALL****MAXIPRINT=*number* | ALL**

specifies the maximum number of observation indices to print in the ODS tables “Missing Response Information” table and “Missing Covariates Information” table. This option applies only to programs that model missing data. The default value is 20. MAXINDEXPRINT=ALL prints all observation indices for every missing variable that is modeled in PROC MCMC.

**MAXSUBVALUEPRINT=*number* | ALL****MAXSVPRINT=*number* | ALL**

specifies the maximum number of subject values to display in the “Subject Values” column of the ODS table “Random Effects Parameters.” This option applies only to programs that have RANDOM statements. The default value is 20. MAXSUBVALUEPRINT=ALL prints all subject values for every random effect in the program.

**MCHISTORY=*keyword*****MCHIST=*keyword***

controls the display of the Markov chain sampling history.

**BRIEF**

produces a summary output for the tuning, burn-in, and sampling history tables. The tables show the following when applicable:

- “RWM Scale” shows the scale, or the range of the scales, used in each random walk Metropolis block that is normal or is based on a *t* distribution.
- “Probability” shows the proposal probability parameter, or the range of the parameters, used in each random walk Metropolis block that is based on a geometric distribution.
- “RWM Acceptance Rate” shows the acceptance rate, or the range of the acceptance rates, for each random walk Metropolis block.
- “IM Acceptance Rate” shows the acceptance rate, or the range of the acceptance rates, for each independent Metropolis block.

**DETAILED**

produces detailed output of the tuning, burn-in, and sampling history tables, including scale values, acceptance probabilities, blocking information, and so on. Use this option with caution, especially in random-effects models that have a large number of random-effects groups. This option can produce copious output.

**NONE**

produces none of the tuning history, burn-in history, and sampling history tables.

The default is MCHISTORY=NONE.

**MINTUNE=*n***

specifies a lower limit for the number of proposal tuning loops. By default, MINTUNE=2. See the section “[Covariance Tuning](#)” on page 4470 for more details.

**MISSING=keyword**

**MISS=keyword**

specifies how missing values are handled (see the section “Handling of Missing Data” on page 4518 for more details). The default is MISSING=COMPLETECASE.

**ALLCASE | AC**

gives you the option to model the missing values in an all-case analysis. You can use any techniques that you see fit, for example, fully Bayesian or multiple imputation.

**COMPLETECASE | CC**

assumes a complete case analysis, so all observations with missing variable values are discarded prior to the simulation.

**MONITOR= (symbol-list)**

outputs analysis for selected symbols of interest in the program. The symbols can be any of the following: model parameters (symbols in the **PARMS** statement), secondary parameters (assigned using the operator “=”), the log of the posterior density (**LOGPOST**), the log of the prior density (**LOGPRIOR**), the log of the hyperprior density (**LOGHYPER**) if the **HYPER** statement is used, or the log of the likelihood function (**LOGLIKE**). You can use the keyword **\_PARMS\_** as a shorthand for all of the model parameters. PROC MCMC performs only posterior analyses (such as plotting, diagnostics, and summaries) on the symbols selected with the **MONITOR=** option. You can also choose to monitor an entire array by specifying the name of the array. By default **MONITOR=\_PARMS\_**.

Posterior samples of any secondary parameters listed in the **MONITOR=** option are saved in the **OUTPOST=** data set. Posterior samples of model parameters are always saved to the **OUTPOST=** data set, regardless of whether they appear in the **MONITOR=** option.

**NBI=*n***

specifies the number of burn-in iterations to perform before beginning to save parameter estimate chains. By default, **NBI=1000**. See the section “Burn-in, Thinning, and Markov Chain Samples” on page 138 for more details.

**NMC=*n***

specifies the number of iterations in the main simulation loop. This is the MCMC sample size if **THIN=1**. By default, **NMC=1000**.

**NOLOGDIST**

omits the calculation of the logarithm of the joint distribution of the model parameters at each iteration. The option applies only if all parameters in the model are updated directly from their target distribution, either from the full conditional posterior via conjugacy or from the marginal distribution. Such algorithms do not require the calculation of the joint posterior distribution; hence PROC MCMC runs faster by avoiding these unnecessary calculations. As a result, the **OUTPOST=** data set does not contain the **LOGPRIOR**, **LOGLIKE**, and **LOGPOST** variables.

**NTU=*n***

specifies the number of iterations to use in each proposal tuning phase. By default, **NTU=500**.

**OUTPOST=SAS-data-set**

specifies an output data set that contains the posterior samples of all model parameters, the iteration numbers (variable name **ITERATION**), the log of the posterior density (**LOGPOST**), the log of the

prior density (LOGPRIOR), the log of the hyperprior density (LOGHYPER), if the **HYPER** statement is used, and the log likelihood (LOGLIKE). Any secondary parameters (assigned using the operator “=”) listed in the **MONITOR=** option are saved to this data set. By default, no **OUTPOST=** data set is created.

**PLOTS**< (*global-plot-options*)>= (*plot-request* <... *plot-request*>)

**PLOT**< (*global-plot-options*)>= (*plot-request* <... *plot-request*>)

controls the display of diagnostic plots. Three types of plots can be requested: trace plots, autocorrelation function plots, and kernel density plots. By default, the plots are displayed in panels unless the global plot option **UNPACK** is specified. Also when more than one type of plot is specified, the plots are grouped by parameter unless the global plot option **GROUPBY=TYPE** is specified. When you specify only one plot request, you can omit the parentheses around the plot-request, as shown in the following example:

```
plots=none
plots(unpack)=trace
plots=(trace density)
```

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;
proc mcmc data=exi seed=7 outpost=p1 plots=all;
 parm mu;
 prior mu ~ normal(0, sd=10);
 model y ~ normal(mu, sd=1);
run;
ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS](#).”

If ODS Graphics is enabled but do not specify the **PLOTS=** option, then PROC MCMC produces, for each parameter, a panel that contains the trace plot, the autocorrelation function plot, and the density plot. This is equivalent to specifying **PLOTS=(TRACE AUTOCORR DENSITY)**.

The *global-plot-options* include the following:

#### **FRINGE**

adds a fringe plot to the horizontal axis of the density plot.

#### **GROUPBY|GROUP=PARAMETER | TYPE**

specifies how the plots are grouped when there is more than one type of plot. **GROUPBY=PARAMETER** is the default. The choices are as follows:

##### **TYPE**

specifies that the plots are grouped by type.

##### **PARAMETER**

specifies that the plots are grouped by parameter.

**LAGS=*n***

specifies the number of autocorrelation lags used in plotting the ACF graph. By default, LAGS=50.

**SMOOTH**

smooths the trace plot with a fitted penalized B-spline curve (Eilers and Marx 1996).

**UNPACKPANEL****UNPACK**

specifies that all paneled plots are to be unpacked, so that each plot in a panel is displayed separately.

The *plot-requests* are as follows:

**ALL**

requests all types of plots. PLOTS=ALL is equivalent to specifying PLOTS=(TRACE AUTO-CORR DENSITY).

**AUTOCORR | ACF**

displays the autocorrelation function plots for the parameters.

**DENSITY | D | KERNEL | K**

displays the kernel density plots for the parameters.

**NONE**

suppresses the display of all plots.

**TRACE | T**

displays the trace plots for the parameters.

Consider a model with four parameters, X1–X4. Displays for various specifications are depicted as follows.

- PLOTS=(TRACE AUTOCORR) displays the trace and autocorrelation plots for each parameter side by side with two parameters per panel:

---

|           |           |              |
|-----------|-----------|--------------|
| Display 1 | Trace(X1) | Autocorr(X1) |
|           | Trace(X2) | Autocorr(X2) |
| Display 2 | Trace(X3) | Autocorr(X3) |
|           | Trace(X4) | Autocorr(X4) |

---

- PLOTS(GROUPBY=TYPE)=(TRACE AUTOCORR) displays all the paneled trace plots, followed by panels of autocorrelation plots:

---

|           |              |              |
|-----------|--------------|--------------|
| Display 1 | Trace(X1)    |              |
|           | Trace(X2)    |              |
| Display 2 | Trace(X3)    |              |
|           | Trace(X4)    |              |
| Display 3 | Autocorr(X1) | Autocorr(X2) |
|           | Autocorr(X3) | Autocorr(X4) |

---

- PLOTS(UNPACK)=(TRACE AUTOCORR) displays a separate trace plot and a separate correlation plot, parameter by parameter:

---

|           |              |
|-----------|--------------|
| Display 1 | Trace(X1)    |
| Display 2 | Autocorr(X1) |
| Display 3 | Trace(X2)    |
| Display 4 | Autocorr(X2) |
| Display 5 | Trace(X3)    |
| Display 6 | Autocorr(X3) |
| Display 7 | Trace(X4)    |
| Display 8 | Autocorr(X4) |

---

- PLOTS(UNPACK GROUPBY=TYPE)=(TRACE AUTOCORR) displays all the separate trace plots followed by the separate autocorrelation plots:

---

|           |              |
|-----------|--------------|
| Display 1 | Trace(X1)    |
| Display 2 | Trace(X2)    |
| Display 3 | Trace(X3)    |
| Display 4 | Trace(X4)    |
| Display 5 | Autocorr(X1) |
| Display 6 | Autocorr(X2) |
| Display 7 | Autocorr(X3) |
| Display 8 | Autocorr(X4) |

---

**PROPCOV=value**

specifies the method used in constructing the initial covariance matrix for the Metropolis-Hastings algorithm. The QUANEW and NMSIMP methods find numerically approximated covariance matrices at the optimum of the posterior density function with respect to all continuous parameters. The optimization does not apply to discrete parameters. The tuning phase starts at the optimized values; in some problems, this can greatly increase convergence performance. If the approximated covariance matrix is not positive definite, then an identity matrix is used instead. Valid values are as follows:

**IND**

uses the identity covariance matrix. This is the default. See the section “[Tuning the Proposal Distribution](#)” on page 4469.

**CONGRA**< (*optimize-options*) >

performs a conjugate-gradient optimization.

**DBLDOG**< (*optimize-options*) >

performs a double-dogleg optimization.

**QUANEW**< (*optimize-options*) >

performs a quasi-Newton optimization.

**NMSIMP | SIMPLEX**< (*optimize-options*) >

performs a Nelder-Mead simplex optimization.

The *optimize-options* are as follows:

**ITPRINT**

prints optimization iteration steps and results.

**PROPDIST**=*value*

specifies a proposal distribution for the Metropolis algorithm. See the section “[Metropolis and Metropolis-Hastings Algorithms](#)” on page 134. You can also use **PARMS** statement option (see the section “[PARMS Statement](#)” on page 4451) to change the proposal distribution for a particular block of parameters. Valid values are as follows:

**NORMAL****N**

specifies a normal distribution as the proposal distribution. This is the default.

**T**< (*df*) >

specifies a *t* distribution with the degrees of freedom *df*. By default, *df* = 3. If *df* > 100, the normal distribution is used since the two distributions are almost identical.

**REOBSINFO** < (*display-options*) >

displays the ODS table “Random Effect Observation Information.” The table lists the name of each random effect, the unique values in the corresponding subject variable, the number of observations in each subject, and the observation indices for each subject value.

To understand how this option works, consider the following statements:

```
data input;
 array names{*} $ n1-n10 ("John" "Mary" "Chris" "Rob" "Greg"
 "Jen" "Henry" "Alice" "James" "Toby");
 call streaminit(17);
 do i = 1 to 20;
 j = ceil(rand("uniform") * 10);
 index = names[j];
 output;
 end;
```

```

drop n: j;
run;

proc print data=input;
run;

```

The input data set (Figure 55.11) contains the index variable, which indicates subjects in a hypothetical random-effects model.

**Figure 55.11** Subject Variable in an Input Data Set

| Obs | i  | index |
|-----|----|-------|
| 1   | 1  | Mary  |
| 2   | 2  | James |
| 3   | 3  | Mary  |
| 4   | 4  | Greg  |
| 5   | 5  | Chris |
| 6   | 6  | James |
| 7   | 7  | James |
| 8   | 8  | Chris |
| 9   | 9  | James |
| 10  | 10 | James |
| 11  | 11 | Chris |
| 12  | 12 | Rob   |
| 13  | 13 | Rob   |
| 14  | 14 | Greg  |
| 15  | 15 | Greg  |
| 16  | 16 | Alice |
| 17  | 17 | Jen   |
| 18  | 18 | Alice |
| 19  | 19 | John  |
| 20  | 20 | Chris |

The following statements illustrate the use of the REOBSINFO option:

```

ods select reobsinfo;
proc mcmc data=input reobsinfo stats=none diag=none;
 random u ~ normal(0, sd=1) subject=index;
 model general(0);
run;

```

Figure 55.12 displays the “Random Effect Observation Information” table. The table contains the name of the random-effect parameter ( $u$ ), the values of the subject variable `index`, the total number of observations, and the row index of these observations in each of the subject values.



Figure 55.12 Random Effect Observation Information

| The MCMC Procedure                    |                |                                   |                     |
|---------------------------------------|----------------|-----------------------------------|---------------------|
| Random Effect Observation Information |                |                                   |                     |
| Parameter                             | Subject Values | Number of Observations in Subject | Observation Indices |
| u                                     | Mary           | 2                                 | 1 3                 |
|                                       | James          | 5                                 | 2 6 7 9 10          |
|                                       | Greg           | 3                                 | 4 14 15             |
|                                       | Chris          | 4                                 | 5 8 11 20           |
|                                       | Rob            | 2                                 | 12 13               |
|                                       | Alice          | 2                                 | 16 18               |
|                                       | Jen            | 1                                 | 17                  |
|                                       | John           | 1                                 | 19                  |

The *display-options* are as follows:

**MAXVALUEPRINT=number | ALL**

**MAXVPRINT=number | ALL**

prints the number of subject values for each random effect (that is, the number of rows that are displayed in the “Random Effect Observation Information” table for each random effect). The default value is 20. MAXVALUEPRINT=ALL displays all subject values.

**MAXOBSPRINT=number | ALL**

**MAXOPRINT=number | ALL**

prints the number of observation indices for each subject value of every random effect (that is, the maximum number of indices that are displayed in the “Observation Indices” column in the “Random Effect Observation Information” table). The default value is 20. MAXOBSPRINT=ALL displays indices for every subject value.

**SCALE=value**

controls the initial multiplicative scale to the covariance matrix of the proposal distribution. By default, SCALE=2.38. See the section “[Scale Tuning](#)” on page 4470 for more details.

**SEED=n**

specifies the random number seed. By default, SEED=0, and PROC MCMC gets a random number seed from the clock.

**SIMREPORT=n**

controls the number of times that PROC MCMC reports the expected run time of the simulation. This can be useful for monitoring the progress of CPU-intensive programs. For example, with SIMREPORT=2, PROC MCMC reports the simulation progress twice. By default, SIMREPORT=0, and there is no reporting. The expected run times are displayed in the log file.

**SINGDEN=***value*

defines the singularity criterion in PROC MCMC. By default, SINGDEN=1E-11. The *value* indicates the exclusion of an endpoint in an interval. The mathematical notation “(0” is equivalent to “[*value*” in PROC MCMC—that is,  $x < 0$  is treated as  $x \leq \textit{value}$  in PROC MCMC. The maximum SINGDEN allowed is 1E-6.

**STATISTICS**< *global-stats-options* > = **NONE** | **ALL** | *stats-request***STATS**< *global-stats-options* > = **NONE** | **ALL** | *stats-request*

specifies options for posterior statistics. By default, PROC MCMC computes the posterior mean, standard deviation, quantiles, and two 95% credible intervals: equal-tail and highest posterior density (HPD). Other available statistics include the posterior correlation and covariance. See the section “[Summary Statistics](#)” on page 153 for more details. You can request all of the posterior statistics by specifying STATS=ALL. You can suppress all the calculations by specifying STATS=NONE.

You can use postprocessing autocall macros to calculate posterior summary statistics of the posterior samples after PROC MCMC has exited. See the section “[Autocall Macros for Postprocessing](#)” on page 4510.

The *global-stats-options* includes the following:

**ALPHA=***numeric-list*

specifies the  $\alpha$  level for the equal-tail and HPD intervals. The value  $\alpha$  must be between 0 and 0.5. By default, ALPHA=0.05.

**PERCENTAGE** | **PERCENT=***numeric-list*

calculates the posterior percentages. The *numeric-list* contains values between 0 and 100. By default, PERCENTAGE=(25 50 75).

The *stats-requests* include the following:

**ALL**

computes all posterior statistics. You can combine the option ALL with any other options. For example STATS(ALPHA=(0.02 0.05 0.1))=ALL computes all statistics with the default settings and intervals at  $\alpha$  levels of 0.02, 0.05, and 0.1.

**CORR**

computes the posterior correlation matrix.

**COV**

computes the posterior covariance matrix.

**SUMMARY****SUM**

computes the posterior means, standard deviations, and percentile points for each variable. By default, the 25th, 50th, and 75th percentile points are produced, but you can use the global PERCENT= option to request specific percentile points.

**INTERVAL****INT**

computes the  $100(1 - \alpha)\%$  equal-tail and HPD credible intervals for each variable. See the sections “[Equal-Tail Credible Interval](#)” on page 154 and “[Highest Posterior Density \(HPD\) Interval](#)” on page 154 for details. By default, ALPHA=0.05, but you can use the global ALPHA= option to request other intervals of any probabilities.

**NONE**

suppresses all of the statistics.

**TARGACCEPT=value**

specifies the target acceptance rate for the random walk based Metropolis algorithm. See the section “[Metropolis and Metropolis-Hastings Algorithms](#)” on page 134. The numeric *value* must be between 0.01 and 0.99. By default, TARGACCEPT=0.45 for models with 1 parameter; TARGACCEPT=0.35 for models with 2, 3, or 4 parameters; and TARGACCEPT=0.234 for models with more than 4 parameters (Roberts, Gelman, and Gilks 1997; Roberts and Rosenthal 2001).

**TARGACCEPTI=value**

specifies the target acceptance rate for the independence sampler algorithm. The independence sampler is used for blocks of binary parameters. See the section “[Independence Sampler](#)” on page 137 for more details. The numeric *value* must be between 0 and 1. By default, TARGACCEPTI=0.6.

**THIN=n****NTHIN=n**

controls the thinning rate of the simulation. PROC MCMC keeps every *n*th simulation sample and discards the rest. All of the posterior statistics and diagnostics are calculated using the thinned samples. By default, THIN=1. See the section “[Burn-in, Thinning, and Markov Chain Samples](#)” on page 138 for more details.

**TRACE**

displays the result of each operation in each statement in the model program as it is executed. This debugging option is very rarely needed, and it produces voluminous output. If you use this option, also use small NMC=, NBI=, MAXTUNE=, and NTU= numbers.

**TUNEWT=value**

specifies the multiplicative weight used in updating the covariance matrix of the proposal distribution. The numeric *value* must be between 0 and 1. By default, TUNEWT=0.75. See the section “[Covariance Tuning](#)” on page 4470 for more details.

---

## ARRAY Statement

```
ARRAY arrayname [dimensions] < $ > < variables-and-constants > ;
```

The ARRAY statement associates a name (of no more than eight characters) with a list of variables and constants. The ARRAY statement is similar to, but not the same as, the ARRAY statement in the DATA step, and it is the same as the ARRAY statements in the NLIN, NLP, NLMIXED, and MODEL procedures. The array name is used with subscripts in the program to refer to the array elements, as illustrated in the following statements:

```
array r[8] r1-r8;

do i = 1 to 8;
 r[i] = 0;
end;
```

The ARRAY statement does not support all the features of the ARRAY statement in the DATA step. Implicit indexing of variables cannot be used; all array references must have explicit subscript expressions. Only exact array dimensions are allowed; lower-bound specifications are not supported. A maximum of six dimensions is allowed.

Both variables and constants can be array elements. Constant array elements cannot have values assigned to them while variables can. Both the dimension specification and the list of elements are optional, but at least one must be specified. When the list of elements is not specified or fewer elements than the size of the array are listed, array variables are created by appending element numbers to the array name to complete the element list. You can index array elements by enclosing a subscript in braces ({} ) or brackets ([ ]), but not in parentheses (( )). The parentheses are reserved for function calls only.

For example, the following statement names an array `day`:

```
array day[365];
```

By default, the variables names are `day1` to `day365`. However, since `day` is a SAS function, any subscript that uses parentheses gives you the wrong results. The expression `day(4)` returns the value 5 and does not reference the array element `day4`.

---

## BEGINCNST/ENDCNST Statement

```
BEGINCNST ;
```

```
ENDCNST ;
```

The BEGINCNST and ENDCNST statements define a block within which PROC MCMC processes the programming statements only during the setup stage of the simulation. You can use the BEGINCNST and ENDCNST statements to define constants or import data set variables into arrays. Storing data in arrays enables you to work with data that are not identically distributed (see the section “[Modeling Joint Likelihood](#)” on page 4504) or to implement your own Markov chain sampler (see the section “[UDS Statement](#)” on page 4462). You can also use the BEGINCNST and ENDCNST statements to assign initial values to the parameters (see the section “[Assignments of Parameters](#)” on page 4474).

### Assign Constants

Whenever you have programming statements that calculate constants that do not need to be evaluated multiple times throughout the simulation, you should put them within the BEGINCNST and ENDCNST statements. Using these statements can reduce redundant processing. For example, you can assign a constant to a symbol or fill in an array with numbers:

```
array cnst[17];
begincnst;
 offset = 17;
 do i = 1 to 17;
 cnst[i] = i * i;
 end;
endcnst;
```

During the setup process, PROC MCMC evaluates the programming statements within the BEGINCNST/ENDCNST once for each observation in the data set and ignores the statements in the rest of the simulation.

## READ\_ARRAY Function

Sometimes you might need to store variables, either from the current input data set or from a different data set, in arrays and use these arrays to specify your model. The READ\_ARRAY function is convenient for that purpose.

The following two forms of the READ\_ARRAY function are available:

```
rc = READ_ARRAY (data-set, array) ;
```

```
rc = READ_ARRAY (data-set, array <, "col-name1"> <, "col-name2"> <, ... >);
```

where

- *rc* returns 0 if the function is able to successfully read the data set.
- *data-set* specifies the name of the data set from which the array data is read. The value specified for *data-set* must be a character literal or a variable that contains the member name (libname.memname) of the data set to be read from.
- *array* specifies the PROC MCMC array variable into which the data is read. The value specified for *array* must be a local temporary array variable because the function might need to grow or shrink its size to accommodate the size of the data set.
- *col-name* specifies optional names for the specific columns of the data set that are read. If specified, *col-name* must be a literal string enclosed in quotation marks. In addition, *col-name* cannot be a PROC MCMC variable. If column names are not specified, PROC MCMC reads all of the columns in the data set.

When SAS translates between an array and a data set, the array is indexed as [row,column].

The READ\_ARRAY function attempts to dynamically resize the array to match the dimensions of the input data set. Therefore, the array must be dynamic; that is, the array must be declared with the /NOSYMBOLS option.

For examples that use the READ\_ARRAY function, see “Modeling Joint Likelihood” on page 4504, “Example 55.14: Time Independent Cox Model” on page 4617, and “Example 55.19: Implement a New Sampling Algorithm” on page 4645.

---

## BEGINNODATA/ENDNODATA Statements

```
BEGINNODATA ;
```

```
ENDNODATA ;
```

```
BEGINPRIOR ;
```

```
ENDPRIOR ;
```

The BEGINNODATA and ENDNODATA statements define a block within which PROC MCMC processes the programming statements without stepping through the entire data set. The programming statements are executed only twice: at the first and the last observation of the data set. The BEGINNODATA and ENDNODATA statements are best used to reduce unnecessary observation-level computations. Any computations that are identical to every observation, such as transformation of parameters, should be enclosed in these statements.

At the first observation, PROC MCMC executes all programming statements, including those that are enclosed by these two statements. This enables a quick update of all the symbols enclosed by the BEGINNODATA and ENDNODATA statements. The goal is to ensure that subsequent statements (for example, the MODEL statement) use symbol values that have been calculated correctly. At the last observation, PROC MCMC executes the enclosed programming statements again and adds the log of the prior density to the log of the posterior density.

The BEGINPRIOR and ENDPRIOR statements are aliases for the BEGINNODATA and ENDNODATA statements, respectively. You can enclose PRIOR statements in the BEGINNODATA and ENDNODATA statements.

---

## BY Statement

**BY** *variables* ;

You can specify a BY statement with PROC MCMC to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the MCMC procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

---

## MODEL Statement

**MODEL** *dependent-variable-list* ~ *distribution* < *options* > ;

The MODEL statement specifies the conditional distribution of the data given the parameters (the likelihood function). You specify a single dependent variable or a list of dependent variables, a tilde ~, and then a

distribution with its arguments. The dependent variables can be variables from the input data set or functions of the symbols in the program. You must specify the dependent variables unless you use the **GENERAL** function or the **DGENERAL** function (see the section “Specifying a New Distribution” on page 4490 for more details).

The **MODEL** statement assumes that the observations are independent of each other, conditional on the model parameters. If you want to model dependent data—that is,  $f(y_i|\theta, y_j)$  for  $j \neq i$ —you can use the **JOINTMODEL** option in the **PROC MCMC** statement. See the section “Modeling Joint Likelihood” on page 4504 for more details. By default, the log-likelihood value is the sum of the individual log-likelihood value for each observation.

You can specify multiple **MODEL** statements. You can define likelihood functions that are independent of each other. For example, in the following statements, the dependent variables **y1** and **y2** are independent of each other:

```
model y1 ~ normal(alpha, var=s21);
model y2 ~ normal(beta, var=s22);
```

Alternatively, you can use marginal and conditional distributions to define a joint log-likelihood function for multiple dependent variables. For example, the following statements jointly define a distribution over (**y1**, **y2**). They specify a marginal distribution for the dependent variable **y1** and a conditional distribution for the dependent variable **y2**:

```
model y1 ~ normal(alpha, var=s21);
model y2 ~ normal(beta * y1, var=s22);
```

Every program must have at least one **MODEL** statement. If you want to run a Monte Carlo simulation that does not require a response variable, use the **GENERAL** function in the **MODEL** statement:

```
model general(0);
```

**PROC MCMC** interprets the statement as a flat likelihood function with a constant log-likelihood value of 0.

**PROC MCMC** is a programming language that is similar to the **DATA** step, and the order of statement evaluation is important. For example, the **MODEL** statement must come after any **SAS** programming statements that define or modify arguments used in the construction of the log likelihood. In **PROC MCMC**, a symbol can be defined multiple times and used at different places. Using an expression out of order produces erroneous results that can also be hard to detect.

Do not embed the **MODEL** statement within programming statements. For example, suppose you have three response variables, **y1**, **y2**, and **y3**, and want to model each with a normal distribution. The following statements lead to erroneous output:

```
array Y[3] y1 y2 y3;
do i = 1 to 3;
 model y[i] ~ normal(mu, sd=s);
end;
```

Instead, you should do one of the following.

- Use separate **MODEL** statements:

```

model y1 ~ normal(mu, sd=s);
model y2 ~ normal(mu, sd=s);
model y3 ~ normal(mu, sd=s);

```

- Use the GENERAL function to construct a joint distribution of the three dependent variables and use a single MODEL statement to specify the log-likelihood function:

```

llike = logpdf("normal", y1, mu, s) +
 logpdf("normal", y2, mu, s) +
 logpdf("normal", y3, mu, s);
model y1 y2 y3 ~ general(llike);

```

See the section “[Specifying a New Distribution](#)” on page 4490 for more information about how to use the GENERAL function to specify an arbitrary distribution.

Missing data are allowed in the response variables; the MODEL statement augments missing data automatically. (In releases before SAS/STAT 12.1, observations with missing values were discarded prior to analysis and PROC MCMC did not attempt to model these values.) In each iteration, PROC MCMC samples missing values from their posterior distributions and incorporates them as part of the simulation. PROC MCMC creates one variable for each missing response value. There are two ways to create the missing value variable names; see the [NAMESUFFIX=](#) option for the naming convention of the variables.

## Distributions in MODEL Statement

Standard distributions that the MODEL statement supports are listed in the [Table 55.2](#) (univariate) and [Table 55.3](#) (multivariate). See the section “[Standard Distributions](#)” on page 4476 for density specifications. You can also specify all distributions except the multinomial distribution in the [PRIOR](#) and [HYPERPRIOR](#) statements. The [RANDOM](#) statement supports only a subset of the distributions (see [Table 55.4](#)).

PROC MCMC allows some distributions to be parameterized in multiple ways. For example, you can specify a normal distribution with a variance, standard deviation, or precision parameter. For distributions that have different parameterizations, you must specify an option to clearly name the ambiguous parameter. For example, in the normal distribution, you must indicate whether the second argument represents variance, standard deviation, or precision.

All univariate distributions, with the exception of binary and uniform, can have the optional LOWER= and UPPER= arguments, which specify a truncated density. See the section “[Truncation and Censoring](#)” on page 4494 for more details. Truncation is not supported for multivariate distributions.

**Table 55.2** Univariate Distributions

| Distribution Name                                                                 | Definition                                                                                                                 |
|-----------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------|
| <b>beta</b> ( $\langle \mathbf{a} = \alpha, \langle \mathbf{b} = \beta \rangle$ ) | Beta distribution with shape parameters $\alpha$ and $\beta$                                                               |
| <b>binary</b> ( $\langle \mathbf{prob p} = p \rangle$ )                           | Binary (Bernoulli) distribution with probability of success $p$ . You can use the alias <b>bern</b> for this distribution. |
| <b>binomial</b> ( $\langle \mathbf{n} = n, \langle \mathbf{prob p} = p \rangle$ ) | Binomial distribution with count $n$ and probability of success $p$                                                        |



Table 55.2 (continued)

| Distribution Name                                                                                                      | Definition                                                                                                                                                                                                                                                                         |
|------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>cauchy</b> (<location loc = > $\theta$ , <scale s = > $\lambda$ )                                                   | Cauchy distribution with location $\theta$ and scale $\lambda$                                                                                                                                                                                                                     |
| <b>chisq</b> (<df=> $\nu$ )                                                                                            | $\chi^2$ distribution with $\nu$ degrees of freedom                                                                                                                                                                                                                                |
| <b>dgeneral</b> (//)                                                                                                   | General log-likelihood function that you construct using SAS programming statements for single or multiple discrete parameters. Also see the function <b>general</b> . The name <b>dlogden</b> is an alias for this function.                                                      |
| <b>expchisq</b> (<df=> $\nu$ )                                                                                         | Log transformation of a $\chi^2$ distribution with $\nu$ degrees of freedom: $\theta \sim \mathbf{chisq}(\nu) \Leftrightarrow \log(\theta) \sim \mathbf{expchisq}(\nu)$ . You can use the alias <b>echisq</b> for this distribution.                                               |
| <b>expexpon</b> (scale s= $\lambda$ )<br><b>expexpon</b> (iscale is= $\lambda$ )                                       | Log transformation of an exponential distribution with scale or inverse-scale parameter $\lambda$ : $\theta \sim \mathbf{expon}(\lambda) \Leftrightarrow \log(\theta) \sim \mathbf{expexpon}(\lambda)$ . You can use the alias <b>eexpon</b> for this distribution.                |
| <b>expGamma</b> (<shape sp=> $a$ , scale s= $\lambda$ )<br><b>expGamma</b> (<shape sp=> $a$ , iscale is= $\lambda$ )   | Log transformation of a gamma distribution with shape $a$ and scale or inverse-scale $\lambda$ : $\theta \sim \mathbf{gamma}(a, \lambda) \Leftrightarrow \log(\theta) \sim \mathbf{expgamma}(a, \lambda)$ . You can use the alias <b>egamma</b> for this distribution.             |
| <b>expichisq</b> (<df=> $\nu$ )                                                                                        | Log transformation of an inverse $\chi^2$ distribution with $\nu$ degrees of freedom: $\theta \sim \mathbf{ichisq}(\nu) \Leftrightarrow \log(\theta) \sim \mathbf{expichisq}(\nu)$ . You can use the alias <b>eichisq</b> for this distribution.                                   |
| <b>expiGamma</b> (<shape sp=> $a$ , scale s= $\lambda$ )<br><b>expiGamma</b> (<shape sp=> $a$ , iscale is= $\lambda$ ) | Log transformation of an inverse-gamma distribution with shape $a$ and scale or inverse-scale $\lambda$ : $\theta \sim \mathbf{igamma}(a, \lambda) \Leftrightarrow \log(\theta) \sim \mathbf{expigamma}(a, \lambda)$ . You can use the alias <b>eigamma</b> for this distribution. |
| <b>expsichisq</b> (<df=> $\nu$ , <scale s=> $s$ )                                                                      | Log transformation of a scaled inverse $\chi^2$ distribution with $\nu$ degrees of freedom and scale parameter $s$ : $\theta \sim \mathbf{sichisq}(\nu) \Leftrightarrow \log(\theta) \sim \mathbf{expsichisq}(\nu)$ . You can use the alias <b>esichisq</b> for this distribution. |
| <b>expon</b> (scale s= $\lambda$ )<br><b>expon</b> (iscale is= $\lambda$ )                                             | Exponential distribution with scale or inverse-scale parameter $\lambda$                                                                                                                                                                                                           |
| <b>gamma</b> (<shape sp=> $a$ , scale s= $\lambda$ )<br><b>gamma</b> (<shape sp=> $a$ , iscale is= $\lambda$ )         | Gamma distribution with shape $a$ and scale or inverse-scale $\lambda$                                                                                                                                                                                                             |

Table 55.2 (continued)

| Distribution Name                                                                                                                                                                                                                                                                     | Definition                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>geo</b> ( <b>&lt; prob p= &gt; p</b> )                                                                                                                                                                                                                                             | Geometric distribution with probability $p$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |
| <b>general</b> ( <i>//</i> )                                                                                                                                                                                                                                                          | General log-likelihood function that you construct using SAS programming statements for a single or multiple continuous parameters. The argument <i>//</i> is an expression for the log of the distribution. If there are multiple variables specified before the tilde in a MODEL, PRIOR, or HYPERPRIOR statement, <i>//</i> is interpreted as the log of the joint distribution for these variables. Note that in the MODEL statement, the response variable specified before the tilde is just a place holder and is of no consequence; the variable must have appeared in the construction of <i>//</i> in the programming statements. <b>general</b> ( <i>constant</i> ) is equivalent to a uniform distribution on the real line. You can use the alias <b>logden</b> for this distribution. |
| <b>ichisq</b> ( <b>&lt; df= &gt; v</b> )                                                                                                                                                                                                                                              | Inverse $\chi^2$ distribution with $v$ degrees of freedom                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
| <b>igamma</b> ( <b>&lt; shape sp= &gt; a, scale s= <math>\lambda</math></b> )<br><b>igamma</b> ( <b>&lt; shape sp= &gt; a, iscale is= <math>\lambda</math></b> )                                                                                                                      | Inverse-gamma distribution with shape $a$ and scale or inverse-scale $\lambda$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
| <b>laplace</b> ( <b>&lt; location loc = &gt; <math>\theta</math>, scale s= <math>\lambda</math></b> )<br><b>laplace</b> ( <b>&lt; location loc = &gt; <math>\theta</math>, iscale is= <math>\lambda</math></b> )                                                                      | Laplace distribution with location $\theta$ and scale or inverse-scale $\lambda$ . This is also known as the <i>double exponential</i> distribution. You can use the alias <b>dexpon</b> for this distribution.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
| <b>logistic</b> ( <b>&lt; location loc = &gt; a, &lt; scale s= &gt; b</b> )                                                                                                                                                                                                           | Logistic distribution with location $a$ and scale $b$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
| <b>lognormal</b> ( <b>&lt; mean m= &gt; <math>\mu</math>, sd= <math>\lambda</math></b> )<br><b>lognormal</b> ( <b>&lt; mean m= &gt; <math>\mu</math>, var v= <math>\lambda</math></b> )<br><b>lognormal</b> ( <b>&lt; mean m= &gt; <math>\mu</math>, prec= <math>\lambda</math></b> ) | Log-normal distribution with mean $\mu$ and a value of $\lambda$ for the standard deviation, variance, or precision. You can use the aliases <b>lognormal</b> or <b>lnorm</b> for this distribution.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
| <b>negbin</b> ( <b>&lt; n= &gt; n, &lt; prob p= &gt; p</b> )                                                                                                                                                                                                                          | Negative binomial distribution with count $n$ and probability of success $p$ . You can use the alias <b>nb</b> for this distribution.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
| <b>normal</b> ( <b>&lt; mean m= &gt; <math>\mu</math>, sd= <math>\lambda</math></b> )<br><b>normal</b> ( <b>&lt; mean m= &gt; <math>\mu</math>, var v= <math>\lambda</math></b> )<br><b>normal</b> ( <b>&lt; mean m= &gt; <math>\mu</math>, prec= <math>\lambda</math></b> )          | Normal (Gaussian) distribution with mean $\mu$ and a value of $\lambda$ for the standard deviation, variance, or precision. You can use the aliases <b>gaussian</b> , <b>norm</b> , or <b>n</b> for this distribution.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
| <b>pareto</b> ( <b>&lt; shape sp= &gt; a, &lt; scale s= &gt; b</b> )                                                                                                                                                                                                                  | Pareto distribution with shape $a$ and scale $b$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |

Table 55.2 (continued)

| Distribution Name                                                                                                                                                                                                                                                                                                                                                                           | Definition                                                                                                                                                                                                        |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>poisson</b> ( <code>&lt;mean m=&gt; <math>\lambda</math></code> )                                                                                                                                                                                                                                                                                                                        | Poisson distribution with mean $\lambda$                                                                                                                                                                          |
| <b>sichisq</b> ( <code>&lt;df=&gt; <math>\nu</math>, &lt;scale s=&gt; <math>s</math></code> )                                                                                                                                                                                                                                                                                               | Scaled inverse $\chi^2$ distribution with $\nu$ degrees of freedom and scale parameter $s$                                                                                                                        |
| <b>t</b> ( <code>&lt;mean m=&gt; <math>\mu</math>, &lt;sd=&gt; <math>\lambda</math>, &lt;df=&gt; <math>\nu</math></code> )<br><b>t</b> ( <code>&lt;mean m=&gt; <math>\mu</math>, &lt;var v=&gt; <math>\lambda</math>, &lt;df=&gt; <math>\nu</math></code> )<br><b>t</b> ( <code>&lt;mean m=&gt; <math>\mu</math>, &lt;prec=&gt; <math>\lambda</math>, &lt;df=&gt; <math>\nu</math></code> ) | $T$ distribution with mean $\mu$ , standard deviation or variance or precision $\lambda$ , and $\nu$ degrees of freedom                                                                                           |
| <b>uniform</b> ( <code>&lt;left l=&gt; <math>a</math>, &lt;right r=&gt; <math>b</math></code> )                                                                                                                                                                                                                                                                                             | Uniform distribution with range $a$ and $b$ . You can use the alias <b>unif</b> for this distribution.                                                                                                            |
| <b>wald</b> ( <code>&lt;mean m=&gt; <math>\mu</math>, &lt;iscale is=&gt; <math>\lambda</math></code> )                                                                                                                                                                                                                                                                                      | Wald distribution with mean parameter $\mu$ and inverse scale parameter $\lambda$ . This is also known as the <i>Inverse Gaussian</i> distribution. You can use the alias <b>igaussian</b> for this distribution. |
| <b>weibull</b> ( <code><math>\mu, c, \sigma</math></code> )                                                                                                                                                                                                                                                                                                                                 | Weibull distribution with location (threshold) parameter $\mu$ , shape parameter $c$ , and scale parameter $\sigma$ .                                                                                             |

Table 55.3 Multivariate Distributions

| Distribution Name                                                                                                                                                                                                                                                                                                                                                                               | Definition                                                                                                                                                                                                                                                                                                            |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>dirichlet</b> ( <code>&lt;alpha=&gt; <math>\alpha</math></code> )                                                                                                                                                                                                                                                                                                                            | Dirichlet distribution with parameter vector $\alpha$ , where $\alpha$ must be a one-dimensional array of length greater than 1                                                                                                                                                                                       |
| <b>iwish</b> ( <code>&lt;df=&gt; <math>\nu</math>, &lt;scale=&gt; <math>S</math></code> )                                                                                                                                                                                                                                                                                                       | Inverse Wishart distribution with $\nu$ degrees of freedom and symmetric positive definite scale array $S$                                                                                                                                                                                                            |
| <b>mvn</b> ( <code>&lt;mu=&gt; <math>\mu</math>, &lt;cov=&gt; <math>\Sigma</math></code> )                                                                                                                                                                                                                                                                                                      | Multivariate normal distribution with mean vector $\mu$ and covariance matrix $\Sigma$                                                                                                                                                                                                                                |
| <b>mvnar</b> ( <code>&lt;mu=&gt; <math>\mu</math>, &lt;sd=&gt; <math>\lambda</math>, &lt;rho=&gt; <math>\rho</math></code> )<br><b>mvnar</b> ( <code>&lt;mu=&gt; <math>\mu</math>, &lt;var=&gt; <math>\lambda</math>, &lt;rho=&gt; <math>\rho</math></code> )<br><b>mvnar</b> ( <code>&lt;mu=&gt; <math>\mu</math>, &lt;prec=&gt; <math>\lambda</math>, &lt;rho=&gt; <math>\rho</math></code> ) | Multivariate normal distribution with mean vector $\mu$ and a covariance matrix $\Sigma$ . The covariance matrix $\Sigma$ is a multiple of the scale and a matrix with a first-order autoregressive structure. When <b>rho=0</b> , this distribution becomes a multivariate normal distribution with shared variance. |
| <b>multinom</b> ( <code>&lt;p=&gt; <math>p</math></code> )                                                                                                                                                                                                                                                                                                                                      | Multinomial distribution with probability vector $p$                                                                                                                                                                                                                                                                  |

## Options for the MODEL Statement

The *options* in the MODEL statement apply only when there are missing values in the response variable. You can specify the following options:

### **INITIAL**=*SAS-data-set* | *constant* | *numeric-list*

specifies the initial values of the missing values. By default, PROC MCMC uses a sample average of the nonmissing values of a response variable as the starting values for all missing values in the simulation for that variable. You can use the INITIAL= option to start the Markov chain at a different place.

If you use a *SAS-data-set* to store initial values, the data set must consist of variable names that agree with the missing variable names that are used by PROC MCMC. The easiest way to find the names of the internally created variables is to run a default analysis with a very small number of simulations and check the variable names in the **OUTPOST**= data set. You can provide a subset of the initial values in the *SAS-data-set*, and PROC MCMC uses a default mechanism to fill in the rest of the missing initial values.

For example, the following statement creates a data set with initial values for the first three missing values of a response variable:

```
data RandomInit;
 input y_1 y_2 y_3;
 datalines;
 2.3 3 -3
;
```

The following MODEL statement uses the values in the RandomInit data set as the initial values of the corresponding missing values in the model:

```
model y ~ normal(0, var=s2u) init=randominit;
```

Specifying a *constant* assigns that constant as the initial value to all missing values in that response variable. For example, the following statement assigns the value 5 to be used as an initial value for all missing  $y_i$  in the model:

```
model y ~ normal(0, var=s2u) init=5;
```

If you have a multidimensional response variable, you can provide a list of numbers that have the same length as the dimension of your response array. Each number is then given to all corresponding missing variables in order. For example, the following statement assigns the value 2 to be used as an initial value for all missing  $w_{1i}$  and the value 3 to be used for all missing  $w_{2i}$  in the model:

```
array w[2] w1 w2;
model w ~ mvn(mu, cov) init=(2 3);
```

### **MONITOR**=(*symbol-list* | *number-list* | **RANDOM**(*number*))

outputs analysis for selected missing data variables. You can choose to monitor the missing values by listing the response variable names, the missing data variable names, or indices, or you can have them randomly selected by PROC MCMC.

For example, suppose that the data set contains 10 observations and the response variable  $y$  has missing values in observations 2, 3, 7, 9, and 10. To monitor all missing data variables (five in total), you specify the response variable name in the `MONITOR=` option:

```
model y ~ normal(0, var=s2u) monitor=(y);
```

Suppose you want to monitor the missing data variables that correspond to the missing values in observations 2, 3, and 10. You have two options: provide either a list of variable names or a list of indices.

The following statement selects monitored variables by their variable names:

```
model y ~ normal(0, var=s2u) monitor=(y_2 y_3 y_10);
```

The variable names must match the internally created variable names for each missing value. See `NAMESUFFIX=` option for the naming convention of the variables. By default, the names are created by concatenating the response variable with the observation index; hence you use the `name_obs` format to construct the names. The numbers 2, 3, and 10 are the corresponding observation indices to the missing values in the input data set.

The following statement selects monitored variables by indices:

```
model y ~ normal(0, var=s2u) monitor=(1 2 5);
```

The indices are not a list of the observation numbers, but rather the order by which the missing values appear in the data set: PROC MCMC reports back the first, the second, and the fifth missing value variables that it creates. The actual variable names that appear in the output are still `y_2`, `y_3`, and `y_10`, honoring the control of the `NAMESUFFIX=` option.

Lastly, PROC MCMC can randomly choose a subset of the variables to monitor. The following statement randomly selects 3 variables to monitor:

```
model y ~ normal(0, var=s2u) monitor=(random(3));
```

The list of the random indices is controlled by the `SEED=` option in the PROC MCMC statement. Therefore, the selected variables will be the same when the `SEED=` option is the same.

### **NAMESUFFIX=OBSERVATION | POSITION | ORDER**

specifies how the names of the missing data variables are created. By default, the names are created by concatenating the response variable symbol, an underscore (“\_”), and the observation number of the missing value.

`NAMESUFFIX=OBSERVATION` constructs the parameter names by appending the observation number to the response variable symbol. This is the default. `NAMESUFFIX=POSITION` or `NAMESUFFIX=ORDER` construct the parameter names by appending the numbers 1, 2, 3, and so on, where the number indicates the order in which the missing values appear in the data set.

For example, suppose you have a response variable  $y$  with 10 observations in total, of which five are missing (observations 2, 3, 7, 9, and 10). By default, PROC MCMC creates five variable names `y_2`, `y_3`, `y_7`, `y_9`, and `y_10`. Using `NAMESUFFIX=POSITION` changes the names to `y_1`, `y_2`, `y_3`, `y_4`, and `y_5`.

## NOOUTPOST

suppresses the output of the posterior samples of missing data variables to the posterior output data set (which is specified in the **OUTPOST=** option in the PROC MCMC statement). In models with a large number of missing values (for example, tens of thousands), PROC MCMC can run faster if it does not save the posterior samples.

When you specify both the NOOUTPOST option and the **MONITOR=** option, PROC MCMC outputs the list of variables that are monitored.

The maximum number of variables that can be saved to an **OUTPOST=** data set is 32,767. If the total number of parameters in your model, including the number of missing data variables, exceeds the limit, the NOOUTPOST option is evoked automatically and PROC MCMC does not save the missing value draws to the posterior output data set. You can use the **MONITOR=** option to select a subset of the parameters to store in the **OUTPOST=** data set.

---

## PARMS Statement

```
PARMS name |(name-list)<=> <{> number | number-list <}>
 < name |(name-list)<=> <{> number | number-list <}> ... >
 </ options> ;
```

The PARS statement lists the names of the parameters in the model and specifies optional initial values for these parameters. These parameters are referred to as the *model parameters*. You can specify multiple PARS statements. Each PARS statement defines a block of parameters, and the blocked Metropolis algorithm updates the parameters in each block simultaneously. See the section “Blocking of Parameters” on page 4466 for more details. PROC MCMC generates missing initial values from the prior distributions whenever needed, as long as they are the standard distributions and not the **GENERAL** or **DGENERAL** function.

If your model contains a multidimensional parameter (for example, a parameter with a multivariate normal prior distribution), you must declare the parameter as an array (using the **ARRAY** statement). You can use braces { } after the parameter name in the PARM statement to assign initial values. For example:

```
array mu[3];
parms mu {1 2 3};
```

You cannot use the **ARRAY** statement to assign initial values. If you use the **ARRAY** statement to store values in array elements, the declared array becomes a constant array and cannot be used as parameters in the PARS statement. For example, the following statement assigns three numbers to mu:

```
array mu[3] (1 2 3);
```

The array mu can no longer be a model parameter.

Every parameter in the PARS statement must have a corresponding prior distribution in the PRIOR statement. The program exits if this one-to-one requirement is not satisfied.

You can specify the following *options* to control different samplers explicitly for that block of parameters.

**NORMAL | N**

uses the normal proposal distribution in the random walk Metropolis. This is the default.

**T <(df)>**

uses the t distribution with  $df$  degrees of freedom as an alternative proposal distribution. A t distribution with a small number of degrees of freedom has thicker tails and can sometimes improve the mixing of the Markov chain. When  $df > 100$ , the normal distribution is used instead.

**SLICE**

applies the slice sampler to each parameter in the PARMS statement individually. See the section “[Slice Sampler](#)” on page 136 for details. PROC MCMC does not implement a multidimensional version of the slice sampler. Because the slice sampler usually requires multiple evaluations of the objective function (the posterior distribution) in each iteration, the associated computational cost could be potentially high with this sampling algorithm.

**UDS**

implements a user-defined sampler for any of the parameters in the block. See the section “[UDS Statement](#)” on page 4462 for details and “[Example 55.19: Implement a New Sampling Algorithm](#)” on page 4645 for a realistic example. When you specify the UDS option, PROC MCMC hands off the sampling of these parameters to you at each iteration and relies on your sampler to return a random draw from the conditional posterior distribution. This option is useful if you have a model-specific sampler that you want to implement or a new algorithm that can improve the convergence and mixing of the Markov chain. This functionality is for advanced users, and you should proceed with caution.

---

## PREDDIST Statement

**PREDDIST** < *label* > **OUTPRED**=*SAS-data-set* < **NSIM**=*n* > < **COVARIATES**=*SAS-data-set* >  
< **STATISTICS**=*options* > ;

The PREDDIST statement creates a new SAS data set that contains random samples from the posterior predictive distribution of the response variable. The posterior predictive distribution is the distribution of unobserved observations (prediction) conditional on the observed data. Let  $\mathbf{y}$  be the observed data,  $\mathbf{X}$  be the covariates,  $\theta$  be the parameter, and  $\mathbf{y}_{\text{pred}}$  be the unobserved data. The posterior predictive distribution is defined to be the following:

$$\begin{aligned} p(\mathbf{y}_{\text{pred}}|\mathbf{y}, \mathbf{X}) &= \int p(\mathbf{y}_{\text{pred}}, \theta|\mathbf{y}, \mathbf{X})d\theta \\ &= \int p(\mathbf{y}_{\text{pred}}|\theta, \mathbf{y}, \mathbf{X})p(\theta|\mathbf{y}, \mathbf{X})d\theta \end{aligned}$$

Given the assumption that the observed and unobserved data are conditional independent given  $\theta$ , the posterior predictive distribution can be further simplified as the following:

$$p(\mathbf{y}_{\text{pred}}|\mathbf{y}, \mathbf{X}) = \int p(\mathbf{y}_{\text{pred}}|\theta)p(\theta|\mathbf{y}, \mathbf{X})d\theta$$

The posterior predictive distribution is an integral of the likelihood function  $p(y_{\text{pred}}|\theta)$  with respect to the posterior distribution  $p(\theta|y)$ . The PREDDIST statement generates samples from a posterior predictive distribution based on draws from the posterior distribution of  $\theta$ .

The PREDDIST statement works only on response variables that have standard distributions, and it does not support either the GENERAL or DGENERAL functions. Multiple PREDDIST statements can be specified, and an optional label (specified as a quoted string) helps identify the output.

The following list explains specifications in the PREDDIST statement:

**COVARIATES=***SAS-data-set*

names the SAS data set that contains the sets of explanatory variable values for which the predictions are established. This data set must contain data with the same variable names as are used in the likelihood function. If you omit the COVARIATES= option, the DATA= data set specified in the PROC MCMC statement is used instead.

**NSIM=***n*

specifies the number of simulated predicted values. By default, NSIM= uses the NMC= option value specified in the PROC MCMC statement.

**OUTPRED=***SAS-data-set*

creates an output data set to contain the samples from the posterior predictive distribution. The output variable names are listed as *resp\_1*–*resp\_m*, where *resp* is the name of the response variable and *m* is the number of observations in the COVARIATES= data set in the PREDDIST statement. If the COVARIATES= data set is not specified, *m* is the number of observations in the DATA= data set specified in the PROC statement.

**STATISTICS**< (*global-stats-options*) > = **NONE** | **ALL** | *stats-request*

**STATS**< (*global-stats-options*) > = **NONE** | **ALL** | *stats-request*

specifies options for calculating posterior statistics. This option works identically to the STATISTICS= option in the PROC statement. By default, this option takes the specification of the STATISTICS= option in the PROC MCMC statement.

For an example that uses the PREDDIST statement, see “[Posterior Predictive Distribution](#)” on page 4514.

---

## PRIOR/HYPERPRIOR Statement

**PRIOR** *parameter-list* ~ *distribution* ;

**HYPERPRIOR** *parameter-list* ~ *distribution* ;

**HYPER** *parameter-list* ~ *distribution* ;

The PRIOR statement specifies the prior distribution of the model parameters. You must specify a single parameter or a list of parameters, a tilde ~, and then a distribution with its parameters.



You can specify multiple **PRIOR** statements to define models with multiple prior components. Your model can have as many hierarchical levels as you want. But in many cases, such as random-effects models, it is better to use the **RANDOM** statements to build up the model hierarchy. The log of the prior is the sum of the log prior values from each of the **PRIOR** statements. Similar to the **MODEL** statement, you can use the **PRIOR** statement to specify marginal or conditional prior distributions. See the section “**MODEL Statement**” on page 4443 for the names of the standard distributions and the section “**Standard Distributions**” on page 4476 for density specification.

The **PRIOR** statements are processed twice at every Markov chain simulation—that is, twice per pass through the data set. The statements are called at the first and the last observation of the data set, just as the **BEGINNODATA** and **ENDNODATA** statements are processed. If you run a Monte Carlo simulation that is data-independent, you can specify the **NOLOGDIST** option in the **PROC MCMC** statement to omit the calculation of the prior distribution. Omitting this calculation enables **PROC MCMC** to run faster.

The **HYPERPRIOR** statement is treated internally the same as the **PRIOR** statement. It provides a notational convenience in case you want to fit a multilevel hierarchical model. It specifies the hyperprior distribution of the prior distribution parameters. The log of the hyperprior is the sum of the log hyperprior values from each of the **HYPERPRIOR** statements.

Parameters in the **PRIOR** statements can appear as hyperparameters in the **RANDOM** statement. The reverse is not allowed: random-effects parameters cannot be hyperparameters in a **PRIOR** statement.

You can have a program that contains a **RANDOM** statement but no **PRIOR** statements. (In SAS 9.3 and earlier, each program had to contain a **PRIOR** statement.) A program that contains a **RANDOM** statement but no **PRIOR** statements could be a random-effects model with no fixed-effects parameters or hyperparameters to the random effects. A **MODEL** statement is still required in every program.

---

## Programming Statements

This section lists the programming statements available in **PROC MCMC** to compute the priors and log-likelihood functions. This section also documents the differences between programming statements in **PROC MCMC** and programming statements in the **DATA** step. The syntax of programming statements used in **PROC MCMC** is identical to that used in the **NLMIXED** procedure (see Chapter 64, “**The NLMIXED Procedure**”) and the **MODEL** procedure (see Chapter 19, “**The MODEL Procedure**” (*SAS/ETS User’s Guide*)). Most of the programming statements that can be used in the **DATA** step can also be used in **PROC MCMC**. See *SAS Language Reference: Dictionary* for a description of SAS programming statements.

There are also a number of unique functions in **PROC MCMC** that calculate the log density of various distributions in the procedure. You can find them at the section “**Using Density Functions in the Programming Statements**” on page 4491.

For the list of matrix-based functions that is supported in **PROC MCMC**, see the section “**Matrix Functions in PROC MCMC**” on page 4498.

The following are valid statements:

```

ABORT;
ARRAY arrayname < [dimensions] > < $ > < variables-and-constants >;
CALL name < (expression < , expression ... >) >;
DELETE;
DO < variable = expression < TO expression > < BY expression > >
 < , expression < TO expression > < BY expression > > ...
 < WHILE expression > < UNTIL expression >;
END;
GOTO statement-label;
IF expression;
IF expression THEN program-statement;
 ELSE program-statement;
variable = expression;
variable + expression;
LINK statement-label;
PUT < variable > < = > ...;
RETURN;
SELECT < (expression) >;
STOP;
SUBSTR(variable, index, length)= expression;
WHEN (expression)program-statement;
 OTHERWISE program-statement;

```

For the most part, the SAS programming statements work the same as they do in the DATA step, as documented in *SAS Language Reference: Concepts*. However, there are several differences:

- The ABORT statement does not allow any arguments.
- The DO statement does not allow a character index variable. Thus

```
do i = 1, 2, 3;
```

is supported; however, the following statement is not supported:

```
do i = 'A', 'B', 'C';
```

- The PUT statement, used mostly for program debugging in PROC MCMC (see the section “[Handling Error Messages](#)” on page 4530), supports only some of the features of the DATA step PUT statement, and it has some features that are not available with the DATA step PUT statement:
  - The PROC MCMC PUT statement does not support line pointers, factored lists, iteration factors, overprinting, \_INFILE\_, \_OBS\_, the colon (:) format modifier, or “\$”.
  - The PROC MCMC PUT statement does support expressions, but the expression must be enclosed in parentheses. For example, the following statement displays the square root of x:

```
put (sqrt(x));
```

- The WHEN and OTHERWISE statements enable you to specify more than one target statement. That is, DO/END groups are not necessary for multiple statement WHENs. For example, the following syntax is valid:

```

select;
 when (exp1) stmt1;
 stmt2;
 when (exp2) stmt3;
 stmt4;
end;

```

You should avoid defining variables that begin with an underscore (\_). They might conflict with internal variables created by PROC MCMC. The **MODEL** statement must come after any SAS programming statements that define or modify terms used in the construction of the log likelihood.

---

## RANDOM Statement

**RANDOM** *random-effect* ~ *distribution* **SUBJECT=***variable* < *options* > ;

The **RANDOM** statement defines a single random effect and its prior distribution or an array of random effects and their prior distribution. The *random-effect* must be represented by either a symbol or an array. The **RANDOM** statement must consist of the *random-effect*, a tilde (~), the distribution for the random effect, and then a **SUBJECT=** variable.

**SUBJECT=***variable* | **\_OBS\_**

identifies the subjects in the random-effects model. The *variable* must be part of the input data set, and it can be either a numeric variable or character literal. The *variable* does not need to be sorted, and the input data set does not need to be clustered according to it. **SUBJECT=\_OBS\_** enables you fit an observation-level random-effects model (each observation has its own random effect) without specifying a subject variable in the input data set.

The random-effects parameters associated with each subject in the same **RANDOM** statement are assumed to be conditionally independent of each other, given other parameters and data set variables in the model. The other parameters include model parameters (declared in the **PARMS** statements), random-effects parameters (from other **RANDOM** statements), and missing data variables.

Table 55.4 shows the distributions that you can specify in the **RANDOM** statement.

**Table 55.4** Valid Distributions in the **RANDOM** Statement

| Distribution Name                                                                                                                                                                    | Definition                                                                                                                 |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------|
| <b>beta</b> (< <b>a</b> => $\alpha$ , < <b>b</b> => $\beta$ )                                                                                                                        | Beta distribution with shape parameters $\alpha$ and $\beta$                                                               |
| <b>binary</b> (< <b>prob</b>   <b>p</b> => $p$ )                                                                                                                                     | Binary (Bernoulli) distribution with probability of success $p$ . You can use the alias <b>bern</b> for this distribution. |
| <b>gamma</b> (< <b>shape</b>   <b>sp</b> => $a$ , <b>scale</b>   <b>s</b> = $\lambda$ )<br><b>gamma</b> (< <b>shape</b>   <b>sp</b> => $a$ , <b>iscale</b>   <b>is</b> = $\lambda$ ) | Gamma distribution with shape $a$ and scale or inverse-scale $\lambda$                                                     |

Table 55.4 (continued)

| Distribution Name                                                                                                                                                                                        | Definition                                                                                                                                                                                                                                |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>dgeneral</b> (//)                                                                                                                                                                                     | General log-prior function that you construct using SAS programming statements for univariate or multivariate discrete random effects. See the section “ <a href="#">Specifying a New Distribution</a> ” on page 4490 for more details.   |
| <b>general</b> (//)                                                                                                                                                                                      | General log-prior function that you construct using SAS programming statements for univariate or multivariate continuous random effects. See the section “ <a href="#">Specifying a New Distribution</a> ” on page 4490 for more details. |
| <b>igamma</b> (< shape sp= > a, scale s= $\lambda$ )<br><b>igamma</b> (< shape sp= > a, iscale is= $\lambda$ )                                                                                           | Inverse-gamma distribution with shape $a$ and scale or inverse-scale $\lambda$                                                                                                                                                            |
| <b>laplace</b> (< location loc = > $\theta$ , scale s= $\lambda$ )<br><b>laplace</b> (< location loc = > $\theta$ , iscale is= $\lambda$ )                                                               | Laplace distribution with location $\theta$ and scale or inverse-scale $\lambda$ . This is also known as the <i>double exponential</i> distribution. You can use the alias <b>dexpon</b> for this distribution.                           |
| <b>normal</b> (< mean m= > $\mu$ , sd= $\lambda$ )<br><b>normal</b> (< mean m= > $\mu$ , var v= $\lambda$ )<br><b>normal</b> (< mean m= > $\mu$ , prec= $\lambda$ )                                      | Normal (Gaussian) distribution with mean $\mu$ and a value of $\lambda$ for the standard deviation, variance, or precision. You can use the aliases <b>gaussian</b> , <b>norm</b> , or <b>n</b> for this distribution.                    |
| <b>poisson</b> (< mean m= > $\lambda$ )                                                                                                                                                                  | Poisson distribution with mean $\lambda$                                                                                                                                                                                                  |
| <b>mvn</b> (< mu= > $\mu$ , < cov= > $\Sigma$ )                                                                                                                                                          | Multivariate normal distribution with mean vector $\mu$ and covariance matrix $\Sigma$                                                                                                                                                    |
| <b>mvnar</b> (< mu= > $\mu$ , sd= $\lambda$ , < rho= > $\rho$ )<br><b>mvnar</b> (< mu= > $\mu$ , var= $\lambda$ , < rho= > $\rho$ )<br><b>mvnar</b> (< mu= > $\mu$ , prec= $\lambda$ , < rho= > $\rho$ ) | Multivariate normal distribution with mean vector $\mu$ and a covariance matrix $\Sigma$ . The covariance matrix $\Sigma$ is a multiple of the scale and a matrix with a first-order autoregressive structure                             |

The following RANDOM statement specifies a scale effect, where `s2u` can be a constant or a model parameter and `index` is a data set variable that indicates group membership of the random effect `u`:

```
random u ~ normal(0,var=s2u) subject=index;
```

The following statements specify multidimensional effects, where `mu` and `cov` can be either parameters in the model or constant arrays:

```
array w[2];
array mu[2];
array cov[2,2];
random w ~ mvn(mu, cov) subject=index;
```

You can specify multiple RANDOM statements. Hyperparameters in the prior distribution of a random effect can be other random effects in the model. For example, the following statements are allowed because the random effect *g* appears in the distribution for the random effect *u*:

```
random g ~ normal(0, var=s2g) subject=month;
random u ~ normal(g, var=s2u) subject=day;
```

These two RANDOM statements specify a nested hierarchical model in which the random-effects *g* is the hyperparameter of the random-effects *u*. You can build the hierarchical structure as deep as you want. You can also use multiple RANDOM statements to build non-nested random-effects models, where the effects could enter the model on different levels but not in the same hierarchy of each other.

The number of random-effects parameters in each RANDOM statement is determined by the number of unique values in the **SUBJECT=** variable, which can be either unsorted numeric or unsorted character literal. Unlike the model parameters that are explicitly declared in the **PARMS** statement (with therefore a fixed total number), the number of random-effects parameters in a program depends on the values of the **SUBJECT=** data set variable. That number can change from one BY group to another.

The names of the random-effects parameters are created internally. See the **NAMESUFFIX=** option for the naming convention of the random-effects parameters. The random-effects parameters are updated conditionally in the simulation. All posterior draws are saved to the **OUTPOST=** output data set by default, and you can use the **MONITOR=** option to monitor any of the parameters. For more information about available sampling algorithms, see the **ALGORITHM=** option. For more information about how to set a random-effects parameter to a constant (also known as corner-point constraint), see the **CONSTRAINT** option.

You can specify the following *options* in the RANDOM statement:

**ALGORITHM=***option*

**ALG=***option*

specifies the algorithm to use to sample the posterior distribution. The following *options* are available:

**RWM**

uses the random-walk Metropolis algorithm with normal proposal.

**SLICE**

uses the slice sampling algorithm.

**GEO**

uses the discrete random-walk Metropolis with symmetric geometric proposal.

When possible, PROC MCMC samples directly from the full conditional distribution. Otherwise, the default sampling algorithm is the RWM.

**CONSTRAINT(VALUE=***value***) =** **FIRST** | **LAST** | **NONE** | '*formatted-value*'

**ZERO=****FIRST** | **LAST** | **NONE** | '*formatted-value*'

sets one of the random-effects parameters to a fixed value. The default is **ZERO=NONE**, which does not fix any of the parameters to be a constant. This option enables you to eliminate one of the parameters.

For example, this option could be useful if you want to fit a regression model with categorical covariates and, instead of creating a design matrix, you treat the parameters as “random effects” and fit an equivalent random-effects model.

Suppose you have a regression that includes a categorical variable  $X$  with  $J$  levels. You can construct a full-rank design matrix with  $J-1$  dummy variables ( $X_2 \cdots X_J$  with  $X_1$  being the base group) and fit a regression such as the following:

$$\mu_i = \beta_0 + \beta_2 \cdot X_2 \cdots \beta_J \cdot X_J$$

The following statements in a PROC MCMC step fit such a hypothetical regression model:

```
parms beta0 betax2 ... betaxJ;
prior beta: ~ n(0, sd=100);
mu = beta0 + betax2 * x2 + ... betaxJ * xJ;
...
```

Equivalently, you can also treat this model as a random-effects model such as the following, where  $\beta_j$  are random effects for each category in  $X$ :

$$\mu_i = \beta_0 + \beta_j \text{ for } j = 1, \dots, J$$

However, this random-effects model is over-parameterized. The ZERO= option rids the model with one random-effects parameter of choice and fixes it to be zero. The following example statements fit such a hypothetical random-effects model:

```
parms beta0;
prior beta0 ~ n(0, sd=100);
random beta ~ n(0, sd=100) subject=x zero=first;
mu = beta0 + beta;
...
```

The specification ZERO=FIRST sets the first random-effects parameter to 0, implying  $\beta_1 = 0$ . This random-effects parameter corresponds to the first category in the SUBJECT= variable. The category is what the first observation of the SUBJECT= variable takes.

The specification ZERO=LAST sets the last random-effects parameter to be 0, implying  $\beta_J = 0$ . This random-effects parameter corresponds to the last category in the SUBJECT= variable. The category is not necessarily the same category that the last observation of the SUBJECT= variable takes because the SUBJECT= variable does not need to be sorted.

The specification ZERO='formatted-value' sets the random-effects parameter for the category (in the SUBJECT= variable) with a formatted value that matches 'formatted-value' to 0. For example, ZERO='3' sets  $\beta_3 = 0$ .

The CONSTRAINT(VALUE=value) option works similarly to the ZERO= option. You can assign an arbitrary value to any one of the random-effects parameter. For example, the specification CONSTRAINT(VALUE=0)=FIRST is equivalent to ZERO=FIRST.

**INITIAL**=*SAS-data-set* | *constant* | *numeric-list*

specifies the initial values of the random-effects parameters. By default, PROC MCMC uses the same option as specified in the **INIT**= option to generate initial values for the random-effects parameter: either it uses the mode of the prior density or it randomly draws a sample from that distribution. You can start the Markov chain at different places by providing a *SAS-data-set*, a constant, or a *numeric-list* for multivariate random-effects parameters.

If you use a *SAS-data-set*, the data set must consist of variable names that agree with the random-effects parameters in the model (see the **NAMESUFFIX**= option for the naming convention of the random-effects parameters). The easiest way to find the names of the internally created parameter names is to run a default analysis with a very small number of simulations and check the variable names in the **OUTPOST**= data set. You can provide a subset of the initial values in the *SAS-data-set* and PROC MCMC will use the default mechanism to fill in the rest of the random-effects parameters.

For example, the following statement creates a data set with initial values for the random-effects parameters `u_1`, `u_2`, and `u_3`:

```
data RandomInit;
 input u_1 u_2 u_3;
 datalines;
 2.3 3 -3
;
```

The following **RANDOM** statement takes the values in the `RandomInit` data set to be the initial values of the corresponding random-effects parameters in the model:

```
random u ~ normal(0,var=s2u) subject=index init=randominit;
```

Specifying a *constant* assigns that constant as the initial value to all random-effects parameters in the statement. For example, the following statement assigns the value 5 to be used as an initial value for all  $u_i$  in the model:

```
random u ~ normal(0,var=s2u) subject=index init=5;
```

If you have multiple effects, you can provide a list of numbers, where the length of the list the same as the dimension of your random-effects array. Each number is then given to all corresponding random-effects parameters in order. For example, the following statement assigns the value 2 to be used as an initial value for all  $w_{1i}$  and the value 3 to be used for all  $w_{2i}$  in the model:

```
array w[2] w1 w2;
random w ~ mvn(mu, cov) subject=index init=(2 3);
```

If you use the **GENERAL** or **DGENERAL** functions in the **RANDOM** statement, you must provide initial values for these parameters.

**MONITOR**=(*symbol-list* | *number-list* | **RANDOM**(*number*))

outputs analysis for selected random-effects parameters. You can choose to monitor the random-effects parameters by listing the effect names or effect indices, or you can have them randomly selected by PROC MCMC.

To monitor all random-effects parameters, you specify the effect name in the **MONITOR**= option:



```
random u ~ normal(0,var=s2u) subject=index monitor=(u);
```

You have three options for monitoring a subset of the random-effects parameters. You can provide a list of the parameter names, you can provide a number list of the parameter indices, or you can have PROC MCMC randomly choose a subset of parameters for you.

For example, if you want to monitor analysis for parameters `u_1` through `u_10`, `u_23`, and `u_57`, you can provide the names as follows:

```
random u ~ normal(0,var=s2u) subject=index monitor=(u_1-u_10 u_23 u_57);
```

The naming convention in the *symbol-list* must agree with the `NAMESUFFIX=` option, which controls how the parameter names of the *random-effect* are created. By default, `NAMESUFFIX=SUBJECT`, and the *symbol-list* must use suffixes that correspond to the formatted values<sup>1</sup> in the `SUBJECT=` data set variable. With the `NAMESUFFIX=POSITION` option, the *symbol-list* must use suffixes that agree with the input order of the `SUBJECT=` variable. If the `SUBJECT=` variable has a character value, you cannot use the hyphen (-) in the *symbol-list* to indicate a range of variables.

To monitor the same list of random-effects parameters, you can provide their indices:

```
random u ~ normal(0,var=s2u) subject=index monitor=(1 to 10 by 1 23 57);
```

PROC MCMC can also randomly choose a subset of the parameters to monitor:

```
random u ~ normal(0,var=s2u) subject=index monitor=(random(12));
```

The sequence of the random indices is controlled by the `SEED=` option in the PROC MCMC statement.

By default, PROC MCMC does not monitor any random-effects parameters. When you specify this option, it takes the specification of the `STATISTICS=` and `PLOTS=` options in the PROC MCMC statement. By default, PROC MCMC outputs all the posterior samples of all random-effects parameters to the `OUTPOST=` output data set. You can use the `NOOUTPOST` option to suppress the saving of the random-effects parameters.

### **NAMESUFFIX=option**

specifies how the names of the random-effects parameters are internally created from the `SUBJECT=variable` that is specified in the RANDOM statement. PROC MCMC creates the names by concatenating the *random-effect* symbol with an underscore and a series of numbers or characters. The following *options* control the type of methods that are used in such construction:

### **SUBJECT**

constructs the parameter names by appending the formatted values of the `SUBJECT=variable` in the input data set<sup>1</sup>.

<sup>1</sup>In SAS/STAT 9.3, the random-effects parameters were created using the unformatted values of the `SUBJECT=variable`.



**POSITION**

constructs the parameter names by appending the numbers 1, 2, 3, and so on, where the number indicates the order in which the **SUBJECT= variable** appears in the data set.

For example, suppose you have an input data set with four observations and the **SUBJECT=** variable `zipcode` has four values (with three of them unique): 27513, 01440, 27513, and 15217. The following SAS statement creates three random-effects parameters named `u_27513`, `u_01440`, and `u_15217`:

```
random u ~ normal(0,var=10) subject=zipcode namesuffix=subject;
```

On the other hand, using **NAMESUFFIX=POSITION** creates three parameters named as `u_1`, `u_2`, and `u_3`:

```
random u ~ normal(0,var=10) subject=zipcode namesuffix=position;
```

By default, **NAMESUFFIX=SUBJECT**.

**NOOUTPOST**

suppresses the output of the posterior samples of random-effects parameters to the **OUTPOST=** data set. In models with a large number of random-effects parameters (for example, tens of thousands), PROC MCMC can run faster if it does not save the posterior samples of the random-effects parameters.

When you specify both the **NOOUTPOST** option and the **MONITOR=** option, PROC MCMC outputs the list of variables that are monitored.

The maximum number of variables that can be saved to an **OUTPOST=** data set is 32,767. If you run a large-scale random-effects model with the number of parameters exceeding the limit, the **NOOUTPOST** option is evoked automatically and PROC MCMC does not save the random-effects parameter draws to the posterior output data set. You can use the **MONITOR=** option to select a subset of the parameters to store in the **OUTPOST=** data set.

**UDS Statement**

```
UDS subroutine-name (subroutine-argument-list) ;
```

UDS stands for user defined sampler. The UDS statement enables you to use a separate algorithm, other than the default random walk Metropolis, to update parameters in the model. The purpose of the UDS statement is to give you a greater amount of flexibility and better control over the updating schemes of the Markov chain. Multiple UDS statements are allowed.

For the UDS statement to work properly, you have to do the following:

- write a subroutine by using PROC FCMP (see the FCMP Procedure in the *Base SAS Procedures Guide*) and save it to a SAS catalog (see the example in this section). The subroutine must update some parameters in the model. These are the UDS parameters. The subroutine is called the UDS subroutine.

- declare any UDS parameters in the **PARMS** statement with a sampling option, as in `</ UDS >` (see the section “**PARMS Statement**” on page 4451).
- specify the prior distributions for all UDS parameters, using the **PRIOR** statements.

**NOTE:** All UDS parameters must appear in three places: the UDS statement, the **PARMS** statement, and the **PRIOR** statement. Otherwise, PROC MCMC exits.

To obtain a valid Markov chain, a UDS subroutine must update a parameter from its full posterior conditional distribution and not the posterior marginal distribution. The posterior conditional is something that you need to provide. This conditional is implicitly based on a prior distribution. PROC MCMC has no means to verify that the implied prior in the UDS subroutine is the same as the prior that you specified in the **PRIOR** statement. You need to make sure that the two distributions agree; otherwise, you will get misleading results.

The priors in the **PRIOR** statements do not directly affect the sampling of the UDS parameters. They could affect the sampling of the other parameters in the model, which, in turn, changes the behavior of the Markov chain. You can see this by noting cases where the hyperparameters of the UDS parameters are model parameters; the priors should be part of the posterior conditional distributions of these hyperparameters, and they cannot be omitted.

Some additional information is listed to help you better understand the UDS statement:

- Most features of the SAS programming language can be used in subroutines processed by PROC FCMP (see the FCMP Procedure in the *Base SAS Procedures Guide*).
- The UDS statement does not support FCMP functions—a FCMP function returns a value, while a subroutine does not. A subroutine updates some of its subroutine arguments. These arguments are called OUTARGS arguments.
- The UDS parameters cannot be in the same block as other parameters. The optional argument `</ UDS >` in the **PARMS** statement prevents parameters that use the default Metropolis from being mixed with those that are updated by the UDS subroutines.
- You can put all the UDS parameters in the same **PARMS** statement or have a separate UDS statement for each of them.
- The same subroutine can be used in multiple UDS statements. This feature comes in handy if you have a generic sampler that can be applied to different parameters.
- PROC MCMC updates the UDS parameters by calling the UDS subroutines directly. At every iteration, PROC MCMC first samples parameters that use the Metropolis algorithm, then the UDS parameters. Sampling of the UDS parameters proceeds in the order in which the UDS statements are listed.
- A UDS subroutine accepts any symbols in the program as well as any input data set variables as its arguments.
- Only the OUTARGS arguments in a UDS subroutine are updated in PROC MCMC. You can modify other arguments in the subroutine, but the changes are not global in PROC MCMC.
- If a UDS subroutine has an argument that is a SAS data set variable, PROC MCMC steps through the data set while updating the UDS parameters. The subroutine is called once per observation in the data set for every iteration.

- If a UDS subroutine does not have any arguments that are data set variables, PROC MCMC does not access the data set while executing the subroutine. The subroutine is called once per iteration.
- To reduce the overhead in calling the UDS subroutine and accessing the data set repeatedly, you might consider reading all the input data set variables into arrays and using the arrays as the subroutine arguments. See the section “[BEGINCNST/ENDCNST Statement](#)” on page 4441 about how to use the [BEGINCNST](#) and [ENDCNST](#) statements to store data set variables.

For an example that uses the UDS statement, see “[Example 55.19: Implement a New Sampling Algorithm](#)” on page 4645.

---

## Details: MCMC Procedure

---

### How PROC MCMC Works

PROC MCMC is a simulation-based procedure that applies a variety of sampling algorithms to the program at hand. The default sampling methods include conjugate sampling (from full conditional), direct sampling from the marginal distribution, inverse cumulative distribution function, random walk Metropolis with normal proposal, and discretized random walk Metropolis with normal proposal. You can request alternate sampling algorithms, such as random walk Metropolis with  $t$  distribution proposal, discretized random walk Metropolis with symmetric geometric proposal, and the slice sampling algorithm.

PROC MCMC applies the more efficient sampling algorithms first, whenever possible. When a parameter does not appear in the conditional distributions of other random variables in the program, PROC MCMC generates samples directly from its prior distribution (which is also its marginal distribution). This usually occurs in data-independent Monte Carlo simulation programs (see “[Example 55.1: Simulating Samples From a Known Density](#)” on page 4540 for an example) or missing data problems, where the missing response variables are generated directly from the conditional sampling distribution (or the conditional likelihood). When conjugacy is detected, PROC MCMC uses random number generators to draw values from the full conditional distribution. (For information about detecting conjugacy, see the section “[Conjugate Sampling](#)” on page 4472.) In other situations, PROC MCMC resorts to the random walk Metropolis with normal proposal to generate posterior samples for continuous parameters and a discretized version for discrete parameters. See the section “[Metropolis and Metropolis-Hastings Algorithms](#)” on page 134 for details about the Metropolis algorithm. For the actual implementation details of the Metropolis algorithm in PROC MCMC, such as tuning of the covariance matrices, see the section “[Tuning the Proposal Distribution](#)” on page 4469.

A key component of the Metropolis algorithm is the calculation of the objective function. In most cases, the objective function that PROC MCMC uses in a Metropolis step is the logarithm of the joint posterior distribution, which is calculated with the inclusion of all data and parameters. The rest of this section describes how PROC MCMC calculates the objective function for parameters that use the Metropolis algorithm.

## Model Parameters

To calculate the log of the posterior density, PROC MCMC assumes that all observations in the data set are independent,

$$\log(p(\theta|\mathbf{y})) = \log(\pi(\theta)) + \sum_{i=1}^n \log(f(y_i|\theta))$$

where  $\theta$  is a parameter or a vector of parameters that are defined in the **PARMS** statements (referred to as the *model parameters*). The term  $\log(\pi(\theta))$  is the sum of the log of the prior densities specified in the **PRIOR** and **HYPERPRIOR** statements. The term  $\log(f(y_i|\theta))$  is the log likelihood specified in the **MODEL** statement. The **MODEL** statement specifies the log likelihood for a single observation in the data set.

If you want to model dependent data—that is,  $\log(f(\mathbf{y}|\theta)) \neq \sum_i \log(f(y_i|\theta))$ —you can use the **JOINT-MODEL** option in the PROC MCMC statement. See the section “**Modeling Joint Likelihood**” on page 4504 for more details.

The statements in PROC MCMC are similar to DATA step statements; PROC MCMC evaluates every statement in order for each observation. At the beginning of the data set, the log likelihood is set to be 0. As PROC MCMC steps through the data set, it cumulatively adds the log likelihood for each observation. Statements between the **BEGINNODATA** and **ENDNODATA** statements are evaluated only at the first and the last observations. At the last observation, the log of the prior and hyperprior distributions is added to the sum of the log likelihood to obtain the log of the posterior distribution.

Calculation of the  $\log(p(\theta|\mathbf{y}))$  objective function involves a complete pass through the data set, making it potentially computationally expensive. If  $\theta = \{\theta_1, \theta_2\}$  is multidimensional, you can choose to update a portion of the parameters at each iteration step by declaring them in separate **PARMS** statements (see the section “**Blocking of Parameters**” on page 4466 for more information). PROC MCMC updates each block of parameters while holding others constant. The objective functions that are used in each update are the same as the log of the joint posterior density:

$$\log(p(\theta_1|\mathbf{y}, \theta_2)) = \log(p(\theta_2|\mathbf{y}, \theta_1)) = \log(p(\theta|\mathbf{y}))$$

In other words, PROC MCMC does not derive the conditional distribution explicitly for each block of parameters, and it uses the full joint distribution in the Metropolis step for every block update.

## Random-Effects Models

For programs that require **RANDOM** statements, PROC MCMC includes the sum of the density evaluation of the random-effects parameters in the calculation of the objective function for  $\theta$ ,

$$\log(p(\theta|\boldsymbol{\gamma}, \mathbf{y})) = \log(\pi(\theta)) + \sum_{j=1}^J \log(\pi(\gamma_j|\theta)) + \sum_{i=1}^n \log(f(y_i|\theta, \boldsymbol{\gamma}))$$

where  $\boldsymbol{\gamma} = \{\gamma_1, \dots, \gamma_J\}$  are random-effects parameters and  $\pi(\gamma_j|\theta)$  is the prior distribution of the random-effects parameters. The likelihood function can be conditional on  $\boldsymbol{\gamma}$ , but the prior distributions of  $\theta$ , which must be independent of  $\boldsymbol{\gamma}$ , cannot.

The objective function used in the Metropolis step for the random-effects parameter  $\gamma_j$  contains only the portion of the data that belong to the  $j$ th cluster:

$$\log(p(\gamma_j|\theta, \mathbf{y})) = \log(\pi(\gamma_j|\theta)) + \sum_{i \in \{j\text{th cluster}\}} \log(f(y_i|\theta, \gamma_j))$$

The calculation does not include  $\log(\theta)$ , the prior density piece, because that is a known constant. Evaluation of this objective function involves only a portion of the data set, making it more computationally efficient. In fact, updating every random-effects parameters in a single **RANDOM** statement involves only one pass through the data set.

You can have multiple **RANDOM** statements in a program, which adds more pieces to the posterior calculation, such as

$$\log(p(\theta|\boldsymbol{\gamma}, \boldsymbol{\alpha}, \mathbf{y})) = \log(\pi(\theta)) + \sum_{j=1}^J \log(\pi(\gamma_j|\theta)) + \sum_{k=1}^K \log(\pi(\alpha_k|\theta)) + \sum_{i=1}^n \log(f(y_i|\theta, \boldsymbol{\gamma}, \boldsymbol{\alpha}))$$

where  $\boldsymbol{\alpha} = \{\alpha_1, \dots, \alpha_K\}$  is another random effect. The random effects  $\boldsymbol{\gamma}$  and  $\boldsymbol{\alpha}$  can form their own hierarchy (as in a nested model), or they can enter the program in a non-nested fashion. The objective functions for  $\gamma_j$  and  $\alpha_k$  are calculated using only observations that belong to their respective clusters.

### Models with Missing Values

Missing values in the response variables of the **MODEL** statement are treated as random variables, and they add another layer in the conditional updates in the simulation. Suppose that

$$\mathbf{y} = \{\mathbf{y}_{\text{obs}}, \mathbf{y}_{\text{mis}}\}$$

The response variable  $\mathbf{y}$  consists of  $n_1$  observed values  $\mathbf{y}_{\text{obs}}$  and  $n_2$  missing values  $\mathbf{y}_{\text{mis}}$ . The log of the posterior distribution is thus formed by

$$\log(p(\theta|\boldsymbol{\gamma}, \mathbf{y}_{\text{mis}}, \mathbf{y}_{\text{obs}})) = \log(\pi(\theta)) + \sum_{j=1}^J \log(\pi(\gamma_j|\theta)) + \sum_{i=1}^{n_2} \log(f(y_{\text{mis},i}|\theta, \boldsymbol{\gamma})) + \sum_{i=1}^{n_1} \log(f(y_{\text{obs},i}|\theta, \boldsymbol{\gamma}))$$

where the expression is evaluated at the drawn  $\boldsymbol{\gamma}$  and  $\mathbf{y}_{\text{obs}}$  values.

The conditional distribution of the random-effects parameter  $\gamma_j$  is

$$\log(p(\gamma_j|\theta, \mathbf{y})) = \log(\pi(\gamma_j|\theta)) + \sum_{i \in \{j\text{th cluster}\}} \log(f(y_i|\theta, \gamma_j))$$

where the  $y_i$  are either the observed or the imputed values of the response variable.

The missing values are usually sampled directly from the sampling distribution and do not require the Metropolis sampler. When a response variable takes on a **GENERAL** function, the objective function is simply the likelihood function:  $\log(f(y_{\text{mis},i}|\theta, \gamma_j))$ .

---

### Blocking of Parameters

In a multivariate parameter model, if all  $k$  parameters are proposed with one joint distribution  $q(\cdot)$ , acceptance or rejection would occur for all of them. This can be rather inefficient, especially when parameters have vastly different scales. A way to avoid this difficulty is to allocate the  $k$  parameters into  $d$  blocks and update them separately. The **PARMS** statement puts model parameters in separate blocks, and each block of parameters is updated sequentially in the procedure.

Suppose you want to sample from a multivariate distribution with probability density function  $p(\theta|\mathbf{y})$  where  $\theta = \{\theta_1, \theta_2, \dots, \theta_k\}$ . Now suppose that these  $k$  parameters are separated into  $d$  blocks—for example,  $p(\theta|\mathbf{x}) = f_d(z)$  where  $z = \{z_1, z_2, \dots, z_d\}$ , where each  $z_j$  contains a nonempty subset of the  $\{\theta_i\}$ , and where each  $\theta_i$  is contained in one and only one  $z_j$ . In the MCMC context, the  $z$ 's are blocks of parameters. In the blocked algorithm, a proposal consists of several parts. Instead of proposing a simultaneous move for all the  $\theta$ 's, a proposal is made for the  $\theta_i$ 's in  $z_1$  only, then for the  $\theta_i$ 's in  $z_2$ , and so on for  $d$  subproposals. Any accepted proposal can involve any number of the blocks moving. The parameters do not necessarily all move at once as in the all-at-once Metropolis algorithm.

Formally, the blocked Metropolis algorithm is as follows. Let  $w_j$  be the collection of  $\theta_i$  that are in block  $z_j$ , and let  $q_j(\cdot|w_j)$  be a symmetric multivariate distribution that is centered at the current values of  $w_j$ .

1. Let  $t = 0$ . Choose points for all  $w_j^t$ . A point can be an arbitrary point as long as  $p(w_j^t|\mathbf{y}) > 0$ .

2. For  $j = 1, \dots, d$ :

a) Generate a new sample,  $w_{j,\text{new}}$ , using the proposal distribution  $q_j(\cdot|w_j^t)$ .

b) Calculate the following quantity:

$$r = \min \left\{ \frac{p(w_{j,\text{new}}|w_1^t, \dots, w_{j-1}^t, w_{j+1}^{t-1}, \dots, w_d^t, \mathbf{y})}{p(w_j^t|w_1^t, \dots, w_{j-1}^t, w_{j-1}^{t+1}, \dots, w_d^t, \mathbf{y})}, 1 \right\}.$$

c) Sample  $u$  from the uniform distribution  $U(0, 1)$ .

d) Set  $w_j^{t+1} = w_{j,\text{new}}$  if  $r < u$ ;  $w_j^{t+1} = w_j^t$  otherwise.

3. Set  $t = t + 1$ . If  $t < T$ , the number of desired samples, go back to Step 2; otherwise, stop.

With PROC MCMC, you can sample all parameters simultaneously by putting them all in a single PARMS statement, you can sample parameters individually by putting each parameter in its own PARMS statement, or you can sample certain subsets of parameters together by grouping each subset in its own PARMS statements. For example, if the model you are interested in has five parameters, alpha, beta, gamma, phi, sigma, the all-at-once strategy is as follows:

```
parms alpha beta gamma phi sigma;
```

The one-at-a-time strategy is as follows:

```
parms alpha;
parms beta;
parms gamma;
parms phi;
parms sigma;
```

A two-block strategy could be as follows:

```
parms alpha beta gamma;
parms phi sigma;
```

The exceptions to the previously described blocking strategies are parameters that are sampled directly (either from their full conditional or marginal distributions) and parameters that are array-based (with multivariate prior distributions). In these cases, the parameters are taken out of an existing block and are updated individually. You can use the sampling options in the **PARMS** statement to override the default behavior.

One of the greatest challenges in MCMC sampling is achieving good mixing of the chains—the chains should quickly traverse the support of the stationary distribution. A number of factors determine the behavior of a Metropolis sampler; blocking is one of them, so you want to be extremely careful when you choose a good design. Generally speaking, forming blocks of parameters has its advantages, but it is not true that the larger the block the faster the convergence.

When simultaneously sampling a large number of parameters, the algorithm might find it difficult to achieve good mixing. As the number of parameters gets large, it is much more likely to have (proposal) samples that fall well into the tails of the target distribution, producing too small a test ratio. As a result, few proposed values are accepted and convergence is slow. On the other hand, when the algorithm samples each parameter individually, the computational cost increases linearly. Each block of Metropolis parameters requires one additional pass through the data set, so a five-block updating strategy could take five times longer than a single-block updating strategy. In addition, there is a chance that the chain might mix far too slowly because the conditional distributions (of  $\theta_i$  given all other  $\theta$ 's) might be very “narrow,” as a result of posterior correlation among the parameters. When that happens, it takes a long time for the chain to fully explore that dimension alone. There are no theoretical results that can help determine an optimal “blocking” for an arbitrary parametric model. A rule followed in practice is to form small groups of correlated parameters that belong to the same context in the formulation of the model. The best mixing is usually obtained with a blocking strategy somewhere between the all-at-once and one-at-a-time strategies.

---

## Sampling Methods

When suitable, PROC MCMC chooses the optimal sampling method for each parameter. That involves direct sampling either from the conditional posterior via conjugacy (see the section “[Conjugate Sampling](#)” on page 4472) or via the marginal posterior (see the section “[Direct Sampling](#)” on page 4472). Alternatively, PROC MCMC samples according to [Table 55.5](#). Each block of parameters is classified by the nature of the prior distributions. “Continuous” means all priors of the parameters in the same block have a continuous distribution. “Discrete” means all priors are discrete. “Mixed” means that some parameters are continuous and others are discrete. Parameters that have binary priors are treated differently, as indicated in the table.

**Table 55.5** Sampling Methods in PROC MCMC

| <b>Blocks</b>                | <b>Default Method</b>     | <b>Alternative Method</b>             |
|------------------------------|---------------------------|---------------------------------------|
| Continuous                   | Multivariate normal (MVN) | Multivariate $t$ (MVT); slice sampler |
| Discrete (other than binary) | Binned MVN                | Binned MVT or symmetric geometric     |
| Mixed                        | MVN                       | MVT                                   |
| Binary (single dimensional)  | Inverse CDF               |                                       |
| Binary (multidimensional)    | Independence sampler      |                                       |

For a block of continuous parameters, PROC MCMC uses a multivariate normal distribution as the default proposal distribution. In the tuning phase, PROC MCMC finds an optimal scale  $c$  and a tuning covariance matrix  $\Sigma$ .



For a discrete block of parameters, PROC MCMC uses a discretized multivariate normal distribution as the default proposal distribution. The scale  $c$  and covariance matrix  $\Sigma$  are tuned. Alternatively, you can use an independent symmetric geometric proposal distribution. The density has form  $\frac{p(1-p)^{|\theta|}}{2(1-p)}$  and has variance  $\frac{(2-p)(1-p)}{p^2}$ . In the tuning phase, the procedure finds an optimal proposal probability  $p$  for every parameter in the block.

You can change the proposal distribution, from the normal to a  $t$  distribution. You can either use the PROC option `PROPDIST=T(df)` or `PARMS` statement option `</ T(df)>` to make the change. The  $t$  distributions have thicker tails, and they can propose to the tail areas more efficiently than the normal distribution. It can help with the mixing of the Markov chain if some of the parameters have a skewed tails. See “[Example 55.6: Nonlinear Poisson Regression Models](#)” on page 4570. The independence sampler (see the section “[Independence Sampler](#)” on page 137) is used for a block of binary parameters. The inverse CDF method is used for a block that consists of a single binary parameter.

For parameters with continuous prior distributions, you can use the slice sampler as an alternative sampling algorithm. To do so, specify the `SLICE` option in the `PARMS`. When you specify the `SLICE` option, all parameters are updated individually. PROC MCMC does not support a multivariate version of the slice sampler. For more in information about the slice sampler, see the section “[Slice Sampler](#)” on page 136.

The sampling algorithms for the random-effects parameters are chosen in a similar fashion. The preferred algorithms are the direct method either from the full conditional or the marginal. When these are not attainable, Metropolis with normal proposal becomes the default for continuous random-effects parameters, and discrete Metropolis with normal proposal becomes the default for discrete random-effects parameters. You can use the `ALGORITHM=` option in the `RANDOM` statement to choose the slice sampler or discrete Metropolis with symmetric geometric as the alternatives.

The sampling preference of the missing data variables is the same as the random-effects parameters. The reserve sampling algorithm is the Metropolis. There is no alternative sampling method available for the missing data variables.

---

## Tuning the Proposal Distribution

One key factor in achieving high efficiency of a Metropolis-based Markov chain is finding a good proposal distribution for each block of parameters. This process is referred to as tuning. The tuning phase consists of a number of loops. The minimum number of loops is controlled by the option `MINTUNE=`, with a default value of 2. The option `MAXTUNE=` controls the maximum number of tuning loops, with a default value of 24. Each loop lasts for `NTU=` iterations, where by default `NTU=` 500. At the end of every loop, PROC MCMC examines the acceptance probability for each block. The acceptance probability is the percentage of `NTU=` proposals that have been accepted. If the probability falls within the acceptance tolerance range (see the section “[Scale Tuning](#)” on page 4470), the current configuration of  $c/\Sigma$  or  $p$  is kept. Otherwise, these parameters are modified before the next tuning loop.

### Continuous Distribution: Normal or $t$ Distribution

A good proposal distribution should resemble the actual posterior distribution of the parameters. Large sample theory states that the posterior distribution of the parameters approaches a multivariate normal distribution (see Gelman et al. 2004, Appendix B, and Schervish 1995, Section 7.4). That is why a normal proposal distribution often works well in practice. The default proposal distribution in PROC MCMC is



the normal distribution:  $q_j(\theta_{\text{new}}|\theta^t) = \text{MVN}(\theta_{\text{new}}|\theta^t, c^2\Sigma)$ . As an alternative, you can choose a multivariate  $t$  distribution as the proposal distribution. It is a good distribution to use if you think that the posterior distribution has thick tails and a  $t$  distribution can improve the mixing of the Markov chain. See “Example 55.6: Nonlinear Poisson Regression Models” on page 4570.

### Scale Tuning

The acceptance rate is closely related to the sampling efficiency of a Metropolis chain. For a random walk Metropolis, high acceptance rate means that most new samples occur right around the current data point. Their frequent acceptance means that the Markov chain is moving rather slowly and not exploring the parameter space fully. On the other hand, a low acceptance rate means that the proposed samples are often rejected; hence the chain is not moving much. An efficient Metropolis sampler has an acceptance rate that is neither too high nor too low. The scale  $c$  in the proposal distribution  $q(\cdot|\cdot)$  effectively controls this acceptance probability. Roberts, Gelman, and Gilks (1997) showed that if both the target and proposal densities are normal, the optimal acceptance probability for the Markov chain should be around 0.45 in a single dimensional problem, and asymptotically approaches 0.234 in higher dimensions. The corresponding optimal scale is 2.38, which is the initial scale set for each block.

Due to the nature of stochastic simulations, it is impossible to fine-tune a set of variables such that the Metropolis chain has the exact desired acceptance rate. In addition, Roberts and Rosenthal (2001) empirically demonstrated that an acceptance rate between 0.15 and 0.5 is at least 80% efficient, so there is really no need to fine-tune the algorithms to reach acceptance probability that is within small tolerance of the optimal values. PROC MCMC works with a probability range, determined by the PROC options `TARGACCEPT ± ACCEPTTOL`. The default value of `TARGACCEPT` is a function of the number of parameters in the model, as outlined in Roberts, Gelman, and Gilks (1997). The default value of `ACCEPTTOL` is 0.075. If the observed acceptance rate in a given tuning loop is less than the lower bound of the range, the scale is reduced; if the observed acceptance rate is greater than the upper bound of the range, the scale is increased. During the tuning phase, a scale parameter in the normal distribution is adjusted as a function of the observed acceptance rate and the target acceptance rate. The following updating scheme is used in PROC MCMC<sup>2</sup>:

$$c_{\text{new}} = \frac{c_{\text{cur}} \cdot \Phi^{-1}(p_{\text{opt}}/2)}{\Phi^{-1}(p_{\text{cur}}/2)}$$

where  $c_{\text{cur}}$  is the current scale,  $p_{\text{cur}}$  is the current acceptance rate,  $p_{\text{opt}}$  is the optimal acceptance probability.

### Covariance Tuning

To tune a covariance matrix, PROC MCMC takes a weighted average of the old proposal covariance matrix and the recent observed covariance matrix, based on `NTU` samples in the current loop. The `TUNEWT=w` option determines how much weight is put on the recently observed covariance matrix. The formula used to update the covariance matrix is as follows:

$$\text{COV}_{\text{new}} = w \text{COV}_{\text{cur}} + (1 - w)\text{COV}_{\text{old}}$$

There are two ways to initialize the covariance matrix:

<sup>2</sup> Roberts, Gelman, and Gilks (1997) and Roberts and Rosenthal (2001) demonstrate that the relationship between acceptance probability and scale in a random walk Metropolis is  $p = 2\Phi(-\sqrt{I}c/2)$ , where  $c$  is the scale,  $p$  is the acceptance rate,  $\Phi$  is the CDF of a standard normal, and  $I \equiv E_f[(f'(x)/f(x))^2]$ ,  $f(x)$  is the density function of samples. This relationship determines the updating scheme, with  $I$  being replaced by the identity matrix to simplify calculation.

- The default is an identity matrix multiplied by the initial scale of 2.38 (controlled by the PROC option `SCALE=`) and divided by the square root of the number of estimated parameters in the model. It can take a number of tuning phases before the proposal distribution is tuned to its optimal stage, since the Markov chain needs to spend time learning about the posterior covariance structure. If the posterior variances of your parameters vary by more than a few orders of magnitude, if the variances of your parameters are much different from 1, or if the posterior correlations are high, then the proposal tuning algorithm might have difficulty with forming an acceptable proposal distribution.
- Alternatively, you can use a numerical optimization routine, such as the quasi-Newton method, to find a starting covariance matrix. The optimization is performed on the joint posterior distribution, and the covariance matrix is a quadratic approximation at the posterior mode. In some cases this is a better and more efficient way of initializing the covariance matrix. However, there are cases, such as when the number of parameters is large, where the optimization could fail to find a matrix that is positive definite. In that case, the tuning covariance matrix is reset to the identity matrix.

A side product of the optimization routine is that it also finds the *maximum a posteriori* (MAP) estimates with respect to the posterior distribution. The MAP estimates are used as the initial values of the Markov chain.

If any of the parameters are discrete, then the optimization is performed conditional on these discrete parameters at their respective fixed initial values. On the other hand, if all parameters are continuous, you can in some cases skip the tuning phase (by setting `MAXTUNE=0`) or the burn-in phase (by setting `NBI=0`).

### Discrete Distribution: Symmetric Geometric

By default, PROC MCMC uses the normal density as the proposal distribution in all Metropolis random walks. For parameters that have discrete prior distributions, PROC MCMC discretizes proposed samples. You can choose an alternative symmetric geometric proposal distribution by specifying the option `DIS-CRETE=GEO`.

The density of the symmetric geometric proposal distribution is as follows:

$$\frac{p_g(1-p_g)^{|\theta|}}{2(1-p_g)}$$

where the symmetry centers at  $\theta$ . The distribution has a variance of

$$\sigma^2 = \frac{(2-p_g)(1-p_g)}{p_g^2}$$

Tuning for the proposal  $p_g$  uses the following formula:

$$\frac{\sigma_{\text{new}}}{\sigma_{\text{cur}}} = \frac{\Phi^{-1}(p_{\text{opt}}/2)}{\Phi^{-1}(p_{\text{cur}}/2)}$$

where  $\sigma_{\text{new}}$  is the standard deviation of the new proposal geometric distribution,  $\sigma_{\text{cur}}$  is the standard deviation of the current proposal distribution,  $p_{\text{opt}}$  is the target acceptance probability, and  $p_{\text{cur}}$  is the current acceptance probability for the discrete parameter block.

The updated  $p_g$  is the solution to the following equation that is between 0 and 1 :

$$\sqrt{\frac{(2-p_g)(1-p_g)}{p_g^2}} = \frac{\sigma_{\text{cur}} \cdot \Phi^{-1}(p_{\text{opt}}/2)}{\Phi^{-1}(p_{\text{cur}}/2)}$$

## Binary Distribution: Independence Sampler

Blocks consisting of a single parameter with a binary prior do not require any tuning; the inverse-CDF method applies. Blocks that consist of multiple parameters with binary prior are sampled by using an independence sampler with binary proposal distributions. See the section “[Independence Sampler](#)” on page 137. During the tuning phase, the success probability  $p$  of the proposal distribution is taken to be the probability of acceptance in the current loop. Ideally, an independence sampler works best if the acceptance rate is 100%, but that is rarely achieved. The algorithm stops when the probability of success exceeds the `TARGACCEPTI=value`, which has a default value of 0.6.

## Direct Sampling

The word “direct” is reserved for sampling that is done directly from the prior distribution of a model or a random-effects parameter or from the sampling distribution of a missing data variable. If the parameter is updated via sampling from its full conditional posterior distribution, the sampling method is referred to as conjugate sampling. (See the section “[Conjugate Sampling](#)” on page 4472.)

Whenever a parameter does not appear in the hierarchy of another parameter in the model, PROC MCMC samples directly from its distribution. For a model parameter or a random-effects parameter, this distribution is its prior distribution. For a missing data variable, this distribution is the sampling distribution of the response variable. Therefore, direct sampling takes place most frequently in data-independent Monte Carlo simulations or the sampling of missing response variables.

## Conjugate Sampling

Conjugate prior is a family of prior distributions in which the prior and the posterior distributions are of the same family of distributions. For example, if you model an independently and identically distributed random variable  $y_i$  using a normal likelihood with known variance  $\sigma^2$ ,

$$y_i \sim \text{normal}(\mu, \sigma^2)$$

a normal prior on  $\mu$

$$\mu \sim \text{normal}(\mu_0, \sigma_0^2)$$

is a conjugate prior because the posterior distribution of  $\mu$  is also a normal distribution given  $y = \{y_i\}$ ,  $\sigma^2$ ,  $\mu_0$ , and  $\sigma_0^2$ :

$$\mu|y \sim \text{normal} \left( \left( \frac{1}{\sigma_0^2} + \frac{n}{\sigma^2} \right)^{-1} \cdot \left( \frac{\mu_0}{\sigma_0^2} + \frac{n \cdot \bar{y}}{\sigma^2} \right), \left( \frac{1}{\sigma_0^2} + \frac{n}{\sigma^2} \right)^{-1} \right)$$

Conjugate sampling is efficient because it enables the Markov chain to obtain samples from the target distribution directly. When appropriate, PROC MCMC uses conjugate sampling methods to draw conditional posterior samples. [Table 55.6](#) lists scenarios that lead to conjugate sampling in PROC MCMC.

**Table 55.6** Conjugate Sampling in PROC MCMC

| Family                                                                  | Parameter               | Prior                |
|-------------------------------------------------------------------------|-------------------------|----------------------|
| Normal with known $\mu$                                                 | Variance $\sigma^2$     | Inverse gamma family |
| Normal with known $\mu$                                                 | Precision $\tau$        | Gamma family         |
| Normal with known scale parameter ( $\sigma^2$ , $\sigma$ , or $\tau$ ) | Mean $\mu$              | Normal               |
| Multivariate normal with known $\Sigma$                                 | Mean $\boldsymbol{\mu}$ | Multivariate normal  |
| Multivariate normal with known $\boldsymbol{\mu}$                       | Covariance $\Sigma$     | Inverse Wishart      |
| Multinomial                                                             | $\mathbf{p}$            | Dirichlet            |
| Binomial/binary                                                         | $p$                     | Beta                 |
| Poisson                                                                 | $\lambda$               | Gamma family         |

In most cases, Family in [Output 55.6](#) refers to the likelihood function. However, it does not necessarily have to be the case. The Family is a distribution that is conditional on the parameter of interest, and it can appear in any level of the hierarchical model, including on the random-effects level.

PROC MCMC can detect conjugacy only if the model parameter (not a function or a transformation of the model parameter) is used in the prior and Family distributions. For example, the following statements lead to a conjugate sampler being used on the parameter mu:

```
parm mu;
prior mu ~ n(0, sd=1000);
model y ~ n(mu, var=s2);
```

However, if you modify the program slightly in the following way, although the conjugacy still holds in theory, PROC MCMC cannot detect conjugacy on mu because the parameter enters the normal likelihood function through the symbol w:

```
parm mu;
prior mu ~ n(0, sd=1000);
w = mu;
model y ~ n(w, var=s2);
```

In this case, PROC MCMC resorts to the default sampling algorithm, which is a random walk Metropolis based on a normal kernel.

Similarly, the following statements also prevent PROC MCMC from detecting conjugacy on the parameter mu:

```
parm mu;
prior mu ~ n(0, sd=1000);
model y ~ n(mu + 2, var=s2);
```

In a normal family, an often-used and often-confused conjugate prior on the variance is the inverse gamma distribution, and a conjugate prior on the precision is the gamma distribution. See “[Gamma and Inverse-Gamma Distributions](#)” on page 4512 for typical usages of these prior distributions.

When conjugacy is detected in a model, PROC MCMC performs a numerical optimization on the joint posterior distribution at the start of the MCMC simulation. If the only sampling methods required in the program are conjugate samplers or direct samplers, PROC MCMC omits this optimization step. To turn off this optimization routine, use the `PROPCOV=IND` option in the PROC MCMC statement.

---

## Initial Values of the Markov Chains

There are three types of parameters in a PROC MCMC program: the *model parameters* in the **PARMS** statement, the *random-effects parameters* in the **RANDOM** statement, and the *missing data variables* in the **MODEL** statement. The last category is used to model missing values in the input data set.

When the model parameters and random-effects parameters have missing initial values, PROC MCMC generates initial values based on the prior distributions. PROC MCMC either uses the mode value (the default) or draws a random number (if the **INIT=****RANDOM** option is specified). For distributions that do not have modes, such as the uniform distribution, PROC MCMC uses the mean instead. In general, PROC MCMC avoids using starting values that are close to the boundary of support of the prior distribution. For example, the exponential prior has a mode at 0, and PROC MCMC starts an initial value at the mean. This avoids some potential numerical problems. If you use the **GENERAL** or **DGENERAL** function in the **PRIOR** statements, you must provide initial values for those parameters.

With missing data variables, PROC MCMC uses the sample average of the nonmissing values (of the response variable) as the initial value. If all values of a particular variable are missing, PROC MCMC resorts to using the mode value or a random number from the sampling distribution (the likelihood), depending on the specification of the **INIT=** option.

To assign a different set of initial values to the model parameters, you use either the **PARMS** statements or programming statements within the **BEGINCNST** and **ENDCNST** statements. See the section “Assignments of Parameters” on page 4474 for more information about how to assign parameter values within the **BEGINCNST** and **ENDCNST** statements.

To assign initial values to the random-effects parameters, you can use the **INIT=** option in the **RANDOM** statement. Either you can give a constant value to all random-effects parameters that are associated with that statement (for example, use **init=3**), or you can assign values individually by providing a data set that stores different values for different parameters.

A mirroring **INIT=** option in the **MODEL** statement enables you to assign different initial values to the missing data variables.

If you use the **PROPCOV=** optimization option in the PROC MCMC statement, PROC MCMC starts the tuning at the optimized values. PROC MCMC overwrites the initial values that you might have provided at the beginning of the Markov chain unless you use the option **INIT=REINIT**.

---

## Assignments of Parameters

In general, you cannot alter the values of any model parameters in PROC MCMC. For example, the following assignment statement produces an error:

```
parms alpha;
alpha = 27;
```

This restriction prevents incorrect calculation of the posterior density—assignments of parameters in the program would override the parameter values generated by PROC MCMC and lead to an incorrect value of the density function.

However, you can modify parameter values and assign initial values to parameters within the block defined by the `BEGINCNST` and `ENDCNST` statements. The following syntax is allowed:

```
parms alpha;
begincnst;
 alpha = 27;
endcnst;
```

The initial value of alpha is 27. Assignments within the `BEGINCNST/ENDCNST` block override initial values specified in the `PARMS` statement. For example, with the following statements, the Markov chain starts at alpha = 27, not 23.

```
parms alpha 23;
begincnst;
 alpha = 27;
endcnst;
```

This feature enables you to systematically assign initial values. Suppose that `z` is an array parameter of the same length as the number of observations in the input data set. You want to start the Markov chain with each  $z_i$  having a different value depending on the data set variable `y`. The following statements set  $z_i = |y|$  for the first half of the observations and  $z_i = 2.3$  for the rest:

```
/* a rather artificial input data set. */
data inputdata;
 do ind = 1 to 10;
 y = rand('normal');
 output;
 end;
run;

proc mcmc data=inputdata;
 array z[10];
 begincnst;
 if ind <= 5 then z[ind] = abs(y);
 else z[ind] = 2.3;
 endcnst;
 parms z;
 prior z: ~ normal(0, sd=1);
 model general(0);
run;
```

Elements of `z` are modified as PROC MCMC executes the programming statements between the `BEGINCNST` and `ENDCNST` statements. This feature could be useful when you use the `GENERAL` function and you find that the `PARMS` statements are too cumbersome for assigning starting values.

## Standard Distributions

The section “Univariate Distributions” on page 4476 (Table 55.7 through Table 55.34) lists all univariate distributions that PROC MCMC recognizes. The section “Multivariate Distributions” on page 4486 (Table 55.35 through Table 55.39) lists all multivariate distributions that PROC MCMC recognizes. With the exception of the multinomial distribution, all these distributions can be used in the MODEL, PRIOR, and HYPERPRIOR statements. The multinomial distribution is supported only in the MODEL statement. The RANDOM statement supports a limited number of distributions; see Table 55.4 for the complete list.

See the section “Using Density Functions in the Programming Statements” on page 4491 for information about how to use distributions in the programming statements. To specify an arbitrary distribution, you can use the GENERAL and DGENERAL functions. See the section “Specifying a New Distribution” on page 4490 for more details. See the section “Truncation and Censoring” on page 4494 for tips about how to work with truncated distributions and censoring data.

## Univariate Distributions

**Table 55.7 Beta Distribution**

|                       |                                                                                                                                                                                                                                                                                                                                           |
|-----------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| PROC specification    | <b>beta</b> ( $a, b$ )                                                                                                                                                                                                                                                                                                                    |
| Density               | $\frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} \theta^{a-1} (1-\theta)^{b-1}$                                                                                                                                                                                                                                                                    |
| Parameter restriction | $a > 0, b > 0$                                                                                                                                                                                                                                                                                                                            |
| Range                 | $\left\{ \begin{array}{ll} [0, 1] & \text{when } a = 1, b = 1 \\ [0, 1) & \text{when } a = 1, b \neq 1 \\ (0, 1] & \text{when } a \neq 1, b = 1 \\ (0, 1) & \text{otherwise} \end{array} \right.$                                                                                                                                         |
| Mean                  | $\frac{a}{a+b}$                                                                                                                                                                                                                                                                                                                           |
| Variance              | $\frac{ab}{(a+b)^2(a+b+1)}$                                                                                                                                                                                                                                                                                                               |
| Mode                  | $\left\{ \begin{array}{ll} \frac{a-1}{a+b-2} & a > 1, b > 1 \\ 0 \text{ and } 1 & a < 1, b < 1 \\ 0 & \left\{ \begin{array}{l} a < 1, b \geq 1 \\ a = 1, b > 1 \end{array} \right. \\ 1 & \left\{ \begin{array}{l} a \geq 1, b < 1 \\ a > 1, b = 1 \end{array} \right. \\ \text{does not exist uniquely} & a = b = 1 \end{array} \right.$ |
| Random number         | If $\min(a, b) > 1$ , see (Cheng 1978); if $\max(a, b) < 1$ , see (Atkinson and Whittaker 1976) and (Atkinson 1979); if $\min(a, b) < 1$ and $\max(a, b) > 1$ , see (Cheng 1978); if $a = 1$ or $b = 1$ , use the inversion method; if $a = b = 1$ , use a uniform random number generator.                                               |

**Table 55.8 Binary Distribution**

|                       |                                                                                                                     |
|-----------------------|---------------------------------------------------------------------------------------------------------------------|
| PROC specification    | <b>binary</b> ( $p$ )                                                                                               |
| Density               | $p^\theta(1-p)^{1-\theta}$                                                                                          |
| Parameter restriction | $0 \leq p \leq 1$                                                                                                   |
| Range                 | $\begin{cases} \{0\} & \text{when } p = 0 \\ \{1\} & \text{when } p = 1 \\ \{0, 1\} & \text{otherwise} \end{cases}$ |
| Mean                  | $\text{round}(p)$                                                                                                   |
| Variance              | $p(1-p)$                                                                                                            |
| Mode                  | $\begin{cases} \{1\} & \text{when } p = 1 \\ \{0\} & \text{otherwise} \end{cases}$                                  |
| Random number         | Generate $u \sim \text{uniform}(0, 1)$ . If $u \leq p$ , $\theta = 1$ ; else, $\theta = 0$ .                        |

**Table 55.9 Binomial Distribution**

|                       |                                               |
|-----------------------|-----------------------------------------------|
| PROC specification    | <b>binomial</b> ( $n, p$ )                    |
| Density               | $\binom{n}{\theta} p^\theta (1-p)^{n-\theta}$ |
| Parameter restriction | $n = 0, 1, 2, \dots, 0 \leq p \leq 1$         |
| Range                 | $\theta \in \{0, \dots, n\}$                  |
| Mean                  | $\lfloor np \rfloor$                          |
| Variance              | $np(1-p)$                                     |
| Mode                  | $\lfloor (n+1)p \rfloor$                      |

**Table 55.10 Cauchy Distribution**

|                       |                                                                                                                                                                                                          |
|-----------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| PROC specification    | <b>cauchy</b> ( $a, b$ )                                                                                                                                                                                 |
| Density               | $\frac{1}{\pi} \left( \frac{b}{b^2 + (\theta - a)^2} \right)$                                                                                                                                            |
| Parameter restriction | $b > 0$                                                                                                                                                                                                  |
| Range                 | $\theta \in (-\infty, \infty)$                                                                                                                                                                           |
| Mean                  | Does not exist.                                                                                                                                                                                          |
| Variance              | Does not exist.                                                                                                                                                                                          |
| Mode                  | $a$                                                                                                                                                                                                      |
| Random number         | Generate $u_1, u_2 \sim \text{uniform}(0, 1)$ ; let $v = 2u_2 - 1$ . Repeat the procedure until $u_1^2 + v^2 < 1$ . $y = v/u_1$ is a draw from the standard Cauchy, and $\theta = a + by$ (Ripley 1987). |



**Table 55.11**  $\chi^2$  Distribution

|                       |                                                                                                                                                   |
|-----------------------|---------------------------------------------------------------------------------------------------------------------------------------------------|
| PROC specification    | <b>chisq</b> ( $\nu$ )                                                                                                                            |
| Density               | $\frac{1}{\Gamma(\nu/2)2^{\nu/2}} \theta^{(\nu/2)-1} e^{-\theta/2}$                                                                               |
| Parameter restriction | $\nu > 0$                                                                                                                                         |
| Range                 | $\theta \in [0, \infty)$ if $\nu = 2$ ; $(0, \infty)$ otherwise.                                                                                  |
| Mean                  | $\nu$                                                                                                                                             |
| Variance              | $2\nu$                                                                                                                                            |
| Mode                  | $\nu - 2$ if $\nu \geq 2$ ; does not exist otherwise.                                                                                             |
| Random number         | $\chi^2$ is a special case of the gamma distribution: $\theta \sim \text{gamma}(\nu/2, \text{scale}=2)$ is a draw from the $\chi^2$ distribution. |

**Table 55.12** Exponential  $\chi^2$  Distribution

|                                           |                                                                                                                  |
|-------------------------------------------|------------------------------------------------------------------------------------------------------------------|
| PROC specification                        | <b>expchisq</b> ( $\nu$ )                                                                                        |
| Density                                   | $\frac{1}{\Gamma(\nu/2)2^{\nu/2}} \exp(\theta)^{\nu/2} \exp(-\exp(\theta)/2)$                                    |
| Parameter restriction                     | $\nu > 0$                                                                                                        |
| Range                                     | $\theta \in (-\infty, \infty)$                                                                                   |
| Mode                                      | $\log(\nu)$                                                                                                      |
| Random number                             | Generate $x_1 \sim \chi^2(\nu)$ , and $\theta = \log(x_1)$ is a draw from the exponential $\chi^2$ distribution. |
| Relationship to the $\chi^2$ distribution | $\theta \sim \chi^2(\nu) \Leftrightarrow \log(\theta) \sim \text{exp } \chi^2(\nu)$                              |

**Table 55.13** Exponential Exponential Distribution

|                                              |                                                                                                                                                                                                                                                |                                                      |
|----------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------|
| PROC specification                           | <b>expexpon</b> (scale = $b$ )                                                                                                                                                                                                                 | <b>expexpon</b> (iscale = $\beta$ )                  |
| Density                                      | $\frac{1}{b} \exp(\theta) \exp(-\exp(\theta)/b)$                                                                                                                                                                                               | $\beta \exp(\theta) \exp(-\exp(\theta) \cdot \beta)$ |
| Parameter restriction                        | $b > 0$                                                                                                                                                                                                                                        | $\beta > 0$                                          |
| Range                                        | $\theta \in (-\infty, \infty)$                                                                                                                                                                                                                 | Same                                                 |
| Mode                                         | $\log(b)$                                                                                                                                                                                                                                      | $\log(1/\beta)$                                      |
| Random number                                | Generate $x_1 \sim \text{expon}(\text{scale}=b)$ , and $\theta = \log(x_1)$ is a draw from the exponential exponential distribution. Note that an exponential exponential distribution is not the same as the double exponential distribution. |                                                      |
| Relationship to the exponential distribution | $\theta \sim \text{expon}(b) \Leftrightarrow \log(\theta) \sim \text{expExpon}(b)$                                                                                                                                                             |                                                      |

**Table 55.14 Exponential Gamma Distribution**

|                                           |                                                                                                                                     |                                                                     |
|-------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------|
| PROC specification                        | <b>expgamma</b> ( $a$ , scale = $b$ )                                                                                               | <b>expgamma</b> ( $a$ , iscale = $\beta$ )                          |
| Density                                   | $\frac{1}{b^a \Gamma(a)} e^{a\theta} \exp(-e^\theta/b)$                                                                             | $\frac{\beta^a}{\Gamma(a)} e^{a\theta} \exp(-e^\theta \cdot \beta)$ |
| Parameter restriction                     | $a > 0, b > 0$                                                                                                                      | $a > 0, \beta > 0$                                                  |
| Range                                     | $\theta \in (-\infty, \infty)$                                                                                                      | Same                                                                |
| Mode                                      | $\log(ab)$                                                                                                                          | $\log(a/\beta)$                                                     |
| Random number                             | Generate $x_1 \sim \text{gamma}(a, \text{scale} = b)$ , and $\theta = \log(x_1)$ is a draw from the exponential gamma distribution. |                                                                     |
| Relationship to the $\Gamma$ distribution | $\theta \sim \text{gamma}(a, b) \Leftrightarrow \log(\theta) \sim \text{expGamma}(a, b)$                                            |                                                                     |

**Table 55.15 Exponential Inverse  $\chi^2$  Distribution**

|                                            |                                                                                                                           |
|--------------------------------------------|---------------------------------------------------------------------------------------------------------------------------|
| PROC specification                         | <b>expichisq</b> ( $\nu$ )                                                                                                |
| Density                                    | $\frac{1}{\Gamma(\frac{\nu}{2}) 2^{\nu/2}} \exp(-\nu\theta/2) \exp(-1/(2 \exp(\theta)))$                                  |
| Parameter restriction                      | $\nu > 0$                                                                                                                 |
| Range                                      | $\theta \in (-\infty, \infty)$                                                                                            |
| Mode                                       | $-\log(\nu)$                                                                                                              |
| Random number                              | Generate $x_1 \sim i\chi^2(\nu)$ , and $\theta = \log(x_1)$ is a draw from the exponential inverse $\chi^2$ distribution. |
| Relationship to the $i\chi^2$ distribution | $\theta \sim i\chi^2(\nu) \Leftrightarrow \log(\theta) \sim \text{exp}i\chi^2(\nu)$                                       |

**Table 55.16 Exponential Inverse-Gamma Distribution**

|                                            |                                                                                                                                              |                                                                                       |
|--------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| PROC specification                         | <b>expigamma</b> ( $a$ , scale = $b$ )                                                                                                       | <b>expigamma</b> ( $a$ , iscale = $\beta$ )                                           |
| Density                                    | $\frac{b^a}{\Gamma(a)} \exp(-\alpha\theta) \exp(-b/\exp(\theta))$                                                                            | $\frac{1}{\beta^a \Gamma(a)} \exp(-\alpha\theta) \exp(-\frac{1}{\beta \exp(\theta)})$ |
| Parameter restriction                      | $a > 0, b > 0$                                                                                                                               | $a > 0, \beta > 0$                                                                    |
| Range                                      | $\theta \in (-\infty, \infty)$                                                                                                               | Same                                                                                  |
| Mode                                       | $-\log(a/b)$                                                                                                                                 | $-\log(a\beta)$                                                                       |
| Random number                              | Generate $x_1 \sim \text{igamma}(a, \text{scale} = b)$ , and $\theta = \log(x_1)$ is a draw from the exponential inverse-gamma distribution. |                                                                                       |
| Relationship to the $i\Gamma$ distribution | $\theta \sim \text{igamma}(a, b) \Leftrightarrow \log(\theta) \sim \text{eigamma}(a, b)$                                                     |                                                                                       |

**Table 55.17 Exponential Scaled Inverse  $\chi^2$  Distribution**

|                                             |                                                                                                                                      |
|---------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------|
| PROC specification                          | <b>expsichisq</b> ( $\nu, s$ )                                                                                                       |
| Density                                     | $\frac{(\frac{\nu}{2})^{\nu/2}}{\Gamma(\frac{\nu}{2})} s^\nu \exp(-\nu\theta/2) \exp(-\nu s^2/(2 \exp(\theta)))$                     |
| Parameter restriction                       | $\nu > 0, s > 0$                                                                                                                     |
| Range                                       | $\theta \in (-\infty, \infty)$                                                                                                       |
| Mode                                        | $\log(s^2)$                                                                                                                          |
| Random number                               | Generate $x_1 \sim si\chi^2(\nu, s)$ , and $\theta = \log(x_1)$ is a draw from the exponential scaled inverse $\chi^2$ distribution. |
| Relationship to the $si\chi^2$ distribution | $\theta \sim si\chi^2(\nu, s) \Leftrightarrow \log(\theta) \sim \text{exp } si\chi^2(\nu, s)$                                        |

**Table 55.18 Exponential Distribution**

|                       |                                                                                                                                                                        |                                  |
|-----------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------|
| PROC specification    | <b>expon</b> (scale = $b$ )                                                                                                                                            | <b>expon</b> (iscale = $\beta$ ) |
| Density               | $\frac{1}{b} e^{-\theta/b}$                                                                                                                                            | $\beta e^{-\beta\theta}$         |
| Parameter restriction | $b > 0$                                                                                                                                                                | $\beta > 0$                      |
| Range                 | $\theta \in [0, \infty)$                                                                                                                                               | Same                             |
| Mean                  | $b$                                                                                                                                                                    | $1/\beta$                        |
| Variance              | $b^2$                                                                                                                                                                  | $1/\beta^2$                      |
| Mode                  | 0                                                                                                                                                                      | 0                                |
| Random number         | The exponential distribution is a special case of the gamma distribution: $\theta \sim \text{gamma}(1, \text{scale} = b)$ is a draw from the exponential distribution. |                                  |

**Table 55.19 Gamma Distribution**

|                       |                                                                |                                                           |
|-----------------------|----------------------------------------------------------------|-----------------------------------------------------------|
| PROC specification    | <b>gamma</b> ( $a, \text{scale} = b$ )                         | <b>gamma</b> ( $a, \text{iscale} = \beta$ )               |
| Density               | $\frac{1}{b^a \Gamma(a)} \theta^{a-1} e^{-\theta/b}$           | $\frac{\beta^a}{\Gamma(a)} \theta^{a-1} e^{-\beta\theta}$ |
| Parameter restriction | $a > 0, b > 0$                                                 | $a > 0, \beta > 0$                                        |
| Range                 | $\theta \in [0, \infty)$ if $a = 1$ ; $(0, \infty)$ otherwise. | Same                                                      |
| Mean                  | $ab$                                                           | $a/\beta$                                                 |
| Variance              | $ab^2$                                                         | $a/\beta^2$                                               |
| Mode                  | $(a-1)b$ if $a \geq 1$                                         | $(a-1)/\beta$ if $a \geq 1$                               |
| Random number         | See (McGrath and Irving 1973).                                 |                                                           |

**Table 55.20 Geometric Distribution**

|                       |                                                                                                       |
|-----------------------|-------------------------------------------------------------------------------------------------------|
| PROC specification    | <b>geo</b> ( $p$ )                                                                                    |
| Density <sup>3</sup>  | $p(1-p)^\theta$                                                                                       |
| Parameter restriction | $0 < p \leq 1$                                                                                        |
| Range                 | $\theta \in \begin{cases} \{0, 1, 2, \dots\} & 0 < p < 1 \\ \{0\} & p = 1 \end{cases}$                |
| Mean                  | $\text{round}(\frac{1-p}{p})$                                                                         |
| Variance              | $\frac{1-p}{p^2}$                                                                                     |
| Mode                  | 0                                                                                                     |
| Random number         | Based on samples obtained from a Bernoulli distribution with probability $p$ until the first success. |

**Table 55.21 Inverse  $\chi^2$  Distribution**

|                       |                                                                                                                                                                               |
|-----------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| PROC specification    | <b>ichisq</b> ( $\nu$ )                                                                                                                                                       |
| Density               | $\frac{1}{\Gamma(\nu/2)2^{\nu/2}} \theta^{-(\nu/2+1)} e^{-1/(2\theta)}$                                                                                                       |
| Parameter restriction | $\nu > 0$                                                                                                                                                                     |
| Range                 | $\theta \in (0, \infty)$                                                                                                                                                      |
| Mean                  | $\frac{1}{\nu-2}$ if $\nu > 2$                                                                                                                                                |
| Variance              | $\frac{2}{(\nu-2)^2(\nu-4)}$ if $\nu > 4$                                                                                                                                     |
| Mode                  | $\frac{1}{\nu+2}$                                                                                                                                                             |
| Random number         | Inverse $\chi^2$ is a special case of the inverse-gamma distribution: $\theta \sim \text{igamma}(\nu/2, \text{iscale} = 2)$ is a draw from the inverse $\chi^2$ distribution. |

**Table 55.22 Inverse-Gamma Distribution**

|                       |                                                                                                                                                     |                                                                  |
|-----------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------|
| PROC specification    | <b>igamma</b> ( $a, \text{scale} = b$ )                                                                                                             | <b>igamma</b> ( $a, \text{iscale} = \beta$ )                     |
| Density               | $\frac{b^a}{\Gamma(a)} \theta^{-(a+1)} e^{-b/\theta}$                                                                                               | $\frac{1}{\beta^a \Gamma(a)} \theta^{-(a+1)} e^{-1/\beta\theta}$ |
| Parameter restriction | $a > 0, b > 0$                                                                                                                                      | $a > 0, \beta > 0$                                               |
| Range                 | $\theta \in (0, \infty)$                                                                                                                            | Same                                                             |
| Mean                  | $\frac{b}{a-1}$ if $a > 1$                                                                                                                          | $\frac{1}{\beta(a-1)}$ if $a > 1$                                |
| Variance              | $\frac{b^2}{(a-1)^2(a-2)}$                                                                                                                          | $\frac{1}{\beta^2(a-1)^2(a-2)}$                                  |
| Mode                  | $\frac{b}{a+1}$                                                                                                                                     | $\frac{1}{\beta(a+1)}$                                           |
| Random number         | Generate $x_1 \sim \text{gamma}(a, \text{scale} = b)$ , and $\theta = 1/x_1$ is a draw from the $\text{igamma}(a, \text{iscale} = b)$ distribution. |                                                                  |

<sup>3</sup>The random variable  $\theta$  is the total number of failures in an experiment *before* the first success. This density function is not to be confused with another popular formulation,  $p(1-p)^{\theta-1}$ , which counts the total number of trials *until* the first success.

Relationship to the gamma distribution  $\theta \sim \text{gamma}(a, \text{iscale} = b) \Leftrightarrow 1/\theta \sim \text{igamma}(a, \text{scale} = b)$

**Table 55.23 Laplace (Double Exponential) Distribution**

|                       |                                                                                                                                                                                                                                                                                                                                                                                   |                                               |
|-----------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------|
| PROC specification    | <b>laplace</b> ( $a, \text{scale} = b$ )                                                                                                                                                                                                                                                                                                                                          | <b>laplace</b> ( $a, \text{iscale} = \beta$ ) |
| Density               | $\frac{1}{2b} e^{- \theta-a /b}$                                                                                                                                                                                                                                                                                                                                                  | $\frac{\beta}{2} e^{-\beta \theta-a }$        |
| Parameter restriction | $b > 0$                                                                                                                                                                                                                                                                                                                                                                           | $\beta > 0$                                   |
| Range                 | $\theta \in (-\infty, \infty)$                                                                                                                                                                                                                                                                                                                                                    | Same                                          |
| Mean                  | $a$                                                                                                                                                                                                                                                                                                                                                                               | $a$                                           |
| Variance              | $2b^2$                                                                                                                                                                                                                                                                                                                                                                            | $2/\beta^2$                                   |
| Mode                  | $a$                                                                                                                                                                                                                                                                                                                                                                               | $a$                                           |
| Random number         | Inverse CDF. $F(\theta) = \begin{cases} \frac{1}{2} \exp\left(-\frac{a-\theta}{b}\right) & \theta < a \\ 1 - \frac{1}{2} \exp\left(-\frac{\theta-a}{b}\right) & \theta \geq a \end{cases}$ .<br>Generate $u_1, u_2 \sim \text{uniform}(0, 1)$ . If $u_1 < 0.5$ , $\theta = a + b \log(u_2)$ ; else $\theta = a - b \log(u_2)$ . $\theta$ is a draw from the Laplace distribution. |                                               |

**Table 55.24 Logistic Distribution**

|                       |                                                                                                                                                                                                                          |
|-----------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| PROC specification    | <b>logistic</b> ( $a, b$ )                                                                                                                                                                                               |
| Density               | $\frac{\exp\left(-\frac{\theta-a}{b}\right)}{b(1+\exp\left(-\frac{\theta-a}{b}\right))^2}$                                                                                                                               |
| Parameter restriction | $b > 0$                                                                                                                                                                                                                  |
| Range                 | $\theta \in (-\infty, \infty)$                                                                                                                                                                                           |
| Mean                  | $a$                                                                                                                                                                                                                      |
| Variance              | $\frac{\pi^2 b^2}{3}$                                                                                                                                                                                                    |
| Mode                  | $a$                                                                                                                                                                                                                      |
| Random number         | Inverse CDF method with $F(\theta) = \left(1 + \exp\left(-\frac{\theta-a}{b}\right)\right)^{-1}$ . Generate $u \sim \text{uniform}(0, 1)$ , and $\theta = a - b \log(1/u - 1)$ is a draw from the logistic distribution. |

**Table 55.25 Lognormal Distribution**

|                       |                                                                                       |                                                                                     |                                                                                                   |
|-----------------------|---------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------|
| PROC specification    | <b>lognormal</b> ( $\mu, \text{sd} = s$ )                                             | <b>lognormal</b> ( $\mu, \text{var} = v$ )                                          | <b>lognormal</b> ( $\mu, \text{prec} = \tau$ )                                                    |
| Density               | $\frac{1}{\theta s \sqrt{2\pi}} \exp\left(-\frac{(\log \theta - \mu)^2}{2s^2}\right)$ | $\frac{1}{\theta \sqrt{2\pi v}} \exp\left(-\frac{(\log \theta - \mu)^2}{2v}\right)$ | $\frac{1}{\theta} \sqrt{\frac{\tau}{2\pi}} \exp\left(-\frac{\tau(\log \theta - \mu)^2}{2}\right)$ |
| Parameter restriction | $s > 0$                                                                               | $v > 0$                                                                             | $\tau > 0$                                                                                        |

|               |                                                                                                                      |                                         |                                                   |
|---------------|----------------------------------------------------------------------------------------------------------------------|-----------------------------------------|---------------------------------------------------|
| Range         | $\theta \in (0, \infty)$                                                                                             | Same                                    | Same                                              |
| Mean          | $\exp(\mu + s^2/2)$                                                                                                  | $\exp(\mu + v/2)$                       | $\exp(\mu + 1/(2\tau))$                           |
| Variance      | $\exp(2(\mu + s^2))$<br>$-\exp(2\mu + s^2)$                                                                          | $\exp(2(\mu + v))$<br>$-\exp(2\mu + v)$ | $\exp(2(\mu + 1/\tau))$<br>$-\exp(2\mu + 1/\tau)$ |
| Mode          | $\exp(\mu - s^2)$                                                                                                    | $\exp(\mu - v)$                         | $\exp(\mu - 1/\tau)$                              |
| Random number | Generate $x_1 \sim \text{normal}(0, 1)$ , and $\theta = \exp(\mu + sx_1)$ is a draw from the lognormal distribution. |                                         |                                                   |

**Table 55.26 Negative Binomial Distribution**

|                       |                                                                                                                |
|-----------------------|----------------------------------------------------------------------------------------------------------------|
| PROC specification    | <b>negbin</b> ( $n, p$ )                                                                                       |
| Density               | $\binom{\theta + n - 1}{n - 1} p^n (1 - p)^\theta$                                                             |
| Parameter restriction | $n = 1, 2, \dots$ , and $0 < p \leq 1$                                                                         |
| Range                 | $\theta \in \begin{cases} \{0, 1, 2, \dots\} & 0 < p < 1 \\ \{0\} & p = 1 \end{cases}$                         |
| Mean                  | $\text{round}\left(\frac{n(1-p)}{p}\right)$                                                                    |
| Variance              | $\frac{n(1-p)}{p^2}$                                                                                           |
| Mode                  | $\begin{cases} 0 & n = 1 \\ \text{round}\left(\frac{(n-1)(1-p)}{p}\right) & n > 1 \end{cases}$                 |
| Random number         | Generate $x_1 \sim \text{gamma}(n, 1)$ , and $\theta \sim \text{Poisson}(x_1 \cdot (1 - p)/p)$ (Fishman 1996). |

**Table 55.27 Normal Distribution**

|                       |                                                                        |                                                                       |                                                                           |
|-----------------------|------------------------------------------------------------------------|-----------------------------------------------------------------------|---------------------------------------------------------------------------|
| PROC specification    | <b>normal</b> ( $\mu, \text{sd} = s$ )                                 | <b>normal</b> ( $\mu, \text{var} = v$ )                               | <b>normal</b> ( $\mu, \text{prec} = \tau$ )                               |
| Density               | $\frac{1}{s\sqrt{2\pi}} \exp\left(-\frac{(\theta-\mu)^2}{2s^2}\right)$ | $\frac{1}{\sqrt{2\pi v}} \exp\left(-\frac{(\theta-\mu)^2}{2v}\right)$ | $\sqrt{\frac{\tau}{2\pi}} \exp\left(-\frac{\tau(\theta-\mu)^2}{2}\right)$ |
| Parameter restriction | $s > 0$                                                                | $v > 0$                                                               | $\tau > 0$                                                                |
| Range                 | $\theta \in (-\infty, \infty)$                                         | Same                                                                  | Same                                                                      |
| Mean                  | $\mu$                                                                  | Same                                                                  | Same                                                                      |
| Variance              | $s^2$                                                                  | $v$                                                                   | $1/\tau$                                                                  |
| Mode                  | $\mu$                                                                  | Same                                                                  | Same                                                                      |

**Table 55.28** Pareto Distribution

|                       |                                                                                                                                                                            |
|-----------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| PROC specification    | <b>pareto</b> ( $a, b$ )                                                                                                                                                   |
| Density               | $\frac{a}{b} \left(\frac{b}{\theta}\right)^{a+1}$                                                                                                                          |
| Parameter restriction | $a > 0, b > 0$                                                                                                                                                             |
| Range                 | $\theta \in [b, \infty)$                                                                                                                                                   |
| Mean                  | $\frac{ab}{a-1}$ if $a > 1$                                                                                                                                                |
| Variance              | $\frac{b^2 a}{(a-1)^2(a-2)}$ if $a > 2$                                                                                                                                    |
| Mode                  | $b$                                                                                                                                                                        |
| Random number         | Inverse CDF method with $F(\theta) = 1 - (b/\theta)^a$ . Generate $u \sim \text{uniform}(0, 1)$ , and $\theta = \frac{b}{u^{1/a}}$ is a draw from the Pareto distribution. |
| Useful transformation | $x = 1/\theta$ is $\text{Beta}(a, 1)\mathbf{I}\{x < 1/b\}$ .                                                                                                               |

**Table 55.29** Poisson Distribution

|                       |                                                                                                                   |
|-----------------------|-------------------------------------------------------------------------------------------------------------------|
| PROC specification    | <b>poisson</b> ( $\lambda$ )                                                                                      |
| Density               | $\frac{\lambda^\theta}{\theta!} \exp(-\lambda)$                                                                   |
| Parameter restriction | $\lambda \geq 0$                                                                                                  |
| Range                 | $\theta \in \begin{cases} \{0, 1, \dots\} & \text{if } \lambda > 0 \\ \{0\} & \text{if } \lambda = 0 \end{cases}$ |
| Mean                  | $\lambda$                                                                                                         |
| Variance              | $\lambda$ , if $\lambda > 0$                                                                                      |
| Mode                  | $\text{round}(\lambda)$                                                                                           |

**Table 55.30** Scaled Inverse  $\chi^2$  Distribution

|                       |                                                                                                                                                                                                      |
|-----------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| PROC specification    | <b>sichisq</b> ( $\nu, s^2$ )                                                                                                                                                                        |
| Density               | $\frac{(s^2\nu/2)^{\nu/2}}{\Gamma(\nu/2)} \theta^{-(\nu/2+1)} e^{-\nu s^2/(2\theta)}$                                                                                                                |
| Parameter restriction | $\nu > 0, s > 0$                                                                                                                                                                                     |
| Range                 | $\theta \in (0, \infty)$                                                                                                                                                                             |
| Mean                  | $\frac{\nu}{\nu-2} s^2$ if $\nu > 2$                                                                                                                                                                 |
| Variance              | $\frac{2\nu^2}{(\nu-2)^2(\nu-4)} s^4$ if $\nu > 4$                                                                                                                                                   |
| Mode                  | $\frac{\nu}{\nu+2} s^2$                                                                                                                                                                              |
| Random number         | Scaled inverse $\chi^2$ is a special case of the inverse-gamma distribution: $\theta \sim \text{igamma}(\nu/2, \text{scale} = (\nu s^2)/2)$ is a draw from the scaled inverse $\chi^2$ distribution. |

**Table 55.31** *t* Distribution

| PROC specification | $\mathbf{t}(\mu, \text{sd} = s, \nu)$                                                                                                     | $\mathbf{t}(\mu, \text{var} = v, \nu)$                                                                                                  | $\mathbf{t}(\mu, \text{prec} = \tau, \nu)$                                                                                                         |
|--------------------|-------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------|
| Density            | $\frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})s\sqrt{\nu\pi}} \left(1 + \frac{(\theta-\mu)^2}{\nu s^2}\right)^{-\frac{\nu+1}{2}}$  | $\frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})\sqrt{\nu\pi v}} \left(1 + \frac{(\theta-\mu)^2}{\nu v}\right)^{-\frac{\nu+1}{2}}$ | $\frac{\Gamma(\frac{\nu+1}{2})\sqrt{\tau}}{\Gamma(\frac{\nu}{2})\sqrt{\nu\pi}} \left(1 + \frac{\tau(\theta-\mu)^2}{\nu}\right)^{-\frac{\nu+1}{2}}$ |
| Parm restriction   | $s > 0, \nu > 0$                                                                                                                          | $v > 0, \nu > 0$                                                                                                                        | $\tau > 0, \nu > 0$                                                                                                                                |
| Range              | $\theta \in (-\infty, \infty)$                                                                                                            | Same                                                                                                                                    | Same                                                                                                                                               |
| Mean               | $\mu$ if $\nu > 1$                                                                                                                        | Same                                                                                                                                    | Same                                                                                                                                               |
| Variance           | $\frac{\nu}{\nu-2}s^2$ if $\nu > 2$                                                                                                       | $\frac{\nu}{\nu-2}v$ if $\nu > 2$                                                                                                       | $\frac{\nu}{\nu-2}\frac{1}{\tau}$ if $\nu > 2$                                                                                                     |
| Mode               | $\mu$                                                                                                                                     | Same                                                                                                                                    | Same                                                                                                                                               |
| Random number      | $x_1 \sim \text{normal}(0, 1), x_2 \sim \chi^2(d)$ , and $\theta = m + \sigma x_1 \sqrt{d/x_2}$ is a draw from the <i>t</i> distribution. |                                                                                                                                         |                                                                                                                                                    |

**Table 55.32** Uniform Distribution

|                       |                                                                                                                          |
|-----------------------|--------------------------------------------------------------------------------------------------------------------------|
| PROC specification    | $\mathbf{uniform}(a, b)$                                                                                                 |
| Density               | $\begin{cases} \frac{1}{a-b} & \text{if } a > b \\ \frac{1}{b-a} & \text{if } b > a \\ 1 & \text{if } a = b \end{cases}$ |
| Parameter restriction | none                                                                                                                     |
| Range                 | $\theta \in [a, b]$                                                                                                      |
| Mean                  | $\frac{a+b}{2}$                                                                                                          |
| Variance              | $\frac{ b-a ^2}{12}$                                                                                                     |
| Mode                  | Does not exist                                                                                                           |
| Random number         | Mersenne Twister (Matsumoto and Kurita 1992, 1994; Matsumoto and Nishimura 1998)                                         |

**Table 55.33** Wald Distribution

|                       |                                                                                                    |
|-----------------------|----------------------------------------------------------------------------------------------------|
| PROC specification    | $\mathbf{wald}(\mu, \lambda)$                                                                      |
| Density               | $\sqrt{\frac{\lambda}{2\pi\theta^3}} \exp\left(\frac{-\lambda(\theta-\mu)^2}{2\mu^2\theta}\right)$ |
| Parameter restriction | $\mu > 0, \lambda > 0$                                                                             |
| Range                 | $\theta \in (0, \infty)$                                                                           |
| Mean                  | $\mu$                                                                                              |
| Variance              | $\mu^3/\lambda$                                                                                    |
| Mode                  | $\mu \left[ \left(1 + \frac{9\mu^2}{4\lambda^2}\right)^{1/2} - \frac{3\mu}{2\lambda} \right]$      |



|               |                                                                                                                                                                                                                                                                                                                                                           |
|---------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Random number | Generate $v_0 \sim \chi^2_{(1)}$ . Let $x_1 = \mu + \frac{\mu^2 v_0}{2\lambda} - \frac{\mu}{2\lambda} \sqrt{4\mu\lambda v_0 + \mu^2 v_0^2}$ and $x_2 = \mu^2/x_1$ . Perform a Bernoulli trial, $w \sim \text{Bernoulli}(\frac{\mu}{\mu+x_1})$ . If $w = 1$ , choose $\theta = x_1$ ; otherwise, choose $\theta = x_2$ (Michael, Schucany, and Haas 1976). |
|---------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|

**Table 55.34 Weibull Distribution**

|                       |                                                                                                                                                                                                                                           |
|-----------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| PROC specification    | <b>weibull</b> ( $\mu, c, \sigma$ )                                                                                                                                                                                                       |
| Density               | $\exp\left(-\left(\frac{\theta-\mu}{\sigma}\right)^c\right) \frac{c}{\sigma} \left(\frac{\theta-\mu}{\sigma}\right)^{c-1}$                                                                                                                |
| Parameter restriction | $c > 0, \sigma > 0$                                                                                                                                                                                                                       |
| Range                 | $\theta \in [\mu, \infty)$ if $c = 1$ ; $(\mu, \infty)$ otherwise                                                                                                                                                                         |
| Mean                  | $\mu + \sigma\Gamma(1 + 1/c)$                                                                                                                                                                                                             |
| Variance              | $\sigma^2[\Gamma(1 + 2/c) - \Gamma^2(1 + 1/c)]$                                                                                                                                                                                           |
| Mode                  | $\mu + \sigma(1 - 1/c)^{1/c}$ if $c > 1$                                                                                                                                                                                                  |
| Random number         | Inverse CDF method with $F(\theta) = 1 - \exp\left(-\left(\frac{\theta-\mu}{\sigma}\right)^c\right)$ . Generate $u \sim \text{uniform}(0, 1)$ , and $\theta = \mu + \sigma \cdot (-\ln u)^{1/c}$ is a draw from the Weibull distribution. |

**Multivariate Distributions**

**Table 55.35 Dirichlet Distribution**

|                       |                                                                                                                                                                         |
|-----------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| PROC specification    | $\boldsymbol{\theta} \sim \text{dirich}(\boldsymbol{\alpha})$ , where $\boldsymbol{\theta} = \{\theta_i\}$ , $\boldsymbol{\alpha} = \{\alpha_i\}$ , for $i = 1 \dots k$ |
| Density               | $\frac{\Gamma(\alpha_0)}{\prod_{i=1}^k \Gamma(\alpha_i)} \prod_{i=1}^k \theta_i^{\alpha_i-1}$ , where $\alpha_0 = \sum_{i=1}^k \alpha_i$                                |
| Parameter restriction | $\alpha_i > 0$                                                                                                                                                          |
| Range                 | $\theta_i > 0, \sum_{i=1}^k \theta_i = 1$                                                                                                                               |
| Mean                  | $\alpha_j / \alpha_0$                                                                                                                                                   |
| Mode                  | $(\alpha_j - 1) / (\alpha_0 - k)$                                                                                                                                       |

**Table 55.36 Inverse Wishart Distribution**

|                       |                                                                                                                                                                                                                                                             |
|-----------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| PROC specification    | $\boldsymbol{\theta} \sim \text{iwishart}(v, \mathbf{S})$ , both $\boldsymbol{\theta}$ and $\mathbf{S}$ are $k \times k$ matrices                                                                                                                           |
| Density               | $\left(2^{\frac{vk}{2}} \pi^{\frac{k(k-1)}{4}} \prod_{i=1}^k \Gamma\left(\frac{v+1-i}{2}\right)\right)^{-1}  \mathbf{S} ^{\frac{v}{2}}  \boldsymbol{\theta} ^{-\frac{v+k+1}{2}} \exp\left(-\frac{1}{2}\text{tr}(\mathbf{S}\boldsymbol{\theta}^{-1})\right)$ |
| Parameter restriction | $\mathbf{S}$ must be symmetric and positive definite; $v > k - 1$                                                                                                                                                                                           |
| Range                 | $\boldsymbol{\theta}$ is symmetric and positive definite                                                                                                                                                                                                    |
| Mean                  | $\mathbf{S} / (v - k - 1)$                                                                                                                                                                                                                                  |
| Mode                  | $\mathbf{S} / (v + k + 1)$                                                                                                                                                                                                                                  |

**Table 55.37 Multivariate Normal Distribution**

|                       |                                                                                                                                                                                                                                                  |
|-----------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| PROC specification    | $\boldsymbol{\theta} \sim \mathbf{mvn}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ , where $\boldsymbol{\theta} = \{\theta_k\}$ , $\boldsymbol{\mu} = \{\mu_k\}$ , for $i = 1 \dots k$ , and $\boldsymbol{\Sigma}$ is a $k \times k$ variance matrix |
| Density               | $\exp\left(-\frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\mu})' \boldsymbol{\Sigma}^{-1}(\boldsymbol{\theta} - \boldsymbol{\mu})\right) / \sqrt{(2\pi)^k  \boldsymbol{\Sigma} }$                                                                |
| Parameter restriction | $\boldsymbol{\Sigma}$ must be symmetric and positive definite                                                                                                                                                                                    |
| Range                 | $-\infty < \theta_i < \infty$                                                                                                                                                                                                                    |
| Mean                  | $\boldsymbol{\mu}$                                                                                                                                                                                                                               |
| Mode                  | $\boldsymbol{\mu}$                                                                                                                                                                                                                               |

**Table 55.38 Autoregressive Multivariate Normal Distribution**

|                       |                                                                                                                                                                                                                                                                                                                                                                            |                                                                                      |                                                                                         |
|-----------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------|
| PROC specification    | $\boldsymbol{\theta} \sim \mathbf{mvn}(\boldsymbol{\mu}, \text{sd}=\sigma, \rho)$                                                                                                                                                                                                                                                                                          | $\boldsymbol{\theta} \sim \mathbf{mvn}(\boldsymbol{\mu}, \text{var}=\sigma^2, \rho)$ | $\boldsymbol{\theta} \sim \mathbf{mvn}(\boldsymbol{\mu}, \text{prec}=1/\sigma^2, \rho)$ |
| Density               | $\exp\left(-\frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\mu})'(\sigma^2 \boldsymbol{\Sigma})^{-1}(\boldsymbol{\theta} - \boldsymbol{\mu})\right) / \sqrt{(2\pi)^k  (\sigma^2 \boldsymbol{\Sigma}) }$ where                                                                                                                                                               |                                                                                      |                                                                                         |
|                       | $\boldsymbol{\Sigma} = \begin{bmatrix} 1 & \rho & \rho^2 & \rho^3 & \dots & \rho^k \\ \rho & 1 & \rho & \rho^2 & \dots & \rho^{k-1} \\ \rho^2 & \rho & 1 & \rho & \dots & \rho^{k-2} \\ \rho^3 & \rho^2 & \rho & 1 & \dots & \rho^{k-3} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \rho^k & \rho^{k-1} & \rho^{k-2} & \rho^{k-3} & \dots & 1 \end{bmatrix}$ |                                                                                      |                                                                                         |
| Parameter restriction | $\sigma > 0$ and $-1 < \rho < 1$                                                                                                                                                                                                                                                                                                                                           |                                                                                      |                                                                                         |
| Range                 | $-\infty < \theta_i < \infty$                                                                                                                                                                                                                                                                                                                                              |                                                                                      |                                                                                         |
| Mean                  | $\boldsymbol{\mu}$                                                                                                                                                                                                                                                                                                                                                         |                                                                                      |                                                                                         |
| Mode                  | $\boldsymbol{\mu}$                                                                                                                                                                                                                                                                                                                                                         |                                                                                      |                                                                                         |
| Special Case          | When $\rho = 0$ , the distribution simplifies to $\mathbf{mvn}(\boldsymbol{\mu}, \sigma^2 \cdot \mathbf{I}_k)$ , where $\mathbf{I}_k$ denotes the $k \times k$ identity matrix                                                                                                                                                                                             |                                                                                      |                                                                                         |

**Table 55.39 Multinomial Distribution**

|                       |                                                                                                                                                        |
|-----------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------|
| PROC specification    | $\boldsymbol{\theta} \sim \mathbf{multinom}(\mathbf{p})$ , where $\boldsymbol{\theta} = \{\theta_i\}$ and $\mathbf{p} = \{p_i\}$ , for $i = 1 \dots k$ |
| Density               | $\frac{n!}{\theta_1 \dots \theta_k} p_1^{\theta_1} \dots p_k^{\theta_k}$ , where $\sum_i \theta_i = n$                                                 |
| Parameter restriction | $\sum_i p_i = 1$ with all $p_i > 0$                                                                                                                    |
| Range                 | $\theta_i \in \{0, \dots, n\}$ , nonnegative integers                                                                                                  |
| Mean                  | $n \cdot \mathbf{p}$                                                                                                                                   |

## Usage of Multivariate Distributions

The following simple example illustrates the usage of the multivariate distributions in PROC MCMC. Suppose you are interested in estimating the mean and covariance of multivariate data using this multivariate normal model:

$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \sim \text{MVN} \left( \boldsymbol{\mu} = \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}, \boldsymbol{\Sigma} = \begin{pmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{21} & \sigma_{22} \end{pmatrix} \right)$$

where

$$\boldsymbol{\mu} = \begin{pmatrix} 1 \\ 2 \end{pmatrix}$$

$$\boldsymbol{\Sigma} = \begin{pmatrix} 2.4 & 3 \\ 3 & 8.1 \end{pmatrix}$$

You can use the following independent prior on  $\boldsymbol{\mu}$  and  $\boldsymbol{\Sigma}$ :

$$\boldsymbol{\mu} \sim \text{MVN} \left( \boldsymbol{\mu}_0 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \boldsymbol{\Sigma}_0 = \begin{pmatrix} 100 & 0 \\ 0 & 100 \end{pmatrix} \right)$$

$$\boldsymbol{\Sigma} \sim \text{iWishart} \left( \nu = 2, \mathbf{S} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right)$$

The following IML procedure statements simulate 100 random multivariate normal samples:

```

title 'An Example that Uses Multivariate Distributions';
proc iml;
 N = 100;
 Mean = {1 2};
 Cov = {2.4 3, 3 8.1};
 call randseed(1);
 x = RANDNORMAL(N, Mean, Cov);

 SampleMean = x[:,];
 n = nrow(x);
 y = x - repeat(SampleMean, n);
 SampleCov = y`*y / (n-1);
 print SampleMean Mean, SampleCov Cov;

 cname = {"x1", "x2"};
 create inputdata from x [colname = cname];
 append from x;
 close inputdata;
quit;

```

Figure 55.13 prints the sample mean and covariance of the simulated data, in addition to the true mean and covariance matrix.

**Figure 55.13** Simulated Multivariate Normal Data

| An Example that Uses Multivariate Distributions |           |             |     |
|-------------------------------------------------|-----------|-------------|-----|
| <b>SampleMean</b>                               |           | <b>Mean</b> |     |
| 0.9987751                                       | 2.115693  | 1           | 2   |
| <b>SampleCov</b>                                |           | <b>Cov</b>  |     |
| 2.8252975                                       | 3.7190704 | 2.4         | 3   |
| 3.7190704                                       | 9.2916805 | 3           | 8.1 |

The following PROC MCMC statements estimate the posterior mean and covariance of the multivariate normal data:

```
proc mcmc data=inputdata seed=17 nmc=3000 diag=none;
 ods select PostSummaries PostIntervals;
 array data[2] x1 x2;
 array mu[2];
 array Sigma[2,2];
 array mu0[2] (0 0);
 array Sigma0[2,2] (100 0 0 100);
 array S[2,2] (1 0 0 1);
 parm mu Sigma;
 prior mu ~ mvn(mu0, Sigma0);
 prior Sigma ~ iwish(2, S);
 model data ~ mvn(mu, Sigma);
run;
```

To use the multivariate distribution, you must specify parameters (or random variables in the MODEL statement) in an array form. The first ARRAY statement creates an one-dimensional array data, which contains two numeric variables, x1 and x2, from the input data set. The data variable is your response variable. The subsequent statements defines two array-parameters (mu and Sigma) and three constant array-hyperparameters (mu0, Sigma0, and S). The PARMs statement declares mu and Sigma to be model parameters. The two PRIOR statements specify the multivariate normal and inverse Wishart distributions as the prior for mu and Sigma, respectively. The MODEL statement specifies the multivariate normal likelihood with data as the random variable, mu as the mean, and Sigma as the covariance matrix.

Figure 55.14 lists the estimated posterior mean and covariance matrix.

Figure 55.14 Estimated Mean and Covariance

| The MCMC Procedure  |      |        |                       |             |        |         |
|---------------------|------|--------|-----------------------|-------------|--------|---------|
| Posterior Summaries |      |        |                       |             |        |         |
| Parameter           | N    | Mean   | Standard<br>Deviation | Percentiles |        |         |
|                     |      |        |                       | 25%         | 50%    | 75%     |
| mu1                 | 3000 | 0.9941 | 0.1763                | 0.8761      | 0.9958 | 1.1136  |
| mu2                 | 3000 | 2.1135 | 0.3112                | 1.9075      | 2.1056 | 2.3254  |
| Sigma1              | 3000 | 2.8726 | 0.4084                | 2.5799      | 2.8347 | 3.1205  |
| Sigma2              | 3000 | 3.7573 | 0.6418                | 3.3090      | 3.7057 | 4.1385  |
| Sigma3              | 3000 | 3.7573 | 0.6418                | 3.3090      | 3.7057 | 4.1385  |
| Sigma4              | 3000 | 9.3987 | 1.3224                | 8.4705      | 9.2507 | 10.1946 |

| Posterior Intervals |       |                     |         |              |         |
|---------------------|-------|---------------------|---------|--------------|---------|
| Parameter           | Alpha | Equal-Tail Interval |         | HPD Interval |         |
| mu1                 | 0.050 | 0.6500              | 1.3356  | 0.6338       | 1.3106  |
| mu2                 | 0.050 | 1.5081              | 2.7405  | 1.4939       | 2.7165  |
| Sigma1              | 0.050 | 2.1725              | 3.8034  | 2.1001       | 3.6723  |
| Sigma2              | 0.050 | 2.6659              | 5.2064  | 2.5791       | 5.0223  |
| Sigma3              | 0.050 | 2.6659              | 5.2064  | 2.5791       | 5.0223  |
| Sigma4              | 0.050 | 7.1260              | 12.3763 | 7.0155       | 12.0969 |

## Specifying a New Distribution

To work with a new density that is not listed in the section “Standard Distributions” on page 4476, you can use the `GENERAL` and `DGENERAL` functions. The letter “D” stands for discrete. The new distributions have to be specified on the logarithm scale.

Suppose you want to use the inverse-beta distribution:

$$p(\alpha|a, b) = \frac{\Gamma(a + b)}{\Gamma(a) + \Gamma(b)} \cdot \alpha^{(a-1)} \cdot (1 + \alpha)^{-(a+b)}$$

The following statements in PROC MCMC define the density on its log scale:

```
a = 3; b = 5;
const = lgamma(a + b) - lgamma(a) - lgamma(b);
lp = const + (a - 1) * log(alpha) - (a + b) * log(1 + alpha);
prior alpha ~ general(lp);
```

The symbol `lp` is the expression for the log of an inverse-beta ( $a = 3$ ,  $b = 5$ ). The function `general(lp)` assigns that distribution to `alpha`. The constant term, `const`, can be omitted because the Markov simulation requires only the log of the density kernel.

You can use the `GENERAL` function to specify a distribution for a single variable or for multiple variables. It is important to emphasize that the argument `lp` is an expression for the log of the joint distribution for

these variables. On the contrary, any standard distribution is applied separately to each random variable in the statement.

When you use the `GENERAL` function in the `MODEL` statement, you do not need to specify the dependent variable on the left of the tilde  $\sim$ . The log-likelihood function takes the dependent variable into account; hence, there is no need to explicitly state the dependent variable in the `MODEL` statement. However, in the `PRIOR` and `RANDOM` statements, you need to explicitly state the parameter names and a tilde with the `GENERAL` function.

You can specify any distribution function by using the `GENERAL` and `DGENERAL` functions as long as the distribution function is programmable with SAS statements. When the function is used in the `PRIOR` statements, you must supply initial values in either the `PARMS` statement or within the `BEGINCNST` and `ENDCNST` statements. See the sections “`PARMS` Statement” on page 4451 and “`BEGINCNST/ENDCNST` Statement” on page 4441. When the function is used in the `RANDOM` statement, you must use the `INITIAL=` option in the `RANDOM` statement to supply initial values

**NOTE:** PROC MCMC does not verify that the `GENERAL` function you specify is a valid distribution—that is, an integrable density. You must use the function with caution.

---

## Using Density Functions in the Programming Statements

### Density Functions in PROC MCMC

PROC MCMC has a number of internally defined log-density functions for univariate and multivariate distributions. These functions have the basic form of `LPDF $dist(x, parm-list)$` , where *dist* is the name of the distribution (see [Table 55.40](#) for univariate distributions and [Table 55.41](#) for multivariate distributions). The argument *x* is the random variable, and *parm-list* is the list of parameters.

In addition, the univariate functions allow for optional boundary arguments, such as `LPDF $dist(x, parm-list, <lower>, <upper>)$` , where *lower* and *upper* are optional but positional boundary arguments. With the exception of the Bernoulli and uniform distribution, you can specify limits on all univariate distributions.

To set a lower bound on the normal density:

```
lpdfnorm(x, 0, 1, -2);
```

To set just an upper bound, specify a missing value for the lower bound argument:

```
lpdfnorm(x, 0, 1, ., 2);
```

Leaving both limits out gives you the unbounded density. You can also specify both bounds:

```
lpdfnorm(x, 0, 1);
lpdfnorm(x, 0, 1, -3, 4);
```

See [Table 55.40](#) for the function names of univariate distributions and [Table 55.41](#) for multivariate distributions.

**Table 55.40** Logarithm of Univariate Density Functions in PROC MCMC

| Distribution Name                   | Function Call                                                                  |
|-------------------------------------|--------------------------------------------------------------------------------|
| Beta                                | <b>lpdfbeta</b> ( <i>x, a, b, &lt; lower &gt;, &lt; upper &gt;</i> );          |
| Binary                              | <b>lpdfbern</b> ( <i>x, p</i> );                                               |
| Binomial                            | <b>lpdfbin</b> ( <i>x, n, p, &lt; lower &gt;, &lt; upper &gt;</i> );           |
| Cauchy                              | <b>lpdfcau</b> ( <i>x, loc, scale, &lt; lower &gt;, &lt; upper &gt;</i> );     |
| $\chi^2$                            | <b>lpdfchisq</b> ( <i>x, df, &lt; lower &gt;, &lt; upper &gt;</i> );           |
| Exponential $\chi^2$                | <b>lpdfechisq</b> ( <i>x, df, &lt; lower &gt;, &lt; upper &gt;</i> );          |
| Exponential gamma                   | <b>lpdfegamma</b> ( <i>x, sp, scale, &lt; lower &gt;, &lt; upper &gt;</i> );   |
| Exponential exponential             | <b>lpdfeexpon</b> ( <i>x, scale, &lt; lower &gt;, &lt; upper &gt;</i> );       |
| Exponential inverse $\chi^2$        | <b>lpdfeichisq</b> ( <i>x, df, &lt; lower &gt;, &lt; upper &gt;</i> );         |
| Exponential inverse-gamma           | <b>lpdfeigamma</b> ( <i>x, sp, scale, &lt; lower &gt;, &lt; upper &gt;</i> );  |
| Exponential scaled inverse $\chi^2$ | <b>lpdfesichisq</b> ( <i>x, df, scale, &lt; lower &gt;, &lt; upper &gt;</i> ); |
| Exponential                         | <b>lpdfexpon</b> ( <i>x, scale, &lt; lower &gt;, &lt; upper &gt;</i> );        |
| Gamma                               | <b>lpdfgamma</b> ( <i>x, sp, scale, &lt; lower &gt;, &lt; upper &gt;</i> );    |
| Geometric                           | <b>lpdfgeo</b> ( <i>x, p, &lt; lower &gt;, &lt; upper &gt;</i> );              |
| Inverse $\chi^2$                    | <b>lpdfichisq</b> ( <i>x, df, &lt; lower &gt;, &lt; upper &gt;</i> );          |
| Inverse-gamma                       | <b>lpdfigamma</b> ( <i>x, sp, scale, &lt; lower &gt;, &lt; upper &gt;</i> );   |
| Laplace                             | <b>lpdfdexp</b> ( <i>x, loc, scale, &lt; lower &gt;, &lt; upper &gt;</i> );    |
| Logistic                            | <b>lpdflogis</b> ( <i>x, loc, scale, &lt; lower &gt;, &lt; upper &gt;</i> );   |
| Lognormal                           | <b>lpdflnorm</b> ( <i>x, loc, sd, &lt; lower &gt;, &lt; upper &gt;</i> );      |
| Negative binomial                   | <b>lpdfnegbin</b> ( <i>x, n, p, &lt; lower &gt;, &lt; upper &gt;</i> );        |
| Normal                              | <b>lpdfnorm</b> ( <i>x, mu, sd, &lt; lower &gt;, &lt; upper &gt;</i> );        |
| Pareto                              | <b>lpdfpareto</b> ( <i>x, sp, scale, &lt; lower &gt;, &lt; upper &gt;</i> );   |

**Table 55.40** (continued)

| Distribution Name       | Function Call                                                                                            |
|-------------------------|----------------------------------------------------------------------------------------------------------|
| Poisson                 | <b>lpdfpoi</b> ( <i>x</i> , <i>mean</i> , < <i>lower</i> >, < <i>upper</i> >);                           |
| Scaled inverse $\chi^2$ | <b>lpdfsichisq</b> ( <i>x</i> , <i>df</i> , <i>scale</i> , < <i>lower</i> >, < <i>upper</i> >);          |
| <i>t</i>                | <b>lpdfft</b> ( <i>x</i> , <i>mu</i> , <i>sd</i> , <i>df</i> , < <i>lower</i> >, < <i>upper</i> >);      |
| Uniform                 | <b>lpdfunif</b> ( <i>x</i> , <i>a</i> , <i>b</i> );                                                      |
| Wald                    | <b>lpdfwald</b> ( <i>x</i> , <i>mean</i> , <i>scale</i> , < <i>lower</i> >, < <i>upper</i> >);           |
| Weibull                 | <b>lpdfwei</b> ( <i>x</i> , <i>loc</i> , <i>sp</i> , <i>scale</i> , < <i>lower</i> >, < <i>upper</i> >); |

In the multivariate log-density functions, arrays must be used in place for the random variable and parameters in the model.

**Table 55.41** Logarithm of Multivariate Density Functions in PROC MCMC

| Distribution Name   | Function Call                                                           |
|---------------------|-------------------------------------------------------------------------|
| Dirichlet           | <b>lpdfdirch</b> ( <i>x_array</i> , <i>alpha_array</i> );               |
| Inverse Wishart     | <b>lpdfiwish</b> ( <i>x_array</i> , <i>df</i> , <i>S_array</i> );       |
| Multivariate normal | <b>lpdfmvn</b> ( <i>x_array</i> , <i>mu_array</i> , <i>cov_array</i> ); |
| Multinomial         | <b>lpdfmnom</b> ( <i>x_array</i> , <i>p_array</i> );                    |

### Standard Distributions, the LOGPDF Functions, and the LPDF $_{dist}$ Functions

Standard distributions listed in the section “Standard Distributions” on page 4476 are *names* only, and they can be used only in the **MODEL**, **PRIOR**, and **HYPERPRIOR** statements to specify either a prior distribution or a conditional distribution of the data given parameters. They do not return any values, and you cannot use them in the programming statements.

The LOGPDF functions are DATA step functions that compute the logarithm of various probability density (mass) functions. For example,

```
logpdf("beta", x, 2, 15);
```

returns the log of a beta density with parameters  $a = 2$  and  $b = 15$ , evaluated at  $x$ . All the LOGPDF functions are supported in PROC MCMC.

The LPDF $_{dist}$  functions are unique to PROC MCMC. They compute the logarithm of various probability density (mass) functions. The functions are the same as the LOGPDF functions when it comes to calculating



the log density. For example,

```
lpdfbeta(x, 2, 15);
```

returns the same value as

```
logpdf("beta", x, 2, 15);
```

The *LPDFdist* functions cover a greater class of probability density functions, and the univariate distribution functions take the optional but positional boundary arguments. There are no corresponding *LCDFdist* or *LSDFdist* functions in PROC MCMC. To work with the cumulative probability function or the survival functions, you need to use the LOGCDF and the LOGSDF DATA step functions.

## Truncation and Censoring

### Truncated Distributions

To specify a truncated distribution, you can use the LOWER= and/or UPPER= options. Almost all of the standard distributions, including the **GENERAL** and **DGENERAL** functions, take these optional truncation arguments. The exceptions are the binary and uniform distributions.

For example, you can specify the following:

```
prior alpha ~ normal(mean = 0, sd = 1, lower = 3, upper = 45);
```

or

```
parms beta;
a = 3; b = 7;
ll = (a + 1) * log(b / beta);
prior beta ~ general(ll, upper = b + 17);
```

The preceding statements state that if beta is less than b+17, the log of the prior density is ll, as calculated by the equation; otherwise, the log of the prior density is missing—the log of zero.

When the same distribution is applied to multiple parameters in a **PRIOR** statement, the LOWER= and UPPER= truncations apply to all parameters in that statement. For example, the following statements define a Poisson density for theta and gamma:

```
parms theta gamma;
lambda = 7;
ll = theta * log(lambda) - lgamma(1 + theta);
l2 = gamma * log(lambda) - lgamma(1 + gamma);
ll = ll + l2;
prior theta gamma ~ dgeneral(ll, lower = 1);
```

The LOWER=1 condition is applied to both theta and gamma, meaning that for the assignment to ll to be meaningful, both theta and gamma have to be greater than 1. If either of the parameters is less than 1, the log of the joint prior density becomes a missing value.

With the exceptions of the normal distribution and the **GENERAL** and **DGENERAL** functions, the LOWER= and UPPER= options cannot be parameters or functions of parameters. The reason is that most

of the truncated distributions are not normalized. Unnormalized densities do not lead to wrong MCMC answers as long as the bounds are constants. However if the bounds involve model parameters, then the normalizing constant, which is a function of these parameters, must be taken into account in the posterior. Without specifying the normalizing constant, inferences on these boundary parameters are incorrect.

It is not difficult to construct a truncated distribution with a normalizing constant. Any truncated distribution has the probability distribution:

$$p(\theta|a < \theta < b) = \frac{p(\theta)}{F(a) - F(b)}$$

where  $p(\cdot)$  is the density function and  $F(\cdot)$  is the cumulative distribution function. In SAS functions,  $p(\cdot)$  is probability density function and  $F(\cdot)$  is cumulative distribution function. The following example shows how to construct a truncated gamma prior on theta, with SHAPE = 3, SCALE = 2, LOWER = a, and UPPER = b:

```
lp = logpdf('gamma', theta, 3, 2)
 - log(cdf('gamma', a, 3, 2) - cdf('gamma', b, 3, 2));
prior theta ~ general(lp);
```

Note the difference from a naive definition of the density, without taking into account of the normalizing constant:

```
lp = logpdf('gamma', theta, 3, 2);
prior theta ~ general(lp, lower=a, upper=b);
```

If a or b are parameters, you get very different results from the two formulations.

## Censoring

There is no built-in mechanism in PROC MCMC that models censoring automatically. You need to construct the density function (using a combination of the LOGPDF, LOGCDF, and LOGSDF functions and IF-ELSE statements) for the censored data.

Suppose you partition the data into four categories: uncensored (with observation x), left censored (with observation xl), right censored (with observation xr), and interval censored (with observations xl and xr). The likelihood is the normal with mean mu and standard deviation s. The following statements construct the corresponding log likelihood for the observed data:

```
if uncensored then
 ll = logpdf('normal', x, mu, s);
else if leftcensored then
 ll = logcdf('normal', x1, mu, s);
else if rightcensored then
 ll = logsdf('normal', xr, mu, s);
else /* this is the case of interval censored. */
 ll = log(cdf('normal', xr, mu, s) - cdf('normal', x1, mu, s));
model general(ll);
```

See “[Example 55.17: Normal Regression with Interval Censoring](#)” on page 4638.

## Some Useful SAS Functions

**Table 55.42** Some Useful SAS Functions

| SAS Function                    | Definition                                                        |
|---------------------------------|-------------------------------------------------------------------|
| <b>abs(x);</b>                  | $ x $                                                             |
| <b>airy(x);</b>                 | Returns the value of the AIRY function.                           |
| <b>beta(x1, x2);</b>            | $\int_0^1 z^{x1-1}(1-z)^{x2-1} dz$                                |
| <b>call logistic(x);</b>        | $\frac{\exp(x)}{1+\exp(x)}$                                       |
| <b>call softmax(x1,...,xn);</b> | Each element is replaced by $\exp(x_j) / \sum \exp(x_j)$          |
| <b>call stdize(x1,...,xn);</b>  | Standardize values                                                |
| <b>cdf();</b>                   | Cumulative distribution function                                  |
| <b>cdf('normal', x, 0, 1);</b>  | Standard normal cumulative distribution function                  |
| <b>comb(x1, x2);</b>            | $\frac{x1!}{x2!(x1-x2)!}$                                         |
| <b>constant('.');</b>           | Calculate commonly used constants                                 |
| <b>cos(x);</b>                  | cosine(x)                                                         |
| <b>css(x1, ..., xn);</b>        | $\sum_i (x_i - \bar{x})^2$                                        |
| <b>cv(x1, ..., xn);</b>         | std(x) / mean(x) * 100                                            |
| <b>dairy(x);</b>                | Derivative of the AIRY function                                   |
| <b>dimN(m);</b>                 | Returns the numbers of elements in the Nth dim of array <i>m</i>  |
| <b>x1 eq x2</b>                 | Returns 1 if x1 = x2; 0 otherwise                                 |
| <b>x1**x2</b>                   | $x1^{x2}$                                                         |
| <b>geomean(x1, ..., xn);</b>    | $\exp\left(\frac{\log(x1)+\dots+\log(xn)}{n}\right)$              |
| <b>difN(x);</b>                 | Returns differences between the argument and its Nth lag          |
| <b>digamma(x1);</b>             | $\frac{\Gamma'(x1)}{\Gamma(x1)}$                                  |
| <b>erf(x);</b>                  | $\frac{2}{\sqrt{\pi}} \int_0^x \exp(-z^2) dz$                     |
| <b>erfc(x);</b>                 | 1 - erf(x)                                                        |
| <b>fact(x);</b>                 | $x!$                                                              |
| <b>floor(x);</b>                | Greatest integer $\leq x$                                         |
| <b>gamma(x);</b>                | $\int_0^\infty z^{x-1} \exp(-1) dz$                               |
| <b>harmean(x1, ..., xn);</b>    | $\frac{n}{1/x1+\dots+1/xn}$                                       |
| <b>ibessel(nu, x, kode);</b>    | Modified Bessel function of order <i>nu</i> evaluated at <i>x</i> |
| <b>jbessel(nu, x);</b>          | Bessel function of order <i>nu</i> evaluated at <i>x</i>          |
| <b>lagN(x);</b>                 | Returns values from a queue                                       |
| <b>largest(k, x1, ..., xn);</b> | Returns the $k^{th}$ largest element                              |
| <b>lgamma(x);</b>               | $\ln(\Gamma(x))$                                                  |
| <b>lgamma(x+1);</b>             | $\ln(x!)$                                                         |
| <b>log(x, logN(x));</b>         | $\ln(x)$                                                          |
| <b>logbeta(x1, x2);</b>         | $\lgamma(x1) + \lgamma(x2) - \lgamma(x1 + x2)$                    |
| <b>logcdf();</b>                | Log of a left cumulative distribution function                    |
| <b>logpdf();</b>                | Log of a probability density (mass) function                      |
| <b>logsdf();</b>                | Log of a survival function                                        |
| <b>max(x1, x2);</b>             | Returns $x_1$ if $x_1 > x_2$ ; $x_2$ otherwise                    |
| <b>mean(of x1-xn);</b>          | $\sum_i x_i / n$                                                  |

Table 55.42 (continued)

| SAS Function                                  | Definition                                                   |
|-----------------------------------------------|--------------------------------------------------------------|
| <b>median</b> (of $x_1$ - $x_n$ );            | Returns the median of nonmissing values                      |
| <b>min</b> ( $x_1$ , $x_2$ );                 | Returns $x_1$ if $x_1 < x_2$ ; $x_2$ otherwise               |
| <b>missing</b> ( $x$ );                       | Returns 1 if $x$ is missing; 0 otherwise                     |
| <b>mod</b> ( $x_1$ , $x_2$ );                 | Returns the remainder from $x_1/x_2$                         |
| <b>n</b> ( $x_1$ , ..., $x_n$ );              | Returns number of nonmissing values                          |
| <b>nmiss</b> (of $y_1$ - $y_n$ );             | Number of missing values                                     |
| <b>quantile</b> ();                           | Computes the quantile from a specific distribution           |
| <b>pdf</b> ();                                | Probability density (mass) functions                         |
| <b>perm</b> ( $n$ , $r$ );                    | $\frac{n!}{(n-r)!}$                                          |
| <b>put</b> ();                                | Returns a value that uses a specified format                 |
| <b>round</b> ( $x$ );                         | Rounds $x$                                                   |
| <b>rms</b> (of $x_1$ - $x_n$ );               | $\sqrt{\frac{x_1^2 + \dots + x_n^2}{n}}$                     |
| <b>sdf</b> ();                                | Survival function                                            |
| <b>sign</b> ( $x$ );                          | Returns -1 if $x < 0$ ; 0 if $x = 0$ ; 1 if $x > 0$          |
| <b>sin</b> ( $x$ );                           | sine( $x$ )                                                  |
| <b>smallest</b> ( $s$ , $x_1$ , ..., $x_n$ ); | Returns the $s^{th}$ smallest component of $x_1, \dots, x_n$ |
| <b>sortn</b> (of $x_1$ - $x_n$ );             | Sorts the values of the variables                            |
| <b>sqrt</b> ( $x$ );                          | $\sqrt{x}$                                                   |
| <b>std</b> ( $x_1$ , ..., $x_n$ );            | Standard deviation of $x_1, \dots, x_n$ (n-1 in denominator) |
| <b>sum</b> (of $x$ );                         | $\sum_i x_i$                                                 |
| <b>trigamma</b> ( $x$ );                      | Derivative of the DIGAMMA( $x$ ) function                    |
| <b>uss</b> (of $x_1$ - $x_n$ );               | Uncorrected sum of squares                                   |

Here are examples of some commonly used transformations:

- logit

```
mu = beta0 + beta1 * z1;
call logistic(mu);
```

- log

```
w = beta0 + beta1 * z1;
mu = exp(w);
```

- probit

```
w = beta0 + beta1 * z1;
mu = cdf('normal', w, 0, 1);
```

- cloglog

```
w = beta0 + beta1 * z1;
mu = 1 - exp(-exp(w));
```

## Matrix Functions in PROC MCMC

The MCMC procedure provides you with a number of CALL routines for performing simple matrix operations on declared arrays. With the exception of FILLMATRIX, IDENTITY, and ZEROMATRIX, the CALL routines listed in Table 55.43 do not support matrices or arrays that contain missing values.

**Table 55.43** Matrix Functions in PROC MCMC

| CALL Routine   | Description                                                                                                                                     |
|----------------|-------------------------------------------------------------------------------------------------------------------------------------------------|
| ADDMATRIX      | Performs an element-wise addition of two matrices or of a matrix and a scalar.                                                                  |
| CHOL           | Calculates the Cholesky decomposition for a particular symmetric matrix.                                                                        |
| DET            | Calculates the determinant of a specified matrix, which must be square.                                                                         |
| ELEMMULT       | Performs an element-wise multiplication of two matrices.                                                                                        |
| FILLMATRIX     | Replaces all of the element values of the input matrix with the specified value. You can use this routine with multidimensional numeric arrays. |
| IDENTITY       | Converts the input matrix to an identity matrix. Diagonal element values of the matrix are set to 1, and the rest of the values are set to 0.   |
| INV            | Calculates a matrix that is the inverse of the input matrix. The input matrix must be a square, nonsingular matrix.                             |
| MULT           | Calculates the matrix product of two input matrices.                                                                                            |
| SUBTRACTMATRIX | Performs an element-wise subtraction of two matrices or of a matrix and a scalar.                                                               |
| TRANSPOSE      | Returns the transpose of a matrix.                                                                                                              |
| ZEROMATRIX     | Replaces all of the element values of the numeric input matrix with 0.                                                                          |

### ADDMATRIX CALL Routine

The ADDMATRIX CALL routine performs an element-wise addition of two matrices or of a matrix and a scalar.

The syntax of the ADDMATRIX CALL routine is

```
CALL ADDMATRIX (X, Y, Z);
```

where

$X$  specifies a scalar or an input matrix with dimensions  $m \times n$  (that is,  $X[m, n]$ )

$Y$  specifies a scalar or an input matrix with dimensions  $m \times n$  (that is,  $Y[m, n]$ )

$Z$  specifies an output matrix with dimensions  $m \times n$  (that is,  $Z[m, n]$ )

such that

$$Z = X + Y$$

## CHOL CALL Routine

The CHOL CALL routine calculates the Cholesky decomposition for a particular symmetric matrix.

The syntax of the CHOL CALL routine is

**CALL CHOL** (*X*, *Y* <, *validate*>) ;

where

*X* specifies a symmetric positive-definite input matrix with dimensions  $m \times m$  (that is,  $X[m, m]$ )

*Y* is a variable that contains the Cholesky decomposition and specifies an output matrix with dimensions  $m \times m$  (that is,  $Y[m, m]$ )

*validate* specifies an optional argument that can increase the processing speed by avoiding error checking:

If *validate* = 0 or is not specified, then the matrix *X* is checked for symmetry.

If *validate* = 1, then the matrix *X* is assumed to be symmetric.

such that

$$X = YY^*$$

where *Y* is a lower triangular matrix with strictly positive diagonal entries and  $Y^*$  denotes the conjugate transpose of *Y*.

Both input and output matrices must be square and have the same dimensions. If *X* is symmetric positive-definite, *Y* is a lower triangle matrix. If *X* is not symmetric positive-definite, *Y* is filled with missing values.

## DET CALL Routine

The determinant, the product of the eigenvalues, is a single numeric value. If the determinant of a matrix is zero, then that matrix is singular (that is, it does not have an inverse). The routine performs an LU decomposition and collects the product of the diagonals.

The syntax of the DET CALL routine is

**CALL DET** (*X*, *a*) ;

where

*X* specifies an input matrix with dimensions  $m \times m$  (that is,  $X[m, m]$ )

*a* specifies the returned determinate value

such that

$$a = |X|$$

**ELEMMULT CALL Routine**

The ELEMMULT CALL routine performs an element-wise multiplication of two matrices.

The syntax of the ELEMMULT CALL routine is

**CALL ELEMMULT (X, Y, Z) ;**

where

$X$  specifies an input matrix with dimensions  $m \times n$  (that is,  $X[m, n]$ )

$Y$  specifies an input matrix with dimensions  $m \times n$  (that is,  $Y[m, n]$ )

$Z$  specifies an output matrix with dimensions  $m \times n$  (that is,  $Z[m, n]$ )

**FILLMATRIX CALL Routine**

The FILLMATRIX CALL routine replaces all of the element values of the input matrix with the specified value. You can use the FILLMATRIX CALL routine with multidimensional numeric arrays.

The syntax of the FILLMATRIX CALL routine is

**CALL FILLMATRIX (X, Y) ;**

where

$X$  specifies an input numeric matrix

$Y$  specifies the numeric value that is used to fill the matrix

**IDENTITY CALL Routine**

The IDENTITY CALL routine converts the input matrix to an identity matrix. Diagonal element values of the matrix are set to 1, and the rest of the values are set to 0.

The syntax of the IDENTITY CALL routine is

**CALL IDENTITY (X) ;**

where

$X$  specifies an input matrix with dimensions  $m \times m$  (that is,  $X[m, m]$ )

**INV CALL Routine**

The INV CALL routine calculates a matrix that is the inverse of the input matrix. The input matrix must be a square, nonsingular matrix.

The syntax of the INV CALL routine is

**CALL INV (X, Y) ;**

where

$X$  specifies an input matrix with dimensions  $m \times m$  (that is,  $X[m, m]$ )

$Y$  specifies an output matrix with dimensions  $m \times m$  (that is,  $Y[m, m]$ )

### MULT CALL Routine

The MULT CALL routine calculates the matrix product of two input matrices.

The syntax of the MULT CALL routine is

**CALL MULT** ( $X, Y, Z$ ) ;

where

$X$  specifies an input matrix with dimensions  $m \times n$  (that is,  $X[m, n]$ )

$Y$  specifies an input matrix with dimensions  $n \times p$  (that is,  $Y[n, p]$ )

$Z$  specifies an output matrix with dimensions  $m \times p$  (that is,  $Z[m, p]$ )

The number of columns for the first input matrix must be the same as the number of rows for the second matrix. The calculated matrix is the last argument.

### SUBTRACTMATRIX CALL Routine

The SUBTRACTMATRIX CALL routine performs an element-wise subtraction of two matrices or of a matrix and a scalar.

The syntax of the SUBTRACTMATRIX CALL routine is

**CALL SUBTRACTMATRIX** ( $X, Y, Z$ ) ;

where

$X$  specifies a scalar or an input matrix with dimensions  $m \times n$  (that is,  $X[m, n]$ )

$Y$  specifies a scalar or an input matrix with dimensions  $m \times n$  (that is,  $Y[m, n]$ )

$Z$  specifies an output matrix with dimensions  $m \times n$  (that is,  $Z[m, n]$ )

such that

$$Z = X - Y$$

### TRANSPOSE CALL Routine

The TRANSPOSE CALL routine returns the transpose of a matrix.

The syntax of the TRANSPOSE CALL routine is

**CALL TRANSPOSE** ( $X, Y$ ) ;

where

$X$  specifies an input matrix with dimensions  $m \times n$  (that is,  $X[m, n]$ )

$Y$  specifies an output matrix with dimensions  $n \times m$  (that is,  $Y[n, m]$ )



## ZEROMATRIX CALL Routine

The ZEROMATRIX CALL routine replaces all of the element values of the numeric input matrix with 0. You can use the ZEROMATRIX CALL routine with multidimensional numeric arrays.

The syntax of the ZEROMATRIX CALL routine is

```
CALL ZEROMATRIX (X) ;
```

where

*X* specifies a numeric input matrix.

## Create Design Matrix

PROC MCMC does not support a CLASS statement; therefore you need to construct the right design matrix (with dummy or indicator variables) prior to calling PROC MCMC. The best tool to use is the TRANSREG procedure (see Chapter 97, “[The TRANSREG Procedure](#)”). This procedure offers both indicator and effects coding methods. You can specify any categorical variables in the CLASS expansion, and use the ZERO= option to select a reference category. You can also specify any other data set variables (predictors, the responses, and so on) to the output data set in the ID statement.

For example, the following statements create a data set that contains two categorical variables (City and G), and two continuous variables (x and resp):

```
title 'Create Design Matrix';
data categorical;
 input City$ G$ x resp @@;
 datalines;
Chicago F 69.0 112.5 Chicago F 56.5 84.0
Chicago M 65.3 98.0 Chicago M 59.8 84.5
NewYork M 62.8 102.5 NewYork M 63.5 102.5
NewYork F 57.3 83.0 NewYork M 57.5 85.0
;
```

Suppose you are interested in creating a design matrix that uses dummy variable coding for the categorical variables City, G and their interaction City \* G. You can use the following PROC TRANSREG statements:

```
proc transreg data=categorical design;
 model class(city g city*g / zero=last);
 id x resp;
 output out=input_mcmc(drop=_: Int:);
run;
```

The DESIGN option specifies that the primary goal is to code the design matrix. The MODEL statement indicates the variable of interest. The CLASS option in the MODEL statement expands the variables of interest to a list of “dummy” variables. The ZERO=LAST option sets the reference level. The ID statement includes x and resp in the OUT= data set. And the OUTPUT statement creates a new data set Input\_MCMC that stores the design matrix and original variables from the original data set.

A quick call of the PRINT procedure shows the output from the PROC TRANSREG call:

```
proc print data=input_mcmc;
run;
```

Figure 55.15 prints the design matrix that is generated by PROC TRANSREG. The Input\_mcmc data set contains all the variables from the original Categorical data set, in addition to corresponding dummy variables (CityChicago, GF, and CityChicagoGF) for the categorical variables.

**Figure 55.15** Design Matrix Generated by PROC TRANSREG

| Create Design Matrix |         |    |         |         |   |      |       |
|----------------------|---------|----|---------|---------|---|------|-------|
| Obs                  | City    | GF | City    | City    | G | x    | resp  |
|                      | Chicago |    | Chicago |         |   |      |       |
| 1                    | 1       | 1  | 1       | Chicago | F | 69.0 | 112.5 |
| 2                    | 1       | 1  | 1       | Chicago | F | 56.5 | 84.0  |
| 3                    | 1       | 0  | 0       | Chicago | M | 65.3 | 98.0  |
| 4                    | 1       | 0  | 0       | Chicago | M | 59.8 | 84.5  |
| 5                    | 0       | 0  | 0       | NewYork | M | 62.8 | 102.5 |
| 6                    | 0       | 0  | 0       | NewYork | M | 63.5 | 102.5 |
| 7                    | 0       | 1  | 0       | NewYork | F | 57.3 | 83.0  |
| 8                    | 0       | 0  | 0       | NewYork | M | 57.5 | 85.0  |

You can now proceed to call PROC MCMC using this input data set Input\_mcmc and the corresponding dummy variables.

PROC TRANSREG automatically creates a macro variable, &\_TRGIND, which contains a list of variable names that it creates. The %put &\_trgind; statement prints the following:

```
CityChicago GF CityChicagoGF
```

The macro variable &\_TRGIND can come handy if you want to build a regression model; you can refer to &\_TRGIND in the following way:

```
proc mcmc data=input_mcmc;
 array data[5] 1 &_trgind x;
 array beta[5] beta0-beta4;
 ...;
 call mult(beta, data, mu);
 ...;
```

The first ARRAY statement defines a one-dimensional array of length 5, and it takes on five values: a constant 1 and variables CityChicago, GF, CityChicagoGF, and x. The second ARRAY statement defines an array of beta, which are the model parameters. Later in the program, you can use the CALL MULT function to calculate the regression mean and store the value in the symbol mu.

## Modeling Joint Likelihood

PROC MCMC assumes that the input observations are independent and that the joint log likelihood is the sum of individual log-likelihood functions. You specify the log likelihood of one observation in the **MODEL** statement. PROC MCMC evaluates that function for each observation in the data set and cumulatively sums them up. If observations are not independent of each other, this summation produces the incorrect log likelihood.

There are two ways to model dependent data. You can either use the DATA step LAG function or use the PROC option **JOINTMODEL**. The LAG function returns values of a variable from a queue. As PROC MCMC steps through the data set, the LAG function queues each data set variable, and you have access to the current value as well as to all previous values of any variable. If the log likelihood for observation  $x_i$  depends only on observations 1 to  $i$  in the data set, you can use this SAS function to construct the log-likelihood function for each observation. Note that the LAG function enables you to access observations from different rows, but the log-likelihood function in the **MODEL** statement must be generic enough that it applies to all observations. See “[Example 55.14: Time Independent Cox Model](#)” on page 4617 and “[Example 55.15: Time Dependent Cox Model](#)” on page 4625 for how to use this LAG function.

A second option is to create arrays, store all relevant variables in the arrays, and construct the joint log likelihood for the entire data set instead of for each observation. Following is a simple example that illustrates the usage of this option. For a more realistic example that models dependent data, see “[Example 55.14: Time Independent Cox Model](#)” on page 4617 and “[Example 55.15: Time Dependent Cox Model](#)” on page 4625.

```
/* allocate the sample size. */
data exi;
 call streaminit(17);
 do ind = 1 to 100;
 y = rand("normal", 2.3, 1);
 output;
 end;
run;
```

The log-likelihood function for each observation is as follows:

$$\log(f(y_i|\mu, \sigma)) = \log(\phi(y_i; \mu, \text{var} = \sigma^2))$$

The joint log-likelihood function is as follows:

$$\log(f(\mathbf{y}|\mu, \sigma)) = \sum_i \log(\phi(y_i; \mu, \text{var} = \sigma^2))$$

The following statements fit a simple model with an unknown mean ( $\mu$ ) in PROC MCMC, with the variance in the likelihood assumed known. The **MODEL** statement indicates a normal likelihood for each observation  $y$ .

```
proc mcmc data=exi seed=7 outpost=p1;
 parm mu;
 prior mu ~ normal(0, sd=10);
 model y ~ normal(mu, sd=1);
run;
```

The following statements show how you can specify the log-likelihood function for the entire data set:

```

data a;
run;

proc mcmc data=a seed=7 outpost=p2 jointmodel;
 array data[1] / nosymbols;
 begincnst;
 rc = read_array("exi", data, "y");
 n = dim(data, 1);
 endcnst;

 parm mu;
 prior mu ~ normal(0, sd=10);
 ll = 0;
 do i = 1 to n;
 ll = ll + lpdfnorm(data[i], mu, 1);
 end;
 model general(ll);
run;

```

The **JOINTMODEL** option indicates that the function used in the **MODEL** statement calculates the log likelihood for the entire data set, rather than just for one observation. Given this option, PROC MCMC no longer steps through the input data during the simulation. Consequently, you can no longer use any data set variables to construct the log-likelihood function. Instead, you store the data set in arrays and use arrays instead of data set variables to calculate the log likelihood.

The **ARRAY** statement allocates a temporary array (data). The **READ\_ARRAY** function selects the y variable from the **exi** data set and stores it in the data array. See the section “**READ\_ARRAY Function**” on page 4442. In the programming statements, you use a **DO** loop to construct the joint log likelihood. The expression **ll** in the **GENERAL** function now takes the value of the joint log likelihood for all data.

You can run the following statements to see that two PROC MCMC runs produce identical results.

```

proc compare data=p1 compare=p2;
 var mu;
run;

```

---

## Regenerating Diagnostics Plots

By default, PROC MCMC generates three plots: the trace plot, the autocorrelation plot, and the kernel density plot. Unless ODS Graphics is enabled before calling the procedure, it is hard to generate the same graph afterwards. Directly using the **Stat.MCMC.Graphics.TraceAutocorrDensity** template is not feasible. The easiest way to regenerate the same graph is with the **%TADPlot** autocall macro. The **%TADPlot** macro requires you to specify an input data set (which usually is the output data set from a previous PROC MCMC call) and a list of variables that you want to plot.

For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

A simple regression example, with three parameters, is used here for illustrational purposes. For an explanation of the regression model and the data involved, see the section “Simple Linear Regression” on page 4408. The following statements generate a SAS data set and fit a regression model:

```

title 'Regenerating Diagnostics Plots';

data Class;
 input Name $ Height Weight @@;
 datalines;
Alfred 69.0 112.5 Alice 56.5 84.0 Barbara 65.3 98.0
Carol 62.8 102.5 Henry 63.5 102.5 James 57.3 83.0
Jane 59.8 84.5 Janet 62.5 112.5 Jeffrey 62.5 84.0
John 59.0 99.5 Joyce 51.3 50.5 Judy 64.3 90.0
Louise 56.3 77.0 Mary 66.5 112.0 Philip 72.0 150.0
Robert 64.8 128.0 Ronald 67.0 133.0 Thomas 57.5 85.0
William 66.5 112.0
;

ods select none;
proc mcmc data=class nmc=50000 thin=5 outpost=classout seed=246810;
 parms beta0 0 beta1 0;
 parms sigma2 1;
 prior beta0 beta1 ~ normal(0, var = 1e6);
 prior sigma2 ~ igamma(3/10, scale = 10/3);
 mu = beta0 + beta1*height;
 model weight ~ normal(mu, var = sigma2);
run;
ods select all;

```

The output data set Classout contains posterior draws for beta0, beta1, and sigma2. It also stores the log of the prior density (LogPrior), log of the likelihood (LogLike), and the log of the posterior density (LogPost). If you want to examine the beta0 and LogPost variable, you can use the following statements to generate the graphs:

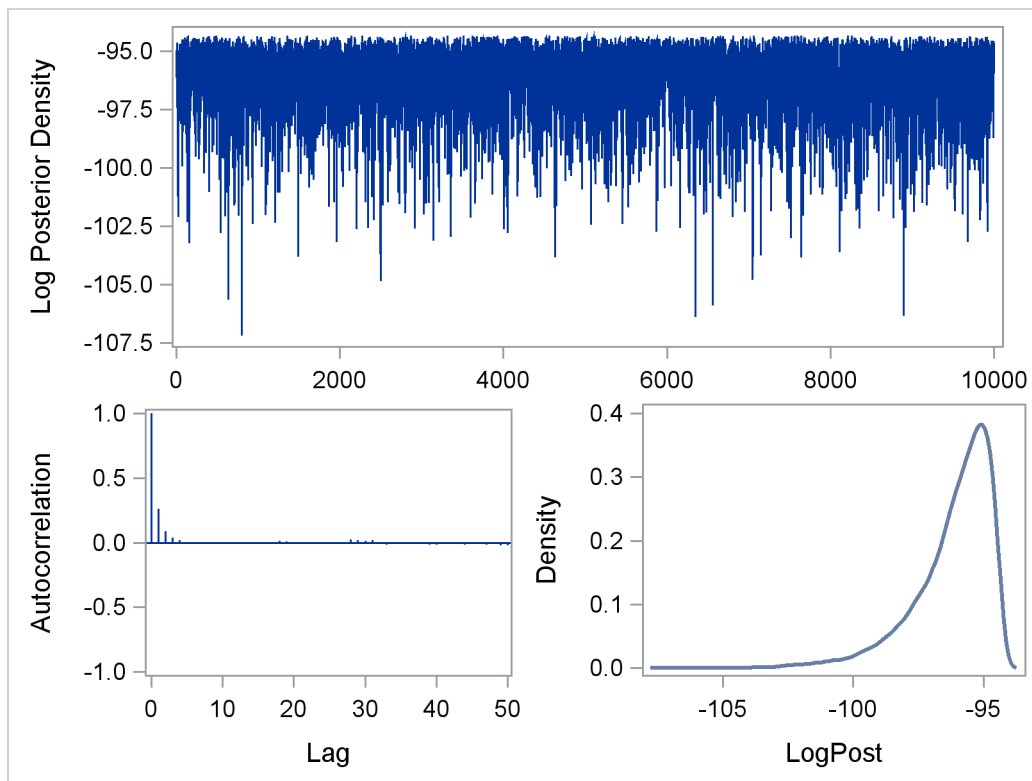
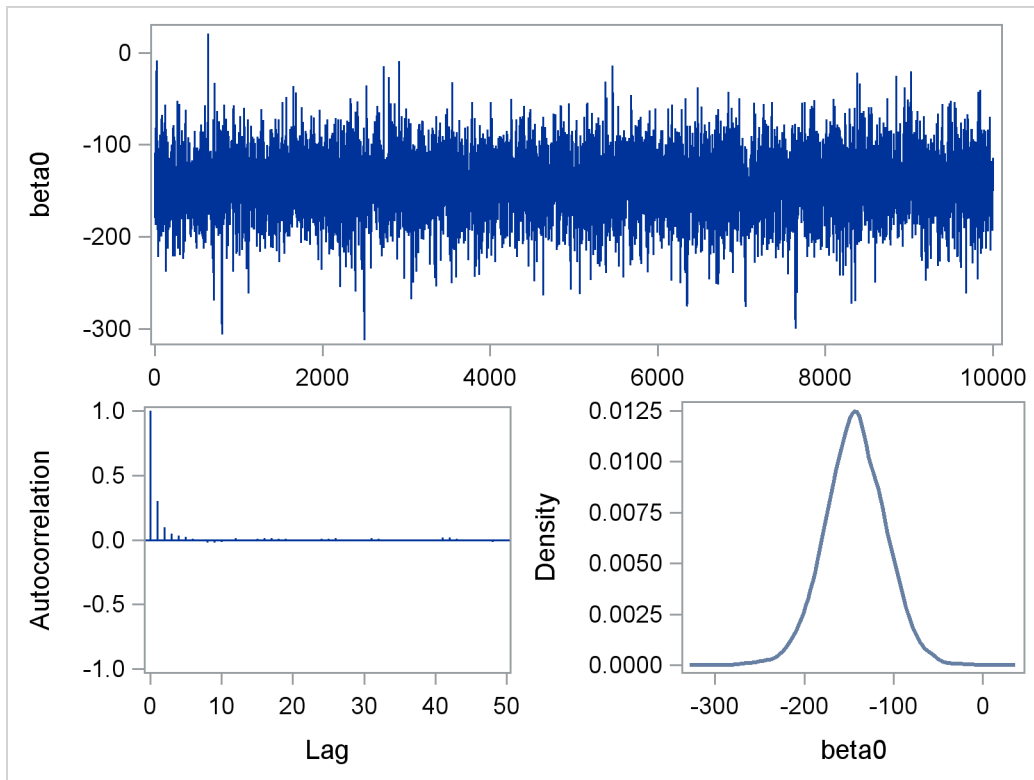
```

ods graphics on;
%tadplot(data=classout, var=beta0 logpost);
ods graphics off;

```

Figure 55.16 displays the regenerated diagnostics plots for variables beta0 and Logpost from the data set Classout.

**Figure 55.16** Regenerated Diagnostics Plots for beta0 and Logpost



## Caterpillar Plot

The caterpillar plot is a side-by-side bar plot of 95% intervals for multiple parameters. Typically, it is used to visualize and compare random-effects parameters, which can come in large numbers in certain models. You can use the %CATER autocall macro to create a caterpillar plot. The %CATER macro requires you specify an input data set and a list of variables that you want to plot.

A random-effects model that has 21 random-effects parameters is used here for illustrational purpose. For an explanation of the random-effects model and the data involved, see “[Example 55.7: Logistic Regression Random-Effects Model](#)” on page 4579. The following statements generate a SAS data set and fit the model:

```

title 'Create a Caterpillar Plot';

data seeds;
 input r n seed extract @@;
 ind = _N_;
 datalines;
10 39 0 0 23 62 0 0 23 81 0 0 26 51 0 0
17 39 0 0 5 6 0 1 53 74 0 1 55 72 0 1
32 51 0 1 46 79 0 1 10 13 0 1 8 16 1 0
10 30 1 0 8 28 1 0 23 45 1 0 0 4 1 0
 3 12 1 1 22 41 1 1 15 30 1 1 32 51 1 1
 3 7 1 1
;

ods select none;
proc mcmc data=seeds outpost=postout seed=332786 nmc=20000;
 parms beta0 0 beta1 0 beta2 0 beta3 0 s2 1;
 prior s2 ~ igamma(0.01, s=0.01);
 prior beta: ~ general(0);
 w = beta0 + beta1*seed + beta2*extract + beta3*seed*extract;
 random delta ~ normal(w, var=s2) subject=ind;
 pi = logistic(delta);
 model r ~ binomial(n = n, p = pi);
run;
ods select all;

```

The output data set Postout contains posterior draws for all 21 random-effects parameters, delta\_1 ... delta\_21. You can use the following statements to generate a caterpillar plot for the 21 parameters:

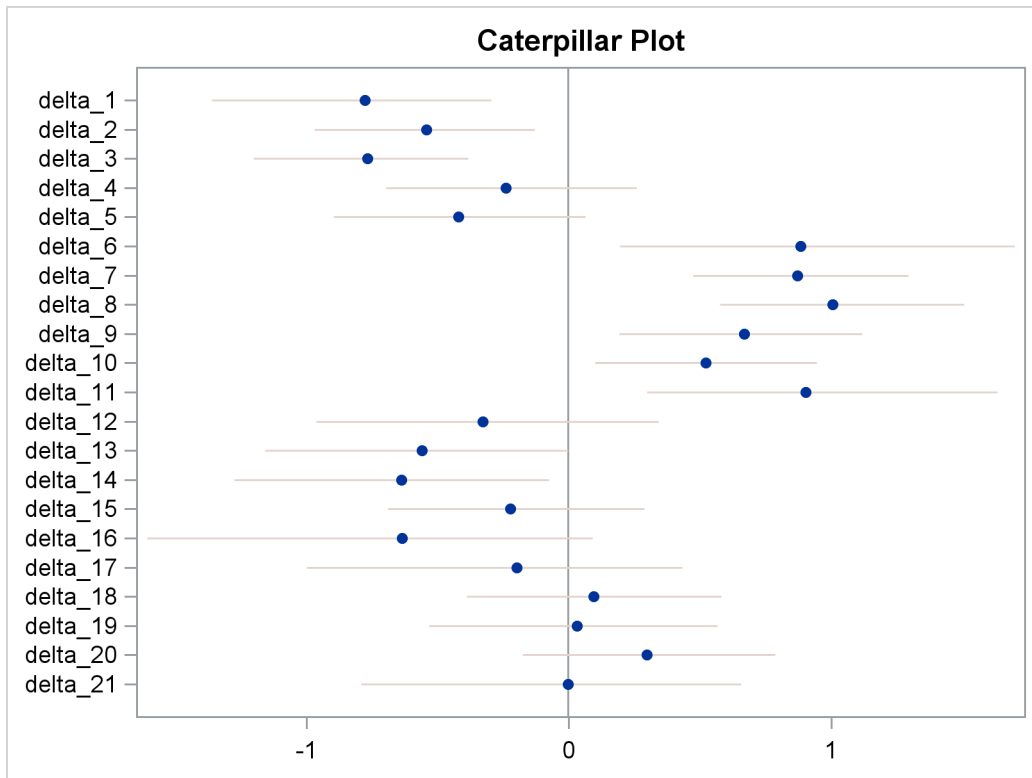
```

ods graphics on;
%CATER(data=postout, var=delta:);
ods graphics off;

```

Figure 55.17 is a caterpillar plot of the random-effects parameters delta\_1–delta\_21.

Figure 55.17 Caterpillar Plot of the Random-Effects Parameters



If you want to change the display of the caterpillar plot, such as using a different line pattern, color, or size of the markers, you need to first modify the `Stat.MCMC.Graphics.Caterpillar` template and then call the `%CATER` macro again.

You can use the following statements to view the source of the `Stat.MCMC.Graphics.Caterpillar` template:

```
proc template;
 path sashelp.tmplmst;
 source Stat.MCMC.Graphics.Caterpillar;
run;
```

Figure 55.18 lists the source statements of the template that is used to generate the template for the caterpillar plot.



**Figure 55.18** Source Statements for Stat.MCMC.Graphics.Caterpillar Template

```

define statgraph Stat.MCMC.Graphics.Caterpillar;
 dynamic _OverallMean _VarName _VarMean _XLower _XUpper _byline_ _bytitle_
 byfootnote;
 begingraph;
 entrytitle "Caterpillar Plot";
 layout overlay / yaxisopts=(offsetmin=0.05 offsetmax=0.05 display=(line
 ticks tickvalues)) xaxisopts=(display=(line ticks tickvalues));
 referenceline x=_OVERALLMEAN / lineattrs=(color=
 GraphReference:ContrastColor);
 HighLowPlot y=_VARNAME high=_XUPPER low=_XLOWER / lineattrs=
 GRAPHCONFIDENCE;
 scatterplot y=_VARNAME x=_VARMEAN / markerattrs=(size=5 symbol=
 circlefilled);
 endlayout;
 if (_BYTITLE_)
 entrytitle _BYLINE_ / textattrs=GRAPHVALUETEXT;
 else
 if (_BYFOOTNOTE_)
 entryfootnote halign=left _BYLINE_;
 endif;
 endif;
endgraph;
end;

```

You can use the `TEMPLATE` procedure (see Chapter 21, “Statistical Graphics Using ODS”) to run any modified SAS/GRAPH graph template definition and then call the `%CATER` macro again. The `%CATER` macro picks up the change you made to the Caterpillar template and displays the new graph accordingly.

## Autocall Macros for Postprocessing

Although PROC MCMC provides a number of convergence diagnostic tests and posterior summary statistics, PROC MCMC performs the calculations only if you specify the options in advance. If you wish to analyze the posterior draws of unmonitored parameters or functions of the parameters that are calculated in later DATA step calls, you can use the autocall macros in Table 55.44.

**Table 55.44** Postprocessing Autocall Macros

| Macro                            | Description                   |
|----------------------------------|-------------------------------|
| <code>%ESS</code>                | Effective sample sizes        |
| <code>%GEWEKE<sup>4</sup></code> | Geweke diagnostic             |
| <code>%HEIDEL<sup>4</sup></code> | Heidelberger-Welch diagnostic |
| <code>%MCSE</code>               | Monte Carlo standard errors   |
| <code>%RAFTERY</code>            | Raftery diagnostic            |
| <code>%POSTACF</code>            | Autocorrelation               |
| <code>%POSTCOR</code>            | Correlation matrix            |

<sup>4</sup>The `%GEWEKE` and `%HEIDEL` macros use a different optimization routine than that used in PROC MCMC. As a result, there might be numerical differences in some cases, especially when the sample size is small.

**Table 55.44** (continued)

| Macro    | Description                  |
|----------|------------------------------|
| %POSTCOV | Covariance matrix            |
| %POSTINT | Equal-tail and HPD intervals |
| %POSTSUM | Summary statistics           |

Table 55.45 lists options that are shared by all postprocessing autocall macros. See Table 55.46 for macro-specific options.

**Table 55.45** Shared Options

| Option            | Description                                                             |
|-------------------|-------------------------------------------------------------------------|
| DATA=SAS-data-set | Input data set that contains posterior samples                          |
| VAR=variable-list | Specifies the variables on which you want to carry out the calculation. |
| PRINT=YES   NO    | Displays the results. The default is YES.                               |
| OUT=SAS-data-set  | Specifies a name for the output SAS data set to contain the results.    |

Suppose that the data set that contains posterior samples is called `post` and that the variables of interest are defined in the macro variable `&PARMS`. The following statements call the `%ESS` macro and calculates the effective sample sizes for each variable:

```
%let parms = alpha beta u_1-u_17;
%ESS(data=post, var=&parms);
```

By default, the ESS estimates are displayed. You can choose not to display the result and save the output to a data set with the following statement:

```
%ESS(data=post, var=&parms, print=NO, out=eout);
```

Some of the macros can take additional options, which are listed in Table 55.46.

**Table 55.46** Macro-Specific Options

| Macro   | Option             | Description                                                                                                                                                                                           |
|---------|--------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| %ESS    | AUTOCORLAG=numeric | Specifies the maximum number of autocorrelation lags used in computing the ESS estimates. By default, AUTOCORLAG=MIN(500, NOBS/4), where NOBS is the sample size of the input data set.               |
|         | HIST=YES NO        | Displays a histogram of all ESS estimates. The default is NO.                                                                                                                                         |
| %HEIDEL | SALPHA=numeric     | Specifies the $\alpha$ level for the stationarity test. By default, SALPHA=0.05.                                                                                                                      |
|         | HALPHA=numeric     | Specifies the $\alpha$ level for the halfwidth test. By default, HALPHA=0.05.                                                                                                                         |
|         | EPS=numeric        | Specifies a small positive number $\epsilon$ such that if the halfwidth is less than $\epsilon$ times the sample mean of the remaining iterations, the halfwidth test is passed. By default, EPS=0.1. |

Table 55.46 (continued)

| Option   | Description                      |                                                                                                                                                                                                                |
|----------|----------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| %GEWEKE  | FRAC1= <i>numeric</i>            | Specifies the earlier portion of the Markov chain used in the test. By default, FRAC1=0.1.                                                                                                                     |
|          | FRAC2= <i>numeric</i>            | Specifies the latter portion of the Markov chain used in the test. By default, FRAC2=0.5.                                                                                                                      |
| %MCSE    | AUTOCORLAG= <i>numeric</i>       | Specifies the maximum number of autocorrelation lags used in computing the Monte Carlo standard error estimates. By default, AUTOCORLAG=MIN(500, NOBS/4), where NOBS is the sample size of the input data set. |
| %RAFTERY | Q= <i>numeric</i>                | Specifies the order of the quantile of interest. By default, Q=0.025.                                                                                                                                          |
|          | R= <i>numeric</i>                | Specifies the margin of error for measuring the accuracy of estimation of the quantile. By default, R=0.005.                                                                                                   |
|          | S= <i>numeric</i>                | Specifies the probability of attaining the accuracy of the estimation of the quantile. By default, S=0.95.                                                                                                     |
|          | EPS= <i>numeric</i>              | Specifies the tolerance level for the stationary test. By default, EPS=0.001.                                                                                                                                  |
| %POSTACF | LAGS=%str( <i>numeric-list</i> ) | Specifies autocorrelation lags calculated. The default values are 1, 5, 10, and 50.                                                                                                                            |
| %POSTINT | ALPHA= <i>value</i>              | Specifies the $\alpha$ level ( $0 < \alpha < 1$ ) for the interval estimates. By default, ALPHA=0.05.                                                                                                          |

For example, the following statement calculates and displays autocorrelation at lags 1, 6, 11, 50, and 100. Note that the lags in the *numeric-list* need to be separated by commas “,”.

```
%PostACF(data=post, var=&parms, lags=%str(1 to 15 by 5, 50, 100));
```

## Gamma and Inverse-Gamma Distributions

The gamma and inverse gamma distributions are widely used in Bayesian analysis. With their respective scale and inverse scale parameterizations, they are a frequent source of confusion in the field. This section aims to clarify their parameterizations and common usages.

The gamma distribution is often used as the conjugate prior for the precision parameter ( $\tau = 1/\sigma^2$ ) in a normal distribution. See Table 55.19 in the section “Standard Distributions” on page 4476 for the density definitions. You can specify the distribution in two ways:

- `gamma(shape=, scale=)` which has mean  $\text{shape} \cdot \text{scale}$  and variance  $\text{shape} \cdot \text{scale}^2$
- `gamma(shape=, iscale=)` which has mean  $\frac{\text{shape}}{\text{iscale}}$  and variance  $\frac{\text{shape}}{\text{iscale}^2}$

The parameterization of the gamma distribution that is preferred by most Bayesian analysts is to have the same number in both hyperparameter positions, which results in a prior distribution that has mean 1. To do this, you should use the `iscale=` parameterization. In addition, if you choose a small value (for example,

0.01), the prior distribution takes on a large variance (100 in this example). To specify this prior in PROC MCMC, use `gamma(shape=0.01, iscale=0.01)`<sup>5</sup>, *not* `gamma(shape=0.01, scale=0.01)`.

If you specify the `scale=` parameterization, as in `gamma(shape=0.01, scale=0.01)`, you would get a prior distribution that has mean 0.0001 and variance 0.000001. This would lead to a completely different posterior inference: the prior would push the precision parameter estimate close to 0, or the variance estimate to a large value.

The inverse-gamma distribution is often used as the conjugate prior of the variance parameter ( $\sigma^2$ ) in a normal distribution. See Table 55.22 in the section “Standard Distributions” on page 4476 for the density definitions. Similar to the gamma distribution, you can specify the inverse-gamma distribution in two ways:

- `igamma(shape=, scale=)`
- `igamma(shape=, iscale=)`

The inverse gamma distribution does not have a mean when the shape parameter is less than or equal to 1 and does not have a variance when the shape parameter is less than or equal to 2.

A gamma prior distribution on the precision is the equivalent to an inverse gamma prior distribution on the variance. The equivalency is the following:

$$\tau \sim \text{gamma}(\text{shape}=0.01, \text{iscale}=0.01) \Leftrightarrow \sigma^2 \sim \text{igamma}(\text{shape}=0.01, \text{scale}=0.01)$$

**NOTE:** This mnemonic might help you remember the parameterization scheme of the distributions. If you prefer to have identical hyperparameter values in the distribution, you should specify one and only one “i.”. When the “i” appears in the `igamma` distribution name for the variance parameter, choose the `scale=` parameterization; when the “i” appears in the `iscale=` parameterization, choose the `gamma` distribution for the precision parameter.

If you are not sure about the choices of other hyperparameter values and what type of prior distributions they induce, you can write a simple PROC MCMC program and see the distributions as in the following example:

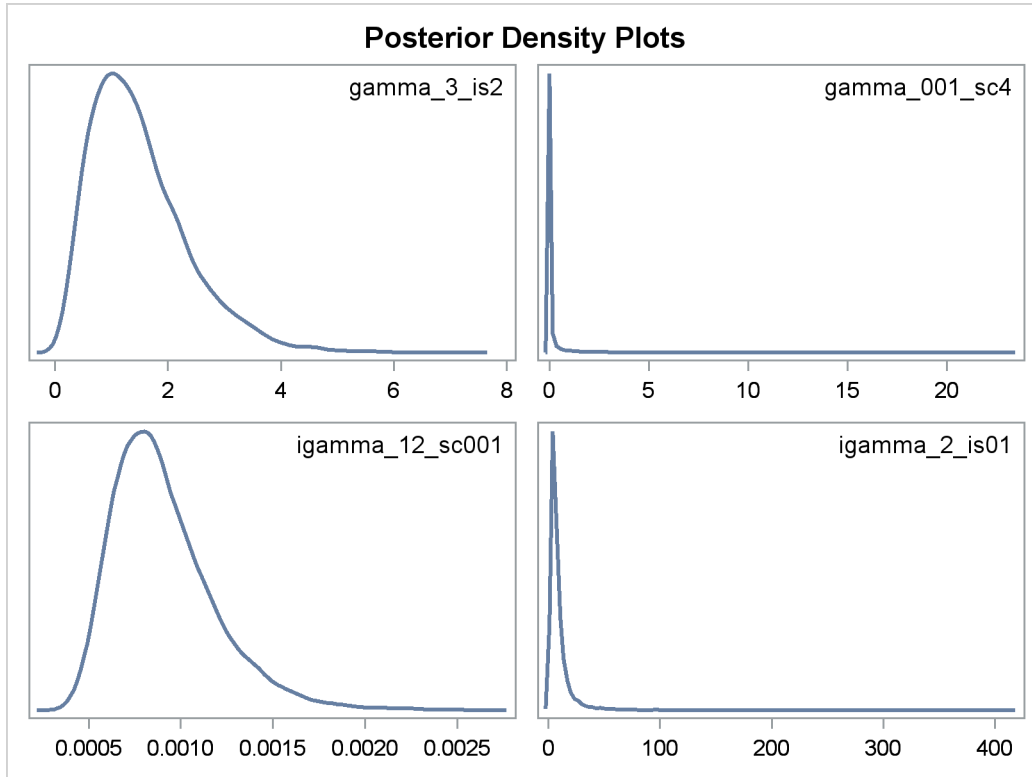
```
data a;
run;

ods graphics on;
ods select DensityPanel;
proc mcmc data=a stats=none diag=none nmc=10000 outpost=gout
 plots=density seed=1;
 parms gamma_3_is2 gamma_001_sc4 igamma_12_sc001 igamma_2_is01;
 prior gamma_3_is2 ~ gamma(shape=3, iscale=2);
 prior gamma_001_sc4 ~ gamma(shape=0.01, scale=4);
 prior igamma_12_sc001 ~ igamma(shape=12, scale=0.01);
 prior igamma_2_is01 ~ igamma(shape=2, iscale=0.1);
 model general(0);
run;
ods graphics off;
```

<sup>5</sup>Specifying the same number at both positions and choosing a small value has been popularized by the WinBUGS software program. The WinBUGS’s distribution specification of `dgamma(0.01, 0.01)` is equivalent to specifying `gamma(shape=0.01, iscale=0.01)` in PROC MCMC.

The preceding statements specify four different gamma and inverse gamma distributions with various scale and inverse scale parameter values. The output of kernel density plots of these four prior distributions is shown in Figure 55.19. Note how the X axis scales vary across different distributions.

**Figure 55.19** Density Plots of Different Gamma and Inverse Gamma Distributions



## Posterior Predictive Distribution

The posterior predictive distribution

$$p(\mathbf{y}_{\text{pred}}|\mathbf{y}) = \int p(\mathbf{y}_{\text{pred}}|\theta)p(\theta|\mathbf{y})d\theta$$

can often be used to check whether the model is consistent with data. For more information about using predictive distribution as a model checking tool, see Gelman et al. 2004, Chapter 6 and the bibliography in that chapter. The idea is to generate replicate data from  $p(\mathbf{y}_{\text{pred}}|\mathbf{y})$ —call them  $\mathbf{y}_{\text{pred}}^i$ , for  $i = 1, \dots, M$ , where  $M$  is the total number of replicates—and compare them to the observed data to see whether there are any large and systematic differences. Large discrepancies suggest a possible model misfit. One way to compare the replicate data to the observed data is to first summarize the data to some test quantities, such as the mean, standard deviation, order statistics, and so on. Then compute the tail-area probabilities of the test statistics (based on the observed data) with respect to the estimated posterior predictive distribution that uses the  $M$  replicate  $\mathbf{y}_{\text{pred}}$  samples.

Let  $T(\cdot)$  denote the function of the test quantity,  $T(\mathbf{y})$  the test quantity that uses the observed data, and  $T(\mathbf{y}_{\text{pred}}^i)$  the test quantity that uses the  $i$ th replicate data from the posterior predictive distribution. You

calculate the tail-area probability by using the following formula:

$$\Pr(T(\mathbf{y}_{\text{pred}}) > T(\mathbf{y})|\theta)$$

The following example shows how you can use PROC MCMC to estimate this probability.

### An Example for the Posterior Predictive Distribution

This example uses a normal mixed model to analyze the effects of coaching programs for the scholastic aptitude test (SAT) in eight high schools. For the original analysis of the data, see Rubin (1981). The presentation here follows the analysis and posterior predictive check presented in Gelman et al. (2004). The data are as follows:

```

title 'An Example for the Posterior Predictive Distribution';

data SAT;
 input effect se @@;
 ind=_n_;
 datalines;
28.39 14.9 7.94 10.2 -2.75 16.3
6.82 11.0 -0.64 9.4 0.63 11.4
18.01 10.4 12.16 17.6
;

```

The variable `effect` is the reported test score difference between coached and uncoached students in eight schools. The variable `se` is the corresponding estimated standard error for each school. In a normal mixed effect model, the variable `effect` is assumed to be normally distributed:

$$\text{effect}_i \sim \text{normal}(\mu_i, \text{se}^2) \quad \text{for } i = 1, \dots, 8$$

The parameter  $\mu_i$  has a normal prior with hyperparameters  $(m, v)$ :

$$\mu_i \sim \text{normal}(m, \text{var} = v)$$

The hyperprior distribution on  $m$  is a uniform prior on the real axis, and the hyperprior distribution on  $v$  is a uniform prior from 0 to infinity.

The following statements fit a normal mixed model and use the `PREDDIST` statement to generate draws from the posterior predictive distribution.

```

ods listing close;
proc mcmc data=SAT outpost=out nmc=40000 seed=12;
 parms m 0;
 parms v 1 /slice;
 prior m ~ general(0);
 prior v ~ general(1, lower=0);
 random mu ~ normal(m, var=v) subject=ind monitor=(mu);
 model effect ~ normal(mu, sd=se);
 preddist outpred=pout nsim=5000;
run;
ods listing;

```

The ODS LISTING CLOSE statement disables the listing output because you are primarily interested in the samples of the predictive distribution. The `HYPER`, `PRIOR`, and `MODEL` statements specify the Bayesian model of interest. The `PREDDIST` statement generates samples from the posterior predictive distribution and stores the samples in the Pout data set. The predictive variables are named `effect_1`, `...`, `effect_8`. When no `COVARIATES` option is specified, the covariates in the original input data set SAT are used in the prediction. The `NSIM=` option specifies the number of predictive simulation iterations.

The following statements use the Pout data set to calculate the four test quantities of interest: the average (mean), the sample standard deviation (sd), the maximum effect (max), and the minimum effect (min). The output is stored in the Pred data set.

```
data pred;
 set pout;
 mean = mean(of effect:);
 sd = std(of effect:);
 max = max(of effect:);
 min = min(of effect:);
run;
```

The following statements compute the corresponding test statistics, the mean, standard deviation, and the minimum and maximum statistics on the real data and store them in macro variables. You then calculate the tail-area probabilities by counting the number of samples in the data set Pred that are greater than the observed test statistics based on the real data.

```
proc means data=SAT noprint;
 var effect;
 output out=stat mean=mean max=max min=min stddev=sd;
run;

data _null_;
 set stat;
 call symputx('mean',mean);
 call symputx('sd',sd);
 call symputx('min',min);
 call symputx('max',max);
run;

data _null_;
 set pred end=eof nobs=nobs;
 ctmean + (mean>&mean);
 ctmin + (min>&min);
 ctmax + (max>&max);
 ctsd + (sd>&sd);
 if eof then do;
 pmean = ctmean/nobs; call symputx('pmean',pmean);
 pmin = ctmin/nobs; call symputx('pmin',pmin);
 pmax = ctmax/nobs; call symputx('pmax',pmax);
 psd = ctsd/nobs; call symputx('psd',psd);
 end;
run;
```

You can plot histograms of each test quantity to visualize the posterior predictive distributions. In addition, you can see where the estimated  $p$ -values fall on these densities. [Figure 55.20](#) shows the histograms. To

put all four histograms on the same panel, you need to use PROC TEMPLATE to define a new graph template. (See Chapter 21, “Statistical Graphics Using ODS.”) The following statements define the template `twobytwo`:

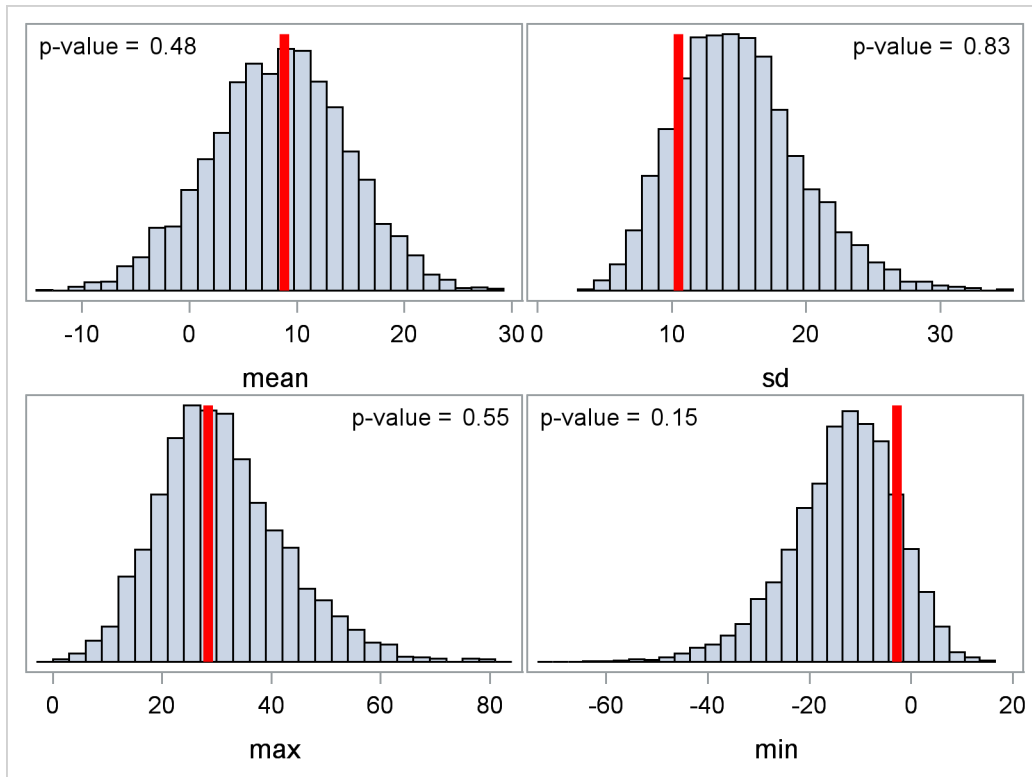
```
proc template;
 define statgraph twobytwo;
 begingraph;
 layout lattice / rows=2 columns=2;
 layout overlay / yaxisopts=(display=none)
 xaxisopts=(label="mean");
 layout gridded / columns=2 border=false
 autoalign=(topleft topright);
 entry halign=right "p-value =";
 entry halign=left eval(strip(put(&pmean, 12.2)));
 endlayout;
 histogram mean / binaxis=false;
 lineparm x=&mean y=0 slope=. /
 lineattrs=(color=red thickness=5);
 endlayout;
 layout overlay / yaxisopts=(display=none)
 xaxisopts=(label="sd");
 layout gridded / columns=2 border=false
 autoalign=(topleft topright);
 entry halign=right "p-value =";
 entry halign=left eval(strip(put(&psd, 12.2)));
 endlayout;
 histogram sd / binaxis=false;
 lineparm x=&sd y=0 slope=. /
 lineattrs=(color=red thickness=5);
 endlayout;
 layout overlay / yaxisopts=(display=none)
 xaxisopts=(label="max");
 layout gridded / columns=2 border=false
 autoalign=(topleft topright);
 entry halign=right "p-value =";
 entry halign=left eval(strip(put(&pmax, 12.2)));
 endlayout;
 histogram max / binaxis=false;
 lineparm x=&max y=0 slope=. /
 lineattrs=(color=red thickness=5);
 endlayout;
 layout overlay / yaxisopts=(display=none)
 xaxisopts=(label="min");
 layout gridded / columns=2 border=false
 autoalign=(topleft topright);
 entry halign=right "p-value =";
 entry halign=left eval(strip(put(&pmin, 12.2)));
 endlayout;
 histogram min / binaxis=false;
 lineparm x=&min y=0 slope=. /
 lineattrs=(color=red thickness=5);
 endlayout;
 endlayout;
 endgraph;
 end;
run;
```



You call PROC SGRENDER to create the graph, which is shown in Figure 55.20. (See the SGRENDER procedure in the *SAS/GRAPH: Statistical Graphics Procedures Guide*.) There are no extreme  $p$ -values observed; this supports the notion that the predicted results are similar to the actual observations and that the model fits the data.

```
proc sgrender data=pred template=twobytwo;
run;
```

**Figure 55.20** Posterior Predictive Distribution Check for the SAT example



Note that the posterior predictive distribution is not the same as the prior predictive distribution. The prior predictive distribution is  $p(\mathbf{y})$ , which is also known as the marginal distribution of the data. The prior predictive distribution is an integral of the likelihood function with respect to the prior distribution

$$p(\mathbf{y}_{\text{pred}}) = \int p(\mathbf{y}_{\text{pred}}|\theta)p(\theta)d\theta$$

and the distribution is not conditional on observed data.

## Handling of Missing Data

PROC MCMC automatically augments missing values<sup>6</sup> via the use of the `MODEL` statement. PROC MCMC treats missing values as unknown parameters, assigns distributions to the variables, and incorporates the sampling of the missing data as part of Markov chain.

<sup>6</sup>A missing value is usually, although not necessarily, represented by a single period (.) in the input data set.

(In SAS/STAT 9.3 and earlier releases, by default, PROC MCMC discarded all observations that had missing or partial missing values. PROC MCMC could not model missing values.)

You can use the `MISSING=` option in the PROC MCMC statement to specify how you want PROC MCMC to handle the missing values. If you specify `MISSING=CC` (CC stands for complete cases), PROC MCMC discards all observations that have missing or partial missing values before carrying out the simulation. If you specify `MISSING=AC` (AC stands for all cases), PROC MCMC neither discards any missing values nor augments them.

Generally speaking, there are three types of missing data models, as discussed by Rubin (1976). Also see Little and Rubin (2002) for a comprehensive treatment of missing data analysis. The rest of this section provides an overview of these three types of missing data models and explains how to use PROC MCMC to fit them.

### Missing Completely at Random (MCAR)

Data are said to be MCAR if the probability of a missing value (or the failure of observing a value) does not depend on any other observations in the data set, regardless of whether they are observed or missing. That is, the observed and unobserved values are independent of each other: if  $y_i$  is missing, it is MCAR if the probability of observing  $y_i$  is independent of other  $y_j$  (and other covariates  $x_i$ ) in the data set. Under this assumption, both the observed and unobserved data are random samples of all the data; hence, fitting a model based only on the observed data does not introduce any biases. This type of analysis is called a complete-case analysis. To carry out a complete-case analysis, you must specify `MISSING=CC` in the PROC MCMC statement. (In SAS/STAT 9.3 and earlier, PROC MCMC performed a complete-case analysis when the data contained missing values.)

### Missing at Random (MAR)

Data are said to be MAR if the probability of a missing value can depend on some observed quantities but does not depend on any unobserved data. For example, suppose that  $x_i$  are completely observed for all observations and some  $y_i$  are missing. MAR states that the probability of observing  $y_i$  is independent of other missing  $y_j$  (values that could have been observed) and that it depends only on  $x_i$  (and, potentially, observed  $y_j$ ).

The MAR assumption states that the missing  $y_i$  are no longer random samples and that they need to be modeled (via the likelihood specification of the missing values). At the same time, the independence assumption of the missing values on the unobserved quantities states that the missing mechanism (usually a binary indicator variable such that  $r_i = 1$  if  $y_i$  is missing and  $r_i = 0$  otherwise) can be ignored and does not need to be taken into account. Hence, MAR is sometimes referred to as *ignorably missing*. It is not the missing values that can be ignored, it is the missing mechanism that can be ignored.

By default, PROC MCMC treats the missing data as MAR (this assumes that you do not input a binary indicator variable  $r_i$  and model it specifically): each missing value becomes an extra parameter and PROC MCMC updates it in every iteration. PROC MCMC assumes that both the missing values and observed values arise from the same distribution (which is specified in the `MODEL` statement),

$$\mathbf{y} = \{\mathbf{y}_{\text{obs}}, \mathbf{y}_{\text{mis}}\} \sim f(\mathbf{y}|\theta)$$

where  $\mathbf{y}$  consists of observed ( $\mathbf{y}_{\text{obs}}$ ) and missing ( $\mathbf{y}_{\text{mis}}$ ) values, and  $f(\mathbf{y}|\theta)$  is the likelihood function with parameters  $\theta$ .

You can use the **MODEL** statement to model missing covariates. Using multiple **MODEL** statements enables you to specify, for example, a marginal distribution for missing values in covariate  $x$  and a conditional distribution for the response variable  $y$  given  $x$  as follows:

```
model x ~ normal(alpha, var=s2_x);
model y ~ normal(beta * x, var=s2_y);
```

In each iteration, PROC MCMC draws samples for every missing value in variable  $x$ , then every missing value in variable  $y$ , conditional on the drawn values of the  $x$  variable.

### Missing Not at Random (MNAR)

Data are said to be MNAR if the probability of a missing value depends on unobserved data (or data that could have been observed): the probability that  $y_i$  is missing depends on the missing values of other  $y_j$ . This is a very general scenario that assumes that the missing mechanism is no longer ignorable (it is sometimes referred to as *nonignorably missing*) and that a model for the missing mechanism is required in order to make correct inferences about the model parameters.

Let  $\mathbf{R} = (r_1, \dots, r_n)$  be the missing value indicator for  $\mathbf{Y} = (y_1, \dots, y_n)$ , where  $r_i = 1$  if  $y_i$  is missing and  $r_i = 0$  otherwise. This  $\mathbf{R}$  is usually part of an input data set where you preprocess the response variable and create this missing value indicator variable. Modeling MNAR data implies that you must specify a joint likelihood function over  $\mathbf{R}$  and  $\mathbf{Y}$ :  $f(\mathbf{R}, \mathbf{Y}|\mathbf{X}, \boldsymbol{\theta})$ , where  $\mathbf{X}$  represents the covariates and  $\boldsymbol{\theta}$  represents the model parameters. This joint distribution can be factored in two ways: a pattern-mixture model and a selection model.

The *selection model* factors the joint distribution  $\mathbf{R}$  and  $\mathbf{Y}$  into a marginal distribution for  $\mathbf{Y}$  and a conditional distribution for  $\mathbf{R}$ ,

$$f(\mathbf{R}, \mathbf{Y}|\mathbf{X}, \boldsymbol{\theta}) \propto f(\mathbf{Y}|\mathbf{X}, \boldsymbol{\alpha}) \cdot f(\mathbf{R}|\mathbf{Y}, \mathbf{X}, \boldsymbol{\beta})$$

where  $\boldsymbol{\theta} = (\boldsymbol{\alpha}, \boldsymbol{\beta})$ ,  $f(\mathbf{R}|\mathbf{Y}, \mathbf{X}, \boldsymbol{\alpha})$  is usually a binary model with a logit or probit link that involves regression parameters  $\boldsymbol{\alpha}$ , and  $f(\mathbf{Y}|\mathbf{X}, \boldsymbol{\beta})$  is the sampling distribution that generates  $y_i$  with model parameters  $\boldsymbol{\beta}$ .

The *pattern-mixture model* factors the opposite way, a marginal distribution for  $\mathbf{R}$  and a conditional distribution for  $\mathbf{Y}$ ,

$$f(\mathbf{R}, \mathbf{Y}|\mathbf{X}, \boldsymbol{\theta}) \propto f(\mathbf{R}|\mathbf{X}, \boldsymbol{\gamma}) \cdot f(\mathbf{Y}|\mathbf{R}, \mathbf{X}, \boldsymbol{\delta})$$

where  $\boldsymbol{\theta} = (\boldsymbol{\gamma}, \boldsymbol{\delta})$ .

You can use PROC MCMC to fit either model by specifying multiple **MODEL** statements: one for the marginal distribution and one for the conditional distribution. Suppose that the variable  $r$  is the missing data indicator, which is modeled using a logit model, and that the response variable  $y$  is a Poisson regression that includes the missing variable indicator as one of its covariates. The following statements are a PROC MCMC program that fits a pattern-mixture model:

```
pi = logistic(alpha * x1);
model r ~ binary(pi);
mu = beta0 + beta1 * x2 + beta3 * r;
model y ~ poisson(exp(mu));
```

The first **MODEL** statement uses a binary model with logit link to model the missing mechanism, and the second **MODEL** statement models the response variable with a Poisson regression that includes the missing

value indicator as one of its covariates. Each of the two sets of regression has its covariates and regression coefficients. If this hypothetical data set contained missing values in covariates  $x_1$  and  $x_2$ , you could add two more **MODEL** statements to handle each variable as follows:

```
model x1 ~ normal(mu1, var=s2_x1);
pi = logistic(alpha * x1);
model r ~ binary(pi);
model x2 ~ normal(mu2, var=s2_x2);
mu = beta0 + beta1 * x2 + beta3 * r;
model y ~ poisson(exp(mu));
```

---

## Functions of Random-Effects Parameters

When you specify a **RANDOM** statement in a program, PROC MCMC internally creates a random-effects parameter for every unique value in the **SUBJECT=** variable. You can calculate any transformations of these random-effects parameters by applying SAS functions to the effect, and you can use the transformed variable in the subsequent statements. For example, the following statements perform a logit transformation of an effect:

```
random u ~ normal(mu, var=s2) subject=students;
p = logistic(u);
...
```

The value of the variable  $p$  changes with  $u$  as the procedure steps through the input data set: for different unique values of the **students** variable,  $u$  takes on a different parameter value, and  $p$  changes accordingly.

To save all the transformed values in  $p$  to the **OUTPOST=** data set, you cannot just specify the **MONITOR=(p)** option in the PROC MCMC statement. With such a specification, PROC MCMC can save only one value of  $p$  (usually the value associated with the last observation in the data set); it cannot save all values. To output all transformed values, you must create an array to store every transformation and use the **MONITOR=** option to save the entire array to the **OUTPOST=** data set. The difficult part of the programming involves the creation of the correct array index to use in different types of the **SUBJECT=** variables. The rest of this section describes how to monitor functions of random-effects parameters in different situations.

### Indexing Subject Variable

This subsection describes how to monitor transformation of an effect  $u$  when the **students** variable is an indexing subject variable. An indexing subject variable is an integer variable that takes value from one to the total number of unique subjects in a variable. In other words, the variable can be used as an index in a SAS array. The indexing subject variable does not need to be sorted for the example code in this section to work. An example of an indexing variable takes the values of (1 2 3 4 5 1 2 3 4 5), where the total number of observation is  $n=10$  and the number of unique values is  $m=5$ .

The following statements create an indexing variable **students** in the data set **a**:

```
data a;
 input students @@;
 datalines;
 1 1 2 2 3 3 4 4 5 5 6 6 7 7 8 8 9 9 10 10
;
```

The following statements run a random-effects model without any response variables. There are only random-effects parameters in the model; the program calculates the logit transformation of each effect, saves the results to the `OUTPOST=` data set, and produces [Figure 55.21](#):

```
proc mcmc data=a monitor=(p) diag=none stats=none outpost=a1
 plots=none seed=1;
 array p[10];
 random u ~ n(0, sd=1) subject=students;
 p[students] = logistic(u);
 model general(0);
run;

proc print data=a1(obs=3);
run;
```

The `ARRAY` statement creates an array `p` of size 10, which is the number of unique values in `students`. The `p` array stores all the transformed values. The `RANDOM` statement declares `u` to be an effect with the subject variable `students`. The `P[STUDENTS]` assignment statement calculates the logit transformations of `u` and saves them in appropriate array elements—this is why the `students` variable must be an indexing variable. Because the `students` variable used in the `p[]` array is also the subject variable in the `RANDOM` statement, PROC MCMC can match each random-effects parameter with the corresponding element in array `p`. The `MONITOR=` option monitors all elements in `p` and saves the output to the `a1` data set. The `a1` data set contains variables `p1–p10`. [Figure 55.21](#) shows the first three observations of the `OUTPOST=` data set.

**Figure 55.21** Monitor Functions of Random Effect `u`

| Obs | Iteration | p1     | p2      | p3      | p4      | p5       | p6      | p7       |         |
|-----|-----------|--------|---------|---------|---------|----------|---------|----------|---------|
| 1   | 1         | 0.5050 | 0.7334  | 0.5375  | 0.5871  | 0.6862   | 0.4944  | 0.5740   |         |
| 2   | 2         | 0.5563 | 0.4254  | 0.7260  | 0.5280  | 0.4593   | 0.5797  | 0.5813   |         |
| 3   | 3         | 0.6132 | 0.8031  | 0.4735  | 0.3135  | 0.7047   | 0.5273  | 0.6761   |         |
| Obs |           | p8     | p9      | p10     | u_1     | u_2      | u_3     | u_4      | u_5     |
| 1   | 0.5991    | 0.6812 | 0.8678  | 0.0198  | 1.0120  | 0.1504   | 0.3521  | 0.7826   |         |
| 2   | 0.7360    | 0.9079 | 0.3351  | 0.2261  | -0.3006 | 0.9742   | 0.1120  | -0.1630  |         |
| 3   | 0.2379    | 0.2938 | 0.3986  | 0.4607  | 1.4058  | -0.1060  | -0.7837 | 0.8698   |         |
| Obs |           | u_6    | u_7     | u_8     | u_9     | u_10     | LogReff | LogLike  | LogPost |
| 1   | -0.0225   | 0.2983 | 0.4019  | 0.7595  | 1.8819  | -12.2658 | 0       | -12.2658 |         |
| 2   | 0.3213    | 0.3281 | 1.0253  | 2.2887  | -0.6854 | -13.2393 | 0       | -13.2393 |         |
| 3   | 0.1092    | 0.7361 | -1.1641 | -0.8772 | -0.4112 | -12.3984 | 0       | -12.3984 |         |

The variable `p1` is the logit transformation of the variable `u_1`, `p2` is the logit transformation of the variable `u_2`, and so on.

The same idea works for a `students` variable that is unsorted. The following statements create an unsorted indexing variable `students` with repeated measures in each subject, fit the same model, and produce [Figure 55.22](#):

```

data a;
 input students @@;
 datalines;
 1 1 1 3 5 3 4 5 3 1 5 5 4 4 2 2 2 2 4 3
;
proc mcmc data=a monitor=(p) diag=none stats=none outpost=a1
 plots=none seed=1;
 array p[5];
 random u ~ n(0, sd=1) subject=students;
 p[students] = logistic(u);
 model general(0);
run;

proc print data=a1(obs=3);
run;

```

**Figure 55.22** Monitor Functions of Random Effect u When the students Variable is Unsorted

| Obs | Iteration | p1     | p2     | p3      | p4      | p5      | u_1     |
|-----|-----------|--------|--------|---------|---------|---------|---------|
| 1   | 1         | 0.5050 | 0.6862 | 0.7334  | 0.5871  | 0.5375  | 0.0198  |
| 2   | 2         | 0.4944 | 0.8678 | 0.5740  | 0.6812  | 0.5991  | -0.0225 |
| 3   | 3         | 0.5563 | 0.4593 | 0.4254  | 0.5280  | 0.7260  | 0.2261  |
| Obs | u_3       | u_5    | u_4    | u_2     | LogReff | LogLike | LogPost |
| 1   | 1.0120    | 0.1504 | 0.3521 | 0.7826  | -5.4865 | 0       | -5.4865 |
| 2   | 0.2983    | 0.4019 | 0.7595 | 1.8819  | -6.7793 | 0       | -6.7793 |
| 3   | -0.3006   | 0.9742 | 0.1120 | -0.1630 | -5.1595 | 0       | -5.1595 |

There are five random-effects parameters in this example, and the array p also has five elements. The values p1–p5 are the transformations of u\_1–u\_5, respectively. The u variables are not sorted from u\_1 to u\_5 because PROC MCMC creates the names according to the order by which the subject variable appears in the input data set. Nevertheless, because students is an indexing variable, the first element p[1] stores the transformation that corresponds to **students=1** (which is u\_1), the second element p[2] stores the transformation that corresponds to **students=2**, and so on.

### Non-Indexing Subject Variable

A non-indexing subject variable can take values of character literals (for example, names) or numerals (for example, ZIP code or a person’s weight). This section illustrates how to monitor functions of random-effects parameters in these situations.

Suppose you have unsorted character literals as the subject variable:

```

data a;
 input students$ @@;
 datalines;
 smith john john mary kay smith lizzy ben ben dylan
 ben toby abby mary kay kay lizzy ben dylan mary
;

```

A statement such as following does not work anymore because a character variable cannot be used as an array index:

```
p[students] = logistic(u);
```

In this situation, you usually need to do two things: (1) find out the number of unique values in the subject variable, and (2) create a numeric index variable that replaces the students array index. You can use the following statements to do the first task:

```

proc sql noprint;
 select count(distinct(students)) into :nuniq from a;
quit;
%put &nuniq;

```

The PROC SQL call counts the distinct values in the students variable and saves the count to the macro variable &nuniq. The macro variable is used later to specify the element size of the p array. In this example, the a data set contains 20 observations and 9 unique elements (the value of &nuniq).

The following statements create an Index variable in the a data set that is in the order by which the students names appear in the data set:

```

proc freq data=a order=data noprint;
 tables students / out=_f(keep=students);
run;

proc print data=_f;
run;

data a(drop=n);
 set a;
 do i = 1 to nobs until(students=n);
 set _f(keep=students rename=(students=n)) point=i nobs=nobs;
 Index = i;
 end;
run;

proc print data=a;
run;

```

The PROC FREQ call identifies the unique students names and saves them to the \_f data set, which is displayed in [Figure 55.23](#).

**Figure 55.23** Unique Names in the Variable Students

| Obs | students |
|-----|----------|
| 1   | smith    |
| 2   | john     |
| 3   | mary     |
| 4   | kay      |
| 5   | lizzy    |
| 6   | ben      |
| 7   | dylan    |
| 8   | toby     |
| 9   | abby     |

The DATA step steps through the a data set and creates an Index variable to match the order in which the students names appear in the data set. The new a data set<sup>7</sup> is displayed in [Figure 55.24](#).

**Figure 55.24** New Index Variable in the a Data Set

| Obs | students | Index |
|-----|----------|-------|
| 1   | smith    | 1     |
| 2   | john     | 2     |
| 3   | john     | 2     |
| 4   | mary     | 3     |
| 5   | kay      | 4     |
| 6   | smith    | 1     |
| 7   | lizzy    | 5     |
| 8   | ben      | 6     |
| 9   | ben      | 6     |
| 10  | dylan    | 7     |
| 11  | ben      | 6     |
| 12  | toby     | 8     |
| 13  | abby     | 9     |
| 14  | mary     | 3     |
| 15  | kay      | 4     |
| 16  | kay      | 4     |
| 17  | lizzy    | 5     |
| 18  | ben      | 6     |
| 19  | dylan    | 7     |
| 20  | mary     | 3     |

Student smith is the first subject, and his Index value is one. The same student appears again in the sixth observation, which is given the same Index value. Now, this Index variable can be used to index the p array, in a similar fashion as demonstrated in previous programs:

<sup>7</sup>The programming code that creates and adds the Index variable to the data set a keeps all variables from the original data set and does not discard them.



```

data _f;
 set _f;
 subj = compress('p_'||students);
run;
proc sql noprint;
 select subj into :pnames separated by ' ' from _f;
quit;
%put &pnames;

proc mcmc data=a monitor=(p) diag=none stats=none outpost=a1
 plots=none seed=1;
 array p[&nuniq] &pnames;
 random u ~ n(0, sd=1) subject=students;
 p[index] = logistic(u);
 model general(0);
run;

proc print data=a1(obs=3);
run;

```

The first part of the DATA step and the PROC SQL call create array names for the `p` array that match the subject names in the `students` variable. It is not necessary to include these steps for the PROC MCMC program to work, but it makes the output more readable. The first DATA step steps through the `_f` data set and creates a `subj` variable that concatenates the prefix characters `p_` with the names of the students. The PROC SQL calls put all the `subj` values to a macro called `&pnames`, which looks like the following:

```
p_smith p_john p_mary p_kay p_lizzy p_ben p_dylan p_toby p_abby
```

In the PROC MCMC program, the `ARRAY` statement defines an `p` array with size `&nuniq` (9), and use the macro variable `&pnames` to name the array elements. The `P[INDEX]` assignment statement uses the `index` variable to find the correct array element to store the transformation. Figure 55.25 displays the first few observations of the `OUTPOST=a1` data set.

**Figure 55.25** First Few Observations of the Outpost Data Set

| Obs | Iteration | p_smith | p_john  | p_mary   | p_kay   | p_lizzy  | p_ben   | p_dylan |
|-----|-----------|---------|---------|----------|---------|----------|---------|---------|
| 1   | 1         | 0.5050  | 0.7334  | 0.5375   | 0.5871  | 0.6862   | 0.4944  | 0.5740  |
| 2   | 2         | 0.8678  | 0.5563  | 0.4254   | 0.7260  | 0.5280   | 0.4593  | 0.5797  |
| 3   | 3         | 0.9079  | 0.3351  | 0.6132   | 0.8031  | 0.4735   | 0.3135  | 0.7047  |
| Obs | p_toby    | p_abby  | u_smith | u_john   | u_mary  | u_kay    | u_lizzy | u_ben   |
| 1   | 0.5991    | 0.6812  | 0.0198  | 1.0120   | 0.1504  | 0.3521   | 0.7826  | -0.0225 |
| 2   | 0.5813    | 0.7360  | 1.8819  | 0.2261   | -0.3006 | 0.9742   | 0.1120  | -0.1630 |
| 3   | 0.5273    | 0.6761  | 2.2887  | -0.6854  | 0.4607  | 1.4058   | -0.1060 | -0.7837 |
| Obs | u_dylan   | u_toby  | u_abby  | LogReff  | LogLike | LogPost  |         |         |
| 1   | 0.2983    | 0.4019  | 0.7595  | -9.5761  | 0       | -9.5761  |         |         |
| 2   | 0.3213    | 0.3281  | 1.0253  | -11.2370 | 0       | -11.2370 |         |         |
| 3   | 0.8698    | 0.1092  | 0.7361  | -13.1867 | 0       | -13.1867 |         |         |

There are nine random-effects parameters ( $u_{\text{smith}}$ ,  $u_{\text{john}}$ , and so on). There are nine elements of the  $p$  array ( $p_{\text{smith}}$ ,  $p_{\text{john}}$ , and so on); each is the logit transformation of corresponding  $u$  elements.

You can use the same statements for subject variables that are numeric non-indexing variables. The following statements create a `students` variable that take large numbers that cannot be used as indices to an array. The rest of the program monitors functions of the effect  $u$ . The output is not displayed here.

```

data a;
 call streaminit(1);
 do i = 1 to 20;
 students = rand("poisson", 20);
 output;
 end;
 drop i;
run;

proc sql noprint;
 select count(distinct(students)) into :nuniq from a;
quit;
%put &nuniq;

proc freq data=a order=data noprint;
 tables students / out=_f(keep=students);
run;

data a(drop=n);
 set a;
 do i = 1 to nobs until(students=n);
 set _f(keep=students rename=(students=n)) point=i nobs=nobs;
 Index = i;
 end;
run;

data _f;
 set _f;
 subj = compress('p_'||students);
proc sql noprint;
 select subj into :pnames separated by ' ' from _f;
quit;
%put &pnames;

proc mcmc data=a monitor=(p) diag=none stats=none outpost=a1
 plots=none seed=1;
 array p[&nuniq] &pnames;
 random u ~ n(0, sd=1) subject=students;
 p[index] = logistic(u);
 model general(0);
run;

proc print data=a1(obs=3);
run;

```

---

## Floating Point Errors and Overflows

When performing a Markov chain Monte Carlo simulation, you must calculate a proposed jump and an objective function (usually a posterior density). These calculations might lead to arithmetic exceptions and overflows. A typical cause of these problems is parameters with widely varying scales. If the posterior variances of your parameters vary by more than a few orders of magnitude, the numerical stability of the optimization problem can be severely reduced and can result in computational difficulties. A simple remedy is to rescale all the parameters so that their posterior variances are all approximately equal. Changing the `SCALE=` option might help if the scale of your parameters is much different than one. Another source of numerical instability is highly correlated parameters. Often a model can be reparameterized to reduce the posterior correlations between parameters.

If parameter rescaling does not help, consider the following actions:

- provide different initial values or try a different seed value
- use boundary constraints to avoid the region where overflows might happen
- change the algorithm (specified in programming statements) that computes the objective function

## Problems Evaluating Code for Objective Function

The initial values must define a point for which the programming statements can be evaluated. However, during simulation, the algorithm might iterate to a point where the objective function cannot be evaluated. If you program your own likelihood, priors, and hyperpriors by using SAS statements and the `GENERAL` function in the `MODEL`, `PRIOR`, and `HYPERPRIOR` statements, you can specify that an expression cannot be evaluated by setting the value you pass back through the `GENERAL` function to missing. This tells the PROC MCMC that the proposed set of parameters is invalid, and the proposal will not be accepted. If you use the shorthand notation that the `MODEL`, `PRIOR`, and `HYPERPRIOR` statements provide, this error checking is done for you automatically.

## Long Run Times

PROC MCMC can take a long time to run for problems with complex models, many parameters, or large input data sets. Although the techniques used by PROC MCMC are some of the best available, they are not guaranteed to converge or proceed quickly for all problems. Ill-posed or misspecified models can cause the algorithms to use more extensive calculations designed to achieve convergence, and this can result in longer run times. You should make sure that your model is specified correctly, that your parameters are scaled to the same order of magnitude, and that your data reasonably match the model that you are specifying.

To speed general computations, you should check over your programming statements to minimize the number of unnecessary operations. For example, you can use the proportional kernel in the priors or the likelihood and not add constants in the densities. You can also use the `BEGINCNST` and `ENDCNST` to reduce unnecessary computations on constants, and the `BEGINNODATA` and `ENDNODATA` statements to reduce observation-level calculations.

Reducing the number of blocks (the number of the `PARMS` statements) can speed up the sampling process. A single-block program is approximately three times faster than a three-block program for the same number

of iterations. On the other hand, you do not want to put too many parameters in a single block, because blocks with large size tend not to produce well-mixed Markov chains.

If some parameters satisfy the conditional independence assumption, such as in the random-effects models or latent variable models, consider using the **RANDOM** statement to model these parameters. This statement takes advantage of the conditional independence assumption and can sample a larger number of parameters at a more efficient pace.

## Slow or No Convergence

If the simulator is slow or fails to converge, you can try changing the model as follows:

- Change the number of Monte Carlo iterations (**NMC=**), or the number of burn-in iterations (**NBI=**), or both. Perhaps the chain just needs to run a little longer. Note that after the simulation, you can always use the **DATA** step or the **FIRSTOBS** data set option to throw away initial observations where the algorithm has not yet burned in, so it is not always necessary to set **NBI=** to a large value.
- Increase the number of tuning. The proposal tuning can often work better in large models (models that have more parameters) with larger values of **NTU=**. The idea of tuning is to find a proposal distribution that is a good approximation to the posterior distribution. Sometimes 500 iterations per tuning phase (the default) is not sufficient to find a good approximating covariance.
- Change the initial values to more feasible starting values. Sometimes the proposal tuning starts badly if the initial values are too far away from the main mass of the posterior density, and it might not be able to recover.
- Use the **PROPCOV=** option to start the Markov chain at better starting values. With the **PROPCOV=QUANEW** option, PROC MCMC optimizes the object function and uses the posterior mode as the starting value of the Markov chain. In addition, a quadrature approximation to the posterior mode is used as the proposal covariance matrix. This option works well in many cases and can improve the mixing of the chain and shorten the tuning and burn-in time.
- Parameterize your model to include conjugacy, such as using the gamma prior on the precision parameter in a normal distribution or using an inverse gamma on the variance parameter. For a list of conjugate sampling methods that PROC MCMC supports, see the section “[Conjugate Sampling](#)” on page 4472.
- Change the blocking by using the **PARMS** statements. Sometimes poor mixing and slow convergence can be attributed to highly correlated parameters being in different parameter blocks.
- Modify the target acceptance rate. A target acceptance rate of about 25% works well for many multi-parameter problems, but if the mixing is slow, a lower target acceptance rate might be better.
- Change the initial scaling or the **TUNEWT=** option to possibly help the proposal tuning.
- Consider using a different proposal distribution. If from a trace plot you see that a chain traverses to the tail area and sometimes takes quite a few simulations before it comes back, you can consider using a  $t$  proposal distribution. You can do this by either using the PROC option **PROPDIST=T** or using a **PARMS** statement option **T**.

- Transform parameters and sample on a different scale. For example, if a parameter has a gamma distribution, sample on the logarithm scale instead. A parameter  $a$  that has a gamma distribution is equivalent to  $\log(a)$  that has an egamma distribution, with the same distribution specification. For example, the following two formulations are equivalent:

```
parm a;
prior a ~ gamma(shape = 0.001, scale = 0.001);
```

and

```
parm la;
prior la ~ egamma(shape = 0.001, scale = 0.001);
a = exp(la);
```

See “[Example 55.6: Nonlinear Poisson Regression Models](#)” on page 4570 and “[Example 55.20: Using a Transformation to Improve Mixing](#)” on page 4654. You can also use the logit transformation on parameters that have  $\text{uniform}(0, 1)$  priors. This prior is often used on probability parameters. The logit transformation is as follows:  $q = \log\left(\frac{p}{1-p}\right)$ . The distribution on  $q$  is the Jacobian of the transformation:  $\exp(-q)(1 + \exp(-q))^{-2}$ . Again, the following two formulations are equivalent:

```
parm p;
prior p ~ uniform(0, 1);
```

and

```
parm q;
lp = -q - 2 * log(1 + exp(-q));
prior q ~ general(lp);
p = 1 / (1 + exp(-q));
```

## Precision of Solution

In some applications, PROC MCMC might produce parameter values that are not precise enough. Usually, this means that there were not enough iterations in the simulation. At best, the precision of MCMC estimates increases with the square of the simulation sample size. Autocorrelation in the parameter values deflate the precision of the estimates. For more information about autocorrelations in Markov chains, see the section “[Autocorrelations](#)” on page 152.

---

## Handling Error Messages

PROC MCMC does not have a debugger. This section covers a few ways to debug and resolve error messages.

## Using the PUT Statement

Adding the PUT statement often helps to find errors in a program. The following statements produce an error:

```
data a;
run;

proc mcmc data=a seed=1;
 parms sigma lt w;

 beginnodata;
 prior sigma ~ unif(0.001,100);
 s2 = sigma*sigma;
 prior lt ~ gamma(shape=1, iscale=0.001);
 t = exp(lt);
 c = t/s2;
 d = 1/(s2);
 prior w ~ gamma(shape=c, iscale=d);
 endnodata;

 model general(0);
run;
```

```
ERROR: PROC MCMC is unable to generate an initial value for the
 parameter w. The first parameter in the prior distribution is
 missing.
```

To find out why the shape parameter *c* is missing, you can add the put statement and examine all the calculations that lead up to the assignment of *c*:

```
proc mcmc data=a seed=1;
 parms sigma lt w;

 beginnodata;
 prior sigma ~ unif(0.001,100);
 s2 = sigma*sigma;
 prior lt ~ gamma(shape=1, iscale=0.001);
 t = exp(lt);
 c = t/s2;
 d = 1/(s2);
 put c= t= s2= lt=; /* display the values of these symbols. */
 prior w ~ gamma(shape=c, iscale=d);
 endnodata;

 model general(0);
run;
```

In the log file, you see the following:

```
c=. t=. s2=. lt=.
c=. t=. s2=2500.0500003 lt=1000
c=. t=. s2=2500.0500003 lt=1000
```

```
ERROR: PROC MCMC is unable to generate an initial value for the parameter w.
 The first parameter in the prior distribution is missing.
```

You can ignore the first few lines. They are the results of initial set up by PROC MCMC. The last line is important. The variable `c` is missing because `t` is the exponential of a very large number, 1000, in `lt`. The value 1000 is assigned to `lt` by PROC MCMC because none was given. The gamma prior with shape of 1 and inverse scale of 0.001 has mode 0 (see “[Standard Distributions](#)” on page 4476 for more details). PROC MCMC avoids starting the Markov chain at the boundary of the support of the distribution, and it uses the mean value here instead. The mean of the gamma prior is 1000, hence the problem. You can change how the initial value is generated by using the PROC statement `INIT=RANDOM`. Remember to take out the `put` statement once you identify the problem. Otherwise, you will see a voluminous output in the log file.

## Using the HYPER Statement

You can use the `HYPER` statement to narrow down possible errors in the prior distribution specification. With multiple `PRIOR` statements in a program, you might see the following error message if one of the prior distributions is not specified correctly:

```
ERROR: The initial prior parameter specifications must yield log
 of positive prior density values.
```

This message is displayed when PROC MCMC detects an error in the prior distribution calculation but cannot pinpoint the specific parameter at fault. It is frequently, although not necessarily, associated with parameters that have `GENERAL` or `DGENERAL` distributions. If you have a complicated model with many `PRIOR` statements, finding the parameter at fault can be time consuming. One way is to change a subset of the `PRIOR` statements to `HYPER` statements. The two statements are treated the same in PROC MCMC and the simulation is not affected, but you get a different message if the hyperprior distributions are calculated incorrectly:

```
ERROR: The initial hyperprior parameter specifications must yield
 log of positive hyperprior density values.
```

This message can help you identify more easily which distributions are producing the error, and you can then use the `PUT` statement to further investigate.

---

## Computational Resources

It is impossible to estimate how long it will take for a general Markov chain to converge to its stationary distribution. It takes a skilled and thoughtful analysis of the chain to decide whether it has converged to the target distribution and whether the chain is mixing rapidly enough. In some cases, you might be able to estimate how long a particular simulation might take. The running time of a program that does not have `RANDOM` statements is approximately linear to the following factors: the number of samples in the input data set, the number of simulations, the number of blocks in the program, and the speed of your computer. For an analysis that uses a data set of size `nsamples`, a simulation length of `nsim`, and a block design of

nblocks, PROC MCMC evaluates the log-likelihood function the following number of times, excluding the tuning phase:

$$\text{nsamples} \times \text{nsim} \times \text{nblocks}$$

The faster your computer evaluates a single log-likelihood function, the faster this program runs. Suppose you have nsamples equal to 200, nsim equal to 55,000, and nblocks equal to 3. PROC MCMC evaluates the log-likelihood function approximately  $3.3 \times 10^7$  times. If your computer can evaluate the log likelihood for one observation  $10^6$  times per second, this program takes approximately a half a minute to run. If you want to increase the number of simulations five-fold, the run time increases approximately five-fold.

Each **RANDOM** statement adds one pass through the input data at each iteration. If the Metropolis algorithm is used to sample the random-effects parameter, the conditional density (objective function) is calculated twice per pass through the data, which requires a computational resource that is approximately equivalent to adding two blocks of parameters.

Of course, larger problems take longer than shorter ones, and if your model is amenable to frequentist treatment, then one of the other SAS procedures might be more suitable. With “regular” likelihoods and a lot of data, the results of standard frequentist analysis are often asymptotically equivalent to a Bayesian approach. If PROC MCMC requires too much CPU time, then perhaps another SAS/STAT tool would be suitable.

## Displayed Output

This section describes the output that PROC MCMC displays. For a quick reference of all ODS table names, see the section “[ODS Table Names](#)” on page 4537. ODS tables are arranged under four groups, which are listed in the following sections: “[Model and Data Related ODS Tables](#)” on page 4533, “[Sampling Related ODS Tables](#)” on page 4534, “[Posterior Statistics Related ODS Tables](#)” on page 4535, “[Convergence Diagnostics Related ODS Tables](#)” on page 4535, and “[Optimization Related ODS Tables](#)” on page 4536.

### Model and Data Related ODS Tables

#### ***Missing Data Information Table***

The “Missing Data Information” table (ODS table name MISSDATAINFO) displays the name of the response variable that contains missing values, the number of missing observations, the corresponding observation indices in the input data set, and the sampling method used in the simulation for the missing values.

#### ***Number of Observation Table***

The “NObs” table (ODS table name NOBS) shows the number of observations that is in the data set and the number of observations that is used in the analysis. By default, observations with missing values are not used (see the section “[Handling of Missing Data](#)” on page 4518 for more details). This table is displayed by default.

#### ***Parameters***

The “Parameters” table (ODS table name Parameters) shows the name of each parameter, the block number of each parameter, the sampling method used for the block, the initial values, and the prior or hyperprior distributions. This table is displayed by default.



**REObsInfo**

The “Random Effect Observation Information” table (ODS table name REObsInfo) lists the name of the random effect, each subject value, the number of observations in each subject, and their corresponding observation indices in the input data set. You can request this table by specifying the **REOBSINFO** option.

**REParameters**

The “REParameters” table (ODS table name REParameters) lists the name of the random effect, sampling algorithm, the subject variable, the number of subjects, unique values of the subject variable, and the prior distribution. This table is displayed by default if a **RANDOM** statement is used in the program.

**Sampling Related ODS Tables****Burn-In History**

The “Burn-In History” table (ODS table name BurnInHistory) shows the scales and acceptance rates for each parameter block in the burn-in phase. The table is not displayed by default and can be requested by specifying the option **MCHISTORY=BRIEF | DETAILED**.

**Parameters Initial Value Table**

The “Parameters Initial” table (ODS table name ParametersInit) shows the value of each parameter after the tuning phase. This table is not displayed by default and can be requested by specifying the option **INIT=PINIT**.

**Posterior Samples**

The “Posterior Samples” table (ODS table name PosteriorSample) stores posterior draws of all parameters. It is not printed by PROC MCMC. You can create an ODS output data set of the chain by specifying the following:

```
ODS OUTPUT PosteriorSample = SAS-data-set;
```

**Sampling History**

The “Sampling History” table (ODS table name SamplingHistory) shows the scales and acceptance rates for each parameter block in the main sampling phase. The table is not displayed by default and can be requested by specifying the option **MCHISTORY=BRIEF | DETAILED**.

**Tuning Covariance**

The “Tuning Covariance” table (ODS table name TuneCov) shows the proposal covariance matrices for each parameter block after the tuning phase. The table is not displayed by default and can be requested by specifying the option **INIT=PINIT**. For more details about proposal tuning, see the section “**Tuning the Proposal Distribution**” on page 4469.

**Tuning History**

The “Tuning History” table (ODS table name TuningHistory) shows the number of tuning phases used in establishing the proposal distribution. The table also displays the scales and acceptance rates for each parameter block at each of the tuning phases. For more information about the self-adapting proposal tuning algorithm used by PROC MCMC, see the section “**Tuning the Proposal Distribution**” on page 4469. The table is not displayed by default and can be requested by specifying the option **MCHISTORY=BRIEF | DETAILED**.

***Tuning Probability Vector***

The “Tuning Probability” table (ODS table name TuneP) shows the proposal probability vector for each discrete parameter block (when the option DISCRETE=GEO is specified and the geometric proposal distribution is used for discrete parameters) after the tuning phase. The table is not displayed by default and can be requested by specifying the option INIT=PINIT. For more information about proposal tuning, see the section “Tuning the Proposal Distribution” on page 4469.

**Posterior Statistics Related ODS Tables**

PROC MCMC calculates some essential posterior statistics and outputs them to a number of ODS tables that you can request and save individually. For details of the calculations, see the section “Summary Statistics” on page 153.

***Summary Statistics***

The “Posterior Summaries” table (ODS table name PostSummaries) contains basic statistics for each parameter. The table lists the number of posterior samples, the posterior mean and standard deviation estimates, and the percentile estimates. This table is displayed by default.

***Correlation Matrix***

The “Posterior Correlation Matrix” table (ODS table name Corr) contains the posterior correlation of model parameters. The table is not displayed by default and can be requested by specifying the option STATS=CORR.

***Covariance Matrix***

The “Posterior Covariance Matrix” table (ODS table name Cov) contains the posterior covariance of model parameters. The table is not displayed by default and can be requested by specifying the option STATISTICS=COV.

***Deviance Information Criterion***

The “Deviance Information Criterion” table (ODS table name DIC) contains the DIC of the model. The table is not displayed by default and can be requested by specifying the option DIC. For details of the calculations, see the section “Deviance Information Criterion (DIC)” on page 155.

***Interval Statistics***

The “Posterior Intervals” table (ODS table name PostIntervals) contains the equal-tail and highest posterior density (HPD) interval estimates for each parameter. The default  $\alpha$  value is 0.05, and you can change it to other levels by using the STATISTICS= option. This table is displayed by default.

**Convergence Diagnostics Related ODS Tables**

PROC MCMC has convergence diagnostic tests that check for Markov chain convergence. PROC MCMC produces a number of ODS tables that you can request and save individually. For details in calculation, see the section “Statistical Diagnostic Tests” on page 144.

***Autocorrelation***

The “Autocorrelations” table (ODS table name AUTOCORR) contains the first order autocorrelations of the posterior samples for each parameter. The “Parameter” column states the name of the parameter. By default,

PROC MCMC displays lag 1, 5, 10, and 50 estimates of the autocorrelations. You can request different autocorrelations by using the `DIAGNOSTICS = AUTOCORR(LAGS=)` option. This table is displayed by default.

### **Effective Sample Size**

The “Effective Sample Sizes” table (ODS table name ESS) calculates the effective sample size of each parameter. See the section “Effective Sample Size” on page 152 for more details. The table is displayed by default.

### **Monte Carlo Standard Errors**

The “Monte Carlo Standard Errors” table (ODS table name MCSE) calculates the standard errors of the posterior mean estimate. See the section “Standard Error of the Mean Estimate” on page 153 for more details. The table is displayed by default.

### **Geweke Diagnostics**

The “Geweke Diagnostics” table (ODS table name Geweke) lists the result of the Geweke diagnostic test. See the section “Geweke Diagnostics” on page 146 for more details. The table is displayed by default.

### **Heidelberger-Welch Diagnostics**

The “Heidelberger-Welch Diagnostics” table (ODS table name Heidelberger) lists the result of the Heidelberger-Welch diagnostic test. The test is consisted of two parts: a stationary test and a half-width test. See the section “Heidelberger and Welch Diagnostics” on page 148 for more details. The table is not displayed by default and can be requested by specifying `DIAGNOSTICS = HEIDEL`.

### **Raftery-Lewis Diagnostics**

The “Raftery-Lewis Diagnostics” table (ODS table name Raftery) lists the result of the Raftery-Lewis diagnostic test. See the section “Raftery and Lewis Diagnostics” on page 149 for more details. The table is not displayed by default and can be requested by specifying `DIAGNOSTICS = RAFTERY`.

### **Summary Statistics for Prediction**

The “Posterior Summaries for Prediction” table (ODS table name PredSummaries) contains basic statistics for each prediction. The table lists the number of posterior samples, the posterior mean and standard deviation estimates, and the percentile estimates. This table is displayed by default if any `PREDDIST` statement is used in the program.

### **Interval Statistics for Prediction**

The “Posterior Intervals for Prediction” table (ODS table name PredIntervals) contains the equal-tail and highest posterior density (HPD) interval estimates for each prediction. The default  $\alpha$  value is 0.05, and you can change it to other levels by using the `STATISTICS` option in a `PREDDIST` statement, or the `STATISTICS=` option in the PROC MCMC statement if the option is not specified in a statement. This table is displayed by default if any `PREDDIST` statement is used in the program.

## **Optimization Related ODS Tables**

PROC MCMC can perform optimization on the joint posterior distribution. This is requested by the `PROPCOV=` option. The most commonly used optimization method is the quasi-Newton method: `PROPCOV=QUANEW(ITPRINT)`. The `ITPRINT` option displays the ODS tables, listed as follows:

**Input Options**

The “Input Options” table (ODS table name InputOptions) lists optimization options used in the procedure.

**Optimization Start**

The “Optimization Start” table (ODS table name ProblemDescription) shows the initial state of the optimization.

**Iteration History**

The “Iteration History” table (ODS table name IterHist) shows iteration history of the optimization.

**Optimization Results**

The “Optimization Results” table (ODS table name IterStop) shows the results of the optimization, includes information about the number of function calls, and the optimized objective function, which is the joint log posterior density.

**Convergence Status**

The “Convergence Status” table (ODS table name ConvergenceStatus) shows whether the convergence criterion is satisfied.

**Parameters Value After Optimization Table**

The “Parameter Values After Optimization” table (ODS table name OptiEstimates) lists the parameter values that maximize the joint log posterior. These are the maximum a posteriori point estimates, and they are used to start the Markov chain.

**Covariance Matrix After Optimization Table**

The “Proposal Covariance” table (ODS table name OptiCov) lists covariance matrices for each block parameter by using quadrature approximation at the posterior mode. These covariance matrices are used in the proposal distribution.

---

## ODS Table Names

PROC MCMC assigns a name to each table it creates. You can use these names to refer to the table when you use the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in Table 55.47. For more information about ODS, see Chapter 21, “Statistical Graphics Using ODS.”

**Table 55.47** ODS Tables Produced in PROC MCMC

| ODS Table Name    | Description                                   | Statement or Option        |
|-------------------|-----------------------------------------------|----------------------------|
| AutoCorr          | Autocorrelation statistics for each parameter | Default                    |
| BurnInHistory     | History of burn-in phase sampling             | MCHISTORY=BRIEF   DETAILED |
| ConvergenceStatus | Optimization convergence status               | PROPCOV=method(ITPRINT)    |
| Corr              | Correlation matrix of the posterior samples   | STATS=CORR                 |

Table 55.47 (continued)

| ODS Table Name     | Description                                                                                                               | Statement or Option                     |
|--------------------|---------------------------------------------------------------------------------------------------------------------------|-----------------------------------------|
| Cov                | Covariance matrix of the posterior samples                                                                                | STATS=COV                               |
| DIC                | Deviance information criterion                                                                                            | DIC                                     |
| ESS                | Effective sample size for each parameter                                                                                  | Default                                 |
| MCSE               | Monte Carlo standard error for each parameter                                                                             | Default                                 |
| Geweke             | Geweke diagnostics for each parameter                                                                                     | Default                                 |
| Heidelberger       | Heidelberger-Welch diagnostics for each parameter                                                                         | DIAGNOSTICS=HEIDEL                      |
| InputOptions       | Optimization input table                                                                                                  | PROPCOV=method(ITPRINT)                 |
| IterHist           | Optimization iteration history                                                                                            | PROPCOV=method(ITPRINT)                 |
| IterStop           | Optimization results table                                                                                                | PROPCOV=method(ITPRINT)                 |
| MissDataInfo       | Response variable, number of missing observations, missing observation indices, and sampling algorithm                    | Default with sampling of missing values |
| NObs               | Number of observations                                                                                                    | Default                                 |
| OptiEstimates      | Parameter values after either optimization                                                                                | PROPCOV=method(ITPRINT)                 |
| OptiCov            | Covariance used in proposal distribution after optimization                                                               | PROPCOV=method(ITPRINT)                 |
| Parameters         | Summary of the PARMS, BLOCKING, PRIOR, sampling method, and initial value specification                                   | Default                                 |
| ParametersInit     | Parameter values after the tuning phase                                                                                   | INIT=PINIT                              |
| PosteriorSample    | Posterior samples for each parameter                                                                                      | (For ODS output data set only)          |
| PostIntervals      | Equal-tail and HPD intervals for each parameter                                                                           | Default                                 |
| PostSummaries      | Basic posterior statistics for each parameter, including sample size, mean, standard deviation, and percentiles           | Default                                 |
| PredIntervals      | Equal-tail and HPD intervals for each prediction                                                                          | Default with any PREDDIST statement     |
| PredSummaries      | Basic posterior statistics for each prediction                                                                            | Default with any PREDDIST statement     |
| ProblemDescription | Optimization table                                                                                                        | PROPCOV=method(ITPRINT)                 |
| REObsInfo          | Random effect, subject values, number of observations in each unique subject value, and corresponding observation indices | REOBSINFO                               |

**Table 55.47** (continued)

| ODS Table Name  | Description                                                                                                                                              | Statement or Option                      |
|-----------------|----------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------|
| REParameters    | Random effect, sampling method, subject variable, number of subjects, unique values of the subject variable, and prior distribution of the random effect | Default with any <b>RANDOM</b> statement |
| Raftery         | Raftery-Lewis diagnostics for each parameter                                                                                                             | DIAGNOSTICS=RAFTERY                      |
| SamplingHistory | History of main phase sampling                                                                                                                           | MCHISTORY=BRIEF   DETAILED               |
| TuneCov         | Proposal covariance matrix (for continuous parameters) after the tuning phase                                                                            | INIT=PINIT                               |
| TuneP           | Proposal probability vector (for discrete parameters) after the tuning phase                                                                             | INIT=PINIT and DISCRETE=GEO              |
| TuningHistory   | History of proposal distribution tuning                                                                                                                  | MCHISTORY=BRIEF   DETAILED               |

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “[Statistical Graphics Using ODS.](#)”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS.](#)”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “[A Primer on ODS Statistical Graphics](#)” on page 599 in Chapter 21, “[Statistical Graphics Using ODS.](#)”

You can reference every graph produced through ODS Graphics with a name. The names of the graphs that PROC MCMC generates are listed in [Table 55.48](#).

**Table 55.48** Graphs Produced by PROC MCMC

| ODS Graph Name | Plot Description                           | Statement & Option       |
|----------------|--------------------------------------------|--------------------------|
| ADPanel        | Autocorrelation function and density panel | PLOTS=(AUTOCORR DENSITY) |
| AutocorrPanel  | Autocorrelation function panel             | PLOTS=AUTOCORR           |
| AutocorrPlot   | Autocorrelation function plot              | PLOTS(UNPACK)=AUTOCORR   |
| DensityPanel   | Density panel                              | PLOTS=DENSITY            |
| DensityPlot    | Density plot                               | PLOTS(UNPACK)=DENSITY    |

Table 55.48 *continued*

| ODS Graph Name | Plot Description                                   | Statement & Option             |
|----------------|----------------------------------------------------|--------------------------------|
| TAPanel        | Trace and autocorrelation function panel           | PLOTS=(TRACE AUTOCORR)         |
| TADPanel       | Trace, density, and autocorrelation function panel | PLOTS=(TRACE AUTOCORR DENSITY) |
| TDPanel        | Trace and density panel                            | PLOTS=(TRACE DENSITY)          |
| TracePanel     | Trace panel                                        | PLOTS=TRACE                    |
| TracePlot      | Trace plot                                         | PLOTS(UNPACK)=TRACE            |

## Examples: MCMC Procedure

### Example 55.1: Simulating Samples From a Known Density

This example illustrates how you can obtain random samples from a known function. The target distributions are the normal distribution (a standard distribution) and a mixture of the normal distributions (a nonstandard distribution). For more information, see the sections “[Standard Distributions](#)” on page 4476 and “[Specifying a New Distribution](#)” on page 4490). This example also shows how you can use PROC MCMC to estimate an integral (area under a curve). Monte Carlo simulation is data-independent; hence, you do not need an input data set from which to draw random samples from the desired distribution.

#### Sampling from a Normal Density

When you run a simulation without an input data set, the posterior distribution is the same as the prior distribution. Hence, if you want to generate samples from a distribution, you declare the distribution in the **PRIOR** statement and set the likelihood function to a constant. Although there is no contribution from any data set variable to the likelihood calculation, you still must specify a data set and the **MODEL** statement needs a distribution. You can input an empty data set and use the **GENERAL** function to provide a flat likelihood. The following statements generate 10,000 samples from a standard normal distribution:

```

title 'Simulating Samples from a Normal Density';
data x;
run;

ods graphics on;
proc mcmc data=x outpost=simout seed=23 nmc=10000
 statistics=(summary interval) diagnostics=none;
 ods exclude nob;
 parm alpha 0;
 prior alpha ~ normal(0, sd=1);
 model general(0);
run;

```

The ODS GRAPHICS ON statement enables ODS Graphics. The PROC MCMC statement specifies the input and output data sets, a random number seed, and the size of the simulation sample. The STATISTICS= option displays only the summary and interval statistics. The ODS EXCLUDE statement excludes the display of the NObs table. PROC MCMC draws independent samples from the normal distribution directly (see Output 55.1.1). Therefore, the simulation does not require any tuning, and PROC MCMC omits the default burn-in phrase.

**Output 55.1.1** Parameters Information

| Simulating Samples from a Normal Density |           |                 |               |                    |
|------------------------------------------|-----------|-----------------|---------------|--------------------|
| The MCMC Procedure                       |           |                 |               |                    |
| Parameters                               |           |                 |               |                    |
| Block                                    | Parameter | Sampling Method | Initial Value | Prior Distribution |
| 1                                        | alpha     | Direct          | 0             | normal(0, sd=1)    |

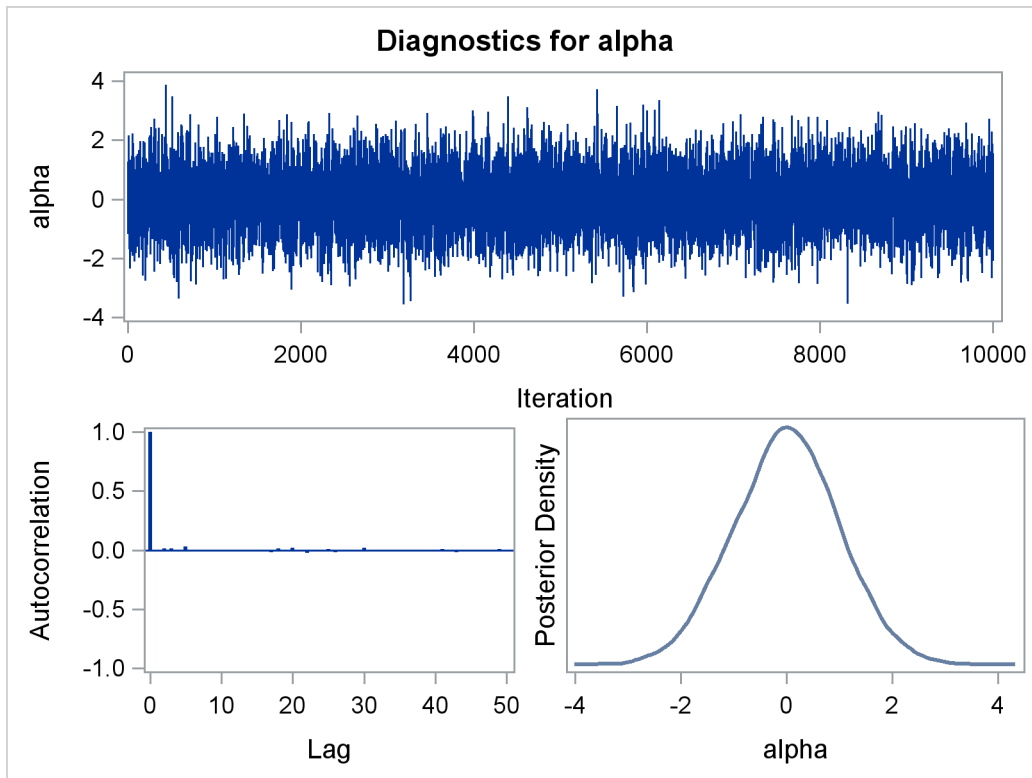
The summary statistics (Output 55.1.2) are what you would expect from a standard normal distribution.

**Output 55.1.2** MCMC Summary and Interval Statistics from a Normal Target Distribution

| Simulating Samples from a Normal Density |       |                     |                    |              |         |        |
|------------------------------------------|-------|---------------------|--------------------|--------------|---------|--------|
| The MCMC Procedure                       |       |                     |                    |              |         |        |
| Posterior Summaries                      |       |                     |                    |              |         |        |
| Parameter                                | N     | Mean                | Standard Deviation | Percentiles  |         |        |
|                                          |       |                     |                    | 25%          | 50%     | 75%    |
| alpha                                    | 10000 | 0.00195             | 0.9949             | -0.6544      | 0.00965 | 0.6709 |
| Posterior Intervals                      |       |                     |                    |              |         |        |
| Parameter                                | Alpha | Equal-Tail Interval |                    | HPD Interval |         |        |
| alpha                                    | 0.050 | -1.9485             | 1.9507             | -1.9664      | 1.9302  |        |

The trace plot (Output 55.1.3) shows perfect mixing with no autocorrelation in the lag plot. This is expected because these are independent draws.



**Output 55.1.3** Diagnostics Plots for  $\alpha$ 

You can overlay the estimated kernel density with the true density to visually compare the densities, as displayed in [Output 55.1.4](#). To create the kernel comparison plot, you first call PROC KDE (see Chapter 48, “The KDE Procedure”) to obtain a kernel density estimate of the posterior density on  $\alpha$ . Then you evaluate a grid of  $\alpha$  values on a normal density. The following statements evaluate kernel density and compute the corresponding normal density:

```
proc kde data=simout;
 ods exclude inputs controls;
 univar alpha /out=sample;
run;

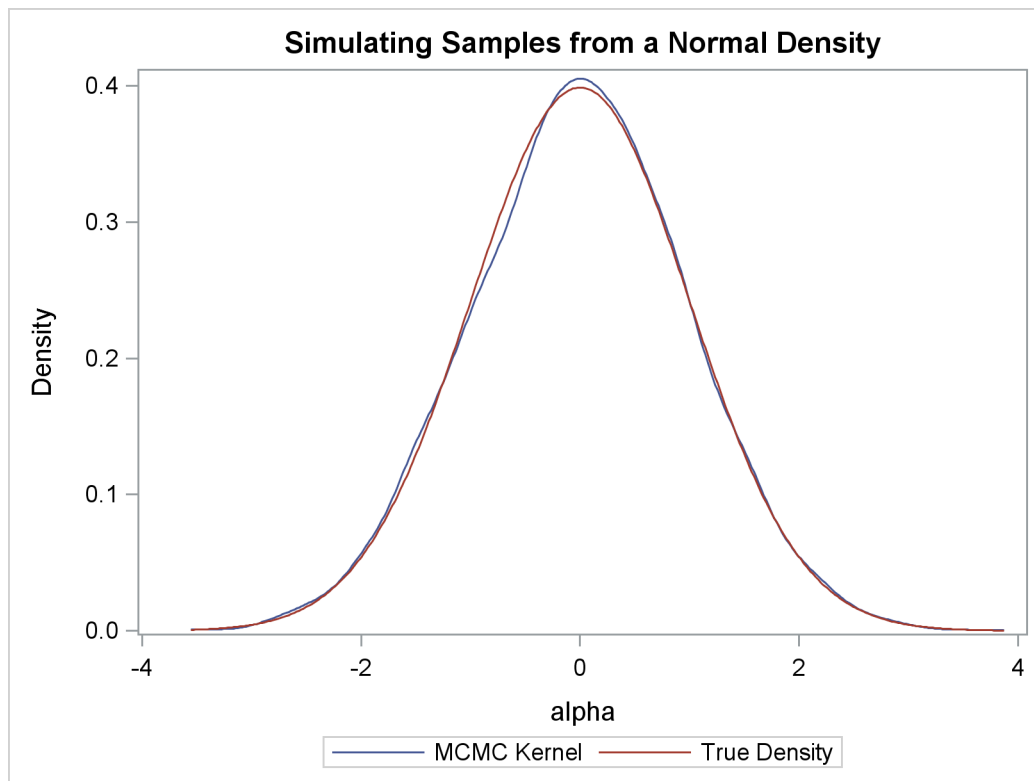
data den;
 set sample;
 alpha = value;
 true = pdf('normal', alpha, 0, 1);
 keep alpha density true;
run;
```

Next you plot the two curves on top of each other by using PROC SGPLOT (see Chapter 21, “Statistical Graphics Using ODS”) as follows:

```
proc sgplot data=den;
 yaxis label="Density";
 series y=density x=alpha / legendlabel = "MCMC Kernel";
 series y=true x=alpha / legendlabel = "True Density";
 discretelegend;
run;
```

Output 55.1.4 shows the result. You can see that the kernel estimate and the true density are very similar to each other.

**Output 55.1.4** Estimated Density versus the True Density



### Density Visualization Macro

In programs that do not involve any data set variables, PROC MCMC samples directly from the (joint) prior distributions of the parameters. The modification makes the sampling from a known distribution more efficient and more precise. For example, you can write simple programs, such as the following macro, to understand different aspects of a prior distribution of interest, such as its moments, intervals, shape, spread, and so on:

```

%macro density(dist=, seed=0);
 %let savenote = %sysfunc(getoption(notes));
 options nonotes;
 title "&dist distribution.";
 data _a;
 run;

 ods select densitypanel postsummaries postintervals;
 proc mcmc data=_a nmc=10000 diag=none nologdist
 plots=density seed=&seed;
 parms alpha;
 prior alpha ~ &dist;
 model general(0);
 run;

 proc datasets nolist;
 delete _a;
 run;
 options &savenote;
%mend;

%density(dist=beta(4, 12), seed=1);

```

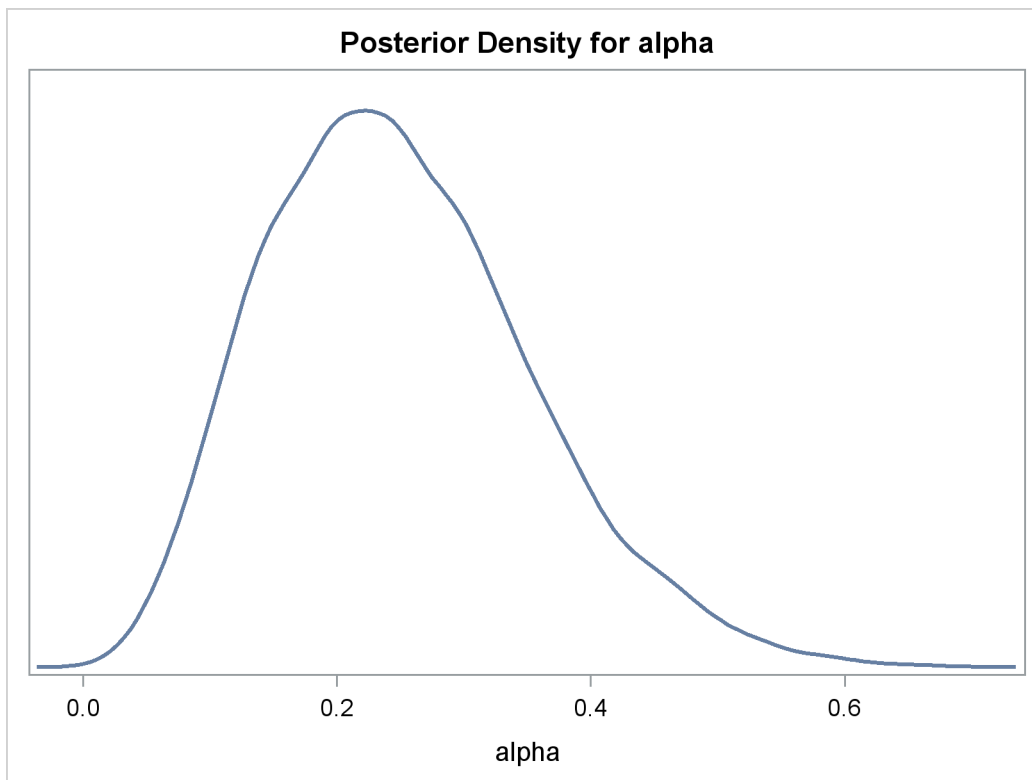
The macro %density creates an empty data set, invokes PROC MCMC, draws 10,000 samples from a beta(4, 12) distribution, displays summary and interval statistics, and generates a kernel density plot. Summary and interval statistics from the beta distribution are displayed in [Output 55.1.5](#).

**Output 55.1.5** Beta Distribution Statistics

| beta(4, 12) distribution. |       |                     |                       |              |        |        |
|---------------------------|-------|---------------------|-----------------------|--------------|--------|--------|
| The MCMC Procedure        |       |                     |                       |              |        |        |
| Posterior Summaries       |       |                     |                       |              |        |        |
| Parameter                 | N     | Mean                | Standard<br>Deviation | Percentiles  |        |        |
|                           |       |                     |                       | 25%          | 50%    | 75%    |
| alpha                     | 10000 | 0.2494              | 0.1039                | 0.1731       | 0.2397 | 0.3148 |
| Posterior Intervals       |       |                     |                       |              |        |        |
| Parameter                 | Alpha | Equal-Tail Interval |                       | HPD Interval |        |        |
| alpha                     | 0.050 | 0.0775              | 0.4800                | 0.0657       | 0.4590 |        |

The distribution is displayed in [Output 55.1.6](#).

Output 55.1.6 Density Plot



## Calculation of Integrals

One advantage of MCMC methods is to estimate any integral under the curve of a target distribution. This can be done fairly easily using the MCMC procedure. Suppose you are interested in estimating the following cumulative probability:

$$\int_{\alpha=0}^{1.3} \phi(\alpha|0, 1) d\alpha$$

To estimate this integral, PROC MCMC draws samples from the distribution and counts the portion of the simulated values that fall within the desired range of [0, 1.3]. This becomes a Monte Carlo estimate of the integral. The following statements simulate samples from a standard normal distribution and estimate the integral:

```
proc mcmc data=x outpost=simout seed=23 nmc=10000 nologdist
 monitor=(int) statistics=(summary) diagnostics=none;
 ods select postsummaries;
 parm alpha 0;
 prior alpha ~ normal(0, sd=1);
 int = (0 <= alpha <= 1.3);
 model general(0);
run;
```

The ODS SELECT statement displays the posterior summary statistics table. The MONITOR= option outputs analysis on the variable int (the integral estimate). The STATISTICS= option computes the summary

statistics. The `NOLOGDIST` option omits the calculation of the log of the prior distribution at each iteration, shortening the simulation time<sup>8</sup>. The `INT` assignment statement sets `int` to be 1 if the simulated alpha value falls between 0 and 1.3, and 0 otherwise. PROC MCMC supports the usage of the IF-ELSE logical control if you need to account for more complex conditions. Output 55.1.7 displays the estimated integral value:

**Output 55.1.7** Monte Carlo Integral from a Normal Distribution

| beta(4, 12) distribution. |       |        |                       |             |     |        |
|---------------------------|-------|--------|-----------------------|-------------|-----|--------|
| The MCMC Procedure        |       |        |                       |             |     |        |
| Posterior Summaries       |       |        |                       |             |     |        |
| Parameter                 | N     | Mean   | Standard<br>Deviation | Percentiles |     |        |
|                           |       |        |                       | 25%         | 50% | 75%    |
| int                       | 10000 | 0.4079 | 0.4915                | 0           | 0   | 1.0000 |

In this simulation, 4079 samples fall between 0 and 1.3, making the expected probability 0.4079. In this example, you can verify the actual cumulative probability by calling the CDF function in the DATA step:

```
data _null_;
 int = cdf("normal", 1.3, 0, 1) - cdf("normal", 0, 0, 1);
 put int=;
run;
```

The value is 0.4032.

## Sampling from a Mixture of Normal Densities

Suppose you are interested in generating samples from a three-component mixture of normal distributions, with the density specified as follows:

$$p(\alpha) = 0.3 \cdot \phi(-3, \sigma = 2) + 0.4 \cdot \phi(2, \sigma = 1) + 0.3 \cdot \phi(10, \sigma = 4)$$

The distribution is not one of the standard distributions that PROC MCMC supports. Hence you need to construct the density function and supply it to the procedure. The following statements generate random samples from this mixture density:

```
title 'Simulating Samples from a Mixture of Normal Densities';
data x;
run;

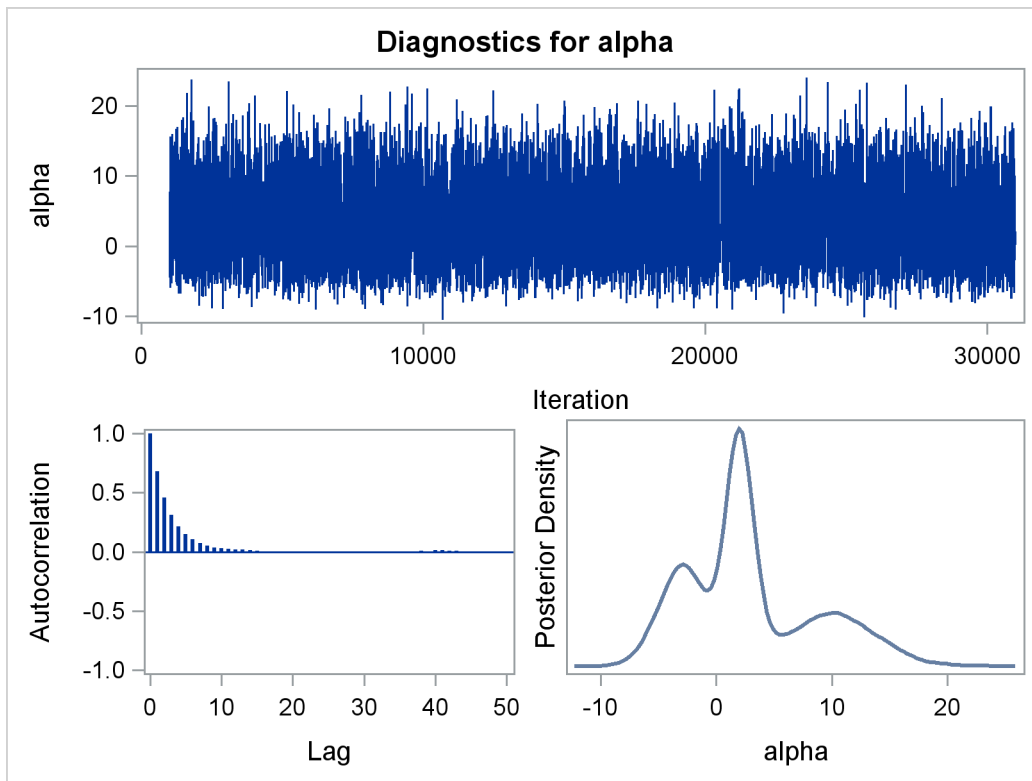
proc mcmc data=x outpost=simout seed=1234 nmc=30000;
 ods select TADpanel;
 parm alpha 0.3;
 lp = logpdf('normalmix', alpha, 3, 0.3, 0.4, 0.3, -3, 2, 10, 2, 1, 4);
 prior alpha ~ general(lp);
 model general(0);
run;
```

<sup>8</sup>In this example, the `NOLOGDIST` option saves only a fraction of the time. But in more complex simulation schemes that involve a larger number of distributions and parameters, the time reduction could be significant.

The ODS SELECT statement displays the diagnostic plots. All other tables, such as the NObs tables, are excluded. The PROC MCMC statement uses the input data set X, saves output to the Simout data set, sets a random number seed, and draws 30,000 samples.

The LP assignment statement evaluates the log density of alpha at the mixture density, using the SAS function LOGPDF. The number 3 after alpha in the LOGPDF function indicates that the density is a three-component normal mixture. The following three numbers, 0.3, 0.4, and 0.3, are the weights in the mixture; -3, 2, and 10 are the means; 2, 1, and 4 are the standard deviations. The PRIOR statement assigns this log density function to alpha as its prior. Note that the GENERAL function interprets the density on the log scale, and not the original scale—you must use the LOGPDF function, not the PDF function. Output 55.1.8 displays the results. The kernel density clearly shows three modes.

**Output 55.1.8** Plots of Posterior Samples from a Mixture Normal Distribution



Using the following set of statements similar to the previous example, you can overlay the estimated kernel density with the true density. The comparison is shown in Output 55.1.9.

```
proc kde data=simout;
 ods exclude inputs controls;
 univar alpha /out=sample;
run;

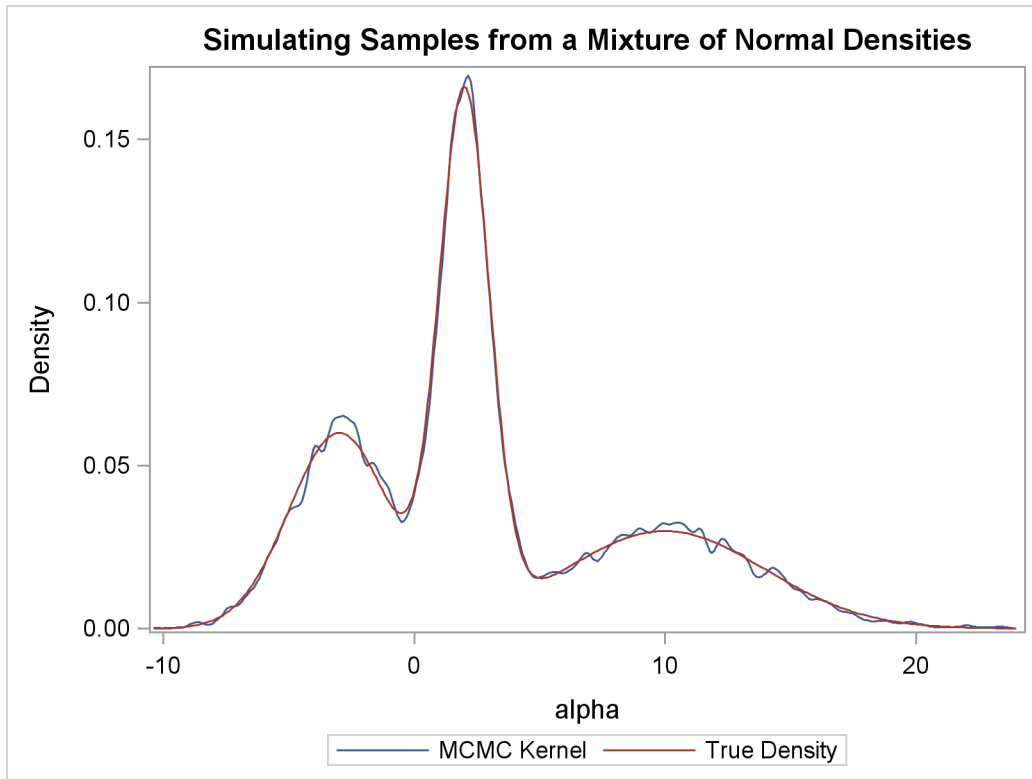
data den;
 set sample;
 alpha = value;
 true = pdf('normalmix', alpha, 3, 0.3, 0.4, 0.3, -3, 2, 10, 2, 1, 4);
 keep alpha density true;
run;
```

```

proc sgplot data=den;
 yaxis label="Density";
 series y=density x=alpha / legendlabel = "MCMC Kernel";
 series y=true x=alpha / legendlabel = "True Density";
 discretelegend;
run;

```

**Output 55.1.9** Estimated Density versus the True Density



## Example 55.2: Box-Cox Transformation

Box-Cox transformations (Box and Cox 1964) are often used to find a power transformation of a dependent variable to ensure the normality assumption in a linear regression model. This example illustrates how you can use PROC MCMC to estimate a Box-Cox transformation for a linear regression model. Two different priors on the transformation parameter  $\lambda$  are considered: a continuous prior and a discrete prior. You can estimate the probability of  $\lambda$  being 0 with a discrete prior but not with a continuous prior. The IF-ELSE statements are demonstrated in the example.

## Using a Continuous Prior on $\lambda$

The following statements create a SAS data set with measurements of  $y$  (the response variable) and  $x$  (a single dependent variable):

```

title 'Box-Cox Transformation, with a Continuous Prior on Lambda';
data boxcox;
 input y x @@;
 datalines;
10.0 3.0 72.6 8.3 59.7 8.1 20.1 4.8 90.1 9.8 1.1 0.9
78.2 8.5 87.4 9.0 9.5 3.4 0.1 1.4 0.1 1.1 42.5 5.1
57.0 7.5 9.9 1.9 0.5 1.0 121.1 9.9 37.5 5.9 49.5 6.7

... more lines ...

2.6 1.8 58.6 7.9 81.2 8.1 37.2 6.9
;

```

The Box-Cox transformation of  $y$  takes on the form of:

$$y(\lambda) = \begin{cases} \frac{y^{\lambda}-1}{\lambda} & \text{if } \lambda \neq 0; \\ \log(y) & \text{if } \lambda = 0. \end{cases}$$

The transformed response  $y(\lambda)$  is assumed to be normally distributed:

$$y_i(\lambda) \sim \text{normal}(\beta_0 + \beta_1 x_i, \sigma^2)$$

The likelihood with respect to the original response  $y_i$  is as follows:

$$p(y_i|\lambda, \beta, \sigma^2, x_i) \propto \phi(y_i|\beta_0 + \beta_1 x_i, \sigma^2) \cdot J(\lambda, y_i)$$

where  $J(\lambda, y_i)$  is the Jacobian:

$$J(\lambda, y) = \begin{cases} y_i^{\lambda-1} & \text{if } \lambda \neq 0; \\ 1/y_i & \text{if } \lambda = 0. \end{cases}$$

And on the log-scale, the Jacobian becomes:

$$\log(J(\lambda, y)) = \begin{cases} (\lambda - 1) \cdot \log(y_i) & \text{if } \lambda \neq 0; \\ -\log(y_i) & \text{if } \lambda = 0. \end{cases}$$

There are four model parameters:  $\lambda$ ,  $\boldsymbol{\beta} = \{\beta_0, \beta_1\}$ , and  $\sigma^2$ . You can consider using a flat prior on  $\boldsymbol{\beta}$  and a gamma prior on  $\sigma^2$ .

To consider only power transformations ( $\lambda \neq 0$ ), you can use a continuous prior (for example, a uniform prior from  $-2$  to  $2$ ) on  $\lambda$ . One issue with using a continuous prior is that you cannot estimate the probability of  $\lambda = 0$ . To do so, you need to consider a discrete prior that places positive probability mass on the point  $0$ . See “[Modeling  \$\lambda = 0\$](#) ” on page 4553.

The following statements fit a Box-Cox transformation model:



```

ods graphics on;
proc mcmc data=boxcox nmc=50000 thin=10 propcov=quanew seed=12567
 monitor=(lda);
 ods select PostSummaries PostIntervals TADpanel;

 parms beta0 0 beta1 0 lda 1 s2 1;

 beginnodata;
 prior beta: ~ general(0);
 prior s2 ~ gamma(shape=3, scale=2);
 prior lda ~ unif(-2,2);
 sd = sqrt(s2);
 endnodata;

 ys = (y**lda-1)/lda;
 mu = beta0+beta1*x;
 ll = (lda-1)*log(y)+lpdfnorm(ys, mu, sd);
 model general(ll);
run;

```

The **PROPCOV=** option initializes the Markov chain at the posterior mode and uses the estimated inverse Hessian matrix as the initial proposal covariance matrix. The **MONITOR=** option selects  $\lambda$  as the variable to report. The ODS SELECT statement displays the summary statistics table, the interval statistics table, and the diagnostic plots.

The **PARMS** statement puts all four parameters,  $\beta_0$ ,  $\beta_1$ ,  $\lambda$ , and  $\sigma^2$ , in a single block and assigns initial values to each of them. Three **PRIOR** statements specify previously stated prior distributions for these parameters. The assignment to **sd** transforms a variance to a standard deviation. It is better to place the transformation inside the **BEGINNODATA** and **ENDNODATA** statements to save computational time.

The assignment to the symbol **ys** evaluates the Box-Cox transformation of  $y$ , where  $\mu$  is the regression mean and  $\ell$  is the log likelihood of the transformed variable  $ys$ . Note that the log of the Jacobian term is included in the calculation of  $\ell$ .

Summary statistics and interval statistics for  $\lambda$  are listed in [Output 55.2.1](#).

### Output 55.2.1 Box-Cox Transformation

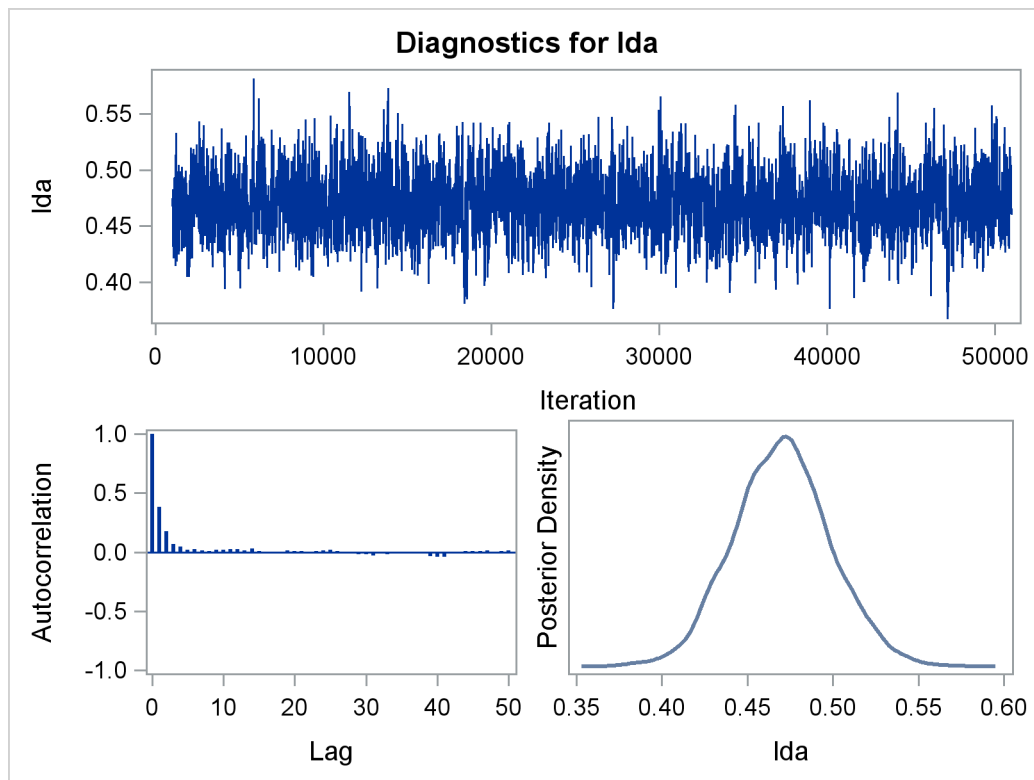
| Box-Cox Transformation, with a Continuous Prior on Lambda |      |        |                       |             |        |        |
|-----------------------------------------------------------|------|--------|-----------------------|-------------|--------|--------|
| The MCMC Procedure                                        |      |        |                       |             |        |        |
| Posterior Summaries                                       |      |        |                       |             |        |        |
| Parameter                                                 | N    | Mean   | Standard<br>Deviation | Percentiles |        |        |
|                                                           |      |        |                       | 25%         | 50%    | 75%    |
| lda                                                       | 5000 | 0.4702 | 0.0284                | 0.4515      | 0.4703 | 0.4884 |

**Output 55.2.1** *continued*

| Parameter | Alpha | Posterior Intervals |        |              |        |
|-----------|-------|---------------------|--------|--------------|--------|
|           |       | Equal-Tail Interval |        | HPD Interval |        |
| lda       | 0.050 | 0.4162              | 0.5269 | 0.4197       | 0.5298 |

The posterior mean of  $\lambda$  is 0.47, with a 95% equal-tail interval of [0.42, 0.53] and a similar HPD interval. The preferred power transformation would be 0.5 (rounding  $\lambda$  up to the square root transformation).

Output 55.2.2 shows diagnostics plots for lda. The chain appears to converge, and you can proceed to make inferences. The density plot shows that the posterior density is relatively symmetric around its mean estimate.

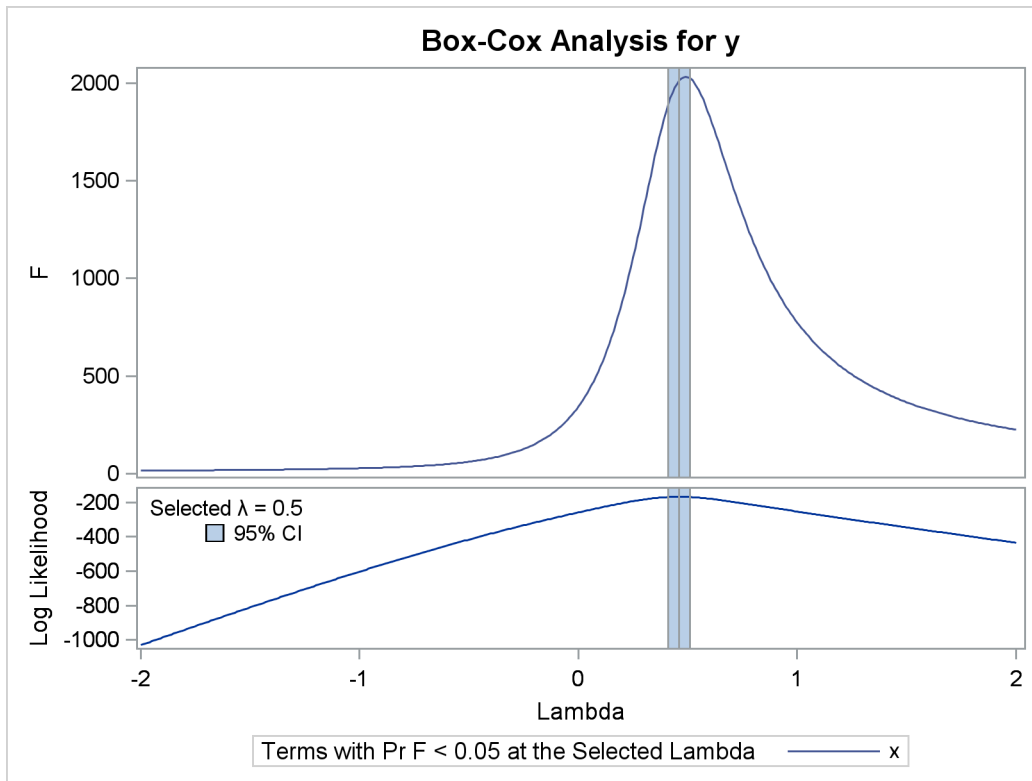
**Output 55.2.2** Diagnostic Plots for  $\lambda$ 

To verify the results, you can use PROC TRANSREG (see Chapter 97, “The TRANSREG Procedure”) to find the estimate of  $\lambda$ .

```
proc transreg data=boxcox details pbo;
 ods output boxcox = bc;
 model boxcox(y / convenient lambda=-2 to 2 by 0.01) = identity(x);
 output out=trans;
run;
```

Output from PROC TRANSREG is shown in [Output 55.2.5](#) and [Output 55.2.4](#). PROC TRANSREG produces a similar point estimate of  $\lambda = 0.46$ , and the 95% confidence interval is shown in [Output 55.2.5](#).

**Output 55.2.3** Box-Cox Transformation Using PROC TRANSREG



**Output 55.2.4** Estimates Reported by PROC TRANSREG

```

Box-Cox Transformation, with a Continuous Prior on Lambda

The TRANSREG Procedure

Model Statement Specification Details

Type DF Variable Description Value
Dep 1 BoxCox(y) Lambda Used 0.5
 Lambda 0.46
 Log Likelihood -167.0
 Conv. Lambda 0.5
 Conv. Lambda LL -168.3
 CI Limit -169.0
 Alpha 0.05
 Options Convenient Lambda Used
Ind 1 Identity(x) DF 1

```

The ODS data set `Bc` contains the 95% confidence interval estimates produced by PROC TRANSREG. This ODS table is rather large, and you want to see only the relevant portion. The following statements generate the part of the table that is important and display [Output 55.2.5](#):

```
proc print noobs label data=bc(drop=rmse);
 title2 'Confidence Interval';
 where ci ne ' ' or abs(lambda - round(lambda, 0.5)) < 1e-6;
 label convenient = '00'x ci = '00'x;
run;
```

The estimated 90% confidence interval is [0.41, 0.51], which is very close to the reported Bayesian credible intervals. The resemblance of the intervals is probably due to the noninformative prior that you used in this analysis.

**Output 55.2.5** Estimated Confidence Interval on  $\lambda$

| Box-Cox Transformation, with a Continuous Prior on Lambda |        |          |                |
|-----------------------------------------------------------|--------|----------|----------------|
| Confidence Interval                                       |        |          |                |
| Dependent                                                 | Lambda | R-Square | Log Likelihood |
| BoxCox (y)                                                | -2.00  | 0.14     | -1030.56       |
| BoxCox (y)                                                | -1.50  | 0.17     | -810.50        |
| BoxCox (y)                                                | -1.00  | 0.22     | -602.53        |
| BoxCox (y)                                                | -0.50  | 0.39     | -415.56        |
| BoxCox (y)                                                | 0.00   | 0.78     | -257.92        |
| BoxCox (y)                                                | 0.41   | 0.95     | -168.40        |
| BoxCox (y)                                                | 0.42   | 0.95     | -167.86        |
| BoxCox (y)                                                | 0.43   | 0.95     | -167.46        |
| BoxCox (y)                                                | 0.44   | 0.95     | -167.19        |
| BoxCox (y)                                                | 0.45   | 0.95     | -167.05        |
| BoxCox (y)                                                | 0.46   | 0.95     | -167.04        |
| BoxCox (y)                                                | 0.47   | 0.95     | -167.16        |
| BoxCox (y)                                                | 0.48   | 0.95     | -167.41        |
| BoxCox (y)                                                | 0.49   | 0.95     | -167.79        |
| BoxCox (y)                                                | 0.50   | 0.95     | -168.28        |
| BoxCox (y)                                                | 0.51   | 0.95     | -168.89        |
| BoxCox (y)                                                | 1.00   | 0.89     | -253.09        |
| BoxCox (y)                                                | 1.50   | 0.79     | -345.35        |
| BoxCox (y)                                                | 2.00   | 0.70     | -435.01        |

### Modeling $\lambda = 0$

With a continuous prior on  $\lambda$ , you can get only a continuous posterior distribution, and this makes the probability of  $\Pr(\lambda = 0|\text{data})$  equal to 0 by definition. To consider  $\lambda = 0$  as a viable solution to the Box-Cox transformation, you need to use a discrete prior that places some probability mass on the point 0 and allows for a meaningful posterior estimate of  $\Pr(\lambda = 0|\text{data})$ .

This example uses a simulation study where the data are generated from an exponential likelihood. The simulation implies that the correct transformation should be the logarithm and  $\lambda$  should be 0. Consider the

following exponential model:

$$y = \exp(x + \epsilon),$$

where  $\epsilon \sim \text{normal}(0, 1)$ . The transformed data can be fitted with a linear model:

$$\log(y) = x + \epsilon$$

The following statements generate a SAS data set with a gridded  $x$  and corresponding  $y$ :

```

title 'Box-Cox Transformation, Modeling Lambda = 0';
data boxcox;
 do x = 1 to 8 by 0.025;
 ly = x + normal(7);
 y = exp(ly);
 output;
 end;
run;

```

The log-likelihood function, after taking the Jacobian into consideration, is as follows:

$$\log p(y_i | \lambda, x_i) = \begin{cases} (\lambda - 1) \log(y_i) - \frac{1}{2} \left( \log \sigma^2 + \frac{(y_i^\lambda - 1)/\lambda - x_i}{\sigma^2} \right)^2 + C_1 & \text{if } \lambda \neq 0; \\ -\log(y_i) - \frac{1}{2} \left( \log \sigma^2 + \frac{(\log(y_i) - x_i)^2}{\sigma^2} \right) + C_2 & \text{if } \lambda = 0. \end{cases}$$

where  $C_1$  and  $C_2$  are two constants.

You can use the function [DGENERAL](#) to place a discrete prior on  $\lambda$ . The function is similar to the function [GENERAL](#), except that it indicates a discrete distribution. For example, you can specify a discrete uniform prior from  $-2$  to  $2$  using

```
prior lda ~ dgeneral(1, lower=-2, upper=2);
```

This places equal probability mass on five points,  $-2$ ,  $-1$ ,  $0$ ,  $1$ , and  $2$ . This prior might not work well here because the grid is too coarse. To consider smaller values of  $\lambda$ , you can sample a parameter that takes a wider range of integer values and transform it back to the  $\lambda$  space. For example, set  $\alpha$  as your model parameter and give it a discrete uniform prior from  $-200$  to  $200$ . Then define  $\lambda$  as  $\alpha/100$  so  $\lambda$  can take values between  $-2$  and  $2$  but on a finer grid.

The following statements fit a Box-Cox transformation by using a discrete prior on  $\lambda$ :

```

proc mcmc data=boxcox outpost=simout nmc=50000 thin=10 seed=12567
 monitor=(lda);

 ods select PostSummaries PostIntervals;
 parms s2 1 alpha 10;

 beginnodata;
 prior s2 ~ gamma(shape=3, scale=2);
 if alpha=0 then lp = log(2);
 else lp = log(1);
 prior alpha ~ dgeneral(lp, lower=-200, upper=200);
 lda = alpha * 0.01;
 sd = sqrt(s2);
endnodata;

```

```

if alpha=0 then
 ll = -ly+lpdfnorm(ly, x, sd);
else do;
 ys = (y**lda - 1)/lda;
 ll = (lda-1)*ly+lpdfnorm(ys, x, sd);
end;
model general(ll);
run;

```

There are two parameters, `s2` and `alpha`, in the model. They are placed in a single **PARMS** statement so that they are sampled in the same block.

The parameter `s2` takes a gamma distribution, and `alpha` takes a discrete prior. The IF-ELSE statements state that `alpha` takes twice as much prior density when it is 0 than otherwise. Note that on the original scale,  $\Pr(\alpha = 0) = 2 \cdot \Pr(\alpha \neq 0)$ . Translating that to the log scale, the densities become  $\log(2)$  and  $\log(1)$ , respectively. The LDA assignment statement transforms `alpha` to the parameter of interest: `lda` takes values between  $-2$  and  $2$ . You can model `lda` on an even smaller scale by dividing `alpha` by a larger constant. However, an increment of 0.01 in the Box-Cox transformation is usually sufficient. The SD assignment statement calculates the square root of the variance term.

The log-likelihood function uses another set of IF-ELSE statements, separating the case of  $\lambda = 0$  from the others. The formulas are stated previously. The output of the program is shown in [Output 55.2.6](#).

#### Output 55.2.6 Box-Cox Transformation

| Box-Cox Transformation, Modeling Lambda = 0 |       |                     |                       |              |     |     |
|---------------------------------------------|-------|---------------------|-----------------------|--------------|-----|-----|
| The MCMC Procedure                          |       |                     |                       |              |     |     |
| Posterior Summaries                         |       |                     |                       |              |     |     |
| Parameter                                   | N     | Mean                | Standard<br>Deviation | Percentiles  |     |     |
|                                             |       |                     |                       | 25%          | 50% | 75% |
| lda                                         | 5000  | -0.00002            | 0.00201               | 0            | 0   | 0   |
| Posterior Intervals                         |       |                     |                       |              |     |     |
| Parameter                                   | Alpha | Equal-Tail Interval |                       | HPD Interval |     |     |
| lda                                         | 0.050 | 0                   | 0                     | 0            | 0   |     |

From the summary statistics table, you see that the point estimate for  $\lambda$  is 0 and both of the 95% equal-tail and HPD credible intervals are 0. This strongly suggests that  $\lambda = 0$  is the best estimate for this problem. In addition, you can also count the frequency of  $\lambda$  among posterior samples to get a more precise estimate on the posterior probability of  $\lambda$  being 0.

The following statements use PROC FREQ to produce [Output 55.2.7](#) and [Output 55.2.8](#):

```

proc freq data=simout;
 ods select onewayfreqs freqplot;
 tables lda /nocum plot=freqplot(scale=percent);
run;
ods graphics off;

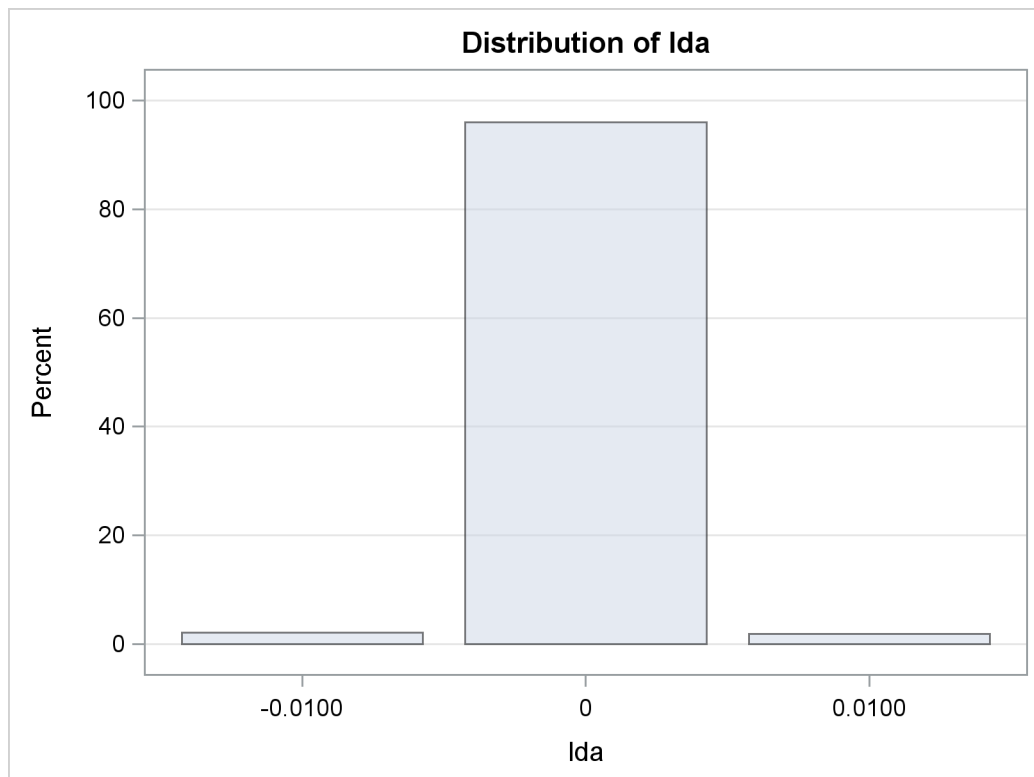
```

Output 55.2.7 shows the frequency count table. An estimate of  $\Pr(\lambda = 0|\text{data})$  is 96%. The conclusion is that the log transformation should be the appropriate transformation used here, which agrees with the simulation setup. Output 55.2.8 shows the histogram of  $\lambda$ .

**Output 55.2.7** Frequency Counts of  $\lambda$

| Box-Cox Transformation, Modeling Lambda = 0 |           |         |
|---------------------------------------------|-----------|---------|
| The FREQ Procedure                          |           |         |
| lda                                         | Frequency | Percent |
| -0.0100                                     | 106       | 2.12    |
| 0                                           | 4798      | 95.96   |
| 0.0100                                      | 96        | 1.92    |

**Output 55.2.8** Histogram of  $\lambda$



## Example 55.3: Logistic Regression Model with a Diffuse Prior

This example illustrates how to fit a logistic regression model with a diffuse prior in PROC MCMC. You can also use the BAYES statement in PROC GENMOD. See Chapter 40, “The GENMOD Procedure.”

The following statements create a SAS data set with measurements of the number of deaths,  $y$ , among  $n$  beetles that have been exposed to an environmental contaminant  $x$ :

```

title 'Logistic Regression Model with a Diffuse Prior';
data beetles;
 input n y x @@;
 datalines;
6 0 25.7 8 2 35.9 5 2 32.9 7 7 50.4 6 0 28.3
7 2 32.3 5 1 33.2 8 3 40.9 6 0 36.5 6 1 36.5
6 6 49.6 6 3 39.8 6 4 43.6 6 1 34.1 7 1 37.4
8 2 35.2 6 6 51.3 5 3 42.5 7 0 31.3 3 2 40.6
;

```

You can model the data points  $y_i$  with a binomial distribution,

$$y_i | p_i \sim \text{binomial}(n_i, p_i)$$

where  $p_i$  is the success probability and links to the regression covariate  $x_i$  through a logit transformation:

$$\text{logit}(p_i) = \log\left(\frac{p_i}{1-p_i}\right) = \alpha + \beta x_i$$

The priors on  $\alpha$  and  $\beta$  are both diffuse normal:

$$\begin{aligned} \alpha &\sim \text{normal}(0, \text{var} = 10000) \\ \beta &\sim \text{normal}(0, \text{var} = 10000) \end{aligned}$$

These statements fit a logistic regression with PROC MCMC:

```

ods graphics on;
proc mcmc data=beetles ntu=1000 nmc=20000 nthin=2 propcov=quanew
 diag=(mcse ess) outpost=beetleout seed=246810;
 ods select PostSummaries PostIntervals mcse ess TADpanel;
 parms (alpha beta) 0;
 prior alpha beta ~ normal(0, var = 10000);
 p = logistic(alpha + beta*x);
 model y ~ binomial(n,p);
run;

```

The key statement in the program is the assignment to  $p$  that calculates the probability of death. The SAS function LOGISTIC does the proper transformation. The MODEL statement specifies that the response variable,  $y$ , is binomially distributed with parameters  $n$  (from the input data set) and  $p$ . The summary statistics table, interval statistics table, the Monte Carlo standard error table, and the effective sample sizes table are shown in [Output 55.3.1](#).



## Output 55.3.1 MCMC Results

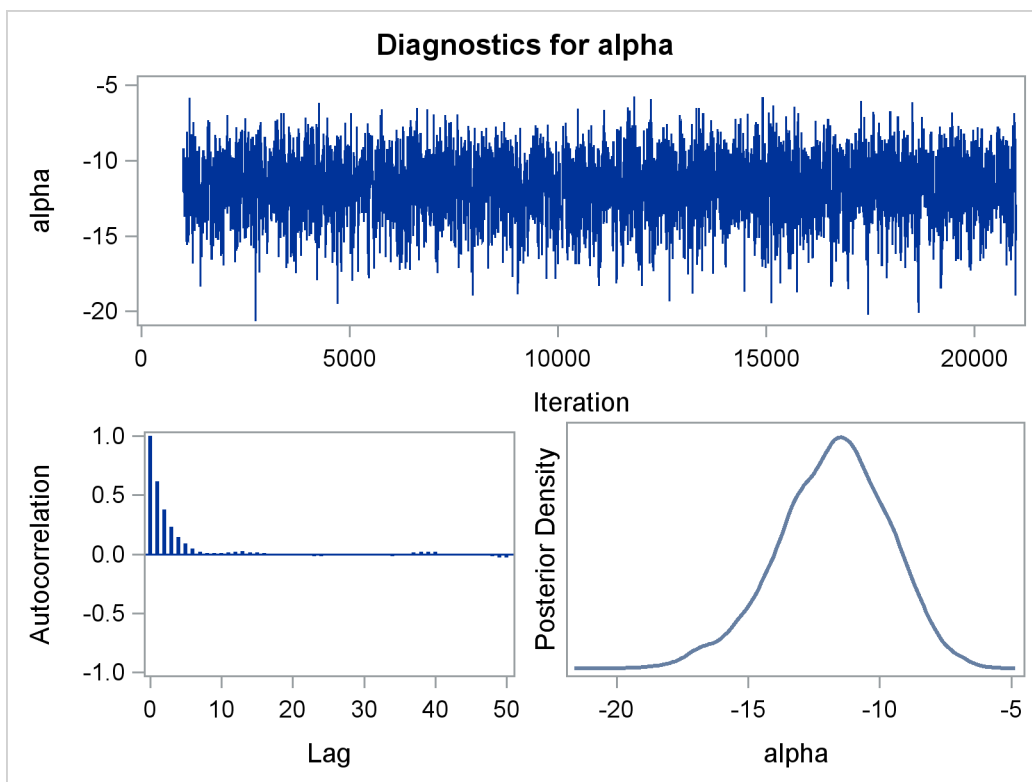
| Logistic Regression Model with a Diffuse Prior |         |                         |                       |              |          |          |
|------------------------------------------------|---------|-------------------------|-----------------------|--------------|----------|----------|
| The MCMC Procedure                             |         |                         |                       |              |          |          |
| Posterior Summaries                            |         |                         |                       |              |          |          |
| Parameter                                      | N       | Mean                    | Standard<br>Deviation | Percentiles  |          |          |
|                                                |         |                         |                       | 25%          | 50%      | 75%      |
| alpha                                          | 10000   | -11.7707                | 2.0997                | -13.1243     | -11.6683 | -10.3003 |
| beta                                           | 10000   | 0.2920                  | 0.0542                | 0.2537       | 0.2889   | 0.3268   |
| Posterior Intervals                            |         |                         |                       |              |          |          |
| Parameter                                      | Alpha   | Equal-Tail Interval     |                       | HPD Interval |          |          |
| alpha                                          | 0.050   | -16.3332                | -7.9675               | -15.8822     | -7.6673  |          |
| beta                                           | 0.050   | 0.1951                  | 0.4087                | 0.1901       | 0.4027   |          |
| Logistic Regression Model with a Diffuse Prior |         |                         |                       |              |          |          |
| The MCMC Procedure                             |         |                         |                       |              |          |          |
| Monte Carlo Standard Errors                    |         |                         |                       |              |          |          |
| Parameter                                      | MCSE    | Standard<br>Deviation   |                       | MCSE/SD      |          |          |
| alpha                                          | 0.0422  | 2.0997                  |                       | 0.0201       |          |          |
| beta                                           | 0.00110 | 0.0542                  |                       | 0.0203       |          |          |
| Effective Sample Sizes                         |         |                         |                       |              |          |          |
| Parameter                                      | ESS     | Autocorrelation<br>Time |                       | Efficiency   |          |          |
| alpha                                          | 2470.1  | 4.0484                  |                       | 0.2470       |          |          |
| beta                                           | 2435.4  | 4.1060                  |                       | 0.2435       |          |          |

The summary statistics table shows that the sample mean of the output chain for the parameter alpha is  $-11.7707$ . This is an estimate of the mean of the marginal posterior distribution for the intercept parameter alpha. The estimated posterior standard deviation for alpha is  $2.0997$ . The two 95% credible intervals for alpha are both negative, which indicates with very high probability that the intercept term is negative. On the other hand, you observe a positive effect on the regression coefficient beta. Exposure to the environment contaminant increases the probability of death.

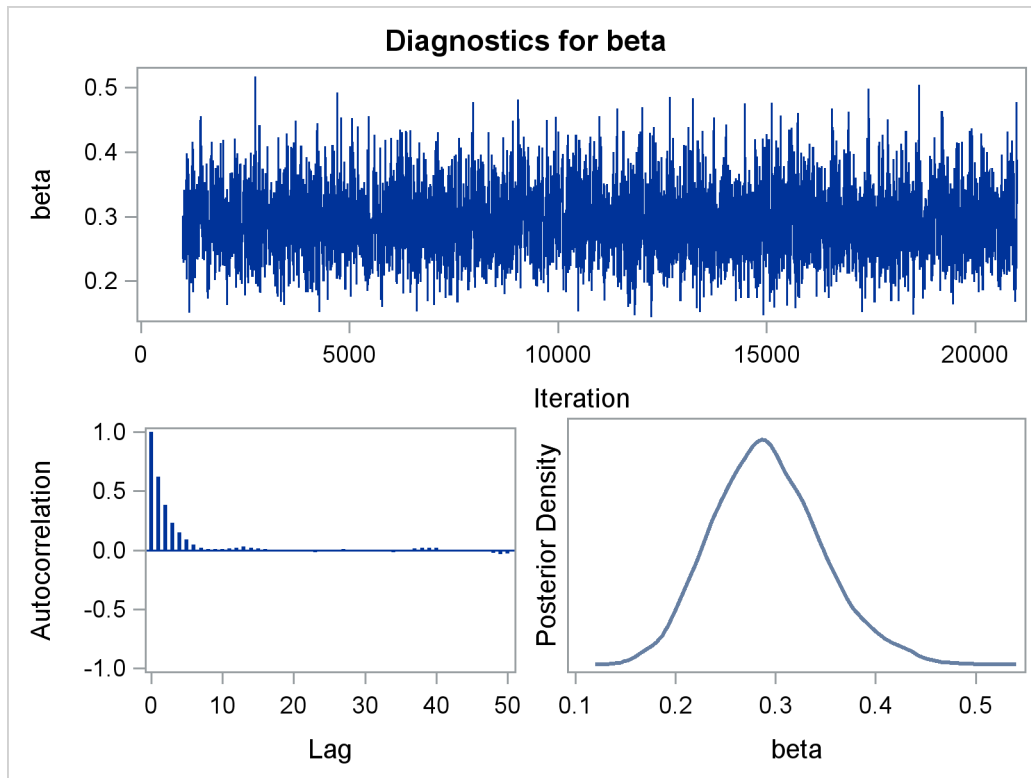
The Monte Carlo standard errors of each parameter are significantly small relative to the posterior standard deviations. A small MCSE/SD ratio indicates that the Markov chain has stabilized and the mean estimates do not vary much over time. Note that the precision in the parameter estimates increases with the square of the MCMC sample size, so if you want to double the precision, you must quadruple the MCMC sample size.

MCMC chains do not produce independent samples. Each sample point depends on the point before it. In this case, the correlation time estimate, read from the effective sample sizes table, is roughly 4. This means that it takes four observations from the MCMC output to make inferences about alpha with the same precision that you would get from using an independent sample. The effective sample size of 2470 reflects this loss of efficiency. The coefficient beta has similar efficiency. You can often observe that some parameters have significantly better mixing (better efficiency) than others, even in a single Markov chain run.

**Output 55.3.2** Plots for Parameters in the Logistic Regression Example



Output 55.3.2 continued



Trace plots and autocorrelation plots of the posterior samples are shown in [Output 55.3.2](#). Convergence looks good in both parameters; there is good mixing in the trace plot and quick drop-off in the ACF plot.

One advantage of Bayesian methods is the ability to directly answer scientific questions. In this example, you might want to find out the posterior probability that the environmental contaminant increases the probability of death—that is,  $\Pr(\beta > 0|y)$ . This can be estimated using the following steps:

```
proc format;
 value betafmt low=0 = 'beta <= 0' 0<-high = 'beta > 0';
run;

proc freq data=beetleout;
 tables beta /nocum;
 format beta betafmt.;
run;
```

Output 55.3.3 Frequency Counts

| Logistic Regression Model with a Diffuse Prior |           |         |
|------------------------------------------------|-----------|---------|
| The FREQ Procedure                             |           |         |
| beta                                           | Frequency | Percent |
| beta > 0                                       | 10000     | 100.00  |

All of the simulated values for  $\beta$  are greater than zero, so the sample estimate of the posterior probability that  $\beta > 0$  is 100%. The evidence overwhelmingly supports the hypothesis that increased levels of the environmental contaminant increase the probability of death.

If you are interested in making inference based on any quantities that are transformations of the random variables, you can either do it directly in PROC MCMC or by using the DATA step after you run the simulation. Transformations sometimes can make parameter inference quite formidable using direct analytical methods, but with simulated chains, it is easy to compute chains for any set of parameters. Suppose you are interested in the lethal dose and want to estimate the level of the covariate  $x$  that corresponds to a probability of death,  $p$ . Abbreviate this quantity as  $ldp$ . In other words, you want to solve the logit transformation with a fixed value  $p$ . The lethal dose is as follows:

$$ldp = \frac{\log\left(\frac{p}{1-p}\right) - \alpha}{\beta}$$

You can obtain an estimate of any  $ldp$  by using the posterior mean estimates for  $\alpha$  and  $\beta$ . For example,  $lp95$ , which corresponds to  $p = 0.95$ , is calculated as follows:

$$lp95 = \frac{\log\left(\frac{0.95}{1-0.95}\right) + 11.77}{0.29} = 50.79$$

where  $-11.77$  and  $0.29$  are the posterior mean estimates of  $\alpha$  and  $\beta$ , respectively, and  $50.79$  is the estimated lethal dose that leads to a 95% death rate.

While it is easy to obtain the point estimates, it is harder to estimate other posterior quantities, such as the standard deviation directly. However, with PROC MCMC, you can trivially get estimates of any posterior quantities of  $lp95$ . Consider the following program in PROC MCMC:

```
proc mcmc data=beetles ntu=1000 nmc=20000 nthin=2 propcov=quanew
 outpost=beetleout seed=246810 plot=density
 monitor=(pi30 ld05 ld50 ld95);
 ods select PostSummaries PostIntervals densitypanel;
 parms (alpha beta) 0;
 begincnst;
 c1 = log(0.05 / 0.95);
 c2 = -c1;
 endcnst;

 beginnodata;
 prior alpha beta ~ normal(0, var = 10000);
 pi30 = logistic(alpha + beta*30);
 ld05 = (c1 - alpha) / beta;
 ld50 = - alpha / beta;
 ld95 = (c2 - alpha) / beta;
 endnodata;
 pi = logistic(alpha + beta*x);
 model y ~ binomial(n,pi);
run;
ods graphics off;
```

The program estimates four additional posterior quantities. The three  $lpd$  quantities,  $ld05$ ,  $ld50$ , and  $ld95$ , are the three levels of the covariate that kills 5%, 50%, and 95% of the population, respectively. The predicted probability when the covariate  $x$  takes the value of 30 is  $\pi_{30}$ . The `MONITOR=` option selects the quantities of interest. The `PLOTS=` option selects kernel density plots as the only ODS graphical output, excluding the trace plot and autocorrelation plot.

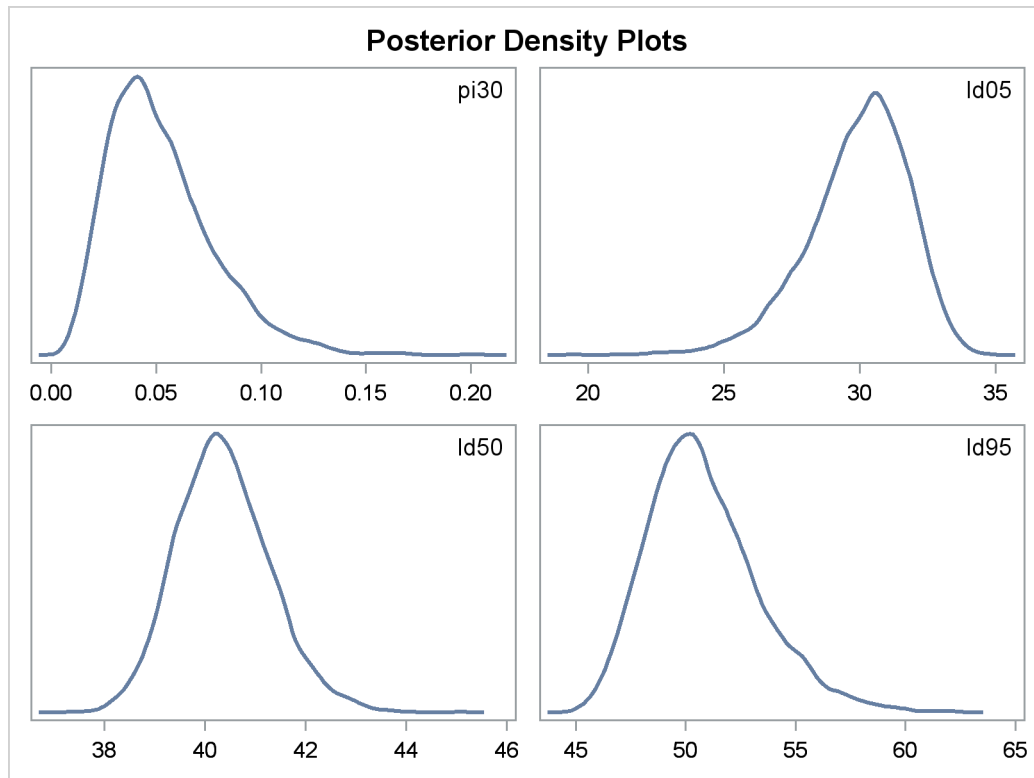
Programming statements between the `BEGINCNST` and `ENDCNST` statements define two constants. These statements are executed once at the beginning of the simulation. The programming statements between the `BEGINNODATA` and `ENDNODATA` statements evaluate the quantities of interest. The symbols,  $\pi_{30}$ ,  $ld05$ ,  $ld50$ , and  $ld95$ , are functions of the parameters  $\alpha$  and  $\beta$  only. Hence, they should not be processed at the observation level and should be included in the `BEGINNODATA` and `ENDNODATA` statements. [Output 55.3.4](#) lists the posterior summary and [Output 55.3.5](#) shows the density plots of these posterior quantities.

#### Output 55.3.4 PROC MCMC Results

| Logistic Regression Model with a Diffuse Prior |       |                     |                       |              |         |         |
|------------------------------------------------|-------|---------------------|-----------------------|--------------|---------|---------|
| The MCMC Procedure                             |       |                     |                       |              |         |         |
| Posterior Summaries                            |       |                     |                       |              |         |         |
| Parameter                                      | N     | Mean                | Standard<br>Deviation | Percentiles  |         |         |
|                                                |       |                     |                       | 25%          | 50%     | 75%     |
| $\pi_{30}$                                     | 10000 | 0.0524              | 0.0253                | 0.0340       | 0.0477  | 0.0662  |
| $ld05$                                         | 10000 | 29.9281             | 1.8814                | 28.8430      | 30.1727 | 31.2563 |
| $ld50$                                         | 10000 | 40.3745             | 0.9377                | 39.7271      | 40.3165 | 40.9612 |
| $ld95$                                         | 10000 | 50.8210             | 2.5353                | 49.0372      | 50.5157 | 52.3100 |
| Posterior Intervals                            |       |                     |                       |              |         |         |
| Parameter                                      | Alpha | Equal-Tail Interval |                       | HPD Interval |         |         |
| $\pi_{30}$                                     | 0.050 | 0.0161              | 0.1133                | 0.0109       | 0.1008  |         |
| $ld05$                                         | 0.050 | 25.6409             | 32.9660               | 26.2193      | 33.2774 |         |
| $ld50$                                         | 0.050 | 38.6706             | 42.3718               | 38.6194      | 42.2811 |         |
| $ld95$                                         | 0.050 | 46.7180             | 56.7667               | 46.3221      | 55.8774 |         |

The posterior mean estimate of  $lp_{95}$  is 50.82, which is close to the estimate of 50.79 by using the posterior mean estimates of the parameters. With PROC MCMC, in addition to the mean estimate, you can get the standard deviation, quantiles, and interval estimates at any level of significance.

From the density plots, you can see, for example, that the sample distribution for  $\pi_{30}$  is skewed to the right, and almost all of your posterior belief concerning  $\pi_{30}$  is concentrated in the region between zero and 0.15.

**Output 55.3.5** Density Plots of Quantities of Interest in the Logistic Regression Example

It is easy to use the DATA step to calculate these quantities of interest. The following DATA step uses the simulated values of  $\alpha$  and  $\beta$  to create simulated values from the posterior distributions of  $ld_{05}$ ,  $ld_{50}$ ,  $ld_{95}$ , and  $\pi_{30}$ :

```
data transout;
 set beetleout;
 pi30 = logistic(alpha + beta*30);
 ld05 = (log(0.05 / 0.95) - alpha) / beta;
 ld50 = (log(0.50 / 0.50) - alpha) / beta;
 ld95 = (log(0.95 / 0.05) - alpha) / beta;
run;
```

Subsequently, you can use SAS/INSIGHT, or the UNIVARIATE, CAPABILITY, or KDE procedures to analyze the posterior sample. If you want to regenerate the default ODS graphs from PROC MCMC, see “Regenerating Diagnostics Plots” on page 4505.

---

### Example 55.4: Logistic Regression Model with Jeffreys' Prior

A controlled experiment was run to study the effect of the rate and volume of air inspired on a transient reflex vasoconstriction in the skin of the fingers. Thirty-nine tests under various combinations of rate and volume of air inspired were obtained (Finney 1947). The result of each test is whether or not vasoconstriction occurred. Pregibon (1981) uses this set of data to illustrate the diagnostic measures he proposes for detecting influential observations and to quantify their effects on various aspects of the maximum likelihood fit. The following statements create the data set Vaso:

```

title 'Logistic Regression Model with Jeffreys Prior';
data vaso;
 input vol rate resp @@;
 lvol = log(vol);
 lrate = log(rate);
 ind = _n_;
 cnst = 1;
 datalines;
3.7 0.825 1 3.5 1.09 1 1.25 2.5 1 0.75 1.5 1
0.8 3.2 1 0.7 3.5 1 0.6 0.75 0 1.1 1.7 0
0.9 0.75 0 0.9 0.45 0 0.8 0.57 0 0.55 2.75 0
0.6 3.0 0 1.4 2.33 1 0.75 3.75 1 2.3 1.64 1
3.2 1.6 1 0.85 1.415 1 1.7 1.06 0 1.8 1.8 1
0.4 2.0 0 0.95 1.36 0 1.35 1.35 0 1.5 1.36 0
1.6 1.78 1 0.6 1.5 0 1.8 1.5 1 0.95 1.9 0
1.9 0.95 1 1.6 0.4 0 2.7 0.75 1 2.35 0.03 0
1.1 1.83 0 1.1 2.2 1 1.2 2.0 1 0.8 3.33 1
0.95 1.9 0 0.75 1.9 0 1.3 1.625 1
;

```

The variable `resp` represents the outcome of a test. The variable `lvol` represents the log of the volume of air intake, and the variable `lrate` represents the log of the rate of air intake. You can model the data by using logistic regression. You can model the response with a binary likelihood:

$$\text{resp}_i \sim \text{binary}(p_i)$$

with

$$p_i = \frac{1}{1 + \exp(-(\beta_0 + \beta_1 \text{lvol}_i + \beta_2 \text{lrate}_i))}$$

Let  $\mathbf{X}$  be the design matrix in the regression. Jeffreys' prior for this model is

$$p(\boldsymbol{\beta}) \propto |\mathbf{X}'\mathbf{M}\mathbf{X}|^{1/2}$$

where  $\mathbf{M}$  is a 39 by 39 matrix with off-diagonal elements being 0 and diagonal elements being  $p_i(1 - p_i)$ . For details on Jeffreys' prior, see "Jeffreys' Prior" on page 129. You can use a number of matrix functions, such as the determinant function, in PROC MCMC to construct Jeffreys' prior. The following statements illustrate how to fit a logistic regression with Jeffreys' prior:

```

%let n = 39;
proc mcmc data=vaso nmc=10000 outpost=mcmcout seed=17;
 ods select PostSummaries PostIntervals;

 array beta[3] beta0 beta1 beta2;
 array m[&n, &n];
 array x[1] / nosymbols;
 array xt[3, &n];
 array xtm[3, &n];
 array xmx[3, 3];
 array p[&n];

 parms beta0 1 beta1 1 beta2 1;

```

```

begincnst;
 if (ind eq 1) then do;
 rc = read_array("vaso", x, "cnst", "lvol", "lrate");
 call transpose(x, xt);
 call zeromatrix(m);
 end;
endcnst;

beginnodata;
call mult(x, beta, p); /* p = x * beta */
do i = 1 to &n;
 p[i] = 1 / (1 + exp(-p[i])); /* p[i] = 1/(1+exp(-x*beta)) */
 m[i,i] = p[i] * (1-p[i]);
end;
call mult (xt, m, xtm); /* xtm = xt * m */
call mult (xtm, x, xmx); /* xmx = xtm * x */
call det (xmx, lp); /* lp = det(xmx) */
lp = 0.5 * log(lp); /* lp = -0.5 * log(lp) */
prior beta: ~ general(lp);
endnodata;

model resp ~ bern(p[ind]);
run;

```

The first `ARRAY` statement defines an array `beta` with three elements: `beta0`, `beta1`, and `beta2`. The subsequent statements define arrays that are used in the construction of Jeffreys' prior. These include `m` (the  $M$  matrix), `x` (the design matrix), `xt` (the transpose of `x`), and some additional work spaces.

The explanatory variables `lvol` and `lrate` are saved in the array `x` in the `BEGINCNST` and `ENDCNST` statements. See “[BEGINCNST/ENDCNST Statement](#)” on page 4441 for details. After all the variables are read into `x`, you transpose the `x` matrix and store it to `xt`. The `ZEROMATRIX` function call assigns all elements in matrix `m` the value zero. To avoid redundant calculation, it is best to perform these calculations as the last observation of the data set is processed—that is, when `ind` is 39.

You calculate Jeffreys' prior in the `BEGINNODATA` and `ENDNODATA` statements. The probability vector `p` is the product of the design matrix `x` and parameter vector `beta`. The diagonal elements in the matrix `m` are  $p_i(1 - p_i)$ . The expression `lp` is the logarithm of Jeffreys' prior. The `PRIOR` statement assigns `lp` as the prior for the  $\beta$  regression coefficients. The `MODEL` statement assigns a binary likelihood to `resp`, with probability `p[ind]`. The `p` array is calculated earlier using the matrix function `MULT`. You use the `ind` variable to pick out the right probability value for each `resp`.

Posterior summary statistics are displayed in [Output 55.4.1](#).



**Output 55.4.1** PROC MCMC Results, Jeffreys' prior

| Logistic Regression Model with Jeffreys Prior |       |                     |                       |              |         |         |
|-----------------------------------------------|-------|---------------------|-----------------------|--------------|---------|---------|
| The MCMC Procedure                            |       |                     |                       |              |         |         |
| Posterior Summaries                           |       |                     |                       |              |         |         |
| Parameter                                     | N     | Mean                | Standard<br>Deviation | Percentiles  |         |         |
|                                               |       |                     |                       | 25%          | 50%     | 75%     |
| beta0                                         | 10000 | -2.9587             | 1.3258                | -3.8117      | -2.7938 | -2.0007 |
| beta1                                         | 10000 | 5.2905              | 1.8193                | 3.9861       | 5.1155  | 6.4145  |
| beta2                                         | 10000 | 4.6889              | 1.8189                | 3.3570       | 4.4914  | 5.8547  |
| Posterior Intervals                           |       |                     |                       |              |         |         |
| Parameter                                     | Alpha | Equal-Tail Interval |                       | HPD Interval |         |         |
| beta0                                         | 0.050 | -5.8247             | -0.7435               | -5.5936      | -0.6027 |         |
| beta1                                         | 0.050 | 2.3001              | 9.3789                | 1.8590       | 8.7222  |         |
| beta2                                         | 0.050 | 1.6788              | 8.6643                | 1.3611       | 8.2490  |         |

You can also use PROC GENMOD to fit the same model by using the following statements:

```
proc genmod data=vaso descending;
 ods select PostSummaries PostIntervals;
 model resp = lvol lrate / d=bin link=logit;
 bayes seed=17 coeffprior=jeffreys nmc=20000 thin=2;
run;
```

The MODEL statement indicates that `resp` is the response variable and `lvol` and `lrate` are the covariates. The options in the MODEL statement specify a binary likelihood and a logit link function. The BAYES statement requests Bayesian capability. The SEED=, NMC=, and THIN= arguments work in the same way as in PROC MCMC. The COEFFPRIOR=JEFFREYS option requests Jeffreys' prior in this analysis.

The PROC GENMOD statements produce [Output 55.4.2](#), with estimates very similar to those reported in [Output 55.4.1](#). Note that you should not expect to see identical output from PROC GENMOD and PROC MCMC, even with the simulation setup and identical random number seed. The two procedures use different sampling algorithms. PROC GENMOD uses the adaptive rejection metropolis algorithm (ARMS) (Gilks and Wild 1992; Gilks 2003) while PROC MCMC uses a random walk Metropolis algorithm. The asymptotic answers, which means that you let both procedures run an very long time, would be the same as they both generate samples from the same posterior distribution.

## Output 55.4.2 PROC GENMOD Results

| Logistic Regression Model with Jeffreys Prior |       |                     |                       |              |         |         |
|-----------------------------------------------|-------|---------------------|-----------------------|--------------|---------|---------|
| The GENMOD Procedure                          |       |                     |                       |              |         |         |
| Bayesian Analysis                             |       |                     |                       |              |         |         |
| Posterior Summaries                           |       |                     |                       |              |         |         |
| Parameter                                     | N     | Mean                | Standard<br>Deviation | Percentiles  |         |         |
|                                               |       |                     |                       | 25%          | 50%     | 75%     |
| Intercept                                     | 10000 | -2.8773             | 1.3213                | -3.6821      | -2.7326 | -1.9097 |
| lvol                                          | 10000 | 5.2059              | 1.8707                | 3.8535       | 4.9574  | 6.3337  |
| lrate                                         | 10000 | 4.5525              | 1.8140                | 3.2281       | 4.3722  | 5.6643  |
| Posterior Intervals                           |       |                     |                       |              |         |         |
| Parameter                                     | Alpha | Equal-Tail Interval |                       | HPD Interval |         |         |
| Intercept                                     | 0.050 | -5.7447             | -0.6877               | -5.4593      | -0.5488 |         |
| lvol                                          | 0.050 | 2.2066              | 9.4415                | 2.0729       | 9.2343  |         |
| lrate                                         | 0.050 | 1.5906              | 8.5272                | 1.3351       | 8.1152  |         |

---

**Example 55.5: Poisson Regression**

You can use the Poisson distribution to model the distribution of cell counts in a multiway contingency table. Aitkin et al. (1989) have used this method to model insurance claims data. Suppose the following hypothetical insurance claims data are classified by two factors: age group (with two levels) and car type (with three levels). The following statements create the data set:

```

title 'Poisson Regression';
data insure;
 input n c car $ age;
 ln = log(n);
 datalines;
500 42 small 0
1200 37 medium 0
100 1 large 0
400 101 small 1
500 73 medium 1
300 14 large 1
;

proc transreg data=insure design;
 model class(car / zero=last);
 id n c age ln;
 output out=input_insure(drop=_: Int:);
run;

```

The variable *n* represents the number of insurance policy holders and the variable *c* represents the number of insurance claims. The variable *car* is the type of car involved (classified into three groups), and it is coded into two levels. The variable *age* is the age group of a policy holder (classified into two groups).

Assume that the number of claims *c* has a Poisson probability distribution and that its mean,  $\mu_i$ , is related to the factors *car* and *age* for observation *i* by

$$\begin{aligned}\log(\mu_i) &= \log(n_i) + \mathbf{x}'\boldsymbol{\beta} \\ &= \log(n_i) + \beta_0 + \\ &\quad \text{car}_i(1)\beta_1 + \text{car}_i(2)\beta_2 + \text{car}_i(3)\beta_3 + \\ &\quad \text{age}_i(1)\beta_4 + \text{age}_i(2)\beta_5\end{aligned}$$

The indicator variables  $\text{car}_i(j)$  is associated with the *j*th level of the variable *car* for observation *i* in the following way:

$$\text{car}_i(j) = \begin{cases} 1 & \text{if } \text{car} = j \\ 0 & \text{if } \text{car} \neq j \end{cases}$$

A similar coding applies to *age*. The  $\boldsymbol{\beta}$ 's are parameters. The logarithm of the variable *n* is used as an offset—that is, a regression variable with a constant coefficient of 1 for each observation. Having the offset constant in the model is equivalent to fitting an expanded data set with 3000 observations, each with response variable *y* observed on an individual level. The log link relates the mean and the factors *car* and *age*.

The following statements run PROC MCMC:

```
proc mcmc data=input_insure outpost=insureout nmc=5000 propcov=quanew
 maxtune=0 seed=7;
 ods select PostSummaries PostIntervals;
 array data[4] 1 &_trgind age;
 array beta[4] alpha beta_car1 beta_car2 beta_age;
 parms alpha beta;
 prior alpha beta: ~ normal(0, prec = 1e-6);
 call mult(data, beta, mu);
 model c ~ poisson(exp(mu+ln));
run;
```

The analysis uses a relatively flat prior on all the regression coefficients, with mean at 0 and precision at  $10^{-6}$ . The option `MAXTUNE=0` skips the tuning phase because the optimization routine (`PROPCOV=QUANEW`) provides good initial values and proposal covariance matrix.

There are four parameters in the model: *alpha* is the intercept; *beta\_car1* and *beta\_car2* are coefficients for the class variable *car*, which has three levels; and *beta\_age* is the coefficient for *age*. The symbol *mu* connects the regression model and the Poisson mean by using the log link. The `MODEL` statement specifies a Poisson likelihood for the response variable *c*.

Posterior summary and interval statistics are shown in [Output 55.5.1](#).

### Output 55.5.1 MCMC Results

| Poisson Regression  |      |         |                       |             |         |         |
|---------------------|------|---------|-----------------------|-------------|---------|---------|
| The MCMC Procedure  |      |         |                       |             |         |         |
| Posterior Summaries |      |         |                       |             |         |         |
| Parameter           | N    | Mean    | Standard<br>Deviation | Percentiles |         |         |
|                     |      |         |                       | 25%         | 50%     | 75%     |
| alpha               | 5000 | -2.6403 | 0.1344                | -2.7261     | -2.6387 | -2.5531 |
| beta_car1           | 5000 | -1.8335 | 0.2917                | -2.0243     | -1.8179 | -1.6302 |
| beta_car2           | 5000 | -0.6931 | 0.1255                | -0.7775     | -0.6867 | -0.6118 |
| beta_age            | 5000 | 1.3151  | 0.1386                | 1.2153      | 1.3146  | 1.4094  |

| Posterior Intervals |       |                     |         |              |         |
|---------------------|-------|---------------------|---------|--------------|---------|
| Parameter           | Alpha | Equal-Tail Interval |         | HPD Interval |         |
| alpha               | 0.050 | -2.9201             | -2.3837 | -2.9133      | -2.3831 |
| beta_car1           | 0.050 | -2.4579             | -1.3036 | -2.4692      | -1.3336 |
| beta_car2           | 0.050 | -0.9462             | -0.4497 | -0.9485      | -0.4589 |
| beta_age            | 0.050 | 1.0442              | 1.5898  | 1.0387       | 1.5812  |

To fit the same model by using PROC GENMOD, you can do the following. Note that the default normal prior on the coefficients  $\beta$  is  $N(0, \text{prec} = 1e - 6)$ , the same as used in the PROC MCMC. The following statements run PROC GENMOD and create [Output 55.5.2](#):

```
proc genmod data=insure;
 ods select PostSummaries PostIntervals;
 class car age(descending);
 model c = car age / dist=poisson link=log offset=ln;
 bayes seed=17 nmc=5000 coeffprior=normal;
run;
```

To compare, posterior summary and interval statistics from PROC GENMOD are reported in [Output 55.5.2](#), and they are very similar to PROC MCMC results in [Output 55.5.1](#).

## Output 55.5.2 PROC GENMOD Results

| Poisson Regression   |      |         |                       |             |         |         |
|----------------------|------|---------|-----------------------|-------------|---------|---------|
| The GENMOD Procedure |      |         |                       |             |         |         |
| Bayesian Analysis    |      |         |                       |             |         |         |
| Posterior Summaries  |      |         |                       |             |         |         |
| Parameter            | N    | Mean    | Standard<br>Deviation | Percentiles |         |         |
|                      |      |         |                       | 25%         | 50%     | 75%     |
| Intercept            | 5000 | -2.6424 | 0.1336                | -2.7334     | -2.6391 | -2.5547 |
| carlarge             | 5000 | -1.8040 | 0.2764                | -1.9859     | -1.7929 | -1.6101 |
| carmedium            | 5000 | -0.6908 | 0.1311                | -0.7797     | -0.6898 | -0.6044 |
| age1                 | 5000 | 1.3207  | 0.1384                | 1.2264      | 1.3209  | 1.4140  |

| Posterior Intervals |       |                     |         |              |         |
|---------------------|-------|---------------------|---------|--------------|---------|
| Parameter           | Alpha | Equal-Tail Interval |         | HPD Interval |         |
| Intercept           | 0.050 | -2.9154             | -2.3893 | -2.8997      | -2.3850 |
| carlarge            | 0.050 | -2.3668             | -1.2891 | -2.2992      | -1.2378 |
| carmedium           | 0.050 | -0.9437             | -0.4231 | -0.9434      | -0.4230 |
| age1                | 0.050 | 1.0455              | 1.5871  | 1.0266       | 1.5629  |

Note that the descending option in the CLASS statement reverses the sort order of the class variable `age` so that the results agree with PROC MCMC. If this option is not used, the estimate for `age` has a reversed sign as compared to [Output 55.5.2](#).

## Example 55.6: Nonlinear Poisson Regression Models

This example illustrates how to fit a nonlinear Poisson regression with PROC MCMC. In addition, it shows how you can improve the mixing of the Markov chain by selecting a different proposal distribution or by sampling on the transformed scale of a parameter. This example shows how to analyze count data for calls to a technical support help line in the weeks immediately following a product release. This information could be used to decide upon the allocation of technical support resources for new products. You can model the number of daily calls as a Poisson random variable, with the average number of calls modeled as a nonlinear function of the number of weeks that have elapsed since the product's release. The data are input into a SAS data set as follows:

```

title 'Nonlinear Poisson Regression';
data calls;
 input weeks calls @@;
 datalines;
1 0 1 2 2 2 1 3 1 3 3
4 5 4 8 5 5 5 9 6 17 6 9
7 24 7 16 8 23 8 27
;

```

During the first several weeks after a new product is released, the number of questions that technical support receives concerning the product increases in a sigmoidal fashion. The expression for the mean value in the classic Poisson regression involves the log link. There is some theoretical justification for this link, but with MCMC methodologies, you are not constrained to exploring only models that are computationally convenient. The number of calls to technical support tapers off after the initial release, so in this example you can use a logistic-type function to model the mean number of calls received weekly for the time period immediately following the initial release. The mean function  $\lambda(t)$  is modeled as follows:

$$\lambda_i = \frac{\gamma}{1 + \exp[-(\alpha + \beta t_i)]}$$

The likelihood for every observation  $\text{calls}_i$  is

$$\text{calls}_i \sim \text{Poisson}(\lambda_i)$$

Past experience with technical support data for similar products suggests the following prior distributions:

$$\begin{aligned} \gamma &\sim \text{gamma}(\text{shape} = 3.5, \text{scale} = 12) \\ \alpha &\sim \text{normal}(-5, \text{sd} = 0.5) \\ \beta &\sim \text{normal}(0.75, \text{sd} = 0.5) \end{aligned}$$

The following PROC MCMC statements fit this model:

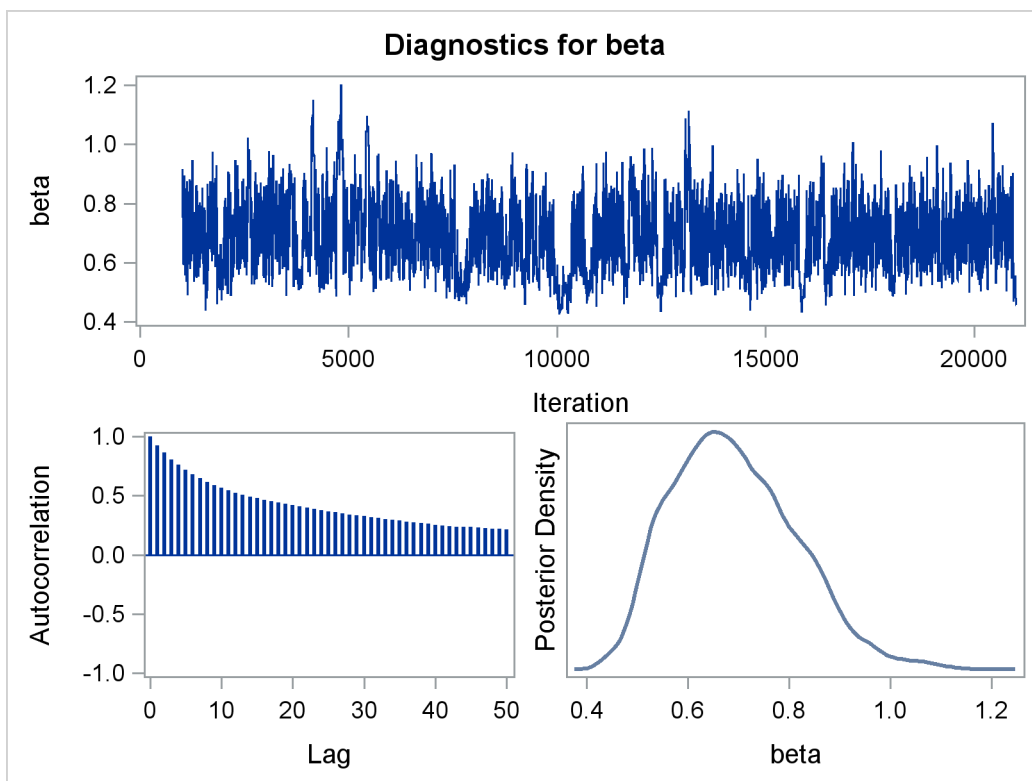
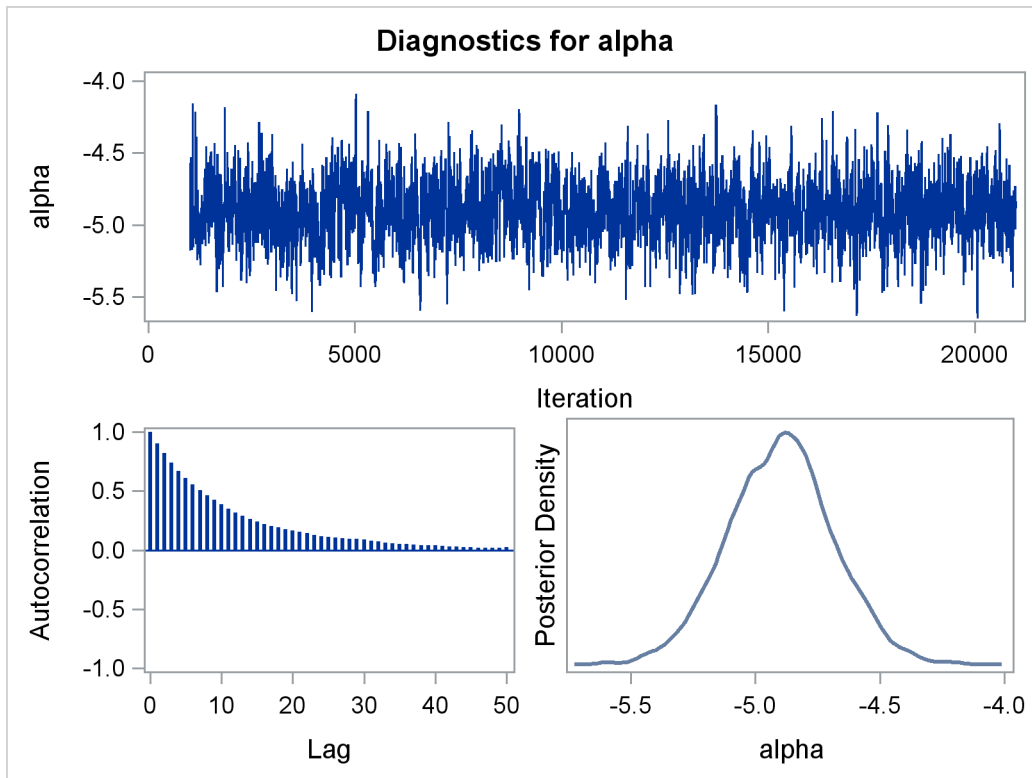
```
ods graphics on;
proc mcmc data=calls outpost=callout seed=53197 ntu=1000 nmc=20000
 propcov=quanew stats=none diag=ess;
 ods select TADpanel ess;
 parms alpha -4 beta 1 gamma 2;
 prior gamma ~ gamma(3.5, scale=12);
 prior alpha ~ normal(-5, sd=0.25);
 prior beta ~ normal(0.75, sd=0.5);
 lambda = gamma*logistic(alpha+beta*weeks);
 model calls ~ poisson(lambda);
run;
```

The one **PARMS** statement defines a block of all parameters and sets their initial values individually. The **PRIOR** statements specify the informative prior distributions for the three parameters. The assignment statement defines  $\lambda$ , the mean number of calls. Instead of using the SAS function LOGISTIC, you can use the following statement to calculate  $\lambda$  and get the same result:

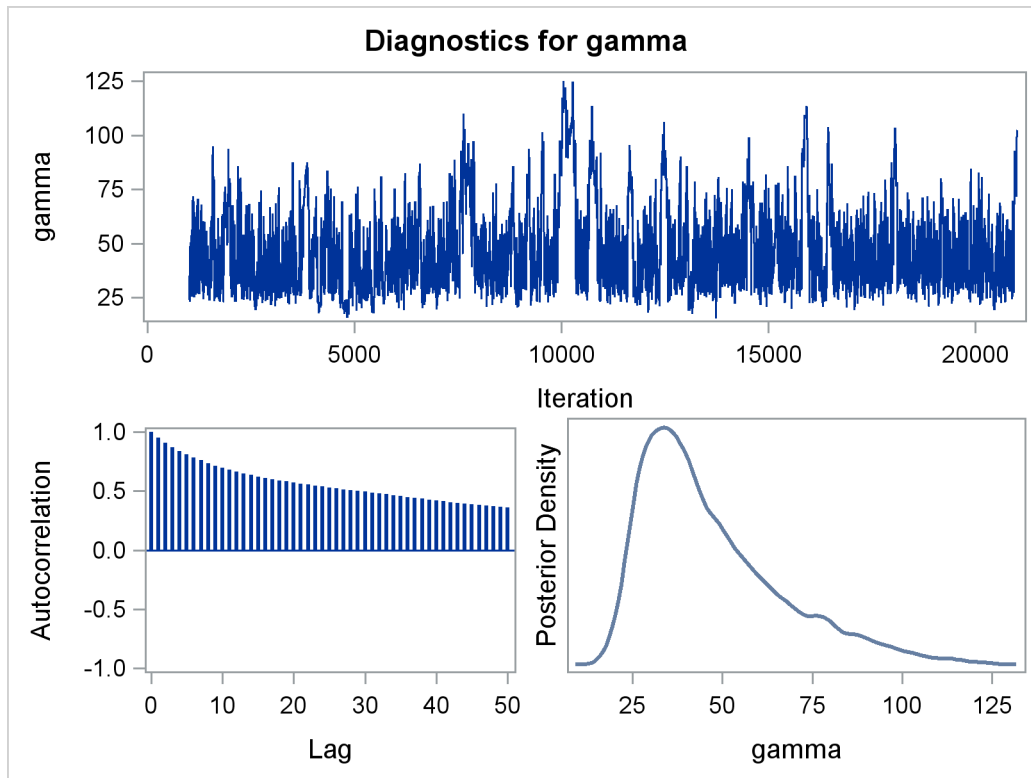
```
lambda = gamma / (1 + exp(-(alpha+beta*weeks)));
```

Mixing is not particularly good with this run of PROC MCMC. The ODS SELECT statement displays the diagnostic graphs and effective sample sizes (ESS) calculation while excluding all other output. The graphical output is shown in [Output 55.6.1](#), and the ESS of each parameters are all relatively low ([Output 55.6.2](#)).

Output 55.6.1 Plots for Parameters



Output 55.6.1 continued



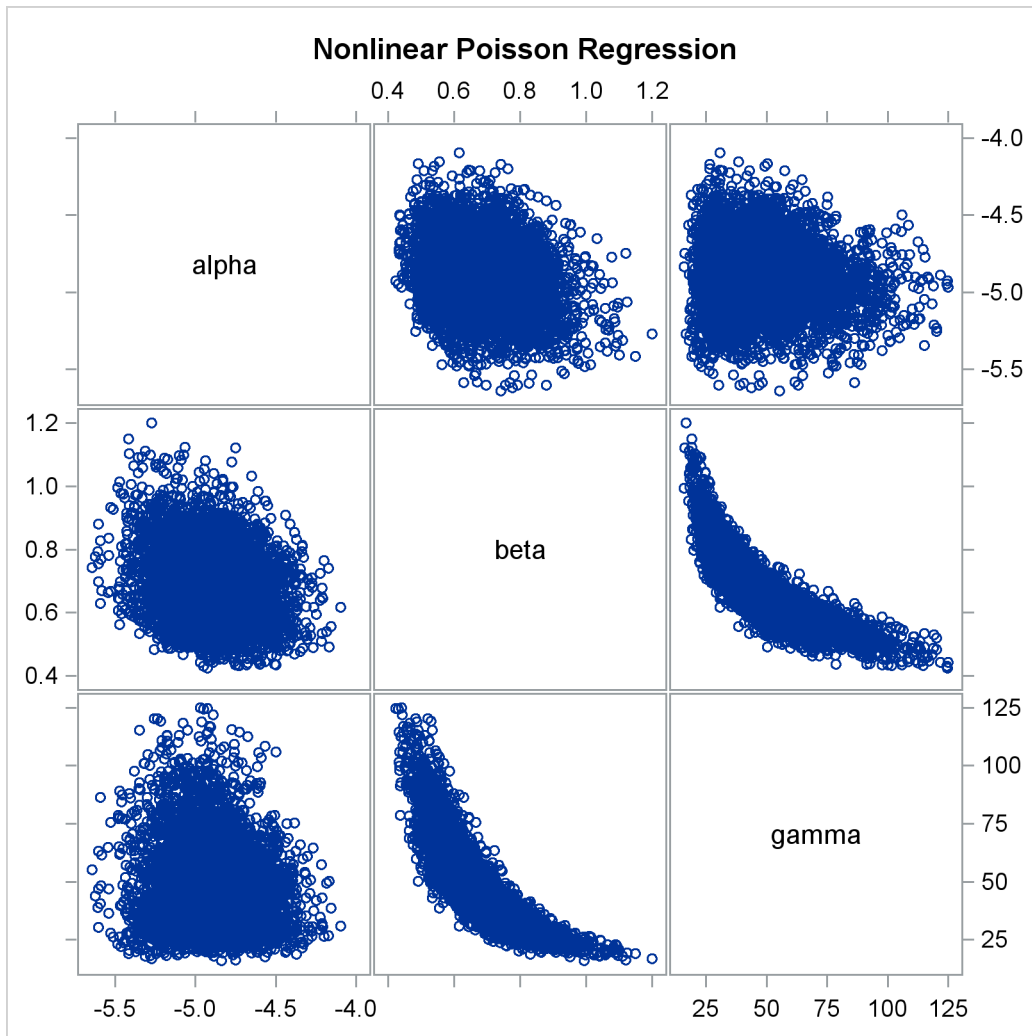
Output 55.6.2 Effective Sample Sizes

| Nonlinear Poisson Regression |       |                 |            |
|------------------------------|-------|-----------------|------------|
| The MCMC Procedure           |       |                 |            |
| Effective Sample Sizes       |       |                 |            |
| Parameter                    | ESS   | Autocorrelation |            |
|                              |       | Time            | Efficiency |
| alpha                        | 897.4 | 22.2870         | 0.0449     |
| beta                         | 231.6 | 86.3540         | 0.0116     |
| gamma                        | 162.9 | 122.8           | 0.0081     |

Often a simple scatter plot of the posterior samples can reveal a potential cause of the bad mixing. You can use PROC SGSCATTER to generate pairwise scatter plots of the three model parameters. The following statements generate Output 55.6.3:

```
proc sgscatter data=callout;
 matrix alpha beta gamma;
run;
```



**Output 55.6.3** Pairwise Scatter Plots of the Parameters

The nonlinearity in parameters **beta** and **gamma** stands out immediately. This explains why a random walk Metropolis with normal proposal has a difficult time exploring the joint distribution efficiently—the algorithm works best when the target distribution is unimodal and symmetric (normal-like). When there is nonlinearity in the parameters, it is impossible to find a single proposal scale parameter that optimally adapts to different regions of the joint parameter space. As a result, the Markov chain can be inefficient in traversing some parts of the distribution. This is evident in examining the trace plot of the **gamma** parameter. You see that the Markov chain sometimes gets stuck in the far-right tail and does not travel back to the high-density area quickly. This effect can be seen around the simulations 8,000 and 18,000 in [Output 55.6.1](#).

Reparameterization can often improve the mixing of the Markov chain. Note that the parameter **gamma** has a positive support and that the posterior distribution is right-skewed. This suggests that the chain might mix more rapidly if you sample on the logarithm of the parameter **gamma**.

Let  $\delta = \log(\gamma)$ , and reparameterize the mean function as follows:

$$\lambda_i = \frac{\exp(\delta)}{1 + \exp[-(\alpha + \beta t_i)]}$$

To obtain the same inference, you use an induced prior on  $\delta$  based on the gamma prior on the gamma parameter. This involves a transformation of variables, and you can obtain the following equivalency, where  $|\exp(\delta)|$  is the Jacobian:

$$\pi(\gamma) = \text{gamma}(\gamma; a, \text{scale} = b) = \frac{1}{b^a \Gamma(a)} \gamma^{a-1} \exp(-\gamma/b)$$

$$\Leftrightarrow \pi(\delta) = \text{gamma}(\gamma = \exp(\delta); a, \text{scale} = b) \cdot |\exp(\delta)|$$

The distribution on  $\delta$  simplifies to the following:

$$\pi(\delta) = \frac{1}{b^a \Gamma(a)} \exp(a\delta) \exp(-\exp(\delta)/b)$$

PROC MCMC supports such a distribution on the logarithm transformation of a gamma random variable. It is called the [ExpGamma](#) distribution.

In the original model, you specify a prior on gamma:

```
prior gamma ~ gamma(3.5, scale=12);
```

You can obtain the same inference by specifying an [ExpGamma](#) prior on delta and take an exponential transformation to get back to gamma:

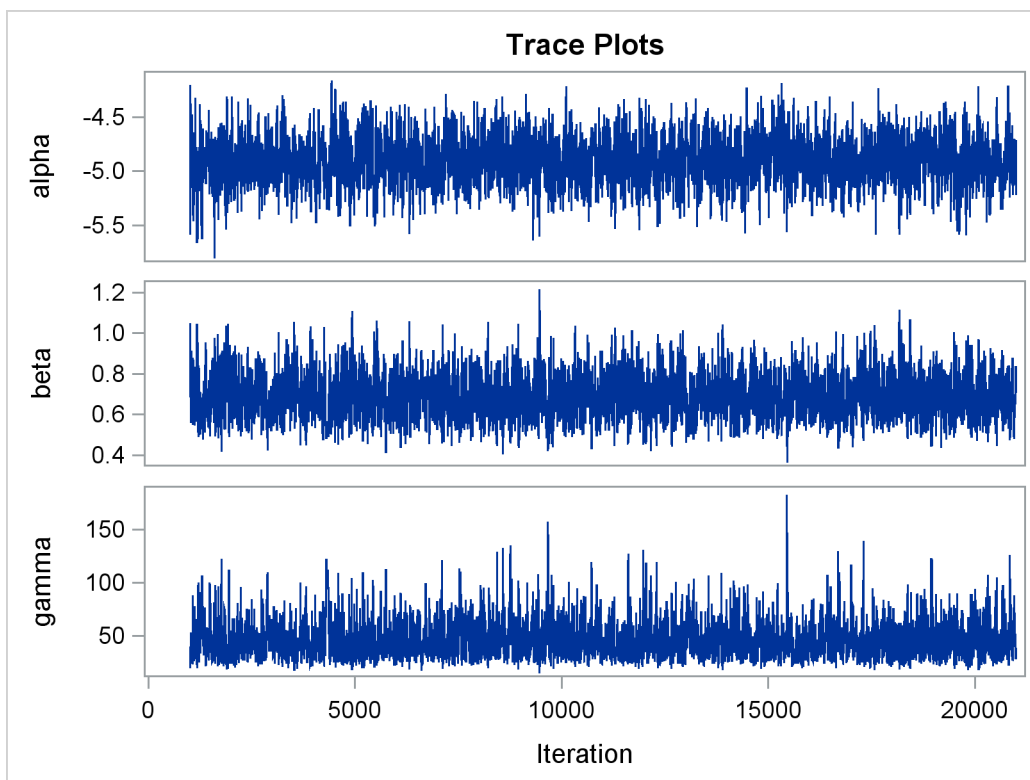
```
prior delta ~ egamma(3.5, scale=12);
gamma = exp(delta);
```

The following statements produce [Output 55.6.6](#) and [Output 55.6.4](#):

```
proc mcmc data=calls outpost=tcallout seed=53197 ntu=1000 nmc=20000
 propcov=quanew diag=ess plots=(trace) monitor=(alpha beta gamma);
 ods select PostSummaries PostIntervals ESS TRACEpanel;
 parms alpha -4 beta 1 delta 2;
 prior alpha ~ normal(-5, sd=0.25);
 prior beta ~ normal(0.75, sd=0.5);
 prior delta ~ egamma(3.5, scale=12);
 gamma = exp(delta);
 lambda = gamma*logistic(alpha+beta*weeks);
 model calls ~ poisson(lambda);
run;
```

The [PARMS](#) statement declares delta, instead of gamma, as a model parameter. The prior distribution of delta is [egamma](#), as opposed to the [gamma](#) distribution. The [GAMMA](#) assignment statement transforms delta to gamma. The [LAMBDA](#) assignment statement calculates the mean for the Poisson by using the gamma parameter. The [MODEL](#) statement specifies a Poisson likelihood for the calls response.

The trace plots in [Output 55.6.4](#) show better mixing of the parameters, and the effective sample sizes in [Output 55.6.5](#) show substantial improvements over the original formulation of the model. The improvements are especially obvious in beta and gamma, where the increase is fivefold to tenfold.

**Output 55.6.4** Plots for Parameters, Sampling on the Log Scale of Gamma**Output 55.6.5** Effective Sample Sizes, Sampling on the Log Scale of Gamma

| Nonlinear Poisson Regression |        |                         |            |
|------------------------------|--------|-------------------------|------------|
| The MCMC Procedure           |        |                         |            |
| Effective Sample Sizes       |        |                         |            |
| Parameter                    | ESS    | Autocorrelation<br>Time | Efficiency |
| alpha                        | 1338.4 | 14.9430                 | 0.0669     |
| beta                         | 1254.9 | 15.9379                 | 0.0627     |
| gamma                        | 1073.4 | 18.6320                 | 0.0537     |

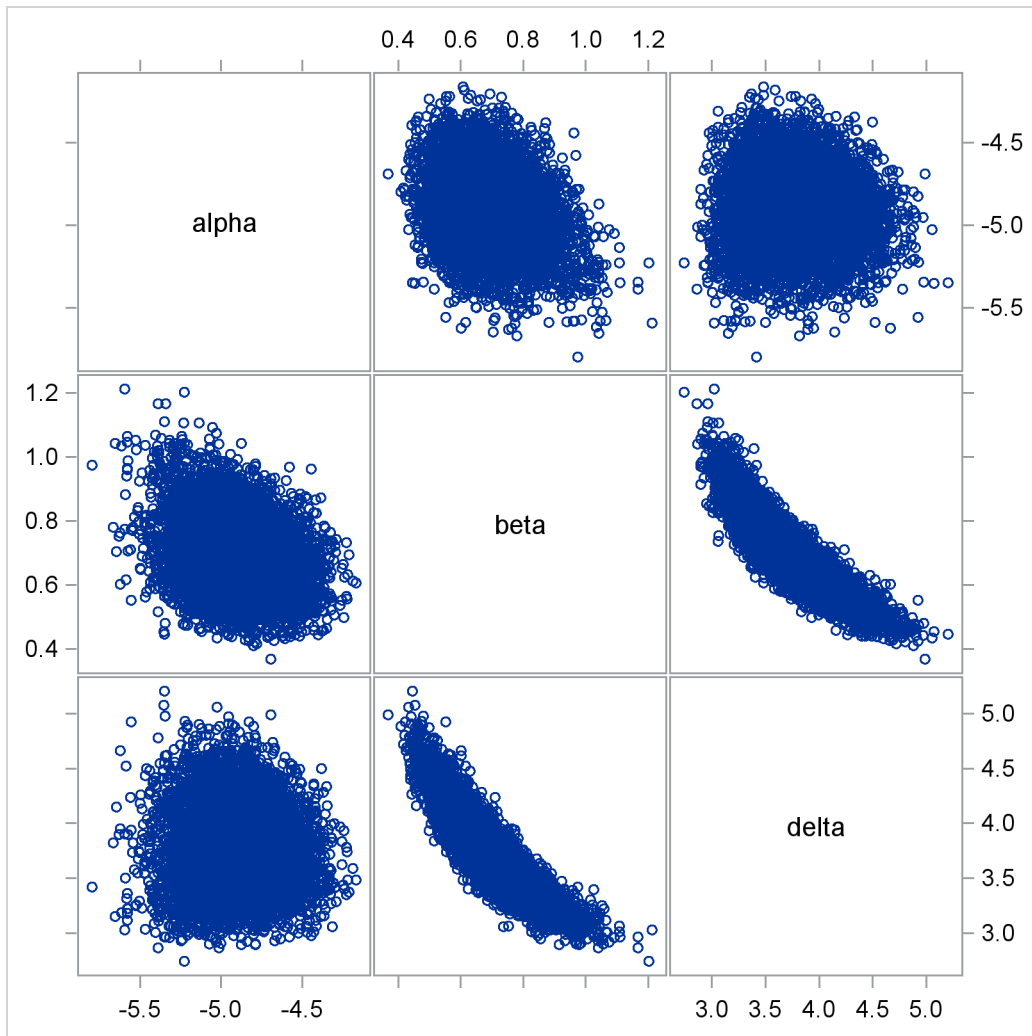
Output 55.6.6 shows the posterior summary and interval statistics of the nonlinear Poisson regression.

**Output 55.6.6** MCMC Results, Sampling on the Log Scale of Gamma

| Nonlinear Poisson Regression |       |                     |                       |              |         |         |
|------------------------------|-------|---------------------|-----------------------|--------------|---------|---------|
| The MCMC Procedure           |       |                     |                       |              |         |         |
| Posterior Summaries          |       |                     |                       |              |         |         |
| Parameter                    | N     | Mean                | Standard<br>Deviation | Percentiles  |         |         |
|                              |       |                     |                       | 25%          | 50%     | 75%     |
| alpha                        | 20000 | -4.9040             | 0.2234                | -5.0555      | -4.9055 | -4.7530 |
| beta                         | 20000 | 0.6899              | 0.1154                | 0.6055       | 0.6787  | 0.7662  |
| gamma                        | 20000 | 46.7199             | 19.4977               | 32.3528      | 41.9888 | 55.4315 |
| Posterior Intervals          |       |                     |                       |              |         |         |
| Parameter                    | Alpha | Equal-Tail Interval |                       | HPD Interval |         |         |
| alpha                        | 0.050 | -5.3392             | -4.4659               | -5.3217      | -4.4544 |         |
| beta                         | 0.050 | 0.4919              | 0.9327                | 0.4841       | 0.9169  |         |
| gamma                        | 0.050 | 23.2996             | 96.7209               | 19.6588      | 86.2425 |         |

Note that the delta parameter has a more symmetric density than the skewed gamma parameter. A pairwise scatter plot (Output 55.6.7) shows a more linear relationship between beta and delta. The Metropolis algorithm always works better if the target distribution is approximately normal.

```
proc sgscatter data=tcallout;
 matrix alpha beta delta;
run;
```

**Output 55.6.7** Pairwise Scatter Plots of the Transformed Parameters

If you are still unsatisfied with the slight nonlinearity in the parameters **beta** and **delta**, you can try another transformation on **beta**. Normally you would not want to do a logarithm transformation on a parameter that has support on the real axis, because you would risk taking the logarithm of negative values. However, because all the **beta** samples are positive and the marginal posterior distribution is away from 0, you can try a such a transformation.

Let  $\kappa = \log(\beta)$ . The prior distribution on  $\kappa$  is the following:

$$\pi(\kappa) = \text{normal}(\beta = \exp(\kappa); \mu, \sigma^2) \cdot |\exp(\kappa)|$$

You can specify the prior distribution in PROC MCMC by using a **GENERAL** function:

```
parms kappa;
lprior = logpdf("normal", exp(kappa), 0.75, 0.5) + kappa;
prior kappa ~ general(lp);
beta = exp(kappa);
```

The **PARMS** statement declares the transformed parameter kappa, which will be sampled. The **LPRIOR** assignment statement defines the logarithm of the prior distribution on kappa. The **LOGPDF** function is used here to simplify the specification of the distribution. The **PRIOR** statement specifies the nonstandard distribution as the prior on kappa. Finally, the **BETA** assignment statement transforms kappa back to the beta parameter.

Applying logarithm transformations on both beta and gamma yields the best mixing. (The results are not shown here, but you can find the code in the file *mcmcex6.sas* in the SAS Sample Library.) The transformed parameters kappa and delta have much clearer linear correlation. However, the improvement over the case where gamma alone is transformed is only marginally significant (50% increase in ESS).

This example illustrates that PROC MCMC can fit Bayesian nonlinear models just as easily as Bayesian linear models. More importantly, transformations can sometimes improve the efficiency of the Markov chain, and that is something to always keep in mind. Also see “[Example 55.20: Using a Transformation to Improve Mixing](#)” on page 4654 for another example of how transformations can improve mixing of the Markov chains.

---

## Example 55.7: Logistic Regression Random-Effects Model

This example illustrates how you can use PROC MCMC to fit random-effects models. In the example “[Random-Effects Model](#)” on page 4419 in “[Getting Started: MCMC Procedure](#)” on page 4408, you already saw PROC MCMC fit a linear random-effects model. This example shows how to fit a logistic random-effects model in PROC MCMC. Although you can use PROC MCMC to analyze random-effects models, you might want to first consider some other SAS procedures. For example, you can use PROC MIXED (see Chapter 59, “[The MIXED Procedure](#)”) to analyze linear mixed effects models, PROC NL MIXED (see Chapter 64, “[The NL MIXED Procedure](#)”) for nonlinear mixed effects models, and PROC GLIMMIX (see Chapter 41, “[The GLIMMIX Procedure](#)”) for generalized linear mixed effects models. In addition, a sampling-based Bayesian analysis is available in the MIXED procedure through the **PRIOR** statement (see “[PRIOR Statement](#)” on page 4935).

The data are taken from Crowder (1978). The *Seeds* data set is a  $2 \times 2$  factorial layout, with two types of seeds, *O. aegyptiaca* 75 and *O. aegyptiaca* 73, and two root extracts, *bean* and *cucumber*. You observe *r*, which is the number of germinated seeds, and *n*, which is the total number of seeds. The independent variables are *seed* and *extract*.

The following statements create the data set:

```

title 'Logistic Regression Random-Effects Model';
data seeds;
 input r n seed extract @@;
 ind = _N_;
 datalines;
10 39 0 0 23 62 0 0 23 81 0 0 26 51 0 0
17 39 0 0 5 6 0 1 53 74 0 1 55 72 0 1
32 51 0 1 46 79 0 1 10 13 0 1 8 16 1 0
10 30 1 0 8 28 1 0 23 45 1 0 0 4 1 0
 3 12 1 1 22 41 1 1 15 30 1 1 32 51 1 1
 3 7 1 1
;

```

You can model each observation  $r_i$  as having its own probability of success  $p_i$ , and the likelihood is as follows:

$$r_i \sim \text{binomial}(n_i, p_i)$$

You can use the logit link function to link the covariates of each observation, `seed` and `extract`, to the probability of success,

$$\begin{aligned}\mu_i &= \beta_0 + \beta_1 \cdot \text{seed}_i + \beta_2 \cdot \text{extract}_i + \beta_3 \cdot \text{seed}_i \cdot \text{extract}_i \\ p_i &= \text{logistic}(\mu_i + \delta_i)\end{aligned}$$

where  $\delta_i$  is assumed to be an iid random effect with a normal prior:

$$\delta_i \sim \text{normal}(0, \text{var} = \sigma^2)$$

The four  $\beta$  regression coefficients and the standard deviation  $\sigma^2$  in the random effects are model parameters; they are given noninformative priors as follows:

$$\begin{aligned}\pi(\beta_0, \beta_1, \beta_2, \beta_3) &\propto 1 \\ \sigma^2 &\sim \text{igamma}(\text{shape} = 0.01, \text{scale} = 0.01)\end{aligned}$$

Another way of expressing the same model is as

$$p_i = \text{logistic}(\delta_i)$$

where

$$\delta_i \sim \text{normal}(\beta_0 + \beta_1 \cdot \text{seed}_i + \beta_2 \cdot \text{extract}_i + \beta_3 \cdot \text{seed}_i \cdot \text{extract}_i, \sigma^2)$$

The two models are equivalent. In the first model, the random effects  $\delta_i$  centers at 0 in the normal distribution, and in the second model,  $\delta_i$  centers at the regression mean. This hierarchical centering can sometimes improve mixing.

The following statements fit the second model and generate [Output 55.7.1](#):

```
proc mcmc data=seeds outpost=postout seed=332786 nmc=20000;
 ods select PostSummaries PostIntervals;
 parms beta0 0 beta1 0 beta2 0 beta3 0 s2 1;
 prior s2 ~ igamma(0.01, s=0.01);
 prior beta: ~ general(0);
 w = beta0 + beta1*seed + beta2*extract + beta3*seed*extract;
 random delta ~ normal(w, var=s2) subject=ind;
 pi = logistic(delta);
 model r ~ binomial(n = n, p = pi);
run;
```

The PROC MCMC statement specifies the input and output data sets, sets a seed for the random number generator, and requests a large simulation size. The ODS SELECT statement displays the summary statistics and interval statistics tables. The PARMs statement declares the model parameters, and the PRIOR statements specify the prior distributions for  $\beta$  and  $\sigma^2$ .

The symbol  $w$  calculates the regression mean, and the **RANDOM** statement specifies the random effect, with a normal prior distribution, centered at  $w$  with variance  $\sigma^2$ . Note that the variable  $w$  is a function of the input data set variables. You can use data set variable in constructing the hyperparameters of the random-effects parameters, as long as the hyperparameters remain constant within each subject group. The **SUBJECT=** option indicates the group index for the random-effects parameters.

The symbol  $\pi$  is the logit transformation. The **MODEL** specifies the response variable  $r$  as a binomial distribution with parameters  $n$  and  $\pi$ .

Output 55.7.1 lists the posterior mean and interval estimates of the regression parameters.

**Output 55.7.1** Logistic Regression Random-Effects Model

| Logistic Regression Random-Effects Model |       |         |                       |             |         |         |
|------------------------------------------|-------|---------|-----------------------|-------------|---------|---------|
| The MCMC Procedure                       |       |         |                       |             |         |         |
| Posterior Summaries                      |       |         |                       |             |         |         |
| Parameter                                | N     | Mean    | Standard<br>Deviation | Percentiles |         |         |
|                                          |       |         |                       | 25%         | 50%     | 75%     |
| beta0                                    | 20000 | -0.5570 | 0.1929                | -0.6842     | -0.5535 | -0.4368 |
| beta1                                    | 20000 | 0.0776  | 0.3276                | -0.1185     | 0.0745  | 0.2765  |
| beta2                                    | 20000 | 1.3667  | 0.2923                | 1.1759      | 1.3453  | 1.5577  |
| beta3                                    | 20000 | -0.8469 | 0.4718                | -1.1487     | -0.8280 | -0.5364 |
| s2                                       | 20000 | 0.1171  | 0.0993                | 0.0497      | 0.0921  | 0.1546  |

| Posterior Intervals |       |                     |         |              |         |
|---------------------|-------|---------------------|---------|--------------|---------|
| Parameter           | Alpha | Equal-Tail Interval |         | HPD Interval |         |
| beta0               | 0.050 | -0.9379             | -0.1753 | -0.9422      | -0.1816 |
| beta1               | 0.050 | -0.6183             | 0.7186  | -0.5690      | 0.7499  |
| beta2               | 0.050 | 0.8326              | 1.9642  | 0.8463       | 1.9724  |
| beta3               | 0.050 | -1.8074             | 0.0604  | -1.7741      | 0.0742  |
| s2                  | 0.050 | 0.0103              | 0.3749  | 0.00163      | 0.3045  |

### Example 55.8: Nonlinear Poisson Regression Multilevel Random-Effects Model

This example uses the pump failure data of Gaver and O’Muircheartaigh (1987) to illustrate how to fit a multilevel random-effects model with PROC MCMC. The number of failures and the time of operation are recorded for 10 pumps. Each of the pumps is classified into one of two groups that correspond to either continuous or intermittent operation. The following statements generate the data set:



```

title 'Nonlinear Poisson Regression Random-Effects Model';
data pump;
 input y t group @@;
 pump = _n_;
 logtstd = log(t) - 2.4564900;
 datalines;
5 94.320 1 1 15.720 2 5 62.880 1
14 125.760 1 3 5.240 2 19 31.440 1
 1 1.048 2 1 1.048 2 4 2.096 2
22 10.480 2
;

```

Each row denotes data for a single pump, and the variable `logtstd` contains the centered operation times. Letting  $y_{ij}$  denote the number of failures for the  $j$ th pump in the  $i$ th group, Draper (1996) considers the following hierarchical model for these data, where the data set variable `logtstd` is  $\log t_{ij} - \overline{\log t}$ :

$$\begin{aligned}
 y_{ij} | \lambda_{ij} &\sim \text{Poisson}(\lambda_{ij}) \\
 \log \lambda_{ij} &= \alpha_i + \beta_i (\log t_{ij} - \overline{\log t}) + e_{ij}
 \end{aligned}$$

This model specifies different intercepts and slopes for each group ( $i = 1, 2$ ), and the random effect  $e_{ij}$  is a mechanism for accounting for overdispersion. You can use noninformative priors on the parameters  $\alpha_i$ ,  $\beta_i$ , and  $\sigma^2$ , and a normal prior on  $e_{ij}$ ,

$$\begin{aligned}
 u_i &= \begin{pmatrix} \alpha_i \\ \beta_i \end{pmatrix} \sim \text{mvn} \left( \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1e6 & 0 \\ 0 & 1e6 \end{pmatrix} \right) \text{ for } i = 1, 2 \\
 \sigma^2 &\sim \text{igamma}(\text{shape} = 0.01, \text{scale} = 0.01) \\
 e_{ij} | \sigma^2 &\sim \text{normal}(0, \sigma^2)
 \end{aligned}$$

where  $u_i$  is a multidimensional random effect. The following statements fit such a random-effects model:

```

ods graphics on;
proc mcmc data=pump outpost=postout seed=248601 nmc=10000
 plots=trace stats=none diag=none;
 ods select tracepanel;
 array u[2] alpha beta;
 array mu[2] (0 0);
 parms s2;
 prior s2 ~ igamma(0.01, scale=0.01);
 random u ~ mvn(mu, sd=1e6, rho=0) subject=group monitor=(u);
 random e ~ normal(0, var=s2) subject=pump monitor=(random(1));
 w = alpha + beta * logtstd;
 lambda = exp(w+e);
 model y ~ poisson(lambda);
run;

```

The PROC MCMC statement specifies the input data set (Pump), the output data set (Postout), a seed for the random number generator, and a simulation sample size of 10,000. The program requests that only trace plots be produced, disabling all posterior calculations and convergence diagnostics tests. The ODS SELECT statement displays the trace plots, which are the primary focus.

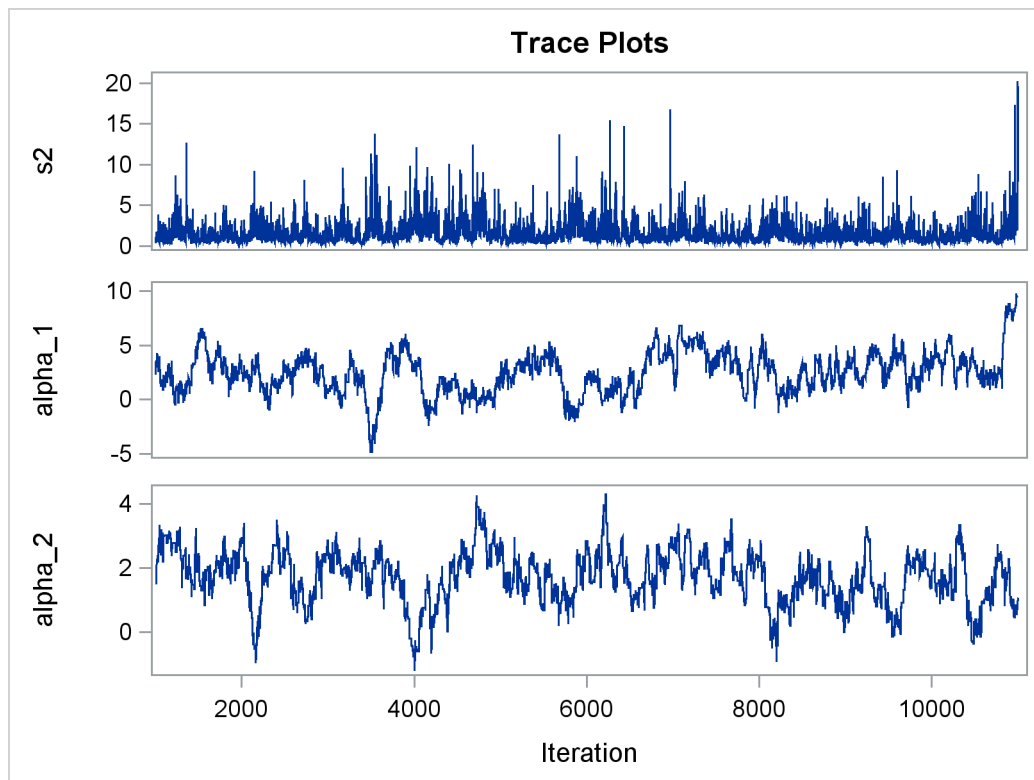
The first **ARRAY** statement declares an array  $u$  of size 2 and names the elements  $\alpha$  and  $\beta$ . The array  $u$  stores the random-effects parameters  $\alpha$  and  $\beta$ . The next **ARRAY** statement defines the mean of the multivariate normal prior on  $u$ .

The **PARMS** statement declares the only model parameter here, the variance  $s^2$  in the prior distribution for the random effect  $e_{ij}$ . The **PRIOR** statement specifies an inverse-gamma prior on the variance. The first **RANDOM** statement specifies a multivariate normal prior on  $u$ . The **mvn** distribution is a multivariate normal distribution with a first-order autoregressive covariance. When the argument  $\rho$  is set to 0, this distribution simplifies to a multivariate normal distribution with a shared variance. The **RANDOM** statement also indicates the group variable as its subject index and monitors all elements  $u$ . The second **RANDOM** statement specifies a normal prior on the effect  $e$ , where the subject index variable is `pump`. The **MONITOR=** option requests that PROC MCMC randomly choose one of the 10  $e$  random-effects parameters to monitor.

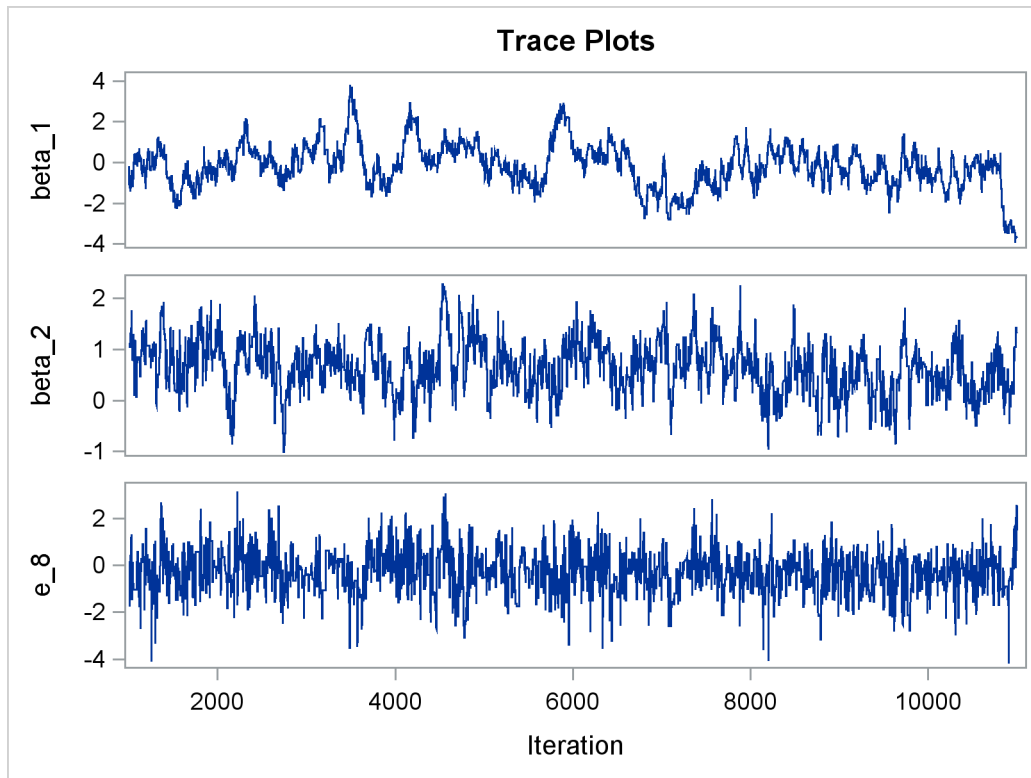
Next, programming statements construct the mean of the Poisson likelihood, and the **MODEL** statement specifies the likelihood function for each observation.

Output 55.8.1 shows trace plots for  $\sigma^2$ ,  $\alpha_1$ ,  $\alpha_2$ ,  $\beta_1$ ,  $\beta_2$ , and  $e_8$ . You can see that the chains are mixing poorly.

**Output 55.8.1** Trace Plots of  $\sigma^2$ ,  $\alpha$ ,  $\beta$ , and  $e_8$  without Hierarchical Centering



Output 55.8.1 continued



To improve mixing, you can repeat the same analysis by using a hierarchical centering technique, where instead of using a normal prior centered at 0 on  $e_{ij}$ , you center the random effects on the group means:

$$y_{ij} | \lambda_{ij} \sim \text{Poisson}(\lambda_{ij})$$

$$\log \lambda_{ij} \sim \text{normal}(\alpha_i + \beta_i (\log t_{ij} - \overline{\log t}), \text{var} = \sigma^2)$$

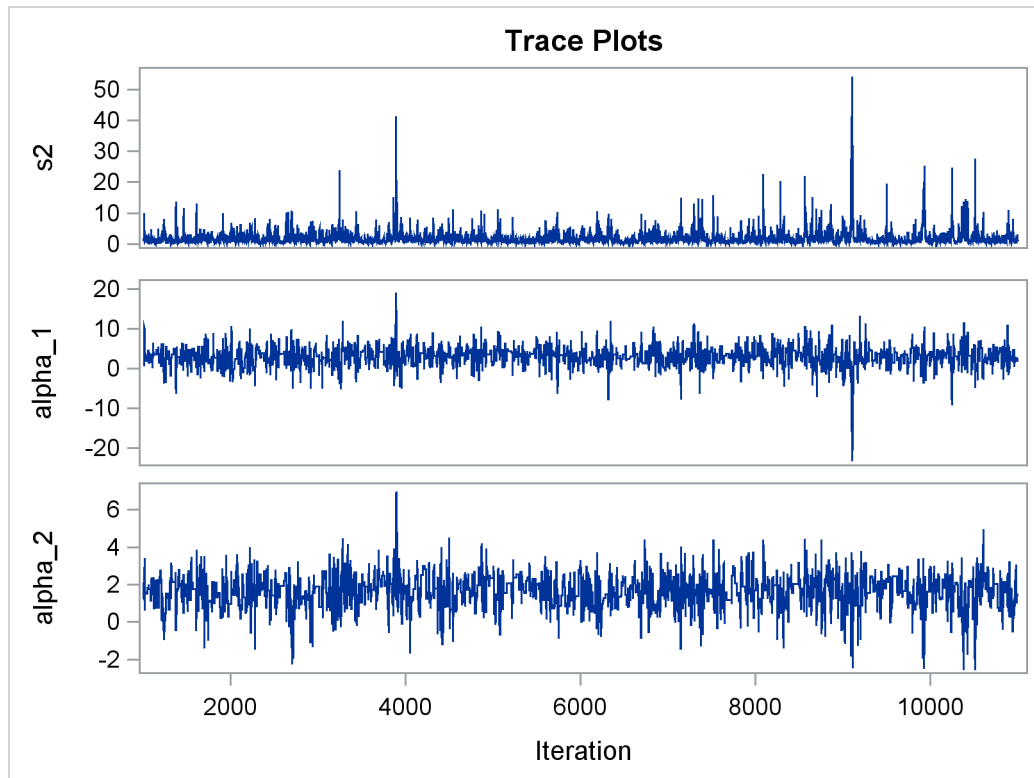
The following statements illustrate how to fit a multilevel hierarchical centering random-effects model:

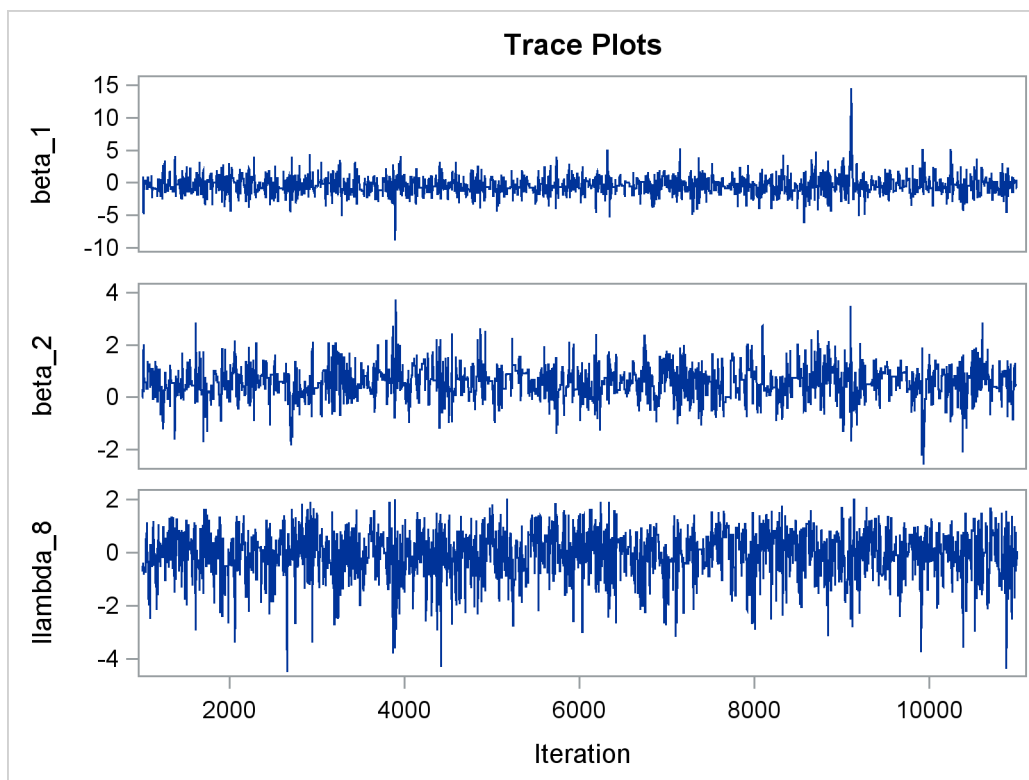
```
proc mcmc data=pump outpost=postout_c seed=248601 nmc=10000
 plots=trace diag=none;
 ods select tracepanel postsummaries postintervals;
 array u[2] alpha beta;
 array mu[2] (0 0);
 parms s2 1;
 prior s2 ~ igamma(0.01, scale=0.01);
 random u ~ mvn(mu, sd=1e6, rho=0) subject=group monitor=(u);
 w = alpha + beta * logtstd;
 random llambda ~ normal(w, var = s2) subject=pump monitor=(random(1));
 lambda = exp(llambda);
 model y ~ poisson(lambda);
run;
```

The difference between these statements and the previous statements on page 4582 is that these statements have the variable  $w$  as the prior mean of the random effect  $\lambda$ . The symbol  $\lambda$  is the exponential of the corresponding  $\log \lambda_{ij}$  ( $\lambda$ ), and the `MODEL` statement assigns the response variable  $y$  a Poisson likelihood with a mean parameter  $\lambda$ , the same way it did in the previous statements.

The trace plots of the monitored parameters are shown in [Output 55.8.2](#). The mixing is significantly improved over the previous model. The posterior summary and interval statistics tables are shown in [Output 55.8.3](#).

**Output 55.8.2** Trace Plots of  $\sigma^2$ ,  $\alpha$ , and  $\beta$  with Hierarchical Centering



Output 55.8.2 *continued*

Output 55.8.3 Posterior Summary Statistics

| Nonlinear Poisson Regression Random-Effects Model |       |         |                       |             |         |        |
|---------------------------------------------------|-------|---------|-----------------------|-------------|---------|--------|
| The MCMC Procedure                                |       |         |                       |             |         |        |
| Posterior Summaries                               |       |         |                       |             |         |        |
| Parameter                                         | N     | Mean    | Standard<br>Deviation | Percentiles |         |        |
|                                                   |       |         |                       | 25%         | 50%     | 75%    |
| s2                                                | 10000 | 1.7606  | 2.2022                | 0.7338      | 1.1862  | 2.0067 |
| alpha_1                                           | 10000 | 2.9286  | 2.4247                | 1.6030      | 3.0767  | 4.2536 |
| alpha_2                                           | 10000 | 1.6105  | 0.8801                | 1.0728      | 1.6514  | 2.1775 |
| beta_1                                            | 10000 | -0.4018 | 1.3110                | -1.1276     | -0.4925 | 0.3198 |
| beta_2                                            | 10000 | 0.5652  | 0.5804                | 0.2198      | 0.5701  | 0.9124 |
| llambda_8                                         | 10000 | -0.0560 | 0.8395                | -0.5437     | 0.0244  | 0.5479 |

**Output 55.8.3** continued

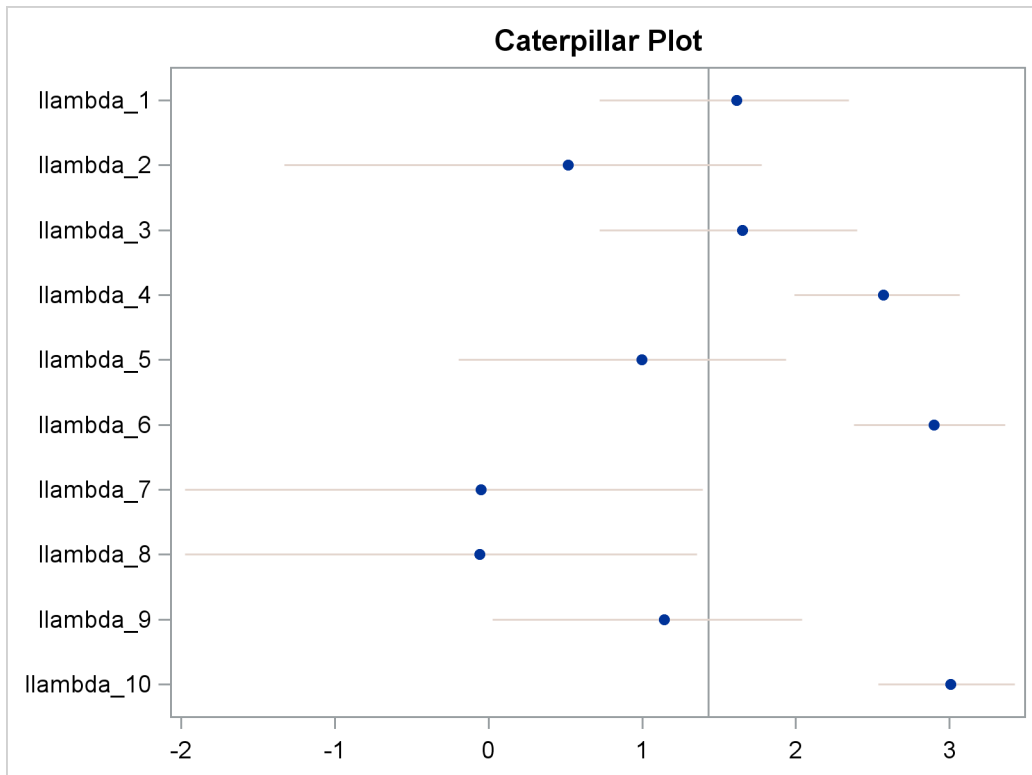
| Parameter | Alpha | Posterior Intervals |        |              |        |
|-----------|-------|---------------------|--------|--------------|--------|
|           |       | Equal-Tail Interval |        | HPD Interval |        |
| s2        | 0.050 | 0.2957              | 6.5641 | 0.1039       | 4.7631 |
| alpha_1   | 0.050 | -1.8812             | 7.5363 | -1.9416      | 7.4115 |
| alpha_2   | 0.050 | -0.2736             | 3.1647 | -0.0436      | 3.2985 |
| beta_1    | 0.050 | -2.8784             | 2.2091 | -2.9323      | 2.0623 |
| beta_2    | 0.050 | -0.5864             | 1.7179 | -0.5469      | 1.7381 |
| llambda_8 | 0.050 | -1.9763             | 1.3552 | -1.6933      | 1.4612 |

You can generate a caterpillar plot (Output 55.8.4) of the random-effects parameters by calling the %CATER macro:

```
%CATER(data=postout_c, var=llambda_);
ods graphics off;
```

Varying llambda indicates nonconstant dispersion in the Poisson model.

**Output 55.8.4** Caterpillar Plots of the Random-Effects Parameters



## Example 55.9: Multivariate Normal Random-Effects Model

Gelfand et al. (1990) use a multivariate normal hierarchical model to estimate growth regression coefficients for the growth of 30 young rats in a control group over a period of 5 weeks. The following statements create a SAS data set with measurements of Weight, Age (in days), and Subject.

```

title 'Multivariate Normal Random-Effects Model';
data rats;
 array days[5] (8 15 22 29 36);
 input weight @@;
 subject = ceil(_n_/5);
 index = mod(_n_-1, 5) + 1;
 age = days[index];
 drop index days;;
 datalines;
151 199 246 283 320 145 199 249 293 354
147 214 263 312 328 155 200 237 272 297
135 188 230 280 323 159 210 252 298 331
141 189 231 275 305 159 201 248 297 338
177 236 285 350 376 134 182 220 260 296
160 208 261 313 352 143 188 220 273 314
154 200 244 289 325 171 221 270 326 358
163 216 242 281 312 160 207 248 288 324
142 187 234 280 316 156 203 243 283 317
157 212 259 307 336 152 203 246 286 321
154 205 253 298 334 139 190 225 267 302
146 191 229 272 302 157 211 250 285 323
132 185 237 286 331 160 207 257 303 345
169 216 261 295 333 157 205 248 289 316
137 180 219 258 291 153 200 244 286 324
;

```

The model assumes normal measurement errors,

$$\text{Weight}_{ij} \sim \text{normal}(\alpha_i + \beta_i \text{Age}_{ij}, \sigma^2), \quad i = 1 \dots 30; j = 1 \dots 5$$

where  $i$  indexes rat (Subject variable),  $j$  indexes the time period,  $\text{Weight}_{ij}$  and  $\text{Age}_{ij}$  denote the weight and age of the  $i$ th rat in week  $j$ , and  $\sigma^2$  is the variance in the normal likelihood. The individual intercept and slope coefficients are modeled as the following:

$$\theta_i = \begin{pmatrix} \alpha_i \\ \beta_i \end{pmatrix} \sim \text{MVN} \left( \theta_c = \begin{pmatrix} \alpha_c \\ \beta_c \end{pmatrix}, \Sigma_c \right), \quad i = 1, \dots, 30$$

You can use the following independent prior distributions on  $\theta_c$ ,  $\Sigma_c$ , and  $\sigma^2$ :

$$\begin{aligned} \theta_c &\sim \text{MVN} \left( \mu_0 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \Sigma_0 = \begin{pmatrix} 1000 & 0 \\ 0 & 1000 \end{pmatrix} \right) \\ \Sigma_c &\sim \text{iwishart} \left( \rho = 2, S = \rho \cdot \begin{pmatrix} 0.01 & 0 \\ 0 & 10 \end{pmatrix} \right) \\ \sigma^2 &\sim \text{igamma}(\text{shape} = 0.01, \text{scale} = 0.01) \end{aligned}$$

The following statements fit this multivariate normal random-effects model:

```
proc mcmc data=rats nmc=10000 outpost=postout
 seed=17 init=random;
 ods select Parameters REParameters PostSummaries;
 array theta[2] alpha beta;
 array theta_c[2];
 array Sig_c[2,2];
 array mu0[2] (0 0);
 array Sig0[2,2] (1000 0 0 1000);
 array S[2,2] (0.02 0 0 20);

 parms theta_c Sig_c {121 0 0 0.26} var_y;
 prior theta_c ~ mvn(mu0, Sig0);
 prior Sig_c ~ iwish(2, S);
 prior var_y ~ igamma(0.01, scale=0.01);

 random theta ~ mvn(theta_c, Sig_c) subject=subject
 monitor=(alpha_9 beta_9 alpha_25 beta_25);
 mu = alpha + beta * age;
 model weight ~ normal(mu, var=var_y);
run;
```

The ODS SELECT statement displays information about model parameters, random-effects parameters, and the posterior summary statistics. The ARRAY statements allocate memory space for the multivariate parameters and hyperparameters in the model. The parameters are  $\theta$  (theta where the variable name of each element is alpha or beta),  $\theta_c$  (theta\_c), and  $\Sigma_c$  (Sig\_c). The hyperparameters are  $\mu_0$  (mu0),  $\Sigma_0$  (Sig0), and S (S). The multivariate hyperparameters are assigned with constant values using parentheses ( ).

The PARMs statement declares model parameters and assigns initial values to Sig\_c using braces { }. The PRIOR statements specify the prior distributions. The RANDOM statement defines an array random effect theta and specifies a multivariate normal prior distribution. The SUBJECT= option indicates cluster membership for each of the random-effects parameter. The MONITOR= option monitors the individual intercept and slope coefficients of subjects 9 and 25.

You can use the following syntax in the RANDOM statement to monitor all parameters in an array random effect:

```
monitor=(theta)
```

This would produce posterior summary statistics on  $\alpha_1 \cdots \alpha_{30}$  and  $\beta_1 \cdots \beta_{30}$ .



The following syntax monitors all  $\alpha_i$  parameters:

```
monitor=(alpha)
```

If you did not name elements of theta to be alpha and beta, the SAS System creates variable names automatically in a consecutive fashion, as in theta1 and theta2.

**Output 55.9.1** Parameter and Random-Effects Parameter Information Table

| Multivariate Normal Random-Effects Model |           |             |                 |               |                          |
|------------------------------------------|-----------|-------------|-----------------|---------------|--------------------------|
| The MCMC Procedure                       |           |             |                 |               |                          |
| Parameters                               |           |             |                 |               |                          |
| Block                                    | Parameter | Array Index | Sampling Method | Initial Value | Prior Distribution       |
| 1                                        | theta_c1  |             | Conjugate       | -4.5834       | MVNormal(mu0, Sig0)      |
|                                          | theta_c2  |             |                 | 5.7930        |                          |
| 2                                        | Sig_c1    | [1,1]       | Conjugate       | 121.0         | iWishart(2, S)           |
|                                          | Sig_c2    | [1,2]       |                 | 0             |                          |
|                                          | Sig_c3    | [2,1]       |                 | 0             |                          |
|                                          | Sig_c4    | [2,2]       |                 | 0.2600        |                          |
| 3                                        | var_y     |             | Conjugate       | 2806714       | igamma(0.01, scale=0.01) |

| Random Effect Parameters |                 |         |                    |                                                                 |                             |
|--------------------------|-----------------|---------|--------------------|-----------------------------------------------------------------|-----------------------------|
| Parameter                | Sampling Method | Subject | Number of Subjects | Subject Values                                                  | Prior Distribution          |
| theta                    | N-Metropolis    | subject | 30                 | 1 2 3 4 5 6 7 8<br>9 10 11 12 13 14<br>15 16 17 18 19<br>20 ... | MVNormal(theta_c,<br>Sig_c) |

Output 55.9.1 displays the parameter and random-effects parameter information tables. The Array Index column in “Parameters” table shows the index reference of the elements in the array parameter Sig\_c. The total number of subjects in the study is 30.

**Output 55.9.2** Multivariate Normal Random-Effects Model

| Multivariate Normal Random-Effects Model |       |         |                       |             |         |         |
|------------------------------------------|-------|---------|-----------------------|-------------|---------|---------|
| The MCMC Procedure                       |       |         |                       |             |         |         |
| Posterior Summaries                      |       |         |                       |             |         |         |
| Parameter                                | N     | Mean    | Standard<br>Deviation | Percentiles |         |         |
|                                          |       |         |                       | 25%         | 50%     | 75%     |
| theta_c1                                 | 10000 | 106.1   | 2.2486                | 104.6       | 106.1   | 107.5   |
| theta_c2                                 | 10000 | 6.1975  | 0.1988                | 6.0639      | 6.1966  | 6.3286  |
| Sig_c1                                   | 10000 | 110.8   | 45.9169               | 78.2354     | 103.6   | 135.9   |
| Sig_c2                                   | 10000 | -1.4267 | 2.3320                | -2.7324     | -1.2288 | 0.0789  |
| Sig_c3                                   | 10000 | -1.4267 | 2.3320                | -2.7324     | -1.2288 | 0.0789  |
| Sig_c4                                   | 10000 | 1.0591  | 0.2979                | 0.8472      | 1.0104  | 1.2145  |
| var_y                                    | 10000 | 37.6855 | 5.9591                | 33.4151     | 36.9994 | 41.2448 |
| alpha_9                                  | 10000 | 119.4   | 5.6756                | 115.6       | 119.2   | 123.2   |
| alpha_25                                 | 10000 | 86.5673 | 6.3694                | 82.4621     | 86.7183 | 90.7307 |
| beta_9                                   | 10000 | 7.4670  | 0.2382                | 7.3109      | 7.4730  | 7.6260  |
| beta_25                                  | 10000 | 6.7804  | 0.2612                | 6.6144      | 6.7756  | 6.9526  |

Output 55.9.2 displays posterior summary statistics for model parameters and the random-effects parameters for subjects 9 and 25. You can see that there is a substantial difference in the intercepts and growth rates between the two rats.

A seemingly confusing message might occur if a symbol name matches an internally generated variable name for elements of an array. For example, if, instead of using the symbol `var_y` in the SAS program for the model variance  $\sigma^2$ , you used `s2`, the SAS System produces the following error message:

```
ERROR: The initial value 0 for the parameter S2 is outside of the prior
distribution support set.
```

This is confusing because the program does not assign an initial value for the parameter `s2` in the `PARMS` statement, and you might expect that PROC MCMC would not generate an invalid initial value. The confusion is caused by the `ARRAY` statement that defines the array variable `S`:

```
array S[2,2] (0.02 0 0 20);
```

Elements of `S` are automatically given names `s1`–`s4`. PROC MCMC interprets `s2` as an element in `S` that was given a value of 0, hence producing this error message.

---

## Example 55.10: Missing at Random Analysis

This example illustrates how PROC MCMC treats missing at random (MAR) data. For a short overview of missing data problems, see the section “Handling of Missing Data” on page 4518.

Researchers studied the effects of air pollution on respiratory disease in children. The response variable ( $y$ ) represented whether a child exhibited wheezing symptoms; it was recorded as 1 for symptoms exhibited and

0 for no symptoms exhibited. City of residency ( $x_1$ ) and maternal smoking status ( $x_2$ ) were the explanatory variables. The variable  $x_1$  was coded as 1 if the child lived in the more polluted city, Steel City, and 0 if the child lived in Green Hills. The variable  $x_2$  was the number of cigarettes the mother reported that she smoked per day. Both the covariates contain missing values: 17 for  $x_1$  and 30 for  $x_2$ , respectively. The total number of observations in the data set is 390. The following statements generate the data set `air`:

```

title 'Missing at Random Analysis';
data air;
 input y x1 x2 @@;
 datalines;
0 0 0 0 0 0 0 1 0 0 0 0 0 0 11 0 1 7
0 0 8 0 1 10 0 1 9 0 0 0 1 1 6 0 1 10
0 1 12 0 0 . 0 0 0 0 1 0 0 1 7 1 1 15
0 0 8 0 0 0 1 1 0 1 0 6 0 0 0 1 1 11
0 0 0 1 0 0 1 0 5 0 0 8 0 0 0 0 1 9

... more lines ...

0 0 11 0 0 0 0 0 6 0 0 12 0 0 10 0 1 10
0 1 11 0 0 9 1 0 11 0 1 7 0 0 7 0 0 0
0 . 11 1 1 6 0 0 8 0 0 0 0 1 12 0 0 0
0 1 0 1 1 8 0 0 0 0 1 11 0 1 0 0 1 8
0 . 0 1 0 0 1 1 10 0 . 4 1 1 16 0 . 13
;

```

Suppose you want to fit a logistic regression model for whether the subject develops wheezing symptoms with density for the  $i = 1, \dots, 390$  subjects as follows:

$$\begin{aligned}
 y_i &\sim \text{binary}(p_i) \\
 \text{logit}(p_i) &= \beta_0 + \beta_1 \cdot x_{1i} + \beta_2 \cdot x_{2i} \\
 \pi(\beta_0), \pi(\beta_1), \pi(\beta_2) &= \text{normal}(0, \sigma^2 = 10)
 \end{aligned}$$

Suppose you specify a joint distribution of  $x_1$  and  $x_2$  in terms of the product of a conditional and marginal distribution; that is,

$$p(x_1, x_2 | \alpha) = p(x_1 | x_2, \alpha_{10}, \alpha_{11}) p(x_2 | \alpha_{20})$$

where  $p(x_1 | x_2, \alpha_{10}, \alpha_{11})$  could be a logistic model and  $p(x_2 | \alpha_{20})$  could be a Poisson distribution that models the following counts:

$$\begin{aligned}
 p(x_1 | x_2, \alpha_{10}, \alpha_{11}) &= \text{binary}(p_{c,i}) \\
 \text{logit}(p_{c,i}) &= \alpha_{10} + \alpha_{11} \cdot x_{2i} \\
 \pi(\alpha_{10}), \pi(\alpha_{11}) &= \text{normal}(0, \sigma^2 = 10) \\
 p(x_2 | \alpha_{20}) &= \text{Poisson}(e^{\alpha_{20}}) \\
 \pi(\alpha_{20}) &= \text{normal}(0, \sigma^2 = 2)
 \end{aligned}$$

The researchers are interested in interpreting how the odds of developing a wheeze changes for a child living in the more polluted city. The odds ratio can be written as the follows:

$$OR_{x1} = \exp(\beta_1)$$

Similarly, the odds ratio for the maternal smoking effect can be written as follows:

$$OR_{x2} = \exp(\beta_2)$$

The following statements fit a Bayesian logistic regression with missing covariates:

```
proc mcmc data=air seed=1181 nmc=10000 monitor=(_parms_ orx1 orx2)
 stats=(summary interval) diag=none plots=none;
 parms beta0 -1 beta1 0.1 beta2 .01;
 parms alpha10 0 alpha11 0 alpha20 0;

 prior beta: alpha1: ~ normal(0,var=10);
 prior alpha20 ~ normal(0,var=2);

 beginnodata;
 pm = exp(alpha20);
 orx1 = exp(beta1);
 orx2 = exp(beta2);
 endnodata;
 model x2 ~ poisson(pm) monitor=(1 3 10);
 p1 = logistic(alpha10 + alpha11 * x2);
 model x1 ~ binary(p1) monitor=(random(3));
 p = logistic(beta0 + beta1*x1 + beta2*x2);
 model y ~ binary(p);
run;
```

The **PARMS** statements specify the parameters in the model and assign initial values to each of them. The **PRIOR** statements specify priors for all the model parameters. The notations **beta:** and **alpha:** in the **PRIOR** statements are shorthand for all variables that start with “beta,” and “alpha,” respectively. The shorthand notation is not necessary, but it keeps your code succinct.

The **BEGINNODATA** and **ENDNODATA** statements enclose three programming statements that calculate the Poisson mean (**pm**) and the two odds ratios (**ORX1** and **ORX2**). These enclosed statements are independent of any data set variables, and they are run only once per iteration to reduce unnecessary observation-level computations.

The first **MODEL** statement assigns a Poisson likelihood with mean **pm** to **x2**. The statement models missing values in **x2** automatically, creating one variable for each of the missing values, and augments them accordingly. By default, PROC MCMC does not output analyses of the posterior samples of the missing values. You can use the **MONITOR=** option to choose the missing values that you want to monitor. In the example, the first, third, and tenth missing values are monitored.

The P1 assignment statement calculates  $p_{c.i}$ . The second **MODEL** statement assigns a binary likelihood with probability p1 and requests a random choice of three missing data variables of x1 to monitor.

The P assignment statement calculates  $p_i$  in the logistic model. The third **MODEL** statement specifies the complete data likelihood function for Y.

**Output 55.10.1** displays the number of observations read from the DATA= data set, the number of observations used in the analysis, and the “Missing Data Information” table. No observations were omitted from the data set in the analysis.

The “Missing Data Information” table lists the variables that contain missing values, which are x1 and x2, the number of missing observations in each variable, the observation indices of these missing values, and the sampling algorithms used. By default, the first 20 observation indices of each variable are printed in the table.

**Output 55.10.1** Observation Information and Missing Data Information

| Missing at Random Analysis     |                       |                          |                 |
|--------------------------------|-----------------------|--------------------------|-----------------|
| The MCMC Procedure             |                       |                          |                 |
| Number of Observations Read    |                       |                          | 390             |
| Number of Observations Used    |                       |                          | 390             |
| Missing Data Information Table |                       |                          |                 |
| Variable                       | Number of Missing Obs | Observation Indices      | Sampling Method |
| x2                             | 30                    | 14 41 50 55 59 66 71 83  | N-Metropolis    |
|                                |                       | 88 90 118 158 174 175    |                 |
|                                |                       | 178 183 196 203 210 212  |                 |
|                                |                       | ...                      |                 |
| x1                             | 17                    | 50 92 93 167 194 231 273 | Inverse CDF     |
|                                |                       | 296 303 304 308 330 349  |                 |
|                                |                       | 373 385 388 390          |                 |
|                                |                       |                          |                 |

There are 30 missing values in the variable x2, and 17 in x1. Internally, PROC MCMC creates 30 and 17 variables for the missing values in x2 and x1, respectively. The default naming convention for these missing values is to concatenate the response variable and the observation number. For example, the first missing value in x2 is the fourteenth observation, and the corresponding variable is x2\_14.

**Output 55.10.2** displays the summary and interval statistics for each parameter, the odds ratios, and the monitored missing values.

## Output 55.10.2 Posterior Summary and Interval Statistics

| Missing at Random Analysis |       |         |                       |             |         |         |
|----------------------------|-------|---------|-----------------------|-------------|---------|---------|
| The MCMC Procedure         |       |         |                       |             |         |         |
| Posterior Summaries        |       |         |                       |             |         |         |
| Parameter                  | N     | Mean    | Standard<br>Deviation | Percentiles |         |         |
|                            |       |         |                       | 25%         | 50%     | 75%     |
| beta0                      | 10000 | -1.3585 | 0.1986                | -1.4891     | -1.3515 | -1.2192 |
| beta1                      | 10000 | 0.4763  | 0.2355                | 0.3195      | 0.4675  | 0.6334  |
| beta2                      | 10000 | 0.0146  | 0.0227                | 0.000049    | 0.0124  | 0.0299  |
| alpha10                    | 10000 | -0.2244 | 0.1446                | -0.3190     | -0.2187 | -0.1273 |
| alpha11                    | 10000 | 0.0140  | 0.0214                | -0.00113    | 0.0136  | 0.0289  |
| alpha20                    | 10000 | 1.5635  | 0.0247                | 1.5466      | 1.5644  | 1.5803  |
| orx1                       | 10000 | 1.6557  | 0.4002                | 1.3765      | 1.5960  | 1.8841  |
| orx2                       | 10000 | 1.0149  | 0.0231                | 1.0000      | 1.0125  | 1.0303  |
| x2_14                      | 10000 | 4.9229  | 2.1745                | 3.0000      | 5.0000  | 6.0000  |
| x2_50                      | 10000 | 4.9569  | 2.1758                | 3.0000      | 5.0000  | 6.0000  |
| x2_90                      | 10000 | 4.9214  | 2.2152                | 3.0000      | 5.0000  | 6.0000  |
| x1_296                     | 10000 | 0.4183  | 0.4933                | 0           | 0       | 1.0000  |
| x1_304                     | 10000 | 0.4569  | 0.4982                | 0           | 0       | 1.0000  |
| x1_373                     | 10000 | 0.4461  | 0.4971                | 0           | 0       | 1.0000  |

| Posterior Intervals |       |                     |         |              |         |
|---------------------|-------|---------------------|---------|--------------|---------|
| Parameter           | Alpha | Equal-Tail Interval |         | HPD Interval |         |
| beta0               | 0.050 | -1.7749             | -0.9914 | -1.7669      | -0.9899 |
| beta1               | 0.050 | 0.0125              | 0.9526  | 0.0481       | 0.9806  |
| beta2               | 0.050 | -0.0295             | 0.0599  | -0.0305      | 0.0580  |
| alpha10             | 0.050 | -0.5175             | 0.0506  | -0.5142      | 0.0508  |
| alpha11             | 0.050 | -0.0271             | 0.0547  | -0.0267      | 0.0549  |
| alpha20             | 0.050 | 1.5137              | 1.6095  | 1.5127       | 1.6078  |
| orx1                | 0.050 | 1.0126              | 2.5924  | 0.9007       | 2.4030  |
| orx2                | 0.050 | 0.9709              | 1.0617  | 0.9699       | 1.0597  |
| x2_14               | 0.050 | 1.0000              | 10.0000 | 1.0000       | 9.0000  |
| x2_50               | 0.050 | 1.0000              | 10.0000 | 1.0000       | 9.0000  |
| x2_90               | 0.050 | 1.0000              | 10.0000 | 1.0000       | 9.0000  |
| x1_296              | 0.050 | 0                   | 1.0000  | 0            | 1.0000  |
| x1_304              | 0.050 | 0                   | 1.0000  | 0            | 1.0000  |
| x1_373              | 0.050 | 0                   | 1.0000  | 0            | 1.0000  |

The odds ratio for x1 is the multiplicative change in the odds of a child wheezing in Steel City compared to the odds of the child wheezing in Green Hills. The estimated odds ratio (ORX1) value is 1.6736 with a corresponding 95% equal-tail credible interval of (1.0248, 2.5939). City of residency is a significant factor in a child's wheezing status. The estimated odds ratio for x2 is the multiplicative change in the odds of developing a wheeze for each additional reported cigarette smoked per day. The odds ratio of ORX2 indicates that the odds of a child developing a wheeze is 1.0150 times higher for each reported cigarette a mother smokes. The corresponding 95% equal-tail credible interval is (0.9695, 1.0619). Since this interval contains the value 1, maternal smoking is not considered to be an influential effect.

## Example 55.11: Nonignorably Missing Data (MNAR) Analysis

This example illustrates how to fit a nonignorably missing data model (MNAR) with PROC MCMC. For a short overview of missing data problems, see the section “Handling of Missing Data” on page 4518.

This data set comes from an environmental study that involve workers in a cotton factory. A similar data set was analyzed from Ibrahim, Chen, and Lipsitz (2001). There are 912 workers in the data set, and the response variable of interest is whether they develop dyspnea (difficult or labored respiration). The data are collected over three time points, and there are six covariates. The following statements create the data set:

```

title 'Nonignorably Missing Data Analysis';
data dyspnea;
 input smoke1 smoke2 smoke3 y1 y2 y3 yrswrk1 yrswrk2 yrswrk3
 age expd sex hgt;
 datalines;
0 0 0 0 0 0 28.1 33.1 39.1 48 1 1 165.0
0 0 0 0 . 0 5.1 10.1 16.1 45 1 0 147.0
0 0 0 0 . 0 26.0 31.0 37.0 46 1 0 156.0

... more lines ...

1 1 1 0 . . 6.0 11.0 17.0 25 0 1 180.0
0 0 0 0 . . 20.0 25.0 31.0 42 0 0 159.0
;

```

The following variables are included in the data set:

- y1, y2, and y3: dichotomous outcome at the three time periods, which takes the value 1 if the worker has dyspnea, 0 if not (there are missing values in y2 and y3)
- smoke1, smoke2, smoke3: smoking status (0=no, and 1=yes)
- yrswrk1, yrswrk2, yrswrk3: years worked at the cotton factory
- age: age of the worker
- expd: cotton dust exposure (0=no, 1=yes)
- sex: gender (0=female, 1=male)
- hgt: height of the worker

Prior to the analysis, three missing data indicator variables (r1, r2, and r3, one for each of the response variables) are created, and they are set to 1 if the response variable is missing, and 0 otherwise. The covariates age, hgt, yrswrk1, yrswrk2, and yrswrk3 are standardized:

```

data dyspnea;
 array y[3] y1-y3;
 array r[3];
 set dyspnea;
 do i = 1 to 3;
 if y[i] = . then r[i] = 1;
 else r[i] = 0;
 end;
 output;
run;

proc standard data=dyspnea out=dyspnea mean=0 std=1;
 var age hgt yrswrk;
run;

```

There are no missing values in response variable  $y_1$ , 128 missing values in  $y_2$ , and 131 in  $y_3$ . Ibrahim, Chen, and Lipsitz (2001) used a logistic regression for each of the response variables, where  $\delta_i$  is a scalar random effect on the observational level:

$$\begin{aligned}
 y_{ki} &\sim \text{binary}(p_{ki}) \quad k = 1, 2, 3; \quad i = 1, \dots, 912 \\
 p_{ki} &= \text{logistic}(\mu_{ki} + \delta_i) \\
 \mu_{ki} &= \beta_1 + \beta_2 \cdot \text{expd}_i + \beta_3 \cdot \text{sex}_i + \beta_4 \cdot \text{hgt}_i + \beta_5 \cdot \text{age}_i + \beta_6 \cdot \text{yrswrk}_{ki} + \beta_7 \cdot \text{smoke}_{ki} \\
 \delta_i &\sim n(0, \sigma^2)
 \end{aligned}$$

Ibrahim, Chen, and Lipsitz (2001) noted that taking  $\delta_i$  to be higher dimensional (3) would make the model either not identifiable or nearly not identifiable because of the multiple missing values for some subjects.

The first response variable  $y_1$  does not contain any missing values, making it meaningless to model the corresponding  $r_1$  because every value is 1. Hence, only  $r_2$  and  $r_3$  are considered in the missing mechanism part of the model. Ibrahim, Chen, and Lipsitz (2001) suggest the following logistic regression for  $r_2$  and  $r_3$ , where the regression mean for each  $r$  depends not only on the current response variable  $y$  but also the response from previous time period:

$$\begin{aligned}
 r_{ki} &\sim \text{binary}(q_{ki}) \quad k = 2, 3; \quad i = 1, \dots, 912 \\
 q_{ki} &= \text{logistic}(v_{ki}) \\
 \mu_c &= \phi_1 + \phi_2 \cdot \text{expd}_i + \phi_3 \cdot \text{sex}_i + \phi_4 \cdot \text{hgt}_i + \phi_5 \cdot \text{age}_i + \phi_6 \cdot \text{yrswrk}_{ki} + \phi_7 \cdot \text{smoke}_{ki} \\
 v_{2i} &= \mu_c + \phi_8 \cdot y_{1i} + \phi_9 \cdot y_{2i} \\
 v_{3i} &= \mu_c + \phi_9 \cdot y_{2i} + \phi_{10} \cdot y_{3i}
 \end{aligned}$$

The missing mechanism model introduces an additional 10 parameters to the model. Normal priors with large standard deviations are used here.

The following statements fit a nonignorably missing model to the dyspnea data set:



```

ods select MissDataInfo REParameters PostSummaries PostIntervals;
proc mcmc data=dyspnea seed=17 outpost=dysp2 nmc=20000
 propcov=simplex diag=none monitor=(beta1-beta7);
 array p[3];
 array yrswrk[3];
 array smoke[3];

 parms beta1-beta7 s2;
 parms phi1-phi10;
 prior beta: phi: ~ n(0, var=1e6);
 prior s2 ~ igamma(2, scale=2);
 random d ~ n(0, var=s2) subject=_obs_;
 mu = beta1 + beta2*expd + beta3*sex + beta4*hgt + beta5*age + d;
 do i = 1 to 3;
 p[i] = logistic(mu + beta6*yrswrk[i] + beta7*smoke[i]);
 end;
 model y1 ~ binary(p1);
 model y2 ~ binary(p2);
 model y3 ~ binary(p3);

 nu = phi1 + phi2*expd + phi3*sex + phi4*hgt + phi5*age;
 q2 = logistic(nu + phi6*yrswrk[2] + phi7*smoke[2] +
 phi8*y1 + phi9*y2);
 model r2 ~ binary(q2);
 q3 = logistic(nu + phi6*yrswrk[3] + phi7*smoke[3] +
 phi9*y2 + phi10*y3);
 model r3 ~ binary(q3);
run;

```

The first **ARRAY** statement declares an array `p` of size 3. This array stores three binary probabilities of the response variables. The next two **ARRAY** statements create storage arrays for some of `yrswrk` and `smoke` variables for later programming convenience. The first **PARMS** statement declares eight parameters,  $\beta_1 - \beta_7$  and  $\sigma^2$ . The second **PARMS** statement declares the 10  $\phi$  parameters for the missing mechanism model. The **PRIOR** statements assign prior distributions to these parameters.

The **RANDOM** statement defines an observational-level random effect `d` that has a normal prior with variance `s2`. The **SUBJECT=\_OBS\_** option enables the specification of individual random effects without an explicit input data set variable.

The **MU** assignment statement and the following **DO** loop statements calculate the binary probabilities for the three response variables. Note that different `yrswrk` and `smoke` variables are used in the **DO** loop for different years. The three **MODEL** statements assign three binary distributions to the response variables.

The **NU** assignment statement starts the calculation for the regression mean in the logistic model for `r2` and `r3`. The variables `q2` and `q3` are the binary probabilities for the missing mechanisms. Note that their calculations are conditional on the response variables `y` (pattern mixture model). The last two **MODEL** statements for `r2` and `r3` complete the specification of the models.

Missing data information and random-effects parameters information are displayed in [Output 55.11.1](#). You can read the total number of missing observations from each variable and its indices from the table. The missing values are sampled using the inverse CDF method. There are 912 random-effects parameters in the model.

**Output 55.11.1** Missing Data and Random-Effects Information

| Nonignorably Missing Data Analysis |                       |                                                                             |                    |                                                                 |                    |  |
|------------------------------------|-----------------------|-----------------------------------------------------------------------------|--------------------|-----------------------------------------------------------------|--------------------|--|
| The MCMC Procedure                 |                       |                                                                             |                    |                                                                 |                    |  |
| Missing Data Information Table     |                       |                                                                             |                    |                                                                 |                    |  |
| Variable                           | Number of Missing Obs | Observation Indices                                                         | Sampling Method    |                                                                 |                    |  |
| y2                                 | 128                   | 2 3 9 11 13 19 20 21 30<br>31 32 35 39 40 43 56 58<br>71 75 95 ...          | Inverse CDF        |                                                                 |                    |  |
| y3                                 | 131                   | 9 14 16 20 21 29 31 32<br>43 45 56 72 86 115 117<br>121 124 142 149 160 ... | Inverse CDF        |                                                                 |                    |  |
| Random Effect Parameters           |                       |                                                                             |                    |                                                                 |                    |  |
| Parameter                          | Sampling Method       | Subject                                                                     | Number of Subjects | Subject Values                                                  | Prior Distribution |  |
| d                                  | N-Metropolis          | _OBS_                                                                       | 912                | 1 2 3 4 5 6 7 8<br>9 10 11 12 13 14<br>15 16 17 18 19<br>20 ... | normal(0, var=s2)  |  |

The posterior summary and interval statistics of all the  $\beta$  parameters are shown in [Output 55.11.2](#). There are a number of significant regression coefficients in modeling the probability of a worker developing dyspnea, including those for  $\text{expd}$  ( $\beta_2$ ),  $\text{sex}$  ( $\beta_3$ ),  $\text{age}$  ( $\beta_5$ ), and  $\text{smoke}$  ( $\beta_7$ ).

**Output 55.11.2** Posterior Summary Statistics for  $\beta$

| Nonignorably Missing Data Analysis |       |         |                    |         |         |         |
|------------------------------------|-------|---------|--------------------|---------|---------|---------|
| The MCMC Procedure                 |       |         |                    |         |         |         |
| Posterior Summaries                |       |         |                    |         |         |         |
| Parameter                          | N     | Mean    | Standard Deviation | 25%     | 50%     | 75%     |
| beta1                              | 20000 | -2.3256 | 0.1771             | -2.4443 | -2.3266 | -2.2069 |
| beta2                              | 20000 | 0.5327  | 0.1530             | 0.4270  | 0.5316  | 0.6352  |
| beta3                              | 20000 | -0.5966 | 0.2593             | -0.7709 | -0.5990 | -0.4244 |
| beta4                              | 20000 | -0.0682 | 0.1061             | -0.1389 | -0.0679 | 0.00196 |
| beta5                              | 20000 | 0.6252  | 0.1640             | 0.5133  | 0.6245  | 0.7324  |
| beta6                              | 20000 | -0.1776 | 0.1574             | -0.2784 | -0.1742 | -0.0693 |
| beta7                              | 20000 | 0.5862  | 0.2214             | 0.4357  | 0.5854  | 0.7285  |

Output 55.11.2 *continued*

| Parameter | Alpha | Posterior Intervals |         |              |         |
|-----------|-------|---------------------|---------|--------------|---------|
|           |       | Equal-Tail Interval |         | HPD Interval |         |
| beta1     | 0.050 | -2.6692             | -1.9826 | -2.6670      | -1.9826 |
| beta2     | 0.050 | 0.2383              | 0.8308  | 0.2306       | 0.8193  |
| beta3     | 0.050 | -1.1085             | -0.0785 | -1.0906      | -0.0691 |
| beta4     | 0.050 | -0.2815             | 0.1400  | -0.2734      | 0.1462  |
| beta5     | 0.050 | 0.3074              | 0.9613  | 0.2992       | 0.9490  |
| beta6     | 0.050 | -0.5047             | 0.1191  | -0.4971      | 0.1218  |
| beta7     | 0.050 | 0.1599              | 1.0301  | 0.1433       | 1.0051  |

**Example 55.12: Change Point Models**

Consider the data set from Bacon and Watts (1971), where  $y_i$  is the logarithm of the height of the stagnant surface layer and the covariate  $x_i$  is the logarithm of the flow rate of water. The following statements create the data set:

```

title 'Change Point Model';
data stagnant;
 input y x @@;
 ind = _n_;
 datalines;
1.12 -1.39 1.12 -1.39 0.99 -1.08 1.03 -1.08
0.92 -0.94 0.90 -0.80 0.81 -0.63 0.83 -0.63
0.65 -0.25 0.67 -0.25 0.60 -0.12 0.59 -0.12
0.51 0.01 0.44 0.11 0.43 0.11 0.43 0.11
0.33 0.25 0.30 0.25 0.25 0.34 0.24 0.34
0.13 0.44 -0.01 0.59 -0.13 0.70 -0.14 0.70
-0.30 0.85 -0.33 0.85 -0.46 0.99 -0.43 0.99
-0.65 1.19
;

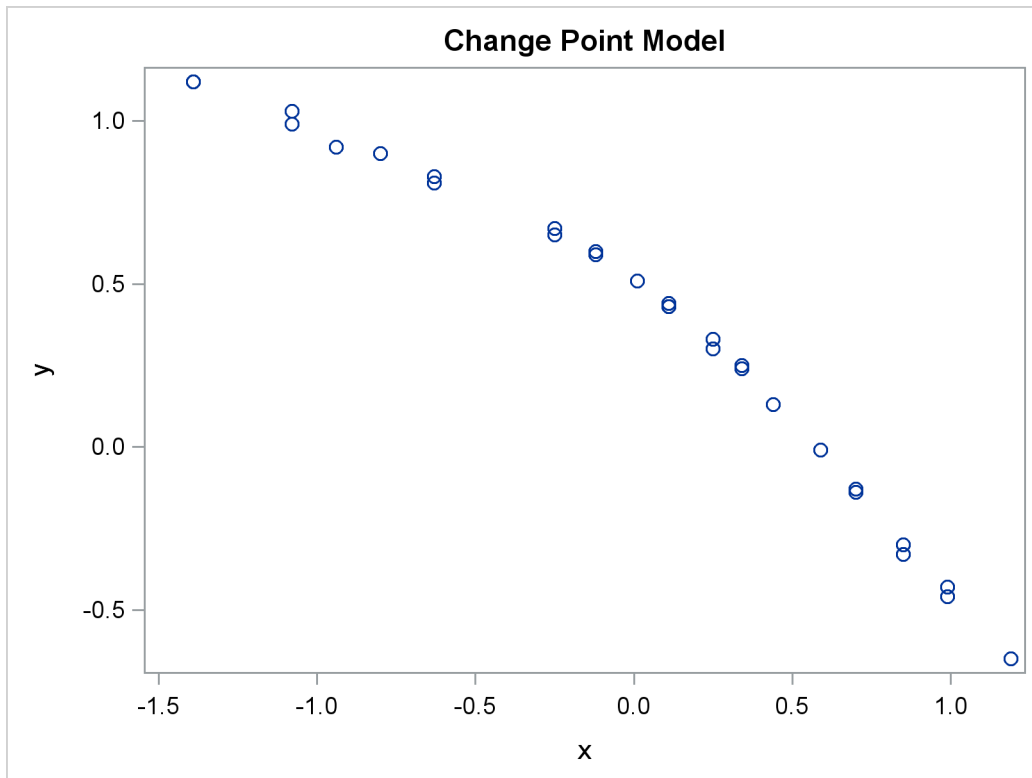
```

A scatter plot (Output 55.12.1) shows the presence of a nonconstant slope in the data. This suggests a change point regression model (Carlin, Gelfand, and Smith 1992). The following statements generate the scatter plot in Output 55.12.1:

```

ods graphics on;
proc sgplot data=stagnant;
 scatter x=x y=y;
run;

```

**Output 55.12.1** Scatter Plot of the Stagnant Data Set

Let the change point be  $cp$ . Following formulation by Spiegelhalter et al. (1996b), the regression model is as follows:

$$y_i \sim \begin{cases} \text{normal}(\alpha + \beta_1(x_i - cp), \sigma^2) & \text{if } x_i < cp \\ \text{normal}(\alpha + \beta_2(x_i - cp), \sigma^2) & \text{if } x_i \geq cp \end{cases}$$

You might consider the following diffuse prior distributions:

$$\begin{aligned} cp &\sim \text{uniform}(-1.3, 1.1) \\ \alpha, \beta_1, \beta_2 &\sim \text{normal}(0, \text{var} = 1e6) \\ \sigma^2 &\sim \text{uniform}(0, 5) \end{aligned}$$

The following statements generate [Output 55.12.2](#):

```
proc mcmc data=stagnant outpost=postout seed=24860 ntu=1000
 nmc=20000;
 ods select PostSummaries;
 ods output PostSummaries=ds;

 array beta[2];
 parms alpha cp beta1 beta2;
 parms s2;

 prior cp ~ unif(-1.3, 1.1);
 prior s2 ~ uniform(0, 5);
```

```

prior alpha beta: ~ normal(0, v = 1e6);

j = 1 + (x >= cp);
mu = alpha + beta[j] * (x - cp);
model y ~ normal(mu, var=s2);
run;

```

The PROC MCMC statement specifies the input data set (Stagnant), the output data set (Postout), a random number seed, a tuning sample of 1000, and an MCMC sample of 20000. The ODS SELECT statement displays only the summary statistics table. The ODS OUTPUT statement saves the summary statistics table to the data set Ds.

The ARRAY statement allocates an array of size 2 for the beta parameters. You can use beta1 and beta2 as parameter names without allocating an array, but having the array makes it easier to construct the likelihood function. The two PARMs statements put the five model parameters in two blocks. The three PRIOR statements specify the prior distributions for these parameters.

The symbol j indicates the segment component of the regression. When x is less than the change point, ( $x < cp$ ) returns 0 and j is assigned the value 1; if x is greater than or equal to the change point, ( $x \geq cp$ ) returns 1 and j is 2. The symbol mu is the mean for the jth segment, and beta[j] changes between the two regression coefficients depending on the segment component. The MODEL statement assigns the normal model to the response variable y.

Posterior summary statistics are shown in [Output 55.12.2](#).

#### Output 55.12.2 MCMC Estimates of the Change Point Regression Model

| Change Point Model  |       |          |                       |             |          |          |
|---------------------|-------|----------|-----------------------|-------------|----------|----------|
| The MCMC Procedure  |       |          |                       |             |          |          |
| Posterior Summaries |       |          |                       |             |          |          |
| Parameter           | N     | Mean     | Standard<br>Deviation | Percentiles |          |          |
|                     |       |          |                       | 25%         | 50%      | 75%      |
| alpha               | 20000 | 0.5349   | 0.0249                | 0.5188      | 0.5341   | 0.5509   |
| cp                  | 20000 | 0.0283   | 0.0314                | 0.00728     | 0.0303   | 0.0493   |
| beta1               | 20000 | -0.4200  | 0.0146                | -0.4293     | -0.4198  | -0.4111  |
| beta2               | 20000 | -1.0136  | 0.0167                | -1.0248     | -1.0136  | -1.0023  |
| s2                  | 20000 | 0.000451 | 0.000145              | 0.000348    | 0.000425 | 0.000522 |

You can use PROC SGPLOT to visualize the model fit. [Output 55.12.3](#) shows the fitted regression lines over the original data. In addition, on the bottom of the plot is the kernel density of the posterior marginal distribution of cp, the change point. The kernel density plot shows the relative variability of the posterior distribution on the data plot. You can use the following statements to create the plot:

```

data _null_;
 set ds;
 call symputx(parameter, mean);
run;

data b;
 missing A;
 input x1 @@;
 if x1 eq .A then x1 = &cp;
 if _n_ <= 2 then y1 = &alpha + &beta1 * (x1 - &cp);
 else y1 = &alpha + &beta2 * (x1 - &cp);
 datalines;
-1.5 A 1.2
;

proc kde data=postout;
 univar cp / out=m1 (drop=count);
run;

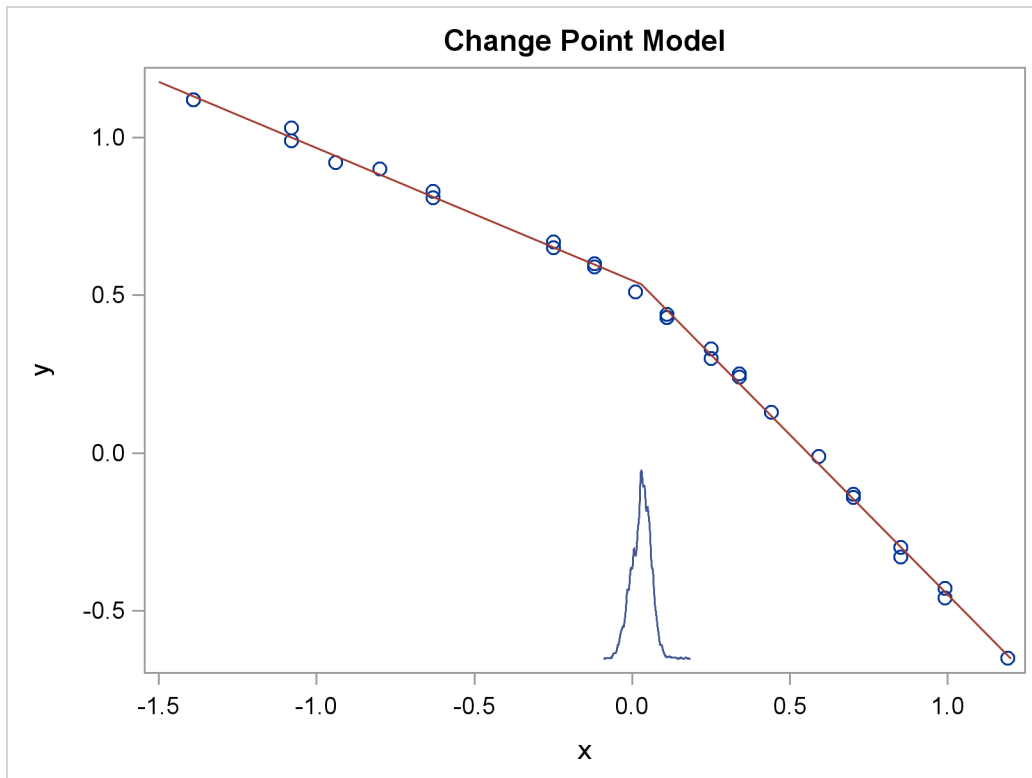
data m1;
 set m1;
 density = (density / 25) - 0.653;
run;

data all;
 set stagnant b m1;
run;

proc sgplot data=all noautolegend;
 scatter x=x y=y;
 series x=x1 y=y1 / lineattrs = graphdata2;
 series x=value y=density / lineattrs = graphdata1;
run;
ods graphics off;

```

The macro variables &alpha, &beta1, &beta2, and &cp store the posterior mean estimates from the data set Ds. The data set b contains three predicted values, at the minimum and maximum values of x and the estimated change point &cp. These input values give you fitted values from the regression model. Data set M1 contains the kernel density estimates of the parameter cp. The density is scaled down so the curve would fit in the plot. Finally, you use PROC SGPLOT to overlay the scatter plot, regression line and kernel density plots in the same graph.

**Output 55.12.3** Estimated Fit to the Stagnant Data Set

---

### Example 55.13: Exponential and Weibull Survival Analysis

This example covers two commonly used survival analysis models: the exponential model and the Weibull model. The deviance information criterion (DIC) is used to do model selections, and you can also find programs that visualize posterior quantities. Exponential and Weibull models are widely used for survival analysis. This example shows you how to use PROC MCMC to analyze the treatment effect for the E1684 melanoma clinical trial data. These data were collected to assess the effectiveness of using interferon alpha-2b in chemotherapeutic treatment of melanoma. The following statements create the data set:

```

data e1684;
 input t t_cen treatment @@;
 if t = . then do;
 t = t_cen;
 v = 0;
 end;
 else
 v = 1;
 ifn = treatment - 1;
 et = exp(t);
 lt = log(t);
 drop t_cen;
 datalines;
1.57808 0.00000 2 1.48219 0.00000 2 . 7.33425 1
2.23288 0.00000 1 . 9.38356 2 3.27671 0.00000 1
. 9.64384 1 1.66575 0.00000 2 0.94247 0.00000 1
1.68767 0.00000 2 2.34247 0.00000 2 0.89863 0.00000 1

... more lines ...

3.39178 0.00000 1 . 4.36164 2 . 4.81918 2
;

```

The data set E1684 contains the following variables:  $t$  is the failure time that equals the censoring time whether the observation was censored,  $v$  indicates whether the observation is an actual failure time or a censoring time,  $treatment$  indicates two levels of treatments, and  $ifn$  indicates the use of interferon as a treatment. The variables  $et$  and  $lt$  are the exponential and logarithm transformation of the time  $t$ . The published data contains other potential covariates that are not listed here. This example concentrates on the effectiveness of the interferon treatment.

## Exponential Survival Model

The density function for exponentially distributed survival times is as follows:

$$p(t_i | \lambda_i) = \lambda_i \exp(-\lambda_i t_i)$$

Note that this formulation of the exponential distribution is different from what is used in the SAS probability function PDF. The definition used in PDF for the exponential distributions is as follows:

$$p(t_i | v_i) = \frac{1}{v_i} \exp\left(-\frac{t_i}{v_i}\right)$$

The relationship between  $\lambda$  and  $v$  is as follows:

$$\lambda_i = \frac{1}{v_i}$$

The corresponding survival function, using the  $\lambda_i$  formulation, is as follows:

$$S(t_i | \lambda_i) = \exp(-\lambda_i t_i)$$



If you have a sample  $\{t_i\}$  of  $n$  independent exponential survival times, each with mean  $\lambda_i$ , then the likelihood function in terms of  $\lambda$  is as follows:

$$\begin{aligned} L(\lambda|t) &= \prod_{i=1}^n p(t_i|\lambda_i)^{v_i} S(t_i|\lambda_i)^{1-v_i} \\ &= \prod_{i=1}^n (\lambda_i \exp(-\lambda_i t_i))^{v_i} (\exp(-\lambda_i t_i))^{1-v_i} \\ &= \prod_{i=1}^n \lambda_i^{v_i} \exp(-\lambda_i t_i) \end{aligned}$$

If you link the covariates to  $\lambda$  with  $\lambda_i = \exp \mathbf{x}_i' \boldsymbol{\beta}$ , where  $\mathbf{x}_i$  is the vector of covariates corresponding to the  $i$ th observation and  $\boldsymbol{\beta}$  is a vector of regression coefficients, then the log-likelihood function is as follows:

$$l(\boldsymbol{\beta}|t, \mathbf{x}) = \sum_{i=1}^n v_i \mathbf{x}_i' \boldsymbol{\beta} - t_i \exp(\mathbf{x}_i' \boldsymbol{\beta})$$

In the absence of prior information about the parameters in this model, you can choose diffuse normal priors for the  $\boldsymbol{\beta}$ :

$$\boldsymbol{\beta} \sim \text{normal}(0, \text{sd}=10000)$$

There are two ways to program the log-likelihood function in PROC MCMC. You can use the SAS functions LOGPDF and LOGSDF. Alternatively, you can use the simplified log-likelihood function, which is more computationally efficient. You get identical results by using either approaches.

The following PROC MCMC statements fit an exponential model with simplified log-likelihood function:

```

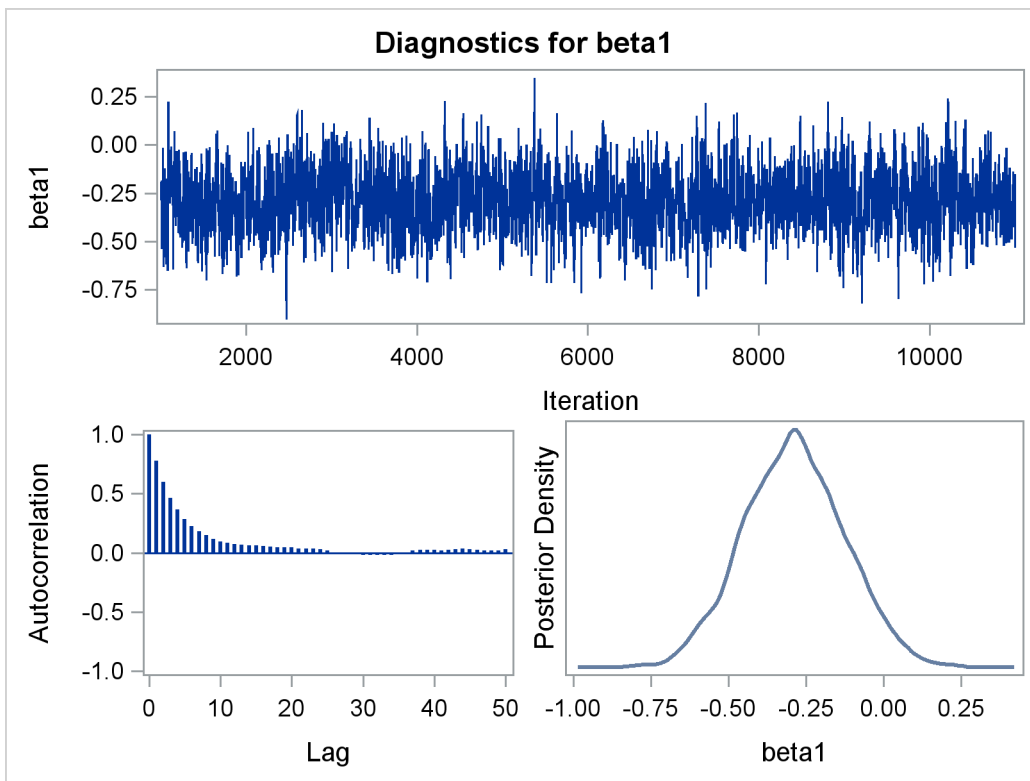
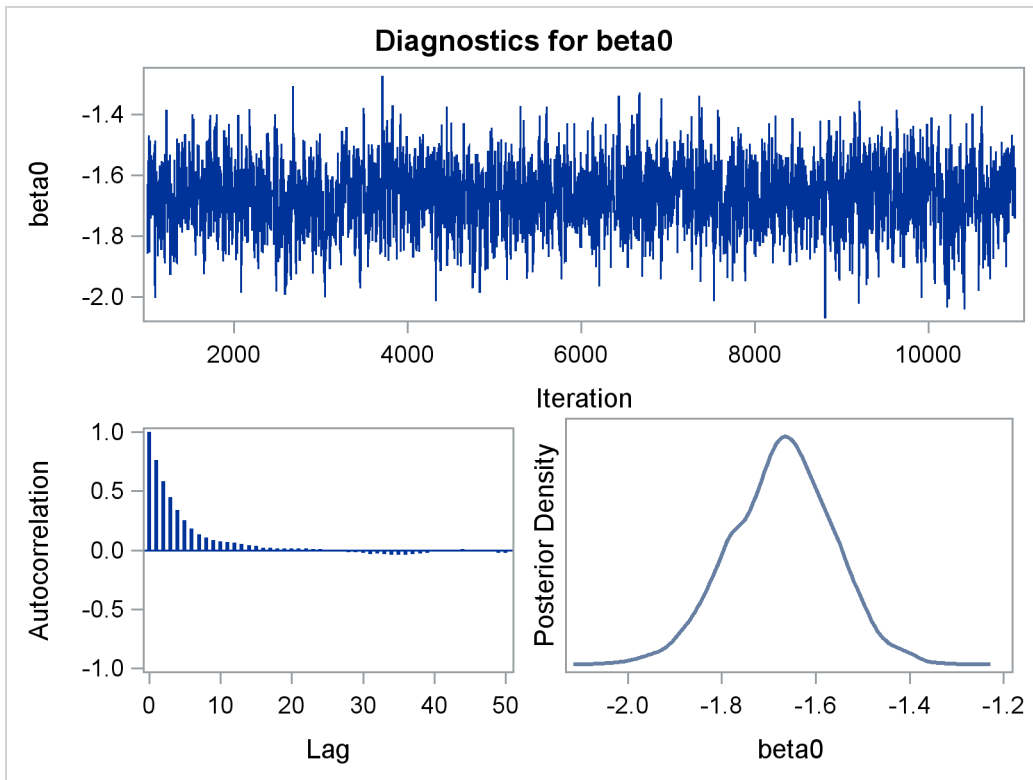
title 'Exponential Survival Model';
ods graphics on;
proc mcmc data=e1684 outpost=expurvout nmc=10000 seed=4861;
 ods select PostSummaries PostIntervals TADpanel
 ess mcse;
 parms (beta0 beta1) 0;
 prior beta: ~ normal(0, sd = 10000);
 /* *****
 /* (1) the logpdf and logsdf functions are not used */
 /* *****
 /* nu = 1/exp(beta0 + beta1*ifn);
 /* llike = v*logpdf("exponential", t, nu) +
 /* (1-v)*logsdf("exponential", t, nu);
 /*
 /* *****
 /* (2) the simplified likelihood formula is used */
 /* *****
 l_h = beta0 + beta1*ifn;
 llike = v*(l_h) - t*exp(l_h);
 model general(llike);
run;

```

The two assignment statements that are commented out calculate the log-likelihood function by using the SAS functions LOGPDF and LOGSDF for the exponential distribution. The next two assignment statements calculate the log likelihood by using the simplified formula. The first approach is slower because of the redundant calculation involved in calling both LOGPDF and LOGSDF.

An examination of the trace plots for  $\beta_0$  and  $\beta_1$  (see [Output 55.13.1](#)) reveals that the sampling has gone well with no particular concerns about the convergence or mixing of the chains.

**Output 55.13.1** Posterior Plots for  $\beta_0$  and  $\beta_1$  in the Exponential Survival Analysis



The MCMC results are shown in [Output 55.13.2](#).

**Output 55.13.2** Posterior Summary and Interval Statistics

| Exponential Survival Model |       |         |                       |             |         |         |
|----------------------------|-------|---------|-----------------------|-------------|---------|---------|
| The MCMC Procedure         |       |         |                       |             |         |         |
| Posterior Summaries        |       |         |                       |             |         |         |
| Parameter                  | N     | Mean    | Standard<br>Deviation | Percentiles |         |         |
|                            |       |         |                       | 25%         | 50%     | 75%     |
| beta0                      | 10000 | -1.6715 | 0.1091                | -1.7426     | -1.6684 | -1.5964 |
| beta1                      | 10000 | -0.2879 | 0.1615                | -0.4001     | -0.2892 | -0.1803 |

| Posterior Intervals |       |                     |         |              |         |
|---------------------|-------|---------------------|---------|--------------|---------|
| Parameter           | Alpha | Equal-Tail Interval |         | HPD Interval |         |
| beta0               | 0.050 | -1.8907             | -1.4639 | -1.8930      | -1.4673 |
| beta1               | 0.050 | -0.5985             | 0.0300  | -0.6104      | 0.0169  |

The Monte Carlo standard errors and effective sample sizes are shown in [Output 55.13.3](#). The posterior means for  $\beta_0$  and  $\beta_1$  are estimated with high precision, with small standard errors with respect to the standard deviation. This indicates that the mean estimates have stabilized and do not vary greatly in the course of the simulation. The effective sample sizes are roughly the same for both parameters.

**Output 55.13.3** MCSE and ESS

| Exponential Survival Model  |         |                       |         |
|-----------------------------|---------|-----------------------|---------|
| The MCMC Procedure          |         |                       |         |
| Monte Carlo Standard Errors |         |                       |         |
| Parameter                   | MCSE    | Standard<br>Deviation | MCSE/SD |
| beta0                       | 0.00302 | 0.1091                | 0.0277  |
| beta1                       | 0.00485 | 0.1615                | 0.0301  |

| Effective Sample Sizes |        |                         |            |
|------------------------|--------|-------------------------|------------|
| Parameter              | ESS    | Autocorrelation<br>Time | Efficiency |
| beta0                  | 1304.1 | 7.6682                  | 0.1304     |
| beta1                  | 1107.2 | 9.0319                  | 0.1107     |

The next part of this example shows fitting a Weibull regression to the data and then comparing the two models with DIC to see which one provides a better fit to the data.

## Weibull Survival Model

The density function for Weibull distributed survival times is as follows:

$$p(t_i | \alpha, \lambda_i) = \alpha t_i^{\alpha-1} \exp(\lambda_i - \exp(\lambda_i) t_i^\alpha)$$

Note that this formulation of the Weibull distribution is different from what is used in the SAS probability function PDF. The definition used in PDF is as follows:

$$p(t_i | \alpha, \gamma_i) = \exp\left(-\left(\frac{t_i}{\gamma_i}\right)^\alpha\right) \frac{\alpha}{\gamma_i} \left(\frac{t_i}{\gamma_i}\right)^{\alpha-1}$$

The relationship between  $\lambda$  and  $\gamma$  in these two parameterizations is as follows:

$$\lambda_i = -\alpha \log \gamma_i$$

The corresponding survival function, using the  $\lambda_i$  formulation, is as follows:

$$S(t_i | \alpha, \lambda_i) = \exp(-\exp(\lambda_i) t_i^\alpha)$$

If you have a sample  $\{t_i\}$  of  $n$  independent Weibull survival times, with parameters  $\alpha$ , and  $\lambda_i$ , then the likelihood function in terms of  $\alpha$  and  $\lambda$  is as follows:

$$\begin{aligned} L(\alpha, \lambda | t) &= \prod_{i=1}^n p(t_i | \alpha, \lambda_i)^{v_i} S(t_i | \alpha, \lambda_i)^{1-v_i} \\ &= \prod_{i=1}^n (\alpha t_i^{\alpha-1} \exp(\lambda_i - \exp(\lambda_i) t_i^\alpha))^{v_i} (\exp(-\exp(\lambda_i) t_i^\alpha))^{1-v_i} \\ &= \prod_{i=1}^n (\alpha t_i^{\alpha-1} \exp(\lambda_i))^{v_i} (\exp(-\exp(\lambda_i) t_i^\alpha)) \end{aligned}$$

If you link the covariates to  $\lambda$  with  $\lambda_i = \mathbf{x}_i' \boldsymbol{\beta}$ , where  $\mathbf{x}_i$  is the vector of covariates corresponding to the  $i$ th observation and  $\boldsymbol{\beta}$  is a vector of regression coefficients, the log-likelihood function becomes this:

$$l(\alpha, \boldsymbol{\beta} | t, \mathbf{x}) = \sum_{i=1}^n v_i (\log(\alpha) + (\alpha - 1) \log(t_i) + \mathbf{x}_i' \boldsymbol{\beta}) - \exp(\mathbf{x}_i' \boldsymbol{\beta}) t_i^\alpha$$

As with the exponential model, in the absence of prior information about the parameters in this model, you can use diffuse normal priors on  $\boldsymbol{\beta}$ . You might want to choose a diffuse gamma distribution for  $\alpha$ . Note that when  $\alpha = 1$ , the Weibull survival likelihood reduces to the exponential survival likelihood. Equivalently, by looking at the posterior distribution of  $\alpha$ , you can conclude whether fitting an exponential survival model would be more appropriate than the Weibull model.

PROC MCMC also enables you to make inference on any functions of the parameters. Quantities of interest in survival analysis include the value of the survival function at specific times for specific treatments and the relationship between the survival curves for different treatments. With PROC MCMC, you can compute a sample from the posterior distribution of the interested survival functions at any number of points. The data in this example range from about 0 to 10 years, and the treatment of interest is the use of interferon.

Like in the previous exponential model example, there are two ways to fit this model: using the SAS functions LOGPDF and LOGSDF, or using the simplified log likelihood functions. The example uses the latter method. The following statements run PROC MCMC and produce [Output 55.13.4](#):

```

title 'Weibull Survival Model';
proc mcmc data=e1684 outpost=weisurvout nmc=10000 seed=1234
 monitor=(_parms_ surv_ifn surv_noifn);
ods select PostSummaries;
ods output PostSummaries=ds PostIntervals=is;
array surv_ifn[10];
array surv_noifn[10];
parms alpha 1 (beta0 betal) 0;
prior beta: ~ normal(0, var=10000);
prior alpha ~ gamma(0.001, is=0.001);

beginnodata;
 do t1 = 1 to 10;
 surv_ifn[t1] = exp(-exp(beta0+betal)*t1**alpha);
 surv_noifn[t1] = exp(-exp(beta0)*t1**alpha);
 end;
endnodata;

lambda = beta0 + betal*ifn;
/*****
/* (1) the logpdf and logsdf functions are not used */
/*****
/* gamma = exp(-lambda /alpha);
 llike = v*logpdf('weibull', t, alpha, gamma) +
 (1-v)*logsdf('weibull', t, alpha, gamma);
*/
/*****
/* (2) the simplified likelihood formula is used */
/*****
llike = v*(log(alpha) + (alpha-1)*log(t) + lambda) -
 exp(lambda)*(t**alpha);
model general(llike);
run;

```

The `MONITOR=` option indicates the parameters and quantities of interest that PROC MCMC tracks. The symbol `_PARMS_` specifies all model parameters. The array `surv_ifn` stores the expected survival probabilities for patients who received interferon over a period of 10 years. Similarly, `surv_noifn` stores the expected survival probabilities for patients who did not received interferon.

The `BEGINNODATA` and `ENDNODATA` statements enclose the calculations for the survival probabilities. The assignment statements proceeding the `MODEL` statement calculate the log likelihood for the Weibull survival model. The `MODEL` statement specifies the log likelihood that you programmed.

An examination of the trace plots for  $\alpha$ ,  $\beta_0$ , and  $\beta_1$  (not displayed here) reveals that the sampling has gone well, with no particular concerns about the convergence or mixing of the chains.

Output 55.13.4 displays the posterior summary statistics.

## Output 55.13.4 Posterior Summary Statistics

| Weibull Survival Model |       |         |                       |             |         |         |
|------------------------|-------|---------|-----------------------|-------------|---------|---------|
| The MCMC Procedure     |       |         |                       |             |         |         |
| Posterior Summaries    |       |         |                       |             |         |         |
| Parameter              | N     | Mean    | Standard<br>Deviation | Percentiles |         |         |
|                        |       |         |                       | 25%         | 50%     | 75%     |
| alpha                  | 10000 | 0.7891  | 0.0539                | 0.7514      | 0.7880  | 0.8260  |
| beta0                  | 10000 | -1.3581 | 0.1369                | -1.4519     | -1.3597 | -1.2624 |
| beta1                  | 10000 | -0.2512 | 0.1541                | -0.3541     | -0.2606 | -0.1521 |
| surv_ifn1              | 10000 | 0.8175  | 0.0227                | 0.8027      | 0.8187  | 0.8331  |
| surv_ifn2              | 10000 | 0.7066  | 0.0291                | 0.6874      | 0.7072  | 0.7265  |
| surv_ifn3              | 10000 | 0.6203  | 0.0331                | 0.5983      | 0.6205  | 0.6436  |
| surv_ifn4              | 10000 | 0.5495  | 0.0360                | 0.5253      | 0.5497  | 0.5747  |
| surv_ifn5              | 10000 | 0.4899  | 0.0381                | 0.4635      | 0.4895  | 0.5170  |
| surv_ifn6              | 10000 | 0.4390  | 0.0396                | 0.4118      | 0.4382  | 0.4666  |
| surv_ifn7              | 10000 | 0.3949  | 0.0406                | 0.3669      | 0.3934  | 0.4223  |
| surv_ifn8              | 10000 | 0.3564  | 0.0413                | 0.3281      | 0.3551  | 0.3840  |
| surv_ifn9              | 10000 | 0.3225  | 0.0416                | 0.2940      | 0.3212  | 0.3505  |
| surv_ifn10             | 10000 | 0.2926  | 0.0416                | 0.2638      | 0.2911  | 0.3208  |
| surv_noifn1            | 10000 | 0.7719  | 0.0274                | 0.7535      | 0.7736  | 0.7913  |
| surv_noifn2            | 10000 | 0.6401  | 0.0339                | 0.6171      | 0.6415  | 0.6635  |
| surv_noifn3            | 10000 | 0.5415  | 0.0374                | 0.5161      | 0.5428  | 0.5662  |
| surv_noifn4            | 10000 | 0.4635  | 0.0395                | 0.4365      | 0.4636  | 0.4890  |
| surv_noifn5            | 10000 | 0.4001  | 0.0406                | 0.3725      | 0.3995  | 0.4261  |
| surv_noifn6            | 10000 | 0.3475  | 0.0411                | 0.3195      | 0.3459  | 0.3745  |
| surv_noifn7            | 10000 | 0.3034  | 0.0411                | 0.2758      | 0.3012  | 0.3299  |
| surv_noifn8            | 10000 | 0.2661  | 0.0406                | 0.2384      | 0.2630  | 0.2921  |
| surv_noifn9            | 10000 | 0.2342  | 0.0399                | 0.2069      | 0.2311  | 0.2592  |
| surv_noifn10           | 10000 | 0.2069  | 0.0389                | 0.1803      | 0.2035  | 0.2312  |

An examination of the  $\alpha$  parameter reveals that the exponential model might not be inappropriate here. The estimated posterior mean of  $\alpha$  is 0.7856 with a posterior standard deviation of 0.0533. As noted previously, if  $\alpha = 1$ , then the Weibull survival distribution is the exponential survival distribution. With these data, you can see that the evidence is in favor of  $\alpha < 1$ . The value 1 is almost 4 posterior standard deviations away from the posterior mean. The following statements compute the posterior probability of the hypothesis that  $\alpha < 1$ .

```
proc format;
 value alphafmt low-<1 = 'alpha < 1' 1-high = 'alpha >= 1';
run;

proc freq data=weisurvout;
 tables alpha /nocum;
 format alpha alphafmt.;
run;
```

The PROC FREQ results are shown in [Output 55.13.5](#).

**Output 55.13.5** Frequency Analysis of  $\alpha$ 

| Weibull Survival Model |           |         |
|------------------------|-----------|---------|
| The FREQ Procedure     |           |         |
| alpha                  | Frequency | Percent |
| alpha < 1              | 9998      | 99.98   |
| alpha >= 1             | 2         | 0.02    |

The output from PROC FREQ shows that 100% of the 10000 simulated values for  $\alpha$  are less than 1. This is a very strong indication that the exponential model is too restrictive to model these data well.

You can examine the estimated survival probabilities over time individually, either through the posterior summary statistics or by looking at the kernel density plots. Alternatively, you might find it more informative to examine these quantities in relation with each other. For example, you can use a side-by-side box plot to display these posterior distributions by using PROC SGPLOT (“[Statistical Graphics Using ODS](#)” on page 579). First you need to take the posterior output data set `Weisurvout` and stack variables that you want to plot. For example, to plot all the survival times for patients who received interferon, you want to stack `surv_inf1–surv_inf10`. The macro `%Stackdata` takes an input data set `dataset`, stacks the wanted variables `vars`, and outputs them into the output data set.

The following statements define the macro `stackdata`:

```

/* define macro stackdata */
%macro StackData(dataset,output,vars);
 data &output;
 length var $ 32;
 if 0 then set &dataset nobs=nnn;
 array l11[*] &vars;
 do jjj=1 to dim(l11);
 do iii=1 to nnn;
 set &dataset point=iii;
 value = l11[jjj];
 call vname(l11[jjj],var);
 output;
 end;
 end;
 stop;
 keep var value;
run;
%mend;

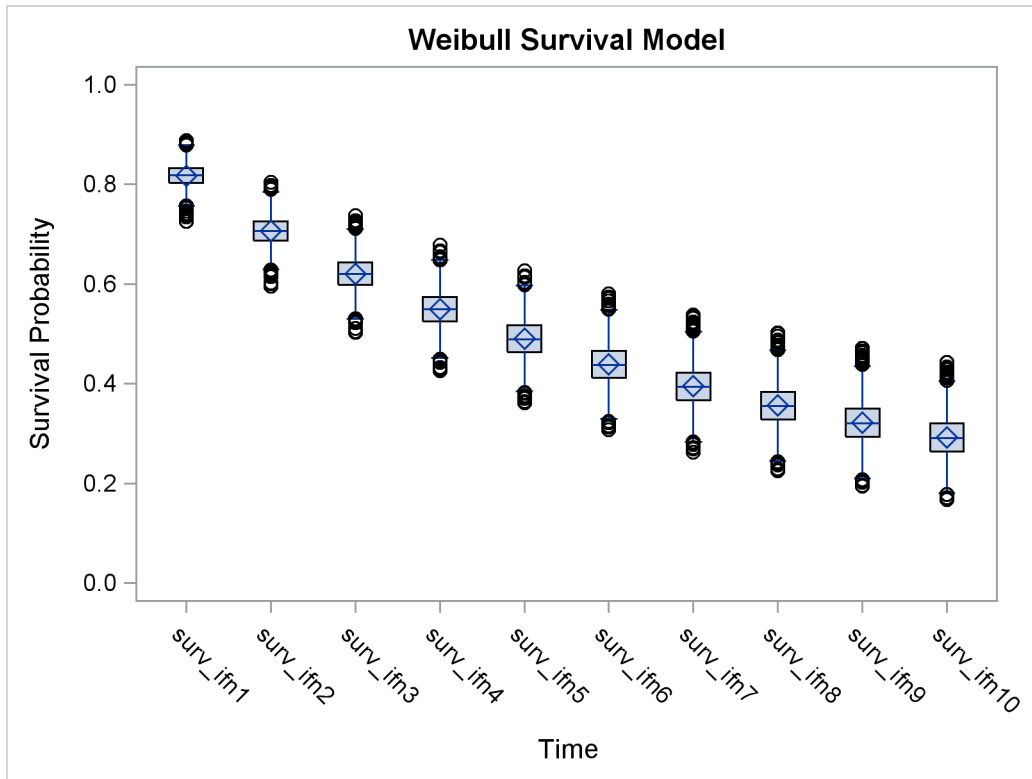
/* stack the surv_ifn variables and saved them to survifn. */
%StackData(weisurvout, survifn, surv_ifn1–surv_ifn10);

```

Once you stack the data, use PROC SGPLOT to create the side-by-side box plots. The following statements generate [Output 55.13.6](#):

```
proc sgplot data=survifn;
 yaxis label='Survival Probability' values=(0 to 1 by 0.2);
 xaxis label='Time' discreteorder=data;
 vbox value / category=var;
run;
```

**Output 55.13.6** Side-by-Side Box Plots of Estimated Survival Probabilities



There is a clear decreasing trend over time of the survival probabilities for patients who receive the treatment. You might ask how does this group compare to those who did not receive the treatment? In this case, you want to overlay the two predicted curves for the two groups of patients and add the corresponding credible interval. See [Output 55.13.7](#). To generate the graph, you first take the posterior mean estimates from the ODS output table ds and the lower and upper HPD interval estimates is, store them in the data set Surv, and draw the figure by using PROC SGPLOT.

The following statements generate data set Surv:

```
data surv;
 set ds;
 if _n_ >= 4 then do;
 set is point=_n_;
 group = 'with interferon ';
 time = _n_ - 3;
 if time > 10 then do;
 time = time - 10;
 group = 'without interferon';
 end;
 end;
```



```

output;
end;
keep time group mean hpdlower hpdupper;
run;

```

The following SGLOT statements generate [Output 55.13.7](#):

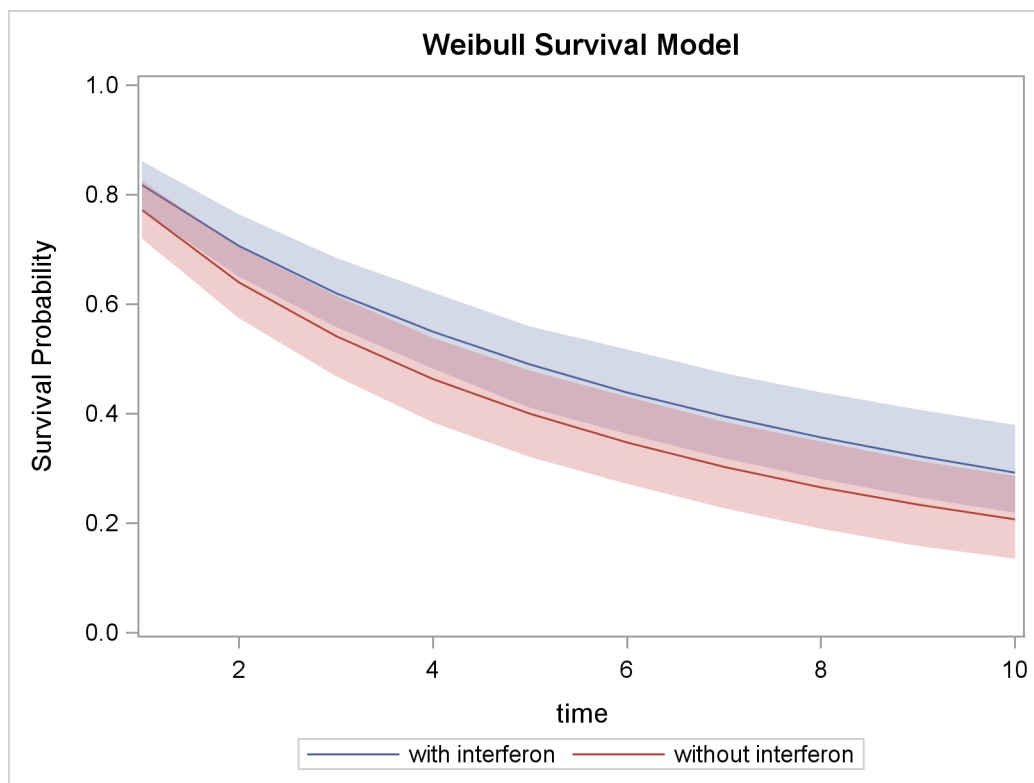
```

proc sgplot data=surv;
 yaxis label="Survival Probability" values=(0 to 1 by 0.2);
 series x=time y=mean / group = group name='i';
 band x=time lower=hpdlower upper=hpdupper / group = group transparency=0.7;
 keylegend 'i';
run;
ods graphics off;

```

In [Output 55.13.7](#), the solid line is the survival curve for patients who received interferon; the shaded region centers at the solid line is the 95% HPD intervals; the medium-dashed line is the survival curve for patients who did not receive interferon; and the shaded region around the dashed line is the corresponding 95% HPD intervals.

**Output 55.13.7** Predicted Survival Probability Curves with 95% HPD Intervals



The plot suggests that there is an effect of using interferon because patients who received interferon have sustained better survival probabilities than those who did not. However, the effect might not be very significant, as the 95% credible intervals of the two groups do overlap. For more on these interferon studies, see Ibrahim, Chen, and Lipsitz (2001).

## Weibull or Exponential?

Although the evidence from the Weibull model fit shows that the posterior distribution of  $\alpha$  has a significant amount of density mass less than 1, suggesting that the Weibull model is a better fit to the data than the exponential model, you might still be interested in comparing the two models more formally. You can use the Bayesian model selection criterion (see the section “[Deviance Information Criterion \(DIC\)](#)” on page 155) to determine which model fits the data better.

The PROC MCMC [DIC](#) option requests the calculation of DIC, and the procedure displays the ODS output table [DIC](#). The table includes the posterior mean of the deviation,  $\overline{D(\theta)}$ , deviation at the estimate,  $D(\hat{\theta})$ , effective number of parameters,  $p_D$ , and DIC. It is important to remember that the standardizing term,  $p(y)$ , which is a function of the data alone, is not taken into account in calculating the DIC. This term is irrelevant only if you compare two models that have the *same* likelihood function. If you do not have identical likelihood functions, using DIC for model selection purposes without taking this standardizing term into account can produce incorrect results. In addition, you want to be careful in interpreting the DIC whenever you use the [GENERAL](#) function to construct the log-likelihood, as the case in this example. Using the [GENERAL](#) function, you can obtain identical posterior samples with two log-likelihood functions that differ only by a constant. This difference translates to a difference in the DIC calculation, which could be very misleading.

If  $\alpha = 1$ , the Weibull likelihood is identical to the exponential likelihood. It is safe in this case to directly compare DICs from these two models. However, if you do not want to work out the mathematical detail or you are uncertain of the equivalence, a better way of comparing the DICs is to run the Weibull model twice: once with  $\alpha$  being a parameter and once with  $\alpha = 1$ . This ensures that the likelihood functions are the same, and the DIC comparison is meaningful.

The following statements fit a Weibull model:

```

title 'Model Comparison between Weibull and Exponential';
proc mcmc data=e1684 outpost=weisurvout nmc=10000 seed=4861 dic;
 ods select dic;
 parms alpha 1 (beta0 beta1) 0;
 prior beta: ~ normal(0, var=10000);
 prior alpha ~ gamma(0.001, is=0.001);

 lambda = beta0 + beta1*ifn;
 llike = v*(log(alpha) + (alpha-1)*log(t) + lambda) -
 exp(lambda)*(t**alpha);
 model general(llike);
run;

```

The DIC option requests the calculation of DIC, and the table is displayed in [Output 55.13.8](#).

**Output 55.13.8** DIC Table from the Weibull Model

| Model Comparison between Weibull and Exponential                                                                                                                                                                                                 |         |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------|
| The MCMC Procedure                                                                                                                                                                                                                               |         |
| Deviance Information Criterion                                                                                                                                                                                                                   |         |
| Dbar (posterior mean of deviance)                                                                                                                                                                                                                | 858.623 |
| Dmean (deviance evaluated at posterior mean)                                                                                                                                                                                                     | 855.633 |
| pD (effective number of parameters)                                                                                                                                                                                                              | 2.990   |
| DIC (smaller is better)                                                                                                                                                                                                                          | 861.614 |
| <p>The GENERAL or DGENERAL function is used in this program. To make meaningful comparisons, you must ensure that all GENERAL or DGENERAL functions include appropriate normalizing constants. Otherwise, DIC comparisons can be misleading.</p> |         |

The note in [Output 55.13.8](#) reminds you of the importance of ensuring identical likelihood functions when you use the GENERAL function. The DIC value is 861.6.

Based on the same set of code, the following statements fit an exponential model by setting  $\alpha = 1$ :

```
proc mcmc data=e1684 outpost=expsurvout nmc=10000 seed=4861 dic;
 ods select dic;
 parms beta0 beta1 0;
 prior beta: ~ normal(0, var=10000);
 begincnst;
 alpha = 1;
 endcnst;

 lambda = beta0 + beta1*ifn;
 llike = v*(log(alpha) + (alpha-1)*log(t) + lambda) -
 exp(lambda)*(t**alpha);
 model general(llike);
run;
```

[Output 55.13.9](#) displays the DIC table.

**Output 55.13.9** DIC Table from the Exponential Model

| Model Comparison between Weibull and Exponential |         |
|--------------------------------------------------|---------|
| The MCMC Procedure                               |         |
| Deviance Information Criterion                   |         |
| Dbar (posterior mean of deviance)                | 870.133 |
| Dmean (deviance evaluated at posterior mean)     | 868.190 |
| pD (effective number of parameters)              | 1.943   |
| DIC (smaller is better)                          | 872.075 |

The GENERAL or DGENERAL function is used in this program. To make meaningful comparisons, you must ensure that all GENERAL or DGENERAL functions include appropriate normalizing constants. Otherwise, DIC comparisons can be misleading.

The DIC value of 872.075 is greater than 861. A smaller DIC indicates a better fit to the data; hence, you can conclude that the Weibull model is more appropriate for this data set. You can see the equivalencing of the exponential model you fitted in “[Exponential Survival Model](#)” on page 4605 by running the following comparison.

The following statements are taken from the section “[Exponential Survival Model](#)” on page 4605, and they fit the same exponential model:

```
proc mcmc data=e1684 outpost=expsurvout1 nmc=10000 seed=4861 dic;
 ods select none;
 parms (beta0 beta1) 0;
 prior beta: ~ normal(0, sd = 10000);
 l_h = beta0 + beta1*ifn;
 llike = v*(l_h) - t*exp(l_h);
 model general(llike);
run;

proc compare data=expsurvout compare=expsurvout1;
 var beta0 beta1;
run;
```

The posterior samples of beta0 and beta1 in the data set Expsurvout1 are identical to those in the data set Expsurvout. The comparison results are not shown here.

---

## Example 55.14: Time Independent Cox Model

This example has two purposes. One is to illustrate how to use PROC MCMC to fit a Cox proportional hazard model. Specifically, the time independent model. See “[Example 55.15: Time Dependent Cox Model](#)” on page 4625 for an example on fitting time dependent Cox model. Note that it is much easier to fit a Bayesian Cox model by specifying the BAYES statement in PROC PHREG (see Chapter 67, “[The PHREG Procedure](#)”). If you are interested only in fitting a Cox regression survival model, you should use PROC PHREG.

The second objective of this example is to demonstrate how to model data that are not independent. That is the case where the likelihood for observation  $i$  depends on other observations in the data set. In other words, if you work with a likelihood function that cannot be broken down simply as  $L(\mathbf{y}) = \prod_i^n L(y_i)$ , you can use this example for illustrative purposes. By default, PROC MCMC assumes that the programming statements and model specification is intended for a single row of observations in the data set. The Cox model is chosen because the complexity in the data structure requires more elaborate coding.

The Cox proportional hazard model is widely used in the analysis of survival time, failure time, or other duration data to explain the effect of exogenous explanatory variables. The data set used in this example is taken from Krall, Uthoff, and Harley (1975), who analyzed data from a study on myeloma in which researchers treated 65 patients with alkylating agents. Of those patients, 48 died during the study and 17 survived. The following statements generate the data set that is used in this example:

```
data Myeloma;
 input Time Vstatus LogBUN HGB Platelet Age LogWBC Frac
 LogPBM Protein SCalc;
 label Time='survival time'
 VStatus='0=alive 1=dead';
 datalines;
 1.25 1 2.2175 9.4 1 67 3.6628 1 1.9542 12 10
 1.25 1 1.9395 12.0 1 38 3.9868 1 1.9542 20 18
 2.00 1 1.5185 9.8 1 81 3.8751 1 2.0000 2 15
 2.00 1 1.7482 11.3 0 75 3.8062 1 1.2553 0 12

 ... more lines ...

 77.00 0 1.0792 14.0 1 60 3.6812 0 0.9542 0 12
;

proc sort data = Myeloma;
 by descending time;
run;

data _null_;
 set Myeloma nobs=_n;
 call symputx('N', _n);
 stop;
run;
```

The variable Time represents the survival time in months from diagnosis. The variable VStatus consists of two values, 0 and 1, indicating whether the patient was alive or dead, respectively, at the end of the study. If the value of VStatus is 0, the corresponding value of Time is censored. The variables thought to be related to survival are LogBUN (log(BUN) at diagnosis), HGB (hemoglobin at diagnosis), Platelet (platelets at diagnosis: 0=abnormal, 1=normal), Age (age at diagnosis in years), LogWBC (log(WBC) at diagnosis), Frac (fractures at diagnosis: 0=none, 1=present), LogPBM (log percentage of plasma cells in bone marrow), Protein (proteinuria at diagnosis), and SCalc (serum calcium at diagnosis). Interest lies in identifying important prognostic factors from these explanatory variables. In addition, there are 65 (&n) observations in the data set Myeloma. The likelihood used in these examples is the Breslow likelihood:

$$L(\boldsymbol{\beta}) = \prod_{i=1}^n \left[ \prod_{j=1}^{d_i} \frac{\exp(\boldsymbol{\beta}'\mathbf{Z}_j(t_i))}{\sum_{l \in \mathcal{R}_i} \exp(\boldsymbol{\beta}'\mathbf{Z}_l(t_i))} \right]^{v_i}$$

where

- $\beta$  is the vector parameters
- $n$  is the total number of observations in the data set
- $t_i$  is the  $i$ th time, which can be either event time or censored time
- $\mathbf{Z}_l(t)$  is the vector explanatory variables for the  $l$ th individual at time  $t$
- $d_i$  is the multiplicity of failures at  $t_i$ . If there are no ties in time,  $d_i$  is 1 for all  $i$ .
- $\mathcal{R}_i$  is the risk set for the  $i$ th time  $t_i$ , which includes all observations that have survival time greater than or equal to  $t_i$
- $v_i$  indicates whether the patient is censored. The value 0 corresponds to censoring. Note that the censored time  $t_i$  enters the likelihood function only through the formation of the risk set  $\mathcal{R}_i$ .

Priors on the coefficients are independent normal priors with very large variance (1e6). Throughout this example, the symbol  $\mathbf{bZ}$  represents the regression term  $\beta' \mathbf{Z}_j(t_i)$  in the likelihood, and the symbol  $\mathbf{S}$  represents the term  $\sum_{l \in \mathcal{R}_i} \exp(\beta' \mathbf{Z}_l(t_i))$ .

The regression model considered in this example uses the following formula:

$$\begin{aligned} \beta' \mathbf{Z}_j = & \beta_1 \text{logbun} + \beta_2 \text{hgb} + \beta_3 \text{platelet} + \beta_4 \text{age} + \\ & \beta_5 \text{logwbc} + \beta_6 \text{frac} + \beta_7 \text{logpbm} + \beta_8 \text{protein} + \beta_9 \text{scal} \end{aligned}$$

The hard part of coding this in PROC MCMC is the construction of the risk set  $\mathcal{R}_i$ .  $\mathcal{R}_i$  contains all observations that have survival time greater than or equal to  $t_i$ . First suppose that there are no ties in time. Sorting the data set by the variable time into descending order gives you  $\mathcal{R}_i$  that is in the right order. Observation  $i$ 's risk set consists of all data points  $j$  such that  $j \leq i$  in the data set. You can cumulatively increment  $\mathbf{S}$  in the SAS statements.

With potential ties in time, at observation  $i$ , you need to know whether any subsequent observations,  $i + 1$  and so on, have the same survival time as  $t_i$ . Suppose that the  $i$ th, the  $i + 1$ , and the  $i + 2$  observations all have the same survival time; all three of them need to be included in the risk set calculation. This means that to calculate the likelihood for some observations, you need to access both the previous and subsequent observations in the data set. There are two ways to do this. One is to use the LAG function; the other is to use the option `JOINTMODEL`.

The LAG function returns values from a queue (see *SAS Language Reference: Dictionary*). So for the  $i$ th observation, you can use LAG1 to access variables from the previous row in the data set. You want to compare the lag1 value of time with the current time value. Depending on whether the two time values are equal, you can add correction terms in the calculation for the risk set  $\mathbf{S}$ .

The following statements sort the data set by time into descending order, with the largest survival time on top:

```

title 'Cox Model with Time Independent Covariates';
proc freq data=myeloma;
 ods select none;
 tables time / out=freqs;
run;

proc sort data = freqs;
 by descending time;
run;

data myelomaM;
 set myeloma;
 ind = _N_;
run;
ods select all;

```

The following statements run PROC MCMC and produce [Output 55.14.1](#):

```

proc mcmc data=myelomaM outpost=outi nmc=50000 ntu=3000 seed=1;
 ods select PostSummaries PostIntervals;
 array beta[9];
 parms beta: 0;
 prior beta: ~ normal(0, var=1e6);

 bZ = beta1 * LogBUN + beta2 * HGB + beta3 * Platelet
 + beta4 * Age + beta5 * LogWBC + beta6 * Frac +
 beta7 * LogPEM + beta8 * Protein + beta9 * SCalc;

 if ind = 1 then do; /* first observation */
 S = exp(bZ);
 l = vstatus * bZ;
 v = vstatus;
 end;
 else if (1 < ind < &N) then do;
 if (lag1(time) ne time) then do;
 l = vstatus * bZ;
 l = l - v * log(S); /* correct the loglike value */
 v = vstatus; /* reset v count value */
 S = S + exp(bZ);
 end;
 else do; /* still a tie */
 l = vstatus * bZ;
 S = S + exp(bZ);
 v = v + vstatus; /* add # of nonsensored values */
 end;
 end;
 else do; /* last observation */
 if (lag1(time) ne time) then do;
 l = - v * log(S); /* correct the loglike value */
 S = S + exp(bZ);
 l = l + vstatus * (bZ - log(S));
 end;
 else do;

```

```

 S = S + exp(bZ) ;
 l = vstatus * bZ - (v + vstatus) * log(S) ;
 end;
 end;
 model general(l) ;
run;

```

The symbol `bZ` is the regression term, which is independent of the time variable. The symbol `ind` indexes observation numbers in the data set. The symbol `S` keeps track of the risk set term for every observation. The symbol `l` calculates the log likelihood for each observation. Note that the value of `l` for observation `ind` is not necessarily the correct log likelihood value for that observation, especially in cases where the observation `ind` is in the tied times. Correction terms are added to subsequent values of `l` when the time variable becomes different in order to make up the difference. The total sum of `l` calculated over the entire data set is correct. The symbol `v` keeps track of the sum of `vstatus`, as censored data do not enter the likelihood and need to be taken out.

You use the function `LAG1` to detect if two adjacent time values are different. If they are, you know that the current observation is in a different risk set than the last one. You then need to add a correction term to the log likelihood value of `l`. The IF-ELSE statements break the observations into three parts: the first observation, the last observation and everything in the middle.

**Output 55.14.1** Summary Statistics on Cox Model with Time Independent Explanatory Variables and Ties in the Survival Time, Using PROC MCMC

| Cox Model with Time Independent Covariates |       |         |                       |             |         |          |
|--------------------------------------------|-------|---------|-----------------------|-------------|---------|----------|
| The MCMC Procedure                         |       |         |                       |             |         |          |
| Posterior Summaries                        |       |         |                       |             |         |          |
| Parameter                                  | N     | Mean    | Standard<br>Deviation | Percentiles |         |          |
|                                            |       |         |                       | 25%         | 50%     | 75%      |
| beta1                                      | 50000 | 1.7600  | 0.6441                | 1.3275      | 1.7651  | 2.1947   |
| beta2                                      | 50000 | -0.1308 | 0.0720                | -0.1799     | -0.1304 | -0.0817  |
| beta3                                      | 50000 | -0.2017 | 0.5148                | -0.5505     | -0.1965 | 0.1351   |
| beta4                                      | 50000 | -0.0126 | 0.0194                | -0.0257     | -0.0128 | 0.000641 |
| beta5                                      | 50000 | 0.3373  | 0.7256                | -0.1318     | 0.3505  | 0.8236   |
| beta6                                      | 50000 | 0.3992  | 0.4337                | 0.0973      | 0.3864  | 0.6804   |
| beta7                                      | 50000 | 0.3749  | 0.4861                | 0.0464      | 0.3636  | 0.6989   |
| beta8                                      | 50000 | 0.0106  | 0.0271                | -0.00723    | 0.0118  | 0.0293   |
| beta9                                      | 50000 | 0.1272  | 0.1064                | 0.0579      | 0.1300  | 0.1997   |



Output 55.14.1 *continued*

| Parameter | Alpha | Posterior Intervals |              |         |         |
|-----------|-------|---------------------|--------------|---------|---------|
|           |       | Equal-Tail Interval | HPD Interval |         |         |
| beta1     | 0.050 | 0.4649              | 3.0214       | 0.5117  | 3.0465  |
| beta2     | 0.050 | -0.2704             | 0.0114       | -0.2746 | 0.00524 |
| beta3     | 0.050 | -1.2180             | 0.8449       | -1.2394 | 0.7984  |
| beta4     | 0.050 | -0.0501             | 0.0257       | -0.0512 | 0.0245  |
| beta5     | 0.050 | -1.1233             | 1.7232       | -1.1124 | 1.7291  |
| beta6     | 0.050 | -0.4136             | 1.2970       | -0.4385 | 1.2575  |
| beta7     | 0.050 | -0.5551             | 1.3593       | -0.5423 | 1.3689  |
| beta8     | 0.050 | -0.0451             | 0.0618       | -0.0451 | 0.0616  |
| beta9     | 0.050 | -0.0933             | 0.3272       | -0.0763 | 0.3406  |

An alternative to using the LAG function is to use the PROC option `JOINTMODEL`. With this option, the log-likelihood function you specify applies not to a single observation but to the entire data set. See “Modeling Joint Likelihood” on page 4504 for details on how to properly use this option. The basic idea is that you store all necessary data set variables in arrays and use only the arrays to construct the log likelihood of the entire data set. This approach works here because for every observation  $i$ , you can use index to access different values of arrays to construct the risk set  $S$ . To use the `JOINTMODEL` option, you need to do some additional data manipulation. You want to create a stop variable for each observation, which indicates the observation number that should be included in  $S$  for that observation. For example, if observations 4, 5, 6 all have the same survival time, the stop value for all of them is 6.

The following statements generate a new data set MyelomaM that contains the stop variable:

```
data myelomaM;
 merge myelomaM freqs(drop=percent);
 by descending time;
 retain stop;
 if first.time then do;
 stop = _n_ + count - 1;
 end;
run;
```

The following SAS program fits the same Cox model by using the `JOINTMODEL` option:

```
data a;
run;

proc mcmc data=a outpost=outa nmc=50000 ntu=3000 seed=1 jointmodel;
 ods select none;
 array beta[9];
 array data[1] / nosymbols;
 array timeA[1] / nosymbols;
 array vstatusA[1] / nosymbols;
 array stopA[1] / nosymbols;
 array bZ[&n];
 array S[&n];

 beginncnst;
```

```

rc = read_array("myelomam", data, "logbun", "hgb", "platelet",
 "age", "logwbc", "frac", "logpbm", "protein", "scalc");
rc = read_array("myelomam", timeA, "time");
rc = read_array("myelomam", vstatusA, "vstatus");
rc = read_array("myelomam", stopA, "stop");
endcnst;

parms (beta:) 0;
prior beta: ~ normal(0, var=1e6);

jl = 0;
/* calculate each bZ and cumulatively adding S as if there are no ties.*/
call mult(data, beta, bZ);
S[1] = exp(bZ[1]);
do i = 2 to &n;
 S[i] = S[i-1] + exp(bZ[i]);
end;

do i = 1 to &n;
 /* correct the S[i] term, when needed. */
 if(stopA[i] > i) then do;
 do j = (i+1) to stopA[i];
 S[i] = S[i] + exp(bZ[j]);
 end;
 end;
 jl = jl + vstatusA[i] * (bZ[i] - log(S[i]));
end;
model general(jl);
run;
ods select all;

```

No output tables were produced because this PROC MCMC run produces identical posterior samples as does the previous example.

Because the `JOINTMODEL` option is specified here, you do not need to specify `myelomaM` as the input data set. An empty data set `a` is used to speed up the procedure run.

Multiple `ARRAY` statements allocate array symbols that are used to store the parameters (`beta`), the response and the covariates (`data`, `timeA`, `vstatusA`, and `stopA`), and the work space (`bZ` and `S`). The `data`, `timeA`, `vstatusA`, and `stopA` arrays are declared with the `/NOSYMBOLS` option. This option enables PROC MCMC to dynamically resize these arrays to match the dimensions of the input data set. See the section “[READ\\_ARRAY Function](#)” on page 4442. The `bZ` and `S` arrays store the regression term and the risk set term for every observation.

The `BEGINCNST` and `ENDCNST` statements enclose programming statements that read the data set variables into these arrays. The rest of the programming statements construct the log likelihood for the entire data set.

The `CALL MULT` function calculates the regression term in the model and stores the result in the array `bZ`. In the first `DO` loop, you sum the risk set term `S` as if there are no ties in time. This underevaluates some of the `S` elements. For observations that have a tied time, you make the necessary correction to the corresponding `S` values. The correction takes place in the second `DO` loop. Any observation that has a tied time also has a `stopA[i]` that is different from `i`. You add the right terms to `S` and sum up the joint log likelihood `jl`. The `MODEL` statement specifies that the log likelihood takes on the value of `jl`.

To see that you get identical results from these two approaches, use PROC COMPARE to compare the posterior samples from two runs:

```
proc compare data=outi compare=outa;
 ods select comparesummary;
 var beta1-beta9;
run;
```

The output is not shown here.

Generally, the **JOINTMODEL** option can be slightly faster than using the default setup. The savings come from avoiding the overhead cost of accessing the data set repeatedly at every iteration. However, the speed gain is not guaranteed because it largely depends on the efficiency of your programs.

PROC PHREG fits the same model, and you get very similar results to PROC MCMC. The following statements fit the model using PROC PHREG and produce [Output 55.14.2](#):

```
proc phreg data=Myeloma;
 ods select PostSummaries PostIntervals;
 model Time*VStatus(0)=LogBUN HGB Platelet Age LogWBC
 Frac LogPBM Protein SCalc;
 bayes seed=1 nmc=10000 outpost=phout;
run;
```

**Output 55.14.2** Summary Statistics for Cox Model with Time Independent Explanatory Variables and Ties in the Survival Time, Using PROC PHREG

| Cox Model with Time Independent Covariates |       |         |                       |             |         |          |
|--------------------------------------------|-------|---------|-----------------------|-------------|---------|----------|
| The PHREG Procedure                        |       |         |                       |             |         |          |
| Bayesian Analysis                          |       |         |                       |             |         |          |
| Posterior Summaries                        |       |         |                       |             |         |          |
| Parameter                                  | N     | Mean    | Standard<br>Deviation | Percentiles |         |          |
|                                            |       |         |                       | 25%         | 50%     | 75%      |
| LogBUN                                     | 10000 | 1.7610  | 0.6593                | 1.3173      | 1.7686  | 2.2109   |
| HGB                                        | 10000 | -0.1279 | 0.0727                | -0.1767     | -0.1287 | -0.0789  |
| Platelet                                   | 10000 | -0.2179 | 0.5169                | -0.5659     | -0.2360 | 0.1272   |
| Age                                        | 10000 | -0.0130 | 0.0199                | -0.0264     | -0.0131 | 0.000492 |
| LogWBC                                     | 10000 | 0.3150  | 0.7451                | -0.1718     | 0.3321  | 0.8253   |
| Frac                                       | 10000 | 0.3766  | 0.4152                | 0.0881      | 0.3615  | 0.6471   |
| LogPBM                                     | 10000 | 0.3792  | 0.4909                | 0.0405      | 0.3766  | 0.7023   |
| Protein                                    | 10000 | 0.0102  | 0.0267                | -0.00745    | 0.0106  | 0.0283   |
| SCalc                                      | 10000 | 0.1248  | 0.1062                | 0.0545      | 0.1273  | 0.1985   |

## Output 55.14.2 continued

| Parameter | Alpha | Posterior Intervals |        |              |         |
|-----------|-------|---------------------|--------|--------------|---------|
|           |       | Equal-Tail Interval |        | HPD Interval |         |
| LogBUN    | 0.050 | 0.4418              | 3.0477 | 0.4107       | 2.9958  |
| HGB       | 0.050 | -0.2718             | 0.0150 | -0.2801      | 0.00599 |
| Platelet  | 0.050 | -1.1952             | 0.8296 | -1.1871      | 0.8341  |
| Age       | 0.050 | -0.0514             | 0.0259 | -0.0519      | 0.0251  |
| LogWBC    | 0.050 | -1.2058             | 1.7228 | -1.1783      | 1.7483  |
| Frac      | 0.050 | -0.3995             | 1.2316 | -0.4273      | 1.2021  |
| LogPBM    | 0.050 | -0.5652             | 1.3671 | -0.5939      | 1.3241  |
| Protein   | 0.050 | -0.0437             | 0.0611 | -0.0405      | 0.0637  |
| SCalc     | 0.050 | -0.0935             | 0.3264 | -0.0846      | 0.3322  |

---

**Example 55.15: Time Dependent Cox Model**

This example uses the same Myeloma data set as in “[Example 55.14: Time Independent Cox Model](#)” on page 4617, and illustrates the fitting of a time dependent Cox model. The following statements generate the data set once again:

```
data Myeloma;
 input Time Vstatus LogBUN HGB Platelet Age LogWBC Frac
 LogPBM Protein SCalc;
 label Time='survival time'
 VStatus='0=alive 1=dead';
 datalines;
 1.25 1 2.2175 9.4 1 67 3.6628 1 1.9542 12 10
 1.25 1 1.9395 12.0 1 38 3.9868 1 1.9542 20 18
 2.00 1 1.5185 9.8 1 81 3.8751 1 2.0000 2 15
 2.00 1 1.7482 11.3 0 75 3.8062 1 1.2553 0 12

 ... more lines ...

 77.00 0 1.0792 14.0 1 60 3.6812 0 0.9542 0 12
;
```

To model  $\mathbf{Z}_i(t_i)$  as a function of the survival time, you can relate time  $t_i$  to covariates by using this formula:

$$\boldsymbol{\beta}'\mathbf{Z}_j(t_i) = (\beta_1 + \beta_2 t_i)\text{logbun} + (\beta_3 + \beta_4 t_i)\text{hgb} + (\beta_5 + \beta_6 t_i)\text{platelet}$$

For illustrational purposes, only three explanatory variables, LOGBUN, HGB, and PLATELET, are used in this example.

Since  $\mathbf{Z}_j(t_i)$  depends on  $t_i$ , every term in the summation of  $\sum_{l \in \mathcal{R}_i} \exp(\boldsymbol{\beta}'\mathbf{Z}_l(t_i))$  is a product of the current time  $t_i$  and all observations that are in the risk set. You can use the **JOINTMODEL** option, as in the last example, or you can modify the input data set such that every row contains not only the current observation but also all observations that are in the corresponding risk set. When you construct the log likelihood for each observation, you have all the relevant data at your disposal.

The following statements illustrate how you can create a new data set with different risk sets at different rows:

```

title 'Cox Model with Time Dependent Covariates';
proc sort data = Myeloma;
 by descending time;
run;

data _null_;
 set Myeloma nobs=_n;
 call symputx('N', _n);
 stop;
run;

ods select none;
proc freq data=myeloma;
 tables time / out=freqs;
run;
ods select all;

proc sort data = freqs;
 by descending time;
run;

data myelomaM;
 set myeloma;
 ind = _N_;
run;

data myelomaM;
 merge myelomaM freqs(drop=percent); by descending time;
 retain stop;
 if first.time then do;
 stop = _n_ + count - 1;
 end;
run;

%macro array(list);
 %global mcmccarray;
 %let mcmccarray = ;
 %do i = 1 %to 32000;
 %let v = %scan(&list, &i, %str());
 %if %nrbquote(&v) ne %then %do;
 array _&v[&n];
 %let mcmccarray = &mcmccarray array _&v[&n] _&v.1 - _&v.&n%str(;;);
 do i = 1 to stop;
 set myelomaM(keep=&v) point=i;
 _&v[i] = &v;
 end;
 %end;
 %else %let i = 32001;
 %end;
%mend;

```

```

data z;
 set myelomaM;
 %array(logbun hgb platelet);
 drop vstatus logbun hgb platelet count stop;
run;

data myelomaM;
 merge myelomaM z; by descending time;
run;

```

The data set MyelomaM contains 65 observations and 209 variables. For each observation, you see added variables stop, \_logbun1 through \_logbun65, \_hgb1 through \_hgb65, and \_platelet1 through \_platelet65. The variable stop indicates the number of observations that are in the risk set of the current observation. The rest are transposed values of model covariates of the entire data set. The data set contains a number of missing values. This is due to the fact that only the relevant observations are kept, such as \_logbun1 to \_logbunstop. The rest of the cells are filled in with missing values. For example, the first observation has a unique survival time of 92 and stop is 1, making it a risk set of itself. You see nonmissing values only in \_logbun1, \_hgb1, and \_platelet1.

The following statements fit the Cox model by using PROC MCMC:

```

proc mcmc data=myelomaM outpost=outi nmc=50000 ntu=3000 seed=17
 missing=ac;
 ods select PostSummaries PostIntervals;
 array beta[6];
 &mcmcarray
 parms (beta:) 0;
 prior beta: ~ normal(0, prec=1e-6);

 b = (beta1 + beta2 * time) * logbun +
 (beta3 + beta4 * time) * hgb +
 (beta5 + beta6 * time) * platelet;
 S = 0;
 do i = 1 to stop;
 S = S + exp((beta1 + beta2 * time) * _logbun[i] +
 (beta3 + beta4 * time) * _hgb[i] +
 (beta5 + beta6 * time) * _platelet[i]);
 end;
 loglike = vstatus * (b - log(S));

 model general(loglike);
run;

```

Note that the option `MISSING=` is set to `AC`. This is due to missing cells in the input data set. You must use this option so that PROC MCMC retains observations that contain missing values.

The macro variable `&mcmcarray` is defined in the earlier part in this example. You can use a `%put` statement to print its value:

```
%put &mcmcarray;
```

This statement prints the following:

```
array _logbun[65] _logbun1 - _logbun65; array _hgb[65] _hgb1 - _hgb65; array
```

```
_platelet[65] _platelet1 - _platelet65;
```

The macro uses the `ARRAY` statement to allocate three arrays, each of which links their corresponding data set variables. This makes it easier to reference these data set variables in the program. The `PARMS` statement puts all the parameters in the same block. The `PRIOR` statement gives them normal priors with large variance. The symbol `b` is the regression term, and `S` is cumulatively added from 1 to stop for each observation in the `DO` loop. The symbol `loglike` completes the construction of log likelihood for each observation and the `MODEL` statement completes the model specification.

Posterior summary and interval statistics are shown in [Output 55.15.1](#).

**Output 55.15.1** Summary Statistics on Cox Model with Time Dependent Explanatory Variables and Ties in the Survival Time, Using PROC MCMC

| Cox Model with Time Dependent Covariates |       |          |                    |             |          |          |
|------------------------------------------|-------|----------|--------------------|-------------|----------|----------|
| The MCMC Procedure                       |       |          |                    |             |          |          |
| Posterior Summaries                      |       |          |                    |             |          |          |
| Parameter                                | N     | Mean     | Standard Deviation | Percentiles |          |          |
|                                          |       |          |                    | 25%         | 50%      | 75%      |
| beta1                                    | 50000 | 3.2397   | 0.8226             | 2.6835      | 3.2413   | 3.7830   |
| beta2                                    | 50000 | -0.1411  | 0.0471             | -0.1722     | -0.1406  | -0.1092  |
| beta3                                    | 50000 | -0.0369  | 0.1017             | -0.1064     | -0.0373  | 0.0315   |
| beta4                                    | 50000 | -0.00409 | 0.00360            | -0.00656    | -0.00408 | -0.00167 |
| beta5                                    | 50000 | 0.3548   | 0.7359             | -0.1634     | 0.3530   | 0.8445   |
| beta6                                    | 50000 | -0.0417  | 0.0359             | -0.0661     | -0.0423  | -0.0181  |

| Posterior Intervals |       |                     |         |              |         |
|---------------------|-------|---------------------|---------|--------------|---------|
| Parameter           | Alpha | Equal-Tail Interval |         | HPD Interval |         |
| beta1               | 0.050 | 1.6399              | 4.8667  | 1.6664       | 4.8752  |
| beta2               | 0.050 | -0.2351             | -0.0509 | -0.2294      | -0.0458 |
| beta3               | 0.050 | -0.2337             | 0.1642  | -0.2272      | 0.1685  |
| beta4               | 0.050 | -0.0111             | 0.00282 | -0.0112      | 0.00264 |
| beta5               | 0.050 | -1.0317             | 1.8202  | -1.0394      | 1.8100  |
| beta6               | 0.050 | -0.1107             | 0.0295  | -0.1122      | 0.0269  |

You can also use the option `JOINTMODEL` to get the same inference and avoid transposing the data for every observation:

```
proc mcmc data=myelomaM outpost=outa nmc=50000 ntu=3000 seed=17 jointmodel;
ods select none;
array beta[6]; array timeA[&n]; array vstatusA[&n];
array logbunA[&n]; array hgbA[&n]; array plateletA[&n];
array stopA[&n]; array bZ[&n]; array S[&n];

beginncst;
timeA[ind]=time; vstatusA[ind]=vstatus;
```

```

 logbunA[ind]=logbun; hgbA[ind]=hgb;
 plateletA[ind]=platelet; stopA[ind]=stop;
endcnst;

parms (beta:) 0;
prior beta: ~ normal(0, prec=1e-6);

j1 = 0;
do i = 1 to &n;
 v1 = beta1 + beta2 * timeA[i];
 v2 = beta3 + beta4 * timeA[i];
 v3 = beta5 + beta6 * timeA[i];
 bZ[i] = v1 * logbunA[i] + v2 * hgbA[i] + v3 * plateletA[i];

 /* sum over risk set without considering ties in time. */
 S[i] = exp(bZ[i]);
 if (i > 1) then do;
 do j = 1 to (i-1);
 b1 = v1 * logbunA[j] + v2 * hgbA[j] + v3 * plateletA[j];
 S[i] = S[i] + exp(b1);
 end;
 end;
end;

/* make correction to the risk set due to ties in time. */
do i = 1 to &n;
 if(stopA[i] > i) then do;
 v1 = beta1 + beta2 * timeA[i];
 v2 = beta3 + beta4 * timeA[i];
 v3 = beta5 + beta6 * timeA[i];
 do j = (i+1) to stopA[i];
 b1 = v1 * logbunA[j] + v2 * hgbA[j] + v3 * plateletA[j];
 S[i] = S[i] + exp(b1);
 end;
 end;
 j1 = j1 + vstatusA[i] * (bZ[i] - log(S[i]));
end;
model general(j1);
run;

```

The multiple **ARRAY** statements allocate array symbols that are used to store the parameters (beta), the response (timeA), the covariates (vstatusA, logbunA, hgbA, plateletA, and stopA), and work space (bZ and S). The bZ and S arrays store the regression term and the risk set term for every observation. Programming statements in the **BEGINCNST** and **ENDCNST** statements input the response and covariates from the data set to the arrays.

Using the same technique shown in the example “[Example 55.14: Time Independent Cox Model](#)” on page 4617, the next **DO** loop calculates the regression term and corresponding S for every observation, pretending that there are no ties in time. This means that the risk set for observation *i* involves only observation 1 to *i*. The correction terms are added to the corresponding S[i] in the second **DO** loop, conditional on whether the stop variable is greater than the observation count itself. The symbol j1 cumulatively adds the log likelihood for the entire data set, and the **MODEL** statement specifies the joint log-likelihood function.



The following statements run PROC COMPARE and show that the output data set outa contains identical posterior samples as outi:

```
proc compare data=outi compare=outa;
 ods select comparesummary;
 var beta1-beta6;
run;
```

The results are not shown here.

The following statements use PROC PHREG to fit the same time dependent Cox model:

```
proc phreg data=Myeloma;
 ods select PostSummaries PostIntervals;
 model Time*VStatus(0)=LogBUN z2 hgb z3 platelet z4;
 z2 = Time*logbun;
 z3 = Time*hgb;
 z4 = Time*platelet;
 bayes seed=1 nmc=10000 outpost=phout;
run;
```

Coding is simpler than PROC MCMC. See [Output 55.15.2](#) for posterior summary and interval statistics:

**Output 55.15.2** Summary Statistics on Cox Model with Time Dependent Explanatory Variables and Ties in the Survival Time, Using PROC PHREG

| Cox Model with Time Dependent Covariates |       |                     |                       |              |          |          |
|------------------------------------------|-------|---------------------|-----------------------|--------------|----------|----------|
| The PHREG Procedure                      |       |                     |                       |              |          |          |
| Bayesian Analysis                        |       |                     |                       |              |          |          |
| Posterior Summaries                      |       |                     |                       |              |          |          |
| Parameter                                | N     | Mean                | Standard<br>Deviation | Percentiles  |          |          |
|                                          |       |                     |                       | 25%          | 50%      | 75%      |
| LogBUN                                   | 10000 | 3.2423              | 0.8311                | 2.6838       | 3.2445   | 3.7929   |
| z2                                       | 10000 | -0.1401             | 0.0482                | -0.1723      | -0.1391  | -0.1069  |
| HGB                                      | 10000 | -0.0382             | 0.1009                | -0.1067      | -0.0385  | 0.0297   |
| z3                                       | 10000 | -0.00407            | 0.00363               | -0.00652     | -0.00404 | -0.00162 |
| Platelet                                 | 10000 | 0.3778              | 0.7524                | -0.1500      | 0.3389   | 0.8701   |
| z4                                       | 10000 | -0.0419             | 0.0364                | -0.0660      | -0.0425  | -0.0178  |
| Posterior Intervals                      |       |                     |                       |              |          |          |
| Parameter                                | Alpha | Equal-Tail Interval |                       | HPD Interval |          |          |
| LogBUN                                   | 0.050 | 1.6059              | 4.8785                | 1.5925       | 4.8582   |          |
| z2                                       | 0.050 | -0.2361             | -0.0494               | -0.2354      | -0.0492  |          |
| HGB                                      | 0.050 | -0.2343             | 0.1598                | -0.2331      | 0.1603   |          |
| z3                                       | 0.050 | -0.0113             | 0.00297               | -0.0109      | 0.00322  |          |
| Platelet                                 | 0.050 | -0.9966             | 1.9464                | -1.1342      | 1.7968   |          |
| z4                                       | 0.050 | -0.1124             | 0.0296                | -0.1142      | 0.0274   |          |

## Example 55.16: Piecewise Exponential Frailty Model

This example illustrates how to fit a piecewise exponential frailty model using PROC MCMC. Part of the notation and presentation in this example follows Clayton (1991) and the Luek example in Spiegelhalter et al. (1996a).

Generally speaking, the proportional hazards model assumes the hazard function,

$$\lambda_i(t|\mathbf{z}_i) = \lambda_0(t) \exp\{\boldsymbol{\beta}'\mathbf{z}_i\}$$

where  $i = 1 \cdots n$  indexes subject,  $\lambda_0(t)$  is the baseline hazard function, and  $\mathbf{z}_i$  are the covariates for subject  $i$ . If you define  $N_i(t)$  to be the number of observed failures of the  $i$ th subject up to time  $t$ , then the hazard function for the  $i$ th subject can be seen as a special case of a *multiplicative intensity model* (Clayton 1991). The intensity process for  $N_i(t)$  becomes

$$I_i(t) = Y_i(t)\lambda_0(t) \exp(\boldsymbol{\beta}'\mathbf{z}_i)$$

where  $Y_i(t)$  indicates observation of the subject at time  $t$  (taking the value of 1 if the subject is observed and 0 otherwise). Under *noninformative censoring*, the corresponding likelihood is proportional to

$$\prod_{i=1}^n \left[ \prod_{t \geq 0} I_i(t) \right]^{dN_i(t)} \exp \left[ - \int_{t \geq 0} I_i(t) dt \right]$$

where  $dN_i(t)$  is the increment of  $N_i(t)$  over the small time interval  $[t, t + dt)$ : it takes a value of 1 if the subject  $i$  fails in the time interval, 0 otherwise. This is a Poisson kernel with the random variable being the increments of  $dN_i$  and the means  $I_i(t)dt$

$$dN_i(t) \sim \text{Poisson}(I_i(t)dt)$$

where

$$I_i(t)dt = Y_i(t) \exp(\boldsymbol{\beta}'\mathbf{z}_i) d\Lambda_0(t)$$

and

$$\Lambda_0(t) = \int_0^t \lambda_0(u) du.$$

The integral is the increment in the integrated baseline hazard function that occurs during the time interval  $[t, t + dt)$ .

This formulation provides an alternative way to fit a piecewise exponential model. You partition the time axis to a few intervals, where each interval has its own hazard rate,  $\Lambda_0(t)$ . You count the  $Y_i(t)$  and  $dN_i(t)$  in each interval, and fit a Poisson model to each count.

The following DATA step creates the data set Blind (Lin 1994) that represents 197 diabetic patients who have a high risk of experiencing blindness in both eyes as defined by DRS criteria:

```

title 'Piecewise Exponential Model';
data Blind;
 input ID Time Status DiabeticType Treatment @@;
 datalines;
 5 46.23 0 1 1 5 46.23 0 1 0 14 42.50 0 0 1 14 31.30 1 0 0
 16 42.27 0 0 1 16 42.27 0 0 0 25 20.60 0 0 1 25 20.60 0 0 0
 29 38.77 0 0 1 29 0.30 1 0 0 46 65.23 0 0 1 46 54.27 1 0 0
 49 63.50 0 0 1 49 10.80 1 0 0 56 23.17 0 0 1 56 23.17 0 0 0

 ... more lines ...

1705 8.00 0 0 1 1705 8.00 0 0 0 1717 51.60 0 1 1 1717 42.33 1 1 0
1727 49.97 0 1 1 1727 2.90 1 1 0 1746 45.90 0 0 1 1746 1.43 1 0 0
1749 41.93 0 1 1 1749 41.93 0 1 0
;

```

One eye of each patient is treated with laser photocoagulation. The hypothesis of interest is whether the laser treatment delays the occurrence of blindness. The following variables are included in `Blind`:

- ID, patient's identification
- Time, failure time
- Status, event indicator (0=censored and 1=uncensored)
- Treatment, treatment received (1=laser photocoagulation and 0=otherwise)
- DiabeticType, type of diabetes (0=juvenile onset with age of onset at 20 or under, and 1= adult onset with age of onset over 20)

For illustrational purposes, a piecewise exponential model that ignores the patient-level frailties is first fit to the entire data set. The formulation of the Poisson counting process makes it straightforward to add the frailty terms, as it is demonstrated later.

The following statements create a partition (of length 8) along the time axis, with  $s_0 < s_1 < s_2 < \dots < s_J$ , with  $s_0 = 0.1 < y_i$  and  $s_J = 80 > y_i$  for all  $i$ . The time intervals are stored in the `Partition` data set:

```

data partition;
 input int_1-int_9;
 datalines;
 0.1 6.545 13.95 26.47 38.8 45.88 54.35 62 80
;

```

To obtain reasonable estimates, placing an equal number of observations in each interval is recommended. You can find the partition points by calculating the percentile statistics of the time variable (for example, by using the `UNIVARIATE` procedure).

The following regression model and prior distributions are used in the analysis:

$$\begin{aligned}\beta'z_i &= \beta_1\text{treatment} + \beta_2\text{diabetictype} + \beta_3\text{treatment} * \text{diabetictype} \\ \beta_1, \beta_2, \beta_3 &\sim \text{normal}(0, \text{var} = 1e6) \\ \lambda_j &\sim \text{gamma}(\text{shape} = 0.01, \text{iscale} = 0.01) \quad \text{for } j = 1 \cdots 8\end{aligned}$$

The following statements calculate  $Y_i(t)$  for each observation  $i$ , at every time point  $t$  in the Partition data set. The statements also find the observed failure time interval,  $dN_i(t)$ , for each observation:

```
%let n = 8;
data _a;
 set blind;
 if _n_ eq 1 then set partition;
 array int[*] int_;
 array Y[&n];
 array dN[&n];
 do k = 1 to (dim(int)-1);
 Y[k] = (time - int[k] + 0.001 >= 0);
 dN[k] = Y[k] * (int[k+1] - time - 0.001 >= 0) * status;
 end;
 output;
 drop int_ : k;
run;
```

The DATA step reads in the Blind data set. At the first observation, it also reads in the Partition data set. The first ARRAY statement creates the int array and name the elements int\_. Because the names match the variable names in the Partition data set, all values of the int\_ variables (there is only one observation) in the Partition data set are therefore stored in the int array. The next two ARRAY statements create arrays Y and dN, each with length 8. They store values of  $Y_i(t)$  and  $dN_i(t)$ , resulting from each failure time in the Blind data set.

The following statements print the first 10 observations of the constructed data set \_a and display them in [Output 55.16.1](#):

```
proc print data=_a(obs=10);
run;
```

**Output 55.16.1** First 10 Observations of the Data Set \_a

| Piecewise Exponential Model |        |                                                                                             |             |             |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
|-----------------------------|--------|---------------------------------------------------------------------------------------------|-------------|-------------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
|                             |        | D<br>i<br>a<br>b T<br>e r<br>t e<br>S i a<br>t c t<br>T a T m<br>i t y e<br>d d d d d d d d |             |             |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| O<br>b<br>s                 | I<br>D | m<br>e                                                                                      | u<br>p<br>s | n<br>e<br>t | Y<br>1 | Y<br>2 | Y<br>3 | Y<br>4 | Y<br>5 | Y<br>6 | Y<br>7 | Y<br>8 | N<br>1 | N<br>2 | N<br>3 | N<br>4 | N<br>5 | N<br>6 | N<br>7 | N<br>8 |
| 1                           | 5      | 46.23                                                                                       | 0           | 1           | 1      | 1      | 1      | 1      | 1      | 1      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      |
| 2                           | 5      | 46.23                                                                                       | 0           | 1           | 0      | 1      | 1      | 1      | 1      | 1      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      |
| 3                           | 14     | 42.50                                                                                       | 0           | 0           | 1      | 1      | 1      | 1      | 1      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      |
| 4                           | 14     | 31.30                                                                                       | 1           | 0           | 0      | 1      | 1      | 1      | 1      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 1      | 0      | 0      | 0      |
| 5                           | 16     | 42.27                                                                                       | 0           | 0           | 1      | 1      | 1      | 1      | 1      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      |
| 6                           | 16     | 42.27                                                                                       | 0           | 0           | 0      | 1      | 1      | 1      | 1      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      |
| 7                           | 25     | 20.60                                                                                       | 0           | 0           | 1      | 1      | 1      | 1      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      |
| 8                           | 25     | 20.60                                                                                       | 0           | 0           | 0      | 1      | 1      | 1      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      |
| 9                           | 29     | 38.77                                                                                       | 0           | 0           | 1      | 1      | 1      | 1      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      | 0      |
| 10                          | 29     | 0.30                                                                                        | 1           | 0           | 0      | 1      | 0      | 0      | 0      | 0      | 0      | 0      | 1      | 0      | 0      | 0      | 0      | 0      | 0      | 0      |

The first subject in `_a` experienced blindness in the left eye at time 46.23, and the time falls in the sixth interval as defined in the Partition data set. Therefore, Y1 through Y6 all take a value of 1, and Y7 and Y8 are 0. The variable `dn#` takes on a value of 1 if the subject is observed to go blind in that interval. Since the first observation is censored (`status == 1`), the actual failure time is unknown. Hence all `dn#` are 0. The first observed failure time occurs in observation number 4 (the right eye of the second subject), where the time variable takes a value of 31.30, Y1 through Y4 are 1, and `dn4` is 1.

Note that each observation in the `_a` data set has 8 Y and 8 `dn`, meaning that you would need eight `MODEL` statements in a PROC MCMC call, each for a Poisson likelihood. Alternatively, you can expand `_a`, put one Y and one `dn` in every observation, and fit the data using a single `MODEL` statement in PROC MCMC. The following statements expand the data set `_a` and save the results in the data set `_b`:

```
data _b;
 set _a;
 array y[*] y;;
 array dn[*] dn;;
 do i = 1 to (dim(y));
 y_val = y[i];
 dn_val = dn[i];
 int_index = i;
 output;
 end;
 keep y_ : dn_ : diabetictype treatment int_index id;
run;
```

```

data _b;
 set _b;
 rename y_val=Y dn_val=dN;
run;

```

You can use the following PROC PRINT statements to see the first few observations in `_b`:

```

proc print data=_b(obs=10);
run;

```

**Output 55.16.2** First 20 Observations of the Data Set `_b`

| Obs | ID | Diabetic<br>Type | Treatment | Y | dN | int_<br>index |
|-----|----|------------------|-----------|---|----|---------------|
| 1   | 5  | 1                | 1         | 1 | 0  | 1             |
| 2   | 5  | 1                | 1         | 1 | 0  | 2             |
| 3   | 5  | 1                | 1         | 1 | 0  | 3             |
| 4   | 5  | 1                | 1         | 1 | 0  | 4             |
| 5   | 5  | 1                | 1         | 1 | 0  | 5             |
| 6   | 5  | 1                | 1         | 1 | 0  | 6             |
| 7   | 5  | 1                | 1         | 0 | 0  | 7             |
| 8   | 5  | 1                | 1         | 0 | 0  | 8             |
| 9   | 5  | 1                | 0         | 1 | 0  | 1             |
| 10  | 5  | 1                | 0         | 1 | 0  | 2             |

The data set `_b` now contains 3,152 observations (see [Output 55.16.2](#) for the first few observations). The Time and Status variables are no longer needed; hence they are discarded from the data set. The `int_index` variable is an index variable that indicates interval membership of each observation.

Because the variable `Y` does not contribute to the likelihood calculation when it takes a value of 0 (it amounts to a Poisson likelihood that has a mean and response variable that are both 0), you can remove these observations. This speeds up the calculation in PROC MCMC:

```

data inputdata;
 set _b;
 if Y > 0;
run;

```

The data set `inputdata` has 1,775 observations, as opposed to 3,152 observations in `_b`. The following statements fit a piecewise exponential model in PROC MCMC:

```

proc mcmc data=inputdata nmc=10000 outpost=postout seed=12351
 maxtune=5 stats=summary diag=none;
ods select PostSummaries;
parms beta1-beta3 0;
prior beta: ~ normal(0, var = 1e6);
random lambda ~ gamma(0.01, iscale = 0.01) subject=int_index;
bZ = beta1*treatment + beta2*diabetictype + beta3*treatment*diabetictype;
idt = exp(bZ) * lambda;
model dN ~ poisson(idt);
run;

```

The **PARMS** statement declares three regression parameters, beta1–beta3. The **PRIOR** statement specifies a noninformative normal prior on the regression coefficients. The **RANDOM** statement specifies the random effect, lambda, its prior distribution, and interval membership which is indexed by the data set variable int\_index.

The symbol bZ calculates the regression mean, and the symbol idt is the mean of the Poisson likelihood. It corresponds to the equation

$$I_i(t)dt = Y_i(t) \exp(\beta'z) d\Lambda_0(t)$$

Note that the  $Y_i(t)$  term is omitted in the assignment statement because Y takes only the value of 1 in the input data set.

Output 55.16.3 displays posterior estimates of the three regression parameters.

**Output 55.16.3** Posterior Summary Statistics

| The MCMC Procedure  |       |         |                       |             |         |         |
|---------------------|-------|---------|-----------------------|-------------|---------|---------|
| Posterior Summaries |       |         |                       |             |         |         |
| Parameter           | N     | Mean    | Standard<br>Deviation | Percentiles |         |         |
|                     |       |         |                       | 25%         | 50%     | 75%     |
| beta1               | 10000 | -0.4174 | 0.2129                | -0.5612     | -0.4282 | -0.2770 |
| beta2               | 10000 | 0.3138  | 0.1956                | 0.1881      | 0.3121  | 0.4387  |
| beta3               | 10000 | -0.7899 | 0.3308                | -0.9999     | -0.7935 | -0.5741 |

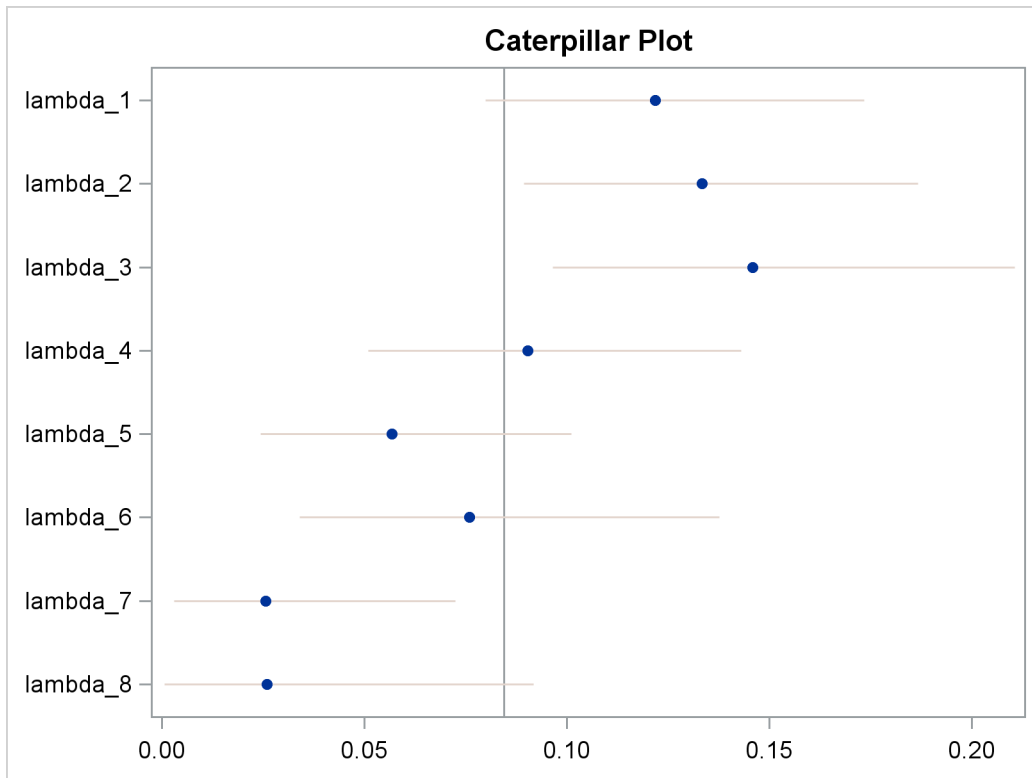
To understand the results, you can create a  $2 \times 2$  table (Table 55.49) and plug in the posterior mean estimates to the regression model. A  $-0.41$  estimate for subjects who received laser treatment and had juvenile diabetes suggests that the laser treatment is effective in delaying blindness. And the effect is much more pronounced ( $-0.80$ ) for adult subjects who have diabetes and received treatment.

**Table 55.49** Estimates of Regression Effects in the Survival Model

| $\hat{\beta}'z$ |   | Diabetic Type |       |
|-----------------|---|---------------|-------|
|                 |   | 0             | 1     |
| Treatment       | 0 | 0             | 0.32  |
|                 | 1 | -0.41         | -0.80 |

You can also use the macro %CATER (“Caterpillar Plot” on page 4508) to draw a caterpillar plot to visualize the eight hazards in the model:

```
ods graphics on;
%cater(data=postout, var=lambda_);
ods graphics off;
```

**Output 55.16.4** Caterpillar Plot of the Hazards in the Piecewise Exponential Model

The fitted hazards show a nonconstant underlying hazard function (read along the y-axis as lambda\_# are hazards along the time-axis) in the model.

Now suppose you want to include patient-level information and fit a frailty model to the blind data set, where the random effect enters the model through the regression term, where the subject is indexed by the variable ID in the data.

$$\begin{aligned}\beta'z_i &= \beta_1\text{treatment} + \beta_2\text{diabetictype} + \beta_3\text{treatment} * \text{diabetictype} + u_{id} \\ u_{id} &\sim \text{normal}(0, \text{var} = \sigma^2) \\ \sigma^2 &\sim \text{igamma}(\text{shape} = 0.01, \text{scale} = 0.01)\end{aligned}$$

where id indexes patient.

The actual coding in PROC MCMC of a piecewise exponential frailty model is rather straightforward:

```
ods select none;
proc mcmc data=inputdata nmc=10000 outpost=postout seed=12351
 stats=summary diag=none;
 parms beta1-beta3 0 s2;
 prior beta: ~ normal(0, var = 1e6);
 prior s2 ~ igamma(0.01, scale=0.01);
 random lambda ~ gamma(0.01, iscale = 0.01) subject=int_index;
 random u ~ normal(0, var=s2) subject=id;
 bZ = beta1*treatment + beta2*diabetictype + beta3*treatment*diabetictype + u;
 idt = exp(bZ) * lambda;
 model dN ~ poisson(idt);
run;
```



A second **RANDOM** statement defines a subject-level random effect  $u$ , and the random-effects parameters enter the model in the term for the regression mean,  $bZ$ . An additional model parameter,  $s2$ , the variance of the random-effects parameters, is needed for the model. The results are not shown here.

### Example 55.17: Normal Regression with Interval Censoring

You can use PROC MCMC to fit failure time data that can be right, left, or interval censored. To illustrate, a normal regression model is used in this example.

Assume that you have the following simple regression model with no covariates:

$$y = \mu + \sigma\epsilon$$

where  $y$  is a vector of response values (the failure times),  $\mu$  is the grand mean,  $\sigma$  is an unknown scale parameter, and  $\epsilon$  are errors from the standard normal distribution. Instead of observing  $y_i$  directly, you only observe a truncated value  $t_i$ . If the true  $y_i$  occurs after the censored time  $t_i$ , it is called *right censoring*. If  $y_i$  occurs before the censored time, it is called *left censoring*. A failure time  $y_i$  can be censored at both ends, and this is called *interval censoring*. The likelihood for  $y_i$  is as follows:

$$p(y_i|\mu) = \begin{cases} \phi(y_i|\mu, \sigma) & \text{if } y_i \text{ is uncensored} \\ S(t_{l,i}|\mu) & \text{if } y_i \text{ is right censored by } t_{l,i} \\ 1 - S(t_{r,i}|\mu) & \text{if } y_i \text{ is left censored by } t_{r,i} \\ S(t_{l,i}|\mu) - S(t_{r,i}|\mu) & \text{if } y_i \text{ is interval censored by } t_{l,i} \text{ and } t_{r,i} \end{cases}$$

where  $S(\cdot)$  is the survival function,  $S(t) = \Pr(T > t)$ .

Gentleman and Geyer (1994) uses the following data on cosmetic deterioration for early breast cancer patients treated with radiotherapy:

```

title 'Normal Regression with Interval Censoring';
data cosmetic;
 label tl = 'Time to Event (Months)';
 input tl tr @@;
 datalines;
45 . 6 10 . 7 46 . 46 . 7 16 17 . 7 14
37 44 . 8 4 11 15 . 11 15 22 . 46 . 46 .
25 37 46 . 26 40 46 . 27 34 36 44 46 . 36 48
37 . 40 . 17 25 46 . 11 18 38 . 5 12 37 .
. 5 18 . 24 . 36 . 5 11 19 35 17 25 24 .
32 . 33 . 19 26 37 . 34 . 36 .
;

```

The data consist of time interval endpoints (in months). Nonmissing equal endpoints ( $tl = tr$ ) indicates noncensoring; a nonmissing lower endpoint ( $tl \neq .$ ) and a missing upper endpoint ( $tr = .$ ) indicates right censoring; a missing lower endpoint ( $tl = .$ ) and a nonmissing upper endpoint ( $tr \neq .$ ) indicates left censoring; and nonmissing unequal endpoints ( $tl \neq tr$ ) indicates interval censoring.

With this data set, you can consider using proper but diffuse priors on both  $\mu$  and  $\sigma$ , for example:

$$\begin{aligned} \mu &\sim \text{normal}(0, \text{sd} = 1000) \\ \sigma &\sim \text{gamma}(0.001, \text{iscale} = 0.001) \end{aligned}$$

The following SAS statements fit an interval censoring model and generate [Output 55.17.1](#):

```
proc mcmc data=cosmetic outpost=postout seed=1 nmc=20000 missing=AC;
 ods select PostSummaries PostIntervals;
 parms mu 60 sigma 50;

 prior mu ~ normal(0, sd=1000);
 prior sigma ~ gamma(shape=0.001, iscale=0.001);

 if (tl^=. and tr^=. and tl=tr) then
 llike = logpdf('normal', tr, mu, sigma);
 else if (tl^=. and tr=.) then
 llike = logsdf('normal', tl, mu, sigma);
 else if (tl=. and tr^=.) then
 llike = logcdf('normal', tr, mu, sigma);
 else
 llike = log(sdf('normal', tl, mu, sigma) -
 sdf('normal', tr, mu, sigma));

 model general(llike);
run;
```

Because there are missing cells in the input data, you want to use the `MISSING=AC` option so that PROC MCMC does not delete any observations that contain missing values. The IF-ELSE statements distinguish different censoring cases for  $y_i$ , according to the likelihood. The SAS functions LOGCDF, LOGSDF, LOGPDF, and SDF are useful here. The `MODEL` statement assigns `llike` as the log likelihood to the response. The Markov chain appears to have converged in this example (evidence not shown here), and the posterior estimates are shown in [Output 55.17.1](#).

**Output 55.17.1** Interval Censoring

| Normal Regression with Interval Censoring |       |                     |                       |              |         |         |
|-------------------------------------------|-------|---------------------|-----------------------|--------------|---------|---------|
| The MCMC Procedure                        |       |                     |                       |              |         |         |
| Posterior Summaries                       |       |                     |                       |              |         |         |
| Parameter                                 | N     | Mean                | Standard<br>Deviation | Percentiles  |         |         |
|                                           |       |                     |                       | 25%          | 50%     | 75%     |
| mu                                        | 20000 | 41.7807             | 5.7882                | 37.7220      | 41.3468 | 45.2249 |
| sigma                                     | 20000 | 29.1122             | 6.0503                | 24.8774      | 28.2210 | 32.4250 |
| Posterior Intervals                       |       |                     |                       |              |         |         |
| Parameter                                 | Alpha | Equal-Tail Interval |                       | HPD Interval |         |         |
| mu                                        | 0.050 | 32.0499             | 54.6104               | 31.3604      | 53.6115 |         |
| sigma                                     | 0.050 | 20.0889             | 43.1335               | 19.4041      | 41.6742 |         |

## Example 55.18: Constrained Analysis

Conjoint analysis uses regression techniques to model consumer preferences and to estimate consumer utility functions. A problem with conventional conjoint analysis is that sometimes your estimated utilities do not make sense. Your results might suggest, for example, that the consumers would prefer to spend more on a product than to spend less. With PROC MCMC, you can specify constraints on the part-worth utilities (parameter estimates). Suppose that the consumer product being analyzed is an off-road motorcycle. The relevant attributes are how large each motorcycle is (less than 300cc, 301–550cc, and more than 551cc), how much it costs (less than \$5000, \$5001–\$6000, \$6001–\$7000, and more than \$7000), whether or not it has an electric starter, whether or not the engine is counter-balanced, and whether the bike is from Japan or Europe. The preference variable is a ranking of the bikes. You could perform an ordinary conjoint analysis with PROC TRANSREG (see Chapter 97, “The TRANSREG Procedure”) as follows:

```
options validvarname=any;
proc format;
 value sizef 1 = '< 300cc' 2 = '300–550cc' 3 = '> 551cc';
 value pricef 1 = '< $5000' 2 = '$5000 - $6000'
 3 = '$6001 - $7000' 4 = '> $7000';
 value startf 1 = 'Electric Start' 2 = 'Kick Start';
 value balf 1 = 'Counter Balanced' 2 = 'Unbalanced';
 value orif 1 = 'Japanese' 2 = 'European';
run;

data bikes;
 input Size Price Start Balance Origin Rank @@;
 format size sizef. price pricef. start startf.
 balance balf. origin orif.;
 datalines;
2 1 2 1 2 3 1 4 2 2 2 7 1 2 1 1 2 6
3 3 1 1 2 1 1 3 2 1 1 5 3 4 2 2 2 12
2 3 2 2 1 9 1 1 1 2 1 8 2 2 1 2 2 10
2 4 1 1 1 4 3 1 1 2 1 11 3 2 2 1 1 2
;

title 'Ordinary Conjoint Analysis by PROC TRANSREG';
proc transreg data=bikes utilities cprefix=0 lprefix=0;
 ods select Utilities;
 model identity(rank / reflect) =
 class(size price start balance origin / zero=sum);
 output out=coded(drop=intercept) replace;
run;
```

The DATA step reads the experimental design and dependent variable Rank and assigns formats to label the factor levels. PROC TRANSREG is run specifying UTILITIES, which requests a conjoint analysis. The rank variable is reflected around its mean ( $1 \rightarrow 12$ ,  $2 \rightarrow 11$ , ...,  $12 \rightarrow 1$ ) so that in the analysis, larger part-worth utilities correspond to higher preference. The OUT=CODED data set contains the reflected ranks and a binary coding of the factors that can be used in other analyses. See Kuhfeld (2004) for more information about conjoint analysis and coding with PROC TRANSREG.

The Utilities table from the conjoint analysis is shown in [Output 55.18.1](#). Notice the part-worth utilities for price. The part-worth utility for < \$5000 is 0.25. As price increases to the \$5000–\$6000 range, utility

decreases to  $-0.5$ . Then as price increases to the \$6001–\$7000 range, part-worth utility *increases* to 0.5. Finally, for the most expensive bikes, utility decreases again to  $-0.25$ . In cases like this, you might want to impose constraints on the solution so that the part-worth utility for price never increases as prices go up.

### Output 55.18.1 Ordinary Conjoint Analysis by PROC TRANSREG

| Ordinary Conjoint Analysis by PROC TRANSREG           |         |                |                              |                        |
|-------------------------------------------------------|---------|----------------|------------------------------|------------------------|
| The TRANSREG Procedure                                |         |                |                              |                        |
| Utilities Table Based on the Usual Degrees of Freedom |         |                |                              |                        |
| Label                                                 | Utility | Standard Error | Importance (% Utility Range) | Variable               |
| Intercept                                             | 6.5000  | 0.95743        |                              | Intercept              |
| < 300cc                                               | -0.0000 | 1.35401        | 0.000                        | Class.< 300cc          |
| 300-550cc                                             | -0.0000 | 1.35401        |                              | Class.300-550cc        |
| > 551cc                                               | 0.0000  | 1.35401        |                              | Class.> 551cc          |
| < \$5000                                              | 0.2500  | 1.75891        | 13.333                       | Class.< \$5000         |
| \$5000 - \$6000                                       | -0.5000 | 1.75891        |                              | Class.\$5000 - \$6000  |
| \$6001 - \$7000                                       | 0.5000  | 1.75891        |                              | Class.\$6001 - \$7000  |
| > \$7000                                              | -0.2500 | 1.75891        |                              | Class.> \$7000         |
| Electric Start                                        | -0.1250 | 1.01550        | 3.333                        | Class.Electric Start   |
| Kick Start                                            | 0.1250  | 1.01550        |                              | Class.Kick Start       |
| Counter Balanced                                      | 3.0000  | 1.01550        | 80.000                       | Class.Counter Balanced |
| Unbalanced                                            | -3.0000 | 1.01550        |                              | Class.Unbalanced       |
| Japanese                                              | -0.1250 | 1.01550        | 3.333                        | Class.Japanese         |
| European                                              | 0.1250  | 1.01550        |                              | Class.European         |

You could run PROC TRANSREG again, specifying monotonicity constraints on the part-worth utilities for price:

```

title 'Constrained Conjoint Analysis by PROC TRANSREG';
proc transreg data=bikes utilities cprefix=0 lprefix=0;
ods select ConservUtilities;
model identity(rank / reflect) =
 monotone(price / tstandard=center)
 class(size start balance origin / zero=sum);
run;

```

The output from this PROC TRANSREG step is shown in [Output 55.18.2](#).

**Output 55.18.2** Constrained Conjoint Analysis by PROC TRANSREG

| Constrained Conjoint Analysis by PROC TRANSREG           |         |                |                              |                        |
|----------------------------------------------------------|---------|----------------|------------------------------|------------------------|
| The TRANSREG Procedure                                   |         |                |                              |                        |
| Utilities Table Based on Conservative Degrees of Freedom |         |                |                              |                        |
| Label                                                    | Utility | Standard Error | Importance (% Utility Range) | Variable               |
| Intercept                                                | 6.5000  | 0.97658        |                              | Intercept              |
| Price                                                    | -0.1581 | .              | 7.143                        | Monotone(Price)        |
| < \$5000                                                 | 0.2500  | .              |                              |                        |
| \$5000 - \$6000                                          | 0.0000  | .              |                              |                        |
| \$6001 - \$7000                                          | 0.0000  | .              |                              |                        |
| > \$7000                                                 | -0.2500 | .              |                              |                        |
| < 300cc                                                  | -0.0000 | 1.38109        | 0.000                        | Class.< 300cc          |
| 300-550cc                                                | 0.0000  | 1.38109        |                              | Class.300-550cc        |
| > 551cc                                                  | 0.0000  | 1.38109        |                              | Class.> 551cc          |
| Electric Start                                           | -0.2083 | 1.00663        | 5.952                        | Class.Electric Start   |
| Kick Start                                               | 0.2083  | 1.00663        |                              | Class.Kick Start       |
| Counter Balanced                                         | 3.0000  | 0.97658        | 85.714                       | Class.Counter Balanced |
| Unbalanced                                               | -3.0000 | 0.97658        |                              | Class.Unbalanced       |
| Japanese                                                 | -0.0417 | 1.00663        | 1.190                        | Class.Japanese         |
| European                                                 | 0.0417  | 1.00663        |                              | Class.European         |

This monotonicity constraint is one of the few constraints on the part-worth utilities that you can specify in PROC TRANSREG. In contrast, PROC MCMC enables you to specify any constraint that can be written in the DATA step language. You can perform the restricted conjoint analysis with PROC MCMC by using the coded factors that were output from PROC TRANSREG. The data set is Coded.

The likelihood is a simple regression model:

$$\text{rank}_i \sim \text{normal}(x_i' \beta, \sigma)$$

where rank is the response, the covariates are '< 300cc'n, '300-500cc'n, '< \$5000'n, '\$5000 - \$6000'n, '\$6001 - \$7000'n, 'Electric Start'n, 'Counter Balanced'n, and Japanese. Note that OPTIONS VALIDVAR-NAME=ANY enables PROC TRANSREG to create names for the coded variables with blanks and special characters. That is why the name-literal notation ('*variable-name*'n) is used for the input data set variables.

Suppose that there are two constraints you want to put on some of the parameters: one is that the parameters for '< \$5000'n, '\$5000 - \$6000'n, and '\$6001 - \$7000'n decrease in order, and the other is that the parameter for 'Counter Balanced'n is strictly positive. You can consider a truncated multivariate normal prior as follows:

$$(\beta_{< \$5000'n}, \beta_{\$5000 - \$6000'n}, \beta_{\$6001 - \$7000'n}, \beta_{\text{Counter Balanced'n}}) \sim \text{MVN}(0, \sigma \mathbf{I})$$

with the following set of constraints:

$$\beta_{< \$5000'n} > \beta_{\$5000 - \$6000'n} > \beta_{\$6001 - \$7000'n} > 0$$

$$\beta_{\text{Counter Balanced'n}} > 0$$

The condition that  $\beta_{\$6001 - \$7000'n} > 0$  reflects an implied constraint that, by definition, 0 is the utility for the highest price range,  $> \$7000$ , which is the reference level for the binary coded price variable. The following statements fit the desired model:

```

title 'Bayesian Constrained Conjoint Analysis by PROC MCMC';
proc mcmc data=coded outpost=bikesout ntu=3000 nmc=50000
 propcov=quanew seed=448 diag=none;
 ods select PostSummaries;
 array pw[4] pw5000 pw5000_6000 pw6001_7000 pwCounterBalanced;
 array sigma[4,4];
 array mu[4];

 begincnst;
 call identity(sigma);
 call mult(sigma, 100, sigma);
 call zeromatrix(mu);
 endcnst;

 parms intercept pw300cc pw300_550cc pwElectricStart pwJapanese tau 1;
 parms pw5000 0.3 pw5000_6000 0.2 pw6001_7000 0.1 pwCounterBalanced 1;

 beginnodata;
 prior intercept pw300: pwE: pwJ: ~ normal(0, var=100);
 if (pw5000 >= pw5000_6000 & pw5000_6000 >= pw6001_7000 &
 pw6001_7000 >= 0 & pwCounterBalanced > 0) then
 lp = lpdfmvn(pw, mu, sigma);
 else
 lp = .;
 prior pw5000 pw5000_6000 pw6001_7000 pwC: ~ general(lp);
 prior tau ~ gamma(0.01, iscale=0.01);
 endnodata;

 mean = intercept +
 pw300cc * '< 300cc'n +
 pw300_550cc * '300-550cc'n +
 pw5000 * '< $5000'n +
 pw5000_6000 * '$5000 - $6000'n +
 pw6001_7000 * '$6001 - $7000'n +
 pwElectricStart * 'Electric Start'n +
 pwCounterBalanced * 'Counter Balanced'n +
 pwJapanese * Japanese;
 model rank ~ normal(mean, prec=tau);
run;

```

The two [ARRAY](#) statements allocate a  $4 \times 4$  dimensional array for the prior covariance and an array of size 4 for the prior means. In the [BEGINCNST](#) and [ENDCNST](#) statements, the [CALL IDENTITY](#) function sets sigma to be an identity matrix; the [CALL MULT](#) function sets sigma's diagonal elements to be 100 (the diagonal variance terms); and the [CALL ZEROMATRIX](#) function sets mu to be a vector of zeros (the prior

means). For matrix functions in PROC MCMC, see the section “Matrix Functions in PROC MCMC” on page 4498.

There are two **PARMS** statements, with each of them naming a block of parameters. The first **PARMS** statement blocks the following: the intercept, the two size parameters, the one start-type parameter, the one origin parameter, and the precision. The second **PARMS** statement blocks the three price parameters and the one balance parameter, parameters that have the constraint multivariate normal prior. The second **PARMS** statement also specifies initial values for the parameter estimates. The initial values reflect the constraints on these parameters. The initial part-worth utilities all decrease from 0.3 to 0.2 to 0.1 to 0.0 (for the implicit reference level) as the prices increase. Also, the initial part-worth utility for the counter-balanced engine is set to a positive value, 1.

In the **PRIOR** statements, regression coefficients without constraints are given an independent normal prior with mean at 0 and variance of 100. The next IF-ELSE construction imposes the constraints. When these constraints are met, pw5000, pw5000\_6000, pw6001\_7000, pwCounterBalanced are jointly distributed as a multivariate normal prior with mean  $\mu$  and covariance  $\sigma$ . Otherwise, the prior is not defined and  $\mu$  is assigned a missing value. The parameter tau is given a gamma prior, which is a conjugate prior for that parameter.

The model specification is linear. The mean is comprised of an intercept and the sum of terms like pw300cc \* '< 300cc'n, which is a parameter times an input data set variable. The **MODEL** statement specifies that the linear model for rank is normally distributed with mean  $\mu$  and precision tau.

The MCMC results are shown in [Output 55.18.3](#).

### Output 55.18.3 MCMC Results

| Bayesian Constrained Conjoint Analysis by PROC MCMC |       |         |                       |             |          |        |
|-----------------------------------------------------|-------|---------|-----------------------|-------------|----------|--------|
| The MCMC Procedure                                  |       |         |                       |             |          |        |
| Posterior Summaries                                 |       |         |                       |             |          |        |
| Parameter                                           | N     | Mean    | Standard<br>Deviation | Percentiles |          |        |
|                                                     |       |         |                       | 25%         | 50%      | 75%    |
| intercept                                           | 50000 | 2.2570  | 2.5131                | 0.8315      | 2.3661   | 3.8234 |
| pw300cc                                             | 50000 | 0.00983 | 2.4903                | -1.4461     | -0.00002 | 1.4821 |
| pw300_550cc                                         | 50000 | 0.0549  | 2.5097                | -1.4175     | 0.0106   | 1.4695 |
| pwElectricStart                                     | 50000 | -1.1319 | 2.1195                | -2.3710     | -1.0665  | 0.1562 |
| pwJapanese                                          | 50000 | -0.4567 | 2.1232                | -1.6836     | -0.4134  | 0.7903 |
| tau                                                 | 50000 | 0.1135  | 0.0765                | 0.0578      | 0.0952   | 0.1499 |
| pw5000                                              | 50000 | 4.1614  | 2.1803                | 2.6082      | 3.7947   | 5.2823 |
| pw5000_6000                                         | 50000 | 2.6147  | 1.6188                | 1.4316      | 2.3400   | 3.4779 |
| pw6001_7000                                         | 50000 | 1.5040  | 1.2530                | 0.5432      | 1.1838   | 2.1456 |
| pwCounterBalanced                                   | 50000 | 5.8880  | 2.0638                | 4.6274      | 5.8946   | 7.1094 |

The estimates of the part-worth utility for the price categories are ordered as expected. This agrees with the intuition that there is a higher preference for a less expensive motor bike when all other things are equal, and that is what you see when you look at the estimated posterior means for the price part-worths. The estimated standard deviations of the price part-worths in this model are of approximately the same order of magnitude as the posterior means. This indicates that the part-worth utilities for this subject are

not significantly far from each other, and that this subject's ranking of the options was not significantly influenced by the difference in price.

One advantage of Bayesian analysis is that you can incorporate prior information in the data analysis. Constraints on the parameter space are one possible source of information that you might have before you examine the data. This example shows that it can be accomplished in PROC MCMC.

---

## Example 55.19: Implement a New Sampling Algorithm

This example illustrates using the UDS statement to implement a new Markov chain sampler. The algorithm demonstrated here is proposed by Holmes and Held (2006), hereafter referred to as HH. They presented a Gibbs sampling algorithm for generating draws from the posterior distribution of the parameters in a probit regression model. The notation follows closely to HH.

The data used here is the remission data set from a PROC LOGISTIC example:

```

title 'Implement a New Sampling Algorithm';
data inputdata;
 input remiss cell smear infil li blast temp;
 ind = _n_;
 cnst = 1;
 label remiss='Complete Remission';
 datalines;
 1 0.8 0.83 0.66 1.9 1.1 0.996
 ... more lines ...
 0 1 0.73 0.73 0.7 0.398 0.986
;

```

The variable `remiss` is the cancer remission indicator variable with a value of 1 for remission and a value of 0 for nonremission. There are six explanatory variables: `cell`, `smear`, `infil`, `li`, `blast`, and `temp`. These variables are the risk factors thought to be related to cancer remission. The binary regression model is as follows:

$$\text{remiss}_i \sim \text{binary}(p_i)$$

where the covariates are linked to  $p_i$  through a probit transformation:

$$\text{probit}(p_i) = \mathbf{x}'\boldsymbol{\beta}$$

$\boldsymbol{\beta}$  are the regression coefficients and  $\mathbf{x}'$  the explanatory variables. Suppose you want to use independent normal priors on the regression coefficients:

$$\beta_i \sim \text{normal}(0, \text{var} = 25)$$

Fitting a probit model with PROC MCMC is straightforward. You can use the following statements:

```

proc mcmc data=inputdata nmc=100000 propcov=quanew seed=17
 outpost=mcmcout;
 ods select PostSummaries ess;
 parms beta0-beta6;

```



```

prior beta: ~ normal(0,var=25);
mu = beta0 + beta1*cell + beta2*smear +
 beta3*infil + beta4*li + beta5*blast + beta6*temp;
p = cdf('normal', mu, 0, 1);
model remiss ~ bern(p);
run;

```

The expression `mu` is the regression mean, and the CDF function links `mu` to the probability of remission `p` in the binary likelihood.

The summary statistics and effective sample sizes tables are shown in [Output 55.19.1](#). There are high autocorrelations among the posterior samples, and efficiency is relatively low. The correlation time is reduced only after a large amount of thinning.

**Output 55.19.1** Random Walk Metropolis

| Implement a New Sampling Algorithm |        |         |                       |             |         |         |
|------------------------------------|--------|---------|-----------------------|-------------|---------|---------|
| The MCMC Procedure                 |        |         |                       |             |         |         |
| Posterior Summaries                |        |         |                       |             |         |         |
| Parameter                          | N      | Mean    | Standard<br>Deviation | Percentiles |         |         |
|                                    |        |         |                       | 25%         | 50%     | 75%     |
| beta0                              | 100000 | -2.0531 | 3.8299                | -4.6418     | -2.0354 | 0.5638  |
| beta1                              | 100000 | 2.6300  | 2.8270                | 0.6563      | 2.5272  | 4.4846  |
| beta2                              | 100000 | -0.8426 | 3.2108                | -3.0270     | -0.8263 | 1.3429  |
| beta3                              | 100000 | 1.5933  | 3.5491                | -0.7993     | 1.6190  | 3.9695  |
| beta4                              | 100000 | 2.0390  | 0.8796                | 1.4312      | 2.0028  | 2.6194  |
| beta5                              | 100000 | -0.3184 | 0.9543                | -0.9613     | -0.3123 | 0.3418  |
| beta6                              | 100000 | -3.2611 | 3.7806                | -5.8050     | -3.2736 | -0.7243 |

| Implement a New Sampling Algorithm |        |                 |            |
|------------------------------------|--------|-----------------|------------|
| The MCMC Procedure                 |        |                 |            |
| Effective Sample Sizes             |        |                 |            |
| Parameter                          | ESS    | Autocorrelation |            |
|                                    |        | Time            | Efficiency |
| beta0                              | 4280.8 | 23.3602         | 0.0428     |
| beta1                              | 4496.5 | 22.2398         | 0.0450     |
| beta2                              | 3434.1 | 29.1199         | 0.0343     |
| beta3                              | 3856.6 | 25.9294         | 0.0386     |
| beta4                              | 3659.7 | 27.3245         | 0.0366     |
| beta5                              | 3229.9 | 30.9610         | 0.0323     |
| beta6                              | 4430.7 | 22.5696         | 0.0443     |

As an alternative to the random walk Metropolis, you can use the Gibbs algorithm to sample from the posterior distribution. The Gibbs algorithm is described in the section “[Gibbs Sampler](#)” on page 135. While the Gibbs algorithm generally applies to a wide range of statistical models, the actual implementation can be problem-specific. In this example, performing a Gibbs sampler involves introducing a class of auxil-

inary variables (also known as latent variables). You first reformulate the model by adding a  $z_i$  for each observation in the data set:

$$\begin{aligned}
 y_i &= \begin{cases} 1 & \text{if } z_i > 0 \\ 0 & \text{otherwise} \end{cases} \\
 z_i &= \mathbf{x}'_i \boldsymbol{\beta} + \epsilon_i \\
 \epsilon &\sim \text{normal}(0, 1) \\
 \boldsymbol{\beta} &\sim \pi(\boldsymbol{\beta})
 \end{aligned}$$

If  $\boldsymbol{\beta}$  has a normal prior, such as  $\pi(\boldsymbol{\beta}) = N(\mathbf{b}, \mathbf{v})$ , you can work out a closed form solution to the full conditional distribution of  $\boldsymbol{\beta}$  given the data and the latent variables  $z_i$ . The full conditional distribution is also a multivariate normal, due to the conjugacy of the problem. See the section “Conjugate Priors” on page 129. The formula is shown here:

$$\begin{aligned}
 \boldsymbol{\beta} | \mathbf{z}, \mathbf{x} &\sim \text{normal}(\mathbf{B}, \mathbf{V}) \\
 \mathbf{B} &= \mathbf{V}((\mathbf{v})^{-1} \mathbf{b} + \mathbf{x}' \mathbf{z}) \\
 \mathbf{V} &= (\mathbf{v}^{-1} + \mathbf{x}' \mathbf{x})^{-1}
 \end{aligned}$$

The advantage of creating the latent variables is that the full conditional distribution of  $\mathbf{z}$  is also easy to work with. The distribution is a truncated normal distribution:

$$z_i | \boldsymbol{\beta}, \mathbf{x}_i, y_i \sim \begin{cases} \text{normal}(\mathbf{x}_i \boldsymbol{\beta}, 1) I(z_i > 0) & \text{if } y_i = 1 \\ \text{normal}(\mathbf{x}_i \boldsymbol{\beta}, 1) I(z_i \leq 0) & \text{otherwise} \end{cases}$$

You can sample  $\boldsymbol{\beta}$  and  $z$  iteratively, by drawing  $\boldsymbol{\beta}$  given  $z$  and vice versa. HH point out that a high degree of correlation could exist between  $\boldsymbol{\beta}$  and  $z$ , and it makes this iterative way of sampling inefficient. As an improvement, HH proposed an algorithm that samples  $\boldsymbol{\beta}$  and  $\mathbf{z}$  jointly. At each iteration, you sample  $z_i$  from the posterior marginal distribution (this is the distribution that is conditional only on the data and not on any parameters) and then sample  $\boldsymbol{\beta}$  from the same posterior full conditional distribution as described previously:

1. Sample  $z_i$  from its posterior marginal distribution:

$$\begin{aligned}
 z_i | \mathbf{z}_{-i}, y_i &\sim \begin{cases} \text{normal}(m_i, v_i) I(z_i > 0) & \text{if } y_i = 1 \\ \text{normal}(m_i, v_i) I(z_i \leq 0) & \text{otherwise} \end{cases} \\
 m_i &= \mathbf{x}_i \mathbf{B} - w_i (z_i - \mathbf{x}_i \mathbf{B}) \\
 v_i &= 1 + w_i \\
 w_i &= h_i / (1 - h_i) \\
 h_i &= (\mathbf{H})_i i, \mathbf{H} = \mathbf{x} \mathbf{V} \mathbf{x}'
 \end{aligned}$$

2. Sample  $\boldsymbol{\beta}$  from the same posterior full conditional distribution described previously.

For a detailed description of each of the conditional terms, refer to the original paper.

PROC MCMC cannot sample from the probit model by using this sampling scheme but you can implement the algorithm by using the UDS statement. To sample  $z_i$  from its marginal, you need a function that draws random variables from a truncated normal distribution. The functions, RLTNORM and RRTNORM, generate left- and right-truncated normal variates, respectively. The algorithm is taken from Robert (1995).

The functions are written in PROC FCMP (see the FCMP Procedure in the *Base SAS Procedures Guide*):

```

proc fcmp outlib=sasuser.funcs.uds;
 /*****
 /* Generate left-truncated normal variate */
 *****/
 function rltnorm(mu, sig, lwr);
 if lwr < mu then do;
 ans = lwr - 1;
 do while (ans < lwr);
 ans = rand('normal', mu, sig);
 end;
 end;
 else do;
 mul = (lwr - mu) / sig;
 alpha = (mul + sqrt(mul**2 + 4)) / 2;
 accept = 0;
 do while (accept = 0);
 z = mul + rand('exponential') / alpha;
 lrho = -(z - alpha)**2 / 2;
 u = rand('uniform');
 lu = log(u);
 if lu <= lrho then accept = 1;
 end;
 ans = sig * z + mu;
 end;
 return(ans);
endsub;

 /*****
 /* Generate right-truncated normal variate */
 *****/
 function rrtnorm(mu, sig, uppr);
 ans = 2 * mu - rltnorm(mu, sig, 2 * mu - uppr);
 return(ans);
endsub;
run;

```

The function call to RLTNORM(mu, sig, lwr) generates a random number from the left-truncated normal distribution:

$$\theta \sim \text{normal}(\mu, \text{sd} = \text{sig}) I(\theta > \text{lwr})$$

Similarly, the function call to `RRTNORM(mu,sig,uppr)` generates a random number from the right-truncated normal distribution:

$$\theta \sim \text{normal}(\mu, \text{sd} = \text{sig})I(\theta < \text{uppr})$$

These functions are used to generate the latent variables  $z_i$ .

Using the algorithm A1 from the HH paper as an example, [Output 55.50](#) lists a line-by-line implementation with the PROC MCMC coding style. The table is broken into three portions: set up the constants, initialize the parameters, and sample one draw from the posterior distribution. The left column of the table is identical to the A1 algorithm stated in the appendix of HH. The right column of the table lists SAS statements.

**Table 55.50** Holmes and Held (2006), algorithm A1. Side-by-Side Comparison to SAS

| Define Constants                                                                         | In the BEGINCNST/ENDCNST Statements                                                                                                                                                                    |
|------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| $V \leftarrow (X'X + v^{-1})^{-1}$                                                       | <pre>call transpose(x,xt); /* xt = transpose(x) */ call mult(xt,x,xtx); call inv(v,v); /* v = inverse(v) */ call addmatrix(xtx,v,xtx); /* xtx = xtx+v */ call inv(xtx,v); /* v = inverse(xtx) */</pre> |
| $L \leftarrow \text{Chol}(V)$                                                            | <pre>call chol(v,L);</pre>                                                                                                                                                                             |
| $S \leftarrow VX'$                                                                       | <pre>call mult(v,xt,S);</pre>                                                                                                                                                                          |
| <pre>FOR j=1 to n   H[j] ← X[j,]S[,j]   W[j] ← H[j]/(1-H[j])   Q[j] ← W[j] + 1 END</pre> | <pre>call mult(x,S,HatMat); do j=1 to &amp;n;   H = HatMat[j,j];   W[j] = H/(1-H);   sQ[j] = sqrt(W[j] + 1); /* use s.d. in SAS */ end;</pre>                                                          |
| Initial Values                                                                           | In the BEGINCNST/ENDCNST Statements                                                                                                                                                                    |
| $Z \sim \text{normal}(0, I_n)\text{Ind}(Y, Z)$                                           | <pre>do j=1 to &amp;n;   if(y[j]=1) then     Z[j] = rlnorm(0,1,0);   else     Z[j] = rrtnorm(0,1,0);   end;</pre>                                                                                      |
| $B \leftarrow SZ$                                                                        | <pre>call mult(S,Z,B);</pre>                                                                                                                                                                           |

| Draw One Sample                                                                                                                                                                                                            | Subroutine HH                                                                                                                                                                                                                                                                                                                                                                                                       |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <pre> FOR j = 1 to n   z<sub>old</sub> ← Z[j]   m ← X[j,]B   m ← m - W[j](Z[j] - m)   Z[j] ~ normal(m, Q[j])Ind(Y[j], Z[j])   B ← B + (Z[j] - z<sub>old</sub>)S[,j] END T ~ normal(0, I<sub>p</sub>) β[,i] ← B + LT </pre> | <pre> do j=1 to &amp;n;   zold = Z[j];   m = 0;   do k= 1 to &amp;p;     m = m + X[j,k] * B[k];   end;   m = m - W[j]*(Z[j]-m);   if (y[j]=1) then     Z[j] = rlnorm(m,sQ[j],0);   else     Z[j] = rrtnorm(m,sQ[j],0);   diff = Z[j] - zold;   do k= 1 to &amp;p;     B[k] = B[k] + diff * S[k,j];   end; end; do j = 1 to &amp;p;   T[j] = rand('normal'); end; call mult(L,T,T); call addmatrix(B,T,beta); </pre> |

The following statements define the subroutine HH (algorithm A1) in PROC FCMP and store it in library `sasuser.funcs.uds`:

```

/* define the HH algorithm in PROC FCMP. */
%let n = 27;
%let p = 7;
options cmplib=sasuser.funcs;
proc fcmp outlib=sasuser.funcs.uds;
 subroutine HH(beta[*],Z[*],B[*],x[*,*],y[*],W[*],sQ[*],S[*,*],L[*,*]);
 outargs beta, Z, B;
 array T[&p] / nosym;
 do j=1 to &n;
 zold = Z[j];
 m = 0;
 do k = 1 to &p;
 m = m + X[j,k] * B[k];
 end;
 m = m - W[j]*(Z[j]-m);
 if (y[j]=1) then
 Z[j] = rlnorm(m,sQ[j],0);
 else
 Z[j] = rrtnorm(m,sQ[j],0);
 diff = Z[j] - zold;
 do k = 1 to &p;
 B[k] = B[k] + diff * S[k,j];
 end;
 end;
 endsubr;
endproc;

```

```

end;
do j=1 to &p;
 T[j] = rand('normal');
end;
call mult(L,T,T);
call addmatrix(B,T,beta);
endsub;
run;

```

Note that one-dimensional array arguments take the form of *name*[\*] and two-dimensional array arguments take the form of *name*[\*,\*]. Three variables, *beta*, *Z*, and *B*, are OUTARGS variables, making them the only arguments that can be modified in the subroutine. For the **UDS** statement to work, all OUTARGS variables have to be model parameters. Technically, only *beta* and *Z* are model parameters, and *B* is not. The reason that *B* is declared as an OUTARGS is because the array must be updated throughout the simulation, and this is the only way to modify its values. The input array *x* contains all of the explanatory variables, and the array *y* stores the response. The rest of the input arrays, *W*, *sQ*, *S*, and *L*, store constants as detailed in the algorithm. The following statements illustrate how to fit a Bayesian probit model by using the HH algorithm:

```

options cmplib=sasuser.funcs;

proc mcmc data=inputdata nmc=5000 monitor=(beta) outpost=hhout;
 ods select PostSummaries ess;
 array xtx[&p,&p]; /* work space */
 array xt[&p,&n]; /* work space */
 array v[&p,&p]; /* work space */
 array HatMat[&n,&n]; /* work space */
 array S[&p,&n]; /* V * Xt */
 array W[&n];
 array y[1]/ nosymbols; /* y stores the response variable */
 array x[1]/ nosymbols; /* x stores the explanatory variables */
 array sQ[&n]; /* sqrt of the diagonal elements of Q */
 array B[&p]; /* conditional mean of beta */
 array L[&p,&p]; /* Cholesky decomp of conditional cov */
 array Z[&n]; /* latent variables Z */
 array beta[&p] beta0-beta6; /* regression coefficients */

 beginncst;
 call streaminit(83101);
 if ind=1 then do;
 rc = read_array("inputdata", x, "cnst", "cell", "smear", "infil",
 "li", "blast", "temp");
 rc = read_array("inputdata", y, "remiss");
 call identity(v);
 call mult(v, 25, v);
 call transpose(x,xt);
 call mult(xt,x,xtx);
 call inv(v,v);
 call addmatrix(xtx,v,xtx);
 call inv(xtx,v);
 call chol(v,L);
 call mult(v,xt,S);
 call mult(x,S,HatMat);
 end;
 end;
run;

```

```

do j=1 to &n;
 H = HatMat[j, j];
 W[j] = H/(1-H);
 sQ[j] = sqrt(W[j] + 1);
end;

do j=1 to &n;
 if(y[j]=1) then
 Z[j] = rltnorm(0,1,0);
 else
 Z[j] = rrtnorm(0,1,0);
 end;
 call mult(S,Z,B);
end;
endcnst;

uds HH(beta,Z,B,x,y,W,sQ,S,L);
parms z: beta: 0 B1-B7 / uds;
prior z: beta: B1-B7 ~ general(0);

model general(0);
run;

```

The `OPTIONS` statement names the catalog of FCMP subroutines to use. The `cmplib` library stores the subroutine `HH`. You do not need to set a random number seed in the `PROC MCMC` statement because all random numbers are generated from the `HH` subroutine. The initialization of the `rand` function is controlled by the `streaminit` function, which is called in the program with a seed value of 83101.

A number of arrays are allocated. Some of them, such as `xtx`, `xt`, `v`, and `HatMat`, allocate work space for constant arrays. Other arrays are used in the subroutine sampling. Explanations of the arrays are shown in comments in the statements.

In the `BEGINCNST` and `ENDCNST` statement block, you read data set variables in the arrays `x` and `y`, calculate all the constant terms, and assign initial values to `Z` and `B`. For the `READ_ARRAY` function, see the section “[READ\\_ARRAY Function](#)” on page 4442. For listings of all array functions and their definitions, see the section “[Matrix Functions in PROC MCMC](#)” on page 4498.

The `UDS` statement declares that the subroutine `HH` is used to sample the parameters `beta`, `Z`, and `B`. You also specify the `UDS` option in the `PARMS` statement. Because all parameters are updated through the `UDS` interface, it is not necessary to declare the actual form of the prior for any of the parameters. Each parameter is declared to have a prior of `general(0)`. Similarly, it is not necessary to declare the actual form of the likelihood. The `MODEL` statement also takes a flat likelihood of the form `general(0)`.

Summary statistics and effective sample sizes are shown in [Output 55.19.2](#). The posterior estimates are very close to what was shown in [Output 55.19.1](#). The `HH` algorithm produces samples that are much less correlated.

**Output 55.19.2** Holms and Held

| Implement a New Sampling Algorithm |      |         |                       |             |         |         |
|------------------------------------|------|---------|-----------------------|-------------|---------|---------|
| The MCMC Procedure                 |      |         |                       |             |         |         |
| Posterior Summaries                |      |         |                       |             |         |         |
| Parameter                          | N    | Mean    | Standard<br>Deviation | Percentiles |         |         |
|                                    |      |         |                       | 25%         | 50%     | 75%     |
| beta0                              | 5000 | -2.0567 | 3.8260                | -4.6537     | -2.0777 | 0.5495  |
| beta1                              | 5000 | 2.7254  | 2.8079                | 0.7812      | 2.6678  | 4.5370  |
| beta2                              | 5000 | -0.8318 | 3.2017                | -2.9987     | -0.8626 | 1.2918  |
| beta3                              | 5000 | 1.6319  | 3.5108                | -0.7481     | 1.6636  | 4.0302  |
| beta4                              | 5000 | 2.0567  | 0.8800                | 1.4400      | 2.0266  | 2.6229  |
| beta5                              | 5000 | -0.3473 | 0.9490                | -0.9737     | -0.3267 | 0.2752  |
| beta6                              | 5000 | -3.3787 | 3.7991                | -5.9089     | -3.3504 | -0.7928 |

| Implement a New Sampling Algorithm |        |                 |            |
|------------------------------------|--------|-----------------|------------|
| The MCMC Procedure                 |        |                 |            |
| Effective Sample Sizes             |        |                 |            |
| Parameter                          | ESS    | Autocorrelation |            |
|                                    |        | Time            | Efficiency |
| beta0                              | 3651.3 | 1.3694          | 0.7303     |
| beta1                              | 1563.8 | 3.1973          | 0.3128     |
| beta2                              | 5005.9 | 0.9988          | 1.0012     |
| beta3                              | 4853.2 | 1.0302          | 0.9706     |
| beta4                              | 2611.2 | 1.9148          | 0.5222     |
| beta5                              | 3049.2 | 1.6398          | 0.6098     |
| beta6                              | 3503.2 | 1.4273          | 0.7006     |

It is interesting to compare the two approaches of fitting a generalized linear model. The random walk Metropolis on a seven-dimensional parameter space produces autocorrelations that are substantially higher than the HH algorithm. A much longer chain is needed to produce roughly equivalent effective sample sizes. On the other hand, the Metropolis algorithm is faster to run. The running time of these two examples is roughly the same, with the random walk Metropolis with 100000 samples, a 20-fold increase over that in the HH algorithm example. The speed difference can be attributed to a number of factors, ranging from the implementation of the software and the overhead cost of calling PROC FCMP subroutine and functions. In addition, the HH algorithm requires more parameters by creating an equal number of latent variables as the sample size. Sampling more parameters takes time. A larger number of parameters also increases the challenge in convergence diagnostics, because it is imperative to have convergence in all parameters before you make valid posterior inferences. Finally, you might feel that coding in PROC MCMC is easier. However, this really is not a fair comparison to make here. Writing a Metropolis algorithm from scratch would have probably taken just as much, if not more, effort than the HH algorithm.



## Example 55.20: Using a Transformation to Improve Mixing

Proper transformations of parameters can often improve the mixing in PROC MCMC. You already saw this in “[Example 55.6: Nonlinear Poisson Regression Models](#)” on page 4570, which sampled using the log scale of parameters that priors that are strictly positive, such as the gamma priors. This example shows another useful transformation: the logit transformation on parameters that take a uniform prior on  $[0, 1]$ .

The data set is taken from Sharples (1990). It is used in Chaloner and Brant (1988) and Chaloner (1994) to identify outliers in the data set in a two-level hierarchical model. Congdon (2003) also uses this data set to demonstrate the same technique. This example uses the data set to illustrate how mixing can be improved using transformation and does not address the question of outlier detection as in those papers. The following statements create the data set:

```
data inputdata;
 input nobobs grp y @@;
 ind = _n_;
 datalines;
1 1 24.80 2 1 26.90 3 1 26.65
4 1 30.93 5 1 33.77 6 1 63.31
1 2 23.96 2 2 28.92 3 2 28.19
4 2 26.16 5 2 21.34 6 2 29.46
1 3 18.30 2 3 23.67 3 3 14.47
4 3 24.45 5 3 24.89 6 3 28.95
1 4 51.42 2 4 27.97 3 4 24.76
4 4 26.67 5 4 17.58 6 4 24.29
1 5 34.12 2 5 46.87 3 5 58.59
4 5 38.11 5 5 47.59 6 5 44.67
;
```

There are five groups ( $\text{grp}$ ,  $j = 1, \dots, 5$ ) with six observations ( $\text{nobobs}$ ,  $i = 1, \dots, 6$ ) in each. The two-level hierarchical model is specified as follows:

$$\begin{aligned}
 y_{ij} &\sim \text{normal}(\theta_j, \text{prec} = \tau_w) \\
 \theta_j &\sim \text{normal}(\mu, \text{prec} = \tau_b) \\
 \mu &\sim \text{normal}(0, \text{prec} = 1e - 6) \\
 \tau &\sim \text{gamma}(0.001, \text{iscale} = 0.001) \\
 p &\sim \text{uniform}(0, 1)
 \end{aligned}$$

with the precision parameters related to each other in the following way:

$$\begin{aligned}
 \tau_b &= \tau/p \\
 \tau_w &= \tau_b - \tau
 \end{aligned}$$

The total number of parameters in this model is eight:  $\theta_1, \dots, \theta_5, \mu, \tau$ , and  $p$ .

The following statements fit the model:

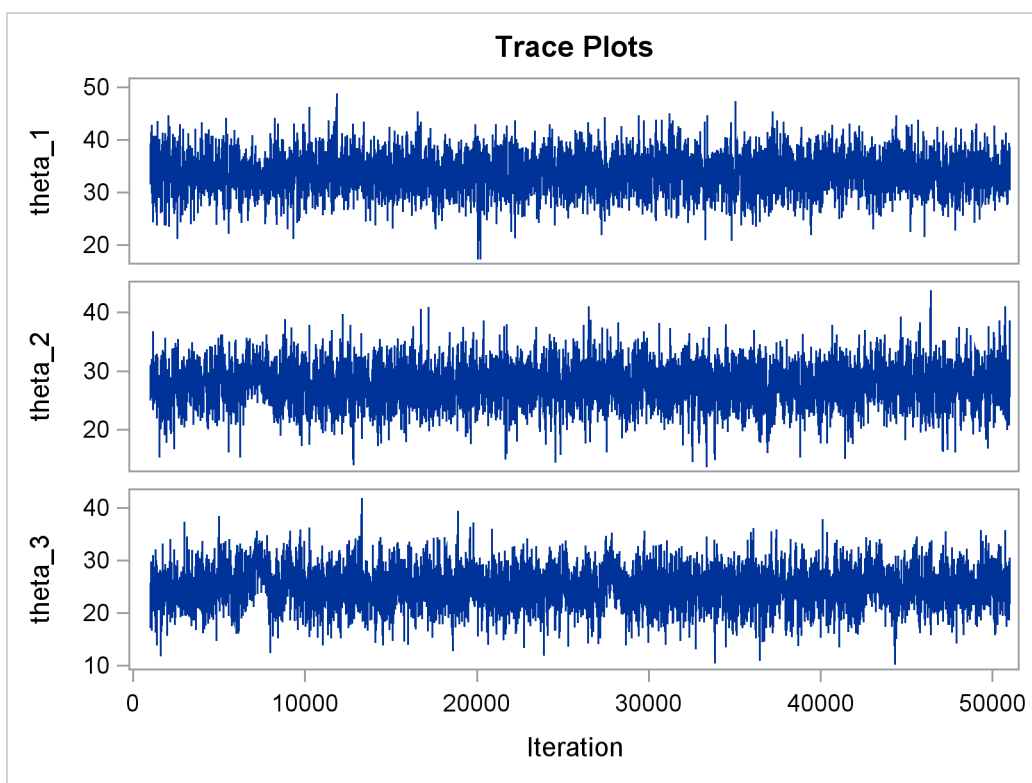
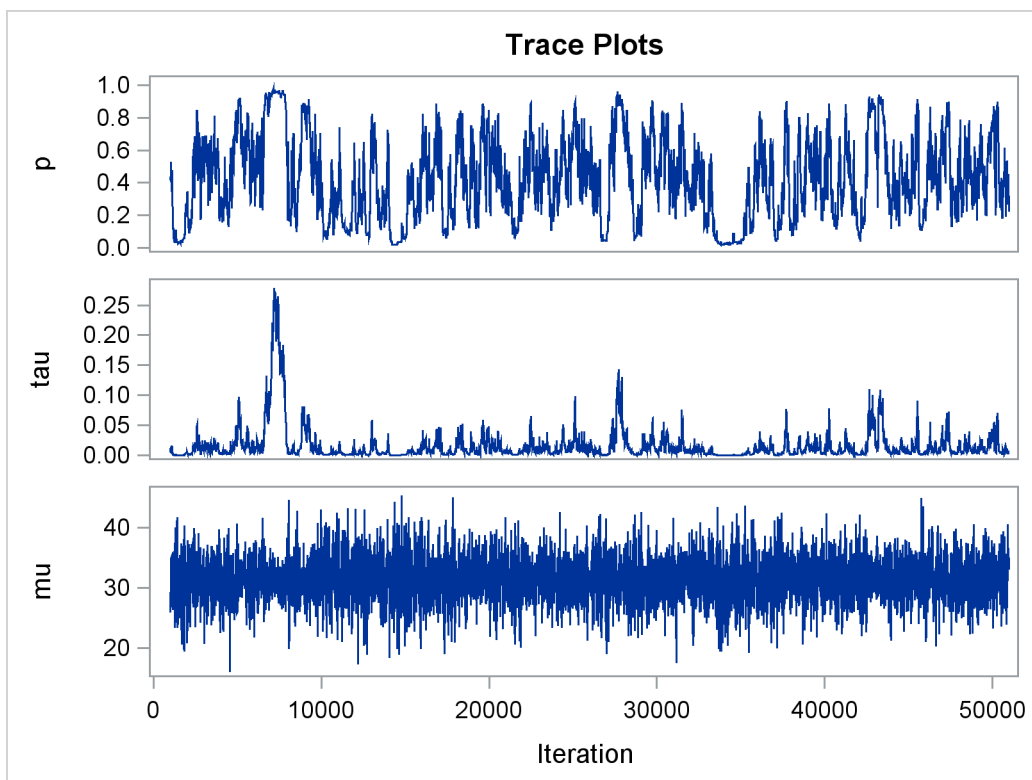
```
ods graphics on;
proc mcmc data=inputdata nmc=50000 thin=10 outpost=m1 seed=17
 plot=trace;
 ods select ess tracepanel;
 parms p;
 parms tau;
 parms mu;

 prior p ~ uniform(0,1);
 prior tau ~ gamma(shape=0.001, iscale=0.001);
 prior mu ~ normal(0, prec=0.00000001);
 beginnodata;
 taub = tau/p;
 tauw = taub-tau;
 endnodata;

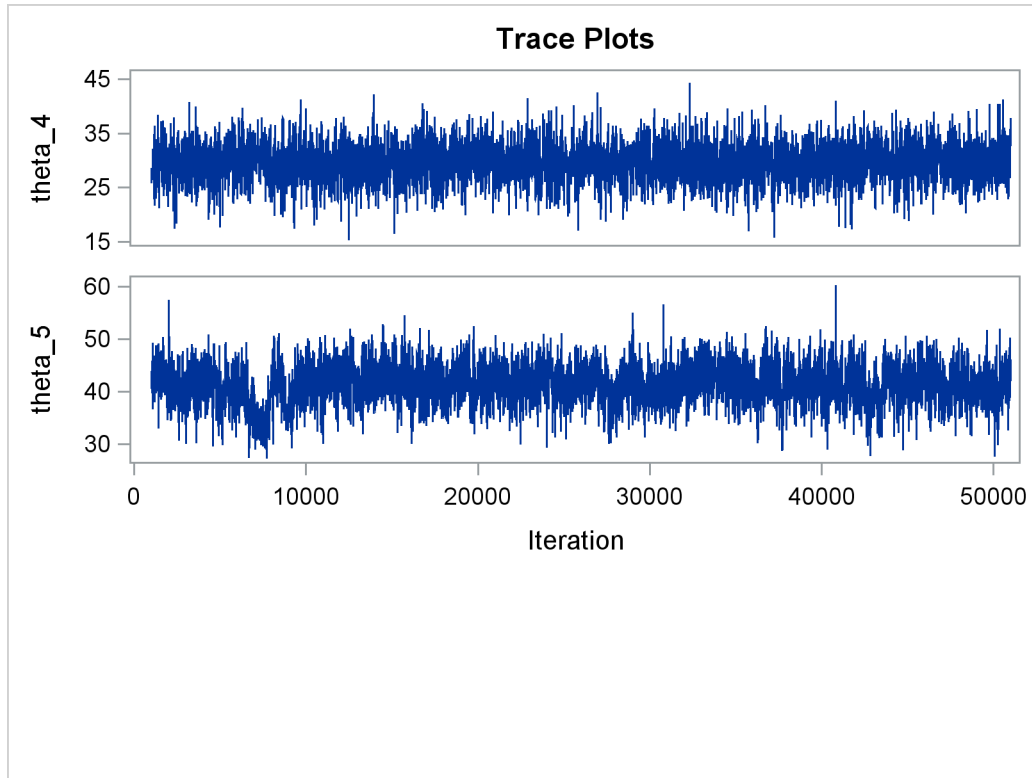
 random theta ~ normal(mu, prec=taub) subject=grp monitor=(theta);
 model y ~ normal(theta, prec=tauw);
run;
```

The ODS SELECT statement displays the effective sample size table and the trace plots. The ODS GRAPHICS ON statement enables ODS Graphics. The PROC MCMC statement specifies the usual options for the procedure run and produces trace plots (**PLOTS=TRACE**). The three **PARMS** statements put three model parameters,  $p$ ,  $\tau$ , and  $\mu$ , in three different blocks. The **PRIOR** statements specify the prior distributions, and the programming statements enclosed with the **BEGINNODATA** and **ENDNODATA** statements calculate the transformation to  $\tau_{\text{aub}}$  and  $\tau_{\text{aw}}$ . The **RANDOM** statement specifies the random effect, its prior distribution, and the subject variable. The resulting trace plots are shown in [Output 55.20.1](#), and the effective sample size table is shown in [Output 55.20.2](#).

Output 55.20.1 Trace Plots



**Output 55.20.1** *continued*



**Output 55.20.2** Bad Effective Sample Sizes

| Implement a New Sampling Algorithm |        |                      |            |
|------------------------------------|--------|----------------------|------------|
| The MCMC Procedure                 |        |                      |            |
| Effective Sample Sizes             |        |                      |            |
| Parameter                          | ESS    | Autocorrelation Time | Efficiency |
| p                                  | 81.3   | 61.5342              | 0.0163     |
| tau                                | 61.2   | 81.7440              | 0.0122     |
| mu                                 | 5000.0 | 1.0000               | 1.0000     |
| theta_1                            | 4839.9 | 1.0331               | 0.9680     |
| theta_2                            | 2739.7 | 1.8250               | 0.5479     |
| theta_3                            | 1346.6 | 3.7130               | 0.2693     |
| theta_4                            | 4897.5 | 1.0209               | 0.9795     |
| theta_5                            | 338.1  | 14.7866              | 0.0676     |

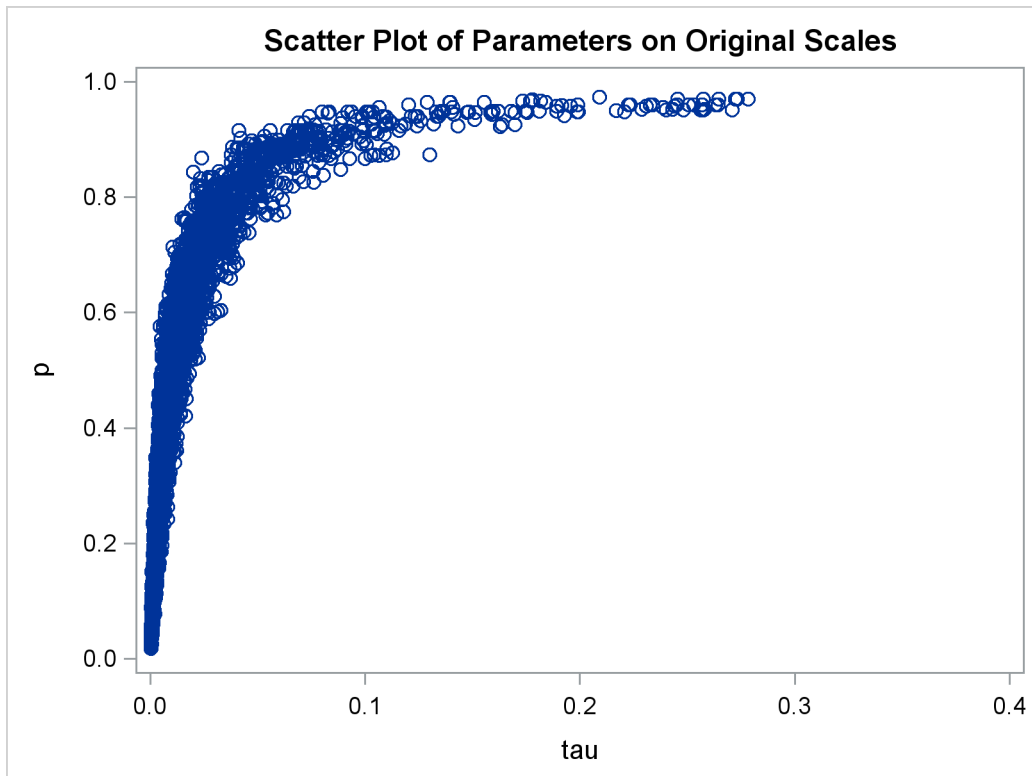
The trace plots show that most parameters have relatively good mixing. Two exceptions appear to be  $p$  and  $\tau$ . The trace plot of  $p$  shows a slow periodic movement. The  $\tau$  parameter does not have good mixing either. When the values are close to zero, the chain stays there for periods of time. An inspection of the effective sample sizes table reveals the same conclusion:  $p$  and  $\tau$  have much smaller ESSs than the rest of the parameters.

A scatter plot of the posterior samples of  $p$  and  $\tau$  reveals why mixing is bad in these two dimensions. The following statements generate the scatter plot in [Output 55.20.3](#):

```
title 'Scatter Plot of Parameters on Original Scales';

proc sgplot data=m1;
 yaxis label = 'p';
 xaxis label = 'tau' values=(0 to 0.4 by 0.1);
 scatter x = tau y = p;
run;
```

**Output 55.20.3** Scatter Plot of  $\tau$  versus  $p$



The two parameters clearly have a nonlinear relationship. It is not surprising that the Metropolis algorithm does not work well here. The algorithm is designed for cases where the parameters are linearly related with each other.

To improve on mixing, you can sample on the log of  $\tau$ , instead of sampling on  $\tau$ . The formulation is:

$$\begin{aligned}\tau &\sim \text{gamma}(\text{shape} = 0.001, \text{iscale} = 0.001) \\ \log(\tau) &\sim \text{egamma}(\text{shape} = 0.001, \text{iscale} = 0.001)\end{aligned}$$

See the section “[Standard Distributions](#)” on page 4476 for the definitions of the [gamma](#) and [egamma](#) distributions. In addition, you can sample on the logit of  $p$ . Note that

$$p \sim \text{uniform}(0, 1)$$

is equivalent to

$$\text{lgp} = \text{logit}(p) \sim \text{logistic}(0, 1)$$

The following statements fit the same model by using transformed parameters:

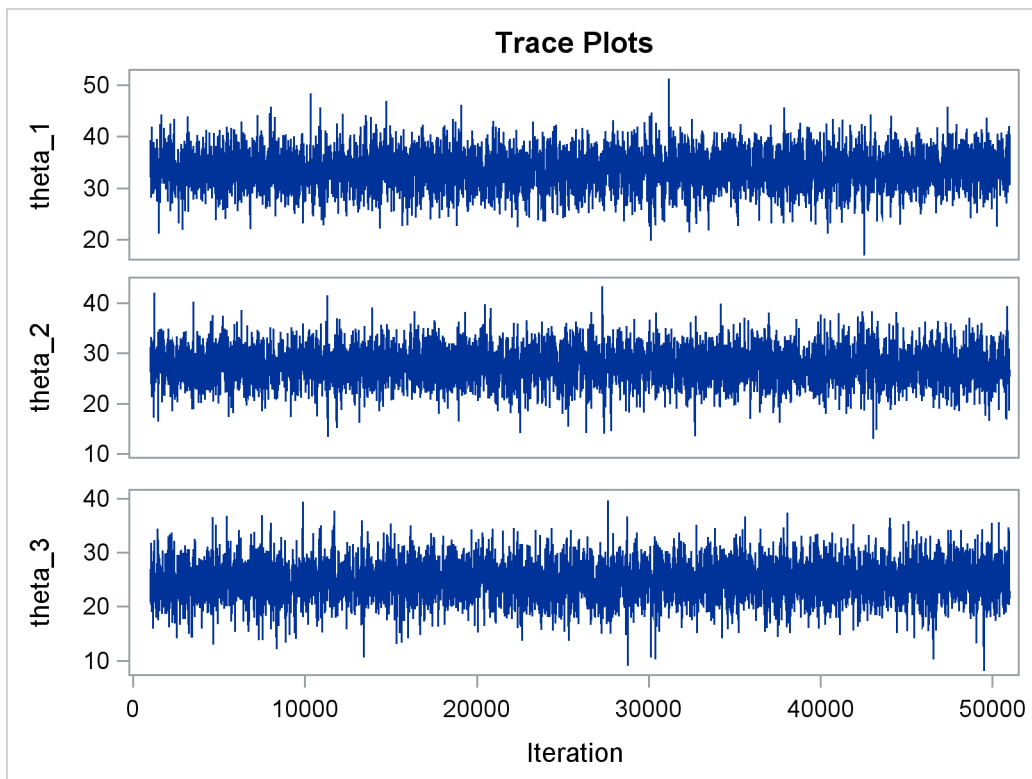
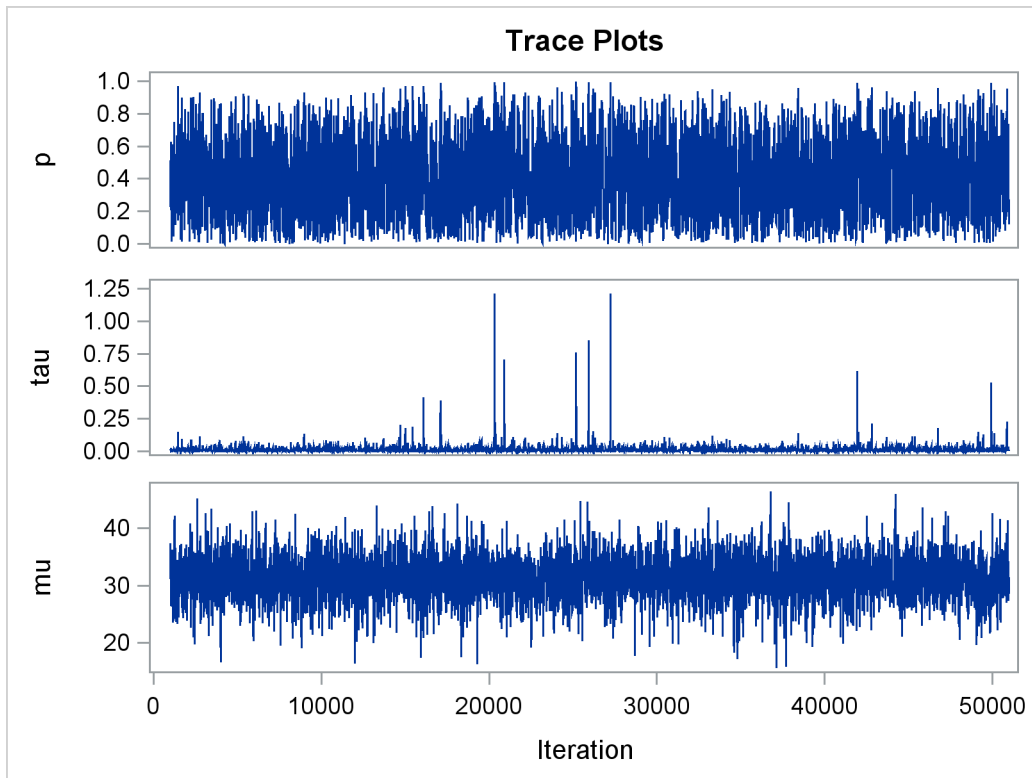
```
proc mcmc data=inputdata nmc=50000 thin=10 outpost=m2 seed=17
 monitor=(p tau mu) plot=trace;
 ods select ess tracepanel;
 parms ltau lgp mu ;

 prior ltau ~ egamma(shape=0.001, iscale=0.001);
 prior lgp ~ logistic(0,1);
 prior mu ~ normal(0, prec=0.00000001);

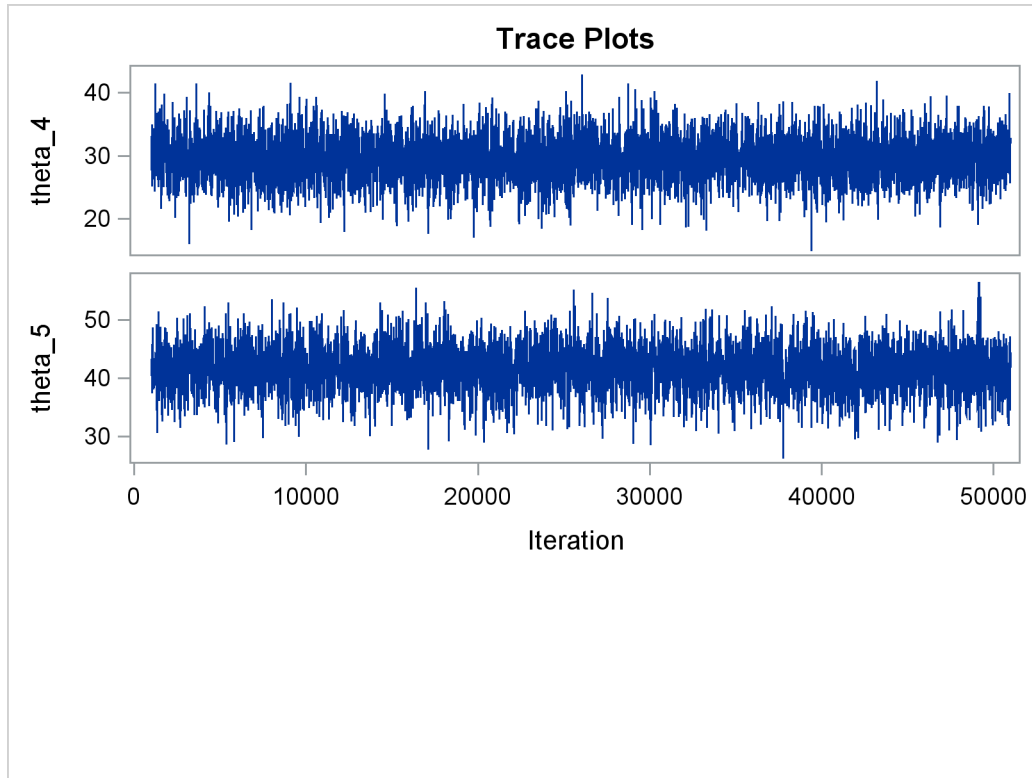
 beginnodata;
 tau = exp(ltau);
 p = logistic(lgp);
 taub = tau/p;
 tauw = taub-tau;
 endnodata;

 random theta ~ normal(mu, prec=taub) subject=grp monitor=(theta);
 model y ~ normal(theta, prec=tauw);
run;
```

The variable `lgp` is the logit transformation of  $p$ , and `ltau` is the log transformation of  $\tau$ . The prior for `ltau` is [egamma](#), and the prior for `lgp` is [logistic](#). The `TAU` and `P` assignment statements transform the parameters back to their original scales. The rest of the programs remain unchanged. Trace plots ([Output 55.20.4](#)) and effective sample size ([Output 55.20.5](#)) both show significant improvements in the mixing for both  $p$  and  $\tau$ .

**Output 55.20.4** Trace Plots after Transformation

**Output 55.20.4** *continued*



**Output 55.20.5** Effective Sample Sizes after Transformation

| The MCMC Procedure     |        |                 |            |
|------------------------|--------|-----------------|------------|
| Effective Sample Sizes |        |                 |            |
| Parameter              | ESS    | Autocorrelation |            |
|                        |        | Time            | Efficiency |
| p                      | 3119.4 | 1.6029          | 0.6239     |
| tau                    | 2588.0 | 1.9320          | 0.5176     |
| mu                     | 5000.0 | 1.0000          | 1.0000     |
| theta_1                | 4866.0 | 1.0275          | 0.9732     |
| theta_2                | 5244.5 | 0.9534          | 1.0489     |
| theta_3                | 5000.0 | 1.0000          | 1.0000     |
| theta_4                | 5000.0 | 1.0000          | 1.0000     |
| theta_5                | 4054.8 | 1.2331          | 0.8110     |



The following statements generate [Output 55.20.6](#) and [Output 55.20.7](#):

```

title 'Scatter Plot of Parameters on Transformed Scales';

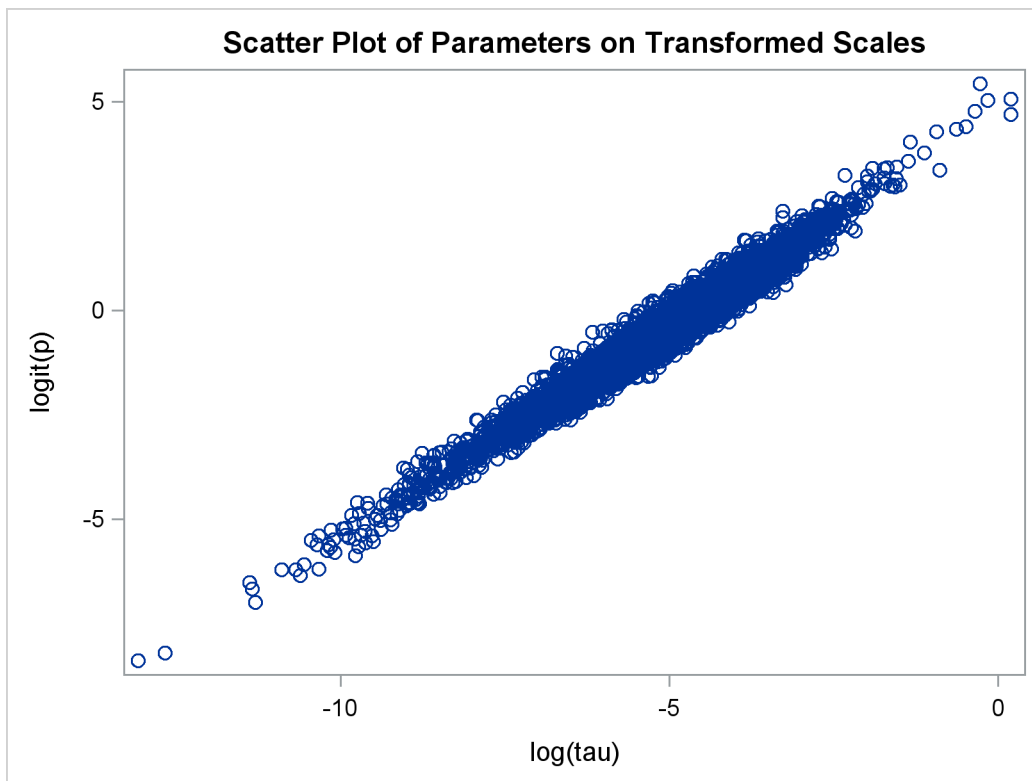
proc sgplot data=m2;
 yaxis label = 'logit(p)';
 xaxis label = 'log(tau)';
 scatter x = ltau y = lgp;
run;

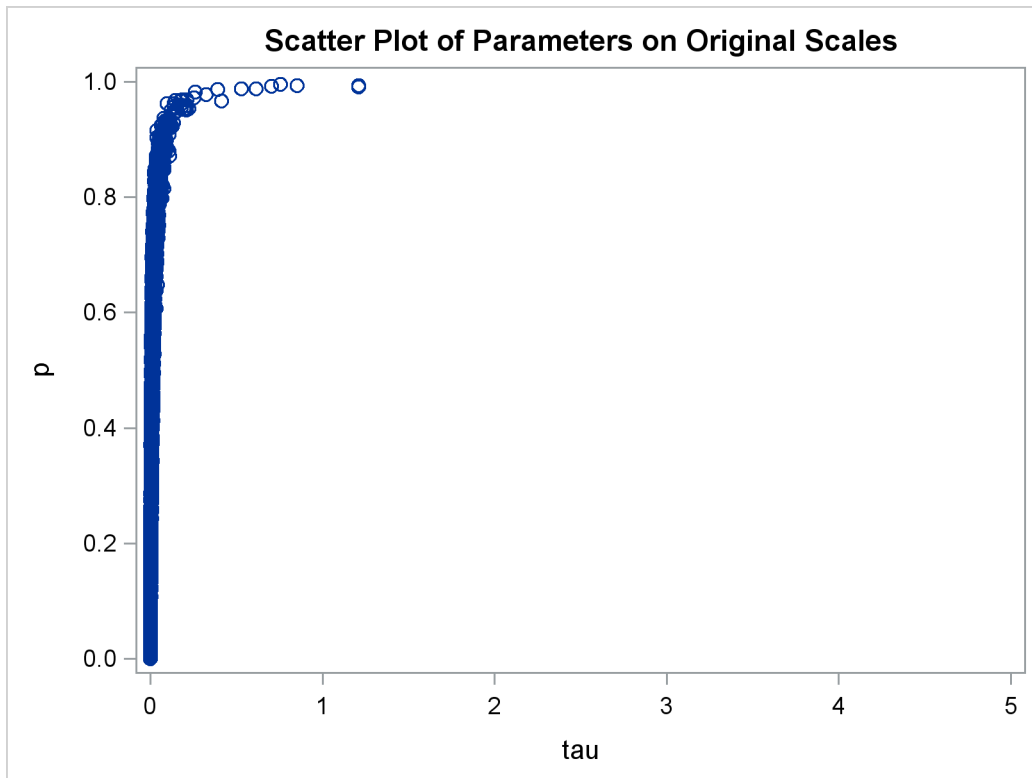
title 'Scatter Plot of Parameters on Original Scales';

proc sgplot data=m2;
 yaxis label = 'p';
 xaxis label = 'tau' values=(0 to 5.0 by 1);
 scatter x = tau y = p;
run;
ods graphics off;

```

**Output 55.20.6** Scatter Plot of  $\log(\tau)$  versus  $\text{logit}(p)$ , After Transformation



**Output 55.20.7** Scatter Plot of  $\tau$  versus  $p$ , After Transformation

The scatter plot of  $\log(\tau)$  versus  $\text{logit}(p)$  shows a linear relationship between the two transformed parameters, and this explains the improvement in mixing. In addition, the transformations also help the Markov chain better explore in the original parameter space. [Output 55.20.7](#) shows a scatter plot of  $\tau$  versus  $p$ . The plot is similar to [Output 55.20.3](#). However, note that  $\tau$  has a far longer tail in [Output 55.20.7](#), extending all the way to 5 as opposed to 0.15 in [Output 55.20.3](#). This means that the second Markov chain can explore this dimension of the parameter more efficiently, and as a result, you are able to draw more precise inference with an equal number of simulations.

---

## Example 55.21: Gelman-Rubin Diagnostics

PROC MCMC does not have the Gelman-Rubin test (see the section “[Gelman and Rubin Diagnostics](#)” on page 145) as a part of its diagnostics. The Gelman-Rubin diagnostics rely on parallel chains to test whether they all converge to the same posterior distribution. This example demonstrates how you can carry out this convergence test. The regression model from the section “[Simple Linear Regression](#)” on page 4408 is used. The model has three parameters:  $\beta_0$  and  $\beta_1$  are the regression coefficients, and  $\sigma^2$  is the variance of the error distribution.

The following statements generate the data set:

```

title 'Simple Linear Regression, Gelman-Rubin Diagnostics';

data Class;
 input Name $ Height Weight @@;
 datalines;
Alfred 69.0 112.5 Alice 56.5 84.0 Barbara 65.3 98.0
Carol 62.8 102.5 Henry 63.5 102.5 James 57.3 83.0
Jane 59.8 84.5 Janet 62.5 112.5 Jeffrey 62.5 84.0
John 59.0 99.5 Joyce 51.3 50.5 Judy 64.3 90.0
Louise 56.3 77.0 Mary 66.5 112.0 Philip 72.0 150.0
Robert 64.8 128.0 Ronald 67.0 133.0 Thomas 57.5 85.0
William 66.5 112.0
;

```

To run a Gelman-Rubin diagnostic test, you want to start Markov chains at different places in the parameter space. Suppose you want to start  $\beta_0$  at 10, -15, and 0;  $\beta_1$  at -5, 10, and 0; and  $\sigma^2$  at 1, 20, and 50. You can put these starting values in the following Init SAS data set:

```

data init;
 input Chain beta0 beta1 sigma2;
 datalines;
1 10 -5 1
2 -15 10 20
3 0 0 50
;

```

The following statements run PROC MCMC three times, each with starting values specified in the data set Init:

```

/* define constants */
%let nchain = 3;
%let nparm = 3;
%let nsim = 50000;
%let var = beta0 beta1 sigma2;

%macro gcmc;
 %do i=1 %to &nchain;
 data _null_;
 set init;
 if Chain=&i;
 %do j = 1 %to &nparm;
 call symputx("init&j", %scan(&var, &j));
 %end;
 stop;
 run;

 proc mcmc data=class outpost=out&i init=reinit nbi=0 nmc=&nsim
 stats=none seed=7;
 parms beta0 &init1 beta1 &init2;
 parms sigma2 &init3 / n;
 prior beta0 beta1 ~ normal(0, var = 1e6);
 prior sigma2 ~ igamma(3/10, scale = 10/3);

```

```

 mu = beta0 + beta1*height;
 model weight ~ normal(mu, var = sigma2);
 run;
%end;
%mend;

ods listing close;
%gcmc;
ods listing;

```

The macro variables `nchain`, `nparm`, `nsim`, and `var` define the number of chains, the number of parameters, the number of Markov chain simulations, and the parameter names, respectively. The macro `GMCMC` gets initial values from the data set `lnit`, assigns them to the macro variables `init1`, `init2` and `init3`, starts the Markov chain at these initial values, and stores the posterior draws to three output data sets: `Out1`, `Out2`, and `Out3`.

In the `PROC MCMC` statement, the `INIT=REINIT` option restarts the Markov chain after tuning at the assigned initial values. No burn-in is requested.

You can use the autocall macro `GELMAN` to calculate the Gelman-Rubin statistics by using the three chains. The `GELMAN` macro has the following arguments:

```
%macro gelman(dset, nparm, var, nsim, nc=3, alpha=0.05);
```

The argument `dset` is the name of the data set that stores the posterior samples from all the runs, `nparm` is the number of parameters, `var` is the name of the parameters, `nsim` is the number of simulations, `nc` is the number of chains with a default value of 3, and `alpha` is the  $\alpha$  significant level in the test with a default value of 0.05. This macro creates two data sets: `_Gelman_Ests` stores the diagnostic estimates and `_Gelman_Parms` stores the names of the parameters.

The following statements calculate the Gelman-Rubin diagnostics:

```

data all;
 set out1(in=in1) out2(in=in2) out3(in=in3);
 if in1 then Chain=1;
 if in2 then Chain=2;
 if in3 then Chain=3;
run;

%gelman(all, &nparm, &var, &nsim);

data GelmanRubin(label='Gelman-Rubin Diagnostics');
 merge _Gelman_Parms _Gelman_Ests;
run;

proc print data=GelmanRubin;
run;

```

The Gelman-Rubin statistics are shown in [Output 55.21.1](#).

**Output 55.21.1** Gelman-Rubin Diagnostics of the Regression Example

| Simple Linear Regression, Gelman-Rubin Diagnostics |           |               |              |          |             |
|----------------------------------------------------|-----------|---------------|--------------|----------|-------------|
| Obs                                                | Parameter | Between-chain | Within-chain | Estimate | Upper Bound |
| 1                                                  | beta0     | 5384.76       | 1168.64      | 1.0002   | 1.0001      |
| 2                                                  | beta1     | 1.20          | 0.30         | 1.0002   | 1.0002      |
| 3                                                  | sigma2    | 8034.41       | 2890.00      | 1.0010   | 1.0011      |

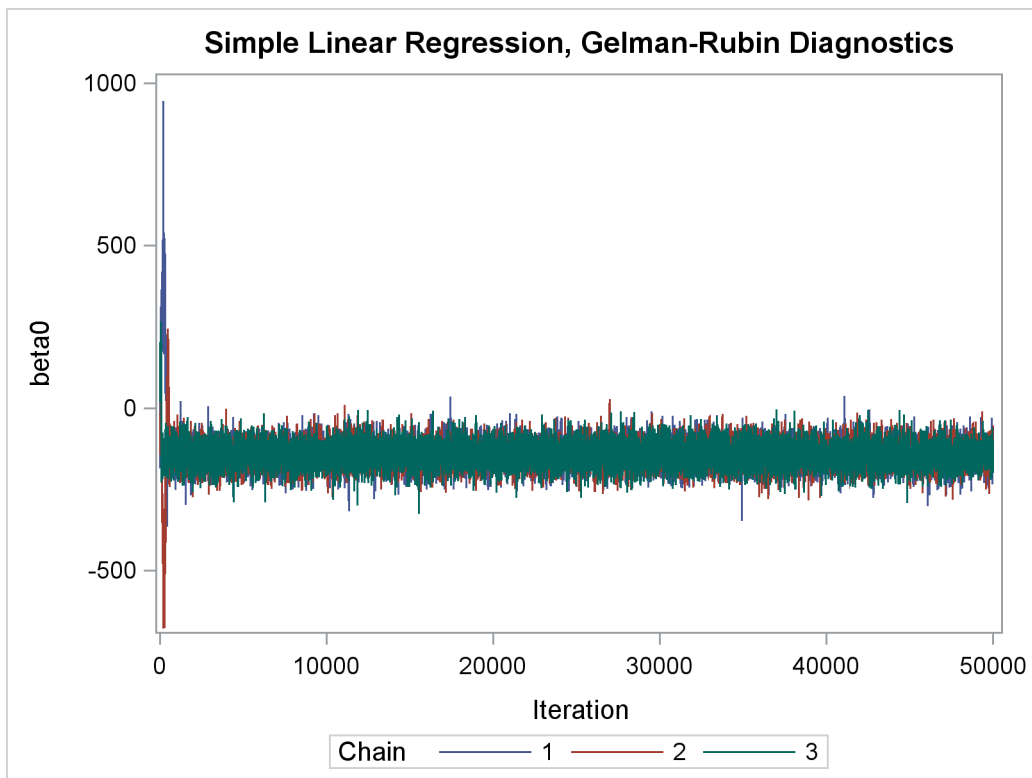
The Gelman-Rubin statistics do not reveal any concerns about the convergence or the mixing of the multiple chains. To get a better visual picture of the multiple chains, you can draw overlapping trace plots of these parameters from the three Markov chains runs.

The following statements create [Output 55.21.2](#):

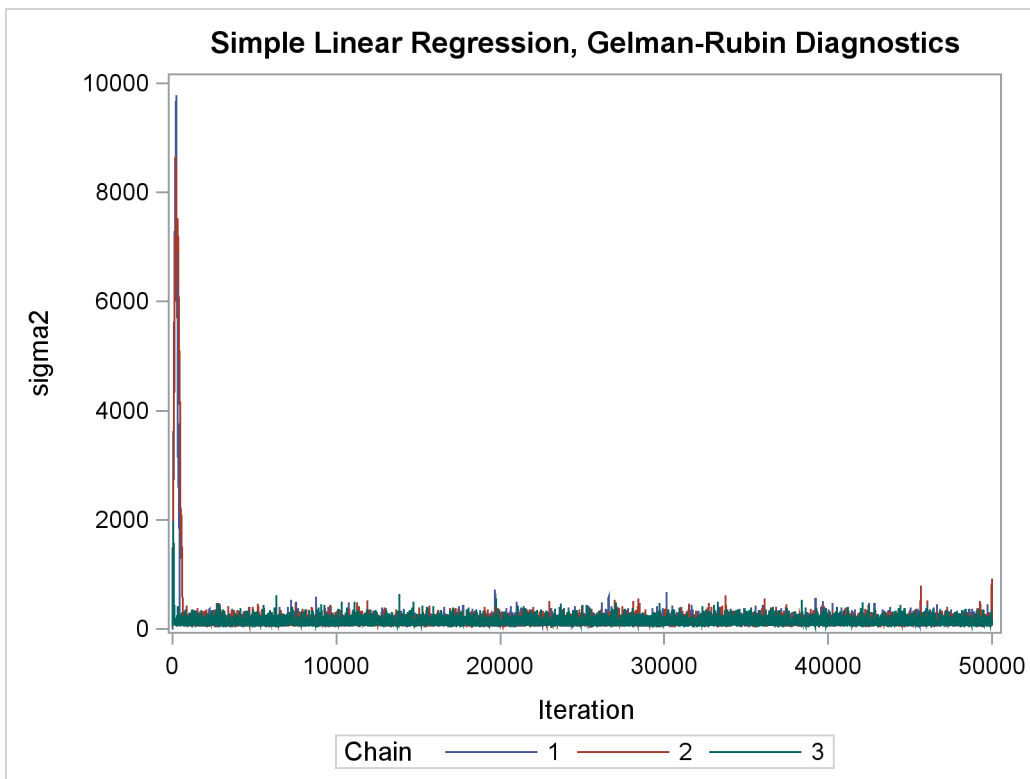
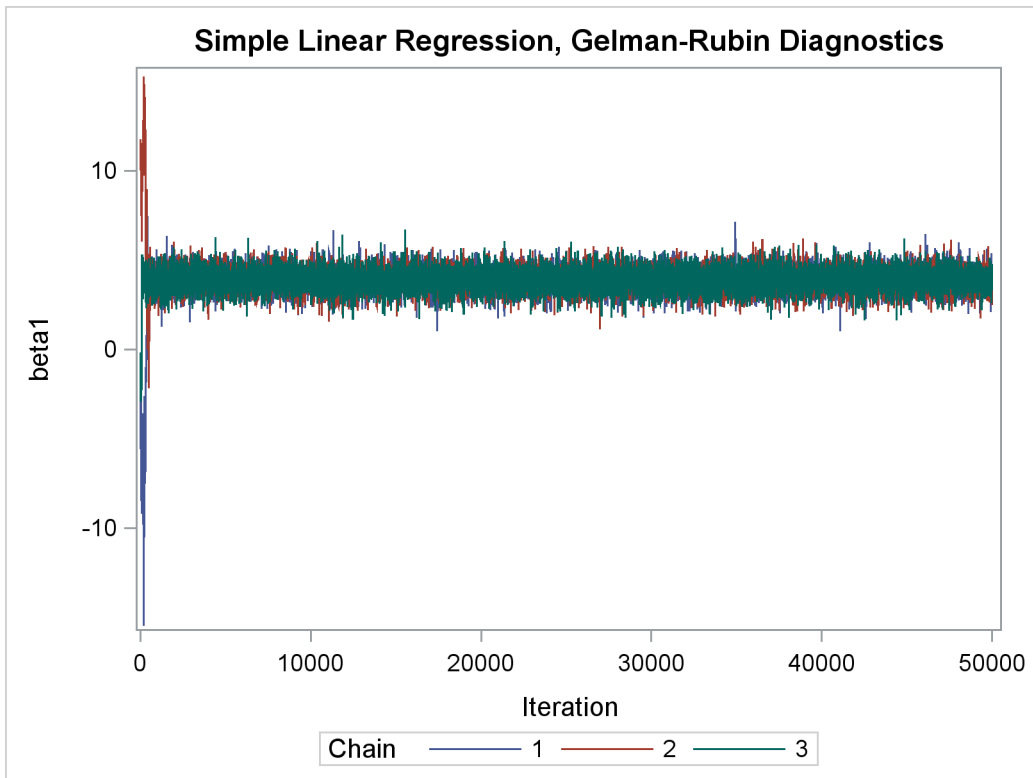
```

/* plot the trace plots of three Markov chains. */
%macro trace;
 %do i = 1 %to &nparm;
 proc sgplot data=all cycleattrs;
 series x=Iteration y=%scan(&var, &i) / group=Chain;
 run;
 %end;
%mend;
%trace;

```

**Output 55.21.2** Trace Plots of Three Chains for Each of the Parameters

Output 55.21.2 continued



The trace plots show that three chains all eventually converge to the same regions even though they started at very different locations. In addition to the trace plots, you can also plot the potential scale reduction factor (PSRF). See the section “[Gelman and Rubin Diagnostics](#)” on page 145 for definition and details.

The following statements calculate PSRF for each parameter. They use the GELMAN macro repeatedly and can take a while to run:

```

/* define sliding window size */
%let nwin = 200;
data PSRF;
run;

%macro PSRF(nsim);
 %do k = 1 %to %sysevalf(&nsim/&nwin, floor);
 %gelman(all, &nparm, &var, nsim=%sysevalf(&k*&nwin));
 data GelmanRubin;
 merge _Gelman_Parms _Gelman_Ests;
 run;

 data PSRF;
 set PSRF GelmanRubin;
 run;
 %end;
%mend PSRF;

options nonotes;
%PSRF(&nsim);
options notes;

data PSRF;
 set PSRF;
 if _n_ = 1 then delete;
run;

proc sort data=PSRF;
 by Parameter;
run;

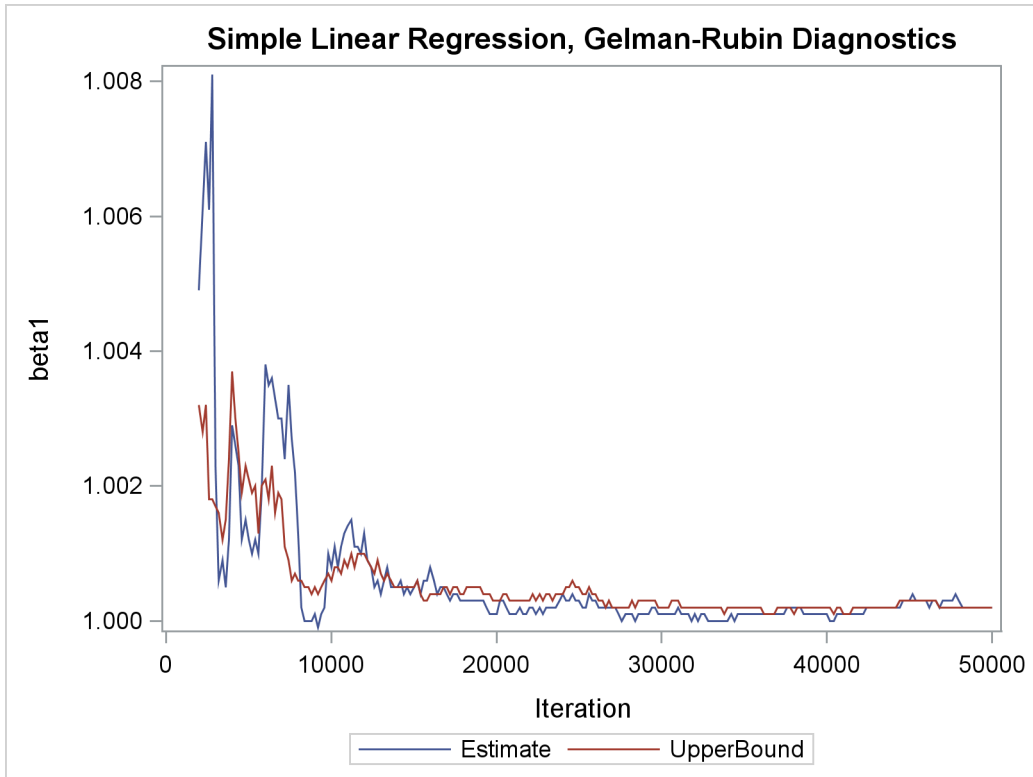
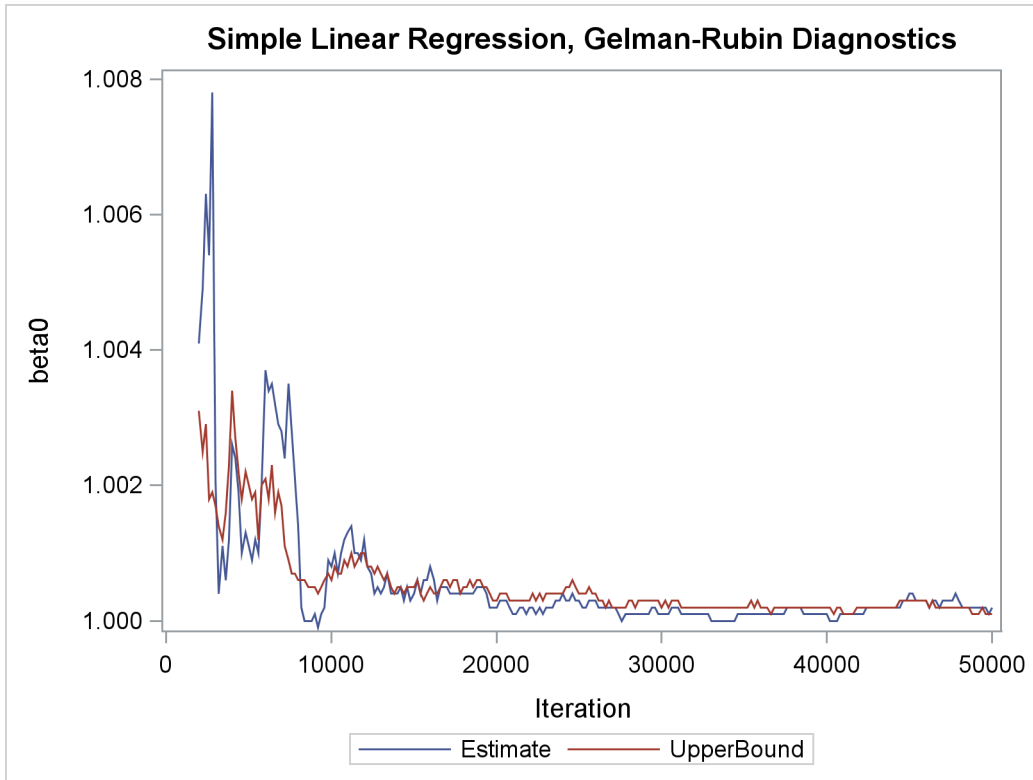
%macro sepPSRF(nparm=, var=, nsim=);
 %do k = 1 %to &nparm;
 data save&k; set PSRF;
 if _n_ > %sysevalf(&k*&nsim/&nwin, floor) then delete;
 if _n_ < %sysevalf((&k-1)*&nsim/&nwin + 1, floor) then delete;
 Iteration + &nwin;
 run;

 proc sgplot data=save&k(firstobs=10) cycleattrs;
 series x=Iteration y=Estimate;
 series x=Iteration y=upperbound;
 yaxis label="%scan(&var, &k)";
 run;
 %end;
%mend sepPSRF;

%sepPSRF(nparm=&nparm, var=&var, nsim=&nsim);

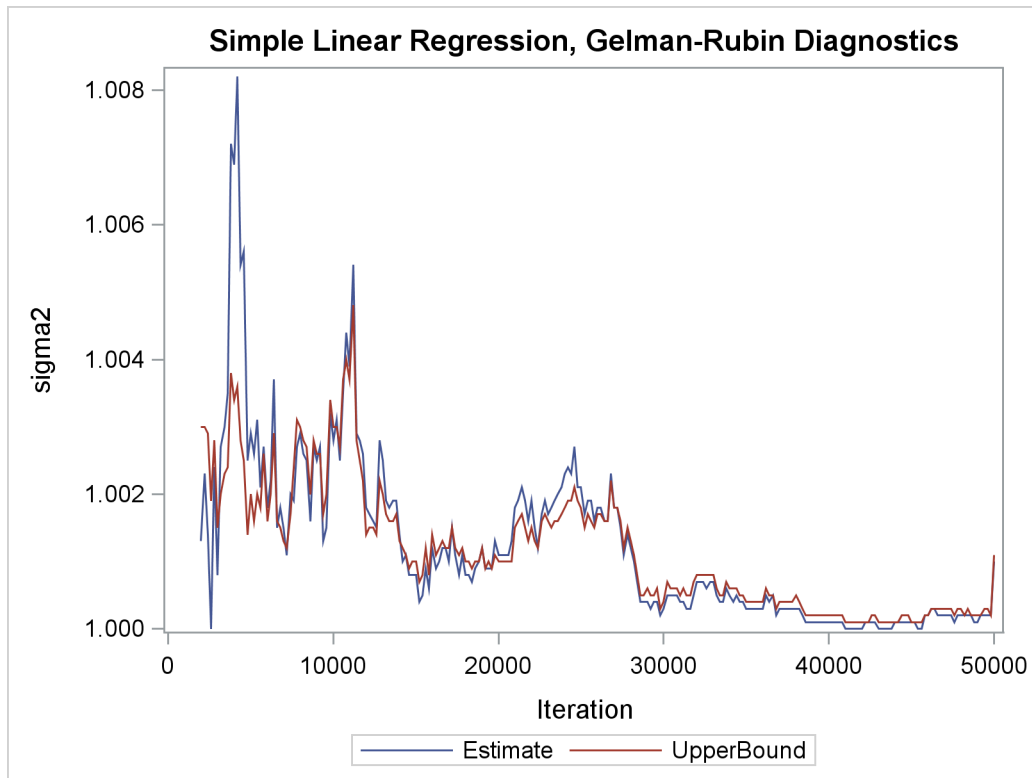
```

Output 55.21.3 PSRF Plot for Each Parameter





## Output 55.21.3 continued



PSRF is the square root of the ratio of the between-chain variance and the within-chain variance. A large PSRF indicates that the between-chain variance is substantially greater than the within-chain variance, so that longer simulation is needed. You want the PSRF to converge to 1 eventually, as it appears to be the case in this simulation study.

---

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# Chapter 56

## The MDS Procedure

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---

## Overview: MDS Procedure

Multidimensional scaling (MDS) refers to a class of methods. These methods estimate coordinates for a set of objects in a space of specified dimensionality. The input data are measurements of distances between pairs of objects. A variety of models can be used that include different ways of computing distances and various functions relating the distances to the actual data. The MDS procedure fits two- and three-way, metric and nonmetric multidimensional scaling models.

The data for the MDS procedure consist of one or more square symmetric or asymmetric matrices of similarities or dissimilarities between *objects* or *stimuli* (Kruskal and Wish 1978, pp. 7–11). Such data are also called *proximity* data. In psychometric applications, each matrix typically corresponds to a *subject*, and models that fit different parameters for each subject are called *individual difference* models.

Missing values are permitted. In particular, if the data are all missing except within some off-diagonal rectangle, the analysis is called *unfolding*. There are, however, many difficulties intrinsic to unfolding models (Heiser 1981). PROC MDS does not perform external unfolding; for analyses requiring external unfolding, use the TRANSREG procedure instead.

The MDS procedure estimates the following parameters by nonlinear least squares:

|                           |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
|---------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| configuration             | the coordinates of each object in a Euclidean (Kruskal and Wish 1978, pp. 17–19) or weighted Euclidean space (Kruskal and Wish 1978, pp. 61–63) of one or more dimensions                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
| dimension coefficients    | for each data matrix, the coefficients that multiply each coordinate of the <i>common</i> or <i>group</i> weighted Euclidean space to yield the <i>individual</i> unweighted Euclidean space. These coefficients are the square roots of the <i>subject weights</i> (Kruskal and Wish 1978, pp. 61–63). A plot of the dimension coefficients is directly interpretable in that it shows how a unit square in the group space is transformed to a rectangle in each individual space. A plot of subject weights has no such simple interpretation. The weighted Euclidean model is related to the INDSCAL model (Carroll and Chang 1970). |
| transformation parameters | intercept, slope, or exponent in a linear, affine, or power transformation relating the distances to the data (Kruskal and Wish 1978, pp. 19–22). For a nonmetric analysis, monotone transformations involving no explicit parameters are used (Kruskal and Wish 1978, pp. 22–25). For a discussion of metric versus nonmetric transformations, see Kruskal and Wish (1978, pp. 76–78).                                                                                                                                                                                                                                                  |

Depending on the LEVEL= option, PROC MDS fits either a regression model of the form

$$fit(datum) = fit(trans(distance)) + error$$

or a measurement model of the form

$$fit(trans(datum)) = fit(distance) + error$$

where

|                 |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |
|-----------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <i>fit</i>      | is a predetermined power or logarithmic transformation specified by the FIT= option.                                                                                                                                                                                                                                                                                                                                                                                                                                             |
| <i>trans</i>    | is an estimated (“optimal”) linear, affine, power, or monotone transformation specified by the LEVEL= option.                                                                                                                                                                                                                                                                                                                                                                                                                    |
| <i>datum</i>    | is a measure of the similarity or dissimilarity of two objects or stimuli.                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
| <i>distance</i> | is a distance computed from the estimated coordinates of the two objects and estimated dimension coefficients in a space of one or more dimensions. If there are no dimension coefficients (COEF=IDENTITY), this is an unweighted Euclidean distance. If dimension coefficients are used (COEF=DIAGONAL), this is a weighted Euclidean distance where the weights are the squares of the dimension coefficients; alternatively, you can multiply each dimension by its coefficient and compute an unweighted Euclidean distance. |
| <i>error</i>    | is an error term assumed to have an approximately normal distribution and to be independently and identically distributed for all data. Under these assumptions, least-squares estimation is statistically appropriate.                                                                                                                                                                                                                                                                                                          |

For an introduction to multidimensional scaling, see Kruskal and Wish (1978) and Arabie, Carroll, and DeSarbo (1987). A more advanced treatment is given by Young (1987). Many practical issues of data collection and analysis are discussed in Schiffman, Reynolds, and Young (1981). The fundamentals of psychological measurement, including both unidimensional and multidimensional scaling, are expounded by Torgerson (1958). Nonlinear least-squares estimation of PROC MDS models is discussed in Null and Sarle (1982).



## Getting Started: MDS Procedure

The simplest application of PROC MDS is to reconstruct a map from a table of distances between points on the map (Kruskal and Wish 1978, pp. 7–9). A data set containing a table of flying mileages between 10 U.S. cities is available in the Sashelp library.

Since the flying mileages are very good approximations to Euclidean distance, no transformation is needed to convert distances from the model to data. The analysis can therefore be done at the absolute level of measurement, as displayed in the following PROC MDS step (LEVEL=ABSOLUTE). The following statements produce Figure 56.1 and Figure 56.2:

```

title 'Analysis of Flying Mileages between Ten U.S. Cities';

ods graphics on;

proc mds data=sashelp.mileages level=absolute;
 id city;
run;

```

PROC MDS first displays the iteration history. In this example, only one iteration is required. The badness-of-fit criterion 0.001689 indicates that the data fit the model extremely well. You can also see that the fit is excellent in the fit plot in Figure 56.2.

**Figure 56.1** Iteration History from PROC MDS

| Analysis of Flying Mileages between Ten U.S. Cities  |         |                                 |                        |                        |
|------------------------------------------------------|---------|---------------------------------|------------------------|------------------------|
| Multidimensional Scaling: Data=SASHELP.MILEAGES.DATA |         |                                 |                        |                        |
| Shape=TRIANGLE Condition=MATRIX Level=ABSOLUTE       |         |                                 |                        |                        |
| Coef=IDENTITY Dimension=2 Formula=1 Fit=1            |         |                                 |                        |                        |
| Gconverge=0.01 Maxiter=100 Over=1 Ridge=0.0001       |         |                                 |                        |                        |
| Iteration                                            | Type    | Badness-<br>of-Fit<br>Criterion | Change in<br>Criterion | Convergence<br>Measure |
| 0                                                    | Initial | 0.003273                        | .                      | 0.8562                 |
| 1                                                    | Lev-Mar | 0.001689                        | 0.001584               | 0.005128               |
| Convergence criterion is satisfied.                  |         |                                 |                        |                        |

While PROC MDS can recover the relative positions of the cities, it cannot determine absolute location or orientation. In this case, north is toward the bottom of the plot. (See the first plot in [Figure 56.2](#).)

**Figure 56.2** Plot of Estimated Configuration and Fit

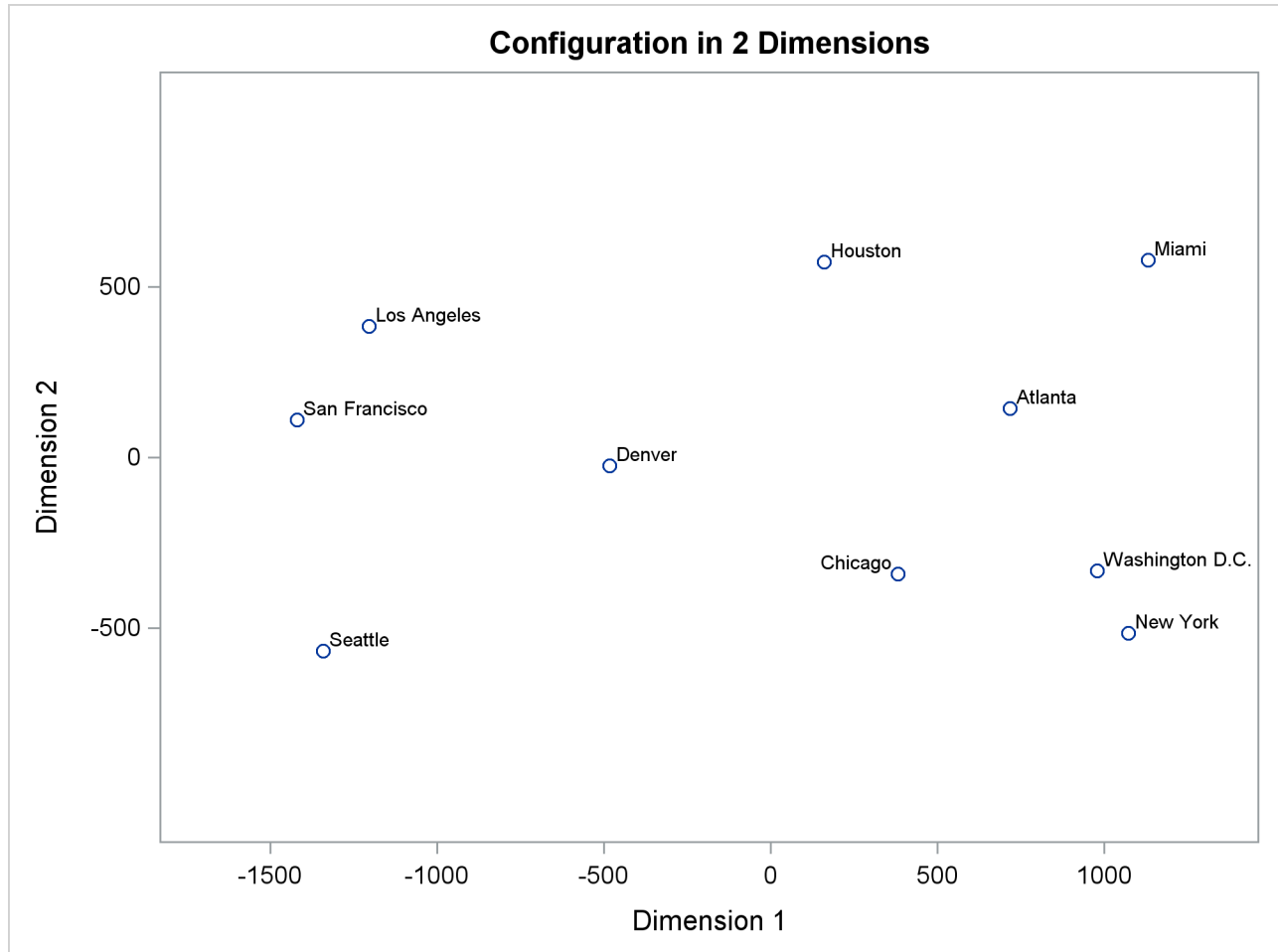
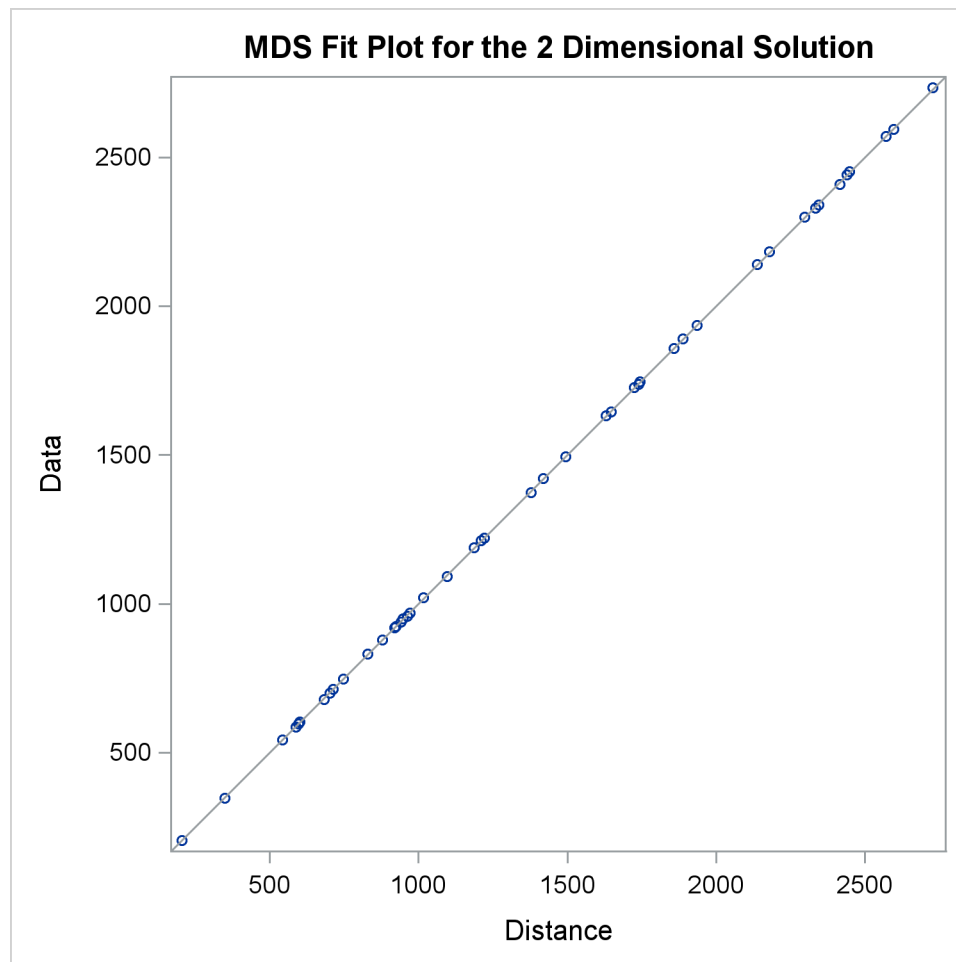


Figure 56.2 continued



---

## Syntax: MDS Procedure

The following statements are available in the MDS procedure:

```
PROC MDS < options > ;
 VAR variables ;
 INVAR variables ;
 ID | OBJECT variable ;
 MATRIX | SUBJECT variable ;
 WEIGHT variables ;
 BY variables ;
```

The PROC MDS statement is required. All other statements are optional.

## PROC MDS Statement

**PROC MDS** < options > ;

The PROC MDS statement invokes the MDS procedure. PROC MDS produces an iteration history by default. Graphical displays are produced when ODS Graphics is enabled. Additional displayed output is controlled by the interaction of the PCONFIG, PCOEF, PTRANS, PFIT, and PFITROW options with the PININ, PINIT, PITER, and PFINAL options. The PCONFIG, PCOEF, PTRANS, PFIT, and PFITROW options specify *which* estimates and fit statistics are to be displayed. The PININ, PINIT, PITER, and PFINAL options specify *when* the estimates and fit statistics are to be displayed. If you specify at least one of the PCONFIG, PCOEF, PTRANS, PFIT, and PFITROW options but none of the PININ, PINIT, PITER, and PFINAL options, the final results (PFINAL) are displayed. If you specify at least one of the PININ, PINIT, PITER, and PFINAL options but none of the PCONFIG, PCOEF, PTRANS, PFIT, and PFITROW options, all estimates (PCONFIG, PCOEF, PTRANS) and the fit statistics for each matrix and for the entire sample (PFIT) are displayed. If you do not specify any of these nine options, no estimates or fit statistics are displayed (except the badness-of-fit criterion in the iteration history).

The types of estimates written to the OUT= data set are determined by the OCONFIG, OCOEF, OTRANS, and OCRIT options. If you do not specify any of these four options, the estimates of all the parameters of the PROC MDS model and the value of the badness-of-fit criterion appear in the OUT= data set. If you specify one or more of these options, only the information requested by the specified options appears in the OUT= data set. Also, the OITER option causes these statistics to be written to the OUT= data set after initialization and on each iteration, as well as after the iterations have terminated.

Table 56.2 summarizes the options available in the PROC MDS statement.

**Table 56.2** Summary of PROC MDS Statement Options

| Option                  | Description                                                |
|-------------------------|------------------------------------------------------------|
| <b>Data Set Options</b> |                                                            |
| DATA=                   | Specifies the input SAS data set                           |
| INITIAL=                | Specifies the input SAS data set containing initial values |
| OUT=                    | Specifies the output data set                              |
| OUTFIT=                 | Specifies the output fit data set                          |
| OUTRES=                 | Specifies the output residual data set                     |
| <b>Input Control</b>    |                                                            |
| CUTOFF=                 | Replaces data values with missing values                   |
| SHAPE=                  | Specifies the shape of the input data matrices             |
| SIMILAR=                | Specifies that the data are similarity measurements        |
| <b>Model</b>            |                                                            |
| COEF=                   | Specifies the type of matrix for the coefficients          |
| CONDITION=              | Specifies the conditionality of the data                   |
| DIMENSION=              | Specifies the number of dimensions                         |
| LEVEL=                  | Specifies the measurement level                            |
| NEGATIVE                | Permits slopes or powers to be negative                    |
| UNTIE                   | Permits tied data to be untied                             |

Table 56.2 *continued*

| Option                                  | Description                                                        |
|-----------------------------------------|--------------------------------------------------------------------|
| <b>Initialization</b>                   |                                                                    |
| INAV=                                   | Affects the computation of initial coordinates                     |
| NOULB                                   | Specifies the missing data initialization                          |
| RANDOM=                                 | Specifies initial random coordinates                               |
| <b>Estimation</b>                       |                                                                    |
| ALTERNATE=                              | Specifies the alternating-least-squares algorithm                  |
| CONVERGE=                               | Specifies the convergence criterion                                |
| EPSILON=                                | Specifies the amount added to squared distances                    |
| FIT=                                    | Specifies a predetermined transformation                           |
| FORMULA=                                | Specifies the badness-of-fit formula                               |
| GCONVERGE=                              | Specifies the gradient convergence criterion                       |
| MAXITER=                                | Specifies the maximum number of iterations                         |
| MCONVERGE=                              | Specifies the monotone convergence criterion                       |
| MINCRIT=                                | Specifies the minimum badness-of-fit criterion                     |
| NONORM                                  | Suppresses normalization of the initial and final estimates        |
| OVER=                                   | Specifies the maximum overrelaxation factor                        |
| RIDGE=                                  | Specifies the initial ridge value                                  |
| SINGULAR=                               | Specifies the singularity criterion                                |
| <b>Control Output Data Set Contents</b> |                                                                    |
| OCOEF                                   | Writes the dimension coefficients to the OUT= data set             |
| ONCONFIG                                | Writes the coordinates of the objects to the OUT= data set         |
| OCRIT                                   | Writes the badness-of-fit criterion to the OUT= data set           |
| OITER                                   | Writes current values after initialization and on every iteration  |
| OTRANS                                  | Writes the transformation parameter estimates to the OUT= data set |
| <b>Control Displayed Output</b>         |                                                                    |
| DECIMALS=                               | Specifies how many decimal places to use                           |
| NOPHIST                                 | Suppresses the iteration history                                   |
| PCOEF                                   | Displays the estimated dimension coefficients                      |
| PCONFIG                                 | Displays the estimated coordinates                                 |
| PDATA                                   | Displays each data matrix                                          |
| PFINAL                                  | Displays final estimates                                           |
| PFIT                                    | Displays the badness-of-fit criterion                              |
| PFITROW                                 | Displays the badness-of-fit criterion for each row                 |
| PINAVDATA                               | Displays INAV= data set information                                |
| PINEIGVAL                               | Displays the initial eigenvalues                                   |
| PINEIGVEC                               | Displays the initial eigenvectors                                  |
| PININ                                   | Displays values read from the INITIAL= data set                    |
| PINIT                                   | Displays initial values                                            |
| PITER                                   | Displays estimates on each iteration                               |
| PLOTS=                                  | Controls the graphical displays                                    |
| PTRANS                                  | Displays the estimated transformation parameters                   |

**ALTERNATE | ALT=NONE | NO | N**

**ALTERNATE | ALT=MATRIX | MAT | M | SUBJECT | SUB | S**

**ALTERNATE | ALT=ROW | R < =n >**

determines what form of alternating-least-squares algorithm is used. The default depends on the amount of memory available. The following ALTERNATE= options are listed in order of decreasing memory requirements:

**ALT=NONE** causes all parameters to be adjusted simultaneously on each iteration. This option is usually best for a small number of subjects and objects.

**ALT=MATRIX** adjusts all the parameters for the first subject, then all the parameters for the second subject, and so on, and finally adjusts all parameters that do not correspond to a subject, such as coordinates and unconditional transformations. This option usually works best for a large number of subjects with a small number of objects.

**ALT=ROW** treats subject parameters the same way as the ALTERNATE=MATRIX option but also includes separate stages for unconditional parameters and for subsets of the objects. The ALT=ROW option usually works best for a large number of objects. Specifying ALT=ROW=*n* divides the objects into subsets of *n* objects each, except possibly for one subset when *n* does not divide the number of objects evenly. If you omit =*n*, the number of objects in the subsets is determined from the amount of memory available. The smaller the value of *n*, the less memory is required.

When you specify the LEVEL=ORDINAL option, the monotone transformation is always computed in a separate stage and is listed as a separate iteration in the iteration history. In this case, estimation is done by iteratively reweighted least squares. The weights are recomputed according to the FORMULA= option on each monotone iteration; hence, it is possible for the badness-of-fit criterion to increase after a monotone iteration.

**COEF=IDENTITY | IDEN | I**

**COEF=DIAGONAL | DIAG | D**

specifies the type of matrix for the dimension coefficients.

**COEF=IDENTITY** is the default, which yields Euclidean distances.

**COEF=DIAGONAL** produces weighted Euclidean distances, in which each subject can have different weights for the dimensions. The dimension coefficients that PROC MDS outputs are related to the square roots of what are called subject weights in PROC ALSCAL; the normalization in PROC MDS also differs from that in PROC ALSCAL. The weighted Euclidean model is related to the INDSCAL model (Carroll and Chang 1970).

**CONDITION | COND=UN | U****CONDITION | COND=MATRIX | MAT | M | SUBJECT | SUB | S****CONDITION | COND=ROW | R**

specifies the conditionality of the data (Young 1987, pp. 60–63). The data are divided into disjoint subsets called *partitions*. Within each partition, a separate transformation is applied, as specified by the LEVEL= option. The three types of conditionality are as follows:

- COND=UN                    (unconditional) puts all the data into a single partition.  
 COND=MATRIX            (matrix conditional) makes each data matrix a partition.  
 COND=ROW                (row conditional) makes each row of each data matrix a partition.

The default is CONDITION=MATRIX. The CONDITION= option also determines the default value for the SHAPE= option. If you specify the CONDITION=ROW option and omit the SHAPE= option, each data matrix is stored as a square and possibly asymmetric matrix. If you specify the CONDITION=UN or CONDITION=MATRIX option and omit the SHAPE= option, only one triangle is stored. See the SHAPE= option for details.

**CONVERGE | CONV= $\rho$** 

sets both the gradient convergence criterion and the monotone convergence criterion to  $\rho$ , where  $0 \leq \rho \leq 1$ . The default is CONVERGE=0.01; smaller values might greatly increase the number of iterations required. Values less than 0.0001 might be impossible to satisfy because of the limits of machine precision. (See the GCONVERGE= and MCONVERGE= options.)

**CUTOFF= $n$** 

replaces data values less than  $n$  with missing values. The default is CUTOFF=0.

**DATA=SAS-data-set**

specifies the SAS data set containing one or more square matrices to be analyzed. In typical psychometric data, each matrix contains judgments from one subject, so there is a one-to-one correspondence between data matrices and subjects.

The data matrices contain similarity or dissimilarity measurements to be modeled and, optionally, weights for these data. The data are generally assumed to be dissimilarities unless you use the SIMILAR option. However, if there are nonmissing diagonal values and these values are predominantly larger than the off-diagonal values, the data are assumed to be similarities and are treated as if the SIMILAR option is specified. The diagonal elements are not otherwise used in fitting the model.

Each matrix must have exactly the same number of observations as the number of variables specified by the VAR statement or determined by defaults. This number is the number of objects or stimuli.

The first observation and variable are assumed to contain data for the first object, the second observation and variable are assumed to contain data for the second object, and so on.

When there are two or more matrices, the observations in each matrix must correspond to the same objects in the same order as in the first matrix.

The matrices can be symmetric or asymmetric, as specified by the SHAPE= option.

**DECIMALS | DEC=*n***

specifies how many decimal places to use when displaying the parameter estimates and fit statistics. The default is DECIMALS=2, which is generally reasonable except in conjunction with the LEVEL=ABSOLUTE option and very large or very small data.

**DIMENSION | DIMENS | DIM=*n* < TO *m* < BY=*i* > >**

specifies the number of dimensions to use in the MDS model, where  $1 \leq n, m < \text{number of objects}$ . The parameter *i* can be either positive or negative but not zero. If you specify different values for *n* and *m*, a separate model is fitted for each requested dimension. If you specify only DIMENSION=*n*, then only *n* dimensions are fitted. The default is DIMENSION=2 if there are three or more objects; otherwise, DIMENSION=1 is the only valid specification. The analyses for each number of dimensions are done independently. For information about choosing the dimensionality, see Kruskal and Wish (1978, pp. 48–60).

**EPSILON | EPS=*n***

specifies a number *n*,  $0 < n < 1$ , that determines the amount added to squared distances computed from the model to avoid numerical problems such as division by 0. This amount is computed as  $\epsilon$  equal to *n* times the mean squared distance in the initial configuration. The distance in the MDS model is thus computed as

$$\text{distance} = \sqrt{\text{sqdist} + \epsilon}$$

where *sqdist* is the squared Euclidean distance or the weighted squared Euclidean distance.

The default is EPSILON=1E-12, which is small enough to have no practical effect on the estimates unless the FIT= value is nonpositive and there are dissimilarities that are very close to 0. Hence, when the FIT= value is nonpositive, dissimilarities less than *n* times 100 times the maximum dissimilarity are not permitted.

**FIT=DISTANCE | DIS | D****FIT=SQUARED | SQU | S****FIT=LOG | L****FIT=*n***

specifies a predetermined (not estimated) transformation to apply to both sides of the MDS model before the error term is added.

The default is FIT=DISTANCE or, equivalently, FIT=1, which fits data to distances.

The option FIT=SQUARED or FIT=2 fits squared data to squared distances. This gives greater importance to large data and distances and lesser importance to small data and distances in fitting the model.

The FIT=LOG or FIT=0 option fits log data to log distances. This gives lesser importance to large data and distances and greater importance to small data and distances in fitting the model.

In general, the FIT=*n* option fits *n*th-power data to *n*th-power distances. Values of *n* that are large in absolute value can cause floating-point overflows.

If the FIT= value is 0 or negative, the data must be strictly positive (see the EPSILON= option). Negative data might produce strange results with any value other than FIT=1.



**FORMULA | FOR=0 | OLS | O****FORMULA | FOR=1 | USS | U****FORMULA | FOR=2 | CSS | C**

determines how the badness-of-fit criterion is standardized in correspondence with stress formulas 1 and 2 (Kruskal and Wish 1978, pp. 24–26). The default is FORMULA=1 unless you specify FIT=LOG, in which case the default is FORMULA=2. Data partitions are defined by the CONDITION= option.

**FORMULA=0** fits a regression model by ordinary least squares (Null and Sarle 1982) without standardizing the partitions; this option cannot be used with the LEVEL=ORDINAL option. The badness-of-fit criterion is the square root of the error sum of squares.

**FORMULA=1** standardizes each partition by the uncorrected sum of squares of the (possibly transformed) data; this option should not be used with the FIT=LOG option. With the FIT=DISTANCE and LEVEL=ORDINAL options, this is equivalent to Kruskal's stress formula 1 or an obvious generalization thereof. With the FIT=SQUARED and LEVEL=ORDINAL options, this is equivalent to Young's s-stress formula 1 or an obvious generalization thereof. The badness-of-fit criterion is analogous to  $\sqrt{1 - R^2}$ , where R is a multiple correlation about the origin.

**FORMULA=2** standardizes each partition by the corrected sum of squares of the (possibly transformed) data; this option is the recommended method for unfolding. With the FIT=DISTANCE and LEVEL=ORDINAL options, this is equivalent to Kruskal's stress formula 2 or an obvious generalization thereof. With the FIT=SQUARED and LEVEL=ORDINAL options, this is equivalent to Young's s-stress formula 2 or an obvious generalization thereof. The badness-of-fit criterion is analogous to  $\sqrt{1 - R^2}$ , where R is a multiple correlation computed with a denominator corrected for the mean.

**GCONVERGE | GCONV= $p$** 

sets the gradient convergence criterion to  $p$ , where  $0 \leq p \leq 1$ . The default is GCONVERGE=0.01; smaller values might greatly increase the number of iterations required. Values less than 0.0001 might be impossible to satisfy because of the limits of machine precision.

The gradient convergence measure is the multiple correlation of the Jacobian matrix with the residual vector, uncorrected for the mean. (See the CONVERGE= and MCONVERGE= options.)

**INAV=DATA | D****INAV=SSCP | S**

affects the computation of initial coordinates. The default is INAV=DATA.

**INAV=DATA** computes a weighted average of the data matrices. Its value is estimated only if an element is missing from every data matrix. The weighted average of the data matrices with missing values filled in is then converted to a scalar products matrix (or what would be a scalar products matrix if the fit were perfect), from which the initial coordinates are computed.

**INAV=SSCP** estimates missing values in each data matrix and converts each data matrix to a scalar products matrix. The initial coordinates are computed from the unweighted average of the scalar products matrices.

**INITIAL** | **IN=SAS-data-set**

specifies a SAS data set containing initial values for some or all of the parameters of the MDS model. If the INITIAL= option is omitted, the initial values are computed from the data.

**LEVEL=ABSOLUTE** | **ABS** | **A****LEVEL=RATIO** | **RAT** | **R****LEVEL=INTERVAL** | **INT** | **I****LEVEL=LOGINTERVAL** | **LOG** | **L****LEVEL=ORDINAL** | **ORD** | **O**

specifies the measurement level of the data and hence the type of estimated (optimal) transformations applied to the data or distances (Young 1987, pp. 57–60; Krantz et al. 1971, pp. 9–12) within each partition as specified by the CONDITION= option. LEVEL=ORDINAL specifies a nonmetric analysis, while all other LEVEL= options specify metric analyses. The default is LEVEL=ORDINAL.

|                   |                                                                                                                                                                                                                                                                      |
|-------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| LEVEL=ABSOLUTE    | permits no optimal transformations. Hence, the distinction between regression and measurement models is irrelevant.                                                                                                                                                  |
| LEVEL=RATIO       | fits a regression model in which the distances are multiplied by a slope parameter in each partition (a linear transformation). In this case, the regression model is equivalent to the measurement model with the slope parameter reciprocated.                     |
| LEVEL=INTERVAL    | fits a regression model in which the distances are multiplied by a slope parameter and added to an intercept parameter in each partition (an affine transformation). In this case, the regression and measurement models differ if there is more than one partition. |
| LEVEL=LOGINTERVAL | fits a regression model in which the distances are raised to a power and multiplied by a slope parameter in each partition (a power transformation).                                                                                                                 |
| LEVEL=ORDINAL     | fits a measurement model in which a least-squares monotone increasing transformation is applied to the data in each partition. At the ordinal measurement level, the regression and measurement models differ.                                                       |

**MAXITER** | **ITER=n**

specifies the maximum number of iterations, where  $n \geq 0$ . The default is MAXITER=100.

**MCONVERGE** | **MCONV=p**

sets the monotone convergence criterion to  $p$ , where  $0 \leq p \leq 1$ , for use with the LEVEL=ORDINAL option. The default is MCONVERGE=0.01; if you want greater precision, MCONVERGE=0.001 is usually reasonable, but smaller values might greatly increase the number of iterations required.

The monotone convergence criterion is the Euclidean norm of the change in the optimally scaled data divided by the Euclidean norm of the optimally scaled data, averaged across partitions defined by the CONDITION= option. (See the CONVERGE= and GCONVERGE= options.)

**MINCRIT** | **CRITMIN=n**

causes iteration to terminate when the badness-of-fit criterion is less than or equal to  $n$ , where  $n \geq 0$ . The default is MINCRIT=1E-6.

**NEGATIVE**

permits slopes or powers to be negative with the LEVEL=RATIO, INTERVAL, or LOGINTERVAL option.

**NONORM**

suppresses normalization of the initial and final estimates.

**NOPHIST | NOPRINT | NOP**

suppresses the output of the iteration history.

**NOULB**

causes missing data to be estimated during initialization by the average nonmissing value, where the average is computed according to the FIT= option. Otherwise, missing data are estimated by interpolating between the Rabinowitz (1976) upper and lower bounds.

**OCOEF**

writes the dimension coefficients to the OUT= data set. See the OUT= option for interactions with other options.

**OCONFIG**

writes the coordinates of the objects to the OUT= data set. See the OUT= option for interactions with other options.

**OCRIT**

writes the badness-of-fit criterion to the OUT= data set. See the OUT= option for interactions with other options.

**OITER | OUTITER**

writes current values to the output data sets after initialization and on every iteration. Otherwise, only the final values are written to any output data sets. (See the OUT=, OUTFIT=, and OUTRES= options.)

**OTRANS**

writes the transformation parameter estimates to the OUT= data set if any such estimates are computed. There are no transformation parameters with the LEVEL=ORDINAL option. See the OUT= option for interactions with other options.

**OUT=SAS-data-set**

creates a SAS data set containing, by default, the estimates of all the parameters of the PROC MDS model and the value of the badness-of-fit criterion. However, if you specify one or more of the OCONFIG, OCOEF, OTRANS, and OCRIT options, only the information requested by the specified options appears in the OUT= data set. (See also the OITER option.)

**OUTFIT=SAS-data-set**

creates a SAS data set containing goodness-of-fit and badness-of-fit measures for each partition as well as for the entire data set. (See also the OITER option.)

**OUTRES=SAS-data-set**

creates a SAS data set containing one observation for each nonmissing data value from the DATA= data set. Each observation contains the original data value, the estimated distance computed from the MDS model, transformed data and distances, and the residual. (See also the OITER option.)

**OVER=*n***

specifies the maximum overrelaxation factor, where  $n \geq 1$ . Values between 1 and 2 are generally reasonable. The default is OVER=2 with the LEVEL=ORDINAL, ALTERNATE=MATRIX, or ALTERNATE=ROW option; otherwise, the default is OVER=1. Use this option only if you have convergence problems.

**PCOEF**

produces the estimated dimension coefficients.

**PCONFIG**

produces the estimated coordinates of the objects in the configuration.

**PDATA**

displays each data matrix.

**PFINAL**

displays final estimates.

**PFIT**

displays the badness-of-fit criterion and various types of correlations between the data and fitted values for each data matrix, as well as for the entire sample.

**PFITROW**

displays the badness-of-fit criterion and various types of correlations between the data and fitted values for each row, as well as for each data matrix and for the entire sample. This option works only with the CONDITION=ROW option.

**PINAVDATA**

displays the sum of the weights and the weighted average of the data matrices computed during initialization with the INAV=DATA option.

**PINEIGVAL**

displays the eigenvalues computed during initialization.

**PINEIGVEC**

displays the eigenvectors computed during initialization.

**PININ**

displays values read from the INITIAL= data set. Since these values might be incomplete, the PFIT and PFITROW options do not apply.

**PINIT**

displays initial values.

**PITER**

displays estimates on each iteration.

**PLOTS**< (*global-plot-option*) > <= *plot-request* < (*options*) > >

**PLOTS**< (*global-plot-options*) > <= (*plot-request* < (*options*) > < ... *plot-request* < (*options*) > > >

specifies options that control the details of the plots. When you specify only one plot request, you can omit the parentheses around the plot request.

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;

proc mds plots(flip);
run;

ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS](#).”

The global plot option is as follows:

#### **FLIP**

flips or interchanges the X-axis and Y-axis dimensions for configuration and coefficient plots.

The plot requests include the following:

#### **COEFFICIENTS(ONE)**

combines the INDSCAL coefficients panel of plots into a single plot. By default, the display consists of a panel with two plots. The vectors are displayed in the left plot, and the labels are displayed in the right plot. The right plot provides a magnification of the region of the vector endpoints. In contrast, the single display, requested by COEFFICIENTS(ONE), is more compact, but there is less room for vector labels. It is often easier to identify the vectors in the default display.

#### **NONE**

suppresses all plots.

By default, a fit plot is produced. When more than one dimension is requested, plots of the configuration are also plotted. For individual differences models with more than one dimension, the subject weights or coefficients are plotted. When more than one value is specified for the DIMENSION= option, the badness-of-fit plot is produced.

#### **PTRANS**

displays the estimated transformation parameters if any are computed. There are no transformation parameters with the LEVEL=ORDINAL option.

#### **RANDOM< =seed >**

causes initial coordinate values to be pseudo-random numbers. In one dimension, the pseudo-random numbers are uniformly distributed on an interval. In two or more dimensions, the pseudo-random numbers are uniformly distributed on the circumference of a circle or the surface of a (hyper)sphere.

**RIDGE=*n***

specifies the initial ridge value, where  $n \geq 0$ . The default is `RIDGE=1E-4`.

If you get a floating-point overflow in the first few iterations, specify a larger value such as `RIDGE=0.01`, `RIDGE=1`, or `RIDGE=100`.

If you know that the initial estimates are very good, using `RIDGE=0` might speed convergence.

**SHAPE=TRIANGULAR | TRIANGLE | TRI | T****SHAPE=SQUARE | SQU | S**

determines whether the entire data matrix for each subject or only one triangle of the matrix is stored and analyzed. If you specify the `CONDITION=ROW` option, the default is `SHAPE=SQUARE`. Otherwise, the default is `SHAPE=TRIANGLE`.

`SHAPE=SQUARE` causes the entire matrix to be stored and analyzed. The matrix can be asymmetric.

`SHAPE=TRIANGLE` causes only one triangle to be stored. However, PROC MDS reads both upper and lower triangles to look for nonmissing values and to symmetrize the data if needed. If corresponding elements in the upper and lower triangles both contain nonmissing values, only the average of the two values is stored and analyzed (Kruskal and Wish 1978, p. 74). Also, if an `OUTRES=` data set is requested, only the average of the two corresponding elements is output.

**SIMILAR | SIM<=*max*>**

causes the data to be treated as similarity measurements rather than dissimilarities. If `=max` is not specified, each data value is converted to a dissimilarity by subtracting it from the maximum value in the data set or BY group. If `=max` is specified, each data value is subtracted from the maximum of `max` and the data. The diagonal data are included in computing these maxima.

By default, the data are assumed to be dissimilarities unless there are nonmissing diagonal values and these values are predominantly larger than the off-diagonal values. In this case, the data are assumed to be similarities and are treated as if the `SIMILAR` option is specified.

**SINGULAR=*p***

specifies the singularity criterion  $p$ ,  $0 \leq p \leq 1$ . The default is `SINGULAR=1E-8`.

**UNTIE**

permits tied data to be assigned different optimally scaled values with the `LEVEL=ORDINAL` option. Otherwise, tied data are assigned equal optimally scaled values. The `UNTIE` option has no effect with values of the `LEVEL=` option other than `LEVEL=ORDINAL`.

---

## BY Statement

**BY variables ;**

You can specify a BY statement with PROC MDS to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the MDS procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

If the INITIAL= data set contains the BY variables, the BY groups must appear in the same order as in the DATA= data set. If the BY variables are not in the INITIAL= data set, the entire data set is used to provide initial values for each BY group in the DATA= data set.

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

---

## ID Statement

**ID | OBJECT | OBJ variable ;**

The ID statement specifies a variable in the DATA= data set that contains descriptive labels for the objects. The labels are used in the output and are copied to the OUT= data set. If there is more than one data matrix, only the ID values from the observations containing the first data matrix are used.

The ID variable is not used to establish any correspondence between observations and variables.

If the ID statement is omitted, the variable labels or names are used as object labels.

---

## INVAR Statement

**INVAR variables ;**

The INVAR statement specifies the numeric variables in the INITIAL= data set that contain initial parameter estimates. The first variable corresponds to the first dimension, the second variable to the second dimension, and so on.

If the INVAR statement is omitted, the variables Dim1, . . . , Dim $m$  are used, where  $m$  is the maximum number of dimensions.

---

## MATRIX Statement

**MATRIX | MAT | SUBJECT | SUB** *variable* ;

The MATRIX statement specifies a variable in the DATA= data set that contains descriptive labels for the data matrices or subjects. The labels are used in the output and are copied to the OUT= and OUTRES= data sets. Only the first observation from each data matrix is used to obtain the label for that matrix.

If the MATRIX statement is omitted, the matrices are labeled 1, 2, 3, and so on.

---

## VAR Statement

**VAR** *variables* ;

The VAR statement specifies the numeric variables in the DATA= data set that contain similarity or dissimilarity measurements on a set of objects or stimuli. Each variable corresponds to one object.

If the VAR statement is omitted, all numeric variables that are not specified in another statement are used.

To analyze a subset of the objects in a data set, you can specify the variable names corresponding to the columns in the subset, but you must also use a DATA step or a WHERE clause to specify the rows in the subset. PROC MDS expects to read one or more square matrices, and you must ensure that the rows in the data set correctly correspond to the columns in number and order.

---

## WEIGHT Statement

**WEIGHT** *variables* ;

The WEIGHT statement specifies numeric variables in the DATA= data set that contain weights for each similarity or dissimilarity measurement. These weights are used to compute weighted least-squares estimates. The number of WEIGHT variables must be the same as the number of VAR variables, and the variables in the WEIGHT statement must be in the same order as the corresponding variables in the VAR statement.

If the WEIGHT statement is omitted, all data within a partition are assigned equal weights.

Data with zero or negative weights are ignored in fitting the model but are included in the OUTRES= data set and in monotone transformations.



---

## Details: MDS Procedure

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### Formulas

The following notation is used:

|              |                                                                                                                                    |
|--------------|------------------------------------------------------------------------------------------------------------------------------------|
| $A_p$        | intercept for partition $p$                                                                                                        |
| $B_p$        | slope for partition $p$                                                                                                            |
| $C_p$        | power for partition $p$                                                                                                            |
| $D_{rcs}$    | distance computed from the model between objects $r$ and $c$ for subject $s$                                                       |
| $F_{rcs}$    | data weight for objects $r$ and $c$ for subject $s$ obtained from the $c$ th WEIGHT variable, or 1 if there is no WEIGHT statement |
| $f$          | value of the FIT= option                                                                                                           |
| $N$          | number of objects                                                                                                                  |
| $O_{rcs}$    | observed dissimilarity between objects $r$ and $c$ for subject $s$                                                                 |
| $P_{rcs}$    | partition index for objects $r$ and $c$ for subject $s$                                                                            |
| $Q_{rcs}$    | dissimilarity after applying any applicable estimated transformation for objects $r$ and $c$ for subject $s$                       |
| $R_{rcs}$    | residual for objects $r$ and $c$ for subject $s$                                                                                   |
| $S_p$        | standardization factor for partition $p$                                                                                           |
| $T_p(\cdot)$ | estimated transformation for partition $p$                                                                                         |
| $V_{sd}$     | coefficient for subject $s$ on dimension $d$                                                                                       |
| $X_{nd}$     | coordinate for object $n$ on dimension $d$                                                                                         |

Summations are taken over nonmissing values.

Distances are computed from the model as

$$\begin{aligned}
 D_{rcs} &= \sqrt{\sum_d (X_{rd} - X_{cd})^2} && \text{for COEF=IDENTITY:} \\
 &&& \text{Euclidean distance} \\
 &= \sqrt{\sum_d V_{sd}^2 (X_{rd} - X_{cd})^2} && \text{for COEF=DIAGONAL:} \\
 &&& \text{weighted Euclidean distance}
 \end{aligned}$$

Partition indexes are

$$\begin{aligned}
 P_{rcs} &= 1 && \text{for CONDITION=UN} \\
 &= s && \text{for CONDITION=MATRIX} \\
 &= (s - 1)N + r && \text{for CONDITION=ROW}
 \end{aligned}$$

The estimated transformation for each partition is

$$\begin{aligned} T_p(d) &= d && \text{for LEVEL=ABSOLUTE} \\ &= B_p d && \text{for LEVEL=RATIO} \\ &= A_p + B_p d && \text{for LEVEL=INTERVAL} \\ &= B_p d^{C_p} && \text{for LEVEL=LOGINTERVAL} \end{aligned}$$

For LEVEL=ORDINAL,  $T_p(\cdot)$  is computed as a least-squares monotone transformation.

For LEVEL=ABSOLUTE, RATIO, or INTERVAL, the residuals are computed as

$$\begin{aligned} Q_{rcs} &= O_{rcs} \\ R_{rcs} &= Q_{rcs}^f - [T_{P_{rcs}}(D_{rcs})]^f \end{aligned}$$

For LEVEL=ORDINAL, the residuals are computed as

$$\begin{aligned} Q_{rcs} &= T_{P_{rcs}}(O_{rcs}) \\ R_{rcs} &= Q_{rcs}^f - D_{rcs}^f \end{aligned}$$

If  $f$  is 0, then natural logarithms are used in place of the  $f$ th powers.

For each partition, let

$$U_p = \frac{\sum_{r,c,s} F_{rcs}}{\sum_{r,c,s|P_{rcs}=p} F_{rcs}}$$

and

$$\bar{Q}_p = \frac{\sum_{r,c,s|P_{rcs}=p} Q_{rcs} F_{rcs}}{\sum_{r,c,s|P_{rcs}=p} F_{rcs}}$$

Then the standardization factor for each partition is

$$\begin{aligned} S_p &= 1 && \text{for FORMULA=0} \\ &= U_p \sum_{r,c,s|P_{rcs}=p} Q_{rcs}^2 F_{rcs} && \text{for FORMULA=1} \\ &= U_p \sum_{r,c,s|P_{rcs}=p} (Q_{rcs} - \bar{Q}_p)^2 F_{rcs} && \text{for FORMULA=2} \end{aligned}$$

The badness-of-fit criterion that the MDS procedure tries to minimize is

$$\sqrt{\sum_{r,c,s} \frac{R_{rcs}^2 F_{rcs}}{S_{P_{rcs}}}}$$

---

## OUT= Data Set

The OUT= data set contains the following variables:

- BY variables, if any
- `_ITER_` (if the OUTITER option is specified), a numeric variable containing the iteration number
- `_DIMENS_`, a numeric variable containing the number of dimensions
- `_MATRIX_` or the variable in the MATRIX statement, identifying the data matrix or subject to which the observation pertains. This variable contains a missing value for observations that pertain to the data set as a whole and not to a particular matrix, such as the coordinates (`_TYPE_='CONFIG'`).
- `_TYPE_`, a character variable of length 10 identifying the type of information in the observation

The values of `_TYPE_` are as follows:

|           |                                                           |
|-----------|-----------------------------------------------------------|
| CONFIG    | the estimated coordinates of the configuration of objects |
| DIAGCOEF  | the estimated dimension coefficients for COEF=DIAGONAL    |
| INTERCEPT | the estimated intercept parameters                        |
| SLOPE     | the estimated slope parameters                            |
| POWER     | the estimated power parameters                            |
| CRITERION | the badness-of-fit criterion                              |

- `_LABEL_` or the variable in the ID statement, containing the variable label or value of the ID variable of the object to which the observation pertains. This variable contains a missing value for observations that do not pertain to a particular object or dimension.
- `_NAME_`, a character variable containing the variable name of the object or dimension to which the observation pertains. This variable contains a missing value for observations that do not pertain to a particular object or dimension.
- Dim1, . . . , Dim $m$ , where  $m$  is the maximum number of dimensions

---

## OUTFIT= Data Set

The OUTFIT= data set contains various measures of goodness and badness of fit. There is one observation for the entire sample plus one observation for each matrix. For the CONDITION=ROW option, there is also one observation for each row.

The OUTFIT= data set contains the following variables:

- BY variables, if any
- `_ITER_` (if the OUTITER option is specified), a numeric variable containing the iteration number

- `_DIMENS_`, a numeric variable containing the number of dimensions
- `_MATRIX_` or the variable in the `MATRIX` statement, identifying the data matrix or subject to which the observation pertains
- `_LABEL_` or the variable in the `ID` statement, containing the variable label or value of the `ID` variable of the object to which the observation pertains when `CONDITION=ROW`
- `_NAME_`, a character variable containing the variable name of the object or dimension to which the observation pertains when `CONDITION=ROW`
- `N`, the number of nonmissing data
- `WEIGHT`, the weight of the partition
- `CRITER`, the badness-of-fit criterion
- `DISCORR`, the correlation between the transformed data and the distances for `LEVEL=ORDINAL` or the correlation between the data and the transformed distances otherwise
- `UDISCORR`, the correlation uncorrected for the mean between the transformed data and the distances for `LEVEL=ORDINAL` or the correlation between the data and the transformed distances otherwise
- `FITCORR`, the correlation between the fit-transformed data and the fit-transformed distances
- `UFITCORR`, the correlation uncorrected for the mean between the fit-transformed data and the fit-transformed distances

---

## OUTRES= Data Set

The `OUTRES=` data set has one observation for each nonmissing data value. It contains the following variables:

- `BY` variables, if any
- `_ITER_` (if the `OUTITER` option is specified), a numeric variable containing the iteration number
- `_DIMENS_`, a numeric variable containing the number of dimensions
- `_MATRIX_` or the variable in the `MATRIX` statement, identifying the data matrix or subject to which the observation pertains
- `_ROW_`, containing the variable label or value of the `ID` variable of the row to which the observation pertains
- `_COL_`, containing the variable label or value of the `ID` variable of the column to which the observation pertains
- `DATA`, the original data value
- `TRANDATA`, the optimally transformed data value when `LEVEL=ORDINAL`

- DISTANCE, the distance computed from the PROC MDS model
- TRANSDIST, the optimally transformed distance when the LEVEL= option is not ORDINAL or ABSOLUTE
- FITDATA, the data value further transformed according to the FIT= option
- FITDIST, the distance further transformed according to the FIT= option
- WEIGHT, the combined weight of the data value based on the WEIGHT variable(s), if any, and the standardization specified by the FORMULA= option
- RESIDUAL, FITDATA minus FITDIST

If you assign a nonmissing data value a weight of zero, PROC MDS will ignore it when the model is fit, but the value will still appear in the OUTRES= data set (see the section “WEIGHT Statement” on page 4693).

---

## INITIAL= Data Set

The INITIAL= data set has the same structure as the OUT= data set but is not required to have all of the variables or observations that appear in the OUT= data set. You can use an OUT= data set previously created by PROC MDS (without the OUTITER option) as an INITIAL= data set in a subsequent invocation of the procedure.

The only variables that are required are Dim1, . . . , Dim $m$  (where  $m$  is the maximum number of dimensions) or equivalent variables specified in the INVAR statement. If these are the only variables, then all the observations are assumed to contain coordinates of the configuration; you cannot read dimension coefficients or transformation parameters.

To read initial values for the dimension coefficients or transformation parameters, the INITIAL= data set must contain the \_TYPE\_ variable and either the variable specified in the ID statement or, if no ID statement is used, the variable \_NAME\_. In addition, if there is more than one data matrix, either the variable specified in the MATRIX statement or, if no MATRIX statement is used, the variable \_MATRIX\_ or \_MATNUM\_ is required.

If the INITIAL= data set contains the variable \_DIMENS\_, initial values are obtained from observations with the corresponding number of dimensions. If there is no \_DIMENS\_ variable, the same observations are used for each number of dimensions analyzed.

If you want PROC MDS to read initial values from some but not all of the observations in the INITIAL= data set, use the WHERE= data set option to select the desired observations.

---

## Missing Values

Missing data in the similarity or dissimilarity matrices are ignored in fitting the model and are omitted from the OUTRES= data set. Any matrix that is completely missing is omitted from the analysis.

Missing weights are treated as 0.

Missing values are also permitted in the INITIAL= data set, but a large number of missing values might yield a degenerate initial configuration.

---

## Normalization of the Estimates

In multidimensional scaling models, the parameter estimates are not uniquely determined; the estimates can be transformed in various ways without changing their badness of fit. The initial and final estimates from PROC MDS are, therefore, normalized (unless you specify the NONORM option) to make it easier to compare results from different analyses.

The configuration always has a mean of 0 for each dimension.

With the COEF=IDENTITY option, the configuration is rotated to a principal-axis orientation. Unless you specify the LEVEL=ABSOLUTE option, the entire configuration is scaled so that the root-mean-square element is 1, and the transformations are adjusted to compensate.

With the COEF=DIAGONAL option, each dimension is scaled to a root-mean-square value of 1, and the dimension coefficients are adjusted to compensate. Unless you specify the LEVEL=ABSOLUTE option, the dimension coefficients are normalized as follows. If you specify the CONDITION=UN option, all of the dimension coefficients are scaled to a root-mean-square value of 1. For other values of the CONDITION= option, the dimension coefficients are scaled separately for each subject to a root-mean-square value of 1. In either case, the transformations are adjusted to compensate.

Each dimension is reflected to give a positive rank correlation with the order of the objects in the data set.

For the LEVEL=ORDINAL option, if the intercept, slope, or power parameters are fitted, the transformed data are normalized to eliminate these parameters if possible.

---

## Comparison with Earlier Procedures

PROC MDS shares many of the features of the ALSCAL procedure (Young, Lewyckyj, and Takane 1986; Young 1982), as well as some features of the MLSCALE procedure (Ramsay 1986). Both PROC ALSCAL and PROC MLSCALE are no longer a part of SAS; however, they are described in the *SUGI Supplemental Library User's Guide, Version 5 Edition*. The MDS procedure generally produces results similar to those from the ALSCAL procedure (Young, Lewyckyj, and Takane 1986; Young 1982) if you use the following options in PROC MDS:

- FIT=SQUARED
- FORMULA=1 except for unfolding data, which require FORMULA=2
- PFINAL to get output similar to that from PROC ALSCAL

Running the MDS procedure with certain options generally produces results similar to those from using the MLSCALE procedure (Ramsay 1986) with other options. This is illustrated with the following statements:

```
proc mds fit=log level=loginterval ... ;
```

```
proc mlscale stvarnce=constant suvarnce=constant ... ;
```

Alternatively, using the FIT=DISTANCE option in the PROC MDS statement produces results similar to those from specifying the NORMAL option in the PROC MLSCALE statement.

## Displayed Output

Unless you specify the NOPHIST option, PROC MDS displays the iteration history containing the following:

- Iteration number
- Type of iteration:
 

|          |                          |
|----------|--------------------------|
| Initial  | initial configuration    |
| Monotone | monotone transformation  |
| Gau-New  | Gauss-Newton step        |
| Lev-Mar  | Levenberg-Marquardt step |
- Badness-of-Fit Criterion
- Change in Criterion
- Convergence Measures:
 

|          |                                                                                                                                                      |
|----------|------------------------------------------------------------------------------------------------------------------------------------------------------|
| Monotone | the Euclidean norm of the change in the optimally scaled data divided by the Euclidean norm of the optimally scaled data, averaged across partitions |
| Gradient | the multiple correlation of the Jacobian matrix with the residual vector, uncorrected for the mean                                                   |

Depending on what options are specified, PROC MDS can also display the following tables:

- Data Matrix and possibly Weight Matrix for each subject
- Eigenvalues from the computation of the initial coordinates
- Sum of Data Weights and Pooled Data Matrix computed during initialization with INAV=DATA
- Configuration, the estimated coordinates of the objects
- Dimension Coefficients
- A table of transformation parameters, including one or more of the following:
 

|           |
|-----------|
| Intercept |
| Slope     |
| Power     |
- A table of fit statistics for each matrix and possibly each row, including the following:
 

|                                                                                              |
|----------------------------------------------------------------------------------------------|
| Number of Nonmissing Data                                                                    |
| Weight of the matrix or row, permitting both observation weights and standardization factors |
| Badness-of-Fit Criterion                                                                     |

Distance Correlation computed between the distances and data with optimal transformation  
 Uncorrected Distance Correlation not corrected for the mean  
 Fit Correlation computed after applying the FIT= transformation to both distances and data  
 Uncorrected Fit Correlation not corrected for the mean

---

## ODS Table Names

PROC MDS assigns a name to each table it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in Table 56.3. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

**Table 56.3** ODS Tables Produced by PROC MDS

| ODS Table Name    | Description                  | Option                                            |
|-------------------|------------------------------|---------------------------------------------------|
| ConvergenceStatus | Convergence status           | default                                           |
| DimensionCoef     | Dimension coefficients       | PCOEF with COEF= not IDENTITY                     |
| FitMeasures       | Measures of fit              | PFIT                                              |
| IterHistory       | Iteration history            | default                                           |
| PConfig           | Configuration of coordinates | PCONFIG                                           |
| PData             | Data matrices                | PDATA                                             |
| PInAvData         | INAV= data set information   | PINAVDATA                                         |
| PInEigval         | Initial eigenvalues          | PINEIGVAL                                         |
| PInEigvec         | Initial eigenvectors         | PINEIGVEC                                         |
| PInWeight         | Initialization weights       | PINWEIGHT                                         |
| Transformations   | Transformation parameters    | PTRANS with LEVEL=RATIO,<br>INTERVAL, LOGINTERVAL |

---

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “Statistical Graphics Using ODS.”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “A Primer on ODS Statistical Graphics” on page 599 in Chapter 21, “Statistical Graphics Using ODS.”

All graphs are produced by default when they are appropriate. You can reference every graph produced through ODS Graphics with a name. The names of the graphs that PROC MDS generates are listed in Table 56.4, along with the required options.



**Table 56.4** Graphs Produced by PROC MDS

| ODS Graph Name   | Plot Description        | Option                                              |
|------------------|-------------------------|-----------------------------------------------------|
| BadnessPlot      | Badness of fit          | DIMENSION= <i>range</i>                             |
| CoefficientsPlot | Individual coefficients | DIMENSION= <i>n</i> , <i>n</i> > 1<br>COEF=DIAGONAL |
| ConfigPlot       | Configuration           | DIMENSION= <i>n</i> , <i>n</i> > 1                  |
| FitPlot          | Fit                     | default                                             |

---

## Example: MDS Procedure

---

### Example 56.1: Jacobowitz Body Parts Data from Children and Adults

Jacobowitz (1975) collected conditional rank-order data regarding perceived similarity of parts of the body from children of ages 6, 8, and 10 years and from college sophomores. The data set includes data from 15 children (6-year-olds) and 15 sophomores. The method of data collection and some results of an analysis are also described by Young (1987, pp. 4–10). The following statements create the input data set:

```

data body;
 title 'Jacobowitz Body Parts Data from 6-Year-Olds and Adults';
 title2 'First 15 Subjects (obs 1–225) Are Children';
 title3 'Second 15 Subjects (obs 226–450) Are Adults';
 input (Cheek Face Mouth Head Ear Body Arm Elbow Hand
 Palm Finger Leg Knee Foot Toe) (2.);
 if _n_ <= 225 then Subject='C'; else subject='A';
 datalines;
0 2 1 3 4 10 5 9 6 7 8 11 12 13 14
2 0 12 1 13 3 8 10 11 9 7 4 5 6 14
3 2 0 1 4 9 5 11 6 7 8 10 13 12 14
2 1 3 0 4 9 5 6 11 7 8 10 12 13 14

... more lines ...

10 12 11 13 9 14 8 7 4 6 2 3 5 1 0
;

```

The data are analyzed as row conditional (CONDITION=ROW) at the ordinal level of measurement (LEVEL=ORDINAL) by using the weighted Euclidean model (COEF=DIAGONAL) in three dimensions (DIMENSION=3). The final estimates are displayed (PFINAL). The estimates (OUT=OUT) and fitted values (OUTRES=RES) are saved in output data sets. The following statements produce [Output 56.1.1](#):

```
ods graphics on;

proc mds data=body condition=row level=ordinal coef=diagonal
 dimension=3 pfinal out=out outres=res;
 subject subject;
 title5 'Nonmetric Weighted MDS';
run;
```

**Output 56.1.1** Analysis of Body Parts Data

| Jacobowitz Body Parts Data from 6-Year-Olds and Adults                         |          |                                 |                        |                      |          |
|--------------------------------------------------------------------------------|----------|---------------------------------|------------------------|----------------------|----------|
| First 15 Subjects (obs 1-225) Are Children                                     |          |                                 |                        |                      |          |
| Second 15 Subjects (obs 226-450) Are Adults                                    |          |                                 |                        |                      |          |
| Nonmetric Weighted MDS                                                         |          |                                 |                        |                      |          |
| Multidimensional Scaling: Data=WORK.BODY.DATA                                  |          |                                 |                        |                      |          |
| Shape=SQUARE Condition=ROW Level=ORDINAL                                       |          |                                 |                        |                      |          |
| Coef=DIAGONAL Dimension=3 Formula=1 Fit=1                                      |          |                                 |                        |                      |          |
| Mconverge=0.01 Gconverge=0.01 Maxiter=100 Over=2 Ridge=0.0001 Alternate=MATRIX |          |                                 |                        |                      |          |
| Iteration                                                                      | Type     | Badness-<br>of-Fit<br>Criterion | Change in<br>Criterion | Convergence Measures |          |
|                                                                                |          |                                 |                        | Monotone             | Gradient |
| 0                                                                              | Initial  | 0.5938                          | .                      | .                    | .        |
| 1                                                                              | Monotone | 0.2344                          | 0.3594                 | 0.4693               | 0.4028   |
| 2                                                                              | Gau-New  | 0.2080                          | 0.0264                 | .                    | .        |
| 3                                                                              | Monotone | 0.1963                          | 0.0118                 | 0.0556               | 0.2630   |
| 4                                                                              | Gau-New  | 0.1927                          | 0.003592               | .                    | .        |
| 5                                                                              | Monotone | 0.1797                          | 0.0130                 | 0.0463               | 0.1544   |
| 6                                                                              | Gau-New  | 0.1779                          | 0.001809               | .                    | .        |
| 7                                                                              | Monotone | 0.1744                          | 0.003430               | 0.0225               | 0.1210   |
| 8                                                                              | Gau-New  | 0.1736                          | 0.000807               | .                    | .        |
| 9                                                                              | Monotone | 0.1717                          | 0.001929               | 0.0161               | 0.1128   |
| 10                                                                             | Gau-New  | 0.1712                          | 0.000474               | .                    | .        |
| 11                                                                             | Monotone | 0.1698                          | 0.001413               | 0.0135               | 0.1119   |
| 12                                                                             | Gau-New  | 0.1696                          | 0.000188               | .                    | .        |
| 13                                                                             | Monotone | 0.1684                          | 0.001261               | 0.0121               | 0.1121   |
| 14                                                                             | Gau-New  | 0.1683                          | 0.000117               | .                    | .        |
| 15                                                                             | Monotone | 0.1672                          | 0.001096               | 0.0111               | 0.1064   |
| 16                                                                             | Gau-New  | 0.1670                          | 0.000131               | .                    | .        |
| 17                                                                             | Monotone | 0.1661                          | 0.000902               | 0.0103               | 0.0965   |
| 18                                                                             | Gau-New  | 0.1660                          | 0.000160               | .                    | .        |
| 19                                                                             | Monotone | 0.1652                          | 0.000736               | 0.009740             | 0.0980   |
| 20                                                                             | Gau-New  | 0.1651                          | 0.000169               | .                    | 0.1062   |
| 21                                                                             | Gau-New  | 0.1645                          | 0.000542               | .                    | 0.0161   |
| 22                                                                             | Gau-New  | 0.1645                          | 4.2645E-6              | .                    | 0.009969 |

Convergence criteria are satisfied.

## Output 56.1.1 continued

| Configuration |       |       |       |
|---------------|-------|-------|-------|
|               | Dim1  | Dim2  | Dim3  |
| Cheek         | 0.25  | 1.47  | 2.06  |
| Face          | 0.36  | 0.32  | 0.33  |
| Mouth         | 0.78  | 0.08  | 1.08  |
| Head          | 2.10  | 1.07  | -0.01 |
| Ear           | 0.26  | 0.72  | -0.34 |
| Body          | 1.51  | -0.61 | -0.68 |
| Arm           | -0.74 | 2.07  | -0.59 |
| Elbow         | -0.51 | -0.21 | 0.01  |
| Hand          | 0.46  | -1.50 | -0.60 |
| Palm          | -1.44 | -0.81 | 1.48  |
| Finger        | -0.24 | -0.24 | -0.81 |
| Leg           | -1.68 | 0.26  | -0.05 |
| Knee          | -1.19 | -1.19 | -1.36 |
| Foot          | 0.16  | -0.03 | -1.56 |
| Toe           | -0.10 | -1.39 | 1.02  |

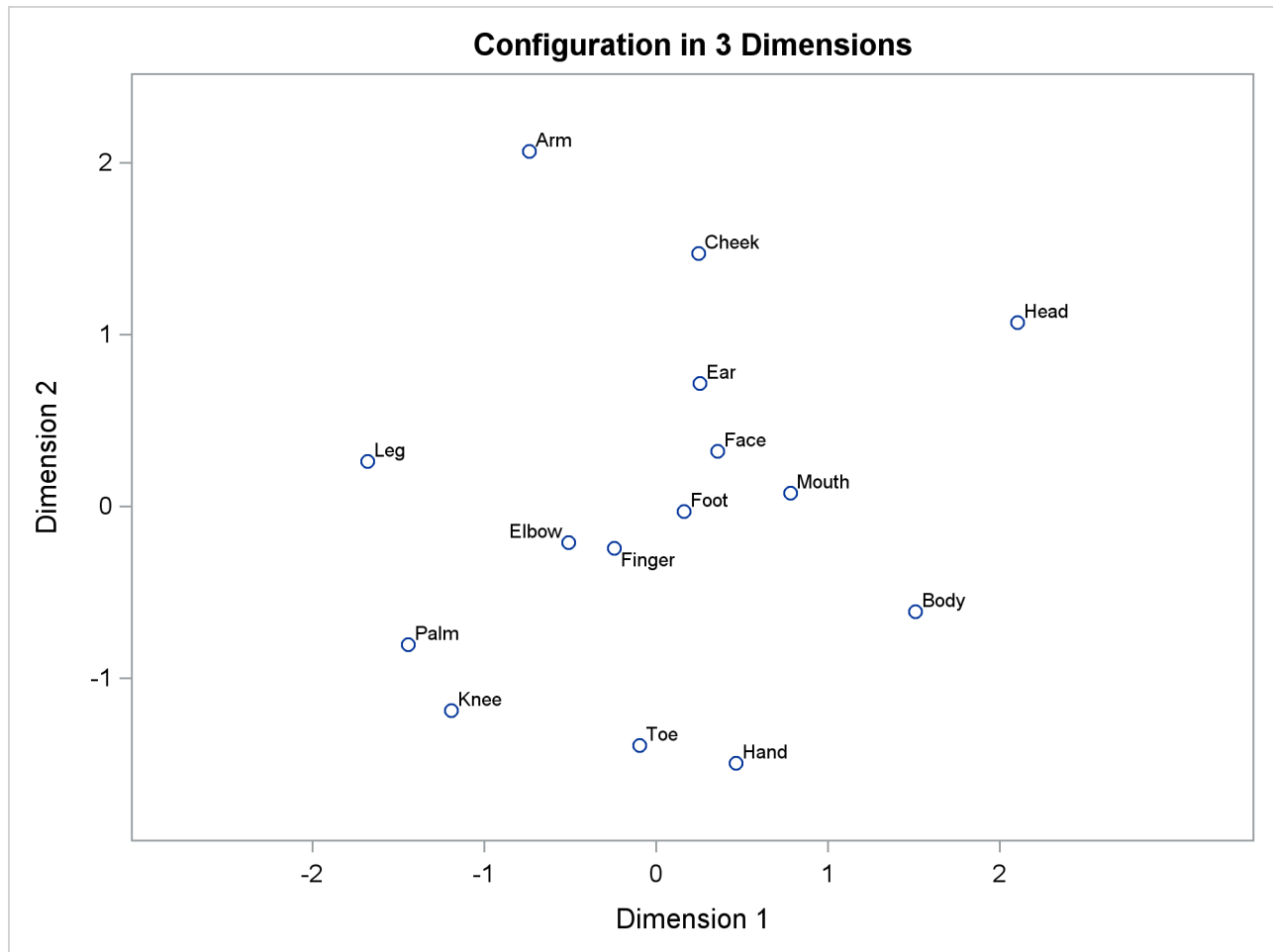
  

| Dimension Coefficients |      |      |      |
|------------------------|------|------|------|
| Subject                | 1    | 2    | 3    |
| C                      | 1.00 | 1.12 | 0.86 |
| C                      | 0.96 | 1.02 | 1.01 |
| C                      | 0.98 | 1.05 | 0.98 |
| C                      | 1.02 | 1.08 | 0.89 |
| C                      | 0.95 | 1.04 | 1.01 |
| C                      | 0.99 | 1.12 | 0.89 |
| C                      | 1.07 | 1.00 | 0.93 |
| C                      | 1.04 | 1.02 | 0.94 |
| C                      | 0.99 | 1.15 | 0.83 |
| C                      | 0.89 | 1.11 | 0.99 |
| C                      | 1.04 | 1.03 | 0.92 |
| C                      | 1.06 | 1.01 | 0.93 |
| C                      | 0.92 | 1.24 | 0.78 |
| C                      | 0.97 | 0.98 | 1.05 |
| C                      | 1.03 | 1.00 | 0.97 |
| A                      | 0.93 | 1.17 | 0.88 |
| A                      | 0.89 | 1.12 | 0.97 |
| A                      | 0.88 | 1.17 | 0.94 |
| A                      | 0.81 | 1.14 | 1.02 |
| A                      | 0.90 | 1.11 | 0.98 |
| A                      | 0.90 | 1.17 | 0.91 |
| A                      | 0.92 | 1.17 | 0.88 |
| A                      | 0.97 | 1.19 | 0.80 |
| A                      | 0.95 | 1.16 | 0.87 |
| A                      | 1.08 | 1.07 | 0.83 |
| A                      | 0.95 | 1.20 | 0.81 |
| A                      | 1.00 | 0.97 | 1.02 |
| A                      | 0.89 | 1.18 | 0.91 |
| A                      | 0.97 | 1.15 | 0.86 |
| A                      | 0.93 | 1.21 | 0.82 |

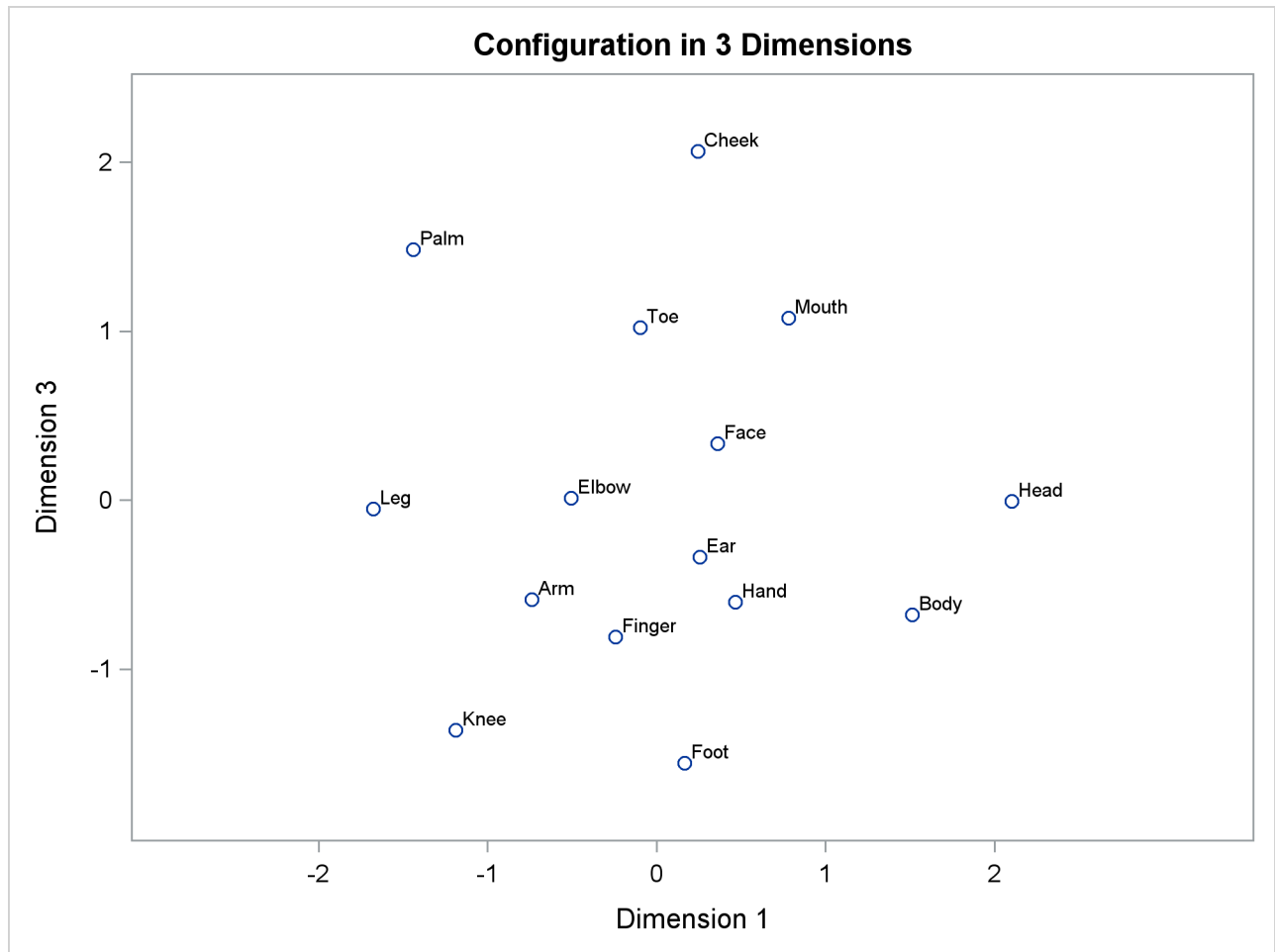
Output 56.1.1 continued

| Subject | Number of<br>Nonmissing<br>Data | Weight | Badness-of-<br>Fit<br>Criterion | Distance<br>Correlation | Uncorrected<br>Distance<br>Correlation |
|---------|---------------------------------|--------|---------------------------------|-------------------------|----------------------------------------|
| C       | 160                             | 0.03   | 0.15                            | 0.86                    | 0.99                                   |
| C       | 163                             | 0.03   | 0.19                            | 0.78                    | 0.98                                   |
| C       | 166                             | 0.03   | 0.20                            | 0.79                    | 0.98                                   |
| C       | 158                             | 0.03   | 0.16                            | 0.84                    | 0.99                                   |
| C       | 173                             | 0.03   | 0.18                            | 0.83                    | 0.98                                   |
| C       | 164                             | 0.03   | 0.14                            | 0.90                    | 0.99                                   |
| C       | 158                             | 0.03   | 0.20                            | 0.77                    | 0.98                                   |
| C       | 170                             | 0.03   | 0.18                            | 0.83                    | 0.98                                   |
| C       | 156                             | 0.03   | 0.15                            | 0.88                    | 0.99                                   |
| C       | 165                             | 0.03   | 0.18                            | 0.79                    | 0.98                                   |
| C       | 153                             | 0.03   | 0.19                            | 0.79                    | 0.98                                   |
| C       | 162                             | 0.03   | 0.17                            | 0.83                    | 0.98                                   |
| C       | 161                             | 0.03   | 0.14                            | 0.90                    | 0.99                                   |
| C       | 164                             | 0.03   | 0.17                            | 0.83                    | 0.99                                   |
| C       | 161                             | 0.03   | 0.18                            | 0.81                    | 0.98                                   |
| A       | 163                             | 0.03   | 0.15                            | 0.87                    | 0.99                                   |
| A       | 174                             | 0.04   | 0.17                            | 0.85                    | 0.99                                   |
| A       | 172                             | 0.03   | 0.15                            | 0.89                    | 0.99                                   |
| A       | 175                             | 0.04   | 0.17                            | 0.85                    | 0.98                                   |
| A       | 171                             | 0.03   | 0.15                            | 0.87                    | 0.99                                   |
| A       | 163                             | 0.03   | 0.16                            | 0.86                    | 0.99                                   |
| A       | 173                             | 0.03   | 0.14                            | 0.90                    | 0.99                                   |
| A       | 160                             | 0.03   | 0.14                            | 0.89                    | 0.99                                   |
| A       | 164                             | 0.03   | 0.14                            | 0.90                    | 0.99                                   |
| A       | 158                             | 0.03   | 0.16                            | 0.86                    | 0.99                                   |
| A       | 165                             | 0.03   | 0.16                            | 0.87                    | 0.99                                   |
| A       | 168                             | 0.03   | 0.18                            | 0.82                    | 0.98                                   |
| A       | 175                             | 0.04   | 0.15                            | 0.89                    | 0.99                                   |
| A       | 172                             | 0.03   | 0.16                            | 0.88                    | 0.99                                   |
| A       | 175                             | 0.04   | 0.15                            | 0.90                    | 0.99                                   |
| - All - | 4962                            | 1.00   | 0.16                            | 0.85                    | 0.99                                   |

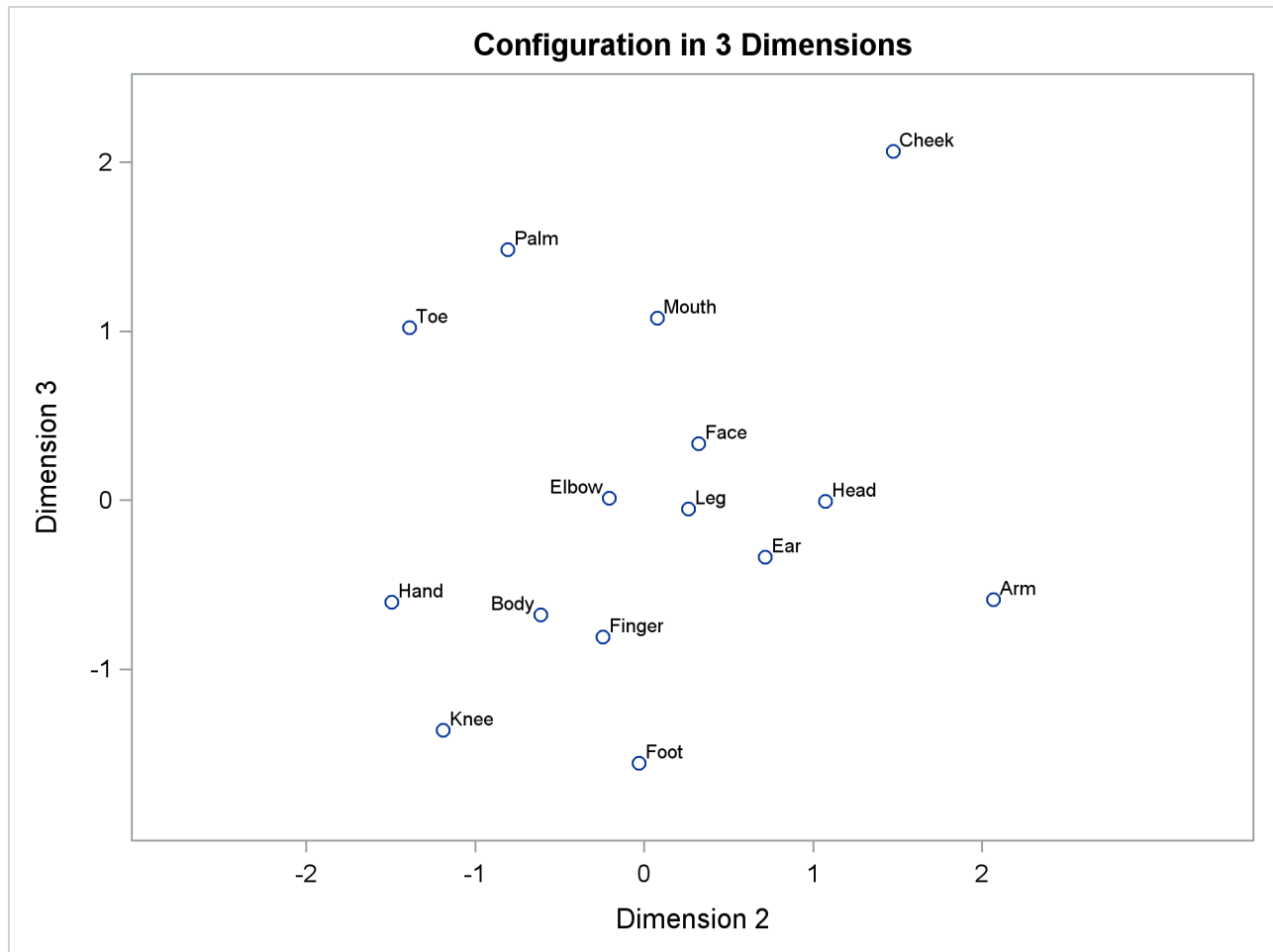
Output 56.1.1 continued



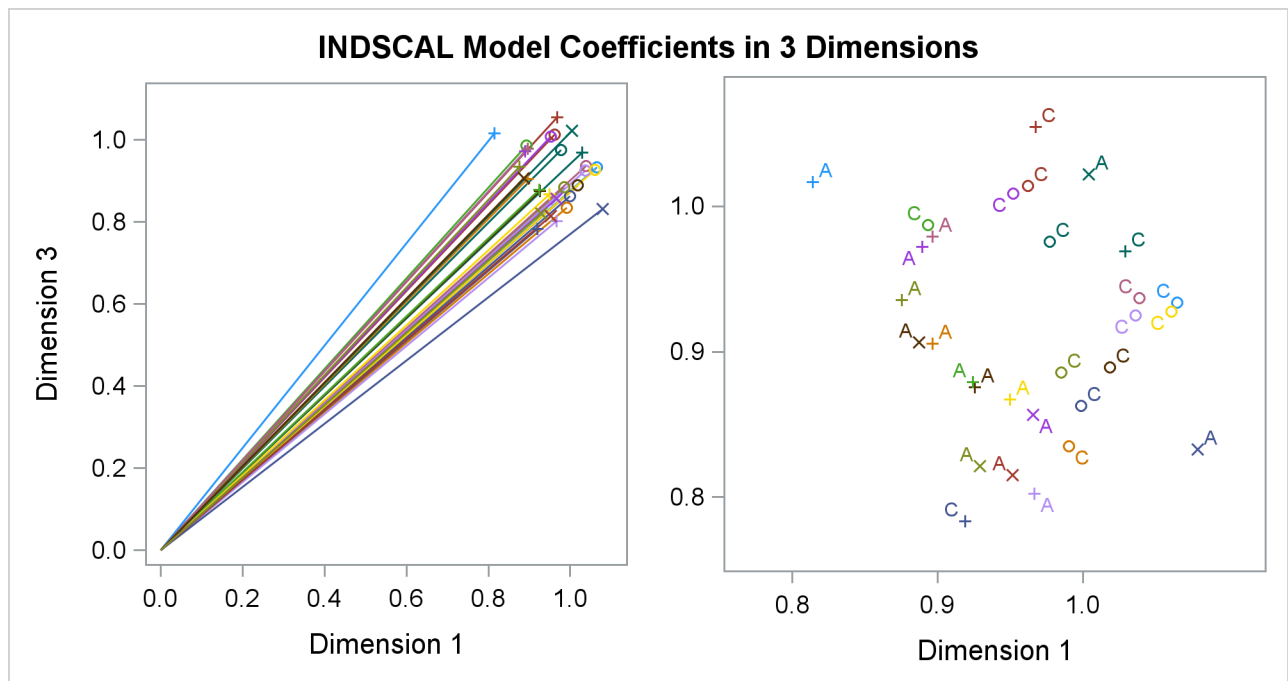
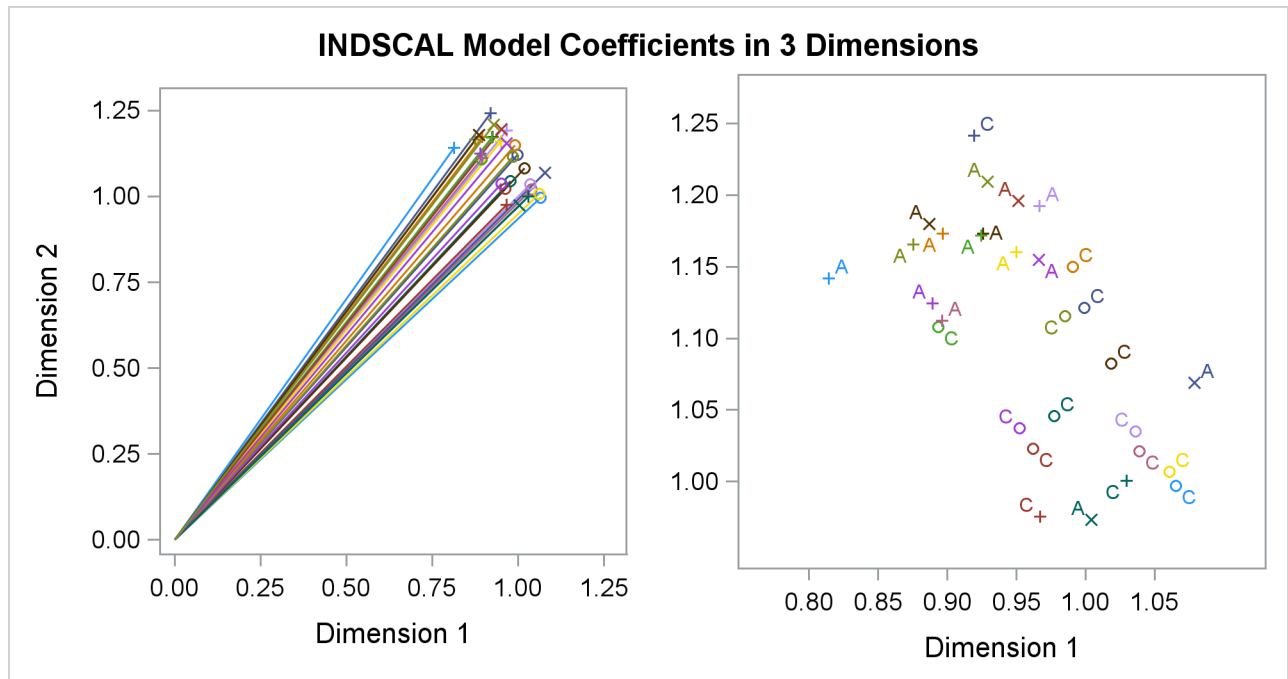
Output 56.1.1 continued



Output 56.1.1 continued

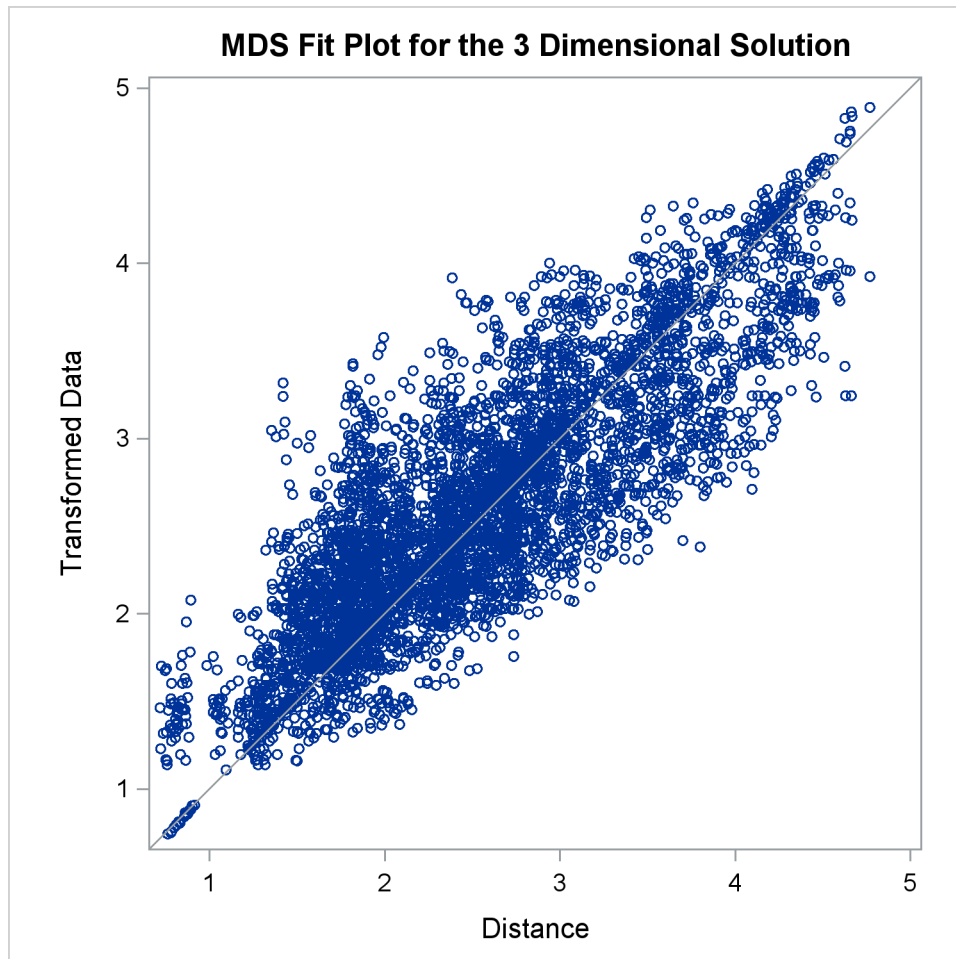
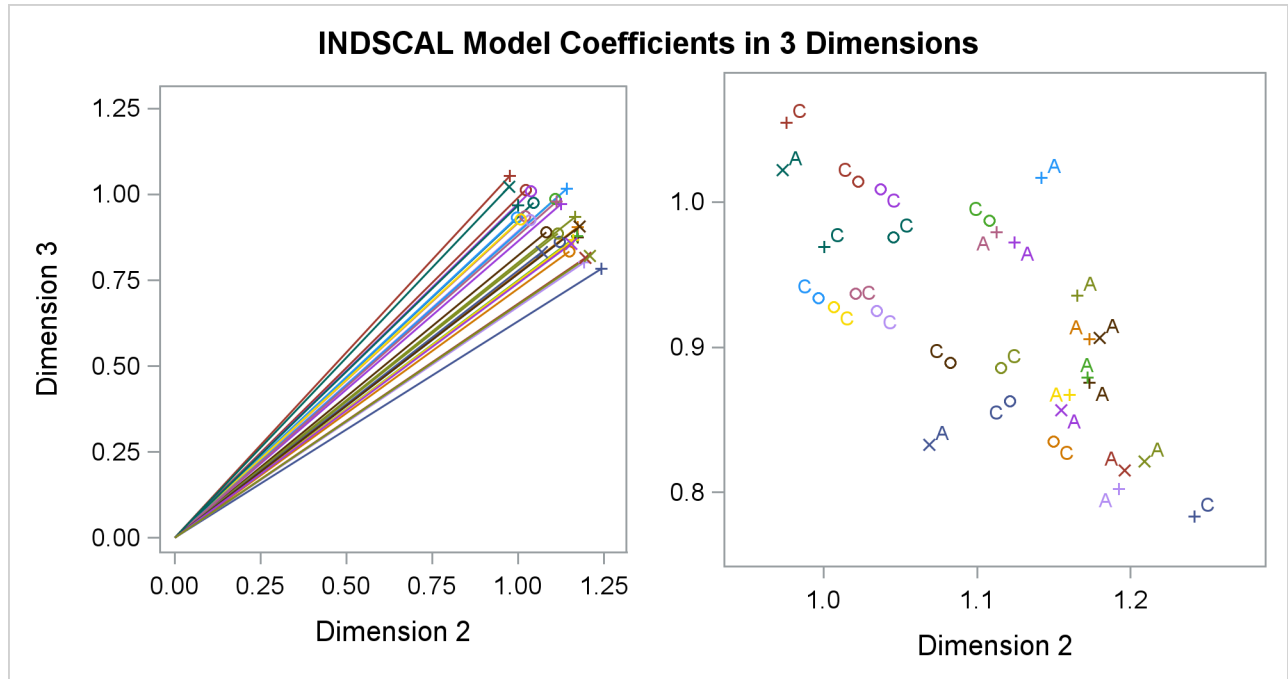


Output 56.1.1 continued





Output 56.1.1 continued



Often the output of greatest interest in an MDS analysis is the graphical output. The first plots show two-dimensional view of the three-dimensional configuration. Next, the coefficients are plotted. The last plot is the fit plot.

In the fit plot, the transformed data are plotted on the vertical axis, and the distances from the model are plotted on the horizontal axis. If the model fits perfectly, all points lie on a diagonal line from lower left to upper right. The vertical departure of each point from this diagonal line represents the residual of the corresponding observation.

The configuration has a tripodal shape with **Body** at the apex. The three legs of the tripod can be distinguished in the plot of dimension 2 by dimension 1, which shows three distinct clusters with **Body** in the center. Dimension 1 separates head parts from arm and leg parts. Dimension 2 separates arm parts from leg parts. The plot of dimension 3 by dimension 1 shows the tripod from the side. Dimension 3 distinguishes the more inclusive body parts (at the top) from the less inclusive body parts (at the bottom).

The plots of dimension coefficients show that children differ from adults primarily in the emphasis given to dimension 2. Children give about the same weight (approximately 1) to each dimension. Adults are much more variable than children, but all have coefficients less than 1.0 for dimension 2, with an average of about 0.7. Referring back to the configuration plot, you can see that adults consider arm parts to be more similar to leg parts than children do. Many adults also give a high weight to dimension 1, indicating that they consider head parts to be more dissimilar from arm and leg parts than children do. Dimension 3 shows considerable variability for both children and adults.

---

## References

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# Chapter 57

## The MI Procedure

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## Overview: MI Procedure

Missing values are an issue in a substantial number of statistical analyses. Most SAS statistical procedures exclude observations with any missing variable values from the analysis. These observations are called incomplete cases. While using only complete cases is simple, you lose information that is in the incomplete cases. Excluding observations with missing values also ignores the possible systematic difference between the complete cases and incomplete cases, and the resulting inference might not be applicable to the population of all cases, especially with a smaller number of complete cases.

Some SAS procedures use all the available cases in an analysis—that is, cases with useful information. For example, the CORR procedure estimates a variable mean by using all cases with nonmissing values for this variable, ignoring the possible missing values in other variables. The CORR procedure also estimates a correlation by using all cases with nonmissing values for this pair of variables. This estimation might make better use of the available data, but the resulting correlation matrix might not be positive definite.

Another strategy is single imputation, in which you substitute a value for each missing value. Standard statistical procedures for complete data analysis can then be used with the filled-in data set. For example, each missing value can be imputed from the variable mean of the complete cases. This approach treats missing values as if they were known in the complete-data analyses. Single imputation does not reflect the uncertainty about the predictions of the unknown missing values, and the resulting estimated variances of the parameter estimates are biased toward zero (Rubin 1987, p. 13).

Instead of filling in a single value for each missing value, multiple imputation replaces each missing value with a set of plausible values that represent the uncertainty about the right value to impute (Rubin 1976, 1987). The multiply imputed data sets are then analyzed by using standard procedures for complete data and combining the results from these analyses. No matter which complete-data analysis is used, the process of combining results from different data sets is essentially the same.

Multiple imputation does not attempt to estimate each missing value through simulated values, but rather to represent a random sample of the missing values. This process results in valid statistical inferences that properly reflect the uncertainty due to missing values; for example, valid confidence intervals for parameters.

Multiple imputation inference involves three distinct phases:

1. The missing data are filled in  $m$  times to generate  $m$  complete data sets.
2. The  $m$  complete data sets are analyzed by using standard procedures.
3. The results from the  $m$  complete data sets are combined for the inference.

The MI procedure is a multiple imputation procedure that creates multiply imputed data sets for incomplete  $p$ -dimensional multivariate data. It uses methods that incorporate appropriate variability across the  $m$  imputations. The imputation method of choice depends on the patterns of missingness in the data and the type of the imputed variable.

A data set with variables  $Y_1, Y_2, \dots, Y_p$  (in that order) is said to have a *monotone missing pattern* when the event that a variable  $Y_j$  is missing for a particular individual implies that all subsequent variables  $Y_k$ ,  $k > j$ , are missing for that individual.

For data sets with monotone missing patterns, the variables with missing values can be imputed sequentially with covariates constructed from their corresponding sets of preceding variables. To impute missing values

for a continuous variable, you can use a regression method (Rubin 1987, pp. 166–167), a predictive mean matching method (Heitjan and Little 1991; Schenker and Taylor 1996), or a propensity score method (Rubin 1987, pp. 124, 158; Lavori, Dawson, and Shera 1995). To impute missing values for a classification variable, you can use a logistic regression method when the classification variable has a binary or ordinal response, or use a discriminant function method when the classification variable has a binary or nominal response.

For data sets with arbitrary missing patterns, you can use either of the following methods to impute missing values: a Markov chain Monte Carlo (MCMC) method (Schafer 1997) that assumes multivariate normality, or a fully conditional specification (FCS) method (Brand 1999; van Buuren 2007) that assumes the existence of a joint distribution for all variables.

You can use the MCMC method to impute either all the missing values or just enough missing values to make the imputed data sets have monotone missing patterns. With a monotone missing data pattern, you have greater flexibility in your choice of imputation models, such as the monotone regression method that do not use Markov chains. You can also specify a different set of covariates for each imputed variable.

An FCS method does not start with an explicitly specified multivariate distribution for all variables, but rather uses a separate conditional distribution for each imputed variable. For each imputation, the process contains two phases: the preliminary filled-in phase followed by the imputation phase. At the filled-in phase, the missing values for all variables are filled in sequentially over the variables taken one at a time. These filled-in values provide starting values for these missing values at the imputation phase. At the imputation phase, the missing values for each variable are imputed sequentially for a number of burn-in iterations before the imputation.

As in methods for data sets with monotone missing patterns, you can use a regression method or a predictive mean matching method to impute missing values for a continuous variable, a logistic regression method to impute missing values for a classification variable with a binary or ordinal response, and a discriminant function method to impute missing values for a classification variable with a binary or nominal response.

After the  $m$  complete data sets are analyzed using standard SAS procedures, the MIANALYZE procedure can be used to generate valid statistical inferences about these parameters by combining results from the  $m$  analyses.

Often, as few as three to five imputations are adequate in multiple imputation (Rubin 1996, p. 480). The relative efficiency of the small  $m$  imputation estimator is high for cases with little missing information (Rubin 1987, p. 114). (Also see the section “[Multiple Imputation Efficiency](#)” on page 4771.)

Multiple imputation inference assumes that the model (variables) you used to analyze the multiply imputed data (the analyst’s model) is the same as the model used to impute missing values in multiple imputation (the imputer’s model). But in practice, the two models might not be the same. The consequences for different scenarios (Schafer 1997, pp. 139–143) are discussed in the section “[Imputer’s Model Versus Analyst’s Model](#)” on page 4771.

---

## Getting Started: MI Procedure

The Fitness data described in the REG procedure are measurements of 31 individuals in a physical fitness course. See Chapter 79, “[The REG Procedure](#),” for more information.

The Fitness1 data set is constructed from the Fitness data set and contains three variables: Oxygen, RunTime, and RunPulse. Some values have been set to missing, and the resulting data set has an arbitrary pattern of missingness in these three variables.

```

-----Data on Physical Fitness-----
| These measurements were made on men involved in a physical fitness |
| course at N.C. State University. Certain values have been set to |
| missing and the resulting data set has an arbitrary missing pattern. |
| Only selected variables of |
| Oxygen (intake rate, ml per kg body weight per minute), |
| Runtime (time to run 1.5 miles in minutes), |
| RunPulse (heart rate while running) are used. |

data Fitness1;
 input Oxygen RunTime RunPulse @@;
 datalines;
44.609 11.37 178 45.313 10.07 185
54.297 8.65 156 59.571 . .
49.874 9.22 . 44.811 11.63 176
. 11.95 176 . 10.85 .
39.442 13.08 174 60.055 8.63 170
50.541 . . 37.388 14.03 186
44.754 11.12 176 47.273 . .
51.855 10.33 166 49.156 8.95 180
40.836 10.95 168 46.672 10.00 .
46.774 10.25 . 50.388 10.08 168
39.407 12.63 174 46.080 11.17 156
45.441 9.63 164 . 8.92 .
45.118 11.08 . 39.203 12.88 168
45.790 10.47 186 50.545 9.93 148
48.673 9.40 186 47.920 11.50 170
47.467 10.50 170
;

```

Suppose that the data are multivariate normally distributed and the missing data are missing at random (MAR). That is, the probability that an observation is missing can depend on the observed variable values of the individual, but not on the missing variable values of the individual. See the section “[Statistical Assumptions for Multiple Imputation](#)” on page 4745 for a detailed description of the MAR assumption.

The following statements invoke the MI procedure and impute missing values for the Fitness1 data set:

```

proc mi data=Fitness1 seed=501213 mu0=50 10 180 out=outmi;
 mcmc;
 var Oxygen RunTime RunPulse;
run;

```

The “Model Information” table in [Figure 57.1](#) describes the method used in the multiple imputation process. By default, the MCMC statement uses the Markov chain Monte Carlo (MCMC) method with a single chain to create five imputations. The posterior mode, the highest observed-data posterior density, with a noninformative prior, is computed from the expectation-maximization (EM) algorithm and is used as the starting value for the chain.



**Figure 57.1** Model Information

| The MI Procedure                 |                   |
|----------------------------------|-------------------|
| Model Information                |                   |
| Data Set                         | WORK.FITNESS1     |
| Method                           | MCMC              |
| Multiple Imputation Chain        | Single Chain      |
| Initial Estimates for MCMC       | EM Posterior Mode |
| Start                            | Starting Value    |
| Prior                            | Jeffreys          |
| Number of Imputations            | 5                 |
| Number of Burn-in Iterations     | 200               |
| Number of Iterations             | 100               |
| Seed for random number generator | 501213            |

The MI procedure takes 200 burn-in iterations before the first imputation and 100 iterations between imputations. In a Markov chain, the information in the current iteration influences the state of the next iteration. The burn-in iterations are iterations in the beginning of each chain that are used both to eliminate the series of dependence on the starting value of the chain and to achieve the stationary distribution. The between-imputation iterations in a single chain are used to eliminate the series of dependence between the two imputations.

The “Missing Data Patterns” table in [Figure 57.2](#) lists distinct missing data patterns with their corresponding frequencies and percentages. An “X” means that the variable is observed in the corresponding group, and a “.” means that the variable is missing. The table also displays group-specific variable means. The MI procedure sorts the data into groups based on whether the analysis variables are observed or missing. For a detailed description of missing data patterns, see the section “[Missing Data Patterns](#)” on page 4746.

**Figure 57.2** Missing Data Patterns

| Missing Data Patterns |        |          |           |      |         |
|-----------------------|--------|----------|-----------|------|---------|
| Group                 | Oxygen | Run Time | Run Pulse | Freq | Percent |
| 1                     | X      | X        | X         | 21   | 67.74   |
| 2                     | X      | X        | .         | 4    | 12.90   |
| 3                     | X      | .        | .         | 3    | 9.68    |
| 4                     | .      | X        | X         | 1    | 3.23    |
| 5                     | .      | X        | .         | 2    | 6.45    |

| Missing Data Patterns |           |           |            |
|-----------------------|-----------|-----------|------------|
| -----Group Means----- |           |           |            |
| Group                 | Oxygen    | RunTime   | RunPulse   |
| 1                     | 46.353810 | 10.809524 | 171.666667 |
| 2                     | 47.109500 | 10.137500 | .          |
| 3                     | 52.461667 | .         | .          |
| 4                     | .         | 11.950000 | 176.000000 |
| 5                     | .         | 9.885000  | .          |

After the completion of  $m$  imputations, the “Variance Information” table in Figure 57.3 displays the between-imputation variance, within-imputation variance, and total variance for combining complete-data inferences. It also displays the degrees of freedom for the total variance. The relative increase in variance due to missing values, the fraction of missing information, and the relative efficiency (in units of variance) for each variable are also displayed. A detailed description of these statistics is provided in the section “Combining Inferences from Multiply Imputed Data Sets” on page 4769.

**Figure 57.3** Variance Information

| Variance Information |                    |          |          |        |
|----------------------|--------------------|----------|----------|--------|
| Variable             | -----Variance----- |          |          | DF     |
|                      | Between            | Within   | Total    |        |
| Oxygen               | 0.056930           | 0.954041 | 1.022356 | 25.549 |
| RunTime              | 0.000811           | 0.064496 | 0.065469 | 27.721 |
| RunPulse             | 0.922032           | 3.269089 | 4.375528 | 15.753 |

| Variance Information |                               |                              |                     |
|----------------------|-------------------------------|------------------------------|---------------------|
| Variable             | Relative Increase in Variance | Fraction Missing Information | Relative Efficiency |
| Oxygen               | 0.071606                      | 0.068898                     | 0.986408            |
| RunTime              | 0.015084                      | 0.014968                     | 0.997015            |
| RunPulse             | 0.338455                      | 0.275664                     | 0.947748            |

The “Parameter Estimates” table in Figure 57.4 displays the estimated mean and standard error of the mean for each variable. The inferences are based on the  $t$  distribution. The table also displays a 95% confidence interval for the mean and a  $t$  statistic with the associated  $p$ -value for the hypothesis that the population mean is equal to the value specified with the MU0= option. A detailed description of these statistics is provided in the section “Combining Inferences from Multiply Imputed Data Sets” on page 4769.

**Figure 57.4** Parameter Estimates

| Parameter Estimates |            |           |                       |          |        |
|---------------------|------------|-----------|-----------------------|----------|--------|
| Variable            | Mean       | Std Error | 95% Confidence Limits |          | DF     |
| Oxygen              | 47.094040  | 1.011116  | 45.0139               | 49.1742  | 25.549 |
| RunTime             | 10.572073  | 0.255870  | 10.0477               | 11.0964  | 27.721 |
| RunPulse            | 171.787793 | 2.091776  | 167.3478              | 176.2278 | 15.753 |

| Parameter Estimates |            |            |            |                       |         |
|---------------------|------------|------------|------------|-----------------------|---------|
| Variable            | Minimum    | Maximum    | Mu0        | t for H0:<br>Mean=Mu0 | Pr >  t |
| Oxygen              | 46.783898  | 47.395550  | 50.000000  | -2.87                 | 0.0081  |
| RunTime             | 10.526392  | 10.599616  | 10.000000  | 2.24                  | 0.0336  |
| RunPulse            | 170.774818 | 173.122002 | 180.000000 | -3.93                 | 0.0012  |

In addition to the output tables, the procedure also creates a data set with imputed values. The imputed data sets are stored in the outmi data set, with the index variable `_Imputation_` indicating the imputation numbers. The data set can now be analyzed using standard statistical procedures with `_Imputation_` as a BY variable.

The following statements list the first 10 observations of data set outmi:

```
proc print data=outmi (obs=10);
 title 'First 10 Observations of the Imputed Data Set';
run;
```

The table in Figure 57.5 shows that the precision of the imputed values differs from the precision of the observed values. You can use the `ROUND=` option to make the imputed values consistent with the observed values.

**Figure 57.5** Imputed Data Set

| First 10 Observations of the Imputed Data Set |              |         |         |              |
|-----------------------------------------------|--------------|---------|---------|--------------|
| Obs                                           | _Imputation_ | Oxygen  | RunTime | Run<br>Pulse |
| 1                                             | 1            | 44.6090 | 11.3700 | 178.000      |
| 2                                             | 1            | 45.3130 | 10.0700 | 185.000      |
| 3                                             | 1            | 54.2970 | 8.6500  | 156.000      |
| 4                                             | 1            | 59.5710 | 8.0747  | 155.925      |
| 5                                             | 1            | 49.8740 | 9.2200  | 176.837      |
| 6                                             | 1            | 44.8110 | 11.6300 | 176.000      |
| 7                                             | 1            | 42.8857 | 11.9500 | 176.000      |
| 8                                             | 1            | 46.9992 | 10.8500 | 173.099      |
| 9                                             | 1            | 39.4420 | 13.0800 | 174.000      |
| 10                                            | 1            | 60.0550 | 8.6300  | 170.000      |

## Syntax: MI Procedure

The following statements are available in the MI procedure:

```
PROC MI < options > ;
 BY variables ;
 CLASS variables ;
 EM < options > ;
 FCS < options > ;
 FREQ variable ;
 MCMC < options > ;
 MONOTONE < options > ;
 TRANSFORM transform (variables< / options >) < . . . transform (variables< / options >) > ;
 VAR variables ;
```

The `BY` statement specifies groups in which separate multiple imputation analyses are performed.

The `CLASS` statement lists the classification variables in the `VAR` statement. Classification variables can be either character or numeric.

The EM statement uses the EM algorithm to compute the maximum likelihood estimate (MLE) of the data with missing values, assuming a multivariate normal distribution for the data.

The FREQ statement specifies the variable that represents the frequency of occurrence for other values in the observation.

For a data set with a monotone missing pattern, you can use the MONOTONE statement to specify applicable monotone imputation methods; otherwise, you can use either the MCMC statement assuming multivariate normality or the FCS method assuming a joint distribution for variables exists. Note that you can specify no more than one of these statements. When none of these three statements is specified, the MCMC method with its default options is used.

The FCS statement uses a multivariate imputation by chained equations method to impute values for a data set with an arbitrary missing pattern, assuming a joint distribution exists for the data.

The MCMC statement uses a Markov chain Monte Carlo method to impute values for a data set with an arbitrary missing pattern, assuming a multivariate normal distribution for the data.

The MONOTONE statement specifies monotone methods to impute continuous and classification variables for a data set with a monotone missing pattern.

The TRANSFORM statement specifies the variables to be transformed before the imputation process; the imputed values of these transformed variables are reverse-transformed to the original forms before the imputation.

The VAR statement lists the numeric variables to be analyzed. If you omit the VAR statement, all numeric variables not listed in other statements are used.

The PROC MI statement is the only required statement for the MI procedure. The rest of this section provides detailed syntax information for each of these statements, beginning with the PROC MI statement. The remaining statements are presented in alphabetical order.

---

## PROC MI Statement

**PROC MI** < options > ;

The PROC MI statement invokes the MI procedure. [Table 57.1](#) summarizes the options available in the PROC MI statement.

**Table 57.1** Summary of PROC MI Options

| Option                    | Description                                          |
|---------------------------|------------------------------------------------------|
| <b>Data Sets</b>          |                                                      |
| DATA=                     | Specifies the input data set                         |
| OUT=                      | Specifies the output data set with imputed values    |
| <b>Imputation Details</b> |                                                      |
| NIMPUTE=                  | Specifies the number of imputations                  |
| SEED=                     | Specifies the seed to begin random number generator  |
| ROUND=                    | Specifies units to round imputed variable values     |
| MAXIMUM=                  | Specifies maximum values for imputed variable values |
| MINIMUM=                  | Specifies minimum values for imputed variable values |

Table 57.1 *continued*

| Option                      | Description                                                                        |
|-----------------------------|------------------------------------------------------------------------------------|
| MINMAXITER=                 | Specifies the maximum number of iterations to impute values in the specified range |
| SINGULAR=                   | Specifies the singularity criterion                                                |
| <b>Statistical Analysis</b> |                                                                                    |
| ALPHA=                      | Specifies the level for the confidence interval, $(1 - \alpha)$                    |
| MU0=                        | Specifies means under the null hypothesis                                          |
| <b>Printed Output</b>       |                                                                                    |
| NOPRINT                     | Suppresses all displayed output                                                    |
| SIMPLE                      | Displays univariate statistics and correlations                                    |

The following options can be used in the PROC MI statement. They are listed in alphabetical order.

**ALPHA= $\alpha$** 

specifies that confidence limits be constructed for the mean estimates with confidence level  $100(1 - \alpha)\%$ , where  $0 < \alpha < 1$ . The default is ALPHA=0.05.

**DATA=SAS-data-set**

names the SAS data set to be analyzed by PROC MI. By default, the procedure uses the most recently created SAS data set.

**MAXIMUM=numbers**

specifies maximum values for imputed variables. When an intended imputed value is greater than the maximum, PROC MI redraws another value for imputation. If only one number is specified, that number is used for all variables. If more than one number is specified, you must use a VAR statement, and the specified numbers must correspond to variables in the VAR statement. The default number is a missing value, which indicates no restriction on the maximum for the corresponding variable

The MAXIMUM= option is related to the MINIMUM= and ROUND= options, which are used to make the imputed values more consistent with the observed variable values. These options are applicable only if you use the MCMC method or the monotone regression method.

When specifying a maximum for the first variable only, you must also specify a missing value after the maximum. Otherwise, the maximum is used for all variables.

For example, the “MAXIMUM= 100 .” option sets a maximum of 100 for the first analysis variable only and no maximum for the remaining variables. The “MAXIMUM= . 100” option sets a maximum of 100 for the second analysis variable only and no maximum for the other variables.

**MINIMUM=numbers**

specifies the minimum values for imputed variables. When an intended imputed value is less than the minimum, PROC MI redraws another value for imputation. If only one number is specified, that number is used for all variables. If more than one number is specified, you must use a VAR statement, and the specified numbers must correspond to variables in the VAR statement. The default number is a missing value, which indicates no restriction on the minimum for the corresponding variable

**MINMAXITER=number**

specifies the maximum number of iterations for imputed values to be in the specified range when the option MINIMUM or MAXIMUM is also specified. The default is MINMAXITER=100.

**MU0=numbers****THETA0=numbers**

specifies the parameter values  $\mu_0$  under the null hypothesis  $\mu = \mu_0$  for the population means corresponding to the analysis variables. Each hypothesis is tested with a  $t$  test. If only one number is specified, that number is used for all variables. If more than one number is specified, you must use a VAR statement, and the specified numbers must correspond to variables in the VAR statement. The default is MU0=0.

If a variable is transformed as specified in a TRANSFORM statement, then the same transformation for that variable is also applied to its corresponding specified MU0= value in the  $t$  test. If the parameter values  $\mu_0$  for a transformed variable are not specified, then a value of zero is used for the resulting  $\mu_0$  after transformation.

**NIMPUTE=number**

specifies the number of imputations. The default is NIMPUTE=5. You can specify NIMPUTE=0 to skip the imputation. In this case, only tables of model information, missing data patterns, descriptive statistics (SIMPLE option), and MLE from the EM algorithm (EM statement) are displayed.

**NOPRINT**

suppresses the display of all output. Note that this option temporarily disables the Output Delivery System (ODS); see Chapter 20, “Using the Output Delivery System,” for more information.

**OUT=SAS-data-set**

creates an output SAS data set that contains imputation results. The data set includes an index variable, `_Imputation_`, to identify the imputation number. For each imputation, the data set contains all variables in the input data set with missing values being replaced by the imputed values. See the section “Output Data Sets” on page 4767 for a description of this data set.

**ROUND=numbers**

specifies the units to round variables in the imputation. If only one number is specified, that number is used for all continuous variables. If more than one number is specified, you must use a VAR statement, and the specified numbers must correspond to variables in the VAR statement. When the classification variables are listed in the VAR statement, their corresponding roundoff units are not used. The default number is a missing value, which indicates no rounding for imputed variables.

When specifying a roundoff unit for the first variable only, you must also specify a missing value after the roundoff unit. Otherwise, the roundoff unit is used for all variables. For example, the option “ROUND= 10 .” sets a roundoff unit of 10 for the first analysis variable only and no rounding for the remaining variables. The option “ROUND= . 10” sets a roundoff unit of 10 for the second analysis variable only and no rounding for other variables.

The ROUND= option sets the precision of imputed values. For example, with a roundoff unit of 0.001, each value is rounded to the nearest multiple of 0.001. That is, each value has three significant digits after the decimal point. See [Example 57.3](#) for an illustration of this option.

**SEED=number**

specifies a positive integer to start the pseudo-random number generator. The default is a value generated from reading the time of day from the computer's clock. However, in order to duplicate the results under identical situations, you must use the same value of the seed explicitly in subsequent runs of the MI procedure.

The seed information is displayed in the "Model Information" table so that the results can be reproduced by specifying this seed with the SEED= option. You need to specify the same seed number in the future to reproduce the results.

**SIMPLE**

displays simple descriptive univariate statistics and pairwise correlations from available cases. For a detailed description of these statistics, see the section "Descriptive Statistics" on page 4743.

**SINGULAR=p**

specifies the criterion for determining the singularity of a covariance matrix based on standardized variables, where  $0 < p < 1$ . The default is SINGULAR=1E-8.

Suppose that  $\mathbf{S}$  is a covariance matrix and  $v$  is the number of variables in  $\mathbf{S}$ . Based on the spectral decomposition  $\mathbf{S} = \mathbf{\Gamma}\mathbf{\Lambda}\mathbf{\Gamma}'$ , where  $\mathbf{\Lambda}$  is a diagonal matrix of eigenvalues  $\lambda_j$ ,  $j = 1, \dots, v$ , where  $\lambda_i \geq \lambda_j$  when  $i < j$ , and  $\mathbf{\Gamma}$  is a matrix with the corresponding orthonormal eigenvectors of  $\mathbf{S}$  as columns,  $\mathbf{S}$  is considered singular when an eigenvalue  $\lambda_j$  is less than  $p\bar{\lambda}$ , where the average  $\bar{\lambda} = \sum_{k=1}^v \lambda_k / v$ .

**BY Statement****BY variables ;**

You can specify a BY statement with PROC MI to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the MI procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

---

## CLASS Statement

**CLASS** *variables* ;

The CLASS statement specifies the classification variables in the VAR statement. Classification variables can be either character or numeric. The CLASS statement must be used in conjunction with either an FCS or MONOTONE statement.

Classification levels are determined from the formatted values of the classification variables. See “The FORMAT Procedure” in the *Base SAS Procedures Guide* for details.

---

## EM Statement

**EM** < *options* > ;

The expectation-maximization (EM) algorithm is a technique for maximum likelihood estimation in parametric models for incomplete data. The EM statement uses the EM algorithm to compute the MLE for  $(\mu, \Sigma)$ , the means and covariance matrix, of a multivariate normal distribution from the input data set with missing values. Either the means and covariances from complete cases or the means and standard deviations from available cases can be used as the initial estimates for the EM algorithm. You can also specify the correlations for the estimates from available cases.

You can also use the EM statement with the NIMPUTE=0 option in the PROC MI statement to compute the EM estimates without multiple imputation, as shown in [Example 57.1](#).

The following seven options are available with the EM statement (in alphabetical order):

**CONVERGE**= $p$

**XCONV**= $p$

sets the convergence criterion. The value must be between 0 and 1. The iterations are considered to have converged when the change in the parameter estimates between iteration steps is less than  $p$  for each parameter—that is, for each of the means and covariances. For each parameter, the change is a relative change if the parameter is greater than 0.01 in absolute value; otherwise, it is an absolute change. By default, CONVERGE=1E-4.

**INITIAL**=CC | AC | AC(R= $r$ )

sets the initial estimates for the EM algorithm. The INITIAL=CC option uses the means and covariances from complete cases; the INITIAL=AC option uses the means and standard deviations from available cases, and the correlations are set to zero; and the INITIAL=AC( R=  $r$ ) option uses the means and standard deviations from available cases with correlation  $r$ , where  $-1/(p - 1) < r < 1$  and  $p$  is the number of variables to be analyzed. The default is INITIAL=AC.

**ITPRINT**

prints the iteration history in the EM algorithm.

**MAXITER**=*number*

specifies the maximum number of iterations used in the EM algorithm. The default is MAXITER=200.



**OUT=SAS-data-set**

creates an output SAS data set that contains results from the EM algorithm. The data set contains all variables in the input data set, with missing values being replaced by the expected values from the EM algorithm. See the section “[Output Data Sets](#)” on page 4767 for a description of this data set.

**OUTEM=SAS-data-set**

creates an output SAS data set of TYPE=COV that contains the MLE of the parameter vector ( $\mu$ ,  $\Sigma$ ). These estimates are computed with the EM algorithm. See the section “[Output Data Sets](#)” on page 4767 for a description of this output data set.

**OUTITER <( options )> =SAS-data-set**

creates an output SAS data set of TYPE=COV that contains parameters for each iteration. The data set includes a variable named `_iteration_` to identify the iteration number. The parameters in the output data set depend on the options specified. You can specify the MEAN and COV options to output the mean and covariance parameters. When no options are specified, the output data set contains the mean parameters for each iteration. See the section “[Output Data Sets](#)” on page 4767 for a description of this data set.

---

## FCS Statement

**FCS** < options > ;

The FCS statement specifies a multivariate imputation by fully conditional specification methods. If you specify an FCS statement, you must also specify a VAR statement.

Table 57.2 summarizes the options available for the FCS statement.

**Table 57.2** Summary of Options in FCS

| Option                     | Description                                    |
|----------------------------|------------------------------------------------|
| <b>Imputation Details</b>  |                                                |
| NBITER=                    | Specifies the number of burn-in iterations     |
| <b>Data Set</b>            |                                                |
| OUTITER=                   | Outputs parameter estimates used in iterations |
| <b>ODS Output Graphics</b> |                                                |
| PLOTS=TRACE                | Displays trace plots                           |
| <b>Imputation Methods</b>  |                                                |
| DISCRIM                    | Specifies the discriminant function method     |
| LOGISTIC                   | Specifies the logistic regression method       |
| REG                        | Specifies the regression method                |
| REGPMM                     | Specifies the predictive mean matching method  |

The following options are available for the FCS statement in addition to the imputation methods specified (in alphabetical order):

**NBITER=number**

specifies the number of burn-in iterations before each imputation. The default is NBITER=20.

**OUTITER <( options )> =SAS-data-set**

creates an output SAS data set of TYPE=COV that contains parameters used in the imputation step for each iteration. The data set includes variables named `_Imputation_` and `_Iteration_` to identify the imputation number and iteration number.

The parameters in the output data set depend on the options specified. You can specify the options MEAN and STD to output parameters of means and standard deviations, respectively. When no options are specified, the output data set contains the mean parameters used in the imputation step for each iteration. See the section “Output Data Sets” on page 4767 for a description of this data set.

**PLOTS <( LOG )> <= TRACE <( trace-options ) >>**

requests statistical graphics of trace plots from iterations via the Output Delivery System (ODS).

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;
proc mi data=Fitness1 seed=501213 mu0=50 10 180;
 mcmc plots=(trace(mean(Oxygen)) acf(mean(Oxygen)));
 var Oxygen RunTime RunPulse;
run;
ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The global plot option LOG requests that the logarithmic transformations of parameters be used. The default is PLOTS=TRACE(MEAN).

The available *trace-options* are as follows:

**MEAN <( variables ) >**

displays plots of means for continuous variables in the list. When the MEAN option is specified without variables, all continuous variables are used.

**STD <( variables ) >**

displays plots of standard deviations for continuous variables in the list. When the STD option is specified without variables, all continuous variables are used.

The discriminant function, logistic regression, regression, and predictive mean matching methods are available in the FCS statement. You specify each method with the syntax

```
method < (<imputed <= effects >> </ options>) >
```

That is, for each method, you can specify the imputed variables and, optionally, a set of effects to impute these variables. Each effect is a variable or a combination of variables in the VAR statement. The syntax for the specification of effects is the same as for the GLM procedure. See Chapter 42, “The GLM Procedure,” for more information.

One general form of an effect involving several variables is

$$X1 * X2 * A * B * C ( D E )$$

where A, B, C, D, and E are classification variables and X1 and X2 are continuous variables.

When an FCS statement is used without specifying any methods, the regression method is used for all continuous variables and the discriminant function method is used for all classification variables. For each imputed variable, all other variables in the VAR statement are used as the covariates.

When a method for continuous variables is specified without imputed variables, the method is used for all continuous variables in the VAR statement that are not specified in other methods. Similarly, when a method for classification variables is specified without imputed variables, the method is used for all classification variables in the VAR statement that are not specified in other methods.

For each imputed variable, if no covariates are specified, then all other variables in the VAR statement are used as the covariates. That is, each continuous variable is used as a regressor effect, and each classification variable is used as a main effect. For the discriminant function method, only the continuous variables can be used as covariate effects.

With an FCS statement, the variables are imputed sequentially in the order specified in the VAR statement. For a continuous variable, you can use a regression method or a regression predicted mean matching method to impute missing values. For a nominal classification variable, you can use a discriminant function method to impute missing values without using the ordering of the class levels. For an ordinal classification variable, you can use a logistic regression method to impute missing values by using the ordering of the class levels. For a binary classification variable, either a discriminant function method or a logistic regression method can be used. By default, a regression method is used for a continuous variable, and a discriminant function method is used for a classification variable.

Note that except for the regression method, all other methods impute values from the observed values. See the section “[FCS Methods for Data Sets with Arbitrary Missing Patterns](#)” on page 4755 for a detailed description of the FCS methods.

You can specify the following imputation methods in an FCS statement (in alphabetical order):

**DISCRIM** *< ( imputed < = effects > < / options > ) >*

specifies the discriminant function method of classification variables. The available options are DETAILS, PCOV=, PRIOR=, and CLASSEFFECTS=. The DETAILS option displays the group means and pooled covariance matrix used in each imputation. The PCOV= option specifies the pooled covariance used in the discriminant method. Valid values for the PCOV= option are as follows:

|           |                                                                      |
|-----------|----------------------------------------------------------------------|
| FIXED     | uses the observed-data pooled covariance matrix for each imputation. |
| POSTERIOR | draws a pooled covariance matrix from its posterior distribution.    |

The default is PCOV=POSTERIOR. See the section “[Monotone and FCS Discriminant Function Methods](#)” on page 4752 for a detailed description of the method.

The PRIOR= option specifies the prior probabilities of group membership. Valid values for the PRIOR= option are as follows:

|              |                                                                    |
|--------------|--------------------------------------------------------------------|
| EQUAL        | sets the prior probabilities equal for all groups.                 |
| PROPORTIONAL | sets the prior probabilities proportion to the group sample sizes. |

JEFFREYS < =*c* > specifies a noninformative prior,  $0 < c < 1$ . If the number *c* is not specified, JEFFREYS=0.5.

RIDGE < =*d* > specifies a ridge prior,  $d > 0$ . If the number *d* is not specified, RIDGE=0.25.

The default is PRIOR=JEFFREYS. See the section “[Monotone and FCS Discriminant Function Methods](#)” on page 4752 for a detailed description of the method.

The CLASSEFFECTS= option specifies whether the CLASS variables are used as covariate effects. Valid values for the CLASSEFFECTS= option are as follows:

EXCLUDE excludes the CLASS variables from covariate effects.

INCLUDE includes the CLASS variables as covariate effects.

The default is CLASSEFFECTS=EXCLUDE.

**LOGISTIC** < ( *imputed* < = *effects* > < / *options* > ) >

specifies the logistic regression method of classification variables. The available options are DETAILS, ORDER=, and DESCENDING. The DETAILS option displays the regression coefficients in the logistic regression model used in each imputation.

When the imputed variable has more than two response levels, the ordinal logistic regression method is used. The ORDER= option specifies the sort order for the levels of the response variable. Valid values for the ORDER= option are as follows:

DATA sorts by the order of appearance in the input data set.

FORMATTED sorts by their external formatted values.

FREQ sorts by the descending frequency counts.

INTERNAL sorts by the unformatted values.

By default, ORDER=FORMATTED.

The option DESCENDING reverses the sort order for the levels of the response variables.

See the section “[Monotone and FCS Logistic Regression Methods](#)” on page 4754 for a detailed description of the method.

**REG | REGRESSION** < ( *imputed* < = *effects* > < / **DETAILS** > ) >

specifies the regression method of continuous variables. The DETAILS option displays the regression coefficients in the regression model used in each imputation.

With a regression method, the MAXIMUM=, MINIMUM=, and ROUND= options can be used to make the imputed values more consistent with the observed variable values.

See the section “[Monotone and FCS Regression Methods](#)” on page 4749 for a detailed description of the method.

**REGPMM** < ( *imputed* < = *effects* > < *options* > ) >

**REGPREDMEANMATCH** < ( *imputed* < = *effects* > < *options* > ) >

specifies the predictive mean matching method for continuous variables. This method is similar to the regression method except that it imputes a value randomly from a set of observed values whose predicted values are closest to the predicted value for the missing value from the simulated regression model (Heitjan and Little 1991; Schenker and Taylor 1996).

The available options are DETAILS and K=. The DETAILS option displays the regression coefficients in the regression model used in each imputation. The K= option specifies the number of closest observations to be used in the selection. The default is K=5.

See the section “[Monotone and FCS Predictive Mean Matching Methods](#)” on page 4750 for a detailed description of the method.

With an FCS statement, the missing values of variables in the VAR statement are imputed. After the initial filled in, these variables with missing values are imputed sequentially in the order specified in the VAR statement. For example, the following MI procedure statements use the regression method to impute variable y1 from effect y2, the regression method to impute variable y3 from effects y1 and y2, the logistic regression method to impute variable c1 from effects y1, y2, and y1 \* y2, and the default regression method for continuous variables to impute variable y2 from effects y1, y3, and c1:

```
proc mi;
 class c1;
 fcs reg(y1= y2) reg(y3= y1 y2) logistic(c1= y1 y2 y1*y2);
 var y1 y2 y3 c1;
run;
```

---

## FREQ Statement

**FREQ** *variable* ;

To run a procedure on an input data set that contains observations that occur multiple times, you can use a variable in the data set to represent how frequently observations occur and specify a FREQ statement with the name of that variable as its argument (*variable*) when you run the procedure.

When you specify a FREQ statement in other SAS procedures, they treat the data set as if each observation appeared *n* times, where *n* is the value of *variable* in the observation. However, PROC MI treats the data set differently because as PROC MI imputes each missing value in each observation, it generates only one imputed value for that missing value. That is, when you specify a FREQ *variable*, each imputed observation (with its imputed value in place of the missing value) is treated as if it appeared *n* times. In contrast, if an observation actually occurs *n* times in the data set, the missing value at each occurrence is imputed separately, and the resulting *n* observations are not identical.

PROC MI uses only the integer portion of each value of *variable*; if any value is less than 1, PROC MI does not use the corresponding observation in the analysis. When PROC MI calculates significance probabilities, it considers the total number of observations to be equal to the sum of the values of *variable*.

---

## MCMC Statement

**MCMC** < options > ;

The MCMC statement specifies the details of the MCMC method for imputation.

Table 57.3 summarizes the options available for the MCMC statement.

**Table 57.3** Summary of Options in MCMC

| Option                      | Description                                                       |
|-----------------------------|-------------------------------------------------------------------|
| <b>Data Sets</b>            |                                                                   |
| INEST=                      | Inputs parameter estimates for imputations                        |
| OUTEST=                     | Outputs parameter estimates used in imputations                   |
| OUTITER=                    | Outputs parameter estimates used in iterations                    |
| <b>Imputation Details</b>   |                                                                   |
| IMPUTE=                     | Specifies monotone or full imputation                             |
| CHAIN=                      | Specifies single or multiple chain                                |
| NBITER=                     | Specifies the number of burn-in iterations for each chain         |
| NITER=                      | Specifies the number of iterations between imputations in a chain |
| INITIAL=                    | Specifies initial parameter estimates for MCMC                    |
| PRIOR=                      | Specifies the prior parameter information                         |
| START=                      | Specifies starting parameters                                     |
| <b>ODS Output Graphics</b>  |                                                                   |
| PLOTS=TRACE                 | Displays trace plots                                              |
| PLOTS=ACF                   | Displays autocorrelation plots                                    |
| <b>Traditional Graphics</b> |                                                                   |
| TIMEPLOT                    | Displays trace plots                                              |
| ACFPLOT                     | Displays autocorrelation plots                                    |
| GOUT=                       | Specifies the graphics catalog name for saving graphics output    |
| <b>Printed Output</b>       |                                                                   |
| WLF                         | Displays the worst linear function                                |
| DISPLAYINIT                 | Displays initial parameter values for MCMC                        |

The following options are available for the MCMC statement (in alphabetical order).

**ACFPLOT** < (options< / display-options >) >

displays the traditional autocorrelation function plots of parameters from iterations. The ACFPLOT option is applicable only if ODS Graphics is not enabled.

The available options are as follows.

**COV** <( < *variables* > < *variable1\*variable2* > < ... *variable1\*variable2* > ) >

displays plots of variances for variables in the list and covariances for pairs of variables in the list. When the option COV is specified without variables, variances for all variables and covariances for all pairs of variables are used.

**MEAN** <( *variables* ) >

displays plots of means for variables in the list. When the option MEAN is specified without variables, all variables are used.

**WLF**

displays the plot for the worst linear function.

When the ACFPLOT is specified without the preceding options, the procedure displays plots of means for all variables that are used.

The display options provide additional information for the autocorrelation function plots. The available display options are as follows:

**CCONF**=*color*

specifies the color of the displayed confidence limits. The default is CCONF=BLACK.

**CFRAME**=*color*

specifies the color for filling the area enclosed by the axes and the frame. By default, this area is not filled.

**CNEEDLES**=*color*

specifies the color of the vertical line segments (needles) that connect autocorrelations to the reference line. The default is CNEEDLES=BLACK.

**CREF**=*color*

specifies the color of the displayed reference line. The default is CREF=BLACK.

**CSYMBOL**=*color*

specifies the color of the displayed data points. The default is CSYMBOL=BLACK.

**HSYMBOL**=*number*

specifies the height of data points in percentage screen units. The default is HSYMBOL=1.

**LCONF**=*linetype*

specifies the line type for the displayed confidence limits. The default is LCONF=1, a solid line.

**LOG**

requests that the logarithmic transformations of parameters be used to compute the autocorrelations; it is generally used for the variances of variables. When a parameter has values less than or equal to zero, the corresponding plot is not created.

**LREF**=*linetype*

specifies the line type for the displayed reference line. The default is LREF=3, a dashed line.

**NAME=***'string'*

specifies a descriptive name, up to eight characters, that appears in the name field of the PROC GREPLAY master menu. The default is NAME='MI'.

**NLAG=***number*

specifies the maximum lag of the series. The default is NLAG=20. The autocorrelations at each lag are displayed in the graph.

**SYMBOL=***value*

specifies the symbol for data points in percentage screen units. The default is SYMBOL=STAR.

**TITLE=***'string'*

specifies the title to be displayed in the autocorrelation function plots. The default is TITLE='Autocorrelation Plot'.

**WCONF=***number*

specifies the width of the displayed confidence limits in percentage screen units. If you specify the WCONF=0 option, the confidence limits are not displayed. The default is WCONF=1.

**WNEEDLES=***number*

specifies the width of the displayed needles that connect autocorrelations to the reference line, in percentage screen units. If you specify the WNEEDLES=0 option, the needles are not displayed. The default is WNEEDLES=1.

**WREF=***number*

specifies the width of the displayed reference line in percentage screen units. If you specify the WREF=0 option, the reference line is not displayed. The default is WREF=1.

For example, the following statement requests autocorrelation function plots for the means and variances of the variable *y1*, respectively:

```
acfplot (mean(y1) cov(y1) /log);
```

Logarithmic transformations of both the means and variances are used in the plots. For a detailed description of the autocorrelation function plot, see the section “[Autocorrelation Function Plot](#)” on page 4765; see also Schafer (1997, pp. 120–126) and the *SAS/ETS User's Guide*.

**CHAIN=SINGLE | MULTIPLE**

specifies whether a single chain is used for all imputations or a separate chain is used for each imputation. The default is CHAIN=SINGLE.

**DISPLAYINIT**

displays initial parameter values in the MCMC method for each imputation.

**GOUT=***graphics-catalog*

specifies the graphics catalog for saving graphics output from PROC MI. The default is WORK.GSEG. For more information, see “The GREPLAY Procedure” in *SAS/GRAPH: Reference*.



**IMPUTE=FULL | MONOTONE**

specifies whether a full-data imputation is used for all missing values or a monotone-data imputation is used for a subset of missing values to make the imputed data sets have a monotone missing pattern. The default is `IMPUTE=FULL`. When `IMPUTE=MONOTONE` is specified, the order in the `VAR` statement is used to complete the monotone pattern.

**INEST=SAS-data-set**

names a SAS data set of `TYPE=EST` that contains parameter estimates for imputations. These estimates are used to impute values for observations in the `DATA=` data set. A detailed description of the data set is provided in the section “[Input Data Sets](#)” on page 4766.

**INITIAL=EM <(options)>****INITIAL=INPUT=SAS-data-set**

specifies the initial mean and covariance estimates for the MCMC method. The default is `INITIAL=EM`.

You can specify `INITIAL=INPUT=SAS-data-set` to read the initial estimates of the mean and covariance matrix for each imputation from a SAS data set. See the section “[Input Data Sets](#)” on page 4766 for a description of this data set.

With `INITIAL=EM`, PROC MI derives parameter estimates for a posterior mode, the highest observed-data posterior density, from the EM algorithm. The MLE from the EM algorithm is used to start the EM algorithm for the posterior mode, and the resulting EM estimates are used to begin the MCMC method. The prior information specified in the `PRIOR=` option is also used in the process to compute the posterior mode.

The following four options are available with `INITIAL=EM`:

**BOOTSTRAP <=number >**

requests bootstrap resampling, which uses a simple random sample with replacement from the input data set for the initial estimate. You can explicitly specify the number of observations in the random sample. Alternatively, you can implicitly specify the number of observations in the random sample by specifying the proportion  $p$ ,  $0 < p \leq 1$ , to request  $[np]$  observations in the random sample, where  $n$  is the number of observations in the data set and  $[np]$  is the integer part of  $np$ . This produces an overdispersed initial estimate that provides different starting values for the MCMC method. If you specify the `BOOTSTRAP` option without the number,  $p = 0.75$  is used by default.

**CONVERGE= $\rho$** **XCONV= $\rho$** 

sets the convergence criterion. The value must be between 0 and 1. The iterations are considered to have converged when the change in the parameter estimates between iteration steps is less than  $\rho$  for each parameter—that is, for each of the means and covariances. For each parameter, the change is a relative change if the parameter is greater than 0.01 in absolute value; otherwise, it is an absolute change. By default, `CONVERGE=1E-4`.

**ITPRINT**

prints the iteration history in the EM algorithm for the posterior mode.

**MAXITER=number**

specifies the maximum number of iterations used in the EM algorithm. The default is MAXITER=200.

**NBITER=number**

specifies the number of burn-in iterations before the first imputation in each chain. The default is NBITER=200.

**NITER=number**

specifies the number of iterations between imputations in a single chain. The default is NITER=100.

**OUTEST=SAS-data-set**

creates an output SAS data set of TYPE=EST. The data set contains parameter estimates used in each imputation. The data set also includes a variable named `_Imputation_` to identify the imputation number. See the section “[Output Data Sets](#)” on page 4767 for a description of this data set.

**OUTITER < ( options ) > =SAS-data-set**

creates an output SAS data set of TYPE=COV that contains parameters used in the imputation step for each iteration. The data set includes variables named `_Imputation_` and `_Iteration_` to identify the imputation number and iteration number.

The parameters in the output data set depend on the options specified. You can specify the options MEAN, STD, COV, LR, LR\_POST, and WLF to output parameters of means, standard deviations, covariances,  $-2 \log$  LR statistic,  $-2 \log$  LR statistic of the posterior mode, and the worst linear function, respectively. When no options are specified, the output data set contains the mean parameters used in the imputation step for each iteration. See the section “[Output Data Sets](#)” on page 4767 for a description of this data set.

**PLOTS < ( LOG ) > < = plot-request >****PLOTS < ( LOG ) > < = ( plot-request < ... plot-request > ) >**

requests statistical graphics via the Output Delivery System (ODS). To request these graphs, ODS Graphics must be enabled and you must specify options in the MCMC statement. For more information about ODS Graphics, see Chapter 21, “[Statistical Graphics Using ODS](#).”

The global plot option LOG requests that the logarithmic transformations of parameters be used. The plot request options include the following:

**ACF < ( acf-options ) >**

displays plots of the autocorrelation function of parameters from iterations. The default is ACF(MEAN).

**ALL**

produces all appropriate plots.

**NONE**

suppresses all plots.

**TRACE < ( trace-options ) >**

displays trace plots of parameters from iterations. The default is TRACE(MEAN).

The available *acf-options* are as follows:

**NLAG=*n***

specifies the maximum lag of the series. The default is NLAG=20. The autocorrelations at each lag are displayed in the graph.

**COV < ( < *variables* > < *variable1\*variable2* > ... ) >**

displays plots of variances for variables in the list and covariances for pairs of variables in the list. When the option COV is specified without variables, variances for all variables and covariances for all pairs of variables are used.

**MEAN < ( *variables* ) >**

displays plots of means for variables in the list. When the option MEAN is specified without variables, all variables are used.

**WLF**

displays the plot for the worst linear function.

The available *trace-options* are as follows:

**COV < ( < *variables* > < *variable1\*variable2* > ... ) >**

displays plots of variances for variables in the list and covariances for pairs of variables in the list. When the option COV is specified without variables, variances for all variables and covariances for all pairs of variables are used.

**MEAN < ( *variables* ) >**

displays plots of means for variables in the list. When the option MEAN is specified without variables, all variables are used.

**WLF**

displays the plot of the worst linear function.

**PRIOR=*name***

specifies the prior information for the means and covariances. Valid values for *name* are as follows:

JEFFREYS specifies a noninformative prior.

RIDGE=*number* specifies a ridge prior.

INPUT=*SAS-data-set* specifies a data set that contains prior information.

For a detailed description of the prior information, see the section “[Bayesian Estimation of the Mean Vector and Covariance Matrix](#)” on page 4759 and the section “[Posterior Step](#)” on page 4759. If you do not specify the PRIOR= option, the default is PRIOR=JEFFREYS.

The PRIOR=INPUT= option specifies a TYPE=COV data set from which the prior information of the mean vector and the covariance matrix is read. See the section “[Input Data Sets](#)” on page 4766 for a description of this data set.

**START=VALUE | DIST**

specifies that the initial parameter estimates are used either as the starting value (START=VALUE) or as the starting distribution (START=DIST) in the first imputation step of each chain. If the IMPUTE=MONOTONE option is specified, then START=VALUE is used in the procedure. The default is START=VALUE.

**TIMEPLOT** < ( *options* < / *display-options* > ) >

displays the traditional trace (time series) plots of parameters from iterations. The TIMEPLOT option is applicable only if ODS Graphics is not enabled.

The available options are as follows:

**COV** < ( < *variables* > < *variable1\*variable2* > ... ) >

displays plots of variances for variables in the list and covariances for pairs of variables in the list. When the option COV is specified without variables, variances for all variables and covariances for all pairs of variables are used.

**MEAN** < (*variables*)>

displays plots of means for variables in the list. When the option MEAN is specified without variables, all variables are used.

**WLF**

displays the plot of the worst linear function.

When the TIMEPLOT is specified without the preceding options, the procedure displays plots of means for all variables that are used.

The display options provide additional information for the trace plots. The available display options are as follows:

**CCONNECT**=*color*

specifies the color of the line segments that connect data points in the trace plots. The default is CCONNECT=BLACK.

**CFRAME**=*color*

specifies the color for filling the area enclosed by the axes and the frame. By default, this area is not filled.

**CSYMBOL**=*color*

specifies the color of the data points to be displayed in the trace plots. The default is CSYMBOL=BLACK.

**HSYMBOL**=*number*

specifies the height of data points in percentage screen units. The default is HSYMBOL=1.

**LCONNECT**=*linetype*

specifies the line type for the line segments that connect data points in the trace plots. The default is LCONNECT=1, a solid line.

**LOG**

requests that the logarithmic transformations of parameters be used; it is generally used for the variances of variables. When a parameter value is less than or equal to zero, the value is not displayed in the corresponding plot.

**NAME=***string*

specifies a descriptive name, up to eight characters, that appears in the name field of the PROC GREPLAY master menu. The default is NAME='MI'.

**SYMBOL=***value*

specifies the symbol for data points in percentage screen units. The default is SYMBOL=PLUS.

**TITLE=***string*

specifies the title to be displayed in the trace plots. The default is TITLE='Trace Plot'.

**WCONNECT=***number*

specifies the width of the line segments that connect data points in the trace plots, in percentage screen units. If you specify the WCONNECT=0 option, the data points are not connected. The default is WCONNECT=1.

For a detailed description of the trace plot, see the section “[Trace Plot](#)” on page 4765 and Schafer (1997, pp. 120–126).

**WLF**

displays the worst linear function of parameters. This scalar function of parameters  $\mu$  and  $\Sigma$  is “worst” in the sense that its values from iterations converge most slowly among parameters. For a detailed description of this statistic, see the section “[Worst Linear Function of Parameters](#)” on page 4764.

---

## MONOTONE Statement

```
MONOTONE <method <(<imputed <= effects>> </options>)>>
 <...method <(<imputed <= effects>> </options>)>> ;
```

The MONOTONE statement specifies imputation methods for data sets with monotone missingness. You must also specify a VAR statement, and the data set must have a monotone missing pattern with variables ordered in the VAR list.

Table 57.4 summarizes the options available for the MONOTONE statement.

**Table 57.4** Summary of Imputation Methods in MONOTONE Statement

| Option     | Description                                   |
|------------|-----------------------------------------------|
| DISCRIM    | Specifies the discriminant function method    |
| LOGISTIC   | Specifies the logistic regression method      |
| PROPENSITY | Specifies the propensity scores method        |
| REG        | Specifies the regression method               |
| REGPMM     | Specifies the predictive mean matching method |

For each method, you can specify the imputed variables and, optionally, a set of the effects to impute these variables. Each effect is a variable or a combination of variables preceding the imputed variable in the VAR statement. The syntax for specification of effects is the same as for the GLM procedure. See Chapter 42, “The GLM Procedure,” for more information.

One general form of an effect involving several variables is

$$X1 * X2 * A * B * C ( D E )$$

where A, B, C, D, and E are classification variables and X1 and X2 are continuous variables.

If no covariates are specified, then all preceding variables are used as the covariates. That is, each preceding continuous variable is used as a regressor effect, and each preceding classification variable is used as a main effect. For the discriminant function method, only the continuous variables can be used as covariate effects.

When a method for continuous variables is specified without imputed variables, the method is used for all continuous variables in the VAR statement that are not specified in other methods. Similarly, when a method for classification variables is specified without imputed variables, the method is used for all classification variables in the VAR statement that are not specified in other methods.

When a MONOTONE statement is used without specifying any methods, the regression method is used for all continuous variables and the discriminant function method is used for all classification variables. The preceding variables of each imputed variable in the VAR statement are used as the covariates.

With a MONOTONE statement, the variables are imputed sequentially in the order given by the VAR statement. For a continuous variable, you can use a regression method, a regression predicted mean matching method, or a propensity score method to impute missing values.

For a nominal classification variable, you can use a discriminant function method to impute missing values without using the ordering of the class levels. For an ordinal classification variable, you can use a logistic regression method to impute missing values by using the ordering of the class levels. For a binary classification variable, either a discriminant function method or a logistic regression method can be used.

Note that except for the regression method, all other methods impute values from the observed observation values. You can specify the following methods in a MONOTONE statement.

**DISCRIM** < ( *imputed* < = *effects* > < / *options* > ) >

specifies the discriminant function method of classification variables. The available options are DETAILS, PCOV=, PRIOR=, and CLASSEFFECTS=. The DETAILS option displays the group means and pooled covariance matrix used in each imputation. The PCOV= option specifies the pooled covariance used in the discriminant method. Valid values for the PCOV= option are as follows:

|           |                                                                      |
|-----------|----------------------------------------------------------------------|
| FIXED     | uses the observed-data pooled covariance matrix for each imputation. |
| POSTERIOR | draws a pooled covariance matrix from its posterior distribution.    |

The default is PCOV=POSTERIOR. See the section “[Monotone and FCS Discriminant Function Methods](#)” on page 4752 for a detailed description of the method.

The PRIOR= option specifies the prior probabilities of group membership. Valid values for the PRIOR= option are as follows:

|              |                                                                    |
|--------------|--------------------------------------------------------------------|
| EQUAL        | sets the prior probabilities equal for all groups.                 |
| PROPORTIONAL | sets the prior probabilities proportion to the group sample sizes. |

**JEFFREYS** < =*c* > specifies a noninformative prior,  $0 < c < 1$ . If the number *c* is not specified, JEFFREYS=0.5.

**RIDGE** < =*d* > specifies a ridge prior,  $d > 0$ . If the number *d* is not specified, RIDGE=0.25.

The default is PRIOR=JEFFREYS. See the section “[Monotone and FCS Discriminant Function Methods](#)” on page 4752 for a detailed description of the method.

The CLASSEFFECTS= option specifies whether the CLASS variables are used as covariate effects. Valid values for the CLASSEFFECTS= option are as follows:

**EXCLUDE** excludes the CLASS variables from covariate effects.

**INCLUDE** includes the CLASS variables as covariate effects.

The default is CLASSEFFECTS=EXCLUDE.

**LOGISTIC** < ( *imputed* < = *effects* > < / *options* > ) >

specifies the logistic regression method of classification variables. The available options are DETAILS, ORDER=, and DESCENDING. The DETAILS option displays the regression coefficients in the logistic regression model used in each imputation.

When the imputed variable has more than two response levels, the ordinal logistic regression method is used. The ORDER= option specifies the sort order for the levels of the response variable. Valid values for the ORDER= option are as follows:

**DATA** sorts by the order of appearance in the input data set.

**FORMATTED** sorts by their external formatted values.

**FREQ** sorts by the descending frequency counts.

**INTERNAL** sorts by the unformatted values.

By default, ORDER=FORMATTED.

The option DESCENDING reverses the sort order for the levels of the response variables.

See the section “[Monotone and FCS Logistic Regression Methods](#)” on page 4754 for a detailed description of the method.

**PROPNENSITY** < ( *imputed* < = *effects* > < / *options* > ) >

specifies the propensity scores method of variables. Each variable is either a classification variable or a continuous variable. The available options are DETAILS and NGROUPS=. The DETAILS option displays the regression coefficients in the logistic regression model for propensity scores. The NGROUPS= option specifies the number of groups created based on propensity scores. The default is NGROUPS=5.

See the section “[Monotone Propensity Score Method](#)” on page 4751 for a detailed description of the method.

**REG | REGRESSION** < ( *imputed* < = *effects* > < / **DETAILS** > ) >

specifies the regression method of continuous variables. The DETAILS option displays the regression coefficients in the regression model used in each imputation.

With a regression method, the MAXIMUM=, MINIMUM=, and ROUND= options can be used to make the imputed values more consistent with the observed variable values.

See the section “[Monotone and FCS Regression Methods](#)” on page 4749 for a detailed description of the method.

**REGPMM** < ( *imputed* < = *effects* > < *options* > ) >

**REGPREDMEANMATCH** < ( *imputed* < = *effects* > < *options* > ) >

specifies the predictive mean matching method for continuous variables. This method is similar to the regression method except that it imputes a value randomly from a set of observed values whose predicted values are closest to the predicted value for the missing value from the simulated regression model (Heitjan and Little 1991; Schenker and Taylor 1996).

The available options are DETAILS and K=. The DETAILS option displays the regression coefficients in the regression model used in each imputation. The K= option specifies the number of closest observations to be used in the selection. The default is K=5.

See the section “[Monotone and FCS Predictive Mean Matching Methods](#)” on page 4750 for a detailed description of the method.

With a MONOTONE statement, the missing values of a variable are imputed when the variable is either explicitly specified in the method or implicitly specified when a method is specified without imputed variables. These variables are imputed sequentially in the order specified in the VAR statement. For example, the following MI procedure statements use the logistic regression method to impute variable c1 from effects y1, y2, and y1 \* y2 first, and then use the regression method to impute variable y3 from effects y1, y2, and c1:

```
proc mi;
 class c1;
 var y1 y2 c1 y3;
 monotone reg(y3= y1 y2 c1) logistic(c1= y1 y2 y1*y2);
run;
```

The variables y1 and y2 are not imputed since y1 is the leading variable in the VAR statement and y2 is not specified as an imputed variable in the MONOTONE statement.

---

## TRANSFORM Statement

**TRANSFORM** *transform* (*variables*</ *options*>)< . . . *transform* (*variables*</ *options*>)> ;

The TRANSFORM statement lists the transformations and their associated variables to be transformed. The options are transformation options that provide additional information for the transformation.

The MI procedure assumes that the data are from a multivariate normal distribution when either the regression method or the MCMC method is used. When some variables in a data set are clearly non-normal, it is useful to transform these variables to conform to the multivariate normality assumption. With a TRANSFORM statement, variables are transformed before the imputation process, and these transformed variable values are displayed in all of the results. When you specify an OUT= option, the variable values are back-transformed to create the imputed data set.



The following transformations can be used in the TRANSFORM statement:

**BOXCOX**

specifies the Box-Cox transformation of variables. The variable  $Y$  is transformed to  $\frac{(Y+c)^\lambda - 1}{\lambda}$ , where  $c$  is a constant such that each value of  $Y + c$  must be positive. If the specified constant  $\lambda = 0$ , the logarithmic transformation is used.

**EXP**

specifies the exponential transformation of variables. The variable  $Y$  is transformed to  $e^{(Y+c)}$ , where  $c$  is a constant.

**LOG**

specifies the logarithmic transformation of variables. The variable  $Y$  is transformed to  $\log(Y + c)$ , where  $c$  is a constant such that each value of  $Y + c$  must be positive.

**LOGIT**

specifies the logit transformation of variables. The variable  $Y$  is transformed to  $\log\left(\frac{Y/c}{1-Y/c}\right)$ , where the constant  $c > 0$  and the values of  $Y/c$  must be between 0 and 1.

**POWER**

specifies the power transformation of variables. The variable  $Y$  is transformed to  $(Y + c)^\lambda$ , where  $c$  is a constant such that each value of  $Y + c$  must be positive and the constant  $\lambda \neq 0$ .

The following options provide the constant  $c$  and  $\lambda$  values in the transformations.

**C=number**

specifies the  $c$  value in the transformation. The default is  $c = 1$  for logit transformation and  $c = 0$  for other transformations.

**LAMBDA=number**

specifies the  $\lambda$  value in the power and Box-Cox transformations. You must specify the  $\lambda$  value for these two transformations.

For example, the following statement requests that variables  $\log(y1)$ , a logarithmic transformation for the variable  $y1$ , and  $\sqrt{y2 + 1}$ , a power transformation for the variable  $y2$ , be used in the imputation:

```
transform log(y1) power(y2/c=1 lambda=.5);
```

If the MU0= option is used to specify a parameter value  $\mu_0$  for a transformed variable, the same transformation for the variable is also applied to its corresponding MU0= value in the  $t$  test. Otherwise,  $\mu_0 = 0$  is used for the transformed variable. See [Example 57.10](#) for a usage of the TRANSFORM statement.

## VAR Statement

**VAR** *variables* ;

The VAR statement lists the variables to be analyzed. The variables can be either character or numeric. If you omit the VAR statement, all continuous variables not mentioned in other statements are used. The VAR statement is required if you specify either an FCS statement, a MONOTONE statement, an IMPUTE=MONOTONE option in the MCMC statement, or more than one number in the MU0=, MAXIMUM=, MINIMUM=, or ROUND= option.

The classification variables in the VAR statement, which can be either character or numeric, are further specified in the CLASS statement.

---

## Details: MI Procedure

---

### Descriptive Statistics

Suppose  $\mathbf{Y} = (\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_n)'$  is the  $(n \times p)$  matrix of complete data, which might not be fully observed,  $n_0$  is the number of observations fully observed, and  $n_j$  is the number of observations with observed values for variable  $Y_j$ .

With complete cases, the sample mean vector is

$$\bar{\mathbf{y}} = \frac{1}{n_0} \sum \mathbf{y}_i$$

and the CSSCP matrix is

$$\sum (\mathbf{y}_i - \bar{\mathbf{y}})(\mathbf{y}_i - \bar{\mathbf{y}})'$$

where each summation is over the fully observed observations.

The sample covariance matrix is

$$\mathbf{S} = \frac{1}{n_0 - 1} \sum (\mathbf{y}_i - \bar{\mathbf{y}})(\mathbf{y}_i - \bar{\mathbf{y}})'$$

and is an unbiased estimate of the covariance matrix.

The correlation matrix  $\mathbf{R}$ , which contains the Pearson product-moment correlations of the variables, is derived by scaling the corresponding covariance matrix:

$$\mathbf{R} = \mathbf{D}^{-1} \mathbf{S} \mathbf{D}^{-1}$$

where  $\mathbf{D}$  is a diagonal matrix whose diagonal elements are the square roots of the diagonal elements of  $\mathbf{S}$ .

With available cases, the corrected sum of squares for variable  $Y_j$  is

$$\sum (y_{ji} - \bar{y}_j)^2$$

where  $\bar{y}_j = \frac{1}{n_j} \sum y_{ji}$  is the sample mean and each summation is over observations with observed values for variable  $Y_j$ .

The variance is

$$s_{jj}^2 = \frac{1}{n_j - 1} \sum (y_{ji} - \bar{y}_j)^2$$

The correlations for available cases contain pairwise correlations for each pair of variables. Each correlation is computed from all observations that have nonmissing values for the corresponding pair of variables.

## EM Algorithm for Data with Missing Values

The EM algorithm (Dempster, Laird, and Rubin 1977) is a technique that finds maximum likelihood estimates in parametric models for incomplete data. For a detailed description and applications of the EM algorithm, see the books by Little and Rubin (2002); Schafer (1997); McLachlan and Krishnan (1997).

The EM algorithm is an iterative procedure that finds the MLE of the parameter vector by repeating the following steps:

### 1. The expectation E-step

Given a set of parameter estimates, such as a mean vector and covariance matrix for a multivariate normal distribution, the E-step calculates the conditional expectation of the complete-data log likelihood given the observed data and the parameter estimates.

### 2. The maximization M-step

Given a complete-data log likelihood, the M-step finds the parameter estimates to maximize the complete-data log likelihood from the E-step.

The two steps are iterated until the iterations converge.

In the EM process, the observed-data log likelihood is nondecreasing at each iteration. For multivariate normal data, suppose there are  $G$  groups with distinct missing patterns. Then the observed-data log likelihood being maximized can be expressed as

$$\log L(\theta|Y_{obs}) = \sum_{g=1}^G \log L_g(\theta|Y_{obs})$$

where  $\log L_g(\theta|Y_{obs})$  is the observed-data log likelihood from the  $g$ th group, and

$$\log L_g(\theta|Y_{obs}) = -\frac{n_g}{2} \log |\Sigma_g| - \frac{1}{2} \sum_{i_g} (\mathbf{y}_{i_g} - \boldsymbol{\mu}_g)' \Sigma_g^{-1} (\mathbf{y}_{i_g} - \boldsymbol{\mu}_g)$$

where  $n_g$  is the number of observations in the  $g$ th group, the summation is over observations in the  $g$ th group,  $\mathbf{y}_{i_g}$  is a vector of observed values corresponding to observed variables,  $\boldsymbol{\mu}_g$  is the corresponding mean vector, and  $\Sigma_g$  is the associated covariance matrix.

A sample covariance matrix is computed at each step of the EM algorithm. If the covariance matrix is singular, the linearly dependent variables for the observed data are excluded from the likelihood function. That is, for each observation with linear dependency among its observed variables, the dependent variables are excluded from the likelihood function. Note that this can result in an unexpected change in the likelihood between iterations prior to the final convergence.

See Schafer (1997, pp. 163–181) for a detailed description of the EM algorithm for multivariate normal data.

PROC MI uses the means and standard deviations from available cases as the initial estimates for the EM algorithm. The correlations are set to zero. These initial estimates provide a good starting value with positive definite covariance matrix. For a discussion of suggested starting values for the algorithm, see Schafer (1997, p. 169).

You can specify the convergence criterion with the `CONVERGE=` option in the EM statement. The iterations are considered to have converged when the maximum change in the parameter estimates between iteration steps is less than the value specified. You can also specify the maximum number of iterations used in the EM algorithm with the `MAXITER=` option.

The MI procedure displays tables of the initial parameter estimates used to begin the EM process and the MLE parameter estimates derived from EM. You can also display the EM iteration history with the `ITPRINT` option. PROC MI lists the iteration number, the likelihood  $-2 \log L$ , and the parameter values  $\mu$  at each iteration. You can also save the MLE derived from the EM algorithm in a SAS data set by specifying the `OUTEM=` option.

---

## Statistical Assumptions for Multiple Imputation

The MI procedure assumes that the data are from a continuous multivariate distribution and contain missing values that can occur for any of the variables. It also assumes that the data are from a multivariate normal distribution when either the regression method or the MCMC method is used.

Suppose  $\mathbf{Y}$  is the  $n \times p$  matrix of complete data, which is not fully observed, and denote the observed part of  $\mathbf{Y}$  by  $\mathbf{Y}_{obs}$  and the missing part by  $\mathbf{Y}_{mis}$ . The MI and MIANALYZE procedures assume that the missing data are missing at random (MAR); that is, the probability that an observation is missing can depend on  $\mathbf{Y}_{obs}$ , but not on  $\mathbf{Y}_{mis}$  (Rubin 1976, 1987, p. 53).

To be more precise, suppose that  $\mathbf{R}$  is the  $n \times p$  matrix of response indicators whose elements are zero or one depending on whether the corresponding elements of  $\mathbf{Y}$  are missing or observed. Then the MAR assumption is that the distribution of  $\mathbf{R}$  can depend on  $\mathbf{Y}_{obs}$  but not on  $\mathbf{Y}_{mis}$ :

$$\text{pr}(\mathbf{R} | \mathbf{Y}_{obs}, \mathbf{Y}_{mis}) = \text{pr}(\mathbf{R} | \mathbf{Y}_{obs})$$

For example, consider a trivariate data set with variables  $Y_1$  and  $Y_2$  fully observed, and a variable  $Y_3$  that has missing values. MAR assumes that the probability that  $Y_3$  is missing for an individual can be related to the individual's values of variables  $Y_1$  and  $Y_2$ , but not to its value of  $Y_3$ . On the other hand, if a complete case and an incomplete case for  $Y_3$  with exactly the same values for variables  $Y_1$  and  $Y_2$  have systematically different values, then there exists a response bias for  $Y_3$ , and MAR is violated.

The MAR assumption is not the same as missing completely at random (MCAR), which is a special case of MAR. Under the MCAR assumption, the missing data values are a simple random sample of all data values; the missingness does not depend on the values of any variables in the data set.

Although the MAR assumption cannot be verified with the data and it can be questionable in some situations, the assumption becomes more plausible as more variables are included in the imputation model (Schafer 1997, pp. 27–28; van Buuren, Boshuizen, and Knook 1999, p. 687).

Furthermore, the MI and MIANALYZE procedures assume that the parameters  $\theta$  of the data model and the parameters  $\phi$  of the model for the missing-data indicators are distinct. That is, knowing the values of  $\theta$  does not provide any additional information about  $\phi$ , and vice versa. If both the MAR and distinctness assumptions are satisfied, the missing-data mechanism is said to be ignorable Rubin 1987, pp. 50–54; Schafer 1997, pp. 10–11).

## Missing Data Patterns

The MI procedure sorts the data into groups based on whether the analysis variables are observed or missing. Note that the input data set does not need to be sorted in any order.

For example, with variables  $Y_1$ ,  $Y_2$ , and  $Y_3$  (in that order) in a data set, up to eight groups of observations can be formed from the data set. Figure 57.6 displays the eight groups of observations and an unique missing pattern for each group.

**Figure 57.6** Missing Data Patterns

| Missing Data Patterns |    |    |    |  |
|-----------------------|----|----|----|--|
| Group                 | Y1 | Y2 | Y3 |  |
| 1                     | X  | X  | X  |  |
| 2                     | X  | X  | .  |  |
| 3                     | X  | .  | X  |  |
| 4                     | X  | .  | .  |  |
| 5                     | .  | X  | X  |  |
| 6                     | .  | X  | .  |  |
| 7                     | .  | .  | X  |  |
| 8                     | .  | .  | .  |  |

Here, an “X” means that the variable is observed in the corresponding group and a “.” means that the variable is missing.

The variable order is used to derive the order of the groups from the data set, and thus determines the order of missing values in the data to be imputed. If you specify a different order of variables in the VAR statement, then the results are different even if the other specifications remain the same.

A data set with variables  $Y_1, Y_2, \dots, Y_p$  (in that order) is said to have a *monotone missing pattern* when the event that a variable  $Y_j$  is missing for a particular individual implies that all subsequent variables  $Y_k, k > j$ , are missing for that individual. Alternatively, when a variable  $Y_j$  is observed for a particular individual, it is assumed that all previous variables  $Y_k, k < j$ , are also observed for that individual.

For example, Figure 57.7 displays a data set of three variables with a monotone missing pattern.

**Figure 57.7** Monotone Missing Patterns

| Monotone Missing Data Patterns |    |    |    |  |
|--------------------------------|----|----|----|--|
| Group                          | Y1 | Y2 | Y3 |  |
| 1                              | X  | X  | X  |  |
| 2                              | X  | X  | .  |  |
| 3                              | X  | .  | .  |  |

Figure 57.8 displays a data set of three variables with a non-monotone missing pattern.

**Figure 57.8** Non-monotone Missing Patterns

| Non-monotone Missing Data Patterns |    |    |    |  |
|------------------------------------|----|----|----|--|
| Group                              | Y1 | Y2 | Y3 |  |
| 1                                  | X  | X  | X  |  |
| 2                                  | X  | .  | X  |  |
| 3                                  | .  | X  | .  |  |
| 4                                  | .  | .  | X  |  |

A data set with an *arbitrary missing pattern* is a data set with either a monotone missing pattern or a non-monotone missing pattern.

## Imputation Methods

This section describes the methods for multiple imputation that are available in the MI procedure. The method of choice depends on the pattern of missingness in the data and the type of the imputed variable, as summarized in Table 57.5.

**Table 57.5** Imputation Methods in PROC MI

| Pattern of Missingness | Type of Imputed Variable | Type of Covariates | Available Methods                                                                                                                                        |
|------------------------|--------------------------|--------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------|
| Monotone               | Continuous               | Arbitrary          | <ul style="list-style-type: none"> <li>• Monotone regression</li> <li>• Monotone predicted mean matching</li> <li>• Monotone propensity score</li> </ul> |
| Monotone               | Classification (ordinal) | Arbitrary          | <ul style="list-style-type: none"> <li>• Monotone logistic regression</li> </ul>                                                                         |
| Monotone               | Classification (nominal) | Arbitrary          | <ul style="list-style-type: none"> <li>• Monotone discriminant function</li> </ul>                                                                       |
| Arbitrary              | Continuous               | Continuous         | <ul style="list-style-type: none"> <li>• MCMC full-data imputation</li> <li>• MCMC monotone-data imputation</li> </ul>                                   |
| Arbitrary              | Continuous               | Arbitrary          | <ul style="list-style-type: none"> <li>• FCS regression</li> <li>• FCS predicted mean matching</li> </ul>                                                |
| Arbitrary              | Classification (ordinal) | Arbitrary          | <ul style="list-style-type: none"> <li>• FCS logistic regression</li> </ul>                                                                              |
| Arbitrary              | Classification (nominal) | Arbitrary          | <ul style="list-style-type: none"> <li>• FCS discriminant function</li> </ul>                                                                            |

To impute missing values for a continuous variable in data sets with monotone missing patterns, you should use either a parametric method that assumes multivariate normality or a nonparametric method that uses propensity scores (Rubin 1987, pp. 124, 158; Lavori, Dawson, and Shera 1995). Parametric methods available include the regression method (Rubin 1987, pp. 166–167) and the predictive mean matching method (Heitjan and Little 1991; Schenker and Taylor 1996).

To impute missing values for a classification variable in data sets with monotone missing patterns, you should use the logistic regression method or the discriminant function method. Use the logistic regression method when the classification variable has a binary or ordinal response, and use the discriminant function method when the classification variable has a binary or nominal response.

For data sets with arbitrary missing patterns, you can use either of the following methods to impute missing values: a Markov chain Monte Carlo (MCMC) method (Schafer 1997) that assumes multivariate normality, or a fully conditional specification (FCS) method (van Buuren 2007; Brand 1999) that assumes the existence of a joint distribution for all variables.

For continuous variables in data sets with arbitrary missing patterns, you can use the MCMC method to impute either all the missing values or just enough missing values to make the imputed data sets have monotone missing patterns. With a monotone missing data pattern, you have greater flexibility in your choice of imputation models. In addition to the MCMC method, you can implement other methods, such as the regression method, that do not use Markov chains. You can also specify a different set of covariates for each imputed variable.

Although the regression and MCMC methods assume multivariate normality, inferences based on multiple imputation can be robust to departures from multivariate normality if the amount of missing information is not large, because the imputation model is effectively applied not to the entire data set but only to its missing part (Schafer 1997, pp.147–148).

To impute missing values for both continuous and classification variables in data sets with arbitrary missing patterns, you can use FCS methods to impute missing values for all variables assuming a joint distribution for these variables exists (Brand 1999; van Buuren 2007). Similar to the methods of imputing missing values for variables in data sets with monotone missing patterns, you can use the regression and predictive mean matching methods to impute missing values for a continuous variable, and use the logistic regression method to impute missing values for a classification variable when the variable has a binary or ordinal response, or use the discriminant function method when the variable has a binary or nominal response.

You can also use a TRANSFORM statement to transform variables to conform to the multivariate normality assumption. Variables are transformed before the imputation process and then are reverse-transformed to create the imputed data set. All continuous variables are standardized before the imputation process and then are transformed back to the original scale after the imputation process.

Li (1988) presents a theoretical argument for convergence of the MCMC method in the continuous case and uses it to create imputations for incomplete multivariate continuous data. In practice, however, it is not easy to check the convergence of a Markov chain, especially for a large number of parameters. PROC MI generates statistics and plots that you can use to check for convergence of the MCMC method. The details are described in the section “[Checking Convergence in MCMC](#)” on page 4764.

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## Monotone Methods for Data Sets with Monotone Missing Patterns

For data sets with monotone missing data patterns, you can use monotone methods to impute missing values for the variables. A monotone method creates multiple imputations by imputing missing values sequentially over the variables taken one at a time.

For example, with variables  $Y_1, Y_2, \dots, Y_p$  (in that order) in the VAR statement, a monotone method sequentially simulates a draw for missing values for variables  $Y_2, \dots, Y_p$ . That is, the missing values are imputed by using the sequence

$$\begin{aligned}
\theta_2^{(*)} &\sim P(\theta_2 | Y_{1(obs)}, Y_{2(obs)}) \\
Y_2^{(*)} &\sim P(Y_2 | \theta_2^{(*)}) \\
&\dots \\
&\dots \\
\theta_p^{(*)} &\sim P(\theta_p | Y_{1(obs)}, \dots, Y_{p(obs)}) \\
Y_p^{(*)} &\sim P(Y_p | \theta_p^{(*)})
\end{aligned}$$

where  $Y_{j(obs)}$  is the set of observed  $Y_j$  values,  $\theta_j^{(*)}$  is the set of simulated parameters for the conditional distribution of  $Y_j$  given covariates constructed from variables  $Y_1, Y_2, \dots, Y_{j-1}$ , and  $Y_j^{(*)}$  is the set of imputed  $Y_j$  values.

The missing values for the leading variable  $Y_1$  are not imputed, and missing values for  $Y_2, \dots, Y_p$  are not imputed for those observations with missing  $Y_1$  values. For each subsequent variable  $Y_j$  with missing values, the corresponding imputation method is used to fit a model with covariates constructed from its preceding variables  $Y_1, Y_2, \dots, Y_{j-1}$ . The observed observations for  $Y_j$ , which include only observations with observed values for  $Y_1, Y_2, \dots, Y_{j-1}$ , are used in the model fitting. With this resulting model, a new model is drawn and then used to impute missing values for  $Y_j$ .

You can specify a separate monotone method for each imputed variable. If a method is not specified for the variable, then the default method is used. That is, a regression method is used for a continuous variable and a discriminant function method is used for a classification variable. For each imputed variable, you can also specify a set of covariates that are constructed from its preceding variables. If a set of covariates is not specified for the variable, all preceding variables in the VAR list are used as covariates.

You can use a regression method, a predictive mean matching method, or a propensity score method to impute missing values for a continuous variable; a logistic regression method for a classification variable with a binary or ordinal response; and a discriminant function method for a classification variable with a binary or nominal response. See the sections “[Monotone and FCS Regression Methods](#)” on page 4749, “[Monotone and FCS Predictive Mean Matching Methods](#)” on page 4750, “[Monotone Propensity Score Method](#)” on page 4751, “[Monotone and FCS Discriminant Function Methods](#)” on page 4752, and “[Monotone and FCS Logistic Regression Methods](#)” on page 4754 for these methods.

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## Monotone and FCS Regression Methods

The regression method is the default imputation method in the MONOTONE and FCS statements for continuous variables.

In the regression method, a regression model is fitted for a continuous variable with the covariates constructed from a set of effects. Based on the fitted regression model, a new regression model is simulated from the posterior predictive distribution of the parameters and is used to impute the missing values for each variable (Rubin 1987, pp. 166–167). That is, for a continuous variable  $Y_j$  with missing values, a model

$$Y_j = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_k X_k$$

is fitted using observations with observed values for the variable  $Y_j$  and its covariates  $X_1, X_2, \dots, X_k$ .



The fitted model includes the regression parameter estimates  $\hat{\boldsymbol{\beta}} = (\hat{\beta}_0, \hat{\beta}_1, \dots, \hat{\beta}_k)$  and the associated covariance matrix  $\hat{\sigma}_j^2 \mathbf{V}_j$ , where  $\mathbf{V}_j$  is the usual  $\mathbf{X}'\mathbf{X}$  inverse matrix derived from the intercept and covariates  $X_1, X_2, \dots, X_k$ .

The following steps are used to generate imputed values for each imputation:

1. New parameters  $\boldsymbol{\beta}_* = (\beta_{*0}, \beta_{*1}, \dots, \beta_{*(k)})$  and  $\sigma_{*j}^2$  are drawn from the posterior predictive distribution of the parameters. That is, they are simulated from  $(\hat{\beta}_0, \hat{\beta}_1, \dots, \hat{\beta}_k)$ ,  $\sigma_j^2$ , and  $\mathbf{V}_j$ . The variance is drawn as

$$\sigma_{*j}^2 = \hat{\sigma}_j^2 (n_j - k - 1) / g$$

where  $g$  is a  $\chi_{n_j - k - 1}^2$  random variate and  $n_j$  is the number of nonmissing observations for  $Y_j$ . The regression coefficients are drawn as

$$\boldsymbol{\beta}_* = \hat{\boldsymbol{\beta}} + \sigma_{*j} \mathbf{V}'_{hj} \mathbf{Z}$$

where  $\mathbf{V}_{hj}$  is the upper triangular matrix in the Cholesky decomposition,  $\mathbf{V}_j = \mathbf{V}'_{hj} \mathbf{V}_{hj}$ , and  $\mathbf{Z}$  is a vector of  $k + 1$  independent random normal variates.

2. The missing values are then replaced by

$$\beta_{*0} + \beta_{*1} x_1 + \beta_{*2} x_2 + \dots + \beta_{*(k)} x_k + z_i \sigma_{*j}$$

where  $x_1, x_2, \dots, x_k$  are the values of the covariates and  $z_i$  is a simulated normal deviate.

## Monotone and FCS Predictive Mean Matching Methods

The predictive mean matching method is also an imputation method available for continuous variables. It is similar to the regression method except that for each missing value, it imputes a value randomly from a set of observed values whose predicted values are closest to the predicted value for the missing value from the simulated regression model (Heitjan and Little 1991; Schenker and Taylor 1996).

Following the description of the model in the section “[Monotone and FCS Regression Methods](#)” on page 4749, the following steps are used to generate imputed values:

1. New parameters  $\boldsymbol{\beta}_* = (\beta_{*0}, \beta_{*1}, \dots, \beta_{*(k)})$  and  $\sigma_{*j}^2$  are drawn from the posterior predictive distribution of the parameters. That is, they are simulated from  $(\hat{\beta}_0, \hat{\beta}_1, \dots, \hat{\beta}_k)$ ,  $\sigma_j^2$ , and  $\mathbf{V}_j$ . The variance is drawn as

$$\sigma_{*j}^2 = \hat{\sigma}_j^2 (n_j - k - 1) / g$$

where  $g$  is a  $\chi_{n_j - k - 1}^2$  random variate and  $n_j$  is the number of nonmissing observations for  $Y_j$ . The regression coefficients are drawn as

$$\boldsymbol{\beta}_* = \hat{\boldsymbol{\beta}} + \sigma_{*j} \mathbf{V}'_{hj} \mathbf{Z}$$

where  $\mathbf{V}_{hj}$  is the upper triangular matrix in the Cholesky decomposition,  $\mathbf{V}_j = \mathbf{V}'_{hj} \mathbf{V}_{hj}$ , and  $\mathbf{Z}$  is a vector of  $k + 1$  independent random normal variates.

2. For each missing value, a predicted value

$$y_{i*} = \beta_{*0} + \beta_{*1} x_1 + \beta_{*2} x_2 + \dots + \beta_{*(k)} x_k$$

is computed with the covariate values  $x_1, x_2, \dots, x_k$ .

3. A set of  $k_0$  observations whose corresponding predicted values are closest to  $y_{i*}$  is generated. You can specify  $k_0$  with the `K=` option.
4. The missing value is then replaced by a value drawn randomly from these  $k_0$  observed values.

The predictive mean matching method requires the number of closest observations to be specified. A smaller  $k_0$  tends to increase the correlation among the multiple imputations for the missing observation and results in a higher variability of point estimators in repeated sampling. On the other hand, a larger  $k_0$  tends to lessen the effect from the imputation model and results in biased estimators (Schenker and Taylor 1996, p. 430).

The predictive mean matching method ensures that imputed values are plausible; it might be more appropriate than the regression method if the normality assumption is violated (Horton and Lipsitz 2001, p. 246).

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## Monotone Propensity Score Method

The propensity score method is another imputation method available for continuous variables when the data set has a monotone missing pattern.

A propensity score is generally defined as the conditional probability of assignment to a particular treatment given a vector of observed covariates (Rosenbaum and Rubin 1983). In the propensity score method, for a variable with missing values, a propensity score is generated for each observation to estimate the probability that the observation is missing. The observations are then grouped based on these propensity scores, and an approximate Bayesian bootstrap imputation (Rubin 1987, p. 124) is applied to each group (Lavori, Dawson, and Shera 1995).

The propensity score method uses the following steps to impute values for variable  $Y_j$  with missing values:

1. Creates an indicator variable  $R_j$  with the value 0 for observations with missing  $Y_j$  and 1 otherwise.
2. Fits a logistic regression model

$$\text{logit}(p_j) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_k X_k$$

where  $X_1, X_2, \dots, X_k$  are covariates for  $Y_j$ ,  $p_j = \Pr(R_j = 0 | X_1, X_2, \dots, X_k)$ , and  $\text{logit}(p) = \log(p/(1-p))$ .

3. Creates a propensity score for each observation to estimate the probability that it is missing.
4. Divides the observations into a fixed number of groups (typically assumed to be five) based on these propensity scores.
5. Applies an approximate Bayesian bootstrap imputation to each group. In group  $k$ , suppose that  $Y_{obs}$  denotes the  $n_1$  observations with nonmissing  $Y_j$  values and  $Y_{mis}$  denotes the  $n_0$  observations with missing  $Y_j$ . The approximate Bayesian bootstrap imputation first draws  $n_1$  observations randomly with replacement from  $Y_{obs}$  to create a new data set  $Y_{obs}^*$ . This is a nonparametric analog of drawing parameters from the posterior predictive distribution of the parameters. The process then draws the  $n_0$  values for  $Y_{mis}$  randomly with replacement from  $Y_{obs}^*$ .

Steps 1 through 5 are repeated sequentially for each variable with missing values.

The propensity score method was originally designed for a randomized experiment with repeated measures on the response variables. The goal was to impute the missing values on the response variables. The method uses only the covariate information that is associated with whether the imputed variable values are missing; it does not use correlations among variables. It is effective for inferences about the distributions of individual imputed variables, such as a univariate analysis, but it is not appropriate for analyses that involve relationship among variables, such as a regression analysis (Schafer 1999, p. 11). It can also produce badly biased estimates of regression coefficients when data on predictor variables are missing (Allison 2000).

## Monotone and FCS Discriminant Function Methods

The discriminant function method is the default imputation method in the MONOTONE and FCS statements for classification variables.

For a nominal classification variable  $Y_j$  with responses  $1, \dots, g$  and a set of effects from its preceding variables, if the covariates  $X_1, X_2, \dots, X_k$  associated with these effects within each group are approximately multivariate normal and the within-group covariance matrices are approximately equal, the discriminant function method (Brand 1999, pp. 95–96) can be used to impute missing values for the variable  $Y_j$ .

Denote the group-specific means for covariates  $X_1, X_2, \dots, X_k$  by

$$\bar{\mathbf{X}}_t = (\bar{X}_{t1}, \bar{X}_{t2}, \dots, \bar{X}_{tk}), t = 1, 2, \dots, g$$

then the pooled covariance matrix is computed as

$$\mathbf{S} = \frac{1}{n - g} \sum_{t=1}^g (n_t - 1) \mathbf{S}_t$$

where  $\mathbf{S}_t$  is the within-group covariance matrix,  $n_t$  is the group-specific sample size, and  $n = \sum_{t=1}^g n_t$  is the total sample size.

In each imputation, new parameters of the group-specific means ( $\mathbf{m}_{*t}$ ), pooled covariance matrix ( $\mathbf{S}_*$ ), and prior probabilities of group membership ( $q_{*t}$ ) can be drawn from their corresponding posterior distributions (Schafer 1997, p. 356).

## Pooled Covariance Matrix and Group-Specific Means

For each imputation, the MI procedure uses either the fixed observed pooled covariance matrix (PCOV=FIXED) or a drawn pooled covariance matrix (PCOV=POSTERIOR) from its posterior distribution with a noninformative prior. That is,

$$\Sigma | \mathbf{X} \sim W^{-1}(n - g, (n - g)\mathbf{S})$$

where  $W^{-1}$  is an inverted Wishart distribution.

The group-specific means are then drawn from their posterior distributions with a noninformative prior

$$\mu_t | (\Sigma, \bar{\mathbf{X}}_t) \sim N\left(\bar{\mathbf{X}}_t, \frac{1}{n_t} \Sigma\right)$$

See the section “Bayesian Estimation of the Mean Vector and Covariance Matrix” on page 4759 for a complete description of the inverted Wishart distribution and posterior distributions that use a noninformative prior.

### Prior Probabilities of Group Membership

The prior probabilities are computed through the drawing of new group sample sizes. When the total sample size  $n$  is considered fixed, the group sample sizes  $(n_1, n_2, \dots, n_g)$  have a multinomial distribution. New multinomial parameters (group sample sizes) can be drawn from their posterior distribution by using a Dirichlet prior with parameters  $(\alpha_1, \alpha_2, \dots, \alpha_g)$ .

After the new sample sizes are drawn from the posterior distribution of  $(n_1, n_2, \dots, n_g)$ , the prior probabilities  $q_{*t}$  are computed proportionally to the drawn sample sizes.

See Schafer (1997, pp. 247–255) for a complete description of the Dirichlet prior.

### Imputation Steps

The discriminant function method uses the following steps in each imputation to impute values for a nominal classification variable  $Y_j$  with  $g$  responses:

1. Draw a pooled covariance matrix  $\mathbf{S}_*$  from its posterior distribution if the PCOV=POSTERIOR option is used.
2. For each group, draw group means  $\mathbf{m}_{*t}$  from the observed group mean  $\bar{\mathbf{X}}_t$  and either the observed pooled covariance matrix (PCOV=FIXED) or the drawn pooled covariance matrix  $\mathbf{S}_*$  (PCOV=POSTERIOR).
3. For each group, compute or draw  $q_{*t}$ , prior probabilities of group membership, based on the PRIOR=option:
  - PRIOR=EQUAL,  $q_{*t} = 1/g$ , prior probabilities of group membership are all equal.
  - PRIOR=PROPORTIONAL,  $q_{*t} = n_t/n$ , prior probabilities are proportional to their group sample sizes.
  - PRIOR=JEFFREYS= $c$ , a noninformative Dirichlet prior with  $\alpha_t = c$  is used.
  - PRIOR=RIDGE= $d$ , a ridge prior is used with  $\alpha_t = d * n_t/n$  for  $d \geq 1$  and  $\alpha_t = d * n_t$  for  $d < 1$ .
4. With the group means  $\mathbf{m}_{*t}$ , the pooled covariance matrix  $\mathbf{S}_*$ , and the prior probabilities of group membership  $q_{*t}$ , the discriminant function method derives linear discriminant function and computes the posterior probabilities of an observation belonging to each group

$$p_t(\mathbf{x}) = \frac{\exp(-0.5D_t^2(\mathbf{x}))}{\sum_{u=1}^g \exp(-0.5D_u^2(\mathbf{x}))}$$

where  $D_t^2(\mathbf{x}) = (\mathbf{x} - \mathbf{m}_{*t})' \mathbf{S}_*^{-1} (\mathbf{x} - \mathbf{m}_{*t}) - 2 \log(q_{*t})$  is the generalized squared distance from  $\mathbf{x}$  to group  $t$ .

5. Draw a random uniform variate  $u$ , between 0 and 1, for each observation with missing group value. With the posterior probabilities,  $p_1(\mathbf{x}) + p_2(\mathbf{x}) + \dots + p_g(\mathbf{x}) = 1$ , the discriminant function method imputes  $Y_j = 1$  if the value of  $u$  is less than  $p_1(\mathbf{x})$ ,  $Y_j = 2$  if the value is greater than or equal to  $p_1(\mathbf{x})$  but less than  $p_1(\mathbf{x}) + p_2(\mathbf{x})$ , and so on.

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## Monotone and FCS Logistic Regression Methods

The logistic regression method is another imputation method available for classification variables. In the logistic regression method, a logistic regression model is fitted for a classification variable with a set of covariates constructed from the effects. For a binary classification variable, based on the fitted regression model, a new logistic regression model is simulated from the posterior predictive distribution of the parameters and is used to impute the missing values for each variable (Rubin 1987, pp. 167–170).

For a binary variable  $Y_j$  with responses 1 and 2, a logistic regression model is fitted using observations with observed values for the imputed variable  $Y_j$  and its covariates  $X_1, X_2, \dots, X_k$ :

$$\text{logit}(p_j) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_k X_k$$

where  $X_1, X_2, \dots, X_k$  are covariates for  $Y_j$ ,  $p_j = \Pr(R_j = 1|X_1, X_2, \dots, X_k)$ , and  $\text{logit}(p) = \log(p/(1-p))$ .

The fitted model includes the regression parameter estimates  $\hat{\boldsymbol{\beta}} = (\hat{\beta}_0, \hat{\beta}_1, \dots, \hat{\beta}_k)$  and the associated covariance matrix  $\mathbf{V}_j$ .

The following steps are used to generate imputed values for a binary variable  $Y_j$  with responses 1 and 2:

1. New parameters  $\boldsymbol{\beta}_* = (\beta_{*0}, \beta_{*1}, \dots, \beta_{*(k)})$  are drawn from the posterior predictive distribution of the parameters.

$$\boldsymbol{\beta}_* = \hat{\boldsymbol{\beta}} + \mathbf{V}'_{hj} \mathbf{Z}$$

where  $\mathbf{V}_{hj}$  is the upper triangular matrix in the Cholesky decomposition,  $\mathbf{V}_j = \mathbf{V}'_{hj} \mathbf{V}_{hj}$ , and  $\mathbf{Z}$  is a vector of  $k+1$  independent random normal variates.

2. For an observation with missing  $Y_j$  and covariates  $x_1, x_2, \dots, x_k$ , compute the expected probability that  $Y_j = 1$ :

$$p_j = \frac{\exp(\mu_j)}{1 + \exp(\mu_j)}$$

where  $\mu_j = \beta_{*0} + \beta_{*1} x_1 + \beta_{*2} x_2 + \dots + \beta_{*(k)} x_k$ .

3. Draw a random uniform variate,  $u$ , between 0 and 1. If the value of  $u$  is less than  $p_j$ , impute  $Y_j = 1$ ; otherwise impute  $Y_j = 2$ .

The preceding logistic regression method can be extended to include the ordinal classification variables with more than two levels of responses. The options ORDER= and DESCENDING can be used to specify the sort order for the levels of the imputed variables.

## FCS Methods for Data Sets with Arbitrary Missing Patterns

For a data set with an arbitrary missing data pattern, you can use FCS methods to impute missing values for all variables, assuming the existence of a joint distribution for these variables (Brand 1999; van Buuren 2007). FCS method involves two phases in each imputation: the preliminary filled-in phase followed by the imputation phase.

At the filled-in phase, the missing values for all variables are filled in sequentially over the variables taken one at a time. The missing values for each variable are filled in using the specified method, or the default method for the variable if a method is not specified, with preceding variables serving as the covariates. These filled-in values provide starting values for these missing values at the imputation phase.

At the imputation phase, the missing values for each variable are imputed using the specified method and covariates at each iteration. The default method for the variable is used if a method is not specified, and the remaining variables are used as covariates if the set of covariates is not specified. After a number of iterations, as specified with the NBITER= option, the imputed values in each variable are used for the imputation. At each iteration, the missing values are imputed sequentially over the variables taken one at a time.

The MI procedure orders the variables as they are ordered in the VAR statement. For example, if the order of the  $p$  variables in the VAR statement is  $Y_1, Y_2, \dots, Y_p$ , then  $Y_1, Y_2, \dots, Y_p$  (in that order) are used in the filled-in and imputation phases.

The filled-in phase replaces missing values with filled-in values for each variable. That is, with  $p$  variables  $Y_1, Y_2, \dots, Y_p$  (in that order), the missing values are filled in by using the sequence,

$$\begin{aligned}
 \theta_1^{(0)} &\sim P(\theta_1 | Y_{1(obs)}) \\
 Y_{1(*)}^{(0)} &\sim P(Y_1 | \theta_1^{(0)}) \\
 Y_1^{(0)} &= (Y_{1(obs)}, Y_{1(*)}^{(0)}) \\
 &\dots \\
 &\dots \\
 \theta_p^{(0)} &\sim P(\theta_p | Y_1^{(0)}, \dots, Y_{p-1}^{(0)}, Y_{p(obs)}) \\
 Y_{p(*)}^{(0)} &\sim P(Y_p | \theta_p^{(0)}) \\
 Y_p^{(0)} &= (Y_{p(obs)}, Y_{p(*)}^{(0)})
 \end{aligned}$$

where  $Y_{j(obs)}$  is the set of observed  $Y_j$  values,  $Y_{j(*)}^{(0)}$  is the set of filled-in  $Y_j$  values,  $Y_j^{(0)}$  is the set of both observed and filled-in  $Y_j$  values, and  $\theta_j^{(0)}$  is the set of simulated parameters for the conditional distribution of  $Y_j$  given variables  $Y_1, Y_2, \dots, Y_{j-1}$ .

For each variable  $Y_j$  with missing values, the corresponding imputation method is used to fit the model with covariates  $Y_1, Y_2, \dots, Y_{j-1}$ . The observed observations for  $Y_j$ , which might include observations with filled-in values for  $Y_1, Y_2, \dots, Y_{j-1}$ , are used in the model fitting. With this resulting model, a new model is drawn and then used to impute missing values for  $Y_j$ .

The imputation phase replaces these filled-in values  $Y_{j(*)}^{(0)}$  with imputed values for each variable sequentially at each iteration. That is, with  $p$  variables  $Y_1, Y_2, \dots, Y_p$  (in that order), the missing values are imputed with the sequence at iteration  $t + 1$ ,

$$\begin{aligned} \theta_1^{(t+1)} &\sim P(\theta_1 | Y_{1(obs)}, Y_2^{(t)}, \dots, Y_p^{(t)}) \\ Y_{1(*)}^{(t+1)} &\sim P(Y_1 | \theta_1^{(t+1)}) \\ Y_1^{(t+1)} &= (Y_{1(obs)}, Y_{1(*)}^{(t+1)}) \\ &\dots \\ &\dots \\ \theta_p^{(t+1)} &\sim P(\theta_p | Y_1^{(t+1)}, \dots, Y_{p-1}^{(t+1)}, Y_{p(obs)}) \\ Y_{p(*)}^{(t+1)} &\sim P(Y_p | \theta_p^{(t+1)}) \\ Y_p^{(t+1)} &= (Y_{p(obs)}, Y_{p(*)}^{(t+1)}) \end{aligned}$$

where  $Y_{j(obs)}$  is the set of observed  $Y_j$  values,  $Y_{j(*)}^{(t+1)}$  is the set of imputed  $Y_j$  values at iteration  $t + 1$ ,  $Y_{j(*)}^{(t)}$  is the set of filled-in  $Y_j$  values ( $t = 0$ ) or the set of imputed  $Y_j$  values at iteration  $t$  ( $t > 0$ ),  $Y_j^{(t+1)}$  is the set of both observed and imputed  $Y_j$  values at iteration  $t + 1$ , and  $\theta_j^{(t+1)}$  is the set of simulated parameters for the conditional distribution of  $Y_j$  given covariates constructed from  $Y_1, \dots, Y_{j-1}, Y_{j+1}, \dots, Y_p$ .

At each iteration, a specified model is fitted for each variable with missing values by using observed observations for that variable, which might include observations with imputed values for other variables. With this resulting model, a new model is drawn and then used to impute missing values for the imputed variable.

The steps are iterated long enough for the results to reliably simulate an approximately independent draw of the missing values for an imputed data set.

The imputation methods used in the filled-in and imputation phases are similar to the corresponding monotone methods for monotone missing data. You can use a regression method or a predictive mean matching method to impute missing values for a continuous variable, a logistic regression method for a classification variable with a binary or ordinal response, and a discriminant function method for a classification variable with a binary or nominal response. See the sections “[Monotone and FCS Regression Methods](#)” on page 4749, “[Monotone and FCS Predictive Mean Matching Methods](#)” on page 4750, “[Monotone and FCS Discriminant Function Methods](#)” on page 4752, and “[Monotone and FCS Logistic Regression Methods](#)” on page 4754 for these methods.

The FCS method requires fewer iterations than the MCMC method (van Buuren 2007). Often, as few as five or 10 iterations are enough to produce satisfactory results (van Buuren 2007; Brand 1999).

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## Checking Convergence in FCS Methods

The parameters used in the imputation step at each iteration can be saved in an output data set with the `OUTITER=` option. These include the means and standard deviations. You can then monitor the convergence by displaying trace plots for those parameter values with the `PLOTS=TRACE` option.

A trace plot for a parameter  $\xi$  is a scatter plot of successive parameter estimates  $\xi_i$  against the iteration number  $i$ . The plot provides a simple way to examine the convergence behavior of the estimation algorithm

for  $\xi$ . Long-term trends in the plot indicate that successive iterations are highly correlated and that the series of iterations has not converged.

You can display trace plots for the variable means and standard deviations. You can also request logarithmic transformations for positive parameters in the plots with the LOG option. With the LOG option, if a parameter value is less than or equal to zero, then the value is not displayed in the corresponding plot.

See [Example 57.8](#) for a usage of the trace plot.

## MCMC Method for Arbitrary Missing Multivariate Normal Data

The Markov chain Monte Carlo (MCMC) method originated in physics as a tool for exploring equilibrium distributions of interacting molecules. In statistical applications, it is used to generate pseudorandom draws from multidimensional and otherwise intractable probability distributions via Markov chains. A Markov chain is a sequence of random variables in which the distribution of each element depends only on the value of the previous element.

In MCMC simulation, you construct a Markov chain long enough for the distribution of the elements to stabilize to a stationary distribution, which is the distribution of interest. Repeatedly simulating steps of the chain simulates draws from the distribution of interest. See Schafer (1997) for a detailed discussion of this method.

In Bayesian inference, information about unknown parameters is expressed in the form of a posterior probability distribution. This posterior distribution is computed using Bayes' theorem,

$$p(\boldsymbol{\theta}|y) = \frac{p(y|\boldsymbol{\theta})p(\boldsymbol{\theta})}{\int p(y|\boldsymbol{\theta})p(\boldsymbol{\theta})d\boldsymbol{\theta}}$$

MCMC has been applied as a method for exploring posterior distributions in Bayesian inference. That is, through MCMC, you can simulate the entire joint posterior distribution of the unknown quantities and obtain simulation-based estimates of posterior parameters that are of interest.

In many incomplete-data problems, the observed-data posterior  $p(\boldsymbol{\theta}|Y_{obs})$  is intractable and cannot easily be simulated. However, when  $Y_{obs}$  is augmented by an estimated or simulated value of the missing data  $Y_{mis}$ , the complete-data posterior  $p(\boldsymbol{\theta}|Y_{obs}, Y_{mis})$  is much easier to simulate. Assuming that the data are from a multivariate normal distribution, data augmentation can be applied to Bayesian inference with missing data by repeating the following steps:

### 1. The imputation I-step

Given an estimated mean vector and covariance matrix, the I-step simulates the missing values for each observation independently. That is, if you denote the variables with missing values for observation  $i$  by  $Y_{i(mis)}$  and the variables with observed values by  $Y_{i(obs)}$ , then the I-step draws values for  $Y_{i(mis)}$  from a conditional distribution for  $Y_{i(mis)}$  given  $Y_{i(obs)}$ .

### 2. The posterior P-step

Given a complete sample, the P-step simulates the posterior population mean vector and covariance matrix. These new estimates are then used in the next I-step. Without prior information about the parameters, a noninformative prior is used. You can also use other informative priors. For example, a prior information about the covariance matrix can help to stabilize the inference about the mean vector for a near singular covariance matrix.



That is, with a current parameter estimate  $\theta^{(t)}$  at the  $t$ th iteration, the I-step draws  $Y_{mis}^{(t+1)}$  from  $p(Y_{mis}|Y_{obs}, \theta^{(t)})$  and the P-step draws  $\theta^{(t+1)}$  from  $p(\theta|Y_{obs}, Y_{mis}^{(t+1)})$ . The two steps are iterated long enough for the results to reliably simulate an approximately independent draw of the missing values for a multiply imputed data set (Schafer 1997).

This creates a Markov chain  $(Y_{mis}^{(1)}, \theta^{(1)})$ ,  $(Y_{mis}^{(2)}, \theta^{(2)})$ , ..., which converges in distribution to  $p(Y_{mis}, \theta|Y_{obs})$ . Assuming the iterates converge to a stationary distribution, the goal is to simulate an approximately independent draw of the missing values from this distribution.

To validate the imputation results, you should repeat the process with different random number generators and starting values based on different initial parameter estimates.

The next three sections provide details for the imputation step, Bayesian estimation of the mean vector and covariance matrix, and the posterior step.

## Imputation Step

In each iteration, starting with a given mean vector  $\mu$  and covariance matrix  $\Sigma$ , the imputation step draws values for the missing data from the conditional distribution  $Y_{mis}$  given  $Y_{obs}$ .

Suppose  $\mu = [\mu'_1, \mu'_2]'$  is the partitioned mean vector of two sets of variables,  $Y_{obs}$  and  $Y_{mis}$ , where  $\mu_1$  is the mean vector for variables  $Y_{obs}$  and  $\mu_2$  is the mean vector for variables  $Y_{mis}$ .

Also suppose

$$\Sigma = \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma'_{12} & \Sigma_{22} \end{bmatrix}$$

is the partitioned covariance matrix for these variables, where  $\Sigma_{11}$  is the covariance matrix for variables  $Y_{obs}$ ,  $\Sigma_{22}$  is the covariance matrix for variables  $Y_{mis}$ , and  $\Sigma_{12}$  is the covariance matrix between variables  $Y_{obs}$  and variables  $Y_{mis}$ .

By using the sweep operator (Goodnight 1979) on the pivots of the  $\Sigma_{11}$  submatrix, the matrix becomes

$$\begin{bmatrix} \Sigma_{11}^{-1} & \Sigma_{11}^{-1}\Sigma_{12} \\ -\Sigma'_{12}\Sigma_{11}^{-1} & \Sigma_{22.1} \end{bmatrix}$$

where  $\Sigma_{22.1} = \Sigma_{22} - \Sigma'_{12}\Sigma_{11}^{-1}\Sigma_{12}$  can be used to compute the conditional covariance matrix of  $Y_{mis}$  after controlling for  $Y_{obs}$ .

For an observation with the preceding missing pattern, the conditional distribution of  $Y_{mis}$  given  $Y_{obs} = \mathbf{y}_1$  is a multivariate normal distribution with the mean vector

$$\mu_{2.1} = \mu_2 + \Sigma'_{12}\Sigma_{11}^{-1}(\mathbf{y}_1 - \mu_1)$$

and the conditional covariance matrix

$$\Sigma_{22.1} = \Sigma_{22} - \Sigma'_{12}\Sigma_{11}^{-1}\Sigma_{12}$$

## Bayesian Estimation of the Mean Vector and Covariance Matrix

Suppose that  $\mathbf{Y} = (\mathbf{y}'_1, \mathbf{y}'_2, \dots, \mathbf{y}'_n)'$  is an  $(n \times p)$  matrix made up of  $n$  ( $p \times 1$ ) independent vectors  $\mathbf{y}_i$ , each of which has a multivariate normal distribution with mean zero and covariance matrix  $\mathbf{\Lambda}$ . Then the SSCP matrix

$$\mathbf{A} = \mathbf{Y}'\mathbf{Y} = \sum_i \mathbf{y}_i \mathbf{y}'_i$$

has a Wishart distribution  $W(n, \mathbf{\Lambda})$ .

When each observation  $\mathbf{y}_i$  is distributed with a multivariate normal distribution with an unknown mean  $\boldsymbol{\mu}$ , then the CSSCP matrix

$$\mathbf{A} = \sum_i (\mathbf{y}_i - \bar{\mathbf{y}})(\mathbf{y}_i - \bar{\mathbf{y}})'$$

has a Wishart distribution  $W(n - 1, \mathbf{\Lambda})$ .

If  $\mathbf{A}$  has a Wishart distribution  $W(n, \mathbf{\Lambda})$ , then  $\mathbf{B} = \mathbf{A}^{-1}$  has an inverted Wishart distribution  $W^{-1}(n, \boldsymbol{\Psi})$ , where  $n$  is the degrees of freedom and  $\boldsymbol{\Psi} = \mathbf{\Lambda}^{-1}$  is the precision matrix (Anderson 1984).

Note that, instead of using the parameter  $\boldsymbol{\Psi} = \mathbf{\Lambda}^{-1}$  for the inverted Wishart distribution, Schafer (1997) uses the parameter  $\mathbf{\Lambda}$ .

Suppose that each observation in the data matrix  $\mathbf{Y}$  has a multivariate normal distribution with mean  $\boldsymbol{\mu}$  and covariance matrix  $\boldsymbol{\Sigma}$ . Then with a prior inverted Wishart distribution for  $\boldsymbol{\Sigma}$  and a prior normal distribution for  $\boldsymbol{\mu}$

$$\begin{aligned} \boldsymbol{\Sigma} &\sim W^{-1}(m, \boldsymbol{\Psi}) \\ \boldsymbol{\mu} | \boldsymbol{\Sigma} &\sim N\left(\boldsymbol{\mu}_0, \frac{1}{\tau} \boldsymbol{\Sigma}\right) \end{aligned}$$

where  $\tau > 0$  is a fixed number.

The posterior distribution (Anderson 1984, p. 270; Schafer 1997, p. 152) is

$$\begin{aligned} \boldsymbol{\Sigma} | \mathbf{Y} &\sim W^{-1}\left(n + m, (n - 1)\mathbf{S} + \boldsymbol{\Psi} + \frac{n\tau}{n + \tau}(\bar{\mathbf{y}} - \boldsymbol{\mu}_0)(\bar{\mathbf{y}} - \boldsymbol{\mu}_0)'\right) \\ \boldsymbol{\mu} | (\boldsymbol{\Sigma}, \mathbf{Y}) &\sim N\left(\frac{1}{n + \tau}(n\bar{\mathbf{y}} + \tau\boldsymbol{\mu}_0), \frac{1}{n + \tau}\boldsymbol{\Sigma}\right) \end{aligned}$$

where  $(n - 1)\mathbf{S}$  is the CSSCP matrix.

## Posterior Step

In each iteration, the posterior step simulates the posterior population mean vector  $\boldsymbol{\mu}$  and covariance matrix  $\boldsymbol{\Sigma}$  from prior information for  $\boldsymbol{\mu}$  and  $\boldsymbol{\Sigma}$ , and the complete sample estimates.

You can specify the prior parameter information by using one of the following methods:

- PRIOR=JEFFREYS, which uses a noninformative prior
- PRIOR=INPUT=, which provides a prior information for  $\boldsymbol{\Sigma}$  in the data set. Optionally, it also provides a prior information for  $\boldsymbol{\mu}$  in the data set.
- PRIOR=RIDGE=, which uses a ridge prior

The next four subsections provide details of the posterior step for different prior distributions.

### 1. A Noninformative Prior

Without prior information about the mean and covariance estimates, you can use a noninformative prior by specifying the PRIOR=JEFFREYS option. The posterior distributions (Schafer 1997, p. 154) are

$$\begin{aligned}\Sigma^{(t+1)}|\mathbf{Y} &\sim W^{-1}(n-1, (n-1)\mathbf{S}) \\ \mu^{(t+1)}|(\Sigma^{(t+1)}, \mathbf{Y}) &\sim N\left(\bar{\mathbf{y}}, \frac{1}{n}\Sigma^{(t+1)}\right)\end{aligned}$$

### 2. An Informative Prior for $\mu$ and $\Sigma$

When prior information is available for the parameters  $\mu$  and  $\Sigma$ , you can provide it with a SAS data set that you specify with the PRIOR=INPUT= option:

$$\begin{aligned}\Sigma &\sim W^{-1}(d^*, d^*\mathbf{S}^*) \\ \mu|\Sigma &\sim N\left(\mu_0, \frac{1}{n_0}\Sigma\right)\end{aligned}$$

To obtain the prior distribution for  $\Sigma$ , PROC MI reads the matrix  $\mathbf{S}^*$  from observations in the data set with \_TYPE\_='COV', and it reads  $n^* = d^* + 1$  from observations with \_TYPE\_='N'.

To obtain the prior distribution for  $\mu$ , PROC MI reads the mean vector  $\mu_0$  from observations with \_TYPE\_='MEAN', and it reads  $n_0$  from observations with \_TYPE\_='N\_MEAN'. When there are no observations with \_TYPE\_='N\_MEAN', PROC MI reads  $n_0$  from observations with \_TYPE\_='N'.

The resulting posterior distribution, as described in the section “Bayesian Estimation of the Mean Vector and Covariance Matrix” on page 4759, is given by

$$\begin{aligned}\Sigma^{(t+1)}|\mathbf{Y} &\sim W^{-1}(n+d^*, (n-1)\mathbf{S} + d^*\mathbf{S}^* + \mathbf{S}_m) \\ \mu^{(t+1)}|(\Sigma^{(t+1)}, \mathbf{Y}) &\sim N\left(\frac{1}{n+n_0}(n\bar{\mathbf{y}} + n_0\mu_0), \frac{1}{n+n_0}\Sigma^{(t+1)}\right)\end{aligned}$$

where

$$\mathbf{S}_m = \frac{nn_0}{n+n_0}(\bar{\mathbf{y}} - \mu_0)(\bar{\mathbf{y}} - \mu_0)'$$

### 3. An Informative Prior for $\Sigma$

When the sample covariance matrix  $\mathbf{S}$  is singular or near singular, prior information about  $\Sigma$  can also be used without prior information about  $\mu$  to stabilize the inference about  $\mu$ . You can provide it with a SAS data set that you specify with the PRIOR=INPUT= option.

To obtain the prior distribution for  $\Sigma$ , PROC MI reads the matrix  $\mathbf{S}^*$  from observations in the data set with \_TYPE\_='COV', and it reads  $n^*$  from observations with \_TYPE\_='N'.

The resulting posterior distribution for  $(\mu, \Sigma)$  (Schafer 1997, p. 156) is

$$\begin{aligned}\Sigma^{(t+1)}|\mathbf{Y} &\sim W^{-1}(n+d^*, (n-1)\mathbf{S} + d^*\mathbf{S}^*) \\ \mu^{(t+1)}|(\Sigma^{(t+1)}, \mathbf{Y}) &\sim N\left(\bar{\mathbf{y}}, \frac{1}{n}\Sigma^{(t+1)}\right)\end{aligned}$$

Note that if the PRIOR=INPUT= data set also contains observations with \_TYPE\_='MEAN', then a complete informative prior for both  $\mu$  and  $\Sigma$  will be used.

#### 4. A Ridge Prior

A special case of the preceding adjustment is a ridge prior with  $\mathbf{S}^* = \text{Diag}(\mathbf{S})$  (Schafer 1997, p. 156). That is,  $\mathbf{S}^*$  is a diagonal matrix with diagonal elements equal to the corresponding elements in  $\mathbf{S}$ .

You can request a ridge prior by using the PRIOR=RIDGE= option. You can explicitly specify the number  $d^* \geq 1$  in the PRIOR=RIDGE= $d^*$  option. Or you can implicitly specify the number by specifying the proportion  $p$  in the PRIOR=RIDGE= $p$  option to request  $d^* = (n - 1)p$ .

The posterior is then given by

$$\begin{aligned} \Sigma^{(t+1)} | \mathbf{Y} &\sim W^{-1} (n + d^*, (n - 1)\mathbf{S} + d^*\text{Diag}(\mathbf{S})) \\ \mu^{(t+1)} | (\Sigma^{(t+1)}, \mathbf{Y}) &\sim N \left( \bar{\mathbf{y}}, \frac{1}{n} \Sigma^{(t+1)} \right) \end{aligned}$$

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## Producing Monotone Missingness with the MCMC Method

The monotone data MCMC method was first proposed by Li (1988) and Liu (1993) described the algorithm. The method is useful especially when a data set is close to having a monotone missing pattern. In this case, the method needs to impute only a few missing values to the data set to have a monotone missing pattern in the imputed data set. Compared to a full data imputation that imputes all missing values, the monotone data MCMC method imputes fewer missing values in each iteration and achieves approximate stationarity in fewer iterations (Schafer 1997, p. 227).

You can request the monotone MCMC method by specifying the option IMPUTE=MONOTONE in the MCMC statement. The “Missing Data Patterns” table now denotes the variables with missing values by “.” or “O”. The value “.” means that the variable is missing and will be imputed, and the value “O” means that the variable is missing and will not be imputed. The “Variance Information” and “Parameter Estimates” tables are not created.

You must specify the variables in the VAR statement. The variable order in the list determines the monotone missing pattern in the imputed data set. With a different order in the VAR list, the results will be different because the monotone missing pattern to be constructed will be different.

Assuming that the data are from a multivariate normal distribution, then like the MCMC method, the monotone MCMC method repeats the following steps:

### 1. The imputation I-step

Given an estimated mean vector and covariance matrix, the I-step simulates the missing values for each observation independently. Only a subset of missing values are simulated to achieve a monotone pattern of missingness.

### 2. The posterior P-step

Given a new sample with a monotone pattern of missingness, the P-step simulates the posterior population mean vector and covariance matrix with a noninformative Jeffreys prior. These new estimates are then used in the next I-step.

## Imputation Step

The I-step is almost identical to the I-step described in the section “MCMC Method for Arbitrary Missing Multivariate Normal Data” on page 4757 except that only a subset of missing values need to be simulated. To state this precisely, denote the variables with observed values for observation  $i$  by  $Y_{i(obs)}$  and the variables with missing values by  $Y_{i(mis)} = (Y_{i(m1)}, Y_{i(m2)})$ , where  $Y_{i(m1)}$  is a subset of the missing variables that will cause a monotone missingness when their values are imputed. Then the I-step draws values for  $Y_{i(m1)}$  from a conditional distribution for  $Y_{i(m1)}$  given  $Y_{i(obs)}$ .

## Posterior Step

The P-step is different from the P-step described in the section “MCMC Method for Arbitrary Missing Multivariate Normal Data” on page 4757. Instead of simulating the  $\mu$  and  $\Sigma$  parameters from the full imputed data set, this P-step simulates the  $\mu$  and  $\Sigma$  parameters through simulated regression coefficients from regression models based on the imputed data set with a monotone pattern of missingness. The step is similar to the process described in the section “Monotone and FCS Regression Methods” on page 4749.

That is, for the variable  $Y_j$ , a model

$$Y_j = \beta_0 + \beta_1 Y_1 + \beta_2 Y_2 + \dots + \beta_{j-1} Y_{j-1}$$

is fitted using  $n_j$  nonmissing observations for variable  $Y_j$  in the imputed data sets.

The fitted model consists of the regression parameter estimates  $\hat{\beta} = (\hat{\beta}_0, \hat{\beta}_1, \dots, \hat{\beta}_{j-1})$  and the associated covariance matrix  $\hat{\sigma}_j^2 \mathbf{V}_j$ , where  $\mathbf{V}_j$  is the usual  $\mathbf{X}'\mathbf{X}$  inverse matrix from the intercept and variables  $Y_1, Y_2, \dots, Y_{j-1}$ .

For each imputation, new parameters  $\beta_* = (\beta_{*0}, \beta_{*1}, \dots, \beta_{*(j-1)})$  and  $\sigma_{*j}^2$  are drawn from the posterior predictive distribution of the parameters. That is, they are simulated from  $(\hat{\beta}_0, \hat{\beta}_1, \dots, \hat{\beta}_{j-1}), \sigma_j^2$ , and  $\mathbf{V}_j$ . The variance is drawn as

$$\sigma_{*j}^2 = \hat{\sigma}_j^2 (n_j - j) / g$$

where  $g$  is a  $\chi_{n_j - p + j - 1}^2$  random variate and  $n_j$  is the number of nonmissing observations for  $Y_j$ . The regression coefficients are drawn as

$$\beta_* = \hat{\beta} + \sigma_{*j} \mathbf{V}_{hj}' \mathbf{Z}$$

where  $\mathbf{V}_{hj}$  is the upper triangular matrix in the Cholesky decomposition,  $\mathbf{V}_j = \mathbf{V}_{hj}' \mathbf{V}_{hj}$ , and  $\mathbf{Z}$  is a vector of  $j$  independent random normal variates.

These simulated values of  $\beta_*$  and  $\sigma_{*j}^2$  are then used to re-create the parameters  $\mu$  and  $\Sigma$ . For a detailed description of how to produce monotone missingness with the MCMC method for a multivariate normal data, see Schafer (1997, pp. 226–235).

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## MCMC Method Specifications

With the MCMC method, you can impute either all missing values (IMPUTE=FULL) or just enough missing values to make the imputed data set have a monotone missing pattern (IMPUTE=MONOTONE). In the process, either a single chain for all imputations (CHAIN=SINGLE) or a separate chain for each imputation

(CHAIN=MULTIPLE) is used. The single chain might be somewhat more precise for estimating a single quantity such as a posterior mean (Schafer 1997, p. 138). See Schafer (1997, pp. 137–138) for a discussion of single versus multiple chains.

You can specify the number of initial burn-in iterations before the first imputation with the NBITER= option. This number is also used for subsequent chains for multiple chains. For a single chain, you can also specify the number of iterations between imputations with the NITER= option.

You can explicitly specify initial parameter values for the MCMC method with the INITIAL=INPUT= data set option. Alternatively, you can use the EM algorithm to derive a set of initial parameter values for MCMC with the option INITIAL=EM. These estimates are used as either the starting value (START=VALUE) or the starting distribution (START=DIST) for the MCMC method. For multiple chains, these estimates are used again as either the starting value (START=VALUE) or the starting distribution (START=DIST) for the subsequent chains.

You can specify the prior parameter information in the PRIOR= option. You can use a noninformative prior (PRIOR=JEFFREYS), a ridge prior (PRIOR=RIDGE), or an informative prior specified in a data set (PRIOR=INPUT).

The parameter estimates used to generate imputed values in each imputation can be saved in a data set with the OUTEST= option. Later, this data set can be read with the INEST= option to provide the reference distribution for imputing missing values for a new data set.

By default, the MCMC method uses a single chain to produce five imputations. It completes 200 burn-in iterations before the first imputation and 100 iterations between imputations. The posterior mode computed from the EM algorithm with a noninformative prior is used as the starting values for the MCMC method.

## INITIAL=EM Specifications

The EM algorithm is used to find the maximum likelihood estimates for incomplete data in the EM statement. You can also use the EM algorithm to find a posterior mode, the parameter estimates that maximize the observed-data posterior density. The resulting posterior mode provides a good starting value for the MCMC method.

With the INITIAL=EM option, PROC MI uses the MLE of the parameter vector as the initial estimates in the EM algorithm for the posterior mode. You can use the ITPRINT option within the INITIAL=EM option to display the iteration history for the EM algorithm.

You can use the CONVERGE= option to specify the convergence criterion in deriving the EM posterior mode. The iterations are considered to have converged when the maximum change in the parameter estimates between iteration steps is less than the value specified. By default, CONVERGE=1E-4.

You can also use the MAXITER= option to specify the maximum number of iterations of the EM algorithm. By default, MAXITER=200.

With the BOOTSTRAP option, you can use overdispersed starting values for the MCMC method. In this case, PROC MI applies the EM algorithm to a bootstrap sample, a simple random sample with replacement from the input data set, to derive the initial estimates for each chain (Schafer 1997, p. 128).

## Checking Convergence in MCMC

The theoretical convergence of the MCMC method has been explored under various conditions, as described in Schafer (1997, p. 70). However, in practice, verification of convergence is not a simple matter.

The parameters used in the imputation step for each iteration can be saved in an output data set with the `OUTITER=` option. These include the means, standard deviations, covariances, worst linear function, and observed-data LR statistics. You can then monitor the convergence in a single chain by displaying trace plots and autocorrelations for those parameter values (Schafer 1997, p. 120). The trace and autocorrelation function plots for parameters such as variable means, covariances, and the worst linear function can be displayed by specifying the `TIMEPLOT` and `ACFPLOT` options, respectively.

You can apply the EM algorithm to a bootstrap sample to obtain overdispersed starting values for multiple chains (Gelman and Rubin 1992). This provides a conservative estimate of the number of iterations needed before each imputation.

The next four subsections describe useful statistics and plots that can be used to check the convergence of the MCMC method.

### LR Statistics

You can save the observed-data likelihood ratio (LR) statistic in each iteration with the `LR` option in the `OUTITER=` data set. The statistic is based on the observed-data likelihood with parameter values used in the iteration and the observed-data maximum likelihood derived from the EM algorithm.

In each iteration, the LR statistic is given by

$$-2 \log \left( \frac{f(\hat{\theta}_i)}{f(\hat{\theta})} \right)$$

where  $f(\hat{\theta})$  is the observed-data maximum likelihood derived from the EM algorithm and  $f(\hat{\theta}_i)$  is the observed-data likelihood for  $\hat{\theta}_i$  used in the iteration.

Similarly, you can also save the observed-data LR posterior mode statistic for each iteration with the `LR_POST` option. This statistic is based on the observed-data posterior density with parameter values used in each iteration and the observed-data posterior mode derived from the EM algorithm for posterior mode.

For large samples, these LR statistics tends to be approximately  $\chi^2$  distributed with degrees of freedom equal to the dimension of  $\theta$  (Schafer 1997, p. 131). For example, with a large number of iterations, if the values of the LR statistic do not behave like a random sample from the described  $\chi^2$  distribution, then there is evidence that the MCMC method has not converged.

### Worst Linear Function of Parameters

The worst linear function (WLF) of parameters (Schafer 1997, pp. 129–131) is a scalar function of parameters  $\mu$  and  $\Sigma$  that is “worst” in the sense that its function values converge most slowly among parameters in the MCMC method. The convergence of this function is evidence that other parameters are likely to converge as well.

For linear functions of parameters  $\theta = (\mu, \Sigma)$ , a worst linear function of  $\theta$  has the highest asymptotic rate of missing information. The function can be derived from the iterative values of  $\theta$  near the posterior mode in the EM algorithm. That is, an estimated worst linear function of  $\theta$  is

$$w(\theta) = \mathbf{v}'(\theta - \hat{\theta})$$

where  $\hat{\theta}$  is the posterior mode and the coefficients  $\mathbf{v} = \hat{\theta}_{(-1)} - \hat{\theta}$  are the difference between the estimated value of  $\theta$  one step prior to convergence and the converged value  $\hat{\theta}$ .

You can display the coefficients of the worst linear function,  $\mathbf{v}$ , by specifying the WLF option in the MCMC statement. You can save the function value from each iteration in an OUTITER= data set by specifying the WLF option within the OUTITER option. You can also display the worst linear function values from iterations in an autocorrelation plot or a trace plot by specifying WLF as an ACFPLOT or TIMEPLOT option, respectively.

Note that when the observed-data posterior is nearly normal, the WLF is one of the slowest functions to approach stationarity. When the posterior is not close to normal, other functions might take much longer than the WLF to converge, as described in Schafer (1997, p.130).

## Trace Plot

A trace plot for a parameter  $\xi$  is a scatter plot of successive parameter estimates  $\xi_i$  against the iteration number  $i$ . The plot provides a simple way to examine the convergence behavior of the estimation algorithm for  $\xi$ . Long-term trends in the plot indicate that successive iterations are highly correlated and that the series of iterations has not converged.

You can display trace plots for worst linear function, variable means, variable variances, and covariances of variables. You can also request logarithmic transformations for positive parameters in the plots with the LOG option. When a parameter value is less than or equal to zero, the value is not displayed in the corresponding plot.

By default, the MI procedure uses solid line segments to connect data points in a trace plot. You can use the CCONNECT=, LCONNECT=, and WCONNECT= options to change the color, line type, and width of the line segments, respectively. When WCONNECT=0 is specified, the data points are not connected, and the procedure uses the plus sign (+) as the plot symbol to display the points with a height of one (percentage screen unit) in a trace plot. You can use the SYMBOL=, CSYMBOL=, and HSYMBOL= options to change the shape, color, and height of the plot symbol, respectively.

By default, the plot title “Trace Plot” is displayed in a trace plot. You can request another title by using the TITLE= option in the TIMEPLOT option. When another title is also specified in a TITLE statement, this title is displayed as the main title and the plot title is displayed as a subtitle in the plot.

You can use options in the GOPTIONS statement to change the color and height of the title. See the chapter “The SAS/GRAPH Statements” in *SAS/GRAPH: Reference* for an illustration of title options. See [Example 57.11](#) for a usage of the trace plot.

## Autocorrelation Function Plot

To examine relationships of successive parameter estimates  $\xi$ , the autocorrelation function (ACF) can be used. For a stationary series,  $\xi_i, i \geq 1$ , in trace data, the autocorrelation function at lag  $k$  is

$$\rho_k = \frac{\text{Cov}(\xi_i, \xi_{i+k})}{\text{Var}(\xi_i)}$$



The sample  $k$ th order autocorrelation is computed as

$$r_k = \frac{\sum_{i=1}^{n-k} (\xi_i - \bar{\xi})(\xi_{i+k} - \bar{\xi})}{\sum_{i=1}^n (\xi_i - \bar{\xi})^2}$$

You can display autocorrelation function plots for the worst linear function, variable means, variable variances, and covariances of variables. You can also request logarithmic transformations for parameters in the plots with the LOG option. When a parameter has values less than or equal to zero, the corresponding plot is not created.

You specify the maximum number of lags of the series with the NLAG= option. The autocorrelations at each lag less than or equal to the specified lag are displayed in the graph. In addition, the plot also displays approximate 95% confidence limits for the autocorrelations. At lag  $k$ , the confidence limits indicate a set of approximate 95% critical values for testing the hypothesis  $\rho_j = 0$ ,  $j \geq k$ .

By default, the MI procedure uses the star (\*) as the plot symbol to display the points with a height of one (percentage screen unit) in the plot, a solid line to display the reference line of zero autocorrelation, vertical line segments to connect autocorrelations to the reference line, and a pair of dashed lines to display approximately 95% confidence limits for the autocorrelations.

You can use the SYMBOL=, CSYMBOL=, and HSYMBOL= options to change the shape, color, and height of the plot symbol, respectively, and the CNEEDLES= and WNEEDLES= options to change the color and width of the needles, respectively. You can also use the LREF=, CREF=, and WREF= options to change the line type, color, and width of the reference line, respectively. Similarly, you can use the LCONF=, CCONF=, and WCONF= options to change the line type, color, and width of the confidence limits, respectively.

By default, the plot title “Autocorrelation Plot” is displayed in an autocorrelation function plot. You can request another title by using the TITLE= option within the ACFPLOT option. When another title is also specified in a TITLE statement, this title is displayed as the main title and the plot title is displayed as a subtitle in the plot.

You can use options in the GOPTIONS statement to change the color and height of the title. See the chapter “The SAS/GRAPH Statements” in *SAS/GRAPH: Reference* for a description of title options. See [Example 57.8](#) for an illustration of the autocorrelation function plot.

## Input Data Sets

You can specify the input data set with missing values by using the DATA= option in the PROC MI statement. When an MCMC method is used, you can specify the data set that contains the reference distribution information for imputation with the INEST= option, the data set that contains initial parameter estimates for the MCMC method with the INITIAL=INPUT= option, and the data set that contains information for the prior distribution with the PRIOR=INPUT= option in the MCMC statement.

### DATA=SAS-data-set

The input DATA= data set is an ordinary SAS data set that contains multivariate data with missing values.

**INEST=SAS-data-set**

The input INEST= data set is a TYPE=EST data set and contains a variable `_Imputation_` to identify the imputation number. For each imputation, PROC MI reads the point estimate from the observations with `_TYPE_='PARM'` or `_TYPE_='PARMS'` and the associated covariances from the observations with `_TYPE_='COV'` or `_TYPE_='COVB'`. These estimates are used as the reference distribution to impute values for observations in the DATA= data set. When the input INEST= data set also contains observations with `_TYPE_='SEED'`, PROC MI reads the seed information for the random number generator from these observations. Otherwise, the SEED= option provides the seed information.

**INITIAL=INPUT=SAS-data-set**

The input INITIAL=INPUT= data set is a TYPE=COV or CORR data set and provides initial parameter estimates for the MCMC method. The covariances derived from the TYPE=COV/CORR data set are divided by the number of observations to get the correct covariance matrix for the point estimate (sample mean).

If TYPE=COV, PROC MI reads the number of observations from the observations with `_TYPE_='N'`, the point estimate from the observations with `_TYPE_='MEAN'`, and the covariances from the observations with `_TYPE_='COV'`.

If TYPE=CORR, PROC MI reads the number of observations from the observations with `_TYPE_='N'`, the point estimate from the observations with `_TYPE_='MEAN'`, the correlations from the observations with `_TYPE_='CORR'`, and the standard deviations from the observations with `_TYPE_='STD'`.

**PRIOR=INPUT=SAS-data-set**

The input PRIOR=INPUT= data set is a TYPE=COV data set that provides information for the prior distribution. You can use the data set to specify a prior distribution for  $\Sigma$  of the form

$$\Sigma \sim W^{-1}(d^*, d^*S^*)$$

where  $d^* = n^* - 1$  is the degrees of freedom. PROC MI reads the matrix  $S^*$  from observations with `_TYPE_='COV'` and reads  $n^*$  from observations with `_TYPE_='N'`.

You can also use this data set to specify a prior distribution for  $\mu$  of the form

$$\mu \sim N\left(\mu_0, \frac{1}{n_0}\Sigma\right)$$

PROC MI reads the mean vector  $\mu_0$  from observations with `_TYPE_='MEAN'` and reads  $n_0$  from observations with `_TYPE_='N_MEAN'`. When there are no observations with `_TYPE_='N_MEAN'`, PROC MI reads  $n_0$  from observations with `_TYPE_='N'`.

---

**Output Data Sets**

You can specify the output data set of imputed values with the OUT= option in the PROC MI statement. When an EM statement is used, you can specify the data set that contains the original data set with missing values being replaced by the expected values from the EM algorithm by using the OUT= option in the EM statement. You can also specify the data set that contains MLE computed with the EM algorithm by using the OUTEM= option.

When an MCMC method is used, you can specify the data set that contains parameter estimates used in each imputation with the `OUTEST=` option in the MCMC statement, and you can specify the data set that contains parameters used in the imputation step for each iteration with the `OUTITER` option in the MCMC statement.

### **OUT=SAS-data-set in the PROC MI statement**

The `OUT=` data set contains all the variables in the original data set and a new variable named `_Imputation_` that identifies the imputation. For each imputation, the data set contains all variables in the input `DATA=` data set with missing values being replaced by imputed values. Note that when the `NIMPUTE=1` option is specified, the variable `_Imputation_` is not created.

### **OUT=SAS-data-set in an EM statement**

The `OUT=` data set contains the original data set with missing values being replaced by expected values from the EM algorithm.

### **OUTEM=SAS-data-set**

The `OUTEM=` data set is a `TYPE=COV` data set and contains the MLE computed with the EM algorithm. The observations with `_TYPE_='MEAN'` contain the estimated mean and the observations with `_TYPE_='COV'` contain the estimated covariances.

### **OUTEST=SAS-data-set**

The `OUTEST=` data set is a `TYPE=EST` data set and contains parameter estimates used in each imputation in the MCMC method. It also includes an index variable named `_Imputation_`, which identifies the imputation.

The observations with `_TYPE_='SEED'` contain the seed information for the random number generator. The observations with `_TYPE_='PARM'` or `_TYPE_='PARMS'` contain the point estimate, and the observations with `_TYPE_='COV'` or `_TYPE_='COVB'` contain the associated covariances. These estimates are used as the parameters of the reference distribution to impute values for observations in the `DATA=` dataset.

Note that these estimates are the values used in the I-step before each imputation. These are not the parameter values simulated from the P-step in the same iteration. See [Example 57.12](#) for a usage of this option.

### **OUTITER <(options)> =SAS-data-set in an EM statement**

The `OUTITER=` data set in an EM statement is a `TYPE=COV` data set and contains parameters for each iteration. It also includes a variable `_Iteration_` that provides the iteration number.

The parameters in the output data set depend on the options specified. You can specify the `MEAN` and `COV` options for `OUTITER`. With the `MEAN` option, the output data set contains the mean parameters in observations with the variable `_TYPE_='MEAN'`. Similarly, with the `COV` option, the output data set contains the covariance parameters in observations with the variable `_TYPE_='COV'`. When no options are specified, the output data set contains the mean parameters for each iteration.

**OUTITER <(options)> =SAS-data-set in an FCS statement**

The OUTITER= data set in an FCS statement is a TYPE=COV data set and contains parameters for each iteration. It also includes variables named `_Imputation_` and `_Iteration_`, which provide the imputation number and iteration number.

The parameters in the output data set depend on the options specified. You can specify the MEAN and STD options for OUTITER. With the MEAN option, the output data set contains the mean parameters used in the imputation in observations with the variable `_TYPE_='MEAN'`. Similarly, with the STD option, the output data set contains the standard deviation parameters used in the imputation in observations with the variable `_TYPE_='STD'`. When no options are specified, the output data set contains the mean parameters for each iteration.

**OUTITER <(options)> =SAS-data-set in an MCMC statement**

The OUTITER= data set in an MCMC statement is a TYPE=COV data set and contains parameters used in the imputation step for each iteration. It also includes variables named `_Imputation_` and `_Iteration_`, which provide the imputation number and iteration number.

The parameters in the output data set depend on the options specified. [Table 57.6](#) summarizes the options available for OUTITER and the corresponding values for the output variable `_TYPE_`.

**Table 57.6** Summary of Options for OUTITER in an MCMC statement

| Option  | Output Parameters                         | _TYPE_   |
|---------|-------------------------------------------|----------|
| MEAN    | mean parameters                           | MEAN     |
| STD     | standard deviations                       | STD      |
| COV     | covariances                               | COV      |
| LR      | -2 log LR statistic                       | LOG_LR   |
| LR_POST | -2 log LR statistic of the posterior mode | LOG_POST |
| WLF     | worst linear function                     | WLF      |

When no options are specified, the output data set contains the mean parameters used in the imputation step for each iteration. For a detailed description of the worst linear function and LR statistics, see the section “[Checking Convergence in MCMC](#)” on page 4764.

---

## Combining Inferences from Multiply Imputed Data Sets

With  $m$  imputations,  $m$  different sets of the point and variance estimates for a parameter  $Q$  can be computed. Suppose  $\hat{Q}_i$  and  $\hat{W}_i$  are the point and variance estimates from the  $i$ th imputed data set,  $i = 1, 2, \dots, m$ . Then the combined point estimate for  $Q$  from multiple imputation is the average of the  $m$  complete-data estimates:

$$\bar{Q} = \frac{1}{m} \sum_{i=1}^m \hat{Q}_i$$

Suppose  $\overline{W}$  is the within-imputation variance, which is the average of the  $m$  complete-data estimates,

$$\overline{W} = \frac{1}{m} \sum_{i=1}^m \hat{W}_i$$

and  $B$  is the between-imputation variance

$$B = \frac{1}{m-1} \sum_{i=1}^m (\hat{Q}_i - \overline{Q})^2$$

Then the variance estimate associated with  $\overline{Q}$  is the total variance (Rubin 1987)

$$T = \overline{W} + \left(1 + \frac{1}{m}\right)B$$

The statistic  $(Q - \overline{Q})T^{-(1/2)}$  is approximately distributed as  $t$  with  $v_m$  degrees of freedom (Rubin 1987), where

$$v_m = (m-1) \left[ 1 + \frac{\overline{W}}{(1+m^{-1})B} \right]^2$$

The degrees of freedom  $v_m$  depend on  $m$  and the ratio

$$r = \frac{(1+m^{-1})B}{\overline{W}}$$

The ratio  $r$  is called the relative increase in variance due to nonresponse (Rubin 1987). When there is no missing information about  $Q$ , the values of  $r$  and  $B$  are both zero. With a large value of  $m$  or a small value of  $r$ , the degrees of freedom  $v_m$  will be large and the distribution of  $(Q - \overline{Q})T^{-(1/2)}$  will be approximately normal.

Another useful statistic is the fraction of missing information about  $Q$ :

$$\hat{\lambda} = \frac{r + 2/(v_m + 3)}{r + 1}$$

Both statistics  $r$  and  $\lambda$  are helpful diagnostics for assessing how the missing data contribute to the uncertainty about  $Q$ .

When the complete-data degrees of freedom  $v_0$  are small, and there is only a modest proportion of missing data, the computed degrees of freedom,  $v_m$ , can be much larger than  $v_0$ , which is inappropriate. For example, with  $m = 5$  and  $r = 10\%$ , the computed degrees of freedom  $v_m = 484$ , which is inappropriate for data sets with complete-data degrees of freedom less than 484.

Barnard and Rubin (1999) recommend the use of adjusted degrees of freedom

$$v_m^* = \left[ \frac{1}{v_m} + \frac{1}{\hat{v}_{obs}} \right]^{-1}$$

where  $\hat{v}_{obs} = (1 - \gamma)v_0(v_0 + 1)/(v_0 + 3)$  and  $\gamma = (1 + m^{-1})B/T$ .

Note that the MI procedure uses the adjusted degrees of freedom,  $v_m^*$ , for inference.

## Multiple Imputation Efficiency

The relative efficiency (RE) of using the finite  $m$  imputation estimator, rather than using an infinite number for the fully efficient imputation, in units of variance, is approximately a function of  $m$  and  $\lambda$  (Rubin 1987, p. 114):

$$\text{RE} = \left(1 + \frac{\lambda}{m}\right)^{-1}$$

Table 57.7 shows relative efficiencies with different values of  $m$  and  $\lambda$ .

**Table 57.7** Relative Efficiencies

| m  | $\lambda$ |        |        |        |        |
|----|-----------|--------|--------|--------|--------|
|    | 10%       | 20%    | 30%    | 50%    | 70%    |
| 3  | 0.9677    | 0.9375 | 0.9091 | 0.8571 | 0.8108 |
| 5  | 0.9804    | 0.9615 | 0.9434 | 0.9091 | 0.8772 |
| 10 | 0.9901    | 0.9804 | 0.9709 | 0.9524 | 0.9346 |
| 20 | 0.9950    | 0.9901 | 0.9852 | 0.9756 | 0.9662 |

The table shows that for situations with little missing information, only a small number of imputations are necessary. In practice, the number of imputations needed can be informally verified by replicating sets of  $m$  imputations and checking whether the estimates are stable between sets (Horton and Lipsitz 2001, p. 246).

## Imputer's Model Versus Analyst's Model

Multiple imputation inference assumes that the model you used to analyze the multiply imputed data (the analyst's model) is the same as the model used to impute missing values in multiple imputation (the imputer's model). But in practice, the two models might not be the same (Schafer 1997, p. 139).

Schafer (1997, pp. 139–143) provides comprehensive coverage of this topic, and the following example is based on his work.

Consider a trivariate data set with variables  $Y_1$  and  $Y_2$  fully observed, and a variable  $Y_3$  with missing values. An imputer creates multiple imputations with the model  $Y_3 = Y_1 Y_2$ . However, the analyst can later use the simpler model  $Y_3 = Y_1$ . In this case, the analyst assumes more than the imputer. That is, the analyst assumes there is no relationship between variables  $Y_3$  and  $Y_2$ .

The effect of the discrepancy between the models depends on whether the analyst's additional assumption is true. If the assumption is true, the imputer's model still applies. The inferences derived from multiple imputations will still be valid, although they might be somewhat conservative because they reflect the additional uncertainty of estimating the relationship between  $Y_3$  and  $Y_2$ .

On the other hand, suppose that the analyst models  $Y_3 = Y_1$ , and there is a relationship between variables  $Y_3$  and  $Y_2$ . Then the model  $Y_3 = Y_1$  will be biased and is inappropriate. Appropriate results can be generated only from appropriate analyst models.

Another type of discrepancy occurs when the imputer assumes more than the analyst. For example, suppose that an imputer creates multiple imputations with the model  $Y_3 = Y_1$ , but the analyst later fits a model  $Y_3 = Y_1 Y_2$ . When the assumption is true, the imputer's model is a correct model and the inferences still hold.

On the other hand, suppose there is a relationship between  $Y_3$  and  $Y_2$ . Imputations created under the incorrect assumption that there is no relationship between  $Y_3$  and  $Y_2$  will make the analyst's estimate of the relationship biased toward zero. Multiple imputations created under an incorrect model can lead to incorrect conclusions.

Thus, generally you should include as many variables as you can when doing multiple imputation. The precision you lose with included unimportant predictors is usually a relatively small price to pay for the general validity of analyses of the resultant multiply imputed data set (Rubin 1996). But at the same time, you need to keep the model building and fitting feasible (Barnard and Meng 1999, pp. 19–20).

To produce high-quality imputations for a particular variable, the imputation model should also include variables that are potentially related to the imputed variable and variables that are potentially related to the missingness of the imputed variable (Schafer 1997, p. 143).

Similar suggestions were also given by van Buuren, Boshuizen, and Knook (1999, p. 687). They recommend that the imputation model include three sets of covariates: variables in the analyst's model, variables associated with the missingness of the imputed variable, and variables correlated with the imputed variable. They also recommend the removal of the covariates not in the analyst's model if they have too many missing values for observations with missing imputed variables.

Note that it is good practice to include a description of the imputer's model with the multiply imputed data set (Rubin 1996, p. 479). That way, the analysts will have information about the variables involved in the imputation and which relationships among the variables have been implicitly set to zero.

---

## Parameter Simulation versus Multiple Imputation

As an alternative to multiple imputation, parameter simulation can also be used to analyze the data for many incomplete-data problems. Although the MI procedure does not offer parameter simulation, the trade-offs between the two methods (Schafer 1997, pp. 89–90, 135–136) are examined in this section.

The parameter simulation method simulates random values of parameters from the observed-data posterior distribution and makes simple inferences about these parameters (Schafer 1997, p. 89). When a set of well-defined population parameters  $\theta$  are of interest, parameter simulation can be used to directly examine and summarize simulated values of  $\theta$ . This usually requires a large number of iterations, and involves calculating appropriate summaries of the resulting dependent sample of the iterates of the  $\theta$ . If only a small set of parameters are involved, parameter simulation is suitable (Schafer 1997).

Multiple imputation requires only a small number of imputations. Generating and storing a few imputations can be more efficient than generating and storing a large number of iterations for parameter simulation.

When fractions of missing information are low, methods that average over simulated values of the missing data, as in multiple imputation, can be much more efficient than methods that average over simulated values of  $\theta$  as in parameter simulation (Schafer 1997).

---

## Summary of Issues in Multiple Imputation

This section summarizes issues that are encountered in applications of the MI procedure.

### The MAR Assumption

The missing at random (MAR) assumption is needed for the imputation methods in the MI procedure. Although this assumption cannot be verified with the data, it becomes more plausible as more variables are included in the imputation model (Schafer 1997, pp. 27–28; van Buuren, Boshuizen, and Knook 1999, p. 687).

### Number of Imputations

Based on the theory of multiple imputation, only a small number of imputations are needed for a data set with little missing information (Rubin 1987, p. 114). The number of imputations can be informally verified by replicating sets of  $m$  imputations and checking whether the estimates are stable (Horton and Lipsitz 2001, p. 246).

### Imputation Model

Generally you should include as many variables as you can in the imputation model (Rubin 1996). At the same time, however, it is important to keep the number of variables in control, as discussed by Barnard and Meng (1999, pp. 19–20). For the imputation of a particular variable, the model should include variables in the complete-data model, variables that are correlated with the imputed variable, and variables that are associated with the missingness of the imputed variable (Schafer 1997, p. 143; van Buuren, Boshuizen, and Knook 1999, p. 687).

### Multivariate Normality Assumption

Although the regression and MCMC methods assume multivariate normality, inferences based on multiple imputation can be robust to departures from the multivariate normality if the amount of missing information is not large (Schafer 1997, pp. 147–148).

You can use variable transformations to make the normality assumption more tenable. Variables are transformed before the imputation process and then back-transformed to create imputed values.

### Monotone Regression Method

With the multivariate normality assumption, either the regression method or the predictive mean matching method can be used to impute continuous variables in data sets with monotone missing patterns.

The predictive mean matching method ensures that imputed values are plausible and might be more appropriate than the regression method if the normality assumption is violated (Horton and Lipsitz 2001, p. 246).

### Monotone Propensity Score Method

The propensity score method can also be used to impute continuous variables in data sets with monotone missing patterns.



The propensity score method does not use correlations among variables and is not appropriate for analyses involving relationship among variables, such as a regression analysis (Schafer 1999, p. 11). It can also produce badly biased estimates of regression coefficients when data on predictor variables are missing (Allison 2000).

### MCMC Monotone-Data Imputation

The MCMC method is used to impute continuous variables in data sets with arbitrary missing patterns, assuming a multivariate normal distribution for the data. It can also be used to impute just enough missing values to make the imputed data sets have a monotone missing pattern. Then, a more flexible monotone imputation method can be used for the remaining missing values.

### Checking Convergence in MCMC

In an MCMC method, parameters are drawn after the MCMC is run long enough to converge to its stationary distribution. In practice, however, it is not simple to verify the convergence of the process, especially for a large number of parameters.

You can check for convergence by examining the observed-data likelihood ratio statistic and worst linear function of the parameters in each iteration. You can also check for convergence by examining a plot of autocorrelation function, as well as a trace plot of parameters (Schafer 1997, p. 120).

### EM Estimates

The EM algorithm can be used to compute the MLE of the mean vector and covariance matrix of the data with missing values, assuming a multivariate normal distribution for the data. However, the covariance matrix associated with the estimate of the mean vector cannot be derived from the EM algorithm.

In the MI procedure, you can use the EM algorithm to compute the posterior mode, which provides a good starting value for the MCMC method (Schafer 1997, p. 169).

---

## ODS Table Names

PROC MI assigns a name to each table it creates. You must use these names to reference tables when using the Output Delivery System (ODS). These names are listed in Table 57.8. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

**Table 57.8** ODS Tables Produced by PROC MI

| ODS Table Name    | Description                   | Statement | Option               |
|-------------------|-------------------------------|-----------|----------------------|
| Corr              | Pairwise correlations         |           | SIMPLE               |
| EMEstimates       | EM (MLE) estimates            | EM        |                      |
| EMInitEstimates   | EM initial estimates          | EM        |                      |
| EMIterHistory     | EM (MLE) iteration history    | EM        | ITPRINT              |
| EMPostEstimates   | EM (posterior mode) estimates | MCMC      | INITIAL=EM           |
| EMPostIterHistory | EM (posterior mode)           | MCMC      | INITIAL=EM (ITPRINT) |

Table 57.8 *continued*

| ODS Table Name     | Description                          | Statement | Option                |
|--------------------|--------------------------------------|-----------|-----------------------|
|                    | iteration history                    |           |                       |
| EMWLF              | Worst linear function                | MCMC      | WLF                   |
| FCSDiscrim         | Discriminant model                   | FCS       | DISCRIM (/DETAILS)    |
|                    | group means                          |           |                       |
| FCSLogistic        | Logistic model                       | FCS       | LOGISTIC (/DETAILS)   |
| FCSModel           | FCS models                           | FCS       |                       |
| FCSReg             | Regression model                     | FCS       | REG (/DETAILS)        |
| FCSRegPMM          | Predicted mean matching model        | FCS       | REGPMM (/DETAILS)     |
| MCMCInitEstimates  | MCMC initial estimates               | MCMC      | DISPLAYINIT           |
| MissPattern        | Missing data patterns                |           |                       |
| ModelInfo          | Model information                    |           |                       |
| MonoDiscrim        | Discriminant model                   | MONOTONE  | DISCRIM (/DETAILS)    |
|                    | group means                          |           |                       |
| MonoLogistic       | Logistic model                       | MONOTONE  | LOGISTIC (/DETAILS)   |
| MonoModel          | Monotone models                      | MONOTONE  |                       |
| MonoPropensity     | Propensity score model               | MONOTONE  | PROPENSITY (/DETAILS) |
|                    | logistic function                    |           |                       |
| MonoReg            | Regression model                     | MONOTONE  | REG (/DETAILS)        |
| MonoRegPMM         | Predicted mean matching model        | MONOTONE  | REGPMM (/DETAILS)     |
| ParameterEstimates | Parameter estimates                  |           |                       |
| Transform          | Variable transformations             | TRANSFORM |                       |
| Univariate         | Univariate statistics                |           | SIMPLE                |
| VarianceInfo       | Between, within, and total variances |           |                       |

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “[Statistical Graphics Using ODS.](#)”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS.](#)”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “[A Primer on ODS Statistical Graphics](#)” on page 599 in Chapter 21, “[Statistical Graphics Using ODS.](#)”

PROC MI assigns a name to each graph it creates using ODS. You can use these names to reference the graphs when using ODS. To request these graphs, ODS Graphics must be enabled and you must specify the options indicated in [Table 57.9](#).

**Table 57.9** Graphs Produced by PROC MI

| ODS Graph Name | Description | Statement | Option       |
|----------------|-------------|-----------|--------------|
| ACFPlot        | ACF plot    | MCMC      | PLOTS=ACF    |
| TracePlot      | Trace plot  | MCMC      | PLOTS= TRACE |
|                |             | FCS       | PLOTS= TRACE |

## Examples: MI Procedure

The Fish data described in the STEPDISC procedure are measurements of 159 fish of seven species caught in Finland’s lake Laengelmavesi. For each fish, the length, height, and width are measured. Three different length measurements are recorded: from the nose of the fish to the beginning of its tail (Length1), from the nose to the notch of its tail (Length2), and from the nose to the end of its tail (Length3). See Chapter 89, “The STEPDISC Procedure,” for more information.

The Fish1 data set is constructed from the Fish data set and contains only one species of the fish and the three length measurements. Some values have been set to missing, and the resulting data set has a monotone missing pattern in the variables Length1, Length2, and Length3. The Fish1 data set is used in [Example 57.2](#) with the propensity score method and in [Example 57.3](#) with the regression method.

The Fish2 data set is also constructed from the Fish data set and contains two species of fish. Some values have been set to missing, and the resulting data set has a monotone missing pattern in the variables Length, Height, Width, and Species. The Fish2 data set is used in [Example 57.4](#) with the logistic regression method and in [Example 57.5](#) with the discriminant function method. Note that some values of the variable Species have also been altered in the data set.

The Fish3 data set is similar to the data set Fish2 except some additional values have been set to missing and the resulting data set has an arbitrary missing pattern. The Fish3 data set is used in [Example 57.7](#) and in [Example 57.8](#).

The Fitness1 data set created in the section “Getting Started: MI Procedure” on page 4716 is used in other examples.

The following statements create the Fish1 data set:

```

-----Fish1 Data-----
| The data set contains one species of the fish (Bream) and |
| three measurements: Length1, Length2, Length3. |
| Some values have been set to missing, and the resulting data set |
| has a monotone missing pattern in the variables |
| Length1, Length2, and Length3. |

data Fish1;
 title 'Fish Measurement Data';
 input Length1 Length2 Length3 @@;
 datalines;
23.2 25.4 30.0 24.0 26.3 31.2 23.9 26.5 31.1
26.3 29.0 33.5 26.5 29.0 . 26.8 29.7 34.7
26.8 . . 27.6 30.0 35.0 27.6 30.0 35.1
28.5 30.7 36.2 28.4 31.0 36.2 28.7 . .
29.1 31.5 . 29.5 32.0 37.3 29.4 32.0 37.2

```

```

29.4 32.0 37.2 30.4 33.0 38.3 30.4 33.0 38.5
30.9 33.5 38.6 31.0 33.5 38.7 31.3 34.0 39.5
31.4 34.0 39.2 31.5 34.5 . 31.8 35.0 40.6
31.9 35.0 40.5 31.8 35.0 40.9 32.0 35.0 40.6
32.7 36.0 41.5 32.8 36.0 41.6 33.5 37.0 42.6
35.0 38.5 44.1 35.0 38.5 44.0 36.2 39.5 45.3
37.4 41.0 45.9 38.0 41.0 46.5
;

```

The Fish2 data set contains two of the seven species in the Fish data set. For each of the two species (Bream and Pike), the length from the nose of the fish to the end of its tail, the height, and the width of each fish are measured.

The following statements create the Fish2 data set:

```

-----Fish2 Data-----
| The data set contains two species of the fish (Bream and Pike) |
| and three measurements: Length, Height, Width. |
| Some values have been set to missing, and the resulting data set |
| has a monotone missing pattern in the variables |
| Length, Height, Width, and Species. |

data Fish2;
 title 'Fish Measurement Data';
 input Species $ Length Height Width @@;
 datalines;
Bream 30.0 11.520 4.020 . 31.2 12.480 4.306
Bream 31.1 12.378 4.696 Bream 33.5 12.730 4.456
. 34.0 12.444 . Bream 34.7 13.602 4.927
Bream 34.5 14.180 5.279 Bream 35.0 12.670 4.690
Bream 35.1 14.005 4.844 Bream 36.2 14.227 4.959
. 36.2 14.263 . Bream 36.2 14.371 4.815
Bream 36.4 13.759 4.368 Bream 37.3 13.913 5.073
Bream 37.2 14.954 5.171 Bream 37.2 15.438 5.580
Bream 38.3 14.860 5.285 Bream 38.5 14.938 5.198
. 38.6 15.633 5.134 Bream 38.7 14.474 5.728
Bream 39.5 15.129 5.570 . 39.2 15.994 .
Bream 39.7 15.523 5.280 Bream 40.6 15.469 6.131
. 40.5 . . Bream 40.9 16.360 6.053
Bream 40.6 16.362 6.090 Bream 41.5 16.517 5.852
Bream 41.6 16.890 6.198 Bream 42.6 18.957 6.603
Bream 44.1 18.037 6.306 Bream 44.0 18.084 6.292
Bream 45.3 18.754 6.750 Bream 45.9 18.635 6.747
Bream 46.5 17.624 6.371
Pike 34.8 5.568 3.376 Pike 37.8 5.708 4.158
Pike 38.8 5.936 4.384 . 39.8 . .
Pike 40.5 7.290 4.577 Pike 41.0 6.396 3.977
. 45.5 7.280 4.323 Pike 45.5 6.825 4.459
Pike 45.8 7.786 5.130 Pike 48.0 6.960 4.896
Pike 48.7 7.792 4.870 Pike 51.2 7.680 5.376
Pike 55.1 8.926 6.171 . 59.7 10.686 .
Pike 64.0 9.600 6.144 Pike 64.0 9.600 6.144
Pike 68.0 10.812 7.480
;

```

The following statements create the Fish3 data set:

```

-----Fish3 Data-----
| The data set contains two species of the fish (Bream and Pike) |
| and three measurements: Length, Height, Width. |
| Some values have been set to missing, and the resulting data set |
| has an arbitrary missing pattern. |

data Fish3;
 title 'Fish Measurement Data';
 input Species $ Length Height Width @@;
 datalines;
Bream 30.0 11.520 4.020 . 31.2 12.480 4.306
Bream 31.1 12.378 4.696 Bream 33.5 12.730 4.456
. . 12.444 . Bream 34.7 13.602 4.927
Bream 34.5 14.180 5.279 . 35.0 . 4.690
Bream 35.1 14.005 4.844 Bream 36.2 14.227 4.959
. 36.2 14.263 . Bream 36.2 14.371 4.815
Bream 36.4 13.759 4.368 Bream 37.3 13.913 5.073
Bream 37.2 14.954 5.171 . 37.2 . 5.580
Bream 38.3 14.860 5.285 Bream 38.5 14.938 5.198
. 38.6 15.633 5.134 Bream 38.7 14.474 5.728
Bream 39.5 15.129 5.570 . 39.2 15.994 .
Bream 39.7 15.523 5.280 Bream 40.6 15.469 6.131
. 40.5 . . Bream 40.9 16.360 6.053
Bream 40.6 16.362 6.090 Bream 41.5 16.517 5.852
Bream 41.6 16.890 6.198 Bream 42.6 18.957 6.603
Bream . 18.037 . Bream . 18.084 6.292
Bream 45.3 18.754 6.750 Bream 45.9 18.635 6.747
Bream 46.5 17.624 6.371
Pike 34.8 5.568 3.376 Pike 37.8 5.708 4.158
Pike 38.8 5.936 4.384 . 39.8 . .
Pike 40.5 7.290 4.577 Pike 41.0 6.396 3.977
. 45.5 7.280 4.323 Pike 45.5 6.825 4.459
Pike 45.8 7.786 5.130 Pike 48.0 6.960 4.896
Pike 48.7 7.792 4.870 Pike 51.2 7.680 5.376
Pike 55.1 8.926 6.171 . 59.7 10.686 .
Pike 64.0 9.600 6.144 Pike 64.0 9.600 6.144
Pike . 10.812 7.480
;

```

### Example 57.1: EM Algorithm for MLE

This example uses the EM algorithm to compute the maximum likelihood estimates for parameters of multivariate normally distributed data with missing values. The following statements invoke the MI procedure and request the EM algorithm to compute the MLE for  $(\mu, \Sigma)$  of a multivariate normal distribution from the input data set Fitness1:

```

proc mi data=Fitness1 seed=1518971 simple nimpute=0;
 em itprint outem=outem;
 var Oxygen RunTime RunPulse;
run;

```

Note that when you specify the NIMPUTE=0 option, the missing values are not imputed.

The “Model Information” table in [Output 57.1.1](#) describes the method and options used in the procedure if a positive number is specified in the NIMPUTE= option.

**Output 57.1.1** Model Information

| The MI Procedure                 |                   |
|----------------------------------|-------------------|
| Model Information                |                   |
| Data Set                         | WORK.FITNESS1     |
| Method                           | MCMC              |
| Multiple Imputation Chain        | Single Chain      |
| Initial Estimates for MCMC       | EM Posterior Mode |
| Start                            | Starting Value    |
| Prior                            | Jeffreys          |
| Number of Imputations            | 0                 |
| Number of Burn-in Iterations     | 200               |
| Number of Iterations             | 100               |
| Seed for random number generator | 1518971           |

The “Missing Data Patterns” table in [Output 57.1.2](#) lists distinct missing data patterns with corresponding frequencies and percentages. Here, a value of “X” means that the variable is observed in the corresponding group and a value of “.” means that the variable is missing. The table also displays group-specific variable means.

**Output 57.1.2** Missing Data Patterns

| Missing Data Patterns |        |          |           |      |         |
|-----------------------|--------|----------|-----------|------|---------|
| Group                 | Oxygen | Run Time | Run Pulse | Freq | Percent |
| 1                     | X      | X        | X         | 21   | 67.74   |
| 2                     | X      | X        | .         | 4    | 12.90   |
| 3                     | X      | .        | .         | 3    | 9.68    |
| 4                     | .      | X        | X         | 1    | 3.23    |
| 5                     | .      | X        | .         | 2    | 6.45    |

| Missing Data Patterns |           |           |            |
|-----------------------|-----------|-----------|------------|
| -----Group Means----- |           |           |            |
| Group                 | Oxygen    | RunTime   | RunPulse   |
| 1                     | 46.353810 | 10.809524 | 171.666667 |
| 2                     | 47.109500 | 10.137500 | .          |
| 3                     | 52.461667 | .         | .          |
| 4                     | .         | 11.950000 | 176.000000 |
| 5                     | .         | 9.885000  | .          |

With the SIMPLE option, the procedure displays simple descriptive univariate statistics for available cases in the “Univariate Statistics” table in [Output 57.1.3](#) and correlations from pairwise available cases in the “Pairwise Correlations” table in [Output 57.1.4](#).

**Output 57.1.3** Univariate Statistics

| Univariate Statistics |    |           |          |           |           |
|-----------------------|----|-----------|----------|-----------|-----------|
| Variable              | N  | Mean      | Std Dev  | Minimum   | Maximum   |
| Oxygen                | 28 | 47.11618  | 5.41305  | 37.38800  | 60.05500  |
| RunTime               | 28 | 10.68821  | 1.37988  | 8.63000   | 14.03000  |
| RunPulse              | 22 | 171.86364 | 10.14324 | 148.00000 | 186.00000 |

| Univariate Statistics |                      |         |  |
|-----------------------|----------------------|---------|--|
| Variable              | ---Missing Values--- |         |  |
|                       | Count                | Percent |  |
| Oxygen                | 3                    | 9.68    |  |
| RunTime               | 3                    | 9.68    |  |
| RunPulse              | 9                    | 29.03   |  |

**Output 57.1.4** Pairwise Correlations

| Pairwise Correlations |              |              |              |  |
|-----------------------|--------------|--------------|--------------|--|
|                       | Oxygen       | RunTime      | RunPulse     |  |
| Oxygen                | 1.000000000  | -0.849118562 | -0.343961742 |  |
| RunTime               | -0.849118562 | 1.000000000  | 0.247258191  |  |
| RunPulse              | -0.343961742 | 0.247258191  | 1.000000000  |  |

When you use the EM statement, the MI procedure displays the initial parameter estimates for the EM algorithm in the “Initial Parameter Estimates for EM” table in [Output 57.1.5](#).

**Output 57.1.5** Initial Parameter Estimates for EM

| Initial Parameter Estimates for EM |          |           |           |            |
|------------------------------------|----------|-----------|-----------|------------|
| _TYPE_                             | _NAME_   | Oxygen    | RunTime   | RunPulse   |
| MEAN                               |          | 47.116179 | 10.688214 | 171.863636 |
| COV                                | Oxygen   | 29.301078 | 0         | 0          |
| COV                                | RunTime  | 0         | 1.904067  | 0          |
| COV                                | RunPulse | 0         | 0         | 102.885281 |

When you use the ITPRINT option in the EM statement, the “EM (MLE) Iteration History” table in [Output 57.1.6](#) displays the iteration history for the EM algorithm.

**Output 57.1.6** EM (MLE) Iteration History

| EM (MLE) Iteration History |                 |               |                |                 |
|----------------------------|-----------------|---------------|----------------|-----------------|
| <u>Iteration</u>           | <u>-2 Log L</u> | <u>Oxygen</u> | <u>RunTime</u> | <u>RunPulse</u> |
| 0                          | 289.544782      | 47.116179     | 10.688214      | 171.863636      |
| 1                          | 263.549489      | 47.116179     | 10.688214      | 171.863636      |
| 2                          | 255.851312      | 47.139089     | 10.603506      | 171.538203      |
| 3                          | 254.616428      | 47.122353     | 10.571685      | 171.426790      |
| 4                          | 254.494971      | 47.111080     | 10.560585      | 171.398296      |
| 5                          | 254.483973      | 47.106523     | 10.556768      | 171.389208      |
| 6                          | 254.482920      | 47.104899     | 10.555485      | 171.385257      |
| 7                          | 254.482813      | 47.104348     | 10.555062      | 171.383345      |
| 8                          | 254.482801      | 47.104165     | 10.554923      | 171.382424      |
| 9                          | 254.482800      | 47.104105     | 10.554878      | 171.381992      |
| 10                         | 254.482800      | 47.104086     | 10.554864      | 171.381796      |
| 11                         | 254.482800      | 47.104079     | 10.554859      | 171.381708      |
| 12                         | 254.482800      | 47.104077     | 10.554858      | 171.381669      |

The “EM (MLE) Parameter Estimates” table in [Output 57.1.7](#) displays the maximum likelihood estimates for  $\mu$  and  $\Sigma$  of a multivariate normal distribution from the data set Fitness1.

**Output 57.1.7** EM (MLE) Parameter Estimates

| EM (MLE) Parameter Estimates |             |               |                |                 |
|------------------------------|-------------|---------------|----------------|-----------------|
| <u>TYPE</u>                  | <u>NAME</u> | <u>Oxygen</u> | <u>RunTime</u> | <u>RunPulse</u> |
| MEAN                         |             | 47.104077     | 10.554858      | 171.381669      |
| COV                          | Oxygen      | 27.797931     | -6.457975      | -18.031298      |
| COV                          | RunTime     | -6.457975     | 2.015514       | 3.516287        |
| COV                          | RunPulse    | -18.031298    | 3.516287       | 97.766857       |

You can also output the EM (MLE) parameter estimates to an output data set with the OUTEM= option. The following statements list the observations in the output data set outem:

```
proc print data=outem;
 title 'EM Estimates';
run;
```

The output data set outem in [Output 57.1.8](#) is a TYPE=COV data set. The observation with TYPE='MEAN' contains the MLE for the parameter  $\mu$ , and the observations with TYPE='COV' contain the MLE for the parameter  $\Sigma$  of a multivariate normal distribution from the data set Fitness1.



**Output 57.1.8** EM Estimates

| EM Estimates |        |          |          |         |          |
|--------------|--------|----------|----------|---------|----------|
| Obs          | _TYPE_ | _NAME_   | Oxygen   | RunTime | RunPulse |
| 1            | MEAN   |          | 47.1041  | 10.5549 | 171.382  |
| 2            | COV    | Oxygen   | 27.7979  | -6.4580 | -18.031  |
| 3            | COV    | RunTime  | -6.4580  | 2.0155  | 3.516    |
| 4            | COV    | RunPulse | -18.0313 | 3.5163  | 97.767   |

## Example 57.2: Monotone Propensity Score Method

This example uses the propensity score method to impute missing values for variables in a data set with a monotone missing pattern. The following statements invoke the MI procedure and request the propensity score method. The resulting data set is named `outex2`.

```
proc mi data=Fish1 seed=899603 out=outex2;
 monotone propensity;
 var Length1 Length2 Length3;
run;
```

Note that the VAR statement is required and the data set must have a monotone missing pattern with variables as ordered in the VAR statement.

The “Model Information” table in [Output 57.2.1](#) describes the method and options used in the multiple imputation process. By default, five imputations are created for the missing data.

**Output 57.2.1** Model Information

| The MI Procedure                 |            |
|----------------------------------|------------|
| Model Information                |            |
| Data Set                         | WORK.FISH1 |
| Method                           | Monotone   |
| Number of Imputations            | 5          |
| Seed for random number generator | 899603     |

When monotone methods are used in the imputation, MONOTONE is displayed as the method. The “Monotone Model Specification” table in [Output 57.2.2](#) displays the detailed model specification. By default, the observations are sorted into five groups based on their propensity scores.

**Output 57.2.2** Monotone Model Specification

| Monotone Model Specification |                   |         |
|------------------------------|-------------------|---------|
| Method                       | Imputed Variables |         |
| Propensity( Groups= 5)       | Length2           | Length3 |

Without covariates specified for imputed variables Length2 and Length3, the variable Length1 is used as the covariate for Length2, and the variables Length1 and Length2 are used as covariates for Length3.

The “Missing Data Patterns” table in [Output 57.2.3](#) lists distinct missing data patterns with corresponding frequencies and percentages. Here, values of “X” and “.” indicate that the variable is observed or missing, respectively, in the corresponding group. The table confirms a monotone missing pattern for these three variables.

**Output 57.2.3** Missing Data Patterns

| Missing Data Patterns |         |         |         |      |         |
|-----------------------|---------|---------|---------|------|---------|
| Group                 | Length1 | Length2 | Length3 | Freq | Percent |
| 1                     | X       | X       | X       | 30   | 85.71   |
| 2                     | X       | X       | .       | 3    | 8.57    |
| 3                     | X       | .       | .       | 2    | 5.71    |

| Missing Data Patterns |                       |           |           |
|-----------------------|-----------------------|-----------|-----------|
| Group                 | -----Group Means----- |           |           |
|                       | Length1               | Length2   | Length3   |
| 1                     | 30.603333             | 33.436667 | 38.720000 |
| 2                     | 29.033333             | 31.666667 | .         |
| 3                     | 27.750000             | .         | .         |

For the imputation process, first, missing values of Length2 in group 3 are imputed using observed values of Length1. Then the missing values of Length3 in group 2 are imputed using observed values of Length1 and Length2. And finally, the missing values of Length3 in group 3 are imputed using observed values of Length1 and imputed values of Length2.

After the completion of  $m$  imputations, the “Variance Information” table in [Output 57.2.4](#) displays the between-imputation variance, within-imputation variance, and total variance for combining complete-data inferences. It also displays the degrees of freedom for the total variance. The relative increase in variance due to missingness, the fraction of missing information, and the relative efficiency for each variable are also displayed. A detailed description of these statistics is provided in the section “[Combining Inferences from Multiply Imputed Data Sets](#)” on page 4769.

**Output 57.2.4** Variance Information

| Variance Information |                    |          |          |        |
|----------------------|--------------------|----------|----------|--------|
| Variable             | -----Variance----- |          |          | DF     |
|                      | Between            | Within   | Total    |        |
| Length2              | 0.001500           | 0.465422 | 0.467223 | 32.034 |
| Length3              | 0.049725           | 0.547434 | 0.607104 | 27.103 |

| Variance Information |                               |                              |                     |
|----------------------|-------------------------------|------------------------------|---------------------|
| Variable             | Relative Increase in Variance | Fraction Missing Information | Relative Efficiency |
| Length2              | 0.003869                      | 0.003861                     | 0.999228            |
| Length3              | 0.108999                      | 0.102610                     | 0.979891            |

The “Parameter Estimates” table in [Output 57.2.5](#) displays the estimated mean and standard error of the mean for each variable. The inferences are based on the  $t$  distributions. For each variable, the table also displays a 95% mean confidence interval and a  $t$  statistic with the associated  $p$ -value for the hypothesis that the population mean is equal to the value specified in the MU0= option, which is zero by default.

**Output 57.2.5** Parameter Estimates

| Parameter Estimates |           |           |                       |          |        |
|---------------------|-----------|-----------|-----------------------|----------|--------|
| Variable            | Mean      | Std Error | 95% Confidence Limits |          | DF     |
| Length2             | 33.006857 | 0.683537  | 31.61460              | 34.39912 | 32.034 |
| Length3             | 38.361714 | 0.779169  | 36.76328              | 39.96015 | 27.103 |

| Parameter Estimates |           |           |           |          |         |
|---------------------|-----------|-----------|-----------|----------|---------|
| Variable            | Minimum   | Maximum   | t for H0: |          |         |
|                     |           |           | Mu0       | Mean=Mu0 | Pr >  t |
| Length2             | 32.957143 | 33.060000 | 0         | 48.29    | <.0001  |
| Length3             | 38.080000 | 38.545714 | 0         | 49.23    | <.0001  |

The following statements list the first 10 observations of the data set outex2, as shown in [Output 57.2.6](#). The missing values are imputed from observed values with similar propensity scores.

```
proc print data=outex2(obs=10);
 title 'First 10 Observations of the Imputed Data Set';
run;
```

**Output 57.2.6** Imputed Data Set

| First 10 Observations of the Imputed Data Set |              |         |         |         |
|-----------------------------------------------|--------------|---------|---------|---------|
| Obs                                           | _Imputation_ | Length1 | Length2 | Length3 |
| 1                                             | 1            | 23.2    | 25.4    | 30.0    |
| 2                                             | 1            | 24.0    | 26.3    | 31.2    |
| 3                                             | 1            | 23.9    | 26.5    | 31.1    |
| 4                                             | 1            | 26.3    | 29.0    | 33.5    |
| 5                                             | 1            | 26.5    | 29.0    | 38.6    |
| 6                                             | 1            | 26.8    | 29.7    | 34.7    |
| 7                                             | 1            | 26.8    | 29.0    | 35.0    |
| 8                                             | 1            | 27.6    | 30.0    | 35.0    |
| 9                                             | 1            | 27.6    | 30.0    | 35.1    |
| 10                                            | 1            | 28.5    | 30.7    | 36.2    |

**Example 57.3: Monotone Regression Method**

This example uses the regression method to impute missing values for all variables in a data set with a monotone missing pattern. The following statements invoke the MI procedure and request the regression method for the variable Length2 and the predictive mean matching method for variable Length3. The resulting data set is named outex3.

```
proc mi data=Fish1 round=.1 mu0= 0 35 45
 seed=13951639 out=outex3;
 monotone reg(Length2/ details)
 regpmm(Length3= Length1 Length2 Length1*Length2/ details);
 var Length1 Length2 Length3;
run;
```

The ROUND= option is used to round the imputed values to the same precision as observed values. The values specified with the ROUND= option are matched with the variables Length1, Length2, and Length3 in the order listed in the VAR statement. The MU0= option requests *t* tests for the hypotheses that the population means corresponding to the variables in the VAR statement are Length2=35 and Length3=45.

The “Missing Data Patterns” table lists distinct missing data patterns with corresponding frequencies and percentages. It is identical to the table in Output 57.2.3 in Example 57.2.

The “Monotone Model Specification” table in [Output 57.3.1](#) displays the model specification.

**Output 57.3.1** Monotone Model Specification

| The MI Procedure             |                   |
|------------------------------|-------------------|
| Monotone Model Specification |                   |
| Method                       | Imputed Variables |
| Regression                   | Length2           |
| Regression-PMM( K= 5)        | Length3           |

When you use the DETAILS option, the parameters estimated from the observed data and the parameters used in each imputation are displayed in [Output 57.3.2](#) and [Output 57.3.3](#).

**Output 57.3.2** Regression Model

| Regression Models for Monotone Method |           |          |                      |           |           |
|---------------------------------------|-----------|----------|----------------------|-----------|-----------|
| Imputed Variable                      | Effect    | Obs-Data | -----Imputation----- |           |           |
|                                       |           |          | 1                    | 2         | 3         |
| Length2                               | Intercept | -0.04249 | -0.049184            | -0.055470 | -0.051346 |
| Length2                               | Length1   | 0.98587  | 1.001934             | 0.995275  | 0.992294  |

| Regression Models for Monotone Method |           |                      |           |
|---------------------------------------|-----------|----------------------|-----------|
| Imputed Variable                      | Effect    | -----Imputation----- |           |
|                                       |           | 4                    | 5         |
| Length2                               | Intercept | -0.064193            | -0.030719 |
| Length2                               | Length1   | 0.983122             | 0.995883  |

**Output 57.3.3** Regression Predicted Mean Matching Model

| Regression Models for Monotone Predicted Mean Matching Method |                 |          |                      |           |           |
|---------------------------------------------------------------|-----------------|----------|----------------------|-----------|-----------|
| Imputed Variable                                              | Effect          | Obs Data | -----Imputation----- |           |           |
|                                                               |                 |          | 1                    | 2         | 3         |
| Length3                                                       | Intercept       | -0.01304 | 0.004134             | -0.011417 | -0.034177 |
| Length3                                                       | Length1         | -0.01332 | 0.025320             | -0.037494 | 0.308765  |
| Length3                                                       | Length2         | 0.98918  | 0.955510             | 1.025741  | 0.673374  |
| Length3                                                       | Length1*Length2 | -0.02521 | -0.034964            | -0.022017 | -0.017919 |

| Regression Models for Monotone Predicted Mean Matching Method |                 |                      |           |
|---------------------------------------------------------------|-----------------|----------------------|-----------|
| Imputed Variable                                              | Effect          | -----Imputation----- |           |
|                                                               |                 | 4                    | 5         |
| Length3                                                       | Intercept       | -0.010532            | 0.004685  |
| Length3                                                       | Length1         | 0.156606             | -0.147118 |
| Length3                                                       | Length2         | 0.828384             | 1.146440  |
| Length3                                                       | Length1*Length2 | -0.029335            | -0.034671 |

After the completion of five imputations by default, the “Variance Information” table in [Output 57.3.4](#) displays the between-imputation variance, within-imputation variance, and total variance for combining complete-data inferences. The relative increase in variance due to missingness, the fraction of missing information, and the relative efficiency for each variable are also displayed. These statistics are described in the section “Combining Inferences from Multiply Imputed Data Sets” on page 4769.

**Output 57.3.4** Variance Information

| Variance Information |                    |          |          |        |
|----------------------|--------------------|----------|----------|--------|
| Variable             | -----Variance----- |          |          | DF     |
|                      | Between            | Within   | Total    |        |
| Length2              | 0.000133           | 0.439512 | 0.439672 | 32.15  |
| Length3              | 0.000386           | 0.486913 | 0.487376 | 32.131 |

| Variance Information |                               |                              |                     |
|----------------------|-------------------------------|------------------------------|---------------------|
| Variable             | Relative Increase in Variance | Fraction Missing Information | Relative Efficiency |
|                      | Length2                       | 0.000363                     | 0.000363            |
| Length3              | 0.000952                      | 0.000951                     | 0.999810            |

The “Parameter Estimates” table in [Output 57.3.5](#) displays a 95% mean confidence interval and a  $t$  statistic with its associated  $p$ -value for each of the hypotheses requested with the MU0= option.

**Output 57.3.5** Parameter Estimates

| Parameter Estimates |           |           |                       |          |        |
|---------------------|-----------|-----------|-----------------------|----------|--------|
| Variable            | Mean      | Std Error | 95% Confidence Limits |          | DF     |
| Length2             | 33.104571 | 0.663078  | 31.75417              | 34.45497 | 32.15  |
| Length3             | 38.424571 | 0.698123  | 37.00277              | 39.84637 | 32.131 |

| Parameter Estimates |           |           |           |                       |         |
|---------------------|-----------|-----------|-----------|-----------------------|---------|
| Variable            | Minimum   | Maximum   | Mu0       | t for H0:<br>Mean=Mu0 | Pr >  t |
| Length2             | 33.088571 | 33.117143 | 35.000000 | -2.86                 | 0.0074  |
| Length3             | 38.397143 | 38.445714 | 45.000000 | -9.42                 | <.0001  |

The following statements list the first 10 observations of the data set outex3 in [Output 57.3.6](#). Note that the imputed values of Length2 are rounded to the same precision as the observed values.

```
proc print data=outex3(obs=10);
 title 'First 10 Observations of the Imputed Data Set';
run;
```

**Output 57.3.6** Imputed Data Set

| First 10 Observations of the Imputed Data Set |              |         |         |         |  |
|-----------------------------------------------|--------------|---------|---------|---------|--|
| Obs                                           | _Imputation_ | Length1 | Length2 | Length3 |  |
| 1                                             | 1            | 23.2    | 25.4    | 30.0    |  |
| 2                                             | 1            | 24.0    | 26.3    | 31.2    |  |
| 3                                             | 1            | 23.9    | 26.5    | 31.1    |  |
| 4                                             | 1            | 26.3    | 29.0    | 33.5    |  |
| 5                                             | 1            | 26.5    | 29.0    | 34.7    |  |
| 6                                             | 1            | 26.8    | 29.7    | 34.7    |  |
| 7                                             | 1            | 26.8    | 28.8    | 34.7    |  |
| 8                                             | 1            | 27.6    | 30.0    | 35.0    |  |
| 9                                             | 1            | 27.6    | 30.0    | 35.1    |  |
| 10                                            | 1            | 28.5    | 30.7    | 36.2    |  |

## Example 57.4: Monotone Logistic Regression Method for CLASS Variables

This example uses logistic regression method to impute values for a binary variable in a data set with a monotone missing pattern.

In the following statements, the logistic regression method is used for the binary CLASS variable Species:

```
proc mi data=Fish2 seed=1305417 out=outex4;
 class Species;
 monotone reg(Length Width/ details)
 logistic(Species= Length Height Width Height*Width/ details);
 var Length Height Width Species;
run;
```

The “Model Information” table in [Output 57.4.1](#) describes the method and options used in the multiple imputation process.

**Output 57.4.1** Model Information

| The MI Procedure                 |            |
|----------------------------------|------------|
| Model Information                |            |
| Data Set                         | WORK.FISH2 |
| Method                           | Monotone   |
| Number of Imputations            | 5          |
| Seed for random number generator | 1305417    |

The “Monotone Model Specification” table in [Output 57.4.2](#) describes methods and imputed variables in the imputation model. The procedure uses the logistic regression method to impute the variable Species in the model. Missing values in other variables are not imputed.

**Output 57.4.2** Monotone Model Specification

| Monotone Model Specification |                   |
|------------------------------|-------------------|
| Method                       | Imputed Variables |
| Regression                   | Height Width      |
| Logistic Regression          | Species           |



The “Missing Data Patterns” table in [Output 57.4.3](#) lists distinct missing data patterns with corresponding frequencies and percentages. The table confirms a monotone missing pattern for these variables.

**Output 57.4.3** Missing Data Patterns

| Missing Data Patterns |        |        |       |         |      |         |
|-----------------------|--------|--------|-------|---------|------|---------|
| Group                 | Length | Height | Width | Species | Freq | Percent |
| 1                     | X      | X      | X     | X       | 43   | 82.69   |
| 2                     | X      | X      | X     | .       | 3    | 5.77    |
| 3                     | X      | X      | .     | .       | 4    | 7.69    |
| 4                     | X      | .      | .     | .       | 2    | 3.85    |

| Missing Data Patterns |           |           |          |
|-----------------------|-----------|-----------|----------|
| -----Group Means----- |           |           |          |
| Group                 | Length    | Height    | Width    |
| 1                     | 41.997674 | 12.819512 | 5.359860 |
| 2                     | 38.433333 | 11.797667 | 4.587667 |
| 3                     | 42.275000 | 13.346750 | .        |
| 4                     | 40.150000 | .         | .        |

When you use the DETAILS option, parameters estimated from the observed data and the parameters used in each imputation are displayed in the “Logistic Models for Monotone Method” table in [Output 57.4.4](#).

**Output 57.4.4** Regression Model

| Regression Models for Monotone Method |           |          |                      |          |           |
|---------------------------------------|-----------|----------|----------------------|----------|-----------|
| Imputed Variable                      | Effect    | Obs-Data | -----Imputation----- |          |           |
|                                       |           |          | 1                    | 2        | 3         |
| Width                                 | Intercept | 0.00682  | 0.054140             | 0.018049 | -0.015137 |
| Width                                 | Length    | 0.75519  | 0.838485             | 0.768945 | 0.789577  |
| Width                                 | Height    | 0.73890  | 0.832117             | 0.831748 | 0.809482  |

| Regression Models for Monotone Method |           |                      |          |
|---------------------------------------|-----------|----------------------|----------|
| Imputed Variable                      | Effect    | -----Imputation----- |          |
|                                       |           | 4                    | 5        |
| Width                                 | Intercept | 0.024027             | 0.084643 |
| Width                                 | Length    | 0.728779             | 0.631217 |
| Width                                 | Height    | 0.747734             | 0.745232 |

**Output 57.4.5** Logistic Regression Model

| Logistic Models for Monotone Method |              |           |                      |            |            |
|-------------------------------------|--------------|-----------|----------------------|------------|------------|
| Imputed Variable                    | Effect       | Obs-Data  | -----Imputation----- |            |            |
|                                     |              |           | 1                    | 2          | 3          |
| Species                             | Intercept    | 22.80713  | 22.807129            | 22.807129  | 22.807129  |
| Species                             | Length       | -14.44698 | -14.446980           | -14.446980 | -14.446980 |
| Species                             | Height       | 43.11236  | 43.112363            | 43.112363  | 43.112363  |
| Species                             | Width        | -9.64352  | -9.643524            | -9.643524  | -9.643524  |
| Species                             | Height*Width | -9.73015  | -9.730154            | -9.730154  | -9.730154  |

| Logistic Models for Monotone Method |              |                      |            |  |
|-------------------------------------|--------------|----------------------|------------|--|
| Imputed Variable                    | Effect       | -----Imputation----- |            |  |
|                                     |              | 4                    | 5          |  |
| Species                             | Intercept    | 22.807129            | 22.807129  |  |
| Species                             | Length       | -14.446980           | -14.446980 |  |
| Species                             | Height       | 43.112363            | 43.112363  |  |
| Species                             | Width        | -9.643524            | -9.643524  |  |
| Species                             | Height*Width | -9.730154            | -9.730154  |  |

The following statements list the first 10 observations of the data set outex4 in [Output 57.4.5](#):

```
proc print data=outex4(obs=10);
 title 'First 10 Observations of the Imputed Data Set';
run;
```

**Output 57.4.6** Imputed Data Set

| First 10 Observations of the Imputed Data Set |              |         |        |        |         |  |
|-----------------------------------------------|--------------|---------|--------|--------|---------|--|
| Obs                                           | _Imputation_ | Species | Length | Height | Width   |  |
| 1                                             | 1            | Bream   | 30.0   | 11.520 | 4.02000 |  |
| 2                                             | 1            | Bream   | 31.2   | 12.480 | 4.30600 |  |
| 3                                             | 1            | Bream   | 31.1   | 12.378 | 4.69600 |  |
| 4                                             | 1            | Bream   | 33.5   | 12.730 | 4.45600 |  |
| 5                                             | 1            | Bream   | 34.0   | 12.444 | 4.62964 |  |
| 6                                             | 1            | Bream   | 34.7   | 13.602 | 4.92700 |  |
| 7                                             | 1            | Bream   | 34.5   | 14.180 | 5.27900 |  |
| 8                                             | 1            | Bream   | 35.0   | 12.670 | 4.69000 |  |
| 9                                             | 1            | Bream   | 35.1   | 14.005 | 4.84400 |  |
| 10                                            | 1            | Bream   | 36.2   | 14.227 | 4.95900 |  |

Note that a missing value of the variable Species is not imputed if the corresponding covariates are missing and not imputed, as shown by observation 4 in the table.

## Example 57.5: Monotone Discriminant Function Method for CLASS Variables

This example uses discriminant monotone methods to impute values of a CLASS variable from the observed observation values in a data set with a monotone missing pattern.

The following statements impute the continuous variables Height and Width with the regression method and the classification variable Species with the discriminant function method:

```
proc mi data=Fish2 seed=7545417 nimpute=3 out=outex5;
 class Species;
 monotone reg(Height Width)
 discrim(Species= Length Height Width/ details);
 var Length Height Width Species;
run;
```

The “Model Information” table in [Output 57.5.1](#) describes the method and options used in the multiple imputation process.

**Output 57.5.1** Model Information

| The MI Procedure                 |            |
|----------------------------------|------------|
| Model Information                |            |
| Data Set                         | WORK.FISH2 |
| Method                           | Monotone   |
| Number of Imputations            | 3          |
| Seed for random number generator | 7545417    |

The “Monotone Model Specification” table in [Output 57.5.2](#) describes methods and imputed variables in the imputation model. The procedure uses the regression method to impute the variables Height and Width, and uses the logistic regression method to impute the variable Species in the model.

**Output 57.5.2** Monotone Model Specification

| Monotone Model Specification |                   |
|------------------------------|-------------------|
| Method                       | Imputed Variables |
| Regression                   | Height Width      |
| Discriminant Function        | Species           |

The “Missing Data Patterns” table in [Output 57.5.3](#) lists distinct missing data patterns with corresponding frequencies and percentages. The table confirms a monotone missing pattern for these variables.

**Output 57.5.3** Missing Data Patterns

| Missing Data Patterns |        |        |       |         |      |         |
|-----------------------|--------|--------|-------|---------|------|---------|
| Group                 | Length | Height | Width | Species | Freq | Percent |
| 1                     | X      | X      | X     | X       | 43   | 82.69   |
| 2                     | X      | X      | X     | .       | 3    | 5.77    |
| 3                     | X      | X      | .     | .       | 4    | 7.69    |
| 4                     | X      | .      | .     | .       | 2    | 3.85    |

| Missing Data Patterns |                       |           |          |
|-----------------------|-----------------------|-----------|----------|
| Group                 | -----Group Means----- |           |          |
|                       | Length                | Height    | Width    |
| 1                     | 41.997674             | 12.819512 | 5.359860 |
| 2                     | 38.433333             | 11.797667 | 4.587667 |
| 3                     | 42.275000             | 13.346750 | .        |
| 4                     | 40.150000             | .         | .        |

When you use the DETAILS option, the parameters estimated from the observed data and the parameters used in each imputation are displayed in [Output 57.5.4](#).

**Output 57.5.4** Discriminant Model

| Group Means for Monotone Discriminant Method |          |          |                      |           |           |
|----------------------------------------------|----------|----------|----------------------|-----------|-----------|
| Species                                      | Variable | Obs-Data | -----Imputation----- |           |           |
|                                              |          |          | 1                    | 2         | 3         |
| Bream                                        | Length   | -0.36712 | -0.198907            | -0.375696 | -0.307771 |
| Bream                                        | Height   | 0.64051  | 0.756448             | 0.684845  | 0.658337  |
| Bream                                        | Width    | 0.20882  | 0.465034             | 0.254438  | 0.252637  |
| Pike                                         | Length   | 0.85554  | 0.656521             | 0.677957  | 1.024069  |
| Pike                                         | Height   | -1.31185 | -1.431954            | -1.436355 | -1.119520 |
| Pike                                         | Width    | -0.25768 | -0.381503            | -0.420441 | -0.136188 |

The following statements list the first 10 observations of the data set outex5 in [Output 57.5.5](#). Note that all missing values of the variables Width and Species are imputed.

```
proc print data=outex5(obs=10);
 title 'First 10 Observations of the Imputed Data Set';
run;
```

**Output 57.5.5** Imputed Data Set

| First 10 Observations of the Imputed Data Set |              |         |        |        |         |
|-----------------------------------------------|--------------|---------|--------|--------|---------|
| Obs                                           | _Imputation_ | Species | Length | Height | Width   |
| 1                                             | 1            | Bream   | 30.0   | 11.520 | 4.02000 |
| 2                                             | 1            | Bream   | 31.2   | 12.480 | 4.30600 |
| 3                                             | 1            | Bream   | 31.1   | 12.378 | 4.69600 |
| 4                                             | 1            | Bream   | 33.5   | 12.730 | 4.45600 |
| 5                                             | 1            | Bream   | 34.0   | 12.444 | 4.46687 |
| 6                                             | 1            | Bream   | 34.7   | 13.602 | 4.92700 |
| 7                                             | 1            | Bream   | 34.5   | 14.180 | 5.27900 |
| 8                                             | 1            | Bream   | 35.0   | 12.670 | 4.69000 |
| 9                                             | 1            | Bream   | 35.1   | 14.005 | 4.84400 |
| 10                                            | 1            | Bream   | 36.2   | 14.227 | 4.95900 |

### Example 57.6: FCS Method for Continuous Variables

This example uses FCS regression methods to impute values for all continuous variables in a data set with an arbitrary missing pattern.

The following statements invoke the MI procedure and impute missing values for the Fitness1 data set:

```
proc mi data=Fitness1 seed=1213 nimpute=4 mu0=50 10 180 out=outex6;
 fcs nbiter=20 reg(/details);
 var Oxygen RunTime RunPulse;
run;
```

The NIMPUTE=4 option specifies the total number of imputations. The FCS statement requests multivariate imputations by FCS methods, and the NBITER=20 option (which is the default) specifies the number of burn-in iterations before each imputation.

The “Model Information” table in [Output 57.6.1](#) describes the method and options used in the multiple imputation process.

**Output 57.6.1** Model Information

| The MI Procedure                 |               |
|----------------------------------|---------------|
| Model Information                |               |
| Data Set                         | WORK.FITNESS1 |
| Method                           | FCS           |
| Number of Imputations            | 4             |
| Number of Burn-in Iterations     | 20            |
| Seed for random number generator | 1213          |

The “FCS Model Specification” table in [Output 57.6.2](#) describes methods and imputed variables in the imputation model. With the REG option in the FCS statement, the procedure uses the regression method to

impute variables RunTime, RunPulse, and Oxygen in the model.

**Output 57.6.2** FCS Model Specification

| FCS Model Specification |                   |         |          |
|-------------------------|-------------------|---------|----------|
| Method                  | Imputed Variables |         |          |
| Regression              | Oxygen            | RunTime | RunPulse |

The “Missing Data Patterns” table in [Output 57.6.3](#) lists distinct missing data patterns with corresponding frequencies and percentages.

**Output 57.6.3** Missing Data Patterns

| Missing Data Patterns |        |          |           |      |         |
|-----------------------|--------|----------|-----------|------|---------|
| Group                 | Oxygen | Run Time | Run Pulse | Freq | Percent |
| 1                     | X      | X        | X         | 21   | 67.74   |
| 2                     | X      | X        | .         | 4    | 12.90   |
| 3                     | X      | .        | .         | 3    | 9.68    |
| 4                     | .      | X        | X         | 1    | 3.23    |
| 5                     | .      | X        | .         | 2    | 6.45    |

| Missing Data Patterns |                       |           |            |
|-----------------------|-----------------------|-----------|------------|
| Group                 | -----Group Means----- |           |            |
|                       | Oxygen                | RunTime   | RunPulse   |
| 1                     | 46.353810             | 10.809524 | 171.666667 |
| 2                     | 47.109500             | 10.137500 | .          |
| 3                     | 52.461667             | .         | .          |
| 4                     | .                     | 11.950000 | 176.000000 |
| 5                     | .                     | 9.885000  | .          |

When you use the DETAILS option, the parameters used in each imputation are displayed in [Output 57.6.4](#), [Output 57.6.5](#), and [Output 57.6.6](#).

**Output 57.6.4** FCS Regression Model for Oxygen

| Regression Models for FCS Method |           |                      |           |           |           |
|----------------------------------|-----------|----------------------|-----------|-----------|-----------|
| Imputed Variable                 | Effect    | -----Imputation----- |           |           |           |
|                                  |           | 1                    | 2         | 3         | 4         |
| Oxygen                           | Intercept | -0.132359            | 0.093555  | 0.078587  | 0.063256  |
| Oxygen                           | RunTime   | -0.908663            | -0.753423 | -1.125549 | -0.634844 |
| Oxygen                           | RunPulse  | -0.134745            | 0.052640  | -0.135864 | -0.158692 |

**Output 57.6.5** FCS Regression Model for RunTime

| The MI Procedure                 |           |                      |           |           |           |
|----------------------------------|-----------|----------------------|-----------|-----------|-----------|
| Regression Models for FCS Method |           |                      |           |           |           |
| Imputed Variable                 | Effect    | -----Imputation----- |           |           |           |
|                                  |           | 1                    | 2         | 3         | 4         |
| RunTime                          | Intercept | -0.127880            | -0.125666 | -0.074802 | 0.058724  |
| RunTime                          | Oxygen    | -0.592047            | -1.067554 | -1.020216 | -0.827592 |
| RunTime                          | RunPulse  | 0.110865             | -0.311273 | -0.158049 | 0.060715  |

**Output 57.6.6** FCS Regression Model for RunPulse

| The MI Procedure                 |           |                      |           |           |           |
|----------------------------------|-----------|----------------------|-----------|-----------|-----------|
| Regression Models for FCS Method |           |                      |           |           |           |
| Imputed Variable                 | Effect    | -----Imputation----- |           |           |           |
|                                  |           | 1                    | 2         | 3         | 4         |
| RunPulse                         | Intercept | -0.072862            | -0.089964 | 0.049778  | 0.082088  |
| RunPulse                         | Oxygen    | 0.226951             | -0.439850 | -0.440705 | -0.353438 |
| RunPulse                         | RunTime   | 0.545914             | 0.067482  | 0.234528  | -0.273761 |

The following statements list the first 10 observations of the data set outex6 in [Output 57.6.7](#). Note that all missing values of all variables are imputed.

```
proc print data=outex6(obs=10);
 title 'First 10 Observations of the Imputed Data Set';
run;
```

**Output 57.6.7** Imputed Data Set

| First 10 Observations of the Imputed Data Set |              |         |         |           |
|-----------------------------------------------|--------------|---------|---------|-----------|
| Obs                                           | _Imputation_ | Oxygen  | RunTime | Run Pulse |
| 1                                             | 1            | 44.6090 | 11.3700 | 178.000   |
| 2                                             | 1            | 45.3130 | 10.0700 | 185.000   |
| 3                                             | 1            | 54.2970 | 8.6500  | 156.000   |
| 4                                             | 1            | 59.5710 | 10.1985 | 185.842   |
| 5                                             | 1            | 49.8740 | 9.2200  | 173.379   |
| 6                                             | 1            | 44.8110 | 11.6300 | 176.000   |
| 7                                             | 1            | 44.6299 | 11.9500 | 176.000   |
| 8                                             | 1            | 47.4258 | 10.8500 | 183.926   |
| 9                                             | 1            | 39.4420 | 13.0800 | 174.000   |
| 10                                            | 1            | 60.0550 | 8.6300  | 170.000   |

After the completion of the specified four imputations, the “Variance Information” table in [Output 57.6.8](#) displays the between-imputation variance, within-imputation variance, and total variance for combining complete-data inferences. The relative increase in variance due to missingness, the fraction of missing information, and the relative efficiency for each variable are also displayed. These statistics are described in the section “Combining Inferences from Multiply Imputed Data Sets” on page 4769.

**Output 57.6.8** Variance Information

| Variance Information |                    |          |          |        |
|----------------------|--------------------|----------|----------|--------|
| Variable             | -----Variance----- |          |          | DF     |
|                      | Between            | Within   | Total    |        |
| Oxygen               | 0.044012           | 0.936794 | 0.991809 | 25.911 |
| RunTime              | 0.002518           | 0.063583 | 0.066730 | 26.328 |
| RunPulse             | 3.552893           | 3.488832 | 7.929948 | 5.3995 |

| Variance Information |                               |                              |                     |
|----------------------|-------------------------------|------------------------------|---------------------|
| Variable             | Relative Increase in Variance | Fraction Missing Information | Relative Efficiency |
| Oxygen               | 0.058727                      | 0.057401                     | 0.985853            |
| RunTime              | 0.049500                      | 0.048575                     | 0.988002            |
| RunPulse             | 1.272952                      | 0.630073                     | 0.863917            |

The “Parameter Estimates” table in [Output 57.6.9](#) displays a 95% mean confidence interval and a *t* statistic with its associated *p*-value for each of the hypotheses requested with the MU0= option.

**Output 57.6.9** Parameter Estimates

| Parameter Estimates |            |           |                       |          |        |
|---------------------|------------|-----------|-----------------------|----------|--------|
| Variable            | Mean       | Std Error | 95% Confidence Limits |          | DF     |
| Oxygen              | 47.200681  | 0.995896  | 45.1532               | 49.2481  | 25.911 |
| RunTime             | 10.578418  | 0.258322  | 10.0478               | 11.1091  | 26.328 |
| RunPulse            | 171.368390 | 2.816016  | 164.2877              | 178.4490 | 5.3995 |

| Parameter Estimates |            |            |            |                    |         |
|---------------------|------------|------------|------------|--------------------|---------|
| Variable            | Minimum    | Maximum    | Mu0        | t for H0: Mean=Mu0 | Pr >  t |
| Oxygen              | 47.075129  | 47.512585  | 50.000000  | -2.81              | 0.0093  |
| RunTime             | 10.526891  | 10.627704  | 10.000000  | 2.24               | 0.0338  |
| RunPulse            | 168.633931 | 172.932612 | 180.000000 | -3.07              | 0.0253  |



## Example 57.7: FCS Method for CLASS Variables

This example uses FCS methods to impute missing values in both continuous and CLASS variables in a data set with an arbitrary missing pattern. The following statements invoke the MI procedure and impute missing values for the Fish3 data set:

```
proc mi data=Fish3 seed=1305417 out=outex7;
 class Species;
 fcs nbiter=10 discrim(Species/details) reg(Height/details);
 var Species Length Height Width;
run;
```

The DISCRIM option uses the discriminant function method to impute the classification variable Species, and the REG option uses the regression method to impute the continuous variable Height. By default, the regression method is also used to impute other continuous variables, Length and Width.

The “Model Information” table in [Output 57.7.1](#) describes the method and options used in the multiple imputation process.

**Output 57.7.1** Model Information

| The MI Procedure                 |            |
|----------------------------------|------------|
| Model Information                |            |
| Data Set                         | WORK.FISH3 |
| Method                           | FCS        |
| Number of Imputations            | 5          |
| Number of Burn-in Iterations     | 10         |
| Seed for random number generator | 1305417    |

The “FCS Model Specification” table in [Output 57.7.2](#) describes methods and imputed variables in the imputation model. The procedure uses the discriminant function method to impute the variable Species, and the regression method to impute other variables.

**Output 57.7.2** FCS Model Specification

| FCS Model Specification |                     |
|-------------------------|---------------------|
| Method                  | Imputed Variables   |
| Regression              | Length Height Width |
| Discriminant Function   | Species             |

The “Missing Data Patterns” table in [Output 57.7.3](#) lists distinct missing data patterns with corresponding frequencies and percentages.

**Output 57.7.3** Missing Data Patterns

| Missing Data Patterns |         |        |        |       |      |         |
|-----------------------|---------|--------|--------|-------|------|---------|
| Group                 | Species | Length | Height | Width | Freq | Percent |
| 1                     | X       | X      | X      | X     | 38   | 73.08   |
| 2                     | X       | .      | X      | X     | 2    | 3.85    |
| 3                     | X       | .      | X      | .     | 1    | 1.92    |
| 4                     | .       | X      | X      | X     | 3    | 5.77    |
| 5                     | .       | X      | X      | .     | 3    | 5.77    |
| 6                     | .       | X      | .      | X     | 2    | 3.85    |
| 7                     | .       | X      | .      | .     | 2    | 3.85    |
| 8                     | .       | .      | X      | .     | 1    | 1.92    |

| Missing Data Patterns |           |           |          |
|-----------------------|-----------|-----------|----------|
| -----Group Means----- |           |           |          |
| Group                 | Length    | Height    | Width    |
| 1                     | 41.515789 | 12.531526 | 5.266474 |
| 2                     | .         | 14.448000 | 6.886000 |
| 3                     | .         | 18.037000 | .        |
| 4                     | 38.433333 | 11.797667 | 4.587667 |
| 5                     | 45.033333 | 13.647667 | .        |
| 6                     | 36.100000 | .         | 5.135000 |
| 7                     | 40.150000 | .         | .        |
| 8                     | .         | 12.444000 | .        |

With the specified DETAILS option for variables Species and Height, parameters used in each imputation for these two variables are displayed in the “Group Means for FCS Discriminant Method” table in [Output 57.7.4](#) and in the “Regression Models for FCS Method” table in [Output 57.7.5](#).

**Output 57.7.4** FCS Discrim Model for Species

| Group Means for FCS Discriminant Method |          |                      |           |           |           |
|-----------------------------------------|----------|----------------------|-----------|-----------|-----------|
| Species                                 | Variable | -----Imputation----- |           |           |           |
|                                         |          | 1                    | 2         | 3         | 4         |
| Bream                                   | Length   | -0.635560            | -0.539102 | -0.183231 | -0.312298 |
| Bream                                   | Height   | 0.505922             | 0.540880  | 0.761373  | 0.736716  |
| Bream                                   | Width    | -0.203055            | 0.030787  | 0.403116  | 0.422214  |
| Pike                                    | Length   | 1.074270             | 0.904169  | 0.409041  | 1.234640  |
| Pike                                    | Height   | -1.293411            | -1.359962 | -1.418251 | -1.177828 |
| Pike                                    | Width    | 0.060791             | -0.463132 | -0.702662 | 0.004479  |

| Group Means for FCS Discriminant Method |          |                      |  |
|-----------------------------------------|----------|----------------------|--|
| Species                                 | Variable | -----Imputation----- |  |
|                                         |          | 5                    |  |
| Bream                                   | Length   | -0.501390            |  |
| Bream                                   | Height   | 0.582379             |  |
| Bream                                   | Width    | 0.080807             |  |
| Pike                                    | Length   | 0.479436             |  |
| Pike                                    | Height   | -1.428490            |  |
| Pike                                    | Width    | -0.659505            |  |

**Output 57.7.5** FCS Regression Model for Height

| Regression Models for FCS Method |           |         |                      |           |           |
|----------------------------------|-----------|---------|----------------------|-----------|-----------|
| Imputed Variable                 | Effect    | Species | -----Imputation----- |           |           |
|                                  |           |         | 1                    | 2         | 3         |
| Height                           | Intercept |         | -0.366066            | -0.359325 | -0.272079 |
| Height                           | Species   | Bream   | 0.973036             | 0.980092  | 0.818649  |
| Height                           | Length    |         | 0.170407             | 0.099879  | -0.018424 |
| Height                           | Width     |         | 0.242966             | 0.382906  | 0.430107  |

| Regression Models for FCS Method |           |                      |           |  |
|----------------------------------|-----------|----------------------|-----------|--|
| Imputed Variable                 | Effect    | -----Imputation----- |           |  |
|                                  |           | 4                    | 5         |  |
| Height                           | Intercept | -0.353772            | -0.357781 |  |
| Height                           | Species   | 1.035374             | 0.963826  |  |
| Height                           | Length    | 0.187469             | 0.090964  |  |
| Height                           | Width     | 0.299173             | 0.325195  |  |

The following statements list the first 10 observations of the data set outex7 in Output 57.7.6:

```
proc print data=outex7(obs=10);
 title 'First 10 Observations of the Imputed Data Set';
run;
```

**Output 57.7.6** Imputed Data Set

| First 10 Observations of the Imputed Data Set |              |         |         |         |         |
|-----------------------------------------------|--------------|---------|---------|---------|---------|
| Obs                                           | _Imputation_ | Species | Length  | Height  | Width   |
| 1                                             | 1            | Bream   | 30.0000 | 11.5200 | 4.02000 |
| 2                                             | 1            | Bream   | 31.2000 | 12.4800 | 4.30600 |
| 3                                             | 1            | Bream   | 31.1000 | 12.3780 | 4.69600 |
| 4                                             | 1            | Bream   | 33.5000 | 12.7300 | 4.45600 |
| 5                                             | 1            | Pike    | 68.6009 | 12.4440 | 7.65040 |
| 6                                             | 1            | Bream   | 34.7000 | 13.6020 | 4.92700 |
| 7                                             | 1            | Bream   | 34.5000 | 14.1800 | 5.27900 |
| 8                                             | 1            | Pike    | 35.0000 | 5.7684  | 4.69000 |
| 9                                             | 1            | Bream   | 35.1000 | 14.0050 | 4.84400 |
| 10                                            | 1            | Bream   | 36.2000 | 14.2270 | 4.95900 |

After the completion of five imputations by default, the “Variance Information” table in [Output 57.7.7](#) displays the between-imputation variance, within-imputation variance, and total variance for combining complete-data inferences for continuous variables. The relative increase in variance due to missingness, the fraction of missing information, and the relative efficiency for each variable are also displayed. These statistics are described in the section “[Combining Inferences from Multiply Imputed Data Sets](#)” on page 4769.

**Output 57.7.7** Variance Information

| Variance Information |                    |          |          |        |
|----------------------|--------------------|----------|----------|--------|
| Variable             | -----Variance----- |          |          | DF     |
|                      | Between            | Within   | Total    |        |
| Length               | 0.076551           | 1.351968 | 1.443828 | 43.942 |
| Height               | 0.024597           | 0.311347 | 0.340863 | 41.379 |
| Width                | 0.000307           | 0.015361 | 0.015730 | 47.645 |

| Variance Information |                               |                              |                     |
|----------------------|-------------------------------|------------------------------|---------------------|
| Variable             | Relative Increase in Variance | Fraction Missing Information | Relative Efficiency |
| Length               | 0.067946                      | 0.065513                     | 0.987067            |
| Height               | 0.094801                      | 0.089997                     | 0.982319            |
| Width                | 0.024018                      | 0.023723                     | 0.995278            |

The “Parameter Estimates” table in [Output 57.7.8](#) displays a 95% mean confidence interval and a  $t$  statistic with its associated  $p$ -value for each of the hypotheses requested with the default  $\text{MU0}=0$  option.

**Output 57.7.8** Parameter Estimates

| Parameter Estimates |           |           |                       |          |        |
|---------------------|-----------|-----------|-----------------------|----------|--------|
| Variable            | Mean      | Std Error | 95% Confidence Limits |          | DF     |
| Length              | 41.952213 | 1.201594  | 39.53047              | 44.37396 | 43.942 |
| Height              | 12.785938 | 0.583835  | 11.60719              | 13.96469 | 41.379 |
| Width               | 5.345132  | 0.125420  | 5.09291               | 5.59735  | 47.645 |

| Parameter Estimates |           |           |           |          |         |
|---------------------|-----------|-----------|-----------|----------|---------|
| Variable            | Minimum   | Maximum   | t for H0: |          |         |
|                     |           |           | Mu0       | Mean=Mu0 | Pr >  t |
| Length              | 41.702410 | 42.286360 | 0         | 34.91    | <.0001  |
| Height              | 12.555560 | 12.988405 | 0         | 21.90    | <.0001  |
| Width               | 5.324639  | 5.366759  | 0         | 42.62    | <.0001  |

### Example 57.8: FCS Method with Trace Plot

This example uses FCS methods to impute missing values in both continuous and classification variables in a data set with an arbitrary missing pattern. The following statements use a logistic regression method to impute values of the classification variable Species:

```
ods graphics on;
proc mi data=Fish3 seed=1305417 out=outex8;
 class Species;
 fcs plots=trace
 logistic(Species= Height Width Height*Width /details);
 var Species Height Width;
run;
ods graphics off;
```

The “Model Information” table in [Output 57.8.1](#) describes the method and options used in the multiple imputation process. By default, a regression method is used to impute missing values in each continuous variable.

**Output 57.8.1** Model Information

| The MI Procedure                 |            |
|----------------------------------|------------|
| Model Information                |            |
| Data Set                         | WORK.FISH3 |
| Method                           | FCS        |
| Number of Imputations            | 5          |
| Number of Burn-in Iterations     | 20         |
| Seed for random number generator | 1305417    |

The “FCS Model Specification” table in [Output 57.8.2](#) describes methods and imputed variables in the imputation model. The procedure uses the logistic regression method to impute the variable Species, and the regression method to impute variables Height and Width.

**Output 57.8.2** FCS Model Specification

| FCS Model Specification |                   |
|-------------------------|-------------------|
| Method                  | Imputed Variables |
| Regression              | Height Width      |
| Logistic Regression     | Species           |

The “Missing Data Patterns” table in [Output 57.8.3](#) lists distinct missing data patterns with corresponding frequencies and percentages.

**Output 57.8.3** Missing Data Patterns

| Missing Data Patterns |         |        |       |      |         |                       |          |
|-----------------------|---------|--------|-------|------|---------|-----------------------|----------|
| Group                 | Species | Height | Width | Freq | Percent | -----Group Means----- |          |
|                       |         |        |       |      |         | Height                | Width    |
| 1                     | X       | X      | X     | 40   | 76.92   | 12.627350             | 5.347450 |
| 2                     | X       | X      | .     | 1    | 1.92    | 18.037000             | .        |
| 3                     | .       | X      | X     | 3    | 5.77    | 11.797667             | 4.587667 |
| 4                     | .       | X      | .     | 4    | 7.69    | 13.346750             | .        |
| 5                     | .       | .      | X     | 2    | 3.85    | .                     | 5.135000 |
| 6                     | O       | O      | O     | 2    | 3.85    | .                     | .        |

When you use the DETAILS keyword in the LOGISTIC option, parameters estimated from the observed data and the parameters used in each imputation are displayed in the “Logistic Models for FCS Method” table in [Output 57.8.4](#).

**Output 57.8.4** FCS Logistic Regression Model for Species

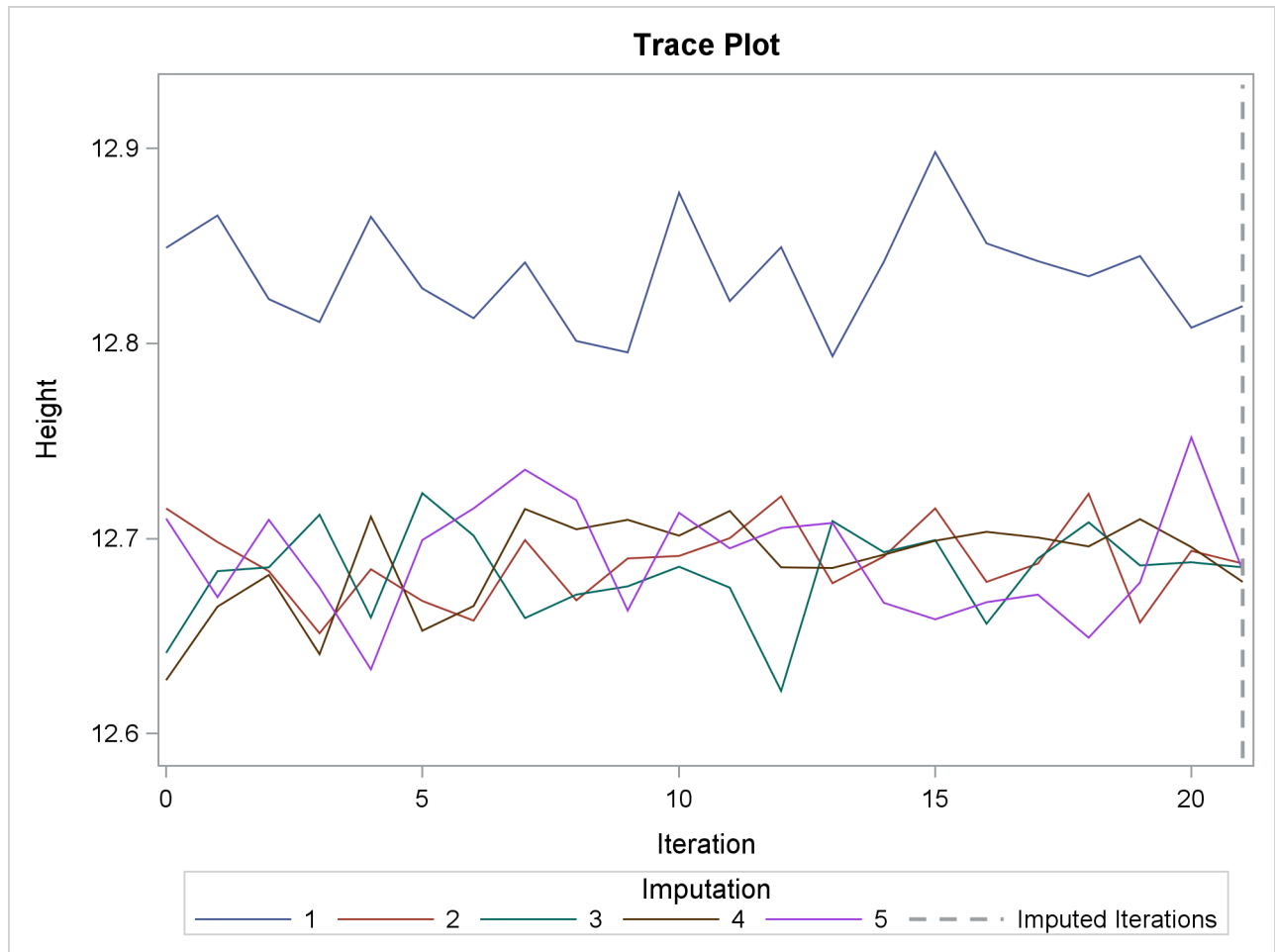
| Logistic Models for FCS Method |              |                      |            |            |            |
|--------------------------------|--------------|----------------------|------------|------------|------------|
| Imputed<br>Variable            | Effect       | -----Imputation----- |            |            |            |
|                                |              | 1                    | 2          | 3          | 4          |
| Species                        | Intercept    | 27.250540            | 27.240843  | 27.242699  | 27.254682  |
| Species                        | Height       | 59.970974            | 59.962249  | 59.964027  | 59.980855  |
| Species                        | Width        | -26.032805           | -26.021304 | -26.023556 | -26.028866 |
| Species                        | Height*Width | -6.760308            | -6.739118  | -6.742934  | -6.754780  |

| Logistic Models for FCS Method |              |                   |
|--------------------------------|--------------|-------------------|
| Imputed<br>Variable            | Effect       | -Imputation-<br>5 |
| Species                        | Intercept    | 27.251468         |
| Species                        | Height       | 59.971742         |
| Species                        | Width        | -26.033865        |
| Species                        | Height*Width | -6.762477         |

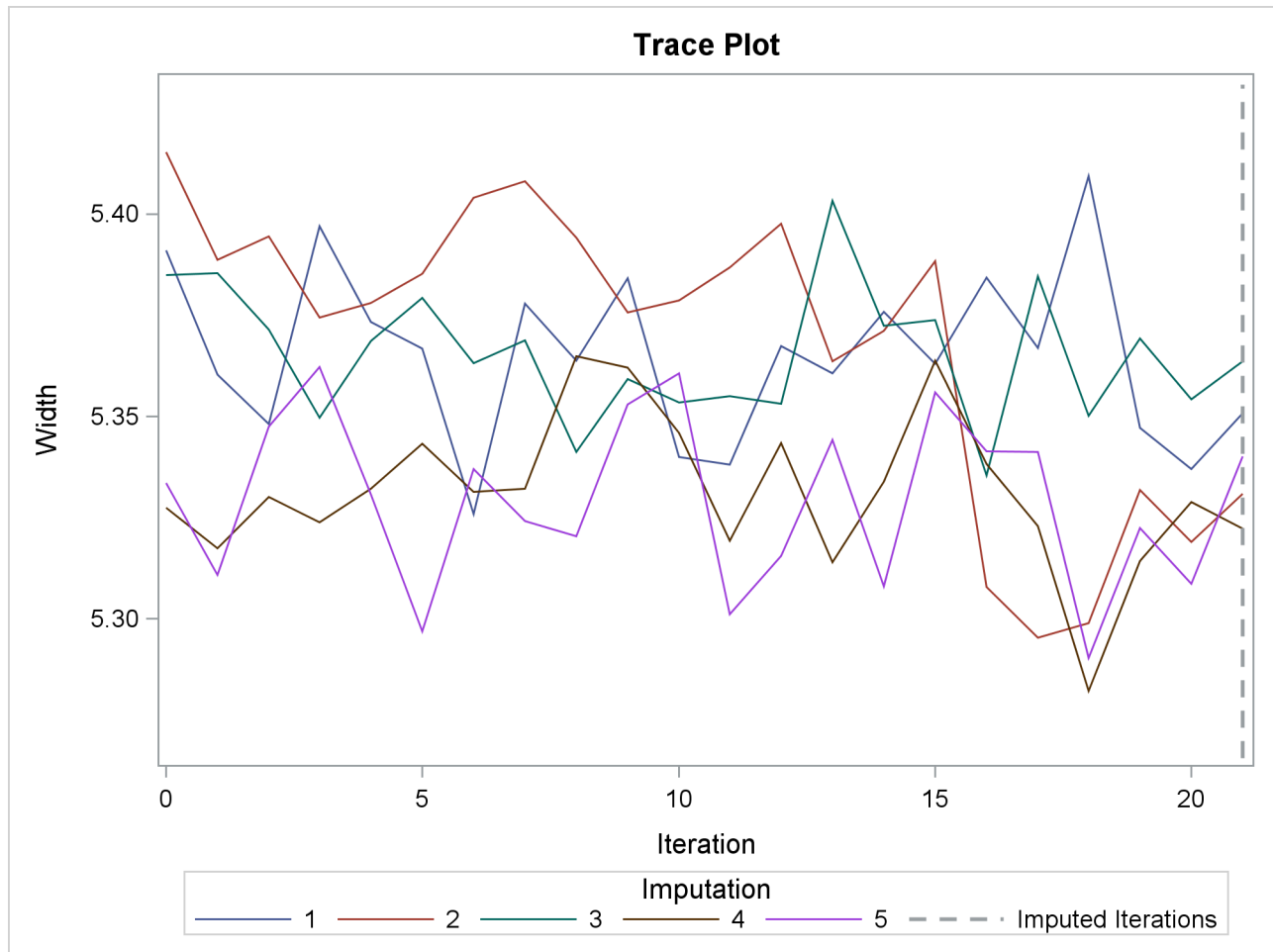
With ODS Graphics enabled, the PLOTS=TRACE option displays trace plots of means for all continuous variables by default, as shown in [Output 57.8.5](#) and [Output 57.8.6](#). The dashed vertical lines indicate the imputed iterations—that is, the variable values used in the imputations. The plot shows no apparent trends for the two variables.

Output 57.8.5 Trace Plot for Height





Output 57.8.6 Trace Plot for Width



The following statements list the first 10 observations of the data set outex8 in Output 57.8.7:

```
proc print data=outex8(obs=10);
 title 'First 10 Observations of the Imputed Data Set';
run;
```

**Output 57.8.7** Imputed Data Set

| First 10 Observations of the Imputed Data Set |              |         |         |         |         |
|-----------------------------------------------|--------------|---------|---------|---------|---------|
| Obs                                           | _Imputation_ | Species | Length  | Height  | Width   |
| 1                                             | 1            | Bream   | 30.0000 | 11.5200 | 4.02000 |
| 2                                             | 1            | Bream   | 31.2000 | 12.4800 | 4.30600 |
| 3                                             | 1            | Bream   | 31.1000 | 12.3780 | 4.69600 |
| 4                                             | 1            | Bream   | 33.5000 | 12.7300 | 4.45600 |
| 5                                             | 1            | Pike    | 68.0455 | 12.4440 | 6.46920 |
| 6                                             | 1            | Bream   | 34.7000 | 13.6020 | 4.92700 |
| 7                                             | 1            | Bream   | 34.5000 | 14.1800 | 5.27900 |
| 8                                             | 1            | Pike    | 35.0000 | 4.9290  | 4.69000 |
| 9                                             | 1            | Bream   | 35.1000 | 14.0050 | 4.84400 |
| 10                                            | 1            | Bream   | 36.2000 | 14.2270 | 4.95900 |

After the completion of five imputations by default, the “Variance Information” table in [Output 57.8.8](#) displays the between-imputation variance, within-imputation variance, and total variance for combining complete-data inferences for continuous variables. The relative increase in variance due to missingness, the fraction of missing information, and the relative efficiency for each variable are also displayed. These statistics are described in the section “[Combining Inferences from Multiply Imputed Data Sets](#)” on page 4769.

**Output 57.8.8** Variance Information

| Variance Information |                    |          |          |        |
|----------------------|--------------------|----------|----------|--------|
| Variable             | -----Variance----- |          |          | DF     |
|                      | Between            | Within   | Total    |        |
| Height               | 0.003691           | 0.318783 | 0.322474 | 46.369 |
| Width                | 0.001464           | 0.017777 | 0.019241 | 39.458 |

| Variance Information |                               |                              |                     |
|----------------------|-------------------------------|------------------------------|---------------------|
| Variable             | Relative Increase in Variance | Fraction Missing Information | Relative Efficiency |
| Height               | 0.013894                      | 0.013797                     | 0.997248            |
| Width                | 0.098807                      | 0.093580                     | 0.981628            |

The “Parameter Estimates” table in [Output 57.8.9](#) displays a 95% mean confidence interval and a  $t$  statistic with its associated  $p$ -value for each of the hypotheses requested with the default  $\text{MU0}=0$  option.

**Output 57.8.9** Parameter Estimates

| Parameter Estimates |           |           |                       |          |        |
|---------------------|-----------|-----------|-----------------------|----------|--------|
| Variable            | Mean      | Std Error | 95% Confidence Limits |          | DF     |
| Height              | 12.710577 | 0.568517  | 11.56646              | 13.85470 | 46.369 |
| Width               | 5.331652  | 0.139764  | 5.04906               | 5.61425  | 39.458 |

| Parameter Estimates |           |           |     |                       |         |
|---------------------|-----------|-----------|-----|-----------------------|---------|
| Variable            | Minimum   | Maximum   | Mu0 | t for H0:<br>Mean=Mu0 | Pr >  t |
| Height              | 12.677842 | 12.819080 | 0   | 22.36                 | <.0001  |
| Width               | 5.287861  | 5.393360  | 0   | 38.15                 | <.0001  |

### Example 57.9: MCMC Method

This example uses the MCMC method to impute missing values for a data set with an arbitrary missing pattern. The following statements invoke the MI procedure and specify the MCMC method with six imputations:

```
proc mi data=Fitness1 seed=21355417 nimpute=6 mu0=50 10 180 ;
 mcmc chain=multiple displayinit initial=em(itprint);
 var Oxygen RunTime RunPulse;
run;
```

The “Model Information” table in [Output 57.9.1](#) describes the method used in the multiple imputation process. When you use the `CHAIN=MULTIPLE` option, the procedure uses multiple chains and completes the default 200 burn-in iterations before each imputation. The 200 burn-in iterations are used to make the iterations converge to the stationary distribution before the imputation.

**Output 57.9.1** Model Information

| The MI Procedure                 |                   |
|----------------------------------|-------------------|
| Model Information                |                   |
| Data Set                         | WORK.FITNESS1     |
| Method                           | MCMC              |
| Multiple Imputation Chain        | Multiple Chains   |
| Initial Estimates for MCMC       | EM Posterior Mode |
| Start                            | Starting Value    |
| Prior                            | Jeffreys          |
| Number of Imputations            | 6                 |
| Number of Burn-in Iterations     | 200               |
| Seed for random number generator | 21355417          |

By default, the procedure uses a noninformative Jeffreys prior to derive the posterior mode from the EM algorithm as the starting values for the MCMC method.

The “Missing Data Patterns” table in [Output 57.9.2](#) lists distinct missing data patterns with corresponding statistics.

**Output 57.9.2** Missing Data Patterns

| Missing Data Patterns |        |          |           |      |         |
|-----------------------|--------|----------|-----------|------|---------|
| Group                 | Oxygen | Run Time | Run Pulse | Freq | Percent |
| 1                     | X      | X        | X         | 21   | 67.74   |
| 2                     | X      | X        | .         | 4    | 12.90   |
| 3                     | X      | .        | .         | 3    | 9.68    |
| 4                     | .      | X        | X         | 1    | 3.23    |
| 5                     | .      | X        | .         | 2    | 6.45    |

| Missing Data Patterns |           |           |            |
|-----------------------|-----------|-----------|------------|
| -----Group Means----- |           |           |            |
| Group                 | Oxygen    | RunTime   | RunPulse   |
| 1                     | 46.353810 | 10.809524 | 171.666667 |
| 2                     | 47.109500 | 10.137500 | .          |
| 3                     | 52.461667 | .         | .          |
| 4                     | .         | 11.950000 | 176.000000 |
| 5                     | .         | 9.885000  | .          |

When you use the `ITPRINT` option within the `INITIAL=EM` option, the procedure displays the “EM (Posterior Mode) Iteration History” table in [Output 57.9.3](#).

**Output 57.9.3** EM (Posterior Mode) Iteration History

| EM (Posterior Mode) Iteration History |                 |                         |               |                |
|---------------------------------------|-----------------|-------------------------|---------------|----------------|
| <u>_Iteration_</u>                    | <u>-2 Log L</u> | <u>-2 Log Posterior</u> | <u>Oxygen</u> | <u>RunTime</u> |
| 0                                     | 254.482800      | 282.909549              | 47.104077     | 10.554858      |
| 1                                     | 255.081168      | 282.051584              | 47.104077     | 10.554857      |
| 2                                     | 255.271408      | 282.017488              | 47.104077     | 10.554857      |
| 3                                     | 255.318622      | 282.015372              | 47.104002     | 10.554523      |
| 4                                     | 255.330259      | 282.015232              | 47.103861     | 10.554388      |
| 5                                     | 255.333161      | 282.015222              | 47.103797     | 10.554341      |
| 6                                     | 255.333896      | 282.015222              | 47.103774     | 10.554325      |
| 7                                     | 255.334085      | 282.015222              | 47.103766     | 10.554320      |

| EM (Posterior Mode) Iteration History |                 |
|---------------------------------------|-----------------|
| <u>_Iteration_</u>                    | <u>RunPulse</u> |
| 0                                     | 171.381669      |
| 1                                     | 171.381652      |
| 2                                     | 171.381644      |
| 3                                     | 171.381842      |
| 4                                     | 171.382053      |
| 5                                     | 171.382150      |
| 6                                     | 171.382185      |
| 7                                     | 171.382196      |

When you use the DISPLAYINIT option in the MCMC statement, the “Initial Parameter Estimates for MCMC” table in [Output 57.9.4](#) displays the starting mean and covariance estimates used in the MCMC method. The same starting estimates are used in the MCMC method for multiple chains because the EM algorithm is applied to the same data set in each chain. You can explicitly specify different initial estimates for different imputations, or you can use the bootstrap method to generate different parameter estimates from the EM algorithm for the MCMC method.

**Output 57.9.4** Initial Parameter Estimates

| Initial Parameter Estimates for MCMC |               |               |                |                 |
|--------------------------------------|---------------|---------------|----------------|-----------------|
| <u>_TYPE_</u>                        | <u>_NAME_</u> | <u>Oxygen</u> | <u>RunTime</u> | <u>RunPulse</u> |
| MEAN                                 |               | 47.103766     | 10.554320      | 171.382196      |
| COV                                  | Oxygen        | 24.549967     | -5.726112      | -15.926036      |
| COV                                  | RunTime       | -5.726112     | 1.781407       | 3.124798        |
| COV                                  | RunPulse      | -15.926036    | 3.124798       | 83.164045       |

[Output 57.9.5](#) and [Output 57.9.6](#) display variance information and parameter estimates, respectively, from the multiple imputation.

**Output 57.9.5** Variance Information

| Variance Information |                    |          |          |        |
|----------------------|--------------------|----------|----------|--------|
| Variable             | -----Variance----- |          |          | DF     |
|                      | Between            | Within   | Total    |        |
| Oxygen               | 0.051560           | 0.928170 | 0.988323 | 25.958 |
| RunTime              | 0.003979           | 0.070057 | 0.074699 | 25.902 |
| RunPulse             | 4.118578           | 4.260631 | 9.065638 | 7.5938 |

| Variance Information |             |             |          |
|----------------------|-------------|-------------|----------|
| Variable             | Relative    | Fraction    | Relative |
|                      | Increase    | Missing     |          |
|                      | in Variance | Information |          |
| Oxygen               | 0.064809    | 0.062253    | 0.989731 |
| RunTime              | 0.066262    | 0.063589    | 0.989513 |
| RunPulse             | 1.127769    | 0.575218    | 0.912517 |

**Output 57.9.6** Parameter Estimates

| Parameter Estimates |            |           |                       |          |        |
|---------------------|------------|-----------|-----------------------|----------|--------|
| Variable            | Mean       | Std Error | 95% Confidence Limits |          | DF     |
| Oxygen              | 47.164819  | 0.994145  | 45.1212               | 49.2085  | 25.958 |
| RunTime             | 10.549936  | 0.273312  | 9.9880                | 11.1118  | 25.902 |
| RunPulse            | 170.969836 | 3.010920  | 163.9615              | 177.9782 | 7.5938 |

| Parameter Estimates |            |            |            |           |         |
|---------------------|------------|------------|------------|-----------|---------|
| Variable            | Minimum    | Maximum    | Mu0        | t for H0: | Pr >  t |
|                     |            |            |            | Mean=Mu0  |         |
| Oxygen              | 46.858020  | 47.363540  | 50.000000  | -2.85     | 0.0084  |
| RunTime             | 10.476886  | 10.659412  | 10.000000  | 2.01      | 0.0547  |
| RunPulse            | 168.252615 | 172.894991 | 180.000000 | -3.00     | 0.0182  |

**Example 57.10: Producing Monotone Missingness with MCMC**

This example uses the MCMC method to impute just enough missing values for a data set with an arbitrary missing pattern so that each imputed data set has a monotone missing pattern based on the order of variables in the VAR statement.

The following statements invoke the MI procedure and specify the IMPUTE=MONOTONE option to create the imputed data set with a monotone missing pattern. You must specify a VAR statement to provide the order of variables in order for the imputed data to achieve a monotone missing pattern.

```
proc mi data=Fitness1 seed=17655417 out=outex10;
 mcmc impute=monotone;
 var Oxygen RunTime RunPulse;
run;
```

The “Model Information” table in [Output 57.10.1](#) describes the method used in the multiple imputation process.

#### Output 57.10.1 Model Information

| The MI Procedure                 |                    |
|----------------------------------|--------------------|
| Model Information                |                    |
| Data Set                         | WORK.FITNESS1      |
| Method                           | Monotone-data MCMC |
| Multiple Imputation Chain        | Single Chain       |
| Initial Estimates for MCMC       | EM Posterior Mode  |
| Start                            | Starting Value     |
| Prior                            | Jeffreys           |
| Number of Imputations            | 5                  |
| Number of Burn-in Iterations     | 200                |
| Number of Iterations             | 100                |
| Seed for random number generator | 17655417           |

The “Missing Data Patterns” table in [Output 57.10.2](#) lists distinct missing data patterns with corresponding statistics. Here, an “X” means that the variable is observed in the corresponding group, a “.” means that the variable is missing and will be imputed to achieve the monotone missingness for the imputed data set, and an “O” means that the variable is missing and will not be imputed. The table also displays group-specific variable means.

**Output 57.10.2** Missing Data Patterns

| Missing Data Patterns |        |          |           |      |         |
|-----------------------|--------|----------|-----------|------|---------|
| Group                 | Oxygen | Run Time | Run Pulse | Freq | Percent |
| 1                     | X      | X        | X         | 21   | 67.74   |
| 2                     | X      | X        | O         | 4    | 12.90   |
| 3                     | X      | O        | O         | 3    | 9.68    |
| 4                     | .      | X        | X         | 1    | 3.23    |
| 5                     | .      | X        | O         | 2    | 6.45    |

| Missing Data Patterns |                       |           |            |
|-----------------------|-----------------------|-----------|------------|
| Group                 | -----Group Means----- |           |            |
|                       | Oxygen                | RunTime   | RunPulse   |
| 1                     | 46.353810             | 10.809524 | 171.666667 |
| 2                     | 47.109500             | 10.137500 | .          |
| 3                     | 52.461667             | .         | .          |
| 4                     | .                     | 11.950000 | 176.000000 |
| 5                     | .                     | 9.885000  | .          |

As shown in the table in [Output 57.10.2](#), the MI procedure needs to impute only three missing values from group 4 and group 5 to achieve a monotone missing pattern for the imputed data set.

When you use the MCMC method to produce an imputed data set with a monotone missing pattern, tables of variance information and parameter estimates are not created.

The following statements are used just to show the monotone missingness of the output data set outex10:

```
proc mi data=outex10 seed=15541 nimpute=0;
 var Oxygen RunTime RunPulse;
run;
```



The “Missing Data Patterns” table in [Output 57.10.3](#) displays a monotone missing data pattern.

**Output 57.10.3** Monotone Missing Data Patterns

| The MI Procedure      |        |          |           |      |         |
|-----------------------|--------|----------|-----------|------|---------|
| Missing Data Patterns |        |          |           |      |         |
| Group                 | Oxygen | Run Time | Run Pulse | Freq | Percent |
| 1                     | X      | X        | X         | 110  | 70.97   |
| 2                     | X      | X        | .         | 30   | 19.35   |
| 3                     | X      | .        | .         | 15   | 9.68    |

| Missing Data Patterns |           |           |            |
|-----------------------|-----------|-----------|------------|
| -----Group Means----- |           |           |            |
| Group                 | Oxygen    | RunTime   | RunPulse   |
| 1                     | 46.152428 | 10.861364 | 171.863636 |
| 2                     | 47.796038 | 10.053333 | .          |
| 3                     | 52.461667 | .         | .          |

The following statements impute one value for each missing value in the monotone missingness data set outex10:

```
proc mi data=outex10 nimpute=1 seed=51343672 out=outex10a;
 monotone method=reg;
 var Oxygen RunTime RunPulse;
 by _Imputation_;
run;
```

You can then analyze these data sets by using other SAS procedures and combine these results by using the MIANALYZE procedure. Note that the VAR statement is required with a MONOTONE statement to provide the variable order for the monotone missing pattern.

---

## Example 57.11: Checking Convergence in MCMC

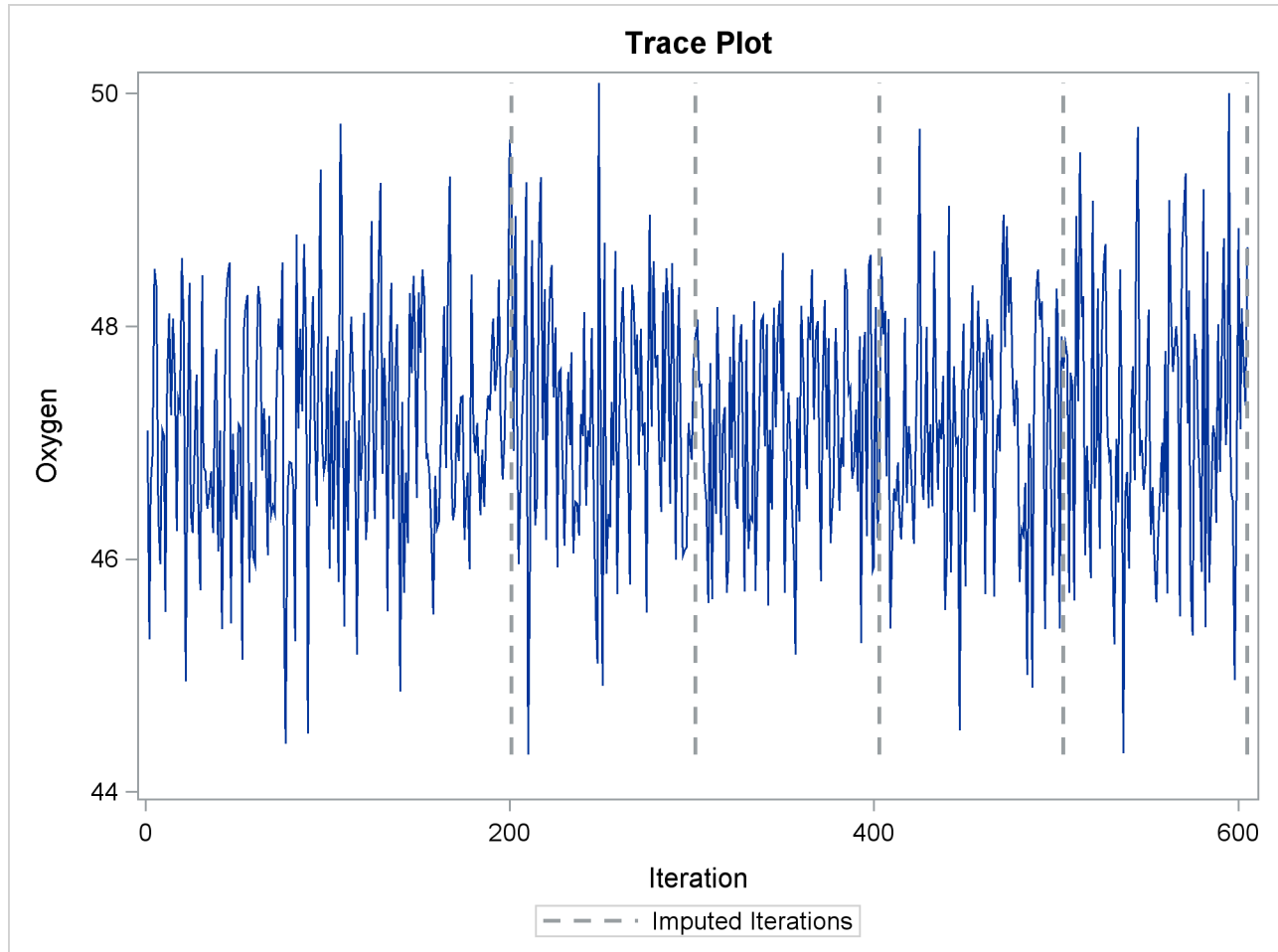
This example uses the MCMC method with a single chain. It also displays trace and autocorrelation plots to check convergence for the single chain.

The following statements use the MCMC method to create an iteration plot for the successive estimates of the mean of Oxygen. These statements also create an autocorrelation function plot for the variable Oxygen.

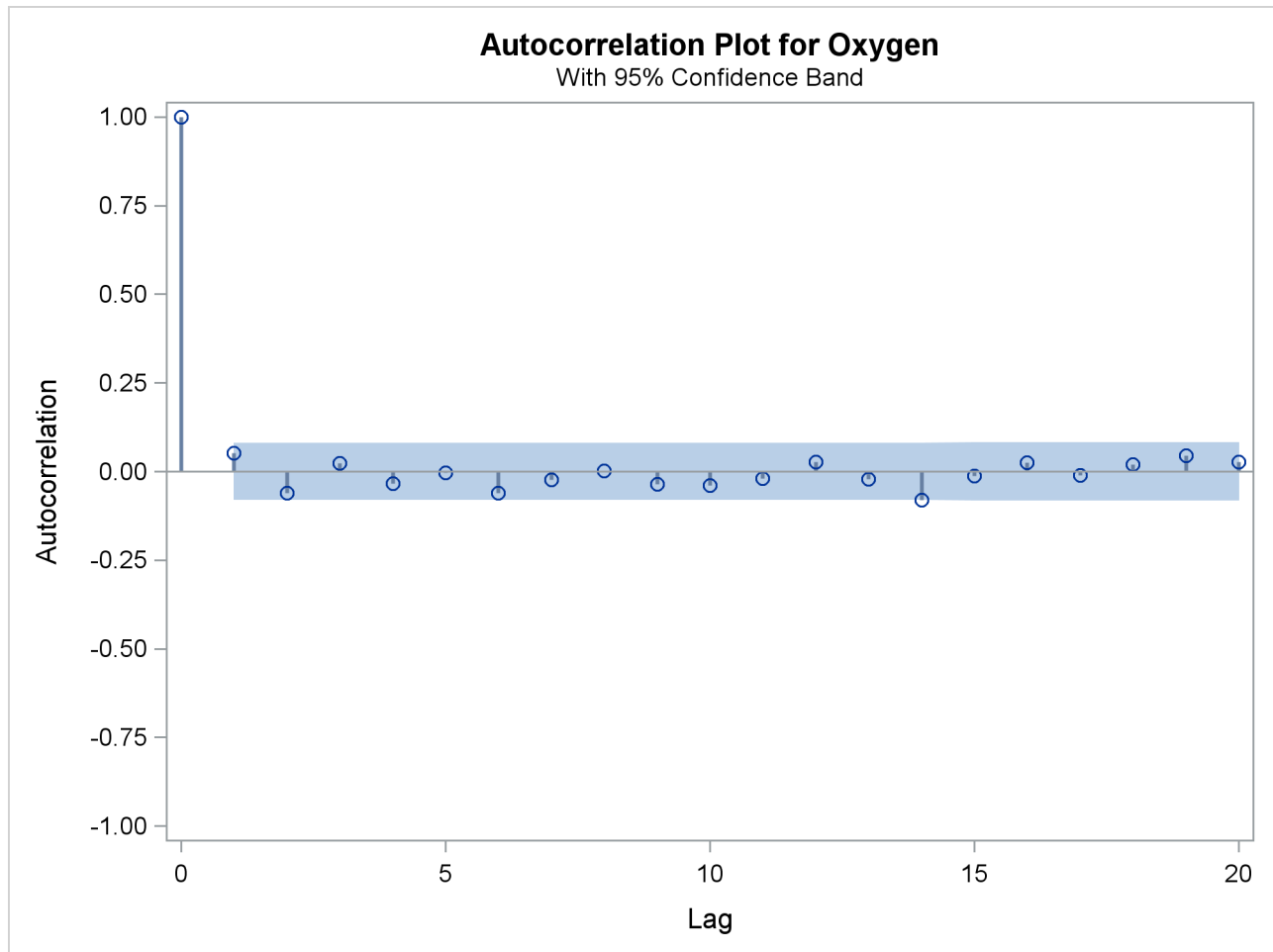
```
ods graphics on;
proc mi data=Fitness1 seed=501213 mu0=50 10 180;
 mcmc plots=(trace(mean(Oxygen)) acf(mean(Oxygen)));
 var Oxygen RunTime RunPulse;
run;
ods graphics off;
```

With ODS Graphics enabled, the TRACE(MEAN(OXYGEN)) option in the PLOTS= option displays the trace plot of means for the variable Oxygen, as shown in [Output 57.11.1](#). The dashed vertical lines indicate the imputed iterations—that is, the Oxygen values used in the imputations. The plot shows no apparent trends for the variable Oxygen.

**Output 57.11.1** Trace Plot for Oxygen



The ACF(MEAN(OXYGEN)) option in the PLOTS= option displays the autocorrelation plot of means for the variable Oxygen, as shown in [Output 57.11.2](#). The autocorrelation function plot shows no significant positive or negative autocorrelation.

**Output 57.11.2** Autocorrelation Function Plot for Oxygen

You can also create plots for the worst linear function, the means of other variables, the variances of variables, and the covariances between variables. Alternatively, you can use the `OUTITER` option to save statistics such as the means, standard deviations, covariances,  $-2 \log LR$  statistic,  $-2 \log LR$  statistic of the posterior mode, and worst linear function from each iteration in an output data set. Then you can do a more in-depth trace (time series) analysis of the iterations with other procedures, such as `PROC AUTOREG` and `PROC ARIMA` in the *SAS/ETS User's Guide*.

For general information about ODS Graphics, see Chapter 21, “[Statistical Graphics Using ODS](#).” For specific information about the graphics available in the MI procedure, see the section “[ODS Graphics](#)” on page 4775.

## Example 57.12: Saving and Using Parameters for MCMC

This example uses the MCMC method with multiple chains as specified in [Example 57.9](#). It saves the parameter values used for each imputation in an output data set of type EST called `miest`. This output data set can then be used to impute missing values in other similar input data sets. The following statements invoke the MI procedure and specify the MCMC method with multiple chains to create three imputations:

```
proc mi data=Fitness1 seed=21355417 nimpute=6 mu0=50 10 180;
 mcmc chain=multiple initial=em outest=miest;
 var Oxygen RunTime RunPulse;
run;
```

The following statements list the parameters used for the imputations in [Output 57.12.1](#). Note that the data set includes observations with `_TYPE_='SEED'` which contains the seed to start the next random number generator.

```
proc print data=miest(obs=15);
 title 'Parameters for the Imputations';
run;
```

**Output 57.12.1** OUTEST Data Set

| Parameters for the Imputations |              |        |          |               |               |               |
|--------------------------------|--------------|--------|----------|---------------|---------------|---------------|
| Obs                            | _Imputation_ | _TYPE_ | _NAME_   | Oxygen        | RunTime       | RunPulse      |
| 1                              | 1            | SEED   |          | 825240167.00  | 825240167.00  | 825240167.00  |
| 2                              | 1            | PARM   |          | 46.77         | 10.47         | 169.41        |
| 3                              | 1            | COV    | Oxygen   | 30.59         | -8.32         | -50.99        |
| 4                              | 1            | COV    | RunTime  | -8.32         | 2.90          | 17.03         |
| 5                              | 1            | COV    | RunPulse | -50.99        | 17.03         | 200.09        |
| 6                              | 2            | SEED   |          | 1895925872.00 | 1895925872.00 | 1895925872.00 |
| 7                              | 2            | PARM   |          | 47.41         | 10.37         | 173.34        |
| 8                              | 2            | COV    | Oxygen   | 22.35         | -4.44         | -21.18        |
| 9                              | 2            | COV    | RunTime  | -4.44         | 1.76          | 1.25          |
| 10                             | 2            | COV    | RunPulse | -21.18        | 1.25          | 125.67        |
| 11                             | 3            | SEED   |          | 137653011.00  | 137653011.00  | 137653011.00  |
| 12                             | 3            | PARM   |          | 48.21         | 10.36         | 170.52        |
| 13                             | 3            | COV    | Oxygen   | 23.59         | -5.25         | -19.76        |
| 14                             | 3            | COV    | RunTime  | -5.25         | 1.66          | 5.00          |
| 15                             | 3            | COV    | RunPulse | -19.76        | 5.00          | 110.99        |

The following statements invoke the MI procedure and use the `INEST=` option in the MCMC statement:

```
proc mi data=Fitness1 mu0=50 10 180;
 mcmc inest=miest;
 var Oxygen RunTime RunPulse;
run;
```

The “Model Information” table in [Output 57.12.2](#) describes the method used in the multiple imputation process. The remaining tables for the example are identical to the tables in [Output 57.9.2](#), [Output 57.9.4](#), [Output 57.9.5](#), and [Output 57.9.6](#) in [Example 57.9](#).

**Output 57.12.2** Model Information

| The MI Procedure      |               |
|-----------------------|---------------|
| Model Information     |               |
| Data Set              | WORK.FITNESS1 |
| Method                | MCMC          |
| INEST Data Set        | WORK.MIEST    |
| Number of Imputations | 6             |

---

### Example 57.13: Transforming to Normality

This example applies the MCMC method to the Fitness1 data set in which the variable Oxygen is transformed. Assume that Oxygen is skewed and can be transformed to normality with a logarithmic transformation. The following statements invoke the MI procedure and specify the transformation. The TRANSFORM statement specifies the log transformation for Oxygen. Note that the values displayed for Oxygen in all of the results correspond to transformed values.

```
proc mi data=Fitness1 seed=32937921 mu0=50 10 180 out=outex13;
 transform log(Oxygen);
 mcmc chain=multiple displayinit;
 var Oxygen RunTime RunPulse;
run;
```

The “Missing Data Patterns” table in [Output 57.13.1](#) lists distinct missing data patterns with corresponding statistics for the Fitness1 data. Note that the values of Oxygen shown in the tables are transformed values.

**Output 57.13.1** Missing Data Patterns

| The MI Procedure      |        |          |           |      |         |
|-----------------------|--------|----------|-----------|------|---------|
| Missing Data Patterns |        |          |           |      |         |
| Group                 | Oxygen | Run Time | Run Pulse | Freq | Percent |
| 1                     | X      | X        | X         | 21   | 67.74   |
| 2                     | X      | X        | .         | 4    | 12.90   |
| 3                     | X      | .        | .         | 3    | 9.68    |
| 4                     | .      | X        | X         | 1    | 3.23    |
| 5                     | .      | X        | .         | 2    | 6.45    |

| Transformed Variables: Oxygen |          |           |            |
|-------------------------------|----------|-----------|------------|
| Missing Data Patterns         |          |           |            |
| -----Group Means-----         |          |           |            |
| Group                         | Oxygen   | RunTime   | RunPulse   |
| 1                             | 3.829760 | 10.809524 | 171.666667 |
| 2                             | 3.851813 | 10.137500 | .          |
| 3                             | 3.955298 | .         | .          |
| 4                             | .        | 11.950000 | 176.000000 |
| 5                             | .        | 9.885000  | .          |

| Transformed Variables: Oxygen |  |
|-------------------------------|--|
|-------------------------------|--|

The “Variable Transformations” table in [Output 57.13.2](#) lists the variables that have been transformed.

**Output 57.13.2** Variable Transformations

| Variable Transformations |             |
|--------------------------|-------------|
| Variable                 | _Transform_ |
| Oxygen                   | LOG         |

The “Initial Parameter Estimates for MCMC” table in [Output 57.13.3](#) displays the starting mean and covariance estimates used in the MCMC method.

**Output 57.13.3** Initial Parameter Estimates

| Initial Parameter Estimates for MCMC |               |           |           |            |
|--------------------------------------|---------------|-----------|-----------|------------|
| <u>_TYPE_</u>                        | <u>_NAME_</u> | Oxygen    | RunTime   | RunPulse   |
| MEAN                                 |               | 3.846122  | 10.557605 | 171.382949 |
| COV                                  | Oxygen        | 0.010827  | -0.120891 | -0.328772  |
| COV                                  | RunTime       | -0.120891 | 1.744580  | 3.011180   |
| COV                                  | RunPulse      | -0.328772 | 3.011180  | 82.747609  |

Transformed Variables: Oxygen

[Output 57.13.4](#) displays variance information from the multiple imputation.

**Output 57.13.4** Variance Information

| Variance Information |                    |          |          |        |
|----------------------|--------------------|----------|----------|--------|
| Variable             | -----Variance----- |          |          | DF     |
|                      | Between            | Within   | Total    |        |
| * Oxygen             | 0.000016175        | 0.000401 | 0.000420 | 26.499 |
| RunTime              | 0.001762           | 0.065421 | 0.067536 | 27.118 |
| RunPulse             | 0.205979           | 3.116830 | 3.364004 | 25.222 |

\* Transformed Variables

| Variance Information |                               |                              |                     |
|----------------------|-------------------------------|------------------------------|---------------------|
| Variable             | Relative Increase in Variance | Fraction Missing Information | Relative Efficiency |
| * Oxygen             | 0.048454                      | 0.047232                     | 0.990642            |
| RunTime              | 0.032318                      | 0.031780                     | 0.993684            |
| RunPulse             | 0.079303                      | 0.075967                     | 0.985034            |

\* Transformed Variables

[Output 57.13.5](#) displays parameter estimates from the multiple imputation. Note that the parameter value of  $\mu_0$  has also been transformed using the logarithmic transformation.

**Output 57.13.5** Parameter Estimates

| Parameter Estimates     |            |            |                       |                       |         |
|-------------------------|------------|------------|-----------------------|-----------------------|---------|
| Variable                | Mean       | Std Error  | 95% Confidence Limits |                       | DF      |
| * Oxygen                | 3.845175   | 0.020494   | 3.8031                | 3.8873                | 26.499  |
| RunTime                 | 10.560131  | 0.259876   | 10.0270               | 11.0932               | 27.118  |
| RunPulse                | 171.802181 | 1.834122   | 168.0264              | 175.5779              | 25.222  |
| * Transformed Variables |            |            |                       |                       |         |
| Parameter Estimates     |            |            |                       |                       |         |
| Variable                | Minimum    | Maximum    | Mu0                   | t for H0:<br>Mean=Mu0 | Pr >  t |
| * Oxygen                | 3.838599   | 3.848456   | 3.912023              | -3.26                 | 0.0030  |
| RunTime                 | 10.493031  | 10.600498  | 10.000000             | 2.16                  | 0.0402  |
| RunPulse                | 171.251777 | 172.498626 | 180.000000            | -4.47                 | 0.0001  |
| * Transformed Variables |            |            |                       |                       |         |

The following statements list the first 10 observations of the data set outex13 in [Output 57.13.6](#). Note that the values for Oxygen are in the original scale.

```
proc print data=outex13(obs=10);
 title 'First 10 Observations of the Imputed Data Set';
run;
```

**Output 57.13.6** Imputed Data Set in Original Scale

| First 10 Observations of the Imputed Data Set |              |         |         |              |
|-----------------------------------------------|--------------|---------|---------|--------------|
| Obs                                           | _Imputation_ | Oxygen  | RunTime | Run<br>Pulse |
| 1                                             | 1            | 44.6090 | 11.3700 | 178.000      |
| 2                                             | 1            | 45.3130 | 10.0700 | 185.000      |
| 3                                             | 1            | 54.2970 | 8.6500  | 156.000      |
| 4                                             | 1            | 59.5710 | 7.1440  | 167.012      |
| 5                                             | 1            | 49.8740 | 9.2200  | 170.092      |
| 6                                             | 1            | 44.8110 | 11.6300 | 176.000      |
| 7                                             | 1            | 38.5834 | 11.9500 | 176.000      |
| 8                                             | 1            | 43.7376 | 10.8500 | 158.851      |
| 9                                             | 1            | 39.4420 | 13.0800 | 174.000      |
| 10                                            | 1            | 60.0550 | 8.6300  | 170.000      |



Note that the results in [Output 57.13.6](#) can also be produced from the following statements without using a TRANSFORM statement. A transformed value of  $\log(50)=3.91202$  is used in the MU0= option.

```
data temp;
 set Fitness1;
 LogOxygen= log(Oxygen);
run;
proc mi data=temp seed=14337921 mu0=3.91202 10 180 out=outtemp;
 mcmc chain=multiple displayinit;
 var LogOxygen RunTime RunPulse;
run;
data outex13;
 set outtemp;
 Oxygen= exp(LogOxygen);
run;
```

---

### Example 57.14: Multistage Imputation

This example uses two separate imputation procedures to complete the imputation process. In the first case, the MI procedure statements use the MCMC method to impute just enough missing values for a data set with an arbitrary missing pattern so that each imputed data set has a monotone missing pattern. In the second case, the MI procedure statements use a MONOTONE statement to impute missing values for data sets with monotone missing patterns.

The following statements are identical to those in [Example 57.10](#). The statements invoke the MI procedure and specify the IMPUTE=MONOTONE option to create the imputed data set with a monotone missing pattern.

```
proc mi data=Fitness1 seed=17655417 out=outex14;
 mcmc impute=monotone;
 var Oxygen RunTime RunPulse;
run;
```

The “Missing Data Patterns” table in [Output 57.14.1](#) lists distinct missing data patterns with corresponding statistics. Here, an “X” means that the variable is observed in the corresponding group, a “.” means that the variable is missing and will be imputed to achieve the monotone missingness for the imputed data set, and an “O” means that the variable is missing and will not be imputed. The table also displays group-specific variable means.

**Output 57.14.1** Missing Data Patterns

| The MI Procedure      |        |          |           |      |         |
|-----------------------|--------|----------|-----------|------|---------|
| Missing Data Patterns |        |          |           |      |         |
| Group                 | Oxygen | Run Time | Run Pulse | Freq | Percent |
| 1                     | X      | X        | X         | 21   | 67.74   |
| 2                     | X      | X        | O         | 4    | 12.90   |
| 3                     | X      | O        | O         | 3    | 9.68    |
| 4                     | .      | X        | X         | 1    | 3.23    |
| 5                     | .      | X        | O         | 2    | 6.45    |

| Missing Data Patterns |           |           |            |
|-----------------------|-----------|-----------|------------|
| -----Group Means----- |           |           |            |
| Group                 | Oxygen    | RunTime   | RunPulse   |
| 1                     | 46.353810 | 10.809524 | 171.666667 |
| 2                     | 47.109500 | 10.137500 | .          |
| 3                     | 52.461667 | .         | .          |
| 4                     | .         | 11.950000 | 176.000000 |
| 5                     | .         | 9.885000  | .          |

As shown in the table, the MI procedure needs to impute only three missing values from group 4 and group 5 to achieve a monotone missing pattern for the imputed data set. When the MCMC method is used to produce an imputed data set with a monotone missing pattern, tables of variance information and parameter estimates are not created.

The following statements impute one value for each missing value in the monotone missingness data set outex14:

```
proc mi data=outex14
 nimpute=1 seed=51343672
 out=outex14a;
 monotone reg;
 var Oxygen RunTime RunPulse;
 by _Imputation_;
run;
```

You can then analyze these data sets by using other SAS procedures and combine these results by using the MIANALYZE procedure. Note that the VAR statement is required with a MONOTONE statement to provide the variable order for the monotone missing pattern.

The “Model Information” table in [Output 57.14.2](#) shows that a monotone method is used to generate imputed values in the first BY group.

**Output 57.14.2** Model Information

```

----- Imputation Number=1 -----
 The MI Procedure
 Model Information
Data Set WORK.OUTEX14
Method Monotone
Number of Imputations 1
Seed for random number generator 51343672

```

The “Monotone Model Specification” table in [Output 57.14.3](#) describes methods and imputed variables in the imputation model. The MI procedure uses the regression method to impute the variables RunTime and RunPulse in the model.

**Output 57.14.3** Monotone Model Specification

```

----- Imputation Number=1 -----
 Monotone Model Specification
Method Imputed
 Variables
Regression RunTime RunPulse

```

The “Missing Data Patterns” table in [Output 57.14.4](#) lists distinct missing data patterns with corresponding statistics. It shows a monotone missing pattern for the imputed data set.

**Output 57.14.4** Missing Data Patterns

```

----- Imputation Number=1 -----
Missing Data Patterns

 Group Oxygen Run Run
 Time Pulse Freq Percent
 1 X X X 22 70.97
 2 X X . 6 19.35
 3 X . . 3 9.68

Missing Data Patterns

-----Group Means-----
 Group Oxygen RunTime RunPulse
 1 46.057479 10.861364 171.863636
 2 46.745227 10.053333 .
 3 52.461667 . .

```

The following statements list the first 10 observations of the data set outex14a in [Output 57.14.5](#):

```

proc print data=outex14a(obs=10);
 title 'First 10 Observations of the Imputed Data Set';
run;

```

**Output 57.14.5** Imputed Data Set

```

First 10 Observations of the Imputed Data Set

 Obs _Imputation_ Oxygen RunTime Run
 Pulse
 1 1 44.6090 11.3700 178.000
 2 1 45.3130 10.0700 185.000
 3 1 54.2970 8.6500 156.000
 4 1 59.5710 7.1569 169.914
 5 1 49.8740 9.2200 159.315
 6 1 44.8110 11.6300 176.000
 7 1 39.8345 11.9500 176.000
 8 1 45.3196 10.8500 151.252
 9 1 39.4420 13.0800 174.000
 10 1 60.0550 8.6300 170.000

```

This example presents an alternative to the full-data MCMC imputation, in which imputation of only a few missing values is needed to achieve a monotone missing pattern for the imputed data set. The example uses a monotone MCMC method that imputes fewer missing values in each iteration and achieves approximate stationarity in fewer iterations (Schafer 1997, p. 227). The example also demonstrates how to combine the monotone MCMC method with a method for monotone missing data, which does not rely on iterations of steps.

---

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# Chapter 58

## The MIANALYZE Procedure

### Contents

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## Overview: MIANALYZE Procedure

The MIANALYZE procedure combines the results of the analyses of imputations and generates valid statistical inferences. Multiple imputation provides a useful strategy for analyzing data sets with missing values. Instead of filling in a single value for each missing value, Rubin's (1976, 1987) multiple imputation strategy replaces each missing value with a set of plausible values that represent the uncertainty about the right value to impute.

Multiple imputation inference involves three distinct phases:

1. The missing data are filled in  $m$  times to generate  $m$  complete data sets.
2. The  $m$  complete data sets are analyzed using standard statistical analyses.
3. The results from the  $m$  complete data sets are combined to produce inferential results.

A companion procedure, PROC MI, creates multiply imputed data sets for incomplete multivariate data. It uses methods that incorporate appropriate variability across the  $m$  imputations.

The analyses of imputations are obtained by using standard SAS procedures (such as PROC REG) for complete data. No matter which complete-data analysis is used, the process of combining results from different imputed data sets is essentially the same and results in valid statistical inferences that properly reflect the uncertainty due to missing values. These results of analyses are combined in the MIANALYZE procedure to derive valid inferences.

The MIANALYZE procedure reads parameter estimates and associated standard errors or covariance matrix that are computed by the standard statistical procedure for each imputed data set. The MIANALYZE procedure then derives valid univariate inference for these parameters. With an additional assumption about the population between and within imputation covariance matrices, multivariate inference based on Wald tests can also be derived.

The MODELEFFECTS statement lists the effects to be analyzed, and the CLASS statement lists the classification variables in the MODELEFFECTS statement. The variables in the MODELEFFECTS statement that are not specified in a CLASS statement are assumed to be continuous.

When each effect in the MODELEFFECTS statement is a continuous variable by itself, a STDERR statement specifies the standard errors when both parameter estimates and associated standard errors are stored as variables in the same data set.

For some parameters of interest, you can use TEST statements to test linear hypotheses about the parameters. For others, it is not straightforward to compute estimates and associated covariance matrices with standard statistical SAS procedures. Examples include correlation coefficients between two variables and ratios of variable means. These special cases are described in the section “[Examples of the Complete-Data Inferences](#)” on page 4848.

## Getting Started: MIANALYZE Procedure

The Fitness data described in the REG procedure are measurements of 31 individuals in a physical fitness course. See Chapter 79, “The REG Procedure,” for more information. The Fitness1 data set is constructed from the Fitness data set and contains three variables: Oxygen, RunTime, and RunPulse. Some values have been set to missing, and the resulting data set has an arbitrary pattern of missingness in these three variables.

```

----- Data on Physical Fitness -----
| These measurements were made on men involved in a physical |
| fitness course at N.C. State University. |
| Only selected variables of |
| Oxygen (oxygen intake, ml per kg body weight per minute), |
| Runtime (time to run 1.5 miles in minutes), and |
| RunPulse (heart rate while running) are used. |
| Certain values were changed to missing for the analysis. |

data Fitness1;
 input Oxygen RunTime RunPulse @@;
 datalines;
44.609 11.37 178 45.313 10.07 185
54.297 8.65 156 59.571 . .
49.874 9.22 . 44.811 11.63 176
. 11.95 176 . 10.85 .
39.442 13.08 174 60.055 8.63 170
50.541 . . 37.388 14.03 186
44.754 11.12 176 47.273 . .
51.855 10.33 166 49.156 8.95 180
40.836 10.95 168 46.672 10.00 .
46.774 10.25 . 50.388 10.08 168
39.407 12.63 174 46.080 11.17 156
45.441 9.63 164 . 8.92 .
45.118 11.08 . 39.203 12.88 168
45.790 10.47 186 50.545 9.93 148
48.673 9.40 186 47.920 11.50 170
47.467 10.50 170
;

```

Suppose that the data are multivariate normally distributed and that the missing data are missing at random (see the “Statistical Assumptions for Multiple Imputation” section in the chapter “The MI Procedure” for a description of these assumptions). The following statements use the MI procedure to impute missing values for the Fitness1 data set:

```

proc mi data=Fitness1 seed=3237851 noprint out=outmi;
 var Oxygen RunTime RunPulse;
run;

```

The MI procedure creates imputed data sets, which are stored in the outmi data set. A variable named `_Imputation_` indicates the imputation numbers. Based on  $m$  imputations,  $m$  different sets of the point and variance estimates for a parameter can be computed. In this example,  $m = 5$  is the default.

The following statements generate regression coefficients for each of the five imputed data sets:

```
proc reg data=outmi outest=outreg covout noprint;
 model Oxygen= RunTime RunPulse;
 by _Imputation_;
run;
```

The following statements display (in Figure 58.1) output parameter estimates and covariance matrices from PROC REG for the first two imputed data sets:

```
proc print data=outreg (obs=8);
 var _Imputation_ _Type_ _Name_
 Intercept RunTime RunPulse;
 title 'Parameter Estimates from Imputed Data Sets';
run;
```

**Figure 58.1** Parameter Estimates

| Parameter Estimates from Imputed Data Sets |              |        |           |           |          |          |
|--------------------------------------------|--------------|--------|-----------|-----------|----------|----------|
| Obs                                        | _Imputation_ | _TYPE_ | _NAME_    | Intercept | RunTime  | RunPulse |
| 1                                          | 1            | PARMS  |           | 86.544    | -2.82231 | -0.05873 |
| 2                                          | 1            | COV    | Intercept | 100.145   | -0.53519 | -0.55077 |
| 3                                          | 1            | COV    | RunTime   | -0.535    | 0.10774  | -0.00345 |
| 4                                          | 1            | COV    | RunPulse  | -0.551    | -0.00345 | 0.00343  |
| 5                                          | 2            | PARMS  |           | 83.021    | -3.00023 | -0.02491 |
| 6                                          | 2            | COV    | Intercept | 79.032    | -0.66765 | -0.41918 |
| 7                                          | 2            | COV    | RunTime   | -0.668    | 0.11456  | -0.00313 |
| 8                                          | 2            | COV    | RunPulse  | -0.419    | -0.00313 | 0.00264  |

The following statements combine the five sets of regression coefficients:

```
proc mianalyze data=outreg;
 modeleffects Intercept RunTime RunPulse;
run;
```

The “Model Information” table in Figure 58.2 lists the input data set(s) and the number of imputations.

**Figure 58.2** Model Information Table

| The MIANALYZE Procedure |             |
|-------------------------|-------------|
| Model Information       |             |
| Data Set                | WORK.OUTREG |
| Number of Imputations   | 5           |

The “Variance Information” table in Figure 58.3 displays the between-imputation, within-imputation, and total variances for combining complete-data inferences. It also displays the degrees of freedom for the total variance, the relative increase in variance due to missing values, the fraction of missing information, and the relative efficiency for each parameter estimate.

Figure 58.3 Variance Information Table

| Variance Information |                    |           |            |        |
|----------------------|--------------------|-----------|------------|--------|
| Parameter            | -----Variance----- |           |            | DF     |
|                      | Between            | Within    | Total      |        |
| Intercept            | 45.529229          | 76.543614 | 131.178689 | 23.059 |
| RunTime              | 0.019390           | 0.106220  | 0.129487   | 123.88 |
| RunPulse             | 0.001007           | 0.002537  | 0.003746   | 38.419 |

| Variance Information |             |             |          |
|----------------------|-------------|-------------|----------|
| Parameter            | Relative    | Fraction    | Relative |
|                      | Increase    | Missing     |          |
|                      | in Variance | Information |          |
| Intercept            | 0.713777    | 0.461277    | 0.915537 |
| RunTime              | 0.219051    | 0.192620    | 0.962905 |
| RunPulse             | 0.476384    | 0.355376    | 0.933641 |

The “Parameter Estimates” table in Figure 58.4 displays a combined estimate and standard error for each regression coefficient (parameter). Inferences are based on  $t$  distributions. The table displays a 95% confidence interval and a  $t$  test with the associated  $p$ -value for the hypothesis that the parameter is equal to the value specified with the THETA0= option (in this case, zero by default). The minimum and maximum parameter estimates from the imputed data sets are also displayed.

Figure 58.4 Parameter Estimates

| Parameter Estimates |           |           |                       |          |        |
|---------------------|-----------|-----------|-----------------------|----------|--------|
| Parameter           | Estimate  | Std Error | 95% Confidence Limits |          | DF     |
| Intercept           | 90.837440 | 11.453327 | 67.14779              | 114.5271 | 23.059 |
| RunTime             | -3.032870 | 0.359844  | -3.74511              | -2.3206  | 123.88 |
| RunPulse            | -0.068578 | 0.061204  | -0.19243              | 0.0553   | 38.419 |

| Parameter Estimates |           |            |
|---------------------|-----------|------------|
| Parameter           | Minimum   | Maximum    |
| Intercept           | 83.020730 | 100.839807 |
| RunTime             | -3.204426 | -2.822311  |
| RunPulse            | -0.112840 | -0.024910  |

| Parameter Estimates |        |                  |         |  |
|---------------------|--------|------------------|---------|--|
| Parameter           | Theta0 | t for H0:        |         |  |
|                     |        | Parameter=Theta0 | Pr >  t |  |
| Intercept           | 0      | 7.93             | <.0001  |  |
| RunTime             | 0      | -8.43            | <.0001  |  |
| RunPulse            | 0      | -1.12            | 0.2695  |  |

## Syntax: MIANALYZE Procedure

The following statements are available in the MIANALYZE procedure:

```
PROC MIANALYZE < options > ;
 BY variables ;
 CLASS variables ;
 MODELEFFECTS effects ;
 < label: > TEST equation1 < , ... , < equationk > > < / options > ;
 STDERR variables ;
```

The BY statement specifies groups in which separate analyses are performed.

The CLASS statement lists the classification variables in the MODELEFFECTS statement. Classification variables can be either character or numeric.

The required MODELEFFECTS statement lists the effects to be analyzed. The variables in the statement that are not specified in a CLASS statement are assumed to be continuous.

The STDERR statement lists the standard errors associated with the effects in the MODELEFFECTS statement when both parameter estimates and standard errors are saved as variables in the same DATA= data set. The STDERR statement can be used only when each effect in the MODELEFFECTS statement is a continuous variable by itself.

The TEST statement tests linear hypotheses about the parameters. An  $F$  statistic is used to jointly test the null hypothesis ( $H_0 : L_c = c$ ) specified in a single TEST statement. Several TEST statements can be used.

The PROC MIANALYZE and MODELEFFECTS statements are required for the MIANALYZE procedure. The rest of this section provides detailed syntax information for each of these statements, beginning with the PROC MIANALYZE statement. The remaining statements are in alphabetical order.

## PROC MIANALYZE Statement

```
PROC MIANALYZE < options > ;
```

The PROC MIANALYZE statement invokes the MIANALYZE procedure. Table 58.1 summarizes the options available in the PROC MIANALYZE statement.

**Table 58.1** Summary of PROC MIANALYZE Options

| Option                 | Description                                                        |
|------------------------|--------------------------------------------------------------------|
| <b>Input Data Sets</b> |                                                                    |
| DATA=                  | Specifies the COV, CORR, or EST type data set                      |
| DATA=                  | Specifies the data set for parameter estimates and standard errors |
| PARMS=                 | Specifies the data set for parameter estimates                     |
| PARMINFO=              | Specifies the data set for parameter information                   |
| COVB=                  | Specifies the data set for covariance matrices                     |
| XPXI=                  | Specifies the data set for $(X'X)^{-1}$ matrices                   |

Table 58.1 *continued*

| Option                      | Description                                       |
|-----------------------------|---------------------------------------------------|
| <b>Statistical Analysis</b> |                                                   |
| THETA0=                     | Specifies parameters under the null hypothesis    |
| ALPHA=                      | Specifies the level for the confidence interval   |
| EDF=                        | Specifies the complete-data degrees of freedom    |
| <b>Printed Output</b>       |                                                   |
| WCOV                        | Displays the within-imputation covariance matrix  |
| BCOV                        | Displays the between-imputation covariance matrix |
| TCOV                        | Displays the total covariance matrix              |
| MULT                        | Displays multivariate inferences                  |

The following options can be used in the PROC MIANALYZE statement. They are listed in alphabetical order.

**ALPHA= $\alpha$** 

specifies that confidence limits are to be constructed for the parameter estimates with confidence level  $100(1 - \alpha)\%$ , where  $0 < \alpha < 1$ . The default is ALPHA=0.05.

**BCOV**

displays the between-imputation covariance matrix.

**COVB <(EFFECTVAR=STACKING | ROWCOL)> =SAS-data-set**

names an input SAS data set that contains covariance matrices of the parameter estimates from imputed data sets. If you provide a COVB= data set, you must also provide a PARMS= data set.

The EFFECTVAR= option identifies the variables for parameters displayed in the covariance matrix and is used only when the PARMINFO= option is not specified. The default is EFFECTVAR= STACKING.

See the section “[Input Data Sets](#)” on page 4840 for a detailed description of the COVB= option.

**DATA=SAS-data-set**

names an input SAS data set.

If the input DATA= data set is not a specially structured SAS data set, the data set contains both the parameter estimates and associated standard errors. The parameter estimates are specified in the MODELEFFECTS statement and the standard errors are specified in the STDERR statement.

If the data set is a specially structured input SAS data set, it must have a TYPE of EST, COV, or CORR that contains estimates from imputed data sets:

- If TYPE=EST, the data set contains the parameter estimates and associated covariance matrices.
- If TYPE=COV, the data set contains the sample means, sample sizes, and covariance matrices. Each covariance matrix for variables is divided by the sample size  $n$  to create the covariance matrix for parameter estimates.
- If TYPE=CORR, the data set contains the sample means, sample sizes, standard errors, and correlation matrices. The covariance matrices are computed from the correlation matrices and associated standard errors. Each covariance matrix for variables is divided by the sample size  $n$  to create the covariance matrix for parameter estimates.

If you do not specify an input data set with the DATA= or PARMS= option, then the most recently created SAS data set is used as an input DATA= data set. See the section “[Input Data Sets](#)” on page 4840 for a detailed description of the input data sets.

**EDF=number**

specifies the complete-data degrees of freedom for the parameter estimates. This is used to compute an adjusted degrees of freedom for each parameter estimate. By default, EDF= $\infty$  and the degrees of freedom for each parameter estimate are not adjusted.

**MULT****MULTIVARIATE**

requests multivariate inference for the parameters. It is based on Wald tests and is a generalization of the univariate inference. See the section “[Multivariate Inferences](#)” on page 4845 for a detailed description of the multivariate inference.

**PARMINFO=SAS-data-set**

names an input SAS data set that contains parameter information associated with variables PRM1, PRM2, . . . , and so on. These variables are used as variables for parameters in a COVB= data set. See the section “[Input Data Sets](#)” on page 4840 for a detailed description of the PARMINFO= option.

**PARMS <(CLASSVAR= ctype)> =SAS-data-set**

names an input SAS data set that contains parameter estimates computed from imputed data sets. When a COVB= data set is not specified, the input PARMS= data set also contains standard errors associated with these parameter estimates. If multivariate inference is requested, you must also provide a COVB= or XPXI= data set.

When the effects contain classification variables, the option CLASSVAR= *ctype* can be used to identify the associated classification variables when reading the classification levels from observations. The available types are FULL, LEVEL, and CLASSVAL. The default is CLASSVAR= FULL. See the section “[Input Data Sets](#)” on page 4840 for a detailed description of the PARMS= option.

**TCOV**

displays the total covariance matrix derived by assuming that the population between-imputation and within-imputation covariance matrices are proportional to each other.

**THETA0=numbers****MU0=numbers**

specifies the parameter values  $\theta_0$  under the null hypothesis  $\theta = \theta_0$  in the  $t$  tests for location for the effects. If only one number  $\theta_0$  is specified, that number is used for all effects. If more than one number is specified, the specified numbers correspond to effects in the MODELEFFECTS statement in the order in which they appear in the statement. When an effect contains classification variables, the corresponding value is not used and the test is not performed.

**WCOV**

displays the within-imputation covariance matrices.

**XPXI=SAS-data-set**

names an input SAS data set that contains the  $(\mathbf{X}'\mathbf{X})^{-1}$  matrices associated with the parameter estimates computed from imputed data sets. If you provide an XPXI= data set, you must also provide a PARMS= data set. In this case, PROC MIANALYZE reads the standard errors of the estimates from the PARMS= data. The standard errors and  $(\mathbf{X}'\mathbf{X})^{-1}$  matrices are used to derive the covariance matrices.

---

## BY Statement

**BY** *variables* ;

You can specify a BY statement with PROC MIANALYZE to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the MIANALYZE procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

---

## CLASS Statement

**CLASS** *variables* ;

The CLASS statement specifies the classification variables in the MODELEFFECTS statement. Classification variables can be either character or numeric. Classification levels are determined from the formatted values of the classification variables. See “The FORMAT Procedure” in the *Base SAS Procedures Guide* for details.

---

## MODELEFFECTS Statement

**MODELEFFECTS** *effects* ;

The MODELEFFECTS statement lists the effects in the data set to be analyzed. Each effect is a variable or a combination of variables, and is specified with a special notation that uses variable names and operators.

Each variable is either a classification (or CLASS) variable or a continuous variable. If a variable is not declared in the CLASS statement, it is assumed to be continuous. Crossing and nesting operators can be used in an effect to create crossed and nested effects.

One general form of an effect involving several variables is

$$X1 * X2 * A * B * C ( D E )$$

where A, B, C, D, and E are classification variables and X1 and X2 are continuous variables.



When the input DATA= data set is not a specially structured SAS data set, you must also specify standard errors of the parameter estimates in an STDERR statement.

---

## STDERR Statement

**STDERR** *variables* ;

The STDERR statement lists standard errors associated with effects in the MODELEFFECTS statement, when the input DATA= data set contains both parameter estimates and standard errors as variables in the data set.

With the STDERR statement, only continuous effects are allowed in the MODELEFFECTS statement. The specified standard errors correspond to parameter estimates in the order in which they appear in the MODELEFFECTS statement.

For example, you can use the following MODELEFFECTS and STDERR statements to identify both the parameter estimates and associated standard errors in a SAS data set:

```
proc mianalyze;
 modeleffects y1-y3;
 stderr sy1-sy3;
run;
```

---

## TEST Statement

*< label: >* **TEST** *equation1 <, ..., < equationk >>* *</ options >* ;

The TEST statement tests linear hypotheses about the parameters  $\beta$ . An  $F$  test is used to jointly test the null hypotheses ( $H_0 : L\beta = c$ ) specified in a single TEST statement in which the MULT option is specified.

Each *equation* specifies a linear hypothesis (a row of the  $L$  matrix and the corresponding element of the  $c$  vector); multiple *equations* are separated by commas. The label, which must be a valid SAS name, is used to identify the resulting output. You can submit multiple TEST statements. When a label is not included in a TEST statement, a label of “Test  $j$ ” is used for the  $j$ th TEST statement.

The form of an *equation* is as follows:

$$term < \pm term \dots > < = \pm term < \pm term \dots > >$$

where *term* is a parameter of the model, or a constant, or a constant times a parameter. When no equal sign appears, the expression is set to 0. Only parameters for regressor effects (continuous variables by themselves) are allowed.

For each TEST statement, PROC MIANALYZE displays a “Test Specification” table of the  $L$  matrix and the  $c$  vector. The procedure also displays a “Variance Information” table of the between-imputation, within-imputation, and total variances for combining complete-data inferences, and a “Parameter Estimates” table of a combined estimate and standard error for each linear component. The linear components are labeled TestPrm1, TestPrm2, ... in the tables.

The following statements illustrate possible uses of the TEST statement:

```

proc mianalyze;
 modeleffects intercept a1 a2 a3;
 test1: test intercept + a2 = 0;
 test2: test intercept + a2;
 test3: test a1=a2=a3;
 test4: test a1=a2, a2=a3;
run;

```

The first and second TEST statements are equivalent and correspond to the specification in Figure 58.5.

**Figure 58.5** Test Specification for test1 and test2

| The MIANALYZE Procedure |           |    |          |    |   |
|-------------------------|-----------|----|----------|----|---|
| Test: test1             |           |    |          |    |   |
| Test Specification      |           |    |          |    |   |
| -----I Matrix-----      |           |    |          |    |   |
| Parameter               | intercept | a1 | a2       | a3 | C |
| TestPrm1                | 1.000000  | 0  | 1.000000 | 0  | 0 |

The third and fourth TEST statements are also equivalent and correspond to the specification in Figure 58.6.

**Figure 58.6** Test Specification for test3 and test4

| The MIANALYZE Procedure |           |          |           |           |   |
|-------------------------|-----------|----------|-----------|-----------|---|
| Test: test3             |           |          |           |           |   |
| Test Specification      |           |          |           |           |   |
| -----I Matrix-----      |           |          |           |           |   |
| Parameter               | intercept | a1       | a2        | a3        | C |
| TestPrm1                | 0         | 1.000000 | -1.000000 | 0         | 0 |
| TestPrm2                | 0         | 0        | 1.000000  | -1.000000 | 0 |

The ALPHA= and EDF options specified in the PROC MIANALYZE statement are also applied to the TEST statement. You can specify the following options in the TEST statement after a slash(/):

#### **BCOV**

displays the between-imputation covariance matrix.

#### **MULT**

displays the multivariate inference for parameters.

#### **TCOV**

displays the total covariance matrix.

**WCOV**

displays the within-imputation covariance matrix.

For more information, see the section “Testing Linear Hypotheses about the Parameters” on page 4847.

## Details: MIANALYZE Procedure

### Input Data Sets

You specify input data sets based on the type of inference you requested. For univariate inference, you can use one of the following options:

- a DATA= data set, which provides both parameter estimates and the associated standard errors
- a DATA=EST, COV, or CORR data set, which provides both parameter estimates and the associated standard errors either explicitly (type CORR) or through the covariance matrix (type EST, COV)
- PARMS= data set, which provides both parameter estimates and the associated standard errors

For multivariate inference, which includes the testing of linear hypotheses about parameters, you can use one of the following option combinations:

- a DATA=EST, COV, or CORR data set, which provides parameter estimates and the associated covariance matrix either explicitly (type EST, COV) or through the correlation matrix and standard errors (type CORR) in a single data set
- PARMS= and COVB= data sets, which provide parameter estimates in a PARMS= data set and the associated covariance matrix in a COVB= data set
- PARMS=, COVB=, and PARMINFO= data sets, which provide parameter estimates in a PARMS= data set, the associated covariance matrix in a COVB= data set with variables named PRM1, PRM2, . . . , and the effects associated with these variables in a PARMINFO= data set
- PARMS= and XPXI= data sets, which provide parameter estimates and the associated standard errors in a PARMS= data set and the associated  $(\mathbf{X}'\mathbf{X})^{-1}$  matrix in an XPXI= data set

The appropriate combination depends on the type of inference and the SAS procedure you used to create the data sets. For instance, if you used PROC REG to create an OUTEST= data set that contains the parameter estimates and covariance matrix, you would use the DATA= option to read the OUTEST= data set.

When the input DATA= data set is a specially structured SAS data set, the data set must contain the variable `_Imputation_` to identify the imputation by number. Otherwise, each observation corresponds to an imputation and contains both parameter estimates and associated standard errors.

If you do not specify an input data set with the DATA= or PARMS= option, then the most recently created SAS data set is used as an input DATA= data set. Note that with a DATA= data set, each effect represents a continuous variable; only regressor effects (continuous variables by themselves) are allowed in the MODELEFFECTS statement.

## DATA= SAS Data Set

The DATA= data set provides both parameter estimates and the associated standard errors computed from imputed data sets. Such data sets are typically created with an OUTPUT statement in procedures such as PROC MEANS and PROC UNIVARIATE.

The MIANALYZE procedure reads parameter estimates from observations with variables in the MODEL-EFFECTS statement, and standard errors for parameter estimates from observations with variables in the STDERR statement. The order of the variables for standard errors must match the order of the variables for parameter estimates.

## DATA=EST, COV, or CORR SAS Data Set

The specially structured DATA= data set provides both parameter estimates and the associated covariance matrix computed from imputed data sets. Such data sets are created by procedures such as PROC CORR (type COV, CORR) and PROC REG (type EST).

With TYPE=EST, the MIANALYZE procedure reads parameter estimates from observations with `_TYPE_='PARM'`, `_TYPE_='PARMS'`, `_TYPE_='OLS'`, or `_TYPE_='FINAL'`, and covariance matrices for parameter estimates from observations with `_TYPE_='COV'` or `_TYPE_='COVB'`.

With TYPE=COV, the procedure reads sample means from observations with `_TYPE_='MEAN'`, sample size  $n$  from observations with `_TYPE_='N'`, and covariance matrices for variables from observations with `_TYPE_='COV'`.

With TYPE=CORR, the procedure reads sample means from observations with `_TYPE_='MEAN'`, sample size  $n$  from observations with `_TYPE_='N'`, correlation matrices for variables from observations with `_TYPE_='CORR'`, and standard errors for variables from observations with `_TYPE_='STD'`. The standard errors and correlation matrix are used to generate a covariance matrix for the variables.

Note that with TYPE=COV or CORR, each covariance matrix for the variables is divided by  $n$  to create the covariance matrix for the sample means.

## PARMS <(CLASSVAR= *ctype*)> = Data Set

The PARMS= data set contains both parameter estimates and the associated standard errors computed from imputed data sets. Such data sets are typically created with an ODS OUTPUT statement in procedures such as PROC GENMOD, PROC GLM, PROC LOGISTIC, and PROC MIXED.

The MIANALYZE procedure reads effect names from observations with the variable Parameter, Effect, Variable, or Parm. It then reads parameter estimates from observations with the variable Estimate and standard errors for parameter estimates from observations with the variable StdErr.

When the effects contain classification variables, the option CLASSVAR= *ctype* can be used to identify associated classification variables when reading the classification levels from observations. The available types are FULL, LEVEL, and CLASSVAL. The default is CLASSVAR= FULL.

With CLASSVAR=FULL, the data set contains the classification variables explicitly. PROC MIANALYZE reads the classification levels from observations with their corresponding classification variables. PROC MIXED generates this type of table.

With CLASSVAR=LEVEL, PROC MIANALYZE reads the classification levels for the effect from observations with variables Level1, Level2, and so on, where the variable Level1 contains the classification level

for the first classification variable in the effect, and the variable `Level2` contains the classification level for the second classification variable in the effect. For each effect, the variables in the crossed list are displayed before the variables in the nested list. The variable order in the `CLASS` statement is used for variables inside each list. PROC GENMOD generates this type of table.

For example, with the following statements, the variable `Level1` has the classification level of the variable `c2` for the effect `c2`:

```
proc mianalyze parms(classvar=Level)= dataparm;
 class c1 c2 c3;
 modeleffects c2 c3(c2 c1);
run;
```

For the effect `c3(c2 c1)`, the variable `Level1` has the classification level of the variable `c3`, `Level2` has the level of `c1`, and `Level3` has the level of `c2`.

Similarly, with `CLASSVAR=CLASSVAL`, PROC MIANALYZE reads the classification levels for the effect from observations with variables `ClassVal0`, `ClassVal1`, and so on, where the variable `ClassVal0` contains the classification level for the first classification variable in the effect, and the variable `ClassVal1` contains the classification level for the second classification variable in the effect. For each effect, the variables in the crossed list are displayed before the variables in the nested list. The variable order in the `CLASS` statement is used for variables inside each list. PROC LOGISTIC generates this type of tables.

### PARMS <(CLASSVAR= *ctype*)> = and COVB= Data Sets

The `PARMS=` data set contains parameter estimates, and the `COVB=` data set contains associated covariance matrices computed from imputed data sets. Such data sets are typically created with an ODS OUTPUT statement in procedures such as PROC LOGISTIC, PROC MIXED, and PROC REG.

With a `PARMS=` data set, the MIANALYZE procedure reads effect names from observations with the variable `Parameter`, `Effect`, `Variable`, or `Parm`. It then reads parameter estimates from observations with the variable `Estimate`.

When the effects contain classification variables, the option `CLASSVAR= ctype` can be used to identify the associated classification variables when reading the classification levels from observations. The available types are `FULL`, `LEVEL`, and `CLASSVAL`, and they are described in the section “`PARMS <(CLASSVAR= ctype)> = Data Set`” on page 4841. The default is `CLASSVAR= FULL`.

The option `EFFECTVAR= etype` identifies the variables for parameters displayed in the covariance matrix. The available types are `STACKING` and `ROWCOL`. The default is `EFFECTVAR= STACKING`.

With `EFFECTVAR= STACKING`, each parameter is displayed by stacking variables in the effect. Begin with the variables in the crossed list, followed by the continuous list, then followed by the nested list. Each classification variable is displayed with its classification level attached. PROC LOGISTIC generates this type of table.

When each effect is a continuous variable by itself, each stacked parameter name reduces to the effect name. PROC REG generates this type of table.

With `EFFECTVAR= STACKING`, the MIANALYZE procedure reads parameter names from observations with the variable `Parameter`, `Effect`, `Variable`, `Parm`, or `RowName`. It then reads covariance matrices from observations with the stacked variables in a `COVB=` data set.

With `EFFECTVAR=ROWCOL`, parameters are displayed by the variables `Col1`, `Col2`, ... The parameter associated with the variable `Col1` is identified by the observation with value 1 for the variable `Row`. The parameter associated with the variable `Col2` is identified by the observation with value 2 for the variable `Row`. `PROC MIXED` generates this type of table.

With `EFFECTVAR=ROWCOL`, the `MIANALYZE` procedure reads the parameter indices from observations with the variable `Row` and the effect names from observations with the variable `Parameter`, `Effect`, `Variable`, `Parm`, or `RowName`. It then reads covariance matrices from observations with the variables `Col1`, `Col2`, and so on in a `COVB=` data set.

When the effects contain classification variables, the data set contains the classification variables explicitly and the `MIANALYZE` procedure also reads the classification levels from their corresponding classification variables.

### **PARMS <(CLASSVAR= *ctype*)> =, PARMINFO=, and COVB= Data Sets**

The input `PARMS=` data set contains parameter estimates and the input `COVB=` data set contains associated covariance matrices computed from imputed data sets. Such data sets are typically created with an `ODS OUTPUT` statement using procedure such as `PROC GENMOD`.

With a `PARMS=` data set, the `MIANALYZE` procedure reads effect names from observations with the variable `Parameter`, `Effect`, `Variable`, or `Parm`. It then reads parameter estimates from observations with the variable `Estimate`.

When the effects contain classification variables, the option `CLASSVAR= ctype` can be used to identify the associated classification variables when reading the classification levels from observations. The available types are `FULL`, `LEVEL`, and `CLASSVAL`, and they are described in the section “`PARMS <(CLASSVAR= ctype)> = Data Set`” on page 4841. The default is `CLASSVAR= FULL`.

With a `COVB=` data set, the `MIANALYZE` procedure reads parameter names from observations with the variable `Parameter`, `Effect`, `Variable`, `Parm`, or `RowName`. It then reads covariance matrices from observations with the variables `Prm1`, `Prm2`, and so on.

The parameters associated with the variables `Prm1`, `Prm2`, and so on are identified in the `PARMINFO=` data set. `PROC MIANALYZE` reads the parameter names from observations with the variable `Parameter` and the corresponding effect from observations with the variable `Effect`. When the effects contain classification variables, the data set contains the classification variables explicitly and the `MIANALYZE` procedure also reads the classification levels from observations with their corresponding classification variables.

### **PARMS= and XPXI= Data Sets**

The input `PARMS=` data set contains parameter estimates, and the input `XPXI=` data set contains associated  $(X'X)^{-1}$  matrices computed from imputed data sets. Such data sets are typically created with an `ODS OUTPUT` statement in a procedure such as `PROC GLM`.

With a `PARMS=` data set, the `MIANALYZE` procedure reads parameter names from observations with the variable `Parameter`, `Effect`, `Variable`, or `Parm`. It then reads parameter estimates from observations with the variable `Estimate` and standard errors for parameter estimates from observations with the variable `StdErr`.

With a `XPXI=` data set, the `MIANALYZE` procedure reads parameter names from observations with the variable `Parameter` and  $(X'X)^{-1}$  matrices from observations with the parameter variables in the data set.

Note that this combination can be used only when each effect is a continuous variable by itself.

## Combining Inferences from Imputed Data Sets

With  $m$  imputations,  $m$  different sets of the point and variance estimates for a parameter  $Q$  can be computed. Suppose that  $\hat{Q}_i$  and  $\hat{W}_i$  are the point and variance estimates, respectively, from the  $i$ th imputed data set,  $i = 1, 2, \dots, m$ . Then the combined point estimate for  $Q$  from multiple imputation is the average of the  $m$  complete-data estimates:

$$\bar{Q} = \frac{1}{m} \sum_{i=1}^m \hat{Q}_i$$

Suppose that  $\bar{W}$  is the within-imputation variance, which is the average of the  $m$  complete-data estimates:

$$\bar{W} = \frac{1}{m} \sum_{i=1}^m \hat{W}_i$$

And suppose that  $B$  is the between-imputation variance:

$$B = \frac{1}{m-1} \sum_{i=1}^m (\hat{Q}_i - \bar{Q})^2$$

Then the variance estimate associated with  $\bar{Q}$  is the total variance (Rubin 1987)

$$T = \bar{W} + \left(1 + \frac{1}{m}\right)B$$

The statistic  $(Q - \bar{Q})T^{-(1/2)}$  is approximately distributed as  $t$  with  $v_m$  degrees of freedom (Rubin 1987), where

$$v_m = (m-1) \left[ 1 + \frac{\bar{W}}{(1+m^{-1})B} \right]^2$$

The degrees of freedom  $v_m$  depend on  $m$  and the ratio

$$r = \frac{(1+m^{-1})B}{\bar{W}}$$

The ratio  $r$  is called the relative increase in variance due to nonresponse (Rubin 1987). When there is no missing information about  $Q$ , the values of  $r$  and  $B$  are both zero. With a large value of  $m$  or a small value of  $r$ , the degrees of freedom  $v_m$  will be large and the distribution of  $(Q - \bar{Q})T^{-(1/2)}$  will be approximately normal.

Another useful statistic is the fraction of missing information about  $Q$ :

$$\hat{\lambda} = \frac{r + 2/(v_m + 3)}{r + 1}$$

Both statistics  $r$  and  $\lambda$  are helpful diagnostics for assessing how the missing data contribute to the uncertainty about  $Q$ .

When the complete-data degrees of freedom  $v_0$  are small, and there is only a modest proportion of missing data, the computed degrees of freedom,  $v_m$ , can be much larger than  $v_0$ , which is inappropriate. For example, with  $m = 5$  and  $r = 10\%$ , the computed degrees of freedom  $v_m = 484$ , which is inappropriate for data sets with complete-data degrees of freedom less than 484.

Barnard and Rubin (1999) recommend the use of adjusted degrees of freedom

$$v_m^* = \left[ \frac{1}{v_m} + \frac{1}{\hat{v}_{obs}} \right]^{-1}$$

where  $\hat{v}_{obs} = (1 - \gamma)v_0(v_0 + 1)/(v_0 + 3)$  and  $\gamma = (1 + m^{-1})B/T$ .

If you specify the complete-data degrees of freedom  $v_0$  with the EDF= option, the MIANALYZE procedure uses the adjusted degrees of freedom,  $v_m^*$ , for inference. Otherwise, the degrees of freedom  $v_m$  are used.

---

## Multiple Imputation Efficiency

The relative efficiency (RE) of using the finite  $m$  imputation estimator, rather than using an infinite number for the fully efficient imputation, in units of variance, is approximately a function of  $m$  and  $\lambda$  (Rubin 1987, p. 114):

$$RE = \left(1 + \frac{\lambda}{m}\right)^{-1}$$

Table 58.2 shows relative efficiencies with different values of  $m$  and  $\lambda$ .

**Table 58.2** Relative Efficiencies

| m  | $\lambda$ |        |        |        |        |
|----|-----------|--------|--------|--------|--------|
|    | 10%       | 20%    | 30%    | 50%    | 70%    |
| 3  | 0.9677    | 0.9375 | 0.9091 | 0.8571 | 0.8108 |
| 5  | 0.9804    | 0.9615 | 0.9434 | 0.9091 | 0.8772 |
| 10 | 0.9901    | 0.9804 | 0.9709 | 0.9524 | 0.9346 |
| 20 | 0.9950    | 0.9901 | 0.9852 | 0.9756 | 0.9662 |

The table shows that for situations with little missing information, only a small number of imputations are necessary. In practice, the number of imputations needed can be informally verified by replicating sets of  $m$  imputations and checking whether the estimates are stable between sets (Horton and Lipsitz 2001, p. 246).

---

## Multivariate Inferences

Multivariate inference based on Wald tests can be done with  $m$  imputed data sets. The approach is a generalization of the approach taken in the univariate case (Rubin 1987, p. 137; Schafer 1997, p. 113). Suppose that  $\hat{Q}_i$  and  $\hat{W}_i$  are the point and covariance matrix estimates for a  $p$ -dimensional parameter  $Q$  (such as a



multivariate mean) from the  $i$ th imputed data set,  $i = 1, 2, \dots, m$ . Then the combined point estimate for  $\mathbf{Q}$  from the multiple imputation is the average of the  $m$  complete-data estimates:

$$\bar{\mathbf{Q}} = \frac{1}{m} \sum_{i=1}^m \hat{\mathbf{Q}}_i$$

Suppose that  $\bar{\mathbf{W}}$  is the within-imputation covariance matrix, which is the average of the  $m$  complete-data estimates:

$$\bar{\mathbf{W}} = \frac{1}{m} \sum_{i=1}^m \hat{\mathbf{W}}_i$$

And suppose that  $\mathbf{B}$  is the between-imputation covariance matrix:

$$\mathbf{B} = \frac{1}{m-1} \sum_{i=1}^m (\hat{\mathbf{Q}}_i - \bar{\mathbf{Q}})(\hat{\mathbf{Q}}_i - \bar{\mathbf{Q}})'$$

Then the covariance matrix associated with  $\bar{\mathbf{Q}}$  is the total covariance matrix

$$\mathbf{T}_0 = \bar{\mathbf{W}} + \left(1 + \frac{1}{m}\right)\mathbf{B}$$

The natural multivariate extension of the  $t$  statistic used in the univariate case is the  $F$  statistic

$$F_0 = (\mathbf{Q} - \bar{\mathbf{Q}})' \mathbf{T}_0^{-1} (\mathbf{Q} - \bar{\mathbf{Q}})$$

with degrees of freedom  $p$  and

$$v = (m-1)(1 + 1/r)^2$$

where

$$r = \left(1 + \frac{1}{m}\right) \text{trace}(\mathbf{B}\bar{\mathbf{W}}^{-1})/p$$

is an average relative increase in variance due to nonresponse (Rubin 1987, p. 137; Schafer 1997, p. 114).

However, the reference distribution of the statistic  $F_0$  is not easily derived. Especially for small  $m$ , the between-imputation covariance matrix  $\mathbf{B}$  is unstable and does not have full rank for  $m \leq p$  (Schafer 1997, p. 113).

One solution is to make an additional assumption that the population between-imputation and within-imputation covariance matrices are proportional to each other (Schafer 1997, p. 113). This assumption implies that the fractions of missing information for all components of  $\mathbf{Q}$  are equal. Under this assumption, a more stable estimate of the total covariance matrix is

$$\mathbf{T} = (1 + r)\bar{\mathbf{W}}$$

With the total covariance matrix  $\mathbf{T}$ , the  $F$  statistic (Rubin 1987, p. 137)

$$F = (\mathbf{Q} - \bar{\mathbf{Q}})' \mathbf{T}^{-1} (\mathbf{Q} - \bar{\mathbf{Q}})/p$$

has an  $F$  distribution with degrees of freedom  $p$  and  $v_1$ , where

$$v_1 = \frac{1}{2}(p+1)(m-1)\left(1 + \frac{1}{r}\right)^2$$

For  $t = p(m-1) \leq 4$ , PROC MIANALYZE uses the degrees of freedom  $v_1$  in the analysis. For  $t = p(m-1) > 4$ , PROC MIANALYZE uses  $v_2$ , a better approximation of the degrees of freedom given by Li, Raghunathan, and Rubin (1991):

$$v_2 = 4 + (t-4) \left[ 1 + \frac{1}{r} \left( 1 - \frac{2}{t} \right) \right]^2$$

## Testing Linear Hypotheses about the Parameters

Linear hypotheses for parameters  $\beta$  are expressed in matrix form as

$$H_0 : \mathbf{L}\beta = \mathbf{c}$$

where  $\mathbf{L}$  is a matrix of coefficients for the linear hypotheses and  $\mathbf{c}$  is a vector of constants.

Suppose that  $\hat{\mathbf{Q}}_i$  and  $\hat{\mathbf{U}}_i$  are the point and covariance matrix estimates, respectively, for a  $p$ -dimensional parameter  $\mathbf{Q}$  from the  $i$ th imputed data set,  $i=1, 2, \dots, m$ . Then for a given matrix  $\mathbf{L}$ , the point and covariance matrix estimates for the linear functions  $\mathbf{LQ}$  in the  $i$ th imputed data set are, respectively,

$$\mathbf{L}\hat{\mathbf{Q}}_i$$

$$\mathbf{L}\hat{\mathbf{U}}_i\mathbf{L}'$$

The inferences described in the section “Combining Inferences from Imputed Data Sets” on page 4844 and the section “Multivariate Inferences” on page 4845 are applied to these linear estimates for testing the null hypothesis  $H_0 : \mathbf{L}\beta = \mathbf{c}$ .

For each TEST statement, the “Test Specification” table displays the  $\mathbf{L}$  matrix and the  $\mathbf{c}$  vector, the “Variance Information” table displays the between-imputation, within-imputation, and total variances for combining complete-data inferences, and the “Parameter Estimates” table displays a combined estimate and standard error for each linear component.

With the WCOV and BCOV options in the TEST statement, the procedure displays the within-imputation and between-imputation covariance matrices, respectively.

With the TCOV option, the procedure displays the total covariance matrix derived under the assumption that the population between-imputation and within-imputation covariance matrices are proportional to each other.

With the MULT option in the TEST statement, the “Multivariate Inference” table displays an  $F$  test for the null hypothesis  $\mathbf{L}\beta = \mathbf{c}$  of the linear components.

## Examples of the Complete-Data Inferences

For a given parameter of interest, it is not always possible to compute the estimate and associated covariance matrix directly from a SAS procedure. This section describes examples of parameters with their estimates and associated covariance matrices, which provide the input to the MIANALYZE procedure. Some are straightforward, and others require special techniques.

### Means

For a population mean vector  $\mu$ , the usual estimate is the sample mean vector

$$\bar{y} = \frac{1}{n} \sum y_i$$

A variance estimate for  $\bar{y}$  is  $\frac{1}{n}S$ , where  $S$  is the sample covariance matrix

$$S = \frac{1}{n-1} \sum (y_i - \bar{y})(y_i - \bar{y})'$$

These statistics can be computed from a procedure such as PROC CORR. This approach is illustrated in [Example 58.2](#).

### Regression Coefficients

Many SAS procedures are available for regression analysis. Among them, PROC REG provides the most general analysis capabilities, and others like PROC LOGISTIC and PROC MIXED provide more specialized analyses.

Some regression procedures, such as REG and LOGISTIC, create an EST type data set that contains both the parameter estimates for the regression coefficients and their associated covariance matrix. You can read an EST type data set in the MIANALYZE procedure with the DATA= option. This approach is illustrated in [Example 58.3](#).

Other procedures, such as GLM, MIXED, and GENMOD, do not generate EST type data sets for regression coefficients. For PROC MIXED and PROC GENMOD, you can use ODS OUTPUT statement to save parameter estimates in a data set and the associated covariance matrix in a separate data set. These data sets are then read in the MIANALYZE procedure with the PARMS= and COVB= options, respectively. This approach is illustrated in [Example 58.4](#) for PROC MIXED and in [Example 58.5](#) for PROC GENMOD.

PROC GLM does not display tables for covariance matrices. However, you can use the ODS OUTPUT statement to save parameter estimates and associated standard errors in a data set and the associated  $(X'X)^{-1}$  matrix in a separate data set. These data sets are then read in the MIANALYZE procedure with the PARMS= and XPXI= options, respectively. This approach is illustrated in [Example 58.6](#).

For univariate inference, only parameter estimates and associated standard errors are needed. You can use the ODS OUTPUT statement to save parameter estimates and associated standard errors in a data set. This data set is then read in the MIANALYZE procedure with the PARMS= option. This approach is illustrated in [Example 58.4](#).

## Correlation Coefficients

For the population correlation coefficient  $\rho$ , a point estimate is the sample correlation coefficient  $r$ . However, for nonzero  $\rho$ , the distribution of  $r$  is skewed.

The distribution of  $r$  can be normalized through Fisher's  $z$  transformation

$$z(r) = \frac{1}{2} \log \left( \frac{1+r}{1-r} \right)$$

$z(r)$  is approximately normally distributed with mean  $z(\rho)$  and variance  $1/(n-3)$ .

With a point estimate  $\hat{z}$  and an approximate 95% confidence interval  $(z_1, z_2)$  for  $z(\rho)$ , a point estimate  $\hat{r}$  and a 95% confidence interval  $(r_1, r_2)$  for  $\rho$  can be obtained by applying the inverse transformation

$$r = \tanh(z) = \frac{e^{2z} - 1}{e^{2z} + 1}$$

to  $z = \hat{z}, z_1,$  and  $z_2$ .

This approach is illustrated in [Example 58.10](#).

## Ratios of Variable Means

For the ratio  $\mu_1/\mu_2$  of means for variables  $Y_1$  and  $Y_2$ , the point estimate is  $\bar{y}_1/\bar{y}_2$ , the ratio of the sample means. The Taylor expansion and delta method can be applied to the function  $y_1/y_2$  to obtain the variance estimate (Schafer 1997, p. 196)

$$\frac{1}{n} \left[ \left( \frac{\bar{y}_1}{\bar{y}_2} \right)^2 s_{22} - 2 \left( \frac{\bar{y}_1}{\bar{y}_2} \right) \left( \frac{1}{\bar{y}_2} \right) s_{12} + \left( \frac{1}{\bar{y}_2} \right)^2 s_{11} \right]$$

where  $s_{11}$  and  $s_{22}$  are the sample variances of  $Y_1$  and  $Y_2$ , respectively, and  $s_{12}$  is the sample covariance between  $Y_1$  and  $Y_2$ .

A ratio of sample means will be approximately unbiased and normally distributed if the coefficient of variation of the denominator (the standard error for the mean divided by the estimated mean) is 10% or less (Cochran 1977, p. 166; Schafer 1997, p. 196).

---

## ODS Table Names

PROC MIANALYZE assigns a name to each table it creates. You must use these names to reference tables when using the Output Delivery System (ODS). These names are listed in [Table 58.3](#). For more information about ODS, see Chapter 20, "Using the Output Delivery System."

**Table 58.3** ODS Tables Produced by PROC MIANALYZE

| ODS Table Name | Description                          | Statement | Option |
|----------------|--------------------------------------|-----------|--------|
| BCov           | Between-imputation covariance matrix |           | BCOV   |
| ModelInfo      | Model information                    |           |        |
| MultStat       | Multivariate inference               |           | MULT   |

Table 58.3 continued

| ODS Table Name         | Description                                       | Statement | Option |
|------------------------|---------------------------------------------------|-----------|--------|
| ParameterEstimates     | Parameter estimates                               |           |        |
| TCov                   | Total covariance matrix                           |           | TCOV   |
| TestBCov               | Between-imputation covariance matrix for $L\beta$ | TEST      | BCOV   |
| TestMultStat           | Multivariate inference for $L\beta$               | TEST      | MULT   |
| TestParameterEstimates | Parameter estimates for $L\beta$                  | TEST      |        |
| TestSpec               | Test specification, $L$ and $c$                   | TEST      |        |
| TestTCov               | Total covariance matrix for $L\beta$              | TEST      | TCOV   |
| TestVarianceInfo       | Variance information for $L\beta$                 | TEST      |        |
| TestWCov               | Within-imputation covariance matrix for $L\beta$  | TEST      | WCOV   |
| VarianceInfo           | Variance information                              |           |        |
| WCov                   | Within-imputation covariance matrix               |           | WCOV   |

## Examples: MIANALYZE Procedure

The following statements generate five imputed data sets to be used in this section. The data set Fitness1 was created in the section “Getting Started: MIANALYZE Procedure” on page 4831. See “The MI Procedure” chapter for details concerning the MI procedure.

```
proc mi data=Fitness1 seed=3237851 noprint out=outmi;
 var Oxygen RunTime RunPulse;
run;
```

The Fish data described in the STEPDISC procedure are measurements of 159 fish of seven species caught in Finland’s lake Laengelmavesi. For each fish, the length, height, and width are measured. See Chapter 89, “The STEPDISC Procedure,” for more information.

The Fish2 data set is constructed from the Fish data set and contains two species of fish. Some values have been set to missing, and the resulting data set has a monotone missing pattern in the variables Length, Height, Width, and Species.

The following statements create the Fish2 data set. It contains two species of fish in the Fish data set.

```
-----Fish2 Data-----
| The data set contains two species of the fish (Bream and Pike) |
| and three measurements: Length, Height, Width. |
| Some values have been set to missing, and the resulting data set |
| has a monotone missing pattern in the variables |
| Length, Height, Width, and Species. |

data Fish2;
 title 'Fish Measurement Data';
 input Species $ Length Height Width @@;
 datalines;
Bream 30.0 11.520 4.020 . 31.2 12.480 4.306
Bream 31.1 12.378 4.696 Bream 33.5 12.730 4.456
```

```

. 34.0 12.444 . Bream 34.7 13.602 4.927
Bream 34.5 14.180 5.279 Bream 35.0 12.670 4.690
Bream 35.1 14.005 4.844 Bream 36.2 14.227 4.959
. 36.2 14.263 . Bream 36.2 14.371 4.815
Bream 36.4 13.759 4.368 Bream 37.3 13.913 5.073
Bream 37.2 14.954 5.171 Bream 37.2 15.438 5.580
Bream 38.3 14.860 5.285 Bream 38.5 14.938 5.198
. 38.6 15.633 5.134 Bream 38.7 14.474 5.728
Bream 39.5 15.129 5.570 . 39.2 15.994 .
Bream 39.7 15.523 5.280 Bream 40.6 15.469 6.131
. 40.5 . . Bream 40.9 16.360 6.053
Bream 40.6 16.362 6.090 Bream 41.5 16.517 5.852
Bream 41.6 16.890 6.198 Bream 42.6 18.957 6.603
Bream 44.1 18.037 6.306 Bream 44.0 18.084 6.292
Bream 45.3 18.754 6.750 Bream 45.9 18.635 6.747
Bream 46.5 17.624 6.371
Pike 34.8 5.568 3.376 Pike 37.8 5.708 4.158
Pike 38.8 5.936 4.384 . 39.8 . .
Pike 40.5 7.290 4.577 Pike 41.0 6.396 3.977
. 45.5 7.280 4.323 Pike 45.5 6.825 4.459
Pike 45.8 7.786 5.130 Pike 48.0 6.960 4.896
Pike 48.7 7.792 4.870 Pike 51.2 7.680 5.376
Pike 55.1 8.926 6.171 . 59.7 10.686 .
Pike 64.0 9.600 6.144 Pike 64.0 9.600 6.144
Pike 68.0 10.812 7.480
;

```

The following statements generate five imputed data sets to be used in this section. The default regression method is used to impute missing values in continuous variables Height and Width, and the discriminant function method is used to impute the variable Species.

```

proc mi data=Fish2 seed=1305417 out=outfish;
 class Species;
 monotone discrim(Species= Length Height Width);
 var Length Height Width Species;
run;

```

Example 58.1 through Example 58.6 use different input option combinations to combine parameter estimates computed from different procedures. Example 58.7 and Example 58.8 combine parameter estimates with classification variables. Example 58.9 shows the use of a TEST statement, and Example 58.10 combines statistics that are not directly derived from procedures.

---

## Example 58.1: Reading Means and Standard Errors from Variables in a DATA= Data Set

This example creates an ordinary SAS data set that contains sample means and standard errors computed from imputed data sets. These estimates are then combined to generate valid univariate inferences about the population means.

The following statements use the UNIVARIATE procedure to generate sample means and standard errors for the variables in each imputed data set:

```
proc univariate data=outmi noprint;
 var Oxygen RunTime RunPulse;
 output out=outuni mean=Oxygen RunTime RunPulse
 stderr=SOxygen SRunTime SRunPulse;
 by _Imputation_;
run;
```

The following statements display the output data set from PROC UNIVARIATE shown in [Output 58.1.1](#):

```
proc print data=outuni;
 title 'UNIVARIATE Means and Standard Errors';
run;
```

**Output 58.1.1** UNIVARIATE Output Data Set

| UNIVARIATE Means and Standard Errors |              |         |         |              |         |              |               |
|--------------------------------------|--------------|---------|---------|--------------|---------|--------------|---------------|
| Obs                                  | _Imputation_ | Oxygen  | RunTime | Run<br>Pulse | SOxygen | SRun<br>Time | SRun<br>Pulse |
| 1                                    | 1            | 47.0120 | 10.4441 | 171.216      | 0.95984 | 0.28520      | 1.59910       |
| 2                                    | 2            | 47.2407 | 10.5040 | 171.244      | 0.93540 | 0.26661      | 1.75638       |
| 3                                    | 3            | 47.4995 | 10.5922 | 171.909      | 1.00766 | 0.26302      | 1.85795       |
| 4                                    | 4            | 47.1485 | 10.5279 | 171.146      | 0.95439 | 0.26405      | 1.75011       |
| 5                                    | 5            | 47.0042 | 10.4913 | 172.072      | 0.96528 | 0.27275      | 1.84807       |

The following statements combine the means and standard errors from imputed data sets. The EDF= option requests that the adjusted degrees of freedom be used in the analysis. For sample means based on 31 observations, the complete-data error degrees of freedom is 30.

```
proc mianalyze data=outuni edf=30;
 modeleffects Oxygen RunTime RunPulse;
 stderr SOxygen SRunTime SRunPulse;
run;
```

The “Model Information” table in [Output 58.1.2](#) lists the input data set(s) and the number of imputations. The “Variance Information” table in [Output 58.1.2](#) displays the between-imputation variance, within-imputation variance, and total variance for each univariate inference. It also displays the degrees of freedom for the total variance. The relative increase in variance due to missing values, the fraction of missing information, and the relative efficiency for each imputed variable are also displayed. A detailed description of these statistics is provided in the section “Combining Inferences from Imputed Data Sets” on page 4844 and the section “Multiple Imputation Efficiency” on page 4845.

**Output 58.1.2** Variance Information

| The MIANALYZE Procedure |                       |             |            |        |
|-------------------------|-----------------------|-------------|------------|--------|
| Model Information       |                       |             |            |        |
|                         | Data Set              | WORK.OUTUNI |            |        |
|                         | Number of Imputations | 5           |            |        |
| Variance Information    |                       |             |            |        |
| Parameter               | -----Variance-----    |             |            | DF     |
|                         | Between               | Within      | Total      |        |
| Oxygen                  | 0.041478              | 0.930853    | 0.980626   | 26.298 |
| RunTime                 | 0.002948              | 0.073142    | 0.076679   | 26.503 |
| RunPulse                | 0.191086              | 3.114442    | 3.343744   | 25.463 |
| Variance Information    |                       |             |            |        |
| Parameter               | Relative              | Fraction    | Relative   |        |
|                         | Increase              | Missing     | Efficiency |        |
|                         | in Variance           | Information |            |        |
| Oxygen                  | 0.053471              | 0.051977    | 0.989712   |        |
| RunTime                 | 0.048365              | 0.047147    | 0.990659   |        |
| RunPulse                | 0.073626              | 0.070759    | 0.986046   |        |

The “Parameter Estimates” table in [Output 58.1.3](#) displays the estimated mean and corresponding standard error for each variable. The table also displays a 95% confidence interval for the mean and a *t* statistic with the associated *p*-value for testing the hypothesis that the mean is equal to the value specified. You can use the THETA0= option to specify the value for the null hypothesis, which is zero by default. The table also displays the minimum and maximum parameter estimates from the imputed data sets.



**Output 58.1.3** Parameter Estimates

| Parameter Estimates |            |           |                       |          |        |
|---------------------|------------|-----------|-----------------------|----------|--------|
| Parameter           | Estimate   | Std Error | 95% Confidence Limits |          | DF     |
| Oxygen              | 47.180993  | 0.990266  | 45.1466               | 49.2154  | 26.298 |
| RunTime             | 10.511906  | 0.276910  | 9.9432                | 11.0806  | 26.503 |
| RunPulse            | 171.517500 | 1.828591  | 167.7549              | 175.2801 | 25.463 |

| Parameter Estimates |            |            |
|---------------------|------------|------------|
| Parameter           | Minimum    | Maximum    |
| Oxygen              | 47.004201  | 47.499541  |
| RunTime             | 10.444149  | 10.592244  |
| RunPulse            | 171.146171 | 172.071730 |

| Parameter Estimates |        |                  |         |  |
|---------------------|--------|------------------|---------|--|
| Parameter           | Theta0 | t for H0:        |         |  |
|                     |        | Parameter=Theta0 | Pr >  t |  |
| Oxygen              | 0      | 47.64            | <.0001  |  |
| RunTime             | 0      | 37.96            | <.0001  |  |
| RunPulse            | 0      | 93.80            | <.0001  |  |

Note that the results in this example could also have been obtained with the MI procedure.

---

## Example 58.2: Reading Means and Covariance Matrices from a DATA= COV Data Set

This example creates a COV-type data set that contains sample means and covariance matrices computed from imputed data sets. These estimates are then combined to generate valid statistical inferences about the population means.

The following statements use the CORR procedure to generate sample means and a covariance matrix for the variables in each imputed data set:

```
proc corr data=outmi cov nocorr noprint out=outcov(type=cov);
 var Oxygen RunTime RunPulse;
 by _Imputation_;
run;
```

The following statements display (in [Output 58.2.1](#)) output sample means and covariance matrices from PROC CORR for the first two imputed data sets:

```
proc print data=outcov(obs=12);
 title 'CORR Means and Covariance Matrices'
 '(First Two Imputations)';
run;
```

## Output 58.2.1 COV Data Set

| CORR Means and Covariance Matrices (First Two Imputations) |              |        |          |          |         |          |
|------------------------------------------------------------|--------------|--------|----------|----------|---------|----------|
| Obs                                                        | _Imputation_ | _TYPE_ | _NAME_   | Oxygen   | RunTime | RunPulse |
| 1                                                          | 1            | COV    | Oxygen   | 28.5603  | -7.2652 | -11.812  |
| 2                                                          | 1            | COV    | RunTime  | -7.2652  | 2.5214  | 2.536    |
| 3                                                          | 1            | COV    | RunPulse | -11.8121 | 2.5357  | 79.271   |
| 4                                                          | 1            | MEAN   |          | 47.0120  | 10.4441 | 171.216  |
| 5                                                          | 1            | STD    |          | 5.3442   | 1.5879  | 8.903    |
| 6                                                          | 1            | N      |          | 31.0000  | 31.0000 | 31.000   |
| 7                                                          | 2            | COV    | Oxygen   | 27.1240  | -6.6761 | -10.217  |
| 8                                                          | 2            | COV    | RunTime  | -6.6761  | 2.2035  | 2.611    |
| 9                                                          | 2            | COV    | RunPulse | -10.2170 | 2.6114  | 95.631   |
| 10                                                         | 2            | MEAN   |          | 47.2407  | 10.5040 | 171.244  |
| 11                                                         | 2            | STD    |          | 5.2081   | 1.4844  | 9.779    |
| 12                                                         | 2            | N      |          | 31.0000  | 31.0000 | 31.000   |

Note that the covariance matrices in the data set outcov are estimated covariance matrices of variables,  $V(\mathbf{y})$ . The estimated covariance matrix of the sample means is  $V(\bar{\mathbf{y}}) = V(\mathbf{y})/n$ , where  $n$  is the sample size, and is not the same as an estimated covariance matrix for variables.

The following statements combine the results for the imputed data sets, and derive both univariate and multivariate inferences about the means. The EDF= option is specified to request that the adjusted degrees of freedom be used in the analysis. For sample means based on 31 observations, the complete-data error degrees of freedom is 30.

```
proc mianalyze data=outcov edf=30;
 modeleffects Oxygen RunTime RunPulse;
run;
```

The “Variance Information” and “Parameter Estimates” tables display the same results as in [Output 58.1.2](#) and [Output 58.1.3](#), respectively, in [Example 58.1](#).

With the WCOV, BCOV, and TCOV options, as in the following statements, the procedure displays the between-imputation covariance matrix, within-imputation covariance matrix, and total covariance matrix assuming that the between-imputation covariance matrix is proportional to the within-imputation covariance matrix in [Output 58.2.2](#).

```
proc mianalyze data=outcov edf=30 wcov bcov tcov mult;
 modeleffects Oxygen RunTime RunPulse;
run;
```

**Output 58.2.2** Covariance Matrices

| The MIANALYZE Procedure              |              |              |              |
|--------------------------------------|--------------|--------------|--------------|
| Within-Imputation Covariance Matrix  |              |              |              |
|                                      | Oxygen       | RunTime      | RunPulse     |
| Oxygen                               | 0.930852655  | -0.226506411 | -0.461022083 |
| RunTime                              | -0.226506411 | 0.073141598  | 0.080316017  |
| RunPulse                             | -0.461022083 | 0.080316017  | 3.114441784  |
| Between-Imputation Covariance Matrix |              |              |              |
|                                      | Oxygen       | RunTime      | RunPulse     |
| Oxygen                               | 0.0414778123 | 0.0099248946 | 0.0183701754 |
| RunTime                              | 0.0099248946 | 0.0029478891 | 0.0091684769 |
| RunPulse                             | 0.0183701754 | 0.0091684769 | 0.1910855259 |
| Total Covariance Matrix              |              |              |              |
|                                      | Oxygen       | RunTime      | RunPulse     |
| Oxygen                               | 1.202882661  | -0.292700068 | -0.595750001 |
| RunTime                              | -0.292700068 | 0.094516313  | 0.103787365  |
| RunPulse                             | -0.595750001 | 0.103787365  | 4.024598310  |

With the MULT option, the procedure assumes that the between-imputation covariance matrix is proportional to the within-imputation covariance matrix and displays a multivariate inference for all the parameters taken jointly.

**Output 58.2.3** Multivariate Inference

| Multivariate Inference                                         |        |        |                            |        |  |
|----------------------------------------------------------------|--------|--------|----------------------------|--------|--|
| Assuming Proportionality of Between/Within Covariance Matrices |        |        |                            |        |  |
| Avg Relative Increase in Variance                              | Num DF | Den DF | F for H0: Parameter=Theta0 | Pr > F |  |
| 0.292237                                                       | 3      | 122.68 | 12519.7                    | <.0001 |  |

The “Multivariate Inference” table in [Output 58.2.3](#) shows a significant  $p$ -value for the null hypothesis that the population means are all equal to zero.

## Example 58.3: Reading Regression Results from a DATA= EST Data Set

This example creates an EST-type data set that contains regression coefficients and their corresponding covariance matrices computed from imputed data sets. These estimates are then combined to generate valid statistical inferences about the regression model.

The following statements use the REG procedure to generate regression coefficients:

```
proc reg data=outmi outest=outreg covout noprint;
 model Oxygen= RunTime RunPulse;
 by _Imputation_;
run;
```

The following statements display (in [Output 58.3.1](#)) output regression coefficients and their covariance matrices from PROC REG for the first two imputed data sets:

```
proc print data=outreg(obs=8);
 var _Imputation_ _Type_ _Name_
 Intercept RunTime RunPulse;
 title 'REG Model Coefficients and Covariance Matrices'
 '(First Two Imputations)';
run;
```

**Output 58.3.1** EST-Type Data Set

| REG Model Coefficients and Covariance Matrices (First Two Imputations) |              |        |           |           |          |          |
|------------------------------------------------------------------------|--------------|--------|-----------|-----------|----------|----------|
| Obs                                                                    | _Imputation_ | _TYPE_ | _NAME_    | Intercept | RunTime  | RunPulse |
| 1                                                                      | 1            | PARMS  |           | 86.544    | -2.82231 | -0.05873 |
| 2                                                                      | 1            | COV    | Intercept | 100.145   | -0.53519 | -0.55077 |
| 3                                                                      | 1            | COV    | RunTime   | -0.535    | 0.10774  | -0.00345 |
| 4                                                                      | 1            | COV    | RunPulse  | -0.551    | -0.00345 | 0.00343  |
| 5                                                                      | 2            | PARMS  |           | 83.021    | -3.00023 | -0.02491 |
| 6                                                                      | 2            | COV    | Intercept | 79.032    | -0.66765 | -0.41918 |
| 7                                                                      | 2            | COV    | RunTime   | -0.668    | 0.11456  | -0.00313 |
| 8                                                                      | 2            | COV    | RunPulse  | -0.419    | -0.00313 | 0.00264  |

The following statements combine the results for the imputed data sets. The EDF= option is specified to request that the adjusted degrees of freedom be used in the analysis. For a regression model with three independent variables (including the Intercept) and 31 observations, the complete-data error degrees of freedom is 28.

```
proc mianalyze data=outreg edf=28;
 modeleffects Intercept RunTime RunPulse;
run;
```

**Output 58.3.2** Variance Information

| The MIANALYZE Procedure |                    |           |            |        |
|-------------------------|--------------------|-----------|------------|--------|
| Variance Information    |                    |           |            |        |
| Parameter               | -----Variance----- |           |            | DF     |
|                         | Between            | Within    | Total      |        |
| Intercept               | 45.529229          | 76.543614 | 131.178689 | 9.1917 |
| RunTime                 | 0.019390           | 0.106220  | 0.129487   | 18.311 |
| RunPulse                | 0.001007           | 0.002537  | 0.003746   | 12.137 |

| Variance Information |                               |                              |                     |
|----------------------|-------------------------------|------------------------------|---------------------|
| Parameter            | Relative Increase in Variance | Fraction Missing Information | Relative Efficiency |
| Intercept            | 0.713777                      | 0.461277                     | 0.915537            |
| RunTime              | 0.219051                      | 0.192620                     | 0.962905            |
| RunPulse             | 0.476384                      | 0.355376                     | 0.933641            |

The “Variance Information” table in [Output 58.3.2](#) displays the between-imputation, within-imputation, and total variances for combining complete-data inferences.

The “Parameter Estimates” table in [Output 58.3.3](#) displays the estimated mean and standard error of the regression coefficients. The inferences are based on the  $t$  distribution. The table also displays a 95% mean confidence interval and a  $t$  test with the associated  $p$ -value for the hypothesis that the regression coefficient is equal to zero. Since the  $p$ -value for RunPulse is 0.1597, this variable can be removed from the regression model.

**Output 58.3.3** Parameter Estimates

| Parameter Estimates |           |           |                       |          |        |
|---------------------|-----------|-----------|-----------------------|----------|--------|
| Parameter           | Estimate  | Std Error | 95% Confidence Limits |          | DF     |
| Intercept           | 90.837440 | 11.453327 | 65.01034              | 116.6645 | 9.1917 |
| RunTime             | -3.032870 | 0.359844  | -3.78795              | -2.2778  | 18.311 |
| RunPulse            | -0.068578 | 0.061204  | -0.20176              | 0.0646   | 12.137 |

| Parameter Estimates |           |            |  |
|---------------------|-----------|------------|--|
| Parameter           | Minimum   | Maximum    |  |
| Intercept           | 83.020730 | 100.839807 |  |
| RunTime             | -3.204426 | -2.822311  |  |
| RunPulse            | -0.112840 | -0.024910  |  |

| Parameter Estimates |        |                  |    |       |
|---------------------|--------|------------------|----|-------|
| Parameter           | Theta0 | t for H0:        |    |       |
|                     |        | Parameter=Theta0 | Pr | >  t  |
| Intercept           | 0      | 7.93             | <  | .0001 |
| RunTime             | 0      | -8.43            | <  | .0001 |
| RunPulse            | 0      | -1.12            | 0. | 2842  |

**Example 58.4: Reading Mixed Model Results from PARMs= and COVB= Data Sets**

This example creates data sets that contains parameter estimates and covariance matrices computed by a mixed model analysis for a set of imputed data sets. These estimates are then combined to generate valid statistical inferences about the parameters.

The following PROC MIXED statements generate the fixed-effect parameter estimates and covariance matrix for each imputed data set:

```
proc mixed data=outmi;
 model Oxygen= RunTime RunPulse RunTime*RunPulse/solution covb;
 by _Imputation_;
 ods output SolutionF=mixparms CovB=mixcovb;
run;
```

The following statements display (in Output 58.4.1) output parameter estimates from PROC MIXED for the first two imputed data sets:

```
proc print data=mixparms (obs=8);
 var _Imputation_ Effect Estimate StdErr;
 title 'MIXED Model Coefficients (First Two Imputations)';
run;
```

**Output 58.4.1** PROC MIXED Model Coefficients

| MIXED Model Coefficients (First Two Imputations) |              |                  |          |         |
|--------------------------------------------------|--------------|------------------|----------|---------|
| Obs                                              | _Imputation_ | Effect           | Estimate | StdErr  |
| 1                                                | 1            | Intercept        | 148.09   | 81.5231 |
| 2                                                | 1            | RunTime          | -8.8115  | 7.8794  |
| 3                                                | 1            | RunPulse         | -0.4123  | 0.4684  |
| 4                                                | 1            | RunTime*RunPulse | 0.03437  | 0.04517 |
| 5                                                | 2            | Intercept        | 64.3607  | 64.6034 |
| 6                                                | 2            | RunTime          | -1.1270  | 6.4307  |
| 7                                                | 2            | RunPulse         | 0.08160  | 0.3688  |
| 8                                                | 2            | RunTime*RunPulse | -0.01069 | 0.03664 |

The following statements display (in [Output 58.4.2](#)) the output covariance matrices associated with the parameter estimates from PROC MIXED for the first two imputed data sets:

```
proc print data=mixcovb (obs=8);
 var _Imputation_ Row Effect Col1 Col2 Col3 Col4;
 title 'Covariance Matrices (First Two Imputations)';
run;
```

**Output 58.4.2** PROC MIXED Covariance Matrices

| Covariance Matrices (First Two Imputations) |              |     |                  |          |         |          |          |
|---------------------------------------------|--------------|-----|------------------|----------|---------|----------|----------|
| Obs                                         | _Imputation_ | Row | Effect           | Col1     | Col2    | Col3     | Col4     |
| 1                                           | 1            | 1   | Intercept        | 6646.01  | -637.40 | -38.1515 | 3.6542   |
| 2                                           | 1            | 2   | RunTime          | -637.40  | 62.0842 | 3.6548   | -0.3556  |
| 3                                           | 1            | 3   | RunPulse         | -38.1515 | 3.6548  | 0.2194   | -0.02099 |
| 4                                           | 1            | 4   | RunTime*RunPulse | 3.6542   | -0.3556 | -0.02099 | 0.002040 |
| 5                                           | 2            | 1   | Intercept        | 4173.59  | -411.46 | -23.7889 | 2.3441   |
| 6                                           | 2            | 2   | RunTime          | -411.46  | 41.3545 | 2.3414   | -0.2353  |
| 7                                           | 2            | 3   | RunPulse         | -23.7889 | 2.3414  | 0.1360   | -0.01338 |
| 8                                           | 2            | 4   | RunTime*RunPulse | 2.3441   | -0.2353 | -0.01338 | 0.001343 |

Note that the variables Col1, Col2, Col3, and Col4 are used to identify the effects Intercept, RunTime, RunPulse, and RunTime\*RunPulse, respectively, through the variable Row.

For univariate inference, only parameter estimates and their associated standard errors are needed. The following statements use the MIANALYZE procedure with the input PARMs= data set to produce univariate results:

```
proc mianalyze parms=mixparms edf=28;
 modeleffects Intercept RunTime RunPulse RunTime*RunPulse;
run;
```

The “Variance Information” table in [Output 58.4.3](#) displays the between-imputation, within-imputation, and total variances for combining complete-data inferences.

**Output 58.4.3** Variance Information

| The MIANALYZE Procedure |                    |             |             |        |
|-------------------------|--------------------|-------------|-------------|--------|
| Variance Information    |                    |             |             |        |
| Parameter               | -----Variance----- |             |             | DF     |
|                         | Between            | Within      | Total       |        |
| Intercept               | 1972.654530        | 4771.948777 | 7139.134213 | 11.82  |
| RunTime                 | 14.712602          | 45.549686   | 63.204808   | 13.797 |
| RunPulse                | 0.062941           | 0.156717    | 0.232247    | 12.046 |
| RunTime*RunPulse        | 0.000470           | 0.001490    | 0.002055    | 13.983 |

| Variance Information |             |             |          |
|----------------------|-------------|-------------|----------|
| Parameter            | Relative    | Fraction    | Relative |
|                      | Increase    | Missing     |          |
|                      | in Variance | Information |          |
| Intercept            | 0.496063    | 0.365524    | 0.931875 |
| RunTime              | 0.387601    | 0.305893    | 0.942348 |
| RunPulse             | 0.481948    | 0.358274    | 0.933136 |
| RunTime*RunPulse     | 0.378863    | 0.300674    | 0.943276 |



The “Parameter Estimates” table in [Output 58.4.4](#) displays the estimated mean and standard error of the regression coefficients.

**Output 58.4.4** Parameter Estimates

| Parameter Estimates |            |           |                       |          |        |
|---------------------|------------|-----------|-----------------------|----------|--------|
| Parameter           | Estimate   | Std Error | 95% Confidence Limits |          | DF     |
| Intercept           | 136.071356 | 84.493397 | -48.3352              | 320.4779 | 11.82  |
| RunTime             | -7.457186  | 7.950145  | -24.5322              | 9.6178   | 13.797 |
| RunPulse            | -0.328104  | 0.481920  | -1.3777               | 0.7215   | 12.046 |
| RunTime*RunPulse    | 0.025364   | 0.045328  | -0.0719               | 0.1226   | 13.983 |

| Parameter Estimates |            |            |  |
|---------------------|------------|------------|--|
| Parameter           | Minimum    | Maximum    |  |
| Intercept           | 64.360719  | 186.549814 |  |
| RunTime             | -11.514341 | -1.127010  |  |
| RunPulse            | -0.602162  | 0.081597   |  |
| RunTime*RunPulse    | -0.010690  | 0.047429   |  |

| Parameter Estimates |        |                  |         |  |
|---------------------|--------|------------------|---------|--|
| Parameter           | Theta0 | t for H0:        |         |  |
|                     |        | Parameter=Theta0 | Pr >  t |  |
| Intercept           | 0      | 1.61             | 0.1337  |  |
| RunTime             | 0      | -0.94            | 0.3644  |  |
| RunPulse            | 0      | -0.68            | 0.5089  |  |
| RunTime*RunPulse    | 0      | 0.56             | 0.5846  |  |

Since each covariance matrix contains variables Row, Col1, Col2, Col3, and Col4 for parameters, the EFFECTVAR=ROWCOL option is needed when you specify the COVB= option. The following statements illustrate the use of the MIANALYZE procedure with input PARMS= and COVB(EFFECTVAR=ROWCOL)= data sets:

```
proc mianalyze parms=mixparms edf=28
 covb(effectvar=rowcol)=mixcovb;
 modeleffects Intercept RunTime RunPulse RunTime*RunPulse;
run;
```

## Example 58.5: Reading Generalized Linear Model Results

This example creates data sets that contains parameter estimates and corresponding covariance matrices computed by a generalized linear model analysis for a set of imputed data sets. These estimates are then combined to generate valid statistical inferences about the model parameters.

The following statements use PROC GENMOD to generate the parameter estimates and covariance matrix for each imputed data set:

```
proc genmod data=outmi;
 model Oxygen= RunTime RunPulse/covb;
 by _Imputation_;
 ods output ParameterEstimates=gmparms
 ParmInfo=gmpinfo
 CovB=gmcovb;
run;
```

The following statements print (in [Output 58.5.1](#)) the output parameter estimates and covariance matrix from PROC GENMOD for the first two imputed data sets:

```
proc print data=gmparms (obs=8);
 var _Imputation_ Parameter Estimate StdErr;
 title 'GENMOD Model Coefficients (First Two Imputations)';
run;
```

**Output 58.5.1** PROC GENMOD Model Coefficients

| GENMOD Model Coefficients (First Two Imputations) |              |           |          |        |
|---------------------------------------------------|--------------|-----------|----------|--------|
| Obs                                               | _Imputation_ | Parameter | Estimate | StdErr |
| 1                                                 | 1            | Intercept | 86.5440  | 9.5107 |
| 2                                                 | 1            | RunTime   | -2.8223  | 0.3120 |
| 3                                                 | 1            | RunPulse  | -0.0587  | 0.0556 |
| 4                                                 | 1            | Scale     | 2.6692   | 0.3390 |
| 5                                                 | 2            | Intercept | 83.0207  | 8.4489 |
| 6                                                 | 2            | RunTime   | -3.0002  | 0.3217 |
| 7                                                 | 2            | RunPulse  | -0.0249  | 0.0488 |
| 8                                                 | 2            | Scale     | 2.5727   | 0.3267 |

The following statements display the parameter information table in [Output 58.5.2](#). The table identifies parameter names used in the covariance matrices. The parameters Prm1, Prm2, and Prm3 are used for the effects Intercept, RunTime, and RunPulse, respectively, in each covariance matrix.

```
proc print data=gmpinfo (obs=6);
 title 'GENMOD Parameter Information (First Two Imputations)';
run;
```

**Output 58.5.2** PROC GENMOD Model Information

| GENMOD Parameter Information (First Two Imputations) |              |           |           |  |
|------------------------------------------------------|--------------|-----------|-----------|--|
| Obs                                                  | _Imputation_ | Parameter | Effect    |  |
| 1                                                    | 1            | Prm1      | Intercept |  |
| 2                                                    | 1            | Prm2      | RunTime   |  |
| 3                                                    | 1            | Prm3      | RunPulse  |  |
| 4                                                    | 2            | Prm1      | Intercept |  |
| 5                                                    | 2            | Prm2      | RunTime   |  |
| 6                                                    | 2            | Prm3      | RunPulse  |  |

The following statements display (in [Output 58.5.3](#)) the output covariance matrices from PROC GENMOD for the first two imputed data sets. Note that the GENMOD procedure computes maximum likelihood estimates for each covariance matrix.

```
proc print data=gmcovb (obs=8);
 var _Imputation_ RowName Prm1 Prm2 Prm3;
 title 'GENMOD Covariance Matrices (First Two Imputations)';
run;
```

**Output 58.5.3** PROC GENMOD Covariance Matrices

| GENMOD Covariance Matrices (First Two Imputations) |              |          |           |           |           |
|----------------------------------------------------|--------------|----------|-----------|-----------|-----------|
| Obs                                                | _Imputation_ | Row Name | Prm1      | Prm2      | Prm3      |
| 1                                                  | 1            | Prm1     | 90.453923 | -0.483394 | -0.497473 |
| 2                                                  | 1            | Prm2     | -0.483394 | 0.0973159 | -0.003113 |
| 3                                                  | 1            | Prm3     | -0.497473 | -0.003113 | 0.0030954 |
| 4                                                  | 1            | Scale    | 1.344E-15 | -1.09E-17 | -6.12E-18 |
| 5                                                  | 2            | Prm1     | 71.383332 | -0.603037 | -0.378616 |
| 6                                                  | 2            | Prm2     | -0.603037 | 0.1034766 | -0.002826 |
| 7                                                  | 2            | Prm3     | -0.378616 | -0.002826 | 0.0023843 |
| 8                                                  | 2            | Scale    | 1.602E-14 | 1.755E-16 | -1.02E-16 |

The following statements use the MIANALYZE procedure with input PARMS=, PARMINFO=, and COVB= data sets:

```
proc mianalyze parms=gmparms covb=gmcovb parminfo=gmpinfo;
 modeleffects Intercept RunTime RunPulse;
run;
```

Since the GENMOD procedure computes maximum likelihood estimates for the covariance matrix, the EDF= option is not used. The resulting model coefficients are identical to the estimates in [Output 58.3.3](#) in [Example 58.3](#). However, the standard errors are slightly different because in this example, maximum likelihood estimates for the standard errors are combined without the EDF= option, whereas in [Example 58.3](#), unbiased estimates for the standard errors are combined with the EDF= option.

## Example 58.6: Reading GLM Results from PARMs= and XPXI= Data Sets

This example creates data sets that contains parameter estimates and corresponding  $(X'X)^{-1}$  matrices computed by a general linear model analysis for a set of imputed data sets. These estimates are then combined to generate valid statistical inferences about the model parameters.

The following statements use PROC GLM to generate the parameter estimates and  $(X'X)^{-1}$  matrix for each imputed data set:

```
proc glm data=outmi;
 model Oxygen= RunTime RunPulse/inverse;
 by _Imputation_;
 ods output ParameterEstimates=glmparms
 InvXPX=glmxpxi;
quit;
```

The following statements display (in [Output 58.6.1](#)) the output parameter estimates and standard errors from PROC GLM for the first two imputed data sets:

```
proc print data=glmparms (obs=6);
 var _Imputation_ Parameter Estimate StdErr;
 title 'GLM Model Coefficients (First Two Imputations)';
run;
```

**Output 58.6.1** PROC GLM Model Coefficients

| GLM Model Coefficients (First Two Imputations) |              |           |            |             |
|------------------------------------------------|--------------|-----------|------------|-------------|
| Obs                                            | _Imputation_ | Parameter | Estimate   | StdErr      |
| 1                                              | 1            | Intercept | 86.5440339 | 10.00726811 |
| 2                                              | 1            | RunTime   | -2.8223108 | 0.32824165  |
| 3                                              | 1            | RunPulse  | -0.0587292 | 0.05854109  |
| 4                                              | 2            | Intercept | 83.0207303 | 8.88996885  |
| 5                                              | 2            | RunTime   | -3.0002288 | 0.33847204  |
| 6                                              | 2            | RunPulse  | -0.0249103 | 0.05137859  |

The following statements display (in [Output 58.6.2](#))  $(X'X)^{-1}$  matrices from PROC GLM for the first two imputed data sets:

```
proc print data=glmxpxi (obs=8);
 var _Imputation_ Parameter Intercept RunTime RunPulse;
 title 'GLM X'X Inverse Matrices (First Two Imputations)';
run;
```

**Output 58.6.2** PROC GLM  $(X'X)^{-1}$  Matrices

| GLM X'X Inverse Matrices (First Two Imputations) |              |           |              |              |              |
|--------------------------------------------------|--------------|-----------|--------------|--------------|--------------|
| Obs                                              | _Imputation_ | Parameter | Intercept    | RunTime      | RunPulse     |
| 1                                                | 1            | Intercept | 12.696250656 | -0.067849956 | -0.069826009 |
| 2                                                | 1            | RunTime   | -0.067849956 | 0.0136594055 | -0.000436938 |
| 3                                                | 1            | RunPulse  | -0.069826009 | -0.000436938 | 0.0004344762 |
| 4                                                | 1            | Oxygen    | 86.544033929 | -2.822310769 | -0.058729234 |
| 5                                                | 2            | Intercept | 10.784620785 | -0.091107072 | -0.057201387 |
| 6                                                | 2            | RunTime   | -0.091107072 | 0.0156332765 | -0.000426902 |
| 7                                                | 2            | RunPulse  | -0.057201387 | -0.000426902 | 0.0003602208 |
| 8                                                | 2            | Oxygen    | 83.020730343 | -3.000228818 | -0.024910305 |

The standard errors for the estimates in the output `glmparms` data set are needed to create the covariance matrix from the  $(X'X)^{-1}$  matrix. The following statements use the MIANALYZE procedure with input `PARMS=` and `XPXI=` data sets to produce the same results as displayed in [Output 58.3.2](#) and [Output 58.3.3](#) in [Example 58.3](#):

```
proc mianalyze parms=glmparms xpxi=glmxpxi edf=28;
 modeleffects Intercept RunTime RunPulse;
run;
```

---

### Example 58.7: Reading Logistic Model Results from `PARMS=` and `COVB=` Data Sets

This example creates data sets that contains parameter estimates and corresponding covariance matrices computed by a logistic regression analysis for a set of imputed data sets. These estimates are then combined to generate valid statistical inferences about the model parameters.

The following statements use PROC LOGISTIC to generate the parameter estimates and covariance matrix for each imputed data set:

```
proc logistic data=outfish;
 class Species;
 model Species= Height Width Height*Width/ covb;
 by _Imputation_;
 ods output ParameterEstimates=lgsparms
 CovB=lgscovb;
run;
```

The following statements display (in [Output 58.7.1](#)) the output logistic regression coefficients from PROC LOGISTIC for the first two imputed data sets:

```
proc print data=lgsparms (obs=8);
 title 'LOGISTIC Model Coefficients (First Two Imputations)';
run;
```

**Output 58.7.1** PROC LOGISTIC Model Coefficients

| LOGISTIC Model Coefficients (First Two Imputations) |              |              |    |          |         |           |               |           |
|-----------------------------------------------------|--------------|--------------|----|----------|---------|-----------|---------------|-----------|
| Obs                                                 | _Imputation_ | Variable     | DF | Estimate | StdErr  | WaldChiSq | Prob<br>ChiSq | _ESTTYPE_ |
| 1                                                   | 1            | Intercept    | 1  | -28.2353 | 316.1   | 0.0080    | 0.9288        | MLE       |
| 2                                                   | 1            | Height       | 1  | 5.3362   | 28.1298 | 0.0360    | 0.8495        | MLE       |
| 3                                                   | 1            | Width        | 1  | -1.0812  | 60.8035 | 0.0003    | 0.9858        | MLE       |
| 4                                                   | 1            | Height*Width | 1  | -0.4304  | 5.1312  | 0.0070    | 0.9332        | MLE       |
| 5                                                   | 2            | Intercept    | 1  | -44.0620 | 262.5   | 0.0282    | 0.8667        | MLE       |
| 6                                                   | 2            | Height       | 1  | 7.3887   | 23.1824 | 0.1016    | 0.7499        | MLE       |
| 7                                                   | 2            | Width        | 1  | 1.6950   | 49.1462 | 0.0012    | 0.9725        | MLE       |
| 8                                                   | 2            | Height*Width | 1  | -0.7692  | 4.0205  | 0.0366    | 0.8483        | MLE       |

The following statements displays the covariance matrices associated with parameter estimates derived from the first two imputations in [Output 58.7.2](#):

```
proc print data=lgscovb (obs=8);
 title 'LOGISTIC Model Covariance Matrices (First Two Imputations)';
run;
```

**Output 58.7.2** PROC LOGISTIC Covariance Matrices

| LOGISTIC Model Covariance Matrices (First Two Imputations) |              |             |           |          |          |                 |
|------------------------------------------------------------|--------------|-------------|-----------|----------|----------|-----------------|
| Obs                                                        | _Imputation_ | Parameter   | Intercept | Height   | Width    | Height<br>Width |
| 1                                                          | 1            | Intercept   | 99938.75  | -8395.34 | -18879.9 | 1556.383        |
| 2                                                          | 1            | Height      | -8395.34  | 791.2859 | 1535.382 | -142.121        |
| 3                                                          | 1            | Width       | -18879.9  | 1535.382 | 3697.064 | -294.815        |
| 4                                                          | 1            | HeightWidth | 1556.383  | -142.121 | -294.815 | 26.32931        |
| 5                                                          | 2            | Intercept   | 68903.42  | -5586.74 | -12603.5 | 1000.283        |
| 6                                                          | 2            | Height      | -5586.74  | 537.4232 | 958.5588 | -91.2266        |
| 7                                                          | 2            | Width       | -12603.5  | 958.5588 | 2415.346 | -180.394        |
| 8                                                          | 2            | HeightWidth | 1000.283  | -91.2266 | -180.394 | 16.16428        |

The following statements use the MIANALYZE procedure with input PARMS= and COVB= data sets:

```
proc mianalyze parms=lgsparms
 covb(effectvar=stacking)=lgscovb;
 modeleffects Intercept Height Width Height*Width;
run;
```

The “Variance Information” table in [Output 58.7.3](#) displays the between-imputation, within-imputation, and total variances for combining complete-data inferences.

**Output 58.7.3** Variance Information

| The MIANALYZE Procedure |                    |             |             |        |
|-------------------------|--------------------|-------------|-------------|--------|
| Variance Information    |                    |             |             |        |
| Parameter               | -----Variance----- |             |             | DF     |
|                         | Between            | Within      | Total       |        |
| Intercept               | 283.306802         | 93045       | 93385       | 301811 |
| Height                  | 4.985634           | 751.535758  | 757.518519  | 64127  |
| Width                   | 6.262249           | 3331.888954 | 3339.403653 | 789905 |
| Height*Width            | 0.113341           | 23.797208   | 23.933217   | 123858 |

| Variance Information |             |             |          |
|----------------------|-------------|-------------|----------|
| Parameter            | Relative    | Fraction    | Relative |
|                      | Increase    | Missing     |          |
|                      | in Variance | Information |          |
| Intercept            | 0.003654    | 0.003647    | 0.999271 |
| Height               | 0.007961    | 0.007929    | 0.998417 |
| Width                | 0.002255    | 0.002253    | 0.999550 |
| Height*Width         | 0.005715    | 0.005699    | 0.998862 |

The “Parameter Estimates” table in [Output 58.7.4](#) displays the combined parameter estimates with associated standard errors.

**Output 58.7.4** Parameter Estimates

| Parameter Estimates |            |            |                       |          |        |
|---------------------|------------|------------|-----------------------|----------|--------|
| Parameter           | Estimate   | Std Error  | 95% Confidence Limits |          | DF     |
| Intercept           | -45.536682 | 305.589037 | -644.483              | 553.4092 | 301811 |
| Height              | 7.452449   | 27.523054  | -46.493               | 61.3977  | 64127  |
| Width               | 1.548439   | 57.787574  | -111.713              | 114.8102 | 789905 |
| Height*Width        | -0.754088  | 4.892159   | -10.343               | 8.8345   | 123858 |

| Parameter Estimates |            |            |
|---------------------|------------|------------|
| Parameter           | Minimum    | Maximum    |
| Intercept           | -73.331892 | -28.235273 |
| Height              | 5.336231   | 11.217552  |
| Width               | -1.081173  | 5.645810   |
| Height*Width        | -1.313883  | -0.430377  |

| Parameter Estimates |        |                  |         |  |
|---------------------|--------|------------------|---------|--|
| Parameter           | Theta0 | t for H0:        |         |  |
|                     |        | Parameter=Theta0 | Pr >  t |  |
| Intercept           | 0      | -0.15            | 0.8815  |  |
| Height              | 0      | 0.27             | 0.7866  |  |
| Width               | 0      | 0.03             | 0.9786  |  |
| Height*Width        | 0      | -0.15            | 0.8775  |  |

## Example 58.8: Reading Mixed Model Results with Classification Variables

This example creates data sets that contains parameter estimates and corresponding covariance matrices with classification variables computed by a mixed regression model analysis for a set of imputed data sets. These estimates are then combined to generate valid statistical inferences about the model parameters.

The following statements use PROC MIXED to generate the parameter estimates and covariance matrix for each imputed data set:

```
proc mixed data=outfish;
 class Species;
 model Length= Species Height Width/ solution covb;
 by _Imputation_;
 ods output SolutionF=mxparms CovB=mxcovb;
run;
```



The following statements display (in [Output 58.8.1](#)) the output mixed model coefficients from PROC MIXED for the first two imputed data sets:

```
proc print data=mxparms (obs=10);
 var _Imputation_ Effect Species Estimate StdErr;
 title 'MIXED Model Coefficients (First Two Imputations)';
run;
```

**Output 58.8.1** PROC MIXED Model Coefficients

| MIXED Model Coefficients (First Two Imputations) |              |           |         |          |        |
|--------------------------------------------------|--------------|-----------|---------|----------|--------|
| Obs                                              | _Imputation_ | Effect    | Species | Estimate | StdErr |
| 1                                                | 1            | Intercept |         | 12.5356  | 2.7808 |
| 2                                                | 1            | Species   | Bream   | -11.9103 | 3.5386 |
| 3                                                | 1            | Species   | Pike    | 0        | .      |
| 4                                                | 1            | Height    |         | -0.1605  | 0.5158 |
| 5                                                | 1            | Width     |         | 7.3962   | 1.1365 |
| 6                                                | 2            | Intercept |         | 13.3607  | 2.7848 |
| 7                                                | 2            | Species   | Bream   | -10.5204 | 3.0517 |
| 8                                                | 2            | Species   | Pike    | 0        | .      |
| 9                                                | 2            | Height    |         | -0.3139  | 0.4384 |
| 10                                               | 2            | Width     |         | 7.4861   | 1.0005 |

The following statements use the MIANALYZE procedure with an input PARMS= data set:

```
proc mianalyze parms(classvar=full)=mxparms;
 class Species;
 modeleffects Intercept Species Height Width;
run;
```

The “Variance Information” table in [Output 58.8.2](#) displays the between-imputation, within-imputation, and total variances for combining complete-data inferences.

**Output 58.8.2** Variance Information

| The MIANALYZE Procedure |         |          |           |           |        |
|-------------------------|---------|----------|-----------|-----------|--------|
| Variance Information    |         |          |           |           |        |
| -----Variance-----      |         |          |           |           |        |
| Parameter               | Species | Between  | Within    | Total     | DF     |
| Intercept               |         | 0.325023 | 7.632716  | 8.022743  | 1692.4 |
| Species                 | Bream   | 0.307202 | 10.394843 | 10.763486 | 3410   |
| Species                 | Pike    | 0        | .         | .         | .      |
| Height                  |         | 0.003686 | 0.217662  | 0.222085  | 10085  |
| Width                   |         | 0.006488 | 1.097103  | 1.104888  | 80560  |

| Variance Information |         |                               |                              |                     |
|----------------------|---------|-------------------------------|------------------------------|---------------------|
| Parameter            | Species | Relative Increase in Variance | Fraction Missing Information | Relative Efficiency |
| Intercept            |         | 0.051099                      | 0.049738                     | 0.990150            |
| Species              | Bream   | 0.035464                      | 0.034815                     | 0.993085            |
| Species              | Pike    | .                             | .                            | .                   |
| Height               |         | 0.020320                      | 0.020110                     | 0.995994            |
| Width                |         | 0.007096                      | 0.007071                     | 0.998588            |

The “Parameter Estimates” table in [Output 58.8.3](#) displays the combined parameter estimates with associated standard errors.

**Output 58.8.3** Parameter Estimates

| Parameter Estimates |         |            |           |                       |          |        |
|---------------------|---------|------------|-----------|-----------------------|----------|--------|
| Parameter           | Species | Estimate   | Std Error | 95% Confidence Limits |          | DF     |
| Intercept           |         | 12.669835  | 2.832445  | 7.1144                | 18.22530 | 1692.4 |
| Species             | Bream   | -11.180159 | 3.280775  | -17.6126              | -4.74767 | 3410   |
| Species             | Pike    | 0          | .         | .                     | .        | .      |
| Height              |         | -0.246488  | 0.471259  | -1.1702               | 0.67727  | 10085  |
| Width               |         | 7.511074   | 1.051137  | 5.4509                | 9.57130  | 80560  |

| Parameter Estimates |           |         |            |            |
|---------------------|-----------|---------|------------|------------|
|                     | Parameter | Species | Minimum    | Maximum    |
|                     | Intercept |         | 12.004593  | 13.360690  |
|                     | Species   | Bream   | -11.910303 | -10.520395 |
|                     | Species   | Pike    | 0          | 0          |
|                     | Height    |         | -0.313882  | -0.160511  |
|                     | Width     |         | 7.396172   | 7.594860   |

| Parameter Estimates |           |         |        |                               |         |
|---------------------|-----------|---------|--------|-------------------------------|---------|
|                     | Parameter | Species | Theta0 | t for H0:<br>Parameter=Theta0 | Pr >  t |
|                     | Intercept |         | 0      | 4.47                          | <.0001  |
|                     | Species   | Bream   | 0      | -3.41                         | 0.0007  |
|                     | Species   | Pike    | 0      | .                             | .       |
|                     | Height    |         | 0      | -0.52                         | 0.6010  |
|                     | Width     |         | 0      | 7.15                          | <.0001  |

### Example 58.9: Using a TEST statement

This example creates an EST-type data set that contains regression coefficients and their corresponding covariance matrices computed from imputed data sets. These estimates are then combined to generate valid statistical inferences about the regression model. A TEST statement is used to test linear hypotheses about the parameters.

The following statements use the REG procedure to generate regression coefficients:

```
proc reg data=outmi outest=outreg covout noprint;
 model Oxygen= RunTime RunPulse;
 by _Imputation_;
run;
```

The following statements combine the results for the imputed data sets. A TEST statement is used to test linear hypotheses of Intercept=0 and RunTime=RunPulse.

```
proc mianalyze data=outreg edf=28;
 modeleffects Intercept RunTime RunPulse;
 test Intercept, RunTime=RunPulse / mult;
run;
```

The “Test Specification” table in [Output 58.9.1](#) displays the L matrix and the c vector in a TEST statement. Since there is no label specified for the TEST statement, “Test 1” is used as the label.

**Output 58.9.1** Test Specification

| The MIANALYZE Procedure |           |          |           |   |
|-------------------------|-----------|----------|-----------|---|
| Test: Test 1            |           |          |           |   |
| Test Specification      |           |          |           |   |
| -----L Matrix-----      |           |          |           |   |
| Parameter               | Intercept | RunTime  | RunPulse  | C |
| TestPrm1                | 1.000000  | 0        | 0         | 0 |
| TestPrm2                | 0         | 1.000000 | -1.000000 | 0 |

The “Variance Information” table in [Output 58.9.2](#) displays the between-imputation variance, within-imputation variance, and total variance for each univariate inference. A detailed description of these statistics is provided in the section “[Combining Inferences from Imputed Data Sets](#)” on page 4844 and the section “[Multiple Imputation Efficiency](#)” on page 4845.

**Output 58.9.2** Variance Information

| Variance Information |           |           |            |        |
|----------------------|-----------|-----------|------------|--------|
| -----Variance-----   |           |           |            |        |
| Parameter            | Between   | Within    | Total      | DF     |
| TestPrm1             | 45.529229 | 76.543614 | 131.178689 | 9.1917 |
| TestPrm2             | 0.014715  | 0.114324  | 0.131983   | 20.598 |

| Variance Information |                               |                              |                     |
|----------------------|-------------------------------|------------------------------|---------------------|
| Parameter            | Relative Increase in Variance | Fraction Missing Information | Relative Efficiency |
| TestPrm1             | 0.713777                      | 0.461277                     | 0.915537            |
| TestPrm2             | 0.154459                      | 0.141444                     | 0.972490            |

The “Parameter Estimates” table in [Output 58.9.3](#) displays the estimated mean and standard error of the linear components. The inferences are based on the  $t$  distribution. The table also displays a 95% mean confidence interval and a  $t$  test with the associated  $p$ -value for the hypothesis that each linear component of  $L\beta$  is equal to zero.

**Output 58.9.3** Parameter Estimates

| Parameter Estimates |           |           |                       |          |        |
|---------------------|-----------|-----------|-----------------------|----------|--------|
| Parameter           | Estimate  | Std Error | 95% Confidence Limits |          | DF     |
| TestPrm1            | 90.837440 | 11.453327 | 65.01034              | 116.6645 | 9.1917 |
| TestPrm2            | -2.964292 | 0.363294  | -3.72070              | -2.2079  | 20.598 |

| Parameter Estimates |           |            |   |             |         |
|---------------------|-----------|------------|---|-------------|---------|
| Parameter           | Minimum   | Maximum    | C | t for H0:   |         |
|                     |           |            |   | Parameter=C | Pr >  t |
| TestPrm1            | 83.020730 | 100.839807 | 0 | 7.93        | <.0001  |
| TestPrm2            | -3.091586 | -2.763582  | 0 | -8.16       | <.0001  |

With the MULT option, the procedure assumes that the between-imputation covariance matrix is proportional to the within-imputation covariance matrix and displays a multivariate inference for all the linear components taken jointly in [Output 58.9.4](#).

**Output 58.9.4** Multivariate Inference

| Multivariate Inference                                         |        |        |                  |        |  |
|----------------------------------------------------------------|--------|--------|------------------|--------|--|
| Assuming Proportionality of Between/Within Covariance Matrices |        |        |                  |        |  |
| Avg Relative Increase in Variance                              | Num DF | Den DF | F for H0:        |        |  |
|                                                                |        |        | Parameter=Theta0 | Pr > F |  |
| 0.419868                                                       | 2      | 35.053 | 60.34            | <.0001 |  |

### Example 58.10: Combining Correlation Coefficients

This example combines sample correlation coefficients computed from a set of imputed data sets by using Fisher’s  $z$  transformation.

Fisher’s  $z$  transformation of the sample correlation  $r$  is

$$z = \frac{1}{2} \log \left( \frac{1+r}{1-r} \right)$$

The statistic  $z$  is approximately normally distributed with mean

$$\log\left(\frac{1+\rho}{1-\rho}\right)$$

and variance  $1/(n-3)$ , where  $\rho$  is the population correlation coefficient and  $n$  is the number of observations.

The following statements use the CORR procedure to compute the correlation  $r$  and its associated Fisher's  $z$  statistic between variables Oxygen and RunTime for each imputed data set. The ODS statement is used to save Fisher's  $z$  statistic in an output data set.

```
proc corr data=outmi fisher(biasadj=no);
 var Oxygen RunTime;
 by _Imputation_;
 ods output FisherPearsonCorr= outz;
run;
```

The following statements display the number of observations and Fisher's  $z$  statistic for each imputed data set in [Output 58.10.1](#):

```
proc print data=outz;
 title 'Fisher's Correlation Statistics';
 var _Imputation_ NObs ZVal;
run;
```

**Output 58.10.1** Output  $z$  Statistics

| Fisher's Correlation Statistics |              |      |          |  |
|---------------------------------|--------------|------|----------|--|
| Obs                             | _Imputation_ | NObs | ZVal     |  |
| 1                               | 1            | 31   | -1.27869 |  |
| 2                               | 2            | 31   | -1.30715 |  |
| 3                               | 3            | 31   | -1.27922 |  |
| 4                               | 4            | 31   | -1.39243 |  |
| 5                               | 5            | 31   | -1.40146 |  |

The following statements generate the standard error associated with the  $z$  statistic,  $1/\sqrt{n-3}$ :

```
data outz;
 set outz;
 StdZ= 1. / sqrt(NObs-3);
run;
```

The following statements use the MIANALYZE procedure to generate a combined parameter estimate  $\hat{z}$  and its variance, as shown in [Output 58.10.2](#). The ODS statement is used to save the parameter estimates in an output data set.

```
proc mianalyze data=outz;
 ods output ParameterEstimates=parms;
 modeleffects ZVal;
 stderr StdZ;
run;
```

**Output 58.10.2** Combining Fisher's  $z$  Statistics

| The MIANALYZE Procedure |           |                               |                       |          |        |
|-------------------------|-----------|-------------------------------|-----------------------|----------|--------|
| Parameter Estimates     |           |                               |                       |          |        |
| Parameter               | Estimate  | Std Error                     | 95% Confidence Limits |          | DF     |
| ZVal                    | -1.331787 | 0.200327                      | -1.72587              | -0.93771 | 330.23 |
| Parameter Estimates     |           |                               |                       |          |        |
| Parameter               | Minimum   | Maximum                       |                       |          |        |
| ZVal                    | -1.401459 | -1.278686                     |                       |          |        |
| Parameter Estimates     |           |                               |                       |          |        |
| Parameter               | Theta0    | t for H0:<br>Parameter=Theta0 |                       | Pr >  t  |        |
| ZVal                    | 0         | -6.65                         |                       | <.0001   |        |

In addition to the estimate for  $z$ , PROC MIANALYZE also generates 95% confidence limits for  $z$ ,  $\hat{z}_{.025}$  and  $\hat{z}_{.975}$ . The following statements print the estimate and 95% confidence limits for  $z$  in [Output 58.10.3](#):

```
proc print data=parms;
 title 'Parameter Estimates with 95% Confidence Limits';
 var Estimate LCLMean UCLMean;
run;
```

**Output 58.10.3** Parameter Estimates with 95% Confidence Limits

| Parameter Estimates with 95% Confidence Limits |           |          |          |
|------------------------------------------------|-----------|----------|----------|
| Obs                                            | Estimate  | LCLMean  | UCLMean  |
| 1                                              | -1.331787 | -1.72587 | -0.93771 |

An estimate of the correlation coefficient with its corresponding 95% confidence limits is then generated from the following inverse transformation as described in the section “[Correlation Coefficients](#)” on page 4849:

$$r = \tanh(z) = \frac{e^{2z} - 1}{e^{2z} + 1}$$

for  $z = \hat{z}$ ,  $\hat{z}_{.025}$ , and  $\hat{z}_{.975}$ .

The following statements generate and display an estimate of the correlation coefficient and its 95% confidence limits, as shown in [Output 58.10.4](#):

```
data corr_ci;
 set parms;
 r= tanh(Estimate);
 r_lower= tanh(LCLMean);
 r_upper= tanh(UCLMean);
run;
proc print data=corr_ci;
 title 'Estimated Correlation Coefficient '
 ' with 95% Confidence Limits';
 var r r_lower r_upper;
run;
```

**Output 58.10.4** Estimated Correlation Coefficient

| Estimated Correlation Coefficient with 95% Confidence Limits |          |          |          |
|--------------------------------------------------------------|----------|----------|----------|
| Obs                                                          | r        | r_lower  | r_upper  |
| 1                                                            | -0.86969 | -0.93857 | -0.73417 |

---

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# Chapter 59

## The MIXED Procedure

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| References . . . . .                                                  | <b>5071</b> |

---

## Overview: MIXED Procedure

The MIXED procedure fits a variety of mixed linear models to data and enables you to use these fitted models to make statistical inferences about the data. A *mixed linear model* is a generalization of the standard linear model used in the GLM procedure, the generalization being that the data are permitted to exhibit correlation and nonconstant variability. The mixed linear model, therefore, provides you with the flexibility of modeling not only the means of your data (as in the standard linear model) but their variances and covariances as well.

The primary assumptions underlying the analyses performed by PROC MIXED are as follows:

- The data are normally distributed (Gaussian).
- The means (expected values) of the data are linear in terms of a certain set of parameters.
- The variances and covariances of the data are in terms of a different set of parameters, and they exhibit a structure matching one of those available in PROC MIXED.

Since Gaussian data can be modeled entirely in terms of their means and variances/covariances, the two sets of parameters in a mixed linear model actually specify the complete probability distribution of the data. The parameters of the mean model are referred to as *fixed-effects parameters*, and the parameters of the variance-covariance model are referred to as *covariance parameters*.

The fixed-effects parameters are associated with known explanatory variables, as in the standard linear model. These variables can be either qualitative (as in the traditional analysis of variance) or quantitative (as in standard linear regression). However, the covariance parameters are what distinguishes the mixed linear model from the standard linear model.

The need for covariance parameters arises quite frequently in applications, the following being the two most typical scenarios:

- The experimental units on which the data are measured can be grouped into clusters, and the data from a common cluster are correlated.
- Repeated measurements are taken on the same experimental unit, and these repeated measurements are correlated or exhibit variability that changes.

The first scenario can be generalized to include one set of clusters nested within another. For example, if students are the experimental unit, they can be clustered into classes, which in turn can be clustered into schools. Each level of this hierarchy can introduce an additional source of variability and correlation. The second scenario occurs in longitudinal studies, where repeated measurements are taken over time. Alternatively, the repeated measures could be spatial or multivariate in nature.

PROC MIXED provides a variety of covariance structures to handle the previous two scenarios. The most common of these structures arises from the use of *random-effects parameters*, which are additional unknown random variables assumed to affect the variability of the data. The variances of the random-effects parameters, commonly known as *variance components*, become the covariance parameters for this particular structure. Traditional mixed linear models contain both fixed- and random-effects parameters, and, in fact, it is the combination of these two types of effects that led to the name *mixed model*. PROC MIXED fits not only these traditional variance component models but numerous other covariance structures as well.

PROC MIXED fits the structure you select to the data by using the method of *restricted maximum likelihood (REML)*, also known as *residual maximum likelihood*. It is here that the Gaussian assumption for the data is exploited. Other estimation methods are also available, including *maximum likelihood* and *MIVQUE0*. The details behind these estimation methods are discussed in subsequent sections.

After a model has been fit to your data, you can use it to draw statistical inferences via both the fixed-effects and covariance parameters. PROC MIXED computes several different statistics suitable for generating hypothesis tests and confidence intervals. The validity of these statistics depends upon the mean and variance-covariance model you select, so it is important to choose the model carefully. Some of the output from PROC MIXED helps you assess your model and compare it with others.

---

## Basic Features

PROC MIXED provides easy accessibility to numerous mixed linear models that are useful in many common statistical analyses. In the style of the GLM procedure, PROC MIXED fits the specified mixed linear model and produces appropriate statistics.

Here are some basic features of PROC MIXED:

- covariance structures, including variance components, compound symmetry, unstructured, AR(1), Toeplitz, spatial, general linear, and factor analytic
- GLM-type grammar, by using **MODEL**, **RANDOM**, and **REPEATED** statements for model specification and **CONTRAST**, **ESTIMATE**, and **LSMEANS** statements for inferences
- appropriate standard errors for all specified estimable linear combinations of fixed and random effects, and corresponding *t* and *F* tests
- subject and group effects that enable blocking and heterogeneity, respectively
- REML and ML estimation methods implemented with a Newton-Raphson algorithm
- capacity to handle unbalanced data
- ability to create a SAS data set corresponding to any table

PROC MIXED uses the Output Delivery System (ODS), a SAS subsystem that provides capabilities for displaying and controlling the output from SAS procedures. ODS enables you to convert any of the output from PROC MIXED into a SAS data set. See the section “ODS Table Names” on page 4987.

The MIXED procedure uses ODS Graphics to create graphs as part of its output. For general information about ODS Graphics, see Chapter 21, “Statistical Graphics Using ODS.” For specific information about the statistical graphics available with the MIXED procedure, see the PLOTS= option in the PROC MIXED statement and the section “ODS Graphics” on page 4992.

---

## Notation for the Mixed Model

This section introduces the mathematical notation used throughout this chapter to describe the mixed linear model. You should be familiar with basic matrix algebra (see Searle 1982). A more detailed description of the mixed model is contained in the section “Mixed Models Theory” on page 4958.

A statistical model is a mathematical description of how data are generated. The standard linear model, as used by the GLM procedure, is one of the most common statistical models:

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

In this expression,  $\mathbf{y}$  represents a vector of observed data,  $\boldsymbol{\beta}$  is an unknown vector of fixed-effects parameters with known design matrix  $\mathbf{X}$ , and  $\boldsymbol{\epsilon}$  is an unknown random error vector modeling the statistical noise around  $\mathbf{X}\boldsymbol{\beta}$ . The focus of the standard linear model is to model the mean of  $\mathbf{y}$  by using the fixed-effects parameters  $\boldsymbol{\beta}$ . The residual errors  $\boldsymbol{\epsilon}$  are assumed to be independent and identically distributed Gaussian random variables with mean 0 and variance  $\sigma^2$ .

The mixed model generalizes the standard linear model as follows:

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\boldsymbol{\gamma} + \boldsymbol{\epsilon}$$

Here,  $\boldsymbol{\gamma}$  is an unknown vector of random-effects parameters with known design matrix  $\mathbf{Z}$ , and  $\boldsymbol{\epsilon}$  is an unknown random error vector whose elements are no longer required to be independent and homogeneous.

To further develop this notion of variance modeling, assume that  $\boldsymbol{\gamma}$  and  $\boldsymbol{\epsilon}$  are Gaussian random variables that are uncorrelated and have expectations  $\mathbf{0}$  and variances  $\mathbf{G}$  and  $\mathbf{R}$ , respectively. The variance of  $\mathbf{y}$  is thus

$$\mathbf{V} = \mathbf{Z}\mathbf{G}\mathbf{Z}' + \mathbf{R}$$

Note that, when  $\mathbf{R} = \sigma^2\mathbf{I}$  and  $\mathbf{Z} = \mathbf{0}$ , the mixed model reduces to the standard linear model.

You can model the variance of the data,  $\mathbf{y}$ , by specifying the structure (or form) of  $\mathbf{Z}$ ,  $\mathbf{G}$ , and  $\mathbf{R}$ . The model matrix  $\mathbf{Z}$  is set up in the same fashion as  $\mathbf{X}$ , the model matrix for the fixed-effects parameters. For  $\mathbf{G}$  and  $\mathbf{R}$ , you must select some *covariance structure*. Possible covariance structures include the following:

- variance components
- compound symmetry (common covariance plus diagonal)
- unstructured (general covariance)
- autoregressive

- spatial
- general linear
- factor analytic

By appropriately defining the model matrices  $\mathbf{X}$  and  $\mathbf{Z}$ , as well as the covariance structure matrices  $\mathbf{G}$  and  $\mathbf{R}$ , you can perform numerous mixed model analyses.

---

## PROC MIXED Contrasted with Other SAS Procedures

PROC MIXED is a generalization of the GLM procedure in the sense that PROC GLM fits standard linear models, and PROC MIXED fits the wider class of mixed linear models. Both procedures have similar **CLASS**, **MODEL**, **CONTRAST**, **ESTIMATE**, and **LSMEANS** statements, but their **RANDOM** and **REPEATED** statements differ (see the following paragraphs). Both procedures use the non-full-rank model parameterization, although the sorting of classification levels can differ between the two. PROC MIXED computes only Type I–Type III tests of fixed effects, while PROC GLM computes Types I–IV.

The **RANDOM** statement in PROC MIXED incorporates random effects constituting the  $\boldsymbol{\gamma}$  vector in the mixed model. However, in PROC GLM, effects specified in the **RANDOM** statement are still treated as fixed as far as the model fit is concerned, and they serve only to produce corresponding expected mean squares. These expected mean squares lead to the traditional ANOVA estimates of variance components. PROC MIXED computes REML and ML estimates of variance parameters, which are generally preferred to the ANOVA estimates (Searle 1988; Harville 1988; Searle, Casella, and McCulloch 1992). Optionally, PROC MIXED also computes MIVQUE0 estimates, which are similar to ANOVA estimates.

The **REPEATED** statement in PROC MIXED is used to specify covariance structures for repeated measurements on subjects, while the **REPEATED** statement in PROC GLM is used to specify various transformations with which to conduct the traditional univariate or multivariate tests. In repeated measures situations, the mixed model approach used in PROC MIXED is more flexible and more widely applicable than either the univariate or multivariate approach. In particular, the mixed model approach provides a larger class of covariance structures and a better mechanism for handling missing values (Wolfinger and Chang 1995).

PROC MIXED subsumes the VARCOMP procedure. PROC MIXED provides a wide variety of covariance structures, while PROC VARCOMP estimates only simple random effects. PROC MIXED carries out several analyses that are absent in PROC VARCOMP, including the estimation and testing of linear combinations of fixed and random effects.

The ARIMA and AUTOREG procedures provide more time series structures than PROC MIXED, although they do not fit variance component models. The CALIS procedure fits general covariance matrices, but the fixed effects structure of the model is formed differently than in PROC MIXED. The LATTICE and NESTED procedures fit special types of mixed linear models that can also be handled in PROC MIXED, although PROC MIXED might run slower because of its more general algorithm. The TSCSREG procedure analyzes time series cross-sectional data, and it fits some structures not available in PROC MIXED.

The GLIMMIX procedure fits generalized linear mixed models (GLMMs). Linear mixed models—where the data are normally distributed, given the random effects—are in the class of GLMMs. The MIXED procedure can estimate covariance parameters with ANOVA methods that are not available in the GLIMMIX procedure (see **METHOD=TYPE1**, **METHOD=TYPE2**, and **METHOD=TYPE3** in the **PROC MIXED**

statement). Also, PROC MIXED can perform a sampling-based Bayesian analysis through the **PRIOR** statement, and the procedure supports certain Kronecker-type covariance structures. These features are not available in the GLIMMIX procedure. The GLIMMIX procedure, on the other hand, accommodates nonnormal data and offers a broader array of post-processing features than the MIXED procedure.

---

## Getting Started: MIXED Procedure

---

### Clustered Data Example

Consider the following SAS data set as an introductory example:

```
data heights;
 input Family Gender$ Height @@;
 datalines;
1 F 67 1 F 66 1 F 64 1 M 71 1 M 72 2 F 63
2 F 63 2 F 67 2 M 69 2 M 68 2 M 70 3 F 63
3 M 64 4 F 67 4 F 66 4 M 67 4 M 67 4 M 69
;
```

The response variable Height measures the heights (in inches) of 18 individuals. The individuals are classified according to Family and Gender. You can perform a traditional two-way analysis of variance of these data with the following PROC MIXED statements:

```
proc mixed data=heights;
 class Family Gender;
 model Height = Gender Family Family*Gender;
run;
```

The **PROC MIXED** statement invokes the procedure. The **CLASS** statement instructs PROC MIXED to consider both Family and Gender as classification variables. Dummy (indicator) variables are, as a result, created corresponding to all of the distinct levels of Family and Gender. For these data, Family has four levels and Gender has two levels.

The **MODEL** statement first specifies the response (dependent) variable Height. The explanatory (independent) variables are then listed after the equal (=) sign. Here, the two explanatory variables are Gender and Family, and these are the main effects of the design. The third explanatory term, Family\*Gender, models an interaction between the two main effects.

PROC MIXED uses the dummy variables associated with Gender, Family, and Family\*Gender to construct the **X** matrix for the linear model. A column of 1s is also included as the first column of **X** to model a global intercept. There are no **Z** or **G** matrices for this model, and **R** is assumed to equal  $\sigma^2\mathbf{I}$ , where **I** is an  $18 \times 18$  identity matrix.

The **RUN** statement completes the specification. The coding is precisely the same as with the GLM procedure. However, much of the output from PROC MIXED is different from that produced by PROC GLM.

The output from PROC MIXED is shown in [Figure 59.1–Figure 59.7](#).

The “Model Information” table in [Figure 59.1](#) describes the model, some of the variables that it involves, and the method used in fitting it. This table also lists the method (profile, factor, parameter, or none) for handling the residual variance.

**Figure 59.1** Model Information

| The Mixed Procedure       |              |
|---------------------------|--------------|
| Model Information         |              |
| Data Set                  | WORK.HEIGHTS |
| Dependent Variable        | Height       |
| Covariance Structure      | Diagonal     |
| Estimation Method         | REML         |
| Residual Variance Method  | Profile      |
| Fixed Effects SE Method   | Model-Based  |
| Degrees of Freedom Method | Residual     |

The “Class Level Information” table in [Figure 59.2](#) lists the levels of all variables specified in the CLASS statement. You can check this table to make sure that the data are correct.

**Figure 59.2** Class Level Information

| Class Level Information |        |         |
|-------------------------|--------|---------|
| Class                   | Levels | Values  |
| Family                  | 4      | 1 2 3 4 |
| Gender                  | 2      | F M     |

The “Dimensions” table in [Figure 59.3](#) lists the sizes of relevant matrices. This table can be useful in determining CPU time and memory requirements.

**Figure 59.3** Dimensions

| Dimensions            |    |
|-----------------------|----|
| Covariance Parameters | 1  |
| Columns in X          | 15 |
| Columns in Z          | 0  |
| Subjects              | 1  |
| Max Obs Per Subject   | 18 |

The “Number of Observations” table in [Figure 59.4](#) displays information about the sample size being processed.



**Figure 59.4** Number of Observations

| Number of Observations          |    |
|---------------------------------|----|
| Number of Observations Read     | 18 |
| Number of Observations Used     | 18 |
| Number of Observations Not Used | 0  |

The “Covariance Parameter Estimates” table in Figure 59.5 displays the estimate of  $\sigma^2$  for the model.

**Figure 59.5** Covariance Parameter Estimates

| Covariance Parameter Estimates |          |
|--------------------------------|----------|
| Cov Parm                       | Estimate |
| Residual                       | 2.1000   |

The “Fit Statistics” table in Figure 59.6 lists several pieces of information about the fitted mixed model, including values derived from the computed value of the restricted/residual likelihood.

**Figure 59.6** Fit Statistics

| Fit Statistics           |      |
|--------------------------|------|
| -2 Res Log Likelihood    | 41.6 |
| AIC (smaller is better)  | 43.6 |
| AICC (smaller is better) | 44.1 |
| BIC (smaller is better)  | 43.9 |

The “Type 3 Tests of Fixed Effects” table in Figure 59.7 displays significance tests for the three effects listed in the MODEL statement. The Type 3  $F$  statistics and  $p$ -values are the same as those produced by the GLM procedure. However, because PROC MIXED uses a likelihood-based estimation scheme, it does not directly compute or display sums of squares for this analysis.

**Figure 59.7** Tests of Fixed Effects

| Type 3 Tests of Fixed Effects |           |           |         |        |
|-------------------------------|-----------|-----------|---------|--------|
| Effect                        | Num<br>DF | Den<br>DF | F Value | Pr > F |
| Gender                        | 1         | 10        | 17.63   | 0.0018 |
| Family                        | 3         | 10        | 5.90    | 0.0139 |
| Family*Gender                 | 3         | 10        | 2.89    | 0.0889 |

The Type 3 test for Family\*Gender effect is not significant at the 5% level, but the tests for both main effects are significant.

The important assumptions behind this analysis are that the data are normally distributed and that they are independent with constant variance. For these data, the normality assumption is probably realistic since the data are observed heights. However, since the data occur in clusters (families), it is very likely that observations from the same family are statistically correlated—that is, not independent.

The methods implemented in PROC MIXED are still based on the assumption of normally distributed data, but you can drop the assumption of independence by modeling statistical correlation in a variety of ways. You can also model variances that are heterogeneous—that is, nonconstant.

For the height data, one of the simplest ways of modeling correlation is through the use of *random effects*. Here the family effect is assumed to be normally distributed with zero mean and some unknown variance. This is in contrast to the previous model in which the family effects are just constants, or *fixed effects*. Declaring Family as a random effect sets up a common correlation among all observations having the same level of Family.

Declaring Family\*Gender as a random effect models an additional correlation between all observations that have the same level of both Family and Gender. One interpretation of this effect is that a female in a certain family exhibits more correlation with the other females in that family than with the other males, and likewise for a male. With the height data, this model seems reasonable.

The statements to fit this correlation model in PROC MIXED are as follows:

```
proc mixed;
 class Family Gender;
 model Height = Gender;
 random Family Family*Gender;
run;
```

Note that Family and Family\*Gender are now listed in the **RANDOM** statement. The dummy variables associated with them are used to construct the **Z** matrix in the mixed model. The **X** matrix now consists of a column of 1s and the dummy variables for Gender.

The **G** matrix for this model is diagonal, and it contains the variance components for both Family and Family\*Gender. The **R** matrix is still assumed to equal  $\sigma^2\mathbf{I}$ , where **I** is an identity matrix.

The output from this analysis is as follows.

**Figure 59.8** Model Information

| The Mixed Procedure       |                     |
|---------------------------|---------------------|
| Model Information         |                     |
| Data Set                  | WORK.HEIGHTS        |
| Dependent Variable        | Height              |
| Covariance Structure      | Variance Components |
| Estimation Method         | REML                |
| Residual Variance Method  | Profile             |
| Fixed Effects SE Method   | Model-Based         |
| Degrees of Freedom Method | Containment         |

The “Model Information” table in Figure 59.8 shows that the containment method is used to compute the degrees of freedom for this analysis. This is the default method when a **RANDOM** statement is used; see the description of the **DDFM=** option for more information.

**Figure 59.9** Class Level Information

| Class Level Information |        |        |       |
|-------------------------|--------|--------|-------|
| Class                   | Levels | Values |       |
| Family                  | 4      | 1      | 2 3 4 |
| Gender                  | 2      | F      | M     |

The “Class Level Information” table in Figure 59.9 is the same as before. The “Dimensions” table in Figure 59.10 displays the new sizes of the **X** and **Z** matrices.

**Figure 59.10** Dimensions and Number of Observations

| Dimensions                      |    |
|---------------------------------|----|
| Covariance Parameters           | 3  |
| Columns in X                    | 3  |
| Columns in Z                    | 12 |
| Subjects                        | 1  |
| Max Obs Per Subject             | 18 |
| Number of Observations          |    |
| Number of Observations Read     | 18 |
| Number of Observations Used     | 18 |
| Number of Observations Not Used | 0  |

The “Iteration History” table in Figure 59.11 displays the results of the numerical optimization of the restricted/residual likelihood. Six iterations are required to achieve the default convergence criterion of  $1E-8$ .

**Figure 59.11** REML Estimation Iteration History

| Iteration History |             |             |          |            |
|-------------------|-------------|-------------|----------|------------|
| Iteration         | Evaluations | -2 Res      | Log Like | Criterion  |
| 0                 | 1           | 74.11074833 |          |            |
| 1                 | 2           | 71.51614003 |          | 0.01441208 |
| 2                 | 1           | 71.13845990 |          | 0.00412226 |
| 3                 | 1           | 71.03613556 |          | 0.00058188 |
| 4                 | 1           | 71.02281757 |          | 0.00001689 |
| 5                 | 1           | 71.02245904 |          | 0.00000002 |
| 6                 | 1           | 71.02245869 |          | 0.00000000 |

**Figure 59.11** *continued*

|                           |
|---------------------------|
| Convergence criteria met. |
|---------------------------|

The “Covariance Parameter Estimates” table in [Figure 59.12](#) displays the results of the REML fit. The Estimate column contains the estimates of the variance components for Family and Family\*Gender, as well as the estimate of  $\sigma^2$ .

**Figure 59.12** Covariance Parameter Estimates (REML)

| Covariance Parameter<br>Estimates |          |
|-----------------------------------|----------|
| Cov Parm                          | Estimate |
| Family                            | 2.4010   |
| Family*Gender                     | 1.7657   |
| Residual                          | 2.1668   |

The “Fit Statistics” table in [Figure 59.13](#) contains basic information about the REML fit.

**Figure 59.13** Fit Statistics

| Fit Statistics           |      |
|--------------------------|------|
| -2 Res Log Likelihood    | 71.0 |
| AIC (smaller is better)  | 77.0 |
| AICC (smaller is better) | 79.0 |
| BIC (smaller is better)  | 75.2 |

The “Type 3 Tests of Fixed Effects” table in [Figure 59.14](#) contains a significance test for the lone fixed effect, Gender. Note that the associated  $p$ -value is not nearly as significant as in the previous analysis. This illustrates the importance of correctly modeling correlation in your data.

**Figure 59.14** Type 3 Tests of Fixed Effects

| Type 3 Tests of Fixed Effects |           |           |         |        |
|-------------------------------|-----------|-----------|---------|--------|
| Effect                        | Num<br>DF | Den<br>DF | F Value | Pr > F |
| Gender                        | 1         | 3         | 7.95    | 0.0667 |

An additional benefit of the random effects analysis is that it enables you to make inferences about gender that apply to an entire population of families, whereas the inferences about gender from the analysis where Family and Family\*Gender are fixed effects apply only to the particular families in the data set.

PROC MIXED thus offers you the ability to model correlation directly and to make inferences about fixed effects that apply to entire populations of random effects.

## Syntax: MIXED Procedure

The following statements are available in the MIXED procedure:

```

PROC MIXED < options > ;
 BY variables ;
 CLASS variable < (REF= option) > ... < variable < (REF= option) > > < / global-options > ;
 CODE < options > ;
 ID variables ;
 MODEL dependent = < fixed-effects > < / options > ;
 RANDOM random-effects < / options > ;
 REPEATED < repeated-effect > < / options > ;
 PARMS (value-list) ... < / options > ;
 PERFORMANCE < options > ;
 PRIOR < distribution > < / options > ;
 CONTRAST 'label' < fixed-effect values ... >
 < | random-effect values ... >, ... < / options > ;
 ESTIMATE 'label' < fixed-effect values ... >
 < | random-effect values ... > < / options > ;
 LSMEANS fixed-effects < / options > ;
 LSMESTIMATE model-effect lsmestimate-specification < / options > ;
 SLICE model-effect < / options > ;
 STORE < OUT= > item-store-name < / LABEL='label' > ;
 WEIGHT variable ;

```

Items within angle brackets (<>) are optional. The **CONTRAST**, **ESTIMATE**, **LSMEANS**, and **RANDOM** statements can appear multiple times; all other statements can appear only once.

The **PROC MIXED** and **MODEL** statements are required, and the **MODEL** statement must appear after the **CLASS** statement if a **CLASS** statement is included. The **CONTRAST**, **ESTIMATE**, **LSMEANS**, **RANDOM**, and **REPEATED** statements must follow the **MODEL** statement. The **CONTRAST** and **ESTIMATE** statements must also follow any **RANDOM** statements. The **LSMESTIMATE**, **SLICE**, and **STORE** statements are shared with many procedures. Summary descriptions of functionality and syntax for these statements are also given after the **PROC MIXED** statement in alphabetical order, but you can find full documentation on them in Chapter 19, “Shared Concepts and Topics.”

Table 59.1 summarizes the basic functions and important options of each PROC MIXED statement. The syntax of each statement in Table 59.1 is described in the following sections in alphabetical order after the description of the **PROC MIXED** statement.

**Table 59.1** Summary of PROC MIXED Statements

| Statement         | Description           | Options                                                                           |
|-------------------|-----------------------|-----------------------------------------------------------------------------------|
| <b>PROC MIXED</b> | Invokes the procedure | <b>DATA=</b> specifies input data set, <b>METHOD=</b> specifies estimation method |

Table 59.1 *continued*

| Statement   | Description                                                                       | Options                                                                                                                                                                                                                                      |
|-------------|-----------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| BY          | Performs multiple PROC MIXED analyses in one invocation                           | None                                                                                                                                                                                                                                         |
| CLASS       | Declares qualitative variables that create indicator variables in design matrices | None                                                                                                                                                                                                                                         |
| CODE        | Requests that the procedure write SAS DATA step code to a file or catalog entry   | FILE= names the file where the generated code is saved, CATALOG= names the catalog entry where the generated code is saved, IMPUTE imputes predicted values for observations with missing or invalid covariates, RESIDUAL computes residuals |
| ID          | Lists additional variables to be included in predicted values tables              | None                                                                                                                                                                                                                                         |
| MODEL       | Specifies dependent variable and fixed effects, setting up X                      | S requests solution for fixed-effects parameters, DDFM= specifies denominator degrees of freedom method, OUTP= outputs predicted values to a data set, INFLUENCE computes influence diagnostics                                              |
| RANDOM      | Specifies random effects, setting up Z and G                                      | SUBJECT= creates block-diagonality, TYPE= specifies covariance structure, S requests solution for random-effects parameters, G displays estimated G                                                                                          |
| REPEATED    | Sets up R                                                                         | SUBJECT= creates block-diagonality, TYPE= specifies covariance structure, R displays estimated blocks of R, GROUP= enables between-subject heterogeneity, LOCAL adds a diagonal matrix to R                                                  |
| PARMS       | Specifies a grid of initial values for the covariance parameters                  | HOLD= and NOITER hold the covariance parameters or their ratios constant, PARMSDATA= reads the initial values from a SAS data set                                                                                                            |
| PERFORMANCE | Specifies the number of threads to use                                            | NTHREADS=                                                                                                                                                                                                                                    |
| PRIOR       | Performs a sampling-based Bayesian analysis for variance component models         | NSAMPLE= specifies the sample size, SEED= specifies the starting seed                                                                                                                                                                        |
| CONTRAST    | Constructs custom hypothesis tests                                                | E displays the L matrix coefficients                                                                                                                                                                                                         |
| ESTIMATE    | Constructs custom scalar estimates                                                | CL produces confidence limits                                                                                                                                                                                                                |

Table 59.1 *continued*

| Statement   | Description                                                    | Options                                                                                                                                                                                                                                                    |
|-------------|----------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| LSMEANS     | Computes least squares means for classification fixed effects  | <b>DIFF</b> computes differences of the least squares means, <b>ADJUST=</b> performs multiple comparisons adjustments, <b>AT</b> changes covariates, <b>OM</b> changes weighting, <b>CL</b> produces confidence limits, <b>SLICE=</b> tests simple effects |
| LSMESTIMATE | Provides custom hypothesis tests among the least squares means | <b>ADJUST=</b> determines the method for multiple comparison adjustment of LS-mean differences, <b>JOINT</b> requests a joint <i>F</i> or chi-square test for the rows of the estimate                                                                     |
| SLICE       | Performs a partitioned analysis of LS-means for an interaction | <b>ADJUST=</b> determines the method for multiple comparison adjustment of LS-mean differences, <b>DIFF</b> requests differences of LS-means                                                                                                               |
| STORE       | Saves the context and results of the analysis                  | <b>LABEL=</b> adds a custom label                                                                                                                                                                                                                          |
| WEIGHT      | Specifies a variable by which to weight <b>R</b>               | None                                                                                                                                                                                                                                                       |

## PROC MIXED Statement

**PROC MIXED** < options > ;

The PROC MIXED statement invokes the MIXED procedure. Table 59.2 summarizes the options available in the PROC MIXED statement. These and other options in the PROC MIXED statement are then described fully in alphabetical order.

Table 59.2 PROC MIXED Statement Options

| Option                  | Description                                                                  |
|-------------------------|------------------------------------------------------------------------------|
| <b>Basic Options</b>    |                                                                              |
| <b>DATA=</b>            | Specifies input data set                                                     |
| <b>METHOD=</b>          | Specifies the estimation method                                              |
| <b>NOPROFILE</b>        | Includes scale parameter in optimization                                     |
| <b>ORDER=</b>           | Determines the sort order of <b>CLASS</b> variables                          |
| <b>Displayed Output</b> |                                                                              |
| <b>ASYCORR</b>          | Displays asymptotic correlation matrix of covariance parameter estimates     |
| <b>ASYCOV</b>           | Displays asymptotic covariance matrix of covariance parameter estimates      |
| <b>CL</b>               | Requests confidence limits for covariance parameter estimates                |
| <b>COVTEST</b>          | Displays asymptotic standard errors and Wald tests for covariance parameters |
| <b>IC</b>               | Displays a table of information criteria                                     |

Table 59.2 *continued*

| Option                       | Description                                                             |
|------------------------------|-------------------------------------------------------------------------|
| ITDETAILS                    | Displays estimates and gradients added to “Iteration History”           |
| LOGNOTE                      | Writes periodic status notes to the log                                 |
| MMEQ                         | Displays mixed model equations                                          |
| MMEQSOL                      | Displays the solution to the mixed model equations                      |
| NOCLPRINT                    | Suppresses “Class Level Information” completely or in parts             |
| NOITPRINT                    | Suppresses “Iteration History” table                                    |
| PLOTS=                       | Produces ODS statistical graphics                                       |
| RATIO                        | Produces ratio of covariance parameter estimates with residual variance |
| <b>Optimization Options</b>  |                                                                         |
| MAXFUNC=                     | Specifies the maximum number of likelihood evaluations                  |
| MAXITER=                     | Specifies the maximum number of iterations                              |
| <b>Computational Options</b> |                                                                         |
| CONVF                        | Requests and tunes the relative function convergence criterion          |
| CONVG                        | Requests and tunes the relative gradient convergence criterion          |
| CONVH                        | Requests and tunes the relative Hessian convergence criterion           |
| DFBW                         | Selects between-within degree of freedom method                         |
| EMPIRICAL                    | Computes empirical (“sandwich”) estimators                              |
| NOBOUND                      | Unbounds covariance parameter estimates                                 |
| RIDGE=                       | Specifies starting value for minimum ridge value                        |
| SCORING=                     | Applies Fisher scoring where applicable                                 |

You can specify the following *options*.

#### **ABSOLUTE**

makes the convergence criterion absolute. By default, it is relative (divided by the current objective function value). See the [CONVF](#), [CONVG](#), and [CONVH](#) options in this section for a description of various convergence criteria.

#### **ALPHA=*number***

requests that confidence limits be constructed for the covariance parameter estimates with confidence level  $1 - \textit{number}$ . The value of *number* must be between 0 and 1; the default is 0.05.

#### **ANOVAF**

The ANOVAF option computes *F* tests in models with REPEATED statement and without RANDOM statement by a method similar to that of Brunner, Domhof, and Langer (2002). The method consists of computing special *F* statistics and adjusting their degrees of freedom. The technique is a generalization of the Greenhouse-Geisser adjustment in MANOVA models (Greenhouse and Geisser 1959). For more details, see the section “[F Tests With the ANOVAF Option](#)” on page 4969.

#### **ASYCORR**

produces the asymptotic correlation matrix of the covariance parameter estimates. It is computed from the corresponding asymptotic covariance matrix (see the description of the [ASYCOV](#) option, which follows). The name of the “Asymptotic Correlation” table is AsyCorr.



**ASYCOV**

requests that the asymptotic covariance matrix of the covariance parameters be displayed. By default, this matrix is the observed inverse Fisher information matrix, which equals  $2\mathbf{H}^{-1}$ , where  $\mathbf{H}$  is the Hessian (second derivative) matrix of the objective function. See the section “Covariance Parameter Estimates” on page 4985 for more information about this matrix. When you use the **SCORING=** option and PROC MIXED converges without stopping the scoring algorithm, PROC MIXED uses the expected Hessian matrix to compute the covariance matrix instead of the observed Hessian. The ODS name of the “Asymptotic Covariance” table is AsyCov.

**CL<=WALD>**

requests confidence limits for the covariance parameter estimates. A Satterthwaite approximation is used to construct limits for all parameters that have a lower boundary constraint of zero. These limits take the form

$$\frac{\nu \hat{\sigma}^2}{\chi_{\nu, 1-\alpha/2}^2} \leq \sigma^2 \leq \frac{\nu \hat{\sigma}^2}{\chi_{\nu, \alpha/2}^2}$$

where  $\nu = 2Z^2$ ,  $Z$  is the Wald statistic  $\hat{\sigma}^2/\text{se}(\hat{\sigma}^2)$ , and the denominators are quantiles of the  $\chi^2$ -distribution with  $\nu$  degrees of freedom. See Milliken and Johnson (1992) and Burdick and Graybill (1992) for similar techniques.

For all other parameters, Wald Z-scores and normal quantiles are used to construct the limits. Wald limits are also provided for variance components if you specify the **NOBOUND** option. The optional **=WALD** specification requests Wald limits for all parameters.

The confidence limits are displayed as extra columns in the “Covariance Parameter Estimates” table. The confidence level is  $1 - \alpha = 0.95$  by default; this can be changed with the **ALPHA=** option.

**CONVF<=number>**

requests the relative function convergence criterion with tolerance *number*. The relative function convergence criterion is

$$\frac{|f_k - f_{k-1}|}{|f_k|} \leq \textit{number}$$

where  $f_k$  is the value of the objective function at iteration  $k$ . To prevent the division by  $|f_k|$ , use the **ABSOLUTE** option. The default convergence criterion is **CONVH**, and the default tolerance is 1E-8.

**CONVG <=number>**

requests the relative gradient convergence criterion with tolerance *number*. The relative gradient convergence criterion is

$$\frac{\max_j |g_{jk}|}{|f_k|} \leq \textit{number}$$

where  $f_k$  is the value of the objective function, and  $g_{jk}$  is the  $j$ th element of the gradient (first derivative) of the objective function, both at iteration  $k$ . To prevent division by  $|f_k|$ , use the **ABSOLUTE** option. The default convergence criterion is **CONVH**, and the default tolerance is 1E-8.

**CONVH**<=*number*>

requests the relative Hessian convergence criterion with tolerance *number*. The relative Hessian convergence criterion is

$$\frac{\mathbf{g}_k' \mathbf{H}_k^{-1} \mathbf{g}_k}{|f_k|} \leq \textit{number}$$

where  $f_k$  is the value of the objective function,  $\mathbf{g}_k$  is the gradient (first derivative) of the objective function, and  $\mathbf{H}_k$  is the Hessian (second derivative) of the objective function, all at iteration  $k$ .

If  $\mathbf{H}_k$  is singular, then PROC MIXED uses the following relative criterion:

$$\frac{\mathbf{g}_k' \mathbf{g}_k}{|f_k|} \leq \textit{number}$$

To prevent the division by  $|f_k|$ , use the **ABSOLUTE** option. The default convergence criterion is **CONVH**, and the default tolerance is 1E-8.

**COVTEST**

produces asymptotic standard errors and Wald Z-tests for the covariance parameter estimates.

**DATA**=SAS-*data-set*

names the SAS data set to be used by PROC MIXED. The default is the most recently created data set.

**DFBW**

has the same effect as the **DDFM**=BW option in the **MODEL** statement.

**EMPIRICAL**

computes the estimated variance-covariance matrix of the fixed-effects parameters by using the asymptotically consistent estimator described in Huber (1967); White (1980); Liang and Zeger (1986); Diggle, Liang, and Zeger (1994). This estimator is commonly referred to as the “sandwich” estimator, and it is computed as follows:

$$(\mathbf{X}'\widehat{\mathbf{V}}^{-1}\mathbf{X})^{-1} \left( \sum_{i=1}^S \mathbf{X}_i' \widehat{\mathbf{V}}_i^{-1} \widehat{\boldsymbol{\epsilon}}_i \widehat{\boldsymbol{\epsilon}}_i' \widehat{\mathbf{V}}_i^{-1} \mathbf{X}_i \right) (\mathbf{X}'\widehat{\mathbf{V}}^{-1}\mathbf{X})^{-1}$$

Here,  $\widehat{\boldsymbol{\epsilon}}_i = y_i - \mathbf{X}_i \widehat{\boldsymbol{\beta}}$ ,  $S$  is the number of subjects, and matrices with an  $i$  subscript are those for the  $i$ th subject. You must include the **SUBJECT**= option in either a **RANDOM** or **REPEATED** statement for this option to take effect.

When you specify the **EMPIRICAL** option, PROC MIXED adjusts all standard errors and test statistics involving the fixed-effects parameters. This changes output in the following tables (listed in [Table 59.26](#)): Contrast, CorrB, CovB, Diffs, Estimates, InvCovB, LSMMeans, Slices, SolutionF, Tests1–Tests3. The **OUTP**= and **OUTPM**= data sets are also affected. Finally, the Satterthwaite and Kenward-Roger degrees of freedom methods are not available if you specify the **EMPIRICAL** option.

**IC**

displays a table of various information criteria. The criteria are all in smaller-is-better form, and are described in [Table 59.3](#).

**Table 59.3** Information Criteria

| Criterion | Formula                               | Reference                                              |
|-----------|---------------------------------------|--------------------------------------------------------|
| AIC       | $-2\ell + 2d$                         | Akaike (1974)                                          |
| AICC      | $-2\ell + 2dn^*/(n^* - d - 1)$        | Hurvich and Tsai (1989)<br>Burnham and Anderson (1998) |
| HQIC      | $-2\ell + 2d \log \log n$ for $n > 1$ | Hannan and Quinn (1979)                                |
| BIC       | $-2\ell + d \log n$ for $n > 0$       | Schwarz (1978)                                         |
| CAIC      | $-2\ell + d(\log n + 1)$ for $n > 0$  | Bozdogan (1987)                                        |

Here  $\ell$  denotes the maximum value of the (possibly restricted) log likelihood,  $d$  the dimension of the model, and  $n$  the number of observations. In SAS 6 of SAS/STAT software,  $n$  equals the number of valid observations for maximum likelihood estimation and  $n - p$  for restricted maximum likelihood estimation, where  $p$  equals the rank of  $\mathbf{X}$ . In later versions,  $n$  equals the number of effective subjects as displayed in the “Dimensions” table, unless this value equals 1, in which case  $n$  equals the number of levels of the first random effect you specify in a **RANDOM** statement. If the number of effective subjects equals 1 and you have no **RANDOM** statements, then  $n$  reverts to the SAS 6 values. For AICC (a finite-sample corrected version of AIC),  $n^*$  equals the SAS 6 values of  $n$ , unless this number is less than  $d + 2$ , in which case it equals  $d + 2$ . When  $n \leq 1$ , the value of the HQIC criterion is  $-2\ell$ . When  $n=0$ , the values of the BIC and CAIC criteria are  $-2\ell$  and  $-2\ell + d$ , respectively.

For restricted likelihood estimation,  $d$  equals  $q$ , the effective number of estimated covariance parameters. In SAS 6, when a parameter estimate lies on a boundary constraint, then it is still included in the calculation of  $d$ , but in later versions it is not. The most common example of this behavior is when a variance component is estimated to equal zero. For maximum likelihood estimation,  $d$  equals  $q + p$ . The value of  $d$  is displayed in the “Information Criteria” table as the value ofParms variable; see [Table 59.27](#).

The ODS name of the “Information Criteria” table is InfoCrit.

### INFO

is a default option. The creation of the “Model Information,” “Dimensions,” and “Number of Observations” tables can be suppressed by using the **NOINFO** option.

Note that in SAS 6 this option displays the “Model Information” and “Dimensions” tables.

### ITDETAILS

displays the parameter values at each iteration and enables the writing of notes to the SAS log pertaining to “infinite likelihood” and “singularities” during Newton-Raphson iterations.

### LOGNOTE

writes periodic notes to the log describing the current status of computations. It is designed for use with analyses requiring extensive CPU resources.

### MAXFUNC=*number*

specifies the maximum number of likelihood evaluations in the optimization process. The default is 150.

**MAXITER=*number***

specifies the maximum number of iterations. The default is 50.

**METHOD=REML | ML | MIVQUE0 | TYPE1 | TYPE2 | TYPE3**

specifies the estimation method for the covariance parameters. The REML specification performs residual (restricted) maximum likelihood, and it is the default method. The ML specification performs maximum likelihood, and the MIVQUE0 specification performs minimum variance quadratic unbiased estimation of the covariance parameters.

The METHOD=TYPE $n$  specifications apply only to variance component models with no **SUBJECT=** effects and no **REPEATED** statement. An analysis of variance table is included in the output, and the expected mean squares are used to estimate the variance components (see Chapter 42, “[The GLM Procedure](#),” for further explanation). The resulting method-of-moment variance component estimates are used in subsequent calculations, including standard errors computed from **ESTIMATE** and **LSMEANS** statements. The ODS table names are Type1, Type2, and Type3, respectively.

**MMEQ**

requests that the coefficient matrix and the right-hand side of the mixed model equations be displayed. If  $\hat{\mathbf{G}}$  is nonsingular, the coefficient matrix and the right-hand side have the following form:

$$\begin{bmatrix} \mathbf{X}'\hat{\mathbf{R}}^{-1}\mathbf{X} & \mathbf{X}'\hat{\mathbf{R}}^{-1}\mathbf{Z} \\ \mathbf{Z}'\hat{\mathbf{R}}^{-1}\mathbf{X} & \mathbf{Z}'\hat{\mathbf{R}}^{-1}\mathbf{Z} + \hat{\mathbf{G}}^{-1} \end{bmatrix} \begin{bmatrix} \hat{\boldsymbol{\beta}} \\ \hat{\boldsymbol{\gamma}} \end{bmatrix} = \begin{bmatrix} \mathbf{X}'\hat{\mathbf{R}}^{-1}\mathbf{y} \\ \mathbf{Z}'\hat{\mathbf{R}}^{-1}\mathbf{y} \end{bmatrix}$$

If  $\hat{\mathbf{G}}$  is singular, the coefficient matrix and right-hand side have the following modified form:

$$\begin{bmatrix} \mathbf{X}'\hat{\mathbf{R}}^{-1}\mathbf{X} & \mathbf{X}'\hat{\mathbf{R}}^{-1}\mathbf{Z}\hat{\mathbf{G}} \\ \hat{\mathbf{G}}'\mathbf{Z}'\hat{\mathbf{R}}^{-1}\mathbf{X} & \hat{\mathbf{G}}'\mathbf{Z}'\hat{\mathbf{R}}^{-1}\mathbf{Z}\hat{\mathbf{G}} + \mathbf{G} \end{bmatrix} \begin{bmatrix} \hat{\boldsymbol{\beta}} \\ \hat{\boldsymbol{\tau}} \end{bmatrix} = \begin{bmatrix} \mathbf{X}'\hat{\mathbf{R}}^{-1}\mathbf{y} \\ \hat{\mathbf{G}}'\mathbf{Z}'\hat{\mathbf{R}}^{-1}\mathbf{y} \end{bmatrix}$$

See the section “[Estimating Fixed and Random Effects in the Mixed Model](#)” on page 4965 for further information about these equations.

**MMEQSOL**

requests that a solution to the mixed model equations be produced, in addition to the inverted coefficients matrix. If  $\hat{\mathbf{G}}$  is nonsingular, the formula is the same as the preceding description of the **MMEQ** option. If  $\hat{\mathbf{G}}$  is singular,  $\hat{\boldsymbol{\beta}}$  and  $\mathbf{G}\hat{\boldsymbol{\tau}}$  are displayed in addition to the inverse of the modified coefficient matrix.

See the section “[Estimating Fixed and Random Effects in the Mixed Model](#)” on page 4965 for further information about these equations and solution transformation.

**NAMELEN<=*number*>**

specifies the length to which long effect names are shortened. The default and minimum value is 20.

**NOBOUND**

has the same effect as the **NOBOUND** option in the **PARMS** statement.

**NOCLPRINT<=*number*>**

suppresses the display of the “Class Level Information” table if you do not specify *number*. If you do specify *number*, only levels with totals that are less than *number* are listed in the table.

**NOINFO**

suppresses the display of the “Model Information,” “Dimensions,” and “Number of Observations” tables.

**NOITPRINT**

suppresses the display of the “Iteration History” table.

**NOPROFILE**

includes the residual variance as part of the Newton-Raphson iterations. This option applies only to models that have a residual variance parameter. By default, this parameter is profiled out of the likelihood calculations, except when you have specified the **HOLD=** option in the **PARMS** statement.

**ORD**

displays ordinates of the relevant distribution in addition to *p*-values. The ordinate can be viewed as an approximate odds ratio of hypothesis probabilities.

**ORDER=DATA | FORMATTED | FREQ | INTERNAL**

specifies the sort order for the levels of the classification variables (which are specified in the **CLASS** statement). This option applies to the levels for all classification variables, except when you use the (default) **ORDER=FORMATTED** option with numeric classification variables that have no explicit format. With this option, the levels of such variables are ordered by their internal value.

The **ORDER=** option can take the following values:

| Value of <b>ORDER=</b> | Levels Sorted By                                                                                                                       |
|------------------------|----------------------------------------------------------------------------------------------------------------------------------------|
| <b>DATA</b>            | Order of appearance in the input data set                                                                                              |
| <b>FORMATTED</b>       | External formatted value, except for numeric variables with no explicit format, which are sorted by their unformatted (internal) value |
| <b>FREQ</b>            | Descending frequency count; levels with the most observations come first in the order                                                  |
| <b>INTERNAL</b>        | Unformatted value                                                                                                                      |

By default, **ORDER=FORMATTED**. For **ORDER=FORMATTED** and **ORDER=INTERNAL**, the sort order is machine-dependent. For more information about sort order, see the chapter on the **SORT** procedure in the *Base SAS Procedures Guide* and the discussion of BY-group processing in *SAS Language Reference: Concepts*.

**PLOTS** <(global-plot-options) > <=plot-request <(options) >>

**PLOTS** <(global-plot-options) > <= (plot-request<(options)><...plot-request<(options)> >>

requests that the MIXED procedure produce statistical graphics via the Output Delivery System, provided that ODS Graphics is enabled.

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;
proc mixed data=heights plots=all;
 class Family Gender;
 model Height = Gender / residual;
 random Family Family*Gender;
run;
ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS](#).”

For examples of the basic statistical graphics produced by the MIXED procedure and aspects of their computation and interpretation, see the section “[ODS Graphics](#)” on page 4992.

The *global-plot-options* apply to all relevant plots generated by the MIXED procedure. The *global-plot-options* supported by the MIXED procedure follow.

## Global Plot Options

### OBSNO

uses the data set observation number to identify observations in tooltips, provided that the observation number can be determined. Otherwise, the number displayed in tooltips is the index of the observation as it is used in the analysis within the BY group.

### ONLY

suppresses the default plots. Only the plots specifically requested are produced.

### UNPACKPANEL

### UNPACK

displays each graph separately. (By default, some graphs can appear together in a single panel.)

### MAXPOINTS=NONE | *number*

specifies that plots with elements that require processing more than *number* points be suppressed. The default is MAXPOINTS=5000. No plots are suppressed if you specify MAXPOINTS=NONE.

## Specific Plot Options

The following listing describes the specific plots and their options.

### ALL

requests that all plots appropriate for the particular analysis be produced.

### BOXPLOT <(boxplot-options)>

requests box plots for the effects in your model that consist of classification effects only. Note that these effects can involve more than one classification variable (interaction and nested effects), but they cannot contain any continuous variables. By default, the BOXPLOT request produces box plots based on (conditional) raw residuals for the qualifying effects in the **MODEL**,

**RANDOM**, and **REPEATED** statements. See the discussion of the *boxplot-options* in a later section for information about how to tune your box plot request.

**DISTANCE<(USEINDEX)>**

requests a plot of the likelihood or restricted likelihood distance. When influence diagnostics are requested with set selection according to an effect, the **USEINDEX** option enables you to replace the formatted tick values on the horizontal axis with integer indices of the effect levels in order to reduce the space taken up by the horizontal plot axis.

**INFLUENCEESTPLOT<(options)>**

requests panels of the deletion estimates in an influence analysis, provided that the **INFLUENCE** option is specified in the **MODEL** statement. No plots are produced for fixed-effects parameters associated with singular columns in the **X** matrix or for covariance parameters associated with singularities in the **ASYCOV** matrix. By default, separate panels are produced for the fixed-effects and covariance parameters delete estimates. The **FIXED** and **RANDOM** options enable you to select these specific panels. The **UNPACK** option produces separate plots for each of the parameter estimates. The **USEINDEX** option replaces formatted tick values for the horizontal axis with integer indices.

**INFLUENCESTATPANEL<(options)>**

requests panels of influence statistics. For iterative influence analysis (see the **INFLUENCE** option in the **MODEL** statement), the panel shows the Cook's *D* and CovRatio statistics for fixed-effects and covariance parameters, enabling you to gauge impact on estimates and precision for both types of estimates. In noniterative analysis, only statistics for the fixed effects are plotted. The **UNPACK** option produces separate plots from the elements in the panel. The **USEINDEX** option replaces formatted tick values for the horizontal axis with integer indices.

**RESIDUALPANEL <(residual-plot-options)>**

requests a panel of raw residuals. By default, the conditional residuals are produced. See the discussion of *residual-plot-options* in a later section for information about how to tune this panel.

**STUDENTPANEL <(residual-plot-options)>**

requests a panel of studentized residuals. By default, the conditional residuals are produced. See the discussion of *residual-plot-options* in a later section for information about how to tune this panel.

**PEARSONPANEL <(residual-plot-options)>**

requests a panel of Pearson residuals. By default, the conditional residuals are produced. See the discussion of *residual-plot-options* in a later section for information about how to tune this panel.

**PRESS<(USEINDEX)>**

requests a plot of PRESS residuals or PRESS statistics. These are based on “leave-one-out” or “leave-set-out” prediction of the marginal mean. When influence diagnostics are requested with set selection according to an effect, the **USEINDEX** option enables you to replace the formatted tick values on the horizontal axis with integer indices of the effect levels in order to reduce the space taken up by the horizontal plot axis.

**VCIRYPANEL** < (*residual-plot-options*) >

requests a panel of residual graphics based on the scaled residuals. See the **VCIRY** option in the **MODEL** statement for details about these scaled residuals. Only the **UNPACK** and **BOX** options of the *residual-plot-options* are available for this type of residual panel.

**NONE**

suppresses all plots.

**Residual Plot Options**

The *residual-plot-options* determine both the composition of the panels and the type of residuals being plotted.

**BOX****BOXPLOT**

replaces the inset of summary statistics in the lower-right corner of the panel with a box plot of the residual (the “PROC GLIMMIX look”).

**CONDITIONAL****BLUP**

constructs plots from conditional residuals.

**MARGINAL****NOBLUP**

constructs plots from marginal residuals.

**UNPACK**

produces separate plots from the elements of the panel. The inset statistics are not part of the unpack operation.

**Box Plot Options**

The *boxplot-options* determine whether box plots are produced for residuals or for residuals and observed values, and for which model effects the box plots are constructed. The available *boxplot-options* are as follows.

**CONDITIONAL****BLUP**

constructs box plots from conditional residuals—that is, residuals using the estimated BLUPs of random effects.

**FIXED**

produces box plots for all fixed effects (**MODEL** statement) consisting entirely of classification variables



**GROUP**

produces box plots for all GROUP= effects (**RANDOM** and **REPEATED** statement) consisting entirely of classification variables

**MARGINAL****NOBLUP**

constructs box plots from marginal residuals.

**NPANEL=number**

provides the ability to break a box plot into multiple graphics. If *number* is negative, no balancing of the number of boxes takes place and *number* is the maximum number of boxes per graphic. If *number* is positive, the number of boxes per graphic is balanced. For example, suppose variable A has 125 levels, and consider the following statements:

```
ods graphics on;
proc mixed plots=boxplot (npanel=20);
 class A;
 model y = A;
run;
```

The box balancing results in six plots with 18 boxes each and one plot with 17 boxes. If *number* is zero, and this is the default, all levels of the effect are displayed in a single plot.

**OBSERVED**

adds box plots of the observed data for the selected effects.

**RANDOM**

produces box plots for all random effects (**RANDOM** statement) consisting entirely of classification variables. This does not include effects specified in the **GROUP=** or **SUBJECT=** options of the **RANDOM** statement.

**REPEATED**

produces box plots for the repeated effects (**REPEATED** statement). This does not include effects specified in the **GROUP=** or **SUBJECT=** options of the **REPEATED** statement.

**STUDENT**

constructs box plots from studentized residuals rather than from raw residuals.

**SUBJECT**

produces box plots for all SUBJECT= effects (**RANDOM** and **REPEATED** statement) consisting entirely of classification variables.

**USEINDEX**

uses as the horizontal axis label the index of the effect level rather than the formatted value(s). For classification variables with many levels or model effects that involve multiple classification variables, the formatted values identifying the effect levels can take up too much space as axis tick values, leading to extensive thinning. The **USEINDEX** option replaces tick values constructed from formatted values with the internal level number.

## Multiple Plot Requests

You can list a plot request one or more times with different options. For example, the following statements request a panel of marginal raw residuals, individual plots generated from a panel of the conditional raw residuals, and a panel of marginal studentized residuals:

```
ods graphics on;
proc mixed plots(only)=(
 ResidualPanel(marginal)
 ResidualPanel(unpack conditional)
 StudentPanel(marginal box));
```

The inset of residual statistics is replaced in this last panel by a box plot of the studentized residuals. Similarly, if you specify the **INFLUENCE** option in the **MODEL** statement, then the following statements request statistical graphics of fixed-effects deletion estimates (in a panel), covariance parameter deletion estimates (unpacked in individual plots), and box plots for the **SUBJECT=** and fixed classification effects based on residuals and observed values:

```
ods graphics on / imagefmt=staticmap;
proc mixed plots(only)=(
 InfluenceEstPlot(fixed)
 InfluenceEstPlot(random unpack)
 BoxPlot(observed fixed subject);
```

The **STATICMAP** image format enables tooltips that show, for example, values of influence diagnostics associated with a particular delete estimate.

This concludes the syntax section for the **PLOTS=** option in the **PROC MIXED** statement.

## RATIO

produces the ratio of the covariance parameter estimates to the estimate of the residual variance when the latter exists in the model.

## RIDGE=*number*

specifies the starting value for the minimum ridge value used in the Newton-Raphson algorithm. The default is 0.3125.

## SCORING<=*number*>

requests that Fisher scoring be used in association with the estimation method up to iteration *number*, which is 0 by default. When you use the **SCORING=** option and **PROC MIXED** converges without stopping the scoring algorithm, **PROC MIXED** uses the expected Hessian matrix to compute approximate standard errors for the covariance parameters instead of the observed Hessian. The output from the **ASYCOV** and **ASYCORR** options is similarly adjusted.

## SIGITER

is an alias for the **NOPROFILE** option.

## UPDATE

is an alias for the **LOGNOTE** option.

---

## BY Statement

**BY** *variables* ;

You can specify a BY statement with PROC MIXED to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the MIXED procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

Because sorting the data changes the order in which PROC MIXED reads observations, the sort order for the levels of the CLASS variable might be affected if you have specified ORDER=DATA in the PROC MIXED statement. This, in turn, affects specifications in the CONTRAST or ESTIMATE statement.

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

---

## CLASS Statement

**CLASS** *variable* < (REF= *option*) > ... < *variable* < (REF= *option*) > > < / *global-options* > ;

The CLASS statement names the classification variables to be used in the model. Typical classification variables are Treatment, Sex, Race, Group, and Replication. If you use the CLASS statement, it must appear before the MODEL statement.

Classification variables can be either character or numeric. By default, class levels are determined from the entire set of formatted values of the CLASS variables.

**NOTE:** Prior to SAS 9, class levels were determined by using no more than the first 16 characters of the formatted values. To revert to this previous behavior, you can use the TRUNCATE option in the CLASS statement.

In any case, you can use formats to group values into levels. See the discussion of the FORMAT procedure in the *Base SAS Procedures Guide* and the discussions of the FORMAT statement and SAS formats in *SAS Formats and Informats: Reference*. You can adjust the order of CLASS variable levels with the ORDER= option in the PROC MIXED statement. You can specify the following REF= option to indicate how the levels of an individual classification variable are to be ordered by enclosing it in parentheses after the variable name:

**REF= 'level' | FIRST | LAST**

specifies a level of the classification variable to be put at the end of the list of levels. This level thus corresponds to the reference level in the usual interpretation of the estimates with PROC MIXED's singular parameterization. You can specify the *level* of the variable to use as the reference level; specify a value that corresponds to the formatted value of the variable if a format is assigned. Alternatively, you can specify REF=FIRST to designate that the first ordered level serve as the reference, or REF=LAST to designate that the last ordered level serve as the reference. To specify that REF=FIRST or REF=LAST be used for all classification variables, use the **REF= global-option** after the slash (/) in the CLASS statement.

You can specify the following *global-options* in the CLASS statement after a slash (/):

**REF=FIRST | LAST**

specifies a level of all classification variables to be put at the end of the list of levels. This level thus corresponds to the reference level in the usual interpretation of the estimates with PROC MIXED's singular parameterization. Specify REF=FIRST to designate that the first ordered level for each classification variable serve as the reference. Specify REF=LAST to designate that the last ordered level serve as the reference. This option applies to all the variables specified in the CLASS statement. To specify different reference levels for different classification variables, use **REF=** options for individual variables.

**TRUNCATE**

specifies that class levels be determined by using only up to the first 16 characters of the formatted values of CLASS variables. When formatted values are longer than 16 characters, you can use this option to revert to the levels as determined in releases prior to SAS 9.

---

## CODE Statement

**CODE** < options > ;

The CODE statement enables you to write SAS DATA step code for computing predicted values of the fitted model either to a file or to a catalog entry. This code can then be included in a DATA step to score new data.

Table 59.4 summarizes the *options* available in the CODE statement.

**Table 59.4** CODE Statement Options

| Option    | Description                                                                  |
|-----------|------------------------------------------------------------------------------|
| CATALOG=  | Names the catalog entry where the generated code is saved                    |
| DUMMIES   | Retains the dummy variables in the data set                                  |
| ERROR     | Computes the error function                                                  |
| FILE=     | Names the file where the generated code is saved                             |
| FORMAT=   | Specifies the numeric format for the regression coefficients                 |
| GROUP=    | Specifies the group identifier for array names and statement labels          |
| IMPUTE    | Imputes predicted values for observations with missing or invalid covariates |
| LINESIZE= | Specifies the line size of the generated code                                |
| LOOKUP=   | Specifies the algorithm for looking up CLASS levels                          |
| RESIDUAL  | Computes residuals                                                           |

For details about the syntax of the CODE statement, see the section “CODE Statement” on page 390 in Chapter 19, “Shared Concepts and Topics.”

## CONTRAST Statement

```
CONTRAST 'label' <fixed-effect values ... >
 <| random-effect values ... >, ... </options>;
```

The CONTRAST statement provides a mechanism for obtaining custom hypothesis tests. It is patterned after the CONTRAST statement in PROC GLM, although it has been extended to include random effects. This enables you to select an appropriate inference space (McLean, Sanders, and Stroup 1991).

You can test the hypothesis  $L'\phi = 0$ , where  $L' = (K' M')$  and  $\phi' = (\beta' \gamma')$ , in several inference spaces. The inference space corresponds to the choice of  $M$ . When  $M = 0$ , your inferences apply to the entire population from which the random effects are sampled; this is known as the *broad* inference space. When all elements of  $M$  are nonzero, your inferences apply only to the observed levels of the random effects. This is known as the *narrow* inference space, and you can also choose it by specifying all of the random effects as fixed. The GLM procedure uses the narrow inference space. Finally, by setting to zero the portions of  $M$  corresponding to selected main effects and interactions, you can choose *intermediate* inference spaces. The broad inference space is usually the most appropriate, and it is used when you do not specify any random effects in the CONTRAST statement.

The CONTRAST statement has the following arguments:

|                      |                                                                                                                                                                                                                                          |
|----------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <i>label</i>         | identifies the contrast in the table. A label is required for every contrast specified. Labels can be up to 200 characters and must be enclosed in quotes.                                                                               |
| <i>fixed-effect</i>  | identifies an effect that appears in the <b>MODEL</b> statement. The keyword INTERCEPT can be used as an effect when an intercept is fitted in the model. You do not need to include all effects that are in the <b>MODEL</b> statement. |
| <i>random-effect</i> | identifies an effect that appears in the <b>RANDOM</b> statement. The first random effect must follow a vertical bar ( ); however, random effects do not have to be specified.                                                           |
| <i>values</i>        | are constants that are elements of the $L$ matrix associated with the fixed and random effects.                                                                                                                                          |

The rows of  $L'$  are specified in order and are separated by commas. The rows of the  $K'$  component of  $L'$  are specified on the left side of the vertical bars (|). These rows test the fixed effects and are, therefore, checked for estimability. The rows of the  $M'$  component of  $L'$  are specified on the right side of the vertical bars. They test the random effects, and no estimability checking is necessary.

If PROC MIXED finds the fixed-effects portion of the specified contrast to be nonestimable (see the **SINGULAR=** option), then it displays a message in the log.

The following CONTRAST statement reproduces the  $F$  test for the effect A in the split-plot example (see Example 59.1):

```
contrast 'A broad'
 A 1 -1 0 A*B .5 .5 -.5 -.5 0 0 ,
 A 1 0 -1 A*B .5 .5 0 0 -.5 -.5 / df=6;
```

Note that no random effects are specified in the preceding contrast; thus, the inference space is broad. The resulting  $F$  test has two numerator degrees of freedom because  $L'$  has two rows. The denominator degrees of freedom is, by default, the residual degrees of freedom (9), but the `DF=` option changes the denominator degrees of freedom to 6.

The following CONTRAST statement reproduces the  $F$  test for A when Block and A\*Block are considered fixed effects (the narrow inference space):

```
contrast 'A narrow'
 A 1 -1 0
 A*B .5 .5 -.5 -.5 0 0 |
 A*Block .25 .25 .25 .25
 -.25 -.25 -.25 -.25
 0 0 0 0 ,
 A 1 0 -1
 A*B .5 .5 0 0 -.5 -.5 |
 A*Block .25 .25 .25 .25
 0 0 0 0
 -.25 -.25 -.25 -.25 ;
```

The preceding contrast does not contain coefficients for B and Block, because they cancel out in estimated differences between levels of A. Coefficients for B and Block are necessary to estimate the mean of one of the levels of A in the narrow inference space (see [Example 59.1](#)).

If the elements of  $L$  are not specified for an effect that contains a specified effect, then the elements of the specified effect are automatically “filled in” over the levels of the higher-order effect. This feature is designed to preserve estimability for cases where there are complex higher-order effects. The coefficients for the higher-order effect are determined by equitably distributing the coefficients of the lower-level effect, as in the construction of least squares means. In addition, if the intercept is specified, it is distributed over all classification effects that are not contained by any other specified effect. If an effect is not specified and does not contain any specified effects, then all of its coefficients in  $L$  are set to 0. You can override this behavior by specifying coefficients for the higher-order effect.

If too many values are specified for an effect, the extra ones are ignored; if too few are specified, the remaining ones are set to 0. If no random effects are specified, the vertical bar can be omitted; otherwise, it must be present. If a `SUBJECT=` effect is used in the `RANDOM` statement, then the coefficients specified for the effects in the `RANDOM` statement are equitably distributed across the levels of the `SUBJECT` effect. You can use the `E` option to see exactly which  $L$  matrix is used.

The `SUBJECT` and `GROUP` options in the `CONTRAST` statement are useful for the case when a `SUBJECT=` or `GROUP=` variable appears in the `RANDOM` statement, and you want to contrast different subjects or groups. By default, `CONTRAST` statement coefficients on random effects are distributed equally across subjects and groups.

`PROC MIXED` handles missing level combinations of classification variables similarly to the way `PROC GLM` does. Both procedures delete fixed-effects parameters corresponding to missing levels in order to preserve estimability. However, `PROC MIXED` does not delete missing level combinations for random-effects parameters because linear combinations of the random-effects parameters are always estimable. These conventions can affect the way you specify your `CONTRAST` coefficients.

The CONTRAST statement computes the statistic

$$F = \frac{\begin{bmatrix} \hat{\beta} \\ \hat{\gamma} \end{bmatrix}' \mathbf{L}(\mathbf{L}'\hat{\mathbf{C}}\mathbf{L})^{-1}\mathbf{L}' \begin{bmatrix} \hat{\beta} \\ \hat{\gamma} \end{bmatrix}}{r}$$

where  $r = \text{rank}(\mathbf{L}'\hat{\mathbf{C}}\mathbf{L})$ , and approximates its distribution with an  $F$  distribution. In this expression,  $\hat{\mathbf{C}}$  is an estimate of the generalized inverse of the coefficient matrix in the mixed model equations. See the section “Inference and Test Statistics” on page 4968 for more information about this  $F$  statistic.

The numerator degrees of freedom in the  $F$  approximation are  $r = \text{rank}(\mathbf{L}'\hat{\mathbf{C}}\mathbf{L})$ , and the denominator degrees of freedom are taken from the “Tests of Fixed Effects” table and corresponds to the final effect you list in the CONTRAST statement. You can change the denominator degrees of freedom by using the **DF=** option.

You can specify the following *options* in the CONTRAST statement after a slash (/).

### CHISQ

requests that chi-square tests be performed in addition to any  $F$  tests. A chi-square statistic equals its corresponding  $F$  statistic times the associate numerator degrees of freedom, and the same degrees of freedom are used to compute the  $p$ -value for the chi-square test. This  $p$ -value is always less than that for the  $F$ -test, as it effectively corresponds to an  $F$  test with infinite denominator degrees of freedom.

### DF=*number*

specifies the denominator degrees of freedom for the  $F$  test. The default is the denominator degrees of freedom taken from the “Tests of Fixed Effects” table and corresponds to the final effect you list in the CONTRAST statement.

### E

requests that the  $\mathbf{L}$  matrix coefficients for the contrast be displayed. The ODS name of the “L Matrix Coefficients” table is Coef.

### GROUP *coeffs*

#### GRP *coeffs*

sets up random-effect contrasts between different groups when a **GROUP=** variable appears in the **RANDOM** statement. By default, CONTRAST statement coefficients on random effects are distributed equally across groups.

### SINGULAR=*number*

tunes the estimability checking. If  $\mathbf{v}$  is a vector, define  $\text{ABS}(\mathbf{v})$  to be the absolute value of the element of  $\mathbf{v}$  with the largest absolute value. If  $\text{ABS}(\mathbf{K}' - \mathbf{K}'\mathbf{T})$  is greater than  $c*\text{number}$  for any row of  $\mathbf{K}'$  in the contrast, then  $\mathbf{K}$  is declared nonestimable. Here  $\mathbf{T}$  is the Hermite form matrix  $(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{X}$ , and  $c$  is  $\text{ABS}(\mathbf{K}')$  except when it equals 0, and then  $c$  is 1. The value for *number* must be between 0 and 1; the default is 1E-4.

### SUBJECT *coeffs*

#### SUB *coeffs*

sets up random-effect contrasts between different subjects when a **SUBJECT=** variable appears in the **RANDOM** statement. By default, CONTRAST statement coefficients on random effects are distributed equally across subjects.

## ESTIMATE Statement

```
ESTIMATE 'label' <fixed-effect values ... >
 <| random-effect values ... > </options>;
```

The ESTIMATE statement is exactly like a **CONTRAST** statement, except only one-row **L** matrices are permitted. The actual estimate,  $L'\hat{p}$ , is displayed along with its approximate standard error. An approximate *t* test that  $L'\hat{p} = 0$  is also produced.

PROC MIXED selects the degrees of freedom to match those displayed in the “Tests of Fixed Effects” table for the final effect you list in the ESTIMATE statement. You can modify the degrees of freedom by using the **DF=** option.

If PROC MIXED finds the fixed-effects portion of the specified estimate to be nonestimable, then it displays “Non-est” for the estimate entries.

The following examples of ESTIMATE statements compute the mean of the first level of A in the split-plot example (see [Example 59.1](#)) for various inference spaces:

```
estimate 'A1 mean narrow' intercept 1
 A 1 B .5 .5 A*B .5 .5 |
 block .25 .25 .25 .25
 A*Block .25 .25 .25 .25
 0 0 0 0
 0 0 0 0;

estimate 'A1 mean intermed' intercept 1
 A 1 B .5 .5 A*B .5 .5 |
 Block .25 .25 .25 .25;

estimate 'A1 mean broad' intercept 1
 A 1 B .5 .5 A*B .5 .5;
```

The construction of the **L** vector for an ESTIMATE statement follows the same rules as listed under the **CONTRAST** statement.

Table 59.5 summarizes the options available in the ESTIMATE statement.

**Table 59.5** ESTIMATE Statement Options

| Option    | Description                                                |
|-----------|------------------------------------------------------------|
| ALPHA=    | Specifies the confidence level                             |
| CL        | Constructs <i>t</i> -type confidence limits                |
| DF=       | Specifies the degrees of freedom                           |
| DIVISOR=  | Specifies a value by which to divide all coefficients      |
| E         | Displays the <b>L</b> matrix coefficients                  |
| GROUP     | Sets up random-effect contrasts between different groups   |
| LOWER     | Performs lower-tailed tests                                |
| SINGULAR= | Tunes the estimability checking                            |
| SUBJECT   | Sets up random-effect contrasts between different subjects |
| UPPER     | Performs upper-tailed tests                                |

You can specify the following *options* in the ESTIMATE statement after a slash (/).



**ALPHA=number**

requests that a  $t$ -type confidence interval be constructed with confidence level  $1 - \text{number}$ . The value of *number* must be between 0 and 1; the default is 0.05.

**CL**

requests that  $t$ -type confidence limits be constructed. The confidence level is 0.95 by default; this can be changed with the **ALPHA=** option.

**DF=number**

specifies the degrees of freedom for the  $t$  test and confidence limits. The default is the denominator degrees of freedom taken from the “Tests of Fixed Effects” table and corresponds to the final effect you list in the ESTIMATE statement.

**DIVISOR=number**

specifies a value by which to divide all coefficients so that fractional coefficients can be entered as integer numerators.

**E**

requests that the **L** matrix coefficients be displayed. The ODS name of this “L Matrix Coefficients” table is “Coef.”

**GROUP coeffs****GRP coeffs**

sets up random-effect contrasts between different groups when a **GROUP=** variable appears in the **RANDOM** statement. By default, ESTIMATE statement coefficients on random effects are distributed equally across groups.

**LOWER****LOWERTAILED**

requests that the  $p$ -value for the  $t$  test be based only on values less than the  $t$  statistic. A two-tailed test is the default. A lower-tailed confidence limit is also produced if you specify the **CL** option.

**SINGULAR=number**

tunes the estimability checking as documented for the **SINGULAR=** option in the **CONTRAST** statement.

**SUBJECT coeffs****SUB coeffs**

sets up random-effect contrasts between different subjects when a **SUBJECT=** variable appears in the **RANDOM** statement. By default, ESTIMATE statement coefficients on random effects are distributed equally across subjects. For example, the ESTIMATE statement in the following code from [Example 59.5](#) constructs the difference between the random slopes of the first two batches.

```
proc mixed data=rc;
 class batch;
 model y = month / s;
 random int month / type=un sub=batch s;
 estimate 'slope b1 - slope b2' | month 1 / subject 1 -1;
run;
```

**UPPER****UPPERTAILED**

requests that the  $p$ -value for the  $t$  test be based only on values greater than the  $t$  statistic. A two-tailed test is the default. An upper-tailed confidence limit is also produced if you specify the **CL** option.

**ID Statement**

**ID** *variables* ;

The ID statement specifies which variables from the input data set are to be included in the **OUTP=** and **OUTPM=** data sets from the **MODEL** statement. If you do not specify an ID statement, then all variables are included in these data sets. Otherwise, only the variables you list in the ID statement are included. Specifying an ID statement with no variables prevents any variables from being included in these data sets.

**LSMEANS Statement**

**LSMEANS** *fixed-effects* < / *options* > ;

The LSMEANS statement computes least squares means (LS-means) of fixed effects. As in the GLM procedure, LS-means are *predicted population margins*—that is, they estimate the marginal means over a balanced population. In a sense, LS-means are to unbalanced designs as class and subclass arithmetic means are to balanced designs. The **L** matrix constructed to compute them is the same as the **L** matrix formed in PROC GLM; however, the standard errors are adjusted for the covariance parameters in the model.

Each LS-mean is computed as  $\mathbf{L}\hat{\boldsymbol{\beta}}$ , where **L** is the coefficient matrix associated with the least squares mean and  $\hat{\boldsymbol{\beta}}$  is the estimate of the fixed-effects parameter vector (see the section “Estimating Fixed and Random Effects in the Mixed Model” on page 4965). The approximate standard errors for the LS-mean is computed as the square root of  $\mathbf{L}(\mathbf{X}'\hat{\mathbf{V}}^{-1}\mathbf{X})^{-1}\mathbf{L}'$ .

LS-means can be computed for any effect in the **MODEL** statement that involves **CLASS** variables. You can specify multiple effects in one LSMEANS statement or in multiple LSMEANS statements, and all LSMEANS statements must appear after the **MODEL** statement. As in the **ESTIMATE** statement, the **L** matrix is tested for estimability, and if this test fails, PROC MIXED displays “Non-est” for the LS-means entries.

Assuming the LS-mean is estimable, PROC MIXED constructs an approximate  $t$  test to test the null hypothesis that the associated population quantity equals zero. By default, the denominator degrees of freedom for this test are the same as those displayed for the effect in the “Tests of Fixed Effects” table (see the section “Default Output” on page 4983).

Table 59.6 summarizes the options available in the LSMEANS statement. All LSMEANS options are subsequently discussed in alphabetical order.

**Table 59.6** Summary of LSMEANS Statement Options

| Option                                          | Description                                    |
|-------------------------------------------------|------------------------------------------------|
| <b>Construction and Computation of LS-Means</b> |                                                |
| <b>AT</b>                                       | Modifies covariate value in computing LS-means |

Table 59.6 continued

| Option                                              | Description                                                                                                                                  |
|-----------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------|
| BYLEVEL                                             | Computes separate margins                                                                                                                    |
| DIFF                                                | Requests differences of LS-means                                                                                                             |
| OM                                                  | Specifies weighting scheme for LS-mean computation                                                                                           |
| SINGULAR=                                           | Tunes estimability checking                                                                                                                  |
| SLICE=                                              | Partitions $F$ tests (simple effects)                                                                                                        |
| <b>Degrees of Freedom and <math>p</math>-values</b> |                                                                                                                                              |
| ADJDFE=                                             | Determines whether to compute row-wise denominator degrees of freedom with <code>DDFM=SATTERTHWAITE</code> or <code>DDFM=KENWARDROGER</code> |
| ADJUST=                                             | Determines the method for multiple comparison adjustment of LS-mean differences                                                              |
| ALPHA= $\alpha$                                     | Determines the confidence level ( $1 - \alpha$ )                                                                                             |
| DF=                                                 | Assigns specific value to degrees of freedom for tests and confidence limits                                                                 |
| <b>Statistical Output</b>                           |                                                                                                                                              |
| CL                                                  | Constructs confidence limits for means and or mean differences                                                                               |
| CORR                                                | Displays correlation matrix of LS-means                                                                                                      |
| COV                                                 | Displays covariance matrix of LS-means                                                                                                       |
| E                                                   | Prints the $L$ matrix                                                                                                                        |

You can specify the following *options* in the LSMEANS statement after a slash (/).

**ADJDFE=SOURCE****ADJDFE=ROW**

specifies how denominator degrees of freedom are determined when  $p$ -values and confidence limits are adjusted for multiple comparisons with the `ADJUST=` option. When you do not specify the `ADJDFE=` option, or when you specify `ADJDFE=SOURCE`, the denominator degrees of freedom for multiplicity-adjusted results are the denominator degrees of freedom for the LS-mean effect in the “Type 3 Tests of Fixed Effects” table. When you specify `ADJDFE=ROW`, the denominator degrees of freedom for multiplicity-adjusted results correspond to the degrees of freedom displayed in the DF column of the “Differences of Least Squares Means” table.

The `ADJDFE=ROW` setting is particularly useful if you want multiplicity adjustments to take into account that denominator degrees of freedom are not constant across LS-mean differences. This can be the case, for example, when the `DDFM=SATTERTHWAITE` or `DDFM=KENWARDROGER` degrees-of-freedom method is in effect.

In one-way models with heterogeneous variance, combining certain `ADJUST=` options with the `ADJDFE=ROW` option corresponds to particular methods of performing multiplicity adjustments in the presence of heteroscedasticity. For example, the following statements fit a heteroscedastic one-way model and perform Dunnett’s T3 method (Dunnett 1980), which is based on the studentized maximum modulus (`ADJUST=SMM`):

```

proc mixed;
 class A;
 model y = A / ddfm=satterth;
 repeated / group=A;
 lsmeans A / adjust=smm adjdfe=row;
run;

```

If you combine the ADJDFE=ROW option with ADJUST=SIDAK, the multiplicity adjustment corresponds to the T2 method of Tamhane (1979), while ADJUST=TUKEY corresponds to the method of Games-Howell (Games and Howell 1976). Note that ADJUST=TUKEY gives the exact results for the case of fractional degrees of freedom in the one-way model, but it does not take into account that the degrees of freedom are subject to variability. A more conservative method, such as ADJUST=SMM, might protect the overall error rate better.

Unless the ADJUST= option of the LSMEANS statement is specified, the ADJDFE= option has no effect.

#### ADJUST=BON

#### ADJUST=DUNNETT

#### ADJUST=SCHEFFE

#### ADJUST=SIDAK

#### ADJUST=SIMULATE<(sim-options)>

#### ADJUST=SMM | GT2

#### ADJUST=TUKEY

requests a multiple comparison adjustment for the  $p$ -values and confidence limits for the differences of LS-means. By default, PROC MIXED adjusts all pairwise differences unless you specify ADJUST=DUNNETT, in which case PROC MIXED analyzes all differences with a control level. The ADJUST= option implies the DIFF option.

The BON (Bonferroni) and SIDAK adjustments involve correction factors described in Chapter 42, “The GLM Procedure,” and Chapter 61, “The MULTTEST Procedure;” also see Westfall and Young (1993) and Westfall et al. (1999). When you specify ADJUST=TUKEY and your data are unbalanced, PROC MIXED uses the approximation described in Kramer (1956). Similarly, when you specify ADJUST=DUNNETT and the LS-means are correlated, PROC MIXED uses the factor-analytic covariance approximation described in Hsu (1992). The preceding references also describe the SCHEFFE and SMM adjustments.

The SIMULATE adjustment computes adjusted  $p$ -values and confidence limits from the simulated distribution of the maximum or maximum absolute value of a multivariate  $t$  random vector. All covariance parameters except the residual variance are fixed at their estimated values throughout the simulation, potentially resulting in some underdispersion. The simulation estimates  $q$ , the true  $(1 - \alpha)$  quantile, where  $1 - \alpha$  is the confidence coefficient. The default  $\alpha$  is 0.05, and you can change this value with the ALPHA= option in the LSMEANS statement.

The number of samples is set so that the tail area for the simulated  $q$  is within  $\gamma$  of  $1 - \alpha$  with  $100(1 - \epsilon)\%$  confidence. In equation form,

$$P(|F(\hat{q}) - (1 - \alpha)| \leq \gamma) = 1 - \epsilon$$

where  $\hat{q}$  is the simulated  $q$  and  $F$  is the true distribution function of the maximum; see Edwards and Berry (1987) for details. By default,  $\gamma = 0.005$  and  $\epsilon = 0.01$ , placing the tail area of  $\hat{q}$  within 0.005 of 0.95 with 99% confidence. The `ACC=` and `EPS=` *sim-options* reset  $\gamma$  and  $\epsilon$ , respectively; the `NSAMP=` *sim-option* sets the sample size directly; and the `SEED=` *sim-option* specifies an integer used to start the pseudo-random number generator for the simulation. If you do not specify a seed, or if you specify a value less than or equal to zero, the seed is generated from reading the time of day from the computer clock. For additional descriptions of these and other simulation options, see the section “[LSMEANS Statement](#)” on page 3293 in Chapter 42, “[The GLM Procedure](#).”

**ALPHA=number**

requests that a  $t$ -type confidence interval be constructed for each of the LS-means with confidence level  $1 - \text{number}$ . The value of *number* must be between 0 and 1; the default is 0.05.

**AT variable = value****AT (variable-list) = (value-list)****AT MEANS**

enables you to modify the values of the covariates used in computing LS-means. By default, all covariate effects are set equal to their mean values for computation of standard LS-means. The AT option enables you to assign arbitrary values to the covariates. Additional columns in the output table indicate the values of the covariates.

If there is an effect containing two or more covariates, the AT option sets the effect equal to the product of the individual means rather than the mean of the product (as with standard LS-means calculations). The AT MEANS option sets covariates equal to their mean values (as with standard LS-means) and incorporates this adjustment to crossproducts of covariates.

As an example, consider the following invocation of PROC MIXED:

```
proc mixed;
 class A;
 model Y = A X1 X2 X1*X2;
 lsmeans A;
 lsmeans A / at means;
 lsmeans A / at X1=1.2;
 lsmeans A / at (X1 X2)=(1.2 0.3);
run;
```

For the first two LSMEANS statements, the LS-means coefficient for X1 is  $\bar{x}_1$  (the mean of X1) and for X2 is  $\bar{x}_2$  (the mean of X2). However, for the first LSMEANS statement, the coefficient for X1\*X2 is  $\bar{x}_1\bar{x}_2$ , but for the second LSMEANS statement, the coefficient is  $\bar{x}_1 \cdot \bar{x}_2$ . The third LSMEANS statement sets the coefficient for X1 equal to 1.2 and leaves it at  $\bar{x}_2$  for X2, and the final LSMEANS statement sets these values to 1.2 and 0.3, respectively.

If a WEIGHT variable is present, it is used in processing AT variables. Also, observations with missing dependent variables are included in computing the covariate means, unless these observations form a missing cell and the `FULLX` option in the `MODEL` statement is not in effect. You can use the `E` option in conjunction with the AT option to check that the modified LS-means coefficients are the ones you want.

The AT option is disabled if you specify the `BYLEVEL` option.

**BYLEVEL**

requests PROC MIXED to process the OM data set by each level of the LS-mean effect (LSMEANS effect) in question. For more details, see the **OM** option later in this section.

**CL**

requests that *t*-type confidence limits be constructed for each of the LS-means. The confidence level is 0.95 by default; this can be changed with the **ALPHA=** option.

**CORR**

displays the estimated correlation matrix of the least squares means as part of the “Least Squares Means” table.

**COV**

displays the estimated covariance matrix of the least squares means as part of the “Least Squares Means” table.

**DF=number**

specifies the degrees of freedom for the *t* test and confidence limits. The default is the denominator degrees of freedom taken from the “Tests of Fixed Effects” table corresponding to the LS-means effect unless the **DDFM=SATTERTHWAITE** or **DDFM=KENWARDROGER** option is in effect in the **MODEL** statement. For these **DDFM=** methods, degrees of freedom are determined separately for each test; see the **DDFM=** option for more information.

**DIFF<=difftype>****PDIFF<=difftype>**

requests that differences of the LS-means be displayed. The optional *difftype* specifies which differences to produce, with possible values being **ALL**, **CONTROL**, **CONTROLL**, and **CONTROLU**. The *difftype* **ALL** requests all pairwise differences, and it is the default. The *difftype* **CONTROL** requests the differences with a control, which, by default, is the first level of each of the specified LSMEANS effects.

To specify which levels of the effects are the controls, list the quoted formatted values in parentheses after the keyword **CONTROL**. For example, if the effects **A**, **B**, and **C** are classification variables, each having two levels, 1 and 2, the following LSMEANS statement specifies the (1,2) level of **A\*B** and the (2,1) level of **B\*C** as controls:

```
lsmeans A*B B*C / diff=control('1' '2' '2' '1');
```

For multiple effects, the results depend upon the order of the list, and so you should check the output to make sure that the controls are correct.

Two-tailed tests and confidence limits are associated with the **CONTROL** *difftype*. For one-tailed results, use either the **CONTROLL** or **CONTROLU** *difftype*. The **CONTROLL** *difftype* tests whether the noncontrol levels are significantly smaller than the control; the upper confidence limits for the control minus the noncontrol levels are considered to be infinity and are displayed as missing. Conversely, the **CONTROLU** *difftype* tests whether the noncontrol levels are significantly larger than the control; the upper confidence limits for the noncontrol levels minus the control are considered to be infinity and are displayed as missing.

If you want to perform multiple comparison adjustments on the differences of LS-means, you must specify the **ADJUST=** option.

The differences of the LS-means are displayed in a table titled “Differences of Least Squares Means.” The ODS table name is `Diff`s.

**E**

requests that the **L** matrix coefficients for all LSMEANS effects be displayed. The ODS name of this “L Matrix Coefficients” table is `Coef`.

**OM**<=*OM-data-set*>

**OBSMARGINS**<=*OM-data-set*>

specifies a potentially different weighting scheme for the computation of LS-means coefficients. The standard LS-means have equal coefficients across classification effects; however, the **OM** option changes these coefficients to be proportional to those found in *OM-data-set*. This adjustment is reasonable when you want your inferences to apply to a population that is not necessarily balanced but has the margins observed in *OM-data-set*.

By default, *OM-data-set* is the same as the analysis data set. You can optionally specify another data set that describes the population for which you want to make inferences. This data set must contain all model variables except for the dependent variable (which is ignored if it is present). In addition, the levels of all **CLASS** variables must be the same as those occurring in the analysis data set. Specifying an *OM-data-set* enables you to construct arbitrarily weighted LS-means.

In computing the observed margins, PROC MIXED uses all observations for which there are no missing or invalid independent variables, including those for which there are missing dependent variables. Also, if *OM-data-set* has a **WEIGHT** variable, PROC MIXED uses weighted margins to construct the LS-means coefficients. If *OM-data-set* is balanced, the LS-means are unchanged by the **OM** option.

The **BYLEVEL** option modifies the observed-margins LS-means. Instead of computing the margins across all of the *OM-data-set*, PROC MIXED computes separate margins for each level of the LSMEANS effect in question. In this case the resulting LS-means are actually equal to raw means for fixed-effects models and certain balanced random-effects models, but their estimated standard errors account for the covariance structure that you have specified. If the **AT** option is specified, the **BYLEVEL** option disables it.

You can use the **E** option in conjunction with either the **OM** or **BYLEVEL** option to check that the modified LS-means coefficients are the ones you want. It is possible that the modified LS-means are not estimable when the standard ones are, or vice versa. Nonestimable LS-means are noted as “Non-est” in the output.

**PDIF**

is the same as the **DIFF** option.

**SINGULAR**=*number*

tunes the estimability checking as documented for the **SINGULAR**= option in the **CONTRAST** statement.

**SLICE**= *fixed-effect*

**SLICE**= (*fixed-effects*)

specifies effects by which to partition interaction LSMEANS effects. This can produce what are known as tests of simple effects (Winer 1971). For example, suppose that **A\*B** is significant, and you want to test the effect of **A** for each level of **B**. The appropriate LSMEANS statement is as follows:

```
lsmeans A*B / slice=B;
```

This code tests for the simple main effects of A for B, which are calculated by extracting the appropriate rows from the coefficient matrix for the A\*B LS-means and by using them to form an  $F$  test. See the section “[Inference and Test Statistics](#)” for more information about this  $F$  test.

The SLICE option produces a table titled “Tests of Effect Slices.” The ODS table name is Slices.

---

## LSMESTIMATE Statement

```
LSMESTIMATE model-effect <'label'> values <divisor=n>
 < , ... <'label'> values <divisor=n> >
 </ options > ;
```

The LSMESTIMATE statement provides a mechanism for obtaining custom hypothesis tests among least squares means.

Table 59.7 summarizes the options available in the LSMESTIMATE statement.

**Table 59.7** LSMESTIMATE Statement Options

| Option                                              | Description                                                                         |
|-----------------------------------------------------|-------------------------------------------------------------------------------------|
| <b>Construction and Computation of LS-Means</b>     |                                                                                     |
| AT                                                  | Modifies covariate values in computing LS-means                                     |
| BYLEVEL                                             | Computes separate margins                                                           |
| DIVISOR=                                            | Specifies a list of values to divide the coefficients                               |
| OM=                                                 | Specifies the weighting scheme for LS-means computation as determined by a data set |
| SINGULAR=                                           | Tunes estimability checking                                                         |
| <b>Degrees of Freedom and <math>p</math>-values</b> |                                                                                     |
| ADJUST=                                             | Determines the method for multiple-comparison adjustment of LS-means differences    |
| ALPHA= $\alpha$                                     | Determines the confidence level ( $1 - \alpha$ )                                    |
| LOWER                                               | Performs one-sided, lower-tailed inference                                          |
| STEPDOWN                                            | Adjusts multiple-comparison $p$ -values further in a step-down fashion              |
| TESTVALUE=                                          | Specifies values under the null hypothesis for tests                                |
| UPPER                                               | Performs one-sided, upper-tailed inference                                          |

---



Table 59.7 continued

| Option                    | Description                                                                            |
|---------------------------|----------------------------------------------------------------------------------------|
| <b>Statistical Output</b> |                                                                                        |
| CL                        | Constructs confidence limits for means and mean differences                            |
| CORR                      | Displays the correlation matrix of LS-means                                            |
| COV                       | Displays the covariance matrix of LS-means                                             |
| E                         | Prints the <b>L</b> matrix                                                             |
| ELSM                      | Prints the <b>K</b> matrix                                                             |
| JOINT                     | Produces a joint <i>F</i> or chi-square test for the LS-means and LS-means differences |
| SEED=                     | Specifies the seed for computations that depend on random numbers                      |

For details about the syntax of the LSMESTIMATE statement, see the section “LSMESTIMATE Statement” on page 470 in Chapter 19, “Shared Concepts and Topics.”

## MODEL Statement

**MODEL** *dependent* = < fixed-effects > < / options > ;

The MODEL statement names a single dependent variable and the fixed effects, which determine the **X** matrix of the mixed model (see the section “Parameterization of Mixed Models” on page 4971 for details). The specification of effects is the same as in the GLM procedure; however, unlike PROC GLM, you do not specify random effects in the MODEL statement. The MODEL statement is required.

An intercept is included in the fixed-effects model by default. If no fixed effects are specified, only this intercept term is fit. The intercept can be removed by using the NOINT option.

Table 59.8 summarizes the options available in the MODEL statement. These are subsequently discussed in detail in alphabetical order.

Table 59.8 Summary of MODEL Statement Options

| Option                          | Description                                                         |
|---------------------------------|---------------------------------------------------------------------|
| <b>Model Building</b>           |                                                                     |
| NOINT                           | Excludes fixed-effect intercept from model                          |
| <b>Statistical Computations</b> |                                                                     |
| ALPHA= $\alpha$                 | Determines the confidence level $(1 - \alpha)$ for fixed effects    |
| ALPHAP= $\alpha$                | Determines the confidence level $(1 - \alpha)$ for predicted values |
| CHISQ                           | Requests chi-square tests                                           |
| DDF=                            | Specifies denominator degrees of freedom (list)                     |
| DDFM=                           | Specifies the method for computing denominator degrees of freedom   |
| HTYPE=                          | Selects the type of hypothesis test                                 |
| INFLUENCE                       | Requests influence and case-deletion diagnostics                    |

Table 59.8 *continued*

| Option                        | Description                                                                    |
|-------------------------------|--------------------------------------------------------------------------------|
| NOTESET                       | Suppresses hypothesis tests for the fixed effects                              |
| OUTP=                         | Specifies output data set for predicted values and related quantities          |
| OUTPM=                        | Specifies output data set for predicted means and related quantities           |
| RESIDUAL                      | Adds Pearson-type and studentized residuals to output data sets                |
| VCIRY                         | Adds scaled marginal residual to output data sets                              |
| <b>Statistical Output</b>     |                                                                                |
| CL                            | Displays confidence limits for fixed-effects parameter estimates               |
| CORRB                         | Displays correlation matrix of fixed-effects parameter estimates               |
| COVB                          | Displays covariance matrix of fixed-effects parameter estimates                |
| COVBI                         | Displays inverse covariance matrix of fixed-effects parameter estimates        |
| E, E1, E2, E3                 | Displays <b>L</b> matrix coefficients                                          |
| INTERCEPT                     | Adds a row for the intercept to test tables                                    |
| SOLUTION                      | Displays fixed-effects parameter estimates (and scale parameter in GLM models) |
| <b>Singularity Tolerances</b> |                                                                                |
| SINGCHOL=                     | Tunes sensitivity in computing Cholesky roots                                  |
| SINGRES=                      | Tunes singularity criterion for residual variance                              |
| SINGULAR=                     | Tunes the sensitivity in sweeping                                              |
| ZETA=                         | Tunes the sensitivity in forming Type 3 functions                              |

You can specify the following *options* in the MODEL statement after a slash (/).

**ALPHA=number**

requests that a *t*-type confidence interval be constructed for each of the fixed-effects parameters with confidence level  $1 - \text{number}$ . The value of *number* must be between 0 and 1; the default is 0.05.

**ALPHAP=number**

requests that a *t*-type confidence interval be constructed for the predicted values with confidence level  $1 - \text{number}$ . The value of *number* must be between 0 and 1; the default is 0.05.

**CHISQ**

requests that chi-square tests be performed for all specified effects in addition to the *F* tests. Type 3 tests are the default; you can produce the Type 1 and Type 2 tests by using the **HTYPE=** option.

**CL**

requests that *t*-type confidence limits be constructed for each of the fixed-effects parameter estimates. The confidence level is 0.95 by default; this can be changed with the **ALPHA=** option.

**CONTAIN**

has the same effect as the **DDFM=CONTAIN** option.

**CORRB**

produces the approximate correlation matrix of the fixed-effects parameter estimates. The ODS name of this table is CorrB.

**COVB**

produces the approximate variance-covariance matrix of the fixed-effects parameter estimates  $\hat{\beta}$ . By default, this matrix equals  $(\mathbf{X}'\hat{\mathbf{V}}^{-1}\mathbf{X})^{-1}$  and results from sweeping  $(\mathbf{X} \ \mathbf{y})'\hat{\mathbf{V}}^{-1}(\mathbf{X} \ \mathbf{y})$  on all but its last pivot and removing the  $y$  border. The **EMPIRICAL** option in the **PROC MIXED** statement changes this matrix into “empirical sandwich” form. The ODS name of this table is CovB. If the degrees-of-freedom method of Kenward and Roger (1997) is in effect (**DDFM=KENWARDROGER**), the COVB matrix changes because the method entails an adjustment of the variance-covariance matrix of the fixed effects by the method proposed by Prasad and Rao (1990); Harville and Jeske (1992). See also Kackar and Harville (1984).

**COVBI**

produces the inverse of the approximate variance-covariance matrix of the fixed-effects parameter estimates. The ODS name of this table is InvCovB.

**DDF=***value-list*

enables you to specify your own denominator degrees of freedom for the fixed effects. The *value-list* specification is a list of numbers or missing values (.) separated by commas. The degrees of freedom should be listed in the order in which the effects appear in the “Tests of Fixed Effects” table. If you want to retain the default degrees of freedom for a particular effect, use a missing value for its location in the list. For example, the following statement assigns 3 denominator degrees of freedom to A and 4.7 to A\*B, while those for B remain the same:

```
model Y = A B A*B / ddf=3, ., 4.7;
```

If you specify **DDFM=SATTERTHWAITE** or **DDFM=KENWARDROGER**, the DDF= option has no effect.

**DDFM=****DDFM=CONTAIN****DDFM=BETWITHIN****DDFM=RESIDUAL****DDFM=SATTERTHWAITE****DDFM=KENWARDROGER<(FIRSTORDER)>****DDFM=KENWARDROGER<(LINEAR)>**

specifies the method for computing the denominator degrees of freedom for the tests of fixed effects resulting from the **MODEL**, **CONTRAST**, **ESTIMATE**, and **LSMEANS** statements.

Table 59.9 lists syntax aliases for the degrees-of-freedom methods.

**Table 59.9** Aliases for DDFM= Option

| DDFM= Option | Alias |
|--------------|-------|
| BETWITHIN    | BW    |
| CONTAIN      | CON   |

Table 59.9 *continued*

| DDFM= Option  | Alias         |
|---------------|---------------|
| KENWARDROGER  | KENROG, KR    |
| RESIDUAL      | RES           |
| SATTERTHWAITE | SATTERTH, SAT |

The DDFM=CONTAIN option invokes the *containment method* to compute denominator degrees of freedom, and it is the default when you specify a **RANDOM** statement. The containment method is carried out as follows: Denote the fixed effect in question **A**, and search the **RANDOM** effect list for the effects that *syntactically* contain **A**. For example, the random effect **B(A)** contains **A**, but the random effect **C** does not, even if it has the same levels as **B(A)**.

Among the random effects that contain **A**, compute their rank contribution to the  $(\mathbf{X} \mathbf{Z})$  matrix. The DDF assigned to **A** is the smallest of these rank contributions. If no effects are found, the DDF for **A** is set equal to the residual degrees of freedom,  $N - \text{rank}(\mathbf{X} \mathbf{Z})$ . This choice of DDF matches the tests performed for balanced split-plot designs and should be adequate for moderately unbalanced designs.

**CAUTION:** If you have a **Z** matrix with a large number of columns, the overall memory requirements and the computing time after convergence can be substantial for the containment method. If it is too large, you might want to use the DDFM=BETWITHIN option.

The DDFM=BETWITHIN option is the default for **REPEATED** statement specifications (with no **RANDOM** statements). It is computed by dividing the residual degrees of freedom into between-subject and within-subject portions. PROC MIXED then checks whether a fixed effect changes within any subject. If so, it assigns within-subject degrees of freedom to the effect; otherwise, it assigns the between-subject degrees of freedom to the effect (see Schluchter and Elashoff 1990). If there are multiple within-subject effects containing classification variables, the within-subject degrees of freedom are partitioned into components corresponding to the subject-by-effect interactions.

One exception to the preceding method is the case where you have specified no **RANDOM** statements and a **REPEATED** statement with the **TYPE=UN** option. In this case, all effects are assigned the between-subject degrees of freedom to provide for better small-sample approximations to the relevant sampling distributions. DDFM=KENWARDROGER might be a better option to try for this case.

The DDFM=RESIDUAL option performs all tests by using the residual degrees of freedom,  $n - \text{rank}(\mathbf{X})$ , where  $n$  is the number of observations.

The DDFM=SATTERTHWAITE option performs a general Satterthwaite approximation for the denominator degrees of freedom, computed as follows. Suppose  $\boldsymbol{\theta}$  is the vector of unknown parameters in **V**, and suppose  $\mathbf{C} = (\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-}$ , where  $^{-}$  denotes a generalized inverse. Let  $\hat{\mathbf{C}}$  and  $\hat{\boldsymbol{\theta}}$  be the corresponding estimates.

Consider the one-dimensional case, and consider  $\ell$  to be a vector defining an estimable linear combination of  $\boldsymbol{\beta}$ . The Satterthwaite degrees of freedom for the  $t$  statistic

$$t = \frac{\ell \hat{\boldsymbol{\beta}}}{\sqrt{\ell \hat{\mathbf{C}} \ell'}}$$

is computed as

$$v = \frac{2(\ell \hat{\mathbf{C}} \ell')^2}{\mathbf{g}' \mathbf{A} \mathbf{g}}$$

where  $\mathbf{g}$  is the gradient of  $\ell\mathbf{C}\ell'$  with respect to  $\boldsymbol{\theta}$ , evaluated at  $\widehat{\boldsymbol{\theta}}$ , and  $\mathbf{A}$  is the asymptotic variance-covariance matrix of  $\widehat{\boldsymbol{\theta}}$  obtained from the second derivative matrix of the likelihood equations.

For the multidimensional case, let  $\mathbf{L}$  be an estimable contrast matrix and denote the rank of  $\mathbf{L}\widehat{\mathbf{C}}\mathbf{L}'$  as  $q > 1$ . The Satterthwaite denominator degrees of freedom for the  $F$  statistic

$$F = \frac{\widehat{\boldsymbol{\beta}}'\mathbf{L}'(\mathbf{L}\widehat{\mathbf{C}}\mathbf{L}')^{-1}\mathbf{L}\widehat{\boldsymbol{\beta}}}{q}$$

are computed by first performing the spectral decomposition  $\mathbf{L}\widehat{\mathbf{C}}\mathbf{L}' = \mathbf{P}'\mathbf{D}\mathbf{P}$ , where  $\mathbf{P}$  is an orthogonal matrix of eigenvectors and  $\mathbf{D}$  is a diagonal matrix of eigenvalues, both of dimension  $q \times q$ . Define  $\ell_m$  to be the  $m$ th row of  $\mathbf{P}\mathbf{L}$ , and let

$$v_m = \frac{2(D_m)^2}{\mathbf{g}_m'\mathbf{A}\mathbf{g}_m}$$

where  $D_m$  is the  $m$ th diagonal element of  $\mathbf{D}$  and  $\mathbf{g}_m$  is the gradient of  $\ell_m\mathbf{C}\ell'_m$  with respect to  $\boldsymbol{\theta}$ , evaluated at  $\widehat{\boldsymbol{\theta}}$ . Then let

$$E = \sum_{m=1}^q \frac{v_m}{v_m - 2} I(v_m > 2)$$

where the indicator function eliminates terms for which  $v_m \leq 2$ . The degrees of freedom for  $F$  are then computed as

$$v = \frac{2E}{E - q}$$

provided  $E > q$ ; otherwise  $v$  is set to zero.

This method is a generalization of the techniques described in Giesbrecht and Burns (1985); McLean and Sanders (1988); Fai and Cornelius (1996). The method can also include estimated random effects. In this case, append  $\widehat{\boldsymbol{\gamma}}$  to  $\widehat{\boldsymbol{\beta}}$  and change  $\widehat{\mathbf{C}}$  to be the inverse of the coefficient matrix in the mixed model equations. The calculations require extra memory to hold  $c$  matrices that are the size of the mixed model equations, where  $c$  is the number of covariance parameters. In the notation of Table 59.29, this is approximately  $8q(p + g)(p + g)/2$  bytes. Extra computing time is also required to process these matrices. The Satterthwaite method implemented here is intended to produce an accurate  $F$  approximation; however, the results can differ from those produced by PROC GLM. Also, the small sample properties of this approximation have not been extensively investigated for the various models available with PROC MIXED.

The DDFM=KENWARDROGER option performs the degrees of freedom calculations detailed by Kenward and Roger (1997). This approximation involves inflating the estimated variance-covariance matrix of the fixed and random effects by the method proposed by Prasad and Rao (1990) and Harville and Jeske (1992), see also Kackar and Harville (1984). Satterthwaite-type degrees of freedom are then computed based on this adjustment. By default, the observed information matrix of the covariance parameter estimates is used in the calculations. For covariance structures that have nonzero second derivatives with respect to the covariance parameters, the Kenward-Roger covariance matrix adjustment includes a second-order term. This term can result in standard error shrinkage. Also, the resulting adjusted covariance matrix can then be indefinite and is not invariant under reparameterization. The FIRSTORDER or LINEAR suboption of the DDFM=KENWARDROGER option

eliminates the second derivatives from the calculation of the covariance matrix adjustment. The `LINEAR` suboption is an alias for `FIRSTORDER`. For the case of scalar estimable functions, the resulting estimator is referred to as the Prasad-Rao estimator  $\tilde{m}^{\circledast}$  in Harville and Jeske (1992). The following are examples of covariance structures that generally lead to nonzero second derivatives: `TYPE=ANTE(1)`, `TYPE=AR(1)`, `TYPE=ARH(1)`, `TYPE=ARMA(1,1)`, `TYPE=CSH`, `TYPE=FA`, `TYPE=FA0(q)`, `TYPE=TOEPH`, `TYPE=UNR`, and all `TYPE=SP()` structures.

When the asymptotic variance matrix of the covariance parameters is found to be singular, a generalized inverse is used. Covariance parameters with zero variance then do not contribute to the degrees-of-freedom adjustment for `DDFM=SATTERTHWAITE` and `DDFM=KENWARDROGER`, and a message is written to the log.

This method changes output in the following tables (listed in [Table 59.26](#)): `Contrast`, `CorrB`, `CovB`, `DiffS`, `Estimates`, `InvCovB`, `LSMeans`, `Slices`, `SolutionF`, `SolutionR`, `Tests1–Tests3`. The `OUTP=` and `OUTPM=` data sets are also affected.

**E**

requests that Type 1, Type 2, and Type 3 `L` matrix coefficients be displayed for all specified effects. The ODS name of the table is `Coef`.

**E1**

requests that Type 1 `L` matrix coefficients be displayed for all specified effects. The ODS name of the table is `Coef`.

**E2**

requests that Type 2 `L` matrix coefficients be displayed for all specified effects. The ODS name of the table is `Coef`.

**E3**

requests that Type 3 `L` matrix coefficients be displayed for all specified effects. The ODS name of the table is `Coef`.

**FULLX**

requests that columns of the `X` matrix that consist entirely of zeros not be eliminated from `X`; otherwise, they are eliminated by default. For a column corresponding to a missing cell to be added to `X`, its particular levels must be present in at least one observation in the analysis data set along with a missing dependent variable. The use of the `FULLX` option can affect coefficient specifications in the `CONTRAST` and `ESTIMATE` statements, as well as covariate coefficients from `LSMEANS` statements specified with the `AT MEANS` option.

**HTYPE=value-list**

indicates the type of hypothesis test to perform on the fixed effects. Valid entries for *values* in the list are 1, 2, and 3; the default value is 3. You can specify several types by separating the values with a comma or a space. The ODS table names are “Tests1” for the Type 1 tests, “Tests2” for the Type 2 tests, and “Tests3” for the Type 3 tests.

**INFLUENCE<(influence-options)>**

specifies that influence and case deletion diagnostics are to be computed.

The `INFLUENCE` option computes influence diagnostics by noniterative or iterative methods. The noniterative diagnostics rely on recomputation formulas under the assumption that covariance parameters or their ratios remain fixed. With the possible exception of a profiled residual variance, no

covariance parameters are updated. This is the default behavior because of its computational efficiency. However, the impact of an observation on the overall analysis can be underestimated if its effect on covariance parameters is not assessed. Toward this end, iterative methods can be applied to gauge the overall impact of observations and to obtain influence diagnostics for the covariance parameter estimates.

If you specify the INFLUENCE option without further suboptions, PROC MIXED computes single-case deletion diagnostics and influence statistics for each observation in the data set by updating estimates for the fixed-effects parameter estimates, and also the residual variance, if it is profiled. The **EFFECT=**, **SELECT=**, **ITER=**, **SIZE=**, and **KEEP=** suboptions provide additional flexibility in the computation and reporting of influence statistics. Table 59.10 briefly describes important suboptions and their effect on the influence analysis.

**Table 59.10** Summary of INFLUENCE Default and Suboptions

| Description                                                                                                                                                    | Suboption                         |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------|
| Compute influence diagnostics for individual observations                                                                                                      | Default                           |
| Measure influence of sets of observations chosen according to a classification variable or effect                                                              | <b>EFFECT=</b>                    |
| Remove pairs of observations and report the results sorted by degree of influence                                                                              | <b>SIZE=2</b>                     |
| Remove triples, quadruples of observations, etc.                                                                                                               | <b>SIZE=</b>                      |
| Allow selection of individual observations, observations sharing specific levels of effects, and construction of tuples from specified subsets of observations | <b>SELECT=</b>                    |
| Update fixed effects and covariance parameters by refitting the mixed model, adding up to $n$ iterations                                                       | <b>ITER=<math>n &gt; 0</math></b> |
| Compute influence diagnostics for the covariance parameters                                                                                                    | <b>ITER=<math>n &gt; 0</math></b> |
| Update only fixed effects and the residual variance, if it is profiled                                                                                         | <b>ITER=0</b>                     |
| Add the reduced-data estimates to the data set created with ODS OUTPUT                                                                                         | <b>ESTIMATES</b>                  |

The modifiers and their default values are discussed in the following paragraphs. The set of computed influence diagnostics varies with the suboptions. The most extensive set of influence diagnostics is obtained when **ITER= $n$**  with  $n > 0$ .

You can produce statistical graphics of influence diagnostics when ODS Graphics is enabled. For general information about ODS Graphics, see Chapter 21, “Statistical Graphics Using ODS.” For specific information about the graphics available in the MIXED procedure, see the section “ODS Graphics” on page 4992.

You can specify the following *influence-options* in parentheses:

**EFFECT=***effect*

specifies an effect according to which observations are grouped. Observations sharing the same level of the *effect* are removed from the analysis as a group. The *effect* must contain only classification variables, but they need not be contained in the model.



Removing observations can change the rank of the  $(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}$  matrix. This is particularly likely to happen when multiple observations are eliminated from the analysis. If the rank of the estimated variance-covariance matrix of  $\hat{\boldsymbol{\beta}}$  changes or its singularity pattern is altered, no influence diagnostics are computed.

## ESTIMATES

### EST

specifies that the updated parameter estimates should be written to the ODS output data set. The values are not displayed in the “Influence” table, but if you use ODS OUTPUT to create a data set from the listing, the estimates are added to the data set. If `ITER=0`, only the fixed-effects estimates are saved. In iterative influence analyses, fixed-effects and covariance parameters are stored. The  $p$  fixed-effects parameter estimates are named `Parm1–Parm $p$` , and the  $q$  covariance parameter estimates are named `CovP1–CovP $q$` . The order corresponds to that in the “Solution for Fixed Effects” and “Covariance Parameter Estimates” tables. If parameter updates fail—for example, because of a loss of rank or a nonpositive definite Hessian—missing values are reported.

### ITER= $n$

controls the maximum number of additional iterations PROC MIXED performs to update the fixed-effects and covariance parameter estimates following data point removal. If you specify  $n > 0$ , then statistics such as DFFITS, MDFFITS, and the likelihood distances measure the impact of observation(s) on all aspects of the analysis. Typically, the influence will grow compared to values at `ITER=0`. In models without `RANDOM` or `REPEATED` effects, the `ITER=` option has no effect.

This documentation refers to analyses when  $n > 0$  simply as iterative influence analysis, even if final covariance parameter estimates can be updated in a single step (for example, when `METHOD=MIVQUE0` or `METHOD=TYPE3`). This nomenclature reflects the fact that only if  $n > 0$  are all model parameters updated, which can require additional iterations. If  $n > 0$  and `METHOD=REML` (default) or `METHOD=ML`, the procedure updates fixed effects *and* variance-covariance parameters after removing the selected observations with additional Newton-Raphson iterations, starting from the converged estimates for the entire data. The process stops for each observation or set of observations if the convergence criterion is satisfied or the number of further iterations exceeds  $n$ . If  $n > 0$  and `METHOD=TYPE1`, `TYPE2`, or `TYPE3`, ANOVA estimates of the covariance parameters are recomputed in a single step.

Compared to noniterative updates, the computations are more involved. In particular for large data sets or a large number of random effects (or both), iterative updates require considerably more resources. A one-step (`ITER=1`) or two-step update might be a good compromise. The output includes the number of iterations performed, which is less than  $n$  if the iteration converges. If the process does not converge in  $n$  iterations, you should be careful in interpreting the results, especially if  $n$  is fairly large.

Bounds and other restrictions on the covariance parameters carry over from the full-data model. Covariance parameters that are not iterated in the model fit to the full data (the `NOITER` or `HOLD=` option in the `PARMS` statement) are likewise not updated in the refit. In certain models, such as random-effects models, the ratios between the covariance parameters and the residual variance are maintained rather than the actual value of the covariance parameter estimate (see the section “Influence Diagnostics” on page 4977).



**KEEP=*n***

determines how many observations are retained for display and in the output data set or how many tuples if you specify **SIZE=**. The output is sorted by an influence statistic as discussed for the **SIZE=** suboption.

**SELECT=*value-list***

specifies which observations or effect levels are chosen for influence calculations. If the **SELECT=** suboption is not specified, diagnostics are computed as follows:

- for all observations, if **EFFECT=** or **SIZE=** are not given
- for all levels of the specified effect, if **EFFECT=** is specified
- for all tuples of size *k* formed from the observations in *value-list*, if **SIZE=*k*** is specified

When you specify an effect with the **EFFECT=** option, the values in *value-list* represent indices of the levels in the order in which PROC MIXED builds classification effects. Which observations in the data set correspond to this index depends on the order of the variables in the **CLASS** statement, not the order in which the variables appear in the interaction effect. See the section “Parameterization of Mixed Models” on page 4971 to understand precisely how the procedure indexes nested and crossed effects and how levels of classification variables are ordered. The actual values of the classification variables involved in the effect are shown in the output so you can determine which observations were removed.

If the **EFFECT=** suboption is not specified, the **SELECT=** value list refers to the sequence in which observations are read from the input data set or from the current BY group if there is a **BY** statement. This indexing is not necessarily the same as the observation numbers in the input data set, for example, if a **WHERE** clause is specified or during BY processing.

**SIZE=*n***

instructs PROC MIXED to remove groups of observations formed as tuples of size *n*. For example, **SIZE=2** specifies all  $n \times (n - 1) / 2$  unique pairs of observations. The number of tuples for **SIZE=*k*** is  $n! / (k!(n - k)!)$  and grows quickly with *n* and *k*. Using the **SIZE=** option can result in considerable computing time. The MIXED procedure displays by default only the 50 tuples with the greatest influence. Use the **KEEP=** option to override this default and to retain a different number of tuples in the listing or ODS output data set. Regardless of the **KEEP=** specification, all tuples are evaluated and the results are ordered according to an influence statistic. This statistic is the (restricted) likelihood distance as a measure of overall influence if **ITER=*n* > 0** or when a residual variance is profiled. When likelihood distances are unavailable, the results are ordered by the PRESS statistic.

To reduce computational burden, the **SIZE=** option can be combined with the **SELECT=*value-list*** modifier. For example, the following statements evaluate all  $15 = 6 \times 5 / 2$  pairs formed from observations 13, 14, 18, 30, 31, and 33 and display the five pairs with the greatest influence:

```
proc mixed;
 class a m f;
 model penetration = a m /
 influence(size=2 keep=5
 select=13,14,18,30,31,33);
 random f(m);
run;
```

If any observation in a tuple contains missing values or has otherwise not contributed to the analysis, the tuple is not evaluated. This guarantees that the displayed results refer to the same number of observations, so that meaningful statistics are available by which to order the results. If computations fail for a particular tuple—for example, because the  $(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}$  matrix changes rank or the  $\mathbf{G}$  matrix is not positive definite—no results are produced. Results are retained when the maximum number of iterative updates is exceeded in iterative influence analyses.

The `SIZE=` suboption cannot be combined with the `EFFECT=` suboption. As in the case of the `EFFECT=` suboption, the statistics being computed are those appropriate for removal of multiple data points, even if `SIZE=1`.

The ODS name of the “Influence Diagnostics” table is `Influence`. The variables in this table depend on whether you specify the `EFFECT=`, `SIZE=`, or `KEEP=` suboption and whether covariance parameters are iteratively updated. When `ITER=0` (the default), certain influence diagnostics are meaningful only if the residual variance is profiled. [Table 59.11](#) and [Table 59.12](#) summarize the statistics obtained depending on the model and modifiers. The last column in these tables gives the variable name in the ODS `OUTPUT INFLUENCE=` data set. Restricted likelihood distances are reported instead of the likelihood distance unless `METHOD=ML`. See the section “[Influence Diagnostics](#)” on page 4977 for details about the individual statistics.

**Table 59.11** Statistics Computed with `INFLUENCE` Option, Noniterative Analysis (`ITER=0`)

| Suboption                                                               | $\sigma^2$<br>Profiled | Statistic                                    | Variable<br>Name    |
|-------------------------------------------------------------------------|------------------------|----------------------------------------------|---------------------|
| Default                                                                 | Yes                    | Observed value                               | Observed            |
|                                                                         |                        | Predicted value                              | Predicted           |
|                                                                         |                        | Marginal residual                            | Residual            |
|                                                                         |                        | Leverage                                     | Leverage            |
|                                                                         |                        | PRESS residual                               | PRESSRes            |
|                                                                         |                        | Internally studentized marginal residual     | Student             |
|                                                                         |                        | Externally studentized marginal residual     | RStudent            |
|                                                                         |                        | RMSE without deleted observations            | RMSE                |
|                                                                         |                        | Cook's <i>D</i>                              | CookD               |
|                                                                         |                        | DFFITS                                       | DFFITS              |
|                                                                         |                        | CovRatio<br>(Restricted) likelihood distance | COVRATIO<br>RLD, LD |
| Default                                                                 | No                     | Observed value                               | Observed            |
|                                                                         |                        | Predicted value                              | Predicted           |
|                                                                         |                        | Marginal residual                            | Residual            |
|                                                                         |                        | Leverage                                     | Leverage            |
|                                                                         |                        | PRESS residual                               | PRESSRes            |
|                                                                         |                        | Internally studentized marginal residual     | Student             |
|                                                                         |                        | Cook's <i>D</i>                              | CookD               |
| <code>EFFECT=</code> ,<br><code>SIZE=</code> ,<br>or <code>KEEP=</code> | Yes                    | Observations in level (tuple)                | Nobs                |
|                                                                         |                        | PRESS statistic                              | PRESS               |
|                                                                         |                        | Cook's <i>D</i>                              | CookD               |

Table 59.11 continued

| Suboption                      | $\sigma^2$<br>Profiled | Statistic                                                              | Variable<br>Name |
|--------------------------------|------------------------|------------------------------------------------------------------------|------------------|
|                                |                        | MDFFITs                                                                | MDFFITs          |
|                                |                        | CovRatio                                                               | COVRATIO         |
|                                |                        | COVTRACE                                                               | COVTRACE         |
|                                |                        | RMSE without deleted level (tuple)<br>(Restricted) likelihood distance | RMSE<br>RLD, LD  |
| EFFECT=,<br>SIZE=,<br>or KEEP= | No                     | Observations in level (tuple)                                          | Nobs             |
|                                |                        | PRESS statistic                                                        | PRESS            |
|                                |                        | Cook's <i>D</i>                                                        | CookD            |

Table 59.12 Statistics Computed with INFLUENCE Option, Iterative Analysis (ITER= $n > 0$ )

| Suboption                      | Statistic                                | Variable<br>Name |
|--------------------------------|------------------------------------------|------------------|
| Default                        | Number of iterations                     | Iter             |
|                                | Observed value                           | Observed         |
|                                | Predicted value                          | Predicted        |
|                                | Marginal residual                        | Residual         |
|                                | Leverage                                 | Leverage         |
|                                | PRESS residual                           | PRESSres         |
|                                | Internally studentized marginal residual | Student          |
|                                | Externally studentized marginal residual | RStudent         |
|                                | RMSE without deleted obs (if possible)   | RMSE             |
|                                | Cook's <i>D</i>                          | CookD            |
|                                | DFFITs                                   | DFFITs           |
|                                | CovRatio                                 | COVRATIO         |
|                                | Cook's <i>D</i> CovParms                 | CookDCP          |
|                                | CovRatio CovParms                        | COVRATIOCP       |
|                                | MDFFITs CovParms                         | MDFFITSCP        |
|                                | (Restricted) likelihood distance         | RLD, LD          |
| EFFECT=,<br>SIZE=,<br>or KEEP= | Observations in level (tuple)            | Nobs             |
|                                | Number of iterations                     | Iter             |
|                                | PRESS statistic                          | PRESS            |
|                                | RMSE without deleted level (tuple)       | RMSE             |
|                                | Cook's <i>D</i>                          | CookD            |
|                                | MDFFITs                                  | MDFFITs          |
|                                | CovRatio                                 | COVRATIO         |
|                                | COVTRACE                                 | COVTRACE         |
|                                | Cook's <i>D</i> CovParms                 | CookDCP          |
|                                | CovRatio CovParms                        | COVRATIOCP       |
|                                | MDFFITs CovParms                         | MDFFITSCP        |
|                                | (Restricted) likelihood distance         | RLD, LD          |

**INTERCEPT**

adds a row to the tables for Type 1, 2, and 3 tests corresponding to the overall intercept.

**LCOMPONENTS**

requests an estimate for each row of the **L** matrix used to form tests of fixed effects. Components corresponding to Type 3 tests are the default; you can produce the Type 1 and Type 2 component estimates with the **HTYPE=** option.

Tests of fixed effects involve testing of linear hypotheses of the form  $\mathbf{L}\boldsymbol{\beta} = \mathbf{0}$ . The matrix **L** is constructed from Type 1, 2, or 3 estimable functions. By default the MIXED procedure constructs Type 3 tests. In many situations, the individual rows of the matrix **L** represent contrasts of interest. For example, in a one-way classification model, the Type 3 estimable functions define differences of factor-level means. In a balanced two-way layout, the rows of **L** correspond to differences of cell means.

For example, suppose factors **A** and **B** have *a* and *b* levels, respectively. The following statements produce (*a* – 1) one degree of freedom tests for the rows of **L** associated with the Type 1 and Type 3 estimable functions for factor **A**, (*b* – 1) tests for the rows of **L** associated with factor **B**, and a single test for the Type 1 and Type 3 coefficients associated with regressor **X**:

```
class A B;
model y = A B x / htype=1,3 lcomponents;
```

The denominator degrees of freedom associated with a row of **L** are the same as those in the corresponding “Tests of Fixed Effects” table, except for **DDFM=KENWARDROGER** and **DDFM=SATTERTHWAITE**. For these degree of freedom methods, the denominator degrees of freedom are computed separately for each row of **L**.

The ODS name of the table containing all requested component tests is **LComponents**. See [Example 59.9](#) for applications of the **LCOMPONENTS** option.

**NOCONTAIN**

has the same effect as the **DDFM=RESIDUAL** option.

**NOINT**

requests that no intercept be included in the model. An intercept is included by default.

**NOTEST**

specifies that no hypothesis tests be performed for the fixed effects.

**OUTP=SAS-data-set****OUTPRED=SAS-data-set**

specifies an output data set containing predicted values and related quantities. This option replaces the **P** option from SAS 6.

Predicted values are formed by using the rows from  $(\mathbf{X} \ \mathbf{Z})$  as **L** matrices. Thus, predicted values from the original data are  $\mathbf{X}\hat{\boldsymbol{\beta}} + \mathbf{Z}\hat{\boldsymbol{\gamma}}$ . Their approximate standard errors of prediction are formed from the quadratic form of **L** with  $\hat{\mathbf{C}}$  defined in the section “Statistical Properties” on page 4967. The **L95** and **U95** variables provide a *t*-type confidence interval for the predicted values, and they correspond to the **L95M** and **U95M** variables from the GLM and REG procedures for fixed-effects models. The residuals are the observed minus the predicted values. Predicted values for data points other than those observed can be obtained by using missing dependent variables in your input data set.

Specifications that have a **REPEATED** statement with the **SUBJECT=** option and missing dependent variables compute predicted values by using empirical best linear unbiased prediction (EBLUP). Using hats ( $\hat{\cdot}$ ) to denote estimates, the EBLUP formula is

$$\hat{\mathbf{m}} = \mathbf{X}_m \hat{\boldsymbol{\beta}} + \hat{\mathbf{C}}_m \hat{\mathbf{V}}^{-1} (\mathbf{y} - \mathbf{X} \hat{\boldsymbol{\beta}})$$

where  $\mathbf{m}$  represents a hypothetical realization of a missing data vector with associated design matrix  $\mathbf{X}_m$ . The matrix  $\mathbf{C}_m$  is the model-based covariance matrix between  $\mathbf{m}$  and the observed data  $\mathbf{y}$ , and other notation is as presented in the section “**Mixed Models Theory**” on page 4958.

The estimated prediction variance is as follows:

$$\widehat{\text{Var}}(\hat{\mathbf{m}} - \mathbf{m}) = \hat{\mathbf{V}}_m - \hat{\mathbf{C}}_m \hat{\mathbf{V}}^{-1} \hat{\mathbf{C}}_m' + [\mathbf{X}_m - \hat{\mathbf{C}}_m \hat{\mathbf{V}}^{-1} \mathbf{X}] (\mathbf{X}' \hat{\mathbf{V}}^{-1} \mathbf{X})^{-1} [\mathbf{X}_m - \hat{\mathbf{C}}_m \hat{\mathbf{V}}^{-1} \mathbf{X}]'$$

where  $\mathbf{V}_m$  is the model-based variance matrix of  $\mathbf{m}$ . For further details, see Henderson (1984) and Harville (1990). This feature can be useful for forecasting time series or for computing spatial predictions.

By default, all variables from the input data set are included in the **OUTP=** data set. You can select a subset of these variables by using the **ID** statement.

#### **OUTPM=SAS-data-set**

#### **OUTPREDM=SAS-data-set**

specifies an output data set containing predicted means and related quantities. This option replaces the **PM** option from SAS 6.

The output data set is of the same form as that resulting from the **OUTP=** option, except that the predicted values do not incorporate the EBLUP values  $\mathbf{Z}\hat{\boldsymbol{\gamma}}$ . They also do not use the EBLUPs for specifications that have a **REPEATED** statement with the **SUBJECT=** option and missing dependent variables. The predicted values are formed as  $\mathbf{X}\hat{\boldsymbol{\beta}}$  in the **OUTPM=** data set, and standard errors are quadratic forms in the approximate variance-covariance matrix of  $\hat{\boldsymbol{\beta}}$  as displayed by the **COVB** option.

By default, all variables from the input data set are included in the **OUTPM=** data set. You can select a subset of these variables by using the **ID** statement.

### **RESIDUAL**

#### **RESIDUALS**

requests that Pearson-type and (internally) studentized residuals be added to the **OUTP=** and **OUTPM=** data sets. Studentized residuals are raw residuals standardized by their estimated standard error. When residuals are internally studentized, the data point in question has contributed to the estimation of the covariance parameter estimates on which the standard error of the residual is based. Externally studentized marginal residuals can be computed with the **INFLUENCE** option. Pearson-type residuals scale the residual by the standard deviation of the response.

The option has no effect unless the **OUTP=** or **OUTPM=** option is specified or unless **ODS Graphics** is enabled. For general information about **ODS Graphics**, see Chapter 21, “**Statistical Graphics Using ODS.**” For specific information about the graphics available in the **MIXED** procedure, see the section “**ODS Graphics**” on page 4992. For computational details about studentized and Pearson residuals in **MIXED**, see the section “**Residual Diagnostics**” on page 4976.

**SINGCHOL=number**

tunes the sensitivity in computing Cholesky roots. If a diagonal pivot element is less than  $D \times \text{number}$  as PROC MIXED performs the Cholesky decomposition on a matrix, the associated column is declared to be linearly dependent upon previous columns and is set to 0. The value  $D$  is the original diagonal element of the matrix. The default for *number* is 1E4 times the machine epsilon; this product is approximately 1E–12 on most computers.

**SINGRES=number**

sets the tolerance for which the residual variance is considered to be zero. The default is 1E4 times the machine epsilon; this product is approximately 1E–12 on most computers.

**SINGULAR=number**

tunes the sensitivity in sweeping. If a diagonal pivot element is less than  $D \times \text{number}$  as PROC MIXED sweeps a matrix, the associated column is declared to be linearly dependent upon previous columns, and the associated parameter is set to 0. The value  $D$  is the original diagonal element of the matrix. The default is 1E4 times the machine epsilon; this product is approximately 1E–12 on most computers.

**SOLUTION****S**

requests that a solution for the fixed-effects parameters be produced. Using notation from the section “Mixed Models Theory” on page 4958, the fixed-effects parameter estimates are  $\hat{\beta}$  and their approximate standard errors are the square roots of the diagonal elements of  $(\mathbf{X}'\hat{\mathbf{V}}^{-1}\mathbf{X})^{-1}$ . You can output this approximate variance matrix with the **COVB** option or modify it with the **EMPIRICAL** option in the PROC MIXED statement or the **DDFM=KENWARDROGER** option in the **MODEL** statement.

Along with the estimates and their approximate standard errors, a  $t$  statistic is computed as the estimate divided by its standard error. The degrees of freedom for this  $t$  statistic matches the one appearing in the “Tests of Fixed Effects” table under the effect containing the parameter. The “Pr > |t|” column contains the two-tailed  $p$ -value corresponding to the  $t$  statistic and associated degrees of freedom. You can use the **CL** option to request confidence intervals for all of the parameters; they are constructed around the estimate by using a radius of the standard error times a percentage point from the  $t$  distribution.

**VCIRY**

requests that responses and marginal residuals be scaled by the inverse Cholesky root of the marginal variance-covariance matrix. The variables **ScaledDep** and **ScaledResid** are added to the **OUTPM=** data set. These quantities can be important in bootstrapping of data or residuals. Examination of the scaled residuals is also helpful in diagnosing departures from normality. Notice that the results of this scaling operation can depend on the order in which the MIXED procedure processes the data.

The **VCIRY** option has no effect unless you also use the **OUTPM=** option or unless ODS Graphics is enabled. For general information about ODS Graphics, see Chapter 21, “Statistical Graphics Using ODS.” For specific information about the graphics available in the MIXED procedure, see the section “ODS Graphics” on page 4992.

**XPVIX**

is an alias for the **COVBI** option.

**XPVIXI**

is an alias for the **COVB** option.

**ZETA=number**

tunes the sensitivity in forming Type 3 functions. Any element in the estimable function basis with an absolute value less than *number* is set to 0. The default is 1E–8.

## PARMS Statement

**PARMS** (*value-list*)...</ options > ;

The **PARMS** statement specifies initial values for the covariance parameters, or it requests a grid search over several values of these parameters. You must specify the values in the order in which they appear in the “Covariance Parameter Estimates” table.

The *value-list* specification can take any of several forms:

|                                  |                                                                                                                          |
|----------------------------------|--------------------------------------------------------------------------------------------------------------------------|
| <i>m</i>                         | a single value                                                                                                           |
| $m_1, m_2, \dots, m_n$           | several values                                                                                                           |
| <i>m</i> to <i>n</i>             | a sequence where <i>m</i> equals the starting value, <i>n</i> equals the ending value, and the increment equals 1        |
| <i>m</i> to <i>n</i> by <i>i</i> | a sequence where <i>m</i> equals the starting value, <i>n</i> equals the ending value, and the increment equals <i>i</i> |
| $m_1, m_2$ to $m_3$              | mixed values and sequences                                                                                               |

You can use the **PARMS** statement to input known parameters. Referring to the split-plot example ([Example 59.1](#)), suppose the three variance components are known to be 60, 20, and 6. The SAS statements to fix the variance components at these values are as follows:

```
proc mixed data=sp noprofile;
 class Block A B;
 model Y = A B A*B;
 random Block A*Block;
 parms (60) (20) (6) / noiter;
run;
```

The **NOPROFILE** option requests PROC MIXED to refrain from profiling the residual variance parameter during its calculations, thereby enabling its value to be held at 6 as specified in the **PARMS** statement. The **NOITER** option prevents any Newton-Raphson iterations so that the subsequent results are based on the given variance components. You can also specify known parameters of **G** by using the **GDATA=** option in the **RANDOM** statement.

If you specify more than one set of initial values, PROC MIXED performs a grid search of the likelihood surface and uses the best point on the grid for subsequent analysis. Specifying a large number of grid points can result in long computing times. The grid search feature is also useful for exploring the likelihood surface. (See [Example 59.3](#).)

The results from the **PARMS** statement are the values of the parameters on the specified grid (denoted by CovP1–CovP*n*), the residual variance (possibly estimated) for models with a residual variance parameter, and various functions of the likelihood.



The ODS name of the “Parameter Search” table is ParmSearch.

Table 59.13 summarizes the options available in the PARMS statement.

**Table 59.13** PARMS Statement Options

| Option            | Description                                                              |
|-------------------|--------------------------------------------------------------------------|
| <b>HOLD=</b>      | Holds parameter values equal to the specified values                     |
| <b>LOGDETH</b>    | Evaluates the log determinant of the Hessian matrix                      |
| <b>LOWERB=</b>    | Specifies lower boundary constraints                                     |
| <b>NOBOUND</b>    | Removes boundary constraints on covariance parameters                    |
| <b>NOITER</b>     | Performs inferences using the best value from the grid search            |
| <b>NOPRINT</b>    | Suppresses the “Parameter Search” table                                  |
| <b>NOPROFILE</b>  | Specifies a different computational method for the residual variance     |
| <b>OLS</b>        | Requests starting values corresponding to the usual general linear model |
| <b>PARMSDATA=</b> | Reads in covariance parameter values from a SAS data set                 |
| <b>RATIOS</b>     | Indicates that ratios with the residual variance are specified           |
| <b>UPPERB=</b>    | Specifies upper boundary constraints                                     |

You can specify the following *options* in the PARMS statement after a slash (/).

**HOLD=***value-list*

**EQCONS=***value-list*

specifies which parameter values PROC MIXED should hold to equal the specified values. For example, the following statement constrains the first and third covariance parameters to equal 5 and 2, respectively:

```
parms (5) (3) (2) (3) / hold=1,3;
```

**LOGDETH**

evaluates the log determinant of the Hessian matrix for each point specified in the PARMS statement. A Log Det H column is added to the “Parameter Search” table.

**LOWERB=***value-list*

enables you to specify lower boundary constraints on the covariance parameters. The *value-list* specification is a list of numbers or missing values (.) separated by commas. You must list the numbers in the order that PROC MIXED uses for the covariance parameters, and each number corresponds to the lower boundary constraint. A missing value instructs PROC MIXED to use its default constraint, and if you do not specify numbers for all of the covariance parameters, PROC MIXED assumes the remaining ones are missing.

An example for which this option is useful is when you want to constrain the **G** matrix to be positive definite in order to avoid the more computationally intensive algorithms required when **G** becomes singular. The corresponding statements for a random coefficients model are as follows:

```
proc mixed;
 class person;
 model y = time;
```



```

 random int time / type=fa0(2) sub=person;
 parms / lowerb=1e-4, ., 1e-4;
run;

```

Here the `TYPE=FA0(2)` structure is used in order to specify a Cholesky root parameterization for the  $2 \times 2$  unstructured blocks in **G**. This parameterization ensures that the **G** matrix is nonnegative definite, and the `PARMS` statement then ensures that it is positive definite by constraining the two diagonal terms to be greater than or equal to  $1E-4$ .

#### **NOBOUND**

requests the removal of boundary constraints on covariance parameters. For example, variance components have a default lower boundary constraint of 0, and the `NOBOUND` option allows their estimates to be negative.

#### **NOITER**

requests that no Newton-Raphson iterations be performed and that PROC MIXED use the best value from the grid search to perform inferences. By default, iterations begin at the best value from the `PARMS` grid search.

#### **NOPRINT**

suppresses the display of the “Parameter Search” table.

#### **NOPROFILE**

specifies a different computational method for the residual variance during the grid search. By default, PROC MIXED estimates this parameter by using the profile likelihood when appropriate. This estimate is displayed in the Variance column of the “Parameter Search” table. The `NOPROFILE` option suppresses the profiling and uses the actual value of the specified variance in the likelihood calculations.

#### **OLS**

requests starting values corresponding to the usual general linear model. Specifically, all variances and covariances are set to zero except for the residual variance, which is set equal to its ordinary least squares (OLS) estimate. This option is useful when the default `MIVQUE0` procedure produces poor starting values for the optimization process.

#### **PARMSDATA=SAS-data-set**

#### **PDATA=SAS-data-set**

reads in covariance parameter values from a SAS data set. The data set should contain the `Est` or `Covp1–Covpn` variables.

#### **RATIOS**

indicates that ratios with the residual variance are specified instead of the covariance parameters themselves. The default is to use the individual covariance parameters.

#### **UPPERB=value-list**

enables you to specify upper boundary constraints on the covariance parameters. The *value-list* specification is a list of numbers or missing values (.) separated by commas. You must list the numbers in the order that PROC MIXED uses for the covariance parameters, and each number corresponds to the upper boundary constraint. A missing value instructs PROC MIXED to use its default constraint, and if you do not specify numbers for all of the covariance parameters, PROC MIXED assumes that the remaining ones are missing.

---

## PERFORMANCE Statement

**PERFORMANCE** < *performance-options* > ;

The PERFORMANCE statement defines performance parameters for multithreaded computing in solving large mixed model equations and other large matrix sweep operations.

You can specify the following *performance-options* in the PERFORMANCE statement:

**CPUCOUNT=ACTUAL** | *num*

specifies how many processors the procedure assumes to be available on the machine. You can specify any integer from 1 to 256 for *num*. CPUCOUNT=ACTUAL is equivalent to setting *num* to be the number of physical processors available. This number can be less than the physical number of CPUs if the SAS process has been restricted by system administration tools. Setting CPUCOUNT= to a number greater than the actual number of available CPUs might result in reduced performance. This option overrides the CPUCOUNT= SAS system option.

**NTHREADS**=*n*

specifies the number of threads for analytic computations and overrides the SAS system option THREADS | NOTHEADS. If you do not specify the NTHREADS= option, the number of threads are determined based on the number of CPUs on the machine by creating one thread per CPU for the analytic computations. The largest number that can be specified for *n* is 256.

By default, PROC MIXED executes in multiple concurrent threads unless you specify the NOTHEADS system option or you force single-threaded execution with NTHREADS=1 or the NOTHEADS options in the PERFORMANCE statement.

**THREADS=YES** | **NO**

specifies whether PROC MIXED executes in multiple concurrent threads. The default is YES.

**NOTHEAD**

turns off the multithreaded computation.

---

## PRIOR Statement

**PRIOR** < *distribution* > < / *options* > ;

The PRIOR statement enables you to carry out a sampling-based Bayesian analysis in PROC MIXED. It currently operates only with variance component models. Other TYPE= structures are not supported. The analysis produces a SAS data set containing a pseudo-random sample from the joint posterior density of the variance components and other parameters in the mixed model.

The posterior analysis is performed after all other PROC MIXED computations. It begins with the “Posterior Sampling Information” table, which provides basic information about the posterior sampling analysis, including the prior densities, sampling algorithm, sample size, and random number seed. The ODS name of this table is Posterior.

By default, PROC MIXED uses an independence chain algorithm in order to generate the posterior sample (Tierney 1994). This algorithm works by generating a pseudo-random proposal from a convenient base distribution, chosen to be as close as possible to the posterior. The proposal is then retained in the sample

with probability proportional to the ratio of weights constructed by taking the ratio of the true posterior to the base density. If a proposal is not accepted, then a duplicate of the previous observation is added to the chain.

In selecting the base distribution, PROC MIXED makes use of the fact that the fixed-effects parameters can be analytically integrated out of the joint posterior, leaving the marginal posterior density of the variance components. In order to better approximate the marginal posterior density of the variance components, PROC MIXED transforms them by using the MIVQUE(0) equations. You can display the selected transformation with the PTRANS option or specify your own with the TDATA= option. The density of the transformed parameters is then approximated by a product of inverted gamma densities (see Gelfand et al. 1990).

To determine the parameters for the inverted gamma densities, PROC MIXED evaluates the logarithm of the posterior density over a grid of points in each of the transformed parameters, and you can display the results of this search with the PSEARCH option. PROC MIXED then performs a linear regression of these values on the logarithm of the inverted gamma density. The resulting base densities are displayed in the “Base Densities” table; for ODS purposes, the name of this table is “Base.” You can input different base densities with the BDATA= option.

At the end of the sampling, the “Acceptance Rates” table displays the acceptance rate computed as the number of accepted samples divided by the total number of samples generated. The ODS name of the “Acceptance Rates” table is AccRates.

The OUT= option specifies the output data set containing the posterior sample. PROC MIXED automatically includes all variance component parameters in this data set (labeled COVP1–COVP $n$ ), the Type 3  $F$  statistics constructed as in Ghosh (1992) discussing Schervish (1992) (labeled T3F $n$ ), the log values of the posterior (labeled LOGF), the log of the base sampling density (labeled LOGG), and the log of their ratio (labeled LOGRATIO). If you specify the SOLUTION option in the MODEL statement, the data set also contains a random sample from the posterior density of the fixed-effects parameters (labeled BETAn); and if you specify the SOLUTION option in the RANDOM statement, the table contains a random sample from the posterior density of the random-effects parameters (labeled GAM $n$ ). PROC MIXED also generates additional variables corresponding to any CONTRAST, ESTIMATE, or LSMEANS statement that you specify.

Subsequently, you can use SAS/INSIGHT or the UNIVARIATE, CAPABILITY, or KDE procedure to analyze the posterior sample.

The prior density of the variance components is, by default, a noninformative version of Jeffreys’ prior (Box and Tiao 1973). You can also specify informative priors with the DATA= option or a flat (equal to 1) prior for the variance components. The prior density of the fixed-effects parameters is assumed to be flat (equal to 1), and the resulting posterior is conditionally multivariate normal (conditioning on the variance component parameters) with mean  $(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}^{-1}\mathbf{y}$  and variance  $(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}$ .

Table 59.14 summarizes the options available in the PRIOR statement.

**Table 59.14** PRIOR Statement Options

| Option   | Description                                                     |
|----------|-----------------------------------------------------------------|
| DATA=    | Inputs the prior densities of the variance components           |
| JEFFREYS | Specifies a noninformative reference version of Jeffreys’ prior |
| FLAT     | Specifies a prior density equal to 1 everywhere                 |

Table 59.14 *continued*

| Option     | Description                                                                             |
|------------|-----------------------------------------------------------------------------------------|
| ALG=       | Specifies the algorithm used for generating the posterior sample                        |
| BDATA=     | Inputs the base densities used by the sampling algorithm                                |
| GRID=      | Specifies a grid of values over which to evaluate the posterior density                 |
| GRIDT=     | Specifies a transformed grid of values over which to evaluate the posterior density     |
| IFACTOR=   | An alias for the SFACTOR= option                                                        |
| LOGNOTE=   | Writes a note to the log after generating the sample                                    |
| LOGRBOUND= | Specifies the bounding constant for rejection sampling                                  |
| NSAMPLE=   | Specifies the number of posterior samples to generate                                   |
| NSEARCH=   | Specifies the number of posterior evaluations                                           |
| OUT=       | Creates an output data set containing the sample from the posterior density             |
| OUTG=      | Creates an output data set from the grid evaluations                                    |
| OUTGT=     | Creates an output data set from the transformed grid evaluations                        |
| PSEARCH    | Displays the search used to determine the parameters for the inverted gamma densities   |
| PTRANS     | Displays the transformation of the variance components                                  |
| SEED=      | Specifies an integer used to start the pseudo-random number generator                   |
| SFACTOR=   | Adjusts the search range of the transformed parameters                                  |
| TDATA=     | Inputs the transformation used by the sampling algorithm                                |
| TRANS=     | Specifies the algorithm that determines the transformation of the covariance parameters |
| UPDATE=    | An alias for the LOGNOTE= option                                                        |

The *distribution* argument in the PRIOR statement determines the prior density for the variance component parameters of your mixed model. Valid values are as follows.

#### DATA=

enables you to input the prior densities of the variance components used by the sampling algorithm. This data set must contain the Type and Parm1–Parm*n* variables, where *n* is the largest number of parameters among each of the base densities. The format of the DATA= data set matches that created by PROC MIXED in the “Base Densities” table, so you can output the densities from one run and use them as input for a subsequent run.

#### JEFFREYS

specifies a noninformative reference version of Jeffreys’ prior constructed by using the square root of the determinant of the expected information matrix as in (1.3.92) of Box and Tiao (1973). This is the default prior.

#### FLAT

specifies a prior density equal to 1 everywhere, making the likelihood function the posterior.

You can specify the following *options* in the PRIOR statement after a slash (/).

**ALG=IC | INDCHAIN****ALG=IS | IMPSAMP****ALG=RS | REJSAMP****ALG=RWC | RWCHAIN**

specifies the algorithm used for generating the posterior sample. The ALG=IC option requests an independence chain algorithm, and it is the default. The option ALG=IS requests importance sampling, ALG=RS requests rejection sampling, and ALG=RWC requests a random walk chain. For more information about these techniques, see Ripley (1987); Smith and Gelfand (1992); Tierney (1994).

**BDATA=**

enables you to input the base densities used by the sampling algorithm. This data set must contain the Type and Parm1–Parm $n$  variables, where  $n$  is the largest number of parameters among each of the base densities. The format of the BDATA= data set matches that created by PROC MIXED in the “Base Densities” table, so you can output the densities from one run and use them as input for a subsequent run.

**GRID=(value-list)**

specifies a grid of values over which to evaluate the posterior density. The *value-list* syntax is the same as in the PARMs statement, and you must specify an output data set name with the OUTG= option.

**GRIDT=(value-list)**

specifies a transformed grid of values over which to evaluate the posterior density. The *value-list* syntax is the same as in the PARMs statement, and you must specify an output data set name with the OUTGT= option.

**IFACTOR=number**

is an alias for the SFACTOR= option.

**LOGNOTE=number**

instructs PROC MIXED to write a note to the SAS log after it generates the sample corresponding to each multiple of *number*. This is useful for monitoring the progress of CPU-intensive runs.

**LOGRBOUND=number**

specifies the bounding constant for rejection sampling. The value of *number* equals the maximum of  $\log\{f/g\}$  over the variance component parameter space, where  $f$  is the posterior density and  $g$  is the product inverted gamma densities used to perform rejection sampling.

When performing the rejection sampling, you might encounter the following message:

```
WARNING: The log ratio bound of LL was violated at sample XX.
```

When this occurs, PROC MIXED reruns an optimization algorithm to determine a new log upper bound and then restarts the rejection sampling. The resulting OUT= data set contains all observations that have been generated; therefore, assuming that you have requested  $N$  samples, you should retain only the final  $N$  observations in this data set for analysis purposes.

**NSAMPLE=***number*

specifies the number of posterior samples to generate. The default is 1000, but more accurate results are obtained with larger samples such as 10000.

**NSEARCH=***number*

specifies the number of posterior evaluations PROC MIXED makes for each transformed parameter in determining the parameters for the inverted gamma densities. The default is 20.

**OUT=***SAS-data-set*

creates an output data set containing the sample from the posterior density.

**OUTG=***SAS-data-set*

creates an output data set from the grid evaluations specified in the **GRID=** option.

**OUTGT=***SAS-data-set*

creates an output data set from the transformed grid evaluations specified in the **GRIDT=** option.

**PSEARCH**

displays the search used to determine the parameters for the inverted gamma densities. The ODS name of the table is Search.

**PTRANS**

displays the transformation of the variance components. For ODS purposes, the name of the table is “Trans.”

**SEED=***number*

specifies an integer used to start the pseudo-random number generator for the simulation. If you do not specify a seed, or if you specify a value less than or equal to zero, the seed is by default generated from reading the time of day from the computer clock. You should use a positive seed (less than  $2^{31} - 1$ ) whenever you want to duplicate the sample in another run of PROC MIXED.

**SFACTOR=***number*

enables you to adjust the range over which PROC MIXED searches the transformed parameters in order to determine the parameters for the inverted gamma densities. PROC MIXED determines the range by first transforming the estimates from the standard PROC MIXED analysis (REML, ML, or MIVQUE0, depending upon which estimation method you select). It then multiplies and divides the transformed estimates by  $2 * \textit{number}$  to obtain upper and lower bounds, respectively. Transformed values that produce negative variance components in the original scale are not included in the search. The default value is 1; *number* must be greater than 0.5.

**TDATA=**

enables you to input the transformation of the covariance parameters used by the sampling algorithm. This data set should contain the CovP1–CovP*n* variables. The format of the TDATA= data set matches that created by PROC MIXED in the “Trans” table, so you can output the transformation from one run and use it as input for a subsequent run.

**TRANS=**EXPECTED | MIVQUE0 | OBSERVED

specifies the particular algorithm used to determine the transformation of the covariance parameters. The default is MIVQUE0, indicating a transformation based on the MIVQUE(0) equations. The other two options indicate the type of Hessian matrix used in constructing the transformation via a Cholesky root.

**UPDATE=number**

is an alias for the **LOGNOTE=** option.

---

## RANDOM Statement

**RANDOM** *random-effects* </ options > ;

The **RANDOM** statement defines the random effects constituting the  $\boldsymbol{\gamma}$  vector in the mixed model. It can be used to specify traditional variance component models (as in the **VARCOMP** procedure) and to specify random coefficients. The random effects can be classification or continuous, and multiple **RANDOM** statements are possible.

Using notation from the section “**Mixed Models Theory**” on page 4958, the purpose of the **RANDOM** statement is to define the **Z** matrix of the mixed model, the random effects in the  $\boldsymbol{\gamma}$  vector, and the structure of **G**. The **Z** matrix is constructed exactly as the **X** matrix for the fixed effects, and the **G** matrix is constructed to correspond with the effects constituting **Z**. The structure of **G** is defined by using the **TYPE=** option.

You can specify **INTERCEPT** (or **INT**) as a random effect to indicate the intercept. **PROC MIXED** does not include the intercept in the **RANDOM** statement by default as it does in the **MODEL** statement.

Table 59.15 summarizes the options available in the **RANDOM** statement. All options are subsequently discussed in alphabetical order.

**Table 59.15** Summary of **RANDOM** Statement Options

| Option                                      | Description                                                                            |
|---------------------------------------------|----------------------------------------------------------------------------------------|
| <b>Construction of Covariance Structure</b> |                                                                                        |
| <b>GDATA=</b>                               | Requests that the <b>G</b> matrix be read from a SAS data set                          |
| <b>GROUP=</b>                               | Varies covariance parameters by groups                                                 |
| <b>LDATA=</b>                               | Specifies data set with coefficient matrices for <b>TYPE=LIN</b>                       |
| <b>NOFULLZ</b>                              | Eliminates columns in <b>Z</b> corresponding to missing values                         |
| <b>RATIOS</b>                               | Indicates that ratios are specified in the <b>GDATA=</b> data set                      |
| <b>SUBJECT=</b>                             | Identifies the subjects in the model                                                   |
| <b>TYPE=</b>                                | Specifies the covariance structure                                                     |
| <b>Statistical Output</b>                   |                                                                                        |
| <b>ALPHA=<math>\alpha</math></b>            | Determines the confidence level ( $1 - \alpha$ )                                       |
| <b>CL</b>                                   | Requests confidence limits for predictors of random effects                            |
| <b>G</b>                                    | Displays the estimated <b>G</b> matrix                                                 |
| <b>GC</b>                                   | Displays the Cholesky root (lower) of estimated <b>G</b> matrix                        |
| <b>GCI</b>                                  | Displays the inverse Cholesky root (lower) of estimated <b>G</b> matrix                |
| <b>GCORR</b>                                | Displays the correlation matrix corresponding to estimated <b>G</b> matrix             |
| <b>GI</b>                                   | Displays the inverse of the estimated <b>G</b> matrix                                  |
| <b>SOLUTION</b>                             | Displays solutions $\hat{\boldsymbol{\gamma}}$ of the G-side random effects            |
| <b>V</b>                                    | Displays blocks of the estimated <b>V</b> matrix                                       |
| <b>VC</b>                                   | Displays the lower-triangular Cholesky root of blocks of the estimated <b>V</b> matrix |



Table 59.15 *continued*

| Option | Description                                                                              |
|--------|------------------------------------------------------------------------------------------|
| VCI    | Displays the inverse Cholesky root of blocks of the estimated <b>V</b> matrix            |
| VCORR  | Displays the correlation matrix corresponding to blocks of the estimated <b>V</b> matrix |
| VI     | Displays the inverse of the blocks of the estimated <b>V</b> matrix                      |

You can specify the following *options* in the RANDOM statement after a slash (/).

**ALPHA=number**

requests that a *t*-type confidence interval be constructed for each of the random-effect estimates with confidence level  $1 - \text{number}$ . The value of *number* must be between 0 and 1; the default is 0.05.

**CL**

requests that *t*-type confidence limits be constructed for each of the random-effect estimates. The confidence level is 0.95 by default; this can be changed with the **ALPHA=** option.

**G**

requests that the estimated **G** matrix be displayed. PROC MIXED displays blanks for values that are 0. If you specify the **SUBJECT=** option, then the block of the **G** matrix corresponding to the first subject is displayed. For ODS purposes, the name of the table is “G.”

**GC**

displays the lower-triangular Cholesky root of the estimated **G** matrix according to the rules listed under the **G** option. The ODS name of the table is CholG.

**GCI**

displays the inverse Cholesky root of the estimated **G** matrix according to the rules listed under the **G** option. The ODS name of the table is InvCholG.

**GCORR**

displays the correlation matrix corresponding to the estimated **G** matrix according to the rules listed under the **G** option. The ODS name of the table is GCorr.

**GDATA=SAS-data-set**

requests that the **G** matrix be read in from a SAS data set. This **G** matrix is assumed to be known; therefore, only **R**-side parameters from effects in the **REPEATED** statement are included in the Newton-Raphson iterations. If no **REPEATED** statement is specified, then only a residual variance is estimated.

The information in the **GDATA=** data set can appear in one of two ways. The first is a sparse representation for which you include **Row**, **Col**, and **Value** variables to indicate the row, column, and value of **G**, respectively. All unspecified locations are assumed to be 0. The second representation is for dense matrices. In it you include **Row** and **Col1–Coln** variables to indicate, respectively, the row and columns of **G**, which is a symmetric matrix of order *n*. For both representations, you must specify effects in the RANDOM statement that generate a **Z** matrix that contains *n* columns. (See Example 59.4.)



If you have more than one RANDOM statement, only one GDATA= option is required in any one of them, and the data set you specify must contain the entire **G** matrix defined by all of the RANDOM statements.

If the GDATA= data set contains variance ratios instead of the variances themselves, then use the **RATIOS** option.

Known parameters of **G** can also be input by using the PARMS statement with the **HOLD=** option.

## GI

displays the inverse of the estimated **G** matrix according to the rules listed under the **G** option. The ODS name of the table is InvG.

## GROUP=effect

### GRP=effect

defines an effect specifying heterogeneity in the covariance structure of **G**. All observations having the same level of the group effect have the same covariance parameters. Each new level of the group effect produces a new set of covariance parameters with the same structure as the original group. You should exercise caution in defining the group effect, because strange covariance patterns can result from its misuse. Also, the group effect can greatly increase the number of estimated covariance parameters, which can adversely affect the optimization process.

Continuous variables are permitted as arguments to the GROUP= option. PROC MIXED does not sort by the values of the continuous variable; rather, it considers the data to be from a new subject or group whenever the value of the continuous variable changes from the previous observation. Using a continuous variable decreases execution time for models with a large number of subjects or groups and also prevents the production of a large “Class Level Information” table.

## LDATA=SAS-data-set

reads the coefficient matrices associated with the **TYPE=LIN(number)** option. The data set must contain the variables Parm, Row, Col1–Col $n$  or Parm, Row, Col, Value. The Parm variable denotes which of the *number* coefficient matrices is currently being constructed, and the Row, Col1–Col $n$ , or Row, Col, Value variables specify the matrix values, as they do with the GDATA= option. Unspecified values of these matrices are set equal to 0.

## NOFULLZ

eliminates the columns in **Z** corresponding to missing levels of random effects involving **CLASS** variables. By default, these columns are included in **Z**.

## RATIOS

indicates that ratios with the residual variance are specified in the GDATA= data set instead of the covariance parameters themselves. The default GDATA= data set contains the individual covariance parameters.

## SOLUTION

### S

requests that the solution for the random-effects parameters be produced. Using notation from the section “Mixed Models Theory” on page 4958, these estimates are the empirical best linear unbiased predictors (EBLUPs)  $\hat{\boldsymbol{y}} = \hat{\mathbf{G}}\mathbf{Z}'\hat{\mathbf{V}}^{-1}(\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}})$ . They can be useful for comparing the random effects from different experimental units and can also be treated as residuals in performing diagnostics for your mixed model.

The numbers displayed in the SE Pred column of the “Solution for Random Effects” table are not the standard errors of the  $\hat{\boldsymbol{\gamma}}$  displayed in the Estimate column; rather, they are the standard errors of predictions  $\hat{\boldsymbol{\gamma}}_i - \boldsymbol{\gamma}_i$ , where  $\hat{\boldsymbol{\gamma}}_i$  is the  $i$ th EBLUP and  $\boldsymbol{\gamma}_i$  is the  $i$ th random-effect parameter.

**SUBJECT=effect**

**SUB=effect**

identifies the subjects in your mixed model. Complete independence is assumed across subjects; thus, for the RANDOM statement, the SUBJECT= option produces a block-diagonal structure in  $\mathbf{G}$  with identical blocks. The  $\mathbf{Z}$  matrix is modified to accommodate this block diagonality. In fact, specifying a subject effect is equivalent to nesting all other effects in the RANDOM statement within the subject effect.

Continuous variables are permitted as arguments to the SUBJECT= option. PROC MIXED does not sort by the values of the continuous variable; rather, it considers the data to be from a new subject or group whenever the value of the continuous variable changes from the previous observation. Using a continuous variable decreases execution time for models with a large number of subjects or groups and also prevents the production of a large “Class Level Information” table.

When you specify the SUBJECT= option and a classification random effect, computations are usually much quicker if the levels of the random effect are duplicated within each level of the SUBJECT= effect.

**TYPE=covariance-structure**

specifies the covariance structure of  $\mathbf{G}$ . Valid values for *covariance-structure* and their descriptions are listed in Table 59.17 and Table 59.18. Although a variety of structures are available, most applications call for either TYPE=VC or TYPE=UN. The TYPE=VC (variance components) option is the default structure, and it models a different variance component for each random effect.

The TYPE=UN (unstructured) option is useful for correlated random coefficient models. For example, the following statement specifies a random intercept-slope model that has different variances for the intercept and slope and a covariance between them:

```
random intercept age / type=un subject=person;
```

You can also use TYPE=FA0(2) here to request a  $\mathbf{G}$  estimate that is constrained to be nonnegative definite.

If you are constructing your own columns of  $\mathbf{Z}$  with continuous variables, you can use the TYPE=TOEP(1) structure to group them together to have a common variance component. If you want to have different covariance structures in different parts of  $\mathbf{G}$ , you must use multiple RANDOM statements with different TYPE= options.

**V<=value-list>**

requests that blocks of the estimated  $\mathbf{V}$  matrix be displayed. The first block determined by the SUBJECT= effect is the default displayed block. PROC MIXED displays entries that are 0 as blanks in the table.

You can optionally use the *value-list* specification, which indicates the subjects for which blocks of  $\mathbf{V}$  are to be displayed. For example, the following statement displays block matrices for the first, third, and seventh persons:

```
random int time / type=un subject=person v=1,3,7;
```

The ODS table name is V.

**VC**<=*value-list*>

displays the Cholesky root of the blocks of the estimated **V** matrix. The *value-list* specification is the same as in the **V** option. The ODS table name is CholV.

**VCI**<=*value-list*>

displays the inverse of the Cholesky root of the blocks of the estimated **V** matrix. The *value-list* specification is the same as in the **V** option. The table name for ODS purposes is “InvCholV.”

**VCORR**<=*value-list*>

displays the correlation matrix corresponding to the blocks of the estimated **V** matrix. The *value-list* specification is the same as in the **V** option. The table name for ODS purposes is “VCorr.”

**VI**<=*value-list*>

displays the inverse of the blocks of the estimated **V** matrix. The *value-list* specification is the same as in the **V** option. The ODS table name is InvV.

---

## REPEATED Statement

**REPEATED** < *repeated-effect* > < / *options* > ;

The REPEATED statement is used to specify the **R** matrix in the mixed model. Its syntax is different from that of the REPEATED statement in PROC GLM. If no REPEATED statement is specified, **R** is assumed to be equal to  $\sigma^2\mathbf{I}$ .

For many repeated measures models, no repeated effect is required in the REPEATED statement. Simply use the **SUBJECT=** option to define the blocks of **R** and the **TYPE=** option to define their covariance structure. In this case, the repeated measures data must be similarly ordered for each subject, and you must indicate all missing response variables with periods in the input data set unless they all fall at the end of a subject’s repeated response profile. These requirements are necessary in order to inform PROC MIXED of the proper location of the observed repeated responses.

Specifying a repeated effect is useful when you do not want to indicate missing values with periods in the input data set. The repeated effect must contain only classification variables. Make sure that the levels of the repeated effect are different for each observation within a subject; otherwise, PROC MIXED constructs identical rows in **R** corresponding to the observations with the same level. This results in a singular **R** and an infinite likelihood.

Whether you specify a REPEATED effect or not, the rows of **R** for each subject are constructed in the order in which they appear in the input data set.

Table 59.16 summarizes the options available in the REPEATED statement. All options are subsequently discussed in alphabetical order.

**Table 59.16** Summary of REPEATED Statement Options

| Option                                      | Description                                                                              |
|---------------------------------------------|------------------------------------------------------------------------------------------|
| <b>Construction of Covariance Structure</b> |                                                                                          |
| GROUP=                                      | Defines an effect specifying heterogeneity in the R-side covariance structure            |
| LDATA=                                      | Specifies data set with coefficient matrices for TYPE=LIN                                |
| LOCAL                                       | Requests that a diagonal matrix be added to <b>R</b>                                     |
| LOCALW                                      | Specifies that only the local effects are weighted                                       |
| NONLOCALW                                   | Specifies that only the nonlocal effects are weighted                                    |
| SUBJECT=                                    | Identifies the subjects in the R-side model                                              |
| TYPE=                                       | Specifies the R-side covariance structure                                                |
| <b>Statistical Output</b>                   |                                                                                          |
| HLM                                         | Produces a table of Hotelling-Lawley-McKeon statistics (McKeon 1974)                     |
| HLPS                                        | Produces a table of Hotelling-Lawley-Pillai-Samson statistics (Pillai and Samson 1959)   |
| R                                           | Displays blocks of the estimated <b>R</b> matrix                                         |
| RC                                          | Display the Cholesky root (lower) of blocks of the estimated <b>R</b> matrix             |
| RCI                                         | Displays the inverse Cholesky root (lower) of blocks of the estimated <b>R</b> matrix    |
| RCORR                                       | Displays the correlation matrix corresponding to blocks of the estimated <b>R</b> matrix |
| RI                                          | Displays the inverse of blocks of the estimated <b>R</b> matrix                          |

You can specify the following *options* in the REPEATED statement after a slash (/).

**GROUP=effect****GRP=effect**

defines an effect that specifies heterogeneity in the covariance structure of **R**. All observations that have the same level of the GROUP effect have the same covariance parameters. Each new level of the GROUP effect produces a new set of covariance parameters with the same structure as the original group. You should exercise caution in properly defining the GROUP effect, because strange covariance patterns can result with its misuse. Also, the GROUP effect can greatly increase the number of estimated covariance parameters, which can adversely affect the optimization process.

Continuous variables are permitted as arguments to the GROUP= option. PROC MIXED does not sort by the values of the continuous variable; rather, it considers the data to be from a new subject or group whenever the value of the continuous variable changes from the previous observation. Using a continuous variable decreases execution time for models with a large number of subjects or groups and also prevents the production of a large “Class Level Information” table.

**HLM**

produces a table of Hotelling-Lawley-McKeon statistics (McKeon 1974) for all fixed effects whose levels change across data having the same level of the SUBJECT= effect (the *within-subject* fixed effects). This option applies only when you specify a REPEATED statement with the TYPE=UN

option and no **RANDOM** statements. For balanced data, this model is equivalent to the multivariate model for repeated measures in PROC GLM.

The Hotelling-Lawley-McKeon statistic has a slightly better  $F$  approximation than the Hotelling-Lawley-Pillai-Samson statistic (see the description of the **HLPS** option, which follows). Both of the Hotelling-Lawley statistics can perform much better in small samples than the default  $F$  statistic (Wright 1994).

Separate tables are produced for Type 1, 2, and 3 tests, according to the ones you select. The ODS table names are HLM1, HLM2, and HLM3, respectively.

## HLPS

produces a table of Hotelling-Lawley-Pillai-Samson statistics (Pillai and Samson 1959) for all fixed effects whose levels change across data having the same level of the **SUBJECT=** effect (the *within-subject* fixed effects). This option applies only when you specify a **REPEATED** statement with the **TYPE=UN** option and no **RANDOM** statements. For balanced data, this model is equivalent to the multivariate model for repeated measures in PROC GLM, and this statistic is the same as the Hotelling-Lawley Trace statistic produced by PROC GLM.

Separate tables are produced for Type 1, 2, and 3 tests, according to the ones you select. The ODS table names are HLPS1, HLPS2, and HLPS3, respectively.

## **LDATA=SAS-data-set**

reads the coefficient matrices associated with the **TYPE=LIN(number)** option. The data set must contain the variables **Parm, Row, Col1–Col $n$**  or **Parm, Row, Col, Value**. The **Parm** variable denotes which of the *number* coefficient matrices is currently being constructed, and the **Row, Col1–Col $n$** , or **Row, Col, Value** variables specify the matrix values, as they do with the **RANDOM** statement option **GDATA=**. Unspecified values of these matrices are set equal to 0.

## LOCAL

### **LOCAL=POM(POM-data-set)**

requests that a diagonal matrix be added to **R**. With just the **LOCAL** option, this diagonal matrix equals  $\sigma^2\mathbf{I}$ , and  $\sigma^2$  becomes an additional variance parameter that PROC MIXED profiles out of the likelihood provided that you do not specify the **NOPROFILE** option in the **PROC MIXED** statement. The **LOCAL** option is useful if you want to add an observational error to a time series structure (Jones and Boadi-Boateng 1991) or a nugget effect to a spatial structure Cressie (1993).

The **LOCAL=EXP(<effects>)** option produces exponential local effects, also known as dispersion effects, in a log-linear variance model. These local effects have the form

$$\sigma^2 \text{diag}[\exp(\mathbf{U}\boldsymbol{\delta})]$$

where **U** is the full-rank design matrix corresponding to the effects that you specify and  $\boldsymbol{\delta}$  are the parameters that PROC MIXED estimates. An intercept is not included in **U** because it is accounted for by  $\sigma^2$ . PROC MIXED constructs the full-rank **U** in terms of 1s and –1s for classification effects. Be sure to scale continuous effects in **U** sensibly.

The **LOCAL=POM(POM-data-set)** option specifies the power-of-the-mean structure. This structure possesses a variance of the form  $\sigma^2|\mathbf{x}'_i\boldsymbol{\beta}^*|^\theta$  for the *i*th observation, where  $\mathbf{x}_i$  is the *i*th row of **X** (the design matrix of the fixed effects) and  $\boldsymbol{\beta}^*$  is an estimate of the fixed-effects parameters that you specify in **POM-data-set**.

The SAS data set specified by *POM-data-set* contains the numeric variable Estimate (in previous releases, the variable name was required to be EST), and it has at least as many observations as there are fixed-effects parameters. The first  $p$  observations of the Estimate variable in *POM-data-set* are taken to be the elements of  $\beta^*$ , where  $p$  is the number of columns of  $\mathbf{X}$ . You must order these observations according to the non-full-rank parameterization of the MIXED procedure. One easy way to set up *POM-data-set* for a  $\beta^*$  corresponding to ordinary least squares is illustrated by the following statements:

```
ods output SolutionF=sf;
proc mixed;
 class a;
 model y = a x / s;
run;

proc mixed;
 class a;
 model y = a x;
 repeated / local=pom(sf);
run;
```

Note that the generalized least squares estimate of the fixed-effects parameters from the second PROC MIXED step usually is not the same as your specified  $\beta^*$ . However, you can iterate the POM fitting until the two estimates agree. Continuing from the previous example, the statements for performing one step of this iteration are as follows:

```
ods output SolutionF=sf1;
proc mixed;
 class a;
 model y = a x / s;
 repeated / local=pom(sf);
run;

proc compare brief data=sf compare=sf1;
 var estimate;
run;

data sf;
 set sf1;
run;
```

Unfortunately, this iterative process does not always converge. For further details, see the description of pseudo-likelihood in Chapter 3 of Carroll and Ruppert (1988).

### LOCALW

specifies that only the local effects and no others be weighted. By default, all effects are weighted. The LOCALW option is used in connection with the WEIGHT statement and the LOCAL option in the REPEATED statement.

**NONLOCALW**

specifies that only the nonlocal effects and no others be weighted. By default, all effects are weighted. The NONLOCALW option is used in connection with the WEIGHT statement and the LOCAL option in the REPEATED statement.

**R<=value-list>**

requests that blocks of the estimated **R** matrix be displayed. The first block determined by the SUBJECT= effect is the default displayed block. PROC MIXED displays blanks for value-lists that are 0.

The *value-list* indicates the subjects for which blocks of **R** are to be displayed. For example, the following statement displays block matrices for the first, third, and fifth persons:

```
repeated / type=cs subject=person r=1,3,5;
```

See the PARMs statement for the possible forms of *value-list*. The ODS table name is R.

**RC<=value-list>**

produces the Cholesky root of blocks of the estimated **R** matrix. The *value-list* specification is the same as with the R option. The ODS table name is CholR.

**RCI<=value-list>**

produces the inverse Cholesky root of blocks of the estimated **R** matrix. The *value-list* specification is the same as with the R option. The ODS table name is InvCholR.

**RCORR<=value-list>**

produces the correlation matrix corresponding to blocks of the estimated **R** matrix. The *value-list* specification is the same as with the R option. The table name for ODS purposes is "RCorr."

**RI<=value-list>**

produces the inverse of blocks of the estimated **R** matrix. The *value-list* specification is the same as with the R option. The ODS table name is InvR.

**SSCP**

requests that an unstructured **R** matrix be estimated from the sum-of-squares-and-crossproducts matrix of the residuals. It applies only when you specify TYPE=UN and have no RANDOM statements. Also, you must have a sufficient number of subjects for the estimate to be positive definite.

This option is useful when the size of the blocks of **R** is large (for example, greater than 10) and you want to use or inspect an unstructured estimate that is much quicker to compute than the default REML estimate. The two estimates will agree for certain balanced data sets when you have a classification fixed effect defined across all time points within a subject.

**SUBJECT=effect****SUB=effect**

identifies the subjects in your mixed model. Complete independence is assumed across subjects; therefore, the SUBJECT= option produces a block-diagonal structure in **R** with identical blocks. When the SUBJECT= effect consists entirely of classification variables, the blocks of **R** correspond to observations sharing the same level of that effect. These blocks are sorted according to this effect as well.



Continuous variables are permitted as arguments to the SUBJECT= option. PROC MIXED does not sort by the values of the continuous variable; rather, it considers the data to be from a new subject or group whenever the value of the continuous variable changes from the previous observation. Using a continuous variable decreases execution time for models with a large number of subjects or groups and also prevents the production of a large “Class Level Information” table.

If you want to model nonzero covariance among all of the observations in your SAS data set, specify SUBJECT=INTERCEPT to treat the data as if they are all from one subject. However, be aware that in this case PROC MIXED manipulates an **R** matrix with dimensions equal to the number of observations. If no SUBJECT= effect is specified, then every observation is assumed to be from a different subject and **R** is assumed to be diagonal. For this reason, you usually want to use the SUBJECT= option in the REPEATED statement.

**TYPE=covariance-structure**

specifies the covariance structure of the **R** matrix. The SUBJECT= option defines the blocks of **R**, and the TYPE= option specifies the structure of these blocks. Valid values for *covariance-structure* and their descriptions are provided in Table 59.17 and Table 59.18. The default structure is VC.

**Table 59.17** Covariance Structures

| Structure | Description          | Parms                         | (i, j) element                                                             |
|-----------|----------------------|-------------------------------|----------------------------------------------------------------------------|
| ANTE(1)   | Antedependence       | $2t - 1$                      | $\sigma_i \sigma_j \prod_{k=i}^{j-1} \rho_k$                               |
| AR(1)     | Autoregressive(1)    | 2                             | $\sigma^2 \rho^{ i-j }$                                                    |
| ARH(1)    | Heterogeneous AR(1)  | $t + 1$                       | $\sigma_i \sigma_j \rho^{ i-j }$                                           |
| ARMA(1,1) | ARMA(1,1)            | 3                             | $\sigma^2 [\gamma \rho^{ i-j -1} 1(i \neq j) + 1(i = j)]$                  |
| CS        | Compound symmetry    | 2                             | $\sigma_1 + \sigma^2 1(i = j)$                                             |
| CSH       | Heterogeneous CS     | $t + 1$                       | $\sigma_i \sigma_j [\rho 1(i \neq j) + 1(i = j)]$                          |
| FA(q)     | Factor analytic      | $\frac{q}{2}(2t - q + 1) + t$ | $\sum_{k=1}^{\min(i,j,q)} \lambda_{ik} \lambda_{jk} + \sigma_i^2 1(i = j)$ |
| FA0(q)    | No diagonal FA       | $\frac{q}{2}(2t - q + 1)$     | $\sum_{k=1}^{\min(i,j,q)} \lambda_{ik} \lambda_{jk}$                       |
| FA1(q)    | Equal diagonal FA    | $\frac{q}{2}(2t - q + 1) + 1$ | $\sum_{k=1}^{\min(i,j,q)} \lambda_{ik} \lambda_{jk} + \sigma^2 1(i = j)$   |
| HF        | Huynh-Feldt          | $t + 1$                       | $(\sigma_i^2 + \sigma_j^2)/2 + \lambda 1(i \neq j)$                        |
| LIN(q)    | General linear       | q                             | $\sum_{k=1}^q \theta_k \mathbf{A}_{ij}$                                    |
| TOEP      | Toeplitz             | t                             | $\sigma_{ i-j +1}$                                                         |
| TOEP(q)   | Banded Toeplitz      | q                             | $\sigma_{ i-j +1} 1( i - j  < q)$                                          |
| TOEPH     | Heterogeneous TOEP   | $2t - 1$                      | $\sigma_i \sigma_j \rho_{ i-j }$                                           |
| TOEPH(q)  | Banded hetero TOEP   | $t + q - 1$                   | $\sigma_i \sigma_j \rho_{ i-j } 1( i - j  < q)$                            |
| UN        | Unstructured         | $t(t + 1)/2$                  | $\sigma_{ij}$                                                              |
| UN(q)     | Banded               | $\frac{q}{2}(2t - q + 1)$     | $\sigma_{ij} 1( i - j  < q)$                                               |
| UNR       | Unstructured corrs   | $t(t + 1)/2$                  | $\sigma_i \sigma_j \rho_{\max(i,j) \min(i,j)}$                             |
| UNR(q)    | Banded correlations  | $\frac{q}{2}(2t - q + 1)$     | $\sigma_i \sigma_j \rho_{\max(i,j) \min(i,j)}$                             |
| UN@AR(1)  | Direct product AR(1) | $t_1(t_1 + 1)/2 + 1$          | $\sigma_{i_1 j_1} \rho^{ i_2 - j_2 }$                                      |



**Table 59.17** continued

| Structure | Description         | Parms                                 | (i, j) element                                                                                                                 |
|-----------|---------------------|---------------------------------------|--------------------------------------------------------------------------------------------------------------------------------|
| UN@CS     | Direct product CS   | $t_1(t_1 + 1)/2 + 1$                  | $\begin{cases} \sigma_{i_1 j_1} & i_2 = j_2 \\ \sigma^2 \sigma_{i_1 j_1} & i_2 \neq j_2 \\ 0 \leq \sigma^2 \leq 1 \end{cases}$ |
| UN@UN     | Direct product UN   | $t_1(t_1 + 1)/2 + t_2(t_2 + 1)/2 - 1$ | $\sigma_{1,i_1 j_1} \sigma_{2,i_2 j_2}$                                                                                        |
| VC        | Variance components | $q$                                   | $\sigma_k^2 1(i = j)$<br>and $i$ corresponds to $k$ th effect                                                                  |

In Table 59.17, “Parms” is the number of covariance parameters in the structure,  $t$  is the overall dimension of the covariance matrix, and  $1(A)$  equals 1 when  $A$  is true and 0 otherwise. For example,  $1(i = j)$  equals 1 when  $i = j$  and 0 otherwise, and  $1(|i - j| < q)$  equals 1 when  $|i - j| < q$  and 0 otherwise. For the TYPE=TOEPH structures,  $\rho_0 = 1$ , and for the TYPE=UNR structures,  $\rho_{ii} = 1$  for all  $i$ . For the direct product structures, the subscripts “1” and “2” see the first and second structure in the direct product, respectively, and  $i_1 = \text{int}((i + t_2 - 1)/t_2)$ ,  $j_1 = \text{int}((j + t_2 - 1)/t_2)$ ,  $i_2 = \text{mod}(i - 1, t_2) + 1$ , and  $j_2 = \text{mod}(j - 1, t_2) + 1$ .

**Table 59.18** Spatial Covariance Structures

| Structure                                 | Description                               | Parms    | (i, j) element                                                                                                                                      |
|-------------------------------------------|-------------------------------------------|----------|-----------------------------------------------------------------------------------------------------------------------------------------------------|
| SP(EXP)(c-list)                           | Exponential                               | 2        | $\sigma^2 \exp\{-d_{ij}/\theta\}$                                                                                                                   |
| SP(EXPA)(c-list)                          | Anisotropic exponential                   | $2c + 1$ | $\sigma^2 \prod_{k=1}^c \exp\{-\theta_k d(i, j, k)^{p_k}\}$                                                                                         |
| SP(EXPGA)(c <sub>1</sub> c <sub>2</sub> ) | 2D exponential, geometrically anisotropic | 4        | $\sigma^2 \exp\{-d_{ij}(\theta, \lambda)/\rho\}$                                                                                                    |
| SP(GAU)(c-list)                           | Gaussian                                  | 2        | $\sigma^2 \exp\{-d_{ij}^2/\rho^2\}$                                                                                                                 |
| SP(GAUGA)(c <sub>1</sub> c <sub>2</sub> ) | 2D Gaussian, geometrically anisotropic    | 4        | $\sigma^2 \exp\{-d_{ij}(\theta, \lambda)^2/\rho^2\}$                                                                                                |
| SP(LIN)(c-list)                           | Linear                                    | 2        | $\sigma^2(1 - \rho d_{ij}) 1(\rho d_{ij} \leq 1)$                                                                                                   |
| SP(LINL)(c-list)                          | Linear log                                | 2        | $\sigma^2(1 - \rho \log(d_{ij})) \times 1(\rho \log(d_{ij}) \leq 1, d_{ij} > 0)$                                                                    |
| SP(MATERN)(c-list)                        | Matérn                                    | 3        | $\sigma^2 \frac{1}{\Gamma(v)} \left(\frac{d_{ij}}{2\rho}\right)^v 2K_v(d_{ij}/\rho)$                                                                |
| SP(MATHSW)(c-list)                        | Matérn (Handcock-Stein-Wallis)            | 3        | $\sigma^2 \frac{1}{\Gamma(v)} \left(\frac{d_{ij}\sqrt{v}}{\rho}\right)^v 2K_v\left(\frac{2d_{ij}\sqrt{v}}{\rho}\right)$                             |
| SP(POW)(c-list)                           | Power                                     | 2        | $\sigma^2 \rho^{d_{ij}}$                                                                                                                            |
| SP(POWA)(c-list)                          | Anisotropic power                         | $c + 1$  | $\sigma^2 \rho_1^{d(i,j,1)} \rho_2^{d(i,j,2)} \dots \rho_c^{d(i,j,c)}$                                                                              |
| SP(SPH)(c-list)                           | Spherical                                 | 2        | $\sigma^2 [1 - (\frac{3d_{ij}}{2\rho}) + (\frac{d_{ij}^3}{2\rho^3})] 1(d_{ij} \leq \rho)$                                                           |
| SP(SPHGA)(c <sub>1</sub> c <sub>2</sub> ) | 2D Spherical, geometrically anisotropic   | 4        | $\sigma^2 [1 - (\frac{3d_{ij}(\theta, \lambda)}{2\rho}) + (\frac{d_{ij}(\theta, \lambda)^3}{2\rho^3})] \times 1(d_{ij}(\theta, \lambda) \leq \rho)$ |

In Table 59.18, *c-list* contains the names of the numeric variables used as coordinates of the location of the observation in space, and  $d_{ij}$  is the Euclidean distance between the  $i$ th and  $j$ th vectors of these coordinates, which correspond to the  $i$ th and  $j$ th observations in the input data set. For SP(POWA) and SP(EXPA),  $c$  is the number of coordinates, and  $d(i, j, k)$  is the absolute distance between the  $k$ th coordinate,  $k = 1, \dots, c$ , of the  $i$ th and  $j$ th observations in the input data set. For the geometrically anisotropic structures SP(EXPGA), SP(GAUGA), and SP(SPHGA), exactly two spatial coordinate variables must be specified as  $c_1$  and  $c_2$ . Geometric anisotropy is corrected by applying a rotation  $\theta$  and scaling  $\lambda$  to the coordinate system, and  $d_{ij}(\theta, \lambda)$  represents the Euclidean distance between two points in the transformed space. SP(MATERN) and SP(MATHSW) represent covariance structures in a class defined by Matérn (see Matérn 1986; Handcock and Stein 1993; Handcock and Wallis 1994). The function  $K_\nu$  is the modified Bessel function of the second kind of (real) order  $\nu > 0$ ; the parameter  $\nu$  governs the smoothness of the process (see below for more details).

Table 59.19 lists some examples of the structures in Table 59.17 and Table 59.18.

**Table 59.19** Covariance Structure Examples

| Description                | Structure    | Example                                                                                                                                                                                                                                                      |
|----------------------------|--------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Variance components        | VC (default) | $\begin{bmatrix} \sigma_B^2 & 0 & 0 & 0 \\ 0 & \sigma_B^2 & 0 & 0 \\ 0 & 0 & \sigma_{AB}^2 & 0 \\ 0 & 0 & 0 & \sigma_{AB}^2 \end{bmatrix}$                                                                                                                   |
| Compound symmetry          | CS           | $\begin{bmatrix} \sigma^2 + \sigma_1 & \sigma_1 & \sigma_1 & \sigma_1 \\ \sigma_1 & \sigma^2 + \sigma_1 & \sigma_1 & \sigma_1 \\ \sigma_1 & \sigma_1 & \sigma^2 + \sigma_1 & \sigma_1 \\ \sigma_1 & \sigma_1 & \sigma_1 & \sigma^2 + \sigma_1 \end{bmatrix}$ |
| Unstructured               | UN           | $\begin{bmatrix} \sigma_1^2 & \sigma_{21} & \sigma_{31} & \sigma_{41} \\ \sigma_{21} & \sigma_2^2 & \sigma_{32} & \sigma_{42} \\ \sigma_{31} & \sigma_{32} & \sigma_3^2 & \sigma_{43} \\ \sigma_{41} & \sigma_{42} & \sigma_{43} & \sigma_4^2 \end{bmatrix}$ |
| Banded main diagonal       | UN(1)        | $\begin{bmatrix} \sigma_1^2 & 0 & 0 & 0 \\ 0 & \sigma_2^2 & 0 & 0 \\ 0 & 0 & \sigma_3^2 & 0 \\ 0 & 0 & 0 & \sigma_4^2 \end{bmatrix}$                                                                                                                         |
| First-order autoregressive | AR(1)        | $\sigma^2 \begin{bmatrix} 1 & \rho & \rho^2 & \rho^3 \\ \rho & 1 & \rho & \rho^2 \\ \rho^2 & \rho & 1 & \rho \\ \rho^3 & \rho^2 & \rho & 1 \end{bmatrix}$                                                                                                    |
| Toeplitz                   | TOEP         | $\begin{bmatrix} \sigma^2 & \sigma_1 & \sigma_2 & \sigma_3 \\ \sigma_1 & \sigma^2 & \sigma_1 & \sigma_2 \\ \sigma_2 & \sigma_1 & \sigma^2 & \sigma_1 \\ \sigma_3 & \sigma_2 & \sigma_1 & \sigma^2 \end{bmatrix}$                                             |
| Toeplitz with two bands    | TOEP(2)      | $\begin{bmatrix} \sigma^2 & \sigma_1 & 0 & 0 \\ \sigma_1 & \sigma^2 & \sigma_1 & 0 \\ 0 & \sigma_1 & \sigma^2 & \sigma_1 \\ 0 & 0 & \sigma_1 & \sigma^2 \end{bmatrix}$                                                                                       |

**Table 59.19** continued

| Description                               | Structure  | Example                                                                                                                                                                                                                                                                                                                                                                                                                              |
|-------------------------------------------|------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Spatial power                             | SP(POW)(c) | $\sigma^2 \begin{bmatrix} 1 & \rho^{d_{12}} & \rho^{d_{13}} & \rho^{d_{14}} \\ \rho^{d_{21}} & 1 & \rho^{d_{23}} & \rho^{d_{24}} \\ \rho^{d_{31}} & \rho^{d_{32}} & 1 & \rho^{d_{34}} \\ \rho^{d_{41}} & \rho^{d_{42}} & \rho^{d_{43}} & 1 \end{bmatrix}$                                                                                                                                                                            |
| Heterogeneous AR(1)                       | ARH(1)     | $\begin{bmatrix} \sigma_1^2 & \sigma_1\sigma_2\rho & \sigma_1\sigma_3\rho^2 & \sigma_1\sigma_4\rho^3 \\ \sigma_2\sigma_1\rho & \sigma_2^2 & \sigma_2\sigma_3\rho & \sigma_2\sigma_4\rho^2 \\ \sigma_3\sigma_1\rho^2 & \sigma_3\sigma_2\rho & \sigma_3^2 & \sigma_3\sigma_4\rho \\ \sigma_4\sigma_1\rho^3 & \sigma_4\sigma_2\rho & \sigma_4\sigma_3\rho & \sigma_4^2 \end{bmatrix}$                                                   |
| First-order autoregressive moving average | ARMA(1,1)  | $\sigma^2 \begin{bmatrix} 1 & \gamma & \gamma\rho & \gamma\rho^2 \\ \gamma & 1 & \gamma & \gamma\rho \\ \gamma\rho & \gamma & 1 & \gamma \\ \gamma\rho^2 & \gamma\rho & \gamma & 1 \end{bmatrix}$                                                                                                                                                                                                                                    |
| Heterogeneous CS                          | CSH        | $\begin{bmatrix} \sigma_1^2 & \sigma_1\sigma_2\rho & \sigma_1\sigma_3\rho & \sigma_1\sigma_4\rho \\ \sigma_2\sigma_1\rho & \sigma_2^2 & \sigma_2\sigma_3\rho & \sigma_2\sigma_4\rho \\ \sigma_3\sigma_1\rho & \sigma_3\sigma_2\rho & \sigma_3^2 & \sigma_3\sigma_4\rho \\ \sigma_4\sigma_1\rho & \sigma_4\sigma_2\rho & \sigma_4\sigma_3\rho & \sigma_4^2 \end{bmatrix}$                                                             |
| First-order factor analytic               | FA(1)      | $\begin{bmatrix} \lambda_1^2 + d_1 & \lambda_1\lambda_2 & \lambda_1\lambda_3 & \lambda_1\lambda_4 \\ \lambda_2\lambda_1 & \lambda_2^2 + d_2 & \lambda_2\lambda_3 & \lambda_2\lambda_4 \\ \lambda_3\lambda_1 & \lambda_3\lambda_2 & \lambda_3^2 + d_3 & \lambda_3\lambda_4 \\ \lambda_4\lambda_1 & \lambda_4\lambda_2 & \lambda_4\lambda_3 & \lambda_4^2 + d_4 \end{bmatrix}$                                                         |
| Huynh-Feldt                               | HF         | $\begin{bmatrix} \sigma_1^2 & \frac{\sigma_1^2 + \sigma_2^2}{2} - \lambda & \frac{\sigma_1^2 + \sigma_3^2}{2} - \lambda \\ \frac{\sigma_2^2 + \sigma_1^2}{2} - \lambda & \sigma_2^2 & \frac{\sigma_2^2 + \sigma_3^2}{2} - \lambda \\ \frac{\sigma_3^2 + \sigma_1^2}{2} - \lambda & \frac{\sigma_3^2 + \sigma_2^2}{2} - \lambda & \sigma_3^2 \end{bmatrix}$                                                                           |
| First-order antedependence                | ANTE(1)    | $\begin{bmatrix} \sigma_1^2 & \sigma_1\sigma_2\rho_1 & \sigma_1\sigma_3\rho_1\rho_2 \\ \sigma_2\sigma_1\rho_1 & \sigma_2^2 & \sigma_2\sigma_3\rho_2 \\ \sigma_3\sigma_1\rho_2\rho_1 & \sigma_3\sigma_2\rho_2 & \sigma_3^2 \end{bmatrix}$                                                                                                                                                                                             |
| Heterogeneous Toeplitz                    | TOEPH      | $\begin{bmatrix} \sigma_1^2 & \sigma_1\sigma_2\rho_1 & \sigma_1\sigma_3\rho_2 & \sigma_1\sigma_4\rho_3 \\ \sigma_2\sigma_1\rho_1 & \sigma_2^2 & \sigma_2\sigma_3\rho_1 & \sigma_2\sigma_4\rho_2 \\ \sigma_3\sigma_1\rho_2 & \sigma_3\sigma_2\rho_1 & \sigma_3^2 & \sigma_3\sigma_4\rho_1 \\ \sigma_4\sigma_1\rho_3 & \sigma_4\sigma_2\rho_2 & \sigma_4\sigma_3\rho_1 & \sigma_4^2 \end{bmatrix}$                                     |
| Unstructured correlations                 | UNR        | $\begin{bmatrix} \sigma_1^2 & \sigma_1\sigma_2\rho_{21} & \sigma_1\sigma_3\rho_{31} & \sigma_1\sigma_4\rho_{41} \\ \sigma_2\sigma_1\rho_{21} & \sigma_2^2 & \sigma_2\sigma_3\rho_{32} & \sigma_2\sigma_4\rho_{42} \\ \sigma_3\sigma_1\rho_{31} & \sigma_3\sigma_2\rho_{32} & \sigma_3^2 & \sigma_3\sigma_4\rho_{43} \\ \sigma_4\sigma_1\rho_{41} & \sigma_4\sigma_2\rho_{42} & \sigma_4\sigma_3\rho_{43} & \sigma_4^2 \end{bmatrix}$ |
| Direct product AR(1)                      | UN@AR(1)   | $\begin{bmatrix} \sigma_1^2 & \sigma_{21} \\ \sigma_{21} & \sigma_2^2 \end{bmatrix} \otimes \begin{bmatrix} 1 & \rho & \rho^2 \\ \rho & 1 & \rho \\ \rho^2 & \rho & 1 \end{bmatrix} =$                                                                                                                                                                                                                                               |

**Table 59.19** *continued*

| Description | Structure | Example                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |
|-------------|-----------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|             |           | $\begin{bmatrix} \sigma_1^2 & \sigma_1^2\rho & \sigma_1^2\rho^2 & \sigma_{21} & \sigma_{21}\rho & \sigma_{21}\rho^2 \\ \sigma_1^2\rho & \sigma_1^2 & \sigma_1^2\rho & \sigma_{21}\rho & \sigma_{21} & \sigma_{21}\rho \\ \sigma_1^2\rho^2 & \sigma_1^2\rho & \sigma_1^2 & \sigma_{21}\rho^2 & \sigma_{21}\rho & \sigma_{21} \\ \sigma_{21} & \sigma_{21}\rho & \sigma_{21}\rho^2 & \sigma_2^2 & \sigma_2^2\rho & \sigma_2^2\rho^2 \\ \sigma_{21}\rho & \sigma_{21} & \sigma_{21}\rho & \sigma_2^2\rho & \sigma_2^2 & \sigma_2^2\rho \\ \sigma_{21}\rho^2 & \sigma_{21}\rho & \sigma_{21} & \sigma_2^2\rho^2 & \sigma_2^2\rho & \sigma_2^2 \end{bmatrix}$ |

The following provides some further information about these covariance structures:

TYPE=ANTE(1) specifies the first-order antedependence structure (see Kenward 1987; Patel 1991; Macchiavelli and Arnold 1994). In Table 59.17,  $\sigma_i^2$  is the  $i$ th variance parameter, and  $\rho_k$  is the  $k$ th autocorrelation parameter satisfying  $|\rho_k| < 1$ .

TYPE=AR(1) specifies a first-order autoregressive structure. PROC MIXED imposes the constraint  $|\rho| < 1$  for stationarity.

TYPE=ARH(1) specifies a heterogeneous first-order autoregressive structure. As with TYPE=AR(1), PROC MIXED imposes the constraint  $|\rho| < 1$  for stationarity.

TYPE=ARMA(1,1) specifies the first-order autoregressive moving-average structure. In Table 59.17,  $\rho$  is the autoregressive parameter,  $\gamma$  models a moving-average component, and  $\sigma^2$  is the residual variance. In the notation of Fuller (1976, p. 68),  $\rho = \theta_1$  and

$$\gamma = \frac{(1 + b_1\theta_1)(\theta_1 + b_1)}{1 + b_1^2 + 2b_1\theta_1}$$

The example in Table 59.19 and  $|b_1| < 1$  imply that

$$b_1 = \frac{\beta - \sqrt{\beta^2 - 4\alpha^2}}{2\alpha}$$

where  $\alpha = \gamma - \rho$  and  $\beta = 1 + \rho^2 - 2\gamma\rho$ . PROC MIXED imposes the constraints  $|\rho| < 1$  and  $|\gamma| < 1$  for stationarity, although for some values of  $\rho$  and  $\gamma$  in this region the resulting covariance matrix is not positive definite. When the estimated value of  $\rho$  becomes negative, the computed covariance is multiplied by  $\cos(\pi d_{ij})$  to account for the negativity.

TYPE=CS specifies the compound-symmetry structure, which has constant variance and constant covariance.

TYPE=CSH specifies the heterogeneous compound-symmetry structure. This structure has a different variance parameter for each diagonal element, and it uses the square roots of these parameters in the off-diagonal entries. In Table 59.17,  $\sigma_i^2$  is the  $i$ th variance parameter, and  $\rho$  is the correlation parameter satisfying  $|\rho| < 1$ .

TYPE=FA( $q$ ) specifies the factor-analytic structure with  $q$  factors (Jennrich and Schluchter 1986). This structure is of the form  $\mathbf{\Lambda}\mathbf{\Lambda}' + \mathbf{D}$ , where  $\mathbf{\Lambda}$  is a  $t \times q$  rectangular matrix and  $\mathbf{D}$  is a  $t \times t$  diagonal matrix with  $t$  different parameters. When  $q > 1$ , the elements of  $\mathbf{\Lambda}$  in its upper-right corner (that is, the elements in the  $i$ th row and  $j$ th column for  $j > i$ ) are set to zero to fix the rotation of the structure.

- TYPE=FA0(*q*)** is similar to the **FA(*q*)** structure except that no diagonal matrix **D** is included. When  $q < t$ —that is, when the number of factors is less than the dimension of the matrix—this structure is nonnegative definite but not of full rank. In this situation, you can use it for approximating an unstructured **G** matrix in the **RANDOM** statement or for combining with the **LOCAL** option in the **REPEATED** statement. When  $q = t$ , you can use this structure to constrain **G** to be nonnegative definite in the **RANDOM** statement.
- TYPE=FA1(*q*)** is similar to the **TYPE=FA(*q*)** structure except that all of the elements in **D** are constrained to be equal. This offers a useful and more parsimonious alternative to the full factor-analytic structure.
- TYPE=HF** specifies the Huynh-Feldt covariance structure (Huynh and Feldt 1970). This structure is similar to the **TYPE=CSH** structure in that it has the same number of parameters and heterogeneity along the main diagonal. However, it constructs the off-diagonal elements by taking arithmetic rather than geometric means.
- You can perform a likelihood ratio test of the Huynh-Feldt conditions by running PROC MIXED twice, once with **TYPE=HF** and once with **TYPE=UN**, and then subtracting their respective values of  $-2$  times the maximized likelihood.
- If PROC MIXED does not converge under your Huynh-Feldt model, you can specify your own starting values with the **PARMS** statement. The default **MIVQUE(0)** starting values can sometimes be poor for this structure. A good choice for starting values is often the parameter estimates corresponding to an initial fit that uses **TYPE=CS**.
- TYPE=LIN(*q*)** specifies the general linear covariance structure with  $q$  parameters. This structure consists of a linear combination of known matrices that are input with the **LDATA=** option. This structure is very general, and you need to make sure that the variance matrix is positive definite. By default, PROC MIXED sets the initial values of the parameters to 1. You can use the **PARMS** statement to specify other initial values.
- TYPE=LINEAR(*q*)** is an alias for **TYPE=LIN(*q*)**.
- TYPE=SIMPLE** is an alias for **TYPE=VC**.
- TYPE=SP(EXPA)(*c-list*)** specifies the spatial anisotropic exponential structure, where *c-list* is a list of variables indicating the coordinates. This structure has (*i, j*) element equal to

$$\sigma^2 \prod_{k=1}^c \exp\{-\theta_k d(i, j, k)^{p_k}\}$$

where  $c$  is the number of coordinates and  $d(i, j, k)$  is the absolute distance between the  $k$ th coordinate ( $k = 1, \dots, c$ ) of the  $i$ th and  $j$ th observations in the input data set. There are  $2c + 1$  parameters to be estimated:  $\theta_k$ ,  $p_k$  ( $k = 1, \dots, c$ ), and  $\sigma^2$ .

You might want to constrain some of the EXPA parameters to known values. For example, suppose you have three coordinate variables **C1**, **C2**, and **C3** and you want to constrain the powers  $p_k$  to equal 2, as in Sacks et al. (1989). Suppose further that you want to model covariance across the entire input data set and you suspect the  $\theta_k$  and  $\sigma^2$  estimates are close to 3, 4, 5, and 1, respectively. Then specify the following statements:

```

repeated / type=sp(expa) (c1 c2 c3)
 subject=intercept;
parms (3) (4) (5) (2) (2) (2) (1) /
 hold=4, 5, 6;

```

TYPE=SP(EXPGA)(c<sub>1</sub> c<sub>2</sub>) specify modification of the isotropic SP(EXP) covariance structure.

TYPE=SP(GAUGA)(c<sub>1</sub> c<sub>2</sub>) specify modification of the isotropic SP(GAU) covariance structure.

TYPE=SP(SPHGA)(c<sub>1</sub> c<sub>2</sub>) specify modification of the isotropic SP(SPH) covariance structure.

These are structures that allow for geometric anisotropy in two dimensions. The coordinates are specified by the variables c<sub>1</sub> and c<sub>2</sub>.

If the spatial process is geometrically anisotropic in  $\mathbf{c} = [c_{i1}, c_{i2}]$ , then it is isotropic in the coordinate system

$$\mathbf{Ac} = \begin{bmatrix} 1 & 0 \\ 0 & \lambda \end{bmatrix} \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix} \mathbf{c} = \mathbf{c}^*$$

for a properly chosen angle  $\theta$  and scaling factor  $\lambda$ . Elliptical isocorrelation contours are thereby transformed to spherical contours, adding two parameters to the respective isotropic covariance structures. Euclidean distances (see Table 59.18) are expressed in terms of  $\mathbf{c}^*$ .

The angle  $\theta$  of the clockwise rotation is reported in radians,  $0 \leq \theta \leq 2\pi$ . The scaling parameter  $\lambda$  represents the ratio of the range parameters in the direction of the major and minor axis of the correlation contours. In other words, following a rotation of the coordinate system by angle  $\theta$ , isotropy is achieved by compressing or magnifying distances in one coordinate by the factor  $\lambda$ .

Fixing  $\lambda = 1.0$  reduces the models to isotropic ones for any angle of rotation. If the scaling parameter is held constant at 1.0, you should also hold constant the angle of rotation, as in the following statements:

```

repeated / type=sp(expga) (gxc gyc)
 subject=intercept;
parms (6) (1.0) (0.0) (1) / hold=2, 3;

```

If  $\lambda$  is fixed at any other value than 1.0, the angle of rotation can be estimated. Specifying a starting grid of angles and scaling factors can considerably improve the convergence properties of the optimization algorithm for these models. Only a single random effect with geometrically anisotropic structure is permitted.

TYPE=SP(MATERN)(c-list) | TYPE=SP(MATHSW)(c-list) specifies covariance structures in the Matérn class of covariance functions (Matérn 1986). Two observations for the same subject (block of  $\mathbf{R}$ ) that are Euclidean distance  $d_{ij}$  apart have covariance

$$\sigma^2 \frac{1}{\Gamma(\nu)} \left( \frac{d_{ij}}{2\rho} \right)^\nu 2K_\nu(d_{ij}/\rho) \quad \nu > 0, \rho > 0$$

where  $K_\nu$  is the modified Bessel function of the second kind of (real) order  $\nu > 0$ . The smoothness (continuity) of a stochastic process with covariance function in this class increases with  $\nu$ . The Matérn class thus enables data-driven estimation

of the smoothness properties. The covariance is identical to the exponential model for  $\nu = 0.5$  (TYPE=SP(EXP)(*c-list*)), while for  $\nu = 1$  the model advocated by Whittle (1954) results. As  $\nu \rightarrow \infty$  the model approaches the gaussian covariance structure (TYPE=SP(GAU)(*c-list*)).

The MATHSW structure represents the Matérn class in the parameterization of Handcock and Stein (1993) and Handcock and Wallis (1994),

$$\sigma^2 \frac{1}{\Gamma(\nu)} \left( \frac{d_{ij} \sqrt{\nu}}{\rho} \right)^\nu 2K_\nu \left( \frac{2d_{ij} \sqrt{\nu}}{\rho} \right)$$

Since computation of the function  $K_\nu$  and its derivatives is numerically very intensive, fitting models with Matérn covariance structures can be more time-consuming than with other spatial covariance structures. Good starting values are essential.

TYPE=SP(POW)(*c-list*) | TYPE=SP(POWA)(*c-list*) specifies the spatial power structures. When the estimated value of  $\rho$  becomes negative, the computed covariance is multiplied by  $\cos(\pi d_{ij})$  to account for the negativity.

TYPE=TOEP(*q*) specifies a banded Toeplitz structure. This can be viewed as a moving-average structure with order equal to  $q - 1$ . The TYPE=TOEP option is a full Toeplitz matrix, which can be viewed as an autoregressive structure with order equal to the dimension of the matrix. The specification TYPE=TOEP(1) is the same as  $\sigma^2 I$ , where  $I$  is an identity matrix, and it can be useful for specifying the same variance component for several effects.

TYPE=TOEPH(*q*) specifies a heterogeneous banded Toeplitz structure. In Table 59.17,  $\sigma_i^2$  is the  $i$ th variance parameter and  $\rho_j$  is the  $j$ th correlation parameter satisfying  $|\rho_j| < 1$ . If you specify the order parameter  $q$ , then PROC MIXED estimates only the first  $q$  bands of the matrix, setting all higher bands equal to 0. The option TOEPH(1) is equivalent to both the TYPE=UN(1) and TYPE=UNR(1) options.

TYPE=UN(*q*) specifies a completely general (unstructured) covariance matrix parameterized directly in terms of variances and covariances. The variances are constrained to be nonnegative, and the covariances are unconstrained. This structure is not constrained to be nonnegative definite in order to avoid nonlinear constraints; however, you can use the TYPE=FA0 structure if you want this constraint to be imposed by a Cholesky factorization. If you specify the order parameter  $q$ , then PROC MIXED estimates only the first  $q$  bands of the matrix, setting all higher bands equal to 0.

TYPE=UNR(*q*) specifies a completely general (unstructured) covariance matrix parameterized in terms of variances and correlations. This structure fits the same model as the TYPE=UN(*q*) option but with a different parameterization. The  $i$ th variance parameter is  $\sigma_i^2$ . The parameter  $\rho_{jk}$  is the correlation between the  $j$ th and  $k$ th measurements; it satisfies  $|\rho_{jk}| < 1$ . If you specify the order parameter  $r$ , then PROC MIXED estimates only the first  $q$  bands of the matrix, setting all higher bands equal to zero.

TYPE=UN@AR(1) | TYPE=UN@CS | TYPE=UN@UN specify direct (Kronecker) product structures designed for multivariate repeated measures (see Galecki 1994). These structures are constructed by taking the Kronecker product of an unstructured matrix

(modeling covariance across the multivariate observations) with an additional covariance matrix (modeling covariance across time or another factor). The upper-left value in the second matrix is constrained to equal 1 to identify the model. See the *SAS/IML User's Guide* for more details about direct products.

To use these structures in the REPEATED statement, you must specify two distinct REPEATED effects, both of which must be included in the CLASS statement. The first effect indicates the multivariate observations, and the second identifies the levels of time or some additional factor. Note that the input data set must still be constructed in “univariate” format; that is, all dependent observations are still listed observation-wise in one single variable. Although this construction provides for general modeling possibilities, it forces you to construct variables indicating both dimensions of the Kronecker product.

For example, suppose your observed data consist of heights and weights of several children measured over several successive years. Your input data set should then contain variables similar to the following:

- Y, all of the heights and weights, with a separate observation for each
- Var, indicating whether the measurement is a height or a weight
- Year, indicating the year of measurement
- Child, indicating the child on which the measurement was taken

Your PROC MIXED statements for a Kronecker AR(1) structure across years would then be as follows:

```
proc mixed;
 class Var Year Child;
 model Y = Var Year Var*Year;
 repeated Var Year / type=un@ar(1)
 subject=Child;
run;
```

You should nearly always want to model different means for the multivariate observations; hence the inclusion of Var in the MODEL statement. The preceding mean model consists of cell means for all combinations of VAR and YEAR.

TYPE=VC specifies standard variance components and is the default structure for both the RANDOM and REPEATED statements. In the RANDOM statement, a distinct variance component is assigned to each effect. In the REPEATED statement, this structure is usually used only with the GROUP= option to specify a heterogeneous variance model.

Jennrich and Schluchter (1986) provide general information about the use of covariance structures, and Wolfinger (1996) presents details about many of the heterogeneous structures. Modeling with spatial covariance structures is discussed in many sources (Marx and Thompson 1987; Zimmerman and Harville 1991; Cressie 1993; Brownie, Bowman, and Burton 1993; Stroup, Baenziger, and Moltipz 1994; Brownie and Gumpertz 1997; Gotway and Stroup 1997; Chilès and Delfiner 1999; Schabenberger and Gotway 2005; Littell et al. 2006).



---

## SLICE Statement

**SLICE** *model-effect* </ options > ;

The SLICE statement provides a general mechanism for performing a partitioned analysis of the LS-means for an interaction. This analysis is also known as an analysis of simple effects.

The SLICE statement uses the same options as the LSMEANS statement, which are summarized in Table 19.21. For details about the syntax of the SLICE statement, see the section “SLICE Statement” on page 498 in Chapter 19, “Shared Concepts and Topics.”

**NOTE:** Use the section “LSMEANS Statement” on page 453 of Chapter 19, “Shared Concepts and Topics.” only for definitions of the options that you can use with the SLICE statement. PROC MIXED uses a slightly different syntax for the LSMEANS, which is described in the section “LSMEANS Statement” on page 491.

---

## STORE Statement

**STORE** < OUT= > *item-store-name* </ LABEL= 'label' > ;

The STORE statement requests that the procedure save the context and results of the statistical analysis. The resulting item store has a binary file format that cannot be modified. The contents of the item store can be processed with the PLM procedure.

For details about the syntax of the STORE statement, see the section “STORE Statement” on page 501 in Chapter 19, “Shared Concepts and Topics.”

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## WEIGHT Statement

**WEIGHT** *variable* ;

If you do not specify a REPEATED statement, the WEIGHT statement operates exactly like the one in PROC GLM. In this case PROC MIXED replaces  $X'X$  and  $Z'Z$  with  $X'WX$  and  $Z'WZ$ , where  $W$  is the diagonal weight matrix. If you specify a REPEATED statement, then the WEIGHT statement replaces  $R$  with  $LRL$ , where  $L$  is a diagonal matrix with elements  $W^{-1/2}$ . Observations with nonpositive or missing weights are not included in the PROC MIXED analysis.

If a computation in PROC MIXED involves  $R$ , then the WEIGHT statement replaces  $R$  with  $W^{-1/2}RW^{-1/2}$ . For example, the covariance matrix  $V$  for the observations usually have the form  $V = ZGZ' + R$ , which with the WEIGHT statement becomes  $V = ZGZ' + W^{-1/2}RW^{-1/2}$ .

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## Details: MIXED Procedure

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### Mixed Models Theory

This section provides an overview of a likelihood-based approach to general linear mixed models. This approach simplifies and unifies many common statistical analyses, including those involving repeated mea-

tures, random effects, and random coefficients. The basic assumption is that the data are linearly related to unobserved multivariate normal random variables. For extensions to nonlinear and nonnormal situations see the documentation of the GLIMMIX and NLMIXED procedures. Additional theory and examples are provided in Littell et al. (2006); Verbeke and Molenberghs (1997, 2000); Brown and Prescott (1999).

## Matrix Notation

Suppose that you observe  $n$  data points  $y_1, \dots, y_n$  and that you want to explain them by using  $n$  values for each of  $p$  explanatory variables  $x_{11}, \dots, x_{1p}, x_{21}, \dots, x_{2p}, \dots, x_{n1}, \dots, x_{np}$ . The  $x_{ij}$  values can be either regression-type continuous variables or dummy variables indicating class membership. The standard linear model for this setup is

$$y_i = \sum_{j=1}^p x_{ij} \beta_j + \epsilon_i \quad i = 1, \dots, n$$

where  $\beta_1, \dots, \beta_p$  are unknown *fixed-effects* parameters to be estimated and  $\epsilon_1, \dots, \epsilon_n$  are unknown independent and identically distributed normal (Gaussian) random variables with mean 0 and variance  $\sigma^2$ .

The preceding equations can be written simultaneously by using vectors and a matrix, as follows:

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} x_{11} & x_{12} & \dots & x_{1p} \\ x_{21} & x_{22} & \dots & x_{2p} \\ \vdots & \vdots & & \vdots \\ x_{n1} & x_{n2} & \dots & x_{np} \end{bmatrix} \begin{bmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_p \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

For convenience, simplicity, and extendability, this entire system is written as

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

where  $\mathbf{y}$  denotes the vector of observed  $y_i$ 's,  $\mathbf{X}$  is the known matrix of  $x_{ij}$ 's,  $\boldsymbol{\beta}$  is the unknown fixed-effects parameter vector, and  $\boldsymbol{\epsilon}$  is the unobserved vector of independent and identically distributed Gaussian random errors.

In addition to denoting data, random variables, and explanatory variables in the preceding fashion, the subsequent development makes use of basic matrix operators such as transpose ( $'$ ), inverse ( $^{-1}$ ), generalized inverse ( $^{-}$ ), determinant ( $|\cdot|$ ), and matrix multiplication. See Searle (1982) for details about these and other matrix techniques.

## Formulation of the Mixed Model

The previous general linear model is certainly a useful one (Searle 1971), and it is the one fitted by the GLM procedure. However, many times the distributional assumption about  $\boldsymbol{\epsilon}$  is too restrictive. The mixed model extends the general linear model by allowing a more flexible specification of the covariance matrix of  $\boldsymbol{\epsilon}$ . In other words, it allows for both correlation and heterogeneous variances, although you still assume normality.

The mixed model is written as

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\boldsymbol{\gamma} + \boldsymbol{\epsilon}$$

where everything is the same as in the general linear model except for the addition of the known design matrix,  $\mathbf{Z}$ , and the vector of unknown *random-effects parameters*,  $\boldsymbol{\gamma}$ . The matrix  $\mathbf{Z}$  can contain either continuous or dummy variables, just like  $\mathbf{X}$ . The name *mixed model* comes from the fact that the model contains both fixed-effects parameters,  $\boldsymbol{\beta}$ , and random-effects parameters,  $\boldsymbol{\gamma}$ . See Henderson (1990) and Searle, Casella, and McCulloch (1992) for historical developments of the mixed model.

A key assumption in the foregoing analysis is that  $\boldsymbol{\gamma}$  and  $\boldsymbol{\epsilon}$  are normally distributed with

$$\begin{aligned} \text{E} \begin{bmatrix} \boldsymbol{\gamma} \\ \boldsymbol{\epsilon} \end{bmatrix} &= \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix} \\ \text{Var} \begin{bmatrix} \boldsymbol{\gamma} \\ \boldsymbol{\epsilon} \end{bmatrix} &= \begin{bmatrix} \mathbf{G} & \mathbf{0} \\ \mathbf{0} & \mathbf{R} \end{bmatrix} \end{aligned}$$

The variance of  $\mathbf{y}$  is, therefore,  $\mathbf{V} = \mathbf{ZGZ}' + \mathbf{R}$ . You can model  $\mathbf{V}$  by setting up the random-effects design matrix  $\mathbf{Z}$  and by specifying covariance structures for  $\mathbf{G}$  and  $\mathbf{R}$ .

Note that this is a general specification of the mixed model, in contrast to many texts and articles that discuss only simple random effects. Simple random effects are a special case of the general specification with  $\mathbf{Z}$  containing dummy variables,  $\mathbf{G}$  containing variance components in a diagonal structure, and  $\mathbf{R} = \sigma^2\mathbf{I}_n$ , where  $\mathbf{I}_n$  denotes the  $n \times n$  identity matrix. The general linear model is a further special case with  $\mathbf{Z} = \mathbf{0}$  and  $\mathbf{R} = \sigma^2\mathbf{I}_n$ .

The following two examples illustrate the most common formulations of the general linear mixed model.

**Example: Growth Curve with Compound Symmetry**

Suppose that you have three growth curve measurements for  $s$  individuals and that you want to fit an overall linear trend in time. Your  $\mathbf{X}$  matrix is as follows:

$$\mathbf{X} = \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \\ \vdots & \vdots \\ 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{bmatrix}$$

The first column (coded entirely with 1s) fits an intercept, and the second column (coded with times of 1, 2, 3) fits a slope. Here,  $n = 3s$  and  $p = 2$ .

Suppose further that you want to introduce a common correlation among the observations from a single individual, with correlation being the same for all individuals. One way of setting this up in the general mixed model is to eliminate the  $\mathbf{Z}$  and  $\mathbf{G}$  matrices and let the  $\mathbf{R}$  matrix be block diagonal with blocks corresponding to the individuals and with each block having the *compound-symmetry* structure. This structure has two unknown parameters, one modeling a common covariance and the other modeling a residual variance. The









In many situations, the best approach is to use *likelihood-based* methods, exploiting the assumption that  $\boldsymbol{\gamma}$  and  $\boldsymbol{\epsilon}$  are normally distributed (Hartley and Rao 1967; Patterson and Thompson 1971; Harville 1977; Laird and Ware 1982; Jennrich and Schluchter 1986). PROC MIXED implements two likelihood-based methods: *maximum likelihood* (ML) and *restricted/residual maximum likelihood* (REML). A favorable theoretical property of ML and REML is that they accommodate data that are missing at random (Rubin 1976; Little 1995).

PROC MIXED constructs an objective function associated with ML or REML and maximizes it over all unknown parameters. Using calculus, it is possible to reduce this maximization problem to one over only the parameters in  $\mathbf{G}$  and  $\mathbf{R}$ . The corresponding log-likelihood functions are as follows:

$$\begin{aligned} \text{ML : } \quad l(\mathbf{G}, \mathbf{R}) &= -\frac{1}{2} \log |\mathbf{V}| - \frac{1}{2} \mathbf{r}' \mathbf{V}^{-1} \mathbf{r} - \frac{n}{2} \log(2\pi) \\ \text{REML : } \quad l_R(\mathbf{G}, \mathbf{R}) &= -\frac{1}{2} \log |\mathbf{V}| - \frac{1}{2} \log |\mathbf{X}' \mathbf{V}^{-1} \mathbf{X}| - \frac{1}{2} \mathbf{r}' \mathbf{V}^{-1} \mathbf{r} - \frac{n-p}{2} \log(2\pi) \end{aligned}$$

where  $\mathbf{r} = \mathbf{y} - \mathbf{X}(\mathbf{X}' \mathbf{V}^{-1} \mathbf{X})^{-1} \mathbf{X}' \mathbf{V}^{-1} \mathbf{y}$  and  $p$  is the rank of  $\mathbf{X}$ . PROC MIXED actually minimizes  $-2$  times these functions by using a ridge-stabilized Newton-Raphson algorithm. Lindstrom and Bates (1988) provide reasons for preferring Newton-Raphson to the Expectation-Maximum (EM) algorithm (Dempster, Laird, and Rubin 1977; Laird, Lange, and Stram 1987), as well as analytical details for implementing a QR-decomposition approach to the problem. Wolfinger, Tobias, and Sall (1994) present the sweep-based algorithms that are implemented in PROC MIXED.

One advantage of using the Newton-Raphson algorithm is that the second derivative matrix of the objective function evaluated at the optima is available upon completion. Denoting this matrix  $\mathbf{H}$ , the asymptotic theory of maximum likelihood (see Serfling 1980) shows that  $2\mathbf{H}^{-1}$  is an asymptotic variance-covariance matrix of the estimated parameters of  $\mathbf{G}$  and  $\mathbf{R}$ . Thus, tests and confidence intervals based on asymptotic normality can be obtained. However, these can be unreliable in small samples, especially for parameters such as variance components that have sampling distributions that tend to be skewed to the right.

If a residual variance  $\sigma^2$  is a part of your mixed model, it can usually be *profiled* out of the likelihood. This means solving analytically for the optimal  $\sigma^2$  and plugging this expression back into the likelihood formula (see Wolfinger, Tobias, and Sall 1994). This reduces the number of optimization parameters by one and can improve convergence properties. PROC MIXED profiles the residual variance out of the log likelihood whenever it appears reasonable to do so. This includes the case when  $\mathbf{R}$  equals  $\sigma^2 \mathbf{I}$  and when it has blocks with a compound symmetry, time series, or spatial structure. PROC MIXED does not profile the log likelihood when  $\mathbf{R}$  has unstructured blocks, when you use the **HOLD=** or **NOITER** option in the **PARMS** statement, or when you use the **NOPROFILE** option in the **PROC MIXED** statement.

Instead of ML or REML, you can use the noniterative MIVQUE0 method to estimate  $\mathbf{G}$  and  $\mathbf{R}$  (Rao 1972; LaMotte 1973; Wolfinger, Tobias, and Sall 1994). In fact, by default PROC MIXED uses MIVQUE0 estimates as starting values for the ML and REML procedures. For variance component models, another estimation method involves equating Type 1, 2, or 3 expected mean squares to their observed values and solving the resulting system. However, Swallow and Monahan (1984) present simulation evidence favoring REML and ML over MIVQUE0 and other method-of-moment estimators.

## Estimating Fixed and Random Effects in the Mixed Model

ML, REML, MIVQUE0, or Type1–Type3 provide estimates of  $\mathbf{G}$  and  $\mathbf{R}$ , which are denoted  $\hat{\mathbf{G}}$  and  $\hat{\mathbf{R}}$ , respectively. To obtain estimates of  $\boldsymbol{\beta}$  and  $\boldsymbol{\gamma}$ , the standard method is to solve the *mixed model equations* (Henderson 1984):



$$\begin{bmatrix} \mathbf{X}'\widehat{\mathbf{R}}^{-1}\mathbf{X} & \mathbf{X}'\widehat{\mathbf{R}}^{-1}\mathbf{Z} \\ \mathbf{Z}'\widehat{\mathbf{R}}^{-1}\mathbf{X} & \mathbf{Z}'\widehat{\mathbf{R}}^{-1}\mathbf{Z} + \widehat{\mathbf{G}}^{-1} \end{bmatrix} \begin{bmatrix} \widehat{\boldsymbol{\beta}} \\ \widehat{\boldsymbol{\gamma}} \end{bmatrix} = \begin{bmatrix} \mathbf{X}'\widehat{\mathbf{R}}^{-1}\mathbf{y} \\ \mathbf{Z}'\widehat{\mathbf{R}}^{-1}\mathbf{y} \end{bmatrix}$$

The solutions can also be written as

$$\begin{aligned} \widehat{\boldsymbol{\beta}} &= (\mathbf{X}'\widehat{\mathbf{V}}^{-1}\mathbf{X})^{-1}\mathbf{X}'\widehat{\mathbf{V}}^{-1}\mathbf{y} \\ \widehat{\boldsymbol{\gamma}} &= \widehat{\mathbf{G}}\mathbf{Z}'\widehat{\mathbf{V}}^{-1}(\mathbf{y} - \mathbf{X}\widehat{\boldsymbol{\beta}}) \end{aligned}$$

and have connections with empirical Bayes estimators (Laird and Ware 1982; Carlin and Louis 1996).

Note that the mixed model equations are extended normal equations and that the preceding expression assumes that  $\widehat{\mathbf{G}}$  is nonsingular. For the extreme case where the eigenvalues of  $\widehat{\mathbf{G}}$  are very large,  $\widehat{\mathbf{G}}^{-1}$  contributes very little to the equations and  $\widehat{\boldsymbol{\gamma}}$  is close to what it would be if  $\boldsymbol{\gamma}$  actually contained fixed-effects parameters. On the other hand, when the eigenvalues of  $\widehat{\mathbf{G}}$  are very small,  $\widehat{\mathbf{G}}^{-1}$  dominates the equations and  $\widehat{\boldsymbol{\gamma}}$  is close to 0. For intermediate cases,  $\widehat{\mathbf{G}}^{-1}$  can be viewed as shrinking the fixed-effects estimates of  $\boldsymbol{\gamma}$  toward 0 (Robinson 1991).

If  $\widehat{\mathbf{G}}$  is singular, then the mixed model equations are modified (Henderson 1984) as follows:

$$\begin{bmatrix} \mathbf{X}'\widehat{\mathbf{R}}^{-1}\mathbf{X} & \mathbf{X}'\widehat{\mathbf{R}}^{-1}\mathbf{Z}\widehat{\mathbf{G}} \\ \widehat{\mathbf{G}}'\mathbf{Z}'\widehat{\mathbf{R}}^{-1}\mathbf{X} & \widehat{\mathbf{G}}'\mathbf{Z}'\widehat{\mathbf{R}}^{-1}\mathbf{Z}\widehat{\mathbf{G}} + \mathbf{G} \end{bmatrix} \begin{bmatrix} \widehat{\boldsymbol{\beta}} \\ \widehat{\boldsymbol{\tau}} \end{bmatrix} = \begin{bmatrix} \mathbf{X}'\widehat{\mathbf{R}}^{-1}\mathbf{y} \\ \widehat{\mathbf{G}}'\mathbf{Z}'\widehat{\mathbf{R}}^{-1}\mathbf{y} \end{bmatrix}$$

Denote the generalized inverses of the nonsingular  $\widehat{\mathbf{G}}$  and singular  $\widehat{\mathbf{G}}$  forms of the mixed model equations by  $\mathbf{C}$  and  $\mathbf{M}$ , respectively. In the nonsingular case, the solution  $\widehat{\boldsymbol{\gamma}}$  estimates the random effects directly, but in the singular case the estimates of random effects are achieved through a back-transformation  $\widehat{\boldsymbol{\gamma}} = \widehat{\mathbf{G}}\widehat{\boldsymbol{\tau}}$  where  $\widehat{\boldsymbol{\tau}}$  is the solution to the modified mixed model equations. Similarly, while in the nonsingular case  $\mathbf{C}$  itself is the estimated covariance matrix for  $(\widehat{\boldsymbol{\beta}}, \widehat{\boldsymbol{\gamma}})$ , in the singular case the covariance estimate for  $(\widehat{\boldsymbol{\beta}}, \widehat{\mathbf{G}}\widehat{\boldsymbol{\tau}})$  is given by  $\mathbf{PMP}$  where

$$\mathbf{P} = \begin{bmatrix} \mathbf{I} & \\ & \widehat{\mathbf{G}} \end{bmatrix}$$

An example of when the singular form of the equations is necessary is when a variance component estimate falls on the boundary constraint of 0.

## Model Selection

The previous section on estimation assumes the specification of a mixed model in terms of  $\mathbf{X}$ ,  $\mathbf{Z}$ ,  $\mathbf{G}$ , and  $\mathbf{R}$ . Even though  $\mathbf{X}$  and  $\mathbf{Z}$  have known elements, their specific form and construction are flexible, and several possibilities can present themselves for a particular data set. Likewise, several different covariance structures for  $\mathbf{G}$  and  $\mathbf{R}$  might be reasonable.

Space does not permit a thorough discussion of model selection, but a few brief comments and references are in order. First, subject matter considerations and objectives are of great importance when selecting a model; see Diggle (1988) and Lindsey (1993).

Second, when the data themselves are looked to for guidance, many of the graphical methods and diagnostics appropriate for the general linear model extend to the mixed model setting as well (Christensen, Pearson, and Johnson 1992).

Finally, a likelihood-based approach to the mixed model provides several statistical measures for model adequacy as well. The most common of these are the likelihood ratio test and Akaike's and Schwarz's criteria (Bozdogan 1987; Wolfinger 1993; Keselman et al. 1998, 1999).

### Statistical Properties

If  $\mathbf{G}$  and  $\mathbf{R}$  are known,  $\hat{\boldsymbol{\beta}}$  is the *best linear unbiased estimator* (BLUE) of  $\boldsymbol{\beta}$ , and  $\hat{\boldsymbol{\gamma}}$  is the *best linear unbiased predictor* (BLUP) of  $\boldsymbol{\gamma}$  (Searle 1971; Harville 1988, 1990; Robinson 1991; McLean, Sanders, and Stroup 1991). Here, "best" means minimum mean squared error. The covariance matrix of  $(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}, \hat{\boldsymbol{\gamma}} - \boldsymbol{\gamma})$  is

$$\mathbf{C} = \begin{bmatrix} \mathbf{X}'\mathbf{R}^{-1}\mathbf{X} & \mathbf{X}'\mathbf{R}^{-1}\mathbf{Z} \\ \mathbf{Z}'\mathbf{R}^{-1}\mathbf{X} & \mathbf{Z}'\mathbf{R}^{-1}\mathbf{Z} + \mathbf{G}^{-1} \end{bmatrix}^{-}$$

where  $^{-}$  denotes a generalized inverse (see Searle 1971).

However,  $\mathbf{G}$  and  $\mathbf{R}$  are usually unknown and are estimated by using one of the aforementioned methods. These estimates,  $\hat{\mathbf{G}}$  and  $\hat{\mathbf{R}}$ , are therefore simply substituted into the preceding expression to obtain

$$\hat{\mathbf{C}} = \begin{bmatrix} \mathbf{X}'\hat{\mathbf{R}}^{-1}\mathbf{X} & \mathbf{X}'\hat{\mathbf{R}}^{-1}\mathbf{Z} \\ \mathbf{Z}'\hat{\mathbf{R}}^{-1}\mathbf{X} & \mathbf{Z}'\hat{\mathbf{R}}^{-1}\mathbf{Z} + \hat{\mathbf{G}}^{-1} \end{bmatrix}^{-}$$

as the approximate variance-covariance matrix of  $(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}, \hat{\boldsymbol{\gamma}} - \boldsymbol{\gamma})$ . In this case, the BLUE and BLUP acronyms no longer apply, but the word *empirical* is often added to indicate such an approximation. The appropriate acronyms thus become EBLUE and EBLUP.

McLean and Sanders (1988) show that  $\hat{\mathbf{C}}$  can also be written as

$$\hat{\mathbf{C}} = \begin{bmatrix} \hat{\mathbf{C}}_{11} & \hat{\mathbf{C}}'_{21} \\ \hat{\mathbf{C}}_{21} & \hat{\mathbf{C}}_{22} \end{bmatrix}$$

where

$$\hat{\mathbf{C}}_{11} = (\mathbf{X}'\hat{\mathbf{V}}^{-1}\mathbf{X})^{-}$$

$$\hat{\mathbf{C}}_{21} = -\hat{\mathbf{G}}\mathbf{Z}'\hat{\mathbf{V}}^{-1}\mathbf{X}\hat{\mathbf{C}}_{11}$$

$$\hat{\mathbf{C}}_{22} = (\mathbf{Z}'\hat{\mathbf{R}}^{-1}\mathbf{Z} + \hat{\mathbf{G}}^{-1})^{-1} - \hat{\mathbf{C}}_{21}\mathbf{X}'\hat{\mathbf{V}}^{-1}\mathbf{Z}\hat{\mathbf{G}}$$

Note that  $\hat{\mathbf{C}}_{11}$  is the familiar estimated generalized least squares formula for the variance-covariance matrix of  $\hat{\boldsymbol{\beta}}$ .

As a cautionary note,  $\hat{\mathbf{C}}$  tends to underestimate the true sampling variability of  $(\hat{\boldsymbol{\beta}}, \hat{\boldsymbol{\gamma}})$  because no account is made for the uncertainty in estimating  $\mathbf{G}$  and  $\mathbf{R}$ . Although inflation factors have been proposed (Kackar and Harville 1984; Kass and Steffey 1989; Prasad and Rao 1990), they tend to be small for data sets that are fairly well balanced. PROC MIXED does not compute any inflation factors by default, but rather accounts for the downward bias by using the approximate  $t$  and  $F$  statistics described subsequently. The `DDFM=KENWARDROGER` option in the `MODEL` statement prompts PROC MIXED to compute a specific inflation factor along with Satterthwaite-based degrees of freedom.

## Inference and Test Statistics

For inferences concerning the covariance parameters in your model, you can use likelihood-based statistics. One common likelihood-based statistic is the *Wald Z*, which is computed as the parameter estimate divided by its asymptotic standard error. The asymptotic standard errors are computed from the inverse of the second derivative matrix of the likelihood with respect to each of the covariance parameters. The *Wald Z* is valid for large samples, but it can be unreliable for small data sets and for parameters such as variance components, which are known to have a skewed or bounded sampling distribution.

A better alternative is the likelihood ratio  $\chi^2$  statistic. This statistic compares two covariance models, one a special case of the other. To compute it, you must run PROC MIXED twice, once for each of the two models, and then subtract the corresponding values of  $-2$  times the log likelihoods. You can use either ML or REML to construct this statistic, which tests whether the full model is necessary beyond the reduced model.

As long as the reduced model does not occur on the boundary of the covariance parameter space, the  $\chi^2$  statistic computed in this fashion has a large-sample  $\chi^2$  distribution that is  $\chi^2$  with degrees of freedom equal to the difference in the number of covariance parameters between the two models. If the reduced model does occur on the boundary of the covariance parameter space, the asymptotic distribution becomes a mixture of  $\chi^2$  distributions (Self and Liang 1987). A common example of this is when you are testing that a variance component equals its lower boundary constraint of 0.

A final possibility for obtaining inferences concerning the covariance parameters is to simulate or resample data from your model and construct empirical sampling distributions of the parameters. The SAS macro language and the ODS system are useful tools in this regard.

### *F* and *t* Tests for Fixed- and Random-Effects Parameters

For inferences concerning the fixed- and random-effects parameters in the mixed model, consider estimable linear combinations of the following form:

$$\mathbf{L} \begin{bmatrix} \boldsymbol{\beta} \\ \boldsymbol{\gamma} \end{bmatrix}$$

The estimability requirement (Searle 1971) applies only to the  $\boldsymbol{\beta}$  portion of  $\mathbf{L}$ , because any linear combination of  $\boldsymbol{\gamma}$  is estimable. Such a formulation in terms of a general  $\mathbf{L}$  matrix encompasses a wide variety of common inferential procedures such as those employed with Type 1–Type 3 tests and LS-means. The **CONTRAST** and **ESTIMATE** statements in PROC MIXED enable you to specify your own  $\mathbf{L}$  matrices. Typically, inference on fixed effects is the focus, and, in this case, the  $\boldsymbol{\gamma}$  portion of  $\mathbf{L}$  is assumed to contain all 0s.

Statistical inferences are obtained by testing the hypothesis

$$H : \mathbf{L} \begin{bmatrix} \boldsymbol{\beta} \\ \boldsymbol{\gamma} \end{bmatrix} = 0$$

or by constructing point and interval estimates.

When  $\mathbf{L}$  consists of a single row, a general *t* statistic can be constructed as follows (see McLean and Sanders 1988; Stroup 1989a):

$$t = \frac{\mathbf{L} \begin{bmatrix} \hat{\boldsymbol{\beta}} \\ \hat{\boldsymbol{\gamma}} \end{bmatrix}}{\sqrt{\mathbf{L}\widehat{\mathbf{C}}\mathbf{L}'}}$$

Under the assumed normality of  $\boldsymbol{\gamma}$  and  $\boldsymbol{\epsilon}$ ,  $t$  has an exact  $t$  distribution only for data exhibiting certain types of balance and for some special unbalanced cases. In general,  $t$  is only approximately  $t$ -distributed, and its degrees of freedom must be estimated. See the `DDFM=` option for a description of the various degrees-of-freedom methods available in PROC MIXED.

With  $\hat{\nu}$  being the approximate degrees of freedom, the associated confidence interval is

$$\mathbf{L} \begin{bmatrix} \hat{\boldsymbol{\beta}} \\ \hat{\boldsymbol{\gamma}} \end{bmatrix} \pm t_{\hat{\nu}, \alpha/2} \sqrt{\mathbf{L}\hat{\mathbf{C}}\mathbf{L}'}$$

where  $t_{\hat{\nu}, \alpha/2}$  is the  $(1 - \alpha/2)100$  percentile of the  $t_{\hat{\nu}}$  distribution.

When the rank of  $\mathbf{L}$  is greater than 1, PROC MIXED constructs the following general  $F$  statistic:

$$F = \frac{\begin{bmatrix} \hat{\boldsymbol{\beta}} \\ \hat{\boldsymbol{\gamma}} \end{bmatrix}' \mathbf{L}'(\mathbf{L}\hat{\mathbf{C}}\mathbf{L}')^{-1} \mathbf{L} \begin{bmatrix} \hat{\boldsymbol{\beta}} \\ \hat{\boldsymbol{\gamma}} \end{bmatrix}}{r}$$

where  $r = \text{rank}(\mathbf{L}\hat{\mathbf{C}}\mathbf{L}')$ . Analogous to  $t$ ,  $F$  in general has an approximate  $F$  distribution with  $r$  numerator degrees of freedom and  $\hat{\nu}$  denominator degrees of freedom.

The  $t$  and  $F$  statistics enable you to make inferences about your fixed effects, which account for the variance-covariance model you select. An alternative is the  $\chi^2$  statistic associated with the likelihood ratio test. This statistic compares two fixed-effects models, one a special case of the other. It is computed just as when comparing different covariance models, although you should use ML and not REML here because the penalty term associated with restricted likelihoods depends upon the fixed-effects specification.

### ***F Tests With the ANOVAF Option***

The ANOVAF option computes  $F$  tests by the following method in models with `REPEATED` statement and without `RANDOM` statement. Let  $\mathbf{L}$  denote the matrix of estimable functions for the hypothesis  $H: \mathbf{L}\boldsymbol{\beta} = \mathbf{0}$ , where  $\boldsymbol{\beta}$  are the fixed-effects parameters. Let  $\mathbf{M} = \mathbf{L}'(\mathbf{L}\mathbf{L}')^{-1}\mathbf{L}$ , and suppose that  $\hat{\mathbf{C}}$  denotes the estimated variance-covariance matrix of  $\hat{\boldsymbol{\beta}}$  (see the section “Statistical Properties” for the construction of  $\hat{\mathbf{C}}$ ).

The ANOVAF  $F$  statistics are computed as

$$F_A = \hat{\boldsymbol{\beta}}' \mathbf{L}' (\mathbf{L}\mathbf{L}')^{-1} \mathbf{L} \hat{\boldsymbol{\beta}} / t_1 = \hat{\boldsymbol{\beta}}' \mathbf{M} \hat{\boldsymbol{\beta}} / t_1$$

Notice that this is a modification of the usual  $F$  statistic where  $(\mathbf{L}\hat{\mathbf{C}}\mathbf{L}')^{-1}$  is replaced with  $(\mathbf{L}\mathbf{L}')^{-1}$  and  $\text{rank}(\mathbf{L})$  is replaced with  $t_1 = \text{trace}(\mathbf{M}\hat{\mathbf{C}})$ ; see, for example, Brunner, Domhof, and Langer (2002, Sec. 5.4). The  $p$ -values for this statistic are computed from either an  $F_{v_1, v_2}$  or an  $F_{v_1, \infty}$  distribution. The respective degrees of freedom are determined by the MIXED procedure as follows:

$$v_1 = \frac{t_1^2}{\text{trace}(\mathbf{M}\hat{\mathbf{C}}\mathbf{M})}$$

$$v_2^* = \frac{2t_1^2}{\mathbf{g}'\mathbf{A}\mathbf{g}}$$

$$v_2 = \begin{cases} \max\{\min\{v_2^*, df_e\}, 1\} & \mathbf{g}'\mathbf{A}\mathbf{g} > 1\text{E}3 \times \text{MACEPS} \\ 1 & \text{otherwise} \end{cases}$$

The term  $\mathbf{g}'\mathbf{A}\mathbf{g}$  in the term  $\nu_2^*$  for the denominator degrees of freedom is based on approximating  $\text{Var}[\text{trace}(\widehat{\mathbf{M}\mathbf{C}})]$  based on a first-order Taylor series about the true covariance parameters. This generalizes results in the appendix of Brunner, Dette, and Munk (1997) to a broader class of models. The vector  $\mathbf{g} = [g_1, \dots, g_q]$  contains the partial derivatives

$$\text{trace} \left( \mathbf{L}' (\mathbf{L}\mathbf{L}')^{-1} \mathbf{L} \frac{\partial \widehat{\mathbf{C}}}{\partial \theta_i} \right)$$

and  $\mathbf{A}$  is the asymptotic variance-covariance matrix of the covariance parameter estimates (`ASYCOV` option).

PROC MIXED reports  $\nu_1$  and  $\nu_2$  as “NumDF” and “DenDF” under the “ANOVA F” heading in the output. The corresponding  $p$ -values are denoted as “Pr > F(DDF)” for  $F_{\nu_1, \nu_2}$  and “Pr > F(infty)” for  $F_{\nu_1, \infty}$ , respectively.

$P$ -values computed with the ANOVAF option can be identical to the nonparametric tests in Akritas, Arnold, and Brunner (1997) and in Brunner, Domhof, and Langer (2002), provided that the response data consist of properly created (and sorted) ranks and that the covariance parameters are estimated by MIVQUE0 in models with `REPEATED` statement and properly chosen `SUBJECT=` and/or `GROUP=` effects.

If you model an unstructured covariance matrix in a longitudinal model with one or more repeated factors, the ANOVAF results are identical to a multivariate MANOVA where degrees of freedom are corrected with the Greenhouse-Geisser adjustment (Greenhouse and Geisser 1959). For example, suppose that factor A has 2 levels and factor B has 4 levels. The following two sets of statements produce the same  $p$ -values:

```
proc mixed data=Mydata anovaf method=mivque0;
 class id A B;
 model score = A | B / chisq;
 repeated / type=un subject=id;
 ods select Tests3;
run;

proc transpose data=MyData out=tdata;
 by id;
 var score;
run;
proc glm data=tdata;
 model col: = / nouni;
 repeated A 2, B 4;
 ods output ModelANOVA=maov epsilons=eps;
run;
proc transpose data=eps(where=(substr(statistic,1,3)='Gre')) out=teps;
 var cvalue1;
run;

data aov; set maov;
 if (_n_ = 1) then merge teps;
 if (Source='A') then do;
 pFddf = ProbF;
 pFinf = 1 - probchi(df*Fvalue,df);
 output;
 end; else if (Source='B') then do;
 pFddf = ProbFGG;
```

```

 pFinf = 1 - probchi(df*col1*Fvalue,df*col1);
 output;
 end; else if (Source='A*B') then do;
 pfddf = ProbFGG;
 pFinf = 1 - probchi(df*col2*Fvalue,df*col2);
 output;
 end;
run;
proc print data=aov label noobs;
 label Source = 'Effect'
 df = 'NumDF'
 Fvalue = 'Value'
 pFddf = 'Pr > F(DDF)'
 pFinf = 'Pr > F(infty)';
 var Source df Fvalue pFddf pFinf;
 format pF: pvalue6.;
run;

```

The PROC GLM code produces  $p$ -values that correspond to the ANOVA  $p$ -values shown as Pr > F(DDF) in the MIXED output. The subsequent DATA step computes the  $p$ -values that correspond to Pr > F(infty) in the PROC MIXED output.

---

## Parameterization of Mixed Models

Recall that a mixed model is of the form

$$y = X\beta + Z\gamma + \epsilon$$

where  $y$  represents univariate data,  $\beta$  is an unknown vector of fixed effects with known model matrix  $X$ ,  $\gamma$  is an unknown vector of random effects with known model matrix  $Z$ , and  $\epsilon$  is an unknown random error vector.

PROC MIXED constructs a mixed model according to the specifications in the **MODEL**, **RANDOM**, and **REPEATED** statements. Each effect in the **MODEL** statement generates one or more columns in the model matrix  $X$ , and each effect in the **RANDOM** statement generates one or more columns in the model matrix  $Z$ . Effects in the **REPEATED** statement do not generate model matrices; they serve only to index observations within subjects. This section shows precisely how PROC MIXED builds  $X$  and  $Z$ .

### Intercept

By default, all models automatically include a column of 1s in  $X$  to estimate a fixed-effect intercept parameter  $\mu$ . You can use the **NOINT** option in the **MODEL** statement to suppress this intercept. The **NOINT** option is useful when you are specifying a classification effect in the **MODEL** statement and you want the parameter estimate to be in terms of the mean response for each level of that effect, rather than in terms of a deviation from an overall mean.

By contrast, the intercept is not included by default in  $Z$ . To obtain a column of 1s in  $Z$ , you must specify in the **RANDOM** statement either the **INTERCEPT** effect or some effect that has only one level.

## Regression Effects

Numeric variables, or polynomial terms involving them, can be included in the model as regression effects (covariates). The actual values of such terms are included as columns of the model matrices **X** and **Z**. You can use the bar operator with a regression effect to generate polynomial effects. For instance,  $X|X|X$  expands to  $X$   $X*X$   $X*X*X$ , a cubic model.

## Main Effects

If a classification variable has  $m$  levels, PROC MIXED generates  $m$  columns in the model matrix for its main effect. Each column is an indicator variable for a given level. The order of the columns is the sort order of the values of their levels and can be controlled with the **ORDER=** option in the PROC MIXED statement. Table 59.20 is an example.

**Table 59.20** Example of Main Effects

| Data |   | I     | A  |    | B  |    |    |
|------|---|-------|----|----|----|----|----|
| A    | B | $\mu$ | A1 | A2 | B1 | B2 | B3 |
| 1    | 1 | 1     | 1  | 0  | 1  | 0  | 0  |
| 1    | 2 | 1     | 1  | 0  | 0  | 1  | 0  |
| 1    | 3 | 1     | 1  | 0  | 0  | 0  | 1  |
| 2    | 1 | 1     | 0  | 1  | 1  | 0  | 0  |
| 2    | 2 | 1     | 0  | 1  | 0  | 1  | 0  |
| 2    | 3 | 1     | 0  | 1  | 0  | 0  | 1  |

Typically, there are more columns for these effects than there are degrees of freedom for them. In other words, PROC MIXED uses an overparameterized model.

## Interaction Effects

Often a model includes interaction (crossed) effects. With an interaction, PROC MIXED first reorders the terms to correspond to the order of the variables in the **CLASS** statement. Thus,  $B*A$  becomes  $A*B$  if **A** precedes **B** in the **CLASS** statement. Then, PROC MIXED generates columns for all combinations of levels that occur in the data. The order of the columns is such that the rightmost variables in the cross index faster than the leftmost variables (Table 59.21). Empty columns (that would contain all 0s) are not generated for **X**, but they are for **Z**.

**Table 59.21** Example of Interaction Effects

| Data |   | I     | A  |    | B  |    |    | A*B  |      |      |      |      |      |
|------|---|-------|----|----|----|----|----|------|------|------|------|------|------|
| A    | B | $\mu$ | A1 | A2 | B1 | B2 | B3 | A1B1 | A1B2 | A1B3 | A2B1 | A2B2 | A2B3 |
| 1    | 1 | 1     | 1  | 0  | 1  | 0  | 0  | 1    | 0    | 0    | 0    | 0    | 0    |
| 1    | 2 | 1     | 1  | 0  | 0  | 1  | 0  | 0    | 1    | 0    | 0    | 0    | 0    |
| 1    | 3 | 1     | 1  | 0  | 0  | 0  | 1  | 0    | 0    | 1    | 0    | 0    | 0    |
| 2    | 1 | 1     | 0  | 1  | 1  | 0  | 0  | 0    | 0    | 0    | 1    | 0    | 0    |
| 2    | 2 | 1     | 0  | 1  | 0  | 1  | 0  | 0    | 0    | 0    | 0    | 1    | 0    |
| 2    | 3 | 1     | 0  | 1  | 0  | 0  | 1  | 0    | 0    | 0    | 0    | 0    | 1    |

In the preceding matrix, main-effects columns are not linearly independent of crossed-effects columns; in fact, the column space for the crossed effects contains the space of the main effect.

When your model contains many interaction effects, you might be able to code them more parsimoniously by using the bar operator ( | ). The bar operator generates all possible interaction effects. For example, A|B|C expands to A B A\*B C A\*C B\*C A\*B\*C. To eliminate higher-order interaction effects, use the at sign (@) in conjunction with the bar operator. For instance, A|B|C|D @2 expands to A B A\*B C A\*C B\*C D A\*D B\*D C\*D.

### Nested Effects

Nested effects are generated in the same manner as crossed effects. Hence, the design columns generated by the following two statements are the same (but the ordering of the columns is different):

```
model Y=A B(A);
```

```
model Y=A A*B;
```

The nesting operator in PROC MIXED is more a notational convenience than an operation distinct from crossing. Nested effects are typically characterized by the property that the nested variables never appear as main effects. The order of the variables within nesting parentheses is made to correspond to the order of these variables in the CLASS statement. The order of the columns is such that variables outside the parentheses index faster than those inside the parentheses, and the rightmost nested variables index faster than the leftmost variables (Table 59.22).

**Table 59.22** Example of Nested Effects

| Data |   | I     | A  |    | B(A) |      |      |      |      |      |
|------|---|-------|----|----|------|------|------|------|------|------|
| A    | B | $\mu$ | A1 | A2 | B1A1 | B2A1 | B3A1 | B1A2 | B2A2 | B3A2 |
| 1    | 1 | 1     | 1  | 0  | 1    | 0    | 0    | 0    | 0    | 0    |
| 1    | 2 | 1     | 1  | 0  | 0    | 1    | 0    | 0    | 0    | 0    |
| 1    | 3 | 1     | 1  | 0  | 0    | 0    | 1    | 0    | 0    | 0    |
| 2    | 1 | 1     | 0  | 1  | 0    | 0    | 0    | 1    | 0    | 0    |
| 2    | 2 | 1     | 0  | 1  | 0    | 0    | 0    | 0    | 1    | 0    |
| 2    | 3 | 1     | 0  | 1  | 0    | 0    | 0    | 0    | 0    | 1    |

Note that nested effects are often distinguished from interaction effects by the implied randomization structure of the design. That is, they usually indicate random effects within a fixed-effects framework. The fact that random effects can be modeled directly in the RANDOM statement might make the specification of nested effects in the MODEL statement unnecessary.

### Continuous-Nesting-Class Effects

When a continuous variable nests with a classification variable, the design columns are constructed by multiplying the continuous values into the design columns for the class effect (Table 59.23).



**Table 59.23** Example of Continuous-Nesting-Class Effects

| Data |   | I     | A  |    | X(A)  |       |
|------|---|-------|----|----|-------|-------|
| X    | A | $\mu$ | A1 | A2 | X(A1) | X(A2) |
| 21   | 1 | 1     | 1  | 0  | 21    | 0     |
| 24   | 1 | 1     | 1  | 0  | 24    | 0     |
| 22   | 1 | 1     | 1  | 0  | 22    | 0     |
| 28   | 2 | 1     | 0  | 1  | 0     | 28    |
| 19   | 2 | 1     | 0  | 1  | 0     | 19    |
| 23   | 2 | 1     | 0  | 1  | 0     | 23    |

This model estimates a separate slope for X within each level of A.

### Continuous-by-Class Effects

Continuous-by-class effects generate the same design columns as continuous-nesting-class effects. The two models are made different by the presence of the continuous variable as a regressor by itself, as well as a contributor to a compound effect. Table 59.24 shows an example.

**Table 59.24** Example of Continuous-by-Class Effects

| Data |   | I     | X  | A  |    | X*A  |      |
|------|---|-------|----|----|----|------|------|
| X    | A | $\mu$ | X  | A1 | A2 | X*A1 | X*A2 |
| 21   | 1 | 1     | 21 | 1  | 0  | 21   | 0    |
| 24   | 1 | 1     | 24 | 1  | 0  | 24   | 0    |
| 22   | 1 | 1     | 22 | 1  | 0  | 22   | 0    |
| 28   | 2 | 1     | 28 | 0  | 1  | 0    | 28   |
| 19   | 2 | 1     | 19 | 0  | 1  | 0    | 19   |
| 23   | 2 | 1     | 23 | 0  | 1  | 0    | 23   |

You can use continuous-by-class effects to test for homogeneity of slopes.

### General Effects

An example that combines all the effects is  $X1*X2*A*B*C$  (D E). The continuous list comes first, followed by the crossed list, followed by the nested list in parentheses. You should be aware of the sequencing of parameters when you use the **CONTRAST** or **ESTIMATE** statement to compute some function of the parameter estimates.

Effects might be renamed by PROC MIXED to correspond to ordering rules. For example,  $B*A(E D)$  might be renamed  $A*B(D E)$  to satisfy the following:

- Classification variables that occur outside parentheses (crossed effects) are sorted in the order in which they appear in the **CLASS** statement.
- Variables within parentheses (nested effects) are sorted in the order in which they appear in the **CLASS** statement.

The sequencing of the parameters generated by an effect can be described by which variables have their levels indexed faster:

- Variables in the crossed list index faster than variables in the nested list.
- Within a crossed or nested list, variables to the right index faster than variables to the left.

For example, suppose a model includes four effects—A, B, C, and D—each having two levels, 1 and 2. Suppose the **CLASS** statement is as follows:

```
class A B C D;
```

Then the order of the parameters for the effect B\*A(C D), which is renamed A\*B (C D), is

$$\begin{aligned} A_1 B_1 C_1 D_1 &\rightarrow A_1 B_2 C_1 D_1 \rightarrow A_2 B_1 C_1 D_1 \rightarrow A_2 B_2 C_1 D_1 \rightarrow \\ A_1 B_1 C_1 D_2 &\rightarrow A_1 B_2 C_1 D_2 \rightarrow A_2 B_1 C_1 D_2 \rightarrow A_2 B_2 C_1 D_2 \rightarrow \\ A_1 B_1 C_2 D_1 &\rightarrow A_1 B_2 C_2 D_1 \rightarrow A_2 B_1 C_2 D_1 \rightarrow A_2 B_2 C_2 D_1 \rightarrow \\ A_1 B_1 C_2 D_2 &\rightarrow A_1 B_2 C_2 D_2 \rightarrow A_2 B_1 C_2 D_2 \rightarrow A_2 B_2 C_2 D_2 \end{aligned}$$

Note that first the crossed effects B and A are sorted in the order in which they appear in the **CLASS** statement so that A precedes B in the parameter list. Then, for each combination of the nested effects in turn, combinations of A and B appear. The B effect moves fastest because it is rightmost in the cross list. Then A moves next fastest, and D moves next fastest. The C effect is the slowest since it is leftmost in the nested list.

When numeric levels are used, levels are sorted by their character format, which might not correspond to their numeric sort sequence (for example, noninteger levels). Therefore, it is advisable to include a desired format for numeric levels or to use the **ORDER=INTERNAL** option in the **PROC MIXED** statement to ensure that levels are sorted by their internal values.

### Implications of the Non-Full-Rank Parameterization

For models with fixed effects involving classification variables, there are more design columns in **X** constructed than there are degrees of freedom for the effect. Thus, there are linear dependencies among the columns of **X**. In this event, all of the parameters are not estimable; there is an infinite number of solutions to the mixed model equations. **PROC MIXED** uses a generalized inverse (a  $g_2$ -inverse, Pringle and Rayner 1971) to obtain values for the estimates (Searle 1971). The solution values are not displayed unless you specify the **SOLUTION** option in the **MODEL** statement. The solution has the characteristic that estimates are 0 whenever the design column for that parameter is a linear combination of previous columns. With this parameterization, hypothesis tests are constructed to test linear functions of the parameters that are estimable.

Some procedures (such as the **CATMOD** procedure) reparameterize models to full rank by using restrictions on the parameters. **PROC GLM** and **PROC MIXED** do not reparameterize, making the hypotheses that are commonly tested more understandable. See Goodnight (1978) for additional reasons for not reparameterizing.

## Missing Level Combinations

PROC MIXED handles missing level combinations of classification variables similarly to the way PROC GLM does. Both procedures delete fixed-effects parameters corresponding to missing levels in order to preserve estimability. However, PROC MIXED does not delete missing level combinations for random-effects parameters because linear combinations of the random-effects parameters are always estimable. These conventions can affect the way you specify your **CONTRAST** and **ESTIMATE** coefficients.

---

## Residuals and Influence Diagnostics

### Residual Diagnostics

Consider a residual vector of the form  $\tilde{\mathbf{e}} = \mathbf{P}\mathbf{Y}$ , where  $\mathbf{P}$  is a projection matrix, possibly an oblique projector. A typical element  $\tilde{e}_i$  with variance  $v_i$  and estimated variance  $\hat{v}_i$  is said to be *standardized* as

$$\frac{\tilde{e}_i}{\sqrt{\text{Var}[\tilde{e}_i]}} = \frac{\tilde{e}_i}{\sqrt{v_i}}$$

and *studentized* as

$$\frac{\tilde{e}_i}{\sqrt{\hat{v}_i}}$$

External studentization uses an estimate of  $\text{Var}[\tilde{e}_i]$  that does not involve the  $i$ th observation. Externally studentized residuals are often preferred over internally studentized residuals because they have well-known distributional properties in standard linear models for independent data.

Residuals that are scaled by the estimated variance of the response, i.e.,  $\tilde{e}_i / \sqrt{\widehat{\text{Var}}[Y_i]}$ , are referred to as Pearson-type residuals.

### Marginal and Conditional Residuals

The marginal and conditional means in the linear mixed model are  $E[\mathbf{Y}] = \mathbf{X}\boldsymbol{\beta}$  and  $E[\mathbf{Y}|\boldsymbol{\gamma}] = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\boldsymbol{\gamma}$ , respectively. Accordingly, the vector  $\mathbf{r}_m$  of marginal residuals is defined as

$$\mathbf{r}_m = \mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}}$$

and the vector  $\mathbf{r}_c$  of conditional residuals is

$$\mathbf{r}_c = \mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}} - \mathbf{Z}\hat{\boldsymbol{\gamma}} = \mathbf{r}_m - \mathbf{Z}\hat{\boldsymbol{\gamma}}$$

Following Gregoire, Schabenberger, and Barrett (1995), let  $\mathbf{Q} = \mathbf{X}(\mathbf{X}'\hat{\mathbf{V}}^{-1}\mathbf{X})^{-1}\mathbf{X}'$  and  $\mathbf{K} = \mathbf{I} - \mathbf{Z}\hat{\mathbf{G}}\mathbf{Z}'\hat{\mathbf{V}}^{-1}$ . Then

$$\widehat{\text{Var}}[\mathbf{r}_m] = \hat{\mathbf{V}} - \mathbf{Q}$$

$$\widehat{\text{Var}}[\mathbf{r}_c] = \mathbf{K}(\hat{\mathbf{V}} - \mathbf{Q})\mathbf{K}'$$

For an individual observation the raw, studentized, and Pearson-type residuals computed by the MIXED procedure are given in Table 59.25.

**Table 59.25** Residual Types Computed by the MIXED Procedure

| Type of Residual | Marginal                                                                | Conditional                                                                                |
|------------------|-------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| Raw              | $r_{mi} = Y_i - \mathbf{x}'_i \hat{\boldsymbol{\beta}}$                 | $r_{ci} = r_{mi} - \mathbf{z}'_i \hat{\boldsymbol{\gamma}}$                                |
| Studentized      | $r_{mi}^{student} = \frac{r_{mi}}{\sqrt{\widehat{\text{Var}}[r_{mi}]}}$ | $r_{ci}^{student} = \frac{r_{ci}}{\sqrt{\widehat{\text{Var}}[r_{ci}]}}$                    |
| Pearson          | $r_{mi}^{pearson} = \frac{r_{mi}}{\sqrt{\widehat{\text{Var}}[Y_i]}}$    | $r_{ci}^{pearson} = \frac{r_{ci}}{\sqrt{\widehat{\text{Var}}[Y_i   \boldsymbol{\gamma}]}}$ |

When the **OUTPM=** option is specified in addition to the **RESIDUAL** option in the **MODEL** statement,  $r_{mi}^{student}$  and  $r_{mi}^{pearson}$  are added to the data set as variables **Resid**, **StudentResid**, and **PearsonResid**, respectively. When the **OUTP=** option is specified,  $r_{ci}^{student}$  and  $r_{ci}^{pearson}$  are added to the data set. Raw residuals are part of the **OUTPM=** and **OUTP=** data sets without the **RESIDUAL** option.

### Scaled Residuals

For correlated data, a set of scaled quantities can be defined through the Cholesky decomposition of the variance-covariance matrix. Since fitted residuals in linear models are rank-deficient, it is customary to draw on the variance-covariance matrix of the data. If  $\text{Var}[\mathbf{Y}] = \mathbf{V}$  and  $\mathbf{C}'\mathbf{C} = \mathbf{V}$ , then  $\mathbf{C}'^{-1}\mathbf{Y}$  has uniform dispersion and its elements are uncorrelated.

Scaled residuals in a mixed model are meaningful for quantities based on the marginal distribution of the data. Let  $\hat{\mathbf{C}}$  denote the Cholesky root of  $\hat{\mathbf{V}}$ , so that  $\hat{\mathbf{C}}'\hat{\mathbf{C}} = \hat{\mathbf{V}}$ , and define

$$\mathbf{Y}_c = \hat{\mathbf{C}}'^{-1}\mathbf{Y}$$

$$\mathbf{r}_{m(c)} = \hat{\mathbf{C}}'^{-1}\mathbf{r}_m$$

By analogy with other scalings, the inverse Cholesky decomposition can also be applied to the residual vector,  $\hat{\mathbf{C}}'^{-1}\mathbf{r}_m$ , although  $\mathbf{V}$  is not the variance-covariance matrix of  $\mathbf{r}_m$ .

To diagnose whether the covariance structure of the model has been specified correctly can be difficult based on  $\mathbf{Y}_c$ , since the inverse Cholesky transformation affects the expected value of  $\mathbf{Y}_c$ . You can draw on  $\mathbf{r}_{m(c)}$  as a vector of (approximately) uncorrelated data with constant mean.

When the **OUTPM=** option in the **MODEL** statement is specified in addition to the **VCIRY** option,  $\mathbf{Y}_c$  is added as variable **ScaledDep** and  $\mathbf{r}_{m(c)}$  is added as **ScaledResid** to the data set.

## Influence Diagnostics

### Basic Idea and Statistics

The general idea of quantifying the influence of one or more observations relies on computing parameter estimates based on all data points, removing the cases in question from the data, refitting the model, and computing statistics based on the change between full-data and reduced-data estimation. Influence statistics can be coarsely grouped by the aspect of estimation that is their primary target:

- overall measures compare changes in objective functions: (restricted) likelihood distance (Cook and Weisberg 1982, Ch. 5.2)
- influence on parameter estimates: Cook's  $D$  (Cook 1977, 1979), MDFFITS (Belsley, Kuh, and Welsch 1980, p. 32)

- influence on precision of estimates: CovRatio and CovTrace
- influence on fitted and predicted values: PRESS residual, PRESS statistic (Allen 1974), DFFITS (Belsley, Kuh, and Welsch 1980, p. 15)
- outlier properties: internally and externally studentized residuals, leverage

For linear models for uncorrelated data, it is not necessary to refit the model after removing a data point in order to measure the impact of an observation on the model. The change in fixed effect estimates, residuals, residual sums of squares, and the variance-covariance matrix of the fixed effects can be computed based on the fit to the full data alone. By contrast, in mixed models several important complications arise. Data points can affect not only the fixed effects but also the covariance parameter estimates on which the fixed-effects estimates depend. Furthermore, closed-form expressions for computing the change in important model quantities might not be available.

This section provides background material for the various influence diagnostics available with the MIXED procedure. See the section “[Mixed Models Theory](#)” on page 4958 for relevant expressions and definitions. The parameter vector  $\theta$  denotes all unknown parameters in the  $\mathbf{R}$  and  $\mathbf{G}$  matrix.

The observations whose influence is being ascertained are represented by the set  $U$  and referred to simply as “the observations in  $U$ .” The estimate of a parameter vector, such as  $\beta$ , obtained from all observations except those in the set  $U$  is denoted  $\hat{\beta}_{(U)}$ . In case of a matrix  $\mathbf{A}$ , the notation  $\mathbf{A}_{(U)}$  represents the matrix with the rows in  $U$  removed; these rows are collected in  $\mathbf{A}_U$ . If  $\mathbf{A}$  is symmetric, then notation  $\mathbf{A}_{(U)}$  implies removal of rows and columns. The vector  $Y_U$  comprises the responses of the data points being removed, and  $\mathbf{V}_{(U)}$  is the variance-covariance matrix of the remaining observations. When  $k = 1$ , lowercase notation emphasizes that single points are removed, such as  $\mathbf{A}_{(u)}$ .

### Managing the Covariance Parameters

An important component of influence diagnostics in the mixed model is the estimated variance-covariance matrix  $\mathbf{V} = \mathbf{ZGZ}' + \mathbf{R}$ . To make the dependence on the vector of covariance parameters explicit, write it as  $\mathbf{V}(\theta)$ . If one parameter,  $\sigma^2$ , is profiled or factored out of  $\mathbf{V}$ , the remaining parameters are denoted as  $\theta^*$ . Notice that in a model where  $\mathbf{G}$  is diagonal and  $\mathbf{R} = \sigma^2\mathbf{I}$ , the parameter vector  $\theta^*$  contains the ratios of each variance component and  $\sigma^2$  (see Wolfinger, Tobias, and Sall 1994). When ITER=0, two scenarios are distinguished:

1. If the residual variance is not profiled, either because the model does not contain a residual variance or because it is part of the Newton-Raphson iterations, then  $\hat{\theta}_{(U)} \equiv \hat{\theta}$ .
2. If the residual variance is profiled, then  $\hat{\theta}_{(U)}^* \equiv \hat{\theta}^*$  and  $\hat{\sigma}_{(U)}^2 \neq \hat{\sigma}^2$ . Influence statistics such as Cook’s  $D$  and internally studentized residuals are based on  $\mathbf{V}(\hat{\theta})$ , whereas externally studentized residuals and the DFFITS statistic are based on  $\mathbf{V}(\hat{\theta}_{(U)}) = \sigma_{(U)}^2 \mathbf{V}(\hat{\theta}^*)$ . In a random components model with uncorrelated errors, for example, the computation of  $\mathbf{V}(\hat{\theta}_{(U)})$  involves scaling of  $\hat{\mathbf{G}}$  and  $\hat{\mathbf{R}}$  by the full-data estimate  $\hat{\sigma}^2$  and multiplying the result with the reduced-data estimate  $\hat{\sigma}_{(U)}^2$ .

Certain statistics, such as MDFFITS, CovRatio, and CovTrace, require an estimate of the variance of the fixed effects that is based on the reduced number of observations. For example,  $\mathbf{V}(\hat{\theta}_{(U)})$  is evaluated at the reduced-data parameter estimates but computed for the entire data set. The matrix  $\mathbf{V}_{(U)}(\hat{\theta}_{(U)})$ , on the other hand, has rows and columns corresponding to the points in  $U$  removed. The resulting matrix is evaluated at the delete-case estimates.

When influence analysis is iterative, the entire vector  $\boldsymbol{\theta}$  is updated, whether the residual variance is profiled or not. The matrices to be distinguished here are  $\mathbf{V}(\hat{\boldsymbol{\theta}})$ ,  $\mathbf{V}(\hat{\boldsymbol{\theta}}_{(U)})$ , and  $\mathbf{V}_{(U)}(\hat{\boldsymbol{\theta}}_{(U)})$ , with unambiguous notation.

### **Predicted Values, PRESS Residual, and PRESS Statistic**

An unconditional predicted value is  $\hat{y}_i = \mathbf{x}_i' \hat{\boldsymbol{\beta}}$ , where the vector  $\mathbf{x}_i$  is the  $i$ th row of  $\mathbf{X}$ . The (raw) residual is given as  $\hat{\epsilon}_i = y_i - \hat{y}_i$ , and the PRESS residual is

$$\hat{\epsilon}_{i(U)} = y_i - \mathbf{x}_i' \hat{\boldsymbol{\beta}}_{(U)}$$

The PRESS statistic is the sum of the squared PRESS residuals,

$$PRESS = \sum_{i \in U} \hat{\epsilon}_{i(U)}^2$$

where the sum is over the observations in  $U$ .

If **EFFECT=**, **SIZE=**, or **KEEP=** is not specified, PROC MIXED computes the PRESS residual for each observation selected through **SELECT=** (or all observations if **SELECT=** is not given). If **EFFECT=**, **SIZE=**, or **KEEP=** is specified, the procedure computes PRESS.

### **Leverage**

For the general mixed model, leverage can be defined through the projection matrix that results from a transformation of the model with the inverse of the Cholesky decomposition of  $\mathbf{V}$ , or through an oblique projector. The MIXED procedure follows the latter path in the computation of influence diagnostics. The leverage value reported for the  $i$ th observation is the  $i$ th diagonal entry of the matrix

$$\mathbf{H} = \mathbf{X}(\mathbf{X}'\mathbf{V}(\hat{\boldsymbol{\theta}})^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}(\hat{\boldsymbol{\theta}})^{-1}$$

which is the weight of the observation in contributing to its own predicted value,  $\mathbf{H} = d\hat{\mathbf{Y}}/d\mathbf{Y}$ .

While  $\mathbf{H}$  is idempotent, it is generally not symmetric and thus not a projection matrix in the narrow sense.

The properties of these leverages are generalizations of the properties in models with diagonal variance-covariance matrices. For example,  $\hat{\mathbf{Y}} = \mathbf{H}\mathbf{Y}$ , and in a model with intercept and  $\mathbf{V} = \sigma^2\mathbf{I}$ , the leverage values

$$h_{ii} = \mathbf{x}_i'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{x}_i$$

are  $h_{ii}^l = 1/n \leq h_{ii} \leq 1 = h_{ii}^u$  and  $\sum_{i=1}^n h_{ii} = \text{rank}(\mathbf{X})$ . The lower bound for  $h_{ii}$  is achieved in an intercept-only model, and the upper bound is achieved in a saturated model. The trace of  $\mathbf{H}$  equals the rank of  $\mathbf{X}$ .

If  $v_{ij}$  denotes the element in row  $i$ , column  $j$  of  $\mathbf{V}^{-1}$ , then for a model containing only an intercept the diagonal elements of  $\mathbf{H}$  are

$$h_{ii} = \frac{\sum_{j=1}^n v_{ij}}{\sum_{i=1}^n \sum_{j=1}^n v_{ij}}$$

Because  $\sum_{j=1}^n v_{ij}$  is a sum of elements in the  $i$ th row of the inverse variance-covariance matrix,  $h_{ii}$  can be negative, even if the correlations among data points are nonnegative. In case of a saturated model with  $\mathbf{X} = \mathbf{I}$ ,  $h_{ii} = 1.0$ .

### Internally and Externally Studentized Residuals

See the section “Residual Diagnostics” on page 4976 for the distinction between standardization, studentization, and scaling of residuals. Internally studentized marginal and conditional residuals are computed with the **RESIDUAL** option of the **MODEL** statement. The **INFLUENCE** option computes internally and externally studentized marginal residuals.

The computation of internally studentized residuals relies on the diagonal entries of  $\mathbf{V}(\hat{\boldsymbol{\theta}}) - \mathbf{Q}(\hat{\boldsymbol{\theta}})$ , where  $\mathbf{Q}(\hat{\boldsymbol{\theta}}) = \mathbf{X}(\mathbf{X}'\mathbf{V}(\hat{\boldsymbol{\theta}})^{-1}\mathbf{X})^{-1}\mathbf{X}'$ . Externally studentized residuals require iterative influence analysis or a profiled residual variance. In the former case the studentization is based on  $\mathbf{V}(\hat{\boldsymbol{\theta}}_U)$ ; in the latter case it is based on  $\sigma_{(U)}^2 \mathbf{V}(\hat{\boldsymbol{\theta}}^*)$ .

### Cook's *D*

Cook's *D* statistic is an invariant norm that measures the influence of observations in  $U$  on a vector of parameter estimates (Cook 1977). In case of the fixed-effects coefficients, let

$$\boldsymbol{\delta}_{(U)} = \hat{\boldsymbol{\beta}} - \hat{\boldsymbol{\beta}}_{(U)}$$

Then the MIXED procedure computes

$$D(\boldsymbol{\beta}) = \boldsymbol{\delta}'_{(U)} \widehat{\text{Var}}[\hat{\boldsymbol{\beta}}]^{-} \boldsymbol{\delta}_{(U)} / \text{rank}(\mathbf{X})$$

where  $\widehat{\text{Var}}[\hat{\boldsymbol{\beta}}]^{-}$  is the matrix that results from sweeping  $(\mathbf{X}'\mathbf{V}(\hat{\boldsymbol{\theta}})^{-1}\mathbf{X})^{-}$ .

If  $\mathbf{V}$  is known, Cook's *D* can be calibrated according to a chi-square distribution with degrees of freedom equal to the rank of  $\mathbf{X}$  (Christensen, Pearson, and Johnson 1992). For estimated  $\mathbf{V}$  the calibration can be carried out according to an  $F(\text{rank}(\mathbf{X}), n - \text{rank}(\mathbf{X}))$  distribution. To interpret *D* on a familiar scale, Cook (1979) and Cook and Weisberg (1982, p. 116) refer to the 50th percentile of the reference distribution. If *D* is equal to that percentile, then removing the points in  $U$  moves the fixed-effects coefficient vector from the center of the confidence region to the 50% confidence ellipsoid (Myers 1990, p. 262).

In the case of iterative influence analysis, the MIXED procedure also computes a *D*-type statistic for the covariance parameters. If  $\boldsymbol{\Gamma}$  is the asymptotic variance-covariance matrix of  $\hat{\boldsymbol{\theta}}$ , then MIXED computes

$$D_{\boldsymbol{\theta}} = (\hat{\boldsymbol{\theta}} - \hat{\boldsymbol{\theta}}_{(U)})' \hat{\boldsymbol{\Gamma}}^{-1} (\hat{\boldsymbol{\theta}} - \hat{\boldsymbol{\theta}}_{(U)})$$

### DFFITS and MDFFITS

A DFFIT measures the change in predicted values due to removal of data points. If this change is standardized by the externally estimated standard error of the predicted value in the full data, the DFFITS statistic of Belsley, Kuh, and Welsch (1980, p. 15) results:

$$\text{DFFITS}_i = (\hat{y}_i - \hat{y}_{i(u)}) / \text{ese}(\hat{y}_i)$$

The MIXED procedure computes DFFITS when the **EFFECT=** or **SIZE=** modifier of the **INFLUENCE** option is not in effect. In general, an external estimate of the estimated standard error is used. When **ITER** > 0, the estimate is

$$\text{ese}(\hat{y}_i) = \sqrt{\mathbf{x}'_i (\mathbf{X}'\mathbf{V}(\hat{\boldsymbol{\theta}}_{(u)})^{-1}\mathbf{X})^{-1} \mathbf{x}_i}$$

When **ITER=0** and  $\sigma^2$  is profiled, then

$$\text{ese}(\hat{y}_i) = \hat{\sigma}_{(u)} \sqrt{\mathbf{x}'_i (\mathbf{X}'\mathbf{V}(\hat{\boldsymbol{\theta}}^*)^{-1}\mathbf{X})^{-1} \mathbf{x}_i}$$

When the **EFFECT=**, **SIZE=**, or **KEEP=** modifier is specified, the MIXED procedure computes a multivariate version suitable for the deletion of multiple data points. The statistic, termed MDFFITS after the MDFFIT statistic of Belsley, Kuh, and Welsch (1980, p. 32), is closely related to Cook's  $D$ . Consider the case  $\mathbf{V} = \sigma^2 \mathbf{V}(\boldsymbol{\theta}^*)$  so that

$$\text{Var}[\widehat{\boldsymbol{\beta}}] = \sigma^2 (\mathbf{X}' \mathbf{V}(\boldsymbol{\theta}^*)^{-1} \mathbf{X})^{-1}$$

and let  $\widetilde{\text{Var}}[\widehat{\boldsymbol{\beta}}_{(U)}]$  be an estimate of  $\text{Var}[\widehat{\boldsymbol{\beta}}_{(U)}]$  that does not use the observations in  $U$ . The MDFFITS statistic is then computed as

$$\text{MDFFITS}(\boldsymbol{\beta}) = \boldsymbol{\delta}'_{(U)} \widetilde{\text{Var}}[\widehat{\boldsymbol{\beta}}_{(U)}]^{-1} \boldsymbol{\delta}_{(U)} / \text{rank}(\mathbf{X})$$

If **ITER=0** and  $\sigma^2$  is profiled, then  $\widetilde{\text{Var}}[\widehat{\boldsymbol{\beta}}_{(U)}]^{-1}$  is obtained by sweeping

$$\widehat{\sigma}^2_{(U)} (\mathbf{X}'_{(U)} \mathbf{V}_{(U)}(\widehat{\boldsymbol{\theta}}^*)^{-1} \mathbf{X}_{(U)})^{-1}$$

The underlying idea is that if  $\boldsymbol{\theta}^*$  were known, then

$$(\mathbf{X}'_{(U)} \mathbf{V}_{(U)}(\boldsymbol{\theta}^*)^{-1} \mathbf{X}_{(U)})^{-1}$$

would be  $\text{Var}[\widehat{\boldsymbol{\beta}}]/\sigma^2$  in a generalized least squares regression with all but the data in  $U$ .

In the case of iterative influence analysis,  $\widetilde{\text{Var}}[\widehat{\boldsymbol{\beta}}_{(U)}]$  is evaluated at  $\widehat{\boldsymbol{\theta}}_{(U)}$ . Furthermore, a MDFFITS-type statistic is then computed for the covariance parameters:

$$\text{MDFFITS}(\boldsymbol{\theta}) = (\widehat{\boldsymbol{\theta}} - \widehat{\boldsymbol{\theta}}_{(U)})' \widetilde{\text{Var}}[\widehat{\boldsymbol{\theta}}_{(U)}]^{-1} (\widehat{\boldsymbol{\theta}} - \widehat{\boldsymbol{\theta}}_{(U)})$$

### Covariance Ratio and Trace

These statistics depend on the availability of an external estimate of  $\mathbf{V}$ , or at least of  $\sigma^2$ . Whereas Cook's  $D$  and MDFFITS measure the impact of data points on a vector of parameter estimates, the covariance-based statistics measure impact on their precision. Following Christensen, Pearson, and Johnson (1992), the MIXED procedure computes

$$\text{CovTrace}(\boldsymbol{\beta}) = |\text{trace}(\widetilde{\text{Var}}[\widehat{\boldsymbol{\beta}}]^{-1} \widetilde{\text{Var}}[\widehat{\boldsymbol{\beta}}_{(U)}]) - \text{rank}(\mathbf{X})|$$

$$\text{CovRatio}(\boldsymbol{\beta}) = \frac{\det_{ns}(\widetilde{\text{Var}}[\widehat{\boldsymbol{\beta}}_{(U)}])}{\det_{ns}(\widetilde{\text{Var}}[\widehat{\boldsymbol{\beta}}])}$$

where  $\det_{ns}(\mathbf{M})$  denotes the determinant of the nonsingular part of matrix  $\mathbf{M}$ .

In the case of iterative influence analysis these statistics are also computed for the covariance parameter estimates. If  $q$  denotes the rank of  $\text{Var}[\widehat{\boldsymbol{\theta}}]$ , then

$$\text{CovTrace}(\boldsymbol{\theta}) = |\text{trace}(\widetilde{\text{Var}}[\widehat{\boldsymbol{\theta}}]^{-1} \widetilde{\text{Var}}[\widehat{\boldsymbol{\theta}}_{(U)}]) - q|$$

$$\text{CovRatio}(\boldsymbol{\theta}) = \frac{\det_{ns}(\widetilde{\text{Var}}[\widehat{\boldsymbol{\theta}}_{(U)}])}{\det_{ns}(\widetilde{\text{Var}}[\widehat{\boldsymbol{\theta}}])}$$



### Likelihood Distances

The log-likelihood function  $l$  and restricted log-likelihood function  $l_R$  of the linear mixed model are given in the section “Estimating Covariance Parameters in the Mixed Model” on page 4964. Denote as  $\psi$  the collection of all parameters, i.e., the fixed effects  $\beta$  and the covariance parameters  $\theta$ . Twice the difference between the (restricted) log-likelihood evaluated at the full-data estimates  $\hat{\psi}$  and at the reduced-data estimates  $\hat{\psi}_{(U)}$  is known as the (restricted) likelihood distance:

$$\begin{aligned} \text{RLD}_{(U)} &= 2\{l_R(\hat{\psi}) - l_R(\hat{\psi}_{(U)})\} \\ \text{LD}_{(U)} &= 2\{l(\hat{\psi}) - l(\hat{\psi}_{(U)})\} \end{aligned}$$

Cook and Weisberg (1982, Ch. 5.2) refer to these differences as *likelihood distances*, Beckman, Nachtsheim, and Cook (1987) call the measures *likelihood displacements*. If the number of elements in  $\psi$  that are subject to updating following point removal is  $q$ , then likelihood displacements can be compared against cutoffs from a chi-square distribution with  $q$  degrees of freedom. Notice that this reference distribution does not depend on the number of observations removed from the analysis, but rather on the number of model parameters that are updated. The likelihood displacement gives twice the amount by which the log likelihood of the full data changes if one were to use an estimate based on fewer data points. It is thus a global, summary measure of the influence of the observations in  $U$  jointly on all parameters.

Unless `METHOD=ML`, the MIXED procedure computes the likelihood displacement based on the residual (=restricted) log likelihood, even if `METHOD=MIVQUE0` or `METHOD=TYPE1`, `TYPE2`, or `TYPE3`.

### Noniterative Update Formulas

Update formulas that do not require refitting of the model are available for the cases where  $\mathbf{V} = \sigma^2\mathbf{I}$ ,  $\mathbf{V}$  is known, or  $\mathbf{V}^*$  is known. When `ITER=0` and these update formulas can be invoked, the MIXED procedure uses the computational devices that are outlined in the following paragraphs. It is then assumed that the variance-covariance matrix of the fixed effects has the form  $(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-}$ . When `DDFM=KENWARDROGER`, this is not the case; the estimated variance-covariance matrix is then inflated to better represent the uncertainty in the estimated covariance parameters. Influence statistics when `DDFM=KENWARDROGER` should iteratively update the covariance parameters (`ITER > 0`). The dependence of  $\mathbf{V}$  on  $\theta$  is suppressed in the sequel for brevity.

**Updating the Fixed Effects** Denote by  $\mathbf{U}$  the  $(n \times k)$  matrix that is assembled from  $k$  columns of the identity matrix. Each column of  $\mathbf{U}$  corresponds to the removal of one data point. The point being targeted by the  $i$ th column of  $\mathbf{U}$  corresponds to the row in which a 1 appears. Furthermore, define

$$\begin{aligned} \mathbf{\Omega} &= (\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-} \\ \mathbf{Q} &= \mathbf{X}\mathbf{\Omega}\mathbf{X}' \\ \mathbf{P} &= \mathbf{V}^{-1}(\mathbf{V} - \mathbf{Q})\mathbf{V}^{-1} \end{aligned}$$

The change in the fixed-effects estimates following removal of the observations in  $U$  is

$$\hat{\beta} - \hat{\beta}_{(U)} = \mathbf{\Omega}\mathbf{X}'\mathbf{V}^{-1}\mathbf{U}(\mathbf{U}'\mathbf{P}\mathbf{U})^{-1}\mathbf{U}'\mathbf{V}^{-1}(\mathbf{y} - \mathbf{X}\hat{\beta})$$

Using results in Cook and Weisberg (1982, A2) you can further compute

$$\tilde{\mathbf{\Omega}} = (\mathbf{X}'_{(U)}\mathbf{V}_{(U)}^{-1}\mathbf{X}_{(U)})^{-} = \mathbf{\Omega} + \mathbf{\Omega}\mathbf{X}'\mathbf{V}^{-1}\mathbf{U}(\mathbf{U}'\mathbf{P}\mathbf{U})^{-1}\mathbf{U}'\mathbf{V}^{-1}\mathbf{X}\mathbf{\Omega}$$

If  $\mathbf{X}$  is  $(n \times p)$  of rank  $m < p$ , then  $\mathbf{\Omega}$  is deficient in rank and the MIXED procedure computes needed quantities in  $\tilde{\mathbf{\Omega}}$  by sweeping (Goodnight 1979). If the rank of the  $(k \times k)$  matrix  $\mathbf{U}'\mathbf{P}\mathbf{U}$  is less than  $k$ , the removal

of the observations introduces a new singularity, whether  $\mathbf{X}$  is of full rank or not. The solution vectors  $\hat{\boldsymbol{\beta}}$  and  $\hat{\boldsymbol{\beta}}_{(U)}$  then do not have the same expected values and should not be compared. When the MIXED procedure encounters this situation, influence diagnostics that depend on the choice of generalized inverse are not computed. The procedure also monitors the singularity criteria when sweeping the rows of  $(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-}$  and of  $(\mathbf{X}'_{(U)}\mathbf{V}_{(U)}^{-1}\mathbf{X}_{(U)})^{-}$ . If a new singularity is encountered or a former singularity disappears, no influence statistics are computed.

**Residual Variance** When  $\sigma^2$  is profiled out of the marginal variance-covariance matrix, a closed-form estimate of  $\sigma^2$  that is based on only the remaining observations can be computed provided  $\mathbf{V}^* = \mathbf{V}(\hat{\boldsymbol{\theta}}^*)$  is known. Hurtado (1993, Thm. 5.2) shows that

$$(n - q - r)\hat{\sigma}_{(U)}^2 = (n - q)\hat{\sigma}^2 - \hat{\boldsymbol{\epsilon}}'_U(\hat{\sigma}^2\mathbf{U}'\mathbf{P}\mathbf{U})^{-1}\hat{\boldsymbol{\epsilon}}_U$$

and  $\hat{\boldsymbol{\epsilon}}_U = \mathbf{U}'\mathbf{V}^{*-1}(\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}})$ . In the case of maximum likelihood estimation  $q = 0$  and for REML estimation  $q = \text{rank}(\mathbf{X})$ . The constant  $r$  equals the rank of  $(\mathbf{U}'\mathbf{P}\mathbf{U})$  for REML estimation and the number of effective observations that are removed if `METHOD=ML`.

**Likelihood Distances** For noniterative methods the following computational devices are used to compute (restricted) likelihood distances provided that the residual variance  $\sigma^2$  is profiled.

The log likelihood function  $l(\hat{\boldsymbol{\theta}})$  evaluated at the full-data and reduced-data estimates can be written as

$$\begin{aligned} l(\hat{\boldsymbol{\psi}}) &= -\frac{n}{2}\log(\hat{\sigma}^2) - \frac{1}{2}\log|\mathbf{V}^*| - \frac{1}{2}(\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}})'\mathbf{V}^{*-1}(\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}})/\hat{\sigma}^2 - \frac{n}{2}\log(2\pi) \\ l(\hat{\boldsymbol{\psi}}_{(U)}) &= -\frac{n}{2}\log(\hat{\sigma}_{(U)}^2) - \frac{1}{2}\log|\mathbf{V}^*| - \frac{1}{2}(\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}}_{(U)})'\mathbf{V}^{*-1}(\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}}_{(U)})/\hat{\sigma}_{(U)}^2 - \frac{n}{2}\log(2\pi) \end{aligned}$$

Notice that  $l(\hat{\boldsymbol{\theta}}_{(U)})$  evaluates the log likelihood for  $n$  data points at the reduced-data estimates. It is not the log likelihood obtained by fitting the model to the reduced data. The likelihood distance is then

$$\text{LD}_{(U)} = n \log \left\{ \frac{\hat{\sigma}_{(U)}^2}{\hat{\sigma}^2} \right\} - n + (\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}}_{(U)})' \mathbf{V}^{*-1} (\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}}_{(U)}) / \hat{\sigma}_{(U)}^2$$

Expressions for  $\text{RLD}_{(U)}$  in noniterative influence analysis are derived along the same lines.

## Default Output

The following sections describe the output PROC MIXED produces by default. This output is organized into various tables, and they are discussed in order of appearance.

## Model Information

The “Model Information” table describes the model, some of the variables it involves, and the method used in fitting it. It also lists the method (profile, factor, parameter, or none) for handling the residual variance in the model. The *profile* method concentrates the residual variance out of the optimization problem, whereas the *parameter* method retains it as a parameter in the optimization. The *factor* method keeps the residual fixed, and *none* is displayed when a residual variance is not part of the model.

The “Model Information” table also has a row labeled Fixed Effects SE Method. This row describes the method used to compute the approximate standard errors for the fixed-effects parameter estimates and related functions of them. The two possibilities for this row are Model-Based, which is the default method, and Empirical, which results from using the **EMPIRICAL** option in the **PROC MIXED** statement.

The ODS name of the “Model Information” table is ModelInfo.

### Class Level Information

The “Class Level Information” table lists the levels of every variable specified in the **CLASS** statement. You should check this information to make sure the data are correct. You can adjust the order of the **CLASS** variable levels with the **ORDER=** option in the **PROC MIXED** statement. The ODS name of the “Class Level Information” table is ClassLevels.

### Dimensions

The “Dimensions” table lists the sizes of relevant matrices. This table can be useful in determining CPU time and memory requirements. The ODS name of the “Dimensions” table is Dimensions.

### Number of Observations

The “Number of Observations” table shows the number of observations read from the data set and the number of observations used in fitting the model.

### Iteration History

The “Iteration History” table describes the optimization of the **residual log likelihood** or **log likelihood**. The function to be minimized (the *objective function*) is  $-2l$  for ML and  $-2l_R$  for REML; the column name of the objective function in the “Iteration History” table is “-2 Log Like” for ML and “-2 Res Log Like” for REML. The minimization is performed by using a ridge-stabilized Newton-Raphson algorithm, and the rows of this table describe the iterations that this algorithm takes in order to minimize the objective function.

The Evaluations column of the “Iteration History” table tells how many times the objective function is evaluated during each iteration.

The Criterion column of the “Iteration History” table is, by default, a relative Hessian convergence quantity given by

$$\frac{\mathbf{g}'_k \mathbf{H}_k^{-1} \mathbf{g}_k}{|f_k|}$$

where  $f_k$  is the value of the objective function at iteration  $k$ ,  $\mathbf{g}_k$  is the gradient (first derivative) of  $f_k$ , and  $\mathbf{H}_k$  is the Hessian (second derivative) of  $f_k$ . If  $\mathbf{H}_k$  is singular, then **PROC MIXED** uses the following relative quantity:

$$\frac{\mathbf{g}'_k \mathbf{g}_k}{|f_k|}$$

To prevent the division by  $|f_k|$ , use the **ABSOLUTE** option in the **PROC MIXED** statement. To use a relative function or gradient criterion, use the **CONVF** or **CONVG** option, respectively.

The Hessian criterion is considered superior to function and gradient criteria because it measures orthogonality rather than lack of progress (Bates and Watts 1988). Provided the initial estimate is feasible and the maximum number of iterations is not exceeded, the Newton-Raphson algorithm is considered to have converged when the criterion is less than the tolerance specified with the `CONVF`, `CONVG`, or `CONVH` option in the `PROC MIXED` statement. The default tolerance is  $1E-8$ . If convergence is not achieved, `PROC MIXED` displays the estimates of the parameters at the last iteration.

A convergence criterion that is missing indicates that a boundary constraint has been dropped; it is usually not a cause for concern.

If you specify the `ITDETAILS` option in the `PROC MIXED` statement, then the covariance parameter estimates at each iteration are included as additional columns in the “Iteration History” table.

The ODS name of the “Iteration History” table is `IterHistory`.

## Convergence Status

The “Convergence Status” table informs about the status of the iterative estimation process at the end of the Newton-Raphson optimization. It appears as a message in the listing, and this message is repeated in the log. The ODS object “ConvergenceStatus” also contains several nonprinting columns that can be helpful in checking the success of the iterative process, in particular during batch processing or when analyzing BY groups. The `Status` variable takes on the value 0 for a successful convergence (even if the Hessian matrix might not be positive definite). The values 1 and 2 of the `Status` variable indicate lack of convergence and infeasible initial parameter values, respectively. The variables `pdG` and `pdH` can be used to check whether the `G` and `H` (Hessian) matrices are positive definite.

For models that are not fit iteratively, such as models without random effects or when the `NOITER` option is in effect, the “Convergence Status” is not produced.

## Covariance Parameter Estimates

The “Covariance Parameter Estimates” table contains the estimates of the parameters in `G` and `R` (see the section “Estimating Covariance Parameters in the Mixed Model” on page 4964). Their values are labeled in the table along with Subject and Group information if applicable. The estimates are displayed in the `Estimate` column and are the results of one of the following estimation methods: `REML`, `ML`, `MIVQUE0`, `SSCP`, `Type1`, `Type2`, or `Type3`.

If you specify the `RATIO` option in the `PROC MIXED` statement, the `Ratio` column is added to the table listing the ratio of each parameter estimate to that of the residual variance.

Specifying the `COVTEST` option in the `PROC MIXED` statement produces the “Std Error,” “Z Value,” and “Pr Z” columns. The “Std Error” column contains the approximate standard errors of the covariance parameter estimates. These are the square roots of the diagonal elements of the observed inverse Fisher information matrix, which equals  $2\mathbf{H}^{-1}$ , where `H` is the Hessian matrix. The `H` matrix consists of the second derivatives of the objective function with respect to the covariance parameters; see Wolfinger, Tobias, and Sall (1994) for formulas. When you use the `SCORING=` option and `PROC MIXED` converges without stopping the scoring algorithm, `PROC MIXED` uses the expected Hessian matrix to compute the covariance matrix instead of the observed Hessian. The observed or expected inverse Fisher information matrix can be viewed as an asymptotic covariance matrix of the estimates.

The “Z Value” column is the estimate divided by its approximate standard error, and the “Pr Z” column is the one- or two-tailed area of the standard Gaussian density outside of the Z-value. The `MIXED` procedure

computes one-sided  $p$ -values for the residual variance and for covariance parameters with a lower bound of 0. The procedure computes two-sided  $p$ -values otherwise. These statistics constitute Wald tests of the covariance parameters, and they are valid only asymptotically.

**CAUTION:** Wald tests can be unreliable in small samples.

The ODS name of the “Covariance Parameter Estimates” table is CovParms.

## Fit Statistics

The “Fit Statistics” table provides some statistics about the estimated mixed model. Expressions for the  $-2$  times the log likelihood are provided in the section “[Estimating Covariance Parameters in the Mixed Model](#)” on page 4964. If the log likelihood is an extremely large number, then PROC MIXED has deemed the estimated  $\mathbf{V}$  matrix to be singular. In this case, all subsequent results should be viewed with caution.

In addition, the “Fit Statistics” table lists three information criteria: AIC, AICC, and BIC, all in smaller-is-better form. Expressions for these criteria are described under the **IC** option.

The ODS name of the “Model Fitting Information” table is FitStatistics.

## Null Model Likelihood Ratio Test

If one covariance model is a submodel of another, you can carry out a likelihood ratio test for the significance of the more general model by computing  $-2$  times the difference between their log likelihoods. Then compare this statistic to the  $\chi^2$  distribution with degrees of freedom equal to the difference in the number of parameters for the two models.

This test is reported in the “Null Model Likelihood Ratio Test” table to determine whether it is necessary to model the covariance structure of the data at all. The “Chi-Square” value is  $-2$  times the log likelihood from the null model minus  $-2$  times the log likelihood from the fitted model, where the null model is the one with only the fixed effects listed in the **MODEL** statement and  $\mathbf{R} = \sigma^2\mathbf{I}$ . This statistic has an asymptotic  $\chi^2$  distribution with  $q - 1$  degrees of freedom, where  $q$  is the effective number of covariance parameters (those not estimated to be on a boundary constraint). The “Pr > ChiSq” column contains the upper-tail area from this distribution. This  $p$ -value can be used to assess the significance of the model fit.

This test is not produced for cases where the null hypothesis lies on the boundary of the parameter space, which is typically for variance component models. This is because the standard asymptotic theory does not apply in this case (Self and Liang 1987, Case 5).

If you specify a **PARMS** statement, PROC MIXED constructs a likelihood ratio test between the best model from the grid search and the final fitted model and reports the results in the “Parameter Search” table.

The ODS name of the “Null Model Likelihood Ratio Test” table is LRT.

## Type 3 Tests of Fixed Effects

The “Type 3 Tests of Fixed Effects” table contains hypothesis tests for the significance of each of the fixed effects—that is, those effects you specify in the **MODEL** statement. By default, PROC MIXED computes these tests by first constructing a Type 3 **L** matrix (see Chapter 15, “[The Four Types of Estimable Functions](#)”) for each effect. This **L** matrix is then used to compute the following  $F$  statistic:

$$F = \frac{\hat{\boldsymbol{\beta}}' \mathbf{L}' [\mathbf{L}(\mathbf{X}' \hat{\mathbf{V}}^{-1} \mathbf{X})^{-1} \mathbf{L}]^{-1} \mathbf{L} \hat{\boldsymbol{\beta}}}{r}$$

where  $r = \text{rank}(\mathbf{L}(\mathbf{X}'\hat{\mathbf{V}}^{-1}\mathbf{X})^{-1}\mathbf{L}')$ . A  $p$ -value for the test is computed as the tail area beyond this statistic from an  $F$  distribution with NDF and DDF degrees of freedom. The numerator degrees of freedom (NDF) are the row rank of  $\mathbf{L}$ , and the denominator degrees of freedom are computed by using one of the methods described under the `DDFM=` option. Small values of the  $p$ -value (typically less than 0.05 or 0.01) indicate a significant effect.

You can use the `HTYPE=` option in the `MODEL` statement to obtain tables of Type 1 (sequential) tests and Type 2 (adjusted) tests in addition to or instead of the table of Type 3 (partial) tests.

You can use the `CHISQ` option in the `MODEL` statement to obtain Wald  $\chi^2$  tests of the fixed effects. These are carried out by using the numerator of the  $F$  statistic and comparing it with the  $\chi^2$  distribution with NDF degrees of freedom. It is more liberal than the  $F$  test because it effectively assumes infinite denominator degrees of freedom.

The ODS names of the “Type 1 Tests of Fixed Effects” through the “Type 3 Tests of Fixed Effects” tables are Tests1 through Tests3, respectively.

## ODS Table Names

Each table created by PROC MIXED has a name associated with it, and you must use this name to reference the table when using ODS statements. These names are listed in Table 59.26.

**Table 59.26** ODS Tables Produced by PROC MIXED

| Table Name  | Description                                                  | Required Statement / Option                                                                                    |
|-------------|--------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------|
| AccRates    | Acceptance rates for posterior sampling                      | PRIOR                                                                                                          |
| AsyCorr     | Asymptotic correlation matrix of covariance parameters       | PROC MIXED ASYCORR                                                                                             |
| AsyCov      | Asymptotic covariance matrix of covariance parameters        | PROC MIXED ASYCOV                                                                                              |
| Base        | Base densities used for posterior sampling                   | PRIOR                                                                                                          |
| Bound       | Computed bound for posterior rejection sampling              | PRIOR                                                                                                          |
| CholG       | Cholesky root of the estimated $\mathbf{G}$ matrix           | RANDOM / GC                                                                                                    |
| CholR       | Cholesky root of blocks of the estimated $\mathbf{R}$ matrix | REPEATED / RC                                                                                                  |
| CholV       | Cholesky root of blocks of the estimated $\mathbf{V}$ matrix | RANDOM / VC                                                                                                    |
| ClassLevels | Level information from the <code>CLASS</code> statement      | Default output                                                                                                 |
| Coef        | $\mathbf{L}$ matrix coefficients                             | E option in <code>MODEL</code> ,<br><code>CONTRAST</code> , <code>ESTIMATE</code> ,<br>or <code>LSMEANS</code> |
| Contrasts   | Results from the <code>CONTRAST</code> statements            | CONTRAST                                                                                                       |

Table 59.26 continued

| Table Name        | Description                                                                   | Required Statement / Option                 |
|-------------------|-------------------------------------------------------------------------------|---------------------------------------------|
| ConvergenceStatus | Convergence status                                                            | Default                                     |
| CorrB             | Approximate correlation matrix of fixed-effects parameter estimates           | MODEL / CORRB                               |
| CovB              | Approximate covariance matrix of fixed-effects parameter estimates            | MODEL / COVB                                |
| CovParms          | Estimated covariance parameters                                               | Default output                              |
| DiffS             | Differences of LS-means                                                       | LSMEANS / DIFF (or PDIFF)                   |
| Dimensions        | Dimensions of the model                                                       | Default output                              |
| Estimates         | Results from ESTIMATE statements                                              | ESTIMATE                                    |
| FitStatistics     | Fit statistics                                                                | Default                                     |
| G                 | Estimated <b>G</b> matrix                                                     | RANDOM / G                                  |
| GCorr             | Correlation matrix from the estimated <b>G</b> matrix                         | RANDOM / GCORR                              |
| HLM1              | Type 1 Hotelling-Lawley-McKeon tests of fixed effects                         | MODEL / HTYPE=1 and REPEATED / HLM TYPE=UN  |
| HLM2              | Type 2 Hotelling-Lawley-McKeon tests of fixed effects                         | MODEL / HTYPE=2 and REPEATED / HLM TYPE=UN  |
| HLM3              | Type 3 Hotelling-Lawley-McKeon tests of fixed effects                         | REPEATED / HLM TYPE=UN                      |
| HLPS1             | Type 1 Hotelling-Lawley-Pillai-Samson tests of fixed effects                  | MODEL / HTYPE=1 and REPEATED / HLPS TYPE=UN |
| HLPS2             | Type 2 Hotelling-Lawley-Pillai-Samson tests of fixed effects                  | MODEL / HTYPE=1 and REPEATED / HLPS TYPE=UN |
| HLPS3             | Type 3 Hotelling-Lawley-Pillai-Samson tests of fixed effects                  | REPEATED / HLPS TYPE=UN                     |
| Influence         | Influence diagnostics                                                         | MODEL / INFLUENCE                           |
| InfoCrit          | Information criteria                                                          | PROC MIXED IC                               |
| InvCholG          | Inverse Cholesky root of the estimated <b>G</b> matrix                        | RANDOM / GCI                                |
| InvCholR          | Inverse Cholesky root of blocks of the estimated <b>R</b> matrix              | REPEATED / RCI                              |
| InvCholV          | Inverse Cholesky root of blocks of the estimated <b>V</b> matrix              | RANDOM / VCI                                |
| InvCovB           | Inverse of approximate covariance matrix of fixed-effects parameter estimates | MODEL / COVBI                               |
| InvG              | Inverse of the estimated <b>G</b> matrix                                      | RANDOM / GI                                 |
| InvR              | Inverse of blocks of the estimated <b>R</b> matrix                            | REPEATED / RI                               |
| InvV              | Inverse of blocks of the estimated <b>V</b> matrix                            | RANDOM / VI                                 |
| IterHistory       | Iteration history                                                             | Default output                              |



Table 59.26 *continued*

| Table Name  | Description                                                                                         | Required Statement / Option |
|-------------|-----------------------------------------------------------------------------------------------------|-----------------------------|
| LComponents | Single-degree-of-freedom estimates that correspond to rows of the <b>L</b> matrix for fixed effects | MODEL / LCOMPONENTS         |
| LRT         | Likelihood ratio test                                                                               | Default output              |
| LSMeans     | LS-means                                                                                            | LSMEANS                     |
| MMEq        | Mixed model equations                                                                               | PROC MIXED MMEQ             |
| MMEqSol     | Mixed model equations solution                                                                      | PROC MIXED MMEQSOL          |
| ModelInfo   | Model information                                                                                   | Default output              |
| NObs        | Number of observations read and used                                                                | Default output              |
| ParmSearch  | Parameter search values                                                                             | PARMS                       |
| Posterior   | Posterior sampling information                                                                      | PRIOR                       |
| R           | Blocks of the estimated <b>R</b> matrix                                                             | REPEATED / R                |
| RCorr       | Correlation matrix from blocks of the estimated <b>R</b> matrix                                     | REPEATED / RCORR            |
| Search      | Posterior density search table                                                                      | PRIOR / PSEARCH             |
| Slices      | Tests of LS-means slices                                                                            | LSMEANS / SLICE=            |
| SolutionF   | Fixed-effects solution vector                                                                       | MODEL / S                   |
| SolutionR   | Random-effects solution vector                                                                      | RANDOM / S                  |
| Tests1      | Type 1 tests of fixed effects                                                                       | MODEL / HTYPE=1             |
| Tests2      | Type 2 tests of fixed effects                                                                       | MODEL / HTYPE=2             |
| Tests3      | Type 3 tests of fixed effects                                                                       | Default output              |
| Type1       | Type 1 analysis of variance                                                                         | PROC MIXED METHOD=TYPE1     |
| Type2       | Type 2 analysis of variance                                                                         | PROC MIXED METHOD=TYPE2     |
| Type3       | Type 3 analysis of variance                                                                         | PROC MIXED METHOD=TYPE3     |
| Trans       | Transformation of covariance parameters                                                             | PRIOR / PTRANS              |
| V           | Blocks of the estimated <b>V</b> matrix                                                             | RANDOM / V                  |
| VCorr       | Correlation matrix from blocks of the estimated <b>V</b> matrix                                     | RANDOM / VCORR              |

In Table 59.26, “Coef” refers to multiple tables produced by the **E**, **E1**, **E2**, or **E3** option in the **MODEL** statement and the **E** option in the **CONTRAST**, **ESTIMATE**, and **LSMEANS** statements. You can create one large data set of these tables with a statement similar to the following:

```
ods output Coef=c;
```

To create separate data sets, use the following statement:

```
ods output Coef(match_all)=c;
```

Here the resulting data sets are named **C**, **C1**, **C2**, etc. The same principles apply to data sets created from the “**R**,” “**CholR**,” “**InvCholR**,” “**RCorr**,” “**InvR**,” “**V**,” “**CholV**,” “**InvCholV**,” “**VCorr**,” and “**InvV**” tables.

In Table 59.26, the following changes have occurred from SAS 6. The “**Predicted**,” “**PredMeans**,” and “**Sample**” tables from SAS 6 no longer exist and have been replaced by output data sets; see descriptions



of the **MODEL** statement options **OUTP=** and **OUTPM=** and the **PRIOR** statement option **OUT=** for more details. The “ML” and “REML” tables from SAS 6 have been replaced by the “IterHistory” table. The “Tests,” “HLM,” and “HLPS” tables from SAS 6 have been renamed “Tests3,” “HLM3,” and “HLPS3,” respectively.

Table 59.27 lists the variable names associated with the data sets created when you use the ODS OUTPUT option in conjunction with the preceding tables. In Table 59.27, *n* is used to denote a generic number that depends on the particular data set and model you select, and it can assume a different value each time it is used (even within the same table). The phrase *model specific* appears in rows of the affected tables to indicate that columns in these tables depend on the variables you specify in the model.

**CAUTION:** There is a danger of name collisions with the variables in the *model specific* tables in Table 59.27 and variables in your input data set. You should avoid using input variables with the same names as the variables in these tables.

**Table 59.27** Variable Names for the ODS Tables Produced in PROC MIXED

| Table Name    | Variables                                                                                                                                                           |
|---------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| AsyCorr       | Row, CovParm, CovP1–CovPn                                                                                                                                           |
| AsyCov        | Row, CovParm, CovP1–CovPn                                                                                                                                           |
| Base          | Type, Parm1–Parmn                                                                                                                                                   |
| Bound         | Technique, Converge, Iterations, Evaluations, LogBound, CovP1–CovPn, TCovP1–TCovPn                                                                                  |
| CholG         | <i>Model specific</i> , Effect, Subject, Sub1–Subn, Group, Group1–Groupn, Row, Col1–Coln                                                                            |
| CholR         | Index, Row, Col1–Coln                                                                                                                                               |
| CholV         | Index, Row, Col1–Coln                                                                                                                                               |
| ClassLevels   | Class, Levels, Values                                                                                                                                               |
| Coef          | <i>Model specific</i> , LMatrix, Effect, Subject, Sub1–Subn, Group, Group1–Groupn, Row1–Rown                                                                        |
| Contrasts     | Label, NumDF, DenDF, ChiSquare, FValue, ProbChiSq, ProbF                                                                                                            |
| CorrB         | <i>Model specific</i> , Effect, Row, Col1–Coln                                                                                                                      |
| CovB          | <i>Model specific</i> , Effect, Row, Col1–Coln                                                                                                                      |
| CovParms      | CovParm, Subject, Group, Estimate, StandardError, ZValue, ProbZ, Alpha, Lower, Upper                                                                                |
| Diffs         | <i>Model specific</i> , Effect, Margins, ByLevel, AT variables, Diff, StandardError, DF, tValue, Tails, Probt, Adjustment, Adj, Alpha, Lower, Upper, AdjLow, AdjUpp |
| Dimensions    | Descr, Value                                                                                                                                                        |
| Estimates     | Label, Estimate, StandardError, DF, tValue, Tails, Probt, Alpha, Lower, Upper                                                                                       |
| FitStatistics | Descr, Value                                                                                                                                                        |
| G             | <i>Model specific</i> , Effect, Subject, Sub1–Subn, Group, Group1–Groupn, Row, Col1–Coln                                                                            |
| GCorr         | <i>Model specific</i> , Effect, Subject, Sub1–Subn, Group, Group1–Groupn, Row, Col1–Coln                                                                            |
| HLM1          | Effect, NumDF, DenDF, FValue, ProbF                                                                                                                                 |
| HLM2          | Effect, NumDF, DenDF, FValue, ProbF                                                                                                                                 |
| HLM3          | Effect, NumDF, DenDF, FValue, ProbF                                                                                                                                 |

Table 59.27 continued

| Table Name  | Variables                                                                                                                                                                                                                                                                                      |
|-------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| HLPS1       | Effect, NumDF, DenDF, FValue, ProbF                                                                                                                                                                                                                                                            |
| HLPS2       | Effect, NumDF, DenDF, FValue, ProbF                                                                                                                                                                                                                                                            |
| HLPS3       | Effect, NumDF, DenDF, FValue, ProbF                                                                                                                                                                                                                                                            |
| Influence   | <i>Dependent on option modifiers</i> , Effect, Tuple, Obs1–Obsk, Level, Iter, Index, Predicted, Residual, Leverage, PressRes, PRESS, Student, RMSE, RStudent, CookD, DFFITS, MDFFITS, CovRatio, CovTrace, CookDCP, MDFFITSCP, CovRatioCP, CovTraceCP, LD, RLD, Parm1–Parmp, CovP1–CovPq, Notes |
| InfoCrit    | Neg2LogLike, Params, AIC, AICC, HQIC, BIC, CAIC                                                                                                                                                                                                                                                |
| InvCholG    | <i>Model specific</i> , Effect, Subject, Sub1–Subn, Group, Group1–Groupn, Row, Col1–Coln                                                                                                                                                                                                       |
| InvCholR    | Index, Row, Col1–Coln                                                                                                                                                                                                                                                                          |
| InvCholV    | Index, Row, Col1–Coln                                                                                                                                                                                                                                                                          |
| InvCovB     | <i>Model specific</i> , Effect, Row, Col1–Coln                                                                                                                                                                                                                                                 |
| InvG        | <i>Model specific</i> , Effect, Subject, Sub1–Subn, Group, Group1–Groupn, Row, Col1–Coln                                                                                                                                                                                                       |
| InvR        | Index, Row, Col1–Coln                                                                                                                                                                                                                                                                          |
| InvV        | Index, Row, Col1–Coln                                                                                                                                                                                                                                                                          |
| IterHistory | CovP1–CovPn, Iteration, Evaluations, M2ResLogLike, M2LogLike, Criterion                                                                                                                                                                                                                        |
| LComponents | Effect, TestType, LIndex, Estimate, StdErr, DF, tValue, Probt                                                                                                                                                                                                                                  |
| LRT         | DF, ChiSquare, ProbChiSq                                                                                                                                                                                                                                                                       |
| LSMeans     | <i>Model specific</i> , Effect, Margins, ByLevel, AT variables, Estimate, StandardError, DF, tValue, Probt, Alpha, Lower, Upper, Cov1–Covn, Corr1–Corrn                                                                                                                                        |
| MMEq        | <i>Model specific</i> , Effect, Subject, Sub1–Subn, Group, Group1–Groupn, Row, Col1–Coln                                                                                                                                                                                                       |
| MMEqSol     | <i>Model specific</i> , Effect, Subject, Sub1–Subn, Group, Group1–Groupn, Row, Col1–Coln                                                                                                                                                                                                       |
| ModelInfo   | Descr, Value                                                                                                                                                                                                                                                                                   |
| Nobs        | Label, N, NObsRead, NObsUsed, SumFreqsRead, SumFreqsUsed                                                                                                                                                                                                                                       |
| ParmSearch  | CovP1–CovPn, Var, ResLogLike, M2ResLogLike2, LogLike, M2LogLike, LogDetH                                                                                                                                                                                                                       |
| Posterior   | Descr, Value                                                                                                                                                                                                                                                                                   |
| R           | Index, Row, Col1–Coln                                                                                                                                                                                                                                                                          |
| RCorr       | Index, Row, Col1–Coln                                                                                                                                                                                                                                                                          |
| Search      | Parm, TCovP1–TCovPn, Posterior                                                                                                                                                                                                                                                                 |
| Slices      | <i>Model specific</i> , Effect, Margins, ByLevel, AT variables, NumDF, DenDF, FValue, ProbF                                                                                                                                                                                                    |
| SolutionF   | <i>Model specific</i> , Effect, Estimate, StandardError, DF, tValue, Probt, Alpha, Lower, Upper                                                                                                                                                                                                |
| SolutionR   | <i>Model specific</i> , Effect, Subject, Sub1–Subn, Group, Group1–Groupn, Estimate, StdErrPred, DF, tValue, Probt, Alpha, Lower, Upper                                                                                                                                                         |
| Tests1      | Effect, NumDF, DenDF, ChiSquare, FValue, ProbChiSq, ProbF                                                                                                                                                                                                                                      |

**Table 59.27** continued

| Table Name | Variables                                                  |
|------------|------------------------------------------------------------|
| Tests2     | Effect, NumDF, DenDF, ChiSquare, FValue, ProbChiSq, ProbF  |
| Tests3     | Effect, NumDF, DenDF, ChiSquare, FValue, ProbChiSq, ProbF  |
| Type1      | Source, DF, SS, MS, EMS, ErrorTerm, ErrorDF, FValue, ProbF |
| Type2      | Source, DF, SS, MS, EMS, ErrorTerm, ErrorDF, FValue, ProbF |
| Type3      | Source, DF, SS, MS, EMS, ErrorTerm, ErrorDF, FValue, ProbF |
| Trans      | Prior, TCovP, CovP1–CovPn                                  |
| V          | Index, Row, Col1–Coln                                      |
| VCorr      | Index, Row, Col1–Coln                                      |

Some of the variables listed in [Table 59.27](#) are created only when you specify certain options in the relevant PROC MIXED statements.

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “[Statistical Graphics Using ODS.](#)”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS.](#)”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “[A Primer on ODS Statistical Graphics](#)” on page 599 in Chapter 21, “[Statistical Graphics Using ODS.](#)”

Some graphs are produced by default; other graphs are produced by using statements and options.

## ODS Graph Names

You can reference every graph produced through ODS Graphics with a name. The names of the graphs that PROC MIXED generates are listed in [Table 59.28](#), along with the required statements and options.

**Table 59.28** Graphs Produced by PROC MIXED

| ODS Graph Name | Plot Description                                               | Statement or Option                                    |
|----------------|----------------------------------------------------------------|--------------------------------------------------------|
| Boxplot        | Box plots                                                      | PLOTS=BOXPLOT                                          |
| CovRatioPlot   | CovRatio statistics for fixed effects or covariance parameters | PLOTS=INFLUENCESTATPANEL(UNPACK) and MODEL / INFLUENCE |
| CooksDPlot     | Cook’s <i>D</i> for fixed effects or covariance parameters     | PLOTS=INFLUENCESTATPANEL(UNPACK) and MODEL / INFLUENCE |
| DistancePlot   | Likelihood or restricted likelihood distance                   | MODEL / INFLUENCE                                      |

Table 59.28 *continued*

| ODS Graph Name      | Plot Description                                                       | Statement or Option                                                          |
|---------------------|------------------------------------------------------------------------|------------------------------------------------------------------------------|
| InfluenceEstPlot    | Panel of deletion estimates                                            | MODEL / INFLUENCE(EST)<br>or PLOTS=INFLUENCEESTPLOT and<br>MODEL / INFLUENCE |
| InfluenceEstPlot    | Parameter estimates after removing observation or sets of observations | PLOTS=INFLUENCEESTPLOT(UNPACK)<br>and MODEL / INFLUENCE                      |
| InfluenceStatPanel  | Panel of influence statistics                                          | MODEL / INFLUENCE                                                            |
| PearsonBoxPlot      | Box plot of Pearson residuals                                          | PLOTS=PEARSONPANEL(UNPACK BOX)                                               |
| PearsonByPredicted  | Pearson residuals vs. predicted                                        | PLOTS=PEARSONPANEL(UNPACK)                                                   |
| PearsonHistogram    | Histogram of Pearson residuals                                         | PLOTS=PEARSONPANEL(UNPACK)                                                   |
| PearsonPanel        | Panel of Pearson residuals                                             | MODEL / RESIDUAL                                                             |
| PearsonQQplot       | $Q-Q$ plot of Pearson residuals                                        | PLOTS=PEARSONPANEL(UNPACK)                                                   |
| PressPlot           | Plot of PRESS residuals or PRESS statistic                             | PLOTS=PRESS and MODEL / INFLUENCE                                            |
| ResidualBoxplot     | Box plot of (raw) residuals                                            | PLOTS=RESIDUALPANEL(UNPACK BOX)                                              |
| ResidualByPredicted | Residuals vs. predicted                                                | PLOTS=RESIDUALPANEL(UNPACK)                                                  |
| ResidualHistogram   | Histogram of raw residuals                                             | PLOTS=RESIDUALPANEL(UNPACK)                                                  |
| ResidualPanel       | Panel of (raw) residuals                                               | MODEL / RESIDUAL                                                             |
| ResidualQQplot      | $Q-Q$ plot of raw residuals                                            | PLOTS=RESIDUALPANEL(UNPACK)                                                  |
| ScaledBoxplot       | Box plot of scaled residuals                                           | PLOTS=VCIRYPANEL(UNPACK BOX)                                                 |
| ScaledByPredicted   | Scaled residuals vs. predicted                                         | PLOTS=VCIRYPANEL(UNPACK)                                                     |
| ScaledHistogram     | Histogram of scaled residuals                                          | PLOTS=VCIRYPANEL(UNPACK)                                                     |
| ScaledQQplot        | $Q-Q$ plot of scaled residuals                                         | PLOTS=VCIRYPANEL(UNPACK)                                                     |
| StudentBoxplot      | Box plot of studentized residuals                                      | PLOTS=STUDENTPANEL(UNPACK BOX)                                               |
| StudentByPredicted  | Studentized residuals vs. predicted                                    | PLOTS=STUDENTPANEL(UNPACK)                                                   |
| StudentHistogram    | Histogram of studentized residuals                                     | PLOTS=STUDENTPANEL(UNPACK)                                                   |
| StudentPanel        | Panel of studentized residuals                                         | MODEL / RESIDUAL                                                             |
| StudentQQplot       | $Q-Q$ plot of studentized residuals                                    | PLOTS=STUDENTPANEL(UNPACK)                                                   |
| VCIRYPanel          | Panel of scaled residuals                                              | MODEL / VCIRY                                                                |

## Residual Plots

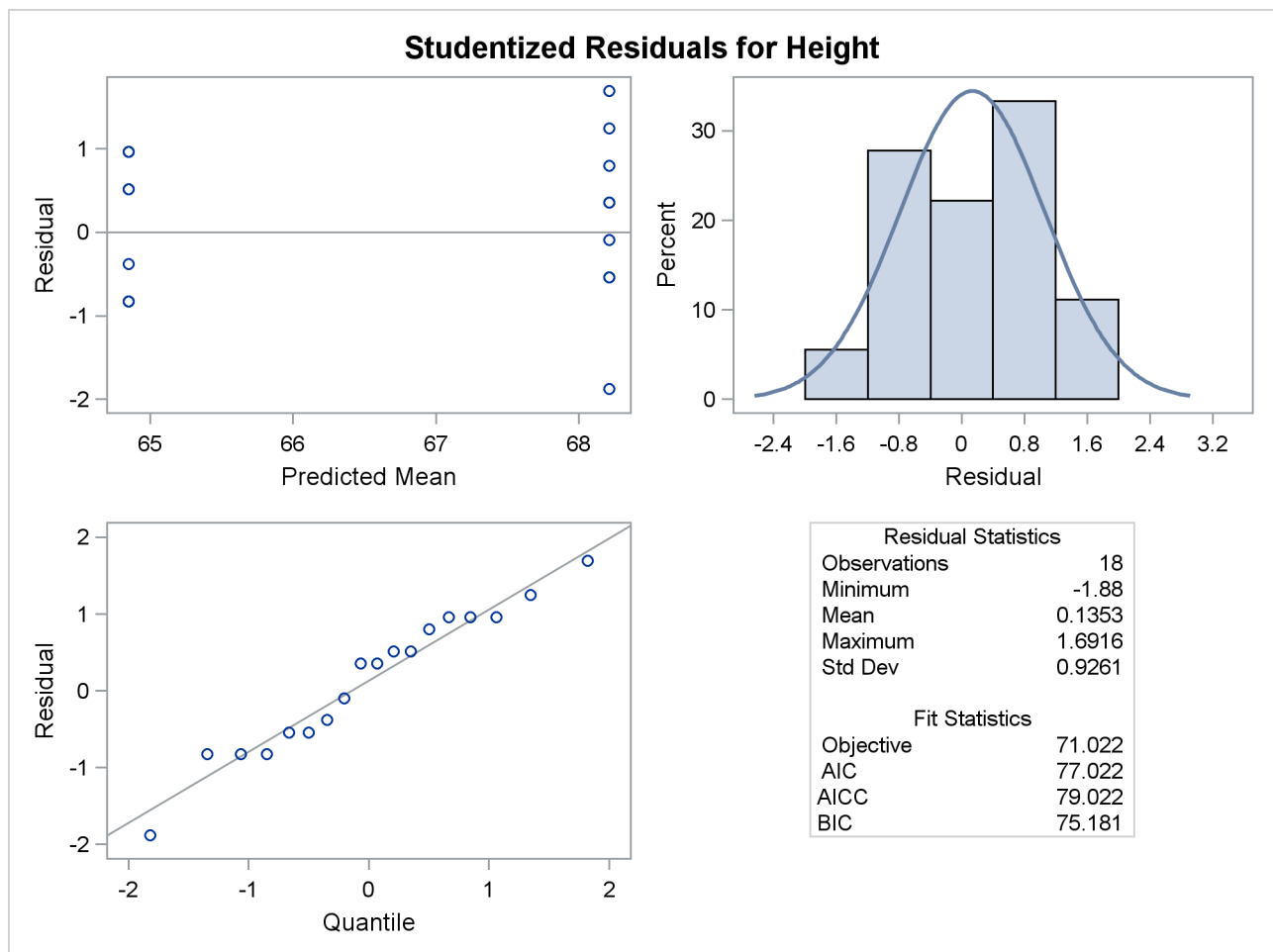
The MIXED procedure can generate panels of residual diagnostics. Each panel consists of a plot of residuals versus predicted values, a histogram with normal density overlaid, a Q-Q plot, and summary residual and fit statistics (Figure 59.15). The plots are produced even if the `OUTP=` and `OUTPM=` options in the `MODEL` statement are not specified. Residual panels can be generated for marginal and conditional raw, studentized, and Pearson residuals as well as for scaled residuals (see the section “Residual Diagnostics” on page 4976).

Recall the example in the section “Getting Started: MIXED Procedure” on page 4884. The following statements generate several  $2 \times 2$  panels of residual graphs:

```
ods graphics on;
proc mixed data=heights plots=studentpanel(marginal conditional);
 class Family Gender;
 model Height = Gender / residual;
 random Family Family*Gender;
run;
ods graphics off;
```

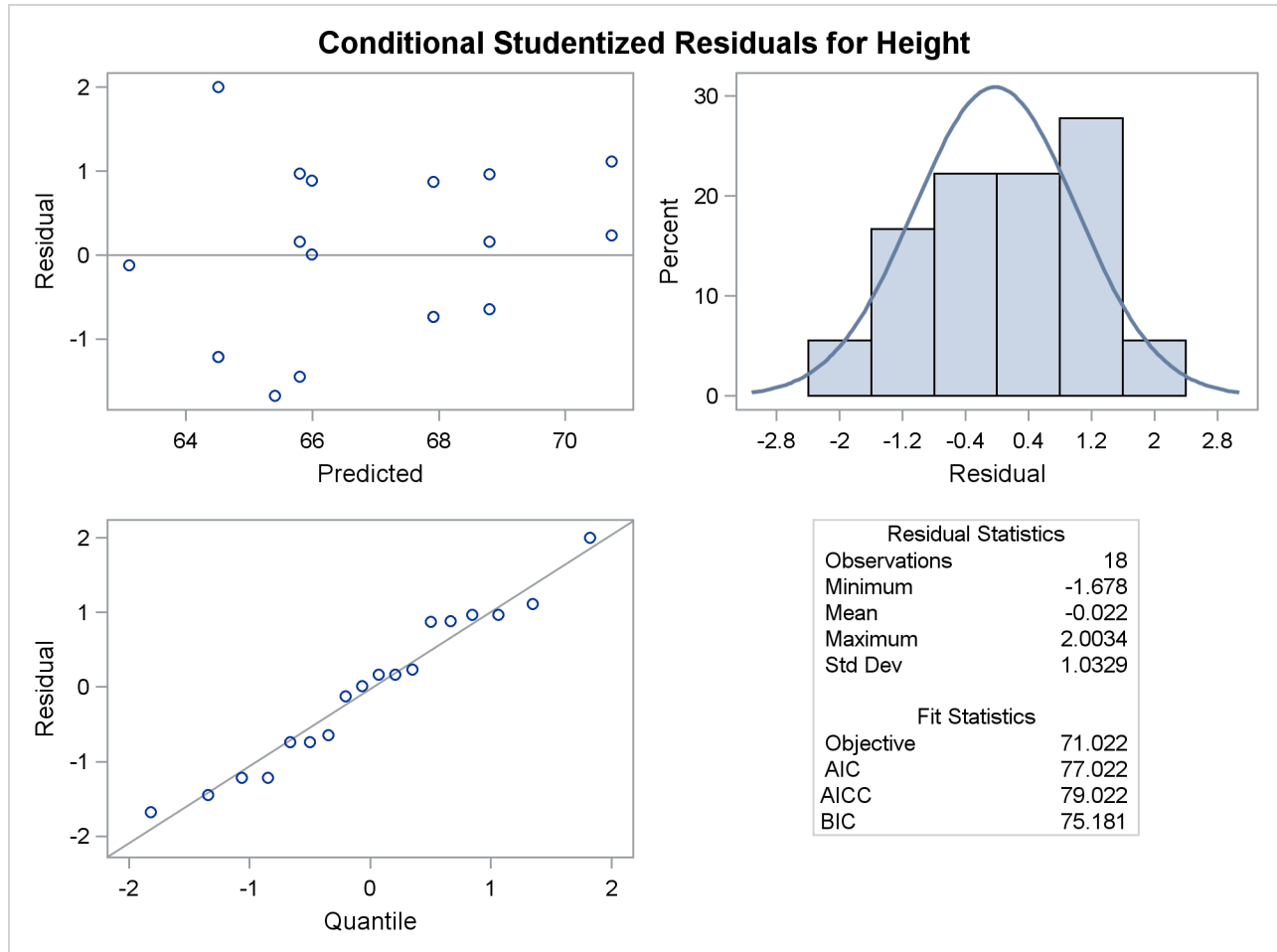
The graphs are created when ODS Graphics is enabled. The panel of the studentized marginal residuals is shown in Figure 59.15, and the panel of the studentized conditional residuals is shown in Figure 59.16.

**Figure 59.15** Panel of the Studentized (Marginal) Residuals



Since the fixed-effects part of the model comprises only an intercept and the gender effect, the marginal mean takes on only two values, one for each gender. The “Residual Statistics” inset in the lower-right corner provides descriptive statistics for the set of residuals that is displayed. Note that residuals in a mixed model do not necessarily sum to zero, even if the model contains an intercept.

**Figure 59.16** Panel of the Conditional Studentized Residuals



### Influence Plots

The graphical features of the MIXED procedure enable you to generate plots of influence diagnostics and of deletion estimates. The type and number of plots produced depend on your modifiers of the **INFLUENCE** option in the **MODEL** statement and on the **PLOTS=** option in the **PROC MIXED** statement. Plots related to covariance parameters are produced only when diagnostics are computed by iterative methods (**ITER=**). The estimates of the fixed effects—and covariance parameters when updates are iterative—are plotted when you specify the **ESTIMATES** modifier or when you request **PLOTS=INFLUENCEESTPLOT**.

Two basic types of influence panels are shown in [Figure 59.17](#) and [Figure 59.18](#). The diagnostics panel shows Cook’s *D* and CovRatio statistics for the fixed effects and the covariance parameters. For the SAS statements that produce these influence panels, see [Example 59.8](#). In this example, the impact of subjects (Person) on the analysis is assessed. The Cook’s *D* statistic measures a subject’s impact on the estimates,

and the CovRatio statistic measures a subject's impact on the precision of the estimates. Separate statistics are computed for the fixed effects and the covariance parameters. The CovRatio statistic has a threshold of 1.0. Values larger than 1.0 indicate that precision of the estimates is lost by exclusion of the observations in question. Values smaller than 1.0 indicate that precision is gained by exclusion of the observations from the analysis. For example, it is evident from [Output 59.17](#) that person 20 has considerable impact on the covariance parameter estimates and moderate influence on the fixed-effects estimates. Furthermore, exclusion of this subject from the analysis increases the precision of the covariance parameters, whereas the effect on the precision of the fixed effects is minor.

[Output 59.18](#) shows another type of influence plot, a panel of the deletion estimates. Each plot within the panel corresponds to one of the model parameters. A reference line is drawn at the estimate based on the full data.

**Figure 59.17** Influence Diagnostics

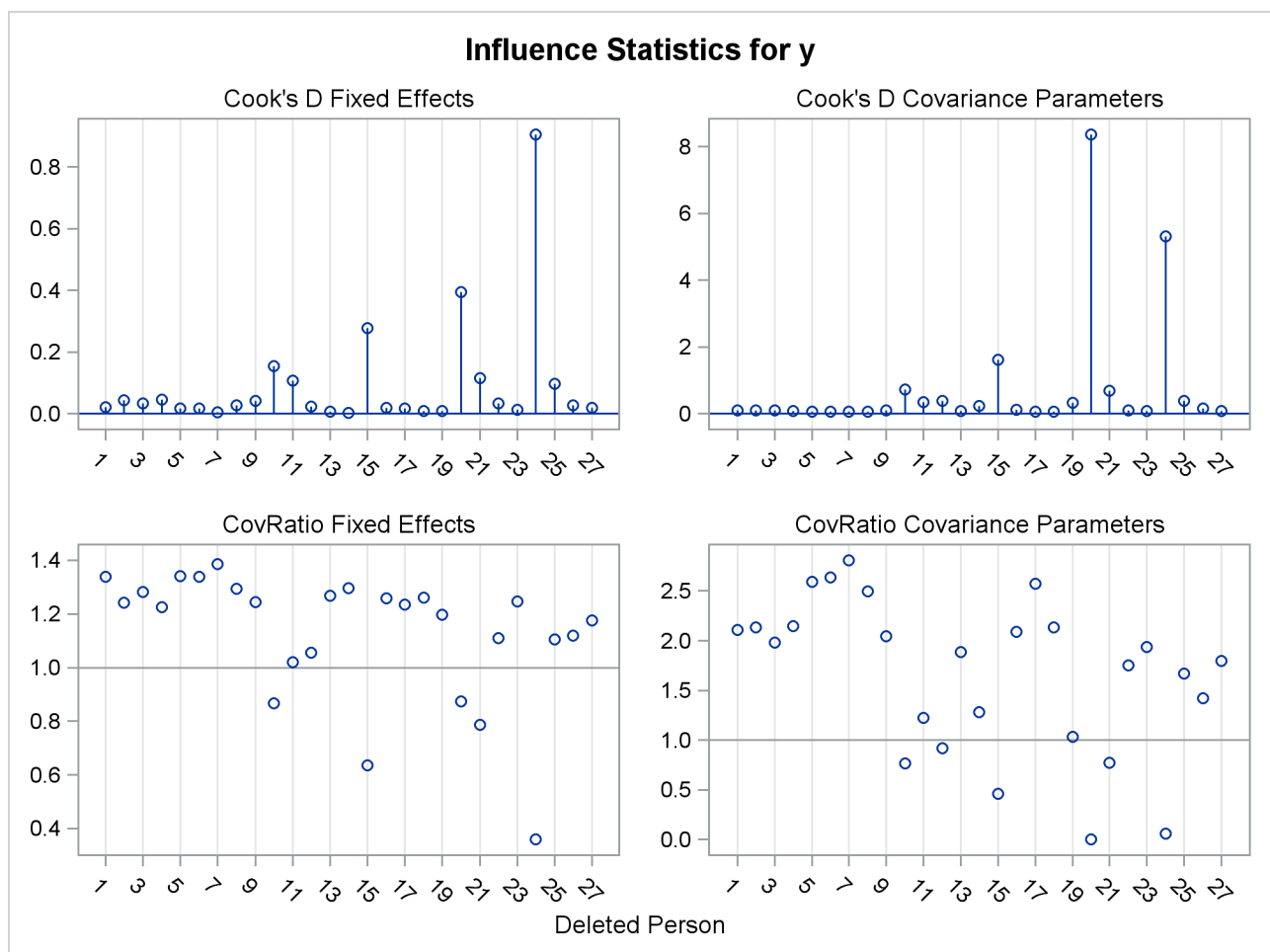
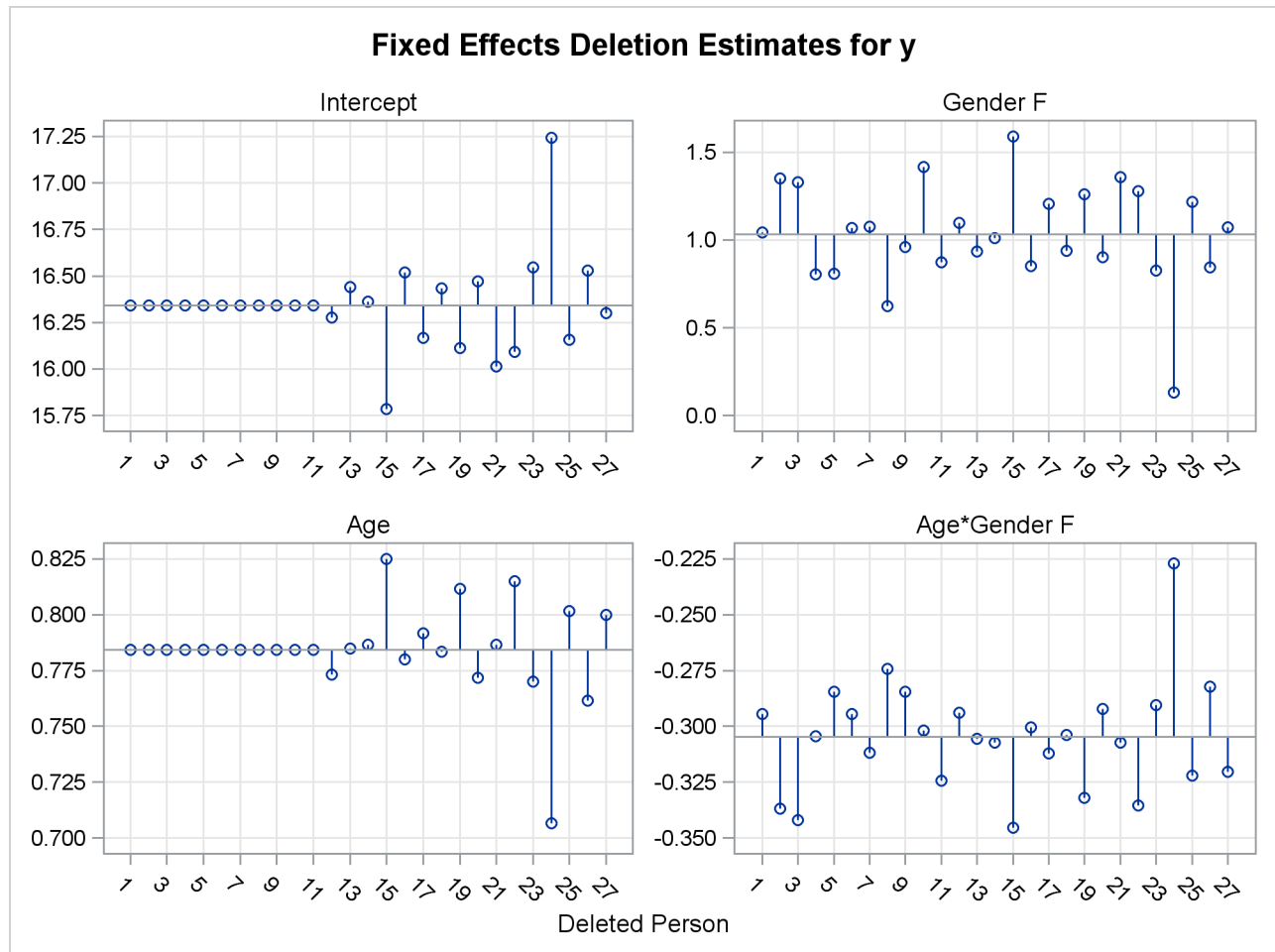


Figure 59.18 Deletion Estimates



## Computational Issues

### Computational Method

In addition to numerous matrix-multiplication routines, PROC MIXED frequently uses the sweep operator (Goodnight 1979) and the Cholesky root (Golub and Van Loan 1989). The routines perform a modified W transformation (Goodnight and Hemmerle 1979) for **G**-side likelihood calculations and a direct method for **R**-side likelihood calculations. For the Type 3 *F* tests, PROC MIXED uses the algorithm described in Chapter 42, “The GLM Procedure.”

PROC MIXED uses a ridge-stabilized Newton-Raphson algorithm to optimize either a full (ML) or residual (REML) likelihood function. The Newton-Raphson algorithm is preferred to the EM algorithm (Lindstrom and Bates 1988). PROC MIXED profiles the likelihood with respect to the fixed effects and also with respect to the residual variance whenever it appears reasonable to do so. The residual profiling can be avoided by using the NOPROFILE option of the PROC MIXED statement. PROC MIXED uses the MIVQUE0 method (Rao 1972; Giesbrecht 1989) to compute initial values.



The likelihoods that PROC MIXED optimizes are usually well-defined continuous functions with a single optimum. The Newton-Raphson algorithm typically performs well and finds the optimum in a few iterations. It is a quadratically converging algorithm, meaning that the error of the approximation near the optimum is squared at each iteration. The quadratic convergence property is evident when the convergence criterion drops to zero by factors of 10 or more.

**Table 59.29** Notation for Order Calculations

| Symbol | Number                           |
|--------|----------------------------------|
| $p$    | Columns of $\mathbf{X}$          |
| $g$    | Columns of $\mathbf{Z}$          |
| $N$    | Observations                     |
| $q$    | Covariance parameters            |
| $t$    | Maximum observations per subject |
| $S$    | Subjects                         |

Using the notation from Table 59.29, the following are estimates of the computational speed of the algorithms used in PROC MIXED. For likelihood calculations, the crossproducts matrix construction is of order  $N(p + g)^2$  and the sweep operations are of order  $(p + g)^3$ . The first derivative calculations for parameters in  $\mathbf{G}$  are of order  $qg^3$  for ML and  $q(g^3 + pg^2 + p^2g)$  for REML. If you specify a subject effect in the **RANDOM** statement and if you are not using the **REPEATED** statement, then replace  $g$  with  $g/S$  and  $q$  with  $qS$  in these calculations. The first derivative calculations for parameters in  $\mathbf{R}$  are of order  $qS(t^3 + gt^2 + g^2t)$  for ML and  $qS(t^3 + (p + g)t^2 + (p^2 + g^2)t)$  for REML. For the second derivatives, replace  $q$  with  $q(q + 1)/2$  in the first derivative expressions. When you specify both **G**- and **R**-side parameters (that is, when you use both the **RANDOM** and **REPEATED** statements), then additional calculations are required of an order equal to the sum of the orders for **G** and **R**. Considerable execution times can result in this case.

For further details about the computational techniques used in PROC MIXED, see Wolfinger, Tobias, and Sall (1994).

## Parameter Constraints

By default, some covariance parameters are assumed to satisfy certain boundary constraints during the Newton-Raphson algorithm. For example, variance components are constrained to be nonnegative, and autoregressive parameters are constrained to be between  $-1$  and  $1$ . You can remove these constraints with the **NOBOUND** option in the **PARMS** statement (or with the **NOBOUND** option in the **PROC MIXED** statement), but this can lead to estimates that produce an infinite likelihood. You can also introduce or change boundary constraints with the **LOWERB=** and **UPPERB=** options in the **PARMS** statement.

During the Newton-Raphson algorithm, a parameter might be set equal to one of its boundary constraints for a few iterations and then it might move away from the boundary. You see a missing value in the Criterion column of the “Iteration History” table whenever a boundary constraint is dropped.

For some data sets the final estimate of a parameter might equal one of its boundary constraints. This is usually not a cause for concern, but it might lead you to consider a different model. For instance, a variance component estimate can equal zero; in this case, you might want to drop the corresponding random effect from the model. However, be aware that changing the model in this fashion can affect degrees-of-freedom calculations.

## Convergence Problems

For some data sets, the Newton-Raphson algorithm can fail to converge. Nonconvergence can result from a number of causes, including flat or ridged likelihood surfaces and ill-conditioned data.

It is also possible for PROC MIXED to converge to a point that is not the global optimum of the likelihood, although this usually occurs only with the spatial covariance structures.

If you experience convergence problems, the following points might be helpful:

- One useful tool is the **PARMS** statement, which lets you input initial values for the covariance parameters and performs a grid search over the likelihood surface.
- Sometimes the Newton-Raphson algorithm does not perform well when two of the covariance parameters are on a different scale—that is, when they are several orders of magnitude apart. This is because the Hessian matrix is processed jointly for the two parameters, and elements of it corresponding to one of the parameters can become close to internal tolerances in PROC MIXED. In this case, you can improve stability by rescaling the effects in the model so that the covariance parameters are on the same scale.
- Data that are extremely large or extremely small can adversely affect results because of the internal tolerances in PROC MIXED. Rescaling it can improve stability.
- For stubborn problems, you might want to specify **ODS OUTPUT COVPARMS=*data-set-name*** to output the “Covariance Parameter Estimates” table as a precautionary measure. That way, if the problem does not converge, you can read the final parameter values back into a new run with the **PARMSDATA=** option in the **PARMS** statement.
- Fisher scoring can be more robust than Newton-Raphson with poor **MIVQUE(0)** starting values. Specifying a **SCORING=** value of 5 or so might help to recover from poor starting values.
- Tuning the singularity options **SINGULAR=**, **SINGCHOL=**, and **SINGRES=** in the **MODEL** statement can improve the stability of the optimization process.
- Tuning the **MAXITER=** and **MAXFUNC=** options in the **PROC MIXED** statement can save resources. Also, the **ITDETAILS** option displays the values of all the parameters at each iteration.
- Using the **NOPROFILE** and **NOBOUND** options in the **PROC MIXED** statement might help convergence, although they can produce unusual results.
- Although the **CONVH** convergence criterion usually gives the best results, you might want to try **CONVF** or **CONVG**, possibly along with the **ABSOLUTE** option.
- If the convergence criterion reaches a relatively small value such as  $1E-7$  but never gets lower than  $1E-8$ , you might want to specify **CONVH=1E-6** in the **PROC MIXED** statement to get results; however, interpret the results with caution.
- An infinite likelihood during the iteration process means that the Newton-Raphson algorithm has stepped into a region where either the **R** or **V** matrix is nonpositive definite. This is usually no cause for concern as long as iterations continue. If PROC MIXED stops because of an infinite likelihood, recheck your model to make sure that no observations from the same subject are producing identical rows in **R** or **V** and that you have enough data to estimate the particular covariance structure you have selected. Any time that the final estimated likelihood is infinite, subsequent results should be interpreted with caution.

- A nonpositive definite Hessian matrix can indicate a surface saddlepoint or linear dependencies among the parameters.
- A warning message about the singularities of  $\mathbf{X}$  changing indicates that there is some linear dependency in the estimate of  $\mathbf{X}'\widehat{\mathbf{V}}^{-1}\mathbf{X}$  that is not found in  $\mathbf{X}'\mathbf{X}$ . This can adversely affect the likelihood calculations and optimization process. If you encounter this problem, make sure that your model specification is reasonable and that you have enough data to estimate the particular covariance structure you have selected. Rearranging effects in the **MODEL** statement so that the most significant ones are first can help, because PROC MIXED sweeps the estimate of  $\mathbf{X}'\mathbf{V}^{-1}\mathbf{X}$  in the order of the **MODEL** effects and the sweep is more stable if larger pivots are dealt with first. If this does not help, specifying starting values with the **PARMS** statement can place the optimization on a different and possibly more stable path.
- Lack of convergence can indicate model misspecification or a violation of the normality assumption.

## Memory

Let  $p$  be the number of columns in  $\mathbf{X}$ , and let  $g$  be the number of columns in  $\mathbf{Z}$ . For large models, most of the memory resources are required for holding symmetric matrices of order  $p$ ,  $g$ , and  $p + g$ . The approximate memory requirement in bytes is

$$40(p^2 + g^2) + 32(p + g)^2$$

If you have a large model that exceeds the memory capacity of your computer, see the suggestions listed under “Computing Time.”

## Computing Time

PROC MIXED is computationally intensive, and execution times can be long. In addition to the CPU time used in collecting sums and crossproducts and in solving the mixed model equations (as in PROC GLM), considerable CPU time is often required to compute the likelihood function and its derivatives. These latter computations are performed for every Newton-Raphson iteration.

If you have a model that takes too long to run, the following suggestions can be helpful:

- Examine the “Model Information” table to find out the number of columns in the  $\mathbf{X}$  and  $\mathbf{Z}$  matrices. A large number of columns in either matrix can greatly increase computing time. You might want to eliminate some higher-order effects if they are too large.
- If you have a  $\mathbf{Z}$  matrix with a lot of columns, use the **DDFM=BW** option in the **MODEL** statement to eliminate the time required for the containment method.
- If possible, “factor out” a common effect from the effects in the **RANDOM** statement and make it the **SUBJECT=** effect. This creates a block-diagonal  $\mathbf{G}$  matrix and can often speed calculations.
- If possible, use the same or nested **SUBJECT=** effects in all **RANDOM** and **REPEATED** statements.
- If your data set is very large, you might want to analyze it in pieces. The **BY** statement can help implement this strategy.

- In general, specify random effects with a lot of levels in the **REPEATED** statement and those with a few levels in the **RANDOM** statement.
- The **METHOD=MIVQUE0** option runs faster than either the **METHOD=REML** or **METHOD=ML** option because it is noniterative.
- You can specify known values for the covariance parameters by using the **HOLD=** or **NOITER** option in the **PARMS** statement or the **GDATA=** option in the **RANDOM** statement. This eliminates the need for iteration.
- The **LOGNOTE** option in the **PROC MIXED** statement writes periodic messages to the SAS log concerning the status of the calculations. It can help you diagnose where the slowdown is occurring.

---

## Examples: MIXED Procedure

The following are basic examples of the use of PROC MIXED. More examples and details can be found in Littell et al. (2006); Wolfinger (1997); Verbeke and Molenberghs (1997, 2000); Murray (1998); Singer (1998); Sullivan, Dukes, and Losina (1999), and Brown and Prescott (1999).

---

### Example 59.1: Split-Plot Design

PROC MIXED can fit a variety of mixed models. One of the most common mixed models is the split-plot design. The split-plot design involves two experimental factors, A and B. Levels of A are randomly assigned to whole plots (main plots), and levels of B are randomly assigned to split plots (subplots) within each whole plot. The design provides more precise information about B than about A, and it often arises when A can be applied only to large experimental units. An example is where A represents irrigation levels for large plots of land and B represents different crop varieties planted in each large plot.

Consider the following data from Stroup (1989a), which arise from a balanced split-plot design with the whole plots arranged in a randomized complete-block design. The variable A is the whole-plot factor, and the variable B is the subplot factor. A traditional analysis of these data involves the construction of the whole-plot error (A\*Block) to test A and the pooled residual error (B\*Block and A\*B\*Block) to test B and A\*B. To carry out this analysis with PROC GLM, you must use a TEST statement to obtain the correct *F* test for A.

Performing a mixed model analysis with PROC MIXED eliminates the need for the error term construction. PROC MIXED estimates variance components for Block, A\*Block, and the residual, and it automatically incorporates the correct error terms into test statistics.

The following statements create a DATA set for a split-plot design with four blocks, three whole-plot levels, and two subplot levels:

```
data sp;
 input Block A B Y @@;
 datalines;
1 1 1 56 1 1 2 41
1 2 1 50 1 2 2 36
```

```

1 3 1 39 1 3 2 35
2 1 1 30 2 1 2 25
2 2 1 36 2 2 2 28
2 3 1 33 2 3 2 30
3 1 1 32 3 1 2 24
3 2 1 31 3 2 2 27
3 3 1 15 3 3 2 19
4 1 1 30 4 1 2 25
4 2 1 35 4 2 2 30
4 3 1 17 4 3 2 18
;

```

The following statements fit the split-plot model assuming random block effects:

```

proc mixed;
 class A B Block;
 model Y = A B A*B;
 random Block A*Block;
run;

```

The variables A, B, and Block are listed as classification variables in the **CLASS** statement. The columns of model matrix **X** consist of indicator variables corresponding to the levels of the fixed effects A, B, and A\*B listed on the right side of the **MODEL** statement. The dependent variable Y is listed on the left side of the **MODEL** statement.

The columns of the model matrix **Z** consist of indicator variables corresponding to the levels of the random effects Block and A\*Block. The **G** matrix is diagonal and contains the variance components of Block and A\*Block. The **R** matrix is also diagonal and contains the residual variance.

The SAS statements produce [Output 59.1.1–Output 59.1.8](#).

The “Model Information” table in [Output 59.1.1](#) lists basic information about the split-plot model. REML is used to estimate the variance components, and the residual variance is profiled from the optimization.

### Output 59.1.1 Results for Split-Plot Analysis

| The Mixed Procedure       |                     |
|---------------------------|---------------------|
| Model Information         |                     |
| Data Set                  | WORK.SP             |
| Dependent Variable        | Y                   |
| Covariance Structure      | Variance Components |
| Estimation Method         | REML                |
| Residual Variance Method  | Profile             |
| Fixed Effects SE Method   | Model-Based         |
| Degrees of Freedom Method | Containment         |

The “Class Level Information” table in [Output 59.1.2](#) lists the levels of all variables specified in the **CLASS** statement. You can check this table to make sure that the data are correct.

**Output 59.1.2** Split-Plot Example (*continued*)

| Class Level Information |        |         |
|-------------------------|--------|---------|
| Class                   | Levels | Values  |
| A                       | 3      | 1 2 3   |
| B                       | 2      | 1 2     |
| Block                   | 4      | 1 2 3 4 |

The “Dimensions” table in [Output 59.1.3](#) lists the magnitudes of various vectors and matrices. The **X** matrix is seen to be  $24 \times 12$ , and the **Z** matrix is  $24 \times 16$ .

**Output 59.1.3** Split-Plot Example (*continued*)

| Dimensions            |    |
|-----------------------|----|
| Covariance Parameters | 3  |
| Columns in X          | 12 |
| Columns in Z          | 16 |
| Subjects              | 1  |
| Max Obs Per Subject   | 24 |

The “Number of Observations” table in [Output 59.1.4](#) shows that all observations read from the data set are used in the analysis.

**Output 59.1.4** Split-Plot Example (*continued*)

| Number of Observations          |    |
|---------------------------------|----|
| Number of Observations Read     | 24 |
| Number of Observations Used     | 24 |
| Number of Observations Not Used | 0  |

PROC MIXED estimates the variance components for Block, A\*Block, and the residual by REML. The REML estimates are the values that maximize the likelihood of a set of linearly independent error contrasts, and they provide a correction for the downward bias found in the usual maximum likelihood estimates. The objective function is  $-2$  times the logarithm of the restricted likelihood, and PROC MIXED minimizes this objective function to obtain the estimates.

The minimization method is the Newton-Raphson algorithm, which uses the first and second derivatives of the objective function to iteratively find its minimum. The “Iteration History” table in [Output 59.1.5](#) records the steps of that optimization process. For this example, only one iteration is required to obtain the estimates. The Evaluations column reveals that the restricted likelihood is evaluated once for each of the iterations. A criterion of 0 indicates that the Newton-Raphson algorithm has converged.

**Output 59.1.5** Split-Plot Analysis (*continued*)

| Iteration History |             |                 |            |
|-------------------|-------------|-----------------|------------|
| Iteration         | Evaluations | -2 Res Log Like | Criterion  |
| 0                 | 1           | 139.81461222    |            |
| 1                 | 1           | 119.76184570    | 0.00000000 |

Convergence criteria met.

The REML estimates for the variance components of Block, A\*Block, and the residual are 62.40, 15.38, and 9.36, respectively, as listed in the Estimate column of the “Covariance Parameter Estimates” table in Output 59.1.6.

**Output 59.1.6** Split-Plot Analysis (*continued*)

| Covariance Parameter Estimates |          |
|--------------------------------|----------|
| Cov Parm                       | Estimate |
| Block                          | 62.3958  |
| A*Block                        | 15.3819  |
| Residual                       | 9.3611   |

The “Fit Statistics” table in Output 59.1.7 lists several pieces of information about the fitted mixed model, including the residual log likelihood. The Akaike (AIC) and Bayesian (BIC) information criteria can be used to compare different models; the ones with smaller values are preferred. The AICC information criteria is a small-sample bias-adjusted form of the Akaike criterion (Hurvich and Tsai 1989).

**Output 59.1.7** Split-Plot Analysis (*continued*)

| Fit Statistics           |       |
|--------------------------|-------|
| -2 Res Log Likelihood    | 119.8 |
| AIC (smaller is better)  | 125.8 |
| AICC (smaller is better) | 127.5 |
| BIC (smaller is better)  | 123.9 |

Finally, the fixed effects are tested by using Type 3 estimable functions (Output 59.1.8).

**Output 59.1.8** Split-Plot Analysis (*continued*)

| Type 3 Tests of Fixed Effects |           |           |         |        |
|-------------------------------|-----------|-----------|---------|--------|
| Effect                        | Num<br>DF | Den<br>DF | F Value | Pr > F |
| A                             | 2         | 6         | 4.07    | 0.0764 |
| B                             | 1         | 9         | 19.39   | 0.0017 |
| A*B                           | 2         | 9         | 4.02    | 0.0566 |

The tests match the one obtained from the following PROC GLM statements:

```
proc glm data=sp;
 class A B Block;
 model Y = A B A*B Block A*Block;
 test h=A e=A*Block;
run;
```

You can continue this analysis by producing solutions for the fixed and random effects and then testing various linear combinations of them by using the **CONTRAST** and **ESTIMATE** statements. If you use the same **CONTRAST** and **ESTIMATE** statements with PROC GLM, the test statistics correspond to the fixed-effects-only model. The test statistics from PROC MIXED incorporate the random effects.

The various “inference space” contrasts given by Stroup (1989a) can be implemented via the **ESTIMATE** statement. Consider the following examples:

```
proc mixed data=sp;
 class A B Block;
 model Y = A B A*B;
 random Block A*Block;
 estimate 'a1 mean narrow'
 intercept 1 A 1 B .5 .5 A*B .5 .5 |
 Block .25 .25 .25 .25
 A*Block .25 .25 .25 .25 0 0 0 0 0 0 0 0;

 estimate 'a1 mean intermed'
 intercept 1 A 1 B .5 .5 A*B .5 .5 |
 Block .25 .25 .25 .25;

 estimate 'a1 mean broad'
 intercept 1 a 1 b .5 .5 A*B .5 .5;
run;
```

These statements result in **Output 59.1.9**.



## Output 59.1.9 Inference Space Results

| The Mixed Procedure |          |                |    |         |         |
|---------------------|----------|----------------|----|---------|---------|
| Estimates           |          |                |    |         |         |
| Label               | Estimate | Standard Error | DF | t Value | Pr >  t |
| a1 mean narrow      | 32.8750  | 1.0817         | 9  | 30.39   | <.0001  |
| a1 mean intermed    | 32.8750  | 2.2396         | 9  | 14.68   | <.0001  |
| a1 mean broad       | 32.8750  | 4.5403         | 9  | 7.24    | <.0001  |

Note that all the estimates are equal, but their standard errors increase with the size of the inference space. The narrow inference space consists of the observed levels of Block and A\*Block, and the  $t$ -statistic value of 30.39 applies only to these levels. This is the same  $t$  statistic computed by PROC GLM, because it computes standard errors from the narrow inference space. The intermediate inference space consists of the observed levels of Block and the entire population of levels from which A\*Block are sampled. The  $t$ -statistic value of 14.68 applies to this intermediate space. The broad inference space consists of arbitrary random levels of both Block and A\*Block, and the  $t$ -statistic value of 7.24 is appropriate. Note that the larger the inference space, the weaker the conclusion. However, the broad inference space is usually the one of interest, and even in this space conclusive results are common. The highly significant  $p$ -value for 'a1 mean broad' is an example. You can also obtain the 'a1 mean broad' result by specifying A in an LSMEANS statement. For more discussion of the inference space concept, see McLean, Sanders, and Stroup (1991).

The following statements illustrate another feature of the RANDOM statement. Recall that the basic statements for a split-plot design with whole plots arranged in randomized blocks are as follows.

```
proc mixed;
 class A B Block;
 model Y = A B A*B;
 random Block A*Block;
run;
```

An equivalent way of specifying this model is as follows:

```
proc mixed data=sp;
 class A B Block;
 model Y = A B A*B;
 random intercept A / subject=Block;
run;
```

In general, if all of the effects in the RANDOM statement can be nested within one effect, you can specify that one effect by using the SUBJECT= option. The subject effect is, in a sense, “factored out” of the random effects. The specification that uses the SUBJECT= effect can result in faster execution times for large problems because PROC MIXED is able to perform the likelihood calculations separately for each subject.

## Example 59.2: Repeated Measures

The following data are from Pothoff and Roy (1964) and consist of growth measurements for 11 girls and 16 boys at ages 8, 10, 12, and 14. Some of the observations are suspect (for example, the third observation for person 20); however, all of the data are used here for comparison purposes.

The analysis strategy employs a linear growth curve model for the boys and girls as well as a variance-covariance model that incorporates correlations for all of the observations arising from the same person. The data are assumed to be Gaussian, and their likelihood is maximized to estimate the model parameters. For overviews of this approach to repeated measures, see Jennrich and Schluchter (1986); Louis (1988); Crowder and Hand (1990); Diggle, Liang, and Zeger (1994); Everitt (1995). Jennrich and Schluchter present results for the Pothoff and Roy data from various covariance structures. The PROC MIXED statements to fit an unstructured variance matrix (their Model 2) are as follows:

```
data pr;
 input Person Gender $ y1 y2 y3 y4;
 y=y1; Age=8; output;
 y=y2; Age=10; output;
 y=y3; Age=12; output;
 y=y4; Age=14; output;
 drop y1-y4;
 datalines;
 1 F 21.0 20.0 21.5 23.0
 2 F 21.0 21.5 24.0 25.5
 3 F 20.5 24.0 24.5 26.0
 4 F 23.5 24.5 25.0 26.5
 5 F 21.5 23.0 22.5 23.5
 6 F 20.0 21.0 21.0 22.5
 7 F 21.5 22.5 23.0 25.0
 8 F 23.0 23.0 23.5 24.0
 9 F 20.0 21.0 22.0 21.5
 10 F 16.5 19.0 19.0 19.5
 11 F 24.5 25.0 28.0 28.0
 12 M 26.0 25.0 29.0 31.0
 13 M 21.5 22.5 23.0 26.5
 14 M 23.0 22.5 24.0 27.5
 15 M 25.5 27.5 26.5 27.0
 16 M 20.0 23.5 22.5 26.0
 17 M 24.5 25.5 27.0 28.5
 18 M 22.0 22.0 24.5 26.5
 19 M 24.0 21.5 24.5 25.5
 20 M 23.0 20.5 31.0 26.0
 21 M 27.5 28.0 31.0 31.5
 22 M 23.0 23.0 23.5 25.0
 23 M 21.5 23.5 24.0 28.0
 24 M 17.0 24.5 26.0 29.5
 25 M 22.5 25.5 25.5 26.0
 26 M 23.0 24.5 26.0 30.0
 27 M 22.0 21.5 23.5 25.0
 ;
```

```

proc mixed data=pr method=ml covtest;
 class Person Gender;
 model y = Gender Age Gender*Age / s;
 repeated / type=un subject=Person r;
run;

```

To follow Jennrich and Schluchter, this example uses maximum likelihood (**METHOD=ML**) instead of the default REML to estimate the unknown covariance parameters. The **COVTEST** option requests asymptotic tests of all the covariance parameters.

The **MODEL** statement first lists the dependent variable *Y*. The fixed effects are then listed after the equal sign. The variable *Gender* requests a different intercept for the girls and boys, *Age* models an overall linear growth trend, and *Gender\*Age* makes the slopes different over time. It is actually not necessary to specify *Age* separately, but doing so enables PROC MIXED to carry out a test for heterogeneous slopes. The **SOLUTION** option requests the display of the fixed-effects solution vector.

The **REPEATED** statement contains no effects, taking advantage of the default assumption that the observations are ordered similarly for each subject. The **TYPE=UN** option requests an unstructured block for each **SUBJECT=Person**. The **R** matrix is, therefore, block diagonal with 27 blocks, each block consisting of identical 4×4 unstructured matrices. The 10 parameters of these unstructured blocks make up the covariance parameters estimated by maximum likelihood. The **R** option requests that the first block of **R** be displayed.

The results from this analysis are shown in [Output 59.2.1–Output 59.2.9](#).

#### Output 59.2.1 Repeated Measures Analysis with Unstructured Covariance Matrix

| The Mixed Procedure       |                |
|---------------------------|----------------|
| Model Information         |                |
| Data Set                  | WORK.PR        |
| Dependent Variable        | y              |
| Covariance Structure      | Unstructured   |
| Subject Effect            | Person         |
| Estimation Method         | ML             |
| Residual Variance Method  | None           |
| Fixed Effects SE Method   | Model-Based    |
| Degrees of Freedom Method | Between-Within |

In [Output 59.2.1](#), the covariance structure is listed as “Unstructured,” and no residual variance is used with this structure. The default degrees-of-freedom method here is “Between-Within.”

**Output 59.2.2** Repeated Measures Analysis (*continued*)

| Class Level Information |        |                                                                               |
|-------------------------|--------|-------------------------------------------------------------------------------|
| Class                   | Levels | Values                                                                        |
| Person                  | 27     | 1 2 3 4 5 6 7 8 9 10 11 12 13<br>14 15 16 17 18 19 20 21 22 23<br>24 25 26 27 |
| Gender                  | 2      | F M                                                                           |

In [Output 59.2.2](#), note that Person has 27 levels and Gender has 2.

**Output 59.2.3** Repeated Measures Analysis (*continued*)

| Dimensions            |    |
|-----------------------|----|
| Covariance Parameters | 10 |
| Columns in X          | 6  |
| Columns in Z          | 0  |
| Subjects              | 27 |
| Max Obs Per Subject   | 4  |

In [Output 59.2.3](#), the 10 covariance parameters result from the  $4 \times 4$  unstructured blocks of **R**. There is no **Z** matrix for this model, and each of the 27 subjects has a maximum of 4 observations.

**Output 59.2.4** Repeated Measures Analysis (*continued*)

| Number of Observations          |     |
|---------------------------------|-----|
| Number of Observations Read     | 108 |
| Number of Observations Used     | 108 |
| Number of Observations Not Used | 0   |

| Iteration History |             |              |            |
|-------------------|-------------|--------------|------------|
| Iteration         | Evaluations | -2 Log Like  | Criterion  |
| 0                 | 1           | 478.24175986 |            |
| 1                 | 2           | 419.47721707 | 0.00000152 |
| 2                 | 1           | 419.47704812 | 0.00000000 |

Convergence criteria met.

Three Newton-Raphson iterations are required to find the maximum likelihood estimates ([Output 59.2.4](#)). The default relative Hessian criterion has a final value less than  $1E-8$ , indicating the convergence of the Newton-Raphson algorithm and the attainment of an optimum.

**Output 59.2.5** Repeated Measures Analysis (*continued*)

| Estimated R Matrix for Person 1 |        |        |        |        |
|---------------------------------|--------|--------|--------|--------|
| Row                             | Col1   | Col2   | Col3   | Col4   |
| 1                               | 5.1192 | 2.4409 | 3.6105 | 2.5222 |
| 2                               | 2.4409 | 3.9279 | 2.7175 | 3.0624 |
| 3                               | 3.6105 | 2.7175 | 5.9798 | 3.8235 |
| 4                               | 2.5222 | 3.0624 | 3.8235 | 4.6180 |

The 4×4 matrix in [Output 59.2.5](#) is the estimated unstructured covariance matrix. It is the estimate of the first block of **R**, and the other 26 blocks all have the same estimate.

**Output 59.2.6** Repeated Measures Analysis (*continued*)

| Covariance Parameter Estimates |         |          |                |         |        |
|--------------------------------|---------|----------|----------------|---------|--------|
| Cov Parm                       | Subject | Estimate | Standard Error | Z Value | Pr Z   |
| UN(1,1)                        | Person  | 5.1192   | 1.4169         | 3.61    | 0.0002 |
| UN(2,1)                        | Person  | 2.4409   | 0.9835         | 2.48    | 0.0131 |
| UN(2,2)                        | Person  | 3.9279   | 1.0824         | 3.63    | 0.0001 |
| UN(3,1)                        | Person  | 3.6105   | 1.2767         | 2.83    | 0.0047 |
| UN(3,2)                        | Person  | 2.7175   | 1.0740         | 2.53    | 0.0114 |
| UN(3,3)                        | Person  | 5.9798   | 1.6279         | 3.67    | 0.0001 |
| UN(4,1)                        | Person  | 2.5222   | 1.0649         | 2.37    | 0.0179 |
| UN(4,2)                        | Person  | 3.0624   | 1.0135         | 3.02    | 0.0025 |
| UN(4,3)                        | Person  | 3.8235   | 1.2508         | 3.06    | 0.0022 |
| UN(4,4)                        | Person  | 4.6180   | 1.2573         | 3.67    | 0.0001 |

The “Covariance Parameter Estimates” table in [Output 59.2.6](#) lists the 10 estimated covariance parameters in order; note their correspondence to the first block of **R** displayed in [Output 59.2.5](#). The parameter estimates are labeled according to their location in the block in the Cov Parm column, and all of these estimates are associated with Person as the subject effect. The Std Error column lists approximate standard errors of the covariance parameters obtained from the inverse Hessian matrix. These standard errors lead to approximate Wald Z statistics, which are compared with the standard normal distribution. The results of these tests indicate that all the parameters are significantly different from 0; however, the Wald test can be unreliable in small samples.

To carry out Wald tests of various linear combinations of these parameters, use the following procedure. First, run the statements again, adding the **ASYCOV** option and an ODS statement:

```
ods output CovParms=cp AsyCov=asy;
proc mixed data=pr method=ml covtest asycov;
 class Person Gender;
 model y = Gender Age Gender*Age / s;
 repeated / type=un subject=Person r;
run;
```

This creates two data sets, `cp` and `asy`, which contain the covariance parameter estimates and their asymptotic variance covariance matrix, respectively. Then read these data sets into the SAS/IML matrix programming language as follows:

```
proc iml;
 use cp;
 read all var {Estimate} into est;
 use asy;
 read all var ('CovP1':'CovP10') into asy;
```

You can then construct your desired linear combinations and corresponding quadratic forms with the `asy` matrix.

### Output 59.2.7 Repeated Measures Analysis (*continued*)

| Fit Statistics                   |            |            |
|----------------------------------|------------|------------|
| -2 Log Likelihood                |            | 419.5      |
| AIC (smaller is better)          |            | 447.5      |
| AICC (smaller is better)         |            | 452.0      |
| BIC (smaller is better)          |            | 465.6      |
| Null Model Likelihood Ratio Test |            |            |
| DF                               | Chi-Square | Pr > ChiSq |
| 9                                | 58.76      | <.0001     |

The null model likelihood ratio test (LRT) in [Output 59.2.7](#) is highly significant for this model, indicating that the unstructured covariance matrix is preferred to the diagonal matrix of the ordinary least squares null model. The degrees of freedom for this test is 9, which is the difference between 10 and the 1 parameter for the null model's diagonal matrix.

### Output 59.2.8 Repeated Measures Analysis (*continued*)

| Solution for Fixed Effects |        |          |                |    |         |         |
|----------------------------|--------|----------|----------------|----|---------|---------|
| Effect                     | Gender | Estimate | Standard Error | DF | t Value | Pr >  t |
| Intercept                  |        | 15.8423  | 0.9356         | 25 | 16.93   | <.0001  |
| Gender                     | F      | 1.5831   | 1.4658         | 25 | 1.08    | 0.2904  |
| Gender                     | M      | 0        | .              | .  | .       | .       |
| Age                        |        | 0.8268   | 0.07911        | 25 | 10.45   | <.0001  |
| Age*Gender                 | F      | -0.3504  | 0.1239         | 25 | -2.83   | 0.0091  |
| Age*Gender                 | M      | 0        | .              | .  | .       | .       |

The “Solution for Fixed Effects” table in [Output 59.2.8](#) lists the solution vector for the fixed effects. The estimate of the boys' intercept is 15.8423, while that for the girls is  $15.8423 + 1.5831 = 17.0654$ . Similarly, the estimate for the boys' slope is 0.8268, while that for the girls is  $0.8268 - 0.3504 = 0.4764$ . Thus the

girls' starting point is larger than that for the boys, but their growth rate is about half that of the boys.

Note that two of the estimates equal 0; this is a result of the overparameterized model used by PROC MIXED. You can obtain a full-rank parameterization by using the following **MODEL** statement:

```
model y = Gender Gender*Age / noint s;
```

Here, the **NOINT** option causes the different intercepts to be fit directly as the two levels of Gender. However, this alternative specification results in different tests for these effects.

**Output 59.2.9** Repeated Measures Analysis (*continued*)

| Type 3 Tests of Fixed Effects |           |           |         |        |
|-------------------------------|-----------|-----------|---------|--------|
| Effect                        | Num<br>DF | Den<br>DF | F Value | Pr > F |
| Gender                        | 1         | 25        | 1.17    | 0.2904 |
| Age                           | 1         | 25        | 110.54  | <.0001 |
| Age*Gender                    | 1         | 25        | 7.99    | 0.0091 |

The “Type 3 Tests of Fixed Effects” table in **Output 59.2.9** displays Type 3 tests for all of the fixed effects. These tests are partial in the sense that they account for all of the other fixed effects in the model. In addition, you can use the **HTYPE=** option in the **MODEL** statement to obtain Type 1 (sequential) or Type 2 (also partial) tests of effects.

It is usually best to consider higher-order terms first, and in this case the **Age\*Gender** test reveals a difference between the slopes that is statistically significant at the 1% level. Note that the  $p$ -value for this test (0.0091) is the same as the  $p$ -value in the “Age\*Gender F” row in the “Solution for Fixed Effects” table (**Output 59.2.8**) and that the  $F$  statistic (7.99) is the square of the  $t$  statistic (−2.83), ignoring rounding error. Similar connections are evident among the other rows in these two tables.

The **Age** test is one for an overall growth curve accounting for possible heterogeneous slopes, and it is highly significant. Finally, the **Gender** row tests the null hypothesis of a common intercept, and this hypothesis cannot be rejected from these data.

As an alternative to the  $F$  tests shown here, you can carry out likelihood ratio tests of various hypotheses by fitting the reduced models, subtracting  $-2 \log$  likelihoods, and comparing the resulting statistics with  $\chi^2$  distributions.

Since the different levels of the repeated effect represent different years, it is natural to try fitting a time series model to the data within each subject. To obtain time series structures in **R**, you can replace **TYPE=UN** with **TYPE=AR(1)** or **TYPE=TOEP** to obtain the first- or  $n$ th-order autoregressive covariance matrices, respectively. For example, the statements to fit an **AR(1)** structure are as follows:

```
/* first-order autoregressive */
proc mixed data=pr method=ml;
 class Person Gender;
 model y = Gender Age Gender*Age / s;
 repeated / type=ar(1) sub=Person r;
run;
```

To fit a random coefficients model, use the following statements:

```
/* random coefficients model */
proc mixed data=pr method=ml;
 class Person Gender;
 model y = Gender Age Gender*Age / s;
 random intercept Age / type=un sub=Person g;
run;
```

This specifies an unstructured covariance matrix for the random intercept and slope. In mixed model notation, **G** is block diagonal with identical 2×2 unstructured blocks for each person. By default, **R** becomes  $\sigma^2\mathbf{I}$ . See [Example 59.5](#) for further information about this model.

Finally, you can fit a compound symmetry structure by using **TYPE=CS**, as follows:

```
proc mixed data=pr method=ml covtest;
 class Person Gender;
 model y = Gender Age Gender*Age / s;
 repeated / type=cs subject=Person r;
run;
```

The results from this analysis are shown in [Output 59.2.10–Output 59.2.17](#).

The “Model Information” table in [Output 59.2.10](#) is the same as before except for the change in “Covariance Structure.”

**Output 59.2.10** Repeated Measures Analysis with Compound Symmetry Structure

| The Mixed Procedure       |                   |
|---------------------------|-------------------|
| Model Information         |                   |
| Data Set                  | WORK.PR           |
| Dependent Variable        | y                 |
| Covariance Structure      | Compound Symmetry |
| Subject Effect            | Person            |
| Estimation Method         | ML                |
| Residual Variance Method  | Profile           |
| Fixed Effects SE Method   | Model-Based       |
| Degrees of Freedom Method | Between-Within    |

The “Dimensions” table in [Output 59.2.11](#) shows that there are only two covariance parameters in the compound symmetry model; this covariance structure has common variance and common covariance.

**Output 59.2.11** Analysis with Compound Symmetry (*continued*)

| Class Level Information |        |                                                                               |
|-------------------------|--------|-------------------------------------------------------------------------------|
| Class                   | Levels | Values                                                                        |
| Person                  | 27     | 1 2 3 4 5 6 7 8 9 10 11 12 13<br>14 15 16 17 18 19 20 21 22 23<br>24 25 26 27 |
| Gender                  | 2      | F M                                                                           |



**Output 59.2.11** *continued*

| Dimensions                      |     |
|---------------------------------|-----|
| Covariance Parameters           | 2   |
| Columns in X                    | 6   |
| Columns in Z                    | 0   |
| Subjects                        | 27  |
| Max Obs Per Subject             | 4   |
| Number of Observations          |     |
| Number of Observations Read     | 108 |
| Number of Observations Used     | 108 |
| Number of Observations Not Used | 0   |

Since the data are balanced, only one step is required to find the estimates ([Output 59.2.12](#)).

**Output 59.2.12** Analysis with Compound Symmetry (*continued*)

| Iteration History         |             |              |            |
|---------------------------|-------------|--------------|------------|
| Iteration                 | Evaluations | -2 Log Like  | Criterion  |
| 0                         | 1           | 478.24175986 |            |
| 1                         | 1           | 428.63905802 | 0.00000000 |
| Convergence criteria met. |             |              |            |

[Output 59.2.13](#) displays the estimated **R** matrix for the first subject. Note the compound symmetry structure here, which consists of a common covariance with a diagonal enhancement.

**Output 59.2.13** Analysis with Compound Symmetry (*continued*)

| Estimated R Matrix for Person 1 |        |        |        |        |
|---------------------------------|--------|--------|--------|--------|
| Row                             | Col1   | Col2   | Col3   | Col4   |
| 1                               | 4.9052 | 3.0306 | 3.0306 | 3.0306 |
| 2                               | 3.0306 | 4.9052 | 3.0306 | 3.0306 |
| 3                               | 3.0306 | 3.0306 | 4.9052 | 3.0306 |
| 4                               | 3.0306 | 3.0306 | 3.0306 | 4.9052 |

The common covariance is estimated to be 3.0306, as listed in the CS row of the “Covariance Parameter Estimates” table in [Output 59.2.14](#), and the residual variance is estimated to be 1.8746, as listed in the Residual row. You can use these two numbers to estimate the intraclass correlation coefficient (ICC) for this model. Here, the ICC estimate equals  $3.0306 / (3.0306 + 1.8746) = 0.6178$ . You can also obtain this

number by adding the `RCORR` option to the `REPEATED` statement.

**Output 59.2.14** Analysis with Compound Symmetry (*continued*)

| Covariance Parameter Estimates |         |          |                |         |        |
|--------------------------------|---------|----------|----------------|---------|--------|
| Cov Parm                       | Subject | Estimate | Standard Error | Z Value | Pr Z   |
| CS                             | Person  | 3.0306   | 0.9552         | 3.17    | 0.0015 |
| Residual                       |         | 1.8746   | 0.2946         | 6.36    | <.0001 |

In the case shown in [Output 59.2.15](#), the null model LRT has only one degree of freedom, corresponding to the common covariance parameter. The test indicates that modeling this extra covariance is superior to fitting the simple null model.

**Output 59.2.15** Analysis with Compound Symmetry (*continued*)

| Fit Statistics           |       |
|--------------------------|-------|
| -2 Log Likelihood        | 428.6 |
| AIC (smaller is better)  | 440.6 |
| AICC (smaller is better) | 441.5 |
| BIC (smaller is better)  | 448.4 |

| Null Model Likelihood Ratio Test |            |            |
|----------------------------------|------------|------------|
| DF                               | Chi-Square | Pr > ChiSq |
| 1                                | 49.60      | <.0001     |

Note that the fixed-effects estimates and their standard errors ([Output 59.2.16](#)) are not very different from those in the preceding unstructured example ([Output 59.2.8](#)).

**Output 59.2.16** Analysis with Compound Symmetry (*continued*)

| Solution for Fixed Effects |        |          |                |    |         |         |
|----------------------------|--------|----------|----------------|----|---------|---------|
| Effect                     | Gender | Estimate | Standard Error | DF | t Value | Pr >  t |
| Intercept                  |        | 16.3406  | 0.9631         | 25 | 16.97   | <.0001  |
| Gender                     | F      | 1.0321   | 1.5089         | 25 | 0.68    | 0.5003  |
| Gender                     | M      | 0        | .              | .  | .       | .       |
| Age                        |        | 0.7844   | 0.07654        | 79 | 10.25   | <.0001  |
| Age*Gender                 | F      | -0.3048  | 0.1199         | 79 | -2.54   | 0.0130  |
| Age*Gender                 | M      | 0        | .              | .  | .       | .       |

The  $F$  tests shown in [Output 59.2.17](#) are also similar to those from the preceding unstructured example ([Output 59.2.9](#)). Again, the slopes are significantly different but the intercepts are not.

**Output 59.2.17** Analysis with Compound Symmetry (*continued*)

| Type 3 Tests of Fixed Effects |           |           |         |        |
|-------------------------------|-----------|-----------|---------|--------|
| Effect                        | Num<br>DF | Den<br>DF | F Value | Pr > F |
| Gender                        | 1         | 25        | 0.47    | 0.5003 |
| Age                           | 1         | 79        | 111.10  | <.0001 |
| Age*Gender                    | 1         | 79        | 6.46    | 0.0130 |

You can fit the same compound symmetry model with the following specification by using the [RANDOM](#) statement:

```
proc mixed data=pr method=ml;
 class Person Gender;
 model y = Gender Age Gender*Age / s;
 random Person;
run;
```

Compound symmetry is the structure that Jennrich and Schluchter deemed best among the ones they fit. To carry the analysis one step further, you can use the [GROUP=](#) option as follows to specify heterogeneity of this structure across girls and boys:

```
proc mixed data=pr method=ml;
 class Person Gender;
 model y = Gender Age Gender*Age / s;
 repeated / type=cs subject=Person group=Gender;
run;
```

The results from this analysis are shown in [Output 59.2.18–Output 59.2.24](#). Note that in [Output 59.2.18](#) Gender is listed as a “Group Effect.”

**Output 59.2.18** Repeated Measures Analysis with Heterogeneous Structures

| The Mixed Procedure       |                   |
|---------------------------|-------------------|
| Model Information         |                   |
| Data Set                  | WORK.PR           |
| Dependent Variable        | y                 |
| Covariance Structure      | Compound Symmetry |
| Subject Effect            | Person            |
| Group Effect              | Gender            |
| Estimation Method         | ML                |
| Residual Variance Method  | None              |
| Fixed Effects SE Method   | Model-Based       |
| Degrees of Freedom Method | Between-Within    |

The four covariance parameters listed in [Output 59.2.19](#) result from the two compound symmetry structures corresponding to the two levels of Gender.

**Output 59.2.19** Analysis with Heterogeneous Structures (*continued*)

| Class Level Information         |        |                                                                               |
|---------------------------------|--------|-------------------------------------------------------------------------------|
| Class                           | Levels | Values                                                                        |
| Person                          | 27     | 1 2 3 4 5 6 7 8 9 10 11 12 13<br>14 15 16 17 18 19 20 21 22 23<br>24 25 26 27 |
| Gender                          | 2      | F M                                                                           |
| Dimensions                      |        |                                                                               |
| Covariance Parameters           |        | 4                                                                             |
| Columns in X                    |        | 6                                                                             |
| Columns in Z                    |        | 0                                                                             |
| Subjects                        |        | 27                                                                            |
| Max Obs Per Subject             |        | 4                                                                             |
| Number of Observations          |        |                                                                               |
| Number of Observations Read     |        | 108                                                                           |
| Number of Observations Used     |        | 108                                                                           |
| Number of Observations Not Used |        | 0                                                                             |

As [Output 59.2.20](#) shows, even with the heterogeneity, only one iteration is required for convergence.

**Output 59.2.20** Analysis with Heterogeneous Structures (*continued*)

| Iteration History         |             |              |            |
|---------------------------|-------------|--------------|------------|
| Iteration                 | Evaluations | -2 Log Like  | Criterion  |
| 0                         | 1           | 478.24175986 |            |
| 1                         | 1           | 408.81297228 | 0.00000000 |
| Convergence criteria met. |             |              |            |

The “Covariance Parameter Estimates” table in [Output 59.2.21](#) lists the heterogeneous estimates. Note that both the common covariance and the diagonal enhancement differ between girls and boys.

**Output 59.2.21** Analysis with Heterogeneous Structures (*continued*)

| Covariance Parameter Estimates |         |          |          |
|--------------------------------|---------|----------|----------|
| Cov Parm                       | Subject | Group    | Estimate |
| Variance                       | Person  | Gender F | 0.5900   |
| CS                             | Person  | Gender F | 3.8804   |
| Variance                       | Person  | Gender M | 2.7577   |
| CS                             | Person  | Gender M | 2.4463   |

As [Output 59.2.22](#) shows, both Akaike's information criterion (424.8) and Schwarz's Bayesian information criterion (435.2) are smaller for this model than for the homogeneous compound symmetry model (440.6 and 448.4, respectively). This indicates that the heterogeneous model is more appropriate. To construct the likelihood ratio test between the two models, subtract the  $-2 \log$  likelihood values:  $428.6 - 408.8 = 19.8$ . Comparing this value with the  $\chi^2$  distribution with two degrees of freedom yields a  $p$ -value less than 0.0001, again favoring the heterogeneous model.

**Output 59.2.22** Analysis with Heterogeneous Structures (*continued*)

| Fit Statistics           |       |
|--------------------------|-------|
| -2 Log Likelihood        | 408.8 |
| AIC (smaller is better)  | 424.8 |
| AICC (smaller is better) | 426.3 |
| BIC (smaller is better)  | 435.2 |

| Null Model Likelihood Ratio Test |            |            |
|----------------------------------|------------|------------|
| DF                               | Chi-Square | Pr > ChiSq |
| 3                                | 69.43      | <.0001     |

Note that the fixed-effects estimates shown in [Output 59.2.23](#) are the same as in the homogeneous case, but the standard errors are different.

**Output 59.2.23** Analysis with Heterogeneous Structures (*continued*)

| Solution for Fixed Effects |        |          |                |    |         |         |
|----------------------------|--------|----------|----------------|----|---------|---------|
| Effect                     | Gender | Estimate | Standard Error | DF | t Value | Pr >  t |
| Intercept                  |        | 16.3406  | 1.1130         | 25 | 14.68   | <.0001  |
| Gender                     | F      | 1.0321   | 1.3890         | 25 | 0.74    | 0.4644  |
| Gender                     | M      | 0        | .              | .  | .       | .       |
| Age                        |        | 0.7844   | 0.09283        | 79 | 8.45    | <.0001  |
| Age*Gender                 | F      | -0.3048  | 0.1063         | 79 | -2.87   | 0.0053  |
| Age*Gender                 | M      | 0        | .              | .  | .       | .       |

The fixed-effects tests shown in [Output 59.2.24](#) are similar to those from previous models, although the  $p$ -values do change as a result of specifying a different covariance structure. It is important for you to select a reasonable covariance structure in order to obtain valid inferences for your fixed effects.

**Output 59.2.24** Analysis with Heterogeneous Structures (*continued*)

| Type 3 Tests of Fixed Effects |           |           |         |        |
|-------------------------------|-----------|-----------|---------|--------|
| Effect                        | Num<br>DF | Den<br>DF | F Value | Pr > F |
| Gender                        | 1         | 25        | 0.55    | 0.4644 |
| Age                           | 1         | 79        | 141.37  | <.0001 |
| Age*Gender                    | 1         | 79        | 8.22    | 0.0053 |

## Example 59.3: Plotting the Likelihood

The data for this example are from Hemmerle and Hartley (1973) and are also used for an example in the VARCOMP procedure. The response variable consists of measurements from an oven experiment, and the model contains a fixed effect A and random effects B and A\*B.

The SAS statements are as follows:

```
data hh;
 input a b y @@;
 datalines;
1 1 237 1 1 254 1 1 246
1 2 178 1 2 179
2 1 208 2 1 178 2 1 187
2 2 146 2 2 145 2 2 141
3 1 186 3 1 183
3 2 142 3 2 125 3 2 136
;

ods output ParmSearch=parms;
proc mixed data=hh asycov mmeq mmeqsol covtest;
 class a b;
 model y = a / outp=predicted;
 random b a*b;
 lsmeans a;
 parms (17 to 20 by .1) (.3 to .4 by .005) (1.0);
run;
proc print data=predicted;
run;
```

The **ASYCOV** option in the **PROC MIXED** statement requests the asymptotic variance matrix of the covariance parameter estimates. This matrix is the observed inverse Fisher information matrix, which equals  $2\mathbf{H}^{-1}$ , where  $\mathbf{H}$  is the Hessian matrix of the objective function evaluated at the final covariance parameter estimates. The **MMEQ** and **MMEQSOL** options in the **PROC MIXED** statement request that the mixed model equations and their solution be displayed.

The `OUTP=` option in the `MODEL` statement produces the data set predicted, containing the predicted values. Least squares means (LSMEANS) are requested for A. The `PARMS` and `ODS` statements are used to construct a data set containing the likelihood surface.

The results from this analysis are shown in [Output 59.3.1–Output 59.3.13](#).

The “Model Information” table in [Output 59.3.1](#) lists details about this variance components model.

**Output 59.3.1** Model Information

| The Mixed Procedure       |                     |
|---------------------------|---------------------|
| Model Information         |                     |
| Data Set                  | WORK.HH             |
| Dependent Variable        | y                   |
| Covariance Structure      | Variance Components |
| Estimation Method         | REML                |
| Residual Variance Method  | Profile             |
| Fixed Effects SE Method   | Model-Based         |
| Degrees of Freedom Method | Containment         |

The “Class Level Information” table in [Output 59.3.2](#) lists the levels for A and B.

**Output 59.3.2** Class Level Information

| Class Level Information |        |        |
|-------------------------|--------|--------|
| Class                   | Levels | Values |
| a                       | 3      | 1 2 3  |
| b                       | 2      | 1 2    |

The “Dimensions” table in [Output 59.3.3](#) reveals that  $\mathbf{X}$  is  $16 \times 4$  and  $\mathbf{Z}$  is  $16 \times 8$ . Since there are no `SUBJECT=` effects, PROC MIXED considers the data to be effectively from one subject with 16 observations.

**Output 59.3.3** Model Dimensions and Number of Observations

| Dimensions            |    |
|-----------------------|----|
| Covariance Parameters | 3  |
| Columns in X          | 4  |
| Columns in Z          | 8  |
| Subjects              | 1  |
| Max Obs Per Subject   | 16 |

**Output 59.3.3** *continued*

| Number of Observations          |    |
|---------------------------------|----|
| Number of Observations Read     | 16 |
| Number of Observations Used     | 16 |
| Number of Observations Not Used | 0  |

Only a portion of the “Parameter Search” table is shown in [Output 59.3.4](#) because the full listing has 651 rows.

**Output 59.3.4** Selected Results of Parameter Search

| The Mixed Procedure |        |        |          |              |                 |
|---------------------|--------|--------|----------|--------------|-----------------|
| CovP1               | CovP2  | CovP3  | Variance | Res Log Like | -2 Res Log Like |
| 17.0000             | 0.3000 | 1.0000 | 80.1400  | -52.4699     | 104.9399        |
| 17.0000             | 0.3050 | 1.0000 | 80.0466  | -52.4697     | 104.9393        |
| 17.0000             | 0.3100 | 1.0000 | 79.9545  | -52.4694     | 104.9388        |
| 17.0000             | 0.3150 | 1.0000 | 79.8637  | -52.4692     | 104.9384        |
| 17.0000             | 0.3200 | 1.0000 | 79.7742  | -52.4691     | 104.9381        |
| 17.0000             | 0.3250 | 1.0000 | 79.6859  | -52.4690     | 104.9379        |
| 17.0000             | 0.3300 | 1.0000 | 79.5988  | -52.4689     | 104.9378        |
| 17.0000             | 0.3350 | 1.0000 | 79.5129  | -52.4689     | 104.9377        |
| 17.0000             | 0.3400 | 1.0000 | 79.4282  | -52.4689     | 104.9377        |
| 17.0000             | 0.3450 | 1.0000 | 79.3447  | -52.4689     | 104.9378        |
| .                   | .      | .      | .        | .            | .               |
| .                   | .      | .      | .        | .            | .               |
| .                   | .      | .      | .        | .            | .               |
| 20.0000             | 0.3550 | 1.0000 | 78.2003  | -52.4683     | 104.9366        |
| 20.0000             | 0.3600 | 1.0000 | 78.1201  | -52.4684     | 104.9368        |
| 20.0000             | 0.3650 | 1.0000 | 78.0409  | -52.4685     | 104.9370        |
| 20.0000             | 0.3700 | 1.0000 | 77.9628  | -52.4687     | 104.9373        |
| 20.0000             | 0.3750 | 1.0000 | 77.8857  | -52.4689     | 104.9377        |
| 20.0000             | 0.3800 | 1.0000 | 77.8096  | -52.4691     | 104.9382        |
| 20.0000             | 0.3850 | 1.0000 | 77.7345  | -52.4693     | 104.9387        |
| 20.0000             | 0.3900 | 1.0000 | 77.6603  | -52.4696     | 104.9392        |
| 20.0000             | 0.3950 | 1.0000 | 77.5871  | -52.4699     | 104.9399        |
| 20.0000             | 0.4000 | 1.0000 | 77.5148  | -52.4703     | 104.9406        |

As [Output 59.3.5](#) shows, convergence occurs quickly because PROC MIXED starts from the best value from the grid search.



**Output 59.3.5** Iteration History and Convergence Status

| Iteration History         |             |                 |            |  |
|---------------------------|-------------|-----------------|------------|--|
| Iteration                 | Evaluations | -2 Res Log Like | Criterion  |  |
| 1                         | 2           | 104.93416367    | 0.00000000 |  |
| Convergence criteria met. |             |                 |            |  |

The “Covariance Parameter Estimates” table in [Output 59.3.6](#) lists the variance components estimates. Note that B is much more variable than A\*B.

**Output 59.3.6** Estimated Covariance Parameters

| Covariance Parameter Estimates |          |                |         |        |
|--------------------------------|----------|----------------|---------|--------|
| Cov Parm                       | Estimate | Standard Error | Z Value | Pr > Z |
| b                              | 1464.36  | 2098.01        | 0.70    | 0.2426 |
| a*b                            | 26.9581  | 59.6570        | 0.45    | 0.3257 |
| Residual                       | 78.8426  | 35.3512        | 2.23    | 0.0129 |

The asymptotic covariance matrix in [Output 59.3.7](#) also reflects the large variability of B relative to A\*B.

**Output 59.3.7** Asymptotic Covariance Matrix of Covariance Parameters

| Asymptotic Covariance Matrix of Estimates |          |         |         |         |
|-------------------------------------------|----------|---------|---------|---------|
| Row                                       | Cov Parm | CovP1   | CovP2   | CovP3   |
| 1                                         | b        | 4401640 | 1.2831  | -273.32 |
| 2                                         | a*b      | 1.2831  | 3558.96 | -502.84 |
| 3                                         | Residual | -273.32 | -502.84 | 1249.71 |

As [Output 59.3.8](#) shows, the PARMS likelihood ratio test (LRT) compares the best model from the grid search with the final fitted model. Since these models are nearly the same, the LRT is not significant.

**Output 59.3.8** Fit Statistics and Likelihood Ratio Test

| Fit Statistics           |       |
|--------------------------|-------|
| -2 Res Log Likelihood    | 104.9 |
| AIC (smaller is better)  | 110.9 |
| AICC (smaller is better) | 113.6 |
| BIC (smaller is better)  | 107.0 |

**Output 59.3.8** *continued*

| PARMS Model Likelihood Ratio Test |            |            |
|-----------------------------------|------------|------------|
| DF                                | Chi-Square | Pr > ChiSq |
| 2                                 | 0.00       | 1.0000     |

The mixed model equations are analogous to the normal equations in the standard linear model. As [Output 59.3.9](#) shows, for this example, rows 1–4 correspond to the fixed effects, rows 5–12 correspond to the random effects, and Col13 corresponds to the dependent variable.

**Output 59.3.9** Mixed Model Equations

| Mixed Model Equations |           |   |   |         |         |         |         |         |         |         |
|-----------------------|-----------|---|---|---------|---------|---------|---------|---------|---------|---------|
| Row                   | Effect    | a | b | Col1    | Col2    | Col3    | Col4    | Col5    | Col6    | Col7    |
| 1                     | Intercept |   |   | 0.2029  | 0.06342 | 0.07610 | 0.06342 | 0.1015  | 0.1015  | 0.03805 |
| 2                     | a         | 1 |   | 0.06342 | 0.06342 |         |         | 0.03805 | 0.02537 | 0.03805 |
| 3                     | a         | 2 |   | 0.07610 |         | 0.07610 |         | 0.03805 | 0.03805 |         |
| 4                     | a         | 3 |   | 0.06342 |         |         | 0.06342 | 0.02537 | 0.03805 |         |
| 5                     | b         |   | 1 | 0.1015  | 0.03805 | 0.03805 | 0.02537 | 0.1022  |         | 0.03805 |
| 6                     | b         |   | 2 | 0.1015  | 0.02537 | 0.03805 | 0.03805 |         | 0.1022  |         |
| 7                     | a*b       | 1 | 1 | 0.03805 | 0.03805 |         |         | 0.03805 |         | 0.07515 |
| 8                     | a*b       | 1 | 2 | 0.02537 | 0.02537 |         |         |         | 0.02537 |         |
| 9                     | a*b       | 2 | 1 | 0.03805 |         | 0.03805 |         | 0.03805 |         |         |
| 10                    | a*b       | 2 | 2 | 0.03805 |         | 0.03805 |         |         | 0.03805 |         |
| 11                    | a*b       | 3 | 1 | 0.02537 |         |         | 0.02537 | 0.02537 |         |         |
| 12                    | a*b       | 3 | 2 | 0.03805 |         |         | 0.03805 |         | 0.03805 |         |

| Mixed Model Equations |         |         |         |         |         |         |
|-----------------------|---------|---------|---------|---------|---------|---------|
| Row                   | Col8    | Col9    | Col10   | Col11   | Col12   | Col13   |
| 1                     | 0.02537 | 0.03805 | 0.03805 | 0.02537 | 0.03805 | 36.4143 |
| 2                     | 0.02537 |         |         |         |         | 13.8757 |
| 3                     |         | 0.03805 | 0.03805 |         |         | 12.7469 |
| 4                     |         |         |         | 0.02537 | 0.03805 | 9.7917  |
| 5                     |         | 0.03805 |         | 0.02537 |         | 21.2956 |
| 6                     | 0.02537 |         | 0.03805 |         | 0.03805 | 15.1187 |
| 7                     |         |         |         |         |         | 9.3477  |
| 8                     | 0.06246 |         |         |         |         | 4.5280  |
| 9                     |         | 0.07515 |         |         |         | 7.2676  |
| 10                    |         |         | 0.07515 |         |         | 5.4793  |
| 11                    |         |         |         | 0.06246 |         | 4.6802  |
| 12                    |         |         |         |         | 0.07515 | 5.1115  |

The solution matrix in [Output 59.3.10](#) results from sweeping all but the last row of the mixed model equations matrix. The final column contains a solution vector for the fixed and random effects. The first four rows correspond to fixed effects and the last eight correspond to random effects.

**Output 59.3.10** Solutions of the Mixed Model Equations

| Mixed Model Equations Solution |           |   |   |          |          |          |      |         |         |          |
|--------------------------------|-----------|---|---|----------|----------|----------|------|---------|---------|----------|
| Row                            | Effect    | a | b | Col1     | Col2     | Col3     | Col4 | Col5    | Col6    | Col7     |
| 1                              | Intercept |   |   | 761.84   | -29.7718 | -29.6578 |      | -731.14 | -733.22 | -0.4680  |
| 2                              | a         | 1 |   | -29.7718 | 59.5436  | 29.7718  |      | -2.0764 | 2.0764  | -14.0239 |
| 3                              | a         | 2 |   | -29.6578 | 29.7718  | 56.2773  |      | -1.0382 | 1.0382  | 0.4680   |
| 4                              | a         | 3 |   |          |          |          |      |         |         |          |
| 5                              | b         |   | 1 | -731.14  | -2.0764  | -1.0382  |      | 741.63  | 722.73  | -4.2598  |
| 6                              | b         |   | 2 | -733.22  | 2.0764   | 1.0382   |      | 722.73  | 741.63  | 4.2598   |
| 7                              | a*b       | 1 | 1 | -0.4680  | -14.0239 | 0.4680   |      | -4.2598 | 4.2598  | 22.8027  |
| 8                              | a*b       | 1 | 2 | 0.4680   | -12.9342 | -0.4680  |      | 4.2598  | -4.2598 | 4.1555   |
| 9                              | a*b       | 2 | 1 | -0.5257  | 1.0514   | -12.9534 |      | -4.7855 | 4.7855  | 2.1570   |
| 10                             | a*b       | 2 | 2 | 0.5257   | -1.0514  | -14.0048 |      | 4.7855  | -4.7855 | -2.1570  |
| 11                             | a*b       | 3 | 1 | -12.4663 | 12.9342  | 12.4663  |      | -4.2598 | 4.2598  | 1.9200   |
| 12                             | a*b       | 3 | 2 | -14.4918 | 14.0239  | 14.4918  |      | 4.2598  | -4.2598 | -1.9200  |

| Mixed Model Equations Solution |          |          |          |          |          |          |
|--------------------------------|----------|----------|----------|----------|----------|----------|
| Row                            | Col8     | Col9     | Col10    | Col11    | Col12    | Col13    |
| 1                              | 0.4680   | -0.5257  | 0.5257   | -12.4663 | -14.4918 | 159.61   |
| 2                              | -12.9342 | 1.0514   | -1.0514  | 12.9342  | 14.0239  | 53.2049  |
| 3                              | -0.4680  | -12.9534 | -14.0048 | 12.4663  | 14.4918  | 7.8856   |
| 4                              |          |          |          |          |          |          |
| 5                              | 4.2598   | -4.7855  | 4.7855   | -4.2598  | 4.2598   | 26.8837  |
| 6                              | -4.2598  | 4.7855   | -4.7855  | 4.2598   | -4.2598  | -26.8837 |
| 7                              | 4.1555   | 2.1570   | -2.1570  | 1.9200   | -1.9200  | 3.0198   |
| 8                              | 22.8027  | -2.1570  | 2.1570   | -1.9200  | 1.9200   | -3.0198  |
| 9                              | -2.1570  | 22.5560  | 4.4021   | 2.1570   | -2.1570  | -1.7134  |
| 10                             | 2.1570   | 4.4021   | 22.5560  | -2.1570  | 2.1570   | 1.7134   |
| 11                             | -1.9200  | 2.1570   | -2.1570  | 22.8027  | 4.1555   | -0.8115  |
| 12                             | 1.9200   | -2.1570  | 2.1570   | 4.1555   | 22.8027  | 0.8115   |

The A factor is significant at the 5% level (Output 59.3.11).

**Output 59.3.11** Tests of Fixed Effects

| Type 3 Tests of Fixed Effects |        |        |         |        |
|-------------------------------|--------|--------|---------|--------|
| Effect                        | Num DF | Den DF | F Value | Pr > F |
| a                             | 2      | 2      | 28.00   | 0.0345 |

Output 59.3.12 shows that the significance of A appears to be from the difference between its first level and its other two levels.

**Output 59.3.12** Least Squares Means for A Effect

| Least Squares Means |   |          |                |    |         |         |
|---------------------|---|----------|----------------|----|---------|---------|
| Effect              | a | Estimate | Standard Error | DF | t Value | Pr >  t |
| a                   | 1 | 212.82   | 27.6014        | 2  | 7.71    | 0.0164  |
| a                   | 2 | 167.50   | 27.5463        | 2  | 6.08    | 0.0260  |
| a                   | 3 | 159.61   | 27.6014        | 2  | 5.78    | 0.0286  |

Output 59.3.13 lists the predicted values from the model. These values are the sum of the fixed-effects estimates and the empirical best linear unbiased predictors (EBLUPs) of the random effects.

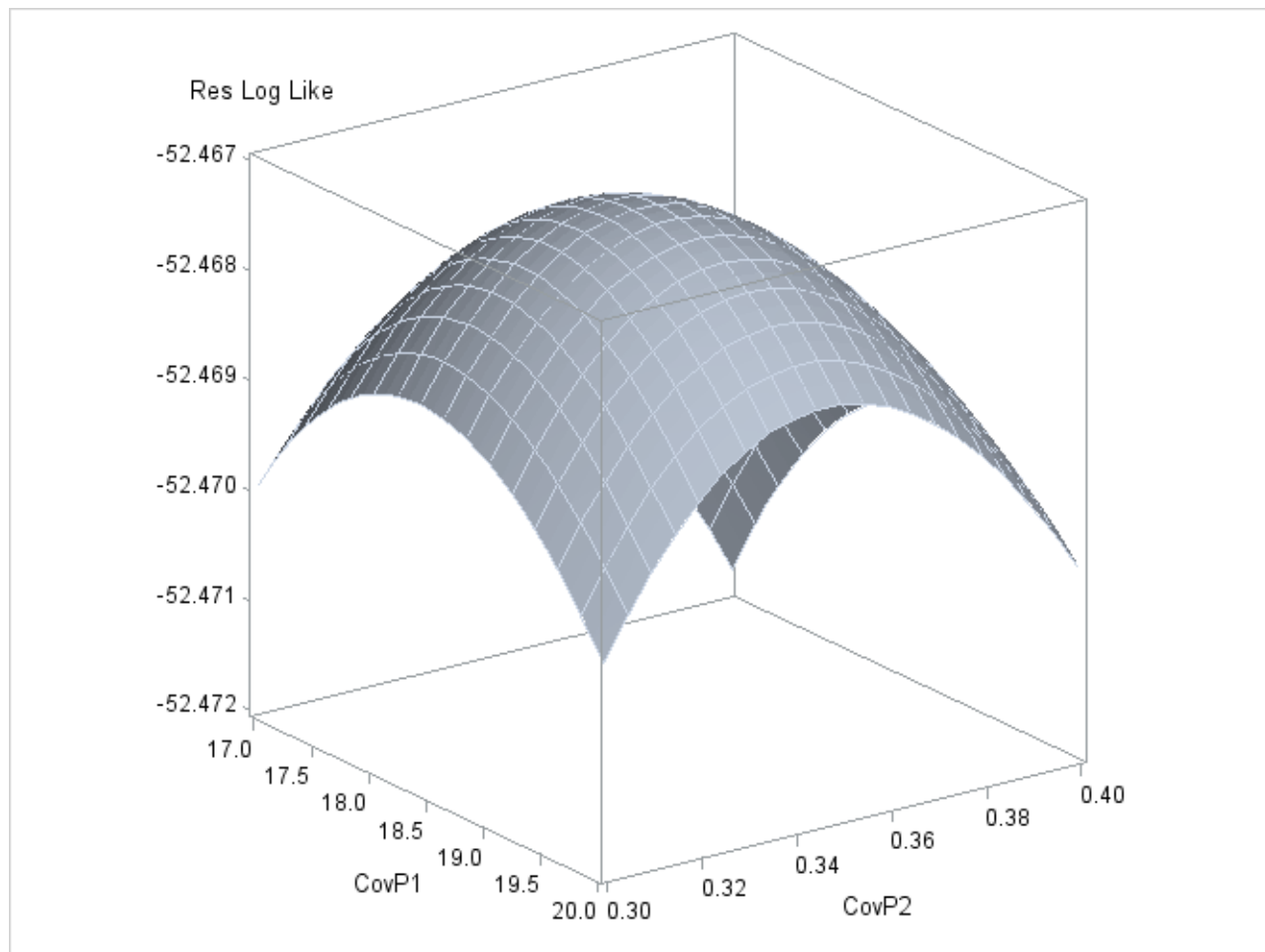
**Output 59.3.13** Predicted Values

| Obs | a | b | y   | Pred    | StdErr  |    | DF   | Alpha   | Lower   | Upper    | Resid |
|-----|---|---|-----|---------|---------|----|------|---------|---------|----------|-------|
|     |   |   |     |         | Pred    | DF |      |         |         |          |       |
| 1   | 1 | 1 | 237 | 242.723 | 4.72563 | 10 | 0.05 | 232.193 | 253.252 | -5.7228  |       |
| 2   | 1 | 1 | 254 | 242.723 | 4.72563 | 10 | 0.05 | 232.193 | 253.252 | 11.2772  |       |
| 3   | 1 | 1 | 246 | 242.723 | 4.72563 | 10 | 0.05 | 232.193 | 253.252 | 3.2772   |       |
| 4   | 1 | 2 | 178 | 182.916 | 5.52589 | 10 | 0.05 | 170.603 | 195.228 | -4.9159  |       |
| 5   | 1 | 2 | 179 | 182.916 | 5.52589 | 10 | 0.05 | 170.603 | 195.228 | -3.9159  |       |
| 6   | 2 | 1 | 208 | 192.670 | 4.70076 | 10 | 0.05 | 182.196 | 203.144 | 15.3297  |       |
| 7   | 2 | 1 | 178 | 192.670 | 4.70076 | 10 | 0.05 | 182.196 | 203.144 | -14.6703 |       |
| 8   | 2 | 1 | 187 | 192.670 | 4.70076 | 10 | 0.05 | 182.196 | 203.144 | -5.6703  |       |
| 9   | 2 | 2 | 146 | 142.330 | 4.70076 | 10 | 0.05 | 131.856 | 152.804 | 3.6703   |       |
| 10  | 2 | 2 | 145 | 142.330 | 4.70076 | 10 | 0.05 | 131.856 | 152.804 | 2.6703   |       |
| 11  | 2 | 2 | 141 | 142.330 | 4.70076 | 10 | 0.05 | 131.856 | 152.804 | -1.3297  |       |
| 12  | 3 | 1 | 186 | 185.687 | 5.52589 | 10 | 0.05 | 173.374 | 197.999 | 0.3134   |       |
| 13  | 3 | 1 | 183 | 185.687 | 5.52589 | 10 | 0.05 | 173.374 | 197.999 | -2.6866  |       |
| 14  | 3 | 2 | 142 | 133.542 | 4.72563 | 10 | 0.05 | 123.013 | 144.072 | 8.4578   |       |
| 15  | 3 | 2 | 125 | 133.542 | 4.72563 | 10 | 0.05 | 123.013 | 144.072 | -8.5422  |       |
| 16  | 3 | 2 | 136 | 133.542 | 4.72563 | 10 | 0.05 | 123.013 | 144.072 | 2.4578   |       |

To plot the likelihood surface by using ODS Graphics, use the following statements:

```
proc template;
 define statgraph surface;
 begingraph;
 layout overlay3d;
 surfaceplotparm x=CovP1 y=CovP2 z=ResLogLike;
 endlayout;
 endgraph;
 end;
run;
proc sgrender data=parms template=surface;
run;
```

The results from this plot are shown in Output 59.3.14. The peak of the surface is the REML estimates for the B and A\*B variance components.

**Output 59.3.14** Plot of Likelihood Surface


---

### Example 59.4: Known G and R

This animal breeding example from Henderson (1984, p. 48) considers multiple traits. The data are artificial and consist of measurements of two traits on three animals, but the second trait of the third animal is missing. Assuming an additive genetic model, you can use PROC MIXED to predict the breeding value of both traits on all three animals and also to predict the second trait of the third animal. The data are as follows:

```
data h;
 input Trait Animal Y;
 datalines;
1 1 6
1 2 8
1 3 7
2 1 9
2 2 5
2 3 .
;
```

Both **G** and **R** are known.

$$\mathbf{G} = \begin{bmatrix} 2 & 1 & 1 & 2 & 1 & 1 \\ 1 & 2 & .5 & 1 & 2 & .5 \\ 1 & .5 & 2 & 1 & .5 & 2 \\ 2 & 1 & 1 & 3 & 1.5 & 1.5 \\ 1 & 2 & .5 & 1.5 & 3 & .75 \\ 1 & .5 & 2 & 1.5 & .75 & 3 \end{bmatrix}$$

$$\mathbf{R} = \begin{bmatrix} 4 & 0 & 0 & 1 & 0 & 0 \\ 0 & 4 & 0 & 0 & 1 & 0 \\ 0 & 0 & 4 & 0 & 0 & 1 \\ 1 & 0 & 0 & 5 & 0 & 0 \\ 0 & 1 & 0 & 0 & 5 & 0 \\ 0 & 0 & 1 & 0 & 0 & 5 \end{bmatrix}$$

In order to read **G** into PROC MIXED by using the **GDATA=** option in the **RANDOM** statement, perform the following DATA step:

```
data g;
 input Row Col1-Col6;
 datalines;
1 2 1 1 2 1 1
2 1 2 .5 1 2 .5
3 1 .5 2 1 .5 2
4 2 1 1 3 1.5 1.5
5 1 2 .5 1.5 3 .75
6 1 .5 2 1.5 .75 3
;
```

The preceding data are in the dense representation for a **GDATA=** data set. You can also construct a data set with the sparse representation by using **Row**, **Col**, and **Value** variables, although this would require 21 observations instead of 6 for this example.

The PROC MIXED statements are as follows:

```
proc mixed data=h mmeq mmeqsol;
 class Trait Animal;
 model Y = Trait / noint s outp=predicted;
 random Trait*Animal / type=un gdata=g g gi s;
 repeated / type=un sub=Animal r ri;
 parms (4) (1) (5) / noiter;
run;
proc print data=predicted;
run;
```

The **MMEQ** and **MMEQSOL** options request the mixed model equations and their solution. The variables **Trait** and **Animal** are classification variables, and **Trait** defines the entire **X** matrix for the fixed-effects portion of the model, since the intercept is omitted with the **NOINT** option. The fixed-effects solution vector and predicted values are also requested by using the **S** and **OUTP=** options, respectively.

The random effect **Trait\*Animal** leads to a **Z** matrix with six columns, the first five corresponding to the identity matrix and the last consisting of 0s. An unstructured **G** matrix is specified by using the **TYPE=UN**

option, and it is read into PROC MIXED from a SAS data set by using the `GDATA=G` specification. The `G` and `GI` options request the display of  $G$  and  $G^{-1}$ , respectively. The `S` option requests that the random-effects solution vector be displayed.

Note that the preceding  $R$  matrix is block diagonal if the data are sorted by animals. The `REPEATED` statement exploits this fact by requesting  $R$  to have unstructured  $2 \times 2$  blocks corresponding to animals, which are the subjects. The `R` and `RI` options request that the estimated  $2 \times 2$  blocks for the first animal and its inverse be displayed. The `PARMS` statement lists the parameters of this  $2 \times 2$  matrix. Note that the parameters from  $G$  are not specified in the `PARMS` statement because they have already been assigned by using the `GDATA=` option in the `RANDOM` statement. The `NOITER` option prevents PROC MIXED from computing residual (restricted) maximum likelihood estimates; instead, the known values are used for inferences.

The results from this analysis are shown in [Output 59.4.1–Output 59.4.12](#).

The “Unstructured” covariance structure ([Output 59.4.1](#)) applies to both  $G$  and  $R$  here. The levels of Trait and Animal have been specified correctly.

**Output 59.4.1** Model and Class Level Information

| The Mixed Procedure       |        |              |
|---------------------------|--------|--------------|
| Model Information         |        |              |
| Data Set                  |        | WORK.H       |
| Dependent Variable        |        | Y            |
| Covariance Structure      |        | Unstructured |
| Subject Effect            |        | Animal       |
| Estimation Method         |        | REML         |
| Residual Variance Method  |        | None         |
| Fixed Effects SE Method   |        | Model-Based  |
| Degrees of Freedom Method |        | Containment  |
| Class Level Information   |        |              |
| Class                     | Levels | Values       |
| Trait                     | 2      | 1 2          |
| Animal                    | 3      | 1 2 3        |

The three covariance parameters indicated in [Output 59.4.2](#) correspond to those from the  $R$  matrix. Those from  $G$  are considered fixed and known because of the `GDATA=` option.

**Output 59.4.2** Model Dimensions and Number of Observations

| Dimensions                      |   |
|---------------------------------|---|
| Covariance Parameters           | 3 |
| Columns in X                    | 2 |
| Columns in Z                    | 6 |
| Subjects                        | 1 |
| Max Obs Per Subject             | 6 |
| Number of Observations          |   |
| Number of Observations Read     | 6 |
| Number of Observations Used     | 5 |
| Number of Observations Not Used | 1 |

Because starting values for the covariance parameters are specified in the **PARMS** statement, the MIXED procedure prints the residual (restricted) log likelihood at the starting values. Because of the **NOITER** option in the **PARMS** statement, this is also the final log likelihood in this analysis (Output 59.4.3).

**Output 59.4.3** REML Log Likelihood

| Parameter Search |        |        |              |                 |
|------------------|--------|--------|--------------|-----------------|
| CovP1            | CovP2  | CovP3  | Res Log Like | -2 Res Log Like |
| 4.0000           | 1.0000 | 5.0000 | -7.3731      | 14.7463         |

The block of **R** corresponding to the first animal and the inverse of this block are shown in Output 59.4.4.

**Output 59.4.4** Inverse R Matrix

| Estimated R Matrix<br>for Animal 1      |          |          |
|-----------------------------------------|----------|----------|
| Row                                     | Col1     | Col2     |
| 1                                       | 4.0000   | 1.0000   |
| 2                                       | 1.0000   | 5.0000   |
| Estimated Inv(R) Matrix<br>for Animal 1 |          |          |
| Row                                     | Col1     | Col2     |
| 1                                       | 0.2632   | -0.05263 |
| 2                                       | -0.05263 | 0.2105   |



The G matrix as specified in the `GDATA=` data set and its inverse are shown in [Output 59.4.5](#) and [Output 59.4.6](#).

**Output 59.4.5** G Matrix

| Estimated G Matrix |              |       |        |        |        |        |        |
|--------------------|--------------|-------|--------|--------|--------|--------|--------|
| Row                | Effect       | Trait | Animal | Col1   | Col2   | Col3   | Col4   |
| 1                  | Trait*Animal | 1     | 1      | 2.0000 | 1.0000 | 1.0000 | 2.0000 |
| 2                  | Trait*Animal | 1     | 2      | 1.0000 | 2.0000 | 0.5000 | 1.0000 |
| 3                  | Trait*Animal | 1     | 3      | 1.0000 | 0.5000 | 2.0000 | 1.0000 |
| 4                  | Trait*Animal | 2     | 1      | 2.0000 | 1.0000 | 1.0000 | 3.0000 |
| 5                  | Trait*Animal | 2     | 2      | 1.0000 | 2.0000 | 0.5000 | 1.5000 |
| 6                  | Trait*Animal | 2     | 3      | 1.0000 | 0.5000 | 2.0000 | 1.5000 |

| Estimated G Matrix |        |        |  |
|--------------------|--------|--------|--|
| Row                | Col15  | Col16  |  |
| 1                  | 1.0000 | 1.0000 |  |
| 2                  | 2.0000 | 0.5000 |  |
| 3                  | 0.5000 | 2.0000 |  |
| 4                  | 1.5000 | 1.5000 |  |
| 5                  | 3.0000 | 0.7500 |  |
| 6                  | 0.7500 | 3.0000 |  |

**Output 59.4.6** Inverse G Matrix

| Estimated Inv(G) Matrix |              |       |        |         |         |         |         |
|-------------------------|--------------|-------|--------|---------|---------|---------|---------|
| Row                     | Effect       | Trait | Animal | Col1    | Col2    | Col3    | Col4    |
| 1                       | Trait*Animal | 1     | 1      | 2.5000  | -1.0000 | -1.0000 | -1.6667 |
| 2                       | Trait*Animal | 1     | 2      | -1.0000 | 2.0000  |         | 0.6667  |
| 3                       | Trait*Animal | 1     | 3      | -1.0000 |         | 2.0000  | 0.6667  |
| 4                       | Trait*Animal | 2     | 1      | -1.6667 | 0.6667  | 0.6667  | 1.6667  |
| 5                       | Trait*Animal | 2     | 2      | 0.6667  | -1.3333 |         | -0.6667 |
| 6                       | Trait*Animal | 2     | 3      | 0.6667  |         | -1.3333 | -0.6667 |

| Estimated Inv(G) Matrix |         |         |  |
|-------------------------|---------|---------|--|
| Row                     | Col15   | Col16   |  |
| 1                       | 0.6667  | 0.6667  |  |
| 2                       | -1.3333 |         |  |
| 3                       |         | -1.3333 |  |
| 4                       | -0.6667 | -0.6667 |  |
| 5                       | 1.3333  |         |  |
| 6                       |         | 1.3333  |  |

The table of covariance parameter estimates in [Output 59.4.7](#) displays only the parameters in **R**. Because of the `GDATA=` option in the `RANDOM` statement, the G-side parameters do not participate in the pa-

parameter estimation process. Because of the **NOITER** option in the **PARMS** statement, however, the R-side parameters in this output are identical to their starting values.

**Output 59.4.7** R-Side Covariance Parameters

| Covariance Parameter Estimates |         |          |
|--------------------------------|---------|----------|
| Cov Parm                       | Subject | Estimate |
| UN(1,1)                        | Animal  | 4.0000   |
| UN(2,1)                        | Animal  | 1.0000   |
| UN(2,2)                        | Animal  | 5.0000   |

The coefficients of the mixed model equations in **Output 59.4.8** agree with Henderson (1984, p. 55). Recall from **Output 59.4.1** that there are 2 columns in **X** and 6 columns in **Z**. The first 8 columns of the mixed model equations correspond to the **X** and **Z** components. Column 9 represents the Y border.

**Output 59.4.8** Mixed Model Equations with Y Border

| Mixed Model Equations |              |       |        |          |          |          |          |
|-----------------------|--------------|-------|--------|----------|----------|----------|----------|
| Row                   | Effect       | Trait | Animal | Col1     | Col2     | Col3     | Col4     |
| 1                     | Trait        | 1     |        | 0.7763   | -0.1053  | 0.2632   | 0.2632   |
| 2                     | Trait        | 2     |        | -0.1053  | 0.4211   | -0.05263 | -0.05263 |
| 3                     | Trait*Animal | 1     | 1      | 0.2632   | -0.05263 | 2.7632   | -1.0000  |
| 4                     | Trait*Animal | 1     | 2      | 0.2632   | -0.05263 | -1.0000  | 2.2632   |
| 5                     | Trait*Animal | 1     | 3      | 0.2500   |          | -1.0000  |          |
| 6                     | Trait*Animal | 2     | 1      | -0.05263 | 0.2105   | -1.7193  | 0.6667   |
| 7                     | Trait*Animal | 2     | 2      | -0.05263 | 0.2105   | 0.6667   | -1.3860  |
| 8                     | Trait*Animal | 2     | 3      |          |          | 0.6667   |          |

| Mixed Model Equations |         |          |          |         |        |
|-----------------------|---------|----------|----------|---------|--------|
| Row                   | Col15   | Col16    | Col17    | Col18   | Col19  |
| 1                     | 0.2500  | -0.05263 | -0.05263 |         | 4.6974 |
| 2                     |         | 0.2105   | 0.2105   |         | 2.2105 |
| 3                     | -1.0000 | -1.7193  | 0.6667   | 0.6667  | 1.1053 |
| 4                     |         | 0.6667   | -1.3860  |         | 1.8421 |
| 5                     | 2.2500  | 0.6667   |          | -1.3333 | 1.7500 |
| 6                     | 0.6667  | 1.8772   | -0.6667  | -0.6667 | 1.5789 |
| 7                     |         | -0.6667  | 1.5439   |         | 0.6316 |
| 8                     | -1.3333 | -0.6667  |          | 1.3333  |        |

The solution to the mixed model equations also matches that given by Henderson (1984, p. 55). After solving the augmented mixed model equations, you can find the solutions for fixed and random effects in the last column (**Output 59.4.9**).

**Output 59.4.9** Solutions of the Mixed Model Equations with Y Border

| Mixed Model Equations Solution |              |       |        |         |         |         |         |
|--------------------------------|--------------|-------|--------|---------|---------|---------|---------|
| Row                            | Effect       | Trait | Animal | Col1    | Col2    | Col3    | Col4    |
| 1                              | Trait        | 1     |        | 2.5508  | 1.5685  | -1.3047 | -1.1775 |
| 2                              | Trait        | 2     |        | 1.5685  | 4.5539  | -1.4112 | -1.3534 |
| 3                              | Trait*Animal | 1     | 1      | -1.3047 | -1.4112 | 1.8282  | 1.0652  |
| 4                              | Trait*Animal | 1     | 2      | -1.1775 | -1.3534 | 1.0652  | 1.7589  |
| 5                              | Trait*Animal | 1     | 3      | -1.1701 | -0.9410 | 1.0206  | 0.7085  |
| 6                              | Trait*Animal | 2     | 1      | -1.3002 | -2.1592 | 1.8010  | 1.0900  |
| 7                              | Trait*Animal | 2     | 2      | -1.1821 | -2.1055 | 1.0925  | 1.7341  |
| 8                              | Trait*Animal | 2     | 3      | -1.1678 | -1.3149 | 1.0070  | 0.7209  |

| Mixed Model Equations Solution |         |         |         |         |          |  |
|--------------------------------|---------|---------|---------|---------|----------|--|
| Row                            | Col5    | Col6    | Col7    | Col8    | Col9     |  |
| 1                              | -1.1701 | -1.3002 | -1.1821 | -1.1678 | 6.9909   |  |
| 2                              | -0.9410 | -2.1592 | -2.1055 | -1.3149 | 6.9959   |  |
| 3                              | 1.0206  | 1.8010  | 1.0925  | 1.0070  | 0.05450  |  |
| 4                              | 0.7085  | 1.0900  | 1.7341  | 0.7209  | -0.04955 |  |
| 5                              | 1.7812  | 1.0095  | 0.7197  | 1.7756  | 0.02230  |  |
| 6                              | 1.0095  | 2.7518  | 1.6392  | 1.4849  | 0.2651   |  |
| 7                              | 0.7197  | 1.6392  | 2.6874  | 0.9930  | -0.2601  |  |
| 8                              | 1.7756  | 1.4849  | 0.9930  | 2.7645  | 0.1276   |  |

The solutions for the fixed and random effects in [Output 59.4.10](#) correspond to the last column in [Output 59.4.9](#). Note that the standard errors for the fixed effects and the prediction standard errors for the random effects are the square root values of the diagonal entries in the solution of the mixed model equations ([Output 59.4.9](#)).

**Output 59.4.10** Solutions for Fixed and Random Effects

| Solution for Fixed Effects |       |          |                |    |         |         |
|----------------------------|-------|----------|----------------|----|---------|---------|
| Effect                     | Trait | Estimate | Standard Error | DF | t Value | Pr >  t |
| Trait                      | 1     | 6.9909   | 1.5971         | 3  | 4.38    | 0.0221  |
| Trait                      | 2     | 6.9959   | 2.1340         | 3  | 3.28    | 0.0465  |

**Output 59.4.10** *continued*

| Solution for Random Effects |       |        |          |         |        |    |         |         |
|-----------------------------|-------|--------|----------|---------|--------|----|---------|---------|
| Effect                      | Trait | Animal | Estimate | Std Err |        | DF | t Value | Pr >  t |
|                             |       |        |          |         | Pred   |    |         |         |
| Trait*Animal                | 1     | 1      | 0.05450  |         | 1.3521 | 0  | 0.04    | .       |
| Trait*Animal                | 1     | 2      | -0.04955 |         | 1.3262 | 0  | -0.04   | .       |
| Trait*Animal                | 1     | 3      | 0.02230  |         | 1.3346 | 0  | 0.02    | .       |
| Trait*Animal                | 2     | 1      | 0.2651   |         | 1.6589 | 0  | 0.16    | .       |
| Trait*Animal                | 2     | 2      | -0.2601  |         | 1.6393 | 0  | -0.16   | .       |
| Trait*Animal                | 2     | 3      | 0.1276   |         | 1.6627 | 0  | 0.08    | .       |

The estimates for the two traits are nearly identical, but the standard error of the second trait is larger because of the missing observation.

The Estimate column in the “Solution for Random Effects” table lists the best linear unbiased predictions (BLUPs) of the breeding values of both traits for all three animals. The *p*-values are missing because the default containment method for computing degrees of freedom results in zero degrees of freedom for the random effects parameter tests.

**Output 59.4.11** Significance Test Comparing Traits

| Type 3 Tests of Fixed Effects |     |     |         |        |
|-------------------------------|-----|-----|---------|--------|
| Effect                        | Num | Den | F Value | Pr > F |
|                               | DF  | DF  |         |        |
| Trait                         | 2   | 3   | 10.59   | 0.0437 |

The two estimated traits are significantly different from zero at the 5% level (Output 59.4.11).

Output 59.4.12 displays the predicted values of the observations based on the trait and breeding value estimates—that is, the fixed and random effects.

**Output 59.4.12** Predicted Observations

| Obs | Trait | Animal | Y | Pred    | StdErr  |    | Alpha | Lower | Upper | Resid    |
|-----|-------|--------|---|---------|---------|----|-------|-------|-------|----------|
|     |       |        |   |         | Pred    | DF |       |       |       |          |
| 1   | 1     | 1      | 6 | 7.04542 | 1.33027 | 0  | 0.05  | .     | .     | -1.04542 |
| 2   | 1     | 2      | 8 | 6.94137 | 1.39806 | 0  | 0.05  | .     | .     | 1.05863  |
| 3   | 1     | 3      | 7 | 7.01321 | 1.41129 | 0  | 0.05  | .     | .     | -0.01321 |
| 4   | 2     | 1      | 9 | 7.26094 | 1.72839 | 0  | 0.05  | .     | .     | 1.73906  |
| 5   | 2     | 2      | 5 | 6.73576 | 1.74077 | 0  | 0.05  | .     | .     | -1.73576 |
| 6   | 2     | 3      | . | 7.12015 | 2.99088 | 0  | 0.05  | .     | .     | .        |

The predicted values are not the predictions of future records in the sense that they do not contain a component corresponding to a new observational error. See Henderson (1984) for information about predicting future records. The Lower and Upper columns usually contain confidence limits for the predicted values; they are missing here because the random-effects parameter degrees of freedom equals 0.

## Example 59.5: Random Coefficients

This example comes from a pharmaceutical stability data simulation performed by Obenchain (1990). The observed responses are replicate assay results, expressed in percent of label claim, at various shelf ages, expressed in months. The desired mixed model involves three batches of product that differ randomly in intercept (initial potency) and slope (degradation rate). This type of model is also known as a hierarchical or multilevel model (Singer 1998; Sullivan, Dukes, and Losina 1999).

The SAS statements are as follows:

```

data rc;
 input Batch Month @@;
 Monthc = Month;
 do i = 1 to 6;
 input Y @@;
 output;
 end;
 datalines;
1 0 101.2 103.3 103.3 102.1 104.4 102.4
1 1 98.8 99.4 99.7 99.5 . .
1 3 98.4 99.0 97.3 99.8 . .
1 6 101.5 100.2 101.7 102.7 . .
1 9 96.3 97.2 97.2 96.3 . .
1 12 97.3 97.9 96.8 97.7 97.7 96.7
2 0 102.6 102.7 102.4 102.1 102.9 102.6
2 1 99.1 99.0 99.9 100.6 . .
2 3 105.7 103.3 103.4 104.0 . .
2 6 101.3 101.5 100.9 101.4 . .
2 9 94.1 96.5 97.2 95.6 . .
2 12 93.1 92.8 95.4 92.2 92.2 93.0
3 0 105.1 103.9 106.1 104.1 103.7 104.6
3 1 102.2 102.0 100.8 99.8 . .
3 3 101.2 101.8 100.8 102.6 . .
3 6 101.1 102.0 100.1 100.2 . .
3 9 100.9 99.5 102.2 100.8 . .
3 12 97.8 98.3 96.9 98.4 96.9 96.5
;

proc mixed data=rc;
 class Batch;
 model Y = Month / s;
 random Int Month / type=un sub=Batch s;
run;

```

In the DATA step, Monthc is created as a duplicate of Month in order to enable both a continuous and a classification version of the same variable. The variable Monthc is used in a subsequent [analysis](#)

In the PROC MIXED statements, Batch is listed as the only classification variable. The fixed effect Month in the MODEL statement is not declared as a classification variable; thus it models a linear trend in time. An intercept is included as a fixed effect by default, and the S option requests that the fixed-effects parameter estimates be produced.

The two random effects are Int and Month, modeling random intercepts and slopes, respectively. Note that Intercept and Month are used as both fixed and random effects. The TYPE=UN option in the RANDOM statement specifies an unstructured covariance matrix for the random intercept and slope effects. In mixed model notation, G is block diagonal with unstructured 2x2 blocks. Each block corresponds to a different level of Batch, which is the SUBJECT= effect. The unstructured type provides a mechanism for estimating the correlation between the random coefficients. The S option requests the production of the random-effects parameter estimates.

The results from this analysis are shown in Output 59.5.1–Output 59.5.9. The “Unstructured” covariance structure in Output 59.5.1 applies to G here.

**Output 59.5.1** Model Information in Random Coefficients Analysis

| The Mixed Procedure       |              |
|---------------------------|--------------|
| Model Information         |              |
| Data Set                  | WORK.RC      |
| Dependent Variable        | Y            |
| Covariance Structure      | Unstructured |
| Subject Effect            | Batch        |
| Estimation Method         | REML         |
| Residual Variance Method  | Profile      |
| Fixed Effects SE Method   | Model-Based  |
| Degrees of Freedom Method | Containment  |

Batch is the only classification variable in this analysis, and it has three levels (Output 59.5.2).

**Output 59.5.2** Random Coefficients Analysis (continued)

| Class Level Information |        |        |
|-------------------------|--------|--------|
| Class                   | Levels | Values |
| Batch                   | 3      | 1 2 3  |

The “Dimensions” table in Output 59.5.3 indicates that there are three subjects (corresponding to batches). The 24 observations not used correspond to the missing values of Y in the input data set.

**Output 59.5.3** Random Coefficients Analysis (*continued*)

| Dimensions                      |     |
|---------------------------------|-----|
| Covariance Parameters           | 4   |
| Columns in X                    | 2   |
| Columns in Z Per Subject        | 2   |
| Subjects                        | 3   |
| Max Obs Per Subject             | 36  |
| Number of Observations          |     |
| Number of Observations Read     | 108 |
| Number of Observations Used     | 84  |
| Number of Observations Not Used | 24  |

As [Output 59.5.4](#) shows, only one iteration is required for convergence.

**Output 59.5.4** Random Coefficients Analysis (*continued*)

| Iteration History         |             |                 |            |
|---------------------------|-------------|-----------------|------------|
| Iteration                 | Evaluations | -2 Res Log Like | Criterion  |
| 0                         | 1           | 367.02768461    |            |
| 1                         | 1           | 350.32813577    | 0.00000000 |
| Convergence criteria met. |             |                 |            |

The Estimate column in [Output 59.5.5](#) lists the estimated elements of the unstructured  $2 \times 2$  matrix comprising the blocks of  $G$ . Note that the random coefficients are negatively correlated.

**Output 59.5.5** Random Coefficients Analysis (*continued*)

| Covariance Parameter Estimates |         |          |
|--------------------------------|---------|----------|
| Cov Parm                       | Subject | Estimate |
| UN(1,1)                        | Batch   | 0.9768   |
| UN(2,1)                        | Batch   | -0.1045  |
| UN(2,2)                        | Batch   | 0.03717  |
| Residual                       |         | 3.2932   |

The null model likelihood ratio test indicates a significant improvement over the null model consisting of no random effects and a homogeneous residual error ([Output 59.5.6](#)).

**Output 59.5.6** Random Coefficients Analysis (*continued*)

| Fit Statistics           |       |
|--------------------------|-------|
| -2 Res Log Likelihood    | 350.3 |
| AIC (smaller is better)  | 358.3 |
| AICC (smaller is better) | 358.8 |
| BIC (smaller is better)  | 354.7 |

| Null Model Likelihood Ratio Test |            |            |
|----------------------------------|------------|------------|
| DF                               | Chi-Square | Pr > ChiSq |
| 3                                | 16.70      | 0.0008     |

The fixed-effects estimates represent the estimated means for the random intercept and slope, respectively ([Output 59.5.7](#)).

**Output 59.5.7** Random Coefficients Analysis (*continued*)

| Solution for Fixed Effects |          |                |    |         |         |
|----------------------------|----------|----------------|----|---------|---------|
| Effect                     | Estimate | Standard Error | DF | t Value | Pr >  t |
| Intercept                  | 102.70   | 0.6456         | 2  | 159.08  | <.0001  |
| Month                      | -0.5259  | 0.1194         | 2  | -4.41   | 0.0478  |

The random-effects estimates represent the estimated deviation from the mean intercept and slope for each batch ([Output 59.5.8](#)). Therefore, the intercept for the first batch is close to  $102.7 - 1 = 101.7$ , while the intercepts for the other two batches are greater than 102.7. The second batch has a slope less than the mean slope of  $-0.526$ , while the other two batches have slopes greater than  $-0.526$ .

**Output 59.5.8** Random Coefficients Analysis (*continued*)

| Solution for Random Effects |       |          |              |    |         |         |
|-----------------------------|-------|----------|--------------|----|---------|---------|
| Effect                      | Batch | Estimate | Std Err Pred | DF | t Value | Pr >  t |
| Intercept                   | 1     | -1.0010  | 0.6842       | 78 | -1.46   | 0.1474  |
| Month                       | 1     | 0.1287   | 0.1245       | 78 | 1.03    | 0.3047  |
| Intercept                   | 2     | 0.3934   | 0.6842       | 78 | 0.58    | 0.5669  |
| Month                       | 2     | -0.2060  | 0.1245       | 78 | -1.65   | 0.1021  |
| Intercept                   | 3     | 0.6076   | 0.6842       | 78 | 0.89    | 0.3772  |
| Month                       | 3     | 0.07731  | 0.1245       | 78 | 0.62    | 0.5365  |

The  $F$  statistic in the “Type 3 Tests of Fixed Effects” table in [Output 59.5.9](#) is the square of the  $t$  statistic



used in the test of Month in the preceding “Solution for Fixed Effects” table (compare [Output 59.5.7](#) and [Output 59.5.9](#)). Both statistics test the null hypothesis that the slope assigned to Month equals 0, and this hypothesis can barely be rejected at the 5% level.

**Output 59.5.9** Random Coefficients Analysis (*continued*)

| Type 3 Tests of Fixed Effects |           |           |         |        |
|-------------------------------|-----------|-----------|---------|--------|
| Effect                        | Num<br>DF | Den<br>DF | F Value | Pr > F |
| Month                         | 1         | 2         | 19.41   | 0.0478 |

It is also possible to fit a random coefficients model with error terms that follow a nested structure (Fuller and Battese 1973). The following SAS statements represent one way of doing this:

```
proc mixed data=rc;
 class Batch Monthc;
 model Y = Month / s;
 random Int Month Monthc / sub=Batch s;
run;
```

The variable Monthc is added to the **CLASS** and **RANDOM** statements, and it models the nested errors. Note that Month and Monthc are continuous and classification versions of the same variable. Also, the **TYPE=UN** option is dropped from the **RANDOM** statement, resulting in the default variance components model instead of correlated random coefficients. The results from this analysis are shown in [Output 59.5.10](#).

**Output 59.5.10** Random Coefficients with Nested Errors Analysis

| The Mixed Procedure       |                     |              |
|---------------------------|---------------------|--------------|
| Model Information         |                     |              |
| Data Set                  | WORK.RC             |              |
| Dependent Variable        | Y                   |              |
| Covariance Structure      | Variance Components |              |
| Subject Effect            | Batch               |              |
| Estimation Method         | REML                |              |
| Residual Variance Method  | Profile             |              |
| Fixed Effects SE Method   | Model-Based         |              |
| Degrees of Freedom Method | Containment         |              |
| Class Level Information   |                     |              |
| Class                     | Levels              | Values       |
| Batch                     | 3                   | 1 2 3        |
| Monthc                    | 6                   | 0 1 3 6 9 12 |

Output 59.5.10 *continued*

| Dimensions                      |             |                 |            |
|---------------------------------|-------------|-----------------|------------|
| Covariance Parameters           |             |                 | 4          |
| Columns in X                    |             |                 | 2          |
| Columns in Z Per Subject        |             |                 | 8          |
| Subjects                        |             |                 | 3          |
| Max Obs Per Subject             |             |                 | 36         |
| Number of Observations          |             |                 |            |
| Number of Observations Read     |             |                 | 108        |
| Number of Observations Used     |             |                 | 84         |
| Number of Observations Not Used |             |                 | 24         |
| Iteration History               |             |                 |            |
| Iteration                       | Evaluations | -2 Res Log Like | Criterion  |
| 0                               | 1           | 367.02768461    |            |
| 1                               | 4           | 277.51945360    | .          |
| 2                               | 1           | 276.97551718    | 0.00104208 |
| 3                               | 1           | 276.90304909    | 0.00003174 |
| 4                               | 1           | 276.90100316    | 0.00000004 |
| 5                               | 1           | 276.90100092    | 0.00000000 |
| Convergence criteria met.       |             |                 |            |
| Covariance Parameter Estimates  |             |                 |            |
| Cov Parm                        | Subject     | Estimate        |            |
| Intercept                       | Batch       | 0               |            |
| Month                           | Batch       | 0.01243         |            |
| Monthc                          | Batch       | 3.7411          |            |
| Residual                        |             | 0.7969          |            |

For this analysis, the Newton-Raphson algorithm requires five iterations and nine likelihood evaluations to achieve convergence. The missing value in the Criterion column in iteration 1 indicates that a boundary constraint has been dropped.

The estimate for the Intercept variance component equals 0. This occurs frequently in practice and indicates that the restricted likelihood is maximized by setting this variance component equal to 0. Whenever a zero variance component estimate occurs, the following note appears in the SAS log:

**NOTE: Estimated G matrix is not positive definite.**

The remaining variance component estimates are positive, and the estimate corresponding to the nested errors (MONTHC) is much larger than the other two.

A comparison of AIC and BIC for this model with those of the previous model favors the nested error model

(compare [Output 59.5.11](#) and [Output 59.5.6](#)). Strictly speaking, a likelihood ratio test cannot be carried out between the two models because one is not contained in the other; however, a cautious comparison of likelihoods can be informative.

**Output 59.5.11** Random Coefficients with Nested Errors Analysis (*continued*)

| Fit Statistics           |       |
|--------------------------|-------|
| -2 Res Log Likelihood    | 276.9 |
| AIC (smaller is better)  | 282.9 |
| AICC (smaller is better) | 283.2 |
| BIC (smaller is better)  | 280.2 |

The better-fitting covariance model affects the standard errors of the fixed-effects parameter estimates more than the estimates themselves ([Output 59.5.12](#)).

**Output 59.5.12** Random Coefficients with Nested Errors Analysis (*continued*)

| Solution for Fixed Effects |          |                |    |         |         |
|----------------------------|----------|----------------|----|---------|---------|
| Effect                     | Estimate | Standard Error | DF | t Value | Pr >  t |
| Intercept                  | 102.56   | 0.7287         | 2  | 140.74  | <.0001  |
| Month                      | -0.5003  | 0.1259         | 2  | -3.97   | 0.0579  |

The random-effects solution provides the empirical best linear unbiased predictions (EBLUPs) for the realizations of the random intercept, slope, and nested errors ([Output 59.5.13](#)). You can use these values to compare batches and months.

**Output 59.5.13** Random Coefficients with Nested Errors Analysis (*continued*)

| Solution for Random Effects |       |        |          |                 |    |         |         |
|-----------------------------|-------|--------|----------|-----------------|----|---------|---------|
| Effect                      | Batch | Monthc | Estimate | Std Err<br>Pred | DF | t Value | Pr >  t |
| Intercept                   | 1     |        | 0        | .               | .  | .       | .       |
| Month                       | 1     |        | -0.00028 | 0.09268         | 66 | -0.00   | 0.9976  |
| Monthc                      | 1     | 0      | 0.2191   | 0.7896          | 66 | 0.28    | 0.7823  |
| Monthc                      | 1     | 1      | -2.5690  | 0.7571          | 66 | -3.39   | 0.0012  |
| Monthc                      | 1     | 3      | -2.3067  | 0.6865          | 66 | -3.36   | 0.0013  |
| Monthc                      | 1     | 6      | 1.8726   | 0.7328          | 66 | 2.56    | 0.0129  |
| Monthc                      | 1     | 9      | -1.2350  | 0.9300          | 66 | -1.33   | 0.1888  |
| Monthc                      | 1     | 12     | 0.7736   | 1.1992          | 66 | 0.65    | 0.5211  |
| Intercept                   | 2     |        | 0        | .               | .  | .       | .       |
| Month                       | 2     |        | -0.07571 | 0.09268         | 66 | -0.82   | 0.4169  |
| Monthc                      | 2     | 0      | -0.00621 | 0.7896          | 66 | -0.01   | 0.9938  |
| Monthc                      | 2     | 1      | -2.2126  | 0.7571          | 66 | -2.92   | 0.0048  |
| Monthc                      | 2     | 3      | 3.1063   | 0.6865          | 66 | 4.53    | <.0001  |
| Monthc                      | 2     | 6      | 2.0649   | 0.7328          | 66 | 2.82    | 0.0064  |
| Monthc                      | 2     | 9      | -1.4450  | 0.9300          | 66 | -1.55   | 0.1250  |
| Monthc                      | 2     | 12     | -2.4405  | 1.1992          | 66 | -2.04   | 0.0459  |
| Intercept                   | 3     |        | 0        | .               | .  | .       | .       |
| Month                       | 3     |        | 0.07600  | 0.09268         | 66 | 0.82    | 0.4152  |
| Monthc                      | 3     | 0      | 1.9574   | 0.7896          | 66 | 2.48    | 0.0157  |
| Monthc                      | 3     | 1      | -0.8850  | 0.7571          | 66 | -1.17   | 0.2466  |
| Monthc                      | 3     | 3      | 0.3006   | 0.6865          | 66 | 0.44    | 0.6629  |
| Monthc                      | 3     | 6      | 0.7972   | 0.7328          | 66 | 1.09    | 0.2806  |
| Monthc                      | 3     | 9      | 2.0059   | 0.9300          | 66 | 2.16    | 0.0347  |
| Monthc                      | 3     | 12     | 0.002293 | 1.1992          | 66 | 0.00    | 0.9985  |

**Output 59.5.14** Random Coefficients with Nested Errors Analysis (*continued*)

| Type 3 Tests of Fixed Effects |           |           |         |        |
|-------------------------------|-----------|-----------|---------|--------|
| Effect                        | Num<br>DF | Den<br>DF | F Value | Pr > F |
| Month                         | 1         | 2         | 15.78   | 0.0579 |

The test of Month is similar to that from the previous model, although it is no longer significant at the 5% level (Output 59.5.14).

## Example 59.6: Line-Source Sprinkler Irrigation

These data appear in Hanks et al. (1980); Johnson, Chaudhuri, and Kanemasu (1983); Stroup (1989b). Three cultivars (Cult) of winter wheat are randomly assigned to rectangular plots within each of three blocks (Block). The nine plots are located side by side, and a line-source sprinkler is placed through the middle. Each plot is subdivided into twelve subplots—six to the north of the line source, six to the south (Dir). The

two plots closest to the line source represent the maximum irrigation level (Irrig=6), the two next-closest plots represent the next-highest level (Irrig=5), and so forth.

This example is a case where both **G** and **R** can be modeled. One of Stroup's models specifies a diagonal **G** containing the variance components for Block, Block\*Dir, and Block\*Irrig, and a Toeplitz **R** with four bands. The SAS statements to fit this model and carry out some further analyses follow.

**CAUTION:** This analysis can require considerable CPU time.

```

data line;
 length Cult$ 8;
 input Block Cult$ @;
 row = _n_;
 do Sbplt=1 to 12;
 if Sbplt le 6 then do;
 Irrig = Sbplt;
 Dir = 'North';
 end; else do;
 Irrig = 13 - Sbplt;
 Dir = 'South';
 end;
 input Y @; output;
 end;
datalines;
1 Luke 2.4 2.7 5.6 7.5 7.9 7.1 6.1 7.3 7.4 6.7 3.8 1.8
1 Nugaines 2.2 2.2 4.3 6.3 7.9 7.1 6.2 5.3 5.3 5.2 5.4 2.9
1 Bridger 2.9 3.2 5.1 6.9 6.1 7.5 5.6 6.5 6.6 5.3 4.1 3.1
2 Nugaines 2.4 2.2 4.0 5.8 6.1 6.2 7.0 6.4 6.7 6.4 3.7 2.2
2 Bridger 2.6 3.1 5.7 6.4 7.7 6.8 6.3 6.2 6.6 6.5 4.2 2.7
2 Luke 2.2 2.7 4.3 6.9 6.8 8.0 6.5 7.3 5.9 6.6 3.0 2.0
3 Nugaines 1.8 1.9 3.7 4.9 5.4 5.1 5.7 5.0 5.6 5.1 4.2 2.2
3 Luke 2.1 2.3 3.7 5.8 6.3 6.3 6.5 5.7 5.8 4.5 2.7 2.3
3 Bridger 2.7 2.8 4.0 5.0 5.2 5.2 5.9 6.1 6.0 4.3 3.1 3.1
;

proc mixed;
 class Block Cult Dir Irrig;
 model Y = Cult|Dir|Irrig@2;
 random Block Block*Dir Block*Irrig;
 repeated / type=toep(4) sub=Block*Cult r;
 lsmeans Cult|Irrig;
 estimate 'Bridger vs Luke' Cult 1 -1 0;
 estimate 'Linear Irrig' Irrig -5 -3 -1 1 3 5;
 estimate 'B vs L x Linear Irrig' Cult*Irrig
 -5 -3 -1 1 3 5 5 3 1 -1 -3 -5;
run;

```

The preceding statements use the bar operator (|) and the at sign (@) to specify all two-factor interactions between Cult, Dir, and Irrig as fixed effects.

The **RANDOM** statement sets up the **Z** and **G** matrices corresponding to the random effects Block, Block\*Dir, and Block\*Irrig.

In the **REPEATED** statement, the **TYPE=TOEP(4)** option sets up the blocks of the **R** matrix to be Toeplitz with four bands below and including the main diagonal. The subject effect is Block\*Cult, and it produces

nine 12×12 blocks. The **R** option requests that the first block of **R** be displayed.

Least squares means (**LSMEANS**) are requested for **Cult**, **Irrig**, and **Cult\*Irrig**, and a few **ESTIMATE** statements are specified to illustrate some linear combinations of the fixed effects.

The results from this analysis are shown in **Output 59.6.1**.

The “Covariance Structures” row in **Output 59.6.1** reveals the two different structures assumed for **G** and **R**.

**Output 59.6.1** Model Information in Line-Source Sprinkler Analysis

| The Mixed Procedure       |                                  |
|---------------------------|----------------------------------|
| Model Information         |                                  |
| Data Set                  | WORK.LINE                        |
| Dependent Variable        | Y                                |
| Covariance Structures     | Variance Components,<br>Toeplitz |
| Subject Effect            | Block*Cult                       |
| Estimation Method         | REML                             |
| Residual Variance Method  | Profile                          |
| Fixed Effects SE Method   | Model-Based                      |
| Degrees of Freedom Method | Containment                      |

The levels of each classification variable are listed as a single string in the **Values** column, regardless of whether the levels are numeric or character (**Output 59.6.2**).

**Output 59.6.2** Class Level Information

| Class Level Information |        |                       |
|-------------------------|--------|-----------------------|
| Class                   | Levels | Values                |
| Block                   | 3      | 1 2 3                 |
| Cult                    | 3      | Bridger Luke Nugaines |
| Dir                     | 2      | North South           |
| Irrig                   | 6      | 1 2 3 4 5 6           |

Even though there is a **SUBJECT=** effect in the **REPEATED** statement, the analysis considers all of the data to be from one subject because there is no corresponding **SUBJECT=** effect in the **RANDOM** statement (**Output 59.6.3**).

**Output 59.6.3** Model Dimensions and Number of Observations

| Dimensions                      |     |
|---------------------------------|-----|
| Covariance Parameters           | 7   |
| Columns in X                    | 48  |
| Columns in Z                    | 27  |
| Subjects                        | 1   |
| Max Obs Per Subject             | 108 |
| Number of Observations          |     |
| Number of Observations Read     | 108 |
| Number of Observations Used     | 108 |
| Number of Observations Not Used | 0   |

The Newton-Raphson algorithm converges successfully in seven iterations ([Output 59.6.4](#)).

**Output 59.6.4** Iteration History and Convergence Status

| Iteration History         |             |              |          |            |
|---------------------------|-------------|--------------|----------|------------|
| Iteration                 | Evaluations | -2 Res       | Log Like | Criterion  |
| 0                         | 1           | 226.25427252 |          |            |
| 1                         | 4           | 187.99336173 |          | .          |
| 2                         | 3           | 186.62579299 |          | 0.10431081 |
| 3                         | 1           | 184.38218213 |          | 0.04807260 |
| 4                         | 1           | 183.41836853 |          | 0.00886548 |
| 5                         | 1           | 183.25111475 |          | 0.00075353 |
| 6                         | 1           | 183.23809997 |          | 0.00000748 |
| 7                         | 1           | 183.23797748 |          | 0.00000000 |
| Convergence criteria met. |             |              |          |            |

The first block of the estimated  $\mathbf{R}$  matrix has the TOEP(4) structure, and the observations that are three plots apart exhibit a negative correlation ([Output 59.6.5](#)).

**Output 59.6.5** Estimated R Matrix for the First Subject

| Estimated R Matrix for Block*Cult 1 Bridger |          |          |          |          |          |          |          |
|---------------------------------------------|----------|----------|----------|----------|----------|----------|----------|
| Row                                         | Col1     | Col2     | Col3     | Col4     | Col5     | Col6     | Col7     |
| 1                                           | 0.2850   | 0.007986 | 0.001452 | -0.09253 |          |          |          |
| 2                                           | 0.007986 | 0.2850   | 0.007986 | 0.001452 | -0.09253 |          |          |
| 3                                           | 0.001452 | 0.007986 | 0.2850   | 0.007986 | 0.001452 | -0.09253 |          |
| 4                                           | -0.09253 | 0.001452 | 0.007986 | 0.2850   | 0.007986 | 0.001452 | -0.09253 |
| 5                                           |          | -0.09253 | 0.001452 | 0.007986 | 0.2850   | 0.007986 | 0.001452 |
| 6                                           |          |          | -0.09253 | 0.001452 | 0.007986 | 0.2850   | 0.007986 |
| 7                                           |          |          |          | -0.09253 | 0.001452 | 0.007986 | 0.2850   |
| 8                                           |          |          |          |          | -0.09253 | 0.001452 | 0.007986 |
| 9                                           |          |          |          |          |          | -0.09253 | 0.001452 |
| 10                                          |          |          |          |          |          |          | -0.09253 |
| 11                                          |          |          |          |          |          |          |          |
| 12                                          |          |          |          |          |          |          |          |

| Estimated R Matrix for Block*Cult 1 Bridger |          |          |          |          |          |
|---------------------------------------------|----------|----------|----------|----------|----------|
| Row                                         | Col8     | Col9     | Col10    | Col11    | Col12    |
| 1                                           |          |          |          |          |          |
| 2                                           |          |          |          |          |          |
| 3                                           |          |          |          |          |          |
| 4                                           |          |          |          |          |          |
| 5                                           | -0.09253 |          |          |          |          |
| 6                                           | 0.001452 | -0.09253 |          |          |          |
| 7                                           | 0.007986 | 0.001452 | -0.09253 |          |          |
| 8                                           | 0.2850   | 0.007986 | 0.001452 | -0.09253 |          |
| 9                                           | 0.007986 | 0.2850   | 0.007986 | 0.001452 | -0.09253 |
| 10                                          | 0.001452 | 0.007986 | 0.2850   | 0.007986 | 0.001452 |
| 11                                          | -0.09253 | 0.001452 | 0.007986 | 0.2850   | 0.007986 |
| 12                                          |          | -0.09253 | 0.001452 | 0.007986 | 0.2850   |

Output 59.6.6 lists the estimated covariance parameters from both **G** and **R**. The first three are the variance components making up the diagonal **G**, and the final four make up the Toeplitz structure in the blocks of **R**. The Residual row corresponds to the variance of the Toeplitz structure, and it represents the parameter profiled out during the optimization process.

**Output 59.6.6** Estimated Covariance Parameters

| Covariance Parameter Estimates |            |          |
|--------------------------------|------------|----------|
| Cov Parm                       | Subject    | Estimate |
| Block                          |            | 0.2194   |
| Block*Dir                      |            | 0.01768  |
| Block*Irrig                    |            | 0.03539  |
| TOEP (2)                       | Block*Cult | 0.007986 |
| TOEP (3)                       | Block*Cult | 0.001452 |
| TOEP (4)                       | Block*Cult | -0.09253 |
| Residual                       |            | 0.2850   |



The “–2 Res Log Likelihood” value in [Output 59.6.7](#) is the same as the final value listed in the “Iteration History” table ([Output 59.6.4](#)).

**Output 59.6.7** Fit Statistics Based on the Residual Log Likelihood

| Fit Statistics           |       |
|--------------------------|-------|
| –2 Res Log Likelihood    | 183.2 |
| AIC (smaller is better)  | 197.2 |
| AICC (smaller is better) | 198.8 |
| BIC (smaller is better)  | 190.9 |

Every fixed effect except for Dir and Cult\*Irrig is significant at the 5% level ([Output 59.6.8](#)).

**Output 59.6.8** Tests for Fixed Effects

| Type 3 Tests of Fixed Effects |           |           |         |        |
|-------------------------------|-----------|-----------|---------|--------|
| Effect                        | Num<br>DF | Den<br>DF | F Value | Pr > F |
| Cult                          | 2         | 68        | 7.98    | 0.0008 |
| Dir                           | 1         | 2         | 3.95    | 0.1852 |
| Cult*Dir                      | 2         | 68        | 3.44    | 0.0379 |
| Irrig                         | 5         | 10        | 102.60  | <.0001 |
| Cult*Irrig                    | 10        | 68        | 1.91    | 0.0580 |
| Dir*Irrig                     | 5         | 68        | 6.12    | <.0001 |

The “Estimates” table lists the results from the various linear combinations of fixed effects specified in the **ESTIMATE** statements ([Output 59.6.9](#)). Bridger is not significantly different from Luke, and Irrig possesses a strong linear component. This strength appears to be influencing the significance of the interaction.

**Output 59.6.9** Estimates

| Estimates             |          |                   |    |         |         |
|-----------------------|----------|-------------------|----|---------|---------|
| Label                 | Estimate | Standard<br>Error | DF | t Value | Pr >  t |
| Bridger vs Luke       | –0.03889 | 0.09524           | 68 | –0.41   | 0.6843  |
| Linear Irrig          | 30.6444  | 1.4412            | 10 | 21.26   | <.0001  |
| B vs L x Linear Irrig | –9.8667  | 2.7400            | 68 | –3.60   | 0.0006  |

The least squares means shown in [Output 59.6.10](#) are useful in comparing the levels of the various fixed effects. For example, it appears that irrigation levels 5 and 6 have virtually the same effect.

**Output 59.6.10** Least Squares Means for Cult, Irrig, and Their Interaction

| Least Squares Means |          |       |          |                |    |         |         |
|---------------------|----------|-------|----------|----------------|----|---------|---------|
| Effect              | Cult     | Irrig | Estimate | Standard Error | DF | t Value | Pr >  t |
| Cult                | Bridger  |       | 5.0306   | 0.2874         | 68 | 17.51   | <.0001  |
| Cult                | Luke     |       | 5.0694   | 0.2874         | 68 | 17.64   | <.0001  |
| Cult                | Nugaines |       | 4.7222   | 0.2874         | 68 | 16.43   | <.0001  |
| Irrig               |          | 1     | 2.4222   | 0.3220         | 10 | 7.52    | <.0001  |
| Irrig               |          | 2     | 3.1833   | 0.3220         | 10 | 9.88    | <.0001  |
| Irrig               |          | 3     | 5.0556   | 0.3220         | 10 | 15.70   | <.0001  |
| Irrig               |          | 4     | 6.1889   | 0.3220         | 10 | 19.22   | <.0001  |
| Irrig               |          | 5     | 6.4000   | 0.3140         | 10 | 20.38   | <.0001  |
| Irrig               |          | 6     | 6.3944   | 0.3227         | 10 | 19.81   | <.0001  |
| Cult*Irrig          | Bridger  | 1     | 2.8500   | 0.3679         | 68 | 7.75    | <.0001  |
| Cult*Irrig          | Bridger  | 2     | 3.4167   | 0.3679         | 68 | 9.29    | <.0001  |
| Cult*Irrig          | Bridger  | 3     | 5.1500   | 0.3679         | 68 | 14.00   | <.0001  |
| Cult*Irrig          | Bridger  | 4     | 6.2500   | 0.3679         | 68 | 16.99   | <.0001  |
| Cult*Irrig          | Bridger  | 5     | 6.3000   | 0.3463         | 68 | 18.19   | <.0001  |
| Cult*Irrig          | Bridger  | 6     | 6.2167   | 0.3697         | 68 | 16.81   | <.0001  |
| Cult*Irrig          | Luke     | 1     | 2.1333   | 0.3679         | 68 | 5.80    | <.0001  |
| Cult*Irrig          | Luke     | 2     | 2.8667   | 0.3679         | 68 | 7.79    | <.0001  |
| Cult*Irrig          | Luke     | 3     | 5.2333   | 0.3679         | 68 | 14.22   | <.0001  |
| Cult*Irrig          | Luke     | 4     | 6.5500   | 0.3679         | 68 | 17.80   | <.0001  |
| Cult*Irrig          | Luke     | 5     | 6.8833   | 0.3463         | 68 | 19.87   | <.0001  |
| Cult*Irrig          | Luke     | 6     | 6.7500   | 0.3697         | 68 | 18.26   | <.0001  |
| Cult*Irrig          | Nugaines | 1     | 2.2833   | 0.3679         | 68 | 6.21    | <.0001  |
| Cult*Irrig          | Nugaines | 2     | 3.2667   | 0.3679         | 68 | 8.88    | <.0001  |
| Cult*Irrig          | Nugaines | 3     | 4.7833   | 0.3679         | 68 | 13.00   | <.0001  |
| Cult*Irrig          | Nugaines | 4     | 5.7667   | 0.3679         | 68 | 15.67   | <.0001  |
| Cult*Irrig          | Nugaines | 5     | 6.0167   | 0.3463         | 68 | 17.37   | <.0001  |
| Cult*Irrig          | Nugaines | 6     | 6.2167   | 0.3697         | 68 | 16.81   | <.0001  |

An interesting exercise is to fit other variance-covariance models to these data and to compare them to this one by using likelihood ratio tests, Akaike's information criterion, or Schwarz's Bayesian information criterion. In particular, some spatial models are worth investigating (Marx and Thompson 1987; Zimmerman and Harville 1991). The following is one example of spatial model statements:

```
proc mixed;
 class Block Cult Dir Irrig;
 model Y = Cult|Dir|Irrig@2;
 repeated / type=sp(pow)(Row Sbplt) sub=intercept;
run;
```

The `TYPE=SP(POW)(Row Sbplt)` option in the `REPEATED` statement requests the spatial power structure, with the two defining coordinate variables being `Row` and `Sbplt`. The `SUBJECT=INTERCEPT` option indicates that the entire data set is to be considered as one subject, thereby modeling **R** as a dense 108×108 covariance matrix. See Wolfinger (1993) for further discussion of this example and additional analyses.

## Example 59.7: Influence in Heterogeneous Variance Model

In this example from Snedecor and Cochran (1976, p. 256), a one-way classification model with heterogeneous variances is fit. The data, shown in the following DATA step, represent amounts of different types of fat absorbed by batches of doughnuts during cooking, measured in grams.

```
data absorb;
 input FatType Absorbed @@;
 datalines;
 1 164 1 172 1 168 1 177 1 156 1 195
 2 178 2 191 2 197 2 182 2 185 2 177
 3 175 3 193 3 178 3 171 3 163 3 176
 4 155 4 166 4 149 4 164 4 170 4 168
 ;
```

The statistical model for these data can be written as

$$Y_{ij} = \mu + \tau_i + \epsilon_{ij}$$

$$i = 1, \dots, t = 4$$

$$j = 1, \dots, r = 6$$

$$\epsilon_{ij} = N(0, \sigma_i^2)$$

where  $Y_{ij}$  is the amount of fat absorbed by the  $j$ th batch of the  $i$ th fat type, and  $\tau_i$  denotes the fat-type effects. A quick glance at the data suggests that observations 6, 9, 14, and 21 might be influential on the analysis, because these are extreme observations for the respective fat types.

The following SAS statements fit this model and request influence diagnostics for the fixed effects and covariance parameters. ODS Graphics is used to create plots of the influence diagnostics in addition to the tabular output. The `ESTIMATES` suboption requests plots of “leave-one-out” estimates for the fixed effects and group variances.

```
ods graphics on;

proc mixed data=absorb asycov;
 class FatType;
 model Absorbed = FatType / s
 influence(iter=10 estimates);
 repeated / group=FatType;
 ods output Influence=inf;
run;

ods graphics off;
```

The “Influence” table is output to the SAS data set `inf` so that parameter estimates can be printed subsequently. Results from this analysis are shown in [Output 59.7.1](#).

**Output 59.7.1** Heterogeneous Variance Analysis

| The Mixed Procedure            |                     |           |                |    |         |         |
|--------------------------------|---------------------|-----------|----------------|----|---------|---------|
| Model Information              |                     |           |                |    |         |         |
| Data Set                       | WORK.ABSORB         |           |                |    |         |         |
| Dependent Variable             | Absorbed            |           |                |    |         |         |
| Covariance Structure           | Variance Components |           |                |    |         |         |
| Group Effect                   | FatType             |           |                |    |         |         |
| Estimation Method              | REML                |           |                |    |         |         |
| Residual Variance Method       | None                |           |                |    |         |         |
| Fixed Effects SE Method        | Model-Based         |           |                |    |         |         |
| Degrees of Freedom Method      | Between-Within      |           |                |    |         |         |
| Covariance Parameter Estimates |                     |           |                |    |         |         |
|                                | Cov Parm            | Group     | Estimate       |    |         |         |
|                                | Residual            | FatType 1 | 178.00         |    |         |         |
|                                | Residual            | FatType 2 | 60.4000        |    |         |         |
|                                | Residual            | FatType 3 | 97.6000        |    |         |         |
|                                | Residual            | FatType 4 | 67.6000        |    |         |         |
| Solution for Fixed Effects     |                     |           |                |    |         |         |
| Effect                         | Fat Type            | Estimate  | Standard Error | DF | t Value | Pr >  t |
| Intercept                      |                     | 162.00    | 3.3566         | 20 | 48.26   | <.0001  |
| FatType                        | 1                   | 10.0000   | 6.3979         | 20 | 1.56    | 0.1337  |
| FatType                        | 2                   | 23.0000   | 4.6188         | 20 | 4.98    | <.0001  |
| FatType                        | 3                   | 14.0000   | 5.2472         | 20 | 2.67    | 0.0148  |
| FatType                        | 4                   | 0         | .              | .  | .       | .       |

The fixed-effects solutions correspond to estimates of the following parameters:

$$\text{Intercept} : \mu + \tau_4$$

$$\text{FatType1} : \tau_1 - \tau_4$$

$$\text{FatType2} : \tau_2 - \tau_4$$

$$\text{FatType3} : \tau_3 - \tau_4$$

$$\text{FatType4} : 0$$

You can easily verify that these estimates are simple functions of the arithmetic means  $\bar{y}_i$  in the groups. For example,  $\widehat{\mu + \tau_4} = \bar{y}_4 = 162.0$ ,  $\widehat{\tau_1 - \tau_4} = \bar{y}_1 - \bar{y}_4 = 10.0$ , and so forth. The covariance parameter estimates are the sample variances in the groups and are uncorrelated.

The variances in the four groups are shown in the “Covariance Parameter Estimates” table (Output 59.7.1). The estimated variance in the first group is two to three times larger than the variance in the other groups.

**Output 59.7.2** Asymptotic Variances of Group Variance Estimates

| Asymptotic Covariance Matrix of Estimates |          |       |         |         |         |
|-------------------------------------------|----------|-------|---------|---------|---------|
| Row                                       | Cov Parm | CovP1 | CovP2   | CovP3   | CovP4   |
| 1                                         | Residual | 12674 |         |         |         |
| 2                                         | Residual |       | 1459.26 |         |         |
| 3                                         | Residual |       |         | 3810.30 |         |
| 4                                         | Residual |       |         |         | 1827.90 |

In groups where the residual variance estimate is large, the precision of the estimate is also small (Output 59.7.2).

The following statements print the “leave-one-out” estimates for fixed effects and covariance parameters that were written to the inf data set with the **ESTIMATES** suboption (Output 59.7.3):

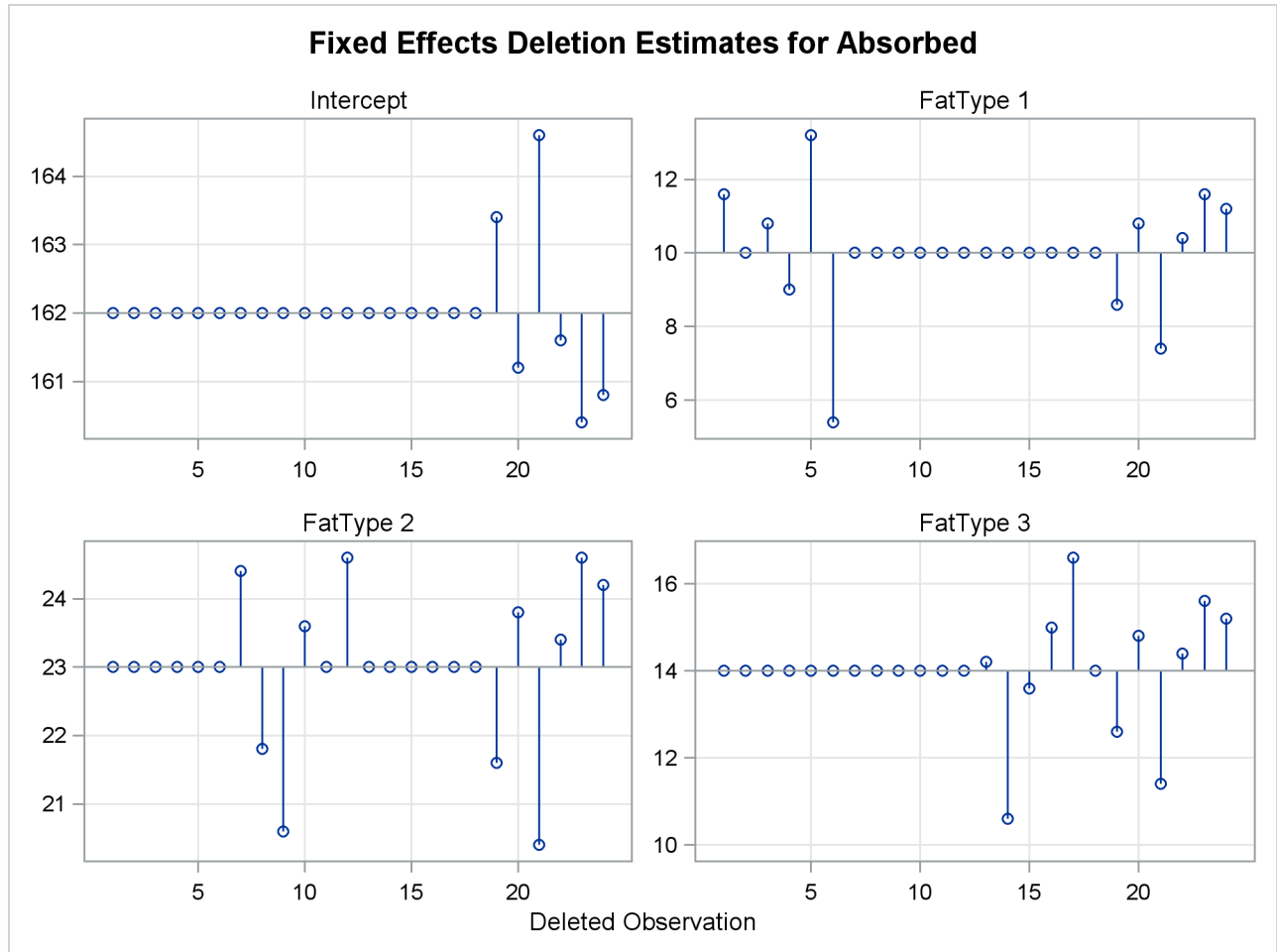
```
proc print data=inf label;
 var parm1-parm5 covp1-covp4;
run;
```

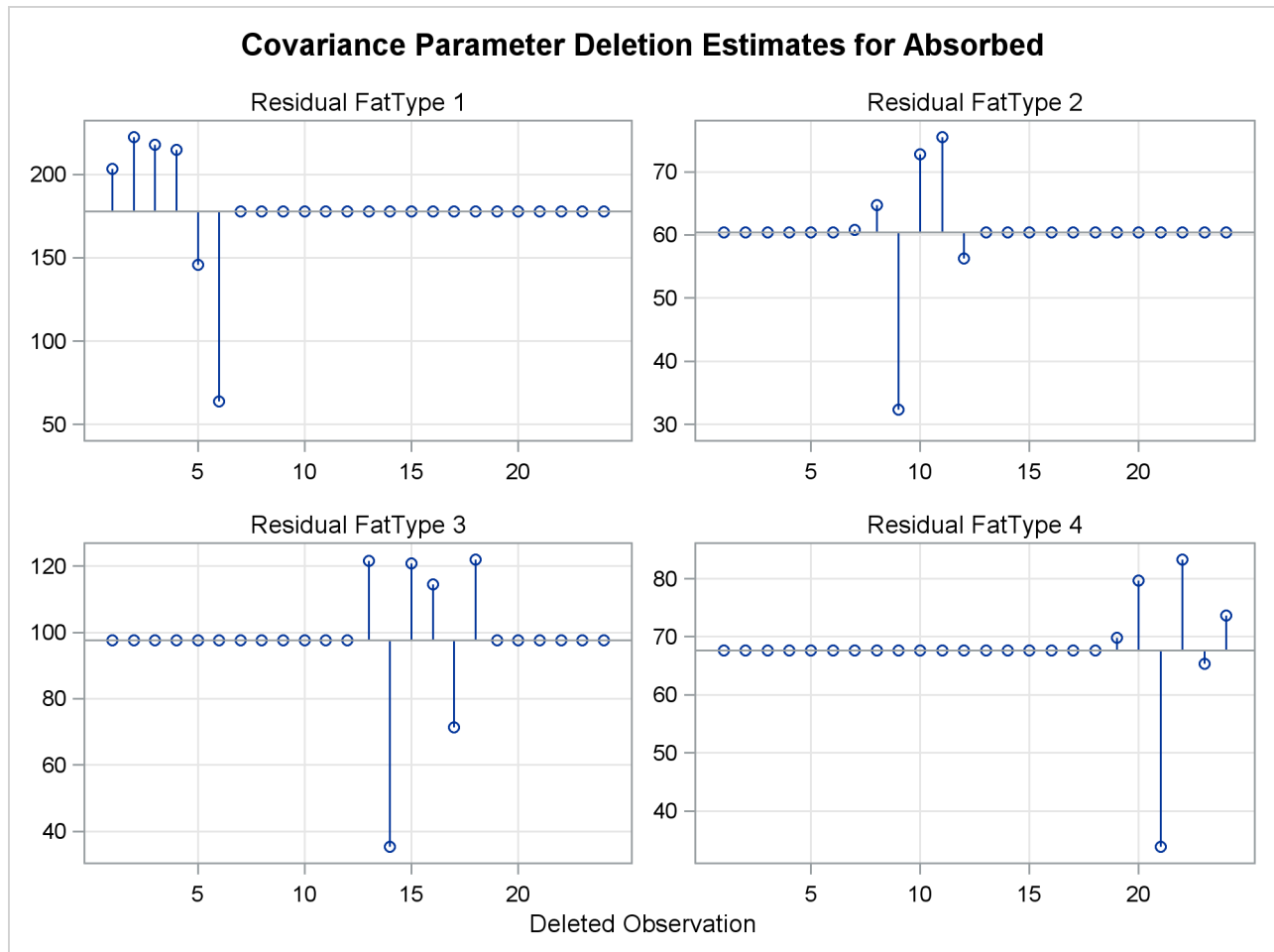
**Output 59.7.3** Leave-One-Out Estimates

| Obs | Intercept | Fat    |        |        |        | Residual  | Residual  | Residual  | Residual  |
|-----|-----------|--------|--------|--------|--------|-----------|-----------|-----------|-----------|
|     |           | Type 1 | Type 2 | Type 3 | Type 4 | FatType 1 | FatType 2 | FatType 3 | FatType 4 |
| 1   | 162.00    | 11.600 | 23.000 | 14.000 | 0      | 203.30    | 60.400    | 97.60     | 67.600    |
| 2   | 162.00    | 10.000 | 23.000 | 14.000 | 0      | 222.47    | 60.400    | 97.60     | 67.600    |
| 3   | 162.00    | 10.800 | 23.000 | 14.000 | 0      | 217.68    | 60.400    | 97.60     | 67.600    |
| 4   | 162.00    | 9.000  | 23.000 | 14.000 | 0      | 214.99    | 60.400    | 97.60     | 67.600    |
| 5   | 162.00    | 13.200 | 23.000 | 14.000 | 0      | 145.70    | 60.400    | 97.60     | 67.600    |
| 6   | 162.00    | 5.400  | 23.000 | 14.000 | 0      | 63.80     | 60.400    | 97.60     | 67.600    |
| 7   | 162.00    | 10.000 | 24.400 | 14.000 | 0      | 178.00    | 60.795    | 97.60     | 67.600    |
| 8   | 162.00    | 10.000 | 21.800 | 14.000 | 0      | 178.00    | 64.691    | 97.60     | 67.600    |
| 9   | 162.00    | 10.000 | 20.600 | 14.000 | 0      | 178.00    | 32.296    | 97.60     | 67.600    |
| 10  | 162.00    | 10.000 | 23.600 | 14.000 | 0      | 178.00    | 72.797    | 97.60     | 67.600    |
| 11  | 162.00    | 10.000 | 23.000 | 14.000 | 0      | 178.00    | 75.490    | 97.60     | 67.600    |
| 12  | 162.00    | 10.000 | 24.600 | 14.000 | 0      | 178.00    | 56.285    | 97.60     | 67.600    |
| 13  | 162.00    | 10.000 | 23.000 | 14.200 | 0      | 178.00    | 60.400    | 121.68    | 67.600    |
| 14  | 162.00    | 10.000 | 23.000 | 10.600 | 0      | 178.00    | 60.400    | 35.30     | 67.600    |
| 15  | 162.00    | 10.000 | 23.000 | 13.600 | 0      | 178.00    | 60.400    | 120.79    | 67.600    |
| 16  | 162.00    | 10.000 | 23.000 | 15.000 | 0      | 178.00    | 60.400    | 114.50    | 67.600    |
| 17  | 162.00    | 10.000 | 23.000 | 16.600 | 0      | 178.00    | 60.400    | 71.30     | 67.600    |
| 18  | 162.00    | 10.000 | 23.000 | 14.000 | 0      | 178.00    | 60.400    | 121.98    | 67.600    |
| 19  | 163.40    | 8.600  | 21.600 | 12.600 | 0      | 178.00    | 60.400    | 97.60     | 69.799    |
| 20  | 161.20    | 10.800 | 23.800 | 14.800 | 0      | 178.00    | 60.400    | 97.60     | 79.698    |
| 21  | 164.60    | 7.400  | 20.400 | 11.400 | 0      | 178.00    | 60.400    | 97.60     | 33.800    |
| 22  | 161.60    | 10.400 | 23.400 | 14.400 | 0      | 178.00    | 60.400    | 97.60     | 83.292    |
| 23  | 160.40    | 11.600 | 24.600 | 15.600 | 0      | 178.00    | 60.400    | 97.60     | 65.299    |
| 24  | 160.80    | 11.200 | 24.200 | 15.200 | 0      | 178.00    | 60.400    | 97.60     | 73.677    |

The graphical displays in [Output 59.7.4](#) and [Output 59.7.5](#) are created when ODS Graphics is enabled. For general information about ODS Graphics, see Chapter 21, “[Statistical Graphics Using ODS](#).” For specific information about the graphics available in the MIXED procedure, see the section “[ODS Graphics](#)” on page 4992.

**Output 59.7.4** Fixed-Effects Deletion Estimates



**Output 59.7.5** Covariance Parameter Deletion Estimates

The estimate of the intercept is affected only when observations from the last group are removed. The estimate of the “FatType 1” effect reacts to removal of observations in the first and last group (Output 59.7.4).

While observations can affect one or more fixed-effects solutions in this model, they can affect only one covariance parameter, the variance in their group (Output 59.7.5). Observations 6, 9, 14, and 21, which are extreme in their group, reduce the group variance considerably.

Diagnostics related to residuals and predicted values are printed with the following statements:

```
proc print data=inf label;
 var observed predicted residual pressres
 student Rstudent;
run;
```

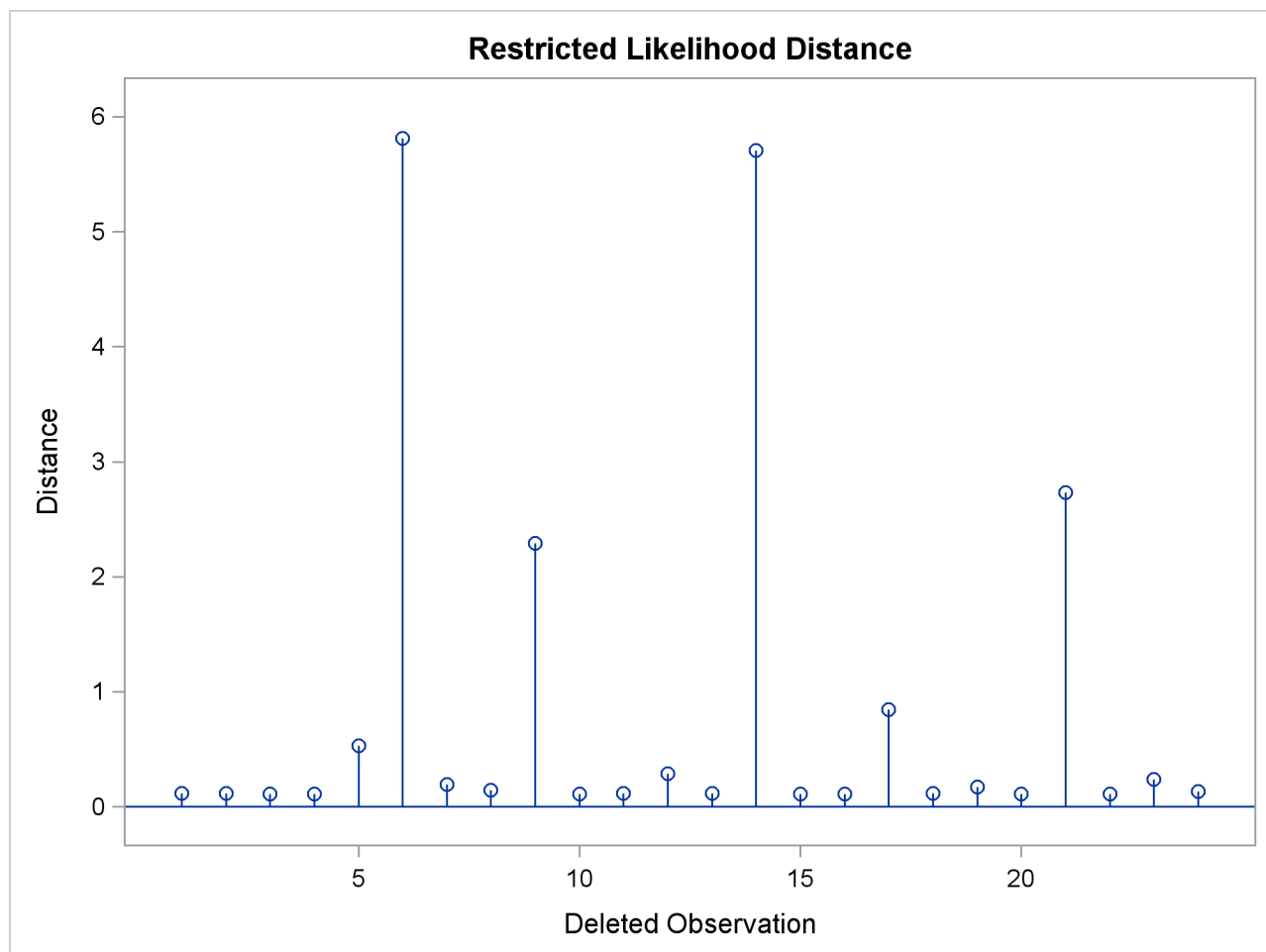
**Output 59.7.6** Residual Diagnostics

| Obs | Observed Value | Predicted Mean | Residual | PRESS Residual | Internally Studentized Residual | Externally Studentized Residual |
|-----|----------------|----------------|----------|----------------|---------------------------------|---------------------------------|
| 1   | 164            | 172.0          | -8.000   | -9.600         | -0.6569                         | -0.6146                         |
| 2   | 172            | 172.0          | 0.000    | 0.000          | 0.0000                          | 0.0000                          |
| 3   | 168            | 172.0          | -4.000   | -4.800         | -0.3284                         | -0.2970                         |
| 4   | 177            | 172.0          | 5.000    | 6.000          | 0.4105                          | 0.3736                          |
| 5   | 156            | 172.0          | -16.000  | -19.200        | -1.3137                         | -1.4521                         |
| 6   | 195            | 172.0          | 23.000   | 27.600         | 1.8885                          | 3.1544                          |
| 7   | 178            | 185.0          | -7.000   | -8.400         | -0.9867                         | -0.9835                         |
| 8   | 191            | 185.0          | 6.000    | 7.200          | 0.8457                          | 0.8172                          |
| 9   | 197            | 185.0          | 12.000   | 14.400         | 1.6914                          | 2.3131                          |
| 10  | 182            | 185.0          | -3.000   | -3.600         | -0.4229                         | -0.3852                         |
| 11  | 185            | 185.0          | 0.000    | -0.000         | 0.0000                          | 0.0000                          |
| 12  | 177            | 185.0          | -8.000   | -9.600         | -1.1276                         | -1.1681                         |
| 13  | 175            | 176.0          | -1.000   | -1.200         | -0.1109                         | -0.0993                         |
| 14  | 193            | 176.0          | 17.000   | 20.400         | 1.8850                          | 3.1344                          |
| 15  | 178            | 176.0          | 2.000    | 2.400          | 0.2218                          | 0.1993                          |
| 16  | 171            | 176.0          | -5.000   | -6.000         | -0.5544                         | -0.5119                         |
| 17  | 163            | 176.0          | -13.000  | -15.600        | -1.4415                         | -1.6865                         |
| 18  | 176            | 176.0          | 0.000    | 0.000          | 0.0000                          | 0.0000                          |
| 19  | 155            | 162.0          | -7.000   | -8.400         | -0.9326                         | -0.9178                         |
| 20  | 166            | 162.0          | 4.000    | 4.800          | 0.5329                          | 0.4908                          |
| 21  | 149            | 162.0          | -13.000  | -15.600        | -1.7321                         | -2.4495                         |
| 22  | 164            | 162.0          | 2.000    | 2.400          | 0.2665                          | 0.2401                          |
| 23  | 170            | 162.0          | 8.000    | 9.600          | 1.0659                          | 1.0845                          |
| 24  | 168            | 162.0          | 6.000    | 7.200          | 0.7994                          | 0.7657                          |

Observations 6, 9, 14, and 21 have large studentized residuals (Output 59.7.6). That the externally studentized residuals are much larger than the internally studentized residuals for these observations indicates that the variance estimate in the group shrinks when the observation is removed. Also important to note is that comparisons based on raw residuals in models with heterogeneous variance can be misleading. Observation 5, for example, has a larger residual but a smaller studentized residual than observation 21. The variance for the first fat type is much larger than the variance in the fourth group. A “large” residual is more “surprising” in the groups with small variance.

A measure of the overall influence on the analysis is the (restricted) likelihood distance, shown in Output 59.7.7. Observations 6, 9, 14, and 21 clearly displace the REML solution more than any other observations.



**Output 59.7.7** Restricted Likelihood Distance

The following statements list the restricted likelihood distance and various diagnostics related to the fixed-effects estimates (Output 59.7.8):

```
proc print data=inf label;
 var leverage observed CookD DFFITS CovRatio RLD;
run;
```

**Output 59.7.8** Restricted Likelihood Distance and Fixed-Effects Diagnostics

| Obs | Leverage | Observed Value | Cook's D | DFFITs   | COVRATIO | Restr. Likelihood Distance |
|-----|----------|----------------|----------|----------|----------|----------------------------|
| 1   | 0.167    | 164            | 0.02157  | -0.27487 | 1.3706   | 0.1178                     |
| 2   | 0.167    | 172            | 0.00000  | -0.00000 | 1.4998   | 0.1156                     |
| 3   | 0.167    | 168            | 0.00539  | -0.13282 | 1.4675   | 0.1124                     |
| 4   | 0.167    | 177            | 0.00843  | 0.16706  | 1.4494   | 0.1117                     |
| 5   | 0.167    | 156            | 0.08629  | -0.64938 | 0.9822   | 0.5290                     |
| 6   | 0.167    | 195            | 0.17831  | 1.41069  | 0.4301   | 5.8101                     |
| 7   | 0.167    | 178            | 0.04868  | -0.43982 | 1.2078   | 0.1935                     |
| 8   | 0.167    | 191            | 0.03576  | 0.36546  | 1.2853   | 0.1451                     |
| 9   | 0.167    | 197            | 0.14305  | 1.03446  | 0.6416   | 2.2909                     |
| 10  | 0.167    | 182            | 0.00894  | -0.17225 | 1.4463   | 0.1116                     |
| 11  | 0.167    | 185            | 0.00000  | -0.00000 | 1.4998   | 0.1156                     |
| 12  | 0.167    | 177            | 0.06358  | -0.52239 | 1.1183   | 0.2856                     |
| 13  | 0.167    | 175            | 0.00061  | -0.04441 | 1.4961   | 0.1151                     |
| 14  | 0.167    | 193            | 0.17766  | 1.40175  | 0.4340   | 5.7044                     |
| 15  | 0.167    | 178            | 0.00246  | 0.08915  | 1.4851   | 0.1139                     |
| 16  | 0.167    | 171            | 0.01537  | -0.22892 | 1.4078   | 0.1129                     |
| 17  | 0.167    | 163            | 0.10389  | -0.75423 | 0.8766   | 0.8433                     |
| 18  | 0.167    | 176            | 0.00000  | 0.00000  | 1.4998   | 0.1156                     |
| 19  | 0.167    | 155            | 0.04349  | -0.41047 | 1.2390   | 0.1710                     |
| 20  | 0.167    | 166            | 0.01420  | 0.21950  | 1.4148   | 0.1124                     |
| 21  | 0.167    | 149            | 0.15000  | -1.09545 | 0.6000   | 2.7343                     |
| 22  | 0.167    | 164            | 0.00355  | 0.10736  | 1.4786   | 0.1133                     |
| 23  | 0.167    | 170            | 0.05680  | 0.48500  | 1.1592   | 0.2383                     |
| 24  | 0.167    | 168            | 0.03195  | 0.34245  | 1.3079   | 0.1353                     |

In this example, observations with large likelihood distances also have large values for Cook's  $D$  and values of CovRatio far less than one ([Output 59.7.8](#)). The latter indicates that the fixed effects are estimated more precisely when these observations are removed from the analysis.

The following statements print the values of the  $D$  statistic and the CovRatio for the covariance parameters:

```
proc print data=inf label;
 var iter CookDCP CovRatioCP;
run;
```

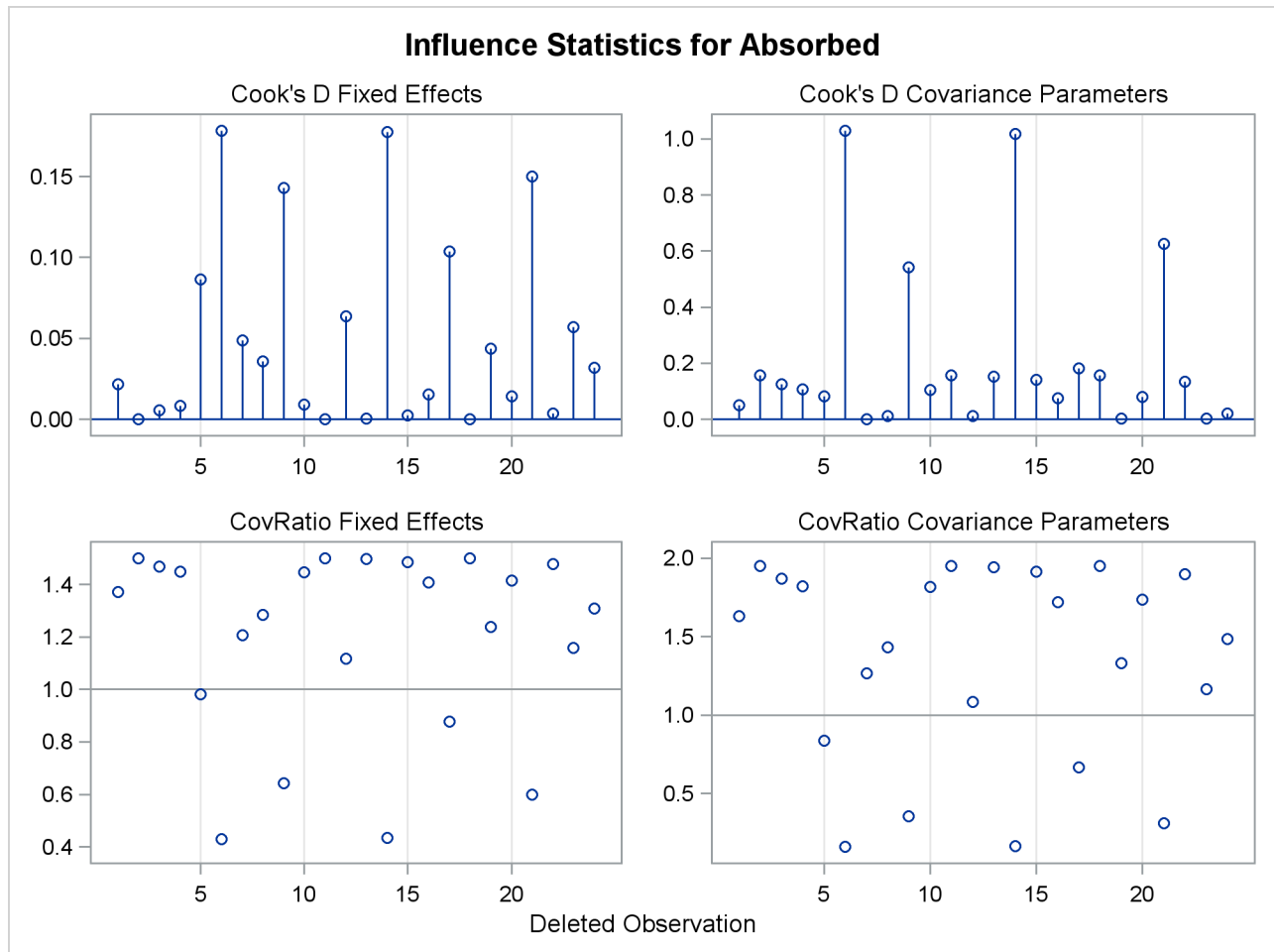
The same conclusions as for the fixed-effects estimates hold for the covariance parameter estimates. Observations 6, 9, 14, and 21 change the estimates and their precision considerably ([Output 59.7.9](#), [Output 59.7.10](#)). All iterative updates converged within at most four iterations.

**Output 59.7.9** Covariance Parameter Diagnostics

| Obs | Iterations | Cook's D<br>CovParms | COVRATIO<br>CovParms |
|-----|------------|----------------------|----------------------|
| 1   | 3          | 0.05050              | 1.6306               |
| 2   | 3          | 0.15603              | 1.9520               |
| 3   | 3          | 0.12426              | 1.8692               |
| 4   | 3          | 0.10796              | 1.8233               |
| 5   | 4          | 0.08232              | 0.8375               |
| 6   | 4          | 1.02909              | 0.1606               |
| 7   | 1          | 0.00011              | 1.2662               |
| 8   | 2          | 0.01262              | 1.4335               |
| 9   | 3          | 0.54126              | 0.3573               |
| 10  | 3          | 0.10531              | 1.8156               |
| 11  | 3          | 0.15603              | 1.9520               |
| 12  | 2          | 0.01160              | 1.0849               |
| 13  | 3          | 0.15223              | 1.9425               |
| 14  | 4          | 1.01865              | 0.1635               |
| 15  | 3          | 0.14111              | 1.9141               |
| 16  | 3          | 0.07494              | 1.7203               |
| 17  | 3          | 0.18154              | 0.6671               |
| 18  | 3          | 0.15603              | 1.9520               |
| 19  | 2          | 0.00265              | 1.3326               |
| 20  | 3          | 0.08008              | 1.7374               |
| 21  | 1          | 0.62500              | 0.3125               |
| 22  | 3          | 0.13472              | 1.8974               |
| 23  | 2          | 0.00290              | 1.1663               |
| 24  | 2          | 0.02020              | 1.4839               |

Output 59.7.10 displays the standard panel of influence diagnostics that is obtained when influence analysis is iterative. The Cook's  $D$  and CovRatio statistics are displayed for each deletion set for both fixed-effects and covariance parameter estimates. This provides a convenient summary of the impact on the analysis for each deletion set, since Cook's  $D$  statistic measures impact on the estimates and the CovRatio statistic measures impact on the precision of the estimates.

**Output 59.7.10** Influence Diagnostics



Observations 6, 9, 14, and 21 have considerable impact on estimates and precision of fixed effects and covariance parameters. This is not necessarily the case. Observations can be influential on only some aspects of the analysis, as shown in the next example.

**Example 59.8: Influence Analysis for Repeated Measures Data**

This example revisits the repeated measures data of Pothoff and Roy (1964) that were analyzed in [Example 59.2](#). Recall that the data consist of growth measurements at ages 8, 10, 12, and 14 for 11 girls and 16 boys. The model being fit contains fixed effects for Gender and Age and their interaction.

The earlier analysis of these data indicated some unusual observations in this data set. Because of the clustered data structure, it is of interest to study the influence of clusters (children) on the analysis rather than the influence of individual observations. A cluster comprises the repeated measurements for each child.

The repeated measures are first modeled with an unstructured within-child variance-covariance matrix. A residual variance is not profiled in this model. A noniterative influence analysis will update the fixed effects only. The following statements request this noniterative maximum likelihood analysis and produce [Output 59.8.1](#):

```

proc mixed data=pr method=ml;
 class person gender;
 model y = gender age gender*age /
 influence(effect=person);
 repeated / type=un subject=person;
 ods select influence;
run;

```

**Output 59.8.1** Default Influence Statistics in Noniterative Analysis

| The Mixed Procedure                        |                                       |                    |             |  |
|--------------------------------------------|---------------------------------------|--------------------|-------------|--|
| Influence Diagnostics for Levels of Person |                                       |                    |             |  |
| Person                                     | Number of<br>Observations<br>in Level | PRESS<br>Statistic | Cook's<br>D |  |
| 1                                          | 4                                     | 10.1716            | 0.01539     |  |
| 2                                          | 4                                     | 3.8187             | 0.03988     |  |
| 3                                          | 4                                     | 10.8448            | 0.02891     |  |
| 4                                          | 4                                     | 24.0339            | 0.04515     |  |
| 5                                          | 4                                     | 1.6900             | 0.01613     |  |
| 6                                          | 4                                     | 11.8592            | 0.01634     |  |
| 7                                          | 4                                     | 1.1887             | 0.00521     |  |
| 8                                          | 4                                     | 4.6717             | 0.02742     |  |
| 9                                          | 4                                     | 13.4244            | 0.03949     |  |
| 10                                         | 4                                     | 85.1195            | 0.13848     |  |
| 11                                         | 4                                     | 67.9397            | 0.09728     |  |
| 12                                         | 4                                     | 40.6467            | 0.04438     |  |
| 13                                         | 4                                     | 13.0304            | 0.00924     |  |
| 14                                         | 4                                     | 6.1712             | 0.00411     |  |
| 15                                         | 4                                     | 24.5702            | 0.12727     |  |
| 16                                         | 4                                     | 20.5266            | 0.01026     |  |
| 17                                         | 4                                     | 9.9917             | 0.01526     |  |
| 18                                         | 4                                     | 7.9355             | 0.01070     |  |
| 19                                         | 4                                     | 15.5955            | 0.01982     |  |
| 20                                         | 4                                     | 42.6845            | 0.01973     |  |
| 21                                         | 4                                     | 95.3282            | 0.10075     |  |
| 22                                         | 4                                     | 13.9649            | 0.03778     |  |
| 23                                         | 4                                     | 4.9656             | 0.01245     |  |
| 24                                         | 4                                     | 37.2494            | 0.15094     |  |
| 25                                         | 4                                     | 4.3756             | 0.03375     |  |
| 26                                         | 4                                     | 8.1448             | 0.03470     |  |
| 27                                         | 4                                     | 20.2913            | 0.02523     |  |

Each observation in the “Influence Diagnostics for Levels of Person” table in [Output 59.8.1](#) represents the removal of four observations. The subjects 10, 15, and 24 have the greatest impact on the fixed effects (Cook’s  $D$ ), and subject 10 and 21 have large PRESS statistics. The 21st child has a large PRESS statistic, and its  $D$  statistic is not that extreme. This is an indication that the model fits rather poorly for this child, whether it is part of the data or not.

The previous analysis does not take into account the effect on the covariance parameters when a subject is removed from the analysis. If you also update the covariance parameters, the impact of observations on

these can amplify or allay their effect on the fixed effects. To assess the overall influence of subjects on the analysis and to compute separate statistics for the fixed effects and covariance parameters, an iterative analysis is obtained by adding the **INFLUENCE** suboption **ITER=**, as follows:

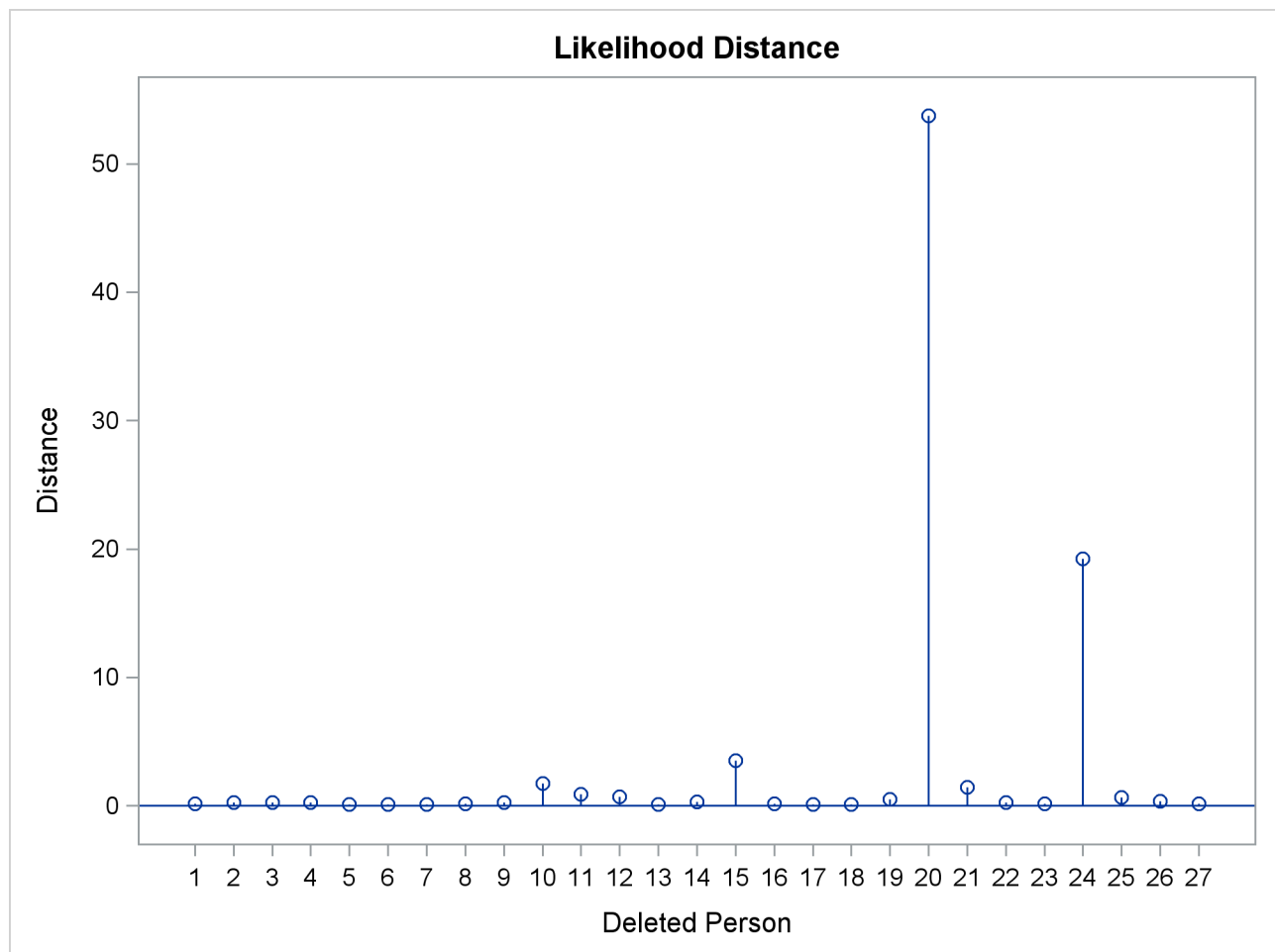
```
ods graphics on;

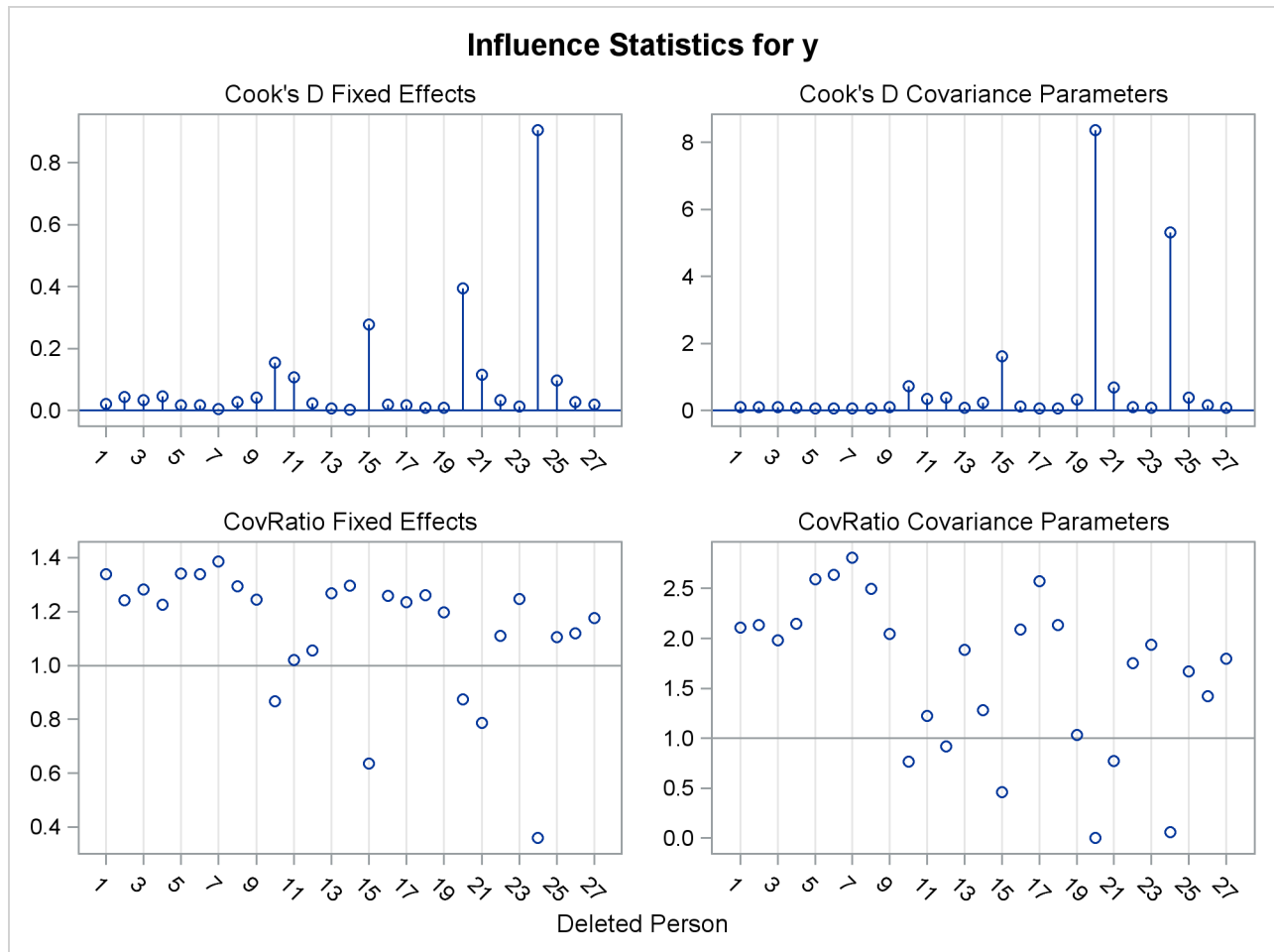
proc mixed data=pr method=ml;
 class person gender;
 model y = gender age gender*age /
 influence(effect=person iter=5);
 repeated / type=un subject=person;
run;
```

The number of additional iterations following removal of the observations for a particular subject is limited to five. Graphical displays of influence diagnostics are created when ODS Graphics is enabled. For general information about ODS Graphics, see Chapter 21, “[Statistical Graphics Using ODS](#).” For specific information about the graphics available in the MIXED procedure, see the section “[ODS Graphics](#)” on page 4992.

The MIXED procedure produces a plot of the restricted likelihood distance ([Output 59.8.2](#)) and a panel of diagnostics for fixed effects and covariance parameters ([Output 59.8.3](#)).

**Output 59.8.2** Restricted Likelihood Distance



**Output 59.8.3** Influence Diagnostics Panel

As judged by the restricted likelihood distance, subjects 20 and 24 clearly have the most influence on the overall analysis (Output 59.8.2).

Output 59.8.3 displays Cook's  $D$  and CovRatio statistics for the fixed effects and covariance parameters. Clearly, subject 20 has a dramatic effect on the estimates of variances and covariances. This subject also affects the precision of the covariance parameter estimates more than any other subject in Output 59.8.3 (CovRatio near 0).

The child who exerts the greatest influence on the fixed effects is subject 24. Maybe surprisingly, this subject affects the variance-covariance matrix of the fixed effects more than subject 20 (small CovRatio in Output 59.8.3).

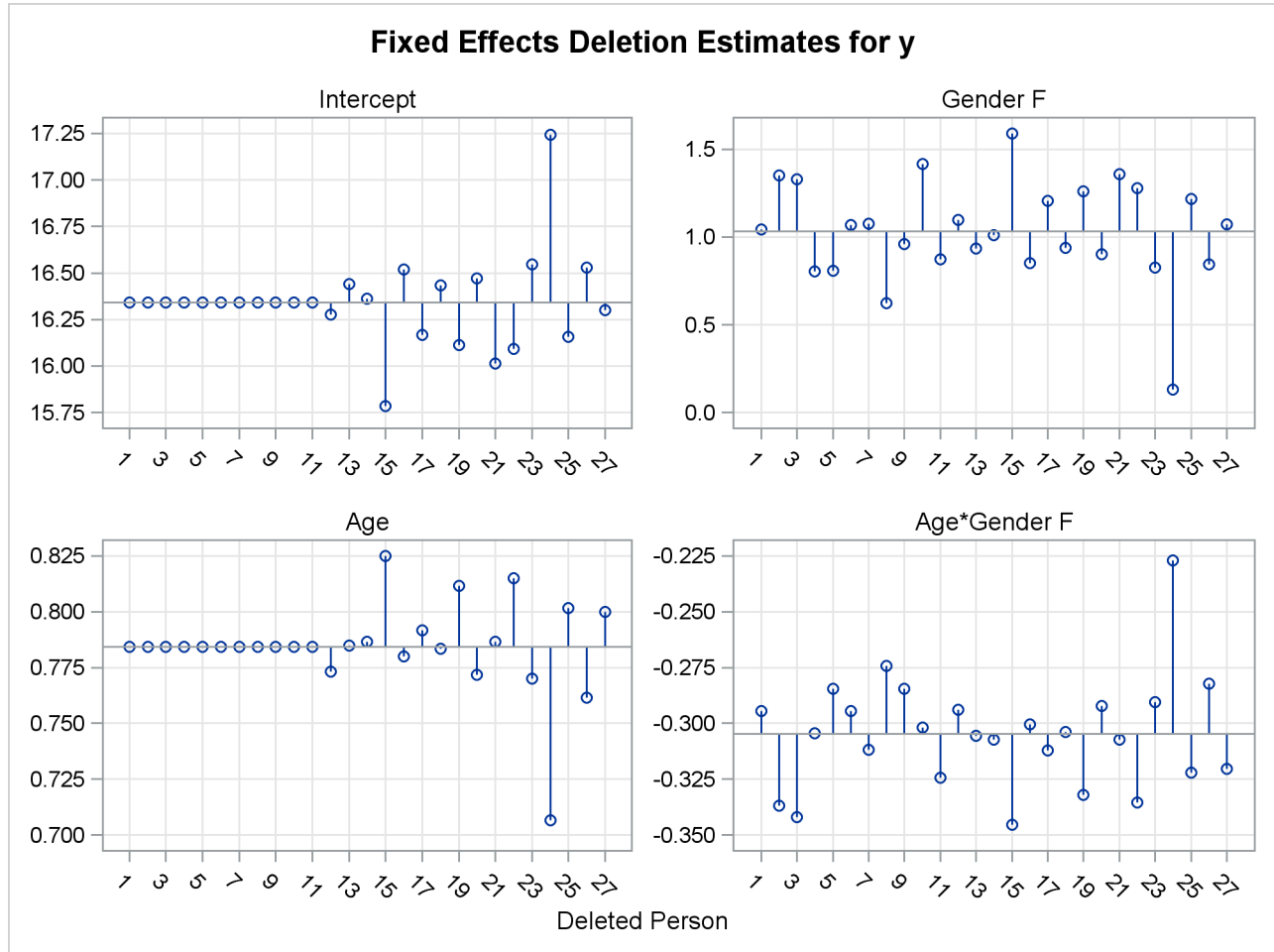
The final model investigated for these data is a random coefficient model as in Stram and Lee (1994) with random effects for the intercept and age effect. The following statements examine the estimates for fixed effects and the entries of the unstructured  $2 \times 2$  variance matrix of the random coefficients graphically:

```
proc mixed data=pr method=ml
 plots (only)=InfluenceEstPlot;
 class person gender;
 model y = gender age gender*age /
```

```
influence(iter=5 effect=person est);
random intercept age / type=un subject=person;
run;
```

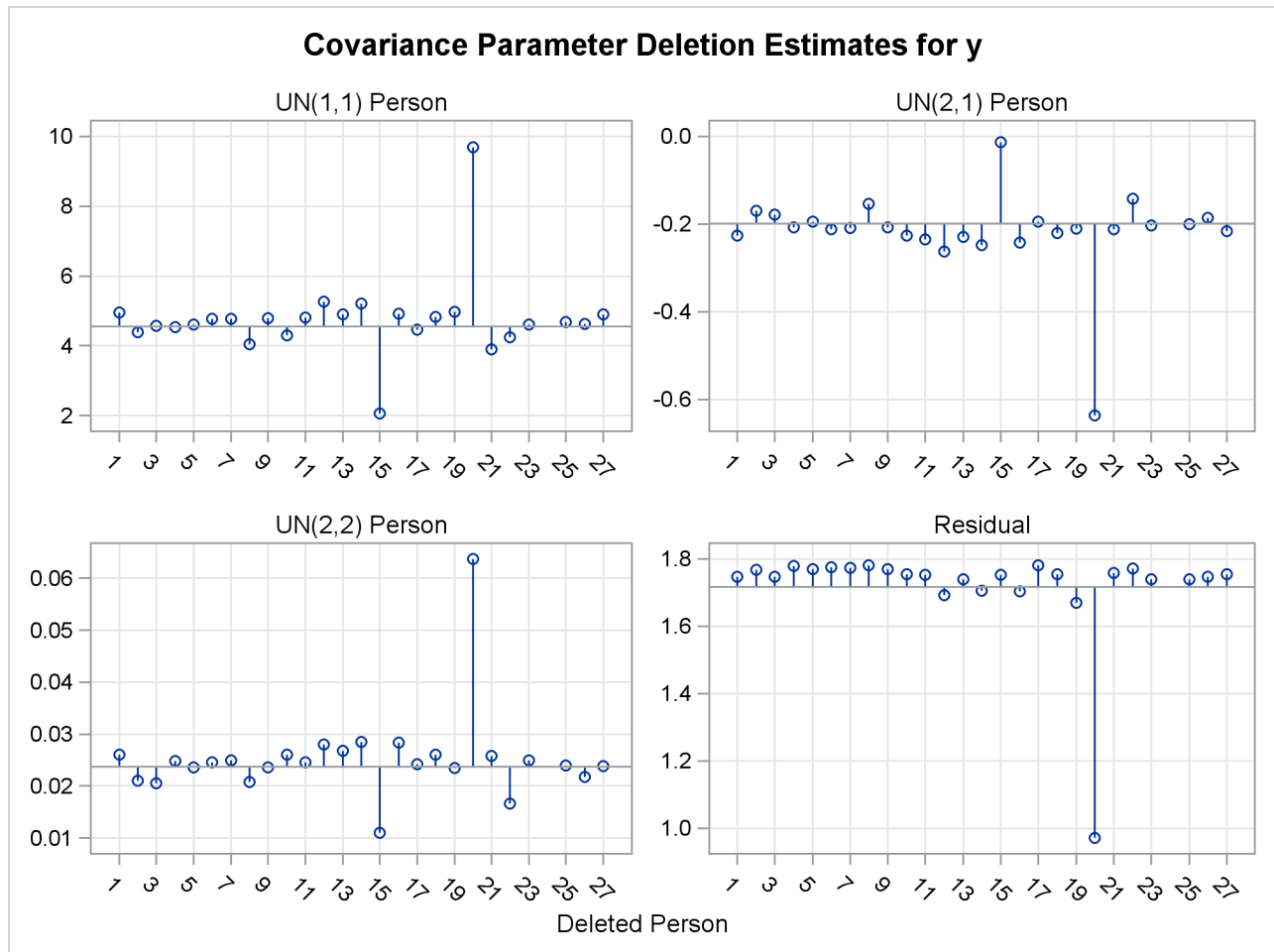
The `PLOTS(ONLY)=INFLUENCEESTPLOT` option restricts the graphical output from this PROC MIXED run to only the panels of deletion estimates (Output 59.8.4 and Output 59.8.5).

**Output 59.8.4** Fixed-Effects Deletion Estimates



In Output 59.8.4 the graphs on the left side of the panel represent the intercept and slope estimate for boys; the graphs on the right side represent the difference in intercept and slope between boys and girls. Removing any one of the first eleven children, who are girls, does not alter the intercept or slope in the group of boys. The difference in these parameters between boys and girls is altered by the removal of any child. Subject 24 changes the fixed effects considerably, subject 20 much less so.



**Output 59.8.5** Covariance Parameter Deletion Estimates

The covariance parameter deletion estimates in [Output 59.8.5](#) show several important features.

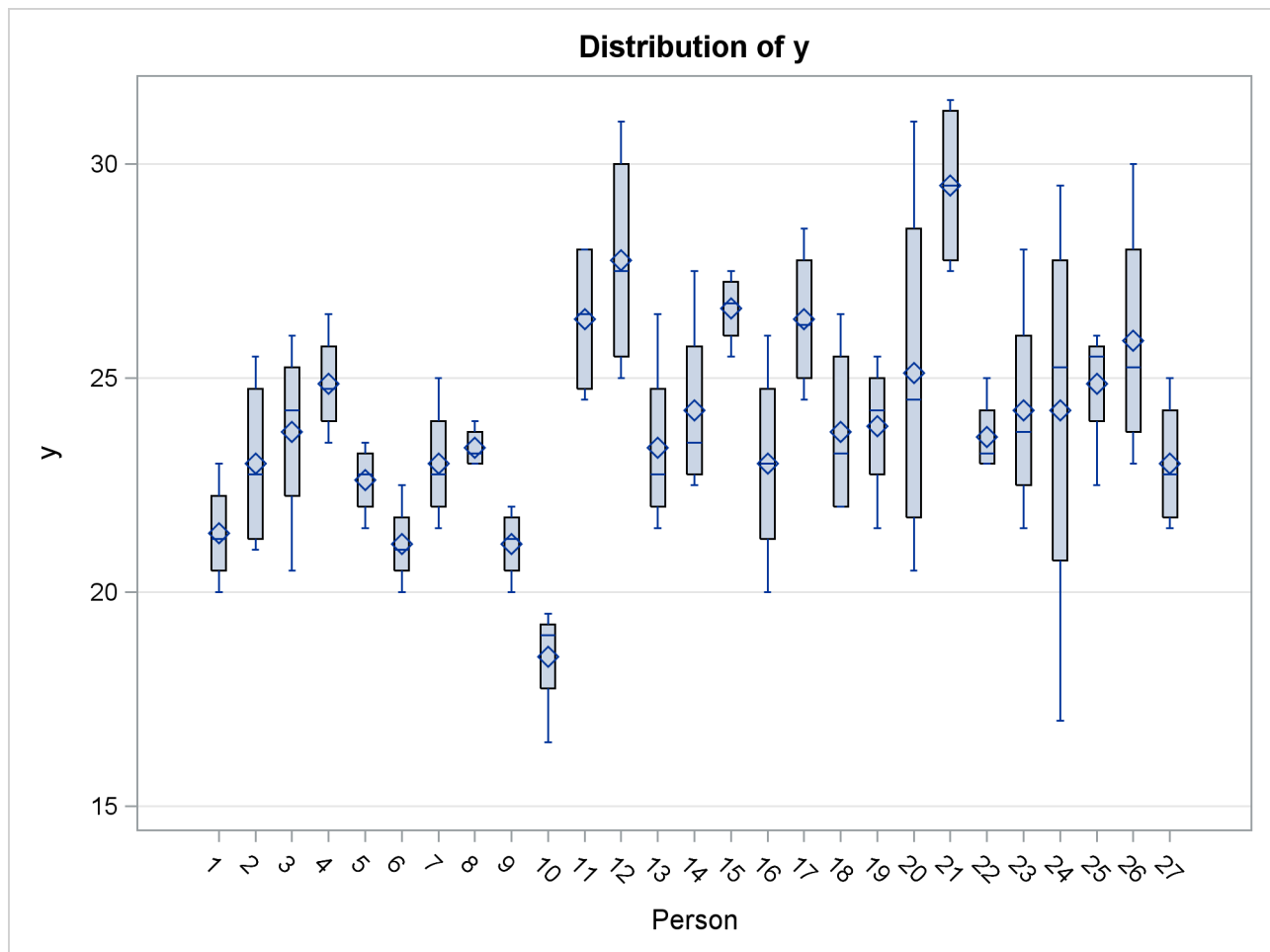
- The panels do not contain information about subject 24. Estimation of the  $G$  matrix following removal of that child did not yield a positive definite matrix. As a consequence, covariance parameter diagnostics are not produced for this subject.
- Subject 20 has great impact on the four covariance parameters. Removing this child from the analysis increases the variance of the random intercept and random slope and reduces the residual variance by almost 80%. The repeated measurements of this child exhibit an up-and-down behavior.
- The variance of the random intercept and slope are reduced when child 15 is removed from the analysis. This child's growth measurements oscillate about 27.0 from age 10 on.

Examining observed and residual values by levels of classification variables is also a useful tool to diagnose the adequacy of the model and unusual observations. Box plots for effects in the model that consist of only classification variables can be requested with the `BOXPLOT` option of the `PLOTS=` option in the `PROC MIXED` statement. For example, the following statements produce box plots for the `SUBJECT=` effects in the model:

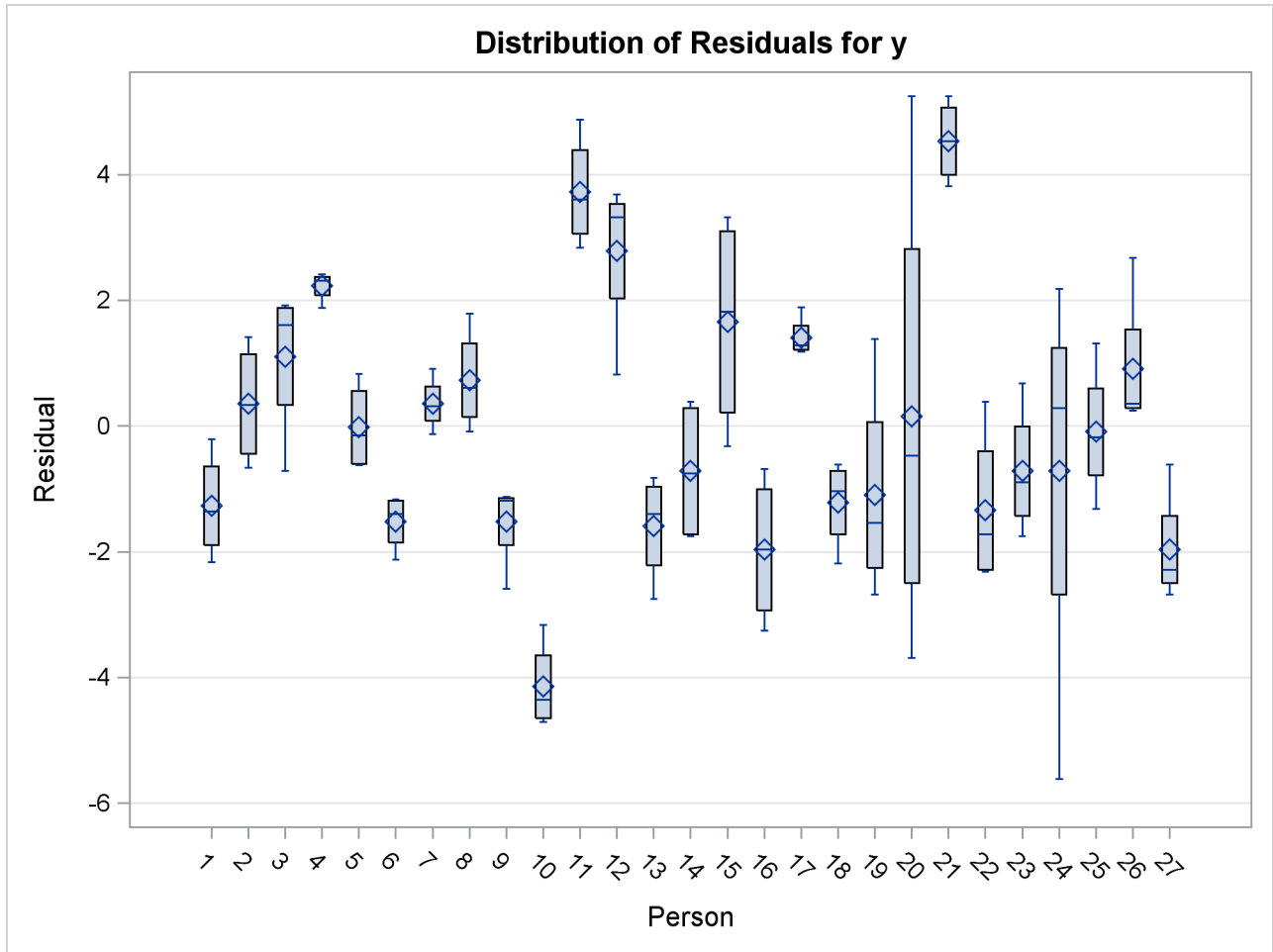
```
ods graphics on;
proc mixed data=pr method=ml
 plot=boxplot(observed marginal conditional subject);
 class person gender;
 model y = gender age gender*age;
 random intercept age / type=un subject=person;
run;
```

The specific boxplot options request a plot of the observed data (Output 59.8.6), the marginal residuals (Output 59.8.7), and the conditional residuals (Output 59.8.8). Box plots of the observed values show the variation within and between children clearly. The group of girls (subjects 1–11) is distinguishable from the group of boys by somewhat lesser average growth and lesser within-child variation (Output 59.8.6). After adjusting for overall (population-averaged) gender and age effects, the residual within-child variation is reduced but substantial differences in the means remain (Output 59.8.7). If child-specific inferences are desired, a model accounting for only Gender, Age, and Gender\*Age effects is not adequate for these data.

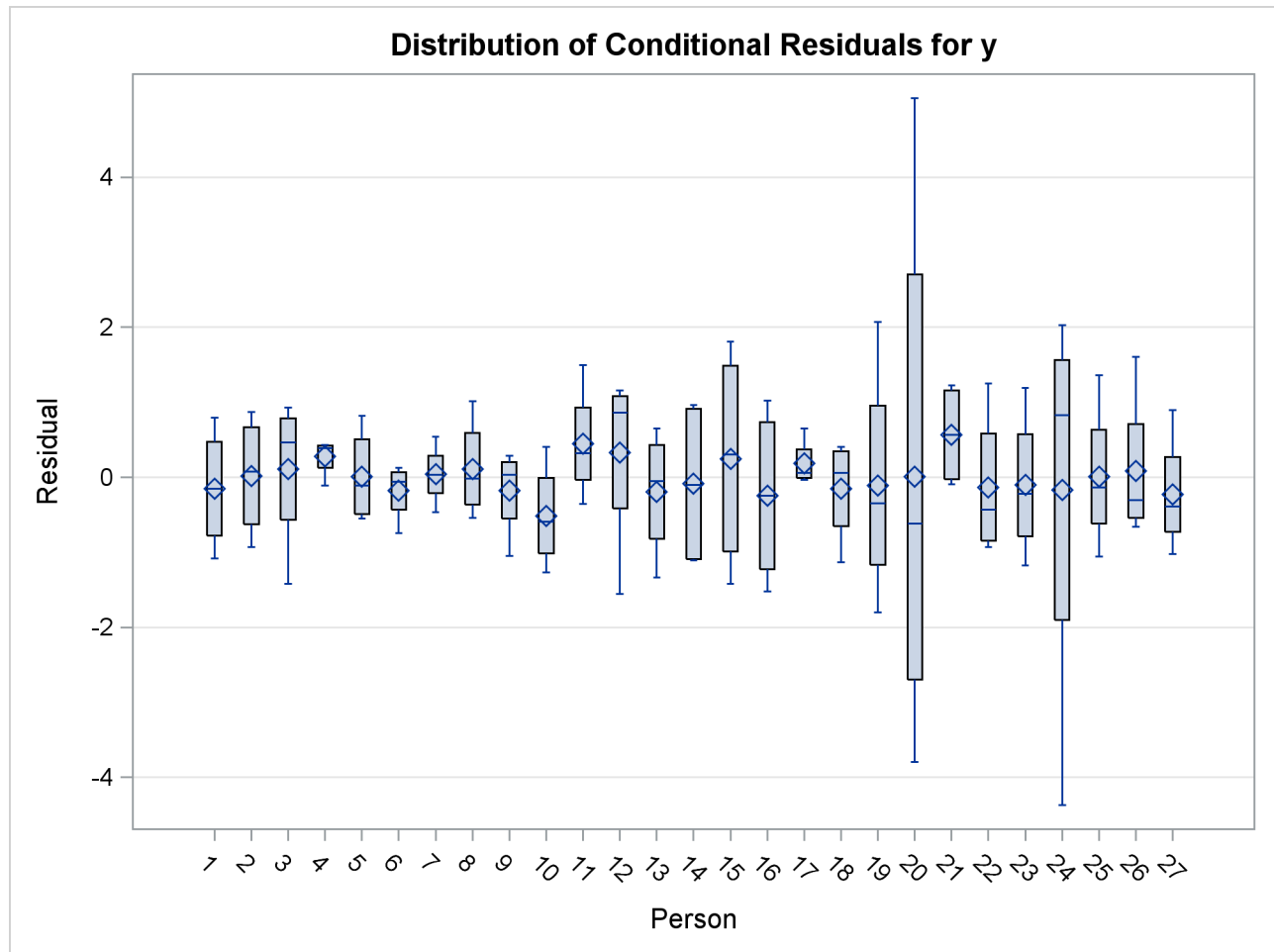
**Output 59.8.6** Distribution of Observed Values



**Output 59.8.7** Distribution of Marginal Residuals



The conditional residuals incorporate the EBLUPs for each child and enable you to examine whether the subject-specific model is adequate (Output 59.8.8). By using each child “as its own control,” the residuals are now centered near zero. Subjects 20 and 24 stand out as unusual in all three sets of box plots.

**Output 59.8.8** Distribution of Conditional Residuals

## Example 59.9: Examining Individual Test Components

The `LCOMPONENTS` option in the `MODEL` statement enables you to perform single-degree-of-freedom tests for individual rows of the `L` matrix. Such tests are useful to identify interaction patterns. In a balanced layout, Type 3 components of `L` associated with `A*B` interactions correspond to simple contrasts of cell mean differences.

The first example revisits the data from the split-plot design by Stroup (1989a) that was analyzed in [Example 59.1](#). Recall that variables `A` and `B` in the following statements represent the whole-plot and subplot factors, respectively:

```
proc mixed data=sp;
 class a b block;
 model y = a b a*b / LComponents e3;
 random block a*block;
run;
```

The `MIXED` procedure constructs a separate `L` matrix for each of the three fixed-effects components. The matrices are displayed in [Output 59.9.1](#). The tests for fixed effects are shown in [Output 59.9.2](#).

## Output 59.9.1 Coefficients of Type 3 Estimable Functions

| The Mixed Procedure         |   |   |        |      |
|-----------------------------|---|---|--------|------|
| Type 3 Coefficients for A   |   |   |        |      |
| Effect                      | A | B | Row1   | Row2 |
| Intercept                   |   |   |        |      |
| A                           | 1 |   | 1      |      |
| A                           | 2 |   |        | 1    |
| A                           | 3 |   | -1     | -1   |
| B                           |   | 1 |        |      |
| B                           |   | 2 |        |      |
| A*B                         | 1 | 1 | 0.5    |      |
| A*B                         | 1 | 2 | 0.5    |      |
| A*B                         | 2 | 1 |        | 0.5  |
| A*B                         | 2 | 2 |        | 0.5  |
| A*B                         | 3 | 1 | -0.5   | -0.5 |
| A*B                         | 3 | 2 | -0.5   | -0.5 |
| Type 3 Coefficients for B   |   |   |        |      |
| Effect                      | A | B | Row1   |      |
| Intercept                   |   |   |        |      |
| A                           | 1 |   |        |      |
| A                           | 2 |   |        |      |
| A                           | 3 |   |        |      |
| B                           |   | 1 |        | 1    |
| B                           |   | 2 |        | -1   |
| A*B                         | 1 | 1 | 0.3333 |      |
| A*B                         | 1 | 2 | -0.333 |      |
| A*B                         | 2 | 1 | 0.3333 |      |
| A*B                         | 2 | 2 | -0.333 |      |
| A*B                         | 3 | 1 | 0.3333 |      |
| A*B                         | 3 | 2 | -0.333 |      |
| Type 3 Coefficients for A*B |   |   |        |      |
| Effect                      | A | B | Row1   | Row2 |
| Intercept                   |   |   |        |      |
| A                           | 1 |   |        |      |
| A                           | 2 |   |        |      |
| A                           | 3 |   |        |      |
| B                           |   | 1 |        |      |
| B                           |   | 2 |        |      |
| A*B                         | 1 | 1 | 1      |      |
| A*B                         | 1 | 2 | -1     |      |
| A*B                         | 2 | 1 |        | 1    |
| A*B                         | 2 | 2 |        | -1   |
| A*B                         | 3 | 1 | -1     | -1   |
| A*B                         | 3 | 2 | 1      | 1    |

**Output 59.9.2** Type 3 Tests in Split-Plot Example

| Type 3 Tests of Fixed Effects |           |           |         |        |
|-------------------------------|-----------|-----------|---------|--------|
| Effect                        | Num<br>DF | Den<br>DF | F Value | Pr > F |
| A                             | 2         | 6         | 4.07    | 0.0764 |
| B                             | 1         | 9         | 19.39   | 0.0017 |
| A*B                           | 2         | 9         | 4.02    | 0.0566 |

If  $\mu_{i.}$  denotes a whole-plot main effect mean,  $\mu_{.j}$  denotes a subplot main effect mean, and  $\mu_{ij}$  denotes a cell mean, the five components shown in [Output 59.9.3](#) correspond to tests of the following:

- $H_0 : \mu_{1.} = \mu_{3.}$
- $H_0 : \mu_{2.} = \mu_{3.}$
- $H_0 : \mu_{.1} = \mu_{.2}$
- $H_0 : \mu_{11} - \mu_{12} = \mu_{31} - \mu_{32}$
- $H_0 : \mu_{21} - \mu_{22} = \mu_{31} - \mu_{32}$

**Output 59.9.3** Type 3 L Components Table

| L Components of Type 3 Tests of Fixed Effects |            |          |                   |    |         |         |
|-----------------------------------------------|------------|----------|-------------------|----|---------|---------|
| Effect                                        | L<br>Index | Estimate | Standard<br>Error | DF | t Value | Pr >  t |
| A                                             | 1          | 7.1250   | 3.1672            | 6  | 2.25    | 0.0655  |
| A                                             | 2          | 8.3750   | 3.1672            | 6  | 2.64    | 0.0383  |
| B                                             | 1          | 5.5000   | 1.2491            | 9  | 4.40    | 0.0017  |
| A*B                                           | 1          | 7.7500   | 3.0596            | 9  | 2.53    | 0.0321  |
| A*B                                           | 2          | 7.2500   | 3.0596            | 9  | 2.37    | 0.0419  |

The first three components are comparisons of marginal means. The fourth component compares the effect of factor B at the first whole-plot level against the effect of B at the third whole-plot level. Finally, the last component tests whether the factor B effect changes between the second and third whole-plot level.

The Type 3 component tests can also be produced with these corresponding `ESTIMATE` statements:

```
proc mixed data=sp;
 class a b block ;
 model y = a b a*b;
 random block a*block;
 estimate 'a' 1' a 1 0 -1;
 estimate 'a' 2' a 0 1 -1;
 estimate 'b' 1' b 1 -1;
```

```

estimate 'a*b 1' a*b 1 -1 0 0 -1 1;
estimate 'a*b 2' a*b 0 0 1 -1 -1 1;
ods select Estimates;
run;

```

The results are shown in [Output 59.9.4](#).

**Output 59.9.4** Results from ESTIMATE Statements

| The Mixed Procedure |   |          |                |    |         |         |
|---------------------|---|----------|----------------|----|---------|---------|
| Estimates           |   |          |                |    |         |         |
| Label               |   | Estimate | Standard Error | DF | t Value | Pr >  t |
| a                   | 1 | 7.1250   | 3.1672         | 6  | 2.25    | 0.0655  |
| a                   | 2 | 8.3750   | 3.1672         | 6  | 2.64    | 0.0383  |
| b                   | 1 | 5.5000   | 1.2491         | 9  | 4.40    | 0.0017  |
| a*b                 | 1 | 7.7500   | 3.0596         | 9  | 2.53    | 0.0321  |
| a*b                 | 2 | 7.2500   | 3.0596         | 9  | 2.37    | 0.0419  |

A second useful application of the **LCOMPONENTS** option is in polynomial models, where Type 1 tests are often used to test the entry of model terms sequentially. The **SOLUTION** option in the **MODEL** statement displays the regression coefficients that correspond to a Type 3 analysis. That is, the coefficients represent the partial coefficients you would get by adding the regressor variable last in a model containing all other effects, and the tests are identical to those in the “Type 3 Tests of Fixed Effects” table.

Consider the following **DATA** step and the fit of a third-order polynomial regression model.

```

data polynomial;
 do x=1 to 20; input y@@; output; end;
 datalines;
1.092 1.758 1.997 3.154 3.880
3.810 4.921 4.573 6.029 6.032
6.291 7.151 7.154 6.469 7.137
6.374 5.860 4.866 4.155 2.711
;

proc mixed data=polynomial;
 model y = x x*x x*x*x / s lcomponents htype=1,3;
run;

```

The *t* tests displayed in the “Solution for Fixed Effects” table are Type 3 tests, sometimes referred to as partial tests. They measure the contribution of a regressor in the presence of all other regressor variables in the model.

**Output 59.9.5** Parameter Estimates in Polynomial Model

| The Mixed Procedure        |          |                |    |         |         |
|----------------------------|----------|----------------|----|---------|---------|
| Solution for Fixed Effects |          |                |    |         |         |
| Effect                     | Estimate | Standard Error | DF | t Value | Pr >  t |
| Intercept                  | 0.7837   | 0.3545         | 16 | 2.21    | 0.0420  |
| x                          | 0.3726   | 0.1426         | 16 | 2.61    | 0.0189  |
| x*x                        | 0.04756  | 0.01558        | 16 | 3.05    | 0.0076  |
| x*x*x                      | -0.00306 | 0.000489       | 16 | -6.27   | <.0001  |

The Type 3 L components are identical to the tests in the “Solutions for Fixed Effects” table shown in Output 59.9.5. The Type 1 table yields the following:

- sequential (Type 1) tests of regression variables that test the significance of a regressor given all other variables preceding it in the model list
- the regression coefficients for sequential submodels

**Output 59.9.6** Type 1 and Type 3 L Components

| L Components of Type 1 Tests of Fixed Effects |         |          |                |    |         |         |
|-----------------------------------------------|---------|----------|----------------|----|---------|---------|
| Effect                                        | L Index | Estimate | Standard Error | DF | t Value | Pr >  t |
| x                                             | 1       | 0.1763   | 0.01259        | 16 | 14.01   | <.0001  |
| x*x                                           | 1       | -0.04886 | 0.002449       | 16 | -19.95  | <.0001  |
| x*x*x                                         | 1       | -0.00306 | 0.000489       | 16 | -6.27   | <.0001  |

| L Components of Type 3 Tests of Fixed Effects |         |          |                |    |         |         |
|-----------------------------------------------|---------|----------|----------------|----|---------|---------|
| Effect                                        | L Index | Estimate | Standard Error | DF | t Value | Pr >  t |
| x                                             | 1       | 0.3726   | 0.1426         | 16 | 2.61    | 0.0189  |
| x*x                                           | 1       | 0.04756  | 0.01558        | 16 | 3.05    | 0.0076  |
| x*x*x                                         | 1       | -0.00306 | 0.000489       | 16 | -6.27   | <.0001  |

The estimate of 0.1763 is the regression coefficient in a simple linear regression of Y on X. The estimate of -0.04886 is the partial coefficient for the quadratic term when it is added to a model containing only a linear component. Similarly, the value -0.00306 is the partial coefficient for the cubic term when it is added to a model containing a linear and quadratic component. The last Type 1 component is always identical to the corresponding Type 3 component.



## Example 59.10: Isotonic Contrasts for Ordered Mean Values

It is often of interest to test whether the mean values of the dependent variable increases or decreases monotonically with certain factors. Hirotsu and Srivastava (2000) demonstrate one approach by using data (Moriguchi 1976). The data consist of ferrite cores subjected to four increasing temperatures. The response variable is the magnetic force of each core.

```
data FerriteCores;
 do Temp = 1 to 4;
 do rep = 1 to 5; drop rep;
 input MagneticForce @@;
 output;
 end;
 end;
 datalines;
10.8 9.9 10.7 10.4 9.7
10.7 10.6 11.0 10.8 10.9
11.9 11.2 11.0 11.1 11.3
11.4 10.7 10.9 11.3 11.7
;
```

The method presented by Hirotsu and Srivastava (2000) to test whether the magnetic force of the cores rises monotonically with temperature depends on the lower confidence limits of the *isotonic contrasts* of the force means at each temperature, adjusted for multiplicity. The corresponding isotonic contrast compares the average of a particular group and the preceding groups with the average of the succeeding groups. You can compute adjusted confidence intervals for isotonic contrasts by using the `LSMESTIMATE` statement.

The following statements analyze the `FerriteCores` data as a one-way design and multiplicity-adjusted lower confidence limits for the isotonic contrasts. For the multiplicity adjustment, the `LSMESTIMATE` statement employs simulation, which provides adjusted  $p$ -values and lower confidence limits that are exact up to Monte Carlo error.

```
proc mixed data=FerriteCores;
 class Temp;
 model MagneticForce = Temp;
 lsestimate Temp
 'avg(1:1)<avg(2:4)' -3 1 1 1 divisor=3,
 'avg(1:2)<avg(3:4)' -1 -1 1 1 divisor=2,
 'avg(1:3)<avg(4:4)' -1 -1 -1 3 divisor=3
 / adjust=simulate(seed=1) cl upper;
 ods select LSMestimates;
run;
```

The results are shown in [Output 59.10.1](#).

### Output 59.10.1 Analysis of LS-Means with Isotonic Contrasts

| The Mixed Procedure                    |                     |          |                |    |         |       |        |
|----------------------------------------|---------------------|----------|----------------|----|---------|-------|--------|
| Least Squares Means Estimates          |                     |          |                |    |         |       |        |
| Adjustment for Multiplicity: Simulated |                     |          |                |    |         |       |        |
| Effect                                 | Label               | Estimate | Standard Error | DF | t Value | Tails | Pr > t |
| Temp                                   | avg(1:1) < avg(2:4) | 0.8000   | 0.1906         | 16 | 4.20    | Upper | 0.0003 |
| Temp                                   | avg(1:2) < avg(3:4) | 0.7000   | 0.1651         | 16 | 4.24    | Upper | 0.0003 |
| Temp                                   | avg(1:3) < avg(4:4) | 0.4000   | 0.1906         | 16 | 2.10    | Upper | 0.0260 |

| Least Squares Means Estimates          |                     |        |       |         |       |
|----------------------------------------|---------------------|--------|-------|---------|-------|
| Adjustment for Multiplicity: Simulated |                     |        |       |         |       |
| Effect                                 | Label               | Adj P  | Alpha | Lower   | Upper |
| Temp                                   | avg(1:1) < avg(2:4) | 0.0010 | 0.05  | 0.4672  | Infty |
| Temp                                   | avg(1:2) < avg(3:4) | 0.0009 | 0.05  | 0.4118  | Infty |
| Temp                                   | avg(1:3) < avg(4:4) | 0.0625 | 0.05  | 0.06721 | Infty |

| Least Squares Means Estimates          |                     |           |           |  |  |
|----------------------------------------|---------------------|-----------|-----------|--|--|
| Adjustment for Multiplicity: Simulated |                     |           |           |  |  |
| Effect                                 | Label               | Adj Lower | Adj Upper |  |  |
| Temp                                   | avg(1:1) < avg(2:4) | 0.3771    | Infty     |  |  |
| Temp                                   | avg(1:2) < avg(3:4) | 0.3337    | Infty     |  |  |
| Temp                                   | avg(1:3) < avg(4:4) | -0.02291  | Infty     |  |  |

With an adjusted  $p$ -value of 0.001, the magnetic force at the first temperature is significantly less than the average of the other temperatures. Likewise, the average of the first two temperatures is significantly less than the average of the last two ( $p = 0.0009$ ). However, the magnetic force at the last temperature is not significantly greater than the average magnetic force of the others ( $p = 0.0625$ ). These results indicate a significant monotone increase over the first three temperatures, but not across all four temperatures.

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# Chapter 60

## The MODECLUS Procedure

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### Overview: MODECLUS Procedure

The MODECLUS procedure clusters observations in a SAS data set by using any of several algorithms based on nonparametric density estimates. The data can be numeric coordinates or distances. PROC MODECLUS can perform approximate significance tests for the number of clusters and can hierarchically join nonsignificant clusters. The significance tests are empirically validated by simulations with sample sizes ranging from 20 to 2000.

PROC MODECLUS produces output data sets containing density estimates and cluster membership, various cluster statistics including approximate  $p$ -values, and a summary of the number of clusters generated by various algorithms, smoothing parameters, and significance levels.

Most clustering methods are biased toward finding clusters possessing certain characteristics related to size (number of members), shape, or dispersion. Methods based on the least squares criterion (Sarle 1982), such as  $k$ -means and Ward's minimum variance method, tend to find clusters with roughly the same number of observations in each cluster. Average linkage (see Chapter 31, "The CLUSTER Procedure") is somewhat biased toward finding clusters of equal variance. Many clustering methods tend to produce compact, roughly hyperspherical clusters and are incapable of detecting clusters with highly elongated or irregular shapes. The methods with the least bias are those based on nonparametric density estimation (Silverman 1986, pp. 130–146; Scott 1992, pp. 125–190) such as density linkage (see Chapter 31, "The CLUSTER Procedure"), Wong and Lane (1983); Wong and Schaack (1982). The biases of many commonly used clustering methods are discussed in Chapter 11, "Introduction to Clustering Procedures."

PROC MODECLUS implements several clustering methods by using nonparametric density estimation. Such clustering methods are referred to hereafter as *nonparametric clustering methods*. The methods in PROC MODECLUS are related to, but not identical to, methods developed by Gitman (1973); Huizinga (1978); Koontz and Fukunaga (1972a, b); Koontz, Narendra, and Fukunaga (1976); Mizoguchi and Shimura (1980); Wong and Lane (1983).

Details of the algorithms are provided in the section "Clustering Methods" on page 5099.

For nonparametric clustering methods, a cluster is loosely defined as a region surrounding a local maximum of the probability density function (see the section "Significance Tests" on page 5101 for a more rigorous definition). Given a sufficiently large sample, nonparametric clustering methods are capable of detecting clusters of unequal size and dispersion and with highly irregular shapes. Nonparametric methods can also obtain good results for compact clusters of equal size and dispersion, but they naturally require larger sample sizes for good recovery than clustering methods that are biased toward finding such "nice" clusters.

For coordinate data, nonparametric clustering methods are less sensitive to changes in scale of the variables or to affine transformations of the variables than are most other commonly used clustering methods. Nevertheless, it is necessary to consider questions of scaling and transformation, since variables with large variances tend to have more of an effect on the resulting clusters than those with small variances. If two or more variables are not measured in comparable units, some type of standardization or scaling is necessary; otherwise, the distances used by the procedure might be based on inappropriate apples-and-oranges computations. For variables with comparable units of measurement, standardization or scaling might still be desirable if the scale estimates of the variables are not related to their expected importance for defining clusters. If you want two variables to have equal importance in the analysis, they should have roughly equal scale estimates. If you want one variable to have more of an effect than another, the former should be scaled to have a greater scale estimate than the latter. The STD option in the PROC MODECLUS statement scales all variables to equal variance. However, the variance is not necessarily the most appropriate scale estimate for cluster analysis. In particular, outliers should be removed before using PROC MODECLUS with the STD option. A variety of scale estimators including robust estimators are provided in the STDIZE procedure (for detailed information, see Chapter 87, "The STDIZE Procedure"). Additionally, the ACECLUS procedure provides another way to transform the variables to try to improve the separation of clusters.

Since clusters are defined in terms of local maxima of the probability density function, nonlinear transformations of the data can change the number of population clusters. The variables should be transformed so that equal differences are of equal practical importance. An interval scale of measurement is required. Or-

dinal or ranked data are generally inappropriate, since monotone transformations can produce any arbitrary number of modes.

Unlike the methods in the CLUSTER procedure, the methods in the MODECLUS procedure are not inherently hierarchical. However, PROC MODECLUS can do approximate nonparametric significance tests for the number of clusters by obtaining an approximate  $p$ -value for each cluster, and it can hierarchically join nonsignificant clusters.

Another important difference between the MODECLUS procedure and many other clustering methods is that you do not tell PROC MODECLUS how many clusters you want. Instead, you specify a *smoothing parameter* (see the section “Density Estimation” on page 5096) and, optionally, a significance level, and PROC MODECLUS determines the number of clusters. You can specify a list of smoothing parameters, and PROC MODECLUS performs a separate cluster analysis for each value in the list.

---

## Getting Started: MODECLUS Procedure

This section illustrates how PROC MODECLUS can be used to examine the clusters of data in the following artificial data set.

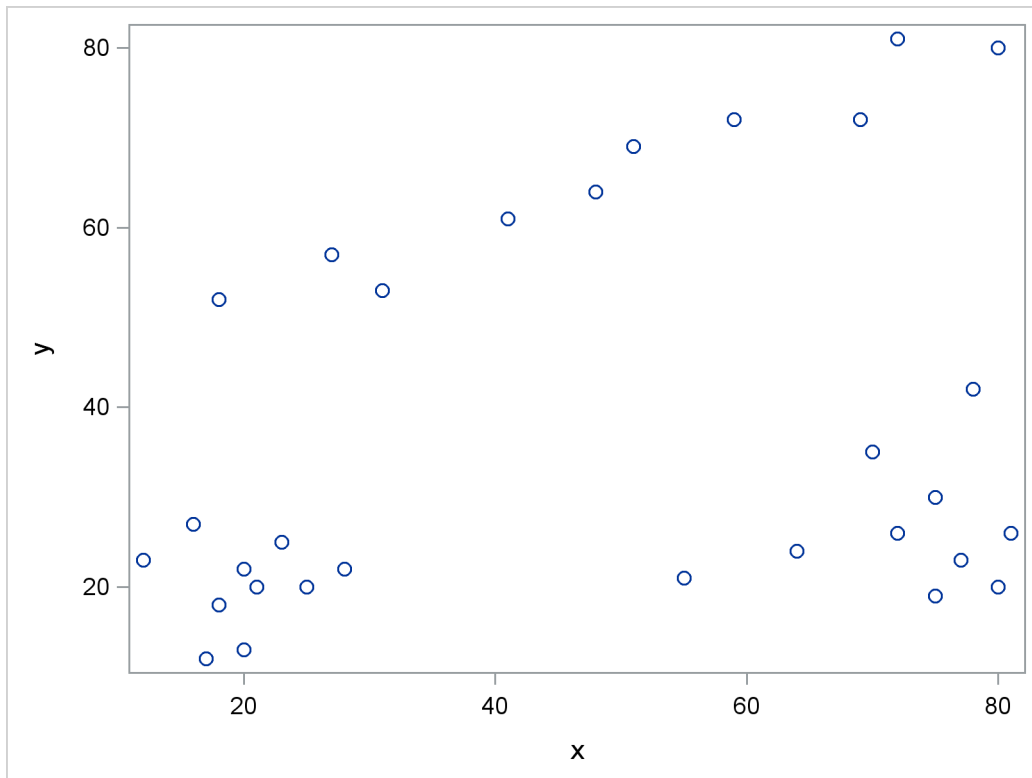
```
data example;
 input x y @@;
 datalines;
18 18 20 22 21 20 12 23 17 12 23 25 25 20 16 27
20 13 28 22 80 20 75 19 77 23 81 26 55 21 64 24
72 26 70 35 75 30 78 42 18 52 27 57 41 61 48 64
59 72 69 72 80 80 31 53 51 69 72 81
;
```

It is a good practice to plot the data to check for obvious clusters or pathologies prior to the analysis. In this example, with only two variables and a small sample size, the SGPLOT procedure in the following statements produces a scatter plot:

```
proc sgplot;
 scatter y=y x=x;
run;
```

Figure 60.1 suggests three clusters. Of these clusters, the one in the lower-left corner is the most compact, while the lower-right cluster is more dispersed.

The upper cluster is elongated and would be difficult for most clustering algorithms to identify as a single cluster. The plot also suggests that a Euclidean distance of 10 or 20 is a good initial guess for the neighborhood size in density estimation and clustering.

**Figure 60.1** Scatter Plot of Data

To obtain a cluster analysis in PROC MODECLUS, you must specify the METHOD= option; for most purposes, METHOD=1 is recommended. The cluster analysis can be performed with a list of radii (R=10 15 35), as shown in the following PROC MODECLUS statement. An output data set containing the cluster membership is created with the OUT= option. The following statements produce Figure 60.2 through Figure 60.5:

```
proc modeclus data=example method=1 r=10 15 35 out=out;
run;
```

For each cluster solution, PROC MODECLUS produces a table of cluster statistics including the cluster number, the number of observations in the cluster, the maximum estimated density within the cluster, the number of observations in the cluster having a neighbor that belongs to a different cluster, and the estimated saddle density of the cluster. The results are displayed in Figure 60.2, Figure 60.3, and Figure 60.4 for three different radii. A smaller radius (R=10) yields a larger number of clusters (6), as displayed in Figure 60.2; a larger radius (R=35) includes all observations in a single cluster, as displayed in Figure 60.4. Note that all clusters in these three figures are “isolated” since their corresponding boundary frequencies are all zeros. Consequently, all the estimated saddle densities are missing. A table summarizing each cluster solution is then produced at the end, as displayed in Figure 60.5.

**Figure 60.2** Results from PROC MODECLUS for METHOD=1 and R=10

| The MODECLUS Procedure |           |                                 |                       |                                |
|------------------------|-----------|---------------------------------|-----------------------|--------------------------------|
| R=10 METHOD=1          |           |                                 |                       |                                |
| Cluster Statistics     |           |                                 |                       |                                |
| Cluster                | Frequency | Maximum<br>Estimated<br>Density | Boundary<br>Frequency | Estimated<br>Saddle<br>Density |
| 1                      | 10        | 0.00106103                      | 0                     | .                              |
| 2                      | 9         | 0.00084883                      | 0                     | .                              |
| 3                      | 7         | 0.00031831                      | 0                     | .                              |
| 4                      | 2         | 0.00021221                      | 0                     | .                              |
| 5                      | 1         | 0.0001061                       | 0                     | .                              |
| 6                      | 1         | 0.0001061                       | 0                     | .                              |

**Figure 60.3** Results from PROC MODECLUS for METHOD=1 and R=15

| The MODECLUS Procedure |           |                                 |                       |                                |
|------------------------|-----------|---------------------------------|-----------------------|--------------------------------|
| R=15 METHOD=1          |           |                                 |                       |                                |
| Cluster Statistics     |           |                                 |                       |                                |
| Cluster                | Frequency | Maximum<br>Estimated<br>Density | Boundary<br>Frequency | Estimated<br>Saddle<br>Density |
| 1                      | 10        | 0.00047157                      | 0                     | .                              |
| 2                      | 10        | 0.00042441                      | 0                     | .                              |
| 3                      | 10        | 0.00023579                      | 0                     | .                              |

**Figure 60.4** Results from PROC MODECLUS for METHOD=1 and R=35

| The MODECLUS Procedure |           |                                 |                       |                                |
|------------------------|-----------|---------------------------------|-----------------------|--------------------------------|
| R=35 METHOD=1          |           |                                 |                       |                                |
| Cluster Statistics     |           |                                 |                       |                                |
| Cluster                | Frequency | Maximum<br>Estimated<br>Density | Boundary<br>Frequency | Estimated<br>Saddle<br>Density |
| 1                      | 30        | 0.00012126                      | 0                     | .                              |

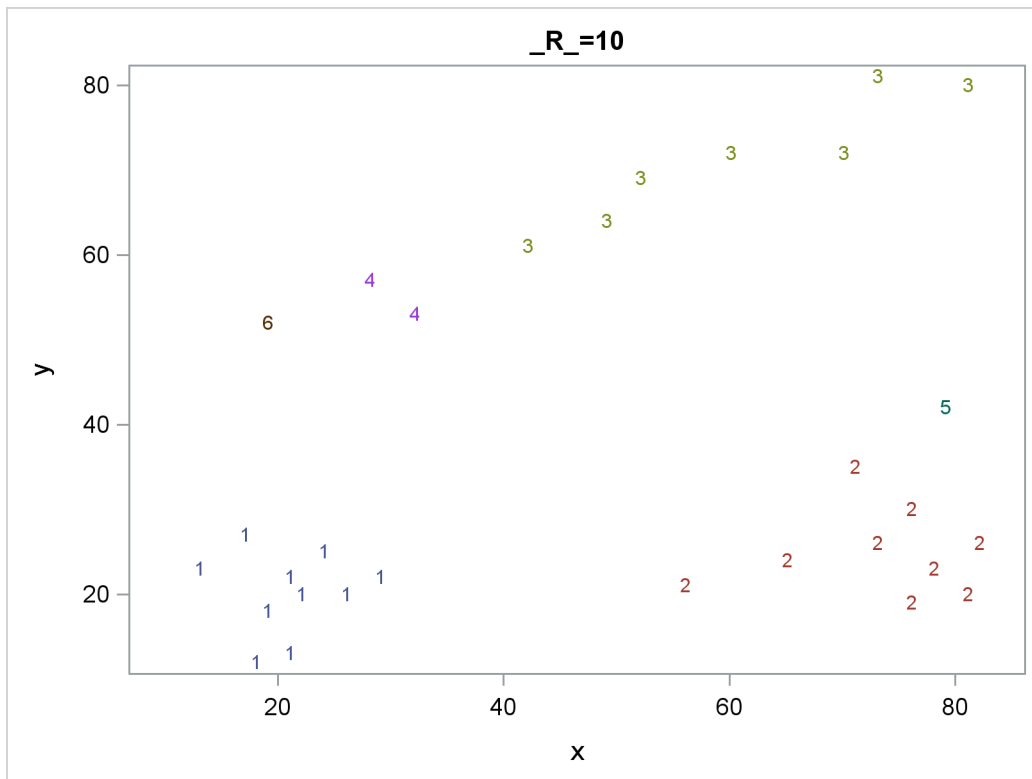


**Figure 60.5** Summary Table

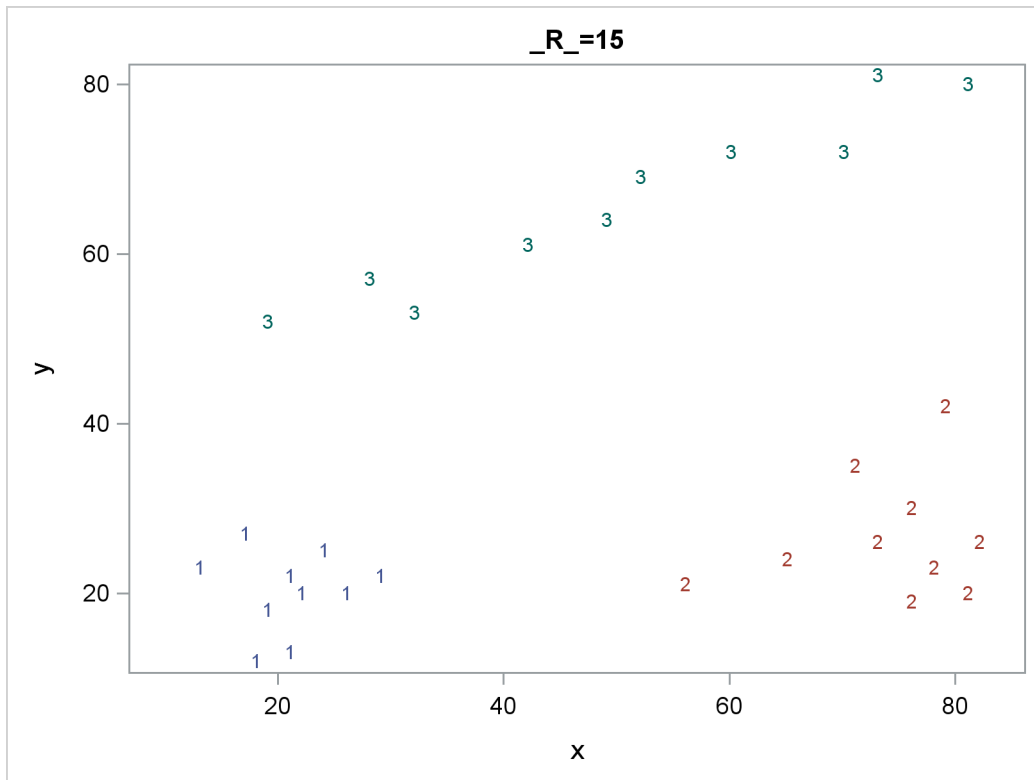
| The MODECLUS Procedure |                    |                                   |
|------------------------|--------------------|-----------------------------------|
| Cluster Summary        |                    |                                   |
| R                      | Number of Clusters | Frequency of Unclassified Objects |
| 10                     | 6                  | 0                                 |
| 15                     | 3                  | 0                                 |
| 35                     | 1                  | 0                                 |

The OUT= data set contains a complete copy of the input data set for each cluster solution. By using a BY statement in the following PROC SGLOT statement, you can examine the differences in cluster memberships for each radius as shown in Figure 60.6 through Figure 60.8:

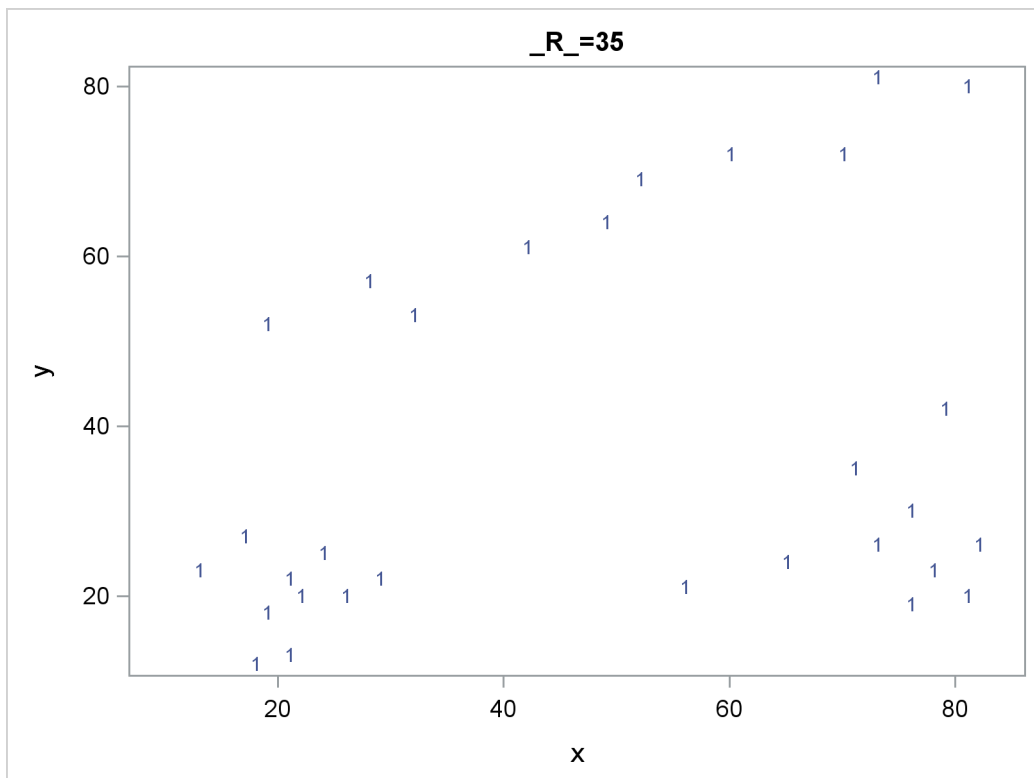
```
proc sgplot data=out noautolegend;
 scatter y=y x=x / group=cluster markerchar=cluster;
 by _r_;
run;
```

**Figure 60.6** Scatter Plots of Cluster Memberships with \_R\_=10

**Figure 60.7** Scatter Plots of Cluster Memberships with  $_R_=15$



**Figure 60.8** Scatter Plots of Cluster Memberships with  $_R_=35$



## Syntax: MODECLUS Procedure

The following statements are available in the MODECLUS procedure:

```
PROC MODECLUS < options > ;
 BY variables ;
 FREQ variable ;
 ID variable ;
 VAR variables ;
```

The PROC MODECLUS statement is required. All other statements are optional.

## PROC MODECLUS Statement

```
PROC MODECLUS < options > ;
```

The PROC MODECLUS statement invokes the MODECLUS procedure. [Table 60.1](#) summarizes the options available in the PROC MODECLUS statement. These options are discussed in the following sections.

**Table 60.1** Summary of PROC MODECLUS Statement Options

| Option                                                         | Description                                                                                                     |
|----------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------|
| <b>Specify input and output data sets</b>                      |                                                                                                                 |
| DATA=                                                          | Specifies input data set name                                                                                   |
| OUT=                                                           | Specifies output data set name for observations                                                                 |
| OUTCLUS=                                                       | Specifies output data set name for clusters                                                                     |
| OUTSUM=                                                        | Specifies output data set name for cluster solutions                                                            |
| <b>Specify variables in output data sets</b>                   |                                                                                                                 |
| CLUSTER=                                                       | Specifies variable in the OUT= and OUTCLUS= data sets identifying clusters                                      |
| DENSITY=                                                       | Specifies variable in the OUT= data set containing density estimates                                            |
| OUTLENGTH=                                                     | Specifies length of variables in the output data sets                                                           |
| <b>Summarize and process coordinate data before clustering</b> |                                                                                                                 |
| SIMPLE                                                         | Requests simple statistics                                                                                      |
| STANDARD                                                       | Standardizes the variables to mean 0 and standard deviation 1                                                   |
| <b>Specify smoothing parameters</b>                            |                                                                                                                 |
| DK=                                                            | Specifies number of neighbors to use for <i>k</i> th-nearest-neighbor density estimation                        |
| CK=                                                            | Specifies number of neighbors to use for clustering                                                             |
| K=                                                             | Specifies number of neighbors to use for <i>k</i> th-nearest-neighbor density estimation and clustering         |
| DR=                                                            | Specifies radius of the sphere of support for uniform-kernel density estimation                                 |
| CR=                                                            | Specifies radius of the neighborhood for clustering                                                             |
| R=                                                             | Specifies radius of the sphere of support for uniform-kernel density estimation and the neighborhood clustering |
| <b>Specify density estimation options</b>                      |                                                                                                                 |
| CASCADE=                                                       | Specifies number of times the density estimates are to be cascaded                                              |

Table 60.1 continued

| Option                                        | Description                                                                                                                                  |
|-----------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------|
| DIMENSION=                                    | Specifies dimensionality to be used when computing density estimates                                                                         |
| AM                                            | Uses arithmetic means for cascading density estimates                                                                                        |
| HM                                            | Uses harmonic means for cascading density estimates                                                                                          |
| SUM                                           | Uses sums for cascading density estimates                                                                                                    |
| <b>Specify clustering methods and options</b> |                                                                                                                                              |
| DOCK=                                         | Dissolves clusters with $n$ or fewer members                                                                                                 |
| EARLY                                         | Stops the analysis after obtaining a solution with either no cluster or a single cluster                                                     |
| JOIN=                                         | Requests that nonsignificant clusters be hierarchically joined                                                                               |
| MAXCLUSTERS=                                  | Specifies maximum number of clusters to be obtained with METHOD=6                                                                            |
| METHOD=                                       | Specifies clustering method to use                                                                                                           |
| MODE=                                         | Specifies minimum members for either cluster to be designated a modal cluster when two clusters are joined using METHOD=5                    |
| POWER=                                        | Specifies power of the density used with METHOD=6                                                                                            |
| TEST                                          | Specifies approximate significance tests for the number of clusters                                                                          |
| THRESHOLD=                                    | Specifies assignment threshold used with METHOD=6                                                                                            |
| <b>Specify the output display options</b>     |                                                                                                                                              |
| ALL                                           | Produces all optional output                                                                                                                 |
| BOUNDARY                                      | Displays the density and cluster membership of observations with neighbors belonging to a different cluster                                  |
| CORE                                          | Retains the neighbor lists for each observation in memory                                                                                    |
| CROSS                                         | Displays the estimated cross validated log density of each observation                                                                       |
| CROSSLIST                                     | Displays the estimated density and cluster membership of each observation                                                                    |
| LOCAL                                         | Displays estimates of local dimensionality and writes them to the OUT=data set                                                               |
| NEIGHBOR                                      | Displays the neighbors of each observation                                                                                                   |
| NOPRINT                                       | Suppresses the display of the output                                                                                                         |
| NOSUMMARY                                     | Suppresses the display of the summary of the number of clusters, number of unassigned observations, and maximum $p$ -value for each analysis |
| SHORT                                         | Suppresses the display of statistics for each cluster                                                                                        |
| TRACE                                         | Traces the cluster assignments when METHOD=6                                                                                                 |

You can specify at least one of the following options for smoothing parameters for density estimation: DK=, K=, DR=, or R=. To obtain a cluster analysis, you can specify the METHOD= option and at least one of the following smoothing parameters for clustering: CK=, K=, CR=, or R=. If you want significance tests for the number of clusters, you should specify either the DR= or R= option. If none of the smoothing parameters is specified, the MODECLUS procedure provides a default value for the R= option. See the section “Density Estimation” on page 5096 for the formula of a reasonable first guess for R= and a discussion of smoothing parameters.

You can specify lists of values for the DK=, CK=, K=, DR=, CR=, and R= options. Numbers in the lists can be separated by blanks or commas. You can include in the lists one or more items of the form *start TO stop BY increment*. Each list can contain either one value or the same number of values as in every other list that contains more than one value. If a list has only one value, that value is used in combination with all

the values in longer lists. If two or more lists have more than one value, then one analysis is done by using the first value in each list, another analysis is done by using the second value in each list, and so on.

You can specify the following options in the PROC MODECLUS statement.

**ALL**

produces all optional output.

**AM**

specifies arithmetic means for cascading density estimates. See the description of the CASCADE= option.

**BOUNDARY**

displays the density and cluster membership of observations with neighbors belonging to a different cluster.

**CASCADE=*n*****CASC=*n***

specifies the number of times the density estimates are to be cascaded (see the section “[Density Estimation](#)” on page 5096). The default value 0 performs no cascading.

You can specify a list of values for the CASCADE= option. Each value in the list is combined with each combination of smoothing parameters to produce a separate analysis.

**CK=*n***

specifies the number of neighbors to use for clustering. The number of neighbors should be at least two but less than the number of observations. See the section “[Density Estimation](#)” on page 5096 for details.

**CLUSTER=*name***

provides a name for the variable in the OUT= and OUTCLUS= data sets identifying clusters. The default name is CLUSTER.

**CORE**

keeps the neighbor lists for each observation in the computer memory to make small problems run faster.

**CR=*n***

specifies the radius of the neighborhood for clustering. See the section “[Density Estimation](#)” on page 5096 for details.

**CROSS**

computes the likelihood cross validation criterion (Silverman 1986, pp. 52–55). This option appears to be of limited usefulness. See the section “[Density Estimation](#)” on page 5096 for details.

**CROSSLIST**

displays the cross validated log density of each observation.

**DATA=*SAS-data-set***

specifies the input data set containing observations to be clustered. If you omit the DATA= option, the most recently created SAS data set is used.

If the data set is TYPE=DISTANCE, the data are interpreted as a distance matrix. The number of variables must equal the number of observations in the data set or in each BY group. The distances are assumed to be Euclidean, but the procedure accepts other types of distances or dissimilarities. Unlike the CLUSTER procedure, PROC MODECLUS uses the entire distance matrix, not just the lower triangle; the distances are not required to be symmetric. The neighbors of a given observation are determined solely from the distances in that observation. Missing values are considered infinite. Various distance measures can be computed from coordinate data by using the DISTANCE procedure (for detailed information, see Chapter 34, “[The DISTANCE Procedure](#)”).

If the data set is not TYPE=DISTANCE, the data are interpreted as coordinates in a Euclidean space, and Euclidean distances are computed. The variables can be discrete or continuous and should be at the interval level of measurement.

Data set types such as TYPE=DISTANCE do not persist when you copy or modify a data set. You must specify the TYPE= data set option for the new data set, as in the following example:

```
data dist2(type=distance);
 set dist;
run;
```

If you do not specify the TYPE=DISTANCE data set option, the new data set is the default TYPE=DATA. If you use the new data set in a procedure that accepts both TYPE=DATA or TYPE=DISTANCE data sets (such as PROC CLUSTER or PROC MODECLUS), the results will be incorrect.

**DENSITY=*name***

provides a name for the variable in the OUT= data set containing density estimates. The default name is DENSITY.

**DIMENSION=*n***

**DIM=*n***

specifies the dimensionality to be used when computing density estimates. The default is the number of variables if the data are coordinates; the default is 1 if the data are distances.

**DK=*n***

specifies the number of neighbors to use for *k*th-nearest-neighbor density estimation. The number of neighbors should be at least two but less than the number of observations. See the section “[Density Estimation](#)” on page 5096 for details.

**DOCK=*n***

dissolves clusters with *n* or fewer members by making the members unassigned.

**DR=*n***

specifies the radius of the sphere of support for uniform-kernel density estimation. See the section “[Density Estimation](#)” on page 5096 for details.

**EARLY**

stops the cluster analysis after obtaining either a solution with no cluster or a solution with one cluster to which all observations are assigned. The smoothing parameters should be specified in increasing order. This can reduce the computer time required for the analysis but might occasionally miss some multiple-cluster solutions.

**HM**

uses harmonic means for cascading density estimates. See the description of the `CASCADE=` option for details.

**JOIN<=*p*>**

requests that nonsignificant clusters be hierarchically joined. The JOIN option implies the TEST option. After each solution is obtained, the cluster with the largest approximate  $p$ -value is either joined to a neighboring cluster or, if there is no neighboring cluster, dissolved by making all of its members unassigned. After two clusters are joined, an analysis of the remaining clusters is displayed.

If you do not specify a  $p$ -value with the JOIN= option, joining continues until only one cluster remains, and the results are written to the output data sets after each analysis. If you specify a  $p$ -value with the JOIN= option, joining continues until the greatest approximate  $p$ -value is less than the value given in the JOIN= option, and only if there is more than one cluster are the results for that analysis written to the output data sets.

Any value of  $p$  less than 1E-8 is set to 1E-8.

**K=*n***

specifies the number of neighbors to use for  $k$ th-nearest-neighbor density estimation and clustering. The number of neighbors should be at least two but less than the number of observations. Specifying `K=n` is equivalent to specifying both `DK=n` and `CK=n`. See the section “Density Estimation” on page 5096 for details.

**LIST**

displays the estimated density and cluster membership of each observation.

**LOCAL**

requests estimates of local dimensionality (Tukey and Tukey 1981, pp. 236–237).

**MAXCLUSTERS=*n*****MAXC=*n***

specifies the maximum number of clusters to be obtained with the `METHOD=6` option. By default, there is no fixed limit.

**METHOD=*n*****MET=*n*****M=*n***

specifies what clustering method to use. Since these methods do not have widely recognized names, the methods are indicated by numbers from 0 to 6. The methods are described in the section “Clustering Methods” on page 5099. For most purposes, `METHOD=1` is recommended, although `METHOD=6` might occasionally produce better results in return for considerably greater computer time and space requirements. `METHOD=1` is not good for discrete coordinate data with only a few equally spaced values. In this case, `METHOD=6` or `METHOD=3` works better. `METHOD=4` or `METHOD=5` is less desirable than other methods when there are ties, since a general characteristic of agglomerative hierarchical clustering methods is that the results are indeterminate in the presence of ties.

You must specify the `METHOD=` option to obtain a cluster analysis.

You can specify a list of values for the `METHOD=` option. Each value in the list is combined with each combination of smoothing and cascading parameters to produce a separate cluster analysis.

**MODE=*n***

specifies that when two clusters are joined using the METHOD=5 option (no other methods are affected by the MODE= option), each must have at least *n* members for either cluster to be designated a modal cluster. In any case, each cluster must also have a maximum density greater than the fusion density for either cluster to be designated a modal cluster. If you specify the K= option, the default value of the MODE= option is the same as the value of the K= option because the use of *k*th-nearest-neighbor density estimation limits the resolution that can be obtained for clusters with fewer than *k* members. If you do not specify the K= option, the default is MODE=2. If you specify MODE=0, the default value is used instead of 0. If you specify a FREQ statement, the MODE= value is compared to the number of observations in each cluster, not to the sum of the frequencies.

**NEIGHBOR**

displays the neighbors of each observation in a table called “Nearest Neighbor List.” See [Nearest Neighbor List](#) for information displayed in the table.

**NOPRINT**

suppresses the display of the output. Note that this option temporarily disables the Output Delivery System (ODS); see Chapter 20, “[Using the Output Delivery System](#),” for more information.

**NOSUMMARY**

suppresses the display of the summary of the number of clusters, number of unassigned observations, and maximum *p*-value for each analysis.

**OUT=*SAS-data-set***

specifies the output data set containing the input data plus density estimates, cluster membership, and variables identifying the type of solution. There is an output observation corresponding to each input observation for each solution. Therefore, the OUT= data set can be very large.

If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*. For details about OUT= data sets, see the section “[Output Data Sets](#)” on page 5107.

**OUTCLUS=*SAS-data-set*****OUTC=*SAS-data-set***

specifies the output data set containing an observation corresponding to each cluster in each solution. The variables identify the solution and contain statistics describing the clusters.

If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*. For details about OUTCLUS= data sets, see the section “[Output Data Sets](#)” on page 5107.

**OUTSUM=*SAS-data-set*****OUTS=*SAS-data-set***

specifies the output data set containing an observation corresponding to each cluster solution, giving the number of clusters and the number of unclassified observations for that solution.

If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*. For details about OUTSUM= data sets, see the section “[Output Data Sets](#)” on page 5107.



**OUTLENGTH=*n*****OUTL=*n***

specifies the length of those output variables that are not copied from the input data set but are created by PROC MODECLUS.

The OUTLENGTH= option applies only to the following variables that appear in all of the output data sets: `_K_`, `_DK_`, `_CK_`, `_R_`, `_DR_`, `_CR_`, `_CASCAD_`, `_METHOD_`, `_NJOIN_`, and `_LOCAL_`.

The minimum value is 2 or 3, depending on the operating system. The maximum value is 8. The default value is 8.

**POWER=*n*****POW=*n***

specifies the power of the density used with the METHOD=6 option. The default value is 2.

**R=*n***

specifies the radius of the sphere of support for uniform-kernel density estimation and the neighborhood for clustering. Specifying R=*n* is equivalent to specifying both DR=*n* and CR=*n*. See the section “Density Estimation” on page 5096 for details.

**SHORT**

suppresses the display of statistics for each cluster.

**SIMPLE****S**

displays means, standard deviations, skewness, kurtosis, and a coefficient of bimodality. The SIMPLE option applies only to coordinate data.

**STANDARD****STD**

standardizes the variables to mean 0 and standard deviation 1. The STANDARD option applies only to coordinate data.

**SUM**

uses sums for cascading density estimates. See the description of the CASCADE= option for details.

**TEST**

performs approximate significance tests for the number of clusters. The R= or DR= option must also be specified with a nonzero value to obtain significance tests.

The significance tests performed by PROC MODECLUS are valid only for simple random samples, and they require at least 20 observations per cluster to have enough power to be of any use. See the section “Significance Tests” on page 5101 for details.

**THRESHOLD=*n*****THR=*n***

specifies the assignment threshold used with the METHOD=6 option. The default is 0.5.

**TRACE**

traces the process of cluster assignments when METHOD=6 is specified.

---

## BY Statement

**BY variables ;**

You can specify a BY statement with PROC MODECLUS to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the MODECLUS procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

---

## FREQ Statement

**FREQ variable ;**

If one variable in the input data set represents the frequency of occurrence for other values in the observation, specify the variable's name in a FREQ statement. PROC MODECLUS then treats the data set as if each observation appeared  $n$  times, where  $n$  is the value of the FREQ variable for the observation. Nonintegral values of the FREQ variable are truncated to the largest integer less than the FREQ value.

---

## ID Statement

**ID variable ;**

The values of the ID variable identify observations in the displayed results and in the OUT= data set. If you omit the ID statement, each observation is identified by its observation number, and a variable called `_OBS_` is written to the OUT= data set containing the original observation numbers.

---

## VAR Statement

**VAR** *variables* ;

The VAR statement specifies numeric variables to be used in the cluster analysis. If you omit the VAR statement, all numeric variables not specified in other statements are used.

---

## Details: MODECLUS Procedure

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### Density Estimation

See Silverman (1986) or Scott (1992) for an introduction to nonparametric density estimation.

PROC MODECLUS uses hyperspherical uniform kernels of fixed or variable radius. The density estimate at a point is computed by dividing the number of observations within a sphere centered at the point by the product of the sample size and the volume of the sphere. The size of the sphere is determined by the smoothing parameters that you are required to specify.

For fixed-radius kernels, specify the radius as a Euclidean distance with either the DR= or R= option. For variable-radius kernels, specify the number of neighbors desired within the sphere with either the DK= or K= option; the radius is then the smallest radius that contains at least the specified number of observations including the observation at which the density is being estimated. If you specify both the DR= or R= option and the DK= or K= option, the radius used is the maximum of the two indicated radii; this is useful for dealing with outliers.

It is convenient to refer to the sphere of support of the kernel at observation  $x_i$  as the *neighborhood* of  $x_i$ . The observations within the neighborhood of  $x_i$  are the *neighbors* of  $x_i$ . In some contexts,  $x_i$  is considered a neighbor of itself, but in other contexts it is not. The following notation is used in this chapter:

|          |                                                                                          |
|----------|------------------------------------------------------------------------------------------|
| $x_i$    | the $i$ th observation                                                                   |
| $d(x,y)$ | the distance between points $x$ and $y$                                                  |
| $n$      | the total number of observations in the sample                                           |
| $n_i$    | the number of observations within the neighborhood of $x_i$ , including $x_i$ itself     |
| $n_i^-$  | the number of observations within the neighborhood of $x_i$ , not including $x_i$ itself |
| $N_i$    | the set of indices of neighbors of $x_i$ , including $i$                                 |
| $N_i^-$  | the set of indices of neighbors of $x_i$ , not including $i$                             |
| $v_i$    | the volume of the neighborhood of $x_i$                                                  |
| $r_i$    | the radius of the neighborhood of $x_i$                                                  |

|               |                                                            |
|---------------|------------------------------------------------------------|
| $\hat{f}_i$   | the estimated density at $x_i$                             |
| $\hat{f}_i^-$ | the cross validated density estimate at $x_i$              |
| $C_k$         | the set of indices of observations assigned to cluster $k$ |
| $v$           | the number of variables or the dimensionality              |
| $s_l$         | standard deviation of the $l$ th variable                  |

The estimated density at  $x_i$  is

$$\hat{f}_i = \frac{n_i}{nv_i}$$

which indicates the number of neighbors of  $x_i$  divided by the product of the sample size and the volume of the neighborhood at  $x_i$ , where

$$v_i = \frac{\pi^{\frac{v}{2}} r_i^v}{\Gamma(\frac{v}{2} + 1)}$$

and  $\Gamma$  can be computed in a DATA step by using the GAMMA function. Note that  $v = 1$  for distance data.

The density estimates provided by uniform kernels are not quite as good as those provided by some other types of kernels, but they are quite satisfactory for clustering. The significance tests for the number of clusters require the use of fixed-size uniform kernels.

There is no simple answer to the question of which smoothing parameter to use (Silverman 1986, pp. 43–61, 84–88, 98–99). It is usually necessary to try several different smoothing parameters. A reasonable first guess for the K= option is in the range of 0.1 to 1 times  $n^{4/(v+4)}$ , smaller values being suitable for higher dimensionalities. A reasonable first guess for the R= option in many coordinate data sets is given by

$$\left[ \frac{2^{v+2}(v+2)\Gamma(\frac{v}{2}+1)}{nv^2} \right]^{1/(v+4)} \sqrt{\sum_{l=1}^v s_l^2}$$

which can be computed in a DATA step by using the GAMMA function for  $\Gamma$ . The MODECLUS procedure also provides this first guess as a default smoothing parameter if none of the options (DR=, CR=, R=, DK=, CK=, and K=) is specified. This formula is derived under the assumption that the data are sampled from a multivariate normal distribution and, therefore, tend to be too large (oversmooth) if the true distribution is multimodal. Robust estimates of the standard deviations might be preferable if there are outliers. If the data are distances, the factor  $\sqrt{\sum s_l^2}$  can be replaced by an average root-mean-squared Euclidean distance divided by  $\sqrt{2}$ . To prevent outliers from appearing as separate clusters, you can also specify K=2 or CK=2 or, more generally, K= $m$  or CK= $m$ ,  $m \geq 2$ , which in most cases forces clusters to have at least  $m$  members.

If the variables all have unit variance (for example, if you specify the STD option), you can use [Table 60.2](#) to obtain an initial guess for the R= option.

**Table 60.2** Reasonable First Guess for R= for Standardized Data

| Number<br>of Obs | Number of Variables |      |      |      |      |      |      |      |      |      |
|------------------|---------------------|------|------|------|------|------|------|------|------|------|
|                  | 1                   | 2    | 3    | 4    | 5    | 6    | 7    | 8    | 9    | 10   |
| 20               | 1.01                | 1.36 | 1.77 | 2.23 | 2.73 | 3.25 | 3.81 | 4.38 | 4.98 | 5.60 |
| 35               | 0.91                | 1.24 | 1.64 | 2.08 | 2.56 | 3.08 | 3.62 | 4.18 | 4.77 | 5.38 |
| 50               | 0.84                | 1.17 | 1.56 | 1.99 | 2.46 | 2.97 | 3.50 | 4.06 | 4.64 | 5.24 |
| 75               | 0.78                | 1.09 | 1.47 | 1.89 | 2.35 | 2.85 | 3.38 | 3.93 | 4.50 | 5.09 |
| 100              | 0.73                | 1.04 | 1.41 | 1.82 | 2.28 | 2.77 | 3.29 | 3.83 | 4.40 | 4.99 |
| 150              | 0.68                | 0.97 | 1.33 | 1.73 | 2.18 | 2.66 | 3.17 | 3.71 | 4.27 | 4.85 |
| 200              | 0.64                | 0.93 | 1.28 | 1.67 | 2.11 | 2.58 | 3.09 | 3.62 | 4.17 | 4.75 |
| 350              | 0.57                | 0.85 | 1.18 | 1.56 | 1.98 | 2.44 | 2.93 | 3.45 | 4.00 | 4.56 |
| 500              | 0.53                | 0.80 | 1.12 | 1.49 | 1.91 | 2.36 | 2.84 | 3.35 | 3.89 | 4.45 |
| 750              | 0.49                | 0.74 | 1.06 | 1.42 | 1.82 | 2.26 | 2.74 | 3.24 | 3.77 | 4.32 |
| 1000             | 0.46                | 0.71 | 1.01 | 1.37 | 1.77 | 2.20 | 2.67 | 3.16 | 3.69 | 4.23 |
| 1500             | 0.43                | 0.66 | 0.96 | 1.30 | 1.69 | 2.11 | 2.57 | 3.06 | 3.57 | 4.11 |
| 2000             | 0.40                | 0.63 | 0.92 | 1.25 | 1.63 | 2.05 | 2.50 | 2.99 | 3.49 | 4.03 |

One data-based method for choosing the smoothing parameter is likelihood cross validation (Silverman 1986, pp. 52–55). The cross validated density estimate at an observation is obtained by omitting the observation from the computations:

$$\hat{f}_i^- = \frac{n_i^-}{nv_i}$$

The (log) likelihood cross validation criterion is then computed as

$$\sum_{i=1}^n \log \hat{f}_i^-$$

The suggested smoothing parameter is the one that maximizes this criterion. With fixed-radius kernels, likelihood cross validation oversmooths long-tailed distributions; for purposes of clustering, it tends to undersmooth short-tailed distributions. With  $k$ -nearest-neighbor density estimation, likelihood cross validation is useless because it almost always indicates  $k=2$ .

Cascaded density estimates are obtained by computing initial kernel density estimates and then, at each observation, taking the arithmetic mean, harmonic mean, or sum of the initial density estimates of the observations within the neighborhood. The cascaded density estimates can, in turn, be cascaded, and so on. Let  ${}_k \hat{f}_i$  be the density estimate at  $x_i$  cascaded  $k$  times. For all types of cascading,  ${}_0 \hat{f}_i = \hat{f}_i$ . If the cascading is done by arithmetic means, then, for  $k \geq 0$ ,

$${}_{k+1} \hat{f}_i = \sum_{j \in N_i} {}_k \hat{f}_j / n_i$$

For harmonic means,

$${}_{k+1} \hat{f}_i = \left( \sum_{j \in N_i} {}_k \hat{f}_j^{-1} / n_i \right)^{-1}$$

and for sums,

$${}_{k+1}\hat{f}_i = \left( \sum_{j \in N_i} {}_k\hat{f}_j^{k+1} \right)^{\frac{1}{k+2}}$$

To avoid cluttering formulas, the symbol  $\hat{f}_i$  is used in the rest of the chapter to denote the density estimate at  $x_i$  whether cascaded or not, since the clustering methods and significance tests do not depend on the degree of cascading.

Cascading increases the smoothness of the estimates with less computation than would be required by increasing the smoothing parameters to yield a comparable degree of smoothness. For population densities with bounded support and discontinuities at the boundaries, cascading improves estimates near the boundaries. Cascaded estimates, especially using sums, might be more sensitive to the local covariance structure of the distribution than are the uncascaded kernel estimates. Cascading seems to be useful for detecting very nonspherical clusters. Cascading was suggested by Tukey and Tukey (1981, p. 237). Additional research into the properties of cascaded density estimates is needed.

---

## Clustering Methods

The number of clusters is a function of the smoothing parameters. The number of clusters tends to decrease as the smoothing parameters increase, but the relationship is not strictly monotonic. Generally, you should specify several different values of the smoothing parameters to see how the number of clusters varies.

The clustering methods used by PROC MODECLUS use spherical clustering neighborhoods of fixed or variable radius that are similar to the spherical kernels used for density estimation. For fixed-radius neighborhoods, specify the radius as a Euclidean distance with either the CR= or R= option. For variable-radius neighborhoods, specify the number of neighbors desired within the sphere with either the CK= or K= option; the radius is then the smallest radius that contains at least the specified number of observations including the observation for which the neighborhood is being determined. However, in the following descriptions of clustering methods, an observation is not considered to be one of its own neighbors. If you specify both the CR= or R= option and the CK= or K= option, the radius used is the maximum of the two indicated radii; this is useful for dealing with outliers. In this section, the symbols  $N_i$ ,  $N_i^-$ ,  $n_i$ , and  $n_i^-$  refer to clustering neighborhoods, not density estimation neighborhoods.

### METHOD=0

Begin with each observation in a separate cluster. For each observation and each of its neighbors, join the cluster to which the observation belongs with the cluster to which the neighbor belongs. This method does not use density estimates. With a fixed clustering radius, the clusters are those obtained by cutting the single linkage tree at the specified radius (see Chapter 31, “The CLUSTER Procedure”).

### METHOD=1

Begin with each observation in a separate cluster. For each observation, find the nearest neighbor with a greater estimated density. If such a neighbor exists, join the cluster to which the observation belongs with the cluster to which the specified neighbor belongs.

Next, consider each observation with density estimates equal to that of one or more neighbors but not less than the estimate at any neighbor. Join the cluster containing the observation with (1) each cluster containing a neighbor of the observation such that the maximum density estimate in the cluster equals the density estimate at the observation and (2) the cluster containing the nearest neighbor of the observation such that the maximum density estimate in the cluster exceeds the density estimate at the observation.

This method is similar to the classification or assignment stage of algorithms described by Gitman (1973) and Huizinga (1978).

## METHOD=2

Begin with each observation in a separate cluster. For each observation, find the neighbor with the greatest estimated density exceeding the estimated density of the observation. If such a neighbor exists, join the cluster to which the observation belongs with the cluster to which the specified neighbor belongs.

Observations with density estimates equal to that of one or more neighbors but not less than the estimate at any neighbor are treated the same way as they are in METHOD=1.

This method is similar to the first stage of an algorithm proposed by Mizoguchi and Shimura (1980).

## METHOD=3

Begin with each observation in a separate cluster. For each observation, find the neighbor with greater estimated density such that the slope of the line connecting the point on the estimated density surface at the observation with the point on the estimated density surface at the neighbor is a maximum. That is, for observation  $x_i$ , find a neighbor  $x_j$  such that  $(\hat{f}_j - \hat{f}_i)/d(x_j, x_i)$  is a maximum. If this slope is positive, join the cluster to which observation  $x_i$  belongs with the cluster to which the specified neighbor  $x_j$  belongs. This method was invented by Koontz, Narendra, and Fukunaga (1976).

Observations with density estimates equal to that of one or more neighbors but not less than the estimate at any neighbor are treated the same way as they are in METHOD=1. The algorithm suggested for this situation by Koontz, Narendra, and Fukunaga (1976) might fail for flat areas in the estimated density that contain four or more observations.

## METHOD=4

This method is equivalent to the first stage of two-stage density linkage (see Chapter 31, “The CLUSTER Procedure”) without the use of the MODE=option.

## METHOD=5

This method is equivalent to the first stage of two-stage density linkage (see Chapter 31, “The CLUSTER Procedure”) with the use of the MODE=option.

## METHOD=6

Begin with all observations unassigned.

**Step 1:** Form a list of seeds, each seed being a single observation such that the estimated density of the observation is not less than the estimated density of any of its neighbors. If you specify the MAXCLUSTERS= $n$  option, retain only the  $n$  seeds with the greatest estimated densities.

**Step 2:** Consider each seed in decreasing order of estimated density, as follows:

1. If the current seed has already been assigned, proceed to the next seed. Otherwise, form a new cluster consisting of the current seed.
2. Add to the cluster any unassigned seed that is a neighbor of a member of the cluster or that shares a neighbor with a member of the cluster; repeat until no unassigned seed satisfies these conditions.
3. Add to the cluster all neighbors of seeds that belong to the cluster.
4. Consider each unassigned observation. Compute the ratio of the sum of the  $p - 1$  powers of the estimated density of the neighbors that belong to the current cluster to the sum of the  $p - 1$  powers of the estimated density of all of its neighbors, where  $p$  is specified by the POWER= option and is 2 by default. Let  $x_i$  be the current observation, and let  $k$  be the index of the current cluster. Then this ratio is

$$r_{ik} = \frac{\sum_{j \in N_i \cap C_k} \hat{f}_j^{p-1}}{\sum_{j \in N_i} \hat{f}_j^{p-1}}$$

(The sum of the  $p - 1$  powers of the estimated density of the neighbors of an observation is an estimate of the integral of the  $p$ th power of the density over the neighborhood.) If  $r_{ik}$  exceeds the maximum of 0.5 and the value of the THRESHOLD= option, add the observation  $x_i$  to the current cluster  $k$ . Repeat until no more observations can be added to the current cluster.

**Step 3:** (This step is performed only if the value of the THRESHOLD= option is less than 0.5.) Form a list of unassigned observations in decreasing order of estimated density. Repeat the following actions until the list is empty:

1. Remove the first observation from the list, such as observation  $x_i$ .
2. For each cluster  $k$ , compute  $r_{ik}$ .
3. If the maximum over clusters of  $r_{ik}$  exceeds the value of the THRESHOLD= option, assign observation  $x_i$  to the corresponding cluster and insert all observations of which the current observation is a neighbor into the list, keeping the list in decreasing order of estimated density.

METHOD=6 is related to a method invented by Koontz and Fukunaga (1972a) and discussed by Koontz and Fukunaga (1972b).

---

## Significance Tests

Significance tests require that a fixed-radius kernel be specified for density estimation via the DR= or R= option. You can also specify the DK= or K= option, but only the fixed radius is used for the significance tests.

The purpose of the significance tests is as follows: given a simple random sample of objects from a population, obtain an estimate of the number of clusters in the population such that the probability in repeated sampling that the estimate exceeds the true number of clusters is not much greater than  $\alpha$ ,  $1\% \leq \alpha \leq 10\%$ . In other words, a sequence of null hypotheses of the form



$H_0^{(i)}$ : The number of population clusters is  $i$  or less

where  $i = 1, 2, \dots, n$ , is tested against the alternatives such as

$H_a^{(i)}$ : The number of population clusters exceeds  $i$

with a maximum experimentwise error rate of approximately  $\alpha$ . The tests protect you from overestimating the number of population clusters. It is impossible to protect against underestimating the number of population clusters without introducing much stronger assumptions than are used here, since the number of population clusters could conceivably exceed the sample size.

The method for conducting significance tests is as follows:

1. Estimate densities by using fixed-radius uniform kernels.
2. Obtain preliminary clusters by a “valley-seeking” method. Other clustering methods could be used but would yield less power.
3. Compute an approximate  $p$ -value for each cluster by comparing the estimated maximum density in the cluster with the estimated maximum density on the cluster boundary.
4. Repeatedly join the least significant cluster with a neighboring cluster until all remaining clusters are significant.
5. Estimate the number of population clusters as the number of significant sample clusters.
6. The preceding steps can be repeated for any number of different radii, and the estimate of the number of population clusters can be taken to be the maximum number of significant sample clusters for any radius.

This method has the following useful features:

- No distributional assumptions are required.
- The choice of smoothing parameter is not critical since you can try any number of different values.
- The data can be coordinates or distances.
- Time and space requirements for the significance tests are no worse than those for obtaining the clusters.
- The power is high enough to be useful for practical purposes.

The method for computing the  $p$ -values is based on a series of plausible approximations. There are as yet no rigorous proofs that the method is infallible. Neither are there any asymptotic results. However, simulations for sample sizes ranging from 20 to 2000 indicate that the  $p$ -values are almost always conservative. The only case discovered so far in which the  $p$ -values are liberal is a uniform distribution in one dimension for

which the simulated error rates exceed the nominal significance level only slightly for a limited range of sample sizes.

To make inferences regarding population clusters, it is first necessary to define what is meant by a cluster. For clustering methods that use nonparametric density estimation, a cluster is usually loosely defined as a region surrounding a local maximum of the probability density function or a maximal connected set of local maxima. This definition might not be satisfactory for very rough densities with many local maxima. It is not applicable at all to discrete distributions for which the density does not exist. As another example in which this definition is not intuitively reasonable, consider a uniform distribution in two dimensions with support in the shape of a figure eight (including the interior). This density might be considered to contain two clusters even though it does not have two distinct modes.

These difficulties can be avoided by defining clusters in terms of the local maxima of a smoothed probability density or mass function. For example, define the neighborhood distribution function (NDF) with radius  $r$  at a point  $x$  as the probability that a randomly selected point will lie within a radius  $r$  of  $x$ —that is, the probability integral over a hypersphere of radius  $r$  centered at  $x$ :

$$s(x) = P(d(x, X) \leq r)$$

where  $X$  is the random variable being sampled,  $r$  is a user-specified radius, and  $d(x,y)$  is the distance between points  $x$  and  $y$ .

The NDF exists for all probability distributions. You can select the radius according to the degree of resolution required. The minimum-variance unbiased estimate of the NDF at a point  $x$  is proportional to the uniform-kernel density estimate with corresponding support.

You can define a *modal region* as a maximal connected set of local maxima of the NDF. A cluster is a connected set containing exactly one modal region. This definition seems to give intuitively reasonable results in most cases. An exception is a uniform density on the perimeter of a square. The NDF has four local maxima. There are eight local maxima along the perimeter, but running PROC MODECLUS with the R= option would yield four clusters since the two local maxima at each corner are separated by a distance equal to the radius. While this density does indeed have four distinctive features (the corners), it is not obvious that each corner should be considered a cluster.

The number of population clusters depends on the radius of the NDF. The significance tests in PROC MODECLUS protect against overestimating the number of clusters at any specified radius. It is often useful to look at the clustering results across a range of radii. A plot of the number of sample clusters as a function of the radius is a useful descriptive display, especially for high-dimensional data (Wong and Schaack 1982).

If a population has two clusters, it must have two modal regions. If there are two modal regions, there must be a “valley” between them. It seems intuitively desirable that the boundary between the two clusters should follow the bottom of this valley. All the clustering methods in PROC MODECLUS are designed to locate the estimated cluster boundaries in this way, although methods 1 and 6 seem to be much more successful at this than the others. Regardless of the precise location of the cluster boundary, it is clear that the maximum of the NDF along the boundary between two clusters must be strictly less than the value of the NDF in either modal region; otherwise, there would be only a single modal region; according to Hartigan and Hartigan (1985), there must be a “dip” between the two modes. PROC MODECLUS assesses the significance of a sample cluster by comparing the NDF in the modal region with the maximum of the NDF along the cluster boundary. If the NDF has second-order derivatives in the region of interest and if the boundary between the two clusters is indeed at the bottom of the valley, then the maximum value of the NDF along the boundary

occurs at a saddle point. Hence, this test is called a *saddle test*. This term is intended to describe any test for clusters that compares modal densities with saddle densities, not just the test currently implemented in the MODECLUS procedure.

The obvious estimate of the maximum NDF in a sample cluster is the maximum estimated NDF at an observation in the cluster. Let  $m(k)$  be the index of the observation for which the maximum is attained in cluster  $k$ .

Estimating the maximum NDF on the cluster boundary is more complicated. One approach is to take the maximum NDF estimate at an observation in the cluster that has a neighbor belonging to another cluster. This method yields excessively large estimates when the neighborhood is large. Another approach is to try to choose an object closer to the boundary by taking the observation with the maximum sum of estimated densities of neighbors belonging to a different cluster. After some experimentation, it is found that a combination of these two methods works well. Let  $B_k$  be the set of indices of observations in cluster  $k$  that have neighbors belonging to a different cluster, and compute

$$\max_{i \in B_k} \left( 0.2 \hat{f}_i n_i + \sum_{j \in N_i - C_k} \hat{f}_j \right)$$

Let  $s(k)$  be the index of the observation for which the maximum is attained.

Using the notation  $\#(S)$  for the cardinality of set  $S$ , let

$$\begin{aligned} n_{ij}^- &= \#(N_i^- \cap N_j^-) \\ c_m(k) &= n_{m(k)}^- - n_{m(k)s(k)}^- \\ c_s(k) &= n_{s(k)}^- - n_{m(k)s(k)}^- \text{ if } B_k \neq \emptyset, \\ &= 0 \text{ otherwise} \\ q_k &= 1/2 \text{ if } B_k \neq \emptyset, \\ &= 2/3 \text{ otherwise} \\ z_k &= \frac{c_m(k) - q_k(c_m(k) + c_s(k)) - 1/2}{\sqrt{q_k(1 - q_k)(c_m(k) + c_s(k))}} \\ u &= \left\lceil (0.2 + 0.05\sqrt{n}) \sum_{i: n_i > 1} \frac{1}{n_i + 1} \right\rceil \end{aligned}$$

Let  $R(u)$  be a random variable distributed as the range of a random sample of  $u$  observations from a standard normal distribution. Then the approximate  $p$ -value  $p_k$  for cluster  $k$  is

$$p_k = \Pr(z_k > R(u)/\sqrt{2})$$

If points  $m(k)$  and  $s(k)$  are fixed a priori,  $z_k$  would be the usual approximately normal test statistic for comparing two binomial random variables. In fact,  $m(k)$  and  $s(k)$  are selected in such a way that  $c_m(k)$  tends to be large and  $c_s(k)$  tends to be small. For this reason, and because there might be a large number of clusters, each with its own  $z_k$  to be tested, each  $z_k$  is referred to the distribution of  $R(u)$  instead of a

standard normal distribution. If the tests are conducted for only one radius and if  $u$  is chosen equal to  $n$ , then the  $p$ -values are very conservative because (1) you are not making all possible pairwise comparisons of observations in the sample and (2)  $n_i^-$  and  $n_j^-$  are positively correlated if the neighborhoods overlap. In the formula for  $u$ , the summation overcorrects somewhat for the conservativeness due to correlated  $n_i^-$ 's. The factor  $0.2 + 0.05\sqrt{n}$  is empirically estimated from simulation results to adjust for the use of more than one radius.

If the JOIN option is specified, the least significant cluster (the cluster with the smallest  $z_k$ ) is either dissolved or joined with a neighboring cluster. If no members of the cluster have neighbors belonging to a different cluster, all members of the cluster are unassigned. Otherwise, the cluster is joined to the neighboring cluster such that the sum of density estimates of neighbors of the estimated saddle point belonging to it is a maximum. Joining clusters increases the power of the saddle test. For example, consider a population with two well-separated clusters. Suppose that, for a certain radius, each population cluster is divided into two sample clusters. None of the four sample clusters is likely to be significant, but after the two sample clusters corresponding to each population cluster are joined, the remaining two clusters can be highly significant.

The saddle test implemented in PROC MODECLUS has been evaluated by simulation from known distributions. Some results are given in the following three tables. In Table 60.3, samples of 20 to 2000 observations are generated from a one-dimensional uniform distribution. For sample sizes of 1000 or less, 2000 samples are generated and analyzed by PROC MODECLUS. For a sample size of 2000, only 1000 samples are generated. The analysis is done with at least 20 different values of the R= option spread across the range of radii most likely to yield significant results. The six central columns of the table give the observed error rates at the nominal error rates ( $\alpha$ ) at the head of each column. The standard errors of the observed error rates are given at the bottom of the table. The observed error rates are conservative for  $\alpha \leq 5\%$ , but they increase with  $\alpha$  and become slightly liberal for sample sizes in the middle of the range tested.

**Table 60.3** Observed Error Rates (%) for Uniform Distribution

| Sample Size     | Nominal Type 1 Error Rate |      |      |       |       |       | Number of Simulations |
|-----------------|---------------------------|------|------|-------|-------|-------|-----------------------|
|                 | 1                         | 2    | 5    | 10    | 15    | 20    |                       |
| 20              | 0.00                      | 0.00 | 0.00 | 0.60  | 11.65 | 27.05 | 2000                  |
| 50              | 0.35                      | 0.70 | 4.50 | 10.95 | 20.55 | 29.80 | 2000                  |
| 100             | 0.35                      | 0.85 | 3.90 | 11.05 | 18.95 | 28.05 | 2000                  |
| 200             | 0.30                      | 1.35 | 4.00 | 10.50 | 18.60 | 27.05 | 2000                  |
| 500             | 0.45                      | 1.05 | 4.35 | 9.80  | 16.55 | 23.55 | 2000                  |
| 1000            | 0.70                      | 1.30 | 4.65 | 9.55  | 15.45 | 19.95 | 2000                  |
| 2000            | 0.40                      | 1.10 | 3.00 | 7.40  | 11.50 | 16.70 | 1000                  |
| <b>Standard</b> | 0.22                      | 0.31 | 0.49 | 0.67  | 0.80  | 0.89  | 2000                  |
| <b>Error</b>    | 0.31                      | 0.44 | 0.69 | 0.95  | 1.13  | 1.26  | 1000                  |

All unimodal distributions other than the uniform that have been tested, including normal, Cauchy, and exponential distributions and uniform mixtures, have produced much more conservative results. Table 60.4 displays results from a unimodal mixture of two normal distributions with equal variances and equal sampling probabilities and with means separated by two standard deviations. Any greater separation would produce a bimodal distribution. The observed error rates are quite conservative.

**Table 60.4** Observed Error Rates (%) for Normal Mixture with  $2\sigma$  Separation

| Sample Size | Nominal Type 1 Error Rate |     |     |     |     |     | Number of Simulations |
|-------------|---------------------------|-----|-----|-----|-----|-----|-----------------------|
|             | 1                         | 2   | 5   | 10  | 15  | 20  |                       |
| 100         | 0.0                       | 0.0 | 0.0 | 1.0 | 2.0 | 4.0 | 200                   |
| 200         | 0.0                       | 0.0 | 0.0 | 2.0 | 3.0 | 3.0 | 200                   |
| 500         | 0.0                       | 0.0 | 0.5 | 0.5 | 0.5 | 0.5 | 200                   |

All distributions in two or more dimensions that have been tested yield extremely conservative results. For example, a uniform distribution on a circle yields observed error rates that are never more than one-tenth of the nominal error rates for sample sizes up to 1000. This conservatism is due to the fact that, as the dimensionality increases, more and more of the probability lies in the tails of the distribution (Silverman 1986, p. 92), and the saddle test used by PROC MODECLUS is more conservative for distributions with pronounced tails. This applies even to a uniform distribution on a hypersphere because, although the density does not have tails, the NDF does.

Since the formulas for the significance tests do not involve the dimensionality, no problems are created when the data are linearly dependent. Simulations of data in nonlinear subspaces (the circumference of a circle or surface of a sphere) have also yielded conservative results.

Table 60.5 displays results in terms of power for identifying two clusters in samples from a bimodal mixture of two normal distributions with equal variances and equal sampling probabilities separated by four standard deviations. In this simulation, PROC MODECLUS never indicated more than two significant clusters.

**Table 60.5** Power (%) for Normal Mixture with  $4\sigma$  Separation

| Sample Size | Nominal Type 1 Error Rate |      |      |       |       |       | Number of Simulations |
|-------------|---------------------------|------|------|-------|-------|-------|-----------------------|
|             | 1                         | 2    | 5    | 10    | 15    | 20    |                       |
| 20          | 0.0                       | 0.0  | 0.0  | 2.0   | 37.5  | 68.5  | 200                   |
| 35          | 0.0                       | 13.5 | 38.5 | 48.5  | 64.0  | 75.5  | 200                   |
| 50          | 17.5                      | 26.0 | 51.5 | 67.0  | 78.5  | 84.0  | 200                   |
| 75          | 25.5                      | 36.0 | 58.5 | 77.5  | 85.5  | 89.5  | 200                   |
| 100         | 40.0                      | 54.5 | 72.5 | 84.5  | 91.5  | 92.5  | 200                   |
| 150         | 70.5                      | 80.0 | 92.0 | 97.0  | 100.0 | 100.0 | 200                   |
| 200         | 89.0                      | 96.0 | 99.5 | 100.0 | 100.0 | 100.0 | 200                   |

The saddle test is not as efficient as excess-mass tests for multimodality (Müller and Sawitzki 1991; Polonik 1993). However, there is not yet a general approximation for the distribution of excess-mass statistics to circumvent the need for simulations to do significance tests. See Minnotte (1992) for a review of tests for multimodality.

---

## Computational Resources

The MODECLUS procedure stores coordinate data in memory if there is enough space. For distance data, only one observation at a time is in memory.

PROC MODECLUS constructs lists of the neighbors of each observation. The total space required is  $12 \sum n_i$  bytes, where  $n_i$  is based on the largest neighborhood required by any analysis. The lists are stored

in a SAS utility data set unless you specify the CORE option. You might get an error message from the SAS System or from the operating system if there is not enough disk space for the utility data set. Clustering method 6 requires a second list that is always stored in memory.

For coordinate data, the time required to construct the neighbor lists is roughly proportional to  $v(\log n)(\sum n_i) \log(\sum n_i/n)$ . For distance data, the time is roughly proportional to  $n^2 \log(\sum n_i/n)$ .

The time required for density estimation is proportional to  $\sum n_i$  and is usually small compared to the time required for constructing the neighbor lists.

Clustering methods 0 through 3 are quite efficient, requiring time proportional to  $\sum n_i$ . Methods 4 and 5 are slower, requiring time roughly proportional to  $(\sum n_i) \log(\sum n_i)$ . Method 6 can also be slow, but the time requirements depend very much on the data and the particular options specified. Methods 4, 5, and 6 also require more memory than the other methods.

The time required for significance tests is roughly proportional to  $g \sum n_i$ , where  $g$  is the number of clusters.

PROC MODECLUS can process data sets of several thousand observations if you specify reasonable smoothing parameters. Very small smoothing values produce many clusters, whereas very large values produce many neighbors; either case can require excessive time or space.

## Missing Values

If the data are coordinates, observations with missing values are excluded from the analysis.

If the data are distances, missing values are treated as infinite. The neighbors of each observation are determined solely by the distances in that observation. The distances are not required to be symmetric, and there is no check for symmetry; the neighbors of each observation are determined only from the distances in that observation. This treatment of missing values is quite different from that of the CLUSTER procedure, which ignores the upper triangle of the distance matrix.

## Output Data Sets

The OUT= data set contains one complete copy of the input data set for each cluster solution. There are additional variables identifying each solution and giving information about individual observations. Solutions with only one remaining cluster when JOIN= $p$  is specified are omitted from the OUT= data set (see the description of the JOIN= option). The OUT= data set can be extremely large, so it is advisable to specify the DROP= data set option to exclude unnecessary variables.

The OUTCLUS= or OUTC= data set contains one observation for each cluster in each cluster solution. The variables identify the solution and provide statistics describing the cluster.

The OUTSUM= or OUTS= data set contains one observation for each cluster solution. The variables identify the solution and provide information about the solution as a whole.

The following variables can appear in all of the output data sets:

- `_K_`, which is the value of the K= option for the current solution. This variable appears only if you specify the K= option.

- `_DK_`, which is the value of the `DK=` option for the current solution. This variable appears only if you specify the `DK=` option.
- `_CK_`, which is the value of the `CK=` option for the current solution. This variable appears only if you specify the `CK=` option.
- `_R_`, which is the value of the `R=` option for the current solution. This variable appears only if you specify the `R=` option.
- `_DR_`, which is the value of the `DR=` option for the current solution. This variable appears only if you specify the `DR=` option.
- `_CR_`, which is the value of the `CR=` option for the current solution. This variable appears only if you specify the `CR=` option.
- `_CASCAD_`, which is the number of times the density estimates have been cascaded for the current solution. This variable appears only if you specify the `CASCADE=` option.
- `_METHOD_`, which is the value of the `METHOD=` option for the current solution. This variable appears only if you specify the `METHOD=` option.
- `_NJOIN_`, which is the number of clusters that are joined or dissolved in the current solution. This variable appears only if you specify the `JOIN` option.
- `_LOCAL_`, which is the local dimensionality estimate of the observation. This variable appears only if you specify the `LOCAL` option.

The `OUT=` data set contains the following variables:

- the variables from the input data set
- `_OBS_`, which is the observation number from the input data set. This variable appears only if you omit the `ID` statement.
- `DENSITY`, which is the estimated density at the observation. This variable can be renamed by the `DENSITY=` option.
- `CLUSTER`, which is the number of the cluster to which the observation is assigned. This variable can be renamed by the `CLUSTER=` option.

The `OUTCLUS=` data set contains the following variables:

- the `BY` variables, if any
- `_NCLUS_`, which is the number of clusters in the solution
- `CLUSTER`, which is the number of the current cluster
- `_FREQ_`, which is the number of observations in the cluster
- `_MODE_`, which is the maximum estimated density in the cluster
- `_BFREQ_`, which is the number of observations in the cluster with neighbors belonging to a different cluster

- `_SADDLE_`, which is the estimated saddle density for the cluster
- `_MC_`, which is the number of observations within the fixed-radius density-estimation neighborhood of the modal observation. This variable appears only if you specify the TEST or JOIN option.
- `_SC_`, which is the number of observations within the fixed-radius density-estimation neighborhood of the saddle observation. This variable appears only if you specify the TEST or JOIN option.
- `_OC_`, which is the number of observations within the overlap of the two previous neighborhoods. This variable appears only if you specify the TEST or JOIN option.
- `_Z_`, which is the approximate  $z$  statistic for the cluster. This variable appears only if you specify the TEST or JOIN option.
- `_P_`, which is the approximate  $p$ -value for the cluster. This variable appears only if you specify the TEST or JOIN option.

The OUTSUM= data set contains the following variables:

- the BY variables, if any
- `_NCLUS_`, which is the number of clusters in the solution
- `_UNCL_`, which is the number of unclassified observations
- `_CROSS_`, which is the likelihood cross validation criterion if you specify the CROSS or CROSSLIST option

---

## Displayed Output

If you specify the SIMPLE option and the data are coordinates, PROC MODECLUS displays the following simple descriptive statistics for each variable:

- the mean
- the standard deviation
- the skewness
- the kurtosis
- a coefficient of bimodality (see Chapter 31, “The CLUSTER Procedure”)

If you specify the NEIGHBOR option, PROC MODECLUS displays a list of neighbors for each observation. The table contains the following items:

- the observation number or ID value of the observation
- the observation number or ID value of each of its neighbors
- the distance to each neighbor

If you specify the CROSSLIST option, PROC MODECLUS produces a table of information regarding cross validation of the density estimates. Each table has a row for each observation. For each observation, the following are displayed:



- the observation number or ID value of the observation
- the radius of the neighborhood
- the number of neighbors
- the estimated log density
- the estimated cross validated log density

If you specify the LOCAL option, PROC MODECLUS produces a table of information regarding estimates of local dimensionality. Each table has a row for each observation. For each observation, the following are displayed:

- the observation number or ID value of the observation
- the radius of the neighborhood
- the estimated local dimensionality

If you specify the LIST option, PROC MODECLUS produces a table listing the observations within each cluster. The table includes the following items:

- the cluster number
- the observation number or ID value of the observation
- the estimated density
- the sum of the density estimates of observations within the neighborhood that belong to the same cluster
- the sum of the density estimates of observations within the neighborhood that belong to a different cluster
- the sum of the density estimates of all the observations within the neighborhood
- the ratio of the sum of the density estimates for the same cluster to the sum of all the density estimates in the neighborhood

If you specify the LIST option and there are unassigned objects, PROC MODECLUS produces a table listing those observations. The table includes the following items:

- the observation number or ID value of the observation
- the estimated density
- the ratio of the sum of the density estimates for the same cluster to the sum of the density estimates in the neighborhood for all other clusters

If you specify the BOUNDARY option, PROC MODECLUS produces a table listing the observations in each cluster that have a neighbor belonging to a different cluster. The table includes the following items:

- the observation number or ID value of the observation
- the estimated density

- the cluster number
- the ratio of the sum of the density estimates for the same cluster to the sum of the density estimates in the neighborhood for all other clusters

If you do not specify the SHORT option, PROC MODECLUS produces a table of cluster statistics including the following items:

- the cluster number
- the cluster frequency (the number of observations in the cluster)
- the maximum estimated density within the cluster
- the number of observations in the cluster having a neighbor that belongs to a different cluster
- the estimated saddle density of the cluster

If you specify the TEST or JOIN option, the table of cluster statistics includes the following items pertaining to the saddle test:

- the number of observations within the fixed-radius density-estimation neighborhood of the modal observation
- the number of observations within the fixed-radius density-estimation neighborhood of the saddle observation
- the number of observations within the overlap of the two preceding neighborhoods
- the  $z$  statistic for comparing the preceding counts
- the approximate  $p$ -value

If you do not specify the NOSUMMARY option, PROC MODECLUS produces a table summarizing each cluster solution containing the following items:

- the smoothing parameters and cascade value
- the number of clusters
- the frequency of unclassified objects
- the likelihood cross validation criterion if you specify the CROSS or CROSSLIST option

If you specify the JOIN option, the summary table also includes the following items:

- the number of clusters joined
- the maximum  $p$ -value of any cluster in the solution

If you specify the TRACE option, PROC MODECLUS produces a table for each cluster solution that lists each observation along with its cluster membership as it is reassigned from the “Old” cluster to the “New” cluster. This reassignment is described in **Step 1** through **Step 3** of the section “METHOD=6” on page 5100. Each table has a row for each observation. For each observation, the following are displayed:

- the observation number or ID value of the observation

- the estimated density
- the “Old” cluster membership. 0 represents an unassigned observation and –1 represents a seed.
- the “New” cluster membership
- “Ratio,” which is documented in the section “METHOD=6” on page 5100. The following character values can also be displayed:

“M” means the observation is a mode

“S” means the observation is a seed

“N” means the neighbor of a mode or seed, for which the ratio is not computed

---

## ODS Table Names

PROC MODECLUS assigns a name to each table it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in Table 60.6.

For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

All of the ODS tables in Table 60.6 are created by specifying the PROC MODECLUS statement.

**Table 60.6** ODS Tables Produced by PROC MODECLUS

| ODS Table Name   | Description                                                                                                   | Option                                            |
|------------------|---------------------------------------------------------------------------------------------------------------|---------------------------------------------------|
| BoundaryFreq     | Boundary objects information                                                                                  | BOUNDARY or ALL                                   |
| ClusterList      | Cluster listing, cluster ID, frequency, density etc.                                                          | LIST or ALL                                       |
| ClusterStats     | Cluster statistics<br>Cluster statistics, significance test statistics                                        | default<br>TEST, JOIN, or ALL                     |
| ClusterSummary   | Cluster summary<br>Cluster summary, crossvalidation criterion<br>Cluster summary, clusters joined information | default<br>CROSS, CROSSLIS, or ALL<br>JOIN or ALL |
| CrossList        | Cross validated log density                                                                                   | CROSSLIST                                         |
| ListLocal        | Local dimensionality estimates                                                                                | LOCAL                                             |
| Neighbor         | Nearest neighbor list                                                                                         | NEIGHBOR or ALL                                   |
| SimpleStatistics | Simple statistics                                                                                             | SIMPLE or ALL                                     |
| Trace            | Trace of clustering algorithm (METHOD=6 only)                                                                 | TRACE or ALL when METHOD=6                        |
| UnassignObjects  | Information about unassigned objects                                                                          | LIST or ALL                                       |

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## Examples: MODECLUS Procedure

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### Example 60.1: Cluster Analysis of Samples from Univariate Distributions

This example uses pseudo-random samples from a uniform distribution, an exponential distribution, and a bimodal mixture of two normal distributions. Results are presented in [Output 60.1.1](#) through [Output 60.1.18](#) as plots displaying both the true density and the estimated density, as well as cluster membership.

The following statements produce [Output 60.1.1](#) through [Output 60.1.4](#):

```
title 'Modeclus Example with Univariate Distributions';
title2 'Uniform Distribution';

data uniform;
 drop n;
 true=1;
 do n=1 to 100;
 x=ranuni(123);
 output;
 end;
run;

proc modeclus data=uniform m=1 k=10 20 40 60 out=out short;
 var x;
run;

proc sgplot data=out noautolegend;
 y2axis label='True' values=(0 to 2 by 1.);
 yaxis values=(0 to 3 by 0.5);
 scatter y=density x=x / markerchar=cluster group=cluster;
 pbspline y=true x=x / y2axis nomarkers lineattrs=(thickness= 1);
 by _K_;
run;

proc modeclus data=uniform m=1 r=.05 .10 .20 .30 out=out short;
 var x;
run;

proc sgplot data=out noautolegend;
 y2axis label='True' values=(0 to 2 by 1.);
 yaxis values=(0 to 2 by 0.5);
 scatter y=density x=x / markerchar=cluster group=cluster;
 pbspline y=true x=x / y2axis nomarkers lineattrs=(thickness= 1);
 by _R_;
run;
```

**Output 60.1.1** Cluster Analysis of Sample from a Uniform Distribution

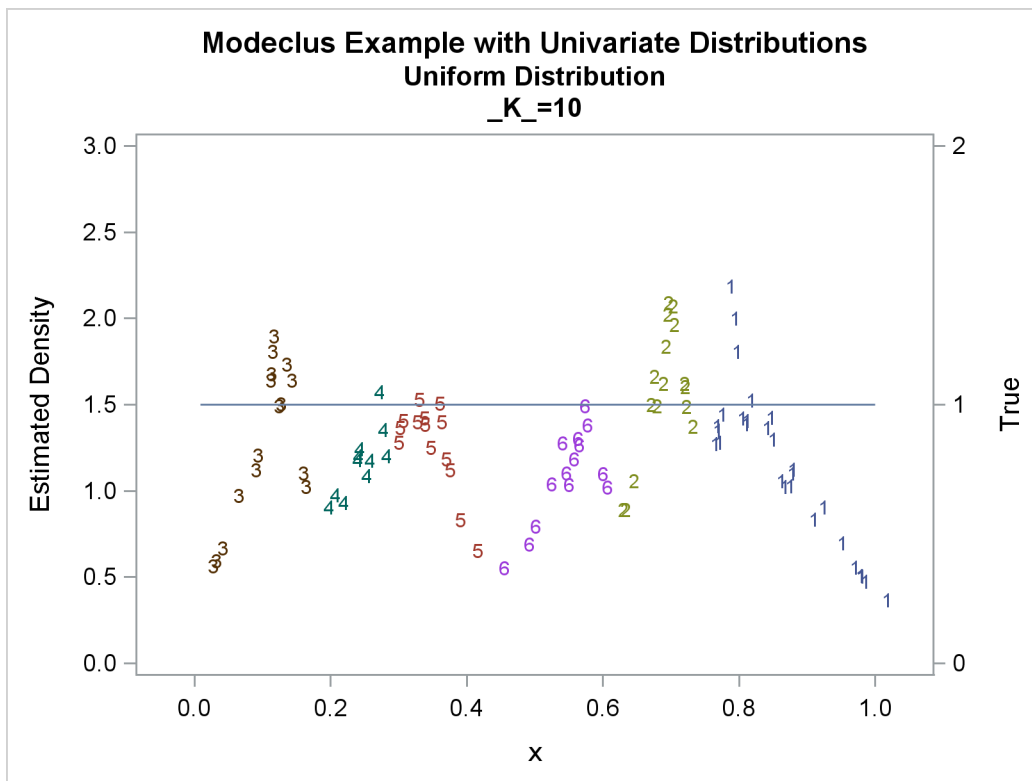
**Modeclus Example with Univariate Distributions**  
**Uniform Distribution**

**The MODECLUS Procedure**

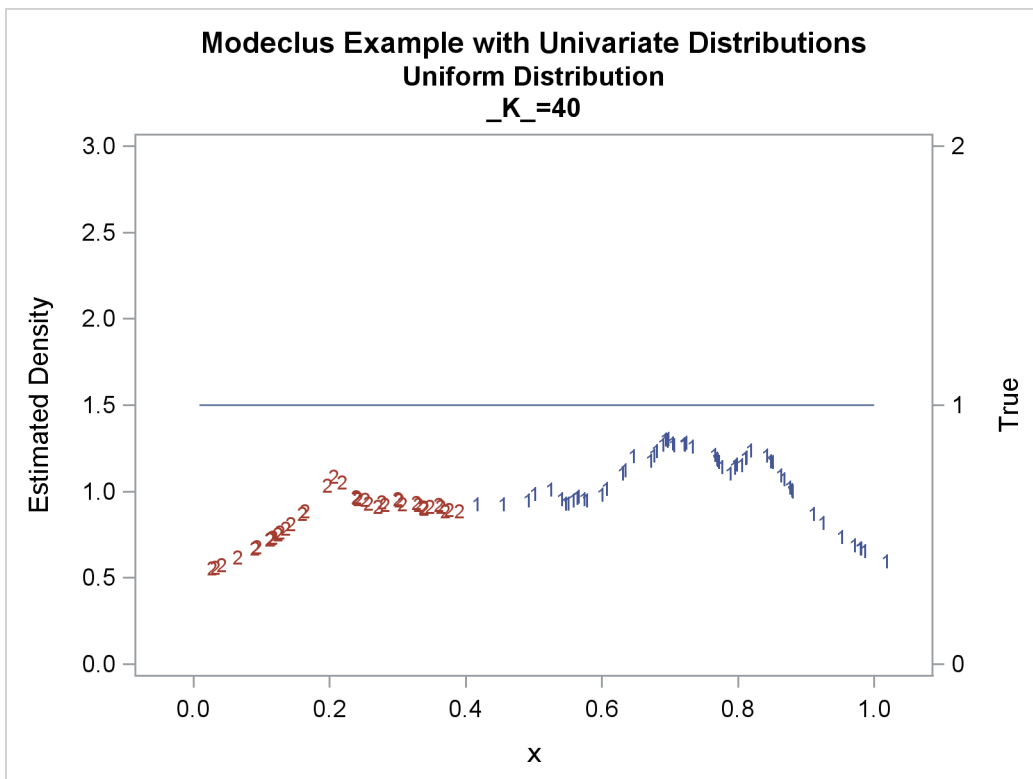
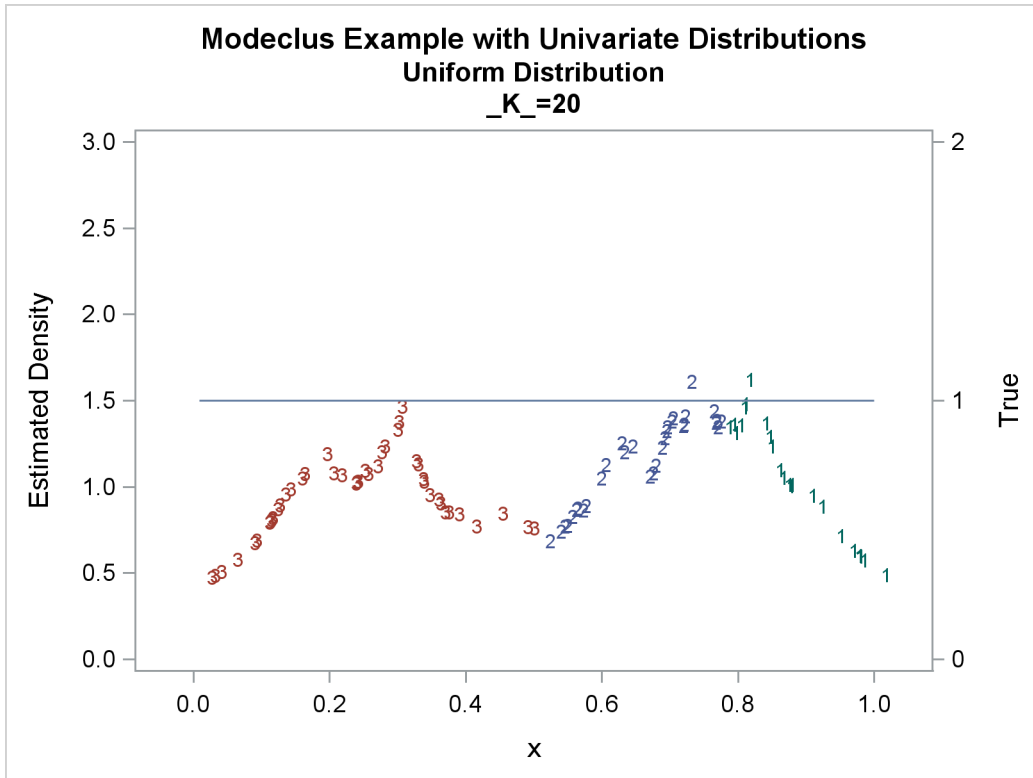
**Cluster Summary**

| K  | Number of<br>Clusters | Frequency of<br>Unclassified<br>Objects |
|----|-----------------------|-----------------------------------------|
| 10 | 6                     | 0                                       |
| 20 | 3                     | 0                                       |
| 40 | 2                     | 0                                       |
| 60 | 1                     | 0                                       |

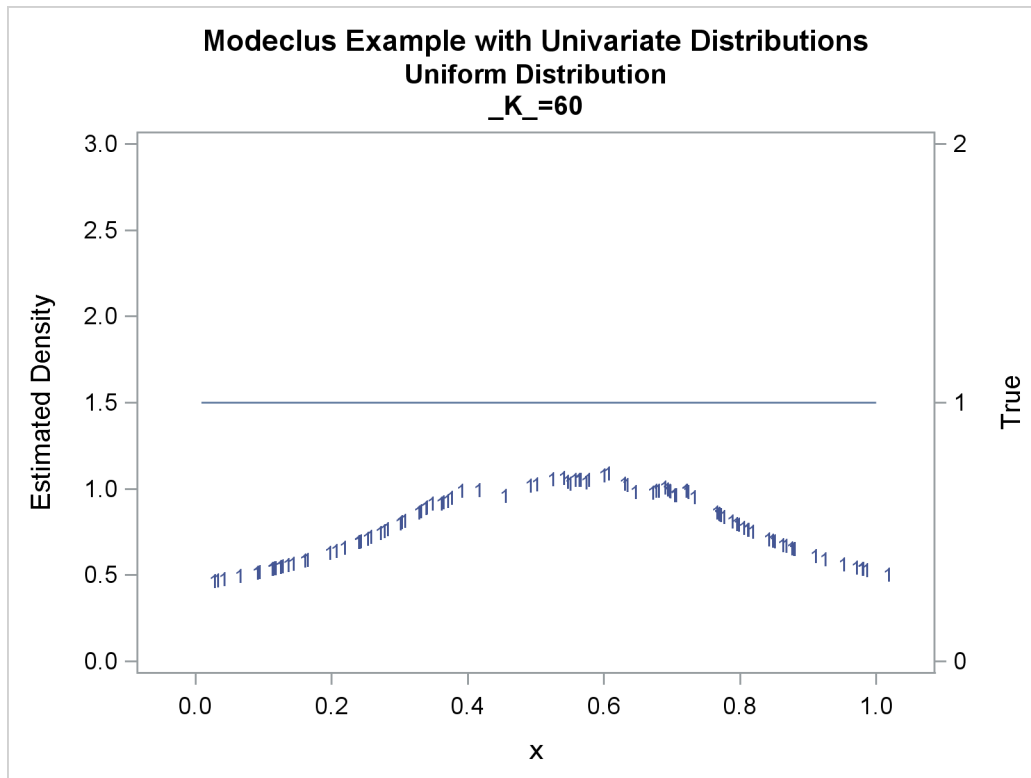
**Output 60.1.2** True Density, Estimated Density, and Cluster Membership by Various K Values



Output 60.1.2 continued



Output 60.1.2 continued



Output 60.1.3 Cluster Analysis of Sample from a Uniform Distribution

```

Modeclus Example with Univariate Distributions
Uniform Distribution

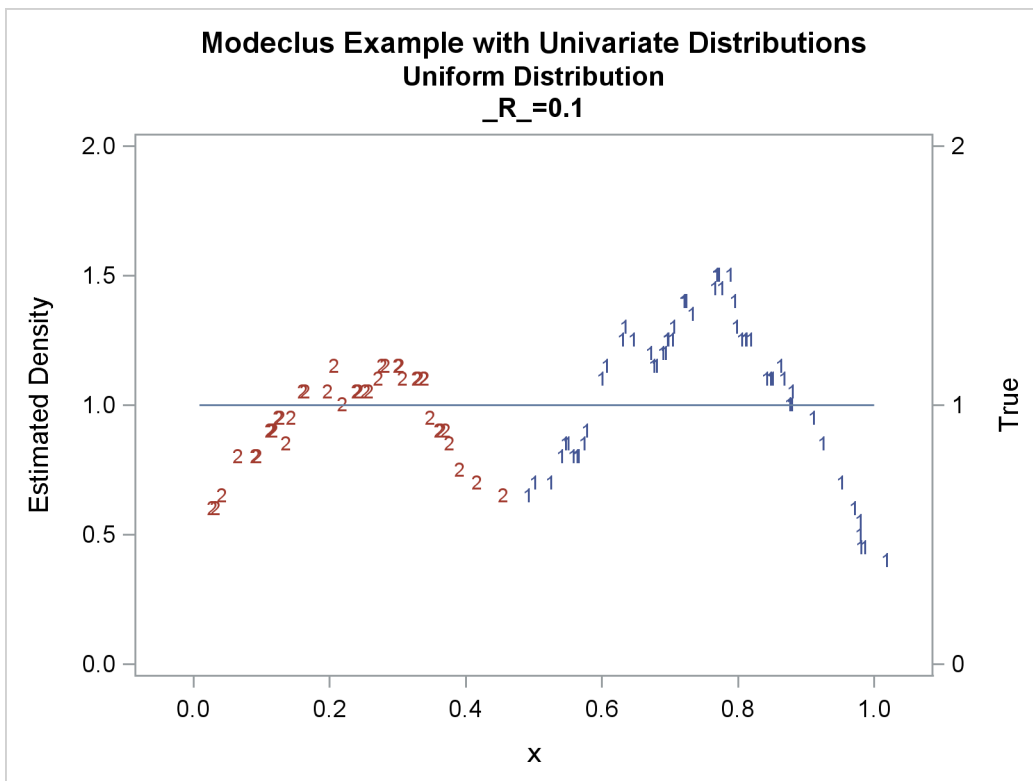
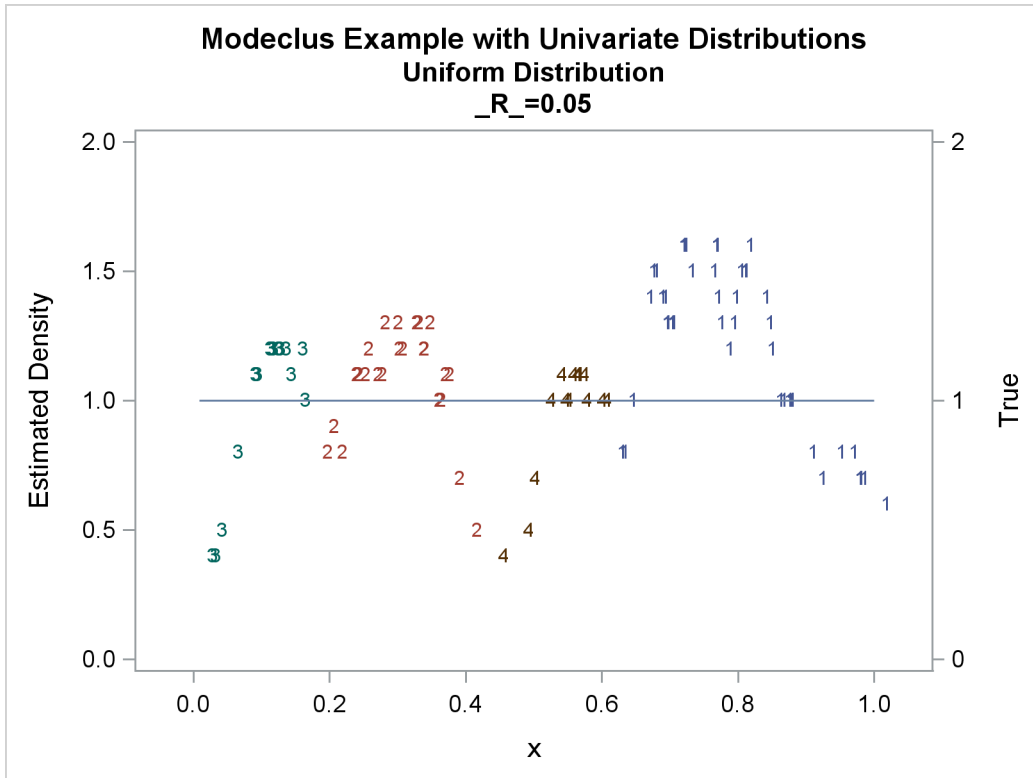
The MODECLUS Procedure

Cluster Summary
Number of Frequency of
R Clusters Unclassified

0.05 4 0
0.1 2 0
0.2 2 0
0.3 1 0

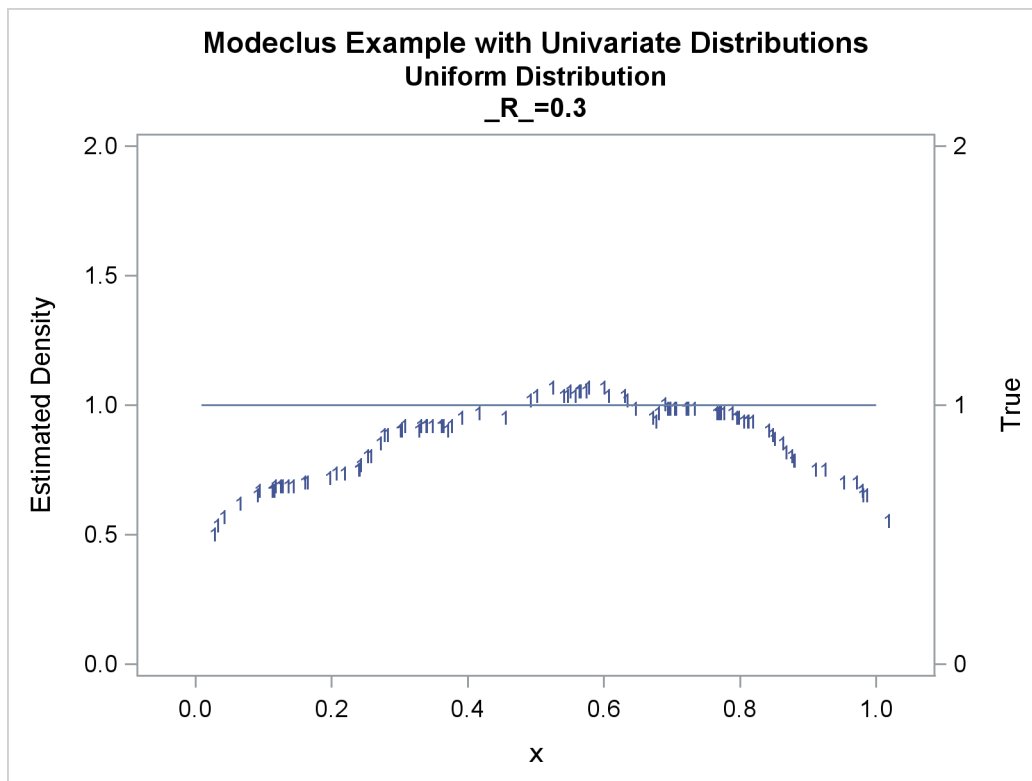
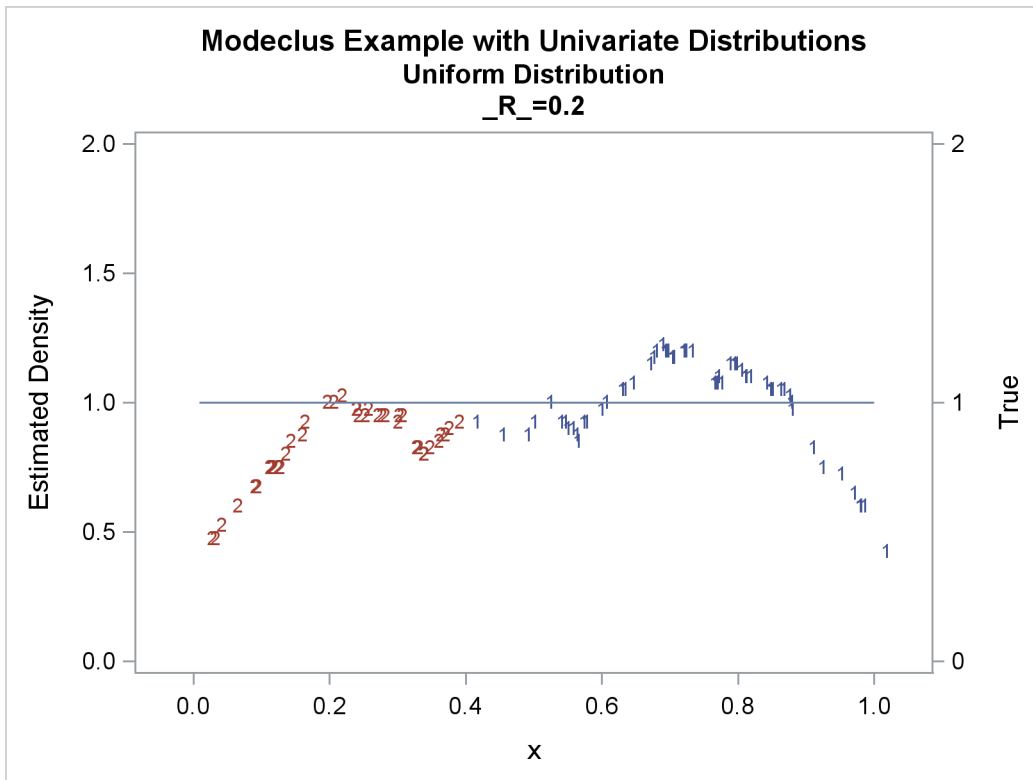
```

**Output 60.1.4** True Density, Estimated Density, and Cluster Membership by Various  $_R_$  Values





Output 60.1.4 continued



The following statements produce [Output 60.1.5](#) through [Output 60.1.12](#):

```

data expon;
 title2 'Exponential Distribution';
 drop n;
 do n=1 to 100;
 x=ranexp(123);
 true=exp(-x);
 output;
 end;
run;

proc modeclus data=expon m=1 k=10 20 40 out=out short;
 var x;
run;

proc sgplot data=out noautolegend;
 y2axis label='True' values=(0 to 1 by .5);
 yaxis values=(0 to 2 by 0.5);
 scatter y=density x=x / markerchar=cluster group=cluster;
 pbspline y=true x=x / y2axis nomarkers lineattrs=(thickness= 1);
 by _K_;
run;

proc modeclus data=expon m=1 r=.20 .40 .80 out=out short;
 var x;
run;

proc sgplot data=out noautolegend;
 y2axis label='True' values=(0 to 1 by .5);
 yaxis values=(0 to 1 by 0.5);
 scatter y=density x=x / markerchar=cluster group=cluster;
 pbspline y=true x=x / y2axis nomarkers lineattrs=(thickness= 1);
 by _R_;
run;

title3 'Different Density-Estimation and Clustering Windows';

proc modeclus data=expon m=1 r=.20 ck=10 20 40
 out=out short;
 var x;
run;

proc sgplot data=out noautolegend;
 y2axis label='True' values=(0 to 1 by .5);
 yaxis values=(0 to 1 by 0.5);
 scatter y=density x=x / markerchar=cluster group=cluster;
 pbspline y=true x=x / y2axis nomarkers lineattrs=(thickness= 1);
 by _CK_;
run;

```

```

title3 'Cascaded Density Estimates Using Arithmetic Means';

proc modeclus data=expon m=1 r=.20 cascade=1 2 4 am out=out short;
 var x;
run;

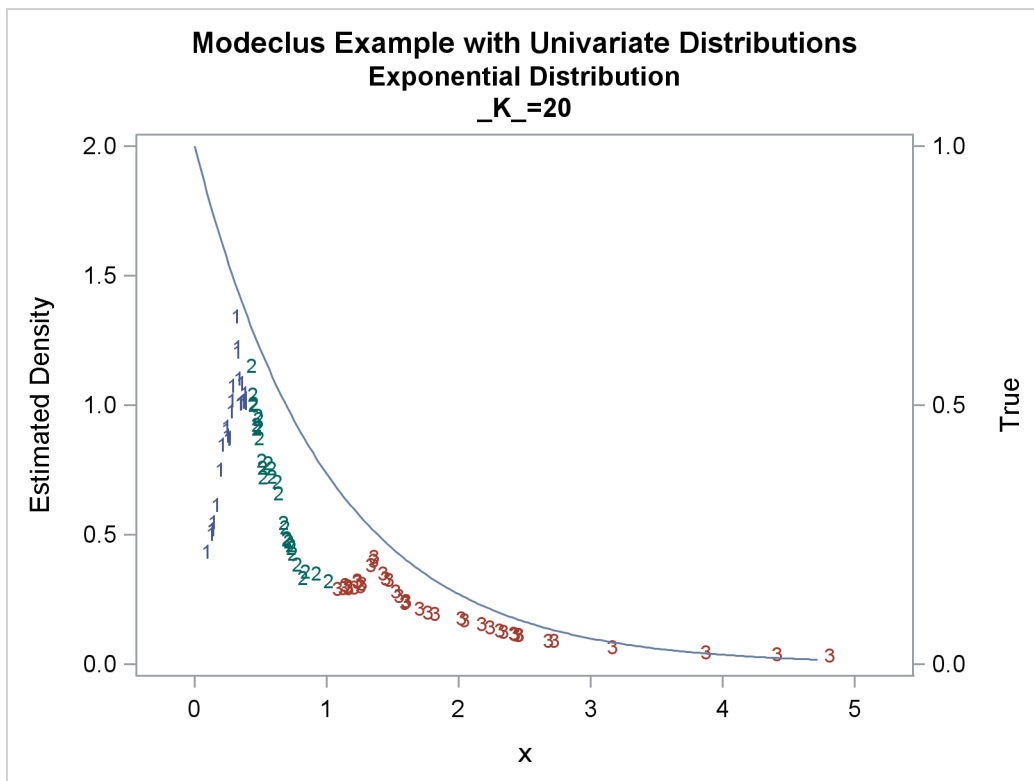
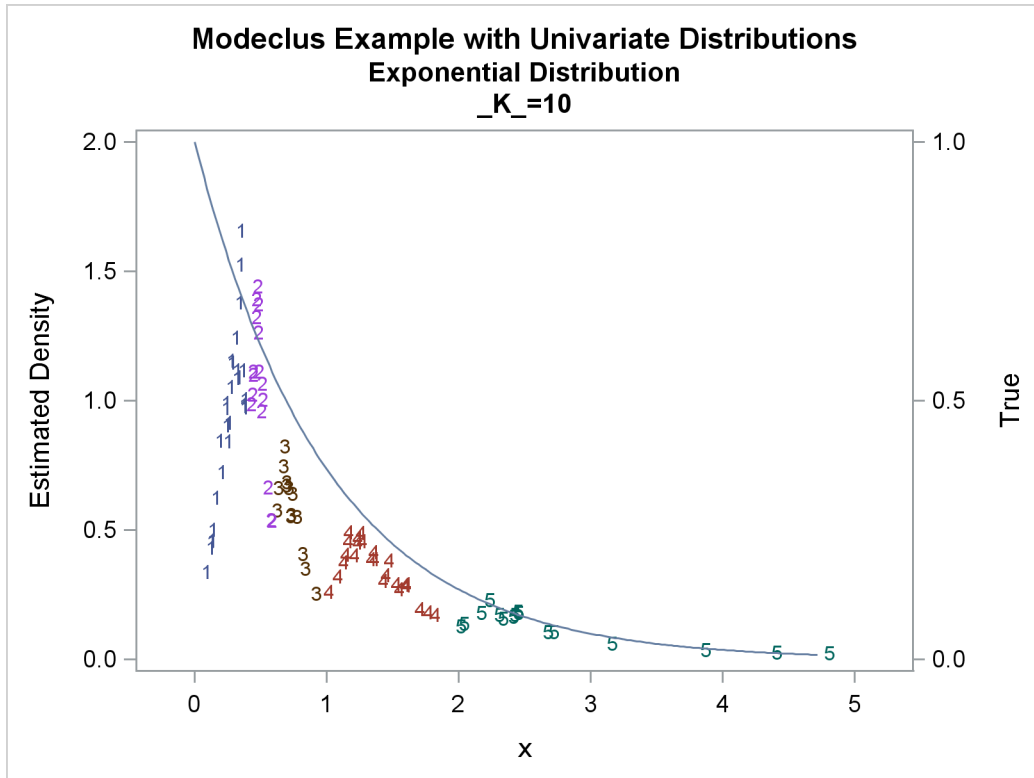
proc sgplot data=out noautolegend;
 y2axis label='True' values=(0 to 1 by .5);
 yaxis values=(0 to 1 by 0.5);
 scatter y=density x=x / markerchar=cluster group=cluster;
 pbspline y=true x=x / y2axis nomarkers lineattrs=(thickness= 1);
 by _R_ _CASCAD_;
run;

```

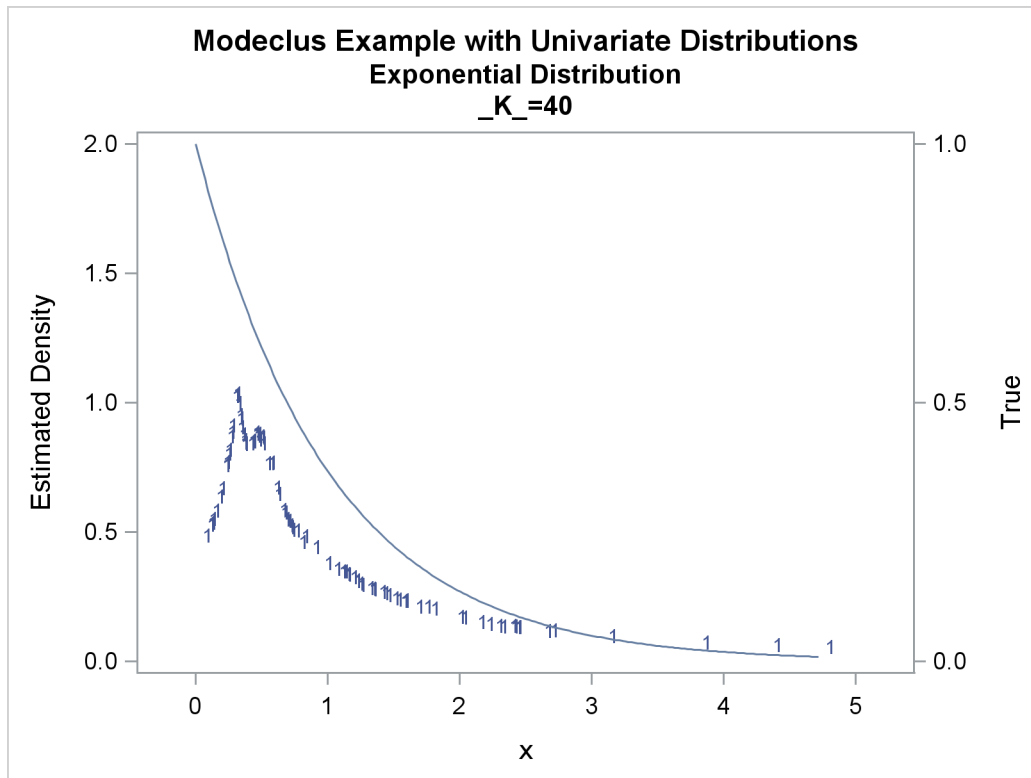
### Output 60.1.5 Cluster Analysis of Sample from an Exponential Distribution

| Modeclus Example with Univariate Distributions<br>Exponential Distribution |                       |                                         |
|----------------------------------------------------------------------------|-----------------------|-----------------------------------------|
| The MODECLUS Procedure                                                     |                       |                                         |
| Cluster Summary                                                            |                       |                                         |
| K                                                                          | Number of<br>Clusters | Frequency of<br>Unclassified<br>Objects |
| 10                                                                         | 5                     | 0                                       |
| 20                                                                         | 3                     | 0                                       |
| 40                                                                         | 1                     | 0                                       |

**Output 60.1.6** True Density, Estimated Density, and Cluster Membership by Various  $_K_$  Values



Output 60.1.6 continued



Output 60.1.7 Cluster Analysis of Sample from an Exponential Distribution

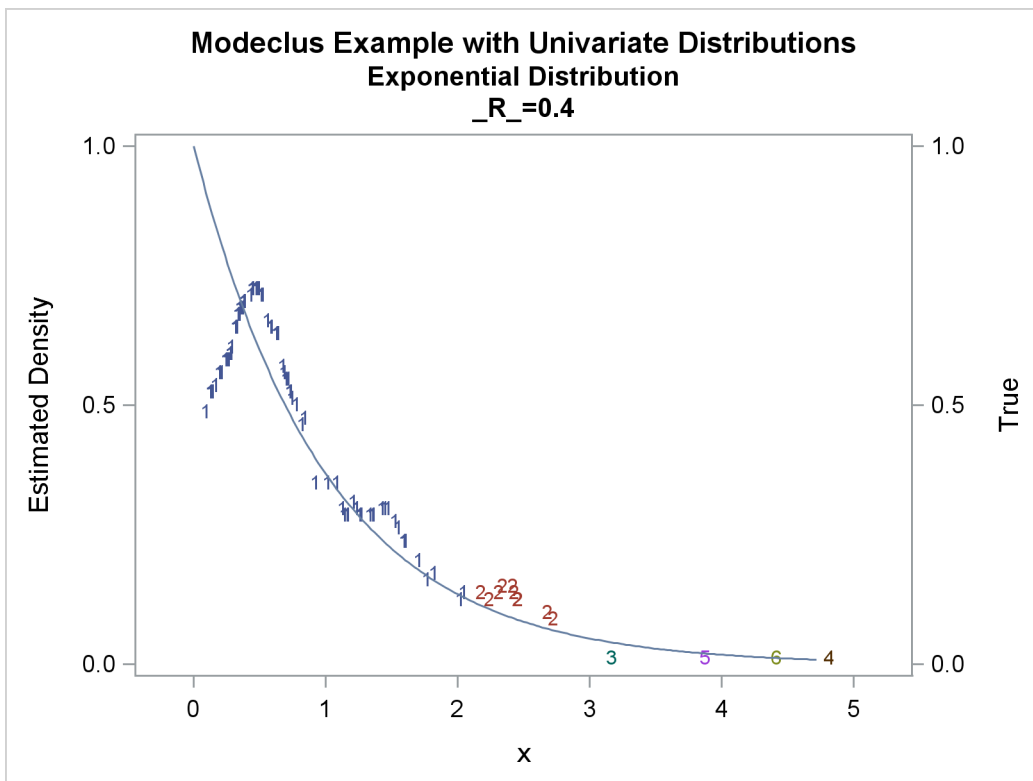
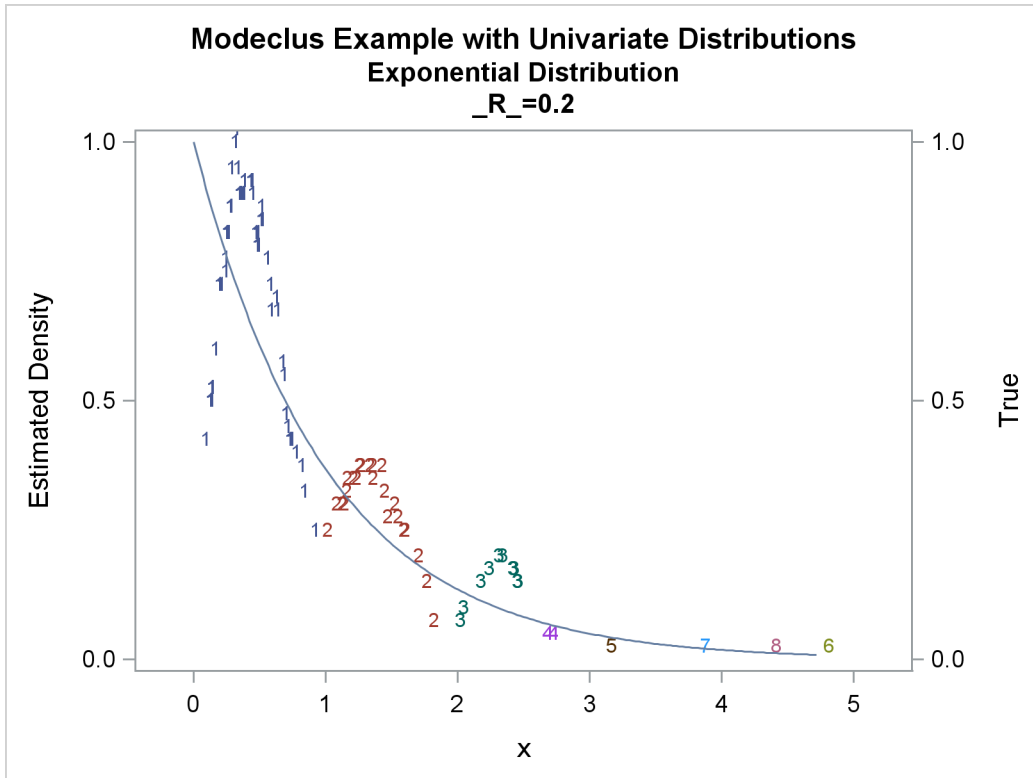
Modeclus Example with Univariate Distributions  
Exponential Distribution

The MODECLUS Procedure

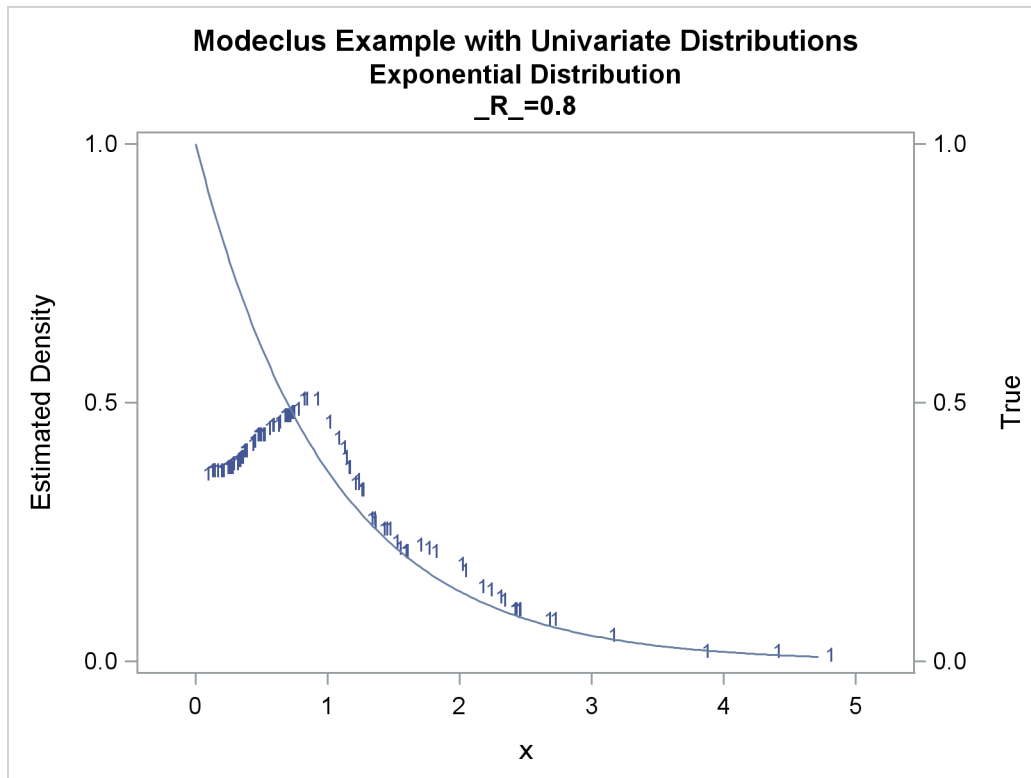
Cluster Summary

| R   | Number of<br>Clusters | Frequency of<br>Unclassified<br>Objects |
|-----|-----------------------|-----------------------------------------|
| 0.2 | 8                     | 0                                       |
| 0.4 | 6                     | 0                                       |
| 0.8 | 1                     | 0                                       |

**Output 60.1.8** True Density, Estimated Density, and Cluster Membership by Various  $_R_$  Values



Output 60.1.8 continued



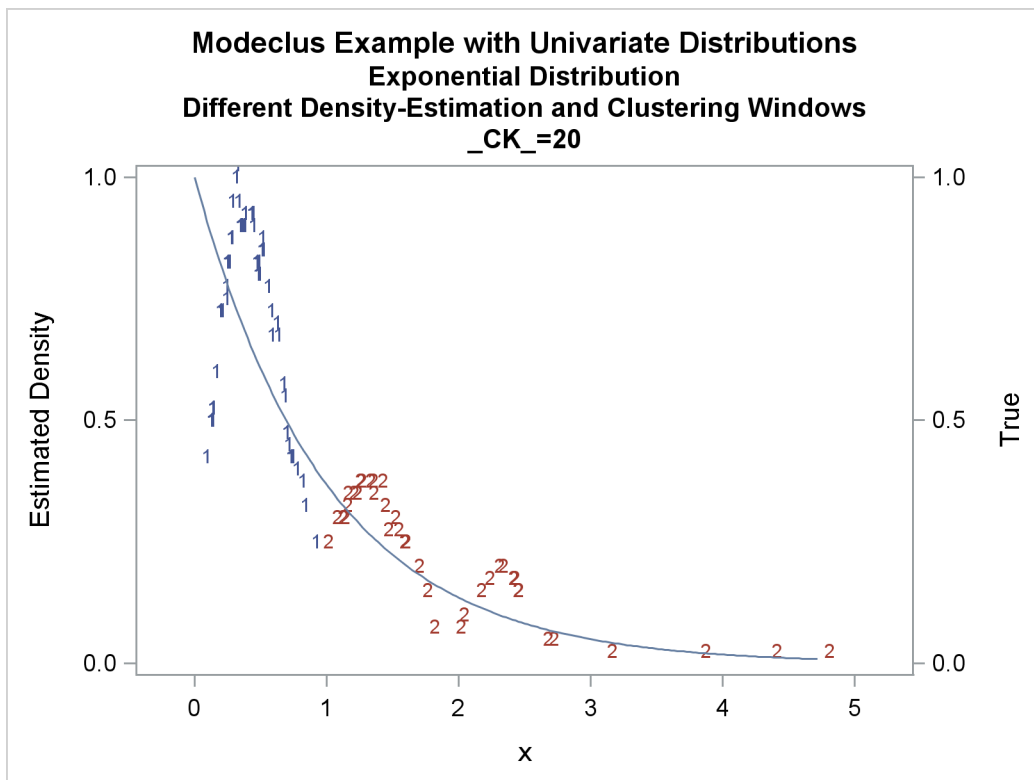
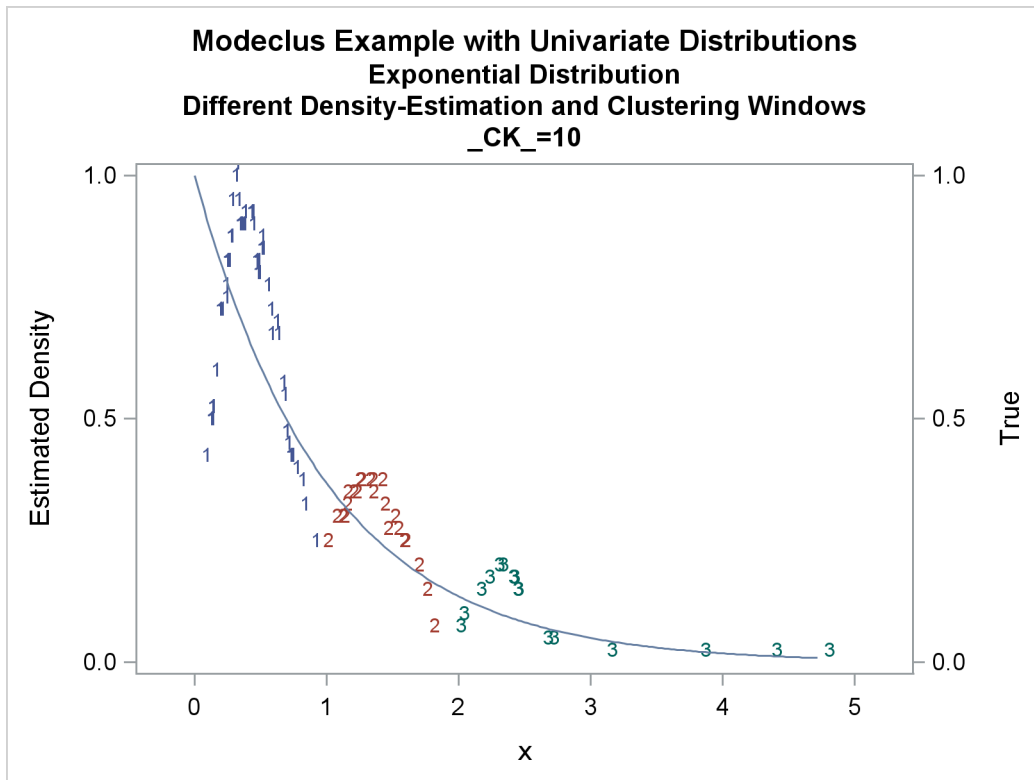
Output 60.1.9 Cluster Analysis of Sample from an Exponential Distribution

Modeclus Example with Univariate Distributions  
Exponential Distribution  
Different Density-Estimation and Clustering Windows

The MODECLUS Procedure

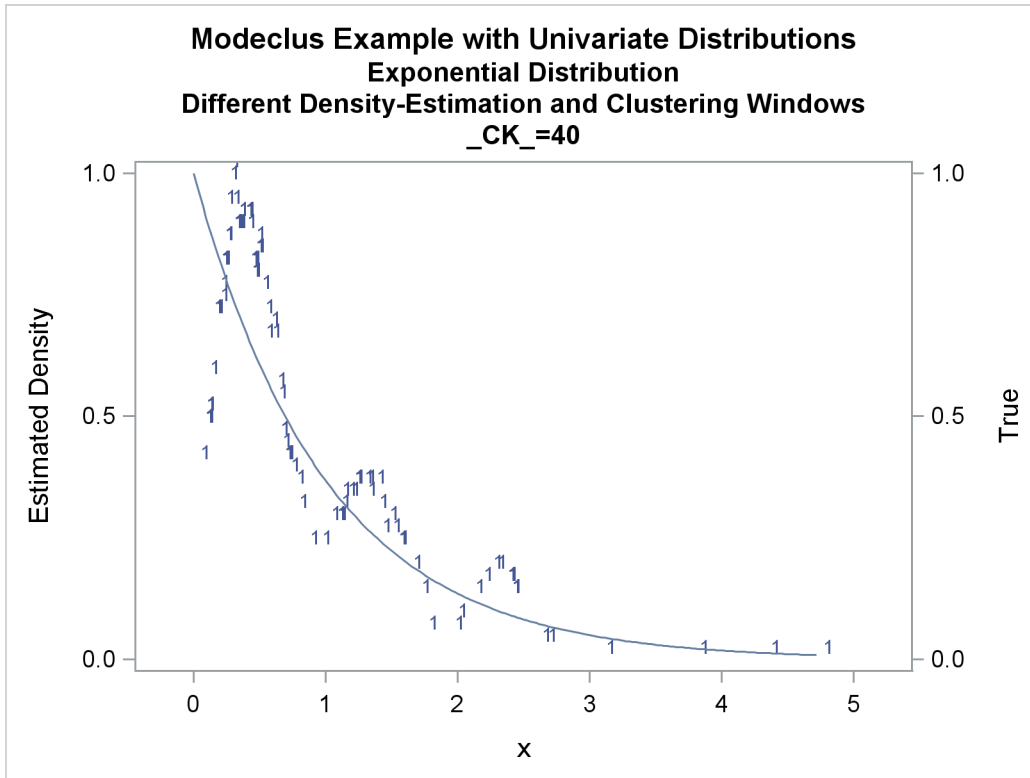
| Cluster Summary |    |                       |                                         |
|-----------------|----|-----------------------|-----------------------------------------|
| R               | CK | Number of<br>Clusters | Frequency of<br>Unclassified<br>Objects |
| 0.2             | 10 | 3                     | 0                                       |
| 0.2             | 20 | 2                     | 0                                       |
| 0.2             | 40 | 1                     | 0                                       |

**Output 60.1.10** True Density, Estimated Density, and Cluster Membership by  $\_R_=0.2$  with Various  $\_CK\_$  Values





Output 60.1.10 continued



Output 60.1.11 Cluster Analysis of Sample from an Exponential Distribution

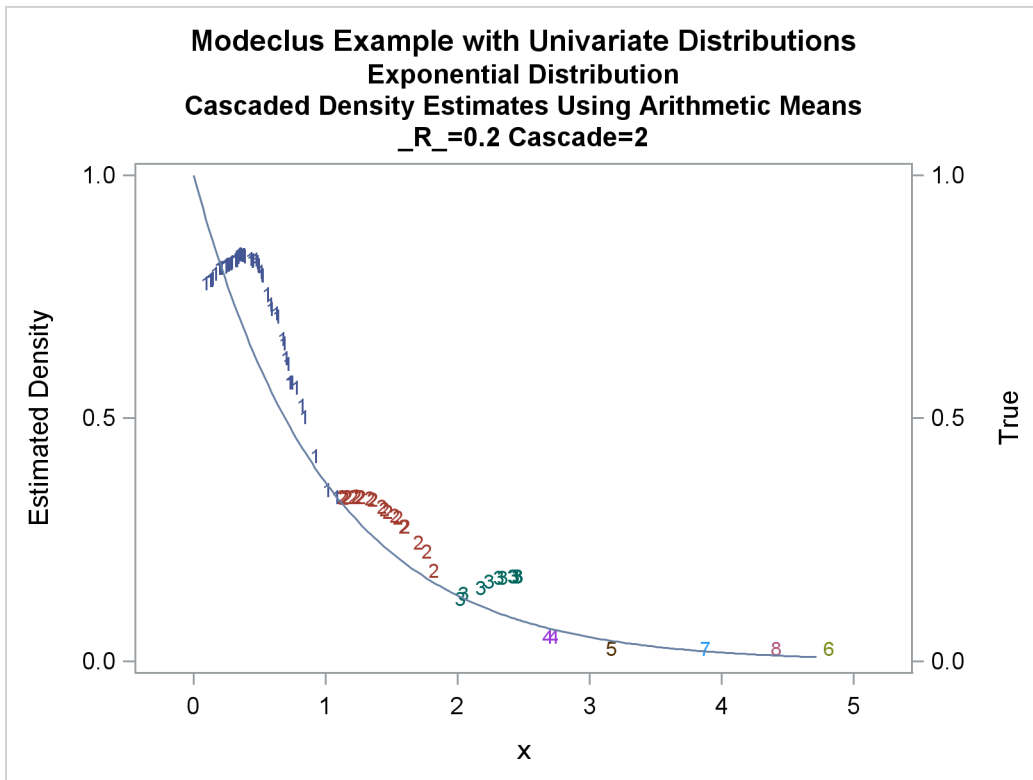
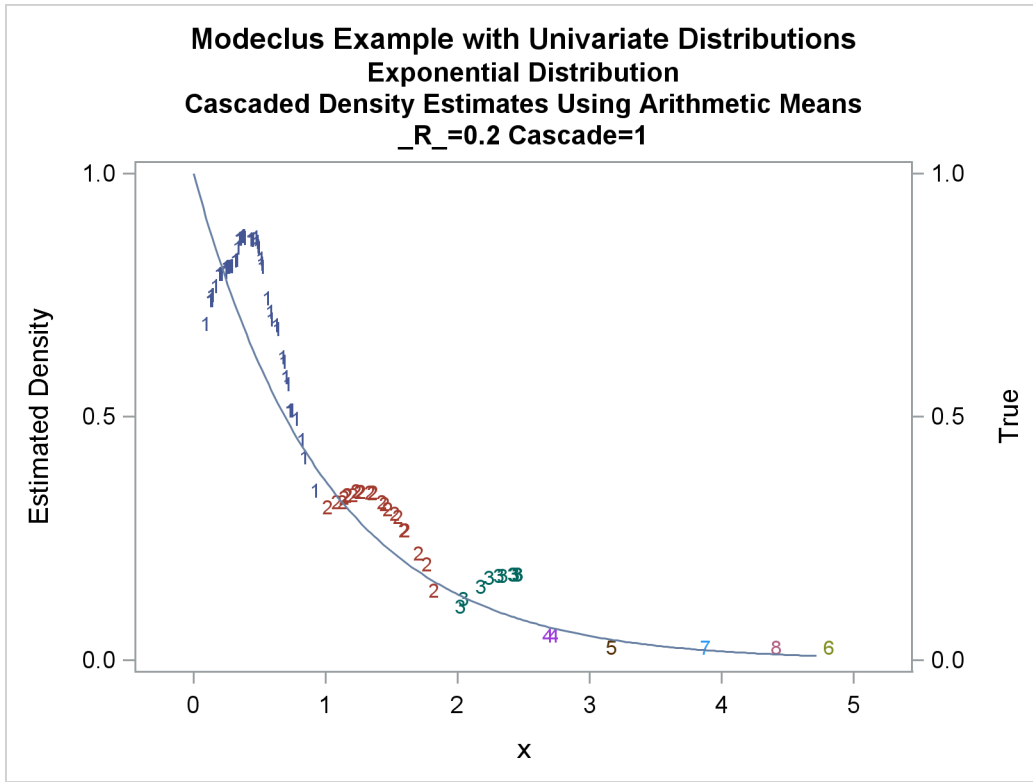
**Modeclus Example with Univariate Distributions**  
**Exponential Distribution**  
**Cascaded Density Estimates Using Arithmetic Means**

The MODECLUS Procedure

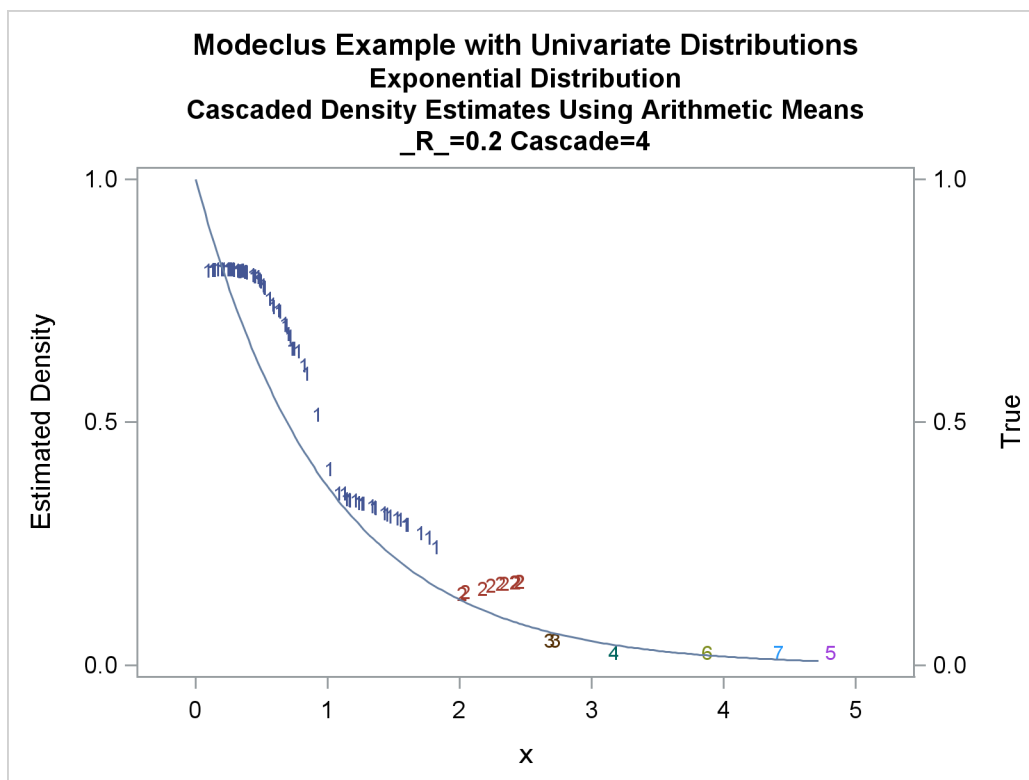
Cluster Summary

| R   | Cascade | Number of<br>Clusters | Frequency of<br>Unclassified<br>Objects |
|-----|---------|-----------------------|-----------------------------------------|
| 0.2 | 1       | 8                     | 0                                       |
| 0.2 | 2       | 8                     | 0                                       |
| 0.2 | 4       | 7                     | 0                                       |

**Output 60.1.12** True Density, Estimated Density, and Cluster Membership by  $\_R_=0.2$  with Various  $\_CAS-$   
 $\_CAD\_Values$



Output 60.1.12 continued



The following statements produce [Output 60.1.13](#) through [Output 60.1.18](#):

```

title2 'Normal Mixture Distribution';

data normix;
 drop n sigma;
 sigma=.125;
 do n=1 to 100;
 x=rannor(456)*sigma+mod(n,2)/2;
 true=exp(-.5*(x/sigma)**2)+exp(-.5*((x-.5)/sigma)**2);
 true=.5*true/(sigma*sqrt(2*3.1415926536));
 output;
 end;
run;

proc modeclus data=normix m=1 k=10 20 40 60 out=out short;
 var x;
run;

proc sgplot data=out noautolegend;
 y2axis label='True' values=(0 to 1.6 by .1);
 yaxis values=(0 to 3 by 0.5);
 scatter y=density x=x / markerchar=cluster group=cluster;
 pbspline y=true x=x / y2axis nomarkers lineattrs=(thickness= 1);
 by _K_;
run;

proc modeclus data=normix m=1 r=.05 .10 .20 .30 out=out short;
 var x;
run;

proc sgplot data=out noautolegend;
 y2axis label='True' values=(0 to 1.6 by .1);
 yaxis values=(0 to 3 by 0.5);
 scatter y=density x=x / markerchar=cluster group=cluster;
 pbspline y=true x=x / y2axis nomarkers lineattrs=(thickness= 1);
 by _R_;
run;

title3 'Cascaded Density Estimates Using Arithmetic Means';

proc modeclus data=normix m=1 r=.05 cascade=1 2 4 am out=out short;
 var x;
run;

proc sgplot data=out noautolegend;
 y2axis label='True' values=(0 to 1.6 by .1);
 yaxis values=(0 to 2 by 0.5);
 scatter y=density x=x / markerchar=cluster group=cluster;
 pbspline y=true x=x / y2axis nomarkers lineattrs=(thickness= 1);
 by _R_ _CASCAD_;
run;

```

**Output 60.1.13** Cluster Analysis of Sample from a Bimodal Mixture of Two Normal Distributions

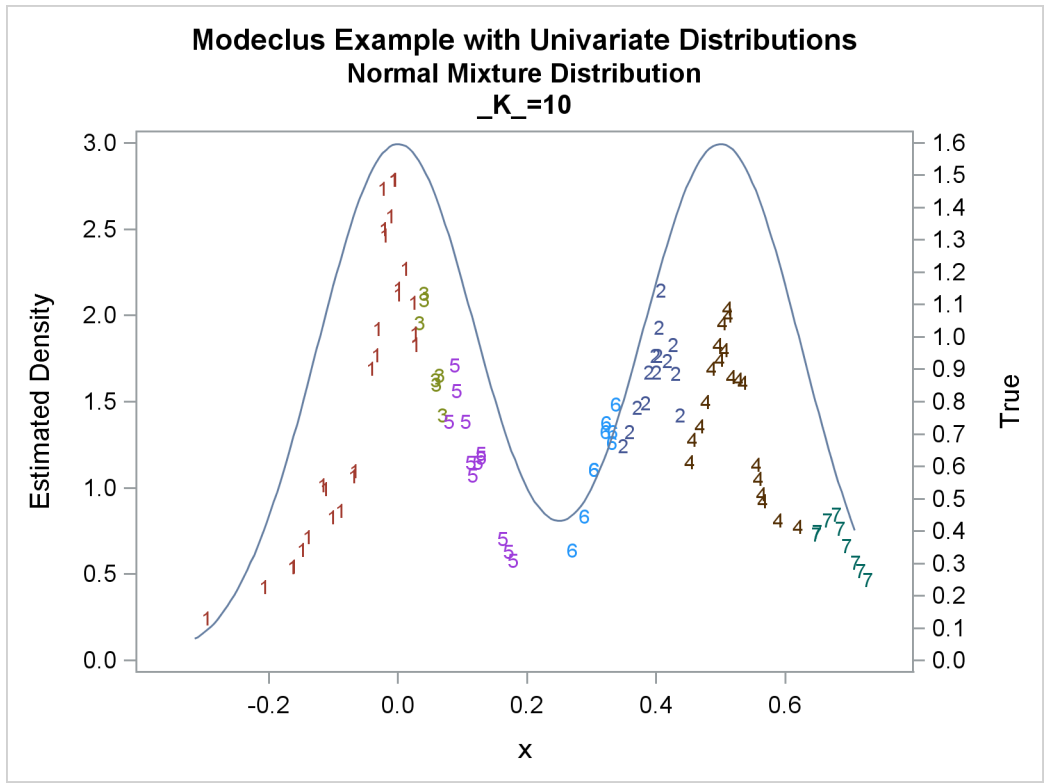
**Modeclus Example with Univariate Distributions  
Normal Mixture Distribution**

**The MODECLUS Procedure**

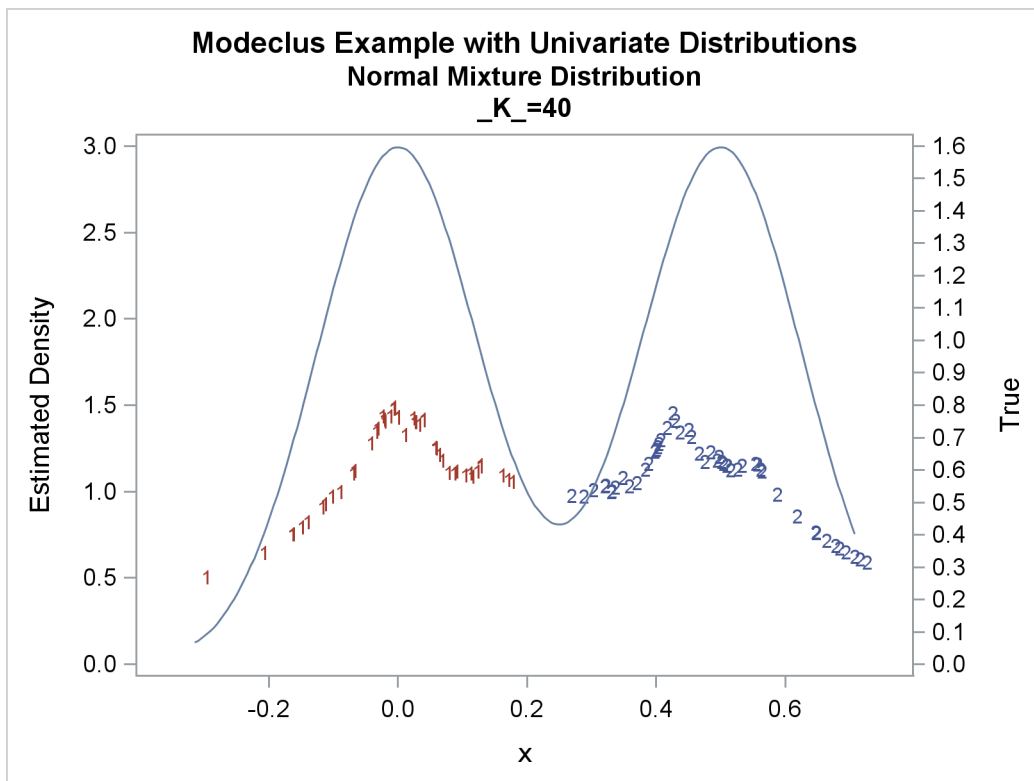
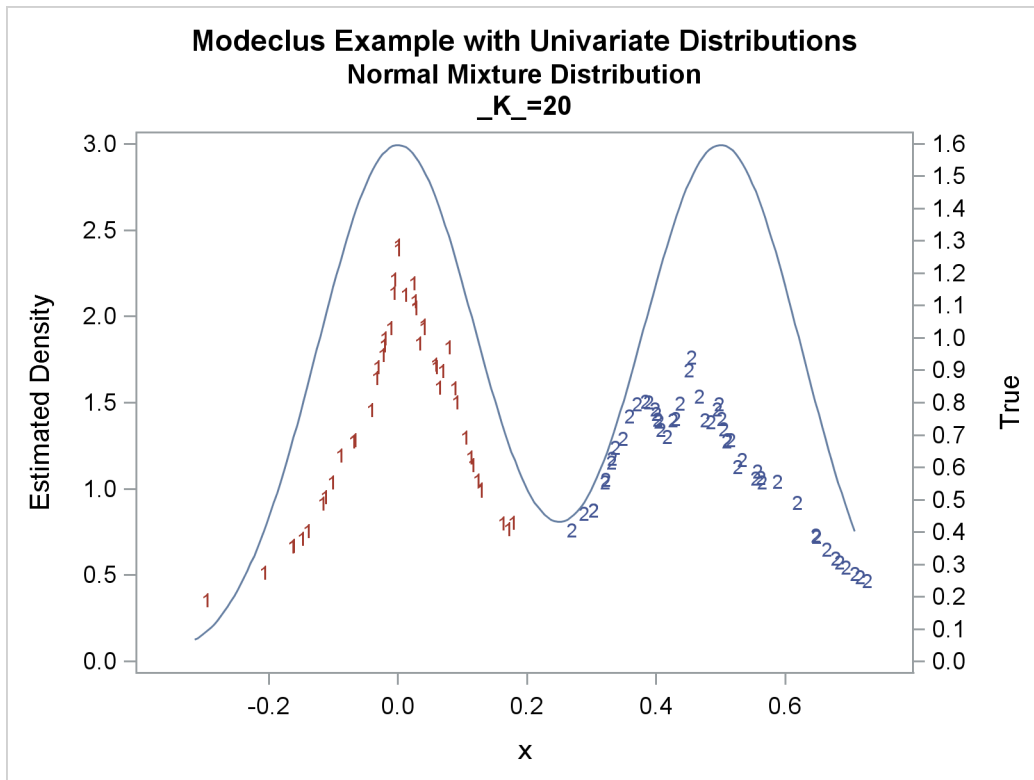
**Cluster Summary**

| K  | Number of<br>Clusters | Frequency of<br>Unclassified<br>Objects |
|----|-----------------------|-----------------------------------------|
| 10 | 7                     | 0                                       |
| 20 | 2                     | 0                                       |
| 40 | 2                     | 0                                       |
| 60 | 1                     | 0                                       |

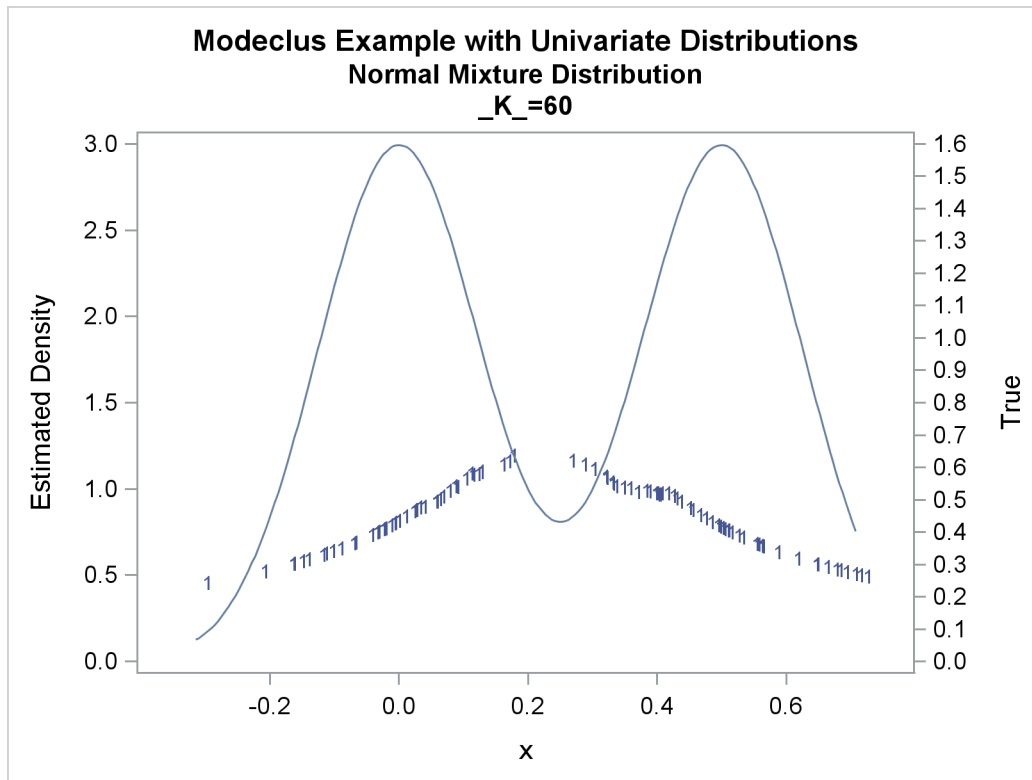
**Output 60.1.14** True Density, Estimated Density, and Cluster Membership by Various \_K\_ Values



Output 60.1.14 continued



Output 60.1.14 continued



Output 60.1.15 Cluster Analysis of Sample from a Bimodal Mixture of Two Normal Distributions

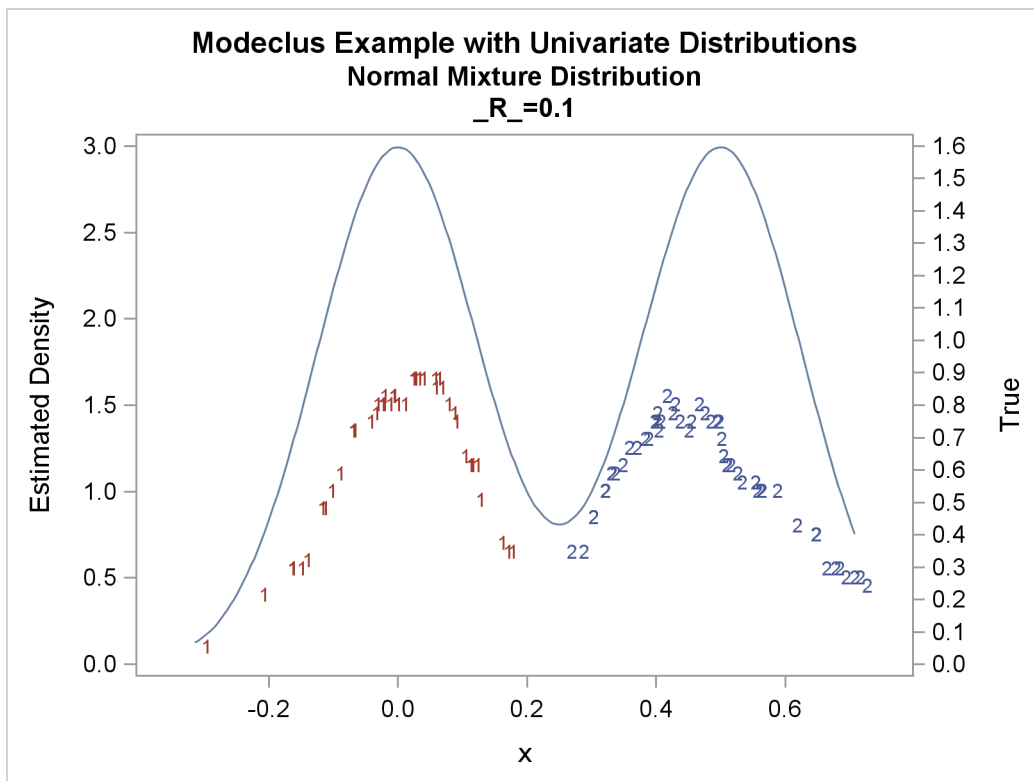
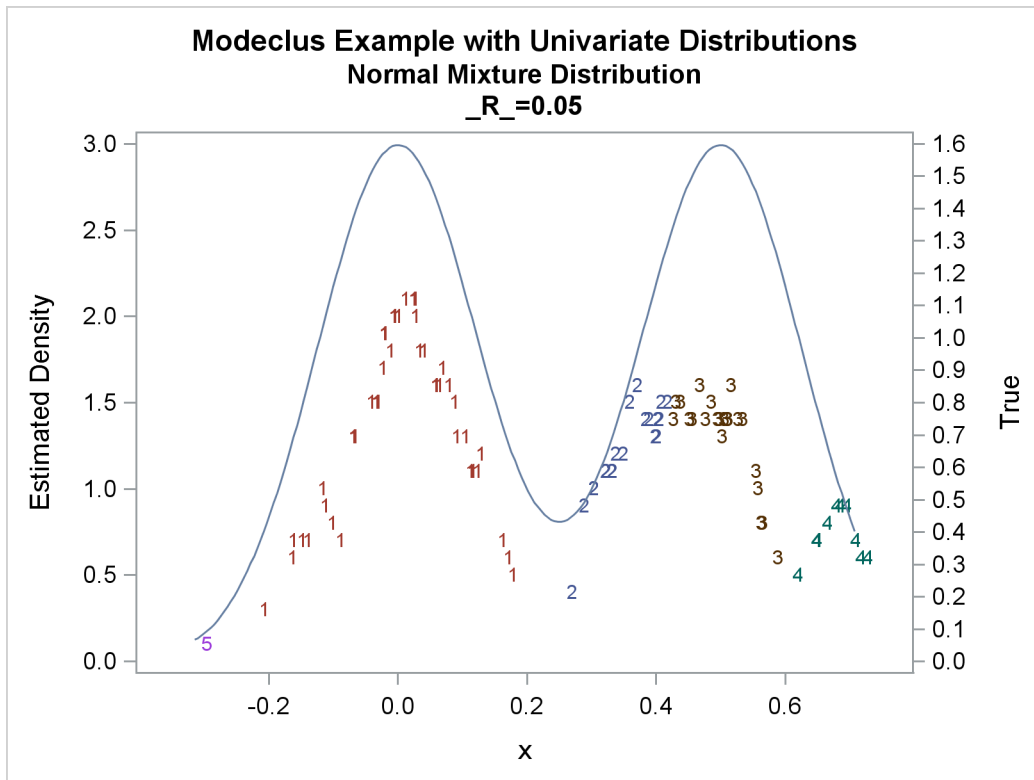
Modeclus Example with Univariate Distributions  
Normal Mixture Distribution

The MODECLUS Procedure

Cluster Summary

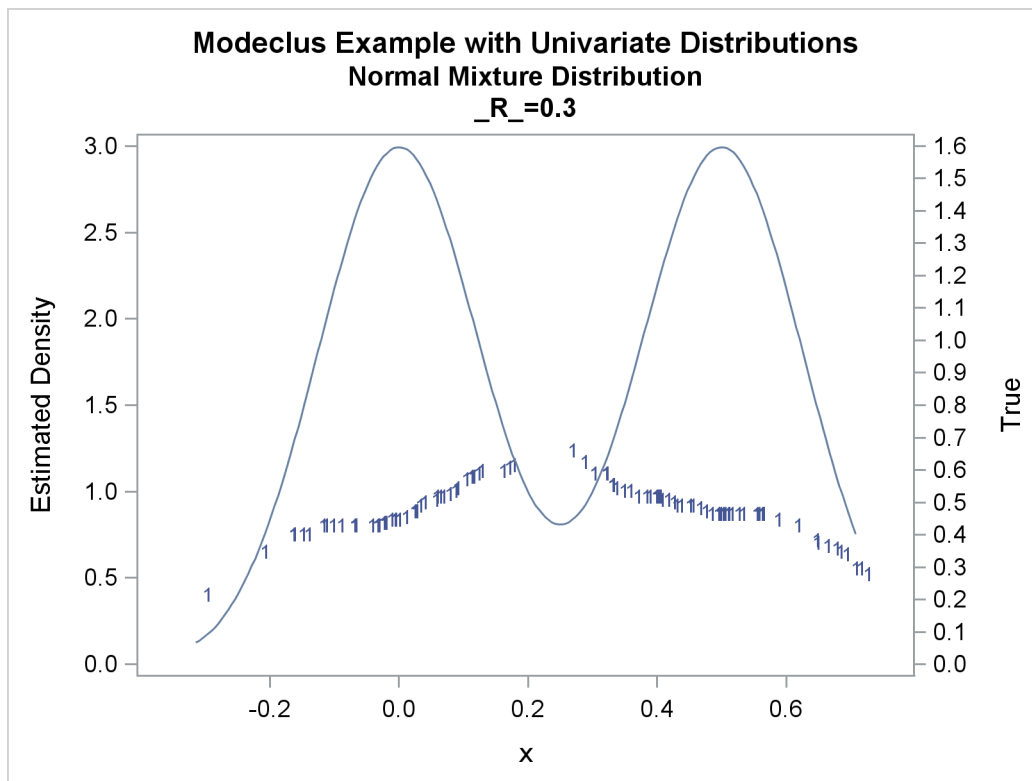
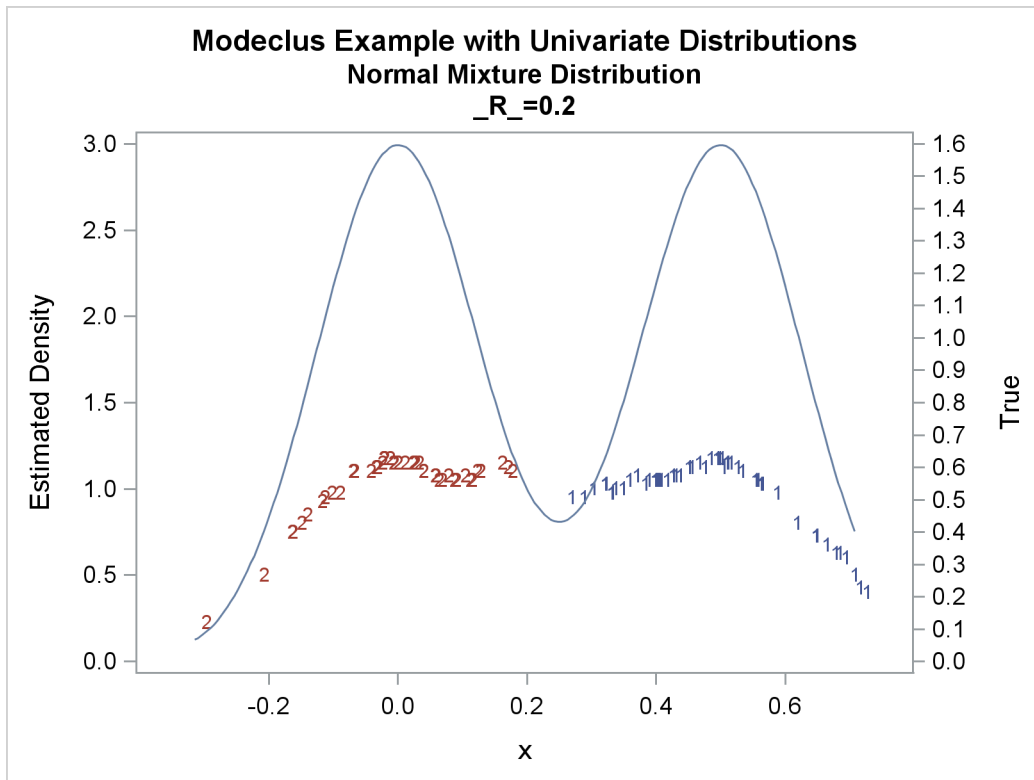
| R    | Number of<br>Clusters | Frequency of<br>Unclassified<br>Objects |
|------|-----------------------|-----------------------------------------|
| 0.05 | 5                     | 0                                       |
| 0.1  | 2                     | 0                                       |
| 0.2  | 2                     | 0                                       |
| 0.3  | 1                     | 0                                       |

**Output 60.1.16** True Density, Estimated Density, and Cluster Membership by Various  $_R_$  = Values





Output 60.1.16 continued



**Output 60.1.17** Cluster Analysis of Sample from a Bimodal Mixture of Two Normal Distributions

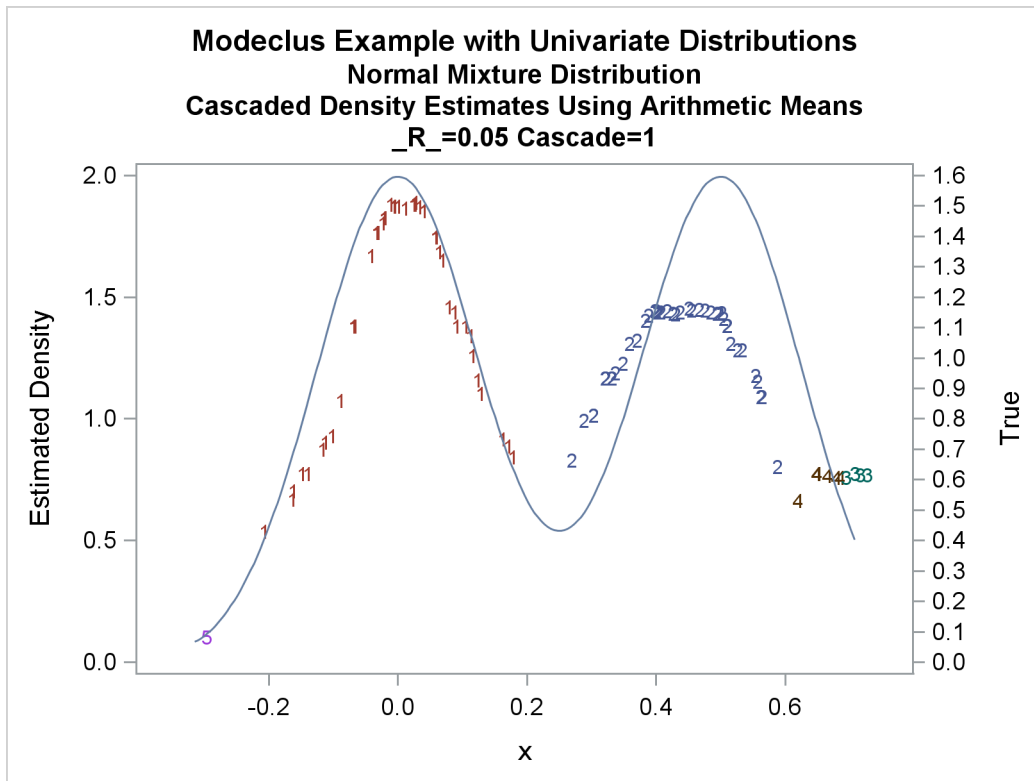
**Modeclus Example with Univariate Distributions**  
**Normal Mixture Distribution**  
**Cascaded Density Estimates Using Arithmetic Means**

**The MODECLUS Procedure**

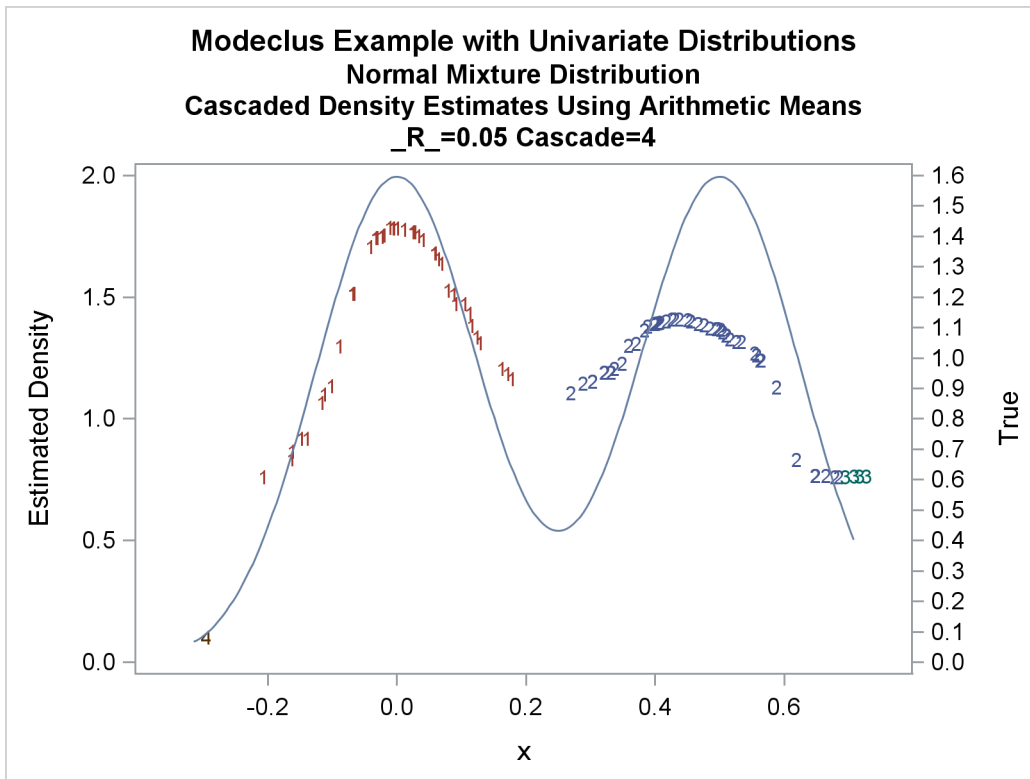
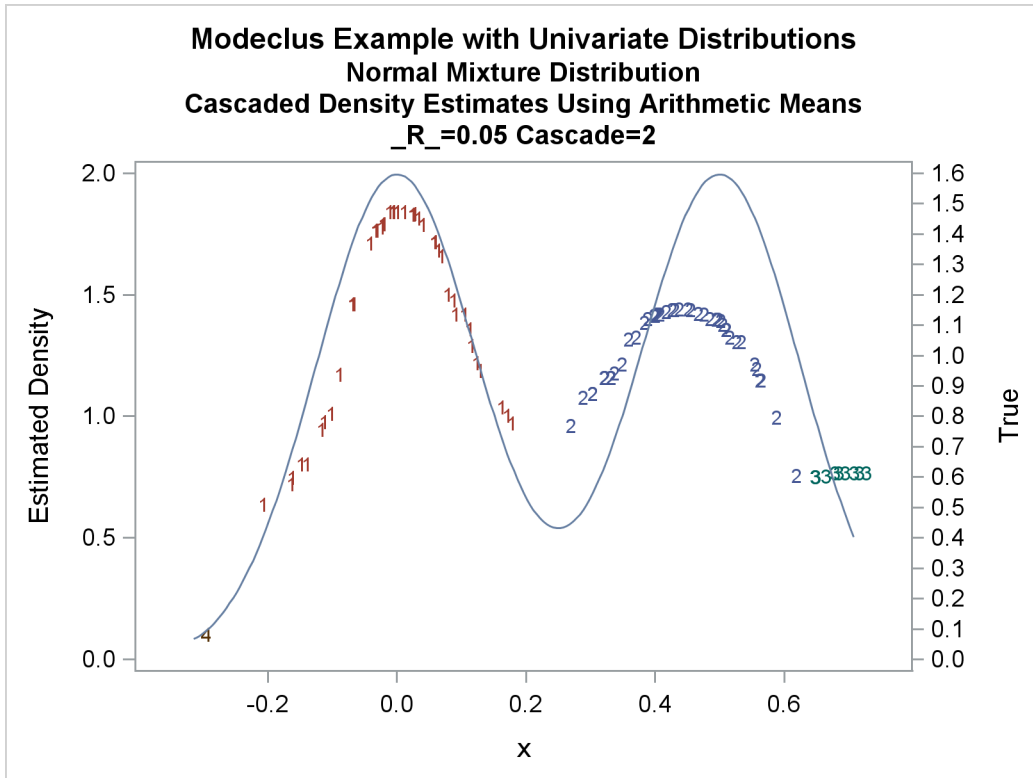
**Cluster Summary**

| R    | Cascade | Number of<br>Clusters | Frequency of<br>Unclassified<br>Objects |
|------|---------|-----------------------|-----------------------------------------|
| 0.05 | 1       | 5                     | 0                                       |
| 0.05 | 2       | 4                     | 0                                       |
| 0.05 | 4       | 4                     | 0                                       |

**Output 60.1.18** True Density, Estimated Density, and Cluster Membership by  $\_R_=0.05$  with Various  $\_CASCAD\_$  Values



Output 60.1.18 continued



---

## Example 60.2: Cluster Analysis of Flying Mileages between Ten American Cities

This example uses distance data and illustrates the use of the TRANSPOSE procedure and the DATA step to fill in the upper triangle of the distance matrix. A data set containing a table of flying mileages between 10 U.S. cities is available in the Sashelp library. The results are displayed in [Output 60.2.1](#) through [Output 60.2.3](#).

The following statements produce [Output 60.2.1](#):

```
title 'Modeclus Analysis of 10 American Cities';
title2 'Based on Flying Mileages';

*-----Fill in Upper Triangle of Distance Matrix-----;
proc transpose data=sashelp.mileages out=tran;
 copy city;
run;

data mileages(type=distance drop=col: _: i);
 merge sashelp.mileages tran;
 array var[10] atlanta--washingtondc;
 array col[10];
 do i = 1 to 10;
 var[i] = sum(var[i], col[i]);
 end;
run;

*-----Clustering with K-Nearest-Neighbor Density Estimates-----;
proc modeclus data=mileages all m=1 k=3;
 id CITY;
run;
```

**Output 60.2.1** Clustering with K-Nearest-Neighbor Density Estimates

| Modeclus Analysis of 10 American Cities<br>Based on Flying Mileages |                 |             |
|---------------------------------------------------------------------|-----------------|-------------|
| The MODECLUS Procedure                                              |                 |             |
| Nearest Neighbor List                                               |                 |             |
| City                                                                | Neighbor        | Distance    |
| Atlanta                                                             | Washington D.C. | 543.0000000 |
|                                                                     | Chicago         | 587.0000000 |
| Chicago                                                             | Atlanta         | 587.0000000 |
|                                                                     | Washington D.C. | 597.0000000 |
| Denver                                                              | Los Angeles     | 831.0000000 |
|                                                                     | Houston         | 879.0000000 |
| Houston                                                             | Atlanta         | 701.0000000 |
|                                                                     | Denver          | 879.0000000 |
| Los Angeles                                                         | San Francisco   | 347.0000000 |
|                                                                     | Denver          | 831.0000000 |
| Miami                                                               | Atlanta         | 604.0000000 |
|                                                                     | Washington D.C. | 923.0000000 |
| New York                                                            | Washington D.C. | 205.0000000 |
|                                                                     | Chicago         | 713.0000000 |
| San Francisco                                                       | Los Angeles     | 347.0000000 |
|                                                                     | Seattle         | 678.0000000 |
| Seattle                                                             | San Francisco   | 678.0000000 |
|                                                                     | Los Angeles     | 959.0000000 |
| Washington D.C.                                                     | New York        | 205.0000000 |
|                                                                     | Atlanta         | 543.0000000 |

**Output 60.2.1** *continued*

| Modeclus Analysis of 10 American Cities<br>Based on Flying Mileages |                 |                                     |                       |                                |            |
|---------------------------------------------------------------------|-----------------|-------------------------------------|-----------------------|--------------------------------|------------|
| The MODECLUS Procedure                                              |                 |                                     |                       |                                |            |
| K=3 METHOD=1                                                        |                 |                                     |                       |                                |            |
| Sums of Density Estimates Within Neighborhood                       |                 |                                     |                       |                                |            |
| Cluster                                                             | City            | Estimated<br>Density                | Same<br>Cluster       | Other<br>Clusters              | Total      |
| 1                                                                   | Atlanta         | 0.00025554                          | 0.0005275             | 0                              | 0.0005275  |
|                                                                     | Chicago         | 0.00025126                          | 0.00053178            | 0                              | 0.00053178 |
|                                                                     | Houston         | 0.00017065                          | 0.00025554            | 0.00017065                     | 0.00042619 |
|                                                                     | Miami           | 0.00016251                          | 0.00053178            | 0                              | 0.00053178 |
|                                                                     | New York        | 0.00021038                          | 0.0005275             | 0                              | 0.0005275  |
|                                                                     | Washington D.C. | 0.00027624                          | 0.00046592            | 0                              | 0.00046592 |
| 2                                                                   | Denver          | 0.00017065                          | 0.00018051            | 0.00017065                     | 0.00035115 |
|                                                                     | Los Angeles     | 0.00018051                          | 0.00039189            | 0                              | 0.00039189 |
|                                                                     | San Francisco   | 0.00022124                          | 0.00033692            | 0                              | 0.00033692 |
|                                                                     | Seattle         | 0.00015641                          | 0.00040174            | 0                              | 0.00040174 |
| Sums of Density Estimates<br>Within Neighborhood                    |                 |                                     |                       |                                |            |
| Cluster                                                             | City            | Cluster<br>Proportion<br>Same/Total |                       |                                |            |
| 1                                                                   | Atlanta         | 1.000                               |                       |                                |            |
|                                                                     | Chicago         | 1.000                               |                       |                                |            |
|                                                                     | Houston         | 0.600                               |                       |                                |            |
|                                                                     | Miami           | 1.000                               |                       |                                |            |
|                                                                     | New York        | 1.000                               |                       |                                |            |
|                                                                     | Washington D.C. | 1.000                               |                       |                                |            |
| 2                                                                   | Denver          | 0.514                               |                       |                                |            |
|                                                                     | Los Angeles     | 1.000                               |                       |                                |            |
|                                                                     | San Francisco   | 1.000                               |                       |                                |            |
|                                                                     | Seattle         | 1.000                               |                       |                                |            |
| Boundary Objects      -Cluster Proportions-                         |                 |                                     |                       |                                |            |
| City                                                                | Density         | Cluster                             | 1                     | 2                              |            |
| Denver                                                              | 0.0001706485    | 2                                   | 0.486                 | 0.514                          |            |
| Houston                                                             | 0.0001706485    | 1                                   | 0.600                 | 0.400                          |            |
| Cluster Statistics                                                  |                 |                                     |                       |                                |            |
| Cluster                                                             | Frequency       | Maximum<br>Estimated<br>Density     | Boundary<br>Frequency | Estimated<br>Saddle<br>Density |            |
| 1                                                                   | 6               | 0.00027624                          | 1                     | 0.00017065                     |            |
| 2                                                                   | 4               | 0.00022124                          | 1                     | 0.00017065                     |            |

**Output 60.2.1** *continued*

```

Modeclus Analysis of 10 American Cities
Based on Flying Mileages

The MODECLUS Procedure

Cluster Summary
 Frequency of
 Number of Unclassified
 K Clusters Objects

 3 2 0

```

The following statements produce **Output 60.2.2**:

```

*-----Clustering with Uniform-Kernel Density Estimates-----;
proc modeclus data=mileages all m=1 r=600 800;
 id CITY;
run;

```

**Output 60.2.2** Clustering with Uniform-Kernel Density Estimates

```

Modeclus Analysis of 10 American Cities
Based on Flying Mileages

The MODECLUS Procedure

Nearest Neighbor List
City Neighbor Distance

Atlanta Washington D.C. 543.0000000
 Chicago 587.0000000
 Miami 604.0000000
 Houston 701.0000000
 New York 748.0000000

Chicago Atlanta 587.0000000
 Washington D.C. 597.0000000
 New York 713.0000000

Houston Atlanta 701.0000000

Los Angeles San Francisco 347.0000000

Miami Atlanta 604.0000000

New York Washington D.C. 205.0000000
 Chicago 713.0000000
 Atlanta 748.0000000

San Francisco Los Angeles 347.0000000
 Seattle 678.0000000

Seattle San Francisco 678.0000000

Washington D.C. New York 205.0000000
 Atlanta 543.0000000
 Chicago 597.0000000

```

**Output 60.2.2** continued

| Modeclus Analysis of 10 American Cities<br>Based on Flying Mileages |                 |                                     |                 |                   |            |
|---------------------------------------------------------------------|-----------------|-------------------------------------|-----------------|-------------------|------------|
| The MODECLUS Procedure                                              |                 |                                     |                 |                   |            |
| R=600 METHOD=1                                                      |                 |                                     |                 |                   |            |
| Sums of Density Estimates Within Neighborhood                       |                 |                                     |                 |                   |            |
| Cluster                                                             | City            | Estimated<br>Density                | Same<br>Cluster | Other<br>Clusters | Total      |
| 1                                                                   | Atlanta         | 0.00025                             | 0.00058333      | 0                 | 0.00058333 |
|                                                                     | Chicago         | 0.00025                             | 0.00058333      | 0                 | 0.00058333 |
|                                                                     | New York        | 0.00016667                          | 0.00033333      | 0                 | 0.00033333 |
|                                                                     | Washington D.C. | 0.00033333                          | 0.00066667      | 0                 | 0.00066667 |
| 2                                                                   | Los Angeles     | 0.00016667                          | 0.00016667      | 0                 | 0.00016667 |
|                                                                     | San Francisco   | 0.00016667                          | 0.00016667      | 0                 | 0.00016667 |
| 3                                                                   | Denver          | 0.00008333                          | 0               | 0                 | 0          |
| 4                                                                   | Houston         | 0.00008333                          | 0               | 0                 | 0          |
| 5                                                                   | Miami           | 0.00008333                          | 0               | 0                 | 0          |
| 6                                                                   | Seattle         | 0.00008333                          | 0               | 0                 | 0          |
| Sums of Density Estimates<br>Within Neighborhood                    |                 |                                     |                 |                   |            |
| Cluster                                                             | City            | Cluster<br>Proportion<br>Same/Total |                 |                   |            |
| 1                                                                   | Atlanta         | 1.000                               |                 |                   |            |
|                                                                     | Chicago         | 1.000                               |                 |                   |            |
|                                                                     | New York        | 1.000                               |                 |                   |            |
|                                                                     | Washington D.C. | 1.000                               |                 |                   |            |
| 2                                                                   | Los Angeles     | 1.000                               |                 |                   |            |
|                                                                     | San Francisco   | 1.000                               |                 |                   |            |
| 3                                                                   | Denver          | .                                   |                 |                   |            |
| 4                                                                   | Houston         | .                                   |                 |                   |            |
| 5                                                                   | Miami           | .                                   |                 |                   |            |
| 6                                                                   | Seattle         | .                                   |                 |                   |            |



**Output 60.2.2** *continued*

| No Boundary Objects |           |                                 |                       |                                |
|---------------------|-----------|---------------------------------|-----------------------|--------------------------------|
| Cluster Statistics  |           |                                 |                       |                                |
| Cluster             | Frequency | Maximum<br>Estimated<br>Density | Boundary<br>Frequency | Estimated<br>Saddle<br>Density |
| 1                   | 4         | 0.00033333                      | 0                     | .                              |
| 2                   | 2         | 0.00016667                      | 0                     | .                              |
| 3                   | 1         | 0.00008333                      | 0                     | .                              |
| 4                   | 1         | 0.00008333                      | 0                     | .                              |
| 5                   | 1         | 0.00008333                      | 0                     | .                              |
| 6                   | 1         | 0.00008333                      | 0                     | .                              |

**Output 60.2.2** *continued*

| Modeclus Analysis of 10 American Cities<br>Based on Flying Mileages |                 |                      |                 |                   |           |
|---------------------------------------------------------------------|-----------------|----------------------|-----------------|-------------------|-----------|
| The MODECLUS Procedure                                              |                 |                      |                 |                   |           |
| R=800 METHOD=1                                                      |                 |                      |                 |                   |           |
| Sums of Density Estimates Within Neighborhood                       |                 |                      |                 |                   |           |
| Cluster                                                             | City            | Estimated<br>Density | Same<br>Cluster | Other<br>Clusters | Total     |
| 1                                                                   | Atlanta         | 0.000375             | 0.001           | 0                 | 0.001     |
|                                                                     | Chicago         | 0.00025              | 0.000875        | 0                 | 0.000875  |
|                                                                     | Houston         | 0.000125             | 0.000375        | 0                 | 0.000375  |
|                                                                     | Miami           | 0.000125             | 0.000375        | 0                 | 0.000375  |
|                                                                     | New York        | 0.00025              | 0.000875        | 0                 | 0.000875  |
|                                                                     | Washington D.C. | 0.00025              | 0.000875        | 0                 | 0.000875  |
| 2                                                                   | Los Angeles     | 0.000125             | 0.0001875       | 0                 | 0.0001875 |
|                                                                     | San Francisco   | 0.0001875            | 0.00025         | 0                 | 0.00025   |
|                                                                     | Seattle         | 0.000125             | 0.0001875       | 0                 | 0.0001875 |
| 3                                                                   | Denver          | 0.0000625            | 0               | 0                 | 0         |

| Sums of Density Estimates<br>Within Neighborhood |                 |                                     |  |
|--------------------------------------------------|-----------------|-------------------------------------|--|
| Cluster                                          | City            | Cluster<br>Proportion<br>Same/Total |  |
| 1                                                | Atlanta         | 1.000                               |  |
|                                                  | Chicago         | 1.000                               |  |
|                                                  | Houston         | 1.000                               |  |
|                                                  | Miami           | 1.000                               |  |
|                                                  | New York        | 1.000                               |  |
|                                                  | Washington D.C. | 1.000                               |  |
| 2                                                | Los Angeles     | 1.000                               |  |
|                                                  | San Francisco   | 1.000                               |  |
|                                                  | Seattle         | 1.000                               |  |
| 3                                                | Denver          | .                                   |  |

No Boundary Objects

| Cluster Statistics |           |                                 |                       |                                |
|--------------------|-----------|---------------------------------|-----------------------|--------------------------------|
| Cluster            | Frequency | Maximum<br>Estimated<br>Density | Boundary<br>Frequency | Estimated<br>Saddle<br>Density |
| 1                  | 6         | 0.000375                        | 0                     | .                              |
| 2                  | 3         | 0.0001875                       | 0                     | .                              |
| 3                  | 1         | 0.0000625                       | 0                     | .                              |

**Output 60.2.2** *continued*

| Modeclus Analysis of 10 American Cities<br>Based on Flying Mileages |                       |                                         |
|---------------------------------------------------------------------|-----------------------|-----------------------------------------|
| The MODECLUS Procedure                                              |                       |                                         |
| Cluster Summary                                                     |                       |                                         |
| R                                                                   | Number of<br>Clusters | Frequency of<br>Unclassified<br>Objects |
| 600                                                                 | 6                     | 0                                       |
| 800                                                                 | 3                     | 0                                       |

The following statements produce [Output 60.2.3](#):

```
*-----Clustering Neighborhoods Extended to Nearest Neighbor-----;
proc modeclus data=mileages list m=1 ck=2 r=600 800;
 id CITY;
run;
```

**Output 60.2.3** Uniform-Kernel Density Estimates, Clustering Neighborhoods Extended to Nearest Neighbor

| Modeclus Analysis of 10 American Cities<br>Based on Flying Mileages |                 |                                     |                       |                                |            |
|---------------------------------------------------------------------|-----------------|-------------------------------------|-----------------------|--------------------------------|------------|
| The MODECLUS Procedure<br>CK=2 R=600 METHOD=1                       |                 |                                     |                       |                                |            |
| Sums of Density Estimates Within Neighborhood                       |                 |                                     |                       |                                |            |
| Cluster                                                             | City            | Estimated<br>Density                | Same<br>Cluster       | Other<br>Clusters              | Total      |
| 1                                                                   | Atlanta         | 0.00025                             | 0.00058333            | 0                              | 0.00058333 |
|                                                                     | Chicago         | 0.00025                             | 0.00058333            | 0                              | 0.00058333 |
|                                                                     | Houston         | 0.00008333                          | 0.00025               | 0                              | 0.00025    |
|                                                                     | Miami           | 0.00008333                          | 0.00025               | 0                              | 0.00025    |
|                                                                     | New York        | 0.00016667                          | 0.00033333            | 0                              | 0.00033333 |
|                                                                     | Washington D.C. | 0.00033333                          | 0.00066667            | 0                              | 0.00066667 |
| 2                                                                   | Denver          | 0.00008333                          | 0.00016667            | 0                              | 0.00016667 |
|                                                                     | Los Angeles     | 0.00016667                          | 0.00016667            | 0                              | 0.00016667 |
|                                                                     | San Francisco   | 0.00016667                          | 0.00016667            | 0                              | 0.00016667 |
|                                                                     | Seattle         | 0.00008333                          | 0.00016667            | 0                              | 0.00016667 |
| Sums of Density Estimates<br>Within Neighborhood                    |                 |                                     |                       |                                |            |
| Cluster                                                             | City            | Cluster<br>Proportion<br>Same/Total |                       |                                |            |
| 1                                                                   | Atlanta         | 1.000                               |                       |                                |            |
|                                                                     | Chicago         | 1.000                               |                       |                                |            |
|                                                                     | Houston         | 1.000                               |                       |                                |            |
|                                                                     | Miami           | 1.000                               |                       |                                |            |
|                                                                     | New York        | 1.000                               |                       |                                |            |
|                                                                     | Washington D.C. | 1.000                               |                       |                                |            |
| 2                                                                   | Denver          | 1.000                               |                       |                                |            |
|                                                                     | Los Angeles     | 1.000                               |                       |                                |            |
|                                                                     | San Francisco   | 1.000                               |                       |                                |            |
|                                                                     | Seattle         | 1.000                               |                       |                                |            |
| Cluster Statistics                                                  |                 |                                     |                       |                                |            |
| Cluster                                                             | Frequency       | Maximum<br>Estimated<br>Density     | Boundary<br>Frequency | Estimated<br>Saddle<br>Density |            |
| 1                                                                   | 6               | 0.00033333                          | 0                     | .                              |            |
| 2                                                                   | 4               | 0.00016667                          | 0                     | .                              |            |

**Output 60.2.3** *continued*

| Modeclus Analysis of 10 American Cities<br>Based on Flying Mileages |                 |                                     |                       |                                |           |
|---------------------------------------------------------------------|-----------------|-------------------------------------|-----------------------|--------------------------------|-----------|
| The MODECLUS Procedure                                              |                 |                                     |                       |                                |           |
| CK=2 R=800 METHOD=1                                                 |                 |                                     |                       |                                |           |
| Sums of Density Estimates Within Neighborhood                       |                 |                                     |                       |                                |           |
| Cluster                                                             | City            | Estimated<br>Density                | Same<br>Cluster       | Other<br>Clusters              | Total     |
| 1                                                                   | Atlanta         | 0.000375                            | 0.001                 | 0                              | 0.001     |
|                                                                     | Chicago         | 0.00025                             | 0.000875              | 0                              | 0.000875  |
|                                                                     | Houston         | 0.000125                            | 0.000375              | 0                              | 0.000375  |
|                                                                     | Miami           | 0.000125                            | 0.000375              | 0                              | 0.000375  |
|                                                                     | New York        | 0.00025                             | 0.000875              | 0                              | 0.000875  |
|                                                                     | Washington D.C. | 0.00025                             | 0.000875              | 0                              | 0.000875  |
| 2                                                                   | Denver          | 0.0000625                           | 0.000125              | 0                              | 0.000125  |
|                                                                     | Los Angeles     | 0.000125                            | 0.0001875             | 0                              | 0.0001875 |
|                                                                     | San Francisco   | 0.0001875                           | 0.00025               | 0                              | 0.00025   |
|                                                                     | Seattle         | 0.000125                            | 0.0001875             | 0                              | 0.0001875 |
| Sums of Density Estimates<br>Within Neighborhood                    |                 |                                     |                       |                                |           |
| Cluster                                                             | City            | Cluster<br>Proportion<br>Same/Total |                       |                                |           |
| 1                                                                   | Atlanta         | 1.000                               |                       |                                |           |
|                                                                     | Chicago         | 1.000                               |                       |                                |           |
|                                                                     | Houston         | 1.000                               |                       |                                |           |
|                                                                     | Miami           | 1.000                               |                       |                                |           |
|                                                                     | New York        | 1.000                               |                       |                                |           |
|                                                                     | Washington D.C. | 1.000                               |                       |                                |           |
| 2                                                                   | Denver          | 1.000                               |                       |                                |           |
|                                                                     | Los Angeles     | 1.000                               |                       |                                |           |
|                                                                     | San Francisco   | 1.000                               |                       |                                |           |
|                                                                     | Seattle         | 1.000                               |                       |                                |           |
| Cluster Statistics                                                  |                 |                                     |                       |                                |           |
| Cluster                                                             | Frequency       | Maximum<br>Estimated<br>Density     | Boundary<br>Frequency | Estimated<br>Saddle<br>Density |           |
| 1                                                                   | 6               | 0.000375                            | 0                     | .                              |           |
| 2                                                                   | 4               | 0.0001875                           | 0                     | .                              |           |

## Output 60.2.3 continued

| Modeclus Analysis of 10 American Cities<br>Based on Flying Mileages |    |                       |                                         |
|---------------------------------------------------------------------|----|-----------------------|-----------------------------------------|
| The MODECLUS Procedure                                              |    |                       |                                         |
| Cluster Summary                                                     |    |                       |                                         |
| R                                                                   | CK | Number of<br>Clusters | Frequency of<br>Unclassified<br>Objects |
| 600                                                                 | 2  | 2                     | 0                                       |
| 800                                                                 | 2  | 2                     | 0                                       |

---

**Example 60.3: Cluster Analysis with Significance Tests**

This example uses artificial data containing two clusters. One cluster is from a circular bivariate normal distribution. The other is a ring-shaped cluster that completely surrounds the first cluster. Without significance tests, the ring is divided into several sample clusters for any degree of smoothing that yields reasonable density estimates. The JOIN= option puts the ring back together. [Output 60.3.1](#) displays a short summary generated from the first PROC MODECLUS statement. [Output 60.3.2](#) contains a series of tables produced from the second PROC MODECLUS statement. The lack of  $p$ -value in the JOIN= option makes joining continue until only one cluster remains (see the description of the JOIN= option). The cluster memberships are then plotted as displayed in [Output 60.3.1](#) through [Output 60.3.8](#).

The following statements produce [Output 60.3.1](#) through [Output 60.3.8](#):

```

title 'Modeclus Analysis with the JOIN= option';
title2 'A Normal Cluster Surrounded by a Ring Cluster';

data circle; keep x y;
 c=1;
 do n=1 to 30;
 x=rannor(5);
 y=rannor(5);
 output;
 end;

 c=2;
 do n=1 to 300;
 x=rannor(5);
 y=rannor(5);
 z=rannor(5)+8;
 l=z/sqrt(x**2+y**2);
 x=x*l;
 y=y*l;
 output;
 end;
run;

```

```

proc modeclus data=circle m=1 r=1 to 3.5 by .25 join=20 short;
run;

proc modeclus data=circle m=1 r=2.5 join out=out;
run;

proc sgplot data=out noautolegend;
 yaxis values=(-10 to 10 by 5);
 xaxis values=(-15 to 15 by 5);
 scatter y=y x=x / group=cluster Markerchar=cluster;
 by _NJOIN_;
run;

```

**Output 60.3.1** Significance Tests with the JOIN=20 and SHORT Options

| Modeclus Analysis with the JOIN= option       |                                 |                    |                       |                                         |
|-----------------------------------------------|---------------------------------|--------------------|-----------------------|-----------------------------------------|
| A Normal Cluster Surrounded by a Ring Cluster |                                 |                    |                       |                                         |
| The MODECLUS Procedure                        |                                 |                    |                       |                                         |
| Cluster Summary                               |                                 |                    |                       |                                         |
| R                                             | Number of<br>Clusters<br>Joined | Maximum<br>P-value | Number of<br>Clusters | Frequency of<br>Unclassified<br>Objects |
| 1                                             | 36                              | 0.9339             | 1                     | 301                                     |
| 1.25                                          | 20                              | 0.7131             | 1                     | 301                                     |
| 1.5                                           | 10                              | 0.3296             | 1                     | 300                                     |
| 1.75                                          | 5                               | 0.1990             | 2                     | 0                                       |
| 2                                             | 5                               | 0.0683             | 2                     | 0                                       |
| 2.25                                          | 3                               | 0.0504             | 2                     | 0                                       |
| 2.5                                           | 4                               | 0.0301             | 2                     | 0                                       |
| 2.75                                          | 3                               | 0.0585             | 2                     | 0                                       |
| 3                                             | 5                               | 0.0003             | 1                     | 0                                       |
| 3.25                                          | 4                               | 0.1923             | 2                     | 0                                       |
| 3.5                                           | 4                               | 0.0000             | 1                     | 0                                       |

**Output 60.3.2** Significance Tests with the JOIN Option

```

Modeclus Analysis with the JOIN= option
A Normal Cluster Surrounded by a Ring Cluster

The MODECLUS Procedure
R=2.5 METHOD=1

Cluster Statistics
Maximum Estimated Boundary Estimated
Cluster Frequency Density Frequency Saddle Density

1 103 0.00617328 22 0.00308664
2 71 0.00571029 20 0.0043213
3 53 0.00509296 18 0.00401263
4 45 0.00478429 19 0.00354964
5 30 0.00462996 0 .
6 28 0.00370397 17 0.00354964

-----Saddle Test: Version 92.7-----
Mode Saddle Overlap Approx
Cluster Count Count Count Z P-value

1 39 19 0 2.495 0.5055
2 36 27 9 1.193 0.999
3 32 25 10 0.986 0.9999
4 30 22 14 1.429 0.9924
5 29 0 . 3.611 0.0301
6 23 22 9 0.000 1

Cluster 6 with P-value 1.0000 will be joined to cluster 4.

Cluster Statistics
Maximum Estimated Boundary Estimated
Cluster Frequency Density Frequency Saddle Density

1 103 0.00617328 22 0.00308664
2 71 0.00571029 20 0.0043213
3 53 0.00509296 18 0.00401263
4 73 0.00478429 13 0.00293231
5 30 0.00462996 0 .

-----Saddle Test: Version 92.7-----
Mode Saddle Overlap Approx
Cluster Count Count Count Z P-value

1 39 19 0 2.495 0.5055
2 36 27 9 1.193 0.999
3 32 25 10 0.986 0.9999
4 30 18 0 1.588 0.9778
5 29 0 . 3.611 0.0301

```



## Output 60.3.2 continued

Cluster 3 with P-value 0.9999 will be joined to cluster 1.

| Cluster Statistics |           |                                 |                       |                                |
|--------------------|-----------|---------------------------------|-----------------------|--------------------------------|
| Cluster            | Frequency | Maximum<br>Estimated<br>Density | Boundary<br>Frequency | Estimated<br>Saddle<br>Density |
| 1                  | 156       | 0.00617328                      | 17                    | 0.00246931                     |
| 2                  | 71        | 0.00571029                      | 20                    | 0.0043213                      |
| 3                  | 73        | 0.00478429                      | 13                    | 0.00293231                     |
| 4                  | 30        | 0.00462996                      | 0                     | .                              |

-----Saddle Test: Version 92.7-----

| Cluster | Mode<br>Count | Saddle<br>Count | Overlap<br>Count | Z     | Approx<br>P-value |
|---------|---------------|-----------------|------------------|-------|-------------------|
| 1       | 39            | 15              | 0                | 3.130 | 0.1318            |
| 2       | 36            | 27              | 9                | 1.193 | 0.999             |
| 3       | 30            | 18              | 0                | 1.588 | 0.9778            |
| 4       | 29            | 0               | .                | 3.611 | 0.0301            |

Cluster 2 with P-value 0.9990 will be joined to cluster 3.

| Cluster Statistics |           |                                 |                       |                                |
|--------------------|-----------|---------------------------------|-----------------------|--------------------------------|
| Cluster            | Frequency | Maximum<br>Estimated<br>Density | Boundary<br>Frequency | Estimated<br>Saddle<br>Density |
| 1                  | 156       | 0.00617328                      | 17                    | 0.00246931                     |
| 2                  | 144       | 0.00571029                      | 14                    | 0.00293231                     |
| 3                  | 30        | 0.00462996                      | 0                     | .                              |

-----Saddle Test: Version 92.7-----

| Cluster | Mode<br>Count | Saddle<br>Count | Overlap<br>Count | Z     | Approx<br>P-value |
|---------|---------------|-----------------|------------------|-------|-------------------|
| 1       | 39            | 15              | 0                | 3.130 | 0.1318            |
| 2       | 36            | 18              | 0                | 2.313 | 0.6447            |
| 3       | 29            | 0               | .                | 3.611 | 0.0301            |

Output 60.3.2 continued

Cluster 2 with P-value 0.6447 will be joined to cluster 1.

| Cluster Statistics |           |            |           |           |
|--------------------|-----------|------------|-----------|-----------|
| Cluster            | Frequency | Maximum    | Boundary  | Estimated |
|                    |           | Estimated  |           | Saddle    |
|                    |           | Density    | Frequency | Density   |
| 1                  | 300       | 0.00617328 | 0         | .         |
| 2                  | 30        | 0.00462996 | 0         | .         |

-----Saddle Test: Version 92.7-----

| Cluster | Mode | Saddle | Overlap | Z     | Approx  |
|---------|------|--------|---------|-------|---------|
|         |      | Count  | Count   |       | P-value |
|         |      | Count  | Count   |       |         |
| 1       | 39   | 0      | .       | 4.246 | 0.0026  |
| 2       | 29   | 0      | .       | 3.611 | 0.0301  |

Cluster 2 with P-value 0.0301 will be dissolved.

| Cluster Statistics |           |            |           |           |
|--------------------|-----------|------------|-----------|-----------|
| Cluster            | Frequency | Maximum    | Boundary  | Estimated |
|                    |           | Estimated  |           | Saddle    |
|                    |           | Density    | Frequency | Density   |
| 1                  | 300       | 0.00617328 | 0         | .         |

-----Saddle Test: Version 92.7-----

| Cluster | Mode | Saddle | Overlap | Z     | Approx  |
|---------|------|--------|---------|-------|---------|
|         |      | Count  | Count   |       | P-value |
|         |      | Count  | Count   |       |         |
| 1       | 39   | 0      | .       | 4.246 | 0.0026  |

30 observations were unassigned.

Cluster 1 with P-value 0.0026 will be dissolved.

**Output 60.3.2** continued

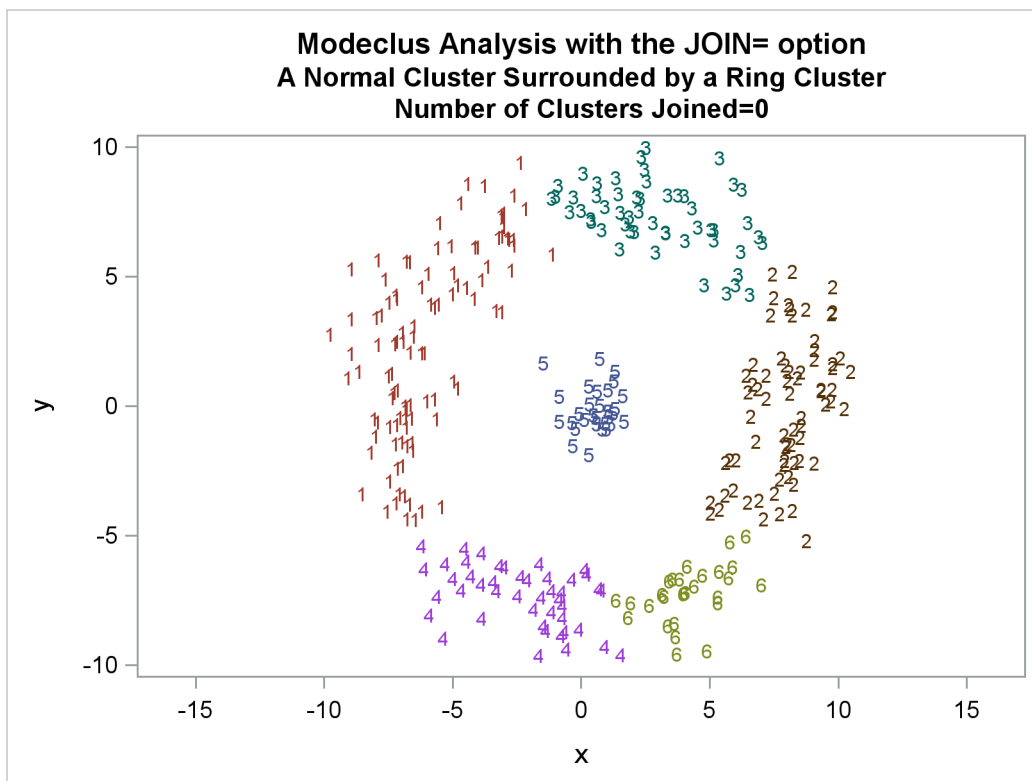
**Modeclus Analysis with the JOIN= option  
A Normal Cluster Surrounded by a Ring Cluster**

**The MODECLUS Procedure**

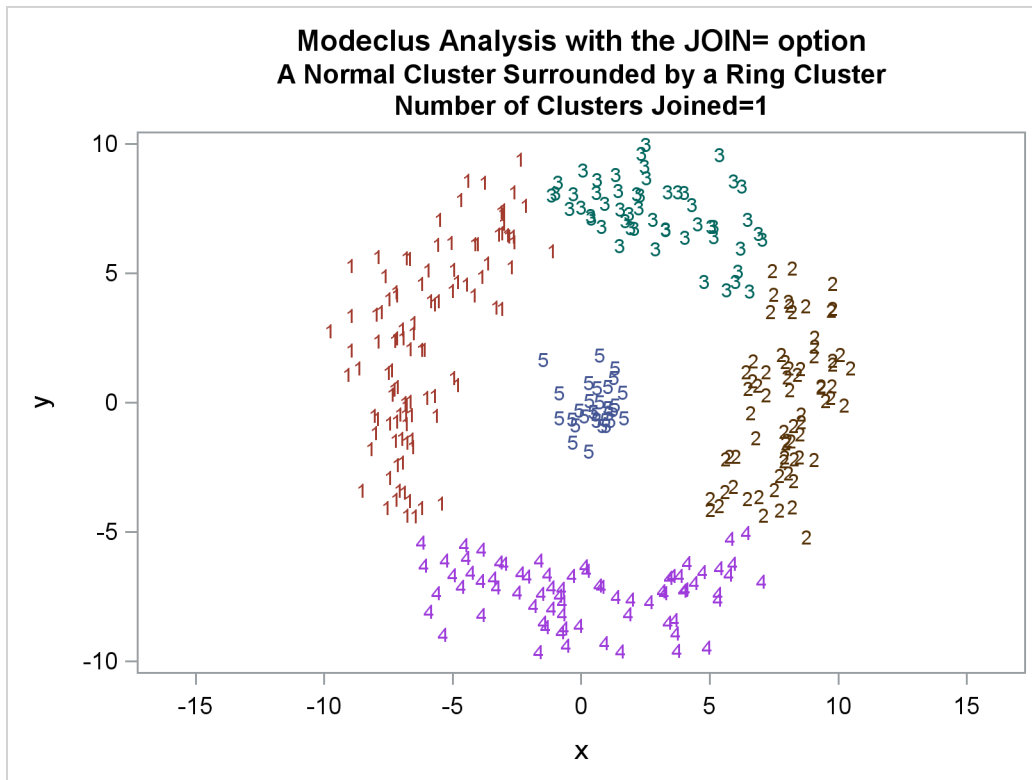
**Cluster Summary**

| R   | Number of Clusters Joined | Maximum P-value | Number of Clusters | Frequency of Unclassified Objects |
|-----|---------------------------|-----------------|--------------------|-----------------------------------|
| 2.5 | 0                         | 1.0000          | 6                  | 0                                 |
| 2.5 | 1                         | 0.9999          | 5                  | 0                                 |
| 2.5 | 2                         | 0.9990          | 4                  | 0                                 |
| 2.5 | 3                         | 0.6447          | 3                  | 0                                 |
| 2.5 | 4                         | 0.0301          | 2                  | 0                                 |
| 2.5 | 5                         | 0.0026          | 1                  | 30                                |

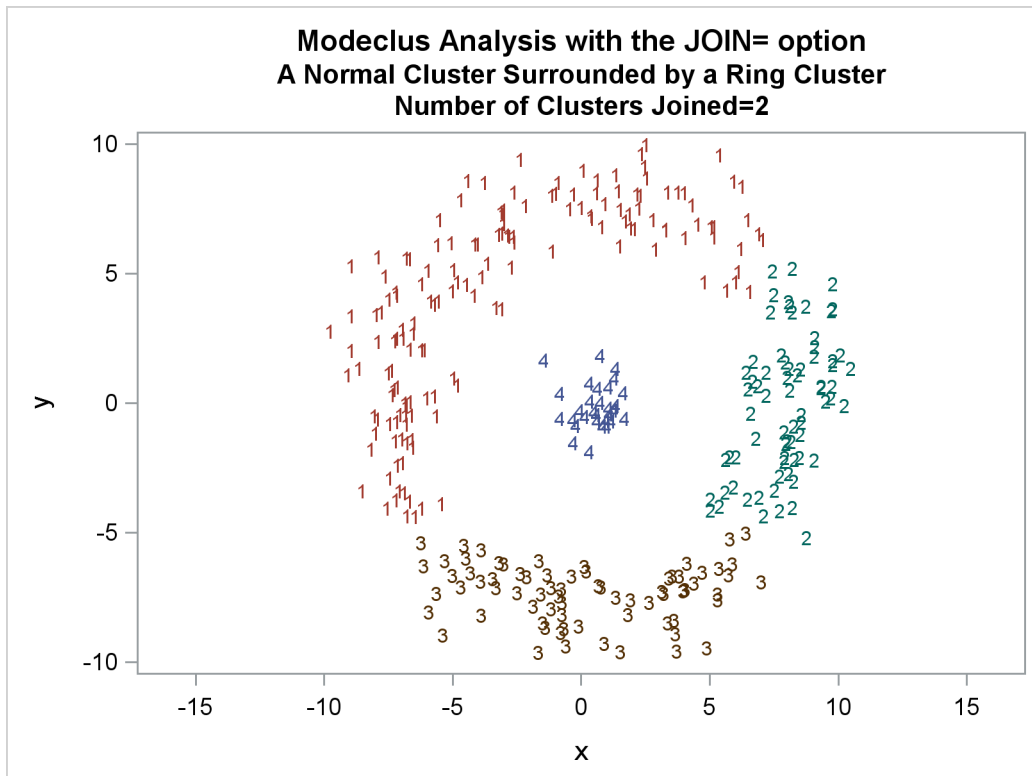
**Output 60.3.3** Cluster Memberships When Number of Clusters Joined=0



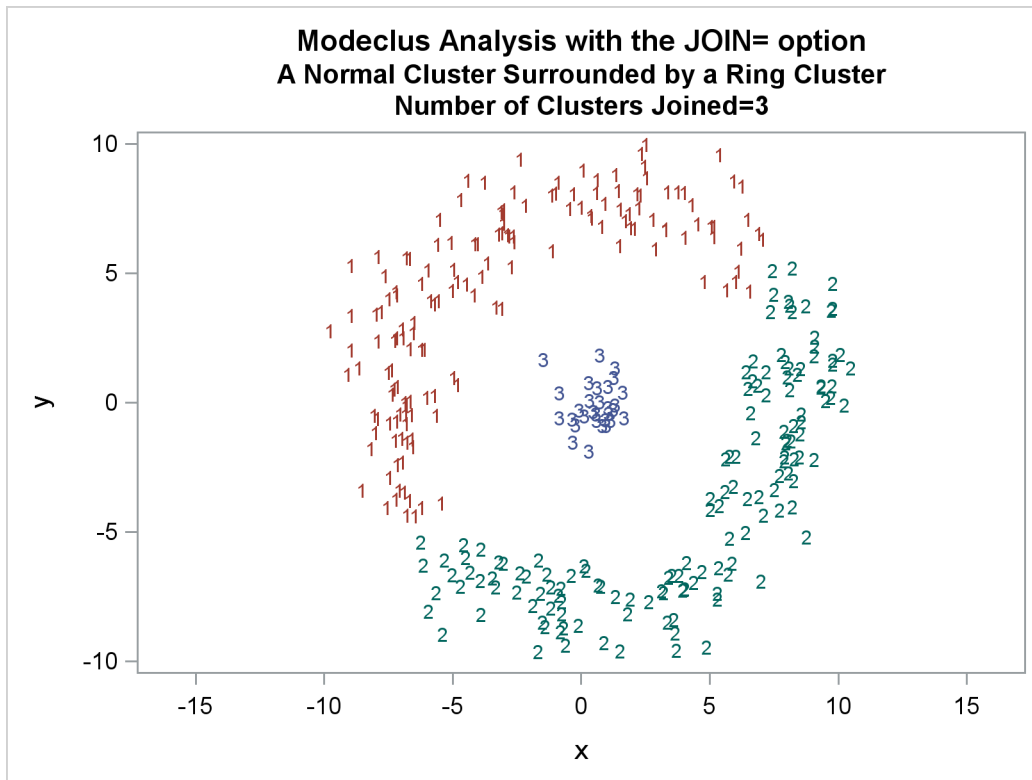
**Output 60.3.4** Cluster Memberships When Number of Clusters Joined=1



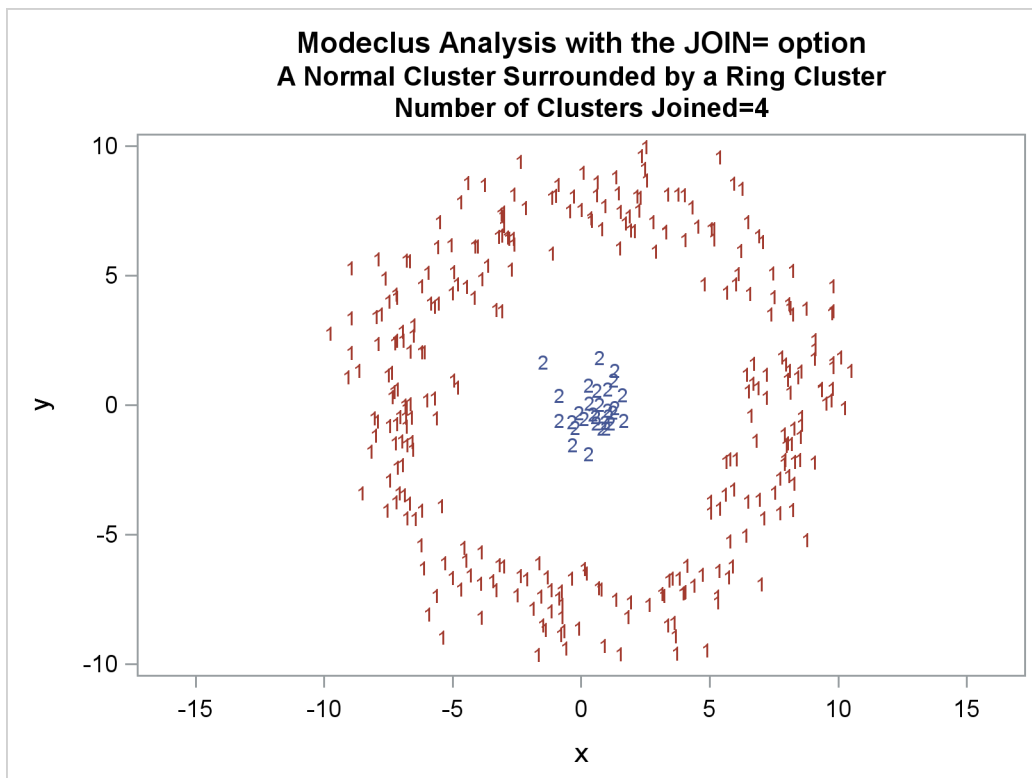
**Output 60.3.5** Cluster Memberships When Number of Clusters Joined=2

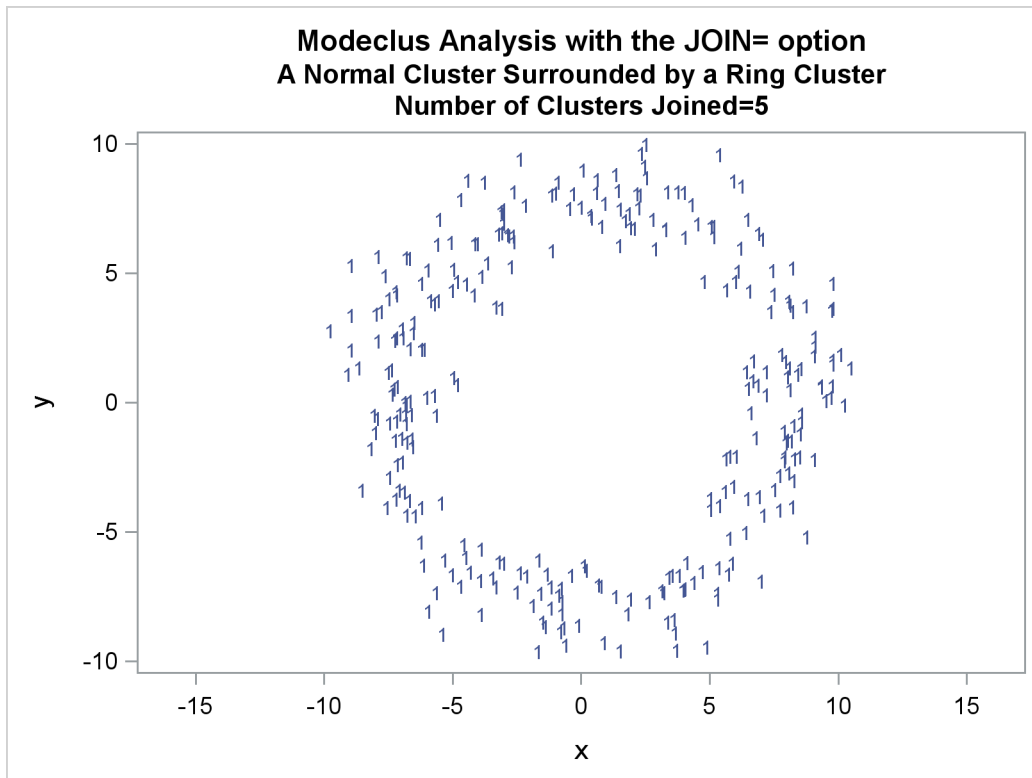


**Output 60.3.6** Cluster Memberships When Number of Clusters Joined=3



**Output 60.3.7** Cluster Memberships When Number of Clusters Joined=4



**Output 60.3.8** Cluster Memberships When Number of Clusters Joined=5**Example 60.4: Cluster Analysis: Hertzsprung-Russell Plot**

This example uses computer-generated data to mimic a Hertzsprung-Russell plot (Struve and Zeberg's 1962, p. 259) of the temperature and luminosity of stars. The data are plotted and displayed in [Output 60.4.1](#). It appears that there are two main groups of stars and a collection of isolated stars. The long straggling group of points appearing diagonally across the figure represents the main group of stars; the more compact group in the top-right corner contains giant stars. The JOIN= option is specified at a 0.05 significance level with various smoothing parameters. The CK=5 option is specified in order to prevent the numerous outliers from forming separate clusters. The results from PROC MODECLUS is displayed in [Output 60.4.2](#). The cluster memberships are then plotted by PROC SGPLOT, as displayed in [Output 60.4.3](#) through [Output 60.4.5](#).

Note that the graphic output from PROC SGPLOT in [Output 60.4.3](#) is not available when `_R_ = 2.5` because only one cluster remains after joining at a 5% significance level, and the results are not written to the OUT= data set. See the description of the JOIN= option). for more information.

The following statements produce [Output 60.4.1](#) through [Output 60.4.5](#):

```

title 'Hertzprung-Russell Plot of Visible Stars';
title2 'Computer-Generated Simulated Data';

data hr;
 input x y @@;
 label x='-Temperature'
 y='-Luminosity';
 datalines;
1.0 12.8 0.9 13.7 0.9 12.9 1.0 12.3 1.0 12.2 2.6 10.9
2.4 10.9 2.5 11.2 2.3 11.5 2.6 12.0 2.4 12.1 2.3 10.9
2.6 11.5 2.5 11.9 2.4 11.0 3.4 11.1 3.3 11.2 3.4 11.1
3.4 9.9 3.2 10.4 3.5 10.8 3.4 11.0 3.3 11.2 3.3 10.8
3.5 10.0 3.5 10.2 3.4 10.2 3.6 10.6 3.7 10.4 3.7 10.1
3.4 10.7 3.4 10.8 3.3 11.0 3.6 10.8 3.5 10.1 4.5 10.3
4.6 9.4 4.3 10.3 4.6 9.4 4.4 9.9 4.5 10.4 4.4 9.9
4.6 9.4 4.4 10.7 4.4 9.3 4.4 9.5 4.1 10.6 4.4 10.6
4.5 10.3 4.4 10.0 4.2 9.8 4.5 9.5 4.2 13.4 4.6 10.4
4.5 9.8 5.8 8.8 5.6 8.4 5.6 13.9 5.7 9.5 5.6 14.5
5.6 9.2 5.7 8.7 5.7 9.4 5.7 9.3 5.6 9.4 5.8 9.8
5.5 8.8 5.8 8.9 5.7 9.4 5.6 12.1 5.4 10.1 5.8 9.3
5.9 9.0 5.7 10.0 5.6 9.3 6.6 8.6 6.7 8.5 6.7 12.5

 ... more lines ...

26.4 14.1 26.6 14.2 27.5 13.7 27.6 14.4 27.8 14.0 27.4 14.7
25.8 13.5 25.6 13.6 26.8 14.4 26.4 19.0 26.0 13.4 27.3 14.0
27.5 14.3 27.4 14.5 26.3 13.8 26.9 13.7 26.3 13.7 27.7 14.3
27.3 14.1 28.3 14.2 17.4 15.5 13.8 15.2 12.0 11.6 14.1 12.8
17.1 10.2 16.9 15.4 18.5 12.6 14.2 16.1 23.2 6.6 11.4 12.4
20.4 11.7 20.9 8.1 18.9 13.7 16.9 9.7 15.5 9.9 18.3 14.2
19.3 13.7 17.0 12.9 10.1 11.6 17.9 13.5 14.3 1.4 13.1 -0.8
8.1 -0.9 20.0 7.0 21.0 8.5 15.6 13.2

;

proc sgplot data=hr;
 scatter y=y x=x;
run;

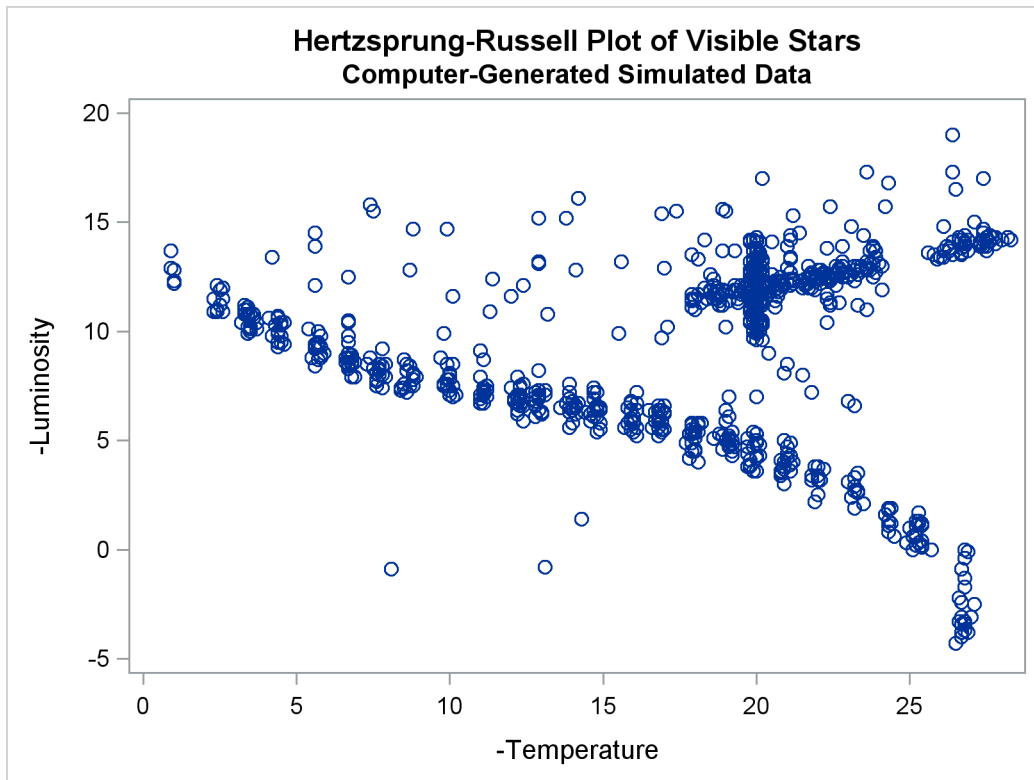
proc modeclus data=hr m=1 r=1 1.5 2 2.5 ck=5
 join=.05 short out=out;
run;

title2 'MODECLUS Analysis';

proc sgplot data=out;
 scatter y=y x=x/group=cluster;
 by _R_;
run;

```

Output 60.4.1 Scatter Plot of Data



Output 60.4.2 Results from PROC MODECLUS

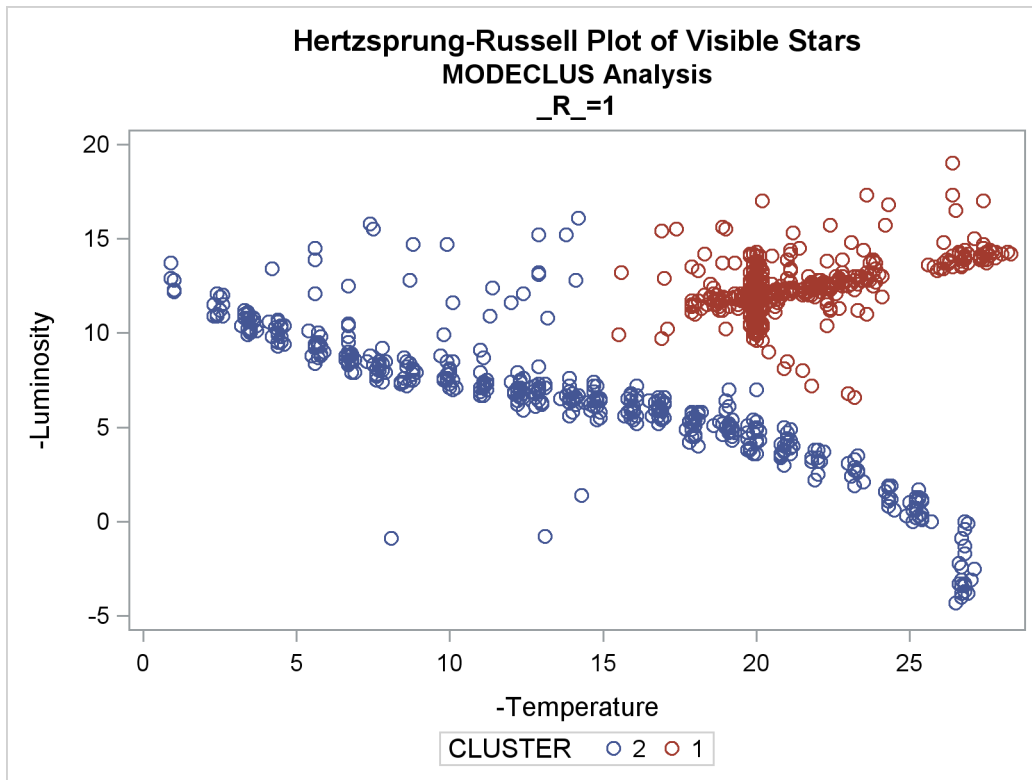
Hertzsprung-Russell Plot of Visible Stars  
Computer-Generated Simulated Data

The MODECLUS Procedure

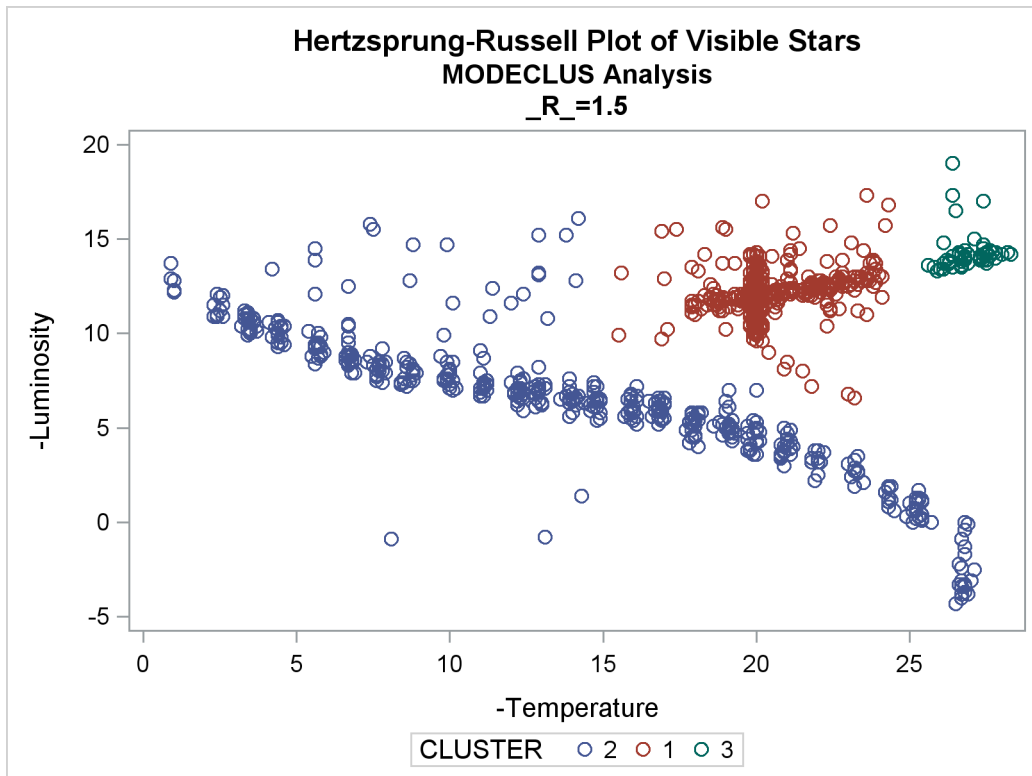
| Cluster Summary |    |                           |                 |                    |                                   |
|-----------------|----|---------------------------|-----------------|--------------------|-----------------------------------|
| R               | CK | Number of Clusters Joined | Maximum P-value | Number of Clusters | Frequency of Unclassified Objects |
| 1               | 5  | 14                        | 0.0001          | 2                  | 0                                 |
| 1.5             | 5  | 6                         | 0.0000          | 3                  | 0                                 |
| 2               | 5  | 4                         | 0.0000          | 2                  | 0                                 |
| 2.5             | 5  | 2                         | 0.0000          | 1                  | 0                                 |

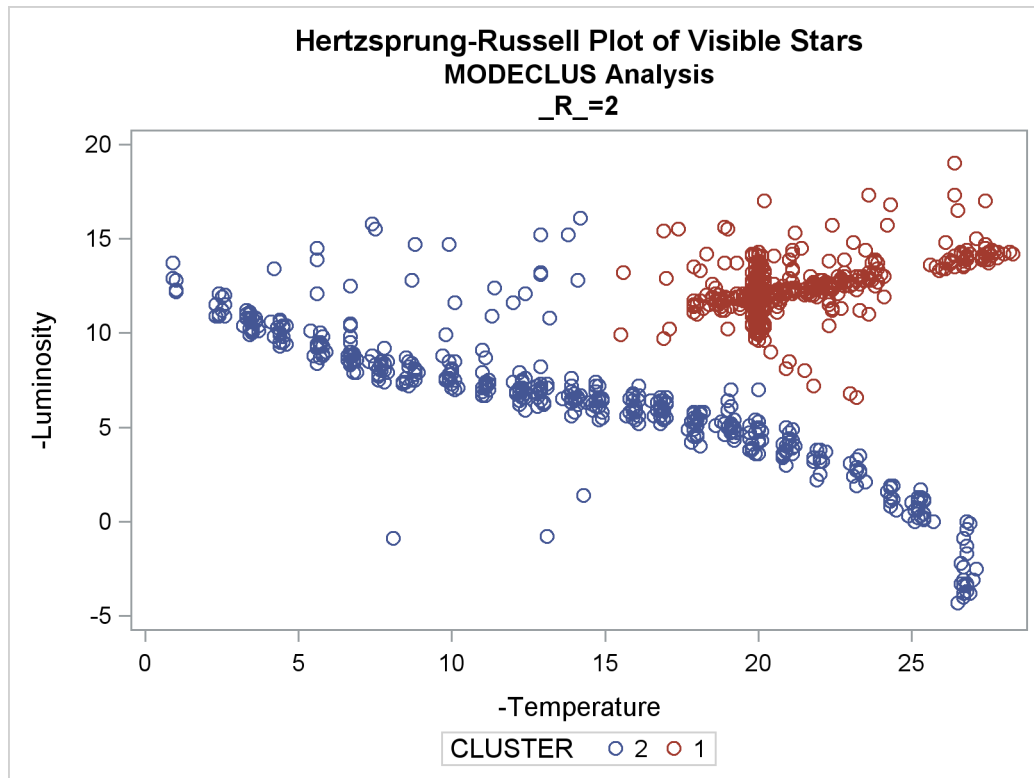


**Output 60.4.3** Scatter Plots of Cluster Memberships by  $\_R\_ = 1$



**Output 60.4.4** Scatter Plots of Cluster Memberships by  $\_R\_ = 1.5$



**Output 60.4.5** Scatter Plots of Cluster Memberships by `_R_=2`**Example 60.5: Using the TRACE Option When METHOD=6**

To illustrate how the TRACE option can help you to understand the clustering process when METHOD=6 is specified, the following data set is created with 12 observations:

```
data test;
 input x @@;
 datalines;
 1 2 3 4 5 7.5 9 11.5 13 14.5 15 16
 ;
```

The first five observations seem to be close to each other, and the last five observations seem to be close to each other. Observation 6 is separated from the first five observations with a (Euclidean) distance of 2.5, and the same distance separates observation 7 from the last five observations. Observations 6 and 7 differ by 1.5.

Suppose METHOD=6 with a radius of 2.5 is chosen for the cluster analysis. You can specify the TRACE option to understand how each observation is assigned.

The following statements produce [Output 60.5.1](#) and [Output 60.5.2](#):

```
/*-- METHOD=6 with TRACE and THRESHOLD=0.5 (default) --*/
title 'METHOD=6 with TRACE and THRESHOLD=0.5 (default)';

proc modeclus data=test method=6 r=2.5 trace short out=out;
 var x;
run;
```

```

title2 'Plot of DENSITY*X=CLUSTER';

proc sgplot data=out;
 scatter y=density x=x / group=cluster datalabel=_obs_;
run;

```

**Output 60.5.1** Partial Output of METHOD=6 with TRACE and Default THRESHOLD=

```

METHOD=6 with TRACE and THRESHOLD=0.5 (default)

 The MODECLUS Procedure
 R=2.5 METHOD=6

 Trace of Clustering Algorithm
 Cluster
Obs Density Old New Ratio

 3 0.0833333 -1 1 M
 2 0.0666667 0 1 N
 4 0.0666667 0 1 N
 1 0.0500000 0 1 N
 5 0.0666667 0 1 N
 6 0.0500000 0 1 0.571
 7 0.0500000 -1 1 0.500
 9 0.0666667 -1 2 M
 8 0.0500000 0 2 N
 11 0.0666667 -1 2 S
 12 0.0500000 0 2 N
 10 0.0666667 -1 2 S

METHOD=6 with TRACE and THRESHOLD=0.5 (default)

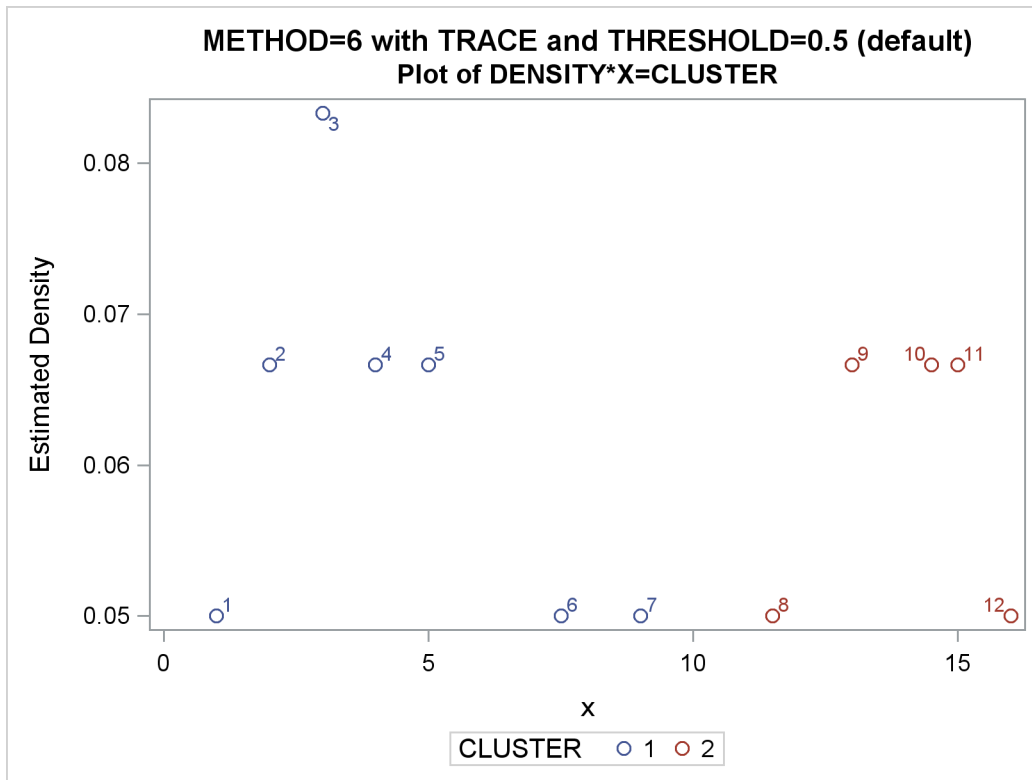
 The MODECLUS Procedure

 Cluster Summary
 Number of Frequency of
 R Clusters Unclassified
 Objects

 2.5 2 0

```

**Output 60.5.2** Density Plot



Note that in [Output 60.5.1](#), observation 7 is originally a seed (indicated by a value of -1 in the “Old” column) and then assigned to cluster 1. This is because the ratio of observation 7 to cluster 1 is 0.5 and is not less than the default value of the THRESHOLD= option (0.5).

If the value of the THRESHOLD= option is increased to 0.55, observation 7 should be excluded from cluster 1 and the cluster membership of observation 7 is changed.

The following statements produce [Output 60.5.3](#) and [Output 60.5.4](#):

```

/*-- METHOD=6 with TRACE and THRESHOLD=0.55 --*/
title 'METHOD=6 with TRACE and THRESHOLD=0.55';

proc modeclus data=test method=6 r=2.5 trace threshold=0.55 short out=out;
 var x;
run;

title2 'Plot of DENSITY*X=CLUSTER with TRACE and THRESHOLD=0.55';

proc sgplot data=out;
 scatter y=density x=x / group=cluster datalabel=_obs_;
run;

```

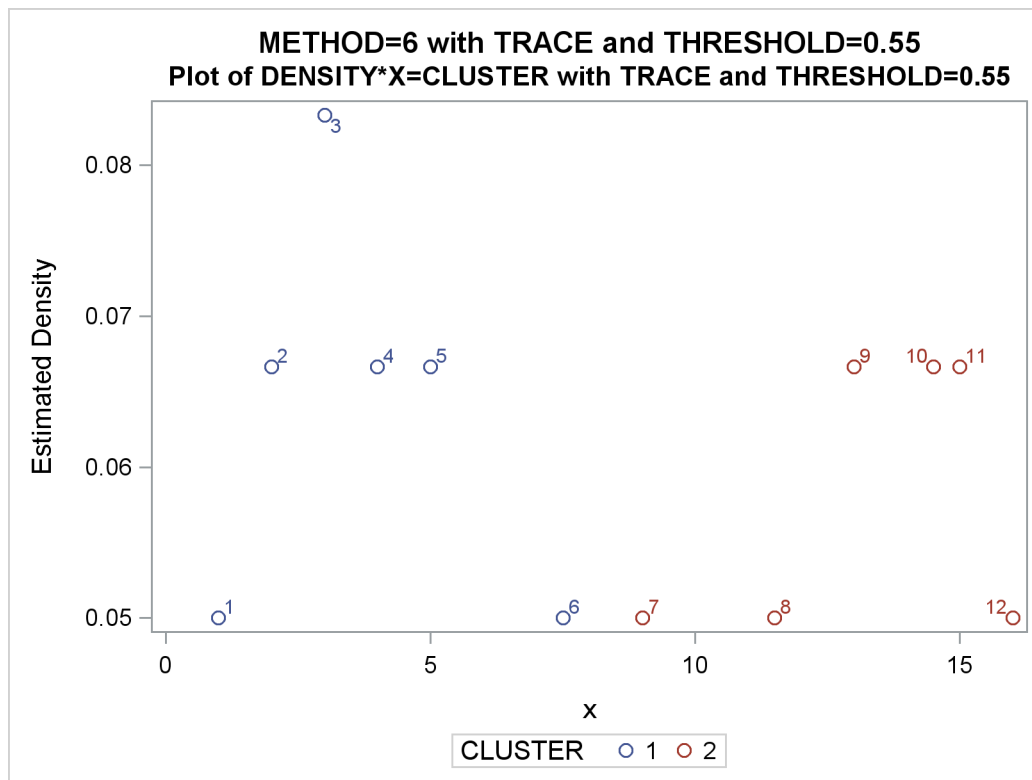
**Output 60.5.3** Partial Output of METHOD=6 with TRACE and THRESHOLD=.55

| METHOD=6 with TRACE and THRESHOLD=0.55 |           |     |     |       |
|----------------------------------------|-----------|-----|-----|-------|
| The MODECLUS Procedure                 |           |     |     |       |
| R=2.5 METHOD=6                         |           |     |     |       |
| Trace of Clustering Algorithm          |           |     |     |       |
| Cluster                                |           |     |     |       |
| Obs                                    | Density   | Old | New | Ratio |
| 3                                      | 0.0833333 | -1  | 1   | M     |
| 2                                      | 0.0666667 | 0   | 1   | N     |
| 4                                      | 0.0666667 | 0   | 1   | N     |
| 1                                      | 0.0500000 | 0   | 1   | N     |
| 5                                      | 0.0666667 | 0   | 1   | N     |
| 6                                      | 0.0500000 | 0   | 1   | 0.571 |
| 9                                      | 0.0666667 | -1  | 2   | M     |
| 8                                      | 0.0500000 | 0   | 2   | N     |
| 11                                     | 0.0666667 | -1  | 2   | S     |
| 12                                     | 0.0500000 | 0   | 2   | N     |
| 10                                     | 0.0666667 | -1  | 2   | S     |
| 7                                      | 0.0500000 | -1  | 2   | S     |

| METHOD=6 with TRACE and THRESHOLD=0.55 |                    |                                   |
|----------------------------------------|--------------------|-----------------------------------|
| The MODECLUS Procedure                 |                    |                                   |
| Cluster Summary                        |                    |                                   |
| R                                      | Number of Clusters | Frequency of Unclassified Objects |
| 2.5                                    | 2                  | 0                                 |

Output 60.5.4 Density Plot



In [Output 60.5.3](#), observation 7 is a seed that is excluded by cluster 1 because its ratio to cluster 1 is less than 0.55. Being a neighbor of a member (observation 8) of cluster 2, observation 7 eventually joins cluster 2 even though it remains a “SEED.” (See [Step 2.2](#) in the section “[METHOD=6](#)” on page 5100.)

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# Chapter 61

## The MULTTEST Procedure

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## Overview: MULTTEST Procedure

The MULTTEST procedure addresses the multiple testing problem. This problem arises when you perform many hypothesis tests on the same data set. Carrying out multiple tests is often reasonable because of the cost of obtaining data, the discovery of new aspects of the data, and the many alternative statistical methods. However, a disadvantage of multiple testing is the greatly increased probability of declaring false significances.

For example, suppose you carry out 10 hypothesis tests at the 5% level, and you assume that the distributions of the  $p$ -values from these tests are uniform and independent. Then, the probability of declaring a particular test significant under its null hypothesis is 0.05, but the probability of declaring at least 1 of the 10 tests significant is 0.401. If you perform 20 hypothesis tests, the latter probability increases to 0.642. These high chances illustrate the danger of multiple testing.

PROC MULTTEST approaches the multiple testing problem by adjusting the  $p$ -values from a family of hypothesis tests. An adjusted  $p$ -value is defined as the smallest significance level for which the given hypothesis would be rejected, when the entire family of tests is considered. The decision rule is to reject the null hypothesis when the adjusted  $p$ -value is less than  $\alpha$ . For most methods, this decision rule controls the *familywise error rate* at or below the  $\alpha$  level. However, the *false discovery rate* controlling procedures control the false discovery rate at or below the  $\alpha$  level.

PROC MULTTEST provides the following  $p$ -value adjustments:

- Bonferroni
- Šidák
- step-down methods
- Hochberg
- Hommel
- Fisher and Stouffer combination
- bootstrap
- permutation
- adaptive methods
- false discovery rate
- positive FDR

The Bonferroni and Šidák adjustments are simple functions of the raw  $p$ -values. They are computationally quick, but they can be too conservative. Step-down methods remove some conservativeness, as do the step-up methods of Hochberg (1988), and the adaptive methods. The bootstrap and permutation adjustments resample the data with and without replacement, respectively, to approximate the distribution of the minimum  $p$ -value of all tests. This distribution is then used to adjust the individual raw  $p$ -values. The bootstrap and permutation methods are computationally intensive but appealing in that, unlike the other methods, correlations and distributional characteristics are incorporated into the adjustments (Westfall and Young 1989; Westfall et al. 1999).

PROC MULTTEST handles data arising from a multivariate one-way ANOVA model, possibly stratified, with continuous and discrete response variables; it can also accept raw  $p$ -values as input data. You can perform a  $t$  test for the mean for continuous data with or without a homogeneity assumption, and the following statistical tests for discrete data:

- Cochran-Armitage linear trend test
- Freeman-Tukey double arcsine test
- Peto mortality-prevalence (log-rank) test
- Fisher exact test

The Cochran-Armitage and Peto tests have exact versions that use permutation distributions and asymptotic versions that use an optional continuity correction. Also, with the exception of the Fisher exact test, you can use a stratification variable to construct Mantel-Haenszel-type tests. All of the previously mentioned tests can be one- or two-sided.

As in the GLM procedure, you can specify linear contrasts that compare means or proportions of the treated groups. The output contains summary statistics and regular and multiplicity-adjusted  $p$ -values. You can create output data sets containing raw and adjusted  $p$ -values, test statistics and other intermediate calculations, permutation distributions, and resampling information.

The MULTTEST procedure uses ODS Graphics to create graphs as part of its output. For general information about ODS Graphics, see Chapter 21, “Statistical Graphics Using ODS.”

The GLIMMIX, GLM, MIXED, and LIFETEST procedures, and other procedures that implement the ESTIMATE, LSMEANS, LSMESTIMATE, and SLICE statements, also adjust their results for multiple tests. For more information, see the documentation for these procedures and statements, and Westfall et al. (1999).

## Getting Started: MULTTEST Procedure

### Drug Example

Suppose you conduct a small study to test the effect of a drug on 15 subjects. You randomly divide the subjects into three balanced groups receiving 0 mg, 1 mg, and 2 mg of the drug, respectively. You carry out the experiment and record the presence or absence of 10 side effects for each subject. Your data set is as follows:

```
data Drug;
 input Dose$ SideEff1-SideEff10;
 datalines;
0MG 0 0 1 0 0 1 0 0 0 0
0MG 0 0 0 0 0 0 0 0 0 1
0MG 0 0 0 0 0 0 0 0 0 0
0MG 0 0 0 0 0 0 0 0 0 0
0MG 0 1 0 0 0 0 0 0 0 0
1MG 1 0 0 1 0 1 0 0 1 0
1MG 0 0 0 1 1 0 0 1 0 1
1MG 0 1 0 0 0 0 1 0 0 0
1MG 0 0 1 0 0 0 0 0 0 1
1MG 1 0 1 0 0 0 0 1 0 0
2MG 0 1 1 1 0 1 1 1 0 1
2MG 1 1 1 1 1 1 0 1 1 0
2MG 1 0 0 1 0 1 1 0 1 0
2MG 0 1 1 1 1 0 1 1 1 1
```

```

2MG 1 0 1 0 1 1 1 0 0 1
;

```

The increasing incidence of 1s for higher dosages in the preceding data set provides an initial visual indication that the drug has an effect. To explore this statistically, you perform an analysis in which the possibility of side effects increases linearly with drug level. You can analyze the data for each side effect separately, but you are concerned that, with so many tests, there might be a high probability of incorrectly declaring some drug effects significant. You want to correct for this multiplicity problem in a way that accounts for the discreteness of the data and for the correlations between observations on the same unit.

PROC MULTTEST addresses these concerns by processing all of the data simultaneously and adjusting the  $p$ -values. The following statements perform a typical analysis:

```

ods graphics on;
proc multtest bootstrap nsample=20000 seed=41287 notables
 plots=PByTest(vref=0.05 0.1);
 class Dose;
 test ca(SideEff1-SideEff10);
 contrast 'Trend' 0 1 2;
run;
ods graphics off;

```

This analysis uses the **BOOTSTRAP** option to adjust the  $p$ -values. The **NSAMPLE=** option requests 20,000 samples for the bootstrap analysis, and the starting seed for the random number generator is 41287. The **NOTABLES** option suppresses the display of summary statistics for each side effect and drug level combination. The **PLOTS=** option displays a visual summary of the unadjusted and adjusted  $p$ -values against each test, and the **VREF=** option adds reference lines to the display.

The **CLASS** statement is used to specify the grouping variable, **Dose**. The **ca(sideeff1-sideeff10)** specification in the **TEST** statement requests a Cochran-Armitage linear trend test for all 10 characteristics. The **CONTRAST** statement gives the coefficients for the linear trend test.

The “Model Information” table in Figure 61.1 describes the statistical tests performed by PROC MULTTEST. For this example, PROC MULTTEST carries out a two-tailed Cochran-Armitage linear trend test with no continuity correction or strata adjustment. This test is performed on the raw data and on 20,000 bootstrap samples.

**Figure 61.1** Output Summary for the MULTTEST Procedure

| The Multtest Procedure      |                  |
|-----------------------------|------------------|
| Model Information           |                  |
| Test for discrete variables | Cochran-Armitage |
| Z-score approximation used  | Everywhere       |
| Continuity correction       | 0                |
| Tails for discrete tests    | Two-tailed       |
| Strata weights              | None             |
| P-value adjustment          | Bootstrap        |
| Number of resamples         | 20000            |
| Seed                        | 41287            |

The “Contrast Coefficients” table in [Figure 61.2](#) displays the coefficients for the Cochran-Armitage test. They are 0, 1, and 2, as specified in the `CONTRAST` statement.

**Figure 61.2** Coefficients Used in the MULTTEST Procedure

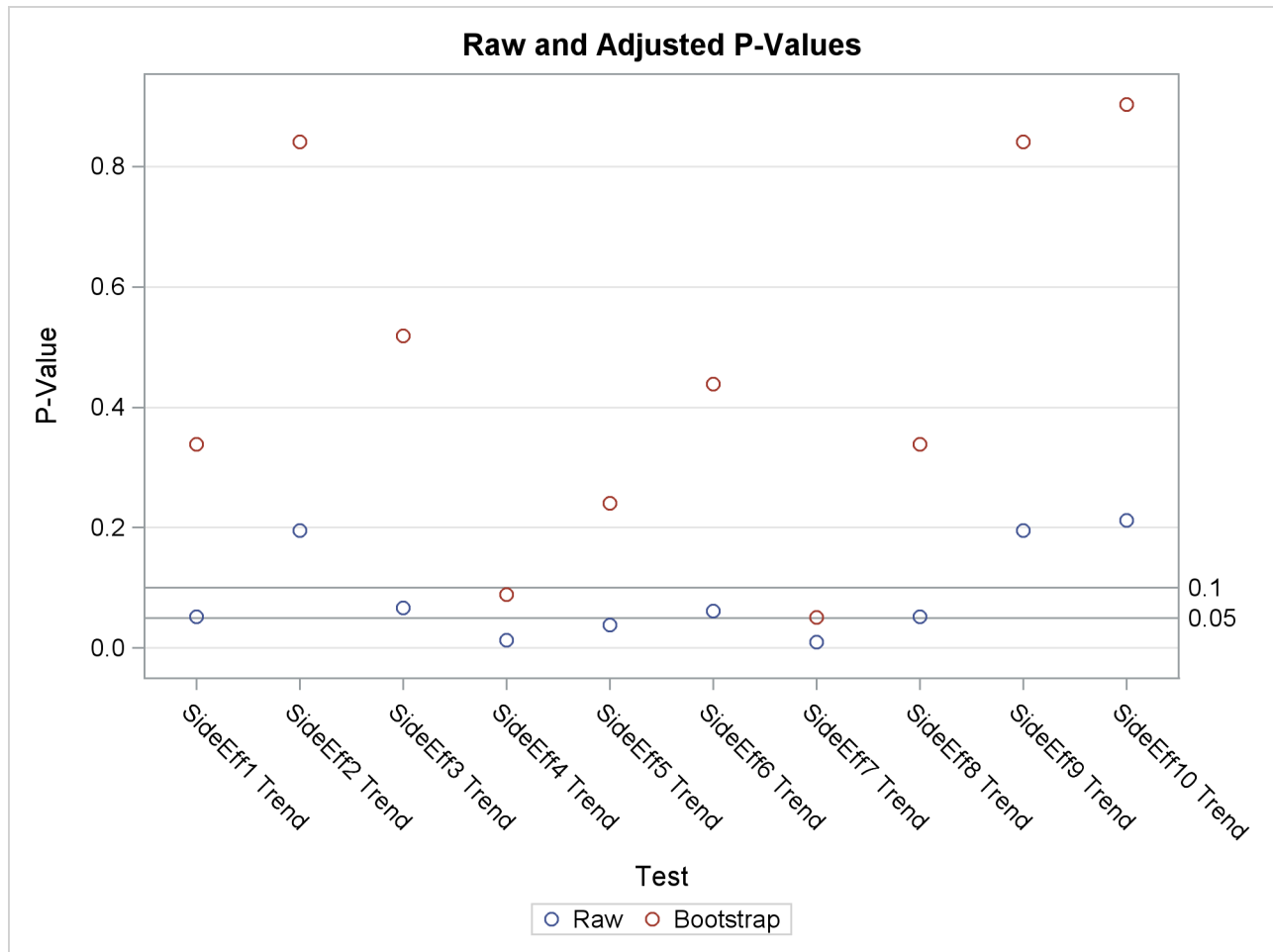
| Contrast Coefficients |      |     |     |
|-----------------------|------|-----|-----|
| Contrast              | Dose |     |     |
|                       | 0MG  | 1MG | 2MG |
| Trend                 | 0    | 1   | 2   |

The “p-Values” table in [Figure 61.3](#) lists the  $p$ -values for the drug example. The Raw column lists the  $p$ -values for the Cochran-Armitage test on the original data, and the Bootstrap column provides the bootstrap adjustment of the raw  $p$ -values.

Note that the raw  $p$ -values lead you to reject the null hypothesis of no linear trend for 3 of the 10 characteristics at the 5% level and 7 of the 10 characteristics at the 10% level. The bootstrap  $p$ -values, however, lead to this conclusion for 0 of the 10 characteristics at the 5% level and only 2 of the 10 characteristics at the 10% level; you can also see this in [Figure 61.4](#).

**Figure 61.3** Summary of  $p$ -Values for the MULTTEST Procedure

| p-Values  |          |        |           |
|-----------|----------|--------|-----------|
| Variable  | Contrast | Raw    | Bootstrap |
| SideEff1  | Trend    | 0.0519 | 0.3388    |
| SideEff2  | Trend    | 0.1949 | 0.8403    |
| SideEff3  | Trend    | 0.0662 | 0.5190    |
| SideEff4  | Trend    | 0.0126 | 0.0884    |
| SideEff5  | Trend    | 0.0382 | 0.2408    |
| SideEff6  | Trend    | 0.0614 | 0.4383    |
| SideEff7  | Trend    | 0.0095 | 0.0514    |
| SideEff8  | Trend    | 0.0519 | 0.3388    |
| SideEff9  | Trend    | 0.1949 | 0.8403    |
| SideEff10 | Trend    | 0.2123 | 0.9030    |

Figure 61.4 Adjusted  $p$ -Values

The bootstrap adjustment gives the probability of observing a  $p$ -value as extreme as each given  $p$ -value, considering all 10 tests simultaneously. This adjustment incorporates the correlation of the raw  $p$ -values, the discreteness of the data, and the multiple testing problem. Failure to account for these issues can certainly lead to misleading inferences for these data.

## Syntax: MULTTEST Procedure

The following statements are available in the MULTTEST procedure:

```

PROC MULTTEST < options > ;
 BY variables ;
 CLASS variable ;
 CONTRAST 'label' values ;
 FREQ variable ;
 ID variables ;
 STRATA variable ;
 TEST name (variables < / options >) ;

```

Statements that follow the PROC MULTTEST statement can appear in any order. The CLASS and TEST statements are required unless the INPVALUES= option is specified in the PROC MULTTEST statement.

The following sections describe the PROC MULTTEST statement and then describe the other statements in alphabetical order.

## PROC MULTTEST Statement

**PROC MULTTEST** < options > ;

The PROC MULTTEST statement invokes the MULTTEST procedure. It also specifies the  $p$ -value adjustments. Table 61.1 summarizes the options available in the PROC MULTTEST statement. These options are described in alphabetical order following the table.

**Table 61.1** PROC MULTTEST Statement Options by Function

| Option                                                  | Description                                                 |
|---------------------------------------------------------|-------------------------------------------------------------|
| <b>FWE-Controlling <math>p</math>-Value Adjustments</b> |                                                             |
| ADAPTIVEHOLM                                            | Computes the adaptive step-down Bonferroni adjustment       |
| ADAPTIVEHOCHBERG                                        | Computes the adaptive step-up Bonferroni adjustment         |
| BONFERRONI                                              | Computes the Bonferroni adjustment                          |
| BOOTSTRAP                                               | Computes the bootstrap min- $p$ adjustment                  |
| FISHER_C                                                | Computes Fisher's combination adjustment                    |
| HOCHBERG                                                | Computes the step-up Bonferroni adjustment                  |
| HOMMEL                                                  | Computes Hommel's adjustment                                |
| HOLM                                                    | Computes the step-down Bonferroni adjustment                |
| PERMUTATION                                             | Computes the permutation min- $p$ adjustment                |
| SIDAK                                                   | Computes Šidák's adjustment                                 |
| STEPBON                                                 | Computes the step-down Bonferroni adjustment                |
| STEPBOOT                                                | Computes the step-down bootstrap adjustment                 |
| STEPPERM                                                | Computes the step-down permutation adjustment               |
| STEPSID                                                 | Computes the step-down Šidák adjustment                     |
| STOUFFER                                                | Computes the Stouffer-Liptak combination adjustment         |
| <b>FDR-Controlling <math>p</math>-Value Adjustments</b> |                                                             |
| ADAPTIVEFDR                                             | Computes the adaptive linear step-up adjustment             |
| DEPENDENTFDR                                            | Computes the linear step-up adjustment under dependence     |
| FDR                                                     | Computes the linear step-up adjustment                      |
| FDRBOOT                                                 | Computes the linear step-up bootstrap min- $p$ adjustment   |
| FDRPERM                                                 | Computes the linear step-up permutation min- $p$ adjustment |
| PFDR                                                    | Computes the positive FDR adjustment                        |
| <b>Input/Output Data Sets</b>                           |                                                             |
| DATA=                                                   | Names the input data set                                    |
| INPVALUES=                                              | Names the input data set of raw $p$ -values                 |
| OUT=                                                    | Names the output data set                                   |
| OUTPERM=                                                | Names the output permutation data set                       |
| OUTSAMP=                                                | Names the output resample data set                          |

Table 61.1 continued

| Option                          | Description                                                      |
|---------------------------------|------------------------------------------------------------------|
| <b>Displayed Output Options</b> |                                                                  |
| NOPRINT                         | Suppresses all tables                                            |
| NOTABLES                        | Suppresses variable tables                                       |
| NOZEROS                         | Suppresses zero tables for CLASS variables                       |
| NOPVALUE                        | Suppresses the “p-Values” table                                  |
| PLOTS                           | Requests ODS Graphics                                            |
| <b>Resampling Options</b>       |                                                                  |
| CENTER                          | Mean-centers continuous variables before resampling              |
| NOCENTER                        | Does not mean-center continuous variables before resampling      |
| NSAMPLE=                        | Specifies the number of resamples                                |
| RANUNI                          | Specifies a different random number generator                    |
| SEED=                           | Specifies the seed for resampling                                |
| <b>CLASS Variable Options</b>   |                                                                  |
| NOZEROS                         | Suppresses zero tables for CLASS variables                       |
| ORDER=                          | Specifies CLASS variable order                                   |
| <b>Computational Options</b>    |                                                                  |
| EPSILON=                        | Specifies the comparison value                                   |
| NTRUENULL=                      | Specifies the estimation method for the number of true nulls     |
| PTRUENULL=                      | Specifies the estimation method for the proportion of true nulls |

You can specify the following options in the PROC MULTTEST statement.

**ADAPTIVEHOCHBERG****AHOC**

requests adjusted  $p$ -values by using the Hochberg and Benjamini (1990) adaptive step-up Bonferroni method. See the section “Adaptive Adjustments” on page 5200 for more details.

**ADAPTIVEHOLM****AHOLM**

requests adjusted  $p$ -values by using the Hochberg and Benjamini (1990) adaptive step-down Bonferroni method. See the section “Adaptive Adjustments” on page 5200 for more details.

**ADAPTIVEFDR<(UNRESTRICT)>****AFDR<(UNRESTRICT)>**

requests adjusted  $p$ -values by using the Benjamini and Hochberg (2000) adaptive linear step-up method (AFDR). The UNRESTRICT option estimates the AFDR as defined in Benjamini and Hochberg (2000), which allows the adjustment to reduce the raw  $p$ -value. By default, the AFDR is constrained to be greater than or equal to the raw  $p$ -value. See the section “Adaptive False Discovery Rate” on page 5202 for more details.

**BONFERRONI****BON**

specifies that the Bonferroni adjustments (number of tests  $\times p$ -value) be computed for each test. These adjustments can be extremely conservative and should be viewed with caution. When exact tests are specified via the PERMUTATION= option in the TEST statement, the actual permutation

distributions are used, resulting in a much less conservative version of this procedure (Westfall and Wolfinger 1997). See the section “[Bonferroni](#)” on page 5197 for more details.

## BOOTSTRAP

### BOOT

specifies that the  $p$ -values be adjusted by using the bootstrap method to resample vectors (Westfall and Young 1993). Resampling is performed with replacement and independently within levels of the [STRATA](#) variable. Continuous variables are mean-centered by default prior to resampling; specify the [NOCENTER](#) option to change this. See the section “[Bootstrap](#)” on page 5197 for more details. The [BOOTSTRAP](#) option is not allowed with the Peto test.

If the [PERMUTATION=](#) suboption is used with the [CA](#) test in the [TEST](#) statement, the exact permutation distribution is recomputed for each bootstrap sample. **CAUTION:** This can be very time-consuming. It is preferable to use permutation resampling when permutation base tests are used.

### CENTER

requests that continuous variables be mean-centered prior to resampling. The default action is to mean-center for bootstrap resampling and not to mean-center for permutation resampling.

### DATA=*SAS-data-set*

names the input SAS data set to be used by PROC MULTTEST. The default is to use the most recently created data set. The [DATA=](#) and [INPVALUES=](#) options cannot both be specified.

## DEPENDENTFDR

### DFDR

requests adjusted  $p$ -values by using the method of Benjamini and Yekateuli (2001). See the section “[Dependent False Discovery Rate](#)” on page 5201 for more details.

### EPSILON=*number*

specifies the amount by which two  $p$ -values must differ to be declared unequal. The value *number* must be between 0 and 1; the default value is 1000 times the machine epsilon, which is approximately  $1\text{E}-12$ . For SAS 9.1 and earlier releases the default value was  $1\text{E}-8$ . See Westfall and Young (1993, pp. 165–166) for more information.

## FDR

### LSU

requests adjusted  $p$ -values by using the linear step-up method of Benjamini and Hochberg (1995). These  $p$ -values do not control the familywise error rate, but they do control the false discovery rate in some cases. See the section “[False Discovery Rate Controlling Adjustments](#)” on page 5200 for more details.

### FDRBOOT< ( $\beta$ ) >

A bootstrap-resampling false discovery rate controlling method due to Yekateuli and Benjamini (1999). This method uses the same resampling algorithm as the [BOOTSTRAP](#) option. Every resample is saved in order to compute a quantile of the resampled  $p$ -values; therefore, this method can use a lot of memory. The parameter  $\beta$  designates that a  $100(1 - \beta)$  quantile is used in the computations for determining the adjustments; by default,  $\beta = 0.05$ . See the section “[False Discovery Rate Resampling Adjustments](#)” on page 5201 for details.



**FDRPERM**< ( $\beta$ ) >

A permutation-resampling false discovery rate controlling method due to Yekateuli and Benjamini (1999). This method uses the same resampling algorithm as the **PERMUTATION** option. Every resample is saved in order to compute a quantile of the resampled  $p$ -values; therefore, this method can use a lot of memory. The parameter  $\beta$  designates that a  $100(1 - \beta)$  quantile is used in the computations for determining the adjustments; by default,  $\beta = 0.05$ . See the section “[False Discovery Rate Resampling Adjustments](#)” on page 5201 for details.

**FISHER\_C****FIC**

requests adjusted  $p$ -values by using Fisher’s combination method. See the section “[Fisher Combination](#)” on page 5199 for more details.

**HOCHBERG****HOC**

requests adjusted  $p$ -values by using the step-up Bonferroni method due to Hochberg (1988). See the section “[Hochberg](#)” on page 5199 for more details.

**HOMMEL****HOM**

requests adjusted  $p$ -values by using the method of Hommel (1988). See the section “[Hommel](#)” on page 5199 for more details.

**HOLM**

is an alias for the [STEPBON](#) adjustment.

**INPVALUES**< (*pvalue-name*) >=*SAS-data-set*

names an input SAS data set that includes a variable containing raw  $p$ -values. The MULTTEST procedure adjusts the collection of raw  $p$ -values for multiplicity. Resampling-based adjustments are not permitted with this type of data input. The **CLASS**, **CONTRAST**, **FREQ**, **STRATA**, and **TEST** statements are ignored when an INPVALUES= data set is specified. The INPVALUES= and **DATA=** options cannot both be specified. The *pvalue-name* enables you to specify the name of the  $p$ -value column from your data set. By default, *pvalue-name*=’raw\_p’. The INPVALUES= data set can contain variables in addition to the raw  $p$ -values variable; see [Example 61.5](#) for an example.

**LIPTAK**

is an alias for the [STOUFFER](#) adjustment.

**NOCENTER**

requests that continuous variables not be mean-centered prior to resampling. The default action is to mean-center for bootstrap resampling and not to mean-center for permutation resampling.

**NOPRINT**

suppresses the normal display of results. Note that this option temporarily disables the Output Delivery System (ODS); see Chapter 20, “[Using the Output Delivery System](#),” for more information.

**NOPVALUE**

suppresses the display of the “ $p$ -Values” table of raw and adjusted  $p$ -values. This option is most useful when you are adjusting many tests and need to create only an **OUT=** data set or display graphics.

**NOTABLES**

suppresses display of the “Discrete Variable Tabulations” and “Continuous Variable Tabulations” tables.

**NOZEROS**

suppresses display of tables having zero occurrences for all **CLASS** levels.

**NSAMPLE=*number*****N=*number***

specifies the number of resamples for use with the resampling methods. The value *number* must be a positive integer; by default, 20,000 resamples are used. Large values of *number* (20,000 or more) are usually recommended for accuracy, but long execution times can result, particularly with large data sets.

**NTRUENULL=*keyword* | *value*****M0=*keyword* | *value***

Controls the method used to estimate the number of true NULL hypotheses ( $m_0$ ) for the adaptive methods. This option is ignored unless one of the adaptive methods is specified. By default, PROC MULTTEST uses the **DECREASESLOPE** method for the **ADAPTIVEHOLM** and **ADAPTIVEHOCHBERG** adjustments, and the **LOWESTSLOPE** method for **ADAPTIVEFDR** adjustment. For the **PFDR** adjustment, the **SPLINE** method is attempted first. If the estimate is nonpositive or if the slope of the spline at the last  $\lambda$  is greater than 0.1 times the range of the fitted spline values, then the **BOOTSTRAP** method is used.

You can specify a positive integer as the *value*, or you can specify one of the *keywords* in the following list. Alternatively, you can specify the proportion of true NULL hypotheses by using the **PTRUENULL=** option. Suppose you have  $m$  tests with ordered  $p$ -values  $p_{(1)} \leq \dots \leq p_{(m)}$ , and define  $q_{(i)} = 1 - p_{(i)}$ .

**BOOTSTRAP<(bootstrap-options)>**

uses the bootstrap method of Storey and Tibshirani (2003). Compute the proportion of true null hypotheses  $\hat{\pi}_0(\lambda) = \frac{m - N(\lambda) + f}{(1 - \lambda)m}$  for  $\lambda \in L = \{0, 0.05, \dots, 0.95\}$ , where  $N(\lambda)$  is the number of  $p$ -values less than or equal to  $\lambda$ , and  $f = 1$  for the finite-sample case; otherwise  $f = 0$ . For each  $\lambda$ , bootstrap on the  $p$ -values to form  $B$  bootstrap versions  $\hat{\pi}_0^b(\lambda)$ ,  $b = 1, \dots, B$ , and choose the  $\lambda$  that yields the minimum  $\widehat{\text{MSE}}(\lambda) = \frac{1}{B} \sum_{b=1}^B (\hat{\pi}_0^b(\lambda) - \min_{\lambda' \in L} \hat{\pi}_0(\lambda'))^2$ . The available *bootstrap-options* are as follows:

**FINITE**

the finite-sample case of the **PFDR** option, described on page 5178.

**NBOOT=*B***

bootstrap resamples of the raw  $p$ -values for the  $\lambda$  computations. **NBOOT=10,000** by default;  $B$  must be a positive integer.

**NLAMBDA=*n***

“optimal”  $\lambda$  is the value in  $\{0, \frac{1}{n}, \dots, \frac{n-1}{n}\}$  that minimizes the MSE. **NLAMBDA=20** by default;  $n$  must be an integer greater than 1.

**DECREASESLOPE**

Schweder and Spjøtvoll (1982) as modified by Hochberg and Benjamini (1990). Let  $b_i$  be the slope of the least squares line fit to  $\{q_{(m)}, \dots, q_{(m-i+1)}\}$  and through the origin, for  $i = 1, \dots, m$ . Find the first  $i = m-1, m-2, \dots, 1$  such that  $b_i < b_{i+1}$ . Then  $\hat{m}_0 = \text{ceil}(\frac{1}{b_{i+1}} - 1)$ .

**KSTEST<( $\beta$ )>**

uses the Kolmogorov-Smirnov uniformity test method of Turkheimer, Smith, and Schmidt (2001). Let  $k_{min} = 1, k_{max} = m$ , and the Kolmogorov-Smirnov statistic  $D = \max(q_{(i)} - i/(m+1)(\sqrt{k} + 0.12 + 0.11/\sqrt{k}))$ . If  $D$  is greater than the upper-tail probability (Press et al. 1992), then  $k_{max} = k, k = \text{floor}((k_{min} + k)/2)$ ; otherwise, let  $k_{min} = k, k = \text{floor}((k + k_{max})/2)$ . Repeat until  $k = k_{min}$ . Next compute the slope  $b$  of the weighted least squares regression line on the  $k$  smallest  $q_{(i)}$  by using weights  $w_i = i(k - i + 1)/((k + 1)^2(k + 2))$ . Then  $\hat{m}_0 = \text{ceil}(\frac{1}{b} - 1)$ .

**LEASTSQUARES**

uses a linear least squares method to search for the correct cutpoint. For each  $i = 0, \dots, m$  compute the SSE of the least squares line through the origin fitting  $\{q_{(m)}, \dots, q_{(m-i+1)}\}$ , let  $b_i$  be the slope of this line, and add the SSE of the unconstrained least squares line through the rest of the  $q$ s. For  $i = 0$  compute the SSE for the unconstrained line. The argument  $i$  that minimizes the SSE is the cutpoint: if  $i = 0$  then  $\hat{m}_0 = 0$ ; if  $i = m$  then  $\hat{m}_0 = m$ ; otherwise  $\hat{m}_0 = \text{ceil}(\frac{1}{b_i} - 1)$ .

**LOWESTSLOPE**

uses the lowest slope method of Benjamini and Hochberg (2000). Find the first  $i = 1, \dots, m$  such that  $b_i = q_{(i)}/(m - i + 1)$  decreases. Then  $\hat{m}_0 = \text{floor}(\min(\frac{1}{b_i} + 1, m))$ .

**MEANDIFF**

uses the mean of differences method of Hsueh, Chen, and Kodell (2003). Let  $\bar{d}_i = \frac{q_{(m-i+1)}}{i}$  and estimate  $\hat{m}_0^i = \frac{1}{\bar{d}_i} - 1$ . Start from  $i = m$  and proceed downward until the first time  $\hat{m}_0^{i-1} \geq \hat{m}_0^i$  occurs.

**SPLINE<(spline-options)>**

uses the cubic spline method of Storey and Tibshirani (2003). For each  $\lambda \in \{0, \frac{1}{n}, \frac{2}{n}, \dots, \frac{n-1}{n}\}$  compute  $\hat{\pi}_0(\lambda) = \frac{\#\{p_i > \lambda\}}{m(1-\lambda)}$ . Let  $\hat{f}(\lambda)$  be the natural cubic spline with 3 degrees of freedom of  $\hat{\pi}_0(\lambda)$  versus  $\lambda$ . Estimate  $\hat{\pi}_0$  by taking the spline value at the last  $\lambda$ :  $\hat{\pi}_0 = \hat{\pi}_0(\frac{n-1}{n})$ , so that  $\hat{m}_0 = m\hat{\pi}_0$ . The available *spline-options* are as follows:

**DF=df**

sets the degrees of freedom of the spline, where *df* is a nonnegative integer. The default is DF=3.

**DFCONV=number**

specifies the absolute change in spline degrees of freedom value for concluding convergence. If  $|df_i - df_{i+1}| < \text{number}$  (or if the **SPCONV=** criterion is satisfied), then convergence is declared. *number* must be between 0 and 1; by default, *number* is 1000 times the square root of machine epsilon, which is about 1E-5.

**FINITE**

computations for the finite-sample case of the [PFDR](#) option, described on page 5178.

**MAXITER=*n***

specifies the maximum number of golden-search iterations used to find a spline with  $DF=df$  degrees of freedom. By default, `MAXITER=100`; *number* must be a nonnegative integer.

**NLAMBDA=*n***

$\hat{\pi}_0(\lambda)$  for  $\lambda \in \{0, \frac{1}{n}, \frac{2}{n}, \dots, \frac{n-1}{n}\}$  for the spline fit. By default, `NLAMBDA=20`; *number* must be an integer greater than 1.

**SPCONV=*number***

specifies the absolute change in smoothing parameter value for concluding convergence of the spline. If  $|sp_i - sp_{i+1}| < number$  (or if the `DFCONV=` criterion is satisfied), then convergence is declared. By default, *number* equals the square root of the machine epsilon, which is about  $1E-8$ .

In all cases  $\hat{m}_0$  is constrained to lie between 0 and  $m$ ; if the computed  $\hat{m}_0 = 0$ , then the adaptive adjustments do not produce results. If you specify  $\hat{m}_0 > m$ , then it is reduced to  $m$ . Values of  $\hat{m}_0$  are displayed in the “Estimated Number of True Null Hypotheses” table.

**ORDER=DATA | FORMATTED | FREQ | INTERNAL**

specifies the sort order for the levels of the classification variables (which are specified in the `CLASS` statement). This option applies to the levels for all classification variables, except when you use the (default) `ORDER=FORMATTED` option with numeric classification variables that have no explicit format. With this option, the levels of such variables are ordered by their internal value.

The `ORDER=` option can take the following values:

| Value of <code>ORDER=</code> | Levels Sorted By                                                                                                                       |
|------------------------------|----------------------------------------------------------------------------------------------------------------------------------------|
| <b>DATA</b>                  | Order of appearance in the input data set                                                                                              |
| <b>FORMATTED</b>             | External formatted value, except for numeric variables with no explicit format, which are sorted by their unformatted (internal) value |
| <b>FREQ</b>                  | Descending frequency count; levels with the most observations come first in the order                                                  |
| <b>INTERNAL</b>              | Unformatted value                                                                                                                      |

By default, `ORDER=FORMATTED`. For `ORDER=FORMATTED` and `ORDER=INTERNAL`, the sort order is machine-dependent. For more information about sort order, see the chapter on the `SORT` procedure in the *Base SAS Procedures Guide* and the discussion of BY-group processing in *SAS Language Reference: Concepts*.

**OUT=*SAS-data-set***

names the output SAS data set containing variable names, contrast names, intermediate calculations, and all associated  $p$ -values. See “[OUT= Data Set](#)” on page 5204 for more information.

**OUTPERM=SAS-data-set**

names the output SAS data set containing entire permutation distributions (upper-tail probabilities) for all tests when the **PERMUTATION=** option is specified. See “**OUTPERM= Data Set**” on page 5205 for more information. **CAUTION:** This data set can be very large.

**OUTSAMP=SAS-data-set**

names the output SAS data set containing information from the resampled data sets when resampling is performed. See “**OUTSAMP= Data Set**” on page 5205 for more information. **CAUTION:** This data set can be very large.

**PDATA=SAS-data-set**

is an alias for the **INPVALUES=** option.

**PERMUTATION****PERM**

computes adjusted  $p$ -values in identical fashion as the **BOOTSTRAP** option, with the exception that PROC MULTTEST resamples without replacement rather than with replacement. Resampling is performed independently within levels of the **STRATA** variable. Continuous variables are not mean-centered prior to resampling; specify the **CENTER** to change this. See the section “**Bootstrap**” on page 5197 for more details. The **PERMUTATION** option is not allowed with the Peto test.

**PFDR<(options)>**

computes the “ $q$ -values”  $\hat{q}_\lambda(p_i)$  of Storey (2002) and Storey, Taylor, and Siegmund (2004). PROC MULTTEST treats these “ $q$ -values” as adjusted  $p$ -values. The computations depend on selecting a parameter  $\lambda$  and an estimation method for the false discovery rate; see the section “**Positive False Discovery Rate**” on page 5202 for computational details. The available *options* for choosing the method are as follows:

**FINITE**

estimates the false discovery rate with  $\widehat{pFDR}$  or  $\widehat{FDR}$  for the finite-sample case with independent null  $p$ -values.

**POSITIVE**

estimates the false discovery rate with  $\widehat{pFDR}$  instead of the default  $\widehat{FDR}$ .

**UNRESTRICT**

estimates the false discovery rate as defined in Storey (2002), which allows the adjustment to reduce the raw  $p$ -value. By default, the PFDR is constrained to be greater than or equal to the raw  $p$ -value.

The available options for controlling the  $\lambda$  search are the *bootstrap-options* (page 5175), the *spline-options* (page 5176), and the following options:

**LAMBDA=number**

specifies a  $\lambda \in [0, 1)$  and does not perform the bootstrap or spline searches for an “optimal”  $\lambda$ .

**MAXLAMBDA=number**

stops the NLAMBDA= search sequence for the **bootstrap** and **spline** searches when this *number* is reached. The *number* must be in  $[0, 1]$ . This option is ignored if the **LAMBDA=** option is specified.

**PLOTS**< (*global-plot-options*) >=*plot-request*< (*options*) >

**PLOTS**< (*global-plot-options*) >=*(plot-request*< (*options*) >< . . . *plot-request*< (*options*) >> )

controls the plots produced through ODS Graphics. If you specify only one *plot-request*, you can omit the parentheses. For example, the following statements are valid specifications of the PLOTS= option:

```
plots = all
plots = (rawprob adjusted)
plots(sigonly) = (rawprob adjusted(unpack))
```

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;
proc multtest plots=adjusted invalues=a pfdr;
run;
ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS](#).”

By default, no graphs are created; you must specify the PLOTS= option to make graphs. You need at least two tests to produce a graph. If you are not using an INPVALUES= data set, then each test is given a name constructed as “variable-name contrast-label”. If you specify a MEAN test in the TEST statement, the *t*-test names are prefixed with “Mean:”. See [Example 61.6](#) for examples of the ODS graphical displays.

The following *global-plot-options* are available:

#### **UNPACKPANELS | UNPACK**

suppresses paneling. By default, the plots produced with the ADJUSTED and RAWPROB options are grouped in a single display, called a *panel*. Specify UNPACK to display each plot separately.

#### **SIGONLY**< =*number* >

displays only those tests with adjusted *p*-values  $\leq$  *number*, where  $0 \leq$  *number*  $\leq$  1. By default, *number* = 0.05.

The following *plot-requests* are available:

#### **ADJUSTED**< (**UNPACK**) >

displays a 2×2 panel of adjusted *p*-value plots similar to those Storey and Tibshirani (2003) developed for use with the PFDR *p*-value adjustment method. The plots of the adjusted *p*-values by the raw *p*-values and the adjusted *p*-values by their rank show the effect of the adjustments. The plot of the proportion of adjusted *p*-values  $\leq$  each adjusted *p*-value and the plot of the expected number of false positives (the proportion significant multiplied by the adjusted *p*-value) versus the proportion significant show the effect of choosing different significance levels. The UNPACK option unpanels the display.

**ALL**

produces all appropriate plots. You can specify other options with ALL; for example, to display all plots and unpack the RAWPROB plots you can specify `plots=(all rawprob(unpack))`.

**LAMBDA**

displays plots of the MSE and the estimated number of true nulls against the  $\lambda$  parameter when the `NTRUENULL=SPLINE` or `NTRUENULL=BOOTSTRAP` option is in effect.

**MANHATTAN**< (options) >

displays the Manhattan plot (a plot of  $-\log_{10}$  of the adjusted  $p$ -values versus the tests). You can specify the following options:

**GROUP**=variable

specifies a variable to group the adjusted  $p$ -values in the display.

**LABEL** < =OBS >

labels the observations that have adjusted  $p$ -values that are less than the value specified in the `VREF=` option. By default, labels are created as follows: if an `INPVALUES=` data set and an `ID` statement are specified, then the observations are labeled with the ID values; if a `DATA=` data set is specified, then the observations are labeled with their constructed test name; otherwise, the observation or test number is displayed.

**NOTESTNAME**

displays the number of the test instead of the test name on the X-axis, which is useful when you have many tests.

**UNPACK**

suppresses paneling. By default, Manhattan plots are created for each requested  $p$ -value adjustment, and the results are grouped in a single display, called a *panel*. Specify UNPACK to display each plot separately.

**VREF**=number | NONE

displays a reference line at  $-\log_{10}(\text{number})$ . The *number* must be between 0 and 1. By default, a reference line at  $-\log_{10}(0.05)$  is displayed; it can be suppressed by specifying `VREF=0` or `VREF=NONE`. If the LABEL option is also specified, then observations above this line are labeled with their ID variables, their observation number, their test name, or their test number.

**NONE**

suppresses all plots.

**PBYTEST**< (options) >

displays the adjusted  $p$ -values for each test. The available options are as follows:

**NOTESTNAME**

displays the number of the test instead of the test name on the axis, which is useful when you have many tests.



**VREF=**

*number-list* displays reference lines at the  $p$ -values specified in the *number-list*. The values in the *number-list* must be between 0 and 1; otherwise they are ignored. You can specify a single value or a list of values; for example, **vref=0.1 0 to 0.05 by 0.01** displays reference lines at each of the values {0.01, 0.02, 0.03, 0.04, 0.05, and 0.1}.

**RAWPROB<(UNPACK)>**

displays a uniform probability plot of 1 minus the raw  $p$ -values (Schweder and Spjøtvoll 1982) along with a histogram. If  $m_0$  is the number of true null hypotheses among the  $m$  tests, the points on the left side of the plot should be approximately linear with slope  $\frac{1}{m_0+1}$ . This graphic is displayed when an adaptive  $p$ -value adjustment method is requested in order to see if the **NTRUENULL=** estimate is appropriate. The UNPACK option unpanels the display.

**PTRUENULL=***keyword* | *value*

**PIO=***keyword* | *value*

is alias for the **NTRUENULL=** option, except that you can specify the proportion of true null hypotheses as a *value* between 0 and 1, instead of specifying the number of true null hypotheses. The available *keywords* are also the **NTRUENULL=** options described on page 5175.

**RANUNI**

requests the random number generator used in releases prior to SAS 9.2. Beginning with SAS 9.2, the random number generator is the Mersenne Twister, which has better performance when bootstrapping. Changes in the **bootstrap-** or **permutation-**adjusted  $p$ -values from prior releases are due to unimportant sampling differences.

**SEED=***number*

**S=***number*

specifies the initial seed for the random number generator used for resampling. The value for *number* must be an integer. If you do not specify a seed, or if you specify a value less than or equal to zero, then PROC MULTTEST uses the time of day from the computer's clock to generate an initial seed. For more details about seed values, see *SAS Language Reference: Concepts*.

**SIDAK****SID**

computes the Šidák adjustment for each test. These adjustments take the form

$$1 - (1 - p)^m$$

where  $p$  is the raw  $p$ -value and  $m$  is the number of tests. These are slightly less conservative than the Bonferroni adjustments, but they still should be viewed with caution. When exact tests are specified via the **PERMUTATION=** option in the **TEST** statement, the actual permutation distributions are used, resulting in a much less conservative version of this procedure (Westfall and Wolfinger 1997). See the section “Šidák” on page 5197 for more details.

**STEPBON****HOLM**

requests adjusted  $p$ -values by using the step-down Bonferroni method of Holm (1979). See the section “Step-Down Methods” on page 5198 for more details.



**STEPBOOT**

requests that adjusted  $p$ -values be computed by using bootstrap resampling as described under the **BOOTSTRAP** option, but in step-down fashion. See the section “[Step-Down Methods](#)” on page 5198 for more details.

**STEPPERM**

requests that adjusted  $p$ -values be computed by using permutation resampling as described under the **PERMUTATION** option, but in step-down fashion. See the section “[Step-Down Methods](#)” on page 5198 for more details.

**STEPSID**

requests adjusted  $p$ -values by using the Šidák method as described in the **SIDAK** option, but in step-down fashion. See the section “[Step-Down Methods](#)” on page 5198 for more details.

**STOUFFER****LIPTAK**

requests adjusted  $p$ -values by using the Stouffer-Liptak combination method. See the section “[Stouffer-Liptak Combination](#)” on page 5199 for more details.

---

## BY Statement

**BY** *variables* ;

You can specify a **BY** statement with PROC MULTTEST to obtain separate analyses of observations in groups that are defined by the **BY** variables. When a **BY** statement appears, the procedure expects the input data set to be sorted in order of the **BY** variables. If you specify more than one **BY** statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar **BY** statement.
- Specify the **NOTSORTED** or **DESCENDING** option in the **BY** statement for the MULTTEST procedure. The **NOTSORTED** option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the **BY** variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the **BY** variables by using the DATASETS procedure (in Base SAS software).

You can specify one or more *variables* in the input data set on the **BY** statement.

Since sorting the data changes the order in which PROC MULTTEST reads observations, this can affect the sort order for the levels of the **CLASS** variable if you have specified **ORDER=DATA** in the PROC MULTTEST statement. This, in turn, affects specifications in the **CONTRAST** statements.

For more information about **BY**-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

---

## CLASS Statement

```
CLASS variable </ TRUNCATE > ;
```

The CLASS statement is required unless the `INPVALUES=` option is specified. The CLASS statement specifies a single variable (character or numeric) used to identify the groups for the analysis. For example, if the variable `Treatment` defines different levels of a treatment that you want to compare, then you would specify the following statements:

```
class Treatment;
```

The CLASS variable can be either character or numeric. By default, class levels are determined from the entire set of formatted values of the CLASS variable. The order of the class levels used by PROC MULTTEST corresponds to the order of their formatted values; this order can be changed with the `ORDER=` option in the PROC MULTTEST statement.

**NOTE:** Prior to SAS 9, class levels were determined by using no more than the first 16 characters of the formatted values. To revert to this previous behavior you can specify the `TRUNCATE` option in the CLASS statement.

In any case, you can use formats to group values into levels. See the discussion of the `FORMAT` procedure in the *Base SAS Procedures Guide* and the discussions of the `FORMAT` statement and SAS formats in *SAS Formats and Informats: Reference*. You can adjust the order of CLASS variable levels with the `ORDER=` option in the PROC MULTTEST statement. You need to be aware of the order when using the `CONTRAST` statement, and you should check the “Contrast Coefficients” table to verify that it is suitable.

You can specify the following option in the CLASS statement after a slash (/):

### TRUNCATE

specifies that class levels should be determined by using only up to the first 16 characters of the formatted values of CLASS variables. When formatted values are longer than 16 characters, you can use this option to revert to the levels as determined in releases prior to SAS 9.

---

## CONTRAST Statement

```
CONTRAST 'label' values ;
```

This statement is used to identify tests between the levels of the CLASS variable; in particular, it is used to specify the coefficients for the trend tests. The *label* is a string naming the contrast; it contains a maximum of 21 characters. The *values* are scoring coefficients across the CLASS variable levels.

You can specify multiple CONTRAST statements, thereby specifying multiple contrasts for each variable. Multiplicity adjustments are computed for all contrasts and all variables simultaneously. The coefficients are applied to the ordered CLASS variables; this order can be changed with the `ORDER=` option in the PROC MULTTEST statement. For example, consider a four-group experiment with CLASS variable levels A1, A2, B1, and B2 denoting two levels of two treatments. The following statements produce three linear trend tests for each variable identified in the TEST statement. PROC MULTTEST computes the multiplicity adjustments over the entire collection of tests, which is three times the number of variables.

```
contrast 'a vs b' -1 -1 1 1;
contrast 'a linear' -1 1 0 0;
contrast 'b linear' 0 0 -1 1;
```

As another example, consider an animal carcinogenicity experiment with dose levels 0, 4, 8, 16, and 50. You can specify a trend test with the indicated scoring coefficients by using the following statement:

```
contrast 'arithmetic trend' 0 4 8 16 50;
```

Multiplicity-adjusted  $p$ -values are then computed over the collection of variables identified in the **TEST** statement. See Lagakos and Louis (1985) for guidelines on the selection of contrast-scoring values.

When a Fisher test is specified in the **TEST** statement, the **CONTRAST** statement coefficients are used to group the **CLASS** variable's levels. Groups with a  $-1$  contrast coefficient are combined and compared with groups with a  $1$  contrast coefficient for each test, and groups with a  $0$  coefficient are not included in the contrast. For example, the following statements compute Fisher exact tests for (a) control versus the combined treatment groups, (b) control versus the first treatment group, and (c) control versus the third treatment group:

```
contrast 'c vs all' 1 -1 -1 -1;
contrast 'c vs t1' 1 -1 0 0;
contrast 'c vs t3' 1 0 0 -1;
```

Multiplicity adjustments are then computed over the entire collection of tests and variables. Only  $-1$ ,  $1$ , and  $0$  are acceptable **CONTRAST** coefficients when the Fisher test is specified; PROC MULTTEST ignores the **CONTRAST** statement if any other coefficients appear.

If you specify the **FISHER** test and no **CONTRAST** statements, then all contrasts of control versus treatment are automatically generated, with the first level of the **CLASS** variable deemed to be the control. In this case, the control level is assigned the value  $1$  in each contrast and the other treatment levels are assigned  $-1$ . You should therefore use the **LOWERTAILED** option to test for higher success rates in the treatment groups.

For tests other than **FISHER**, **CONTRAST** values are  $0, 1, 2, \dots$  by default. If you specify the **CA** or **PETO** test with the **PERMUTATION=** option, then your **CONTRAST** coefficients must be integer valued.

For  $t$  tests for the mean of continuous data (and for the **FT** tests), the contrast coefficients are centered to have mean  $= 0$ . The resulting centered scoring coefficients are then applied to the sample means (or to the double-arcsine-transformed proportions in the case of the **FT** tests).

## FREQ Statement

**FREQ** *variable* ;

The **FREQ** statement names a variable that provides frequencies for each observation in the **DATA=** data set. Specifically, if  $n$  is the value of the **FREQ** variable for a given observation, then that observation is used  $n$  times.

If the value of the **FREQ** variable is missing or is less than  $1$ , the observation is not used in the analysis. If the value is not an integer, only the integer portion is used.

---

## ID Statement

**ID** *variables* ;

The ID statement names one or more variables for identifying observations in the output and in the plots. The statement requires an **INPVALUES=** data set. All ID variables are displayed in the “pValues” table. The ID variables are used as the X axis for the plots requested by the **PLOTS=PBYTEST** and **PLOTS=MANHATTAN** options in the PROC MULTTEST statement; they are also used to label points on the Manhattan plots. This option has no effect on the **OUT=** data set.

---

## STRATA Statement

**STRATA** *variable* ;

The STRATA statement identifies a single variable to use as a stratification variable in the analysis. This yields tests similar to those discussed in Mantel and Haenszel (1959) and Hoel and Walburg (1972) for binary data and pooled-means tests for continuous data. For example, when you test for prevalence in a carcinogenicity study, it is common to stratify on intervals of the time of death; the first level of the stratification variable might represent weeks 0–52, the second might represent weeks 53–80, and so on. In multicenter clinical studies, each level of the stratification variable might represent a particular center.

The following option is available in the STRATA statement after a slash (/):

**WEIGHT=***keyword*

specifies the type of strata weighting to use when computing the Freeman-Tukey and *t* tests. Valid *keywords* are SAMPLESIZE, HARMONIC, and EQUAL. SAMPLESIZE requests weights proportional to the within-stratum sample sizes, and is the default method even if the WEIGHT= option is not specified. HARMONIC sets up weights equal to the harmonic mean of the nonmissing within-stratum CLASS sizes, and is similar to a Type 2 analysis in PROC GLM. EQUAL specifies equal weights, and is similar to a Type 3 analysis in PROC GLM.

---

## TEST Statement

**TEST** *name (variables </ options>)* ;

The TEST statement is required unless the **INPVALUES=** option is specified. The TEST statement identifies statistical tests to be performed and the discrete and continuous variables to be tested. [Table 61.2](#) summarizes the names and options available in the TEST statement.

**Table 61.2** TEST Statement Names and Options

| Option              | Description                                                                                  |
|---------------------|----------------------------------------------------------------------------------------------|
| <b>TEST Names</b>   |                                                                                              |
| CA                  | Requests the Cochran-Armitage linear trend tests for group comparisons                       |
| FISHER              | Requests Fisher exact tests                                                                  |
| FT                  | Requests Z-score CA tests based upon the Freeman-Tukey double arcsine transformation         |
| MEAN                | Requests the <i>t</i> test for the mean                                                      |
| PETO                | Requests the Peto mortality-prevalence test                                                  |
| <b>TEST Options</b> |                                                                                              |
| BINOMIAL            | Uses the binomial variance estimate for CA and Peto tests                                    |
| CONTINUITY=         | Specifies a continuity correction                                                            |
| DDFM=               | Specifies whether to use homogeneous or heterogeneous variances                              |
| LOWERTAILED         | Makes all tests lower-tailed                                                                 |
| PERMUTATION=        | Computes <i>p</i> -values for the CA and Peto tests by using exact permutation distributions |
| TIME=               | Identifies the Peto test variable containing the age at death                                |
| UPPERTAILED         | Makes all tests upper-tailed                                                                 |

The following tests are permitted as *name* in the TEST statement.

**CA**

requests the Cochran-Armitage linear trend tests for group comparisons. The test variables should take the value 0 for a failure and 1 for a success. **PERMUTATION=** option can be used to request an exact permutation test; otherwise, a Z-score approximation is used. The **CONTINUITY=** option can be used to specify a continuity correction for the Z-score approximation.

**FISHER**

requests Fisher exact tests for comparing two treatment groups. The test variables should take the value 0 for a failure and 1 for a success.

**FT**

requests Z-score CA tests based upon the Freeman-Tukey double arcsine transformation of the frequencies. The test variables should take the value 0 for a failure and 1 for a success.

**MEAN**

requests the *t* test for the mean. The test variables can take on any numeric values.

**PETO**

requests the Peto mortality-prevalence test. The test variables should take the value 0 for a nonoccurrence, 1 for an incidental occurrence, and 2 for a fatal occurrence. The **TIME=** option should be used with the Peto test to specify an integer-valued variable giving the age at death. The **CONTINUITY=** option can be used to specify a continuity correction for the test.

If the value of a TEST variable is invalid, the observation is not used in the analysis. You can specify two tests only if one of them is **MEAN**. For example, the following statement is valid:

```
test ca (d1-d2) mean (c1-c2);
```

But specifying both CA and FT, as shown in the following statement, is invalid:

```
test ca (d1-d2) ft (d1-d2);
```

You can specify the following options in the TEST statement (some apply to only one test).

#### **BINOMIAL**

uses the binomial variance estimate for CA and Peto tests in their asymptotic normal approximations. The default is to use the hypergeometric variance.

#### **CONTINUITY=number**

##### **C=number**

specifies *number* as a particular continuity correction for the Z-score approximation in the CA and Peto tests. The default is 0.

#### **LOWERTAILED**

##### **LOWER**

is used to make all tests lower-tailed. All tests are two-tailed by default.

#### **PERMUTATION=number**

##### **PERM=number**

computes *p*-values for the CA and Peto tests by using exact permutation distributions when marginal success or failure totals within a stratum are *number* or less. You can specify *number* as a nonnegative integer. For totals greater than *number* (or when the PERMUTATION= option is omitted), PROC MULTTEST uses standard normal approximations with a continuity correction chosen to approximate the permutation distribution. PROC MULTTEST computes the appropriate convolution distributions when you use the [STRATA](#) statement along with the PERMUTATION= option.

#### **DDFM= POOLED | SATTERTHWAITE**

specifies whether the [MEAN](#) test uses a homogeneity assumption (DDFM=POOLED, the default) or deals with heterogeneous variances (DDFM=SATTERTHWAITE). See “[t Test for the Mean](#)” on page 5194 for more information.

#### **TIME=variable**

identifies the Peto test variable containing the age at death, which must be integer valued. If the TIME= option is omitted, all ages are assumed to equal 1.

#### **UPPERTAILED**

##### **UPPER**

is used to make all tests upper-tailed. All tests are two-tailed by default.

---

## Details: MULTTEST Procedure

---

### Statistical Tests

The following section discusses the statistical tests performed in the MULTTEST procedure. For continuous data, a  $t$  test for the mean (**MEAN**) is available. For discrete variables, available tests are the Cochran-Armitage linear trend test (**CA**), the Freeman-Tukey double arcsine test (**FT**), the Peto mortality-prevalence test (**PETO**), and the Fisher exact test (**FISHER**).

Throughout this section, the discrete and continuous variables are denoted by  $S_{vgsr}$  and  $X_{vgsr}$ , respectively, where  $v$  is the variable,  $g$  is the treatment group,  $s$  is the stratum, and  $r$  is the replication. Let  $m_{vgs}$  denote the sample size for a binary variable  $v$  within group  $g$  and stratum  $s$ . A plus sign (+) subscript denotes summation over an index. Note that the tests are invariant to the location and scale of the contrast coefficients  $t_g$ .

### Cochran-Armitage Linear Trend Test

The Cochran-Armitage linear trend test (Cochran 1954; Armitage 1955; Agresti 2002) is implemented by using a  $Z$ -score approximation, an exact permutation distribution, or a combination of both.

#### Z-Score Approximation

The pooled probability estimate for variable  $v$  and stratum  $s$  is

$$p_{vs} = \frac{S_{v+s+}}{m_{v+s}}$$

The expected value (under constant within-stratum treatment probabilities) for variable  $v$ , group  $g$ , and stratum  $s$  is

$$E_{vgs} = m_{vgs} p_{vs}$$

Letting  $t_g$  denote the contrast trend coefficients specified by the **CONTRAST** statement, the test statistic for variable  $v$  has numerator

$$N_v = \sum_s \sum_g t_g (S_{vgs+} - E_{vgs})$$

The binomial variance estimate for this statistic is

$$V_v = \sum_s p_{vs}(1 - p_{vs}) \sum_g m_{vgs} (t_g - \bar{t}_{vs})^2$$

where

$$\bar{t}_{vs} = \sum_g \frac{m_{vgs} t_g}{m_{v+s}}$$

The hypergeometric variance estimate (the default) is

$$V_v = \sum_s \{m_{v+s}/(m_{v+s} - 1)\} p_{vs}(1 - p_{vs}) \sum_g m_{vgs} (t_g - \bar{t}_{vs})^2$$

For any strata  $s$  with  $m_{v+s} \leq 1$ , the contribution to the variance is taken to be zero.

PROC MULTTEST computes the  $Z$ -score statistic

$$Z_v = \frac{N_v}{\sqrt{V_v}}$$

The  $p$ -value for this statistic comes from the standard normal distribution. Whenever a 0 is computed for the denominator, the  $p$ -value is set to 1. This  $p$ -value approximates the probability obtained from the exact permutation distribution, discussed in the following text.

The  $Z$ -score statistic can be continuity-corrected to better approximate the permutation distribution. With continuity correction  $c$ , the upper-tailed  $p$ -value is computed from

$$Z_v = \frac{N_v - c}{\sqrt{V_v}}$$

For two-tailed, noncontinuity-corrected tests, PROC MULTTEST reports the  $p$ -value as  $2 \min(p, 1 - p)$ , where  $p$  is the upper-tailed  $p$ -value. The same formula holds for the continuity-corrected test, with the exception that when the noncontinuity-corrected  $Z$  and the continuity-corrected  $Z$  have opposite signs, the two-tailed  $p$ -value is 1.

When the `PERMUTATION=` option is specified and no `STRATA` variable is specified, PROC MULTTEST uses a continuity correction selected to optimally approximate the upper-tail probability of permutation distributions with smaller marginal totals (Westfall and Lin 1988). Otherwise, the continuity correction is specified by the `CONTINUITY=` option in the `TEST` statement.

The `CA`  $Z$ -score statistic is the Hoel-Walburg (Mantel-Haenszel) statistic reported by Dinse (1985).

### Exact Permutation Test

When you use the `PERMUTATION=` option for `CA` in the `TEST` statement, PROC MULTTEST computes the exact permutation distribution of the trend score

$$T_v = \sum_s \sum_g t_g S_{vgs+}$$

where the contrast trend coefficients  $t_g$  must be integer valued. The observed value of this trend is compared to the permutation distribution to obtain the  $p$ -value

$$p_v = \Pr(X \geq \text{observed } T_v)$$

where  $X$  is a random variable from the permutation distribution and where upper-tailed tests are requested. This probability can be viewed as a binomial probability, where the within-stratum probabilities are constant and where the probability is conditional with respect to the marginal totals  $S_{v+s+}$ . It also can be considered a rerandomization probability.

Because the computations can be quite time-consuming with large data sets, specifying the `PERMUTATION=number` option in the `TEST` statement limits the situations where PROC MULTTEST computes the exact permutation distribution. When marginal total success or total failure frequencies exceed `number` for a particular stratum, the permutation distribution is approximated by a continuity-corrected normal distribution. You should be cautious when using the `PERMUTATION=` option in conjunction with bootstrap resampling because the permutation distribution is recomputed for each bootstrap sample. This recomputation is not necessary with permutation resampling.



The permutation distribution is computed in two steps:

1. The permutation distributions of the trend scores are computed within each stratum.
2. The distributions are convolved to obtain the distribution of the total trend.

As long as the total success or failure frequency does not exceed *number* for any stratum, the computed distributions are exact. In other words, if  $S_{v+s+} \leq \text{number}$  or  $(m_{v+s} - S_{v+s+}) \leq \text{number}$  for all  $s$ , then the permutation trend distribution for variable  $v$  is computed exactly.

In step 1, the distribution of the within-stratum trend

$$\sum_g t_g S_{vg s+}$$

is computed by using the multivariate hypergeometric distribution of the  $S_{vg s+}$ , provided *number* is not exceeded. This distribution can be written as

$$\Pr(S_{v1s+}, S_{v2s+}, \dots, S_{vGs+}) = \prod_{g=1}^G \frac{\binom{m_{vgs}}{S_{vgs+}}}{\binom{m_{v+s}}{S_{v+s+}}}$$

The distribution of the within-stratum trend is then computed by summing these probabilities over appropriate configurations. For further information about this technique, see Bickis and Krewski (1986) and Westfall and Lin (1988). In step 2, the exact convolution distribution is obtained for the trend statistic summed over all strata having totals that meet the threshold criterion. This distribution is obtained by applying the fast Fourier transform to the exact within-stratum distributions. A description of this general method can be found in Pagano and Tritchler (1983) and Good (1987).

The convolution distribution of the overall trend is then computed by convolving the exact distribution with the distribution of the continuity-corrected standard normal approximation. To be more specific, let  $S_1$  denote the subset of stratum indices that satisfy the threshold criterion, and let  $S_2$  denote the subset of indices that do not satisfy the criterion. Let  $T_{v1}$  denote the combined trend statistic from the set  $S_1$ , which has an exact distribution obtained from Fourier analysis as previously outlined, and let  $T_{v2}$  denote the combined trend statistic from the set  $S_2$ . Then the distribution of the overall trend  $T_v = T_{v1} + T_{v2}$  is obtained by convolving the analytic distribution of  $T_{v1}$  with the continuity-corrected normal approximation for  $T_{v2}$ . Using the notation from the section “Z-Score Approximation” on page 5188, this convolution can be written as

$$\begin{aligned} \Pr(T_{v1} + T_{v2} \geq u) &= \sum_{u1} \Pr(T_{v1} + T_{v2} \geq u \mid T_{v1} = u1) \Pr(T_{v1} = u1) \\ &\approx \sum_{u1} \Pr(Z \geq z) \Pr(T_{v1} = u1) \end{aligned}$$

where  $Z$  is a standard normal random variable, and

$$z = \frac{1}{\sqrt{V_v}} \left( u - u1 - \sum_{S_2} p_{vs} \sum_g t_g m_{vgs} - c \right)$$

In this expression, the summation of  $s$  in  $V_v$  is over  $S_2$ , and  $c$  is the continuity correction discussed under the  $Z$ -score approximation.

When a two-tailed test is requested, the expected trend is computed

$$E_v = \sum_s \sum_g t_g E_{vgs}$$

The two-tailed  $p$ -value is reported as the permutation tail probability for the observed trend  $T_v$  plus the permutation tail probability for  $2E_v - T_v$ , the reflected trend.

### Freeman-Tukey Double Arcsine Test

For this test, the contrast trend coefficients  $t_1, \dots, t_G$  are centered to the values  $c_1, \dots, c_G$ , where  $c_g = t_g - \bar{t}$ ,  $\bar{t} = \sum_g t_g / G$ , and  $G$  is the number of groups. The numerator of this test statistic is

$$N_v = \sum_s w_{vs} \sum_g c_g f(S_{vgs+}, m_{vgs})$$

where the weights  $w_{vs}$  take on three different types of values depending upon your specification of the **WEIGHT=** option in the **STRATA** statement. The default value is the within-strata sample size  $m_{v+s}$ , ensuring comparability with the ordinary CA trend statistic. **WEIGHT=HARMONIC** sets  $w_{vs}$  equal to the harmonic mean

$$\left[ \left( \sum_g \frac{1}{m_{vgs}} \right) / G^* \right]^{-1}$$

where  $G^*$  is the number of nonmissing groups and the summation is over only the nonmissing elements. The harmonic means analysis places more weight on the smaller sample sizes than does the default sample size method, and is similar to a Type 2 analysis in PROC GLM. **WEIGHT=EQUAL** sets  $w_{vs} = 1$  for all  $v$  and  $s$ , and is similar to a Type 3 analysis in PROC GLM.

The function  $f(r, n)$  is the double arcsine transformation:

$$f(r, n) = \arcsin \left( \sqrt{\frac{r}{n+1}} \right) + \arcsin \left( \sqrt{\frac{r+1}{n+1}} \right)$$

The variance estimate is

$$V_v = \sum_s w_{vs}^2 \sum_g \frac{c_g^2}{m_{vgs} + \frac{1}{2}}$$

The test statistic is

$$Z_v = \frac{N_v}{\sqrt{V_v}}$$

The Freeman-Tukey transformation and its variance are described by Freeman and Tukey (1950) and Miller (1978). Since its variance is not weighted by the pooled probabilities, as is the CA test, the **FT** test can be more useful than the CA test for tests involving only a subset of the groups.

### Peto Mortality-Prevalence Trend Test

The Peto test is a modified Cochran-Armitage procedure incorporating mortality and prevalence information. The Peto test is computed like two Cochran-Armitage Z-score approximations, one for prevalence and one for mortality (Peto, Pike, and Day 1980). It represents a special case in PROC MULTTEST because the data structure requirements are different, and the resampling methods used for adjusting  $p$ -values are not valid. The `TIME=` option variable is required to specify “death” times or, more generally, times of occurrence. In addition, the test variables must assume one of the following three values:

- 0 = no occurrence
- 1 = incidental occurrence
- 2 = fatal occurrence

Use the `TIME=` option variable to define the mortality strata, and use the `STRATA` statement variable to define the prevalence strata.

In the following notation, the subscript  $v$  represents the variable,  $g$  represents the treatment group,  $s$  represents the stratum, and  $t$  represents the time. Recall that a plus sign (+) in a subscript location denotes summation over that subscript.

Let  $S_{vgs}^P$  be the number of incidental occurrences, and let  $m_{vgs}^P$  be the total sample size for variable  $v$  in group  $g$ , stratum  $s$ , excluding fatal tumors.

Let  $S_{vgt}^F$  be the number of fatal occurrences in time period  $t$ , and let  $m_{vgt}^F$  be the number of patients alive at the end of time  $t - 1$ .

The pooled probability estimates are given by

$$p_{vs}^P = \frac{S_{v+s}^P}{m_{v+s}^P}$$

$$p_{vt}^F = \frac{S_{v+t}^F}{m_{v+t}^F}$$

The expected values are

$$E_{vgs}^P = m_{vgs}^P p_{vs}^P$$

$$E_{vgt}^F = m_{vgt}^F p_{vt}^F$$

Let  $t_g$  denote a contrast trend coefficient, and define the numerator terms as follows:

$$N_v^P = \sum_s \sum_g t_g (S_{vgs}^P - E_{vgs}^P)$$

$$N_v^F = \sum_t \sum_g t_g (S_{vgt}^F - E_{vgt}^F)$$

Define the denominator variance terms by using the binomial variance:

$$V_v^P = \sum_s p_{vs}^P (1 - p_{vs}^P) \left[ \left( \sum_g m_{vgs}^P t_g^2 \right) - \frac{1}{m_{v+s}^P} \left( \sum_g m_{vgs}^P t_g \right)^2 \right]$$

$$V_v^F = \sum_s p_{vt}^F (1 - p_{vt}^F) \left[ \left( \sum_g m_{vgt}^F t_g^2 \right) - \frac{1}{m_{v+t}^F} \left( \sum_g m_{vgt}^F t_g \right)^2 \right]$$

The hypergeometric variances (the default) are calculated by weighting the within-strata variances as discussed in the section “Z-Score Approximation” on page 5188.

The Peto statistic is computed as

$$Z_v = \frac{N_v^P + N_v^F - c}{\sqrt{V_v^P + V_v^F}}$$

where  $c$  is a continuity correction. The  $p$ -value is determined from the standard normal distribution unless the `PERMUTATION=number` option is used. When you use the `PERMUTATION=` option for `PETO` in the `TEST` statement, PROC MULTTEST computes the “discrete approximation” permutation distribution described by Mantel (1980) and Soper and Tonkonoh (1993). Specifically, the permutation distribution of  $\sum_s \sum_g t_g S_{vgs}^P + \sum_t \sum_g t_g S_{vgt}^F$  is computed, assuming that  $\{\sum_g t_g S_{vgs}^P\}$  and  $\{\sum_g t_g S_{vgt}^F\}$  are independent over all  $s$  and  $t$ . Note that the contrast trend coefficients  $t_g$  must be integer valued. The  $p$ -values are exact under this independence assumption. However, the independence assumption is valid only asymptotically, which is why these  $p$ -values are called “approximate.”

An exact permutation distribution is available only under the assumption of equal risk of censoring in all treatment groups; even then, computing this distribution can be cumbersome. Soper and Tonkonoh (1993) describe situations where the discrete approximation distribution closely fits the exact permutation distribution.

### Fisher Exact Test

The `CONTRAST` statement in PROC MULTTEST enables you to compute Fisher exact tests for two-group comparisons. No stratification variable is allowed for this test. Note, however, that the `FISHER` exact test is a special case of the exact permutation tests performed by PROC MULTTEST and that these permutation tests allow a stratification variable. Recall that contrast coefficients can be  $-1$ ,  $0$ , or  $1$  for the Fisher test. The frequencies and sample sizes of the groups scored as  $-1$  are combined, as are the frequencies and sample sizes of the groups scored as  $1$ . Groups scored as  $0$  are excluded. The  $-1$  group is then compared with the  $1$  group by using the Fisher exact test.

Letting  $x$  and  $m$  denote the frequency and sample size of the  $1$  group, and letting  $y$  and  $n$  denote those of the  $-1$  group, the  $p$ -value is calculated as

$$\Pr(X \geq x \mid X + Y = x + y) = \sum_{i=x}^m \frac{\binom{m}{i} \binom{n}{x+y-i}}{\binom{m+n}{x+y}}$$

where  $X$  and  $Y$  are independent binomially distributed random variables with sample sizes  $m$  and  $n$  and common probability parameters. The hypergeometric distribution is used to determine the stated probability; Yates (1984) discusses this technique. PROC MULTTEST computes the two-tailed  $p$ -values by adding probabilities from both tails of the hypergeometric distribution. The first tail is from the observed  $x$  and  $y$ , and the other tail is chosen so that the resulting probability is as large as possible without exceeding the probability from the first tail. If the variable being tested has only one level, then the  $p$ -value is set to 1.

### ***t* Test for the Mean**

For continuous variables, PROC MULTTEST automatically centers the contrast trend coefficients, as in the Freeman-Tukey test. These centered coefficients  $c_g$  are then used to form a  $t$  statistic contrasting the within-group means. Let  $n_{vgs}$  denote the sample size within group  $g$  and stratum  $s$ ; it depends on variable  $v$  only when there are missing values. Determine the weights  $w_{vs}$  as in the Freeman-Tukey test with  $n_{vgs}$  replacing  $m_{vgs}$ . Define

$$\bar{X}_{vgs+} = \frac{1}{n_{vgs}} \sum_r X_{vgsr}$$

as the sample mean within a group-and-stratum combination, and let  $\mu_{vgs}$  denote the treatment means. Write the null hypothesis as

$$\sum_s w_{vs} \sum_g c_g \mu_{vgs} = 0$$

Also define

$$s_v^2 = \frac{\sum_s \sum_g \sum_r (X_{vgsr} - \bar{X}_{vgs+})^2}{\sum_s \sum_g (n_{vgs} - 1)}$$

as the pooled sample variance.

### ***Homogeneous Variance***

Assuming constant variance for all group-and-stratum combinations, the  $t$  statistic for the mean is

$$M_v = \frac{\sum_s w_{vs} \sum_g c_g \bar{X}_{vgs+}}{\sqrt{s_v^2 \left( \sum_s w_{vs}^2 \sum_g \frac{c_g^2}{n_{vgs}} \right)}}$$

Then under the null hypothesis and assuming normality, independence, and homoscedasticity,  $M_v$  follows a  $t$  distribution with  $df_p = \sum_s \sum_g (n_{vgs} - 1)$  degrees of freedom.

Whenever a denominator of 0 is computed, the  $p$ -value is set to 1. When missing data force  $n_{vgs} = 0$ , the contribution to the denominator of the pooled variance is 0 and not  $-1$ . This is also true for the degrees of freedom.

### Heterogeneous Variance

If you do not assume constant variance for all group-and-stratum combinations, then the approximate  $t$  test is

$$M_v = \frac{\sum_s w_{vs} \sum_g c_g \bar{X}_{vgs} +}{\sqrt{\sum_s w_{vs}^2 \sum_g c_g^2 \frac{s_{vgs}^2}{n_{vgs}}}}$$

Under the null hypothesis and assuming normality and independence, the Satterthwaite (1946) approximation for the degrees of freedom of the  $t$  test is given by

$$df_s = \frac{\left(\sum_s w_{vs}^2 \sum_g c_g^2 \frac{s_{vgs}^2}{n_{vgs}}\right)^2}{\sum_s \sum_g \frac{\left(w_{vs}^2 c_g^2 \frac{s_{vgs}^2}{n_{vgs}}\right)^2}{n_{vgs} - 1}}$$

under the restriction  $1 \leq df_s \leq \sum_s \sum_g n_{vgs}$ .

Whenever a denominator of 0 for  $M_v$  is computed, the  $p$ -value is set to 1. If the denominator for  $df_s$  is computed as 0, then set  $df_s = df_p$ . When missing data force  $n_{vgs} \leq 1$ , that group-and-stratum combination does not contribute to the  $df_s$  computation.

## p-Value Adjustments

Suppose you test  $m$  null hypotheses,  $H_{01}, \dots, H_{0m}$ , and obtain the  $p$ -values  $p_1, \dots, p_m$ . Denote the ordered  $p$ -values as  $p_{(1)} \leq \dots \leq p_{(m)}$  and order the tests appropriately:  $H_{0(1)}, \dots, H_{0(m)}$ . Suppose you know  $m_0$  of the null hypotheses are true and  $m_1 = m - m_0$  are false. Let  $R$  indicate the number of null hypotheses rejected by the tests, where  $V$  of these are incorrectly rejected (that is,  $V$  tests are Type I errors) and  $R - V$  are correctly rejected (so  $m_1 - R + V$  tests are Type II errors). This information is summarized in the following table:

|               | Null is Rejected | Null is Not Rejected | Total |
|---------------|------------------|----------------------|-------|
| Null is True  | $V$              | $m_0 - V$            | $m_0$ |
| Null is False | $R - V$          | $m_1 - R + V$        | $m_1$ |
| Total         | $R$              | $m - R$              | $m$   |

The *familywise error rate* (FWE) is the overall Type I error rate for all the comparisons (possibly under some restrictions); that is, it is the maximum probability of incorrectly rejecting one or more null hypotheses:

$$\text{FWE} = \Pr(V > 0)$$

The FWE is also known as the *maximum experimentwise error rate* (MEER), as discussed in the section “Pairwise Comparisons” on page 3351 of Chapter 42, “The GLM Procedure.”

The *false discovery rate* (FDR) is the expected proportion of incorrectly rejected hypotheses among all rejected hypotheses:

$$\begin{aligned} \text{FDR} &= E\left(\frac{V}{R}\right) \quad \text{where } \frac{V}{R} = 0 \text{ when } V = R = 0 \\ &= E\left(\frac{V}{R} \mid R > 0\right) \Pr(R > 0) \end{aligned}$$

Under the overall null hypothesis (all the null hypotheses are true), the FDR=FWE since  $V = R$  gives  $E\left(\frac{V}{R}\right) = 1 \times \Pr\left(\frac{V}{R} = 1\right) = \Pr(V > 0)$ . Otherwise, FDR is always less than FWE, and an FDR-controlling adjustment also controls the FWE. Another definition used is the *positive* false discovery rate:

$$\text{pFDR} = E\left(\frac{V}{R} \mid R > 0\right)$$

The  $p$ -value adjustment methods discussed in the following sections attempt to correct the raw  $p$ -values while controlling either the FWE or the FDR. Note that the methods might impose some restrictions in order to achieve this; restrictions are discussed along with the methods in the following sections. Discussions and comparisons of some of these methods are given in Dmitrienko et al. (2005), Dudoit, Shaffer, and Boldrick (2003), Westfall et al. (1999), and Brown and Russell (1997).

## Familywise Error Rate Controlling Adjustments

PROC MULTTEST provides several  $p$ -value adjustments to control the familywise error rate. *Single-step* adjustment methods are computed without reference to the other hypothesis tests under consideration. The available single-step methods are the Bonferroni and Šidák adjustments, which are simple functions of the raw  $p$ -values that try to distribute the significance level  $\alpha$  across all the tests, and the bootstrap and permutation resampling adjustments, which require the raw data. The Bonferroni and Šidák methods are calculated from the permutation distributions when exact permutation tests are used with the **CA** or **Peto** test.

*Stepwise* tests, or *sequentially rejective* tests, order the hypotheses in *step-up* (least significant to most significant) or *step-down* fashion, then sequentially determine acceptance or rejection of the nulls. These tests are more powerful than the single-step tests, and they do not always require you to perform every test. However, PROC MULTTEST still adjusts every  $p$ -value. PROC MULTTEST provides the following stepwise  $p$ -value adjustments: step-down Bonferroni (Holm), step-down Šidák, step-down bootstrap and permutation resampling, Hochberg's (1988) step-up, Hommel's (1988), Fisher's combination method, and the Stouffer-Liptak combination method. Adaptive versions of Holm's step-down Bonferroni and Hochberg's step-up Bonferroni methods, which require an estimate of the number of true null hypotheses, are also available.

Liu (1996) shows that all single-step and stepwise tests based on marginal  $p$ -values can be used to construct a *closed* test (Marcus, Peritz, and Gabriel 1976; Dmitrienko et al. 2005). Closed testing methods not only control the familywise error rate at size  $\alpha$ , but are also more powerful than the tests on which they are based. Westfall and Wolfinger (2000) note that several of the methods available in PROC MULTTEST are closed—namely, the **step-down methods**, **Hommel's method**, and **Fisher's combination**; see that reference for conditions and exceptions.

All methods except the resampling methods are calculated by simple functions of the raw  $p$ -values or marginal permutation distributions; the permutation and bootstrap adjustments require the raw data. Because the resampling techniques incorporate distributional and correlational structures, they tend to be less conservative than the other methods.

When a resampling (bootstrap or permutation) method is used with only one test, the adjusted  $p$ -value is the bootstrap or permutation  $p$ -value for that test, with no adjustment for multiplicity, as described by Westfall and Soper (1994).

### **Bonferroni**

The Bonferroni  $p$ -value for test  $i$ ,  $i = 1, \dots, m$  is simply  $\tilde{p}_i = mp_i$ . If the adjusted  $p$ -value exceeds 1, it is set to 1. The Bonferroni test is conservative but always controls the familywise error rate.

If the unadjusted  $p$ -values are computed by using exact permutation distributions, then the Bonferroni adjustment for  $p_i$  is  $\tilde{p}_i = p_1^* + \dots + p_m^*$ , where  $p_j^*$  is the largest  $p$ -value from the permutation distribution of test  $j$  satisfying  $p_j^* \leq p_i$ , or 0 if all permutational  $p$ -values of test  $j$  are greater than  $p_i$ . These adjustments are much less conservative than the ordinary Bonferroni adjustments because they incorporate the discrete distributional characteristics. However, they remain conservative in that they do not incorporate correlation structures between multiple contrasts and multiple variables (Westfall and Wolfinger 1997).

### **Šidák**

A technique slightly less conservative than Bonferroni is the Šidák  $p$ -value (Šidák 1967), which is  $\tilde{p}_i = 1 - (1 - p_i)^m$ . It is exact when all of the  $p$ -values are uniformly distributed and independent, and it is conservative when the test statistics satisfy the positive orthant dependence condition (Holland and Copenhaver 1987).

If the unadjusted  $p$ -values are computed by using exact permutation distributions, then the Šidák adjustment for  $p_i$  is  $\tilde{p}_i = 1 - (1 - p_1^*) \dots (1 - p_m^*)$ , where the  $p_j^*$  are as described previously. These adjustments are less conservative than the corresponding Bonferroni adjustments, but they do not incorporate correlation structures between multiple contrasts and multiple variables (Westfall and Wolfinger 1997).

### **Bootstrap**

The bootstrap method creates pseudo-data sets by sampling observations with replacement from each within-stratum pool of observations. An entire data set is thus created, and  $p$ -values for all tests are computed on this pseudo-data set. A counter records whether the minimum  $p$ -value from the pseudo-data set is less than or equal to the actual  $p$ -value for each base test. (If there are  $m$  tests, then there are  $m$  such counters.) This process is repeated a large number of times, and the proportion of resampled data sets where the minimum pseudo- $p$ -value is less than or equal to an actual  $p$ -value is the adjusted  $p$ -value reported by PROC MULTTEST. The algorithms are described in Westfall and Young (1993).

In the case of continuous data, the pooling of the groups is not likely to re-create the shape of the null hypothesis distribution, since the pooled data are likely to be multimodal. For this reason, PROC MULTTEST automatically mean-centers all continuous variables prior to resampling. Such mean-centering is akin to resampling residuals in a regression analysis, as discussed by Freedman (1981). You can specify the **NO-CENTER** option if you do not want to center the data.

The bootstrap method implicitly incorporates all sources of correlation, from both the multiple contrasts and the multivariate structure. The adjusted  $p$ -values incorporate all correlations and distributional characteristics. This method always provides weak control of the familywise error rate, and it provides strong control when the *subset pivotality* condition holds; that is, for any subset of the null hypotheses, the joint distribution of the  $p$ -values for the subset is identical to that under the complete null (Westfall and Young 1993).



### Permutation

The permutation-style-adjusted  $p$ -values are computed in identical fashion as the **bootstrap**-adjusted  $p$ -values, with the exception that the within-stratum resampling is performed without replacement instead of with replacement. This produces a rerandomization analysis such as in Brown and Fears (1981) and Heyse and Rom (1988). In the spirit of rerandomization analyses, the continuous variables are not centered prior to resampling. This default can be overridden by using the **CENTER** option.

The permutation method implicitly incorporates all sources of correlation, from both the multiple contrasts and the multivariate structure. The adjusted  $p$ -values incorporate all correlations and distributional characteristics. This method always provides weak control of the familywise error rate, and it provides strong control of the familywise error rate under the *subset pivotality* condition, as described in the preceding section.

### Step-Down Methods

Step-down testing is available for the Bonferroni, Šidák, bootstrap, and permutation methods. The benefit of using step-down methods is that the tests are made more powerful (smaller adjusted  $p$ -values) while, in most cases, maintaining strong control of the familywise error rate. The step-down method was pioneered by Holm (1979) and further developed by Shaffer (1986), Holland and Copenhaver (1987), and Hochberg and Tamhane (1987).

The Bonferroni step-down (Holm)  $p$ -values  $\tilde{p}_{(1)}, \dots, \tilde{p}_{(m)}$  are obtained from

$$\tilde{p}_{(i)} = \begin{cases} mp_{(1)} & \text{for } i = 1 \\ \max(\tilde{p}_{(i-1)}, (m - i + 1)p_{(i)}) & \text{for } i = 2, \dots, m \end{cases}$$

As always, if any adjusted  $p$ -value exceeds 1, it is set to 1.

The Šidák step-down  $p$ -values are determined similarly:

$$\tilde{p}_{(i)} = \begin{cases} 1 - (1 - p_{(1)})^m & \text{for } i = 1 \\ \max(\tilde{p}_{(i-1)}, 1 - (1 - p_{(i)})^{m-i+1}) & \text{for } i = 2, \dots, m \end{cases}$$

Step-down Bonferroni adjustments that use exact tests are defined as

$$\tilde{p}_{(i)} = \begin{cases} p_{(1)}^* + \dots + p_{(m)}^* & \text{for } i = 1 \\ \max(\tilde{p}_{(i-1)}, p_{(i)}^* + \dots + p_{(m)}^*) & \text{for } i = 2, \dots, m \end{cases}$$

where the  $p_j^*$  are defined as before. Note that  $p_j^*$  is taken from the permutation distribution corresponding to the  $j$ th-smallest unadjusted  $p$ -value. Also, any  $\tilde{p}_j$  greater than 1.0 is reduced to 1.0.

Step-down Šidák adjustments for exact tests are defined analogously by substituting  $1 - (1 - p_{(j)}^*) \cdots (1 - p_{(m)}^*)$  for  $p_{(j)}^* + \dots + p_{(m)}^*$ .

The resampling-style step-down methods are analogous to the preceding step-down methods; the most extreme  $p$ -value is adjusted according to all  $m$  tests, the second-most extreme  $p$ -value is adjusted according to  $(m - 1)$  tests, and so on. The difference is that all correlational and distributional characteristics are incorporated when you use resampling methods. More specifically, assuming the same ordering of  $p$ -values as discussed previously, the resampling-style step-down-adjusted  $p$ -value for test  $i$  is the probability that the minimum pseudo- $p$ -value of tests  $i, \dots, m$  is less than or equal to  $p_i$ .

This probability is evaluated by using Monte Carlo simulation, as are the previously described resampling-style-adjusted *p*-values. In fact, the computations for step-down-adjusted *p*-values are essentially no more time-consuming than the computations for the non-step-down-adjusted *p*-values. After Monte Carlo, the step-down-adjusted *p*-values are corrected to ensure monotonicity; this correction leaves the first adjusted *p*-values alone, then corrects the remaining ones as needed. The step-down method approximately controls the familywise error rate, and it is described in more detail by Westfall and Young (1993), Westfall et al. (1999), and Westfall and Wolfinger (2000).

**Hommel**

Hommel’s (1988) method is a closed testing procedure based on Simes’ test (Simes 1986). The Simes *p*-value for a joint test of any set of *S* hypotheses with *p*-values  $p_{(1)} \leq p_{(2)} \leq \dots \leq p_{(S)}$  is  $\min((S/1)p_{(1)}, (S/2)p_{(2)}, \dots, (S/S)p_{(S)})$ . The Hommel-adjusted *p*-value for test *j* is the maximum of all such Simes *p*-values, taken over all joint tests that include *j* as one of their components.

Hochberg-adjusted *p*-values are always as large or larger than Hommel-adjusted *p*-values. Sarkar and Chang (1997) shows that Simes’ method is valid under independent or positively dependent *p*-values, so Hommel’s and Hochberg’s methods are also valid in such cases by the closure principle.

**Hochberg**

Assuming *p*-values are independent and uniformly distributed under their respective null hypotheses, Hochberg (1988) demonstrates that Holm’s step-down adjustments control the familywise error rate even when calculated in *step-up* fashion. Since the adjusted *p*-values are uniformly smaller for Hochberg’s method than for Holm’s method, the Hochberg method is more powerful. However, this improved power comes at the cost of having to make the assumption of independence. Hochberg’s method can be derived from Hommel’s (Liu 1996), and is thus also derived from Simes’ test (Simes 1986).

Hochberg-adjusted *p*-values are always as large or larger than Hommel-adjusted *p*-values. Sarkar and Chang (1997) showed that Simes’ method is valid under independent or positively dependent *p*-values, so Hommel’s and Hochberg’s methods are also valid in such cases by the closure principle.

The Hochberg-adjusted *p*-values are defined in reverse order of the step-down Bonferroni:

$$\tilde{p}_{(i)} = \begin{cases} p_{(m)} & \text{for } i = m \\ \min(\tilde{p}_{(i+1)}, (m - i + 1)p_{(i)}) & \text{for } i = m - 1, \dots, 1 \end{cases}$$

**Fisher Combination**

The FISHER\_C option requests adjusted *p*-values by using closed tests, based on the idea of Fisher’s combination test. The Fisher combination test for a joint test of any set of *S* hypotheses with *p*-values uses the chi-square statistic  $\chi^2 = -2 \sum \log(p_i)$ , with  $2S$  degrees of freedom. The FISHER\_C adjusted *p*-value for test *j* is the maximum of all *p*-values for the combination tests, taken over all joint tests that include *j* as one of their components. Independence of *p*-values is required for the validity of this method.

**Stouffer-Liptak Combination**

The STOUFFER option requests adjusted *p*-values by using closed tests, based on the Stouffer-Liptak combination test. The Stouffer combination joint test of any set of *S* one-sided hypotheses with *p*-values,  $p_1, \dots, p_S$ , yields the *p*-value,  $1 - \Phi\left(\frac{1}{\sqrt{S}} \sum_i \Phi^{-1}(1 - p_i)\right)$ . The STOUFFER adjusted *p*-value for test *j* is the maximum of all *p*-values for the combination tests, taken over all joint tests that include *j* as one of their components.

Independence of the one-sided  $p$ -values is required for the validity of this method. Westfall (2005) shows that the Stouffer-Liptak adjustment might have more power than the Fisher combination and Simes' adjustments when the test results reinforce each other.

### Adaptive Adjustments

*Adaptive* adjustments modify the FWE- and FDR-controlling procedures by taking an estimate of the number  $m_0$  or proportion  $\pi_0$  of true null hypotheses into account. The adjusted  $p$ -values for Holm's and Hochberg's methods involve the number of unadjusted  $p$ -values larger than ( $i$ ),  $m - i + 1$ . So the minimal significance level at which the  $i$ th ordered  $p$ -value is rejected implies that the number of true null hypotheses is  $m - i + 1$ . However, if you know  $m_0$ , then you can replace  $m - i + 1$  with  $\min(m_0, m - i + 1)$ , thereby obtaining more power while maintaining the original  $\alpha$ -level significance.

Since  $m_0$  is unknown, there are several methods used to estimate the value—see the `NTRUENULL=` option for more information. The estimation method described by Hochberg and Benjamini (1990) considers the graph of  $1 - p_{(i)}$  versus  $i$ , where the  $p_{(i)}$  are the ordered  $p$ -values of your tests. See [Output 61.6.4](#) for an example. If all null hypotheses are actually true ( $m_0 = m$ ), then the  $p$ -values behave like a sample from a uniform distribution and this graph should be a straight line through the origin. However, if points in the upper-right corner of this plot do not follow the initial trend, then some of these null hypotheses are probably false and  $0 < m_0 < m$ .

The `ADAPTIVEHOLM` option uses this estimate of  $m_0$  to adjust the step-up Bonferroni method while the `ADAPTIVEHOCHBERG` option adjusts the step-down Bonferroni method. Both of these methods are due to Hochberg and Benjamini (1990). When  $m_0$  is known, these procedures control the familywise error rate in the same manner as their nonadaptive versions but with more power; however, since  $m_0$  must be estimated, the FWE control is only approximate. The `ADAPTIVEFDR` and `PFDR` options also use  $\hat{m}_0$ , and are described in the following section.

The adjusted  $p$ -values for the `ADAPTIVEHOLM` method are computed by

$$\tilde{p}_{(i)} = \begin{cases} \min(m, \hat{m}_0) p_{(1)} & \text{for } i = 1 \\ \max[\tilde{p}_{(i-1)}, \min(m - i + 1, \hat{m}_0) p_{(i)}] & \text{for } i = 2, \dots, m \end{cases}$$

The adjusted  $p$ -values for the `ADAPTIVEHOCHBERG` method are computed by

$$\tilde{p}_{(i)} = \begin{cases} \min(1, \hat{m}_0) p_{(m)} & \text{for } i = m \\ \min[\tilde{p}_{(i+1)}, \min(m - i + 1, \hat{m}_0) p_{(i)}] & \text{for } i = m - 1, \dots, 1 \end{cases}$$

### False Discovery Rate Controlling Adjustments

Methods that control the *false discovery rate* (FDR) were described by Benjamini and Hochberg (1995). These adjustments do not necessarily control the familywise error rate (FWE). However, FDR-controlling methods are more powerful and more liberal, and hence reject more null hypotheses, than adjustments protecting the FWE. FDR-controlling methods are often used when you have a large number of null hypotheses. To control the FDR, Benjamini and Hochberg's (1995) linear step-up method is provided, as well as an adaptive version, a dependence version, and bootstrap and permutation resampling versions. Storey's (2002) pFDR methods are also provided.

The `FDR` option requests  $p$ -values that control the "false discovery rate" described by Benjamini and Hochberg (1995). These *linear step-up* adjustments are potentially much less conservative than the `Hochberg` adjustments.

The FDR-adjusted *p*-values are defined in step-up fashion, like the Hochberg adjustments, but with less conservative multipliers:

$$\tilde{p}^{(i)} = \begin{cases} p^{(m)} & \text{for } i = m \\ \min(\tilde{p}^{(i+1)}, \frac{m}{i} p^{(i)}) & \text{for } i = m - 1, \dots, 1 \end{cases}$$

The FDR method is guaranteed to control the false discovery rate at level  $\leq \frac{m_0}{m} \alpha \leq \alpha$  when you have independent *p*-values that are uniformly distributed under their respective null hypotheses. Benjamini and Yekateuli (2001) show that the false discovery rate is also controlled at level  $\leq \frac{m_0}{m} \alpha$  when the *positive regression dependent* condition holds on the set of the true null hypotheses, and they provide several examples where this condition is true.

**NOTE:** The positive regression dependent condition on the set of the true null hypotheses holds if the joint distribution of the test statistics  $\mathbf{X} = (X_1, \dots, X_m)$  for the null hypotheses  $H_{01}, \dots, H_{0m}$  satisfies:  $\Pr(\mathbf{X} \in A | X_i = x)$  is nondecreasing in *x* for each  $X_i$  where  $H_{0i}$  is true, for any increasing set *A*. The set *A* is increasing if  $\mathbf{x} \in A$  and  $\mathbf{y} \geq \mathbf{x}$  implies  $\mathbf{y} \in A$ .

**Dependent False Discovery Rate**

The DEPENDENTFDR option requests a false discovery rate controlling method that is always valid for *p*-values under any kind of dependency (Benjamini and Yekateuli 2001), but is thus quite conservative. Let  $\gamma = \sum_{i=1}^m \frac{1}{i}$ . The DEPENDENTFDR procedure always controls the false discovery rate at level  $\leq \frac{m_0}{m} \alpha \gamma$ . The adjusted *p*-values are computed as

$$\tilde{p}^{(i)} = \begin{cases} \gamma p^{(m)} & \text{for } i = m \\ \min(\tilde{p}^{(i+1)}, \gamma \frac{m}{i} p^{(i)}) & \text{for } i = m - 1, \dots, 1 \end{cases}$$

**False Discovery Rate Resampling Adjustments**

Bootstrap and permutation resampling methods to control the false discovery rate are available with the FDRBOOT and FDRPERM options (Yekateuli and Benjamini 1999). These methods approximately control the false discovery rate when the *subset pivotality* condition holds, as discussed in the section “Bootstrap” on page 5197, and when the *p*-values corresponding to the true null hypotheses are independent of those for the false null hypotheses.

The resampling methodology for the BOOTSTRAP and PERMUTATION methods is used to create *B* resamples. For the *b*th resample, let  $R^b(p)$  denote the number of *p*-values that are less than or equal to the observed *p*-value *p*. Let  $r_\beta(p)$  be the  $100(1 - \beta)$  quantile of  $\{R^1(p) \dots R^b(p) \dots R^B(p)\}$ , and let  $r(p)$  be the number of observed *p*-values less than or equal to *p*. Compute one of the following estimators:

$$\begin{aligned} \text{local estimator} \quad Q_1(p) &= \begin{cases} \frac{1}{B} \sum_{b=1}^B \frac{R^b(p)}{R^b(p) + r(p) - pm} & \text{if } r(p) - r_\beta(p) \geq pm \\ \#\{R^b(p) \geq 1\} / B & \text{otherwise} \end{cases} \\ \text{upper limit estimator} \quad Q_\beta(p) &= \begin{cases} \sup_{x \in [0, p]} \left( \frac{1}{B} \sum_{b=1}^B \frac{R^b(x)}{R^b(x) + r(x) - r_\beta(x)} \right) & \text{if } r(x) - r_\beta(x) \geq 0 \\ \#\{R^b(p) \geq 1\} / B & \text{otherwise} \end{cases} \end{aligned}$$

where  $m$  is the number of tests and  $B$  is the number of resamples. Then for  $Q = Q_1$  or  $Q_\beta$ , the adjusted  $p$ -values are computed as

$$\tilde{p}^{(i)} = \begin{cases} Q(p^{(m)}) & \text{for } i = m \\ \min(\tilde{p}^{(i+1)}, Q(p^{(i)})) & \text{for } i = m - 1, \dots, 1 \end{cases}$$

### Adaptive False Discovery Rate

Since the FDR method controls the false discovery rate at  $\leq \frac{m_0}{m}\alpha \leq \alpha$ , knowledge of  $m_0$  allows improvement of the power of the adjustment while still maintaining control of the false discovery rate. The ADAPTIVEFDR option requests adaptive adjusted  $p$ -values for approximate control of the false discovery rate, as discussed in Benjamini and Hochberg (2000). See the section “Adaptive Adjustments” on page 5200 for more details. These adaptive adjustments are also defined in step-up fashion but use an estimate  $\hat{m}_0$  of the number of true null hypotheses:

$$\tilde{p}^{(i)} = \begin{cases} \frac{\hat{m}_0}{m} p^{(m)} & \text{for } i = m \\ \min(\tilde{p}^{(i+1)}, \frac{\hat{m}_0}{i} p^{(i)}) & \text{for } i = m - 1, \dots, 1 \end{cases}$$

Since  $\hat{m}_0 \leq m$ , the larger  $p$ -values are adjusted down. This means that, as defined, controlling the false discovery rate enables you to reject these tests at a level less than the observed  $p$ -value. However, by default, this reduction is prevented with an additional restriction:  $\tilde{p}^{(i)} = \max\{\tilde{p}^{(i)}, p^{(i)}\}$ .

To use this adjustment, Benjamini and Hochberg (2000) suggest first specifying the FDR option—if at least one test is rejected at your level, then apply the ADAPTIVEFDR adjustment. Alternatively, Benjamini, Krieger, and Yekutieli (2006) apply the FDR adjustment at level  $\frac{\alpha}{\alpha+1}$ , then specify the resulting number of true hypotheses with the NTRUENULL= option and apply the ADAPTIVEFDR adjustment; they show that this *two-stage linear step-up* procedure controls the false discovery rate at level  $\alpha$  for independent test statistics.

### Positive False Discovery Rate

The PFDR option computes the “ $q$ -values”  $\hat{q}_\lambda(p_i)$  (Storey 2002; Storey, Taylor, and Siegmund 2004), which are adaptive adjusted  $p$ -values for strong control of the false discovery rate when the  $p$ -values corresponding to the true null hypotheses are independent and uniformly distributed. There are four versions of the PFDR available. Let  $N(\lambda)$  be the number of observed  $p$ -values that are less than or equal to  $\lambda$ ; let  $m$  be the number of tests; let  $f = 1$  if the FINITE option is specified, and otherwise set  $f = 0$ ; and denote the estimated proportion of true null hypotheses by

$$\hat{\pi}_0(\lambda) = \frac{m - N(\lambda) + f}{(1 - \lambda)m}$$

The default estimate of FDR is

$$\widehat{\text{FDR}}_\lambda(p) = \frac{\hat{\pi}_0(\lambda)p}{\max(N(p), 1)/m}$$

If you set  $\lambda = 0$ , then this is identical to the FDR adjustment.

The positive FDR is estimated by

$$\widehat{\text{pFDR}}_\lambda(p) = \frac{\widehat{\text{FDR}}_\lambda(p)}{1 - (1 - p)^m}$$

The finite-sample versions of these two estimators for independent null  $p$ -values are given by

$$\widehat{\text{FDR}}_{\lambda}^*(p) = \begin{cases} \frac{\hat{\pi}_0^*(\lambda)p}{\max(N(p), 1)/m} & \text{if } p \leq \lambda \\ 1 & \text{if } p > \lambda \end{cases}$$

$$\widehat{\text{pFDR}}_{\lambda}^*(p) = \frac{\widehat{\text{FDR}}_{\lambda}^*(p)}{1 - (1 - p)^m}$$

Finally, the adjusted  $p$ -values are computed as

$$\tilde{p}_i = \hat{q}_{\lambda}(p_i) = \inf_{p \geq p_i} \widehat{\text{FDR}}_{\lambda}(p) \quad i = 1, \dots, m$$

This method can produce adjusted  $p$ -values that are smaller than the raw  $p$ -values. This means that, as defined, controlling the false discovery rate enables you to reject these tests at a level less than the observed  $p$ -value. However, by default, this reduction is prevented with an additional restriction:  $\tilde{p}_i = \max\{\tilde{p}_i, p_i\}$ .

## Missing Values

If a **CLASS** or **STRATA** variable has a missing value, then PROC MULTTEST removes that observation from the analysis.

When there are missing values for test variables, the within-group-and-stratum sample sizes can differ from variable to variable. In most cases this is not a problem; however, it is possible for all data to be missing for a particular group within a particular stratum. For continuous variables and Freeman-Tukey tests, PROC MULTTEST re-centers the contrast trend coefficients within strata where all data for a particular group are missing. Re-centering the **MEAN** tests could redefine your  $t$  tests in an undesirable fashion; for example, if you specify coefficients to contrast the first and third groups (**contrast -1 0 1**) but the third group is missing, then the re-centered coefficients become  $-0.5$  and  $0.5$ , thus contrasting the first and second groups. If this is the case, you can run your  $t$  tests in separate PROC MULTTEST invocations, then combine the data and adjust the  $p$ -values by using the **INPVALUES=** option. However, you might find this re-centering acceptable for the Freeman-Tukey trend tests, since the contrast still tests for an increasing trend. The Cochran-Armitage and Peto tests are unaffected by this situation.

PROC MULTTEST uses missing values for resampling if they exist in the original data set. If all variables have missing values for any observation, then PROC MULTTEST removes the observation prior to resampling. Otherwise, PROC MULTTEST treats all missing values as ordinary observations in the resampling. This means that different resampled data sets can have different group sizes. In some cases it means that a resampled data set can have all missing values for a particular variable in a particular group/stratum combination, even when values exist for that combination in the original data. For this reason, PROC MULTTEST recomputes all quantities within each pseudo-data set, including such items as centered scoring coefficients and degrees of freedom for  $p$ -values.

While PROC MULTTEST does provide analyses in missing value cases, you should not feel that it completely solves the missing-value problem. If you are concerned about the adverse effects of missing data on a particular analysis, you should consider using imputation and sensitivity analyses to assess the effects of the missing data.



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## Computational Resources

PROC MULTTEST keeps all of the data in memory to expedite resampling. A large portion of the memory requirement is thus  $8 \times \text{NOBS} \times \text{NVAR}$  bytes, where NOBS is the number of observations in the data set, and NVAR is the number of variables analyzed, including CLASS, FREQ, and STRATA variables.

If you specify PERMUTATION=*number* (for exact permutation distributions), then PROC MULTTEST requires additional memory. This requirement is approximately  $4 \times \text{NTEST} \times \text{NSTRATA} \times \text{CMAX} \times \text{number} \times (\text{number} + 1)$  bytes, where NTEST is the number of contrasts, NSTRATA is the number of STRATA levels, and CMAX is the maximum contrast coefficient.

If you specify the FDRBOOT or FDRPERM option, then saving all the resamples in memory requires  $8 \times \text{NSAMPLE} \times \text{NOBS}$  bytes, where NSAMPLE is the number of resamples used.

The execution time is linear in the number of resamples; that is, 10,000 resamples will take 10 times longer than 1,000 resamples. The execution time is also linear in the sample size; that is, 100 resamples of size  $N$  will take 10 times longer than 100 resamples of size  $10N$ .

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## Output Data Sets

### OUT= Data Set

The OUT= data set contains contrast names (`_test_`), variable names (`_var_`), the contrast label (`_contrast_`), raw  $p$ -values (`raw_p` or the value specified in the INPVALUES= option), and all requested adjusted  $p$ -values (`bon_p`, `sid_p`, `boot_p`, `perm_p`, `stpbon_p`, `stpsid_p`, `stpbootp`, `stppermp`, `hom_p`, `hoc_p`, `fic_p`, `stouffer_p`, `aholm_p`, `ahoc_p`, `fdr_p`, `dfdr_p`, `fdrbootp`, `ufdbootp`, `fdrpermp`, `ufdpermp`, `afdr_p`, or `pfdr_p`).

If a resampling-based adjusted  $p$ -value is requested, then the simulation standard error is included as either `sim_se`, `stpsimse`, `fdrsimse`, or `ufdsimse`, depending on whether single-step, step-down, or FDR adjustments are requested. The simulation standard errors are used to bound the true resampling-based adjusted  $p$ -value. For example, if the resampling-based estimate is 0.0312 and the simulation standard error is 0.00123, then a 95% confidence interval for the true adjusted  $p$ -value is  $0.0312 \pm 1.96(0.00123)$ , or 0.0288 to 0.0336.

Intermediate statistics used to calculate the  $p$ -values are also written to the OUT= data set. The statistics are separated by the `_strat_` level. When `_strat_` is reported as missing, the statistics refer to the pooled analysis over all `_strat_` levels. The  $p$ -values are provided only for the pooled analyses and are therefore reported as missing for the strata-specific statistics.

For the Peto test, an additional variable, `_tstrat_`, is included to indicate whether the stratum is an incidental occurrence stratum (`_tstrat_=0`) or a fatal occurrence stratum (`_tstrat_=1`).

The statistic `_value_` is the per-strata contribution to the numerator of the overall test statistic. In the case of the MEAN test, this is the contrast function of the sample means multiplied by the total number of observations within the stratum. For the FT test, `_value_` is the contrast function of the double-arcsine transformed proportions, again multiplied by the total number of observations within the stratum. For the CA and Peto tests, `_value_` is the observed value of the trend statistic within that stratum.

When either PETO or CA is requested, the variable `_exp_` is included; this variable contains the expected value of the trend statistic for the given stratum.

The statistic `_se_` is the square root of the variance of the per-strata `_value_` statistic for any of the tests.

For **MEAN** tests, the variable `_nval_` is included. When reported with an individual stratum level (that is, when the `_strat_` value is nonmissing), the value `_nval_` refers to the within-stratum sample size. For the combined analysis (that is, the value of the `_strat_` is missing), the value `_nval_` contains degrees of freedom of the  $t$  distribution used to compute the unadjusted  $p$ -value.

When the **FISHER** test is requested, the `OUT=` data set contains the variables `_xval_`, `_mval_`, `_yval_`, and `_nval_`, which define observations and sample sizes in the two groups defined by the **CONTRAST** statement.

For example, the `OUT=` data set from the drug example in the section “Getting Started: **MULTTEST** Procedure” on page 5167 is displayed in [Figure 61.5](#).

**Figure 61.5** Output Data for the **MULTTEST** Procedure

| Obs | _test_ | _var_     | _contrast_ | _value_ | _exp_ | _se_    | raw_p   | boot_p  | sim_se     |
|-----|--------|-----------|------------|---------|-------|---------|---------|---------|------------|
| 1   | CA     | SideEff1  | Trend      | 8       | 5     | 1.54303 | 0.05187 | 0.33880 | .003346749 |
| 2   | CA     | SideEff2  | Trend      | 7       | 5     | 1.54303 | 0.19492 | 0.84030 | .002590327 |
| 3   | CA     | SideEff3  | Trend      | 10      | 7     | 1.63299 | 0.06619 | 0.51895 | .003532994 |
| 4   | CA     | SideEff4  | Trend      | 10      | 6     | 1.60357 | 0.01262 | 0.08840 | .002007305 |
| 5   | CA     | SideEff5  | Trend      | 7       | 4     | 1.44749 | 0.03821 | 0.24080 | .003023370 |
| 6   | CA     | SideEff6  | Trend      | 9       | 6     | 1.60357 | 0.06137 | 0.43825 | .003508468 |
| 7   | CA     | SideEff7  | Trend      | 9       | 5     | 1.54303 | 0.00953 | 0.05135 | .001560660 |
| 8   | CA     | SideEff8  | Trend      | 8       | 5     | 1.54303 | 0.05187 | 0.33880 | .003346749 |
| 9   | CA     | SideEff9  | Trend      | 7       | 5     | 1.54303 | 0.19492 | 0.84030 | .002590327 |
| 10  | CA     | SideEff10 | Trend      | 8       | 6     | 1.60357 | 0.21232 | 0.90300 | .002092737 |

## OUTPERM= Data Set

The `OUTPERM=` data set contains contrast names (`_contrast_`), variable names (`_var_`), and the associated permutation distributions (`_value_` and `upper_p`). **PROC MULTTEST** computes the permutation distributions when you use the **PERMUTATION=** option with the **CA** or Peto test. The `_value_` variable represents the support of the distributions, and `upper_p` represents their cumulative upper-tail probabilities. The size of this data set depends on the number of variables and the support of their permutation distributions.

For information about how this distribution is computed, see the section “Exact Permutation Test” on page 5189. For an illustration, see [Example 61.1](#).

## OUTSAMP= Data Set

The `OUTSAMP=` data set contains the data sets used in the resampling analysis, if such an analysis is requested. The variable `_sample_` indicates the number of the resampled data set. This variable ranges from 1 to the value of the **NSAMPLE=** option. For each value of the `_sample_` variable, an entire resampled data set is included, with `_stratum_`, `_class_`, and all other variables in the original data set. The values of the original variables are mean-centered for the mean test, if requested. The variable `_obs_` indicates the observation’s position in the original data set.

Each new data set is randomly drawn from the original data set, either with (bootstrap) or without (permutation) replacement. The size of this data set is, thus, the number of observations in the original data set times the number of samples.



---

## Displayed Output

The output produced by PROC MULTTEST is divided into several tables. If the `DATA=` data set is specified, then the following tables are displayed:

- The “Model Information” table provides a list of the options and settings used for that particular invocation of the procedure. This table is not displayed if the `INPVALUES=` data set is specified. Included in this list are the following items:
  - statistical tests
  - support of the exact permutation distribution for the `CA` and `Peto` tests
  - continuity corrections used for the `CA` test
  - test tails
  - strata adjustment
  - $p$ -value adjustments and specified suboptions
  - centering of continuous variables
  - number of samples and seed
- The “Contrast Coefficients” table lists the coefficients used in constructing the statistical tests. These coefficients are either specified in `CONTRAST` statements or generated by default. The coefficients apply to the levels of the `CLASS` statement variable. If a `MEAN` or `FT` test is specified in the `TEST` statement, the centered coefficients are displayed. Patterns of missing values in your data set might affect the coefficients used in your analysis; the displayed contrasts take missing value patterns into account. See the section “Missing Values” on page 5203 for more information.
- The “Variable Tabulations” tables provide summary statistics for each variable listed in the `TEST` statement. Included for discrete variables are the count, sample size, and percentage of occurrences. For continuous variables, the mean, sample standard deviation, and sample size are displayed. All of the previously mentioned statistics are computed for distinct combinations of the `CLASS` and `STRATA` statement variables.

If the `INPVALUES=` data set is specified, then the following tables are displayed:

- The “P-Value Adjustment Information” table provides a list of the specified  $p$ -value adjustments. If an adaptive adjustment is specified (see section “Adaptive Adjustments” on page 5200), then the following settings are also displayed when appropriate:
  - whether the finite-sample version of the PFDR is used (`FINITE`)
  - the number of tuning parameters to check (`NLAMBDA=`), the maximum tuning parameter (`MAXLAMBDA=`), or the specified tuning parameter (`LAMBDA=`)
  - the degrees of freedom of the spline (`DF=`) and the smoothing parameter
  - the number of bootstrap resamples (`NBOOT=`) and the seed (`SEED=`)

- If the `bootstrap` or `spline` method for estimating the number of true null hypotheses  $m_0$  is used and the `PLOTS=` option is specified, the “Lambda Values” table displays the  $m_0$  estimates as a function of the tuning parameter  $\lambda$ . If the `bootstrap` method is used, the table also displays the mean-squared errors, the minimum of which is used to select a specific  $\lambda$ . This table contains the values used in the “Lambda Functions” plot.
- The “Estimated Number of True Null Hypotheses” table displays the  $p$ -value adjustment, the method used to estimate the number of true nulls, and an estimate of the number and proportion of true null hypotheses in the data set.

The following table is displayed unless the `NOPVALUE` option is specified:

- The “p-Values” table is a collection of the raw and adjusted  $p$ -values from the run of PROC MULTTEST. The  $p$ -values are identified by variable and test.

---

## ODS Table Names

PROC MULTTEST assigns a name to each table it creates, and you must use this name to reference the table when using the Output Delivery System (ODS). These names are listed in the following table. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

**Table 61.3** ODS Tables Produced by PROC MULTTEST

| ODS Table Name | Description                       | Statement or Option               |
|----------------|-----------------------------------|-----------------------------------|
| Continuous     | Continuous variable tabulations   | TEST with MEAN                    |
| Contrasts      | Contrast coefficients             | default                           |
| Discrete       | Discrete variable tabulations     | TEST with CA, FT, PETO, or FISHER |
| LambdaValues   | True null estimates               | AHOLM, AHOC, AFDR, or PFDR        |
| ModelInfo      | Model information                 | default                           |
| NumTrueNull    | Estimates of number of true nulls | AHOLM, AHOC, AFDR, or PFDR        |
| pValues        | $p$ -values from the tests        | default                           |
| pValueInfo     | $p$ -value adjustment information | INPVALUES=                        |

---

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “Statistical Graphics Using ODS.”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “A Primer on ODS Statistical Graphics” on page 599 in Chapter 21, “Statistical Graphics Using ODS.”

You must also specify the options in the PROC MULTTEST statement that are indicated in Table 61.4.

PROC MULTTEST assigns a name to each graph it creates using ODS. You can use these names to reference the graphs when using ODS. The names are listed in Table 61.4.

**Table 61.4** Graphs Produced by PROC MULTTEST

| ODS Graph Name        | Plot Description                                             | Option                                                                      |
|-----------------------|--------------------------------------------------------------|-----------------------------------------------------------------------------|
| AdjPlots              | Panel of adjusted $p$ -value plots                           | PLOTS=ADJUSTED                                                              |
| AdjByRawRank          | Adjusted by rank of raw $p$ -values                          | PLOTS=ADJUSTED(UNPACK)                                                      |
| AdjbyRawP             | Adjusted by raw $p$ -values                                  | PLOTS=ADJUSTED(UNPACK)                                                      |
| AdjBySignificant      | Proportion significant by adjusted                           | PLOTS=ADJUSTED(UNPACK)                                                      |
| FalsePosBySignificant | Expected number of false positives by proportion significant | PLOTS=ADJUSTED(UNPACK)                                                      |
| PByTest               | $p$ -values by test                                          | PLOTS=PBYTEST                                                               |
| LambdaPlot            | MSE or NTRUENULL by lambda                                   | PLOTS=LAMBDA and<br>(NTRUENULL=BOOTSTRAP<br>or NTRUENULL=SPLINE<br>or PFDR) |
| ManhattanPlots        | $-\log_{10}$ (adjusted $p$ -values) by test                  | PLOTS=MANHATTAN                                                             |
| ManhattanPanel        | Panel of Manhattan plots                                     | PLOTS=MANHATTAN                                                             |
| RawUniformPlot        | Raw $p$ -values by rank and histogram                        | PLOTS=RAWPROB or<br>AHOLM or AHOC or AFDR or PFDR                           |
| RawUniformPlot        | Raw $p$ -values by rank                                      | PLOTS=RAWPROB(UNPACK) and<br>AHOLM or AHOC or AFDR or PFDR                  |
| RawUniformHist        | Histogram of raw $p$ -values                                 | PLOTS=RAWPROB(UNPACK) and<br>AHOLM or AHOC or AFDR or PFDR                  |

## Examples: MULTTEST Procedure

### Example 61.1: Cochran-Armitage Test with Permutation Resampling

This example, from Keith Soper at Merck, illustrates the exact permutation Cochran-Armitage test carried out on permutation resamples. In the following data set, each observation represents an animal. The binary variables S1 and S2 indicate two tumor types, with 0s indicating no tumor (failure) and 1 indicating a tumor (success); note that they have perfect negative association. The grouping variable is Dose.

```
data a;
 input S1 S2 Dose @@;
 datalines;
0 1 1 1 0 1 0 1 1
0 1 1 0 1 1 1 0 1
1 0 2 1 0 2 0 1 2
1 0 2 0 1 2 1 0 2
```

```

1 0 3 1 0 3 1 0 3
0 1 3 0 1 3 1 0 3
;

proc multtest data=a permutation nsample=10000 seed=36607 outperm=pmt;
 test ca(S1 S2 / permutation=10 uppertailed);
 class Dose;
 contrast 'CA Linear Trend' 0 1 2;
run;
proc print data=pmt;
run;

```

The PROC MULTTEST statement requests 10,000 permutation resamples. The **OUTPERM=** option creates an output SAS data set **pmt** used for the exact permutation distribution computed for the **CA** test.

The **TEST** statement specifies an upper-tailed Cochran-Armitage linear trend test for **S1** and **S2**. The cutoff for exact permutation calculations is 10, as specified with the **PERMUTATION=** option in the **TEST** statement. Since **S1** and **S2** have 10 and 8 successes, respectively, PROC MULTTEST uses exact permutation distributions to compute the *p*-values for both variables.

The groups for the **CA** test are the levels of **Dose** from the **CLASS** statement. The trend coefficients applied to these groups are 0, 1, and 2, respectively, as specified in the **CONTRAST** statement.

Finally, the PROC PRINT statement displays the SAS data set **pmt**, which contains the permutation distributions.

The results from this analysis are displayed in [Output 61.1.1](#) through [Output 61.1.5](#). You should check the “Model Information” table to verify that the analysis specifications are correct.

### Output 61.1.1 Cochran-Armitage Test with Permutation Resampling

| The Multtest Procedure              |                  |
|-------------------------------------|------------------|
| Model Information                   |                  |
| Test for discrete variables         | Cochran-Armitage |
| Exact permutation distribution used | Everywhere       |
| Tails for discrete tests            | Upper-tailed     |
| Strata weights                      | None             |
| P-value adjustment                  | Permutation      |
| Number of resamples                 | 10000            |
| Seed                                | 36607            |

The label and coefficients from the **CONTRAST** statement are shown in [Output 61.1.2](#).

**Output 61.1.2** Contrast Coefficients

| Contrast Coefficients |      |   |   |
|-----------------------|------|---|---|
|                       | Dose |   |   |
| Contrast              | 1    | 2 | 3 |
| CA Linear Trend       | 0    | 1 | 2 |

Output 61.1.3 displays summary statistics for the two test variables, S1 and S2. The Count column lists the number of successes for each level of the CLASS variable, Dose. The NumObs column lists the sample size, and the Percent column lists the percentage of successes in the sample.

**Output 61.1.3** Summary Statistics

| Discrete Variable Tabulations |      |       |        |         |
|-------------------------------|------|-------|--------|---------|
| Variable                      | Dose | Count | NumObs | Percent |
| S1                            | 1    | 2     | 6      | 33.33   |
| S1                            | 2    | 4     | 6      | 66.67   |
| S1                            | 3    | 4     | 6      | 66.67   |
| S2                            | 1    | 4     | 6      | 66.67   |
| S2                            | 2    | 2     | 6      | 33.33   |
| S2                            | 3    | 2     | 6      | 33.33   |

The Raw column in Output 61.1.4 contains the  $p$ -values from the CA test, and the Permutation column contains the permutation-adjusted  $p$ -values.

**Output 61.1.4** Resulting  $p$ -Values

| p-Values |                 |        |             |
|----------|-----------------|--------|-------------|
| Variable | Contrast        | Raw    | Permutation |
| S1       | CA Linear Trend | 0.1993 | 0.4009      |
| S2       | CA Linear Trend | 0.9220 | 1.0000      |

This table shows that, for S1, the adjusted  $p$ -value is approximately twice the raw  $p$ -value. In fact, resamples with small (large)  $p$ -values for S1 have large (small)  $p$ -values for S2 due to the perfect negative association of the variables, and hence the permutation-adjusted  $p$ -value for S1 should be  $2 \times 0.1993 = 0.3986$ ; the difference is due to resampling error. For the same reason, since the raw  $p$ -value for S2 is 0.9220, the adjusted  $p$ -value equals 1. The permutation  $p$ -values for S1 and S2 also happen to be the Bonferroni-adjusted  $p$ -values for this example.

The OUTPERM= data set is displayed in Output 61.1.5, which contains the exact permutation distributions for S1 and S2 in terms of cumulative probabilities.

**Output 61.1.5** Exact Permutation Distribution

| Obs | _contrast_      | _var_ | _value_ | upper_p |
|-----|-----------------|-------|---------|---------|
| 1   | CA Linear Trend | S1    | 0       | 1.00000 |
| 2   | CA Linear Trend | S1    | 1       | 1.00000 |
| 3   | CA Linear Trend | S1    | 2       | 1.00000 |
| 4   | CA Linear Trend | S1    | 3       | 1.00000 |
| 5   | CA Linear Trend | S1    | 4       | 1.00000 |
| 6   | CA Linear Trend | S1    | 5       | 0.99966 |
| 7   | CA Linear Trend | S1    | 6       | 0.99609 |
| 8   | CA Linear Trend | S1    | 7       | 0.97827 |
| 9   | CA Linear Trend | S1    | 8       | 0.92205 |
| 10  | CA Linear Trend | S1    | 9       | 0.80070 |
| 11  | CA Linear Trend | S1    | 10      | 0.61011 |
| 12  | CA Linear Trend | S1    | 11      | 0.38989 |
| 13  | CA Linear Trend | S1    | 12      | 0.19930 |
| 14  | CA Linear Trend | S1    | 13      | 0.07795 |
| 15  | CA Linear Trend | S1    | 14      | 0.02173 |
| 16  | CA Linear Trend | S1    | 15      | 0.00391 |
| 17  | CA Linear Trend | S1    | 16      | 0.00034 |
| 18  | CA Linear Trend | S1    | 17      | 0.00000 |
| 19  | CA Linear Trend | S1    | 18      | 0.00000 |
| 20  | CA Linear Trend | S1    | 19      | 0.00000 |
| 21  | CA Linear Trend | S1    | 20      | 0.00000 |
| 22  | CA Linear Trend | S2    | 0       | 1.00000 |
| 23  | CA Linear Trend | S2    | 1       | 1.00000 |
| 24  | CA Linear Trend | S2    | 2       | 1.00000 |
| 25  | CA Linear Trend | S2    | 3       | 0.99966 |
| 26  | CA Linear Trend | S2    | 4       | 0.99609 |
| 27  | CA Linear Trend | S2    | 5       | 0.97827 |
| 28  | CA Linear Trend | S2    | 6       | 0.92205 |
| 29  | CA Linear Trend | S2    | 7       | 0.80070 |
| 30  | CA Linear Trend | S2    | 8       | 0.61011 |
| 31  | CA Linear Trend | S2    | 9       | 0.38989 |
| 32  | CA Linear Trend | S2    | 10      | 0.19930 |
| 33  | CA Linear Trend | S2    | 11      | 0.07795 |
| 34  | CA Linear Trend | S2    | 12      | 0.02173 |
| 35  | CA Linear Trend | S2    | 13      | 0.00391 |
| 36  | CA Linear Trend | S2    | 14      | 0.00034 |
| 37  | CA Linear Trend | S2    | 15      | 0.00000 |
| 38  | CA Linear Trend | S2    | 16      | 0.00000 |

## Example 61.2: Freeman-Tukey and $t$ Tests with Bootstrap Resampling

The data for this example are the same as for [Example 61.1](#), except that a continuous variable T, which indicates the time of death of the animal, has been added.

```
data a;
 input S1 S2 T Dose @@;
 datalines;
0 1 104 1 1 0 80 1 0 1 104 1
0 1 104 1 0 1 100 1 1 0 104 1
1 0 85 2 1 0 60 2 0 1 89 2
1 0 96 2 0 1 96 2 1 0 99 2
1 0 60 3 1 0 50 3 1 0 80 3
0 1 98 3 0 1 99 3 1 0 50 3
;

proc multtest data=a bootstrap nsample=10000 seed=37081 outsamp=res;
 test ft(S1 S2 / lowertailed) mean(T / lowertailed);
 class Dose;
 contrast 'Linear Trend' 0 1 2;
run;

proc print data=res(obs=36);
run;
```

The **BOOTSTRAP** option in the PROC MULTTEST statement requests bootstrap resampling, and **NSAMPLE=10000** requests 10,000 bootstrap samples. The **SEED=37081** option provides a starting value for the random number generator. The **OUTSAMP=res** option creates an output SAS data set res containing the 10,000 bootstrap samples.

The **TEST** statement specifies the Freeman-Tukey test for S1 and S2 and specifies the  $t$  test for T. Both tests are lower-tailed. The grouping variable in the **CLASS** statement is Dose, and the coefficients across the levels of Dose are 0, 1, and 2, as specified in the **CONTRAST** statement. The PROC PRINT statement displays the first 36 observations of the res data set containing the bootstrap samples.

The results from this analysis are listed in [Output 61.2.1](#) through [Output 61.2.5](#).

The “Model Information” table in [Output 61.2.1](#) corresponds to the specifications in the invocation of PROC MULTTEST.

**Output 61.2.1** FT and *t* tests with Bootstrap Resampling

| The Multtest Procedure        |               |
|-------------------------------|---------------|
| Model Information             |               |
| Test for discrete variables   | Freeman-Tukey |
| Test for continuous variables | Mean t-test   |
| Degrees of Freedom Method     | Pooled        |
| Tails for discrete tests      | Lower-tailed  |
| Tails for continuous tests    | Lower-tailed  |
| Strata weights                | None          |
| P-value adjustment            | Bootstrap     |
| Center continuous variables   | Yes           |
| Number of resamples           | 10000         |
| Seed                          | 37081         |

The “Contrast Coefficients” table in [Output 61.2.2](#) shows the coefficients from the `CONTRAST` statement after centering, and they model a linear trend.

**Output 61.2.2** Contrast Coefficients

| Contrast Coefficients |          |      |   |   |
|-----------------------|----------|------|---|---|
|                       |          | Dose |   |   |
| Contrast              |          | 1    | 2 | 3 |
| Linear Trend          | Centered | -1   | 0 | 1 |

The summary statistics are displayed in [Output 61.2.3](#). The values for the discrete variables S1 and S2 are the same as those from [Example 61.1](#). The mean, standard deviation, and sample size for the continuous variable T at each level of Dose are displayed in the “Continuous Variable Tabulations” table.

**Output 61.2.3** Summary Statistics

| Discrete Variable Tabulations |      |       |        |         |
|-------------------------------|------|-------|--------|---------|
| Variable                      | Dose | Count | NumObs | Percent |
| S1                            | 1    | 2     | 6      | 33.33   |
| S1                            | 2    | 4     | 6      | 66.67   |
| S1                            | 3    | 4     | 6      | 66.67   |
| S2                            | 1    | 4     | 6      | 66.67   |
| S2                            | 2    | 2     | 6      | 33.33   |
| S2                            | 3    | 2     | 6      | 33.33   |



**Output 61.2.3** *continued*

| Continuous Variable Tabulations |      |        |         |                    |
|---------------------------------|------|--------|---------|--------------------|
| Variable                        | Dose | NumObs | Mean    | Standard Deviation |
| T                               | 1    | 6      | 99.3333 | 9.6056             |
| T                               | 2    | 6      | 87.5000 | 14.4326            |
| T                               | 3    | 6      | 72.8333 | 22.7017            |

The  $p$ -values, displayed in [Output 61.2.4](#), are from the Freeman-Tukey test for S1 and S2, and are from the  $t$  test for T.

**Output 61.2.4**  $p$ -Values

| p-Values |              |        |           |
|----------|--------------|--------|-----------|
| Variable | Contrast     | Raw    | Bootstrap |
| S1       | Linear Trend | 0.8547 | 1.0000    |
| S2       | Linear Trend | 0.1453 | 0.4605    |
| T        | Linear Trend | 0.0070 | 0.0281    |

The Raw column in [Output 61.2.4](#) contains the results from the tests on the original data, while the Bootstrap column contains the bootstrap resampled adjustment to raw\_p. Note that the adjusted  $p$ -values are larger than the raw  $p$ -values for all three variables. The adjusted  $p$ -values more accurately reflect the correlation of the raw  $p$ -values, the small size of the data, and the multiple testing.

[Output 61.2.5](#) displays the first 36 observations of the SAS data set resulting from the OUTSAMP=RES option in the PROC MULTTEST statement. The entire data set has 180,000 observations, which is 10,000 times the number of observations in the data set.

**Output 61.2.5** Resampling Data Set

| Obs | _sample_ | _class_ | _obs_ | S1 | S2 | T        |
|-----|----------|---------|-------|----|----|----------|
| 1   | 1        | 1       | 17    | 0  | 1  | 26.1667  |
| 2   | 1        | 1       | 8     | 1  | 0  | -27.5000 |
| 3   | 1        | 1       | 5     | 0  | 1  | 0.6667   |
| 4   | 1        | 1       | 9     | 0  | 1  | 1.5000   |
| 5   | 1        | 1       | 7     | 1  | 0  | -2.5000  |
| 6   | 1        | 1       | 3     | 0  | 1  | 4.6667   |
| 7   | 1        | 2       | 12    | 1  | 0  | 11.5000  |
| 8   | 1        | 2       | 12    | 1  | 0  | 11.5000  |
| 9   | 1        | 2       | 14    | 1  | 0  | -22.8333 |
| 10  | 1        | 2       | 17    | 0  | 1  | 26.1667  |
| 11  | 1        | 2       | 1     | 0  | 1  | 4.6667   |
| 12  | 1        | 2       | 15    | 1  | 0  | 7.1667   |
| 13  | 1        | 3       | 4     | 0  | 1  | 4.6667   |
| 14  | 1        | 3       | 17    | 0  | 1  | 26.1667  |
| 15  | 1        | 3       | 14    | 1  | 0  | -22.8333 |
| 16  | 1        | 3       | 15    | 1  | 0  | 7.1667   |
| 17  | 1        | 3       | 15    | 1  | 0  | 7.1667   |
| 18  | 1        | 3       | 6     | 1  | 0  | 4.6667   |
| 19  | 2        | 1       | 6     | 1  | 0  | 4.6667   |
| 20  | 2        | 1       | 17    | 0  | 1  | 26.1667  |
| 21  | 2        | 1       | 8     | 1  | 0  | -27.5000 |
| 22  | 2        | 1       | 13    | 1  | 0  | -12.8333 |
| 23  | 2        | 1       | 9     | 0  | 1  | 1.5000   |
| 24  | 2        | 1       | 8     | 1  | 0  | -27.5000 |
| 25  | 2        | 2       | 9     | 0  | 1  | 1.5000   |
| 26  | 2        | 2       | 18    | 1  | 0  | -22.8333 |
| 27  | 2        | 2       | 15    | 1  | 0  | 7.1667   |
| 28  | 2        | 2       | 14    | 1  | 0  | -22.8333 |
| 29  | 2        | 2       | 9     | 0  | 1  | 1.5000   |
| 30  | 2        | 2       | 17    | 0  | 1  | 26.1667  |
| 31  | 2        | 3       | 16    | 0  | 1  | 25.1667  |
| 32  | 2        | 3       | 11    | 0  | 1  | 8.5000   |
| 33  | 2        | 3       | 14    | 1  | 0  | -22.8333 |
| 34  | 2        | 3       | 18    | 1  | 0  | -22.8333 |
| 35  | 2        | 3       | 18    | 1  | 0  | -22.8333 |
| 36  | 2        | 3       | 10    | 1  | 0  | 8.5000   |

The `_sample_` variable is the sample indicator and `_class_` indicates the resampling group—that is, the level of the `CLASS` variable Dose assigned to the new observation. The number of the observation in the original data set is represented by `_obs_`. Also listed are the values of the original test variables, S1 and S2, and the mean-centered values of T.

### Example 61.3: Peto Mortality-Prevalence Test

This example illustrates the use of the Peto mortality-prevalence test. The test is a combination of analyses about the prevalence of incidental tumors in the population and mortality due to fatal tumors.

In the following data set, each observation represents an animal. The variables S1–S3 are three tumor types, with a value of 0 indicating no tumor, 1 indicating an incidental (nonlethal) tumor, and 2 indicating a lethal tumor. The time variable T indicates the time of death of the animal, a strata variable B is constructed from T, and the grouping variable Dose is drug dosage.

```
data a;
 input S1-S3 T Dose @@;
 if T<=90 then B=1; else B=2;
 datalines;
0 0 0 104 0 2 0 1 80 0 0 0 1 104 0
0 0 0 104 0 0 2 0 100 0 1 0 0 104 0
2 0 0 85 1 2 1 0 60 1 0 1 0 89 1
2 0 1 96 1 0 0 0 96 1 2 0 1 99 1
2 1 1 60 2 2 0 0 50 2 2 0 1 80 2
0 0 2 98 2 0 0 1 99 2 2 1 1 50 2
;

proc multtest data=a notables out=p stepsid;
 test peto(S1-S3 / permutation=20 time=T uppertailed);
 class Dose;
 strata B;
 contrast 'mort-prev' 0 1 2;
run;
proc print data=p;
run;
```

The **NOTABLES** option in the PROC MULTTEST statement suppresses the display of the summary statistics for each variable. The **OUT=** option creates an output SAS data set *p* containing all *p*-values and intermediate statistics. The **STEPSID** option is used to adjust the *p*-values.

The **TEST** statement specifies an upper-tailed Peto test for S1–S3. The mortality strata are defined by **TIME=T**, the death times. The **CLASS** statement contains the grouping variable Dose. The prevalence strata are defined by the **STRATA** statement as the blocking variable B. The **CONTRAST** statement lists the default linear trend coefficients. The PROC PRINT statement displays the requested *p*-value data set.

The results from this analysis are listed in [Output 61.3.1](#) through [Output 61.3.4](#).

The “Model Information” table in [Output 61.3.1](#) displays information corresponding to the PROC MULTTEST invocation. In this case the totals for all prevalence and fatality strata are less than 20, so exact permutation tests are used everywhere, and the STEPSID adjustments are computed from these permutation distributions.

**Output 61.3.1** Peto Test

| The Multtest Procedure              |                |
|-------------------------------------|----------------|
| Model Information                   |                |
| Test for discrete variables         | Peto           |
| Exact permutation distribution used | Everywhere     |
| Tails for discrete tests            | Upper-tailed   |
| Strata weights                      | Sample size    |
| P-value adjustment                  | Stepdown Sidak |

The contrast trend coefficients are listed in [Output 61.3.2](#). They happen to be the same as the levels of the Dose variable.

**Output 61.3.2** Contrast Coefficients

| Contrast Coefficients |      |   |   |
|-----------------------|------|---|---|
|                       | Dose |   |   |
| Contrast              | 0    | 1 | 2 |
| mort-prev             | 0    | 1 | 2 |

In the “*p*-Values” table in [Output 61.3.3](#), the *p*-values for the Peto tests are listed in the Raw column, and the step-down Šidák adjusted *p*-values are in the Stepdown Šidák column.

**Output 61.3.3** *p*-Values

| p-Values |           |        |                |
|----------|-----------|--------|----------------|
| Variable | Contrast  | Raw    | Stepdown Sidak |
| S1       | mort-prev | 0.0681 | 0.0814         |
| S2       | mort-prev | 0.5000 | 0.5000         |
| S3       | mort-prev | 0.0363 | 0.0781         |

Significant *p*-values in the preceding table support the claim that higher dosage levels lead to higher mortality and prevalence. The raw Peto test is significant at the 5% level for S3, but the adjusted S3 test is no longer significant at 5%. The raw and adjusted *p*-values for S2 are the same because of the step-down technique.

The OUT= data set is displayed in [Output 61.3.4](#).

## Output 61.3.4 OUT= Data Set

|     | <u>t</u> | <u>v</u> | <u>a</u>  | <u>s</u> | <u>t</u> | <u>s</u> | <u>v</u> | <u>e</u> | <u>s</u> | <u>r</u> | <u>s</u> | <u>t</u> |
|-----|----------|----------|-----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| Obs | test     | var      | contrast  | strat    | tsrat    | value    | exp      | se       | raw_p    | stpsid_p |          |          |
| 1   | PETO     | S1       | mort-prev | 1        | 0        | 0        | 0.00000  | 0.00000  | .        | .        |          |          |
| 2   | PETO     | S1       | mort-prev | 2        | 0        | 0        | 0.62500  | 0.85696  | .        | .        |          |          |
| 3   | PETO     | S1       | mort-prev | 50       | 1        | 4        | 2.00000  | 1.12022  | .        | .        |          |          |
| 4   | PETO     | S1       | mort-prev | 60       | 1        | 3        | 1.75000  | 1.06654  | .        | .        |          |          |
| 5   | PETO     | S1       | mort-prev | 80       | 1        | 2        | 1.57143  | 1.04978  | .        | .        |          |          |
| 6   | PETO     | S1       | mort-prev | 85       | 1        | 1        | 0.75000  | 0.72169  | .        | .        |          |          |
| 7   | PETO     | S1       | mort-prev | 96       | 1        | 1        | 0.70000  | 0.78102  | .        | .        |          |          |
| 8   | PETO     | S1       | mort-prev | 98       | 1        | 0        | 0.00000  | 0.00000  | .        | .        |          |          |
| 9   | PETO     | S1       | mort-prev | 99       | 1        | 1        | 0.42857  | 0.72843  | .        | .        |          |          |
| 10  | PETO     | S1       | mort-prev | 100      | 1        | 0        | 0.00000  | 0.00000  | .        | .        |          |          |
| 11  | PETO     | S2       | mort-prev | 1        | 0        | 6        | 5.50000  | 1.05221  | .        | .        |          |          |
| 12  | PETO     | S2       | mort-prev | 2        | 0        | 0        | 0.00000  | 0.00000  | .        | .        |          |          |
| 13  | PETO     | S2       | mort-prev | 50       | 1        | 0        | 0.00000  | 0.00000  | .        | .        |          |          |
| 14  | PETO     | S2       | mort-prev | 60       | 1        | 0        | 0.00000  | 0.00000  | .        | .        |          |          |
| 15  | PETO     | S2       | mort-prev | 80       | 1        | 0        | 0.00000  | 0.00000  | .        | .        |          |          |
| 16  | PETO     | S2       | mort-prev | 85       | 1        | 0        | 0.00000  | 0.00000  | .        | .        |          |          |
| 17  | PETO     | S2       | mort-prev | 96       | 1        | 0        | 0.00000  | 0.00000  | .        | .        |          |          |
| 18  | PETO     | S2       | mort-prev | 98       | 1        | 0        | 0.00000  | 0.00000  | .        | .        |          |          |
| 19  | PETO     | S2       | mort-prev | 99       | 1        | 0        | 0.00000  | 0.00000  | .        | .        |          |          |
| 20  | PETO     | S2       | mort-prev | 100      | 1        | 0        | 0.00000  | 0.00000  | .        | .        |          |          |
| 21  | PETO     | S3       | mort-prev | 1        | 0        | 6        | 5.50000  | 1.05221  | .        | .        |          |          |
| 22  | PETO     | S3       | mort-prev | 2        | 0        | 4        | 2.22222  | 1.08298  | .        | .        |          |          |
| 23  | PETO     | S3       | mort-prev | 50       | 1        | 0        | 0.00000  | 0.00000  | .        | .        |          |          |
| 24  | PETO     | S3       | mort-prev | 60       | 1        | 0        | 0.00000  | 0.00000  | .        | .        |          |          |
| 25  | PETO     | S3       | mort-prev | 80       | 1        | 0        | 0.00000  | 0.00000  | .        | .        |          |          |
| 26  | PETO     | S3       | mort-prev | 85       | 1        | 0        | 0.00000  | 0.00000  | .        | .        |          |          |
| 27  | PETO     | S3       | mort-prev | 96       | 1        | 0        | 0.00000  | 0.00000  | .        | .        |          |          |
| 28  | PETO     | S3       | mort-prev | 98       | 1        | 2        | 0.62500  | 0.85696  | .        | .        |          |          |
| 29  | PETO     | S3       | mort-prev | 99       | 1        | 0        | 0.00000  | 0.00000  | .        | .        |          |          |
| 30  | PETO     | S3       | mort-prev | 100      | 1        | 0        | 0.00000  | 0.00000  | .        | .        |          |          |
| 31  | PETO     | S1       | mort-prev | .        | .        | 12       | 7.82500  | 2.42699  | 0.06808  | 0.08140  |          |          |
| 32  | PETO     | S2       | mort-prev | .        | .        | 6        | 5.50000  | 1.05221  | 0.50000  | 0.50000  |          |          |
| 33  | PETO     | S3       | mort-prev | .        | .        | 12       | 8.34722  | 1.73619  | 0.03627  | 0.07811  |          |          |

The first 30 observations correspond to intermediate statistics used to compute the Peto  $p$ -values. The `_test_` variable lists the name of the test, the `_var_` variable lists the name of the TEST variables, and the `_contrast_` variable lists the CONTRAST label. The `_strat_` variable lists the level of the STRATA variable, and the `_tsrat_` variable indicates whether or not the stratum corresponds to values of the TIME= variable. The `_value_` variable is the observed contrast for a stratum, and the `_exp_` variable is its expected value. The variable `_se_` contains the square root of the variance terms summed to form the denominator of the Peto statistics.

The final three observations correspond to the three Peto tests, with their  $p$ -values listed under the `raw_p` variable. The `stpsid_p` variable contains the step-down Šidák-adjusted  $p$ -values.

## Example 61.4: Fisher Test with Permutation Resampling

The following data, from Brown and Fears (1981), are the results of an 80-week carcinogenesis bioassay with female mice. Six tissue sites are examined at necropsy; 1 indicates the presence of a tumor and 0 the absence. A frequency variable Freq is included. A control and four different doses of a drug (in parts per milliliter) make up the levels of the grouping variable Dose.

```
data a;
 input Liver Lung Lymph Cardio Pitui Ovary Freq Dose$ @@;
 datalines;
1 0 0 0 0 0 8 CTRL 0 1 0 0 0 0 7 CTRL 0 0 1 0 0 0 6 CTRL
0 0 0 1 0 0 1 CTRL 0 0 0 0 0 1 2 CTRL 1 1 0 0 0 0 4 CTRL
1 0 1 0 0 0 1 CTRL 1 0 0 0 0 1 1 CTRL 0 1 1 0 0 0 1 CTRL
0 0 0 0 0 0 18 CTRL
1 0 0 0 0 0 9 4PPM 0 1 0 0 0 0 4 4PPM 0 0 1 0 0 0 7 4PPM
0 0 0 1 0 0 1 4PPM 0 0 0 0 1 0 2 4PPM 0 0 0 0 0 1 1 4PPM
1 1 0 0 0 0 4 4PPM 1 0 1 0 0 0 3 4PPM 1 0 0 0 1 0 1 4PPM
0 1 1 0 0 0 1 4PPM 0 1 0 1 0 0 1 4PPM 1 0 1 1 0 0 1 4PPM
0 0 0 0 0 0 15 4PPM
1 0 0 0 0 0 8 8PPM 0 1 0 0 0 0 3 8PPM 0 0 1 0 0 0 6 8PPM
0 0 0 1 0 0 3 8PPM 1 1 0 0 0 0 1 8PPM 1 0 1 0 0 0 2 8PPM
1 0 0 1 0 0 1 8PPM 1 0 0 0 1 0 1 8PPM 1 1 0 1 0 0 2 8PPM
1 1 0 0 0 1 2 8PPM 0 0 0 0 0 0 19 8PPM
1 0 0 0 0 0 4 16PPM 0 1 0 0 0 0 2 16PPM 0 0 1 0 0 0 9 16PPM
0 0 0 0 1 0 1 16PPM 0 0 0 0 0 1 1 16PPM 1 1 0 0 0 0 4 16PPM
1 0 1 0 0 0 1 16PPM 0 1 1 0 0 0 1 16PPM 0 1 0 1 0 0 1 16PPM
0 1 0 0 0 1 1 16PPM 0 0 1 1 0 0 1 16PPM 0 0 1 0 1 0 1 16PPM
1 1 1 0 0 0 2 16PPM 0 0 0 0 0 0 14 16PPM
1 0 0 0 0 0 8 50PPM 0 1 0 0 0 0 4 50PPM 0 0 1 0 0 0 8 50PPM
0 0 0 1 0 0 1 50PPM 0 0 0 0 0 1 4 50PPM 1 1 0 0 0 0 3 50PPM
1 0 1 0 0 0 1 50PPM 0 1 1 0 0 0 1 50PPM 0 1 0 0 1 1 1 50PPM
0 0 0 0 0 0 19 50PPM
;

proc multtest data=a order=data notables out=p
 permutation nsample=1000 seed=764511;
 test fisher(Liver Lung Lymph Cardio Pitui Ovary /
 lowertailed);
 class Dose;
 freq Freq;
run;
proc print data=p;
run;
```

In the PROC MULTTEST statement, the **ORDER=DATA** option is required to keep the levels of Dose in the order in which they appear in the data set. Without this option, the levels are sorted by their formatted value, resulting in an alphabetic ordering. The **NOTABLES** option suppresses the display of summary statistics, and the **OUT=** option produces an output data set p containing the  $p$ -values. The **PERMUTATION** option specifies permutation resampling, **NSAMPLE=1000** requests 1000 samples, and **SEED=764511** option provides a starting value for the random number generator. You should specify a seed if you need to duplicate resampling results.

To test for higher rates of tumor occurrence in the treatment groups compared to the control group, the **LOWERTAILED** option is specified in the **FISHER** option of the **TEST** statement to produce a lower-tailed Fisher exact test for the six tissue sites. The Fisher test is appropriate for comparing a treatment and a control, but multiple testing can be a problem. Brown and Fears (1981) use a multivariate permutation to evaluate the entire collection of tests. PROC MULTTEST adjusts the  $p$ -values by simulation.

The treatments make up the levels of the grouping variable Dose, listed in the **CLASS** statement. Since no **CONTRAST** statement is specified, PROC MULTTEST uses the default pairwise contrasts with the first level of Dose. The **FREQ** statement is used since these are summary data containing frequency counts of occurrences.

The results from this analysis are listed in [Output 61.4.1](#) through [Output 61.4.4](#). First, the PROC MULTTEST specifications are displayed in [Output 61.4.1](#).

**Output 61.4.1** Fisher Test with Permutation Resampling

| The Multtest Procedure      |              |
|-----------------------------|--------------|
| Model Information           |              |
| Test for discrete variables | Fisher       |
| Tails for discrete tests    | Lower-tailed |
| Strata weights              | None         |
| P-value adjustment          | Permutation  |
| Number of resamples         | 1000         |
| Seed                        | 764511       |

The default contrasts for the Fisher test are displayed in [Output 61.4.2](#). Note that each dose is compared with the control.

**Output 61.4.2** Default Contrast Coefficients

| Contrast       | Contrast Coefficients |      |      |       |       |
|----------------|-----------------------|------|------|-------|-------|
|                | Dose                  |      |      |       |       |
|                | CTRL                  | 4PPM | 8PPM | 16PPM | 50PPM |
| CTRL vs. 4PPM  | 1                     | -1   | 0    | 0     | 0     |
| CTRL vs. 8PPM  | 1                     | 0    | -1   | 0     | 0     |
| CTRL vs. 16PPM | 1                     | 0    | 0    | -1    | 0     |
| CTRL vs. 50PPM | 1                     | 0    | 0    | 0     | -1    |

The “p-Values” table in [Output 61.4.3](#) displays  $p$ -values for the Fisher exact tests and their permutation-based adjustments.

**Output 61.4.3** *p*-Values

| p-Values |                |        |             |  |
|----------|----------------|--------|-------------|--|
| Variable | Contrast       | Raw    | Permutation |  |
| Liver    | CTRL vs. 4PPM  | 0.2828 | 0.9610      |  |
| Liver    | CTRL vs. 8PPM  | 0.3069 | 0.9670      |  |
| Liver    | CTRL vs. 16PPM | 0.7102 | 1.0000      |  |
| Liver    | CTRL vs. 50PPM | 0.7718 | 1.0000      |  |
| Lung     | CTRL vs. 4PPM  | 0.7818 | 1.0000      |  |
| Lung     | CTRL vs. 8PPM  | 0.8858 | 1.0000      |  |
| Lung     | CTRL vs. 16PPM | 0.5469 | 0.9990      |  |
| Lung     | CTRL vs. 50PPM | 0.8498 | 1.0000      |  |
| Lymph    | CTRL vs. 4PPM  | 0.2423 | 0.9280      |  |
| Lymph    | CTRL vs. 8PPM  | 0.5898 | 1.0000      |  |
| Lymph    | CTRL vs. 16PPM | 0.0350 | 0.2680      |  |
| Lymph    | CTRL vs. 50PPM | 0.4161 | 0.9930      |  |
| Cardio   | CTRL vs. 4PPM  | 0.3163 | 0.9710      |  |
| Cardio   | CTRL vs. 8PPM  | 0.0525 | 0.3710      |  |
| Cardio   | CTRL vs. 16PPM | 0.4506 | 0.9960      |  |
| Cardio   | CTRL vs. 50PPM | 0.7576 | 1.0000      |  |
| Pitui    | CTRL vs. 4PPM  | 0.1250 | 0.7540      |  |
| Pitui    | CTRL vs. 8PPM  | 0.4948 | 0.9970      |  |
| Pitui    | CTRL vs. 16PPM | 0.2157 | 0.9080      |  |
| Pitui    | CTRL vs. 50PPM | 0.5051 | 0.9970      |  |
| Ovary    | CTRL vs. 4PPM  | 0.9437 | 1.0000      |  |
| Ovary    | CTRL vs. 8PPM  | 0.8126 | 1.0000      |  |
| Ovary    | CTRL vs. 16PPM | 0.7760 | 1.0000      |  |
| Ovary    | CTRL vs. 50PPM | 0.3689 | 0.9930      |  |

As noted by Brown and Fears, only one of the 24 tests is significant at the 5% level (Lymph, CTRL vs. 16PPM). Brown and Fears report a 12% chance of observing at least one significant raw *p*-value for 16PPM and a 9% chance of observing at least one significant raw *p*-value for Lymph (both at the 5% level). Adjusted *p*-values exhibit much lower chances of false significances. For this example, none of the adjusted *p*-values are close to significant.

The OUT= data set is displayed in [Output 61.4.4](#).



## Output 61.4.4 OUT= Data Set

|     | <u>t</u> | <u>v</u> | <u>r</u>       | <u>x</u> | <u>m</u> | <u>y</u> | <u>n</u> | <u>r</u> | <u>p</u> | <u>s</u> |
|-----|----------|----------|----------------|----------|----------|----------|----------|----------|----------|----------|
| Obs | test     | var      | contrast       | val      | mval     | yval     | nval     | raw      | perm     | sim      |
| 1   | 2        | 3        | 4              | 5        | 6        | 7        | 8        | 9        | 10       | 11       |
| 1   | FISHER   | Liver    | CTRL vs. 4PPM  | 14       | 49       | 18       | 50       | 0.28282  | 0.961    | 0.006122 |
| 2   | FISHER   | Liver    | CTRL vs. 8PPM  | 14       | 49       | 17       | 48       | 0.30688  | 0.967    | 0.005649 |
| 3   | FISHER   | Liver    | CTRL vs. 16PPM | 14       | 49       | 11       | 43       | 0.71022  | 1.000    | 0.000000 |
| 4   | FISHER   | Liver    | CTRL vs. 50PPM | 14       | 49       | 12       | 50       | 0.77175  | 1.000    | 0.000000 |
| 5   | FISHER   | Lung     | CTRL vs. 4PPM  | 12       | 49       | 10       | 50       | 0.78180  | 1.000    | 0.000000 |
| 6   | FISHER   | Lung     | CTRL vs. 8PPM  | 12       | 49       | 8        | 48       | 0.88581  | 1.000    | 0.000000 |
| 7   | FISHER   | Lung     | CTRL vs. 16PPM | 12       | 49       | 11       | 43       | 0.54685  | 0.999    | 0.000999 |
| 8   | FISHER   | Lung     | CTRL vs. 50PPM | 12       | 49       | 9        | 50       | 0.84978  | 1.000    | 0.000000 |
| 9   | FISHER   | Lymph    | CTRL vs. 4PPM  | 8        | 49       | 12       | 50       | 0.24228  | 0.928    | 0.008174 |
| 10  | FISHER   | Lymph    | CTRL vs. 8PPM  | 8        | 49       | 8        | 48       | 0.58977  | 1.000    | 0.000000 |
| 11  | FISHER   | Lymph    | CTRL vs. 16PPM | 8        | 49       | 15       | 43       | 0.03498  | 0.268    | 0.014006 |
| 12  | FISHER   | Lymph    | CTRL vs. 50PPM | 8        | 49       | 10       | 50       | 0.41607  | 0.993    | 0.002636 |
| 13  | FISHER   | Cardio   | CTRL vs. 4PPM  | 1        | 49       | 3        | 50       | 0.31631  | 0.971    | 0.005307 |
| 14  | FISHER   | Cardio   | CTRL vs. 8PPM  | 1        | 49       | 6        | 48       | 0.05254  | 0.371    | 0.015276 |
| 15  | FISHER   | Cardio   | CTRL vs. 16PPM | 1        | 49       | 2        | 43       | 0.45061  | 0.996    | 0.001996 |
| 16  | FISHER   | Cardio   | CTRL vs. 50PPM | 1        | 49       | 1        | 50       | 0.75758  | 1.000    | 0.000000 |
| 17  | FISHER   | Pitui    | CTRL vs. 4PPM  | 0        | 49       | 3        | 50       | 0.12496  | 0.754    | 0.013619 |
| 18  | FISHER   | Pitui    | CTRL vs. 8PPM  | 0        | 49       | 1        | 48       | 0.49485  | 0.997    | 0.001729 |
| 19  | FISHER   | Pitui    | CTRL vs. 16PPM | 0        | 49       | 2        | 43       | 0.21572  | 0.908    | 0.009140 |
| 20  | FISHER   | Pitui    | CTRL vs. 50PPM | 0        | 49       | 1        | 50       | 0.50505  | 0.997    | 0.001729 |
| 21  | FISHER   | Ovary    | CTRL vs. 4PPM  | 3        | 49       | 1        | 50       | 0.94372  | 1.000    | 0.000000 |
| 22  | FISHER   | Ovary    | CTRL vs. 8PPM  | 3        | 49       | 2        | 48       | 0.81260  | 1.000    | 0.000000 |
| 23  | FISHER   | Ovary    | CTRL vs. 16PPM | 3        | 49       | 2        | 43       | 0.77596  | 1.000    | 0.000000 |
| 24  | FISHER   | Ovary    | CTRL vs. 50PPM | 3        | 49       | 5        | 50       | 0.36889  | 0.993    | 0.002636 |

The test, var, and contrast variables provide the TEST name, TEST variable, and CONTRAST label, respectively. The xval, mval, yval, and nval variables contain the components used to compute the Fisher exact tests from the hypergeometric distribution. The raw\_p variable contains the  $p$ -values from the Fisher exact tests, and the perm\_p variable contains their permutation-based adjustments. The variable sim\_se is the simulation standard error from the permutation resampling.

## Example 61.5: Inputting Raw $p$ -Values

This example illustrates how to use PROC MULTTEST to multiplicity-adjust a collection of raw  $p$ -values obtained from some other source. This is a valuable option for those cases where PROC MULTTEST cannot compute the raw  $p$ -values directly. The data set `a`, which follows, contains the unadjusted  $p$ -values computed in Example 61.4. Note that the data set needs to have one variable containing the  $p$ -values, but the data set can contain other variables as well.

```
data a;
 input Test$ Raw_P @@;
 datalines;
test01 0.28282 test02 0.30688 test03 0.71022
test04 0.77175 test05 0.78180 test06 0.88581
test07 0.54685 test08 0.84978 test09 0.24228
test10 0.58977 test11 0.03498 test12 0.41607
test13 0.31631 test14 0.05254 test15 0.45061
test16 0.75758 test17 0.12496 test18 0.49485
test19 0.21572 test20 0.50505 test21 0.94372
test22 0.81260 test23 0.77596 test24 0.36889
;

proc multtest inpvalues=a holm hoc fdr;
run;
```

Note that the PROC MULTTEST statement is the only statement that can be specified with the  $p$ -value input mode. In this example, the raw  $p$ -values are adjusted by the [Holm](#), [Hochberg](#), and [FDR](#) methods.

The “P-Value Adjustment Information” table, displayed in [Output 61.5.1](#), provides information about the requested adjustments and replaces the usual “Model Information” table. The adjusted  $p$ -values are displayed in [Output 61.5.2](#)

### Output 61.5.1 Inputting Raw $p$ -Values

| The Multtest Procedure         |                      |
|--------------------------------|----------------------|
| P-Value Adjustment Information |                      |
| P-Value Adjustment             | Stepdown Bonferroni  |
| P-Value Adjustment             | Hochberg             |
| P-Value Adjustment             | False Discovery Rate |

Output 61.5.2  $p$ -Values

| Test | p-Values |                        |          | False<br>Discovery<br>Rate |
|------|----------|------------------------|----------|----------------------------|
|      | Raw      | Stepdown<br>Bonferroni | Hochberg |                            |
| 1    | 0.2828   | 1.0000                 | 0.9437   | 0.9243                     |
| 2    | 0.3069   | 1.0000                 | 0.9437   | 0.9243                     |
| 3    | 0.7102   | 1.0000                 | 0.9437   | 0.9243                     |
| 4    | 0.7718   | 1.0000                 | 0.9437   | 0.9243                     |
| 5    | 0.7818   | 1.0000                 | 0.9437   | 0.9243                     |
| 6    | 0.8858   | 1.0000                 | 0.9437   | 0.9243                     |
| 7    | 0.5469   | 1.0000                 | 0.9437   | 0.9243                     |
| 8    | 0.8498   | 1.0000                 | 0.9437   | 0.9243                     |
| 9    | 0.2423   | 1.0000                 | 0.9437   | 0.9243                     |
| 10   | 0.5898   | 1.0000                 | 0.9437   | 0.9243                     |
| 11   | 0.0350   | 0.8395                 | 0.8395   | 0.6305                     |
| 12   | 0.4161   | 1.0000                 | 0.9437   | 0.9243                     |
| 13   | 0.3163   | 1.0000                 | 0.9437   | 0.9243                     |
| 14   | 0.0525   | 1.0000                 | 0.9437   | 0.6305                     |
| 15   | 0.4506   | 1.0000                 | 0.9437   | 0.9243                     |
| 16   | 0.7576   | 1.0000                 | 0.9437   | 0.9243                     |
| 17   | 0.1250   | 1.0000                 | 0.9437   | 0.9243                     |
| 18   | 0.4949   | 1.0000                 | 0.9437   | 0.9243                     |
| 19   | 0.2157   | 1.0000                 | 0.9437   | 0.9243                     |
| 20   | 0.5051   | 1.0000                 | 0.9437   | 0.9243                     |
| 21   | 0.9437   | 1.0000                 | 0.9437   | 0.9437                     |
| 22   | 0.8126   | 1.0000                 | 0.9437   | 0.9243                     |
| 23   | 0.7760   | 1.0000                 | 0.9437   | 0.9243                     |
| 24   | 0.3689   | 1.0000                 | 0.9437   | 0.9243                     |

Note that the adjusted  $p$ -values for the Hochberg method are less than or equal to those for the Holm (Step-down Bonferroni) method. In turn, the adjusted  $p$ -values for the FDR method (False Discovery Rate) are less than or equal to those for the Hochberg method. These comparisons hold generally for all  $p$ -value configurations. The FDR method controls the false discovery rate and not the familywise error rate. The Hochberg method controls the familywise error rate under independence. The Holm method controls the familywise error rate without assuming independence.

---

### Example 61.6: Adaptive Adjustments and ODS Graphics

An experiment was performed using Affymetrix<sup>®</sup> gene chips on the CD4 lymphocyte white blood cells of patients with and without a hereditary allergy (atopy) and possibly with asthma. The Asthma-Atopy microarray data set and analysis are discussed in Gibson and Wolfinger (2004): a one-way ANOVA model of the  $\log_2\text{mas5}$  variable ( $\log_2(\text{MAS 5.0 summary statistics})$ ) is fit against a classification variable  $\text{trt}$  describing different asthma-atopy combinations in the patients, and the least squares means of the  $\text{trt}$  variable are computed.

For this example, a 1% random sample of least squares means having  $p$ -values exceeding  $1E-6$  is taken. The resulting data are recorded in the test data set, where the Probe\_Set\_ID variable identifies the probe and the Probt variable contains the  $p$ -values for the  $m = 121$  tests, as follows:

```
data test;
 length Probe_Set_ID $9.;
 input Probe_Set_ID $ Probt @@;
 datalines;
200973_s_ .963316 201059_at .462754 201563_at .000409 201733_at .000819
201951_at .000252 202944_at .106550 203107_x_ .040396 203372_s_ .010911
203469_s_ .987234 203641_s_ .019296 203795_s_ .002276 204055_s_ .002328
205020_s_ .008628 205199_at .608129 205373_at .005209 205384_at .742381
205428_s_ .870533 205653_at .621671 205686_s_ .396440 205760_s_ .000002
206032_at .024661 206159_at .997627 206223_at .003702 206398_s_ .191682
206623_at .010030 206852_at .000004 207072_at .000214 207371_at .000013
207789_s_ .023623 207861_at .000002 207897_at .000007 208022_s_ .251999
208086_s_ .000361 208406_s_ .040182 208464_at .161468 209055_s_ .529824
209125_at .142276 209369_at .240079 209748_at .071750 209894_at .000042
209906_at .223282 210130_s_ .192187 210199_at .101623 210477_x_ .300038
210491_at .000078 210531_at .000784 210734_x_ .202931 210755_at .009644
210782_x_ .000011 211320_s_ .022896 211329_x_ .486869 211362_s_ .881798
211369_at .000030 211399_at .000008 211572_s_ .269788 211647_x_ .001301
213072_at .005019 213143_at .008711 213238_at .004824 213391_at .316133
213468_at .000172 213636_at .097133 213823_at .001678 213854_at .001921
213976_at .000299 214006_s_ .014616 214063_s_ .000361 214407_x_ .609880
214445_at .000009 214570_x_ .000002 214648_at .001255 214684_at .288156
214991_s_ .006695 215012_at .000499 215117_at .000136 215201_at .045235
215304_at .000816 215342_s_ .973786 215392_at .112937 215557_at .000007
215608_at .006204 215935_at .000027 215980_s_ .037382 216010_x_ .000354
216051_x_ .000003 216086_at .002310 216092_s_ .000056 216511_s_ .294776
216733_s_ .004823 216747_at .002902 216874_at .000117 216969_s_ .001614
217133_x_ .056851 217198_x_ .169196 217557_s_ .002966 217738_at .000005
218601_at .023817 218818_at .027554 219302_s_ .000039 219441_s_ .000172
219574_at .193737 219612_s_ .000075 219697_at .046476 219700_at .003049
219945_at .000066 219964_at .000684 220234_at .130064 220473_s_ .000017
220575_at .030223 220633_s_ .058460 220925_at .252465 221256_s_ .721731
221314_at .002307 221589_s_ .001810 221995_s_ .350859 222071_s_ .000062
222113_s_ .000023 222208_s_ .100961 222303_at .049265 37226_at .000749
60474_at .000423
run;
```

The following statements adjust the  $p$ -values in the test data set by using the adaptive adjustments ([ADAPTIVEHOLM](#), [ADAPTIVEHOCHBERG](#), [ADAPTIVEFDR](#), and [PFDR](#)), which require an estimate of the number of true null hypotheses ( $\hat{m}_0$ ) or proportion of true null hypotheses ( $\hat{\pi}_0$ ). This example illustrates some of the features and graphics for computing and evaluating these estimates. The [NOPVALUE](#) option is specified to suppress the display of the “p-Values” table.

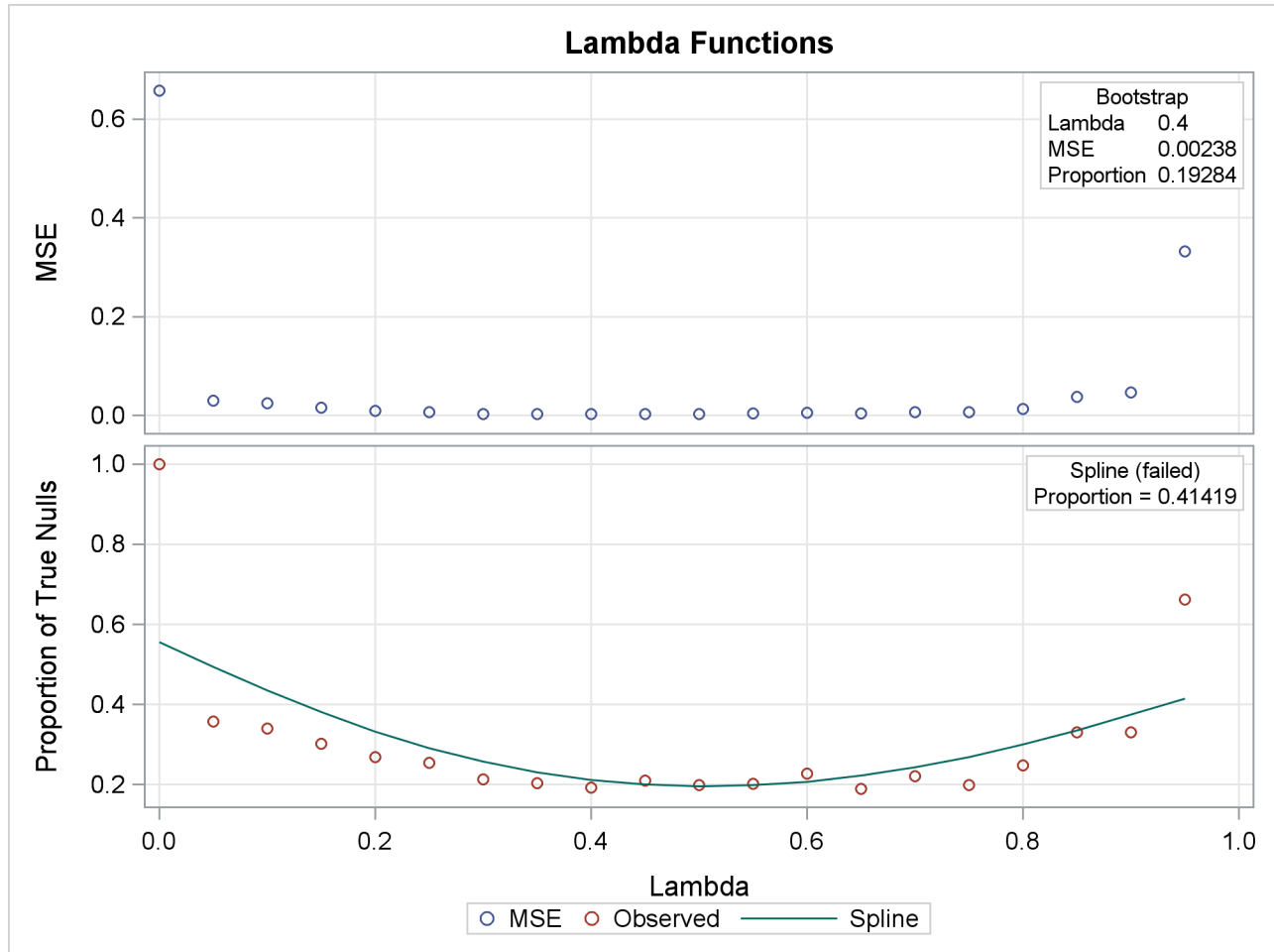
```
ods graphics on;
proc multtest inpvalues(Probt)=test plots=all seed=518498000
 aholm ahoc afdr pfdr(positive) nopvalue;
 id Probe_Set_ID;
run;
ods graphics off;
```

Output 61.6.1 lists the requested  $p$ -value adjustments, along with the selected value of the “Lambda” tuning parameter and the seed (specified with the `SEED=` option) used in the `bootstrap` method of estimating the number of true null hypotheses. The “Lambda Values” table lists the estimated number of true nulls for each value of  $\lambda$ , where you can see that the minimum MSE (0.002315) occurs at  $\lambda = 0.4$ . Output 61.6.2 shows that the `SPLINE` method failed due to a large slope at  $\lambda = 0.95$ , so the bootstrap method is used and the MSE plot is displayed.

**Output 61.6.1**  $p$  and Lambda Values

| The Multtest Procedure         |          |                       |                     |
|--------------------------------|----------|-----------------------|---------------------|
| P-Value Adjustment Information |          |                       |                     |
| P-Value Adjustment             |          | Adaptive Holm         |                     |
| P-Value Adjustment             |          | Adaptive Hochberg     |                     |
| P-Value Adjustment             |          | Adaptive FDR          |                     |
| P-Value Adjustment             |          | pFDR Q-Value          |                     |
| Lambda                         |          | 0.4                   |                     |
| Seed                           |          | 518498000             |                     |
| Lambda Values                  |          |                       |                     |
| Lambda                         | MSE      | NTrueNull<br>Observed | NTrueNull<br>Spline |
| 0                              | 0.657880 | 121.000000            | 67.318707           |
| 0.050000                       | 0.030212 | 43.157895             | 59.812885           |
| 0.100000                       | 0.024897 | 41.111111             | 52.636271           |
| 0.150000                       | 0.014904 | 36.470588             | 46.033846           |
| 0.200000                       | 0.008580 | 32.500000             | 40.172642           |
| 0.250000                       | 0.006476 | 30.666667             | 35.157768           |
| 0.300000                       | 0.002719 | 25.714286             | 31.046105           |
| 0.350000                       | 0.002471 | 24.615385             | 27.861153           |
| 0.400000                       | 0.002378 | 23.333333             | 25.595089           |
| 0.450000                       | 0.003285 | 25.454545             | 24.217908           |
| 0.500000                       | 0.003036 | 24.000000             | 23.687690           |
| 0.550000                       | 0.003567 | 24.444444             | 23.965745           |
| 0.600000                       | 0.005813 | 27.500000             | 25.016579           |
| 0.650000                       | 0.004118 | 22.857143             | 26.809774           |
| 0.700000                       | 0.006647 | 26.666667             | 29.321876           |
| 0.750000                       | 0.006260 | 24.000000             | 32.512203           |
| 0.800000                       | 0.013242 | 30.000000             | 36.315191           |
| 0.850000                       | 0.037624 | 40.000000             | 40.618909           |
| 0.900000                       | 0.046906 | 40.000000             | 45.274355           |
| 0.950000                       | 0.332183 | 80.000000             | 50.117369           |

**Output 61.6.2** Tuning Parameter Plots



Output 61.6.3 also shows that the bootstrap estimate is used for the PFDR adjustment. The other adjustments have different default methods for estimating the number of true nulls.

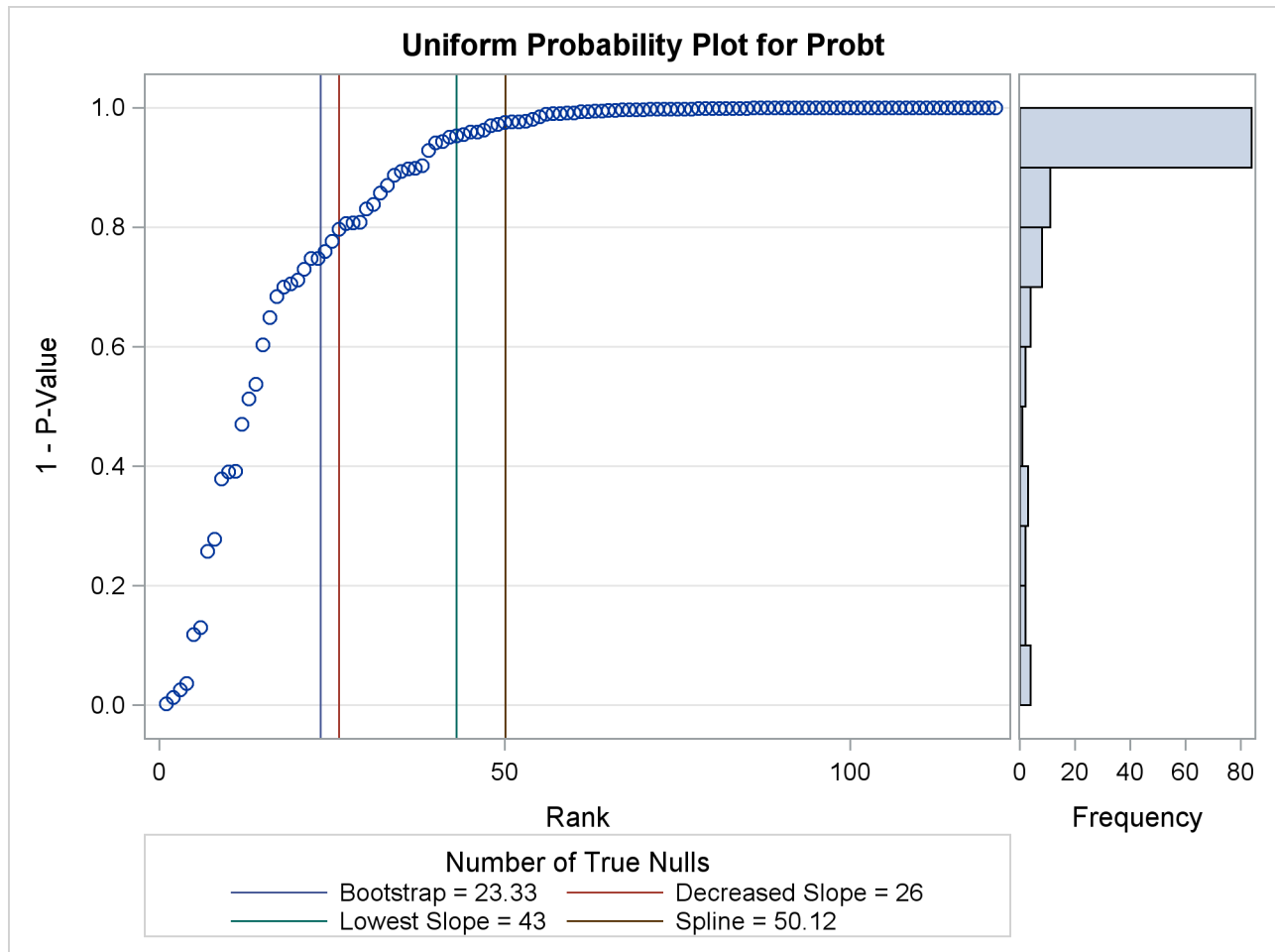
**Output 61.6.3** Adjustments and Their Default Estimation Method

| Estimated Number of True Null Hypotheses |                 |          |            |
|------------------------------------------|-----------------|----------|------------|
| P-Value Adjustment                       | Method          | Estimate | Proportion |
| Adaptive Holm                            | Decreased Slope | 26       | 0.21488    |
| Adaptive Hochberg                        | Decreased Slope | 26       | 0.21488    |
| Adaptive FDR                             | Lowest Slope    | 43       | 0.35537    |
| Positive FDR                             | Bootstrap       | 23.3333  | 0.19284    |

Output 61.6.4 displays the estimated number of true nulls  $\hat{m}_0$  against a uniform probability plot of the unadjusted  $p$ -values (if the  $p$ -values are distributed uniformly, the points on the plot will all lie on a straight line). According to Schweder and Spjøtvoll (1982) and Hochberg and Benjamini (1990), the points on the

left side of the plot should be approximately linear with slope  $\frac{1}{m_0+1}$ , so you can use this plot to evaluate whether your estimate of  $\hat{m}_0$  seems reasonable.

**Output 61.6.4** *p*-Value Distribution



The `NTRUENULL=` option provides several methods for estimating the number of true null hypotheses; the following table displays each method and its estimate for this example:

| <code>NTRUENULL=</code> | Estimate |
|-------------------------|----------|
| BOOTSTRAP               | 23.3     |
| DECREASESLOPE           | 26       |
| KSTEST                  | 35       |
| LEASTSQUARES            | 28       |
| LOWESTSLOPE             | 43       |
| MEANDIFF                | 42       |
| SPLINE                  | 50.1     |

Another method of estimating the number of true null hypotheses fits a finite mixture model (mixing a uniform with a beta) to the distribution of the unadjusted  $p$ -values (Allison et al. 2002). Osborne (2006) provides the following PROC NLMIXED statements to fit this model:

```
proc nlmixed data=test;
 parameters pi0=0.5 a=.1 b=.1;
 pi1= 1-pi0;
 bounds 0 <= pi0 <= 1;
 loglikelihood= log(pi0+pi1*pdf('beta',Probt,a,b));
 model Probt ~ general(loglikelihood);
run;
```

You might have to change the initial parameter values in the PARAMETERS statement to achieve convergence; see Chapter 64, “The NLMIXED Procedure,” for more information. This mixture model estimates  $\hat{\pi}_0 = 0$ , meaning that the distribution of  $p$ -values is completely specified by a single beta distribution. If the estimate were, say,  $\hat{\pi}_0 = 0.10$ , you could then specify it as follows:

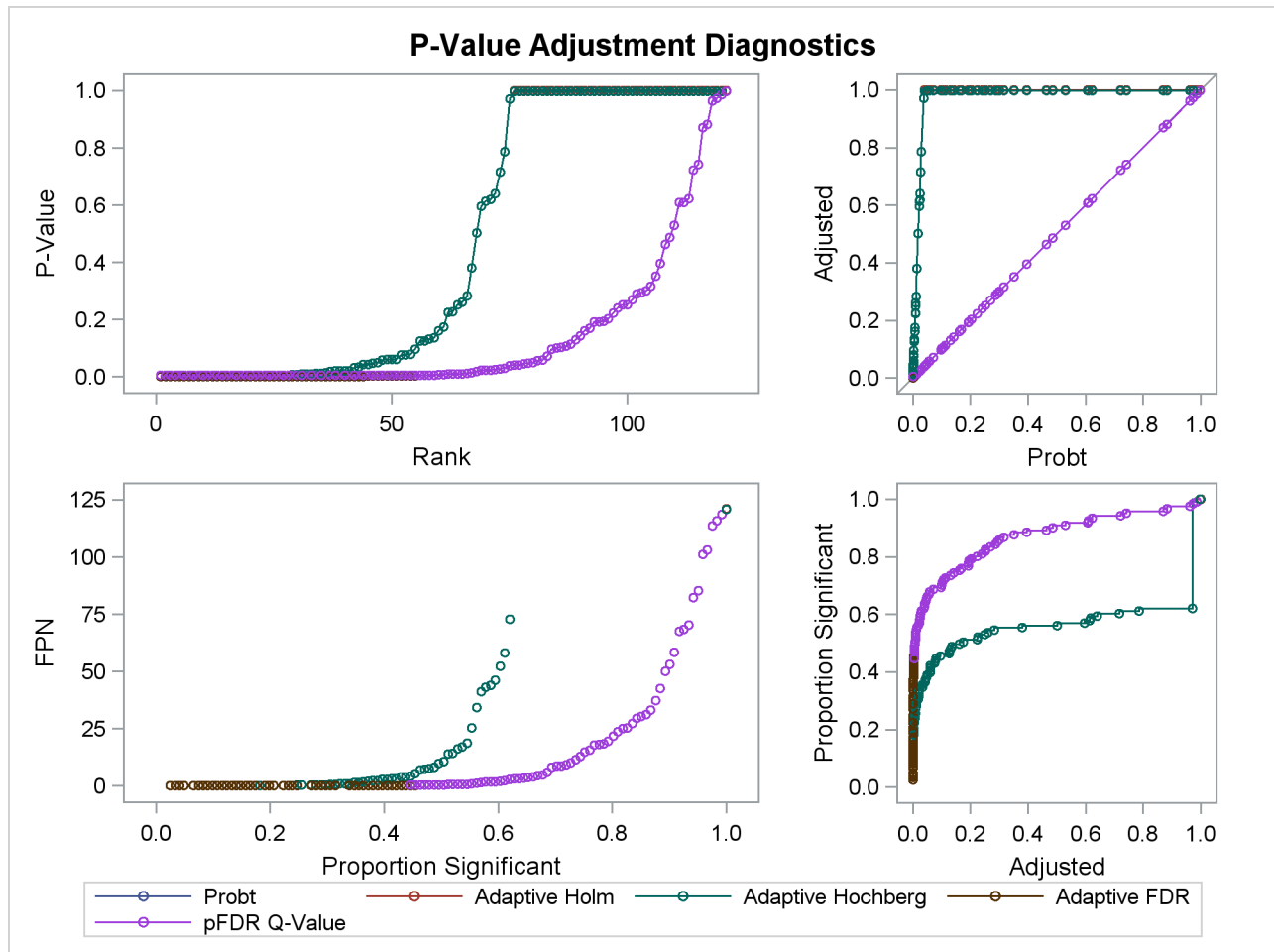
```
proc multtest invalues(Probt)=test ptruennull=0.10
 aholm ahoc afdr pfdr(positive) nopvalue;
 id Probe_Set_ID;
run;
```

A plot of the unadjusted and adjusted  $p$ -values for each test is also produced. Due to the large number of tests and adjustments, the plot is not very informative and is not displayed here.

The top two plots in [Output 61.6.5](#) show how the adjusted values compare with each other and the unadjusted  $p$ -values. The PFDR and AFDR adjustments are eventually smaller than the unadjusted  $p$ -values since they control the false discovery rate. The adaptive Holm and Hochberg adjustments are almost identical, so the adaptive Holm values are mostly obscured in all four plots. The plot of the Proportion Significant versus the Adjusted  $p$ -values tells you how many of the tests are significant for each cutoff, while the plot of the number of false positives (FPN) versus the Proportion Significant tells you how many false positives you can expect for that cutoff.



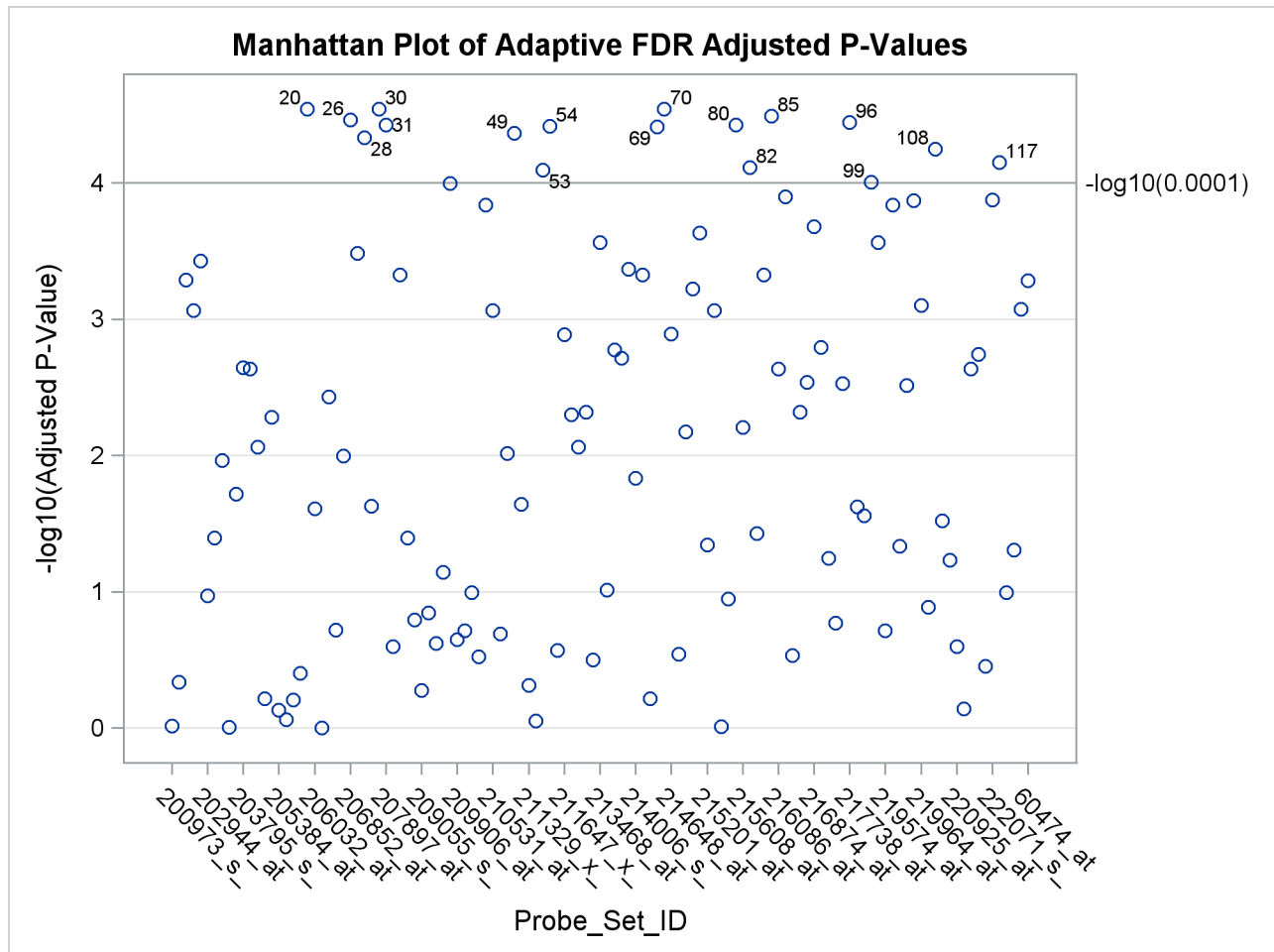
## Output 61.6.5 Adjustment Diagnostics



A Manhattan plot displays  $-\log_{10}$  of the adjusted  $p$ -values, so the most significant tests stand out at the top of the plot. The default plot is not displayed here. The following statements create a Manhattan plot of the adaptive FDR  $p$ -values, with the most significant tests labeled with their observation number. The ID values are displayed on the X axis, and the `VREF=` option specifies the significance level. This plot is typically created with many more  $p$ -values, and special ODS Graphics options such as the `LABELMAX=` option might be required to display the graph. If memory usage is an issue, you might want to store your  $p$ -values and use the `SGPLOT` procedure to create a similar graph.

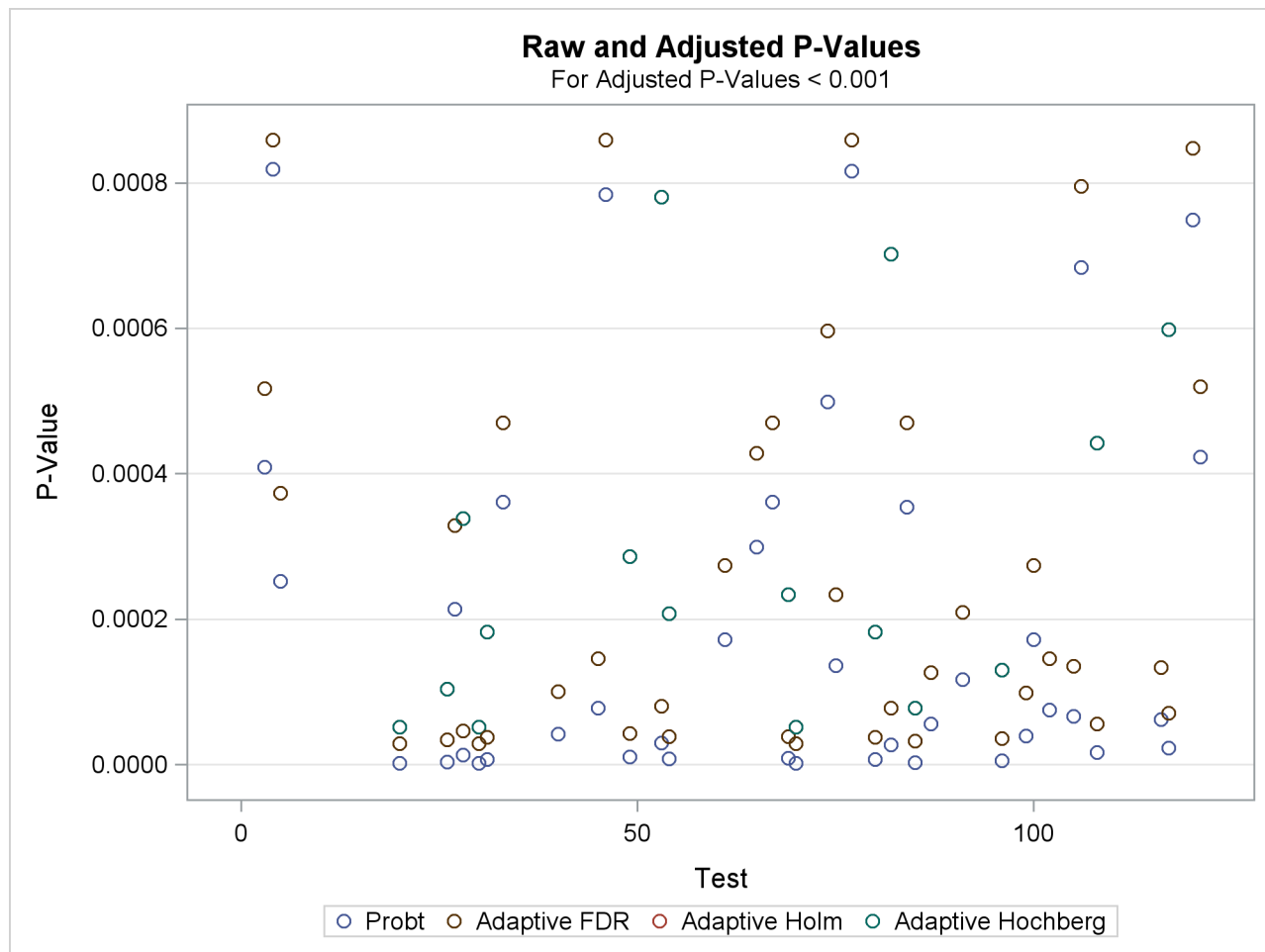
```
ods graphics on / labelmax=1000;
proc multtest inpvalues(Probt)=test afdr nopvalue
 plots=Manhattan(label=obs vref=0.0001);
 id Probe_Set_ID;
run;
ods graphics off;
```

Output 61.6.6 Manhattan Plot



If you have a lot of tests, the “Raw and Adjusted  $p$ -Values” and “P-Value Adjustment Diagnostics” plots can be more informative if you suppress some of the tests. In the following statements, the SIGONLY=0.001 option selects tests with adjusted  $p$ -values < 0.001 for display. Output 61.6.7 displays tests with their “significant” adjusted  $p$ -values:

```
ods graphics on;
proc multtest invalues(Probt)=test plots(sigonly=0.001)=PByTest
 aholm ahoc afdr pfdr(positive) nopvalue;
run;
ods graphics off;
```

Output 61.6.7 Raw and Adjusted  $p$ -Values

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# Chapter 62

## The NESTED Procedure

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## Overview: NESTED Procedure

The NESTED procedure performs random-effects analysis of variance for data from an experiment with a nested (hierarchical) structure.<sup>1</sup> A random-effects model for data from a completely nested design with two factors has the form

$$y_{ijr} = \mu + \alpha_i + \beta_{ij} + \epsilon_{ijr}$$

---

<sup>1</sup>PROC NESTED is modeled after the General Purpose Nested Analysis of Variance program of the Dairy Cattle Research Branch of the United States Department of Agriculture. That program was originally written by M. R. Swanson, Statistical Reporting Service, United States Department of Agriculture.



where

- $y_{ijr}$  is the value of the dependent variable observed at the  $r$ th replication with the first factor at its  $i$ th level and the second factor at its  $j$ th level.
- $\mu$  is the overall (fixed) mean of the sampling population.
- $\alpha_i, \beta_{ij}, \epsilon_{ijr}$  are mutually uncorrelated random effects with zero means and respective variances  $\sigma_\alpha^2, \sigma_\beta^2$ , and  $\sigma_\epsilon^2$  (the variance components).

This model is appropriate for an experiment with a multistage nested sampling design. An example of this is given in [Example 62.1](#), where four turnip plants are randomly chosen (the first factor), then three leaves are randomly chosen from each plant (the second factor nested within the first), and then two samples are taken from each leaf (the different replications at fixed levels of the two factors).

Note that PROC NESTED is appropriate for models with only classification effects; it does not handle models that contain continuous covariates. For random effects models with covariates, use either the GLM or MIXED procedure.

---

## Contrasted with Other SAS Procedures

The NESTED procedure performs a computationally efficient analysis of variance for data with a nested design, estimating the different components of variance and also testing for their significance if the design is balanced (see the section “[Unbalanced Data](#)” on page 5243). Although other procedures (such as GLM and MIXED) provide similar analyzes, PROC NESTED is both easier to use and computationally more efficient for this special type of design. This is especially true when the design involves a large number of factors, levels, or observations.

For example, to specify a four-factor completely nested design in the GLM procedure, you use the following form:

```
class a b c d;
model y=a b(a) c(a b) d(a b c);
```

However, to specify the same design in PROC NESTED, you simply use the following form:

```
class a b c d;
var y;
```

In addition, other procedures require TEST statements to perform appropriate tests, whereas the NESTED procedure produces the appropriate tests automatically. However, PROC NESTED makes one assumption about the input data that the other procedures do not: **PROC NESTED assumes that the input data set is sorted by the classification (CLASS) variables defining the effects.** If you use PROC NESTED on data that are not sorted by the CLASS variables, then the results might not be valid.

---

## Getting Started: NESTED Procedure

---

### Reliability of Automobile Models

A study is performed to compare the reliability of several models of automobiles. Three different automobile models (Model) from each of four U.S. automobile manufacturers (Make) are tested. Three different cars of each make and model are subjected to a reliability test and given a score between 1 and 100 (Score), where higher scores indicate greater reliability.

The following statements create the SAS data set auto.

```

title1 'Reliability of Automobile Models';
data auto;
 input Make $ Model Score @@;
 datalines;
a 1 62 a 2 77 a 3 59
a 1 67 a 2 73 a 3 64
a 1 60 a 2 79 a 3 60
b 1 72 b 2 58 b 3 80
b 1 75 b 2 63 b 3 84
b 1 69 b 2 57 b 3 89
c 1 94 c 2 76 c 3 81
c 1 90 c 2 75 c 3 85
c 1 88 c 2 78 c 3 85
d 1 69 d 2 73 d 3 90
d 1 72 d 2 88 d 3 87
d 1 76 d 2 87 d 3 92
;

```

The Make variable contains the make of the automobile, represented here by 'a', 'b', 'c', or 'd', while the Model variable represents the automobile model with a '1', '2', or '3'. The Score variable contains the reliability scores given to the three sampled cars from each Make-Model group. Since the automobile models are nested within their makes, the NESTED procedure is used to analyze these data. The NESTED procedure requires the data to be sorted by Make and, within Make, by Model, so the following statements execute a PROC SORT before completing the analysis.

```

proc sort data=auto;
 by Make Model;
run;

title1 'Reliability of Automobile Models';
proc nested data=auto;
 class Make Model;
 var Score;
run;

```

The Model variable appears after the Make variable in the CLASS statement because it is nested within Make. The VAR statement specifies the response variable. The output is displayed in [Figure 62.1](#).

Figure 62.1 Output from PROC NESTED

| Reliability of Automobile Models                              |      |                |         |        |            |             |                    |                  |
|---------------------------------------------------------------|------|----------------|---------|--------|------------|-------------|--------------------|------------------|
| The NESTED Procedure                                          |      |                |         |        |            |             |                    |                  |
| Coefficients of Expected Mean Squares                         |      |                |         |        |            |             |                    |                  |
| Source                                                        | Make | Model          | Error   |        |            |             |                    |                  |
| Make                                                          | 9    | 3              | 1       |        |            |             |                    |                  |
| Model                                                         | 0    | 3              | 1       |        |            |             |                    |                  |
| Error                                                         | 0    | 0              | 1       |        |            |             |                    |                  |
| Nested Random Effects Analysis of Variance for Variable Score |      |                |         |        |            |             |                    |                  |
| Variance Source                                               | DF   | Sum of Squares | F Value | Pr > F | Error Term | Mean Square | Variance Component | Percent of Total |
| Total                                                         | 35   | 4177.888889    |         |        |            | 119.368254  | 131.876543         | 100.0000         |
| Make                                                          | 3    | 1709.000000    | 2.15    | 0.1719 | Model      | 569.666667  | 33.867284          | 25.6811          |
| Model                                                         | 8    | 2118.888889    | 18.16   | <.0001 | Error      | 264.861111  | 83.425926          | 63.2606          |
| Error                                                         | 24   | 350.000000     |         |        |            | 14.583333   | 14.583333          | 11.0583          |
| Score Mean                                                    |      |                |         |        |            | 75.94444444 |                    |                  |
| Standard Error of Score Mean                                  |      |                |         |        |            | 3.97794848  |                    |                  |

Figure 62.1 first displays the coefficients of the variance components that make up each of the expected mean squares, and then it displays the ANOVA table. The results do not indicate significant variation between the different automobile makes ( $F = 2.15$ ,  $p = 0.1719$ ). However, they do suggest that there is significant variation between the different models within the makes ( $F = 18.16$ ,  $p < 0.0001$ ). This is evident in the fact that the make of car accounts for only 25.7% of the total variation in the data, while the car model accounts for 63.3% (as shown in the Percent of Total column). The estimated variance components are shown in the Variance Component column.

## Syntax: NESTED Procedure

The following statements are available in the NESTED procedure:

```
PROC NESTED < options > ;
 CLASS variables < / option > ;
 VAR variables ;
 BY variables ;
```

The PROC NESTED and CLASS statements are required. The BY, CLASS, and VAR statements are described after the PROC NESTED statement.

---

## PROC NESTED Statement

**PROC NESTED** < options > ;

The PROC NESTED statement invokes the NESTED procedure. Table 62.1 summarizes the options available in the PROC NESTED statement.

**Table 62.1** PROC NESTED Statement Options

| Option | Description                                       |
|--------|---------------------------------------------------|
| AOV    | Displays only the analysis of variance statistics |
| DATA=  | Names the SAS data set                            |

The PROC NESTED statement has the following options:

### AOV

displays only the analysis of variance statistics when there is more than one dependent variable. The “analysis of covariation” statistics are suppressed (see the section “[Analysis of Covariation](#)” on page 5244).

### DATA=SAS-data-set

names the SAS data set to be used by PROC NESTED. By default, the procedure uses the most recently created SAS data set.

---

## BY Statement

**BY** variables ;

You can specify a BY statement with PROC NESTED to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the NESTED procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

---

## CLASS Statement

**CLASS** *variables* </ option > ;

You must include a CLASS statement with PROC NESTED specifying the classification variables for the analysis.

Values of a variable in the CLASS statement denote the levels of an effect. The name of that variable is also the name of the corresponding effect. The second effect is assumed to be nested within the first effect, the third effect is assumed to be nested within the second effect, and so on.

By default, class levels are determined from the entire formatted values of the CLASS variables. Note that this represents a slight change from previous releases in the way in which class levels are determined. Prior to SAS 9, class levels were determined using no more than the first eight characters of the formatted values, except for numeric variables with no explicit format, for which class levels were determined from the raw numeric values. If you want to revert to this previous behavior, you can use the TRUNCATE option in the CLASS statement. In any case, you can use formats to group values into levels. See the discussion of the FORMAT procedure in the *Base SAS Procedures Guide*, and the discussions for the FORMAT statement and SAS formats in *SAS Statements: Reference*.

**NOTE:** The data set must be sorted by the classification variables in the order in which they are given in the CLASS statement. Use PROC SORT to sort the data if they are not already sorted.

You can specify the following option in the CLASS statement after a slash (/):

### TRUNCATE

specifies that class levels should be determined by using only up to the first 16 characters of the formatted values of CLASS variables. When formatted values are longer than 16 characters, you can use this option to revert to the levels as determined in releases prior to SAS 9.

---

## VAR Statement

**VAR** *variables* ;

The VAR statement lists the dependent variables for the analysis. The dependent variables must be numeric variables. If you do not specify a VAR statement, PROC NESTED performs an analysis of variance for all numeric variables in the data set, except those already specified in the CLASS statement.

---

## Details: NESTED Procedure

---

### Missing Values

An observation with missing values for any of the variables used by PROC NESTED is omitted from the analysis. Blank values of CLASS character variables are treated as missing values.

---

### Unbalanced Data

A completely nested design is defined to be unbalanced if the groups corresponding to the levels of some classification variable are not all of the same size. The NESTED procedure can compute unbiased estimates for the variance components in an unbalanced design, but because the sums of squares on which these estimates are based no longer have  $\chi^2$  distributions under a Gaussian model for the data,  $F$  tests for the significance of the variance components cannot be computed. PROC NESTED checks to see that the design is balanced. If it is not, a warning to that effect appears in the log, and the columns corresponding to the  $F$  tests in the analysis of variance are left blank.

---

### General Random-Effects Model

A random-effects model for data from a completely nested design with  $n$  factors has the general form

$$y_{i_1 i_2 \dots i_n r} = \mu + \alpha_{i_1} + \beta_{i_1 i_2} + \dots + \epsilon_{i_1 i_2 \dots i_n r}$$

where

$y_{i_1 i_2 \dots i_n r}$  is the value of the dependent variable observed at the  $r$ th replication with factor  $j$  at level  $i_j$ , for  $j = 1, \dots, n$ .

$\mu$  is the overall (fixed) mean of the sampled population.

$\alpha_{i_1}, \beta_{i_1 i_2}, \dots, \epsilon_{i_1 i_2 \dots i_n r}$  are mutually uncorrelated random effects with zero means and respective variances  $\sigma_\alpha^2, \sigma_\beta^2, \dots, \sigma_\epsilon^2$ .

---

## Analysis of Covariation

When you specify more than one dependent variable, the NESTED procedure produces a descriptive analysis of the covariance between each pair of dependent variables in addition to a separate analysis of variance for each variable. The analysis of covariation is computed under the basic random-effects model for each pair of dependent variables:

$$y_{i_1 i_2 \dots i_n r} = \mu + \alpha_{i_1} + \beta_{i_1 i_2} + \dots + \epsilon_{i_1 i_2 \dots i_n r}$$

$$y'_{i_1 i_2 \dots i_n r} = \mu' + \alpha'_{i_1} + \beta'_{i_1 i_2} + \dots + \epsilon'_{i_1 i_2 \dots i_n r}$$

where the notation is the same as that used in the preceding general random-effects model.

There is an additional assumption that all the random effects in the two models are mutually uncorrelated except for corresponding effects, for which

$$\begin{aligned} \text{Corr}(\alpha_{i_1}, \alpha'_{i_1}) &= \rho_\alpha \\ \text{Corr}(\beta_{i_1 i_2}, \beta'_{i_1 i_2}) &= \rho_\beta \\ &\vdots \\ \text{Corr}(\epsilon_{i_1 i_2 \dots i_n r}, \epsilon'_{i_1 i_2 \dots i_n r}) &= \rho_\epsilon \end{aligned}$$

---

## Error Terms in *F* Tests

Random-effects ANOVAs are distinguished from fixed-effects ANOVAs by which error mean squares are used as the denominator for *F* tests. Under a fixed-effects model, there is only one true error term in the model, and the corresponding mean square is used as the denominator for all tests. This is how the usual analysis is computed in PROC ANOVA, for example. However, in a random-effects model for a nested experiment, mean squares are compared sequentially. The correct denominator in the test for the first factor is the mean square due to the second factor; the correct denominator in the test for the second factor is the mean square due to the third factor; and so on. Only the mean square due to the last factor, the one at the bottom of the nesting order, should be compared to the error mean square.

## Computational Method

The building blocks of the analysis are the sums of squares for the dependent variables for each classification variable within the factors that precede it in the model, corrected for the factors that follow it. For example, for a two-factor nested design, PROC NESTED computes the following sums of squares:

$$\begin{aligned} \text{Total SS} & \quad \sum_{ijr} (y_{ijr} - y_{\dots})^2 \\ \text{SS for Factor 1} & \quad \sum_i n_{i\cdot} \left( \frac{y_{i\cdot}}{n_{i\cdot}} - \frac{y_{\dots}}{n_{\dots}} \right)^2 \\ \text{SS for Factor 2 within Factor 1} & \quad \sum_{ij} n_{ij} \left( \frac{y_{ij\cdot}}{n_{ij}} - \frac{y_{i\cdot}}{n_{i\cdot}} \right)^2 \\ \text{Error SS} & \quad \sum_{ijr} \left( y_{ijr} - \frac{y_{ij\cdot}}{n_{ij}} \right)^2 \end{aligned}$$

where  $y_{ijr}$  is the  $r$ th replication,  $n_{ij}$  is the number of replications at level  $i$  of the first factor and level  $j$  of the second, and a dot as a subscript indicates summation over the corresponding index. If there is more than one dependent variable, PROC NESTED also computes the corresponding sums of crossproducts for each pair. The expected value of the sum of squares for a given classification factor is a linear combination of the variance components corresponding to this factor and to the factors that are nested within it. For each factor, the coefficients of this linear combination are computed. (The efficiency of PROC NESTED is partly due to the fact that these various sums can be accumulated with just one pass through the data, assuming that the data have been sorted by the classification variables.) Finally, estimates of the variance components are derived as the solution to the set of linear equations that arise from equating the mean squares to their expected values.

## Displayed Output

PROC NESTED displays the following items for each dependent variable:

- Coefficients of Expected Mean Squares, which are the coefficients of the  $n + 1$  variance components making up the expected mean square. Denoting the element in the  $i$ th row and  $j$ th column of this matrix by  $C_{ij}$ , the expected value of the mean square due to the  $i$ th classification factor is

$$C_{i1}\sigma_1^2 + \cdots + C_{in}\sigma_n^2 + C_{i,n+1}\sigma_\epsilon^2$$

$C_{ij}$  is always zero for  $i > j$ , and if the design is balanced,  $C_{ij}$  is equal to the common size of all classification groups of the  $j$ th factor for  $i \leq j$ . Finally, the mean square for error is always an unbiased estimate of  $\sigma_\epsilon^2$ . In other words,  $C_{n+1,n+1} = 1$ .



For every dependent variable, PROC NESTED displays an analysis of variance table. Each table contains the following:

- each Variance Source in the model (the different components of variance) and the total variance
- degrees of freedom (DF) for the corresponding sum of squares
- Sum of Squares for each classification factor. The sum of squares for a given classification factor is the sum of squares in the dependent variable within the factors that precede it in the model, corrected for the factors that follow it. (See the section “[Computational Method](#)” on page 5245.)
- *F* Value for a factor, which is the ratio of its mean square to the appropriate error mean square. The next column, labeled *PR > F*, gives the significance levels that result from testing the hypothesis that each variance component equals zero.
- the appropriate Error Term for an *F* test, which is the mean square due to the next classification factor in the nesting order. (See the section “[Error Terms in \*F\* Tests](#)” on page 5244.)
- Mean Square due to a factor, which is the corresponding sum of squares divided by the degrees of freedom
- estimates of the Variance Components. These are computed by equating the mean squares to their expected values and solving for the variance terms. (See the section “[Computational Method](#)” on page 5245.)
- Percent of Total, the proportion of variance due to each source. For the *i*th factor, the value is

$$100 \times \frac{\text{source variance component}}{\text{total variance component}}$$

- Mean, the overall average of the dependent variable. This gives an unbiased estimate of the mean of the population. Its variance is estimated by a certain linear combination of the estimated variance components, which is identical to the mean square due to the first factor in the model divided by the total number of observations when the design is balanced.

If there is more than one dependent variable, then the NESTED procedure displays an “analysis of covariation” table for each pair of dependent variables (unless the AOV option is specified in the PROC NESTED statement). See the section “[Analysis of Covariation](#)” on page 5244 for details. For each source of variation, this table includes the following:

- Degrees of Freedom
- Sum of Products

- Mean Products
- Covariance Component, the estimate of the covariance component

Items in the analysis of covariation table are computed analogously to their counterparts in the analysis of variance table. The analysis of covariation table also includes the following:

- Variance Component Correlation for a given factor. This is an estimate of the correlation between corresponding effects due to this factor. This correlation is the ratio of the covariance component for this factor to the square root of the product of the variance components for the factor for the two different dependent variables. (See the section “[Analysis of Covariation](#)” on page 5244.)
- Mean Square Correlation for a given classification factor. This is the ratio of the Mean Products for this factor to the square root of the product of the Mean Squares for the factor for the two different dependent variables.

---

## ODS Table Names

PROC NESTED assigns a name to each table it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in the following table. For more information about ODS, see Chapter 20, “[Using the Output Delivery System.](#)”

**Table 62.2** ODS Tables Produced by PROC NESTED

| ODS Table Name | Description                           | Statement                                     |
|----------------|---------------------------------------|-----------------------------------------------|
| ANCOVA         | Analysis of covariance                | default with more than one dependent variable |
| ANOVA          | Analysis of variance                  | default                                       |
| EMSCoef        | Coefficients of expected mean squares | default                                       |
| Statistics     | Overall statistics for fit            | default                                       |

## Example: NESTED Procedure

### Example 62.1: Variability of Calcium Concentration in Turnip Greens

In the following example from Snedecor and Cochran (1976), an experiment is conducted to study the variability of calcium concentration in turnip greens. Four plants are selected at random; then three leaves are randomly selected from each plant. Two 100-mg samples are taken from each leaf. The amount of calcium is determined by microchemical methods.

Because the data are read in sorted order, it is not necessary to use PROC SORT on the CLASS variables. Leaf is nested in Plant; Sample is nested in Leaf and is left for the residual term. All the effects are random effects. The following statements read the data and invoke PROC NESTED. These statements produce Output 62.1.1.

```

title 'Calcium Concentration in Turnip Leaves--Nested Random Model';
title2 'Snedecor and Cochran, 'Statistical Methods', 1976, p. 286';
data Turnip;
 do Plant=1 to 4;
 do Leaf=1 to 3;
 do Sample=1 to 2;
 input Calcium @@;
 output;
 end;
 end;
 end;
 datalines;
3.28 3.09 3.52 3.48 2.88 2.80 2.46 2.44
1.87 1.92 2.19 2.19 2.77 2.66 3.74 3.44
2.55 2.55 3.78 3.87 4.07 4.12 3.31 3.31
;

proc nested data=Turnip;
 class plant leaf;
 var calcium;
run;

```

**Output 62.1.1** Analysis of Calcium Concentration in Turnip Greens Using PROC NESTED

Calcium Concentration in Turnip Leaves--Nested Random Model  
Snedecor and Cochran, 'Statistical Methods', 1976, p. 286

The NESTED Procedure

Coefficients of Expected Mean Squares

| Source | Plant | Leaf | Error |
|--------|-------|------|-------|
| Plant  | 6     | 2    | 1     |
| Leaf   | 0     | 2    | 1     |
| Error  | 0     | 0    | 1     |

Output 62.1.1 *continued*

| Nested Random Effects Analysis of Variance for Variable Calcium |    |                |         |        |            |             |                    |                  |
|-----------------------------------------------------------------|----|----------------|---------|--------|------------|-------------|--------------------|------------------|
| Variance Source                                                 | DF | Sum of Squares | F Value | Pr > F | Error Term | Mean Square | Variance Component | Percent of Total |
| Total                                                           | 23 | 10.270396      |         |        |            | 0.446539    | 0.532938           | 100.0000         |
| Plant                                                           | 3  | 7.560346       | 7.67    | 0.0097 | Leaf       | 2.520115    | 0.365223           | 68.5302          |
| Leaf                                                            | 8  | 2.630200       | 49.41   | <.0001 | Error      | 0.328775    | 0.161060           | 30.2212          |
| Error                                                           | 12 | 0.079850       |         |        |            | 0.006654    | 0.006654           | 1.2486           |
| Calcium Mean                                                    |    |                |         |        |            | 3.01208333  |                    |                  |
| Standard Error of Calcium Mean                                  |    |                |         |        |            | 0.32404445  |                    |                  |

The results indicate that there is significant (nonzero) variation from plant to plant ( $Pr > F$  is 0.0097) and from leaf to leaf within a plant ( $Pr > F$  is less than 0.0001). Notice that the variance component for Plant uses the Leaf mean square as an error term in the model rather than the error mean square.

---

## References

- Snedecor, G. W. and Cochran, W. G. (1976), *Statistical Methods*, Sixth Edition, Ames: Iowa State University Press.
- Steel, R. G. D. and Torrie, J. H. (1980), *Principles and Procedures of Statistics*, Second Edition, New York: McGraw-Hill.



# Chapter 63

## The NLIN Procedure

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| References . . . . .                                                 | <b>5344</b> |

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## Overview: NLIN Procedure

The NLIN procedure fits nonlinear regression models and estimates the parameters by nonlinear least squares or weighted nonlinear least squares. You specify the model with programming statements. This gives you great flexibility in modeling the relationship between the response variable and independent (regressor) variables. It does, however, require additional coding compared to model specifications in linear modeling procedures such as the REG, GLM, and MIXED procedures.

Estimating parameters in a nonlinear model is an iterative process that commences from starting values. You need to declare the parameters in your model and supply their initial values for the NLIN procedure. You do not need to specify derivatives of the model equation with respect to the parameters. Although facilities for specifying first and second derivatives exist in the NLIN procedure, it is not recommended that you specify derivatives this way. Obtaining derivatives from user-specified expressions predates the high-quality automatic differentiator that is now used by the NLIN procedure.

Nonlinear least-squares estimation involves finding those values in the parameter space that minimize the (weighted) residual sum of squares. In a sense, this is a “distribution-free” estimation criterion since the distribution of the data does not need to be fully specified. Instead, the assumption of homoscedastic and uncorrelated model errors with zero mean is sufficient. You can relax the homoscedasticity assumption by using a weighted residual sum of squares criterion. The assumption of uncorrelated errors (independent observations) cannot be relaxed in the NLIN procedure. In summary, the primary assumptions for analyses with the NLIN procedure are as follows:

- The structure in the response variable can be decomposed additively into a mean function and an error component.
- The model errors are uncorrelated and have zero mean. Unless a weighted analysis is performed, the errors are also assumed to be homoscedastic (have equal variance).
- The mean function consists of known regressor (independent) variables and unknown constants (the parameters).

Fitting nonlinear models can be a difficult undertaking. There is no closed-form solution for the parameter estimates, and the process is iterative. There can be one or more local minima in the residual sum of squares surface, and the process depends on the starting values supplied by the user. You can reduce the dependence on the starting values and reduce the chance to arrive at a local minimum by specifying a grid of starting values. The NLIN procedure then computes the residual sum of squares at each point on the grid and starts the iterative process from the point that yields the lowest sum of squares. Even in this case, however, convergence does not guarantee that a global minimum has been found.

The numerical behavior of a model and a model–data combination can depend on the way in which you parameterize the model—for example, whether parameters are expressed on the logarithmic scale or not. Parameterization also has bearing on the interpretation of the estimated quantities and the statistical properties of the parameter estimators. Inferential procedures in nonlinear regression models are typically approximate in that they rely on the asymptotic properties of the parameter estimators that are obtained as the sample size grows without bound. Such asymptotic inference can be questionable in small samples, especially if the behavior of the parameter estimators is “far-from-linear.” Reparameterization of the model can yield parameters whose behavior is akin to that of estimators in linear models. These parameters exhibit close-to-linear behavior.

The NLIN procedure solves the nonlinear least squares problem by one of the following four algorithms (methods):

- steepest-descent or gradient method
- Newton method
- modified Gauss-Newton method
- Marquardt method

These methods use derivatives or approximations to derivatives of the SSE with respect to the parameters to guide the search for the parameters producing the smallest SSE. Derivatives computed automatically by the NLIN procedure are analytic, unless the model contains functions for which an analytic derivative is not available.

Using PROC NLIN, you can also do the following:

- confine the estimation procedure to a certain range of values of the parameters by imposing bounds on the estimates
- produce new SAS data sets containing predicted values, parameter estimates, residuals and other model diagnostics, estimates at each iteration, and so forth.

You can use the NLIN procedure for segmented models (see [Example 63.1](#)) or robust regression (see [Example 63.2](#)). You can also use it to compute maximum-likelihood estimates for certain models (see Jennrich and Moore 1975; Charnes, Frome, and Yu 1976). For maximum likelihood estimation in a model with a linear predictor and binomial error distribution, see the LOGISTIC, PROBIT, GENMOD, GLIMMIX, and CATMOD procedures. For a linear model with a Poisson, gamma, or inverse Gaussian error distribution, see the GENMOD and GLIMMIX procedures. For likelihood estimation in a linear model with a normal error distribution, see the MIXED, GENMOD, and GLIMMIX procedures. The PHREG and LIFEREG procedures fit survival models by maximum likelihood. For general maximum likelihood estimation, see the NLP procedure in the *SAS/OR User's Guide: Mathematical Programming* and the NLMIXED procedure. These procedures are recommended over the NLIN procedure for solving maximum likelihood problems.

PROC NLIN uses the Output Delivery System (ODS). ODS enables you to convert any of the output from PROC NLIN into a SAS data set. See the section “[ODS Table Names](#)” on page 5305 for a listing of the ODS tables that are produced by the NLIN procedure.

In addition, PROC NLIN can produce graphs when ODS Graphics is enabled. For more information, see the [PLOTS](#) option and the section “[ODS Graphics](#)” on page 5305 for a listing of the ODS graphs.



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## Getting Started: NLIN Procedure

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### Nonlinear or Linear Model

The NLIN procedure performs univariate nonlinear regression by using the least squares method. Nonlinear regression analysis is indicated when the functional relationship between the response variable and the predictor variables is nonlinear. Nonlinearity in this context refers to a nonlinear relationship in the *parameters*. Many linear regression models exhibit a relationship in the regressor (predictor) variables that is not simply a straight line. This does not make the models nonlinear. A model is nonlinear in the parameters if the derivative of the model with respect to a parameter depends on this or other parameters.

Consider, for example the models

$$E[Y|x] = \beta_0 + \beta_1 x$$

$$E[Y|x] = \beta_0 + \beta_1 x + \beta_2 x^2$$

$$E[Y|x] = \beta + x/\alpha$$

In these expressions,  $E[Y|x]$  denotes the expected value of the response variable  $Y$  at the fixed value of  $x$ . (The conditioning on  $x$  simply indicates that the predictor variables are assumed to be non-random in models fit by the NLIN procedure. Conditioning is often omitted for brevity in this chapter.)

Only the third model is a nonlinear model. The first model is a simple linear regression. It is linear in the parameters  $\beta_0$  and  $\beta_1$  since the model derivatives do not depend on unknowns:

$$\frac{\partial}{\partial \beta_0} (\beta_0 + \beta_1 x) = 1$$

$$\frac{\partial}{\partial \beta_1} (\beta_0 + \beta_1 x) = x$$

The model is also linear in its relationship with  $x$  (a straight line). The second model is also linear in the parameters, since

$$\frac{\partial}{\partial \beta_0} (\beta_0 + \beta_1 x + \beta_2 x^2) = 1$$

$$\frac{\partial}{\partial \beta_1} (\beta_0 + \beta_1 x + \beta_2 x^2) = x$$

$$\frac{\partial}{\partial \beta_2} (\beta_0 + \beta_1 x + \beta_2 x^2) = x^2$$

It is a *curvilinear* model since it exhibits a curved relationship when plotted against  $x$ . The third model, finally, is a nonlinear model since

$$\frac{\partial}{\partial \beta} (\beta + x/\alpha) = 1$$

$$\frac{\partial}{\partial \alpha} (\beta + x/\alpha) = -\frac{x}{\alpha^2}$$

The second of these derivatives depends on a parameter  $\alpha$ . A model is nonlinear if it is not linear in at least one parameter.

---

## Notation for Nonlinear Regression Models

This section briefly introduces the basic notation for nonlinear regression models that applies in this chapter. Additional notation is introduced throughout as needed.

The  $(n \times 1)$  vector of observed responses is denoted as  $\mathbf{y}$ . This vector is the realization of an  $(n \times 1)$  random vector  $\mathbf{Y}$ . The NLIN procedure assumes that the variance matrix of this random vector is  $\sigma^2\mathbf{I}$ . In other words, the observations have equal variance (are homoscedastic) and are uncorrelated. By defining the special variable `_WEIGHT_` in your NLIN programming statements, you can introduce heterogeneous variances. If a `_WEIGHT_` variable is present, then  $\text{Var}[\mathbf{Y}] = \sigma^2\mathbf{W}^{-1}$ , where  $\mathbf{W}$  is a diagonal matrix containing the values of the `_WEIGHT_` variable.

The mean of the random vector is represented by a nonlinear model that depends on parameters  $\beta_1, \dots, \beta_p$  and regressor (independent) variables  $z_1, \dots, z_k$ :

$$E[Y_i] = f(\beta_1, \beta_2, \dots, \beta_p; z_{i1}, \dots, z_{ik})$$

In contrast to linear models, the number of regressor variables ( $k$ ) does not necessarily equal the number of parameters ( $p$ ) in the mean function  $f(\cdot)$ . For example, the model fitted in the next subsection contains a single regressor and two parameters.

To represent the mean of the vector of observations, boldface notation is used in an obvious extension of the previous equation:

$$E[\mathbf{Y}] = \mathbf{f}(\boldsymbol{\beta}; \mathbf{z}_1, \dots, \mathbf{z}_k)$$

The vector  $\mathbf{z}_1$ , for example, is an  $(n \times 1)$  vector of the values for the first regressor variables. The explicit dependence of the mean function on  $\boldsymbol{\beta}$  and/or the  $\mathbf{z}$  vectors is often omitted for brevity.

In summary, the stochastic structure of models fit with the NLIN procedure is mathematically captured by

$$\begin{aligned} \mathbf{Y} &= \mathbf{f}(\boldsymbol{\beta}; \mathbf{z}_1, \dots, \mathbf{z}_k) + \boldsymbol{\epsilon} \\ E[\boldsymbol{\epsilon}] &= \mathbf{0} \\ \text{Var}[\boldsymbol{\epsilon}] &= \sigma^2\mathbf{I} \end{aligned}$$

Note that the residual variance  $\sigma^2$  is typically also unknown. Since it is not estimated in the same fashion as the other  $p$  parameters, it is often not counted in the number of parameters of the nonlinear regression. An estimate of  $\sigma^2$  is obtained after the model fit by the method of moments based on the residual sum of squares.

A matrix that plays an important role in fitting nonlinear regression models is the  $(n \times p)$  matrix of the first partial derivatives of the mean function  $\mathbf{f}$  with respect to the  $p$  model parameters. It is frequently denoted as

$$\mathbf{X} = \frac{\partial \mathbf{f}(\boldsymbol{\beta}; \mathbf{z}_1, \dots, \mathbf{z}_k)}{\partial \boldsymbol{\beta}}$$

The use of the symbol  $\mathbf{X}$ —common in linear statistical modeling—is no accident here. The first derivative matrix plays a similar role in nonlinear regression to that of the  $\mathbf{X}$  matrix in a linear model. For example, the

asymptotic variance of the nonlinear least-squares estimators is proportional to  $(\mathbf{X}'\mathbf{X})^{-1}$ , and projection-type matrices in nonlinear regressions are based on  $\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'$ . Also, fitting a nonlinear regression model can be cast as an iterative process where a nonlinear model is approximated by a series of linear models in which the derivative matrix is the regressor matrix. An important difference between linear and nonlinear models is that the derivatives in a linear model do not depend on any parameters (see previous subsection). In contrast, the derivative matrix  $\partial f(\boldsymbol{\beta})/\partial \boldsymbol{\beta}$  is a function of at least one element of  $\boldsymbol{\beta}$ . It is this dependence that lies at the core of the fact that estimating the parameters in a nonlinear model cannot be accomplished in closed form, but it is an iterative process that commences with user-supplied starting values and attempts to continually improve on the parameter estimates.

---

## Estimating the Parameters in the Nonlinear Model

As an example of a nonlinear regression analysis, consider the following theoretical model of enzyme kinetics. The model relates the initial velocity of an enzymatic reaction to the substrate concentration.

$$f(\mathbf{x}, \boldsymbol{\theta}) = \frac{\theta_1 x_i}{\theta_2 + x_i}, \quad \text{for } i = 1, 2, \dots, n$$

where  $x_i$  represents the amount of substrate for  $n$  trials and  $f(\mathbf{x}, \boldsymbol{\theta})$  is the velocity of the reaction. The vector  $\boldsymbol{\theta}$  contains the rate parameters. This model is known as the Michaelis-Menten model in biochemistry (Ratkowsky 1990, p. 59). The model exists in many parameterizations. In the form shown here,  $\theta_1$  is the maximum velocity of the reaction that is theoretically attainable. The parameter  $\theta_2$  is the substrate concentration at which the velocity is 50% of the maximum.

Suppose that you want to study the relationship between concentration and velocity for a particular enzyme/substrate pair. You record the reaction rate (velocity) observed at different substrate concentrations.

A SAS data set is created for this experiment in the following DATA step:

```
data Enzyme;
 input Concentration Velocity @@;
 datalines;
0.26 124.7 0.30 126.9
0.48 135.9 0.50 137.6
0.54 139.6 0.68 141.1
0.82 142.8 1.14 147.6
1.28 149.8 1.38 149.4
1.80 153.9 2.30 152.5
2.44 154.5 2.48 154.7
;
```

The SAS data set Enzyme contains the two variables Concentration (substrate concentration) and Velocity (reaction rate). The following statements fit the Michaelis-Menten model by nonlinear least squares:

```
proc nlin data=Enzyme method=marquardt hougard;
 parms theta1=155
 theta2=0 to 0.07 by 0.01;
 model Velocity = theta1*Concentration / (theta2 + Concentration);
run;
```

The **DATA=** option specifies that the SAS data set `Enzyme` be used in the analysis. The **METHOD=** option directs PROC NLIN to use the MARQUARDT iterative method. The **HOUGAARD** option requests that a skewness measure be calculated for the parameters.

The **PARMS** statement declares the parameters and specifies their initial values. Suppose that  $V$  represents the velocity and  $C$  represents the substrate concentration. In this example, the initial estimates listed in the **PARMS** statement for  $\theta_1$  and  $\theta_2$  are obtained as follows:

$\theta_1$ : Because the model is a monotonic increasing function in  $C$ , and because

$$\lim_{C \rightarrow \infty} \left( \frac{\theta_1 C}{\theta_2 + C} \right) = \theta_1$$

you can take the largest observed value of the variable `Velocity` (154.7) as the initial value for the parameter `Theta1`. Thus, the **PARMS** statement specifies 155 as the initial value for `Theta1`, which is approximately equal to the maximum observed velocity.

$\theta_2$ : To obtain an initial value for the parameter  $\theta_2$ , first rearrange the model equation to solve for  $\theta_2$ :

$$\theta_2 = \frac{\theta_1 C}{V} - C$$

By substituting the initial value of `Theta1` for  $\theta_1$  and taking each pair of observed values of `Concentration` and `Velocity` for  $C$  and  $V$ , respectively, you obtain a set of possible starting values for `Theta2` ranging from about 0.01 to 0.07.

You can choose any value within this range as a starting value for `Theta2`, or you can direct PROC NLIN to perform a preliminary search for the best initial `Theta2` value within that range of values. The **PARMS** statement specifies a range of values for `Theta2`, resulting in a search over the grid points from 0 to 0.07 in increments of 0.01.

The **MODEL** statement specifies the enzymatic reaction model

$$V = \frac{\theta_1 C}{\theta_2 + C}$$

in terms of the data set variables `Velocity` and `Concentration` and in terms of the parameters in the **PARMS** statement.

The results from this PROC NLIN invocation are displayed in the following figures.

PROC NLIN evaluates the model at each point on the specified grid for the `Theta2` parameter. [Figure 63.1](#) displays the calculations resulting from the grid search.

**Figure 63.1** Nonlinear Least-Squares Grid Search

| The NLIN Procedure          |        |                |
|-----------------------------|--------|----------------|
| Dependent Variable Velocity |        |                |
| Grid Search                 |        |                |
| theta1                      | theta2 | Sum of Squares |
| 155.0                       | 0      | 3075.4         |
| 155.0                       | 0.0100 | 2074.1         |
| 155.0                       | 0.0200 | 1310.3         |
| 155.0                       | 0.0300 | 752.0          |
| 155.0                       | 0.0400 | 371.9          |
| 155.0                       | 0.0500 | 147.2          |
| 155.0                       | 0.0600 | 58.1130        |
| 155.0                       | 0.0700 | 87.9662        |

The parameter Theta1 is held constant at its specified initial value of 155, the grid is traversed, and the residual sum of squares is computed at each point. The “best” starting value is the point that corresponds to the smallest value of the residual sum of squares. The best set of starting values is obtained for  $\theta_1 = 155$ ,  $\theta_2 = 0.06$  (Figure 63.1). PROC NLIN uses this point from which to start the following, iterative phase of nonlinear least-squares estimation.

Figure 63.2 displays the iteration history. Note that the first entry in the “Iterative Phase” table echoes the starting values and the residual sum of squares for the best value combination in Figure 63.1. The subsequent rows of the table show the updates of the parameter estimates and the improvement (decrease) in the residual sum of squares. For this data-and-model combination, the first iteration yielded a large improvement in the sum of squares (from 58.113 to 19.7017). Further steps were necessary to improve the estimates in order to achieve the convergence criterion. The NLIN procedure by default determines convergence by using R, the relative offset measure of Bates and Watts (1981). Convergence is declared when this measure is less than  $10^{-5}$ —in this example, after three iterations.

**Figure 63.2** Iteration History and Convergence Status

| The NLIN Procedure          |        |        |                |
|-----------------------------|--------|--------|----------------|
| Dependent Variable Velocity |        |        |                |
| Method: Marquardt           |        |        |                |
| Iterative Phase             |        |        |                |
| Iter                        | theta1 | theta2 | Sum of Squares |
| 0                           | 155.0  | 0.0600 | 58.1130        |
| 1                           | 158.0  | 0.0736 | 19.7017        |
| 2                           | 158.1  | 0.0741 | 19.6606        |
| 3                           | 158.1  | 0.0741 | 19.6606        |

**NOTE:** Convergence criterion met.

**Figure 63.3** Estimation Summary

| Estimation Summary   |           |
|----------------------|-----------|
| Method               | Marquardt |
| Iterations           | 3         |
| R                    | 5.861E-6  |
| PPC(theta2)          | 8.569E-7  |
| RPC(theta2)          | 0.000078  |
| Object               | 2.902E-7  |
| Objective            | 19.66059  |
| Observations Read    | 14        |
| Observations Used    | 14        |
| Observations Missing | 0         |

A summary of the estimation including several convergence measures (R, PPC, RPC, and Object) is displayed in Figure 63.3.

The “R” measure in Figure 63.3 is the relative offset convergence measure of Bates and Watts. A “PPC” value of 8.569E-7 indicates that the parameter Theta2 (which has the largest PPC value of the parameters) would change by that relative amount, if PROC NLIN were to take an additional iteration step. The “RPC” value indicates that Theta2 changed by 0.000078, relative to its value in the last iteration. These changes are measured before step length adjustments are made. The “Object” measure indicates that the objective function changed by 2.902E-7 in relative value from the last iteration.

Figure 63.4 displays the analysis of variance table for the model. The table displays the degrees of freedom, sums of squares, and mean squares along with the model *F* test.

**Figure 63.4** Nonlinear Least-Squares Analysis of Variance

NOTE: An intercept was not specified for this model.

| Source            | DF | Sum of Squares | Mean Square | F Value | Approx Pr > F |
|-------------------|----|----------------|-------------|---------|---------------|
| Model             | 2  | 290116         | 145058      | 88537.2 | <.0001        |
| Error             | 12 | 19.6606        | 1.6384      |         |               |
| Uncorrected Total | 14 | 290135         |             |         |               |

**Figure 63.5** Parameter Estimates and Approximate 95% Confidence Intervals

| Parameter | Estimate | Approx Std Error | Approximate 95% Confidence Limits |        | Skewness |
|-----------|----------|------------------|-----------------------------------|--------|----------|
| theta1    | 158.1    | 0.6737           | 156.6                             | 159.6  | 0.0152   |
| theta2    | 0.0741   | 0.00313          | 0.0673                            | 0.0809 | 0.0362   |

Figure 63.5 displays the estimates for each parameter, the associated asymptotic standard error, and the upper and lower values for the asymptotic 95% confidence interval. PROC NLIN also displays the asymptotic

correlations between the estimated parameters (not shown).

The skewness measures of 0.0152 and 0.0362 indicate that the parameter estimators exhibit close-to-linear behavior and that their standard errors and confidence intervals can be safely used for inferences.

Thus, the estimated nonlinear model relating reaction velocity and substrate concentration can be written as

$$\hat{V} = \frac{158.1C}{0.0741 + C}$$

where  $\hat{V}$  represents the predicted velocity or rate of the reaction, and  $C$  represents the substrate concentration.

## Syntax: NLIN Procedure

The following statements are available in the NLIN procedure:

```

PROC NLIN < options > ;
 BOUNDS inequality < , ... , inequality > ;
 BY variables ;
 CONTROL variable < =values > < ... variable < =values > > ;
 DER. parameter=expression ;
 DER. parameter.parameter=expression ;
 ID variables ;
 MODEL dependent = expression ;
 OUTPUT OUT=SAS-data-set keyword=names < ... keyword=names > ;
 PARAMETERS < parameter-specification > < , ... , parameter-specification >
 < / PDATA=SAS-data-set > ;
 PROFILE parameter < ... parameter > < / options > ;
 RETAIN variable < =values > < ... variable < =values > > ;
 Programming statements ;

```

The statements in the NLIN procedure, in addition to the **PROC NLIN** statement, are as follows:

|                               |                                                                                                                                                                    |
|-------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>BOUNDS</b>                 | constrains the parameter estimates within specified bounds                                                                                                         |
| <b>BY</b>                     | specifies variables to define subgroups for the analysis                                                                                                           |
| <b>DER</b>                    | specifies the first or second partial derivatives                                                                                                                  |
| <b>ID</b>                     | specifies additional variables to add to the output data set                                                                                                       |
| <b>MODEL</b>                  | defines the relationship between the dependent and independent variables (the mean function)                                                                       |
| <b>OUTPUT</b>                 | creates an output data set containing observation-wise statistics                                                                                                  |
| <b>PARAMETERS</b>             | identifies parameters to be estimated and their starting values                                                                                                    |
| <b>PROFILE</b>                | identifies parameters to be profiled                                                                                                                               |
| <i>Programming Statements</i> | includes assignment statements, <b>ARRAY</b> statements, <b>DO</b> loops, and other program control statements. These are valid SAS expressions that can appear in |

the DATA step. PROC NLIN enables you to create new variables within the procedure and use them in the nonlinear analysis. These programming statements can appear anywhere in the PROC NLIN code, but new variables must be created before they appear in other statements. The NLIN procedure automatically creates several variables that are also available for use in the analysis. See the section “Special Variables” on page 5291 for more information.

The PROC NLIN, PARAMETERS, and MODEL statements are required.

---

## PROC NLIN Statement

**PROC NLIN** < options > ;

The PROC NLIN statement invokes the NLIN procedure.

Table 63.1 summarizes the options available in the PROC NLIN statement. All options are subsequently discussed in alphabetical order.

**Table 63.1** Summary of Options in PROC NLIN Statement

| Option                                      | Description                                                                                     |
|---------------------------------------------|-------------------------------------------------------------------------------------------------|
| <b>Options Related to Data Sets</b>         |                                                                                                 |
| DATA=                                       | Specifies the input data set                                                                    |
| OUTEST=                                     | Specifies the output data set for parameter estimates, covariance matrix, and so on             |
| SAVE                                        | Requests that final estimates be added to the OUTEST= data set                                  |
| <b>Optimization Options</b>                 |                                                                                                 |
| BEST=                                       | Limits display of grid search                                                                   |
| METHOD=                                     | Chooses the optimization method                                                                 |
| MAXITER=                                    | Specifies the maximum number of iterations                                                      |
| MAXSUBIT=                                   | Specifies the maximum number of step halvings                                                   |
| NOHALVE                                     | Allows the objective function to increase between iterations                                    |
| RHO=                                        | Controls the step-size search                                                                   |
| SMETHOD=                                    | Specifies the step-size search method                                                           |
| TAU=                                        | Controls the step-size search                                                                   |
| G4                                          | Uses the Moore-Penrose inverse                                                                  |
| UNCORRECTEDDF                               | Does not expense degrees of freedom when bounds are active                                      |
| SIGSQ=                                      | Specifies the fixed value for residual variance                                                 |
| <b>Singularity and Convergence Criteria</b> |                                                                                                 |
| CONVERGE=                                   | Tunes the convergence criterion                                                                 |
| CONVERGEOBJ=                                | Uses the change in loss function as the convergence criterion and tunes its value               |
| CONVERGEPARM=                               | Uses the maximum change in parameter estimates as the convergence criterion and tunes its value |
| SINGULAR=                                   | Tunes the singularity criterion used in matrix inversions                                       |

---



Table 63.1 *continued*

| Option                       | Description                                                                              |
|------------------------------|------------------------------------------------------------------------------------------|
| <b>ODS Graphics Options</b>  |                                                                                          |
| PLOTS=                       | Produces ODS graphical displays                                                          |
| <b>Displayed Output</b>      |                                                                                          |
| HOUGAARD                     | Adds Hougaard's skewness measure to the "Parameter Estimates" table                      |
| BIAS                         | Adds Box's bias measure to the "Parameter Estimates" table                               |
| NOITPRINT                    | Suppresses the "Iteration History" table                                                 |
| NOPRINT                      | Suppresses displayed output                                                              |
| LIST                         | Displays the model program and variable list                                             |
| LISTALL                      | Selects the LIST, LISTDEP, LISTDER, and LISTCODE options                                 |
| LISTCODE                     | Displays the model program code                                                          |
| LISTDEP                      | Displays dependencies of model variables                                                 |
| LISTDER                      | Displays the derivative table                                                            |
| NLINMEASURES                 | Displays the global nonlinearity measures table                                          |
| TOTALSS                      | Adds the uncorrected or corrected total sum of squares to the analysis of variance table |
| XREF                         | Displays the cross-reference of variables                                                |
| <b>Trace Model Execution</b> |                                                                                          |
| FLOW                         | Displays execution messages for program statements                                       |
| PRINT                        | Displays results of statements in model program                                          |
| TRACE                        | Displays results of operations in model program                                          |

**ALPHA= $\alpha$** 

specifies the level of significance  $\alpha$  used in the construction of  $100(1 - \alpha)\%$  confidence intervals. The value must be strictly between 0 and 1; the default value of  $\alpha = 0.05$  results in 95% intervals. This value is used as the default confidence level for limits computed in the "Parameter Estimates" table and with the LCLM, LCL, UCLM, and UCL options in the OUTPUT statement.

**BEST= $n$** 

requests that PROC NLIN display the residual sums of squares only for the best  $n$  combinations of possible starting values from the grid. If you do not specify the BEST= option, PROC NLIN displays the residual sum of squares for every combination of possible parameter starting values.

**BIAS**

adds Box's bias and percentage bias measures to the "Parameter Estimates" table (Box 1971). Box's bias measure, along with Hougaard's measure of skewness, is used for assessing a parameter estimator's close-to-linear behavior (Ratkowsky 1983, 1990). Hence, it is useful for identifying problematic parameters (Seber and Wild 1989, sec. 4.7.1). When you specify the BIAS option, Box's bias measure (Box 1971) and the percentage bias (the bias expressed as a percentage of the least-squares estimator) are added for each parameter to the "Parameter Estimates" table. Ratkowsky (1983, p. 21) takes a percentage bias in excess of 1% to be a good rule of thumb for indicating nonlinear behavior.

See the section "Box's Measure of Bias" on page 5286 for further details. Example 63.4 shows how to use this measure, along with Hougaard's measure of skewness, to evaluate changes in the

parameterization of a nonlinear model. Computation of the Box's bias measure requires first and second derivatives. If you do not provide derivatives with the **DER** statement—and it is recommended that you do not—the analytic derivatives are computed for you.

### **CONVERGE=c**

specifies the convergence criterion for PROC NLIN. For all iterative methods the relative offset convergence measure of Bates and Watts is used by default to determine convergence. This measure is labeled “R” in the “Estimation Summary” table. The iterations are said to have converged for **CONVERGE=c** if

$$\sqrt{\frac{\mathbf{r}'\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{r}}{\text{LOSS}^{(i)}}} < c$$

where  $\mathbf{r}$  is the residual vector and  $\mathbf{X}$  is the  $(n \times p)$  matrix of first derivatives with respect to the parameters. The default LOSS function is the sum of squared errors (SSE), and  $\text{LOSS}^{(i)}$  denotes the value of the loss function at the  $i$ th iteration. By default, **CONVERGE**= $10^{-5}$ . The R convergence measure cannot be computed accurately in the special case of a perfect fit (residuals close to zero). When the SSE is less than the value of the **SINGULAR=** criterion, convergence is assumed.

### **CONVERGEOBJ=c**

uses the change in the LOSS function as the convergence criterion and tunes the criterion. The iterations are said to have converged for **CONVERGEOBJ=c** if

$$\frac{|\text{LOSS}^{(i-1)} - \text{LOSS}^{(i)}|}{|\text{LOSS}^{(i-1)} + 10^{-6}|} < c$$

where  $\text{LOSS}^{(i)}$  is the LOSS for the  $i$ th iteration. The default LOSS function is the sum of squared errors (SSE), the residual sum of squares. The constant  $c$  should be a small positive number. For more details about the LOSS function, see the section “[Special Variable Used to Determine Convergence Criteria](#)” on page 5292. For more details about the computational methods in the NIN procedure, see the section “[Computational Methods](#)” on page 5294.

Note that in SAS 6 the **CONVERGE=** and **CONVERGEOBJ=** options both requested that convergence be tracked by the relative change in the loss function. If you specify the **CONVERGEOBJ=** option in newer releases, the **CONVERGE=** option is disabled. This enables you to track convergence as in SAS 6.

### **CONVERGEPARM=c**

uses the maximum change among parameter estimates as the convergence criterion and tunes the criterion. The iterations are said to have converged for **CONVERGEPARM=c** if

$$\max_j \left( \frac{|\beta_j^{(i-1)} - \beta_j^{(i)}|}{|\beta_j^{(i-1)}|} \right) < c$$

where  $\beta_j^{(i)}$  is the value of the  $j$ th parameter at the  $i$ th iteration.

The default convergence criterion is **CONVERGE**. If you specify **CONVERGEPARM=c**, the maximum change in parameters is used as the convergence criterion. If you specify both the **CONVERGEOBJ=** and **CONVERGEPARM=** options, PROC NLIN continues to iterate until the decrease in LOSS is sufficiently small (as determined by the **CONVERGEOBJ=** option) and the maximum change among the parameters is sufficiently small (as determined by the **CONVERGEPARM=** option).

**DATA=SAS-data-set**

specifies the input SAS data set to be analyzed by PROC NLIN. If you omit the DATA= option, the most recently created SAS data set is used.

**FLOW**

displays a message for each statement in the model program as it is executed. This debugging option is rarely needed, and it produces large amounts of output.

**G4**

uses a Moore-Penrose inverse ( $g_4$ -inverse) in parameter estimation. See Kennedy and Gentle (1980) for details.

**HOUGAARD**

adds Hougaard's measure of skewness to the "Parameter Estimates" table (Hougaard 1982, 1985). The skewness measure is one method of assessing a parameter estimator's close-to-linear behavior in the sense of Ratkowsky (1983, 1990). The behavior of estimators that are close to linear approaches that of least squares estimators in linear models, which are unbiased and have minimum variance. When you specify the HOUGAARD option, the standardized skewness measure of Hougaard (1985) is added for each parameter to the "Parameter Estimates" table. Because of the linkage between nonlinear behavior of a parameter estimator in nonlinear regression and the nonnormality of the estimator's sampling distribution, Ratkowsky (1990, p. 28) provides the following rules to interpret the (standardized) Hougaard skewness measure:

- Values less than 0.1 in absolute value indicate very close-to-linear behavior.
- Values between 0.1 and 0.25 in absolute value indicate reasonably close-to-linear behavior.
- The nonlinear behavior is apparent for absolute values above 0.25 and is considerable for absolute values above 1.

See the section "[Hougaard's Measure of Skewness](#)" on page 5286 for further details. [Example 63.4](#) shows how to use this measure to evaluate changes in the parameterization of a nonlinear model. Computation of the Hougaard skewness measure requires first and second derivatives. If you do not provide derivatives with the [DER](#) statement—and it is recommended that you do not—the analytic derivatives are computed for you.

**LIST**

displays the model program and variable lists, including the statements added by macros. Note that the expressions displayed by the LIST option do not necessarily represent the way the expression is actually calculated—because intermediate results for common subexpressions can be reused—but are shown in expanded form. To see how the expression is actually evaluated, use the [LISTCODE](#) option.

**LISTALL**

selects the [LIST](#), [LISTDEP](#), [LISTDER](#), and [LISTCODE](#) options.

**LISTCODE**

displays the derivative tables and the compiled model program code. The LISTCODE option is a debugging feature and is not normally needed.

**LISTDEP**

produces a report that lists, for each variable in the model program, the variables that depend on it and the variables on which it depends.

**LISTDER**

displays a table of derivatives. The derivatives table lists each nonzero derivative computed for the problem. The derivative listed can be a constant, a variable in the model program, or a special derivative variable created to hold the result of an expression.

**MAXITER=*n***

specifies the maximum number *n* of iterations in the optimization process. The default is *n* = 100.

**MAXSUBIT=*n***

places a limit on the number of step halvings. The value of MAXSUBIT must be a positive integer and the default value is *n* = 30.

**METHOD=GAUSS****METHOD=MARQUARDT****METHOD=NEWTON****METHOD=GRADIENT**

specifies the iterative method employed by the NLIN procedure in solving the nonlinear least squares problem. The GAUSS, MARQUARDT, and NEWTON methods are more robust than the GRADIENT method. If you omit the METHOD= option, METHOD=GAUSS is used. See the section “Computational Methods” on page 5294 for more information.

**NLINMEASURES**

displays the global nonlinearity measures table. These measures include the maximum intrinsic and parameter-effects curvatures (Bates and Watts 1980), the root mean square (RMS) intrinsic and parameter-effects curvatures and the critical curvature value (Bates and Watts 1980). In addition, the variances of the ordinary and projected residuals are included. According to Bates and Watts (1980), both intrinsic and parameter-effects curvatures are deemed negligible if they are less than the critical curvature value. This critical value is given by  $1/(\sqrt{F})$  where  $F = F(p, n - p; \alpha)$ . The value  $1/\sqrt{F}$  can be considered as the radius of curvature of the 100(1 -  $\alpha$ ) percent confidence region (Bates and Watts 1980).

**NOITPRINT**

suppresses the display of the “Iteration History” table.

**NOHALVE**

removes the restriction that the objective value must decrease at every iteration. Step halving is still used to satisfy **BOUNDS** and to ensure that the number of observations that can be evaluated does not decrease. The NOHALVE option can be useful in weighted nonlinear least squares problems where the weights depend on the parameters, such as in iteratively reweighted least squares (IRLS) fitting. See [Example 63.2](#) for an application of IRLS fitting.

**NOPRINT**

suppresses the display of the output. Note that this option temporarily disables the Output Delivery System (ODS). For more information, see Chapter 20, “Using the Output Delivery System.”

**OUTEST=SAS-data-set**

specifies an output data set that contains the parameter estimates produced at each iteration. See the section “[Output Data Sets](#)” for details. If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*.

**PLOTS** <(global-plot-option)> <= (plot-request <(options)> <... plot-request <(options)> >)>

controls most of the plots that are produced through ODS Graphics (other plots are controlled by the [PROFILE](#) statement). When you specify only one *plot-request*, you can omit the parentheses around it. Here are some examples:

```
plots
plots = none
plots = diagnostics(unpack)
plots = fit(stats=none)
plots = residuals(residualtype=proj unpack smooth)
plots(stats=all) = (diagnostics(stats=(maxincurv maxpecurv)) fit)
```

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;

proc nlin plots=diagnostics(stats=all);
 model y = alpha - beta*(gamma**x);
run;

ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS](#).”

If ODS Graphics is enabled and if you specify the PLOTS option without any *global-plot-option* or *plot-requests*, PROC NLIN produces the plots listed in [Table 63.2](#) with the default set of statistics and options. If you do not specify the PLOTS option, PROC NLIN does not produce any of these graphs.

**Table 63.2** Graphs Produced When the PLOTS Option Is Specified

| Plot                | Conditional On            |
|---------------------|---------------------------|
| ContourFitPlot      | Model with two regressors |
| FitDiagnosticsPanel | Unconditional             |
| FitPlot             | Model with one regressor  |
| LeveragePlot        | Unconditional             |
| LocalInfluencePlot  | Unconditional             |
| ResidualPanel       | Unconditional             |

You can request additional plots by specifying *plot-requests*. For a listing of all the plots that PROC NLIN produces, see the section “[ODS Graphics](#)” on page 5305. Each *global-plot-option* applies to all plots that are generated by the NLIN procedure except for plots that are controlled by the **PROFILE** statement. The *global-plot-option* can be overridden by a specific *option* after a *plot-request*.

The following *global-plot-options* are available:

**RESIDUALTYPE=RAW | PROJ | BOTH**

specifies the residual type to be plotted in the fit diagnostics and residual plots. RESIDUALTYPE=RAW requests that only the ordinary residuals be included in the plots; RESIDUALTYPE=PROJ sets the choice to projected residuals. By default, both residual types are included, which can also be effected by setting RESIDUALTYPE=BOTH. See the section “[Residuals in Nonlinear Regression](#)” on page 5289 for details about the properties of ordinary and projected residuals in nonlinear regression.

**STATS=ALL | DEFAULT | NONE | (*plot-statistics*)**

requests the statistics to be included in all plots, except the ResidualPlots and the unpacked diagnostics plots. [Table 63.3](#) lists the statistics that you can request. STATS=ALL requests all these statistics, STATS=NONE suppresses all statistics, and STATS=DEFAULT selects the default statistics. You request statistics in addition to the default set by including the keyword DEFAULT in the *plot-statistics* list.

**Table 63.3** Statistics Available in Plots

| Keyword    | Default | Description                                                              |
|------------|---------|--------------------------------------------------------------------------|
| DEFAULT    |         | All default statistics                                                   |
| MAXINCURV  |         | Maximum intrinsic curvature                                              |
| MAXPECURV  |         | Maximum parameter-effects curvature                                      |
| MSE        | x       | Mean squared error, estimated or set by the <a href="#">SIGSQ</a> option |
| NOBS       | x       | Number of observations used                                              |
| NPARAM     | x       | Number of parameters in the model                                        |
| PVAR       | x       | Estimated variance of the projected residuals                            |
| RMSNINCURV |         | Root mean square intrinsic curvature                                     |
| RMSPECURV  |         | Root mean square parameter-effects curvature                             |
| VAR        | x       | Estimated variance of the ordinary residuals                             |

Along with the maximum intrinsic and parameter-effects curvatures, the critical curvature (CURVCRIT) value,  $1/\sqrt{F}$  where  $F = F(p, n - p; \alpha)$ , is also displayed. You do not need to specify any option for it. See the section “[Relative Curvature Measures of Nonlinearity](#)” on page 5287 for details about curvature measures of nonlinearity.

**UNPACK**

suppresses paneling.

You can specify the following *plot-requests* in the PLOTS= option:

**ALL**

produces all appropriate plots.

**NONE**

suppresses all plots.

**DIAGNOSTICS** < (*diagnostics-options*) >

produces a summary panel of fit diagnostics, leverage plots, and local-influence plots. The fit diagnostics panel includes:

- histogram of the ordinary residuals
- histogram of the projected residuals
- response variable values versus the predicted values
- expectation or mean of the ordinary residuals versus the predicted values
- ordinary and projected residuals versus the predicted values
- standardized ordinary and projected residuals versus the predicted values
- standardized ordinary and projected residuals versus the tangential leverage
- standardized ordinary and projected residuals versus the Jacobian leverage
- box plot of the ordinary and projected residuals if you specify the STATS=NONE suboption

The leverage and local influence plots are produced separately. The leverage plot is an index plot of the tangential and Jacobian leverages (by observation), and the local-influence plot contains the local influence by observation for a perturbation of the response variable. See the sections “[Leverage in Nonlinear Regression](#)” on page 5288 and “[Local Influence in Nonlinear Regression](#)” on page 5288 for a some details about leverages and local-influence in nonlinear regression.

You can specify the following *diagnostics-options*:

**RESIDUALTYPE=RAW | PROJ | BOTH**

specifies the residual type to be plotted in the panel. See the RESIDUALTYPE= *global-plot-option* for details. This *diagnostics-option* overrides the PLOTS RESIDUALTYPE *global-plot-option*. Only the plots that overlay both ordinary and projected residuals in the same plot are affected by this option.

**LEVERAGETYPE=TAN | JAC | BOTH**

specifies the leverage type to be plotted in the leverage plot. LEVERAGETYPE=TAN specifies that only the tangential leverage be included in the leverage plot, and LEVERAGETYPE=JAC specifies that only the Jacobian leverage be included. By default, both are displayed in the leverage plot. The same result can be effected by setting LEVERAGETYPE=BOTH. Only the leverage plot is affected by this option.

**LABELOBS**

specifies that the leverage and local-influence plots be labeled with the observation number. Only these two plots are affected by this option.

**STATS=stats-options**

determines which statistics are included in the panel. See the *STATS= global-plot-option* for details. This *diagnostics-option* overrides the *PLOTS STATS global-plot-option*.

**UNPACK**

produces the plots in the diagnostics panel as individual plots. The statistics panel is not included in the individual plots, even if *STATS= global-plot-option* or *STATS= diagnostics-option* or both are specified.

**FITPLOT | FIT <(fit-options)>**

produces, depending on the number of regressors, a scatter or contour fit plot. For a single-regressor model, a scatter plot of the data overlaid with the regression curve, confidence, and prediction bands is produced. For two-regressor models, a contour fit plot of the model with overlaid data is produced. If the model contains more than two regressors, no fit plot is produced.

You can specify the following *fit-options*:

**NOCLI**

suppresses the prediction limits for single-regressor models.

**NOCLM**

suppresses the confidence limits for single-regressor models.

**NOLIMITS**

suppresses the confidence and prediction limits for single-regressor models.

**OBS=GRADIENT | NONE | OUTLINE | OUTLINEGRADIENT**

controls how the observations are displayed. The suboptions are as follows:

**OBS=GRADIENT** specifies that observations be displayed as circles colored by the observed response. The same color gradient is used to display the fitted surface and the observations. Observations for which the predicted response is close to the observed response have similar colors—the greater the contrast between the color of an observation and the surface, the larger the residual is at that point. **OBS=GRADIENT** is the default.

**OBS=NONE** suppresses the observations.

**OBS=OUTLINE** specifies that observations be displayed as circles with a border but with a completely transparent fill.

**OBS=OUTLINEGRADIENT** is the same as **OBS=GRADIENT** except that a border is shown around each observation. This option is useful for identifying the location observations for which the residuals are small, because at these points the color of the observations and the color of the surface are indistinguishable.

**CONTLEG**

specifies that a continuous legend be included in the contour fit plot of a two-regressor model.



**STATS=stats-options**

determines which model fit statistics are included in the panel. See the `STATS= global-plot-option` for details. This *fit-option* overrides the `PLOTS STATS global-plot-option`.

**RESIDUALS < residual-options >**

produces panels of the ordinary and projected residuals versus the regressors in the model. Each panel contains at most six plots, and multiple panels are used in the case where there are more than six regressors in the model.

The following *residual-options* are available:

**RESIDUALTYPE=RAW | PROJ | BOTH**

specifies the residual type to be plotted in the panel. See the `RESIDUALTYPE= global-plot-option` for details. This *residual-option* overrides the `PLOTS RESIDUALTYPE global-plot-option`.

**SMOOTH**

requests a nonparametric smooth of the residuals for each regressor. Each nonparametric fit is a loess fit that uses local linear polynomials, linear interpolation, and a smoothing parameter selected that yields a local minimum of the corrected Akaike information criterion (AICC). See Chapter 53, “[The LOESS Procedure](#),” for details.

**UNPACK**

suppresses paneling.

**PRINT**

displays the result of each statement in the program as it is executed. This option is a debugging feature that produces large amounts of output and is normally not needed.

**RHO=value**

specifies a value that controls the step-size search. By default `RHO=0.1`, except when `METHOD=MARQUARDT`. In that case, `RHO=10`. See the section “[Step-Size Search](#)” on page 5299 for more details.

**SAVE**

specifies that, when the iteration limit is exceeded, the parameter estimates from the final iteration be output to the `OUTEST=` data set. These parameter estimates are associated with the observation for which `_TYPE_="FINAL"`. If you omit the `SAVE` option, the parameter estimates from the final iteration are not output to the data set unless convergence has been attained.

**SIGSQ=value**

specifies a value to use as the estimate of the residual variance in lieu of the estimated mean-squared error. This value is used in computing the standard errors of the estimates. Fixing the value of the residual variance can be useful, for example, in maximum likelihood estimation.

**SINGULAR=s**

specifies the singularity criterion, `s`, which is the absolute magnitude of the smallest pivot value allowed when inverting the Hessian or the approximation to the Hessian. The default value is `1E4` times the machine epsilon; this product is approximately `1E-12` on most computers.

**SMETHOD=HALVE****SMETHOD=GOLDEN****SMETHOD=CUBIC**

specifies the step-size search method. The default is **SMETHOD=HALVE**. See the section “[Step-Size Search](#)” on page 5299 for details.

**TAU=value**

specifies a value that is used to control the step-size search. The default is **TAU=1**, except when **METHOD=MARQUARDT**. In that case the default is **TAU=0.01**. See the section “[Step-Size Search](#)” on page 5299 for details.

**TOTALSS**

adds to the analysis of variance table the uncorrected total sum of squares in models that have an (implied) intercept, and adds the corrected total sum of squares in models that do not have an (implied) intercept.

**TRACE**

displays the result of each operation in each statement in the model program as it is executed, in addition to the information displayed by the **FLOW** and **PRINT** options. This debugging option is needed very rarely, and it produces even more output than the **FLOW** and **PRINT** options.

**XREF**

displays a cross-reference of the variables in the model program showing where each variable is referenced or given a value. The XREF listing does not include derivative variables.

**UNCORRECTEDDF**

specifies that no degrees of freedom be lost when a bound is active. When the **UNCORRECTEDDF** option is not specified, an active bound is treated as if a restriction were applied to the set of parameters, so one parameter degree of freedom is deducted.

---

## BOUNDS Statement

**BOUNDS** *inequality* <, ..., *inequality* > ;

The **BOUNDS** statement restricts the parameter estimates so that they lie within specified regions. In each **BOUNDS** statement, you can specify a series of boundary values separated by commas. The series of bounds is applied simultaneously. Each boundary specification consists of a list of parameters, an inequality comparison operator, and a value. In a single-bounded expression, these three elements follow one another in the order described. The following are examples of valid single-bounded expressions:

```
bounds a1-a10 <= 20;
bounds c > 30;
bounds a b c > 0;
```

Multiple-bounded expressions are also permitted. For example:

```
bounds 0 <= B<= 10;
bounds 15 < x1 <= 30;
bounds r <= s <= p < q;
```

If you need to restrict an expression involving several parameters (for example,  $\alpha + \beta < 1$ ), you can reparameterize the model so that the expression becomes a parameter or so that the boundary constraint can be expressed as a simple relationship between two parameters. For example, the boundary constraint  $\alpha + \beta < 1$  in the model

```
model y = alpha + beta*x;
```

can be achieved by parameterizing  $\theta = 1 - \beta$  as follows:

```
bounds alpha < theta;
model y = alpha + (1-theta)*x;
```

Starting with SAS 7.01, Lagrange multipliers are reported for all bounds that are enforced (active) when the estimation terminates. In the “Parameter Estimates” table, the Lagrange multiplier estimates are identified with names *Bound1*, *Bound2*, and so forth. An active bound is treated as if a restriction were applied to the set of parameters so that one parameter degree of freedom is deducted. You can use the `UNCORRECTEDDF` option to prevent the loss of degrees of freedom when bounds are active.

## BY Statement

**BY** *variables* ;

You can specify a BY statement with PROC NLIN to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the NLIN procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

## CONTROL Statement

**CONTROL** *variable* <=*values*> <... *variable* <=*values*>> ;

The CONTROL statement declares control variables and specifies their values. A control variable is like a retained variable (see the section “RETAIN Statement” on page 5282) except that it is retained *across* iterations, and the derivative of the model with respect to a control variable is always zero.

---

## DER Statement

**DER.** *parameter=expression ;*

**DER.** *parameter.parameter=expression ;*

The DER statement specifies first or second partial derivatives. By default, analytical derivatives are automatically computed. However, you can specify the derivatives yourself by using the DER.parm syntax. Use the first form shown to specify first partial derivatives, and use the second form to specify second partial derivatives. Note that the DER.parm syntax is retained for backward compatibility. The automatic analytical derivatives are, in general, a better choice. For additional information about automatic analytical derivatives, see the section “Automatic Derivatives” on page 5284.

For most of the computational methods, you need only specify the first partial derivative with respect to each parameter to be estimated. For the NEWTON method, specify both the first and the second derivatives. If any needed derivatives are not specified, they are automatically computed.

The expression can be an algebraic representation of the partial derivative of the expression in the MODEL statement with respect to the parameter or parameters that appear on the left side of the DER statement. Numerical derivatives can also be used. The expression in the DER statement must conform to the rules for a valid SAS expression, and it can include any quantities that the MODEL statement expression contains.

---

## ID Statement

**ID** *variables ;*

The ID statement specifies additional variables to place in the output data set created by the OUTPUT statement. Any variable on the left side of any assignment statement is eligible. Also, the special variables created by the procedure can be specified. Variables in the input data set do not need to be specified in the ID statement since they are automatically included in the output data set.

---

## MODEL Statement

**MODEL** *dependent = expression ;*

The MODEL statement defines the prediction equation by declaring the dependent variable and defining an expression that evaluates predicted values. The expression can be any valid SAS expression that yields a numeric result. The expression can include parameter names, variables in the data set, and variables created by programming statements in the NLIN procedure. Any operators or functions that can be used in a DATA step can also be used in the MODEL statement.

A statement such as

```
model y=expression;
```

is translated into the form

```
model .y=expression;
```

using the compound variable name `model.y` to hold the predicted value. You can use this assignment directly as an alternative to the `MODEL` statement. Either a `MODEL` statement or an assignment to a compound variable such as `model.y` must appear.

## OUTPUT Statement

**OUTPUT** **OUT**=*SAS-data-set keyword=names* <... *keyword=names*> </ *options* > ;

The `OUTPUT` statement specifies an output data set to contain statistics calculated for each observation. For each statistic, specify the keyword, an equal sign, and a variable name for the statistic in the output data set. All of the names appearing in the `OUTPUT` statement must be valid SAS names, and none of the new variable names can match a variable already existing in the data set to which `PROC NLIN` is applied.

If an observation includes a missing value for one of the independent variables, both the predicted value and the residual value are missing for that observation. If the iterations fail to converge, all the values of all the variables named in the `OUTPUT` statement are missing values.

Table 63.4 summarizes the options available in the `OUTPUT` statement.

**Table 63.4** OUTPUT Statement Options

| Option                                              | Description                                                                                      |
|-----------------------------------------------------|--------------------------------------------------------------------------------------------------|
| <b>Output data set and OUTPUT statement options</b> |                                                                                                  |
| <code>ALPHA=</code>                                 | Specifies the level of significance $\alpha$                                                     |
| <code>DER</code>                                    | Saves the first derivatives of the model                                                         |
| <code>OUT=</code>                                   | Specifies the output data set                                                                    |
| <b>Keyword options</b>                              |                                                                                                  |
| <code>H=</code>                                     | Specifies the tangential leverage                                                                |
| <code>J=</code>                                     | Specifies the Jacobian leverage                                                                  |
| <code>L95=</code>                                   | Specifies the lower bound of an approximate 95% prediction interval                              |
| <code>L95M=</code>                                  | Specifies the lower bound of an approximate 95% confidence interval for the mean                 |
| <code>LCL=</code>                                   | Specifies the lower bound of an approximate $100(1 - \alpha)\%$ prediction interval              |
| <code>LCLM=</code>                                  | Specifies the lower bound of an approximate $100(1 - \alpha)\%$ confidence interval for the mean |
| <code>LMAX=</code>                                  | Specifies the direction of maximum local influence                                               |
| <code>PARMS=</code>                                 | Specifies the parameter estimates                                                                |
| <code>PREDICTED=</code>                             | Specifies the predicted values                                                                   |
| <code>PROJRES=</code>                               | Specifies the projected residuals                                                                |
| <code>PROJSTUDENT=</code>                           | Specifies the standardized projected residuals                                                   |
| <code>RESEXPEC=</code>                              | Specifies the mean of the residuals                                                              |
| <code>RESIDUAL=</code>                              | Specifies the residuals                                                                          |
| <code>SSE=</code>                                   | Specifies the residual sum of squares                                                            |
| <code>STDI=</code>                                  | Specifies the standard error of the individual predicted value                                   |
| <code>STDP=</code>                                  | Specifies the standard error of the mean predicted value                                         |
| <code>STDR=</code>                                  | Specifies the standard error of the residual                                                     |
| <code>STUDENT=</code>                               | Specifies the standardized residuals                                                             |

Table 63.4 *continued*

| Option  | Description                                                                                      |
|---------|--------------------------------------------------------------------------------------------------|
| U95=    | Specifies the upper bound of an approximate 95% prediction interval                              |
| U95M=   | Specifies the upper bound of an approximate 95% confidence interval for the mean                 |
| UCL=    | Specifies the upper bound of an approximate $100(1 - \alpha)\%$ prediction interval              |
| UCLM=   | Specifies the upper bound of an approximate $100(1 - \alpha)\%$ confidence interval for the mean |
| WEIGHT= | Specifies the special variable <code>_WEIGHT_</code>                                             |

You can specify the following options in the OUTPUT statement. For a description of computational formulas, see Chapter 4, “Introduction to Regression Procedures.”

**OUT=SAS-data-set**

specifies the SAS data set to be created by PROC NLIN when an OUTPUT statement is included. The new data set includes the variables in the input data set. Also included are any **ID** variables specified in the **ID** statement, plus new variables with names that are specified in the OUTPUT statement.

The following values can be calculated and output to the new data set.

**H=name**

specifies a variable that contains the tangential leverage. See the section “Leverage in Nonlinear Regression” on page 5288 for details.

**J=name**

specifies a variable that contains the Jacobian leverage. See the section “Leverage in Nonlinear Regression” on page 5288 for details.

**L95=name**

specifies a variable that contains the lower bound of an approximate 95% confidence interval for an individual prediction. This includes the variance of the error as well as the variance of the parameter estimates. See also the description for the **U95=** option later in this section.

**L95M=name**

specifies a variable that contains the lower bound of an approximate 95% confidence interval for the expected value (mean). See also the description for the **U95M=** option later in this section.

**LCL=name**

specifies a variable that contains the lower bound of an approximate  $100(1 - \alpha)\%$  confidence interval for an individual prediction. The  $\alpha$  level is equal to the value of the **ALPHA=** option in the OUTPUT statement or, if this option is not specified, to the value of the **ALPHA=** option in the **PROC NLIN** statement. If neither of these options is specified, then  $\alpha = 0.05$  by default, resulting in a lower bound for an approximate 95% confidence interval. For the corresponding upper bound, see the **UCL** keyword.

**LCLM=***name*

specifies a variable that contains the lower bound of an approximate  $100(1 - \alpha)\%$  confidence interval for the expected value (mean). The  $\alpha$  level is equal to the value of the **ALPHA=** option in the **OUTPUT** statement or, if this option is not specified, to the value of the **ALPHA=** option in the **PROC NLIN** statement. If neither of these options is specified, then  $\alpha = 0.05$  by default, resulting in a lower bound for an approximate 95% confidence interval. For the corresponding lower bound, see the **UCLM** keyword.

**LMAX=***name*

specifies a variable that contains the direction of maximum local influence of an additive perturbation of the response variable. See the section “[Local Influence in Nonlinear Regression](#)” on page 5288 for details.

**PARMS=***names*

specifies variables in the output data set that contains parameter estimates. These can be the same variable names that are listed in the **PARAMETERS** statement; however, you can choose new names for the parameters identified in the sequence from the parameter estimates table. A note in the log indicates which variable in the output data set is associated with which parameter name. Note that, for each of these new variables, the values are the same for every observation in the new data set.

**PREDICTED=***name***P=***name*

specifies a variable in the output data set that contains the predicted values of the dependent variable.

**PROJRES=***name*

specifies a variable that contains the projected residuals obtained by projecting the residuals (ordinary residuals) into the null space of  $(X|H)$ . For the ordinary residuals, see the **RESIDUAL=** option later in this section. The section “[Residuals in Nonlinear Regression](#)” on page 5289 describes the statistical properties of projected residuals in nonlinear regression.

**PROJSTUDENT=***name*

specifies a variable that contains the standardized projected residuals. See the section “[Residuals in Nonlinear Regression](#)” on page 5289 for details and the **STUDENT=** option later in this section.

**RESEXPEC=***name*

specifies a variable that contains the mean of the residuals. In contrast to linear regressions where the mean of the residuals is zero, in nonlinear regression the residuals have a nonzero mean value and show a negative covariance with the mean response. See the section “[Residuals in Nonlinear Regression](#)” on page 5289 for details.

**RESIDUAL=***name***R=***name*

specifies a variable in the output data set that contains the residuals. See also the description of **PROJRES=** option stated previously in this section and the section “[Residuals in Nonlinear Regression](#)” on page 5289 for the statistical properties of residuals and projected residuals.

**SSE=***name***ESS=***name*

specifies a variable in the output data set that contains the residual sum of squares finally determined by the procedure. The value of the variable is the same for every observation in the new data set.

**STDI=***name*

specifies a variable that contains the standard error of the individual predicted value.

**STDP=***name*

specifies a variable that contains the standard error of the mean predicted value.

**STDR=***name*

specifies a variable that contains the standard error of the residual.

**STUDENT=***name*

specifies a variable that contains the standardized residuals. These are residuals divided by their estimated standard deviation. See the **PROJSTUDENT=** option defined previously in this section and the section “Residuals in Nonlinear Regression” on page 5289 for the statistical properties of residuals and projected residuals.

**U95=***name*

specifies a variable that contains the upper bound of an approximate 95% confidence interval for an individual prediction. See also the description for the **L95=** option.

**U95M=***name*

specifies a variable that contains the upper bound of an approximate 95% confidence interval for the expected value (mean). See also the description for the **L95M=** option.

**UCL=***name*

specifies a variable that contains the upper bound of an approximate  $100(1 - \alpha)\%$  confidence interval for an individual prediction. The  $\alpha$  level is equal to the value of the **ALPHA=** option in the **OUTPUT** statement or, if this option is not specified, to the value of the **ALPHA=** option in the **PROC NLIN** statement. If neither of these options is specified, then  $\alpha = 0.05$  by default, resulting in an upper bound for an approximate 95% confidence interval. For the corresponding lower bound, see the **LCL** keyword.

**UCLM=***name*

specifies a variable that contains the upper bound of an approximate  $100(1 - \alpha)\%$  confidence interval for the expected value (mean). The  $\alpha$  level is equal to the value of the **ALPHA=** option in the **OUTPUT** statement or, if this option is not specified, to the value of the **ALPHA=** option in the **PROC NLIN** statement. If neither of these options is specified, then  $\alpha = 0.05$  by default, resulting in an upper bound for an approximate 95% confidence interval. For the corresponding lower bound, see the **LCLM** keyword.

**WEIGHT=***name*

specifies a variable in the output data set that contains values of the special variable **\_WEIGHT\_**.

You can specify the following options in the **OUTPUT** statement after a slash (/):



**ALPHA= $\alpha$** 

specifies the level of significance  $\alpha$  for  $100(1 - \alpha)\%$  confidence intervals. By default,  $\alpha$  is equal to the value of the **ALPHA=** option in the **PROC NLIN** statement or 0.05 if that option is not specified. You can supply values that are strictly between 0 and 1.

**DER**

saves the first derivatives of the model with respect to the parameters to the **OUTPUT** data set. The derivatives are named **DER\_parmname**, where “parmname” is the name of the model parameter in your **NLIN** statements. You can use the **DER** option to extract the  $\mathbf{X} = \partial f / \partial \boldsymbol{\beta}$  matrix into a SAS data set. For example, the following statements create the data set **nlinX**, which contains the **X** matrix:

```
proc nlin;
 parms theta1=155 theta3=0.04;
 model v = theta1*c / (theta3 + c);
 output out=nlinout / der;
run;

data nlinX;
 set nlinout (keep=DER_);
run;
```

The derivatives are evaluated at the final parameter estimates.

---

## PARAMETERS Statement

**PARAMETERS** < *parameter-specification* > < , ... , *parameter-specification* >  
< / **PDATA=SAS-data-set** > ;

**PARMS** < *parameter-specification* > < , ... , *parameter-specification* >  
< / **PDATA=SAS-data-set** > ;

A **PARAMETERS** (or **PARMS**) statement is required. The purpose of this statement is to provide starting values for the **NLIN** procedure. You can provide values that define a point in the parameter space or a set of points.

All parameters must be assigned starting values through the **PARAMETERS** statement. The **NLIN** procedure does not assign default starting values to parameters in your model that do not appear in the **PARAMETERS** statement. However, it is not necessary to supply parameters and starting values explicitly through a *parameter-specification*. Starting values can also be provided through a data set. The names assigned to parameters must be valid SAS names and must not coincide with names of variables in the input data set (see the **DATA=** option in the **PROC NLIN** statement). Parameters that are assigned starting values through the **PARAMETERS** statement can be omitted from the estimation, for example, if the expression in the **MODEL** statement does not depend on them.

### Assigning Starting Values with Parameter-Specification

A *parameter-specification* has the general form

*name* = *value-list*

where *name* identifies the parameter and *value-list* provides the set of starting values for the parameter.

Very often, the *value-list* contains only a single value, but more general and flexible list specifications are possible:

|                                                   |                                                                                                                      |
|---------------------------------------------------|----------------------------------------------------------------------------------------------------------------------|
| <i>m</i>                                          | a single value                                                                                                       |
| <i>m</i> 1, <i>m</i> 2, . . . , <i>m</i> <i>n</i> | several values                                                                                                       |
| <i>m</i> TO <i>n</i>                              | a sequence where <i>m</i> equals the starting value, <i>n</i> equals the ending value, and the increment equals 1    |
| <i>m</i> TO <i>n</i> BY <i>i</i>                  | a sequence where <i>m</i> equals the starting value, <i>n</i> equals the ending value, and the increment is <i>i</i> |
| <i>m</i> 1, <i>m</i> 2 TO <i>m</i> 3              | mixed values and sequences                                                                                           |

When you specify more than one value for a parameter, PROC NLIN sorts the values in ascending sequence and removes duplicate values from the parameter list before forming the grid for the parameter search. If you specify several values for each parameter, PROC NLIN evaluates the model at each point on the grid. The iterations then commence from the point on the grid that yields the smallest objective function value.

For example, the following PARMs statement specifies five parameters and sets their possible starting values as shown in the table:

```
parms b0 = 0
 b1 = 4 to 8
 b2 = 0 to .6 by .2
 b3 = 1, 10, 100
 b4 = 0, .5, 1 to 4;
```

| Possible starting values |    |     |     |     |
|--------------------------|----|-----|-----|-----|
| B0                       | B1 | B2  | B3  | B4  |
| 0                        | 4  | 0.0 | 1   | 0.0 |
|                          | 5  | 0.2 | 10  | 0.5 |
|                          | 6  | 0.4 | 100 | 1.0 |
|                          | 7  | 0.6 |     | 2.0 |
|                          | 8  |     |     | 3.0 |
|                          |    |     |     | 4.0 |

Residual sums of squares are calculated for each of the  $1 \times 5 \times 4 \times 3 \times 6 = 360$  combinations of possible starting values. (Specifying a large grid of values can take considerable computing time.)

If you specify a starting value with a *parameter-specification*, any starting values provided for this parameter through the PDATA= data set are ignored. The *parameter-specification* overrides the information in the PDATA= data set. When you specify a BY statement, the same *parameter-specification* is applied in each BY group. To vary starting values with BY groups, use the PDATA= option in the PARAMETERS statement as described in the following paragraphs.

## Assigning Starting Values from a SAS Data Set

The PDATA= option in the PARAMETERS statement enables you to assign starting values for parameters through a SAS data set. The data set must contain at least two variables that identify the parameter and contain starting values, respectively. The *character* variable identifying the parameters must be named Parameter or Parm. The *numeric* variable containing the starting value must be named Estimate or Est. This enables you, for example, to use the contents of the “ParameterEstimates” table from one PROC NLIN run to supply starting values for a subsequent run, as in the following example:

```
proc nlin data=FirstData;
 parameters alpha=100 beta=3 gamma=4;
 < other NLIN statements >
 model y = ... ;
 ods output ParameterEstimates=pest;
run;

proc nlin data=SecondData;
 parameters / pdata=pest;
 Switch = 1/(1+gamma*exp(beta*log(dose)));
 model y = alpha*Switch;
run;
```

You can specify multiple values for a parameter in the PDATA= data set, and the parameters can appear in any order. The starting values are collected by parameter and arranged in ascending order, and duplicate values are removed. The parameter names in the PDATA= data set are not case sensitive. For example, the following DATA step defines starting values for three parameters and a starting grid with  $1 \times 3 \times 1 = 3$  points:

```
data test;
 input Parameter $ Estimate;
 datalines;
alpha 100
BETA 4
beta 4.1
beta 4.2
beta 4.1
gamma 30
;
```

If starting values for a parameter are provided through the PDATA= data set and through an explicit *parameter-specification*, the latter takes precedence.

When you specify a BY statement, you can control whether the same starting values are applied to each BY group or whether the starting values are varied. If the BY variables are not present in the PDATA= data set, the entire contents of the PDATA= data set are applied in each BY group. If the BY variables are present in the PDATA= data set, then BY-group-specific starting values are assigned.

## PROFILE Statement

**PROFILE** *parameter* <...*parameter*> </*options*> ;

A PROFILE statement selects parameters for profiling to assess their nonlinear characteristics. It can also gauge the influence of each observation on the selected parameters. To produce the plots that are controlled by the PROFILE statement, ODS Graphics must be enabled. PROC NLIN ignores PROFILE statements for nonconvergent and singular models.

Table 63.6 summarizes the *options* available in the PROFILE statement.

**Table 63.6** Summary of Options in PROFILE Statement

| Option    | Description                                                                                        |
|-----------|----------------------------------------------------------------------------------------------------|
| ALL       | Produces all profiling related plots and statistics                                                |
| CONFCURV  | Produces confidence curves for the listed parameters                                               |
| JACKKNIFE | Produces plots of the absolute relative percentage change by observation for the listed parameters |
| PROFDATA= | Specifies the profile output data set                                                              |
| RANGE=    | Specifies a profiling range                                                                        |
| TPLOT     | Produces profile <i>t</i> plots for the listed parameters                                          |

### ALL

produces all appropriate plots for the parameters that are listed in the PROFILE statement. This option overrides all other *options*. If the PROFDATA= option is specified, the values of the corresponding statistics are written to the data set.

### CONFCURV

produces confidence curves for each parameter listed in the PROFILE statement. If the PROFDATA= option is specified, the values of the corresponding statistics are written to the data set. See the section “Profiling Parameters and Assessing the Influence of Observations on Parameter Estimates” on page 5290 for details.

### JACKKNIFE

produces, for each parameter listed in the PROFILE statement, plots of absolute relative percentage change in the value of the parameter that results from a fit to a jackknife-resampled datum versus observation number. The jackknife resampling is performed with a leave-one-out method. If the PROFDATA= option is specified, the values of the corresponding statistics are written to the data set. See the section “Profiling Parameters and Assessing the Influence of Observations on Parameter Estimates” on page 5290 for details.

### PROFDATA=*SAS-data-set*

specifies the SAS data set to be created by PROC NLIN when a PROFILE statement is included. See the section “Output Data Sets” on page 5299 for details about this data set.

**RANGE=** $\beta_f$  to  $\beta_t$  by  $\beta_b$ 

specifies a profiling range for each parameter listed in the PROFILE statement.  $\beta_f$ ,  $\beta_t$  and  $\beta_b$  represent the starting, final, and consecutive incremental values of the range in terms of the standard errors of the parameters to be profiled. If you do not specify the RANGE= option, PROC NLIN uses  $-2$ ,  $2$ , and  $0.2$  as default values for  $\beta_f$ ,  $\beta_t$ , and  $\beta_b$ , respectively. For example, if parameter  $\theta$  is in the PROFILE statement, then during the profiling of  $\theta$ , PROC NLIN performs approximately  $(\beta_t - \beta_f)/\beta_b$  number of constrained optimizations. At the  $i$ th constrained optimization, the value of  $\theta$  is constrained to  $\theta_i$ ,

$$\theta_i = \hat{\theta} + \text{stderr}_\theta \left( \beta_f + i \frac{(\beta_t - \beta_f)}{\beta_b} \right)$$

and the rest of the parameters are freely optimized. In the preceding expression,  $\hat{\theta}$  and  $\text{stderr}_\theta$  are the estimated value and standard error, respectively, for  $\theta$ . If parameter bounds are specified with BOUNDS statements, PROC NLIN enforces those bounds during the profiling optimizations.

**NOTE:** The profiling optimizations are performed using quasi-Newton algorithm. During these optimizations, any optimization options specified in the PROC NLIN statement and the `_LOSS_` variable are ignored.

**TPLOT**

produces profile  $t$  plots for each parameter listed in the PROFILE statement. If the PROFDATA= option is specified, the values of the corresponding statistics are written to the data set. See the section “Profiling Parameters and Assessing the Influence of Observations on Parameter Estimates” on page 5290 for details.

**RETAIN Statement**

**RETAIN** *variable* <=*values*> <... *variable* <=*values*>> ;

The RETAIN statement declares retained variables and specifies their values. A retained variable is like a control variable (see the section “CONTROL Statement” on page 5272) except that it is retained only *within* iterations. An iteration involves a single pass through the data set.

**Other Programming Statements**

PROC NLIN supports many statements that are similar to SAS programming statements used in a DATA step. However, there are some differences in capabilities; for additional information, see also the section “Incompatibilities with SAS 6.11 and Earlier Versions of PROC NLIN” on page 5303.

Several SAS programming statements can be used after the PROC NLIN statement. These statements can appear anywhere in the PROC NLIN code, but new variables must be created before they appear in other statements. For example, the following statements are valid since they create the variable `temp` before it is used in the MODEL statement:

```
proc nlin;
 parms b0=0 to 2 by 0.5 b1=0.01 to 0.09 by 0.01;
 temp = exp(-b1*x);
 model y=b0*(1-temp);
run;
```

The following statements result in missing values for y because the variable temp is undefined before it is used:

```
proc nlin;
 parms b0=0 to 2 by 0.5 b1=0.01 to 0.09 by 0.01;
 model y = b0*(1-temp);
 temp = exp(-b1*x);
run;
```

PROC NLIN can process assignment statements, explicitly or implicitly subscripted ARRAY statements, explicitly or implicitly subscripted array references, IF statements, SAS functions, and program control statements. You can use programming statements to create new SAS variables for the duration of the procedure. These variables are not included in the data set to which PROC NLIN is applied. Program statements can include variables in the **DATA=** data set, parameter names, variables created by preceding programming statements within PROC NLIN, and special variables used by PROC NLIN. The following SAS programming statements can be used in PROC NLIN:

```
ABORT;
ARRAY arrayname < [dimensions] > < $ > < variables-and-constants >;
CALL name < (expression < , expression ... >) >;
DELETE;
DO < variable = expression < TO expression > < BY expression > >
 < , expression < TO expression > < BY expression > > ...
 < WHILE expression > < UNTIL expression >;
END;
GOTO statement-label;
IF expression;
IF expression THEN program-statement;
 ELSE program-statement;
variable = expression;
variable + expression;
LINK statement-label;
PUT < variable > < = > ...;
RETURN;
SELECT < (expression) >;
STOP;
SUBSTR(variable, index, length)= expression;
WHEN (expression)program-statement;
 OTHERWISE program-statement;
```

These statements can use the special variables created by PROC NLIN. See the section “Special Variables” on page 5291 for more information.

## Details: NLIN Procedure

### Automatic Derivatives

Depending on the optimization method you select, analytical first- and second-order derivatives are computed automatically. Derivatives can still be supplied using the DER.parm syntax. These DER.parm derivatives are not verified by the differentiator. If any needed derivatives are not supplied, they are computed and added to the programming statements. To view the computed derivatives, use the [LISTDER](#) or [LIST](#) option.

The following model is solved using Newton's method. Analytical first- and second-order derivatives are automatically computed. The compiled program code is shown in [Figure 63.6](#).

```
proc nlin data=Enzyme method=newton list;
 parms x1=4 x2=2;
 model Velocity = x1 * exp (x2 * Concentration);
run;
```

**Figure 63.6** Model and Derivative Code Output

| The NLIN Procedure               |          |                                                                                                |
|----------------------------------|----------|------------------------------------------------------------------------------------------------|
| Listing of Compiled Program Code |          |                                                                                                |
| Stmt                             | Line:Col | Statement as Parsed                                                                            |
| 1                                | 1429:4   | MODEL.Velocity = x1 * EXP(x2<br>* Concentration);                                              |
| 1                                | 1429:4   | @MODEL.Velocity/@x1 = EXP(x2<br>* Concentration);                                              |
| 1                                | 1429:4   | @MODEL.Velocity/@x2 = x1 * Concentration<br>* EXP(x2 * Concentration);                         |
| 1                                | 1429:4   | @@MODEL.Velocity/@x1/@x2 = Concentration<br>* EXP(x2 * Concentration);                         |
| 1                                | 1429:4   | @@MODEL.Velocity/@x2/@x1 = Concentration<br>* EXP(x2 * Concentration);                         |
| 1                                | 1429:4   | @@MODEL.Velocity/@x2/@x2 = x1<br>* Concentration * Concentration<br>* EXP(x2 * Concentration); |

Note that all the derivatives require the evaluation of EXP(X2 \* Concentration). The actual machine-level code is displayed if you specify the [LISTCODE](#) option, as in the following statements:

```
proc nlin data=Enzyme method=newton listcode;
 parms x1=4 x2=2;
 model Velocity = x1 * exp (x2 * Concentration);
run;
```

Note that, in the generated code, only one exponentiation is performed ([Figure 63.7](#)). The generated code reuses previous operations to be more efficient.

Figure 63.7 LISTCODE Output

```

 The NLIN Procedure

 Code Listing

1 Stmt MODEL line 1436 column
 4. (1)
 arg=MODEL.Velocity
 argsave=MODEL.
 Velocity
 Source Text:
 model Velocity = x1 * exp
 (x2 * Concentration);
Oper * at 1436:34 (30,0,2). * : _temp1 <- x2 Concentration
Oper EXP at 1436:30 EXP : _temp2 <- _temp1
 (103,0,1) .
Oper * at 1436:24 (30,0,2). * : MODEL.Velocity <- x1 _temp2
Oper eeocf at 1436:24 (18,0,1). eeocf : _DER_ <- _DER_
Oper = at 1436:24 (1,0,1). = : @MODEL.Velocity/@x1 <- _temp2
Oper * at 1436:30 (30,0,2). * : @1dt1_1 <- Concentration _temp2
Oper * at 1436:24 (30,0,2). * : @MODEL.Velocity/@x2
 <- x1 @1dt1_1
Oper = at 1436:24 (1,0,1). = : @@MODEL.Velocity/@x1/@x2
 <- @1dt1_1
Oper = at 1436:24 (1,0,1). = : @@MODEL.Velocity/@x2/@x1
 <- @1dt1_1
Oper * at 1436:30 (30,0,2). * : @2dt1_1 <- Concentration
 @1dt1_1
Oper * at 1436:24 (30,0,2). * : @@MODEL.Velocity/@x2/@x2
 <- x1 @2dt1_1

```

## Measures of Nonlinearity and Diagnostics

A “close-to-linear” nonlinear regression model, in the sense of Ratkowsky (1983, 1990), is a model in which parameter estimators have properties similar to those in a linear regression model. That is, the least squares estimators of the parameters are close to being unbiased and normally distributed, and they have minimum variance.

A nonlinear regression model sometimes fails to be close to linear due to the properties of one or several parameters. When this occurs, bias in the parameter estimates can render inferences that use the reported standard errors and confidence limits invalid.

PROC NLIN provides various measures of nonlinearity. To assess the nonlinearity of a model-data combination, you can use both of the following complementary sets of measures:

- Box’s bias (Box 1971) and Hougaard’s skewness (Hougaard 1982, 1985) of the least squares parameter estimates
- curvature measures of nonlinearity (Bates and Watts 1980).



Furthermore, PROC NLIN provides residual, leverage, and local-influence diagnostics (St. Laurent and Cook 1993).

In the following several sections, these nonlinearity measures and diagnostics are discussed. For this material, several basic definitions are required. Let  $\mathbf{X}$  be the Jacobian matrix for the model,  $\mathbf{X} = \frac{\partial \mathbf{f}}{\partial \boldsymbol{\beta}}$ , and let  $\mathbf{Q}$  and  $\mathbf{R}$  be the components of the QR decomposition of  $\mathbf{X} = \mathbf{QR}$  of  $\mathbf{X}$ , where  $\mathbf{Q}$  is an  $(n \times n)$  orthogonal matrix. Finally, let  $\mathbf{B}$  be the inverse of the matrix constructed from the first  $p$  rows of the  $(n \times p)$  dimensional matrix  $\mathbf{R}$  (that is,  $\mathbf{B} = \mathbf{R}_p^{-1}$ ). Next define

$$\begin{aligned} [\mathbf{H}_j]_{kl} &= \frac{\partial^2 f_j}{\partial \beta_k \partial \beta_l} \\ [\mathbf{U}_j]_{kl} &= \sum_{mn} \mathbf{B}'_{km} [\mathbf{H}_j]_{mn} \mathbf{B}_{nl} \\ [\mathbf{A}_j]_{kl} &= \sqrt{p \times \text{mse}} \sum_m \mathbf{Q}'_{jm} [\mathbf{U}_m]_{kl}, \end{aligned}$$

where  $\mathbf{H}$ ,  $\mathbf{U}$  and the acceleration array  $\mathbf{A}$  are three-dimensional  $(n \times p \times p)$  matrices. The first  $p$  faces of the acceleration array constitute a  $(p \times p \times p)$  parameter-effects array and the last  $(n - p)$  faces constitute the  $(n - p \times p \times p)$  intrinsic curvature array (Bates and Watts 1980). The previous and subsequent quantities are computed at the least squares parameter estimators.

### Box's Measure of Bias

The degree to which parameter estimators exhibit close-to-linear behavior can be assessed with Box's bias (Box 1971) and Hougaard's measure of skewness (Hougaard 1982, 1985). The bias and percentage bias measures are available through the **BIAS** option in the **PROC NLIN** statement. Box's bias measure is defined as

$$\widehat{\text{E}}[\widehat{\theta} - \theta] = -\frac{\sigma^2}{2} (\mathbf{X}'\mathbf{W}\mathbf{X})^{-1} \sum_{i=1}^n w_i \mathbf{x}'_i \text{Tr} \left( (\mathbf{X}'\mathbf{W}\mathbf{X})^{-1} [\mathbf{H}_i] \right)$$

where  $\sigma^2 = \text{mse}$  if the **SIGSQ** option is not set. Otherwise,  $\sigma^2$  is the value you set with the **SIGSQ** option.  $\mathbf{W}$  is the diagonal weight matrix specified with the **\_WEIGHT\_** variable (or the identity matrix if **\_WEIGHT\_** is not defined) and  $[\mathbf{H}_i]$  is the  $(p \times p)$  Hessian matrix at the  $i$ th observation. In the case of unweighted least squares, the bias formula can be expressed in terms of the acceleration array  $\mathbf{A}$ ,

$$\widehat{\text{E}}[\widehat{\theta}_i - \theta_i] = -\frac{\sigma^2}{2p \times \text{mse}} \sum_{j,k=1}^p \mathbf{B}_{ij} [\mathbf{A}_j]_{kk}$$

As the preceding formulas illustrate, the bias depends solely on the parameter-effects array, thereby permitting its reduction through reparameterization. **Example 63.4** shows how changing the parameterization of a four-parameter logistic model can reduce the bias. Ratkowsky (1983, p. 21) recommends that you consider reparameterization if the percentage bias exceeds 1%.

### Hougaard's Measure of Skewness

In addition to Box's bias, Hougaard's measure of skewness,  $g_{1i}$  (Hougaard 1982, 1985), is also provided in PROC NLIN to assess the close-to-linear behavior of parameter estimators. This measure is available

through the **HOUGAARD** option in the **PROC NLIN** statement. Hougaard's skewness measure for the  $i$ th parameter is based on the third central moment, defined as

$$E \left[ \widehat{\theta}_i - E(\widehat{\theta}_i) \right]^3 = -(\sigma^2)^2 \sum_{jkl} [\mathbf{L}]_{ij} [\mathbf{L}]_{ik} [\mathbf{L}]_{il} \left( [\mathbf{V}_j]_{kl} + [\mathbf{V}_k]_{jl} + [\mathbf{V}_l]_{jk} \right)$$

where the sum is a triple sum over the number of parameters and

$$\mathbf{L} = (\mathbf{X}'\mathbf{X})^{-1} = \left( \frac{\partial \mathbf{f}}{\partial \boldsymbol{\beta}'} \frac{\partial \mathbf{f}}{\partial \boldsymbol{\beta}} \right)^{-1}$$

The term  $[\mathbf{L}]_{ij}$  denotes the value in row  $i$ , column  $j$  of the matrix  $\mathbf{L}$ . (Hougaard (1985) uses superscript notation to denote elements in this inverse.) The matrix  $\mathbf{V}$  is a three-dimensional ( $p \times p \times p$ ) array

$$[\mathbf{V}_j]_{kl} = \sum_{m=1}^n \frac{\partial F_m}{\partial \beta_j} \frac{\partial^2 F_m}{\partial \beta_k \partial \beta_l}$$

The third central moment is then normalized using the standard error as

$$G_{1i} = E \left[ \widehat{\theta}_i - E(\widehat{\theta}_i) \right]^3 / (\sigma^2 \times [\mathbf{L}]_{ii})^{3/2}$$

The previous expressions depend on the unknown values of the parameters and on the residual variance  $\sigma^2$ . In order to evaluate the Hougaard measure in a particular data set, the NLIN procedure computes

$$g_{1i} = \widehat{E} \left[ \widehat{\theta}_i - E(\widehat{\theta}_i) \right]^3 / \left( \text{mse} \times [\widehat{\mathbf{L}}]_{ii} \right)^{3/2}$$

$$\widehat{E} \left[ \widehat{\theta}_i - E(\widehat{\theta}_i) \right]^3 = -\text{mse}^2 \sum_{jkl} [\widehat{\mathbf{L}}]_{ij} [\widehat{\mathbf{L}}]_{ik} [\widehat{\mathbf{L}}]_{il} \left( [\widehat{\mathbf{V}}_j]_{kl} + [\widehat{\mathbf{V}}_k]_{jl} + [\widehat{\mathbf{V}}_l]_{jk} \right)$$

Following Ratkowsky (1990, p. 28), the parameter  $\theta_i$  is considered to be very close to linear, reasonably close, skewed, or quite nonlinear according to the absolute value of the Hougaard measure  $|g_{1i}|$  being less than 0.1, between 0.1 and 0.25, between 0.25 and 1, or greater than 1, respectively.

## Relative Curvature Measures of Nonlinearity

Bates and Watts (1980) formulated the maximum parameter-effects and maximum intrinsic curvature measures of nonlinearity to assess the close-to-linear behavior of nonlinear models. Ratkowsky (1990) notes that of the two curvature components in a nonlinear model, the parameter-effects curvature is typically larger. It is this component that you can affect by changing the parameterization of a model. PROC NLIN provides these two measures of curvature both through the **STATS plot-option** and through the **NLINMEASURES** option in the **PROC NLIN** statement.

The maximum parameter-effects and intrinsic curvatures are defined, in a compact form, as

$$\mathbf{T}^\tau = \max_{\boldsymbol{\theta}} \left\| \boldsymbol{\theta}' \mathbf{A}^\tau \boldsymbol{\theta} \right\|$$

$$\mathbf{T}^\eta = \max_{\boldsymbol{\theta}} \left\| \boldsymbol{\theta}' \mathbf{A}^\eta \boldsymbol{\theta} \right\|$$

where  $\mathbf{T}^\tau$  and  $\mathbf{T}^\eta$  denote the maximum parameter-effects and intrinsic curvatures, while  $\mathbf{A}^\tau$  and  $\mathbf{A}^\eta$  stand for the parameter-effects and intrinsic curvature arrays. The maximization is carried out over a unit-vector

of the parameter values (Bates and Watts 1980). In line with Bates and Watts (1980), PROC NLIN takes  $10^{-4}$  as the convergence tolerance for the maximum intrinsic and parameter-effects curvatures. Note that the preceding matrix products involve contraction of the faces of the three-dimensional acceleration arrays with the normalized parameter vector,  $\theta$ . The corresponding expressions for the RMS (root mean square) parameter-effects and intrinsic curvatures can be found in Bates and Watts (1980).

The statistical significance of  $T^\tau$  and  $T^\eta$  and the corresponding RMS values can be assessed by comparing these values with  $1/\sqrt{F}$ , where  $F$  is the upper  $\alpha \times 100\%$  quantile of an  $F$  distribution with  $p$  and  $n - p$  degrees of freedom (Bates and Watts 1980).

One motivation for fitting a nonlinear model in a different parameterization is to obtain a particular interpretation and to give parameter estimators more close-to-linear behavior. [Example 63.4](#) shows how changing the parameterization of a four-parameter logistic model can reduce the parameter-effects curvature and can yield a useful parameter interpretation at the same time. In addition, [Example 63.6](#) shows a nonlinear model with a high intrinsic curvature and the corresponding diagnostics.

## Leverage in Nonlinear Regression

In contrast to linear regression, there are several measures of leverage in nonlinear regression. Furthermore, in nonlinear regression, the effect of a change in the  $i$ th response on the  $i$ th predicted value might depend on both the size of the change and the  $i$ th response itself (St. Laurent and Cook 1992). As a result, some observations might show superleverage —namely, leverages in excess of one (St. Laurent and Cook 1992).

PROC NLIN provides two measures of leverages: tangential and Jacobian leverages through the PLOTS option in the PROC NLIN statement and the H= and J= options of OUTPUT statement. Tangential leverage,  $H_i$ , is based on approximating the nonlinear model with a linear model that parameterizes the tangent plane at the least squares parameter estimators. In contrast, Jacobian leverage,  $J_i$ , is simply defined as the instantaneous rate of change in the  $i$ th predicted value with respect to the  $i$ th response (St. Laurent and Cook 1992).

The mathematical formulas for tangential and Jacobian leverages are

$$H_i = w_i \mathbf{x}_i (\mathbf{X}'\mathbf{W}\mathbf{X})^{-1} \mathbf{x}_i'$$

$$J_i = w_i \mathbf{x}_i (\mathbf{X}'\mathbf{W}\mathbf{X} - [\mathbf{W} \mathbf{e}] [\mathbf{H}])^{-1} \mathbf{x}_i',$$

where  $\mathbf{e}$  is the vector of residuals,  $\mathbf{W}$  is the diagonal weight matrix if you specify the special variable `_WEIGHT_` and otherwise the identity matrix, and  $i$  indexes the corresponding quantities for the  $i$ th observation. The brackets `[.][.]` indicate column multiplication as defined in Bates and Watts (1980). The preceding formula for tangential leverage holds if the gradient, Marquardt, or Gauss methods are used. For the Newton method, the tangential leverage is set equal to the Jacobian leverage.

In a model with a large intrinsic curvature, the Jacobian and tangential leverages can be very different. In fact, the two leverages are identical only if the model provides an exact fit to the data ( $\mathbf{e} = 0$ ) or the model is intrinsically linear (St. Laurent and Cook 1993). This is also illustrated by the leverage plot and nonlinearity measures provided in [Example 63.6](#).

## Local Influence in Nonlinear Regression

St. Laurent and Cook (1993) suggest using  $l_{\max}$ , the direction that yields the maximum normal curvature, to assess the local influence of an additive perturbation to the response variable on the estimation of the

parameters and variance of a nonlinear model. Defining the normal curvature components

$$C_\theta = \max_l \frac{2}{\sigma^2} l' \mathbf{J} l$$

$$C_\sigma = \max_l \frac{4}{\sigma^2} l' \mathbf{P}_e l$$

where  $\mathbf{J}$  is the Jacobian leverage matrix and  $\mathbf{P}_e = \mathbf{e}\mathbf{e}'/(\mathbf{e}'\mathbf{e})$ , you choose the  $l_{\max}$  that results in the maximum of the two curvature components (St. Laurent and Cook 1993). PROC NLIN provides  $l_{\max}$  through the PLOTS option in the PROC NLIN statement and the LMAX= option in the OUTPUT statement. Example 63.6 shows a plot of  $l_{\max}$  for a model with high intrinsic curvature.

## Residuals in Nonlinear Regression

If a nonlinear model is intrinsically nonlinear, using the residuals  $\mathbf{e} = \mathbf{y} - \hat{\mathbf{y}}$  for diagnostics can be misleading (Cook and Tsai 1985). This is due to the fact that in correctly specified intrinsically nonlinear models, the residuals have nonzero means and different variances, even when the original error terms have identical variances. Furthermore, the covariance between the residuals and the predicted values tends to be negative semidefinite, complicating the interpretation of plots based on  $\mathbf{e}$  (Cook and Tsai 1985).

Projected residuals are proposed by Cook and Tsai (1985) to overcome these shortcomings of residuals, which are henceforth called raw (ordinary) residuals to differentiate them from their projected counterparts. Projected residuals have zero means and are uncorrelated with the predicted values. In fact, projected residuals are identical to the raw residuals in intrinsically linear models.

PROC NLIN provides raw and projected residuals, along with their standardized forms. In addition, the mean or expectation of the raw residuals is available. These can be accessed with the PLOTS option in the PROC NLIN statement and the OUTPUT statement options PROJRES=, PROJSTUDENT=, RESEXPEC=, RESIDUAL= and STUDENT=.

Denote the projected residuals by  $\mathbf{e}_p$  and the expectation of the raw residuals by  $E[\mathbf{e}]$ . Then

$$\mathbf{e}_p = (\mathbf{I}_n - \mathbf{P}_{xh}) \mathbf{e}$$

$$E[\mathbf{e}_i] = -\frac{\sigma^2}{2} \sum_{j=1}^n \tilde{\mathbf{P}}_{x,ij} \text{Tr} \left( [\mathbf{H}_j] (\mathbf{X}'\mathbf{X})^{-1} \right)$$

where  $\mathbf{e}_i$  is the  $i$ th observation raw residual,  $\mathbf{I}_n$  is an  $n$ -dimensional identity matrix,  $\mathbf{P}_{xh}$  is the projector onto the column space of  $(\mathbf{X}|\mathbf{H})$ , and  $\tilde{\mathbf{P}}_x = \mathbf{I}_n - \mathbf{P}_x$ . The preceding formulas are general with the projectors defined accordingly to take the weighting into consideration. In unweighted least squares,  $E[\mathbf{e}]$  reduces to

$$E[\mathbf{e}] = -\frac{1}{2} \sigma^2 \tilde{\mathbf{Q}} \mathbf{a}$$

with  $\tilde{\mathbf{Q}}$  being the last  $n - p$  columns of the  $\mathbf{Q}$  matrix in the QR decomposition of  $\mathbf{X}$  and the  $(n - p)$  dimensional vector  $\mathbf{a}$  being defined in terms of the intrinsic acceleration array

$$\mathbf{a}_i = \sum_{j=1}^p [\mathbf{A}_{i+p}]_{jj}$$

Standardization of the projected residuals requires the variance of the projected residuals. This is estimated using the formula (Cook and Tsai 1985)

$$\sigma_p^2 = \frac{\mathbf{e}_p' \mathbf{e}_p}{\text{Tr}(\mathbf{I}_n - \mathbf{P}_{xh})}$$

The standardized raw and projected residuals, denoted by  $\tilde{\mathbf{e}}$  and  $\tilde{\mathbf{e}}_p$  respectively, are given by

$$\tilde{\mathbf{e}} = \frac{\sqrt{w_i} \mathbf{e}}{\sigma \sqrt{1 - \mathbf{P}_{x,ii}}}$$

$$\tilde{\mathbf{e}}_p = \frac{\sqrt{w_i} \mathbf{e}_p}{\sigma \sqrt{1 - \mathbf{P}_{xh,ii}}}$$

The use of raw and projected residuals for diagnostics in nonlinear regression is illustrated in [Example 63.6](#).

### Profiling Parameters and Assessing the Influence of Observations on Parameter Estimates

The global measures of nonlinearity, discussed in the preceding section, are very useful for assessing the overall nonlinearity of the model. However, the impact of global nonlinearity on inference regarding subsets of the parameter set cannot be easily determined (Cook and Tsai 1985). The impact of the nonlinearity on the uncertainty of individual parameters can be efficiently described by profile  $t$  plots and confidence curves (Bates and Watts 1988; Cook and Weisberg 1990).

A profile  $t$  plot for parameter  $\theta$  is a plot of the likelihood ratio pivotal statistic,  $\tau(\theta)$ , and the corresponding Wald pivotal statistic,  $\sigma(\theta)$  (Bates and Watts 1988). The likelihood ratio pivotal statistic is defined as

$$\tau(\theta) = \text{sign}(\theta - \hat{\theta}) L(\theta)$$

with

$$L(\theta) = \left( \frac{\text{SSE}(\theta, \tilde{\Theta}) - \text{SSE}(\hat{\theta}, \hat{\Theta})}{\text{mse}} \right)^{1/2}$$

where  $\theta$  is the profile parameter and  $\Theta$  refers to the remaining parameters.  $\text{SSE}(\theta, \tilde{\Theta})$  is the sum of square errors where the profile parameter  $\theta$  is constrained at a given value and  $\tilde{\Theta}$  is the least squares estimate of  $\Theta$  conditional on a given value of  $\theta$ . In contrast,  $\text{SSE}(\hat{\theta}, \hat{\Theta})$  is the sum of square errors for the full model. For linear models,  $\tau(\theta)$  matches  $\sigma(\theta)$ , which is defined as

$$\sigma(\theta) = \frac{\theta - \hat{\theta}}{\text{stderr}_\theta}$$

where  $\theta$  is the constrained value,  $\hat{\theta}$  is the estimated value for the parameter, and  $\text{stderr}_\theta$  is the standard error for the parameter. Usually a profile  $t$  plot is overlaid with a reference line that passes through the origin and has a slope of 1. PROC NLIN follows this convention.

A confidence curve for a particular parameter is useful for validating Wald-based confidence intervals for the parameter against likelihood-based confidence intervals (Cook and Weisberg 1990). A confidence curve contains a scatter plot of the constrained parameter value versus  $L(\theta)$ . The Wald-based confidence intervals are overlaid as two straight lines that pass through  $(0, \hat{\theta})$  with a slope of  $\pm \text{stderr}_\theta$ . Hence, for different levels of significance, you can easily compare the Wald-based confidence intervals against the corresponding confidence intervals that are based on the likelihood ratio. Cook and Weisberg (1990) recommend that you report a single Wald-based confidence interval only if there is a good agreement between the Wald and likelihood intervals up to at least the 99% confidence level.

Compared to local influence, the leave-one-out method performs a more complete analysis of the influence of observations on the values of parameter estimates. In this method, jackknife resampling removes each

observation in turn and fits the model to the remaining data set. Hence, a data set with  $n$  observations will have  $n$  corresponding data sets with  $n-1$  observations. The impact of each observation on a parameter is assessed by the absolute relative percentage change in the value of the parameter compared with the reference value from the full data.

---

## Missing Values

If the value of any one of the SAS variables involved in the model is missing from an observation, that observation is omitted from the analysis. If only the value of the dependent variable is missing, that observation has a predicted value calculated for it when you use an **OUTPUT** statement and specify the **PREDICTED=** option.

If an observation includes a missing value for one of the independent variables, both the predicted value and the residual value are missing for that observation. If the iterations fail to converge, the values for all variables named in the **OUTPUT** statement are set to missing.

---

## Special Variables

Several special variables are created automatically and can be used in PROC NLIN programming statements.

### Special Variables with Values That Are Set by PROC NLIN

The values of the following six special variables are set by PROC NLIN and should not be reset to a different value by programming statements:

- \_ERROR\_** is set to 1 if a numerical error or invalid argument to a function occurs during the current execution of the program. It is reset to 0 before each new execution.
- \_ITER\_** represents the current iteration number. The variable **\_ITER\_** is set to -1 during the grid search phase.
- \_MODEL\_** is set to 1 for passes through the data when only the predicted values are needed, and not the derivatives. It is 0 when both predicted values and derivatives are needed. If your derivative calculations consume a lot of time, you can save resources by using the following statement after your **MODEL** statement but before your derivative calculations:

```
if _model_ then return;
```

The derivatives generated by PROC NLIN do this automatically.

- \_N\_** indicates the number of times the PROC NLIN step has been executed. It is never reset for successive passes through the data set.
- \_OBS\_** indicates the observation number in the data set for the current program execution. It is reset to 1 to start each pass through the data set (unlike the **\_N\_** variable).
- \_SSE\_** contains the error sum of squares of the last iteration. During the grid search phase, the **\_SSE\_** variable is set to 0. For iteration 0, the **\_SSE\_** variable is set to the SSE associated with the point chosen from the grid search.

`_P_WEIGHTED_SSE_` contains the error sum of squares for the optimization tasks that are required for profiling parameters and assessing the influence of each observation on the estimate of each profiled parameter.

### Special Variable Used to Determine Convergence Criteria

The special variable `_LOSS_` can be used to determine the criterion function for convergence and step shortening. PROC NLIN looks for the variable `_LOSS_` in the programming statements and, if it is defined, uses the (weighted) sum of this value instead of the residual sum of squares to determine the criterion function for convergence and step shortening. This feature is useful in certain types of maximum-likelihood estimation.

**NOTE:** Even if you specify the `_LOSS_` variable in your programming statements, the NLIN procedure continues to solve a least squares problem. The specified `_LOSS_` variable does **not** define or alter the objective function for parameter estimation.

### Weighted Regression with the Special Variable `_WEIGHT_`

To obtain weighted nonlinear least squares estimates of parameters, make an assignment to the `_WEIGHT_` variable as in the following statement:

```
weight = expression;
```

When this statement is included, the expression on the right side of the assignment statement is evaluated for each observation in the data set. The values multiplied by  $1/\sigma^2$  are then taken as inverse elements of the diagonal variance-covariance matrix of the dependent variable.

When a variable name is given after the equal sign, the values of the variable are taken as the inverse elements of the variance-covariance matrix. The larger the `_WEIGHT_` value, the more importance the observation is given.

The `_WEIGHT_` variable can be a function of the estimated parameters. For estimation purposes, the derivative of the `_WEIGHT_` variable with respect to the parameters is not included in the gradient and the Hessian of the loss function. This is normally the desired approach for iteratively reweighted least squares estimation. When the `_WEIGHT_` variable is a function of the parameters, the gradient and the Hessian used can lead to poor convergence or nonconvergence of the requested estimation. To have the derivative of the `_WEIGHT_` variable with respect to the parameters included in the gradient and the Hessian of the loss function, do not use the `_WEIGHT_` variable. Instead, redefine the model as

$$(y - f(x, \beta)) \times \sqrt{\text{wgt}(\beta)}$$

where  $y$  is the original dependent variable,  $f(x, \beta)$  is the nonlinear model, and  $\text{wgt}(\beta)$  is the weight that is a function of the parameters.

If the `_WEIGHT_ =` statement is not used, the default value of 1 is used, and regular least squares estimates are obtained.

---

## Troubleshooting

This section describes a number of problems that might occur in your analysis with PROC NLIN.

## Excessive Computing Time

If you specify a grid of starting values that contains many points, the analysis might take excessive time since the procedure must go through the entire data set for each point on the grid.

The analysis might also take excessive time if your problem takes many iterations to converge, since each iteration requires as much time as a linear regression with predicted values and residuals calculated.

## Dependencies

The matrix of partial derivatives can be singular, possibly indicating an overparameterized model. For example, if  $b_0$  starts at zero in the following model, the derivatives for  $b_1$  are all zero for the first iteration:

```
parms b0=0 b1=.022;
model pop=b0*exp(b1*(year-1790));
der.b0=exp(b1*(year-1790));
der.b1=(year-1790)*b0*exp(b1*(year-1790));
```

The first iteration changes a subset of the parameters; then the procedure can make progress in succeeding iterations. This singularity problem is local. The next example displays a global problem. The term  $b_2$  in the exponent is not identifiable since it trades roles with  $b_0$ .

```
parms b0=3.9 b1=.022 b2=0;
model pop=b0*exp(b1*(year-1790)+b2);
der.b0 = exp(b1*(year-1790)+b2);
der.b1 = (year-1790)*b0*exp(b1*(year-1790)+b2);
der.b2 = b0*exp(b1*(year-1790)+b2);
```

## Unable to Improve

The method can lead to steps that do not improve the estimates even after a series of step halvings. If this happens, the procedure issues a message stating that it is unable to make further progress, but it then displays the following warning message:

```
PROC NLIN failed to converge
```

Then it displays the results. This often means that the procedure has not converged at all. If you provided your own derivatives, check them carefully and then examine the residual sum of squares surface. If PROC NLIN has not converged, try a different set of starting values, a different METHOD= specification, the G4 option, or a different model.

## Divergence

The iterative process might diverge, resulting in overflows in computations. It is also possible that parameters enter a space where arguments to such functions as LOG and SQRT become invalid. For example, consider the following model:

```
parms b=0;
model y = x / b;
```



Suppose that  $y$  contains only zeros, and suppose that the values for variable  $x$  are not zero. There is no least squares estimate for  $b$  since the SSE declines as  $b$  approaches infinity or minus infinity. To avoid the problem, the same model could be parameterized as  $y = a \cdot x$ .

If you have divergence problems, try reparameterizing the model, selecting different starting values, increasing the maximum allowed number of iterations (the `MAXITER=` option), specifying an alternative `METHOD=` option, or including a `BOUNDS` statement.

## Local Minimum

The program might converge to a local rather than a global minimum. For example, consider the following model:

```
parms a=1 b=-1;
model y=(1-a*x) * (1-b*x);
```

Once a solution is found, an equivalent solution with the same SSE can be obtained by swapping the values of  $a$  and  $b$ .

## Discontinuities

The computational methods assume that the model is a continuous and smooth function of the parameters. If this is not true, the method does not work. For example, the following models do not work:

```
model y=a+int(b*x);

model y=a+b*x+4*(z>c);
```

## Responding to Trouble

PROC NLIN does not necessarily produce a good solution the first time. Much depends on specifying good initial values for the parameters. You can specify a grid of values in the `PARMS` statement to search for good starting values. While most practical models should give you no trouble, other models can require switching to a different iteration method or a different computational method for matrix inversion. Specifying the option `METHOD=MARQUARDT` sometimes works when the default method (Gauss-Newton) does not work.

## Computational Methods

### Nonlinear Least Squares

Recall the basic notation for the nonlinear regression model from the section “Notation for Nonlinear Regression Models” on page 5255. The parameter vector  $\beta$  belongs to  $\Omega$ , a subset of  $R^p$ . Two points of this set are of particular interest: the true value  $\tilde{\beta}$  and the least squares estimate  $\hat{\beta}$ . The general nonlinear model fit with the NLIN procedure is represented by the equation

$$Y = f(\tilde{\beta}_0, \tilde{\beta}_1, \dots, \tilde{\beta}_p; z_1, z_2, \dots, z_k) + \epsilon = f(\tilde{\beta}; z_1, z_2, \dots, z_k) + \epsilon$$

where  $z_j$  denotes the  $(n \times 1)$  vector of the  $j$ th regressor (independent) variable,  $\tilde{\beta}$  is the true value of the parameter vector, and  $\epsilon$  is the  $(n \times 1)$  vector of homoscedastic and uncorrelated model errors with zero mean.

To write the model for the  $i$ th observation, the  $i$ th elements of  $\mathbf{z}_1, \dots, \mathbf{z}_k$  are collected in the row vector  $\mathbf{z}'_i$ , and the model equation becomes

$$Y_i = f(\boldsymbol{\beta}; \mathbf{z}'_i) + \epsilon_i$$

The shorthand  $f_i(\boldsymbol{\beta})$  will also be used throughout to denote the mean of the  $i$ th observation.

For any given value  $\boldsymbol{\beta}$  we can compute the residual sum of squares

$$\begin{aligned} \text{SSE}(\boldsymbol{\beta}) &= \sum_{i=1}^n (y_i - f(\boldsymbol{\beta}; \mathbf{z}'_i))^2 \\ &= \sum_{i=1}^n (y_i - f_i(\boldsymbol{\beta}))^2 = \mathbf{r}(\boldsymbol{\beta})' \mathbf{r}(\boldsymbol{\beta}) \end{aligned}$$

The aim of nonlinear least squares estimation is to find the value  $\widehat{\boldsymbol{\beta}}$  that minimizes  $\text{SSE}(\boldsymbol{\beta})$ . Because  $\mathbf{f}$  is a nonlinear function of  $\boldsymbol{\beta}$ , a closed-form solution does not exist for this minimization problem. An iterative process is used instead. The iterative techniques that PROC NLIN uses are similar to a series of linear regressions involving the matrix  $\mathbf{X}$  and the residual vector  $\mathbf{r} = \mathbf{y} - \mathbf{f}(\boldsymbol{\beta})$ , evaluated at the current values of  $\boldsymbol{\beta}$ .

It is more insightful, however, to describe the algorithms in terms of their approach to minimizing the residual sum of squares and in terms of their updating formulas. If  $\widehat{\boldsymbol{\beta}}^{(u)}$  denotes the value of the parameter estimates at the  $u$ th iteration, and  $\widehat{\boldsymbol{\beta}}^{(0)}$  are your starting values, then the NLIN procedure attempts to find values  $k$  and  $\boldsymbol{\Delta}$  such that

$$\widehat{\boldsymbol{\beta}}^{(u+1)} = \widehat{\boldsymbol{\beta}}^{(u)} + k \boldsymbol{\Delta}$$

and

$$\text{SSE}(\widehat{\boldsymbol{\beta}}^{(u+1)}) < \text{SSE}(\widehat{\boldsymbol{\beta}}^{(u)})$$

The various methods to fit a nonlinear regression model—which you can select with the `METHOD=` option in the `PROC NLIN` statement—differ in the calculation of the update vector  $\boldsymbol{\Delta}$ .

The gradient and Hessian of the residual sum of squares with respect to individual parameters and pairs of parameters are, respectively,

$$\begin{aligned} \mathbf{g}(\boldsymbol{\beta}_j) &= \frac{\partial \text{SSE}(\boldsymbol{\beta})}{\partial \beta_j} = -2 \sum_{i=1}^n (y_i - f_i(\boldsymbol{\beta})) \frac{\partial f_i(\boldsymbol{\beta})}{\partial \beta_j} \\ [\mathbf{H}(\boldsymbol{\beta})]_{jk} &= \frac{\partial^2 \text{SSE}(\boldsymbol{\beta})}{\partial \beta_j \partial \beta_k} = 2 \sum_{i=1}^n \frac{\partial f_i(\boldsymbol{\beta})}{\partial \beta_j} \frac{\partial f_i(\boldsymbol{\beta})}{\partial \beta_k} - (y_i - f_i(\boldsymbol{\beta})) \frac{\partial^2 f_i(\boldsymbol{\beta})}{\partial \beta_j \partial \beta_k} \end{aligned}$$

Denote as  $\mathbf{H}_i^*(\boldsymbol{\beta})$  the Hessian matrix of the mean function,

$$[\mathbf{H}_i^*(\boldsymbol{\beta})]_{jk} = \left[ \frac{\partial^2 f_i(\boldsymbol{\beta})}{\partial \beta_j \partial \beta_k} \right]_{jk}$$

Collecting the derivatives across all parameters leads to the expressions

$$\mathbf{g}(\boldsymbol{\beta}) = \frac{\partial \text{SSE}(\boldsymbol{\beta})}{\partial \boldsymbol{\beta}} = -2\mathbf{X}'\mathbf{r}(\boldsymbol{\beta})$$

$$\mathbf{H}(\boldsymbol{\beta}) = \frac{\partial^2 \text{SSE}(\boldsymbol{\beta})}{\partial \boldsymbol{\beta} \partial \boldsymbol{\beta}'} = 2 \left( \mathbf{X}'\mathbf{X} - \sum_{i=1}^n r_i(\boldsymbol{\beta}) \mathbf{H}_i^*(\boldsymbol{\beta}) \right)$$

The change in the vector of parameter estimates is computed as follows, depending on the estimation method:

$$\text{Gauss-Newton: } \boldsymbol{\Delta} = (-\mathbf{E}[\mathbf{H}(\boldsymbol{\beta})])^{-1} \mathbf{g}(\boldsymbol{\beta}) = (\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}'\mathbf{r}$$

$$\text{Marquardt: } \boldsymbol{\Delta} = (\mathbf{X}'\mathbf{X} + \lambda \text{diag}(\mathbf{X}'\mathbf{X}))^{-1} \mathbf{X}'\mathbf{r}$$

$$\text{Newton: } \boldsymbol{\Delta} = -\mathbf{H}(\boldsymbol{\beta})^{-1} \mathbf{g}(\boldsymbol{\beta}) = \mathbf{H}(\boldsymbol{\beta})^{-1} \mathbf{X}'\mathbf{r}$$

$$\text{Steepest descent: } \boldsymbol{\Delta} = -\frac{1}{2} \frac{\partial \text{SSE}(\boldsymbol{\beta})}{\partial \boldsymbol{\beta}} = \mathbf{X}'\mathbf{r}$$

The Gauss-Newton and Marquardt iterative methods regress the residuals onto the partial derivatives of the model with respect to the parameters until the estimates converge. You can view the Marquardt algorithm as a Gauss-Newton algorithm with a ridgeing penalty. The Newton iterative method regresses the residuals onto a function of the first and second derivatives of the model with respect to the parameters until the estimates converge. Analytical first- and second-order derivatives are automatically computed as needed.

The default method used to compute  $(\mathbf{X}'\mathbf{X})^{-1}$  is the sweep (Goodnight 1979). It produces a reflexive generalized inverse (a  $g_2$ -inverse, Pringle and Rayner 1971). In some cases it might be preferable to use a Moore-Penrose inverse (a  $g_4$ -inverse) instead. If you specify the **G4** option in the **PROC NLIN** statement, a  $g_4$ -inverse is used to calculate  $\boldsymbol{\Delta}$  on each iteration.

The four algorithms are now described in greater detail.

## Algorithmic Details

### **Gauss-Newton and Newton Methods**

From the preceding set of equations you can see that the Marquardt method is a ridged version of the Gauss-Newton method. If the ridge parameter  $\lambda$  equals zero, the Marquardt step is identical to the Gauss-Newton step. An important difference between the Newton methods and the Gauss-Newton-type algorithms lies in the use of second derivatives. To motivate this distinctive element between Gauss-Newton and the Newton method, focus first on the objective function in nonlinear least squares. To numerically find the minimum of

$$\text{SSE}(\boldsymbol{\beta}) = \mathbf{r}(\boldsymbol{\beta})'\mathbf{r}(\boldsymbol{\beta})$$

you can approach the problem by approximating the sum of squares criterion by a criterion for which you can compute a closed-form solution. Following Seber and Wild (1989, Sect. 2.1.3), we can achieve that by doing the following:

- approximating the model and substituting the approximation into  $SSE(\boldsymbol{\beta})$
- approximating  $SSE(\boldsymbol{\beta})$  directly

The first method, approximating the nonlinear model with a first-order Taylor series, is the purview of the Gauss-Newton method. Approximating the residual sum of squares directly is the realm of the Newton method.

The first-order Taylor series of the residual  $\mathbf{r}(\boldsymbol{\beta})$  at the point  $\hat{\boldsymbol{\beta}}$  is

$$\mathbf{r}(\boldsymbol{\beta}) \approx \mathbf{r}(\hat{\boldsymbol{\beta}}) - \hat{\mathbf{X}}(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})$$

Substitution into  $SSE(\boldsymbol{\beta})$  leads to the objective function for the Gauss-Newton step:

$$SSE(\boldsymbol{\beta}) \approx S_G(\boldsymbol{\beta}) = \mathbf{r}(\hat{\boldsymbol{\beta}})' - 2\mathbf{r}'(\hat{\boldsymbol{\beta}})\hat{\mathbf{X}}(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}}) + (\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})'(\hat{\mathbf{X}}'\hat{\mathbf{X}})(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})$$

“Hat” notation is used here to indicate that the quantity in question is evaluated at  $\hat{\boldsymbol{\beta}}$ .

To motivate the Newton method, take a second-order Taylor series of  $SSE(\boldsymbol{\beta})$  around the value  $\hat{\boldsymbol{\beta}}$ :

$$SSE(\boldsymbol{\beta}) \approx S_N(\boldsymbol{\beta}) = SSE(\hat{\boldsymbol{\beta}}) + \mathbf{g}(\hat{\boldsymbol{\beta}})'(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}}) + \frac{1}{2}(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})' \mathbf{H}(\hat{\boldsymbol{\beta}})(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})$$

Both  $S_G(\boldsymbol{\beta})$  and  $S_N(\boldsymbol{\beta})$  are quadratic functions in  $\boldsymbol{\beta}$  and are easily minimized. The minima occur when

$$\text{Gauss-Newton: } \boldsymbol{\beta} - \hat{\boldsymbol{\beta}} = (\hat{\mathbf{X}}'\hat{\mathbf{X}})^{-1} \hat{\mathbf{X}}'\mathbf{r}(\hat{\boldsymbol{\beta}})$$

$$\text{Newton: } \boldsymbol{\beta} - \hat{\boldsymbol{\beta}} = -\mathbf{H}(\hat{\boldsymbol{\beta}})^{-1} \mathbf{g}(\hat{\boldsymbol{\beta}})$$

and these terms define the preceding  $\boldsymbol{\Delta}$  update vectors.

### **Gauss-Newton Method**

Since the Gauss-Newton method is based on an approximation of the model, you can also derive the update vector by first considering the “normal” equations of the nonlinear model

$$\mathbf{X}'\mathbf{f}(\boldsymbol{\beta}) = \mathbf{X}'\mathbf{Y}$$

and then substituting the Taylor approximation

$$\mathbf{f}(\boldsymbol{\beta}) \approx \mathbf{f}(\hat{\boldsymbol{\beta}}) + \mathbf{X}(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})$$

for  $\mathbf{f}(\boldsymbol{\beta})$ . This leads to

$$\mathbf{X}'(\mathbf{f}(\hat{\boldsymbol{\beta}}) + \mathbf{X}(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})) = \mathbf{X}'\mathbf{Y}$$

$$(\mathbf{X}'\mathbf{X})(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}}) = \mathbf{X}'\mathbf{Y} - \mathbf{X}'\mathbf{f}(\hat{\boldsymbol{\beta}})$$

$$(\mathbf{X}'\mathbf{X})\boldsymbol{\Delta} = \mathbf{X}'\mathbf{r}(\hat{\boldsymbol{\beta}})$$

and the update vector becomes

$$\boldsymbol{\Delta} = (\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}'\mathbf{r}(\hat{\boldsymbol{\beta}})$$

**NOTE:** If  $\mathbf{X}'\mathbf{X}$  is singular or becomes singular, PROC NLIN computes  $\boldsymbol{\Delta}$  by using a generalized inverse for the iterations after singularity occurs. If  $\mathbf{X}'\mathbf{X}$  is still singular for the last iteration, the solution should be examined.

**Newton Method**

The Newton method uses the second derivatives and solves the equation

$$\Delta = \mathbf{H}^{-1} \mathbf{X}' \mathbf{r}$$

If the automatic variables `_WEIGHT_`, `_WGTJPJ_`, and `_RESID_` are used, then

$$\Delta = \mathbf{H}^{-1} \mathbf{X}' \mathbf{W}^{\text{SSE}} \mathbf{r}^*$$

is the direction, where

$$\mathbf{H} = \mathbf{X}' \mathbf{W}^{\text{XPX}} \mathbf{X} - \sum_{i=1}^n \mathbf{H}_i^*(\boldsymbol{\beta}) w_i^{\text{XPX}} r_i^*$$

and

$\mathbf{W}^{\text{SSE}}$  is an  $n \times n$  diagonal matrix with elements  $w_i^{\text{SSE}}$  of weights from the `_WEIGHT_` variable. Each element  $w_i^{\text{SSE}}$  contains the value of `_WEIGHT_` for the  $i$ th observation.

$\mathbf{W}^{\text{XPX}}$  is an  $n \times n$  diagonal matrix with elements  $w_i^{\text{XPX}}$  of weights from the `_WGTJPJ_` variable. Each element  $w_i^{\text{XPX}}$  contains the value of `_WGTJPJ_` for the  $i$ th observation.

$\mathbf{r}^*$  is a vector with elements  $r_i^*$  from the `_RESID_` variable. Each element  $r_i^*$  contains the value of `_RESID_` evaluated for the  $i$ th observation.

**Marquardt Method**

The updating formula for the Marquardt method is as follows:

$$\Delta = (\mathbf{X}' \mathbf{X} + \lambda \text{diag}(\mathbf{X}' \mathbf{X}))^{-1} \mathbf{X}' \mathbf{e}$$

The Marquardt method is a compromise between the Gauss-Newton and steepest descent methods (Marquardt 1963). As  $\lambda \rightarrow 0$ , the direction approaches Gauss-Newton. As  $\lambda \rightarrow \infty$ , the direction approaches steepest descent.

Marquardt's studies indicate that the average angle between Gauss-Newton and steepest descent directions is about  $90^\circ$ . A choice of  $\lambda$  between 0 and infinity produces a compromise direction.

By default, PROC NLIN chooses  $\lambda = 10^{-7}$  to start and computes  $\Delta$ . If  $\text{SSE}(\boldsymbol{\beta}_0 + \Delta) < \text{SSE}(\boldsymbol{\beta}_0)$ , then  $\lambda = \lambda/10$  for the next iteration. Each time  $\text{SSE}(\boldsymbol{\beta}_0 + \Delta) > \text{SSE}(\boldsymbol{\beta}_0)$ , then  $\lambda = 10\lambda$ .

**NOTE:** If the SSE decreases on each iteration, then  $\lambda \rightarrow 0$ , and you are essentially using the Gauss-Newton method. If SSE does not improve, then  $\lambda$  is increased until you are moving in the steepest descent direction.

Marquardt's method is equivalent to performing a series of ridge regressions, and it is useful when the parameter estimates are highly correlated or the objective function is not well approximated by a quadratic.

**Steepest Descent (Gradient) Method**

The steepest descent method is based directly on the gradient of  $0.5\mathbf{r}(\boldsymbol{\beta})' \mathbf{r}(\boldsymbol{\beta})$ :

$$\frac{1}{2} \frac{\partial \text{SSE}(\boldsymbol{\beta})}{\partial \boldsymbol{\beta}} = -\mathbf{X}' \mathbf{r}$$

The quantity  $-\mathbf{X}'\mathbf{r}$  is the gradient along which  $\epsilon'\epsilon$  increases. Thus  $\mathbf{\Delta} = \mathbf{X}'\mathbf{r}$  is the direction of steepest descent.

If the automatic variables `_WEIGHT_` and `_RESID_` are used, then

$$\mathbf{\Delta} = \mathbf{X}'\mathbf{W}^{\text{SSE}}\mathbf{r}^*$$

is the direction, where

$\mathbf{W}^{\text{SSE}}$  is an  $n \times n$  diagonal matrix with elements  $w_i^{\text{SSE}}$  of weights from the `_WEIGHT_` variable. Each element  $w_i^{\text{SSE}}$  contains the value of `_WEIGHT_` for the  $i$ th observation.

$\mathbf{r}^*$  is a vector with elements  $r_i^*$  from `_RESID_`. Each element  $r_i^*$  contains the value of `_RESID_` evaluated for the  $i$ th observation.

Using the method of steepest descent, let

$$\boldsymbol{\beta}^{(k+1)} = \boldsymbol{\beta}^{(k)} + \alpha \mathbf{\Delta}$$

where the scalar  $\alpha$  is chosen such that

$$\text{SSE}(\boldsymbol{\beta}_i + \alpha \mathbf{\Delta}) < \text{SSE}(\boldsymbol{\beta}_i)$$

**NOTE:** The steepest-descent method can converge very slowly and is therefore not generally recommended. It is sometimes useful when the initial values are poor.

### Step-Size Search

The default method of finding the step size  $k$  is step halving by using `SMETHOD=HALVE`. If  $\text{SSE}(\boldsymbol{\beta}^{(u)} + \mathbf{\Delta}) > \text{SSE}(\boldsymbol{\beta}^{(u)})$ , compute  $\text{SSE}(\boldsymbol{\beta}^{(u)} + 0.5\mathbf{\Delta})$ ,  $\text{SSE}(\boldsymbol{\beta}^{(u)} + 0.25\mathbf{\Delta})$ , . . . , until a smaller SSE is found.

If you specify `SMETHOD=GOLDEN`, the step size  $k$  is determined by a golden section search. The parameter `TAU` determines the length of the initial interval to be searched, with the interval having length `TAU` (or  $2 \times \text{TAU}$ ), depending on  $\text{SSE}(\boldsymbol{\beta}^{(u)} + \mathbf{\Delta})$ . The `RHO` parameter specifies how fine the search is to be. The SSE at each endpoint of the interval is evaluated, and a new subinterval is chosen. The size of the interval is reduced until its length is less than `RHO`. One pass through the data is required each time the interval is reduced. Hence, if `RHO` is very small relative to `TAU`, a large amount of time can be spent determining a step size. For more information about the golden section search, see Kennedy and Gentle (1980).

If you specify `SMETHOD=CUBIC`, the NLIN procedure performs a cubic interpolation to estimate the step size. If the estimated step size does not result in a decrease in SSE, step halving is used.

---

## Output Data Sets

The data set produced by the `OUTEST=` option in the `PROC NLIN` statement contains the parameter estimates on each iteration, including the grid search.

The variable `_ITER_` contains the iteration number. The variable `_TYPE_` denotes whether the observation contains iteration parameter estimates (“ITER”), final parameter estimates (“FINAL”), or covariance estimates (“COVB”). The variable `_NAME_` contains the parameter name for covariances, and the variable

`_SSE_` contains the objective function value for the parameter estimates. The variable `_STATUS_` indicates whether the estimates have converged.

The data set produced by the `OUTPUT` statement contains statistics calculated for each observation. In addition, the data set contains the variables from the input data set and any `ID` variables that are specified in the `ID` statement.

The data set that is produced by the `PROFDATA=` option in the `PROFILE` statement contains statistics that are calculated during parameter profiling. The variable `_TYPE_` denotes whether the observation is from a profiling task (set as `PROF`) or jackknife resampling task (set as `JACK`). The variable `_PROF_PARM_` refers to the name of the profiled parameter for profiling tasks. The variable `_OBS_INF_MEAS_` is the observation index of the deleted observation for jackknife resampling tasks, and the variables `_L_STAT_` and `_W_STAT_` contain the likelihood ratio pivotal statistic and the Wald pivotal statistic, respectively. The rest of the variables are the parameter estimates.

## Confidence Intervals

### Parameter Confidence Intervals

The parameter confidence intervals are computed using the Wald-based formula:

$$\hat{\beta}_i \pm \text{stderr}_i \times t(n - p, 1 - \alpha/2)$$

where  $\hat{\beta}_i$  is the  $i$ th parameter estimate,  $\text{stderr}_i$  is its estimated approximate standard error,  $t(n - p, 1 - \alpha/2)$  is a  $t$  statistic with  $n - p$  degrees of freedom,  $n$  is the number of observations, and  $p$  is the number of parameters. You can specify the significance level  $\alpha$  used in the construction of these confidence limits with the `ALPHA=` option in the `PROC NLIN` statement; the default value is  $\alpha = 0.05$ . Because Wald-based confidence intervals are only asymptotically valid, you should use confidence curves for a more accurate and complete inference on confidence intervals. See the section “[Profiling Parameters and Assessing the Influence of Observations on Parameter Estimates](#)” on page 5290 for details.

### Model Confidence Intervals

Model confidence intervals are output when an `OUT=` data set is specified and one or more of the keywords `LCLM`, `UCLM`, `LCL`, `UCL`, `L95M=`, `U95M=`, `L95=`, and `U95=` is specified. The expressions for these terms are as follows:

$$\text{LCLM} = f(\boldsymbol{\beta}, \mathbf{z}_i) - \sqrt{\text{MSE} \times h_i/w_i} \times t(n - p, 1 - \alpha/2)$$

$$\text{UCLM} = f(\boldsymbol{\beta}, \mathbf{z}_i) + \sqrt{\text{MSE} \times h_i/w_i} \times t(n - p, 1 - \alpha/2)$$

$$\text{LCL} = f(\boldsymbol{\beta}, \mathbf{z}_i) - \sqrt{\text{MSE}(h_i + 1/w_i)} \times t(n - p, 1 - \alpha/2)$$

$$\text{UCL} = f(\boldsymbol{\beta}, \mathbf{z}_i) + \sqrt{\text{MSE}(h_i + 1/w_i)} \times t(n - p, 1 - \alpha/2)$$

$$\text{L95M} = f(\boldsymbol{\beta}, \mathbf{z}_i) - \sqrt{\text{MSE} \times h_i/w_i} \times t(n - p, 1 - 0.05/2)$$

$$\text{U95M} = f(\boldsymbol{\beta}, \mathbf{z}_i) + \sqrt{\text{MSE} \times h_i/w_i} \times t(n - p, 1 - 0.05/2)$$

$$\text{L95} = f(\boldsymbol{\beta}, \mathbf{z}_i) - \sqrt{\text{MSE}(h_i + 1/w_i)} \times t(n - p, 1 - 0.05/2)$$

$$\text{U95} = f(\boldsymbol{\beta}, \mathbf{z}_i) + \sqrt{\text{MSE}(h_i + 1/w_i)} \times t(n - p, 1 - 0.05/2)$$

where  $h_i = w_i x_i (\mathbf{X}'\mathbf{W}\mathbf{X})^{-1} \mathbf{x}'_i$  is the leverage,  $\mathbf{X} = \partial \mathbf{f} / \partial \boldsymbol{\beta}$ , and  $\mathbf{x}_i$  is the  $i$ th row of  $\mathbf{X}$ . These results are derived for linear systems. The intervals are approximate for nonlinear models. The value  $\alpha$  in the preceding formulas for **LCLM**, **UCLM**, **LCL**, and **UCL** can be set with the **ALPHA=** option in the **PROC NLIN** statement or with the **ALPHA=** option in the **OUTPUT** statement. If both **ALPHA=** options are specified, the option in the **OUTPUT** takes precedence.

---

## Covariance Matrix of Parameter Estimates

For unconstrained estimates (no active bounds), the covariance matrix of the parameter estimates is

$$\text{mse} \times (\mathbf{X}'\mathbf{X})^{-1}$$

for the gradient, Marquardt, and Gauss methods and

$$\text{mse} \times \mathbf{H}^{-1}$$

for the Newton method. Recall that  $\mathbf{X}$  is the matrix of the first partial derivatives of the nonlinear model with respect to the parameters. The matrices are evaluated at the final parameter estimates. The mean squared error, the estimate of the residual variance  $\sigma^2$ , is computed as

$$\text{mse} = \mathbf{r}'\mathbf{r} / (n - p)$$

where  $n$  is the number of nonmissing (used) observations and  $p$  is the number of estimable parameters. The standard error reported for the parameter estimates is the square root of the corresponding diagonal element of this matrix. If you specify a value for the residual variance with the **SIGSQ=** option, then that value replaces **mse** in the preceding expressions.

Now suppose that restrictions or bounds are active. Equality restrictions can be written as a vector function,  $h(\boldsymbol{\theta}) = \mathbf{0}$ . Inequality restrictions are either active or inactive. When an inequality restriction is active, it is treated as an equality restriction.

Assume that the vector  $h(\boldsymbol{\theta})$  contains the current active restrictions. The constraint matrix  $\mathbf{A}$  is then

$$\mathbf{A}(\hat{\boldsymbol{\theta}}) = \frac{\partial h(\hat{\boldsymbol{\theta}})}{\partial \hat{\boldsymbol{\theta}}}$$

The covariance matrix for the restricted parameter estimates is computed as

$$\mathbf{Z}(\mathbf{Z}'\mathbf{H}\mathbf{Z})^{-1}\mathbf{Z}'$$

where  $\mathbf{H}$  is the Hessian (or approximation to the Hessian) and  $\mathbf{Z}$  collects the last  $(p - n_c)$  columns of  $\mathbf{Q}$  from an LQ factorization of the constraint matrix. Further,  $n_c$  is the number of active constraints, and  $p$  denotes the number of parameters. See Gill, Murray, and Wright (1981) for more details about the LQ factorization. The covariance matrix for the Lagrange multipliers is computed as

$$(\mathbf{A}\mathbf{H}^{-1}\mathbf{A}')^{-1}$$



## Convergence Measures

The NLIN procedure computes and reports four convergence measures, labeled R, PPC, RPC, and OBJECT.

**R** is the primary convergence measure for the parameters. It measures the degree to which the residuals are orthogonal to the columns of  $\mathbf{X}$ , and it approaches 0 as the gradient of the objective function becomes small. R is defined as

$$\sqrt{\frac{\mathbf{r}'\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{r}}{\text{LOSS}^i}}$$

**PPC** is the prospective parameter change measure. PPC measures the maximum relative change in the parameters implied by the parameter-change vector computed for the next iteration. At the  $k$ th iteration, PPC is the maximum over the parameters

$$\frac{|\widehat{\theta}_i^{(k+1)} - \widehat{\theta}_i^{(k)}|}{|\widehat{\theta}_i^{(k)}| + 1\text{E} - 6}$$

where  $\widehat{\theta}_i^{(k)}$  is the current value of the  $i$ th parameter and  $\widehat{\theta}_i^{(k+1)}$  is the prospective value of this parameter after adding the change vector computed for the next iteration. These changes are measured before step length adjustments are made. The parameter with the maximum prospective relative change is displayed with the value of PPC, unless the PPC is nearly 0.

**RPC** is the retrospective parameter change measure. RPC measures the maximum relative change in the parameters from the previous iteration. At the  $k$ th iteration, RPC is the maximum over  $i$  of

$$\frac{|\widehat{\theta}_i^{(k)} - \widehat{\theta}_i^{(k-1)}|}{|\widehat{\theta}_i^{(k-1)}| + 1\text{E} - 6}$$

where  $\widehat{\theta}_i^{(k)}$  is the current value of the  $i$ th parameter and  $\widehat{\theta}_i^{(k-1)}$  is the previous value of this parameter. These changes are measured before step length adjustments are made. The name of the parameter with the maximum retrospective relative change is displayed with the value of RPC, unless the RPC is nearly 0.

**OBJECT** measures the relative change in the objective function value between iterations:

$$\frac{|O^{(k)} - O^{(k-1)}|}{|O^{(k-1)}| + 1\text{E} - 6}$$

where  $O^{(k-1)}$  is the value of the objective function ( $O^{(k)}$ ) from the previous iteration. This is the old **CONVERGEOBJ=** criterion.

---

## Displayed Output

In addition to the output data sets, PROC NLIN also produces the following output objects:

- the residual sums of squares associated with all or some of the combinations of possible starting values of the parameters
- the estimates of the parameters and the residual sums of squares at each iteration
- the estimation summary table, which displays information about the estimation method, the number of observations in the analysis, the objective function, and convergence measures
- the analysis of variance table, including sums of squares for the “Model,” “Residual,” and “Total” sources of variation (“Corrected Total” or “Uncorrected Total”), and the model  $F$  test. Note that beginning in SAS<sup>®</sup> 9, only the uncorrected total SS is reported and the respective  $F$  test is based on the uncorrected total SS if PROC NLIN determines the model does not include an intercept. If PROC NLIN determines the model does include an intercept, only the corrected total SS is reported and the respective  $F$  test is based on the corrected total SS.
- the table of parameter estimates, which contains for each parameter in the model its estimate, the approximate standard error of the estimate, and a 95% confidence interval based on the approximate standard error. The confidence level can be changed with the `ALPHA=` option in the `PROC NLIN` statement. The `HOUGAARD` option in the `PROC NLIN` statement requests that Hougaard’s skewness measure be added for each parameter. The standard errors and confidence limits are labeled approximate because they are valid asymptotically as the number of observations grows. If your model is linear in the parameters, the standard errors and confidence intervals are not approximate.
- the approximate correlation matrix of the parameter estimates. This correlation matrix is labeled approximate because it is computed from the approximate covariance matrix of the parameter estimates. If your model is linear in the parameters, the correlation matrix is not approximate.

---

## Incompatibilities with SAS 6.11 and Earlier Versions of PROC NLIN

The NLIN procedure now uses a compiler that is different from the DATA step compiler. The compiler was changed so that analytical derivatives could be computed automatically. For the most part, the syntax accepted by the old NLIN procedure can be used in the new NLIN procedure. However, there are several differences that should be noted:

- You cannot specify a character index variable in the DO statement, and you cannot specify a character test in the IF statement. Thus `do i=1,2,3;` is supported, but `do i='ONE','TWO','THREE';` is not supported. And `if 'THIS' < 'THAT' then ...;` is supported, but `if 'THIS' THEN ...;` is not supported.
- The PUT statement, which is used mostly for program debugging in PROC NLIN, supports only some of the features of the DATA step PUT statement, and it has some new features that the DATA step PUT statement does not.

- The PUT statement does not support line pointers, factored lists, iteration factors, overprinting, the `_INFILE_` option, the ‘.’ format modifier, or the symbol ‘\$’.
  - The PUT statement does support expressions inside of parentheses. For example, `put (sqrt(x));` produces the square root of X.
  - The PUT statement also supports the option `_PDV_` to display a formatted listing of all the variables in the program. The statement `put _pdv_;` prints a much more readable listing of the variables than `put _all_;` does.
- You cannot use the ‘\*’ subscript, but you can specify an array name in a PUT statement without subscripts. Thus, `array a ...; put a;` is acceptable, but `put a[*];` is not. The statement `put a;` displays all the elements of the array a. The `put a=;` statement displays all the elements of A with each value labeled by the name of the element variable.
  - You cannot specify arguments in the ABORT statement.
  - You can specify more than one target statement in the WHEN and OTHERWISE statements. That is, DO/END groups are not necessary for multiple WHEN statements, such as `select; when(exp1); stmt1; stmt2; when(exp2); stmt3; stmt4; end;`
  - You can specify only the options LOG, PRINT, and LIST in the FILE statement.
  - The RETAIN statement retains only values across one pass through the data set. If you need to retain values across iterations, use the CONTROL statement to make a control variable.

The ARRAY statement in PROC NLIN is similar to, but not the same as, the ARRAY statement in the DATA step. The ARRAY statement is used to associate a name (of no more than 8 characters) with a list of variables and constants. The array name can then be used with subscripts in the program to refer to the items in the list.

The ARRAY statement supported by PROC NLIN does not support all the features of the DATA step ARRAY statement. You cannot specify implicit indexing variables; all array references must have explicit subscript expressions. You can specify simple array dimensions; lower bound specifications are not supported. A maximum of six dimensions are accepted.

On the other hand, the ARRAY statement supported by PROC NLIN does accept both variables and constants as array elements. In the following statements, b is a constant array and c is a variable array. Note that the constant array elements cannot be changed with assignment statements.

```
proc nlin data=nld;
array b[4] 1 2 3 4; /* Constant array */
array c[4] (1 2 3 4); /* Numeric array with initial values */

b[1] = 2; /* This is an ERROR, b is a constant array*/
c[2] = 7.5; /* This is allowed */
```

Both dimension specification and the list of elements are optional, but at least one must be specified. When the list of elements is not specified, or fewer elements than the size of the array are listed, array variables are created by suffixing element numbers to the array name to complete the element list.

If the array is used as a pure array in the program rather than a list of symbols (the individual symbols of the array are not referenced in the code), the array is converted to a numerical array. A pure array is literally

a vector of numbers that are accessed only by index. Using these types of arrays results in faster derivatives and compiled code. The assignment to `c1` in the following statements forces the array to be treated as a list of symbols:

```
proc nlin data=nld;
 array c[4] (1 2 3 4); /* Numeric array with initial values */

 c[2] = 7.5; /* This is C used as a pure array */
 c1 = -92.5; /* This forces C to be a list of symbols */
```

---

## ODS Table Names

PROC NLIN assigns a name to each table it creates. You can use these names to refer to the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in Table 63.7. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

**Table 63.7** ODS Tables Produced by PROC NLIN

| ODS Table Name       | Description                             | Statement    |
|----------------------|-----------------------------------------|--------------|
| ANOVA                | Analysis of variance                    | default      |
| CodeDependency       | Variable cross reference                | LISTDEP      |
| CodeList             | Listing of program statements           | LISTCODE     |
| ConvergenceStatus    | Convergence status                      | default      |
| CorrB                | Correlation of the parameters           | default      |
| EstSummary           | Summary of the estimation               | default      |
| FirstDerivatives     | First derivative table                  | LISTDER      |
| IterHistory          | Iteration output                        | default      |
| MissingValues        | Missing values generated by the program | default      |
| NonlinearityMeasures | Global nonlinearity measures            | NLINMEASURES |
| ParameterEstimates   | Parameter estimates                     | default      |

---

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “Statistical Graphics Using ODS.”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “A Primer on ODS Statistical Graphics” on page 599 in Chapter 21, “Statistical Graphics Using ODS.”

PROC NLIN assigns a name to each graph it creates using ODS. You can use these names to refer to the graphs when using ODS. The graphs that are controlled by the **PLOTS** option in the **PROC NLIN** statement are listed in Table 63.8 and those that are controlled by the options in **PROFILE** statement are in Table 63.9.

**Table 63.8** Graphs Controlled by the PLOTS option in the PROC NLIN Statement

| ODS Graph Name             | Plot Description                                                     | PLOTS Option        |
|----------------------------|----------------------------------------------------------------------|---------------------|
| ContourFitPlot             | Contour fit plot for models with two regressors                      | FIT                 |
| FitPlot                    | Fit plot for models with one regressor                               | FIT                 |
| FitDiagnosticsPanel        | Panel of fit diagnostics                                             | DIAGNOSTICS         |
| LeveragePlot               | Tangential and Jacobian leverages versus observation number          | DIAGNOSTICS         |
| LocalInfluencePlot         | Local influence versus observation number                            | DIAGNOSTICS         |
| ObservedByPredictedPlot    | Dependent variable versus predicted values                           | DIAGNOSTICS(UNPACK) |
| ProjectedResidualHistogram | A histogram of the projected residuals                               | DIAGNOSTICS(UNPACK) |
| RawResidualExpectationPlot | Raw residual expectation versus predicted values                     | DIAGNOSTICS(UNPACK) |
| RawResidualHistogram       | A histogram of the raw residuals                                     | DIAGNOSTICS(UNPACK) |
| ResidualBoxPlot            | A box plot of the raw and projected residuals                        | DIAGNOSTICS(UNPACK) |
| ResidualPanel              | A panel of the raw and projected residuals versus the regressors     | RESIDUALS           |
| ResidualPlot               | A plot of the raw and projected residuals versus the regressors      | RESIDUALS(UNPACK)   |
| ResidualByPredictedPlot    | Raw and projected residuals versus the predicted values              | DIAGNOSTICS(UNPACK) |
| RStudentByJacLeveragePlot  | Standardized raw and projected residuals versus Jacobian leverage    | DIAGNOSTICS(UNPACK) |
| RStudentByPredictedPlot    | Standardized raw and projected residuals versus the predicted values | DIAGNOSTICS(UNPACK) |
| RStudentByTanLeveragePlot  | Standardized raw and projected residuals versus tangential leverage  | DIAGNOSTICS(UNPACK) |

**Table 63.9** Graphs Controlled by the PROFILE Statement

| ODS Graph Name  | Plot Description                                                  | PROFILE Option |
|-----------------|-------------------------------------------------------------------|----------------|
| ConfidenceCurve | Parameter value versus $t$ value                                  | CONF CURV      |
| JackknifePlot   | Absolute relative percentage difference versus observation number | JACKKNIFE      |
| ProfiletPlot    | Likelihood ratio pivotal statistic versus Wald pivotal statistic  | T PLOT         |

## Convergence Status Table

The “Convergence Status” table can be used to programmatically check the status of an estimation. This table contains the `Status` variable that takes on the value 0, 1, 2, or 3. If `Status` takes on a value less than 3, the convergence criterion was met. Specifically, the values mean the following:

|          |                                                                                                                                                                                                  |
|----------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Status=0 | indicates that the convergence criterion was met and no warning or error messages were issued during the PROC NLIN run. Also, no notes that could indicate a problem with the model were issued. |
| Status=1 | indicates that the convergence criterion was met and notes were written to the log that might indicate a problem with the model.                                                                 |
| Status=2 | indicates that the convergence criterion was met and one or more warning messages were produced during the PROC NLIN run.                                                                        |
| Status=3 | indicates that the convergence criterion was not met.                                                                                                                                            |

The following sample program demonstrates how the “Convergence Status” table can be used:

```
ods output ConvergenceStatus=ConvStatus;
proc nlin data=YourData;
 parameters a=1 b=1 c=1;
 model wgt = a + x / (b*y+c*z);
run;

data _null_;
 set ConvStatus;
 if status > 0 then put "A problem occurred";
run;
```

---

## Examples: NLIN Procedure

---

### Example 63.1: Segmented Model

Suppose you are interested in fitting a model that consists of two segments that connect in a smooth fashion. For example, the following model states that for values of  $x$  less than  $x_0$  the mean of  $Y$  is a quadratic function in  $x$ , and for values of  $x$  greater than  $x_0$  the mean of  $Y$  is constant:

$$E[Y|x] = \begin{cases} \alpha + \beta x + \gamma x^2 & \text{if } x < x_0 \\ c & \text{if } x \geq x_0 \end{cases}$$

In this model equation  $\alpha$ ,  $\beta$ , and  $\gamma$  are the coefficients of the quadratic segment, and  $c$  is the plateau of the mean function. The NLIN procedure can fit such a segmented model even when the join point,  $x_0$ , is unknown.

We also want to impose conditions on the two segments of the model. First, the curve should be continuous—that is, the quadratic and the plateau section need to meet at  $x_0$ . Second, the curve should be smooth—that is, the first derivative of the two segments with respect to  $x$  need to coincide at  $x_0$ .

The continuity condition requires that

$$p = E[Y|x_0] = \alpha + \beta x_0 + \gamma x_0^2$$

The smoothness condition requires that

$$\frac{\partial E[Y|x_0]}{\partial x} = \beta + 2\gamma x_0 \equiv 0$$

If you solve for  $x_0$  and substitute into the expression for  $c$ , the two conditions jointly imply that

$$\begin{aligned} x_0 &= -\beta/2\gamma \\ c &= \alpha - \beta^2/4\gamma \end{aligned}$$

Although there are apparently four unknowns, the model contains only three parameters. The continuity and smoothness restrictions together completely determine one parameter given the other three.

The following DATA step creates the SAS data set for this example:

```
data a;
 input y x @@;
 datalines;
.46 1 .47 2 .57 3 .61 4 .62 5 .68 6 .69 7
.78 8 .70 9 .74 10 .77 11 .78 12 .74 13 .80 13
.80 15 .78 16
;
```

The following PROC NLIN statements fit this segmented model:

```
title 'Quadratic Model with Plateau';
proc nlin data=a;
 parms alpha=.45 beta=.05 gamma=-.0025;

 x0 = -.5*beta / gamma;

 if (x < x0) then
 mean = alpha + beta*x + gamma*x*x;
 else mean = alpha + beta*x0 + gamma*x0*x0;
 model y = mean;

 if _obs_=1 and _iter_ =. then do;
 plateau =alpha + beta*x0 + gamma*x0*x0;
 put / x0= plateau= ;
 end;
 output out=b predicted=yp;
run;
```

The parameters of the model are  $\alpha$ ,  $\beta$ , and  $\gamma$ , respectively. They are represented in the PROC NLIN statements by the variables alpha, beta, and gamma, respectively. In order to model the two segments, a conditional statement is used that assigns the appropriate expression to the mean function depending on the value of  $x_0$ . A PUT statement is used to print the constrained parameters every time the program is executed for the first observation. The OUTPUT statement computes predicted values for plotting and saves them to data set b.

Note that there are other ways in which you can write the conditional expressions for this model. For example, you could formulate a condition with two model statements, as follows:

```
proc nlin data=a;
 parms alpha=.45 beta=.05 gamma=-.0025;
 x0 = -.5*beta / gamma;
 if (x < x0) then
 model y = alpha+beta*x+gamma*x*x;
 else model y = alpha+beta*x0+gamma*x0*x0;
run;
```

Or you could use a single expression with a conditional evaluation, as in the following statements:

```
proc nlin data=a;
 parms alpha=.45 beta=.05 gamma=-.0025;
 x0 = -.5*beta / gamma;
 model y = (x <x0)*(alpha+beta*x +gamma*x*x) +
 (x>=x0)*(alpha+beta*x0+gamma*x0*x0);
run;
```

The results from fitting this model with PROC NLIN are shown in [Output 63.1.1–Output 63.1.3](#). The iterative optimization converges after six iterations ([Output 63.1.1](#)). [Output 63.1.1](#) indicates that the join point is 12.747 and the plateau value is 0.777.

**Output 63.1.1** Nonlinear Least-Squares Iterative Phase

| Quadratic Model with Plateau |        |        |          |                |
|------------------------------|--------|--------|----------|----------------|
| The NLIN Procedure           |        |        |          |                |
| Dependent Variable y         |        |        |          |                |
| Method: Gauss-Newton         |        |        |          |                |
| Iterative Phase              |        |        |          |                |
| Iter                         | alpha  | beta   | gamma    | Sum of Squares |
| 0                            | 0.4500 | 0.0500 | -0.00250 | 0.0562         |
| 1                            | 0.3881 | 0.0616 | -0.00234 | 0.0118         |
| 2                            | 0.3930 | 0.0601 | -0.00234 | 0.0101         |
| 3                            | 0.3922 | 0.0604 | -0.00237 | 0.0101         |
| 4                            | 0.3921 | 0.0605 | -0.00237 | 0.0101         |
| 5                            | 0.3921 | 0.0605 | -0.00237 | 0.0101         |
| 6                            | 0.3921 | 0.0605 | -0.00237 | 0.0101         |

NOTE: Convergence criterion met.



**Output 63.1.2** Results from Put Statement

```
x0=12.747669162 plateau=0.7774974276
```

**Output 63.1.3** Least-Squares Analysis for the Quadratic Model

| Source          | DF | Sum of Squares | Mean Square | F Value | Approx Pr > F |
|-----------------|----|----------------|-------------|---------|---------------|
| Model           | 2  | 0.1769         | 0.0884      | 114.22  | <.0001        |
| Error           | 13 | 0.0101         | 0.000774    |         |               |
| Corrected Total | 15 | 0.1869         |             |         |               |

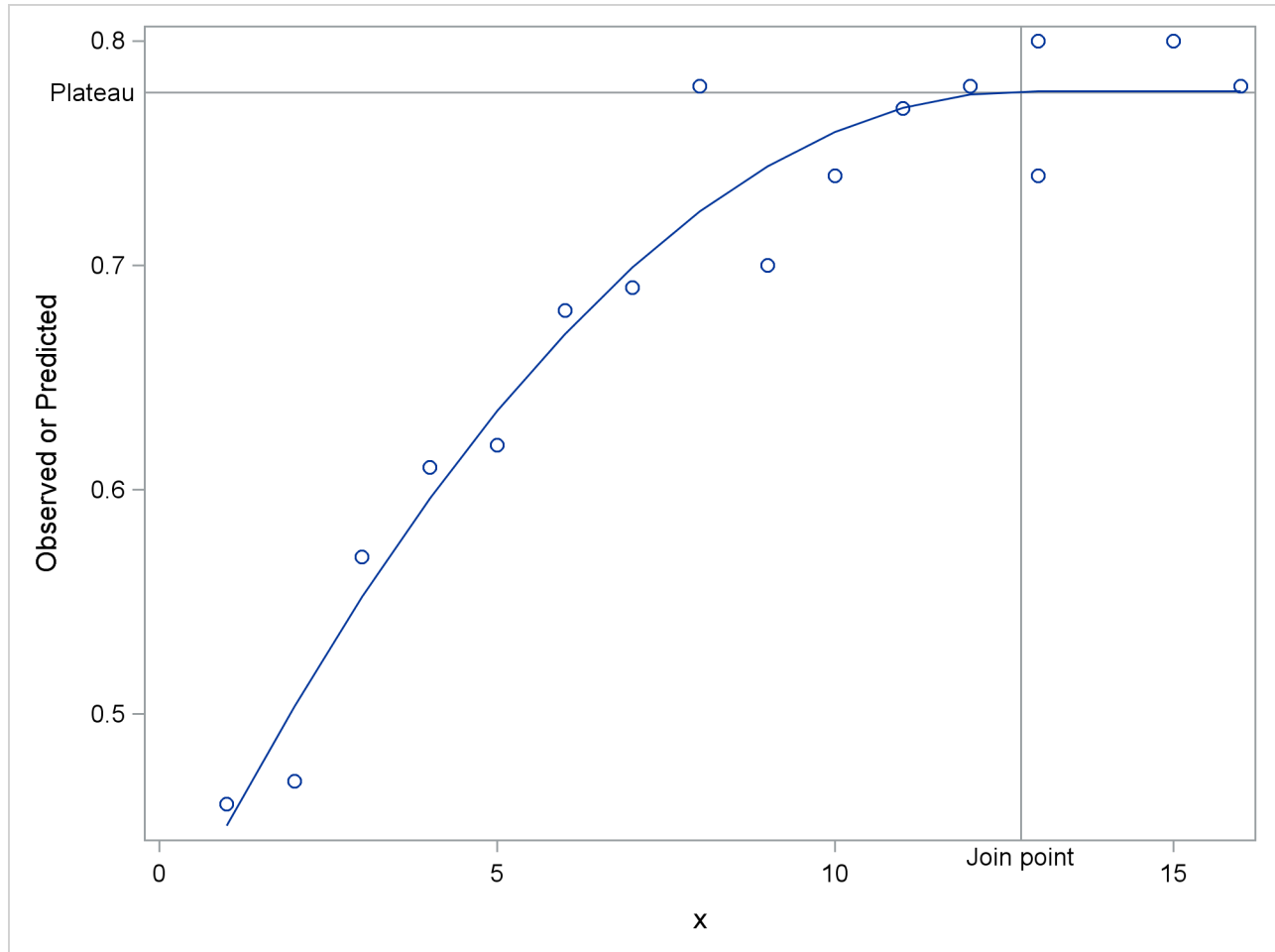
  

| Parameter | Estimate | Approx Std Error | Approximate 95% Confidence Limits |          |
|-----------|----------|------------------|-----------------------------------|----------|
| alpha     | 0.3921   | 0.0267           | 0.3345                            | 0.4497   |
| beta      | 0.0605   | 0.00842          | 0.0423                            | 0.0787   |
| gamma     | -0.00237 | 0.000551         | -0.00356                          | -0.00118 |

The following statements produce a graph of the observed and predicted values with reference lines for the join point and plateau estimates ([Output 63.1.4](#)):

```
proc sgplot data=b noautolegend;
 yaxis label='Observed or Predicted';
 refline 0.777 / axis=y label="Plateau" labelpos=min;
 refline 12.747 / axis=x label="Join point" labelpos=min;
 scatter y=y x=x;
 series y=yp x=x;
run;
```

**Output 63.1.4** Observed and Predicted Values for the Quadratic Model



If you want to estimate the join point directly, you can use the relationship between the parameters to change the parameterization of the model in such a way that the mean function depends directly on  $x_0$ . Using the smoothness condition that relates  $x_0$  to  $\gamma$ ,

$$x_0 = -\beta/2\gamma$$

you can express  $\gamma$  as a function of  $\beta$  and  $x_0$ :

$$\gamma = -\beta/(2x_0)$$

Substituting for  $\gamma$  in the model equation

$$E[Y|x] = \begin{cases} \alpha + \beta x + \gamma x^2 & \text{if } x < x_0 \\ \alpha - \beta^2/(4\gamma) & \text{if } x \geq x_0 \end{cases}$$

yields the reparameterized model

$$E[Y|x] = \begin{cases} \alpha + \beta x(1 - x/(2x_0)) & \text{if } x < x_0 \\ \alpha + \beta x_0/2 & \text{if } x \geq x_0 \end{cases}$$

This model is fit with the following PROC NLIN statements:

```

proc nlin data=a;
 parms alpha=.45 beta=.05 x0=10;
 if (x<x0) then
 mean = alpha + beta*x *(1-x/(2*x0));
 else mean = alpha + beta*x0/2;
 model y = mean;
run;

```

**Output 63.1.5** Results from Reparameterized Model

| The NLIN Procedure               |          |                  |                                   |         |               |
|----------------------------------|----------|------------------|-----------------------------------|---------|---------------|
| Dependent Variable y             |          |                  |                                   |         |               |
| Method: Gauss-Newton             |          |                  |                                   |         |               |
| NOTE: Convergence criterion met. |          |                  |                                   |         |               |
| Source                           | DF       | Sum of Squares   | Mean Square                       | F Value | Approx Pr > F |
| Model                            | 2        | 0.1769           | 0.0884                            | 114.22  | <.0001        |
| Error                            | 13       | 0.0101           | 0.000774                          |         |               |
| Corrected Total                  | 15       | 0.1869           |                                   |         |               |
| Parameter                        | Estimate | Approx Std Error | Approximate 95% Confidence Limits |         |               |
| alpha                            | 0.3921   | 0.0267           | 0.3345                            | 0.4497  |               |
| beta                             | 0.0605   | 0.00842          | 0.0423                            | 0.0787  |               |
| x0                               | 12.7477  | 1.2781           | 9.9864                            | 15.5089 |               |

The analysis of variance table in the reparameterized model is the same as in the earlier analysis (compare [Output 63.1.5](#) and [Output 63.1.3](#)). Changing the parameterization of a model does not affect the fit. The “Parameter Estimates” table now shows  $x_0$  as a parameter in the model. The estimate agrees with the earlier result that uses the PUT statement ([Output 63.1.2](#)). Since  $x_0$  is now a model parameter, the NLIN procedure also reports its asymptotic standard error and its approximate 95% confidence interval.

## Example 63.2: Iteratively Reweighted Least Squares

With the NLIN procedure you can perform weighted nonlinear least squares regression in situations where the weights are functions of the parameters. To minimize a weighted sum of squares, you assign an expression to the `_WEIGHT_` variable in your PROC NLIN statements. When the `_WEIGHT_` variable depends on the model parameters, the estimation technique is known as iteratively reweighted least squares (IRLS). In this situation you should employ the `NOHALVE` option in the PROC NLIN statement. Because the weights change from iteration to iteration, it is not reasonable to expect the *weighted* residual sum of squares to decrease between iterations. The `NOHALVE` option removes that restriction.

Examples where IRLS estimation is used include robust regression via M-estimation (Huber 1964, 1973), generalized linear models (McCullagh and Nelder 1989), and semivariogram fitting in spatial statistics (Schabenberger and Pierce 2002, Sect. 9.2). There are dedicated SAS/STAT procedures for robust regression (the ROBUSTREG procedure) and generalized linear models (the GENMOD and GLIMMIX procedures). Examples of weighted least squares fitting of a semivariogram function can be found in Chapter 102, “The VARIOGRAM Procedure.”

In this example we show an application of PROC NLIN for M-estimation only to illustrate the connection between robust regression and weighted least squares. The ROBUSTREG procedure is the appropriate tool to fit these models with SAS/STAT software.

M-estimation was introduced by Huber (1964, 1973) to estimate location parameters robustly. Beaton and Tukey (1974) applied the idea of M-estimation in regression models and introduced the biweight (or bisquare) weight function. See Holland and Welsch (1977) for this and other robust methods. Consider a linear regression model of the form

$$E[Y_i|x] = \mathbf{x}'_i \boldsymbol{\beta} + \epsilon_i$$

In weighted least squares estimation you seek the parameters  $\hat{\boldsymbol{\beta}}$  that minimize

$$\sum_{i=1}^n w_i (y_i - \mathbf{x}'_i \boldsymbol{\beta})^2 = \sum_{i=1}^n w_i e_i^2$$

where  $w_i$  is the weight associated with the  $i$ th observation. The *normal* equations of this minimization problem can be written as

$$\sum_{i=1}^n w_i e_i \mathbf{x}_i = \mathbf{0}$$

In M-estimation the corresponding equations take on the form

$$\sum_{i=1}^n \psi(e_i) \mathbf{x}_i = \mathbf{0}$$

where  $\psi(\cdot)$  is a weighing function. The Beaton-Tukey biweight, for example, can be written as

$$\psi(e_i) = \begin{cases} e_i \left(1 - \left(\frac{e_i}{\sigma k}\right)^2\right)^2 & |e_i/\sigma| \leq k \\ 0 & |e_i/\sigma| > k \end{cases}$$

Substitution into the estimating equation for M-estimation yields weighted least squares equations

$$\sum_{i=1}^n \psi(e_i) \mathbf{x}_i = \sum_{i=1}^n w_i e_i \mathbf{x}_i = \mathbf{0}$$

$$w_i = \begin{cases} \left(1 - \left(\frac{e_i}{\sigma k}\right)^2\right)^2 & |e_i/\sigma| \leq k \\ 0 & |e_i/\sigma| > k \end{cases}$$

The biweight function involves two constants,  $\sigma$  and  $k$ . The scale  $\sigma$  can be fixed or estimated from the fit in the previous iteration. If  $\sigma$  is estimated, a robust estimator of scale is typically used. In this example  $\sigma$  is fixed at 2. A common value for the constant  $k$  is  $k = 4.685$ .

The following DATA step creates a SAS data set of the population of the United States (in millions), recorded at 10-year intervals starting in 1790 and ending in 1990. The aim is to fit a quadratic linear model to the population over time.

```

title 'U.S. Population Growth';
data uspop;
 input pop :6.3 @@;
 retain year 1780;
 year = year+10;
 yearsq = year*year;
 datalines;
3929 5308 7239 9638 12866 17069 23191 31443 39818 50155
62947 75994 91972 105710 122775 131669 151325 179323 203211
226542 248710
;

```

The PROC NLIN code that follows fits this linear model by M-estimation and IRLS. The weight function is set to a zero or nonzero value depending on the value of the scaled residual. The **NOHALVE** option removes the requirement that the (weighted) residual sum of squares must decrease between iterations.

```

title 'Beaton/Tukey Biweight Robust Regression using IRLS';
proc nlin data=uspop nohalve;
 parms b0=20450.43 b1=-22.7806 b2=.0063456;
 model pop=b0+b1*year+b2*year*year;
 resid = pop-model.pop;
 sigma = 2;
 k = 4.685;
 if abs(resid/sigma)<=k then _weight_=(1-(resid / (sigma*k))**2)**2;
 else _weight_=0;
 output out=c r=rbi;
run;

```

Parameter estimates from this fit are shown in [Output 63.2.1](#), and the computed weights at the final iteration are displayed in [Output 63.2.2](#). The observations for 1940 and 1950 are highly discounted because of their large residuals.

**Output 63.2.1** Nonlinear Least-Squares Analysis

| Beaton/Tukey Biweight Robust Regression using IRLS |    |                |             |         |               |
|----------------------------------------------------|----|----------------|-------------|---------|---------------|
| The NLIN Procedure                                 |    |                |             |         |               |
| Source                                             | DF | Sum of Squares | Mean Square | F Value | Approx Pr > F |
| Model                                              | 2  | 113564         | 56782.0     | 49454.5 | <.0001        |
| Error                                              | 18 | 20.6670        | 1.1482      |         |               |
| Corrected Total                                    | 20 | 113585         |             |         |               |

| Parameter | Estimate | Approx Std Error | Approximate 95% Confidence Limits |          |
|-----------|----------|------------------|-----------------------------------|----------|
| b0        | 20828.7  | 259.4            | 20283.8                           | 21373.6  |
| b1        | -23.2004 | 0.2746           | -23.7773                          | -22.6235 |
| b2        | 0.00646  | 0.000073         | 0.00631                           | 0.00661  |

**Output 63.2.2** Listing of Computed Weights from PROC NLIN

| Obs | pop     | year | yearsq  | rbi      | sigma | k     | _weight_ |
|-----|---------|------|---------|----------|-------|-------|----------|
| 1   | 3.929   | 1790 | 3204100 | -0.93711 | 2     | 4.685 | 0.98010  |
| 2   | 5.308   | 1800 | 3240000 | 0.46091  | 2     | 4.685 | 0.99517  |
| 3   | 7.239   | 1810 | 3276100 | 1.11853  | 2     | 4.685 | 0.97170  |
| 4   | 9.638   | 1820 | 3312400 | 0.95176  | 2     | 4.685 | 0.97947  |
| 5   | 12.866  | 1830 | 3348900 | 0.32159  | 2     | 4.685 | 0.99765  |
| 6   | 17.069  | 1840 | 3385600 | -0.62597 | 2     | 4.685 | 0.99109  |
| 7   | 23.191  | 1850 | 3422500 | -0.94692 | 2     | 4.685 | 0.97968  |
| 8   | 31.443  | 1860 | 3459600 | -0.43027 | 2     | 4.685 | 0.99579  |
| 9   | 39.818  | 1870 | 3496900 | -1.08302 | 2     | 4.685 | 0.97346  |
| 10  | 50.155  | 1880 | 3534400 | -1.06615 | 2     | 4.685 | 0.97427  |
| 11  | 62.947  | 1890 | 3572100 | 0.11332  | 2     | 4.685 | 0.99971  |
| 12  | 75.994  | 1900 | 3610000 | 0.25539  | 2     | 4.685 | 0.99851  |
| 13  | 91.972  | 1910 | 3648100 | 2.03607  | 2     | 4.685 | 0.90779  |
| 14  | 105.710 | 1920 | 3686400 | 0.28436  | 2     | 4.685 | 0.99816  |
| 15  | 122.775 | 1930 | 3724900 | 0.56725  | 2     | 4.685 | 0.99268  |
| 16  | 131.669 | 1940 | 3763600 | -8.61325 | 2     | 4.685 | 0.02403  |
| 17  | 151.325 | 1950 | 3802500 | -8.32415 | 2     | 4.685 | 0.04443  |
| 18  | 179.323 | 1960 | 3841600 | -0.98543 | 2     | 4.685 | 0.97800  |
| 19  | 203.211 | 1970 | 3880900 | 0.95088  | 2     | 4.685 | 0.97951  |
| 20  | 226.542 | 1980 | 3920400 | 1.03780  | 2     | 4.685 | 0.97562  |
| 21  | 248.710 | 1990 | 3960100 | -1.33067 | 2     | 4.685 | 0.96007  |

You can obtain this analysis more conveniently with PROC ROBUSTREG. The procedure re-estimates the scale parameter robustly between iterations. To obtain an analysis with a fixed scale parameter as in this example, use the following PROC ROBUSTREG statements:

```

proc robustreg data=uspop method=m(scale=2);
 model pop = year year*year;
 output out=weights weight=w;
run;

proc print data=weights;
run;

```

Note that the computation of standard errors in the ROBUSTREG procedure is different from the calculations in the NLIN procedure.

---

### Example 63.3: Probit Model with Likelihood Function

The data in this example, taken from Lee (1974), consist of patient characteristics and a variable indicating whether cancer remission occurred. This example demonstrates how to use PROC NLIN with a likelihood function. In this case, twice the negative of the log-likelihood function is to be minimized. This is the objective function for the analysis:

$$-2 \log L = -2 \sum_{i=1}^n \log \{ \pi_i(y_i, \mathbf{x}_i) \}$$

In this expression,  $\pi_i$  denotes the success probability of the  $n$  Bernoulli trials, and  $\log L$  is the log likelihood of  $n$  independent binary (Bernoulli) observations. The probability  $\pi_i$  depends on the observations through the linear predictor  $\eta_i$ ,

$$\pi_i(y_i, \mathbf{x}_i) = \begin{cases} 1 - \Phi(\eta_i) & y_i = 1 \\ \Phi(\eta_i) & y_i = 0 \end{cases}$$

The linear predictor takes the form of a regression equation that is linear in the parameters,

$$\eta_i = \beta_0 + \beta_1 z_{1i} + \beta_2 z_{2i} + \cdots + \beta_k z_{ki} = \mathbf{z}_i \boldsymbol{\beta}$$

Despite this linearity of  $\eta$  in the  $z$  variables, the probit model is nonlinear, because the linear predictor appears inside the nonlinear probit function.

In order to use the NLIN procedure to minimize the function, the estimation problem must be cast in terms of a nonlinear least squares problem with objective function

$$\sum_{i=1}^n (y_i - f(\boldsymbol{\beta}, \mathbf{z}'_i))^2$$

This can be accomplished by setting  $y_i = 0$  and  $f(\boldsymbol{\beta}, \mathbf{z}'_i) = \sqrt{-2 \log \{ \pi_i \}}$ . Because  $0 \leq \pi \leq 1$ , the function  $-2 \log \{ \pi_i \}$  is strictly positive and the square root can be taken safely.

The following DATA step creates the data for the probit analysis. The variable like is created in the DATA step, and it contains the value 0 throughout. This variable serves as the “dummy” response variable in the PROC NLIN step. The variable remiss indicates whether cancer remission occurred. It is the binary outcome variable of interest and is used to determine the relevant probability for observation  $i$  as the success or failure probability of a Bernoulli experiment.

```

data remiss;
 input remiss cell smear infil li blast temp;
 label remiss = 'complete remission';
 like = 0;
 label like = 'dummy variable for nlin';
 datalines;
1 0.8 .83 .66 1.9 1.10 .996
1 0.9 .36 .32 1.4 0.74 .992
0 0.8 .88 .70 0.8 0.176 .982
0 1 .87 .87 0.7 1.053 .986
1 0.9 .75 .68 1.3 0.519 .980
0 1 .65 .65 0.6 0.519 .982
1 0.95 .97 .92 1 1.23 .992
0 0.95 .87 .83 1.9 1.354 1.020
0 1 .45 .45 0.8 0.322 .999
0 0.95 .36 .34 0.5 0 1.038
0 0.85 .39 .33 0.7 0.279 .988
0 0.7 .76 .53 1.2 0.146 .982
0 0.8 .46 .37 0.4 0.38 1.006
0 0.2 .39 .08 0.8 0.114 .990
0 1 .90 .90 1.1 1.037 .990
1 1 .84 .84 1.9 2.064 1.020
0 0.65 .42 .27 0.5 0.114 1.014
0 1 .75 .75 1 1.322 1.004
0 0.5 .44 .22 0.6 0.114 .990
1 1 .63 .63 1.1 1.072 .986
0 1 .33 .33 0.4 0.176 1.010
0 0.9 .93 .84 0.6 1.591 1.020
1 1 .58 .58 1 0.531 1.002
0 0.95 .32 .30 1.6 0.886 .988
1 1 .60 .60 1.7 0.964 .990
1 1 .69 .69 0.9 0.398 .986
0 1 .73 .73 0.7 0.398 .986
;

```

The following NLIN statements fit the probit model:

```

proc nlin data=remiss method=newton sigsq=1;
 parms int=-10 a = -2 b = -1 c=6;

 linp = int + a*cell + b*li + c*temp;
 p = probnorm(linp);

 if (remiss = 1) then pi = 1-p;
 else pi = p;

 model.like = sqrt(- 2 * log(pi));
 output out=p p=predict;
run;

```

The assignment to the variable `linp` creates the linear predictor of the generalized linear model,

$$\eta = \beta_0 + \beta_1 \text{cell}_i + \beta_2 \text{li}_i + \beta_3 * \text{temp}_i$$



In this example, the variables cell, li, and temp are used as regressors.

By default, the NLIN procedure computes the covariance matrix of the parameter estimates based on the nonlinear least squares assumption. That is, the procedure computes the estimate of the residual variance as the mean squared error and uses that to multiply the inverse crossproduct matrix or the inverse Hessian matrix. (See the section “Covariance Matrix of Parameter Estimates” on page 5301 for details.) In the probit model, there is no residual variance. In addition, standard errors in maximum likelihood estimation are based on the inverse Hessian matrix. The `METHOD=NEWTON` option in the `PROC NLIN` statement is used to employ the Hessian matrix in computing the covariance matrix of the parameter estimates. The `SIGSQ=1` option replaces the residual variance estimate that PROC NLIN would use by default as a multiplier of the inverse Hessian with the value 1.0.

**Output 63.3.1** shows the results of this analysis. The analysis of variance table shows an apparently strange result. The total sum of squares is zero, and the model sum of squares is negative. Recall that the values of the response variable were set to zero and the mean function was constructed as  $-2 \log\{\pi_i\}$  in order for the NLIN procedure to minimize a log-likelihood function in terms of a nonlinear least squares problem. The value 21.9002 shown as the “Error” sum of squares is the value of the function  $-2 \log L$ .

**Output 63.3.1** Nonlinear Least-Squares Analysis from PROC NLIN

| The NLIN Procedure                                   |    |                |             |         |               |
|------------------------------------------------------|----|----------------|-------------|---------|---------------|
| NOTE: An intercept was not specified for this model. |    |                |             |         |               |
| Source                                               | DF | Sum of Squares | Mean Square | F Value | Approx Pr > F |
| Model                                                | 4  | -21.9002       | -5.4750     | -5.75   | .             |
| Error                                                | 23 | 21.9002        | 0.9522      |         |               |
| Uncorrected Total                                    | 27 | 0              |             |         |               |

| Parameter | Estimate | Approx Std Error | Approximate 95% Confidence Limits |         |
|-----------|----------|------------------|-----------------------------------|---------|
| int       | -36.7548 | 32.3607          | -103.7                            | 30.1885 |
| a         | -5.6298  | 4.6376           | -15.2235                          | 3.9639  |
| b         | -2.2513  | 0.9790           | -4.2764                           | -0.2262 |
| c         | 45.1815  | 34.9095          | -27.0343                          | 117.4   |

The problem can be more simply solved using dedicated procedures for generalized linear models:

```
proc glimmix data=remiss;
 model remiss = cell li temp / dist=binary link=probit s;
run;

proc genmod data=remiss;
 model remiss = cell li temp / dist=bin link=probit;
run;

proc logistic data=remiss;
 model remiss = cell li temp / link=probit technique=newton;
run;
```

---

### Example 63.4: Affecting Curvature through Parameterization

The work of Ratkowsky (1983, 1990) has brought into focus the importance of close-to-linear behavior of parameters in nonlinear regression models. The curvature in a nonlinear model consists of two components: the intrinsic curvature and the parameter-effects curvature. See the section “[Relative Curvature Measures of Nonlinearity](#)” on page 5287 for details. Intrinsic curvature expresses the degree to which the nonlinear model bends as values of the *parameters* change. This is not the same as the curviness of the model as a function of the covariates (the  $x$  variables). Intrinsic curvature is a function of the type of model you are fitting and the data. This curvature component cannot be affected by reparameterization of the model. According to Ratkowsky (1983), the intrinsic curvature component is typically smaller than the parameter-effects curvature, which can be affected by altering the parameterization of the model.

In models with low curvature, the nonlinear least squares parameter estimators behave similarly to least squares estimators in linear regression models, which have a number of desirable properties. If the model is correct, they are best linear unbiased estimators and are normally distributed if the model errors are normal (otherwise they are asymptotically normal). As you lower the curvature of a nonlinear model, you can expect that the parameter estimators approach the behavior of the linear regression model estimators: they behave “close to linear.”

This example uses a simple data set and a commonly applied model for dose-response relationships to examine how the parameter-effects curvature can be reduced. The statistics by which an estimator’s behavior is judged are Box’s bias (Box 1971) and Hougaard’s measure of skewness (Hougaard 1982, 1985).

The log-logistic model

$$E[Y|x] = \delta + \frac{\alpha - \delta}{1 + \gamma \exp\{\beta \ln(x)\}}$$

is a popular model to express the response  $Y$  as a function of dose  $x$ . The response is bounded between the asymptotes  $\alpha$  and  $\delta$ . The term in the denominator governs the transition between the asymptotes and depends on two parameters,  $\gamma$  and  $\beta$ . The log-logistic model can be viewed as a member of a broader class of dose-response functions, those relying on *switch-on* or *switch-off* mechanisms (see, for example, Schabenberger and Pierce 2002, sec. 5.8.6). A switch function is usually a monotonic function  $S(x, \boldsymbol{\theta})$  that takes values between 0 and 1. A switch-on function increases in  $x$ ; a switch-off function decreases in  $x$ . In the log-logistic case, the function

$$S(x, [\beta, \gamma]) = \frac{1}{1 + \gamma \exp\{\beta \ln(x)\}}$$

is a switch-off function for  $\beta > 0$  and a switch-on function for  $\beta < 0$ . You can write general dose-response functions with asymptotes simply as

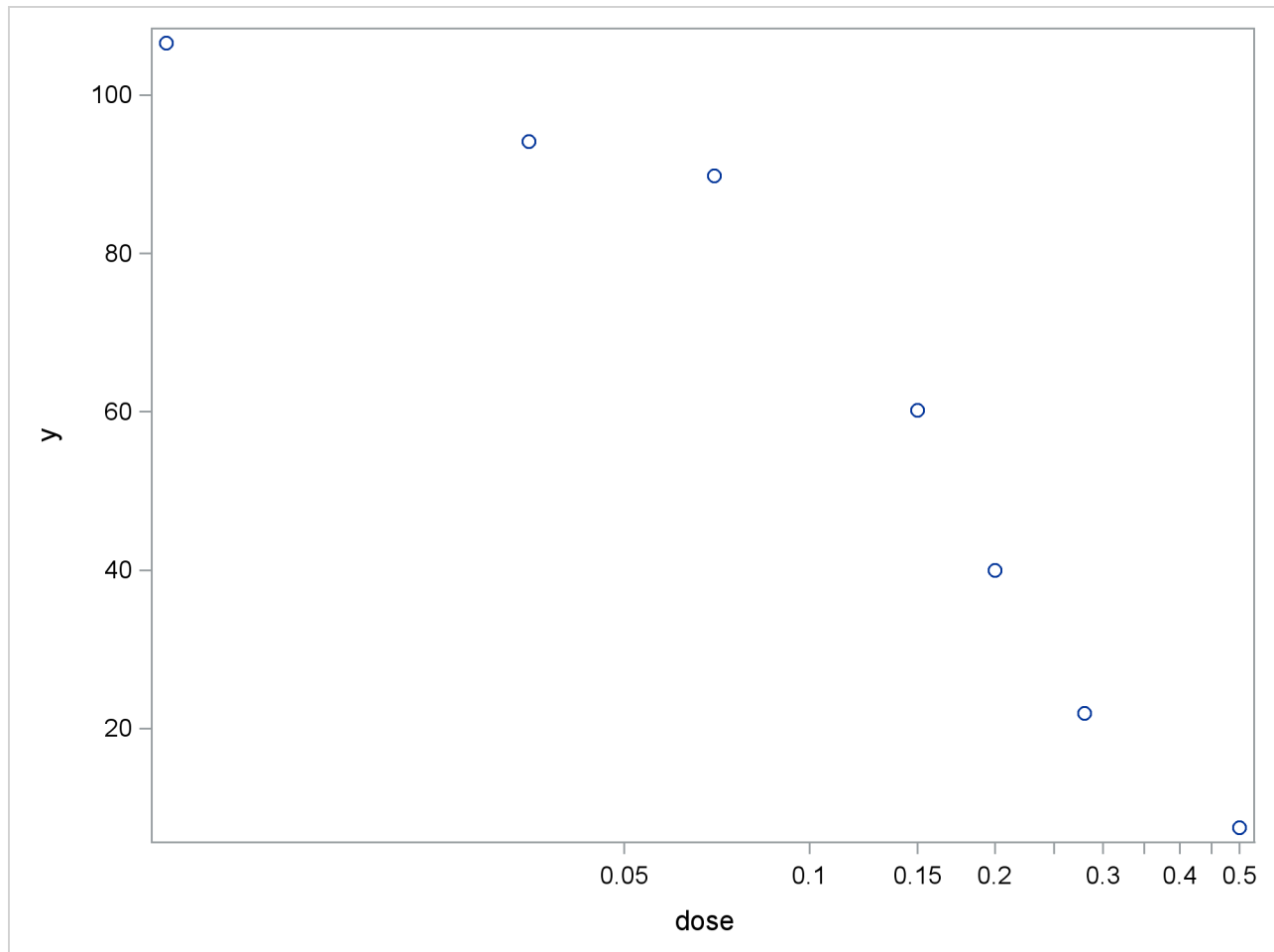
$$E[Y|x] = \mu_{\min} + (\mu_{\max} - \mu_{\min})S(x, \theta)$$

The following DATA step creates a small data set from a dose-response experiment with response y:

```
data logistic;
 input dose y;
 logdose = log(dose);
 datalines;
0.009 106.56
0.035 94.12
0.07 89.76
0.15 60.21
0.20 39.95
0.28 21.88
0.50 7.46
;
```

A graph of these data is produced with the following statements:

```
proc sgplot data=logistic;
 scatter y=y x=dose;
 xaxis type=log logstyle=linear;
run;
```

**Output 63.4.1** Observed Data in Dose-Response Experiment

When dose is expressed on the log scale, the sigmoidal shape of the dose-response relationship is clearly visible (Output 63.4.1). The log-logistic switching model in the preceding parameterization is fit with the following statements in the NLIN procedure:

```
proc nlin data=logistic bias hougaard nlinmeasures;
 parameters alpha=100 beta=3 gamma=300;
 delta = 0;
 Switch = 1/(1+gamma*exp(beta*log(dose)));
 model y = delta + (alpha - delta)*Switch;
run;
```

The lower asymptote  $\delta$  is assumed to be 0 in this case. Since  $\delta$  is not listed in the **PARAMETERS** statement and is assigned a value in the program, it is assumed to be constant. Note that the term **Switch** is the switch-off function in the log-logistic model. The **BIAS** and **HOUGAARD** options in the **PROC NLIN** statement request that Box's bias, percentage bias, and Hougaard's skewness measure be added to the table of parameter estimates, and the **NLINMEASURES** option requests that the global nonlinearity measures be produced.

The NLIN procedure converges after 10 iterations and achieves a residual mean squared error of 15.1869 (Output 63.4.2). This value is not that important by itself, but it is worth noting since this model fit is compared to the fit with other parameterizations later on.

#### Output 63.4.2 Iteration History and Analysis of Variance

| The NLIN Procedure   |       |        |         |                |
|----------------------|-------|--------|---------|----------------|
| Dependent Variable y |       |        |         |                |
| Method: Gauss-Newton |       |        |         |                |
| Iterative Phase      |       |        |         |                |
| Iter                 | alpha | beta   | gamma   | Sum of Squares |
| 0                    | 100.0 | 3.0000 | 300.0   | 386.4          |
| 1                    | 100.4 | 2.8011 | 162.8   | 129.1          |
| 2                    | 100.8 | 2.6184 | 101.4   | 69.2710        |
| 3                    | 101.3 | 2.4266 | 69.7579 | 68.2167        |
| 4                    | 101.7 | 2.3790 | 69.0358 | 60.8223        |
| 5                    | 101.8 | 2.3621 | 67.3709 | 60.7516        |
| 6                    | 101.8 | 2.3582 | 67.0044 | 60.7477        |
| 7                    | 101.8 | 2.3573 | 66.9150 | 60.7475        |
| 8                    | 101.8 | 2.3571 | 66.8948 | 60.7475        |
| 9                    | 101.8 | 2.3570 | 66.8902 | 60.7475        |
| 10                   | 101.8 | 2.3570 | 66.8892 | 60.7475        |

NOTE: Convergence criterion met.

NOTE: An intercept was not specified for this model.

| Source            | DF | Sum of Squares | Mean Square | F Value | Approx Pr > F |
|-------------------|----|----------------|-------------|---------|---------------|
| Model             | 3  | 33965.4        | 11321.8     | 745.50  | <.0001        |
| Error             | 4  | 60.7475        | 15.1869     |         |               |
| Uncorrected Total | 7  | 34026.1        |             |         |               |

The table of parameter estimates displays the estimates of the three model parameters, their approximate standard errors, 95% confidence limits, Hougaard's skewness measure, Box's bias, and percentage bias (Output 63.4.3). Parameters for which the skewness measure is less than 0.1 in absolute value and with percentage bias less than 1% exhibit very close-to-linear behavior, and skewness values less than 0.25 in absolute value indicate reasonably close-to-linear behavior (Ratkowsky 1990). According to these rules, the estimators  $\hat{\beta}$  and  $\hat{\gamma}$  suffer from substantial curvature. The estimator  $\hat{\gamma}$  is especially "far-from-linear." Inferences that involve  $\hat{\gamma}$  and rely on the reported standard errors or confidence limits (or both) for this parameter might be questionable.

**Output 63.4.3** Parameter Estimates, Hougaard’s Skewness, and Box’s Bias

| Parameter | Estimate | Approx Std Error | Approximate 95% Confidence Limits | Skewness | Bias    | Percent Bias |
|-----------|----------|------------------|-----------------------------------|----------|---------|--------------|
| alpha     | 101.8    | 3.0034           | 93.4751 110.2                     | 0.1415   | 0.1512  | 0.15         |
| beta      | 2.3570   | 0.2928           | 1.5440 3.1699                     | 0.4987   | 0.0303  | 1.29         |
| gamma     | 66.8892  | 31.6146          | -20.8870 154.7                    | 1.9200   | 10.9230 | 16.3         |

The related global nonlinearity measures output table (Output 63.4.4) shows that both the maximum and RMS parameter-effects curvature are substantially larger than the critical curvature value recommended by Bates and Watts (1980). In contrast, the intrinsic curvatures of the model are less than the critical value. This implies that most of the nonlinearity can be removed by reparameterization.

**Output 63.4.4** Global Nonlinearity Measures

| Global Nonlinearity Measures    |        |
|---------------------------------|--------|
| Max Intrinsic Curvature         | 0.2397 |
| RMS Intrinsic Curvature         | 0.1154 |
| Max Parameter-Effects Curvature | 4.0842 |
| RMS Parameter-Effects Curvature | 1.8198 |
| Curvature Critical Value        | 0.3895 |
| Raw Residual Variance           | 15.187 |
| Projected Residual Variance     | 5.922  |

One method of reducing the parameter-effects curvature, and thereby reduce the bias and skewness of the parameter estimators, is to replace a parameter with its expected-value parameterization. Schabenberger et al. (1999) and Schabenberger and Pierce (2002, sec. 5.7.2) refer to this method as *reparameterization through defining relationships*. A defining relationship is obtained by equating the mean response at a chosen value of  $x$  (say,  $x^*$ ) to the model:

$$E[Y|x^*] = \delta + \frac{\alpha - \delta}{1 + \gamma \exp\{\beta \ln(x^*)\}}$$

This equation is then solved for a parameter that is subsequently replaced in the original equation. This method is particularly useful if  $x^*$  has an interesting interpretation. For example, let  $\lambda_K$  denote the value that reduces the response by  $K \times 100\%$ ,

$$E[Y|\lambda_K] = \delta + \left(\frac{100 - K}{100}\right)(\alpha - \delta)$$

Because  $\gamma$  exhibits large bias and skewness, it is the target in the first round of reparameterization. Setting the expression for the conditional mean at  $\lambda_K$  equal to the mean function when  $x = \lambda_K$  yields the following expression:

$$\delta + \left(\frac{100 - K}{100}\right)(\alpha - \delta) = \delta + \frac{\alpha - \delta}{1 + \gamma \exp\{\beta \ln(\lambda_K)\}}$$

This expression is solved for  $\gamma$ , and the result is substituted back into the model equation. This leads to a log-logistic model in which  $\gamma$  is replaced by the parameter  $\lambda_K$ , the dose at which the response was reduced by  $K \times 100\%$ . The new model equation is

$$E[Y|x] = \delta + \frac{\alpha - \delta}{1 + K/(100 - K) \exp\{\beta \ln(x/\lambda_K)\}}$$

A particularly interesting choice is  $K = 50$ , since  $\lambda_{50}$  is the dose at which the response is halved. In studies of mortality, this concentration is also known as the LD50. For the special case of  $\lambda_{50}$  the model equation becomes

$$E[Y|x] = \delta + \frac{\alpha - \delta}{1 + \exp\{\beta \ln(x/\lambda_{50})\}}$$

You can fit the model in the LD50 parameterization with the following statements:

```
proc nlin data=logistic bias hougard;
 parameters alpha=100 beta=3 LD50=0.15;
 delta = 0;
 Switch = 1/(1+exp(beta*log(dose/LD50)));
 model y = delta + (alpha - delta)*Switch;
 output out=nlinout pred=p lcl=lcl ucl=ucl;
run;
```

Partial results from this NLIN run are shown in [Output 63.4.5](#). The analysis of variance tables in [Output 63.4.2](#) and [Output 63.4.5](#) are identical. Changing the parameterization of a model does not affect the model fit. It does, however, affect the interpretation of the parameters and the statistical properties (close-to-linear behavior) of the parameter estimators. The skewness and bias measures of the parameter LD50 is considerably reduced compared to those values for the parameter  $\gamma$  in the previous parameterization. Also,  $\gamma$  has been replaced by a parameter with a useful interpretation, the dose that yields a 50% reduction in mean response. Also notice that the bias and skewness measures of  $\alpha$  and  $\beta$  are not affected by the  $\gamma \rightarrow$  LD50 reparameterization.

**Output 63.4.5** ANOVA Table and Parameter Estimates in LD50 Parameterization

| The NLIN Procedure                                   |    |                |             |         |               |
|------------------------------------------------------|----|----------------|-------------|---------|---------------|
| Dependent Variable y                                 |    |                |             |         |               |
| Method: Gauss-Newton                                 |    |                |             |         |               |
| NOTE: Convergence criterion met.                     |    |                |             |         |               |
| NOTE: An intercept was not specified for this model. |    |                |             |         |               |
| Source                                               | DF | Sum of Squares | Mean Square | F Value | Approx Pr > F |
| Model                                                | 3  | 33965.4        | 11321.8     | 745.50  | <.0001        |
| Error                                                | 4  | 60.7475        | 15.1869     |         |               |
| Uncorrected Total                                    | 7  | 34026.1        |             |         |               |

## Output 63.4.5 continued

| Parameter | Estimate | Approx Std Error | Approximate 95% Confidence Limits | Skewness | Bias     | Percent Bias |
|-----------|----------|------------------|-----------------------------------|----------|----------|--------------|
| alpha     | 101.8    | 3.0034           | 93.4752 110.2                     | 0.1415   | 0.1512   | 0.15         |
| beta      | 2.3570   | 0.2928           | 1.5440 3.1699                     | 0.4987   | 0.0303   | 1.29         |
| LD50      | 0.1681   | 0.00915          | 0.1427 0.1935                     | -0.0605  | -0.00013 | -0.08        |

To reduce the parameter-effects curvature of the  $\beta$  parameter, you can use the technique of defining relationships again. This can be done generically, by solving

$$\mu^* = \delta + \frac{\alpha - \delta}{1 + \exp\{\beta \ln(x/\lambda)\}}$$

for  $\beta$ , treating  $\mu^*$  as the new parameter (in lieu of  $\beta$ ), and choosing a value for  $x^*$  that leads to low skewness. This results in the expected-value parameterization of  $\beta$ . Solving for  $\beta$  yields

$$\beta = \frac{\log\left(\frac{\alpha - \mu^*}{\mu^* - \delta}\right)}{\log(x^*/\lambda)}$$

The interpretation of the parameter  $\mu^*$  that replaces  $\beta$  in the model equation is simple: it is the mean dose response when the dose is  $x^*$ . Fixing  $x^* = 0.3$ , the following PROC NLIN statements fit this model:

```
proc nlin data=logistic bias hougaard nlinmeasures;
 parameters alpha=100 mustar=20 LD50=0.15;
 delta = 0;
 xstar = 0.3;
 beta = log((alpha - mustar)/(mustar - delta)) / log(xstar/LD50);
 Switch = 1/(1+exp(beta*log(dose/LD50)));
 model y = delta + (alpha - delta)*Switch;
 output out=nlinout pred=p lcl=lcl ucl=ucl;
run;
```

Note that the switch-off function continues to be written in terms of  $\beta$  and the LD50. The only difference from the previous model is that  $\beta$  is now expressed as a function of the parameter  $\mu^*$ . Using expected-value parameterizations is a simple mechanism to lower the curvature in a model and to arrive at starting values. The starting value for  $\mu^*$  can be gleaned from [Output 63.4.1](#) at  $x = 0.3$ .

[Output 63.4.6](#) shows selected results from this NLIN run. The ANOVA table is again unaffected by the change in parameterization. The skewness for  $\mu^*$  is significantly reduced in comparison to those of the  $\beta$  parameter in the previous model (compare [Output 63.4.6](#) and [Output 63.4.5](#)), while its bias remains on the same scale from [Output 63.4.5](#) to [Output 63.4.6](#). Also note the substantial reduction in the parameter-effects curvature values. As expected, the intrinsic curvature values remain intact.



**Output 63.4.6** ANOVA Table and Parameter Estimates in Expected-Value Parameterization

| The NLIN Procedure                                   |          |                  |                                   |         |               |          |              |
|------------------------------------------------------|----------|------------------|-----------------------------------|---------|---------------|----------|--------------|
| Dependent Variable y                                 |          |                  |                                   |         |               |          |              |
| Method: Gauss-Newton                                 |          |                  |                                   |         |               |          |              |
| NOTE: Convergence criterion met.                     |          |                  |                                   |         |               |          |              |
| NOTE: An intercept was not specified for this model. |          |                  |                                   |         |               |          |              |
| Source                                               | DF       | Sum of Squares   | Mean Square                       | F Value | Approx Pr > F |          |              |
| Model                                                | 3        | 33965.4          | 11321.8                           | 745.50  | <.0001        |          |              |
| Error                                                | 4        | 60.7475          | 15.1869                           |         |               |          |              |
| Uncorrected Total                                    | 7        | 34026.1          |                                   |         |               |          |              |
| Parameter                                            | Estimate | Approx Std Error | Approximate 95% Confidence Limits |         | Skewness      | Bias     | Percent Bias |
| alpha                                                | 101.8    | 3.0034           | 93.4752                           | 110.2   | 0.1415        | 0.1512   | 0.15         |
| mustar                                               | 20.7073  | 2.6430           | 13.3693                           | 28.0454 | -0.0572       | -0.0983  | -0.47        |
| LD50                                                 | 0.1681   | 0.00915          | 0.1427                            | 0.1935  | -0.0605       | -0.00013 | -0.08        |
| Global Nonlinearity Measures                         |          |                  |                                   |         |               |          |              |
| Max Intrinsic Curvature                              |          |                  |                                   |         | 0.2397        |          |              |
| RMS Intrinsic Curvature                              |          |                  |                                   |         | 0.1154        |          |              |
| Max Parameter-Effects Curvature                      |          |                  |                                   |         | 0.2925        |          |              |
| RMS Parameter-Effects Curvature                      |          |                  |                                   |         | 0.1500        |          |              |
| Curvature Critical Value                             |          |                  |                                   |         | 0.3895        |          |              |
| Raw Residual Variance                                |          |                  |                                   |         | 15.187        |          |              |
| Projected Residual Variance                          |          |                  |                                   |         | 5.9219        |          |              |

**Example 63.5: Comparing Nonlinear Trends among Groups**

When you model nonlinear trends in the presence of group (classification) variables, two questions often arise: whether the trends should be varied by group, and how to decide which parameters should be varied across groups. A large battery of tools is available on linear statistical models to test hypotheses involving the model parameters, especially to test linear hypotheses. To test similar hypotheses in nonlinear models, you can draw on analogous tools. Especially important in this regard are comparisons of nested models by contrasting their residual sums of squares.

In this example, a two-group model from a pharmacokinetic application is fit to data that are in part based on the theophylline data from Pinheiro and Bates (1995) and the first example in the documentation for the NLMIXED procedure. In a pharmacokinetic application you study how a drug is dispersed through a living organism. The following data represent concentrations of the drug theophylline over a 25-hour period following oral administration. The data are derived by collapsing and averaging the subject-specific data from Pinheiro and Bates (1995) in a particular, yet unimportant, way. The purpose of arranging the data in this way is purely to demonstrate the methodology.

```

data theop;
 input time dose conc @@;
 if (dose = 4) then group=1; else group=2;
 datalines;
0.00 4 0.1633 0.25 4 2.045
0.27 4 4.4 0.30 4 7.37
0.35 4 1.89 0.37 4 2.89
0.50 4 3.96 0.57 4 6.57
0.58 4 6.9 0.60 4 4.6
0.63 4 9.03 0.77 4 5.22
1.00 4 7.82 1.02 4 7.305
1.05 4 7.14 1.07 4 8.6
1.12 4 10.5 2.00 4 9.72
2.02 4 7.93 2.05 4 7.83
2.13 4 8.38 3.50 4 7.54
3.52 4 9.75 3.53 4 5.66
3.55 4 10.21 3.62 4 7.5
3.82 4 8.58 5.02 4 6.275
5.05 4 9.18 5.07 4 8.57
5.08 4 6.2 5.10 4 8.36
7.02 4 5.78 7.03 4 7.47
7.07 4 5.945 7.08 4 8.02
7.17 4 4.24 8.80 4 4.11
9.00 4 4.9 9.02 4 5.33
9.03 4 6.11 9.05 4 6.89
9.38 4 7.14 11.60 4 3.16
11.98 4 4.19 12.05 4 4.57
12.10 4 5.68 12.12 4 5.94
12.15 4 3.7 23.70 4 2.42
24.15 4 1.17 24.17 4 1.05
24.37 4 3.28 24.43 4 1.12
24.65 4 1.15 0.00 5 0.025
0.25 5 2.92 0.27 5 1.505
0.30 5 2.02 0.50 5 4.795
0.52 5 5.53 0.58 5 3.08
0.98 5 7.655 1.00 5 9.855
1.02 5 5.02 1.15 5 6.44
1.92 5 8.33 1.98 5 6.81
2.02 5 7.8233 2.03 5 6.32
3.48 5 7.09 3.50 5 7.795
3.53 5 6.59 3.57 5 5.53
3.60 5 5.87 5.00 5 5.8
5.02 5 6.2867 5.05 5 5.88
6.98 5 5.25 7.00 5 4.02
7.02 5 7.09 7.03 5 4.925
7.15 5 4.73 9.00 5 4.47
9.03 5 3.62 9.07 5 4.57
9.10 5 5.9 9.22 5 3.46
12.00 5 3.69 12.05 5 3.53
12.10 5 2.89 12.12 5 2.69
23.85 5 0.92 24.08 5 0.86
24.12 5 1.25 24.22 5 1.15
24.30 5 0.9 24.35 5 1.57

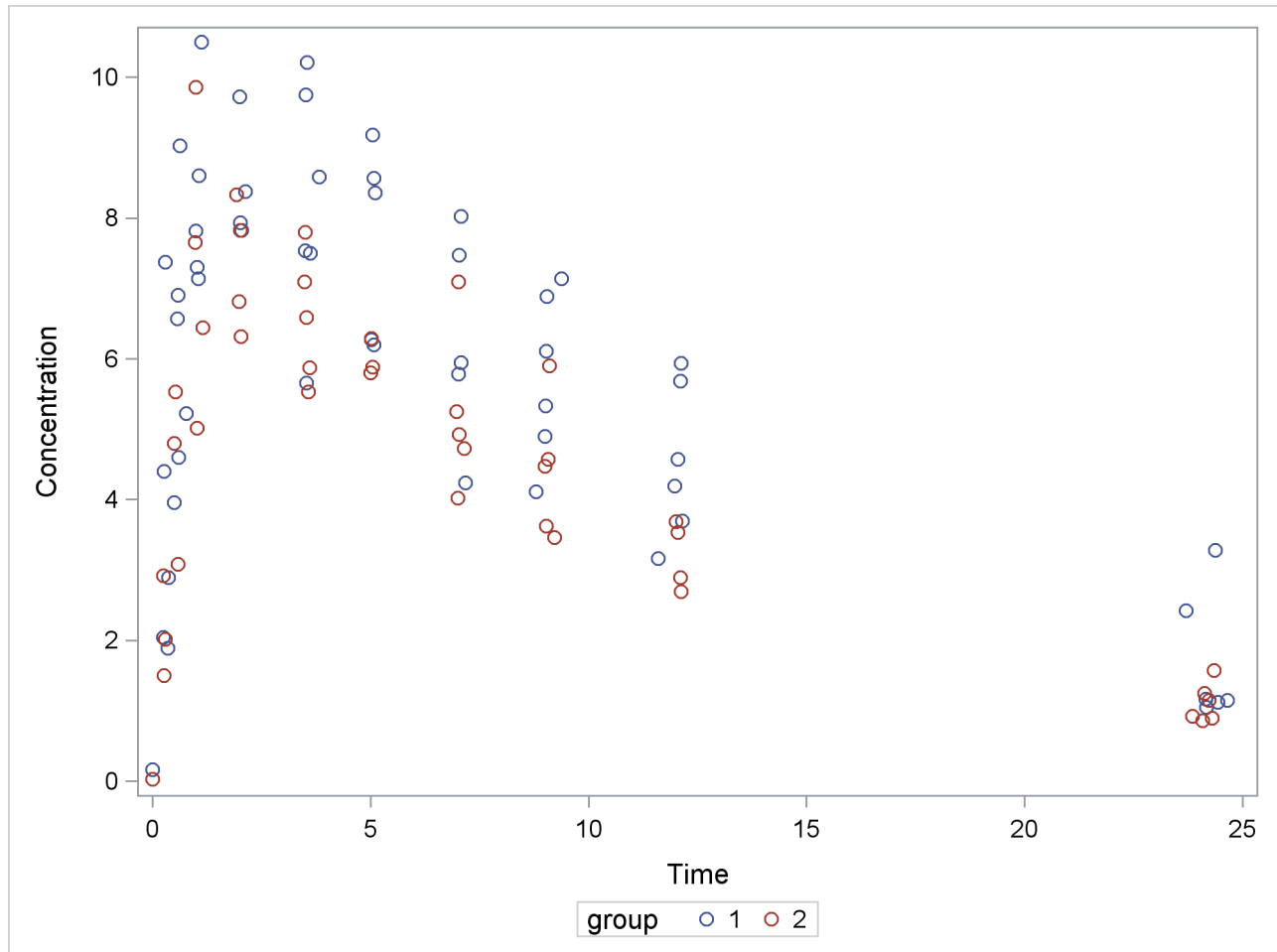
```

;

The following code plots the theophylline concentration data over time for the two groups (Output 63.5.1). In each group the concentration tends to rise sharply right after the drug is administered, followed by a prolonged tapering of the concentration.

```
proc sgplot data=theop;
 scatter x=time y=conc / group=group;
 yaxis label='Concentration';
 xaxis label='Time';
run;
```

**Output 63.5.1** Observed Responses in Two Groups



In the context of nonlinear mixed models, Pinheiro and Bates (1995) consider a first-order compartment model for these data. In terms of two fixed treatment groups, the model can be written as

$$C_{it} = \frac{Dk_{e_i}k_{a_i}}{Cl_i(k_{a_i} - k_{e_i})} [\exp(-k_{e_i}t) - \exp(-k_{a_i}t)] + \epsilon_{it}$$

where  $C_{it}$  is the observed concentration in group  $i$  at time  $t$ ,  $D$  is the dose of theophylline,  $k_{e_i}$  is the elimination rate in group  $i$ ,  $k_{a_i}$  is the absorption rate in group  $i$ ,  $Cl_i$  is the clearance in group  $i$ , and  $\epsilon_{it}$

denotes the model error. Because the rates and the clearance must be positive, you can parameterize the model in terms of log rates and the log clearance:

$$\begin{aligned} Cl_i &= \exp\{\beta_{1i}\} \\ k_{a_i} &= \exp\{\beta_{2i}\} \\ k_{e_i} &= \exp\{\beta_{3i}\} \end{aligned}$$

In this parameterization the model contains six parameters, and the rates and clearance vary by group. This produces two separate response profiles, one for each group. On the other extreme, you could model the trends as if there were no differences among the groups:

$$\begin{aligned} Cl_i &= \exp\{\beta_1\} \\ k_{a_i} &= \exp\{\beta_2\} \\ k_{e_i} &= \exp\{\beta_3\} \end{aligned}$$

In between these two extremes lie other models, such as a model where both groups have the same absorption and elimination rate, but different clearances. The question then becomes how to go about building a model in an organized manner.

To test hypotheses about nested nonlinear models, you can apply the idea of a “Sum of Squares Reduction Test.” A reduced model is nested within a full model if you can impose  $q$  constraints on the full model to obtain the reduced model. Then, if  $SSE_r$  and  $SSE_f$  denote the residual sum of squares in the reduced and the full model, respectively, the test statistic is

$$F_R = \frac{(SSE_r - SSE_f) / q}{SSE_f / (n - p)} = \frac{(SSE_r - SSE_f) / q}{MSE_f}$$

where  $n$  are the number of observations used and  $p$  are the number of parameters in the full model. The numerator of the  $F_R$  statistic is the average reduction in residual sum of squares per constraint. The mean squared error of the full model is used to scale this average because it is less likely to be a biased estimator of the residual variance than the variance estimate from a constrained (reduced) model. The  $F_R$  statistic is then compared against quantiles from an  $F$  distribution with  $q$  numerator and  $n - p$  denominator degrees of freedom. Schabenberger and Pierce (2002) discuss the justification for this test and compare it to other tests in nonlinear models.

In the present application we might phrase the initial question akin to the overall  $F$  test for a factor in a linear model: Should any parameters be varied between the two groups? The corresponding null hypothesis is

$$H: \begin{cases} \beta_{11} = \beta_{12} \\ \beta_{21} = \beta_{22} \\ \beta_{31} = \beta_{32} \end{cases}$$

where the first subscript identifies the type of the parameter and the second subscript identifies the group. Note that this hypothesis implies

$$H: \begin{cases} Cl_1 = Cl_2 \\ k_{a_1} = k_{a_2} \\ k_{e_1} = k_{e_2} \end{cases}$$

If you fail to reject this hypothesis, there is no need to further examine individual parameter differences.

The reduced model—the model subject to the null hypothesis—is fit with the following PROC NLIN statements:

```
proc nlin data=theop;
 parms beta1=-3.22 beta2=0.47 beta3=-2.45;
 c1 = exp(beta1);
 ka = exp(beta2);
 ke = exp(beta3);
 mean = dose*ke*ka*(exp(-ke*time)-exp(-ka*time))/c1/(ka-ke);
 model conc = mean;
 ods output Anova=aovred(rename=(ss=ssred ms=msred df=dfred));
run;
```

The clearance, the rates, and the mean function are formed independently of the group membership. The analysis of variance table is saved to the data set aovred, and some of its variables are renamed. This is done so that the data set can be merged easily with the analysis of variance table for the full model (see following).

The converged model has a residual sum of square of  $SSE_r = 286.4$  and a mean squared error of 3.0142 (Output 63.5.2). The table of parameter estimates gives the values for the estimated log clearance ( $\hat{\beta}_1 = -3.2991$ ), the estimated log absorption rate ( $\hat{\beta}_2 = 0.4769$ ), and the estimated log elimination rate ( $\hat{\beta}_3 = -2.5555$ ).

#### Output 63.5.2 Fit Results for the Reduced Model

| The NLIN Procedure                                   |          |                  |                                   |         |               |
|------------------------------------------------------|----------|------------------|-----------------------------------|---------|---------------|
| Dependent Variable conc                              |          |                  |                                   |         |               |
| Method: Gauss-Newton                                 |          |                  |                                   |         |               |
| NOTE: Convergence criterion met.                     |          |                  |                                   |         |               |
| NOTE: An intercept was not specified for this model. |          |                  |                                   |         |               |
| Source                                               | DF       | Sum of Squares   | Mean Square                       | F Value | Approx Pr > F |
| Model                                                | 3        | 3100.5           | 1033.5                            | 342.87  | <.0001        |
| Error                                                | 95       | 286.4            | 3.0142                            |         |               |
| Uncorrected Total                                    | 98       | 3386.8           |                                   |         |               |
| Parameter                                            | Estimate | Approx Std Error | Approximate 95% Confidence Limits |         |               |
| beta1                                                | -3.2991  | 0.0956           | -3.4888                           | -3.1094 |               |
| beta2                                                | 0.4769   | 0.1640           | 0.1512                            | 0.8025  |               |
| beta3                                                | -2.5555  | 0.1410           | -2.8354                           | -2.2755 |               |

The full model, in which all three parameters are varied by group, can be fit with the following statements in the NLIN procedure:

```
proc nlin data=theop;
 parms beta1_1=-3.22 beta2_1=0.47 beta3_1=-2.45
 beta1_2=-3.22 beta2_2=0.47 beta3_2=-2.45;
 if (group=1) then do;
 c1 = exp(beta1_1);
 ka = exp(beta2_1);
 ke = exp(beta3_1);
 end; else do;
 c1 = exp(beta1_2);
 ka = exp(beta2_2);
 ke = exp(beta3_2);
 end;
 mean = dose*ke*ka*(exp(-ke*time)-exp(-ka*time))/c1/(ka-ke);
 model conc = mean;
 ods output Anova=aovfull;
run;
```

Separate parameters for the groups are now specified in the **PARMS** statement, and the value of the model variables *c1*, *ka*, and *ke* is assigned conditional on the group membership of an observation. Notice that the same expression as in the previous run can be used to model the mean function.

The results from this PROC NLIN run are shown in **Output 63.5.3**. The residual sum of squares in the full model is only  $SSE_f = 138.9$ , compared to  $SSE_r = 286.4$  in the reduced model (**Output 63.5.3**).

**Output 63.5.3** Fit Results for the Full Model

| The NLIN Procedure                                   |          |                  |                                   |         |               |
|------------------------------------------------------|----------|------------------|-----------------------------------|---------|---------------|
| Dependent Variable conc                              |          |                  |                                   |         |               |
| Method: Gauss-Newton                                 |          |                  |                                   |         |               |
| NOTE: Convergence criterion met.                     |          |                  |                                   |         |               |
| NOTE: An intercept was not specified for this model. |          |                  |                                   |         |               |
| Source                                               | DF       | Sum of Squares   | Mean Square                       | F Value | Approx Pr > F |
| Model                                                | 6        | 3247.9           | 541.3                             | 358.56  | <.0001        |
| Error                                                | 92       | 138.9            | 1.5097                            |         |               |
| Uncorrected Total                                    | 98       | 3386.8           |                                   |         |               |
| Parameter                                            | Estimate | Approx Std Error | Approximate 95% Confidence Limits |         |               |
| beta1_1                                              | -3.5671  | 0.0864           | -3.7387                           | -3.3956 |               |
| beta2_1                                              | 0.4421   | 0.1349           | 0.1742                            | 0.7101  |               |
| beta3_1                                              | -2.6230  | 0.1265           | -2.8742                           | -2.3718 |               |
| beta1_2                                              | -3.0111  | 0.1061           | -3.2219                           | -2.8003 |               |
| beta2_2                                              | 0.3977   | 0.1987           | 0.00305                           | 0.7924  |               |
| beta3_2                                              | -2.4442  | 0.1618           | -2.7655                           | -2.1229 |               |

Whether this reduction in sum of squares is sufficient to declare that the full model provides a significantly better fit than the reduced model depends on the number of constraints imposed on the full model and on the variability in the data. In other words, before drawing any conclusions, you have to take into account how many parameters have been dropped from the model and how much variation around the regression trends the data exhibit. The  $F_R$  statistic sets these quantities into relation. The following macro merges the analysis of variance tables from the full and reduced model, and computes  $F_R$  and its  $p$ -value:

```
%macro SSReductionTest;
 data aov; merge aovred aovfull;
 if (Source='Error') then do;
 Fstat = ((SSred-SS)/(dfred-df))/ms;
 pvalue = 1-ProbF(Fstat,dfred-df,df);
 output;
 end;
run;
proc print data=aov label noobs;
 label Fstat = 'F Value'
 pValue = 'Prob > F';
 format pvalue pvalue8.;
 var Fstat pValue;
run;
%mend;
%SSReductionTest;
```

#### Output 63.5.4 F Statistic and P-value for Hypothesis of Equal Trends

|  | F Value | Prob > F |
|--|---------|----------|
|  | 32.5589 | <.000001 |

There is clear evidence that the model with separate trends fits these data significantly better (Output 63.5.4). To decide whether all parameters should be varied between the groups or only one or two of them, we first refit the model in a slightly different parameterization:

```
proc nlin data=theop;
 parms beta1_1=-3.22 beta2_1=0.47 beta3_1=-2.45
 beta1_diff=0 beta2_diff=0 beta3_diff=0;
 if (group=1) then do;
 c1 = exp(beta1_1);
 ka = exp(beta2_1);
 ke = exp(beta3_1);
 end; else do;
 c1 = exp(beta1_1 + beta1_diff);
 ka = exp(beta2_1 + beta2_diff);
 ke = exp(beta3_1 + beta3_diff);
 end;
 mean = dose*ke*ka*(exp(-ke*time)-exp(-ka*time))/c1/(ka-ke);
 model conc = mean;
run;
```

In the preceding statements, the parameters in the second group were expressed using offsets from parameters in the first group. For example, the parameter `beta1_diff` measures the change in log clearance between group 2 and group 1.

This simple reparameterization does not affect the model fit. The analysis of variance tables in [Output 63.5.5](#) and [Output 63.5.3](#) are identical. It does, however, affect the interpretation of the estimated quantities. Since the parameter `beta1_diff` measures the change in the log clearance rates between the groups, you can use the approximate 95% confidence limits in [Output 63.5.5](#) to assess whether that quantity in the pharmacokinetic equation varies between groups. Only the confidence interval for the difference in the log clearances excludes 0. The intervals for `beta2_diff` and `beta3_diff` include 0.

**Output 63.5.5** Fit Results for the Full Model in Difference Parameterization

| The NLIN Procedure                                   |          |                  |                                   |         |               |
|------------------------------------------------------|----------|------------------|-----------------------------------|---------|---------------|
| Dependent Variable conc                              |          |                  |                                   |         |               |
| Method: Gauss-Newton                                 |          |                  |                                   |         |               |
| NOTE: Convergence criterion met.                     |          |                  |                                   |         |               |
| NOTE: An intercept was not specified for this model. |          |                  |                                   |         |               |
| Source                                               | DF       | Sum of Squares   | Mean Square                       | F Value | Approx Pr > F |
| Model                                                | 6        | 3247.9           | 541.3                             | 358.56  | <.0001        |
| Error                                                | 92       | 138.9            | 1.5097                            |         |               |
| Uncorrected Total                                    | 98       | 3386.8           |                                   |         |               |
| Parameter                                            | Estimate | Approx Std Error | Approximate 95% Confidence Limits |         |               |
| <code>beta1_1</code>                                 | -3.5671  | 0.0864           | -3.7387                           | -3.3956 |               |
| <code>beta2_1</code>                                 | 0.4421   | 0.1349           | 0.1742                            | 0.7101  |               |
| <code>beta3_1</code>                                 | -2.6230  | 0.1265           | -2.8742                           | -2.3718 |               |
| <code>beta1_diff</code>                              | 0.5560   | 0.1368           | 0.2842                            | 0.8278  |               |
| <code>beta2_diff</code>                              | -0.0444  | 0.2402           | -0.5214                           | 0.4326  |               |
| <code>beta3_diff</code>                              | 0.1788   | 0.2054           | -0.2291                           | 0.5866  |               |

This suggests as the final model one where the absorption and elimination rates are the same for both groups and only the clearances are varied. The following statements fit this model and perform the sum of squares reduction test:

```
proc nlin data=theop;
 parms beta1_1=-3.22 beta2_1=0.47 beta3_1=-2.45
 beta1_diff=0;
 ka = exp(beta2_1);
 ke = exp(beta3_1);
 if (group=1) then do;
 cl = exp(beta1_1);
 end; else do;
 cl = exp(beta1_1 + beta1_diff);
 end;
 mean = dose*ke*ka*(exp(-ke*time)-exp(-ka*time))/cl/(ka-ke);
 model conc = mean;
 ods output Anova=aovred(rename=(ss=ssred ms=msred df=dfred));
```



```

output out=predvals predicted=p;
run;
%SSReductionTest;

```

The results for this model with common absorption and elimination rates are shown in [Output 63.5.6](#). The sum-of-squares reduction test comparing this model against the full model with six parameters shows—as expected—that the full model does not fit the data significantly better ( $p = 0.6193$ , [Output 63.5.7](#)).

**Output 63.5.6** Fit Results for Model with Common Rates

| The NLIN Procedure                                   |          |                  |                                   |         |               |
|------------------------------------------------------|----------|------------------|-----------------------------------|---------|---------------|
| Dependent Variable conc                              |          |                  |                                   |         |               |
| Method: Gauss-Newton                                 |          |                  |                                   |         |               |
| NOTE: Convergence criterion met.                     |          |                  |                                   |         |               |
| NOTE: An intercept was not specified for this model. |          |                  |                                   |         |               |
| Source                                               | DF       | Sum of Squares   | Mean Square                       | F Value | Approx Pr > F |
| Model                                                | 4        | 3246.5           | 811.6                             | 543.60  | <.0001        |
| Error                                                | 94       | 140.3            | 1.4930                            |         |               |
| Uncorrected Total                                    | 98       | 3386.8           |                                   |         |               |
| Parameter                                            | Estimate | Approx Std Error | Approximate 95% Confidence Limits |         |               |
| beta1_1                                              | -3.5218  | 0.0681           | -3.6570                           | -3.3867 |               |
| beta2_1                                              | 0.4226   | 0.1107           | 0.2028                            | 0.6424  |               |
| beta3_1                                              | -2.5571  | 0.0988           | -2.7532                           | -2.3610 |               |
| beta1_diff                                           | 0.4346   | 0.0454           | 0.3444                            | 0.5248  |               |

**Output 63.5.7** F Statistic and P-value for Hypothesis of Common Rates

| F Value | Prob > F |
|---------|----------|
| 0.48151 | 0.619398 |

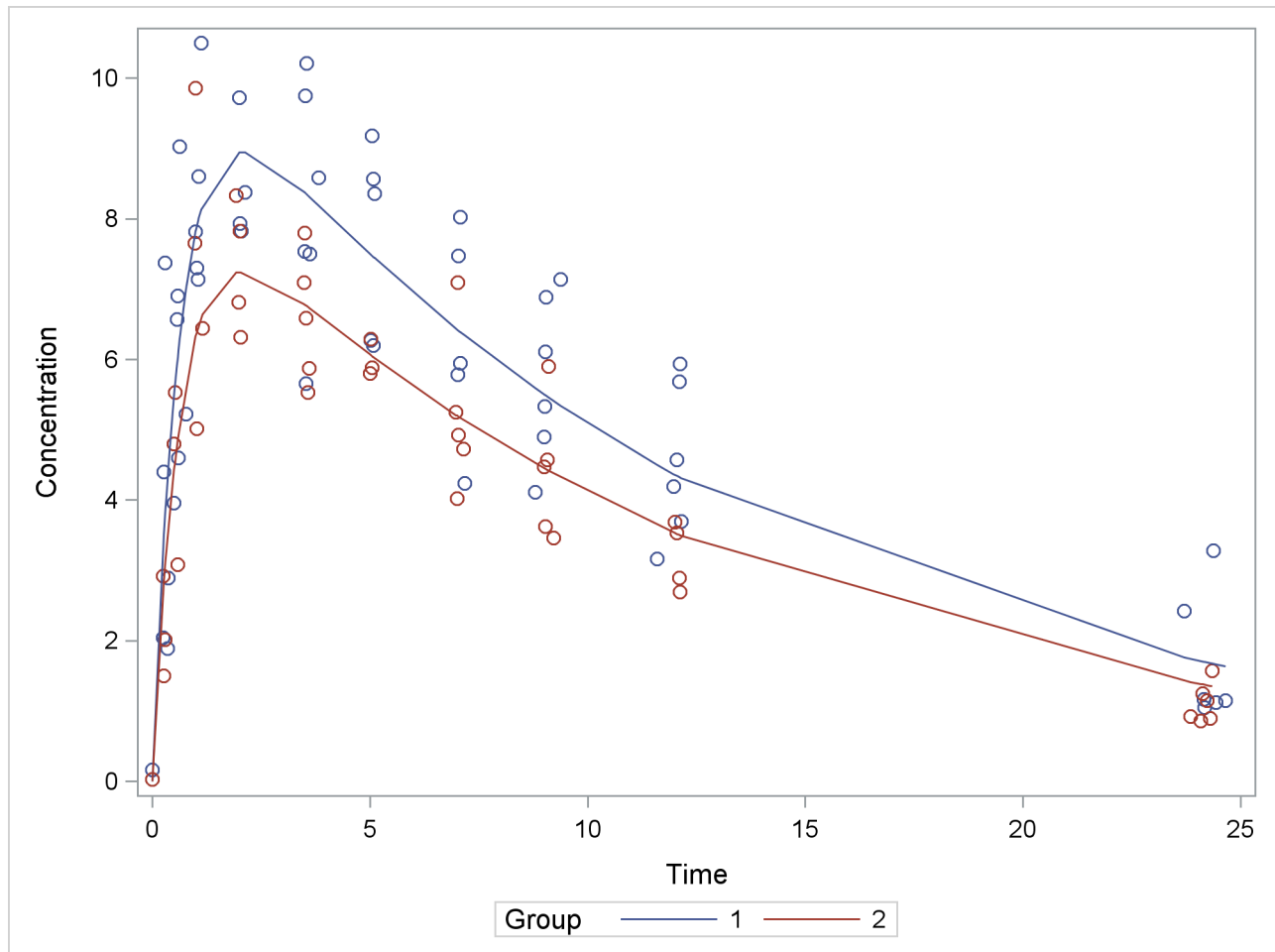
A plot of the observed and predicted values for this final model is obtained with the following statements:

```

proc sgplot data=predvals;
 scatter x=time y=conc / group=group;
 series x=time y=p / group=group name='fit';
 keylegend 'fit' / across=2 title='Group';
 yaxis label='Concentration';
 xaxis label='Time';
run;

```

The plot is shown in [Output 63.5.8](#).

**Output 63.5.8** Observed and Fitted Values for Theophylline Data

The sum-of-squares reduction test is not the only possibility of performing linear-model style hypothesis testing in nonlinear models. You can also perform Wald-type testing of linear hypotheses about the parameter estimates. See [Example 41.17](#) in Chapter 41, “The GLIMMIX Procedure,” for an application of this example that uses the NLIN and GLIMMIX procedures to compare the parameters across groups and adjusts  $p$ -values for multiplicity.

## Example 63.6: ODS Graphics and Diagnostics

The model in this example, taken from St. Laurent and Cook (1993), shows an unusual behavior in that the intrinsic curvature is substantially larger than the parameter-effects curvature. This example demonstrates how the diagnostics features of PROC NLIN can be used to perform postconvergence diagnostics.

The model takes the form

$$E[Y|x_1, x_2] = \alpha x_1 + \exp\{\gamma x_2\}$$

The following DATA step creates a small data set to be used in this example:

```

data contrived;
 input x1 x2 y;
 datalines;
-4.0 -2.5 -10.0
-3.0 -2.0 -5.0
-2.0 -1.5 -2.0
-1.0 -1.0 -1.0
 0.0 0.0 1.5
 1.0 1.0 4.0
 2.0 1.5 5.0
 3.0 2.0 6.0
 4.0 2.5 7.0
-3.5 -2.2 -7.1
-3.5 -1.7 -5.1
 3.5 0.7 6.1
 2.5 1.2 7.5
;

```

The model is fit with the following statements in the NLIN procedure:

```

ods graphics on;
proc nlin data=contrived bias hougaard
 NLINMEASURES plots(stats=all)=(diagnostics);
 parms alpha=2.0
 gamma=0.0;
 model y = alpha*x1 + exp(gamma*x2);
run;
ods graphics off;

```

#### Output 63.6.1 Bias, Skewness, and Global Nonlinearity Measures

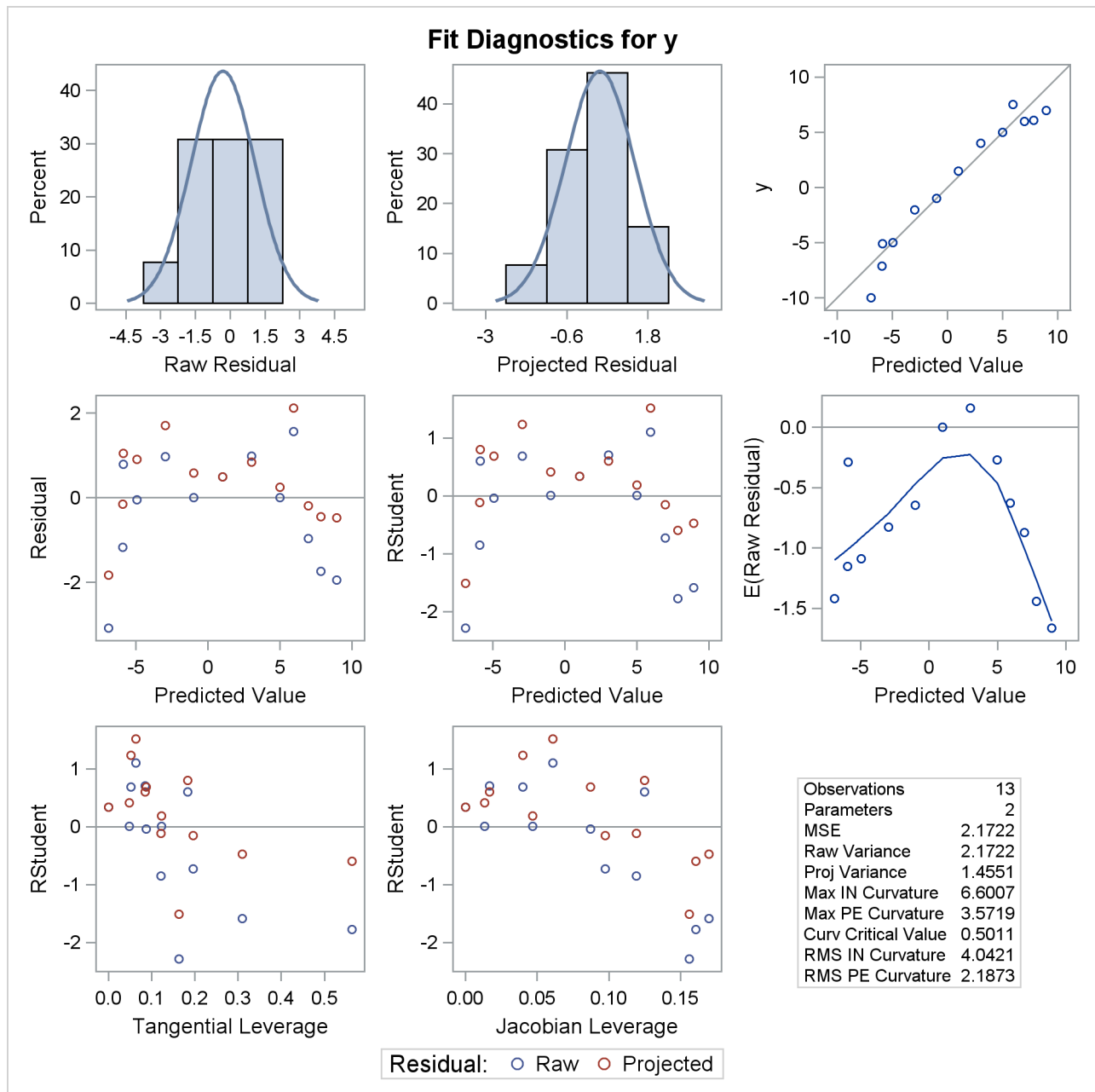
| The NLIN Procedure           |                                 |                  |                                   |        |          |         |              |
|------------------------------|---------------------------------|------------------|-----------------------------------|--------|----------|---------|--------------|
| Parameter                    | Estimate                        | Approx Std Error | Approximate 95% Confidence Limits |        | Skewness | Bias    | Percent Bias |
| alpha                        | 1.9378                          | 0.4704           | 0.9024                            | 2.9733 | 6.6491   | 0.5763  | 29.7         |
| gamma                        | 0.0718                          | 0.7923           | -1.6720                           | 1.8156 | -7.5596  | -0.9982 | -1390        |
| Global Nonlinearity Measures |                                 |                  |                                   |        |          |         |              |
|                              | Max Intrinsic Curvature         |                  |                                   |        | 6.6007   |         |              |
|                              | RMS Intrinsic Curvature         |                  |                                   |        | 4.0421   |         |              |
|                              | Max Parameter-Effects Curvature |                  |                                   |        | 3.5719   |         |              |
|                              | RMS Parameter-Effects Curvature |                  |                                   |        | 2.1873   |         |              |
|                              | Curvature Critical Value        |                  |                                   |        | 0.5011   |         |              |
|                              | Raw Residual Variance           |                  |                                   |        | 2.1722   |         |              |
|                              | Projected Residual Variance     |                  |                                   |        | 1.4551   |         |              |

The bias, skewness, and both the maximum and RMS intrinsic curvatures, compared to the critical curvature value, show that the model is highly nonlinear (Output 63.6.1). As such, performing diagnostics with the

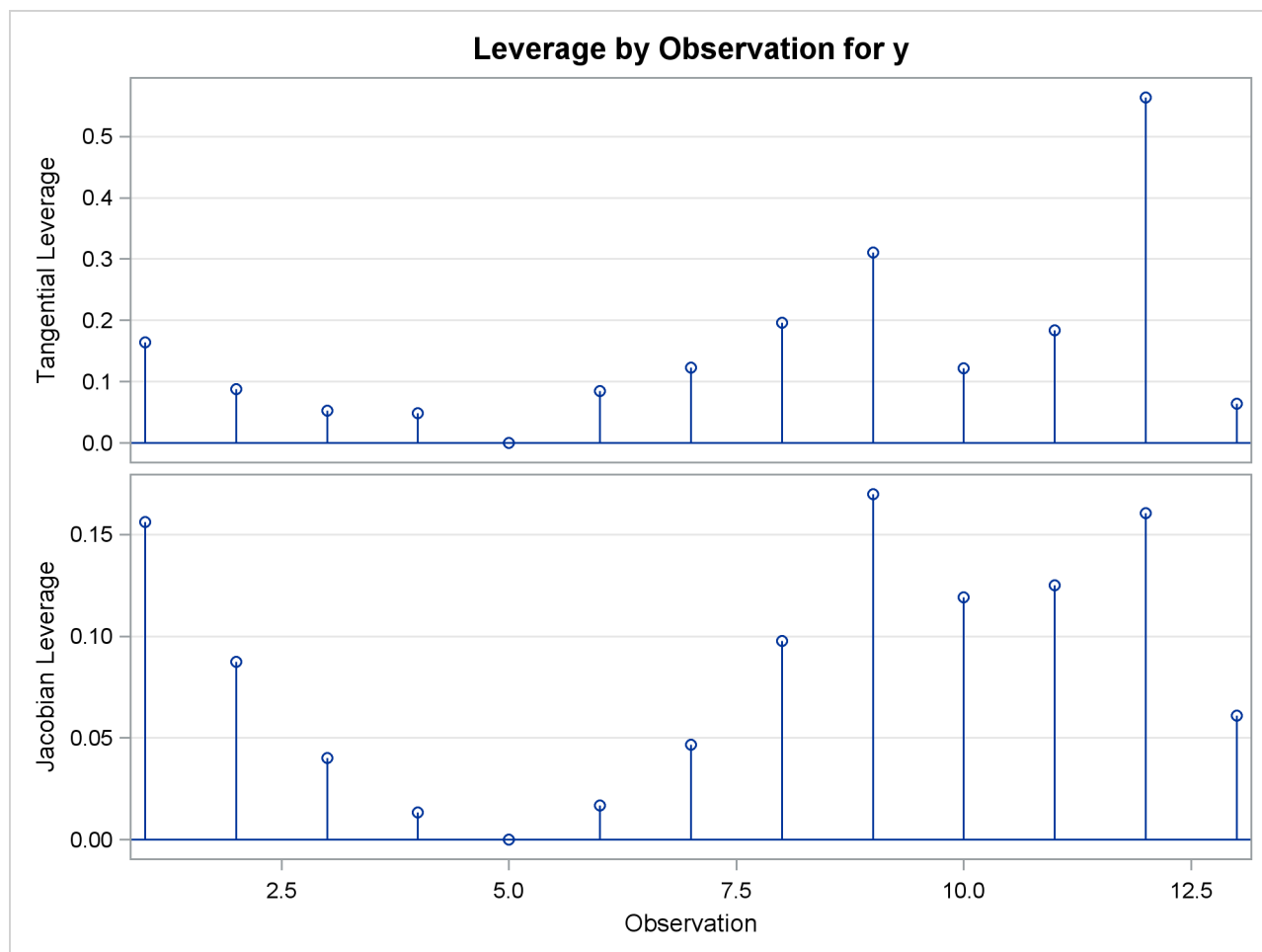
raw residuals can be problematic because they might have undesirable statistical properties: a nonzero mean and a negative semidefinite (instead of zero) covariance with the predicted values and different variances. In addition, the use of tangential leverage is questionable in this case.

The partial results from this NLIN run are shown in [Output 63.6.2](#), [Output 63.6.3](#), and [Output 63.6.4](#). The diagnostics plots corroborate the previously mentioned expectations: highly correlated raw residuals (with the predicted values), significant differences between tangential and Jacobian leverages and projected residuals which overcome some of the shortcomings of the raw residuals. Finally, considering the large intrinsic curvature, reparameterization might not make the model close-to-linear, perhaps necessitating the construction of another model.

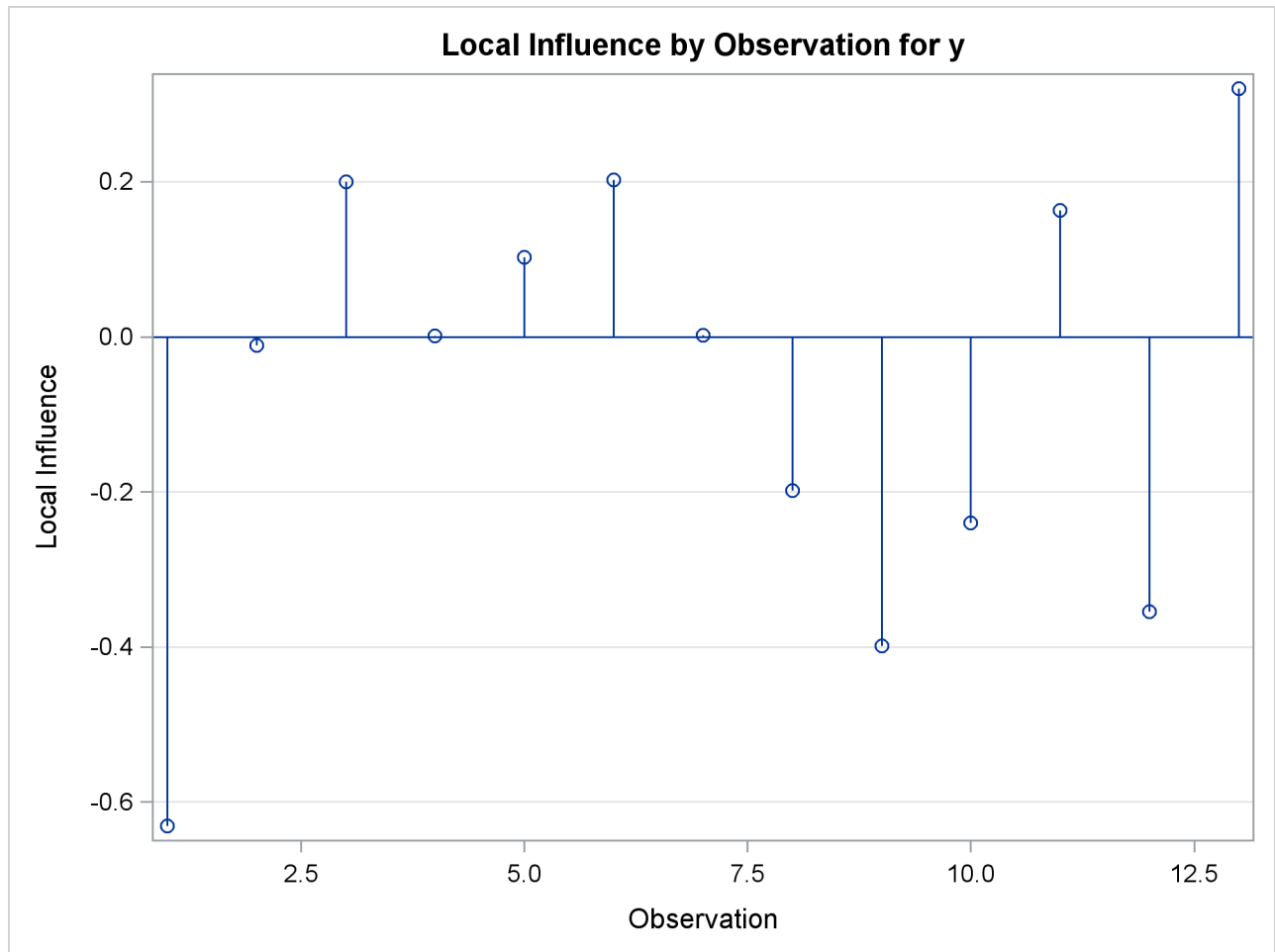
**Output 63.6.2** Diagnostics Panel



Output 63.6.3 Leverage Plots



Output 63.6.4 Local Influence Plot



## Example 63.7: Parameter Profiling

The following model, taken from Clarke (1987a), demonstrates the benefits of parameter profiling and confidence curves to identify the nonlinear characteristics of parameters that occur in the model. The profiling is also augmented with a plot that shows the influence of each observation on the parameter estimates.

The model takes the form

$$E[Y|x] = \theta_3 + \theta_2 \exp\{\theta_1 x\}$$

The data set used in this example is taken from Clarke (1987a). The following DATA step creates this data set:

```
data clarke1987a;
 input x y;
 datalines;
1 3.183
2 3.059
3 2.871
4 2.622
5 2.541
6 2.184
7 2.110
8 2.075
9 2.018
10 1.903
11 1.770
12 1.762
13 1.550
;
```

The model is fit with the following statements in the NLIN procedure:

```
ods graphics on;
proc nlin data=clarke1987a plots(stats=none)=diagnostics;
 parms theta1=-0.15
 theta2=2.0
 theta3=0.80;
 profile theta3 / range = -6 to 2 by 0.2 all;
 model y = theta3 + theta2*exp(theta1*x);
run;
ods graphics off;
```

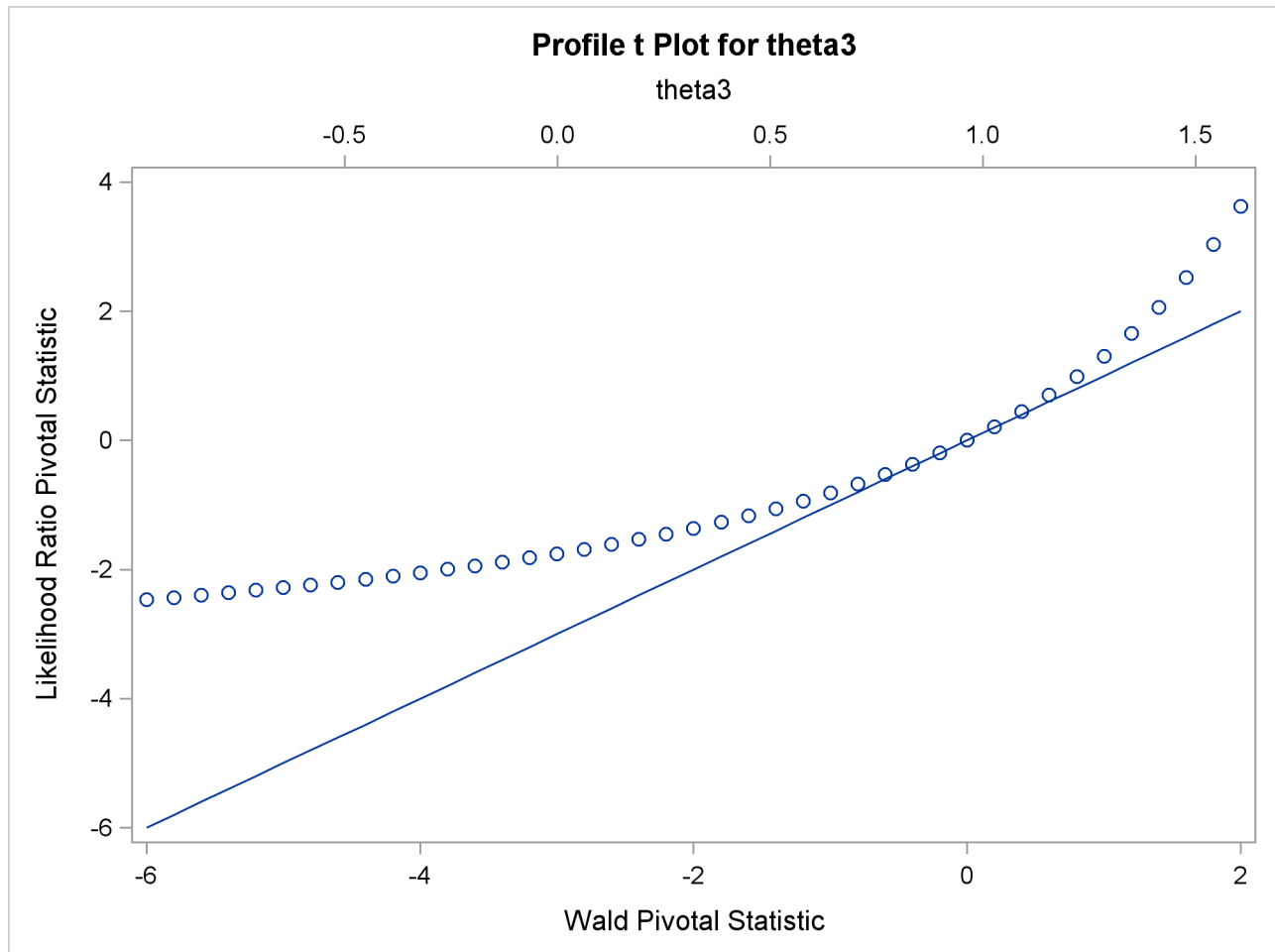
The profile  $t$  plot, [Output 63.7.1](#), for parameter  $\theta_3$  shows a definite deviation from the linear reference line that has a slope of 1 and passes through the origin. Hence, Wald-based inference for  $\theta_3$  is not appropriate. The confidence curve for  $\theta_3$  validates this conclusion.

[Output 63.7.2](#) shows the confidence curve for  $\theta_3$ . You can see that there is a significant difference between the Wald-based confidence interval and the corresponding likelihood-based interval. In such cases, the likelihood-based intervals are preferred because their coverage rate is much closer to the nominal values than the coverage rate of the Wald-based intervals (Donaldson and Schnabel 1987; Cook and Weisberg 1990). Furthermore, this example shows that the adequacy of a linear approximation with regards to a certain parameter cannot be inferred directly from the model. If it could,  $\theta_3$ , which enters the model linearly,

would have a completely linear behavior. For a detailed discussion about this issue, see Cook and Weisberg (1990).

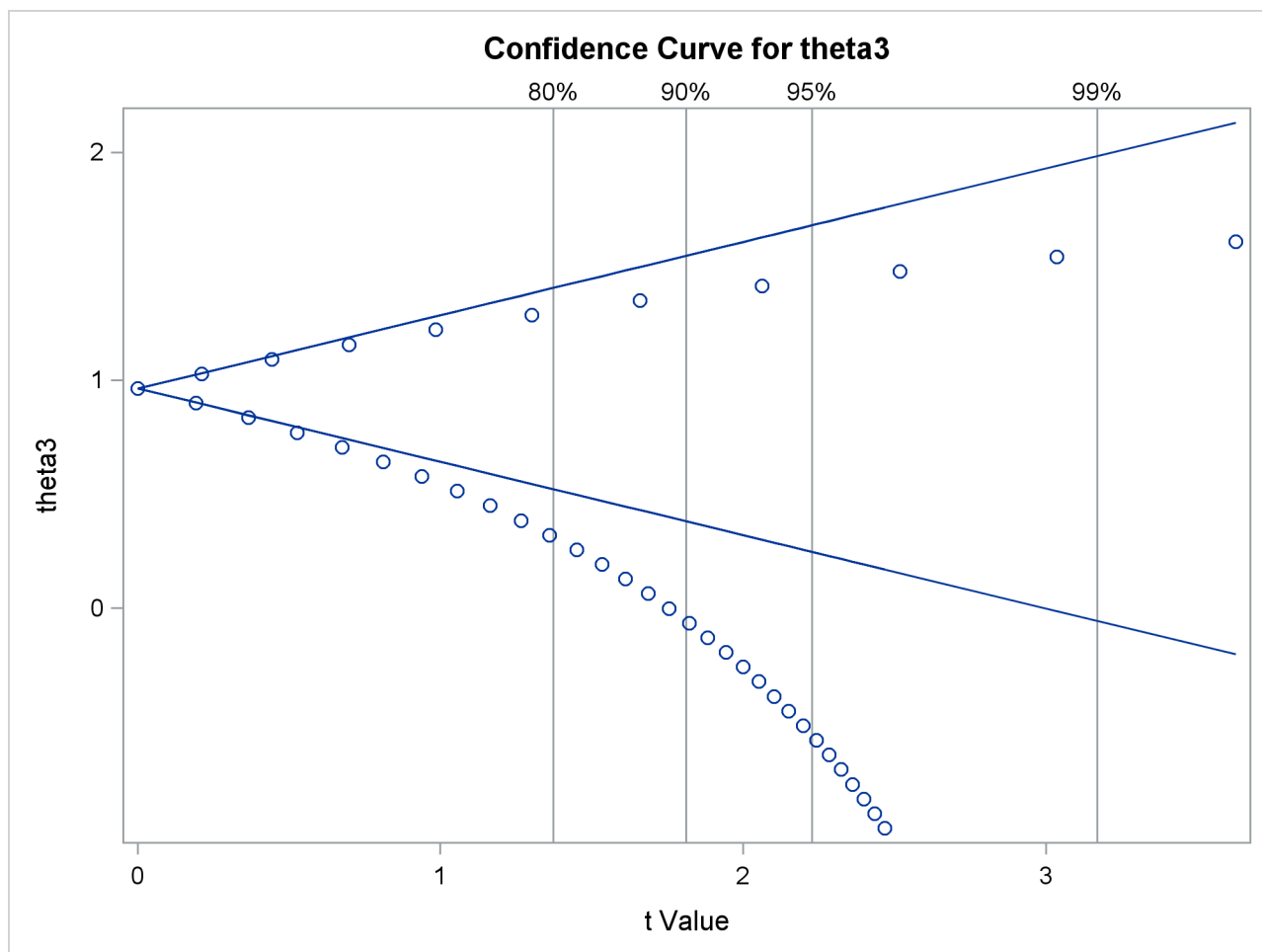
Finally, [Output 63.7.3](#) depicts the influence of each observation on the value of  $\theta_3$ . Observations 6 and 13 have the most influence on the value of this parameter. The plot is generated using the leave-one-out method and should be contrasted with the local influence plot, [Output 63.7.4](#), which is based on assessing the influence of an additive perturbation of the response variable.

**Output 63.7.1** Profile  $t$  Plot

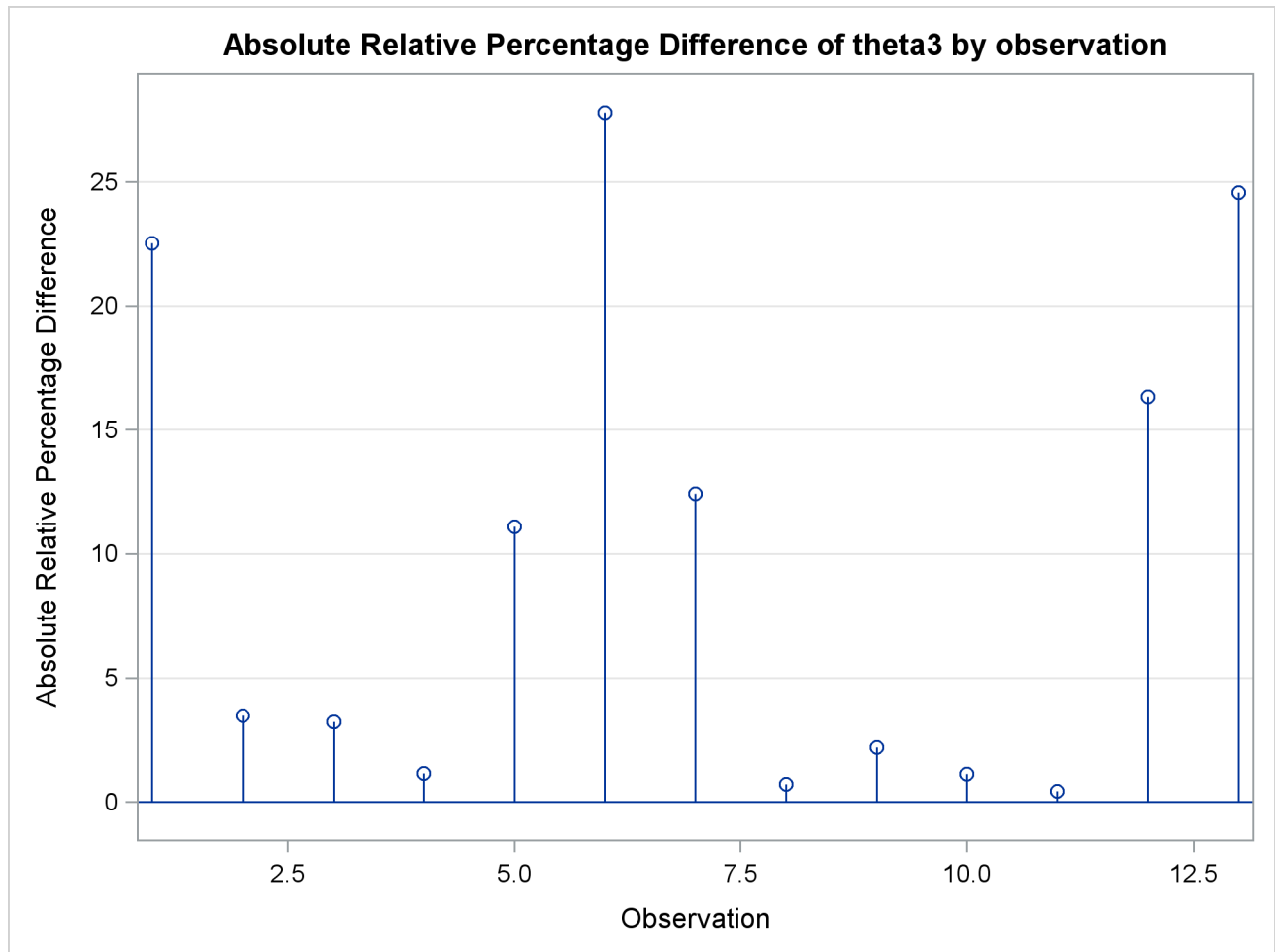


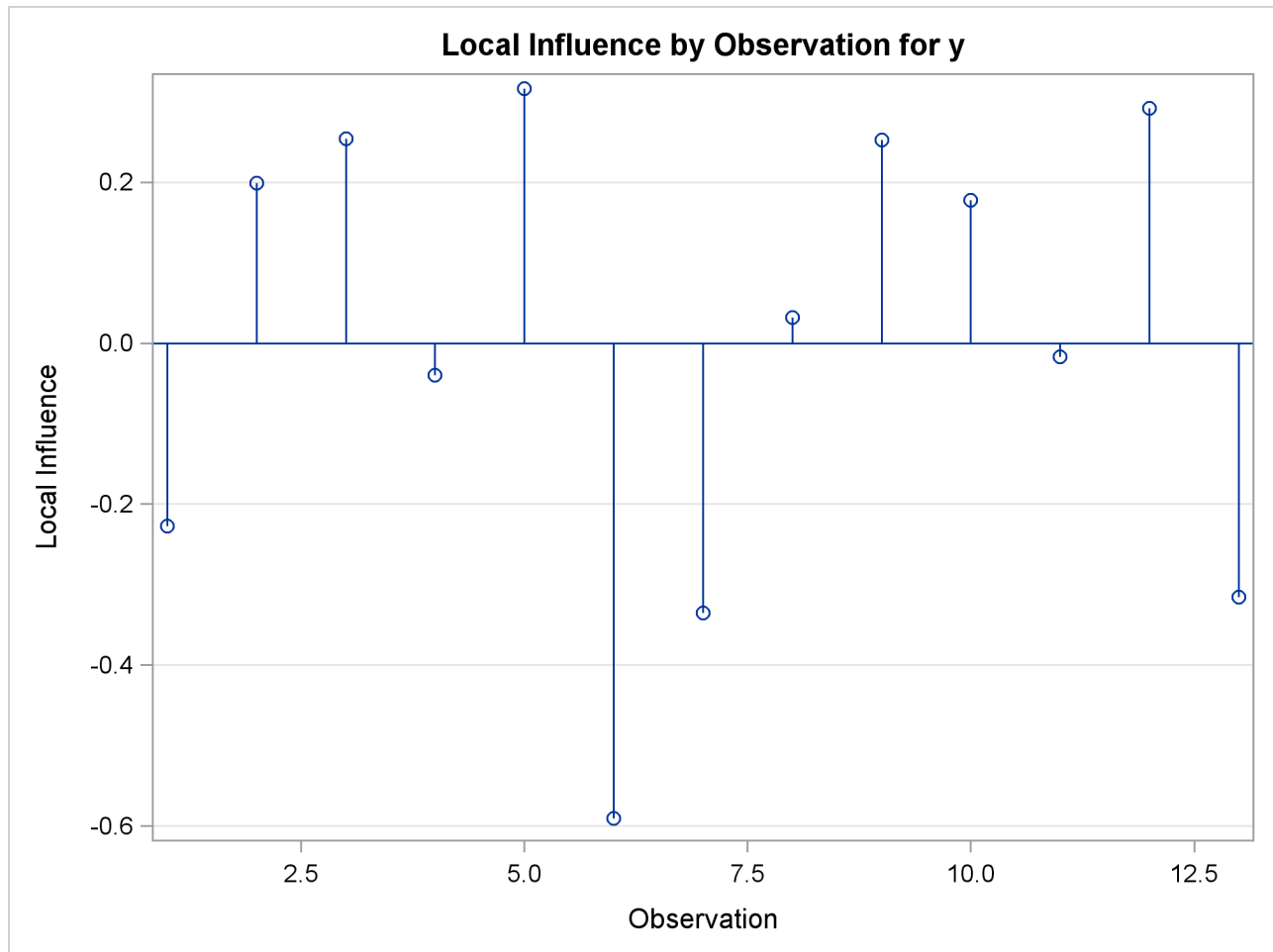


Output 63.7.2 Confidence Curve



**Output 63.7.3** Observation Influence on Parameter Estimate



**Output 63.7.4** Local Influence Plot

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# Chapter 64

## The NLMIXED Procedure

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## Overview: NLMIXED Procedure

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### Introduction

The NLMIXED procedure fits nonlinear mixed models—that is, models in which both fixed and random effects enter nonlinearly. These models have a wide variety of applications, two of the most common being pharmacokinetics and overdispersed binomial data. PROC NLMIXED enables you to specify a conditional distribution for your data (given the random effects) having either a standard form (normal, binomial, Poisson) or a general distribution that you code using SAS programming statements.

PROC NLMIXED fits nonlinear mixed models by maximizing an approximation to the likelihood integrated over the random effects. Different integral approximations are available, the principal ones being adaptive Gaussian quadrature and a first-order Taylor series approximation. A variety of alternative optimization techniques are available to carry out the maximization; the default is a dual quasi-Newton algorithm.

Successful convergence of the optimization problem results in parameter estimates along with their approximate standard errors based on the second derivative matrix of the likelihood function. PROC NLMIXED enables you to use the estimated model to construct predictions of arbitrary functions by using empirical Bayes estimates of the random effects. You can also estimate arbitrary functions of the nonrandom parameters, and PROC NLMIXED computes their approximate standard errors by using the delta method.

### Literature on Nonlinear Mixed Models

Davidian and Giltinan (1995) and Vonesh and Chinchilli (1997) provide good overviews as well as general theoretical developments and examples of nonlinear mixed models. Pinheiro and Bates (1995) is a primary reference for the theory and computational techniques of PROC NLMIXED. They describe and compare several different integrated likelihood approximations and provide evidence that adaptive Gaussian quadrature is one of the best methods. Davidian and Gallant (1993) also use Gaussian quadrature for nonlinear mixed models, although the smooth nonparametric density they advocate for the random effects is currently not available in PROC NLMIXED.

Traditional approaches to fitting nonlinear mixed models involve Taylor series expansions, expanding around either zero or the empirical best linear unbiased predictions of the random effects. The former is the basis for the well-known first-order method (Beal and Sheiner 1982, 1988; Sheiner and Beal 1985),

and it is optionally available in PROC NL MIXED. The latter is the basis for the estimation method of Lindstrom and Bates (1990), and it is not available in PROC NL MIXED. However, the closely related Laplacian approximation is an option; it is equivalent to adaptive Gaussian quadrature with only one quadrature point. The Laplacian approximation and its relationship to the Lindstrom-Bates method are discussed by: Beal and Sheiner (1992); Wolfinger (1993); Vonesh (1992, 1996); Vonesh and Chinchilli (1997); Wolfinger and Lin (1997).

A parallel literature exists in the area of generalized linear mixed models, in which random effects appear as a part of the linear predictor inside a link function. Taylor-series methods similar to those just described are discussed in articles such as: Harville and Mee (1984); Stiratelli, Laird, and Ware (1984); Gilmour, Anderson, and Rae (1985); Goldstein (1991); Schall (1991); Engel and Keen (1992); Breslow and Clayton (1993); Wolfinger and O'Connell (1993); McGilchrist (1994), but such methods have not been implemented in PROC NL MIXED because they can produce biased results in certain binary data situations (Rodriguez and Goldman 1995; Lin and Breslow 1996). Instead, a numerical quadrature approach is available in PROC NL MIXED, as discussed in: Pierce and Sands (1975); Anderson and Aitkin (1985); Hedeker and Gibbons (1994); Crouch and Spiegelman (1990); Longford (1994); McCulloch (1994); Liu and Pierce (1994); Diggle, Liang, and Zeger (1994).

Nonlinear mixed models have important applications in pharmacokinetics, and Roe (1997) provides a wide-ranging comparison of many popular techniques. Yuh et al. (1994) provide an extensive bibliography on nonlinear mixed models and their use in pharmacokinetics.

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## PROC NL MIXED Compared with Other SAS Procedures and Macros

The models fit by PROC NL MIXED can be viewed as generalizations of the random coefficient models fit by the MIXED procedure. This generalization allows the random coefficients to enter the model nonlinearly, whereas in PROC MIXED they enter linearly. With PROC MIXED you can perform both maximum likelihood and restricted maximum likelihood (REML) estimation, whereas PROC NL MIXED implements only maximum likelihood. This is because the analog to the REML method in PROC NL MIXED would involve a high-dimensional integral over all of the fixed-effects parameters, and this integral is typically not available in closed form. Finally, PROC MIXED assumes the data to be normally distributed, whereas PROC NL MIXED enables you to analyze data that are normal, binomial, or Poisson or that have any likelihood programmable with SAS statements.

PROC NL MIXED does not implement the same estimation techniques available with the NLINMIX macro or the default estimation method of the GLIMMIX procedure. These are based on the estimation methods of: Lindstrom and Bates (1990); Breslow and Clayton (1993); Wolfinger and O'Connell (1993), and they iteratively fit a set of generalized estimating equations (see Chapters 14 and 15 of Littell et al. 2006; Wolfinger 1997). In contrast, PROC NL MIXED directly maximizes an approximate integrated likelihood. This remark also applies to the SAS/IML macros MIXNLIN (Vonesh and Chinchilli 1997) and NLMEM (Galecki 1998).

The GLIMMIX procedure also fits mixed models for nonnormal data with nonlinearity in the conditional mean function. In contrast to the NL MIXED procedure, PROC GLIMMIX assumes that the model contains a linear predictor that links covariates to the conditional mean of the response. The NL MIXED procedure is designed to handle general conditional mean functions, whether they contain a linear component or not. As mentioned earlier, the GLIMMIX procedure by default estimates parameters in generalized linear mixed models by pseudo-likelihood techniques, whereas PROC NL MIXED by default performs maximum likeli-



hood estimation by adaptive Gauss-Hermite quadrature. This estimation method is also available with the GLIMMIX procedure (METHOD=QUAD in the PROC GLIMMIX statement).

PROC NLMIXED has close ties with the NLP procedure in SAS/OR software. PROC NLMIXED uses a subset of the optimization code underlying PROC NLP and has many of the same optimization-based options. Also, the programming statement functionality used by PROC NLMIXED is the same as that used by PROC NLP and the MODEL procedure in SAS/ETS software.

## Getting Started: NLMIXED Procedure

### Nonlinear Growth Curves with Gaussian Data

As an introductory example, consider the orange tree data of Draper and Smith (1981). These data consist of seven measurements of the trunk circumference (in millimeters) on each of five orange trees. You can input these data into a SAS data set as follows:

```
data tree;
 input tree day y;
 datalines;
1 118 30
1 484 58
1 664 87

... more lines ...

5 1582 177
;
```

Lindstrom and Bates (1990) and Pinheiro and Bates (1995) propose the following logistic nonlinear mixed model for these data:

$$y_{ij} = \frac{b_1 + u_{i1}}{1 + \exp[-(d_{ij} - b_2)/b_3]} + e_{ij}$$

Here,  $y_{ij}$  represents the  $j$ th measurement on the  $i$ th tree ( $i = 1, \dots, 5; j = 1, \dots, 7$ ),  $d_{ij}$  is the corresponding day,  $b_1, b_2, b_3$  are the fixed-effects parameters,  $u_{i1}$  are the random-effect parameters assumed to be iid  $N(0, \sigma_u^2)$ , and  $e_{ij}$  are the residual errors assumed to be iid  $N(0, \sigma_e^2)$  and independent of the  $u_{i1}$ . This model has a logistic form, and the random-effect parameters  $u_{i1}$  enter the model linearly.

The statements to fit this nonlinear mixed model are as follows:

```
proc nlmixed data=tree;
 parms b1=190 b2=700 b3=350 s2u=1000 s2e=60;
 num = b1+u1;
 ex = exp(-(day-b2)/b3);
 den = 1 + ex;
 model y ~ normal(num/den, s2e);
 random u1 ~ normal(0, s2u) subject=tree;
run;
```

The **PROC NLMIXED** statement invokes the procedure and inputs the tree data set. The **PARMS** statement identifies the unknown parameters and their starting values. Here there are three fixed-effects parameters ( $b_1$ ,  $b_2$ ,  $b_3$ ) and two variance components ( $s^2u$ ,  $s^2e$ ).

The next three statements are SAS programming statements specifying the logistic mixed model. A new variable  $u_1$  is included to identify the random effect. These statements are evaluated for every observation in the data set when the NLMIXED procedure computes the log likelihood function and its derivatives.

The **MODEL** statement defines the dependent variable and its conditional distribution given the random effects. Here a normal (Gaussian) conditional distribution is specified with mean  $\text{num}/\text{den}$  and variance  $s^2e$ .

The **RANDOM** statement defines the single random effect to be  $u_1$ , and specifies that it follow a normal distribution with mean 0 and variance  $s^2u$ . The **SUBJECT=** argument in the **RANDOM** statement defines a variable indicating when the random effect obtains new realizations; in this case, it changes according to the values of the *tree* variable. PROC NLMIXED assumes that the input data set is clustered according to the levels of the *tree* variable; that is, all observations from the same tree occur sequentially in the input data set.

The output from this analysis is as follows.

**Figure 64.1** Model Specifications

| The NLMIXED Procedure               |                                 |
|-------------------------------------|---------------------------------|
| Specifications                      |                                 |
| Data Set                            | WORK.TREE                       |
| Dependent Variable                  | Y                               |
| Distribution for Dependent Variable | Normal                          |
| Random Effects                      | $u_1$                           |
| Distribution for Random Effects     | Normal                          |
| Subject Variable                    | tree                            |
| Optimization Technique              | Dual Quasi-Newton               |
| Integration Method                  | Adaptive Gaussian<br>Quadrature |

The “Specifications” table lists basic information about the nonlinear mixed model you have specified (Figure 64.1). Included are the input data set, the dependent and subject variables, the random effects, the relevant distributions, and the type of optimization. The “Dimensions” table lists various counts related to the model, including the number of observations, subjects, and parameters (Figure 64.2). These quantities are useful for checking that you have specified your data set and model correctly. Also listed is the number of quadrature points that PROC NLMIXED has selected based on the evaluation of the log likelihood at the starting values of the parameters. Here, only one quadrature point is necessary because the random-effect parameters  $u_{i1}$  enter the model linearly. (The Gauss-Hermite quadrature with a single quadrature point results in the Laplace approximation of the log likelihood.)

**Figure 64.2** Dimensions Table for Growth Curve Model

| Dimensions            |    |
|-----------------------|----|
| Observations Used     | 35 |
| Observations Not Used | 0  |
| Total Observations    | 35 |
| Subjects              | 5  |
| Max Obs Per Subject   | 7  |
| Parameters            | 5  |
| Quadrature Points     | 1  |

**Figure 64.3** Starting Values of Parameter Estimates and Negative Log Likelihood

| Parameters |     |     |      |     |            |
|------------|-----|-----|------|-----|------------|
| b1         | b2  | b3  | s2u  | s2e | NegLogLike |
| 190        | 700 | 350 | 1000 | 60  | 132.491787 |

The “Parameters” table lists the parameters to be estimated, their starting values, and the negative log likelihood evaluated at the starting values (Figure 64.3).

**Figure 64.4** Iteration History for Growth Curve Model

| Iteration History |       |            |          |          |          |
|-------------------|-------|------------|----------|----------|----------|
| Iter              | Calls | NegLogLike | Diff     | MaxGrad  | Slope    |
| 1                 | 4     | 131.686742 | 0.805045 | 0.010269 | -0.633   |
| 2                 | 6     | 131.64466  | 0.042082 | 0.014783 | -0.0182  |
| 3                 | 8     | 131.614077 | 0.030583 | 0.009809 | -0.02796 |
| 4                 | 10    | 131.572522 | 0.041555 | 0.001186 | -0.01344 |
| 5                 | 11    | 131.571895 | 0.000627 | 0.0002   | -0.00121 |
| 6                 | 13    | 131.571889 | 5.549E-6 | 0.000092 | -7.68E-6 |
| 7                 | 15    | 131.571888 | 1.096E-6 | 6.097E-6 | -1.29E-6 |

NOTE: GCONV convergence criterion satisfied.

The “Iteration History” table records the history of the minimization of the negative log likelihood (Figure 64.4). For each iteration of the quasi-Newton optimization, values are listed for the number of function calls, the value of the negative log likelihood, the difference from the previous iteration, the absolute value of the largest gradient, and the slope of the search direction. The note at the bottom of the table indicates that the algorithm has converged successfully according to the **GCONV** convergence criterion, a standard criterion computed using a quadratic form in the gradient and the inverse Hessian.

The final maximized value of the log likelihood as well as the information criterion of Akaike (AIC), its small sample bias corrected version (AICC), and the Bayesian information criterion (BIC) in the “smaller is better” form appear in the “Fit Statistics” table (Figure 64.5). These statistics can be used to compare different nonlinear mixed models.

**Figure 64.5** Fit Statistics for Growth Curve Model

| Fit Statistics           |       |
|--------------------------|-------|
| -2 Log Likelihood        | 263.1 |
| AIC (smaller is better)  | 273.1 |
| AICC (smaller is better) | 275.2 |
| BIC (smaller is better)  | 271.2 |

**Figure 64.6** Parameter Estimates at Convergence

| Parameter Estimates |          |                |    |         |         |       |         |
|---------------------|----------|----------------|----|---------|---------|-------|---------|
| Parameter           | Estimate | Standard Error | DF | t Value | Pr >  t | Alpha | Lower   |
| b1                  | 192.05   | 15.6473        | 4  | 12.27   | 0.0003  | 0.05  | 148.61  |
| b2                  | 727.90   | 35.2472        | 4  | 20.65   | <.0001  | 0.05  | 630.04  |
| b3                  | 348.07   | 27.0790        | 4  | 12.85   | 0.0002  | 0.05  | 272.88  |
| s2u                 | 999.88   | 647.44         | 4  | 1.54    | 0.1974  | 0.05  | -797.70 |
| s2e                 | 61.5139  | 15.8831        | 4  | 3.87    | 0.0179  | 0.05  | 17.4153 |

| Parameter Estimates |         |          |
|---------------------|---------|----------|
| Parameter           | Upper   | Gradient |
| b1                  | 235.50  | 1.154E-6 |
| b2                  | 825.76  | 5.289E-6 |
| b3                  | 423.25  | -6.1E-6  |
| s2u                 | 2797.45 | -3.84E-6 |
| s2e                 | 105.61  | 2.892E-6 |

The maximum likelihood estimates of the five parameters and their approximate standard errors computed using the final Hessian matrix are displayed in the “Parameter Estimates” table (Figure 64.6). Approximate *t*-values and Wald-type confidence limits are also provided, with degrees of freedom equal to the number of subjects minus the number of random effects. You should interpret these statistics cautiously for variance parameters like s2u and s2e. The final column in the output shows the gradient vector at the optimization solution. Each element appears to be sufficiently small to indicate a stationary point.

Since the random-effect parameters  $u_{i1}$  enter the model linearly, you can obtain equivalent results by using the first-order method (specify `METHOD=FIRO` in the `PROC NL MIXED` statement).

## Logistic-Normal Model with Binomial Data

This example analyzes the data from Beitler and Landis (1985), which represent results from a multi-center clinical trial investigating the effectiveness of two topical cream treatments (active drug, control) in curing an infection. For each of eight clinics, the number of trials and favorable cures are recorded for each treatment. The SAS data set is as follows.

```
data infection;
 input clinic t x n;
 datalines;
1 1 11 36
1 0 10 37
2 1 16 20
2 0 22 32
3 1 14 19
3 0 7 19
4 1 2 16
4 0 1 17
5 1 6 17
5 0 0 12
6 1 1 11
6 0 0 10
7 1 1 5
7 0 1 9
8 1 4 6
8 0 6 7
;
```

Suppose  $n_{ij}$  denotes the number of trials for the  $i$ th clinic and the  $j$ th treatment ( $i = 1, \dots, 8; j = 0, 1$ ), and  $x_{ij}$  denotes the corresponding number of favorable cures. Then a reasonable model for the preceding data is the following logistic model with random effects:

$$x_{ij}|u_i \sim \text{Binomial}(n_{ij}, p_{ij})$$

and

$$\eta_{ij} = \log\left(\frac{p_{ij}}{1 - p_{ij}}\right) = \beta_0 + \beta_1 t_j + u_i$$

The notation  $t_j$  indicates the  $j$ th treatment, and the  $u_i$  are assumed to be iid  $N(0, \sigma_u^2)$ .

The PROC NLMIXED statements to fit this model are as follows:

```
proc nlmixed data=infection;
 parms beta0=-1 beta1=1 s2u=2;
 eta = beta0 + beta1*t + u;
 expeta = exp(eta);
 p = expeta/(1+expeta);
 model x ~ binomial(n,p);
 random u ~ normal(0,s2u) subject=clinic;
 predict eta out=eta;
 estimate '1/beta1' 1/beta1;
run;
```

The **PROC NL MIXED** statement invokes the procedure, and the **PARMS** statement defines the parameters and their starting values. The next three statements define  $p_{ij}$ , and the **MODEL** statement defines the conditional distribution of  $x_{ij}$  to be binomial. The **RANDOM** statement defines  $u$  to be the random effect with subjects defined by the clinic variable.

The **PREDICT** statement constructs predictions for each observation in the input data set. For this example, predictions of  $\eta_{ij}$  and approximate standard errors of prediction are output to a data set named eta. These predictions include empirical Bayes estimates of the random effects  $u_i$ .

The **ESTIMATE** statement requests an estimate of the reciprocal of  $\beta_1$ .

The output for this model is as follows.

**Figure 64.7** Model Information and Dimensions for Logistic-Normal Model

| The NL MIXED Procedure              |                              |
|-------------------------------------|------------------------------|
| Specifications                      |                              |
| Data Set                            | WORK.INFECTION               |
| Dependent Variable                  | x                            |
| Distribution for Dependent Variable | Binomial                     |
| Random Effects                      | u                            |
| Distribution for Random Effects     | Normal                       |
| Subject Variable                    | clinic                       |
| Optimization Technique              | Dual Quasi-Newton            |
| Integration Method                  | Adaptive Gaussian Quadrature |
| Dimensions                          |                              |
| Observations Used                   | 16                           |
| Observations Not Used               | 0                            |
| Total Observations                  | 16                           |
| Subjects                            | 8                            |
| Max Obs Per Subject                 | 2                            |
| Parameters                          | 3                            |
| Quadrature Points                   | 5                            |

The “Specifications” table provides basic information about the nonlinear mixed model (Figure 64.7). For example, the distribution of the response variable, conditional on normally distributed random effects, is binomial. The “Dimensions” table provides counts of various variables. You should check this table to make sure the data set and model have been entered properly. PROC NL MIXED selects five quadrature points to achieve the default accuracy in the likelihood calculations.

**Figure 64.8** Starting Values of Parameter Estimates

| Parameters |       |     |            |
|------------|-------|-----|------------|
| beta0      | beta1 | s2u | NegLogLike |
| -1         | 1     | 2   | 37.5945925 |

The “Parameters” table lists the starting point of the optimization and the negative log likelihood at the starting values (Figure 64.8).

**Figure 64.9** Iteration History and Fit Statistics for Logistic-Normal Model

| Iteration History |       |            |          |          |          |
|-------------------|-------|------------|----------|----------|----------|
| Iter              | Calls | NegLogLike | Diff     | MaxGrad  | Slope    |
| 1                 | 2     | 37.3622692 | 0.232323 | 2.882077 | -19.3762 |
| 2                 | 3     | 37.1460375 | 0.216232 | 0.921926 | -0.82852 |
| 3                 | 5     | 37.0300936 | 0.115944 | 0.315897 | -0.59175 |
| 4                 | 6     | 37.0223017 | 0.007792 | 0.01906  | -0.01615 |
| 5                 | 7     | 37.0222472 | 0.000054 | 0.001743 | -0.00011 |
| 6                 | 9     | 37.0222466 | 6.57E-7  | 0.000091 | -1.28E-6 |
| 7                 | 11    | 37.0222466 | 5.38E-10 | 2.078E-6 | -1.1E-9  |

NOTE: GCONV convergence criterion satisfied.

| Fit Statistics           |      |
|--------------------------|------|
| -2 Log Likelihood        | 74.0 |
| AIC (smaller is better)  | 80.0 |
| AICC (smaller is better) | 82.0 |
| BIC (smaller is better)  | 80.3 |

The “Iteration History” table indicates successful convergence in seven iterations (Figure 64.9). The “Fit Statistics” table lists some useful statistics based on the maximized value of the log likelihood.

**Figure 64.10** Parameter Estimates for Logistic-Normal Model

| Parameter Estimates |          |                |    |         |         |       |         |
|---------------------|----------|----------------|----|---------|---------|-------|---------|
| Parameter           | Estimate | Standard Error | DF | t Value | Pr >  t | Alpha | Lower   |
| beta0               | -1.1974  | 0.5561         | 7  | -2.15   | 0.0683  | 0.05  | -2.5123 |
| beta1               | 0.7385   | 0.3004         | 7  | 2.46    | 0.0436  | 0.05  | 0.02806 |
| s2u                 | 1.9591   | 1.1903         | 7  | 1.65    | 0.1438  | 0.05  | -0.8554 |

| Parameter Estimates |        |          |
|---------------------|--------|----------|
| Parameter           | Upper  | Gradient |
| beta0               | 0.1175 | -3.1E-7  |
| beta1               | 1.4488 | -2.08E-6 |
| s2u                 | 4.7736 | -2.48E-7 |

The “Parameter Estimates” table indicates marginal significance of the two fixed-effects parameters (Figure 64.10). The positive value of the estimate of  $\beta_1$  indicates that the treatment significantly increases the chance of a favorable cure.

**Figure 64.11** Table of Additional Estimates

| Additional Estimates |          |                |    |         |         |       |         |        |
|----------------------|----------|----------------|----|---------|---------|-------|---------|--------|
| Label                | Estimate | Standard Error | DF | t Value | Pr >  t | Alpha | Lower   | Upper  |
| 1/beta1              | 1.3542   | 0.5509         | 7  | 2.46    | 0.0436  | 0.05  | 0.05146 | 2.6569 |

The “Additional Estimates” table displays results from the `ESTIMATE` statement (Figure 64.11). The estimate of  $1/\beta_1$  equals  $1/0.7385 = 1.3542$  and its standard error equals  $0.3004/0.7385^2 = 0.5509$  by the delta method (Billingsley 1986; Cox 1998). Note that this particular approximation produces a  $t$ -statistic identical to that for the estimate of  $\beta_1$ .

Not shown is the eta data set, which contains the original 16 observations and predictions of the  $\eta_{ij}$ .

---

## Syntax: NLMIXED Procedure

The following statements are available in the NLMIXED procedure:

```

PROC NLMIXED < options > ;
 ARRAY array-specification ;
 BOUNDS boundary-constraints ;
 BY variables ;
 CONTRAST 'label' expression <, expression > < options > ;
 ESTIMATE 'label' expression < options > ;
 ID names ;
 MODEL model-specification ;
 PARMS parameters-and-starting-values ;
 PREDICT expression OUT=SAS-data-set < options > ;
 RANDOM random-effects-specification ;
 REPLICATE variable ;
 Programming statements ;

```

The following sections provide a detailed description of each of these statements.

---

## PROC NLMIXED Statement

```

PROC NLMIXED < options > ;

```

The `PROC NLMIXED` statement invokes the NLMIXED procedure. Table 64.1 summarizes the options available in the `PROC NLMIXED` statement.



**Table 64.1** PROC NLMIXED Statement Options

| Option                                 | Description                                                            |
|----------------------------------------|------------------------------------------------------------------------|
| <b>Basic Options</b>                   |                                                                        |
| DATA=                                  | Specifies the input data set                                           |
| METHOD=                                | Specifies the integration method                                       |
| <b>Displayed Output Specifications</b> |                                                                        |
| ALPHA=                                 | Specifies $\alpha$ for confidence limits                               |
| CORR                                   | Requests the correlation matrix                                        |
| COV                                    | Requests the covariance matrix                                         |
| DF=                                    | Specifies the degrees of freedom for $p$ -values and confidence limits |
| ECORR                                  | Requests the correlation matrix of additional estimates                |
| ECOV                                   | Requests the covariance matrix of additional estimates                 |
| EDER                                   | Requests derivatives of additional estimates                           |
| EMPIRICAL                              | Requests the empirical (“sandwich”) estimator of covariance matrix     |
| HESS                                   | Requests the Hessian matrix                                            |
| ITDETAILS                              | Requests iteration details                                             |
| START                                  | Specifies the gradient at starting values                              |
| <b>Debugging Output</b>                |                                                                        |
| FLOW                                   | Displays the model execution messages                                  |
| LISTCODE                               | Displays compiled model program                                        |
| LISTDEP                                | Produces a model dependency listing                                    |
| LISTDER                                | Displays the model derivatives                                         |
| LIST                                   | Displays the model program and variables                               |
| TRACE                                  | Displays detailed model execution messages                             |
| XREF                                   | Displays the model cross references                                    |
| <b>Quadrature Options</b>              |                                                                        |
| NOADSCALE                              | Requests no adaptive scaling                                           |
| NOAD                                   | Requests no adaptive centering                                         |
| OUTQ=                                  | Displays output data set                                               |
| QFAC=                                  | Specifies the search factor                                            |
| QMAX=                                  | Specifies the maximum points                                           |
| QPOINTS=                               | Specifies the number of points                                         |
| QSCALEFAC=                             | Specifies the scale factor                                             |
| QTOL=                                  | Specifies the tolerance                                                |
| <b>Empirical Bayes Options</b>         |                                                                        |
| EBOPT                                  | Requests comprehensive optimization                                    |
| EBSSFRAC=                              | Specifies the step-shortening fraction                                 |
| EBSTOL=                                | Specifies the step-shortening tolerance                                |
| EBSTEPS=                               | Specifies the number of Newton steps                                   |
| EBSUBSTEPS=                            | Specifies the number of substeps                                       |
| EBTOL=                                 | Specifies the convergence tolerance                                    |
| EBZSTART                               | Requests zero as the starting values                                   |

Table 64.1 *continued*

| Option                                     | Description                                                                                       |
|--------------------------------------------|---------------------------------------------------------------------------------------------------|
| <b>Optimization Specifications</b>         |                                                                                                   |
| HESCAL=                                    | Specifies the type of Hessian scaling                                                             |
| INHESIAN<=>                                | Specifies the start for approximated Hessian                                                      |
| LINESEARCH=                                | Specifies the line-search method                                                                  |
| LSPRECISION=                               | Specifies the line-search precision                                                               |
| OPTCHECK<=>                                | Checks optimality in a neighborhood                                                               |
| RESTART=                                   | Specifies the iteration number for update restart                                                 |
| TECHNIQUE=                                 | Specifies the minimization technique                                                              |
| UPDATE=                                    | Specifies the update technique                                                                    |
| <b>Derivatives Specifications</b>          |                                                                                                   |
| DIAHES                                     | Uses only the diagonal of Hessian                                                                 |
| FDHESSIAN<=>                               | Specifies the finite-difference second derivatives                                                |
| FD<=>                                      | Specifies the finite-difference derivatives                                                       |
| <b>Constraint Specifications</b>           |                                                                                                   |
| LCDEACT=                                   | Specifies the Lagrange multiplier tolerance for deactivating                                      |
| LCEPSILON=                                 | Specifies the range for active constraints                                                        |
| LCSINGULAR=                                | Specifies the tolerance for dependent constraints                                                 |
| <b>Termination Criteria Specifications</b> |                                                                                                   |
| ABSCONV=                                   | Specifies the absolute function convergence criterion                                             |
| ABSFCONV=                                  | Specifies the absolute function difference convergence criterion                                  |
| ABSGCONV=                                  | Specifies the absolute gradient convergence criterion                                             |
| ABSXCONV=                                  | Specifies the absolute parameter convergence criterion                                            |
| FCONV=                                     | Specifies the relative function convergence criterion                                             |
| FCONV2=                                    | Specifies another relative function convergence criterion                                         |
| FDIGITS=                                   | Specifies the number accurate digits in objective function                                        |
| FSIZE=                                     | Specifies the FSIZE parameter of the relative function and relative gradient termination criteria |
| GCONV=                                     | Specifies the relative gradient convergence criterion                                             |
| MAXFUNC=                                   | Specifies the maximum number of function calls                                                    |
| MAXITER=                                   | Specifies the maximum number of iterations                                                        |
| MAXTIME=                                   | Specifies the upper limit seconds of CPU time                                                     |
| MINITER=                                   | Specifies the minimum number of iterations                                                        |
| XCONV=                                     | Specifies the relative parameter convergence criterion                                            |
| XSIZE=                                     | Used in XCONV criterion                                                                           |
| <b>Step Length Specifications</b>          |                                                                                                   |
| DAMPSTEP<=>                                | Specifies the damped steps in line search                                                         |
| INSTEP=                                    | Specifies the initial trust-region radius                                                         |
| MAXSTEP=                                   | Specifies the maximum trust-region radius                                                         |
| <b>Singularity Tolerances</b>              |                                                                                                   |
| SINGCHOL=                                  | Specifies the tolerance for Cholesky roots                                                        |

Table 64.1 *continued*

| Option                              | Description                                        |
|-------------------------------------|----------------------------------------------------|
| SINGHESS=                           | Specifies the tolerance for Hessian                |
| SINGSWEEP=                          | Specifies the tolerance for sweep                  |
| SINGVAR=                            | Specifies the tolerance for variances              |
| <b>Covariance Matrix Tolerances</b> |                                                    |
| ASINGULAR=                          | Specifies the absolute singularity for inertia     |
| CFACTOR=                            | Specifies the multiplication factor for COV matrix |
| COVSING=                            | Specifies the tolerance for singular COV matrix    |
| G4=                                 | Specifies the threshold for Moore-Penrose inverse  |
| MSINGULAR=                          | Specifies the relative M singularity for inertia   |
| VSINGULAR=                          | Specifies the relative V singularity for inertia   |

These options are described in alphabetical order. For a description of the mathematical notation used in the following sections, see the section “[Modeling Assumptions and Notation](#)” on page 5383.

**ABSCONV=r**

**ABSTOL=r**

specifies an absolute function convergence criterion. For minimization, termination requires  $f(\boldsymbol{\theta}^{(k)}) \leq r$ . The default value of  $r$  is the negative square root of the largest double-precision value, which serves only as a protection against overflows.

**ABSFCONV=r<[n]>**

**ABSFTOL=r<[n]>**

specifies an absolute function difference convergence criterion. For all techniques except NMSIMP, termination requires a small change of the function value in successive iterations:

$$|f(\boldsymbol{\theta}^{(k-1)}) - f(\boldsymbol{\theta}^{(k)})| \leq r$$

The same formula is used for the NMSIMP technique, but  $\boldsymbol{\theta}^{(k)}$  is defined as the vertex with the lowest function value, and  $\boldsymbol{\theta}^{(k-1)}$  is defined as the vertex with the highest function value in the simplex. The default value is  $r = 0$ . The optional integer value  $n$  specifies the number of successive iterations for which the criterion must be satisfied before the process can be terminated.

**ABSGCONV=r<[n]>**

**ABSGTOL=r<[n]>**

specifies an absolute gradient convergence criterion. Termination requires the maximum absolute gradient element to be small:

$$\max_j |g_j(\boldsymbol{\theta}^{(k)})| \leq r$$

This criterion is not used by the NMSIMP technique. The default value is  $r = 1\text{E-}5$ . The optional integer value  $n$  specifies the number of successive iterations for which the criterion must be satisfied before the process can be terminated.

**ABSXCONV**= $r < [n] >$ **ABSXTOL**= $r < [n] >$ 

specifies an absolute parameter convergence criterion. For all techniques except NMSIMP, termination requires a small Euclidean distance between successive parameter vectors,

$$\| \boldsymbol{\theta}^{(k)} - \boldsymbol{\theta}^{(k-1)} \|_2 \leq r$$

For the NMSIMP technique, termination requires either a small length  $\alpha^{(k)}$  of the vertices of a restart simplex,

$$\alpha^{(k)} \leq r$$

or a small simplex size,

$$\delta^{(k)} \leq r$$

where the simplex size  $\delta^{(k)}$  is defined as the L1 distance from the simplex vertex  $\boldsymbol{\xi}^{(k)}$  with the smallest function value to the other  $n$  simplex points  $\boldsymbol{\theta}_l^{(k)} \neq \boldsymbol{\xi}^{(k)}$ :

$$\delta^{(k)} = \sum_{\boldsymbol{\theta}_l^{(k)} \neq \boldsymbol{\xi}^{(k)}} \| \boldsymbol{\theta}_l^{(k)} - \boldsymbol{\xi}^{(k)} \|_1$$

The default is  $r = 1\text{E-}8$  for the NMSIMP technique and  $r = 0$  otherwise. The optional integer value  $n$  specifies the number of successive iterations for which the criterion must be satisfied before the process can terminate.

**ALPHA**= $\alpha$ 

specifies the alpha level to be used in computing confidence limits. The default value is 0.05.

**ASINGULAR**= $r$ **ASING**= $r$ 

specifies an absolute singularity criterion for the computation of the inertia (number of positive, negative, and zero eigenvalues) of the Hessian and its projected forms. The default value is the square root of the smallest positive double-precision value.

**CFACTOR**= $f$ 

specifies a multiplication factor  $f$  for the estimated covariance matrix of the parameter estimates.

**COV**

requests the approximate covariance matrix for the parameter estimates.

**CORR**

requests the approximate correlation matrix for the parameter estimates.

**COVSING**= $r > 0$ 

specifies a nonnegative threshold that determines whether the eigenvalues of a singular Hessian matrix are considered to be zero.

**DAMPSTEP** $\langle =r \rangle$ **DS** $\langle =r \rangle$ 

specifies that the initial step-size value  $\alpha^{(0)}$  for each line search (used by the QUANEW, CONGRA, or NEWRAP technique) cannot be larger than  $r$  times the step-size value used in the former iteration. If you specify the DAMPSTEP option without factor  $r$ , the default value is  $r = 2$ . The DAMPSTEP= $r$  option can prevent the line-search algorithm from repeatedly stepping into regions where some objective functions are difficult to compute or where they could lead to floating-point overflows during the computation of objective functions and their derivatives. The DAMPSTEP= $r$  option can save time-costly function calls that result in very small step sizes  $\alpha$ . For more details on setting the start values of each line search, see the section “Restricting the Step Length” on page 5398.

**DATA**=SAS-data-set

specifies the input data set. Observations in this data set are used to compute the log likelihood function that you specify with PROC NLMIXED statements.

**NOTE:** If you are using a **RANDOM** statement, the input data set must be clustered according to the **SUBJECT=** variable. One easy way to accomplish this is to sort your data by the **SUBJECT=** variable prior to calling PROC NLMIXED. PROC NLMIXED does not sort the input data set for you.

**DF**= $d$ 

specifies the degrees of freedom to be used in computing  $p$  values and confidence limits. The default value is the number of subjects minus the number of random effects for random effects models, and the number of observations otherwise.

**DIAHES**

specifies that only the diagonal of the Hessian is used.

**EBOPT**

requests that a more comprehensive optimization be carried out if the default empirical Bayes optimization fails to converge.

**EBSSFRAC**= $r > 0$ 

specifies the step-shortening fraction to be used while computing empirical Bayes estimates of the random effects. The default value is 0.8.

**EBSSTOL**= $r \geq 0$ 

specifies the objective function tolerance for determining the cessation of step-shortening while computing empirical Bayes estimates of the random effects. The default value is  $r = 1\text{E}-8$ .

**EBSTEPS**= $n \geq 0$ 

specifies the maximum number of Newton steps for computing empirical Bayes estimates of random effects. The default value is  $n = 50$ .

**EBSUBSTEPS**= $n \geq 0$ 

specifies the maximum number of step-shortenings for computing empirical Bayes estimates of random effects. The default value is  $n = 20$ .

**EBTOL**= $r \geq 0$ 

specifies the convergence tolerance for empirical Bayes estimation. The default value is  $r = \epsilon\text{E}4$ , where  $\epsilon$  is the machine precision. This default value equals approximately  $1\text{E}-12$  on most machines.

**EBZSTART**

requests that a zero be used as starting values during empirical Bayes estimation. By default, the starting values are set equal to the estimates from the previous iteration (or zero for the first iteration).

**ECOV**

requests the approximate covariance matrix for all expressions specified in **ESTIMATE** statements.

**ECORR**

requests the approximate correlation matrix for all expressions specified in **ESTIMATE** statements.

**EDER**

requests the derivatives of all expressions specified in **ESTIMATE** statements with respect to each of the model parameters.

**EMPIRICAL**

requests that the covariance matrix of the parameter estimates be computed as a likelihood-based empirical (“sandwich”) estimator (White 1982). If  $f(\boldsymbol{\theta}) = -\log\{m(\boldsymbol{\theta})\}$  is the objective function for the optimization and  $m(\boldsymbol{\theta})$  denotes the marginal log likelihood (see the section “**Modeling Assumptions and Notation**” on page 5383 for notation and further definitions) the empirical estimator is computed as

$$\mathbf{H}(\hat{\boldsymbol{\theta}})^{-1} \left( \sum_{i=1}^s \mathbf{g}_i(\hat{\boldsymbol{\theta}}) \mathbf{g}_i(\hat{\boldsymbol{\theta}})' \right) \mathbf{H}(\hat{\boldsymbol{\theta}})^{-1}$$

where  $\mathbf{H}$  is the second derivative matrix of  $f$  and  $\mathbf{g}_i$  is the first derivative of the contribution to  $f$  by the  $i$ th subject. If you choose the **EMPIRICAL** option, this estimator of the covariance matrix of the parameter estimates replaces the model-based estimator  $\mathbf{H}(\hat{\boldsymbol{\theta}})^{-1}$  in subsequent calculations. You can output the subject-specific gradients  $\mathbf{g}_i$  to a SAS data set with the **SUBGRADIENT** option in the **PROC NL MIXED** statement.

The **EMPIRICAL** option requires the presence of a **RANDOM** statement and is available for **METHOD=GAUSS** and **METHOD=ISAMP** only.

**FCONV=r<[n]>****FTOL=r<[n]>**

specifies a relative function convergence criterion. For all techniques except **NMSIMP**, termination requires a small relative change of the function value in successive iterations,

$$\frac{|f(\boldsymbol{\theta}^{(k)}) - f(\boldsymbol{\theta}^{(k-1)})|}{\max(|f(\boldsymbol{\theta}^{(k-1)})|, \text{FSIZE})} \leq r$$

where **FSIZE** is defined by the **FSIZE=** option. The same formula is used for the **NMSIMP** technique, but  $\boldsymbol{\theta}^{(k)}$  is defined as the vertex with the lowest function value, and  $\boldsymbol{\theta}^{(k-1)}$  is defined as the vertex with the highest function value in the simplex. The default is  $r = 10^{-\text{FDIGITS}}$ , where **FDIGITS** is the value of the **FDIGITS=** option. The optional integer value  $n$  specifies the number of successive iterations for which the criterion must be satisfied before the process can terminate.

**FCONV2**= $r$ <[ $n$ ]>

**FTOL2**= $r$ <[ $n$ ]>

specifies another function convergence criterion. For all techniques except NMSIMP, termination requires a small predicted reduction

$$df^{(k)} \approx f(\boldsymbol{\theta}^{(k)}) - f(\boldsymbol{\theta}^{(k)} + \mathbf{s}^{(k)})$$

of the objective function. The predicted reduction

$$\begin{aligned} df^{(k)} &= -\mathbf{g}^{(k)'} \mathbf{s}^{(k)} - \frac{1}{2} \mathbf{s}^{(k)'} \mathbf{H}^{(k)} \mathbf{s}^{(k)} \\ &= -\frac{1}{2} \mathbf{s}^{(k)'} \mathbf{g}^{(k)} \\ &\leq r \end{aligned}$$

is computed by approximating the objective function  $f$  by the first two terms of the Taylor series and substituting the Newton step:

$$\mathbf{s}^{(k)} = -[\mathbf{H}^{(k)}]^{-1} \mathbf{g}^{(k)}$$

For the NMSIMP technique, termination requires a small standard deviation of the function values of the  $n + 1$  simplex vertices  $\boldsymbol{\theta}_l^{(k)}$ ,  $l = 0, \dots, n$ ,

$$\sqrt{\frac{1}{n+1} \sum_l \left[ f(\boldsymbol{\theta}_l^{(k)}) - \bar{f}(\boldsymbol{\theta}^{(k)}) \right]^2} \leq r$$

where  $\bar{f}(\boldsymbol{\theta}^{(k)}) = \frac{1}{n+1} \sum_l f(\boldsymbol{\theta}_l^{(k)})$ . If there are  $n_{act}$  boundary constraints active at  $\boldsymbol{\theta}^{(k)}$ , the mean and standard deviation are computed only for the  $n + 1 - n_{act}$  unconstrained vertices. The default value is  $r = 1\text{E-}6$  for the NMSIMP technique and  $r = 0$  otherwise. The optional integer value  $n$  specifies the number of successive iterations for which the criterion must be satisfied before the process can terminate.

**FD** <= **FORWARD** | **CENTRAL** |  $r$ >

specifies that all derivatives be computed using finite difference approximations. The following specifications are permitted:

**FD** is equivalent to **FD**=100.

**FD**=**CENTRAL** uses central differences.

**FD**=**FORWARD** uses forward differences.

**FD**= $r$  uses central differences for the initial and final evaluations of the gradient and for the Hessian. During iteration, start with forward differences and switch to a corresponding central-difference formula during the iteration process when one of the following two criteria is satisfied:

- The absolute maximum gradient element is less than or equal to  $r$  times the **ABSGCONV**= threshold.
- The normalized predicted function reduction (see the **GTOL** option) is less than or equal to  $\max(1\text{E-}6, r \times \text{GTOL})$ . The  $1\text{E-}6$  ensures that the switch is done, even if you set the **GTOL** threshold to zero.

Note that the FD and FDHESSIAN options cannot apply at the same time. The FDHESSIAN option is ignored when only first-order derivatives are used. See the section “[Finite-Difference Approximations of Derivatives](#)” on page 5393 for more information.

**FDHESSIAN**<=**FORWARD** | **CENTRAL**>

**FDHES**<=**FORWARD** | **CENTRAL**>

**FDH**<=**FORWARD** | **CENTRAL**>

specifies that second-order derivatives be computed using finite difference approximations based on evaluations of the gradients.

FDHESSIAN=FORWARD uses forward differences.

FDHESSIAN=CENTRAL uses central differences.

FDHESSIAN uses forward differences for the Hessian except for the initial and final output.

Note that the FD and FDHESSIAN options cannot apply at the same time. See the section “[Finite-Difference Approximations of Derivatives](#)” on page 5393 for more information.

**FDIGITS**=*r*

specifies the number of accurate digits in evaluations of the objective function. Fractional values such as FDIGITS=4.7 are allowed. The default value is  $r = -\log_{10} \epsilon$ , where  $\epsilon$  is the machine precision. The value of  $r$  is used to compute the interval size  $h$  for the computation of finite-difference approximations of the derivatives of the objective function and for the default value of the **FCONV**= option.

**FLOW**

displays a message for each statement in the model program as it is executed. This debugging option is very rarely needed and produces voluminous output.

**FSIZE**=*r*

specifies the FSIZE parameter of the relative function and relative gradient termination criteria. The default value is  $r = 0$ . For more details, see the **FCONV**= and **GCONV**= options.

**G4**= $n > 0$

specifies a dimension to determine the type of generalized inverse to use when the approximate covariance matrix of the parameter estimates is singular. The default value of  $n$  is 60. See the section “[Covariance Matrix](#)” on page 5402 for more information.

**GCONV**=*r*< [*n*]>

**GTOL**=*r*< [*n*]>

specifies a relative gradient convergence criterion. For all techniques except CONGRA and NMSIMP, termination requires that the normalized predicted function reduction is small,

$$\frac{\mathbf{g}(\boldsymbol{\theta}^{(k)})' [\mathbf{H}^{(k)}]^{-1} \mathbf{g}(\boldsymbol{\theta}^{(k)})}{\max(|f(\boldsymbol{\theta}^{(k)})|, \text{FSIZE})} \leq r$$

where FSIZE is defined by the FSIZE= option. For the CONGRA technique (where a reliable Hessian estimate  $H$  is not available), the following criterion is used:

$$\frac{\|\mathbf{g}(\boldsymbol{\theta}^{(k)})\|_2^2 \|\mathbf{s}(\boldsymbol{\theta}^{(k)})\|_2}{\|\mathbf{g}(\boldsymbol{\theta}^{(k)}) - \mathbf{g}(\boldsymbol{\theta}^{(k-1)})\|_2 \max(|f(\boldsymbol{\theta}^{(k)})|, \text{FSIZE})} \leq r$$



This criterion is not used by the NMSIMP technique.

The default value is  $r = 1\text{E-}8$ . The optional integer value  $n$  specifies the number of successive iterations for which the criterion must be satisfied before the process can terminate.

**HESCAL=0|1|2|3**

**HS=0|1|2|3**

specifies the scaling version of the Hessian matrix used in NRRIDG, TRUREG, NEWRAP, or DBLDOG optimization.

If HS is not equal to 0, the first iteration and each restart iteration sets the diagonal scaling matrix  $\mathbf{D}^{(0)} = \text{diag}(d_i^{(0)})$ :

$$d_i^{(0)} = \sqrt{\max(|H_{i,i}^{(0)}|, \epsilon)}$$

where  $H_{i,i}^{(0)}$  are the diagonal elements of the Hessian. In every other iteration, the diagonal scaling matrix  $\mathbf{D}^{(0)} = \text{diag}(d_i^{(0)})$  is updated depending on the HS option:

HS=0 specifies that no scaling is done.

HS=1 specifies the Moré (1978) scaling update:

$$d_i^{(k+1)} = \max \left[ d_i^{(k)}, \sqrt{\max(|H_{i,i}^{(k)}|, \epsilon)} \right]$$

HS=2 specifies the Dennis, Gay, and Welsch (1981) scaling update:

$$d_i^{(k+1)} = \max \left[ 0.6 * d_i^{(k)}, \sqrt{\max(|H_{i,i}^{(k)}|, \epsilon)} \right]$$

HS=3 specifies that  $d_i$  is reset in each iteration:

$$d_i^{(k+1)} = \sqrt{\max(|H_{i,i}^{(k)}|, \epsilon)}$$

In each scaling update,  $\epsilon$  is the relative machine precision. The default value is HS=0. Scaling of the Hessian can be time-consuming in the case where general linear constraints are active.

## HESS

requests the display of the final Hessian matrix after optimization. If you also specify the **START** option, then the Hessian at the starting values is also printed.

**INHESIAN<=r>**

**INHES<=r>**

specifies how the initial estimate of the approximate Hessian is defined for the quasi-Newton techniques QUANEW and DBLDOG. There are two alternatives:

- If you do not use the  $r$  specification, the initial estimate of the approximate Hessian is set to the Hessian at  $\theta^{(0)}$ .
- If you do use the  $r$  specification, the initial estimate of the approximate Hessian is set to the multiple of the identity matrix,  $r\mathbf{I}$ .

By default, if you do not specify the option **INHESIAN=r**, the initial estimate of the approximate Hessian is set to the multiple of the identity matrix  $r\mathbf{I}$ , where the scalar  $r$  is computed from the magnitude of the initial gradient.

**INSTEP=*r***

reduces the length of the first trial step during the line search of the first iterations. For highly nonlinear objective functions, such as the EXP function, the default initial radius of the trust-region algorithm TRUREG or DBLDOG or the default step length of the line-search algorithms can result in arithmetic overflows. If this occurs, you should specify decreasing values of  $0 < r < 1$  such as INSTEP=1E-1, INSTEP=1E-2, INSTEP=1E-4, and so on, until the iteration starts successfully.

- For trust-region algorithms (TRUREG, DBLDOG), the INSTEP= option specifies a factor  $r > 0$  for the initial radius  $\Delta^{(0)}$  of the trust region. The default initial trust-region radius is the length of the scaled gradient. This step corresponds to the default radius factor of  $r = 1$ .
- For line-search algorithms (NEWRAP, CONGRA, QUANEW), the INSTEP= option specifies an upper bound for the initial step length for the line search during the first five iterations. The default initial step length is  $r = 1$ .
- For the Nelder-Mead simplex algorithm, using TECH=NMSIMP, the INSTEP=*r* option defines the size of the start simplex.

For more details, see the section “[Computational Problems](#)” on page 5399.

**ITDETAILS**

requests a more complete iteration history, including the current values of the parameter estimates, their gradients, and additional optimization statistics. For further details, see the section “[Iterations](#)” on page 5405.

**LCDEACT=*r*****LCD=*r***

specifies a threshold  $r$  for the Lagrange multiplier that determines whether an active inequality constraint remains active or can be deactivated. During minimization, an active inequality constraint can be deactivated only if its Lagrange multiplier is less than the threshold value  $r < 0$ . The default value is

$$r = -\min(0.01, \max(0.1 \times \text{ABSGCONV}, 0.001 \times \text{gmax}^{(k)}))$$

where ABSGCONV is the value of the absolute gradient criterion, and  $\text{gmax}^{(k)}$  is the maximum absolute element of the (projected) gradient  $\mathbf{g}^{(k)}$  or  $\mathbf{Z}'\mathbf{g}^{(k)}$ . (See the section “[Active Set Methods](#)” for a definition of  $\mathbf{Z}$ .)

**LCEPSILON=*r* > 0****LCEPS=*r* > 0****LCE=*r* > 0**

specifies the range for active and violated boundary constraints. The default value is  $r = 1\text{E}-8$ . During the optimization process, the introduction of rounding errors can force PROC NL MIXED to increase the value of  $r$  by a factor of 10, 100, . . . . If this happens, it is indicated by a message displayed in the log.

**LCSINGULAR= $r > 0$** **LCSING= $r > 0$** **LCS= $r > 0$** 

specifies a criterion  $r$ , used in the update of the QR decomposition, that determines whether an active constraint is linearly dependent on a set of other active constraints. The default value is  $r = 1\text{E-}8$ . The larger  $r$  becomes, the more the active constraints are recognized as being linearly dependent. If the value of  $r$  is larger than 0.1, it is reset to 0.1.

**LINESEARCH= $i$** **LIS= $i$** 

specifies the line-search method for the CONGRA, QUANEW, and NEWRAP optimization techniques. See Fletcher (1987) for an introduction to line-search techniques. The value of  $i$  can be  $1, \dots, 8$ . For CONGRA, QUANEW and NEWRAP, the default value is  $i = 2$ .

- |       |                                                                                                                                                                                                                                                                                 |
|-------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| LIS=1 | specifies a line-search method that needs the same number of function and gradient calls for cubic interpolation and cubic extrapolation; this method is similar to one used by the Harwell subroutine library.                                                                 |
| LIS=2 | specifies a line-search method that needs more function than gradient calls for quadratic and cubic interpolation and cubic extrapolation; this method is implemented as shown in Fletcher (1987) and can be modified to an exact line search by using the LSPRECISION= option. |
| LIS=3 | specifies a line-search method that needs the same number of function and gradient calls for cubic interpolation and cubic extrapolation; this method is implemented as shown in Fletcher (1987) and can be modified to an exact line search by using the LSPRECISION= option.  |
| LIS=4 | specifies a line-search method that needs the same number of function and gradient calls for stepwise extrapolation and cubic interpolation.                                                                                                                                    |
| LIS=5 | specifies a line-search method that is a modified version of LIS=4.                                                                                                                                                                                                             |
| LIS=6 | specifies golden section line search (Polak 1971), which uses only function values for linear approximation.                                                                                                                                                                    |
| LIS=7 | specifies bisection line search (Polak 1971), which uses only function values for linear approximation.                                                                                                                                                                         |
| LIS=8 | specifies the Armijo line-search technique (Polak 1971), which uses only function values for linear approximation.                                                                                                                                                              |

**LIST**

displays the model program and variable lists. The LIST option is a debugging feature and is not normally needed.

**LISTCODE**

displays the derivative tables and the compiled program code. The LISTCODE option is a debugging feature and is not normally needed.

**LISTDEP**

produces a report that lists, for each variable in the program, the variables that depend on it and on which it depends. The LISTDEP option is a debugging feature and is not normally needed.

**LISTDER**

displays a table of derivatives. This table lists each nonzero derivative computed for the problem. The LISTDER option is a debugging feature and is not normally needed.

**LOGNOTE**<=*n*>

writes periodic notes to the log that describe the current status of computations. It is designed for use with analyses requiring extensive CPU resources. The optional integer value *n* specifies the desired level of reporting detail. The default is *n* = 1. Choosing *n* = 2 adds information about the objective function values at the end of each iteration. The most detail is obtained with *n* = 3, which also reports the results of function evaluations within iterations.

**LSPRECISION**=*r***LSP**=*r*

specifies the degree of accuracy that should be obtained by the line-search algorithms LIS=2 and LIS=3. Usually an imprecise line search is inexpensive and successful. For more difficult optimization problems, a more precise and expensive line search might be necessary (Fletcher 1987). The second line-search method (which is the default for the NEWRAP, QUANEW, and CONGRA techniques) and the third line-search method approach exact line search for small LSPRECISION= values. If you have numerical problems, you should try to decrease the LSPRECISION= value to obtain a more precise line search. The default values are shown in the following table.

| <b>TECH=</b> | <b>UPDATE=</b> | <b>LSP default</b> |
|--------------|----------------|--------------------|
| QUANEW       | DBFGS, BFGS    | <i>r</i> = 0.4     |
| QUANEW       | DDFP, DFP      | <i>r</i> = 0.06    |
| CONGRA       | all            | <i>r</i> = 0.1     |
| NEWRAP       | no update      | <i>r</i> = 0.9     |

For more details, see Fletcher (1987).

**MAXFUNC**=*i***MAXFU**=*i*

specifies the maximum number *i* of function calls in the optimization process. The default values are as follows:

- TRUREG, NRRIDG, NEWRAP: 125
- QUANEW, DBLDOG: 500
- CONGRA: 1000
- NMSIMP: 3000

Note that the optimization can terminate only after completing a full iteration. Therefore, the number of function calls that is actually performed can exceed the number that is specified by the MAXFUNC= option.

**MAXITER=*i*****MAXIT=*i***

specifies the maximum number *i* of iterations in the optimization process. The default values are as follows:

- TRUREG, NRRIDG, NEWRAP: 50
- QUANEW, DBLDOG: 200
- CONGRA: 400
- NMSIMP: 1000

These default values are also valid when *i* is specified as a missing value.

**MAXSTEP=*r*<[*n*]>**

specifies an upper bound for the step length of the line-search algorithms during the first *n* iterations. By default, *r* is the largest double-precision value and *n* is the largest integer available. Setting this option can improve the speed of convergence for the CONGRA, QUANEW, and NEWRAP techniques.

**MAXTIME=*r***

specifies an upper limit of *r* seconds of CPU time for the optimization process. The default value is the largest floating-point double representation of your computer. Note that the time specified by the MAXTIME= option is checked only once at the end of each iteration. Therefore, the actual running time can be much longer than that specified by the MAXTIME= option. The actual running time includes the rest of the time needed to finish the iteration and the time needed to generate the output of the results.

**METHOD=*value***

specifies the method for approximating the integral of the likelihood over the random effects. Valid values are as follows:

**FIRO**

specifies the first-order method of Beal and Sheiner (1982). When using METHOD=FIRO, you must specify the NORMAL distribution in the MODEL statement and you must also specify a RANDOM statement.

**GAUSS**

specifies adaptive Gauss-Hermite quadrature (Pinheiro and Bates 1995). You can prevent the adaptation with the NOAD option or prevent adaptive scaling with the NOADSCALE option. This is the default integration method.

**HARDY**

specifies Hardy quadrature based on an adaptive trapezoidal rule. This method is available only for one-dimensional integrals; that is, you must specify only one random effect.

**ISAMP**

specifies adaptive importance sampling (Pinheiro and Bates 1995). You can prevent the adaptation with the NOAD option or prevent adaptive scaling with the NOADSCALE option. You can use the SEED= option to specify a starting seed for the random number generation used in the importance sampling. If you do not specify a seed, or if you specify a value less than or equal to zero, the seed is generated from reading the time of day from the computer clock.

**MINITER=*i*****MINIT=*i***

specifies the minimum number of iterations. The default value is 0. If you request more iterations than are actually needed for convergence to a stationary point, the optimization algorithms can behave strangely. For example, the effect of rounding errors can prevent the algorithm from continuing for the required number of iterations.

**MSINGULAR= $r > 0$** **MSING= $r > 0$** 

specifies a relative singularity criterion for the computation of the inertia (number of positive, negative, and zero eigenvalues) of the Hessian and its projected forms. The default value is  $1E-12$  if you do not specify the SINGHESS= option; otherwise, the default value is  $\max(10\epsilon, (1E-4) \times \text{SINGHESS})$ . See the section “Covariance Matrix” on page 5402 for more information.

**NOAD**

requests that the Gaussian quadrature be nonadaptive; that is, the quadrature points are centered at zero for each of the random effects and the current random-effects variance matrix is used as the scale matrix.

**NOADSCALE**

requests nonadaptive scaling for adaptive Gaussian quadrature; that is, the quadrature points are centered at the empirical Bayes estimates for the random effects, but the current random-effects variance matrix is used as the scale matrix. By default, the observed Hessian from the current empirical Bayes estimates is used as the scale matrix.

**OPTCHECK $\langle =r > 0 \rangle$** 

computes the function values  $f(\theta_l)$  of a grid of points  $\theta_l$  in a ball of radius of  $r$  about  $\theta^*$ . If you specify the OPTCHECK option without factor  $r$ , the default value is  $r = 0.1$  at the starting point and  $r = 0.01$  at the terminating point. If a point  $\theta_l^*$  is found with a better function value than  $f(\theta^*)$ , then optimization is restarted at  $\theta_l^*$ .

**OUTQ=*SAS-data-set***

specifies an output data set containing the quadrature points used for numerical integration.

**QFAC= $r > 0$** 

specifies the additive factor used to adaptively search for the number of quadrature points. For **METHOD=GAUSS**, the search sequence is 1, 3, 5, 7, 9, 11,  $11 + r$ ,  $11 + 2r$ , ..., where the default value of  $r$  is 10. For **METHOD=ISAMP**, the search sequence is 10,  $10 + r$ ,  $10 + 2r$ , ..., where the default value of  $r$  is 50.

**QMAX= $r > 0$** 

specifies the maximum number of quadrature points permitted before the adaptive search is aborted. The default values are 31 for adaptive Gaussian quadrature, 61 for nonadaptive Gaussian quadrature, 160 for adaptive importance sampling, and 310 for nonadaptive importance sampling.

**QPOINTS= $n > 0$** 

specifies the number of quadrature points to be used during evaluation of integrals. For **METHOD=GAUSS**,  $n$  equals the number of points used in each dimension of the random effects, resulting in a total of  $n^r$  points, where  $r$  is the number of dimensions. For **METHOD=ISAMP**,  $n$  specifies the total number of quadrature points regardless of the dimension of the random effects.

By default, the number of quadrature points is selected adaptively, and this option disables the adaptive search.

**QSCALEFAC= $r > 0$** 

specifies a multiplier for the scale matrix used during quadrature calculations. The default value is 1.0.

**QTOL= $r > 0$** 

specifies the tolerance used to adaptively select the number of quadrature points. When the relative difference between two successive likelihood calculations is less than  $r$ , then the search terminates and the lesser number of quadrature points is used during the subsequent optimization process. The default value is  $1E-4$ .

**RESTART= $i > 0$** **REST= $i > 0$** 

specifies that the QUANEW or CONGRA algorithm is restarted with a steepest descent/ascent search direction after, at most,  $i$  iterations. Default values are as follows:

- CONGRA: UPDATE=PB: restart is performed automatically,  $i$  is not used.
- CONGRA: UPDATE $\neq$ PB:  $i = \min(10n, 80)$ , where  $n$  is the number of parameters.
- QUANEW:  $i$  is the largest integer available.

**SEED= $i$** 

specifies the random number seed for **METHOD=ISAMP**. If you do not specify a seed, or if you specify a value less than or equal to zero, the seed is generated from reading the time of day from the computer clock. The value must be less than  $2^{31} - 1$ .

**SINGCHOL= $r > 0$** 

specifies the singularity criterion  $r$  for Cholesky roots of the random-effects variance matrix and scale matrix for adaptive Gaussian quadrature. The default value is  $1E4$  times the machine epsilon; this product is approximately  $1E-12$  on most computers.

**SINGHESS= $r > 0$** 

specifies the singularity criterion  $r$  for the inversion of the Hessian matrix. The default value is  $1E-8$ . See the ASINGULAR, MSINGULAR=, and VSINGULAR= options for more information.

**SINGSWEEP= $r > 0$** 

specifies the singularity criterion  $r$  for inverting the variance matrix in the first-order method and the empirical Bayes Hessian matrix. The default value is  $1E4$  times the machine epsilon; this product is approximately  $1E-12$  on most computers.

**SINGVAR= $r > 0$** 

specifies the singularity criterion  $r$  below which statistical variances are considered to equal zero. The default value is  $1E4$  times the machine epsilon; this product is approximately  $1E-12$  on most computers.

**START**

requests that the gradient of the log likelihood at the starting values be displayed. If you also specify the **HESS** option, then the starting Hessian is displayed as well.

**SUBGRADIENT**=*SAS-data-set*

**SUBGRAD**=*SAS-data-set*

specifies a SAS data set to save in models with **RANDOM** statement the subject-specific gradients of the integrated, marginal log-likelihood with respect to all parameters. The sum of the subject-specific gradients equals the gradient reported in the “Parameter Estimates” table. The data set contains a variable identifying the subjects.

In models without **RANDOM** statement the **SUBGRADIENT**= data set contains the observation-wise gradient. The variable identifying the **SUBJECT**= is then replaced with the Observation. This observation counter includes observations not used in the analysis and is reset in each **BY**-group.

Saving disaggregated gradient information with the **SUBGRADIENT**= option requires **METHOD**=**GAUSS** or **METHOD**=**ISAMP**.

**TECHNIQUE**=*value*

**TECH**=*value*

specifies the optimization technique. By default, **TECH** = **QUANEW**. Valid values are as follows:

- **CONGRA**  
performs a conjugate-gradient optimization, which can be more precisely specified with the **UPDATE**= option and modified with the **LINESEARCH**= option. When you specify this option, **UPDATE**=**PB** by default.
- **DBLDOG**  
performs a version of double-dogleg optimization, which can be more precisely specified with the **UPDATE**= option. When you specify this option, **UPDATE**=**DBFGS** by default.
- **NMSIMP**  
performs a Nelder-Mead simplex optimization.
- **NONE**  
does not perform any optimization. This option can be used as follows:
  - to perform a grid search without optimization
  - to compute estimates and predictions that cannot be obtained efficiently with any of the optimization techniques
- **NEWRAP**  
performs a Newton-Raphson optimization combining a line-search algorithm with ridging. The line-search algorithm **LIS**=**2** is the default method.
- **NRRIDG**  
performs a Newton-Raphson optimization with ridging.
- **QUANEW**  
performs a quasi-Newton optimization, which can be defined more precisely with the **UPDATE**= option and modified with the **LINESEARCH**= option. This is the default estimation method.
- **TRUREG**  
performs a trust region optimization.



**TRACE**

displays the result of each operation in each statement in the model program as it is executed. This debugging option is very rarely needed, and it produces voluminous output.

**UPDATE=method****UPD=method**

specifies the update method for the quasi-Newton, double-dogleg, or conjugate-gradient optimization technique. Not every update method can be used with each optimizer. See the section “[Optimization Algorithms](#)” on page 5388 for more information.

Valid methods are as follows:

- **BFGS**  
performs the original Broyden, Fletcher, Goldfarb, and Shanno (BFGS) update of the inverse Hessian matrix.
- **DBFGS**  
performs the dual BFGS update of the Cholesky factor of the Hessian matrix. This is the default update method.
- **DDFP**  
performs the dual Davidon, Fletcher, and Powell (DFP) update of the Cholesky factor of the Hessian matrix.
- **DFP**  
performs the original DFP update of the inverse Hessian matrix.
- **PB**  
performs the automatic restart update method of Powell (1977) and Beale (1972).
- **FR**  
performs the Fletcher-Reeves update (Fletcher 1987).
- **PR**  
performs the Polak-Ribiere update (Fletcher 1987).
- **CD**  
performs a conjugate-descent update of Fletcher (1987).

**VSINGULAR=r > 0****VSING=r > 0**

specifies a relative singularity criterion for the computation of the inertia (number of positive, negative, and zero eigenvalues) of the Hessian and its projected forms. The default value is  $r = 1\text{E-}8$  if the **SINGHESS=** option is not specified, and it is the value of **SINGHESS=** option otherwise. See the section “[Covariance Matrix](#)” on page 5402 for more information.

**XCONV=r < [n] >****XTOL=r < [n] >**

specifies the relative parameter convergence criterion. For all techniques except NMSIMP, termination requires a small relative parameter change in subsequent iterations:

$$\frac{\max_j |\theta_j^{(k)} - \theta_j^{(k-1)}|}{\max(|\theta_j^{(k)}|, |\theta_j^{(k-1)}|, \text{XSIZE})} \leq r$$

For the NMSIMP technique, the same formula is used, but  $\theta^{(k)}$  is defined as the vertex with the lowest function value and  $\theta^{(k-1)}$  is defined as the vertex with the highest function value in the simplex.

The default value is  $r = 1E-8$  for the NMSIMP technique and  $r = 0$  otherwise. The optional integer value  $n$  specifies the number of successive iterations for which the criterion must be satisfied before the process can be terminated.

#### **XREF**

displays a cross-reference of the variables in the program showing where each variable is referenced or given a value. The XREF listing does not include derivative variables. This option is a debugging feature and is not normally needed.

#### **XSIZE= $r > 0$**

specifies the XSIZE parameter of the relative parameter termination criterion. The default value is  $r = 0$ . For more details, see the **XCONV=** option.

---

## **ARRAY Statement**

**ARRAY** *arrayname* [ *dimensions* ] <\$> <*variables-and-constants*> ;

The ARRAY statement is similar to, but not exactly the same as, the ARRAY statement in the SAS DATA step, and it is exactly the same as the ARRAY statements in the NLIN, NLP, and MODEL procedures. The ARRAY statement is used to associate a name (of no more than eight characters) with a list of variables and constants. The array name is used with subscripts in the program to refer to the array elements. The following statements illustrate this:

```
array r[8] r1-r8;

do i = 1 to 8;
 r[i] = 0;
end;
```

The ARRAY statement does not support all the features of the ARRAY statement in the DATA step. It cannot be used to assign initial values to array elements. Implicit indexing of variables cannot be used; all array references must have explicit subscript expressions. Only exact array dimensions are allowed; lower-bound specifications are not supported. A maximum of six dimensions is allowed.

On the other hand, the ARRAY statement does allow both variables and constants to be used as array elements. (Constant array elements cannot have values assigned to them.) Both dimension specification and the list of elements are optional, but at least one must be specified. When the list of elements is not specified or fewer elements than the size of the array are listed, array variables are created by suffixing element numbers to the array name to complete the element list.

---

## BOUNDS Statement

**BOUNDS** *b-con* <, *b-con* ... >;

where *b-con* := number *operator* parameter\_list *operator* number  
 or *b-con* := number *operator* parameter\_list  
 or *b-con* := parameter\_list *operator* number  
 and *operator* := <=, <, >=, or >

Boundary constraints are specified with a BOUNDS statement. One- or two-sided boundary constraints are allowed. The list of boundary constraints are separated by commas. For example:

```
bounds 0 <= a1-a9 x <= 1, -1 <= c2-c5;
bounds b1-b10 y >= 0;
```

You can specify more than one BOUNDS statement. If you specify more than one lower (upper) bound for the same parameter, the maximum (minimum) of these is taken.

If the maximum  $l_j$  of all lower bounds is larger than the minimum of all upper bounds  $u_j$  for the same parameter  $\theta_j$ , the boundary constraint is replaced by  $\theta_j := l_j := \min(u_j)$  defined by the minimum of all upper bounds specified for  $\theta_j$ .

---

## BY Statement

**BY** *variables* ;

You can specify a BY statement with PROC NLMIXED to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the NLMIXED procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

An optimization problem is solved for each BY group separately unless the **TECH=NONE** option is specified.

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

---

## CONTRAST Statement

**CONTRAST** *'label'* *expression* < , *expression* > < *options* > ;

The CONTRAST statement enables you to conduct a statistical test that several expressions simultaneously equal zero. The expressions are typically contrasts—that is, differences whose expected values equal zero under the hypothesis of interest.

In the CONTRAST statement you must provide a quoted string to identify the contrast and then a list of valid SAS expressions separated by commas. Multiple CONTRAST statements are permitted, and results from all statements are listed in a common table. PROC NL MIXED constructs approximate  $F$  tests for each statement using the delta method (Cox 1998) to approximate the variance-covariance matrix of the constituent expressions.

The following option is available in the CONTRAST statement:

**DF=*d***

specifies the denominator degrees of freedom to be used in computing  $p$  values for the  $F$  statistics. The default value corresponds to the **DF=** option in the PROC NL MIXED statement.

---

## ESTIMATE Statement

**ESTIMATE** *'label'* *expression* < *options* > ;

The ESTIMATE statement enables you to compute an additional estimate that is a function of the parameter values. You must provide a quoted string to identify the estimate and then a valid SAS expression. Multiple ESTIMATE statements are permitted, and results from all statements are listed in a common table. PROC NL MIXED computes approximate standard errors for the estimates using the delta method (Billingsley 1986). It uses these standard errors to compute corresponding  $t$  statistics,  $p$ -values, and confidence limits.

The **ECOV** option in the PROC NL MIXED statement produces a table containing the approximate covariance matrix of all the additional estimates you specify. The **ECORR** option produces the corresponding correlation matrix. The **EDER** option produces a table of the derivatives of the additional estimates with respect to each of the model parameters.

The following options are available in the ESTIMATE statement:

**ALPHA= $\alpha$**

specifies the alpha level to be used in computing confidence limits. The default value corresponds to the **ALPHA=** option in the PROC NL MIXED statement.

**DF=*d***

specifies the degrees of freedom to be used in computing  $p$ -values and confidence limits. The default value corresponds to the **DF=** option in the PROC NL MIXED statement.

---

## ID Statement

**ID** *names* ;

The ID statement identifies additional quantities to be included in the **OUT=** data set of the **PREDICT** statement. These can be any symbols you have defined with SAS programming statements.

---

## MODEL Statement

**MODEL** *dependent-variable* ~ *distribution* ;

The MODEL statement is the mechanism for specifying the conditional distribution of the data given the random effects. You must specify a single dependent variable from the input data set, a tilde ~, and then a distribution with its parameters. Valid distributions are as follows.

- *normal(m,v)* specifies a normal (Gaussian) distribution with mean *m* and variance *v*.
- *binary(p)* specifies a binary (Bernoulli) distribution with probability *p*.
- *binomial(n,p)* specifies a binomial distribution with count *n* and probability *p*.
- *gamma(a,b)* specifies a gamma distribution with shape *a* and scale *b*.
- *negbin(n,p)* specifies a negative binomial distribution with count *n* and probability *p*.
- *poisson(m)* specifies a Poisson distribution with mean *m*.
- *general(ll)* specifies a general log likelihood function that you construct using SAS programming statements.

The MODEL statement must follow any SAS programming statements you specify for computing parameters of the preceding distributions. See the section “[Built-in Log-Likelihood Functions](#)” on page 5386 for expressions of the built-in conditional log-likelihood functions.

---

## PARMS Statement

**PARMS** < *name-list* <=*numbers*> > < , *name-list* <=*numbers*> ... >  
< / *options* > ;

The PARMS statement lists names of parameters and specifies initial values, possibly over a grid. You can specify the parameters and values directly in a list, or you can provide the name of a SAS data set that contains them by using the **DATA=** option.

While the PARMS statement is not required, you are encouraged to use it to provide PROC NLMIXED with accurate starting values. Parameters not listed in the PARMS statement are assigned an initial value of 1.

PROC NLMIXED considers all symbols not assigned values to be parameters, so you should specify your modeling statements carefully and check the output from the “Parameters” table to make sure the proper parameters are identified.

A list of parameter names in the PARMs statement is not separated by commas and is followed by an equal sign and a list of numbers. If the number list consists of only one number, this number defines the initial value for all the parameters listed to the left of the equal sign.

If the number list consists of more than one number, these numbers specify the grid locations for each of the parameters listed to the left of the equal sign. You can use the TO and BY keywords to specify a number list for a grid search. If you specify a grid of points in a PARMs statement, PROC NLMIXED computes the objective function value at each grid point and chooses the best (feasible) grid point as an initial point for the optimization process. You can use the BEST= option to save memory for the storing and sorting of all grid point information.

The following options are available in the PARMs statement after a slash (/):

**BEST=*i* > 0**

specifies the maximum number of points displayed in the “Parameters” table, selected as the points with the maximum likelihood values. By default, all grid values are displayed.

**BYDATA**

enables you to assign different starting values for each BY group by using the DATA=SAS-*data-set* option during BY processing. By default, BY groups are ignored in the PARMs data set. For the BYDATA option to be effective, the DATA= data set must contain the BY variables and the same BY groups as the primary input data set. When you supply a grid of starting values with the DATA= data set and the BYDATA option is in effect, the size of the grid is determined by the first BY group.

**DATA=SAS-*data-set***

specifies a SAS data set containing parameter names and starting values. The data set should be in one of two forms: narrow or wide. The narrow-form data set contains the variables Parameter and Estimate, with parameters and values listed as distinct observations. The wide-form data set has the parameters themselves as variables, and each observation provides a different set of starting values. By default, BY groups are ignored in this data set, so the same starting grid is evaluated for each BY group. You can vary the starting values for BY groups by using the BYDATA option.

---

## PREDICT Statement

**PREDICT** *expression* **OUT=SAS-*data-set*** < *options* > ;

The PREDICT statement enables you to construct predictions of an expression across all of the observations in the input data set. Any valid SAS programming expression involving the input data set variables, parameters, and random effects is valid. Predicted values are computed using the parameter estimates and empirical Bayes estimates of the random effects. Standard errors of prediction are computed using the delta method (Billingsley 1986; Cox 1998). Results are placed in an output data set that you specify with the OUT= option. Besides all variables from the input data set, the OUT= data set contains the following variables: Pred, StdErrPred, DF, tValue, Probt, Alpha, Lower, Upper. You can also add other computed quantities to this data set with the ID statement.

The following options are available in the PREDICT statement:

**ALPHA= $\alpha$** 

specifies the alpha level to be used in computing  $t$  statistics and intervals. The default value corresponds to the ALPHA= option in the PROC NLMIXED statement.

**DER**

requests that derivatives of the predicted expression with respect to all parameters be included in the OUT= data set. The variable names for the derivatives are the same as the parameter names with the prefix “Der\_” appended. All of the derivatives are evaluated at the final estimates of the parameters and the empirical Bayes estimates of the random effects.

**DF= $d$** 

specifies the degrees of freedom to be used in computing  $t$  statistics and intervals in the OUT= data set. The default value corresponds to the DF= option in the PROC NLMIXED statement.

---

## RANDOM Statement

**RANDOM** *random-effects* ~ *distribution* **SUBJECT=***variable* < *options* > ;

The RANDOM statement defines the random effects and their distribution. The random effects must be represented by symbols that appear in your SAS programming statements. They typically influence the mean value of the distribution specified in the MODEL statement. The RANDOM statement consists of a list of the random effects (usually just one or two symbols), a tilde ~, the distribution for the random effects, and then a SUBJECT= variable.

**NOTE:** The input data set must be clustered according to the SUBJECT= variable. One easy way to accomplish this is to sort your data by the SUBJECT= variable prior to calling PROC NLMIXED. PROC NLMIXED does not sort the input data set for you; rather, it processes the data sequentially and considers an observation to be from a new subject whenever the value of its SUBJECT= variable changes from the previous observation.

The only distribution available for the random effects is normal( $m,v$ ) with mean  $m$  and variance  $v$ .

This syntax is illustrated as follows for one effect:

```
random u ~ normal(0,s2u) subject=clinic;
```

For multiple effects, you should specify bracketed vectors for  $m$  and  $v$ , the latter consisting of the lower triangle of the random-effects variance matrix listed in row order. This is illustrated for two and three random effects as follows:

```
random b1 b2 ~ normal([0,0],[g11,g21,g22]) subject=person;
random b1 b2 b3 ~ normal([0,0,0],[g11,g21,g22,g31,g32,g33])
subject=person;
```

The SUBJECT= variable determines when new realizations of the random effects are assumed to occur. PROC NLMIXED assumes that a new realization occurs whenever the value of the SUBJECT= variable changes from the previous observation, so your input data set should be clustered according to this variable. One easy way to accomplish this is to run PROC SORT prior to calling PROC NLMIXED by using the SUBJECT= variable as the BY variable.

Only one RANDOM statement is permitted, so multilevel nonlinear mixed models are not accommodated. However, you can specify certain nested random effects structure with a single RANDOM statement (see Chapter 15 of Littell et al. (2006) for an example).

The following options are available in the RANDOM statement:

**ALPHA= $\alpha$**

specifies the alpha level to be used in computing  $t$  statistics and intervals. The default value corresponds to the ALPHA= option in the PROC NL MIXED statement.

**DF= $d$**

specifies the degrees of freedom to be used in computing  $t$  statistics and intervals in the OUT= data set. The default value corresponds to the DF= option in the PROC NL MIXED statement.

**OUT=*SAS-data-set***

requests an output data set containing empirical Bayes estimates of the random effects and their approximate standard errors of prediction.

---

## REPLICATE Statement

**REPLICATE** *variable* ;

The REPLICATE statement provides a way to accommodate models in which different subjects have identical data. This occurs most commonly when the dependent variable is binary. When you specify a REPLICATE variable, PROC NL MIXED treats its value as the number of subjects that have data identical to the data for the current value of the SUBJECT= variable (specified in the RANDOM statement). Only the last observation of the REPLICATE variable for each subject is used, and the replicate variable must have only positive values.

The function of a REPLICATE statement is related to but not quite the same as the function of either a FREQ or a WEIGHT statement in other statistical modeling procedures, such as the GLM, GENMOD, GLIMMIX, and LOGISTIC procedures. A FREQ or a WEIGHT value essentially multiplies the log likelihood or sum of squares contribution for each observation. On the other hand, a REPLICATE value multiplies the log likelihood contribution of each subject, which consists of one or more observations. When no SUBJECT= variable is specified, the REPLICATE value behaves like a weight, multiplying each observation's log likelihood contribution.

---

## Programming Statements

This section lists the programming statements used to code the log-likelihood function in PROC NL MIXED. It also documents the differences between programming statements in PROC NL MIXED and programming statements in the SAS DATA step. The syntax of programming statements used in PROC NL MIXED is identical to that used in the CALIS and GENMOD procedures (see Chapter 27 and Chapter 40, respectively), and the MODEL procedure (see the *SAS/ETS User's Guide*). Most of the programming statements that can be used in the SAS DATA step can also be used in the NL MIXED procedure. See *SAS Language Reference: Dictionary* for a description of SAS programming statements. The following are valid statements:



```

ABORT;
ARRAY arrayname < [dimensions] > < $ > < variables-and-constants >;
CALL name < (expression < , expression ... >) >;
DELETE;
DO < variable = expression < TO expression > < BY expression > >
 < , expression < TO expression > < BY expression > > ...
 < WHILE expression > < UNTIL expression >;
END;
GOTO statement-label;
IF expression;
IF expression THEN program-statement;
 ELSE program-statement;
variable = expression;
variable + expression;
LINK statement-label;
PUT < variable > < = > ...;
RETURN;
SELECT < (expression) >;
STOP;
SUBSTR(variable, index, length)= expression;
WHEN (expression)program-statement;
 OTHERWISE program-statement;

```

For the most part, the SAS programming statements work the same as they do in the SAS DATA step, as documented in *SAS Language Reference: Concepts*; however, there are the following differences:

- The ABORT statement does not allow any arguments.
- The DO statement does not allow a character index variable. Thus

```
do i = 1,2,3;
```

is supported, but the following statement is not supported:

```
do i = 'A', 'B', 'C';
```

- The LAG function does work appropriately with PROC NLMIXED, but you can use the ZLAG function instead.
- The PUT statement, used mostly for program debugging in PROC NLMIXED, supports only some of the features of the DATA step PUT statement, and it has some new features that the DATA step PUT statement does not.
  - The PROC NLMIXED PUT statement does not support line pointers, factored lists, iteration factors, overprinting, `_INFILE_`, the colon (:) format modifier, or “\$”.
  - The PROC NLMIXED PUT statement does support expressions, but the expression must be enclosed in parentheses. For example, the following statement displays the square root of x:
 

```
put (sqrt(x));
```

- The PROC NLMIXED PUT statement supports the item `_PDV_` to display a formatted listing of all variables in the program. For example, the following statement displays a much more readable listing of the variables than the `_ALL_` print item:

```
put _pdv_;
```

- The WHEN and OTHERWISE statements enable you to specify more than one target statement. That is, DO/END groups are not necessary for multiple statement WHENs. For example, the following syntax is valid:

```
select;
 when (exp1) stmt1;
 stmt2;
 when (exp2) stmt3;
 stmt4;
end;
```

When coding your programming statements, you should avoid defining variables that begin with an underscore (`_`), because they might conflict with internal variables created by PROC NLMIXED. The `MODEL` statement must come after any SAS programming statements that define or modify terms used in the construction of the log-likelihood.

## Details: NLMIXED Procedure

This section contains details about the underlying theory and computations of PROC NLMIXED.

### Modeling Assumptions and Notation

PROC NLMIXED operates under the following general framework for nonlinear mixed models. Assume that you have an observed data vector  $\mathbf{y}_i$  for each of  $i$  subjects,  $i = 1, \dots, s$ . The  $\mathbf{y}_i$  are assumed to be independent across  $i$ , but within-subject covariance is likely to exist because each of the elements of  $\mathbf{y}_i$  is measured on the same subject. As a statistical mechanism for modeling this within-subject covariance, assume that there exist latent random-effect vectors  $\mathbf{u}_i$  of small dimension (typically one or two) that are also independent across  $i$ . Assume also that an appropriate model linking  $\mathbf{y}_i$  and  $\mathbf{u}_i$  exists, leading to the joint probability density function

$$p(\mathbf{y}_i | \mathbf{X}_i, \boldsymbol{\phi}, \mathbf{u}_i)q(\mathbf{u}_i | \boldsymbol{\xi})$$

where  $\mathbf{X}_i$  is a matrix of observed explanatory variables and  $\boldsymbol{\phi}$  and  $\boldsymbol{\xi}$  are vectors of unknown parameters.

Let  $\boldsymbol{\theta} = [\boldsymbol{\phi}, \boldsymbol{\xi}]$  and assume that it is of dimension  $n$ . Then inferences about  $\boldsymbol{\theta}$  are based on the marginal likelihood function

$$m(\boldsymbol{\theta}) = \prod_{i=1}^s \int p(\mathbf{y}_i | \mathbf{X}_i, \boldsymbol{\phi}, \mathbf{u}_i)q(\mathbf{u}_i | \boldsymbol{\xi})d\mathbf{u}_i$$

In particular, the function

$$f(\boldsymbol{\theta}) = -\log m(\boldsymbol{\theta})$$

is minimized over  $\boldsymbol{\theta}$  numerically in order to estimate  $\boldsymbol{\theta}$ , and the inverse Hessian (second derivative) matrix at the estimates provides an approximate variance-covariance matrix for the estimate of  $\boldsymbol{\theta}$ . The function  $f(\boldsymbol{\theta})$  is referred to both as the negative log likelihood function and as the objective function for optimization.

As an example of the preceding general framework, consider the nonlinear growth curve example in the section “Getting Started: NLMIXED Procedure” on page 5350. Here, the conditional distribution  $p(y_i | \mathbf{X}_i, \boldsymbol{\phi}, u_i)$  is normal with mean

$$\frac{b_1 + u_{i1}}{1 + \exp[-(d_{ij} - b_2)/b_3]}$$

and variance  $\sigma_e^2$ ; thus  $\boldsymbol{\phi} = [b_1, b_2, b_3, \sigma_e^2]$ . Also,  $u_i$  is a scalar and  $q(u_i | \xi)$  is normal with mean 0 and variance  $\sigma_u^2$ ; thus  $\xi = \sigma_u^2$ .

The following additional notation is also found in this chapter. The quantity  $\boldsymbol{\theta}^{(k)}$  refers to the parameter vector at the  $k$ th iteration, the vector  $\mathbf{g}(\boldsymbol{\theta})$  refers to the gradient vector  $\nabla f(\boldsymbol{\theta})$ , and the matrix  $\mathbf{H}(\boldsymbol{\theta})$  refers to the Hessian  $\nabla^2 f(\boldsymbol{\theta})$ . Other symbols are used to denote various constants or option values.

## Integral Approximations

An important part of the marginal maximum likelihood method described previously is the computation of the integral over the random effects. The default method in PROC NLMIXED for computing this integral is adaptive Gaussian quadrature as described in Pinheiro and Bates (1995). Another approximation method is the first-order method of Beal and Sheiner (1982, 1988). A description of these two methods follows.

### Adaptive Gaussian Quadrature

A quadrature method approximates a given integral by a weighted sum over predefined abscissas for the random effects. A good approximation can usually be obtained with an adequate number of quadrature points as well as appropriate centering and scaling of the abscissas. Adaptive Gaussian quadrature for the integral over  $\mathbf{u}_i$  centers the integral at the empirical Bayes estimate of  $\mathbf{u}_i$ , defined as the vector  $\hat{\mathbf{u}}_i$  that minimizes

$$-\log [p(y_i | \mathbf{X}_i, \boldsymbol{\phi}, \mathbf{u}_i)q(\mathbf{u}_i | \boldsymbol{\xi})]$$

with  $\boldsymbol{\phi}$  and  $\boldsymbol{\xi}$  set equal to their current estimates. The final Hessian matrix from this optimization can be used to scale the quadrature abscissas.

Suppose  $(z_j, w_j; j = 1, \dots, p)$  denote the standard Gauss-Hermite abscissas and weights (Golub and Welsch 1969, or Table 25.10 of Abramowitz and Stegun 1972). The adaptive Gaussian quadrature integral approximation is as follows:

$$\int p(y_i | \mathbf{X}_i, \boldsymbol{\phi}, \mathbf{u}_i)q(\mathbf{u}_i | \boldsymbol{\xi})d\mathbf{u}_i \approx 2^{r/2} |\boldsymbol{\Gamma}(\mathbf{X}_i, \boldsymbol{\theta})|^{-1/2} \sum_{j_1=1}^p \cdots \sum_{j_r=1}^p \left[ p(y_i | \mathbf{X}_i, \boldsymbol{\phi}, \mathbf{a}_{j_1, \dots, j_r})q(\mathbf{a}_{j_1, \dots, j_r} | \boldsymbol{\xi}) \prod_{k=1}^r w_{j_k} \exp z_{j_k}^2 \right]$$

where  $r$  is the dimension of  $u_i$ ,  $\Gamma(\mathbf{X}_i, \boldsymbol{\theta})$  is the Hessian matrix from the empirical Bayes minimization,  $\mathbf{z}_{j_1, \dots, j_r}$  is a vector with elements  $(z_{j_1}, \dots, z_{j_r})$ , and

$$\mathbf{a}_{j_1, \dots, j_r} = \hat{\mathbf{u}}_i + 2^{1/2} \Gamma(\mathbf{X}_i, \boldsymbol{\theta})^{-1/2} \mathbf{z}_{j_1, \dots, j_r}$$

PROC NL MIXED selects the number of quadrature points adaptively by evaluating the log-likelihood function at the starting values of the parameters until two successive evaluations have a relative difference less than the value of the QTOL= option. The specific search sequence is described under the QFAC= option. Using the QPOINTS= option, you can adjust the number of quadrature points  $p$  to obtain different levels of accuracy. Setting  $p = 1$  results in the Laplacian approximation as described in: Beal and Sheiner (1992); Wolfinger (1993); Vonesh (1992, 1996); Vonesh and Chinchilli (1997); Wolfinger and Lin (1997).

The NOAD option in the PROC NL MIXED statement requests nonadaptive Gaussian quadrature. Here all  $\hat{\mathbf{u}}_i$  are set equal to zero, and the Cholesky root of the estimated variance matrix of the random effects is substituted for  $\Gamma(\mathbf{X}_i, \boldsymbol{\theta})^{-1/2}$  in the preceding expression for  $\mathbf{a}_{j_1, \dots, j_r}$ . In this case derivatives are computed using the algorithm of Smith (1995). The NOADSCALE option requests the same scaling substitution but with the empirical Bayes  $\hat{\mathbf{u}}_i$ .

PROC NL MIXED computes the derivatives of the adaptive Gaussian quadrature approximation when carrying out the default dual quasi-Newton optimization.

## First-Order Method

Another integral approximation available in PROC NL MIXED is the first-order method of Beal and Sheiner (1982, 1988) and Sheiner and Beal (1985). This approximation is used only in the case where  $p(\mathbf{y}_i | \mathbf{X}_i, \boldsymbol{\phi}, \mathbf{u}_i)$  is normal—that is,

$$p(\mathbf{y}_i | \mathbf{X}_i, \boldsymbol{\phi}, \mathbf{u}_i) = (2\pi)^{-n_i/2} |\mathbf{R}_i(\mathbf{X}_i, \boldsymbol{\phi})|^{-1/2} \exp \left\{ -(1/2) [\mathbf{y}_i - \mathbf{m}_i(\mathbf{X}_i, \boldsymbol{\phi}, \mathbf{u}_i)]' \mathbf{R}_i(\mathbf{X}_i, \boldsymbol{\phi})^{-1} [\mathbf{y}_i - \mathbf{m}_i(\mathbf{X}_i, \boldsymbol{\phi}, \mathbf{u}_i)] \right\}$$

where  $n_i$  is the dimension of  $\mathbf{y}_i$ ,  $\mathbf{R}_i$  is a diagonal variance matrix, and  $\mathbf{m}_i$  is the conditional mean vector of  $\mathbf{y}_i$ .

The first-order approximation is obtained by expanding  $\mathbf{m}_i(\mathbf{X}_i, \boldsymbol{\phi}, \mathbf{u}_i)$  with a one-term Taylor series expansion about  $\mathbf{u}_i = \mathbf{0}$ , resulting in the approximation

$$p(\mathbf{y}_i | \mathbf{X}_i, \boldsymbol{\phi}, \mathbf{u}_i) \approx (2\pi)^{-n_i/2} |\mathbf{R}_i(\mathbf{X}_i, \boldsymbol{\phi})|^{-1/2} \exp \left( -(1/2) [\mathbf{y}_i - \mathbf{m}_i(\mathbf{X}_i, \boldsymbol{\phi}, \mathbf{0}) - \mathbf{Z}_i(\mathbf{X}_i, \boldsymbol{\phi}) \mathbf{u}_i]' \mathbf{R}_i(\mathbf{X}_i, \boldsymbol{\phi})^{-1} [\mathbf{y}_i - \mathbf{m}_i(\mathbf{X}_i, \boldsymbol{\phi}, \mathbf{0}) - \mathbf{Z}_i(\mathbf{X}_i, \boldsymbol{\phi}) \mathbf{u}_i] \right)$$

where  $\mathbf{Z}_i(\mathbf{X}_i, \boldsymbol{\phi})$  is the Jacobian matrix  $\partial \mathbf{m}_i(\mathbf{X}_i, \boldsymbol{\phi}, \mathbf{u}_i) / \partial \mathbf{u}_i$  evaluated at  $\mathbf{u}_i = \mathbf{0}$ .

Assuming that  $q(\mathbf{u}_i | \boldsymbol{\xi})$  is normal with mean  $\mathbf{0}$  and variance matrix  $\mathbf{G}(\boldsymbol{\xi})$ , the first-order integral approximation is computable in closed form after completing the square:

$$\int p(\mathbf{y}_i | \mathbf{X}_i, \boldsymbol{\phi}, \mathbf{u}_i) q(\mathbf{u}_i | \boldsymbol{\xi}) d\mathbf{u}_i \approx (2\pi)^{-n_i/2} |\mathbf{V}_i(\mathbf{X}_i, \boldsymbol{\theta})|^{-1/2} \exp \left( -(1/2) [\mathbf{y}_i - \mathbf{m}_i(\mathbf{X}_i, \boldsymbol{\phi}, \mathbf{0})]' \mathbf{V}_i(\mathbf{X}_i, \boldsymbol{\theta})^{-1} [\mathbf{y}_i - \mathbf{m}_i(\mathbf{X}_i, \boldsymbol{\phi}, \mathbf{0})] \right)$$

where  $\mathbf{V}_i(\mathbf{X}_i, \boldsymbol{\theta}) = \mathbf{Z}_i(\mathbf{X}_i, \boldsymbol{\phi}) \mathbf{G}(\boldsymbol{\xi}) \mathbf{Z}_i(\mathbf{X}_i, \boldsymbol{\phi})' + \mathbf{R}_i(\mathbf{X}_i, \boldsymbol{\phi})$ . The resulting approximation for  $f(\boldsymbol{\theta})$  is then minimized over  $\boldsymbol{\theta} = [\boldsymbol{\phi}, \boldsymbol{\xi}]$  to obtain the first-order estimates. PROC NL MIXED uses finite-difference derivatives of the first-order integral approximation when carrying out the default dual quasi-Newton optimization.

## Built-in Log-Likelihood Functions

This section displays the basic formulas used by the NLMIXED procedure to compute the conditional log-likelihood functions of the data given the random effects. Note, however, that in addition to these basic equations, the NLMIXED procedure employs a number of checks for missing values and floating-point arithmetic. You can see the entire program used by the NLMIXED procedure to compute the conditional log-likelihood functions  $l(\phi; y)$  by adding the **LIST** debugging option to the **PROC NLMIXED** statement.

$Y \sim \text{normal}(m, v)$

$$l(m, v; y) = -\frac{1}{2} \left( \log\{2\pi\} + \frac{(y - m)^2}{v} + \log\{v\} \right)$$

$$E[Y] = m$$

$$\text{Var}[Y] = v$$

$$v > 0$$

$Y \sim \text{binary}(p)$

$$l_1(p; y) = \begin{cases} y \log\{p\} & y > 0 \\ 0 & \text{otherwise} \end{cases}$$

$$l_2(p; y) = \begin{cases} (1 - y) \log\{1 - p\} & y < 1 \\ 0 & \text{otherwise} \end{cases}$$

$$l(p; y) = l_1(p; y) + l_2(p; y)$$

$$E[Y] = p$$

$$\text{Var}[Y] = p(1 - p)$$

$$0 < p < 1$$

$Y \sim \text{binomial}(n, p)$

$$l_c = \log\{\Gamma(n + 1)\} - \log\{\Gamma(y + 1)\} - \log\{\Gamma(n - y + 1)\}$$

$$l_1(n, p; y) = \begin{cases} y \log\{p\} & y > 0 \\ 0 & \text{otherwise} \end{cases}$$

$$l_2(n, p; y) = \begin{cases} (n - y) \log\{1 - p\} & n - y > 0 \\ 0 & \text{otherwise} \end{cases}$$

$$l(n, p; y) = l_c + l_1(n, p; y) + l_2(n, p; y)$$

$$E[Y] = n p$$

$$\text{Var}[Y] = n p(1 - p)$$

$$0 < p < 1$$

$Y \sim \text{gamma}(a, b)$

$$l(a, b; y) = -a \log\{b\} - \log\{\Gamma(a)\} + (a - 1) \log\{y\} - y/b$$

$$E[Y] = ab$$

$$\text{Var}[Y] = ab^2$$

$$a > 0$$

$$b > 0$$

This parameterization of the gamma distribution differs from the parameterization used in the GLIMMIX and GENMOD procedures. The following statements show the equivalent reparameterization in the NLMIXED procedure that fits a generalized linear model for gamma-distributed data in the parameterization of the GLIMMIX procedure:

```
proc glimmix;
 model y = x / dist=gamma s;
run;

proc nlmixed;
 parms b0=1 b1=0 scale=14;
 linp = b0 + b1*x;
 mu = exp(linp);
 b = mu/scale;
 model y ~ gamma(scale,b);
run;
```

$Y \sim \text{negbin}(n, p)$

$$l(n, p; y) = \log\{\Gamma(n + y)\} - \log\{\Gamma(n)\} - \log\{\Gamma(y + 1)\} \\ + n \log\{p\} + y \log\{1 - p\}$$

$$E[Y] = nP = n \left( \frac{1 - p}{p} \right)$$

$$\text{Var}[Y] = nP(1 - P) = n \left( \frac{1 - p}{p} \right) \frac{1}{p}$$

$$n \geq 0$$

$$0 < p < 1$$

This form of the negative binomial distribution is one of the many parameterizations in which the mass function or log-likelihood function appears. Another common parameterization uses

$$l(n, p; y) = \log\{\Gamma(n + y)\} - \log\{\Gamma(n)\} - \log\{\Gamma(y + 1)\} \\ + n \log\{1 - P/(1 + P)\} + y \log\{P/(1 + P)\}$$

with  $P = (1 - p)/p$ ,  $P > 0$ .

Note that the parameter  $n$  can be real-numbered; it does not have to be integer-valued. The parameterization of the negative binomial distribution in the NLMIXED procedure differs from that in the GLIMMIX and GENMOD procedures. The following statements show the equivalent formulations for maximum likelihood estimation in the GLIMMIX and NLMIXED procedures in a negative binomial regression model:

```
proc glimmix;
 model y = x / dist=negbin s;
run;
```

```

proc nlmixed;
 parms b0=3, b1=1, k=0.8;
 linp = b0 + b1*x;
 mu = exp(linp);
 p = 1/(1+mu*k);
 model y ~ negbin(1/k, p);
run;

```

$Y \sim \text{Poisson}(m)$

$$l(m; y) = y \log\{m\} - m - \log\{\Gamma(y + 1)\}$$

$$E[Y] = m$$

$$\text{Var}[Y] = m$$

$$m > 0$$

---

## Optimization Algorithms

There are several optimization techniques available in PROC NLMIXED. You can choose a particular optimizer with the **TECH=** option in the **PROC NLMIXED** statement.

| Algorithm                                     | TECH=  |
|-----------------------------------------------|--------|
| trust region method                           | TRUREG |
| Newton-Raphson method with line search        | NEWRAP |
| Newton-Raphson method with ridging            | NRRIDG |
| quasi-Newton methods (DBFGS, DDFP, BFGS, DFP) | QUANEW |
| double-dogleg method (DBFGS, DDFP)            | DBLDOG |
| conjugate gradient methods (PB, FR, PR, CD)   | CONGRA |
| Nelder-Mead simplex method                    | NMSIMP |

No algorithm for optimizing general nonlinear functions exists that always finds the global optimum for a general nonlinear minimization problem in a reasonable amount of time. Since no single optimization technique is invariably superior to others, PROC NLMIXED provides a variety of optimization techniques that work well in various circumstances. However, you can devise problems for which none of the techniques in PROC NLMIXED can find the correct solution. Moreover, nonlinear optimization can be computationally expensive in terms of time and memory, so you must be careful when matching an algorithm to a problem.

All optimization techniques in PROC NLMIXED use  $O(n^2)$  memory except the conjugate gradient methods, which use only  $O(n)$  of memory and are designed to optimize problems with many parameters. Since the techniques are iterative, they require the repeated computation of the following:

- the function value (optimization criterion)
- the gradient vector (first-order partial derivatives)
- for some techniques, the (approximate) Hessian matrix (second-order partial derivatives)

However, since each of the optimizers requires different derivatives, some computational efficiencies can be gained. The following table shows, for each optimization technique, which derivatives are required (FOD: first-order derivatives; SOD: second-order derivatives).

| Algorithm | FOD | SOD |
|-----------|-----|-----|
| TRUREG    | x   | x   |
| NEWRAP    | x   | x   |
| NRRIDG    | x   | x   |
| QUANEW    | x   | -   |
| DBLDOG    | x   | -   |
| CONGRA    | x   | -   |
| NMSIMP    | -   | -   |

Each optimization method employs one or more convergence criteria that determine when it has converged. The various termination criteria are listed and described in the “**PROC NLMIXED Statement**” section. An algorithm is considered to have converged when any one of the convergence criteria is satisfied. For example, under the default settings, the QUANEW algorithm will converge if  $ABSGCONV < 1E-5$ ,  $FCONV < 10^{-FDIGITS}$ , or  $GCONV < 1E-8$ .

### Choosing an Optimization Algorithm

The factors that go into choosing a particular optimization technique for a particular problem are complex and can involve trial and error.

For many optimization problems, computing the gradient takes more computer time than computing the function value, and computing the Hessian sometimes takes *much* more computer time and memory than computing the gradient, especially when there are many decision variables. Unfortunately, optimization techniques that do not use some kind of Hessian approximation usually require many more iterations than techniques that do use a Hessian matrix, and as a result the total run time of these techniques is often longer. Techniques that do not use the Hessian also tend to be less reliable. For example, they can more easily terminate at stationary points rather than at global optima.

A few general remarks about the various optimization techniques follow:

- The second-derivative methods TRUREG, NEWRAP, and NRRIDG are best for small problems where the Hessian matrix is not expensive to compute. Sometimes the NRRIDG algorithm can be faster than the TRUREG algorithm, but TRUREG can be more stable. The NRRIDG algorithm requires only one matrix with  $n(n + 1)/2$  double words; TRUREG and NEWRAP require two such matrices.
- The first-derivative methods QUANEW and DBLDOG are best for medium-sized problems where the objective function and the gradient are much faster to evaluate than the Hessian. The QUANEW and DBLDOG algorithms, in general, require more iterations than TRUREG, NRRIDG, and NEWRAP, but each iteration can be much faster. The QUANEW and DBLDOG algorithms require only the gradient to update an approximate Hessian, and they require slightly less memory than TRUREG or NEWRAP (essentially one matrix with  $n(n + 1)/2$  double words). QUANEW is the default optimization method.



- The first-derivative method CONGRA is best for large problems where the objective function and the gradient can be computed much faster than the Hessian and where too much memory is required to store the (approximate) Hessian. The CONGRA algorithm, in general, requires more iterations than QUANEW or DBLDOG, but each iteration can be much faster. Since CONGRA requires only a factor of  $n$  double-word memory, many large applications of PROC NLMIXED can be solved only by CONGRA.
- The no-derivative method NMSIMP is best for small problems where derivatives are not continuous or are very difficult to compute.

## Algorithm Descriptions

Some details about the optimization techniques follow.

### **Trust Region Optimization (TRUREG)**

The trust region method uses the gradient  $\mathbf{g}(\boldsymbol{\theta}^{(k)})$  and the Hessian matrix  $\mathbf{H}(\boldsymbol{\theta}^{(k)})$ ; thus, it requires that the objective function  $f(\boldsymbol{\theta})$  have continuous first- and second-order derivatives inside the feasible region.

The trust region method iteratively optimizes a quadratic approximation to the nonlinear objective function within a hyperelliptic trust region with radius  $\Delta$  that constrains the step size corresponding to the quality of the quadratic approximation. The trust region method is implemented using: Dennis, Gay, and Welsch (1981); Gay (1983); Moré and Sorensen (1983).

The trust region method performs well for small- to medium-sized problems, and it does not need many function, gradient, and Hessian calls. However, if the computation of the Hessian matrix is computationally expensive, one of the (dual) quasi-Newton or conjugate gradient algorithms might be more efficient.

### **Newton-Raphson Optimization with Line Search (NEWRAP)**

The NEWRAP technique uses the gradient  $\mathbf{g}(\boldsymbol{\theta}^{(k)})$  and the Hessian matrix  $\mathbf{H}(\boldsymbol{\theta}^{(k)})$ ; thus, it requires that the objective function have continuous first- and second-order derivatives inside the feasible region. If second-order derivatives are computed efficiently and precisely, the NEWRAP method can perform well for medium-sized to large problems, and it does not need many function, gradient, and Hessian calls.

This algorithm uses a pure Newton step when the Hessian is positive definite and when the Newton step reduces the value of the objective function successfully. Otherwise, a combination of ridging and line search is performed to compute successful steps. If the Hessian is not positive definite, a multiple of the identity matrix is added to the Hessian matrix to make it positive definite (Eskow and Schnabel 1991).

In each iteration, a line search is performed along the search direction to find an approximate optimum of the objective function. The default line-search method uses quadratic interpolation and cubic extrapolation (LINESEARCH=2).

### **Newton-Raphson Ridge Optimization (NRRIDG)**

The NRRIDG technique uses the gradient  $\mathbf{g}(\boldsymbol{\theta}^{(k)})$  and the Hessian matrix  $\mathbf{H}(\boldsymbol{\theta}^{(k)})$ ; thus, it requires that the objective function have continuous first- and second-order derivatives inside the feasible region.

This algorithm uses a pure Newton step when the Hessian is positive definite and when the Newton step reduces the value of the objective function successfully. If at least one of these two conditions is not satisfied, a multiple of the identity matrix is added to the Hessian matrix.

The NRRIDG method performs well for small- to medium-sized problems, and it does not require many function, gradient, and Hessian calls. However, if the computation of the Hessian matrix is computationally expensive, one of the (dual) quasi-Newton or conjugate gradient algorithms might be more efficient.

Since the NRRIDG technique uses an orthogonal decomposition of the approximate Hessian, each iteration of NRRIDG can be slower than that of the NEWRAP technique, which works with Cholesky decomposition. Usually, however, NRRIDG requires fewer iterations than NEWRAP.

### **Quasi-Newton Optimization (QUANEW)**

The (dual) quasi-Newton method uses the gradient  $g(\theta^{(k)})$ , and it does not need to compute second-order derivatives since they are approximated. It works well for medium to moderately large optimization problems where the objective function and the gradient are much faster to compute than the Hessian; but, in general, it requires more iterations than the TRUREG, NEWRAP, and NRRIDG techniques, which compute second-order derivatives. QUANEW is the default optimization algorithm because it provides an appropriate balance between the speed and stability required for most nonlinear mixed model applications.

The QUANEW technique is one of the following, depending on the value of the `UPDATE=` option.

- the original quasi-Newton algorithm, which updates an approximation of the inverse Hessian
- the dual quasi-Newton algorithm, which updates the Cholesky factor of an approximate Hessian (default)

You can specify four update formulas with the `UPDATE=` option:

- DBFGS performs the dual Broyden, Fletcher, Goldfarb, and Shanno (BFGS) update of the Cholesky factor of the Hessian matrix. This is the default.
- DDFP performs the dual Davidon, Fletcher, and Powell (DFP) update of the Cholesky factor of the Hessian matrix.
- BFGS performs the original BFGS update of the inverse Hessian matrix.
- DFP performs the original DFP update of the inverse Hessian matrix.

In each iteration, a line search is performed along the search direction to find an approximate optimum. The default line-search method uses quadratic interpolation and cubic extrapolation to obtain a step size  $\alpha$  satisfying the Goldstein conditions. One of the Goldstein conditions can be violated if the feasible region defines an upper limit of the step size. Violating the left-side Goldstein condition can affect the positive definiteness of the quasi-Newton update. In that case, either the update is skipped or the iterations are restarted with an identity matrix, resulting in the steepest descent or ascent search direction. You can specify line-search algorithms other than the default with the `LINESEARCH=` option.

The QUANEW algorithm uses its own line-search technique. No options and parameters (except the `INSTEP=` option) controlling the line search in the other algorithms apply here. In several applications, large steps in the first iterations are troublesome. You can use the `INSTEP=` option to impose an upper bound for the step size  $\alpha$  during the first five iterations. You can also use the `INHESIAN=r` option to specify a different starting approximation for the Hessian. If you specify only the `INHESIAN` option, the Cholesky factor of a (possibly ridged) finite difference approximation of the Hessian is used to initialize the quasi-Newton update process. The values of the `LCSINGULAR=`, `LCEPSILON=`, and `LCDEACT=`

options, which control the processing of linear and boundary constraints, are valid only for the quadratic programming subroutine used in each iteration of the QUANEW algorithm.

### **Double-Dogleg Optimization (DBLDOG)**

The double-dogleg optimization method combines the ideas of the quasi-Newton and trust region methods. In each iteration, the double-dogleg algorithm computes the step  $s^{(k)}$  as the linear combination of the steepest descent or ascent search direction  $s_1^{(k)}$  and a quasi-Newton search direction  $s_2^{(k)}$ :

$$s^{(k)} = \alpha_1 s_1^{(k)} + \alpha_2 s_2^{(k)}$$

The step is requested to remain within a prespecified trust region radius; see Fletcher (1987, p. 107). Thus, the DBLDOG subroutine uses the dual quasi-Newton update but does not perform a line search. You can specify two update formulas with the `UPDATE=` option:

- DBFGS performs the dual Broyden, Fletcher, Goldfarb, and Shanno update of the Cholesky factor of the Hessian matrix. This is the default.
- DDFP performs the dual Davidon, Fletcher, and Powell update of the Cholesky factor of the Hessian matrix.

The double-dogleg optimization technique works well for medium to moderately large optimization problems where the objective function and the gradient are much faster to compute than the Hessian. The implementation is based on Dennis and Mei (1979) and Gay (1983), but it is extended for dealing with boundary and linear constraints. The DBLDOG technique generally requires more iterations than the TRUREG, NEWRAP, and NRRIDG techniques, which require second-order derivatives; however, each of the DBLDOG iterations is computationally cheap. Furthermore, the DBLDOG technique requires only gradient calls for the update of the Cholesky factor of an approximate Hessian.

### **Conjugate Gradient Optimization (CONGRA)**

Second-order derivatives are not required by the CONGRA algorithm and are not even approximated. The CONGRA algorithm can be expensive in function and gradient calls, but it requires only  $O(n)$  memory for unconstrained optimization. In general, many iterations are required to obtain a precise solution, but each of the CONGRA iterations is computationally cheap. You can specify four different update formulas for generating the conjugate directions by using the `UPDATE=` option:

- PB performs the automatic restart update method of Powell (1977) and Beale (1972). This is the default.
- FR performs the Fletcher-Reeves update (Fletcher 1987).
- PR performs the Polak-Ribiere update (Fletcher 1987).
- CD performs a conjugate-descent update of Fletcher (1987).

The default, `UPDATE=PB`, behaved best in most test examples. You are advised to avoid the option `UPDATE=CD`, which behaved worst in most test examples.

The CONGRA subroutine should be used for optimization problems with large  $n$ . For the unconstrained or boundary constrained case, CONGRA requires only  $O(n)$  bytes of working memory, whereas all other

optimization methods require order  $O(n^2)$  bytes of working memory. During  $n$  successive iterations, uninterrupted by restarts or changes in the working set, the conjugate gradient algorithm computes a cycle of  $n$  conjugate search directions. In each iteration, a line search is performed along the search direction to find an approximate optimum of the objective function. The default line-search method uses quadratic interpolation and cubic extrapolation to obtain a step size  $\alpha$  satisfying the Goldstein conditions. One of the Goldstein conditions can be violated if the feasible region defines an upper limit for the step size. Other line-search algorithms can be specified with the `LINESEARCH=` option.

### **Nelder-Mead Simplex Optimization (NMSIMP)**

The Nelder-Mead simplex method does not use any derivatives and does not assume that the objective function has continuous derivatives. The objective function itself needs to be continuous. This technique is quite expensive in the number of function calls, and it might be unable to generate precise results for  $n \gg 40$ .

The original Nelder-Mead simplex algorithm is implemented and extended to boundary constraints. This algorithm does not compute the objective for infeasible points, but it changes the shape of the simplex adapting to the nonlinearities of the objective function, which contributes to an increased speed of convergence. It uses a special termination criterion.

---

## **Finite-Difference Approximations of Derivatives**

The `FD=` and `FDHESSIAN=` options specify the use of finite-difference approximations of the derivatives. The `FD=` option specifies that all derivatives are approximated using function evaluations, and the `FDHESSIAN=` option specifies that second-order derivatives are approximated using gradient evaluations.

Computing derivatives by finite-difference approximations can be very time-consuming, especially for second-order derivatives based only on values of the objective function (`FD=` option). If analytical derivatives are difficult to obtain (for example, if a function is computed by an iterative process), you might consider one of the optimization techniques that use first-order derivatives only (`QUANEW`, `DBLDOG`, or `CONGRA`). In the expressions that follow,  $\boldsymbol{\theta}$  denotes the parameter vector,  $h_i$  denotes the step size for the  $i$ th parameter, and  $\mathbf{e}_i$  is a vector of zeros with a 1 in the  $i$ th position.

### **Forward-Difference Approximations**

The forward-difference derivative approximations consume less computer time, but they are usually not as precise as approximations that use central-difference formulas.

- For first-order derivatives,  $n$  additional function calls are required:

$$g_i = \frac{\partial f}{\partial \theta_i} \approx \frac{f(\boldsymbol{\theta} + h_i \mathbf{e}_i) - f(\boldsymbol{\theta})}{h_i}$$

- For second-order derivatives based on function calls only (Dennis and Schnabel 1983, p. 80),  $n + n^2/2$  additional function calls are required for dense Hessian:

$$\frac{\partial^2 f}{\partial \theta_i \partial \theta_j} \approx \frac{f(\boldsymbol{\theta} + h_i \mathbf{e}_i + h_j \mathbf{e}_j) - f(\boldsymbol{\theta} + h_i \mathbf{e}_i) - f(\boldsymbol{\theta} + h_j \mathbf{e}_j) + f(\boldsymbol{\theta})}{h_i h_j}$$

- For second-order derivatives based on gradient calls (Dennis and Schnabel 1983, p. 103),  $n$  additional gradient calls are required:

$$\frac{\partial^2 f}{\partial \theta_i \partial \theta_j} \approx \frac{g_i(\boldsymbol{\theta} + h_j \mathbf{e}_j) - g_i(\boldsymbol{\theta})}{2h_j} + \frac{g_j(\boldsymbol{\theta} + h_i \mathbf{e}_i) - g_j(\boldsymbol{\theta})}{2h_i}$$

### Central-Difference Approximations

Central-difference approximations are usually more precise, but they consume more computer time than approximations that use forward-difference derivative formulas.

- For first-order derivatives,  $2n$  additional function calls are required:

$$g_i = \frac{\partial f}{\partial \theta_i} \approx \frac{f(\boldsymbol{\theta} + h_i \mathbf{e}_i) - f(\boldsymbol{\theta} - h_i \mathbf{e}_i)}{2h_i}$$

- For second-order derivatives based on function calls only (Abramowitz and Stegun 1972, p. 884),  $2n + 4n^2/2$  additional function calls are required.

$$\frac{\partial^2 f}{\partial \theta_i^2} \approx \frac{-f(\boldsymbol{\theta} + 2h_i \mathbf{e}_i) + 16f(\boldsymbol{\theta} + h_i \mathbf{e}_i) - 30f(\boldsymbol{\theta}) + 16f(\boldsymbol{\theta} - h_i \mathbf{e}_i) - f(\boldsymbol{\theta} - 2h_i \mathbf{e}_i)}{12h_i^2}$$

$$\frac{\partial^2 f}{\partial \theta_i \partial \theta_j} \approx \frac{f(\boldsymbol{\theta} + h_i \mathbf{e}_i + h_j \mathbf{e}_j) - f(\boldsymbol{\theta} + h_i \mathbf{e}_i - h_j \mathbf{e}_j) - f(\boldsymbol{\theta} - h_i \mathbf{e}_i + h_j \mathbf{e}_j) + f(\boldsymbol{\theta} - h_i \mathbf{e}_i - h_j \mathbf{e}_j)}{4h_i h_j}$$

- For second-order derivatives based on gradient calls,  $2n$  additional gradient calls are required:

$$\frac{\partial^2 f}{\partial \theta_i \partial \theta_j} \approx \frac{g_i(\boldsymbol{\theta} + h_j \mathbf{e}_j) - g_i(\boldsymbol{\theta} - h_j \mathbf{e}_j)}{4h_j} + \frac{g_j(\boldsymbol{\theta} + h_i \mathbf{e}_i) - g_j(\boldsymbol{\theta} - h_i \mathbf{e}_i)}{4h_i}$$

You can use the `FDIGITS=` option to specify the number of accurate digits in the evaluation of the objective function. This specification is helpful in determining an appropriate interval size  $h$  to be used in the finite-difference formulas.

The step sizes  $h_j$ ,  $j = 1, \dots, n$  are defined as follows:

- For the forward-difference approximation of first-order derivatives that use function calls and second-order derivatives that use gradient calls,  $h_j = \sqrt[2]{\eta}(1 + |\theta_j|)$ .
- For the forward-difference approximation of second-order derivatives that use only function calls and all central-difference formulas,  $h_j = \sqrt[3]{\eta}(1 + |\theta_j|)$ .

The value of  $\eta$  is defined by the `FDIGITS=` option:

- If you specify the number of accurate digits by using `FDIGITS=r`,  $\eta$  is set to  $10^{-r}$ .
- If you do not specify the `FDIGITS=` option,  $\eta$  is set to the machine precision  $\epsilon$ .

## Hessian Scaling

The rows and columns of the Hessian matrix can be scaled when you use the trust region, Newton-Raphson, and double-dogleg optimization techniques. Each element  $H_{i,j}$ ,  $i, j = 1, \dots, n$  is divided by the scaling factor  $d_i d_j$ , where the scaling vector  $d = (d_1, \dots, d_n)$  is iteratively updated in a way specified by the HESCAL= $i$  option, as follows:

$i = 0$  : No scaling is done (equivalent to  $d_i = 1$ ).

$i \neq 0$  : First iteration and each restart iteration sets:

$$d_i^{(0)} = \sqrt{\max(|H_{i,i}^{(0)}|, \epsilon)}$$

$i = 1$  : See Moré (1978):

$$d_i^{(k+1)} = \max \left[ d_i^{(k)}, \sqrt{\max(|H_{i,i}^{(k)}|, \epsilon)} \right]$$

$i = 2$  : See Dennis, Gay, and Welsch (1981):

$$d_i^{(k+1)} = \max \left[ 0.6d_i^{(k)}, \sqrt{\max(|H_{i,i}^{(k)}|, \epsilon)} \right]$$

$i = 3$  :  $d_i$  is reset in each iteration:

$$d_i^{(k+1)} = \sqrt{\max(|H_{i,i}^{(k)}|, \epsilon)}$$

In the preceding equations,  $\epsilon$  is the relative machine precision or, equivalently, the largest double-precision value that, when added to 1, results in 1.

## Active Set Methods

The parameter vector  $\theta \in \mathcal{R}^n$  can be subject to a set of  $m$  linear equality and inequality constraints:

$$\begin{aligned} \sum_{j=1}^n a_{ij} \theta_j &= b_i & i = 1, \dots, m_e \\ \sum_{j=1}^n a_{ij} \theta_j &\geq b_i & i = m_e + 1, \dots, m \end{aligned}$$

The coefficients  $a_{ij}$  and right-hand sides  $b_i$  of the equality and inequality constraints are collected in the  $m \times n$  matrix  $\mathbf{A}$  and the  $m$  vector  $\mathbf{b}$ .

The  $m$  linear constraints define a feasible region  $\mathcal{G}$  in  $\mathcal{R}^n$  that must contain the point  $\theta_*$  that minimizes the problem. If the feasible region  $\mathcal{G}$  is empty, no solution to the optimization problem exists.

In PROC NLMIXED, all optimization techniques use *active set methods*. The iteration starts with a feasible point  $\theta^{(0)}$ , which you can provide or which can be computed by the Schittkowski and Stoer (1979) algorithm

implemented in PROC NLMIXED. The algorithm then moves from one feasible point  $\theta^{(k-1)}$  to a better feasible point  $\theta^{(k)}$  along a feasible search direction  $s^{(k)}$ ,

$$\theta^{(k)} = \theta^{(k-1)} + \alpha^{(k)} s^{(k)}, \quad \alpha^{(k)} > 0$$

Theoretically, the path of points  $\theta^{(k)}$  never leaves the feasible region  $\mathcal{G}$  of the optimization problem, but it can reach its boundaries. The active set  $\mathcal{A}^{(k)}$  of point  $\theta^{(k)}$  is defined as the index set of all linear equality constraints and those inequality constraints that are satisfied at  $\theta^{(k)}$ . If no constraint is active at  $\theta^{(k)}$ , the point is located in the interior of  $\mathcal{G}$ , and the active set  $\mathcal{A}^{(k)} = \emptyset$  is empty. If the point  $\theta^{(k)}$  in iteration  $k$  hits the boundary of inequality constraint  $i$ , this constraint  $i$  becomes active and is added to  $\mathcal{A}^{(k)}$ . Each equality constraint and each active inequality constraint reduce the dimension (degrees of freedom) of the optimization problem.

In practice, the active constraints can be satisfied only with finite precision. The `LCEPSILON=r` option specifies the range for active and violated linear constraints. If the point  $\theta^{(k)}$  satisfies the condition

$$\left| \sum_{j=1}^n a_{ij} \theta_j^{(k)} - b_i \right| \leq t$$

where  $t = r(|b_i| + 1)$ , the constraint  $i$  is recognized as an active constraint. Otherwise, the constraint  $i$  is either an inactive inequality or a violated inequality or equality constraint. Due to rounding errors in computing the projected search direction, error can be accumulated so that an iterate  $\theta^{(k)}$  steps out of the feasible region.

In those cases, PROC NLMIXED might try to pull the iterate  $\theta^{(k)}$  back into the feasible region. However, in some cases the algorithm needs to increase the feasible region by increasing the `LCEPSILON=r` value. If this happens, a message is displayed in the log output.

If the algorithm cannot improve the value of the objective function by moving from an active constraint back into the interior of the feasible region, it makes this inequality constraint an equality constraint in the next iteration. This means that the active set  $\mathcal{A}^{(k+1)}$  still contains the constraint  $i$ . Otherwise, it releases the active inequality constraint and increases the dimension of the optimization problem in the next iteration.

A serious numerical problem can arise when some of the active constraints become (nearly) linearly dependent. PROC NLMIXED removes linearly dependent equality constraints before starting optimization. You can use the `LCSINGULAR=` option to specify a criterion  $r$  used in the update of the QR decomposition that determines whether an active constraint is linearly dependent relative to a set of other active constraints.

If the solution  $\theta^*$  is subjected to  $n_{act}$  linear equality or active inequality constraints, the QR decomposition of the  $n \times n_{act}$  matrix  $\hat{\mathbf{A}}'$  of the linear constraints is computed by  $\hat{\mathbf{A}}' = \mathbf{QR}$ , where  $\mathbf{Q}$  is an  $n \times n$  orthogonal matrix and  $\mathbf{R}$  is an  $n \times n_{act}$  upper triangular matrix. The  $n$  columns of matrix  $\mathbf{Q}$  can be separated into two matrices,  $\mathbf{Q} = [\mathbf{Y}, \mathbf{Z}]$ , where  $\mathbf{Y}$  contains the first  $n_{act}$  orthogonal columns of  $\mathbf{Q}$  and  $\mathbf{Z}$  contains the last  $n - n_{act}$  orthogonal columns of  $\mathbf{Q}$ . The  $n \times (n - n_{act})$  column-orthogonal matrix  $\mathbf{Z}$  is also called the *null-space matrix* of the active linear constraints  $\hat{\mathbf{A}}'$ . The  $n - n_{act}$  columns of the  $n \times (n - n_{act})$  matrix  $\mathbf{Z}$  form a basis orthogonal to the rows of the  $n_{act} \times n$  matrix  $\hat{\mathbf{A}}$ .

At the end of the iterating, PROC NLMIXED computes the *projected gradient*  $\mathbf{gz}$ ,

$$\mathbf{gz} = \mathbf{Z}'\mathbf{g}$$

In the case of boundary-constrained optimization, the elements of the projected gradient correspond to the gradient elements of the free parameters. A necessary condition for  $\theta^*$  to be a local minimum of the optimization problem is

$$\mathbf{gz}(\theta^*) = \mathbf{Z}'\mathbf{g}(\theta^*) = \mathbf{0}$$



The symmetric  $n_{act} \times n_{act}$  matrix  $\mathbf{G}_Z$ ,

$$\mathbf{G}_Z = \mathbf{Z}'\mathbf{G}\mathbf{Z}$$

is called a *projected Hessian matrix*. A second-order necessary condition for  $\boldsymbol{\theta}^*$  to be a local minimizer requires that the projected Hessian matrix is positive semidefinite.

Those elements of the  $n_{act}$  vector of first-order estimates of *Lagrange multipliers*,

$$\lambda = (\hat{\mathbf{A}}\hat{\mathbf{A}}')^{-1}\hat{\mathbf{A}}\mathbf{Z}\mathbf{Z}'\mathbf{g}$$

that correspond to active inequality constraints indicate whether an improvement of the objective function can be obtained by releasing this active constraint. For minimization, a significant negative Lagrange multiplier indicates that a possible reduction of the objective function can be achieved by releasing this active linear constraint. The `LCDEACT=r` option specifies a threshold  $r$  for the Lagrange multiplier that determines whether an active inequality constraint remains active or can be deactivated. (In the case of boundary-constrained optimization, the Lagrange multipliers for active lower (upper) constraints are the negative (positive) gradient elements corresponding to the active parameters.)

## Line-Search Methods

In each iteration  $k$ , the (dual) quasi-Newton, conjugate gradient, and Newton-Raphson minimization techniques use iterative line-search algorithms that try to optimize a linear, quadratic, or cubic approximation of  $f$  along a feasible descent search direction  $\mathbf{s}^{(k)}$ ,

$$\boldsymbol{\theta}^{(k+1)} = \boldsymbol{\theta}^{(k)} + \alpha^{(k)}\mathbf{s}^{(k)}, \quad \alpha^{(k)} > 0$$

by computing an approximately optimal scalar  $\alpha^{(k)}$ .

Therefore, a line-search algorithm is an iterative process that optimizes a nonlinear function  $f(\alpha)$  of one parameter ( $\alpha$ ) within each iteration  $k$  of the optimization technique. Since the outside iteration process is based only on the approximation of the objective function, the inside iteration of the line-search algorithm does not have to be perfect. Usually, it is satisfactory that the choice of  $\alpha$  significantly reduces (in a minimization) the objective function. Criteria often used for termination of line-search algorithms are the Goldstein conditions (see Fletcher 1987).

You can select various line-search algorithms by specifying the `LINESEARCH=` option. The line-search method `LINESEARCH=2` seems to be superior when function evaluation consumes significantly less computation time than gradient evaluation. Therefore, `LINESEARCH=2` is the default method for Newton-Raphson, (dual) quasi-Newton, and conjugate gradient optimizations.

You can modify the line-search methods `LINESEARCH=2` and `LINESEARCH=3` to be exact line searches by using the `LSPRECISION=` option and specifying the  $\sigma$  parameter described in Fletcher (1987). The line-search methods `LINESEARCH=1`, `LINESEARCH=2`, and `LINESEARCH=3` satisfy the left-side and right-side Goldstein conditions (see Fletcher 1987). When derivatives are available, the line-search methods `LINESEARCH=6`, `LINESEARCH=7`, and `LINESEARCH=8` try to satisfy the right-side Goldstein condition; if derivatives are not available, these line-search algorithms use only function calls.



## Restricting the Step Length

Almost all line-search algorithms use iterative extrapolation techniques that can easily lead them to (feasible) points where the objective function  $f$  is no longer defined or is difficult to compute. Therefore, PROC NLMIXED provides options restricting the step length  $\alpha$  or trust region radius  $\Delta$ , especially during the first main iterations.

The inner product  $\mathbf{g}'\mathbf{s}$  of the gradient  $\mathbf{g}$  and the search direction  $\mathbf{s}$  is the slope of  $f(\alpha) = f(\boldsymbol{\theta} + \alpha\mathbf{s})$  along the search direction  $\mathbf{s}$ . The default starting value  $\alpha^{(0)} = \alpha^{(k,0)}$  in each line-search algorithm ( $\min_{\alpha>0} f(\boldsymbol{\theta} + \alpha\mathbf{s})$ ) during the main iteration  $k$  is computed in three steps:

1. The first step uses either the difference  $|\Delta f| = |f^{(k)} - f^{(k-1)}|$  of the function values during the last two consecutive iterations or the final step-size value  $\alpha^-$  of the last iteration  $k - 1$  to compute a first value of  $\alpha_1^{(0)}$ .

- If the **DAMPSTEP** option is not used,

$$\alpha_1^{(0)} = \begin{cases} \text{step} & \text{if } 0.1 \leq \text{step} \leq 10 \\ 10 & \text{if } \text{step} > 10 \\ 0.1 & \text{if } \text{step} < 0.1 \end{cases}$$

with

$$\text{step} = \begin{cases} |\Delta f|/|\mathbf{g}'\mathbf{s}| & \text{if } |\mathbf{g}'\mathbf{s}| \geq \epsilon \max(100 \times |\Delta f|, 1) \\ 1 & \text{otherwise} \end{cases}$$

This value of  $\alpha_1^{(0)}$  can be too large and can lead to a difficult or impossible function evaluation, especially for highly nonlinear functions such as the EXP function.

- If the **DAMPSTEP=r** option is used,

$$\alpha_1^{(0)} = \min(1, r\alpha^-)$$

The initial value for the new step length can be no larger than  $r$  times the final step length  $\alpha^-$  of the former iteration. The default value is  $r = 2$ .

2. During the first five iterations, the second step enables you to reduce  $\alpha_1^{(0)}$  to a smaller starting value  $\alpha_2^{(0)}$  by using the **INSTEP=r** option:

$$\alpha_2^{(0)} = \min(\alpha_1^{(0)}, r)$$

After more than five iterations,  $\alpha_2^{(0)}$  is set to  $\alpha_1^{(0)}$ .

3. The third step can further reduce the step length by

$$\alpha_3^{(0)} = \min(\alpha_2^{(0)}, \min(10, u))$$

where  $u$  is the maximum length of a step inside the feasible region.

The `INSTEP=r` option enables you to specify a smaller or larger radius  $\Delta$  of the trust region used in the first iteration of the trust region and double-dogleg algorithms. The default initial trust region radius  $\Delta^{(0)}$  is the length of the scaled gradient (Moré 1978). This step corresponds to the default radius factor of  $r = 1$ . In most practical applications of the TRUREG and DBLDOG algorithms, this choice is successful. However, for bad initial values and highly nonlinear objective functions (such as the EXP function), the default start radius can result in arithmetic overflows. If this happens, you can try decreasing values of `INSTEP=r`,  $0 < r < 1$ , until the iteration starts successfully. A small factor  $r$  also affects the trust region radius  $\Delta^{(k+1)}$  of the next steps because the radius is changed in each iteration by a factor  $0 < c \leq 4$ , depending on the ratio  $\rho$  expressing the goodness of quadratic function approximation. Reducing the radius  $\Delta$  corresponds to increasing the ridge parameter  $\lambda$ , producing smaller steps aimed more closely toward the (negative) gradient direction.

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## Computational Problems

### Floating-Point Errors and Overflows

Numerical optimization of a numerically integrated function is a difficult task, and the computation of the objective function and its derivatives can lead to arithmetic exceptions and overflows. A typical cause of these problems is parameters with widely varying scales. If the scaling of your parameters varies by more than a few orders of magnitude, the numerical stability of the optimization problem can be seriously reduced and can result in computational difficulties. A simple remedy is to rescale each parameter so that its final estimated value has a magnitude near 1.

If parameter rescaling does not help, consider the following actions:

- Specify the `ITDETAILS` option in the `PROC NLMIXED` statement to obtain more detailed information about when and where the problem is occurring.
- Provide different initial values or try a grid search of values.
- Use boundary constraints to avoid the region where overflows can happen.
- Delete outlying observations or subjects from the input data, if this is reasonable.
- Change the algorithm (specified in programming statements) that computes the objective function.

The line-search algorithms that work with cubic extrapolation are especially sensitive to arithmetic overflows. If an overflow occurs during a line search, you can use the `INSTEP=` option to reduce the length of the first trial step during the first five iterations, or you can use the `DAMPSTEP` or `MAXSTEP` option to restrict the step length of the initial  $\alpha$  in subsequent iterations. If an arithmetic overflow occurs in the first iteration of the trust region or double-dogleg algorithm, you can use the `INSTEP=` option to reduce the default trust region radius of the first iteration. You can also change the optimization technique or the line-search method.

### Long Run Times

`PROC NLMIXED` can take a long time to run for problems involving complex models, many parameters, or large input data sets. Although the optimization techniques used by `PROC NLMIXED` are some of the best ones available, they are not guaranteed to converge quickly for all problems. Ill-posed or misspecified

models can cause the algorithms to use more extensive calculations designed to achieve convergence, and this can result in longer run times. So first make sure that your model is specified correctly, that your parameters are scaled to be of the same order of magnitude, and that your data reasonably match the model you are contemplating.

If you are using the default adaptive Gaussian quadrature algorithm and no iteration history is printing at all, then PROC NLMIXED might be bogged down trying to determine the number of quadrature points at the first set of starting values. Specifying the `QPOINTS=` option will bypass this stage and proceed directly to iterations; however, be aware that the likelihood approximation might not be accurate if there are too few quadrature points.

PROC NLMIXED can also have difficulty determining the number of quadrature points if the initial starting values are far from the optimum values. To obtain more accurate starting values for the model parameters, one easy method is to fit a model with no `RANDOM` statement. You can then use these estimates as starting values, although you will still need to specify values for the random-effects distribution. For normal-normal models, another strategy is to use `METHOD=FIRO`. If you can obtain estimates by using this approximate method, then they can be used as starting values for more accurate likelihood approximations.

If you are running PROC NLMIXED multiple times, you will probably want to include a statement like the following in your program:

```
ods output ParameterEstimates=pe;
```

This statement creates a SAS data set named PE upon completion of the run. In your next invocation of PROC NLMIXED, you can then specify

```
parms / data=pe;
```

to read in the previous estimates as starting values.

To speed general computations, you should double-check your programming statements to minimize the number of floating-point operations. Using auxiliary variables and factoring amenable expressions can be useful changes in this regard.

## Problems Evaluating Code for Objective Function

The starting point  $\theta^{(0)}$  must be a point for which the programming statements can be evaluated. However, during optimization, the optimizer might iterate to a point  $\theta^{(k)}$  where the objective function or its derivatives cannot be evaluated. In some cases, the specification of boundary for parameters can avoid such situations. In many other cases, you can indicate that the point  $\theta^{(0)}$  is a bad point simply by returning an extremely large value for the objective function. In these cases, the optimization algorithm reduces the step length and stays closer to the point that has been evaluated successfully in the former iteration.

## No Convergence

There are a number of things to try if the optimizer fails to converge.

- Change the initial values by using a grid search specification to obtain a set of good feasible starting values.
- Change or modify the update technique or the line-search algorithm.

This method applies only to `TECH=QUANEW` and `TECH=CONGRA`. For example, if you use the default update formula and the default line-search algorithm, you can do the following:

- change the update formula with the `UPDATE=` option
  - change the line-search algorithm with the `LINESEARCH=` option
  - specify a more precise line search with the `LSPRECISION=` option, if you use `LINESEARCH=2` or `LINESEARCH=3`
- Change the optimization technique.  
For example, if you use the default option, `TECH=QUANEW`, you can try one of the second-derivative methods if your problem is small or the conjugate gradient method if it is large.
  - Adjust finite-difference derivatives.  
The forward-difference derivatives specified with the `FD=` or `FDHESSIAN=` option might not be precise enough to satisfy strong gradient termination criteria. You might need to specify the more expensive central-difference formulas. The finite-difference intervals might be too small or too big, and the finite-difference derivatives might be erroneous.
  - Double-check the data entry and program specification.

### Convergence to Stationary Point

The gradient at a stationary point is the null vector, which always leads to a zero search direction. This point satisfies the first-order termination criterion. Search directions that are based on the gradient are zero, so the algorithm terminates. There are two ways to avoid this situation:

- Use the `PARMS` statement to specify a grid of feasible initial points.
- Use the `OPTCHECK=r` option to avoid terminating at the stationary point.

The signs of the eigenvalues of the (reduced) Hessian matrix contain the following information regarding a stationary point:

- If all of the eigenvalues are positive, the Hessian matrix is positive definite, and the point is a minimum point.
- If some of the eigenvalues are positive and all remaining eigenvalues are zero, the Hessian matrix is positive semidefinite, and the point is a minimum or saddle point.
- If all of the eigenvalues are negative, the Hessian matrix is negative definite, and the point is a maximum point.
- If some of the eigenvalues are negative and all remaining eigenvalues are zero, the Hessian matrix is negative semidefinite, and the point is a maximum or saddle point.
- If all of the eigenvalues are zero, the point can be a minimum, maximum, or saddle point.

## Precision of Solution

In some applications, PROC NLMIXED can result in parameter values that are not precise enough. Usually, this means that the procedure terminated at a point too far from the optimal point. The termination criteria define the size of the termination region around the optimal point. Any point inside this region can be accepted for terminating the optimization process. The default values of the termination criteria are set to satisfy a reasonable compromise between the computational effort (computer time) and the precision of the computed estimates for the most common applications. However, there are a number of circumstances in which the default values of the termination criteria specify a region that is either too large or too small.

If the termination region is too large, then it can contain points with low precision. In such cases, you should determine which termination criterion stopped the optimization process. In many applications, you can obtain a solution with higher precision simply by using the old parameter estimates as starting values in a subsequent run in which you specify a smaller value for the termination criterion that was satisfied at the former run.

If the termination region is too small, the optimization process might take longer to find a point inside such a region, or it might not even find such a point due to rounding errors in function values and derivatives. This can easily happen in applications in which finite-difference approximations of derivatives are used and the `GCONV` and `ABSGCONV` termination criteria are too small to respect rounding errors in the gradient values.

---

## Covariance Matrix

The estimated covariance matrix of the parameter estimates is computed as the inverse Hessian matrix, and for unconstrained problems it should be positive definite. If the final parameter estimates are subjected to  $n_{act} > 0$  active linear inequality constraints, the formulas of the covariance matrices are modified similar to Gallant (1987) and Cramer (1986, p. 38) and additionally generalized for applications with singular matrices.

There are several steps available that enable you to tune the rank calculations of the covariance matrix.

1. You can use the `ASINGULAR=`, `MSINGULAR=`, and `VSINGULAR=` options to set three singularity criteria for the inversion of the Hessian matrix **H**. The singularity criterion used for the inversion is

$$|d_{j,j}| \leq \max(\text{ASING}, \text{VSING} * |H_{j,j}|, \text{MSING} * \max(|H_{1,1}|, \dots, |H_{n,n}|))$$

where  $d_{j,j}$  is the diagonal pivot of the matrix **H**, and `ASING`, `VSING`, and `MSING` are the specified values of the `ASINGULAR=`, `VSINGULAR=`, and `MSINGULAR=` options, respectively. The default values are as follows:

- `ASING`: the square root of the smallest positive double-precision value
- `MSING`:  $1\text{E}-12$  if you do not specify the `SINGHESS=` option and  $\max(10\epsilon, 1\text{E} - 4 \times \text{SINGHESS})$  otherwise, where  $\epsilon$  is the machine precision
- `VSING`:  $1\text{E}-8$  if you do not specify the `SINGHESS=` option and the value of `SINGHESS` otherwise

Note that, in many cases, a normalized matrix  $\mathbf{D}^{-1}\mathbf{AD}^{-1}$  is decomposed, and the singularity criteria are modified correspondingly.

2. If the matrix  $\mathbf{H}$  is found to be singular in the first step, a generalized inverse is computed. Depending on the `G4=` option, either a generalized inverse satisfying all four Moore-Penrose conditions is computed (a  $g_4$ -inverse) or a generalized inverse satisfying only two Moore-Penrose conditions is computed (a  $g_2$ -inverse, Pringle and Rayner 1971). If the number of parameters  $n$  of the application is less than or equal to `G4=i`, a  $g_4$ -inverse is computed; otherwise, only a  $g_2$ -inverse is computed. The  $g_4$ -inverse is computed by the (computationally very expensive but numerically stable) eigenvalue decomposition, and the  $g_2$ -inverse is computed by Gauss transformation. The  $g_4$ -inverse is computed using the eigenvalue decomposition  $\mathbf{A} = \mathbf{Z}\mathbf{\Lambda}\mathbf{Z}'$ , where  $\mathbf{Z}$  is the orthogonal matrix of eigenvectors and  $\mathbf{\Lambda}$  is the diagonal matrix of eigenvalues,  $\mathbf{\Lambda} = \text{diag}(\lambda_1, \dots, \lambda_n)$ . The  $g_4$ -inverse of  $\mathbf{H}$  is set to

$$\mathbf{A}^- = \mathbf{Z}\mathbf{\Lambda}^- \mathbf{Z}'$$

where the diagonal matrix  $\mathbf{\Lambda}^- = \text{diag}(\lambda_1^-, \dots, \lambda_n^-)$  is defined using the `COVSING=` option:

$$\lambda_i^- = \begin{cases} 1/\lambda_i & \text{if } |\lambda_i| > \text{COVSING} \\ 0 & \text{if } |\lambda_i| \leq \text{COVSING} \end{cases}$$

If you do not specify the `COVSING=` option, the  $nr$  smallest eigenvalues are set to zero, where  $nr$  is the number of rank deficiencies found in the first step.

For optimization techniques that do not use second-order derivatives, the covariance matrix is computed using finite-difference approximations of the derivatives.

---

## Prediction

The nonlinear mixed model is a useful tool for statistical prediction. Assuming a prediction is to be made regarding the  $i$ th subject, suppose that  $f(\boldsymbol{\theta}, \mathbf{u}_i)$  is a differentiable function predicting some quantity of interest. Recall that  $\boldsymbol{\theta}$  denotes the vector of unknown parameters and  $\mathbf{u}_i$  denotes the vector of random effects for the  $i$ th subject. A natural point prediction is  $f(\hat{\boldsymbol{\theta}}, \hat{\mathbf{u}}_i)$ , where  $\hat{\boldsymbol{\theta}}$  is the maximum likelihood estimate of  $\boldsymbol{\theta}$  and  $\hat{\mathbf{u}}_i$  is the empirical Bayes estimate of  $\mathbf{u}_i$  described previously in the section “Integral Approximations” on page 5384.

An approximate prediction variance matrix for  $(\hat{\boldsymbol{\theta}}, \hat{\mathbf{u}}_i)$  is

$$\mathbf{P} = \begin{bmatrix} \hat{\mathbf{H}}^{-1} & \hat{\mathbf{H}}^{-1} \left( \frac{\partial \hat{\mathbf{u}}_i}{\partial \boldsymbol{\theta}} \right)' \\ \left( \frac{\partial \hat{\mathbf{u}}_i}{\partial \boldsymbol{\theta}} \right) \hat{\mathbf{H}}^{-1} & \hat{\mathbf{\Gamma}}^{-1} + \left( \frac{\partial \hat{\mathbf{u}}_i}{\partial \boldsymbol{\theta}} \right) \hat{\mathbf{H}}^{-1} \left( \frac{\partial \hat{\mathbf{u}}_i}{\partial \boldsymbol{\theta}} \right)' \end{bmatrix}$$

where  $\hat{\mathbf{H}}$  is the approximate Hessian matrix from the optimization for  $\hat{\boldsymbol{\theta}}$ ,  $\hat{\mathbf{\Gamma}}$  is the approximate Hessian matrix from the optimization for  $\hat{\mathbf{u}}_i$ , and  $(\partial \hat{\mathbf{u}}_i / \partial \boldsymbol{\theta})$  is the derivative of  $\hat{\mathbf{u}}_i$  with respect to  $\boldsymbol{\theta}$ , evaluated at  $(\hat{\boldsymbol{\theta}}, \hat{\mathbf{u}}_i)$ . The approximate variance matrix for  $\hat{\boldsymbol{\theta}}$  is the standard one discussed in the previous section, and that for  $\hat{\mathbf{u}}_i$  is an approximation to the conditional mean squared error of prediction described by Booth and Hobert (1998).

The prediction variance for a general scalar function  $f(\boldsymbol{\theta}, \mathbf{u}_i)$  is defined as the expected squared difference  $E[f(\hat{\boldsymbol{\theta}}, \hat{\mathbf{u}}_i) - f(\boldsymbol{\theta}, \mathbf{u}_i)]^2$ . PROC NL MIXED computes an approximation to it as follows. The derivative of  $f(\boldsymbol{\theta}, \mathbf{u}_i)$  is computed with respect to each element of  $(\boldsymbol{\theta}, \mathbf{u}_i)$  and evaluated at  $(\hat{\boldsymbol{\theta}}, \hat{\mathbf{u}}_i)$ . If  $\mathbf{a}_i$  is the resulting vector, then the approximate prediction variance is  $\mathbf{a}_i' \mathbf{P} \mathbf{a}_i$ . This approximation is known as the delta method (Billingsley 1986; Cox 1998).

## Computational Resources

Since nonlinear optimization is an iterative process that depends on many factors, it is difficult to estimate how much computer time is necessary to find an optimal solution satisfying one of the termination criteria. You can use the `MAXTIME=`, `MAXITER=`, and `MAXFUNC=` options to restrict the amount of CPU time, the number of iterations, and the number of function calls in a single run of PROC NLMIXED.

In each iteration  $k$ , the NRRIDG technique uses a symmetric Householder transformation to decompose the  $n \times n$  Hessian matrix  $\mathbf{H}$ ,

$$\mathbf{H} = \mathbf{V}'\mathbf{T}\mathbf{V}, \quad \mathbf{V}: \text{orthogonal}, \quad \mathbf{T}: \text{tridiagonal}$$

to compute the (Newton) search direction  $\mathbf{s}$ ,

$$\mathbf{s}^{(k)} = -[\mathbf{H}^{(k)}]^{-1}\mathbf{g}^{(k)} \quad k = 1, 2, 3, \dots$$

The TRUREG and NEWRAP techniques use the Cholesky decomposition to solve the same linear system while computing the search direction. The QUANEW, DBLDOG, CONGRA, and NMSIMP techniques do not need to invert or decompose a Hessian matrix; thus, they require less computational resources than the other techniques.

The larger the problem, the more time is needed to compute function values and derivatives. Therefore, you might want to compare optimization techniques by counting and comparing the respective numbers of function, gradient, and Hessian evaluations.

Finite-difference approximations of the derivatives are expensive because they require additional function or gradient calls:

- forward-difference formulas
  - For first-order derivatives,  $n$  additional function calls are required.
  - For second-order derivatives based on function calls only, for a dense Hessian,  $n + n^2/2$  additional function calls are required.
  - For second-order derivatives based on gradient calls,  $n$  additional gradient calls are required.
- central-difference formulas
  - For first-order derivatives,  $2n$  additional function calls are required.
  - For second-order derivatives based on function calls only, for a dense Hessian,  $2n + 2n^2$  additional function calls are required.
  - For second-order derivatives based on gradient calls,  $2n$  additional gradient calls are required.

Many applications need considerably more time for computing second-order derivatives (Hessian matrix) than for computing first-order derivatives (gradient). In such cases, a dual quasi-Newton technique is recommended, which does not require second-order derivatives.

---

## Displayed Output

This section describes the displayed output from PROC NLMIXED. See the section “ODS Table Names” on page 5407 for details about how this output interfaces with the Output Delivery System.

### **Specifications**

The NLMIXED procedure first displays the “Specifications” table, listing basic information about the nonlinear mixed model that you have specified. It includes the principal variables and estimation methods.

### **Dimensions**

The “Dimensions” table lists counts of important quantities in your nonlinear mixed model, including the number of observations, subjects, parameters, and quadrature points.

### **Parameters**

The “Parameters” table displays the information you provided with the **PARMS** statement and the value of the negative log-likelihood function evaluated at the starting values.

### **Starting Gradient and Hessian**

The **START** option in the **PROC NLMIXED** statement displays the gradient of the negative log-likelihood function at the starting values of the parameters. If you also specify the **HESS** option, then the starting Hessian is displayed as well.

### **Iterations**

The iteration history consists of one line of output for each iteration in the optimization process. The iteration history is displayed by default because it is important that you check for possible convergence problems. The default iteration history includes the following variables:

- Iter, the iteration number
- Calls, the number of function calls
- NegLogLike, the value of the objective function
- Diff, the difference between adjacent function values
- MaxGrad, the maximum of the absolute (projected) gradient components (except NMSIMP)
- Slope, the slope  $g'$ s of the search direction  $s$  at the current parameter iterate  $\theta^{(k)}$  (QUANEW only)
- Rho, the ratio between the achieved and predicted values of Diff (NRRIDG only)
- Radius, the radius of the trust region (TRUREG only)
- StdDev, the standard deviation of the simplex values (NMSIMP only)
- Delta, the vertex length of the simplex (NMSIMP only)
- Size, the size of the simplex (NMSIMP only)



For the QUANEW method, the value of Slope should be significantly negative. Otherwise, the line-search algorithm has difficulty reducing the function value sufficiently. If this difficulty is encountered, an asterisk (\*) appears after the iteration number. If there is a tilde ~ after the iteration number, the BFGS update is skipped, and very high values of the Lagrange function are produced. A backslash ( \ ) after the iteration number indicates that Powell's correction for the BFGS update is used.

For methods using second derivatives, an asterisk (\*) after the iteration number means that the computed Hessian approximation was singular and had to be ridged with a positive value.

For the NMSIMP method, only one line is displayed for several internal iterations. This technique skips the output for some iterations because some of the termination tests (StdDev and Size) are rather time-consuming compared to the simplex operations, and they are performed only every five simplex operations.

The ITDETAILS option in the PROC NLMIXED statement provides a more detailed iteration history. Besides listing the current values of the parameters and their gradients, the ITDETAILS option provides the following values in addition to the default output:

- Restart, the number of iteration restarts
- Active, the number of active constraints
- Lambda, the value of the Lagrange multiplier (TRUREG and DBLDOG only)
- Ridge, the ridge value (NRRIDG only)
- Alpha, the line-search step size (QUANEW only)

An apostrophe (') trailing the number of active constraints indicates that at least one of the active constraints was released from the active set due to a significant Lagrange multiplier.

### Convergence Status

The "Convergence Status" table contains a status message describing the reason for termination of the optimization. The ODS name of this table is ConvergenceStatus, and you can query the nonprinting numeric variable Status to check for a successful optimization. This is useful in batch processing, or when processing BY groups, for example, in simulations. Successful convergence is indicated by Status=0.

### Fitting Information

The "Fitting Information" table lists the final minimized value of  $-2$  times the log likelihood as well as the information criteria of Akaike (AIC) and Schwarz (BIC), as well as a finite-sample corrected version of AIC (AICC). The criteria are computed as follows:

$$\text{AIC} = 2f(\hat{\theta}) + 2p$$

$$\text{AICC} = 2f(\hat{\theta}) + 2pn/(n - p - 1)$$

$$\text{BIC} = 2f(\hat{\theta}) + p \log(s)$$

where  $f()$  is the negative of the marginal log-likelihood function,  $\hat{\theta}$  is the vector of parameter estimates,  $p$  is the number of parameters,  $n$  is the number of observations, and  $s$  is the number of subjects. See Hurvich and Tsai (1989) and Burnham and Anderson (1998) for additional details.

### Parameter Estimates

The “Parameter Estimates” table lists the estimates of the parameter values after successful convergence of the optimization problem or the final values of the parameters under nonconvergence. If the problem did converge, standard errors are computed from the final Hessian matrix. The ratio of the estimate with its standard error produces a  $t$  value, with approximate degrees of freedom computed as the number of subjects minus the number of random effects. A  $p$ -value and confidence limits based on this  $t$  distribution are also provided. Finally, the gradient of the negative log-likelihood function is displayed for each parameter, and you should verify that they each are sufficiently small for unconstrained parameters.

### Covariance and Correlation Matrices

Following standard maximum likelihood theory (for example, Serfling 1980), the asymptotic variance-covariance matrix of the parameter estimates equals the inverse of the Hessian matrix. You can display this matrix with the **COV** option in the **PROC NL MIXED** statement. The corresponding correlation form is available with the **CORR** option.

### Additional Estimates

The “Additional Estimates” table displays the results of all **ESTIMATE** statements that you specify, with the same columns as the “Parameter Estimates” table. The **ECOV** and **ECORR** options in the **PROC NL MIXED** statement produce tables displaying the approximate covariance and correlation matrices of the additional estimates. They are computed using the delta method (Billingsley 1986; Cox 1998). The **EDER** option in the **PROC NL MIXED** statement produces a table that displays the derivatives of the additional estimates with respect to the model parameters evaluated at their final estimated values.

---

## ODS Table Names

**PROC NL MIXED** assigns a name to each table it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in Table 64.2. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

**Table 64.2** ODS Tables Produced by **PROC NL MIXED**

| ODS Table Name      | Description                                | Statement or Option |
|---------------------|--------------------------------------------|---------------------|
| AdditionalEstimates | Results from <b>ESTIMATE</b> statements    | <b>ESTIMATE</b>     |
| Contrasts           | Results from <b>CONTRAST</b> statements    | <b>CONTRAST</b>     |
| ConvergenceStatus   | Convergence status                         | default             |
| CorrMatAddEst       | Correlation matrix of additional estimates | <b>ECORR</b>        |
| CorrMatParmEst      | Correlation matrix of parameter estimates  | <b>CORR</b>         |
| CovMatAddEst        | Covariance matrix of additional estimates  | <b>ECOV</b>         |
| CovMatParmEst       | Covariance matrix of parameter estimates   | <b>COV</b>          |
| DerAddEst           | Derivatives of additional estimates        | <b>EDER</b>         |
| Dimensions          | Dimensions of the problem                  | default             |
| FitStatistics       | Fit statistics                             | default             |
| Hessian             | Second derivative matrix                   | <b>HESS</b>         |
| IterHistory         | Iteration history                          | default             |
| Parameters          | Parameters                                 | default             |
| ParameterEstimates  | Parameter estimates                        | default             |

Table 64.2 continued

| ODS Table Name  | Description                  | Statement or Option |
|-----------------|------------------------------|---------------------|
| Specifications  | Model specifications         | default             |
| StartingHessian | Starting Hessian matrix      | START HESS          |
| StartingValues  | Starting values and gradient | START               |

## Examples: NLMIXED Procedure

### Example 64.1: One-Compartment Model with Pharmacokinetic Data

A popular application of nonlinear mixed models is in the field of pharmacokinetics, which studies how a drug disperses through a living individual. This example considers the theophylline data from Pinheiro and Bates (1995). Serum concentrations of the drug theophylline are measured in 12 subjects over a 25-hour period after oral administration. The data are as follows.

```
data theoph;
 input subject time conc dose wt;
 datalines;
 1 0.00 0.74 4.02 79.6
 1 0.25 2.84 4.02 79.6
 1 0.57 6.57 4.02 79.6
 1 1.12 10.50 4.02 79.6
 1 2.02 9.66 4.02 79.6
 1 3.82 8.58 4.02 79.6
 1 5.10 8.36 4.02 79.6
 1 7.03 7.47 4.02 79.6

 ... more lines ...

12 24.15 1.17 5.30 60.5
;
```

Pinheiro and Bates (1995) consider the following first-order compartment model for these data:

$$C_{it} = \frac{Dk_{e_i}k_{a_i}}{Cl_i(k_{a_i} - k_{e_i})} [\exp(-k_{e_i}t) - \exp(-k_{a_i}t)] + e_{it}$$

where  $C_{it}$  is the observed concentration of the  $i$ th subject at time  $t$ ,  $D$  is the dose of theophylline,  $k_{e_i}$  is the elimination rate constant for subject  $i$ ,  $k_{a_i}$  is the absorption rate constant for subject  $i$ ,  $Cl_i$  is the clearance for subject  $i$ , and  $e_{it}$  are normal errors. To allow for random variability between subjects, they assume

$$\begin{aligned} Cl_i &= \exp(\beta_1 + b_{i1}) \\ k_{a_i} &= \exp(\beta_2 + b_{i2}) \\ k_{e_i} &= \exp(\beta_3) \end{aligned}$$

where the  $\beta$ s denote fixed-effects parameters and the  $b_i$ s denote random-effects parameters with an unknown covariance matrix.

The PROC NL MIXED statements to fit this model are as follows:

```
proc nlmixed data=theoph;
 parms beta1=-3.22 beta2=0.47 beta3=-2.45
 s2b1 =0.03 cb12 =0 s2b2 =0.4 s2=0.5;
 cl = exp(beta1 + b1);
 ka = exp(beta2 + b2);
 ke = exp(beta3);
 pred = dose*ke*ka*(exp(-ke*time)-exp(-ka*time))/cl/(ka-ke);
 model conc ~ normal(pred,s2);
 random b1 b2 ~ normal([0,0],[s2b1,cb12,s2b2]) subject=subject;
run;
```

The **PARMS** statement specifies starting values for the three  $\beta$ s and four variance-covariance parameters. The clearance and rate constants are defined using SAS programming statements, and the conditional model for the data is defined to be normal with mean `pred` and variance `s2`. The two random effects are `b1` and `b2`, and their joint distribution is defined in the **RANDOM** statement. Brackets are used in defining their mean vector (two zeros) and the lower triangle of their variance-covariance matrix (a general  $2 \times 2$  matrix). The **SUBJECT=** variable is `subject`.

The results from this analysis are as follows.

#### Output 64.1.1 Model Specification for One-Compartment Model

| The NL MIXED Procedure              |                                 |
|-------------------------------------|---------------------------------|
| Specifications                      |                                 |
| Data Set                            | WORK.THEOPH                     |
| Dependent Variable                  | conc                            |
| Distribution for Dependent Variable | Normal                          |
| Random Effects                      | b1 b2                           |
| Distribution for Random Effects     | Normal                          |
| Subject Variable                    | subject                         |
| Optimization Technique              | Dual Quasi-Newton               |
| Integration Method                  | Adaptive Gaussian<br>Quadrature |

The “Specifications” table lists the setup of the model (Output 64.1.1). The “Dimensions” table indicates that there are 132 observations, 12 subjects, and 7 parameters. PROC NL MIXED selects 5 quadrature points for each random effect, producing a total grid of 25 points over which quadrature is performed (Output 64.1.2).

**Output 64.1.2** Dimensions Table for One-Compartment Model

| Dimensions            |     |
|-----------------------|-----|
| Observations Used     | 132 |
| Observations Not Used | 0   |
| Total Observations    | 132 |
| Subjects              | 12  |
| Max Obs Per Subject   | 11  |
| Parameters            | 7   |
| Quadrature Points     | 5   |

The “Parameters” table lists the 7 parameters, their starting values, and the initial evaluation of the negative log likelihood using adaptive Gaussian quadrature (Output 64.1.3). The “Iteration History” table indicates that 10 steps are required for the dual quasi-Newton algorithm to achieve convergence.

**Output 64.1.3** Starting Values and Iteration History

| Parameters |       |       |      |      |      |                |
|------------|-------|-------|------|------|------|----------------|
| beta1      | beta2 | beta3 | s2b1 | cb12 | s2b2 | s2 NegLogLike  |
| -3.22      | 0.47  | -2.45 | 0.03 | 0    | 0.4  | 0.5 177.789945 |

| Iteration History |       |            |          |          |          |
|-------------------|-------|------------|----------|----------|----------|
| Iter              | Calls | NegLogLike | Diff     | MaxGrad  | Slope    |
| 1                 | 5     | 177.776248 | 0.013697 | 2.873367 | -63.0744 |
| 2                 | 8     | 177.7643   | 0.011948 | 1.698144 | -4.75239 |
| 3                 | 10    | 177.757264 | 0.007036 | 1.297439 | -1.97311 |
| 4                 | 12    | 177.755688 | 0.001576 | 1.441408 | -0.49772 |
| 5                 | 14    | 177.7467   | 0.008988 | 1.132279 | -0.8223  |
| 6                 | 17    | 177.746401 | 0.000299 | 0.831293 | -0.00244 |
| 7                 | 19    | 177.746318 | 0.000083 | 0.724198 | -0.00789 |
| 8                 | 21    | 177.74574  | 0.000578 | 0.180018 | -0.00583 |
| 9                 | 23    | 177.745736 | 3.88E-6  | 0.017958 | -8.25E-6 |
| 10                | 25    | 177.745736 | 3.222E-8 | 0.000143 | -6.51E-8 |

NOTE: GCONV convergence criterion satisfied.

**Output 64.1.4** Fit Statistics for One-Compartment Model

| Fit Statistics           |       |
|--------------------------|-------|
| -2 Log Likelihood        | 355.5 |
| AIC (smaller is better)  | 369.5 |
| AICC (smaller is better) | 370.4 |
| BIC (smaller is better)  | 372.9 |

The “Fit Statistics” table lists the final optimized values of the log-likelihood function and information criteria in the “smaller is better” form (Output 64.1.4).

**Output 64.1.5** Parameter Estimates for One-Compartment Model

| Parameter Estimates |          |                |    |         |         |       |          |
|---------------------|----------|----------------|----|---------|---------|-------|----------|
| Parameter           | Estimate | Standard Error | DF | t Value | Pr >  t | Alpha | Lower    |
| beta1               | -3.2268  | 0.05950        | 10 | -54.23  | <.0001  | 0.05  | -3.3594  |
| beta2               | 0.4806   | 0.1989         | 10 | 2.42    | 0.0363  | 0.05  | 0.03745  |
| beta3               | -2.4592  | 0.05126        | 10 | -47.97  | <.0001  | 0.05  | -2.5734  |
| s2b1                | 0.02803  | 0.01221        | 10 | 2.30    | 0.0445  | 0.05  | 0.000833 |
| cb12                | -0.00127 | 0.03404        | 10 | -0.04   | 0.9710  | 0.05  | -0.07712 |
| s2b2                | 0.4331   | 0.2005         | 10 | 2.16    | 0.0560  | 0.05  | -0.01353 |
| s2                  | 0.5016   | 0.06837        | 10 | 7.34    | <.0001  | 0.05  | 0.3493   |

| Parameter Estimates |         |          |
|---------------------|---------|----------|
| Parameter           | Upper   | Gradient |
| beta1               | -3.0942 | -0.00009 |
| beta2               | 0.9238  | 3.645E-7 |
| beta3               | -2.3449 | 0.000039 |
| s2b1                | 0.05523 | -0.00014 |
| cb12                | 0.07458 | -0.00007 |
| s2b2                | 0.8798  | -6.98E-6 |
| s2                  | 0.6540  | 6.133E-6 |

The “Parameter Estimates” table contains the maximum likelihood estimates of the parameters (Output 64.1.5). Both s2b1 and s2b2 are marginally significant, indicating between-subject variability in the clearances and absorption rate constants, respectively. There does not appear to be a significant covariance between them, as seen by the estimate of cb12.

The estimates of  $\beta_1$ ,  $\beta_2$ , and  $\beta_3$  are close to the adaptive quadrature estimates listed in Table 3 of Pinheiro and Bates (1995). However, Pinheiro and Bates use a Cholesky-root parameterization for the random-effects variance matrix and a logarithmic parameterization for the residual variance. The PROC NL MIXED statements using their parameterization are as follows, and results are similar.

```

proc nlmixed data=theoph;
 parms l11=-1.5 l2=0 l13=-0.1 beta1=-3 beta2=0.5 beta3=-2.5 ls2=-0.7;
 s2 = exp(ls2);
 l1 = exp(l11);
 l3 = exp(l13);
 s2b1 = l1*l1*s2;
 cb12 = l2*l1*s2;
 s2b2 = (l2*l2 + l3*l3)*s2;
 c1 = exp(beta1 + b1);
 ka = exp(beta2 + b2);
 ke = exp(beta3);
 pred = dose*ke*ka*(exp(-ke*time)-exp(-ka*time))/c1/(ka-ke);
 model conc ~ normal(pred, s2);
 random b1 b2 ~ normal([0,0], [s2b1, cb12, s2b2]) subject=subject;
run;

```

## Example 64.2: Probit-Normal Model with Binomial Data

For this example, consider the data from Weil (1970), also studied by: Williams (1975); Ochi and Prentice (1984); McCulloch (1994). In this experiment 16 pregnant rats receive a control diet and 16 receive a chemically treated diet, and the litter size for each rat is recorded after 4 and 21 days. The SAS data set follows:

```

data rats;
 input trt $ m x @@;
 if (trt='c') then do;
 x1 = 1;
 x2 = 0;
 end;
 else do;
 x1 = 0;
 x2 = 1;
 end;
 litter = _n_;
 datalines;
c 13 13 c 12 12 c 9 9 c 9 9 c 8 8 c 8 8 c 13 12 c 12 11
c 10 9 c 10 9 c 9 8 c 13 11 c 5 4 c 7 5 c 10 7 c 10 7
t 12 12 t 11 11 t 10 10 t 9 9 t 11 10 t 10 9 t 10 9 t 9 8
t 9 8 t 5 4 t 9 7 t 7 4 t 10 5 t 6 3 t 10 3 t 7 0
;

```

Here,  $m$  represents the size of the litter after 4 days, and  $x$  represents the size of the litter after 21 days. Also, indicator variables  $x_1$  and  $x_2$  are constructed for the two treatment levels.

Following McCulloch (1994), assume a latent survival model of the form

$$y_{ijk} = t_i + \alpha_{ij} + e_{ijk}$$

where  $i$  indexes treatment,  $j$  indexes litter, and  $k$  indexes newborn rats within a litter. The  $t_i$  represent treatment means, the  $\alpha_{ij}$  represent random litter effects assumed to be iid  $N(0, s_i^2)$ , and the  $e_{ijk}$  represent iid residual errors, all on the latent scale.

Instead of observing the survival times  $y_{ijk}$ , assume that only the binary variable indicating whether  $y_{ijk}$  exceeds 0 is observed. If  $x_{ij}$  denotes the sum of these binary variables for the  $i$ th treatment and the  $j$ th litter,

then the preceding assumptions lead to the following generalized linear mixed model:

$$x_{ij} | \alpha_{ij} \sim \text{Binomial}(m_{ij}, p_{ij})$$

where  $m_{ij}$  is the size of each litter after 4 days and

$$p_{ij} = \Phi(t_i + \alpha_{ij})$$

The PROC NLMIXED statements to fit this model are as follows:

```
proc nlmixed data=rats;
 parms t1=1 t2=1 s1=.05 s2=1;
 eta = x1*t1 + x2*t2 + alpha;
 p = probnorm(eta);
 model x ~ binomial(m,p);
 random alpha ~ normal(0,x1*s1*s1+x2*s2*s2) subject=litter;
 estimate 'gamma2' t2/sqrt(1+s2*s2);
 predict p out=p;
run;
```

As in [Example 64.1](#), the PROC NLMIXED statement invokes the procedure and the PARMS statement defines the parameters. The parameters for this example are the two treatment means,  $t_1$  and  $t_2$ , and the two random-effect standard deviations,  $s_1$  and  $s_2$ .

The indicator variables  $x_1$  and  $x_2$  are used in the program to assign the proper mean to each observation in the input data set as well as the proper variance to the random effects. Note that programming expressions are permitted inside the distributional specifications, as illustrated by the random-effects variance specified here.

The ESTIMATE statement requests an estimate of  $\gamma_2 = t_2 / \sqrt{1 + s_2^2}$ , which is a location-scale parameter from Ochi and Prentice (1984).

The PREDICT statement constructs predictions for each observation in the input data set. For this example, predictions of  $p$  and approximate standard errors of prediction are output to a SAS data set named P. These predictions are functions of the parameter estimates and the empirical Bayes estimates of the random effects  $\alpha_i$ .

The output for this model is as follows.

#### Output 64.2.1 Specifications, Dimensions, and Starting Values

| The NLMIXED Procedure               |                              |
|-------------------------------------|------------------------------|
| Specifications                      |                              |
| Data Set                            | WORK.RATS                    |
| Dependent Variable                  | x                            |
| Distribution for Dependent Variable | Binomial                     |
| Random Effects                      | alpha                        |
| Distribution for Random Effects     | Normal                       |
| Subject Variable                    | litter                       |
| Optimization Technique              | Dual Quasi-Newton            |
| Integration Method                  | Adaptive Gaussian Quadrature |



**Output 64.2.1** *continued*

| Dimensions            |    |      |    |            |    |
|-----------------------|----|------|----|------------|----|
| Observations Used     |    |      |    |            | 32 |
| Observations Not Used |    |      |    |            | 0  |
| Total Observations    |    |      |    |            | 32 |
| Subjects              |    |      |    |            | 32 |
| Max Obs Per Subject   |    |      |    |            | 1  |
| Parameters            |    |      |    |            | 4  |
| Quadrature Points     |    |      |    |            | 7  |
| Parameters            |    |      |    |            |    |
| t1                    | t2 | s1   | s2 | NegLogLike |    |
| 1                     | 1  | 0.05 | 1  | 54.9362323 |    |

The “Specifications” table provides basic information about this nonlinear mixed model (Output 64.2.1). The “Dimensions” table provides counts of various variables. Note that each observation in the data comprises a separate subject. Using the starting values in the “Parameters” table, PROC NLMIXED determines that the log-likelihood function can be approximated with sufficient accuracy with a seven-point quadrature rule.

**Output 64.2.2** Iteration History for Probit-Normal Model

| Iteration History                            |       |            |          |          |          |
|----------------------------------------------|-------|------------|----------|----------|----------|
| Iter                                         | Calls | NegLogLike | Diff     | MaxGrad  | Slope    |
| 1                                            | 2     | 53.9933934 | 0.942839 | 11.03261 | -81.9428 |
| 2                                            | 3     | 52.875353  | 1.11804  | 2.148952 | -2.86277 |
| 3                                            | 5     | 52.6350386 | 0.240314 | 0.329957 | -1.05049 |
| 4                                            | 6     | 52.6319939 | 0.003045 | 0.122926 | -0.00672 |
| 5                                            | 8     | 52.6313583 | 0.000636 | 0.028246 | -0.00352 |
| 6                                            | 11    | 52.6313174 | 0.000041 | 0.013551 | -0.00023 |
| 7                                            | 13    | 52.6313115 | 5.839E-6 | 0.000603 | -0.00001 |
| 8                                            | 15    | 52.6313115 | 9.45E-9  | 0.000022 | -1.68E-8 |
| NOTE: GCONV convergence criterion satisfied. |       |            |          |          |          |

The “Iteration History” table indicates successful convergence in 8 iterations (Output 64.2.2).

**Output 64.2.3** Fit Statistics for Probit-Normal Model

| Fit Statistics           |       |
|--------------------------|-------|
| -2 Log Likelihood        | 105.3 |
| AIC (smaller is better)  | 113.3 |
| AICC (smaller is better) | 114.7 |
| BIC (smaller is better)  | 119.1 |

The “Fit Statistics” table lists useful statistics based on the maximized value of the log likelihood (Output 64.2.3).

**Output 64.2.4** Parameter Estimates for Probit-Normal Model

| Parameter Estimates |          |                |    |         |         |       |         |
|---------------------|----------|----------------|----|---------|---------|-------|---------|
| Parameter           | Estimate | Standard Error | DF | t Value | Pr >  t | Alpha | Lower   |
| t1                  | 1.3063   | 0.1685         | 31 | 7.75    | <.0001  | 0.05  | 0.9626  |
| t2                  | 0.9475   | 0.3055         | 31 | 3.10    | 0.0041  | 0.05  | 0.3244  |
| s1                  | 0.2403   | 0.3015         | 31 | 0.80    | 0.4315  | 0.05  | -0.3746 |
| s2                  | 1.0292   | 0.2988         | 31 | 3.44    | 0.0017  | 0.05  | 0.4198  |

| Parameter Estimates |        |          |
|---------------------|--------|----------|
| Parameter           | Upper  | Gradient |
| t1                  | 1.6499 | -0.00002 |
| t2                  | 1.5705 | 9.283E-6 |
| s1                  | 0.8552 | 0.000014 |
| s2                  | 1.6385 | -3.16E-6 |

The “Parameter Estimates” table indicates significance of all the parameters except S1 (Output 64.2.4).

**Output 64.2.5** Additional Estimates

| Additional Estimates |          |                |    |         |         |       |        |        |
|----------------------|----------|----------------|----|---------|---------|-------|--------|--------|
| Label                | Estimate | Standard Error | DF | t Value | Pr >  t | Alpha | Lower  | Upper  |
| gamma2               | 0.6603   | 0.2165         | 31 | 3.05    | 0.0047  | 0.05  | 0.2186 | 1.1019 |

The “Additional Estimates” table displays results from the ESTIMATE statement (Output 64.2.5). The estimate of  $\gamma_2$  equals 0.66, agreeing with that obtained by McCulloch (1994). The standard error 0.22 is computed using the delta method (Billingsley 1986; Cox 1998).

Not shown is the P data set, which contains the original 32 observations and predictions of the  $p_{ij}$ .

### Example 64.3: Probit-Normal Model with Ordinal Data

The data for this example are from Ezzet and Whitehead (1991), who describe a crossover experiment on two groups of patients using two different inhaler devices (A and B). Patients from group 1 used device A for one week and then device B for another week. Patients from group 2 used the devices in reverse order. The data entered as a SAS data set are as follows:

```
data inhaler;
 input clarity group time freq @@;
 gt = group*time;
 sub = floor((_n_+1)/2);
 datalines;
1 0 0 59 1 0 1 59 1 0 0 35 2 0 1 35 1 0 0 3 3 0 1 3 1 0 0 2
4 0 1 2 2 0 0 11 1 0 1 11 2 0 0 27 2 0 1 27 2 0 0 2 3 0 1 2
2 0 0 1 4 0 1 1 4 0 0 1 1 0 1 1 4 0 0 1 2 0 1 1 1 1 0 63
1 1 1 63 1 1 0 13 2 1 1 13 2 1 0 40 1 1 1 40 2 1 0 15 2 1 1 15
3 1 0 7 1 1 1 7 3 1 0 2 2 1 1 2 3 1 0 1 3 1 1 1 4 1 0 2
1 1 1 2 4 1 0 1 3 1 1 1
;
```

The response measurement, clarity, is the patients' assessment on the clarity of the leaflet instructions for the devices. The clarity variable is on an ordinal scale, with 1=easy, 2=only clear after rereading, 3=not very clear, and 4=confusing. The group variable indicates the treatment group, and the time variable indicates the time of measurement. The freq variable indicates the number of patients with exactly the same responses. A variable gt is created to indicate a group-by-time interaction, and a variable sub is created to indicate patients.

As in the previous example and in Hedeker and Gibbons (1994), assume an underlying latent continuous variable, here with the form

$$y_{ij} = \beta_0 + \beta_1 g_i + \beta_2 t_j + \beta_3 g_i t_j + u_i + e_{ij}$$

where  $i$  indexes patient and  $j$  indexes the time period,  $g_i$  indicates groups,  $t_j$  indicates time,  $u_i$  is a patient-level normal random effect, and  $e_{ij}$  are iid normal errors. The  $\beta$ s are unknown coefficients to be estimated.

Instead of observing  $y_{ij}$ , however, you observe only whether it falls in one of the four intervals:  $(-\infty, 0)$ ,  $(0, I_1)$ ,  $(I_1, I_1 + I_2)$ , or  $(I_1 + I_2, \infty)$ , where  $I_1$  and  $I_2$  are both positive. The resulting category is the value assigned to the clarity variable.

The following code sets up and fits this ordinal probit model:

```
proc nlmixed data=inhaler corr ecorr;
 parms b0=0 b1=0 b2=0 b3=0 sd=1 i1=1 i2=1;
 bounds i1 > 0, i2 > 0;
 eta = b0 + b1*group + b2*time + b3*gt + u;
 if (clarity=1) then p = probnorm(-eta);
 else if (clarity=2) then
 p = probnorm(i1-eta) - probnorm(-eta);
 else if (clarity=3) then
 p = probnorm(i1+i2-eta) - probnorm(i1-eta);
 else p = 1 - probnorm(i1+i2-eta);
 if (p > 1e-8) then ll = log(p);
 else ll = -1e20;
```

```

model clarity ~ general(11);
random u ~ normal(0,sd*sd) subject=sub;
replicate freq;
estimate 'thresh2' i1;
estimate 'thresh3' i1 + i2;
estimate 'icc' sd*sd/(1+sd*sd);
run;

```

The **PROC NLMIXED** statement specifies the input data set and requests correlations both for the parameter estimates (**CORR** option) and for the additional estimates specified with **ESTIMATE** statements (**ECORR** option).

The parameters as defined in the **PARMS** statement are as follows: **b0** (overall intercept), **b1** (group main effect), **B2** (time main effect), **b3** (group-by-time interaction), **sd** (standard deviation of the random effect), **i1** (increment between first and second thresholds), and **i2** (increment between second and third thresholds). The **BOUNDS** statement restricts **i1** and **i2** to be positive.

The SAS programming statements begin by defining the linear predictor **eta**, which is a linear combination of the **b** parameters and a single random effect **u**. The next statements define the ordinal likelihood according to the **clarity** variable, **eta**, and the increment variables. An error trap is included in case the likelihood becomes too small.

A general log-likelihood specification is used in the **MODEL** statement, and the **RANDOM** statement defines the random effect **u** to have standard deviation **sd** and subject variable **sub**. The **REPLICATE** statement indicates that data for each subject should be replicated according to the **freq** variable.

The **ESTIMATE** statements specify the second and third thresholds in terms of the increment variables (the first threshold is assumed to equal zero for model identifiability). Also computed is the intraclass correlation.

The output is as follows.

### Output 64.3.1 Specifications for Ordinal Data Model

| The NLMIXED Procedure               |                              |
|-------------------------------------|------------------------------|
| Specifications                      |                              |
| Data Set                            | WORK.INHALER                 |
| Dependent Variable                  | clarity                      |
| Distribution for Dependent Variable | General                      |
| Random Effects                      | u                            |
| Distribution for Random Effects     | Normal                       |
| Subject Variable                    | sub                          |
| Replicate Variable                  | freq                         |
| Optimization Technique              | Dual Quasi-Newton            |
| Integration Method                  | Adaptive Gaussian Quadrature |

The “Specifications” table echoes some primary information specified for this nonlinear mixed model (Output 64.3.1). Because the log-likelihood function was expressed with SAS programming statements, the distribution is displayed as *General* in the “Specifications” table.

The “Dimensions” table reveals a total of 286 subjects, which is the sum of the values of the FREQ variable for the second time point. Five quadrature points are selected for log-likelihood evaluation (Output 64.3.2).

**Output 64.3.2** Dimensions Table for Ordinal Data Model

| Dimensions            |     |
|-----------------------|-----|
| Observations Used     | 38  |
| Observations Not Used | 0   |
| Total Observations    | 38  |
| Subjects              | 286 |
| Max Obs Per Subject   | 2   |
| Parameters            | 7   |
| Quadrature Points     | 5   |

**Output 64.3.3** Parameter Starting Values and Negative Log Likelihood

| Parameters |    |    |    |    |    |    |            |
|------------|----|----|----|----|----|----|------------|
| b0         | b1 | b2 | b3 | sd | i1 | i2 | NegLogLike |
| 0          | 0  | 0  | 0  | 1  | 1  | 1  | 538.484276 |

The “Parameters” table lists the simple starting values for this problem (Output 64.3.3). The “Iteration History” table indicates successful convergence in 13 iterations (Output 64.3.4).

**Output 64.3.4** Iteration History

| Iteration History |       |            |          |          |          |
|-------------------|-------|------------|----------|----------|----------|
| Iter              | Calls | NegLogLike | Diff     | MaxGrad  | Slope    |
| 1                 | 2     | 476.382511 | 62.10176 | 43.75062 | -1431.4  |
| 2                 | 4     | 463.228197 | 13.15431 | 14.24648 | -106.753 |
| 3                 | 5     | 458.528118 | 4.70008  | 48.31316 | -33.0389 |
| 4                 | 6     | 450.975735 | 7.552383 | 22.60098 | -40.9954 |
| 5                 | 8     | 448.012701 | 2.963033 | 14.86877 | -16.7453 |
| 6                 | 10    | 447.245153 | 0.767549 | 7.774189 | -2.26743 |
| 7                 | 11    | 446.72767  | 0.517483 | 3.793533 | -1.59278 |
| 8                 | 13    | 446.518273 | 0.209396 | 0.868638 | -0.37801 |
| 9                 | 16    | 446.514528 | 0.003745 | 0.328568 | -0.02356 |
| 10                | 18    | 446.513341 | 0.001187 | 0.056778 | -0.00183 |
| 11                | 20    | 446.513314 | 0.000027 | 0.010785 | -0.00004 |
| 12                | 22    | 446.51331  | 3.956E-6 | 0.004922 | -5.41E-6 |
| 13                | 24    | 446.51331  | 1.989E-7 | 0.00047  | -4E-7    |

NOTE: GCONV convergence criterion satisfied.

**Output 64.3.5** Fit Statistics for Ordinal Data Model

| Fit Statistics           |       |
|--------------------------|-------|
| -2 Log Likelihood        | 893.0 |
| AIC (smaller is better)  | 907.0 |
| AICC (smaller is better) | 910.8 |
| BIC (smaller is better)  | 932.6 |

The “Fit Statistics” table lists the log likelihood and information criteria for model comparisons (Output 64.3.5).

**Output 64.3.6** Parameter Estimates at Convergence

| Parameter Estimates |          |                |     |         |         |       |         |
|---------------------|----------|----------------|-----|---------|---------|-------|---------|
| Parameter           | Estimate | Standard Error | DF  | t Value | Pr >  t | Alpha | Lower   |
| b0                  | -0.6364  | 0.1342         | 285 | -4.74   | <.0001  | 0.05  | -0.9006 |
| b1                  | 0.6007   | 0.1770         | 285 | 3.39    | 0.0008  | 0.05  | 0.2523  |
| b2                  | 0.6015   | 0.1582         | 285 | 3.80    | 0.0002  | 0.05  | 0.2900  |
| b3                  | -1.4817  | 0.2385         | 285 | -6.21   | <.0001  | 0.05  | -1.9512 |
| sd                  | 0.6599   | 0.1312         | 285 | 5.03    | <.0001  | 0.05  | 0.4017  |
| i1                  | 1.7450   | 0.1474         | 285 | 11.84   | <.0001  | 0.05  | 1.4548  |
| i2                  | 0.5985   | 0.1427         | 285 | 4.19    | <.0001  | 0.05  | 0.3177  |

| Parameter Estimates |         |          |
|---------------------|---------|----------|
| Parameter           | Upper   | Gradient |
| b0                  | -0.3722 | 0.00047  |
| b1                  | 0.9491  | 0.000265 |
| b2                  | 0.9129  | 0.00008  |
| b3                  | -1.0122 | 0.000102 |
| sd                  | 0.9181  | -0.00009 |
| i1                  | 2.0352  | 0.000202 |
| i2                  | 0.8794  | 0.000087 |

The “Parameter Estimates” table indicates significance of all the parameters (Output 64.3.6).

**Output 64.3.7** Threshold and Intraclass Correlation Estimates

| Additional Estimates |          |                |     |         |         |       |        |        |
|----------------------|----------|----------------|-----|---------|---------|-------|--------|--------|
| Label                | Estimate | Standard Error | DF  | t Value | Pr >  t | Alpha | Lower  | Upper  |
| thresh2              | 1.7450   | 0.1474         | 285 | 11.84   | <.0001  | 0.05  | 1.4548 | 2.0352 |
| thresh3              | 2.3435   | 0.2073         | 285 | 11.31   | <.0001  | 0.05  | 1.9355 | 2.7515 |
| icc                  | 0.3034   | 0.08402        | 285 | 3.61    | 0.0004  | 0.05  | 0.1380 | 0.4687 |

The “Additional Estimates” table displays results from the ESTIMATE statements (Output 64.3.7).

### Example 64.4: Poisson-Normal Model with Count Data

This example uses the pump failure data of Gaver and O’Muircheartaigh (1987). The number of failures and the time of operation are recorded for 10 pumps. Each of the pumps is classified into one of two groups corresponding to either continuous or intermittent operation. The data are as follows:

```
data pump;
 input y t group;
 pump = _n_;
 logtstd = log(t) - 2.4564900;
 datalines;
5 94.320 1
1 15.720 2
5 62.880 1
14 125.760 1
3 5.240 2
19 31.440 1
1 1.048 2
1 1.048 2
4 2.096 2
22 10.480 2
;
```

Each row denotes data for a single pump, and the variable logtstd contains the centered operation times.

Letting  $y_{ij}$  denote the number of failures for the  $j$ th pump in the  $i$ th group, Draper (1996) considers the following hierarchical model for these data:

$$y_{ij} | \lambda_{ij} \sim \text{Poisson}(\lambda_{ij})$$

$$\log \lambda_{ij} = \alpha_i + \beta_i (\log t_{ij} - \overline{\log t}) + e_{ij}$$

$$e_{ij} | \sigma^2 \sim \text{Normal}(0, \sigma^2)$$

The model specifies different intercepts and slopes for each group, and the random effect is a mechanism for accounting for overdispersion.

The corresponding PROC NL MIXED statements are as follows:

```
proc nlmixed data=pump;
 parms logsig 0 beta1 1 beta2 1 alpha1 1 alpha2 1;
 if (group = 1) then eta = alpha1 + beta1*logtstd + e;
 else eta = alpha2 + beta2*logtstd + e;
 lambda = exp(eta);
 model y ~ poisson(lambda);
 random e ~ normal(0,exp(2*logsig)) subject=pump;
 estimate 'alpha1-alpha2' alpha1-alpha2;
 estimate 'beta1-beta2' beta1-beta2;
run;
```

The selected output is as follows.

**Output 64.4.1** Dimensions Table for Poisson-Normal Model

| The NL MIXED Procedure |    |
|------------------------|----|
| Dimensions             |    |
| Observations Used      | 10 |
| Observations Not Used  | 0  |
| Total Observations     | 10 |
| Subjects               | 10 |
| Max Obs Per Subject    | 1  |
| Parameters             | 5  |
| Quadrature Points      | 5  |

The “Dimensions” table indicates that data for 10 pumps are used with one observation for each (Output 64.4.1).

**Output 64.4.2** Iteration History for Poisson-Normal Model

| Iteration History |       |            |          |          |          |
|-------------------|-------|------------|----------|----------|----------|
| Iter              | Calls | NegLogLike | Diff     | MaxGrad  | Slope    |
| 1                 | 2     | 30.6986932 | 2.162768 | 5.107253 | -91.602  |
| 2                 | 5     | 30.0255468 | 0.673146 | 2.761738 | -11.0489 |
| 3                 | 7     | 29.726325  | 0.299222 | 2.990401 | -2.36048 |
| 4                 | 9     | 28.7390263 | 0.987299 | 2.074431 | -3.93678 |
| 5                 | 10    | 28.3161933 | 0.422833 | 0.612531 | -0.63084 |
| 6                 | 12    | 28.09564   | 0.220553 | 0.462162 | -0.52684 |
| 7                 | 14    | 28.0438024 | 0.051838 | 0.405047 | -0.10018 |
| 8                 | 16    | 28.0357134 | 0.008089 | 0.135059 | -0.01875 |
| 9                 | 18    | 28.033925  | 0.001788 | 0.026279 | -0.00514 |
| 10                | 20    | 28.0338744 | 0.000051 | 0.00402  | -0.00012 |
| 11                | 22    | 28.0338727 | 1.681E-6 | 0.002864 | -5.09E-6 |
| 12                | 24    | 28.0338724 | 3.199E-7 | 0.000147 | -6.87E-7 |
| 13                | 26    | 28.0338724 | 2.532E-9 | 0.000017 | -5.75E-9 |

NOTE: GCONV convergence criterion satisfied.



The “Iteration History” table indicates successful convergence in 13 iterations (Output 64.4.2).

#### Output 64.4.3 Fit Statistics for Poisson-Normal Model

| Fit Statistics           |      |
|--------------------------|------|
| -2 Log Likelihood        | 56.1 |
| AIC (smaller is better)  | 66.1 |
| AICC (smaller is better) | 81.1 |
| BIC (smaller is better)  | 67.6 |

The “Fit Statistics” table lists the final log likelihood and associated information criteria (Output 64.4.3).

#### Output 64.4.4 Parameter Estimates and Additional Estimates

| Parameter Estimates |          |                |    |         |         |       |         |
|---------------------|----------|----------------|----|---------|---------|-------|---------|
| Parameter           | Estimate | Standard Error | DF | t Value | Pr >  t | Alpha | Lower   |
| logsig              | -0.3161  | 0.3213         | 9  | -0.98   | 0.3508  | 0.05  | -1.0429 |
| beta1               | -0.4256  | 0.7473         | 9  | -0.57   | 0.5829  | 0.05  | -2.1162 |
| beta2               | 0.6097   | 0.3814         | 9  | 1.60    | 0.1443  | 0.05  | -0.2530 |
| alpha1              | 2.9644   | 1.3826         | 9  | 2.14    | 0.0606  | 0.05  | -0.1632 |
| alpha2              | 1.7992   | 0.5492         | 9  | 3.28    | 0.0096  | 0.05  | 0.5568  |

| Parameter Estimates |        |          |
|---------------------|--------|----------|
| Parameter           | Upper  | Gradient |
| logsig              | 0.4107 | -0.00002 |
| beta1               | 1.2649 | -0.00002 |
| beta2               | 1.4724 | -1.61E-6 |
| alpha1              | 6.0921 | -5.25E-6 |
| alpha2              | 3.0415 | -5.73E-6 |

| Additional Estimates |          |                |    |         |         |       |         |
|----------------------|----------|----------------|----|---------|---------|-------|---------|
| Label                | Estimate | Standard Error | DF | t Value | Pr >  t | Alpha | Lower   |
| alpha1-alpha2        | 1.1653   | 1.4855         | 9  | 0.78    | 0.4529  | 0.05  | -2.1952 |
| beta1-beta2          | -1.0354  | 0.8389         | 9  | -1.23   | 0.2484  | 0.05  | -2.9331 |

| Additional Estimates |        |
|----------------------|--------|
| Label                | Upper  |
| alpha1-alpha2        | 4.5257 |
| beta1-beta2          | 0.8623 |

The “Parameter Estimates” and “Additional Estimates” tables list the maximum likelihood estimates for each of the parameters and two differences (Output 64.4.4). The point estimates for the mean parameters agree fairly closely with the Bayesian posterior means reported by Draper (1996); however, the likelihood-based standard errors are roughly half the Bayesian posterior standard deviations. This is most likely due to the fact that the Bayesian standard deviations account for the uncertainty in estimating  $\sigma^2$ , whereas the likelihood values plug in its estimated value. This downward bias can be corrected somewhat by using the  $t_9$  distribution shown here.

## Example 64.5: Failure Time and Frailty Model

In this example an accelerated failure time model with proportional hazard is fitted with and without random effects. The data are from the “Getting Started” example of PROC LIFEREG; see Chapter 51, “The LIFEREG Procedure.” Thirty-eight patients are divided into two groups of equal size, and different pain relievers are assigned to each group. The outcome reported is the time in minutes until headache relief. The variable `sensor` indicates whether relief was observed during the course of the observation period (`sensor = 0`) or whether the observation is censored (`sensor = 1`). The SAS DATA step for these data is as follows:

```
data headache;
 input minutes group sensor @@;
 patient = _n_;
 datalines;
11 1 0 12 1 0 19 1 0 19 1 0
19 1 0 19 1 0 21 1 0 20 1 0
21 1 0 21 1 0 20 1 0 21 1 0
20 1 0 21 1 0 25 1 0 27 1 0
30 1 0 21 1 1 24 1 1 14 2 0
16 2 0 16 2 0 21 2 0 21 2 0
23 2 0 23 2 0 23 2 0 23 2 0
25 2 1 23 2 0 24 2 0 24 2 0
26 2 1 32 2 1 30 2 1 30 2 0
32 2 1 20 2 1
;
```

In modeling survival data, censoring of observations must be taken into account carefully. In this example, only right censoring occurs. If  $g(t, \boldsymbol{\beta})$ ,  $h(t, \boldsymbol{\beta})$ , and  $G(t, \boldsymbol{\beta})$  denote the density of failure, the hazard function, and the survival distribution function at time  $t$ , respectively, then the log likelihood can be written as

$$\begin{aligned} l(\boldsymbol{\beta}; \mathbf{t}) &= \sum_{i \in U_u} \log g(t_i, \boldsymbol{\beta}) + \sum_{i \in U_c} \log G(t_i, \boldsymbol{\beta}) \\ &= \sum_{i \in U_u} \log h(t_i, \boldsymbol{\beta}) + \sum_{i=1}^n \log G(t_i, \boldsymbol{\beta}) \end{aligned}$$

(See Cox and Oakes 1984, Ch. 3.) In these expressions  $U_u$  is the set of uncensored observations,  $U_c$  is the set of censored observations, and  $n$  denotes the total sample size.

The proportional hazards specification expresses the hazard in terms of a baseline hazard, multiplied by a constant. In this example the hazard is that of a Weibull model and is parameterized as  $h(t, \boldsymbol{\beta}) = \gamma \alpha (\alpha t)^{\gamma-1}$  and  $\alpha = \exp\{-\mathbf{x}'\boldsymbol{\beta}\}$ .

The linear predictor is set equal to the intercept in the reference group (`group = 2`); this defines the baseline hazard. The corresponding distribution of survival past time  $t$  is  $G(t, \beta) = \exp\{-(\alpha t)^\gamma\}$ . See Cox and Oakes (1984, Table 2.1) and the section “Supported Distributions” in Chapter 51, “The LIFEREG Procedure,” for this and other survival distribution models and various parameterizations.

The following NLMIXED statements fit this accelerated failure time model and estimate the cumulative distribution function of time to headache relief:

```
proc nlmixed data=headache;
 bounds gamma > 0;
 linp = b0 - b1*(group-2);
 alpha = exp(-linp);
 G_t = exp(-(alpha*minutes)**gamma);
 g = gamma*alpha*(alpha*minutes)**(gamma-1)*G_t;
 ll = (censor=0)*log(g) + (censor=1)*log(G_t);
 model minutes ~ general(ll);
 predict 1-G_t out=cdf;
run;
```

**Output 64.5.1** Specifications Table for Fixed-Effects Failure Time Model

| The NLMIXED Procedure               |                   |
|-------------------------------------|-------------------|
| Specifications                      |                   |
| Data Set                            | WORK.HEADACHE     |
| Dependent Variable                  | minutes           |
| Distribution for Dependent Variable | General           |
| Optimization Technique              | Dual Quasi-Newton |
| Integration Method                  | None              |

The “Specifications” table shows that no integration is required, since the model does not contain random effects (Output 64.5.1).

**Output 64.5.2** Negative Log Likelihood with Default Starting Values

| Parameters |    |    |            |
|------------|----|----|------------|
| gamma      | b0 | b1 | NegLogLike |
| 1          | 1  | 1  | 263.990327 |

No starting values were given for the three parameters. The NLMIXED procedure assigns the default value of 1.0 in this case. The negative log likelihood based on these starting values is shown in Output 64.5.2.

**Output 64.5.3** Iteration History for Fixed-Effects Failure Time Model

| Iteration History |       |            |          |          |          |
|-------------------|-------|------------|----------|----------|----------|
| Iter              | Calls | NegLogLike | Diff     | MaxGrad  | Slope    |
| 1                 | 2     | 169.244311 | 94.74602 | 22.5599  | -2230.83 |
| 2                 | 4     | 142.873508 | 26.3708  | 14.88631 | -3.64643 |
| 3                 | 6     | 140.633695 | 2.239814 | 11.25234 | -9.49454 |
| 4                 | 8     | 122.890659 | 17.74304 | 19.44959 | -2.50807 |
| 5                 | 9     | 121.396959 | 1.493699 | 13.85584 | -4.55427 |
| 6                 | 11    | 120.623843 | 0.773116 | 13.67062 | -1.38064 |
| 7                 | 12    | 119.278196 | 1.345647 | 15.78014 | -1.69072 |
| 8                 | 14    | 116.271325 | 3.006871 | 26.94029 | -3.2529  |
| 9                 | 16    | 109.427401 | 6.843925 | 19.88382 | -6.9289  |
| 10                | 19    | 103.298102 | 6.129298 | 12.15647 | -4.96054 |
| 11                | 22    | 101.686239 | 1.611863 | 14.24868 | -4.34059 |
| 12                | 23    | 100.027875 | 1.658364 | 11.69853 | -13.2049 |
| 13                | 26    | 99.9189048 | 0.108971 | 3.602552 | -0.55176 |
| 14                | 28    | 99.8738836 | 0.045021 | 0.170712 | -0.16645 |
| 15                | 30    | 99.8736392 | 0.000244 | 0.050822 | -0.00041 |
| 16                | 32    | 99.8736351 | 4.071E-6 | 0.000705 | -6.9E-6  |
| 17                | 34    | 99.8736351 | 6.1E-10  | 4.768E-6 | -1.23E-9 |

NOTE: GCONV convergence criterion satisfied.

The “Iteration History” table shows that the procedure converges after 17 iterations and 34 evaluations of the objective function (Output 64.5.3).

**Output 64.5.4** Fit Statistics and Parameter Estimates

| Fit Statistics |                          |  |  |  |  |  |       |
|----------------|--------------------------|--|--|--|--|--|-------|
|                | -2 Log Likelihood        |  |  |  |  |  | 199.7 |
|                | AIC (smaller is better)  |  |  |  |  |  | 205.7 |
|                | AICC (smaller is better) |  |  |  |  |  | 206.5 |
|                | BIC (smaller is better)  |  |  |  |  |  | 210.7 |

| Parameter Estimates |          |                |    |         |         |       |         |
|---------------------|----------|----------------|----|---------|---------|-------|---------|
| Parameter           | Estimate | Standard Error | DF | t Value | Pr >  t | Alpha | Lower   |
| gamma               | 4.7128   | 0.6742         | 38 | 6.99    | <.0001  | 0.05  | 3.3479  |
| b0                  | 3.3091   | 0.05885        | 38 | 56.23   | <.0001  | 0.05  | 3.1900  |
| b1                  | -0.1933  | 0.07856        | 38 | -2.46   | 0.0185  | 0.05  | -0.3523 |

| Parameter Estimates |          |          |
|---------------------|----------|----------|
| Parameter           | Upper    | Gradient |
| gamma               | 6.0777   | 5.327E-8 |
| b0                  | 3.4283   | -4.77E-6 |
| b1                  | -0.03426 | -1.22E-6 |

The parameter estimates and their standard errors shown in [Output 64.5.4](#) are identical to those obtained with the LIFEREG procedure and the following statements:

```
proc lifereg data=headache;
 class group;
 model minutes*censor(1) = group / dist=weibull;
 output out=new cdf=prob;
run;
```

The  $t$  statistic and confidence limits are based on 38 degrees of freedom. The LIFEREG procedure computes  $z$  intervals for the parameter estimates.

For the two groups you obtain

$$\hat{\alpha}(\text{group} = 1) = \exp\{-3.3091 + 0.1933\} = 0.04434$$

$$\hat{\alpha}(\text{group} = 2) = \exp\{-3.3091\} = 0.03655$$

The probabilities of headache relief by  $t$  minutes are estimated as

$$1 - G(t, \text{group} = 1) = 1 - \exp\{-(0.04434 * t)^{4.7128}\}$$

$$1 - G(t, \text{group} = 2) = 1 - \exp\{-(0.03655 * t)^{4.7128}\}$$

These probabilities, calculated at the observed times, are shown for the two groups in [Output 64.5.5](#) and printed with the following statements:

```
proc print data=cdf;
 var group censor patient minutes pred;
run;
```

Since the slope estimate is negative with  $p$ -value of 0.0185, you can infer that pain reliever 1 leads to overall significantly faster relief, but the estimated probabilities give no information about patient-to-patient variation within and between groups. For example, while pain reliever 1 provides faster relief overall, some patients in group 2 might respond more quickly than some patients in group 1. A frailty model enables you to accommodate and estimate patient-to-patient variation in health status by introducing random effects into a subject's hazard function.

**Output 64.5.5** Estimated Cumulative Distribution Function

| Obs | group | ensor | patient | minutes | Pred    |
|-----|-------|-------|---------|---------|---------|
| 1   | 1     | 0     | 1       | 11      | 0.03336 |
| 2   | 1     | 0     | 2       | 12      | 0.04985 |
| 3   | 1     | 0     | 3       | 19      | 0.35975 |
| 4   | 1     | 0     | 4       | 19      | 0.35975 |
| 5   | 1     | 0     | 5       | 19      | 0.35975 |
| 6   | 1     | 0     | 6       | 19      | 0.35975 |
| 7   | 1     | 0     | 7       | 21      | 0.51063 |
| 8   | 1     | 0     | 8       | 20      | 0.43325 |
| 9   | 1     | 0     | 9       | 21      | 0.51063 |
| 10  | 1     | 0     | 10      | 21      | 0.51063 |
| 11  | 1     | 0     | 11      | 20      | 0.43325 |
| 12  | 1     | 0     | 12      | 21      | 0.51063 |
| 13  | 1     | 0     | 13      | 20      | 0.43325 |
| 14  | 1     | 0     | 14      | 21      | 0.51063 |
| 15  | 1     | 0     | 15      | 25      | 0.80315 |
| 16  | 1     | 0     | 16      | 27      | 0.90328 |
| 17  | 1     | 0     | 17      | 30      | 0.97846 |
| 18  | 1     | 1     | 18      | 21      | 0.51063 |
| 19  | 1     | 1     | 19      | 24      | 0.73838 |
| 20  | 2     | 0     | 20      | 14      | 0.04163 |
| 21  | 2     | 0     | 21      | 16      | 0.07667 |
| 22  | 2     | 0     | 22      | 16      | 0.07667 |
| 23  | 2     | 0     | 23      | 21      | 0.24976 |
| 24  | 2     | 0     | 24      | 21      | 0.24976 |
| 25  | 2     | 0     | 25      | 23      | 0.35674 |
| 26  | 2     | 0     | 26      | 23      | 0.35674 |
| 27  | 2     | 0     | 27      | 23      | 0.35674 |
| 28  | 2     | 0     | 28      | 23      | 0.35674 |
| 29  | 2     | 1     | 29      | 25      | 0.47982 |
| 30  | 2     | 0     | 30      | 23      | 0.35674 |
| 31  | 2     | 0     | 31      | 24      | 0.41678 |
| 32  | 2     | 0     | 32      | 24      | 0.41678 |
| 33  | 2     | 1     | 33      | 26      | 0.54446 |
| 34  | 2     | 1     | 34      | 32      | 0.87656 |
| 35  | 2     | 1     | 35      | 30      | 0.78633 |
| 36  | 2     | 0     | 36      | 30      | 0.78633 |
| 37  | 2     | 1     | 37      | 32      | 0.87656 |
| 38  | 2     | 1     | 38      | 20      | 0.20414 |

The following statements model the hazard for patient  $i$  in terms of  $\alpha_i = \exp\{-\mathbf{x}_i' \boldsymbol{\beta} - z_i\}$ , where  $z_i$  is a (normal) random patient effect. Notice that the only difference from the previous NLMIXED statements are the **RANDOM** statement and the addition of  $z$  in the linear predictor. The empirical Bayes estimates of the random effect (**RANDOM** statement), the parameter estimates (**ODS OUTPUT** statement), and the estimated cumulative distribution function (**PREDICT** statement) are saved to subsequently graph the patient-specific distribution functions.

```
ods output ParameterEstimates=est;
proc nlmixed data=headache;
 bounds gamma > 0;
 linp = b0 - b1*(group-2) + z;
 alpha = exp(-linp);
 G_t = exp(-(alpha*minutes)**gamma);
 g = gamma*alpha*((alpha*minutes)**(gamma-1))*G_t;
 ll = (censor=0)*log(g) + (censor=1)*log(G_t);
 model minutes ~ general(ll);
 random z ~ normal(0,exp(2*logsig)) subject=patient out=EB;
 predict 1-G_t out=cdf;
run;
```

### Output 64.5.6 Specifications for Random Frailty Model

| The NL MIXED Procedure              |                              |
|-------------------------------------|------------------------------|
| Specifications                      |                              |
| Data Set                            | WORK.HEADACHE                |
| Dependent Variable                  | minutes                      |
| Distribution for Dependent Variable | General                      |
| Random Effects                      | z                            |
| Distribution for Random Effects     | Normal                       |
| Subject Variable                    | patient                      |
| Optimization Technique              | Dual Quasi-Newton            |
| Integration Method                  | Adaptive Gaussian Quadrature |

The “Specifications” table shows that the objective function is computed by adaptive Gaussian quadrature because of the presence of random effects (compare [Output 64.5.6](#) and [Output 64.5.1](#)). The “Dimensions” table reports that nine quadrature points are being used to integrate over the random effects ([Output 64.5.7](#)).

### Output 64.5.7 Dimensions Table for Random Frailty Model

| Dimensions            |    |
|-----------------------|----|
| Observations Used     | 38 |
| Observations Not Used | 0  |
| Total Observations    | 38 |
| Subjects              | 38 |
| Max Obs Per Subject   | 1  |
| Parameters            | 4  |
| Quadrature Points     | 9  |

**Output 64.5.8** Iteration History for Random Frailty Model

| Iteration History |       |            |          |          |          |
|-------------------|-------|------------|----------|----------|----------|
| Iter              | Calls | NegLogLike | Diff     | MaxGrad  | Slope    |
| 1                 | 5     | 142.121411 | 28.82225 | 12.14484 | -88.8664 |
| 2                 | 7     | 136.440369 | 5.681042 | 25.93096 | -65.7217 |
| 3                 | 9     | 122.972041 | 13.46833 | 46.56546 | -146.887 |
| 4                 | 11    | 120.904825 | 2.067216 | 23.77936 | -94.2862 |
| 5                 | 13    | 109.224144 | 11.68068 | 57.65493 | -92.4075 |
| 6                 | 15    | 105.064733 | 4.159411 | 4.824649 | -19.5879 |
| 7                 | 16    | 101.902207 | 3.162526 | 14.1287  | -6.33767 |
| 8                 | 18    | 99.6907395 | 2.211468 | 7.676822 | -3.42364 |
| 9                 | 20    | 99.3654033 | 0.325336 | 5.689204 | -0.93978 |
| 10                | 22    | 99.2602178 | 0.105185 | 0.317643 | -0.23408 |
| 11                | 24    | 99.254434  | 0.005784 | 1.17351  | -0.00556 |
| 12                | 25    | 99.2456973 | 0.008737 | 0.247412 | -0.00871 |
| 13                | 27    | 99.2445445 | 0.001153 | 0.104942 | -0.00218 |
| 14                | 29    | 99.2444958 | 0.000049 | 0.005646 | -0.0001  |
| 15                | 31    | 99.2444957 | 9.147E-8 | 0.000271 | -1.84E-7 |

NOTE: GCONV convergence criterion satisfied.

The procedure converges after 15 iterations (Output 64.5.8). The achieved  $-2$  log likelihood is only 1.2 less than that in the model without random effects (compare Output 64.5.9 and Output 64.5.4). Compared to a chi-square distribution with one degree of freedom, the addition of the random effect appears not to improve the model significantly. You must exercise care, however, in interpreting likelihood ratio tests when the value under the null hypothesis falls on the boundary of the parameter space (see, for example, Self and Liang 1987).

**Output 64.5.9** Fit Statistics for Random Frailty Model

| Fit Statistics           |       |
|--------------------------|-------|
| -2 Log Likelihood        | 198.5 |
| AIC (smaller is better)  | 206.5 |
| AICC (smaller is better) | 207.7 |
| BIC (smaller is better)  | 213.0 |



**Output 64.5.10** Parameter Estimates

| Parameter Estimates |          |                |    |         |         |       |         |
|---------------------|----------|----------------|----|---------|---------|-------|---------|
| Parameter           | Estimate | Standard Error | DF | t Value | Pr >  t | Alpha | Lower   |
| gamma               | 6.2867   | 2.1334         | 37 | 2.95    | 0.0055  | 0.05  | 1.9641  |
| b0                  | 3.2786   | 0.06576        | 37 | 49.86   | <.0001  | 0.05  | 3.1453  |
| b1                  | -0.1761  | 0.08264        | 37 | -2.13   | 0.0398  | 0.05  | -0.3436 |
| logsig              | -1.9027  | 0.5273         | 37 | -3.61   | 0.0009  | 0.05  | -2.9711 |

| Parameter Estimates |          |          |
|---------------------|----------|----------|
| Parameter           | Upper    | Gradient |
| gamma               | 10.6093  | -1.89E-7 |
| b0                  | 3.4118   | 0.000271 |
| b1                  | -0.00868 | 0.000111 |
| logsig              | -0.8343  | 0.000027 |

The estimate of the Weibull parameter has changed drastically from the model without random effects (compare [Output 64.5.10](#) and [Output 64.5.4](#)). The variance of the patient random effect is  $\exp\{-2 \times 1.9027\} = 0.02225$ . The listing in [Output 64.5.11](#) shows the empirical Bayes estimates of the random effects. These are the adjustments made to the linear predictor in order to obtain a patient's survival distribution. The listing is produced with the following statements:

```
proc print data=eb;
 var Patient Effect Estimate StdErrPred;
run;
```

**Output 64.5.11** Empirical Bayes Estimates of Random Effects

| Obs | patient | Effect | Estimate | StdErr<br>Pred |
|-----|---------|--------|----------|----------------|
| 1   | 1       | z      | -0.13597 | 0.23249        |
| 2   | 2       | z      | -0.13323 | 0.22793        |
| 3   | 3       | z      | -0.06294 | 0.13813        |
| 4   | 4       | z      | -0.06294 | 0.13813        |
| 5   | 5       | z      | -0.06294 | 0.13813        |
| 6   | 6       | z      | -0.06294 | 0.13813        |
| 7   | 7       | z      | -0.02568 | 0.11759        |
| 8   | 8       | z      | -0.04499 | 0.12618        |
| 9   | 9       | z      | -0.02568 | 0.11759        |
| 10  | 10      | z      | -0.02568 | 0.11759        |
| 11  | 11      | z      | -0.04499 | 0.12618        |
| 12  | 12      | z      | -0.02568 | 0.11759        |
| 13  | 13      | z      | -0.04499 | 0.12618        |
| 14  | 14      | z      | -0.02568 | 0.11759        |
| 15  | 15      | z      | 0.05980  | 0.11618        |
| 16  | 16      | z      | 0.10458  | 0.12684        |
| 17  | 17      | z      | 0.17147  | 0.14550        |
| 18  | 18      | z      | 0.06471  | 0.13807        |
| 19  | 19      | z      | 0.11157  | 0.14604        |
| 20  | 20      | z      | -0.13406 | 0.22899        |
| 21  | 21      | z      | -0.12698 | 0.21667        |
| 22  | 22      | z      | -0.12698 | 0.21667        |
| 23  | 23      | z      | -0.08506 | 0.15701        |
| 24  | 24      | z      | -0.08506 | 0.15701        |
| 25  | 25      | z      | -0.05797 | 0.13294        |
| 26  | 26      | z      | -0.05797 | 0.13294        |
| 27  | 27      | z      | -0.05797 | 0.13294        |
| 28  | 28      | z      | -0.05797 | 0.13294        |
| 29  | 29      | z      | 0.06420  | 0.13956        |
| 30  | 30      | z      | -0.05797 | 0.13294        |
| 31  | 31      | z      | -0.04266 | 0.12390        |
| 32  | 32      | z      | -0.04266 | 0.12390        |
| 33  | 33      | z      | 0.07618  | 0.14132        |
| 34  | 34      | z      | 0.16292  | 0.16460        |
| 35  | 35      | z      | 0.13193  | 0.15528        |
| 36  | 36      | z      | 0.06327  | 0.12124        |
| 37  | 37      | z      | 0.16292  | 0.16460        |
| 38  | 38      | z      | 0.02074  | 0.14160        |

The predicted values and patient-specific survival distributions can be plotted with the SAS code that follows:

```
proc transpose data=est(keep=estimate)
 out=trest(rename=(col1=gamma col2=b0 col3=b1));
run;

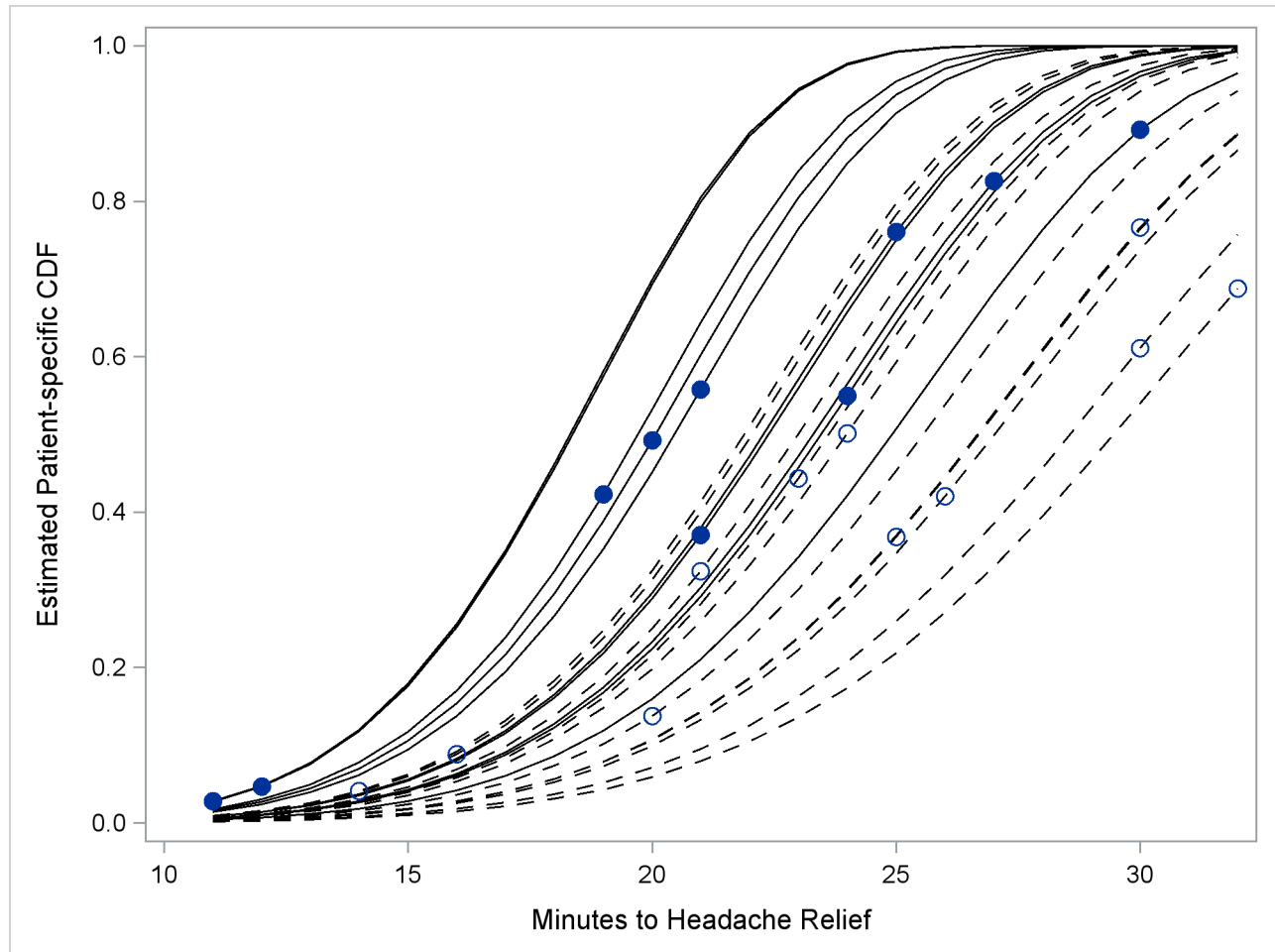
data pred;
 merge eb(keep=estimate) headache(keep=patient group);
 array pp{2} pred1-pred2;
 if _n_ = 1 then set trest(keep=gamma b0 b1);
 do time=11 to 32;
 linp = b0 - b1*(group-2) + estimate;
 pp{group} = 1-exp(- (exp(-linp)*time)**gamma);
 symbolid = patient+1;
 output;
 end;
 keep pred1 pred2 time patient;
run;

data pred;
 merge pred
 cdf(where = (group=1)
 rename = (pred=pcdf1 minutes=minutes1)
 keep = pred minutes group)
 cdf(where = (group=2)
 rename = (pred=pcdf2 minutes=minutes2)
 keep = pred minutes group);
 drop group;
run;

proc sgplot data=pred noautolegend;
 label minutes1='Minutes to Headache Relief'
 pcdf1 ='Estimated Patient-specific CDF';
 series x=time y=pred1 /
 group=patient
 lineattrs=(pattern=solid color=black);
 series x=time y=pred2 /
 group=patient
 lineattrs=(pattern=dash color=black);
 scatter x=minutes1 y=pcdf1 /
 markerattrs=(symbol=CircleFilled size=9);
 scatter x=minutes2 y=pcdf2 /
 markerattrs=(symbol=Circle size=9);
run;
```

The separation of the distribution functions by groups is evident in [Output 64.5.12](#). Most of the distributions of patients in the first group are to the left of the distributions in the second group. The separation is not complete, however. Several patients who are assigned the second pain reliever experience headache relief more quickly than patients assigned to the first group.

**Output 64.5.12** Patient-Specific CDFs and Predicted Values. Pain Reliever 1: Solid Lines, Closed Circles; Pain Reliever 2: Dashed Lines, Open Circles.



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# Chapter 65

## The NPAR1WAY Procedure

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## Overview: NPAR1WAY Procedure

The NPAR1WAY procedure performs nonparametric tests for location and scale differences across a one-way classification. PROC NPAR1WAY also provides a standard analysis of variance on the raw data and tests based on the empirical distribution function.

PROC NPAR1WAY performs tests for location and scale differences based on the following scores of a response variable: Wilcoxon, median, Van der Waerden (normal), Savage, Siegel-Tukey, Ansari-Bradley, Klotz, Mood, and Conover. Additionally, PROC NPAR1WAY provides tests that use the raw input data as scores. When the data are classified into two samples, tests are based on simple linear rank statistics. When the data are classified into more than two samples, tests are based on one-way ANOVA statistics. Both asymptotic and exact  $p$ -values are available for these tests. PROC NPAR1WAY also provides Hodges-Lehmann estimation, including exact confidence limits for the location shift.

PROC NPAR1WAY computes empirical distribution function (EDF) statistics, which test whether the distribution of a variable is the same across different groups. These include the Kolmogorov-Smirnov test, the Cramer-von Mises test, and, when the data are classified into only two samples, the Kuiper test. Exact  $p$ -values are available for the two-sample Kolmogorov-Smirnov test.

PROC NPAR1WAY uses the Output Delivery System (ODS), a SAS subsystem that provides capabilities for displaying and controlling the output from SAS procedures. ODS enables you to convert any of the output from PROC NPAR1WAY into a SAS data set. See the section “[ODS Table Names](#)” on page 5493 for more information.

PROC NPAR1WAY uses ODS Graphics to create graphs as part of its output. For general information about ODS Graphics, see Chapter 21, “[Statistical Graphics Using ODS](#).” For specific information about the statistical graphics available with the NPAR1WAY procedure, see the `PLOTS=` option in the PROC NPAR1WAY statement and the section “[ODS Graphics](#)” on page 5495.

## Getting Started: NPAR1WAY Procedure

This example illustrates how you can use PROC NPAR1WAY to perform a one-way nonparametric analysis. The data from Halverson and Sherwood (1930) consist of weight gain measurements for five different levels of gossypol additive in animal feed. Gossypol is a substance contained in cottonseed shells, and these data were collected to study the effect of gossypol on animal nutrition.

The following DATA step statements create the SAS data set Gossypol:

```
data Gossypol;
 input Dose n;
 do i=1 to n;
 input Gain @@;
 output;
 end;
 datalines;
0 16
228 229 218 216 224 208 235 229 233 219 224 220 232 200 208 232
.04 11
186 229 220 208 228 198 222 273 216 198 213
.07 12
179 193 183 180 143 204 114 188 178 134 208 196
.10 17
130 87 135 116 118 165 151 59 126 64 78 94 150 160 122 110 178
.13 11
154 130 130 118 118 104 112 134 98 100 104
;
```

The data set Gossypol contains the variable Dose, which represents the amount of gossypol additive, and the variable Gain, which represents the weight gain.

Researchers are interested in whether there is a difference in weight gain among animals receiving the different dose levels of gossypol. The following statements invoke the NPAR1WAY procedure to perform a nonparametric analysis of this problem:

```
proc npar1way data=Gossypol;
 class Dose;
 var Gain;
run;
```

The variable Dose is the CLASS variable, and the VAR statement specifies the variable Gain is the response variable. The CLASS statement is required, and you must name only one CLASS variable. You can name one or more analysis variables in the VAR statement. If you omit the VAR statement, PROC NPAR1WAY analyzes all numeric variables in the data set except for the CLASS variable, the FREQ variable, and the BY variables.

When no analysis options are specified in the PROC NPAR1WAY statement, the ANOVA, WILCOXON, MEDIAN, VW, SAVAGE, and EDF options are invoked by default. The tables in the following figures show the results of these analyses.

The tables in Figure 65.1 are produced with the ANOVA option. For each level of the CLASS variable Dose, PROC NPAR1WAY displays the number of observations and the mean of the analysis variable Gain. PROC NPAR1WAY displays a standard analysis of variance on the raw data. This gives the same results as the GLM and ANOVA procedures. The  $p$ -value for the  $F$  test is  $<0.0001$ , which indicates that Dose accounts for a significant portion of the variability of the dependent variable Gain.

**Figure 65.1** Analysis of Variance

| The NPAR1WAY Procedure                 |      |                |             |         |        |
|----------------------------------------|------|----------------|-------------|---------|--------|
| Analysis of Variance for Variable Gain |      |                |             |         |        |
| Classified by Variable Dose            |      |                |             |         |        |
|                                        | Dose | N              | Mean        |         |        |
|                                        | 0    | 16             | 222.187500  |         |        |
|                                        | 0.04 | 11             | 217.363636  |         |        |
|                                        | 0.07 | 12             | 175.000000  |         |        |
|                                        | 0.1  | 17             | 120.176471  |         |        |
|                                        | 0.13 | 11             | 118.363636  |         |        |
| Source                                 | DF   | Sum of Squares | Mean Square | F Value | Pr > F |
| Among                                  | 4    | 140082.986077  | 35020.74652 | 55.8143 | <.0001 |
| Within                                 | 62   | 38901.998997   | 627.45160   |         |        |
| Average scores were used for ties.     |      |                |             |         |        |

The WILCOXON option produces the output in Figure 65.2. PROC NPAR1WAY first provides a summary of the Wilcoxon scores for the analysis variable Gain by class level. For each level of the CLASS variable Dose, PROC NPAR1WAY displays the following information: number of observations, sum of the Wilcoxon scores, expected sum under the null hypothesis of no difference among class levels, standard deviation under the null hypothesis, and mean score.

Next PROC NPAR1WAY displays the one-way ANOVA statistic, which for Wilcoxon scores is known as the Kruskal-Wallis test. The statistic equals 52.6656, with four degrees of freedom, which is the number of class levels minus one. The  $p$ -value (probability of a larger statistic under the null hypothesis) is  $<0.0001$ . This leads to rejection of the null hypothesis that there is no difference in location for Gain among the levels of Dose. This  $p$ -value is asymptotic, computed from the asymptotic chi-square distribution of the test statistic. For certain data sets it might also be useful to compute the exact  $p$ -value—for example, for small data sets or for data sets that are sparse, skewed, or heavily tied. You can use the EXACT statement to request exact  $p$ -values for any of the location or scale tests available in PROC NPAR1WAY.

**Figure 65.2** Wilcoxon Score Analysis

| Wilcoxon Scores (Rank Sums) for Variable Gain<br>Classified by Variable Dose |    |                  |                      |                     |               |
|------------------------------------------------------------------------------|----|------------------|----------------------|---------------------|---------------|
| Dose                                                                         | N  | Sum of<br>Scores | Expected<br>Under H0 | Std Dev<br>Under H0 | Mean<br>Score |
| 0                                                                            | 16 | 890.50           | 544.0                | 67.978966           | 55.656250     |
| 0.04                                                                         | 11 | 555.00           | 374.0                | 59.063588           | 50.454545     |
| 0.07                                                                         | 12 | 395.50           | 408.0                | 61.136622           | 32.958333     |
| 0.1                                                                          | 17 | 275.50           | 578.0                | 69.380741           | 16.205882     |
| 0.13                                                                         | 11 | 161.50           | 374.0                | 59.063588           | 14.681818     |

Average scores were used for ties.

**Kruskal-Wallis Test**

|                 |         |
|-----------------|---------|
| Chi-Square      | 52.6656 |
| DF              | 4       |
| Pr > Chi-Square | <.0001  |

Figure 65.3 through Figure 65.5 display the analyses produced by the MEDIAN, VW, and SAVAGE options. For each score type, PROC NPAR1WAY provides a summary of scores and the one-way ANOVA statistic, as previously described for Wilcoxon scores. Other score types available in PROC NPAR1WAY are Siegel-Tukey, Ansari-Bradley, Klotz, and Mood, which can be used to test for scale differences. Conover scores can be used to test for differences in both location and scale. Additionally, you can specify the SCORES=DATA option, which uses the input data as scores. This option gives you the flexibility to construct any scores for your data with the DATA step and then analyze these scores with PROC NPAR1WAY.

**Figure 65.3** Median Score Analysis

| Median Scores (Number of Points Above Median) for Variable Gain<br>Classified by Variable Dose |    |                  |                      |                     |               |
|------------------------------------------------------------------------------------------------|----|------------------|----------------------|---------------------|---------------|
| Dose                                                                                           | N  | Sum of<br>Scores | Expected<br>Under H0 | Std Dev<br>Under H0 | Mean<br>Score |
| 0                                                                                              | 16 | 16.0             | 7.880597             | 1.757902            | 1.00          |
| 0.04                                                                                           | 11 | 11.0             | 5.417910             | 1.527355            | 1.00          |
| 0.07                                                                                           | 12 | 6.0              | 5.910448             | 1.580963            | 0.50          |
| 0.1                                                                                            | 17 | 0.0              | 8.373134             | 1.794152            | 0.00          |
| 0.13                                                                                           | 11 | 0.0              | 5.417910             | 1.527355            | 0.00          |

Average scores were used for ties.

**Median One-Way Analysis**

|                 |         |
|-----------------|---------|
| Chi-Square      | 54.1765 |
| DF              | 4       |
| Pr > Chi-Square | <.0001  |

**Figure 65.4** Van der Waerden (Normal) Score Analysis

| Van der Waerden Scores (Normal) for Variable Gain<br>Classified by Variable Dose |    |                  |                      |                     |               |
|----------------------------------------------------------------------------------|----|------------------|----------------------|---------------------|---------------|
| Dose                                                                             | N  | Sum of<br>Scores | Expected<br>Under H0 | Std Dev<br>Under H0 | Mean<br>Score |
| 0                                                                                | 16 | 16.116474        | 0.0                  | 3.325957            | 1.007280      |
| 0.04                                                                             | 11 | 8.340899         | 0.0                  | 2.889761            | 0.758264      |
| 0.07                                                                             | 12 | -0.576674        | 0.0                  | 2.991186            | -0.048056     |
| 0.1                                                                              | 17 | -14.688921       | 0.0                  | 3.394540            | -0.864054     |
| 0.13                                                                             | 11 | -9.191777        | 0.0                  | 2.889761            | -0.835616     |

Average scores were used for ties.

| Van der Waerden One-Way Analysis |         |
|----------------------------------|---------|
| Chi-Square                       | 47.2972 |
| DF                               | 4       |
| Pr > Chi-Square                  | <.0001  |

**Figure 65.5** Savage Score Analysis

| Savage Scores (Exponential) for Variable Gain<br>Classified by Variable Dose |    |                  |                      |                     |               |
|------------------------------------------------------------------------------|----|------------------|----------------------|---------------------|---------------|
| Dose                                                                         | N  | Sum of<br>Scores | Expected<br>Under H0 | Std Dev<br>Under H0 | Mean<br>Score |
| 0                                                                            | 16 | 16.074391        | 0.0                  | 3.385275            | 1.004649      |
| 0.04                                                                         | 11 | 7.693099         | 0.0                  | 2.941300            | 0.699373      |
| 0.07                                                                         | 12 | -3.584958        | 0.0                  | 3.044534            | -0.298746     |
| 0.1                                                                          | 17 | -11.979488       | 0.0                  | 3.455082            | -0.704676     |
| 0.13                                                                         | 11 | -8.203044        | 0.0                  | 2.941300            | -0.745731     |

Average scores were used for ties.

| Savage One-Way Analysis |         |
|-------------------------|---------|
| Chi-Square              | 39.4908 |
| DF                      | 4       |
| Pr > Chi-Square         | <.0001  |

The tables in Figure 65.6 display the empirical distribution function statistics, comparing the distribution of Gain for the different levels of Dose. These tables are produced by the EDF option, and they include Kolmogorov-Smirnov statistics and Cramér-von Mises statistics.

**Figure 65.6** Empirical Distribution Function Analysis

| Kolmogorov-Smirnov Test for Variable Gain<br>Classified by Variable Dose |    |                   |                                   |
|--------------------------------------------------------------------------|----|-------------------|-----------------------------------|
| Dose                                                                     | N  | EDF at<br>Maximum | Deviation from Mean<br>at Maximum |
| 0                                                                        | 16 | 0.000000          | -1.910448                         |
| 0.04                                                                     | 11 | 0.000000          | -1.584060                         |
| 0.07                                                                     | 12 | 0.333333          | -0.499796                         |
| 0.1                                                                      | 17 | 1.000000          | 2.153861                          |
| 0.13                                                                     | 11 | 1.000000          | 1.732565                          |
| Total                                                                    | 67 | 0.477612          |                                   |

Maximum Deviation Occurred at Observation 36  
Value of Gain at Maximum = 178.0

| Kolmogorov-Smirnov Statistics (Asymptotic) |          |     |     |
|--------------------------------------------|----------|-----|-----|
| KS                                         | KSa      | KSb | KSd |
| 0.457928                                   | 3.748300 |     |     |

| Cramer-von Mises Test for Variable Gain<br>Classified by Variable Dose |    |                               |                          |
|------------------------------------------------------------------------|----|-------------------------------|--------------------------|
| Dose                                                                   | N  | Summed Deviation<br>from Mean | Summed Squared Deviation |
| 0                                                                      | 16 | 2.165210                      | 4.697243                 |
| 0.04                                                                   | 11 | 0.918280                      | 0.843166                 |
| 0.07                                                                   | 12 | 0.348227                      | 0.121261                 |
| 0.1                                                                    | 17 | 1.497542                      | 2.242627                 |
| 0.13                                                                   | 11 | 1.335745                      | 1.784237                 |

| Cramer-von Mises Statistics (Asymptotic) |          |     |     |
|------------------------------------------|----------|-----|-----|
| CM                                       | CMa      | CMb | CMd |
| 0.093508                                 | 6.265003 |     |     |



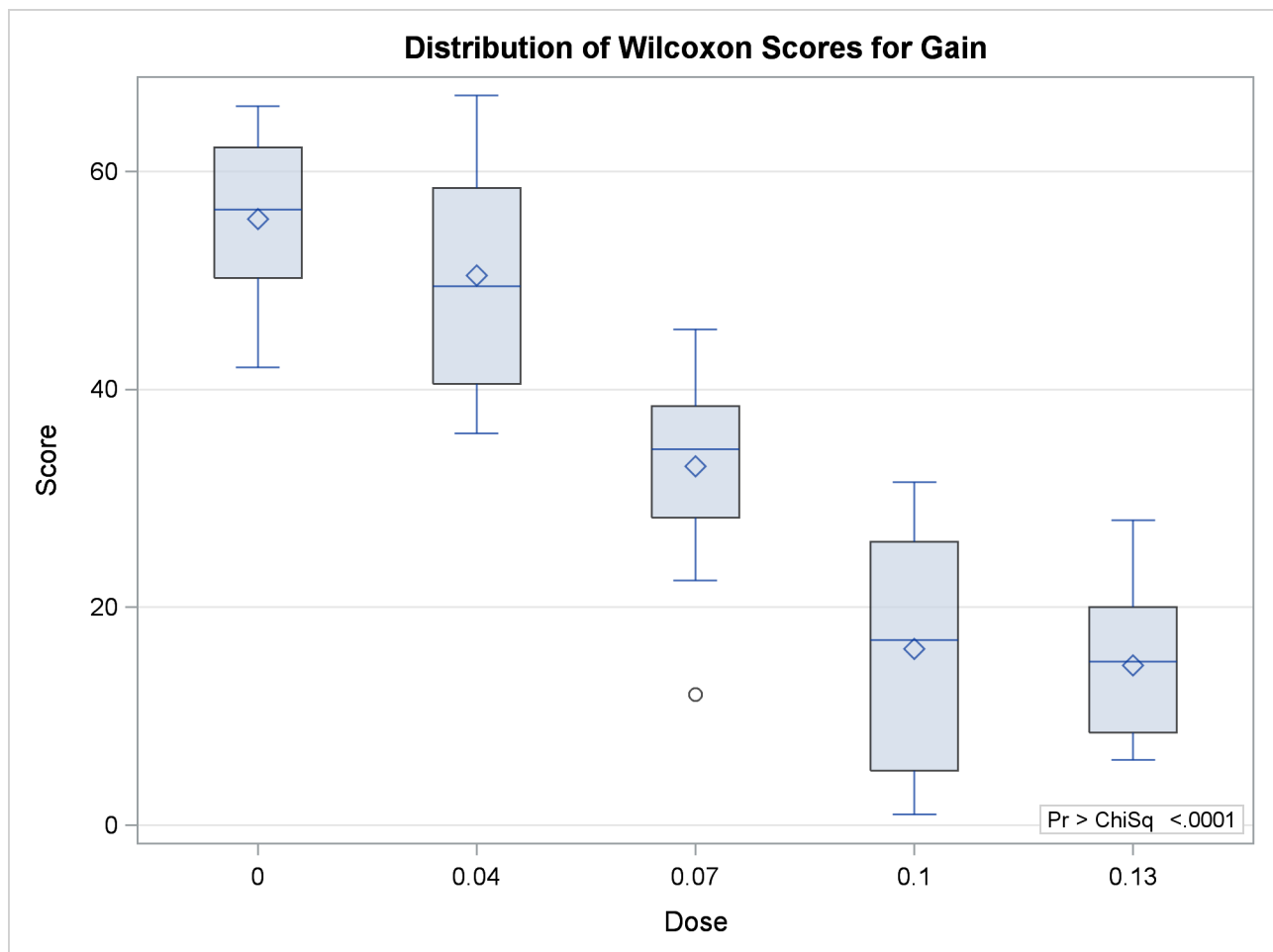
PROC NPAR1WAY uses ODS Graphics to create graphs as part of its output. The following statements produce a box plot of Wilcoxon scores for Gain classified by Dose. ODS Graphics must be enabled before producing graphs.

```
ods graphics on;
proc npar1way data=Gossypol plots(only)=wilcoxonboxplot;
 class Dose;
 var Gain;
run;
ods graphics off;
```

Figure 65.7 displays the box plot of Wilcoxon scores. This graph corresponds to the Wilcoxon scores analysis shown in Figure 65.2. To remove the  $p$ -value from the box plot display, you can specify the NOSTATS plot option in parentheses following the WILCOXONBOXPLOT option.

Box plots are available for all PROC NPAR1WAY score types except median scores, which are displayed in a stacked bar chart. If ODS Graphics is enabled but you do not specify the PLOTS= option, then PROC NPAR1WAY produces all plots that are associated with the analyses that you request.

**Figure 65.7** Box Plot of Wilcoxon Scores



In the preceding example, the CLASS variable Dose has five levels, and the analyses examine possible differences among these five levels (samples). The following statements invoke the NPAR1WAY procedure to perform a nonparametric analysis of the two lowest levels of Dose:

```
proc npar1way data=Gossypol;
 where Dose <= .04;
 class Dose;
 var Gain;
run;
```

The tables in the following figures show the results of this two-sample analysis. The tables in [Figure 65.8](#) are produced by the ANOVA option.

**Figure 65.8** Analysis of Variance for Two-Sample Data

| The NPAR1WAY Procedure                 |      |                |             |         |        |
|----------------------------------------|------|----------------|-------------|---------|--------|
| Analysis of Variance for Variable Gain |      |                |             |         |        |
| Classified by Variable Dose            |      |                |             |         |        |
|                                        | Dose | N              | Mean        |         |        |
|                                        | 0    | 16             | 222.187500  |         |        |
|                                        | 0.04 | 11             | 217.363636  |         |        |
| Source                                 | DF   | Sum of Squares | Mean Square | F Value | Pr > F |
| Among                                  | 1    | 151.683712     | 151.683712  | 0.5587  | 0.4617 |
| Within                                 | 25   | 6786.982955    | 271.479318  |         |        |
| Average scores were used for ties.     |      |                |             |         |        |

[Figure 65.9](#) displays the output produced by the WILCOXON option. PROC NPAR1WAY provides a summary of the Wilcoxon scores for the analysis variable Gain for each of the two class levels. Since there are only two levels, PROC NPAR1WAY displays the two-sample test, based on the simple linear rank statistic with Wilcoxon scores. The normal approximation includes a continuity correction. To remove the continuity correction, you can specify the CORRECT=NO option. PROC NPAR1WAY also gives a *t* approximation for the Wilcoxon two-sample test. Like the multisample analysis, PROC NPAR1WAY computes a one-way ANOVA statistic, which for Wilcoxon scores is known as the Kruskal-Wallis test. All these *p*-values show no difference in Gain for the two Dose levels at the 0.05 level of significance.

[Figure 65.10](#) through [Figure 65.12](#) display the two-sample analyses produced by the MEDIAN, VW, and SAVAGE options.

Figure 65.9 Wilcoxon Two-Sample Analysis

| Wilcoxon Scores (Rank Sums) for Variable Gain<br>Classified by Variable Dose |    |                  |                      |                     |               |
|------------------------------------------------------------------------------|----|------------------|----------------------|---------------------|---------------|
| Dose                                                                         | N  | Sum of<br>Scores | Expected<br>Under H0 | Std Dev<br>Under H0 | Mean<br>Score |
| 0                                                                            | 16 | 253.50           | 224.0                | 20.221565           | 15.843750     |
| 0.04                                                                         | 11 | 124.50           | 154.0                | 20.221565           | 11.318182     |

Average scores were used for ties.

Wilcoxon Two-Sample Test

|           |          |
|-----------|----------|
| Statistic | 124.5000 |
|-----------|----------|

Normal Approximation

|                   |         |
|-------------------|---------|
| Z                 | -1.4341 |
| One-Sided Pr < Z  | 0.0758  |
| Two-Sided Pr >  Z | 0.1515  |

t Approximation

|                   |        |
|-------------------|--------|
| One-Sided Pr < Z  | 0.0817 |
| Two-Sided Pr >  Z | 0.1635 |

Z includes a continuity correction of 0.5.

Kruskal-Wallis Test

|                 |        |
|-----------------|--------|
| Chi-Square      | 2.1282 |
| DF              | 1      |
| Pr > Chi-Square | 0.1446 |

Figure 65.10 Median Two-Sample Analysis

| Median Scores (Number of Points Above Median) for Variable Gain<br>Classified by Variable Dose |    |                  |                      |                     |               |
|------------------------------------------------------------------------------------------------|----|------------------|----------------------|---------------------|---------------|
| Dose                                                                                           | N  | Sum of<br>Scores | Expected<br>Under H0 | Std Dev<br>Under H0 | Mean<br>Score |
| 0                                                                                              | 16 | 9.0              | 7.703704             | 1.299995            | 0.562500      |
| 0.04                                                                                           | 11 | 4.0              | 5.296296             | 1.299995            | 0.363636      |

Average scores were used for ties.

**Median Two-Sample Test**

|                   |         |
|-------------------|---------|
| Statistic         | 4.0000  |
| Z                 | -0.9972 |
| One-Sided Pr < Z  | 0.1593  |
| Two-Sided Pr >  Z | 0.3187  |

**Median One-Way Analysis**

|                 |        |
|-----------------|--------|
| Chi-Square      | 0.9943 |
| DF              | 1      |
| Pr > Chi-Square | 0.3187 |

Figure 65.11 Van der Waerden (Normal) Two-Sample Analysis

| Van der Waerden Scores (Normal) for Variable Gain<br>Classified by Variable Dose |    |                  |                      |                     |               |
|----------------------------------------------------------------------------------|----|------------------|----------------------|---------------------|---------------|
| Dose                                                                             | N  | Sum of<br>Scores | Expected<br>Under H0 | Std Dev<br>Under H0 | Mean<br>Score |
| 0                                                                                | 16 | 3.346520         | 0.0                  | 2.320336            | 0.209157      |
| 0.04                                                                             | 11 | -3.346520        | 0.0                  | 2.320336            | -0.304229     |

Average scores were used for ties.

**Van der Waerden Two-Sample Test**

|                   |         |
|-------------------|---------|
| Statistic         | -3.3465 |
| Z                 | -1.4423 |
| One-Sided Pr < Z  | 0.0746  |
| Two-Sided Pr >  Z | 0.1492  |

**Van der Waerden One-Way Analysis**

|                 |        |
|-----------------|--------|
| Chi-Square      | 2.0801 |
| DF              | 1      |
| Pr > Chi-Square | 0.1492 |

**Figure 65.12** Savage Two-Sample Analysis

| Savage Scores (Exponential) for Variable Gain<br>Classified by Variable Dose |    |                  |                      |                     |               |
|------------------------------------------------------------------------------|----|------------------|----------------------|---------------------|---------------|
| Dose                                                                         | N  | Sum of<br>Scores | Expected<br>Under H0 | Std Dev<br>Under H0 | Mean<br>Score |
| 0                                                                            | 16 | 1.834554         | 0.0                  | 2.401839            | 0.114660      |
| 0.04                                                                         | 11 | -1.834554        | 0.0                  | 2.401839            | -0.166778     |

Average scores were used for ties.

**Savage Two-Sample Test**

|                   |         |
|-------------------|---------|
| Statistic         | -1.8346 |
| Z                 | -0.7638 |
| One-Sided Pr < Z  | 0.2225  |
| Two-Sided Pr >  Z | 0.4450  |

**Savage One-Way Analysis**

|                 |        |
|-----------------|--------|
| Chi-Square      | 0.5834 |
| DF              | 1      |
| Pr > Chi-Square | 0.4450 |

The tables in [Figure 65.13](#) display the empirical distribution function statistics, comparing the distribution of Gain for the two levels of Dose. The  $p$ -value for the Kolmogorov-Smirnov two-sample test is 0.6199, which indicates no rejection of the null hypothesis that the Gain distributions are identical for the two levels of Dose.

Figure 65.13 Two-Sample EDF Tests

| Kolmogorov-Smirnov Test for Variable Gain<br>Classified by Variable Dose        |          |                               |                                   |
|---------------------------------------------------------------------------------|----------|-------------------------------|-----------------------------------|
| Dose                                                                            | N        | EDF at<br>Maximum             | Deviation from Mean<br>at Maximum |
| 0                                                                               | 16       | 0.250000                      | -0.481481                         |
| 0.04                                                                            | 11       | 0.545455                      | 0.580689                          |
| Total                                                                           | 27       | 0.370370                      |                                   |
| Maximum Deviation Occurred at Observation 4<br>Value of Gain at Maximum = 216.0 |          |                               |                                   |
| Kolmogorov-Smirnov Two-Sample Test (Asymptotic)                                 |          |                               |                                   |
| KS                                                                              | 0.145172 | D                             | 0.295455                          |
| KSa                                                                             | 0.754337 | Pr > KSa                      | 0.6199                            |
| Cramer-von Mises Test for Variable Gain<br>Classified by Variable Dose          |          |                               |                                   |
| Dose                                                                            | N        | Summed Deviation<br>from Mean |                                   |
| 0                                                                               | 16       | 0.098638                      |                                   |
| 0.04                                                                            | 11       | 0.143474                      |                                   |
| Cramer-von Mises Statistics (Asymptotic)                                        |          |                               |                                   |
| CM                                                                              | 0.008967 | CMa                           | 0.242112                          |
| Kuiper Test for Variable Gain<br>Classified by Variable Dose                    |          |                               |                                   |
| Dose                                                                            | N        | Deviation<br>from Mean        |                                   |
| 0                                                                               | 16       | 0.090909                      |                                   |
| 0.04                                                                            | 11       | 0.295455                      |                                   |
| Kuiper Two-Sample Test (Asymptotic)                                             |          |                               |                                   |
| K                                                                               | 0.386364 | Ka                            | 0.986440                          |
|                                                                                 |          | Pr > Ka                       | 0.8383                            |

---

## Syntax: NPAR1WAY Procedure

The following statements are available in the NPAR1WAY procedure:

```
PROC NPAR1WAY < options > ;
 BY variables ;
 CLASS variable ;
 EXACT statistic-options < / computation-options > ;
 FREQ variable ;
 OUTPUT < OUT=SAS-data-set > < options > ;
 VAR variables ;
```

The **PROC NPAR1WAY** statement invokes the NPAR1WAY procedure. The **PROC NPAR1WAY** and **CLASS** statements are required. Table 65.1 summarizes the statements available in the NPAR1WAY procedure.

The rest of this section gives detailed syntax information for the **BY**, **CLASS**, **EXACT**, **FREQ**, **OUTPUT**, and **VAR** statements in alphabetical order after the description of the **PROC NPAR1WAY** statement.

**Table 65.1** Summary of PROC NPAR1WAY Statements

| Statement     | Description                                  |
|---------------|----------------------------------------------|
| <b>BY</b>     | Provides separate analyses for each BY group |
| <b>CLASS</b>  | Identifies the classification variable       |
| <b>EXACT</b>  | Requests exact tests                         |
| <b>FREQ</b>   | Identifies a frequency variable              |
| <b>OUTPUT</b> | Requests an output data set                  |
| <b>VAR</b>    | Identifies analysis variables                |

---

## PROC NPAR1WAY Statement

```
PROC NPAR1WAY < options > ;
```

The **PROC NPAR1WAY** statement invokes the NPAR1WAY procedure. Optionally, it identifies the input data set and requests analyses. By default, the procedure uses the most recently created SAS data set and omits missing values from the analysis. If you do not specify any analysis *options*, **PROC NPAR1WAY** performs an analysis of variance (**ANOVA** option), tests for location differences (**WILCOXON**, **MEDIAN**, **SAVAGE**, and **VW** options), and empirical distribution function tests (**EDF** option).

Table 65.2 summarizes the *options* available in the **PROC NPAR1WAY** statement. Descriptions of the *options* follow in alphabetical order.

**Table 65.2** PROC NPAR1WAY Statement Options

| Option                  | Description                                                                         |
|-------------------------|-------------------------------------------------------------------------------------|
| <b>Input Data Set</b>   |                                                                                     |
| DATA=                   | Names the input SAS data set                                                        |
| <b>Missing Values</b>   |                                                                                     |
| MISSING                 | Treats missing CLASS values as a valid class                                        |
| <b>Analyses</b>         |                                                                                     |
| AB                      | Requests analysis of Ansari-Bradley scores                                          |
| ANOVA                   | Requests standard analysis of variance                                              |
| CONOVER                 | Requests analysis of Conover scores                                                 |
| D                       | Requests one-sided Kolmogorov-Smirnov statistics                                    |
| DSCF                    | Requests pairwise multiple comparison analysis                                      |
| EDF                     | Requests empirical distribution function statistics                                 |
| FP                      | Requests the Fligner-Policello test                                                 |
| HL                      | Requests Hodges-Lehmann estimation for two-sample data                              |
| KLOTZ                   | Requests analysis of Klotz scores                                                   |
| MEDIAN                  | Requests analysis of median scores                                                  |
| MOOD                    | Requests analysis of Mood scores                                                    |
| SAVAGE                  | Requests analysis of Savage scores                                                  |
| SCORES=DATA             | Requests analysis of input data scores                                              |
| ST                      | Requests analysis of Siegel-Tukey scores                                            |
| VW   NORMAL             | Requests analysis of Van der Waerden (normal) scores                                |
| WILCOXON                | Requests analysis of Wilcoxon scores                                                |
| <b>Analysis Details</b> |                                                                                     |
| ADJUST                  | Requests median adjustment for scale analyses                                       |
| ALPHA=                  | Specifies the confidence level for Hodges-Lehmann estimation                        |
| CORRECT=NO              | Suppresses the continuity correction for Wilcoxon and Siegel-Tukey two-sample tests |
| <b>Displayed Output</b> |                                                                                     |
| NOPRINT                 | Suppresses the display of all output                                                |
| <b>Plots</b>            |                                                                                     |
| PLOTS=                  | Requests plots from ODS Graphics                                                    |

You can specify the following *options* in the PROC NPAR1WAY statement.

**AB < (ADJUST) >**

requests an analysis of Ansari-Bradley scores. See the section “[Ansari-Bradley Scores](#)” on page 5472 for more information. The ADJUST option subtracts class medians from the input observations before performing the analysis.



**ADJUST**

adjusts for location differences among classes before performing tests for scale differences. The ADJUST option applies to the following analyses: Ansari-Bradley (**AB**), Klotz (**KLOTZ**), Mood (**MOOD**), and Siegel-Tukey (**ST**). If you specify the ADJUST option, PROC NPAR1WAY subtracts the corresponding class median from each observation before scoring the data and performing the scale tests that you request.

You can also request adjustment for an individual scale test by specifying ADJUST in parentheses after the scale test option; for example, you can specify **ST(ADJUST)** to adjust by class medians before performing the Siegel-Tukey test.

**ALPHA= $\alpha$** 

specifies the level of the confidence limits for location shift, which you request with the **HL** option. The value of  $\alpha$  must be between 0 and 1, and the default is 0.05. A confidence level of  $\alpha$  produces  $100(1 - \alpha)\%$  confidence limits. The default of ALPHA=0.05 produces 95% confidence limits for the Hodges-Lehmann estimate.

**ANOVA**

requests a standard analysis of variance on the raw data.

**CONOVER**

requests an analysis of Conover scores. See the section “[Conover Scores](#)” on page 5472 for more information.

**CORRECT=NO**

suppresses the continuity correction for the Wilcoxon two-sample test and the Siegel-Tukey two-sample test. See the section “[Continuity Correction](#)” on page 5469 for more information.

**D**

requests the one-sided Kolmogorov-Smirnov  $D+$  and  $D-$  statistics and their asymptotic  $p$ -values, in addition to the two-sided  $D$  statistic produced by the **EDF** option for two-sample data. The **D** option invokes the **EDF** option. The statistics  $D+$  and  $D-$  are provided by default if you request exact Kolmogorov-Smirnov statistics with the **KS** option in the **EXACT** statement for two-sample data. See the section “[Tests Based on the Empirical Distribution Function](#)” on page 5477 for details about Kolmogorov-Smirnov statistics.

**DATA=SAS-data-set**

names the SAS data set to be analyzed by PROC NPAR1WAY. If you omit the DATA= option, the procedure uses the most recently created SAS data set.

**DSCF**

requests the Dwass, Steel, Critchlow-Fligner multiple comparison procedure, which is based on pairwise two-sample rankings. This procedure is available for multisample data, where the number of **CLASS** variable levels is greater than 2. See the section “[Multiple Comparisons Based on Pairwise Rankings](#)” on page 5476 for more information.

**EDF**

requests statistics based on the empirical distribution function. These include the Kolmogorov-Smirnov and Cramér-von Mises tests and, if there are only two classification levels, the Kuiper test. See the section “[Tests Based on the Empirical Distribution Function](#)” on page 5477 for more information.

The EDF option produces the Kolmogorov-Smirnov  $D$  statistic for two-sample data. You can request the one-sided  $D+$  and  $D-$  statistics for two-sample data with the **D** option.

**FP < (REFCLASS = class-number | 'class-value' ) >**

requests the Fligner-Policello test for two-sample data. See the section “[Fligner-Policello Test](#)” on page 5475 for more information.

The REFCLASS= option specifies which of the two **CLASS** variable levels (samples) to use as the reference class  $X$  for the difference between class placement sums,  $P_Y - P_X$ . REFCLASS=1 refers to the first class that is listed in the “Fligner-Policello Placements” table, and REFCLASS=2 refers to the second class listed. The table displays class levels in the order in which they appear in the input data set. REFCLASS=*class-value* identifies the reference class by the formatted value of the **CLASS** variable. By default, the reference class is the second class listed in the “Fligner-Policello Placements” table (REFCLASS=2).

**HL < (REFCLASS = class-number | 'class-value' ) >**

requests Hodges-Lehmann estimation of the location shift for two-sample data. The HL option provides asymptotic confidence limits for the location shift. These are sometimes known as Moses confidence limits. See the section “[Hodges-Lehmann Estimation of Location Shift](#)” on page 5473 for details. You can specify the level of the confidence limits by using the **ALPHA=** option. The default of ALPHA=0.5 produces 95% confidence limits for the location shift.

The REFCLASS= option specifies which of the two **CLASS** variable levels (samples) to use as the reference class  $X$  for the location shift,  $Y - X$ . REFCLASS=1 refers to the first class that is listed in the “Wilcoxon Scores” table, and REFCLASS=2 refers to the second class listed. The table displays class levels in the order in which they appear in the input data set. REFCLASS=*class-value* identifies the reference class by the formatted value of the **CLASS** variable.

By default, PROC NPAR1WAY uses the larger of the two classes as the reference class  $X$  to compute the Hodges-Lehmann location shift,  $Y - X$ . If both class have the same number of observations, PROC NPAR1WAY uses the class that appears second in the input data set as the reference class.

**KLOTZ < (ADJUST) >**

requests an analysis of Klotz scores. See the section “[Klotz Scores](#)” on page 5472 for more information. The ADJUST option subtracts class medians from the input observations before performing the analysis.

**MEDIAN**

requests an analysis of median scores. When there are two classification levels, this option produces the two-sample median test. When there are more than two samples, this option produces the multi-sample median test, which is also known as the Brown-Mood test. See the section “[Median Scores](#)” on page 5471 for more information.

**MISSING**

treats missing values of the **CLASS** variable as a valid class level.

**MOOD < (ADJUST) >**

requests an analysis of Mood scores. See the section “[Mood Scores](#)” on page 5472 for more information. The ADJUST option subtracts class medians from the input observations before performing the analysis.

**NOPRINT**

suppresses the display of all output. You can use the NOPRINT option when you only want to create an output data set. Note that this option temporarily disables the Output Delivery System (ODS). For more information, see Chapter 20, “Using the Output Delivery System.”

**PLOTS** < ( *global-plot-options* ) > < = *plot-request* < ( *plot-option* ) > >

**PLOTS** < ( *global-plot-options* ) > < = ( *plot-request* < ( *plot-option* ) > <...*plot-request* < ( *plot-option* ) >> ) >

controls the plots that are produced through ODS Graphics. *Plot-requests* specify the plots to produce, and *plot-options* control the appearance and content of the plots. You can specify *plot-options* in parentheses after a *plot-request*. A *global-plot-option* applies to all plots for which it is available, unless it is altered by a specific *plot-option*. You can specify *global-plot-options* in parentheses after the PLOTS option.

When you specify only one *plot-request*, you can omit the parentheses around the request. For example:

```
plots=all
plots=wilcoxonboxplot
plots=(wilcoxonboxplot edfplot)
plots(only)=(medianplot normalboxplot)
```

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;
proc npar1way plots=wilcoxonboxplot;
 variable response;
 class treatment;
run;
ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

If ODS Graphics is enabled but you do not specify the PLOTS= option, PROC NPAR1WAY produces all plots that are associated with the analyses that you request. If you request a plot with the PLOTS= option but do not request the corresponding analysis, PROC NPAR1WAY automatically invokes that analysis. For example, if you specify PLOTS=CONOVERBOXPLOT but do not also specify the CONOVER option in the PROC NPAR1WAY statement, PROC NPAR1WAY produces the Conover scores analysis in addition to the box plot.

You can suppress default plots and request specific plots by using the PLOTS(ONLY)= option; PLOTS(ONLY)=(*plot-requests*) produces only the plots that are specified as *plot-requests*. You can suppress all plots with the PLOTS=NONE option. The PLOTS= option has no effect when you specify the NOPRINT option.

PROC NPAR1WAY provides box plots of scored data, median plots, and empirical distribution plots. See Figure 65.7, Output 65.1.2, Output 65.1.4, and Output 65.2.2 for examples of plots that PROC NPAR1WAY produces. For general information about ODS Graphics, see Chapter 21, “Statistical Graphics Using ODS.”

**Global Plot Options**

A *Global-plot-option* applies to all plots for which the option is available unless it is altered by a specific *plot-option*. You can specify the following *global-plot-options* in parentheses after the PLOTS option. You cannot specify both STATS and NOSTATS as *global-plot-options* in the same statement.

**NOSTATS**

suppresses the  $p$ -values that are displayed by default in the plots.

**ONLY**

suppresses the default plots and requests only the plots that are specified as *plot-requests*.

**STATS**

displays  $p$ -values in the plots. This is the default.

**Plot Requests**

The following *plot-requests* are available with the PLOTS= option.

**ABBOXPLOT | AB**

requests a box plot of Ansari-Bradley scores. This plot is associated with the Ansari-Bradley analysis, which you request by specifying the **AB** option.

**ALL**

requests all plots that are associated with the specified analyses. This is the default if you do not specify the **ONLY** *global-plot-option*.

**ANOVABOXPLOT | ANOVA**

requests a box plot of the raw data. This plot is associated with the analysis of variance based on the raw data, which you request by specifying the **ANOVA** option.

**CONOVERBOXPLOT | CONOVER**

requests a box plot of Conover scores. This plot is associated with the Conover analysis, which you request by specifying the **CONOVER** option.

**DATASCORESBXPLOT | DATASCORES**

requests a box plot of raw data scores. This plot is associated with the analysis that uses input data as scores, which you request by specifying the **SCORES=DATA** option.

**EDFPLOT | EDF**

requests an empirical distribution plot. This plot is associated with the analyses based on the empirical distribution function, which you request by specifying the **EDF** option.

**FPBOXPLOT | FP**

requests a box plot of Fligner-Policello placements. This plot is associated with the Fligner-Policello analysis, which you request by specifying the **FP** option.

**KLOTZBOXPLOT | KLOTZ**

requests a box plot of Klotz scores. This plot is associated with the Klotz analysis, which you request by specifying the **KLOTZ** option.

**MEDIANPLOT | MEDIAN**

requests a stacked bar chart showing the frequencies above and below the overall median. This plot is associated with the median score analysis, which you request by specifying the **MEDIAN** option.

**MOODBOXPLOT | MOOD**

requests a box plot of Mood scores. This plot is associated with the Mood analysis, which you request by specifying the **MOOD** option.

**NONE**

suppresses all plots.

**SAVAGEBOXPLOT | SAVAGE**

requests a box plot of Savage scores. This plot is associated with the Savage analysis, which you request by specifying the **SAVAGE** option.

**STBOXPLOT | ST**

requests a box plot of Siegel-Tukey scores. This plot is associated with the Siegel-Tukey analysis, which you request by specifying the **ST** option.

**VWBOXPLOT | VW****NORMALBOXPLOT | NORMAL**

requests a box plot of Van der Waerden (normal) scores. This plot is associated with the Van der Waerden analysis, which you request by specifying the **VW** or **NORMAL** option.

**WILCOXONBOXPLOT | WILCOXON**

requests a box plot of Wilcoxon scores. This plot is associated with the Wilcoxon analysis, which you request by specifying the **WILCOXON** option.

**Plot Options**

The following *plot-options* are available for any *plot-request*. You cannot specify both **STATS** and **NOSTATS** as *plot-options* for the same plot. If you specify **NOSTATS** as a *global-plot-option*, specifying **STATS** as an individual *plot-option* overrides the *global-plot-option* for the individual plot and displays statistics in the plot.

**NOSTATS**

suppresses the *p*-values that are displayed in the plot by default.

**STATS**

displays *p*-values in the plot. This is the default.

**SAVAGE**

requests an analysis of Savage scores. See the section “[Savage Scores](#)” on page 5471 for more information.

**SCORES=DATA**

requests an analysis that uses input data as scores. This option gives you the flexibility to construct any scores for your data with the **DATA** step and then analyze these scores with PROC NPAR1WAY. See the section “[Scores for Linear Rank and One-Way ANOVA Tests](#)” on page 5470 for more information.

To produce the two-sample permutation test that is known as Pitman's test, provide raw (unscored) data in the input data set and specify the SCORES=DATA option in the EXACT statement. See the section "Exact Tests" on page 5479 for more information.

#### ST < (ADJUST) >

requests an analysis of Siegel-Tukey scores. See the section "Siegel-Tukey Scores" on page 5472 for more information. The ADJUST option subtracts class medians from the input observations before performing the analysis.

#### VW | NORMAL

requests an analysis of Van der Waerden (normal) scores. See the section "Van der Waerden (Normal) Scores" on page 5471 for more information.

#### WILCOXON

requests an analysis of Wilcoxon scores. When there are two classification levels (samples), this option produces the Wilcoxon rank-sum test. For any number of classification levels, this option produces the Kruskal-Wallis test. See the section "Wilcoxon Scores" on page 5471 for more information.

---

## BY Statement

**BY variables ;**

You can specify a BY statement with PROC NPARIWAY to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the NPARIWAY procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

---

## CLASS Statement

**CLASS** *variable* ;

The CLASS statement, which is required, names one and only one classification variable. The variable can be character or numeric. The CLASS variable identifies groups (samples) in the data, and PROC NPAR1WAY provides analyses to examine differences among these groups. There can be two or more groups in the data.

---

## EXACT Statement

**EXACT** *statistic-options* < / *computation-options* > ;

The EXACT statement requests exact tests and confidence limits for selected statistics. The *statistic-options* identify which statistics to compute, and the *computation-options* specify options for computing exact statistics. See the section “Exact Tests” on page 5479 for details.

**NOTE:** PROC NPAR1WAY computes exact tests by using fast and efficient algorithms that are superior to direct enumeration. Exact tests are appropriate when a data set is small, sparse, skewed, or heavily tied. For some large problems, computation of exact tests might require a large amount of time and memory. Consider using asymptotic tests for such problems. Alternatively, when asymptotic methods might not be sufficient for such large problems, consider using Monte Carlo estimation of exact  $p$ -values. You can request Monte Carlo estimation by specifying the **MC** *computation-option* in the EXACT statement. See the section “Computational Resources” on page 5481 for more information.

## Statistic Options

The *statistic-options* specify which exact tests to compute. Table 65.3 lists the available *statistic-options* and the exact statistics that are computed. Descriptions of the *statistic-options* follow Table 65.3 in alphabetical order.

Exact  $p$ -values are available for all nonparametric tests of location and scale differences that are produced by PROC NPAR1WAY. These include tests based on the following scores: Wilcoxon, median, Van der Waerden (normal), Savage, Siegel-Tukey, Ansari-Bradley, Klotz, Mood, and Conover. Additionally, exact  $p$ -values are available for tests that use the raw input data as scores. The procedure computes exact  $p$ -values when the data are classified into two levels (two-sample tests) and when the data are classified into more than two levels (multisample tests). Two-sample tests are based on simple linear rank statistics. Multisample tests are based on one-way ANOVA statistics.

Exact  $p$ -values are also available for the two-sample Kolmogorov-Smirnov test. Exact confidence limits are available for the Hodges-Lehmann estimate of location shift.

If you list no *statistic-options* in the EXACT statement, then PROC NPAR1WAY computes all available exact  $p$ -values for those tests that you request in the PROC NPAR1WAY statement.



**Table 65.3** EXACT Statement Statistic Options

| Statistic Option | Exact Test                                                                       |
|------------------|----------------------------------------------------------------------------------|
| AB               | Ansari-Bradley test                                                              |
| CONOVER          | Conover test                                                                     |
| HL               | Hodges-Lehmann confidence limits                                                 |
| KLOTZ            | Klotz test                                                                       |
| KS   EDF         | Two-sample Kolmogorov-Smirnov test                                               |
| MEDIAN           | Median test                                                                      |
| MOOD             | Mood test                                                                        |
| SAVAGE           | Savage test                                                                      |
| SCORES=DATA      | Test with input data as scores                                                   |
| ST               | Siegel-Tukey test                                                                |
| VW   NORMAL      | Van der Waerden (normal scores) test                                             |
| WILCOXON         | Wilcoxon test for two-sample data or<br>Kruskal-Wallis test for multisample data |

You can specify the following *statistic-options* in the EXACT statement.

**AB**

requests the exact Ansari-Bradley test. See the sections “[Ansari-Bradley Scores](#)” on page 5472 and “[Exact Tests](#)” on page 5479 for details. The **AB** option in the PROC NPAR1WAY statement provides Ansari-Bradley score analysis and asymptotic tests.

**CONOVER**

requests the exact Conover test. See the sections “[Conover Scores](#)” on page 5472 and “[Exact Tests](#)” on page 5479 for details. The **CONOVER** option in the PROC NPAR1WAY statement provides Conover score analysis and asymptotic tests.

**HL**

requests exact Hodges-Lehmann confidence limits for the location shift for two-sample data. See the section “[Hodges-Lehmann Estimation of Location Shift](#)” on page 5473 for details. The **HL** option in the PROC NPAR1WAY statement provides asymptotic Hodges-Lehmann confidence limits.

You can specify the level of the confidence limits by using the **ALPHA=** option in the PROC NPAR1WAY statement. The default of ALPHA=0.5 produces 95% confidence limits for the location shift.

**KLOTZ**

requests the exact Klotz test. See the sections “[Klotz Scores](#)” on page 5472 and “[Exact Tests](#)” on page 5479 for details. The **KLOTZ** option in the PROC NPAR1WAY statement provides Klotz score analysis and asymptotic tests.

**KS | EDF**

requests the exact Kolmogorov-Smirnov two-sample test. See the section “[Tests Based on the Empirical Distribution Function](#)” on page 5477 for details. The **EDF** option in the PROC NPAR1WAY statement provides the asymptotic Kolmogorov-Smirnov test and other statistics that are based on the empirical distribution function. The **D** option in the PROC NPAR1WAY statement provides the asymptotic one-sided Kolmogorov-Smirnov tests for two-sample data.



**MEDIAN**

requests the exact median test. See the sections “Median Scores” on page 5471 and “Exact Tests” on page 5479 for details. The **MEDIAN** option in the PROC NPAR1WAY statement provides median score analysis and asymptotic tests.

**MOOD**

requests the exact Mood test. See the sections “Mood Scores” on page 5472 and “Exact Tests” on page 5479 for details. The **MOOD** option in the PROC NPAR1WAY statement provides Mood score analysis and asymptotic tests.

**SAVAGE**

requests the exact Savage test. See the sections “Savage Scores” on page 5471 and “Exact Tests” on page 5479 for details. The **SAVAGE** option in the PROC NPAR1WAY statement provides Savage score analysis and asymptotic tests.

**SCORES=DATA**

requests the exact test that uses the input data as scores. For two-sample data, the test is based on the rank-sum statistic. For multisample data, the test is based on the one-way ANOVA statistic. See the sections “Scores for Linear Rank and One-Way ANOVA Tests” on page 5470 and “Exact Tests” on page 5479 for details. The **SCORES=DATA** option in the PROC NPAR1WAY statement provides analysis of the data scores and the corresponding asymptotic test.

**ST**

requests the exact Siegel-Tukey test. See the sections “Siegel-Tukey Scores” on page 5472 and “Exact Tests” on page 5479 for details. The **ST** option in the PROC NPAR1WAY statement provides analysis of Siegel-Tukey scores and asymptotic tests.

**VW | NORMAL**

requests the exact Van der Waerden (normal scores) test. See the sections “Van der Waerden (Normal Scores)” on page 5471 and “Exact Tests” on page 5479 for details. The **VW** option in the PROC NPAR1WAY statement provides analysis of Van der Waerden (normal) scores and asymptotic tests.

**WILCOXON**

requests the exact Wilcoxon test. When the data consist of two classification levels (samples), the exact test is based on the Wilcoxon rank-sum statistic. When the data consist of more than two levels (multisample data), the exact test is based on the one-way ANOVA statistic for Wilcoxon scores, which is the Kruskal-Wallis statistic. See the sections “Wilcoxon Scores” on page 5471 and “Exact Tests” on page 5479 for details. The **WILCOXON** option in the PROC NPAR1WAY statement provides analysis of Wilcoxon scores and the asymptotic Wilcoxon and Kruskal-Wallis tests.

**Computation Options**

*Computation-options* specify options for computing exact statistics. You can specify the following *computation-options* in the EXACT statement after a slash (/).

**ALPHA= $\alpha$** 

specifies the level of the confidence limits for Monte Carlo  $p$ -value estimates. The value of  $\alpha$  must be between 0 and 1, and the default is 0.01. A confidence level of  $\alpha$  produces  $100(1 - \alpha)\%$  confidence limits. The default of ALPHA=0.01 produces 99% confidence limits for the Monte Carlo estimates.

The ALPHA= option invokes the **MC** option.

**MAXTIME=***value*

specifies the maximum clock time (in seconds) that PROC NPAR1WAY can use to compute an exact  $p$ -value. If the procedure does not complete the computation within the specified time, the computation terminates. The value of MAXTIME= must be a positive number. The MAXTIME= option is valid for Monte Carlo estimation of exact  $p$ -values as well as direct exact  $p$ -value computation. See the section “[Computational Resources](#)” on page 5481 for more information.

**MC**

requests Monte Carlo estimation of exact  $p$ -values instead of direct exact  $p$ -value computation. Monte Carlo estimation can be useful for large problems that require a considerable amount of time and memory for exact computations but for which asymptotic approximations might not be sufficient. See the section “[Monte Carlo Estimation](#)” on page 5481 for more information.

The MC option is available for all EXACT *statistic-options* except the HL option, which produces exact Hodges-Lehmann confidence limits. The ALPHA=, N=, and SEED= options also invoke the MC option.

**N=***n*

specifies the number of samples for Monte Carlo estimation. The value of  $n$  must be a positive integer, and the default is 10,000 samples. Larger values of  $n$  produce more precise estimates of exact  $p$ -values. Because larger values of  $n$  generate more samples, the computation time increases.

The N= option invokes the MC option.

**POINT**

requests exact point probabilities for the test statistics.

The POINT option is available for all EXACT statement *statistic-options* except the HL option, which produces exact Hodges-Lehmann confidence limits. The POINT option is not available with the MC option.

**SEED=***number*

specifies the initial seed for random number generation for Monte Carlo estimation. The value of the SEED= option must be an integer. If you do not specify the SEED= option or if the SEED= value is negative or zero, PROC NPAR1WAY uses the time of day from the computer’s clock to obtain the initial seed.

The SEED= option invokes the MC option.

**FREQ Statement**

**FREQ** *variable* ;

The FREQ statement names a numeric variable that provides a frequency for each observation in the input data set. If you use a FREQ statement, PROC NPAR1WAY assumes that an observation occurs  $n$  times, where  $n$  is the value of the FREQ variable for the observation. The sum of the FREQ variable values represents the total number of observations, and the analysis is based on this expanded number of observations.

If the value of the FREQ variable is missing or is less than one, PROC NPAR1WAY does not use that observation in the analysis. If the value of the FREQ variable is not an integer, PROC NPAR1WAY uses only the integer portion as the frequency of the observation.

---

## OUTPUT Statement

**OUTPUT** < **OUT=SAS-data-set** > < *output-options* > ;

The OUTPUT statement creates a SAS data set that contains statistics that PROC NPAR1WAY computes. Table 65.4 lists the statistics that can be stored in the output data set. You identify which statistics to include by specifying *output-options*.

The output data set contains one observation for each analysis variable that you name in the VAR statement. If you use a BY statement, the output data set contains an observation or set of observations for each BY group. See the section “Contents of the Output Data Set” on page 5483 for more information.

As an alternative to the OUTPUT statement, you can use the Output Delivery System (ODS) to store statistics that PROC NPAR1WAY computes. ODS can create a SAS data set from any table that PROC NPAR1WAY produces. For more information, see the section “ODS Table Names” on page 5493 and Chapter 20, “Using the Output Delivery System.”

You can specify the following *options* in the OUTPUT statement:

### **OUT=SAS-data-set**

names the output data set. When you use an OUTPUT statement but do not specify the OUT= option, PROC NPAR1WAY creates a data set and names it by using the DATA*n* convention.

### *output-options*

specifies the statistics to include in the output data set. Table 65.4 lists the *output-options* that are available in the OUTPUT statement. Descriptions of the *output-options* follow the table in alphabetical order.

When you specify an *output-option*, the output data set includes the test statistic and associated values from the analysis that you specify. The associated values might include standardized statistics, one- and two-sided *p*-values, exact *p*-values, degrees of freedom, and confidence limits. See the section “Contents of the Output Data Set” on page 5483 for a list of output data set variables that each *output-option* produces.

If you do not specify any *output-options* in the OUTPUT statement, the output data set includes all available statistics from the analyses that you request in the PROC NPAR1WAY statement. If you request a statistic in the OUTPUT statement but do not request the corresponding analysis in the PROC NPAR1WAY statement, PROC NPAR1WAY performs the corresponding analysis.

**Table 65.4** OUTPUT Statement Output Options

| Output Option | Output Data Set Statistics                                                                |
|---------------|-------------------------------------------------------------------------------------------|
| AB            | Ansari-Bradley test                                                                       |
| ANOVA         | Analysis of variance                                                                      |
| CONOVER       | Conover test                                                                              |
| EDF           | Kolmogorov-Smirnov test,<br>Cramér-von Mises test, and<br>Kuiper test for two-sample data |
| FP            | Fligner-Policello test                                                                    |
| HL            | Hodges-Lehmann estimates                                                                  |
| KLOTZ         | Klotz test                                                                                |
| MEDIAN        | Median test                                                                               |
| MOOD          | Mood test                                                                                 |
| SAVAGE        | Savage test                                                                               |
| SCORES=DATA   | Test with input data as scores                                                            |
| ST            | Siegel-Tukey test                                                                         |
| VW   NORMAL   | Van der Waerden (normal scores) test                                                      |
| WILCOXON      | Wilcoxon test for two-sample data and<br>Kruskal-Wallis test                              |

You can specify the following *output-options* in the OUTPUT statement.

**AB**

includes statistics from the Ansari-Bradley analysis in the output data set. The **AB** option in the PROC NPAR1WAY statement requests analysis of Ansari-Bradley scores. See the section “[Ansari-Bradley Scores](#)” on page 5472 for more information.

**ANOVA**

includes analysis of variance statistics in the output data set. The **ANOVA** option in the PROC NPAR1WAY statement requests a standard analysis of variance for the raw data.

**CONOVER**

includes statistics from the Conover analysis in the output data set. The **CONOVER** option in the PROC NPAR1WAY statement requests analysis of Conover scores. See the section “[Conover Scores](#)” on page 5472 for more information.

**EDF**

includes empirical distribution function statistics in the output data set. The **EDF** option in the PROC NPAR1WAY statement requests computation of these statistics, which include the Kolmogorov-Smirnov test, the Cramér-von Mises test, and the Kuiper test for two sample-data. See the section “[Tests Based on the Empirical Distribution Function](#)” on page 5477 for more information.

**FP**

includes the Fligner-Policello test in the output data set. The **FP** option in the PROC NPAR1WAY statement requests the Fligner-Policello test, which is available for two-sample data. See the section “[Fligner-Policello Test](#)” on page 5475 for more information.

**HL**

includes the Hodges-Lehmann estimate and confidence limits in the output data set. The **HL** option in the PROC NPAR1WAY statement requests Hodges-Lehmann estimation, which is available for two-sample data. See the section “[Hodges-Lehmann Estimation of Location Shift](#)” on page 5473 for more information.

**KLOTZ**

includes statistics from the Klotz analysis in the output data set. The **KLOTZ** option in the PROC NPAR1WAY statement requests analysis of Klotz scores. See the section “[Klotz Scores](#)” on page 5472 for more information.

**MEDIAN**

includes statistics from the median analysis in the output data set. The **MEDIAN** option in the PROC NPAR1WAY statement requests analysis of median scores. See the section “[Median Scores](#)” on page 5471 for more information.

**MOOD**

includes statistics from the Mood analysis in the output data set. The **MOOD** option in the PROC NPAR1WAY statement requests analysis of Mood scores. See the section “[Mood Scores](#)” on page 5472 for more information.

**SAVAGE**

includes statistics from the Savage analysis in the output data set. The **SAVAGE** option in the PROC NPAR1WAY statement requests analysis of SAVAGE scores. See the section “[Savage Scores](#)” on page 5471 for more information.

**SCORES=DATA**

includes statistics from the analysis of data scores in the output data set. The **SCORES=DATA** option in the PROC NPAR1WAY statement requests an analysis that uses the raw input data as scores.

**ST**

includes statistics from the Siegel-Tukey analysis in the output data set. The **ST** option in the PROC NPAR1WAY statement requests analysis of Siegel-Tukey scores. See the section “[Siegel-Tukey Scores](#)” on page 5472 for more information.

**VW | NORMAL**

includes statistics from the Van der Waerden (normal scores) analysis in the output data set. The **VW** option in the PROC NPAR1WAY statement requests analysis of Van der Waerden scores. See the section “[Van der Waerden \(Normal\) Scores](#)” on page 5471 for more information.

**WILCOXON**

includes statistics from the Wilcoxon analysis in the output data set. The **WILCOXON** option in the PROC NPAR1WAY statement requests analysis of Wilcoxon scores. For two-sample data, this analysis includes the Wilcoxon rank-sum test. For all data (two-sample and multisample), the analysis includes the Kruskal-Wallis test. See the section “[Wilcoxon Scores](#)” on page 5471 for more information.

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## VAR Statement

**VAR** *variables* ;

The VAR statement names the response (dependent) variables to be included in the analysis. These variables must be numeric. If you omit the VAR statement, the procedure includes all numeric variables in the data set except for the CLASS variable, the FREQ variable, and the BY variables.

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## Details: NPAR1WAY Procedure

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### Missing Values

If an observation has a missing value for a response (VAR) variable, PROC NPAR1WAY excludes that observation from the analysis. Any observation with a missing or nonpositive value for the FREQ variable is also excluded from the analysis.

By default, PROC NPAR1WAY also excludes observations with missing values of the CLASS variable. If you specify the MISSING option, PROC NPAR1WAY treats missing values of the CLASS variable as a valid class level and includes these observations in the analysis.

PROC NPAR1WAY treats missing BY variable values like any other BY variable value. The missing values form a separate, valid BY group.

---

### Tied Values

*Tied values* occur when two or more observations are equal, whether the observations occur in the same sample or in different samples. In theory, nonparametric tests were developed for continuous distributions where the probability of a tie is zero. In practice, however, ties often occur. PROC NPAR1WAY uses the same method to handle ties for all score types. The procedure computes the scores as if there were no ties, averages the scores for tied observations, and assigns this average score to each observation with the same value.

When there are tied values, PROC NPAR1WAY first sorts the observations in ascending order and assigns ranks as if there were no ties. Then the procedure computes the scores based on these ranks by using the formula for the specified score type. The procedure averages the scores for tied observations and assigns this average score to each of the tied observations. Thus, all equal data values have the same score value. PROC NPAR1WAY then computes the test statistic from these scores.

Note that the asymptotic tests might be less accurate when the distribution of the data is heavily tied. For such data, it might be appropriate to use the exact tests provided by PROC NPAR1WAY as described in the section “Exact Tests” on page 5479.

When computing empirical distribution function statistics for data with ties, PROC NPAR1WAY uses the formulas given in the section “Tests Based on the Empirical Distribution Function” on page 5477. No special handling of ties is necessary.

PROC NPAR1WAY bases its computations on the internal numeric values of the analysis variables; the procedure does not format or round these values before analysis. When values differ in their internal representation, even slightly, PROC NPAR1WAY does not treat them as tied values. If this is a concern for your data, then round the analysis variables by an appropriate amount before invoking PROC NPAR1WAY. For information about the ROUND function, see the discussion in *SAS Language Reference: Dictionary*.

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## Statistical Computations

### Simple Linear Rank Tests for Two-Sample Data

Statistics of the form

$$S = \sum_{j=1}^n c_j a(R_j)$$

are called *simple linear rank statistics*, where

$R_j$  is the rank of observation  $j$

$a(R_j)$  is the score based on the rank of observation  $j$

$c_j$  is an indicator variable denoting the class to which the  $j$ th observation belongs

$n$  is the total number of observations

For two-sample data (where the observations are classified into two levels), PROC NPAR1WAY calculates simple linear rank statistics for the scores that you specify. The section “[Scores for Linear Rank and One-Way ANOVA Tests](#)” on page 5470 describes the available scores, which you can use to test for differences in location and differences in scale.

To compute the linear rank statistic  $S$ , PROC NPAR1WAY sums the scores of the observations in the smaller of the two samples. If both samples have the same number of observations, PROC NPAR1WAY sums those scores for the sample that appears first in the input data set.

For each score that you specify, PROC NPAR1WAY computes an asymptotic test of the null hypothesis of no difference between the two classification levels. Exact tests are also available for these two-sample linear rank statistics. PROC NPAR1WAY computes exact tests for each score type that you specify in the **EXACT** statement. See the section “[Exact Tests](#)” on page 5479 for details.

To compute an asymptotic test for a linear rank sum statistic, PROC NPAR1WAY uses a standardized test statistic  $z$ , which has an asymptotic standard normal distribution under the null hypothesis. The standardized test statistic is computed as

$$z = (S - E_0(S)) / \sqrt{\text{Var}_0(S)}$$

where  $E_0(S)$  is the expected value of  $S$  under the null hypothesis, and  $\text{Var}_0(S)$  is the variance under the null hypothesis. As shown in Randles and Wolfe (1979),

$$E_0(S) = \frac{n_1}{n} \sum_{j=1}^n a(R_j)$$



where  $n_1$  is the number of observations in the first (smaller) class level (sample),  $n_2$  is the number of observations in the other class level, and

$$\text{Var}_0(S) = \frac{n_1 n_2}{n(n-1)} \sum_{j=1}^n (a(R_j) - \bar{a})^2$$

where  $\bar{a}$  is the average score,

$$\bar{a} = \frac{1}{n} \sum_{j=1}^n a(R_j)$$

### Definition of $p$ -Values

PROC NPAR1WAY computes one-sided and two-sided asymptotic  $p$ -values for each two-sample linear rank test. When the test statistic  $z$  is greater than its null hypothesis expected value of zero, PROC NPAR1WAY computes the right-sided  $p$ -value, which is the probability of a larger value of the statistic occurring under the null hypothesis. When the test statistic is less than or equal to zero, PROC NPAR1WAY computes the left-sided  $p$ -value, which is the probability of a smaller value of the statistic occurring under the null hypothesis. The one-sided  $p$ -value  $P_1(z)$  can be expressed as

$$P_1(z) = \begin{cases} \text{Prob}(Z > z) & \text{if } z > 0 \\ \text{Prob}(Z < z) & \text{if } z \leq 0 \end{cases}$$

where  $Z$  has a standard normal distribution. The two-sided  $p$ -value  $P_2(z)$  is computed as

$$P_2(z) = \text{Prob}(|Z| > |z|)$$

### Continuity Correction

PROC NPAR1WAY uses a continuity correction for the asymptotic two-sample Wilcoxon and Siegel-Tukey tests by default. You can remove the continuity correction by specifying the `CORRECT=NO` option. PROC NPAR1WAY incorporates the continuity correction when computing the standardized test statistic  $z$  by subtracting 0.5 from the numerator ( $S - E_0(S)$ ) if it is greater than zero. If the numerator is less than zero, PROC NPAR1WAY adds 0.5. Some sources recommend a continuity correction for nonparametric tests that use a continuous distribution to approximate a discrete distribution. (See Sheskin 1997.)

If you specify `CORRECT=NO`, PROC NPAR1WAY does not use a continuity correction for any test.

## One-Way ANOVA Tests

PROC NPAR1WAY computes a one-way ANOVA test for each score type that you specify. Under the null hypothesis of no difference among class levels (samples), this test statistic has an asymptotic chi-square distribution with  $r - 1$  degrees of freedom, where  $r$  is the number of class levels. For Wilcoxon scores, this test is known as the Kruskal-Wallis test.

Exact one-way ANOVA tests are also available for multisample data (where the data are classified into more than two levels). For two-sample data, exact simple linear rank tests are available. PROC NPAR1WAY computes exact tests for each score type that you specify in the `EXACT` statement. See the section “Exact Tests” on page 5479 for details.



PROC NPAR1WAY computes the one-way ANOVA test statistic as

$$C = \left( \sum_{i=1}^r (T_i - E_0(T_i))^2 / n_i \right) / S^2$$

where  $T_i$  is the total of scores for class level  $i$ ,  $E_0(T_i)$  is the expected total for level  $i$  under the null hypothesis of no difference among levels,  $n_i$  is the number of observations in level  $i$ , and  $S^2$  is the sample variance of the scores. The total of scores for class level  $i$  is given by

$$T_i = \sum_{j=1}^n c_{ij} a(R_j)$$

where  $a(R_j)$  is the score for observation  $j$ , and  $c_{ij}$  indicates whether observation  $j$  is in level  $i$ . The expected total of scores for class level  $i$  under the null hypothesis is equal to

$$E_0(T_i) = \frac{n_i}{n} \sum_{j=1}^n a(R_j)$$

The sample variance of the scores is computed as

$$S^2 = \frac{1}{(n-1)} \sum_{j=1}^n (a(R_j) - \bar{a})^2$$

where  $\bar{a}$  is the average score,

$$\bar{a} = \frac{1}{n} \sum_{j=1}^n a(R_j)$$

### Scores for Linear Rank and One-Way ANOVA Tests

For each score type that you specify, PROC NPAR1WAY computes a one-way ANOVA statistic and also a linear rank statistic for two-sample data. The following score types are used primarily to test for differences in location: Wilcoxon, median, Van der Waerden (normal), and Savage. The following scores types are used to test for scale differences: Siegel-Tukey, Ansari-Bradley, Klotz, and Mood. Conover scores can be used to test for differences in both location and scale. This section gives formulas for the score types available in PROC NPAR1WAY. For further information about the formulas and the applicability of each score, see Randles and Wolfe (1979); Gibbons and Chakraborti (2010); Conover (1999); Hollander and Wolfe (1999).

In addition to the score types described in this section, you can specify the **SCORES=DATA** option to use the input data observations as scores. This enables you to produce a wide variety of tests. You can construct any scores by using the DATA step, and then you can use PROC NPAR1WAY to compute the corresponding linear rank and one-way ANOVA tests for these scores. You can also analyze raw (unscored) data with the **SCORES=DATA** option; for two-sample data, the corresponding exact test is a permutation test that is known as Pitman's test.

**Wilcoxon Scores**

Wilcoxon scores are the ranks of the observations, which can be written as

$$a(R_j) = R_j$$

where  $R_j$  is the rank of observation  $j$ , and  $a(R_j)$  is the score of observation  $j$ .

Using Wilcoxon scores in the linear rank statistic for two-sample data produces the rank sum statistic of the Mann-Whitney-Wilcoxon test. Using Wilcoxon scores in the one-way ANOVA statistic produces the Kruskal-Wallis test. Wilcoxon scores are locally most powerful for location shifts of a logistic distribution.

When computing the asymptotic Wilcoxon two-sample test, PROC NPAR1WAY uses a continuity correction by default, as described in the section “[Continuity Correction](#)” on page 5469. If you specify the `CORRECT=NO` option in the PROC NPAR1WAY statement, the procedure does not use a continuity correction.

**Median Scores**

Median scores equal 1 for observations greater than the median, and 0 otherwise. In terms of the observation ranks, median scores are defined as

$$a(R_j) = \begin{cases} 1 & \text{if } R_j > (n + 1)/2 \\ 0 & \text{if } R_j \leq (n + 1)/2 \end{cases}$$

Using median scores in the linear rank statistic for two-sample data produces the two-sample median test. The one-way ANOVA statistic with median scores is equivalent to the Brown-Mood test. Median scores are particularly powerful for distributions that are symmetric and heavy-tailed.

**Van der Waerden (Normal) Scores**

Van der Waerden scores are the quantiles of a standard normal distribution and are also known as *quantile normal scores*. Van der Waerden scores are computed as

$$a(R_j) = \Phi^{-1} \left( \frac{R_j}{n + 1} \right)$$

where  $\Phi$  is the cumulative distribution function of a standard normal distribution. These scores are powerful for normal distributions.

**Savage Scores**

Savage scores are expected values of order statistics from the exponential distribution, with 1 subtracted to center the scores around 0. Savage scores are computed as

$$a(R_j) = \sum_{i=1}^{R_j} \left( \frac{1}{n - i + 1} \right) - 1$$

Savage scores are powerful for comparing scale differences in exponential distributions or location shifts in extreme value distributions (Hajek 1969, p. 83).

**Siegel-Tukey Scores**

Siegel-Tukey scores are defined as

$$\begin{aligned} a(1) &= 1, & a(n) &= 2, & a(n-1) &= 3, & a(2) &= 4, \\ a(3) &= 5, & a(n-2) &= 6, & a(n-3) &= 7, & a(4) &= 8, \dots \end{aligned}$$

where the score values continue to increase in this pattern toward the middle ranks until all observations have been assigned a score.

When computing the asymptotic Siegel-Tukey two-sample test, PROC NPAR1WAY uses a continuity correction by default, as described in the section “[Continuity Correction](#)” on page 5469. If you specify the `CORRECT=NO` option in the PROC NPAR1WAY statement, the procedure does not use a continuity correction.

**Ansari-Bradley Scores**

Ansari-Bradley scores are similar to Siegel-Tukey scores, but Ansari-Bradley scoring assigns the same score value to corresponding extreme ranks. (Siegel-Tukey scores are a permutation of the ranks  $1, 2, \dots, n$ .) Ansari-Bradley scores are defined as

$$\begin{aligned} a(1) &= 1, & a(n) &= 1, \\ a(2) &= 2, & a(n-1) &= 2, \dots \end{aligned}$$

Equivalently, Ansari-Bradley scores are equal to

$$a(R_j) = \frac{n+1}{2} - \left| R_j - \frac{n+1}{2} \right|$$

**Klotz Scores**

Klotz scores are the squares of the Van der Waerden (normal) scores. Klotz scores are computed as

$$a(R_j) = \left( \Phi^{-1} \left( \frac{R_j}{n+1} \right) \right)^2$$

where  $\Phi$  is the cumulative distribution function of a standard normal distribution.

**Mood Scores**

Mood scores are computed as the square of the difference between the observation rank and the average rank. Mood scores can be written as

$$a(R_j) = \left( R_j - \frac{n+1}{2} \right)^2$$

**Conover Scores**

Conover scores are based on the squared ranks of the absolute deviations from the sample means. For observation  $j$  the absolute deviation from the mean is computed as

$$U_j = |X_{j(i)} - \bar{X}_i|$$

where  $X_{j(i)}$  is the value of observation  $j$ , observation  $j$  belongs to sample  $i$ , and  $\bar{X}_i$  is the mean of sample  $i$ . The values of  $U_j$  are ranked, and the Conover score for observation  $j$  is computed as

$$\text{Score}_j = (\text{Rank}(U_j))^2$$

Following Conover (1999), when there are ties among the values of  $U_j$ , PROC NPAR1WAY assigns the average rank to each of the tied observations. To compute the average rank, PROC NPAR1WAY ranks the  $U_j$  as if there were no ties, and then averages the ranks of the tied observations.

The Conover score test is also known as the squared ranks test for variances. See Conover (1999) for more information.

### Hodges-Lehmann Estimation of Location Shift

If you specify the **HL** option, PROC NPAR1WAY computes the Hodges-Lehmann estimate of location shift for two-sample data. PROC NPAR1WAY also provides confidence limits for the location shift. These confidence limits are sometimes called Moses confidence limits. You can set the level of the confidence limits with the **ALPHA=** option. The default is ALPHA=0.05, which produces 95% confidence limits. Additionally, you can request exact confidence limits for the location shift by specifying the HL option in the **EXACT** statement.

The Hodges-Lehmann estimator of location shift is associated with the Wilcoxon linear rank statistic. See Hollander and Wolfe (1999) and Hodges and Lehmann (1983) for details.

PROC NPAR1WAY computes the Hodges-Lehmann estimate  $\hat{\Delta}$  as the median of all paired differences between observations in the two samples (classes), which can be written as

$$\hat{\Delta} = \text{median} \left( (Y_j - X_i) \quad \text{where } j = 1, 2, \dots, n_1; i = 1, 2, \dots, n_2 \right)$$

The  $Y_j$  are observations in class 1, the  $X_i$  are observations in class 2, and  $n_1$  and  $n_2$  denote the number of observations in class 1 and class 2, respectively.

By default, PROC NPAR1WAY uses the larger of the two classes as the reference class  $X$  (class 2). If both classes have the same number of observations, PROC NPAR1WAY uses the class that appears second in the input data set as the reference class. You can specify the reference class by using the **HL(REFCLASS=)** option. REFCLASS=1 refers to the first class that is listed in the “Wilcoxon Scores” table, and REFCLASS=2 refers to the second class in the table. REFCLASS=*class-value* identifies the reference class by the formatted value of the **CLASS** variable.

Let  $m$  denote the total number of differences ( $n_1 \times n_2$ ), and let  $U^{(k)}$  denote the  $k$ th value of  $(Y_j - X_i)$  among the ordered differences. When  $m$  is an odd number, then the median difference is the value with rank  $(m + 1)/2$ ,

$$\hat{\Delta} = U^{(k)} \quad \text{where } k = (m + 1)/2$$

When  $m$  is an even number, the median difference is the average of the values with ranks  $(m/2)$  and  $((m/2) + 1)$ ,

$$\hat{\Delta} = \left( U^{(k)} + U^{(k+1)} \right) / 2 \quad \text{where } k = m/2$$

Following Hollander and Wolfe (1999), the asymptotic lower and upper confidence limits for the location shift are

$$\left( \Delta_L = U^{(C_\alpha)}, \quad \Delta_U = U^{(m+1-C_\alpha)} \right)$$

where  $C_\alpha$  is the largest integer less than or equal to  $C_\alpha^*$ , which is computed as

$$C_\alpha^* = E_0(S) - z_{\alpha/2} \sqrt{\text{Var}_0(S)}$$

where  $E_0(S)$  and  $\text{Var}_0(S)$  are the expected value and variance, respectively, of the Wilcoxon statistic  $S$  under the null hypothesis (as described in the section “Simple Linear Rank Tests for Two-Sample Data” on page 5468), and  $z_{\alpha/2}$  is the  $100(1 - \alpha/2)$  percentile of the standard normal distribution. For Wilcoxon rank scores,

$$E_0(S) = n_1 n_2 / 2$$

When there are no tied values,  $\text{Var}_0(S)$  for Wilcoxon scores equals

$$\text{Var}_0(S) = n_1 n_2 (n_1 + n_2 + 1) / 12$$

PROC NPAR1WAY displays the midpoint of the confidence interval  $(\Delta_L, \Delta_U)$ , which can also be used as an estimate of location shift. See Lehmann (1963) for details. Additionally, PROC NPAR1WAY provides an estimate of the asymptotic standard error of  $\hat{\Delta}$  based on the length of the confidence interval, which is computed as

$$\text{se}(\hat{\Delta}) = (\Delta_U - \Delta_L) / (2 z_{\alpha/2})$$

### Exact Confidence Limits

If you specify the HL option in the EXACT statement, PROC NPAR1WAY computes exact confidence limits for the location shift between the two samples. As for the asymptotic confidence limits, you can set the confidence level with the ALPHA= option. The default is ALPHA=0.05, which produces 95% confidence limits.

PROC NPAR1WAY computes exact confidence limits for the location shift as described in Randles and Wolfe (1979, p. 180). PROC NPAR1WAY first generates the exact conditional distribution of the Mann-Whitney  $U$  statistic, which equals the number of pairwise differences  $(Y_i - X_j)$  that are positive, plus half the number of pairwise differences that are zero. The Mann-Whitney statistic is defined as

$$MW = \sum_{i=1}^{n_1} \sum_{j=i}^{n_2} \phi(X_i - Y_j)$$

where

$$\phi(Y_i, X_j) = \begin{cases} 1 & \text{if } Y_i > X_j \\ 1/2 & \text{if } Y_i = X_j \\ 0 & \text{otherwise} \end{cases}$$

From the exact conditional distribution of the Mann-Whitney statistic  $MW$ , PROC NPAR1WAY chooses  $C_{L,\alpha}^*$  as the largest value such that  $\text{Prob}(MW \geq C_{L,\alpha}^*) \geq \alpha/2$ . Rounding  $C_{L,\alpha}^*$  up to the nearest integer  $C_{L,\alpha}$ , the lower confidence limit equals the difference  $(Y_i - X_j)$  that has a rank of  $(n_1 n_2 - C_{L,\alpha} + 1)$ .

To find the upper confidence limit, PROC NPAR1WAY chooses  $C_{U,\alpha}^*$  as the smallest value such that  $\text{Prob}(MW \leq C_{U,\alpha}^*) \geq \alpha/2$ . Rounding  $C_{U,\alpha}^*$  down to the nearest integer  $C_{U,\alpha}$ , the upper confidence limit equals the difference  $(Y_i - X_j)$  that has a rank of  $(n_1 n_2 - C_{U,\alpha})$ .

Because this is a discrete problem, the confidence coefficient for these exact confidence limits is not exactly  $(1 - \alpha)$  but is at least  $(1 - \alpha)$ . Thus, these confidence limits are conservative.

## Fligner-Policello Test

If you specify the `FP` option, PROC `NPARIWAY` computes the Fligner-Policello location test for two-sample data (Fligner and Policello 1981). The null hypothesis for the test is  $H_0 : \theta_X = \theta_Y$ , where  $\theta_X$  and  $\theta_Y$  are the population medians of the two classes. The Fligner-Policello test assumes that the distribution in each class is symmetric around the class median, but it does not require that the two class distributions have the same form or that the class variances be equal. See Hollander and Wolfe (1999) and Juneau (2007) for more information.

The Fligner-Policello test is based on placement scores (Orban and Wolfe 1979). The placement of an observation  $X_i$  from class  $X$ ,  $P(X_i)$ , is defined as the number of observations in class  $Y$  that are less than  $X_i$ . If there are ties, the placement of  $X_i$  is adjusted by adding half the number of observations in class  $Y$  that are equal to  $X_i$ . The placement of an observation  $Y_j$  from class  $Y$ ,  $P(Y_j)$ , is defined in the same way. The placements can be expressed as

$$P(X_i) = \sum_{j=1}^{n_y} (I(Y_j < X_i) + 0.5I(Y_j = X_i))$$

$$P(Y_j) = \sum_{i=1}^{n_x} (I(X_i < Y_j) + 0.5I(X_i = Y_j))$$

where  $I(\cdot)$  is an indicator function and  $n_x$  and  $n_y$  denote the number of observations in class  $X$  and class  $Y$ , respectively.

The average placements for class  $X$  and class  $Y$  are computed as

$$\bar{P}_x = \left( \sum_{i=1}^{n_x} P(X_i) \right) / n_x$$

$$\bar{P}_y = \left( \sum_{j=1}^{n_y} P(Y_j) \right) / n_y$$

The Fligner-Policello test statistic is computed as

$$z = \left( \sum_{j=1}^{n_y} P(Y_j) - \sum_{i=1}^{n_x} P(X_i) \right) / \left( 2\sqrt{V_x + V_y + \bar{P}_x \bar{P}_y} \right)$$

where

$$V_x = \sum_{i=1}^{n_x} (P(X_i) - \bar{P}_x)^2$$

$$V_y = \sum_{j=1}^{n_y} (P(Y_j) - \bar{P}_y)^2$$

and the standard deviation of the placements is  $\sqrt{V_x/(n_x - 1)}$  for class  $X$  and  $\sqrt{V_y/(n_y - 1)}$  for class  $Y$ .

Under the null hypothesis, the Fligner-Policello statistic has an asymptotic standard normal distribution. PROC NPAR1WAY provides one- and two-sided asymptotic  $p$ -values for the Fligner-Policello test. For the one-sided test, PROC NPAR1WAY displays the right-sided  $p$ -value when the test statistic  $z$  is greater than its null hypothesis expected value of zero. PROC NPAR1WAY displays the left-sided  $p$ -value when the test statistic  $z$  is less than or equal to zero. The one-sided  $p$ -value  $P_1(z)$  can be expressed as

$$P_1(z) = \begin{cases} \text{Prob}(Z > z) & \text{if } z > 0 \\ \text{Prob}(Z < z) & \text{if } z \leq 0 \end{cases}$$

where  $Z$  has a standard normal distribution. The two-sided  $p$ -value  $P_2(z)$  is computed as  $\text{Prob}(|Z| > |z|)$ .

When you specify the FP option, PROC NPAR1WAY displays a “Fligner-Policello Placements” table and a “Fligner-Policello Test” table. The “Fligner-Policello Placements” table contains the following information for each of the two classes: number of observations, sum of the placements, average placement, and standard deviation of the placements. The “Fligner-Policello Test” table contains the test statistic  $z$  and the corresponding one- and two-sided  $p$ -values. This table also displays the difference between the class placement sums, which is the numerator of the test statistic. When ODS Graphics is enabled and you specify the FP or PLOTS=FPBOXPLOT option, PROC NPAR1WAY provides a box plot of the Fligner-Policello placements.

PROC NPAR1WAY computes the Fligner-Policello difference (the numerator of the test statistic) as the placement sum for class  $Y$  minus the placement sum for class  $X$  (the reference class). By default, PROC NPAR1WAY uses the first class that is listed in the “Fligner-Policello Placements” table as class  $Y$  and the second class as the reference class  $X$ . The table displays class levels in the order in which they appear in the input data set. To use the first class (instead of the second class) as the reference class for the Fligner-Policello test, you can specify the FP(REFCLASS=1) option. Or you can specify the FP(REFCLASS=*class-value*) option to identify the reference class by the formatted value of the CLASS variable.

## Multiple Comparisons Based on Pairwise Rankings

If you specify the DSCF option, PROC NPAR1WAY computes the Dwass, Steel, Critchlow-Fligner (DSCF) multiple comparison analysis, which is based on pairwise two-sample Wilcoxon comparisons (Dwass 1960; Steel 1960; Critchlow and Fligner 1991). The DSCF analysis is available when the number of CLASS variable levels (samples) is greater than 2. There are  $r(r-1)/2$  pairs of samples, where  $r$  is the total number of samples.

For each pair of samples, PROC NPAR1WAY ranks the observations and computes the standardized Wilcoxon test statistic, which is described in the sections “Simple Linear Rank Tests for Two-Sample Data” on page 5468 and “Wilcoxon Scores” on page 5471. The procedure does not include a continuity correction in the Wilcoxon test statistics that it computes for the DSCF analysis. The DSCF statistic for a pair of samples is computed as  $\sqrt{2}z$ , where  $z$  is the two-sample standardized Wilcoxon statistic. Under the null hypothesis of no location differences among the  $r$  samples, the distribution of the DSCF statistics can be approximated by the studentized range distribution for  $r$  independent standard normal variables. The  $p$ -value for a two-sample DSCF comparison is the percentile of the studentized range distribution that corresponds to the value of the DSCF statistic. See Hollander and Wolfe (1999) and Juneau (2007, 2004) for more information.

When you specify the DSCF option, PROC NPAR1WAY displays the “Pairwise Two-Sided Multiple Comparison Analysis” table, which contains the following information for each two-sample comparison: comparison identification (two class variable levels), two-sample Wilcoxon test statistic, DSCF statistic, and

two-sided DSCF  $p$ -value. You can store these statistics in a SAS data set by using the Output Delivery System (ODS). The ODS name for this table is DSCF. For more information, see the section “ODS Table Names” on page 5493 and Chapter 20, “Using the Output Delivery System.”

## Tests Based on the Empirical Distribution Function

If you specify the **EDF** option, PROC NPAR1WAY computes tests based on the empirical distribution function. These include the Kolmogorov-Smirnov and Cramér–von Mises tests, and also the Kuiper test for two-sample data. This section gives formulas for these test statistics. For further information about the formulas and the interpretation of EDF statistics, see Hollander and Wolfe (1999) and Gibbons and Chakraborti (2010). For details about the  $k$ -sample analogs of the Kolmogorov-Smirnov and Cramér–von Mises statistics, see Kiefer (1959).

The *empirical distribution function* (EDF) of a sample  $\{x_j\}$ ,  $j = 1, 2, \dots, n$ , is defined as

$$F(x) = \frac{1}{n}(\text{number of } x_j \leq x) = \frac{1}{n} \sum_{j=1}^n I(x_j \leq x)$$

where  $I(\cdot)$  is an indicator function. PROC NPAR1WAY uses the subsample of values within the  $i$ th class level to generate an EDF for the class,  $F_i$ . The EDF for the overall sample, pooled over classes, can also be expressed as

$$F(x) = \frac{1}{n} \sum_i (n_i F_i(x))$$

where  $n_i$  is the number of observations in the  $i$ th class level, and  $n$  is the total number of observations.

### Kolmogorov-Smirnov Test

The Kolmogorov-Smirnov statistic measures the maximum deviation of the EDF within the classes from the pooled EDF. PROC NPAR1WAY computes the Kolmogorov-Smirnov statistic as

$$KS = \max_j \sqrt{\frac{1}{n} \sum_i n_i (F_i(x_j) - F(x_j))^2} \quad \text{where } j = 1, 2, \dots, n$$

The asymptotic Kolmogorov-Smirnov statistic is computed as

$$KS_a = KS \times \sqrt{n}$$

For each class level  $i$  and overall, PROC NPAR1WAY displays the value of  $F_i$  at the maximum deviation from  $F$  and the value  $\sqrt{n_i} (F_i - F)$  at the maximum deviation from  $F$ . PROC NPAR1WAY also gives the observation where the maximum deviation occurs.

If there are only two class levels, PROC NPAR1WAY computes the two-sample Kolmogorov-Smirnov test statistic  $D$  as

$$D = \max_j |F_1(x_j) - F_2(x_j)| \quad \text{where } j = 1, 2, \dots, n$$

The  $p$ -value for this test is the probability that  $D$  is greater than the observed value  $d$  under the null hypothesis of no difference between class levels (samples). PROC NPAR1WAY computes the asymptotic  $p$ -value for



$D$  with the approximation

$$\text{Prob}(D > d) = 2 \sum_{i=1}^{\infty} (-1)^{(i-1)} e^{(-2i^2 z^2)}$$

where

$$z = d \sqrt{n_1 n_2 / n}$$

See Hodges (1957) for information about this approximation.

If you specify the **D** option, or if you request exact Kolmogorov-Smirnov  $p$ -values with the **KS** option in the **EXACT** statement, PROC NPAR1WAY also computes the one-sided Kolmogorov-Smirnov statistics  $D+$  and  $D-$  for two-sample data as

$$D+ = \max_j (F_1(x_j) - F_2(x_j)) \quad \text{where } j = 1, 2, \dots, n$$

$$D- = \max_j (F_2(x_j) - F_1(x_j)) \quad \text{where } j = 1, 2, \dots, n$$

The asymptotic probability that  $D+$  is greater than the observed value  $d^+$ , under the null hypothesis of no difference between the two class levels, is computed as

$$\text{Prob}(D+ > d^+) = e^{-2z^2} \quad \text{where } z = d^+ \sqrt{n_1 n_2 / n}$$

Similarly, the asymptotic probability that  $D-$  is greater than the observed value  $d^-$  is computed as

$$\text{Prob}(D- > d^-) = e^{-2z^2} \quad \text{where } z = d^- \sqrt{n_1 n_2 / n}$$

To request exact  $p$ -values for the Kolmogorov-Smirnov statistics, you can specify the **KS** option in the **EXACT** statement. See the section “Exact Tests” on page 5479 for more information.

### **Cramér–von Mises Test**

The Cramér–von Mises statistic is defined as

$$CM = \frac{1}{n^2} \sum_i \left( n_i \sum_{j=1}^p t_j (F_i(x_j) - F(x_j))^2 \right)$$

where  $t_j$  is the number of ties at the  $j$ th distinct value and  $p$  is the number of distinct values. The asymptotic value is computed as

$$CM_a = CM \times n$$

PROC NPAR1WAY displays the contribution of each class level to the sum  $CM_a$ .

**Kuiper Test**

For data with two class levels, PROC NPAR1WAY computes the Kuiper statistic, its scaled value for the asymptotic distribution, and the asymptotic  $p$ -value. The Kuiper statistic is computed as

$$K = \max_j (F_1(x_j) - F_2(x_j)) - \min_j (F_1(x_j) - F_2(x_j)) \quad \text{where } j = 1, 2, \dots, n$$

The asymptotic value is

$$K_a = K \sqrt{n_1 n_2 / n}$$

PROC NPAR1WAY displays the value of  $(\max_j |F_1(x_j) - F_2(x_j)|)$  for each class level.

The  $p$ -value for the Kuiper test is the probability of observing a larger value of  $K_a$  under the null hypothesis of no difference between the two classes. PROC NPAR1WAY computes this  $p$ -value according to Owen (1962, p. 441).

**Exact Tests**

PROC NPAR1WAY provides exact  $p$ -values for tests for location and scale differences based on the following scores: Wilcoxon, median, van der Waerden (normal), Savage, Siegel-Tukey, Ansari-Bradley, Klotz, Mood, and Conover. Additionally, PROC NPAR1WAY provides exact  $p$ -values for tests that use the raw data as scores. Exact tests are available for two-sample and multisample data. When the data are classified into two samples, tests are based on simple linear rank statistics. When the data are classified into more than two samples, tests are based on one-way ANOVA statistics.

Exact tests can be useful in situations where the asymptotic assumptions are not met and the asymptotic  $p$ -values are not close approximations for the true  $p$ -values. Standard asymptotic methods involve the assumption that the test statistic follows a particular distribution when the sample size is sufficiently large. When the sample size is not large, asymptotic results might not be valid, with the asymptotic  $p$ -values differing perhaps substantially from the exact  $p$ -values. Asymptotic results might also be unreliable when the distribution of the data is sparse, skewed, or heavily tied. See Agresti (2007) and Bishop, Fienberg, and Holland (1975). Exact computations are based on the statistical theory of exact conditional inference for contingency tables, reviewed by Agresti (1992).

In addition to computation of exact  $p$ -values, PROC NPAR1WAY provides the option of estimating exact  $p$ -values by Monte Carlo simulation. This can be useful for problems that are so large that exact computations require a great amount of time and memory, but for which asymptotic approximations might not be sufficient.

The following sections summarize the exact computational algorithms, define the exact  $p$ -values that PROC NPAR1WAY computes, discuss the computational resource requirements, and describe the Monte Carlo estimation option.

**Computational Algorithms**

PROC NPAR1WAY computes exact  $p$ -values by using the network algorithm developed by Mehta and Patel (1983). This algorithm provides a substantial advantage over direct enumeration, which can be very time-consuming and feasible only for small problems. See Agresti (1992) for a review of algorithms for computation of exact  $p$ -values, and see Mehta, Patel, and Tsiatis (1984) and Mehta, Patel, and Senchaudhuri (1991) for information about the performance of the network algorithm.

PROC NPAR1WAY constructs a contingency table from the input data, with rows formed by the levels of the classification variable and columns formed by the response variable values. The reference set for a given contingency table is the set of all contingency tables with the observed marginal row and column sums. Corresponding to this reference set, the network algorithm forms a directed acyclic network consisting of nodes in a number of stages. A path through the network corresponds to a distinct table in the reference set. The distances between nodes are defined so that the total distance of a path through the network is the corresponding value of the test statistic. At each node, the algorithm computes the shortest and longest path distances for all the paths that pass through that node. For the two-sample linear rank statistics, which can be expressed as linear combinations of cell frequencies multiplied by increasing row and column scores, PROC NPAR1WAY computes shortest and longest path distances by using the algorithm given by Agresti, Mehta, and Patel (1990). For the multisample one-way test statistics, PROC NPAR1WAY computes an upper bound for the longest path and a lower bound for the shortest path by following the approach of Valz and Thompson (1994).

The longest and shortest path distances (bounds) for a node are compared to the value of the test statistic to determine whether all paths through the node contribute to the  $p$ -value, none of the paths through the node contribute to the  $p$ -value, or neither of these situations occurs. If all paths through the node contribute, the  $p$ -value is incremented accordingly, and these paths are eliminated from further analysis. If no paths contribute, these paths are eliminated from the analysis. Otherwise, the algorithm continues, still processing this node and the associated paths. The algorithm finishes when all nodes have been accounted for.

In applying the network algorithm, PROC NPAR1WAY uses full numerical precision to represent all statistics, row and column scores, and other quantities involved in the computations. Although it is possible to use rounding to improve the speed and memory requirements of the algorithm, PROC NPAR1WAY does not do this because it can result in reduced accuracy of the  $p$ -values.

### Definition of $p$ -Values

For two-sample linear rank tests, PROC NPAR1WAY computes exact one-sided and two-sided  $p$ -values for each test that is specified in the EXACT statement. For the one-sided test, PROC NPAR1WAY displays the right-sided  $p$ -value when the observed value of the test statistic is greater than its expected value. The right-sided  $p$ -value is the sum of probabilities for those tables having a test statistic greater than or equal to the observed test statistic. Otherwise, when the test statistic is less than or equal to its expected value, PROC NPAR1WAY displays the left-sided  $p$ -value. The left-sided  $p$ -value is the sum of probabilities for those tables having a test statistic less than or equal to the one observed. The one-sided  $p$ -value  $P_1$  can be expressed as

$$P_1(t) = \begin{cases} \text{Prob}(\text{Test Statistic} \geq t) & \text{if } t > E_0(T) \\ \text{Prob}(\text{Test Statistic} \leq t) & \text{if } t \leq E_0(T) \end{cases}$$

where  $t$  is the observed value of the test statistic and  $E_0(T)$  is the expected value of the test statistic under the null hypothesis. PROC NPAR1WAY computes the two-sided  $p$ -value as the sum of the one-sided  $p$ -value and the corresponding area in the opposite tail of the distribution of the statistic, equidistant from the expected value. The two-sided  $p$ -value  $P_2$  can be expressed as

$$P_2(t) = \text{Prob}(|\text{Test Statistic} - E_0(T)| \geq |t - E_0(T)|)$$

For multisample data, the tests are based on one-way ANOVA statistics. For a test of this form, large values of the test statistic indicate a departure from the null hypothesis; the test is inherently two-sided. The exact

$p$ -value is the sum of probabilities for those tables having a test statistic greater than or equal to the value of the observed test statistic.

If you specify the **POINT** option in the EXACT statement, PROC NPAR1WAY also displays exact point probabilities for the test statistics. The exact point probability is the exact probability that the test statistic equals the observed value.

### **Computational Resources**

PROC NPAR1WAY uses relatively fast and efficient algorithms for exact computations. These algorithms, together with improvements in computer power, now make it feasible to perform exact computations for data sets where previously only asymptotic methods could be applied. Nevertheless, there are still large problems that might require a prohibitive amount of time and memory for exact computations, depending on the speed and memory available on your computer. For large problems, consider whether exact methods are really needed or whether asymptotic methods might give results quite close to the exact results while requiring much less computer time and memory. When asymptotic methods might not be sufficient for such large problems, consider using Monte Carlo estimation of exact  $p$ -values, as described in the section “**Monte Carlo Estimation**” on page 5481.

A formula does not exist that can predict in advance how much time and memory are needed to compute an exact  $p$ -value for a certain problem. The time and memory required depend on several factors, including which test is being performed, the total sample size, the number of rows and columns, and the specific arrangement of the observations into table cells. Generally, larger problems (in terms of total sample size, number of rows, and number of columns) tend to require more time and memory. Additionally, for a fixed total sample size, time and memory requirements tend to increase as the number of rows and columns increase, since this corresponds to an increase in the number of tables in the reference set. Also for a fixed sample size, time and memory requirements increase as the marginal row and column totals become more homogeneous. See Agresti, Mehta, and Patel (1990) and Gail and Mantel (1977) for details.

At any time while PROC NPAR1WAY is computing exact  $p$ -values, you can terminate the computations by pressing the system interrupt key sequence (see the *SAS Companion* for your system) and choosing to stop computations. After you terminate exact computations, PROC NPAR1WAY completes all other remaining tasks. The procedure produces the requested output and reports missing values for any exact  $p$ -values not computed by the time of termination.

You can also use the **MAXTIME=** option in the EXACT statement to limit the amount of time PROC NPAR1WAY uses for exact computations. You specify a **MAXTIME=** value that is the maximum amount of time (in seconds) that PROC NPAR1WAY can use to compute an exact  $p$ -value. If PROC NPAR1WAY does not finish computing the exact  $p$ -value within that time, it terminates the computation and completes all other remaining tasks.

### **Monte Carlo Estimation**

If you specify the **MC** option in the EXACT statement, PROC NPAR1WAY computes Monte Carlo estimates of the exact  $p$ -values instead of directly computing the exact  $p$ -values. Monte Carlo estimation can be useful for large problems that require a great amount of time and memory for exact computations but for which asymptotic approximations might not be sufficient. To describe the precision of each Monte Carlo estimate, PROC NPAR1WAY provides the asymptotic standard error and  $100(1 - \alpha)\%$  confidence limits. The confidence level  $\alpha$  is determined by the **ALPHA=** option in the EXACT statement, which, by default, equals 0.01 and produces 99% confidence limits. The **N=** option in the EXACT statement specifies the

number of samples PROC NPAR1WAY uses for Monte Carlo estimation; the default is 10,000 samples. You can specify a larger value for  $n$  to improve the precision of the Monte Carlo estimates. Because larger values of  $n$  generate more samples, the computation time increases. Or you can specify a smaller value of  $n$  to reduce the computation time.

To compute a Monte Carlo estimate of an exact  $p$ -value, PROC NPAR1WAY generates a random sample of tables with the same total sample size, row totals, and column totals as the observed table. PROC NPAR1WAY uses the algorithm of Agresti, Wackerly, and Boyett (1979), which generates tables in proportion to their hypergeometric probabilities conditional on the marginal frequencies. For each sample table, PROC NPAR1WAY computes the value of the test statistic and compares it to the value for the observed table. When estimating a right-sided  $p$ -value, PROC NPAR1WAY counts all sample tables for which the test statistic is greater than or equal to the observed test statistic. Then the  $p$ -value estimate equals the number of these tables divided by the total number of tables sampled, which can be written as

$$\begin{aligned}\hat{P}_{MC} &= M / N \\ M &= \text{number of samples with (Test Statistic} \geq t) \\ N &= \text{total number of samples} \\ t &= \text{observed Test Statistic}\end{aligned}$$

PROC NPAR1WAY computes left-sided and two-sided  $p$ -value estimates in a similar manner. For left-sided  $p$ -values, PROC NPAR1WAY evaluates whether the test statistic for each sampled table is less than or equal to the observed test statistic. For two-sided  $p$ -values, PROC NPAR1WAY examines the sample test statistics according to the expression for  $P_2(t)$  given in the section “[Definition of  \$p\$ -Values](#)” on page 5480.

The variable  $M$  is a binomial variable with  $N$  trials and success probability  $p$ . It follows that the asymptotic standard error of the Monte Carlo estimate is

$$se(\hat{P}_{MC}) = \sqrt{\hat{P}_{MC} (1 - \hat{P}_{MC}) / (N - 1)}$$

PROC NPAR1WAY constructs asymptotic confidence limits for the  $p$ -values according to

$$\hat{P}_{MC} \pm (z_{\alpha/2} \times se(\hat{P}_{MC}))$$

where  $z_{\alpha/2}$  is the  $100(1 - \alpha/2)$  percentile of the standard normal distribution, and the confidence level  $\alpha$  is determined by the ALPHA= option in the EXACT statement.

When the Monte Carlo estimate  $\hat{P}_{MC}$  equals 0, PROC NPAR1WAY computes confidence limits for the  $p$ -value as

$$(0, 1 - \alpha^{(1/N)})$$

When the Monte Carlo estimate  $\hat{P}_{MC}$  equals 1, PROC NPAR1WAY computes the confidence limits as

$$(\alpha^{(1/N)}, 1)$$

## Contents of the Output Data Set

The **OUTPUT** statement creates a SAS data set that contains statistics that PROC NPAR1WAY computes. You identify which statistics to store in the output data set by specifying *output-options* in the OUTPUT statement. See the description of the **OUTPUT** statement for more information.

The output data set contains one observation for each analysis variable for each **BY** group. (You can specify the analysis variables in the **VAR** statement.) The OUTPUT data set includes the following variables:

- BY variables, if you use a **BY** statement
- **\_VAR\_**, which identifies the analysis variable
- variables that contain the statistics

When you specify an *output-option* in the OUTPUT statement, the output data set contains the test statistic and associated values from the analysis that you specify. The associated values might include standardized statistics, one- and two-sided *p*-values, exact *p*-values, degrees of freedom, and confidence limits. If you request an exact test for the specified analysis by using the **EXACT** statement, the output data set includes the exact *p*-values. The statistics that are included also depend on the classification of the data. Some statistics are available only for two-sample data (where the **CLASS** variable groups the data into two classes); other statistics are available only for multisample data.

Table 65.5 lists variable names and descriptions for the statistics that are available in the output data set.

Monte Carlo estimates of exact *p*-values are not available in this output data set. You can store Monte Carlo estimates in a SAS data set by using the Output Delivery System (ODS). ODS can create a SAS data set from any table that PROC NPAR1WAY produces. For more information, see the section “ODS Table Names” on page 5493 and Chapter 20, “Using the Output Delivery System.”

**Table 65.5** Output Data Set Variable Names and Descriptions

| Output Option   | Output Variables                                      | Variable Descriptions                                      |
|-----------------|-------------------------------------------------------|------------------------------------------------------------|
| AB              | <b>_AB_</b>                                           | * Two-sample Ansari-Bradley statistic                      |
|                 | <b>Z_AB</b>                                           | * Ansari-Bradley statistic, standardized                   |
|                 | <b>PL_AB</b>                                          | * <i>p</i> -value (left-sided), Ansari-Bradley test        |
|                 | <b>PR_AB</b>                                          | * <i>p</i> -value (right-sided), Ansari-Bradley test       |
|                 | <b>P2_AB</b>                                          | * <i>p</i> -value (two-sided), Ansari-Bradley test         |
|                 | <b>XPL_AB</b>                                         | * Exact <i>p</i> -value (left-sided), Ansari-Bradley test  |
|                 | <b>XPR_AB</b>                                         | * Exact <i>p</i> -value (right-sided), Ansari-Bradley test |
|                 | <b>XPT_AB</b>                                         | * Exact point probability, Ansari-Bradley test             |
|                 | <b>XP2_AB</b>                                         | * Exact <i>p</i> -value (two-sided), Ansari-Bradley test   |
|                 | <b>_CHAB_</b>                                         | Ansari-Bradley chi-square                                  |
|                 | <b>DF_CHAB</b>                                        | Degrees of freedom, Ansari-Bradley chi-square              |
|                 | <b>P_CHAB</b>                                         | <i>p</i> -value, Ansari-Bradley chi-square test            |
|                 | <b>XP_CHAB</b>                                        | ** Exact <i>p</i> -value, Ansari-Bradley chi-square test   |
| <b>XPT_CHAB</b> | ** Exact point probability, Ansari-Bradley chi-square |                                                            |

Table 65.5 continued

| Output Option | Output Variables | Variable Descriptions                              |
|---------------|------------------|----------------------------------------------------|
| ANOVA         | _MSA_            | ANOVA effect mean square, among MS                 |
|               | _MSE_            | ANOVA error mean square, within MS                 |
|               | _F_              | $F$ statistic for ANOVA                            |
|               | P_F              | $p$ -value, $F$ statistic for ANOVA                |
| CONOVER       | _CON_            | * Two-sample Conover statistic                     |
|               | Z_CON            | * Conover statistic, standardized                  |
|               | PL_CON           | * $p$ -value (left-sided), Conover test            |
|               | PR_CON           | * $p$ -value (right-sided), Conover test           |
|               | P2_CON           | * $p$ -value (two-sided), Conover test             |
|               | XPL_CON          | * Exact $p$ -value (left-sided), Conover test      |
|               | XPR_CON          | * Exact $p$ -value (right-sided), Conover test     |
|               | XPT_CON          | * Exact point probability, Conover test            |
|               | XP2_CON          | * Exact $p$ -value (two-sided), Conover test       |
|               | _CHCON_          | Conover chi-square                                 |
|               | DF_CHCON         | Degrees of freedom, Conover chi-square             |
|               | P_CHCON          | $p$ -value, Conover chi-square test                |
|               | XP_CHCON         | ** Exact $p$ -value, Conover chi-square test       |
|               | XPT_CHCO         | ** Exact point probability, Conover chi-square     |
|               | EDF              | _KS_                                               |
| _KSA_         |                  | Kolmogorov-Smirnov statistic (asymptotic)          |
| _Dp_          |                  | * Two-sample Kolmogorov-Smirnov $D+$               |
| P_Dp          |                  | * $p$ -value, $D+$                                 |
| _Dm_          |                  | * Two-sample Kolmogorov-Smirnov $D-$               |
| P_Dm          |                  | * $p$ -value, $D-$                                 |
| _D_           |                  | * Two-sample Kolmogorov-Smirnov statistic $D$      |
| P_KSA         |                  | * $p$ -value, $D$                                  |
| XP_Dp         |                  | * Exact $p$ -value, $D+$                           |
| XPT_Dp        |                  | * Exact point probability, $D+$                    |
| XP_Dm         |                  | * Exact $p$ -value, $D-$                           |
| XPT_Dm        |                  | * Exact point probability, $D-$                    |
| XP_D          |                  | * Exact $p$ -value, $D$                            |
| XPT_D         |                  | * Exact point probability, $D$                     |
| _CM_          |                  | Cramér-von Mises statistic                         |
| _CMA_         |                  | Cramér-von Mises statistic (asymptotic)            |
| _K_           |                  | * Kuiper two-sample statistic                      |
| _KA_          |                  | * Kuiper two-sample statistic (asymptotic)         |
| P_KA          |                  | * $p$ -value, two-sample Kuiper test               |
| FP            |                  | _FP_                                               |
|               | PL_FP            | * $p$ -value (left-sided), Fligner-Policello test  |
|               | PR_FP            | * $p$ -value (right-sided), Fligner-Policello test |
|               | P2_FP            | * $p$ -value (two-sided), Fligner-Policello test   |



Table 65.5 continued

| Output Option | Output Variables | Variable Descriptions                          |
|---------------|------------------|------------------------------------------------|
| HL            | _HL_             | * Hodges-Lehmann estimate, location shift      |
|               | L_HL             | * Lower confidence limit, Hodges-Lehmann       |
|               | U_HL             | * Upper confidence limit, Hodges-Lehmann       |
|               | M_HL             | * Confidence limit midpoint, Hodges-Lehmann    |
|               | E_HL             | * ASE of Hodges-Lehmann estimate               |
|               | XL_HL            | * Exact lower confidence limit, Hodges-Lehmann |
|               | XU_HL            | * Exact upper confidence limit, Hodges-Lehmann |
|               | XM_HL            | * Exact confidence limit midpoint              |
| KLOTZ         | _KLOTZ_          | * Two-sample Klotz statistic                   |
|               | Z_K              | * Klotz statistic, standardized                |
|               | PL_K             | * $p$ -value (left-sided), Klotz test          |
|               | PR_K             | * $p$ -value (right-sided), Klotz test         |
|               | P2_K             | * $p$ -value (two-sided), Klotz test           |
|               | XPL_K            | * Exact $p$ -value (left-sided), Klotz test    |
|               | XPR_K            | * Exact $p$ -value (right-sided), Klotz test   |
|               | XPT_K            | * Exact point probability, Klotz test          |
|               | XP2_K            | * Exact $p$ -value (two-sided), Klotz test     |
|               | _CHK_            | Klotz chi-square                               |
|               | DF_CHK           | Degrees of freedom, Klotz chi-square           |
|               | P_CHK            | $p$ -value, Klotz chi-square test              |
|               | XP_CHK           | ** Exact $p$ -value, Klotz chi-square test     |
|               | XPT_CHK          | ** Exact point probability, Klotz chi-square   |
| MEDIAN        | _MED_            | * Two-sample median statistic                  |
|               | Z_MED            | * Median statistic, standardized               |
|               | PL_MED           | * $p$ -value (left-sided), median test         |
|               | PR_MED           | * $p$ -value (right-sided), median test        |
|               | P2_MED           | * $p$ -value (two-sided), median test          |
|               | XPL_MED          | * Exact $p$ -value (left-sided), median test   |
|               | XPR_MED          | * Exact $p$ -value (right-sided), median test  |
|               | XPT_MED          | * Exact point probability, median test         |
|               | XP2_MED          | * Exact $p$ -value (two-sided), median test    |
|               | _CHMED_          | Median chi-square (Brown-Mood test)            |
|               | DF_CHMED         | Degrees of freedom, median chi-square          |
|               | P_CHMED          | $p$ -value, median chi-square test             |
|               | XP_CHMED         | ** Exact $p$ -value, median chi-square test    |
|               | XPT_CHME         | ** Exact point probability, median chi-square  |



Table 65.5 continued

| Output Option | Output Variables | Variable Descriptions                         |                                        |
|---------------|------------------|-----------------------------------------------|----------------------------------------|
| MOOD          | _MOOD_           | * Two-sample Mood statistic                   |                                        |
|               | Z_MOOD           | * Mood statistic, standardized                |                                        |
|               | PL_MOOD          | * $p$ -value (left-sided), Mood test          |                                        |
|               | PR_MOOD          | * $p$ -value (right-sided), Mood test         |                                        |
|               | P2_MOOD          | * $p$ -value (two-sided), Mood test           |                                        |
|               | XPL_MOOD         | * Exact $p$ -value (left-sided), Mood test    |                                        |
|               | XPR_MOOD         | * Exact $p$ -value (right-sided), Mood test   |                                        |
|               | XPT_MOOD         | * Exact point probability, Mood test          |                                        |
|               | XP2_MOOD         | * Exact $p$ -value (two-sided), Mood test     |                                        |
|               | _CHMOOD_         | Mood chi-square                               |                                        |
|               | DF_CHMOO         | Degrees of Freedom, Mood chi-square           |                                        |
|               | P_CHMOOD         | $p$ -value, Mood chi-square test              |                                        |
|               | XP_CHMOO         | ** Exact $p$ -value, Mood chi-square test     |                                        |
|               | XPT_CHMO         | ** Exact point probability, Mood chi-square   |                                        |
|               | SAVAGE           | _SAV_                                         | * Two-sample Savage statistic          |
|               |                  | Z_SAV                                         | * Savage statistic, standardized       |
|               |                  | PL_SAV                                        | * $p$ -value (left-sided), Savage test |
| PR_SAV        |                  | * $p$ -value (right-sided), Savage test       |                                        |
| P2_SAV        |                  | * $p$ -value (two-sided), Savage test         |                                        |
| XPL_SAV       |                  | * Exact $p$ -value (left-sided), Savage test  |                                        |
| XPR_SAV       |                  | * Exact $p$ -value (right-sided), Savage test |                                        |
| XPT_SAV       |                  | * Exact point probability, Savage test        |                                        |
| XP2_SAV       |                  | * Exact $p$ -value (two-sided), Savage test   |                                        |
| _CHSAV_       |                  | Savage chi-square                             |                                        |
| DF_CHSAV      |                  | Degrees of freedom, Savage chi-square         |                                        |
| P_CHSAV       |                  | $p$ -value, Savage chi-square test            |                                        |
| XP_CHSAV      |                  | ** Exact $p$ -value, Savage chi-square test   |                                        |
| XPT_CHSA      |                  | ** Exact point probability, Savage chi-square |                                        |

Table 65.5 continued

| Output Option | Output Variables | Variable Descriptions                                       |
|---------------|------------------|-------------------------------------------------------------|
| SCORES=DATA   | _DATA_           | * Two-sample data scores statistic                          |
|               | Z_DATA           | * Data scores statistic, standardized                       |
|               | PL_DATA          | * <i>p</i> -value (left-sided), data scores test            |
|               | PR_DATA          | * <i>p</i> -value (right-sided), data scores test           |
|               | P2_DATA          | * <i>p</i> -value (two-sided), data scores test             |
|               | XPL_DATA         | * Exact <i>p</i> -value (left-sided), data scores test      |
|               | XPR_DATA         | * Exact <i>p</i> -value (right-sided), data scores test     |
|               | XPT_DATA         | * Exact point probability, data scores test                 |
|               | XP2_DATA         | * Exact <i>p</i> -value (two-sided), data scores test       |
|               | _CHDATA_         | Data scores chi-square                                      |
|               | DF_CHDAT         | Degrees of freedom, data scores chi-square                  |
|               | P_CHDATA         | <i>p</i> -value, data scores chi-square test                |
|               | XP_CHDAT         | ** Exact <i>p</i> -value, data scores chi-square test       |
|               | XPT_CHDA         | ** Exact point probability, data scores chi-square          |
|               | ST               | _ST_                                                        |
| Z_ST          |                  | * Siegel-Tukey statistic, standardized                      |
| PL_ST         |                  | * <i>p</i> -value (left-sided), Siegel-Tukey test           |
| PR_ST         |                  | * <i>p</i> -value (right-sided), Siegel-Tukey test          |
| P2_ST         |                  | * <i>p</i> -value (two-sided), Siegel-Tukey test            |
| XPL_ST        |                  | * Exact <i>p</i> -value (left-sided), Siegel-Tukey test     |
| XPR_ST        |                  | * Exact <i>p</i> -value (right-sided), Siegel-Tukey test    |
| XPT_ST        |                  | * Exact point probability, Siegel-Tukey test                |
| XP2_ST        |                  | * Exact <i>p</i> -value (two-sided), Siegel-Tukey test      |
| _CHST_        |                  | Siegel-Tukey chi-square                                     |
| DF_CHST       |                  | Degrees of freedom, Siegel-Tukey chi-square                 |
| P_CHST        |                  | <i>p</i> -value, Siegel-Tukey chi-square test               |
| XP_CHST       |                  | ** Exact <i>p</i> -value, Siegel-Tukey chi-square test      |
| XPT_CHST      |                  | ** Exact point probability, Siegel-Tukey chi-square         |
| VW   NORMAL   |                  | _VW_                                                        |
|               | Z_VW             | * Van der Waerden statistic, standardized                   |
|               | PL_VW            | * <i>p</i> -value (left-sided), Van der Waerden test        |
|               | PR_VW            | * <i>p</i> -value (right-sided), Van der Waerden test       |
|               | P2_VW            | * <i>p</i> -value (two-sided), Van der Waerden test         |
|               | XPL_VW           | * Exact <i>p</i> -value (left-sided), Van der Waerden test  |
|               | XPR_VW           | * Exact <i>p</i> -value (right-sided), Van der Waerden test |
|               | XPT_VW           | * Exact point probability, Van der Waerden test             |
|               | XP2_VW           | * Exact <i>p</i> -value (two-sided), Van der Waerden test   |
|               | _CHVW_           | Van der Waerden chi-square                                  |
|               | DF_CHVW          | Degrees of freedom, Van der Waerden chi-square              |
|               | P_CHVW           | <i>p</i> -value, Van der Waerden chi-square test            |
|               | XP_CHVW          | ** Exact <i>p</i> -value, Van der Waerden chi-square test   |
|               | XPT_CHVW         | ** Exact point probability, Van der Waerden chi-square      |

Table 65.5 continued

| Output Option | Output Variables                                | Variable Descriptions                                  |
|---------------|-------------------------------------------------|--------------------------------------------------------|
| WILCOXON      | _WIL_                                           | * Two-sample Wilcoxon statistic                        |
|               | Z_WIL                                           | * Wilcoxon statistic, standardized                     |
|               | PL_WIL                                          | * $p$ -value (left-sided), Wilcoxon test               |
|               | PR_WIL                                          | * $p$ -value (right-sided), Wilcoxon test              |
|               | P2_WIL                                          | * $p$ -value (two-sided), Wilcoxon test                |
|               | PTL_WIL                                         | * $p$ -value (left-sided), Wilcoxon $t$ approximation  |
|               | PTR_WIL                                         | * $p$ -value (right-sided), Wilcoxon $t$ approximation |
|               | PT2_WIL                                         | * $p$ -value (two-sided), Wilcoxon $t$ approximation   |
|               | XPL_WIL                                         | * Exact $p$ -value (left-sided), Wilcoxon test         |
|               | XPR_WIL                                         | * Exact $p$ -value (right-sided), Wilcoxon test        |
|               | XPT_WIL                                         | * Exact point probability, Wilcoxon test               |
|               | XP2_WIL                                         | * Exact $p$ -value (two-sided), Wilcoxon test          |
|               | _KW_                                            | Kruskal-Wallis statistic                               |
|               | DF_KW                                           | Degrees of freedom, Kruskal-Wallis test                |
|               | P_KW                                            | $p$ -value, Kruskal-Wallis test                        |
|               | XP_KW                                           | ** Exact $p$ -value, Kruskal-Wallis test               |
| XPT_KW        | ** Exact point probability, Kruskal-Wallis test |                                                        |

\*Statistic included only for two-sample cases.

\*\*Statistic included only for multisample cases.

## Displayed Output

If you specify the ANOVA option, PROC NPAR1WAY displays a “Class Means” table and an “Analysis of Variance” table for each response variable. The “Class Means” table includes the following information for each CLASS variable value (level):

- N, which is the number of observations
- Mean of the response variable

The “Analysis of Variance” table includes the following information for each Source of variation (Among classes and Within classes):

- DF, which is the degrees of freedom associated with the source
- Sum of Squares
- Mean Square, which is the sum of squares divided by the degrees of freedom

The “Analysis of Variance” table also includes the following:

- F Value for testing the hypothesis that the class means are equal, which is computed by dividing the Mean Square (Among) by the Mean Square (Within)
- $Pr > F$ , which is the significance probability corresponding to the F Value

For each score type that you specify, PROC NPAR1WAY displays a “Class Scores” table. The available score types include Wilcoxon, median, Van der Waerden (normal), Savage, Siegel-Tukey, Ansari-Bradley, Klotz, Mood, Conover, and raw data scores. PROC NPAR1WAY computes the scores for the response variable values and classifies the scored observations according to the CLASS variable values. The “Class Scores” table includes the following information for each CLASS variable level:

- N, which is the number of observations
- Sum of Scores
- Expected Under H0, which is the expected sum of scores under the null hypothesis of no difference among classes
- Std Dev Under H0, which is the standard deviation under the null hypothesis
- Mean Score

When there are two levels of the CLASS variable, PROC NPAR1WAY displays a “Two-Sample Test” table for each analysis of scores. The “Two-Sample Test” table includes the following information:

- Statistic, which is the sum of scores for the class with the smaller sample size
- Z, which is the standardized test statistic and has an asymptotic standard normal distribution under the null hypothesis
- One-Sided  $Pr < Z$  or One-Sided  $Pr > Z$ , which is the asymptotic one-sided  $p$ -value. This is displayed as  $Pr < Z$  or  $Pr > Z$ , depending on whether Z is  $\leq 0$  or  $> 0$ .
- Two-Sided  $Pr > |Z|$ , which is the asymptotic two-sided  $p$ -value

For Wilcoxon scores, the “Two-Sample Test” table also includes a  $t$  Approximation for the Wilcoxon two-sample test.

If you request an exact test by specifying the score type in the EXACT statement, the “Two-Sample Test” table also includes the following exact  $p$ -values:

- One-Sided  $Pr \leq S$  or One-Sided  $Pr \geq S$ , which is the exact one-sided  $p$ -value. This is displayed as  $Pr \leq S$  or  $Pr \geq S$ , depending on whether  $S \leq \text{Mean}$  or  $S > \text{Mean}$ , where S is the test statistic and Mean is its expected value under the null hypothesis.

- Point  $Pr = S$ , which is the point probability. This is displayed if you specify the **POINT** option in the **EXACT** statement.
- Two-Sided  $Pr \geq |S - \text{Mean}|$ , which is the exact two-sided  $p$ -value

If you request Monte Carlo estimates for a two-sample exact test by specifying the **MC** option in the **EXACT** statement, PROC NPAR1WAY displays the “Monte Carlo Estimates for the Exact Test” table, which includes the following information:

- Estimate of One-Sided  $Pr \leq S$  or One-Sided  $Pr \geq S$ , which is the exact one-sided  $p$ -value, together with its Lower and Upper Confidence Limits
- Estimate of Two-Sided  $Pr \geq |S - \text{Mean}|$ , which is the exact two-sided  $p$ -value, together with its Lower and Upper Confidence Limits
- Number of Samples used to compute the Monte Carlo estimates
- Initial Seed used to compute the Monte Carlo estimates

For both two-sample and multisample data, PROC NPAR1WAY displays a “One-Way Analysis” table, which includes the following information:

- Chi-Square, which is the one-way ANOVA statistic for testing the null hypothesis of no difference among classes
- DF, which is the degrees of freedom
- $Pr > \text{Chi-Square}$ , which is the asymptotic  $p$ -value

For multisample data, if you request an exact test by specifying the score type in the **EXACT** statement, the “One-Way Analysis” table also displays the exact  $p$ -value as follows:

- Exact  $Pr \geq \text{Chi-Square}$
- Exact  $Pr = \text{Chi-Square}$ , which is the point probability. This is displayed if you specify the **POINT** option in the **EXACT** statement.

For multisample data, if you specify the **MC** option in the **EXACT** statement, PROC NPAR1WAY displays the following information in the “Monte Carlo Estimate for the Exact Test” table:

- Estimate of Exact  $Pr \geq \text{Chi-Square}$ , together with its Lower and Upper Confidence Limits
- Number of Samples used to compute the Monte Carlo estimate
- Initial Seed used to compute the Monte Carlo estimate

If you specify the **HL** option for two-sample data, PROC NPAR1WAY produces a “Hodges-Lehmann Estimation” table, which includes the following information:

- Location Shift estimate
- Confidence Limits for the Location Shift
- Confidence Interval Midpoint
- Asymptotic Standard Error estimate, which is based on the confidence interval

If you request exact Hodges-Lehmann confidence limits by specifying the HL option in the **EXACT** statement, the “Hodges-Lehmann Estimation” table also includes Exact Confidence Limits and the exact Interval Midpoint.

If you specify the **FP** option for two-sample data, PROC NPAR1WAY produces the “Fligner-Policello Placements” table and the “Fligner-Policello Test” table. The “Fligner-Policello Placements” table includes the following information for each **CLASS** variable level:

- N, which is the number of observations
- Sum, which is the sum of the placements
- Mean, which is the average placement
- Std Dev, which is the standard deviation of the placements

The “Fligner-Policello Test” table includes the following information:

- Difference, which is the difference in placement sums between the two **CLASS** levels (samples)
- Statistic ( $Z$ ), which is the standardized test statistic and has an asymptotic standard normal distribution under the null hypothesis
- One-Sided  $\Pr < Z$  or One-Sided  $\Pr > Z$ , which is the one-sided  $p$ -value. This is displayed as  $\Pr < Z$  or  $\Pr > Z$ , depending on whether  $Z$  is  $\leq 0$  or  $> 0$ .
- Two-Sided  $\Pr > |Z|$ , which is the two-sided  $p$ -value

If you specify the **DSCF** option for multisample data, PROC NPAR1WAY produces the “Pairwise Two-Sided Multiple Comparison Analysis” table, which includes the following information for each two-sample comparison:

- Comparison, which identifies the two **CLASS** levels that are compared
- Wilcoxon  $Z$ , which is the standardized two-sample Wilcoxon statistic
- DSCF Value, which is the Dwass, Steel, Critchlow-Fligner statistic
- $\Pr > \text{DSCF}$ , which is the two-sided  $p$ -value

If you specify the **EDF** option, PROC NPAR1WAY produces tables for the Kolmogorov-Smirnov test, the Cramér-von Mises test, and for two-sample data only, the Kuiper test.

The “Kolmogorov-Smirnov Test” table includes the following information for each **CLASS** variable level:

- N, which is the number of observations
- EDF at Maximum, which is the value of the class EDF (empirical distribution function) at its maximum deviation from the pooled EDF
- Deviation from Mean at Maximum, which is the value of  $\sqrt{n_i} \sqrt{F_i - F}$  at its maximum, where  $n_i$  is the class sample size,  $F_i$  is the class EDF, and  $F$  is the pooled EDF

The “Kolmogorov-Smirnov Test” table displays the following statistics:

- KS, which is the Kolmogorov-Smirnov statistic
- KSa, which is the asymptotic Kolmogorov-Smirnov statistic,  $KSa = \sqrt{n}$  KS

For two-sample data, the “Kolmogorov-Smirnov Test” table also displays the following statistics:

- Pr > KSa, which is the asymptotic  $p$ -value for KSa and equals Pr > D
- D, which is the two-sample Kolmogorov-Smirnov statistic,  $\max_j |F_1(x_j) - F_2(x_j)|$

If you specify the **D** option for two-sample data, PROC NPAR1WAY displays the following one-sided Kolmogorov-Smirnov statistics and their asymptotic  $p$ -values in the “Kolmogorov-Smirnov Two-Sample Test” table:

- D+, which is  $\max_j (F_1(x_j) - F_2(x_j))$
- Pr > D+
- D-, which is  $\max_j (F_2(x_j) - F_1(x_j))$
- Pr > D-

For two-sample data, if you request an exact Kolmogorov-Smirnov test by specifying the **KS** option in the **EXACT** statement, PROC NPAR1WAY displays the following exact  $p$ -values in the “Kolmogorov-Smirnov Two-Sample Test” table:

- Exact Pr  $\geq$  D
- Exact Pr  $\geq$  D+
- Exact Pr  $\geq$  D-
- Exact Point Pr = D, Exact Point Pr = D+, and Exact Point Pr = D-, if you specify the **POINT** option in the **EXACT** statement

If you request Monte Carlo estimates for the two-sample exact Kolmogorov-Smirnov test, PROC NPAR1WAY displays the following information in the “Kolmogorov-Smirnov Two-Sample Test” table:

- Estimate of Exact  $\Pr \geq D$ , together with its Lower and Upper Confidence Limits
- Estimate of Exact  $\Pr \geq D+$ , together with its Lower and Upper Confidence Limits
- Estimate of Exact  $\Pr \geq D-$ , together with its Lower and Upper Confidence Limits
- Number of Samples used to compute the Monte Carlo estimates
- Initial Seed used to compute the Monte Carlo estimates

The “Cramér–von Mises Test” table includes the following information for each CLASS variable level:

- N, which is the number of observations
- Summed Deviation from Mean, which is  $(n_i/n) \sum_{j=1}^p t_j (F_i(x_j) - F(x_j))^2$

The “Cramér–von Mises Statistics” table displays the following statistics:

- CM, which is the Cramér–von Mises statistic
- CMa, which is the asymptotic Cramér–von Mises statistic,  $CMa = n CM$

For two-sample data, PROC NPAR1WAY displays the “Kuiper Test” table, which includes the following information for each CLASS variable level:

- N, which is the number of observations
- Deviation from Mean, which is  $\max_j |F_1(x_j) - F_2(x_j)|$

The “Kuiper Two-Sample Statistics” table displays the following statistics:

- K, which is the Kuiper two-sample test statistic
- Ka, which is the asymptotic Kuiper two-sample test statistic,  $Ka = K \sqrt{n_1 n_2 / n}$
- $\Pr > Ka$

---

## ODS Table Names

PROC NPAR1WAY assigns a name to each table that it creates. You can use these names to refer to tables when you use the Output Delivery System (ODS) to select tables and create output data sets. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

Table 65.6 lists the ODS table names together with their descriptions and the options required to produce the tables. If you do not specify any analysis options in the PROC NPAR1WAY statement, the procedure provides the ANOVA, WILCOXON, MEDIAN, VW (NORMAL), SAVAGE, and EDF analyses by default.



**Table 65.6** ODS Tables Produced by PROC NPAR1WAY

| ODS Table Name     | Description                                                 | Statement | Option           |
|--------------------|-------------------------------------------------------------|-----------|------------------|
| ANOVA              | Analysis of variance                                        | PROC      | ANOVA            |
| ABAnalysis         | Ansari-Bradley one-way analysis                             | PROC      | AB               |
| ABMC               | Monte Carlo estimates for the Ansari-Bradley exact test     | EXACT     | AB / MC          |
| ABScores           | Ansari-Bradley scores                                       | PROC      | AB               |
| ABTest*            | Ansari-Bradley two-sample test                              | PROC      | AB               |
| ClassMeans         | Class means                                                 | PROC      | ANOVA            |
| ConoverAnalysis    | Conover one-way analysis                                    | PROC      | CONOVER          |
| ConoverMC          | Monte Carlo estimates for the Conover exact test            | EXACT     | CONOVER / MC     |
| ConoverScores      | Conover scores                                              | PROC      | CONOVER          |
| ConoverTest*       | Conover two-sample test                                     | PROC      | CONOVER          |
| CVMStats           | Cramér-von Mises statistics                                 | PROC      | EDF              |
| CVMTest            | Cramér-von Mises test                                       | PROC      | EDF              |
| DataScores         | Data scores                                                 | PROC      | SCORES=DATA      |
| DataScoresAnalysis | Data scores one-way analysis                                | PROC      | SCORES=DATA      |
| DataScoresMC       | Monte Carlo estimates for the data scores exact test        | EXACT     | SCORES=DATA / MC |
| DataScoresTest*    | Data scores two-sample test                                 | PROC      | SCORES=DATA      |
| DSCF**             | DSCF multiple comparison analysis                           | PROC      | DSCF             |
| FPPlacements*      | Fligner-Policello placements                                | PROC      | FP               |
| FPTest*            | Fligner-Policello test                                      | PROC      | FP               |
| HodgesLehmann*     | Hodges-Lehmann estimation                                   | PROC      | HL               |
| KlotzAnalysis      | Klotz one-way analysis                                      | PROC      | KLOTZ            |
| KlotzMC            | Monte Carlo estimates for the Klotz exact test              | EXACT     | KLOTZ / MC       |
| KlotzScores        | Klotz scores                                                | PROC      | KLOTZ            |
| KlotzTest*         | Klotz two-sample test                                       | PROC      | KLOTZ            |
| KolSmir2Stats*     | Kolmogorov-Smirnov two-sample statistics                    | PROC      | EDF              |
| KolSmirExactTest*  | Kolmogorov-Smirnov exact test                               | EXACT     | KS   EDF         |
| KolSmirStats**     | Kolmogorov-Smirnov statistics                               | PROC      | EDF              |
| KolSmirTest        | Kolmogorov-Smirnov test                                     | PROC      | EDF              |
| KruskalWallisMC**  | Monte Carlo estimates for the Kruskal-Wallis exact test     | EXACT     | WILCOXON / MC    |
| KruskalWallisTest  | Kruskal-Wallis test                                         | PROC      | WILCOXON         |
| KSMC*              | Monte Carlo estimates for the Kolmogorov-Smirnov exact test | EXACT     | KS   EDF / MC    |
| KuiperStats*       | Kuiper two-sample statistics                                | PROC      | EDF              |
| KuiperTest*        | Kuiper test                                                 | PROC      | EDF              |
| MedianAnalysis     | Median one-way analysis                                     | PROC      | MEDIAN           |
| MedianMC           | Monte Carlo estimates for the median exact test             | EXACT     | MEDIAN / MC      |
| MedianScores       | Median scores                                               | PROC      | MEDIAN           |

Table 65.6 *continued*

| ODS Table Name | Description                                                  | Statement | Option           |
|----------------|--------------------------------------------------------------|-----------|------------------|
| MedianTest*    | Median two-sample test                                       | PROC      | MEDIAN           |
| MoodAnalysis   | Mood one-way analysis                                        | PROC      | MOOD             |
| MoodMC         | Monte Carlo estimates for the Mood exact test                | EXACT     | MOOD / MC        |
| MoodScores     | Mood scores                                                  | PROC      | MOOD             |
| MoodTest*      | Mood two-sample test                                         | PROC      | MOOD             |
| SavageAnalysis | Savage one-way analysis                                      | PROC      | SAVAGE           |
| SavageMC       | Monte Carlo estimates for the Savage exact test              | EXACT     | SAVAGE / MC      |
| SavageScores   | Savage scores                                                | PROC      | SAVAGE           |
| SavageTest*    | Savage two-sample test                                       | PROC      | SAVAGE           |
| STAnalysis     | Siegel-Tukey one-way analysis                                | PROC      | ST               |
| STMC           | Monte Carlo estimates for the Siegel-Tukey exact test        | EXACT     | ST / MC          |
| STScores       | Siegel-Tukey scores                                          | PROC      | ST               |
| STTest*        | Siegel-Tukey two-sample test                                 | PROC      | ST               |
| VWAnalysis     | Van der Waerden one-way analysis                             | PROC      | VW   NORMAL      |
| VWMC           | Monte Carlo estimates for the Van der Waerden exact test     | EXACT     | VW   NORMAL / MC |
| VWScores       | Van der Waerden scores                                       | PROC      | VW   NORMAL      |
| VWTest*        | Van der Waerden two-sample test                              | PROC      | VW   NORMAL      |
| WilcoxonMC*    | Monte Carlo estimates for the Wilcoxon two-sample exact test | EXACT     | WILCOXON / MC    |
| WilcoxonScores | Wilcoxon scores                                              | PROC      | WILCOXON         |
| WilcoxonTest*  | Wilcoxon two-sample test                                     | PROC      | WILCOXON         |

\*PROC NPAR1WAY produces this table only for two-sample data.

\*\*PROC NPAR1WAY produces this table only for multisample data.

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “Statistical Graphics Using ODS.”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “A Primer on ODS Statistical Graphics” on page 599 in Chapter 21, “Statistical Graphics Using ODS.”

When ODS Graphics is enabled, you can request specific plots with the PLOTS= option in the PROC NPAR1WAY statement. If you do not specify the PLOTS= option but have enabled ODS Graphics, PROC NPAR1WAY produces all plots that are associated with the analyses that you request.

PROC NPAR1WAY assigns a name to each graph that it creates with ODS Graphics. You can use these names to refer to the graphs. Table 65.7 lists the names of the graphs that PROC NPAR1WAY generates together with their descriptions and the options that are required to produce the graphs.

**Table 65.7** Graphs Produced by PROC NPAR1WAY

| ODS Graph Name    | Description                              | Option      |
|-------------------|------------------------------------------|-------------|
| ABBoxPlot         | Box plot of Ansari-Bradley scores        | AB          |
| ANOVABoxPlot      | Box plot of raw data                     | ANOVA       |
| ConoverBoxPlot    | Box plot of Conover scores               | CONOVER     |
| DataScoresBoxPlot | Box plot of data scores                  | SCORES=DATA |
| EDFPlot           | Empirical distribution function plot     | EDF         |
| FPBoxPlot         | Box plot of Fligner-Policello placements | FP          |
| KlotzBoxPlot      | Box plot of Klotz scores                 | KLOTZ       |
| MedianPlot        | Median plot                              | MEDIAN      |
| MoodBoxPlot       | Box plot of Mood scores                  | MOOD        |
| SavageBoxPlot     | Box plot of Savage scores                | SAVAGE      |
| STBoxPlot         | Box plot of Siegel-Tukey scores          | ST          |
| VWBoxPlot         | Box plot of Van der Waerden scores       | VW   NORMAL |
| WilcoxonBoxPlot   | Box plot of Wilcoxon scores              | WILCOXON    |

## Examples: NPAR1WAY Procedure

### Example 65.1: Two-Sample Location Tests and Plots

Fifty-nine female patients with rheumatoid arthritis who participated in a clinical trial were assigned to two groups, active and placebo. The response status (excellent=5, good=4, moderate=3, fair=2, poor=1) of each patient was recorded.

The following SAS statements create the data set *Arthritis*, which contains the observed status values for all the patients. The variable *Treatment* denotes the treatment received by a patient, and the variable *Response* contains the response status of the patient. The variable *Freq* contains the frequency of the observation, which is the number of patients with the *Treatment* and *Response* combination.

```
data Arthritis;
 input Treatment $ Response Freq @@;
 datalines;
 Active 5 5 Active 4 11 Active 3 5 Active 2 1 Active 1 5
 Placebo 5 2 Placebo 4 4 Placebo 3 7 Placebo 2 7 Placebo 1 12
 ;
```

The following PROC NPAR1WAY statements test the null hypothesis that there is no difference in the patient response status against the alternative hypothesis that the patient response status differs in the two treatment groups. The WILCOXON option requests the Wilcoxon test for difference in location, and the MEDIAN option requests the median test for difference in location. The variable *Treatment* is the CLASS variable, and the VAR statement specifies that the variable *Response* is the analysis variable.

The PLOTS= option requests a box plot of the Wilcoxon scores and a median plot for Response classified by Treatment. ODS Graphics must be enabled before producing plots.

```
ods graphics on;
proc nparlway data=Arthritis wilcoxon median
 plots=(wilcoxonboxplot medianplot);
 class Treatment;
 var Response;
 freq Freq;
run;
ods graphics off;
```

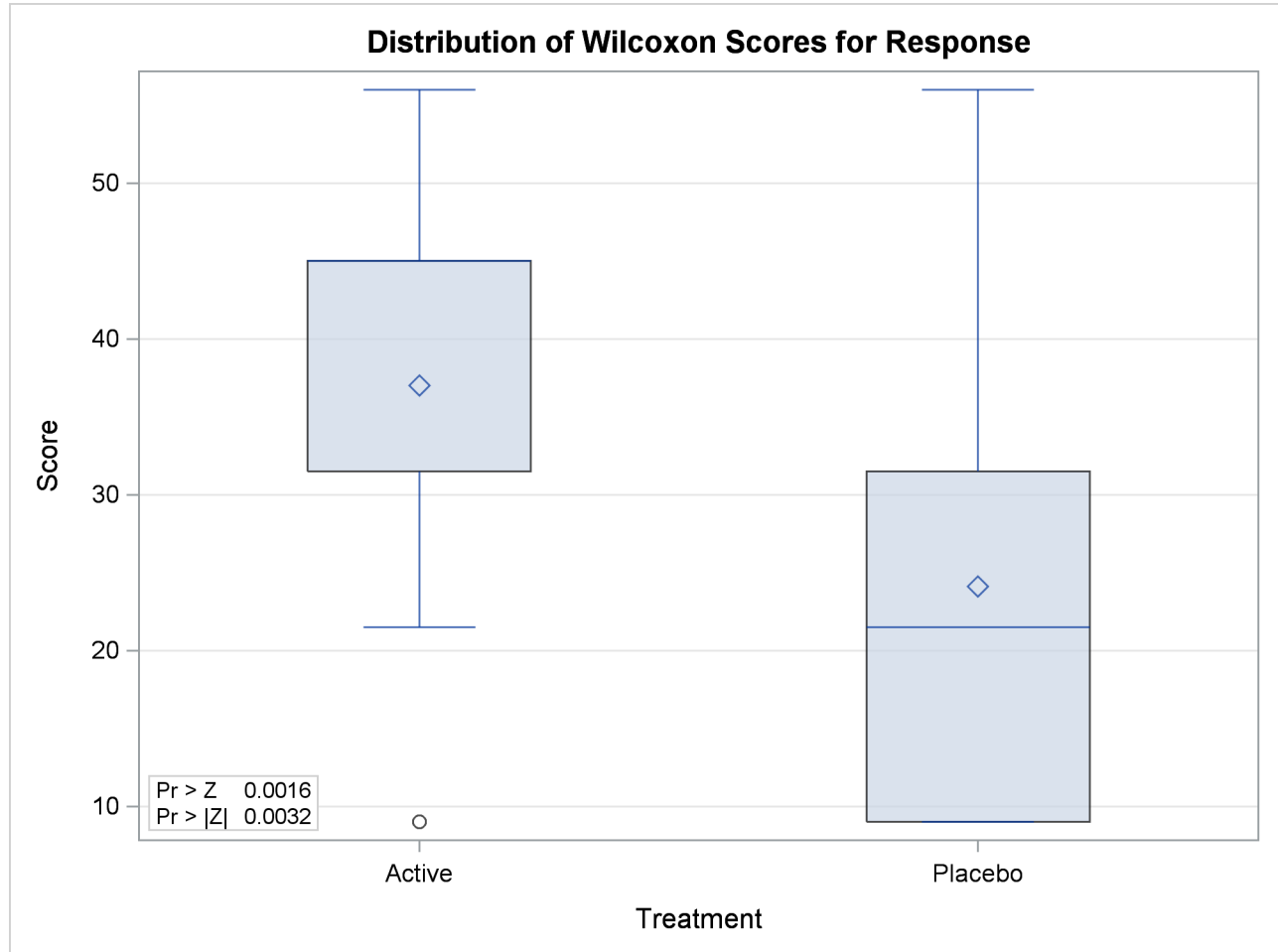
Output 65.1.1 shows the results of the Wilcoxon analysis. The Wilcoxon two-sample test statistic equals 999.0, which is the sum of the Wilcoxon scores for the smaller sample (Active). This sum is greater than 810.0, which is the expected value under the null hypothesis of no difference between the two samples, Active and Placebo. The one-sided  $p$ -value is 0.0016, which indicates that the patient response for the Active treatment is significantly more than for the Placebo group.

### Output 65.1.1 Wilcoxon Two-Sample Test

| The NPAR1WAY Procedure                                                                |    |                  |                      |                     |               |
|---------------------------------------------------------------------------------------|----|------------------|----------------------|---------------------|---------------|
| Wilcoxon Scores (Rank Sums) for Variable Response<br>Classified by Variable Treatment |    |                  |                      |                     |               |
| Treatment                                                                             | N  | Sum of<br>Scores | Expected<br>Under H0 | Std Dev<br>Under H0 | Mean<br>Score |
| Active                                                                                | 27 | 999.0            | 810.0                | 63.972744           | 37.000000     |
| Placebo                                                                               | 32 | 771.0            | 960.0                | 63.972744           | 24.093750     |
| Average scores were used for ties.                                                    |    |                  |                      |                     |               |
| Wilcoxon Two-Sample Test                                                              |    |                  |                      |                     |               |
| Statistic                                                                             |    | 999.0000         |                      |                     |               |
| Normal Approximation                                                                  |    |                  |                      |                     |               |
| Z                                                                                     |    | 2.9466           |                      |                     |               |
| One-Sided Pr > Z                                                                      |    | 0.0016           |                      |                     |               |
| Two-Sided Pr >  Z                                                                     |    | 0.0032           |                      |                     |               |
| t Approximation                                                                       |    |                  |                      |                     |               |
| One-Sided Pr > Z                                                                      |    | 0.0023           |                      |                     |               |
| Two-Sided Pr >  Z                                                                     |    | 0.0046           |                      |                     |               |
| Z includes a continuity correction of 0.5.                                            |    |                  |                      |                     |               |
| Kruskal-Wallis Test                                                                   |    |                  |                      |                     |               |
| Chi-Square                                                                            |    | 8.7284           |                      |                     |               |
| DF                                                                                    |    | 1                |                      |                     |               |
| Pr > Chi-Square                                                                       |    | 0.0031           |                      |                     |               |

Output 65.1.2 displays the box plot of Wilcoxon scores classified by Treatment, which corresponds to the Wilcoxon analysis in Output 65.1.1. To remove the  $p$ -values from the box plot display, you can specify the NOSTATS plot option in parentheses after the WILCOXONBOXPLOT option.

**Output 65.1.2** Box Plot of Wilcoxon Scores



Output 65.1.3 shows the results of the median two-sample test. The test statistic equals 18.9167, and its standardized  $Z$  value is 3.2667. The one-sided  $p$ -value  $\Pr > Z$  equals 0.0005. This supports the alternative hypothesis that the effect of the Active treatment is greater than that of the Placebo.

Output 65.1.4 displays the median plot for the analysis of Response classified by Treatment. The median plot is a stacked bar chart showing the frequencies above and below the overall median. This plot corresponds to the median scores analysis in Output 65.1.3.

**Output 65.1.3** Median Two-Sample Test

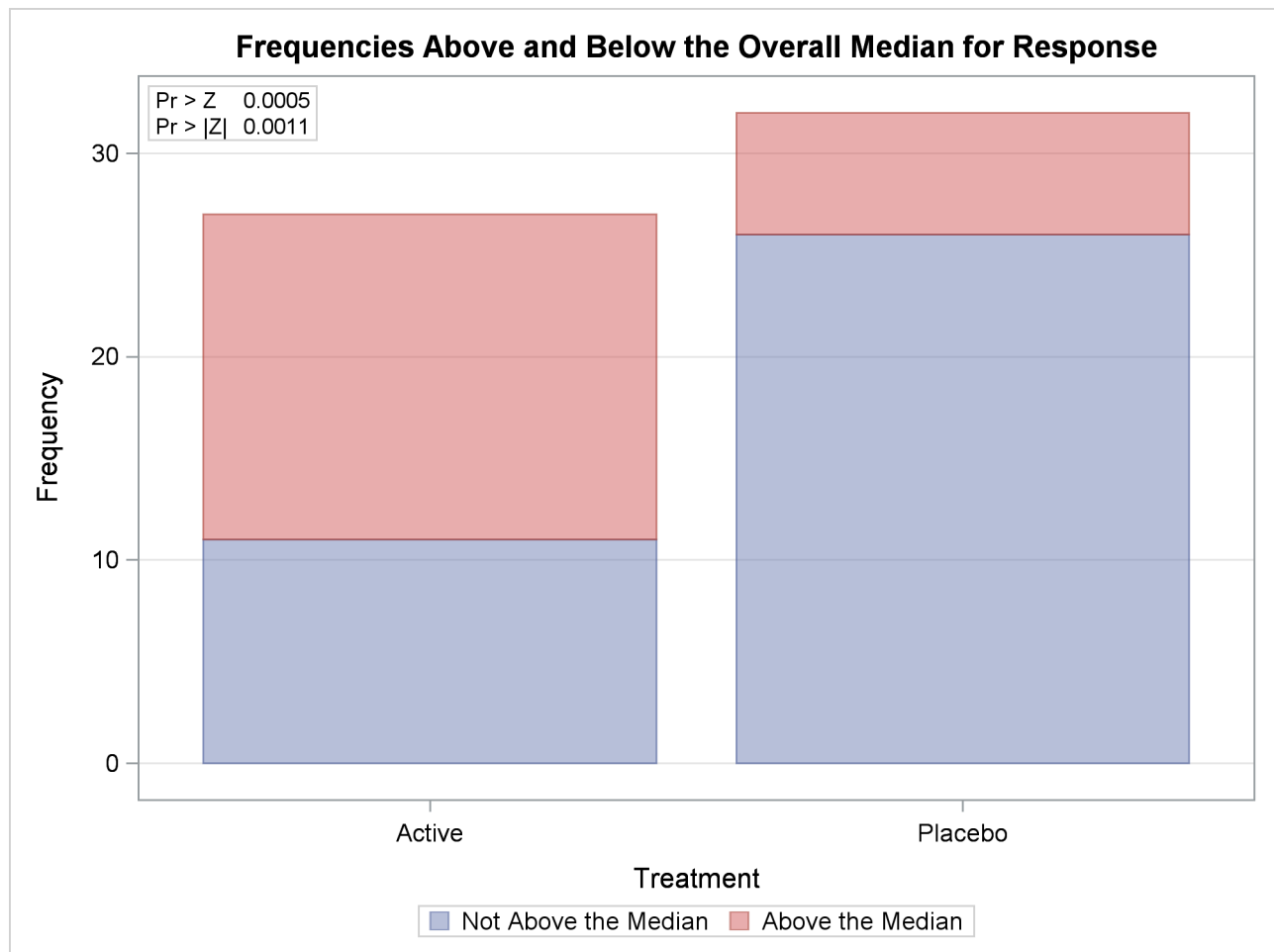
| Median Scores (Number of Points Above Median) for Variable Response<br>Classified by Variable Treatment |    |                  |                      |                     |               |
|---------------------------------------------------------------------------------------------------------|----|------------------|----------------------|---------------------|---------------|
| Treatment                                                                                               | N  | Sum of<br>Scores | Expected<br>Under H0 | Std Dev<br>Under H0 | Mean<br>Score |
| Active                                                                                                  | 27 | 18.916667        | 13.271186            | 1.728195            | 0.700617      |
| Placebo                                                                                                 | 32 | 10.083333        | 15.728814            | 1.728195            | 0.315104      |

Average scores were used for ties.

| Median Two-Sample Test |         |
|------------------------|---------|
| Statistic              | 18.9167 |
| Z                      | 3.2667  |
| One-Sided Pr > Z       | 0.0005  |
| Two-Sided Pr >  Z      | 0.0011  |

| Median One-Way Analysis |         |
|-------------------------|---------|
| Chi-Square              | 10.6713 |
| DF                      | 1       |
| Pr > Chi-Square         | 0.0011  |

Output 65.1.4 Median Plot



## Example 65.2: EDF Statistics and EDF Plot

This example uses the SAS data set *Arthritis* created in [Example 65.1](#). The data set contains the variable *Treatment*, which denotes the treatment received by a patient, and the variable *Response*, which contains the response status of the patient. The variable *Freq* contains the frequency of the observation, which is the number of patients with the *Treatment* and *Response* combination.

The following statements request empirical distribution function (EDF) statistics, which test whether the distribution of a variable is the same across different groups. The *EDF* option requests the EDF analysis. The variable *Treatment* is the *CLASS* variable, and the variable *Response* specified in the *VAR* statement is the analysis variable. The *FREQ* statement names *Freq* as the frequency variable.

The *PLOTS=* option requests an EDF plot for *Response* classified by *Treatment*. ODS Graphics must be enabled before producing plots.

```
ods graphics on;
proc npar1way edf plots=edfplot data=Arthritis;
 class Treatment;
 var Response;
 freq Freq;
run;
ods graphics off;
```

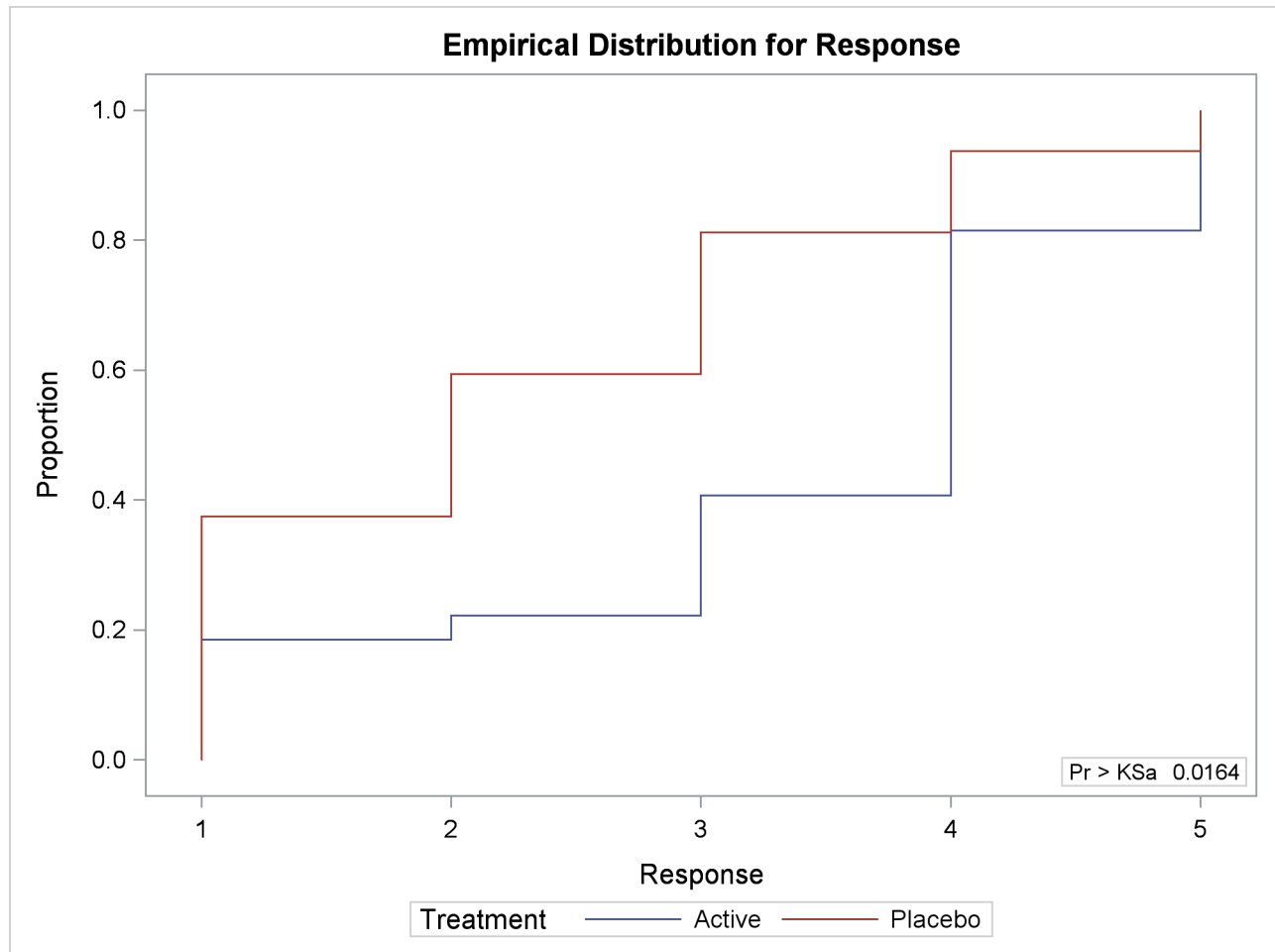
[Output 65.2.1](#) shows EDF statistics that compare the two levels of *Treatment*, *Active* and *Placebo*. The asymptotic *p*-value for the Kolmogorov-Smirnov test is 0.0164. This supports rejection of the null hypothesis that the distributions are the same for the two samples.

[Output 65.2.2](#) shows the EDF plot for *Response* classified by *Treatment*.

### Output 65.2.1 Empirical Distribution Function Statistics

| The NPAR1WAY Procedure                                                            |          |                   |                                   |
|-----------------------------------------------------------------------------------|----------|-------------------|-----------------------------------|
| Kolmogorov-Smirnov Test for Variable Response<br>Classified by Variable Treatment |          |                   |                                   |
| Treatment                                                                         | N        | EDF at<br>Maximum | Deviation from Mean<br>at Maximum |
| Active                                                                            | 27       | 0.407407          | -1.141653                         |
| Placebo                                                                           | 32       | 0.812500          | 1.048675                          |
| Total                                                                             | 59       | 0.627119          |                                   |
| Maximum Deviation Occurred at Observation 3<br>Value of Response at Maximum = 3.0 |          |                   |                                   |
| Kolmogorov-Smirnov Two-Sample Test (Asymptotic)                                   |          |                   |                                   |
| KS                                                                                | 0.201818 | D                 | 0.405093                          |
| KSa                                                                               | 1.550191 | Pr > KSa          | 0.0164                            |



**Output 65.2.2** Empirical Distribution Function Plot

### Example 65.3: Exact Wilcoxon Two-Sample Test

Researchers conducted an experiment to compare the effects of two stimulants. Thirteen randomly selected subjects received the first stimulant, and six randomly selected subjects received the second stimulant. The reaction times (in minutes) were measured while the subjects were under the influence of the stimulants.

The following SAS statements create the data set `React`, which contains the observed reaction times for each stimulant. The variable `Stim` represents Stimulant 1 or 2. The variable `Time` contains the reaction times observed for subjects under the stimulant.

```
data React;
 input Stim Time @@;
 datalines;
 1 1.94 1 1.94 1 2.92 1 2.92 1 2.92 1 2.92 1 3.27
 1 3.27 1 3.27 1 3.27 1 3.70 1 3.70 1 3.74
 2 3.27 2 3.27 2 3.27 2 3.70 2 3.70 2 3.74
 ;
```

The following statements request a Wilcoxon test of the null hypothesis that there is no difference between the effects of the two stimulants. `Stim` is the CLASS variable, and `Time` is the analysis variable. The

WILCOXON option requests an analysis of Wilcoxon scores. The CORRECT=NO option removes the continuity correction from the computation of the standardized  $z$  test statistic. The WILCOXON option in the EXACT statement requests exact  $p$ -values for the Wilcoxon test. Because the sample size is small, the large-sample normal approximation might not be adequate, and it is appropriate to compute the exact test. These statements produce the results shown in Output 65.3.1.

```
proc npar1way wilcoxon correct=no data=React;
 class Stim;
 var Time;
 exact wilcoxon;
run;
```

Output 65.3.1 displays the results of the Wilcoxon two-sample test. The Wilcoxon statistic equals 79.50. Since this value is greater than 60.0, the expected value under the null hypothesis, PROC NPAR1WAY displays the right-sided  $p$ -values. The normal approximation for the Wilcoxon two-sample test yields a one-sided  $p$ -value of 0.0382 and a two-sided  $p$ -value of 0.0764. For the exact Wilcoxon test, the one-sided  $p$ -value is 0.0527, and the two-sided  $p$ -value is 0.1054.

**Output 65.3.1** Wilcoxon Two-Sample Test

| The NPAR1WAY Procedure                                                       |    |                  |                      |                     |               |
|------------------------------------------------------------------------------|----|------------------|----------------------|---------------------|---------------|
| Wilcoxon Scores (Rank Sums) for Variable Time<br>Classified by Variable Stim |    |                  |                      |                     |               |
| Stim                                                                         | N  | Sum of<br>Scores | Expected<br>Under H0 | Std Dev<br>Under H0 | Mean<br>Score |
| 1                                                                            | 13 | 110.50           | 130.0                | 11.004784           | 8.500         |
| 2                                                                            | 6  | 79.50            | 60.0                 | 11.004784           | 13.250        |
| Average scores were used for ties.                                           |    |                  |                      |                     |               |
| Wilcoxon Two-Sample Test                                                     |    |                  |                      |                     |               |
| Statistic (S)                                                                |    | 79.5000          |                      |                     |               |
| Normal Approximation                                                         |    |                  |                      |                     |               |
| Z                                                                            |    | 1.7720           |                      |                     |               |
| One-Sided Pr > Z                                                             |    | 0.0382           |                      |                     |               |
| Two-Sided Pr >  Z                                                            |    | 0.0764           |                      |                     |               |
| t Approximation                                                              |    |                  |                      |                     |               |
| One-Sided Pr > Z                                                             |    | 0.0467           |                      |                     |               |
| Two-Sided Pr >  Z                                                            |    | 0.0933           |                      |                     |               |
| Exact Test                                                                   |    |                  |                      |                     |               |
| One-Sided Pr >= S                                                            |    | 0.0527           |                      |                     |               |
| Two-Sided Pr >=  S - Mean                                                    |    | 0.1054           |                      |                     |               |
| Kruskal-Wallis Test                                                          |    |                  |                      |                     |               |
| Chi-Square                                                                   |    | 3.1398           |                      |                     |               |
| DF                                                                           |    | 1                |                      |                     |               |
| Pr > Chi-Square                                                              |    | 0.0764           |                      |                     |               |

## Example 65.4: Hodges-Lehmann Estimation

This example uses the SAS data set `React` created in [Example 65.3](#). The data set contains the variable `Stim`, which represents Stimulant 1 or 2, and the variable `Time`, which contains the reaction times observed for subjects under the stimulant.

The following statements request Hodges-Lehmann estimation of the location shift between the two groups. `Stim` is the CLASS variable, and `Time` is the analysis variable. The `HL` option requests Hodges-Lehmann estimation. The `ALPHA=` option sets the confidence level for the Hodges-Lehmann confidence limits. The `HL` option in the `EXACT` statement requests exact confidence limits for the estimate of location shift. The `ODS SELECT` statement selects which tables to display. [Output 65.4.1](#) shows the Hodges-Lehmann results.

```
proc npar1way hl alpha=.02 data=React;
 class Stim;
 var Time;
 exact hl;
 ods select WilcoxonScores HodgesLehmann;
run;
```

The `HL` option invokes the `WILCOXON` option, which produces a table of Wilcoxon scores ([Output 65.4.1](#)). The Hodges-Lehmann estimate of location shift is 0.35, and the asymptotic confidence limits are 0.00 and 0.82. The confidence interval midpoint equals 0.41, which can also be used as an estimate of the location shift. The ASE estimate of 0.1762 is based on the length of the confidence interval. The exact confidence limits are 0.00 and 1.33.

**Output 65.4.1** Hodges-Lehmann Estimate of Location Shift

| The NPAR1WAY Procedure                                                       |                       |                  |                      |                              |               |
|------------------------------------------------------------------------------|-----------------------|------------------|----------------------|------------------------------|---------------|
| Wilcoxon Scores (Rank Sums) for Variable Time<br>Classified by Variable Stim |                       |                  |                      |                              |               |
| Stim                                                                         | N                     | Sum of<br>Scores | Expected<br>Under H0 | Std Dev<br>Under H0          | Mean<br>Score |
| 1                                                                            | 13                    | 110.50           | 130.0                | 11.004784                    | 8.500         |
| 2                                                                            | 6                     | 79.50            | 60.0                 | 11.004784                    | 13.250        |
| Average scores were used for ties.                                           |                       |                  |                      |                              |               |
| Hodges-Lehmann Estimation                                                    |                       |                  |                      |                              |               |
| Location Shift (2 - 1)                                                       |                       |                  |                      | 0.3500                       |               |
| Type                                                                         | 98% Confidence Limits |                  | Interval<br>Midpoint | Asymptotic<br>Standard Error |               |
| Asymptotic (Moses)                                                           | 0.0000                | 0.8200           | 0.4100               | 0.1762                       |               |
| Exact                                                                        | 0.0000                | 1.3300           | 0.6650               |                              |               |

## Example 65.5: Exact Savage Multisample Test

A researcher conducting a laboratory experiment randomly assigned 15 mice to receive one of three drugs. The survival time (in days) was then recorded.

The following SAS statements create the data set `Mice`, which contains the observed survival times for the mice. The variable `Treatment` denotes the treatment received. The variable `Days` contains the number of days the mouse survived.

```
data Mice;
 input Treatment $ Days @@;
 datalines;
1 1 1 1 1 3 1 3 1 4
2 3 2 4 2 4 2 4 2 15
3 4 3 4 3 10 3 10 3 26
;
```

The following statements request a Savage test of the null hypothesis that there is no difference in survival time among the three drugs. `Treatment` is the CLASS variable, and `Days` is the analysis variable. The SAVAGE option requests an analysis of Savage scores. The SAVAGE option in the EXACT statement requests exact  $p$ -values for the Savage test. Because the sample size is small, the large-sample normal approximation might not be adequate, and it is appropriate to compute the exact test.

PROC NPAR1WAY tests the null hypothesis that there is no difference in the survival times among the three drugs against the alternative hypothesis of difference among the drugs. The SAVAGE option specifies an analysis based on Savage scores. The variable `Treatment` is the CLASS variable, and the variable `Days` is the response variable. The EXACT statement requests the exact Savage test.

```
proc npar1way savage data=Mice;
 class Treatment;
 var Days;
 exact savage;
run;
```

Output 65.5.1 shows the results of the Savage test. The exact  $p$ -value is 0.0445, which supports a difference in survival times among the drugs at the 0.05 level. The asymptotic  $p$ -value based on the chi-square approximation is 0.0638.

## Output 65.5.1 Savage Multisample Exact Test

| The NPAR1WAY Procedure                                                            |   |                  |                      |                     |               |
|-----------------------------------------------------------------------------------|---|------------------|----------------------|---------------------|---------------|
| Savage Scores (Exponential) for Variable Days<br>Classified by Variable Treatment |   |                  |                      |                     |               |
| Treatment                                                                         | N | Sum of<br>Scores | Expected<br>Under H0 | Std Dev<br>Under H0 | Mean<br>Score |
| 1                                                                                 | 5 | -3.367980        | 0.0                  | 1.634555            | -0.673596     |
| 2                                                                                 | 5 | 0.095618         | 0.0                  | 1.634555            | 0.019124      |
| 3                                                                                 | 5 | 3.272362         | 0.0                  | 1.634555            | 0.654472      |

Average scores were used for ties.

| Savage One-Way Analysis |            |            |        |
|-------------------------|------------|------------|--------|
| Chi-Square              |            |            | 5.5047 |
| DF                      |            |            | 2      |
| Asymptotic Pr >         | Chi-Square |            | 0.0638 |
| Exact                   | Pr >=      | Chi-Square | 0.0445 |

---

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# Chapter 66

## The ORTHOREG Procedure

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### Overview: ORTHOREG Procedure

The ORTHOREG procedure fits general linear models by the method of least squares. Other SAS/STAT software procedures, such as the GLM and REG procedures, fit the same types of models, but PROC



ORTHOREG can produce more accurate estimates than other regression procedures when your data are ill-conditioned. Instead of collecting crossproducts, PROC ORTHOREG uses Gentleman-Givens transformations to update and compute the upper triangular matrix  $\mathbf{R}$  of the QR decomposition of the data matrix, with special care for scaling (Gentleman 1972, 1973). This method has the advantage over other orthogonalization methods (for example, Householder transformations) of not requiring the data matrix to be stored in memory.

The standard SAS regression procedures (PROC REG and PROC GLM) are very accurate for most problems. However, if you have very ill-conditioned data, these procedures can produce estimates that yield an error sum of squares very close to the minimum but still different from the exact least squares estimates. Normally, this coincides with estimates that have very high standard errors. In other words, the numerical error is much smaller than the statistical standard error.

PROC ORTHOREG fits models by the method of linear least squares, minimizing the sum of the squared residuals for predicting the responses—that is, the distance between the regression line and the observed  $Y$ s. The “ORTHO” in the name of the procedure refers to the orthogonalization approach to solving the least squares equations. In particular, PROC ORTHOREG does *not* perform the modeling method known as “orthogonal regression,” which minimizes a different criterion (namely, the distance between the regression line and the  $X/Y$  points taken together.)

---

## Getting Started: ORTHOREG Procedure

---

### Longley Data

The labor statistics data set of Longley (1967) is noted for being ill-conditioned. Both the ORTHOREG and GLM procedures are applied for comparison (only portions of the PROC GLM results are shown).

**NOTE:** The results from this example vary from machine to machine, depending on floating-point configuration.

The following statements read the data into the SAS data set Longley:

```

title 'PROC ORTHOREG used with Longley data';
data Longley;
 input Employment Prices GNP Jobless Military PopSize Year;
 datalines;
60323 83.0 234289 2356 1590 107608 1947
61122 88.5 259426 2325 1456 108632 1948
60171 88.2 258054 3682 1616 109773 1949
61187 89.5 284599 3351 1650 110929 1950
63221 96.2 328975 2099 3099 112075 1951
63639 98.1 346999 1932 3594 113270 1952
64989 99.0 365385 1870 3547 115094 1953
63761 100.0 363112 3578 3350 116219 1954
66019 101.2 397469 2904 3048 117388 1955
67857 104.6 419180 2822 2857 118734 1956
68169 108.4 442769 2936 2798 120445 1957
66513 110.8 444546 4681 2637 121950 1958
68655 112.6 482704 3813 2552 123366 1959

```

```

69564 114.2 502601 3931 2514 125368 1960
69331 115.7 518173 4806 2572 127852 1961
70551 116.9 554894 4007 2827 130081 1962
;

```

The data set contains one dependent variable, Employment (total derived employment), and six independent variables: Prices (GNP implicit price deflator normalized to the value 100 in 1954), GNP (gross national product), Jobless (unemployment), Military (size of armed forces), PopSize (noninstitutional population aged 14 and over), and Year (year).

The following statements use the ORTHOREG procedure to model the Longley data by using a quadratic model in each independent variable, without interaction:

```

proc orthoreg data=Longley;
 model Employment = Prices Prices*Prices
 GNP GNP*GNP
 Jobless Jobless*Jobless
 Military Military*Military
 PopSize PopSize*PopSize
 Year Year*Year;
run;

```

Figure 66.1 shows the resulting analysis.

**Figure 66.1** PROC ORTHOREG Results

| PROC ORTHOREG used with Longley data |    |                |              |         |        |
|--------------------------------------|----|----------------|--------------|---------|--------|
| The ORTHOREG Procedure               |    |                |              |         |        |
| Dependent Variable: Employment       |    |                |              |         |        |
| Source                               | DF | Sum of Squares | Mean Square  | F Value | Pr > F |
| Model                                | 12 | 184864508.5    | 15405375.709 | 320.24  | 0.0003 |
| Error                                | 3  | 144317.49568   | 48105.831895 |         |        |
| Corrected Total                      | 15 | 185008826      |              |         |        |
|                                      |    | Root MSE       | 219.33041717 |         |        |
|                                      |    | R-Square       | 0.9992199426 |         |        |

Figure 66.1 continued

| Parameter   | DF | Parameter Estimate | Standard Error | t Value | Pr >  t |
|-------------|----|--------------------|----------------|---------|---------|
| Intercept   | 1  | 186931078.640216   | 154201839.66   | 1.21    | 0.3122  |
| Prices      | 1  | 1324.50679362506   | 916.17455832   | 1.45    | 0.2440  |
| Prices**2   | 1  | -6.61923922845539  | 4.7891445654   | -1.38   | 0.2609  |
| GNP         | 1  | -0.12768642156232  | 0.0738897784   | -1.73   | 0.1824  |
| GNP**2      | 1  | 3.1369569286212E-8 | 8.7167753E-8   | 0.36    | 0.7428  |
| Jobless     | 1  | -4.35507653558708  | 1.3851792402   | -3.14   | 0.0515  |
| Jobless**2  | 1  | 0.00022132944101   | 0.0001763541   | 1.26    | 0.2983  |
| Military    | 1  | 4.91162014560828   | 1.826715856    | 2.69    | 0.0745  |
| Military**2 | 1  | -0.00113707146734  | 0.0003539971   | -3.21   | 0.0489  |
| PopSize     | 1  | -0.0303997234299   | 5.9272538242   | -0.01   | 0.9962  |
| PopSize**2  | 1  | -1.212511414607E-6 | 0.0000237262   | -0.05   | 0.9625  |
| Year        | 1  | -194907.139041839  | 157739.28757   | -1.24   | 0.3045  |
| Year**2     | 1  | 50.8067603538501   | 40.279878943   | 1.26    | 0.2963  |

The estimates in Figure 66.1 compare very well with the best estimates available; for additional information, see Longley (1967) and Beaton, Rubin, and Barone (1976).

The following statements request the same analysis from the GLM procedure:

```
proc glm data=Longley;
 model Employment = Prices Prices*Prices
 GNP GNP*GNP
 Jobless Jobless*Jobless
 Military Military*Military
 PopSize PopSize*PopSize
 Year Year*Year;
 ods select OverallANOVA
 FitStatistics
 ParameterEstimates
 Notes;
run;
```

Figure 66.2 contains the overall ANOVA table and the parameter estimates produced by PROC GLM. Notice that the PROC ORTHOREG fit achieves a somewhat smaller root mean square error (RMSE) and also that the GLM procedure detects spurious singularities.

Figure 66.2 Partial PROC GLM Results

PROC ORTHOREG used with Longley data

The GLM Procedure

Dependent Variable: Employment

| Source          | DF | Sum of Squares | Mean Square | F Value | Pr > F |
|-----------------|----|----------------|-------------|---------|--------|
| Model           | 11 | 184791061.6    | 16799187.4  | 308.58  | <.0001 |
| Error           | 4  | 217764.4       | 54441.1     |         |        |
| Corrected Total | 15 | 185008826.0    |             |         |        |

| R-Square | Coeff Var | Root MSE | Employment Mean |
|----------|-----------|----------|-----------------|
| 0.998823 | 0.357221  | 233.3262 | 65317.00        |

| Parameter         | Estimate       | Standard Error | t Value | Pr >  t |
|-------------------|----------------|----------------|---------|---------|
| Intercept         | -3598851.899 B | 1327335.652    | -2.71   | 0.0535  |
| Prices            | 523.802        | 688.979        | 0.76    | 0.4894  |
| Prices*Prices     | -2.326         | 3.507          | -0.66   | 0.5434  |
| GNP               | -0.138         | 0.078          | -1.76   | 0.1526  |
| GNP*GNP           | 0.000          | 0.000          | 0.24    | 0.8218  |
| Jobless           | -4.599         | 1.459          | -3.15   | 0.0344  |
| Jobless*Jobless   | 0.000          | 0.000          | 1.14    | 0.3183  |
| Military          | 4.994          | 1.942          | 2.57    | 0.0619  |
| Military*Military | -0.001         | 0.000          | -3.15   | 0.0346  |
| PopSize           | -4.246         | 5.156          | -0.82   | 0.4565  |
| PopSize*PopSize   | 0.000 B        | 0.000          | 0.81    | 0.4655  |
| Year              | 0.000 B        | .              | .       | .       |
| Year*Year         | 1.038          | 0.419          | 2.48    | 0.0683  |

NOTE: The X'X matrix has been found to be singular, and a generalized inverse was used to solve the normal equations. Terms whose estimates are followed by the letter 'B' are not uniquely estimable.

## Syntax: ORTHOREG Procedure

The following statements are available in the ORTHOREG procedure:

```

PROC ORTHOREG < options > ;
 CLASS variables < / option > ;
 MODEL dependent-variable = independent-effects < / option > ;
 BY variables ;
 EFFECT name = effect-type (variables < / options >) ;
 EFFECTPLOT < plot-type < (plot-definition-options) > > < / options > ;
 ESTIMATE < 'label' > estimate-specification < / options > ;
 LSMEANS < model-effects > < / options > ;
 LSMESTIMATE model-effect lsmestimate-specification < / options > ;
 SLICE model-effect < / options > ;
 STORE < OUT= > item-store-name < / LABEL= 'label' > ;
 TEST < model-effects > < / options > ;
 WEIGHT variable ;

```

The **BY**, **CLASS**, **MODEL**, and **WEIGHT** statements are described in full after the **PROC ORTHOREG** statement in alphabetical order. The **EFFECT**, **EFFECTPLOT**, **ESTIMATE**, **LSMEANS**, **LSMESTIMATE**, **SLICE**, **STORE**, and **TEST** statements are common to many procedures. Summary descriptions of functionality and syntax for these statements are also given after the **PROC ORTHOREG** statement in alphabetical order, and full documentation about them is available in Chapter 19, “Shared Concepts and Topics.”

## PROC ORTHOREG Statement

```
PROC ORTHOREG < options > ;
```

The **PROC ORTHOREG** statement invokes the ORTHOREG procedure. Table 66.1 summarizes the options available in the **PROC ORTHOREG** statement.

**Table 66.1** PROC ORTHOREG Statement Options

| Option           | Description                                       |
|------------------|---------------------------------------------------|
| <b>DATA=</b>     | Specifies the input SAS data set                  |
| <b>NOPRINT</b>   | Suppresses the normal display of results          |
| <b>ORDER=</b>    | Specifies the order in which to sort class levels |
| <b>OUTEST=</b>   | Produces an output data set                       |
| <b>SINGULAR=</b> | Specifies the singularity criterion               |

The **PROC ORTHOREG** statement has the following options:

**DATA=SAS-data-set**

specifies the input SAS data set to use. By default, the procedure uses the most recently created SAS data set. The data set specified cannot be a **TYPE=CORR**, **TYPE=COV**, or **TYPE=SSCP** data set.

**NOPRINT**

suppresses the normal display of results. This option temporarily disables the Output Delivery System (ODS); see Chapter 20, “Using the Output Delivery System” for more information.

**ORDER=DATA | FORMATTED | FREQ | INTERNAL**

specifies the sort order for the levels of the classification variables (which are specified in the **CLASS** statement). This ordering determines which parameters in the model correspond to each level in the data, so the **ORDER=** option may be useful when you use **ESTIMATE** statement. This option applies to the levels for all classification variables, except when you use the (default) **ORDER=FORMATTED** option with numeric classification variables that have no explicit format. With this option, the levels of such variables are ordered by their internal value.

The **ORDER=** option can take the following values:

| Value of <b>ORDER=</b> | Levels Sorted By                                                                                                                       |
|------------------------|----------------------------------------------------------------------------------------------------------------------------------------|
| <b>DATA</b>            | Order of appearance in the input data set                                                                                              |
| <b>FORMATTED</b>       | External formatted value, except for numeric variables with no explicit format, which are sorted by their unformatted (internal) value |
| <b>FREQ</b>            | Descending frequency count; levels with the most observations come first in the order                                                  |
| <b>INTERNAL</b>        | Unformatted value                                                                                                                      |

By default, **ORDER=FORMATTED**. For **ORDER=FORMATTED** and **ORDER=INTERNAL**, the sort order is machine-dependent.

For more information about sort order, see the chapter on the **SORT** procedure in the *Base SAS Procedures Guide* and the discussion of **BY**-group processing in *SAS Language Reference: Concepts*.

**OUTEST=SAS-data-set**

produces an output data set that contains the parameter estimates, the **BY** variables, and the special variables **\_TYPE\_** (value “**PARMS**”), **\_NAME\_** (blank), and **\_RMSE\_** (root mean squared error).

**SINGULAR=s**

specifies a singularity criterion ( $s \geq 0$ ) for the inversion of the triangular matrix **R**. By default, **SINGULAR=1E-12**.

---

## BY Statement

**BY variables ;**

You can specify a **BY** statement with **PROC ORTHOREG** to obtain separate analyses of observations in groups that are defined by the **BY** variables. When a **BY** statement appears, the procedure expects the input data set to be sorted in order of the **BY** variables. If you specify more than one **BY** statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the ORTHOREG procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

---

## CLASS Statement

**CLASS** *variable* <(REF= *option*)> ... <*variable* <(REF= *option*)>> </ *global-options* > ;

The CLASS statement names the classification variables to be used in the model. Typical classification variables are Treatment, Sex, Race, Group, and Replication. If you use the CLASS statement, it must appear before the MODEL statement.

Classification variables can be either character or numeric. By default, class levels are determined from the entire set of formatted values of the CLASS variables.

**NOTE:** Prior to SAS 9, class levels were determined by using no more than the first 16 characters of the formatted values. To revert to this previous behavior, you can use the TRUNCATE option in the CLASS statement.

In any case, you can use formats to group values into levels. See the discussion of the FORMAT procedure in the *Base SAS Procedures Guide* and the discussions of the FORMAT statement and SAS formats in *SAS Formats and Informats: Reference*. You can adjust the order of CLASS variable levels with the ORDER= option in the PROC ORTHOREG statement. You can specify the following REF= option to indicate how the levels of an individual classification variable are to be ordered by enclosing it in parentheses after the variable name:

### REF= '*level*' | FIRST | LAST

specifies a level of the classification variable to be put at the end of the list of levels. This level thus corresponds to the reference level in the usual interpretation of the estimates with PROC ORTHOREG's singular parameterization. You can specify the *level* of the variable to use as the reference level; specify a value that corresponds to the formatted value of the variable if a format is assigned. Alternatively, you can specify REF=FIRST to designate that the first ordered level serve as the reference, or REF=LAST to designate that the last ordered level serve as the reference. To specify that REF=FIRST or REF=LAST be used for all classification variables, use the REF= *global-option* after the slash (/) in the CLASS statement.

You can specify the following *global-options* in the CLASS statement after a slash (/):

**REF=FIRST | LAST**

specifies a level of all classification variables to be put at the end of the list of levels. This level thus corresponds to the reference level in the usual interpretation of the estimates with PROC ORTHOREG's singular parameterization. Specify REF=FIRST to designate that the first ordered level for each classification variable serve as the reference. Specify REF=LAST to designate that the last ordered level serve as the reference. This option applies to all the variables specified in the CLASS statement. To specify different reference levels for different classification variables, use REF= options for individual variables.

**TRUNCATE**

specifies that class levels be determined by using only up to the first 16 characters of the formatted values of CLASS variables. When formatted values are longer than 16 characters, you can use this option to revert to the levels as determined in releases prior to SAS 9.

---

## EFFECT Statement

**EFFECT** *name=effect-type* (*variables* < / *options* >);

The EFFECT statement enables you to construct special collections of columns for design matrices. These collections are referred to as *constructed effects* to distinguish them from the usual model effects that are formed from continuous or classification variables, as discussed in the section “GLM Parameterization of Classification Variables and Effects” on page 383 in Chapter 19, “Shared Concepts and Topics.”

You can specify the following *effect-types*:

|                          |                                                                                                                                                                                                           |
|--------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>COLLECTION</b>        | is a collection effect that defines one or more variables as a single effect with multiple degrees of freedom. The variables in a collection are considered as a unit for estimation and inference.       |
| <b>LAG</b>               | is a classification effect in which the level that is used for a given period corresponds to the level in the preceding period.                                                                           |
| <b>MULTIMEMBER   MM</b>  | is a multimember classification effect whose levels are determined by one or more variables that appear in a CLASS statement.                                                                             |
| <b>POLYNOMIAL   POLY</b> | is a multivariate polynomial effect in the specified numeric variables.                                                                                                                                   |
| <b>SPLINE</b>            | is a regression spline effect whose columns are univariate spline expansions of one or more variables. A spline expansion replaces the original variable with an expanded or larger set of new variables. |

Table 66.2 summarizes the *options* available in the EFFECT statement.

**Table 66.2** EFFECT Statement Options

| Option                            | Description                                        |
|-----------------------------------|----------------------------------------------------|
| <b>Collection Effects Options</b> |                                                    |
| <b>DETAILS</b>                    | Displays the constituents of the collection effect |



Table 66.2 continued

| Option                             | Description                                                                                                                                          |
|------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Lag Effects Options</b>         |                                                                                                                                                      |
| DESIGNROLE=                        | Names a variable that controls to which lag design an observation is assigned                                                                        |
| DETAILS                            | Displays the lag design of the lag effect                                                                                                            |
| NLAG=                              | Specifies the number of periods in the lag                                                                                                           |
| PERIOD=                            | Names the variable that defines the period                                                                                                           |
| WITHIN=                            | Names the variable or variables that define the group within which each period is defined                                                            |
| <b>Multimember Effects Options</b> |                                                                                                                                                      |
| NOEFFECT                           | Specifies that observations with all missing levels for the multimember variables should have zero values in the corresponding design matrix columns |
| WEIGHT=                            | Specifies the weight variable for the contributions of each of the classification effects                                                            |
| <b>Polynomial Effects Options</b>  |                                                                                                                                                      |
| DEGREE=                            | Specifies the degree of the polynomial                                                                                                               |
| MDEGREE=                           | Specifies the maximum degree of any variable in a term of the polynomial                                                                             |
| STANDARDIZE=                       | Specifies centering and scaling suboptions for the variables that define the polynomial                                                              |
| <b>Spline Effects Options</b>      |                                                                                                                                                      |
| BASIS=                             | Specifies the type of basis (B-spline basis or truncated power function basis) for the spline expansion                                              |
| DEGREE=                            | Specifies the degree of the spline transformation                                                                                                    |
| KNOTMETHOD=                        | Specifies how to construct the knots for spline effects                                                                                              |

For more information about the syntax of these *effect-types* and how columns of constructed effects are computed, see the section “EFFECT Statement” on page 393 in Chapter 19, “Shared Concepts and Topics.”

## EFFECTPLOT Statement

**EFFECTPLOT** < *plot-type* < (*plot-definition-options*) > > < / *options* > ;

The EFFECTPLOT statement produces a display of the fitted model and provides options for changing and enhancing the displays. Table 66.3 describes the available *plot-types* and their *plot-definition-options*.

**Table 66.3** *Plot-Types and Plot-Definition-Options*

| <b>Plot-Type and Description</b>                                                                                                                                                                                                          | <b>Plot-Definition-Options</b>                                                                                                     |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------|
| <p><b>BOX</b><br/>Displays a box plot of continuous response data at each level of a CLASS effect, with predicted values superimposed and connected by a line. This is an alternative to the <b>INTERACTION</b> <i>plot-type</i>.</p>     | <p><b>PLOTBY=</b> variable or CLASS effect<br/><b>X=</b> CLASS variable or effect</p>                                              |
| <p><b>CONTOUR</b><br/>Displays a contour plot of predicted values against two continuous covariates.</p>                                                                                                                                  | <p><b>PLOTBY=</b> variable or CLASS effect<br/><b>X=</b> continuous variable<br/><b>Y=</b> continuous variable</p>                 |
| <p><b>FIT</b><br/>Displays a curve of predicted values versus a continuous variable.</p>                                                                                                                                                  | <p><b>PLOTBY=</b> variable or CLASS effect<br/><b>X=</b> continuous variable</p>                                                   |
| <p><b>INTERACTION</b><br/>Displays a plot of predicted values (possibly with error bars) versus the levels of a CLASS effect. The predicted values are connected with lines and can be grouped by the levels of another CLASS effect.</p> | <p><b>PLOTBY=</b> variable or CLASS effect<br/><b>SLICEBY=</b> variable or CLASS effect<br/><b>X=</b> CLASS variable or effect</p> |
| <p><b>SLICEFIT</b><br/>Displays a curve of predicted values versus a continuous variable grouped by the levels of a CLASS effect.</p>                                                                                                     | <p><b>PLOTBY=</b> variable or CLASS effect<br/><b>SLICEBY=</b> variable or CLASS effect<br/><b>X=</b> continuous variable</p>      |

For full details about the syntax and options of the EFFECTPLOT statement, see the section “EFFECTPLOT Statement” on page 411 in Chapter 19, “Shared Concepts and Topics.”

## ESTIMATE Statement

```
ESTIMATE <'label'> estimate-specification <(divisor=n)>
 <, ... <'label'> estimate-specification <(divisor=n)>>
 </options>;
```

The ESTIMATE statement provides a mechanism for obtaining custom hypothesis tests. Estimates are formed as linear estimable functions of the form  $\mathbf{L}\boldsymbol{\beta}$ . You can perform hypothesis tests for the estimable functions, construct confidence limits, and obtain specific nonlinear transformations.

Table 66.4 summarizes the options available in the ESTIMATE statement.

**Table 66.4** ESTIMATE Statement Options

| Option                                                     | Description                                                               |
|------------------------------------------------------------|---------------------------------------------------------------------------|
| <b>Construction and Computation of Estimable Functions</b> |                                                                           |
| DIVISOR=                                                   | Specifies a list of values to divide the coefficients                     |
| NOFILL                                                     | Suppresses the automatic fill-in of coefficients for higher-order effects |
| SINGULAR=                                                  | Tunes the estimability checking difference                                |
| <b>Degrees of Freedom and <math>p</math>-values</b>        |                                                                           |
| ADJUST=                                                    | Determines the method for multiple comparison adjustment of estimates     |
| ALPHA= $\alpha$                                            | Determines the confidence level ( $1 - \alpha$ )                          |
| LOWER                                                      | Performs one-sided, lower-tailed inference                                |
| STEPDOWN                                                   | Adjusts multiplicity-corrected $p$ -values further in a step-down fashion |
| TESTVALUE=                                                 | Specifies values under the null hypothesis for tests                      |
| UPPER                                                      | Performs one-sided, upper-tailed inference                                |
| <b>Statistical Output</b>                                  |                                                                           |
| CL                                                         | Constructs confidence limits                                              |
| CORR                                                       | Displays the correlation matrix of estimates                              |
| COV                                                        | Displays the covariance matrix of estimates                               |
| E                                                          | Prints the $\mathbf{L}$ matrix                                            |
| JOINT                                                      | Produces a joint $F$ or chi-square test for the estimable functions       |
| SEED=                                                      | Specifies the seed for computations that depend on random numbers         |

For details about the syntax of the ESTIMATE statement, see the section “ESTIMATE Statement” on page 437 in Chapter 19, “Shared Concepts and Topics.”

## LSMEANS Statement

**LSMEANS** < model-effects > < / options > ;

The LSMEANS statement computes and compares least squares means (LS-means) of fixed effects. LS-means are *predicted population margins*—that is, they estimate the marginal means over a balanced population. In a sense, LS-means are to unbalanced designs as class and subclass arithmetic means are to balanced designs.

Table 66.5 summarizes the options available in the LSMEANS statement.

**Table 66.5** LSMEANS Statement Options

| Option                                          | Description                                                                                 |
|-------------------------------------------------|---------------------------------------------------------------------------------------------|
| <b>Construction and Computation of LS-Means</b> |                                                                                             |
| AT                                              | Modifies the covariate value in computing LS-means                                          |
| BYLEVEL                                         | Computes separate margins                                                                   |
| DIFF                                            | Requests differences of LS-means                                                            |
| OM=                                             | Specifies the weighting scheme for LS-means computation as determined by the input data set |
| SINGULAR=                                       | Tunes estimability checking                                                                 |
| <b>Degrees of Freedom and <i>p</i>-values</b>   |                                                                                             |
| ADJUST=                                         | Determines the method for multiple-comparison adjustment of LS-means differences            |
| ALPHA= $\alpha$                                 | Determines the confidence level $(1 - \alpha)$                                              |
| STEPDOWN                                        | Adjusts multiple-comparison <i>p</i> -values further in a step-down fashion                 |
| <b>Statistical Output</b>                       |                                                                                             |
| CL                                              | Constructs confidence limits for means and mean differences                                 |
| CORR                                            | Displays the correlation matrix of LS-means                                                 |
| COV                                             | Displays the covariance matrix of LS-means                                                  |
| E                                               | Prints the L matrix                                                                         |
| LINES                                           | Produces a “Lines” display for pairwise LS-means differences                                |
| MEANS                                           | Prints the LS-means                                                                         |
| PLOTS=                                          | Requests graphs of means and mean comparisons                                               |
| SEED=                                           | Specifies the seed for computations that depend on random numbers                           |

For details about the syntax of the LSMEANS statement, see the section “LSMEANS Statement” on page 453 in Chapter 19, “Shared Concepts and Topics.”

## LSMESTIMATE Statement

```
LSMESTIMATE model-effect <'label'> values <divisor=n>
 < , ... <'label'> values <divisor=n> >
 </options> ;
```

The LSMESTIMATE statement provides a mechanism for obtaining custom hypothesis tests among least squares means.

Table 66.6 summarizes the options available in the LSMESTIMATE statement.

**Table 66.6** LSMESTIMATE Statement Options

| Option                                              | Description                                                                         |
|-----------------------------------------------------|-------------------------------------------------------------------------------------|
| <b>Construction and Computation of LS-Means</b>     |                                                                                     |
| AT                                                  | Modifies covariate values in computing LS-means                                     |
| BYLEVEL                                             | Computes separate margins                                                           |
| DIVISOR=                                            | Specifies a list of values to divide the coefficients                               |
| OM=                                                 | Specifies the weighting scheme for LS-means computation as determined by a data set |
| SINGULAR=                                           | Tunes estimability checking                                                         |
| <b>Degrees of Freedom and <math>p</math>-values</b> |                                                                                     |
| ADJUST=                                             | Determines the method for multiple-comparison adjustment of LS-means differences    |
| ALPHA= $\alpha$                                     | Determines the confidence level $(1 - \alpha)$                                      |
| LOWER                                               | Performs one-sided, lower-tailed inference                                          |
| STEPDOWN                                            | Adjusts multiple-comparison $p$ -values further in a step-down fashion              |
| TESTVALUE=                                          | Specifies values under the null hypothesis for tests                                |
| UPPER                                               | Performs one-sided, upper-tailed inference                                          |
| <b>Statistical Output</b>                           |                                                                                     |
| CL                                                  | Constructs confidence limits for means and mean differences                         |
| CORR                                                | Displays the correlation matrix of LS-means                                         |
| COV                                                 | Displays the covariance matrix of LS-means                                          |
| E                                                   | Prints the <b>L</b> matrix                                                          |
| ELSM                                                | Prints the <b>K</b> matrix                                                          |
| JOINT                                               | Produces a joint $F$ or chi-square test for the LS-means and LS-means differences   |
| SEED=                                               | Specifies the seed for computations that depend on random numbers                   |

For details about the syntax of the LSMESTIMATE statement, see the section “LSMESTIMATE Statement” on page 470 in Chapter 19, “Shared Concepts and Topics.”

---

## MODEL Statement

**MODEL** *dependent-variable = independent-effects* </ option > ;

The MODEL statement names the dependent variable and the independent effects. Only one MODEL statement is allowed. The [specification of effects](#) and the parameterization of the linear model are the same as in the GLM procedure; see Chapter 42, “[The GLM Procedure](#)” for further details.

The following option can be used in the MODEL statement:

### NOINT

omits the intercept term from the model. Often, this omission also changes the total sum of squares in the ANOVA and the value of R square to forms of these statistics that are not corrected for the mean. However, if the model is determined to contain an implicit intercept, in the sense that the all-ones intercept vector is in the column space of the design, then the usual mean-corrected forms of these statistics are used.

---

## SLICE Statement

**SLICE** *model-effect* </ options > ;

The SLICE statement provides a general mechanism for performing a partitioned analysis of the LS-means for an interaction. This analysis is also known as an analysis of simple effects.

The SLICE statement uses the same options as the [LSMEANS](#) statement, which are summarized in [Table 19.21](#). For details about the syntax of the SLICE statement, see the section “[SLICE Statement](#)” on page 498 in Chapter 19, “[Shared Concepts and Topics](#).”

---

## STORE Statement

**STORE** < **OUT=** > *item-store-name* </ **LABEL=** 'label' > ;

The STORE statement requests that the procedure save the context and results of the statistical analysis. The resulting item store has a binary file format that cannot be modified. The contents of the item store can be processed with the PLM procedure.

For details about the syntax of the STORE statement, see the section “[STORE Statement](#)” on page 501 in Chapter 19, “[Shared Concepts and Topics](#).”

---

## TEST Statement

**TEST** < *model-effects* > </ options > ;

The TEST statement enables you to perform  $F$  tests for model effects that test Type I, Type II, or Type III hypotheses. See Chapter 15, “[The Four Types of Estimable Functions](#),” for details about the construction of Type I, II, and III estimable functions.

[Table 66.7](#) summarizes the options available in the TEST statement.

**Table 66.7** TEST Statement Options

| Option    | Description                                                |
|-----------|------------------------------------------------------------|
| CHISQ     | Requests chi-square tests                                  |
| DDF=      | Specifies denominator degrees of freedom for fixed effects |
| E         | Requests Type I, Type II, and Type III coefficients        |
| E1        | Requests Type I coefficients                               |
| E2        | Requests Type II coefficients                              |
| E3        | Requests Type III coefficients                             |
| HTYPE=    | Indicates the type of hypothesis test to perform           |
| INTERCEPT | Adds a row that corresponds to the overall intercept       |

For details about the syntax of the TEST statement, see the section “TEST Statement” on page 502 in Chapter 19, “Shared Concepts and Topics.”

---

## WEIGHT Statement

**WEIGHT** *variable* ;

A WEIGHT statement names a variable in the input data set whose values are relative weights for a weighted least squares regression. If the weight value is proportional to the reciprocal of the variance for each observation, the weighted estimates are the best linear unbiased estimates (BLUE). For a more complete description of the WEIGHT statement, see the section “WEIGHT Statement” on page 3323 in the GLM procedure.

---

## Details: ORTHOREG Procedure

---

### Missing Values

If there is a missing value for any model variable in an observation, the entire observation is dropped from the analysis.

---

### Output Data Set

The OUTEST= option produces a TYPE=EST output SAS data set that contains the BY variables, parameter estimates, and four special variables. For each new value of the BY variables, PROC ORTHOREG outputs an observation to the OUTEST= data set. The variables in the data set are as follows:

- parameter estimates for all variables listed in the MODEL statement
- BY variables
- \_TYPE\_, which is a character variable with the value PARMS for every observation

- `_NAME_`, which is a character variable left blank for every observation
- `_RMSE_`, which is the root mean square error (the estimate of the standard deviation of the true errors)
- Intercept, which is the estimated intercept. This variable does not exist in the OUTEST= data set if the `NOINT` option is specified.

---

## Displayed Output

PROC ORTHOREG displays the parameter estimates and associated statistics. These include the following:

- overall model analysis of variance, including the error mean square, which is an estimate of  $\sigma^2$  (the variance of the true errors), and the overall  $F$  test for a model effect.
- root mean square error, which is an estimate of the standard deviation of the true errors. It is calculated as the square root of the mean squared error.
- R square ( $R^2$ ) measures how much variation in the dependent variable can be accounted for by the model. R square, which can range from 0 to 1, is the ratio of the sum of squares for the model to the corrected total sum of squares. In general, the larger the value of R square, the better the model's fit.
- estimates for the parameters in the linear model

The table of parameter estimates consists of the following:

- the terms used as regressors, including the intercept.
- degrees of freedom (DF) for the variable. There is one degree of freedom for each parameter being estimated unless the model is not full rank.
- estimated linear coefficients.
- estimates of the standard errors of the parameter estimates.
- the critical  $t$  values for testing whether the parameters are This is computed as the parameter estimate divided by its standard error.
- the two-sided  $p$ -value for the  $t$  test, which is the probability that a  $t$  statistic would obtain a greater absolute value than that observed given that the true parameter is zero.

---

## ODS Table Names

PROC ORTHOREG assigns a name to each table it creates. You can use these names to reference the table when you use the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in [Table 66.8](#). For more information about ODS, see Chapter 20, “[Using the Output Delivery System.](#)”



Each of the EFFECT, ESTIMATE, LSMEANS, LSMESTIMATE, and SLICE statements also creates tables, which are not listed in Table 66.8. For information about these tables, see the corresponding sections of Chapter 19, “Shared Concepts and Topics.”

**Table 66.8** ODS Tables Produced by PROC ORTHOREG

| ODS Table Name     | Description                | Statement       |
|--------------------|----------------------------|-----------------|
| ANOVA              | Analysis of variance       | Default         |
| FitStatistics      | Overall statistics for fit | Default         |
| Levels             | Table of class levels      | CLASS statement |
| ParameterEstimates | Parameter estimates        | Default         |

---

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “Statistical Graphics Using ODS.”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “A Primer on ODS Statistical Graphics” on page 599 in Chapter 21, “Statistical Graphics Using ODS.”

When ODS Graphics is enabled, then each of the EFFECT, ESTIMATE, LSMEANS, LSMESTIMATE, and SLICE statements can produce plots associated with their analyses. For information about these plots, see the corresponding sections of Chapter 19, “Shared Concepts and Topics.”

---

## Examples: ORTHOREG Procedure

---

### Example 66.1: Precise Analysis of Variance

The data for the following example are from Powell, Murphy, and Gramlich (1982). In order to calibrate an instrument for measuring atomic weight, 24 replicate measurements of the atomic weight of silver (chemical symbol Ag) are made with the new instrument and with a reference instrument.

**NOTE:** The results from this example vary from machine to machine, depending on floating-point configuration.

The following statements read the measurements for the two instruments into the SAS data set AgWeight:

```

title 'Atomic Weight of Silver by Two Different Instruments';
data AgWeight;
 input Instrument AgWeight @@;
 datalines;
1 107.8681568 1 107.8681465 1 107.8681572 1 107.8681785
1 107.8681446 1 107.8681903 1 107.8681526 1 107.8681494
1 107.8681616 1 107.8681587 1 107.8681519 1 107.8681486
1 107.8681419 1 107.8681569 1 107.8681508 1 107.8681672
1 107.8681385 1 107.8681518 1 107.8681662 1 107.8681424
1 107.8681360 1 107.8681333 1 107.8681610 1 107.8681477
2 107.8681079 2 107.8681344 2 107.8681513 2 107.8681197
2 107.8681604 2 107.8681385 2 107.8681642 2 107.8681365
2 107.8681151 2 107.8681082 2 107.8681517 2 107.8681448
2 107.8681198 2 107.8681482 2 107.8681334 2 107.8681609
2 107.8681101 2 107.8681512 2 107.8681469 2 107.8681360
2 107.8681254 2 107.8681261 2 107.8681450 2 107.8681368
;

```

Notice that the variation in the atomic weight measurements is several orders of magnitude less than their mean. This is a situation that can be difficult for standard, regression-based analysis-of-variance procedures to handle correctly.

The following statements invoke the ORTHOREG procedure to perform a simple one-way analysis of variance, testing for differences between the two instruments:

```

proc orthoreg data=AgWeight;
 class Instrument;
 model AgWeight = Instrument;
run;

```

Output 66.1.1 shows the resulting analysis.

#### Output 66.1.1 PROC ORTHOREG Results for Atomic Weight Example

| Atomic Weight of Silver by Two Different Instruments |        |          |
|------------------------------------------------------|--------|----------|
| The ORTHOREG Procedure                               |        |          |
| Class Level Information                              |        |          |
| Factor                                               | Levels | -Values- |
| Instrument                                           | 2      | 1 2      |

Output 66.1.1 *continued*

| Atomic Weight of Silver by Two Different Instruments |    |                    |                |         |         |
|------------------------------------------------------|----|--------------------|----------------|---------|---------|
| The ORTHOREG Procedure                               |    |                    |                |         |         |
| Dependent Variable: AgWeight                         |    |                    |                |         |         |
| Source                                               | DF | Sum of Squares     | Mean Square    | F Value | Pr > F  |
| Model                                                | 1  | 3.6383419E-9       | 3.6383419E-9   | 15.95   | 0.0002  |
| Error                                                | 46 | 1.0495173E-8       | 2.281559E-10   |         |         |
| Corrected Total                                      | 47 | 1.4133515E-8       |                |         |         |
|                                                      |    | Root MSE           | 0.0000151048   |         |         |
|                                                      |    | R-Square           | 0.2574265445   |         |         |
| Parameter                                            | DF | Parameter Estimate | Standard Error | t Value | Pr >  t |
| Intercept                                            | 1  | 107.868136354166   | 3.0832608E-6   | 3.499E7 | <.0001  |
| (Instrument='1')                                     | 1  | 0.00001741249999   | 4.3603893E-6   | 3.99    | 0.0002  |
| (Instrument='2')                                     | 0  | 0                  | .              | .       | .       |

The mean difference between instruments is about  $1.74 \times 10^{-5}$  (the value of the `(Instrument='1')` parameter in the parameter estimates table), whereas the level of background variation in the measurements is about  $1.51 \times 10^{-5}$  (the value of the root mean square error). At this level of error, the difference is significant, with a  $p$ -value of 0.0002.

The National Institute of Standards and Technology (1998) has provided certified ANOVA values for this data set. The following statements use ODS to examine the ANOVA values produced by both the ORTHOREG and GLM procedures more precisely for comparison with the NIST-certified values:

```

ods listing close;

proc orthoreg data=AgWeight;
 class Instrument;
 model AgWeight = Instrument;
 ods output ANOVA = OrthoregANOVA
 FitStatistics = OrthoregFitStat;
run;

proc glm data=AgWeight;
 class Instrument;
 model AgWeight = Instrument;
 ods output OverallANOVA = GLMANOVA
 FitStatistics = GLMFitStat;
run;
ods listing;

data _null_;
 set OrthoregANOVA (in=inANOVA)
 OrthoregFitStat(in=inFitStat);
 if (inANOVA) then do;
 if (Source = 'Model') then put "Model SS: " ss e20.;
 if (Source = 'Error') then put "Error SS: " ss e20.;
 end;
 if (inFitStat) then do;
 if (Statistic = 'Root MSE') then
 put "Root MSE: " nValue1 e20.;
 if (Statistic = 'R-Square') then
 put "R-Square: " nValue1 best20.;
 end;
run;

data _null_;
 set GLMANOVA (in=inANOVA)
 GLMFitStat(in=inFitStat);
 if (inANOVA) then do;
 if (Source = 'Model') then put "Model SS: " ss e20.;
 if (Source = 'Error') then put "Error SS: " ss e20.;
 end;
 if (inFitStat) then put "Root MSE: " RootMSE e20.;
 if (inFitStat) then put "R-Square: " RSquare best20.;
run;

```

In SAS/STAT software prior to SAS 8, PROC GLM gave much less accurate results than PROC ORTHOREG. Table 66.9 and Table 66.10 compare the ANOVA values certified by NIST with those produced by the two procedures.

**Table 66.9** Accuracy Comparison for Sums of Squares

| Values         | Model SS            | Error SS            |
|----------------|---------------------|---------------------|
| NIST-certified | 3.6383418750000E-09 | 1.0495172916667E-08 |
| ORTHOREG       | 3.6383418747907E-09 | 1.0495172916797E-08 |

**Table 66.9** *continued*

| Values            | Model SS            | Error SS            |
|-------------------|---------------------|---------------------|
| GLM, since SAS 8  | 3.6383418747907E-09 | 1.0495172916797E-08 |
| GLM, before SAS 8 | 0                   | 1.0331496763990E-08 |

**Table 66.10** Accuracy Comparison for Fit Statistics

| Values            | Root MSE            | R Square         |
|-------------------|---------------------|------------------|
| NIST-certified    | 1.5104831444641E-05 | 0.25742654453832 |
| ORTHOREG          | 1.5104831444735E-05 | 0.25742654452494 |
| GLM, since SAS 8  | 1.5104831444735E-05 | 0.25742654452494 |
| GLM, before SAS 8 | 1.4986585859992E-05 | 0                |

Although the PROC ORTHOREG values and the PROC GLM values for the current version are quite close to the certified ones, the PROC GLM values for releases prior to SAS 8 are not. In fact, since the model sum of squares is so small, in prior releases the GLM procedure set it (and consequently R square) to zero.

## Example 66.2: Wampler Data

This example applies the ORTHOREG procedure to a collection of data sets noted for being ill-conditioned. The `OUTEST=` data set is used to collect the results for comparison with values certified to be correct by the National Institute of Standards and Technology (1998).

**NOTE:** The results from this example vary from machine to machine, depending on floating-point configuration.

The data are from Wampler (1970). The independent variates for all five data sets are  $x^i$ ,  $i = 1, \dots, 5$ , for  $x = 0, 1, \dots, 20$ . Two of the five dependent variables are exact linear functions of the independent terms:

$$y_1 = 1 + x + x^2 + x^3 + x^4 + x^5$$

$$y_2 = 1 + 0.1x + 0.01x^2 + 0.001x^3 + 0.0001x^4 + 0.00001x^5$$

The other three dependent variables have the same mean value as  $y_1$ , but with nonzero errors:

$$y_3 = y_1 + e$$

$$y_4 = y_1 + 100e$$

$$y_5 = y_1 + 10000e$$

where  $e$  is a vector of values with standard deviation  $\sim 2044$ , chosen to be orthogonal to the mean model for  $y_1$ .

The following statements create a SAS data set Wampler that contains the Wampler data, run a SAS macro program that uses PROC ORTHOREG to fit a fifth-order polynomial in  $x$  to each of the Wampler dependent variables, and collect the results in a data set named ParmEst:

```

data Wampler;
 do x=0 to 20;
 input e @@;
 y1 = 1 + x + x**2 + x**3
 + x**4 + x**5;
 y2 = 1 + .1 *x + .01 *x**2 + .001*x**3
 + .0001*x**4 + .00001*x**5;
 y3 = y1 + e;
 y4 = y1 + 100*e;
 y5 = y1 + 10000*e;
 output;
 end;
 datalines;
759 -2048 2048 -2048 2523 -2048 2048 -2048 1838 -2048 2048
-2048 1838 -2048 2048 -2048 2523 -2048 2048 -2048 759
;

%macro WTest;
 data ParmEst; if (0); run;
 %do i = 1 %to 5;
 proc orthoreg data=Wampler outest=ParmEst&i noprint;
 model y&i = x *x *x*x*x *x*x*x*x*x *x*x*x*x*x*x;
 data ParmEst&i; set ParmEst&i; Dep = "y&i";
 data ParmEst; set ParmEst ParmEst&i;
 label Col1='x' Col2='x**2' Col3='x**3'
 Col4='x**4' Col5='x**5';
 run;
 %end;
%mend;
%WTest;

```

Instead of displaying the raw values of the RMSE and parameter estimates, use an additional DATA step as follows to compute the deviations from the values certified to be correct by the National Institute of Standards and Technology (1998):

```

data ParmEst; set ParmEst;
 if (Dep = 'y1') then
 RMSE = _RMSE_ - 0.000000000000000;
 else if (Dep = 'y2') then
 RMSE = _RMSE_ - 0.000000000000000;
 else if (Dep = 'y3') then
 RMSE = _RMSE_ - 2360.14502379268;
 else if (Dep = 'y4') then
 RMSE = _RMSE_ - 236014.502379268;
 else if (Dep = 'y5') then
 RMSE = _RMSE_ - 23601450.2379268;
 if (Dep ^= 'y2') then do;

```

```

Intercept = Intercept - 1.000000000000000;
Col1 = Col1 - 1.000000000000000;
Col2 = Col2 - 1.000000000000000;
Col3 = Col3 - 1.000000000000000;
Col4 = Col4 - 1.000000000000000;
Col5 = Col5 - 1.000000000000000;
end;
else do;
Intercept = Intercept - 1.000000000000000;
Col1 = Col1 - 0.100000000000000;
Col2 = Col2 - 0.100000000000000e-1;
Col3 = Col3 - 0.100000000000000e-2;
Col4 = Col4 - 0.100000000000000e-3;
Col5 = Col5 - 0.100000000000000e-4;
end;
run;

proc print data=ParmEst label noobs;
 title 'Wampler data: Deviations from Certified Values';
 format _RMSE_ Intercept Col1-Col5 e9.;
 var Dep _RMSE_ Intercept Col1-Col5;
run;

```

The results, shown in [Output 66.2.1](#), indicate that the values computed by PROC ORTHOREG are quite close to the NIST-certified values.

**Output 66.2.1** Wampler Data: Deviations from Certified Values

| Wampler data: Deviations from Certified Values |           |           |           |           |           |           |           |
|------------------------------------------------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| Dep                                            | _RMSE_    | Intercept | x         | x**2      | x**3      | x**4      | x**5      |
| y1                                             | 0.00E+00  | 5.46E-12  | -9.82E-11 | 1.55E-11  | -5.68E-13 | 3.55E-14  | -6.66E-16 |
| y2                                             | 0.00E+00  | 8.88E-16  | -3.19E-15 | 1.24E-15  | -1.88E-16 | 1.20E-17  | -2.57E-19 |
| y3                                             | -2.09E-11 | -7.73E-11 | 1.46E-11  | -2.09E-11 | 2.50E-12  | -1.28E-13 | 2.66E-15  |
| y4                                             | -4.07E-10 | -5.38E-10 | 8.99E-10  | -3.29E-10 | 4.23E-11  | -2.27E-12 | 4.35E-14  |
| y5                                             | -3.35E-08 | -4.10E-08 | 8.07E-08  | -2.77E-08 | 3.54E-09  | -1.90E-10 | 3.64E-12  |

### Example 66.3: Fitting Polynomials

The extra accuracy of the regression algorithm used by PROC ORTHOREG is most useful when the model contains near-singularities that you want to be able to distinguish from true singularities. This example demonstrates this usefulness in the context of fitting polynomials of high degree.

**NOTE:** The results from this example vary from machine to machine, depending on floating-point configuration.

The following DATA step computes a response  $y$  as an exact ninth-degree polynomial function of a predictor  $x$  evaluated at 0, 0.01, 0.02, ..., 1.

```

title 'Polynomial Data';
data Polynomial;
 do i = 1 to 101;
 x = (i-1)/(101-1);
 y = 10**(9/2);
 do j = 0 to 8;
 y = y * (x - j/8);
 end;
 output;
 end;
run;

```

The polynomial is constructed in such a way that its zeros lie at  $x = i/8$  for  $i = 0, \dots, 8$ . The following statements use the EFFECT statement to fit a ninth-degree polynomial to this data with PROC ORTHOREG. The EFFECT statement makes it easy to specify complicated polynomial models.

```

ods graphics on;

proc orthoreg data=Polynomial;
 effect xMod = polynomial(x / degree=9);
 model y = xMod;
 effectplot fit / obs;
 store OStore;
run;

ods graphics off;

```

The effect xMod defined by the EFFECT statement refers to all nine degrees of freedom in the ninth-degree polynomial (excluding the intercept term). The resulting output is shown in [Output 66.3.1](#). Note that the R square for the fit is 1, indicating that the ninth-degree polynomial has been correctly fit.

**Output 66.3.1** PROC ORTHOREG Results for Ninth-Degree Polynomial

| Polynomial Data        |     |                |              |         |        |
|------------------------|-----|----------------|--------------|---------|--------|
| The ORTHOREG Procedure |     |                |              |         |        |
| Dependent Variable: y  |     |                |              |         |        |
| Source                 | DF  | Sum of Squares | Mean Square  | F Value | Pr > F |
| Model                  | 9   | 15.527180055   | 1.7252422284 | 1.65E22 | <.0001 |
| Error                  | 91  | 9.496616E-21   | 1.043584E-22 |         |        |
| Corrected Total        | 100 | 15.527180055   |              |         |        |
|                        |     | Root MSE       | 1.02156E-11  |         |        |
|                        |     | R-Square       | 1            |         |        |

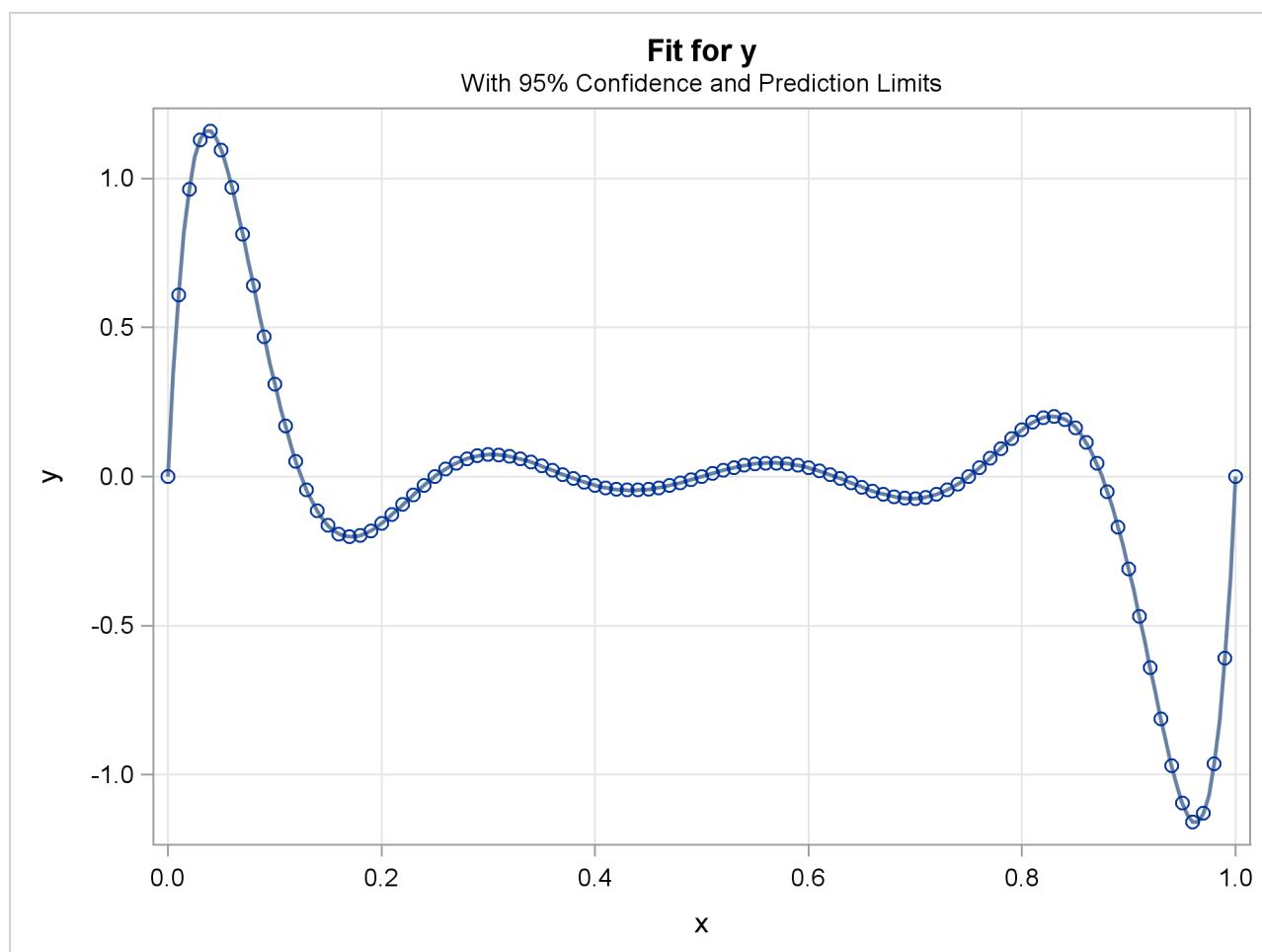


## Output 66.3.1 continued

| Parameter | DF | Parameter Estimate | Standard Error | t Value | Pr >  t |
|-----------|----|--------------------|----------------|---------|---------|
| Intercept | 1  | -3.24572035915E-11 | 8.114115E-12   | -4.00   | 0.0001  |
| x         | 1  | 75.9977312440678   | 4.898326E-10   | 1.55E11 | <.0001  |
| x^2       | 1  | -1652.40781362191  | 9.5027919E-9   | -174E9  | <.0001  |
| x^3       | 1  | 14249.4539769783   | 8.3110512E-8   | 1.71E11 | <.0001  |
| x^4       | 1  | -64932.461575205   | 3.8997072E-7   | -167E9  | <.0001  |
| x^5       | 1  | 173315.359360779   | 1.066611E-6    | 1.62E11 | <.0001  |
| x^6       | 1  | -280158.03646002   | 1.7523078E-6   | -16E10  | <.0001  |
| x^7       | 1  | 269781.812887653   | 1.7021134E-6   | 1.58E11 | <.0001  |
| x^8       | 1  | -142302.494710055  | 9.0027891E-7   | -158E9  | <.0001  |
| x^9       | 1  | 31622.7766022468   | 1.997493E-7    | 1.58E11 | <.0001  |

The fit plot produced by the EFFECTPLOT statement, [Output 66.3.2](#), also demonstrates the perfect fit.

## Output 66.3.2 PROC ORTHOREG Fit Plot for Ninth-Degree Polynomial



Finally, you can use the PLM procedure with the fit model saved by the STORE statement in the item store

OStore to check the predicted values for the known zeros of the polynomial, as shown in the following statements:

```
data Zeros(keep=x);
 do j = 0 to 8;
 x = j/8;
 output;
 end;
run;

proc plm restore=OStore noprint;
 score data=Zeros out=OZeros pred=OPred;
run;

proc print noobs;
run;
```

The predicted values of the zeros, shown in [Output 66.3.3](#), are again all miniscule.

**Output 66.3.3** Predicted Zeros for Ninth-Degree Polynomial

| Polynomial Data |             |
|-----------------|-------------|
| x               | OPred       |
| 0.000           | -3.2457E-11 |
| 0.125           | -2.1262E-11 |
| 0.250           | -9.5867E-12 |
| 0.375           | -2.2895E-11 |
| 0.500           | -5.2154E-11 |
| 0.625           | -1.2329E-10 |
| 0.750           | -2.5329E-10 |
| 0.875           | -3.9836E-10 |
| 1.000           | -5.9663E-10 |

To compare these results with those from a least squares fit produced by an alternative algorithm, consider fitting a polynomial to this data using the GLM procedure. PROC GLM does not have an EFFECT statement, but the familiar bar notation can still be used to specify a ninth-degree polynomial fairly succinctly, as shown in the following statements:

```
proc glm data=Polynomial;
 model y = x|x|x|x|x|x|x|x|x;
 store GStore;
run;
```

Partial results are shown in [Output 66.3.4](#). In this case, the R square for the fit is only about 0.83, indicating that the full ninth-degree polynomial was not correctly fit.

**Output 66.3.4** PROC GLM for Ninth-Degree Polynomial

| Polynomial Data       |          |                |             |           |        |
|-----------------------|----------|----------------|-------------|-----------|--------|
| The GLM Procedure     |          |                |             |           |        |
| Dependent Variable: y |          |                |             |           |        |
| Source                | DF       | Sum of Squares | Mean Square | F Value   | Pr > F |
| Model                 | 8        | 12.91166643    | 1.61395830  | 56.77     | <.0001 |
| Error                 | 92       | 2.61551363     | 0.02842950  |           |        |
| Corrected Total       | 100      | 15.52718006    |             |           |        |
|                       | R-Square | Coeff Var      | Root MSE    | y Mean    |        |
|                       | 0.831553 | -6.6691E17     | 0.168610    | -0.000000 |        |

The following statements, which use the PLM procedure to compute predictions based on the GLM fit at the true zeros of the polynomial, also confirm that PROC GLM is not able to correctly fit a polynomial of this degree, as shown in [Output 66.3.5](#).

```
proc plm restore=GStore noprint;
 score data=Zeros out=GZeros pred=GPred;
run;

data Zeros;
 merge OZeros GZeros;
run;

proc print noobs;
run;
```

**Output 66.3.5** Predicted Zeros for Ninth-Degree Polynomial

| Polynomial Data |             |          |
|-----------------|-------------|----------|
| x               | OPred       | GPred    |
| 0.000           | -3.2457E-11 | 0.44896  |
| 0.125           | -2.1262E-11 | 0.22087  |
| 0.250           | -9.5867E-12 | -0.19037 |
| 0.375           | -2.2895E-11 | 0.12710  |
| 0.500           | -5.2154E-11 | 0.00000  |
| 0.625           | -1.2329E-10 | -0.12710 |
| 0.750           | -2.5329E-10 | 0.19037  |
| 0.875           | -3.9836E-10 | -0.22087 |
| 1.000           | -5.9663E-10 | -0.44896 |

---

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# Chapter 67

## The PHREG Procedure

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## Overview: PHREG Procedure

The analysis of survival data requires special techniques because the data are almost always incomplete and familiar parametric assumptions might be unjustifiable. Investigators follow subjects until they reach a prespecified endpoint (for example, death). However, subjects sometimes withdraw from a study, or the study is completed before the endpoint is reached. In these cases, the survival times (also known as failure times) are *censored*; subjects survived to a certain time beyond which their status is unknown. The uncensored survival times are sometimes referred to as *event* times. Methods of survival analysis must account for both censored and uncensored data.

Many types of models have been used for survival data. Two of the more popular types of models are the accelerated failure time model (Kalbfleisch and Prentice 1980) and the Cox proportional hazards model (Cox 1972). Each has its own assumptions about the underlying distribution of the survival times. Two closely related functions often used to describe the distribution of survival times are the survivor function and the hazard function. See the section “[Failure Time Distribution](#)” on page 5608 for definitions. The accelerated failure time model assumes a parametric form for the effects of the explanatory variables and usually assumes a parametric form for the underlying survivor function. The Cox proportional hazards model also assumes a parametric form for the effects of the explanatory variables, but it allows an unspecified form for the underlying survivor function.

The PHREG procedure performs regression analysis of survival data based on the Cox proportional hazards model. Cox’s semiparametric model is widely used in the analysis of survival data to explain the effect of explanatory variables on hazard rates.

The survival time of each member of a population is assumed to follow its own hazard function,  $\lambda_i(t)$ , expressed as

$$\lambda_i(t) = \lambda(t; \mathbf{Z}_i) = \lambda_0(t) \exp(\mathbf{Z}_i' \boldsymbol{\beta})$$

where  $\lambda_0(t)$  is an arbitrary and unspecified baseline hazard function,  $\mathbf{Z}_i$  is the vector of explanatory variables for the  $i$ th individual, and  $\boldsymbol{\beta}$  is the vector of unknown regression parameters that is associated with the explanatory variables. The vector  $\boldsymbol{\beta}$  is assumed to be the same for all individuals. The survivor function can be expressed as

$$S(t; \mathbf{Z}_i) = [S_0(t)]^{\exp(\mathbf{Z}_i' \boldsymbol{\beta})}$$

where  $S_0(t) = \exp(-\int_0^t \lambda_0(u) du)$  is the baseline survivor function. To estimate  $\boldsymbol{\beta}$ , Cox (1972, 1975) introduced the partial likelihood function, which eliminates the unknown baseline hazard  $\lambda_0(t)$  and accounts for censored survival times.

The partial likelihood of Cox also allows time-dependent explanatory variables. An explanatory variable is time-dependent if its value for any given individual can change over time. Time-dependent variables have many useful applications in survival analysis. You can use a time-dependent variable to model the effect of subjects changing treatment groups. Or you can include time-dependent variables such as blood pressure or blood chemistry measures that vary with time during the course of a study. You can also use time-dependent variables to test the validity of the proportional hazards model.

An alternative way to fit models with time-dependent explanatory variables is to use the counting process style of input. The counting process formulation enables PROC PHREG to fit a superset of the Cox model,



known as the multiplicative hazards model. This extension also includes recurrent events data and left-truncation of failure times. The theory of these models is based on the counting process pioneered by Andersen and Gill (1982), and the model is often referred to as the Andersen-Gill model.

Multivariate failure-time data arise when each study subject can potentially experience several events (for example, multiple infections after surgery) or when there exists some natural or artificial clustering of subjects (for example, a litter of mice) that induces dependence among the failure times of the same cluster. Data in the former situation are referred to as multiple events data, which include recurrent events data as a special case; data in the latter situation are referred to as clustered data. You can use PROC PHREG to carry out various methods of analyzing these data.

The population under study can consist of a number of subpopulations, each of which has its own baseline hazard function. PROC PHREG performs a stratified analysis to adjust for such subpopulation differences. Under the stratified model, the hazard function for the  $j$ th individual in the  $i$ th stratum is expressed as

$$\lambda_{ij}(t) = \lambda_{i0}(t) \exp(\mathbf{Z}'_{ij}\boldsymbol{\beta})$$

where  $\lambda_{i0}(t)$  is the baseline hazard function for the  $i$ th stratum and  $\mathbf{Z}_{ij}$  is the vector of explanatory variables for the individual. The regression coefficients are assumed to be the same for all individuals across all strata.

Ties in the failure times can arise when the time scale is genuinely discrete or when survival times that are generated from the continuous-time model are grouped into coarser units. The PHREG procedure includes four methods of handling ties. The *discrete* logistic model is available for discrete time-scale data. The other three methods apply to continuous time-scale data. The *exact* method computes the exact conditional probability under the model that the set of observed tied event times occurs before all the censored times with the same value or before larger values. *Breslow* and *Efron* methods provide approximations to the exact method.

Variable selection is a typical exploratory exercise in multiple regression when the investigator is interested in identifying important prognostic factors from a large number of candidate variables. The PHREG procedure provides four selection methods: forward selection, backward elimination, stepwise selection, and best subset selection. The best subset selection method is based on the likelihood score statistic. This method identifies a specified number of best models that contain one, two, or three variables and so on, up to the single model that contains all of the explanatory variables.

The PHREG procedure also enables you to do the following: include an offset variable in the model; weight the observations in the input data; test linear hypotheses about the regression parameters; perform conditional logistic regression analysis for matched case-control studies; output survivor function estimates, residuals, and regression diagnostics; and estimate and plot the survivor function for a new set of covariates.

PROC PHREG can also be used to fit the multinomial logit choice model to discrete choice data. See [http://support.sas.com/resources/papers/tnote/tnote\\_marketresearch.html](http://support.sas.com/resources/papers/tnote/tnote_marketresearch.html) for more information about discrete choice modeling and the multinomial logit model. Look for the “Discrete Choice” report.

The PHREG procedure uses ODS Graphics to create graphs as part of its output. For example, the ASSESS statement uses a graphical method that uses ODS Graphics to check the adequacy of the model. See Chapter 21, “Statistical Graphics Using ODS,” for general information about ODS Graphics.

For both the BASELINE and OUTPUT statements, the default method of estimating a survivor function has changed to the Breslow (1972) estimator—that is, METHOD=CH. The option NOMEAN that was available

in the BASELINE statement prior to SAS/STAT 9.2 has become obsolete—that is, requested statistics at the sample average values of the covariates are no longer computed and added to the OUT= data set. However, if the COVARIATES= data set is not specified, the requested statistics are computed and output for the covariate set that consists of the reference levels for the CLASS variables and sample averages for the continuous variable. In addition to the requested statistics, the OUT= data set also contains all variables in the COVARIATES= data set.

The remaining sections of this chapter contain information about how to use PROC PHREG, information about the underlying statistical methodology, and some sample applications of the procedure. The section “Getting Started: PHREG Procedure” on page 5543 introduces PROC PHREG with two examples. The section “Syntax: PHREG Procedure” on page 5553 describes the syntax of the procedure. The section “Details: PHREG Procedure” on page 5608 summarizes the statistical techniques used in PROC PHREG. The section “Examples: PHREG Procedure” on page 5678 includes eight additional examples of useful applications. Experienced SAS/STAT software users might decide to proceed to the “Syntax” section, while other users might choose to read both the “Getting Started” and “Examples” sections before proceeding to “Syntax” and “Details.”

---

## Getting Started: PHREG Procedure

This section uses the two-sample vaginal cancer mortality data from Kalbfleisch and Prentice (1980, p. 2) in two examples to illustrate some of the basic features of PROC PHREG. The first example carries out a classical Cox regression analysis and the second example performs a Bayesian analysis of the Cox model.

Two groups of rats received different pretreatment regimes and then were exposed to a carcinogen. Investigators recorded the survival times of the rats from exposure to mortality from vaginal cancer. Four rats died of other causes, so their survival times are censored. Interest lies in whether the survival curves differ between the two groups.

The following DATA step creates the data set Rats, which contains the variable Days (the survival time in days), the variable Status (the censoring indicator variable: 0 if censored and 1 if not censored), and the variable Group (the pretreatment group indicator).

```
data Rats;
 label Days = 'Days from Exposure to Death';
 input Days Status Group @@;
 datalines;
143 1 0 164 1 0 188 1 0 188 1 0
190 1 0 192 1 0 206 1 0 209 1 0
213 1 0 216 1 0 220 1 0 227 1 0
230 1 0 234 1 0 246 1 0 265 1 0
304 1 0 216 0 0 244 0 0 142 1 1
156 1 1 163 1 1 198 1 1 205 1 1
232 1 1 232 1 1 233 1 1 233 1 1
233 1 1 233 1 1 239 1 1 240 1 1
261 1 1 280 1 1 280 1 1 296 1 1
296 1 1 323 1 1 204 0 1 344 0 1
;
```

By using ODS Graphics, PROC PHREG allows you to plot the survival curve for Group=0 and the survival curve for Group=1, but first you must save these two covariate values in a SAS data set as in the following DATA step:

```
data Regimes;
 Group=0;
 output;
 Group=1;
 output;
run;
```

---

## Classical Method of Maximum Likelihood

PROC PHREG fits the Cox model by maximizing the partial likelihood and computes the baseline survivor function by using the Breslow (1972) estimate. The following statements produce [Figure 67.1](#) and [Figure 67.2](#):

```
ods graphics on;
proc phreg data=Rats plot(overlay)=survival;
 model Days*Status(0)=Group;
 baseline covariates=regimes out=_null_;
run;
ods graphics off;
```

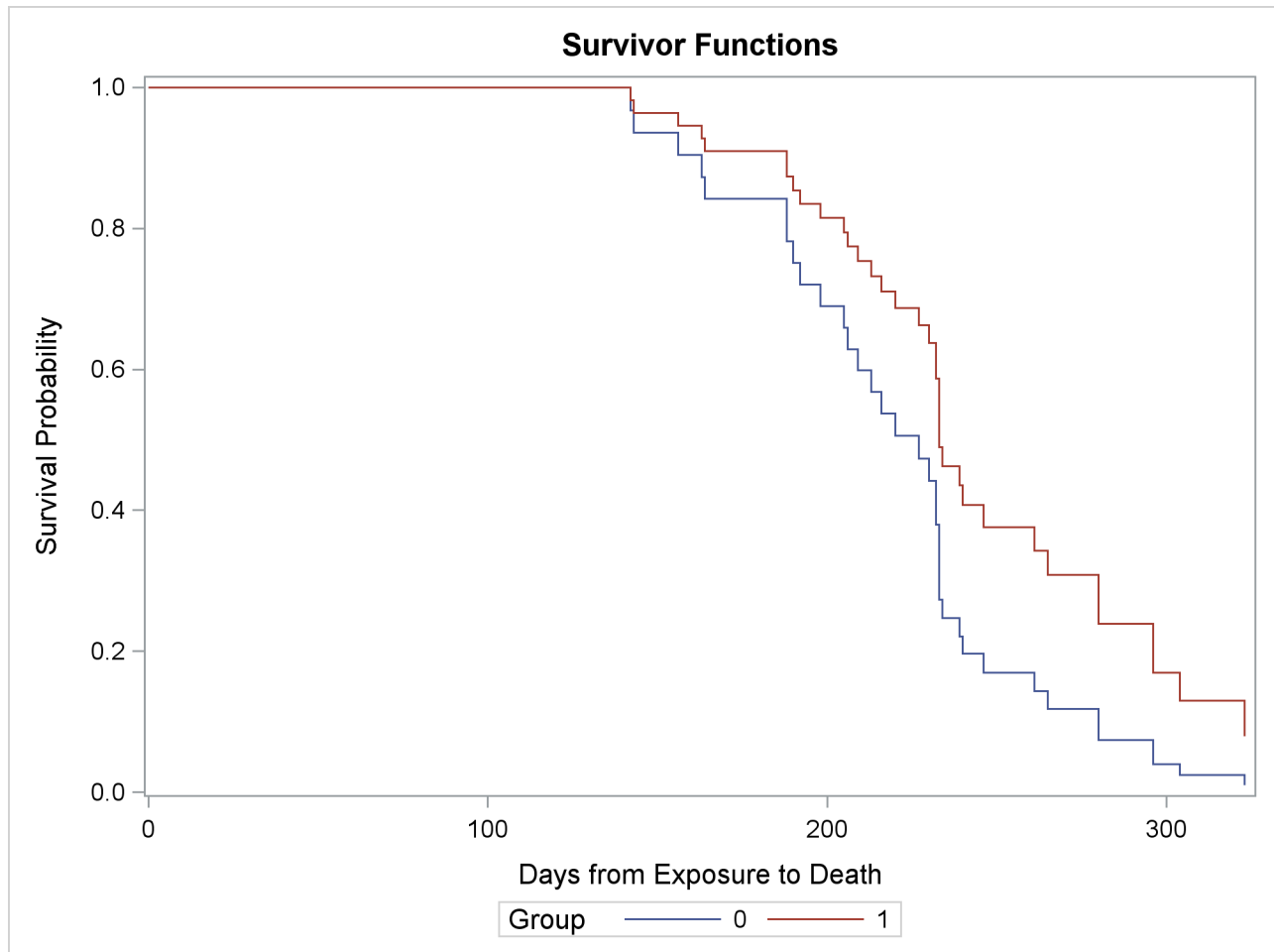
In the MODEL statement, the response variable, Days, is crossed with the censoring variable, Status, with the value that indicates censoring is enclosed in parentheses. The values of Days are considered censored if the value of Status is 0; otherwise, they are considered event times.

Graphs are produced when ODS Graphics is enabled. The survival curves for the two observations in the data set Regime, specified in the COVARIATES= option in the BASELINE statement, are requested through the PLOTS= option with the OVERLAY option for overlaying both survival curves in the same plot.

[Figure 67.2](#) shows a typical printed output of a classical analysis. Since Group takes only two values, the null hypothesis for no difference between the two groups is identical to the null hypothesis that the regression coefficient for Group is 0. All three tests in the “Testing Global Null Hypothesis: BETA=0” table (see the section “Testing the Global Null Hypothesis” on page 5625) suggest that the survival curves for the two pretreatment groups might not be the same. In this model, the hazard ratio (or risk ratio) for Group, defined as the exponentiation of the regression coefficient for Group, is the ratio of the hazard functions between the two groups. The estimate is 0.551, implying that the hazard function for Group=1 is smaller than that for Group=0. In other words, rats in Group=1 lived longer than those in Group=0. This conclusion is also revealed in the plot of the survivor functions in [Figure 67.2](#).

**Figure 67.1** Comparison of Two Survival Curves

| The PHREG Procedure                                |                  |                             |                 |                  |            |              |
|----------------------------------------------------|------------------|-----------------------------|-----------------|------------------|------------|--------------|
| Model Information                                  |                  |                             |                 |                  |            |              |
| Data Set                                           | WORK.RATS        |                             |                 |                  |            |              |
| Dependent Variable                                 | Days             | Days from Exposure to Death |                 |                  |            |              |
| Censoring Variable                                 | Status           |                             |                 |                  |            |              |
| Censoring Value(s)                                 | 0                |                             |                 |                  |            |              |
| Ties Handling                                      | BRESLOW          |                             |                 |                  |            |              |
| Number of Observations Read                        |                  | 40                          |                 |                  |            |              |
| Number of Observations Used                        |                  | 40                          |                 |                  |            |              |
| Summary of the Number of Event and Censored Values |                  |                             |                 |                  |            |              |
|                                                    | Total            | Event                       | Censored        | Percent Censored |            |              |
|                                                    | 40               | 36                          | 4               | 10.00            |            |              |
| Convergence Status                                 |                  |                             |                 |                  |            |              |
| Convergence criterion (GCONV=1E-8) satisfied.      |                  |                             |                 |                  |            |              |
| Model Fit Statistics                               |                  |                             |                 |                  |            |              |
|                                                    | Criterion        | Without Covariates          | With Covariates |                  |            |              |
|                                                    | -2 LOG L         | 204.317                     | 201.438         |                  |            |              |
|                                                    | AIC              | 204.317                     | 203.438         |                  |            |              |
|                                                    | SBC              | 204.317                     | 205.022         |                  |            |              |
| Testing Global Null Hypothesis: BETA=0             |                  |                             |                 |                  |            |              |
|                                                    | Test             | Chi-Square                  | DF              | Pr > ChiSq       |            |              |
|                                                    | Likelihood Ratio | 2.8784                      | 1               | 0.0898           |            |              |
|                                                    | Score            | 3.0001                      | 1               | 0.0833           |            |              |
|                                                    | Wald             | 2.9254                      | 1               | 0.0872           |            |              |
| Analysis of Maximum Likelihood Estimates           |                  |                             |                 |                  |            |              |
| Parameter                                          | DF               | Parameter Estimate          | Standard Error  | Chi-Square       | Pr > ChiSq | Hazard Ratio |
| Group                                              | 1                | -0.59590                    | 0.34840         | 2.9254           | 0.0872     | 0.551        |

**Figure 67.2** Survivorship for the Two Pretreatment Regimes

In this example, the comparison of two survival curves is put in the form of a proportional hazards model. This approach is essentially the same as the log-rank (Mantel-Haenszel) test. In fact, if there are no ties in the survival times, the likelihood score test in the Cox regression analysis is identical to the log-rank test. The advantage of the Cox regression approach is the ability to adjust for the other variables by including them in the model. For example, the present model could be expanded by including a variable that contains the initial body weights of the rats.

Next, consider a simple test of the validity of the proportional hazards assumption. The proportional hazards model for comparing the two pretreatment groups is given by the following:

$$\lambda(t) = \begin{cases} \lambda_0(t) & \text{if GROUP} = 0 \\ \lambda_0(t)e^{\beta_1} & \text{if GROUP} = 1 \end{cases}$$

The ratio of hazards is  $e^{\beta_1}$ , which does not depend on time. If the hazard ratio changes with time, the proportional hazards model assumption is invalid. Simple forms of departure from the proportional hazards model can be investigated with the following time-dependent explanatory variable  $x = x(t)$ :

$$x(t) = \begin{cases} 0 & \text{if GROUP} = 0 \\ \log(t) - 5.4 & \text{if GROUP} = 1 \end{cases}$$

Here,  $\log(t)$  is used instead of  $t$  to avoid numerical instability in the computation. The constant, 5.4, is the average of the logs of the survival times and is included to improve interpretability. The hazard ratio in the two groups then becomes  $e^{\beta_1 - 5.4\beta_2 t^{\beta_2}}$ , where  $\beta_2$  is the regression parameter for the time-dependent variable  $x$ . The term  $e^{\beta_1}$  represents the hazard ratio at the geometric mean of the survival times. A nonzero value of  $\beta_2$  would imply an increasing ( $\beta_2 > 0$ ) or decreasing ( $\beta_2 < 0$ ) trend in the hazard ratio with time.

The following statements implement this simple test of the proportional hazards assumption. The MODEL statement includes the time-dependent explanatory variable X, which is defined subsequently by the programming statement. At each event time, subjects in the risk set (those alive just before the event time) have their X values changed accordingly.

```
proc phreg data=Rats;
 model Days*Status(0)=Group X;
 X=Group*(log(Days) - 5.4);
run;
```

The analysis of the parameter estimates is displayed in [Figure 67.3](#). The Wald chi-square statistic for testing the null hypothesis that  $\beta_2 = 0$  is 0.0158. The statistic is not statistically significant when compared to a chi-square distribution with one degree of freedom ( $p = 0.8999$ ). Thus, you can conclude that there is no evidence of an increasing or decreasing trend over time in the hazard ratio.

**Figure 67.3** A Simple Test of Trend in the Hazard Ratio

| The PHREG Procedure                      |    |                    |                |            |            |              |
|------------------------------------------|----|--------------------|----------------|------------|------------|--------------|
| Analysis of Maximum Likelihood Estimates |    |                    |                |            |            |              |
| Parameter                                | DF | Parameter Estimate | Standard Error | Chi-Square | Pr > ChiSq | Hazard Ratio |
| Group                                    | 1  | -0.59976           | 0.34837        | 2.9639     | 0.0851     | 0.549        |
| X                                        | 1  | -0.22952           | 1.82489        | 0.0158     | 0.8999     | 0.795        |

## Bayesian Analysis

PROC PHREG uses the partial likelihood of the Cox model as the likelihood and generates a chain of posterior distribution samples by the Gibbs Sampler. Summary statistics, convergence diagnostics, and diagnostic plots are provided for each parameter. The following statements generate [Figure 67.4](#)–[Figure 67.10](#):

```
ods graphics on;
proc phreg data=Rats;
 model Days*Status(0)=Group;
 bayes seed=1 outpost=Post;
run;
ods graphics off;
```

The BAYES statement invokes the Bayesian analysis. The SEED= option is specified to maintain reproducibility; the OUTPOST= option saves the posterior distribution samples in a SAS data set for post-

processing; no other options are specified in the BAYES statement. By default, a uniform prior distribution is assumed on the regression coefficient Group. The uniform prior is a flat prior on the real line with a distribution that reflects ignorance of the location of the parameter, placing equal probability on all possible values the regression coefficient can take. Using the uniform prior in the following example, you would expect the Bayesian estimates to resemble the classical results of maximizing the likelihood. If you can elicit an informative prior on the regression coefficients, you should use the COEFFPRIOR= option to specify it.

You should make sure that the posterior distribution samples have achieved convergence before using them for Bayesian inference. PROC PHREG produces three convergence diagnostics by default. If ODS Graphics is enabled before calling PROC PHREG as in the preceding program, diagnostics plots are also displayed.

The results of this analysis are shown in the following figures.

The “Model Information” table in Figure 67.4 summarizes information about the model you fit and the size of the simulation.

**Figure 67.4** Model Information

| The PHREG Procedure |           |                             |
|---------------------|-----------|-----------------------------|
| Bayesian Analysis   |           |                             |
| Model Information   |           |                             |
| Data Set            | WORK.RATS |                             |
| Dependent Variable  | Days      | Days from Exposure to Death |
| Censoring Variable  | Status    |                             |
| Censoring Value(s)  | 0         |                             |
| Model               | Cox       |                             |
| Ties Handling       | BRESLOW   |                             |
| Sampling Algorithm  | ARMS      |                             |
| Burn-In Size        | 2000      |                             |
| MC Sample Size      | 10000     |                             |
| Thinning            | 1         |                             |

PROC PHREG first fits the Cox model by maximizing the partial likelihood. The only parameter in the model is the regression coefficient of Group. The maximum likelihood estimate (MLE) of the parameter and its 95% confidence interval are shown in Figure 67.5.

**Figure 67.5** Classical Parameter Estimates

| Maximum Likelihood Estimates |    |          |                |                       |        |
|------------------------------|----|----------|----------------|-----------------------|--------|
| Parameter                    | DF | Estimate | Standard Error | 95% Confidence Limits |        |
| Group                        | 1  | -0.5959  | 0.3484         | -1.2788               | 0.0870 |

Since no prior is specified for the regression coefficient, the default uniform prior is used. This information is displayed in the “Uniform Prior for Regression Coefficients” table in Figure 67.6.

**Figure 67.6** Coefficient Prior

| Uniform Prior for Regression Coefficients |          |
|-------------------------------------------|----------|
| Parameter                                 | Prior    |
| Group                                     | Constant |

The “Fit Statistics” table in [Figure 67.7](#) lists information about the fitted model. The table displays the DIC (deviance information criterion) and pD (effective number of parameters). See the section “Fit Statistics” on page 5662 for details.

**Figure 67.7** Fit Statistics

| Fit Statistics                      |         |
|-------------------------------------|---------|
| DIC (smaller is better)             | 203.444 |
| pD (Effective Number of Parameters) | 1.003   |

Summary statistics of the posterior samples are displayed in the “Posterior Summaries” table and “Posterior Intervals” table as shown in [Figure 67.8](#). Note that the mean and standard deviation of the posterior samples are comparable to the MLE and its standard error, respectively, due to the use of the uniform prior.

**Figure 67.8** Summary Statistics

| The PHREG Procedure |       |                     |                    |              |         |         |
|---------------------|-------|---------------------|--------------------|--------------|---------|---------|
| Bayesian Analysis   |       |                     |                    |              |         |         |
| Posterior Summaries |       |                     |                    |              |         |         |
| Parameter           | N     | Mean                | Standard Deviation | Percentiles  |         |         |
|                     |       |                     |                    | 25%          | 50%     | 75%     |
| Group               | 10000 | -0.5998             | 0.3511             | -0.8326      | -0.5957 | -0.3670 |
| Posterior Intervals |       |                     |                    |              |         |         |
| Parameter           | Alpha | Equal-Tail Interval |                    | HPD Interval |         |         |
| Group               | 0.050 | -1.3042             | 0.0721             | -1.2984      | 0.0756  |         |

PROC PHREG provides diagnostics to assess the convergence of the generated Markov chain. [Figure 67.9](#) shows three of these diagnostics: the lag1, lag5, lag10, and lag50 autocorrelations; the Geweke diagnostic; and the effective sample size. There is no indication that the Markov chain has not reached convergence. See the section “Statistical Diagnostic Tests” on page 144 for information about interpreting these diagnostics.

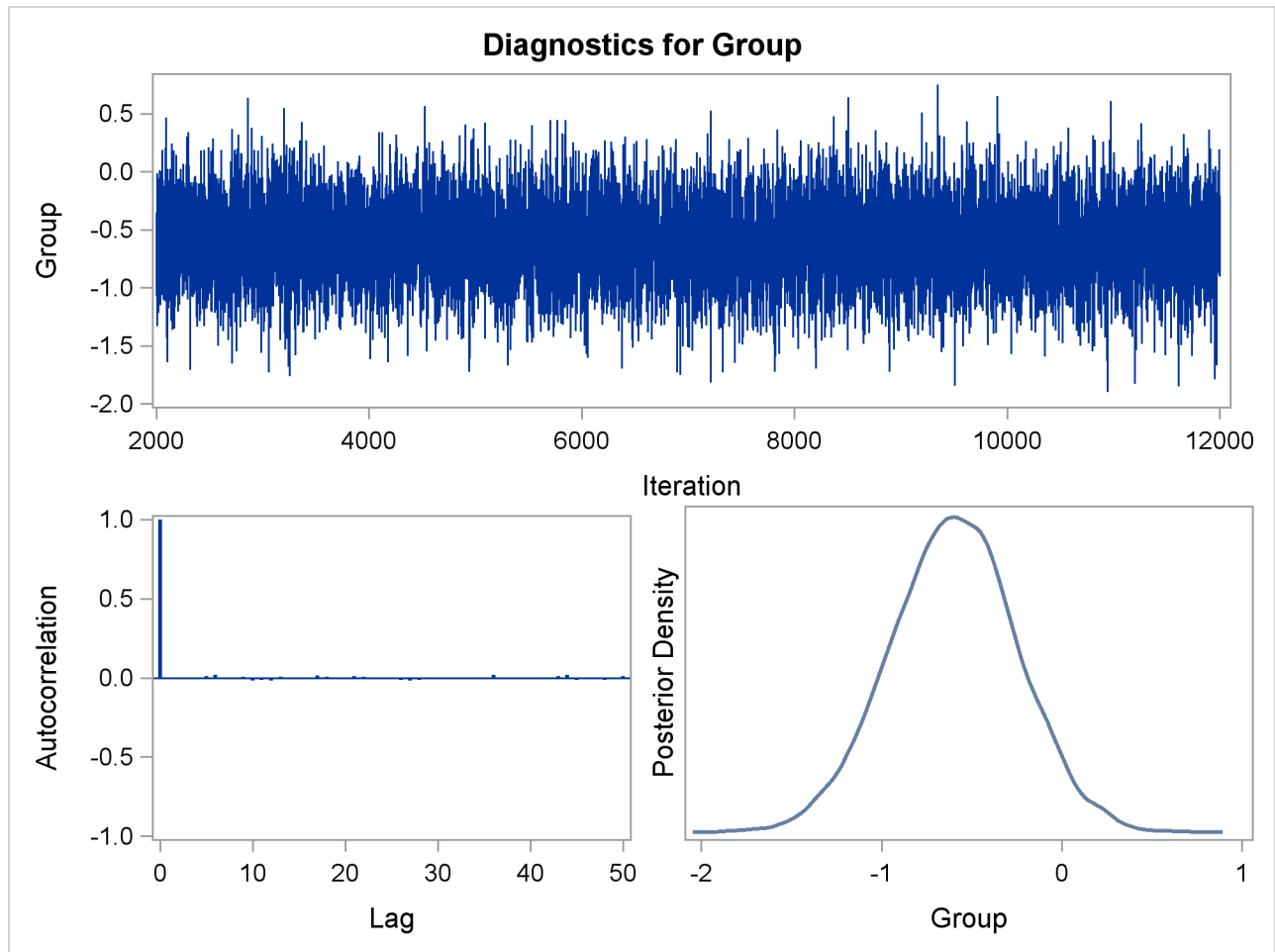


**Figure 67.9** Convergence Diagnostics

| The PHREG Procedure        |         |                      |            |        |
|----------------------------|---------|----------------------|------------|--------|
| Bayesian Analysis          |         |                      |            |        |
| Posterior Autocorrelations |         |                      |            |        |
| Parameter                  | Lag 1   | Lag 5                | Lag 10     | Lag 50 |
| Group                      | -0.0079 | 0.0091               | -0.0161    | 0.0101 |
| Geweke Diagnostics         |         |                      |            |        |
| Parameter                  | z       | Pr >  z              |            |        |
| Group                      | 0.0149  | 0.9881               |            |        |
| Effective Sample Sizes     |         |                      |            |        |
| Parameter                  | ESS     | Autocorrelation Time | Efficiency |        |
| Group                      | 10000.0 | 1.0000               | 1.0000     |        |

You can also assess the convergence of the generated Markov chain by examining the trace plot, the autocorrelation function plot, and the posterior density plot. [Figure 67.10](#) displays a panel of these three plots for the parameter Group. This graphical display is automatically produced when ODS Graphics is enabled. Note that the trace of the samples centers on  $-0.6$  with only small fluctuations, the autocorrelations are quite small, and the posterior density appears bell-shaped—all exemplifying the behavior of a converged Markov chain.

Figure 67.10 Diagnostic Plots



The proportional hazards model for comparing the two pretreatment groups is

$$\lambda(t) = \begin{cases} \lambda_0(t) & \text{if Group}=0 \\ \lambda_0(t)e^\beta & \text{if Group}=1 \end{cases}$$

The probability that the hazard of Group=0 is greater than that of Group=1 is

$$\Pr(\lambda_0(t) > \lambda_0(t)e^\beta) = \Pr(\beta < 0)$$

This probability can be enumerated from the posterior distribution samples by computing the fraction of samples with a coefficient less than 0. The following DATA step and PROC MEANS perform this calculation:

```
data New;
 set Post;
 Indicator=(Group < 0);
 label Indicator='Group < 0';
run;
proc means data=New(keep=Indicator) n mean;
run;
```

**Figure 67.11** Prob(Hazard(Group=0) > Hazard(Group=1))

| The MEANS Procedure                     |           |
|-----------------------------------------|-----------|
| Analysis Variable : Indicator Group < 0 |           |
| N                                       | Mean      |
| 10000                                   | 0.9581000 |

The PROC MEANS results are displayed in [Figure 67.11](#). There is a 95.8% chance that the hazard rate of Group=0 is greater than that of Group=1. The result is consistent with the fact that the average survival time of Group=0 is less than that of Group=1.

## Syntax: PHREG Procedure

The following statements are available in the PHREG procedure. Items within < > are optional.

```

PROC PHREG < options > ;
 ASSESS keyword < / options > ;
 BASELINE < OUT=SAS-data-set > < COVARIATES=SAS-data-set >
 < keyword=name ... keyword=name > < / options > ;
 BAYES < options > ;
 BY variables ;
 CLASS variable < (options) > < ... variable < (options) > > < / options > ;
 CONTRAST < 'label' > effect values < , ... , effect values > < / options > ;
 FREQ variable ;
 EFFECT name = effect-type (variables < / options >) ;
 ESTIMATE < 'label' > estimate-specification < / options > ;
 HAZARDRATIO < 'label' > variable < / options > ;
 ID variables ;
 LSMEANS < model-effects > < / options > ;
 LSMESTIMATE model-effect lsmestimate-specification < / options > ;
 MODEL response < * censor(list) > = < effects > < / options > ;
 OUTPUT < OUT=SAS-data-set > < keyword=name ... keyword=name > < / options > ;
 Programming statements ;
 RANDOM variable < / options > ;
 SLICE model-effect < / options > ;
 STORE < OUT= > item-store-name < / LABEL='label' > ;
 STRATA variable < (list) > < ... variable < (list) > > < / option > ;
 < label: > TEST equation < , ... , equation > < / options > ;
 WEIGHT variable < / option > ;

```

The PROC PHREG and MODEL statements are required. The CLASS statement, if present, must precede the MODEL statement, and the ASSESS or CONTRAST statement, if present, must come after the MODEL statement. The BAYES statement, that invokes a Bayesian analysis, is not compatible with the ASSESS, CONTRAST, ID, OUTPUT, and TEST statements, as well as a number of options in the PROC PHREG and MODEL statements. See the section “[Specifics for Bayesian Analysis](#)” on page 5653 for details.

The rest of this section provides detailed syntax information for each statement, beginning with the PROC PHREG statement. The remaining statements are covered in alphabetical order.

## PROC PHREG Statement

**PROC PHREG** < options > ;

The PROC PHREG statement invokes the PHREG procedure. Table 67.1 summarizes the options available in the PROC PHREG statement.

**Table 67.1** PROC PHREG Statement Options

| Option      | Description                                                                                                |
|-------------|------------------------------------------------------------------------------------------------------------|
| ALPHA=      | Specifies the level of significance                                                                        |
| ATRISK      | Displays a table that contains the number of units and the corresponding number of events in the risk sets |
| COVM        | Uses the model-based covariance matrix in the analysis                                                     |
| COVOUT      | Adds the estimated covariance matrix to the OUTEST= data set                                               |
| COVSANDWICH | Requests the robust sandwich estimate for the covariance matrix                                            |
| DATA=       | Names the SAS data set to be analyzed                                                                      |
| INEST=      | Names the SAS data set that contains initial estimates                                                     |
| MULTIPASS   | Recompiles the risk sets                                                                                   |
| NAMELEN=    | Specifies the length of effect names                                                                       |
| NOPRINT     | Suppresses all displayed output                                                                            |
| NOSUMMARY   | Suppresses the summary display observation frequencies                                                     |
| OUTEST=     | Creates an output SAS data set containing estimates of the regression coefficients                         |
| PLOTS       | Controls the plots produced through ODS Graphics                                                           |
| SIMPLE      | Displays simple descriptive statistics                                                                     |

You can specify the following *options* in the PROC PHREG statement.

### ALPHA=*number*

specifies the level of significance  $\alpha$  for  $100(1 - \alpha)\%$  confidence intervals. The value *number* must be between 0 and 1; the default value is 0.05, which results in 95% intervals. This value is used as the default confidence level for limits computed by the BASELINE, BAYES, CONTRAST, HAZARDRATIO, and MODEL statements. You can override this default by specifying the ALPHA= option in the separate statements.

### ATRISK

displays a table that contains the number of units at risk at each event time and the corresponding number of events in the risk sets. For example, the following risk set information is displayed if the ATRISK option is specified in the example in the section “Getting Started: PHREG Procedure” on page 5543.

| Risk Set Information |         |       |
|----------------------|---------|-------|
| Number of Units      |         |       |
| Days                 | At Risk | Event |
| 142                  | 40      | 1     |
| 143                  | 39      | 1     |
| 156                  | 38      | 1     |
| ⋮                    | ⋮       | ⋮     |
| 296                  | 5       | 2     |
| 304                  | 3       | 1     |
| 323                  | 2       | 1     |

**COVOUT**

adds the estimated covariance matrix of the parameter estimates to the OUTEST= data set. The COVOUT option has no effect unless the OUTEST= option is specified.

**COVM**

requests that the model-based covariance matrix (which is the inverse of the observed information matrix) be used in the analysis if the COVS option is also specified. The COVM option has no effect if the COVS option is not specified.

**COVSANDWICH <(AGGREGATE)>****COVS <(AGGREGATE)>**

requests the robust sandwich estimate of Lin and Wei (1989) for the covariance matrix. When this option is specified, this robust sandwich estimate is used in the Wald tests for testing the global null hypothesis, null hypotheses of individual parameters, and the hypotheses in the CONTRAST and TEST statements. In addition, a modified score test is computed in the testing of the global null hypothesis, and the parameter estimates table has an additional StdErrRatio column, which contains the ratios of the robust estimate of the standard error relative to the corresponding model-based estimate. Optionally, you can specify the keyword AGGREGATE enclosed in parentheses after the COVSANDWICH (or COVS) option, which requests a summing up of the score residuals for each distinct ID pattern in the computation of the robust sandwich covariance estimate. This AGGREGATE option has no effect if the ID statement is not specified.

**DATA=SAS-data-set**

names the SAS data set that contains the data to be analyzed. If you omit the DATA= option, the procedure uses the most recently created SAS data set.

**INEST=SAS-data-set**

names the SAS data set that contains initial estimates for all the parameters in the model. BY-group processing is allowed in setting up the INEST= data set. See the section “[INEST= Input Data Set](#)” on page 5665 for more information.

**MULTIPASS**

requests that, for each Newton-Raphson iteration, PROC PHREG recompile the risk sets corresponding to the event times for the (start,stop) style of response and recomputes the values of the time-dependent variables defined by the programming statements for each observation in the risk sets. If the MULTIPASS option is not specified, PROC PHREG computes all risk sets and all the variable values and saves them in a utility file. The MULTIPASS option decreases required disk space at the

expense of increased execution time; however, for very large data, it might actually save time since it is time-consuming to write and read large utility files. This option has an effect only when the (start,stop) style of response is used or when there are time-dependent explanatory variables.

**NAMELEN=*n***

specifies the length of effect names in tables and output data sets to be *n* characters, where *n* is a value between 20 and 200. The default length is 20 characters.

**NOPRINT**

suppresses all displayed output. Note that this option temporarily disables the Output Delivery System (ODS); see Chapter 20, “Using the Output Delivery System,” for more information.

**NOSUMMARY**

suppresses the summary display of the event and censored observation frequencies.

**OUTEST=*SAS-data-set***

creates an output SAS data set that contains estimates of the regression coefficients. The data set also contains the convergence status and the log likelihood. If you use the COVOUT option, the data set also contains the estimated covariance matrix of the parameter estimators. See the section “**OUTEST= Output Data Set**” on page 5664 for more information.

**PLOTS<(global-plot-options)> = *plot-request*****PLOTS<(global-plot-options)> = (*plot-request* <...<*plot-request*>>)**

controls the baseline functions plots produced through ODS Graphics. Each observation in the COVARIATES= data set in the BASELINE statement represents a set of covariates for which a curve is produced for each *plot-request* and for each stratum. You can use the ROWID= option in the BASELINE statement to specify a variable in the COVARIATES= data set for identifying the curves produced for the covariate sets. If the ROWID= option is not specified, the curves produced are identified by the covariate values if there is only a single covariate or by the observation numbers of the COVARIATES= data set if the model has two or more covariates. If the COVARIATES= data set is not specified, a reference set of covariates consisting of the reference levels for the CLASS variables and the average values for the continuous variables is used. For plotting more than one curve, you can use the OVERLAY= option to group the curves in separate plots. When you specify one *plot-request*, you can omit the parentheses around the plot request. Here are some examples:

```
plots=survival
plots=(survival cumhaz)
```

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;

proc phreg plots(cl)=survival;
 model Time*Status(0)=X1-X5;
 baseline covariates=One;
run;

ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The *global-plot-options* include the following:

**CL=<EQTAIL | HPD>**

displays the pointwise interval limits for the specified curves. For the classical analysis, CL displays the confidence limits. For the Bayesian analysis, CL=EQTAIL displays the equal-tail credible limits and CL=HPD displays the HPD limits. Specifying just CL in a Bayesian analysis defaults to CL=HPD.

**OVERLAY <=overlay-option>**

specifies how the curves for the various strata and covariate sets are overlaid. If the STRATA statement is not specified, specifying OVERLAY without any option will overlay the curves for all the covariate sets. The available *overlay-options* are as follows:

**BYGROUP**

**GROUP**

overlays, for each stratum, all curves for the covariate sets that have the same **GROUP=** value in the COVARIATES= data set in the same plot.

**INDIVIDUAL**

**IND**

displays, for each stratum, a separate plot for each covariate set.

**BYROW**

**ROW**

displays, for each covariate set, a separate plot containing the curves for all the strata.

**BYSTRATUM**

**STRATUM**

displays, for each stratum, a separate plot containing the curves for all sets of covariates.

The default is OVERLAY=BYGROUP if the **GROUP=** option is specified in the BASELINE statement or if the COVARIATES= data set contains the `_GROUP_` variable; otherwise the default is OVERLAY=INDIVIDUAL.

**TIMERANGE=(<min> <,max>)**

**TIMERANGE=<min> <,max>**

**RANGE=(<min> <,max>)**

**RANGE=<min> <,max>**

specifies the range of values on the time axis to clip the display. The *min* and *max* values are the lower and upper bounds of the range. By default, *min* is 0 and *max* is the largest event time.

The *plot-requests* include the following:

**CUMHAZ**

plots the estimated cumulative hazard function for each set of covariates in the COVARIATES= data set in the BASELINE statement. If the COVARIATES= data set is not specified, the estimated cumulative hazard function is plotted for the reference set of covariates consisting of reference levels for the CLASS variables and average values for the continuous variables.



**MCF**

plots the estimated mean cumulative function for each set of covariates in the COVARIATES= data set in the BASELINE statement. If the COVARIATES= data set is not specified, the estimated mean cumulative function is plotted for the reference set of covariates consisting of reference levels for the CLASS variables and average values for the continuous variables.

**NONE**

suppresses all the plots in the procedure. Specifying this option is equivalent to disabling ODS Graphics for the entire procedure.

**SURVIVAL**

plots the estimated survivor function for each set of covariates in the COVARIATES= data set in the BASELINE statement. If COVARIATES= data set is not specified, the estimated survivor function is plotted for the reference set of covariates consisting of reference levels for the CLASS variables and average values for the continuous variables.

**SIMPLE**

displays simple descriptive statistics (mean, standard deviation, minimum, and maximum) for each explanatory variable in the MODEL statement.

**ASSESS Statement**

**ASSESS** < VAR=(list) > < PH > < / options > ;

The ASSESS statement performs the graphical and numerical methods of Lin, Wei, and Ying (1993) for checking the adequacy of the Cox regression model. The methods are derived from cumulative sums of martingale residuals over follow-up times or covariate values. You can assess the functional form of a covariate or you can check the proportional hazards assumption for each covariate in the Cox model. PROC PHREG uses ODS Graphics for the graphical displays. You must specify at least one of the following options to create an analysis.

**VAR=(variable-list)**

specifies the list of explanatory variables for which their functional forms are assessed. For each variable on the list, the observed cumulative martingale residuals are plotted against the values of the explanatory variable along with 20 (or  $n$  if NPATHS= $n$  is specified) simulated residual patterns.

**PROPORTIONALHAZARDS****PH**

requests the checking of the proportional hazards assumption. For each explanatory variable in the model, the observed score process component is plotted against the follow-up time along with 20 (or  $n$  if NPATHS= $n$  is specified) simulated patterns.

The following options can be specified after a slash (/):

**NPATHS= $n$** 

specifies the number of simulated residual patterns to be displayed in a cumulative martingale residual plot or a score process plot. The default is  $n=20$ .

**CRPANEL**

requests that a plot with four panels, each containing the observed cumulative martingale residuals and two simulated residual patterns, be created.

**RESAMPLE <=n>**

requests that the Kolmogorov-type supremum test be computed on 1,000 simulated patterns or on *n* simulated patterns if *n* is specified.

**SEED=*n***

specifies an integer seed for the random number generator used in creating simulated realizations for plots and for the Kolmogorov-type supremum tests. Specifying a seed enables you to reproduce identical graphs and *p*-values for the model assessments from the same PHREG specification. If the SEED= option is not specified, or if you specify a nonpositive seed, a random seed is derived from the time of day.

**BASELINE Statement**

**BASELINE** <OUT=SAS-data-set> <OUTDIFF=SAS-data-set> <COVARIATES=SAS-data-set>  
<TIMELIST=list> <keyword=name . . . keyword=name> </ options> ;

The BASELINE statement creates a SAS data set (named by the OUT= option) that contains the baseline function estimates at the event times of each stratum for every set of covariates in the COVARIATES= data set. If the COVARIATES= data set is not specified, a reference set of covariates consisting of the reference levels for the CLASS variables and the average values for the continuous variables is used. You can use the DIRADJ option to obtain the direct adjusted survival curve that averages the estimated survival curves for the observations in the COVARIATES= data set. No BASELINE data set is created if the model contains a time-dependent variable defined by means of programming statement.

Table 67.2 summarizes the options available in the BASELINE statement.

**Table 67.2** BASELINE Statement Options

| Option                                | Description                                                                                |
|---------------------------------------|--------------------------------------------------------------------------------------------|
| <b>Data Set and Time List Options</b> |                                                                                            |
| OUT=                                  | Specifies the output BASELINE data set                                                     |
| OUTDIFF=                              | Specifies the output data set that contains differences of direct adjusted survival curves |
| COVARIATES=                           | Specifies the SAS data set that contains the explanatory variables                         |
| TIMELIST=                             | Specifies a list of time points for Bayesian computation of survival estimates.            |
| <b>Keyword Options</b>                |                                                                                            |
| CMF=                                  | Specifies the cumulative mean function estimate                                            |
| CUMHAZ=                               | Specifies the cumulative hazard function estimate                                          |
| LOGLOGS=                              | Specifies the log of the negative log of SURVIVAL                                          |
| LOGSURV=                              | Specifies the log of SURVIVAL                                                              |
| LOWERCMF=                             | Specifies the lower pointwise confidence limit for CMF                                     |
| LOWERCUMHAZ=                          | specifies the lower pointwise confidence limit for CUMHAZ                                  |

Table 67.2 continued

| Options              | Description                                                                                               |
|----------------------|-----------------------------------------------------------------------------------------------------------|
| LOWERHPDCUMHAZ=      | Specifies the lower limit of the HPD interval for CUMHAZ                                                  |
| LOWERHPD=            | Specifies the lower limit of the HPD interval for SURVIVAL                                                |
| LOWER=               | Specifies the lower pointwise confidence limit for SURVIVAL                                               |
| STDCMF=              | Specifies the estimated standard error of CMF                                                             |
| STDCUMHAZ=           | Specifies the estimated standard error of CUMHAZ                                                          |
| STDERR=              | Specifies the standard error of SURVIVAL                                                                  |
| STDXBETA=            | Specifies the estimated standard error of the linear predictor estimator                                  |
| SURVIVAL=            | Specifies the survivor function estimate                                                                  |
| UPPERCMF=            | Specifies the upper pointwise confidence limit for CMF                                                    |
| UPPERCUMHAZ=         | Specifies the upper pointwise confidence limit for CUMHAZ                                                 |
| UPPERHPDCUMHAZ=      | Specifies the upper limit of the HPD interval for CUMHAZ                                                  |
| UPPERHPD=            | Specifies the upper limit of the HPD interval for SURVIVAL                                                |
| UPPER=               | Specifies the upper pointwise confidence limit for SURVIVAL                                               |
| XBETA=               | Specifies the estimate of the linear predictor $\mathbf{x}'\boldsymbol{\beta}$                            |
| <b>Other Options</b> |                                                                                                           |
| ALPHA=               | Specifies the significance level of the confidence interval for the survivor function                     |
| CLTYPE=              | Specifies the method used to compute the confidence limits                                                |
| DIRADJ               | Computes direct adjusted survival curves                                                                  |
| GROUP=               | Names a variable whose values are used to identify or group the survival curves                           |
| METHOD=              | Specifies the method used to compute the survivor function estimates                                      |
| ROWID=               | Names the variable in the COVARIATES= data set for identifying the baseline functions curves in the plots |

The following options are available in the BASELINE statement.

**OUT=SAS-data-set**

names the output BASELINE data set. If you omit the OUT= option, the data set is created and given a default name by using the DATA*n* convention. See the section “OUT= Output Data Set in the BASELINE Statement” on page 5665 for more information.

**OUTDIFF=SAS-data-set**

names the output data set that contains all pairwise differences of direct adjusted probabilities between groups if the GROUP= variable is specified, or between strata if the GROUP= variable is not specified. It is required that the DIRADJ option be specified to use the OUTDIFF= option.

**COVARIATES=SAS-data-set**

names the SAS data set that contains the sets of explanatory variable values for which the quantities of interest are estimated. All variables in the COVARIATES= data set are copied to the OUT= data set. Thus, any variable in the COVARIATES= data set can be used to identify the covariate sets in the OUT= data set.

**TIMELIST=*list***

specifies a list of time points at which the survival function estimates and cumulative hazard function estimates are computed. The following specifications are equivalent:

```
timelist=5,20 to 50 by 10
timelist=5 20 30 40 50
```

If the TIMELIST= option is not specified, the default is to carry out the prediction at all event times and at time 0. This option can be used only for the Bayesian analysis.

**keyword=*name***

specifies the statistics to be included in the OUT= data set and assigns names to the variables that contain these statistics. Specify a *keyword* for each desired statistic, an equal sign, and the name of the variable for the statistic. Not all *keywords* listed in Table 67.3 (and discussed in the text that follows) are appropriate for both the classical analysis and the Bayesian analysis; and the table summarizes the choices for each analysis.

**Table 67.3** Summary of the Keyword Choices

| <b>Keyword</b>                    | <b>Classical</b> | <b>Bayesian</b> |
|-----------------------------------|------------------|-----------------|
| <b>Survivor Function</b>          |                  |                 |
| SURVIVAL=                         | X                | X               |
| STDERR=                           | X                | X               |
| LOWER=                            | X                | X               |
| UPPER=                            | X                | X               |
| LOWERHPD=                         |                  | X               |
| UPPERHPD=                         |                  | X               |
| <b>Cumulative Hazard Function</b> |                  |                 |
| CUMHAZ=                           | X                | X               |
| STDCUMHAZ=                        | X                | X               |
| LOWERCUMHAZ=                      | X                | X               |
| UPPERCUMHAZ=                      | X                | X               |
| LOWERHPDCUMHAZ=                   |                  | X               |
| UPPERHPDCUMHAZ=                   |                  | X               |
| <b>Cumulative Mean Function</b>   |                  |                 |
| CMF=                              | X                |                 |
| STDCMF=                           | X                |                 |
| LOWERCMF=                         | X                |                 |
| UPPERCMF=                         | X                |                 |
| <b>Others</b>                     |                  |                 |
| XBETA=                            | X                | X               |
| STDXBETA=                         | X                | X               |
| LOGSURV=                          | X                |                 |
| LOGLOGS=                          | X                |                 |

The available *keywords* are as follows.

**CMF=****MCF=**

specifies the cumulative mean function estimate for recurrent events data. Specifying `CMF=_ALL_` is equivalent to specifying `CMF=CMF`, `STDCMF=StdErrCMF`, `LOWERCMF=LowerCMF`, and `UPPERCMF=UpperCMF`. Nelson (2002) refers to the mean function estimate as MCF (mean cumulative function).

**CUMHAZ=**

specifies the cumulative hazard function estimate. Specifying `CUMHAZ=_ALL_` is equivalent to specifying `CUMHAZ=CumHaz`, `STDCUMHAZ=StdErrCumHaz`, `LOWERCUMHAZ=LowerCumHaz`, and `UPPERCUMHAZ=UpperCumHaz`. For a Bayesian analysis, `CUMHAZ=_ALL_` also includes `LOWERHPDCUMHAZ=LowerHPDCumHaz` and `UpperHPDCUMHAZ=UpperHPDCumHaz`.

**LOGLOGS=**

specifies the log of the negative log of `SURVIVAL`.

**LOGSURV=**

specifies the log of `SURVIVAL`.

**LOWER=****L=**

specifies the lower pointwise confidence limit for the survivor function. For a Bayesian analysis, this is the lower limit of the equal-tail credible interval for the survivor function. The confidence level is determined by the `ALPHA=` option.

**LOWERCMF=****LOWERMCF=**

specifies the lower pointwise confidence limit for the cumulative mean function. The confidence level is determined by the `ALPHA=` option.

**LOWERHPD=**

specifies the lower limit of the HPD interval for the survivor function. The confidence level is determined by the `ALPHA=` option.

**LOWERHPDCUMHAZ=**

specifies the lower limit of the HPD interval for the cumulative hazard function. The confidence level is determined by the `ALPHA=` option.

**LOWERCUMHAZ=**

specifies the lower pointwise confidence limit for the cumulative hazard function. For a Bayesian analysis, this is the lower limit of the equal-tail credible interval for the cumulative hazard function. The confidence level is determined by the `ALPHA=` option.

**STDERR=**

specifies the standard error of the survivor function estimator. For a Bayesian analysis, this is the standard deviation of the posterior distribution of the survivor function.

**STDCMF=**

**STDMCF=**

specifies the estimated standard error of the cumulative mean function estimator.

**STDCUMHAZ=**

specifies the estimated standard error of the cumulative hazard function estimator. For a Bayesian analysis, this is the standard deviation of the posterior distribution of the cumulative hazard function.

**STDXBETA=**

specifies the estimated standard error of the linear predictor estimator. For a Bayesian analysis, this is the standard deviation of the posterior distribution of the linear predictor.

**SURVIVAL=**

specifies the survivor function ( $S(t) = [S_0(t)]^{\exp(\beta'x)}$ ) estimate. Specifying SURVIVAL=\_ALL\_ is equivalent to specifying SURVIVAL=Survival, STDERR=StdErrSurvival, LOWER=LowerSurvival, and UPPER=UpperSurvival; and for a Bayesian analysis, SURVIVAL=\_ALL\_ also specifies LOWERHPD= LowerHPDSurvival and UPPERHPD=UpperHPDSurvival.

**UPPER=**

**U=**

specifies the upper pointwise confidence limit for the survivor function. For a Bayesian analysis, this is the upper limit of the equal-tail credible interval for the survivor function. The confidence level is determined by the ALPHA= option.

**UPPERCMF=**

**UPPERMCF=**

specifies the upper pointwise confidence limit for the cumulative mean function. The confidence level is determined by the ALPHA= option.

**UPPERCUMHAZ=**

specifies the upper pointwise confidence limit for the cumulative hazard function. For a Bayesian analysis, this is the upper limit of the equal-tail credible interval for the cumulative hazard function. The confidence level is determined by the ALPHA= option.

**UPPERHPD=**

specifies the upper limit of the equal-tail credible interval for the survivor function. The confidence level is determined by the ALPHA= option.

**UPPERHPDCUMHAZ=**

specifies the upper limit of the equal-tail credible interval for the cumulative hazard function. The confidence level is determined by the ALPHA= option.

**XBETA=**

specifies the estimate of the linear predictor  $x'\beta$ .

The following options can appear in the BASELINE statement after a slash (/). The METHOD= and CLTYPE= options apply only to the estimate of the survivor function in the classical analysis. For the Bayesian analysis, the survivor function is estimated by the Breslow (1972) method.

**ALPHA=***value*

specifies the significance level of the confidence interval for the survivor function. The value must be between 0 and 1. The default is the value of the ALPHA= option in the PROC PHREG statement, or 0.05 if that option is not specified.

**CLTYPE=***method*

specifies the method used to compute the confidence limits for  $S(t, \mathbf{z})$ , the survivor function for a subject with a fixed covariate vector  $\mathbf{z}$  at event time  $t$ . The CLTYPE= option can take the following values:

**LOG**

specifies that the confidence limits for  $\log(S(t, \mathbf{z}))$  be computed using the normal theory approximation. The confidence limits for  $S(t, \mathbf{z})$  are obtained by back-transforming the confidence limits for  $\log(S(t, \mathbf{z}))$ . The default is CLTYPE=LOG.

**LOGLOG**

specifies that the confidence limits for the  $\log(-\log(S(t, \mathbf{z})))$  be computed using normal theory approximation. The confidence limits for  $S(t, \mathbf{z})$  are obtained by back-transforming the confidence limits for  $\log(-\log(S(t, \mathbf{z})))$ .

**NORMAL**

<LINEAR> specifies that the confidence limits for  $S(t, \mathbf{z})$  be computed directly using normal theory approximation.

**DIRADJ**

computes direct adjusted survival curves (Makuch 1982; Gail and Byar 1986; Zhang et al. 2007) by averaging the estimated survival curves for the observations in the COVARIATES= data set. See the section “Direct Adjusted Survival Curves” on page 5646 and Example 67.8 for the computation and specific details. If the COVARIATES= data set is not specified, the input data set specified in the DATA= option in the PROC PHREG statement is used instead. If you also specify the GROUP= option, PROC PHREG computes an adjusted survival curve for each value of the GROUP= variable.

**GROUP=***variable*

names a variable whose values identify or group the estimated survival curves. The behavior of this option depends on whether you also specify the DIRADJ option:

- If you also specify the DIRADJ option, *variable* must be a CLASS variable in the model. A direct adjusted survival curve is computed for each value of *variable* in the input data. The *variable* does not have to be a variable in the COVARIATES= data set. Each direct adjusted survival curve is the average of the survival curves of all individuals in the COVARIATES= data set with their value of *variable* set to a specific value.
- If you do not specify the DIRADJ option, *variable* is required to be a numeric variable in the COVARIATES= data set. Survival curves for the observations with the same value of the *variable* are overlaid in the same plot.

**METHOD=***method*

specifies the method used to compute the survivor function estimates. See the section “Survivor Function Estimators” on page 5643 for details. You can specify the following *methods*:

**BRESLOW****CH****EMP**

specifies that the Breslow (1972) estimator be used to compute the survivor function—that is, that the survivor function be estimated by exponentiating the negative empirical cumulative hazard function.

**FH**

specifies that the Fleming-Harrington (FH) estimates be computed. The FH estimator is a tie-breaking modification of the Breslow estimator. If there are no tied event times, this estimator is the same as the Breslow estimator.

**PL**

specifies that the product-limit estimates of the survivor function be computed. This estimator is not available if you use the model syntax that allows two time variables for counting process style of input; in such a case the Breslow estimator (METHOD=BRESLOW) is used instead.

The default is METHOD=BRESLOW.

**ROWID=***variable*

**ID=***variable*

**ROW=***variable*

names a variable in the COVARIATES= data set for identifying the baseline function curves in the plots. This option has no effect if the PLOTS= option in the PROC PHREG statement is not specified. Values of this variable are used to label the curves for the corresponding rows in the COVARIATES= data set. You can specify ROWID=\_OBS\_ to use the observation numbers in the COVARIATES= data set for identification.

For recurrent events data, both CMF= and CUMHAZ= statistics are the Nelson estimators, but their standard error are not the same. Confidence limits for the cumulative mean function and cumulative hazard function are based on the log transform.

---

## BAYES Statement

**BAYES** < *options* > ;

The BAYES statement requests a Bayesian analysis of the regression model by using Gibbs sampling. The Bayesian posterior samples (also known as the chain) for the regression parameters can be output to a SAS data set. Table 67.4 summarizes the options available in the BAYES statement.

**Table 67.4** BAYES Statement Options

| Option                     | Description                                      |
|----------------------------|--------------------------------------------------|
| <b>Monte Carlo Options</b> |                                                  |
| INITIAL=                   | Specifies initial values of the chain            |
| NBI=                       | Specifies the number of burn-in iterations       |
| NMC=                       | Specifies the number of iterations after burn-in |
| SAMPLING=                  | Specifies the sampling algorithm                 |



Table 67.4 continued

| Option                                                    | Description                                                   |
|-----------------------------------------------------------|---------------------------------------------------------------|
| SEED=                                                     | Specifies the random number generator seed                    |
| THINNING=                                                 | Controls the thinning of the Markov chain                     |
| <b>Model and Prior Options</b>                            |                                                               |
| COEFFPRIOR=                                               | Specifies the prior of the regression coefficients            |
| DISPERSIONPRIOR=                                          | Specifies the prior of the dispersion parameter for frailties |
| PIECEWISE=                                                | Specifies details of the piecewise exponential model          |
| <b>Summaries and Diagnostics of the Posterior Samples</b> |                                                               |
| DIAGNOSTICS=                                              | Displays convergence diagnostics                              |
| PLOTS=                                                    | Displays diagnostic plots                                     |
| STATISTICS=                                               | Displays summary statistics                                   |
| <b>Posterior Samples</b>                                  |                                                               |
| OUTPOST=                                                  | Names a SAS data set for the posterior samples                |

The following list describes these options and their suboptions.

**COEFFPRIOR=UNIFORM | NORMAL** <(normal-option)> | **ZELLNER** <(zellner-option)>

**CPRIOR=UNIFORM | NORMAL** <(normal-option)> | **ZELLNER** <(zellner-option)>

**COEFF=UNIFORM | NORMAL** <(normal-option)> | **ZELLNER** <(zellner-option)>

specifies the prior distribution for the regression coefficients. The default is COEFFPRIOR=UNIFORM.

The following prior distributions are available:

#### UNIFORM

specifies a flat prior—that is, the prior that is proportional to a constant ( $p(\beta_1, \dots, \beta_k) \propto 1$  for all  $-\infty < \beta_i < \infty$ ).

**NORMAL**<(normal-option)>

specifies a normal distribution. The *normal-options* include the following:

**INPUT=SAS-data-set**

specifies a SAS data set that contains the mean and covariance information of the normal prior. The data set must contain the `_TYPE_` variable to identify the observation type, and it must contain a variable to represent each regression coefficient. If the data set also contains the `_NAME_` variable, values of this variable are used to identify the covariances for the `_TYPE_='COV'` observations; otherwise, the `_TYPE_='COV'` observations are assumed to be in the same order as the explanatory variables in the MODEL statement. PROC PHREG reads the mean vector from the observation with `_TYPE_='MEAN'` and the covariance matrix from observations with `_TYPE_='COV'`. For an independent normal prior, the variances can be specified with `_TYPE_='VAR'`; alternatively, the precisions (inverse of the variances) can be specified with `_TYPE_='PRECISION'`.

**RELVAR** <=c>

specifies a normal prior  $N(\mathbf{0}, c\mathbf{J})$ , where  $\mathbf{J}$  is a diagonal matrix with diagonal elements equal to the variances of the corresponding ML estimator. By default,  $c=1E6$ .

**VAR=c**

specifies the normal prior  $N(\mathbf{0}, c\mathbf{I})$ , where  $\mathbf{I}$  is the identity matrix.

If you do not specify a *normal-option*, the normal prior  $N(\mathbf{0}, 10^6\mathbf{I})$ , where  $\mathbf{I}$  is the identity matrix, is used. See the section “Normal Prior” on page 5658 for details.

**ZELLNER< (zellner-option) >**

specifies the Zellner g-prior for the regression coefficients. The g-prior is a normal prior distribution with mean zero and covariance matrix equal to  $(g\mathbf{X}'\mathbf{X})^{-1}$ , where  $\mathbf{X}$  is the design matrix and  $g$  can be a constant or a parameter with a gamma prior. The *zellner-options* include the following:

**G=number**

specifies a constant *number* for  $g$ .

**GAMMA < (SHAPE=a ISCALE=b) >**

specifies that  $g$  has a gamma prior distribution  $G(a, b)$  with density  $f(t) = \frac{b(bt)^{a-1}e^{-bt}}{\Gamma(a)}$ .  
By default,  $a=b=1E-4$ .

If you do not specify a *zellner-option*, the default is ZELLNER( $g=1E-6$ ).

**DISPERSIONPRIOR=GAMMA< (gamma-options) > | IGAMMA< (igamma-options) > | IMPROPER****DPRIOR=GAMMA< (gamma-options) > | IGAMMA< (igamma-options) > | IMPROPER**

specifies the prior distribution of the dispersion parameter. For gamma frailty, the dispersion parameter is the variance of the gamma frailty; for lognormal frailty, the dispersion parameter is the variance of the normal random component. The default is DISPERSIONPRIOR=IMPROPER.

You can specify the following values for this options:

**GAMMA< (gamma-options) >**

specifies the gamma prior. A gamma prior  $G(a, b)$  with hyperparameters  $a$  and  $b$  has density  $f(\theta) = \frac{b^a \theta^{a-1} e^{-b\theta}}{\Gamma(a)}$ , where  $a$  is the shape parameter and  $b$  is the inverse-scale parameter. You can use the following *gamma-options* enclosed in parentheses to specify the hyperparameters:

**SHAPE=a****ISCALE=b**

results in a  $G(a, b)$  prior when both *gamma-options* are specified.

**SHAPE=c**

results in a  $G(c, c)$  prior when specified alone.

**ISCALE=c**

results in a  $G(c, c)$  prior when specify alone.

The default is SHAPE=1E-4 and ISCALE=1E-4.

**IGAMMA< (igamma-options) >**

specifies the inverse-gamma prior. An inverse-gamma prior  $IG(a, b)$  with hyperparameters  $a$  and  $b$  has a density  $f(\theta) = \frac{b^a \theta^{-(a+1)} e^{-\frac{b}{\theta}}}{\Gamma(a)}$ , where  $a$  is the shape parameter and  $b$  is the scale parameter. You can use the following *igamma-options* enclosed in parentheses to specify the hyperparameters:

**SHAPE=*a*****SCALE=*b***

results in a  $IG(a, b)$  prior when both *igamma-options* are specified.

**SHAPE=*c***

results in a  $IG(c, c)$  prior when specified alone.

**SCALE=*c***

results in a  $IG(c, c)$  prior when specified alone.

The default is SHAPE=2.001 AND SCALE=0.01.

**IMPROPER**

specifies the improper prior, which has a density  $f(\theta)$  proportional to  $\theta^{-1}$ .

**DIAGNOSTICS=ALL | NONE | *keyword* | (*keyword-list*)****DIAG=ALL | NONE | *keyword* | (*keyword-list*)**

controls the number of diagnostics produced. You can request all the diagnostics in the following list by specifying DIAGNOSTICS=ALL. If you do not want any of these diagnostics, you specify DIAGNOSTICS=NONE. If you want some but not all of the diagnostics, or if you want to change certain settings of these diagnostics, you specify a subset of the following keywords. The default is DIAGNOSTICS=(AUTOCORR GEWEKE ESS).

**AUTOCORR <(LAGS= *numeric-list*)>**

computes the autocorrelations of lags given by LAGS= list for each parameter. Elements in the list are truncated to integers and repeated values are removed. If the LAGS= option is not specified, autocorrelations of lags 1, 5, 10, and 50 are computed for each variable. See the section “[Autocorrelations](#)” on page 152 for details.

**ESS**

computes the effective sample size of Kass et al. (1998), the correlation time, and the efficiency of the chain for each parameter. See the section “[Effective Sample Size](#)” on page 152 for details.

**MCSE****MCERROR**

computes the Monte Carlo standard error for each parameter. The Monte Carlo standard error, which measures the simulation accuracy, is the standard error of the posterior mean estimate and is calculated as the posterior standard deviation divided by the square root of the effective sample size. See the section “[Standard Error of the Mean Estimate](#)” on page 153 for details.

**HEIDELBERGER <(heidel-options)>**

computes the Heidelberg and Welch tests for each parameter. See the section “[Heidelberg and Welch Diagnostics](#)” on page 148 for details. The tests consist of a stationary test and a halfwidth test. The former tests the null hypothesis that the sample values form a stationary process. If the stationarity test is passed, a halfwidth test is then carried out. Optionally, you can specify one or more of the following *heidel-options*:

**SALPHA=***value*

specifies the  $\alpha$  level ( $0 < \alpha < 1$ ) for the stationarity test. The default is the value of the **ALPHA=** option in the PROC PHREG statement, or 0.05 if that option is not specified.

**HALPHA=***value*

specifies the  $\alpha$  level ( $0 < \alpha < 1$ ) for the halfwidth test. The default is the value of the **ALPHA=** option in the PROC PHREG statement, or 0.05 if that option is not specified.

**EPS=***value*

specifies a small positive number  $\epsilon$  such that if the halfwidth is less than  $\epsilon$  times the sample mean of the retaining samples, the halfwidth test is passed.

**GELMAN** <*gelman-options*>

computes the Gelman and Rubin convergence diagnostics. See the section “[Gelman and Rubin Diagnostics](#)” on page 145 for details. You can specify one or more of the following *gelman-options*:

**NCHAIN=***number***N=***number*

specifies the number of parallel chains used to compute the diagnostic and has to be 2 or larger. The default is NCHAIN=3. The NCHAIN= option is ignored when the INITIAL= option is specified in the BAYES statement, and in such a case, the number of parallel chains is determined by the number of valid observations in the INITIAL= data set.

**ALPHA=***value*

specifies the significance level for the upper bound. The default is the value of the **ALPHA=** option in the PROC PHREG statement, or 0.05 if that option is not specified (resulting in a 97.5% bound).

**GEWEKE** <*geweke-options*>

computes the Geweke diagnostics. See the section “[Geweke Diagnostics](#)” on page 146 for details. The diagnostic is essentially a two-sample *t*-test between the first  $f_1$  portion and the last  $f_2$  portion of the chain. The default is  $f_1=0.1$  and  $f_2=0.5$ , but you can choose other fractions by using the following *geweke-options*:

**FRAC1=***value*

specifies the early  $f_1$  fraction of the Markov chain.

**FRAC2=***value*

specifies the latter  $f_2$  fraction of the Markov chain.

**RAFTERY** <*raftery-options*>

computes the Raftery and Lewis diagnostics. See the section “[Raftery and Lewis Diagnostics](#)” on page 149 for details. The diagnostic evaluates the accuracy of the estimated quantile ( $\hat{\theta}_Q$  for a given  $Q \in (0, 1)$ ) of a chain.  $\hat{\theta}_Q$  can achieve any degree of accuracy when the chain is allowed to run for a long time. A stopping criterion is when the estimated probability  $\hat{P}_Q = \Pr(\theta \leq \hat{\theta}_Q)$  reaches within  $\pm R$  of the value  $Q$  with probability  $S$ ; that is,  $\Pr(Q - R \leq \hat{P}_Q \leq Q + R) = S$ . The following *raftery-options* enable you to specify  $Q$ ,  $R$ ,  $S$ , and a precision level  $\epsilon$  for a stationary test.

**QUANTILE=***value***Q=***value*

specifies the order (a value between 0 and 1) of the quantile of interest. The default is 0.025.

**ACCURACY=***value***R=***value*

specifies a small positive number as the margin of error for measuring the accuracy of estimation of the quantile. The default is 0.005.

**PROBABILITY=***value***S=***value*

specifies the probability of attaining the accuracy of the estimation of the quantile. The default is 0.95.

**EPSILON=***value***EPS=***value*

specifies the tolerance level (a small positive number) for the test. The default is 0.001.

**INITIAL=***SAS-data-set*

specifies the SAS data set that contains the initial values of the Markov chains. The INITIAL= data set must contain a variable for each parameter in the model. You can specify multiple rows as the initial values of the parallel chains for the Gelman-Rubin statistics, but posterior summary statistics, diagnostics, and plots are computed only for the first chain.

**NBI=***number*

specifies the number of burn-in iterations before the chains are saved. The default is 2000.

**NMC=***number*

specifies the number of iterations after the burn-in. The default is 10000.

**OUTPOST=***SAS-data-set***OUT=***SAS-data-set*names the SAS data set that contains the posterior samples. See the section “[OUTPOST= Output Data Set in the BAYES Statement](#)” on page 5665 for more information. Alternatively, you can output the posterior samples into a data set, as shown in the following example in which the data set is named PostSamp.

```
ODS OUTPUT PosteriorSample = PostSamp;
```

**PIECEWISE** <=*keyword* <(< **NINTERVAL=***number* > < **INTERVALS=**(*numeric-list*) > < **PRIOR=***option* >)>>specifies that the piecewise constant baseline hazard model be used in the Bayesian analysis. You can specify one of the following two *keywords*:**HAZARD**

models the baseline hazard parameters in the original scale. The hazard parameters are named Lambda1, Lambda2, . . . , and so on.

**LOGHAZARD**

models the baseline hazard parameters in the log scale. The log-hazard parameters are named Alpha1, Alpha2, . . . , and so on.

Specifying PIECEWISE by itself is the same as specifying PIECEWISE=LOGHAZARD.

You can choose one of the following two options to specify the partition of the time axis into intervals of constant baseline hazards:

**NINTERVAL=***number*

**N=***number*

specifies the number of intervals with constant baseline hazard rates. PROC PHREG partitions the time axis into the given number of intervals with approximately equal number of events in each interval.

**INTERVALS=***(numeric-list)*

**INTERVAL=***(numeric-list)*

specifies the list of numbers that partition the time axis into disjoint intervals with constant baseline hazard in each interval. For example, INTERVALS=(100, 150, 200, 250, 300) specifies a model with a constant hazard in the intervals [0,100), [100,150), [150,200), [200,250), [250,300), and [300,∞). Each interval must contain at least one event; otherwise, the posterior distribution can be improper, and inferences cannot be derived from an improper posterior distribution.

If neither **NINTERVAL=** nor **INTERVAL=** is specified, the default is **NINTERVAL=8**.

To specify the prior for the baseline hazards  $(\lambda_1, \dots, \lambda_J)$  in the original scale, you specify the following:

**PRIOR = IMPROPER | UNIFORM | GAMMA***<(gamma-option)>* | **ARGAMMA***<(arggamma-option)>*

The default is **PRIOR=IMPROPER**. The available prior options include the following:

**IMPROPER**

specifies the noninformative and improper prior  $p(\lambda_1, \dots, \lambda_J) \propto \prod_i \lambda_i^{-1}$  for all  $\lambda_i > 0$ .

**UNIFORM**

specifies a uniform prior on the real line; that is,  $p(\lambda_i) \propto 1$  for all  $\lambda_i > 0$ .

**GAMMA** *<(gamma-option)>*

specifies an independent gamma prior  $G(a, b)$  with density  $f(t) = \frac{b(bt)^{a-1}e^{-bt}}{\Gamma(a)}$ , which can be followed by one of the following *gamma-options* enclosed in parentheses. The hyperparameters  $a$  and  $b$  are the shape and inverse-scale parameters of the gamma distribution, respectively. See the section “[Independent Gamma Prior](#)” on page 5657 for details. The default is  $G(10^{-4}, 10^{-4})$  for each  $\lambda_j$ , setting the prior mean to 1 with variance 1E4. This prior is proper and reasonably noninformative.

**INPUT=SAS-data-set**

specifies a data set containing the hyperparameters of the independent gamma prior. The data set must contain the `_TYPE_` variable to identify the observation type, and it must contain the variables named Lambda1, Lambda2, . . . , and so forth, to represent

the hazard parameters. The observation with `_TYPE_='SHAPE'` identifies the shape parameters, and the observation with `_TYPE_='ISCALE'` identifies the inverse-scale parameters.

**RELSHAPE=<c>**

specifies independent  $G(c\hat{\lambda}_j, c)$  distribution, where  $\hat{\lambda}_j$ 's are the MLEs of the hazard rates. This prior has mean  $\hat{\lambda}_j$  and variance  $\frac{\hat{\lambda}_j}{c}$ . By default,  $c=1E-4$ .

**SHAPE=a and ISCALE=b**

together specify the  $G(a, b)$  prior.

**SHAPE=c****ISCALE=c**

specifies the  $G(c, c)$  prior.

**ARGAMMA <(argamma-option)>**

specifies an autoregressive gamma prior of order 1, which can be followed by one of the following *argamma-options*. See the section “AR1 Prior” on page 5657 for details.

**INPUT=SAS-data-set**

specifies a data set containing the hyperparameters of the correlated gamma prior. The data set must contain the `_TYPE_` variable to identify the observation type, and it must contain the variables named `Lambda1`, `Lambda2`, `...`, and so forth, to represent the hazard parameters. The observation with `_TYPE_='SHAPE'` identifies the shape parameters, and the observation with `_TYPE_='ISCALE'` identifies the *relative* inverse-scale parameters; that is, if  $a_j$  and  $b_j$  are, respectively, the SHAPE and ISCALE values for  $\lambda_j$ ,  $1 \leq j \leq J$ , then  $\lambda_1 \sim G(a_1, b_1)$ , and  $\lambda_j \sim G(a_j, b_j/\lambda_{j-1})$  for  $2 \leq j \leq J$ .

**SHAPE=a and SCALE=b**

together specify that  $\lambda_1 \sim G(a, b)$  and  $\lambda_j \sim G(a, b/\lambda_{j-1})$  for  $2 \leq j \leq J$ .

**SHAPE=c****ISCALE=c**

specifies that  $\lambda_1 \sim G(c, c)$  and  $\lambda_j \sim G(c, c/\lambda_{j-1})$  for  $2 \leq j \leq J$ .

To specify the prior for  $\alpha_1, \dots, \alpha_J$ , the hazard parameters in the log scale, you specifying the following:

**PRIOR=UNIFORM | NORMAL<(normal-option)>**

specifies the prior for the loghazard parameters. The default is `PRIOR=UNIFORM`. The available `PRIOR=` options are as follows:

**UNIFORM**

specifies the uniform prior on the real line; that is,  $\alpha_i \propto 1$  for all  $-\infty < \alpha_i < \infty$ .

**NORMAL<(normal-option)>**

specifies a normal prior distribution on the log-hazard parameters. The *normal-options* include the following. If you do not specify a *normal-option*, the normal prior  $N(\mathbf{0}, 10^6\mathbf{I})$ , where  $\mathbf{I}$  is the identity matrix, is used.

**INPUT=SAS-data-set**

specifies a SAS data set containing the mean and covariance information of the normal prior. The data set must contain the `_TYPE_` variable to identify the observation type, and it must contain variables named `Alpha1`, `Alpha2`, ..., and so forth, to represent the log-hazard parameters. If the data set also contains the `_NAME_` variable, the value of this variable will be used to identify the covariances for the `_TYPE_='COV'` observations; otherwise, the `_TYPE_='COV'` observations are assumed to be in the same order as the explanatory variables in the MODEL statement. PROC PHREG reads the mean vector from the observation with `_TYPE_='MEAN'` and the covariance matrix from observations with `_TYPE_='COV'`. See the section “Normal Prior” on page 5658 for details. For an independent normal prior, the variances can be specified with `_TYPE_='VAR'`; alternatively, the precisions (inverse of the variances) can be specified with `_TYPE_='PRECISION'`.

If you have a joint normal prior for the log-hazard parameters and the regression coefficients, specify the same data set containing the mean and covariance information of the multivariate normal distribution in both the `COEFFPRIOR=NORMAL(INPUT=)` and the `PIECEWISE=LOGHAZARD(PRIOR=NORMAL(INPUT=))` options. See the section “Joint Multivariate Normal Prior for Log-Hazards and Regression Coefficients” on page 5658 for details.

**RELVAR <c>**

specifies the normal prior  $N(\mathbf{0}, \mathbf{cJ})$ , where  $\mathbf{J}$  is a diagonal matrix with diagonal elements equal to the variances of the corresponding ML estimator. By default,  $\mathbf{c}=1E6$ .

**VAR=c**

specifies the normal prior  $N(\mathbf{0}, \mathbf{cI})$ , where  $\mathbf{I}$  is the identity matrix.

**PLOTS <(global-plot-options)> = plot-request****PLOTS <(global-plot-options)> = (plot-requests)**

controls the diagnostic plots produced through ODS Graphics. Three types of plots can be requested: trace plots, autocorrelation function plots, and kernel density plots. By default, the plots are displayed in panels unless the global plot option `UNPACK` is specified. If you specify more than one type of plots, the plots are displayed by parameters unless the global plot option `GROUPBY=TYPE` is specified. When you specify only one plot request, you can omit the parentheses around the plot request. For example:

```
plots=none
plots(unpack)=trace
plots=(trace autocorr)
```

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;
proc phreg;
 model y=x;
 bayes plots=trace;
run;
ods graphics off;
```



If ODS Graphics is enabled but you do not specify the PLOTS= option in the BAYES statement, then PROC PHREG produces, for each parameter, a panel that contains the trace plot, the autocorrelation function plot, and the density plot. This is equivalent to specifying `plots=(trace autocorr density)`.

The *global-plot-options* include the following:

**FRINGE**

creates a fringe plot on the X axis of the density plot.

**GROUPBY = PARAMETER | TYPE**

specifies how the plots are to be grouped when there is more than one type of plots. The choices are as follows:

**TYPE**

specifies that the plots be grouped by type.

**PARAMETER**

specifies that the plots be grouped by parameter.

GROUPBY=PARAMETER is the default.

**SMOOTH**

displays a fitted penalized B-spline curve each trace plot.

**UNPACKPANEL**

**UNPACK**

specifies that all paneled plots be unpacked, meaning that each plot in a panel is displayed separately.

The *plot-requests* include the following:

**ALL**

specifies all types of plots. PLOTS=ALL is equivalent to specifying PLOTS=(TRACE AUTOCORR DENSITY).

**AUTOCORR**

displays the autocorrelation function plots for the parameters.

**DENSITY**

displays the kernel density plots for the parameters.

**NONE**

suppresses all diagnostic plots.

**TRACE**

displays the trace plots for the parameters. See the section “[Visual Analysis via Trace Plots](#)” on page 139 for details.

Consider a model with four parameters, X1–X4. Displays for various specification are depicted as follows.

1. PLOTS=(TRACE AUTOCORR) displays the trace and autocorrelation plots for each parameter side by side with two parameters per panel:

---

|           |           |              |
|-----------|-----------|--------------|
| Display 1 | Trace(X1) | Autocorr(X1) |
|           | Trace(X2) | Autocorr(X2) |

|           |           |              |
|-----------|-----------|--------------|
| Display 2 | Trace(X3) | Autocorr(X3) |
|           | Trace(X4) | Autocorr(X4) |

---

2. PLOTS(GROUPBY=TYPE)=(TRACE AUTOCORR) displays all the paneled trace plots, followed by panels of autocorrelation plots:

---

|           |           |
|-----------|-----------|
| Display 1 | Trace(X1) |
|           | Trace(X2) |

|           |           |
|-----------|-----------|
| Display 2 | Trace(X3) |
|           | Trace(X4) |

|           |              |              |
|-----------|--------------|--------------|
| Display 3 | Autocorr(X1) | Autocorr(X2) |
|           | Autocorr(X3) | Autocorr(X4) |

---

3. PLOTS(UNPACK)=(TRACE AUTOCORR) displays a separate trace plot and a separate correlation plot, parameter by parameter:

---

|           |           |
|-----------|-----------|
| Display 1 | Trace(X1) |
|-----------|-----------|

|           |              |
|-----------|--------------|
| Display 2 | Autocorr(X1) |
|-----------|--------------|

|           |           |
|-----------|-----------|
| Display 3 | Trace(X2) |
|-----------|-----------|

|           |              |
|-----------|--------------|
| Display 4 | Autocorr(X2) |
|-----------|--------------|

|           |           |
|-----------|-----------|
| Display 5 | Trace(X3) |
|-----------|-----------|

|           |              |
|-----------|--------------|
| Display 6 | Autocorr(X3) |
|-----------|--------------|

|           |           |
|-----------|-----------|
| Display 7 | Trace(X4) |
|-----------|-----------|

|           |              |
|-----------|--------------|
| Display 8 | Autocorr(X4) |
|-----------|--------------|

---

4. PLOTS(UNPACK GROUPBY=TYPE) = (TRACE AUTOCORR) displays all the separate trace plots followed by the separate autocorrelation plots:

---

|           |              |
|-----------|--------------|
| Display 1 | Trace(X1)    |
| Display 2 | Trace(X2)    |
| Display 3 | Trace(X3)    |
| Display 4 | Trace(X4)    |
| Display 5 | Autocorr(X1) |
| Display 6 | Autocorr(X2) |
| Display 7 | Autocorr(X3) |
| Display 8 | Autocorr(X4) |

---

**SAMPLING=keyword**

specifies the sampling algorithm used in the Markov chain Monte Carlo (MCMC) simulations. Two sampling algorithms are available:

**ARMS****GIBBS**

requests the use of the adaptive rejection Metropolis sampling (ARMS) algorithm to draw the Gibbs samples. ALGORITHM=ARMS is the default.

**RWM**

requests the use of the random walk Metropolis (RWM) algorithm to draw the samples.

For details about the MCMC sampling algorithms, see the section “[Markov Chain Monte Carlo Method](#)” on page 133 in Chapter 7, “[Introduction to Bayesian Analysis Procedures](#).”

**SEED=number**

specifies an integer seed ranging from 1 to  $2^{31}-1$  for the random number generator in the simulation. Specifying a seed enables you to reproduce identical Markov chains for the same specification. If the SEED= option is not specified, or if you specify a nonpositive seed, a random seed is derived from the time of day.

**STATISTICS <(global-options)> = ALL | NONE | keyword | (keyword-list)****STATS <(global-statoptions)> = ALL | NONE | keyword | (keyword-list)**

controls the number of posterior statistics produced. Specifying STATISTICS=ALL is equivalent to specifying STATISTICS=(SUMMARY INTERVAL COV CORR). If you do not want any posterior statistics, you specify STATISTICS=NONE. The default is STATISTICS=(SUMMARY INTERVAL). See the section “[Summary Statistics](#)” on page 153 for details. The *global-options* include the following:

**ALPHA=***numeric-list*

controls the probabilities of the credible intervals. The ALPHA= values must be between 0 and 1. Each ALPHA= value produces a pair of 100(1–ALPHA)% equal-tail and HPD intervals for each parameters. The default is the value of the ALPHA= option in the PROC PHREG statement, or 0.05 if that option is not specified (yielding the 95% credible intervals for each parameter).

**PERCENT=***numeric-list*

requests the percentile points of the posterior samples. The PERCENT= values must be between 0 and 100. The default is PERCENT= 25, 50, 75, which yield the 25th, 50th, and 75th percentile points for each parameter.

You can specify the following values for a *keyword* or as part of a *keyword-list*. To specify a list, place parentheses around multiple keywords that are separated by spaces.

**CORR**

produces the posterior correlation matrix.

**COV**

produces the posterior covariance matrix.

**SUMMARY**

produces the means, standard deviations, and percentile points for the posterior samples. The default is to produce the 25th, 50th, and 75th percentile points, but you can use the global PERCENT= option to request specific percentile points.

**INTERVAL**

produces equal-tail credible intervals and HPD intervals. The default is to produce the 95% equal-tail credible intervals and 95% HPD intervals, but you can use the global ALPHA= option to request intervals of any probabilities.

**THINNING=***number***THIN=***number*

controls the thinning of the Markov chain. Only one in every  $k$  samples is used when THINNING= $k$ , and if NBI= $n_0$  and NMC= $n$ , the number of samples kept is

$$\left[ \frac{n_0 + n}{k} \right] - \left[ \frac{n_0}{k} \right]$$

where  $[a]$  represents the integer part of the number  $a$ . The default is THINNING=1.

**BY Statement****BY variables ;**

You can specify a BY statement with PROC PHREG to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the PHREG procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

---

## CLASS Statement

**CLASS** *variable* < (*options*) > ... < *variable* < (*options*) > > < / *global-options* > ;

The CLASS statement names the classification variables to be used as explanatory variables in the analysis.

The CLASS statement must precede the MODEL statement. Most options can be specified either as individual variable *options* or as *global-options*. You can specify *options* for each variable by enclosing the options in parentheses after the variable name. You can also specify *global-options* for the CLASS statement by placing them after a slash (/). *Global-options* are applied to all the variables specified in the CLASS statement. If you specify more than one CLASS statement, the *global-options* specified in any one CLASS statement apply to all CLASS statements. However, individual CLASS variable *options* override the *global-options*. You can specify the following values for either an *option* or a *global-option*:

### CPREFIX=*n*

specifies that, at most, the first *n* characters of a CLASS variable name be used in creating names for the corresponding design variables. The default is  $32 - \min(32, \max(2, f))$ , where *f* is the formatted length of the CLASS variable.

### DESCENDING

#### DESC

reverses the sort order of the classification variable. If both the DESCENDING and ORDER= options are specified, PROC PHREG orders the categories according to the ORDER= option and then reverses that order.

### LPREFIX=*n*

specifies that, at most, the first *n* characters of a CLASS variable label be used in creating labels for the corresponding design variables. The default is  $256 - \min(256, \max(2, f))$ , where *f* is the formatted length of the CLASS variable.

### MISSING

treats missing values ('.', '.\_', '.A', ..., '.Z' for numeric variables and blanks for character variables) as valid values for the CLASS variable.

**ORDER=DATA | FORMATTED | FREQ | INTERNAL**

specifies the sort order for the levels of classification variables. This ordering determines which parameters in the model correspond to each level in the data, so the ORDER= option can be useful when you use the CONTRAST statement. By default, ORDER=FORMATTED. For ORDER=FORMATTED and ORDER=INTERNAL, the sort order is machine-dependent. When ORDER=FORMATTED is in effect for numeric variables for which you have supplied no explicit format, the levels are ordered by their internal values.

The following table shows how PROC PHREG interprets values of the ORDER= option.

| Value of ORDER= | Levels Sorted By                                                                                                                         |
|-----------------|------------------------------------------------------------------------------------------------------------------------------------------|
| DATA            | Order of appearance in the input data set                                                                                                |
| FORMATTED       | External formatted values, except for numeric variables with no explicit format, which are sorted by their unformatted (internal) values |
| FREQ            | Descending frequency count; levels with more observations come earlier in the order                                                      |
| INTERNAL        | Unformatted value                                                                                                                        |

For more information about sort order, see the chapter on the SORT procedure in the *Base SAS Procedures Guide* and the discussion of BY-group processing in *SAS Language Reference: Concepts*.

**PARAM=keyword**

specifies the parameterization method for the classification variable or variables. You can specify any of the *keywords* shown in the following table; the default is PARAM=REF. Design matrix columns are created from CLASS variables according to the corresponding coding schemes:

| Value of PARAM=           | Coding                                                                                              |
|---------------------------|-----------------------------------------------------------------------------------------------------|
| EFFECT                    | Effect coding                                                                                       |
| GLM                       | Less-than-full-rank reference cell coding (this <i>keyword</i> can be used only in a global option) |
| ORDINAL<br>THERMOMETER    | Cumulative parameterization for an ordinal CLASS variable                                           |
| POLYNOMIAL<br>POLY        | Polynomial coding                                                                                   |
| REFERENCE<br>REF          | Reference cell coding                                                                               |
| ORTHEFFECT                | Orthogonalizes PARAM=EFFECT coding                                                                  |
| ORTHORDINAL<br>ORTHOTHERM | Orthogonalizes PARAM=ORDINAL coding                                                                 |
| ORTHPOLY                  | Orthogonalizes PARAM=POLYNOMIAL coding                                                              |
| ORTHREF                   | Orthogonalizes PARAM=REFERENCE coding                                                               |

All parameterizations are full rank, except for the GLM parameterization. The **REF=** option in the CLASS statement determines the reference level for EFFECT and REFERENCE coding and for their orthogonal parameterizations. It also indirectly determines the reference level for a singular GLM parameterization through the order of levels.

If **PARAM=ORTHPOLY** or **PARAM=POLY** and the classification variable is numeric, then the **ORDER=** option in the CLASS statement is ignored, and the internal unformatted values are used. See the section “[Other Parameterizations](#)” on page 387 of Chapter 19, “[Shared Concepts and Topics](#),” for further details.

**REF=** *'level' | keyword*

specifies the reference level for **PARAM=EFFECT**, **PARAM=REFERENCE**, and their orthogonalizations. For **PARAM=GLM**, the **REF=** option specifies a level of the classification variable to be put at the end of the list of levels. This level thus corresponds to the reference level in the usual interpretation of the linear estimates with a singular parameterization.

For an individual variable **REF=** option (but not for a global **REF=** option), you can specify the *level* of the variable to use as the reference level. Specify the formatted value of the variable if a format is assigned. For a global or individual variable **REF=** option, you can use one of the following *keywords*. The default is **REF=LAST**.

**FIRST**     designates the first ordered level as reference.

**LAST**      designates the last ordered level as reference.

**TRUNCATE**<=*n*>

specifies the length *n* of CLASS variable values to use in determining CLASS variable levels. The default is to use the full formatted length of the CLASS variable. If you specify **TRUNCATE** without the length *n*, the first 16 characters of the formatted values are used. When formatted values are longer than 16 characters, you can use this option to revert to the levels as determined in releases before SAS 9. The **TRUNCATE** option is available only as a global option.

## Class Variable Naming Convention

Parameter names for a CLASS predictor variable are constructed by concatenating the CLASS variable name with the CLASS levels. However, for the POLYNOMIAL and orthogonal parameterizations, parameter names are formed by concatenating the CLASS variable name and keywords that reflect the parameterization. See the section “[Other Parameterizations](#)” on page 387 in Chapter 19, “[Shared Concepts and Topics](#),” for examples and further details.

## Class Variable Parameterization with Unbalanced Designs

PROC PHREG initially parameterizes the CLASS variables by looking at the levels of the variables across the complete data set. If you have an *unbalanced* replication of levels across variables or BY groups, then the design matrix and the parameter interpretation might be different from what you expect. For instance, suppose you have a model with one CLASS variable A with three levels (1, 2, and 3), and another CLASS variable B with two levels (1 and 2). If the third level of A occurs only with the first level of B, if you use the EFFECT parameterization, and if your model contains the effect A(B) and an intercept, then the design for A within the second level of B is not a differential effect. In particular, the design looks like the following:

|   |   | Design Matrix |    |        |    |
|---|---|---------------|----|--------|----|
|   |   | A(B=1)        |    | A(B=2) |    |
| B | A | A1            | A2 | A1     | A2 |
| 1 | 1 | 1             | 0  | 0      | 0  |
| 1 | 2 | 0             | 1  | 0      | 0  |
| 1 | 3 | -1            | -1 | 0      | 0  |
| 2 | 1 | 0             | 0  | 1      | 0  |
| 2 | 2 | 0             | 0  | 0      | 1  |

PROC PHREG detects linear dependency among the last two design variables and sets the parameter for A2(B=2) to zero, resulting in an interpretation of these parameters as if they were reference- or dummy-coded. The REFERENCE or GLM parameterization might be more appropriate for such problems.

## CONTRAST Statement

**CONTRAST** *'label'* *row-description* <, ... *row-description*> </ *options*> ;

The CONTRAST statement provides a mechanism for obtaining customized hypothesis tests. It is similar to the CONTRAST statement in PROC GLM and PROC CATMOD, depending on the coding schemes used with any categorical variables involved.

The CONTRAST statement enables you to specify a matrix,  $\mathbf{L}$ , for testing the hypothesis  $\mathbf{L}\boldsymbol{\beta} = \mathbf{0}$ . You must be familiar with the details of the model parameterization that PROC PHREG uses (for more information, see the PARAM= option in the section “CLASS Statement” on page 5578). Optionally, the CONTRAST statement enables you to estimate each row,  $\mathbf{L}'_i\boldsymbol{\beta}$ , of  $\mathbf{L}\boldsymbol{\beta}$  and test the hypothesis  $\mathbf{L}'_i\boldsymbol{\beta} = 0$ . Computed statistics are based on the asymptotic chi-square distribution of the Wald statistic.

There is no limit to the number of CONTRAST statements that you can specify, but they must appear after the MODEL statement.

The syntax of a *row-description* is:

*effect values* <, ... , *effect values*>

The following parameters are specified in the CONTRAST statement:

- label* identifies the contrast on the output. A label is required for every contrast specified, and it must be enclosed in quotes.
- effect* identifies an effect that appears in the MODEL statement. You do not need to include all effects that are included in the MODEL statement.
- values* are constants that are elements of the  $\mathbf{L}$  matrix associated with the effect. To correctly specify your contrast, it is crucial to know the ordering of parameters within each effect and the variable levels associated with any parameter. The “Class Level Information” table shows the ordering of levels within variables. The E option, described later in this section, enables you to verify the proper correspondence of *values* to parameters.

The rows of  $\mathbf{L}$  are specified in order and are separated by commas. Multiple degree-of-freedom hypotheses can be tested by specifying multiple *row-descriptions*. For any of the full-rank parameterizations, if an effect



is not specified in the CONTRAST statement, all of its coefficients in the **L** matrix are set to 0. If too many values are specified for an effect, the extra ones are ignored. If too few values are specified, the remaining ones are set to 0.

When you use effect coding (by specifying PARAM=EFFECT in the CLASS statement), all parameters are directly estimable (involve no other parameters). For example, suppose an effect coded CLASS variable **A** has four levels. Then there are three parameters ( $\alpha_1, \alpha_2, \alpha_3$ ) representing the first three levels, and the fourth parameter is represented by

$$-\alpha_1 - \alpha_2 - \alpha_3$$

To test the first versus the fourth level of **A**, you would test

$$\alpha_1 = -\alpha_1 - \alpha_2 - \alpha_3$$

or, equivalently,

$$2\alpha_1 + \alpha_2 + \alpha_3 = 0$$

which, in the form  $\mathbf{L}\boldsymbol{\beta} = 0$ , is

$$\begin{bmatrix} 2 & 1 & 1 \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{bmatrix} = 0$$

Therefore, you would use the following CONTRAST statement:

```
contrast '1 vs. 4' A 2 1 1;
```

To contrast the third level with the average of the first two levels, you would test

$$\frac{\alpha_1 + \alpha_2}{2} = \alpha_3$$

or, equivalently,

$$\alpha_1 + \alpha_2 - 2\alpha_3 = 0$$

Therefore, you would use the following CONTRAST statement:

```
contrast '1&2 vs. 3' A 1 1 -2;
```

Other CONTRAST statements involving classification variables with PARAM=EFFECT are constructed similarly. For example:

```
contrast '1 vs. 2' A 1 -1 0;
contrast '1&2 vs. 4' A 3 3 2;
contrast '1&2 vs. 3&4' A 2 2 0;
contrast 'Main Effect' A 1 0 0,
A 0 1 0,
A 0 0 1;
```

When you use the less-than-full-rank parameterization (by specifying PARAM=GLM in the CLASS statement), each row is checked for estimability. If PROC PHREG finds a contrast to be nonestimable, it displays missing values in corresponding rows in the results. PROC PHREG handles missing level combinations of categorical variables in the same manner as PROC GLM. Parameters corresponding to missing level combinations are not included in the model. This convention can affect the way in which you specify the **L** matrix in your CONTRAST statement. If the elements of **L** are not specified for an effect that contains a specified effect, then the elements of the specified effect are distributed over the levels of the higher-order effect just as the GLM procedure does for its CONTRAST and ESTIMATE statements. For example, suppose that the model contains effects A and B and their interaction A\*B. If you specify a CONTRAST statement involving A alone, the **L** matrix contains nonzero terms for both A and A\*B, since A\*B contains A.

The Cox model contains no explicit intercept parameter, so it is not valid to specify one in the CONTRAST statement. As a consequence, you can test or estimate only homogeneous linear combinations (those with zero-intercept coefficients, such as contrasts that represent group differences) for the GLM parameterization.

The degrees of freedom are the number of linearly independent constraints implied by the CONTRAST statement—that is, the rank of **L**.

You can specify the following *options* after a slash (/).

**ALPHA=** *p*

specifies the level of significance *p* for the  $100(1 - p)\%$  confidence interval for each contrast when the ESTIMATE option is specified. The value *p* must be between 0 and 1. By default, *p* is equal to the value of the ALPHA= option in the PROC PHREG statement, or 0.05 if that option is not specified.

**E**

requests that the **L** matrix be displayed.

**ESTIMATE=***keyword*

requests that each individual contrast (that is, each row,  $l'_i\beta$ , of **L** $\beta$ ) or exponentiated contrast ( $e^{l'_i\beta}$ ) be estimated and tested. PROC PHREG displays the point estimate, its standard error, a Wald confidence interval, and a Wald chi-square test for each contrast. The significance level of the confidence interval is controlled by the ALPHA= option. You can estimate the contrast or the exponentiated contrast ( $e^{l'_i\beta}$ ), or both, by specifying one of the following *keywords*:

|      |                                                                               |
|------|-------------------------------------------------------------------------------|
| PARM | specifies that the contrast itself be estimated.                              |
| EXP  | specifies that the exponentiated contrast be estimated.                       |
| BOTH | specifies that both the contrast and the exponentiated contrast be estimated. |

**SINGULAR=***number*

tunes the estimability check. This option is ignored when the full-rank parameterization is used. If **v** is a vector, define ABS(**v**) to be the largest absolute value of the elements of **v**. For a row vector  $l'$  of the contrast matrix **L**, define *c* to be equal to ABS( $l'$ ) if ABS( $l'$ ) is greater than 0; otherwise, *c* equals 1. If  $\text{ABS}(l' - l'\mathbf{T})$  is greater than  $c * \text{number}$ , then  $l'$  is declared nonestimable. The **T** matrix is the Hermite form matrix  $\mathbf{I}_0^{-1}\mathbf{I}_0$ , where  $\mathbf{I}_0^{-1}$  represents a generalized inverse of the information matrix  $\mathbf{I}_0$  of the null model. The value for *number* must be between 0 and 1; the default value is 1E-4.

**TEST**< (*keywords*)>

requests a Type 3 test for each contrast. The default is to use the Wald statistic, but you can request other statistics by specifying one or more of the following *keywords*:

**ALL**

requests the likelihood ratio tests, the score tests, and the Wald tests. Specifying TEST(ALL) is equivalent to specifying TEST=(LR SCORE WALD).

**NONE**

suppresses the Type 3 analysis. Even if the TEST option is not specified, PROC PHREG displays the Wald test results for each model effect if a CLASS variable is involved in a MODEL effect. The NONE option can be used to suppress such display.

**LR**

requests the likelihood ratio tests. This request is not honored if the COVS option is also specified.

**SCORE**

requests the score tests. This request is not honored if the COVS option is also specified.

**WALD**

requests the Wald tests.

\*

## EFFECT Statement

**EFFECT** *name*=*effect-type* (*variables* < / *options*>);

The EFFECT statement enables you to construct special collections of columns for design matrices. These collections are referred to as *constructed effects* to distinguish them from the usual model effects that are formed from continuous or classification variables, as discussed in the section “GLM Parameterization of Classification Variables and Effects” on page 383 in Chapter 19, “Shared Concepts and Topics.”

You can specify the following *effect-types*:

|                          |                                                                                                                                                                                                           |
|--------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>COLLECTION</b>        | is a collection effect that defines one or more variables as a single effect with multiple degrees of freedom. The variables in a collection are considered as a unit for estimation and inference.       |
| <b>LAG</b>               | is a classification effect in which the level that is used for a given period corresponds to the level in the preceding period.                                                                           |
| <b>MULTIMEMBER   MM</b>  | is a multimember classification effect whose levels are determined by one or more variables that appear in a CLASS statement.                                                                             |
| <b>POLYNOMIAL   POLY</b> | is a multivariate polynomial effect in the specified numeric variables.                                                                                                                                   |
| <b>SPLINE</b>            | is a regression spline effect whose columns are univariate spline expansions of one or more variables. A spline expansion replaces the original variable with an expanded or larger set of new variables. |

Table 67.5 summarizes the *options* available in the EFFECT statement.

**Table 67.5** EFFECT Statement Options

| Option                             | Description                                                                                                                                           |
|------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Collection Effects Options</b>  |                                                                                                                                                       |
| DETAILS                            | Displays the constituents of the collection effect                                                                                                    |
| <b>Lag Effects Options</b>         |                                                                                                                                                       |
| DESIGNROLE=                        | Names a variable that controls to which lag design an observation is assigned                                                                         |
| DETAILS                            | Displays the lag design of the lag effect                                                                                                             |
| NLAG=                              | Specifies the number of periods in the lag                                                                                                            |
| PERIOD=                            | Names the variable that defines the period                                                                                                            |
| WITHIN=                            | Names the variable or variables that define the group within which each period is defined                                                             |
| <b>Multimember Effects Options</b> |                                                                                                                                                       |
| NOEFFECT                           | Specifies that observations with all missing levels for the multi-member variables should have zero values in the corresponding design matrix columns |
| WEIGHT=                            | Specifies the weight variable for the contributions of each of the classification effects                                                             |
| <b>Polynomial Effects Options</b>  |                                                                                                                                                       |
| DEGREE=                            | Specifies the degree of the polynomial                                                                                                                |
| MDEGREE=                           | Specifies the maximum degree of any variable in a term of the polynomial                                                                              |
| STANDARDIZE=                       | Specifies centering and scaling suboptions for the variables that define the polynomial                                                               |
| <b>Spline Effects Options</b>      |                                                                                                                                                       |
| BASIS=                             | Specifies the type of basis (B-spline basis or truncated power function basis) for the spline expansion                                               |
| DEGREE=                            | Specifies the degree of the spline transformation                                                                                                     |
| KNOTMETHOD=                        | Specifies how to construct the knots for spline effects                                                                                               |

For more information about the syntax of these *effect-types* and how columns of constructed effects are computed, see the section “EFFECT Statement” on page 393 in Chapter 19, “Shared Concepts and Topics.”

## ESTIMATE Statement

```
ESTIMATE <'label'> estimate-specification <(divisor=n)>
 < , <'label'> estimate-specification <(divisor=n)> > < , ... >
 </ options > ;
```

The ESTIMATE statement provides a mechanism for obtaining custom hypothesis tests. Estimates are formed as linear estimable functions of the form  $\mathbf{L}\boldsymbol{\beta}$ . You can perform hypothesis tests for the estimable functions, construct confidence limits, and obtain specific nonlinear transformations.

Table 67.6 summarizes *options* available in the ESTIMATE statement. If the BAYES statement is specified, the ADJUST=, STEPDOWN, TESTVALUE, LOWER, UPPER, and JOINT options are ignored. The PLOTS= option is not available for the maximum likelihood analysis. It is available only for the Bayesian analysis.

**Table 67.6** ESTIMATE Statement Options

| Option                                                     | Description                                                                    |
|------------------------------------------------------------|--------------------------------------------------------------------------------|
| <b>Construction and Computation of Estimable Functions</b> |                                                                                |
| DIVISOR=                                                   | Specifies a list of values to divide the coefficients                          |
| NOFILL                                                     | Suppresses the automatic fill-in of coefficients for higher-order effects      |
| SINGULAR=                                                  | Tunes the estimability checking difference                                     |
| <b>Degrees of Freedom and <i>p</i>-values</b>              |                                                                                |
| ADJUST=                                                    | Determines the method for multiple comparison adjustment of estimates          |
| ALPHA= $\alpha$                                            | Determines the confidence level ( $1 - \alpha$ )                               |
| LOWER                                                      | Performs one-sided, lower-tailed inference                                     |
| STEPDOWN                                                   | Adjusts multiplicity-corrected <i>p</i> -values further in a step-down fashion |
| TESTVALUE=                                                 | Specifies values under the null hypothesis for tests                           |
| UPPER                                                      | Performs one-sided, upper-tailed inference                                     |
| <b>Statistical Output</b>                                  |                                                                                |
| CL                                                         | Constructs confidence limits                                                   |
| CORR                                                       | Displays the correlation matrix of estimates                                   |
| COV                                                        | Displays the covariance matrix of estimates                                    |
| E                                                          | Prints the $\mathbf{L}$ matrix                                                 |
| JOINT                                                      | Produces a joint <i>F</i> or chi-square test for the estimable functions       |
| PLOTS=                                                     | Requests ODS statistical graphics if the analysis is sampling-based            |
| SEED=                                                      | Specifies the seed for computations that depend on random numbers              |

For details about the syntax of the ESTIMATE statement, see the section “ESTIMATE Statement” on page 437 of Chapter 19, “Shared Concepts and Topics.”

---

## FREQ Statement

**FREQ** *variable* </ option > ;

The FREQ statement identifies the *variable* (in the input data set) that contains the frequency of occurrence of each observation. PROC PHREG treats each observation as if it appears  $n$  times, where  $n$  is the value of the FREQ variable for the observation. If not an integer, the frequency value is truncated to an integer. If the frequency value is missing, the observation is not used in the estimation of the regression parameters.

The following option can be specified in the FREQ statement after a slash (/):

**NOTRUNCATE**

**NOTRUNC**

specifies that frequency values are not truncated to integers.

---

## HAZARDRATIO Statement

**HAZARDRATIO** < 'label' > *variable* </ options > ;

The HAZARDRATIO statement enables you to request hazard ratios for any variable in the model at customized settings. For example, if the model contains the interaction of a CLASS variable A and a continuous variable X, the following specification displays a table of hazard ratios comparing the hazards of each pair of levels of A at X=3:

```
hazardratio A / at (X=3) diff=ALL;
```

The HAZARDRATIO statement identifies the variable whose hazard ratios are to be evaluated. If the variable is a continuous variable, the hazard ratio compares the hazards for a given change (by default, a increase of 1 unit) in the variable. For a CLASS variable, a hazard ratio compares the hazards of two levels of the variable. More than one HAZARDRATIO statement can be specified, and an optional label (specified as a quoted string) helps identify the output.

Table 67.7 summarizes the options available in the HAZARDRATIO statement.

**Table 67.7** HAZARDRATIO Statement Options

| Option      | Description                                                           |
|-------------|-----------------------------------------------------------------------|
| ALPHA=      | Specifies the alpha level                                             |
| AT          | Specifies the variables that interact with the variable of interest   |
| CL=         | Specifies confidence limits                                           |
| DIFF=       | Specifies which differences to consider                               |
| E           | Displays the log-hazard ratio                                         |
| PLCONV=     | Controls the convergence criterion                                    |
| PLMAXIT=    | Specifies the maximum number of iterations to achieve the convergence |
| PLSINGULAR= | Specifies the tolerance for testing the singularity                   |
| UNITS=      | Specifies the units of change                                         |

Options for the HAZARDRATIO statement are as follows.

**ALPHA=number**

specifies the alpha level of the interval estimates for the hazard ratios. The value must be between 0 and 1. The default is the value of the ALPHA= option in the PROC PHREG statement, or 0.05 if that option is not specified.

**AT (variable=ALL | REF | list <... variable=ALL | REF | list > )**

specifies the variables that interact with the variable of interest and the corresponding values of the interacting variables. If the interacting variable is continuous and a numeric list is specified after the equal sign, hazard ratios are computed for each value in the list. If the interacting variable is a CLASS variable, you can specify, after the equal sign, a list of quoted strings corresponding to various levels of the CLASS variable, or you can specify the keyword ALL or REF. Hazard ratios are computed at each value of the list if the list is specified, or at each level of the interacting variable if ALL is specified, or at the reference level of the interacting variable if REF is specified.

If this option is not specified, PROC PHREG finds all the variables that interact with the variable of interest. If an interacting variable is a CLASS variable, *variable= ALL* is the default; if the interacting variable is continuous, *variable=m* is the default, where *m* is the average of all the sampled values of the continuous variable.

Suppose the model contains two interactions: an interaction A\*B of CLASS variables A and B, and another interaction A\*X of A with a continuous variable X. If 3.5 is the average of the sampled values of X, the following two HAZARDRATIO statements are equivalent:

```
hazardratio A;
hazardratio A / at (B=ALL X=3.5);
```

**CL=WALD | PL | BOTH**

specifies whether to create the Wald or profile-likelihood confidence limits, or both for the classical analysis. By default, Wald confidence limits are produced. This option is not applicable to a Bayesian analysis.

**DIFF=ALL | REF**

specifies which differences to consider for the level comparisons of a CLASS variable. The default is DIFF=ALL. This option is ignored in the estimation of hazard ratios for a continuous variable. DIFF=ALL requests all differences, and DIFF=REF requests comparisons between the reference level and all other levels of the CLASS variable.

**E**

displays the vector **h** of linear coefficients such that  $\mathbf{h}'\boldsymbol{\beta}$  is the log-hazard ratio, with  $\boldsymbol{\beta}$  being the vector of regression coefficients.

**PLCONV=value**

controls the convergence criterion for the profile-likelihood confidence limits. The quantity *value* must be a positive number, with a default value of 1E-4. The PLCONV= option has no effect if profile-likelihood confidence intervals (CL=PL) are not requested.

**PLMAXIT=*n***

specifies the maximum number of iterations to achieve the convergence of the profile-likelihood confidence limits. By default, PLMAXITER=25. If convergence is not attained in *n* iterations, the corresponding profile-likelihood confidence limit for the hazard ratio is set to missing. The PLMAXITER= option has no effect if profile-likelihood confidence intervals (CL=PL) are not requested.

**PLSINGULAR=*value***

specifies the tolerance for testing the singularity of the Hessian matrix in the computation of the profile-likelihood confidence limits. The test requires that a pivot for sweeping this matrix be at least this number times a norm of the matrix. Values of the PLSINGULAR= option must be numeric. By default, *value* is the machine epsilon times 1E7, which is approximately 1E-9. The PLSINGULAR= option has no effect if profile-likelihood confidence intervals (CL=PL) are not requested.

**UNITS=*value***

specifies the units of change in the continuous explanatory variable for which the customized hazard ratio is estimated. The default is UNITS=1. This option is ignored in the computation of the hazard ratios for a CLASS variable.

---

## ID Statement

**ID** *variables* ;

The ID statement specifies additional variables for identifying observations in the input data. These variables are placed in the OUT= data set created by the OUTPUT statement. In the computation of the COVSANDWICH estimate, you can aggregate over distinct values of these ID variables.

Only variables in the input data set can be included in the ID statement.

---

## LSMEANS Statement

**LSMEANS** < *model-effects* > < / *options* > ;

The LSMEANS statement compares least squares means (LS-means) of fixed effects. LS-means are *predicted population margins*—that is, they estimate the marginal means over a balanced population. In a sense, LS-means are to unbalanced designs as class and subclass arithmetic means are to balanced designs.

Table 67.8 summarizes the options available in the LSMEANS statement. If the BAYES statement is specified, the ADJUST=, STEPDOWN, and LINES options are ignored. The PLOTS= option is not available for the maximum likelihood analysis. It is available only for the Bayesian analysis.



**Table 67.8** LSMEANS Statement Options

| Option                                              | Description                                                                                 |
|-----------------------------------------------------|---------------------------------------------------------------------------------------------|
| <b>Construction and Computation of LS-Means</b>     |                                                                                             |
| AT                                                  | Modifies the covariate value in computing LS-means                                          |
| BYLEVEL                                             | Computes separate margins                                                                   |
| DIFF                                                | Requests differences of LS-means                                                            |
| OM=                                                 | Specifies the weighting scheme for LS-means computation as determined by the input data set |
| SINGULAR=                                           | Tunes estimability checking                                                                 |
| <b>Degrees of Freedom and <math>p</math>-values</b> |                                                                                             |
| ADJUST=                                             | Determines the method for multiple-comparison adjustment of LS-means differences            |
| ALPHA= $\alpha$                                     | Determines the confidence level ( $1 - \alpha$ )                                            |
| STEPDOWN                                            | Adjusts multiple-comparison $p$ -values further in a step-down fashion                      |
| <b>Statistical Output</b>                           |                                                                                             |
| CL                                                  | Constructs confidence limits for means and mean differences                                 |
| CORR                                                | Displays the correlation matrix of LS-means                                                 |
| COV                                                 | Displays the covariance matrix of LS-means                                                  |
| E                                                   | Prints the L matrix                                                                         |
| LINES                                               | Produces a “Lines” display for pairwise LS-means differences                                |
| MEANS                                               | Prints the LS-means                                                                         |
| PLOTS=                                              | Requests graphs of means and mean comparisons                                               |
| SEED=                                               | Specifies the seed for computations that depend on random numbers                           |

For details about the syntax of the LSMEANS statement, see the section “LSMEANS Statement” on page 453 of Chapter 19, “Shared Concepts and Topics.”

## LSMESTIMATE Statement

```
LSMESTIMATE model-effect < 'label' > values < divisor=n >
 < , < 'label' > values < divisor=n > > < , ... >
 < / options > ;
```

The LSMESTIMATE statement provides a mechanism for obtaining custom hypothesis tests among least squares means.

Table 67.9 summarizes the options available in the LSMESTIMATE statement. If the BAYES statement is specified, the ADJUST=, STEPDOWN, TESTVALUE, LOWER, UPPER, and JOINT options are ignored. The PLOTS= option is not available for the maximum likelihood analysis. It is available only for the Bayesian analysis.

**Table 67.9** LSMESTIMATE Statement Options

| Option                                              | Description                                                                         |
|-----------------------------------------------------|-------------------------------------------------------------------------------------|
| <b>Construction and Computation of LS-Means</b>     |                                                                                     |
| AT                                                  | Modifies covariate values in computing LS-means                                     |
| BYLEVEL                                             | Computes separate margins                                                           |
| DIVISOR=                                            | Specifies a list of values to divide the coefficients                               |
| OM=                                                 | Specifies the weighting scheme for LS-means computation as determined by a data set |
| SINGULAR=                                           | Tunes estimability checking                                                         |
| <b>Degrees of Freedom and <math>p</math>-values</b> |                                                                                     |
| ADJUST=                                             | Determines the method for multiple-comparison adjustment of LS-means differences    |
| ALPHA= $\alpha$                                     | Determines the confidence level ( $1 - \alpha$ )                                    |
| LOWER                                               | Performs one-sided, lower-tailed inference                                          |
| STEPDOWN                                            | Adjusts multiple-comparison $p$ -values further in a step-down fashion              |
| TESTVALUE=                                          | Specifies values under the null hypothesis for tests                                |
| UPPER                                               | Performs one-sided, upper-tailed inference                                          |
| <b>Statistical Output</b>                           |                                                                                     |
| CL                                                  | Constructs confidence limits for means and mean differences                         |
| CORR                                                | Displays the correlation matrix of LS-means                                         |
| COV                                                 | Displays the covariance matrix of LS-means                                          |
| E                                                   | Prints the <b>L</b> matrix                                                          |
| ELSM                                                | Prints the <b>K</b> matrix                                                          |
| JOINT                                               | Produces a joint $F$ or chi-square test for the LS-means and LS-means differences   |
| PLOTS=                                              | Requests graphs of means and mean comparisons                                       |
| SEED=                                               | Specifies the seed for computations that depend on random numbers                   |

For details about the syntax of the LSMESTIMATE statement, see the section “LSMESTIMATE Statement” on page 470 of Chapter 19, “Shared Concepts and Topics.”

## MODEL Statement

**MODEL** *response* < \* *censor (list)* > = *effects* < / *options* > ;

**MODEL** (*t1*, *t2*) < \* *censor (list)* > = *effects* < / *options* > ;

The MODEL statement identifies the variables to be used as the failure time variables, the optional censoring variable, and the explanatory effects, including covariates, main effects, interactions, nested effects; see the section “Specification of Effects” on page 3324 of Chapter 42, “The GLM Procedure,” for more information. A note of caution: specifying the effect T\*A in the MODEL statement, where T is the time variable and A is

a CLASS variable, does not make the effect time-dependent. See the section “Time and CLASS Variables Usage” on page 5609 for more information.

Two forms of MODEL syntax can be specified; the first form allows one time variable, and the second form allows two time variables for the counting process style of input (see the section “Counting Process Style of Input” on page 5615 for more information).

In the first MODEL statement, the name of the failure time variable precedes the equal sign. This name can optionally be followed by an asterisk, the name of the censoring variable, and a list of censoring values (separated by blanks or commas if there is more than one) enclosed in parentheses. If the censoring variable takes on one of these values, the corresponding failure time is considered to be censored. Following the equal sign are the explanatory effects (sometimes called independent variables or covariates) for the model.

Instead of a single failure-time variable, the second MODEL statement identifies a pair of failure-time variables. Their names are enclosed in parentheses, and they signify the endpoints of a semiclosed interval  $(t1, t2]$  during which the subject is at risk. If the censoring variable takes on one of the censoring values, the time  $t2$  is considered to be censored.

The censoring variable must be numeric and the failure-time variables must contain nonnegative values. Any observation with a negative failure time is excluded from the analysis, as is any observation with a missing value for any of the variables listed in the MODEL statement. Failure-time variables with a SAS date format are not recommended because the dates might be translated into negative numbers and consequently the corresponding observation would be discarded.

Table 67.10 summarizes the *options* available in the MODEL statement. These *options* can be specified after a slash (/). Four convergence criteria are allowed for the maximum likelihood optimization: ABSFCONV=, FCONV=, GCONV=, and XCONV=. If you specify more than one convergence criterion, the optimization is terminated as soon as one of the criteria is satisfied. If none of the criteria is specified, the default is GCONV=1E-8.

**Table 67.10** MODEL Statement Options

| Option                             | Description                                                                                                                                        |
|------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Model Specification Options</b> |                                                                                                                                                    |
| NOFIT                              | Suppresses model fitting                                                                                                                           |
| OFFSET=                            | Specifies offset variable                                                                                                                          |
| SELECTION=                         | Specifies effect selection method                                                                                                                  |
| <b>Effect Selection Options</b>    |                                                                                                                                                    |
| BEST=                              | Controls the number of models displayed for SCORE selection                                                                                        |
| DETAILS                            | Requests detailed results at each step                                                                                                             |
| HIERARCHY=                         | Specifies whether and how hierarchy is maintained and whether a single effect or multiple effects are allowed to enter or leave the model per step |
| INCLUDE=                           | Specifies number of effects included in every model                                                                                                |
| MAXSTEP=                           | Specifies maximum number of steps for STEPWISE selection                                                                                           |
| SEQUENTIAL                         | Adds or deletes effects in sequential order                                                                                                        |
| SLENTRY=                           | Specifies significance level for entering effects                                                                                                  |
| SLSTAY=                            | Specifies significance level for removing effects                                                                                                  |

Table 67.10 *continued*

| Option                                         | Description                                                                                                           |
|------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------|
| START=                                         | Specifies number of variables in first model                                                                          |
| STOP=                                          | Specifies number of variables in final model                                                                          |
| STOPRES                                        | Adds or deletes variables by residual chi-square criterion                                                            |
| <b>Maximum Likelihood Optimization Options</b> |                                                                                                                       |
| ABSFCONV=                                      | Specifies absolute function convergence criterion                                                                     |
| FCONV=                                         | Specifies relative function convergence criterion                                                                     |
| FIRTH                                          | Specifies Firth's penalized likelihood method                                                                         |
| GCONV=                                         | Specifies relative gradient convergence criterion                                                                     |
| XCONV=                                         | Specifies relative parameter convergence criterion                                                                    |
| MAXITER=                                       | Specifies maximum number of iterations                                                                                |
| RIDGEINIT=                                     | Specifies the initial ridging value                                                                                   |
| RIDGING=                                       | Specifies the technique to improve the log likelihood function when its value is worse than that of the previous step |
| SINGULAR=                                      | Specifies tolerance for testing singularity                                                                           |
| <b>Confidence Interval Options</b>             |                                                                                                                       |
| ALPHA=                                         | Specifies $\alpha$ for the $100(1 - \alpha)\%$ confidence intervals                                                   |
| PLCONV=                                        | Specifies profile-likelihood convergence criterion                                                                    |
| RISKLIMITS=                                    | Computes confidence intervals for hazard ratios                                                                       |
| <b>Display Options</b>                         |                                                                                                                       |
| CORRB                                          | Displays correlation matrix                                                                                           |
| COVB                                           | Displays covariance matrix                                                                                            |
| ITPRINT                                        | Displays iteration history                                                                                            |
| NODUMMYPRINT                                   | Suppresses "Class Level Information" table                                                                            |
| TYPE1                                          | Displays Type 1 analysis                                                                                              |
| TYPE3                                          | Displays Type 3 analysis                                                                                              |
| <b>Miscellaneous Options</b>                   |                                                                                                                       |
| ENTRYTIME=                                     | Specifies the delayed entry time variable                                                                             |
| TIES=                                          | Specifies the method of handling ties in failure times                                                                |

**ALPHA=value**

sets the significance level used for the confidence limits for the hazard ratios. The quantity *value* must be between 0 and 1. The default is the value of the ALPHA= option in the PROC PHREG statement, or 0.05 if that option is not specified. This option has no effect unless the RISKLIMITS option is specified.

**ABSFCONV=value****CONVERGELIKE=value**

specifies the absolute function convergence criterion. Termination requires a small change in the objective function (log partial likelihood function) in subsequent iterations,

$$|l_k - l_{k-1}| < \text{value}$$

where  $l_k$  is the value of the objective function at iteration  $k$ .

**BEST=*n***

is used exclusively with the SCORE model selection method. The BEST=*n* option specifies that *n* models with the highest-score chi-square statistics are to be displayed for each model size. If the option is omitted and there are no more than 10 explanatory variables, then all possible models are listed for each model size. If the option is omitted and there are more than 10 explanatory variables, then the number of models selected for each model size is, at most, equal to the number of explanatory variables listed in the MODEL statement.

See [Example 67.2](#) for an illustration of the SCORE selection method and the BEST= option.

**CORRB**

displays the estimated correlation matrix of the parameter estimates.

**COVB**

displays the estimated covariance matrix of the parameter estimates.

**DETAILS**

produces a detailed display at each step of the model-building process. It produces an “Analysis of Variables Not in the Model” table before displaying the variable selected for entry for FORWARD or STEPWISE selection. For each model fitted, it produces the “Analysis of Maximum Likelihood Estimates” table.

See [Example 67.1](#) for a discussion of these tables.

**ENTRYTIME=*variable*****ENTRY=*variable***

specifies the name of the variable that represents the left-truncation time. This option has no effect when the counting process style of input is specified. See the section “[Left-Truncation of Failure Times](#)” on page 5617 for more information.

**FCONV=*value***

specifies the relative function convergence criterion. Termination requires a small relative change in the objective function (log partial likelihood function) in subsequent iterations,

$$\frac{|l_k - l_{k-1}|}{|l_{k-1}| + 1\text{E} - 6} < \textit{value}$$

where  $l_k$  is the value of the objective function at iteration  $k$ .

**FIRTH**

performs Firth’s penalized maximum likelihood estimation to reduce bias in the parameter estimates (Heinze and Schemper 2001; Firth 1993). This method is useful when the likelihood is monotone—that is, the likelihood converges to finite value while at least one estimate diverges to infinity.

**GCONV=*value***

specifies the relative gradient convergence criterion. Termination requires that the normalized prediction function reduction is small,

$$\frac{\mathbf{g}_k \mathbf{H}_k^{-1} \mathbf{g}_k}{|l_k| + 1\text{E} - 6} < \textit{value}$$

where  $l_k$  is the log partial likelihood,  $\mathbf{g}_k$  is the gradient vector (first partial derivatives of the log partial likelihood), and  $\mathbf{H}_k$  is the negative Hessian matrix (second partial derivatives of the log partial likelihood), all at iteration  $k$ .

**HIERARCHY=***keyword*

**HIER=***keyword*

specifies whether and how the model hierarchy requirement is applied and whether a single effect or multiple effects are allowed to enter or leave the model in one step. You can specify that only CLASS variable effects, or both CLASS and continuous variable effects, be subject to the hierarchy requirement. The HIERARCHY= option is ignored unless you also specify the FORWARD, BACKWARD, or STEPWISE selection method.

Model hierarchy refers to the requirement that, for any term to be in the model, all effects contained in the term must be present in the model. For example, in order for the interaction A\*B to enter the model, the main effects A and B must be in the model. Likewise, neither effect A nor B can leave the model while the interaction A\*B is in the model.

You can specify any of the following *keywords* in the HIERARCHY= option:

**NONE**

indicates that the model hierarchy is not maintained. Any single effect can enter or leave the model at any given step of the selection process.

**SINGLE**

indicates that only one effect can enter or leave the model at one time, subject to the model hierarchy requirement. For example, suppose that you specify the main effects A and B and the interaction of A\*B in the model. In the first step of the selection process, either A or B can enter the model. In the second step, the other main effect can enter the model. The interaction effect can enter the model only when both main effects have already been entered. Also, before A or B can be removed from the model, the A\*B interaction must first be removed. All effects (CLASS and continuous variables) are subject to the hierarchy requirement.

**SINGLECLASS**

is the same as HIERARCHY=SINGLE except that only CLASS effects are subject to the hierarchy requirement.

**MULTIPLE**

indicates that more than one effect can enter or leave the model at one time, subject to the model hierarchy requirement. In a forward selection step, a single main effect can enter the model, or an interaction can enter the model together with all the effects that are contained in the interaction. In a backward elimination step, an interaction itself, or the interaction together with all the effects that the interaction contains, can be removed. All effects (CLASS and continuous variable) are subject to the hierarchy requirement.

**MULTIPLECLASS**

is the same as HIERARCHY=MULTIPLE except that only CLASS effects are subject to the hierarchy requirement.

The default value is HIERARCHY=SINGLE, which means that model hierarchy is to be maintained for all effects (that is, both CLASS and continuous variable effects) and that only a single effect can enter or leave the model at each step.

**INCLUDE=*n***

includes the first *n* effects in the MODEL statement in every model. By default, INCLUDE=0. The INCLUDE= option has no effect when SELECTION=NONE.

**ITPRINT**

displays the iteration history, including the last evaluation of the gradient vector.

**MAXITER=*n***

specifies the maximum number of iterations allowed. The default value for *n* is 25. If convergence is not attained in *n* iterations, the displayed output and all data sets created by PROC PHREG contain results that are based on the last maximum likelihood iteration.

**MAXSTEP=*n***

specifies the maximum number of times the explanatory variables can move in and out of the model before the STEPWISE model-building process ends. The default value for *n* is twice the number of explanatory variables in the MODEL statement. The option has no effect for other model selection methods.

**NODUMMYPRINT****NODESIGNPRINT****NODP**

suppresses the “Class Level Information” table, which shows how the design matrix columns for the CLASS variables are coded.

**NOFIT**

performs the global score test, which tests the joint significance of all the explanatory variables in the MODEL statement. No parameters are estimated. If the NOFIT option is specified along with other MODEL statement options, NOFIT takes precedence, and all other options are ignored except the TIES= option.

**OFFSET=*name***

specifies the name of an offset variable, which is an explanatory variable with a regression coefficient fixed as one. This option can be used to incorporate risk weights for the likelihood function.

**PLCONV=*value***

controls the convergence criterion for confidence intervals based on the profile-likelihood function. The quantity *value* must be a positive number, with a default value of 1E-4. The PLCONV= option has no effect if profile-likelihood based confidence intervals are not requested.

**RIDGING=*keyword***

specifies the technique to improve the log likelihood when its value is worse than that of the previous step. The available *keywords* are as follows:

**ABSOLUTE**

specifies that the diagonal elements of the negative (expected) Hessian be inflated by adding the ridge value.

**RELATIVE**

specifies that the diagonal elements be inflated by the factor equal to 1 plus the ridge value.

**NONE**

specifies the crude line-search method of taking half a step be used instead of ridging.

The default is RIDGING=RELATIVE.

**RIDGEINIT=***value*

specifies the initial ridge value. The maximum ridge value is 2000 times the maximum of 1 and the initial ridge value. The initial ridge value is raised to 1E-4 if it is less than 1E-4. By default, RIDGEINIT=1E-4. This option has no effect for RIDGING=ABSOLUTE.

**RISKLIMITS**< =*keyword* >**RL**< =*keyword* >

produces confidence intervals for hazard ratios of main effects not involved in interactions or nestings. Computation of these confidence intervals is based on the profile likelihood or based on individual Wald tests. The confidence coefficient can be specified with the ALPHA= option. You can specify one of the following keywords:

**PL**

requests profile-likelihood confidence limits.

**WALD**

requests confidence limits based on the Wald tests.

**BOTH**

request both profile-likelihood and Wald confidence limits.

Classification main effects that use parameterizations other than REF, EFFECT, or GLM are ignored. If you need to compute hazard ratios for an effect involved in interactions or nestings, or using some other parameterization, then you should specify a HAZARDRATIO statement for that effect.

**SELECTION**=*method*

specifies the method used to select the model. The *methods* available are as follows:

**BACKWARD****B**

requests backward elimination.

**FORWARD****F**

requests forward selection.

**NONE****N**

fits the complete model specified in the MODEL statement. This is the default value.

**SCORE**

requests best subset selection. It identifies a specified number of models with the highest-score chi-square statistic for all possible model sizes ranging from one explanatory variable to the total number of explanatory variables listed in the MODEL statement. This option is not allowed if an explanatory effect in the MODEL statement contains a CLASS variable.



**STEPWISE****S**

requests stepwise selection.

For more information, see the section “[Effect Selection Methods](#)” on page 5648.

**SEQUENTIAL**

forces variables to be added to the model in the order specified in the MODEL statement or to be eliminated from the model in the reverse order of that specified in the MODEL statement.

**SINGULAR=value**

specifies the singularity criterion for determining linear dependencies in the set of explanatory variables. The default value is 1E-12.

**SLENTRY=value****SLE=value**

specifies the significance level (a value between 0 and 1) for entering an explanatory variable into the model in the FORWARD or STEPWISE method. For all variables not in the model, the one with the smallest  $p$ -value is entered if the  $p$ -value is less than or equal to the specified significance level. The default value is 0.05.

**SLSTAY=value****SLS=value**

specifies the significance level (a value between 0 and 1) for removing an explanatory variable from the model in the BACKWARD or STEPWISE method. For all variables in the model, the one with the largest  $p$ -value is removed if the  $p$ -value exceeds the specified significance level. The default value is 0.05.

**START=n**

begins the FORWARD, BACKWARD, or STEPWISE selection process with the first  $n$  effects listed in the MODEL statement. The value of  $n$  ranges from 0 to  $s$ , where  $s$  is the total number of effects in the MODEL statement. The default value of  $n$  is  $s$  for the BACKWARD method and 0 for the FORWARD and STEPWISE methods. Note that  $START=n$  specifies only that the first  $n$  effects appear in the first model, while  $INCLUDE=n$  requires that the first  $n$  effects be included in every model. For the SCORE method,  $START=n$  specifies that the smallest models contain  $n$  effects, where  $n$  ranges from 1 to  $s$ ; the default value is 1. The  $START=$  option has no effect when  $SELECTION=NONE$ .

**STOP=n**

specifies the maximum (FORWARD method) or minimum (BACKWARD method) number of effects to be included in the final model. The effect selection process is stopped when  $n$  effects are found. The value of  $n$  ranges from 0 to  $s$ , where  $s$  is the total number of effects in the MODEL statement. The default value of  $n$  is  $s$  for the FORWARD method and 0 for the BACKWARD method. For the SCORE method,  $STOP=n$  specifies that the smallest models contain  $n$  effects, where  $n$  ranges from 1 to  $s$ ; the default value of  $n$  is  $s$ . The  $STOP=$  option has no effect when  $SELECTION=NONE$  or  $STEPWISE$ .

**STOPRES****SR**

specifies that the addition and deletion of variables be based on the result of the likelihood score test for testing the joint significance of variables not in the model. This score chi-square statistic is referred to as the residual chi-square. In the FORWARD method, the STOPRES option enters the explanatory variables into the model one at a time until the residual chi-square becomes insignificant (that is, until the  $p$ -value of the residual chi-square exceeds the SLENTY= value). In the BACKWARD method, the STOPRES option removes variables from the model one at a time until the residual chi-square becomes significant (that is, until the  $p$ -value of the residual chi-square becomes less than the SLSTAY= value). The STOPRES option has no effect for the STEPWISE method.

**TYPE1**

requests that a Type 1 (sequential) analysis of likelihood ratio test be performed. This consists of sequentially fitting models, beginning with the null model and continuing up to the model specified in the MODEL statement. The likelihood ratio statistic for each successive pair of models is computed and displayed in a table.

**TYPE3** <(keywords)>

requests a Type 3 test for each effect that is specified in the MODEL statement. The default is to use the Wald statistic, but you can request other statistics by specifying one or more of the following keywords:

**ALL**

requests the likelihood ratio tests, the score tests, and the Wald tests. Specifying TYPE3(ALL) is equivalent to specifying TYPE3=(LR SCORE WALD).

**NONE**

suppresses the Type 3 analysis. Even if the TYPE3 option is not specified, PROC PHREG displays the Wald test results for each model effect if a CLASS variable is involved in a MODEL effect. The NONE option can be used to suppress such display.

**LR**

requests the likelihood ratio tests. This request is not honored if the COVS option is also specified.

**SCORE**

requests the score tests. This request is not honored if the COVS option is also specified.

**WALD**

requests the Wald tests.

**TIES=method**

specifies how to handle ties in the failure time. The following *methods* are available:

**BRESLOW**

uses the approximate likelihood of Breslow (1974). This is the default value.

**DISCRETE**

replaces the proportional hazards model by the discrete logistic model

$$\frac{\lambda(t; \mathbf{z})}{1 - \lambda(t; \mathbf{z})} = \frac{\lambda_0(t)}{1 - \lambda_0(t)} \exp(\mathbf{z}'\boldsymbol{\beta})$$

where  $\lambda_0(t)$  and  $h(t; \mathbf{z})$  are discrete hazard functions.

**EFRON**

uses the approximate likelihood of Efron (1977).

**EXACT**

computes the exact conditional probability under the proportional hazards assumption that all tied event times occur before censored times of the same value or before larger values. This is equivalent to summing all terms of the marginal likelihood for  $\beta$  that are consistent with the observed data (Kalbfleisch and Prentice 1980; DeLong, Guirguis, and So 1994).

The EXACT method can take a considerable amount of computer resources. If ties are not extensive, the EFRON and BRESLOW methods provide satisfactory approximations to the EXACT method for the continuous time-scale model. In general, Efron's approximation gives results that are much closer to the EXACT method results than Breslow's approximation does. If the time scale is genuinely discrete, you should use the DISCRETE method. The DISCRETE method is also required in the analysis of case-control studies when there is more than one case in a matched set. If there are no ties, all four methods result in the same likelihood and yield identical estimates. The default, TIES=BRESLOW, is the most efficient method when there are no ties.

**XCONV=value**

**CONVEREPARM=value**

specifies the relative parameter convergence criterion. Termination requires a small relative parameter change in subsequent iterations,

$$\max_i |\delta_k^{(i)}| < value$$

where

$$\delta_k^{(i)} = \begin{cases} \theta_k^{(i)} - \theta_{k-1}^{(i)} & |\theta_{k-1}^{(i)}| < .01 \\ \frac{\theta_k^{(i)} - \theta_{k-1}^{(i)}}{\theta_{k-1}^{(i)}} & \text{otherwise} \end{cases}$$

where  $\theta_k^{(i)}$  is the estimate of the  $i$ th parameter at iteration  $k$ .

**OUTPUT Statement**

**OUTPUT < OUT=SAS-data-set > < keyword=name ... keyword=name > < / options > ;**

The OUTPUT statement creates a new SAS data set containing statistics calculated for each observation. These can include the estimated linear predictor ( $\mathbf{z}'_j \hat{\beta}$ ) and its standard error, survival distribution estimates, residuals, and influence statistics. In addition, this data set includes the time variable, the explanatory variables listed in the MODEL statement, the censoring variable (if specified), and the BY, STRATA, FREQ, and ID variables (if specified).

For observations with missing values in the time variable or any explanatory variables, the output statistics are set to missing. However, for observations with missing values only in the censoring variable or the FREQ variable, survival estimates are still computed. Therefore, by adding observations with missing values in the FREQ variable or the censoring variable, you can compute the survivor function estimates for new observations or for settings of explanatory variables not present in the data without affecting the model fit.

No OUTPUT data set is created if the model contains a time-dependent variable defined by means of programming statements.

The following list explains specifications in the OUTPUT statement.

**OUT=SAS-data-set**

names the output data set. If you omit the OUT= option, the OUTPUT data set is created and given a default name by using the DATA $n$  convention. See the section “OUT= Output Data Set in the OUTPUT Statement” on page 5665 for more information.

**keyword=name**

specifies the statistics included in the OUTPUT data set and names the new variables that contain the statistics. Specify a keyword for each desired statistic (see the following list of keywords), an equal sign, and either a variable or a list of variables to contain the statistic. The keywords that accept a list of variables are DFBETA, RESSCH, RESSCO, and WTRESSCH. For these keywords, you can specify as many names in *name* as the number of explanatory variables specified in the MODEL statement. If you specify  $k$  names and  $k$  is less than the total number of explanatory variables, only the changes for the first  $k$  parameter estimates are output. The keywords and the corresponding statistics are as follows:

**ATRISK**

specifies the number of subjects at risk at the observation time  $\tau_j$  (or at the right endpoint of the at-risk interval when a counting process MODEL specification is used).

**DFBETA**

specifies the approximate changes in the parameter estimates ( $\hat{\beta} - \hat{\beta}_{(j)}$ ) when the  $j$ th observation is omitted. These variables are a weighted transform of the score residual variables and are useful in assessing local influence and in computing robust variance estimates.

**LD**

specifies the approximate likelihood displacement when the observation is left out. This diagnostic can be used to assess the impact of each observation on the overall fit of the model.

**LMAX**

specifies the relative influence of observations on the overall fit of the model. This diagnostic is useful in assessing the sensitivity of the fit of the model to each observation.

**LOGLOGS**

specifies the log of the negative log of SURVIVAL.

**LOGSURV**

specifies the log of SURVIVAL.

**RESDEV**

specifies the deviance residual  $\hat{D}_j$ . This is a transform of the martingale residual to achieve a more symmetric distribution.

**RESMART**

specifies the martingale residual  $\hat{M}_j$ . The residual at the observation time  $\tau_j$  can be interpreted as the difference over  $[0, \tau_j]$  in the observed number of events minus the expected number of events given by the model.

**RESSCH**

specifies the Schoenfeld residuals. These residuals are useful in assessing the proportional hazards assumption.

**RESSCO**

specifies the score residuals. These residuals are a decomposition of the first partial derivative of the log likelihood. They can be used to assess the leverage exerted by each subject in the parameter estimation. They are also useful in constructing robust sandwich variance estimators.

**STDXBETA**

specifies the standard error of the **XBETA** predictor,  $\sqrt{\mathbf{z}'_j \hat{\mathbf{V}}(\hat{\boldsymbol{\beta}}) \mathbf{z}_j}$ .

**SURVIVAL**

specifies the survivor function estimate  $\hat{S}_j = [\hat{S}_0(\tau_j)]^{\exp(\mathbf{z}'_j \hat{\boldsymbol{\beta}})}$ , where  $\tau_j$  is the observation time.

**WTRESSCH**

specifies the weighted Schoenfeld residuals. These residuals are useful in investigating the nature of nonproportionality if the proportional hazard assumption does not hold.

**XBETA**

specifies the estimate of the linear predictor,  $\mathbf{z}'_j \hat{\boldsymbol{\beta}}$ .

The following *options* can appear in the OUTPUT statement after a slash (/) as follows:

**ORDER=value**

specifies the order of the observations in the OUTPUT data set. The following *values* are available:

- DATA** requests that the output observations be sorted the same as the input data set.
- SORTED** requests that the output observations be sorted by strata and descending order of the time variable within each stratum.

The default is ORDER=DATA.

**METHOD=method**

specifies the method used to compute the survivor function estimates. See the section “Survivor Function Estimators” on page 5643 for details. The following *methods* are available:

**BRESLOW****CH****EMP**

specifies that the empirical cumulative hazard function estimate of the survivor function be computed; that is, the survivor function is estimated by exponentiating the negative empirical cumulative hazard function.

**FH**

specifies that the Fleming-Harrington (FH) estimates be computed. The FH estimator is a tie-breaking modification of the Breslow estimator. If there are no tied event times, this estimator is the same as the Breslow estimator.

**PL**

specifies that the product-limit estimates of the survivor function be computed. This estimator is not available if you use the model syntax that allows two time variables for the counting process style of input; in such a case, the Breslow estimator (METHOD=BRESLOW) is used instead.

The default is METHOD=BRESLOW.

---

## Programming Statements

Programming statements are used to create or modify the values of the explanatory variables in the MODEL statement. They are especially useful in fitting models with time-dependent explanatory variables. Programming statements can also be used to create explanatory variables that are not time dependent. For example, you can create indicator variables from a categorical variable and incorporate them into the model. PROC PHREG programming statements cannot be used to create or modify the values of the response variable, the censoring variable, the frequency variable, or the strata variables.

The following DATA step statements are available in PROC PHREG:

```

ABORT;
ARRAY arrayname < [dimensions] > < $ > < variables-and-constants >;
CALL name < (expression < , expression ... >) >;
DELETE;
DO < variable = expression < TO expression > < BY expression > >
 < , expression < TO expression > < BY expression > > ...
 < WHILE expression > < UNTIL expression >;
END;
GOTO statement-label;
IF expression;
IF expression THEN program-statement;
 ELSE program-statement;
variable = expression;
variable + expression;
LINK statement-label;
PUT < variable > < = > ...;
RETURN;
SELECT < (expression) >;
STOP;
SUBSTR(variable, index, length) = expression;
WHEN (expression) program-statement;
 OTHERWISE program-statement;

```

By default, the PUT statement in PROC PHREG writes results to the Output window instead of the Log window. If you want the results of the PUT statements to go to the Log window, add the following statement before the PUT statements:

```
FILE LOG;
```

DATA step functions are also available. Use these programming statements the same way you use them in the DATA step. For detailed information, see *SAS Statements: Reference*.

Consider the following example of using programming statements in PROC PHREG. Suppose blood pressure is measured at multiple times during the course of a study investigating the effect of blood pressure on some survival time. By treating the blood pressure as a time-dependent explanatory variable, you are able to use the value of the most recent blood pressure at each specific point of time in the modeling process rather than using the initial blood pressure or the final blood pressure. The values of the following variables are recorded for each patient, if they are available. Otherwise, the variables contain missing values.

|        |                                                     |
|--------|-----------------------------------------------------|
| Time   | survival time                                       |
| Censor | censoring indicator (with 0 as the censoring value) |
| BP0    | blood pressure on entry to the study                |
| T1     | time 1                                              |
| BP1    | blood pressure at T1                                |
| T2     | time 2                                              |
| BP2    | blood pressure at T2                                |

The following programming statements create a variable BP. At each time T, the value of BP is the blood pressure reading for that time, if available. Otherwise, it is the last blood pressure reading.

```
proc phreg;
 model Time*Censor(0)=BP;
 BP = BP0;
 if Time>=T1 and T1^=. then BP=BP1;
 if Time>=T2 and T2^=. then BP=BP2;
run;
```

For other illustrations of using programming statements, see the section “Classical Method of Maximum Likelihood” on page 5544 and Example 67.6.

---

## RANDOM Statement

**RANDOM** *variable* </ options > ;

The RANDOM statement enables you to fit a shared frailty model for clustered data (see the section “The Frailty Model” on page 5618 for details). The *variable* that represents the clusters must be a CLASS variable (declared in the CLASS statement).

The following *options* can be specified in the RANDOM statement:

### **ABSPCONV=***r*

specifies an absolute variance estimate convergence criterion for the doubly iterative estimation process. The PHREG procedure applies this criterion to the variance parameter estimate of the random effects. Suppose  $\hat{\theta}^{(j)}$  denotes the estimate of the variance parameter at the *j*th optimization. By default, PROC PHREG examines the relative change in the variance estimate between optimizations (see the PCONV= option). The purpose of the ABSPCONV= criterion is to stop the doubly iterative process when the absolute change  $|\hat{\theta}^{(j)} - \hat{\theta}^{(j-1)}|$  is less than the tolerance criterion *r*. This convergence criterion does not affect the convergence criteria applied within any individual optimization. In order to change the convergence behavior within an individual optimization, you can use the

ABSCONV=, ABSFCONV=, ABSGCONV=, ABSXCONV=, FCONV=, or GCONV= option in the NLOPTIONS statement.

**ALPHA=value**

specifies the  $\alpha$  level of the confidence limits for the random effects. The default is the value of the ALPHA= option in the PROC PHREG statement, or 0.05 if that option is not specified. This option is ignored if the SOLUTION option is not also specified.

**DIST=GAMMA | LOGNORMAL**

specifies the distribution of the shared frailty. DIST=GAMMA specifies a gamma frailty model. DIST=LOGNORMAL specifies a lognormal frailty model; that is, the log-frailty random variable has a normal distribution with mean zero. The default is DIST=LOGNORMAL.

**METHOD=REML | ML**

specifies the estimation method for the variance parameter of the normal random effects. METHOD=REML performs the residual maximum likelihood; METHOD=ML performs maximum likelihood. This option is ignored for the gamma frailty model. The default is METHOD=REML.

**NOCLPRINT**

suppresses the display of the “Class Level Information for Random Effects” table.

**PCONV=r**

specifies the variance estimate convergence criterion for the doubly iterative estimation process. The PHREG procedure applies this criterion to the variance estimate of the random effects. Suppose  $\hat{\theta}^{(j)}$  denotes the estimate of variance at the  $j$ th optimization. The procedure terminates the doubly iterative process if the relative change

$$2 \times \frac{|\hat{\theta}^{(j)} - \hat{\theta}^{(j-1)}|}{|\hat{\theta}^{(j)}| + |\hat{\theta}^{(j-1)}|}$$

is less than  $r$ . To check an absolute convergence criterion in addition, you can specify the ABSPCONV= option in the RANDOM statement. The default value for  $r$  is 1E-4. This convergence criterion does not affect the convergence criteria applied within any individual optimization. In order to change the convergence behavior within an individual optimization, you can use the ABSCONV=, ABSFCONV=, ABSGCONV=, ABSXCONV=, FCONV=, or GCONV= option in the NLOPTIONS statement.

**SOLUTION < (number-list) >**

displays statistical measures of the random-effect parameters. The behavior of this option depends on whether you also specify the BAYES statement:

- When you do not specify a BAYES statement, this option displays point estimates and confidence intervals for the random components and for the frailties.
- When you also specify a BAYES statement, this option displays the summary statistics and diagnostics of the random-effect parameters. Optionally, you can specify a *number-list* of indices of the random-effect parameters for which the summary statistics and diagnostics are to be displayed. For example, to display the summary statistics and diagnostics for the second to the fifth random-effect parameters, specify

**SOLUTION(2 to 5)**

If you specify SOLUTION without a list, summary statistics and diagnostics are displayed for each random-effect parameter.



**INITIALVARIANCE**=*value*

**INITIAL**=*value*

specifies an initial value of the dispersion parameter. For the lognormal frailty model, the dispersion parameter represents the variance of the normal random effect; for the gamma frailty model, it represents the variance of the gamma frailty. The default is INITIAL=1.

## STRATA Statement

**STRATA** *variable* <(list)> <... *variable* <(list)>> </option> ;

The proportional hazards assumption might not be realistic for all data. If so, it might still be reasonable to perform a stratified analysis. The STRATA statement names the variables that determine the stratification. Strata are formed according to the nonmissing values of the STRATA variables unless the MISSING option is specified. In the STRATA statement, *variable* is a variable with values that are used to determine the strata levels, and *list* is an optional list of values for a numeric variable. Multiple variables can appear in the STRATA statement.

The values for *variable* can be formatted or unformatted. If the variable is a character variable, or if the variable is numeric and no list appears, then the strata are defined by the unique values of the variable. If the variable is numeric and is followed by a list, then the levels for that variable correspond to the intervals defined by the list. The corresponding strata are formed by the combination of levels and unique values. The list can include numeric values separated by commas or blanks, *value* to *value* by *value* range specifications, or combinations of these.

For example, the specification

```
strata age (5, 10 to 40 by 10) sex;
```

indicates that the levels for *age* are to be less than 5, 5 to 10, 10 to 20, 20 to 30, 30 to 40, and greater than 40. (Note that observations with exactly the cutpoint value fall into the interval preceding the cutpoint.) Thus, with the *sex* variable, this STRATA statement specifies 12 strata altogether.

The following option can be specified in the STRATA statement after a slash (/):

### MISSING

allows missing values (‘.’ for numeric variables and blanks for character variables) as valid STRATA variable values. Otherwise, observations with missing STRATA variable values are deleted from the analysis.

## SLICE Statement

**SLICE** *model-effect* </options> ;

The SLICE statement provides a general mechanism for performing a partitioned analysis of the LS-means for an interaction. This analysis is also known as an analysis of simple effects.

The SLICE statement uses the same options as the LSMEANS statement, which are summarized in Table 19.21. For details about the syntax of the SLICE statement, see the section “SLICE Statement” on page 498 in Chapter 19, “Shared Concepts and Topics.”

---

## STORE Statement

**STORE** <OUT=>*item-store-name* </ LABEL='label'> ;

The STORE statement requests that the procedure save the context and results of the statistical analysis. The resulting item store has a binary file format that cannot be modified. The contents of the item store can be processed with the PLM procedure.

For details about the syntax of the STORE statement, see the section “STORE Statement” on page 501 in Chapter 19, “Shared Concepts and Topics.”

---

## TEST Statement

<label:> **TEST** *equation* <, ..., *equation*> </ options> ;

The TEST statement tests linear hypotheses about the regression coefficients. PROC PHREG performs a Wald test for the joint hypothesis specified in a single TEST statement. Each equation specifies a linear hypothesis; multiple equations (rows of the joint hypothesis) are separated by commas. The *label*, which must be a valid SAS name, is used to identify the resulting output and should always be included. You can submit multiple TEST statements.

The form of an equation is as follows:

*term* < ± *term* ... > <= < ± *term* < ± *term* ... >>>

where *term* is a variable or a constant or a constant times a variable. The variable is any explanatory variable in the MODEL statement. When no equal sign appears, the expression is set to 0. The following program illustrates possible uses of the TEST statement:

```
proc phreg;
 model time= A1 A2 A3 A4;
 Test1: test A1, A2;
 Test2: test A1=0,A2=0;
 Test3: test A1=A2=A3;
 Test4: test A1=A2,A2=A3;
run;
```

Note that the first and second TEST statements are equivalent, as are the third and fourth TEST statements.

The following *options* can be specified in the TEST statement after a slash (/):

### AVERAGE

enables you to assess the average effect of the variables in the given TEST statement. An overall estimate of the treatment effect is computed as a weighted average of the treatment coefficients as illustrated in the following statement:

```
TREATMENT: test trt1, trt2, trt3, trt4 / average;
```

Let  $\beta_1, \beta_2, \beta_3,$  and  $\beta_4$  be corresponding parameters for trt1, trt2, trt3, and trt4, respectively. Let  $\hat{\beta} = (\hat{\beta}_1, \hat{\beta}_2, \hat{\beta}_3, \hat{\beta}_4)'$  be the estimated coefficient vector and let  $\hat{V}(\hat{\beta})$  be the corresponding variance estimate. Assuming  $\beta_1 = \beta_2 = \beta_3 = \beta_4$ , let  $\bar{\beta}$  be the average treatment effect. The effect is

estimated by  $\mathbf{c}'\hat{\boldsymbol{\beta}}$ , where  $\mathbf{c} = [\mathbf{1}'_4 \hat{\mathbf{V}}^{-1}(\hat{\boldsymbol{\beta}}) \mathbf{1}_4]^{-1} \hat{\mathbf{V}}^{-1}(\hat{\boldsymbol{\beta}}) \mathbf{1}_4$  and  $\mathbf{1}_4 = (1, 1, 1, 1)'$ . A test of the null hypothesis  $H_0 : \bar{\beta} = 0$  is also included, which is more sensitive than the multivariate test for testing the null hypothesis  $H_0 : \beta_1 = \beta_2 = \beta_3 = \beta_4 = 0$ .

**E**

specifies that the linear coefficients and constants be printed. When the AVERAGE option is specified along with the E option, the optimal weights of the average effect are also printed in the same tables as the coefficients.

**PRINT**

displays intermediate calculations. This includes  $\mathbf{L}\hat{\mathbf{V}}(\hat{\boldsymbol{\beta}})\mathbf{L}'$  bordered by  $(\mathbf{L}\hat{\boldsymbol{\beta}} - \mathbf{c})$ , and  $[\mathbf{L}\hat{\mathbf{V}}(\hat{\boldsymbol{\beta}})\mathbf{L}']^{-1}$  bordered by  $[\mathbf{L}\hat{\mathbf{V}}(\hat{\boldsymbol{\beta}})\mathbf{L}']^{-1}(\mathbf{L}\hat{\boldsymbol{\beta}} - \mathbf{c})$ , where  $\mathbf{L}$  is a matrix of linear coefficients and  $\mathbf{c}$  is a vector of constants.

See the section “Using the TEST Statement to Test Linear Hypotheses” on page 5628 for details.

## WEIGHT Statement

**WEIGHT** *variable* </option> ;

The *variable* in the WEIGHT statement identifies the variable in the input data set that contains the case weights. When the WEIGHT statement appears, each observation in the input data set is weighted by the value of the WEIGHT variable. The WEIGHT values can be nonintegral and are not truncated. Observations with negative, zero, or missing values for the WEIGHT variable are not used in the model fitting. When the WEIGHT statement is not specified, each observation is assigned a weight of 1. The WEIGHT statement is available for TIES=BRESLOW and TIES=EFRON only.

The following *option* can be specified in the WEIGHT statement after a slash (/):

**NORMALIZE****NORM**

causes the weights specified by the WEIGHT *variable* to be normalized so that they add up the actual sample size. With this option, the estimated covariance matrix of the parameter estimators is invariant to the scale of the WEIGHT variable.

## Details: PHREG Procedure

### Failure Time Distribution

Let  $T$  be a nonnegative random variable representing the failure time of an individual from a homogeneous population. The survival distribution function (also known as the survivor function) of  $T$  is written as

$$S(t) = \Pr(T \geq t)$$

A mathematically equivalent way of specifying the distribution of  $T$  is through its hazard function. The hazard function  $\lambda(t)$  specifies the instantaneous failure rate at  $t$ . If  $T$  is a continuous random variable,  $\lambda(t)$  is expressed as

$$\lambda(t) = \lim_{\Delta t \rightarrow 0^+} \frac{\Pr(t \leq T < t + \Delta t \mid T \geq t)}{\Delta t} = \frac{f(t)}{S(t)}$$

where  $f(t)$  is the probability density function of  $T$ . If  $T$  is discrete with masses at  $x_1 < x_2 < \dots$ , then survivor function is given by

$$S(t) = \sum_{x_j \leq t} \Pr(T = x_j) = \sum_j \Pr(T = j) \delta(t - x_j)$$

where  $\delta(u)=0$  if  $u < 0$  and  $\delta(u)=1$  otherwise. The discrete hazards are given by

$$\lambda_j = \Pr(T = x_j \mid T \geq x_j) = \frac{\Pr(T = x_j)}{S(x_j)} \quad j = 1, 2, \dots$$

---

## Time and CLASS Variables Usage

The following DATA step creates an artificial data set, `Test`, to be used in this section. There are four variables in `Test`: the variable `T` contains the failure times; the variable `Status` is the censoring indicator variable with the value 1 for an uncensored failure time and the value 0 for a censored time; the variable `A` is a categorical variable with values 1, 2, and 3 representing three different categories; and the variable `MirrorT` is an exact copy of `T`.

```
data Test;
 input T Status A @@;
 MirrorT = T;
 datalines;
23 1 1 7 0 1
23 1 1 10 1 1
20 0 1 13 0 1
24 1 1 10 1 1
18 1 2 6 1 2
18 0 2 6 1 2
13 0 2 13 1 2
 9 0 2 15 1 2
 8 1 3 6 1 3
12 0 3 4 1 3
11 1 3 8 1 1
 6 1 3 7 1 3
 7 1 3 12 1 3
 9 1 2 15 1 2
 3 1 2 14 0 3
 6 1 1 13 1 2
;
```

### Time Variable on the Right Side of the MODEL Statement

When the time variable is explicitly used in an explanatory effect in the MODEL statement, the effect is *not* time-dependent. In the following specification, T is the time variable, but T does not play the role of the time variable in the explanatory effect T\*A:

```
proc phreg data=Test;
 class A;
 model T*Status(0)=T*A;
run;
```

The parameter estimates of this model are shown in Figure 67.12.

**Figure 67.12** T\*A Effect

| The PHREG Procedure                      |     |                    |                |            |            |              |         |  |
|------------------------------------------|-----|--------------------|----------------|------------|------------|--------------|---------|--|
| Analysis of Maximum Likelihood Estimates |     |                    |                |            |            |              |         |  |
| Parameter                                | DF  | Parameter Estimate | Standard Error | Chi-Square | Pr > ChiSq | Hazard Ratio | Label   |  |
| T*A                                      | 1 1 | -0.16549           | 0.05042        | 10.7734    | 0.0010     | .            | A 1 * T |  |
| T*A                                      | 2 1 | -0.11852           | 0.04181        | 8.0344     | 0.0046     | .            | A 2 * T |  |

To verify that the effect T\*A in the MODEL statement is not time-dependent, T is replaced by MirrorT, which is an exact copy of T, as in the following statements:

```
proc phreg data=Test;
 class A;
 model T*Status(0)=A*MirrorT;
run;
```

The results of fitting this model (Figure 67.13) are identical to those of the previous model (Figure 67.12), except for the parameter names and labels. The effect A\*MirrorT is not time-dependent, so neither is A\*T.

Figure 67.13 T\*A Effect

| The PHREG Procedure                      |    |                    |                |            |            |
|------------------------------------------|----|--------------------|----------------|------------|------------|
| Analysis of Maximum Likelihood Estimates |    |                    |                |            |            |
| Parameter                                | DF | Parameter Estimate | Standard Error | Chi-Square | Pr > ChiSq |
| MirrorT*A 1                              | 1  | -0.16549           | 0.05042        | 10.7734    | 0.0010     |
| MirrorT*A 2                              | 1  | -0.11852           | 0.04181        | 8.0344     | 0.0046     |

| Analysis of Maximum Likelihood Estimates |              |               |
|------------------------------------------|--------------|---------------|
| Parameter                                | Hazard Ratio | Label         |
| MirrorT*A 1                              | .            | A 1 * MirrorT |
| MirrorT*A 2                              | .            | A 2 * MirrorT |

## CLASS Variables and Programming Statements

In PROC PHREG, the levels of CLASS variables are determined by the CLASS statement and the input data and are not affected by user-supplied programming statements. Consider the following statements, which produce the results in Figure 67.14. Variable A is declared as a CLASS variable in the CLASS statement. By default, the reference parameterization is used with A=3 as the reference level. Two regression coefficients are estimated for the two dummy variables of A.

```
proc phreg data=Test;
 class A;
 model T*Status(0)=A;
run;
```

Figure 67.14 shows the dummy variables of A and the regression coefficients estimates.

Figure 67.14 Design Variable and Regression Coefficient Estimates

| The PHREG Procedure     |       |                  |   |
|-------------------------|-------|------------------|---|
| Class Level Information |       |                  |   |
| Class                   | Value | Design Variables |   |
| A                       | 1     | 1                | 0 |
|                         | 2     | 0                | 1 |
|                         | 3     | 0                | 0 |

Figure 67.14 continued

| Analysis of Maximum Likelihood Estimates |    |                    |                |            |            |              |           |
|------------------------------------------|----|--------------------|----------------|------------|------------|--------------|-----------|
| Parameter                                | DF | Parameter Estimate | Standard Error | Chi-Square | Pr > ChiSq | Hazard Ratio | Label     |
| A                                        | 1  | 1                  | -1.40925       | 0.64802    | 4.7293     | 0.0297       | 0.244 A 1 |
| A                                        | 2  | 1                  | -0.65705       | 0.51764    | 1.6112     | 0.2043       | 0.518 A 2 |

Now consider the programming statement that attempts to change the value of the CLASS variable A as in the following specification:

```
proc phreg data=Test;
 class A;
 model T*Status(0)=A;
 if A=3 then A=2;
run;
```

Results of this analysis are shown in Figure 67.15 and are identical to those in Figure 67.14. The `if A=3 then A=2` programming statement has no effects on the design variables for A, which have already been determined.

Figure 67.15 Design Variable and Regression Coefficient Estimates

| The PHREG Procedure                      |       |                    |                |            |            |              |           |
|------------------------------------------|-------|--------------------|----------------|------------|------------|--------------|-----------|
| Class Level Information                  |       |                    |                |            |            |              |           |
| Class                                    | Value | Design Variables   |                |            |            |              |           |
| A                                        | 1     | 1                  | 0              |            |            |              |           |
|                                          | 2     | 0                  | 1              |            |            |              |           |
|                                          | 3     | 0                  | 0              |            |            |              |           |
| Analysis of Maximum Likelihood Estimates |       |                    |                |            |            |              |           |
| Parameter                                | DF    | Parameter Estimate | Standard Error | Chi-Square | Pr > ChiSq | Hazard Ratio | Label     |
| A                                        | 1     | 1                  | -1.40925       | 0.64802    | 4.7293     | 0.0297       | 0.244 A 1 |
| A                                        | 2     | 1                  | -0.65705       | 0.51764    | 1.6112     | 0.2043       | 0.518 A 2 |

Additionally any variable used in a programming statement that has already been declared in the CLASS statement is *not* treated as a collection of the corresponding design variables. Consider the following statements:

```

proc phreg data=Test;
 class A;
 model T*Status(0)=A X;
 X=T*A;
run;

```

The CLASS variable A generates two design variables as explanatory variables. The variable X created by the `X=T*A` programming statement is a single time-dependent covariate whose values are evaluated using the exact values of A given in the data, not the dummy-coded values that represent the levels of A. In data set Test, A assumes the values of 1, 2, and 3, and these are the exact values that are used in producing X. If A were a character variable with values ‘Bird’, ‘Cat’, and ‘Dog’, the programming statement `X=T*A` would have produced an error in the attempt to multiply a number with a character value.

**Figure 67.16** Single Time-Dependent Variable X\*A

| The PHREG Procedure                      |    |                    |                |            |            |              |       |     |
|------------------------------------------|----|--------------------|----------------|------------|------------|--------------|-------|-----|
| Analysis of Maximum Likelihood Estimates |    |                    |                |            |            |              |       |     |
| Parameter                                | DF | Parameter Estimate | Standard Error | Chi-Square | Pr > ChiSq | Hazard Ratio | Label |     |
| A                                        | 1  | 1                  | 0.15798        | 1.69338    | 0.0087     | 0.9257       | 1.171 | A 1 |
| A                                        | 2  | 1                  | 0.00898        | 0.87573    | 0.0001     | 0.9918       | 1.009 | A 2 |
| X                                        |    | 1                  | 0.09268        | 0.09535    | 0.9448     | 0.3311       | 1.097 |     |

To generalize the simple test of proportional hazard assumption for the design variables of A (as in the section the “[Classical Method of Maximum Likelihood](#)” on page 5544), you specify the following statements, which are not the same as in the preceding program or as in the specification in the section “[Time Variable on the Right Side of the MODEL Statement](#)” on page 5610:

```

proc phreg data=Test;
 class A;
 model T*Status(0)=A X1 X2;
 X1= T*(A=1);
 X2= T*(A=2);
run;

```

The Boolean parenthetical expressions (A=1) and (A=2) resolve to a value of 1 or 0, depending on whether the expression is true or false, respectively.

Results of this test are shown in [Figure 67.17](#).



**Figure 67.17** Simple Test of Proportional Hazards Assumption

| The PHREG Procedure                      |    |                    |                |            |            |              |       |     |
|------------------------------------------|----|--------------------|----------------|------------|------------|--------------|-------|-----|
| Analysis of Maximum Likelihood Estimates |    |                    |                |            |            |              |       |     |
| Parameter                                | DF | Parameter Estimate | Standard Error | Chi-Square | Pr > ChiSq | Hazard Ratio | Label |     |
| A                                        | 1  | 1                  | -0.00766       | 1.69435    | 0.0000     | 0.9964       | 0.992 | A 1 |
| A                                        | 2  | 1                  | -0.88132       | 1.64298    | 0.2877     | 0.5917       | 0.414 | A 2 |
| X1                                       |    | 1                  | -0.15522       | 0.20174    | 0.5920     | 0.4417       | 0.856 |     |
| X2                                       |    | 1                  | 0.01155        | 0.18858    | 0.0037     | 0.9512       | 1.012 |     |

In general, when your model contains a categorical explanatory variable that is time-dependent, it might be necessary to use hardcoded dummy variables to represent the categories of the categorical variable. Alternatively, you might consider using the counting-process style of input where you break up the covariate history of an individual into a number of records with nonoverlapping start and stop times and declare the categorical time-dependent variable in the CLASS statement.

## Partial Likelihood Function for the Cox Model

Let  $\mathbf{Z}_l(t)$  denote the vector explanatory variables for the  $l$ th individual at time  $t$ . Let  $t_1 < t_2 < \dots < t_k$  denote the  $k$  distinct, ordered event times. Let  $d_i$  denote the multiplicity of failures at  $t_i$ ; that is,  $d_i$  is the size of the set  $\mathcal{D}_i$  of individuals that fail at  $t_i$ . Let  $w_l$  be the weight associated with the  $l$ th individual. Using this notation, the likelihood functions used in PROC PHREG to estimate  $\boldsymbol{\beta}$  are described in the following sections.

### Continuous Time Scale

Let  $\mathcal{R}_i$  denote the risk set just before the  $i$ th ordered event time  $t_i$ . Let  $\mathcal{R}_i^*$  denote the set of individuals whose event or censored times exceed  $t_i$  or whose censored times are equal to  $t_i$ .

#### Exact Likelihood

$$L_1(\boldsymbol{\beta}) = \prod_{i=1}^k \left\{ \int_0^{\infty} \prod_{j \in \mathcal{D}_i} \left[ 1 - \exp \left( - \frac{e^{\boldsymbol{\beta}' \mathbf{Z}_j(t_i)}}{\sum_{l \in \mathcal{R}_i^*} e^{\boldsymbol{\beta}' \mathbf{Z}_l(t_i)} t} \right) \right] \exp(-t) dt \right\}$$

#### Breslow Likelihood

$$L_2(\boldsymbol{\beta}) = \prod_{i=1}^k \frac{e^{\boldsymbol{\beta}' \sum_{j \in \mathcal{D}_i} \mathbf{Z}_j(t_i)}}{\left[ \sum_{l \in \mathcal{R}_i} e^{\boldsymbol{\beta}' \mathbf{Z}_l(t_i)} \right]^{d_i}}$$

Incorporating weights, the Breslow likelihood becomes

$$L_2(\boldsymbol{\beta}) = \prod_{i=1}^k \frac{e^{\boldsymbol{\beta}' \sum_{j \in \mathcal{D}_i} w_j \mathbf{Z}_j(t_i)}}{\left[ \sum_{l \in \mathcal{R}_i} w_l e^{\boldsymbol{\beta}' \mathbf{Z}_l(t_i)} \right]^{\sum_{j \in \mathcal{D}_i} w_j}}$$

### Efron Likelihood

$$L_3(\boldsymbol{\beta}) = \prod_{i=1}^k \frac{e^{\boldsymbol{\beta}' \sum_{j \in \mathcal{D}_i} \mathbf{Z}_j(t_i)}}{\prod_{j=1}^{d_i} \left( \sum_{l \in \mathcal{R}_i} e^{\boldsymbol{\beta}' \mathbf{Z}_l(t_i)} - \frac{j-1}{d_i} \sum_{l \in \mathcal{D}_i} e^{\boldsymbol{\beta}' \mathbf{Z}_l(t_i)} \right)}$$

Incorporating weights, the Efron likelihood becomes

$$L_3(\boldsymbol{\beta}) = \prod_{i=1}^k \frac{e^{\boldsymbol{\beta}' \sum_{j \in \mathcal{D}_i} w_j \mathbf{Z}_j(t_i)}}{\left[ \prod_{j=1}^{d_i} \left( \sum_{l \in \mathcal{R}_i} w_l e^{\boldsymbol{\beta}' \mathbf{Z}_l(t_i)} - \frac{j-1}{d_i} \sum_{l \in \mathcal{D}_i} w_l e^{\boldsymbol{\beta}' \mathbf{Z}_l(t_i)} \right) \right]^{\frac{1}{d_i} \sum_{j \in \mathcal{D}_i} w_j}}$$

## Discrete Time Scale

Let  $\mathcal{Q}_i$  denote the set of all subsets of  $d_i$  individuals from the risk set  $\mathcal{R}_i$ . For each  $\mathbf{q} \in \mathcal{Q}_i$ ,  $\mathbf{q}$  is a  $d_i$ -tuple  $(q_1, q_2, \dots, q_{d_i})$  of individuals who might have failed at  $t_i$ .

### Discrete Logistic Likelihood

$$L_4(\boldsymbol{\beta}) = \prod_{i=1}^k \frac{e^{\boldsymbol{\beta}' \sum_{j \in \mathcal{D}_i} \mathbf{Z}_j(t_i)}}{\sum_{\mathbf{q} \in \mathcal{Q}_i} e^{\boldsymbol{\beta}' \sum_{l=1}^{d_i} \mathbf{Z}_{q_l}(t_i)}}$$

The computation of  $L_4(\boldsymbol{\beta})$  and its derivatives is based on an adaptation of the recurrence algorithm of Gail, Lubin, and Rubinstein (1981) to the logarithmic scale. When there are no ties on the event times (that is,  $d_i \equiv 1$ ), all four likelihood functions  $L_1(\boldsymbol{\beta})$ ,  $L_2(\boldsymbol{\beta})$ ,  $L_3(\boldsymbol{\beta})$ , and  $L_4(\boldsymbol{\beta})$  reduce to the same expression. In a stratified analysis, the partial likelihood is the product of the partial likelihood functions for the individual strata.

---

## Counting Process Style of Input

In the counting process formulation, data for each subject are identified by a triple  $\{N, Y, \mathbf{Z}\}$  of counting, at-risk, and covariate processes. Here,  $N(t)$  indicates the number of events that the subject experiences over the time interval  $(0, t]$ ;  $Y(t)$  indicates whether the subject is at risk at time  $t$  (one if at risk and zero otherwise);

and  $\mathbf{Z}(t)$  is a vector of explanatory variables for the subject at time  $t$ . The sample path of  $N$  is a step function with jumps of size +1 at the event times, and  $N(0) = 0$ . Unless  $\mathbf{Z}(t)$  changes continuously with time, the data for each subject can be represented by multiple observations, each identifying a semiclosed time interval  $(t_1, t_2]$ , the values of the explanatory variables over that interval, and the event status at  $t_2$ . The subject remains at risk during the interval  $(t_1, t_2]$ , and an event might occur at  $t_2$ . Values of the explanatory variables for the subject remain unchanged in the interval. This style of data input was originated by Therneau (1994).

For example, a patient has a tumor recurrence at weeks 3, 10, and 15 and is followed up to week 23. Consider three fixed explanatory variables Trt (treatment), Number (initial tumor number), and Size (initial tumor size), and one time-dependent covariate Z that represents a hormone level. The value of Z might change during the follow-up period. The data for this patient are represented by the following four observations:

| T1 | T2 | Status | Trt | Number | Size | Z    |
|----|----|--------|-----|--------|------|------|
| 0  | 3  | 1      | 1   | 1      | 3    | 12.3 |
| 3  | 10 | 1      | 1   | 1      | 3    | 14.7 |
| 10 | 15 | 1      | 1   | 1      | 3    | 13.8 |
| 15 | 23 | 0      | 1   | 1      | 3    | 15.5 |

Here (T1,T2] contains the at-risk intervals. The variable Event indicates whether a recurrence has occurred at T2; a value of 1 indicates a tumor recurrence, and a value of 0 indicates nonrecurrence. The following statements fit a multiplicative hazards model with baseline covariates Trt, Number, and Size, and a time-varying covariate Z.

```
proc phreg;
 model (T1,T2) * Status(0) = Trt Z1 Z2 Z3;
run;
```

Another useful application of the counting process formulation is delayed entry of subjects into the risk set. For example, in studying the mortality of workers exposed to a carcinogen, the survival time is chosen to be the worker's age at death by malignant neoplasm. Any worker joining the workplace at a later age than a given event failure time is not included in the corresponding risk set. The variables of a worker consist of Entry (age at which the worker entered the workplace), Age (age at death or age censored), Status (an indicator of whether the observation time is censored, with the value 0 identifying a censored time), and X1 and X2 (explanatory variables thought to be related to survival). The specification for such an application is as follows:

```
proc phreg;
 model (Entry, Age) * Status(0) = X1 X2;
run;
```

Alternatively, you can use a time-dependent variable to control the risk set, as illustrated in the following specification:

```
proc phreg;
 model Age * Status(0) = X1 X2;
 if Age < Entry then X1= .;
run;
```

Here, X1 becomes a time-dependent variable. At a given death time  $t$ , the value of X1 is reevaluated for each subject with  $\text{Age} \geq t$ ; subjects with  $\text{Entry} > t$  are given a missing value in X1 and are subsequently removed

from the risk set. Computationally, this approach is not as efficient as the one that uses the counting process formulation.

---

## Left-Truncation of Failure Times

Left-truncation occurs when individuals are not observed at the natural time origin of the phenomenon under study but come under observation at some known later time (called the left-truncation time). The risk set just prior to an event time does not include individuals whose left-truncation times exceed the given event time. Thus, any contribution to the likelihood must be conditional on the truncation limit having been exceeded.

You use the `ENTRY=` option to specify the variable that represents the left-truncation time. Suppose `T1` and `T2` represent the left-truncation time and the survival time, respectively. To account for left-truncation, you specify the following statements:

```
proc phreg;
 model T2*Dead(0)=X1-X10/entry=T1;
 title 'The ENTRY= option is Specified';
run;
```

Equivalently, you can use the counting process style of input for left-truncation:

```
proc phreg;
 model (T1, T2)*Dead(0)=X1-X10;
 title 'Counting Process Style of Input';
run;
```

Since the product-limit estimator of the survivor function is not available for the counting process style of input, you cannot use PROC PHREG to obtain the product-limit estimate of the survivor function if you have data with left-truncation times. In the preceding PROC PHREG calls, if you also specify `METHOD=PL` in a `BASELINE` statement or an `OUTPUT` statement, it is defaulted to `METHOD=BRESLOW`.

---

## The Multiplicative Hazards Model

Consider a set of  $n$  subjects such that the counting process  $N_i \equiv \{N_i(t), t \geq 0\}$  for the  $i$ th subject represents the number of observed events experienced over time  $t$ . The sample paths of the process  $N_i$  are step functions with jumps of size  $+1$ , with  $N_i(0) = 0$ . Let  $\boldsymbol{\beta}$  denote the vector of unknown regression coefficients. The multiplicative hazards function  $\Lambda(t, \mathbf{Z}_i(t))$  for  $N_i$  is given by

$$Y_i(t)d\Lambda(t, \mathbf{Z}_i(t)) = Y_i(t) \exp(\boldsymbol{\beta}'\mathbf{Z}_i(t))d\Lambda_0(t)$$

where

- $Y_i(t)$  indicates whether the  $i$ th subject is at risk at time  $t$  (specifically,  $Y_i(t) = 1$  if at risk and  $Y_i(t) = 0$  otherwise)
- $\mathbf{Z}_i(t)$  is the vector of explanatory variables for the  $i$ th subject at time  $t$
- $\Lambda_0(t)$  is an unspecified baseline hazard function

See Fleming and Harrington (1991) and Andersen et al. (1992). The Cox model is a special case of this multiplicative hazards model, where  $Y_i(t) = 1$  until the first event or censoring, and  $Y_i(t) = 0$  thereafter.

The partial likelihood for  $n$  independent triplets  $(N_i, Y_i, \mathbf{Z}_i), i = 1, \dots, n$ , has the form

$$\mathcal{L}(\boldsymbol{\beta}) = \prod_{i=1}^n \prod_{t \geq 0} \left\{ \frac{Y_i(t) \exp(\boldsymbol{\beta}' \mathbf{Z}_i(t))}{\sum_{j=1}^n Y_j(t) \exp(\boldsymbol{\beta}' \mathbf{Z}_j(t))} \right\}^{\Delta N_i(t)}$$

where  $\Delta N_i(t) = 1$  if  $N_i(t) - N_i(t-) = 1$ , and  $\Delta N_i(t) = 0$  otherwise.

## The Frailty Model

You can use the frailty model to model correlations between failures of the same cluster. The hazard rate for the  $j$ th individual in the  $i$ th cluster is

$$\lambda_{ij}(t) = \lambda_0(t) e^{\boldsymbol{\beta}' \mathbf{Z}_{ij}(t) + \gamma_i}$$

where  $\lambda_0(t)$  is an arbitrary baseline hazard rate,  $\mathbf{Z}_{ij}$  is the vector of (fixed-effect) covariates,  $\boldsymbol{\beta}$  is the vector of regression coefficients, and  $\gamma_i$  is the random effect for cluster  $i$ .

Frailties are the exponential transformations of the random components, and the frailty model can be written as

$$\lambda_{ij}(t) = \lambda_0(t) e^{\gamma_i} e^{\boldsymbol{\beta}' \mathbf{Z}_{ij}(t)}$$

The random components  $\gamma_1, \dots, \gamma_s$  (alternatively, the frailties  $e^{\gamma_1}, \dots, e^{\gamma_s}$ ) are assumed to be independent and identically distributed. Modeling is based on the random effects rather than on the frailties.

Two frailty distributions are available in PROC PHREG: gamma and lognormal. Use the DIST= option in the RANDOM statement to choose the distribution. Let  $\theta$  be an unknown parameter. The frailty distributions are listed in Table 67.11.

**Table 67.11** Frailty Distributions

| Frailty Option | Distribution                                                         | Density $f(\boldsymbol{\gamma}_i)$                                                                                                                    | Mean and Variance                                |
|----------------|----------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------|
| DIST=GAMMA     | $e^{\gamma_i} \sim G\left(\frac{1}{\theta}, \frac{1}{\theta}\right)$ | $\frac{\exp(\frac{\gamma_i}{\theta}) \exp\left(-\frac{\exp(\gamma_i)}{\theta}\right)}{\theta^{\frac{1}{\theta}} \Gamma\left(\frac{1}{\theta}\right)}$ | $E(e^{\gamma_i})=1 \quad V(e^{\gamma_i})=\theta$ |
| DIST=LOGNORMAL | $\gamma_i \sim N(0, \theta)$                                         | $\frac{1}{\sqrt{(2\pi\theta)}} \exp\left(-\frac{\gamma_i^2}{2\theta}\right)$                                                                          | $E(\gamma_i)=0 \quad V(\gamma_i)=\theta$         |

The unknown parameter  $\theta$  is a dispersion parameter. Each frailty distribution has a central tendency of 1 (the gamma frailty has a mean of 1, and the lognormal frailty has a median of 1). Thus, you can infer that individuals in cluster  $i$  with frailty  $e^{\gamma_i} > 1$  (or  $e^{\gamma_i} < 1$ ) tend to fail at a faster (or slower) rate than they fail under an independence model.

PROC PHREG estimates the regression coefficients  $\boldsymbol{\beta}$ , the random effects  $\gamma_1, \dots, \gamma_s$ , and the dispersion parameter  $\theta$ . The RANDOM statement in PROC PHREG enables you to fit a shared frailty model by a

penalized partial likelihood approach. If you also specify the BAYES statement, PROC PHREG performs a Bayesian analysis of the shared frailty model.

If the RANDOM statement is specified, any ASSESS, BASELINE, and OUTPUT statements are ignored. Also ignored are the COVS options in the PROC PHREG statement and the following options in the MODEL statement: BEST=, DETAILS, HIERARCHY=, INCLUDE=, NOFIT, PLCONV=, SELECTION=, SEQUENTIAL, SLENTY=, SLSTAY=, TYPE1, and TYPE3(ALL, LR, SCORE). Profile likelihood confidence intervals for the hazard ratios are not available for the frailty model analysis.

---

## Hazard Ratios

Consider a dichotomous risk factor variable  $X$  that takes the value 1 if the risk factor is present and 0 if the risk factor is absent. The log-hazard function is given by

$$\log[\lambda(t|X)] = \log[\lambda_0(t)] + \beta_1 X$$

where  $\lambda_0(t)$  is the baseline hazard function.

The hazard ratio  $\psi$  is defined as the ratio of the hazard for those with the risk factor ( $X = 1$ ) to the hazard without the risk factor ( $X = 0$ ). The log of the hazard ratio is given by

$$\log(\psi) \equiv \log[\psi(X = 1, X = 0)] = \log[\lambda(t|X = 1)] - \log[\lambda(t|X = 0)] = \beta_1$$

In general, the hazard ratio can be computed by exponentiating the difference of the log-hazard between any two population profiles. This is the approach taken by the HAZARDRATIO statement, so the computations are available regardless of parameterization, interactions, and nestings. However, as shown in the preceding equation for  $\log(\psi)$ , hazard ratios of main effects can be computed as functions of the parameter estimates, and the remainder of this section is concerned with this methodology.

The parameter,  $\beta_1$ , associated with  $X$  represents the change in the log-hazard from  $X = 0$  to  $X = 1$ . So the hazard ratio is obtained by simply exponentiating the value of the parameter associated with the risk factor. The hazard ratio indicates how the hazard change as you change  $X$  from 0 to 1. For instance,  $\psi = 2$  means that the hazard when  $X = 1$  is twice the hazard when  $X = 0$ .

Suppose the values of the dichotomous risk factor are coded as constants  $a$  and  $b$  instead of 0 and 1. The hazard when  $X = a$  becomes  $\lambda(t) \exp(a\beta_1)$ , and the hazard when  $X = b$  becomes  $\lambda(t) \exp(b\beta_1)$ . The hazard ratio corresponding to an increase in  $X$  from  $a$  to  $b$  is

$$\psi = \exp[(b - a)\beta_1] = [\exp(\beta_1)]^{b-a} \equiv [\exp(\beta_1)]^c$$

Note that for any  $a$  and  $b$  such that  $c = b - a = 1$ ,  $\psi = \exp(\beta_1)$ . So the hazard ratio can be interpreted as the change in the hazard for any increase of one unit in the corresponding risk factor. However, the change in hazard for some amount other than one unit is often of greater interest. For example, a change of one pound in body weight might be too small to be considered important, while a change of 10 pounds might be more meaningful. The hazard ratio for a change in  $X$  from  $a$  to  $b$  is estimated by raising the hazard ratio estimate for a unit change in  $X$  to the power of  $c = b - a$  as shown previously.

For a polytomous risk factor, the computation of hazard ratios depends on how the risk factor is parameterized. For illustration, suppose that Cell is a risk factor with four categories: Adeno, Large, Small, and Squamous.

For the effect parameterization scheme (PARAM=EFFECT) with Squamous as the reference group, the design variables for Cell are as follows:

| Cell     | Design Variables |       |       |
|----------|------------------|-------|-------|
|          | $X_1$            | $X_2$ | $X_3$ |
| Adeno    | 1                | 0     | 0     |
| Large    | 0                | 1     | 0     |
| Small    | 0                | 0     | 1     |
| Squamous | -1               | -1    | -1    |

The log-hazard for Adeno is

$$\begin{aligned}\log[\lambda(t|\text{Adeno})] &= \log[\lambda_0(t)] + \beta_1(X_1 = 1) + \beta_2(X_2 = 0) + \beta_3(X_3 = 0) \\ &= \lambda_0(t) + \beta_1\end{aligned}$$

The log-hazard for Squamous is

$$\begin{aligned}\log[\lambda(t|\text{Squamous})] &= \log[\lambda_0(t)] + \beta_1(X_1 = -1) + \beta_2(X_2 = -1) + \beta_3(X_3 = -1) \\ &= \log[\lambda_0(t)] - \beta_1 - \beta_2 - \beta_3\end{aligned}$$

Therefore, the log-hazard ratio of Adeno versus Squamous

$$\begin{aligned}\log[\psi(\text{Adeno, Squamous})] &= \log[\lambda(t|\text{Adeno})] - \log[\lambda(t|\text{Squamous})] \\ &= 2\beta_1 + \beta_2 + \beta_3\end{aligned}$$

For the reference cell parameterization scheme (**PARAM=REF**) with Squamous as the reference cell, the design variables for Cell are as follows:

| Cell     | Design Variables |       |       |
|----------|------------------|-------|-------|
|          | $X_1$            | $X_2$ | $X_3$ |
| Adeno    | 1                | 0     | 0     |
| Large    | 0                | 1     | 0     |
| Small    | 0                | 0     | 1     |
| Squamous | 0                | 0     | 0     |

The log-hazard ratio of Adeno versus Squamous is given by

$$\begin{aligned}\log(\psi(\text{Adeno, Squamous})) &= \log[\lambda(t|\text{Adeno})] - \log[\lambda(t|\text{Squamous})] \\ &= (\log[\lambda_0(t)] + \beta_1(X_1 = 1) + \beta_2(X_2 = 0) + \beta_3(X_3 = 0)) - \\ &\quad (\log[\lambda_0(t)] + \beta_1(X_1 = 0) + \beta_2(X_2 = 0) + \beta_3(X_3 = 0)) \\ &= \beta_1\end{aligned}$$

For the GLM parameterization scheme (PARAM=GLM), the design variables are as follows:

| Cell     | Design Variables |       |       |       |
|----------|------------------|-------|-------|-------|
|          | $X_1$            | $X_2$ | $X_3$ | $X_4$ |
| Adeno    | 1                | 0     | 0     | 0     |
| Large    | 0                | 1     | 0     | 0     |
| Small    | 0                | 0     | 1     | 0     |
| Squamous | 0                | 0     | 0     | 1     |

The log-hazard ratio of Adeno versus Squamous is

$$\begin{aligned}
 & \log(\psi(\text{Adeno}, \text{Squamous})) \\
 &= \log[\lambda(t|\text{Adeno})] - \log[\lambda(t|\text{Squamous})] \\
 &= \log[\lambda_0(t) + \beta_1(X_1 = 1) + \beta_2(X_2 = 0) + \beta_3(X_3 = 0) + \beta_4(X_4 = 0)] - \\
 & \quad (\log(\lambda_0(t)) + \beta_1(X_1 = 0) + \beta_2(X_2 = 0) + \beta_3(X_3 = 0) + \beta_4(X_4 = 1)) \\
 &= \beta_1 - \beta_4
 \end{aligned}$$

Consider Cell as the only risk factor in the Cox regression in [Example 67.3](#). The computation of hazard ratio of Adeno versus Squamous for various parameterization schemes is tabulated in [Table 67.12](#).

**Table 67.12** Hazard Ratio Comparing Adeno to Squamous

| PARAM= | Parameter Estimates |                 |                 |                 | Hazard Ratio Estimates                            |
|--------|---------------------|-----------------|-----------------|-----------------|---------------------------------------------------|
|        | $\hat{\beta}_1$     | $\hat{\beta}_2$ | $\hat{\beta}_3$ | $\hat{\beta}_4$ |                                                   |
| EFFECT | 0.5772              | -0.2115         | 0.2454          |                 | $\exp(2 \times 0.5772 - 0.2115 + 0.2454) = 3.281$ |
| REF    | 1.8830              | 0.3996          | 0.8565          |                 | $\exp(1.8830) = 3.281$                            |
| GLM    | 1.8830              | 0.3996          | 0.8565          | 0.0000          | $\exp(1.8830) = 3.281$                            |

The fact that the log-hazard ratio ( $\log(\psi)$ ) is a linear function of the parameters enables the **HAZARDRATIO** statement to compute the hazard ratio of the main effect even in the presence of interactions and nest effects. The section “[Hazard Ratios](#)” on page 5619 details the estimation of the hazard ratios in a classical analysis.

To customize hazard ratios for specific units of change for a continuous risk factor, you can use the **UNITS=** option in a **HAZARDRATIO** statement to specify a list of relevant units for each explanatory variable in the model. Estimates of these customized hazard ratios are given in a separate table. Let  $(L_j, U_j)$  be a confidence interval for  $\log(\psi)$ . The corresponding lower and upper confidence limits for the customized hazard ratio  $\exp(c\beta_j)$  are  $\exp(cL_j)$  and  $\exp(cU_j)$ , respectively (for  $c > 0$ ), or  $\exp(cU_j)$  and  $\exp(cL_j)$ , respectively (for  $c < 0$ ).

## Proportional Rates/Means Models for Recurrent Events

Let  $N(t)$  be the number of events experienced by a subject over the time interval  $(0, t]$ . Let  $dN(t)$  be the increment of the counting process  $N$  over  $[t, t + dt)$ . The rate function is given by

$$d\mu_{\mathbf{Z}}(t) = E[dN(t)|Z(t)] = e^{\beta' \mathbf{Z}(t)} d\mu_0(t)$$



where  $\mu_0(\cdot)$  is an unknown continuous function. If the  $\mathbf{Z}$  are time independent, the rate model is reduced to the mean model

$$\mu_{\mathbf{Z}}(t) = e^{\boldsymbol{\beta}'\mathbf{Z}} \mu_0(t)$$

The partial likelihood for  $n$  independent triplets  $(N_i, Y_i, \mathbf{Z}_i)$ ,  $i = 1, \dots, n$ , of counting, at-risk, and covariate processes is the same as that of the multiplicative hazards model. However, a robust sandwich estimate is used for the covariance matrix of the parameter estimator instead of the model-based estimate.

Let  $T_{ki}$  be the  $k$ th event time of the  $i$ th subject. Let  $C_i$  be the censoring time of the  $i$ th subject. The at-risk indicator and the failure indicator are, respectively,

$$Y_i(t) = I(C_i \geq t) \text{ and } \Delta_{ki} = I(T_{ki} \leq C_i)$$

Denote

$$S^{(0)}(\boldsymbol{\beta}, t) = \sum_{i=1}^n Y_i(t) e^{\boldsymbol{\beta}'\mathbf{Z}_i(t)} \text{ and } \bar{\mathbf{Z}}(\boldsymbol{\beta}, t) = \frac{\sum_{i=1}^n Y_i(t) e^{\boldsymbol{\beta}'\mathbf{Z}_i(t)} \mathbf{Z}_i(t)}{S^{(0)}(\boldsymbol{\beta}, t)}$$

Let  $\hat{\boldsymbol{\beta}}$  be the maximum likelihood estimate of  $\boldsymbol{\beta}$ , and let  $\mathcal{I}(\hat{\boldsymbol{\beta}})$  be the observed information matrix. The robust sandwich covariance matrix estimate is given by

$$\mathcal{I}^{-1}(\hat{\boldsymbol{\beta}}) \sum_{i=1}^n \left[ W_i(\hat{\boldsymbol{\beta}}) W_i'(\hat{\boldsymbol{\beta}}) \right] \mathcal{I}^{-1}(\hat{\boldsymbol{\beta}})$$

where

$$W_i(\boldsymbol{\beta}) = \sum_k \Delta_{ki} \left\{ Z_i(T_{ki}) - \bar{\mathbf{Z}}(\boldsymbol{\beta}, T_{ki}) \right\} - \sum_{i=1}^n \sum_l \frac{\Delta_{lj} Y_i(T_{lj}) e^{\boldsymbol{\beta}'\mathbf{Z}_i(T_{lj})}}{S^{(0)}(\boldsymbol{\beta}, T_{lj})} \left\{ Z_i(T_{lj}) - \bar{\mathbf{Z}}(\boldsymbol{\beta}, T_{lj}) \right\}$$

For a given realization of the covariates  $\boldsymbol{\xi}$ , the Nelson estimator is used to predict the mean function

$$\hat{\mu}_{\boldsymbol{\xi}}(t) = e^{\hat{\boldsymbol{\beta}}'\boldsymbol{\xi}} \sum_{i=1}^n \sum_k \frac{I(T_{ki} \leq t) \Delta_{ki}}{S^{(0)}(\hat{\boldsymbol{\beta}}, T_{ki})}$$

with standard error estimate given by

$$\hat{\sigma}^2(\hat{\mu}_{\boldsymbol{\xi}}(t)) = \sum_{i=1}^n \left( \frac{1}{n} \hat{\Psi}_i(t, \boldsymbol{\xi}) \right)^2$$

where

$$\begin{aligned} \frac{1}{n} \hat{\Psi}_i(t, \boldsymbol{\xi}) &= e^{\hat{\boldsymbol{\beta}}'\boldsymbol{\xi}} \left\{ \sum_k \frac{I(T_{ki} \leq t) \Delta_{ik}}{S^{(0)}(\hat{\boldsymbol{\beta}}, T_{ki})} - \sum_{j=1}^n \sum_k \frac{Y_i(T_{kj}) e^{\hat{\boldsymbol{\beta}}'\mathbf{Z}_i(T_{kj})} I(T_{kj} \leq t) \Delta_{kj}}{[S^{(0)}(\hat{\boldsymbol{\beta}}, T_{kj})]^2} \right. \\ &\quad \left[ \sum_{i=1}^n \sum_k \frac{I(T_{ki} \leq t) \Delta_{ik} [\bar{\mathbf{Z}}(\hat{\boldsymbol{\beta}}, T_{ki}) - \boldsymbol{\xi}]}{S^{(0)}(\hat{\boldsymbol{\beta}}, T_{ki})} \right] \\ &\quad \left. \times \mathcal{I}^{-1}(\hat{\boldsymbol{\beta}}) \int_0^{\tau} [\mathbf{Z}_i(u) - \bar{\mathbf{Z}}(\hat{\boldsymbol{\beta}}, u)] d\hat{M}_i(u) \right\} \end{aligned}$$

Since the cumulative mean function is always nonnegative, the log transform is used to compute confidence intervals. The  $100(1 - \alpha)\%$  pointwise confidence limits for  $\mu_{\xi}(t)$  are

$$\hat{\mu}_{\xi}(t) e^{\pm z_{\alpha/2} \frac{\hat{\sigma}(\hat{\mu}_{\xi}(t))}{\hat{\mu}_{\xi}(t)}}$$

where  $z_{\alpha/2}$  is the upper  $100\alpha/2$  percentage point of the standard normal distribution.

## Newton-Raphson Method

Let  $L(\boldsymbol{\beta})$  be one of the likelihood functions described in the previous subsections. Let  $l(\boldsymbol{\beta}) = \log L(\boldsymbol{\beta})$ . Finding  $\boldsymbol{\beta}$  such that  $L(\boldsymbol{\beta})$  is maximized is equivalent to finding the solution  $\hat{\boldsymbol{\beta}}$  to the likelihood equations

$$\frac{\partial l(\boldsymbol{\beta})}{\partial \boldsymbol{\beta}} = 0$$

With  $\hat{\boldsymbol{\beta}}^0 = \mathbf{0}$  as the initial solution, the iterative scheme is expressed as

$$\hat{\boldsymbol{\beta}}^{j+1} = \hat{\boldsymbol{\beta}}^j - \left[ \frac{\partial^2 l(\hat{\boldsymbol{\beta}}^j)}{\partial \boldsymbol{\beta}^2} \right]^{-1} \frac{\partial l(\hat{\boldsymbol{\beta}}^j)}{\partial \boldsymbol{\beta}}$$

The term after the minus sign is the Newton-Raphson step. If the likelihood function evaluated at  $\hat{\boldsymbol{\beta}}^{j+1}$  is less than that evaluated at  $\hat{\boldsymbol{\beta}}^j$ , then  $\hat{\boldsymbol{\beta}}^{j+1}$  is recomputed using half the step size. The iterative scheme continues until convergence is obtained—that is, until  $\hat{\boldsymbol{\beta}}_{j+1}$  is sufficiently close to  $\hat{\boldsymbol{\beta}}^j$ . Then the maximum likelihood estimate of  $\boldsymbol{\beta}$  is  $\hat{\boldsymbol{\beta}} = \hat{\boldsymbol{\beta}}_{j+1}$ .

The model-based variance estimate of  $\hat{\boldsymbol{\beta}}$  is obtained by inverting the information matrix  $\mathcal{I}(\hat{\boldsymbol{\beta}})$

$$\hat{\mathbf{V}}_m(\hat{\boldsymbol{\beta}}) = \mathcal{I}^{-1}(\hat{\boldsymbol{\beta}}) = - \left[ \frac{\partial^2 l(\hat{\boldsymbol{\beta}})}{\partial \boldsymbol{\beta}^2} \right]^{-1}$$

## Firth's Modification for Maximum Likelihood Estimation

In fitting a Cox model, the phenomenon of monotone likelihood is observed if the likelihood converges to a finite value while at least one parameter diverges (Heinze and Schemper 2001).

Let  $\mathbf{x}_l(t)$  denote the vector explanatory variables for the  $l$ th individual at time  $t$ . Let  $t_1 < t_2 < \dots < t_m$  denote the  $k$  distinct, ordered event times. Let  $d_j$  denote the multiplicity of failures at  $t_j$ ; that is,  $d_j$  is the size of the set  $\mathcal{D}_j$  of individuals that fail at  $t_j$ . Let  $\mathcal{R}_j$  denote the risk set just before  $t_j$ . Let  $\boldsymbol{\beta} = (\beta_1, \dots, \beta_k)'$  be the vector of regression parameters. The Breslow log partial likelihood is given by

$$l(\boldsymbol{\beta}) = \log L(\boldsymbol{\beta}) = \sum_{j=1}^m \left\{ \boldsymbol{\beta}' \sum_{l \in \mathcal{D}_j} \mathbf{x}_l(t_j) - d_j \log \sum_{h \in \mathcal{R}_j} e^{\boldsymbol{\beta}' \mathbf{x}_h(t_j)} \right\}$$

Denote

$$\mathbf{S}_j^{(a)}(\boldsymbol{\beta}) = \sum_{h \in \mathcal{R}_j} e^{\boldsymbol{\beta}' \mathbf{x}_h(t_j)} [\mathbf{x}_h(t_j)]^{\otimes a} \quad a = 0, 1, 2$$

Then the score function is given by

$$\begin{aligned} \mathbf{U}(\boldsymbol{\beta}) &\equiv (U(\beta_1), \dots, U(\beta_k))' \\ &= \frac{\partial l(\boldsymbol{\beta})}{\partial \boldsymbol{\beta}} \\ &= \sum_{j=1}^m \left\{ \sum_{l \in \mathcal{D}_j} \mathbf{x}_l(t_j) - d_j \frac{\mathbf{S}_j^{(1)}(\boldsymbol{\beta})}{S_j^{(0)}(\boldsymbol{\beta})} \right\} \end{aligned}$$

and the Fisher information matrix is given by

$$\begin{aligned} \mathcal{I}(\boldsymbol{\beta}) &= -\frac{\partial^2 l(\boldsymbol{\beta})}{\partial \boldsymbol{\beta}^2} \\ &= \sum_{j=1}^m d_j \left\{ \frac{\mathbf{S}_j^{(2)}(\boldsymbol{\beta})}{S_j^{(0)}(\boldsymbol{\beta})} - \left[ \frac{\mathbf{S}_j^{(1)}(\boldsymbol{\beta})}{S_j^{(0)}(\boldsymbol{\beta})} \right] \left[ \frac{\mathbf{S}_j^{(1)}(\boldsymbol{\beta})}{S_j^{(0)}(\boldsymbol{\beta})} \right]' \right\} \end{aligned}$$

Heinze (1999); Heinze and Schemper (2001) applied the idea of Firth (1993) by maximizing the penalized partial likelihood

$$l^*(\boldsymbol{\beta}) = l(\boldsymbol{\beta}) + 0.5 \log(|\mathcal{I}(\boldsymbol{\beta})|)$$

The score function  $\mathbf{U}(\boldsymbol{\beta})$  is replaced by the modified score function by  $\mathbf{U}^*(\boldsymbol{\beta}) \equiv (U^*(\beta_1), \dots, U^*(\beta_k))'$ , where

$$U^*(\beta_r) = U(\beta_r) + 0.5 \text{tr} \left\{ \mathcal{I}^{-1}(\boldsymbol{\beta}) \frac{\partial \mathcal{I}(\boldsymbol{\beta})}{\partial \beta_r} \right\} \quad r = 1, \dots, k$$

The Firth estimate is obtained iteratively as

$$\boldsymbol{\beta}^{(s+1)} = \boldsymbol{\beta}^{(s)} + \mathcal{I}^{-1}(\boldsymbol{\beta}^{(s)}) \mathbf{U}^*(\boldsymbol{\beta}^{(s)})$$

The covariance matrix  $\hat{\mathbf{V}}$  is computed as  $\mathcal{I}^{-1}(\hat{\boldsymbol{\beta}})$ , where  $\hat{\boldsymbol{\beta}}$  is the maximum penalized partial likelihood estimate.

### Explicit formulae for $\frac{\partial \mathcal{I}(\boldsymbol{\beta})}{\partial \beta_r}$ , $r = 1, \dots, k$

Denote

$$\begin{aligned} \mathbf{x}_h(t) &= (x_{h1}(t), \dots, x_{hk}(t))' \\ \mathbf{Q}_{jr}^{(a)}(\boldsymbol{\beta}) &= \sum_{h \in \mathcal{R}_j} e^{\boldsymbol{\beta}' \mathbf{x}_h(t_j)} x_{hr}(t_j) [\mathbf{x}_h(t_j)]^{\otimes a} \quad a = 0, 1, 2; r = 1, \dots, k \end{aligned}$$

Then

$$\frac{\partial \mathcal{I}(\boldsymbol{\beta})}{\partial \beta_r} = \sum_{j=1}^m d_j \left\{ \left[ \frac{\mathbf{Q}_{jr}^{(2)}(\boldsymbol{\beta})}{S_j^{(0)}(\boldsymbol{\beta})} - \frac{\mathbf{Q}_{jr}^{(0)}(\boldsymbol{\beta}) S_j^{(2)}(\boldsymbol{\beta})}{S_j^{(0)}(\boldsymbol{\beta}) S_j^{(0)}(\boldsymbol{\beta})} \right] - \left[ \frac{\mathbf{Q}_{jr}^{(1)}(\boldsymbol{\beta})}{S_j^{(0)}(\boldsymbol{\beta})} - \frac{\mathbf{Q}_{jr}^{(0)}(\boldsymbol{\beta}) S_j^{(1)}(\boldsymbol{\beta})}{S_j^{(0)}(\boldsymbol{\beta}) S_j^{(0)}(\boldsymbol{\beta})} \right] \left[ \frac{S_j^{(1)}(\boldsymbol{\beta})}{S_j^{(0)}(\boldsymbol{\beta})} \right]' - \left[ \frac{S_j^{(1)}(\boldsymbol{\beta})}{S_j^{(0)}(\boldsymbol{\beta})} \right] \left[ \frac{\mathbf{Q}_{jr}^{(1)}(\boldsymbol{\beta})}{S_j^{(0)}(\boldsymbol{\beta})} - \frac{\mathbf{Q}_{jr}^{(0)}(\boldsymbol{\beta}) S_j^{(1)}(\boldsymbol{\beta})}{S_j^{(0)}(\boldsymbol{\beta}) S_j^{(0)}(\boldsymbol{\beta})} \right]' \right\} \quad r = 1, \dots, k$$

---

## Robust Sandwich Variance Estimate

For the  $i$ th subject,  $i = 1, \dots, n$ , let  $X_i$ ,  $w_i$ , and  $\mathbf{Z}_i(t)$  be the observed time, weight, and the covariate vector at time  $t$ , respectively. Let  $\Delta_i$  be the event indicator and let  $Y_i(t) = I(X_i \geq t)$ . Let

$$S^{(r)}(\boldsymbol{\beta}, t) = \sum_{j=1}^n w_j Y_j(t) e^{\boldsymbol{\beta}' \mathbf{Z}_j(t)} \mathbf{Z}_j^{\otimes r}(t), \quad r = 0, 1$$

Let  $\bar{\mathbf{Z}}(\boldsymbol{\beta}, t) = \frac{S^{(1)}(\boldsymbol{\beta}, t)}{S^{(0)}(\boldsymbol{\beta}, t)}$ . The score residual for the  $i$ th subject is

$$\mathbf{L}_i(\boldsymbol{\beta}) = \Delta_i \left\{ \mathbf{Z}_i(X_i) - \bar{\mathbf{Z}}(\boldsymbol{\beta}, X_i) \right\} - \sum_{j=1}^n \Delta_j \frac{w_j Y_j(X_j) e^{\boldsymbol{\beta}' \mathbf{Z}_j(X_j)}}{S^{(0)}(\boldsymbol{\beta}, X_j)} \left\{ \mathbf{Z}_j(X_j) - \bar{\mathbf{Z}}(\boldsymbol{\beta}, X_j) \right\}$$

For TIES=EFRON, the computation of the score residuals is modified to comply with the Efron partial likelihood. See the section “Residuals” on page 5639 for more information.

The robust sandwich variance estimate of  $\hat{\boldsymbol{\beta}}$  derived by Binder (1992), who incorporated weights into the analysis, is

$$\hat{\mathbf{V}}_s(\hat{\boldsymbol{\beta}}) = \mathcal{I}^{-1}(\hat{\boldsymbol{\beta}}) \left[ \sum_{j=1}^n (w_j \mathbf{L}_j(\hat{\boldsymbol{\beta}}))^{\otimes 2} \right] \mathcal{I}^{-1}(\hat{\boldsymbol{\beta}})$$

where  $\mathcal{I}(\hat{\boldsymbol{\beta}})$  is the observed information matrix, and  $\mathbf{a}^{\otimes 2} = \mathbf{a}\mathbf{a}'$ . Note that when  $w_i \equiv 1$ ,

$$\hat{\mathbf{V}}_s(\hat{\boldsymbol{\beta}}) = \mathbf{D}'\mathbf{D}$$

where  $\mathbf{D}$  is the matrix of DFBETA residuals. This robust variance estimate was proposed by Lin and Wei (1989) and Reid and Crèpeau (1985).

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## Testing the Global Null Hypothesis

The following statistics can be used to test the global null hypothesis  $H_0: \boldsymbol{\beta} = \mathbf{0}$ . Under mild assumptions, each statistic has an asymptotic chi-square distribution with  $p$  degrees of freedom given the null hypothesis. The value  $p$  is the dimension of  $\boldsymbol{\beta}$ . For clustered data, the likelihood ratio test, the score test, and the Wald test assume independence of observations within a cluster, while the robust Wald test and the robust score test do not need such an assumption.

**Likelihood Ratio Test**

$$\chi_{LR}^2 = 2 \left[ l(\hat{\boldsymbol{\beta}}) - l(\mathbf{0}) \right]$$

**Score Test**

$$\chi_S^2 = \left[ \frac{\partial l(\mathbf{0})}{\partial \boldsymbol{\beta}} \right]' \left[ -\frac{\partial^2 l(\mathbf{0})}{\partial \boldsymbol{\beta}^2} \right]^{-1} \left[ \frac{\partial l(\mathbf{0})}{\partial \boldsymbol{\beta}} \right]$$

**Wald's Test**

$$\chi_W^2 = \hat{\boldsymbol{\beta}}' \left[ -\frac{\partial^2 l(\hat{\boldsymbol{\beta}})}{\partial \boldsymbol{\beta}^2} \right] \hat{\boldsymbol{\beta}}$$

**Robust Score Test**

$$\chi_{RS}^2 = \left[ \sum_i \mathbf{L}_i^0 \right]' \left[ \sum_i \mathbf{L}_i^0 \mathbf{L}_i^{0'} \right]^{-1} \left[ \sum_i \mathbf{L}_i^0 \right]$$

where  $\mathbf{L}_i^0$  is the score residual of the  $i$ th subject at  $\boldsymbol{\beta} = \mathbf{0}$ ; that is,  $\mathbf{L}_i^0 = \mathbf{L}_i(\mathbf{0}, \infty)$ , where the score process  $\mathbf{L}_i(\boldsymbol{\beta}, t)$  is defined in the section “Residuals” on page 5639.

**Robust Wald's Test**

$$\chi_{RW}^2 = \hat{\boldsymbol{\beta}}' [\hat{\mathbf{V}}_s(\hat{\boldsymbol{\beta}})]^{-1} \hat{\boldsymbol{\beta}}$$

where  $\hat{\mathbf{V}}_s(\hat{\boldsymbol{\beta}})$  is the sandwich variance estimate (see the section “Robust Sandwich Variance Estimate” on page 5625 for details).

**Type 3 Tests**

The following statistics can be used to test the null hypothesis  $H_{0L}: \mathbf{L}\boldsymbol{\beta} = \mathbf{0}$ , where  $\mathbf{L}$  is a matrix of known coefficients. Under mild assumptions, each of the following statistics has an asymptotic chi-square distribution with  $p$  degrees of freedom, where  $p$  is the rank of  $\mathbf{L}$ . Let  $\tilde{\boldsymbol{\beta}}_L$  be the maximum likelihood of  $\boldsymbol{\beta}$  under the null hypothesis  $H_{0L}$ ; that is,

$$l(\tilde{\boldsymbol{\beta}}_L) = \max_{\mathbf{L}\boldsymbol{\beta}=\mathbf{0}} l(\boldsymbol{\beta})$$

**Likelihood Ratio Statistic**

$$\chi_{LR}^2 = 2 \left[ l(\hat{\boldsymbol{\beta}}) - l(\tilde{\boldsymbol{\beta}}_L) \right]$$

### Score Statistic

$$\chi_S^2 = \left[ \frac{\partial l(\tilde{\boldsymbol{\beta}}_L)}{\partial \boldsymbol{\beta}} \right]' \left[ -\frac{\partial^2 l(\tilde{\boldsymbol{\beta}}_L)}{\partial \boldsymbol{\beta}^2} \right]^{-1} \left[ \frac{\partial l(\tilde{\boldsymbol{\beta}}_L)}{\partial \boldsymbol{\beta}} \right]$$

### Wald's Statistic

$$\chi_W^2 = (\mathbf{L}\hat{\boldsymbol{\beta}})' [\mathbf{L}\hat{\mathbf{V}}(\hat{\boldsymbol{\beta}})\mathbf{L}']^{-1} (\mathbf{L}\hat{\boldsymbol{\beta}})$$

where  $\hat{\mathbf{V}}(\hat{\boldsymbol{\beta}})$  is the estimated covariance matrix, which can be the model-based covariance matrix  $\left[ -\frac{\partial^2 l(\hat{\boldsymbol{\beta}})}{\partial \boldsymbol{\beta}^2} \right]^{-1}$  or the sandwich covariance matrix  $V_S(\hat{\boldsymbol{\beta}})$  (see the section “Robust Sandwich Variance Estimate” on page 5625 for details).

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## Confidence Limits for a Hazard Ratio

Let  $\mathbf{e}_j$  be the  $j$ th unit vector—that is, the  $j$ th entry of the vector is 1 and all other entries are 0. The hazard ratio for the explanatory variable with regression coefficient  $\beta_j = \mathbf{e}_j' \boldsymbol{\beta}$  is defined as  $\exp(\beta_j)$ . In general, a log-hazard ratio can be written as  $\mathbf{h}' \boldsymbol{\beta}$ , a linear combination of the regression coefficients, and the hazard ratio  $\exp(\mathbf{h}' \boldsymbol{\beta})$  is obtained by replacing  $\mathbf{e}_j$  with  $\mathbf{h}$ .

### Point Estimate

The hazard ratio  $\exp(\mathbf{e}_j' \boldsymbol{\beta})$  is estimated by  $\exp(\mathbf{e}_j' \hat{\boldsymbol{\beta}})$ , where  $\hat{\boldsymbol{\beta}}$  is the maximum likelihood estimate of the  $\boldsymbol{\beta}$ .

### Wald's Confidence Limits

The  $100(1 - \alpha)\%$  confidence limits for the hazard ratio are calculated as

$$\exp \left( \mathbf{e}_j' \hat{\boldsymbol{\beta}} \pm z_{\alpha/2} \sqrt{\mathbf{e}_j' \hat{\mathbf{V}}(\hat{\boldsymbol{\beta}}) \mathbf{e}_j} \right)$$

where  $\hat{\mathbf{V}}(\hat{\boldsymbol{\beta}})$  is estimated covariance matrix, and  $z_{\alpha/2}$  is the  $100(1 - \alpha/2)$  percentile point of the standard normal distribution.

### Profile-Likelihood Confidence Limits

The construction of the profile-likelihood-based confidence interval is derived from the asymptotic  $\chi^2$  distribution of the generalized likelihood ratio test of Venzon and Moolgavkar (1988). Suppose that the parameter vector is  $\boldsymbol{\beta} = (\beta_1, \dots, \beta_k)'$  and you want to compute a confidence interval for  $\beta_j$ . The profile-likelihood function for  $\beta_j = \gamma$  is defined as

$$l_j^*(\gamma) = \max_{\boldsymbol{\beta} \in \mathcal{B}_j(\gamma)} l(\boldsymbol{\beta})$$

where  $\mathcal{B}_j(\gamma)$  is the set of all  $\boldsymbol{\beta}$  with the  $j$ th element fixed at  $\gamma$ , and  $l(\boldsymbol{\beta})$  is the log-likelihood function for  $\boldsymbol{\beta}$ . If  $l_{\max} = l(\hat{\boldsymbol{\beta}})$  is the log likelihood evaluated at the maximum likelihood estimate  $\hat{\boldsymbol{\beta}}$ , then  $2(l_{\max} - l_j^*(\beta_j))$

has a limiting chi-square distribution with one degree of freedom if  $\beta_j$  is the true parameter value. Let  $l_0 = l_{\max} - 0.5\chi_1^2(1 - \alpha)$ , where  $\chi_1^2(1 - \alpha)$  is the  $100(1 - \alpha)$  percentile of the chi-square distribution with one degree of freedom. A  $100(1 - \alpha)\%$  confidence interval for  $\beta_j$  is

$$\{\gamma : l_j^*(\gamma) \geq l_0\}$$

The endpoints of the confidence interval are found by solving numerically for values of  $\beta_j$  that satisfy equality in the preceding relation. To obtain an iterative algorithm for computing the confidence limits, the log-likelihood function in a neighborhood of  $\beta$  is approximated by the quadratic function

$$\tilde{l}(\beta + \delta) = l(\beta) + \delta' \mathbf{g} + \frac{1}{2} \delta' \mathbf{V} \delta$$

where  $\mathbf{g} = \mathbf{g}(\beta)$  is the gradient vector and  $\mathbf{V} = \mathbf{V}(\beta)$  is the Hessian matrix. The increment  $\delta$  for the next iteration is obtained by solving the likelihood equations

$$\frac{d}{d\delta} \{\tilde{l}(\beta + \delta) + \lambda(\mathbf{e}'_j \delta - \gamma)\} = \mathbf{0}$$

where  $\lambda$  is the Lagrange multiplier,  $\mathbf{e}_j$  is the  $j$ th unit vector, and  $\gamma$  is an unknown constant. The solution is

$$\delta = -\mathbf{V}^{-1}(\mathbf{g} + \lambda \mathbf{e}_j)$$

By substituting this  $\delta$  into the equation  $\tilde{l}(\beta + \delta) = l_0$ , you can estimate  $\lambda$  as

$$\lambda = \pm \left( \frac{2(l_0 - l(\beta) + \frac{1}{2} \mathbf{g}' \mathbf{V}^{-1} \mathbf{g})}{\mathbf{e}'_j \mathbf{V}^{-1} \mathbf{e}_j} \right)^{\frac{1}{2}}$$

The upper confidence limit for  $\beta_j$  is computed by starting at the maximum likelihood estimate of  $\beta$  and iterating with positive values of  $\lambda$  until convergence is attained. The process is repeated for the lower confidence limit, using negative values of  $\lambda$ .

Convergence is controlled by value  $\epsilon$  specified with the PLCONV= option in the MODEL statement (the default value of  $\epsilon$  is  $1\text{E-}4$ ). Convergence is declared on the current iteration if the following two conditions are satisfied:

$$|l(\beta) - l_0| \leq \epsilon$$

and

$$(\mathbf{g} + \lambda \mathbf{e}_j)' \mathbf{V}^{-1} (\mathbf{g} + \lambda \mathbf{e}_j) \leq \epsilon$$

The profile-likelihood confidence limits for the hazard ratio  $\exp(\mathbf{e}'_j \beta)$  are obtained by exponentiating these confidence limits.

## Using the TEST Statement to Test Linear Hypotheses

Linear hypotheses for  $\beta$  are expressed in matrix form as

$$H_0: \mathbf{L}\beta = \mathbf{c}$$

where  $\mathbf{L}$  is a matrix of coefficients for the linear hypotheses, and  $\mathbf{c}$  is a vector of constants. The Wald chi-square statistic for testing  $H_0$  is computed as

$$\chi_W^2 = (\mathbf{L}\hat{\beta} - \mathbf{c})' [\mathbf{L}\hat{\mathbf{V}}(\hat{\beta})\mathbf{L}']^{-1} (\mathbf{L}\hat{\beta} - \mathbf{c})$$

where  $\hat{\mathbf{V}}(\hat{\beta})$  is the estimated covariance matrix. Under  $H_0$ ,  $\chi_W^2$  has an asymptotic chi-square distribution with  $r$  degrees of freedom, where  $r$  is the rank of  $\mathbf{L}$ .

### Optimal Weights for the AVERAGE option in the TEST Statement

Let  $\beta_0 = (\beta_{i_1}, \dots, \beta_{i_s})'$ , where  $\{\beta_{i_1}, \dots, \beta_{i_s}\}$  is a subset of  $s$  regression coefficients. For any vector  $\mathbf{e} = (e_1, \dots, e_s)'$  of length  $s$ ,

$$\mathbf{e}'\hat{\beta}_0 \sim N(\mathbf{e}'\beta_0, \mathbf{e}'\hat{\mathbf{V}}(\hat{\beta}_0)\mathbf{e})$$

To find  $\mathbf{e}$  such that  $\mathbf{e}'\hat{\beta}_0$  has the minimum variance, it is necessary to minimize  $\mathbf{e}'\hat{\mathbf{V}}(\hat{\beta}_0)\mathbf{e}$  subject to  $\sum_{i=1}^s e_i = 1$ . Let  $\mathbf{1}_s$  be a vector of 1's of length  $s$ . The expression to be minimized is

$$\mathbf{e}'\hat{\mathbf{V}}(\hat{\beta}_0)\mathbf{e} - \lambda(\mathbf{e}'\mathbf{1}_s - 1)$$

where  $\lambda$  is the Lagrange multiplier. Differentiating with respect to  $\mathbf{e}$  and  $\lambda$ , respectively, yields

$$\begin{aligned} \hat{\mathbf{V}}(\hat{\beta}_0)\mathbf{e} - \lambda\mathbf{1}_s &= \mathbf{0} \\ \mathbf{e}'\mathbf{1}_s - 1 &= 0 \end{aligned}$$

Solving these equations gives

$$\mathbf{e} = [\mathbf{1}'_s \hat{\mathbf{V}}^{-1}(\hat{\beta}_0) \mathbf{1}_s]^{-1} \hat{\mathbf{V}}^{-1}(\hat{\beta}_0) \mathbf{1}_s$$

This provides a one degree-of-freedom test for testing the null hypothesis  $H_0 : \beta_{i_1} = \dots = \beta_{i_s} = 0$  with normal test statistic

$$Z = \frac{\mathbf{e}'\hat{\beta}_0}{\sqrt{\mathbf{e}'\hat{\mathbf{V}}(\hat{\beta}_0)\mathbf{e}}}$$

This test is more sensitive than the multivariate test specified by the TEST statement

**Multivariate: test X1, ..., Xs;**

where X1, ..., Xs are the variables with regression coefficients  $\beta_{i_1}, \dots, \beta_{i_s}$ , respectively.

## Analysis of Multivariate Failure Time Data

Multivariate failure time data arise when each study subject can potentially experience several events (for instance, multiple infections after surgery) or when there exists some natural or artificial clustering of subjects (for instance, a litter of mice) that induces dependence among the failure times of the same cluster. Data in the former situation are referred to as multiple events data, and data in the latter situation are referred to as clustered data. The multiple events data can be further classified into ordered and unordered data. For ordered data, there is a natural ordering of the multiple failures within a subject, which includes recurrent events data as a special case. For unordered data, the multiple event times result from several concurrent failure processes.

Multiple events data can be analyzed by the Wei, Lin, and Weissfeld (1989), or WLW, method based on the marginal Cox models. For the special case of recurrent events data, you can fit the intensity model (Andersen and Gill 1982), the proportional rates/means model (Pepe and Cai 1993; Lawless and Nadeau 1995; Lin et al. 2000), or the stratified models for total time and gap time proposed by Prentice, Williams,



and Peterson (1981), or PWP. For clustered data, you can carry out the analysis of Lee, Wei, and Amato (1992) based on the marginal Cox model. To use PROC PHREG to perform these analyses correctly and effectively, you have to array your data in a specific way to produce the correct risk sets.

All examples described in this section can be found in the program *phrmult.sas* in the SAS/STAT sample library. Furthermore, the “Examples” section in this chapter contains two examples to illustrate the methods of analyzing recurrent events data and clustered data.

### Marginal Cox Models for Multiple Events Data

Suppose there are  $n$  subjects and each subject can experience up to  $K$  potential events. Let  $\mathbf{Z}_{ki}(\cdot)$  be the covariate process associated with the  $k$ th event for the  $i$ th subject. The marginal Cox models are given by

$$\lambda_k(t; \mathbf{Z}_{ki}) = \lambda_{k0} e^{\boldsymbol{\beta}'_k \mathbf{Z}_{ki}(t)}, k = 1, \dots, K; i = 1, \dots, n$$

where  $\lambda_{k0}(t)$  is the (event-specific) baseline hazard function for the  $k$ th event and  $\boldsymbol{\beta}_k$  is the (event-specific) column vector of regression coefficients for the  $k$ th event. WLW estimates  $\boldsymbol{\beta}_1, \dots, \boldsymbol{\beta}_K$  by the maximum partial likelihood estimates  $\hat{\boldsymbol{\beta}}_1, \dots, \hat{\boldsymbol{\beta}}_K$ , respectively, and uses a robust sandwich covariance matrix estimate for  $(\hat{\boldsymbol{\beta}}'_1, \dots, \hat{\boldsymbol{\beta}}'_K)'$  to account for the dependence of the multiple failure times.

By using a properly prepared input data set, you can estimate the regression parameters for all the marginal Cox models and compute the robust sandwich covariance estimates in one PROC PHREG invocation. For convenience of discussion, suppose each subject can potentially experience  $K = 3$  events and there are two explanatory variables Z1 and Z2. The event-specific parameters to be estimated are  $\boldsymbol{\beta}_1 = (\beta_{11}, \beta_{21})'$  for the first marginal model,  $\boldsymbol{\beta}_2 = (\beta_{12}, \beta_{22})'$  for the second marginal model, and  $\boldsymbol{\beta}_3 = (\beta_{13}, \beta_{23})'$  for the third marginal model. Inference of these parameters is based on the robust sandwich covariance matrix estimate of the parameter estimators. It is necessary that each row of the input data set represent the data for a potential event of a subject. The input data set should contain the following:

- an ID variable for identifying the subject so that all observations of the same subject have the same ID value
- an Enum variable to index the multiple events. For example, Enum=1 for the first event, Enum=2 for the second event, and so on.
- a Time variable to represent the observed time from some time origin for the event. For recurrence events data, it is the time from the study entry to each recurrence.
- a Status variable to indicate whether the Time value is a censored or uncensored time. For example, Status=1 indicates an uncensored time and Status=0 indicates a censored time.
- independent variables (Z1 and Z2)

The WLW analysis can be carried out by specifying the following:

```
proc phreg covs(aggregate);
 model Time*Status(0)=Z11 Z12 Z13 Z21 Z22 Z23;
 strata Enum;
 id ID;
 Z11= Z1 * (Enum=1);
 Z12= Z1 * (Enum=2);
```

```

Z13= Z1 * (Enum=3);
Z21= Z2 * (Enum=1);
Z22= Z2 * (Enum=2);
Z23= Z2 * (Enum=3);
run;

```

The variable Enum is specified in the STRATA statement so that there is one marginal Cox model for each distinct value of Enum. The variables Z11, Z12, Z13, Z21, Z22, and Z23 in the MODEL statement are event-specific variables derived from the independent variables Z1 and Z2 by the given programming statements. In particular, the variables Z11, Z12, and Z13 are event-specific variables for the explanatory variable Z1; the variables Z21, Z22, and Z23 are event-specific variables for the explanatory variable Z2. For  $j = 1, 2$ , and  $k = 1, 2, 3$ , variable Zjk contains the same values as the explanatory variable Zj for the rows that correspond to  $k$ th marginal model and the value 0 for all other rows; as such,  $\beta_{jk}$  is the regression coefficient for Zjk. You can avoid using the programming statements in PROC PHREG if you create these event-specific variables in the input data set by using the same programming statements in a DATA step.

The option COVS(AGGREGATE) is specified in the PROC PHREG statement to obtain the robust sandwich estimate of the covariance matrix, and the score residuals used in computing the middle part of the sandwich estimate are aggregated over identical ID values. You can also include TEST statements in the PROC PHREG code to test various linear hypotheses of the regression parameters based on the robust sandwich covariance matrix estimate.

Consider the AIDS study data in Wei, Lin, and Weissfeld (1989) from a randomized clinical trial to assess the antiretroviral capacity of ribavirin over time in AIDS patients. Blood samples were collected at weeks 4, 8, and 12 from each patient in three treatment groups (placebo, low dose of ribavirin, and high dose). For each serum sample, the failure time is the number of days before virus positivity was detected. If the sample was contaminated or it took a longer period of time than was achievable in the laboratory, the sample was censored. For example:

- Patient #1 in the placebo group has uncensored times 9, 6, and 7 days (that is, it took 9 days to detect viral positivity in the first blood sample, 6 days for the second blood sample, and 7 days for the third blood sample).
- Patient #14 in the low-dose group of ribavirin has uncensored times of 16 and 17 days for the first and second sample, respectively, and a censored time of 21 days for the third blood sample.
- Patient #28 in the high-dose group has an uncensored time of 21 days for the first sample, no measurement for the second blood sample, and a censored time of 25 days for the third sample.

For a full-rank parameterization, two design variables are sufficient to represent three treatment groups. Based on the reference coding with placebo as the reference, the values of the two dummy explanatory variables Z1 and Z2 representing the treatments are as follows:

| Treatment Group     | Z1 | Z2 |
|---------------------|----|----|
| Placebo             | 0  | 0  |
| Low dose ribavirin  | 1  | 0  |
| High dose ribavirin | 0  | 1  |

The bulk of the task in using PROC PHREG to perform the WLW analysis lies in the preparation of the input data set. As discussed earlier, the input data set should contain the ID, Enum, Time, and Status variables,

and event-specific independent variables Z11, Z12, Z13, Z21, Z22, and Z23. Data for the three patients described earlier are arrayed as follows:

| ID | Time | Status | Enum | Z1 | Z2 |
|----|------|--------|------|----|----|
| 1  | 9    | 1      | 1    | 0  | 0  |
| 1  | 6    | 1      | 2    | 0  | 0  |
| 1  | 7    | 1      | 3    | 0  | 0  |
| 14 | 16   | 1      | 1    | 1  | 0  |
| 14 | 17   | 1      | 2    | 1  | 0  |
| 14 | 21   | 0      | 3    | 1  | 0  |
| 28 | 21   | 1      | 1    | 0  | 1  |
| 28 | 25   | 0      | 3    | 0  | 1  |

The first three rows are data for Patient #1 with event times at 9, 6, and 7 days, one row for each event. The next three rows are data for Patient #14, who has an uncensored time of 16 days for the first serum sample, an uncensored time of 17 days for the second sample, and a censored time of 21 days for the third sample. The last two rows are data for Patient #28 of the high-dose group (Z1=0 and Z2=1). Since the patient did not have a second serum sample, there are only two rows of data.

To perform the WLW analysis, you specify the following statements:

```
proc phreg covs(aggregate);
 model Time*Status(0)=Z11 Z12 Z13 Z21 Z22 Z23;
 strata Enum;
 id ID;
 Z11= Z1 * (Enum=1);
 Z12= Z1 * (Enum=2);
 Z13= Z1 * (Enum=3);
 Z21= Z2 * (Enum=1);
 Z22= Z2 * (Enum=2);
 Z23= Z2 * (Enum=3);
 EqualLowDose: test Z11=Z12, Z12=Z23;
 AverageLow: test Z11,Z12,Z13 / e average;
run;
```

Two linear hypotheses are tested using the TEST statements. The specification

```
EqualLowDose: test Z11=Z12, Z12=Z13;
```

tests the null hypothesis  $\beta_{11} = \beta_{12} = \beta_{13}$  of identical low-dose effects across three marginal models. The specification

```
AverageLow: test Z11,Z12,Z13 / e average;
```

tests the null hypothesis of no low-dose effects (that is,  $\beta_{11} = \beta_{12} = \beta_{13} = 0$ ). The AVERAGE option computes the optimal weights for estimating the average low-dose effect  $\beta_1^* = \beta_{11} = \beta_{12} = \beta_{13}$  and performs a 1 DF test for testing the null hypothesis that  $\beta_1^* = 0$ . The E option displays the coefficients for the linear hypotheses, including the optimal weights.

## Marginal Cox Models for Clustered Data

Suppose there are  $n$  clusters with  $K_i$  members in the  $i$ th cluster,  $i = 1, \dots, n$ . Let  $\mathbf{Z}_{ki}(\cdot)$  be the covariate process associated with the  $k$ th member of the  $i$ th cluster. The marginal Cox model is given by

$$\lambda(t; \mathbf{Z}_{ki}) = \lambda_0(t) e^{\boldsymbol{\beta}' \mathbf{Z}_{ki}(t)} \quad k = 1, \dots, K_i; i = 1, \dots, n$$

where  $\lambda_0(t)$  is an arbitrary baseline hazard function and  $\boldsymbol{\beta}$  is the vector of regression coefficients. Lee, Wei, and Amato (1992) estimate  $\boldsymbol{\beta}$  by the maximum partial likelihood estimate  $\hat{\boldsymbol{\beta}}$  under the independent working assumption, and use a robust sandwich covariance estimate to account for the intracluster dependence.

To use PROC PHREG to analyze the clustered data, each member of a cluster is represented by an observation in the input data set. The input data set to PROC PHREG should contain the following:

- an ID variable to identify the cluster so that members of the same cluster have the same ID value
- a Time variable to represent the observed survival time of a member of a cluster
- a Status variable to indicate whether the Time value is an uncensored or censored time. For example, Status=1 indicates an uncensored time and Status=0 indicates a censored time.
- the explanatory variables thought to be related to the failure time

Consider a tumor study in which one of three female rats of the same litter was randomly subjected to a drug treatment. The failure time is the time from randomization to the detection of tumor. If a rat died before the tumor was detected, the failure time was censored. For example:

- In litter #1, the drug-treated rat has an uncensored time of 101 days, one untreated rat has a censored time of 49 days, and the other untreated rat has a failure time of 104 days.
- In litter #3, the drug-treated rat has a censored time of 104 days, one untreated rat has a censored time of 102 days, and the other untreated rat has a censored time of 104 days.

In this example, a litter is a cluster and the rats of the same litter are members of the cluster. Let Trt be a 0-1 variable representing the treatment a rat received, with value 1 for drug treatment and 0 otherwise. Data for the two litters of rats described earlier contribute six observations to the input data set:

| Litter | Time | Status | Trt |
|--------|------|--------|-----|
| 1      | 101  | 1      | 1   |
| 1      | 49   | 0      | 0   |
| 1      | 104  | 1      | 0   |
| 3      | 104  | 0      | 1   |
| 3      | 102  | 0      | 0   |
| 3      | 104  | 0      | 0   |

The analysis of Lee, Wei, and Amato (1992) can be performed by PROC PHREG as follows:

```
proc phreg covs(aggregate);
 model Time*Status(0)=Treatment;
 id Litter;
run;
```

## Intensity and Rate/Mean Models for Recurrent Events Data

Suppose each subject experiences recurrences of the same phenomenon. Let  $N(t)$  be the number of events a subject experiences over the interval  $[0, t]$  and let  $\mathbf{Z}(\cdot)$  be the covariate process of the subject.

The intensity model (Andersen and Gill 1982) is given by

$$\lambda_{\mathbf{Z}}(t)dt = E\{dN(t)|\mathcal{F}_{t-}\} = \lambda_0(t)e^{\boldsymbol{\beta}'\mathbf{Z}(t)}dt$$

where  $\mathcal{F}_t$  represents all the information of the processes  $N$  and  $\mathbf{Z}$  up to time  $t$ ,  $\lambda_0(t)$  is an arbitrary baseline intensity function, and  $\boldsymbol{\beta}$  is the vector of regression coefficients. This model consists of two components: (1) all the influence of the prior events on future recurrences, if there is any, is mediated through the time-dependent covariates, and (2) the covariates have multiplicative effects on the instantaneous rate of the counting process. If the covariates are time invariant, the risk of recurrences is unaffected by the past events.

The proportional rates and means models (Pepe and Cai 1993; Lawless and Nadeau 1995; Lin et al. 2000) assume that the covariates have multiplicative effects on the mean and rate functions of the counting process. The rate function is given by

$$d\mu_{\mathbf{Z}}(t) = E\{dN(t)|\mathbf{Z}(t)\} = e^{\boldsymbol{\beta}'\mathbf{Z}(t)}d\mu_0(t)$$

where  $\mu_0(t)$  is an unknown continuous function and  $\boldsymbol{\beta}$  is the vector of regression parameters. If  $\mathbf{Z}$  is time invariant, the mean function is given by

$$\mu_{\mathbf{Z}}(t) = E\{N(t)|\mathbf{Z}\} = e^{\boldsymbol{\beta}'\mathbf{Z}}\mu_0(t)$$

For both the intensity and the proportional rates/means models, estimates of the regression coefficients are obtained by solving the partial likelihood score function. However, the covariance matrix estimate for the intensity model is computed as the inverse of the observed information matrix, while that for the proportional rates/means model is given by a sandwich estimate. For a given pattern of fixed covariates, the Nelson estimate for the cumulative intensity function is the same for the cumulative mean function, but their standard errors are not the same.

To fit the intensity or rate/mean model by using PROC PHREG, the counting process style of input is needed. A subject with  $K$  events contributes  $K + 1$  observations to the input data set. The  $k$ th observation of the subject identifies the time interval from the  $(k - 1)$  event or time 0 (if  $k = 1$ ) to the  $k$ th event,  $k = 1, \dots, K$ . The  $(K + 1)$  observation represents the time interval from the  $K$ th event to time of censorship. The input data set should contain the following variables:

- a TStart variable to represent the  $(k - 1)$  recurrence time or the value 0 if  $k = 1$
- a TStop variable to represent the  $k$ th recurrence time or the follow-up time if  $k = K + 1$

- a `Status` variable indicating whether the `TStop` time is a recurrence time or a censored time; for example, `Status=1` for a recurrence time and `Status=0` for censored time
- explanatory variables thought to be related to the recurrence times

If the rate/mean model is used, the input data should also contain an `ID` variable for identifying the subjects.

Consider the chronic granulomatous disease (CGD) data listed in Fleming and Harrington (1991). The disease is a rare disorder characterized by recurrent pyrogenic infections. The study is a placebo-controlled randomized clinical trial conducted by the International CGD Cooperative Study to assess the effect of gamma interferon to reduce the rate of infection. For each study patient the times of recurrent infections along with a number of prognostic factors were collected. For example:

- Patient #17404, age 38, in the gamma interferon group had a follow-up time of 293 without any infection.
- Patient #204001, age 12, in the placebo group had an infection at 219 days, a recurrent infection at 373 days, and was followed up to 414 days.

Let `Trt` be the variable representing the treatment status with value 1 for gamma interferon and value 2 for placebo. Let `Age` be a covariate representing the age of the CGD patient. Data for the two CGD patients described earlier are given in the following table.

| <code>ID</code> | <code>TStart</code> | <code>TStop</code> | <code>Status</code> | <code>Trt</code> | <code>Age</code> |
|-----------------|---------------------|--------------------|---------------------|------------------|------------------|
| 174054          | 0                   | 293                | 0                   | 1                | 38               |
| 204001          | 0                   | 219                | 1                   | 2                | 12               |
| 204001          | 219                 | 373                | 1                   | 2                | 12               |
| 204001          | 373                 | 414                | 0                   | 2                | 12               |

Since Patient #174054 had no infection through the end of the follow-up period (293 days), there is only one observation representing the period from time 0 to the end of the follow-up. Data for Patient #204001 are broken into three observations, since there are two infections. The first observation represents the period from time 0 to the first infection, the second observation represents the period from the first infection to the second infection, and the third time period represents the period from the second infection to the end of the follow-up.

The following specification fits the intensity model:

```
proc phreg;
 model (TStart, TStop)*Status(0)=Trt Age;
run;
```

You can predict the cumulative intensity function for a given pattern of fixed covariates by specifying the `CUMHAZ=` option in the `BASELINE` statement. Suppose you are interested in two fixed patterns, one for patients of age 30 in the gamma interferon group and the other for patients of age 1 in the placebo group. You first create the SAS data set as follows:

```

data Pattern;
 Trt=1; Age=30;
 output;
 Trt=2; Age=1;
 output;
run;

```

You then include the following BASELINE statement in the PROC PHREG specification. The CUMHAZ=\_all\_ option produces the cumulative hazard function estimates, the standard error estimates, and the lower and upper pointwise confidence limits.

```
baseline covariates=Pattern out=out1 cumhaz=_all_;
```

The following specification of PROC PHREG fits the mean model and predicts the cumulative mean function for the two patterns of covariates in the Pattern data set:

```

proc phreg covs(aggregate);
 model (Tstart,Tstop)*Status(0)=Trt Age;
 baseline covariates=Pattern out=out2 cmf=_all_;
 id ID;
run;

```

The COV(AGGREGATE) option, along with the ID statement, computes the robust sandwich covariance matrix estimate. The CMF=\_ALL\_ option adds the cumulative mean function estimates, the standard error estimates, and the lower and upper pointwise confidence limits to the OUT=Out2 data set.

## PWP Models for Recurrent Events Data

Let  $N(t)$  be the number of events a subject experiences by time  $t$ . Let  $\mathbf{Z}(t)$  be the covariate vectors of the subject at time  $t$ . For a subject who has  $K$  events before censorship takes place, let  $t_0 = 0$ , let  $t_k$  be the  $k$ th recurrence time,  $k = 1, \dots, K$ , and let  $t_{K+1}$  be the censored time. Prentice, Williams, and Peterson (1981) consider two time scales, a total time from the beginning of the study and a gap time from immediately preceding failure. The PWP models are stratified Cox-type models that allow the shape of the hazard function to depend on the number of preceding events and possibly on other characteristics of  $\{N(t)$  and  $\mathbf{Z}(t)\}$ . The total time and gap time models are given, respectively, as follows:

$$\begin{aligned} \lambda(t|\mathcal{F}_{t-}) &= \lambda_{0k}(t)e^{\beta_k' \mathbf{Z}(t)}, & t_{k-1} < t \leq t_k \\ \lambda(t|\mathcal{F}_{t-}) &= \lambda_{0k}(t - t_{k-1})e^{\beta_k' \mathbf{Z}(t)}, & t_{k-1} < t \leq t_k \end{aligned}$$

where  $\lambda_{0k}$  is an arbitrary baseline intensity functions, and  $\beta_k$  is a vector of stratum-specific regression coefficients. Here, a subject moves to the  $k$ th stratum immediately after his  $(k - 1)$  recurrence time and remains there until the  $k$ th recurrence occurs or until censorship takes place. For instance, a subject who experiences only one event moves from the first stratum to the second stratum after the event occurs and remains in the second stratum until the end of the follow-up.

You can use PROC PHREG to carry out the analyses of the PWP models, but you have to prepare the input data set to provide the correct risk sets. The input data set for analyzing the total time is the same as the AG model with an additional variable to represent the stratum that the subject is in. A subject with  $K$  events contributes  $K + 1$  observations to the input data set, one for each stratum that the subject moves to. The input data should contain the following variables:

- a TStart variable to represent the  $(k - 1)$  recurrence time or the value 0 if  $k = 1$
- a TStop variable to represent the  $k$ th recurrence time or the time of censorship if  $k = K + 1$
- a Status variable with value 1 if the Time value is a recurrence time and value 0 if the Time value is a censored time
- an Enum variable representing the index of the stratum that the subject is in. For a subject who has only one event at  $t_1$  and is followed to time  $t_c$ , Enum=1 for the first observation (where Time= $t_1$  and Status=1) and Enum=2 for the second observation (where Time= $t_c$  and Status=0).
- explanatory variables thought to be related to the recurrence times

To analyze gap times, the input data set should also include a GapTime variable that is equal to (TStop – TStart).

Consider the data of two subjects in CGD data described in the previous section:

- Patients #174054, age 38, in the gamma interferon group had a follow-up time of 293 without any infection.
- Patient #204001, age 12, in the placebo group had an infection at 219 days, a recurrent infection at 373 days, and a follow-up time of 414 days.

To illustrate, suppose all subjects have at most two observed events. The data for the two subjects in the input data set are as follows:

| ID     | TStart | TStop | Gaptime | Status | Enum | Trt | Age |
|--------|--------|-------|---------|--------|------|-----|-----|
| 174054 | 0      | 293   | 293     | 0      | 1    | 1   | 38  |
| 204001 | 0      | 219   | 219     | 1      | 1    | 2   | 12  |
| 204001 | 219    | 373   | 154     | 1      | 2    | 2   | 12  |
| 204001 | 373    | 414   | 41      | 0      | 3    | 2   | 12  |

Subject #174054 contributes only one observation to the input data, since there is no observed event. Subject #204001 contributes three observations, since there are two observed events.

To fit the total time model of PWP with stratum-specific slopes, either you can create the stratum-specific explanatory variables (Trt1, Trt2, and Trt3 for Trt, and Age1, Age2, and Age3 for Age) in a DATA step, or you can specify them in PROC PHREG by using programming statements as follows:

```
proc phreg;
 model (TStart,TStop)*Status(0)=Trt1 Trt2 Trt3 Age1 Age2 Age3;
 strata Enum;
 Trt1= Trt * (Enum=1);
 Trt2= Trt * (Enum=2);
 Trt3= Trt * (Enum=3);
 Age1= Age * (Enum=1);
 Age2= Age * (Enum=2);
 Age3= Age * (Enum=3);
run;
```



To fit the total time model of PWP with the common regression coefficients, you specify the following:

```
proc phreg;
 model (TStart, TStop)*Status(0)=Trt Age;
 strata Enum;
run;
```

To fit the gap time model of PWP with stratum-specific regression coefficients, you specify the following:

```
proc phreg;
 model Gaptime*Status(0)=Trt1 Trt2 Trt3 Age1 Age2 Age3;
 strata Enum;
 Trt1= Trt * (Enum=1);
 Trt2= Trt * (Enum=2);
 Trt3= Trt * (Enum=3);
 Age1= Age * (Enum=1);
 Age2= Age * (Enum=2);
 Age3= Age * (Enum=3);
run;
```

To fit the gap time model of PWP with common regression coefficients, you specify the following:

```
proc phreg;
 model Gaptime*Status(0)=Trt Age;
 strata Enum;
run;
```

---

## Model Fit Statistics

Suppose the model contains  $p$  regression parameters. Let  $\Delta_j$  and  $f_j$  be the event indicator and the frequency, respectively, of the  $j$ th observation. The three criteria displayed by the PHREG procedure are calculated as follows:

- $-2$  Log Likelihood:

$$-2 \text{ Log L} = -2 \log(L_n(\hat{\beta}))$$

where  $L_n(\cdot)$  is a partial likelihood function for the corresponding TIES= option as described in the section “[Partial Likelihood Function for the Cox Model](#)” on page 5614, and  $\hat{\beta}$  is the maximum likelihood estimate of the regression parameter vector.

- Akaike’s Information Criterion:

$$\text{AIC} = -2 \text{ Log L} + 2p$$

- Schwarz Bayesian (Information) Criterion:

$$\text{SBC} = -2 \text{ Log L} + p \log\left(\sum_j f_j \Delta_j\right)$$

The  $-2$  Log Likelihood statistic has a chi-square distribution under the null hypothesis (that all the explanatory effects in the model are zero) and the procedure produces a  $p$ -value for this statistic. The AIC and SBC statistics give two different ways of adjusting the  $-2$  Log Likelihood statistic for the number of terms in the model and the number of observations used. These statistics should be used when comparing different models for the same data (for example, when you use the METHOD=STEPWISE option in the MODEL statement); lower values of the statistic indicate a more desirable model.

## Residuals

This section describes the computation of residuals (RESMART=, RESDEV=, RESSCH=, and RESSCO=) in the OUTPUT statement.

First, consider TIES=BRESLOW. Let

$$\begin{aligned} S^{(0)}(\boldsymbol{\beta}, t) &= \sum_i Y_i(t) e^{\boldsymbol{\beta}' \mathbf{Z}_i(t)} \\ S^{(1)}(\boldsymbol{\beta}, t) &= \sum_i Y_i(t) e^{\boldsymbol{\beta}' \mathbf{Z}_i(t)} \mathbf{Z}_i(t) \\ \bar{\mathbf{Z}}(\boldsymbol{\beta}, t) &= \frac{S^{(1)}(\boldsymbol{\beta}, t)}{S^{(0)}(\boldsymbol{\beta}, t)} \\ d\Lambda_0(\boldsymbol{\beta}, t) &= \sum_i \frac{dN_i(t)}{S^{(0)}(\boldsymbol{\beta}, t)} \\ dM_i(\boldsymbol{\beta}, t) &= dN_i(t) - Y_i(t) e^{\boldsymbol{\beta}' \mathbf{Z}_i(t)} d\Lambda_0(\boldsymbol{\beta}, t) \end{aligned}$$

The martingale residual at  $t$  is defined as

$$\hat{M}_i(t) = \int_0^t dM_i(\hat{\boldsymbol{\beta}}, s) = N_i(t) - \int_0^t Y_i(s) e^{\hat{\boldsymbol{\beta}}' \mathbf{Z}_i(s)} d\Lambda_0(\hat{\boldsymbol{\beta}}, s)$$

Here  $\hat{M}_i(t)$  estimates the difference over  $(0, t]$  between the observed number of events for the  $i$ th subject and a conditional expected number of events. The quantity  $\hat{M}_i \equiv \hat{M}_i(\infty)$  is referred to as the martingale residual for the  $i$ th subject. When the counting process MODEL specification is used, the RESMART= variable contains the component  $(\hat{M}_i(t_2) - \hat{M}_i(t_1))$  instead of the martingale residual at  $t_2$ . The martingale residual for a subject can be obtained by summing up these component residuals within the subject. For the Cox model with no time-dependent explanatory variables, the martingale residual for the  $i$ th subject with observation time  $t_i$  and event status  $\Delta_i$  is

$$\hat{M}_i = \Delta_i - e^{\hat{\boldsymbol{\beta}}' \mathbf{Z}_i} \int_0^{t_i} d\Lambda_0(\hat{\boldsymbol{\beta}}, s)$$

The deviance residuals  $D_i$  are a transform of the martingale residuals:

$$D_i = \text{sign}(\hat{M}_i) \sqrt{2 \left[ -\hat{M}_i - N_i(\infty) \log \left( \frac{N_i(\infty) - \hat{M}_i}{N_i(\infty)} \right) \right]}$$

The square root shrinks large negative martingale residuals, while the logarithmic transformation expands martingale residuals that are close to unity. As such, the deviance residuals are more symmetrically distributed around zero than the martingale residuals. For the Cox model, the deviance residual reduces to the form

$$D_i = \text{sign}(\hat{M}_i) \sqrt{2[-\hat{M}_i - \Delta_i \log(\Delta_i - \hat{M}_i)]}$$

When the counting process MODEL specification is used, values of the RESDEV= variable are set to missing because the deviance residuals can be calculated only on a per-subject basis.

The Schoenfeld (1982) residual vector is calculated on a per-event-time basis. At the  $j$ th event time  $t_{ij}$  of the  $i$ th subject, the Schoenfeld residual

$$\hat{U}_i(t_{ij}) = \mathbf{Z}_i(t_{ij}) - \bar{\mathbf{Z}}(\hat{\boldsymbol{\beta}}, t_{ij})$$

is the difference between the  $i$ th subject covariate vector at  $t_{ij}$  and the average of the covariate vectors over the risk set at  $t_{ij}$ . Under the proportional hazards assumption, the Schoenfeld residuals have the sample path of a random walk; therefore, they are useful in assessing time trend or lack of proportionality. Harrell (1986) proposed a  $z$ -transform of the Pearson correlation between these residuals and the rank order of the failure time as a test statistic for nonproportional hazards. Therneau, Grambsch, and Fleming (1990) considered a Kolmogorov-type test based on the cumulative sum of the residuals.

The score process for the  $i$ th subject at time  $t$  is

$$\mathbf{L}_i(\boldsymbol{\beta}, t) = \int_0^t [\mathbf{Z}_i(s) - \bar{\mathbf{Z}}(\boldsymbol{\beta}, s)] dM_i(\boldsymbol{\beta}, s)$$

The vector  $\hat{\mathbf{L}}_i \equiv \mathbf{L}_i(\hat{\boldsymbol{\beta}}, \infty)$  is the score residual for the  $i$ th subject. When the counting process MODEL specification is used, the RESSCO= variables contain the components of  $(\mathbf{L}_i(\hat{\boldsymbol{\beta}}, t_2) - \mathbf{L}_i(\hat{\boldsymbol{\beta}}, t_1))$  instead of the score process at  $t_2$ . The score residual for a subject can be obtained by summing up these component residuals within the subject.

The score residuals are a decomposition of the first partial derivative of the log likelihood. They are useful in assessing the influence of each subject on individual parameter estimates. They also play an important role in the computation of the robust sandwich variance estimators of Lin and Wei (1989) and Wei, Lin, and Weissfeld (1989).

For TIES=EFRON, the preceding computation is modified to comply with the Efron partial likelihood. For a given time  $t$ , let  $\Delta_i(t)=1$  if the  $t$  is an event time of the  $i$ th subject and 0 otherwise. Let  $d(t) = \sum_i \Delta_i(t)$ , which is the number of subjects that have an event at  $t$ . For  $1 \leq k \leq d(t)$ , let

$$\begin{aligned} S^{(0)}(\boldsymbol{\beta}, k, t) &= \sum_i Y_i(t) \left\{ 1 - \frac{k-1}{d(t)} \Delta_i(t) \right\} e^{\boldsymbol{\beta}' \mathbf{Z}_i(t)} \\ S^{(1)}(\boldsymbol{\beta}, k, t) &= \sum_i Y_i(t) \left\{ 1 - \frac{k-1}{d(t)} \Delta_i(t) \right\} e^{\boldsymbol{\beta}' \mathbf{Z}_i(t)} \mathbf{Z}_i(t) \\ \bar{\mathbf{Z}}(\boldsymbol{\beta}, k, t) &= \frac{S^{(1)}(\boldsymbol{\beta}, k, t)}{S^{(0)}(\boldsymbol{\beta}, k, t)} \\ d\Lambda_0(\boldsymbol{\beta}, k, t) &= \sum_i \frac{dN_i(t)}{S^{(0)}(\boldsymbol{\beta}, k, t)} \\ dM_i(\boldsymbol{\beta}, k, t) &= dN_i(t) - Y_i(t) \left( 1 - \Delta_i(t) \frac{k-1}{d(t)} \right) e^{\boldsymbol{\beta}' \mathbf{Z}_i(t)} d\Lambda_0(\boldsymbol{\beta}, k, t) \end{aligned}$$

The martingale residual at  $t$  for the  $i$ th subject is defined as

$$\hat{M}_i(t) = \int_0^t \frac{1}{d(s)} \sum_{k=1}^{d(s)} dM_i(\hat{\beta}, k, s) = N_i(t) - \int_0^t \frac{1}{d(s)} \sum_{k=1}^{d(s)} Y_i(s) \left( 1 - \Delta_i(s) \frac{k-1}{d(s)} \right) e^{\hat{\beta}' \mathbf{Z}_i(s)} d\Lambda_0(\hat{\beta}, k, s)$$

Deviance residuals are computed by using the same transform on the corresponding martingale residuals as in TIES=BRESLOW.

The Schoenfeld residual vector for the  $i$ th subject at event time  $t_{ij}$  is

$$\hat{U}_i(t_{ij}) = \mathbf{Z}_i(t_{ij}) - \frac{1}{d(t_{ij})} \sum_{k=1}^{d(t_{ij})} \bar{\mathbf{Z}}(\hat{\beta}, k, t_{ij})$$

The score process for the  $i$ th subject at time  $t$  is given by

$$\mathbf{L}_i(\beta, t) = \int_0^t \frac{1}{d(s)} \sum_{k=1}^{d(s)} \left( \mathbf{Z}_i(s) - \bar{\mathbf{Z}}(\beta, k, s) \right) dM_i(\beta, k, s)$$

For TIES=DISCRETE or TIES=EXACT, it is difficult to come up with modifications that are consistent with the corresponding partial likelihood. Residuals for these TIES= methods are computed by using the same formulae as in TIES=BRESLOW.

## Diagnostics Based on Weighted Residuals

The vector of weighted Schoenfeld residuals,  $\mathbf{r}_i$ , is computed as

$$\mathbf{r}_i = n_e \mathcal{I}^{-1}(\hat{\beta}) \hat{U}_i(t_i)$$

where  $n_e$  is the total number of events and  $\hat{U}_i(t_i)$  is the vector of Schoenfeld residuals at the event time  $t_i$ . The components of  $\mathbf{r}_i$  are output to the WTRESSCH= variables.

The weighted Schoenfeld residuals are useful in assessing the proportional hazards assumption. The idea is that most of the common alternatives to the proportional hazards can be cast in terms of a time-varying coefficient model

$$\lambda(t, \mathbf{Z}) = \lambda_0(t) \exp(\beta_1(t)Z_1 + \beta_2(t)Z_2 + \dots)$$

where  $\lambda(t, \mathbf{Z})$  and  $\lambda_0(t)$  are hazard rates. Let  $\hat{\beta}_j$  and  $r_{ij}$  be the  $j$ th component of  $\hat{\beta}$  and  $\mathbf{r}_i$ , respectively. Grambsch and Therneau (1994) suggest using a smoothed plot of  $(\hat{\beta}_j + r_{ij})$  versus  $t_i$  to discover the functional form of the time-varying coefficient  $\beta_j(t)$ . A zero slope indicates that the coefficient is not varying with time.

The weighted score residuals are used more often than their unscaled counterparts in assessing local influence. Let  $\hat{\beta}_{(i)}$  be the estimate of  $\beta$  when the  $i$ th subject is left out, and let  $\delta \hat{\beta}_i = \hat{\beta} - \hat{\beta}_{(i)}$ . The  $j$ th component of  $\delta \hat{\beta}_i$  can be used to assess any untoward effect of the  $i$ th subject on  $\hat{\beta}_j$ . The exact computation of  $\delta \hat{\beta}_i$

involves refitting the model each time a subject is omitted. Cain and Lange (1984) derived the following approximation of  $\Delta_i$  as weighted score residuals:

$$\delta \hat{\beta}_i = \mathcal{I}^{-1}(\hat{\beta}) \hat{\mathbf{L}}_i$$

Here,  $\hat{\mathbf{L}}_i$  is the vector of the score residuals for the  $i$ th subject. Values of  $\delta \hat{\beta}_i$  are output to the DFBETA= variables. Again, when the counting process MODEL specification is used, the DFBETA= variables contain the component  $\mathcal{I}^{-1}(\hat{\beta})(\mathbf{L}_i(\hat{\beta}, t_2) - \mathbf{L}_i(\hat{\beta}, t_1))$ , where the score process  $\mathbf{L}_i(\beta, t)$  is defined in the section “Residuals” on page 5639. The vector  $\delta \hat{\beta}_i$  for the  $i$ th subject can be obtained by summing these components within the subject.

Note that these DFBETA statistics are a transform of the score residuals. In computing the robust sandwich variance estimators of Lin and Wei (1989) and Wei, Lin, and Weissfeld (1989), it is more convenient to use the DFBETA statistics than the score residuals (see Example 67.10).

## Influence of Observations on Overall Fit of the Model

The LD statistic approximates the likelihood displacement, which is the amount by which minus twice the log likelihood ( $-2 \log L(\hat{\beta})$ ), under a fitted model, changes when each subject in turn is left out. When the  $i$ th subject is omitted, the likelihood displacement is

$$2 \log L(\hat{\beta}) - 2 \log L(\hat{\beta}_{(i)})$$

where  $\hat{\beta}_{(i)}$  is the vector of parameter estimates obtained by fitting the model without the  $i$ th subject. Instead of refitting the model without the  $i$ th subject, Pettitt and Bin Daud (1989) propose that the likelihood displacement for the  $i$ th subject be approximated by

$$\text{LD}_i = \hat{\mathbf{L}}_i' \mathcal{I}^{-1}(\hat{\beta}) \hat{\mathbf{L}}_i$$

where  $\hat{\mathbf{L}}_i$  is the score residual vector of the  $i$ th subject. This approximation is output to the LD= variable.

The LMAX statistic is another global influence statistic. This statistic is based on the symmetric matrix

$$\mathbf{B} = \mathbf{L} \mathcal{I}^{-1}(\hat{\beta}) \mathbf{L}'$$

where  $\mathbf{L}$  is the matrix with rows that are the score residual vectors  $\hat{\mathbf{L}}_i$ . The elements of the eigenvector associated with the largest eigenvalue of the matrix  $\mathbf{B}$ , standardized to unit length, give a measure of the sensitivity of the fit of the model to each observation in the data. The influence of the  $i$ th subject on the global fit of the model is proportional to the magnitude of  $\zeta_i$ , where  $\zeta_i$  is the  $i$ th element of the vector  $\boldsymbol{\zeta}$  that satisfies

$$\mathbf{B} \boldsymbol{\zeta} = \lambda_{\max} \boldsymbol{\zeta} \quad \text{and} \quad \boldsymbol{\zeta}' \boldsymbol{\zeta} = 1$$

with  $\lambda_{\max}$  being the largest eigenvalue of  $\mathbf{B}$ . The sign of  $\zeta_i$  is irrelevant, and its absolute value is output to the LMAX= variable.

When the counting process MODEL specification is used, the LD= and LMAX= variables are set to missing, because these two global influence statistics can be calculated on a per-subject basis only.

## Survivor Function Estimators

Three estimators of the survivor function are available: the Breslow (1972) estimator, which is based on the empirical cumulative hazard function, the Fleming and Harrington (1984) estimator, which is a tie-breaking modification of the Breslow estimator, and the product-limit estimator (Kalbfleisch and Prentice 1980, pp. 84–86).

Let  $\{t_1 < \dots < t_k\}$  be the distinct uncensored times of the survival data.

### Breslow Estimator

To select this estimator, specify the METHOD=BRESLOW option in the BASELINE statement or OUTPUT statement. For the  $j$ th subject, let  $\{(X_j, \Delta_j, \mathbf{Z}_j(\cdot))\}$  represent the failure time, the event indicator, and the vector of covariate values, respectively. For  $t \geq 0$ , let

$$\begin{aligned} Y_j(t) &= I(X_j \geq t) \\ \Delta_j(t) &= \begin{cases} 1 & X_j = t \text{ \& } \Delta_j = 1 \\ 0 & \text{otherwise} \end{cases} \\ d(t) &= \sum_j \Delta_j(t) \end{aligned}$$

Note that  $d(t)$  is the number of subjects that have an event at  $t$ . Let

$$\begin{aligned} S^{(0)}(\boldsymbol{\beta}, t) &= \sum_j Y_j(t) e^{\boldsymbol{\beta}' \mathbf{Z}_j(t)} \\ S^{(1)}(\boldsymbol{\beta}, t) &= \sum_j Y_j(t) e^{\boldsymbol{\beta}' \mathbf{Z}_j(t)} \mathbf{Z}_j(t) \\ \bar{\mathbf{Z}}(\boldsymbol{\beta}, t) &= \frac{S^{(1)}(\boldsymbol{\beta}, t)}{S^{(0)}(\boldsymbol{\beta}, t)} \end{aligned}$$

For a given realization of the explanatory variables  $\boldsymbol{\xi}$ , the cumulative hazard function estimator at  $\boldsymbol{\xi}$  is

$$\hat{\Lambda}_B(t, \boldsymbol{\xi}) = e^{\hat{\boldsymbol{\beta}}' \boldsymbol{\xi}} \sum_{t_i \leq t} \frac{d(t_i)}{S^{(0)}(\hat{\boldsymbol{\beta}}, t_i)}$$

with variance estimated by

$$\hat{\sigma}^2(\hat{\Lambda}_B(t, \boldsymbol{\xi})) = e^{2\hat{\boldsymbol{\beta}}' \boldsymbol{\xi}} \sum_{t_i \leq t} \frac{d(t_i)}{[S^{(0)}(\hat{\boldsymbol{\beta}}, t_i)]^2} + H(t, \boldsymbol{\xi})' [\mathcal{I}(\hat{\boldsymbol{\beta}})]^{-1} H(t, \boldsymbol{\xi})$$

where

$$H(t, \boldsymbol{\xi}) = e^{\hat{\boldsymbol{\beta}}' \boldsymbol{\xi}} \sum_{t_i \leq t} \frac{d(t_i)}{S^{(0)}(\hat{\boldsymbol{\beta}}, t_i)} \left( \bar{\mathbf{Z}}(\hat{\boldsymbol{\beta}}, t_i) - \boldsymbol{\xi} \right)$$

For the marginal model, the variance estimator computation follows Spiekerman and Lin (1998).

The Breslow estimate of the survivor function for  $\mathbf{Z} = \boldsymbol{\xi}$  is

$$\hat{S}_B(t, \boldsymbol{\xi}) = \exp(-\hat{\Lambda}_B(t, \boldsymbol{\xi}))$$

By the delta method, the standard error of  $\hat{S}_B(t, \boldsymbol{\xi})$  is approximated by

$$\hat{\sigma}(\hat{S}_B(t, \boldsymbol{\xi})) = \hat{S}_B(t, \boldsymbol{\xi}) \hat{\sigma}(\hat{\Lambda}_B(t, \boldsymbol{\xi}))$$

### Fleming-Harrington Estimator

To select this estimator, specify the METHOD=FH option in the BASELINE statement or OUTPUT statement. With  $Y_j(t)$  and  $d(t)$  as defined in the section “Breslow Estimator” on page 5643 and for  $1 \leq k \leq d(t)$ , let

$$\begin{aligned} S_E^{(0)}(\boldsymbol{\beta}, k, t) &= \sum_j Y_j(t) \left\{ 1 - \frac{k-1}{d(t)} \Delta_j(t) \right\} e^{\boldsymbol{\beta}' \mathbf{Z}_j(t)} \\ S_E^{(1)}(\boldsymbol{\beta}, k, t) &= \sum_j Y_j(t) \left\{ 1 - \frac{k-1}{d(t)} \Delta_j(t) \right\} e^{\boldsymbol{\beta}' \mathbf{Z}_j(t)} \mathbf{Z}_j(t) \\ \bar{\mathbf{Z}}_E \boldsymbol{\beta}, k, t &= \frac{S_E^{(1)}(\boldsymbol{\beta}, k, t)}{S_E^{(0)}(\boldsymbol{\beta}, k, t)} \end{aligned}$$

For a given realization of the explanatory variables, the Fleming-Harrington adjustment of the cumulative hazard function is

$$\hat{\Lambda}_F(t, \boldsymbol{\xi}) = e^{\hat{\boldsymbol{\beta}}' \boldsymbol{\xi}} \sum_{t_i \leq t} \left\{ \sum_{k=1}^{d(t_i)} \frac{1}{S_E^{(0)}(\hat{\boldsymbol{\beta}}, k, t_i)} \right\}$$

with variance estimated by

$$\hat{\sigma}^2(\hat{\Lambda}_F(t, \boldsymbol{\xi})) = e^{2\hat{\boldsymbol{\beta}}' \boldsymbol{\xi}} \sum_{t_i \leq t} \left\{ \sum_{k=1}^{d(t_i)} \frac{1}{[S_E^{(0)}(\hat{\boldsymbol{\beta}}, k, t_i)]^2} \right\} + H_E(t, \boldsymbol{\xi})' [\mathcal{I}(\hat{\boldsymbol{\beta}})]^{-1} H_E(t, \boldsymbol{\xi})$$

where

$$H_E(t, \boldsymbol{\xi}) = e^{\hat{\boldsymbol{\beta}}' \boldsymbol{\xi}} \left\{ \left[ \sum_{t_i \leq t} \sum_{k=1}^{d(t_i)} \frac{1}{S_E^{(0)}(\hat{\boldsymbol{\beta}}, k, t_i)} \bar{\mathbf{Z}}_E(\hat{\boldsymbol{\beta}}, k, t_i) \right] - \hat{\Lambda}_F(t, \mathbf{0}) \boldsymbol{\xi} \right\}$$

The Fleming-Harrington estimate of the survivor function for  $\mathbf{Z} = \boldsymbol{\xi}$  is

$$\hat{S}_F(t, \boldsymbol{\xi}) = \exp(-\hat{\Lambda}_F(t, \boldsymbol{\xi}))$$

By the delta method, the standard error of  $\hat{S}_F(t, \boldsymbol{\xi})$  is approximated by

$$\hat{\sigma}(\hat{S}_F(t, \boldsymbol{\xi})) = \hat{S}_F(t, \boldsymbol{\xi}) \hat{\sigma}(\hat{\Lambda}_F(t, \boldsymbol{\xi}))$$

## Product-Limit Estimator

To select this estimator, specify the METHOD=PL option in the BASELINE statement or OUTPUT statement. Let  $\mathcal{D}_i$  denote the set of individuals that fail at  $t_i$ . Let  $\mathcal{C}_i$  denote the set of individuals that are censored in the half-open interval  $[t_i, t_{i+1})$ , where  $t_0 = 0$  and  $t_{k+1} = \infty$ . Let  $\gamma_l$  denote the censoring times in  $[t_i, t_{i+1})$ , where  $l$  ranges over  $\mathcal{C}_i$ .

The likelihood function for all individuals is given by

$$\mathcal{L} = \prod_{i=0}^k \left\{ \prod_{l \in \mathcal{D}_i} \left( [S_0(t_i)]^{\exp(\mathbf{Z}'_l \boldsymbol{\beta})} - [S_0(t_i + 0)]^{\exp(\mathbf{Z}'_l \boldsymbol{\beta})} \right) \prod_{l \in \mathcal{C}_i} [S_0(\gamma_l + 0)]^{\exp(\mathbf{Z}'_l \boldsymbol{\beta})} \right\}$$

where  $\mathcal{D}_0$  is empty. The likelihood  $\mathcal{L}$  is maximized by taking  $S_0(t) = S_0(t_i + 0)$  for  $t_i < t \leq t_{i+1}$  and allowing the probability mass to fall only on the observed event times  $t_1, \dots, t_k$ . By considering a discrete model with hazard contribution  $1 - \alpha_i$  at  $t_i$ , you take  $S_0(t_i) = S_0(t_{i-1} + 0) = \prod_{j=0}^{i-1} \alpha_j$ , where  $\alpha_0 = 1$ . Substitution into the likelihood function produces

$$\mathcal{L} = \prod_{i=0}^k \left\{ \prod_{j \in \mathcal{D}_i} \left( 1 - \alpha_i^{\exp(\mathbf{Z}'_j \boldsymbol{\beta})} \right) \prod_{l \in \mathcal{R}_i - \mathcal{D}_i} \alpha_i^{\exp(\mathbf{Z}'_l \boldsymbol{\beta})} \right\}$$

If you replace  $\boldsymbol{\beta}$  with  $\hat{\boldsymbol{\beta}}$  estimated from the partial likelihood function and then maximize with respect to  $\alpha_1, \dots, \alpha_k$ , the maximum likelihood estimate  $\hat{\alpha}_i$  of  $\alpha_i$  becomes a solution of

$$\sum_{j \in \mathcal{D}_i} \frac{\exp(\mathbf{Z}'_j \hat{\boldsymbol{\beta}})}{1 - \hat{\alpha}_i^{\exp(\mathbf{Z}'_j \hat{\boldsymbol{\beta}})}} = \sum_{l \in \mathcal{R}_i} \exp(\mathbf{Z}'_l \hat{\boldsymbol{\beta}})$$

When only a single failure occurs at  $t_i$ ,  $\hat{\alpha}_i$  can be found explicitly. Otherwise, an iterative solution is obtained by the Newton method.

The baseline survival function is estimated by

$$\hat{S}_0(t) = \hat{S}_0(t_{i-1} + 0) = \prod_{j=0}^{i-1} \hat{\alpha}_j, t_{i-1} < t \leq t_i$$

For a given realization of the explanatory variables  $\boldsymbol{\xi}$ , the product-limit estimate of the survival function at  $\mathbf{Z} = \boldsymbol{\xi}$  is

$$\hat{S}_P(t, \boldsymbol{\xi}) = [\hat{S}_0(t)]^{\exp(\boldsymbol{\beta}' \boldsymbol{\xi})}$$

Approximating the variance of  $-\log(\hat{S}_P(t, \boldsymbol{\xi}))$  by the variance estimate of the Breslow estimator of the cumulative hazard function, the variance of the product-limit estimator at  $\mathbf{Z} = \boldsymbol{\xi}$  is given by

$$\hat{\sigma}(\hat{S}_P(t, \boldsymbol{\xi})) = \hat{S}_P(t, \boldsymbol{\xi}) \hat{\sigma}(\hat{\Lambda}_B(t, \boldsymbol{\xi}))$$



### Direct Adjusted Survival Curves

Consider the Breslow estimator of the survival function. For  $j = 1, \dots, n$ , let  $\xi_j$  represent the covariate set of the  $j$ th patient. The direct adjusted survival curve averages the estimated survival curves for each patient:

$$\bar{S}(t) = \frac{1}{n} \sum_{j=1}^n \hat{S}(t, \xi_j)$$

The variance of  $\bar{S}(t)$  can be estimated by

$$\hat{\sigma}^2(\bar{S}(t)) = \frac{1}{n^2} \left( V^{(1)}(t) + V^{(2)}(t) \right)$$

where

$$V^{(1)}(t) = \left( \sum_{j=1}^n e^{\hat{\beta}' \xi_j} \hat{S}(t, \xi_j) \right)^2 \sum_{t_i \leq t} \frac{d(t_i)}{[S^{(0)}(\hat{\beta}, t_i)]^2}$$

$$V^{(2)}(t) = \left( \sum_{j=1}^n \hat{S}(t, \xi_j) H(t, \xi_j) \right)' \left[ \mathcal{I}(\hat{\beta}) \right]^{-1} \left( \sum_{j=1}^n \hat{S}(t, \xi_j) H(t, \xi_j) \right)$$

### Comparison of Direct Adjusted Probabilities of Two Strata

For a stratified Cox model, let  $k$  index the strata. For the  $j$ th patient, let  $\hat{S}_k(t, \xi_j)$  and  $H_k(t, \xi_j)$  be the estimated survival function and the  $\mathbf{H}$  vector for the  $k$ th stratum. The direct adjusted survival curve for the  $k$ th stratum is

$$\bar{S}_k(t) = \frac{1}{n} \sum_{j=1}^n \hat{S}_k(t, \xi_j)$$

The variance of  $\bar{S}_1(t) - \bar{S}_2(t)$  can be estimated by

$$\hat{\sigma}^2(\bar{S}_1(t) - \bar{S}_2(t)) = \frac{1}{n^2} \left( U_1^{(1)}(t) + U_2^{(1)} + U_{12}^{(2)}(t) \right)$$

where

$$U_k^{(1)}(t) = \left( \sum_{j=1}^n e^{\hat{\beta}' \xi_j} \hat{S}_k(t, \xi_j) \right)^2 \sum_{t_i \leq t} \frac{d(t_i)}{[S^{(0)}(\hat{\beta}, t_i)]^2} \quad k = 1, 2$$

$$U_{12}^{(2)}(t) = \left\{ \sum_{j=1}^n \left[ \hat{S}_1(t, \xi_j) H_1(t, \xi_j) - \hat{S}_2(t, \xi_j) H_2(t, \xi_j) \right] \right\}' \mathcal{I}^{-1}(\hat{\beta}) \left\{ \sum_{j=1}^n \left[ \hat{S}_1(t, \xi_j) H_2(t, \xi_j) - \hat{S}_2(t, \xi_j) H_1(t, \xi_j) \right] \right\}$$

### Comparison of Direct Adjusted Survival Probabilities of Two Treatments

For  $j = 1, \dots, n$ , let  $\xi_{jk}$  represent the covariate set of the  $j$ th patient with the  $k$ th treatment,  $k = 1, 2$ . The direct adjusted survival curve for the  $k$ th treatment is

$$\bar{S}_k(t) = \frac{1}{n} \sum_{i=j}^n \hat{S}(t, \xi_{jk})$$

The variance of  $\bar{S}_1(t) - \bar{S}_2(t)$  can be estimated by

$$\hat{\sigma}^2(\bar{S}_1(t) - \bar{S}_2(t)) = \frac{1}{n^2} \left( V_{12}^{(1)}(t) + V_{12}^{(2)}(t) \right)$$

where

$$V_{12}^{(1)}(t) = \left\{ \sum_{j=1}^n \left[ e^{\beta' \xi_{1j}} \hat{S}(t, \xi_{1j}) - e^{\beta' \xi_{2j}} \hat{S}(t, \xi_{2j}) \right] \right\}^2 \sum_{t_i \leq t} \frac{d(t_i)}{[S^{(0)}(\hat{\beta}, t_i)]^2}$$

$$V_{12}^{(2)}(t) = \left\{ \sum_{j=1}^n \left[ \hat{S}(t, \xi_{1j}) H(t, \xi_{1j}) - \hat{S}(t, \xi_{2j}) H(t, \xi_{2j}) \right] \right\}' \mathcal{I}^{-1}(\hat{\beta})$$

$$\left\{ \sum_{j=1}^n \left[ \hat{S}(t, \xi_{1j}) H(t, \xi_{1j}) - \hat{S}(t, \xi_{2j}) H(t, \xi_{2j}) \right] \right\}$$

### Confidence Intervals for the Survivor Function

When the computation of confidence limits for the survivor function  $S(t)$  is based on the asymptotic normality of the survival estimator  $\hat{S}(t)$ —which can be the Breslow estimator  $\hat{S}_B(t)$ , the Fleming-Harrington estimator  $\hat{S}_F(t)$ , or the product-limit estimator  $\hat{S}_P(t)$ —the approximate confidence interval might include impossible values outside the range  $[0, 1]$  at extreme values of  $t$ . This problem can be avoided by applying the asymptotic normality to a transformation of  $S(t)$  for which the range is unrestricted. In addition, certain transformed confidence intervals for  $S(t)$  perform better than the usual linear confidence intervals (Borgan and Liestøl 1990). The CLTYPE= option in the BASELINE statement enables you to choose one of the following transformations: the log-log function, the log function, and the linear function.

Let  $g$  be the transformation that is being applied to the survivor function  $S(t)$ . By the delta method, the standard error of  $g(\hat{S}(t))$  is estimated by

$$\tau(t) = \hat{\sigma} \left[ g(\hat{S}(t)) \right] = g'(\hat{S}(t)) \hat{\sigma}[\hat{S}(t)]$$

where  $g'$  is the first derivative of the function  $g$ . The  $100(1-\alpha)\%$  confidence interval for  $S(t)$  is given by

$$g^{-1} \left\{ g[\hat{S}(t)] \pm z_{\frac{\alpha}{2}} g'[\hat{S}(t)] \hat{\sigma}[\hat{S}(t)] \right\}$$

where  $g^{-1}$  is the inverse function of  $g$ . The choices for the transformation  $g$  are as follows:

- CLTYPE=NORMAL specifies linear transformation, which is the same as having no transformation in which  $g$  is the identity. The  $100(1-\alpha)\%$  confidence interval for  $S(t)$  is given by

$$\hat{S}(t) - z_{\frac{\alpha}{2}} \hat{\sigma} \left[ \hat{S}(t) \right] \leq S(t) \leq \hat{S}(t) + z_{\frac{\alpha}{2}} \hat{\sigma} \left[ \hat{S}(t) \right]$$

- CLTYPE=LOG specifies log transformation. The estimated variance of  $\log(\hat{S}(t))$  is  $\hat{\tau}^2(t) = \frac{\hat{\sigma}^2(\hat{S}(t))}{\hat{S}^2(t)}$ . The  $100(1-\alpha)\%$  confidence interval for  $S(t)$  is given by

$$\hat{S}(t) \exp\left(-z_{\frac{\alpha}{2}} \hat{\tau}(t)\right) \leq S(t) \leq \hat{S}(t) \exp\left(z_{\frac{\alpha}{2}} \hat{\tau}(t)\right)$$

- CLTYPE=LOGLOG specifies log-log transformation. The estimated variance of  $\log(-\log(\hat{S}(t)))$  is  $\hat{\tau}^2(t) = \frac{\hat{\sigma}^2[\hat{S}(t)]}{[\hat{S}(t) \log(\hat{S}(t))]^2}$ . The  $100(1-\alpha)\%$  confidence interval for  $S(t)$  is given by

$$\left[ \hat{S}(t) \right]^{\exp\left(z_{\frac{\alpha}{2}} \hat{\tau}(t)\right)} \leq S(t) \leq \left[ \hat{S}(t) \right]^{\exp\left(-z_{\frac{\alpha}{2}} \hat{\tau}(t)\right)}$$

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## Effect Selection Methods

Five effect selection methods are available. The simplest method (and the default) is SELECTION=NONE, for which PROC PHREG fits the complete model as specified in the MODEL statement. The other four methods are FORWARD for forward selection, BACKWARD for backward elimination, STEPWISE for stepwise selection, and SCORE for best subsets selection. These methods are specified with the SELECTION= option in the MODEL statement and are based on the score test or Wald test as described in the section “Type 3 Tests” on page 5626.

When SELECTION=FORWARD, PROC PHREG first estimates parameters for effects that are forced into the model. These are the first  $n$  effects in the MODEL statement, where  $n$  is the number specified by the START= or INCLUDE= option in the MODEL statement ( $n$  is zero by default). Next, the procedure computes the score statistic for each effect that is not in the model. Each score statistic is the chi-square statistic of the score test for testing the null hypothesis that the corresponding effect that is not in the model is null. If the largest of these statistics is significant at the SLSENTRY= level, the effect with the largest score statistic is added to the model. After an effect is entered in the model, it is never removed from the model. The process is repeated until none of the remaining effects meet the specified level for entry or until the STOP= value is reached.

When SELECTION=BACKWARD, parameters for the complete model as specified in the MODEL statement are estimated unless the START= option is specified. In that case, only the parameters for the first  $n$  effects in the MODEL statement are estimated, where  $n$  is the number specified by the START= option. Next, the procedure computes the Wald statistic of each effect in the model. Each Wald’s statistic is the chi-square statistic of the Wald test for testing the null hypothesis that the corresponding effect is null. If the smallest of these statistics is not significant at the SLSTAY= level, the effect with the smallest Wald statistic is removed. After an effect is removed from the model, it remains excluded. The process is repeated until no other variable in the model meets the specified level for removal or until the STOP= value is reached.

The SELECTION=STEPWISE option is similar to the SELECTION=FORWARD option except that effects already in the model do not necessarily remain. Effects are entered into and removed from the model in such

a way that each forward selection step can be followed by one or more backward elimination steps. The stepwise selection process terminates if no further effect can be added to the model or if the effect just entered into the model is the only effect that is removed in the subsequent backward elimination.

For SELECTION=SCORE, PROC PHREG uses the branch-and-bound algorithm of Furnival and Wilson (1974) to find a specified number of models with the highest score (chi-square) statistic for all possible model sizes, from 1, 2, or 3 variables, and so on, up to the single model that contains all of the explanatory variables. The number of models displayed for each model size is controlled by the BEST= option. You can use the START= option to impose a minimum model size, and you can use the STOP= option to impose a maximum model size. For instance, with BEST=3, START=2, and STOP=5, the SCORE selection method displays the best three models (that is, the three models with the highest score chi-squares) that contain 2, 3, 4, and 5 variables. One of the limitations of the branch-and-bound algorithm is that it works only when each explanatory effect contains exactly one parameter—the SELECTION=SCORE option is not allowed when an explanatory effect in the MODEL statement contains a CLASS variable.

The SEQUENTIAL and STOPRES options can alter the default criteria for adding variables to or removing variables from the model when they are used with the FORWARD, BACKWARD, or STEPWISE selection method.

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## Assessment of the Proportional Hazards Model

The proportional hazards model specifies that the hazard function for the failure time  $T$  associated with a  $p \times 1$  column covariate vector  $\mathbf{Z}$  takes the form

$$\lambda(t; \mathbf{Z}) = \lambda_0(t)e^{\boldsymbol{\beta}'\mathbf{Z}}$$

where  $\lambda_0(\cdot)$  is an unspecified baseline hazard function and  $\boldsymbol{\beta}$  is a  $p \times 1$  column vector of regression parameters. Lin, Wei, and Ying (1993) present graphical and numerical methods for model assessment based on the cumulative sums of martingale residuals and their transforms over certain coordinates (such as covariate values or follow-up times). The distributions of these stochastic processes under the assumed model can be approximated by the distributions of certain zero-mean Gaussian processes whose realizations can be generated by simulation. Each observed residual pattern can then be compared, both graphically and numerically, with a number of realizations from the null distribution. Such comparisons enable you to assess objectively whether the observed residual pattern reflects anything beyond random fluctuation. These procedures are useful in determining appropriate functional forms of covariates and assessing the proportional hazards assumption. You use the ASSESS statement to carry out these model-checking procedures.

For a sample of  $n$  subjects, let  $(X_i, \Delta_i, \mathbf{Z}_i)$  be the data of the  $i$ th subject; that is,  $X_i$  represents the observed failure time,  $\Delta_i$  has a value of 1 if  $X_i$  is an uncensored time and 0 otherwise, and  $\mathbf{Z}_i = (Z_{1i}, \dots, Z_{pi})'$  is a  $p$ -vector of covariates. Let  $N_i(t) = \Delta_i I(X_i \leq t)$  and  $Y_i(t) = I(X_i \geq t)$ . Let

$$S^{(0)}(\boldsymbol{\beta}, t) = \sum_{i=1}^n Y_i(t)e^{\boldsymbol{\beta}'\mathbf{Z}_i} \quad \text{and} \quad \mathbf{Z}(\boldsymbol{\beta}, t) = \frac{\sum_{i=1}^n Y_i(t)e^{\boldsymbol{\beta}'\mathbf{Z}_i} \mathbf{Z}_i}{S^{(0)}(\boldsymbol{\beta}, t)}$$

Let  $\hat{\boldsymbol{\beta}}$  be the maximum partial likelihood estimate of  $\boldsymbol{\beta}$ , and let  $\mathcal{I}(\hat{\boldsymbol{\beta}})$  be the observed information matrix.

The martingale residuals are defined as

$$\hat{M}_i(t) = N_i(t) - \int_0^t Y_i(u)e^{\hat{\boldsymbol{\beta}}'\mathbf{Z}_i} d\hat{\Lambda}_0(u), \quad i = 1, \dots, n$$

where  $\hat{\Lambda}_0(t) = \int_0^t \frac{\sum_{i=1}^n dN_i(u)}{S^{(0)}(\hat{\beta}, u)}$ .

The empirical score process  $\mathbf{U}(\hat{\beta}, t) = (U_1(\hat{\beta}, t), \dots, U_p(\hat{\beta}, t))'$  is a transform of the martingale residuals:

$$\mathbf{U}(\hat{\beta}, t) = \sum_{i=1}^n \mathbf{Z}_i \hat{M}_i(t)$$

### Checking the Functional Form of a Covariate

To check the functional form of the  $j$ th covariate, consider the partial-sum process of  $\hat{M}_i = \hat{M}_i(\infty)$ :

$$W_j(z) = \sum_{i=1}^n I(Z_{ji} \leq z) \hat{M}_i$$

Under that null hypothesis that the model holds,  $W_j(z)$  can be approximated by the zero-mean Gaussian process

$$\begin{aligned} \hat{W}_j(z) &= \sum_{l=1}^n \Delta_l \left\{ I(Z_{jl} \leq z) - \frac{\sum_{i=1}^n Y_i(X_l) e^{\hat{\beta}' \mathbf{Z}_i} I(Z_{ij} \leq z)}{S^{(0)}(\hat{\beta}, X_l)} \right\} G_l - \\ &\quad \sum_{k=1}^n \int_0^\infty Y_k(s) e^{\hat{\beta}' \mathbf{Z}_k} I(Z_{jk} \leq z) [\mathbf{Z}_k - \bar{\mathbf{Z}}(\hat{\beta}, s)]' d\hat{\Lambda}_0(s) \\ &\quad \times \mathcal{I}^{-1}(\hat{\beta}) \sum_{l=1}^n \Delta_l [\mathbf{Z}_l - \bar{\mathbf{Z}}(\hat{\beta}, X_l)] G_l \end{aligned}$$

where  $(G_1, \dots, G_n)$  are independent standard normal variables that are independent of  $(X_i, \Delta_i, \mathbf{Z}_i)$ ,  $i = 1, \dots, n$ .

You can assess the functional form of the  $j$ th covariate by plotting a small number of realizations (the default is 20) of  $\hat{W}_j(z)$  on the same graph as the observed  $W_j(z)$  and visually comparing them to see how typical the observed pattern of  $W_j(z)$  is of the null distribution samples. You can supplement the graphical inspection method with a Kolmogorov-type supremum test. Let  $s_j$  be the observed value of  $S_j = \sup_z |W_j(z)|$  and let  $\hat{S}_j = \sup_z |\hat{W}_j(z)|$ . The  $p$ -value  $\Pr(S_j \geq s_j)$  is approximated by  $\Pr(\hat{S}_j \geq s_j)$ , which in turn is approximated by generating a large number of realizations (1000 is the default) of  $\hat{W}_j(\cdot)$ .

### Checking the Proportional Hazards Assumption

Consider the standardized empirical score process for the  $j$ th component of  $\mathbf{Z}$

$$U_j^*(t) = [\mathcal{I}^{-1}(\hat{\beta})_{jj}]^{\frac{1}{2}} U_j(\hat{\beta}, t),$$

Under the null hypothesis that the model holds,  $U_j^*(t)$  can be approximated by

$$\begin{aligned} \hat{U}_j^*(t) &= [\mathcal{I}^{-1}(\hat{\boldsymbol{\beta}})_{jj}]^{\frac{1}{2}} \left\{ \sum_{l=1}^n I(X_l \leq t) \Delta_l [Z_{jl} - \bar{Z}_j(\hat{\boldsymbol{\beta}}, t)] G_l - \right. \\ &\quad \sum_{k=1}^n \int_0^t Y_k(s) e^{\hat{\boldsymbol{\beta}}' \mathbf{Z}_k} Z_{jk} [\mathbf{Z}_k - \bar{\mathbf{Z}}(\hat{\boldsymbol{\beta}}, s)]' d\hat{\Lambda}_0(s) \\ &\quad \left. \times \mathcal{I}^{-1}(\hat{\boldsymbol{\beta}}) \sum_{l=1}^n \Delta_l [\mathbf{Z}_l - \bar{\mathbf{Z}}(\hat{\boldsymbol{\beta}}, X_l)] G_l \right\} \end{aligned}$$

where  $\bar{Z}_j(\hat{\boldsymbol{\beta}}, t)$  is the  $j$ th component of  $\bar{\mathbf{Z}}(\hat{\boldsymbol{\beta}}, t)$ , and  $(G_1, \dots, G_n)$  are independent standard normal variables that are independent of  $(X_i, \Delta_i, \mathbf{Z}_i, (i = 1, \dots, n))$ .

You can assess the proportional hazards assumption for the  $j$ th covariate by plotting a few realizations of  $\hat{U}_j^*(t)$  on the same graph as the observed  $U_j^*(t)$  and visually comparing them to see how typical the observed pattern of  $U_j^*(t)$  is of the null distribution samples. Again you can supplement the graphical inspection method with a Kolmogorov-type supremum test. Let  $s_j^*$  be the observed value of  $S_j^* = \sup_t |U_j^*(t)|$  and let  $\hat{S}_j^* = \sup_t |\hat{U}_j^*(t)|$ . The  $p$ -value  $\Pr[S_j^* \geq s_j^*]$  is approximated by  $\Pr[\hat{S}_j^* \geq s_j^*]$ , which in turn is approximated by generating a large number of realizations (1000 is the default) of  $\hat{U}_j^*(\cdot)$ .

## The Penalized Partial Likelihood Approach for Fitting Frailty Models

Let  $\boldsymbol{\gamma} = (\gamma_1, \dots, \gamma_s)'$  be the vector of random components for the  $s$  clusters.

### Gamma Frailty Model

Assume each  $e^{\gamma_i}$  has an independent and identically distributed gamma distribution with mean 1 and a common unknown variance  $\theta$ ; that is,  $e^{\gamma_i}$  is iid  $G(\frac{1}{\theta}, \frac{1}{\theta})$ . The penalty function is

$$-\frac{1}{\theta} \sum_{i=1}^s (\gamma_i - e^{\gamma_i})$$

plus a function of  $\theta$ . The penalized partial log likelihood is given by

$$l_p(\boldsymbol{\beta}, \boldsymbol{\gamma}, \theta) = l_{\text{partial}}(\boldsymbol{\beta}, \boldsymbol{\gamma}) + \frac{1}{\theta} \sum_{i=1}^s (\gamma_i - e^{\gamma_i})$$

where  $l_{\text{partial}}(\boldsymbol{\beta}, \boldsymbol{\gamma})$  is the log of any of the partial likelihoods in the sections “Partial Likelihood Function for the Cox Model” on page 5614 and “The Multiplicative Hazards Model” on page 5617.

The profile marginal log-likelihood of this shared frailty model (Therneau and Grambsch 2000, pp. 257–258) is

$$l_m(\theta) = l_p(\hat{\boldsymbol{\beta}}(\theta), \hat{\boldsymbol{\gamma}}(\theta), \theta) + \sum_{i=1}^s \left\{ \theta^{-1} - (\theta^{-1} + d_i) \log[\theta^{-1} + d_i] + \theta^{-1} \log(\theta^{-1}) + \log \left[ \frac{\Gamma(\theta^{-1} + d_i)}{\Gamma(\theta^{-1})} \right] \right\}$$

where  $d_i$  is the number of events in the  $i$ th cluster.

The maximization of this approximate likelihood is a doubly iterative process that alternates between the following two steps:

- For a provisional value of  $\theta$ , the best linear unbiased predictors (BLUP) of  $\boldsymbol{\beta}$  and  $\boldsymbol{\gamma}$  are computed by maximizing the penalized partial log-likelihood  $l_p(\boldsymbol{\beta}, \boldsymbol{\gamma}, \theta)$ . The marginal likelihood is evaluated. This constitutes the inner loop.
- A new value of  $\theta$  is obtained by the golden section search based on the marginal likelihood of all the previous iterations. This constitutes the outer loop.

The outer loop is iterated until the bracketing interval of  $\theta$  is small.

### Lognormal Frailty Model

With each  $\gamma_i$  having a zero-mean normal distribution and a common variance  $\theta$ , the penalty function is

$$\frac{1}{2\theta} \boldsymbol{\gamma}' \boldsymbol{\gamma}$$

plus a function of  $\theta$ . The penalized partial log likelihood is given by

$$l_p(\boldsymbol{\beta}, \boldsymbol{\gamma}, \theta) = l_{\text{partial}}(\boldsymbol{\beta}, \boldsymbol{\gamma}) - \frac{1}{2\theta} \boldsymbol{\gamma}' \boldsymbol{\gamma}$$

where  $l_{\text{partial}}(\boldsymbol{\beta}, \boldsymbol{\gamma})$  is the log of any of the partial likelihoods in the sections “[Partial Likelihood Function for the Cox Model](#)” on page 5614 and “[The Multiplicative Hazards Model](#)” on page 5617.

For a given  $\theta$ , let  $\mathbf{H}$  be the negative Hessian of the penalized partial log likelihood  $l_p(\boldsymbol{\beta}, \boldsymbol{\gamma}, \theta)$ ; that is,

$$\mathbf{H} = \mathbf{H}(\boldsymbol{\beta}, \boldsymbol{\gamma}) = \begin{bmatrix} \mathbf{H}_{11} & \mathbf{H}_{12} \\ \mathbf{H}_{21} & \mathbf{H}_{22} \end{bmatrix}$$

where  $\mathbf{H}_{11} = -\frac{\partial^2 l_p(\boldsymbol{\beta}, \boldsymbol{\gamma}, \theta)}{\partial \boldsymbol{\beta}^2}$ ,  $\mathbf{H}_{12} = \mathbf{H}'_{21} = -\frac{\partial^2 l_p(\boldsymbol{\beta}, \boldsymbol{\gamma}, \theta)}{\partial \boldsymbol{\beta} \partial \boldsymbol{\gamma}}$ , and  $\mathbf{H}_{22} = -\frac{\partial^2 l_p(\boldsymbol{\beta}, \boldsymbol{\gamma}, \theta)}{\partial \boldsymbol{\gamma}^2}$ .

The marginal log likelihood of this shared frailty model is

$$l_m(\boldsymbol{\beta}, \theta) = -\frac{1}{2} \log(\theta^s) + \log \left[ \int e^{l_p(\boldsymbol{\beta}, \boldsymbol{\gamma}, \theta)} d\boldsymbol{\gamma} \right]$$

Using a Laplace approximation to the integral as in Breslow and Clayton (1993), an approximate marginal log likelihood (Ripatti and Palmgren 2000; Therneau and Grambsch 2000) is given by

$$l_m(\boldsymbol{\beta}, \theta) \approx -\frac{1}{2} \log(\theta^s) - \frac{1}{2} \log(|\mathbf{H}_{22}(\boldsymbol{\beta}, \tilde{\boldsymbol{\gamma}}, \theta)|) - l_p(\boldsymbol{\beta}, \tilde{\boldsymbol{\gamma}}, \theta)$$

The maximization of this approximate likelihood is a doubly iterative process that alternates between the following two steps:

- For a provisional value of  $\theta$ , PROC PHREG computes the best linear unbiased predictors (BLUP) of  $\boldsymbol{\beta}$  and  $\boldsymbol{\gamma}$  by maximizing the penalized partial log likelihood  $l_p(\boldsymbol{\beta}, \boldsymbol{\gamma}, \theta)$ . This constitutes the inner loop.

- For  $\boldsymbol{\beta}$  and  $\boldsymbol{\gamma}$  fixed at the BLUP values, PROC PHREG estimates  $\theta$  by maximizing the approximate marginal likelihood  $l_m(\boldsymbol{\beta}, \theta)$ . This constitutes the outer loop.

The outer loop is iterated until the difference between two successive estimates of  $\theta$  is small.

The ML estimate of  $\theta$  is

$$\hat{\theta} = \frac{\hat{\boldsymbol{\gamma}}' \hat{\boldsymbol{\gamma}} + \text{trace}(\mathbf{H}_{22}^{-1})}{s}$$

The variance for  $\hat{\theta}$  is

$$\text{var}(\hat{\theta}) = 2\hat{\theta} \left[ s + \frac{1}{\hat{\theta}^2} \text{trace}(\mathbf{H}_{22}^{-1} \mathbf{H}_{22}^{-1}) - \frac{2}{\hat{\theta}} \text{trace}(\mathbf{H}_{22}^{-1}) \right]^{-1}$$

The REML estimation of  $\theta$  is obtained by replacing  $(\mathbf{H}_{22})^{-1}$  by  $(\mathbf{H}^{-1})_{22}$ .

The inverse of the final  $\mathbf{H}$  matrix is used as the variance estimate of  $(\hat{\boldsymbol{\beta}}, \hat{\boldsymbol{\gamma}})'$ .

The final BLUP estimates of the random components  $\gamma_1, \dots, \gamma_s$  can be displayed by using the SOLUTION option in the RANDOM statement. Also displayed are estimates of the lognormal frailties, which are the exponentiated estimates of the BLUP estimates.

### Wald-Type Tests for Penalized Models

Let  $\mathbf{I}$  be the negative Hessian of the partial log likelihood  $l_{\text{partial}}(\boldsymbol{\beta}, \boldsymbol{\gamma})$ :

$$\mathbf{I} = \begin{bmatrix} \mathbf{I}_{11} & \mathbf{I}_{12} \\ \mathbf{I}_{21} & \mathbf{I}_{22} \end{bmatrix}$$

where  $\mathbf{I}_{11} = -\frac{\partial^2 l_{\text{partial}}(\boldsymbol{\beta}, \boldsymbol{\gamma})}{\partial \boldsymbol{\beta}^2}$ ,  $\mathbf{I}_{12} = \mathbf{I}_{21}' = -\frac{\partial^2 l_{\text{partial}}(\boldsymbol{\beta}, \boldsymbol{\gamma})}{\partial \boldsymbol{\beta} \partial \boldsymbol{\gamma}}$ , and  $\mathbf{I}_{22} = -\frac{\partial^2 l_{\text{partial}}(\boldsymbol{\beta}, \boldsymbol{\gamma})}{\partial \boldsymbol{\gamma}^2}$ . Write  $\boldsymbol{\tau}' = (\boldsymbol{\beta}', \boldsymbol{\gamma}')'$ . The Wald-type chi-square statistic for testing  $H_0 : \mathbf{C}\boldsymbol{\tau} = \mathbf{0}$  is

$$(\mathbf{C}\hat{\boldsymbol{\tau}})'(\mathbf{C}\mathbf{H}^{-1}\mathbf{C}')^{-1}(\mathbf{C}\hat{\boldsymbol{\tau}})$$

Let  $\mathbf{H}$  be the negative Hessian of the penalized partial log likelihood  $l_p(\boldsymbol{\beta}, \boldsymbol{\gamma}, \theta)$  at the ML estimate  $\theta$ ; that is,  $\mathbf{H} = \frac{\partial^2}{\partial \boldsymbol{\beta} \partial \boldsymbol{\gamma}} l_p(\boldsymbol{\beta}, \boldsymbol{\gamma}, \hat{\theta})$ . Let  $\mathbf{V} = \mathbf{H}^{-1} \mathbf{I} \mathbf{H}^{-1}$ . Gray (1992) recommends the following generalized degrees of freedom for the Wald test:

$$\text{DF} = \text{trace}[(\mathbf{C}\mathbf{H}^{-1}\mathbf{C}')^{-1} \mathbf{C}\mathbf{V}\mathbf{C}']$$

See Therneau and Grambsch (2000, Section 5.8) for a discussion of this Wald-type test.

PROC PHREG uses the label "Adjusted DF" to represent this generalized degrees of freedom in the output.

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## Specifics for Bayesian Analysis

To request a Bayesian analysis, you specify the new BAYES statement in addition to the PROC PHREG statement and the MODEL statement. You include a CLASS statement if you have effects that involve categorical variables. The FREQ or WEIGHT statement can be included if you have a frequency or weight



variable, respectively, in the input data. The STRATA statement can be used to carry out a stratified analysis for the Cox model, but it is not allowed in the piecewise constant baseline hazard model. Programming statements can be used to create time-dependent covariates for the Cox model, but they are not allowed in the piecewise constant baseline hazard model. However, you can use the counting process style of input to accommodate time-dependent covariates that are not continuously changing with time for the piecewise constant baseline hazard model and the Cox model as well. The HAZARDRATIO statement enables you to request a hazard ratio analysis based on the posterior samples. The ASSESS, CONTRAST, ID, OUTPUT, and TEST statements, if specified, are ignored. Also ignored are the COVM and COVS options in the PROC PHREG statement and the following options in the MODEL statement: BEST=, CORRB, COVB, DETAILS, HIERARCHY=, INCLUDE=, MAXSTEP=, NOFIT, PLCONV=, SELECTION=, SEQUENTIAL, SLENTY=, and SLSTAY=.

## Piecewise Constant Baseline Hazard Model

### Single Failure Time Variable

Let  $\{(t_i, \mathbf{x}_i, \delta_i), i = 1, 2, \dots, n\}$  be the observed data. Let  $a_0 = 0 < a_1 < \dots < a_{J-1} < a_J = \infty$  be a partition of the time axis.

**Hazards in Original Scale** The hazard function for subject  $i$  is

$$h(t|\mathbf{x}_i; \boldsymbol{\theta}) = h_0(t) \exp(\boldsymbol{\beta}'\mathbf{x}_i)$$

where

$$h_0(t) = \lambda_j \text{ if } a_{j-1} \leq t < a_j, j = 1, \dots, J$$

The baseline cumulative hazard function is

$$H_0(t) = \sum_{j=1}^J \lambda_j \Delta_j(t)$$

where

$$\Delta_j(t) = \begin{cases} 0 & t < a_{j-1} \\ t - a_{j-1} & a_{j-1} \leq t < a_j \\ a_j - a_{j-1} & t \geq a_j \end{cases}$$

The log likelihood is given by

$$\begin{aligned} l(\boldsymbol{\lambda}, \boldsymbol{\beta}) &= \sum_{i=1}^n \delta_i \left[ \sum_{j=1}^J I(a_{j-1} \leq t_i < a_j) \log \lambda_j + \boldsymbol{\beta}'\mathbf{x}_i \right] - \sum_{i=1}^n \left[ \sum_{j=1}^J \Delta_j(t_i) \lambda_j \right] \exp(\boldsymbol{\beta}'\mathbf{x}_i) \\ &= \sum_{j=1}^J d_j \log \lambda_j + \sum_{i=1}^n \delta_i \boldsymbol{\beta}'\mathbf{x}_i - \sum_{j=1}^J \lambda_j \left[ \sum_{i=1}^n \Delta_j(t_i) \exp(\boldsymbol{\beta}'\mathbf{x}_i) \right] \end{aligned}$$

where  $d_j = \sum_{i=1}^n \delta_i I(a_{j-1} \leq t_i < a_j)$ .

Note that for  $1 \leq j \leq J$ , the full conditional for  $\lambda_j$  is log-concave only when  $d_j > 0$ , but the full conditionals for the  $\beta$ 's are always log-concave.

For a given  $\beta$ ,  $\frac{\partial l}{\partial \lambda} = 0$  gives

$$\tilde{\lambda}_j(\beta) = \frac{d_j}{\sum_{i=1}^n \Delta_j(t_i) \exp(\beta' \mathbf{x}_i)}, \quad j = 1, \dots, J$$

Substituting these values into  $l(\lambda, \beta)$  gives the profile log likelihood for  $\beta$

$$l_p(\beta) = \sum_{i=1}^n \delta_i \beta' \mathbf{x}_i - \sum_{j=1}^J d_j \log \left[ \sum_{l=1}^n \Delta_j(t_l) \exp(\beta' \mathbf{x}_l) \right] + c$$

where  $c = \sum_j (d_j \log d_j - d_j)$ . Since the constant  $c$  does not depend on  $\beta$ , it can be discarded from  $l_p(\beta)$  in the optimization.

The MLE  $\hat{\beta}$  of  $\beta$  is obtained by maximizing

$$l_p(\beta) = \sum_{i=1}^n \delta_i \beta' \mathbf{x}_i - \sum_{j=1}^J d_j \log \left[ \sum_{l=1}^n \Delta_j(t_l) \exp(\beta' \mathbf{x}_l) \right]$$

with respect to  $\beta$ , and the MLE  $\hat{\lambda}$  of  $\lambda$  is given by

$$\hat{\lambda} = \tilde{\lambda}(\hat{\beta})$$

For  $j = 1, \dots, J$ , let

$$\begin{aligned} \mathbf{S}_j^{(r)}(\beta) &= \sum_{l=1}^n \Delta_j(t_l) e^{\beta' \mathbf{x}_l} \mathbf{x}_l^{\otimes r}, \quad r = 0, 1, 2 \\ \mathbf{E}_j(\beta) &= \frac{\mathbf{S}_j^{(1)}(\beta)}{S_j^{(0)}(\beta)} \end{aligned}$$

The partial derivatives of  $l_p(\beta)$  are

$$\begin{aligned} \frac{\partial l_p(\beta)}{\partial \beta} &= \sum_{i=1}^n \delta_i \mathbf{x}_i - \sum_{j=1}^J d_j \mathbf{E}_j(\beta) \\ -\frac{\partial^2 l_p(\beta)}{\partial \beta^2} &= \sum_{j=1}^J d_j \left\{ \frac{\mathbf{S}_j^{(2)}(\beta)}{S_j^{(0)}(\beta)} - \left[ \mathbf{E}_j(\beta) \right] \left[ \mathbf{E}_j(\beta) \right]' \right\} \end{aligned}$$

The asymptotic covariance matrix for  $(\hat{\lambda}, \hat{\beta})$  is obtained as the inverse of the information matrix given by

$$\begin{aligned} -\frac{\partial^2 l(\hat{\lambda}, \hat{\beta})}{\partial \lambda^2} &= \mathcal{D} \left( \frac{d_1}{\hat{\lambda}_1^2}, \dots, \frac{d_J}{\hat{\lambda}_J^2} \right) \\ -\frac{\partial^2 l(\hat{\lambda}, \hat{\beta})}{\partial \beta^2} &= \sum_{j=1}^J \hat{\lambda}_j \mathbf{S}_j^{(2)}(\hat{\beta}) \\ -\frac{\partial^2 l(\hat{\lambda}, \hat{\beta})}{\partial \lambda \partial \beta} &= (\mathbf{S}_1^{(1)}(\hat{\beta}), \dots, \mathbf{S}_J^{(1)}(\hat{\beta})) \end{aligned}$$

See Example 6.5.1 in Lawless (2003) for details.

**Hazards in Log Scale** By letting

$$\alpha_j = \log(\lambda_j), \quad j = 1, \dots, J$$

you can build a prior correlation among the  $\lambda_j$ 's by using a correlated prior  $\boldsymbol{\alpha} \sim N(\boldsymbol{\alpha}_0, \Sigma_\alpha)$ , where  $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_J)'$ .

The log likelihood is given by

$$l(\boldsymbol{\alpha}, \boldsymbol{\beta}) = \sum_{j=1}^J d_j \alpha_j + \sum_{i=1}^n \delta_i \boldsymbol{\beta}' \mathbf{x}_i - \sum_{j=1}^J e^{\alpha_j} S_j^{(0)}(\boldsymbol{\beta})$$

Then the MLE of  $\lambda_j$  is given by

$$e^{\hat{\alpha}_j} = \hat{\lambda}_j = \frac{d_j}{S_j^0(\hat{\boldsymbol{\beta}})}$$

Note that the full conditionals for  $\alpha$ 's and  $\beta$ 's are always log-concave.

The asymptotic covariance matrix for  $(\hat{\boldsymbol{\alpha}}, \hat{\boldsymbol{\beta}})$  is obtained as the inverse of the information matrix formed by

$$\begin{aligned} -\frac{\partial^2 l(\hat{\boldsymbol{\alpha}}, \hat{\boldsymbol{\beta}})}{\partial \boldsymbol{\alpha}^2} &= \mathcal{D}\left(e^{\hat{\alpha}_1} S_1^0(\hat{\boldsymbol{\beta}}), \dots, e^{\hat{\alpha}_J} S_J^0(\hat{\boldsymbol{\beta}})\right) \\ -\frac{\partial^2 l(\hat{\boldsymbol{\alpha}}, \hat{\boldsymbol{\beta}})}{\partial \boldsymbol{\beta}^2} &= \sum_{j=1}^J e^{\hat{\alpha}_j} \mathbf{S}_j^{(2)}(\hat{\boldsymbol{\beta}}) \\ -\frac{\partial^2 l(\hat{\boldsymbol{\alpha}}, \hat{\boldsymbol{\beta}})}{\partial \boldsymbol{\alpha} \partial \boldsymbol{\beta}} &= (e^{\hat{\alpha}_1} \mathbf{S}_1^{(1)}(\hat{\boldsymbol{\beta}}), \dots, e^{\hat{\alpha}_J} \mathbf{S}_J^{(1)}(\hat{\boldsymbol{\beta}})) \end{aligned}$$

### Counting Process Style of Input

Let  $\{(s_i, t_i], \mathbf{x}_i, \delta_i\}, i = 1, 2, \dots, n\}$  be the observed data. Let  $a_0 = 0 < a_1 < \dots < a_k$  be a partition of the time axis, where  $a_k > t_i$  for all  $i = 1, 2, \dots, n$ .

Replacing  $\Delta_j(t_i)$  with

$$\Delta_j((s_i, t_i]) = \begin{cases} 0 & t_i < a_{j-1} \vee s_i > a_j \\ t_i - \max(s_i, a_{j-1}) & a_{j-1} \leq t_i < a_j \\ a_j - \max(s_i, a_{j-1}) & t_i \geq a_j \end{cases}$$

the formulation for the single failure time variable applies.

### Priors for Model Parameters

For a Cox model, the model parameters are the regression coefficients. For a piecewise exponential model, the model parameters consist of the regression coefficients and the hazards or log-hazards. The priors for the hazards and the priors for the regression coefficients are assumed to be independent, while you can have a joint multivariate normal prior for the log-hazards and the regression coefficients.

**Hazard Parameters**

Let  $\lambda_1, \dots, \lambda_J$  be the constant baseline hazards.

**Improper Prior** The joint prior density is given by

$$p(\lambda_1, \dots, \lambda_J) = \prod_{j=1}^J \frac{1}{\lambda_j}, \forall \lambda_j > 0$$

This prior is improper (nonintegrable), but the posterior distribution is proper as long as there is at least one event time in each of the constant hazard intervals.

**Uniform Prior** The joint prior density is given by

$$p(\lambda_1, \dots, \lambda_J) \propto 1, \forall \lambda_j > 0$$

This prior is improper (nonintegrable), but the posteriors are proper as long as there is at least one event time in each of the constant hazard intervals.

**Gamma Prior** The gamma distribution  $G(a, b)$  has a PDF

$$f_{a,b}(t) = \frac{b(bt)^{a-1}e^{-bt}}{\Gamma(a)}, t > 0$$

where  $a$  is the shape parameter and  $b^{-1}$  is the scale parameter. The mean is  $\frac{a}{b}$  and the variance is  $\frac{a}{b^2}$ .

**Independent Gamma Prior** Suppose for  $j = 1, \dots, J$ ,  $\lambda_j$  has an independent  $G(a_j, b_j)$  prior. The joint prior density is given by

$$p(\lambda_1, \dots, \lambda_J) \propto \prod_{j=1}^J \left\{ \lambda_j^{a_j-1} e^{-b_j \lambda_j} \right\}, \forall \lambda_j > 0$$

**AR1 Prior**  $\lambda_1, \dots, \lambda_J$  are correlated as follows:

$$\begin{aligned} \lambda_1 &\sim G(a_1, b_1) \\ \lambda_2 &\sim G\left(a_2, \frac{b_2}{\lambda_1}\right) \\ \dots &\dots \\ \lambda_J &\sim G\left(a_J, \frac{b_J}{\lambda_{J-1}}\right) \end{aligned}$$

The joint prior density is given by

$$p(\lambda_1, \dots, \lambda_J) \propto \lambda_1^{a_1-1} e^{-b_1 \lambda_1} \prod_{j=2}^J \left( \frac{b_j}{\lambda_{j-1}} \right)^{a_j} \lambda_j^{a_j-1} e^{-\frac{b_j}{\lambda_{j-1}} \lambda_j}$$

**Log-Hazard Parameters**

Write  $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_J)' \equiv (\log \lambda_1, \dots, \log \lambda_J)'$ .

**Uniform Prior** The joint prior density is given by

$$p(\alpha_1 \dots \alpha_J) \propto 1, \forall -\infty < \alpha_i < \infty$$

Note that the uniform prior for the log-hazards is the same as the improper prior for the hazards.

**Normal Prior** Assume  $\boldsymbol{\alpha}$  has a multivariate normal prior with mean vector  $\boldsymbol{\alpha}_0$  and covariance matrix  $\boldsymbol{\Psi}_0$ . The joint prior density is given by

$$p(\boldsymbol{\alpha}) \propto e^{-\frac{1}{2}(\boldsymbol{\alpha}-\boldsymbol{\alpha}_0)'\boldsymbol{\Psi}_0^{-1}(\boldsymbol{\alpha}-\boldsymbol{\alpha}_0)}$$

**Regression Coefficients**

Let  $\boldsymbol{\beta} = (\beta_1, \dots, \beta_k)'$  be the vector of regression coefficients.

**Uniform Prior** The joint prior density is given by

$$p(\beta_1, \dots, \beta_k) \propto 1, \forall -\infty < \beta_i < \infty$$

This prior is improper, but the posterior distributions for  $\boldsymbol{\beta}$  are proper.

**Normal Prior** Assume  $\boldsymbol{\beta}$  has a multivariate normal prior with mean vector  $\boldsymbol{\beta}_0$  and covariance matrix  $\boldsymbol{\Sigma}_0$ . The joint prior density is given by

$$p(\boldsymbol{\beta}) \propto e^{-\frac{1}{2}(\boldsymbol{\beta}-\boldsymbol{\beta}_0)'\boldsymbol{\Sigma}_0^{-1}(\boldsymbol{\beta}-\boldsymbol{\beta}_0)}$$

**Joint Multivariate Normal Prior for Log-Hazards and Regression Coefficients** Assume  $(\boldsymbol{\alpha}', \boldsymbol{\beta}')$  has a multivariate normal prior with mean vector  $(\boldsymbol{\alpha}'_0, \boldsymbol{\beta}'_0)'$  and covariance matrix  $\boldsymbol{\Phi}_0$ . The joint prior density is given by

$$p(\boldsymbol{\alpha}, \boldsymbol{\beta}) \propto e^{-\frac{1}{2}[(\boldsymbol{\alpha}-\boldsymbol{\alpha}_0)', (\boldsymbol{\beta}-\boldsymbol{\beta}_0)']\boldsymbol{\Phi}_0^{-1}[(\boldsymbol{\alpha}-\boldsymbol{\alpha}_0)', (\boldsymbol{\beta}-\boldsymbol{\beta}_0)']}$$

**Zellner's g-Prior** Assume  $\boldsymbol{\beta}$  has a multivariate normal prior with mean vector  $\mathbf{0}$  and covariance matrix  $(g\mathbf{X}'\mathbf{X})^{-1}$ , where  $\mathbf{X}$  is the design matrix and  $g$  is either a constant or it follows a gamma prior with density  $f(\tau) = \frac{b(b\tau)^{a-1}e^{-b\tau}}{\Gamma(a)}$  where  $a$  and  $b$  are the SHAPE= and ISCALE= parameters. Let  $k$  be the rank of  $\mathbf{X}$ . The joint prior density with  $g$  being a constant  $c$  is given by

$$p(\boldsymbol{\beta}) \propto c^{\frac{k}{2}} e^{-\frac{1}{2}\boldsymbol{\beta}'(c\mathbf{X}'\mathbf{X})^{-1}\boldsymbol{\beta}}$$

The joint prior density with  $g$  having a gamma prior is given by

$$p(\boldsymbol{\beta}, \tau) \propto \tau^{\frac{k}{2}} e^{-\frac{1}{2}\boldsymbol{\beta}'(\tau\mathbf{X}'\mathbf{X})^{-1}\boldsymbol{\beta}} \frac{b(b\tau)^{a-1}e^{-b\tau}}{\Gamma(a)}$$

**Dispersion Parameter for Frailty Model**

**Improper Prior** The density is

$$p(\theta) = \frac{1}{\theta}$$

**Inverse Gamma Prior** The inverse gamma distribution  $IG(a, b)$  has a density

$$p(\theta|a, b) = \frac{b^a \theta^{-(a+1)} e^{-\frac{b}{\theta}}}{\Gamma(a)}$$

where  $a$  and  $b$  are the SHAPE= and SCALE= parameters.

**Gamma Prior** The gamma distribution  $G(a, b)$  has a density

$$p(\theta|a, b) = \frac{b^a \theta^{a-1} e^{-b\theta}}{\Gamma(a)}$$

where  $a$  and  $b$  are the SHAPE= and ISCALE= parameters.

**Posterior Distribution**

Denote the observed data by  $D$ .

**Cox Model**

$$\pi(\boldsymbol{\beta}|D) \propto \underbrace{L(D|\boldsymbol{\beta})}_{\text{partial likelihood}} \overbrace{p(\boldsymbol{\beta})}^{\text{prior}}$$

**Frailty Model**

Based on the framework of Sargent (1998),

$$\pi(\boldsymbol{\beta}, \boldsymbol{\gamma}, \theta|D) \propto \underbrace{L(D|\boldsymbol{\beta}, \boldsymbol{\gamma})}_{\text{partial likelihood}} \overbrace{g(\boldsymbol{\gamma}|\theta)}^{\text{random effects}} \underbrace{p(\boldsymbol{\beta})p(\theta)}_{\text{priors}}$$

where the joint density of the random effects  $\boldsymbol{\gamma} = (\gamma_1, \dots, \gamma_s)'$  is given by

$$g(\boldsymbol{\gamma}|\theta) \propto \begin{cases} \prod_i \exp\left(\frac{\gamma_i}{\theta}\right) \exp\left(-\exp\left(\frac{\gamma_i}{\theta}\right)\right) & \text{gamma frailty} \\ \prod_i \exp\left(-\frac{\gamma_i^2}{2\theta}\right) & \text{lognormal frailty} \end{cases}$$

**Piecewise Exponential Model****Hazard Parameters**

$$\pi(\boldsymbol{\lambda}, \boldsymbol{\beta} | D) \propto L_H(D | \boldsymbol{\lambda}, \boldsymbol{\beta}) p(\boldsymbol{\lambda}) p(\boldsymbol{\beta})$$

where  $L_H(D | \boldsymbol{\lambda}, \boldsymbol{\beta})$  is the likelihood function with hazards  $\boldsymbol{\lambda}$  and regression coefficients  $\boldsymbol{\beta}$  as parameters.

**Log-Hazard Parameters**

$$\pi(\boldsymbol{\alpha}, \boldsymbol{\beta} | D) \propto \begin{cases} L_{LH}(D | \boldsymbol{\alpha}, \boldsymbol{\beta}) p(\boldsymbol{\alpha}, \boldsymbol{\beta}) & \text{if } (\boldsymbol{\alpha}', \boldsymbol{\beta}')' \sim \text{MVN} \\ L_{LH}(D | \boldsymbol{\alpha}, \boldsymbol{\beta}) p(\boldsymbol{\alpha}) p(\boldsymbol{\beta}) & \text{otherwise} \end{cases}$$

where  $L_{LH}(D | \boldsymbol{\alpha}, \boldsymbol{\beta})$  is the likelihood function with log-hazards  $\boldsymbol{\alpha}$  and regression coefficients  $\boldsymbol{\beta}$  as parameters.

**Sampling from the Posterior Distribution**

For the Gibbs sampler, PROC PHREG uses the ARMS (adaptive rejection Metropolis sampling) algorithm of Gilks, Best, and Tan (1995) to sample from the full conditionals. This is the default sampling scheme. Alternatively, you can request the random walk Metropolis (RWM) algorithm to sample an entire parameter vector from the posterior distribution. For a general discussion of these algorithms, see section “[Markov Chain Monte Carlo Method](#)” on page 133.

You can output these posterior samples into a SAS data set by using the OUTPOST= option in the BAYES statement, or you can use the following SAS statement to output the posterior samples into the SAS data set Post:

```
ods output PosteriorSample=Post;
```

The output data set also includes the variables LogLike and LogPost, which represent the log of the likelihood and the log of the posterior log density, respectively.

Let  $\boldsymbol{\theta} = (\theta_1, \dots, \theta_k)'$  be the parameter vector. For the Cox model, the  $\theta_i$ 's are the regression coefficients  $\beta_i$ 's, and for the piecewise constant baseline hazard model, the  $\theta_i$ 's consist of the baseline hazards  $\lambda_i$ 's (or log baseline hazards  $\alpha_i$ 's) and the regression coefficients  $\beta_j$ 's. Let  $L(D | \boldsymbol{\theta})$  be the likelihood function, where  $D$  is the observed data. Note that for the Cox model, the likelihood contains the infinite-dimensional baseline hazard function, and the gamma process is perhaps the most commonly used prior process (Ibrahim, Chen, and Sinha 2001). However, Sinha, Ibrahim, and Chen (2003) justify using the partial likelihood as the likelihood function for the Bayesian analysis. Let  $p(\boldsymbol{\theta})$  be the prior distribution. The posterior  $f\pi(\boldsymbol{\theta} | D)$  is proportional to the joint distribution  $L(D | \boldsymbol{\theta}) p(\boldsymbol{\theta})$ .

**Gibbs Sampler**

The full conditional distribution of  $\theta_i$  is proportional to the joint distribution; that is,

$$\pi(\theta_i | \theta_j, i \neq j, D) \propto L(D | \boldsymbol{\theta}) p(\boldsymbol{\theta})$$

For example, the one-dimensional conditional distribution of  $\theta_1$ , given  $\theta_j = \theta_j^*, 2 \leq j \leq k$ , is computed as

$$\pi(\theta_1 | \theta_j = \theta_j^*, 2 \leq j \leq k, D) = L(D | \boldsymbol{\theta} = (\theta_1, \theta_2^*, \dots, \theta_k^*)') p(\boldsymbol{\theta} = (\theta_1, \theta_2^*, \dots, \theta_k^*)')$$

Suppose you have a set of arbitrary starting values  $\{\theta_1^{(0)}, \dots, \theta_k^{(0)}\}$ . Using the ARMS algorithm, an iteration of the Gibbs sampler consists of the following:

- draw  $\theta_1^{(1)}$  from  $\pi(\theta_1|\theta_2^{(0)}, \dots, \theta_k^{(0)}, D)$
- draw  $\theta_2^{(1)}$  from  $\pi(\theta_2|\theta_1^{(1)}, \theta_3^{(0)}, \dots, \theta_k^{(0)}, D)$
- $\vdots$
- draw  $\theta_k^{(1)}$  from  $\pi(\theta_k|\theta_1^{(1)}, \dots, \theta_{k-1}^{(1)}, D)$

After one iteration, you have  $\{\theta_1^{(1)}, \dots, \theta_k^{(1)}\}$ . After  $n$  iterations, you have  $\{\theta_1^{(n)}, \dots, \theta_k^{(n)}\}$ . Cumulatively, a chain of  $n$  samples is obtained.

### Random Walk Metropolis Algorithm

PROC PHREG uses a multivariate normal proposal distribution  $q(\cdot|\theta)$  centered at  $\theta$ . With an initial parameter vector  $\theta^{(0)}$ , a new sample  $\theta^{(1)}$  is obtained as follows:

- sample  $\theta^*$  from  $q(\cdot|\theta^{(0)})$
- calculate the quantity  $r = \min \left\{ \frac{\pi(\theta^*|D)}{\pi(\theta^{(0)}|D)}, 1 \right\}$
- sample  $u$  from the uniform distribution  $U(0, 1)$
- set  $\theta^{(1)} = \theta^*$  if  $u < r$ ; otherwise set  $\theta^{(1)} = \theta^{(0)}$

With  $\theta^{(1)}$  taking the role of  $\theta^{(0)}$ , the previous steps are repeated to generate the next sample  $\theta^{(2)}$ . After  $n$  iterations, a chain of  $n$  samples  $\{\theta^{(1)}, \dots, \theta^{(n)}\}$  is obtained.

### Starting Values of the Markov Chains

When the BAYES statement is specified, PROC PHREG generates one Markov chain that contains the approximate posterior samples of the model parameters. Additional chains are produced when the Gelman-Rubin diagnostics are requested. Starting values (initial values) can be specified in the INITIAL= data set in the BAYES statement. If the INITIAL= option is not specified, PROC PHREG picks its own initial values for the chains based on the maximum likelihood estimates of  $\theta$  and the prior information of  $\theta$ .

Denote  $[x]$  as the integral value of  $x$ .

### Constant Baseline Hazards $\lambda_i$ 's

For the first chain that the summary statistics and diagnostics are based on, the initial values are

$$\lambda_i^{(0)} = \hat{\lambda}_i$$

For subsequent chains, the starting values are picked in two different ways according to the total number of chains specified. If the total number of chains specified is less than or equal to 10, initial values of the  $r$ th chain ( $2 \leq r \leq 10$ ) are given by

$$\lambda_i^{(0)} = \hat{\lambda}_i e^{\pm \left( \left[ \frac{r}{2} \right] + 2 \right) \hat{s}(\hat{\lambda}_i)}$$



with the plus sign for odd  $r$  and minus sign for even  $r$ . If the total number of chains is greater than 10, initial values are picked at random over a wide range of values. Let  $u_i$  be a uniform random number between 0 and 1; the initial value for  $\lambda_i$  is given by

$$\lambda_i^{(0)} = \hat{\lambda}_i e^{16(u_i - 0.5)\hat{s}(\hat{\lambda}_i)}$$

### Regression Coefficients and Log-Hazard Parameters $\theta_i$ 's

The  $\theta_i$ 's are the regression coefficients  $\beta_i$ 's, and in the piecewise exponential model, include the log-hazard parameters  $\alpha_i$ 's. For the first chain that the summary statistics and regression diagnostics are based on, the initial values are

$$\theta_i^{(0)} = \hat{\theta}_i$$

If the number of chains requested is less than or equal to 10, initial values for the  $r$ th chain ( $2 \leq r \leq 10$ ) are given by

$$\theta_i^{(0)} = \hat{\theta}_i \pm \left(2 + \left\lceil \frac{r}{2} \right\rceil\right) \hat{s}(\hat{\theta}_i)$$

with the plus sign for odd  $r$  and minus sign for even  $r$ . When there are more than 10 chains, the initial value for the  $\theta_i$  is picked at random over the range  $(\hat{\theta}_i - 8\hat{s}(\hat{\theta}_i), \hat{\theta}_i + 8\hat{s}(\hat{\theta}_i))$ ; that is,

$$\theta_i^{(0)} = \hat{\theta}_i + 16(u_i - 0.5)\hat{s}(\hat{\theta}_i)$$

where  $u_i$  is a uniform random number between 0 and 1.

### Fit Statistics

Denote the observed data by  $D$ . Let  $\boldsymbol{\theta}$  be the vector of parameters of length  $k$ . Let  $L(D|\boldsymbol{\theta})$  be the likelihood. The deviance information criterion (DIC) proposed in Spiegelhalter et al. (2002) is a Bayesian model assessment tool. Let  $\text{Dev}(\boldsymbol{\theta}) = -2 \log L(D|\boldsymbol{\theta})$ . Let  $\overline{\text{Dev}(\boldsymbol{\theta})}$  and  $\bar{\boldsymbol{\theta}}$  be the corresponding posterior means of  $\text{Dev}(\boldsymbol{\theta})$  and  $\boldsymbol{\theta}$ , respectively. The deviance information criterion is computed as

$$\text{DIC} = 2\overline{\text{Dev}(\boldsymbol{\theta})} - \text{Dev}(\bar{\boldsymbol{\theta}})$$

Also computed is

$$pD = \overline{\text{Dev}(\boldsymbol{\theta})} - \text{Dev}(\bar{\boldsymbol{\theta}})$$

where  $pD$  is interpreted as the effective number of parameters.

Note that  $\text{Dev}(\boldsymbol{\theta})$  defined here does not have the standardizing term as in the section “Deviance Information Criterion (DIC)” on page 155. Nevertheless, the DIC calculated here is still useful for variable selection.

### Posterior Distribution for Quantities of Interest

Let  $\boldsymbol{\theta} = (\theta_1, \dots, \theta_k)'$  be the parameter vector. For the Cox model, the  $\theta_i$ 's are the regression coefficients  $\beta_i$ 's; for the piecewise constant baseline hazard model, the  $\theta_i$ 's consist of the baseline hazards  $\lambda_i$ 's (or log baseline hazards  $\alpha_i$ 's) and the regression coefficients  $\beta_j$ 's. Let  $\mathcal{S} = \{\boldsymbol{\theta}^{(r)}, r = 1, \dots, N\}$  be the chain that represents the posterior distribution for  $\boldsymbol{\theta}$ .

Consider a quantity of interest  $\tau$  that can be expressed as a function  $f(\boldsymbol{\theta})$  of the parameter vector  $\boldsymbol{\theta}$ . You can construct the posterior distribution of  $\tau$  by evaluating the function  $f(\boldsymbol{\theta}^{(r)})$  for each  $\boldsymbol{\theta}^{(r)}$  in  $\mathcal{S}$ . The posterior chain for  $\tau$  is  $\{f(\boldsymbol{\theta}^{(r)}), r = 1, \dots, N\}$ . Summary statistics such as mean, standard deviation, percentiles, and credible intervals are used to describe the posterior distribution of  $\tau$ .

### Hazard Ratio

As shown in the section “Hazard Ratios” on page 5619, a log-hazard ratio is a linear combination of the regression coefficients. Let  $\mathbf{h}$  be the vector of linear coefficients. The posterior sample for this hazard ratio is the set  $\{\exp(\mathbf{h}'\boldsymbol{\beta}^{(r)}), r = 1, \dots, N\}$ .

### Survival Distribution

Let  $\mathbf{x}$  be a covariate vector of interest.

**Cox Model** Let  $\{(t_i, \mathbf{z}_i, \delta_i), i = 1, 2, \dots, n\}$  be the observed data. Define

$$Y_i(t) = \begin{cases} 1 & t < t_i \\ 0 & \text{otherwise} \end{cases}$$

Consider the  $r$ th draw  $\boldsymbol{\beta}^{(r)}$  of  $\mathcal{S}$ . The baseline cumulative hazard function at time  $t$  is given by

$$H_0(t|\boldsymbol{\beta}^{(r)}) = \sum_{i:t_i \leq t} \frac{\delta_i}{\sum_{l=1}^n Y_l(t_i) \exp(\mathbf{z}_l' \boldsymbol{\beta}^{(r)})}$$

For the given covariate vector  $\mathbf{x}$ , the cumulative hazard function at time  $t$  is

$$H(t; \mathbf{x}|\boldsymbol{\beta}^{(r)}) = H_0(t|\boldsymbol{\beta}^{(r)}) \exp(\mathbf{x}' \boldsymbol{\beta}^{(r)})$$

and the survival function at time  $t$  is

$$S(t; \mathbf{x}|\boldsymbol{\beta}^{(r)}) = \exp[-H^{(r)}(t; \mathbf{x}|\boldsymbol{\beta}^{(r)})]$$

**Piecewise Exponential Model** Let  $0 = a_0 < a_1 < \dots < a_J < \infty$  be a partition of the time axis. Consider the  $r$ th draw  $\boldsymbol{\theta}^{(r)}$  in  $\mathcal{S}$ , where  $\boldsymbol{\theta}^{(r)}$  consists of  $\boldsymbol{\lambda}^{(r)} = (\lambda_1^{(r)}, \dots, \lambda_J^{(r)})'$  and  $\boldsymbol{\beta}^{(r)}$ . The baseline cumulative hazard function at time  $t$  is

$$H_0(t|\boldsymbol{\lambda}^{(r)}) = \sum_{j=1}^J \lambda_j^{(r)} \Delta_j(t)$$

where

$$\Delta_j(t) = \begin{cases} 0 & t < a_{j-1} \\ t - a_{j-1} & a_{j-1} \leq t < a_j \\ a_j - a_{j-1} & t \geq a_j \end{cases}$$

For the given covariate vector  $\mathbf{x}$ , the cumulative hazard function at time  $t$  is

$$H(t; \mathbf{x}|\boldsymbol{\lambda}^{(r)}, \boldsymbol{\beta}^{(r)}) = H_0(t|\boldsymbol{\lambda}^{(r)}) \exp(\mathbf{x}' \boldsymbol{\beta}^{(r)})$$

and the survival function at time  $t$  is

$$S(t; \mathbf{x}|\boldsymbol{\lambda}^{(r)}, \boldsymbol{\beta}^{(r)}) = \exp[-H(t; \mathbf{x}|\boldsymbol{\lambda}^{(r)}, \boldsymbol{\beta}^{(r)})]$$

---

## Computational Resources

Let  $n$  be the number of observations in a BY group. Let  $p$  be the number of explanatory variables. The minimum working space (in bytes) needed to process the BY group is

$$\max\{12n, 24p^2 + 160p\}$$

Extra memory is needed for certain TIES= options. Let  $k$  be the maximum multiplicity of tied times. The TIES=DISCRETE option requires extra memory (in bytes) of

$$4k(p^2 + 4p)$$

The TIES=EXACT option requires extra memory (in bytes) of

$$24(k^2 + 5k)$$

If sufficient space is available, the input data are also kept in memory. Otherwise, the input data are reread from the utility file for each evaluation of the likelihood function and its derivatives, with the resulting execution time substantially increased.

---

## Input and Output Data Sets

### OUTEST= Output Data Set

The OUTEST= data set contains one observation for each BY group containing the maximum likelihood estimates of the regression coefficients. If you also use the COVOUT option in the PROC PHREG statement, there are additional observations containing the rows of the estimated covariance matrix. If you specify SELECTION=FORWARD, BACKWARD, or STEPWISE, only the estimates of the parameters and covariance matrix for the final model are output to the OUTEST= data set.

#### *Variables in the OUTEST= Data Set*

The OUTEST= data set contains the following variables:

- any BY variables specified
- `_TIES_`, a character variable of length 8 with four possible values: BRESLOW, DISCRETE, EFRON, and EXACT. These are the four values of the TIES= option in the MODEL statement.
- `_TYPE_`, a character variable of length 8 with two possible values: PARMS for parameter estimates or COV for covariance estimates. If both the COVM and COVS options are specified in the PROC PHREG statement along with the COVOUT option, `_TYPE_='COVM'` for the model-based covariance estimates and `_TYPE_='COVS'` for the robust sandwich covariance estimates.
- `_STATUS_`, a character variable indicating whether the estimates have converged
- `_NAME_`, a character variable containing the name of the TIME variable for the row of parameter estimates and the name of each explanatory variable to label the rows of covariance estimates

- one variable for each regression coefficient and one variable for the offset variable if the **OFFSET=** option is specified. If an explanatory variable is not included in the final model in a variable selection process, the corresponding parameter estimates and covariances are set to missing.
- **\_LNLIKE\_**, a numeric variable containing the last computed value of the log likelihood

### **Parameter Names in the **OUTEST=** Data Set**

For continuous explanatory variables, the names of the parameters are the same as the corresponding variables. For CLASS variables, the parameter names are obtained by concatenating the corresponding CLASS variable name with the CLASS category; see the **PARAM=** option in the **CLASS** statement for more details. For interaction and nested effects, the parameter names are created by concatenating the names of each component effect.

### **INEST= Input Data Set**

You can specify starting values for the maximum likelihood iterative algorithm in the **INEST=** data set. The **INEST=** data set has the same structure as the **OUTEST=** data set but is not required to have all the variables or observations that appear in the **OUTEST=** data set.

The **INEST=** data set must contain variables that represent the regression coefficients of the model. If BY processing is used, the **INEST=** data set should also include the BY variables, and there must be one observation for each BY group. If the **INEST=** data set also contains the **\_TYPE\_** variable, only observations with **\_TYPE\_** value 'PARMS' are used as starting values.

### **OUT= Output Data Set in the **OUTPUT** Statement**

The **OUT=** data set in the **OUTPUT** statement contains all the variables in the input data set, along with statistics you request by specifying *keyword=name* options. The new variables contain a variety of diagnostics that are calculated for each observation in the input data set.

### **OUT= Output Data Set in the **BASELINE** Statement**

The **OUT=** data set in the **BASELINE** statement contains all the variables in the **COVARIATES=** data set, along with statistics you request by specifying *keyword=name* options. For unstratified input data, there are  $1 + n$  observations in the **OUT=** data set for each observation in the **COVARIATES=** data set, where  $n$  is the number of distinct event times in the input data. For input data that are stratified into  $k$  strata, with  $n_i$  distinct events in the  $i$ th stratum,  $i = 1, \dots, k$ , there are  $1+n_i$  observations for the  $i$ th stratum in the **OUT=** data set for each observation in the **COVARIATES=** data set.

### **OUTDIFF= Output Data Set in the **BASELINE** Statement**

The **OUTDIFF=** data set contains the differences of the direct adjusted survival probabilities between two treatments or two strata and their standard errors.

### **OUTPOST= Output Data Set in the **BAYES** Statement**

The **OUTPOST=** data set contains the generated posterior samples. There are  $3+n$  variables, where  $n$  is the number of model parameters. The variable **Iteration** represents the iteration number, the variable **LogLike** contains the log-likelihood values, and the variable **LogPost** contains the log-posterior-density values. The other  $n$  variables represent the draws of the Markov chain for the model parameters.

---

## Displayed Output

If you use the NOPRINT option in the PROC PHREG statement, the procedure does not display any output. Otherwise, PROC PHREG displays results of the analysis in a collection of tables. The tables are listed separately for the maximum likelihood analysis and for the Bayesian analysis.

### Maximum Likelihood Analysis Displayed Output

#### ***Model Information***

The “Model Information” table displays the two-level name of the input data set, the name and label of the failure time variable, the name and label of the censoring variable and the values indicating censored times, the model (either the Cox model or the piecewise constant baseline hazard model), the name and label of the OFFSET variable, the name and label of the FREQ variable, the name and label of the WEIGHT variable, and the method of handling ties in the failure time for the Cox model. The ODS name of the “Model Information” table is ModelInfo.

#### ***Number of Observations***

The “Number of Observations” table displays the number of observations read and used in the analysis. The ODS name of the “Number of Observations” is NObs.

#### ***Class Level Information***

The “Class Level Information” table is displayed when there are CLASS variables in the model. The table lists the categories of every CLASS variable that is used in the model and the corresponding design variable values. The ODS name of the “Class Level Information” table is ClassLevelInfo.

#### ***Class Level Information for Random Effects***

The “Class Level Information for Random Effects” table is displayed when the RANDOM statement is specified. The table lists the categories of the classification variable specified in the RANDOM statement. The ODS name of the “Class Level Information for Random Effects” table is ClassLevelInfoR.

#### ***Summary of the Number of Event and Censored Values***

The “Summary of the Number of Event and Censored Values” table displays, for each stratum, the breakdown of the number of events and censored values. The ODS name of the “Summary of the Number of Event and Censored Values” table is CensoredSummary.

#### ***Risk Sets Information***

The “Risk Sets Information” table is displayed if you specify the ATRISK option in the PROC PHREG statement. The table displays, for each event time, the number of units at-risk and the number of units that experience the event. The ODS name of the “Risk Sets Information” table is RiskSetInfo.

#### ***Descriptive Statistics for Continuous Explanatory Variables***

The “Simple Statistics for Continuous Explanatory Variables” table is displayed when you specify the SIMPLE option in the PROC PHREG statement. The table contains, for each stratum, the mean, standard deviation, and minimum and maximum for each continuous explanatory variable in the MODEL statement. For ODS purposes, the name of the “Descriptive Statistics for Continuous Explanatory Variables” table is “SimpleStatistics.”

**Frequency Distribution of CLASS Variables**

The “Frequency Distribution of CLASS Variables” table is displayed if you specify the SIMPLE option in the PROC PHREG statement and there are CLASS variables in the model. The table lists the frequency of the levels of the CLASS variables. The ODS name of the “Frequency Distribution of CLASS Variables” table is ClassLevelFreq.

**Maximum Likelihood Iteration History**

The “Maximum Likelihood Iteration History” table is displayed if you specify the ITPRINT option in the MODEL statement. The table contains the iteration number, ridge value or step size, log likelihood, and parameter estimates at each iteration. The ODS name of the “Maximum Likelihood Iteration History” table is IterHistory.

**Gradient of Last Iteration**

The “Gradient of Last Iteration” table is displayed if you specify the ITPRINT option in the MODEL statement. The ODS name of the “Gradient of Last Iteration” table is LastGradient.

**Convergence Status**

The “Convergence Status” table displays the convergence status of the Newton-Raphson maximization. The ODS name of the “Convergence Status” table is ConvergenceStatus.

**Model Fit Statistics**

The “Model Fit Statistics” table displays the values of  $-2 \log$  likelihood for the null model and the fitted model, the AIC, and SBC. The ODS name of the “Model Fit Statistics” table is FitStatistics.

**Covariance Parameter Estimates**

The “Covariance Parameter Estimates” table displays the estimate of the variance parameter of the random effect and the standard error estimate of the variance parameter estimator. The ODS name of the “Covariance Parameter Estimates” table is CovParms.

**Testing Global Null Hypothesis: BETA=0**

The “Testing Global Null Hypothesis: BETA=0” table displays results of the likelihood ratio test, the score test, and the Wald test for testing the hypothesis that all parameters are zero. For the frailty model, the score test is not displayed and an adjusted degrees of freedom is used (see the section “Wald-Type Tests for Penalized Models” on page 5653 for more information.) For ODS purpose, the name of the “Testing Global Null Hypothesis: BETA=0” table is “GlobalTests.”

**Likelihood Ratio Statistics for Type 1 Analysis**

The “Likelihood Ratio Statistics for Type 1 Analysis” table is displayed if the TYPE1 option is specified in the MODEL statement. The table displays the degrees of freedom, the likelihood ratio chi-square statistic, and the  $p$ -value for each effect in the model. The ODS name of “Likelihood Ratio Statistics for Type 1 Analysis” is Type1.

**Type 3 Tests**

The “Type 3 Tests” table is displayed if the model contains a CLASS variable or if the TYPE3 option is specified in the MODEL statement. The table displays, for each specified statistic, the Type 3 chi-square, the degrees of freedom, and the  $p$ -value for each effect in the model. For the frailty model, the table also

displays the adjusted Wald-type test results (see the section “Wald-Type Tests for Penalized Models” on page 5653 for details.) The ODS name of “Type 3 Tests” is Type3.

### ***Analysis of Maximum Likelihood Estimates***

The “Analysis of Maximum Likelihood Estimates” table displays the maximum likelihood estimate of the parameter; the estimated standard error, computed as the square root of the corresponding diagonal element of the estimated covariance matrix; the ratio of the robust standard error estimate to the model-based standard error estimate if you specify the COVS option in the PROC PHREG statement; the Wald Chi-Square statistic, computed as the square of the parameter estimate divided by its standard error estimate; the degrees of freedom of the Wald chi-square statistic, which has a value of 1 unless the corresponding parameter is redundant or infinite, in which case the value is 0; the  $p$ -value of the Wald chi-square statistic with respect to a chi-square distribution with one degree of freedom; the hazard ratio estimate; and the confidence limits for the hazard ratio if you specified the RISKLIMITS option in the MODEL statement. The ODS name of the “Analysis of Maximum Likelihood Estimates” table is ParameterEstimates.

### ***Solution for Random Effects***

The “Solution for Random Effects” table displays the BLUP estimates of the random effects, the estimated standard errors, the confidence intervals for the random effects, the exponentiated values of the BLUP estimates, and confidence intervals for the exponentiated random effects. The ODS name of the “Solution for Random Effects” table is SolutionR.

### ***Regression Models Selected by Score Criterion***

The “Regression Models Selected by Score Criterion” table is displayed if you specify SELECTION=SCORE in the MODEL statement. The table contains the number of explanatory variables in each model, the score chi-square statistic, and the names of the variables included in the model. The ODS name of the “Regression Models Selected by Score Criterion” table is BestSubsets.

### ***Analysis of Effects Eligible for Entry***

The “Analysis of Effects Eligible for Entry” table is displayed if you use the FORWARD or STEPWISE selection method and you specify the DETAILS option in the MODEL statement. The table contains the score chi-square statistic for testing the significance of each variable not in the model (after adjusting for the variables already in the model), and the  $p$ -value of the chi-square statistic with respect to a chi-square distribution with one degree of freedom. This table is produced before a variable is selected for entry in a forward selection step. The ODS name of the “Analysis of Effects Eligible for Entry” table is EffectsToEntry.

### ***Analysis of Effects Eligible for Removal***

The “Analysis of Effects Eligible for Removal” table is displayed if you use the BACKWARD or STEPWISE selection method and you specify the DETAILS option in the MODEL statement. The table contains the Wald chi-square statistic for testing the significance of each candidate effect for removal, the degrees of freedom of the Wald chi-square, and the corresponding  $p$ -value. This table is produced before an effect is selected for removal. The ODS name of the “Analysis of Effects Eligible for Removal” table is EffectsToRemoval.

### ***Summary of Backward Elimination***

The “Summary of Backward Elimination” table is displayed if you specify the SELECTION=BACKWARD option in the MODEL statement. The table contains the step number, the effects removed at each step, the



corresponding chi-square statistic, the degrees of freedom, and the  $p$ -value. For ODS purpose, the name of the “Summary of Backward Elimination” table is “ModelBuildingSummary.”

### **Summary of Forward Selection**

The “Summary of Forward Selection” table is displayed if you specify the SELECTION=FORWARD option in the MODEL statement. The table contains the step number, the effects entered at each step, the corresponding chi-square statistic, the degrees of freedom, and the  $p$ -value. For ODS purpose, the name of the “Summary of Forward Selection” table is “ModelBuildingSummary.”

### **Summary of Stepwise Selection**

The “Summary of Stepwise Selection” table is displayed if you specify SELECTION=STEPWISE is specified in the MODEL statement. The table contains the step number, the effects entered or removed at each step, the corresponding chi-square statistic, the degrees of freedom, and the corresponding  $p$ -value. For ODS purpose, the name of the “Summary of Stepwise Selection” table is “ModelBuildingSummary.”

### **Covariance Matrix**

The “Covariance Matrix” table is displayed if you specify the COVB option in the MODEL statement. The table contains the estimated covariance matrix for the parameter estimates. For ODS purposes, the name of the “Covariance Matrix” table is “CovB.”

### **Correlation Matrix**

The “Correlation Matrix” table is displayed if you specify the COVB option in the MODEL statement. The table contains the estimated correlation matrix for the parameter estimates. For ODS purposes, the name of the “Correlation Matrix” table is “CorrB.”

### **Hazard Ratios for *label***

The “Hazard Ratios for *label*” table is displayed if you specify the HAZARDRATIO statement. The table displays the estimate and confidence limits for each hazard ratio. The ODS name of the “Hazard Ratios for *label*” table is HazardRatios.

### **Coefficients of Contrast *label***

The “Coefficients of Contrast *label*” table is displayed if you specify the E option in the CONTRAST statement. The table displays the parameter names and the corresponding coefficients of each row of contrast *label*. The ODS name of the “Coefficients of Contrast *label*” table is ContrastCoeff.

### **Contrast Test Results**

The “Contrast Test Results” table is displayed if you specify the CONTRAST statement. The table displays the degrees of freedom, test statistics, and the  $p$ -values for testing each contrast. The ODS name of the “Contrast Test Results” table is ContrastTest.

### **Contrast Estimation and Testing Results by Row**

The “Contrast Estimation and Testing Results by Row” table is displayed if you specify the ESTIMATE option in the CONTRAST statement. The table displays, for each row, the estimate of the linear function of the coefficients, its standard error, and the confidence limits for the linear function. The ODS name of the “Contrast Estimation and Testing Results by Row” table is ContrastEstimate.



**Linear Coefficients for *label***

The “Linear Coefficients *label*” table is displayed if you specify the E option in the TEST statement with *label* being the TEST statement label. The table contains the coefficients and constants of the linear hypothesis. For ODS purposes, the name of the “Linear Coefficients for *label*” table is “TestCoeff.”

**L[cov(b)]L' and Lb-c**

The “L[cov(b)]L' and Lb-c” table is displayed if you specified the PRINT option in a TEST statement with *label* being the TEST statement label. The table displays the intermediate calculations of the Wald test. The ODS name of the “L[cov(b)]L' and Lb-c” table is TestPrint1.

**Ginv(L[cov(b)]L') and Ginv(L[cov(b)]L')(Lb-c)**

The “Ginv(L[cov(b)]L') and Ginv(L[cov(b)]L')(Lb-c)” table is displayed if you specified the PRINT option in a TEST statement with *label* being the TEST statement label. The table displays the intermediate calculations of the Wald test. The ODS name of the “Ginv(L[cov(b)]L') and Ginv(L[cov(b)]L')(Lb-c)” table is TestPrint2.

***label* Test Results**

The “*label* Test Results” table is displayed if you specify a TEST statement with *label* being the TEST statement label. The table contains the Wald chi-square statistic, the degrees of freedom, and the *p*-value. The ODS name of “*label* Test Results” table is TestStmts.

**Average Effect for *label***

The “Average Effect for *label*” table is displayed if the AVERAGE option is specified in a TEST statement with *label* being the TEST statement label. The table contains the weighted average of the parameter estimates for the variables in the TEST statement, the estimated standard error, the z-score, and the *p*-value. The ODS name of the “Average Effect for *label*” is TestAverage.

**Reference Set of Covariates for Plotting**

The “Reference Set of Covariates for Plotting” table is displayed if the PLOTS= option is requested without specifying the COVARIATES= data set in the BASELINE statement. The tables contains the values of the covariates for the reference set, where the reference levels are used for the CLASS variables and the sample averages for the continuous variables.

**Bayesian Analysis Displayed Output****Model Information**

The “Model Information” table displays the two-level name of the input data set, the name and label of the failure time variable, the name and label of the censoring variable and the values indicating censored times, the model (either the Cox model or the piecewise constant baseline hazard model), the name and label of the OFFSET variable, the name and label of the FREQ variable, the name and label of the WEIGHT variable, the method of handling ties in the failure time, the number of burn-in iterations, the number of iterations after the burn-in, and the number of thinning iterations. The ODS name of the “Model Information” table is ModelInfo.

**Number of Observations**

The “Number of Observations” table displays the number of observations read and used in the analysis. The ODS name of the “Number of Observations” is NObs.

### ***Summary of the Number of Event and Censored Values***

The “Summary of the Number of Event and Censored Values” table displays, for each stratum, the breakdown of the number of events and censored values. This table is not produced if the NONSUMMARY option is specified in the PROC PHREG statement. The ODS name of the “Summary of the Number of Event and Censored Values” table is CensoredSummary.

### ***Descriptive Statistics for Continuous Explanatory Variables***

The “Simple Statistics for Continuous Explanatory Variables” table is displayed when you specify the SIMPLE option in the PROC PHREG statement. The table contains, for each stratum, the mean, standard deviation, and minimum and maximum for each continuous explanatory variable in the MODEL statement. For ODS purposes, the name of the “Descriptive Statistics for Continuous Explanatory Variables” table is “SimpleStatistics.”

### ***Class Level Information***

The “Class Level Information” table is displayed if there are CLASS variables in the model. The table lists the categories of every CLASS variable in the model and the corresponding design variable values. The ODS name of the “Class Level Information” table is ClassLevelInfo.

### ***Frequency Distribution of CLASS Variables***

The “Frequency Distribution of CLASS Variables” table is displayed if you specify the SIMPLE option in the PROC PHREG statement and there are CLASS variables in the model. The table lists the frequency of the levels of the CLASS variables. The ODS name of the “Frequency Distribution of CLASS Variables” table is ClassLevelFreq.

### ***Regression Parameter Information***

The “Regression Parameter Information” table displays the names of the parameters and the corresponding level information of effects containing the CLASS variables. The ODS name of the “Regression Parameter Information” table is ParmInfo.

### ***Constant Baseline Hazard Time Intervals***

The “Constant Baseline Hazard Time Intervals” table displays the intervals of constant baseline hazard and the corresponding numbers of failure times and event times. This table is produced only if you specify the PIECEWISE option in the BAYES statement. The ODS name of the “Constant Baseline Hazard Time Intervals” table is Interval.

### ***Maximum Likelihood Estimates***

The “Maximum Likelihood Estimates” table displays, for each parameter, the maximum likelihood estimate, the estimated standard error, and the 95% confidence limits. The ODS name of the “Maximum Likelihood Estimates” table is ParameterEstimates.

### ***Hazard Prior***

The “Hazard Prior” table is displayed if you specify the PIECEWISE=HAZARD option in the BAYES statement. It describes the prior distribution of the hazard parameters. The ODS name of the “Hazard Prior” table is HazardPrior.

**Log-Hazard Prior**

The “Log-Hazard Prior” table is displayed if you specify the `PIECEWISE=LOGHAZARD` option in the `BAYES` statement. It describes the prior distribution of the log-hazard parameters. The ODS name of the “Log-Hazard Prior” table is `HazardPrior`.

**Coefficient Prior**

The “Coefficient Prior” table displays the prior distribution of the regression coefficients. The ODS name of the “Coefficient Prior” table is `CoeffPrior`.

**Initial Values**

The “Initial Values” table is displayed if you specify the `INITIAL` option in the `BAYES` statement. The table contains the initial values of the parameters for the Gibbs sampling. The ODS name of the “Initial Values” table is `InitialValues`.

**Fit Statistics**

The “Fit Statistics” table displays the DIC and pD statistics for each parameter. The ODS name of the “Fit Statistics” table is `FitStatistics`.

**Posterior Summaries**

The “Posterior Summaries” table displays the size of the posterior sample, the mean, the standard error, and the percentiles for each model parameter. The ODS name of the “Posterior Summaries” table is `PostSummaries`.

**Posterior Intervals**

The “Posterior Intervals” table displays the equal-tail interval and the HPD interval for each model parameter. The ODS name of the “Posterior Intervals” table is `PostIntervals`.

**Posterior Covariance Matrix**

The “Posterior Covariance Matrix” table is produced if you include `COV` in the `SUMMARY=` option in the `BAYES` statement. This table displays the sample covariance of the posterior samples. The ODS name of the “Posterior Covariance Matrix” table is `Cov`.

**Posterior Correlation Matrix**

The “Posterior Correlation Matrix” table is displayed if you include `CORR` in the `SUMMARY=` option in the `BAYES` statement. The table contains the sample correlation of the posterior samples. The ODS name of the “Posterior Correlation Matrix” table is `Corr`.

**Posterior Autocorrelations**

The “Posterior Autocorrelations” table displays the lag 1, lag 5, lag 10, and lag 50 autocorrelations for each parameter. The ODS name of the “Posterior Autocorrelations” table is `AutoCorr`.

**Gelman-Rubin Diagnostics**

The “Gelman-Rubin Diagnostics” table is produced if you include `GELMAN` in the `DIAGNOSTIC=` option in the `BAYES` statement. This table displays the estimate of the potential scale reduction factor and its 97.5% upper confidence limit for each parameter. The ODS name of the “Gelman-Rubin Diagnostics” table is `Gelman`.

**Geweke Diagnostics**

The “Geweke Diagnostics” table displays the Geweke statistic and its  $p$ -value for each parameter. The ODS name of the “Geweke Diagnostics” table is Geweke.

**Raftery-Lewis Diagnostics**

The “Raftery-Lewis Diagnostics” tables is produced if you include RAFTERY in the DIAGNOSTIC= option in the BAYES statement. This table displays the Raftery and Lewis diagnostics for each variable. For ODS purposes, the name of the “Raftery-Diagnostics” table is “Raftery.”

**Heidelberger-Welch Diagnostics**

The “Heidelberger-Welch Diagnostics” table is displayed if you include HEIDELBERGER in the DIAGNOSTIC= option in the BAYES statement. This table describes the results of a stationary test and a halfwidth test for each parameter. The ODS name of the “Heidelberger-Welch Diagnostics” table is Heidelberg.

**Effective Sample Sizes**

The “Effective Sample Sizes” table displays, for each parameter, the effective sample size, the correlation time, and the efficiency. The ODS name of the “Effective Sample Sizes” table is ESS.

**Hazard Ratios for label**

The “Hazard Ratios for *label*” table is displayed if you specify the HAZARDRATIO statement. The table displays the posterior summary for each hazard ratio. The summary includes the mean, standard error, quartiles, and equal-tailed and HPD intervals. The ODS name of the “Hazard Ratios for *label*” table is HazardRatios.

**Reference Set of Covariates for Plotting**

The “Reference Set of Covariates for Plotting” table is displayed if the PLOTS= option is requested without specifying the COVARIATES= data set in the BASELINE statement. The table contains the values of the covariates for the reference set, where the reference levels are used for the CLASS variables and the sample averages for the continuous variables.

---

## ODS Table Names

PROC PHREG assigns a name to each table it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed separately in Table 67.13 for the maximum likelihood analysis and in Table 67.14 for the Bayesian analysis. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

Each of the EFFECT, ESTIMATE, LSMEANS, LSMESTIMATE, and SLICE statements creates ODS tables, which are not listed in Table 67.13 and Table 67.14. For information about these tables, see the corresponding sections of Chapter 19, “Shared Concepts and Topics.”

**Table 67.13** ODS Tables for a Maximum Likelihood Analysis Produced by PROC PHREG

| ODS Table Name | Description           | Statement / Option      |
|----------------|-----------------------|-------------------------|
| BestSubsets    | Best subset selection | MODEL / SELECTION=SCORE |

Table 67.13 continued

| ODS Table Name             | Description                                                  | Statement / Option      |
|----------------------------|--------------------------------------------------------------|-------------------------|
| CensoredSummary            | Summary of event and censored observations                   | Default                 |
| ClassLevelFreq             | Frequency distribution of CLASS variables                    | CLASS, PROC / SIMPLE    |
| ClassLevelInfo             | CLASS variable levels and design variables                   | CLASS                   |
| ClassLevelInfoR            | Class levels for random effects                              | RANDOM                  |
| ContrastCoeff              | L matrix for contrasts                                       | CONTRAST / E            |
| ContrastEstimate           | Individual contrast estimates                                | CONTRAST / ESTIMATE=    |
| ContrastTest               | Wald test for contrasts                                      | CONTRAST                |
| ConvergenceStatus          | Convergence status                                           | Default                 |
| CorrB                      | Estimated correlation matrix of parameter estimators         | MODEL / CORRB           |
| CovB                       | Estimated covariance matrix of parameter estimators          | MODEL / COVB            |
| CovParms                   | Variance estimates of the random effects                     | RANDOM                  |
| EffectsToEnter             | Analysis of effects for entry                                | MODEL / SELECTION=FIS   |
| EffectsToRemove            | Analysis of effects for removal                              | MODEL / SELECTION=BIS   |
| FitStatistics              | Model fit statistics                                         | Default                 |
| FunctionalFormSupTest      | Supremum test for functional form                            | ASSESS / VAR=           |
| GlobalScore                | Global chi-square test                                       | MODEL / NOFIT           |
| GlobalTests                | Tests of the global null hypothesis                          | Default                 |
| HazardRatios               | Hazard ratios and confidence limits                          | HAZARDRATIO             |
| IterHistory                | Iteration history                                            | MODEL / ITPRINT         |
| LastGradient               | Last evaluation of gradient                                  | MODEL / ITPRINT         |
| ModelBuildingSummary       | Summary of model building                                    | MODEL / SELECTION=BIFIS |
| ModelInfo                  | Model information                                            | Default                 |
| NObs                       | Number of observations                                       | Default                 |
| ParameterEstimates         | Maximum likelihood estimates of model parameters             | Default                 |
| ProportionalHazardsSupTest | Supremum test for proportional hazards assumption            | ASSESS / PH             |
| ResidualChiSq              | Residual chi-square                                          | MODEL / SELECTION=FIB   |
| ReferenceSet               | Reference set of covariates for plotting                     | PROC / PLOTS=           |
| RiskSetInfo                | Risk set information                                         | PROC / ATRISK           |
| SimpleStatistics           | Summary statistics of input continuous explanatory variables | PROC / SIMPLE           |
| SolutionR                  | Solutions for random effects                                 | RANDOM / SOLUTION       |
| TestAverage                | Average effect for test                                      | TEST / AVERAGE          |
| TestCoeff                  | Coefficients for linear hypotheses                           | TEST / E                |
| TestPrint1                 | $L[\text{cov}(\mathbf{b})]L'$ and $L\mathbf{b}-\mathbf{c}$   | TEST / PRINT            |

**Table 67.13** *continued*

| ODS Table Name | Description                                                                                                                                                             | Statement / Option    |
|----------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------|
| TestPrint2     | $G_{\text{inv}}(\mathbf{L}[\text{cov}(\mathbf{b})]\mathbf{L}')$ and<br>$G_{\text{inv}}(\mathbf{L}[\text{cov}(\mathbf{b})]\mathbf{L}')(\mathbf{L}\mathbf{b}-\mathbf{c})$ | TEST / PRINT          |
| TestStmtns     | Linear hypotheses testing results                                                                                                                                       | TEST                  |
| Type1          | Type 1 likelihood ratio tests                                                                                                                                           | MODEL / TYPE1         |
| Type3          | Type 3 chi-square tests                                                                                                                                                 | MODEL / TYPE3   CLASS |

**Table 67.14** ODS Table for a Bayesian Analysis Produced by PROC PHREG

| ODS Table Name     | Description                                       | Statement / Option                  |
|--------------------|---------------------------------------------------|-------------------------------------|
| AutoCorr           | Autocorrelations of the posterior samples         | BAYES                               |
| CensoredSummary    | Numbers of the event and censored observations    | PROC                                |
| ClassLevelFreq     | Frequency distribution of CLASS variables         | CLASS, PROC / SIMPLE                |
| ClassLevelInfo     | CLASS variable levels and design variables        | CLASS                               |
| CoeffPrior         | Prior distribution of the regression coefficients | BAYES                               |
| Corr               | Posterior correlation matrix                      | BAYES / SUMMARY=CORR                |
| Cov                | Posterior covariance Matrix                       | BAYES / SUMMARY=COV                 |
| ESS                | Effective sample sizes                            | BAYES / DIAGNOSTICS=ESS             |
| FitStatistics      | Fit statistics                                    | BAYES                               |
| Gelman             | Gelman-Rubin convergence diagnostics              | BAYES /<br>DIAGNOSTICS=GELMAN       |
| Geweke             | Geweke convergence diagnostics                    | BAYES                               |
| HazardPrior        | Prior distribution of the baseline hazards        | BAYES / PIECEWISE                   |
| HazardRatios       | Posterior summary statistics for hazard ratios    | HAZARDRATIO                         |
| Heidelberger       | Heidelberger-Welch convergence diagnostics        | BAYES /<br>DIAGNOSTICS=HEIDELBERGER |
| InitialValues      | Initial values of the Markov chains               | BAYES                               |
| ModelInfo          | Model information                                 | Default                             |
| NObs               | Number of observations                            | Default                             |
| MError             | Monte Carlo standard errors                       | BAYES /<br>DIAGNOSTICS=MCERROR      |
| ParameterEstimates | Maximum likelihood estimates of model parameters  | Default                             |
| ParmInfo           | Names of regression coefficients                  | CLASS,BAYES                         |
| Partition          | Partition of constant baseline hazard intervals   | BAYES / PIECEWISE                   |

**Table 67.14** *continued*

| ODS Table Name   | Description                                                                | Statement / Option                     |
|------------------|----------------------------------------------------------------------------|----------------------------------------|
| PostIntervals    | Equal-tail and high probability density intervals of the posterior samples | BAYES                                  |
| PosteriorSample  | Posterior samples                                                          | BAYES / (for ODS output data set only) |
| PostSummaries    | Summary statistics of the posterior samples                                | BAYES                                  |
| Raftery          | Raftery-Lewis convergence diagnostics                                      | BAYES /<br>DIAGNOSTICS=RAFTERY         |
| ReferenceSet     | Reference set of covariates for plotting                                   | PROC / PLOTS=                          |
| SimpleStatistics | Summary statistics of input continuous explanatory variables               | PROC / SIMPLE                          |

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “[Statistical Graphics Using ODS.](#)”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS.](#)”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “[A Primer on ODS Statistical Graphics](#)” on page 599 in Chapter 21, “[Statistical Graphics Using ODS.](#)”

You can reference every graph produced through ODS Graphics with a name. The names of the graphs that PROC PHREG generates are listed separately in [Table 67.15](#) for the maximum likelihood analysis and in [Table 67.16](#) for the Bayesian analysis. When the ODS Graphics are in effect in a Bayesian analysis, each of the ESTIMATE, LSMEANS, LSMESTIMATE, and SLICE statements can produce plots associated with their analyses. For information of these plots, see the corresponding sections of Chapter 19, “[Shared Concepts and Topics.](#)”

**Table 67.15** Graphs for a Maximum Likelihood Analysis Produced by PROC PHREG

| ODS Graph Name      | Plot Description                              | Statement / Option     |
|---------------------|-----------------------------------------------|------------------------|
| CumhazPlot          | Cumulative hazard function plot               | PROC / PLOTS=CUMHAZ    |
| CumulativeResiduals | Cumulative martingale residual plot           | ASSESS / VAR=          |
| CumResidPanel       | Panel plot of cumulative martingale residuals | ASSESS / VAR=, CRPANEL |
| MCFPlot             | Mean cumulative function plot                 | PROC / PLOTS=MCF       |
| ScoreProcess        | Standardized score process plot               | ASSESS / PH            |
| SurvivalPlot        | Survivor function plot                        | PROC / PLOTS=SURVIVAL  |

**Table 67.16** Graphs for a Bayesian Analysis Produced by PROC PHREG

| ODS Graph Name | Plot Description                                   | Statement / Option                     |
|----------------|----------------------------------------------------|----------------------------------------|
| ADPanel        | Autocorrelation function and density panel         | BAYES / PLOTS=(AUTOCORR DENSITY)       |
| AutocorrPanel  | Autocorrelation function panel                     | BAYES / PLOTS= AUTOCORR                |
| AutocorrPlot   | Autocorrelation function plot                      | BAYES / PLOTS(UNPACK)=AUTOCORR         |
| CumhazPlot     | Cumulative hazard function plot                    | PROC / PLOTS=CUMHAZ                    |
| DensityPanel   | Density panel                                      | BAYES / PLOTS=DENSITY                  |
| DensityPlot    | Density plot                                       | BAYES / PLOTS(UNPACK)=DENSITY          |
| SurvivalPlot   | Survivor function plot                             | PROC / PLOTS=SURVIVAL                  |
| TAPanel        | Trace and autocorrelation function panel           | BAYES / PLOTS=(TRACE AUTOCORR)         |
| TADPanel       | Trace, density, and autocorrelation function panel | BAYES / PLOTS=(TRACE AUTOCORR DENSITY) |
| TDPanel        | Trace and density panel                            | BAYES / PLOTS=(TRACE DENSITY)          |
| TracePanel     | Trace panel                                        | BAYES / PLOTS=TRACE                    |
| TracePlot      | Trace plot                                         | BAYES / PLOTS(UNPACK)=TRACE            |



## Examples: PHREG Procedure

This section contains 14 examples of PROC PHREG applications. The first 12 examples use the classical method of maximum likelihood, while the last two examples illustrate the Bayesian methodology.

### Example 67.1: Stepwise Regression

Krall, Uthoff, and Harley (1975) analyzed data from a study on multiple myeloma in which researchers treated 65 patients with alkylating agents. Of those patients, 48 died during the study and 17 survived. The following DATA step creates the data set Myeloma. The variable Time represents the survival time in months from diagnosis. The variable VStatus consists of two values, 0 and 1, indicating whether the patient was alive or dead, respectively, at the end of the study. If the value of VStatus is 0, the corresponding value of Time is censored. The variables thought to be related to survival are LogBUN (log(BUN) at diagnosis), HGB (hemoglobin at diagnosis), Platelet (platelets at diagnosis: 0=abnormal, 1=normal), Age (age at diagnosis, in years), LogWBC (log(WBC) at diagnosis), Frac (fractures at diagnosis: 0=none, 1=present), LogPBM (log percentage of plasma cells in bone marrow), Protein (proteinuria at diagnosis), and SCalc (serum calcium at diagnosis). Interest lies in identifying important prognostic factors from these nine explanatory variables.

```
data Myeloma;
 input Time VStatus LogBUN HGB Platelet Age LogWBC Frac
 LogPBM Protein SCalc;
 label Time='Survival Time'
 VStatus='0=Alive 1=Dead';
 datalines;
1.25 1 2.2175 9.4 1 67 3.6628 1 1.9542 12 10
1.25 1 1.9395 12.0 1 38 3.9868 1 1.9542 20 18
2.00 1 1.5185 9.8 1 81 3.8751 1 2.0000 2 15
2.00 1 1.7482 11.3 0 75 3.8062 1 1.2553 0 12
2.00 1 1.3010 5.1 0 57 3.7243 1 2.0000 3 9
3.00 1 1.5441 6.7 1 46 4.4757 0 1.9345 12 10
5.00 1 2.2355 10.1 1 50 4.9542 1 1.6628 4 9
5.00 1 1.6812 6.5 1 74 3.7324 0 1.7324 5 9
6.00 1 1.3617 9.0 1 77 3.5441 0 1.4624 1 8
6.00 1 2.1139 10.2 0 70 3.5441 1 1.3617 1 8
6.00 1 1.1139 9.7 1 60 3.5185 1 1.3979 0 10
6.00 1 1.4150 10.4 1 67 3.9294 1 1.6902 0 8
7.00 1 1.9777 9.5 1 48 3.3617 1 1.5682 5 10
7.00 1 1.0414 5.1 0 61 3.7324 1 2.0000 1 10
7.00 1 1.1761 11.4 1 53 3.7243 1 1.5185 1 13
9.00 1 1.7243 8.2 1 55 3.7993 1 1.7404 0 12
11.00 1 1.1139 14.0 1 61 3.8808 1 1.2788 0 10
11.00 1 1.2304 12.0 1 43 3.7709 1 1.1761 1 9
11.00 1 1.3010 13.2 1 65 3.7993 1 1.8195 1 10
11.00 1 1.5682 7.5 1 70 3.8865 0 1.6721 0 12
11.00 1 1.0792 9.6 1 51 3.5051 1 1.9031 0 9
13.00 1 0.7782 5.5 0 60 3.5798 1 1.3979 2 10
14.00 1 1.3979 14.6 1 66 3.7243 1 1.2553 2 10
15.00 1 1.6021 10.6 1 70 3.6902 1 1.4314 0 11
16.00 1 1.3424 9.0 1 48 3.9345 1 2.0000 0 10
```

```

16.00 1 1.3222 8.8 1 62 3.6990 1 0.6990 17 10
17.00 1 1.2304 10.0 1 53 3.8808 1 1.4472 4 9
17.00 1 1.5911 11.2 1 68 3.4314 0 1.6128 1 10
18.00 1 1.4472 7.5 1 65 3.5682 0 0.9031 7 8
19.00 1 1.0792 14.4 1 51 3.9191 1 2.0000 6 15
19.00 1 1.2553 7.5 0 60 3.7924 1 1.9294 5 9
24.00 1 1.3010 14.6 1 56 4.0899 1 0.4771 0 9
25.00 1 1.0000 12.4 1 67 3.8195 1 1.6435 0 10
26.00 1 1.2304 11.2 1 49 3.6021 1 2.0000 27 11
32.00 1 1.3222 10.6 1 46 3.6990 1 1.6335 1 9
35.00 1 1.1139 7.0 0 48 3.6532 1 1.1761 4 10
37.00 1 1.6021 11.0 1 63 3.9542 0 1.2041 7 9
41.00 1 1.0000 10.2 1 69 3.4771 1 1.4771 6 10
41.00 1 1.1461 5.0 1 70 3.5185 1 1.3424 0 9
51.00 1 1.5682 7.7 0 74 3.4150 1 1.0414 4 13
52.00 1 1.0000 10.1 1 60 3.8573 1 1.6532 4 10
54.00 1 1.2553 9.0 1 49 3.7243 1 1.6990 2 10
58.00 1 1.2041 12.1 1 42 3.6990 1 1.5798 22 10
66.00 1 1.4472 6.6 1 59 3.7853 1 1.8195 0 9
67.00 1 1.3222 12.8 1 52 3.6435 1 1.0414 1 10
88.00 1 1.1761 10.6 1 47 3.5563 0 1.7559 21 9
89.00 1 1.3222 14.0 1 63 3.6532 1 1.6232 1 9
92.00 1 1.4314 11.0 1 58 4.0755 1 1.4150 4 11
 4.00 0 1.9542 10.2 1 59 4.0453 0 0.7782 12 10
 4.00 0 1.9243 10.0 1 49 3.9590 0 1.6232 0 13
 7.00 0 1.1139 12.4 1 48 3.7993 1 1.8573 0 10
 7.00 0 1.5315 10.2 1 81 3.5911 0 1.8808 0 11
 8.00 0 1.0792 9.9 1 57 3.8325 1 1.6532 0 8
12.00 0 1.1461 11.6 1 46 3.6435 0 1.1461 0 7
11.00 0 1.6128 14.0 1 60 3.7324 1 1.8451 3 9
12.00 0 1.3979 8.8 1 66 3.8388 1 1.3617 0 9
13.00 0 1.6628 4.9 0 71 3.6435 0 1.7924 0 9
16.00 0 1.1461 13.0 1 55 3.8573 0 0.9031 0 9
19.00 0 1.3222 13.0 1 59 3.7709 1 2.0000 1 10
19.00 0 1.3222 10.8 1 69 3.8808 1 1.5185 0 10
28.00 0 1.2304 7.3 1 82 3.7482 1 1.6721 0 9
41.00 0 1.7559 12.8 1 72 3.7243 1 1.4472 1 9
53.00 0 1.1139 12.0 1 66 3.6128 1 2.0000 1 11
57.00 0 1.2553 12.5 1 66 3.9685 0 1.9542 0 11
77.00 0 1.0792 14.0 1 60 3.6812 0 0.9542 0 12
;
```

The stepwise selection process consists of a series of alternating forward selection and backward elimination steps. The former adds variables to the model, while the latter removes variables from the model.

The following statements use PROC PHREG to produce a stepwise regression analysis. Stepwise selection is requested by specifying the SELECTION=STEPWISE option in the MODEL statement. The option SLENTRY=0.25 specifies that a variable has to be significant at the 0.25 level before it can be entered into the model, while the option SLSTAY=0.15 specifies that a variable in the model has to be significant at the 0.15 level for it to remain in the model. The DETAILS option requests detailed results for the variable selection process.

```

proc phreg data=Myeloma;
 model Time*VStatus(0)=LogBUN HGB Platelet Age LogWBC
 Frac LogPBM Protein SCalc
 / selection=stepwise slentry=0.25
 slstay=0.15 details;
run;

```

Results of the stepwise regression analysis are displayed in [Output 67.1.1](#) through [Output 67.1.7](#).

Individual score tests are used to determine which of the nine explanatory variables is first selected into the model. In this case, the score test for each variable is the global score test for the model containing that variable as the only explanatory variable. [Output 67.1.1](#) displays the chi-square statistics and the corresponding  $p$ -values. The variable LogBUN has the largest chi-square value (8.5164), and it is significant ( $p = 0.0035$ ) at the SLENTY=0.25 level. The variable LogBUN is thus entered into the model.

**Output 67.1.1** Individual Score Test Results for All Variables

| The PHREG Procedure                                |              |                |            |                  |
|----------------------------------------------------|--------------|----------------|------------|------------------|
| Model Information                                  |              |                |            |                  |
| Data Set                                           | WORK.MYELOMA |                |            |                  |
| Dependent Variable                                 | Time         | Survival Time  |            |                  |
| Censoring Variable                                 | VStatus      | 0=Alive 1=Dead |            |                  |
| Censoring Value(s)                                 | 0            |                |            |                  |
| Ties Handling                                      | BRESLOW      |                |            |                  |
| Summary of the Number of Event and Censored Values |              |                |            |                  |
|                                                    | Total        | Event          | Censored   | Percent Censored |
|                                                    | 65           | 48             | 17         | 26.15            |
| Analysis of Effects Eligible for Entry             |              |                |            |                  |
| Effect                                             | DF           | Score          |            |                  |
|                                                    |              | Chi-Square     | Pr > ChiSq |                  |
| LogBUN                                             | 1            | 8.5164         | 0.0035     |                  |
| HGB                                                | 1            | 5.0664         | 0.0244     |                  |
| Platelet                                           | 1            | 3.1816         | 0.0745     |                  |
| Age                                                | 1            | 0.0183         | 0.8924     |                  |
| LogWBC                                             | 1            | 0.5658         | 0.4519     |                  |
| Frac                                               | 1            | 0.9151         | 0.3388     |                  |
| LogPBM                                             | 1            | 0.5846         | 0.4445     |                  |
| Protein                                            | 1            | 0.1466         | 0.7018     |                  |
| SCalc                                              | 1            | 1.1109         | 0.2919     |                  |

**Output 67.1.1** *continued*

| Residual Chi-Square Test |    |            |
|--------------------------|----|------------|
| Chi-Square               | DF | Pr > ChiSq |
| 18.4550                  | 9  | 0.0302     |

Output 67.1.2 displays the results of the first model. Since the Wald chi-square statistic is significant ( $p = 0.0039$ ) at the SLSTAY=0.15 level, LogBUN stays in the model.

**Output 67.1.2** First Model in the Stepwise Selection Process

```

Step 1. Effect LogBUN is entered. The model contains the following effects:

 LogBUN

 Convergence Status

 Convergence criterion (GCONV=1E-8) satisfied.

 Model Fit Statistics

 Criterion Without With
 Covariates Covariates
-2 LOG L 309.716 301.959
AIC 309.716 303.959
SBC 309.716 305.830

 Testing Global Null Hypothesis: BETA=0

 Test Chi-Square DF Pr > ChiSq
Likelihood Ratio 7.7572 1 0.0053
Score 8.5164 1 0.0035
Wald 8.3392 1 0.0039

 Analysis of Maximum Likelihood Estimates

 Parameter DF Parameter Estimate Standard Error Chi-Square Pr > ChiSq Hazard Ratio
LogBUN 1 1.74595 0.60460 8.3392 0.0039 5.731

```

The next step consists of selecting another variable to add to the model. Output 67.1.3 displays the chi-square statistics and  $p$ -values of individual score tests (adjusted for LogBUN) for the remaining eight variables. The score chi-square for a given variable is the value of the likelihood score test for testing the

significance of the variable in the presence of LogBUN. The variable HGB is selected because it has the highest chi-square value (4.3468), and it is significant ( $p = 0.0371$ ) at the SLENTRY=0.25 level.

### Output 67.1.3 Score Tests Adjusted for the Variable LogBUN

| Analysis of Effects Eligible for Entry |    |            |            |
|----------------------------------------|----|------------|------------|
| Effect                                 | DF | Score      |            |
|                                        |    | Chi-Square | Pr > ChiSq |
| HGB                                    | 1  | 4.3468     | 0.0371     |
| Platelet                               | 1  | 2.0183     | 0.1554     |
| Age                                    | 1  | 0.7159     | 0.3975     |
| LogWBC                                 | 1  | 0.0704     | 0.7908     |
| Frac                                   | 1  | 1.0354     | 0.3089     |
| LogPBM                                 | 1  | 1.0334     | 0.3094     |
| Protein                                | 1  | 0.5214     | 0.4703     |
| SCalc                                  | 1  | 1.4150     | 0.2342     |

| Residual Chi-Square Test |    |            |
|--------------------------|----|------------|
| Chi-Square               | DF | Pr > ChiSq |
| 9.3164                   | 8  | 0.3163     |

Output 67.1.4 displays the fitted model containing both LogBUN and HGB. Based on the Wald statistics, neither LogBUN nor HGB is removed from the model.

### Output 67.1.4 Second Model in the Stepwise Selection Process

Step 2. Effect HGB is entered. The model contains the following effects:

LogBUN HGB

Convergence Status

Convergence criterion (GCONV=1E-8) satisfied.

Model Fit Statistics

| Criterion | Without Covariates | With Covariates |
|-----------|--------------------|-----------------|
| -2 LOG L  | 309.716            | 297.767         |
| AIC       | 309.716            | 301.767         |
| SBC       | 309.716            | 305.509         |

**Output 67.1.4** *continued*

| Testing Global Null Hypothesis: BETA=0   |    |                    |                |            |            |              |
|------------------------------------------|----|--------------------|----------------|------------|------------|--------------|
| Test                                     |    | Chi-Square         | DF             | Pr > ChiSq |            |              |
| Likelihood Ratio                         |    | 11.9493            | 2              | 0.0025     |            |              |
| Score                                    |    | 12.7252            | 2              | 0.0017     |            |              |
| Wald                                     |    | 12.1900            | 2              | 0.0023     |            |              |
| Analysis of Maximum Likelihood Estimates |    |                    |                |            |            |              |
| Parameter                                | DF | Parameter Estimate | Standard Error | Chi-Square | Pr > ChiSq | Hazard Ratio |
| LogBUN                                   | 1  | 1.67440            | 0.61209        | 7.4833     | 0.0062     | 5.336        |
| HGB                                      | 1  | -0.11899           | 0.05751        | 4.2811     | 0.0385     | 0.888        |

Output 67.1.5 shows Step 3 of the selection process, in which the variable SCalc is added, resulting in the model with LogBUN, HGB, and SCalc as the explanatory variables. Note that SCalc has the smallest Wald chi-square statistic, and it is not significant ( $p = 0.1782$ ) at the SLSTAY=0.15 level.

**Output 67.1.5** Third Model in the Stepwise Regression

| Step 3. Effect SCalc is entered. The model contains the following effects: |     |                    |    |                 |  |  |
|----------------------------------------------------------------------------|-----|--------------------|----|-----------------|--|--|
| LogBUN                                                                     | HGB | SCalc              |    |                 |  |  |
| Convergence Status                                                         |     |                    |    |                 |  |  |
| Convergence criterion (GCONV=1E-8) satisfied.                              |     |                    |    |                 |  |  |
| Model Fit Statistics                                                       |     |                    |    |                 |  |  |
| Criterion                                                                  |     | Without Covariates |    | With Covariates |  |  |
| -2 LOG L                                                                   |     | 309.716            |    | 296.078         |  |  |
| AIC                                                                        |     | 309.716            |    | 302.078         |  |  |
| SBC                                                                        |     | 309.716            |    | 307.692         |  |  |
| Testing Global Null Hypothesis: BETA=0                                     |     |                    |    |                 |  |  |
| Test                                                                       |     | Chi-Square         | DF | Pr > ChiSq      |  |  |
| Likelihood Ratio                                                           |     | 13.6377            | 3  | 0.0034          |  |  |
| Score                                                                      |     | 15.3053            | 3  | 0.0016          |  |  |
| Wald                                                                       |     | 14.4542            | 3  | 0.0023          |  |  |

Output 67.1.5 *continued*

| Analysis of Maximum Likelihood Estimates |    |                    |                |            |            |              |
|------------------------------------------|----|--------------------|----------------|------------|------------|--------------|
| Parameter                                | DF | Parameter Estimate | Standard Error | Chi-Square | Pr > ChiSq | Hazard Ratio |
| LogBUN                                   | 1  | 1.63593            | 0.62359        | 6.8822     | 0.0087     | 5.134        |
| HGB                                      | 1  | -0.12643           | 0.05868        | 4.6419     | 0.0312     | 0.881        |
| SCalc                                    | 1  | 0.13286            | 0.09868        | 1.8127     | 0.1782     | 1.142        |

The variable SCalc is then removed from the model in a step-down phase in Step 4 (Output 67.1.6). The removal of SCalc brings the stepwise selection process to a stop in order to avoid repeatedly entering and removing the same variable.

## Output 67.1.6 Final Model in the Stepwise Regression

| Step 4. Effect SCalc is removed. The model contains the following effects: |                  |                    |                |            |            |              |
|----------------------------------------------------------------------------|------------------|--------------------|----------------|------------|------------|--------------|
| LogBUN HGB                                                                 |                  |                    |                |            |            |              |
| Convergence Status                                                         |                  |                    |                |            |            |              |
| Convergence criterion (GCONV=1E-8) satisfied.                              |                  |                    |                |            |            |              |
| Model Fit Statistics                                                       |                  |                    |                |            |            |              |
|                                                                            |                  | Without            | With           |            |            |              |
|                                                                            | Criterion        | Covariates         | Covariates     |            |            |              |
|                                                                            | -2 LOG L         | 309.716            | 297.767        |            |            |              |
|                                                                            | AIC              | 309.716            | 301.767        |            |            |              |
|                                                                            | SBC              | 309.716            | 305.509        |            |            |              |
| Testing Global Null Hypothesis: BETA=0                                     |                  |                    |                |            |            |              |
|                                                                            | Test             | Chi-Square         | DF             | Pr > ChiSq |            |              |
|                                                                            | Likelihood Ratio | 11.9493            | 2              | 0.0025     |            |              |
|                                                                            | Score            | 12.7252            | 2              | 0.0017     |            |              |
|                                                                            | Wald             | 12.1900            | 2              | 0.0023     |            |              |
| Analysis of Maximum Likelihood Estimates                                   |                  |                    |                |            |            |              |
| Parameter                                                                  | DF               | Parameter Estimate | Standard Error | Chi-Square | Pr > ChiSq | Hazard Ratio |
| LogBUN                                                                     | 1                | 1.67440            | 0.61209        | 7.4833     | 0.0062     | 5.336        |
| HGB                                                                        | 1                | -0.11899           | 0.05751        | 4.2811     | 0.0385     | 0.888        |

**Output 67.1.6** *continued*

**NOTE:** Model building terminates because the effect to be entered is the effect that was removed in the last step.

The procedure also displays a summary table of the steps in the stepwise selection process, as shown in Output 67.1.7.

**Output 67.1.7** Model Selection Summary

| Summary of Stepwise Selection |         |         |    |        |            |            |            |
|-------------------------------|---------|---------|----|--------|------------|------------|------------|
| Step                          | Effect  |         | DF | Number |            | Wald       |            |
|                               | Entered | Removed |    | In     | Chi-Square | Chi-Square | Pr > ChiSq |
| 1                             | LogBUN  |         | 1  | 1      | 8.5164     |            | 0.0035     |
| 2                             | HGB     |         | 1  | 2      | 4.3468     |            | 0.0371     |
| 3                             | SCalc   |         | 1  | 3      | 1.8225     |            | 0.1770     |
| 4                             |         | SCalc   | 1  | 2      |            | 1.8127     | 0.1782     |

The stepwise selection process results in a model with two explanatory variables, LogBUN and HGB.

---

## Example 67.2: Best Subset Selection

An alternative to stepwise selection of variables is best subset selection. This method uses the branch-and-bound algorithm of Furnival and Wilson (1974) to find a specified number of best models containing one, two, or three variables, and so on, up to the single model containing all of the explanatory variables. The criterion used to determine the “best” subset is based on the global score chi-square statistic. For two models A and B, each having the same number of explanatory variables, model A is considered to be better than model B if the global score chi-square statistic for A exceeds that for B.

In the following statements, best subset selection analysis is requested by specifying the SELECTION=SCORE option in the MODEL statement. The BEST=3 option requests the procedure to identify only the three best models for each size. In other words, PROC PHREG will list the three models having the highest score statistics of all the models possible for a given number of covariates.

```
proc phreg data=Myeloma;
 model Time*VStatus(0)=LogBUN HGB Platelet Age LogWBC
 Frac LogPBM Protein SCalc
 / selection=score best=3;
run;
```

Output 67.2.1 displays the results of this analysis. The number of explanatory variables in the model is given in the first column, and the names of the variables are listed on the right. The models are listed in descending order of their score chi-square values within each model size. For example, among all models containing two explanatory variables, the model that contains the variables LogBUN and HGB has the largest score value (12.7252), the model that contains the variables LogBUN and Platelet has the second-largest score



value (11.1842), and the model that contains the variables LogBUN and SCalc has the third-largest score value (9.9962).

### Output 67.2.1 Best Variable Combinations

| The PHREG Procedure                           |                  |                                                          |  |
|-----------------------------------------------|------------------|----------------------------------------------------------|--|
| Regression Models Selected by Score Criterion |                  |                                                          |  |
| Number of Variables                           | Score Chi-Square | Variables Included in Model                              |  |
| 1                                             | 8.5164           | LogBUN                                                   |  |
| 1                                             | 5.0664           | HGB                                                      |  |
| 1                                             | 3.1816           | Platelet                                                 |  |
| 2                                             | 12.7252          | LogBUN HGB                                               |  |
| 2                                             | 11.1842          | LogBUN Platelet                                          |  |
| 2                                             | 9.9962           | LogBUN SCalc                                             |  |
| 3                                             | 15.3053          | LogBUN HGB SCalc                                         |  |
| 3                                             | 13.9911          | LogBUN HGB Age                                           |  |
| 3                                             | 13.5788          | LogBUN HGB Frac                                          |  |
| 4                                             | 16.9873          | LogBUN HGB Age SCalc                                     |  |
| 4                                             | 16.0457          | LogBUN HGB Frac SCalc                                    |  |
| 4                                             | 15.7619          | LogBUN HGB LogPBM SCalc                                  |  |
| 5                                             | 17.6291          | LogBUN HGB Age Frac SCalc                                |  |
| 5                                             | 17.3519          | LogBUN HGB Age LogPBM SCalc                              |  |
| 5                                             | 17.1922          | LogBUN HGB Age LogWBC SCalc                              |  |
| 6                                             | 17.9120          | LogBUN HGB Age Frac LogPBM SCalc                         |  |
| 6                                             | 17.7947          | LogBUN HGB Age LogWBC Frac SCalc                         |  |
| 6                                             | 17.7744          | LogBUN HGB Platelet Age Frac SCalc                       |  |
| 7                                             | 18.1517          | LogBUN HGB Platelet Age Frac LogPBM SCalc                |  |
| 7                                             | 18.0568          | LogBUN HGB Age LogWBC Frac LogPBM SCalc                  |  |
| 7                                             | 18.0223          | LogBUN HGB Platelet Age LogWBC Frac SCalc                |  |
| 8                                             | 18.3925          | LogBUN HGB Platelet Age LogWBC Frac LogPBM SCalc         |  |
| 8                                             | 18.1636          | LogBUN HGB Platelet Age Frac LogPBM Protein SCalc        |  |
| 8                                             | 18.1309          | LogBUN HGB Platelet Age LogWBC Frac Protein SCalc        |  |
| 9                                             | 18.4550          | LogBUN HGB Platelet Age LogWBC Frac LogPBM Protein SCalc |  |

### Example 67.3: Modeling with Categorical Predictors

Consider the data for the Veterans Administration lung cancer trial presented in Appendix 1 of Kalbfleisch and Prentice (1980). In this trial, males with advanced inoperable lung cancer were randomized to a standard therapy and a test chemotherapy. The primary endpoint for the therapy comparison was time to death in days, represented by the variable Time. Negative values of Time are censored values. The data include information about a number of explanatory variables: Therapy (type of therapy: standard or test), Cell (type

of tumor cell: adeno, large, small, or squamous), Prior (prior therapy: 0=no, 10=yes), Age (age, in years), Duration (months from diagnosis to randomization), and Kps (Karnofsky performance scale). A censoring indicator variable, Censor, is created from the data, with the value 1 indicating a censored time and the value 0 indicating an event time. The following DATA step saves the data in the data set VALung.

```
proc format;
 value yesno 0='no' 10='yes';
run;

data VALung;
 drop check m;
 retain Therapy Cell;
 infile cards column=column;
 length Check $ 1;
 label Time='time to death in days'
 Kps='Karnofsky performance scale'
 Duration='months from diagnosis to randomization'
 Age='age in years'
 Prior='prior therapy'
 Cell='cell type'
 Therapy='type of treatment';
 format Prior yesno.;
 M=Column;
 input Check $ @@;
 if M>Column then M=1;
 if Check='s'|Check='t' then do;
 input @M Therapy $ Cell $;
 delete;
 end;
 else do;
 input @M Time Kps Duration Age Prior @@;
 Status=(Time>0);
 Time=abs(Time);
 end;
 datalines;
standard squamous
 72 60 7 69 0 411 70 5 64 10 228 60 3 38 0 126 60 9 63 10
 118 70 11 65 10 10 20 5 49 0 82 40 10 69 10 110 80 29 68 0
 314 50 18 43 0 -100 70 6 70 0 42 60 4 81 0 8 40 58 63 10
 144 30 4 63 0 -25 80 9 52 10 11 70 11 48 10
standard small
 30 60 3 61 0 384 60 9 42 0 4 40 2 35 0 54 80 4 63 10
 13 60 4 56 0 -123 40 3 55 0 -97 60 5 67 0 153 60 14 63 10
 59 30 2 65 0 117 80 3 46 0 16 30 4 53 10 151 50 12 69 0
 22 60 4 68 0 56 80 12 43 10 21 40 2 55 10 18 20 15 42 0
 139 80 2 64 0 20 30 5 65 0 31 75 3 65 0 52 70 2 55 0
 287 60 25 66 10 18 30 4 60 0 51 60 1 67 0 122 80 28 53 0
 27 60 8 62 0 54 70 1 67 0 7 50 7 72 0 63 50 11 48 0
 392 40 4 68 0 10 40 23 67 10
standard adeno
 8 20 19 61 10 92 70 10 60 0 35 40 6 62 0 117 80 2 38 0
 132 80 5 50 0 12 50 4 63 10 162 80 5 64 0 3 30 3 43 0
 95 80 4 34 0
```

```

standard large
177 50 16 66 10 162 80 5 62 0 216 50 15 52 0 553 70 2 47 0
278 60 12 63 0 12 40 12 68 10 260 80 5 45 0 200 80 12 41 10
156 70 2 66 0 -182 90 2 62 0 143 90 8 60 0 105 80 11 66 0
103 80 5 38 0 250 70 8 53 10 100 60 13 37 10

test squamous
999 90 12 54 10 112 80 6 60 0 -87 80 3 48 0 -231 50 8 52 10
242 50 1 70 0 991 70 7 50 10 111 70 3 62 0 1 20 21 65 10
587 60 3 58 0 389 90 2 62 0 33 30 6 64 0 25 20 36 63 0
357 70 13 58 0 467 90 2 64 0 201 80 28 52 10 1 50 7 35 0
 30 70 11 63 0 44 60 13 70 10 283 90 2 51 0 15 50 13 40 10

test small
25 30 2 69 0 -103 70 22 36 10 21 20 4 71 0 13 30 2 62 0
87 60 2 60 0 2 40 36 44 10 20 30 9 54 10 7 20 11 66 0
24 60 8 49 0 99 70 3 72 0 8 80 2 68 0 99 85 4 62 0
61 70 2 71 0 25 70 2 70 0 95 70 1 61 0 80 50 17 71 0
51 30 87 59 10 29 40 8 67 0

test adeno
24 40 2 60 0 18 40 5 69 10 -83 99 3 57 0 31 80 3 39 0
51 60 5 62 0 90 60 22 50 10 52 60 3 43 0 73 60 3 70 0
 8 50 5 66 0 36 70 8 61 0 48 10 4 81 0 7 40 4 58 0
140 70 3 63 0 186 90 3 60 0 84 80 4 62 10 19 50 10 42 0
45 40 3 69 0 80 40 4 63 0

test large
52 60 4 45 0 164 70 15 68 10 19 30 4 39 10 53 60 12 66 0
15 30 5 63 0 43 60 11 49 10 340 80 10 64 10 133 75 1 65 0
111 60 5 64 0 231 70 18 67 10 378 80 4 65 0 49 30 3 37 0
;

```

The following statements use the PHREG procedure to fit the Cox proportional hazards model to these data. The variables `Prior`, `Cell`, and `Therapy`, which are categorical variables, are declared in the `CLASS` statement. By default, PROC PHREG parameterizes the `CLASS` variables by using the reference coding with the last category as the reference category. However, you can explicitly specify the reference category of your choice. Here, `Prior=no` is chosen as the reference category for prior therapy, `Cell=large` is chosen as the reference category for type of tumor cell, and `Therapy=standard` is chosen as the reference category for the type of therapy. In the `MODEL` statement, the term `Prior|Therapy` is just another way of specifying the main effects `Prior`, `Therapy`, and the `Prior*Therapy` interaction.

```

proc phreg data=VALung;
 class Prior(ref='no') Cell(ref='large') Therapy(ref='standard');
 model Time*Status(0) = Kps Duration Age Cell Prior|Therapy;
run;

```

Coding of the `CLASS` variables is displayed in [Output 67.3.1](#). There is one dummy variable for `Prior` and one for `Therapy`, since both variables are binary. The dummy variable has a value of 0 for the reference category (`Prior=no`, `Therapy=standard`). The variable `Cell` has four categories and is represented by three dummy variables. Note that the reference category, `Cell=large`, has a value of 0 for all three dummy variables.

**Output 67.3.1** Reference Coding of CLASS Variables

| The PHREG Procedure     |          |                  |   |   |
|-------------------------|----------|------------------|---|---|
| Class Level Information |          |                  |   |   |
| Class                   | Value    | Design Variables |   |   |
| Prior                   | no       | 0                |   |   |
|                         | yes      | 1                |   |   |
| Cell                    | adeno    | 1                | 0 | 0 |
|                         | large    | 0                | 0 | 0 |
|                         | small    | 0                | 1 | 0 |
|                         | squamous | 0                | 0 | 1 |
| Therapy                 | standard | 0                |   |   |
|                         | test     | 1                |   |   |

The test results of individual model effects are shown in [Output 67.3.2](#). There is a strong prognostic effect of Kps on patient's survivorship ( $p < 0.0001$ ), and the survival times for patients of different Cell types differ significantly ( $p = 0.0003$ ). The Prior\*Therapy interaction is marginally significant ( $p = 0.0416$ )—that is, prior therapy might play a role in whether one treatment is more effective than the other.

**Output 67.3.2** Wald Tests of Individual Effects

| Type 3 Tests  |    |                    |            |
|---------------|----|--------------------|------------|
| Effect        | DF | Wald<br>Chi-Square | Pr > ChiSq |
| Kps           | 1  | 35.5051            | <.0001     |
| Duration      | 1  | 0.1159             | 0.7335     |
| Age           | 1  | 1.9772             | 0.1597     |
| Cell          | 3  | 18.5339            | 0.0003     |
| Prior         | 1  | 2.5296             | 0.1117     |
| Therapy       | 1  | 5.2349             | 0.0221     |
| Prior*Therapy | 1  | 4.1528             | 0.0416     |

In the Cox proportional hazards model, the effects of the covariates are to act multiplicatively on the hazard of the survival time, and therefore it is a little easier to interpret the corresponding hazard ratios than the regression parameters. For a parameter that corresponds to a continuous variable, the hazard ratio is the ratio of hazard rates for an increase of one unit of the variable. From [Output 67.3.3](#), the hazard ratio estimate for Kps is 0.968, meaning that an increase of 10 units in Karnofsky performance scale will shrink the hazard rate by  $1 - (0.968)^{10} = 28\%$ . For a CLASS variable parameter, the hazard ratio presented in the [Output 67.3.3](#) is the ratio of the hazard rates between the given category and the reference category. The hazard rate of

Cell=adeno is 219% that of Cell=large, the hazard rate of Cell=small is 62% that of Cell=large, and the hazard rate of Cell=squamous is only 66% that of Cell=large. Hazard ratios for Prior and Therapy are missing since the model contains the Prior\*Therapy interaction. You can use the HAZARDRATIO statement to obtain the hazard ratios for a main effect in the presence of interaction as shown later in this example.

### Output 67.3.3 Parameters Estimates with Reference Coding

| Analysis of Maximum Likelihood Estimates |          |    |                    |                |                       |
|------------------------------------------|----------|----|--------------------|----------------|-----------------------|
| Parameter                                |          | DF | Parameter Estimate | Standard Error | Chi-Square Pr > ChiSq |
| Kps                                      |          | 1  | -0.03300           | 0.00554        | 35.5051 <.0001        |
| Duration                                 |          | 1  | 0.00323            | 0.00949        | 0.1159 0.7335         |
| Age                                      |          | 1  | -0.01353           | 0.00962        | 1.9772 0.1597         |
| Cell                                     | adeno    | 1  | 0.78356            | 0.30382        | 6.6512 0.0099         |
| Cell                                     | small    | 1  | 0.48230            | 0.26537        | 3.3032 0.0691         |
| Cell                                     | squamous | 1  | -0.40770           | 0.28363        | 2.0663 0.1506         |
| Prior                                    | yes      | 1  | 0.45914            | 0.28868        | 2.5296 0.1117         |
| Therapy                                  | test     | 1  | 0.56662            | 0.24765        | 5.2349 0.0221         |
| Prior*Therapy                            | yes test | 1  | -0.87579           | 0.42976        | 4.1528 0.0416         |

| Analysis of Maximum Likelihood Estimates |          |              |
|------------------------------------------|----------|--------------|
| Parameter                                |          | Hazard Ratio |
| Kps                                      |          | 0.968        |
| Duration                                 |          | 1.003        |
| Age                                      |          | 0.987        |
| Cell                                     | adeno    | 2.189        |
| Cell                                     | small    | 1.620        |
| Cell                                     | squamous | 0.665        |
| Prior                                    | yes      | .            |
| Therapy                                  | test     | .            |
| Prior*Therapy                            | yes test | .            |

| Analysis of Maximum Likelihood Estimates |          |                                            |
|------------------------------------------|----------|--------------------------------------------|
| Parameter                                |          | Label                                      |
| Kps                                      |          | Karnofsky performance scale                |
| Duration                                 |          | months from diagnosis to randomization     |
| Age                                      |          | age in years                               |
| Cell                                     | adeno    | cell type adeno                            |
| Cell                                     | small    | cell type small                            |
| Cell                                     | squamous | cell type squamous                         |
| Prior                                    | yes      | prior therapy yes                          |
| Therapy                                  | test     | type of treatment test                     |
| Prior*Therapy                            | yes test | prior therapy yes * type of treatment test |

The following PROC PHREG statements illustrate the use of the backward elimination process to identify the effects that affect the survivorship of the lung cancer patients. The option **SELECTION=BACKWARD** is specified to carry out the backward elimination. The option **SLSTAY=0.1** specifies the significant level for retaining the effects in the model.

```
proc phreg data=VALung;
 class Prior(ref='no') Cell(ref='large') Therapy(ref='standard');
 model Time*Status(0) = Kps Duration Age Cell Prior|Therapy
 / selection=backward slstay=0.1;
run;
```

Results of the backward elimination process are summarized in **Output 67.3.4**. The effect Duration was eliminated first and was followed by Age.

**Output 67.3.4** Effects Eliminated from the Model

| The PHREG Procedure             |                                        |    |           |                 |            |  |
|---------------------------------|----------------------------------------|----|-----------|-----------------|------------|--|
| Summary of Backward Elimination |                                        |    |           |                 |            |  |
| Step                            | Effect Removed                         | DF | Number In | Wald Chi-Square | Pr > ChiSq |  |
| 1                               | Duration                               | 1  | 6         | 0.1159          | 0.7335     |  |
| 2                               | Age                                    | 1  | 5         | 2.0458          | 0.1526     |  |
| Summary of Backward Elimination |                                        |    |           |                 |            |  |
| Step                            | Effect Label                           |    |           |                 |            |  |
| 1                               | months from diagnosis to randomization |    |           |                 |            |  |
| 2                               | age in years                           |    |           |                 |            |  |

**Output 67.3.5** shows the Type 3 analysis of effects and the maximum likelihood estimates of the regression coefficients of the model. Without controlling for Age and Duration, KPS and Cell remain significant, but the Prior\*Therapy interaction is less prominent than before ( $p = 0.0871$ ) though still significant at 0.1 level.

**Output 67.3.5** Type 3 Effects and Parameter Estimates for the Selected Model

| Type 3 Tests  |    |                 |            |  |
|---------------|----|-----------------|------------|--|
| Effect        | DF | Wald Chi-Square | Pr > ChiSq |  |
| Kps           | 1  | 35.9218         | <.0001     |  |
| Cell          | 3  | 17.4134         | 0.0006     |  |
| Prior         | 1  | 2.3113          | 0.1284     |  |
| Therapy       | 1  | 3.8030          | 0.0512     |  |
| Prior*Therapy | 1  | 2.9269          | 0.0871     |  |

Output 67.3.5 *continued*

| Analysis of Maximum Likelihood Estimates |          |    |                    |                |            |            |
|------------------------------------------|----------|----|--------------------|----------------|------------|------------|
| Parameter                                |          | DF | Parameter Estimate | Standard Error | Chi-Square | Pr > ChiSq |
| Kps                                      |          | 1  | -0.03111           | 0.00519        | 35.9218    | <.0001     |
| Cell                                     | adeno    | 1  | 0.74907            | 0.30465        | 6.0457     | 0.0139     |
| Cell                                     | small    | 1  | 0.44265            | 0.26168        | 2.8614     | 0.0907     |
| Cell                                     | squamous | 1  | -0.41145           | 0.28309        | 2.1125     | 0.1461     |
| Prior                                    | yes      | 1  | 0.41755            | 0.27465        | 2.3113     | 0.1284     |
| Therapy                                  | test     | 1  | 0.45670            | 0.23419        | 3.8030     | 0.0512     |
| Prior*Therapy                            | yes test | 1  | -0.69443           | 0.40590        | 2.9269     | 0.0871     |

| Analysis of Maximum Likelihood Estimates |          |              |
|------------------------------------------|----------|--------------|
| Parameter                                |          | Hazard Ratio |
| Kps                                      |          | 0.969        |
| Cell                                     | adeno    | 2.115        |
| Cell                                     | small    | 1.557        |
| Cell                                     | squamous | 0.663        |
| Prior                                    | yes      | .            |
| Therapy                                  | test     | .            |
| Prior*Therapy                            | yes test | .            |

| Analysis of Maximum Likelihood Estimates |          |                                            |
|------------------------------------------|----------|--------------------------------------------|
| Parameter                                |          | Label                                      |
| Kps                                      |          | Karnofsky performance scale                |
| Cell                                     | adeno    | cell type adeno                            |
| Cell                                     | small    | cell type small                            |
| Cell                                     | squamous | cell type squamous                         |
| Prior                                    | yes      | prior therapy yes                          |
| Therapy                                  | test     | type of treatment test                     |
| Prior*Therapy                            | yes test | prior therapy yes * type of treatment test |

Finally, the following statements refit the previous model and computes hazard ratios at settings beyond those displayed in the “Analysis of Maximum Likelihood Estimates” table. You can use either the HAZARDRATIO statement or the CONTRAST statement to obtain hazard ratios. Using the CONTRAST statement to compute hazard ratios for CLASS variables can be a daunting task unless you are familiar with the parameterization schemes (see the section “Parameterization of Model Effects” on page 383 of Chapter 19, “Shared Concepts and Topics,” for details), but you have control over which specific hazard ratios you want to compute. HAZARDRATIO statements, on the other hand, are designed specifically to provide hazard ratios. They are easy to use and you can also request both the Wald confidence limits and the profile-likelihood confidence limits; the latter is not available for the CONTRAST statements. Three HAZARDRATIO statements are specified; each has the CL=BOTH option to request both the Wald confidence limits and the profile-likelihood limits. The first HAZARDRATIO statement, labeled ‘H1’, estimates the hazard ratio for an increase of 10 units in the KPS; the UNITS= option specifies the number of units increase. The second HAZARDRATIO statement, labeled ‘H2’ computes the hazard ratios for comparing any pairs of tumor Cell

types. The third HAZARDRATIO statement, labeled 'H3', compares the test therapy with the standard therapy. The DIFF=REF option specifies that each nonreference category is compared to the reference category. The purpose of using DIFF=REF here is to ensure that the hazard ratio is comparing the test therapy to the standard therapy instead of the other way around. Three CONTRAST statements, labeled 'C1', 'C2', and 'C3', parallel to the HAZARDRATIO statements 'H1', 'H2', and 'H3', respectively, are specified. The ESTIMATE=EXP option specifies that the linear predictors be estimated in the exponential scale, which are precisely the hazard ratios.

```
proc phreg data=VALung;
 class Prior(ref='no') Cell(ref='large') Therapy(ref='standard');
 model Time*Status(0) = Kps Cell Prior|Therapy;
 hazardratio 'H1' Kps / units=10 cl=both;
 hazardratio 'H2' Cell / cl=both;
 hazardratio 'H3' Therapy / diff=ref cl=both;
 contrast 'C1' Kps 10 / estimate=exp;
 contrast 'C2' cell 1 0 0, /* adeno vs large */
 cell 1 -1 0, /* adeno vs small */
 cell 1 0 -1, /* adeno vs squamous */
 cell 0 -1 0, /* large vs small */
 cell 0 0 -1, /* large vs Squamous */
 cell 0 1 -1 /* small vs squamous */
 / estimate=exp;
 contrast 'C3' Prior 0 Therapy 1 Prior*Therapy 0,
 Prior 0 Therapy 1 Prior*Therapy 1 / estimate=exp;
run;
```

Output 67.3.6 displays the results of the three HAZARDRATIO statements in separate tables. Results of the three CONTRAST statements are shown in one table in Output 67.3.7. However, point estimates and the Wald confidence limits for the hazard ratio agree in between the two outputs.

**Output 67.3.6** Results from HAZARDRATIO Statements

| The PHREG Procedure       |                |                            |       |                                          |       |
|---------------------------|----------------|----------------------------|-------|------------------------------------------|-------|
| H1: Hazard Ratios for Kps |                |                            |       |                                          |       |
| Description               | Point Estimate | 95% Wald Confidence Limits |       | 95% Profile Likelihood Confidence Limits |       |
| Kps Unit=10               | 0.733          | 0.662                      | 0.811 | 0.662                                    | 0.811 |



## Output 67.3.6 continued

| H2: Hazard Ratios for Cell |                |                            |       |                                          |       |
|----------------------------|----------------|----------------------------|-------|------------------------------------------|-------|
| Description                | Point Estimate | 95% Wald Confidence Limits |       | 95% Profile Likelihood Confidence Limits |       |
| Cell adeno vs large        | 2.115          | 1.164                      | 3.843 | 1.162                                    | 3.855 |
| Cell adeno vs small        | 1.359          | 0.798                      | 2.312 | 0.791                                    | 2.301 |
| Cell adeno vs squamous     | 3.192          | 1.773                      | 5.746 | 1.770                                    | 5.768 |
| Cell large vs small        | 0.642          | 0.385                      | 1.073 | 0.380                                    | 1.065 |
| Cell large vs squamous     | 1.509          | 0.866                      | 2.628 | 0.863                                    | 2.634 |
| Cell small vs squamous     | 2.349          | 1.387                      | 3.980 | 1.399                                    | 4.030 |

| H3: Hazard Ratios for Therapy         |                |                            |       |  |
|---------------------------------------|----------------|----------------------------|-------|--|
| Description                           | Point Estimate | 95% Wald Confidence Limits |       |  |
| Therapy test vs standard At Prior=no  | 1.579          | 0.998                      | 2.499 |  |
| Therapy test vs standard At Prior=yes | 0.788          | 0.396                      | 1.568 |  |

| H3: Hazard Ratios for Therapy |  |                                          |       |  |
|-------------------------------|--|------------------------------------------|-------|--|
|                               |  | 95% Profile Likelihood Confidence Limits |       |  |
|                               |  | 0.998                                    | 2.506 |  |
|                               |  | 0.390                                    | 1.560 |  |

**Output 67.3.7** Results from CONTRAST Statements

| Contrast Estimation and Testing Results by Row |      |     |          |                |       |                   |        |
|------------------------------------------------|------|-----|----------|----------------|-------|-------------------|--------|
| Contrast                                       | Type | Row | Estimate | Standard Error | Alpha | Confidence Limits |        |
| C1                                             | EXP  | 1   | 0.7326   | 0.0380         | 0.05  | 0.6618            | 0.8111 |
| C2                                             | EXP  | 1   | 2.1150   | 0.6443         | 0.05  | 1.1641            | 3.8427 |
| C2                                             | EXP  | 2   | 1.3586   | 0.3686         | 0.05  | 0.7982            | 2.3122 |
| C2                                             | EXP  | 3   | 3.1916   | 0.9575         | 0.05  | 1.7727            | 5.7462 |
| C2                                             | EXP  | 4   | 0.6423   | 0.1681         | 0.05  | 0.3846            | 1.0728 |
| C2                                             | EXP  | 5   | 1.5090   | 0.4272         | 0.05  | 0.8664            | 2.6282 |
| C2                                             | EXP  | 6   | 2.3493   | 0.6318         | 0.05  | 1.3868            | 3.9797 |
| C3                                             | EXP  | 1   | 1.5789   | 0.3698         | 0.05  | 0.9977            | 2.4985 |
| C3                                             | EXP  | 2   | 0.7884   | 0.2766         | 0.05  | 0.3964            | 1.5680 |

| Contrast Estimation and Testing Results by Row |      |     |                 |            |  |
|------------------------------------------------|------|-----|-----------------|------------|--|
| Contrast                                       | Type | Row | Wald Chi-Square | Pr > ChiSq |  |
| C1                                             | EXP  | 1   | 35.9218         | <.0001     |  |
| C2                                             | EXP  | 1   | 6.0457          | 0.0139     |  |
| C2                                             | EXP  | 2   | 1.2755          | 0.2587     |  |
| C2                                             | EXP  | 3   | 14.9629         | 0.0001     |  |
| C2                                             | EXP  | 4   | 2.8614          | 0.0907     |  |
| C2                                             | EXP  | 5   | 2.1125          | 0.1461     |  |
| C2                                             | EXP  | 6   | 10.0858         | 0.0015     |  |
| C3                                             | EXP  | 1   | 3.8030          | 0.0512     |  |
| C3                                             | EXP  | 2   | 0.4593          | 0.4980     |  |

**Example 67.4: Firth's Correction for Monotone Likelihood**

In fitting the Cox regression model by maximizing the partial likelihood, the estimate of an explanatory variable X will be infinite if the value of X at each uncensored failure time is the largest of all the values of X in the risk set at that time (Tsiatis 1981; Bryson and Johnson 1981). You can exploit this information to artificially create a data set that has the condition of monotone likelihood for the Cox regression. The following DATA step modifies the Myeloma data in Example 67.1 to create a new explanatory variable, Contrived, which has the value 1 if the observed time is less than or equal to 65 and has the value 0 otherwise. The phenomenon of monotone likelihood will be demonstrated in the new data set Myeloma2.

```
data Myeloma2;
 set Myeloma;
 Contrived= (Time <= 65);
run;
```

For illustration purposes, consider a Cox model with three explanatory variables, one of which is the variable Contrived. The following statements invoke PROC PHREG to perform the Cox regression. The IPRINT option is specified in the MODEL statement to print the iteration history of the optimization.

```
proc phreg data=Myeloma2;
 model Time*Vstatus(0)=LOGbun HGB Contrived / itprint;
run;
```

The symptom of monotony is demonstrated in [Output 67.4.1](#). The log likelihood converges to the value of  $-136.56$  while the coefficient for `Contrived` diverges. Although the Newton-Raphson optimization process did not fail, it is obvious that convergence is questionable. A close examination of the standard errors in the “Analysis of Maximum Likelihood Estimates” table reveals a very large value for the coefficient of `Contrived`. This is very typical of a diverged estimate.

**Output 67.4.1** Monotone Likelihood Behavior Displayed

| The PHREG Procedure                  |       |                 |              |              |              |  |
|--------------------------------------|-------|-----------------|--------------|--------------|--------------|--|
| Maximum Likelihood Iteration History |       |                 |              |              |              |  |
| Iter                                 | Ridge | Log Likelihood  | LogBUN       | HGB          | Contrived    |  |
| 0                                    | 0     | -154.8579914384 | 0.0000000000 | 0.0000000000 | 0.0000000000 |  |
| 1                                    | 0     | -140.6934052686 | 1.9948819671 | -0.084318519 | 1.466331269  |  |
| 2                                    | 0     | -137.7841629416 | 1.6794678962 | -0.109067888 | 2.778361123  |  |
| 3                                    | 0     | -136.9711897754 | 1.7140611684 | -0.111564202 | 3.938095086  |  |
| 4                                    | 0     | -136.7078932606 | 1.7181735043 | -0.112273248 | 5.003053568  |  |
| 5                                    | 0     | -136.6164264879 | 1.7187547532 | -0.112369756 | 6.027435769  |  |
| 6                                    | 0     | -136.5835200895 | 1.7188294108 | -0.112382079 | 7.036444978  |  |
| 7                                    | 0     | -136.5715152788 | 1.7188392687 | -0.112383700 | 8.039763533  |  |
| 8                                    | 0     | -136.5671126045 | 1.7188405904 | -0.112383917 | 9.040984886  |  |
| 9                                    | 0     | -136.5654947987 | 1.7188407687 | -0.112383947 | 10.041434266 |  |
| 10                                   | 0     | -136.5648998913 | 1.7188407928 | -0.112383950 | 11.041599592 |  |
| 11                                   | 0     | -136.5646810709 | 1.7188407960 | -0.112383951 | 12.041660414 |  |
| 12                                   | 0     | -136.5646005760 | 1.7188407965 | -0.112383951 | 13.041682789 |  |
| 13                                   | 0     | -136.5645709642 | 1.7188407965 | -0.112383951 | 14.041691020 |  |
| 14                                   | 0     | -136.5645600707 | 1.7188407965 | -0.112383951 | 15.041694049 |  |
| 15                                   | 0     | -136.5645560632 | 1.7188407965 | -0.112383951 | 16.041695162 |  |
| 16                                   | 0     | -136.5645545889 | 1.7188407965 | -0.112383951 | 17.041695572 |  |

| Analysis of Maximum Likelihood Estimates |    |                    |                |            |            |              |
|------------------------------------------|----|--------------------|----------------|------------|------------|--------------|
| Parameter                                | DF | Parameter Estimate | Standard Error | Chi-Square | Pr > ChiSq | Hazard Ratio |
| LogBUN                                   | 1  | 1.71884            | 0.58376        | 8.6697     | 0.0032     | 5.578        |
| HGB                                      | 1  | -0.11238           | 0.06090        | 3.4053     | 0.0650     | 0.894        |
| Contrived                                | 1  | 17.04170           | 1080           | 0.0002     | 0.9874     | 25183399     |

Next, the Firth correction was applied as shown in the following statements. Also, the profile-likelihood confidence limits for the hazard ratios are requested by using the `RISKLIMITS=PL` option.

```
proc phreg data=Myeloma2;
 model Time*Vstatus(0)=LogBUN HGB Contrived /
 firth risklimits=pl itprint;
run;
```

PROC PHREG uses the penalized likelihood maximum to obtain a finite estimate for the coefficient of Contrived (Output 67.4.2). The much preferred profile-likelihood confidence limits, as shown in (Heinze and Schemper 2001), are also displayed.

**Output 67.4.2** Convergence Obtained with the Firth Correction

| The PHREG Procedure                  |       |                 |              |              |              |
|--------------------------------------|-------|-----------------|--------------|--------------|--------------|
| Maximum Likelihood Iteration History |       |                 |              |              |              |
| Iter                                 | Ridge | Log Likelihood  | LogBUN       | HGB          | Contrived    |
| 0                                    | 0     | -150.7361197494 | 0.0000000000 | 0.0000000000 | 0.0000000000 |
| 1                                    | 0     | -136.9933949142 | 2.0262484120 | -0.086519138 | 1.4338859318 |
| 2                                    | 0     | -134.5796594364 | 1.6770836974 | -0.109172604 | 2.6221444778 |
| 3                                    | 0     | -134.1572923217 | 1.7163408994 | -0.111166227 | 3.4458043289 |
| 4                                    | 0     | -134.1229607193 | 1.7209210332 | -0.112007726 | 3.7923555412 |
| 5                                    | 0     | -134.1228364805 | 1.7219588214 | -0.112178328 | 3.8174197804 |
| 6                                    | 0     | -134.1228355256 | 1.7220081673 | -0.112187764 | 3.8151642206 |

| Analysis of Maximum Likelihood Estimates |    |                    |                |            |            |
|------------------------------------------|----|--------------------|----------------|------------|------------|
| Parameter                                | DF | Parameter Estimate | Standard Error | Chi-Square | Pr > ChiSq |
| LogBUN                                   | 1  | 1.72201            | 0.58379        | 8.7008     | 0.0032     |
| HGB                                      | 1  | -0.11219           | 0.06059        | 3.4279     | 0.0641     |
| Contrived                                | 1  | 3.81516            | 1.55812        | 5.9955     | 0.0143     |

| Analysis of Maximum Likelihood Estimates |              |                                                       |          |       |
|------------------------------------------|--------------|-------------------------------------------------------|----------|-------|
| Parameter                                | Hazard Ratio | 95% Hazard Ratio Profile Likelihood Confidence Limits |          |       |
|                                          |              | Lower                                                 | Upper    | Upper |
| LogBUN                                   | 5.596        | 1.761                                                 | 17.231   |       |
| HGB                                      | 0.894        | 0.794                                                 | 1.007    |       |
| Contrived                                | 45.384       | 5.406                                                 | 6005.404 |       |

**Example 67.5: Conditional Logistic Regression for m:n Matching**

Conditional logistic regression is used to investigate the relationship between an outcome and a set of prognostic factors in matched case-control studies. The outcome is whether the subject is a case or a control. If there is only one case and one control, the matching is 1:1. The m:n matching refers to the situation in which there is a varying number of cases and controls in the matched sets. You can perform conditional logistic regression with the PHREG procedure by using the discrete logistic model and forming a stratum for each matched set. In addition, you need to create dummy survival times so that all the cases in a matched set have the same event time value, and the corresponding controls are censored at later times.

Consider the following set of low infant birth-weight data extracted from Appendix 1 of Hosmer and Lemeshow (1989). These data represent 189 women, of whom 59 had low-birth-weight babies and 130

had normal-weight babies. Under investigation are the following risk factors: weight in pounds at the last menstrual period (LWT), presence of hypertension (HT), smoking status during pregnancy (Smoke), and presence of uterine irritability (UI). For HT, Smoke, and UI, a value of 1 indicates a “yes” and a value of 0 indicates a “no.” The woman’s age (Age) is used as the matching variable. The SAS data set LBW contains a subset of the data corresponding to women between the ages of 16 and 32.

```

data LBW;
 input id Age Low LWT Smoke HT UI @@;
 Time=2-Low;
 datalines;
 25 16 1 130 0 0 0 143 16 0 110 0 0 0
 166 16 0 112 0 0 0 167 16 0 135 1 0 0
 189 16 0 135 1 0 0 206 16 0 170 0 0 0
 216 16 0 95 0 0 0 37 17 1 130 1 0 1
 45 17 1 110 1 0 0 68 17 1 120 1 0 0
 71 17 1 120 0 0 0 83 17 1 142 0 1 0
 93 17 0 103 0 0 0 113 17 0 122 1 0 0
 116 17 0 113 0 0 0 117 17 0 113 0 0 0
 147 17 0 119 0 0 0 148 17 0 119 0 0 0
 180 17 0 120 1 0 0 49 18 1 148 0 0 0
 50 18 1 110 1 0 0 89 18 0 107 1 0 1
 100 18 0 100 1 0 0 101 18 0 100 1 0 0
 132 18 0 90 1 0 1 133 18 0 90 1 0 1
 168 18 0 229 0 0 0 205 18 0 120 1 0 0
 208 18 0 120 0 0 0 23 19 1 91 1 0 1
 33 19 1 102 0 0 0 34 19 1 112 1 0 1
 85 19 0 182 0 0 1 96 19 0 95 0 0 0
 97 19 0 150 0 0 0 124 19 0 138 1 0 0
 129 19 0 189 0 0 0 135 19 0 132 0 0 0
 142 19 0 115 0 0 0 181 19 0 105 0 0 0
 187 19 0 235 1 1 0 192 19 0 147 1 0 0
 193 19 0 147 1 0 0 197 19 0 184 1 1 0
 224 19 0 120 1 0 0 27 20 1 150 1 0 0
 31 20 1 125 0 0 1 40 20 1 120 1 0 0
 44 20 1 80 1 0 1 47 20 1 109 0 0 0
 51 20 1 121 1 0 1 60 20 1 122 1 0 0
 76 20 1 105 0 0 0 87 20 0 105 1 0 0
 104 20 0 120 0 0 1 146 20 0 103 0 0 0
 155 20 0 169 0 0 1 160 20 0 141 0 0 1
 172 20 0 121 1 0 0 177 20 0 127 0 0 0
 201 20 0 120 0 0 0 211 20 0 170 1 0 0
 217 20 0 158 0 0 0 20 21 1 165 1 1 0
 28 21 1 200 0 0 1 30 21 1 103 0 0 0
 52 21 1 100 0 0 0 84 21 1 130 1 1 0
 88 21 0 108 1 0 1 91 21 0 124 0 0 0
 128 21 0 185 1 0 0 131 21 0 160 0 0 0
 144 21 0 110 1 0 1 186 21 0 134 0 0 0
 219 21 0 115 0 0 0 42 22 1 130 1 0 1
 67 22 1 130 1 0 0 92 22 0 118 0 0 0
 98 22 0 95 0 1 0 137 22 0 85 1 0 0
 138 22 0 120 0 1 0 140 22 0 130 1 0 0
 161 22 0 158 0 0 0 162 22 0 112 1 0 0
 174 22 0 131 0 0 0 184 22 0 125 0 0 0

```

```

204 22 0 169 0 0 0 220 22 0 129 0 0 0
 17 23 1 97 0 0 1 59 23 1 187 1 0 0
 63 23 1 120 0 0 0 69 23 1 110 1 0 0
 82 23 1 94 1 0 0 130 23 0 130 0 0 0
139 23 0 128 0 0 0 149 23 0 119 0 0 0
164 23 0 115 1 0 0 173 23 0 190 0 0 0
179 23 0 123 0 0 0 182 23 0 130 0 0 0
200 23 0 110 0 0 0 18 24 1 128 0 0 0
 19 24 1 132 0 1 0 29 24 1 155 1 0 0
 36 24 1 138 0 0 0 61 24 1 105 1 0 0
118 24 0 90 1 0 0 136 24 0 115 0 0 0
150 24 0 110 0 0 0 156 24 0 115 0 0 0
185 24 0 133 0 0 0 196 24 0 110 0 0 0
199 24 0 110 0 0 0 225 24 0 116 0 0 0
 13 25 1 105 0 1 0 15 25 1 85 0 0 1
 24 25 1 115 0 0 0 26 25 1 92 1 0 0
 32 25 1 89 0 0 0 46 25 1 105 0 0 0
103 25 0 118 1 0 0 111 25 0 120 0 0 1
120 25 0 155 0 0 0 121 25 0 125 0 0 0
169 25 0 140 0 0 0 188 25 0 95 1 0 1
202 25 0 241 0 1 0 215 25 0 120 0 0 0
221 25 0 130 0 0 0 35 26 1 117 1 0 0
 54 26 1 96 0 0 0 75 26 1 154 0 1 0
 77 26 1 190 1 0 0 95 26 0 113 1 0 0
115 26 0 168 1 0 0 154 26 0 133 1 0 0
218 26 0 160 0 0 0 16 27 1 150 0 0 0
 43 27 1 130 0 0 1 125 27 0 124 1 0 0
 4 28 1 120 1 0 1 79 28 1 95 1 0 0
105 28 0 120 1 0 0 109 28 0 120 0 0 0
112 28 0 167 0 0 0 151 28 0 140 0 0 0
159 28 0 250 1 0 0 212 28 0 134 0 0 0
214 28 0 130 0 0 0 10 29 1 130 0 0 1
 94 29 0 123 1 0 0 114 29 0 150 0 0 0
123 29 0 140 1 0 0 190 29 0 135 0 0 0
191 29 0 154 0 0 0 209 29 0 130 1 0 0
 65 30 1 142 1 0 0 99 30 0 107 0 0 1
141 30 0 95 1 0 0 145 30 0 153 0 0 0
176 30 0 110 0 0 0 195 30 0 137 0 0 0
203 30 0 112 0 0 0 56 31 1 102 1 0 0
107 31 0 100 0 0 1 126 31 0 215 1 0 0
163 31 0 150 1 0 0 222 31 0 120 0 0 0
 22 32 1 105 1 0 0 106 32 0 121 0 0 0
134 32 0 132 0 0 0 170 32 0 134 1 0 0
175 32 0 170 0 0 0 207 32 0 186 0 0 0
;

```

The variable Low is used to determine whether the subject is a case (Low=1, low-birth-weight baby) or a control (Low=0, normal-weight baby). The dummy time variable Time takes the value 1 for cases and 2 for controls.

The following statements produce a conditional logistic regression analysis of the data. The variable Time is the response, and Low is the censoring variable. Note that the data set is created so that all the cases have the same event time and the controls have later censored times. The matching variable Age is used in the STRATA statement so that each unique age value defines a stratum. The variables LWT, Smoke, HT, and UI are specified as explanatory variables. The TIES=DISCRETE option requests the discrete logistic model.

```
proc phreg data=LBW;
 model Time*Low(0)= LWT Smoke HT UI / ties=discrete;
 strata Age;
run;
```

The procedure displays a summary of the number of event and censored observations for each stratum. These are the number of cases and controls for each matched set shown in [Output 67.5.1](#).

**Output 67.5.1** Summary of Number of Case and Controls

| The PHREG Procedure                                |     |       |          |          |                  |  |
|----------------------------------------------------|-----|-------|----------|----------|------------------|--|
| Model Information                                  |     |       |          |          |                  |  |
| Data Set                                           |     |       | WORK.LBW |          |                  |  |
| Dependent Variable                                 |     |       | Time     |          |                  |  |
| Censoring Variable                                 |     |       | Low      |          |                  |  |
| Censoring Value(s)                                 |     |       | 0        |          |                  |  |
| Ties Handling                                      |     |       | DISCRETE |          |                  |  |
| Summary of the Number of Event and Censored Values |     |       |          |          |                  |  |
| Stratum                                            | Age | Total | Event    | Censored | Percent Censored |  |
| 1                                                  | 16  | 7     | 1        | 6        | 85.71            |  |
| 2                                                  | 17  | 12    | 5        | 7        | 58.33            |  |
| 3                                                  | 18  | 10    | 2        | 8        | 80.00            |  |
| 4                                                  | 19  | 16    | 3        | 13       | 81.25            |  |
| 5                                                  | 20  | 18    | 8        | 10       | 55.56            |  |
| 6                                                  | 21  | 12    | 5        | 7        | 58.33            |  |
| 7                                                  | 22  | 13    | 2        | 11       | 84.62            |  |
| 8                                                  | 23  | 13    | 5        | 8        | 61.54            |  |
| 9                                                  | 24  | 13    | 5        | 8        | 61.54            |  |
| 10                                                 | 25  | 15    | 6        | 9        | 60.00            |  |
| 11                                                 | 26  | 8     | 4        | 4        | 50.00            |  |
| 12                                                 | 27  | 3     | 2        | 1        | 33.33            |  |
| 13                                                 | 28  | 9     | 2        | 7        | 77.78            |  |
| 14                                                 | 29  | 7     | 1        | 6        | 85.71            |  |
| 15                                                 | 30  | 7     | 1        | 6        | 85.71            |  |
| 16                                                 | 31  | 5     | 1        | 4        | 80.00            |  |
| 17                                                 | 32  | 6     | 1        | 5        | 83.33            |  |
| Total                                              |     | 174   | 54       | 120      | 68.97            |  |

Results of the conditional logistic regression analysis are shown in [Output 67.5.2](#). Based on the Wald test for individual variables, the variables LWT, Smoke, and HT are statistically significant while UI is marginal.

The hazard ratios, computed by exponentiating the parameter estimates, are useful in interpreting the results of the analysis. If the hazard ratio of a prognostic factor is larger than 1, an increment in the factor increases the hazard rate. If the hazard ratio is less than 1, an increment in the factor decreases the hazard rate. Results indicate that women were more likely to have low-birth-weight babies if they were underweight in the last menstrual cycle, were hypertensive, smoked during pregnancy, or suffered uterine irritability.

**Output 67.5.2** Conditional Logistic Regression Analysis for the Low-Birth-Weight Study

| Convergence Status                            |                    |                    |                |            |            |              |
|-----------------------------------------------|--------------------|--------------------|----------------|------------|------------|--------------|
| Convergence criterion (GCONV=1E-8) satisfied. |                    |                    |                |            |            |              |
| Model Fit Statistics                          |                    |                    |                |            |            |              |
| Criterion                                     | Without Covariates | With Covariates    |                |            |            |              |
| -2 LOG L                                      | 159.069            | 141.108            |                |            |            |              |
| AIC                                           | 159.069            | 149.108            |                |            |            |              |
| SBC                                           | 159.069            | 157.064            |                |            |            |              |
| Testing Global Null Hypothesis: BETA=0        |                    |                    |                |            |            |              |
| Test                                          | Chi-Square         | DF                 | Pr > ChiSq     |            |            |              |
| Likelihood Ratio                              | 17.9613            | 4                  | 0.0013         |            |            |              |
| Score                                         | 17.3152            | 4                  | 0.0017         |            |            |              |
| Wald                                          | 15.5577            | 4                  | 0.0037         |            |            |              |
| Analysis of Maximum Likelihood Estimates      |                    |                    |                |            |            |              |
| Parameter                                     | DF                 | Parameter Estimate | Standard Error | Chi-Square | Pr > ChiSq | Hazard Ratio |
| LWT                                           | 1                  | -0.01498           | 0.00706        | 4.5001     | 0.0339     | 0.985        |
| Smoke                                         | 1                  | 0.80805            | 0.36797        | 4.8221     | 0.0281     | 2.244        |
| HT                                            | 1                  | 1.75143            | 0.73932        | 5.6120     | 0.0178     | 5.763        |
| UI                                            | 1                  | 0.88341            | 0.48032        | 3.3827     | 0.0659     | 2.419        |

For matched case-control studies with one case per matched set (1:n matching), the likelihood function for the conditional logistic regression reduces to that of the Cox model for the continuous time scale. For this situation, you can use the default TIES=BRESLOW.

---

**Example 67.6: Model Using Time-Dependent Explanatory Variables**

Time-dependent variables can be used to model the effects of subjects transferring from one treatment group to another. One example of the need for such strategies is the Stanford heart transplant program. Patients are accepted if physicians judge them suitable for heart transplant. Then, when a donor becomes available, physicians choose transplant recipients according to various medical criteria. A patient’s status can be changed during the study from waiting for a transplant to being a transplant recipient. Transplant status can be defined by the time-dependent covariate function  $z = z(t)$  as

$$z(t) = \begin{cases} 0 & \text{if the patient has not received the transplant at time } t \\ 1 & \text{if the patient has received the transplant at time } t \end{cases}$$



The Stanford heart transplant data that appear in Crowley and Hu (1977) consist of 103 patients, 69 of whom received transplants. The data are saved in a SAS data set called Heart in the following DATA step. For each patient in the program, there is a birth date (Bir\_Date), a date of acceptance (Acc\_Date), and a date last seen (Ter\_Date). The survival time (Time) in days is defined as  $\text{Time} = \text{Ter\_Date} - \text{Acc\_Date}$ . The survival time is said to be uncensored (Status=1) or censored (Status=0), depending on whether Ter\_Date is the date of death or the closing date of the study. The age, in years, at acceptance into the program is  $\text{Acc\_Age} = (\text{Acc\_Date} - \text{Bir\_Date}) / 365$ . Previous open-heart surgery for each patient is indicated by the variable PrevSurg. For each transplant recipient, there is a date of transplant (Xpl\_Date) and three measures (NMismatch, Antigen, Mismatch) of tissue-type mismatching. The waiting period (WaitTime) in days for a transplant recipient is calculated as  $\text{WaitTime} = \text{Xpl\_Date} - \text{Acc\_Date}$ , and the age (in years) at transplant is  $\text{Xpl\_Age} = (\text{Xpl\_Date} - \text{Bir\_Date}) / 365$ . For those who do not receive heart transplants, the WaitTime, Xpl\_Age, NMismatch, Antigen, and Mismatch variables contain missing values.

The input data contain dates that have a two-digit year representation. The SAS option YEARCUTOFF=1900 is specified to ensure that a two-digit year xx is year 19xx.

```
options yearcutoff=1900;
data Heart;
 input ID
 @5 Bir_Date mmddyy8.
 @14 Acc_Date mmddyy8.
 @23 Xpl_Date mmddyy8.
 @32 Ter_Date mmddyy8.
 @41 Status 1.
 @43 PrevSurg 1.
 @45 NMismatch 1.
 @47 Antigen 1.
 @49 Mismatch 4.
 @54 Reject 1.
 @56 NotTyped $1.;
 label Bir_Date = 'Date of birth'
 Acc_Date = 'Date of acceptance'
 Xpl_Date = 'Date of transplant'
 Ter_Date = 'Date last seen'
 Status = 'Dead=1 Alive=0'
 PrevSurg = 'Previous surgery'
 NMismatch= 'No of mismatches'
 Antigen = 'HLA-A2 antigen'
 Mismatch = 'Mismatch score'
 NotTyped = 'y=not tissue-typed';
 Time= Ter_Date - Acc_Date;
 Acc_Age=int((Acc_Date - Bir_Date)/365);
 if (Xpl_Date ne .) then do;
 WaitTime= Xpl_Date - Acc_Date;
 Xpl_Age= int((Xpl_Date - Bir_Date)/365);
 end;
 datalines;
1 01 10 37 11 15 67 01 03 68 1 0
2 03 02 16 01 02 68 01 07 68 1 0
3 09 19 13 01 06 68 01 06 68 01 21 68 1 0 2 0 1.11 0
4 12 23 27 03 28 68 05 02 68 05 05 68 1 0 3 0 1.66 0
5 07 28 47 05 10 68 05 27 68 1 0
6 11 08 13 06 13 68 06 15 68 1 0
```

```

7 08 29 17 07 12 68 08 31 68 05 17 70 1 0 4 0 1.32 1
8 03 27 23 08 01 68 09 09 68 1 0
9 06 11 21 08 09 68 11 01 68 1 0
10 02 09 26 08 11 68 08 22 68 10 07 68 1 0 2 0 0.61 1
11 08 22 20 08 15 68 09 09 68 01 14 69 1 0 1 0 0.36 0
12 07 09 15 09 17 68 09 24 68 1 0
13 02 22 14 09 19 68 10 05 68 12 08 68 1 0 3 0 1.89 1
14 09 16 14 09 20 68 10 26 68 07 07 72 1 0 1 0 0.87 1
15 12 04 14 09 27 68 09 27 68 1 1
16 05 16 19 10 26 68 11 22 68 08 29 69 1 0 2 0 1.12 1
17 06 29 48 10 28 68 12 02 68 1 0
18 12 27 11 11 01 68 11 20 68 12 13 68 1 0 3 0 2.05 0
19 10 04 09 11 18 68 12 24 68 1 0
20 10 19 13 01 29 69 02 15 69 02 25 69 1 0 3 1 2.76 1
21 09 29 25 02 01 69 02 08 69 11 29 71 1 0 2 0 1.13 1
22 06 05 26 03 18 69 03 29 69 05 07 69 1 0 3 0 1.38 1
23 12 02 10 04 11 69 04 13 69 04 13 71 1 0 3 0 0.96 1
24 07 07 17 04 25 69 07 16 69 11 29 69 1 0 3 1 1.62 1
25 02 06 36 04 28 69 05 22 69 04 01 74 0 0 2 0 1.06 0
26 10 18 38 05 01 69 03 01 73 0 0
27 07 21 60 05 04 69 01 21 70 1 0
28 05 30 15 06 07 69 08 16 69 08 17 69 1 0 2 0 0.47 0
29 02 06 19 07 14 69 08 17 69 1 0
30 09 20 24 08 19 69 09 03 69 12 18 71 1 0 4 0 1.58 1
31 10 04 14 08 23 69 09 07 69 1 0
32 04 02 05 08 29 69 09 14 69 11 13 69 1 0 4 0 0.69 1
33 01 01 21 11 27 69 01 16 70 04 01 74 0 0 3 0 0.91 0
34 05 24 29 12 12 69 01 03 70 04 01 74 0 0 2 0 0.38 0
35 08 04 26 01 21 70 02 01 70 1 0
36 05 01 21 04 04 70 05 19 70 07 12 70 1 0 2 0 2.09 1
37 10 24 08 04 25 70 05 13 70 06 29 70 1 0 3 1 0.87 1
38 11 14 28 05 05 70 05 09 70 05 09 70 1 0 3 0 0.87 0
39 11 12 19 05 20 70 05 21 70 07 11 70 1 0 y
40 11 30 21 05 25 70 07 04 70 04 01 74 0 1 4 0 0.75 0
41 04 30 25 08 19 70 10 15 70 04 01 74 0 1 2 0 0.98 0
42 03 13 34 08 21 70 08 23 70 1 0
43 06 01 27 10 22 70 10 23 70 1 1
44 05 02 28 11 30 70 01 08 71 1 1
45 10 30 34 01 05 71 01 05 71 02 18 71 1 0 1 0 0.0 0
46 06 01 22 01 10 71 01 11 71 10 01 73 1 1 2 0 0.81 1
47 12 28 23 02 02 71 02 22 71 04 14 71 1 0 3 0 1.38 1
48 01 23 15 02 05 71 02 13 71 1 0
49 06 21 34 02 15 71 03 22 71 04 01 74 0 1 4 0 1.35 0
50 03 28 25 02 15 71 05 08 71 10 21 73 1 1 y
51 06 29 22 03 24 71 04 24 71 01 02 72 1 0 4 1 1.08 1
52 01 24 30 04 25 71 08 04 71 1 0
53 02 27 24 07 02 71 08 11 71 01 05 72 1 0 y
54 09 16 23 07 02 71 07 04 71 1 0
55 02 24 19 08 09 71 08 18 71 10 08 71 1 0 2 0 1.51 1
56 12 05 32 09 03 71 11 08 71 04 01 74 0 0 4 0 0.98 0
57 06 08 30 09 13 71 02 08 72 1 0
58 09 17 23 09 23 71 10 13 71 08 30 72 1 1 2 1 1.82 1
59 05 12 30 09 29 71 12 15 71 04 01 74 0 1 2 0 0.19 0
60 10 29 22 11 18 71 11 20 71 01 24 72 1 0 3 0 0.66 1

```

```

61 05 12 19 12 04 71 12 05 71 1 0
62 08 01 32 12 09 71 02 15 72 1 0
63 04 15 39 12 12 71 01 07 72 04 01 74 0 0 3 1 1.93 0
64 04 09 23 02 01 72 03 04 72 09 06 73 1 1 1 0 0.12 0
65 11 19 20 03 06 72 03 17 72 05 22 72 1 0 2 0 1.12 1
66 01 02 19 03 20 72 04 20 72 1 0
67 09 03 52 03 23 72 05 18 72 01 01 73 1 0 3 0 1.02 0
68 01 10 27 04 07 72 04 09 72 06 13 72 1 0 3 1 1.68 1
69 06 05 24 06 01 72 06 10 72 04 01 74 0 0 2 0 1.20 0
70 06 17 19 06 17 72 06 21 72 07 16 72 1 0 3 1 1.68 1
71 02 22 25 07 21 72 08 20 72 04 01 74 0 0 3 0 0.97 0
72 11 22 45 08 14 72 08 17 72 04 01 74 0 0 3 1 1.46 0
73 05 13 16 09 11 72 10 07 72 12 09 72 1 0 3 1 2.16 1
74 07 20 43 09 18 72 09 22 72 10 04 72 1 0 1 0 0.61 0
75 07 25 20 09 29 72 09 30 72 1 0
76 09 03 20 10 04 72 11 18 72 04 01 74 0 1 3 1 1.70 0
77 08 27 31 10 06 72 10 26 72 1 0
78 02 20 24 11 03 72 05 31 73 04 01 74 0 0 3 0 0.81 0
79 02 18 19 11 30 72 02 04 73 03 05 73 1 0 2 0 1.08 1
80 06 27 26 12 06 72 12 31 72 04 01 74 0 1 3 0 1.41 0
81 02 21 20 01 12 73 01 17 73 04 01 74 0 0 4 1 1.94 0
82 08 19 42 11 01 71 01 01 73 0 0
83 10 04 19 01 24 73 02 24 73 04 13 73 1 0 4 0 3.05 0
84 05 13 30 01 30 73 03 07 73 12 29 73 1 0 4 0 0.60 1
85 02 13 25 02 06 73 02 10 73 1 0
86 03 30 24 03 01 73 03 08 73 04 01 74 0 0 3 1 1.44 0
87 12 19 26 03 21 73 05 19 73 07 08 73 1 0 2 0 2.25 1
88 11 16 18 03 28 73 04 27 73 04 01 74 0 0 3 0 0.68 0
89 03 19 22 04 05 73 08 21 73 10 28 73 1 0 4 1 1.33 1
90 03 25 21 04 06 73 09 12 73 10 08 73 1 1 3 1 0.82 0
91 09 08 25 04 13 73 03 18 74 1 0
92 05 03 28 04 27 73 03 02 74 04 01 74 0 0 1 0 0.16 0
93 10 10 25 07 11 73 08 07 73 04 01 74 0 0 2 0 0.33 0
94 11 11 29 09 14 73 09 17 73 02 25 74 1 1 3 0 1.20 1
95 06 11 33 09 22 73 09 23 73 10 07 73 1 0
96 02 09 47 10 04 73 10 16 73 04 01 74 0 0 2 0 0.46 0
97 04 11 50 11 22 73 12 12 73 04 01 74 0 0 3 1 1.78 0
98 04 28 45 12 14 73 03 19 74 04 01 74 0 0 4 1 0.77 0
99 02 24 24 12 25 73 01 14 74 1 0
100 01 31 39 02 22 74 03 31 74 04 01 74 0 1 3 0 0.67 0
101 08 25 24 03 02 74 04 01 74 0 0
102 10 30 33 03 22 74 04 01 74 0 0
103 05 20 28 09 13 67 09 18 67 1 0
;

```

Crowley and Hu (1977) have presented a number of analyses to assess the effects of various explanatory variables on the survival of patients. This example fits two of the models that they have considered.

The first model consists of two explanatory variables—the transplant status and the age at acceptance. The transplant status (XStatus) is a time-dependent variable defined by the programming statements between the MODEL statement and the RUN statement. The XStatus variable takes the value 1 or 0 at time  $t$  (measured from the date of acceptance), depending on whether or not the patient has received a transplant at that time. Note that the value of XStatus changes for subjects in each risk set (subjects still alive just before each distinct event time); therefore, the variable cannot be created in the DATA step. The variable

Acc\_Age, which is not time dependent, accounts for the possibility that pretransplant risks vary with age. The following statements fit this model:

```
proc phreg data= Heart;
 model Time*Status(0)= XStatus Acc_Age;
 if (WaitTime = . or Time < WaitTime) then XStatus=0.;
 else XStatus= 1.0;
run;
```

Results of this analysis are shown in [Output 67.6.1](#). Transplantation appears to be associated with a slight decrease in risk, although the effect is not significant ( $p = 0.8261$ ). The age at acceptance as a pretransplant risk factor adds significantly to the model ( $p = 0.0289$ ). The risk increases significantly with age at acceptance.

**Output 67.6.1** Heart Transplant Study Analysis I

| The PHREG Procedure                                |                    |                 |                  |
|----------------------------------------------------|--------------------|-----------------|------------------|
| Model Information                                  |                    |                 |                  |
| Data Set                                           | WORK.HEART         |                 |                  |
| Dependent Variable                                 | Time               |                 |                  |
| Censoring Variable                                 | Status             | Dead=1 Alive=0  |                  |
| Censoring Value(s)                                 | 0                  |                 |                  |
| Ties Handling                                      | BRESLOW            |                 |                  |
| Number of Observations Read                        |                    | 103             |                  |
| Number of Observations Used                        |                    | 103             |                  |
| Summary of the Number of Event and Censored Values |                    |                 |                  |
|                                                    | Total              | Event           | Censored         |
|                                                    | 103                | 75              | 28               |
|                                                    |                    |                 | Percent Censored |
|                                                    |                    |                 | 27.18            |
| Convergence Status                                 |                    |                 |                  |
| Convergence criterion (GCONV=1E-8) satisfied.      |                    |                 |                  |
| Model Fit Statistics                               |                    |                 |                  |
| Criterion                                          | Without Covariates | With Covariates |                  |
| -2 LOG L                                           | 596.651            | 591.292         |                  |
| AIC                                                | 596.651            | 595.292         |                  |
| SBC                                                | 596.651            | 599.927         |                  |

## Output 67.6.1 continued

| Testing Global Null Hypothesis: BETA=0   |    |                    |                |            |            |              |
|------------------------------------------|----|--------------------|----------------|------------|------------|--------------|
| Test                                     |    | Chi-Square         | DF             | Pr > ChiSq |            |              |
| Likelihood Ratio                         |    | 5.3593             | 2              | 0.0686     |            |              |
| Score                                    |    | 4.8093             | 2              | 0.0903     |            |              |
| Wald                                     |    | 4.7999             | 2              | 0.0907     |            |              |
| Analysis of Maximum Likelihood Estimates |    |                    |                |            |            |              |
| Parameter                                | DF | Parameter Estimate | Standard Error | Chi-Square | Pr > ChiSq | Hazard Ratio |
| XStatus                                  | 1  | -0.06720           | 0.30594        | 0.0482     | 0.8261     | 0.935        |
| Acc_Age                                  | 1  | 0.03158            | 0.01446        | 4.7711     | 0.0289     | 1.032        |

The second model consists of three explanatory variables—the transplant status, the transplant age, and the mismatch score. Four transplant recipients who were not typed have no Mismatch values; they are excluded from the analysis by the use of a WHERE clause. The transplant age (XAge) and the mismatch score (XScore) are also time dependent and are defined in a fashion similar to that of XStatus. While the patient is waiting for a transplant, XAge and XScore have a value of 0. After the patient has migrated to the recipient population, XAge takes on the value of Xpl\_Age (transplant age for the recipient), and XScore takes on the value of Mismatch (a measure of the degree of dissimilarity between donor and recipient). The following statements fit this model:

```
proc phreg data= Heart;
 model Time*Status(0)= XStatus XAge XScore;
 where NotTyped ^= 'y';
 if (WaitTime = . or Time < WaitTime) then do;
 XStatus=0.;
 XAge=0.;
 XScore= 0.;
 end;
 else do;
 XStatus= 1.0;
 XAge= Xpl_Age;
 XScore= Mismatch;
 end;
run;
```

Results of the analysis are shown in [Output 67.6.2](#). Note that only 99 patients are included in this analysis, instead of 103 patients as in the previous analysis, since four transplant recipients who were not typed are excluded. The variable XAge is statistically significant ( $p = 0.0143$ ), with a hazard ratio exceeding 1. Therefore, patients who had a transplant at younger ages lived longer than those who received a transplant later in their lives. The variable XScore has only minimal effect on the survival ( $p = 0.1121$ ).

**Output 67.6.2** Heart Transplant Study Analysis II

| The PHREG Procedure                                |                  |                    |                 |                  |            |              |
|----------------------------------------------------|------------------|--------------------|-----------------|------------------|------------|--------------|
| Model Information                                  |                  |                    |                 |                  |            |              |
| Data Set                                           | WORK.HEART       |                    |                 |                  |            |              |
| Dependent Variable                                 | Time             |                    |                 |                  |            |              |
| Censoring Variable                                 | Status           | Dead=1 Alive=0     |                 |                  |            |              |
| Censoring Value(s)                                 | 0                |                    |                 |                  |            |              |
| Ties Handling                                      | BRESLOW          |                    |                 |                  |            |              |
|                                                    |                  |                    |                 |                  |            |              |
| Number of Observations Read                        |                  |                    |                 |                  |            | 99           |
| Number of Observations Used                        |                  |                    |                 |                  |            | 99           |
|                                                    |                  |                    |                 |                  |            |              |
| Summary of the Number of Event and Censored Values |                  |                    |                 |                  |            |              |
|                                                    | Total            | Event              | Censored        | Percent Censored |            |              |
|                                                    | 99               | 71                 | 28              | 28.28            |            |              |
|                                                    |                  |                    |                 |                  |            |              |
| Convergence Status                                 |                  |                    |                 |                  |            |              |
| Convergence criterion (GCONV=1E-8) satisfied.      |                  |                    |                 |                  |            |              |
|                                                    |                  |                    |                 |                  |            |              |
| Model Fit Statistics                               |                  |                    |                 |                  |            |              |
|                                                    | Criterion        | Without Covariates | With Covariates |                  |            |              |
|                                                    | -2 LOG L         | 561.680            | 551.874         |                  |            |              |
|                                                    | AIC              | 561.680            | 557.874         |                  |            |              |
|                                                    | SBC              | 561.680            | 564.662         |                  |            |              |
|                                                    |                  |                    |                 |                  |            |              |
| Testing Global Null Hypothesis: BETA=0             |                  |                    |                 |                  |            |              |
|                                                    | Test             | Chi-Square         | DF              | Pr > ChiSq       |            |              |
|                                                    | Likelihood Ratio | 9.8059             | 3               | 0.0203           |            |              |
|                                                    | Score            | 9.0521             | 3               | 0.0286           |            |              |
|                                                    | Wald             | 9.0554             | 3               | 0.0286           |            |              |
|                                                    |                  |                    |                 |                  |            |              |
| Analysis of Maximum Likelihood Estimates           |                  |                    |                 |                  |            |              |
| Parameter                                          | DF               | Parameter Estimate | Standard Error  | Chi-Square       | Pr > ChiSq | Hazard Ratio |
| XStatus                                            | 1                | -3.19837           | 1.18746         | 7.2547           | 0.0071     | 0.041        |
| XAge                                               | 1                | 0.05544            | 0.02263         | 6.0019           | 0.0143     | 1.057        |
| XScore                                             | 1                | 0.44490            | 0.28001         | 2.5245           | 0.1121     | 1.560        |

## Example 67.7: Time-Dependent Repeated Measurements of a Covariate

Repeated determinations can be made during the course of a study of variables thought to be related to survival. Consider an experiment to study the dosing effect of a tumor-promoting agent. Forty-five rodents initially exposed to a carcinogen were randomly assigned to three dose groups. After the first death of an animal, the rodents were examined every week for the number of papillomas. Investigators were interested in determining the effects of dose on the carcinoma incidence after adjusting for the number of papillomas.

The input data set TUMOR consists of the following 19 variables:

- ID (subject identification)
- Time (survival time of the subject)
- Dead (censoring status where 1=dead and 0=censored)
- Dose (dose of the tumor-promoting agent)
- P1–P15 (number of papillomas at the 15 times that animals died. These 15 death times are weeks 27, 34, 37, 41, 43, 45, 46, 47, 49, 50, 51, 53, 65, 67, and 71. For instance, subject 1 died at week 47; it had no papilloma at week 27, five papillomas at week 34, six at week 37, eight at week 41, and 10 at weeks 43, 45, 46, and 47. For an animal that died before week 71, the number of papillomas is missing for those times beyond its death.)

The following SAS statements create the data set TUMOR:

```
data Tumor;
 infile datalines missover;
 input ID Time Dead Dose P1-P15;
 label ID='Subject ID';
 datalines;
1 47 1 1.0 0 5 6 8 10 10 10 10
2 71 1 1.0 0 0 0 0 0 0 0 0 1 1 1 1 1 1 1
3 81 0 1.0 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1
4 81 0 1.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
5 81 0 1.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
6 65 1 1.0 0 0 0 1 1 1 1 1 1 1 1 1 1 1
7 71 0 1.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
8 69 0 1.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
9 67 1 1.0 0 0 1 1 2 2 2 2 3 3 3 3 3 3
10 81 0 1.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
11 37 1 1.0 9 9 9
12 81 0 1.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
13 77 0 1.0 0 0 0 0 1 1 1 1 1 1 1 1 1 1 1
14 81 0 1.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
15 81 0 1.0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16 54 0 2.5 0 1 1 1 2 2 2 2 2 2 2 2
17 53 0 2.5 0 0 0 0 0 0 0 0 0 0 0 0
18 38 0 2.5 5 13 14
19 54 0 2.5 2 6 6 6 6 6 6 6 6 6 6 6
20 51 1 2.5 15 15 15 16 16 17 17 17 17 17
21 47 1 2.5 13 20 20 20 20 20 20
```

```

22 27 1 2.5 22
23 41 1 2.5 6 13 13 13
24 49 1 2.5 0 3 3 3 3 3 3 3 3
25 53 0 2.5 0 0 1 1 1 1 1 1 1 1 1
26 50 1 2.5 0 0 2 3 4 6 6 6 6 6
27 37 1 2.5 3 15 15
28 49 1 2.5 2 3 3 3 3 4 4 4 4
29 46 1 2.5 4 6 7 9 9 9 9
30 48 0 2.5 15 26 26 26 26 26 26
31 54 0 10.0 12 14 15 15 15 15 15 15 15 15 15
32 37 1 10.0 12 16 17
33 53 1 10.0 3 6 6 6 6 6 6 6 6 6 6
34 45 1 10.0 4 12 15 20 20 20
35 53 0 10.0 6 10 13 13 13 15 15 15 15 15 20
36 49 1 10.0 0 2 2 2 2 2 2 2
37 39 0 10.0 7 8 8
38 27 1 10.0 17
39 49 1 10.0 0 6 9 14 14 14 14 14
40 43 1 10.0 14 18 20 20 20
41 28 0 10.0 8
42 34 1 10.0 11 18
43 45 1 10.0 10 12 16 16 16 16
44 37 1 10.0 0 1 1
45 43 1 10.0 9 19 19 19 19
;

```

The number of papillomas (NPap) for each animal in the study was measured repeatedly over time. One way of handling time-dependent repeated measurements in the PHREG procedure is to use programming statements to capture the appropriate covariate values of the subjects in each risk set. In this example, NPap is a time-dependent explanatory variable with values that are calculated by means of the programming statements shown in the following SAS statements:

```

proc phreg data=Tumor;
 model Time*Dead(0)=Dose NPap;
 array pp{*} P1-P14;
 array tt{*} t1-t15;
 t1=27; t2=34; t3=37; t4=41; t5=43;
 t6=45; t7=46; t8=47; t9=49; t10=50;
 t11=51; t12=53; t13=65; t14=67; t15=71;
 if Time < tt[1] then NPap=0;
 else if time >= tt[15] then NPap=P15;
 else do i=1 to dim(pp);
 if tt[i] <= Time < tt[i+1] then NPap= pp[i];
 end;
run;

```

At each death time, the NPap value of each subject in the risk set is recalculated to reflect the actual number of papillomas at the given death time. For instance, subject one in the data set Tumor was in the risk sets at weeks 27 and 34; at week 27, the animal had no papilloma, while at week 34, it had five papillomas. Results of the analysis are shown in [Output 67.7.1](#). After the number of papillomas is adjusted for, the dose effect of the tumor-promoting agent is not statistically significant.



## Output 67.7.1 Cox Regression Analysis on the Survival of Rodents

| The PHREG Procedure                                |                  |                    |                 |                  |            |              |
|----------------------------------------------------|------------------|--------------------|-----------------|------------------|------------|--------------|
| Model Information                                  |                  |                    |                 |                  |            |              |
| Data Set                                           | WORK.TUMOR       |                    |                 |                  |            |              |
| Dependent Variable                                 | Time             |                    |                 |                  |            |              |
| Censoring Variable                                 | Dead             |                    |                 |                  |            |              |
| Censoring Value(s)                                 | 0                |                    |                 |                  |            |              |
| Ties Handling                                      | BRESLOW          |                    |                 |                  |            |              |
|                                                    |                  |                    |                 |                  |            |              |
| Number of Observations Read                        | 45               |                    |                 |                  |            |              |
| Number of Observations Used                        | 45               |                    |                 |                  |            |              |
|                                                    |                  |                    |                 |                  |            |              |
| Summary of the Number of Event and Censored Values |                  |                    |                 |                  |            |              |
|                                                    | Total            | Event              | Censored        | Percent Censored |            |              |
|                                                    | 45               | 25                 | 20              | 44.44            |            |              |
|                                                    |                  |                    |                 |                  |            |              |
| Convergence Status                                 |                  |                    |                 |                  |            |              |
| Convergence criterion (GCONV=1E-8) satisfied.      |                  |                    |                 |                  |            |              |
|                                                    |                  |                    |                 |                  |            |              |
| Model Fit Statistics                               |                  |                    |                 |                  |            |              |
|                                                    | Criterion        | Without Covariates | With Covariates |                  |            |              |
|                                                    | -2 LOG L         | 166.793            | 143.269         |                  |            |              |
|                                                    | AIC              | 166.793            | 147.269         |                  |            |              |
|                                                    | SBC              | 166.793            | 149.707         |                  |            |              |
|                                                    |                  |                    |                 |                  |            |              |
| Testing Global Null Hypothesis: BETA=0             |                  |                    |                 |                  |            |              |
|                                                    | Test             | Chi-Square         | DF              | Pr > ChiSq       |            |              |
|                                                    | Likelihood Ratio | 23.5243            | 2               | <.0001           |            |              |
|                                                    | Score            | 28.0498            | 2               | <.0001           |            |              |
|                                                    | Wald             | 21.1646            | 2               | <.0001           |            |              |
|                                                    |                  |                    |                 |                  |            |              |
| Analysis of Maximum Likelihood Estimates           |                  |                    |                 |                  |            |              |
| Parameter                                          | DF               | Parameter Estimate | Standard Error  | Chi-Square       | Pr > ChiSq | Hazard Ratio |
| Dose                                               | 1                | 0.06885            | 0.05620         | 1.5010           | 0.2205     | 1.071        |
| NPap                                               | 1                | 0.11714            | 0.02998         | 15.2705          | <.0001     | 1.124        |

Another way to handle time-dependent repeated measurements in the PHREG procedure is to use the counting process style of input. Multiple records are created for each subject, one record for each distinct pattern of the time-dependent measurements. Each record contains a T1 value and a T2 value representing the time interval (T1,T2] during which the values of the explanatory variables remain unchanged. Each record also contains the censoring status at T2.

One advantage of using the counting process formulation is that you can easily obtain various residuals and influence statistics that are not available when programming statements are used to compute the values of the time-dependent variables. On the other hand, creating multiple records for the counting process formulation requires extra effort in data manipulation.

Consider a counting process style of input data set named Tumor1. It contains multiple observations for each subject in the data set Tumor. In addition to variables ID, Time, Dead, and Dose, four new variables are generated:

- T1 (left endpoint of the risk interval)
- T2 (right endpoint of the risk interval)
- NPap (number of papillomas in the time interval (T1,T2])
- Status (censoring status at T2)

For example, five observations are generated for the rodent that died at week 47 and that had no papilloma at week 27, five papillomas at week 34, six at week 37, eight at week 41, and 10 at weeks 43, 45, 46, and 47. The values of T1, T2, NPap, and Status for these five observations are (0,27,0,0), (27,34,5,0), (34,37,6,0), (37,41,8,0), and (41,47,10,1). Note that the variables ID, Time, and Dead are not needed for the estimation of the regression parameters, but they are useful for plotting the residuals.

The following SAS statements create the data set Tumor1:

```
data Tumor1(keep=ID Time Dead Dose T1 T2 NPap Status);
 array pp{*} P1-P14;
 array qq{*} P2-P15;
 array tt{1:15} _temporary_
 (27 34 37 41 43 45 46 47 49 50 51 53 65 67 71);
 set Tumor;
 T1 = 0;
 T2 = 0;
 Status = 0;
 if (Time = tt[1]) then do;
 T2 = tt[1];
 NPap = p1;
 Status = Dead;
 output;
 end;
 else do _i_=1 to dim(pp);
 if (tt[_i_] = Time) then do;
 T2= Time;
 NPap = pp[_i_];
 Status = Dead;
 output;
 end;
 end;
```

```

 else if (tt[_i_] < Time) then do;
 if (pp[_i_] ^= qq[_i_]) then do;
 if qq[_i_] = . then T2= Time;
 else T2= tt[_i_];
 NPap= pp[_i_];
 Status= 0;
 output;
 T1 = T2;
 end;
 end;
 end;
end;
if (Time >= tt[15]) then do;
 T2 = Time;
 NPap = P15;
 Status = Dead;
 output;
end;
run;

```

In the following SAS statements, the counting process MODEL specification is used. The DFBETA statistics are output to a SAS data set named Out1. Note that Out1 contains multiple observations for each subject—that is, one observation for each risk interval (T1,T2).

```

proc phreg data=Tumor1;
 model (T1,T2)*Status(0)=Dose NPap;
 output out=Out1 resmart=Mart dfbeta=db1-db2;
 id ID Time Dead;
run;

```

The output from PROC PHREG (not shown) is identical to [Output 67.7.1](#) except for the “Summary of the Number of Event and Censored Values” table. The number of event observations remains unchanged between the two specifications of PROC PHREG, but the number of censored observations differs due to the splitting of each subject’s data into multiple observations for the counting process style of input.

Next, the MEANS procedure sums up the component statistics for each subject and outputs the results to a SAS data set named Out2:

```

proc means data=Out1 noprint;
 by ID Time Dead;
 var Mart db1-db2;
 output out=Out2 sum=Mart db_Dose db_NPap;
run;

```

Finally, DFBETA statistics are plotted against subject ID for easy identification of influential points:

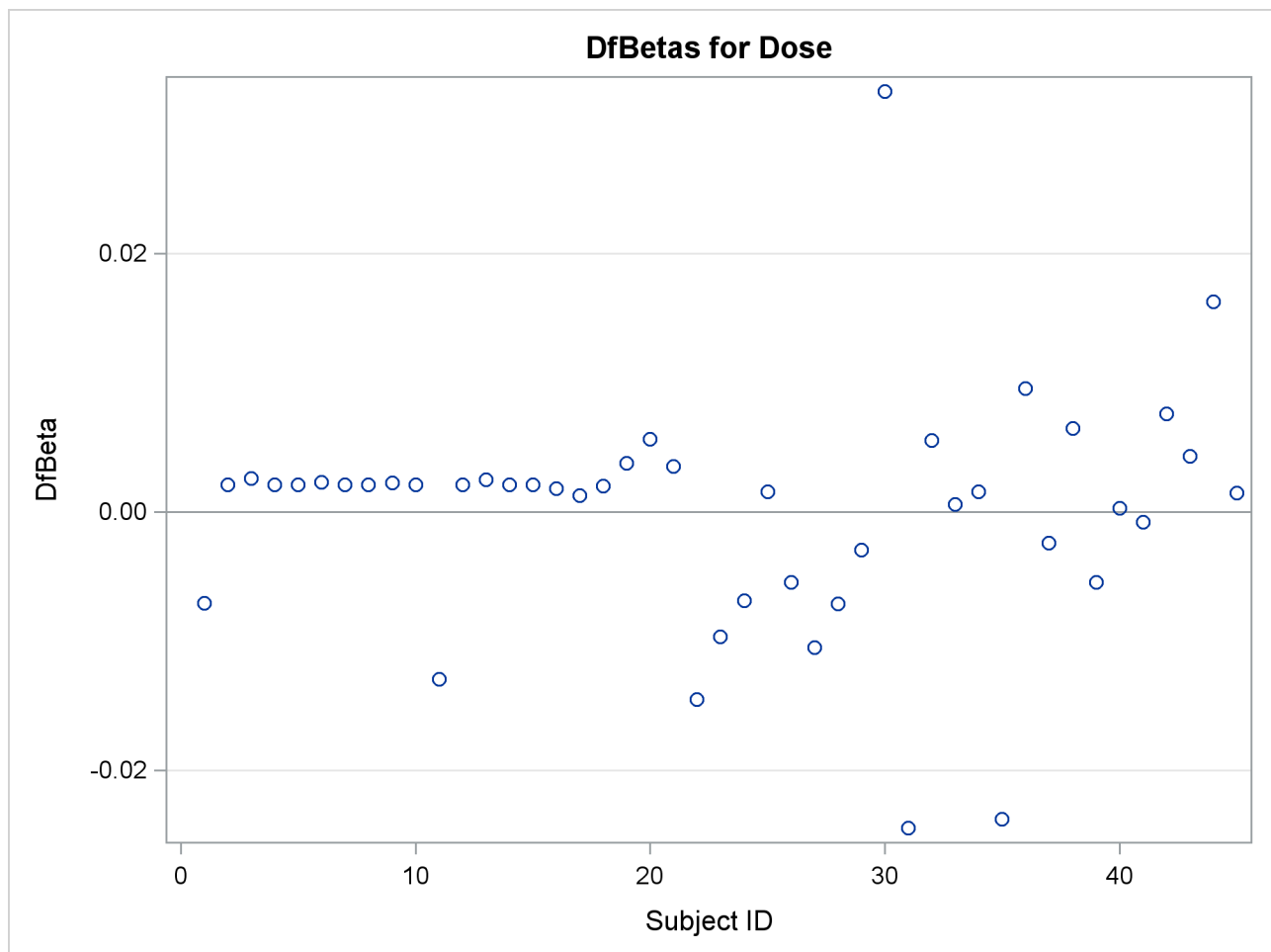
```

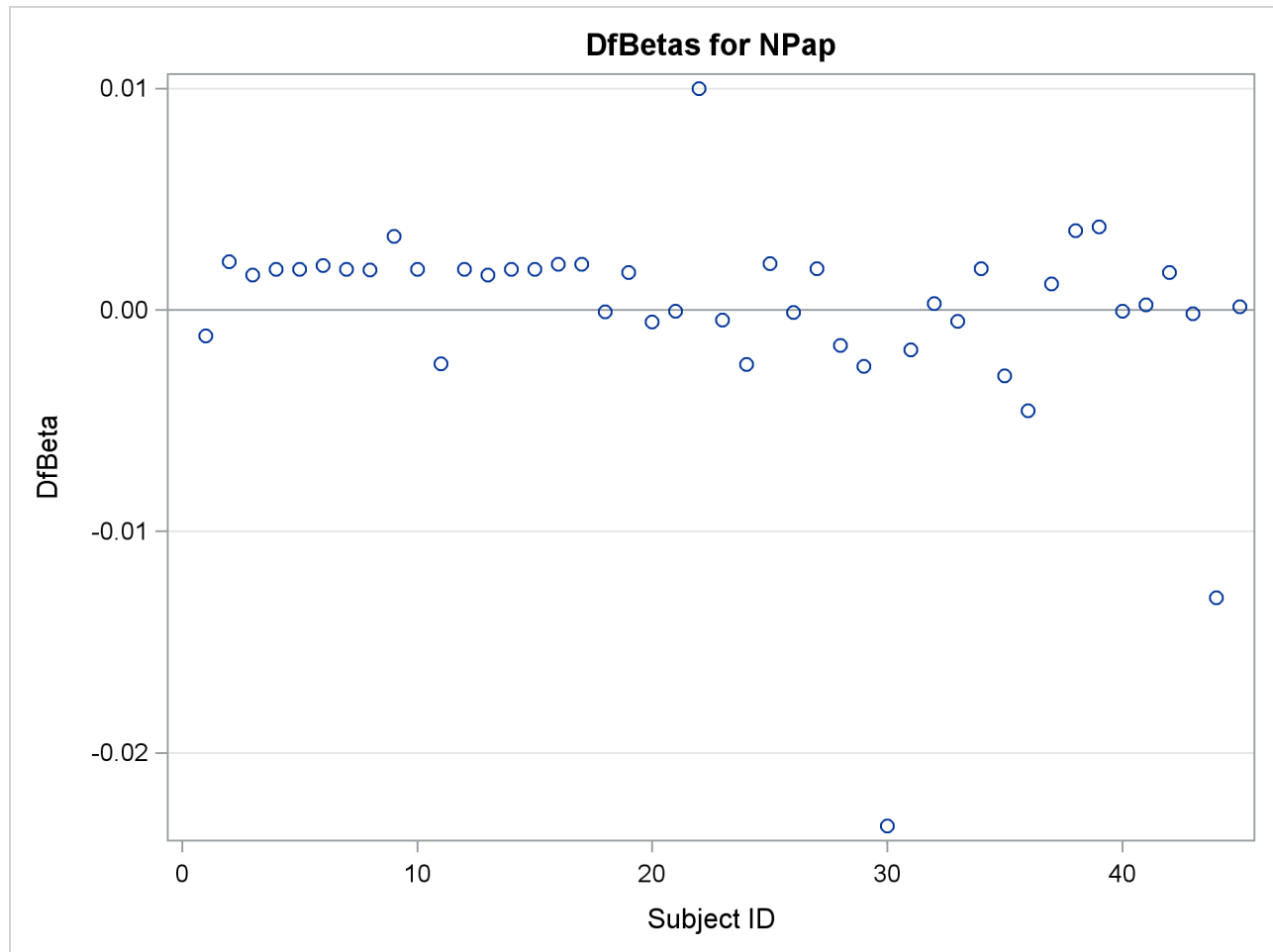
title 'DfBetas for Dose';
proc sgplot data=Out2;
 yaxis label="DfBeta" grid;
 refline 0 / axis=y;
 scatter y=db_Dose x=ID;
run;
title 'DfBetas for NPap';
proc sgplot data=Out2;
 yaxis label="DfBeta" grid;
 refline 0 / axis=y;
 scatter y=db_NPap x=ID;
run;

```

The plots of the DFBETA statistics are shown in [Output 67.7.2](#) and [Output 67.7.3](#). Subject 30 appears to have a large influence on both the Dose and NPap coefficients. Subjects 31 and 35 have considerable influences on the DOSE coefficient, while subjects 22 and 44 have rather large influences on the NPap coefficient.

**Output 67.7.2** Plot of DFBETA Statistic for DOSE versus Subject Number



**Output 67.7.3** Plot of DFBETA Statistic for NPAP versus Subject Number

### Example 67.8: Survival Curves

You might want to use your regression analysis results to predict the survivorship of subjects of specific covariate values. The `COVARIATES=` data set in the `BASELINE` statement enables you to specify the sets of covariate values for the prediction. On the other hand, you might want to summarize the survival experience of an average patient for a given population. The `DIRADJ` option in the `BASELINE` statement computes the direct adjusted survival curve that averages the estimated survival curves for patients whose covariates are represented in the `COVARIATES=` data set. By using the `PLOTS=` option in the `PROC PHREG` statement, you can use ODS Graphics to display the predicted survival curves. You can elect to output the predicted survival curves in a SAS data set by optionally specifying the `OUT=` option in the `BASELINE` statement. This example illustrates how to obtain the covariate-specific survival curves and the direct adjusted survival curve by using the Myeloma data set in [Example 67.1](#), where variables `LogBUN` and `HGB` were identified as the most important prognostic factors.

Suppose you want to compute the predicted survival curves for two sets of covariate values: (LogBUN=1.0, HGB=10) and (LogBUN=1.8, HGB=12). These values are saved in the data set `Inrisks` in the following DATA step. Also created in this data set is the variable `Id`, whose values will be used in identifying the covariate sets in the survival plot.

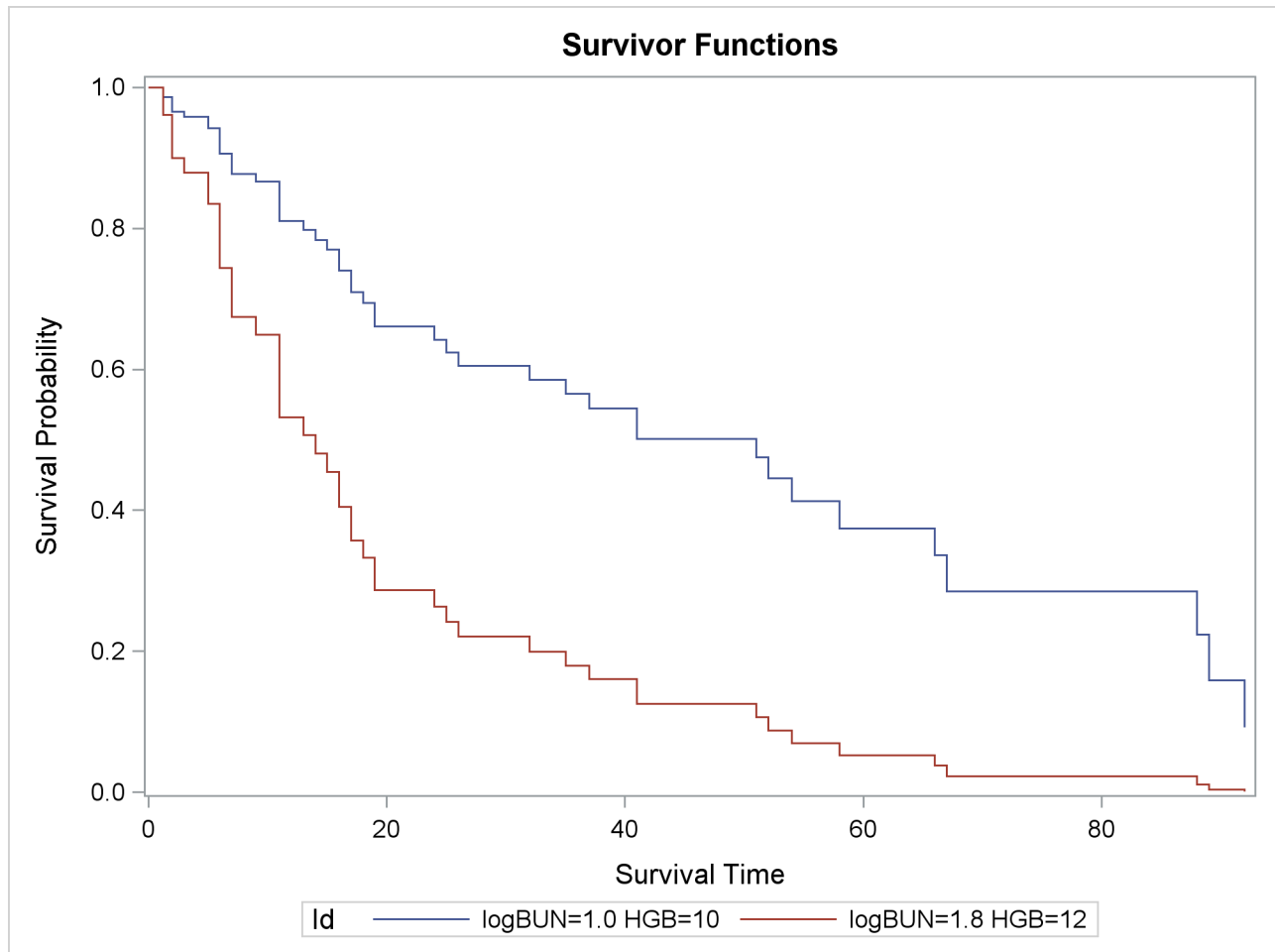
```
data Inrisks;
 length Id $20;
 input LogBUN HGB Id $12-31;
 datalines;
1.00 10.0 logBUN=1.0 HGB=10
1.80 12.0 logBUN=1.8 HGB=12
;
```

The following statements plot the survival functions in [Output 67.8.1](#) and save the survival estimates in the data set `Pred1`:

```
ods graphics on;
proc phreg data=Myeloma plots(overlay)=survival;
 model Time*VStatus(0)=LogBUN HGB;
 baseline covariates=Inrisks out=Pred1 survival=_all_/rowid=Id;
run;
```

The `COVARIATES=` option in the `BASELINE` statement specifies the data set that contains the set of covariates of interest. The `PLOTS=` option in the `PROC PHREG` statement creates the survival plot. The `OVERLAY` suboption overlays the two curves in the same plot. If the `OVERLAY` suboption is not specified, each curve is displayed in a separate plot. The `ROWID=` option in the `BASELINE` statement specifies that the values of the variable `Id` in the `COVARIATES=` data set be used to identify the curves in the plot. The `SURVIVAL=_ALL_` option in the `BASELINE` statement requests that the estimated survivor function, standard error, and lower and upper confidence limits for the survivor function be output into the SAS data set that is specified in the `OUT=` option.

The survival Plot ([Output 67.8.1](#)) contains two curves, one for each of row of covariates in the data set `Inrisks`.

**Output 67.8.1** Estimated Survivor Function Plot

The following statements print out the observations in the data set `Pred1` for the realization `LogBUN=1.00` and `HGB=10.0`:

```
proc print data=Pred1(where=(logBUN=1 and HGB=10));
run;
```

As shown in [Output 67.8.2](#), 32 observations represent the survivor function for the realization `LogBUN=1.00` and `HGB=10.0`. The first observation has survival time 0 and survivor function estimate 1.0. Each of the remaining 31 observations represents a distinct event time in the input data set `Myeloma`. These observations are presented in ascending order of the event times. Note that all the variables in the `COVARIATES=InRisks` data set are included in the `OUT=Pred1` data set. Likewise, you can print out the observations that represent the survivor function for the realization `LogBUN=1.80` and `HGB=12.0`.

**Output 67.8.2** Survivor Function Estimates for LogBUN=1.0 and HGB=10.0

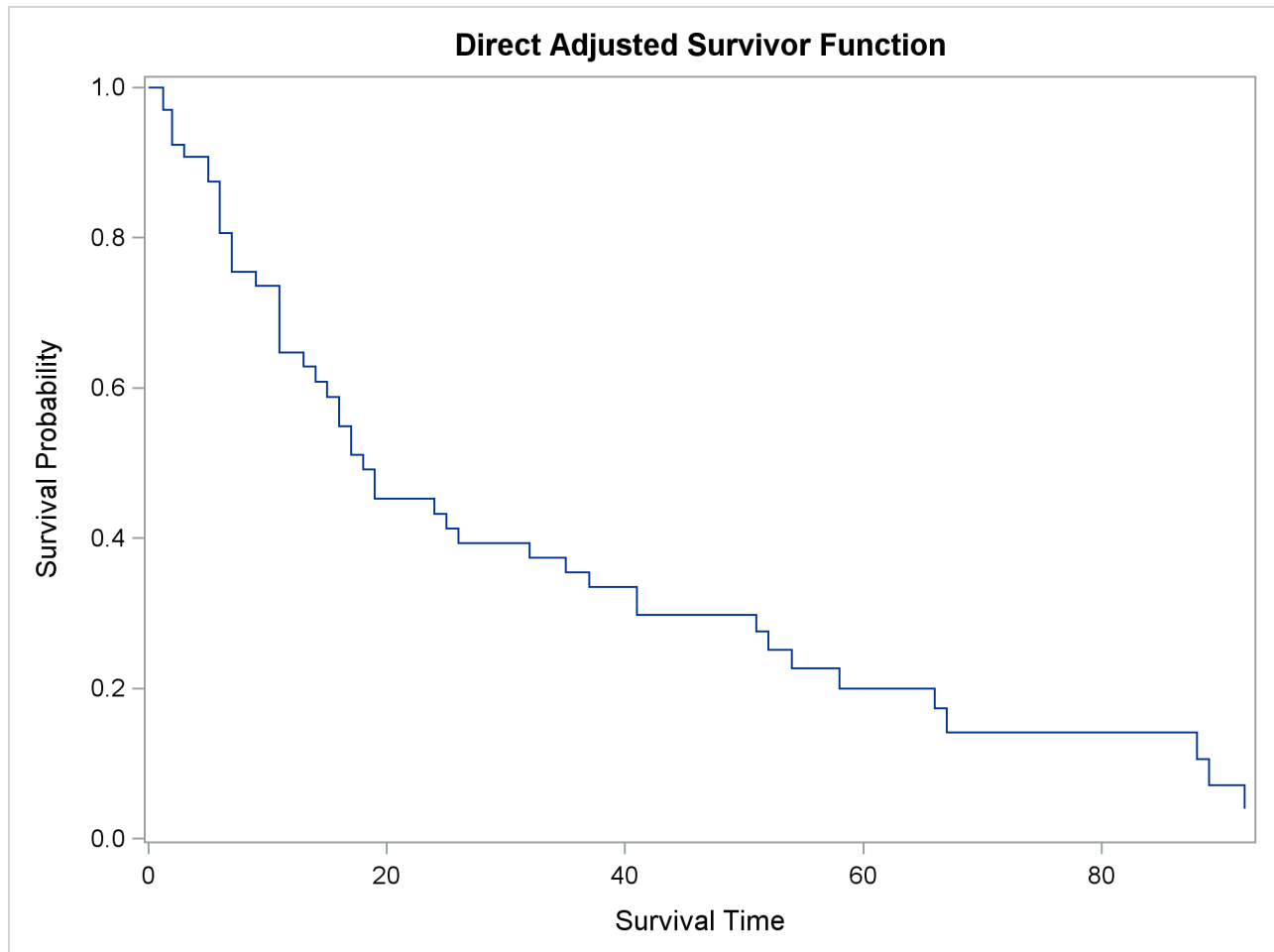
| Obs | Id                | Log<br>BUN | HGB | Time  | Survival | StdErr<br>Survival | Lower<br>Survival | Upper<br>Survival |
|-----|-------------------|------------|-----|-------|----------|--------------------|-------------------|-------------------|
| 1   | logBUN=1.0 HGB=10 | 1          | 10  | 0.00  | 1.00000  | .                  | .                 | .                 |
| 2   | logBUN=1.0 HGB=10 | 1          | 10  | 1.25  | 0.98678  | 0.01043            | 0.96655           | 1.00000           |
| 3   | logBUN=1.0 HGB=10 | 1          | 10  | 2.00  | 0.96559  | 0.01907            | 0.92892           | 1.00000           |
| 4   | logBUN=1.0 HGB=10 | 1          | 10  | 3.00  | 0.95818  | 0.02180            | 0.91638           | 1.00000           |
| 5   | logBUN=1.0 HGB=10 | 1          | 10  | 5.00  | 0.94188  | 0.02747            | 0.88955           | 0.99729           |
| 6   | logBUN=1.0 HGB=10 | 1          | 10  | 6.00  | 0.90635  | 0.03796            | 0.83492           | 0.98389           |
| 7   | logBUN=1.0 HGB=10 | 1          | 10  | 7.00  | 0.87742  | 0.04535            | 0.79290           | 0.97096           |
| 8   | logBUN=1.0 HGB=10 | 1          | 10  | 9.00  | 0.86646  | 0.04801            | 0.77729           | 0.96585           |
| 9   | logBUN=1.0 HGB=10 | 1          | 10  | 11.00 | 0.81084  | 0.05976            | 0.70178           | 0.93686           |
| 10  | logBUN=1.0 HGB=10 | 1          | 10  | 13.00 | 0.79800  | 0.06238            | 0.68464           | 0.93012           |
| 11  | logBUN=1.0 HGB=10 | 1          | 10  | 14.00 | 0.78384  | 0.06515            | 0.66601           | 0.92251           |
| 12  | logBUN=1.0 HGB=10 | 1          | 10  | 15.00 | 0.76965  | 0.06779            | 0.64762           | 0.91467           |
| 13  | logBUN=1.0 HGB=10 | 1          | 10  | 16.00 | 0.74071  | 0.07269            | 0.61110           | 0.89781           |
| 14  | logBUN=1.0 HGB=10 | 1          | 10  | 17.00 | 0.71005  | 0.07760            | 0.57315           | 0.87966           |
| 15  | logBUN=1.0 HGB=10 | 1          | 10  | 18.00 | 0.69392  | 0.07998            | 0.55360           | 0.86980           |
| 16  | logBUN=1.0 HGB=10 | 1          | 10  | 19.00 | 0.66062  | 0.08442            | 0.51425           | 0.84865           |
| 17  | logBUN=1.0 HGB=10 | 1          | 10  | 24.00 | 0.64210  | 0.08691            | 0.49248           | 0.83717           |
| 18  | logBUN=1.0 HGB=10 | 1          | 10  | 25.00 | 0.62360  | 0.08921            | 0.47112           | 0.82542           |
| 19  | logBUN=1.0 HGB=10 | 1          | 10  | 26.00 | 0.60523  | 0.09136            | 0.45023           | 0.81359           |
| 20  | logBUN=1.0 HGB=10 | 1          | 10  | 32.00 | 0.58549  | 0.09371            | 0.42784           | 0.80122           |
| 21  | logBUN=1.0 HGB=10 | 1          | 10  | 35.00 | 0.56534  | 0.09593            | 0.40539           | 0.78840           |
| 22  | logBUN=1.0 HGB=10 | 1          | 10  | 37.00 | 0.54465  | 0.09816            | 0.38257           | 0.77542           |
| 23  | logBUN=1.0 HGB=10 | 1          | 10  | 41.00 | 0.50178  | 0.10166            | 0.33733           | 0.74639           |
| 24  | logBUN=1.0 HGB=10 | 1          | 10  | 51.00 | 0.47546  | 0.10368            | 0.31009           | 0.72901           |
| 25  | logBUN=1.0 HGB=10 | 1          | 10  | 52.00 | 0.44510  | 0.10522            | 0.28006           | 0.70741           |
| 26  | logBUN=1.0 HGB=10 | 1          | 10  | 54.00 | 0.41266  | 0.10689            | 0.24837           | 0.68560           |
| 27  | logBUN=1.0 HGB=10 | 1          | 10  | 58.00 | 0.37465  | 0.10891            | 0.21192           | 0.66232           |
| 28  | logBUN=1.0 HGB=10 | 1          | 10  | 66.00 | 0.33626  | 0.10980            | 0.17731           | 0.63772           |
| 29  | logBUN=1.0 HGB=10 | 1          | 10  | 67.00 | 0.28529  | 0.11029            | 0.13372           | 0.60864           |
| 30  | logBUN=1.0 HGB=10 | 1          | 10  | 88.00 | 0.22412  | 0.10928            | 0.08619           | 0.58282           |
| 31  | logBUN=1.0 HGB=10 | 1          | 10  | 89.00 | 0.15864  | 0.10317            | 0.04435           | 0.56750           |
| 32  | logBUN=1.0 HGB=10 | 1          | 10  | 92.00 | 0.09180  | 0.08545            | 0.01481           | 0.56907           |

Next, the DIRADJ option in the BASELINE statement is used to request a survival curve that represents the survival experience of an average patient in the population in which the COVARIATES= data set is sampled. When the DIRADJ option is specified, PROC PHREG computes the direct adjusted survival function by averaging the predicted survival functions for the rows in the COVARIATES= data set. The following statements plot the direct adjusted survival function in [Output 67.8.3](#).

```
proc phreg data=Myeloma plots=survival;
 model Time*VStatus(0)=LogBUN HGB;
 baseline covariates=Myeloma survival=_all_/diradj;
run;
```

When the DIRADJ option is specified in the BASELINE statement, the default COVARIATES= data set is the input data set. For clarity, the COVARIATES=MYELOMA is specified in the BASELINE statement in the preceding PROC PHREG call.



**Output 67.8.3** Average Survival Function for the Myeloma Data

If neither the COVARIATES= data set nor the DIRADJ option is specified in the BASELINE statement, PROC PHREG computes a predicted survival curve based on  $\bar{\mathbf{Z}}$ , the average values of the covariate vectors in the input data (Neuberger et al. 1986). This curve represents the survival experience of a patient with an average prognostic index  $\beta'\bar{\mathbf{Z}}$  equal to the average prognostic index of all patients. This approach has a couple of drawbacks: it is possible that no patient could ever have such an average index, and it does not account for the variability in the prognostic factor from patient to patient.

The DIRADJ option is particularly useful if the model contains a categorical explanatory variable that represents different treatments of interest. By specifying this categorical variable in the GROUP= option, you obtain a direct adjusted survival curve for each category of the variable. In addition, you can use the OUTDIFF= option to save all pairwise differences of these direct adjusted survival probabilities in a data set. For illustration, consider a model that also includes the categorical variable Frac, which has a value 0 if a patient did not have a fracture at diagnosis and 1 otherwise, as an explanatory variable. The following statements plot the adjusted survival curves in [Output 67.8.4](#) and save the differences of the direct adjusted survival probabilities in the data set Diff1:

```

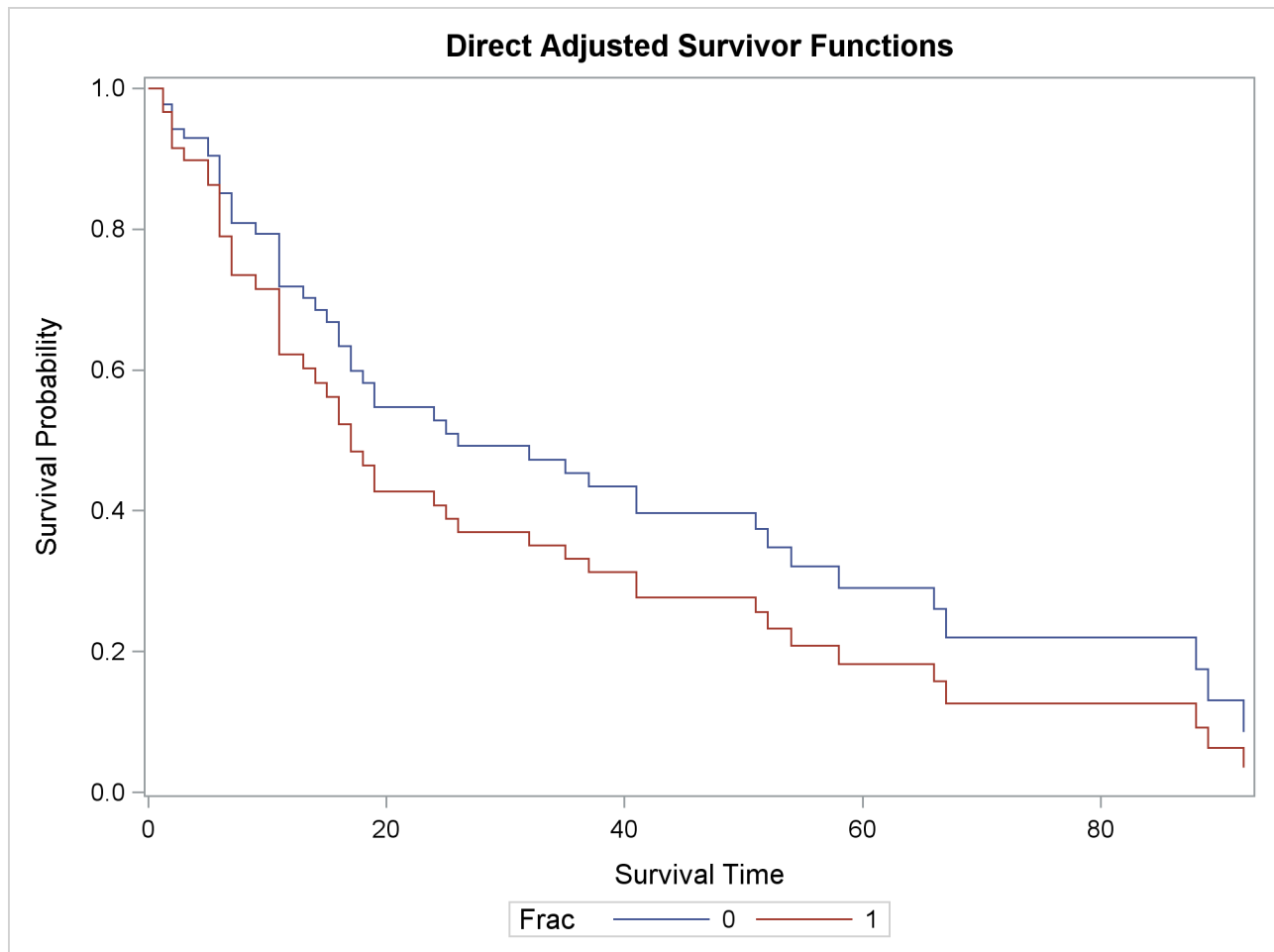
proc phreg data=Myeloma plots(overlay)=survival;
 class Frac;
 model Time*VStatus(0)=LogBUN HGB Frac;
 baseline covariates=Myeloma outdiff=Diff1 survival=_all_/diradj group=Frac;
run;

```

Because the CLASS variable Frac is specified as the GROUP= variable, a separate direct adjusted survival curve is computed for each value of the variable Frac. Each direct adjusted survival curve is the average of the predicted survival curves for all the patients in the entire Myeloma data set with their Frac value set to a specific constant. For example, the direct adjusted survival curve for Frac=0 (no fracture at diagnosis) is computed as follows:

1. The value of the variable Frac is set to 0 for all observations in the Myeloma data set.
2. The survival curve for each observation in the modified data set is computed.
3. All the survival curves computed in step 2 are averaged.

**Output 67.8.4** Average Survival by Fracture Status



Output 67.8.4 shows that patients without fracture at diagnosis have better survival than those with fractures. Differences in the survival probabilities and their standard errors are displayed in Output 67.8.5.

```
proc print data=Diff1;
run;
ods graphics off;
```

**Output 67.8.5** Differences in the Survival between Fracture and Nonfracture

| Obs | Frac | Frac2 | Time  | Surv<br>Diff | StdErr  |
|-----|------|-------|-------|--------------|---------|
| 1   | 0    | 1     | 1.25  | 0.01074      | 0.01199 |
| 2   | 0    | 1     | 2.00  | 0.02653      | 0.02605 |
| 3   | 0    | 1     | 3.00  | 0.03165      | 0.03063 |
| 4   | 0    | 1     | 5.00  | 0.04191      | 0.03963 |
| 5   | 0    | 1     | 6.00  | 0.06115      | 0.05669 |
| 6   | 0    | 1     | 7.00  | 0.07416      | 0.06853 |
| 7   | 0    | 1     | 9.00  | 0.07854      | 0.07261 |
| 8   | 0    | 1     | 11.00 | 0.09669      | 0.09002 |
| 9   | 0    | 1     | 13.00 | 0.09998      | 0.09327 |
| 10  | 0    | 1     | 14.00 | 0.10319      | 0.09644 |
| 11  | 0    | 1     | 15.00 | 0.10611      | 0.09937 |
| 12  | 0    | 1     | 16.00 | 0.11117      | 0.10464 |
| 13  | 0    | 1     | 17.00 | 0.11532      | 0.10922 |
| 14  | 0    | 1     | 18.00 | 0.11704      | 0.11120 |
| 15  | 0    | 1     | 19.00 | 0.11969      | 0.11447 |
| 16  | 0    | 1     | 24.00 | 0.12072      | 0.11593 |
| 17  | 0    | 1     | 25.00 | 0.12145      | 0.11713 |
| 18  | 0    | 1     | 26.00 | 0.12189      | 0.11808 |
| 19  | 0    | 1     | 32.00 | 0.12208      | 0.11883 |
| 20  | 0    | 1     | 35.00 | 0.12197      | 0.11933 |
| 21  | 0    | 1     | 37.00 | 0.12155      | 0.11956 |
| 22  | 0    | 1     | 41.00 | 0.11983      | 0.11924 |
| 23  | 0    | 1     | 51.00 | 0.11821      | 0.11850 |
| 24  | 0    | 1     | 52.00 | 0.11580      | 0.11714 |
| 25  | 0    | 1     | 54.00 | 0.11262      | 0.11507 |
| 26  | 0    | 1     | 58.00 | 0.10824      | 0.11203 |
| 27  | 0    | 1     | 66.00 | 0.10301      | 0.10814 |
| 28  | 0    | 1     | 67.00 | 0.09451      | 0.10130 |
| 29  | 0    | 1     | 88.00 | 0.08248      | 0.09133 |
| 30  | 0    | 1     | 89.00 | 0.06847      | 0.08033 |
| 31  | 0    | 1     | 92.00 | 0.05038      | 0.06515 |

## Example 67.9: Analysis of Residuals

Residuals are used to investigate the lack of fit of a model to a given subject. You can obtain martingale and deviance residuals for the Cox proportional hazards regression analysis by requesting that they be included in the OUTPUT data set. You can plot these statistics and look for outliers.

Consider the stepwise regression analysis performed in [Example 67.1](#). The final model included variables LogBUN and HGB. You can generate residual statistics for this analysis by refitting the model containing those variables and including an OUTPUT statement as in the following invocation of PROC PHREG. The keywords XBETA, RESMART, and RESDEV identify new variables that contain the linear predictor scores  $z_j'\hat{\beta}$ , martingale residuals, and deviance residuals. These variables are xb, mart, and dev, respectively.

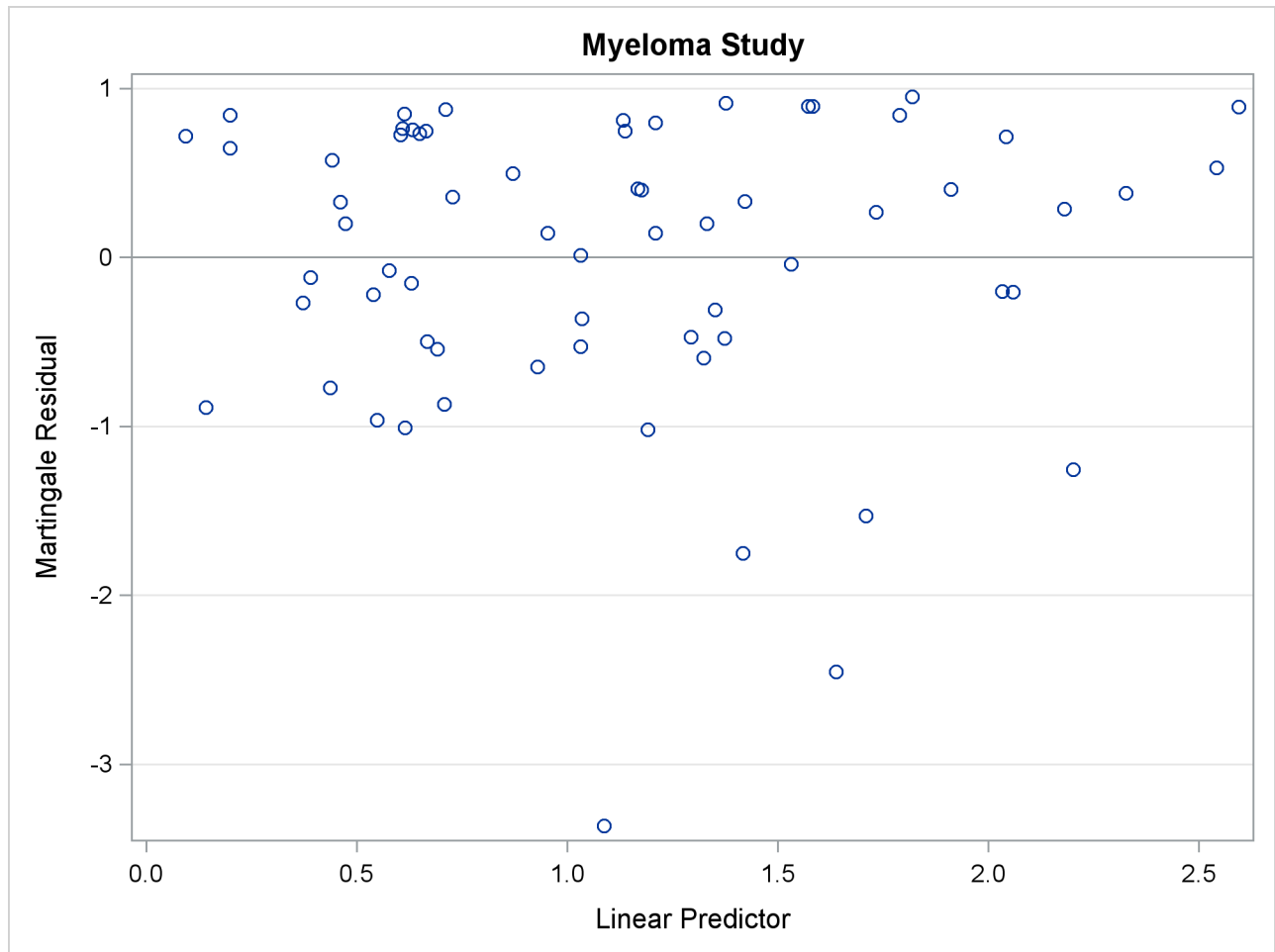
```
proc phreg data=Myeloma noprint;
 model Time*Vstatus(0)=LogBUN HGB;
 output out=Outp xbeta=Xb resmart=Mart resdev=Dev;
run;
```

The following statements plot the residuals against the linear predictor scores:

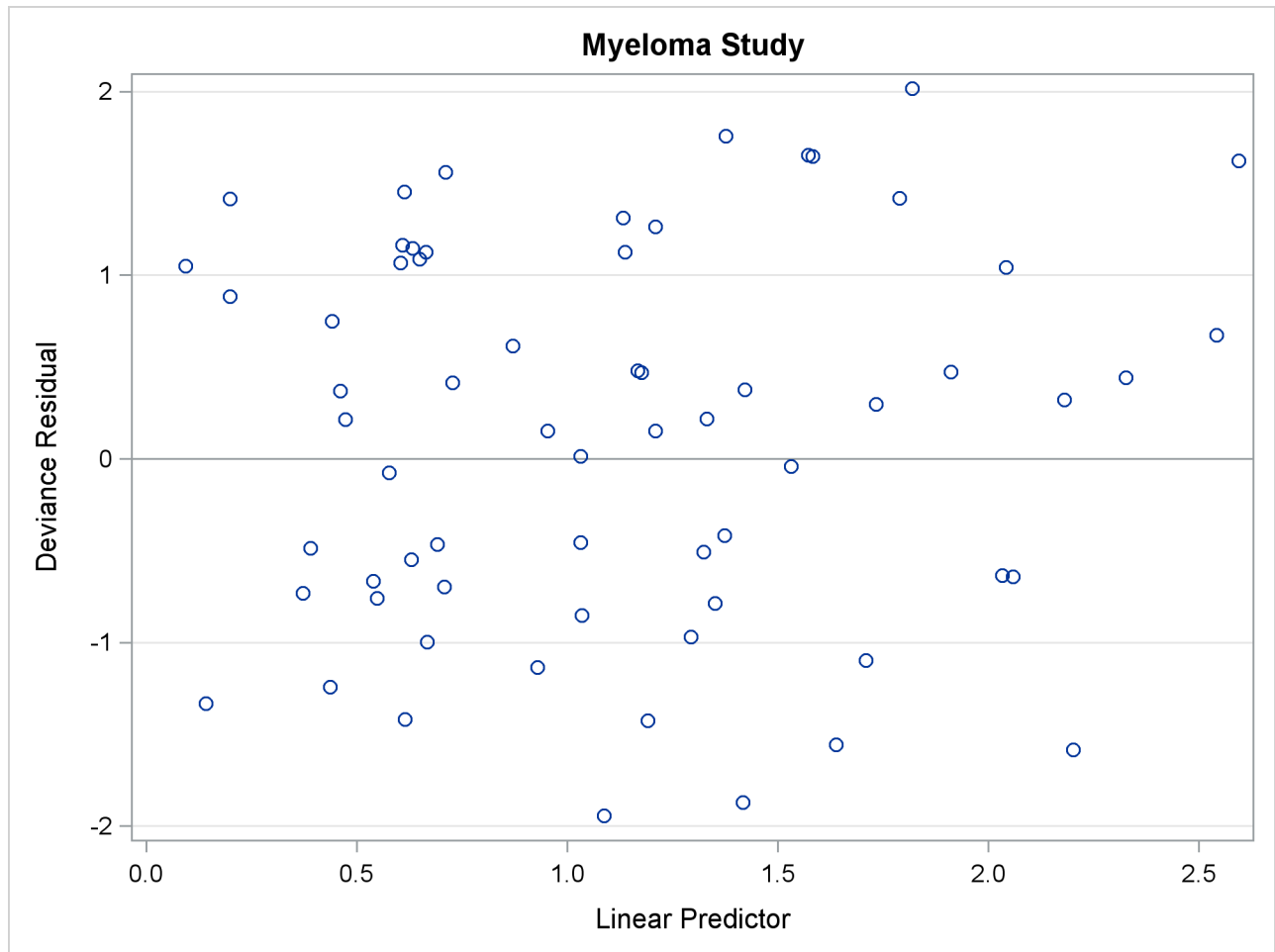
```
title "Myeloma Study";
proc sgplot data=Outp;
 yaxis grid;
 refline 0 / axis=y;
 scatter y=Mart x=Xb;
run;
proc sgplot data=Outp;
 yaxis grid;
 refline 0 / axis=y;
 scatter y=Dev x=Xb;
run;
```

The resulting plots are shown in [Output 67.9.1](#) and [Output 67.9.2](#). The martingale residuals are skewed because of the single event setting of the Cox model. The martingale residual plot shows an isolation point (with linear predictor score 1.09 and martingale residual  $-3.37$ ), but this observation is no longer distinguishable in the deviance residual plot. In conclusion, there is no indication of a lack of fit of the model to individual observations.

**Output 67.9.1** Martingale Residual Plot



Output 67.9.2 Deviance Residual Plot



## Example 67.10: Analysis of Recurrent Events Data

Recurrent events data consist of times to a number of repeated events for each sample unit—for example, times of recurrent episodes of a disease in patients. Various ways of analyzing recurrent events data are described in the section “[Analysis of Multivariate Failure Time Data](#)” on page 5629. The bladder cancer data listed in Wei, Lin, and Weissfeld (1989) are used here to illustrate these methods.

The data consist of 86 patients with superficial bladder tumors, which were removed when the patients entered the study. Of these patients, 48 were randomized into the placebo group, and 38 were randomized into the group receiving thiotepa. Many patients had multiple recurrences of tumors during the study, and new tumors were removed at each visit. The data set contains the first four recurrences of the tumor for each patient, and each recurrence time was measured from the patient’s entry time into the study.

The data consist of the following eight variables:

- Trt, treatment group (1=placebo and 2=thiotepa)
- Time, follow-up time
- Number, number of initial tumors
- Size, initial tumor size
- T1, T2, T3, and T4, times of the four potential recurrences of the bladder tumor. A patient with only two recurrences has missing values in T3 and T4.

In the data set Bladder, four observations are created for each patient, one for each of the four potential tumor recurrences. In addition to values of Trt, Number, and Size for the patient, each observation contains the following variables:

- ID, patient’s identification (which is the sequence number of the subject)
- Visit, visit number (with value  $k$  for the  $k$ th potential tumor recurrence)
- TStart, time of the  $(k - 1)$  recurrence for Visit= $k$ , or the entry time 0 if VISIT=1, or the follow-up time if the  $(k - 1)$  recurrence does not occur
- TStop, time of the  $k$ th recurrence if Visit= $k$  or follow-up time if the  $k$ th recurrence does not occur
- Status, event status of TStop (1=recurrence and 0=censored)

For instance, a patient with only one recurrence time at month 6 who was followed until month 10 will have values for Visit, TStart, TStop, and Status of (1,0,6,1), (2,6,10,0), (3,10,10,0), and (4,10,10,0), respectively. The last two observations are redundant for the intensity model and the proportional means model, but they are important for the analysis of the marginal Cox models. If the follow-up time is beyond the time of the fourth tumor recurrence, it is tempting to create a fifth observation with the time of the fourth tumor recurrence as the TStart value, the follow-up time as the TStop value, and a Status value of 0. However, Therneau and Grambsch (2000, Section 8.5) have warned against incorporating such observations into the analysis.

The following SAS statements create the data set Bladder:

```

data Bladder;
 keep ID TStart TStop Status Trt Number Size Visit;
 retain ID TStart 0;
 array tt T1-T4;
 infile datalines missover;
 input Trt Time Number Size T1-T4;
 ID + 1;
 TStart=0;
 do over tt;
 Visit=_i_;
 if tt = . then do;
 TStop=Time;
 Status=0;
 end;
 else do;
 TStop=tt;
 Status=1;
 end;
 output;
 TStart=TStop;
end;
if (TStart < Time) then delete;
datalines;
1 0 1 1
1 1 1 3
1 4 2 1
1 7 1 1
1 10 5 1
1 10 4 1 6
1 14 1 1
1 18 1 1
1 18 1 3 5
1 18 1 1 12 16
1 23 3 3
1 23 1 3 10 15
1 23 1 1 3 16 23
1 23 3 1 3 9 21
1 24 2 3 7 10 16 24
1 25 1 1 3 15 25
1 26 1 2
1 26 8 1 1
1 26 1 4 2 26
1 28 1 2 25
1 29 1 4
1 29 1 2
1 29 4 1
1 30 1 6 28 30
1 30 1 5 2 17 22
1 30 2 1 3 6 8 12
1 31 1 3 12 15 24
1 32 1 2
1 34 2 1

```



|   |    |   |   |    |    |    |    |  |
|---|----|---|---|----|----|----|----|--|
| 1 | 36 | 2 | 1 |    |    |    |    |  |
| 1 | 36 | 3 | 1 | 29 |    |    |    |  |
| 1 | 37 | 1 | 2 |    |    |    |    |  |
| 1 | 40 | 4 | 1 | 9  | 17 | 22 | 24 |  |
| 1 | 40 | 5 | 1 | 16 | 19 | 23 | 29 |  |
| 1 | 41 | 1 | 2 |    |    |    |    |  |
| 1 | 43 | 1 | 1 | 3  |    |    |    |  |
| 1 | 43 | 2 | 6 | 6  |    |    |    |  |
| 1 | 44 | 2 | 1 | 3  | 6  | 9  |    |  |
| 1 | 45 | 1 | 1 | 9  | 11 | 20 | 26 |  |
| 1 | 48 | 1 | 1 | 18 |    |    |    |  |
| 1 | 49 | 1 | 3 |    |    |    |    |  |
| 1 | 51 | 3 | 1 | 35 |    |    |    |  |
| 1 | 53 | 1 | 7 | 17 |    |    |    |  |
| 1 | 53 | 3 | 1 | 3  | 15 | 46 | 51 |  |
| 1 | 59 | 1 | 1 |    |    |    |    |  |
| 1 | 61 | 3 | 2 | 2  | 15 | 24 | 30 |  |
| 1 | 64 | 1 | 3 | 5  | 14 | 19 | 27 |  |
| 1 | 64 | 2 | 3 | 2  | 8  | 12 | 13 |  |
| 2 | 1  | 1 | 3 |    |    |    |    |  |
| 2 | 1  | 1 | 1 |    |    |    |    |  |
| 2 | 5  | 8 | 1 | 5  |    |    |    |  |
| 2 | 9  | 1 | 2 |    |    |    |    |  |
| 2 | 10 | 1 | 1 |    |    |    |    |  |
| 2 | 13 | 1 | 1 |    |    |    |    |  |
| 2 | 14 | 2 | 6 | 3  |    |    |    |  |
| 2 | 17 | 5 | 3 | 1  | 3  | 5  | 7  |  |
| 2 | 18 | 5 | 1 |    |    |    |    |  |
| 2 | 18 | 1 | 3 | 17 |    |    |    |  |
| 2 | 19 | 5 | 1 | 2  |    |    |    |  |
| 2 | 21 | 1 | 1 | 17 | 19 |    |    |  |
| 2 | 22 | 1 | 1 |    |    |    |    |  |
| 2 | 25 | 1 | 3 |    |    |    |    |  |
| 2 | 25 | 1 | 5 |    |    |    |    |  |
| 2 | 25 | 1 | 1 |    |    |    |    |  |
| 2 | 26 | 1 | 1 | 6  | 12 | 13 |    |  |
| 2 | 27 | 1 | 1 | 6  |    |    |    |  |
| 2 | 29 | 2 | 1 | 2  |    |    |    |  |
| 2 | 36 | 8 | 3 | 26 | 35 |    |    |  |
| 2 | 38 | 1 | 1 |    |    |    |    |  |
| 2 | 39 | 1 | 1 | 22 | 23 | 27 | 32 |  |
| 2 | 39 | 6 | 1 | 4  | 16 | 23 | 27 |  |
| 2 | 40 | 3 | 1 | 24 | 26 | 29 | 40 |  |
| 2 | 41 | 3 | 2 |    |    |    |    |  |
| 2 | 41 | 1 | 1 |    |    |    |    |  |
| 2 | 43 | 1 | 1 | 1  | 27 |    |    |  |
| 2 | 44 | 1 | 1 |    |    |    |    |  |
| 2 | 44 | 6 | 1 | 2  | 20 | 23 | 27 |  |
| 2 | 45 | 1 | 2 |    |    |    |    |  |
| 2 | 46 | 1 | 4 | 2  |    |    |    |  |
| 2 | 46 | 1 | 4 |    |    |    |    |  |
| 2 | 49 | 3 | 3 |    |    |    |    |  |
| 2 | 50 | 1 | 1 |    |    |    |    |  |
| 2 | 50 | 4 | 1 | 4  | 24 | 47 |    |  |

```

2 54 3 4
2 54 2 1 38
2 59 1 3
;

```

First, consider fitting the intensity model (Andersen and Gill 1982) and the proportional means model (Lin et al. 2000). The counting process style of input is used in the PROC PHREG specification. For the proportional means model, inference is based on the robust sandwich covariance estimate, which is requested by the COVS(AGGREGATE) option in the PROC PHREG statement. The COVM option is specified for the analysis of the intensity model to use the model-based covariance estimate. Note that some of the observations in the data set `Bladder` have a degenerated interval of risk. The presence of these observations does not affect the results of the analysis since none of these observations are included in any of the risk sets. However, the procedure will run more efficiently without these observations; consequently, in the following SAS statements, the WHERE clause is used to eliminate these redundant observations:

```

title 'Intensity Model and Proportional Means Model';
proc phreg data=Bladder covm covs(aggregate);
 model (TStart, TStop) * Status(0) = Trt Number Size;
 id id;
 where TStart < TStop;
run;

```

Results of fitting the intensity model and the proportional means model are shown in [Output 67.10.1](#) and [Output 67.10.2](#), respectively. The robust sandwich standard error estimate for `Trt` is larger than its model-based counterpart, rendering the effect of thiotepa less significant in the proportional means model ( $p = 0.0747$ ) than in the intensity model ( $p = 0.0215$ ).

**Output 67.10.1** Analysis of the Intensity Model

| Intensity Model and Proportional Means Model                                   |    |                       |                   |            |            |                 |
|--------------------------------------------------------------------------------|----|-----------------------|-------------------|------------|------------|-----------------|
| The PHREG Procedure                                                            |    |                       |                   |            |            |                 |
| Analysis of Maximum Likelihood Estimates<br>with Model-Based Variance Estimate |    |                       |                   |            |            |                 |
| Parameter                                                                      | DF | Parameter<br>Estimate | Standard<br>Error | Chi-Square | Pr > ChiSq | Hazard<br>Ratio |
| Trt                                                                            | 1  | -0.45979              | 0.19996           | 5.2873     | 0.0215     | 0.631           |
| Number                                                                         | 1  | 0.17165               | 0.04733           | 13.1541    | 0.0003     | 1.187           |
| Size                                                                           | 1  | -0.04256              | 0.06903           | 0.3801     | 0.5375     | 0.958           |

**Output 67.10.2** Analysis of the Proportional Means Model

| Analysis of Maximum Likelihood Estimates<br>with Sandwich Variance Estimate |    |                    |                |              |            |            |              |
|-----------------------------------------------------------------------------|----|--------------------|----------------|--------------|------------|------------|--------------|
| Parameter                                                                   | DF | Parameter Estimate | Standard Error | StdErr Ratio | Chi-Square | Pr > ChiSq | Hazard Ratio |
| Trt                                                                         | 1  | -0.45979           | 0.25801        | 1.290        | 3.1757     | 0.0747     | 0.631        |
| Number                                                                      | 1  | 0.17165            | 0.06131        | 1.296        | 7.8373     | 0.0051     | 1.187        |
| Size                                                                        | 1  | -0.04256           | 0.07555        | 1.094        | 0.3174     | 0.5732     | 0.958        |

Next, consider the conditional models of Prentice, Williams, and Peterson (1981). In the PWP models, the risk set for the  $(k + 1)$  recurrence is restricted to those patients who have experienced the first  $k$  recurrences. For example, a patient who experienced only one recurrence is an event observation for the first recurrence; this patient is a censored observation for the second recurrence and should not be included in the risk set for the third or fourth recurrence. The following DATA step eliminates those observations that should not be in the risk sets, forming a new input data set (named Bladder2) for fitting the PWP models. The variable Gaptime, representing the gap times between successive recurrences, is also created.

```
data Bladder2(drop=LastStatus);
 retain LastStatus;
 set Bladder;
 by ID;
 if first.id then LastStatus=1;
 if (Status=0 and LastStatus=0) then delete;
 LastStatus=Status;
 Gaptime=Tstop-Tstart;
run;
```

The following statements fit the PWP total time model. The variables Trt1, Trt2, Trt3, and Trt4 are visit-specific variables for Trt; the variables Number1, Number2, Number3, and Number4 are visit-specific variables for Number; and the variables Size1, Size2, Size3, and Size4 are visit-specific variables for Size.

```
title 'PWP Total Time Model with Noncommon Effects';
proc phreg data=Bladder2;
 model (Tstart,Tstop) * Status(0) = Trt1-Trt4 Number1-Number4
 Size1-Size4;

 Trt1= Trt * (Visit=1);
 Trt2= Trt * (Visit=2);
 Trt3= Trt * (Visit=3);
 Trt4= Trt * (Visit=4);
 Number1= Number * (Visit=1);
 Number2= Number * (Visit=2);
 Number3= Number * (Visit=3);
 Number4= Number * (Visit=4);
 Size1= Size * (Visit=1);
 Size2= Size * (Visit=2);
 Size3= Size * (Visit=3);
 Size4= Size * (Visit=4);
 strata Visit;
run;
```

Results of the analysis of the PWP total time model are shown in [Output 67.10.3](#). There is no significant treatment effect on the total time in any of the four tumor recurrences.

**Output 67.10.3** Analysis of the PWP Total Time Model with Noncommon Effects

| PWP Total Time Model with Noncommon Effects        |       |                    |                |            |                  |              |
|----------------------------------------------------|-------|--------------------|----------------|------------|------------------|--------------|
| The PHREG Procedure                                |       |                    |                |            |                  |              |
| Summary of the Number of Event and Censored Values |       |                    |                |            |                  |              |
| Stratum                                            | Visit | Total              | Event          | Censored   | Percent Censored |              |
| 1                                                  | 1     | 85                 | 47             | 38         | 44.71            |              |
| 2                                                  | 2     | 46                 | 29             | 17         | 36.96            |              |
| 3                                                  | 3     | 27                 | 22             | 5          | 18.52            |              |
| 4                                                  | 4     | 20                 | 14             | 6          | 30.00            |              |
| -----                                              |       |                    |                |            |                  |              |
| Total                                              |       | 178                | 112            | 66         | 37.08            |              |
| Analysis of Maximum Likelihood Estimates           |       |                    |                |            |                  |              |
| Parameter                                          | DF    | Parameter Estimate | Standard Error | Chi-Square | Pr > ChiSq       | Hazard Ratio |
| Trt1                                               | 1     | -0.51757           | 0.31576        | 2.6868     | 0.1012           | 0.596        |
| Trt2                                               | 1     | -0.45967           | 0.40642        | 1.2792     | 0.2581           | 0.631        |
| Trt3                                               | 1     | 0.11700            | 0.67183        | 0.0303     | 0.8617           | 1.124        |
| Trt4                                               | 1     | -0.04059           | 0.79251        | 0.0026     | 0.9592           | 0.960        |
| Number1                                            | 1     | 0.23605            | 0.07607        | 9.6287     | 0.0019           | 1.266        |
| Number2                                            | 1     | -0.02044           | 0.09052        | 0.0510     | 0.8213           | 0.980        |
| Number3                                            | 1     | 0.01219            | 0.18208        | 0.0045     | 0.9466           | 1.012        |
| Number4                                            | 1     | 0.18915            | 0.24443        | 0.5989     | 0.4390           | 1.208        |
| Size1                                              | 1     | 0.06790            | 0.10125        | 0.4498     | 0.5024           | 1.070        |
| Size2                                              | 1     | -0.15425           | 0.12300        | 1.5728     | 0.2098           | 0.857        |
| Size3                                              | 1     | 0.14891            | 0.26299        | 0.3206     | 0.5713           | 1.161        |
| Size4                                              | 1     | 0.0000732          | 0.34297        | 0.0000     | 0.9998           | 1.000        |

The following statements fit the PWP gap-time model:

```

title 'PWP Gap-Time Model with Noncommon Effects';
proc phreg data=Bladder2;
 model Gaptime * Status(0) = Trt1-Trt4 Number1-Number4
 Size1-Size4;

 Trt1= Trt * (Visit=1);
 Trt2= Trt * (Visit=2);
 Trt3= Trt * (Visit=3);
 Trt4= Trt * (Visit=4);
 Number1= Number * (Visit=1);
 Number2= Number * (Visit=2);
 Number3= Number * (Visit=3);
 Number4= Number * (Visit=4);

```

```

Size1= Size * (Visit=1);
Size2= Size * (Visit=2);
Size3= Size * (Visit=3);
Size4= Size * (Visit=4);
strata Visit;
run;

```

Results of the analysis of the PWP gap-time model are shown in [Output 67.10.4](#). Note that the regression coefficients for the first tumor recurrence are the same as those of the total time model, since the total time and the gap time are the same for the first recurrence. There is no significant treatment effect on the gap times for any of the four tumor recurrences.

**Output 67.10.4** Analysis of the PWP Gap-Time Model with Noncommon Effects

| PWP Gap-Time Model with Noncommon Effects |    |                    |                |            |            |              |
|-------------------------------------------|----|--------------------|----------------|------------|------------|--------------|
| The PHREG Procedure                       |    |                    |                |            |            |              |
| Analysis of Maximum Likelihood Estimates  |    |                    |                |            |            |              |
| Parameter                                 | DF | Parameter Estimate | Standard Error | Chi-Square | Pr > ChiSq | Hazard Ratio |
| Trt1                                      | 1  | -0.51757           | 0.31576        | 2.6868     | 0.1012     | 0.596        |
| Trt2                                      | 1  | -0.25911           | 0.40511        | 0.4091     | 0.5224     | 0.772        |
| Trt3                                      | 1  | 0.22105            | 0.54909        | 0.1621     | 0.6873     | 1.247        |
| Trt4                                      | 1  | -0.19498           | 0.64184        | 0.0923     | 0.7613     | 0.823        |
| Number1                                   | 1  | 0.23605            | 0.07607        | 9.6287     | 0.0019     | 1.266        |
| Number2                                   | 1  | -0.00571           | 0.09667        | 0.0035     | 0.9529     | 0.994        |
| Number3                                   | 1  | 0.12935            | 0.15970        | 0.6561     | 0.4180     | 1.138        |
| Number4                                   | 1  | 0.42079            | 0.19816        | 4.5091     | 0.0337     | 1.523        |
| Size1                                     | 1  | 0.06790            | 0.10125        | 0.4498     | 0.5024     | 1.070        |
| Size2                                     | 1  | -0.11636           | 0.11924        | 0.9524     | 0.3291     | 0.890        |
| Size3                                     | 1  | 0.24995            | 0.23113        | 1.1695     | 0.2795     | 1.284        |
| Size4                                     | 1  | 0.03557            | 0.29043        | 0.0150     | 0.9025     | 1.036        |

You can fit the PWP total time model with common effects by using the following SAS statements. However, the analysis is not shown here.

```

title2 'PWP Total Time Model with Common Effects';
proc phreg data=Bladder2;
 model (tstart,tstop) * status(0) = Trt Number Size;
 strata Visit;
run;

```

You can fit the PWP gap-time model with common effects by using the following statements. Again, the analysis is not shown here.

```

title2 'PWP Gap Time Model with Common Effects';
proc phreg data=Bladder2;
 model Gaptime * Status(0) = Trt Number Size;
 strata Visit;
run;

```

Recurrent events data are a special case of multiple events data in which the recurrence times are regarded as multivariate failure times and the marginal approach of Wei, Lin, and Weissfeld (1989) can be used. WLW fits a Cox model to each of the component times and makes statistical inference of the regression parameters based on a robust sandwich covariance matrix estimate. No specific correlation structure is imposed on the multivariate failure times. For the  $k$ th marginal model, let  $\beta_k$  denote the row vector of regression parameters, let  $\hat{\beta}_k$  denote the maximum likelihood estimate of  $\beta_k$ , let  $\hat{A}_k$  denote the covariance matrix obtained by inverting the observed information matrix, and let  $R_k$  denote the matrix of score residuals. WLW showed that the joint distribution of  $(\hat{\beta}_1, \dots, \hat{\beta}_4)'$  can be approximated by a multivariate normal distribution with mean vector  $(\beta_1, \dots, \beta_4)'$  and robust covariance matrix

$$\begin{pmatrix} \mathbf{V}_{11} & \mathbf{V}_{12} & \mathbf{V}_{13} & \mathbf{V}_{14} \\ \mathbf{V}_{21} & \mathbf{V}_{22} & \mathbf{V}_{23} & \mathbf{V}_{24} \\ \mathbf{V}_{31} & \mathbf{V}_{32} & \mathbf{V}_{33} & \mathbf{V}_{34} \\ \mathbf{V}_{41} & \mathbf{V}_{42} & \mathbf{V}_{43} & \mathbf{V}_{44} \end{pmatrix}$$

with the submatrix  $V_{ij}$  given by

$$V_{ij} = \hat{A}_i (\mathbf{R}'_i \mathbf{R}_j) \hat{A}_j$$

In this example, there are four marginal proportional hazards models, one for each potential recurrence time. Instead of fitting one model at a time, you can fit all four marginal models in one analysis by using the STRATA statement and model-specific covariates as in the following statements. Using Visit as the STRATA variable on the input data set Bladder, PROC PHREG simultaneously fits all four marginal models, one for each Visit value. The COVS(AGGREGATE) option is specified to compute the robust sandwich variance estimate by summing up the score residuals for each distinct pattern of ID value. The TEST statement TREATMENT is used to perform the global test of no treatment effect for each tumor recurrence, the AVERAGE option is specified to estimate the parameter for the common treatment effect, and the E option displays the optimal weights for the common treatment effect.

```

title 'Wei-Lin-Weissfeld Model';
proc phreg data=Bladder covs(aggregate);
 model TStop*Status(0)=Trt1-Trt4 Number1-Number4 Size1-Size4;
 Trt1= Trt * (Visit=1);
 Trt2= Trt * (Visit=2);
 Trt3= Trt * (Visit=3);
 Trt4= Trt * (Visit=4);
 Number1= Number * (Visit=1);
 Number2= Number * (Visit=2);
 Number3= Number * (Visit=3);
 Number4= Number * (Visit=4);
 Size1= Size * (Visit=1);
 Size2= Size * (Visit=2);
 Size3= Size * (Visit=3);
 Size4= Size * (Visit=4);
 strata Visit;
 id ID;
 TREATMENT: test trt1,trt2,trt3,trt4/average e;
run;

```

Out of the 86 patients, 47 patients have only one tumor recurrence, 29 patients have two recurrences, 22 patients have three recurrences, and 14 patients have four recurrences (Output 67.10.5). Parameter estimates for the four marginal models are shown in Output 67.10.6. The 4 DF Wald test (Output 67.10.7) indicates a lack of evidence of a treatment effect in any of the four recurrences ( $p = 0.4105$ ). The optimal weights for estimating the parameter of the common treatment effect are 0.67684, 0.25723,  $-0.07547$ , and 0.14140 for Trt1, Trt2, Trt3, and Trt4, respectively, which gives a parameter estimate of  $-0.5489$  with a standard error estimate of 0.2853. A more sensitive test for a treatment effect is the 1 DF test based on this common parameter; however, there is still insufficient evidence for such effect at the 0.05 level ( $p = 0.0543$ ).

**Output 67.10.5** Summary of Bladder Tumor Recurrences in 86 Patients

| Wei-Lin-Weissfeld Model                            |       |       |       |          |                  |
|----------------------------------------------------|-------|-------|-------|----------|------------------|
| The PHREG Procedure                                |       |       |       |          |                  |
| Summary of the Number of Event and Censored Values |       |       |       |          |                  |
| Stratum                                            | Visit | Total | Event | Censored | Percent Censored |
| 1                                                  | 1     | 86    | 47    | 39       | 45.35            |
| 2                                                  | 2     | 86    | 29    | 57       | 66.28            |
| 3                                                  | 3     | 86    | 22    | 64       | 74.42            |
| 4                                                  | 4     | 86    | 14    | 72       | 83.72            |
| -----                                              |       |       |       |          |                  |
| Total                                              |       | 344   | 112   | 232      | 67.44            |

**Output 67.10.6** Analysis of Marginal Cox Models

| Analysis of Maximum Likelihood Estimates |    |                    |                |              |            |            |              |
|------------------------------------------|----|--------------------|----------------|--------------|------------|------------|--------------|
| Parameter                                | DF | Parameter Estimate | Standard Error | StdErr Ratio | Chi-Square | Pr > ChiSq | Hazard Ratio |
| Trt1                                     | 1  | -0.51762           | 0.30750        | 0.974        | 2.8336     | 0.0923     | 0.596        |
| Trt2                                     | 1  | -0.61944           | 0.36391        | 0.926        | 2.8975     | 0.0887     | 0.538        |
| Trt3                                     | 1  | -0.69988           | 0.41516        | 0.903        | 2.8419     | 0.0918     | 0.497        |
| Trt4                                     | 1  | -0.65079           | 0.48971        | 0.848        | 1.7661     | 0.1839     | 0.522        |
| Number1                                  | 1  | 0.23599            | 0.07208        | 0.947        | 10.7204    | 0.0011     | 1.266        |
| Number2                                  | 1  | 0.13756            | 0.08690        | 0.946        | 2.5059     | 0.1134     | 1.147        |
| Number3                                  | 1  | 0.16984            | 0.10356        | 0.984        | 2.6896     | 0.1010     | 1.185        |
| Number4                                  | 1  | 0.32880            | 0.11382        | 0.909        | 8.3453     | 0.0039     | 1.389        |
| Size1                                    | 1  | 0.06789            | 0.08529        | 0.842        | 0.6336     | 0.4260     | 1.070        |
| Size2                                    | 1  | -0.07612           | 0.11812        | 0.881        | 0.4153     | 0.5193     | 0.927        |
| Size3                                    | 1  | -0.21131           | 0.17198        | 0.943        | 1.5097     | 0.2192     | 0.810        |
| Size4                                    | 1  | -0.20317           | 0.19106        | 0.830        | 1.1308     | 0.2876     | 0.816        |

**Output 67.10.7** Tests of Treatment Effects

| Wei-Lin-Weissfeld Model                |       |       |       |       |                |
|----------------------------------------|-------|-------|-------|-------|----------------|
| The PHREG Procedure                    |       |       |       |       |                |
| Linear Coefficients for Test TREATMENT |       |       |       |       |                |
| Parameter                              | Row 1 | Row 2 | Row 3 | Row 4 | Average Effect |
| Trt1                                   | 1     | 0     | 0     | 0     | 0.67684        |
| Trt2                                   | 0     | 1     | 0     | 0     | 0.25723        |
| Trt3                                   | 0     | 0     | 1     | 0     | -0.07547       |
| Trt4                                   | 0     | 0     | 0     | 1     | 0.14140        |
| Number1                                | 0     | 0     | 0     | 0     | 0.00000        |
| Number2                                | 0     | 0     | 0     | 0     | 0.00000        |
| Number3                                | 0     | 0     | 0     | 0     | 0.00000        |
| Number4                                | 0     | 0     | 0     | 0     | 0.00000        |
| Size1                                  | 0     | 0     | 0     | 0     | 0.00000        |
| Size2                                  | 0     | 0     | 0     | 0     | 0.00000        |
| Size3                                  | 0     | 0     | 0     | 0     | 0.00000        |
| Size4                                  | 0     | 0     | 0     | 0     | 0.00000        |
| CONSTANT                               | 0     | 0     | 0     | 0     | 0.00000        |

| Test TREATMENT Results |    |            |  |
|------------------------|----|------------|--|
| Wald                   |    |            |  |
| Chi-Square             | DF | Pr > ChiSq |  |
| 3.9668                 | 4  | 0.4105     |  |

| Average Effect for Test TREATMENT |                |         |         |
|-----------------------------------|----------------|---------|---------|
| Estimate                          | Standard Error | z-Score | Pr >  z |
| -0.5489                           | 0.2853         | -1.9240 | 0.0543  |

**Example 67.11: Analysis of Clustered Data**

When experimental units are naturally or artificially clustered, failure times of experimental units within a cluster are correlated. Two approaches can be taken to adjust for the intracluster correlation. In the marginal Cox model approach, Lee, Wei, and Amato (1992) estimate the regression parameters in the Cox model by the maximum partial likelihood estimates under an independent working assumption and use a robust sandwich covariance matrix estimate to account for the intracluster dependence. Lin (1994) illustrates this methodology by using a subset of data from the Diabetic Retinopathy Study (DRS). An alternative approach to account for the within-cluster correlation is to use a shared frailty model where cluster effects are incorporated into the model as independent and identically distributed random variables.



The following DATA step creates the data set Blind that represents 197 diabetic patients who have a high risk of experiencing blindness in both eyes as defined by DRS criteria. One eye of each patient is treated with laser photocoagulation. The hypothesis of interest is whether the laser treatment delays the occurrence of blindness. Since juvenile and adult diabetes have very different courses, it is also desirable to examine how the age of onset of diabetes might affect the time of blindness. Since there are no biological differences between the left eye and the right eye, it is natural to assume a common baseline hazard function for the failure times of the left and right eyes.

Each patient is a cluster that contributes two observations to the input data set, one for each eye. The following variables are in the input data set Blind:

- ID, patient's identification
- Time, time to blindness
- Status, blindness indicator (0:censored and 1:blind)
- Treat, treatment received (Laser or Others)
- Type, type of diabetes (Juvenile: onset at age  $\leq 20$  or Adult: onset at age  $> 20$ )

```
proc format;
 value type 0='Juvenile' 1='Adult';
 value Rx 1='Laser' 0='Others';
run;

data Blind;
 input ID Time Status dtypes trt @@;
 Type= put(dtypes, type.);
 Treat= put(trt, Rx.);
 datalines;
 5 46.23 0 1 1 5 46.23 0 1 0 14 42.50 0 0 1 14 31.30 1 0 0
 16 42.27 0 0 1 16 42.27 0 0 0 25 20.60 0 0 1 25 20.60 0 0 0
 29 38.77 0 0 1 29 0.30 1 0 0 46 65.23 0 0 1 46 54.27 1 0 0

 ... more lines ...

 1705 8.00 0 0 1 1705 8.00 0 0 0 1717 51.60 0 1 1 1717 42.33 1 1 0
 1727 49.97 0 1 1 1727 2.90 1 1 0 1746 45.90 0 0 1 1746 1.43 1 0 0
 1749 41.93 0 1 1 1749 41.93 0 1 0
 ;
```

As a preliminary analysis, PROC FREQ is used to summarize the number of eyes that developed blindness.

```
proc freq data=Blind;
 table Treat*Status;
run;
```

By the end of the study, 54 eyes treated with laser photocoagulation and 101 eyes treated by other means have developed blindness (Output 67.11.1).

**Output 67.11.1** Distribution of Blindness

| The FREQ Procedure       |        |       |        |  |
|--------------------------|--------|-------|--------|--|
| Table of Treat by Status |        |       |        |  |
| Treat                    | Status |       |        |  |
| Frequency                |        |       |        |  |
| Percent                  |        |       |        |  |
| Row Pct                  |        |       |        |  |
| Col Pct                  | 0      | 1     | Total  |  |
| Laser                    | 143    | 54    | 197    |  |
|                          | 36.29  | 13.71 | 50.00  |  |
|                          | 72.59  | 27.41 |        |  |
|                          | 59.83  | 34.84 |        |  |
| Others                   | 96     | 101   | 197    |  |
|                          | 24.37  | 25.63 | 50.00  |  |
|                          | 48.73  | 51.27 |        |  |
|                          | 40.17  | 65.16 |        |  |
| Total                    | 239    | 155   | 394    |  |
|                          | 60.66  | 39.34 | 100.00 |  |

The following statements use PROC PHREG to carry out the analysis of Lee, Wei, and Amato (1992). The explanatory variables in this Cox model are Treat, Type, and the Treat  $\times$  Type interaction. The COVS(AGGREGATE) option is specified to compute the robust sandwich covariance matrix estimate. The ID statement identifies the variable that represents the clusters. The HAZARDRATIO statement requests hazard ratios for the treatments be displayed.

```
proc phreg data=Blind covs(aggregate);
 class Treat Type;
 model Time*Status(0)=Treat|Type;
 id ID;
 hazardratio 'Marginal Model Analysis' Treat;
run;
```

Results of the marginal model analysis are displayed in [Output 67.11.2](#). The robust standard error estimates are smaller than the model-based counterparts, since the ratio of the robust standard error estimate relative to the model-based estimate is less than 1 for each parameter. Laser photocoagulation appears to be effective ( $p = 0.0217$ ) in delaying the occurrence of blindness, although there is also a significant interaction effect between treatment and type of diabetes ( $p = 0.0053$ ).

**Output 67.11.2** Inference Based the Marginal Model

| The PHREG Procedure                      |             |    |                    |                |              |            |
|------------------------------------------|-------------|----|--------------------|----------------|--------------|------------|
| Analysis of Maximum Likelihood Estimates |             |    |                    |                |              |            |
| Parameter                                |             | DF | Parameter Estimate | Standard Error | StdErr Ratio | Chi-Square |
| Treat                                    | Laser       | 1  | -0.42467           | 0.18497        | 0.850        | 5.2713     |
| Type                                     | Adult       | 1  | 0.34084            | 0.19558        | 0.982        | 3.0371     |
| Treat*Type                               | Laser Adult | 1  | -0.84566           | 0.30353        | 0.865        | 7.7622     |

| Analysis of Maximum Likelihood Estimates |             |            |              |                          |  |  |
|------------------------------------------|-------------|------------|--------------|--------------------------|--|--|
| Parameter                                |             | Pr > ChiSq | Hazard Ratio | Label                    |  |  |
| Treat                                    | Laser       | 0.0217     | .            | Treat Laser              |  |  |
| Type                                     | Adult       | 0.0814     | .            | Type Adult               |  |  |
| Treat*Type                               | Laser Adult | 0.0053     | .            | Treat Laser * Type Adult |  |  |

Hazard ratio estimates of the laser treatment relative to nonlaser treatment are displayed in [Output 67.11.3](#). For both types of diabetes, the 95% confidence interval for the hazard ratio lies below 1. This indicates that laser-photocoagulation treatment is more effective in delaying blindness regardless of the type of diabetes. However, the effect is more prominent for adult-onset diabetes than for juvenile-onset diabetes since the hazard ratio estimates for the former are less than those of the latter.

**Output 67.11.3** Hazard Ratio Estimates for Marginal Model

| Marginal Model Analysis: Hazard Ratios for Treat |                |                                   |       |
|--------------------------------------------------|----------------|-----------------------------------|-------|
| Description                                      | Point Estimate | 95% Wald Robust Confidence Limits |       |
| Treat Laser vs Others At Type=Adult              | 0.281          | 0.175                             | 0.451 |
| Treat Laser vs Others At Type=Juvenile           | 0.654          | 0.455                             | 0.940 |

Next, you analyze the same data by using a shared frailty model. The following statements use PROC PHREG to fit a shared frailty model to the Blind data set. The RANDOM statement identifies the variable ID as the variable that represents the clusters. You must declare the cluster variable as a classification variable in the CLASS statement.

```
proc phreg data=Blind;
 class ID Treat Type;
 model Time*Status(0)=Treat|Type;
 random ID;
 hazardratio 'Frailty Model Analysis' Treat;
run;
```

Selected results of this analysis are displayed in [Output 67.11.4](#) to [Output 67.11.6](#).

The “Random Class Level Information” table in [Output 67.11.4](#) displays the 197 ID values of the patients. You can suppress the display of this table by using the NOCLPRINT option in the RANDOM statement.

#### Output 67.11.4 Unique Cluster Identification Values

| The PHREG Procedure                        |        |        |      |      |      |      |      |      |      |      |      |     |     |     |     |
|--------------------------------------------|--------|--------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|
| Class Level Information for Random Effects |        |        |      |      |      |      |      |      |      |      |      |     |     |     |     |
| Class                                      | Levels | Values |      |      |      |      |      |      |      |      |      |     |     |     |     |
| ID                                         | 197    | 5      | 14   | 16   | 25   | 29   | 46   | 49   | 56   | 61   | 71   | 100 | 112 | 120 | 127 |
|                                            |        | 133    | 150  | 167  | 176  | 185  | 190  | 202  | 214  | 220  | 243  | 255 |     |     |     |
|                                            |        | 264    | 266  | 284  | 295  | 300  | 302  | 315  | 324  | 328  | 335  | 342 |     |     |     |
|                                            |        | 349    | 357  | 368  | 385  | 396  | 405  | 409  | 419  | 429  | 433  | 445 |     |     |     |
|                                            |        | 454    | 468  | 480  | 485  | 491  | 503  | 515  | 522  | 538  | 547  | 550 |     |     |     |
|                                            |        | 554    | 557  | 561  | 568  | 572  | 576  | 581  | 606  | 610  | 615  | 618 |     |     |     |
|                                            |        | 624    | 631  | 636  | 645  | 653  | 662  | 664  | 683  | 687  | 701  | 706 |     |     |     |
|                                            |        | 717    | 722  | 731  | 740  | 749  | 757  | 760  | 766  | 769  | 772  | 778 |     |     |     |
|                                            |        | 780    | 793  | 800  | 804  | 810  | 815  | 832  | 834  | 838  | 857  | 866 |     |     |     |
|                                            |        | 887    | 903  | 910  | 920  | 925  | 931  | 936  | 945  | 949  | 952  | 962 |     |     |     |
|                                            |        | 964    | 971  | 978  | 983  | 987  | 1002 | 1017 | 1029 | 1034 | 1037 |     |     |     |     |
|                                            |        | 1042   | 1069 | 1074 | 1098 | 1102 | 1112 | 1117 | 1126 | 1135 |      |     |     |     |     |
|                                            |        | 1145   | 1148 | 1167 | 1184 | 1191 | 1205 | 1213 | 1228 | 1247 |      |     |     |     |     |
|                                            |        | 1250   | 1253 | 1267 | 1281 | 1287 | 1293 | 1296 | 1309 | 1312 |      |     |     |     |     |
|                                            |        | 1317   | 1321 | 1333 | 1347 | 1361 | 1366 | 1373 | 1397 | 1410 |      |     |     |     |     |
|                                            |        | 1413   | 1425 | 1447 | 1461 | 1469 | 1480 | 1487 | 1491 | 1499 |      |     |     |     |     |
|                                            |        | 1503   | 1513 | 1524 | 1533 | 1537 | 1552 | 1554 | 1562 | 1572 |      |     |     |     |     |
|                                            |        | 1581   | 1585 | 1596 | 1600 | 1603 | 1619 | 1627 | 1636 | 1640 |      |     |     |     |     |
|                                            |        | 1643   | 1649 | 1666 | 1672 | 1683 | 1688 | 1705 | 1717 | 1727 |      |     |     |     |     |
|                                            |        | 1746   | 1749 |      |      |      |      |      |      |      |      |     |     |     |     |

The “Covariance Parameter Estimates” table in [Output 67.11.5](#) displays the estimate and asymptotic estimated standard error of the common variance parameter of the normal random effects.

#### Output 67.11.5 Variance Estimate of the Normal Random Effects

| Covariance Parameter Estimates |                  |                   |
|--------------------------------|------------------|-------------------|
| Cov<br>Parm                    | REML<br>Estimate | Standard<br>Error |
| ID                             | 0.8308           | 0.2145            |

[Output 67.11.6](#) displays the Wald tests for both the fixed effects and the random effects. The random effects are statistically significant ( $p = 0.0042$ ). Results of testing the fixed effects are very similar to those based on the robust variance estimates. Laser photocoagulation appears to be effective ( $p = 0.0252$ ) in delaying the occurrence of blindness, although there is also a significant treatment by diabetes type interaction effect ( $p = 0.0071$ ).

**Output 67.11.6** Inference Based on the Frailty Model

| Type 3 Tests |                    |    |            |                |                        |  |
|--------------|--------------------|----|------------|----------------|------------------------|--|
| Effect       | Wald<br>Chi-Square | DF | Pr > ChiSq | Adjusted<br>DF | Adjusted<br>Pr > ChiSq |  |
| Treat        | 4.8964             | 1  | 0.0269     | 0.9587         | 0.0252                 |  |
| Type         | 2.6386             | 1  | 0.1043     | 0.6795         | 0.0629                 |  |
| Treat*Type   | 7.1336             | 1  | 0.0076     | 0.9644         | 0.0071                 |  |
| ID           | 110.3916           | .  | .          | 74.2776        | 0.0042                 |  |

| Analysis of Maximum Likelihood Estimates |             |    |                       |                   |            |            |
|------------------------------------------|-------------|----|-----------------------|-------------------|------------|------------|
| Parameter                                |             | DF | Parameter<br>Estimate | Standard<br>Error | Chi-Square | Pr > ChiSq |
| Treat                                    | Laser       | 1  | -0.49849              | 0.22528           | 4.8964     | 0.0269     |
| Type                                     | Adult       | 1  | 0.39781               | 0.24490           | 2.6386     | 0.1043     |
| Treat*Type                               | Laser Adult | 1  | -0.96530              | 0.36142           | 7.1336     | 0.0076     |

| Analysis of Maximum Likelihood Estimates |             |       |                 |                          |  |  |
|------------------------------------------|-------------|-------|-----------------|--------------------------|--|--|
| Parameter                                |             |       | Hazard<br>Ratio | Label                    |  |  |
| Treat                                    | Laser       |       | .               | Treat Laser              |  |  |
| Type                                     | Adult       |       | .               | Type Adult               |  |  |
| Treat*Type                               | Laser Adult | Adult | .               | Treat Laser * Type Adult |  |  |

Estimates of hazard ratios of the laser treatment relative to nonlaser treatment are displayed in [Output 67.11.7](#). These estimates closely resemble those computed in analysis based on the marginal Cox model in [Output 67.11.3](#), which leads to the same conclusion that laser photocoagulation is effective in delaying blindness for both types of diabetes, and more effective for the adult-onset diabetes than for juvenile-onset diabetes.

**Output 67.11.7** Hazard Ratio Estimates for Frailty Model

| Frailty Model Analysis: Hazard Ratios for Treat |                   |                               |       |
|-------------------------------------------------|-------------------|-------------------------------|-------|
| Description                                     | Point<br>Estimate | 95% Wald Confidence<br>Limits |       |
| Treat Laser vs Others At Type=Adult             | 0.231             | 0.133                         | 0.403 |
| Treat Laser vs Others At Type=Juvenile          | 0.607             | 0.391                         | 0.945 |

## Example 67.12: Model Assessment Using Cumulative Sums of Martingale Residuals

The Mayo liver disease example of Lin, Wei, and Ying (1993) is reproduced here to illustrate the checking of the functional form of a covariate and the assessment of the proportional hazards assumption. The data represent 418 patients with primary biliary cirrhosis (PBC), among whom 161 had died as of the date of data listing. A subset of the variables is saved in the SAS data set Liver. The data set contains the following variables:

- Time, follow-up time, in years
- Status, event indicator with value 1 for death time and value 0 for censored time
- Age, age in years from birth to study registration
- Albumin, serum albumin level, in gm/dl
- Bilirubin, serum bilirubin level, in mg/dl
- Edema, edema presence
- Prottime, prothrombin time, in seconds

The following statements create the data set Liver:

```
data Liver;
 input Time Status Age Albumin Bilirubin Edema Prottime @@;
 label Time="Follow-up Time in Years";
 Time= Time / 365.25;
 datalines;
 400 1 58.7652 2.60 14.5 1.0 12.2 4500 0 56.4463 4.14 1.1 0.0 10.6
 1012 1 70.0726 3.48 1.4 0.5 12.0 1925 1 54.7406 2.54 1.8 0.5 10.3
 1504 0 38.1054 3.53 3.4 0.0 10.9 2503 1 66.2587 3.98 0.8 0.0 11.0
 1832 0 55.5346 4.09 1.0 0.0 9.7 2466 1 53.0568 4.00 0.3 0.0 11.0
 2400 1 42.5079 3.08 3.2 0.0 11.0 51 1 70.5599 2.74 12.6 1.0 11.5
 3762 1 53.7139 4.16 1.4 0.0 12.0 304 1 59.1376 3.52 3.6 0.0 13.6
 3577 0 45.6893 3.85 0.7 0.0 10.6 1217 1 56.2218 2.27 0.8 1.0 11.0
 3584 1 64.6461 3.87 0.8 0.0 11.0 3672 0 40.4435 3.66 0.7 0.0 10.8

 ... more lines ...

 989 0 35.0000 3.23 0.7 0.0 10.8 681 1 67.0000 2.96 1.2 0.0 10.9
 1103 0 39.0000 3.83 0.9 0.0 11.2 1055 0 57.0000 3.42 1.6 0.0 9.9
 691 0 58.0000 3.75 0.8 0.0 10.4 976 0 53.0000 3.29 0.7 0.0 10.6
;
```

Consider fitting a Cox model for the survival time of the PCB patients with the covariates Bilirubin,  $\log(\text{Prottime})$ ,  $\log(\text{Albumin})$ , Age, and Edema. The log transform, which is often applied to blood chemistry measurements, is deliberately not employed for Bilirubin. It is of interest to assess the functional form of the variable Bilirubin in the Cox model. The specifications are as follows:

```
ods graphics on;
proc phreg data=Liver;
 model Time*Status(0)=Bilirubin logProttime logAlbumin Age Edema;
 logProttime=log(Prottime);
 logAlbumin=log(Albumin);
 assess var=(Bilirubin) / resample seed=7548;
run;
```

The ASSESS statement creates a plot of the cumulative martingale residuals against the values of the covariate Bilirubin, which is specified in the VAR= option. The RESAMPLE option computes the  $p$ -value of a Kolmogorov-type supremum test based on a sample of 1,000 simulated residual patterns.

Parameter estimates of the model fit are shown in [Output 67.12.1](#). The plot in [Output 67.12.2](#) displays the observed cumulative martingale residual process for Bilirubin together with 20 simulated realizations from the null distribution. When ODS Graphics is enabled, this graphical display is requested by specifying the ASSESS statement. It is obvious that the observed process is atypical compared to the simulated realizations. Also, none of the 1,000 simulated realizations has an absolute maximum exceeding that of the observed cumulative martingale residual process. Both the graphical and numerical results indicate that a transform is deemed necessary for Bilirubin in the model.

**Output 67.12.1** Cox Model with Bilirubin as a Covariate

| The PHREG Procedure                      |    |                    |                |            |            |              |
|------------------------------------------|----|--------------------|----------------|------------|------------|--------------|
| Analysis of Maximum Likelihood Estimates |    |                    |                |            |            |              |
| Parameter                                | DF | Parameter Estimate | Standard Error | Chi-Square | Pr > ChiSq | Hazard Ratio |
| Bilirubin                                | 1  | 0.11733            | 0.01298        | 81.7567    | <.0001     | 1.124        |
| logProttime                              | 1  | 2.77581            | 0.71482        | 15.0794    | 0.0001     | 16.052       |
| logAlbumin                               | 1  | -3.17195           | 0.62945        | 25.3939    | <.0001     | 0.042        |
| Age                                      | 1  | 0.03779            | 0.00805        | 22.0288    | <.0001     | 1.039        |
| Edema                                    | 1  | 0.84772            | 0.28125        | 9.0850     | 0.0026     | 2.334        |





```

 x1 = 1 + (x1 - 1) / 10;
 x2= x1 * x1;
 x3= x1 * x2;
 status= rantbl(seed, .8);
 tmp= log(1-ranuni(seed));
 t1= -exp(-log(x1)) * tmp;
 t2= -exp(-.1*(x1+x2)) * tmp;
 t3= -exp(-.01*(x1+x2+x3)) * tmp;
 tt= -exp(-(x1>5)) * tmp;
 output;
 end;
run;

proc sort data=sim;
 by x1;
run;

proc phreg data=sim noprint;
 model t1*status(2)=x1;
 output out=out1 resmart=resmart;
run;

proc phreg data=sim noprint;
 model t2*status(2)=x1;
 output out=out2 resmart=resmart;
run;

proc phreg data=sim noprint;
 model t3*status(2)=x1 x2;
 output out=out3 resmart=resmart;
run;

proc phreg data=sim noprint;
 model tt*status(2)=x1;
 output out=out4 resmart=resmart;
run;

data out1(keep=x1 cresid1);
 retain cresid1 0;
 set out1;
 by x1;
 cresid1 + resmart;
 if last.x1 then output;
run;

data out2(keep=x1 cresid2);
 retain cresid2 0;
 set out2;
 by x1;
 cresid2 + resmart;
 if last.x1 then output;
run;

```

```

data out3(keep=x1 cresid3);
 retain cresid3 0;
 set out3;
 by x1;
 cresid3 + resmart;
 if last.x1 then output;
run;

data out4(keep=x1 cresid4);
 retain cresid4 0;
 set out4;
 by x1;
 cresid4 + resmart;
 if last.x1 then output;
run;

data all;
 set out1;
 set out2;
 set out3;
 set out4;
run;

proc template;
 define statgraph MisSpecification;
 BeginGraph;
 entrytitle "Covariate Misspecification";
 layout lattice / columns=2 rows=2 columndatarange=unionall;

 columnaxes;
 columnaxis / display=(ticks tickvalues label) label="x";
 columnaxis / display=(ticks tickvalues label) label="x";
 endcolumnaxes;

 cell;
 cellheader;
 entry "(a) Data: log(X), Model: X";
 endcellheader;
 layout overlay / xaxisopts=(display=none)
 yaxisopts=(label="Cumulative Residual");
 seriesplot y=cresid1 x=x1 / lineattrs=GraphFit;
 endlayout;
 endcell;

 cell;
 cellheader;
 entry "(b) Data: X*X, Model: X";
 endcellheader;
 layout overlay / xaxisopts=(display=none)
 yaxisopts=(label=" ");
 seriesplot y=cresid2 x=x1 / lineattrs=GraphFit;
 endlayout;
 endcell;
 end;
 end;

```

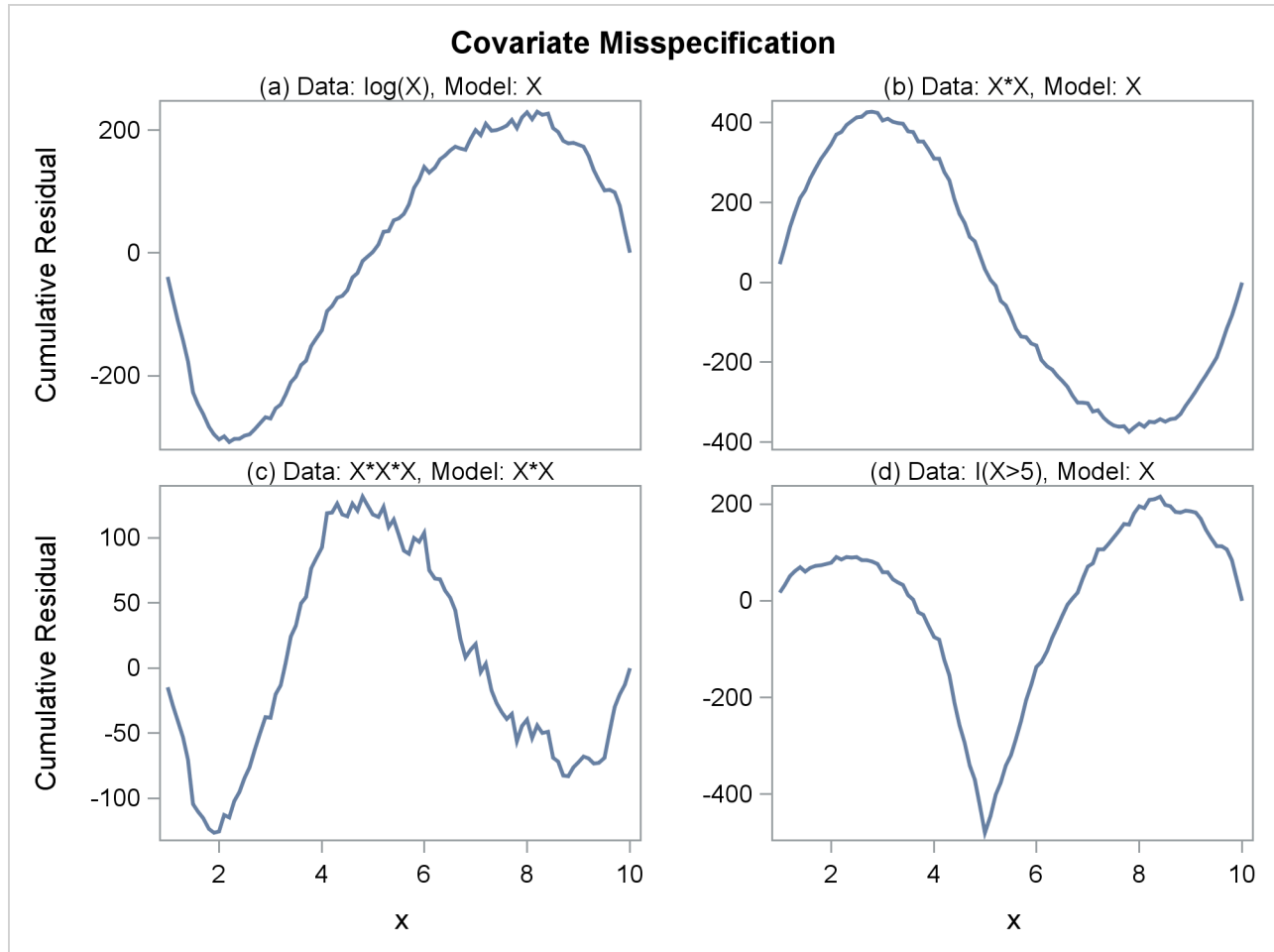
```
cell;
 cellheader;
 entry "(c) Data: X*X*X, Model: X*X";
 endcellheader;
 layout overlay / xaxisopts=(display=none)
 yaxisopts=(label="Cumulative Residual");
 seriesplot y=cresid3 x=x1 / lineattrs=GraphFit;
 endlayout;
endcell;

cell;
 cellheader;
 entry "(d) Data: I(X>5), Model: X";
 endcellheader;
 layout overlay / xaxisopts=(display=none)
 yaxisopts=(label=" ");
 seriesplot y=cresid4 x=x1 / lineattrs=GraphFit;
 endlayout;
endcell;

 endlayout;
EndGraph;
end;
run;

proc sgrender data=all template=MisSpecification;
run;
```

**Output 67.12.3** Typical Cumulative Residual Plot Patterns



**Table 67.17** Model Misspecifications

| Plot | Data              | Fitted Model |
|------|-------------------|--------------|
| (a)  | $\log(X)$         | $X$          |
| (b)  | $\{X, X^2\}$      | $X$          |
| (c)  | $\{X, X^2, X^3\}$ | $\{X, X^2\}$ |
| (d)  | $I(X > 5)$        | $X$          |

The curve of observed cumulative martingale residuals in [Output 67.12.2](#) most resembles the behavior of the curve in plot (a) of [Output 67.12.3](#), indicating that  $\log(\text{Bilirubin})$  might be a more appropriate term in the model than Bilirubin.

Next, the analysis of the natural history of the PBC is repeated with  $\log(\text{Bilirubin})$  replacing Bilirubin, and the functional form of  $\log(\text{Bilirubin})$  is assessed. Also assessed is the proportional hazards assumption for the Cox model. The analysis is carried out by the following statements:

```

proc phreg data=Liver;
 model Time*Status(0)=logBilirubin logProttime logAlbumin Age Edema;
 logBilirubin=log(Bilirubin);
 logProttime=log(Prottime);
 logAlbumin=log(Albumin);
 assess var=(logBilirubin) ph / crpanel resample seed=19;
run;
ods graphics off;

```

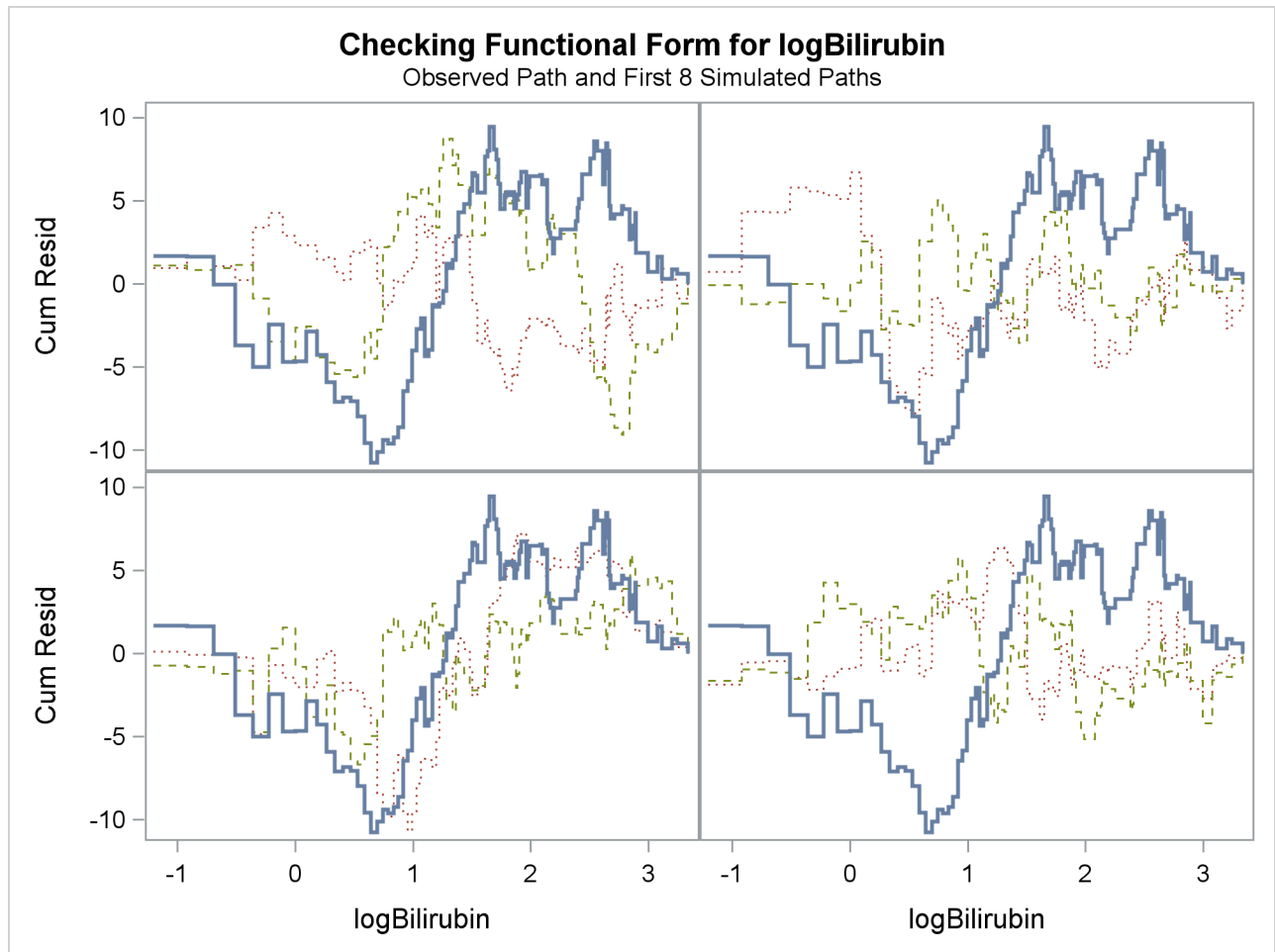
The SEED= option specifies a integer seed for generating random numbers. The CRPANEL option in the ASSESS statement requests a panel of four plots. Each plot displays the observed cumulative martingale residual process along with two simulated realizations. The PH option checks the proportional hazards assumption of the model by plotting the observed standardized score process with 20 simulated realizations for each covariate in the model.

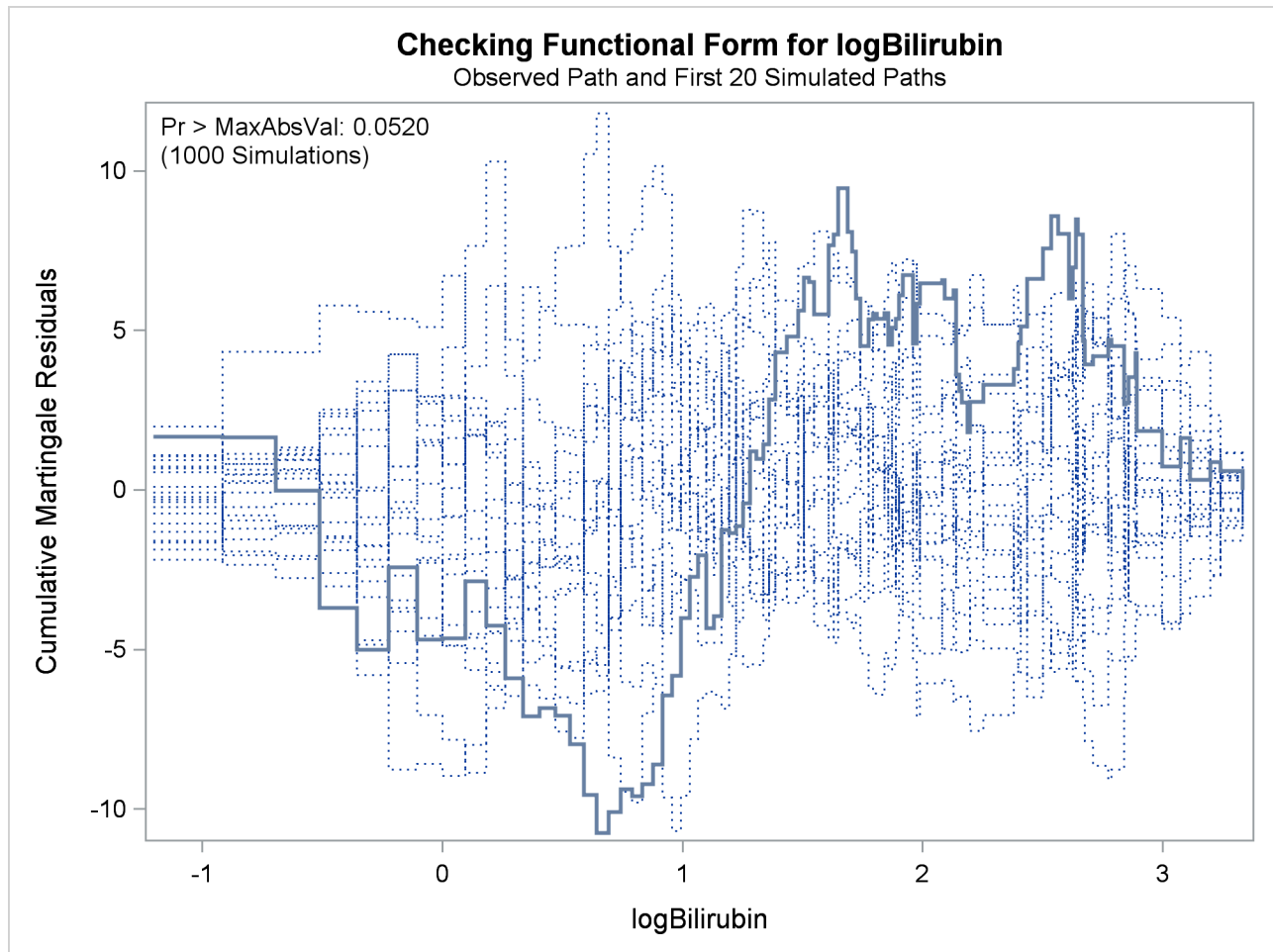
Output 67.12.4 displays the parameter estimates of the fitted model. The cumulative martingale residual plots in Output 67.12.5 and Output 67.12.6 show that the observed martingale residual process is more typical of the simulated realizations. The  $p$ -value for the Kolmogorov-type supremum test based on 1,000 simulations is 0.052, indicating that the log transform is a much improved functional form for Bilirubin.

**Output 67.12.4** Model with log(Bilirubin) as a Covariate

| The PHREG Procedure                      |    |                    |                |            |            |              |
|------------------------------------------|----|--------------------|----------------|------------|------------|--------------|
| Analysis of Maximum Likelihood Estimates |    |                    |                |            |            |              |
| Parameter                                | DF | Parameter Estimate | Standard Error | Chi-Square | Pr > ChiSq | Hazard Ratio |
| logBilirubin                             | 1  | 0.87072            | 0.08263        | 111.0484   | <.0001     | 2.389        |
| logProttime                              | 1  | 2.37789            | 0.76674        | 9.6181     | 0.0019     | 10.782       |
| logAlbumin                               | 1  | -2.53264           | 0.64819        | 15.2664    | <.0001     | 0.079        |
| Age                                      | 1  | 0.03940            | 0.00765        | 26.5306    | <.0001     | 1.040        |
| Edema                                    | 1  | 0.85934            | 0.27114        | 10.0447    | 0.0015     | 2.362        |

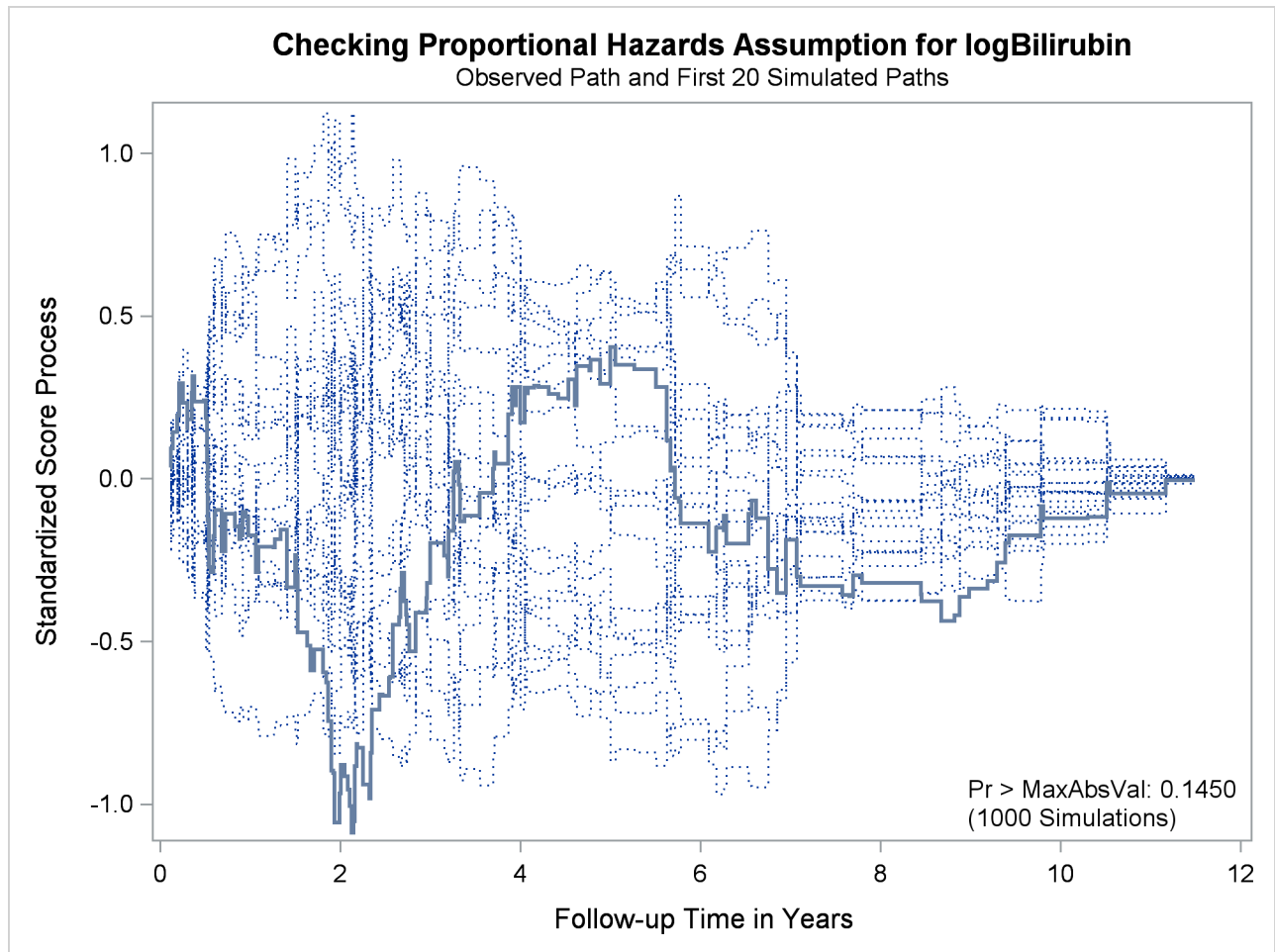
**Output 67.12.5** Panel Plot of Cumulative Martingale Residuals versus log(Bilirubin)



**Output 67.12.6** Cumulative Martingale Residuals versus log(Bilirubin)

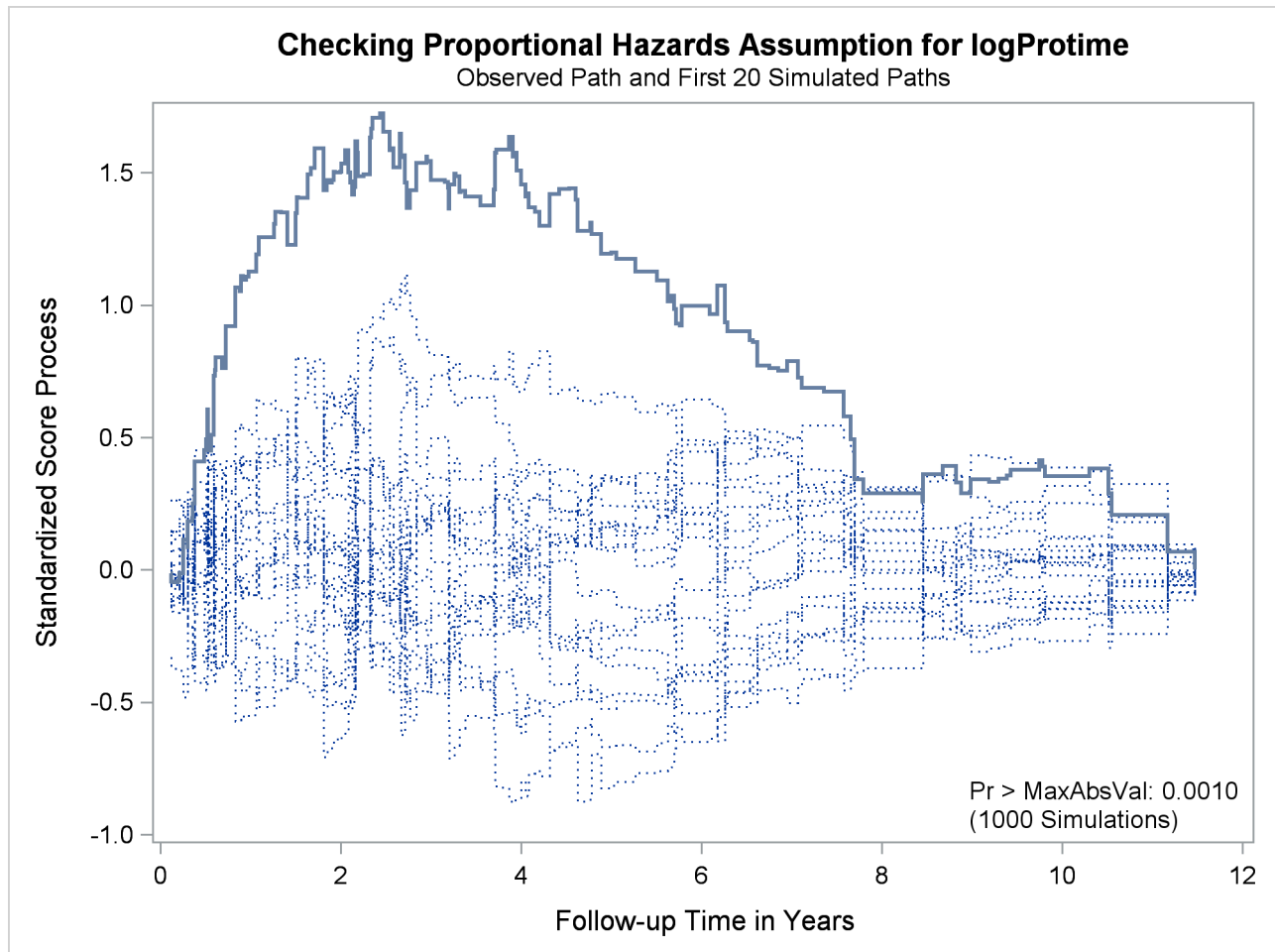
Output 67.12.7 and Output 67.12.8 display the results of proportional hazards assumption assessment for log(Bilirubin) and log(Prottime), respectively. The latter plot reveals nonproportional hazards for log(Prottime).

**Output 67.12.7** Standardized Score Process for log(Bilirubin)



[



**Output 67.12.8** Standardized Score Process for log(Prottime)

Plots for log(Albumin), Age, and Edema are not shown here. The Kolmogorov-type supremum test results for all the covariates are shown in [Output 67.12.9](#). In addition to log(Prottime), the proportional hazards assumption appears to be violated for Edema.

**Output 67.12.9** Kolmogorov-Type Supremum Tests for Proportional Hazards Assumption

| Supremum Test for Proportionals Hazards Assumption |                              |              |      |                   |
|----------------------------------------------------|------------------------------|--------------|------|-------------------|
| Variable                                           | Maximum<br>Absolute<br>Value | Replications | Seed | Pr ><br>MaxAbsVal |
| logBilirubin                                       | 1.0880                       | 1000         | 19   | 0.1450            |
| logProttime                                        | 1.7243                       | 1000         | 19   | 0.0010            |
| logAlbumin                                         | 0.8443                       | 1000         | 19   | 0.4330            |
| Age                                                | 0.7387                       | 1000         | 19   | 0.4620            |
| Edema                                              | 1.4350                       | 1000         | 19   | 0.0330            |

## Example 67.13: Bayesian Analysis of the Cox Model

This example illustrates the use of an informative prior. Hazard ratios, which are transformations of the regression parameters, are useful for interpreting survival models. This example also demonstrates the use of the HAZARDRATIO statement to obtain customized hazard ratios.

Consider the VALung data set in [Example 67.3](#). In this example, the Cox model is used for the Bayesian analysis. The parameters are the coefficients of the continuous explanatory variables (Kps, Duration, and Age) and the coefficients of the design variables for the categorical explanatory variables (Prior, Cell, and Therapy). You use the CLASS statement in PROC PHREG to specify the categorical variables and their reference levels. Using the default reference parameterization, the design variables for the categorical variables are Prioryes (for Prior with Prior='no' as reference), Celladeno, Cellsmall, Cellsquamous (for Cell with Cell='large' as reference), and Therapytest (for Therapy='standard' as reference).

Consider the explanatory variable Kps. The Karnofsky performance scale index enables patients to be classified according to their functional impairment. The scale can range from 0 to 100—0 for dead, and 100 for a normal, healthy person with no evidence of disease. Recall that a flat prior was used for the regression coefficient in the example in the section “[Bayesian Analysis](#)” on page 5547. A flat prior on the Kps coefficient implies that the coefficient is as likely to be 0.1 as it is to be  $-100000$ . A coefficient of  $-5$  means that a decrease of 20 points in the scale increases the hazard by  $e^{-20 \times -5} (=2.68 \times 10^{43})$ -fold, which is a rather unreasonable and unrealistic expectation for the effect of the Karnofsky index, much less than the value of  $-100000$ . Suppose you have a more realistic expectation: the effect is somewhat small and is more likely to be negative than positive, and a decrease of 20 points in the Karnofsky index will change the hazard from 0.9-fold (some minor positive effect) to 4-fold (a large negative effect). You can convert this opinion to a more informative prior on the Kps coefficient  $\beta_1$ . Mathematically,

$$0.9 < e^{-20\beta_1} < 4$$

which is equivalent to

$$-0.0693 < \beta_1 < 0.0053$$

This becomes the plausible range that you believe the Kps coefficient can take. Now you can find a normal distribution that best approximates this belief by placing the majority of the prior distribution mass within this range. Assuming this interval is  $\mu \pm 2\sigma$ , where  $\mu$  and  $\sigma$  are the mean and standard deviation of the normal prior, respectively, the hyperparameters  $\mu$  and  $\sigma$  are computed as follows:

$$\begin{aligned}\mu &= \frac{-0.0693 + 0.0053}{2} = -0.032 \\ \sigma &= \frac{0.0053 - (-0.0693)}{4} = 0.0186\end{aligned}$$

Note that a normal prior distribution with mean  $-0.0320$  and standard deviation  $0.0186$  indicates that you believe, before looking at the data, that a decrease of 20 points in the Karnofsky index will probably change the hazard rate by 0.9-fold to 4-fold. This does not rule out the possibility that the Kps coefficient can take a more extreme value such as  $-5$ , but the probability of having such extreme values is very small.

Assume the prior distributions are independent for all the parameters. For the coefficient of Kps, you use a normal prior distribution with mean  $-0.0320$  and variance  $0.0186^2 (=0.00035)$ . For other parameters, you resort to using a normal prior distribution with mean 0 and variance 1E6, which is fairly noninformative. Means and variances of these independent normal distributions are saved in the data set Prior as follows:

```

proc format;
 value yesno 0='no' 10='yes';
run;

data VALung;
 drop check m;
 retain Therapy Cell;
 infile cards column=column;
 length Check $ 1;
 label Time='time to death in days'
 Kps='Karnofsky performance scale'
 Duration='months from diagnosis to randomization'
 Age='age in years'
 Prior='prior therapy'
 Cell='cell type'
 Therapy='type of treatment';
 format Prior yesno.;
 M=Column;
 input Check $ @@;
 if M>Column then M=1;
 if Check='s'|Check='t' then do;
 input @M Therapy $ Cell $;
 delete;
 end;
 else do;
 input @M Time Kps Duration Age Prior @@;
 Status=(Time>0);
 Time=abs(Time);
 end;
 datalines;
standard squamous
 72 60 7 69 0 411 70 5 64 10 228 60 3 38 0 126 60 9 63 10
118 70 11 65 10 10 20 5 49 0 82 40 10 69 10 110 80 29 68 0
314 50 18 43 0 -100 70 6 70 0 42 60 4 81 0 8 40 58 63 10
144 30 4 63 0 -25 80 9 52 10 11 70 11 48 10
standard small
 30 60 3 61 0 384 60 9 42 0 4 40 2 35 0 54 80 4 63 10
 13 60 4 56 0 -123 40 3 55 0 -97 60 5 67 0 153 60 14 63 10
 59 30 2 65 0 117 80 3 46 0 16 30 4 53 10 151 50 12 69 0
 22 60 4 68 0 56 80 12 43 10 21 40 2 55 10 18 20 15 42 0
139 80 2 64 0 20 30 5 65 0 31 75 3 65 0 52 70 2 55 0
287 60 25 66 10 18 30 4 60 0 51 60 1 67 0 122 80 28 53 0
 27 60 8 62 0 54 70 1 67 0 7 50 7 72 0 63 50 11 48 0
392 40 4 68 0 10 40 23 67 10
standard adeno
 8 20 19 61 10 92 70 10 60 0 35 40 6 62 0 117 80 2 38 0
132 80 5 50 0 12 50 4 63 10 162 80 5 64 0 3 30 3 43 0
 95 80 4 34 0
standard large
177 50 16 66 10 162 80 5 62 0 216 50 15 52 0 553 70 2 47 0
278 60 12 63 0 12 40 12 68 10 260 80 5 45 0 200 80 12 41 10
156 70 2 66 0 -182 90 2 62 0 143 90 8 60 0 105 80 11 66 0
103 80 5 38 0 250 70 8 53 10 100 60 13 37 10

```

```

test squamous
999 90 12 54 10 112 80 6 60 0 -87 80 3 48 0 -231 50 8 52 10
242 50 1 70 0 991 70 7 50 10 111 70 3 62 0 1 20 21 65 10
587 60 3 58 0 389 90 2 62 0 33 30 6 64 0 25 20 36 63 0
357 70 13 58 0 467 90 2 64 0 201 80 28 52 10 1 50 7 35 0
30 70 11 63 0 44 60 13 70 10 283 90 2 51 0 15 50 13 40 10
test small
25 30 2 69 0 -103 70 22 36 10 21 20 4 71 0 13 30 2 62 0
87 60 2 60 0 2 40 36 44 10 20 30 9 54 10 7 20 11 66 0
24 60 8 49 0 99 70 3 72 0 8 80 2 68 0 99 85 4 62 0
61 70 2 71 0 25 70 2 70 0 95 70 1 61 0 80 50 17 71 0
51 30 87 59 10 29 40 8 67 0
test adeno
24 40 2 60 0 18 40 5 69 10 -83 99 3 57 0 31 80 3 39 0
51 60 5 62 0 90 60 22 50 10 52 60 3 43 0 73 60 3 70 0
8 50 5 66 0 36 70 8 61 0 48 10 4 81 0 7 40 4 58 0
140 70 3 63 0 186 90 3 60 0 84 80 4 62 10 19 50 10 42 0
45 40 3 69 0 80 40 4 63 0
test large
52 60 4 45 0 164 70 15 68 10 19 30 4 39 10 53 60 12 66 0
15 30 5 63 0 43 60 11 49 10 340 80 10 64 10 133 75 1 65 0
111 60 5 64 0 231 70 18 67 10 378 80 4 65 0 49 30 3 37 0
;

data Prior;
input _TYPE_ $ Kps Duration Age Prioryes Celladeno Cellsmall
 Cellsquamous Therapytest;
datalines;
Mean -0.0320 0 0 0 0 0 0 0 0
Var 0.00035 1e6 1e6 1e6 1e6 1e6 1e6 1e6
run;

```

In the following BAYES statement, COEFFPRIOR=NORMAL(INPUT=Prior) specifies the normal prior distribution for the regression coefficients with details contained in the data set Prior. Summary statistics of the posterior distribution are produced by default. Autocorrelations and effective sample size are requested as convergence diagnostics as well as the trace plots for visual analysis. For comparisons of hazards, three HAZARDRATIO statements are specified—one for the variable Therapy, one for the variable Age, and one for the variable Cell.

```

ods graphics on;
proc phreg data=VALung;
class Prior(ref='no') Cell(ref='large') Therapy(ref='standard');
model Time*Status(0) = Kps Duration Age Prior Cell Therapy;
bayes seed=1 coeffprior=normal(input=Prior) diagnostic=(autocorr ess)
 plots=trace;
hazardratio 'Hazard Ratio Statement 1' Therapy;
hazardratio 'Hazard Ratio Statement 2' Age / unit=10;
hazardratio 'Hazard Ratio Statement 3' Cell;
run;
ods graphics off;

```

This analysis generates a posterior chain of 10,000 iterations after 2,000 iterations of burn-in, as depicted in Output 67.13.1.

**Output 67.13.1** Model Information

| The PHREG Procedure |             |                       |
|---------------------|-------------|-----------------------|
| Bayesian Analysis   |             |                       |
| Model Information   |             |                       |
| Data Set            | WORK.VALUNG |                       |
| Dependent Variable  | Time        | time to death in days |
| Censoring Variable  | Status      |                       |
| Censoring Value(s)  | 0           |                       |
| Model               | Cox         |                       |
| Ties Handling       | BRESLOW     |                       |
| Sampling Algorithm  | ARMS        |                       |
| Burn-In Size        | 2000        |                       |
| MC Sample Size      | 10000       |                       |
| Thinning            | 1           |                       |

Output 67.13.2 displays the names of the parameters and their corresponding effects and categories.

**Output 67.13.2** Parameter Names

| Regression Parameter Information |          |       |          |         |
|----------------------------------|----------|-------|----------|---------|
| Parameter                        | Effect   | Prior | Cell     | Therapy |
| Kps                              | Kps      |       |          |         |
| Duration                         | Duration |       |          |         |
| Age                              | Age      |       |          |         |
| Prioryes                         | Prior    | yes   |          |         |
| Celladeno                        | Cell     |       | adeno    |         |
| Cellsmall                        | Cell     |       | small    |         |
| Cellsquamous                     | Cell     |       | squamous |         |
| Therapytest                      | Therapy  |       |          | test    |

PROC PHREG computes the maximum likelihood estimates of regression parameters (Output 67.13.3). These estimates are used as the starting values for the simulation of posterior samples.

**Output 67.13.3** Parameter Estimates

| Maximum Likelihood Estimates |    |          |                |                       |         |
|------------------------------|----|----------|----------------|-----------------------|---------|
| Parameter                    | DF | Estimate | Standard Error | 95% Confidence Limits |         |
| Kps                          | 1  | -0.0326  | 0.00551        | -0.0434               | -0.0218 |
| Duration                     | 1  | -0.00009 | 0.00913        | -0.0180               | 0.0178  |
| Age                          | 1  | -0.00855 | 0.00930        | -0.0268               | 0.00969 |
| Prioryes                     | 1  | 0.0723   | 0.2321         | -0.3826               | 0.5273  |
| Celladeno                    | 1  | 0.7887   | 0.3027         | 0.1955                | 1.3819  |
| Cellsmall                    | 1  | 0.4569   | 0.2663         | -0.0650               | 0.9787  |
| Cellsquamous                 | 1  | -0.3996  | 0.2827         | -0.9536               | 0.1544  |
| Therapytest                  | 1  | 0.2899   | 0.2072         | -0.1162               | 0.6961  |

Output 67.13.4 displays the independent normal prior for the analysis.

**Output 67.13.4** Coefficient Prior

| Independent Normal Prior for Regression Coefficients |        |           |
|------------------------------------------------------|--------|-----------|
| Parameter                                            | Mean   | Precision |
| Kps                                                  | -0.032 | 2857.143  |
| Duration                                             | 0      | 1E-6      |
| Age                                                  | 0      | 1E-6      |
| Prioryes                                             | 0      | 1E-6      |
| Celladeno                                            | 0      | 1E-6      |
| Cellsmall                                            | 0      | 1E-6      |
| Cellsquamous                                         | 0      | 1E-6      |
| Therapytest                                          | 0      | 1E-6      |

Fit statistics are displayed in Output 67.13.5. These statistics are useful for variable selection.

**Output 67.13.5** Fit Statistics

| Fit Statistics                      |         |
|-------------------------------------|---------|
| DIC (smaller is better)             | 966.260 |
| pD (Effective Number of Parameters) | 7.934   |

Summary statistics of the posterior samples are shown in Output 67.13.6 and Output 67.13.7. These results are quite comparable to the classical results based on maximizing the likelihood as shown in Output 67.13.3, since the prior distribution for the regression coefficients is relatively flat.

**Output 67.13.6** Summary Statistics

| The PHREG Procedure |       |          |                       |             |          |          |
|---------------------|-------|----------|-----------------------|-------------|----------|----------|
| Bayesian Analysis   |       |          |                       |             |          |          |
| Posterior Summaries |       |          |                       |             |          |          |
| Parameter           | N     | Mean     | Standard<br>Deviation | Percentiles |          |          |
|                     |       |          |                       | 25%         | 50%      | 75%      |
| Kps                 | 10000 | -0.0326  | 0.00523               | -0.0362     | -0.0326  | -0.0291  |
| Duration            | 10000 | -0.00159 | 0.00954               | -0.00756    | -0.00093 | 0.00504  |
| Age                 | 10000 | -0.00844 | 0.00928               | -0.0147     | -0.00839 | -0.00220 |
| Priories            | 10000 | 0.0742   | 0.2348                | -0.0812     | 0.0737   | 0.2337   |
| Celladeno           | 10000 | 0.7881   | 0.3065                | 0.5839      | 0.7876   | 0.9933   |
| Cellsmall           | 10000 | 0.4639   | 0.2709                | 0.2817      | 0.4581   | 0.6417   |
| Cellsquamous        | 10000 | -0.4024  | 0.2862                | -0.5927     | -0.4025  | -0.2106  |
| Therapytest         | 10000 | 0.2892   | 0.2038                | 0.1528      | 0.2893   | 0.4240   |

**Output 67.13.7** Interval Statistics

| Posterior Intervals |       |                     |         |              |         |
|---------------------|-------|---------------------|---------|--------------|---------|
| Parameter           | Alpha | Equal-Tail Interval |         | HPD Interval |         |
| Kps                 | 0.050 | -0.0429             | -0.0222 | -0.0433      | -0.0226 |
| Duration            | 0.050 | -0.0220             | 0.0156  | -0.0210      | 0.0164  |
| Age                 | 0.050 | -0.0263             | 0.00963 | -0.0265      | 0.00941 |
| Priories            | 0.050 | -0.3936             | 0.5308  | -0.3832      | 0.5384  |
| Celladeno           | 0.050 | 0.1879              | 1.3920  | 0.1764       | 1.3755  |
| Cellsmall           | 0.050 | -0.0571             | 1.0167  | -0.0888      | 0.9806  |
| Cellsquamous        | 0.050 | -0.9687             | 0.1635  | -0.9641      | 0.1667  |
| Therapytest         | 0.050 | -0.1083             | 0.6930  | -0.1284      | 0.6710  |

With autocorrelations retreating quickly to 0 ([Output 67.13.8](#)) and large effective sample sizes ([Output 67.13.9](#)), both diagnostics indicate a reasonably good mixing of the Markov chain. The trace plots in [Output 67.13.10](#) also confirm the convergence of the Markov chain.

**Output 67.13.8** Autocorrelation Diagnostics

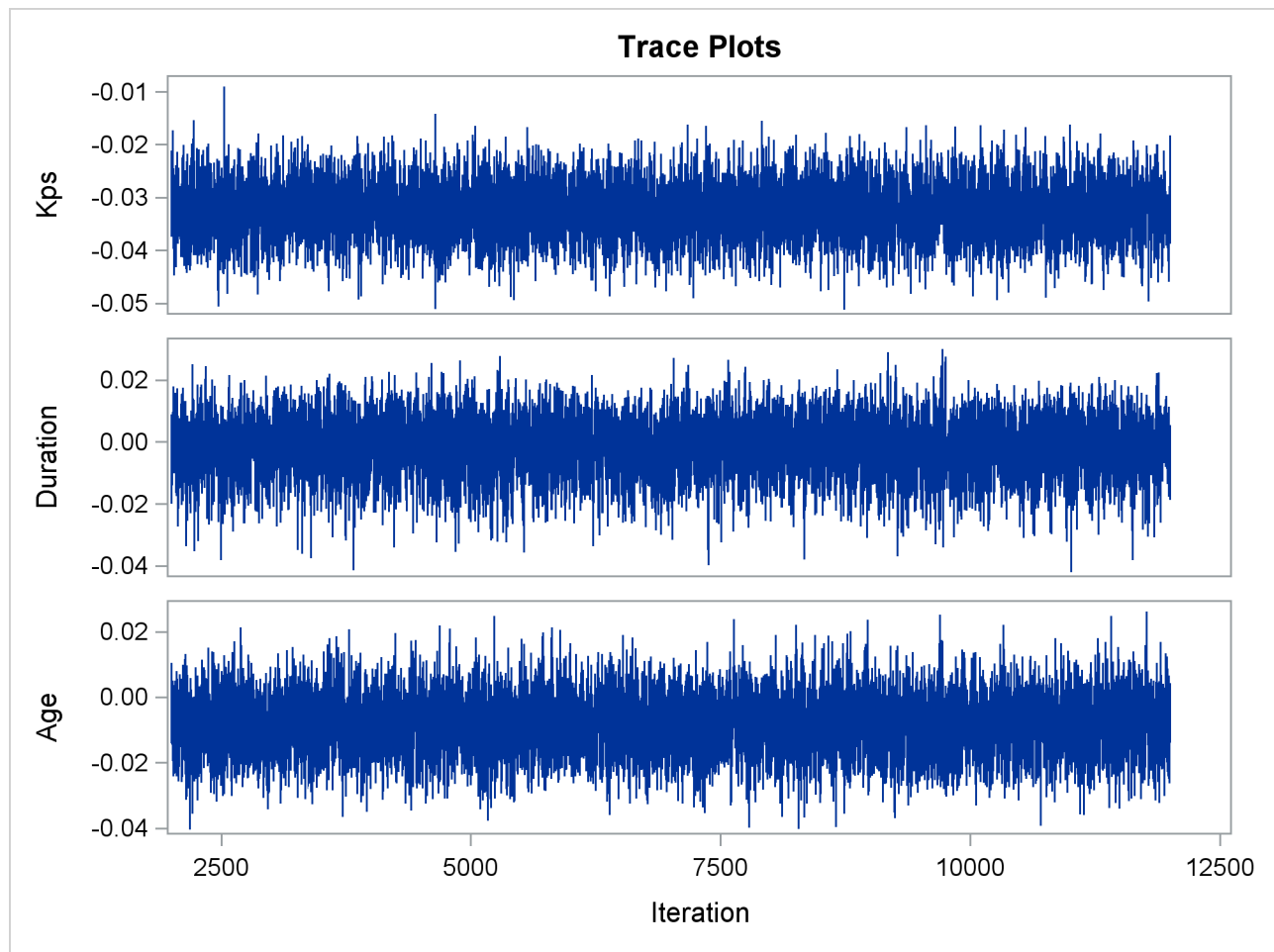
| The PHREG Procedure        |        |         |         |         |
|----------------------------|--------|---------|---------|---------|
| Bayesian Analysis          |        |         |         |         |
| Posterior Autocorrelations |        |         |         |         |
| Parameter                  | Lag 1  | Lag 5   | Lag 10  | Lag 50  |
| Kps                        | 0.1442 | -0.0016 | 0.0096  | -0.0013 |
| Duration                   | 0.2672 | -0.0054 | -0.0004 | -0.0011 |
| Age                        | 0.1374 | -0.0044 | 0.0129  | 0.0084  |
| Priories                   | 0.2507 | -0.0271 | -0.0012 | 0.0004  |
| Celladeno                  | 0.4160 | 0.0265  | -0.0062 | 0.0190  |
| Cellsmall                  | 0.5055 | 0.0277  | -0.0011 | 0.0271  |
| Cellsquamous               | 0.3586 | 0.0252  | -0.0044 | 0.0107  |
| Therapytest                | 0.2063 | 0.0199  | -0.0047 | -0.0166 |

**Output 67.13.9** Effective Sample Size Diagnostics

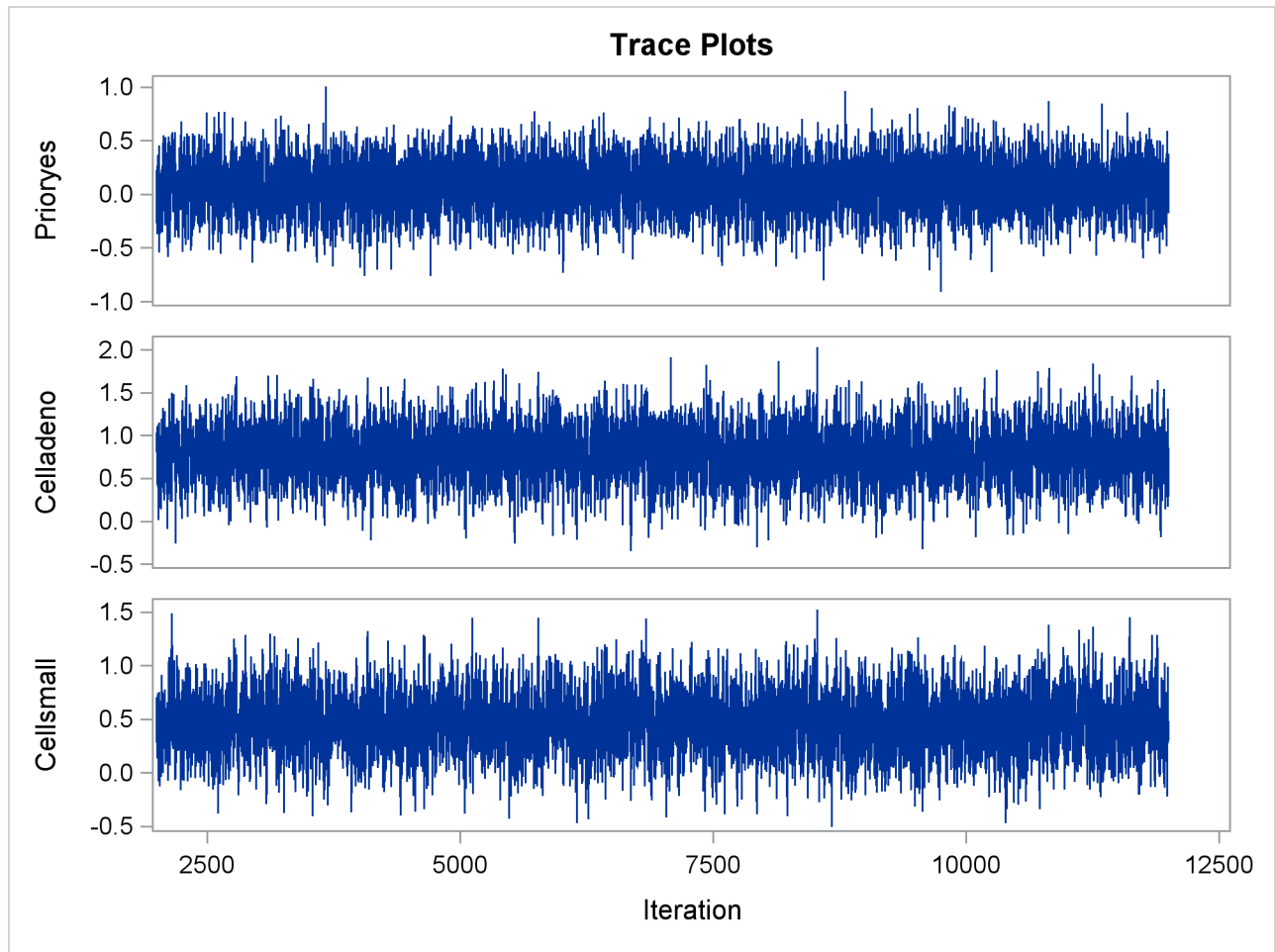
| Effective Sample Sizes |        |                 |            |
|------------------------|--------|-----------------|------------|
| Parameter              | ESS    | Autocorrelation |            |
|                        |        | Time            | Efficiency |
| Kps                    | 7046.7 | 1.4191          | 0.7047     |
| Duration               | 5790.0 | 1.7271          | 0.5790     |
| Age                    | 7426.1 | 1.3466          | 0.7426     |
| Priories               | 6102.2 | 1.6388          | 0.6102     |
| Celladeno              | 3673.4 | 2.7223          | 0.3673     |
| Cellsmall              | 3346.4 | 2.9883          | 0.3346     |
| Cellsquamous           | 4052.8 | 2.4674          | 0.4053     |
| Therapytest            | 6870.8 | 1.4554          | 0.6871     |



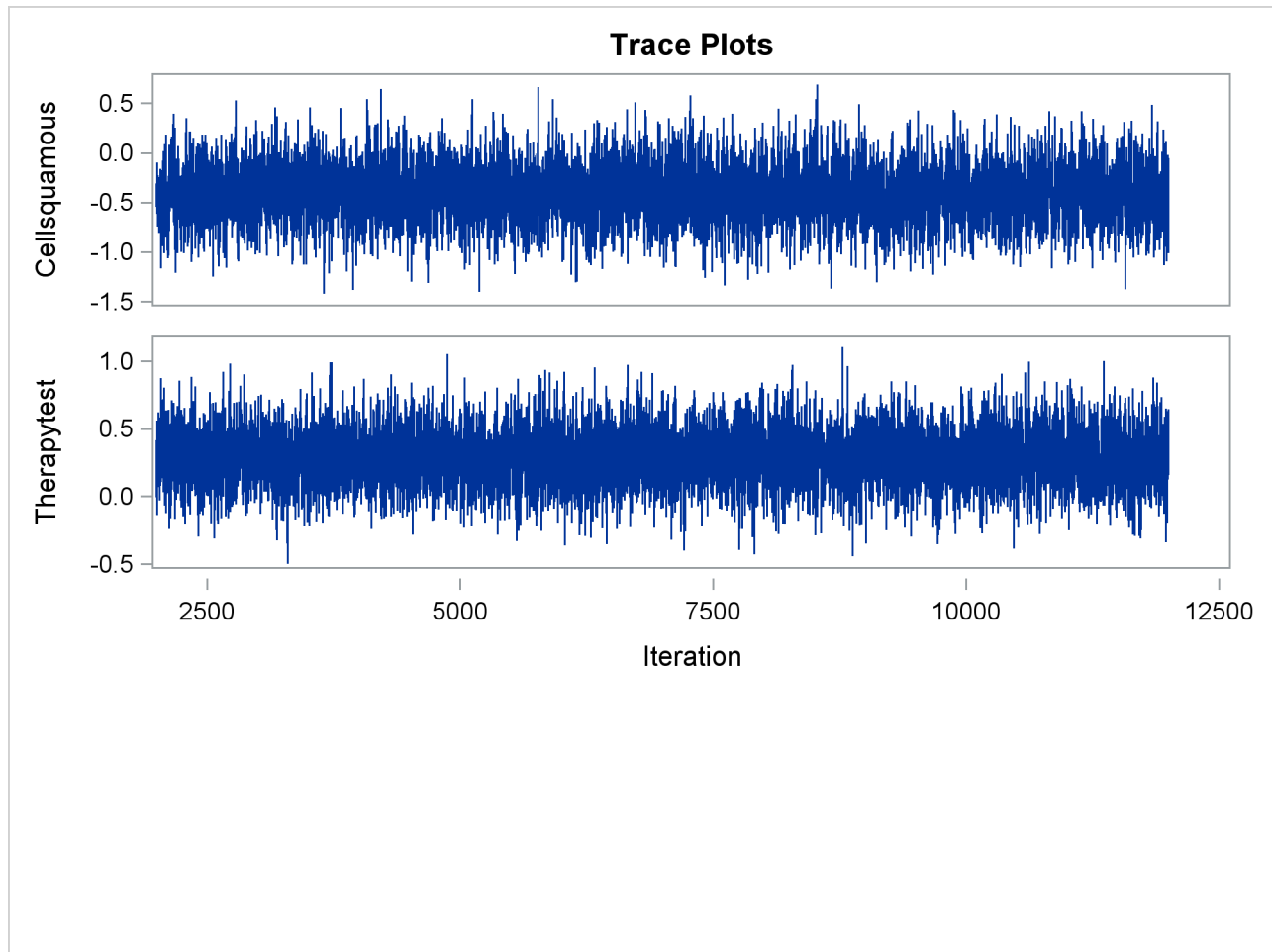
Output 67.13.10 Trace Plots



Output 67.13.10 continued



Output 67.13.10 continued



The first HAZARDRATIO statement compares the hazards between the standard therapy and the test therapy. Summaries of the posterior distribution of the corresponding hazard ratio are shown in Output 67.13.11. There is a 95% chance that the hazard ratio of standard therapy versus test therapy lies between 0.5 and 1.1.

Output 67.13.11 Hazard Ratio for Treatment

| Hazard Ratio Statement 1: Hazard Ratios for Therapy |           |        |                         |        |                  |        |
|-----------------------------------------------------|-----------|--------|-------------------------|--------|------------------|--------|
| Description                                         | N         | Mean   | Standard Deviation      |        |                  |        |
| Therapy standard vs test                            | 10000     | 0.7645 | 0.1573                  |        |                  |        |
| Hazard Ratio Statement 1: Hazard Ratios for Therapy |           |        |                         |        |                  |        |
| 25%                                                 | Quantiles |        | 95% Equal-Tail Interval |        | 95% HPD Interval |        |
| 0.6544                                              | 50%       | 75%    | Interval                |        |                  |        |
|                                                     | 0.7488    | 0.8583 | 0.5001                  | 1.1143 | 0.4788           | 1.0805 |

The second HAZARDRATIO statement assesses the change of hazards for an increase in Age of 10 years. Summaries of the posterior distribution of the corresponding hazard ratio are shown in [Output 67.13.12](#).

**Output 67.13.12** Hazard Ratio for Age

| Hazard Ratio Statement 2: Hazard Ratios for Age |       |                         |                    |                  |        |        |
|-------------------------------------------------|-------|-------------------------|--------------------|------------------|--------|--------|
| Description                                     | N     | Mean                    | Standard Deviation | 25%              | 50%    | 75%    |
| Age Unit=10                                     | 10000 | 0.9230                  | 0.0859             | 0.8635           | 0.9195 | 0.9782 |
| Hazard Ratio Statement 2: Hazard Ratios for Age |       |                         |                    |                  |        |        |
|                                                 |       | 95% Equal-Tail Interval |                    | 95% HPD Interval |        |        |
|                                                 |       | 0.7685                  | 1.1011             | 0.7650           | 1.0960 |        |

The third HAZARDRATIO statement compares the changes of hazards between two types of cells. For four types of cells, there are six different pairs of cell comparisons. The results are shown in [Output 67.13.13](#).

**Output 67.13.13** Hazard Ratios for Cell

| Hazard Ratio Statement 3: Hazard Ratios for Cell |           |        |                         |        |                  |        |        |
|--------------------------------------------------|-----------|--------|-------------------------|--------|------------------|--------|--------|
| Description                                      | N         | Mean   | Standard Deviation      |        |                  |        |        |
| Cell adeno vs large                              | 10000     | 2.3048 | 0.7224                  |        |                  |        |        |
| Cell adeno vs small                              | 10000     | 1.4377 | 0.4078                  |        |                  |        |        |
| Cell adeno vs squamous                           | 10000     | 3.4449 | 1.0745                  |        |                  |        |        |
| Cell large vs small                              | 10000     | 0.6521 | 0.1780                  |        |                  |        |        |
| Cell large vs squamous                           | 10000     | 1.5579 | 0.4548                  |        |                  |        |        |
| Cell small vs squamous                           | 10000     | 2.4728 | 0.7081                  |        |                  |        |        |
| Hazard Ratio Statement 3: Hazard Ratios for Cell |           |        |                         |        |                  |        |        |
|                                                  | Quantiles |        | 95% Equal-Tail Interval |        | 95% HPD Interval |        |        |
|                                                  | 25%       | 50%    | 75%                     |        |                  |        |        |
|                                                  | 1.7929    | 2.1982 | 2.7000                  | 1.2067 | 4.0227           | 1.0053 | 3.7057 |
|                                                  | 1.1522    | 1.3841 | 1.6704                  | 0.7930 | 2.3999           | 0.7309 | 2.2662 |
|                                                  | 2.6789    | 3.2941 | 4.0397                  | 1.8067 | 5.9727           | 1.6303 | 5.5946 |
|                                                  | 0.5264    | 0.6325 | 0.7545                  | 0.3618 | 1.0588           | 0.3331 | 1.0041 |
|                                                  | 1.2344    | 1.4955 | 1.8089                  | 0.8492 | 2.6346           | 0.7542 | 2.4575 |
|                                                  | 1.9620    | 2.3663 | 2.8684                  | 1.3789 | 4.1561           | 1.2787 | 3.9263 |

## Example 67.14: Bayesian Analysis of Piecewise Exponential Model

This example illustrates using a piecewise exponential model in a Bayesian analysis. Consider the Rats data set in the section “Getting Started: PHREG Procedure” on page 5543. In the following statements, PROC PHREG is used to carry out a Bayesian analysis for the piecewise exponential model. In the BAYES statement, the option `PIECEWISE` stipulates a piecewise exponential model, and `PIECEWISE=HAZARD` requests that the constant hazards be modeled in the original scale. By default, eight intervals of constant hazards are used, and the intervals are chosen such that each has roughly the same number of events.

```
data Rats;
 label Days = 'Days from Exposure to Death';
 input Days Status Group @@;
 datalines;
143 1 0 164 1 0 188 1 0 188 1 0
190 1 0 192 1 0 206 1 0 209 1 0
213 1 0 216 1 0 220 1 0 227 1 0
230 1 0 234 1 0 246 1 0 265 1 0
304 1 0 216 0 0 244 0 0 142 1 1
156 1 1 163 1 1 198 1 1 205 1 1
232 1 1 232 1 1 233 1 1 233 1 1
233 1 1 233 1 1 239 1 1 240 1 1
261 1 1 280 1 1 280 1 1 296 1 1
296 1 1 323 1 1 204 0 1 344 0 1
;

proc phreg data=Rats;
 model Days*Status(0)=Group;
 bayes seed=1 piecewise=hazard;
run;
```

The “Model Information” table in [Output 67.14.1](#) shows that the piecewise exponential model is being used.

**Output 67.14.1** Model Information

| The PHREG Procedure |                       |                             |
|---------------------|-----------------------|-----------------------------|
| Bayesian Analysis   |                       |                             |
| Model Information   |                       |                             |
| Data Set            | WORK.RATS             |                             |
| Dependent Variable  | Days                  | Days from Exposure to Death |
| Censoring Variable  | Status                |                             |
| Censoring Value(s)  | 0                     |                             |
| Model               | Piecewise Exponential |                             |
| Sampling Algorithm  | ARMS                  |                             |
| Burn-In Size        | 2000                  |                             |
| MC Sample Size      | 10000                 |                             |
| Thinning            | 1                     |                             |

By default the time axis is partitioned into eight intervals of constant hazard. [Output 67.14.2](#) details the number of events and observations in each interval. Note that the constant hazard parameters are named  $\text{Lambda1}, \dots, \text{Lambda8}$ . You can supply your own partition by using the `INTERVALS=` suboption within the `PIECEWISE=HAZARD` option.

**Output 67.14.2** Interval Partition

| Constant Hazard Time Intervals |        |   |       |                  |  |
|--------------------------------|--------|---|-------|------------------|--|
| Interval                       |        | N | Event | Hazard           |  |
| [Lower,                        | Upper) |   |       | Parameter        |  |
| 0                              | 176    | 5 | 5     | $\text{Lambda1}$ |  |
| 176                            | 201.5  | 5 | 5     | $\text{Lambda2}$ |  |
| 201.5                          | 218    | 7 | 5     | $\text{Lambda3}$ |  |
| 218                            | 232.5  | 5 | 5     | $\text{Lambda4}$ |  |
| 232.5                          | 233.5  | 4 | 4     | $\text{Lambda5}$ |  |
| 233.5                          | 253.5  | 5 | 4     | $\text{Lambda6}$ |  |
| 253.5                          | 288    | 4 | 4     | $\text{Lambda7}$ |  |
| 288                            | Infty  | 5 | 4     | $\text{Lambda8}$ |  |

The model parameters consist of the eight hazard parameters  $\text{Lambda1}, \dots, \text{Lambda8}$ , and the regression coefficient `Group`. The maximum likelihood estimates are displayed in [Output 67.14.3](#). Again, these estimates are used as the starting values for simulation of the posterior distribution.

**Output 67.14.3** Maximum Likelihood Estimates

| Maximum Likelihood Estimates |    |          |                |                       |         |
|------------------------------|----|----------|----------------|-----------------------|---------|
| Parameter                    | DF | Estimate | Standard Error | 95% Confidence Limits |         |
| $\text{Lambda1}$             | 1  | 0.000953 | 0.000443       | 0.000084              | 0.00182 |
| $\text{Lambda2}$             | 1  | 0.00794  | 0.00371        | 0.000672              | 0.0152  |
| $\text{Lambda3}$             | 1  | 0.0156   | 0.00734        | 0.00120               | 0.0300  |
| $\text{Lambda4}$             | 1  | 0.0236   | 0.0115         | 0.00112               | 0.0461  |
| $\text{Lambda5}$             | 1  | 0.3669   | 0.1959         | -0.0172               | 0.7509  |
| $\text{Lambda6}$             | 1  | 0.0276   | 0.0148         | -0.00143              | 0.0566  |
| $\text{Lambda7}$             | 1  | 0.0262   | 0.0146         | -0.00233              | 0.0548  |
| $\text{Lambda8}$             | 1  | 0.0545   | 0.0310         | -0.00626              | 0.1152  |
| <code>Group</code>           | 1  | -0.6223  | 0.3468         | -1.3020               | 0.0573  |

Without using the `PRIOR=` suboption within the `PIECEWISE=HAZARD` option to specify the prior of the hazard parameters, the default is to use the noninformative and improper prior displayed in [Output 67.14.4](#).

**Output 67.14.4** Hazard Prior

| Improper Prior for Hazards |             |
|----------------------------|-------------|
| Parameter                  | Prior       |
| Lambda1                    | 1 / Lambda1 |
| Lambda2                    | 1 / Lambda2 |
| Lambda3                    | 1 / Lambda3 |
| Lambda4                    | 1 / Lambda4 |
| Lambda5                    | 1 / Lambda5 |
| Lambda6                    | 1 / Lambda6 |
| Lambda7                    | 1 / Lambda7 |
| Lambda8                    | 1 / Lambda8 |

The noninformative uniform prior is used for the regression coefficient Group (Output 67.14.5), as in the section “Bayesian Analysis” on page 5547.

**Output 67.14.5** Coefficient Prior

| Uniform Prior for Regression Coefficients |          |
|-------------------------------------------|----------|
| Parameter                                 | Prior    |
| Group                                     | Constant |

Summary statistics for all model parameters are shown in Output 67.14.6 and Output 67.14.7.

**Output 67.14.6** Summary Statistics

| The PHREG Procedure |       |          |                       |             |          |         |
|---------------------|-------|----------|-----------------------|-------------|----------|---------|
| Bayesian Analysis   |       |          |                       |             |          |         |
| Posterior Summaries |       |          |                       |             |          |         |
| Parameter           | N     | Mean     | Standard<br>Deviation | Percentiles |          |         |
|                     |       |          |                       | 25%         | 50%      | 75%     |
| Lambda1             | 10000 | 0.000945 | 0.000444              | 0.000624    | 0.000876 | 0.00118 |
| Lambda2             | 10000 | 0.00782  | 0.00363               | 0.00519     | 0.00724  | 0.00979 |
| Lambda3             | 10000 | 0.0155   | 0.00735               | 0.0102      | 0.0144   | 0.0195  |
| Lambda4             | 10000 | 0.0236   | 0.0116                | 0.0152      | 0.0217   | 0.0297  |
| Lambda5             | 10000 | 0.3634   | 0.1965                | 0.2186      | 0.3266   | 0.4685  |
| Lambda6             | 10000 | 0.0278   | 0.0153                | 0.0166      | 0.0249   | 0.0356  |
| Lambda7             | 10000 | 0.0265   | 0.0151                | 0.0157      | 0.0236   | 0.0338  |
| Lambda8             | 10000 | 0.0558   | 0.0323                | 0.0322      | 0.0488   | 0.0721  |
| Group               | 10000 | -0.6154  | 0.3570                | -0.8569     | -0.6186  | -0.3788 |

**Output 67.14.7** Interval Statistics

| Parameter | Alpha | Posterior Intervals |         |              |         |
|-----------|-------|---------------------|---------|--------------|---------|
|           |       | Equal-Tail Interval |         | HPD Interval |         |
| Lambda1   | 0.050 | 0.000289            | 0.00199 | 0.000208     | 0.00182 |
| Lambda2   | 0.050 | 0.00247             | 0.0165  | 0.00194      | 0.0152  |
| Lambda3   | 0.050 | 0.00484             | 0.0331  | 0.00341      | 0.0301  |
| Lambda4   | 0.050 | 0.00699             | 0.0515  | 0.00478      | 0.0462  |
| Lambda5   | 0.050 | 0.0906              | 0.8325  | 0.0541       | 0.7469  |
| Lambda6   | 0.050 | 0.00676             | 0.0654  | 0.00409      | 0.0580  |
| Lambda7   | 0.050 | 0.00614             | 0.0648  | 0.00421      | 0.0569  |
| Lambda8   | 0.050 | 0.0132              | 0.1368  | 0.00637      | 0.1207  |
| Group     | 0.050 | -1.3190             | 0.0893  | -1.3379      | 0.0652  |

The default diagnostics—namely, lag1, lag5, lag10, lag50 autocorrelations (Output 67.14.8), the Geweke diagnostics (Output 67.14.9), and the effective sample size diagnostics (Output 67.14.10)—show a good mixing of the Markov chain.

**Output 67.14.8** Autocorrelations

| The PHREG Procedure        |        |         |         |         |
|----------------------------|--------|---------|---------|---------|
| Bayesian Analysis          |        |         |         |         |
| Posterior Autocorrelations |        |         |         |         |
| Parameter                  | Lag 1  | Lag 5   | Lag 10  | Lag 50  |
| Lambda1                    | 0.0705 | 0.0015  | 0.0017  | -0.0076 |
| Lambda2                    | 0.0909 | 0.0206  | -0.0013 | -0.0039 |
| Lambda3                    | 0.0861 | -0.0072 | 0.0011  | 0.0002  |
| Lambda4                    | 0.1447 | -0.0023 | 0.0081  | 0.0082  |
| Lambda5                    | 0.1086 | 0.0072  | -0.0038 | -0.0028 |
| Lambda6                    | 0.1281 | 0.0049  | -0.0036 | 0.0048  |
| Lambda7                    | 0.1925 | -0.0011 | 0.0094  | -0.0011 |
| Lambda8                    | 0.2128 | 0.0322  | -0.0042 | -0.0045 |
| Group                      | 0.5638 | 0.0410  | -0.0003 | -0.0071 |



**Output 67.14.9** Geweke Diagnostics

| Geweke Diagnostics |         |         |
|--------------------|---------|---------|
| Parameter          | z       | Pr >  z |
| Lambda1            | -0.0705 | 0.9438  |
| Lambda2            | -0.4936 | 0.6216  |
| Lambda3            | 0.5751  | 0.5652  |
| Lambda4            | 1.0514  | 0.2931  |
| Lambda5            | 0.8910  | 0.3729  |
| Lambda6            | 0.2976  | 0.7660  |
| Lambda7            | 1.6543  | 0.0981  |
| Lambda8            | 0.6686  | 0.5038  |
| Group              | -1.2621 | 0.2069  |

**Output 67.14.10** Effective Sample Size

| Parameter | ESS    | Autocorrelation |            |
|-----------|--------|-----------------|------------|
|           |        | Time            | Efficiency |
| Lambda1   | 7775.3 | 1.2861          | 0.7775     |
| Lambda2   | 6874.8 | 1.4546          | 0.6875     |
| Lambda3   | 7655.7 | 1.3062          | 0.7656     |
| Lambda4   | 6337.1 | 1.5780          | 0.6337     |
| Lambda5   | 6563.3 | 1.5236          | 0.6563     |
| Lambda6   | 6720.8 | 1.4879          | 0.6721     |
| Lambda7   | 5968.7 | 1.6754          | 0.5969     |
| Lambda8   | 5137.2 | 1.9466          | 0.5137     |
| Group     | 2980.4 | 3.3553          | 0.2980     |

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# Chapter 68

## The PLAN Procedure

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### Overview: PLAN Procedure

The PLAN procedure constructs designs and randomizes plans for factorial experiments, especially nested and crossed experiments and randomized block designs. PROC PLAN can also be used for generating lists of permutations and combinations of numbers. The PLAN procedure can construct the following types of experimental designs:

- full factorial designs, with and without randomization
- certain balanced and partially balanced incomplete block designs
- generalized cyclic incomplete block designs
- Latin square designs

For other kinds of experimental designs, especially fractional factorial, response surface, and orthogonal array designs, see the FACTEX and OPTTEX procedures and the ADX Interface in SAS/QC software.

PROC PLAN generates designs by first generating a selection of the levels for the first factor. Then, for the second factor, PROC PLAN generates a selection of its levels for each level of the first factor. In general, for a given factor, the PLAN procedure generates a selection of its levels for all combinations of levels for the factors that precede it.

The selection can be done in five different ways:

- randomized selection, for which the levels are returned in a random order
- ordered selection, for which the levels are returned in a standard order every time a selection is generated
- cyclic selection, for which the levels returned are computed by cyclically permuting the levels of the previous selection
- permuted selection, for which the levels are a permutation of the integers  $1, \dots, n$
- combination selection, for which the  $m$  levels are selected as a combination of the integers  $1, \dots, n$  taken  $m$  at a time

The randomized selection method can be used to generate randomized plans. Also, by appropriate use of cyclic selection, any of the designs in the very wide class of generalized cyclic block designs (Jarrett and Hall 1978) can be generated.

There is no limit to the depth to which the different factors can be nested, and any number of randomized plans can be generated.

You can also declare a list of factors to be selected simultaneously with the lowest (that is, the most nested) factor. The levels of the factors in this list can be seen as constituting the treatment to be applied to the cells of the design. For this reason, factors in this list are called *treatments*. With this list, you can generate and randomize plans in one run of PROC PLAN.

## Getting Started: PLAN Procedure

### Three Replications with Four Factors

Suppose you want to determine if the order in which four drugs are given affects the response of a subject. If you have only three subjects to test, you can use the following statements to design the experiment.

```
proc plan seed=27371;
 factors Replicate=3 ordered Drug=4;
run;
```

These statements produce a design with three replicates of the four levels of the factor Drug arranged in random order. The three levels of Replicate are arranged in order, as shown in [Figure 68.1](#).

**Figure 68.1** Three Replications and Four Factors

| The PLAN Procedure |           |          |         |
|--------------------|-----------|----------|---------|
| Factor             | Select    | Levels   | Order   |
| Replicate          | 3         | 3        | Ordered |
| Drug               | 4         | 4        | Random  |
|                    | Replicate | --Drug-- |         |
|                    | 1         | 3 2 4 1  |         |
|                    | 2         | 1 2 4 3  |         |
|                    | 3         | 4 1 2 3  |         |

You might also want to apply one of four different treatments to each cell of this plan (for example, applying different amounts of each drug). The following additional statements create the output shown in [Figure 68.2](#):

```
factors Replicate=3 ordered Drug=4;
treatments Treatment=4;
run;
```

**Figure 68.2** Using the TREATMENTS Statement

| The PLAN Procedure |        |        |         |
|--------------------|--------|--------|---------|
| Plot Factors       |        |        |         |
| Factor             | Select | Levels | Order   |
| Replicate          | 3      | 3      | Ordered |
| Drug               | 4      | 4      | Random  |
| Treatment Factors  |        |        |         |
| Factor             | Select | Levels | Order   |
| Treatment          | 4      | 4      | Random  |



Figure 68.2 continued

| Replicate | --Drug-- | --Treatment-- |   |   |   |
|-----------|----------|---------------|---|---|---|
| 1         | 3 1 2 4  | 2             | 1 | 3 | 4 |
| 2         | 4 3 2 1  | 4             | 1 | 2 | 3 |
| 3         | 3 2 4 1  | 1             | 4 | 2 | 3 |

## Randomly Assigning Subjects to Treatments

You can use the PLAN procedure to design a completely randomized design. Suppose you have 12 experimental units, and you want to assign one of two treatments to each unit. Use a DATA step to store the unrandomized design in a SAS data set, and then call PROC PLAN to randomize it by specifying one factor with the default type of RANDOM, having 12 levels. The following statements produce Figure 68.3 and Figure 68.4:

```

title 'Completely Randomized Design';
/* The unrandomized design */

data Unrandomized;
 do Unit=1 to 12;
 if (Unit <= 6) then Treatment=1;
 else Treatment=2;
 output;
 end;
run;

/* Randomize the design */

proc plan seed=27371;
 factors Unit=12;
 output data=Unrandomized out=Randomized;
run;

proc sort data=Randomized;
 by Unit;
run;
proc print;
run;

```

Figure 68.3 shows that the 12 levels of the unit factor have been randomly reordered and then lists the new ordering.

**Figure 68.3** A Completely Randomized Design for Two Treatments

| Completely Randomized Design |        |        |        |
|------------------------------|--------|--------|--------|
| The PLAN Procedure           |        |        |        |
| Factor                       | Select | Levels | Order  |
| Unit                         | 12     | 12     | Random |
| -----Unit-----               |        |        |        |
| 8                            | 5      | 1      | 4      |
| 6                            | 2      | 12     | 7      |
| 3                            | 9      | 10     | 11     |

After the data set is sorted by the unit variable, the randomized design is displayed (Figure 68.4).

**Figure 68.4** A Completely Randomized Design for Two Treatments

| Completely Randomized Design |      |           |
|------------------------------|------|-----------|
| Obs                          | Unit | Treatment |
| 1                            | 1    | 1         |
| 2                            | 2    | 1         |
| 3                            | 3    | 2         |
| 4                            | 4    | 1         |
| 5                            | 5    | 1         |
| 6                            | 6    | 1         |
| 7                            | 7    | 2         |
| 8                            | 8    | 1         |
| 9                            | 9    | 2         |
| 10                           | 10   | 2         |
| 11                           | 11   | 2         |
| 12                           | 12   | 2         |

You can also generate the plan by using a **TREATMENTS** statement instead of a DATA step. The following statements generate the same plan.

```
proc plan seed=27371;
 factors Unit=12;
 treatments Treatment=12 cyclic (1 1 1 1 1 1 2 2 2 2 2 2);
 output out=Randomized;
run;
```

## Syntax: PLAN Procedure

The following statements are available in the PLAN procedure:

```
PROC PLAN < options > ;
 FACTORS factor-selections < / NOPRINT > ;
 OUTPUT OUT=SAS-data-set < factor-value-settings > ;
 TREATMENTS factor-selections ;
```

To use PROC PLAN, you need to specify the PROC PLAN statement and at least one FACTORS statement before the first RUN statement. The TREATMENTS statement, OUTPUT statement, and additional FACTORS statements can appear either before the first RUN statement or after it.

The rest of this section gives detailed syntax information for each of the statements, beginning with the PROC PLAN statement. The remaining statements are described in alphabetical order.

You can use PROC PLAN interactively by specifying multiple groups of statements, separated by RUN statements. For details, see the section “Using PROC PLAN Interactively” on page 5782.

## PROC PLAN Statement

```
PROC PLAN < options > ;
```

The PROC PLAN statement invokes the PLAN procedure. Optionally, you can also specify a random number seed or a default method for selecting levels of factors. By default, the procedure uses a random number seed generated from reading the time of day from the computer’s clock and randomly selects levels of factors. These defaults can be modified with the SEED= and ORDERED options, respectively. Unlike many SAS/STAT procedures, the PLAN procedure does not have a DATA= option in the PROC PLAN statement; in this procedure, both the input and output data sets are specified in the OUTPUT statement.

Table 68.1 summarizes the options available in the PROC PLAN statement.

**Table 68.1** PROC PLAN Statement Options

| Option  | Description                                                                   |
|---------|-------------------------------------------------------------------------------|
| ORDERED | Selects the levels of the factor as the integers 1, 2, . . . , $m$ , in order |
| SEED=   | Specifies an integer used to start the pseudo-random number generator         |

You can specify the following options in the PROC PLAN statement:

### ORDERED

selects the levels of the factor as the integers 1, 2, . . . ,  $m$ , in order. For more detail, see “*Selection-Types*” on page 5777 and “*Specifying Factor Structures*” on page 5784.

### SEED=*number*

specifies an integer used to start the pseudo-random number generator for selecting factor levels randomly. If you do not specify a seed, or if you specify a value less than or equal to zero, the seed is by default generated from reading the time of day from the computer’s clock.

## FACTORS Statement

**FACTORS** *factor-selections* </ **NOPRINT** > ;

The FACTORS statement specifies the factors of the plan and generates the plan. Taken together, the *factor-selections* specify the plan to be generated; more than one *factor-selection* request can be used in a FACTORS statement. The form of a *factor-selection* is

*name* = *m* < **OF** *n* > < *selection-type* > ;

where

- name* is a valid SAS name. This gives the name of a factor in the design.
- m* is a positive integer that gives the number of values to be selected. If *n* is specified, the value of *m* must be less than or equal to *n*.
- n* is a positive integer that gives the number of values to be selected from.
- selection-type* specifies one of five methods for selecting *m* values. Possible values are COMB, CYCLIC, ORDERED, PERM, and RANDOM. The CYCLIC *selection-type* has additional optional specifications that enable you to specify an initial block of numbers to be cyclically permuted and an increment used to permute the numbers. By default, the *selection-type* is RANDOM, unless you use the ORDERED option in the PROC PLAN statement. In this case, the default *selection-type* is ORDERED. For details, see the following section, “[Selection-Types](#)”; for examples, see the section “[Syntax Examples](#)” on page 5778.

The following option can appear in the FACTORS statement after the slash:

### **NOPRINT**

suppresses the display of the plan. This is particularly useful when you require only an output data set. Note that this option temporarily disables the Output Delivery System (ODS); see Chapter 20, “[Using the Output Delivery System](#),” for more information.

### **Selection-Types**

PROC PLAN interprets *selection-type* as follows:

- RANDOM** selects the *m* levels of the factor randomly without replacement from the integers 1, 2, . . . , *n*. Or, if *n* is not specified, RANDOM selects levels by randomly ordering the integers 1, 2, . . . , *m*.
- ORDERED** selects the levels of the factor as the integers 1, 2, . . . , *m*, in that order.
- PERM** selects the *m* levels of the factor as a permutation of the integers 1, . . . , *m* according to an algorithm that cycles through all *m*! permutations. The permutations are produced in a sorted standard order; see [Example 68.6](#).
- COMB** selects the *m* levels of the factor as a combination of the integers 1, . . . , *n* taken *m* at a time, according to an algorithm that cycles through all  $n!/(m!(n - m)!)$  combinations. The combinations are produced in a sorted standard order; see [Example 68.6](#).

**CYCLIC** *<(initial-block)>* *<increment>* selects the levels of the factor by cyclically permuting the integers 1, 2, . . . , *n*. Wrapping occurs at *m* if *n* is not specified, and at *n* if *n* is specified. Additional optional specifications are as follows.

With the *selection-type* CYCLIC, you can optionally specify an *initial-block* and an *increment*. The *Argument* *initial-block* must be specified within parentheses, and it specifies the block of numbers to permute. The first permutation is the block you specify, the second is the block permuted by 1 (or by the *increment* you specify), and so on. By default, the *initial-block* is the integers 1, 2, . . . , *m*. If you specify an *initial-block*, it must have *m* values. Values specified in the *initial-block* do not have to be given in increasing order.

The *increment* specifies the increment by which to permute the block of numbers. By default, the *increment* is 1.

## Syntax Examples

This section gives some simple syntax examples. For more complex examples and details on how to generate various designs, see “[Specifying Factor Structures](#)” on page 5784. The examples in this section assume that you use the default random selection method and do not use the **ORDERED** option in the **PROC PLAN** statement.

The following specification generates a random permutation of the numbers 1, 2, 3, 4, and 5.

```
factors A=5;
```

The following specification generates a random permutation of five of the integers from 1 to 8, selected without replacement.

```
factors A=5 of 8;
```

Adding the **ORDERED** *selection-type* to the two previous specifications generates an ordered list of the integers 1 to 5. The following specification cyclically permutes the integers 1, 2, 3, and 4.

```
factors A=4 cyclic;
```

Since this simple request generates only one permutation of the numbers, the procedure generates an ordered list of the integers 1 to 4. The following specification cyclically permutes the integers 5 to 8.

```
factors A=4 of 8 cyclic (5 6 7 8);
```

In this case, since only one permutation is performed, the procedure generates an ordered list of the integers 5 to 8. The following specification produces an ordered list for A, with values 1 and 2.

```
factors A=2 ordered B=4 of 8 cyclic (5 6 7 8) 2;
```

The associated factor levels for B are 5, 6, 7, 8 for level 1 of A, and 7, 8, 1, 2 for level 2 of A.

## Handling More Than One Factor-Selection

For cases with more than one *factor-selection* in the same **FACTORS** statement, **PROC PLAN** constructs the design as follows:

1. **PROC PLAN** first generates levels for the first *factor-selection*. These levels are permutations of integers (1, 2, and so on) appropriate for the selection type chosen. If you do not specify a selection

type, PROC PLAN uses the default (RANDOM); if you specify the **ORDERED** option in the **PROC PLAN** statement, the procedure uses **ORDERED** as the default selection type.

2. For every integer generated for the first *factor-selection*, levels are generated for the second *factor-selection*. These levels are generated according to the specifications following the second equal sign.
3. This process is repeated until levels for all *factor-selections* have been generated.

The following statements give an example of generating a design with two random factors:

```
proc plan;
 factors One=4 Two=3;
run;
```

The procedure first generates a random permutation of the integers 1 to 4 and then, for each of these, generates a random permutation of the integers 1 to 3. You can think of factor Two as being nested within factor One, where the levels of factor One are to be randomly assigned to 4 units.

As another example, six random permutations of the numbers 1, 2, 3 can be generated by specifying the following statements:

```
proc plan;
 factors a=6 ordered b=3;
run;
```

---

## OUTPUT Statement

**OUTPUT** **OUT=SAS-data-set** < **DATA=SAS-data-set** > < *factor-value-settings* > ;

The OUTPUT statement applies only to the last plan generated. If you use PROC PLAN interactively, the OUTPUT statement for a given plan must be immediately preceded by the **FACTORS** statement (and the **TREATMENTS** statement, if appropriate) for the plan.

See “Output Data Sets” on page 5783 for more information about how output data sets are constructed.

You can specify the following options in the OUTPUT statement:

**OUT=SAS-data-set**

**DATA=SAS-data-set**

You can use the OUTPUT statement both to output the last plan generated and to use the last plan generated to randomize another SAS data set.

When you specify only the OUT= option in the OUTPUT statement, PROC PLAN saves the last plan generated to the specified data set. The output data set contains one variable for each factor in the plan and one observation for each cell in the plan. The value of a variable in a given observation is the level of the corresponding factor for that cell. The OUT= option is required.

When you specify both the DATA= and OUT= options in the OUTPUT statement, then PROC PLAN uses the last plan generated to randomize the input data set (DATA=), saving the results to the output data set (OUT=). The output data set has the same form as the input data set but has modified values for the variables that correspond to factors (see the section “Output Data Sets” on page 5783 for details). Values for variables not corresponding to factors are transferred without change.

*factor-value-settings*

specify the values input or output for the factors in the design. The form for *factor-value-settings* is different when only an `OUT=` data set is specified and when both `OUT=` and `DATA=` data sets are specified.

Both forms are discussed in the following section.

**Factor-Value-Settings with Only an `OUT=` Data Set**

When you specify only an `OUT=` data set, the form for each *factor-value-setting* specification is one of the following:

```
factor-name < NVALS=list-of-n-numbers > < ORDERED | RANDOM > ;
```

or

```
factor-name < CVALS=list-of-n-strings > < ORDERED | RANDOM > ;
```

where

- factor-name* is a factor in the last **FACTORS** statement preceding the **OUTPUT** statement.
- NVALS=** lists *n* numeric values for the factor. By default, the procedure uses `NVALS=(1 2 3 ... n)`.
- CVALS=** lists *n* character strings for the factor. Each string can have up to 40 characters, and each string must be enclosed in quotes. **CAUTION:** When you use the `CVALS=` option, the variable created in the output data set has a length equal to the length of the longest string given as a value; shorter strings are padded with trailing blanks. For example, the values output for the first level of a two-level factor with the following two different specifications are not the same.

```
CVALS=('String 1' "String 2")
```

```
CVALS=('String 1' "A longer string")
```

The value output with the second specification is 'String 1' followed by seven blanks. In order to match two such values (for example, when merging two plans), you must use the `TRIM` function in the **DATA** step (see *SAS Functions and CALL Routines: Reference*).

- ORDERED | RANDOM** specifies how values (those given with the `NVALS=` or `CVALS=` option, or the default values) are associated with the levels of a factor (the integers 1, 2, ..., *n*). The default association type is **ORDERED**, for which the first value specified is output for a factor level setting of 1, the second value specified is output for a level of 2, and so on. You can also specify an association type of **RANDOM**, for which the levels are associated with the values in a random order. Specifying **RANDOM** is useful for randomizing crossed experiments (see the section "[Randomizing Designs](#)" on page 5786).

The following statements give an example of using the **OUTPUT** statement with only an `OUT=` data set and with both the `NVALS=` and `CVALS=` specifications.

```
proc plan;
 factors a=6 ordered b=3;
 output out=design a nvals=(10 to 60 by 10)
 b cvals=('HSX' 'SB2' 'DNY');
run;
```

The DESIGN data set contains two variables, a and b. The values of the variable a are 10 when factor a equals 1, 20 when factor a equals 2, and so on. Values of the variable b are ‘HSX’ when factor b equals 1, ‘SB2’ when factor b equals 2, and ‘DNY’ when factor b equals 3.

### Factor-Value-Settings with OUT= and DATA= Data Sets

If you specify an input data set with **DATA=**, then PROC PLAN assumes that each factor in the last plan generated corresponds to a variable in the input set. If the variable name is different from the name of the factor to which it corresponds, the two can be associated in the values specification by

*input-variable-name = factor-name ;*

Then, the **NVALS=** or **CVALS=** specification can be used. The values given by **NVALS=** or **CVALS=** specify the input values as well as the output values for the corresponding variable.

Since the procedure assumes that the collection of input factor values constitutes a plan position description (see the section “**Output Data Sets**” on page 5783), the values must correspond to integers less than or equal to *m*, the number of values selected for the associated factor. If any input values do not correspond, then the collection does not define a plan position, and the corresponding observation is output without changing the values of any of the factor variables.

The following statements demonstrate the use of *factor-value-settings*. The input SAS data set a contains variables Block and Plot, which are renamed Day and Hour, respectively.

```
proc plan;
 factors Day=7 Hour=6;
 output data=a out=b
 Block = Day cvals=('Mon' 'Tue' 'Wed' 'Thu'
 'Fri' 'Sat' 'Sun')
 Plot = Hour;
run;
```

For another example of using both a **DATA=** and **OUT=** data set, see the section “**Randomly Assigning Subjects to Treatments**” on page 5774.

---

## TREATMENTS Statement

**TREATMENTS** *factor-selections ;*

The TREATMENTS statement specifies the treatments of the plan to generate, but it does not generate a plan. If you supply several **FACTORS** and TREATMENTS statements before the first RUN statement, the procedure uses only the last TREATMENTS specification and applies it to the plans that are generated by each of the **FACTORS** statements. The TREATMENTS statement must follow a **FACTORS** statement. The TREATMENTS statement has the same syntax as the **FACTORS** statement. The individual *factor-selections* also have the same form as in the **FACTORS** statement:



```
name = m <OF n> <selection-type> ;
```

The procedure generates each treatment simultaneously with the lowest (that is, the most nested) factor in the last **FACTORS** statement. The  $m$  value for each treatment must be at least as large as the  $m$  for the most nested factor.

The following statements use both a **FACTORS** and a **TREATMENTS** statement. First the **FACTORS** statement sets up the rows and columns of a  $3 \times 3$  square (factors  $r$  and  $c$ ). Then, the **TREATMENTS** statement augments the square with two cyclic treatments. The resulting design is a  $3 \times 3$  Graeco-Latin square, a type of design useful in main-effects factorial experiments.

```
proc plan;
 factors r=3 ordered c=3 ordered;
 treatments a=3 cyclic
 b=3 cyclic 2;
run;
```

The resulting Graeco-Latin square design is shown in [Figure 68.5](#). Notice how the values of  $r$  and  $c$  are ordered (1, 2, 3) as requested.

**Figure 68.5** A  $3 \times 3$  Graeco-Latin Square

| The PLAN Procedure |       |       |       |     |
|--------------------|-------|-------|-------|-----|
| r                  | --c-- | --a-- | --b-- |     |
| 1                  | 1 2 3 | 1 2 3 | 1     | 2 3 |
| 2                  | 1 2 3 | 2 3 1 | 3     | 1 2 |
| 3                  | 1 2 3 | 3 1 2 | 2     | 3 1 |

---

## Details: PLAN Procedure

---

### Using PROC PLAN Interactively

After specifying a design with a **FACTORS** statement and running PROC PLAN with a **RUN** statement, you can generate additional plans and output data sets without invoking PROC PLAN again.

In PROC PLAN, all statements can be used interactively. You can execute statements singly or in groups by following the single statement or group of statements with a **RUN** statement.

If you use PROC PLAN interactively, you can end the procedure with a **DATA** step, another PROC step, an **ENDSAS** statement, or a **QUIT** statement. The syntax of the **QUIT** statement is

```
quit;
```

When you use PROC PLAN interactively, additional **RUN** statements do not end the procedure but tell PROC PLAN to execute additional statements.

## Output Data Sets

To understand how PROC PLAN creates output data sets, you need to look at how the procedure represents a plan. A plan is a list of values for all the factors, the values being chosen according to the *factor-selection* requests you specify. For example, consider the plan produced by the following statements:

```
proc plan seed=12345;
 factors a=3 b=2;
run;
```

The plan as displayed by PROC PLAN is shown in Figure 68.6.

**Figure 68.6** A Simple Plan

| The PLAN Procedure |        |        |        |   |
|--------------------|--------|--------|--------|---|
| Factor             | Select | Levels | Order  |   |
| a                  | 3      | 3      | Random |   |
| b                  | 2      | 2      | Random |   |
|                    |        | a      | -b-    |   |
|                    |        | 2      | 2      | 1 |
|                    |        | 1      | 1      | 2 |
|                    |        | 3      | 2      | 1 |

The first cell of the plan has a=2 and b=2, the second has a=2 and b=1, the third has a=1 and b=1, and so on. If you output the plan to a data set with the OUTPUT statement, by default the output data set contains a numeric variable with that factor's name; the values of this numeric variable are the numbers of the successive levels selected for the factor in the plan. For example, the following statements produce Figure 68.7.

```
proc plan seed=12345;
 factors a=3 b=2;
 output out=out;
run;
proc print data=out;
run;
```

**Figure 68.7** Output Data Set from Simple Plan

| Obs | a | b |
|-----|---|---|
| 1   | 2 | 2 |
| 2   | 2 | 1 |
| 3   | 1 | 1 |
| 4   | 1 | 2 |
| 5   | 3 | 2 |
| 6   | 3 | 1 |

Alternatively, you can specify the values that are output for a factor with the `CVALS=` or `NVALS=` option. Also, you can specify that the internal values be associated with the output values in random order with the `RANDOM` option. See the section “[OUTPUT Statement](#)” on page 5779.

If you also specify an input data set (`DATA=`), each factor is associated with a variable in the `DATA=` data set. This occurs either implicitly by the factor and variable having the same name or explicitly as described in the specifications for the `OUTPUT` statement. In this case, the values of the variables corresponding to the factors are first read and then interpreted as describing the position of a cell in the plan. Then the respective values taken by the factors at that position are assigned to the variables in the `OUT=` data set. For example, consider the data set defined by the following statements.

```
data in;
 input a b;
 datalines;
1 1
2 1
3 1
;
```

Suppose you specify this data set as an input data set for the `OUTPUT` statement.

```
proc plan seed=12345;
 factors a=3 b=2;
 output out=out data=in;
run;
proc print data=out;
run;
```

PROC PLAN interprets the first observation as referring to the cell in the first row and column of the plan, since `a=1` and `b=1`; likewise, the second observation is interpreted as the cell in the second row and first column, and the third observation as the cell in the third row and first column. In the output data set, `a` and `b` have the values they have in the plan at these positions, as shown in [Figure 68.8](#).

**Figure 68.8** Output Form of Input Data Set from Simple Plan

| Obs | a | b |
|-----|---|---|
| 1   | 2 | 2 |
| 2   | 1 | 1 |
| 3   | 3 | 2 |

When the factors are random, this has the effect of randomizing the input data set in the same manner as the plan produced (see the sections “[Randomizing Designs](#)” on page 5786 and “[Randomly Assigning Subjects to Treatments](#)” on page 5774).

---

## Specifying Factor Structures

By appropriately combining features of the PLAN procedure, you can construct an extensive set of designs. The basic tools are the *factor-selections*, which are used in the `FACTORS` and `TREATMENTS` statements.

Table 68.2 summarizes how the procedure interprets various *factor-selections* (assuming that the **ORDERED** option is not specified in the **PROC PLAN** statement).

**Table 68.2** *Factor-Selection Interpretation*

| <b>Form of Request</b>                                                              | <b>Interpretation</b>                                                                                                                                 | <b>Example</b>                                     | <b>Results</b>                                                                                                                                                                                      |
|-------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <i>name=m</i>                                                                       | produce a random permutation of the integers $1, 2, \dots, m$                                                                                         | <b>t=15</b>                                        | lists a random ordering of the numbers $1, 2, \dots, 15$                                                                                                                                            |
| <i>name=m</i><br>cyclic                                                             | cyclically permute the integers $1, 2, \dots, m$                                                                                                      | <b>t=5 cyclic</b>                                  | selects the integers 1 to 5. On the next iteration, selects 2,3,4,5,1; then 3,4,5,1,2; and so on.                                                                                                   |
| <i>name=m</i> of <i>n</i>                                                           | choose a random sample of <i>m</i> integers (without replacement) from the set of integers $1, 2, \dots, n$                                           | <b>t=5 of 15</b>                                   | lists a random selection of 5 numbers from 1 to 15. First, the procedure selects 5 numbers and then arranges them in random order.                                                                  |
| <i>name=m</i> of <i>n</i><br>ordered                                                | has the same effect as <i>name=m</i> ordered                                                                                                          | <b>t=5 of 15<br/>ordered</b>                       | lists the integers 1 to 5 in increasing order (same as t=5 ordered)                                                                                                                                 |
| <i>name=m</i> of <i>n</i><br>cyclic                                                 | permute <i>m</i> of the <i>n</i> integers                                                                                                             | <b>t=5 of 30<br/>cyclic</b>                        | selects the integers 1 to 5. On the next iteration, selects 2,3,4,5,6; then 3,4,5,6,7; and so on. The 30th iteration produces 30,1,2,3,4; the 31st iteration produces 1,2,3,4,5; and so on.         |
| <i>name=m</i><br>perm                                                               | produce a list of all permutations of <i>m</i> integers                                                                                               | <b>t=5 perm</b>                                    | lists the integers 1,2,3,4,5 on the first iteration; on the second lists 1,2,3,5,4; on the 119th iteration lists 5,4,3,1,2; and on the last (120th) lists 5,4,3,2,1.                                |
| <i>name=m</i> of <i>n</i><br>comb                                                   | choose combinations of <i>m</i> integers from <i>n</i> integers                                                                                       | <b>t=3 of 5<br/>comb</b>                           | lists all combinations of 5 choose 3 integers. The first iteration is 1,2,3; the second is 1,2,4; the third is 1,2,5; and so on until the last iteration 3,4,5.                                     |
| <i>name=m</i> of <i>n</i><br>cyclic<br>( <i>initial-block</i> )                     | permute <i>m</i> of the <i>n</i> integers, starting with the values specified in the <i>initial-block</i>                                             | <b>t=4 of 30<br/>cyclic<br/>(2 10 15 18)</b>       | selects the integers 2,10,15,18. On the next iteration, selects 3,11,16,19; then 4,12,17,20; and so on. The thirteenth iteration is 14,22,27,30; the fourteenth iteration is 15,23,28,1; and so on. |
| <i>name=m</i> of <i>n</i><br>cyclic<br>( <i>initial-block</i> )<br><i>increment</i> | permute <i>m</i> of the <i>n</i> integers. Start with the values specified in the <i>initial-block</i> , then add the <i>increment</i> to each value. | <b>t=4 of 30<br/>cyclic<br/>(2 10 15 18)<br/>2</b> | selects the integers 2,10,15,18. On the next iteration, selects 4,12,17,20; then 6,14,19,22; and so on. The wrap occurs at the eighth iteration. The eighth iteration is 16,24,29,2; and so on.     |

In Table 68.2, in order for more than one iteration to appear in the plan, another *name=j* factor selection (with  $j > 1$ ) must precede the example factor selection. For example, the following statements produce six of the iterations described in the last entry of Table 68.2.

```
proc plan;
 factors c=6 ordered t=4 of 30 cyclic (2 10 15 18) 2;
run;
```

The following statements create a randomized complete block design and output the design to a data set.

```
proc plan ordered;
 factors blocks=3 cell=5;
 treatments t=5 random;
 output out=rcdb;
run;
```

---

## Randomizing Designs

In many situations, proper randomization is crucial for the validity of any conclusions to be drawn from an experiment. Randomization is used both to neutralize the effect of any unknown systematic biases that might be involved in the design and to provide a basis for the assumptions underlying the analysis.

You can use PROC PLAN to randomize an already existing design: one produced by a previous call to PROC PLAN, perhaps, or a more specialized design taken from a standard reference such as Cochran and Cox (1957). The method is to specify the appropriate block structure in the **FACTORS** statement and then to specify the data set where the design is stored with the **DATA=** option in the **OUTPUT** statement. For an illustration of this method, see the section “Randomly Assigning Subjects to Treatments” on page 5774).

Two sorts of randomization are provided for, corresponding to the **RANDOM** factor selection and association types in the **FACTORS** and **OUTPUT** statements, respectively. Designs in which factors are completely nested (for example, block designs) should be randomized by specifying that the selection type of each factor is **RANDOM** in the **FACTORS** statement, which is the default (see Example 68.3). On the other hand, if the factors are crossed (for example, row-and-column designs), they should be randomized by one random reassignment of their values for the whole design. To do this, specify that the association type of each factor is **RANDOM** in the **OUTPUT** statement (see Example 68.4).

---

## Displayed Output

The PLAN procedure displays the following output:

- the  $m$  value for each factor, which is the number of values to be selected
- the  $n$  value for each factor, which is the number of values to be selected from
- the selection type for each factor, as specified in the **FACTORS** statement
- the initial block and increment number for cyclic factors
- the *factor-value-selections* making up each plan

In addition, notes are written to the log that give the starting and ending values of the random number seed for each call to PROC PLAN.

---

## ODS Table Names

PROC PLAN assigns a name to each table it creates. You can use these names to reference the table in the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in the following table. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

**Table 68.3** ODS Tables Produced by PROC PLAN

| ODS Table Name | Description                  | Statements                |
|----------------|------------------------------|---------------------------|
| FInfo          | General factor information   | FACTORS and no TREATMENTS |
| PFInfo         | Plot factor information      | FACTORS and TREATMENTS    |
| Plan           | Computed plan                | default                   |
| TFInfo         | Treatment factor information | FACTORS and TREATMENTS    |

---

## Examples: PLAN Procedure

---

### Example 68.1: A Split-Plot Design

This plan is appropriate for a split-plot design with main plots forming a randomized complete block design. In this example, there are three blocks, four main plots per block, and two subplots per main plot. First, three random permutations (one for each of the blocks) of the integers 1, 2, 3, and 4 are produced. The four integers correspond to the four levels of the main plot factor *a*; the permutation determines how the levels of *a* are assigned to the main plots within a block. For each of these 12 numbers (four numbers per block for three blocks), a random permutation of the integers 1 and 2 is produced. Each two-integer permutation determines the assignment of the two levels of the subplot factor *b* within a main plot. The following statements produce Output 68.1.1:

```
title 'Split Plot Design';
proc plan seed=37277;
 factors Block=3 ordered a=4 b=2;
run;
```

**Output 68.1.1** A Split-Plot Design

| Split Plot Design  |        |        |         |
|--------------------|--------|--------|---------|
| The PLAN Procedure |        |        |         |
| Factor             | Select | Levels | Order   |
| Block              | 3      | 3      | Ordered |
| a                  | 4      | 4      | Random  |
| b                  | 2      | 2      | Random  |

| Block | a | -b- |
|-------|---|-----|
| 1     | 4 | 2 1 |
|       | 3 | 2 1 |
|       | 1 | 2 1 |
|       | 2 | 2 1 |
| 2     | 4 | 1 2 |
|       | 3 | 1 2 |
|       | 1 | 2 1 |
|       | 2 | 1 2 |
| 3     | 4 | 2 1 |
|       | 2 | 2 1 |
|       | 3 | 2 1 |
|       | 1 | 2 1 |

**Example 68.2: A Hierarchical Design**

In this example, three plants are nested within four pots, which are nested within three houses. The **FACTORS** statement requests a random permutation of the numbers 1, 2, and 3 to choose Houses randomly. The second step requests a random permutation of the numbers 1, 2, 3, and 4 for each of those first three numbers to randomly assign Pots to Houses. Finally, the **FACTORS** statement requests a random permutation of 1, 2, and 3 for each of the 12 integers in the second set of permutations. This last step randomly assigns Plants to Pots. The following statements produce **Output 68.2.1**:

```

title 'Hierarchical Design';
proc plan seed=17431;
 factors Houses=3 Pots=4 Plants=3 / noprint;
 output out=nested;
run;

proc print data=nested;
run;

```

**Output 68.2.1** A Hierarchical Design

| Hierarchical Design |        |      |        |
|---------------------|--------|------|--------|
| Obs                 | Houses | Pots | Plants |
| 1                   | 1      | 3    | 2      |
| 2                   | 1      | 3    | 3      |
| 3                   | 1      | 3    | 1      |
| 4                   | 1      | 1    | 3      |
| 5                   | 1      | 1    | 1      |
| 6                   | 1      | 1    | 2      |
| 7                   | 1      | 2    | 2      |
| 8                   | 1      | 2    | 3      |
| 9                   | 1      | 2    | 1      |
| 10                  | 1      | 4    | 3      |
| 11                  | 1      | 4    | 2      |
| 12                  | 1      | 4    | 1      |
| 13                  | 2      | 4    | 1      |
| 14                  | 2      | 4    | 3      |
| 15                  | 2      | 4    | 2      |
| 16                  | 2      | 2    | 2      |
| 17                  | 2      | 2    | 1      |
| 18                  | 2      | 2    | 3      |
| 19                  | 2      | 3    | 2      |
| 20                  | 2      | 3    | 3      |
| 21                  | 2      | 3    | 1      |
| 22                  | 2      | 1    | 2      |
| 23                  | 2      | 1    | 3      |
| 24                  | 2      | 1    | 1      |
| 25                  | 3      | 4    | 1      |
| 26                  | 3      | 4    | 3      |
| 27                  | 3      | 4    | 2      |
| 28                  | 3      | 1    | 3      |
| 29                  | 3      | 1    | 2      |
| 30                  | 3      | 1    | 1      |
| 31                  | 3      | 2    | 1      |
| 32                  | 3      | 2    | 2      |
| 33                  | 3      | 2    | 3      |
| 34                  | 3      | 3    | 3      |
| 35                  | 3      | 3    | 2      |
| 36                  | 3      | 3    | 1      |

**Example 68.3: An Incomplete Block Design**

Jarrett and Hall (1978) give an example of a generalized cyclic design with good efficiency characteristics. The design consists of two replicates of 52 treatments in 13 blocks of size 8. The following statements use the PLAN procedure to generate this design in an appropriately randomized form and store it in a SAS data set GCBD. Then the design is sorted and transposed to display in randomized order. The following statements produce Output 68.3.1 and Output 68.3.2:



```

title 'Generalized Cyclic Block Design';
proc plan seed=33373;
 factors Block=13 Plot=8;
 treatments Treatment=8 of 52 cyclic (1 2 3 4 32 43 46 49) 4;
 output out=GCBD;
quit;
proc sort data=GCBD out=GCBD;
 by Block Plot;
run;
proc transpose data= GCBD(rename=(Plot=_NAME_))
 out =tGCBD(drop=_NAME_);
 by Block;
 var Treatment;
run;
proc print data=tGCBD noobs;
run;

```

Output 68.3.1 A Generalized Cyclic Block Design

| Generalized Cyclic Block Design |                 |                         |                     |                           |
|---------------------------------|-----------------|-------------------------|---------------------|---------------------------|
| The PLAN Procedure              |                 |                         |                     |                           |
| Plot Factors                    |                 |                         |                     |                           |
| Factor                          | Select          | Levels                  | Order               |                           |
| Block                           | 13              | 13                      | Random              |                           |
| Plot                            | 8               | 8                       | Random              |                           |
| Treatment Factors               |                 |                         |                     |                           |
| Factor                          | Select          | Levels                  | Order               | Initial Block / Increment |
| Treatment                       | 8               | 52                      | Cyclic              | (1 2 3 4 32 43 46 49) / 4 |
| Block                           | -----Plot-----  |                         | -----Treatment----- |                           |
| 10                              | 7 4 8 1 2 3 5 6 | 1 2 3 4 32 43 46 49     |                     |                           |
| 8                               | 1 2 4 3 8 6 5 7 | 5 6 7 8 36 47 50 1      |                     |                           |
| 9                               | 2 5 4 7 3 1 8 6 | 9 10 11 12 40 51 2 5    |                     |                           |
| 6                               | 4 2 6 8 3 7 1 5 | 13 14 15 16 44 3 6 9    |                     |                           |
| 7                               | 4 7 6 3 1 2 8 5 | 17 18 19 20 48 7 10 13  |                     |                           |
| 4                               | 4 8 1 5 3 6 7 2 | 21 22 23 24 52 11 14 17 |                     |                           |
| 2                               | 6 2 3 8 7 5 1 4 | 25 26 27 28 4 15 18 21  |                     |                           |
| 3                               | 6 2 3 1 7 4 5 8 | 29 30 31 32 8 19 22 25  |                     |                           |
| 1                               | 1 2 7 8 5 6 3 4 | 33 34 35 36 12 23 26 29 |                     |                           |
| 5                               | 5 7 6 8 4 3 1 2 | 37 38 39 40 16 27 30 33 |                     |                           |
| 12                              | 5 8 1 4 7 3 6 2 | 41 42 43 44 20 31 34 37 |                     |                           |
| 13                              | 3 5 1 8 4 2 6 7 | 45 46 47 48 24 35 38 41 |                     |                           |
| 11                              | 4 1 5 2 3 8 6 7 | 49 50 51 52 28 39 42 45 |                     |                           |

**Output 68.3.2** A Generalized Cyclic Block Design

| Generalized Cyclic Block Design |    |    |    |    |    |    |    |    |
|---------------------------------|----|----|----|----|----|----|----|----|
| Block                           | _1 | _2 | _3 | _4 | _5 | _6 | _7 | _8 |
| 1                               | 33 | 34 | 26 | 29 | 12 | 23 | 35 | 36 |
| 2                               | 18 | 26 | 27 | 21 | 15 | 25 | 4  | 28 |
| 3                               | 32 | 30 | 31 | 19 | 22 | 29 | 8  | 25 |
| 4                               | 23 | 17 | 52 | 21 | 24 | 11 | 14 | 22 |
| 5                               | 30 | 33 | 27 | 16 | 37 | 39 | 38 | 40 |
| 6                               | 6  | 14 | 44 | 13 | 9  | 15 | 3  | 16 |
| 7                               | 48 | 7  | 20 | 17 | 13 | 19 | 18 | 10 |
| 8                               | 5  | 6  | 8  | 7  | 50 | 47 | 1  | 36 |
| 9                               | 51 | 9  | 40 | 11 | 10 | 5  | 12 | 2  |
| 10                              | 4  | 32 | 43 | 2  | 46 | 49 | 1  | 3  |
| 11                              | 50 | 52 | 28 | 49 | 51 | 42 | 45 | 39 |
| 12                              | 43 | 37 | 31 | 44 | 41 | 34 | 20 | 42 |
| 13                              | 47 | 35 | 45 | 24 | 46 | 38 | 41 | 48 |

**Example 68.4: A Latin Square Design**

All of the preceding examples involve designs with completely nested block structures, for which PROC PLAN was especially designed. However, by appropriate coordination of its facilities, PROC PLAN can accommodate a much wider class of designs. A Latin square design is based on experimental units that have a row-and-column block structure. The following statements use the **CYCLIC** option in the **TREATMENTS** statement to generate a simple  $4 \times 4$  Latin square. The **RANDOM** option in the **OUTPUT** statement randomizes the generated Latin square by randomly permuting the row, column, and treatment values independently. This example also uses *factor-value-settings* in the **OUTPUT** statement.

```

title 'Latin Square Design';
proc plan seed=37430;
 factors Row=4 ordered Col=4 ordered / noprint;
 treatments Tmt=4 cyclic;
 output out=LatinSquare
 Row cvals=('Day 1' 'Day 2' 'Day 3' 'Day 4') random
 Col cvals=('Lab 1' 'Lab 2' 'Lab 3' 'Lab 4') random
 Tmt nvals=(0 100 250 450) random;
quit;

proc sort data=LatinSquare out=LatinSquare;
 by Row Col;
run;
proc transpose data= LatinSquare(rename=(Col=_NAME_))
 out =tLatinSquare(drop=_NAME_);
 by Row;
 var Tmt;
run;
proc print data=tLatinSquare noobs;
run;

```

The preceding statements produce [Output 68.4.1](#).

**Output 68.4.1** A Randomized Latin Square Design

| Latin Square Design |       |       |       |       |
|---------------------|-------|-------|-------|-------|
| Row                 | Lab_1 | Lab_2 | Lab_3 | Lab_4 |
| Day 1               | 0     | 250   | 100   | 450   |
| Day 2               | 250   | 450   | 0     | 100   |
| Day 3               | 100   | 0     | 450   | 250   |
| Day 4               | 450   | 100   | 250   | 0     |

You can use the PLAN procedure to randomize Latin squares from any transformation sets. See Kempthorne (1952) for definitions of transformation sets. In particular, the following DATA step and PROC PLAN statements demonstrate how to randomize a Latin square from the second transformation set defined in Kempthorne (1952). The following DATA step creates a  $4 \times 4$  Latin square from the transformation set 2:

```
data Unrandomized;
 do Row = 1 to 4;
 do Col = 1 to 4;
 input Tmt @@;
 output;
 end;
 end;
 datalines;
1 2 3 4
2 1 4 3
3 4 1 2
4 3 2 1
;
```

The following PROC PLAN statements permute the rows and columns and randomly assign treatment levels.

```
proc plan;
 factors Row = 4;
 output data= Unrandomized out=Randomized1;
run;
 factors Col = 4;
 output data= Randomized1 out=Randomized2;
run;
 factors Tmt = 4;
 output data= Randomized2 out=Randomized3;
run;

proc sort data=Randomized3;
 by Row Col;
run;
proc transpose data= Randomized3 out =tLatinSquare2(drop=_NAME_);
 by Row;
 var Tmt;
run;
proc print data=tLatinSquare2 noobs;
run;
```

**Output 68.4.2** A Randomized Latin Square from a Different Transformation Set

```

The PLAN Procedure
Factor Select Levels Order
Row 4 4 Random

--Row--

3 2 4 1

The PLAN Procedure
Factor Select Levels Order
Col 4 4 Random

--Col--

2 4 1 3

The PLAN Procedure
Factor Select Levels Order
Tmt 4 4 Random

--Tmt--

1 2 3 4

Row COL1 COL2 COL3 COL4
1 2 4 1 3
2 4 2 3 1
3 3 1 4 2
4 1 3 2 4

```

**Example 68.5: A Generalized Cyclic Incomplete Block Design**

The following statements depict how to create an appropriately randomized generalized cyclic incomplete block design for  $v$  treatments (given by the value of  $t$ ) in  $b$  blocks (given by the value of  $b$ ) of size  $k$  (with values of  $p$  indexing the cells within a block) with initial block  $(e_1 e_2 \dots e_k)$  and increment number  $i$ .

```

factors b=b p=k ;
treatments t=k of v cyclic (e1 e2 ... ek) i ;

```

For example, the specification

```
proc plan seed=37430;
 factors b=10 p=4;
 treatments t=4 of 30 cyclic (1 3 4 26) 2;
run;
```

generates the generalized cyclic incomplete block design given in Example 1 of Jarrett and Hall (1978), which is given by the rows and columns of the plan associated with the treatment factor *t* in [Output 68.5.1](#).

**Output 68.5.1** A Generalized Cyclic Incomplete Block Design

| The PLAN Procedure |        |         |             |                           |
|--------------------|--------|---------|-------------|---------------------------|
| Plot Factors       |        |         |             |                           |
| Factor             | Select | Levels  | Order       |                           |
| b                  | 10     | 10      | Random      |                           |
| p                  | 4      | 4       | Random      |                           |
| Treatment Factors  |        |         |             |                           |
| Factor             | Select | Levels  | Order       | Initial Block / Increment |
| t                  | 4      | 30      | Cyclic      | (1 3 4 26) / 2            |
|                    | b      | ---p--- | -----t----- |                           |
|                    | 2      | 2 3 1 4 | 1 3 4 26    |                           |
|                    | 1      | 3 2 4 1 | 3 5 6 28    |                           |
|                    | 3      | 2 3 4 1 | 5 7 8 30    |                           |
|                    | 10     | 4 2 3 1 | 7 9 10 2    |                           |
|                    | 9      | 4 1 2 3 | 9 11 12 4   |                           |
|                    | 4      | 1 3 2 4 | 11 13 14 6  |                           |
|                    | 5      | 1 2 4 3 | 13 15 16 8  |                           |
|                    | 8      | 3 2 4 1 | 15 17 18 10 |                           |
|                    | 7      | 2 4 1 3 | 17 19 20 12 |                           |
|                    | 6      | 2 1 4 3 | 19 21 22 14 |                           |

## Example 68.6: Permutations and Combinations

Occasionally, you might need to generate all possible permutations of  $n$  things, or all possible combinations of  $n$  things taken  $m$  at a time.

For example, suppose you are planning an experiment in cognitive psychology where you want to present four successive stimuli to each subject. You want to observe each permutation of the four stimuli. The following statements use PROC PLAN to create a data set containing all possible permutations of four numbers in random order.

```

title 'All Permutations of 1,2,3,4';
proc plan seed=60359;
 factors Subject = 24
 Order = 4 ordered;
 treatments Stimulus = 4 perm;
 output out=Psych;
run;

proc sort data=Psych out=Psych;
 by Subject Order;
run;

proc transpose data= Psych(rename=(Order=_NAME_))
 out =tPsych(drop=_NAME_);
 by Subject;
 var Stimulus;
run;

proc print data=tPsych noobs;
run;

```

The variable Subject is set at 24 levels because there are  $4! = 24$  total permutations to be listed. If Subject > 24, the list repeats. [Output 68.6.1](#) displays the PROC PLAN output. Note that the variable Subject is listed in random order.

**Output 68.6.1** List of Permutations

| All Permutations of 1,2,3,4 |        |        |         |
|-----------------------------|--------|--------|---------|
| The PLAN Procedure          |        |        |         |
| Plot Factors                |        |        |         |
| Factor                      | Select | Levels | Order   |
| Subject                     | 24     | 24     | Random  |
| Order                       | 4      | 4      | Ordered |
| Treatment Factors           |        |        |         |
| Factor                      | Select | Levels | Order   |
| Stimulus                    | 4      | 4      | Perm    |

**Output 68.6.1** *continued*

| Subject | -Order- | -Stimulus- |
|---------|---------|------------|
| 4       | 1 2 3 4 | 1 2 3 4    |
| 15      | 1 2 3 4 | 1 2 4 3    |
| 24      | 1 2 3 4 | 1 3 2 4    |
| 1       | 1 2 3 4 | 1 3 4 2    |
| 5       | 1 2 3 4 | 1 4 2 3    |
| 17      | 1 2 3 4 | 1 4 3 2    |
| 19      | 1 2 3 4 | 2 1 3 4    |
| 14      | 1 2 3 4 | 2 1 4 3    |
| 6       | 1 2 3 4 | 2 3 1 4    |
| 23      | 1 2 3 4 | 2 3 4 1    |
| 8       | 1 2 3 4 | 2 4 1 3    |
| 2       | 1 2 3 4 | 2 4 3 1    |
| 13      | 1 2 3 4 | 3 1 2 4    |
| 16      | 1 2 3 4 | 3 1 4 2    |
| 12      | 1 2 3 4 | 3 2 1 4    |
| 18      | 1 2 3 4 | 3 2 4 1    |
| 21      | 1 2 3 4 | 3 4 1 2    |
| 9       | 1 2 3 4 | 3 4 2 1    |
| 22      | 1 2 3 4 | 4 1 2 3    |
| 10      | 1 2 3 4 | 4 1 3 2    |
| 7       | 1 2 3 4 | 4 2 1 3    |
| 11      | 1 2 3 4 | 4 2 3 1    |
| 3       | 1 2 3 4 | 4 3 1 2    |
| 20      | 1 2 3 4 | 4 3 2 1    |

The output data set Psych contains 96 observations of the 3 variables (Subject, Order, and Stimulus). Sorting the output data set by Subject and by Order within Subject results in all possible permutations of Stimulus in random order. PROC TABULATE displays these permutations in [Output 68.6.2](#).

**Output 68.6.2** Randomized Permutations

| All Permutations of 1,2,3,4 |    |    |    |    |
|-----------------------------|----|----|----|----|
| Subject                     | _1 | _2 | _3 | _4 |
| 1                           | 1  | 3  | 4  | 2  |
| 2                           | 2  | 4  | 3  | 1  |
| 3                           | 4  | 3  | 1  | 2  |
| 4                           | 1  | 2  | 3  | 4  |
| 5                           | 1  | 4  | 2  | 3  |
| 6                           | 2  | 3  | 1  | 4  |
| 7                           | 4  | 2  | 1  | 3  |
| 8                           | 2  | 4  | 1  | 3  |
| 9                           | 3  | 4  | 2  | 1  |
| 10                          | 4  | 1  | 3  | 2  |
| 11                          | 4  | 2  | 3  | 1  |
| 12                          | 3  | 2  | 1  | 4  |
| 13                          | 3  | 1  | 2  | 4  |
| 14                          | 2  | 1  | 4  | 3  |
| 15                          | 1  | 2  | 4  | 3  |
| 16                          | 3  | 1  | 4  | 2  |
| 17                          | 1  | 4  | 3  | 2  |
| 18                          | 3  | 2  | 4  | 1  |
| 19                          | 2  | 1  | 3  | 4  |
| 20                          | 4  | 3  | 2  | 1  |
| 21                          | 3  | 4  | 1  | 2  |
| 22                          | 4  | 1  | 2  | 3  |
| 23                          | 2  | 3  | 4  | 1  |
| 24                          | 1  | 3  | 2  | 4  |

As another example, suppose you have six alternative treatments, any four of which can occur together in a block (in no particular order). The following statements use PROC PLAN to create a data set containing all possible combinations of six numbers taken four at a time. In this case, you use ODS to create the data set.

```

title 'All Combinations of (6 Choose 4) Integers';
proc plan;
 factors Block=15 ordered
 Treat= 4 of 6 comb;
 ods output Plan=Combinations;
run;

proc print data=Combinations noobs;
run;

```

The variable Block has 15 levels since there are a total of  $6!/(4!2!) = 15$  combinations of four integers chosen from six integers. The data set formed by ODS from the displayed plan has one row for each block, with the four values of Treat corresponding to four different variables, as shown in [Output 68.6.3](#) and [Output 68.6.4](#).



**Output 68.6.3** List of Combinations

| All Combinations of (6 Choose 4) Integers |        |         |         |
|-------------------------------------------|--------|---------|---------|
| The PLAN Procedure                        |        |         |         |
| Factor                                    | Select | Levels  | Order   |
| Block                                     | 15     | 15      | Ordered |
| Treat                                     | 4      | 6       | Comb    |
|                                           | Block  | -Treat- |         |
|                                           | 1      | 1 2 3 4 |         |
|                                           | 2      | 1 2 3 5 |         |
|                                           | 3      | 1 2 3 6 |         |
|                                           | 4      | 1 2 4 5 |         |
|                                           | 5      | 1 2 4 6 |         |
|                                           | 6      | 1 2 5 6 |         |
|                                           | 7      | 1 3 4 5 |         |
|                                           | 8      | 1 3 4 6 |         |
|                                           | 9      | 1 3 5 6 |         |
|                                           | 10     | 1 4 5 6 |         |
|                                           | 11     | 2 3 4 5 |         |
|                                           | 12     | 2 3 4 6 |         |
|                                           | 13     | 2 3 5 6 |         |
|                                           | 14     | 2 4 5 6 |         |
|                                           | 15     | 3 4 5 6 |         |

**Output 68.6.4** Combinations Data Set Created by ODS

| All Combinations of (6 Choose 4) Integers |        |        |        |        |
|-------------------------------------------|--------|--------|--------|--------|
| Block                                     | Treat1 | Treat2 | Treat3 | Treat4 |
| 1                                         | 1      | 2      | 3      | 4      |
| 2                                         | 1      | 2      | 3      | 5      |
| 3                                         | 1      | 2      | 3      | 6      |
| 4                                         | 1      | 2      | 4      | 5      |
| 5                                         | 1      | 2      | 4      | 6      |
| 6                                         | 1      | 2      | 5      | 6      |
| 7                                         | 1      | 3      | 4      | 5      |
| 8                                         | 1      | 3      | 4      | 6      |
| 9                                         | 1      | 3      | 5      | 6      |
| 10                                        | 1      | 4      | 5      | 6      |
| 11                                        | 2      | 3      | 4      | 5      |
| 12                                        | 2      | 3      | 4      | 6      |
| 13                                        | 2      | 3      | 5      | 6      |
| 14                                        | 2      | 4      | 5      | 6      |
| 15                                        | 3      | 4      | 5      | 6      |

## Example 68.7: Crossover Designs

In *crossover* experiments, the same experimental units or subjects are given multiple treatments in sequence, and the model for the response at any one period includes an effect for the treatment applied in the previous period. A good design for a crossover experiment is therefore one that balances how often each treatment is preceded by each other treatment. Cox (1992) gives the following example of a balanced crossover experiment for paper production. In this experiment, the subjects are production runs of the mill, with the treatments being six different concentrations of pulp used in sequence. The following statements construct this design in a standard form:

```
proc plan;
 factors Run=6 ordered Period=6 ordered;
 treatments Treatment=6 cyclic (1 2 6 3 5 4);
run;
```

Output 68.7.1 shows the results of the preceding statements.

**Output 68.7.1** Crossover Design for Six Treatments

| The PLAN Procedure |        |             |         |                           |
|--------------------|--------|-------------|---------|---------------------------|
| Plot Factors       |        |             |         |                           |
| Factor             | Select | Levels      | Order   |                           |
| Run                | 6      | 6           | Ordered |                           |
| Period             | 6      | 6           | Ordered |                           |
| Treatment Factors  |        |             |         |                           |
| Factor             | Select | Levels      | Order   | Initial Block / Increment |
| Treatment          | 6      | 6           | Cyclic  | (1 2 6 3 5 4) / 1         |
|                    | Run    | ---Period-- |         | -Treatment-               |
|                    | 1      | 1 2 3 4 5 6 |         | 1 2 6 3 5 4               |
|                    | 2      | 1 2 3 4 5 6 |         | 2 3 1 4 6 5               |
|                    | 3      | 1 2 3 4 5 6 |         | 3 4 2 5 1 6               |
|                    | 4      | 1 2 3 4 5 6 |         | 4 5 3 6 2 1               |
|                    | 5      | 1 2 3 4 5 6 |         | 5 6 4 1 3 2               |
|                    | 6      | 1 2 3 4 5 6 |         | 6 1 5 2 4 3               |

The construction method for this example is due to Williams (1949). The initial block for the treatment variable Treatment is defined as follows for  $n = 6$ :

$$(1 \quad 2 \quad n \quad 3 \quad n - 1 \quad \dots \quad n/2 \quad n/2 + 2 \quad n/2)$$

This general form serves to generate a balanced crossover design for  $n$  treatments and  $n$  subjects in  $n$  periods when  $n$  is even. When  $n$  is odd,  $2n$  subjects are required, with the following initial blocks, respectively for odd and even  $n$ :

$$\begin{pmatrix} 1 & 2 & n & 3 & n-1 & \dots & n/2+1 & n/2 \\ n/2 & n/2+1 & \dots & n-1 & 3 & n & 2 & 1 \end{pmatrix}$$

In order to randomize Williams' crossover designs, the following statements randomly permute the subjects and treatments:

```
proc plan seed=136149876;
 factors Run=6 ordered Period=6 ordered / noprint;
 treatments Treatment=6 cyclic (1 2 6 3 5 4);
 output out=RandomizedDesign
 Run random
 Treatment random
 ;
run;

/*
/ Relabel Period to obtain the same design as in Cox (1992) .
/-----*/
data RandomizedDesign;
 set RandomizedDesign;
 Period = mod(Period+2,6)+1;
run;

proc sort data=RandomizedDesign;
 by Run Period;
run;

proc transpose data=RandomizedDesign out=tDesign(drop=_name_);
 by notsorted Run;
 var Treatment;
run;

data tDesign;
 set tDesign;
 rename COL1-COL6 = Period_1-Period_6;
run;

proc print data=tDesign noobs;
run;
```

In the preceding statements, Run and Treatment are randomized by using the **RANDOM** option in the **OUTPUT** statement, and new labels for Period are obtained in a subsequent **DATA** step. This Period relabeling is not necessary and might not be valid for Williams' designs in general; it is used in this example only to match results with those of Cox (1992). The **SORT** and **TRANSPOSE** steps then prepare the design to be printed in a standard form, shown in [Output 68.7.2](#).

**Output 68.7.2** Randomized Crossover Design

| Run | Period_1 | Period_2 | Period_3 | Period_4 | Period_5 | Period_6 |
|-----|----------|----------|----------|----------|----------|----------|
| 1   | 3        | 6        | 2        | 5        | 4        | 1        |
| 2   | 5        | 3        | 4        | 6        | 1        | 2        |
| 3   | 1        | 4        | 5        | 2        | 6        | 3        |
| 4   | 2        | 1        | 6        | 4        | 3        | 5        |
| 5   | 6        | 5        | 1        | 3        | 2        | 4        |
| 6   | 4        | 2        | 3        | 1        | 5        | 6        |

The analysis of a crossover experiment requires for each observation a *carryover* variable whose values are the treatment in the preceding period. The following statements add such a variable to the randomized design constructed previously:

```
proc sort data=RandomizedDesign;
 by Run Period;
run;
data RandomizedDesign;
 set RandomizedDesign;
 by Run period;
 LagTreatment = lag(Treatment);
 if (first.Run) then LagTreatment = .;
run;

proc transpose data=RandomizedDesign out=tDesign(drop=_name_);
 by notsorted Run;
 var LagTreatment;
run;
data tDesign;
 set tDesign;
 rename COL1-COL6 = Period_1-Period_6;
run;
proc print data=tDesign noobs;
run;
```

Output 68.7.3 displays the values of the carryover variable for each run and period.

**Output 68.7.3** Lag Treatment Effect in Crossover Design

| Run | Period_1 | Period_2 | Period_3 | Period_4 | Period_5 | Period_6 |
|-----|----------|----------|----------|----------|----------|----------|
| 1   | .        | 3        | 6        | 2        | 5        | 4        |
| 2   | .        | 5        | 3        | 4        | 6        | 1        |
| 3   | .        | 1        | 4        | 5        | 2        | 6        |
| 4   | .        | 2        | 1        | 6        | 4        | 3        |
| 5   | .        | 6        | 5        | 1        | 3        | 2        |
| 6   | .        | 4        | 2        | 3        | 1        | 5        |

Of course, the carryover variable has no effect in the first period, which is why it is coded with a missing value in this case.

The experimental LAG effect in the EFFECT statement in PROC ORTHOREG provides a convenient mechanism for incorporating the carryover effect into the analysis. The following statements first add the observed data to the design to create the Mills data set. Then PROC ORTHOREG is invoked, and the carryover effect is defined as a lag effect with the relevant period and subject information specified. ODS is used to trim down the results to show only the parts that are usually of interest in crossover analysis. For more information about the EFFECTS statement in PROC ORTHOREG, see the section “EFFECT Statement” on page 5517.

```

data Responses;
 input Response @@;
 datalines;
56.7 53.8 54.4 54.4 58.9 54.5
58.5 60.2 61.3 54.4 59.1 59.8
55.7 60.7 56.7 59.9 56.6 59.6
57.3 57.7 55.2 58.1 60.2 60.2
53.7 57.1 59.2 58.9 58.9 59.6
58.1 55.7 58.9 56.6 59.6 57.5
;
data Mills;
 merge RandomizedDesign Responses;
run;

proc orthoreg data=Mills;
 class Run Period Treatment;
 effect CarryOver = lag(Treatment / period=Period within=Run);
 model Response = Run Period Treatment CarryOver;
 test Run Period Treatment CarryOver / htype=1;
 lsmeans Treatment CarryOver / diff=anom;
 ods select Tests1 LSMeans Diffs;
run;

```

Output 68.7.4 shows the carryover analysis that results from the preceding statements.

**Output 68.7.4** Carryover Analysis for Crossover Experiment

| The ORTHOREG Procedure        |           |           |         |        |
|-------------------------------|-----------|-----------|---------|--------|
| Dependent Variable: Response  |           |           |         |        |
| Type I Tests of Model Effects |           |           |         |        |
| Effect                        | Num<br>DF | Den<br>DF | F Value | Pr > F |
| Run                           | 5         | 15        | 13.76   | <.0001 |
| Period                        | 5         | 15        | 7.19    | 0.0013 |
| Treatment                     | 5         | 15        | 22.95   | <.0001 |
| CarryOver                     | 5         | 15        | 7.76    | 0.0009 |

Output 68.7.4 continued

| Treatment Least Squares Means |          |                |    |         |         |  |
|-------------------------------|----------|----------------|----|---------|---------|--|
| Treatment                     | Estimate | Standard Error | DF | t Value | Pr >  t |  |
| 1                             | 57.1954  | 0.3220         | 15 | 177.65  | <.0001  |  |
| 2                             | 57.6204  | 0.3220         | 15 | 178.97  | <.0001  |  |
| 3                             | 59.1919  | 0.3220         | 15 | 183.85  | <.0001  |  |
| 4                             | 59.2288  | 0.3220         | 15 | 183.97  | <.0001  |  |
| 5                             | 57.9829  | 0.3220         | 15 | 180.10  | <.0001  |  |
| 6                             | 55.0639  | 0.3220         | 15 | 171.03  | <.0001  |  |

| Differences of Treatment Least Squares Means |            |          |                |    |         |         |
|----------------------------------------------|------------|----------|----------------|----|---------|---------|
| Treatment                                    | _Treatment | Estimate | Standard Error | DF | t Value | Pr >  t |
| 1                                            | Avg        | -0.5185  | 0.2948         | 15 | -1.76   | 0.0990  |
| 2                                            | Avg        | -0.09345 | 0.2948         | 15 | -0.32   | 0.7556  |
| 3                                            | Avg        | 1.4780   | 0.2948         | 15 | 5.01    | 0.0002  |
| 4                                            | Avg        | 1.5149   | 0.2948         | 15 | 5.14    | 0.0001  |
| 5                                            | Avg        | 0.2690   | 0.2948         | 15 | 0.91    | 0.3758  |
| 6                                            | Avg        | -2.6500  | 0.2948         | 15 | -8.99   | <.0001  |

| CarryOver Least Squares Means |          |                |    |         |         |  |
|-------------------------------|----------|----------------|----|---------|---------|--|
| Carry Over                    | Estimate | Standard Error | DF | t Value | Pr >  t |  |
| 1                             | Non-est  | .              | .  | .       | .       |  |
| 2                             | Non-est  | .              | .  | .       | .       |  |
| 3                             | Non-est  | .              | .  | .       | .       |  |
| 4                             | Non-est  | .              | .  | .       | .       |  |
| 5                             | Non-est  | .              | .  | .       | .       |  |
| 6                             | Non-est  | .              | .  | .       | .       |  |

| Differences of CarryOver Least Squares Means |              |          |                |    |         |         |
|----------------------------------------------|--------------|----------|----------------|----|---------|---------|
| Carry Over                                   | — Carry Over | Estimate | Standard Error | DF | t Value | Pr >  t |
| 1                                            | Avg          | 0.3726   | 0.3284         | 15 | 1.13    | 0.2743  |
| 2                                            | Avg          | -0.2774  | 0.3284         | 15 | -0.84   | 0.4116  |
| 3                                            | Avg          | 0.6512   | 0.3284         | 15 | 1.98    | 0.0660  |
| 4                                            | Avg          | -1.3274  | 0.3284         | 15 | -4.04   | 0.0011  |
| 5                                            | Avg          | 1.3976   | 0.3284         | 15 | 4.26    | 0.0007  |
| 6                                            | Avg          | -0.8167  | 0.3284         | 15 | -2.49   | 0.0252  |

The Type I analysis of variance indicates that all effects are significant—in particular, both the direct and the carryover effects of the treatment. In the presence of carryover effects, the LS-means need to be defined

with some care. The LS-means for treatments computed using balanced margins for the carryover effect are inestimable; so the OBSMARGINS option is specified in the LSMEANS statement in order to use the observed margins instead. The observed margins take the absence of a carryover effect in the first period into account. Note that the LS-means themselves of the carryover effect are inestimable, but their differences are estimable. The LS-means of the direct effect of the treatment and the ANOM differences for the LS-means of their carryover effect match the “adjusted direct effects” and “adjusted residual effects,” respectively, of Cox (1992).

---

## References

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# Chapter 69

## The PLM Procedure

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## Overview: PLM Procedure

The PLM procedure performs postfitting statistical analyses for the contents of a SAS item store that was previously created with the STORE statement in some other SAS/STAT procedure. An item store is a special SAS-defined binary file format used to store and restore information with a hierarchical structure.

The statements available in the PLM procedure are designed to reveal the contents of the source item store via the Output Delivery System (ODS) and to perform postfitting tasks such as the following:

- testing hypotheses
- computing confidence intervals
- producing prediction plots
- scoring a new data set

The use of item stores and PROC PLM enables you to separate common postprocessing tasks, such as testing for treatment differences and predicting new observations under a fitted model, from the process of model building and fitting. A numerically expensive model fitting technique can be applied once to produce a source item store. The PLM procedure can then be called multiple times and the results of the fitted model analyzed without incurring the model fitting expenditure again.

The PLM procedure offers the most advanced postprocessing techniques available in SAS/STAT software. These techniques include step-down multiplicity adjustments for  $p$ -values,  $F$  tests with order restrictions, analysis of means (ANOM), and sampling-based linear inference based on Bayes posterior estimates.

The following procedures support the STORE statement for the generation of item stores that can be processed with the PLM procedure: GENMOD, GLIMMIX, GLM, GLMSELECT, LIFEREG, LOGISTIC, MIXED, ORTHOREG, PHREG, PROBIT, SURVEYLOGISTIC, SURVEYPHREG, and SURVEYREG. The RELIABILITY procedure in SAS/QC software also supports the STORE statement. For details about the STORE statement, see the section “STORE Statement” on page 501 of Chapter 19, “Shared Concepts and Topics.”

---

## Basic Features

The PLM procedure, unlike most SAS/STAT procedures, does not operate primarily on an input data set. Instead, the procedure requires you to specify an item store with the RESTORE= option in the PROC PLM statement. The item store contains the necessary information and context about the statistical model that was fit when the store was created. SAS data sets are used only to provide input information in some circumstances. For example, when scoring a data set or when computing least squares means with specially defined population margins. In other words, instead of reading raw data and fitting a model, the PLM procedure reads the results of a model having been fit.

In order to interact with the item store and to reveal its contents, the PLM procedure supports the SHOW statement which converts item store information into standard ODS tables for viewing and further processing.

The PLM procedure is sensitive to the contents of the item store. For example, if a BAYES statement was in effect when the item store was created, the posterior parameter estimates are saved to the item store so that the PLM procedure can perform postprocessing tasks by taking the posterior distribution of estimable functions into account. As another example, for item stores that are generated by a mixed model procedure using the Satterthwaite or Kenward-Roger (Kenward and Roger 1997) degrees-of-freedom method, these methods continue to be available when the item store contents are processed with the PLM procedure.

Because the PLM procedure does not read data and does not fit a model, the processing time of this procedure is usually considerably less than the processing time of the procedure that generates the item store.

## PROC PLM Contrasted with Other SAS Procedures

In contrast to other analytic procedures in SAS/STAT software, the PLM procedure does not use an input data set. Instead, it retrieves information from an item store.

Some of the statements in the PLM procedure are also available as postprocessing statements in other procedures. Table 69.1 lists SAS/STAT procedures that support the same postprocessing statements as PROC PLM does.

**Table 69.1** SAS/STAT Procedures with Postprocessing Statements Similar to PROC PLM

|                | EFFECTPLOT | ESTIMATE | LSMEANS | LSMESTIMATE | SLICE | TEST |
|----------------|------------|----------|---------|-------------|-------|------|
| GENMOD         | ✓          | ✓*       | ✓       | ✓           | ✓     |      |
| GLIMMIX        |            | ✓*       | ✓*      | ✓*          | ✓     |      |
| GLM            |            | ✓*       | ✓*      |             |       | ✓*   |
| LIFEREG        | ✓          | ✓        | ✓       | ✓           | ✓     | ✓    |
| LOGISTIC       | ✓          | ✓        | ✓       | ✓           | ✓     | ✓*   |
| MIXED          |            | ✓*       | ✓*      | ✓           | ✓     |      |
| ORTHOREG       | ✓          | ✓        | ✓       | ✓           | ✓     | ✓    |
| PHREG          |            | ✓        | ✓       | ✓           | ✓     | ✓*   |
| PROBIT         | ✓          | ✓        | ✓       | ✓           | ✓     | ✓    |
| SURVEYLOGISTIC |            | ✓        | ✓       | ✓           | ✓     | ✓*   |
| SURVEYPHREG    |            | ✓        | ✓       | ✓           | ✓     | ✓    |
| SURVEYREG      |            | ✓        | ✓       | ✓           | ✓     | ✓    |

Table entries marked with ✓ indicate procedures that support statements with the same functionality as in PROC PLM. Those entries marked with ✓\* indicate procedures that support statements with same names but different syntaxes from PROC PLM. You can find the most comprehensive set of features for these statements in the PLM procedure. For example, the LSMEANS statement is available in all of the listed procedures. For example, the ESTIMATE statement available in the GENMOD, GLIMMIX, GLM and MIXED procedures does not support all options that PROC PLM supports, such as multiple rows and multiplicity adjustments.

The WHERE statement in other procedures enables you to conditionally select a subset of the observations from the input data set so that the procedure processes only the observations that meet the specified conditions. Since the PLM procedure does not use an input data set, the WHERE statement in the PLM procedure has different functionality. If the item store contains information about BY groups—that is, a BY statement

was in effect when the item store was created—you can use the **WHERE** statement to select specific BY groups for the analysis. You can also use the **FILTER** statement in the PLM procedure to filter results from the ODS output and output data sets.

## Getting Started: PLM Procedure

The following DATA step creates a data set from a randomized block experiment with a factorial treatment structure of factors A and B:

```
data BlockDesign;
 input block a b y @@;
 datalines;
 1 1 1 56 1 1 2 41
 1 2 1 50 1 2 2 36
 1 3 1 39 1 3 2 35
 2 1 1 30 2 1 2 25
 2 2 1 36 2 2 2 28
 2 3 1 33 2 3 2 30
 3 1 1 32 3 1 2 24
 3 2 1 31 3 2 2 27
 3 3 1 15 3 3 2 19
 4 1 1 30 4 1 2 25
 4 2 1 35 4 2 2 30
 4 3 1 17 4 3 2 18
 ;
```

The GLM procedure is used in the following statements to fit the model and to create a source item store for the PLM procedure:

```
proc glm data=BlockDesign;
 class block a b;
 model y = block a b a*b / solution;
 store sasuser.BlockAnalysis / label='PLM: Getting Started';
run;
```

The CLASS statement identifies the variables Block, A, and B as classification variables. The MODEL statement specifies the response variable and the model effects. The block effect models the design effect, and the a, b, and a\*b effects model the factorial treatment structure. The STORE statement requests that the context and results of this analysis be saved to an item store named sasuser.BlockAnalysis. Because the SASUSER library is specified as the library name of the item store, the store will be available after the SAS session completes. The optional label in the STORE statement identifies the store in subsequent analyses with the PLM procedure.

Note that having BlockDesign as the name of the output store would not create a conflict with the input data set name, because data sets and item stores are saved as files of different types.

Figure 69.1 displays the results from the GLM procedure. The “Class Level Information” table shows the number of levels and their values for the three classification variables. The “Parameter Estimates” table shows the estimates and their standard errors along with *t* tests.

**Figure 69.1** Class Variable Information, Fit Statistics, and Parameter Estimates

| The GLM Procedure       |     |               |                |          |         |
|-------------------------|-----|---------------|----------------|----------|---------|
| Class Level Information |     |               |                |          |         |
| Class                   |     | Levels        | Values         |          |         |
| block                   |     | 4             | 1              | 2        | 3 4     |
| a                       |     | 3             | 1              | 2        | 3       |
| b                       |     | 2             | 1              | 2        |         |
| R-Square                |     | Coeff Var     | Root MSE       | y Mean   |         |
| 0.848966                |     | 15.05578      | 4.654747       | 30.91667 |         |
| Parameter               |     | Estimate      | Standard Error | t Value  | Pr >  t |
| Intercept               |     | 20.41666667 B | 2.85043856     | 7.16     | <.0001  |
| block                   | 1   | 17.00000000 B | 2.68741925     | 6.33     | <.0001  |
| block                   | 2   | 4.50000000 B  | 2.68741925     | 1.67     | 0.1148  |
| block                   | 3   | -1.16666667 B | 2.68741925     | -0.43    | 0.6704  |
| block                   | 4   | 0.00000000 B  | .              | .        | .       |
| a                       | 1   | 3.25000000 B  | 3.29140294     | 0.99     | 0.3391  |
| a                       | 2   | 4.75000000 B  | 3.29140294     | 1.44     | 0.1695  |
| a                       | 3   | 0.00000000 B  | .              | .        | .       |
| b                       | 1   | 0.50000000 B  | 3.29140294     | 0.15     | 0.8813  |
| b                       | 2   | 0.00000000 B  | .              | .        | .       |
| a*b                     | 1 1 | 7.75000000 B  | 4.65474668     | 1.66     | 0.1167  |
| a*b                     | 1 2 | 0.00000000 B  | .              | .        | .       |
| a*b                     | 2 1 | 7.25000000 B  | 4.65474668     | 1.56     | 0.1402  |
| a*b                     | 2 2 | 0.00000000 B  | .              | .        | .       |
| a*b                     | 3 1 | 0.00000000 B  | .              | .        | .       |
| a*b                     | 3 2 | 0.00000000 B  | .              | .        | .       |

The following statements invoke the PLM procedure and use `sasuser.BlockAnalysis` as the source item store:

```
proc plm restore=sasuser.BlockAnalysis;
run;
```

These statements produce [Figure 69.2](#). The “Store Information” table displays information that is gleaned from the source item store. For example, the store was created by the GLM procedure at the indicated time and date, and the input data set for the analysis was `WORK.BLOCKDESIGN`. The label used earlier in the `STORE` statement of the GLM procedure also appears as a descriptor in [Figure 69.2](#).

Figure 69.2 Default Information

| The PLM Procedure       |                         |
|-------------------------|-------------------------|
| Store Information       |                         |
| Item Store              | SASUSER.BLOCKANALYSIS   |
| Label                   | PLM: Getting Started    |
| Data Set Created From   | WORK.BLOCKDESIGN        |
| Created By              | PROC GLM                |
| Date Created            | 13JUN12:12:33:28        |
| Response Variable       | y                       |
| Class Variables         | block a b               |
| Model Effects           | Intercept block a b a*b |
| Class Level Information |                         |
| Class                   | Levels Values           |
| block                   | 4 1 2 3 4               |
| a                       | 3 1 2 3                 |
| b                       | 2 1 2                   |

The “Store Information” table also echoes partial information about the variables and model effects that are used in the analysis. The “Class Level Information” table is produced by the PLM procedure by default whenever the model contains effects that depend on CLASS variables.

The following statements request a display of the fit statistics and the parameter estimates from the source item store and a test of the treatment main effects and their interactions:

```
proc plm restore=sasuser.BlockAnalysis;
 show fit parms;
 test a b a*b;
run;
```

The statements produce Figure 69.3. Notice that the estimates and standard errors in the “Parameter Estimates” table agree with the results displayed earlier by the GLM procedure, except for small differences in formatting.

Figure 69.3 Fit Statistics, Parameter Estimates, and Tests of Effects

| The PLM Procedure |          |
|-------------------|----------|
| Fit Statistics    |          |
| MSE               | 21.66667 |
| Error df          | 15       |

Figure 69.3 continued

| Parameter Estimates |       |   |   |          |                |
|---------------------|-------|---|---|----------|----------------|
| Effect              | block | a | b | Estimate | Standard Error |
| Intercept           |       |   |   | 20.4167  | 2.8504         |
| block               | 1     |   |   | 17.0000  | 2.6874         |
| block               | 2     |   |   | 4.5000   | 2.6874         |
| block               | 3     |   |   | -1.1667  | 2.6874         |
| block               | 4     |   |   | 0        | .              |
| a                   |       | 1 |   | 3.2500   | 3.2914         |
| a                   |       | 2 |   | 4.7500   | 3.2914         |
| a                   |       | 3 |   | 0        | .              |
| b                   |       |   | 1 | 0.5000   | 3.2914         |
| b                   |       |   | 2 | 0        | .              |
| a*b                 |       | 1 | 1 | 7.7500   | 4.6547         |
| a*b                 |       | 1 | 2 | 0        | .              |
| a*b                 |       | 2 | 1 | 7.2500   | 4.6547         |
| a*b                 |       | 2 | 2 | 0        | .              |
| a*b                 |       | 3 | 1 | 0        | .              |
| a*b                 |       | 3 | 2 | 0        | .              |

| Type III Tests of Model Effects |        |        |         |        |
|---------------------------------|--------|--------|---------|--------|
| Effect                          | Num DF | Den DF | F Value | Pr > F |
| a                               | 2      | 15     | 7.54    | 0.0054 |
| b                               | 1      | 15     | 8.38    | 0.0111 |
| a*b                             | 2      | 15     | 1.74    | 0.2097 |

Since the main effects, but not the interaction are significant in this experiment, the subsequent analysis focuses on the main effects, in particular on the effect of variable A.

The following statements request the least squares means of the A effect along with their pairwise differences:

```
proc plm restore=sasuser.BlockAnalysis seed=3;
 lsmeans a / diff;
 lsmestimate a -1 1,
 1 1 -2 / uppertailed ftest;
run;
```

The **LSMESTIMATE** statement tests two linear combinations of the A least squares means: equality of the first two levels and whether the sum of the first two level effects equals twice the effect of the third level. The **FTEST** option in the **LSMESTIMATE** statement requests a joint *F* test for this two-row contrast. The **UPPERTAILED** option requests that the *F* test also be carried out under one-sided order restrictions. Since *F* tests under order restrictions (chi-bar-square statistic) require a simulation-based approach for the calculation of *p*-values, the random number stream is initialized with a seed value through the **SEED=** option in the **PROC PLM** statement.

The results of the **LSMEANS** and the **LSMESTIMATE** statement are shown in Figure 69.4.

Figure 69.4 LS-Means Related Inference for A Effect

| The PLM Procedure                        |        |          |                |        |                 |               |        |
|------------------------------------------|--------|----------|----------------|--------|-----------------|---------------|--------|
| a Least Squares Means                    |        |          |                |        |                 |               |        |
| a                                        |        | Estimate | Standard Error | DF     | t Value         | Pr >  t       |        |
| 1                                        |        | 32.8750  | 1.6457         | 15     | 19.98           | <.0001        |        |
| 2                                        |        | 34.1250  | 1.6457         | 15     | 20.74           | <.0001        |        |
| 3                                        |        | 25.7500  | 1.6457         | 15     | 15.65           | <.0001        |        |
| Differences of a Least Squares Means     |        |          |                |        |                 |               |        |
| a                                        | _a     | Estimate | Standard Error | DF     | t Value         | Pr >  t       |        |
| 1                                        | 2      | -1.2500  | 2.3274         | 15     | -0.54           | 0.5991        |        |
| 1                                        | 3      | 7.1250   | 2.3274         | 15     | 3.06            | 0.0079        |        |
| 2                                        | 3      | 8.3750   | 2.3274         | 15     | 3.60            | 0.0026        |        |
| Least Squares Means Estimates            |        |          |                |        |                 |               |        |
| Effect                                   | Label  | Estimate | Standard Error | DF     | t Value         | Tails         | Pr > t |
| a                                        | Row 1  | 1.2500   | 2.3274         | 15     | 0.54            | Upper         | 0.2995 |
| a                                        | Row 2  | 15.5000  | 4.0311         | 15     | 3.85            | Upper         | 0.0008 |
| F Test for Least Squares Means Estimates |        |          |                |        |                 |               |        |
| Effect                                   | Num DF | Den DF   | F Value        | Pr > F | ChiBar Sq Value | Pr > ChiBarSq |        |
| a                                        | 2      | 15       | 7.54           | 0.0054 | 15.07           | 0.0001        |        |

The least squares means for the three levels of variable A are 32.875, 34.125, and 25.75. The differences between the third level and the first and second levels are statistically significant at the 5% level ( $p$ -values of 0.0079 and 0.0026, respectively). There is no significant difference between the first two levels. The first row of the “Least Squares Means Estimates” table also displays the difference between the first two levels of factor A. Although the (absolute value of the) estimate and its standard error are identical to those in the “Differences of a Least Squares Means” table, the  $p$ -values do not agree because one-sided tests were requested in the LSMESTIMATE statement.

The “F Test” table in Figure 69.4 shows the two degree-of-freedom test for the linear combinations of the LS-means. The  $F$  value of 7.54 with  $p$ -value of 0.0054 represents the usual (two-sided)  $F$  test. Under the one-sided right-tailed order restriction imposed by the UPPERTAILED option, the ChiBarSq value of 15.07 represents the observed value of the chi-bar-square statistic of Silvapulle and Sen (2004). The associated  $p$ -value of 0.0001 was obtained by simulation.

Now suppose that you are interested in analyzing the relationship of the interaction cell means. (Typically this would not be the case in this example since the  $a*b$  interaction is not significant; see [Figure 69.3](#).) The `SLICE` statement in the following PROC PLM run produces an  $F$  test of equality and all pair-wise differences of the interaction means for the subset (partition) where variable B is at level '1'. With ODS Graphics enabled, the pairwise differences are displayed in a diffogram.

```
ods graphics on;
proc plm restore=sasuser.BlockAnalysis;
 slice a*b / sliceby(b='1') diff;
run;
ods graphics off;
```

The results are shown in [Figure 69.5](#). Since variable A has three levels, the test of equality of the A means at level '1' of B is a two-degree comparison. This comparison is statistically significant ( $p$ -value equals 0.0040). You can conclude that the three levels of A are not the same for the first level of B.

**Figure 69.5** Results from Analyzing an Interaction Partition

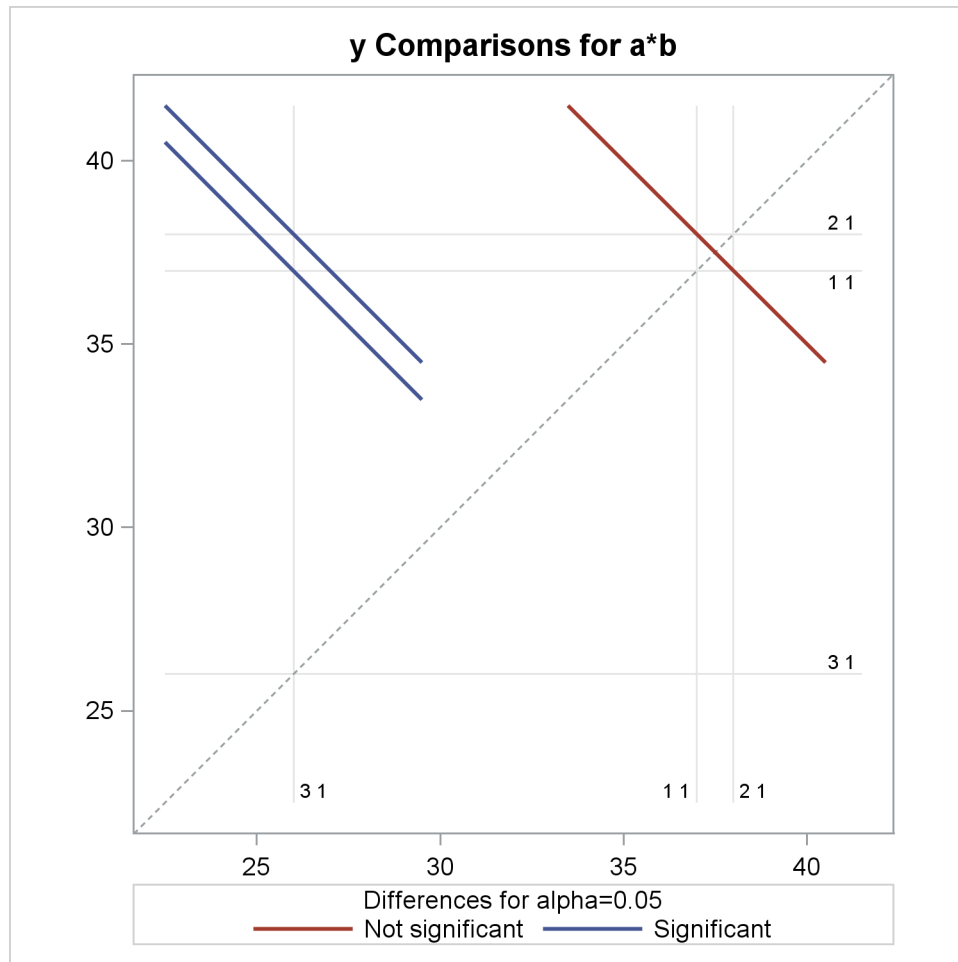
| The PLM Procedure                             |   |           |           |                   |    |         |         |
|-----------------------------------------------|---|-----------|-----------|-------------------|----|---------|---------|
| F Test for a*b Least Squares Means Slice      |   |           |           |                   |    |         |         |
| Slice                                         |   | Num<br>DF | Den<br>DF | F Value           |    | Pr > F  |         |
| b 1                                           |   | 2         | 15        | 8.18              |    | 0.0040  |         |
| Simple Differences of a*b Least Squares Means |   |           |           |                   |    |         |         |
| Slice                                         | a | _a        | Estimate  | Standard<br>Error | DF | t Value | Pr >  t |
| b 1                                           | 1 | 2         | -1.0000   | 3.2914            | 15 | -0.30   | 0.7654  |
| b 1                                           | 1 | 3         | 11.0000   | 3.2914            | 15 | 3.34    | 0.0045  |
| b 1                                           | 2 | 3         | 12.0000   | 3.2914            | 15 | 3.65    | 0.0024  |

The table of “Simple Differences” was produced by the `DIFF` option in the `SLICE` statement. As is the case with the marginal comparisons in [Figure 69.4](#), there are significant differences against the third level of A if variable B is held fixed at '1'.

[Figure 69.6](#) shows the diffogram that displays the three pairwise least squares mean differences and their significance. Each line segment corresponds to a comparison. It centers at the least squares means in the pair with its length corresponding to the projected width of a confidence interval for the difference. If the variable B is held fixed at '1', both the first two levels are significantly different from the third level, but the difference between the first and the second level is not significant.



**Figure 69.6** LS-Means Difference Diffogram



## Syntax: PLM Procedure

The following statements are available in the PLM procedure:

```

PROC PLM RESTORE=item-store-specification < options > ;
 CODE < options > ;
 EFFECTPLOT < plot-type < (plot-definition-options) > > < / options > ;
 ESTIMATE < 'label' > estimate-specification < (divisor=n) >
 < , ... < 'label' > estimate-specification < (divisor=n) > > < / options > ;
 FILTER expression ;
 LSMEANS < model-effects > < / options > ;
 LSMESTIMATE model-effect < 'label' > values < divisor=n >
 < , ... < 'label' > values < divisor=n > > < / options > ;
 SCORE DATA=SAS-data-set < OUT=SAS-data-set >
 < keyword<=name> > ...
 < keyword<=name> > < / options > ;
 SHOW options ;
 SLICE model-effect < / options > ;
 TEST < model-effects > < / options > ;
 WHERE expression ;

```

With the exception of the **PROC PLM** statement and the **FILTER** statement, any statement can appear multiple times and in any order. The default order in which the statements are processed by the PLM procedure depends on the specification in the item store and can be modified with the **STMTORDER=** option in the **PROC PLM** statement.

In contrast to many other SAS/STAT modeling procedures, the PLM procedure does not have common modeling statements such as the **CLASS** and **MODEL** statements. This is because the information about classification variables and model effects is contained in the source item store that is passed to the procedure in the **PROC PLM** statement. All subsequent statements are checked for consistency with the stored model. For example, the statement

```
lsmeans c / diff;
```

is detected as not valid unless one of the following conditions was true at the time when the source store was created:

- The effect C was used in the model.
- C was specified in the **CLASS** statement.
- The **CLASS** variables in the model had a GLM parameterization.

The **FILTER**, **SCORE**, **SHOW**, and **WHERE** statements are described in full after the **PROC PLM** statement in alphabetical order. The **CODE**, **EFFECTPLOT**, **ESTIMATE**, **LSMEANS**, **LSMESTIMATE**, **SLICE**, and **TEST** statements are also used by many other procedures. Summary descriptions of functionality and syntax for these statements are also given after the **PROC PLM** statement in alphabetical order, but full documentation about them is available in Chapter 19, “Shared Concepts and Topics.”

## PROC PLM Statement

**PROC PLM RESTORE=***item-store-specification* < options > ;

The PROC PLM statement invokes the PLM procedure. The **RESTORE=** option with *item-store-specification* is required. Table 69.2 summarizes the options available in the PROC PLM statement.

**Table 69.2** PROC PLM Statement Options

| Option                        | Description                                                                                    |
|-------------------------------|------------------------------------------------------------------------------------------------|
| <b>Basic Options</b>          |                                                                                                |
| <b>RESTORE=</b>               | Specifies the source item store for processing                                                 |
| <b>SEED=</b>                  | Specifies the random number seed                                                               |
| <b>STMTORDER=</b>             | Affects the order in which statements are grouped during processing                            |
| <b>FORMAT=</b>                | Specifies how the PLM procedure handles user-defined formats                                   |
| <b>WHEREFORMAT</b>            | Specifies the constants (literals) in terms of the formatted values of the BY variables        |
| <b>Computational Options</b>  |                                                                                                |
| <b>ALPHA=</b>                 | Specifies the nominal significance level                                                       |
| <b>DDFMETHOD=</b>             | Specifies the method for determining denominator degrees of freedom                            |
| <b>PERCENTILES=</b>           | Supplies a list of percentiles for the construction of HPD intervals                           |
| <b>Displayed Output</b>       |                                                                                                |
| <b>MAXLEN=</b>                | Determines the maximum length of informational strings                                         |
| <b>NOCLPRINT</b>              | Suppresses the display of the “Class Level Information” table                                  |
| <b>NOINFO</b>                 | Suppresses the display of the “Store Information” table                                        |
| <b>NOPRINT</b>                | Suppresses tabular and graphical output                                                        |
| <b>PLOT</b>                   | Controls the plots produced through ODS Graphics                                               |
| <b>Singularity Tolerances</b> |                                                                                                |
| <b>ESTEPS=</b>                | Specifies the tolerance value used in determining the estimability of linear functions         |
| <b>SINGCHOL=</b>              | Tunes the singularity criterion in Cholesky decompositions                                     |
| <b>SINGRES=</b>               | Sets the tolerance for which the residual variance or scale parameter is considered to be zero |
| <b>SINGULAR=</b>              | Tunes the general singularity criterion                                                        |
| <b>ZETA=</b>                  | Tunes the sensitivity in forming Type III functions                                            |

You can specify the following *options*:

### **ALPHA=** $\alpha$

specifies the nominal significance level for multiplicity corrections and for the construction of confidence intervals. The value of  $\alpha$  must be between 0 and 1. The default is the value specified in the source item store, or 0.05 if the item store does not provide a value. The confidence level based on  $\alpha$  is  $1 - \alpha$ .

**DDFMETHOD=RESIDUAL | RES | ERROR****DDFMETHOD=NONE****DDFMETHOD=KENROG | KR | KENWARDROGER****DDFMETHOD=SATTERTH | SAT | SATTERTHWAITE**

specifies the method for determining denominator degrees of freedom for tests and confidence intervals. The default degree-of-freedom method is determined by the contents of the item store. You can override the default to some extent with the DDFMETHOD= option.

If you choose DDFMETHOD=NONE, then infinite denominator degrees of freedom are assumed for tests and confidence intervals. This essentially produces  $z$  tests and intervals instead of  $t$  tests and intervals and chi-square tests instead of  $F$  tests.

The KENWARDROGER and SATTERTHWAITE methods require that the source item store contain information about these methods. This information is currently available for item stores that were created with the MIXED or GLIMMIX procedures when the appropriate DDFM= option was in effect.

**ESTEPS= $\epsilon$** 

specifies the tolerance value used in determining the estimability of linear functions. The default value is determined by the contents of the source item store; it is usually 1E-4.

**FORMAT=NOLOAD | RELOAD**

specifies how the PLM procedure handles user-defined formats, which are not permanent. When the item store is created, user-defined formats are stored. When the PLM procedure opens an item store, it uses this option as follows. If FORMAT=RELOAD (the default), the stored formats are loaded again from the item store and formats that already exist in your SAS session are replaced by the reloaded formats. If FORMAT=NOLOAD, stored formats are not loaded from the item store and existing formats are not replaced.

With FORMAT=NOLOAD, you prevent the PLM procedure from reloading the format from the item store. As a consequence, PLM statements might fail if a format was present at the item store creation and is not available in your SAS session. Also, if you modify the format that was used in the item store creation and use FORMAT=NOLOAD, you might obtain unexpected results because levels of classification variables are remapped.

The “Class Level Information” table always displays the formatted values of classification variables that were used in fitting the model, regardless of the FORMAT= option. For more details about using formats with the PLM procedure, see “[User-Defined Formats and the PLM Procedure](#)” on page 5834.

**MAXLEN= $n$** 

determines the maximum length of informational strings in the “Store Information” table. This table displays, for example, lists of classification or BY variables and lists of model effects. The value of  $n$  determines the truncation length for these strings. The minimum and maximum values for  $n$  are 20 and 256, respectively. The default is  $n = 100$ .

**NOCLPRINT<= $number$ >**

suppresses the display of the “Class Level Information” table if you do not specify  $number$ . If you specify  $number$ , only levels with totals that are less than  $number$  are listed in the table. The PLM procedure produces the “Class Level Information” table by default when the model contains effects that depend on classification variables.

**NOINFO**

suppresses the display of the “Store Information” table.

**NOPRINT**

suppresses the generation of tabular and graphical output. When the NOPRINT option is in effect, ODS tables are also not produced.

**PERCENTILES=***value-list***PERCENTILE=***value-list*

supplies a list of percentiles for the construction of highest posterior density (HPD) intervals when the PLM procedure performs a sampling-based analysis (for example, when processing an item store that contains posterior parameter estimates from a Bayesian analysis). The default set of percentiles depends on the contents of the source item store; it is typically PERCENTILES=25, 50, 75. The entries in *value-list* must be strictly between 0 and 100.

**PLOTS** <(*global-plot-option*)> <=*specific-plot-options*>

controls the plots produced through ODS Graphics. ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;

proc plm plots=all;
 lsmeans a/diff;
run;

ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS](#).”

**Global Plot Option**

The following *global-plot-option* applies to all plots produced by PROC PLM.

**UNPACKPANEL****UNPACK**

suppresses paneling. (By default, multiple plots can appear in some output panels.) Specify UNPACK to display each plot separately.

**Specific Plot Options**

You can specify the following *specific-plot-options*:

**ALL**

requests that all the appropriate plots be produced.

**NONE**

suppresses all plots.

**SEED=number**

specifies the random number seed for analyses that depend on a random number stream. You can also specify the random number seed through some PLM statements (for example, through the SEED= options in the ESTIMATE, LSMEANS, and LSMESTIMATE statements). However, note that there is only a single random number stream per procedure run. Specifying the SEED= option in the PROC PLM statement initializes the stream for all subsequent statements. If you do not specify a random number seed, the source item store might supply one for you. If a seed is in effect when the PLM procedure opens the source store, the “Store Information” table displays its value.

If the random number seed is less than or equal to zero, the seed is generated from reading the time of day from the computer clock and a log message indicates the chosen seed value.

**SINGCHOL=number**

tunes the singularity criterion in Cholesky decompositions. The default value depends on the contents of the source item store. The default value is typically 1E4 times the machine epsilon; this product is approximately 1E–12 on most computers.

**SINGRES=number**

sets the tolerance for which the residual variance or scale parameter is considered to be zero. The default value depends on the contents of the source item store. The default value is typically 1E4 times the machine epsilon; this product is approximately 1E–12 on most computers.

**SINGULAR=number**

tunes the general singularity criterion applied by the PLM procedure in divisions and inversions. The default value used by the PLM procedure depends on the contents of the item store. The default value is typically 1E4 times the machine epsilon; this product is approximately 1E–12 on most computers.

**RESTORE=item-store-specification**

specifies the source item store for processing. This option is required because, in contrast to SAS data sets, there is no default item store. An *item-store-specification* consists of a one- or two-level name as with SAS data sets. As with data sets, the default library association of an item store is with the WORK library, and any stores created in this library are deleted when the SAS session concludes.

**STMTORDER=SYNTAX | GROUP****STMT=SYNTAX | GROUP**

affects the order in which statements are grouped during processing. The default behavior depends on the contents of the source item store and can be modified with the STMTORDER= option. If STMTORDER=SYNTAX is in effect, the statements are processed in the order in which they appear. Note that this precludes the hierarchical grouping of ODS objects. If STMTORDER=GROUP is in effect, the statements are processed in groups and in the following order: **SHOW**, **TEST**, **LSMEANS**, **SLICE**, **LSMESTIMATE**, **ESTIMATE**, **SCORE**, **EFFECTPLOT**, and **CODE**.

**WHEREFORMAT**

specifies that the constants (literals) specified in **WHERE** expressions for group selection are in terms of the formatted values of the BY variables. By default, WHERE expressions are specified in terms of the unformatted (raw) values of the BY variables, as in the SAS DATA step.

**ZETA=number**

tunes the sensitivity in forming Type III functions. Any element in the estimable function basis with an absolute value less than *number* is set to 0. The default depends on the contents of the source item store; it usually is 1E-8.

---

## CODE Statement

**CODE** < options > ;

The CODE statement enables you to write SAS DATA step code for computing predicted values of the fitted model either to a file or to a catalog entry. This code can then be included in a DATA step to score new data.

Table 69.3 summarizes the *options* available in the CODE statement.

**Table 69.3** CODE Statement Options

| Option    | Description                                                                  |
|-----------|------------------------------------------------------------------------------|
| CATALOG=  | Names the catalog entry where the generated code is saved                    |
| DUMMIES   | Retains the dummy variables in the data set                                  |
| ERROR     | Computes the error function                                                  |
| FILE=     | Names the file where the generated code is saved                             |
| FORMAT=   | Specifies the numeric format for the regression coefficients                 |
| GROUP=    | Specifies the group identifier for array names and statement labels          |
| IMPUTE    | Imputes predicted values for observations with missing or invalid covariates |
| LINESIZE= | Specifies the line size of the generated code                                |
| LOOKUP=   | Specifies the algorithm for looking up CLASS levels                          |
| RESIDUAL  | Computes residuals                                                           |

For details about the syntax of the CODE statement, see the section “CODE Statement” on page 390 in Chapter 19, “Shared Concepts and Topics.”

---

## EFFECTPLOT Statement

**EFFECTPLOT** < plot-type < (plot-definition-options) > > < / options > ;

The EFFECTPLOT statement produces a display of the fitted model and provides options for changing and enhancing the displays. Table 69.4 describes the available *plot-types* and their *plot-definition-options*.

**Table 69.4** *Plot-Types and Plot-Definition-Options*

| <b>Plot-Type and Description</b>                                                                                                                                                                                                             | <b>Plot-Definition-Options</b>                                                                                                       |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------|
| <p><b>BOX</b></p> <p>Displays a box plot of continuous response data at each level of a CLASS effect, with predicted values superimposed and connected by a line. This is an alternative to the <b>INTERACTION</b> <i>plot-type</i>.</p>     | <p><b>PLOTBY=</b> variable or CLASS effect<br/> <b>X=</b> CLASS variable or effect</p>                                               |
| <p><b>CONTOUR</b></p> <p>Displays a contour plot of predicted values against two continuous covariates.</p>                                                                                                                                  | <p><b>PLOTBY=</b> variable or CLASS effect<br/> <b>X=</b> continuous variable<br/> <b>Y=</b> continuous variable</p>                 |
| <p><b>FIT</b></p> <p>Displays a curve of predicted values versus a continuous variable.</p>                                                                                                                                                  | <p><b>PLOTBY=</b> variable or CLASS effect<br/> <b>X=</b> continuous variable</p>                                                    |
| <p><b>INTERACTION</b></p> <p>Displays a plot of predicted values (possibly with error bars) versus the levels of a CLASS effect. The predicted values are connected with lines and can be grouped by the levels of another CLASS effect.</p> | <p><b>PLOTBY=</b> variable or CLASS effect<br/> <b>SLICEBY=</b> variable or CLASS effect<br/> <b>X=</b> CLASS variable or effect</p> |
| <p><b>SLICEFIT</b></p> <p>Displays a curve of predicted values versus a continuous variable grouped by the levels of a CLASS effect.</p>                                                                                                     | <p><b>PLOTBY=</b> variable or CLASS effect<br/> <b>SLICEBY=</b> variable or CLASS effect<br/> <b>X=</b> continuous variable</p>      |

For full details about the syntax and options of the EFFECTPLOT statement, see the section “EFFECTPLOT Statement” on page 411 in Chapter 19, “Shared Concepts and Topics.”

---

## ESTIMATE Statement

```
ESTIMATE <'label'> estimate-specification <(divisor=n)>
 < , ... <'label'> estimate-specification <(divisor=n)> >
 </ options > ;
```

The ESTIMATE statement provides a mechanism for obtaining custom hypothesis tests. Estimates are formed as linear estimable functions of the form  $L\beta$ . You can perform hypothesis tests for the estimable functions, construct confidence limits, and obtain specific nonlinear transformations.

Table 69.5 summarizes the options available in the ESTIMATE statement.



**Table 69.5** ESTIMATE Statement Options

| Option                                                     | Description                                                                     |
|------------------------------------------------------------|---------------------------------------------------------------------------------|
| <b>Construction and Computation of Estimable Functions</b> |                                                                                 |
| DIVISOR=                                                   | Specifies a list of values to divide the coefficients                           |
| NOFILL                                                     | Suppresses the automatic fill-in of coefficients for higher-order effects       |
| SINGULAR=                                                  | Tunes the estimability checking difference                                      |
| <b>Degrees of Freedom and <math>p</math>-values</b>        |                                                                                 |
| ADJUST=                                                    | Determines the method for multiple comparison adjustment of estimates           |
| ALPHA= $\alpha$                                            | Determines the confidence level ( $1 - \alpha$ )                                |
| LOWER                                                      | Performs one-sided, lower-tailed inference                                      |
| STEPDOWN                                                   | Adjusts multiplicity-corrected $p$ -values further in a step-down fashion       |
| TESTVALUE=                                                 | Specifies values under the null hypothesis for tests                            |
| UPPER                                                      | Performs one-sided, upper-tailed inference                                      |
| <b>Statistical Output</b>                                  |                                                                                 |
| CL                                                         | Constructs confidence limits                                                    |
| CORR                                                       | Displays the correlation matrix of estimates                                    |
| COV                                                        | Displays the covariance matrix of estimates                                     |
| E                                                          | Prints the L matrix                                                             |
| JOINT                                                      | Produces a joint $F$ or chi-square test for the estimable functions             |
| PLOTS=                                                     | Requests ODS statistical graphics if the analysis is sampling-based             |
| SEED=                                                      | Specifies the seed for computations that depend on random numbers               |
| <b>Generalized Linear Modeling</b>                         |                                                                                 |
| CATEGORY=                                                  | Specifies how to construct estimable functions with multinomial data            |
| EXP                                                        | Exponentiates and displays estimates                                            |
| ILINK                                                      | Computes and displays estimates and standard errors on the inverse linked scale |

For details about the syntax of the ESTIMATE statement, see the section “ESTIMATE Statement” on page 437 in Chapter 19, “Shared Concepts and Topics.”

## FILTER Statement

**FILTER** *expression* ;

The FILTER statement enables you to filter the results of the PLM procedure, specifically the contents of ODS tables and the output data sets. There can be at most one FILTER statement per PROC PLM run, and the filter is applied to all BY groups and to all queries generated through WHERE expressions.

A filter *expression* follows the same pattern as a *where-expression* in the **WHERE** statement. The expressions consist of operands and operators. For more information about specifying *where-expressions*, see the **WHERE** statement for the PLM procedure and *SAS Language Reference: Concepts*.

Valid keywords for the formation of operands in the FILTER statement are shown in Table 69.6.

**Table 69.6** Keywords for Filtering Results

| Keyword    | Description                                                                                                  |
|------------|--------------------------------------------------------------------------------------------------------------|
| Prob       | Regular (unadjusted) $p$ -values from $t$ , $F$ , or chi-square tests                                        |
| ProbChi    | Regular (unadjusted) $p$ -values from chi-square tests                                                       |
| ProbF      | Regular (unadjusted) $p$ -values from $F$ tests                                                              |
| ProbT      | Regular (unadjusted) $p$ -values from $t$ tests                                                              |
| AdjP       | Adjusted $p$ -values                                                                                         |
| Estimate   | Results displayed in “Estimates” column of ODS tables                                                        |
| Pred       | Predicted values in <b>SCORE</b> output data sets                                                            |
| Resid      | Residuals in <b>SCORE</b> output data sets.                                                                  |
| Std        | Standard errors in ODS tables and in <b>SCORE</b> results                                                    |
| Mu         | Results displayed in the “Mean” column of ODS tables (this column is typically produced by the ILINK option) |
| tValue     | The value of the usual $t$ statistic                                                                         |
| FValue     | The value of the usual $F$ statistic                                                                         |
| Chisq      | The value of the chi-square statistic                                                                        |
| testStat   | The value of the test statistic (a generic keyword for the ‘tValue’, ‘FValue’, and ‘Chisq’ tokens)           |
| Lower      | The lower confidence limit displayed in ODS tables                                                           |
| Upper      | The upper confidence limit displayed in ODS tables                                                           |
| AdjLower   | The adjusted lower confidence limit displayed in ODS tables                                                  |
| AdjUpper   | The adjusted upper confidence limit displayed in ODS tables                                                  |
| LowerMu    | The lower confidence limit for the mean displayed in ODS tables                                              |
| UpperMu    | The upper confidence limit for the mean displayed in ODS tables                                              |
| AdjLowerMu | The adjusted lower confidence limit for the mean displayed in ODS tables                                     |
| AdjUpperMu | The adjusted upper confidence limit for the mean displayed in ODS tables                                     |

When you write filtering expressions, be advised that filtering variables that are not used in the results are typically set to missing values. For example, the following statements select all results (filter nothing) because no adjusted  $p$ -values are computed:

```
proc plm restore=MyStore;
 lsmeans a / diff;
 filter adjp < 0.05;
run;
```

If the adjusted  $p$ -values are set to missing values, the condition `adjp < 0.05` is true in each case (missing values always compare smaller than the smallest nonmissing value).

See “Example 69.6: Comparing Multiple B-Splines” on page 5853 for an example of using the `FILTER` statement.

Filtering results has no effect on the item store contents that are displayed with the `SHOW` statement. However, BY-group selection with the `WHERE` statement can limit the amount of information that is displayed by the `SHOW` statements.

---

## LSMEANS Statement

**LSMEANS** < model-effects > < / options > ;

The LSMEANS statement computes and compares least squares means (LS-means) of fixed effects. LS-means are *predicted population margins*—that is, they estimate the marginal means over a balanced population. In a sense, LS-means are to unbalanced designs as class and subclass arithmetic means are to balanced designs.

Table 69.7 summarizes the options available in the LSMEANS statement.

**Table 69.7** LSMEANS Statement Options

| Option                                              | Description                                                                                 |
|-----------------------------------------------------|---------------------------------------------------------------------------------------------|
| <b>Construction and Computation of LS-Means</b>     |                                                                                             |
| <code>AT</code>                                     | Modifies the covariate value in computing LS-means                                          |
| <code>BYLEVEL</code>                                | Computes separate margins                                                                   |
| <code>DIFF</code>                                   | Requests differences of LS-means                                                            |
| <code>OM=</code>                                    | Specifies the weighting scheme for LS-means computation as determined by the input data set |
| <code>SINGULAR=</code>                              | Tunes estimability checking                                                                 |
| <b>Degrees of Freedom and <math>p</math>-values</b> |                                                                                             |
| <code>ADJUST=</code>                                | Determines the method for multiple-comparison adjustment of LS-means differences            |
| <code>ALPHA=<math>\alpha</math></code>              | Determines the confidence level $(1 - \alpha)$                                              |
| <code>STEPDOWN</code>                               | Adjusts multiple-comparison $p$ -values further in a step-down fashion                      |
| <b>Statistical Output</b>                           |                                                                                             |
| <code>CL</code>                                     | Constructs confidence limits for means and mean differences                                 |
| <code>CORR</code>                                   | Displays the correlation matrix of LS-means                                                 |
| <code>COV</code>                                    | Displays the covariance matrix of LS-means                                                  |
| <code>E</code>                                      | Prints the <b>L</b> matrix                                                                  |
| <code>LINES</code>                                  | Produces a “Lines” display for pairwise LS-means differences                                |
| <code>MEANS</code>                                  | Prints the LS-means                                                                         |
| <code>PLOTS=</code>                                 | Requests graphs of means and mean comparisons                                               |
| <code>SEED=</code>                                  | Specifies the seed for computations that depend on random numbers                           |

---

Table 69.7 *continued*

| Option                             | Description                                                                                                       |
|------------------------------------|-------------------------------------------------------------------------------------------------------------------|
| <b>Generalized Linear Modeling</b> |                                                                                                                   |
| EXP                                | Exponentiates and displays estimates of LS-means or LS-means differences                                          |
| ILINK                              | Computes and displays estimates and standard errors of LS-means (but not differences) on the inverse linked scale |
| ODDSRATIO                          | Reports (simple) differences of least squares means in terms of odds ratios if permitted by the link function     |

For details about the syntax of the LSMEANS statement, see the section “LSMEANS Statement” on page 453 in Chapter 19, “Shared Concepts and Topics.”

## LSMESTIMATE Statement

```
LSMESTIMATE model-effect <'label'> values <divisor=n>
 < , ... <'label'> values <divisor=n> >
 </options> ;
```

The LSMESTIMATE statement provides a mechanism for obtaining custom hypothesis tests among least squares means.

Table 69.8 summarizes the options available in the LSMESTIMATE statement.

Table 69.8 LSMESTIMATE Statement Options

| Option                                              | Description                                                                         |
|-----------------------------------------------------|-------------------------------------------------------------------------------------|
| <b>Construction and Computation of LS-Means</b>     |                                                                                     |
| AT                                                  | Modifies covariate values in computing LS-means                                     |
| BYLEVEL                                             | Computes separate margins                                                           |
| DIVISOR=                                            | Specifies a list of values to divide the coefficients                               |
| OM=                                                 | Specifies the weighting scheme for LS-means computation as determined by a data set |
| SINGULAR=                                           | Tunes estimability checking                                                         |
| <b>Degrees of Freedom and <math>p</math>-values</b> |                                                                                     |
| ADJUST=                                             | Determines the method for multiple-comparison adjustment of LS-means differences    |
| ALPHA= $\alpha$                                     | Determines the confidence level $(1 - \alpha)$                                      |
| LOWER                                               | Performs one-sided, lower-tailed inference                                          |
| STEPDOWN                                            | Adjusts multiple-comparison $p$ -values further in a step-down fashion              |
| TESTVALUE=                                          | Specifies values under the null hypothesis for tests                                |
| UPPER                                               | Performs one-sided, upper-tailed inference                                          |

Table 69.8 *continued*

| Option                             | Description                                                                                                       |
|------------------------------------|-------------------------------------------------------------------------------------------------------------------|
| <b>Statistical Output</b>          |                                                                                                                   |
| CL                                 | Constructs confidence limits for means and mean differences                                                       |
| CORR                               | Displays the correlation matrix of LS-means                                                                       |
| COV                                | Displays the covariance matrix of LS-means                                                                        |
| E                                  | Prints the <b>L</b> matrix                                                                                        |
| ELSM                               | Prints the <b>K</b> matrix                                                                                        |
| JOINT                              | Produces a joint <i>F</i> or chi-square test for the LS-means and LS-means differences                            |
| PLOTS=                             | Requests graphs of means and mean comparisons                                                                     |
| SEED=                              | Specifies the seed for computations that depend on random numbers                                                 |
| <b>Generalized Linear Modeling</b> |                                                                                                                   |
| CATEGORY=                          | Specifies how to construct estimable functions with multinomial data                                              |
| EXP                                | Exponentiates and displays LS-means estimates                                                                     |
| ILINK                              | Computes and displays estimates and standard errors of LS-means (but not differences) on the inverse linked scale |

For details about the syntax of the LSMESTIMATE statement, see the section “[LSMESTIMATE Statement](#)” on page 470 in Chapter 19, “[Shared Concepts and Topics](#).”

## SCORE Statement

```
SCORE DATA=SAS-data-set < OUT=SAS-data-set >
 < keyword< =name> > ...
 < keyword< =name> > < / options > ;
```

The SCORE statement applies the contents of the source item store to compute predicted values and other observation-wise statistics for a SAS data set.

You can specify the following syntax elements in the SCORE statement before the option slash (/):

### **DATA=SAS-data-set**

specifies the input data set for scoring. This option is required, and the data set is examined for congruity with the previously fitted (and stored) model. For example, all necessary variables to form a row of the **X** matrix must be present in the input data set and must be of the correct type and format. The following variables do not have to be present in the input data set:

- the response variable
- the *events* and *trials* variables used in the *events/trials* syntax for binomial data
- variables used in WEIGHT or FREQ statements

**OUT=SAS-data-set**

specifies the name of the output data set. If you do not specify an output data set with the OUT= option, the PLM procedure uses the DATA*n* convention to name the output data set.

**keyword<=name>**

specifies a statistic to be included in the OUT= data set and optionally assigns the statistic the variable name *name*. Table 69.9 lists the keywords and the default names assigned by the PLM procedure if you do not specify a *name*.

**Table 69.9** Keywords for Output Statistics

| Keyword   | Description                                     | Expression                                        | Name      |
|-----------|-------------------------------------------------|---------------------------------------------------|-----------|
| PREDICTED | Linear predictor                                | $\hat{\eta} = \mathbf{x}\hat{\boldsymbol{\beta}}$ | Predicted |
| STDERR    | Standard deviation of linear predictor          | $\sqrt{\text{Var}(\hat{\eta})}$                   | StdErr    |
| RESIDUAL  | Residual                                        | $y - g^{-1}(\hat{\eta})$                          | Resid     |
| LCLM      | Lower confidence limit for the linear predictor |                                                   | LCLM      |
| UCLM      | Upper confidence limit for the linear predictor |                                                   | UCLM      |
| LCL       | Lower prediction limit for the linear predictor |                                                   | LCL       |
| UCL       | Upper prediction limit for the linear predictor |                                                   | UCL       |

Prediction limits (LCL, UCL) are available only for statistical models that allow such limits, typically regression-type models for normally distributed data with an identity link function.

You can specify the following options in the SCORE statement after a slash (/):

**ALPHA=number**

determines the coverage probability for two-sided confidence and prediction intervals. The coverage probability is computed as  $1 - \text{number}$ . The value of *number* must be between 0 and 1; the default is 0.05.

**DF=number**

specifies the degrees of freedom to use in the construction of prediction and confidence limits.

**ILINK**

requests that predicted values be inversely linked to produce predictions on the data scale. By default, predictions are produced on the linear scale where covariate effects are additive.

**NOUNIQUE**

requests that names not be made unique in the case of naming conflicts. By default, the PLM procedure avoids naming conflicts by assigning a unique name to each output variable. If you specify the NOUNIQUE option, variables with conflicting names are not renamed. In that case, the first variable added to the output data set takes precedence.

**NOVAR**

requests that variables from the input data set not be added to the output data set.

**OBSCAT**

requests that statistics in models for multinomial data be written to the output data set only for the response level that corresponds to the observed level of the observation.

**SAMPLE**

requests that the sample of parameter estimates in the item store be used to form scoring statistics. This option is useful when the item store contains the results of a Bayesian analysis and a posterior sample of parameter estimates. The predicted value is then computed as the average predicted value across the posterior estimates, and the standard error measures the standard deviation of these estimates. For example, let  $\widehat{\beta}_1, \dots, \widehat{\beta}_k$  denote the  $k$  posterior sample estimates of  $\beta$ , and let  $\mathbf{x}_i$  denote the  $x$ -vector for the  $i$ th observation in the scoring data set. If the **SAMPLE** option is in effect, the output statistics for the predicted value, the standard error, and the residual of the  $i$ th observation are computed as

$$\begin{aligned}\eta_{ij} &= \mathbf{x}_i \widehat{\beta}_j \\ \text{PRED}_i &= \bar{\eta}_i = \frac{1}{k} \sum_{j=1}^k \eta_{ij} \\ \text{STDERR}_i &= \left( \frac{1}{k-1} \sum_{j=1}^k (\eta_{ij} - \bar{\eta}_i)^2 \right)^{1/2} \\ \text{RESIDUAL}_i &= y_i - g^{-1}(\bar{\eta}_i)\end{aligned}$$

where  $g^{-1}(\cdot)$  denotes the inverse link function.

If, in addition, the **ILINK** option is in effect, the calculations are as follows:

$$\begin{aligned}\eta_{ij} &= \mathbf{x}_i \widehat{\beta}_j \\ \text{PRED}_i &= \frac{1}{k} \sum_{j=1}^k g^{-1}(\eta_{ij}) \\ \text{STDERR}_i &= \left( \frac{1}{k-1} \sum_{j=1}^k (g^{-1}(\eta_{ij}) - \text{PRED}_i)^2 \right)^{1/2} \\ \text{RESIDUAL}_i &= y_i - \text{PRED}_i\end{aligned}$$

The LCL and UCL statistics are not available with the **SAMPLE** option. When the LCLM and UCLM statistics are requested, the **SAMPLE** option yields the lower  $100 \times \alpha/2\%$  and upper  $100 \times (1 - \alpha/2)\%$  percentiles of the predicted values under the sample (posterior) distribution. When you request residuals with the **SAMPLE** option, the calculation depends on whether the **ILINK** option is specified.

## SHOW Statement

**SHOW** *options* ;

The SHOW statement uses the Output Delivery System to display contents of the item store. This statement is useful for verifying that the contents of the item store apply to the analysis and for generating ODS tables. Table 69.10 summarizes the options available in the SHOW statement.

**Table 69.10** SHOW Statement Options

| Option      | Description                                                                                     |
|-------------|-------------------------------------------------------------------------------------------------|
| ALL         | Displays all applicable contents                                                                |
| BYVAR       | Displays information about the BY variables                                                     |
| CLASSLEVELS | Displays the “Class Level Information” table                                                    |
| CORRELATION | Produces the correlation matrix of the parameter estimates                                      |
| COVARIANCE  | Produces the covariance matrix of the parameter estimates                                       |
| EFFECTS     | Displays information about the constructed effects                                              |
| FITSTATS    | Displays the fit statistics                                                                     |
| HESSIAN     | Displays the Hessian matrix                                                                     |
| HERMITE     | Generates the Hermite matrix $\mathbf{H} = (\mathbf{X}'\mathbf{X})^{-1}(\mathbf{X}'\mathbf{X})$ |
| PARAMETERS  | Displays the parameter estimates                                                                |
| PROGRAM     | Displays the SAS program that generated the item store                                          |
| XPX         | Displays the crossproduct matrix $\mathbf{X}'\mathbf{X}$                                        |
| XPXI        | Displays the generalized inverse of the crossproduct matrix $\mathbf{X}'\mathbf{X}$             |

You can specify the following options after the SHOW statement:

**ALL | \_ALL\_**

displays all applicable contents.

**BYVAR | BY**

displays information about the BY variables in the source item store. If a BY statement was present when the item store was created, the PLM procedure performs the analysis separately for each BY group.

**CLASSLEVELS | CLASS**

displays the “Class Level Information” table. This table is produced by the PLM procedure by default if the model contains effects that depend on classification variables.

**CORRELATION | CORR | CORRB**

produces the correlation matrix of the parameter estimates. If the source item store contains a posterior sample of parameter estimates, the computed matrix is the correlation matrix of the sample covariance matrix.

**COVARIANCE | COV | COVB**

produces the covariance matrix of the parameter estimates. If the source item store contains a posterior sample of parameter estimates, the PLM procedure computes the empirical sample covariance matrix from the posterior estimates. You can convert this matrix into a sample correlation matrix with the CORRELATION option in the SHOW statement.



**EFFECTS**

displays information about the constructed effects in the model. Constructed effects are those that were created with the EFFECT statement in the procedure run that generated the source item store.

**FITSTATS | FIT**

displays the fit statistics from the item store.

**HESSIAN | HESS**

displays the Hessian matrix.

**HERMITE | HERM**

generates the Hermite matrix  $\mathbf{H} = (\mathbf{X}'\mathbf{X})^{-1}(\mathbf{X}'\mathbf{X})$ . The PLM procedure chooses a reflexive,  $g_2$ -inverse for the generalized inverse of the crossproduct matrix  $\mathbf{X}'\mathbf{X}$ . See “Important Linear Algebra Concepts” on page 44 of Chapter 3, “Introduction to Statistical Modeling with SAS/STAT Software,” for information about generalized inverses and the sweep operator.

**PARAMETERS<=n>****PARMS<=n>**

displays the parameter estimates. The structure of the display depends on whether a posterior sample of parameter estimates is available in the source item store. If such a sample is present, up to the first 20 parameter vectors are shown in wide format. You can modify this number with the  $n$  argument.

If no posterior sample is present, the single vector of parameter estimates is shown in narrow format. If the store contains information about the covariance matrix of the parameter estimates, then standard errors are added.

**PROGRAM<(WIDTH=n)>****PROG<(WIDTH=n)>**

displays the SAS program that generated the item store, provided that this was stored at store generation time. The program does not include comments, titles, or some other global statements. The optional width parameter  $n$  determines the display width of the source code.

**XPX | CROSSPRODUCT**

displays the crossproduct matrix  $\mathbf{X}'\mathbf{X}$ .

**XPXI**

displays the generalized inverse of the crossproduct matrix  $\mathbf{X}'\mathbf{X}$ . The PLM procedure obtains a reflexive  $g_2$ -inverse by sweeping. See “Important Linear Algebra Concepts” on page 44 of Chapter 3, “Introduction to Statistical Modeling with SAS/STAT Software,” for information about generalized inverses and the sweep operator.

**SLICE Statement**

**SLICE** *model-effect* </options> ;

The SLICE statement provides a general mechanism for performing a partitioned analysis of the LS-means for an interaction. This analysis is also known as an analysis of simple effects.

The SLICE statement uses the same options as the LSMEANS statement, which are summarized in Table 19.21. For details about the syntax of the SLICE statement, see the section “SLICE Statement” on page 498 in Chapter 19, “Shared Concepts and Topics.”

---

## TEST Statement

**TEST** < *model-effects* > < / *options* > ;

The TEST statement enables you to perform  $F$  tests for model effects that test Type I, Type II, or Type III hypotheses. See Chapter 15, “The Four Types of Estimable Functions,” for details about the construction of Type I, II, and III estimable functions.

Table 69.11 summarizes the options available in the TEST statement.

**Table 69.11** TEST Statement Options

| Option    | Description                                                |
|-----------|------------------------------------------------------------|
| CHISQ     | Requests chi-square tests                                  |
| DDF=      | Specifies denominator degrees of freedom for fixed effects |
| E         | Requests Type I, Type II, and Type III coefficients        |
| E1        | Requests Type I coefficients                               |
| E2        | Requests Type II coefficients                              |
| E3        | Requests Type III coefficients                             |
| HTYPE=    | Indicates the type of hypothesis test to perform           |
| INTERCEPT | Adds a row that corresponds to the overall intercept       |

For details about the syntax of the TEST statement, see the section “TEST Statement” on page 502 in Chapter 19, “Shared Concepts and Topics.”

---

## WHERE Statement

**WHERE** *expression* ;

You can use the WHERE statement in the PLM procedure when the item store contains BY-variable information and you want to apply the PROC PLM statements to only a subset of the BY groups.

A WHERE expression is a type of SAS expression that defines a condition. In the DATA step and in procedures that use SAS data sets as the input source, the WHERE expression is used to select observations for inclusion in the DATA step or in the analysis. In the PLM procedure, which does not accept a SAS data set but rather takes an item store that was created by a qualifying SAS/STAT procedure, the WHERE statement is also used to specify conditions. The conditional selection does not apply to observations in PROC PLM, however. Instead, you use the WHERE statement in the PLM procedure to select a subset of BY groups from the item store to which to apply the PROC PLM statements.

The general syntax of the WHERE statement is

**WHERE** *operand* < *operator operand* > < **AND** | **OR** *operand* < *operator operand* > . . . > ;

where

*operand* is something to be operated on. The operand can be the name of a BY variable in the item store, a SAS function, a constant, or a predefined name to identify columns in result tables.

*operator* is a symbol that requests a comparison, logical operation, or arithmetic calculation. All SAS expression operators are valid for a WHERE expression.

For more details about how to specify general WHERE expressions, see *SAS Language Reference: Concepts*. Notice that the **FILTER** statement accepts similar expressions that are specified in terms of predefined keywords. Expressions in the WHERE statement of the PLM procedure are written in terms of BY variables.

There is no limit to the number of WHERE statements in the PLM procedure. When you specify multiple WHERE statements, the statements are *not* cumulative. Each WHERE statement is executed separately. You can think of each selection WHERE statement as one analytic query to the item store: the WHERE statement defines the query, and the PLM procedure is the querying engine. For example, suppose that the item store contains results for the numeric BY variables A and B. The following statements define two separate queries of the item store:

```
WHERE a = 4;
WHERE (b < 3) and (a > 4);
```

The PLM procedure first applies the requested analysis to all BY groups where a equals 4 (irrespective of the value of variable b). The analysis is then repeated for all BY groups where b is less than 3 and a is greater than 4.

Group selection with WHERE statements is possible only if the item store contains BY variables. You can use the **BYVAR** option in the **SHOW** statement to display the BY variables in the item store.

Note that WHERE expressions in the SAS DATA step and in many procedures are specified in terms of the unformatted values of data set variables, even if a format was applied to the variable. If you specify the **WHEREFORMAT** option in the **PROC PLM** statement, the PLM procedure evaluates WHERE expressions for BY variables in terms of the formatted values. For example, assume that the following format was applied to the variable tx when the item store was created:

```
proc format;
 value bf 1 = 'Control'
 2 = 'Treated';
run;
```

Then the following two PROC PLM runs are equivalent:

```
proc plm restore=MyStore;
 show parms;
 where b = 2;
run;

proc plm restore=MyStore whereformat;
 show parms;
 where b = 'Treated';
run;
```

---

## Details: PLM Procedure

---

### BY Processing and the PLM Procedure

When a BY statement is in effect for the analysis that creates an item store, the information about BY variables and BY-group-specific modeling results are transferred to the item store. In this case, the PLM procedure automatically assumes a processing mode for the item store that is akin to BY processing, with the PLM statements being applied in turn for each of the BY groups. Also, you can then obtain a table of BY groups with the **BYVAR** option in the **SHOW** statement. The “Source Information” table also displays the variable names of the BY variables if BY groups are present. The **WHERE** statement can be used to restrict the analysis to specific BY groups that meet the conditions of the **WHERE** expression.

See [Example 69.4](#) for an example that uses BY-group-specific information in the source item store.

As with procedures that operate on input data sets, the BY variable information is added automatically to any output data sets and ODS tables produced by the PLM procedure.

When you score a data set with the **SCORE** statement and the item store contains BY variables, three situations can arise:

- None of the BY variables are present in the scoring data set. In this situation the results of the BY groups in the item store are applied in turn to the entire scoring data set. For example, if the scoring data set contains 50 observations and no BY-variable information, the number of observations in the output data set of the **SCORE** statement equals 50 times the number of BY groups.
- The scoring data set contains only a part of the BY variables, or the variables have different type or format. The PLM procedure does not process such an incompatible scoring data set.
- All BY variables are in the scoring data set in the same type and format as when the item store was created. The BY-group-specific results are applied to each observation in the scoring data set. The scoring data set does not have to be sorted or grouped by the BY variables. However, it is computationally more efficient if the scoring data set is arranged by groups of the BY variables.

---

### Analysis Based on Posterior Estimates

If an item store is saved from a Bayesian analysis (by PROC GENMOD or PROC PHREG or PROC LIFEREG), then PROC PLM can perform sampling-based inference based on Bayes posterior estimates that are saved in the item store. For example, the following statements request a Bayesian analysis and save the results to an item store named `sasuser.gmd`. For the Bayesian analysis, the random number generator seed is set to 1. By default, a noninformative distribution is set as the prior distribution for the regression coefficients and the posterior sample size is 10,000.

```
proc genmod data=gs;
 class a b;
 model y = a b;
 bayes seed=1;
 store sasuser.gmd / label='Bayesian Analysis';
run;
```

When the PLM procedure opens the item store `sasuser.gmd`, it detects that the results were saved from a Bayesian analysis. The posterior sample of regression coefficient estimates are then loaded to perform statistical inference tasks.

The majority of postprocessing tasks involve inference based on an estimable linear function  $\mathbf{L}\widehat{\boldsymbol{\beta}}$ , which often requires its mean and variance. When the standard frequentist analyses are performed, the mean and variance have explicit forms because the parameter estimate  $\widehat{\boldsymbol{\beta}}$  is analytically tractable. However, explicit forms are not usually available when Bayesian models are fitted. Instead, empirical means and variance-covariance matrices for the estimable function are constructed from the posterior sample.

Let  $\widehat{\boldsymbol{\beta}}_i, i = 1, \dots, N_p$  denote the  $N_p$  vectors of posterior sample estimates of  $\boldsymbol{\beta}$  saved in `sasuser.gmd`. Use these vectors to construct the posterior sample of estimable functions  $\mathbf{L}\widehat{\boldsymbol{\beta}}_i$ . The posterior mean of the estimable function is thus

$$\overline{\mathbf{L}\widehat{\boldsymbol{\beta}}} = \frac{1}{N_p} \sum_{i=1}^{N_p} \mathbf{L}\widehat{\boldsymbol{\beta}}_i$$

and the posterior variance of the estimable function is

$$\mathbf{V}(\mathbf{L}\widehat{\boldsymbol{\beta}}) = \frac{1}{N_p - 1} \sum_{i=1}^{N_p} (\mathbf{L}\widehat{\boldsymbol{\beta}}_i - \overline{\mathbf{L}\widehat{\boldsymbol{\beta}}})^2$$

Sometimes statistical inference on a transformation of  $\mathbf{L}\widehat{\boldsymbol{\beta}}$  is requested. For example, the EXP option for the ESTIMATE and LSMESTIMATE statements requests analysis based on  $\exp(\mathbf{L}\widehat{\boldsymbol{\beta}})$ , exponentiation of the estimable function. If this type of analysis is requested, the posterior sample of transformed estimable functions is constructed by transforming each of the estimable function evaluated at the posterior sample:  $f(\mathbf{L}\widehat{\boldsymbol{\beta}}_i), i = 1, \dots, N_p$ . The posterior mean and variance for  $f(\mathbf{L}\widehat{\boldsymbol{\beta}})$  are then computed from the constructed sample to make the inference:

$$\overline{f(\mathbf{L}\widehat{\boldsymbol{\beta}})} = \frac{1}{N_p} \sum_{i=1}^{N_p} f(\mathbf{L}\widehat{\boldsymbol{\beta}}_i)$$

$$\mathbf{V}(f(\mathbf{L}\widehat{\boldsymbol{\beta}})) = \frac{1}{N_p - 1} \sum_{i=1}^{N_p} (f(\mathbf{L}\widehat{\boldsymbol{\beta}}_i) - \overline{f(\mathbf{L}\widehat{\boldsymbol{\beta}})})^2$$

After obtaining the posterior mean and variance, the PLM procedure proceeds to perform statistical inference based on them.

---

## User-Defined Formats and the PLM Procedure

The PLM procedure does not support a FORMAT statement because it operates without an input data set, and also because changing the format properties of variables could alter the interpretation of parameter estimates, thus creating a dissonance with variable properties in effect when the item store was created. Instead, user-defined formats that are applied to classification variables when the item store is created are saved to the store and are by default reloaded by the PLM procedure. When the PLM procedure loads a format, notes are issued to the log.

You can change the load behavior for formats with the `FORMAT=` option in the `PROC PLM` statement.

User-defined formats do not need to be supplied in a new SAS session. However, when a user-defined format with the same name as a stored format exists and the default `FORMAT=RELOAD` option is in effect, the format definition loaded from the item store replaces the format currently in effect.

In the following statements, the format `AFORM` is created and applied to the variable `a` in the `PROC GLM` step. This format definition is transferred to the item store `sasuser.glm` through the `STORE` statement.

```
proc format;
 value aform 1='One' 2='Two' 3='Three';
run;
proc glm data=sp;
 format a aform.;
 class block a b;
 model y = block a b x;
 store sasuser.glm;
 weight x;
run;
```

The following statements replace the format definition of the `AFORM` format. The `PLM` step then reloads the `AFORM` format (from the item store) and thereby restores its original state.

```
proc format;
 value aform 1='Un' 2='Deux' 3='Trois';
run;
proc plm restore=sasuser.glm;
 show class;
 score data=sp out=plmout lcl lclm ucl uclm;
run;
```

The following notes, issued by the `PLM` procedure, inform you that the procedure loaded the format, the format already existed, and the existing format was replaced:

```
NOTE: The format AFORM was loaded from item store SASUSER.GLM.
NOTE: Format AFORM is already on the library.
NOTE: Format AFORM has been output.
```

After the `PROC PLM` run, the definition that is in effect for the format `AFORM` corresponds to the following SAS statements:

```
proc format;
 value aform 1='One' 2='Two' 3='Three';
run;
```

---

## ODS Table Names

`PROC PLM` assigns a name to each table it creates. You can use these names to refer to the table when you use the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in Table 69.12. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

Each of the EFFECTPLOT, ESTIMATE, LSMEANS, LSMESTIMATE, and SLICE statements also creates tables, which are not listed in Table 69.12. For information about these tables, see the corresponding sections of Chapter 19, “Shared Concepts and Topics.”

**Table 69.12** ODS Tables Produced by PROC PLM

| Table Name         | Description                                                      | Required Option                                             |
|--------------------|------------------------------------------------------------------|-------------------------------------------------------------|
| ByVarInfo          | Information about BY variables in source item store (if present) | SHOW BYVAR                                                  |
| ClassLevels        | Level information from the CLASS statement                       | Default output when model effects depend on CLASS variables |
| Corr               | Correlation matrix of parameter estimates                        | SHOW CORR                                                   |
| Cov                | Covariance matrix of parameter estimates                         | SHOW COV                                                    |
| FitStatistics      | Fit statistics                                                   | SHOW FIT                                                    |
| Hessian            | Hessian matrix                                                   | SHOW HESSIAN                                                |
| Hermite            | Hermite matrix                                                   | SHOW HERMITE                                                |
| ParameterEstimates | Parameter estimates                                              | SHOW PARMS                                                  |
| ParameterSample    | Sampled (posterior) parameter estimates                          | SHOW PARMS                                                  |
| Program            | Originating source code                                          | SHOW PROGRAM                                                |
| StoreInfo          | Information about source item store                              | Default                                                     |
| XpX                | $\mathbf{X}'\mathbf{X}$ matrix                                   | SHOW XPX                                                    |
| XpXI               | $(\mathbf{X}'\mathbf{X})^{-1}$ matrix                            | SHOW XPXI                                                   |

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “Statistical Graphics Using ODS.”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “A Primer on ODS Statistical Graphics” on page 599 in Chapter 21, “Statistical Graphics Using ODS.”

When ODS Graphics is enabled, then each of the EFFECTPLOT, ESTIMATE, LSMEANS, LSMESTIMATE, and SLICE statements can produce plots associated with their analyses. For information about these plots, see the corresponding sections of Chapter 19, “Shared Concepts and Topics.”

---

## Examples: PLM Procedure

---

### Example 69.1: Scoring with PROC PLM

Logistic regression with model selection is often used to extract useful information and build interpretable models for classification problems with many variables. This example demonstrates how you can use PROC LOGISTIC to build a spline model on a simulated data set and how you can later use the fitted model to classify new observations.

The following DATA step creates a data set named SimuData, which contains 5,000 observations and 100 continuous variables:

```
%let nObs = 5000;
%let nVars = 100;
data SimuData;
 array x{&nVars};
 do obsNum=1 to &nObs;
 do j=1 to &nVars;
 x{j}=ranuni(1);
 end;

 linp = 10 + 11*x1 - 10*sqrt(x2) + 2/x3 - 8*exp(x4) + 7*x5*x5
 - 6*x6**1.5 + 5*log(x7) - 4*sin(3.14*x8) + 3*x9 - 2*x10;
 TrueProb = 1/(1+exp(-linp));

 if ranuni(1) < TrueProb then y=1;
 else y=0;

 output;
 end;
run;
```

The response is binary based on the inversely transformed logit values. The true logit is a function of only 10 of the 100 variables, including nonlinear transformations of seven variables, as follows:

$$\text{logit}(p) = 10 + 11x_1 - 10\sqrt{x_2} + \frac{2}{x_3} - 8 \exp(x_4) + 7x_5^2 - 6x_6^{1.5} + 5 \log(x_7) - 4 \sin(3.14x_8) + 3x_9 - 2x_{10}$$

Now suppose the true model is not known. With some exploratory data analysis, you determine that the dependency of the logit on some variables is nonlinear. Therefore, you decide to use splines to model this nonlinear dependence. Also, you want to use stepwise regression to remove unimportant variable transformations. The following statements perform the task:

```
proc logistic data=SimuData;
 effect splines = spline(x1-x&nVars/separate);
 model y = splines/selection=stepwise;
 store sasuser.SimuModel;
run;
```

By default, PROC LOGISTIC models the probability that  $y = 0$ . The EFFECT statement requests an effect named splines constructed by all predictors in the data. The SEPARATE option specifies that the spline



basis for each variable be treated as a separate set so that model selection applies to each individual set. The `SELECTION=STEPWISE` specifies the stepwise regression as the model selection technique. The `STORE` statement requests that the fitted model be saved to an item store `sasuser.SimuModel`. See “[Example 69.2: Working with Item Stores](#)” on page 5838 for an example with more details about working with item stores.

The spline effect for each predictor produces seven columns in the design matrix, making stepwise regression computationally intensive. For example, a typical Pentium 4 workstation takes around ten minutes to run the preceding statements. Real data sets for classification can be much larger. See examples at UCI Machine Learning Repository (Asuncion and Newman 2007). If new observations about which you want to make predictions are available at model fitting time, you can add the `SCORE` statement in the `LOGISTIC` procedure. Consider the case in which observations to predict become available after fitting the model. With `PROC PLM`, you do not have to repeat the computationally intensive model-fitting processes multiple times. You can use the `SCORE` statement in the `PLM` procedure to score new observations based on the item store `sasuser.SimuModel` that was created during the initial model building. For example, to compute the probability of  $y = 0$  for one new observation with all predictor values equal to 0.15 in the data set `test`, you can use the following statements:

```
data test;
 array x{&nVars};
 do j=1 to &nVars;
 x{j}=0.15;
 end;
 drop j;
 output;
run;

proc plm restore=sasuser.SimuModel;
 score data=test out=testout predicted / ilink;
run;
```

The `ILINK` option in the `SCORE` statement requests that predicted values be inversely transformed to the response scale. In this case, it is the predicted probability of  $y = 0$ . [Output 69.1.1](#) shows the predicted probability for the new observation.

**Output 69.1.1** Predicted Probability for One New Observation

| Obs | Predicted |
|-----|-----------|
| 1   | 0.56649   |

---

## Example 69.2: Working with Item Stores

This example demonstrates how procedures save statistical analysis context and results into item stores and how you can use `PROC PLM` to make post hoc inference based on saved item stores. The data are taken from McCullagh and Nelder (1989) and concern the effects on taste of various cheese additives. Four cheese additives were tested, and 52 response ratings for each additive were obtained. The response was measured on a scale of nine categories that range from strong dislike (1) to excellent taste (9). The following program

saves the data in the data set Cheese. The variable *y* contains the taste rating, the variable *Additive* contains cheese additive types, and the variable *freq* contains the frequencies with which each additive received each rating.

```
data Cheese;
 do Additive = 1 to 4;
 do y = 1 to 9;
 input freq @@;
 output;
 end;
 end;
 label y='Taste Rating';
 datalines;
0 0 1 7 8 8 19 8 1
6 9 12 11 7 6 1 0 0
1 1 6 8 23 7 5 1 0
0 0 0 1 3 7 14 16 11
;
```

The response *y* is a categorical variable that contains nine ordered levels. You can use PROC LOGISTIC to fit an ordinal model to investigate the effects of the cheese additive types on taste ratings. Suppose you also want to save the ordinal model into an item store so that you can make statistical inference later. You can use the following statements to perform the tasks:

```
proc logistic data=cheese;
 freq freq;
 class additive y / param=glm;
 model y=additive;
 store sasuser.cheese;
 title 'Ordinal Model on Cheese Additives';
run;
```

By default, PROC LOGISTIC uses the cumulative logit model for the ordered categorical response. The STORE statement saves the fitted model to a SAS item store named *sasuser.cheese*. The name is a two-level SAS name of the form *libname.membername*. If *libname* is not specified in the STORE statement, the fitted results are saved in *work.membername* and the item store is deleted after the current SAS session ends. With this example, the fitted model is saved to an item store named *sasuser.cheese* in the *Sasuser* library. It is not deleted after the current SAS session ends. You can use PROC PLM to restore the results later.

The following statements use PROC PLM to load the saved model context and results by specifying RESTORE= with the target item store *sasuser.cheese*. Then they use two SHOW statements to display separate information saved in the item store. The first SHOW statement with the PROGRAM option displays the program that was used to generate the item store *sasuser.cheese*. The second SHOW statement with the PARMS option displays parameter estimates and associated statistics of the fitted ordinal model.

```
proc plm restore=sasuser.cheese;
 show program;
 show parms;
run;
```

Output 69.2.1 displays the program that generated the item store *sasuser.cheese*. Except for the title information, it matches the original program.

**Output 69.2.1** Program Information from sasuser.cheese

```

Ordinal Model on Cheese Additives

The PLM Procedure

SAS Program Information

proc logistic data=cheese;
 freq freq;
 class additive y / param=glm;
 model y=additive;
 store sasuser.cheese;
run;

```

Output 69.2.2 displays estimates of the intercept terms and covariates and associated statistics. The intercept terms correspond to eight cumulative logits defined on taste ratings; that is, the  $i$ th intercept for  $i$ th logit is

$$\log\left(\frac{\sum_{j \leq i} p_j}{1 - \sum_{j \leq i} p_j}\right)$$

**Output 69.2.2** Parameter Estimates of the Ordinal Model

| Parameter Estimates |              |          |                |
|---------------------|--------------|----------|----------------|
| Parameter           | Taste Rating | Estimate | Standard Error |
| Intercept           | 1            | -7.0801  | 0.5624         |
| Intercept           | 2            | -6.0249  | 0.4755         |
| Intercept           | 3            | -4.9254  | 0.4272         |
| Intercept           | 4            | -3.8568  | 0.3902         |
| Intercept           | 5            | -2.5205  | 0.3431         |
| Intercept           | 6            | -1.5685  | 0.3086         |
| Intercept           | 7            | -0.06688 | 0.2658         |
| Intercept           | 8            | 1.4930   | 0.3310         |
| Additive 1          |              | 1.6128   | 0.3778         |
| Additive 2          |              | 4.9645   | 0.4741         |
| Additive 3          |              | 3.3227   | 0.4251         |
| Additive 4          |              | 0        | .              |

You can perform various statistical inference tasks from a saved item store, as long as the task is applicable under the model context. For example, you can perform group comparisons between different cheese additive types. See the next example for details.

---

### Example 69.3: Group Comparisons in an Ordinal Model

This example continues the study of the effects on taste of various cheese additives. You have finished fitting an ordinal logistic model and saved it to an item store named `sasuser.cheese` in the previous example. Suppose you want to make comparisons between any pair of cheese additives. You can conduct the analysis by using the ESTIMATE statement and constructing an appropriate L matrix, or by using the LSMEANS statement to compute least squares means differences. For an ordinal logistic model with the cumulative logit link, the least squares means are predicted population margins of the cumulative logits. The following statements compute and display differences between least squares means of cheese additive:

```
ods graphics on;
proc plm restore=sasuser.cheese;
 lsmeans additive / cl diff oddsratio plot=diff;
run;
ods graphics off;
```

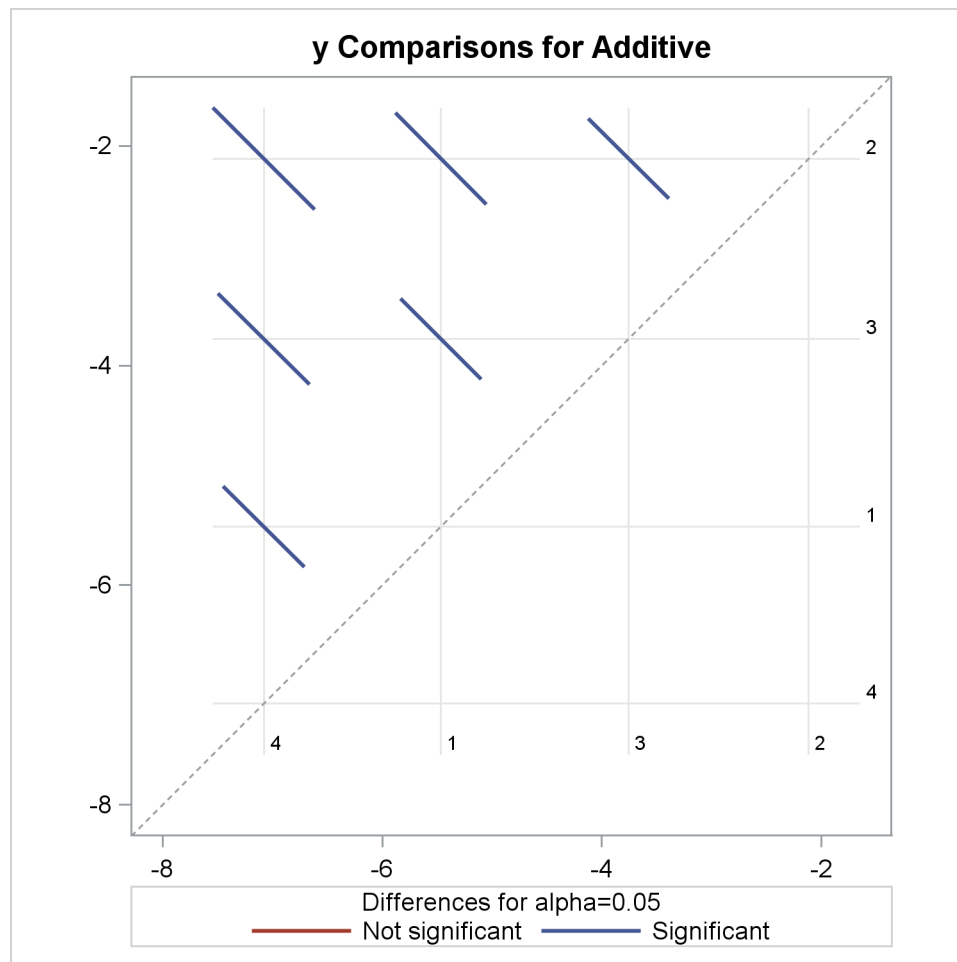
The LSMEANS statement contains four options. The DIFF option requests least squares means differences for cheese additives. Since the fitted model is an ordinal logistic model with the cumulative logit link, the least squares means differences represent log cumulative odds ratios. The ODDSRATIO option requests exponentiation of the LS-means differences which produces cumulative odds ratios. The CL option constructs confidence limits for the LS-means differences. When ODS Graphics is enabled, the PLOTS=DIFF option requests a display of all pairwise least squares means differences and their significance.

Output 69.3.1 displays the LS-means differences. The reported log odds ratios indicate the relative difference among the cheese additives. A negative log odds ratio indicates that the first category (displayed in the Additive column) having a lower taste rating is less likely than the second category (displayed in the \_Additive column) having a lower taste rating. For example, the log odds ratio between cheese additive 1 and 2 is  $-3.3517$  and the corresponding odds ratio is  $0.035$ . This means the odds of cheese additive 1 receiving a poor rating is  $0.035$  times the odds of cheese additive 2 receiving a poor rating. In addition to the highly significant  $p$ -value ( $< 0.0001$ ), the confidence limits for both the log odds ratio and the odds ratio indicate that you can reject the null hypothesis that the odds of cheese additive 1 having a lower taste rating is the same as that of cheese additive 2 having a lower rating. Similarly, the odds of cheese additive 2 having a lower rating is  $143.241$  (with 95% confidence limits  $(56.558, 362.777)$ ) times the odds of cheese additive 4 having a lower rating. With the same logic, you can conclude that the preference order for the four cheese types from the most favorable to the least favorable is: 4, 1, 3 and 2.

**Output 69.3.1** LS-Means Differences of Additive

| Ordinal Model on Cheese Additives           |           |          |                |            |                                       |                                       |
|---------------------------------------------|-----------|----------|----------------|------------|---------------------------------------|---------------------------------------|
| The PLM Procedure                           |           |          |                |            |                                       |                                       |
| Differences of Additive Least Squares Means |           |          |                |            |                                       |                                       |
| Additive                                    | _Additive | Estimate | Standard Error | z Value    | Pr >  z                               | Alpha                                 |
| 1                                           | 2         | -3.3517  | 0.4235         | -7.91      | <.0001                                | 0.05                                  |
| 1                                           | 3         | -1.7098  | 0.3731         | -4.58      | <.0001                                | 0.05                                  |
| 1                                           | 4         | 1.6128   | 0.3778         | 4.27       | <.0001                                | 0.05                                  |
| 2                                           | 3         | 1.6419   | 0.3738         | 4.39       | <.0001                                | 0.05                                  |
| 2                                           | 4         | 4.9645   | 0.4741         | 10.47      | <.0001                                | 0.05                                  |
| 3                                           | 4         | 3.3227   | 0.4251         | 7.82       | <.0001                                | 0.05                                  |
| Differences of Additive Least Squares Means |           |          |                |            |                                       |                                       |
| Additive                                    | _Additive | Lower    | Upper          | Odds Ratio | Lower Confidence Limit for Odds Ratio | Upper Confidence Limit for Odds Ratio |
| 1                                           | 2         | -4.1818  | -2.5216        | 0.035      | 0.015                                 | 0.080                                 |
| 1                                           | 3         | -2.4410  | -0.9787        | 0.181      | 0.087                                 | 0.376                                 |
| 1                                           | 4         | 0.8724   | 2.3532         | 5.017      | 2.393                                 | 10.520                                |
| 2                                           | 3         | 0.9092   | 2.3746         | 5.165      | 2.482                                 | 10.746                                |
| 2                                           | 4         | 4.0353   | 5.8938         | 143.241    | 56.558                                | 362.777                               |
| 3                                           | 4         | 2.4895   | 4.1558         | 27.734     | 12.055                                | 63.805                                |

Output 69.3.2 displays the DiffPlot. This shows that all pairs of LS-means differences, equivalent to log odds ratios in this case, are significant at the level of  $\alpha = 0.05$ . This means that the preference between any pair of the four cheese additive types are statistically significantly different.

**Output 69.3.2** LS-Means Plot of Pairwise Differences

## Example 69.4: Posterior Inference for Binomial Data

This example demonstrates how you can use PROC PLM to perform posterior inference from a Bayesian analysis. The data for this example are taken from Weisberg (1985) and concern the effect of small electrical currents on farm animals. The ultimate goal of the experiment was to understand the effects of high-voltage power lines on livestock and to better protect farm animals. Seven cows and six shock intensities were used in two experiments. In one experiment, each cow was given 30 electrical shocks with five at each shock intensity in random order. The number of shock responses was recorded for each cow at each shock level. The experiment was then repeated to investigate whether the response diminished due to fatigue of cows, or due to learning. So each cow received a total of 60 shocks. For the following analysis, the cow difference is ignored. The following DATA step lists the data where the variable `current` represents the shock level, the variable `response` represents the number of shock responses, the variable `trial` represents the total number of trials at each shock level, and the variable `experiment` represents the experiment number (1 for the initial experiment and 2 for the repeated one):

```

data cow;
 input current response trial experiment;
 datalines;
0 0 35 1
0 0 35 2
1 6 35 1
1 3 35 2
2 13 35 1
2 8 35 2
3 26 35 1
3 21 35 2
4 33 35 1
4 27 35 2
5 34 35 1
5 29 35 2
;

```

Suppose you are interested in modeling the distribution of the shock response based on the level of the current and the experiment number. You can use the GENMOD procedure to fit a frequentist logistic model for the data. However, if you have some prior information about parameter estimates, you can fit a Bayesian logistic regression model to take this prior information into account. In this case, suppose you believe the logit of response has a positive association with the shock level but you are uncertain about the ranges of other regression coefficients. To incorporate this prior information in the regression model, you can use the following statements:

```

data prior;
 input _type_$ current;
 datalines;
mean 100
var 50
;

proc genmod data=cow;
 class experiment;
 bayes coeffprior=normal(input=prior) seed=1;
 model response/trial = current|experiment / dist=binomial;
 store cowgmd;
 title 'Bayesian Logistic Model on Cow';
run;

```

The DATA step creates a data set prior that specifies the prior distribution for the variable current, which in this case is a normal distribution with mean 100 and variance 50. This reflects a rough belief in a positive coefficient in a moderate range for current. The prior distribution parameters are not specified for experiment and the interaction between experiment and current, and so PROC GENMOD assigns a default prior for them, which is a normal distribution with mean 0 and variance 1E6.

The BAYES statement in PROC GENMOD specifies that the regression coefficients follow a normal distribution with mean and variance specified in the input data set named prior. It also specifies 1 as the seed for the random number generator in the simulation of the posterior sample. The MODEL statement requests a logistic regression model with a logit link. The STORE statement requests that the fitted results be saved into an item store named cowgmd.

The convergence diagnostics in the output of PROC GENMOD indicate that the Markov chain has converged. [Output 69.4.1](#) displays summaries on the posterior sample of the regression coefficients. The posterior mean for the intercept is  $-3.5857$  with a 95% HPD interval  $(-4.5226, -2.6303)$ . The posterior mean of the coefficient for current is  $1.1893$  with a 95% HPD interval  $(0.8950, 1.4946)$ , which indicates a positive association between the logit of response and the shock level. Further investigation about whether shock reaction was different between two experiment is warranted.

**Output 69.4.1** Posterior Summaries on the Bayesian Logistic Model

| Bayesian Logistic Model on Cow |       |         |                       |             |         |         |
|--------------------------------|-------|---------|-----------------------|-------------|---------|---------|
| The GENMOD Procedure           |       |         |                       |             |         |         |
| Bayesian Analysis              |       |         |                       |             |         |         |
| Posterior Summaries            |       |         |                       |             |         |         |
| Parameter                      | N     | Mean    | Standard<br>Deviation | Percentiles |         |         |
|                                |       |         |                       | 25%         | 50%     | 75%     |
| Intercept                      | 10000 | -3.6047 | 0.4906                | -3.9281     | -3.5842 | -3.2679 |
| current                        | 10000 | 1.1966  | 0.1561                | 1.0873      | 1.1927  | 1.2996  |
| experiment1                    | 10000 | 0.0350  | 0.7014                | -0.4206     | 0.0347  | 0.4987  |
| experiment1current             | 10000 | 0.3574  | 0.2503                | 0.1906      | 0.3520  | 0.5235  |

| Posterior Intervals |       |                     |         |              |         |
|---------------------|-------|---------------------|---------|--------------|---------|
| Parameter           | Alpha | Equal-Tail Interval |         | HPD Interval |         |
| Intercept           | 0.050 | -4.6233             | -2.7074 | -4.5611      | -2.6581 |
| current             | 0.050 | 0.9073              | 1.5152  | 0.9028       | 1.5064  |
| experiment1         | 0.050 | -1.3651             | 1.4004  | -1.2995      | 1.4370  |
| experiment1current  | 0.050 | -0.1293             | 0.8580  | -0.1287      | 0.8580  |

Bayesian model fitting typically involves a large amount of simulation. Using the item store and PROC PLM, you do not need to refit the model to perform further posterior inference. Suppose you want to determine whether the shock reaction for the current level is different between the two experiments. You can use PROC PLM with the ESTIMATE statement in the following statements:

```
proc plm restore=cowgmd;
 estimate
 'Diff at current 0' experiment 1 -1 current*experiment [1, 0 1] [-1, 0 2],
 'Diff at current 1' experiment 1 -1 current*experiment [1, 1 1] [-1, 1 2],
 'Diff at current 2' experiment 1 -1 current*experiment [1, 2 1] [-1, 2 2],
 'Diff at current 3' experiment 1 -1 current*experiment [1, 3 1] [-1, 3 2],
 'Diff at current 4' experiment 1 -1 current*experiment [1, 4 1] [-1, 4 2],
 'Diff at current 5' experiment 1 -1 current*experiment [1, 5 1] [-1, 5 2]
 / exp cl;
run;
```

Each line in the ESTIMATE statement compares the fits between the two groups at each current level. The nonpositional syntax is used for the interaction effect current\*experiment. For example, the first line requests coefficient 1 for the interaction effect at current level 0 for the initial experiment, and coefficient



-1 for the effect at current level 0 for the repeated experiment. The two terms are then added to derive the difference. For more details about the nonpositional syntax, see “Positional and Nonpositional Syntax for Coefficients in Linear Functions” on page 448 of Chapter 19, “Shared Concepts and Topics.”

The EXP option exponentiates log odds ratios to produce odds ratios. The CL option requests that confidence limits be constructed for both log odds ratios and odds ratios. Output 69.4.2 lists the posterior sample estimates for differences between experiments at different current levels.

**Output 69.4.2** Comparisons between Experiments at Different Current Levels

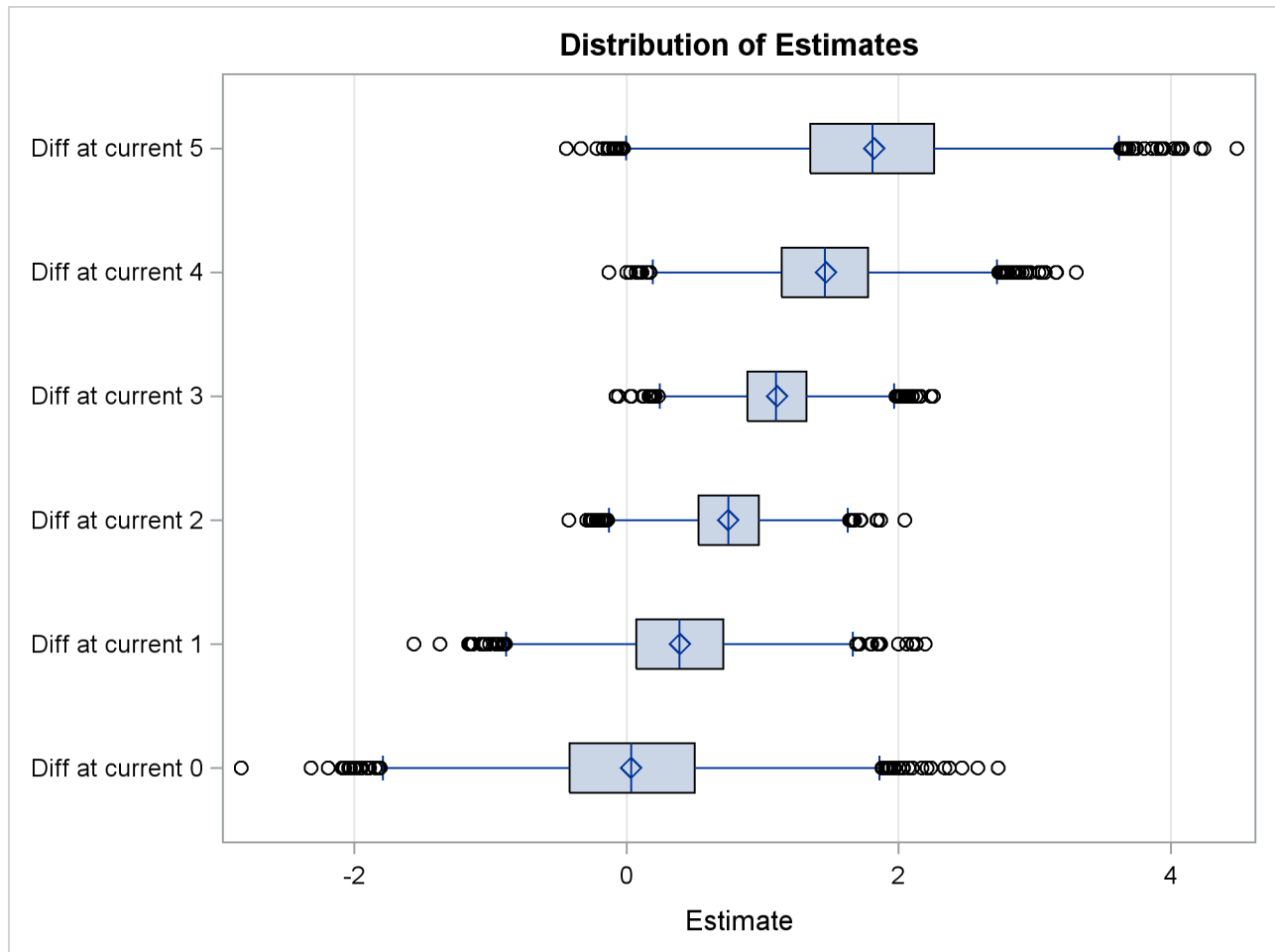
| Bayesian Logistic Model on Cow |                                         |           |                    |                            |                                     |        |
|--------------------------------|-----------------------------------------|-----------|--------------------|----------------------------|-------------------------------------|--------|
| The PLM Procedure              |                                         |           |                    |                            |                                     |        |
| Sample Estimates               |                                         |           |                    |                            |                                     |        |
| Label                          | N                                       | Estimate  | Standard Deviation | -----Percentiles-----      |                                     |        |
|                                |                                         |           |                    | 25th                       | 50th                                | 75th   |
| Diff at current 0              | 10000                                   | 0.03500   | 0.7014             | -0.4206                    | 0.0347                              | 0.4987 |
| Diff at current 1              | 10000                                   | 0.3924    | 0.4865             | 0.0700                     | 0.3884                              | 0.7096 |
| Diff at current 2              | 10000                                   | 0.7498    | 0.3266             | 0.5283                     | 0.7468                              | 0.9719 |
| Diff at current 3              | 10000                                   | 1.1072    | 0.3194             | 0.8901                     | 1.1001                              | 1.3220 |
| Diff at current 4              | 10000                                   | 1.4646    | 0.4718             | 1.1387                     | 1.4559                              | 1.7756 |
| Diff at current 5              | 10000                                   | 1.8219    | 0.6844             | 1.3508                     | 1.8079                              | 2.2601 |
| Sample Estimates               |                                         |           |                    |                            |                                     |        |
| Label                          | Alpha                                   | Lower HPD | Upper HPD          | Exponentiated              | Standard Deviation of Exponentiated |        |
| Diff at current 0              | 0.05                                    | -1.2995   | 1.4370             | 1.3258                     | 1.080632                            |        |
| Diff at current 1              | 0.05                                    | -0.5287   | 1.3599             | 1.6672                     | 0.873185                            |        |
| Diff at current 2              | 0.05                                    | 0.1300    | 1.3827             | 2.2328                     | 0.753450                            |        |
| Diff at current 3              | 0.05                                    | 0.4772    | 1.7182             | 3.1863                     | 1.068673                            |        |
| Diff at current 4              | 0.05                                    | 0.5369    | 2.3694             | 4.8511                     | 2.562732                            |        |
| Diff at current 5              | 0.05                                    | 0.4881    | 3.1505             | 7.8941                     | 6.668085                            |        |
| Sample Estimates               |                                         |           |                    |                            |                                     |        |
| Label                          | -----Percentiles for Exponentiated----- |           |                    | Lower HPD of Exponentiated | Upper HPD of Exponentiated          |        |
|                                | 25th                                    | 50th      | 75th               |                            |                                     |        |
| Diff at current 0              | 0.6566                                  | 1.0353    | 1.6466             | 0.1263                     | 3.3077                              |        |
| Diff at current 1              | 1.0725                                  | 1.4746    | 2.0331             | 0.3809                     | 3.3011                              |        |
| Diff at current 2              | 1.6961                                  | 2.1101    | 2.6429             | 1.0081                     | 3.7135                              |        |
| Diff at current 3              | 2.4353                                  | 3.0045    | 3.7509             | 1.3990                     | 5.1655                              |        |
| Diff at current 4              | 3.1227                                  | 4.2885    | 5.9040             | 1.3083                     | 9.6902                              |        |
| Diff at current 5              | 3.8606                                  | 6.0976    | 9.5838             | 0.9081                     | 19.4638                             |        |

The sample statistics are constructed from the posterior sample saved in the item store `cowgmd`. From the output, the odds of a cow showing shock reaction at level 0 in the initial experiment is 1.2811 (with a 95% HPD interval (0.07387, 3.1001)) times the odds in the repeated experiment. The HPD interval for the odds ratio is constructed based on the mean and variance of the sample of the exponentiated log odds ratios, instead of based on the exponentiated mean and variance of the posterior sample of log odds ratios. The HPD interval suggests that there is not much evidence that the cows responded differently at current level 0 between the two experiments. Similar conclusions can be drawn for current level 1, 2, and 5. However, there is strong evidence that cows responded differently at current level 3 and 4 between the two experiments. The possible explanation is that, if the current level is so small that cows could hardly feel it or the current level is so strong that cows could hardly bear it, cows would respond consistently in the two experiment. If the current level is moderate, cows might get used to it and their response diminished in the repeated experiment.

You can visualize the distribution of the posterior sample of log odds ratios by specifying the `PLOTS=` option in the `ESTIMATE` statement. In the following statements, ODS Graphics is enabled by the `ODS GRAPHICS ON` statement, the `PLOTS=BOXPLOT` option requests a box plot of posterior distribution of log odds ratios. The suboption `ORIENT=HORIZONTAL` specifies a horizontal orientation of the boxes.

```
ods graphics on;
proc plm restore=cowgmd;
 estimate
 'Diff at current 0' experiment 1 -1 current*experiment [1, 0 1] [-1, 0 2],
 'Diff at current 1' experiment 1 -1 current*experiment [1, 1 1] [-1, 1 2],
 'Diff at current 2' experiment 1 -1 current*experiment [1, 2 1] [-1, 2 2],
 'Diff at current 3' experiment 1 -1 current*experiment [1, 3 1] [-1, 3 2],
 'Diff at current 4' experiment 1 -1 current*experiment [1, 4 1] [-1, 4 2],
 'Diff at current 5' experiment 1 -1 current*experiment [1, 5 1] [-1, 5 2]
 / plots=boxplot(orient=horizontal);
run;
ods graphics off;
```

Output 69.4.3 displays the box plot of the posterior sample of log odds ratios. The two boxes for differences at current level 3 and 4 show that the corresponding log odds ratios are significantly larger than the reference value  $x = 0$ . This indicate that there is obvious evidence that the probability of cow response is larger in the initial experiment than in the repeated one at the two current levels. The other four boxes show that the corresponding log odds ratios are not significantly different from 0, which suggests that there is no obvious reaction difference at current level 0, 1, 2, and 5 between the two experiments.

**Output 69.4.3** Box Plot of Difference between Two Experiments

### Example 69.5: BY-Group Processing

This example uses a data set on a study of the analgesic effects of treatments on elderly patients with neuralgia. The purpose of this example is to show how PROC PLM behaves under different situations when BY-group processing is present. Two test treatments and a placebo are compared to test whether the patient reported pain or not. For each patient, the information of age, gender, and the duration of complaint before the treatment began were recorded. The following DATA step creates the data set named Neuralgia:

```

Data Neuralgia;
 input Treatment $ Sex $ Age Duration Pain $ @@;
 datalines;
P F 68 1 No B M 74 16 No P F 67 30 No
P M 66 26 Yes B F 67 28 No B F 77 16 No
A F 71 12 No B F 72 50 No B F 76 9 Yes
A M 71 17 Yes A F 63 27 No A F 69 18 Yes
B F 66 12 No A M 62 42 No P F 64 1 Yes
A F 64 17 No P M 74 4 No A F 72 25 No
P M 70 1 Yes B M 66 19 No B M 59 29 No
A F 64 30 No A M 70 28 No A M 69 1 No

```

```

B F 78 1 No P M 83 1 Yes B F 69 42 No
B M 75 30 Yes P M 77 29 Yes P F 79 20 Yes
A M 70 12 No A F 69 12 No B F 65 14 No
B M 70 1 No B M 67 23 No A M 76 25 Yes
P M 78 12 Yes B M 77 1 Yes B F 69 24 No
P M 66 4 Yes P F 65 29 No P M 60 26 Yes
A M 78 15 Yes B M 75 21 Yes A F 67 11 No
P F 72 27 No P F 70 13 Yes A M 75 6 Yes
B F 65 7 No P F 68 27 Yes P M 68 11 Yes
P M 67 17 Yes B M 70 22 No A M 65 15 No
P F 67 1 Yes A M 67 10 No P F 72 11 Yes
A F 74 1 No B M 80 21 Yes A F 69 3 No
;

```

The data set contains five variables. Treatment is a classification variable that has three levels: A and B represent the two test treatments, and P represents the placebo treatment. Sex is a classification variable that indicates each patient's gender. Age is a continuous variable that indicates the age in years of each patient when a treatment began. Duration is a continuous variable that indicates the duration of complaint in months. The last variable Pain is the response variable with two levels: 'Yes' if pain was reported, 'No' if no pain was reported.

Suppose there is some preliminary belief that the dependency of pain on the explanatory variables is different for male and female patients, leading to separate models between genders. You believe there might be redundant information for predicting the probability of Pain. Thus, you want to perform model selection to eliminate unnecessary effects. You can use the following statements:

```

proc sort data=Neuralgia;
 by sex;
run;

proc logistic data=Neuralgia;
 class Treatment / param=glm;
 model pain = Treatment Age Duration / selection=backward;
 by sex;
 store painmodel;
 title 'Logistic Model on Neuralgia';
run;

```

PROC SORT is called to sort the data by variable Sex. The LOGISTIC procedure is then called to fit the probability of no pain. Three variables are specified for the full model: Treatment, Age, and Duration. Backward elimination is used as the model selection method. The BY statement fits separate models for male and female patients. Finally, the STORE statement specifies that the fitted results be saved to an item store named painmodel.

Output 69.5.1 lists parameter estimates from the two models after backward elimination is performed. From the model for female patients, Treatment is the only factor that affects the probability of no pain, and Treatment A and B have the same positive effect in predicting the probability of no pain. From the model for male patients, both Treatment and Age are included in the selected model. Treatment A and B have different positive effects, while Age has a negative effect in predicting the probability of no pain.

**Output 69.5.1** Parameter Estimates for Male and Female Patients

| Logistic Model on Neuralgia              |    |          |                |                 |            |
|------------------------------------------|----|----------|----------------|-----------------|------------|
| ----- Sex=F -----                        |    |          |                |                 |            |
| The LOGISTIC Procedure                   |    |          |                |                 |            |
| Analysis of Maximum Likelihood Estimates |    |          |                |                 |            |
| Parameter                                | DF | Estimate | Standard Error | Wald Chi-Square | Pr > ChiSq |
| Intercept                                | 1  | -0.4055  | 0.6455         | 0.3946          | 0.5299     |
| Treatment A                              | 1  | 2.6027   | 1.2360         | 4.4339          | 0.0352     |
| Treatment B                              | 1  | 2.6027   | 1.2360         | 4.4339          | 0.0352     |
| Treatment P                              | 0  | 0        | .              | .               | .          |
| ----- Sex=M -----                        |    |          |                |                 |            |
| Analysis of Maximum Likelihood Estimates |    |          |                |                 |            |
| Parameter                                | DF | Estimate | Standard Error | Wald Chi-Square | Pr > ChiSq |
| Intercept                                | 1  | 20.6178  | 9.1638         | 5.0621          | 0.0245     |
| Treatment A                              | 1  | 3.9982   | 1.7333         | 5.3208          | 0.0211     |
| Treatment B                              | 1  | 4.5556   | 1.9252         | 5.5993          | 0.0180     |
| Treatment P                              | 0  | 0        | .              | .               | .          |
| Age                                      | 1  | -0.3416  | 0.1408         | 5.8869          | 0.0153     |

Now the fitted models are saved to the item store `painmodel`. Suppose you want to use it to score several new observations. The following DATA steps create three data sets for scoring:

```
data score1;
 input Treatment $ Sex $ Age;
 datalines;
A F 20
B F 30
P F 40
A M 20
B M 30
P M 40
;

data score2;
 set score1(drop=sex);
run;

data score3;
 set score2(drop=Age);
run;
```

The first score data set `score1` contains six observations and all the variables that are specified in the full model. The second score data set `score2` is a duplicate of `score1` except that `Sex` is dropped. The third score data set `score3` is a duplicate of `score2` except that `Age` is dropped. You can use the following statements to score the three data sets:

```
proc plm restore=painmodel;
 score data=score1 out=score1out predicted;
 score data=score2 out=score2out predicted;
 score data=score3 out=score3out predicted;
run;
```

Output 69.5.2 lists the store information that PROC PLM reads from the item store `painmodel`. The “Model Effects” entry lists all three variables that are specified in the full model before the BY-group processing.

**Output 69.5.2** Item Store Information for `painmodel`

| Logistic Model on Neuralgia |                                  |
|-----------------------------|----------------------------------|
| The PLM Procedure           |                                  |
| Store Information           |                                  |
| Item Store                  | WORK.PAINMODEL                   |
| Data Set Created From       | WORK.NEURALGIA                   |
| Created By                  | PROC LOGISTIC                    |
| Date Created                | 13JUN12:12:38:48                 |
| By Variable                 | Sex                              |
| Response Variable           | Pain                             |
| Link Function               | Logit                            |
| Distribution                | Binary                           |
| Class Variables             | Treatment Pain                   |
| Model Effects               | Intercept Treatment Age Duration |

With the three SCORE statements, three data sets are thus produced: `score1out`, `score2out`, and `score3out`. They contain the linear predictors in addition to all original variables. The data set `score1out` contains the values shown in Output 69.5.3.

**Output 69.5.3** Values of Data Set `score1out`

| Logistic Model on Neuralgia |           |     |     |           |
|-----------------------------|-----------|-----|-----|-----------|
| Obs                         | Treatment | Sex | Age | Predicted |
| 1                           | A         | F   | 20  | 2.1972    |
| 2                           | B         | F   | 30  | 2.1972    |
| 3                           | P         | F   | 40  | -0.4055   |
| 4                           | A         | M   | 20  | 17.7850   |
| 5                           | B         | M   | 30  | 14.9269   |
| 6                           | P         | M   | 40  | 6.9557    |

Linear predictors are computed for all six observations. Because the BY variable Sex is available in score1, PROC PLM uses separate models to score observations of male and female patients. So an observation with the same Treatment and Age has different linear predictors for different genders.

The data set score2out contains the values shown in [Output 69.5.4](#).

**Output 69.5.4** Values of Data Set score2out

| Logistic Model on Neuralgia |     |           |     |           |
|-----------------------------|-----|-----------|-----|-----------|
| Obs                         | Sex | Treatment | Age | Predicted |
| 1                           | F   | A         | 20  | 2.1972    |
| 2                           | F   | B         | 30  | 2.1972    |
| 3                           | F   | P         | 40  | -0.4055   |
| 4                           | F   | A         | 20  | 2.1972    |
| 5                           | F   | B         | 30  | 2.1972    |
| 6                           | F   | P         | 40  | -0.4055   |
| 7                           | M   | A         | 20  | 17.7850   |
| 8                           | M   | B         | 30  | 14.9269   |
| 9                           | M   | P         | 40  | 6.9557    |
| 10                          | M   | A         | 20  | 17.7850   |
| 11                          | M   | B         | 30  | 14.9269   |
| 12                          | M   | P         | 40  | 6.9557    |

The second score data set score2 does not contain the BY variable Sex. PROC PLM continues to score the full data set two times. Each time the scoring is based on the fitted model for each corresponding BY-group. In the output data set, Sex is added at the first column as the BY-group indicator. The first six entries correspond to the model for female patients, and the next six entries correspond to the model for male patients. Age is not included in the first model, and Treatment A and B have the same parameter estimates, so observations 1, 2, 4, and 5 have the same linear predicted value.

The data set score3out contains the values shown in [Output 69.5.5](#).

**Output 69.5.5** Values of Data Set score3out

| Logistic Model on Neuralgia |     |           |           |
|-----------------------------|-----|-----------|-----------|
| Obs                         | Sex | Treatment | Predicted |
| 1                           | F   | A         | 2.19722   |
| 2                           | F   | B         | 2.19722   |
| 3                           | F   | P         | -0.40547  |
| 4                           | F   | A         | 2.19722   |
| 5                           | F   | B         | 2.19722   |
| 6                           | F   | P         | -0.40547  |
| 7                           | M   | A         | .         |
| 8                           | M   | B         | .         |
| 9                           | M   | P         | .         |
| 10                          | M   | A         | .         |
| 11                          | M   | B         | .         |
| 12                          | M   | P         | .         |

The third score data set `score3` does not contain the BY variable `Sex`. PROC PLM scores the full data twice with separate models. Furthermore, it does not contain the variable `Age`, which is a selected variable for predicting the probability of no pain for male patients. Thus, PROC PLM computes linear predictor values for `score3` by using the first model for female patients, and sets the linear predictor to missing when using the second model for male patients to score the data set.

## Example 69.6: Comparing Multiple B-Splines

This example conducts an analysis similar to Example 15 in Chapter 41.33, “Examples: GLIMMIX Procedure.” It uses simulated data to perform multiple comparisons among predicted values in a model with group-specific trends that are modeled through regression splines. The estimable functions are formed using nonpositional syntax with constructed effects. Consider the data in the following DATA step. Each of the 100 observations for the continuous response variable `y` is associated with one of two groups.

```
data spline;
 input group y @@;
 x = _n_;
 datalines;
1 -.020 1 0.199 2 -1.36 1 -.026
2 -.397 1 0.065 2 -.861 1 0.251
1 0.253 2 -.460 2 0.195 2 -.108
1 0.379 1 0.971 1 0.712 2 0.811
2 0.574 2 0.755 1 0.316 2 0.961
2 1.088 2 0.607 2 0.959 1 0.653
1 0.629 2 1.237 2 0.734 2 0.299
2 1.002 2 1.201 1 1.520 1 1.105
1 1.329 1 1.580 2 1.098 1 1.613
2 1.052 2 1.108 2 1.257 2 2.005
2 1.726 2 1.179 2 1.338 1 1.707
2 2.105 2 1.828 2 1.368 1 2.252
1 1.984 2 1.867 1 2.771 1 2.052
2 1.522 2 2.200 1 2.562 1 2.517
1 2.769 1 2.534 2 1.969 1 2.460
1 2.873 1 2.678 1 3.135 2 1.705
1 2.893 1 3.023 1 3.050 2 2.273
2 2.549 1 2.836 2 2.375 2 1.841
1 3.727 1 3.806 1 3.269 1 3.533
1 2.948 2 1.954 2 2.326 2 2.017
1 3.744 2 2.431 2 2.040 1 3.995
2 1.996 2 2.028 2 2.321 2 2.479
2 2.337 1 4.516 2 2.326 2 2.144
2 2.474 2 2.221 1 4.867 2 2.453
1 5.253 2 3.024 2 2.403 1 5.498
;
```

The following statements fit a model with separate trends for the two groups; the trends are modeled as B-splines.



```

proc orthoreg data=spline;
 class group;
 effect spl = spline(x);
 model y = group spl*group / noint;
 store ortho_spline;
 title 'B-splines Comparisons';
run;

```

Results from this analysis are shown in [Output 69.6.1](#). The “Parameter Estimates” table shows the estimates for the spline coefficients in the two groups.

**Output 69.6.1** Results for Group-Specific Spline Model

| B-splines Comparisons  |    |                    |                |         |         |
|------------------------|----|--------------------|----------------|---------|---------|
| The ORTHOREG Procedure |    |                    |                |         |         |
| Dependent Variable: y  |    |                    |                |         |         |
| Source                 | DF | Sum of Squares     | Mean Square    | F Value | Pr > F  |
| Model                  | 13 | 153.0175561        | 11.770581238   | 160.11  | <.0001  |
| Error                  | 86 | 6.3223804119       | 0.0735160513   |         |         |
| Corrected Total        | 99 | 159.33993651       |                |         |         |
|                        |    | Root MSE           | 0.2711384357   |         |         |
|                        |    | R-Square           | 0.9603214326   |         |         |
| Parameter              | DF | Parameter Estimate | Standard Error | t Value | Pr >  t |
| (group='1')            | 1  | 9.70265463962039   | 3.1341899987   | 3.10    | 0.0026  |
| (group='2')            | 1  | 6.30619220563569   | 2.6299147768   | 2.40    | 0.0187  |
| spl*group 1 1          | 1  | -11.1786451718041  | 3.7008097395   | -3.02   | 0.0033  |
| spl*group 1 2          | 1  | -20.1946092746139  | 3.9765046236   | -5.08   | <.0001  |
| spl*group 2 1          | 1  | -9.53273697995301  | 3.2575832048   | -2.93   | 0.0044  |
| spl*group 2 2          | 1  | -5.85652496534967  | 2.7906116773   | -2.10   | 0.0388  |
| spl*group 3 1          | 1  | -8.96118371893294  | 3.0717508806   | -2.92   | 0.0045  |
| spl*group 3 2          | 1  | -5.55671605245205  | 2.5716715573   | -2.16   | 0.0335  |
| spl*group 4 1          | 1  | -7.26153231478755  | 3.243690314    | -2.24   | 0.0278  |
| spl*group 4 2          | 1  | -4.36778889738236  | 2.7246809593   | -1.60   | 0.1126  |
| spl*group 5 1          | 1  | -6.44615256510896  | 2.9616955361   | -2.18   | 0.0323  |
| spl*group 5 2          | 1  | -4.03801618914902  | 2.4588839125   | -1.64   | 0.1042  |
| spl*group 6 1          | 1  | -4.63816959094139  | 3.7094636319   | -1.25   | 0.2146  |
| spl*group 6 2          | 1  | -4.30290104395061  | 3.0478540171   | -1.41   | 0.1616  |
| spl*group 7 1          | 0  | 0                  | .              | .       | .       |
| spl*group 7 2          | 0  | 0                  | .              | .       | .       |

By default, the ORTHOREG procedure constructs B-splines with seven knots. Since B-spline coefficients satisfy a sum-to-one constraint and since the model contains group-specific intercepts, the last spline coefficient for each group is redundant and is set to 0.

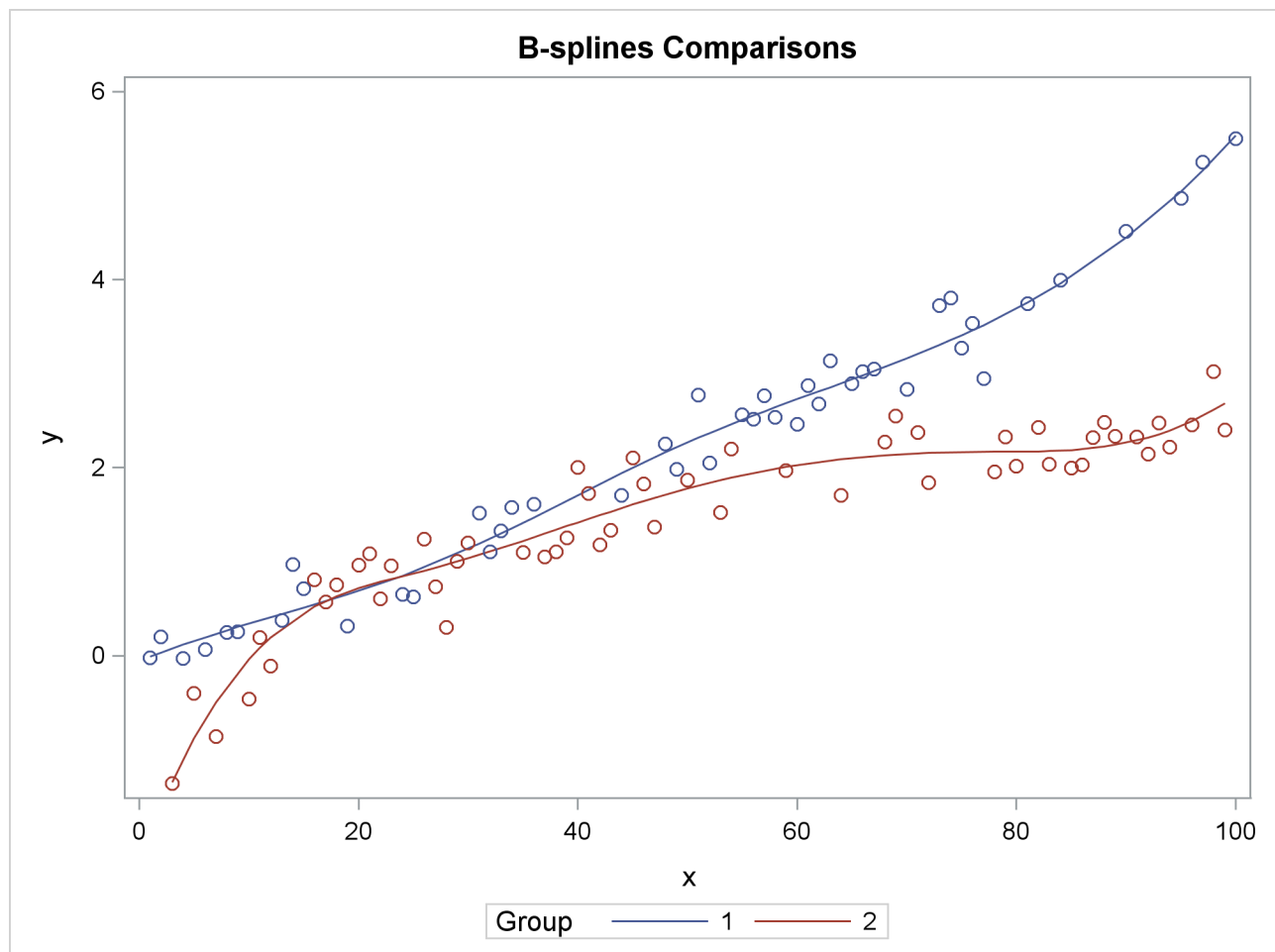
The following statements make a prediction for the input data set by using the SCORE statement with PROC PLM and graph the observed and predicted values in the two groups:

```
proc plm restore=ortho_spline;
 score data=spline out=ortho_pred predicted=p;
run;

proc sgplot data=ortho_pred;
 series y=p x=x / group=group name="fit";
 scatter y=y x=x / group=group;
 keylegend "fit" / title="Group";
run;
```

The prediction plot in [Output 69.6.2](#) suggests that there is some separation of the group trends for small values of  $x$  and for values that exceed about  $x = 40$ .

**Output 69.6.2** Observed Data and Predicted Values by Group



In order to determine the range on which the trends separate significantly, the PLM procedure is executed in the following statements with an [ESTIMATE](#) statement that applies group comparisons at a number of values for the spline variable  $x$ :

```

%macro GroupDiff;
 %do x=0 %to 75 %by 5;
 "Diff at x=&x" group 1 -1 group*spl [1,1 &x] [-1,2 &x],
 %end;
 'Diff at x=80' group 1 -1 group*spl [1,1 80] [-1,2 80]
%mend;

proc plm restore=ortho_spline;
 show effects;
 estimate %GroupDiff / adjust=simulate seed=1 stepdown;
run;

```

For example, the following ESTIMATE statement compares the trends between the two groups at  $x = 25$ :

```
estimate 'Diff at x=25' group 1 -1 group*spl [1,1 25] [-1,2 25];
```

The nonpositional syntax is used for the `group*spl` effect. For example, the specification `[-1, 2 25]` requests that the spline be computed at  $x = 25$  for the second level of variable `group`. The resulting coefficients are added to the  $L$  vector for the estimate after being multiplied with  $-1$ .

Because comparisons are made at a large number of values for  $x$ , a multiplicity correction is in order to adjust the  $p$ -values to reflect familywise error control. Simulated  $p$ -values with step-down adjustment are used here.

Output 69.6.3 displays the “Store Information” for the item store and information about the spline effect (the result of the `SHOW` statement).

**Output 69.6.3** Spline Details

| B-splines Comparisons |                   |
|-----------------------|-------------------|
| The PLM Procedure     |                   |
| Store Information     |                   |
| Item Store            | WORK.ORTHO_SPLINE |
| Data Set Created From | WORK.SPLINE       |
| Created By            | PROC ORTHOREG     |
| Date Created          | 13JUN12:12:38:57  |
| Response Variable     | y                 |
| Class Variable        | group             |
| Constructed Effect    | spl               |
| Model Effects         | group spl*group   |

**Output 69.6.3** *continued*

| B-splines Comparisons       |          |           |
|-----------------------------|----------|-----------|
| The PLM Procedure           |          |           |
| Knots for Spline Effect spl |          |           |
| Knot<br>Number              | Boundary | x         |
| 1                           | *        | -48.50000 |
| 2                           | *        | -23.75000 |
| 3                           | *        | 1.00000   |
| 4                           |          | 25.75000  |
| 5                           |          | 50.50000  |
| 6                           |          | 75.25000  |
| 7                           | *        | 100.00000 |
| 8                           | *        | 124.75000 |
| 9                           | *        | 149.50000 |

| B-splines Comparisons               |                    |                  |
|-------------------------------------|--------------------|------------------|
| The PLM Procedure                   |                    |                  |
| Basis Details for Spline Effect spl |                    |                  |
| Column                              | -----Support-----  | Support<br>Knots |
| 1                                   | -48.50000 25.75000 | 1-4              |
| 2                                   | -48.50000 50.50000 | 1-5              |
| 3                                   | -23.75000 75.25000 | 2-6              |
| 4                                   | 1.00000 100.00000  | 3-7              |
| 5                                   | 25.75000 124.75000 | 4-8              |
| 6                                   | 50.50000 149.50000 | 5-9              |
| 7                                   | 75.25000 149.50000 | 6-9              |

Output 69.6.4 displays the results from the `ESTIMATE` statement.

**Output 69.6.4** Estimate Results with Multiplicity Correction

| Estimates                                   |          |                |    |         |         |        |
|---------------------------------------------|----------|----------------|----|---------|---------|--------|
| Adjustment for Multiplicity: Holm-Simulated |          |                |    |         |         |        |
| Label                                       | Estimate | Standard Error | DF | t Value | Pr >  t | Adj P  |
| Diff at x=0                                 | 12.4124  | 4.2130         | 86 | 2.95    | 0.0041  | 0.0206 |
| Diff at x=5                                 | 1.0376   | 0.1759         | 86 | 5.90    | <.0001  | <.0001 |
| Diff at x=10                                | 0.3778   | 0.1540         | 86 | 2.45    | 0.0162  | 0.0545 |
| Diff at x=15                                | 0.05822  | 0.1481         | 86 | 0.39    | 0.6952  | 0.9101 |
| Diff at x=20                                | -0.02602 | 0.1243         | 86 | -0.21   | 0.8346  | 0.9565 |
| Diff at x=25                                | 0.02014  | 0.1312         | 86 | 0.15    | 0.8783  | 0.9565 |
| Diff at x=30                                | 0.1023   | 0.1378         | 86 | 0.74    | 0.4600  | 0.7418 |
| Diff at x=35                                | 0.1924   | 0.1236         | 86 | 1.56    | 0.1231  | 0.2925 |
| Diff at x=40                                | 0.2883   | 0.1114         | 86 | 2.59    | 0.0113  | 0.0450 |
| Diff at x=45                                | 0.3877   | 0.1195         | 86 | 3.24    | 0.0017  | 0.0096 |
| Diff at x=50                                | 0.4885   | 0.1308         | 86 | 3.74    | 0.0003  | 0.0024 |
| Diff at x=55                                | 0.5903   | 0.1231         | 86 | 4.79    | <.0001  | <.0001 |
| Diff at x=60                                | 0.7031   | 0.1125         | 86 | 6.25    | <.0001  | <.0001 |
| Diff at x=65                                | 0.8401   | 0.1203         | 86 | 6.99    | <.0001  | <.0001 |
| Diff at x=70                                | 1.0147   | 0.1348         | 86 | 7.52    | <.0001  | <.0001 |
| Diff at x=75                                | 1.2400   | 0.1326         | 86 | 9.35    | <.0001  | <.0001 |
| Diff at x=80                                | 1.5237   | 0.1281         | 86 | 11.89   | <.0001  | <.0001 |

Notice that the “Store Information” in [Output 69.6.3](#) displays the classification variables (from the CLASS statement in PROC ORTHOREG), the constructed effects (from the EFFECT statement in PROC ORTHOREG), and the model effects (from the MODEL statement in PROC ORTHOREG). [Output 69.6.4](#) shows that at the 5% significance level the trends are significantly different for  $x \leq 10$  and for  $x \geq 40$ . Between those values you cannot reject the hypothesis of trend congruity.

To see this effect more clearly, you can filter the results by adding the a filtering statement to the previous PROC PLM step:

```
proc plm restore=ortho_spline;
 estimate %GroupDiff / adjust=simulate seed=1 stepdown;
 filter adjp > 0.05;
run;
```

This produces [Output 69.6.5](#), which displays the subset of the results in [Output 69.6.4](#) that meets the condition in the `FILTER` expression.

**Output 69.6.5** Filtered Estimate Results

| B-splines Comparisons                       |          |                |    |         |         |        |
|---------------------------------------------|----------|----------------|----|---------|---------|--------|
| The PLM Procedure                           |          |                |    |         |         |        |
| Estimates                                   |          |                |    |         |         |        |
| Adjustment for Multiplicity: Holm-Simulated |          |                |    |         |         |        |
| Label                                       | Estimate | Standard Error | DF | t Value | Pr >  t | Adj P  |
| Diff at x=10                                | 0.3778   | 0.1540         | 86 | 2.45    | 0.0162  | 0.0545 |
| Diff at x=15                                | 0.05822  | 0.1481         | 86 | 0.39    | 0.6952  | 0.9101 |
| Diff at x=20                                | -0.02602 | 0.1243         | 86 | -0.21   | 0.8346  | 0.9565 |
| Diff at x=25                                | 0.02014  | 0.1312         | 86 | 0.15    | 0.8783  | 0.9565 |
| Diff at x=30                                | 0.1023   | 0.1378         | 86 | 0.74    | 0.4600  | 0.7418 |
| Diff at x=35                                | 0.1924   | 0.1236         | 86 | 1.56    | 0.1231  | 0.2925 |

## Example 69.7: Linear Inference with Arbitrary Estimates

Suppose that you have calculated a vector of parameter estimates of dimension  $(p \times 1)$  and its associated variance-covariance matrix by some statistical method. You might want to use these results to perform linear inference, or to score a data set and calculate predicted values and their standard errors.

The following DATA steps create two SAS data sets. The first, called `parms`, contains six estimates that represent two uncorrelated groups. The data set `cov` contains the covariance matrix of the estimates. The lack of correlation between the two sets of three parameters is evident in the block-diagonal structure of the covariance matrix.

```

data parms;
 length name $6;
 input Name$ Value;
 datalines;
alpha1 -3.5671
beta1 0.4421
gamma1 -2.6230
alpha2 -3.0111
beta2 0.3977
gamma2 -2.4442
;

data cov;
 input Parm row col1-col6;
 datalines;
1 1 0.007462 -0.005222 0.010234 0.000000 0.000000 0.000000
1 2 -0.005222 0.048197 -0.010590 0.000000 0.000000 0.000000
1 3 0.010234 -0.010590 0.215999 0.000000 0.000000 0.000000
1 4 0.000000 0.000000 0.000000 0.031261 -0.009096 0.015785
1 5 0.000000 0.000000 0.000000 -0.009096 0.039487 -0.019996
1 6 0.000000 0.000000 0.000000 0.015785 -0.019996 0.126172
;

```

Suppose that you are interested in testing whether the parameters are homogeneous across groups—that is, whether  $\alpha_1 = \alpha_2$ ,  $\beta_1 = \beta_2$ ,  $\gamma_1 = \gamma_2$ . You are interested in testing the hypothesis jointly and separately with multiplicity adjustment.

To use the PLM procedure, you first need to create an item store that contains the necessary information as if the preceding parameter vector and covariance matrix were the result of a statistical modeling procedure. The following statements use the GLIMMIX procedure to create such an item store, by fitting a saturated linear model with the data set that contains the parameter estimates serving as the input data set:

```

proc glimmix data=parms order=data;
 class Name;
 model Value = Name / noint ddfm=none s;
 random _residual_ / type=lin(1) ldata=cov v;
 parms (1) / noiter;
 store ArtificialModel;
 title 'Linear Inference';
run;

```

The RANDOM statement is used to form the covariance structure for the estimates. The PARMs statement prevents iterative updates of the covariance parameters. The resulting marginal covariance matrix of the “data” is thus identical to the covariance matrix in the data set cov. The ORDER=DATA option in the PROC GLIMMIX statement is used to arrange the levels of the classification variable Name in the order in which they appear in the data set so that the order of the parameters matches that of the covariance matrix.

The results of this analysis are shown in [Output 69.7.1](#). Note that the parameter estimates are identical to the values passed in the input data set and their standard errors equal the square root of the diagonal elements of the cov data set.

**Output 69.7.1** “Fitted” Parameter Estimates and Covariance Matrix

| Linear Inference                 |          |          |          |          |          |          |
|----------------------------------|----------|----------|----------|----------|----------|----------|
| The GLIMMIX Procedure            |          |          |          |          |          |          |
| Estimated V Matrix for Subject 1 |          |          |          |          |          |          |
| Row                              | Col1     | Col2     | Col3     | Col4     | Col5     | Col6     |
| 1                                | 0.007462 | -0.00522 | 0.01023  |          |          |          |
| 2                                | -0.00522 | 0.04820  | -0.01059 |          |          |          |
| 3                                | 0.01023  | -0.01059 | 0.2160   |          |          |          |
| 4                                |          |          |          | 0.03126  | -0.00910 | 0.01579  |
| 5                                |          |          |          | -0.00910 | 0.03949  | -0.02000 |
| 6                                |          |          |          | 0.01579  | -0.02000 | 0.1262   |

| Solutions for Fixed Effects |        |          |                |       |         |         |
|-----------------------------|--------|----------|----------------|-------|---------|---------|
| Effect                      | name   | Estimate | Standard Error | DF    | t Value | Pr >  t |
| name                        | alpha1 | -3.5671  | 0.08638        | Infty | -41.29  | <.0001  |
| name                        | beta1  | 0.4421   | 0.2195         | Infty | 2.01    | 0.0440  |
| name                        | gamma1 | -2.6230  | 0.4648         | Infty | -5.64   | <.0001  |
| name                        | alpha2 | -3.0111  | 0.1768         | Infty | -17.03  | <.0001  |
| name                        | beta2  | 0.3977   | 0.1987         | Infty | 2.00    | 0.0454  |
| name                        | gamma2 | -2.4442  | 0.3552         | Infty | -6.88   | <.0001  |

There are other ways to fit a saturated model with the GLIMMIX procedure. For example, you can use the TYPE=UN covariance structure in the RANDOM statement with a properly prepared input data set for the PDATA= option in the PARMS statement. See Example 17 in Chapter 41.33, “Examples: GLIMMIX Procedure,” for details.

Once the item store exists, you can apply the linear inference capabilities of the PLM procedure. For example, the ESTIMATE statement in the following statements test the hypothesis of parameter homogeneity across groups:

```
proc plm restore=ArtificialModel;
 estimate
 'alpha1 = alpha2' Name 1 0 0 -1 0 0,
 'beta1 = beta2 ' Name 0 1 0 0 -1 0,
 'gamma1 = gamma2' Name 0 0 1 0 0 -1 /
 adjust=bon stepdown ftest(label='Homogeneity');
run;
```



**Output 69.7.2** Results from the PLM Procedure

| Linear Inference                  |          |                |         |         |         |        |
|-----------------------------------|----------|----------------|---------|---------|---------|--------|
| The PLM Procedure                 |          |                |         |         |         |        |
| Estimates                         |          |                |         |         |         |        |
| Adjustment for Multiplicity: Holm |          |                |         |         |         |        |
| Label                             | Estimate | Standard Error | DF      | t Value | Pr >  t | Adj P  |
| alpha1 = alpha2                   | -0.5560  | 0.1968         | Infty   | -2.83   | 0.0047  | 0.0142 |
| beta1 = beta2                     | 0.04440  | 0.2961         | Infty   | 0.15    | 0.8808  | 1.0000 |
| gamma1 = gamma2                   | -0.1788  | 0.5850         | Infty   | -0.31   | 0.7599  | 1.0000 |
| F Test for Estimates              |          |                |         |         |         |        |
| Label                             | Num DF   | Den DF         | F Value | Pr > F  |         |        |
| Homogeneity                       | 3        | Infty          | 2.79    | 0.0389  |         |        |

The  $F$  test in [Output 69.7.2](#) shows that the joint test of homogeneity is rejected. The individual tests with familywise control of the Type I error show that the overall difference is due to a significant change in the  $\alpha$  parameters. The hypothesis of homogeneity across the two groups cannot be rejected for the  $\beta$  and  $\gamma$  parameters.

---

## References

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# Chapter 70

## The PLS Procedure

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## Overview: PLS Procedure

The PLS procedure fits models by using any one of a number of linear predictive methods, including *partial least squares* (PLS). Ordinary least squares regression, as implemented in SAS/STAT procedures such as PROC GLM and PROC REG, has the single goal of minimizing sample response prediction error, seeking linear functions of the predictors that explain as much variation in each response as possible. The techniques implemented in the PLS procedure have the additional goal of accounting for variation in the predictors, under the assumption that directions in the predictor space that are well sampled should provide better prediction for *new* observations when the predictors are highly correlated. All of the techniques implemented in the PLS procedure work by extracting successive linear combinations of the predictors, called *factors* (also called *components*, *latent vectors*, or *latent variables*), which optimally address one or both of these two goals—explaining response variation and explaining predictor variation. In particular, the method of partial least squares balances the two objectives, seeking factors that explain both response and predictor variation.

Note that the name “partial least squares” also applies to a more general statistical method that is *not* implemented in this procedure. The partial least squares method was originally developed in the 1960s by the econometrician Herman Wold (1966) for modeling “paths” of causal relation between any number of “blocks” of variables. However, the PLS procedure fits only *predictive* partial least squares models, with one “block” of predictors and one “block” of responses. If you are interested in fitting more general path models, you should consider using the CALIS procedure.

---

## Basic Features

The techniques implemented by the PLS procedure are as follows:

- principal components regression, which extracts factors to explain as much predictor sample variation as possible
- reduced rank regression, which extracts factors to explain as much response variation as possible. This technique, also known as (maximum) redundancy analysis, differs from multivariate linear regression only when there are multiple responses.
- partial least squares regression, which balances the two objectives of explaining response variation and explaining predictor variation. Two different formulations for partial least squares are available: the original predictive method of Wold (1966) and the SIMPLS method of de Jong (1993).

The number of factors to extract depends on the data. Basing the model on more extracted factors improves the model fit to the observed data, but extracting too many factors can cause *overfitting*—that is, tailoring the model too much to the current data, to the detriment of future predictions. The PLS procedure enables you to choose the number of extracted factors by *cross validation*—that is, fitting the model to part of the data, minimizing the prediction error for the unfitted part, and iterating with different portions of the data in the roles of fitted and unfitted. Various methods of cross validation are available, including one-at-a-time validation and splitting the data into blocks. The PLS procedure also offers test set validation, where the model is fit to the entire primary input data set and the fit is evaluated over a distinct test data set.

You can use the general linear modeling approach of the GLM procedure to specify a model for your design, allowing for general polynomial effects as well as classification or ANOVA effects. You can save the model fit by the PLS procedure in a data set and apply it to new data by using the SCORE procedure.

The PLS procedure uses ODS Graphics to create graphs as part of its output. For general information about ODS Graphics, see Chapter 21, “Statistical Graphics Using ODS.” For specific information about the statistical graphics available with the PLS procedure, see the PLOTS options in the PROC PLS statements and the section “ODS Graphics” on page 5891.

## Getting Started: PLS Procedure

### Spectrometric Calibration

The example in this section illustrates basic features of the PLS procedure. The data are reported in Umetrics (1995); the original source is Lindberg, Persson, and Wold (1983). Suppose that you are researching pollution in the Baltic Sea, and you would like to use the spectra of samples of seawater to determine the amounts of three compounds present in samples from the Baltic Sea: lignin sulfonate (ls: pulp industry pollution), humic acids (ha: natural forest products), and optical whitener from detergent (dt). Spectrometric calibration is a type of problem in which partial least squares can be very effective. The predictors are the spectra emission intensities at different frequencies in sample spectrum, and the responses are the amounts of various chemicals in the sample.

For the purposes of calibrating the model, samples with known compositions are used. The calibration data consist of 16 samples of known concentrations of ls, ha, and dt, with spectra based on 27 frequencies (or, equivalently, wavelengths). The following statements create a SAS data set named Sample for these data.

```

data Sample;
 input obsnam $ v1-v27 ls ha dt @@;
 datalines;
EM1 2766 2610 3306 3630 3600 3438 3213 3051 2907 2844 2796
 2787 2760 2754 2670 2520 2310 2100 1917 1755 1602 1467
 1353 1260 1167 1101 1017 3.0110 0.0000 0.00
EM2 1492 1419 1369 1158 958 887 905 929 920 887 800
 710 617 535 451 368 296 241 190 157 128 106
 89 70 65 56 50 0.0000 0.4005 0.00
EM3 2450 2379 2400 2055 1689 1355 1109 908 750 673 644
 640 630 618 571 512 440 368 305 247 196 156
 120 98 80 61 50 0.0000 0.0000 90.63
EM4 2751 2883 3492 3570 3282 2937 2634 2370 2187 2070 2007
 1974 1950 1890 1824 1680 1527 1350 1206 1080 984 888
 810 732 669 630 582 1.4820 0.1580 40.00
EM5 2652 2691 3225 3285 3033 2784 2520 2340 2235 2148 2094
 2049 2007 1917 1800 1650 1464 1299 1140 1020 909 810
 726 657 594 549 507 1.1160 0.4104 30.45
EM6 3993 4722 6147 6720 6531 5970 5382 4842 4470 4200 4077
 4008 3948 3864 3663 3390 3090 2787 2481 2241 2028 1830
 1680 1533 1440 1314 1227 3.3970 0.3032 50.82
EM7 4032 4350 5430 5763 5490 4974 4452 3990 3690 3474 3357

```

```

 3300 3213 3147 3000 2772 2490 2220 1980 1779 1599 1440
 1320 1200 1119 1032 957 2.4280 0.2981 70.59
EM8 4530 5190 6910 7580 7510 6930 6150 5490 4990 4670 4490
 4370 4300 4210 4000 3770 3420 3060 2760 2490 2230 2060
 1860 1700 1590 1490 1380 4.0240 0.1153 89.39
EM9 4077 4410 5460 5857 5607 5097 4605 4170 3864 3708 3588
 3537 3480 3330 3192 2910 2610 2325 2064 1830 1638 1476
 1350 1236 1122 1044 963 2.2750 0.5040 81.75
EM10 3450 3432 3969 4020 3678 3237 2814 2487 2205 2061 2001
 1965 1947 1890 1776 1635 1452 1278 1128 981 867 753
 663 600 552 507 468 0.9588 0.1450 101.10
EM11 4989 5301 6807 7425 7155 6525 5784 5166 4695 4380 4197
 4131 4077 3972 3777 3531 3168 2835 2517 2244 2004 1809
 1620 1470 1359 1266 1167 3.1900 0.2530 120.00
EM12 5340 5790 7590 8390 8310 7670 6890 6190 5700 5380 5200
 5110 5040 4900 4700 4390 3970 3540 3170 2810 2490 2240
 2060 1870 1700 1590 1470 4.1320 0.5691 117.70
EM13 3162 3477 4365 4650 4470 4107 3717 3432 3228 3093 3009
 2964 2916 2838 2694 2490 2253 2013 1788 1599 1431 1305
 1194 1077 990 927 855 2.1600 0.4360 27.59
EM14 4380 4695 6018 6510 6342 5760 5151 4596 4200 3948 3807
 3720 3672 3567 3438 3171 2880 2571 2280 2046 1857 1680
 1548 1413 1314 1200 1119 3.0940 0.2471 61.71
EM15 4587 4200 5040 5289 4965 4449 3939 3507 3174 2970 2850
 2814 2748 2670 2529 2328 2088 1851 1641 1431 1284 1134
 1020 918 840 756 714 1.6040 0.2856 108.80
EM16 4017 4725 6090 6570 6354 5895 5346 4911 4611 4422 4314
 4287 4224 4110 3915 3600 3240 2913 2598 2325 2088 1917
 1734 1587 1452 1356 1257 3.1620 0.7012 60.00
;

```

## Fitting a PLS Model

To isolate a few underlying spectral factors that provide a good predictive model, you can fit a PLS model to the 16 samples by using the following SAS statements:

```

proc pls data=sample;
 model ls ha dt = v1-v27;
run;

```

By default, the PLS procedure extracts at most 15 factors. The procedure lists the amount of variation accounted for by each of these factors, both individual and cumulative; this listing is shown in [Figure 70.1](#).

**Figure 70.1** PLS Variation Summary

| The PLS Procedure                                                   |               |          |                     |          |
|---------------------------------------------------------------------|---------------|----------|---------------------|----------|
| Percent Variation Accounted for<br>by Partial Least Squares Factors |               |          |                     |          |
| Number of<br>Extracted<br>Factors                                   | Model Effects |          | Dependent Variables |          |
|                                                                     | Current       | Total    | Current             | Total    |
| 1                                                                   | 97.4607       | 97.4607  | 41.9155             | 41.9155  |
| 2                                                                   | 2.1830        | 99.6436  | 24.2435             | 66.1590  |
| 3                                                                   | 0.1781        | 99.8217  | 24.5339             | 90.6929  |
| 4                                                                   | 0.1197        | 99.9414  | 3.7898              | 94.4827  |
| 5                                                                   | 0.0415        | 99.9829  | 1.0045              | 95.4873  |
| 6                                                                   | 0.0106        | 99.9935  | 2.2808              | 97.7681  |
| 7                                                                   | 0.0017        | 99.9952  | 1.1693              | 98.9374  |
| 8                                                                   | 0.0010        | 99.9961  | 0.5041              | 99.4415  |
| 9                                                                   | 0.0014        | 99.9975  | 0.1229              | 99.5645  |
| 10                                                                  | 0.0010        | 99.9985  | 0.1103              | 99.6747  |
| 11                                                                  | 0.0003        | 99.9988  | 0.1523              | 99.8270  |
| 12                                                                  | 0.0003        | 99.9991  | 0.1291              | 99.9561  |
| 13                                                                  | 0.0002        | 99.9994  | 0.0312              | 99.9873  |
| 14                                                                  | 0.0004        | 99.9998  | 0.0065              | 99.9938  |
| 15                                                                  | 0.0002        | 100.0000 | 0.0062              | 100.0000 |

Note that all of the variation in both the predictors and the responses is accounted for by only 15 factors; this is because there are only 16 sample observations. More important, almost all of the variation is accounted for with even fewer factors—one or two for the predictors and three to eight for the responses.

### Selecting the Number of Factors by Cross Validation

A PLS model is not complete until you choose the number of factors. You can choose the number of factors by using cross validation, in which the data set is divided into two or more groups. You fit the model to all groups except one, and then you check the capability of the model to predict responses for the group omitted. Repeating this for each group, you then can measure the overall capability of a given form of the model. The predicted residual sum of squares (PRESS) statistic is based on the residuals generated by this process.

To select the number of extracted factors by cross validation, you specify the **CV=** option with an argument that says which cross validation method to use. For example, a common method is split-sample validation, in which the different groups are composed of every  $n$ th observation beginning with the first, every  $n$ th observation beginning with the second, and so on. You can use the **CV=SPLIT** option to specify split-sample validation with  $n = 7$  by default, as in the following SAS statements:

```
proc pls data=sample cv=split;
 model ls ha dt = v1-v27;
run;
```

The resulting output is shown in [Figure 70.2](#) and [Figure 70.3](#).

**Figure 70.2** Split-Sample Validated PRESS Statistics for Number of Factors

| The PLS Procedure                                           |                       |        |
|-------------------------------------------------------------|-----------------------|--------|
| Split-sample Validation for the Number of Extracted Factors |                       |        |
| Number of<br>Extracted<br>Factors                           | Root<br>Mean<br>PRESS |        |
| 0                                                           | 1.107747              |        |
| 1                                                           | 0.957983              |        |
| 2                                                           | 0.931314              |        |
| 3                                                           | 0.520222              |        |
| 4                                                           | 0.530501              |        |
| 5                                                           | 0.586786              |        |
| 6                                                           | 0.475047              |        |
| 7                                                           | 0.477595              |        |
| 8                                                           | 0.483138              |        |
| 9                                                           | 0.485739              |        |
| 10                                                          | 0.48946               |        |
| 11                                                          | 0.521445              |        |
| 12                                                          | 0.525653              |        |
| 13                                                          | 0.531049              |        |
| 14                                                          | 0.531049              |        |
| 15                                                          | 0.531049              |        |
| Minimum root mean PRESS                                     |                       | 0.4750 |
| Minimizing number of factors                                |                       | 6      |

**Figure 70.3** PLS Variation Summary for Split-Sample Validated Model

| Number of<br>Extracted<br>Factors | Percent Variation Accounted for<br>by Partial Least Squares Factors |         |                     |         |
|-----------------------------------|---------------------------------------------------------------------|---------|---------------------|---------|
|                                   | Model Effects                                                       |         | Dependent Variables |         |
|                                   | Current                                                             | Total   | Current             | Total   |
| 1                                 | 97.4607                                                             | 97.4607 | 41.9155             | 41.9155 |
| 2                                 | 2.1830                                                              | 99.6436 | 24.2435             | 66.1590 |
| 3                                 | 0.1781                                                              | 99.8217 | 24.5339             | 90.6929 |
| 4                                 | 0.1197                                                              | 99.9414 | 3.7898              | 94.4827 |
| 5                                 | 0.0415                                                              | 99.9829 | 1.0045              | 95.4873 |
| 6                                 | 0.0106                                                              | 99.9935 | 2.2808              | 97.7681 |

The absolute minimum PRESS is achieved with six extracted factors. Notice, however, that this is not much smaller than the PRESS for three factors. By using the **CVTEST** option, you can perform a statistical model comparison suggested by van der Voet (1994) to test whether this difference is significant, as shown in the following SAS statements:

```
proc pls data=sample cv=split cvtest (seed=12345);
 model ls ha dt = v1-v27;
run;
```

The model comparison test is based on a rerandomization of the data. By default, the seed for this randomization is based on the system clock, but it is specified here. The resulting output is shown in Figure 70.4 and Figure 70.5.

**Figure 70.4** Testing Split-Sample Validation for Number of Factors

| The PLS Procedure                                           |                       |          |                |  |
|-------------------------------------------------------------|-----------------------|----------|----------------|--|
| Split-sample Validation for the Number of Extracted Factors |                       |          |                |  |
| Number of<br>Extracted<br>Factors                           | Root<br>Mean<br>PRESS | T**2     | Prob ><br>T**2 |  |
| 0                                                           | 1.107747              | 9.272858 | 0.0010         |  |
| 1                                                           | 0.957983              | 10.62305 | <.0001         |  |
| 2                                                           | 0.931314              | 8.950878 | 0.0010         |  |
| 3                                                           | 0.520222              | 5.133259 | 0.1440         |  |
| 4                                                           | 0.530501              | 5.168427 | 0.1340         |  |
| 5                                                           | 0.586786              | 6.437266 | 0.0150         |  |
| 6                                                           | 0.475047              | 0        | 1.0000         |  |
| 7                                                           | 0.477595              | 2.809763 | 0.4750         |  |
| 8                                                           | 0.483138              | 7.189526 | 0.0110         |  |
| 9                                                           | 0.485739              | 7.931726 | 0.0070         |  |
| 10                                                          | 0.48946               | 6.612597 | 0.0150         |  |
| 11                                                          | 0.521445              | 6.666235 | 0.0130         |  |
| 12                                                          | 0.525653              | 7.092861 | 0.0080         |  |
| 13                                                          | 0.531049              | 7.538298 | 0.0030         |  |
| 14                                                          | 0.531049              | 7.538298 | 0.0030         |  |
| 15                                                          | 0.531049              | 7.538298 | 0.0030         |  |
| Minimum root mean PRESS                                     |                       |          | 0.4750         |  |
| Minimizing number of factors                                |                       |          | 6              |  |
| Smallest number of factors with p > 0.1                     |                       |          | 3              |  |

**Figure 70.5** PLS Variation Summary for Tested Split-Sample Validated Model

| Percent Variation Accounted for<br>by Partial Least Squares Factors |               |         |                     |         |
|---------------------------------------------------------------------|---------------|---------|---------------------|---------|
| Number of<br>Extracted<br>Factors                                   | Model Effects |         | Dependent Variables |         |
|                                                                     | Current       | Total   | Current             | Total   |
| 1                                                                   | 97.4607       | 97.4607 | 41.9155             | 41.9155 |
| 2                                                                   | 2.1830        | 99.6436 | 24.2435             | 66.1590 |
| 3                                                                   | 0.1781        | 99.8217 | 24.5339             | 90.6929 |



The  $p$ -value of 0.1430 in comparing the cross validated residuals from models with 6 and 3 factors indicates that the difference between the two models is insignificant; therefore, the model with fewer factors is preferred. The variation summary shows that over 99% of the predictor variation and over 90% of the response variation are accounted for by the three factors.

## Predicting New Observations

Now that you have chosen a three-factor PLS model for predicting pollutant concentrations based on sample spectra, suppose that you have two new samples. The following SAS statements create a data set containing the spectra for the new samples:

```
data newobs;
 input obsnam $ v1-v27 @@;
 datalines;
EM17 3933 4518 5637 6006 5721 5187 4641 4149 3789
 3579 3447 3381 3327 3234 3078 2832 2571 2274
 2040 1818 1629 1470 1350 1245 1134 1050 987
EM25 2904 2997 3255 3150 2922 2778 2700 2646 2571
 2487 2370 2250 2127 2052 1713 1419 1200 984
 795 648 525 426 351 291 240 204 162
;
```

You can apply the PLS model to these samples to estimate pollutant concentration. To do so, append the new samples to the original 16, and specify that the predicted values for all 18 be output to a data set, as shown in the following statements:

```
data all;
 set sample newobs;
run;

proc pls data=all nfac=3;
 model ls ha dt = v1-v27;
 output out=pred p=p_ls p_ha p_dt;
run;

proc print data=pred;
 where (obsnam in ('EM17','EM25'));
 var obsnam p_ls p_ha p_dt;
run;
```

The new observations are not used in calculating the PLS model, since they have no response values. Their predicted concentrations are shown in [Figure 70.6](#).

**Figure 70.6** Predicted Concentrations for New Observations

| Obs | obsnam | p_ls     | p_ha    | p_dt    |
|-----|--------|----------|---------|---------|
| 17  | EM17   | 2.54261  | 0.31877 | 81.4174 |
| 18  | EM25   | -0.24716 | 1.37892 | 46.3212 |

Finally, if ODS Graphics is enabled, PLS also displays by default a plot of the amount of variation accounted for by each factor, as well as a correlations loading plot that summarizes the first two dimensions of the PLS model. The following statements, which are the same as the previous split-sample validation analysis but with ODS Graphics enabled, additionally produce [Figure 70.7](#) and [Figure 70.8](#):

```
ods graphics on;

proc pls data=sample cv=split cvtest(seed=12345);
 model ls ha dt = v1-v27;
run;

ods graphics off;
```

**Figure 70.7** Split-Sample Cross Validation Plot

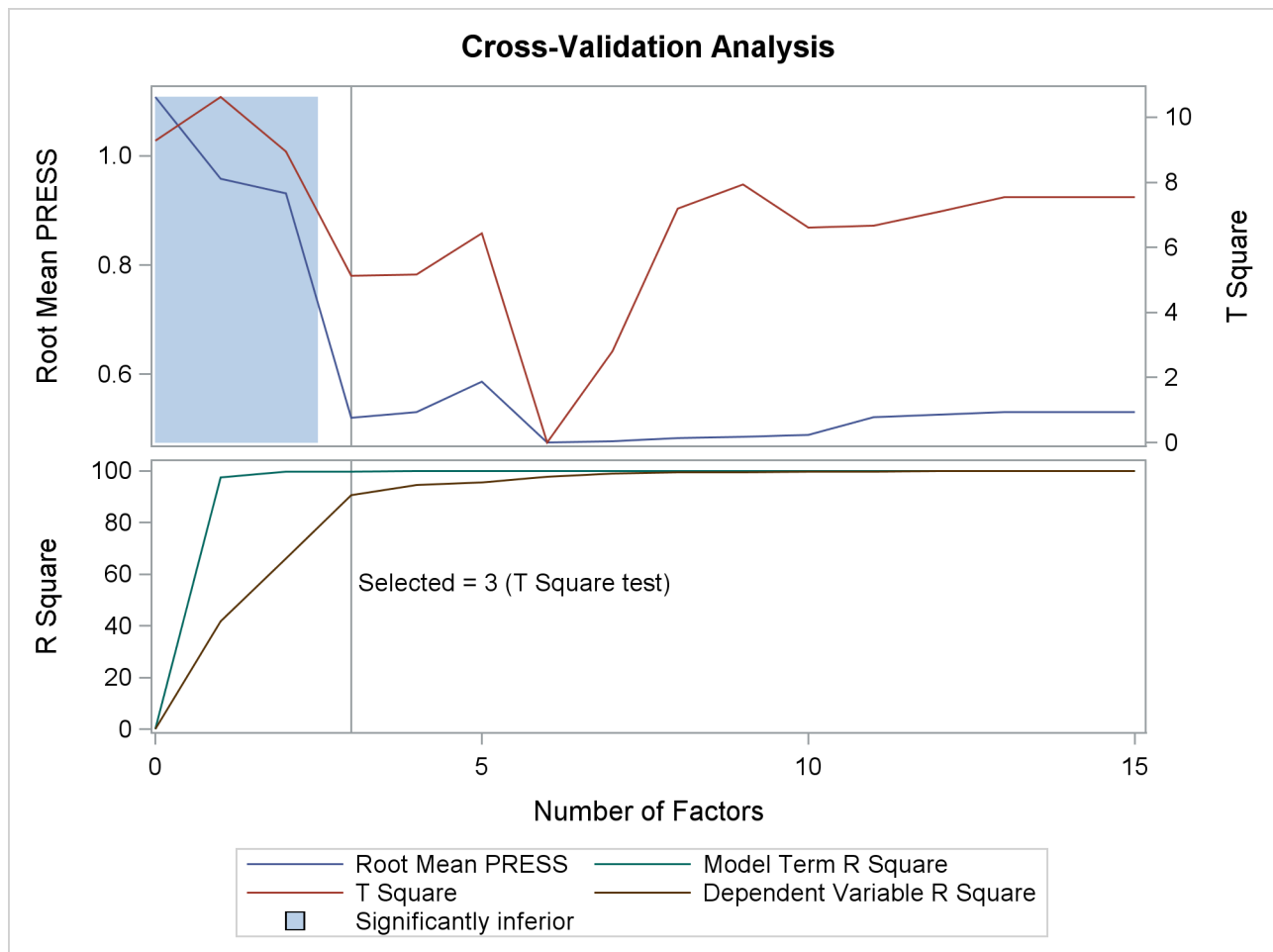
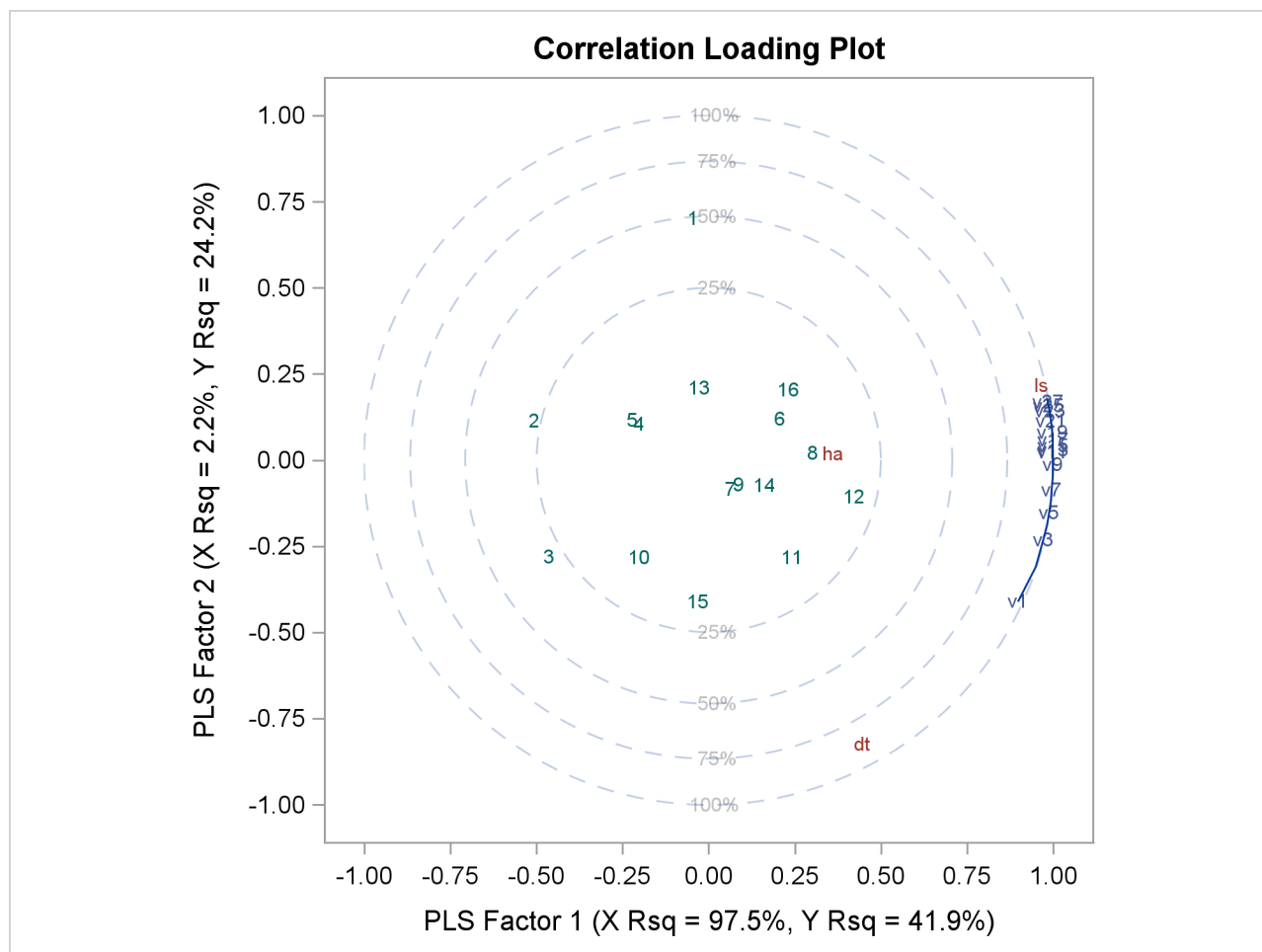


Figure 70.8 Correlation Loadings Plot



The cross validation plot in [Figure 70.7](#) gives a visual representation of the selection of the optimum number of factors discussed previously. The correlation loadings plot is a compact summary of many features of the PLS model. For example, it shows that the first factor is highly positively correlated with all spectral values, indicating that it is approximately an average of them all; the second factor is positively correlated with the lowest frequencies and negatively correlated with the highest, indicating that it is approximately a contrast between the two ends of the spectrum. The observations, represented by their number in the data set on this plot, are generally spaced well apart, indicating that the data give good information about these first two factors. For more details on the interpretation of the correlation loadings plot, see the section “[ODS Graphics](#)” on page 5891 and [Example 70.1](#).

## Syntax: PLS Procedure

The following statements are available in the PLS procedure. Items within the angle brackets are optional.

```
PROC PLS < options > ;
 BY variables ;
 CLASS variables < / option > ;
 EFFECT name=effect-type (variables < / options >) ;
 ID variables ;
 MODEL dependent-variables = effects < / options > ;
 OUTPUT OUT=SAS-data-set < options > ;
```

To analyze a data set, you must use the **PROC PLS** and **MODEL** statements. You can use the other statements as needed. **CLASS** and **EFFECT** statements, if present, must precede the **MODEL** statement.

## PROC PLS Statement

```
PROC PLS < options > ;
```

The PROC PLS statement invokes the PLS procedure. Optionally, you can also indicate the analysis data and method in the PROC PLS statement. [Table 70.1](#) summarizes the options available in the PROC PLS statement.

**Table 70.1** PROC PLS Statement Options

| Option     | Description                                                                                 |
|------------|---------------------------------------------------------------------------------------------|
| CENSCALE   | Displays the centering and scaling information                                              |
| CV=ONE     | Specifies the cross validation method to be used                                            |
| CVTEST     | Specifies that van der Voet's (1994) randomization-based model comparison test be performed |
| DATA=      | Names the SAS data set                                                                      |
| DETAILS    | Displays the details of the fitted model                                                    |
| METHOD=PLS | Specifies the general factor extraction method to be used                                   |
| MISSING=   | Specifies how observations with missing values are to be handled in computing the fit       |
| NFAC=      | Specifies the number of factors to extract                                                  |
| NOCENTER   | Suppresses centering of the responses and predictors before fitting                         |
| NOCVSTDIZE | Suppresses re-centering and rescaling of the responses and predictors when cross-validating |
| NOPRINT    | Suppresses the normal display of results                                                    |
| NOSCALE    | Suppresses scaling of the responses and predictors before fitting                           |
| PLOTS      | Controls the plots produced through ODS Graphics                                            |
| VARSCALE   | Specifies that continuous model variables be centered and scaled                            |
| VARSS      | Displays the amount of variation accounted for in each response and predictor               |

The following options are available.

**CENSCALE**

lists the centering and scaling information for each response and predictor.

**CV=ONE**

**CV=SPLIT** <(*n*)>

**CV=BLOCK** <(*n*)>

**CV=RANDOM** <(*cv-random-opts*)>

**CV=TESTSET**(*SAS-data-set*)

specifies the cross validation method to be used. By default, no cross validation is performed. The method **CV=ONE** requests one-at-a-time cross validation, **CV=SPLIT** requests that every *n*th observation be excluded, **CV=BLOCK** requests that *n* blocks of consecutive observations be excluded, **CV=RANDOM** requests that observations be excluded at random, and **CV=TESTSET**(*SAS-data-set*) specifies a test set of observations to be used for validation (formally, this is called “test set validation” rather than “cross validation”). You can, optionally, specify *n* for **CV=SPLIT** and **CV=BLOCK**; the default is *n* = 7. You can also specify the following optional *cv-random-options* in parentheses after the **CV=RANDOM** option:

**NITER**=*n*

specifies the number of random subsets to exclude. The default value is 10.

**NTEST**=*n*

specifies the number of observations in each random subset chosen for exclusion. The default value is one-tenth of the total number of observations.

**SEED**=*n*

specifies an integer used to start the pseudo-random number generator for selecting the random test set. If you do not specify a seed, or specify a value less than or equal to zero, the seed is by default generated from reading the time of day from the computer’s clock.

**CVTEST** <(*cvtest-options*)>

specifies that van der Voet’s (1994) randomization-based model comparison test be performed to test models with different numbers of extracted factors against the model that minimizes the predicted residual sum of squares; see the section “[Cross Validation](#)” on page 5887 for more information. You can also specify the following *cv-test-options* in parentheses after the **CVTEST** option:

**PVAL**=*n*

specifies the cutoff probability for declaring an insignificant difference. The default value is 0.10.

**STAT**=*test-statistic*

specifies the test statistic for the model comparison. You can specify either T2, for Hotelling’s  $T^2$  statistic, or PRESS, for the predicted residual sum of squares. The default value is T2.

**NSAMP**=*n*

specifies the number of randomizations to perform. The default value is 1000.

**SEED=*n***

specifies the seed value for randomization generation (the clock time is used by default).

**DATA=*SAS-data-set***

names the SAS data set to be used by PROC PLS. The default is the most recently created data set.

**DETAILS**

lists the details of the fitted model for each successive factor. The details listed are different for different extraction methods; see the section “[Displayed Output](#)” on page 5890 for more information.

**METHOD=PLS < ( *PLS-options* )>****METHOD=SIMPLS****METHOD=PCR****METHOD=RRR**

specifies the general factor extraction method to be used. The value PLS requests partial least squares, SIMPLS requests the SIMPLS method of de Jong (1993), PCR requests principal components regression, and RRR requests reduced rank regression. The default is METHOD=PLS. You can also specify the following optional *PLS-options* in parentheses after METHOD=PLS:

**ALGORITHM=NIPALS | SVD | EIG | RLGW**

names the specific algorithm used to compute extracted PLS factors. NIPALS requests the usual iterative NIPALS algorithm, SVD bases the extraction on the singular value decomposition of  $\mathbf{X}'\mathbf{Y}$ , EIG bases the extraction on the eigenvalue decomposition of  $\mathbf{Y}'\mathbf{X}\mathbf{X}'\mathbf{Y}$ , and RLGW is an iterative approach that is efficient when there are many predictors. ALGORITHM=SVD is the most accurate but least efficient approach; the default is ALGORITHM=NIPALS.

**MAXITER=*n***

specifies the maximum number of iterations for the NIPALS and RLGW algorithms. The default value is 200.

**EPSILON=*n***

specifies the convergence criterion for the NIPALS and RLGW algorithms. The default value is  $10^{-12}$ .

**MISSING=NONE****MISSING=AVG****MISSING=EM < ( *EM-options* )>**

specifies how observations with missing values are to be handled in computing the fit. The default is MISSING=NONE, for which observations with any missing variables (dependent or independent) are excluded from the analysis. MISSING=AVG specifies that the fit be computed by filling in missing values with the average of the nonmissing values for the corresponding variable. If you specify MISSING=EM, then the procedure first computes the model with MISSING=AVG and then fills in missing values by their predicted values based on that model and computes the model again. For both methods of imputation, the imputed values contribute to the centering and scaling values, and the difference between the imputed values and their final predictions contributes to the percentage of variation explained. You can also specify the following optional *EM-options* in parentheses after MISSING=EM:

**MAXITER=*n***

specifies the maximum number of iterations for the imputation/fit loop. The default value is 1. If you specify a large value of MAXITER=, then the loop will iterate until it converges (as controlled by the EPSILON= option).

**EPSILON=*n***

specifies the convergence criterion for the imputation/fit loop. The default value is  $10^{-8}$ . This option is effective only if you specify a large value for the MAXITER= option.

**NFAC=*n***

specifies the number of factors to extract. The default is  $\min\{15, p, N\}$ , where  $p$  is the number of predictors (the number of dependent variables for METHOD=RRR) and  $N$  is the number of runs (observations). This is probably more than you need for most applications. Extracting too many factors can lead to an overfit model, one that matches the training data too well, sacrificing predictive ability. Thus, if you use the default NFAC= specification, you should also either use the CV= option to select the appropriate number of factors for the final model or consider the analysis to be preliminary and examine the results to determine the appropriate number of factors for a subsequent analysis.

**NOCENTER**

suppresses centering of the responses and predictors before fitting. This is useful if the analysis variables are already centered and scaled. See the section “Centering and Scaling” on page 5889 for more information.

**NOCVSTDIZE**

suppresses re-centering and rescaling of the responses and predictors before each model is fit in the cross validation. See the section “Centering and Scaling” on page 5889 for more information.

**NOPRINT**

suppresses the normal display of results. This is useful when you want only the output statistics saved in a data set. Note that this option temporarily disables the Output Delivery System (ODS); see Chapter 20, “Using the Output Delivery System” for more information.

**NOSCALE**

suppresses scaling of the responses and predictors before fitting. This is useful if the analysis variables are already centered and scaled. See the section “Centering and Scaling” on page 5889 for more information.

**PLOTS** <(global-plot-options)> <= plot-request <(options)>>

**PLOTS** <(global-plot-options)> <= (plot-request <(options)> <... plot-request <(options)>>>

controls the plots produced through ODS Graphics. When you specify only one plot request, you can omit the parentheses from around the plot request. For example:

```
plots=none
plots=cvplot
plots=(diagnostics cvplot)
plots(unpack)=diagnostics
plots(unpack)=(diagnostics corrload(trace=off))
```

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;
proc pls data=pentaTrain;
 model log_RAI = S1-S5 L1-L5 P1-P5;
run;
ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS](#).”

If ODS Graphics is enabled but you do not specify the PLOTS= option, then PROC PLS produces by default a plot of the R-square analysis and a correlation loading plot summarizing the first two factors.

The global plot options include the following:

#### **FLIP**

interchanges the X-axis and Y-axis dimensions for the score, weight, and loading plots.

#### **ONLY**

suppresses the default plots. Only plots specifically requested are displayed.

#### **UNPACKPANEL**

##### **UNPACK**

suppresses paneling. By default, multiple plots can appear in some output panels. Specify UNPACKPANEL to get each plot in a separate panel. You can specify PLOTS(UNPACKPANEL) to unpack only the default plots. You can also specify UNPACKPANEL as a suboption for certain specific plots, as discussed in the following.

The plot requests include the following:

#### **ALL**

produces all appropriate plots. You can specify other options with ALL—for example, to request all plots and unpack only the residuals, specify PLOTS=(ALL RESIDUALS(UNPACK)).

#### **CORRLOAD <(TRACE = ON | OFF)>**

produces a correlation loading plot (default). The TRACE= option controls how points corresponding to the X-loadings in the correlation loadings plot are depicted. By default, these points are depicted by the name of the corresponding model effect if there are 20 or fewer of them; otherwise, they are depicted by a connected “trace” through the points. You can use this option to change this behavior.

#### **CVPLOT**

produces a cross validation and R-square analysis. This plot requires the CV= option to be specified, and is displayed by default in this case.

#### **DIAGNOSTICS <(UNPACK)>**

produces a summary panel of the fit for each dependent variable. The summary by default consists of a panel for each dependent variable, with plots depicting the distribution of residuals and predicted values. You can use the UNPACK suboption to specify that the subplots be produced separately.



**DMOD**

produces the DMODX, DMODY, and DMODXY plots.

**DMODX**

produces a plot of the distance of each observation to the X model.

**DMODXY**

produces plots of the distance of each observation to the X and Y models.

**DMODY**

produces a plot of the distance of each observation to the Y model.

**FIT**

produces both the fit diagnostic panel and the ParmProfiles plot.

**NONE**

suppresses the display of graphics.

**PARMPROFILES**

produces profiles of the regression coefficients.

**SCORES <(UNPACK | FLIP)>**

produces the XScores, YScores, XYScores, and DModXY plots. You can use the UNPACK suboption to specify that the subplots for scores be produced separately, and the FLIP option to interchange their default X-axis and Y-axis dimensions.

**RESIDUALS <(UNPACK)>**

plots the residuals for each dependent variable against each independent variable. Residual plots are by default composed of multiple plots combined into a single panel. You can use the UNPACK suboption to specify that the subplots be produced separately.

**VIP**

produces profiles of variable importance factors.

**WEIGHTS <(UNPACK | FLIP)>**

produces all X and Y loading and weight plots, as well as the VIP plot. You can use the UNPACK suboption to specify that the subplots for weights and loadings be produced separately, and the FLIP option to interchange their default X-axis and Y-axis dimensions.

**XLOADINGPLOT <(UNPACK | FLIP)>**

produces a scatter plot matrix of X-loadings against each other. Loading scatter plot matrices are by default composed of multiple plots combined into a single panel. You can use the UNPACK suboption to specify that the subplots be produced separately, and the FLIP option to interchange the default X-axis and Y-axis dimensions.

**XLOADINGPROFILES**

produces profiles of the X-loadings.

**XSCORES <(UNPACK | FLIP)>**

produces a scatter plot matrix of X-scores against each other. Score scatter plot matrices are by default composed of multiple plots combined into a single panel. You can use the UNPACK suboption to specify that the subplots be produced separately, and the FLIP option to interchange the default X-axis and Y-axis dimensions.

**XWEIGHTPLOT <(UNPACK | FLIP)>**

produces a scatter plot matrix of X-weights against each other. Weight scatter plot matrices are by default composed of multiple plots combined into a single panel. You can use the UNPACK suboption to specify that the subplots be produced separately, and the FLIP option to interchange the default X-axis and Y-axis dimensions.

**XWEIGHTPROFILES**

produces profiles of the X-weights.

**XYScores <(UNPACK)>**

produces a scatter plot matrix of X-scores against Y-scores. Score scatter plot matrices are by default composed of multiple plots combined into a single panel. You can use the UNPACK suboption to specify that the subplots be produced separately.

**YScores <(UNPACK | FLIP)>**

produces a scatter plot matrix of Y-scores against each other. Score scatter plot matrices are by default composed of multiple plots combined into a single panel. You can use the UNPACK suboption to specify that the subplots be produced separately, and the FLIP option to interchange the default X-axis and Y-axis dimensions.

**YWEIGHTPLOT <(UNPACK | FLIP)>**

produces a scatter plot matrix of Y-weights against each other. Weight scatter plot matrices are by default composed of multiple plots combined into a single panel. You can use the UNPACK suboption to specify that the subplots be produced separately, and the FLIP option to interchange the default X-axis and Y-axis dimensions.

**VARSCALE**

specifies that continuous model variables be centered and scaled prior to centering and scaling the model effects in which they are involved. The rescaling specified by the VARSCALE option is sometimes more appropriate if the model involves crossproducts between model variables; however, the VARSCALE option still might not produce the model you expect. See the section “[Centering and Scaling](#)” on page 5889 for more information.

**VARSS**

lists, in addition to the average response and predictor sum of squares accounted for by each successive factor, the amount of variation accounted for in each response and predictor.

---

## BY Statement

**BY** *variables* ;

You can specify a BY statement with PROC PLS to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.

- Specify the `NOTSORTED` or `DESCENDING` option in the `BY` statement for the PLS procedure. The `NOTSORTED` option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the `BY` variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the `BY` variables by using the `DATASETS` procedure (in Base SAS software).

For more information about `BY`-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the `DATASETS` procedure, see the discussion in the *Base SAS Procedures Guide*.

## CLASS Statement

**CLASS** *variables* </ **TRUNCATE** > ;

The `CLASS` statement names the classification variables to be used in the model. Typical classification variables are `Treatment`, `Sex`, `Race`, `Group`, and `Replication`. If you use the `CLASS` statement, it must appear before the `MODEL` statement.

Classification variables can be either character or numeric. By default, class levels are determined from the entire set of formatted values of the `CLASS` variables.

**NOTE:** Prior to SAS 9, class levels were determined by using no more than the first 16 characters of the formatted values. To revert to this previous behavior, you can use the `TRUNCATE` option in the `CLASS` statement.

In any case, you can use formats to group values into levels. See the discussion of the `FORMAT` procedure in the *Base SAS Procedures Guide* and the discussions of the `FORMAT` statement and SAS formats in *SAS Language Reference: Dictionary*.

You can specify the following option in the `CLASS` statement after a slash (/):

### **TRUNCATE**

specifies that class levels should be determined by using only up to the first 16 characters of the formatted values of `CLASS` variables. When formatted values are longer than 16 characters, you can use this option to revert to the levels as determined in releases prior to SAS 9.

## EFFECT Statement

**EFFECT** *name=effect-type* (*variables*</ *options*>) ;

The `EFFECT` statement enables you to construct special collections of columns for design matrices. These collections are referred to as *constructed effects* to distinguish them from the usual model effects formed from continuous or classification variables, as discussed in the section “[GLM Parameterization of Classification Variables and Effects](#)” on page 383 of Chapter 19, “[Shared Concepts and Topics](#).”

The following *effect-types* are available.

### **COLLECTION**

is a collection effect that defines one or more variables as a single effect with multiple degrees of freedom. The variables in a collection are considered as a unit for estimation and inference.

|                          |                                                                                                                                                                                                           |
|--------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>LAG</b>               | is a classification effect in which the level that is used for a given period corresponds to the level in the preceding period.                                                                           |
| <b>MULTIMEMBER   MM</b>  | is a multimember classification effect whose levels are determined by one or more variables that appear in a CLASS statement.                                                                             |
| <b>POLYNOMIAL   POLY</b> | is a multivariate polynomial effect in the specified numeric variables.                                                                                                                                   |
| <b>SPLINE</b>            | is a regression spline effect whose columns are univariate spline expansions of one or more variables. A spline expansion replaces the original variable with an expanded or larger set of new variables. |

Table 70.2 summarizes the *options* available in the EFFECT statement.

**Table 70.2** EFFECT Statement Options

| Option                             | Description                                                                                                                                          |
|------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Collection Effects Options</b>  |                                                                                                                                                      |
| DETAILS                            | Displays the constituents of the collection effect                                                                                                   |
| <b>Lag Effects Options</b>         |                                                                                                                                                      |
| DESIGNROLE=                        | Names a variable that controls to which lag design an observation is assigned                                                                        |
| DETAILS                            | Displays the lag design of the lag effect                                                                                                            |
| NLAG=                              | Specifies the number of periods in the lag                                                                                                           |
| PERIOD=                            | Names the variable that defines the period                                                                                                           |
| WITHIN=                            | Names the variable or variables that define the group within which each period is defined                                                            |
| <b>Multimember Effects Options</b> |                                                                                                                                                      |
| NOEFFECT                           | Specifies that observations with all missing levels for the multimember variables should have zero values in the corresponding design matrix columns |
| WEIGHT=                            | Specifies the weight variable for the contributions of each of the classification effects                                                            |
| <b>Polynomial Effects Options</b>  |                                                                                                                                                      |
| DEGREE=                            | Specifies the degree of the polynomial                                                                                                               |
| MDEGREE=                           | Specifies the maximum degree of any variable in a term of the polynomial                                                                             |
| STANDARDIZE=                       | Specifies centering and scaling suboptions for the variables that define the polynomial                                                              |
| <b>Spline Effects Options</b>      |                                                                                                                                                      |
| BASIS=                             | Specifies the type of basis (B-spline basis or truncated power function basis) for the spline expansion                                              |
| DEGREE=                            | Specifies the degree of the spline transformation                                                                                                    |
| KNOTMETHOD=                        | Specifies how to construct the knots for spline effects                                                                                              |

For further details about the syntax of these *effect-types* and how columns of constructed effects are computed, see the section “[EFFECT Statement](#)” on page 393 of Chapter 19, “[Shared Concepts and Topics](#).”

## ID Statement

**ID** *variables* ;

The ID statement names variables whose values are used to label observations in plots. If you do not specify an ID statement, then each observations is labeled in plots by its corresponding observation number.

## MODEL Statement

**MODEL** *response-variables = predictor-effects < / options >* ;

The MODEL statement names the responses and the predictors, which determine the **Y** and **X** matrices of the model, respectively. Usually you simply list the names of the predictor variables as the model effects, but you can also use the effects notation of PROC GLM to specify polynomial effects and interactions; see the section “[Specification of Effects](#)” on page 3324 in Chapter 42, “[The GLM Procedure](#)” for further details. The MODEL statement is required. You can specify only one MODEL statement (in contrast to the REG procedure, for example, which allows several MODEL statements in the same PROC REG run).

You can specify the following options in the MODEL statement after a slash (/).

### INTERCEPT

By default, the responses and predictors are centered; thus, no intercept is required in the model. You can specify the INTERCEPT option to override the default.

### SOLUTION

lists the coefficients of the final predictive model for the responses. The coefficients for predicting the centered and scaled responses based on the centered and scaled predictors are displayed, as well as the coefficients for predicting the raw responses based on the raw predictors.

## OUTPUT Statement

**OUTPUT** **OUT=***SAS-data-set keyword=names < . . . keyword=names >* ;

You use the OUTPUT statement to specify a data set to receive quantities that can be computed for every input observation, such as extracted factors and predicted values. The following *keywords* are available:

|           |                                                                           |
|-----------|---------------------------------------------------------------------------|
| PREDICTED | predicted values for responses                                            |
| YRESIDUAL | residuals for responses                                                   |
| XRESIDUAL | residuals for predictors                                                  |
| XSCORE    | extracted factors (X-scores, latent vectors, latent variables, <i>T</i> ) |
| YSCORE    | extracted responses (Y-scores, <i>U</i> )                                 |
| STDY      | standardized (centered and scaled) responses                              |

|         |                                                         |
|---------|---------------------------------------------------------|
| STDY    | standardized (centered and scaled) predictors           |
| H       | approximate leverage                                    |
| PRESS   | approximate predicted residuals                         |
| TSQUARE | scaled sum of squares of score values                   |
| STDXSSE | sum of squares of residuals for standardized predictors |
| STDYSSE | sum of squares of residuals for standardized responses  |

Suppose that there are  $N_x$  predictors and  $N_y$  responses and that the model has  $N_f$  selected factors.

- The keywords XRESIDUAL and STDY define an output variable for each predictor, so  $N_x$  names are required after each one.
- The keywords PREDICTED, YRESIDUAL, STDY, and PRESS define an output variable for each response, so  $N_y$  names are required after each of these keywords.
- The keywords XSCORE and YSCORE specify an output variable for each selected model factor. For these keywords, you provide only one base name, and the variables corresponding to each successive factor are named by appending the factor number to the base name. For example, if  $N_f = 3$ , then a specification of XSCORE=T would produce the variables T1, T2, and T3.
- Finally, the keywords H, TSQUARE, STDXSSE, and STDYSSE each specify a single output variable, so only one name is required after each of these keywords.

---

## Details: PLS Procedure

---

### Regression Methods

All of the predictive methods implemented in PROC PLS work essentially by finding linear combinations of the predictors (factors) to use to predict the responses linearly. The methods differ only in how the factors are derived, as explained in the following sections.

### Partial Least Squares

Partial least squares (PLS) works by extracting one factor at a time. Let  $\mathbf{X} = \mathbf{X}_0$  be the centered and scaled matrix of predictors and let  $\mathbf{Y} = \mathbf{Y}_0$  be the centered and scaled matrix of response values. The PLS method starts with a linear combination  $\mathbf{t} = \mathbf{X}_0\mathbf{w}$  of the predictors, where  $\mathbf{t}$  is called a *score* vector and  $\mathbf{w}$  is its associated *weight* vector. The PLS method predicts both  $\mathbf{X}_0$  and  $\mathbf{Y}_0$  by regression on  $\mathbf{t}$ :

$$\begin{aligned}\hat{\mathbf{X}}_0 &= \mathbf{t}\mathbf{p}', \quad \text{where } \mathbf{p}' = (\mathbf{t}'\mathbf{t})^{-1}\mathbf{t}'\mathbf{X}_0 \\ \hat{\mathbf{Y}}_0 &= \mathbf{t}\mathbf{c}', \quad \text{where } \mathbf{c}' = (\mathbf{t}'\mathbf{t})^{-1}\mathbf{t}'\mathbf{Y}_0\end{aligned}$$

The vectors  $\mathbf{p}$  and  $\mathbf{c}$  are called the *X-* and *Y-loadings*, respectively.

The specific linear combination  $\mathbf{t} = \mathbf{X}_0\mathbf{w}$  is the one that has maximum covariance  $\mathbf{t}'\mathbf{u}$  with some response linear combination  $\mathbf{u} = \mathbf{Y}_0\mathbf{q}$ . Another characterization is that the X- and Y-weights  $\mathbf{w}$  and  $\mathbf{q}$  are proportional to the first left and right singular vectors of the covariance matrix  $\mathbf{X}'_0\mathbf{Y}_0$  or, equivalently, the first eigenvectors of  $\mathbf{X}'_0\mathbf{Y}_0\mathbf{Y}'_0\mathbf{X}_0$  and  $\mathbf{Y}'_0\mathbf{X}_0\mathbf{X}'_0\mathbf{Y}_0$ , respectively.

This accounts for how the first PLS factor is extracted. The second factor is extracted in the same way by replacing  $\mathbf{X}_0$  and  $\mathbf{Y}_0$  with the X- and Y-residuals from the first factor:

$$\begin{aligned}\mathbf{X}_1 &= \mathbf{X}_0 - \hat{\mathbf{X}}_0 \\ \mathbf{Y}_1 &= \mathbf{Y}_0 - \hat{\mathbf{Y}}_0\end{aligned}$$

These residuals are also called the *deflated* X and Y blocks. The process of extracting a score vector and deflating the data matrices is repeated for as many extracted factors as are wanted.

## SIMPLS

Note that each extracted PLS factor is defined in terms of different X-variables  $\mathbf{X}_i$ . This leads to difficulties in comparing different scores, weights, and so forth. The SIMPLS method of de Jong (1993) overcomes these difficulties by computing each score  $t_i = \mathbf{X}\mathbf{r}_i$  in terms of the original (centered and scaled) predictors  $\mathbf{X}$ . The SIMPLS X-weight vectors  $\mathbf{r}_i$  are similar to the eigenvectors of  $\mathbf{S}\mathbf{S}' = \mathbf{X}'\mathbf{Y}\mathbf{Y}'\mathbf{X}$ , but they satisfy a different orthogonality condition. The  $\mathbf{r}_1$  vector is just the first eigenvector  $\mathbf{e}_1$  (so that the first SIMPLS score is the same as the first PLS score), but whereas the second eigenvector maximizes

$$\mathbf{e}'_1\mathbf{S}\mathbf{S}'\mathbf{e}_2 \text{ subject to } \mathbf{e}'_1\mathbf{e}_2 = 0$$

the second SIMPLS weight  $\mathbf{r}_2$  maximizes

$$\mathbf{r}'_1\mathbf{S}\mathbf{S}'\mathbf{r}_2 \text{ subject to } \mathbf{r}'_1\mathbf{X}'\mathbf{X}\mathbf{r}_2 = \mathbf{t}'_1\mathbf{t}_2 = 0$$

The SIMPLS scores are identical to the PLS scores for one response but slightly different for more than one response; see de Jong (1993) for details. The X- and Y-loadings are defined as in PLS, but since the scores are all defined in terms of  $\mathbf{X}$ , it is easy to compute the overall model coefficients  $\mathbf{B}$ :

$$\begin{aligned}\hat{\mathbf{Y}} &= \sum_i \mathbf{t}_i\mathbf{c}'_i \\ &= \sum_i \mathbf{X}\mathbf{r}_i\mathbf{c}'_i \\ &= \mathbf{X}\mathbf{B}, \text{ where } \mathbf{B} = \mathbf{R}\mathbf{C}'\end{aligned}$$

## Principal Components Regression

Like the SIMPLS method, principal components regression (PCR) defines all the scores in terms of the original (centered and scaled) predictors  $\mathbf{X}$ . However, unlike both the PLS and SIMPLS methods, the PCR method chooses the X-weights/X-scores without regard to the response data. The X-scores are chosen to explain as much variation in  $\mathbf{X}$  as possible; equivalently, the X-weights for the PCR method are the eigenvectors of the predictor covariance matrix  $\mathbf{X}'\mathbf{X}$ . Again, the X- and Y-loadings are defined as in PLS; but, as in SIMPLS, it is easy to compute overall model coefficients for the original (centered and scaled) responses  $\mathbf{Y}$  in terms of the original predictors  $\mathbf{X}$ .

## Reduced Rank Regression

As discussed in the preceding sections, partial least squares depends on selecting factors  $\mathbf{t} = \mathbf{X}\mathbf{w}$  of the predictors and  $\mathbf{u} = \mathbf{Y}\mathbf{q}$  of the responses that have maximum covariance, whereas principal components regression effectively ignores  $\mathbf{u}$  and selects  $\mathbf{t}$  to have maximum variance, subject to orthogonality constraints. In contrast, reduced rank regression selects  $\mathbf{u}$  to account for as much variation in the *predicted* responses as possible, effectively ignoring the predictors for the purposes of factor extraction. In reduced rank regression, the Y-weights  $\mathbf{q}_j$  are the eigenvectors of the covariance matrix  $\hat{\mathbf{Y}}'_{LS}\hat{\mathbf{Y}}_{LS}$  of the responses predicted by ordinary least squares regression; the X-scores are the projections of the Y-scores  $\mathbf{Y}\mathbf{q}_j$  onto the X space.

## Relationships between Methods

When you develop a predictive model, it is important to consider not only the explanatory power of the model for current responses, but also how well sampled the predictive functions are, since this affects how well the model can extrapolate to future observations. All of the techniques implemented in the PLS procedure work by extracting successive factors, or linear combinations of the predictors, that optimally address one or both of these two goals—explaining response variation and explaining predictor variation. In particular, principal components regression selects factors that explain as much predictor variation as possible, reduced rank regression selects factors that explain as much response variation as possible, and partial least squares balances the two objectives, seeking for factors that explain both response and predictor variation.

To see the relationships between these methods, consider how each one extracts a single factor from the following artificial data set consisting of two predictors and one response:

```
data data;
 input x1 x2 y;
 datalines;
 3.37651 2.30716 0.75615
 0.74193 -0.88845 1.15285
 4.18747 2.17373 1.42392
 0.96097 0.57301 0.27433
 -1.11161 -0.75225 -0.25410
 -1.38029 -1.31343 -0.04728
 1.28153 -0.13751 1.00341
 -1.39242 -2.03615 0.45518
 0.63741 0.06183 0.40699
 -2.52533 -1.23726 -0.91080
 2.44277 3.61077 -0.82590
 ;

proc pls data=data nfac=1 method=rrr;
 model y = x1 x2;
run;

proc pls data=data nfac=1 method=pcr;
 model y = x1 x2;
run;

proc pls data=data nfac=1 method=pls;
 model y = x1 x2;
run;
```



The amount of model and response variation explained by the first factor for each method is shown in Figure 70.9 through Figure 70.11.

**Figure 70.9** Variation Explained by First Reduced Rank Regression Factor

| The PLS Procedure                                                     |               |         |                     |          |
|-----------------------------------------------------------------------|---------------|---------|---------------------|----------|
| Percent Variation Accounted for by<br>Reduced Rank Regression Factors |               |         |                     |          |
| Number of<br>Extracted<br>Factors                                     | Model Effects |         | Dependent Variables |          |
|                                                                       | Current       | Total   | Current             | Total    |
| 1                                                                     | 15.0661       | 15.0661 | 100.0000            | 100.0000 |

**Figure 70.10** Variation Explained by First Principal Components Regression Factor

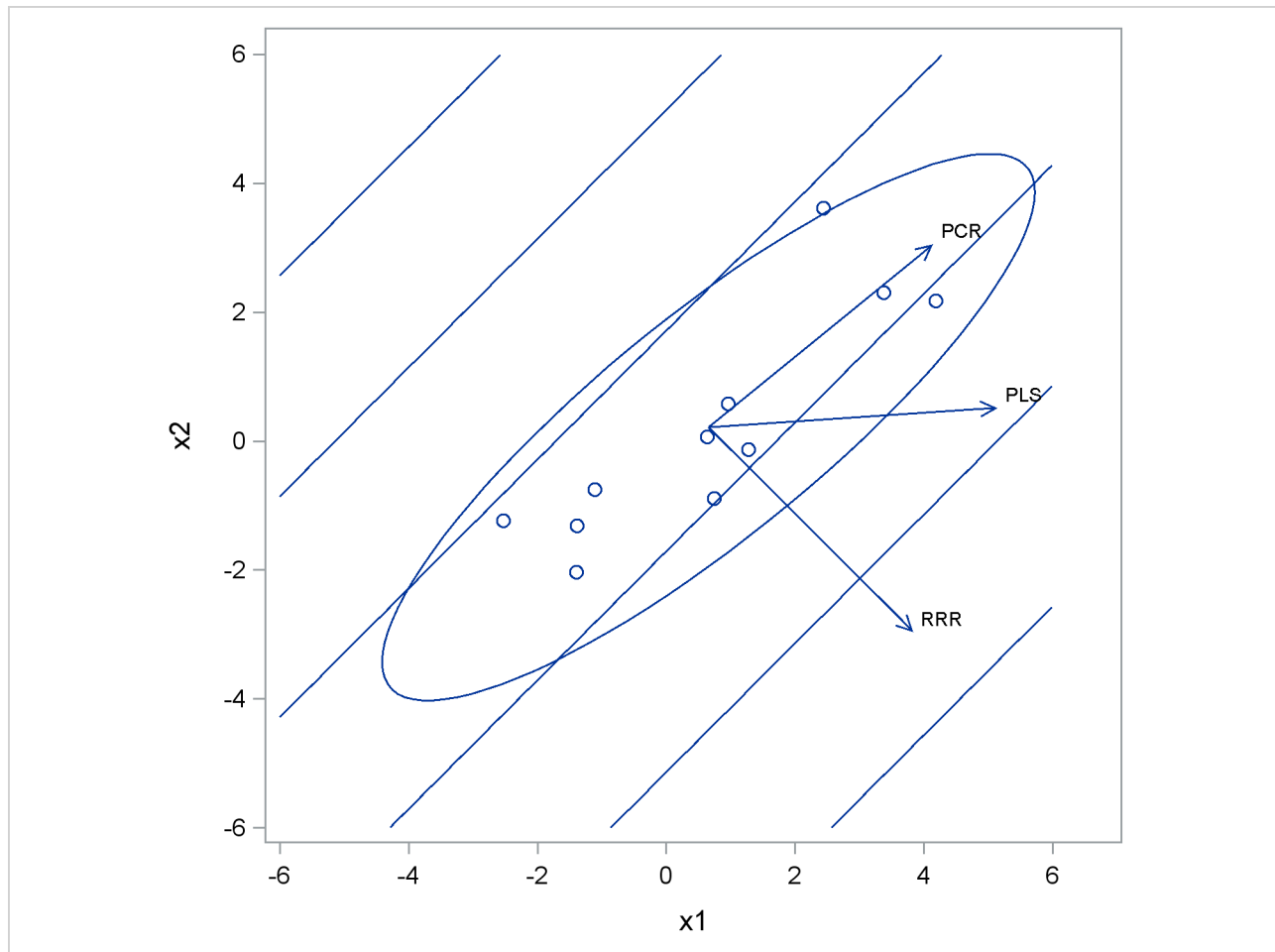
| The PLS Procedure                                       |               |         |                     |        |
|---------------------------------------------------------|---------------|---------|---------------------|--------|
| Percent Variation Accounted for by Principal Components |               |         |                     |        |
| Number of<br>Extracted<br>Factors                       | Model Effects |         | Dependent Variables |        |
|                                                         | Current       | Total   | Current             | Total  |
| 1                                                       | 92.9996       | 92.9996 | 9.3787              | 9.3787 |

**Figure 70.11** Variation Explained by First Partial Least Squares Regression Factor

| The PLS Procedure                                                   |               |         |                     |         |
|---------------------------------------------------------------------|---------------|---------|---------------------|---------|
| Percent Variation Accounted for<br>by Partial Least Squares Factors |               |         |                     |         |
| Number of<br>Extracted<br>Factors                                   | Model Effects |         | Dependent Variables |         |
|                                                                     | Current       | Total   | Current             | Total   |
| 1                                                                   | 88.5357       | 88.5357 | 26.5304             | 26.5304 |

Notice that, while the first reduced rank regression factor explains *all* of the response variation, it accounts for only about 15% of the predictor variation. In contrast, the first principal components regression factor accounts for most of the predictor variation (93%) but only 9% of the response variation. The first partial least squares factor accounts for only slightly less predictor variation than principal components but about three times as much response variation.

Figure 70.12 illustrates how partial least squares balances the goals of explaining response and predictor variation in this case.

**Figure 70.12** Depiction of First Factors for Three Different Regression Methods

The ellipse shows the general shape of the 11 observations in the predictor space, with the contours of increasing  $y$  overlaid. Also shown are the directions of the first factor for each of the three methods. Notice that, while the predictors vary most in the  $x_1 = x_2$  direction, the response changes most in the orthogonal  $x_1 = -x_2$  direction. This explains why the first principal component accounts for little variation in the response and why the first reduced rank regression factor accounts for little variation in the predictors. The direction of the first partial least squares factor represents a compromise between the other two directions.

---

## Cross Validation

None of the regression methods implemented in the PLS procedure fit the observed data any better than ordinary least squares (OLS) regression; in fact, all of the methods approach OLS as more factors are extracted. The crucial point is that, when there are many predictors, OLS can *overfit* the observed data; biased regression methods with fewer extracted factors can provide better predictability of *future* observations. However, as the preceding observations imply, the quality of the observed data fit cannot be used to choose the number of factors to extract; the number of extracted factors must be chosen on the basis of how well the model fits observations not involved in the modeling procedure itself.

One method of choosing the number of extracted factors is to fit the model to only part of the available data (the *training set*) and to measure how well models with different numbers of extracted factors fit the other part of the data (the *test set*). This is called *test set validation*. However, it is rare that you have enough data to make both parts large enough for pure test set validation to be useful. Alternatively, you can make several different divisions of the observed data into training set and test set. This is called *cross validation*, and there are several different types. In *one-at-a-time* cross validation, the first observation is held out as a single-element test set, with all other observations as the training set; next, the second observation is held out, then the third, and so on. Another method is to hold out successive blocks of observations as test sets—for example, observations 1 through 7, then observations 8 through 14, and so on; this is known as *blocked* validation. A similar method is *split-sample* cross validation, in which successive groups of widely separated observations are held out as the test set—for example, observations {1, 11, 21, ...}, then observations {2, 12, 22, ...}, and so on. Finally, test sets can be selected from the observed data randomly; this is known as *random sample* cross validation.

Which validation you should use depends on your data. Test set validation is preferred when you have enough data to make a division into a sizable training set and test set that represent the predictive population well. You can specify that the number of extracted factors be selected by test set validation by using the `CV=TESTSET(data set)` option, where *data set* is the name of the data set containing the test set. If you do not have enough data for test set validation, you can use one of the cross validation techniques. The most common technique is one-at-a-time validation (which you can specify with the `CV=ONE` option or just the `CV` option), unless the observed data are serially correlated, in which case either blocked or split-sample validation might be more appropriate (`CV=BLOCK` or `CV=SPLIT`); you can specify the number of test sets in blocked or split-sample validation with a number in parentheses after the `CV=` option. Note that `CV=ONE` is the most computationally intensive of the cross validation methods, since it requires a recomputation of the PLS model for every input observation. Also, note that using random subset selection with `CV=RANDOM` might lead two different researchers to produce different PLS models on the same data (unless the same seed is used).

Whichever validation method you use, the number of factors chosen is usually the one that minimizes the predicted residual sum of squares (PRESS); this is the default choice if you specify any of the CV methods with PROC PLS. However, often models with fewer factors have PRESS statistics that are only marginally larger than the absolute minimum. To address this, van der Voet (1994) has proposed a statistical test for comparing the predicted residuals from different models; when you apply van der Voet's test, the number of factors chosen is the fewest with residuals that are insignificantly larger than the residuals of the model with minimum PRESS.

To see how van der Voet's test works, let  $R_{i,jk}$  be the  $j$ th predicted residual for response  $k$  for the model with  $i$  extracted factors; the PRESS statistic is  $\sum_{jk} R_{i,jk}^2$ . Also, let  $i_{\min}$  be the number of factors for which PRESS is minimized. The critical value for van der Voet's test is based on the differences between squared predicted residuals

$$D_{i,jk} = R_{i,jk}^2 - R_{i_{\min},jk}^2$$

One alternative for the critical value is  $C_i = \sum_{jk} D_{i,jk}$ , which is just the difference between the PRESS statistics for  $i$  and  $i_{\min}$  factors; alternatively, van der Voet suggests Hotelling's  $T^2$  statistic  $C_i = \mathbf{d}'_i \mathbf{S}_i^{-1} \mathbf{d}_i$ , where  $\mathbf{d}_i$  is the sum of the vectors  $\mathbf{d}_{i,j} = \{D_{i,j1}, \dots, D_{i,jN_y}\}'$  and  $\mathbf{S}_i$  is the sum of squares and crossproducts matrix

$$\mathbf{S}_i = \sum_j \mathbf{d}_{i,j} \mathbf{d}'_{i,j}$$

Virtually, the significance level for van der Voet's test is obtained by comparing  $C_i$  with the distribution of values that result from randomly exchanging  $R_{i,jk}^2$  and  $R_{i_{\min},jk}^2$ . In practice, a Monte Carlo sample of such values is simulated and the significance level is approximated as the proportion of simulated critical values that are greater than  $C_i$ . If you apply van der Voet's test by specifying the **CVTEST** option, then, by default, the number of extracted factors chosen is the least number with an approximate significance level that is greater than 0.10.

## Centering and Scaling

By default, the predictors and the responses are centered and scaled to have mean 0 and standard deviation 1. Centering the predictors and the responses ensures that the criterion for choosing successive factors is based on how much *variation* they explain, in either the predictors or the responses or both. (See the section “Regression Methods” on page 5883 for more details on how different methods explain variation.) Without centering, both the mean variable value and the variation around that mean are involved in selecting factors. Scaling serves to place all predictors and responses on an equal footing relative to their variation in the data. For example, if Time and Temp are two of the predictors, then scaling says that a change of  $\text{std}(\text{Time})$  in Time is roughly equivalent to a change of  $\text{std}(\text{Temp})$  in Temp.

Usually, both the predictors and responses should be centered and scaled. However, if their values already represent variation around a nominal or target value, then you can use the **NOCENTER** option in the **PROC PLS** statement to suppress centering. Likewise, if the predictors or responses are already all on comparable scales, then you can use the **NOSCALE** option to suppress scaling.

Note that, if the predictors involve crossproduct terms, then, by default, the variables are *not* standardized before standardizing the crossproduct. That is, if the  $i$ th values of two predictors are denoted  $x_i^1$  and  $x_i^2$ , then the default standardized  $i$ th value of the crossproduct is

$$\frac{x_i^1 x_i^2 - \text{mean}_j(x_j^1 x_j^2)}{\text{std}_j(x_j^1 x_j^2)}$$

If you want the crossproduct to be based instead on standardized variables

$$\frac{x_i^1 - m^1}{s^1} \times \frac{x_i^2 - m^2}{s^2}$$

where  $m^k = \text{mean}_j(x_j^k)$  and  $s^k = \text{std}_j(x_j^k)$  for  $k = 1, 2$ , then you should use the **VARSCALE** option in the **PROC PLS** statement. Standardizing the variables separately is usually a good idea, but unless the model also contains all crossproducts nested within each term, the resulting model might not be equivalent to a simple linear model in the same terms. To see this, note that a model involving the crossproduct of two standardized variables

$$\frac{x_i^1 - m^1}{s^1} \times \frac{x_i^2 - m^2}{s^2} = x_i^1 x_i^2 \frac{1}{s^1 s^2} - x_i^1 \frac{m^2}{s^1 s^2} - x_i^2 \frac{m^1}{s^1 s^2} + \frac{m^1 m^2}{s^1 s^2}$$

involves both the crossproduct term and the linear terms for the unstandardized variables.

When cross validation is performed for the number of effects, there is some disagreement among practitioners as to whether each cross validation training set should be retransformed. By default, **PROC PLS** does so, but you can suppress this behavior by specifying the **NOCVSTDIZE** option in the **PROC PLS** statement.

---

## Missing Values

By default, PROC PLS handles missing values very simply. Observations with any missing independent variables (including all classification variables) are excluded from the analysis, and no predictions are computed for such observations. Observations with no missing independent variables but any missing dependent variables are also excluded from the analysis, but predictions are computed.

However, the **MISSING=** option in the **PROC PLS** statement provides more sophisticated ways of modeling in the presence of missing values. If you specify **MISSING=AVG** or **MISSING=EM**, then all observations in the input data set contribute to both the analysis and the **OUTPUT OUT=** data set. With **MISSING=AVG**, the fit is computed by filling in missing values with the average of the nonmissing values for the corresponding variable. With **MISSING=EM**, the procedure first computes the model with **MISSING=AVG**, then fills in missing values with their predicted values based on that model and computes the model again. Alternatively, you can specify **MISSING=EM(MAXITER=*n*)** with a large value of *n* in order to perform this imputation/fit loop until convergence.

---

## Displayed Output

By default, PROC PLS displays just the amount of predictor and response variation accounted for by each factor.

If you perform a cross validation for the number of factors by specifying the **CV** option in the **PROC PLS** statement, then the procedure displays a summary of the cross validation for each number of factors, along with information about the optimal number of factors.

If you specify the **DETAILS** option in the **PROC PLS** statement, then details of the fitted model are displayed for each successive factor. These details for each number of factors include the following:

- the predictor loadings
- the predictor weights
- the response weights
- the coded regression coefficients (for **METHOD=SIMPLS**, **PCR**, or **RRR**)

If you specify the **CENSCALE** option in the **PROC PLS** statement, then centering and scaling information for each response and predictor is displayed.

If you specify the **VARSS** option in the **PROC PLS** statement, the procedure displays, in addition to the average response and predictor sum of squares accounted for by each successive factor, the amount of variation accounted for in each response and predictor.

If you specify the **SOLUTION** option in the **MODEL** statement, then PROC PLS displays the coefficients of the final predictive model for the responses. The coefficients for predicting the centered and scaled responses based on the centered and scaled predictors are displayed, as well as the coefficients for predicting the raw responses based on the raw predictors.

## ODS Table Names

PROC PLS assigns a name to each table it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in Table 70.3. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

**Table 70.3** ODS Tables Produced by PROC PLS

| ODS Table Name     | Description                                               | Statement | Option                |
|--------------------|-----------------------------------------------------------|-----------|-----------------------|
| CVResults          | Results of cross validation                               | PROC      | CV                    |
| CenScaleParms      | Parameter estimates for centered and scaled data          | MODEL     | SOLUTION              |
| CodedCoef          | Coded coefficients                                        | PROC      | DETAILS               |
| MissingIterations  | Iterations for missing value imputation                   | PROC      | MISSING=EM            |
| ModelInfo          | Model information                                         | PROC      | default               |
| NObs               | Number of observations                                    | PROC      | default               |
| ParameterEstimates | Parameter estimates for raw data                          | MODEL     | SOLUTION              |
| PercentVariation   | Variation accounted for by each factor                    | PROC      | default               |
| ResidualSummary    | Residual summary from cross validation                    | PROC      | CV                    |
| XEffectCenScale    | Centering and scaling information for predictor effects   | PROC      | CENSACLE              |
| XLoadings          | Loadings for independents                                 | PROC      | DETAILS               |
| XVariableCenScale  | Centering and scaling information for predictor variables | PROC      | CENSACLE and VARSCALE |
| XWeights           | Weights for independents                                  | PROC      | DETAILS               |
| YVariableCenScale  | Centering and scaling information for responses           | PROC      | CENSACLE              |
| YWeights           | Weights for dependents                                    | PROC      | DETAILS               |

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “Statistical Graphics Using ODS.”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “A Primer on ODS Statistical Graphics” on page 599 in Chapter 21, “Statistical Graphics Using ODS.”

When ODS Graphics is enabled, by default the PLS procedure produces a plot of the variation accounted for by each extracted factor, as well as a *correlation loading plot* for the first two extracted factors (if the final model has at least two factors). The plot of the variation accounted for can take several forms:

- If the PLS analysis does not include cross validation, then the plot shows the total R square for both model effects and the dependent variables against the number of factors.
- If you specify the **CV=** option to select the number of factors in the final model by cross validation, then the plot shows the R-square analysis discussed previously as well as the root mean PRESS from the cross validation analysis, with the selected number of factors identified by a vertical line.

The correlation loading plot for the first two factors summarizes many aspects of the two most significant dimensions of the model. It consists of overlaid scatter plots of the scores of the first two factors, the loadings of the model effects, and the loadings of the dependent variables. The loadings are scaled so that the amount of variation in the variables that is explained by the model is proportional to the distance from the origin; circles indicating various levels of explained variation are also overlaid on the correlation loading plot. Also, the correlation between the model approximations for any two variables is proportional to the length of the projection of the point corresponding to one variable on a line through the origin passing through the point corresponding to the other variable; the sign of the correlation corresponds to which side of the origin the projected point falls on.

The R square and the first two correlation loadings are plotted by default when ODS Graphics is enabled, but you can produce many other plots for the PROC PLS analysis.

## ODS Graph Names

PROC PLS assigns a name to each graph it creates using ODS. You can use these names to reference the graphs when using ODS. The names are listed in [Table 70.4](#).

**Table 70.4** Graphs Produced by PROC PLS

| ODS Graph Name         | Plot Description                                                 | Option                         |
|------------------------|------------------------------------------------------------------|--------------------------------|
| CorrLoadPlot           | Correlation loading plot (default)                               | PLOT=CORRLOAD( <i>option</i> ) |
| CVPlot                 | Cross validation and R-square analysis (default, as appropriate) | CV=                            |
| DModXPlot              | Distance of each observation to the X model                      | PLOT=DMODX                     |
| DModXYPlot             | Distance of each observation to the X and Y models               | PLOT=DMODXY                    |
| DModYPlot              | Distance of each observation to the Y model                      | PLOT=DMODY                     |
| DiagnosticsPanel       | Panel of diagnostic plots for the fit                            | PLOT=DIAGNOSTICS               |
| AbsResidualByPredicted | Absolute residual by predicted values                            | PLOT=DIAGNOSTICS(UNPACK)       |
| ObservedByPredicted    | Observed by predicted                                            | PLOT=DIAGNOSTICS(UNPACK)       |
| QQPlot                 | Residual Q-Q plot                                                | PLOT=DIAGNOSTICS(UNPACK)       |
| ResidualByPredicted    | Residual by predicted values                                     | PLOT=DIAGNOSTICS(UNPACK)       |
| ResidualHistogram      | Residual histogram                                               | PLOT=DIAGNOSTICS(UNPACK)       |
| RFPlot                 | RF plot                                                          | PLOT=DIAGNOSTICS(UNPACK)       |

Table 70.4 *continued*

| ODS Graph Name         | Plot Description                                     | Option                |
|------------------------|------------------------------------------------------|-----------------------|
| ParmProfiles           | Profiles of regression coefficients                  | PLOT=PARMPROFILES     |
| R2Plot                 | R-square analysis (default, as appropriate)          |                       |
| ResidualPlots          | Residuals for each dependent variable                | PLOT=RESIDUALS        |
| VariableImportancePlot | Profile of variable importance factors               | PLOT=VIP              |
| XLoadingPlot           | Scatter plot matrix of X-loadings against each other | PLOT=XLOADINGPLOT     |
| XLoadingProfiles       | Profiles of the X-loadings                           | PLOT=XLOADINGPROFILES |
| XScorePlot             | Scatter plot matrix of X-scores against each other   | PLOT=XSCORES          |
| XWeightPlot            | Scatter plot matrix of X-weights against each other  | PLOT=XWEIGHTPLOT      |
| XWeightProfiles        | Profiles of the X-weights                            | PLOT=XWEIGHTPROFILES  |
| XYScorePlot            | Scatter plot matrix of X-scores against Y-scores     | PLOT=XYSCORES         |
| YScorePlot             | Scatter plot matrix of Y-scores against each other   | PLOT=YSCORES          |
| YWeightPlot            | Scatter plot matrix of Y-weights against each other  | PLOT=YWEIGHTPLOT      |

---

## Examples: PLS Procedure

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### Example 70.1: Examining Model Details

This example, from Umetrics (1995), demonstrates different ways to examine a PLS model. The data come from the field of drug discovery. New drugs are developed from chemicals that are biologically active. Testing a compound for biological activity is an expensive procedure, so it is useful to be able to predict biological activity from cheaper chemical measurements. In fact, computational chemistry makes it possible to calculate certain chemical measurements without even making the compound. These measurements include size, lipophilicity, and polarity at various sites on the molecule. The following statements create a data set named `pentaTrain`, which contains these data.



```

data pentaTrain;
 input obsnam $ S1 L1 P1 S2 L2 P2
 S3 L3 P3 S4 L4 P4
 S5 L5 P5 log_RAI @@;

 n = _n_;
 datalines;
VESSK -2.6931 -2.5271 -1.2871 3.0777 0.3891 -0.0701
 1.9607 -1.6324 0.5746 1.9607 -1.6324 0.5746
 2.8369 1.4092 -3.1398 0.00
VESAK -2.6931 -2.5271 -1.2871 3.0777 0.3891 -0.0701
 1.9607 -1.6324 0.5746 0.0744 -1.7333 0.0902
 2.8369 1.4092 -3.1398 0.28
VEASK -2.6931 -2.5271 -1.2871 3.0777 0.3891 -0.0701
 0.0744 -1.7333 0.0902 1.9607 -1.6324 0.5746
 2.8369 1.4092 -3.1398 0.20
VEAAK -2.6931 -2.5271 -1.2871 3.0777 0.3891 -0.0701
 0.0744 -1.7333 0.0902 0.0744 -1.7333 0.0902
 2.8369 1.4092 -3.1398 0.51
VKAAK -2.6931 -2.5271 -1.2871 2.8369 1.4092 -3.1398
 0.0744 -1.7333 0.0902 0.0744 -1.7333 0.0902
 2.8369 1.4092 -3.1398 0.11
VEWAK -2.6931 -2.5271 -1.2871 3.0777 0.3891 -0.0701
 -4.7548 3.6521 0.8524 0.0744 -1.7333 0.0902
 2.8369 1.4092 -3.1398 2.73
VEAAP -2.6931 -2.5271 -1.2871 3.0777 0.3891 -0.0701
 0.0744 -1.7333 0.0902 0.0744 -1.7333 0.0902
 -1.2201 0.8829 2.2253 0.18
VEHAK -2.6931 -2.5271 -1.2871 3.0777 0.3891 -0.0701
 2.4064 1.7438 1.1057 0.0744 -1.7333 0.0902
 2.8369 1.4092 -3.1398 1.53
VAAAK -2.6931 -2.5271 -1.2871 0.0744 -1.7333 0.0902
 0.0744 -1.7333 0.0902 0.0744 -1.7333 0.0902
 2.8369 1.4092 -3.1398 -0.10
GEAAK 2.2261 -5.3648 0.3049 3.0777 0.3891 -0.0701
 0.0744 -1.7333 0.0902 0.0744 -1.7333 0.0902
 2.8369 1.4092 -3.1398 -0.52
LEAAK -4.1921 -1.0285 -0.9801 3.0777 0.3891 -0.0701
 0.0744 -1.7333 0.0902 0.0744 -1.7333 0.0902
 2.8369 1.4092 -3.1398 0.40
FEAAK -4.9217 1.2977 0.4473 3.0777 0.3891 -0.0701
 0.0744 -1.7333 0.0902 0.0744 -1.7333 0.0902
 2.8369 1.4092 -3.1398 0.30
VEGGK -2.6931 -2.5271 -1.2871 3.0777 0.3891 -0.0701
 2.2261 -5.3648 0.3049 2.2261 -5.3648 0.3049
 2.8369 1.4092 -3.1398 -1.00
VEFAK -2.6931 -2.5271 -1.2871 3.0777 0.3891 -0.0701
 -4.9217 1.2977 0.4473 0.0744 -1.7333 0.0902
 2.8369 1.4092 -3.1398 1.57
VELAK -2.6931 -2.5271 -1.2871 3.0777 0.3891 -0.0701
 -4.1921 -1.0285 -0.9801 0.0744 -1.7333 0.0902
 2.8369 1.4092 -3.1398 0.59
;

```

You would like to study the relationship between these measurements and the activity of the compound, represented by the logarithm of the relative Bradykinin activating activity (log\_RAI). Notice that these data consist of many predictors relative to the number of observations. Partial least squares is especially appropriate in this situation as a useful tool for finding a few underlying predictive factors that account for most of the variation in the response. Typically, the model is fit for part of the data (the “training” or “work” set), and the quality of the fit is judged by how well it predicts the other part of the data (the “test” or “prediction” set). For this example, the first 15 observations serve as the training set and the rest constitute the test set (see Ufkes et al. 1978, 1982).

When you fit a PLS model, you hope to find a few PLS factors that explain most of the variation in both predictors and responses. Factors that explain response variation provide good predictive models for new responses, and factors that explain predictor variation are well represented by the observed values of the predictors. The following statements fit a PLS model with two factors and save predicted values, residuals, and other information for each data point in a data set named outpls.

```
proc pls data=pentaTrain;
 model log_RAI = S1-S5 L1-L5 P1-P5;
run;
```

The PLS procedure displays a table, shown in [Output 70.1.1](#), showing how much predictor and response variation is explained by each PLS factor.

**Output 70.1.1** Amount of Training Set Variation Explained

| The PLS Procedure                                                   |               |          |                     |         |  |
|---------------------------------------------------------------------|---------------|----------|---------------------|---------|--|
| Percent Variation Accounted for<br>by Partial Least Squares Factors |               |          |                     |         |  |
| Number of<br>Extracted<br>Factors                                   | Model Effects |          | Dependent Variables |         |  |
|                                                                     | Current       | Total    | Current             | Total   |  |
| 1                                                                   | 16.9014       | 16.9014  | 89.6399             | 89.6399 |  |
| 2                                                                   | 12.7721       | 29.6735  | 7.8368              | 97.4767 |  |
| 3                                                                   | 14.6554       | 44.3289  | 0.4636              | 97.9403 |  |
| 4                                                                   | 11.8421       | 56.1710  | 0.2485              | 98.1889 |  |
| 5                                                                   | 10.5894       | 66.7605  | 0.1494              | 98.3383 |  |
| 6                                                                   | 5.1876        | 71.9481  | 0.2617              | 98.6001 |  |
| 7                                                                   | 6.1873        | 78.1354  | 0.2428              | 98.8428 |  |
| 8                                                                   | 7.2252        | 85.3606  | 0.1926              | 99.0354 |  |
| 9                                                                   | 6.7285        | 92.0891  | 0.0725              | 99.1080 |  |
| 10                                                                  | 7.9076        | 99.9967  | 0.0000              | 99.1080 |  |
| 11                                                                  | 0.0033        | 100.0000 | 0.0099              | 99.1179 |  |
| 12                                                                  | 0.0000        | 100.0000 | 0.0000              | 99.1179 |  |
| 13                                                                  | 0.0000        | 100.0000 | 0.0000              | 99.1179 |  |
| 14                                                                  | 0.0000        | 100.0000 | 0.0000              | 99.1179 |  |
| 15                                                                  | 0.0000        | 100.0000 | 0.0000              | 99.1179 |  |

From [Output 70.1.1](#), note that 97% of the response variation is already explained by just two factors, but only 29% of the predictor variation is explained.

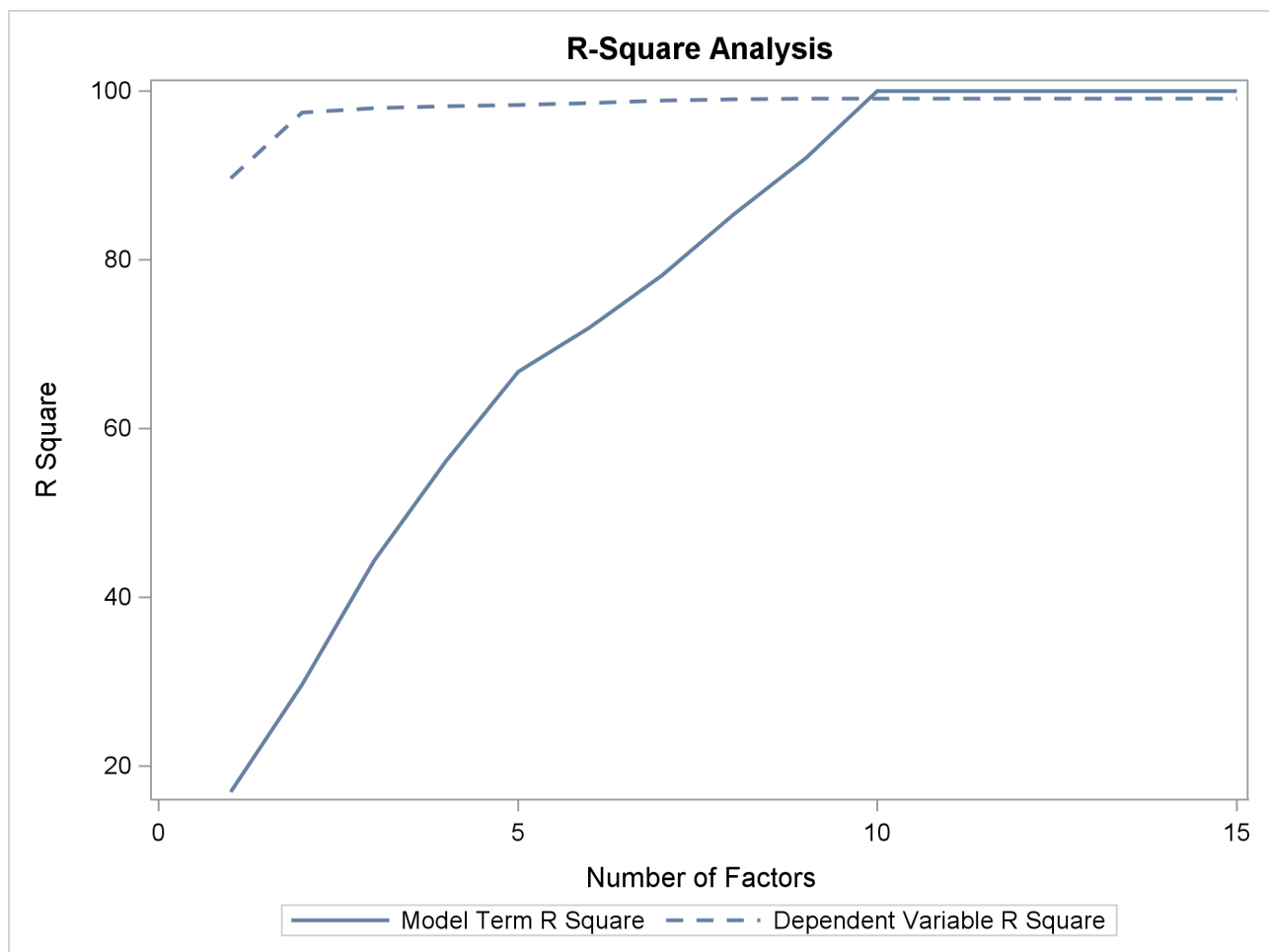
The graphics in PROC PLS, available when ODS Graphics is enabled, make it easier to see features of the PLS model.

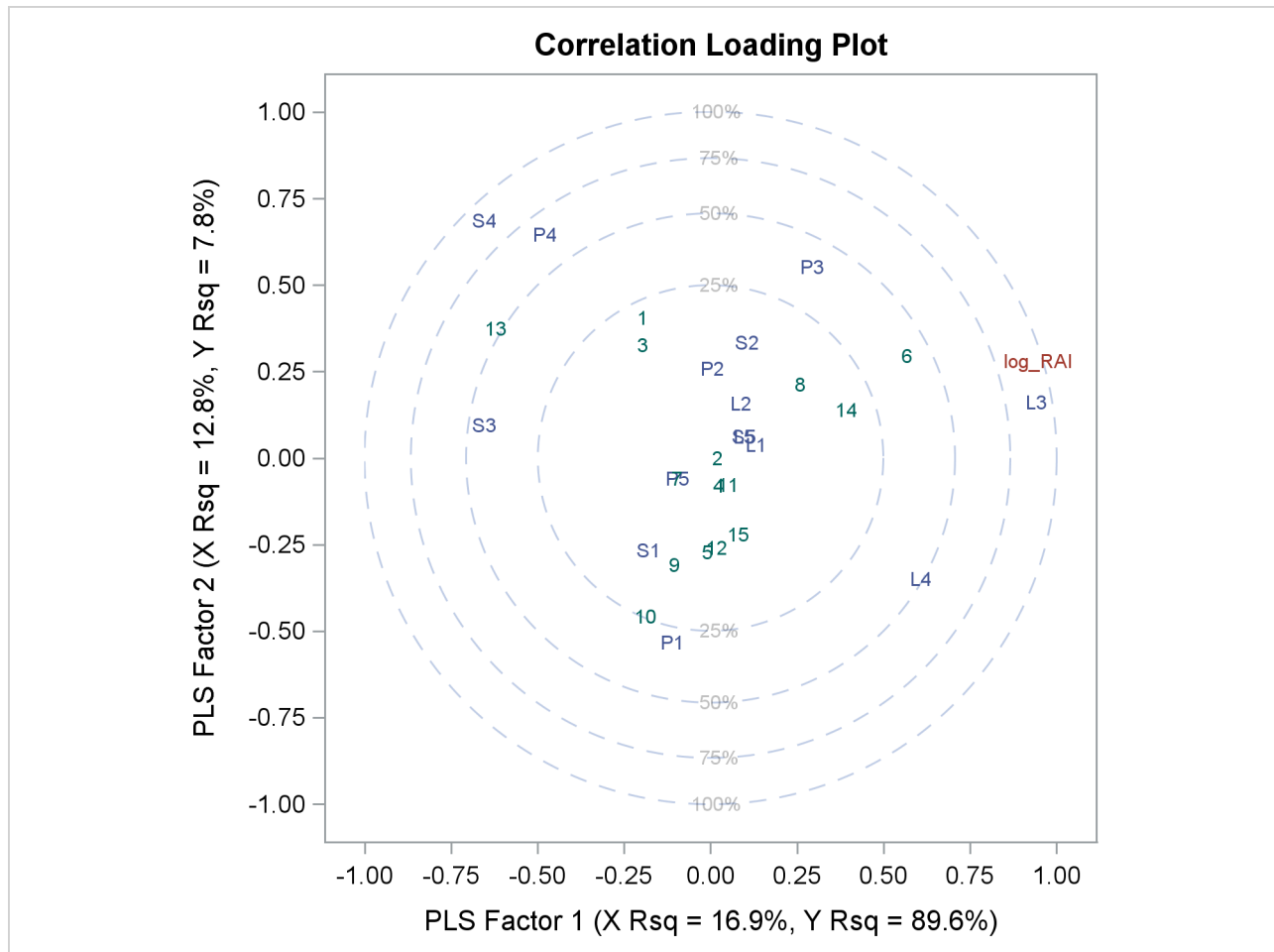
If ODS Graphics is enabled, then in addition to the tables discussed previously, PROC PLS displays a graphical depiction of the R-square analysis as well as a correlation loadings plot summarizing the model based on the first two PLS factors. The following statements perform the previous analysis with ODS Graphics enabled, producing [Output 70.1.2](#) and [Output 70.1.3](#).

```
ods graphics on;

proc pls data=pentaTrain;
 model log_RAI = S1-S5 L1-L5 P1-P5;
run;
```

**Output 70.1.2** Plot of Proportion of Variation Accounted For



**Output 70.1.3** Correlation Loadings Plot

The plot in [Output 70.1.2](#) of the proportion of variation explained (or R square) makes it clear that there is a plateau in the response variation after two factors are included in the model. The correlation loading plot in [Output 70.1.3](#) summarizes many features of this two-factor model, including the following:

- The X-scores are plotted as numbers for each observation. You should look for patterns or clearly grouped observations. If you see a curved pattern, for example, you might want to add a quadratic term. Two or more groupings of observations indicate that it might be better to analyze the groups separately, perhaps by including classification effects in the model. This plot appears to show most of the observations close together, with a few being more spread out with larger positive X-scores for factor 2. There are no clear grouping patterns, but observation 13 stands out.
- The loadings show how much variation in each variable is accounted for by the first two factors, jointly by the distance of the corresponding point from the origin and individually by the distance for the projections of this point onto the horizontal and vertical axes. That the dependent variable is well explained by the model is reflected in the fact that the point for `log_RAI` is near the 100% circle.
- You can also use the projection interpretation to relate variables to each other. For example, projecting other variables' points onto the line that runs through the `log_RAI` point and the origin, you can see that the PLS approximation for the predictor `L3` is highly positively correlated with `log_RAI`, `S3` is

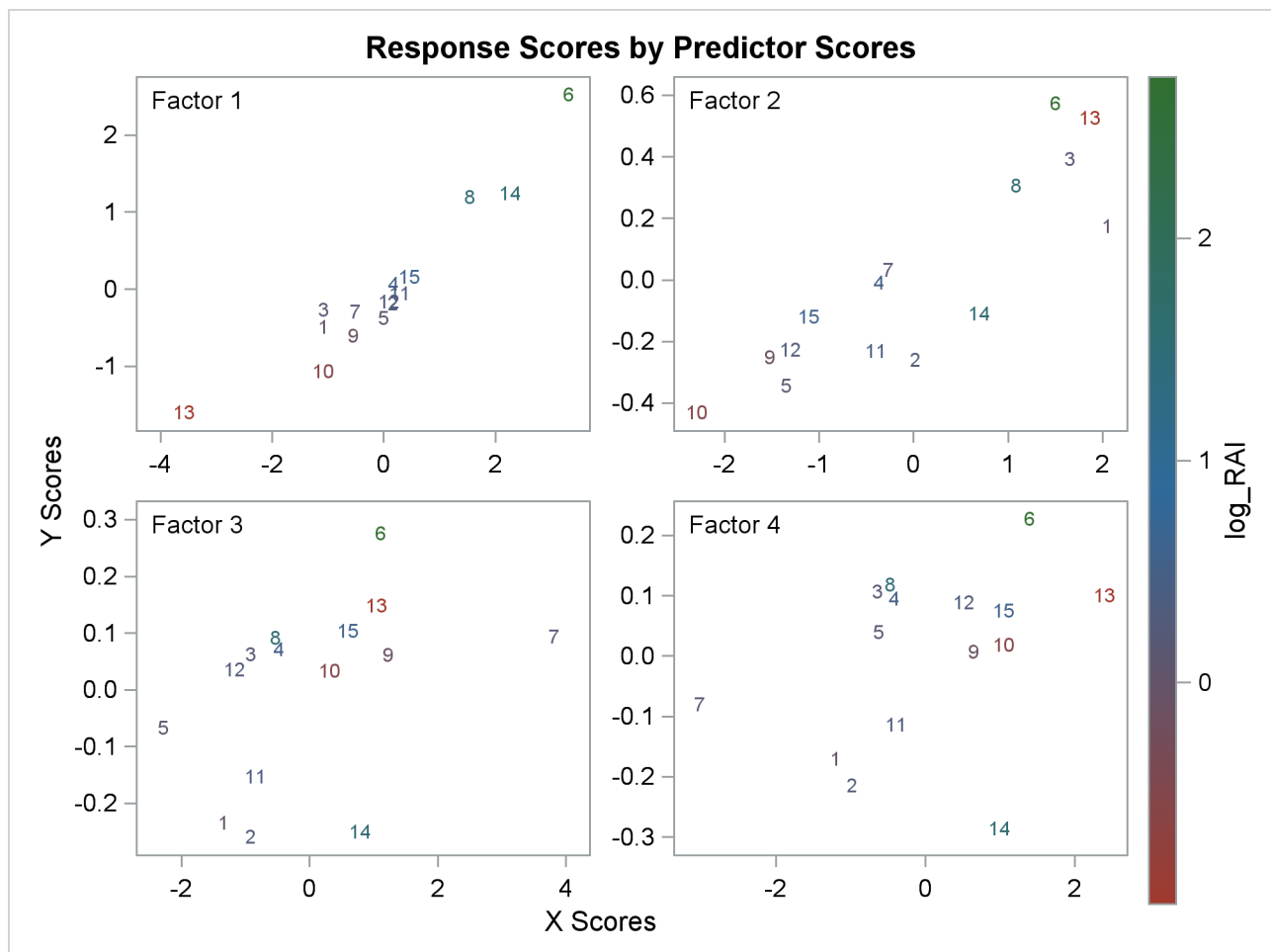
somewhat less correlated but in the negative direction, and several predictors including L1, L5, and S5 have very little correlation with log\_RAI.

Other graphics enable you to explore more of the features of the PLS model. For example, you can examine the X-scores versus the Y-scores to explore how partial least squares chooses successive factors. For a good PLS model, the first few factors show a high correlation between the X- and Y-scores. The correlation usually decreases from one factor to the next. When ODS Graphics is enabled, you can plot the X-scores versus the Y-scores by using the `PLOT=XYSCORES` option, as shown in the following statements.

```
proc pls data=pentaTrain nfac=4 plot=XYScores;
 model log_RAI = S1-S5 L1-L5 P1-P5;
run;
```

The plot of the X-scores versus the Y-scores for the first four factors is shown in [Output 70.1.4](#).

**Output 70.1.4** X-Scores versus Y-Scores



For this example, [Output 70.1.4](#) shows high correlation between X- and Y-scores for the first factor but somewhat lower correlation for the second factor and sharply diminishing correlation after that. This adds strength to the judgment that `NFAC=2` is the right number of factors for these data and this model. Note that observation 13 is again extreme in the first two plots. This run might be overly influential for the PLS analysis; thus, you should check to make sure it is reliable.

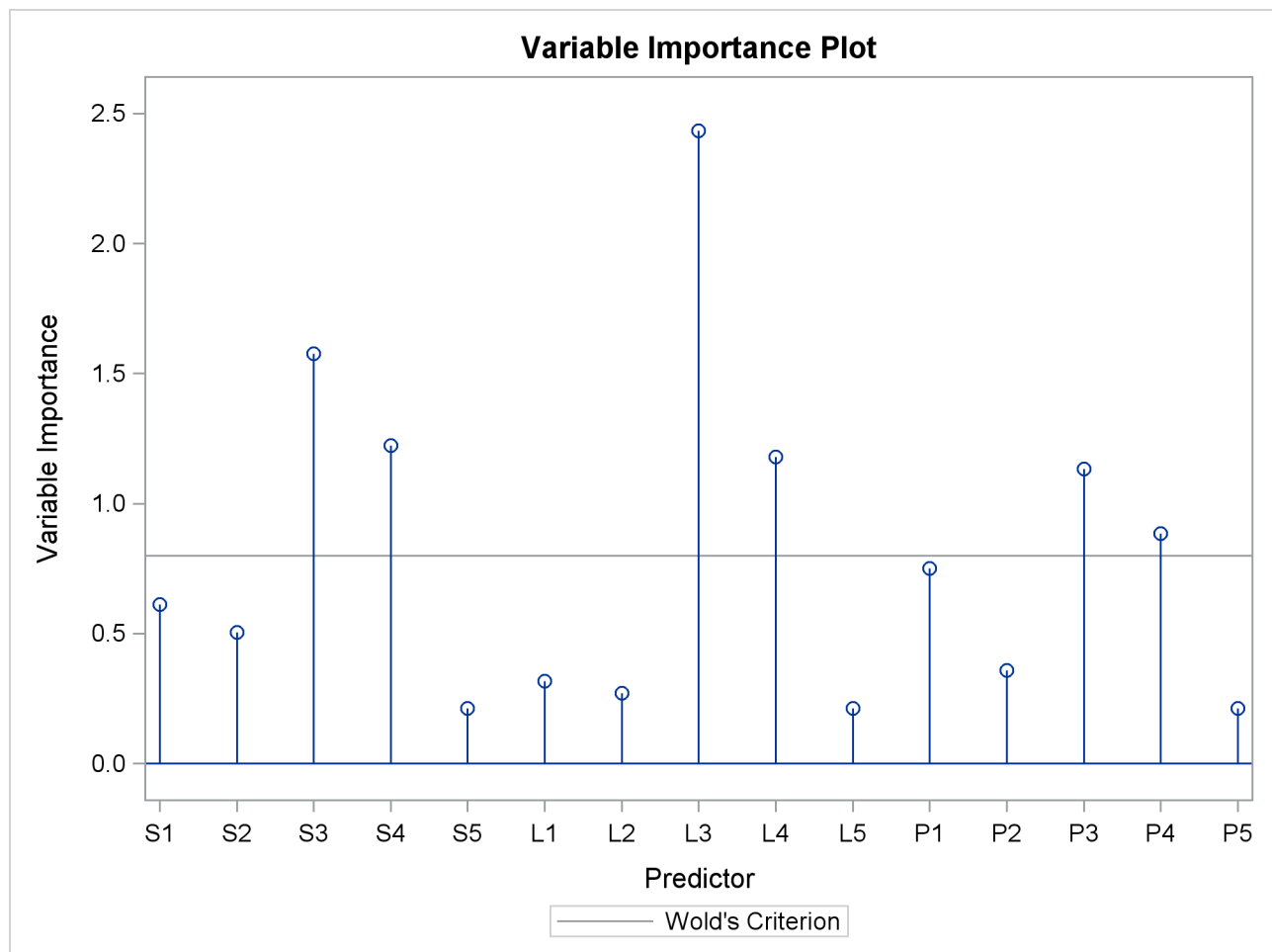
As explained earlier, you can draw some inferences about the relationship between individual predictors and the dependent variable from the correlation loading plot. However, the regression coefficient profile and the variable importance plot give a more direct indication of which predictors are most useful for predicting the dependent variable. The regression coefficients represent the importance each predictor has in the prediction of just the response. The variable importance plot, on the other hand, represents the contribution of each predictor in fitting the PLS model for both predictors and response. It is based on the *Variable Importance for Projection* (VIP) statistic of Wold (1994), which summarizes the contribution a variable makes to the model. If a predictor has a relatively small coefficient (in absolute value) *and* a small value of VIP, then it is a prime candidate for deletion. Wold in Umetrics (1995) considers a value less than 0.8 to be “small” for the VIP. The following statements fit a two-factor PLS model and display these two additional plots.

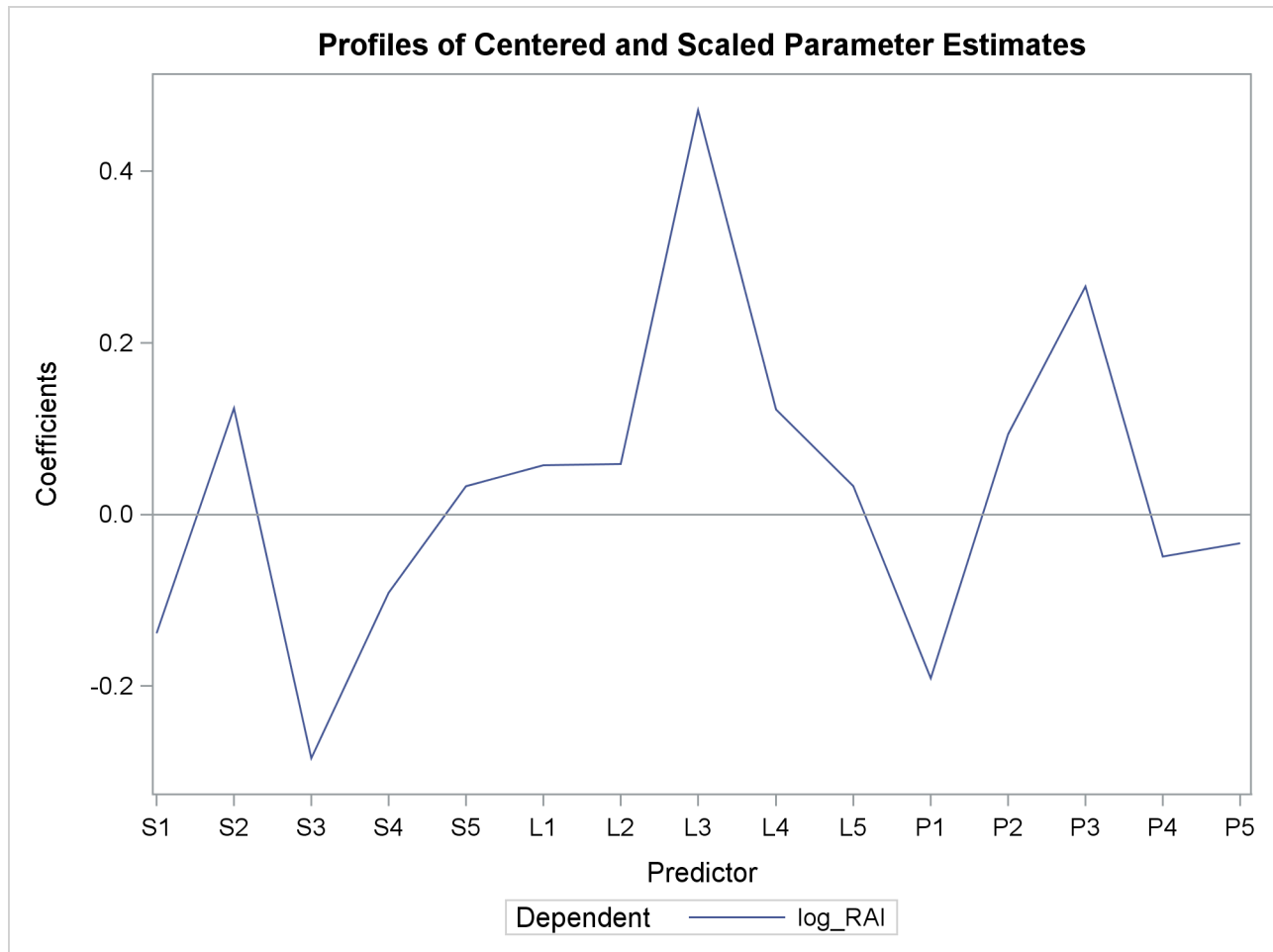
```
proc pls data=pentaTrain nfac=2 plot=(ParmProfiles VIP);
 model log_RAI = S1-S5 L1-L5 P1-P5;
run;

ods graphics off;
```

The additional graphics are shown in [Output 70.1.5](#) and [Output 70.1.6](#).

**Output 70.1.5** Variable Importance Plots



**Output 70.1.6** Regression Parameter Profile

In these two plots, the variables L1, L2, P2, S5, L5, and P5 have small absolute coefficients and small VIP. Looking back at the correlation loadings plot in [Output 70.1.2](#), you can see that these variables tend to be the ones near zero for both PLS factors. You should consider dropping these variables from the model.

## Example 70.2: Examining Outliers

This example is a continuation of [Example 70.1](#).

Standard diagnostics for statistical models focus on the response, allowing you to look for patterns that indicate the model is inadequate or for outliers that do not seem to follow the trend of the rest of the data. However, partial least squares effectively models the predictors as well as the responses, so you should consider the pattern of the fit for both. The DModX and DModY statistics give the distance from each point to the PLS model with respect to the predictors and the responses, respectively, and ODS Graphics enables you to plot these values. No point should be dramatically farther from the model than the rest. If there is a group of points that are all farther from the model than the rest, they might have something in common, in which case they should be analyzed separately.

The following statements fit a reduced model to the data discussed in [Example 70.1](#) and plot a panel of standard diagnostics as well as the distances of the observations to the model.

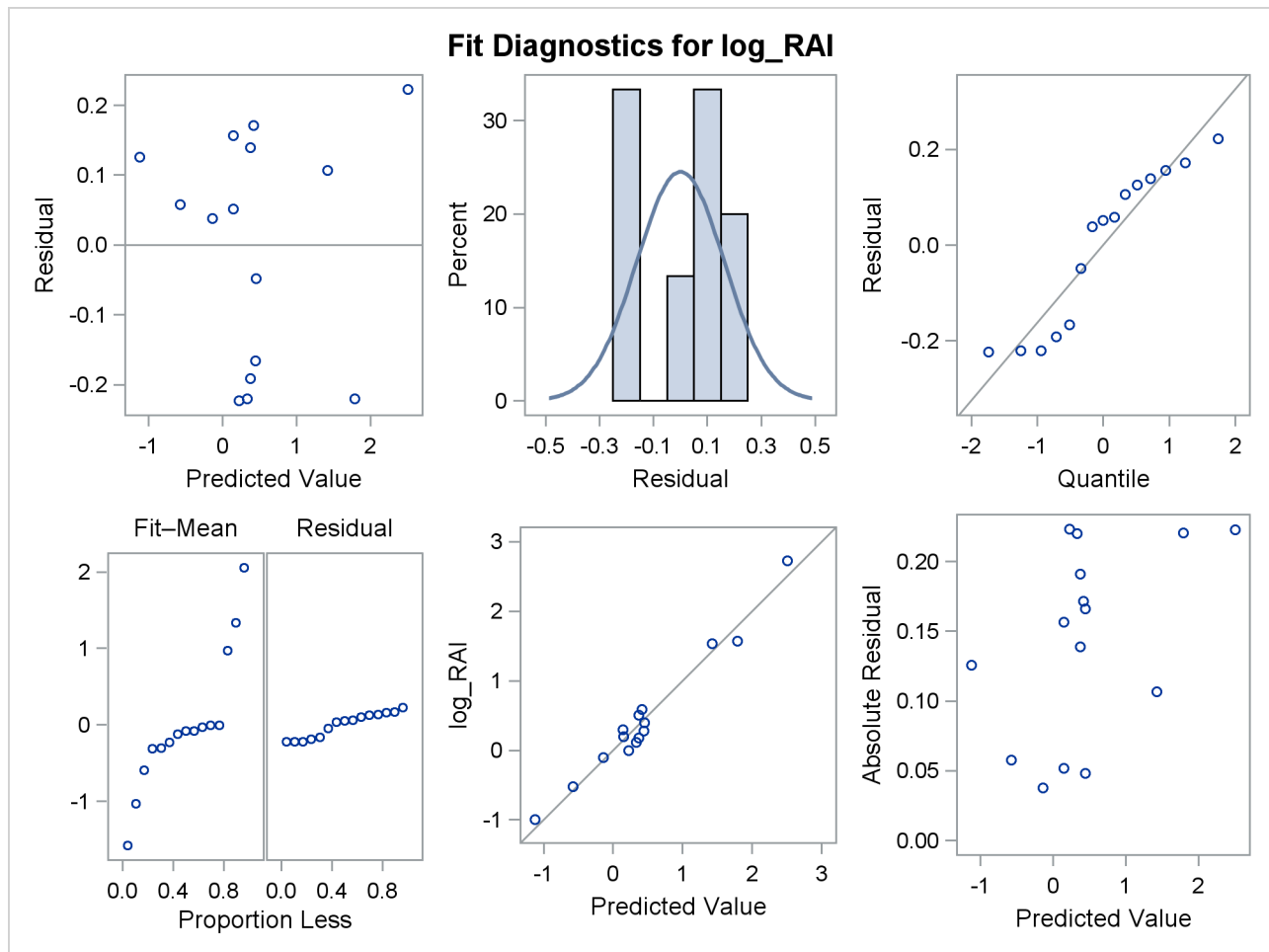
```
ods graphics on;

proc pls data=pentaTrain nfac=2 plot=(diagnostics dmod);
 model log_RAI = S1 P1
 S2
 S3 L3 P3
 S4 L4 ;
run;

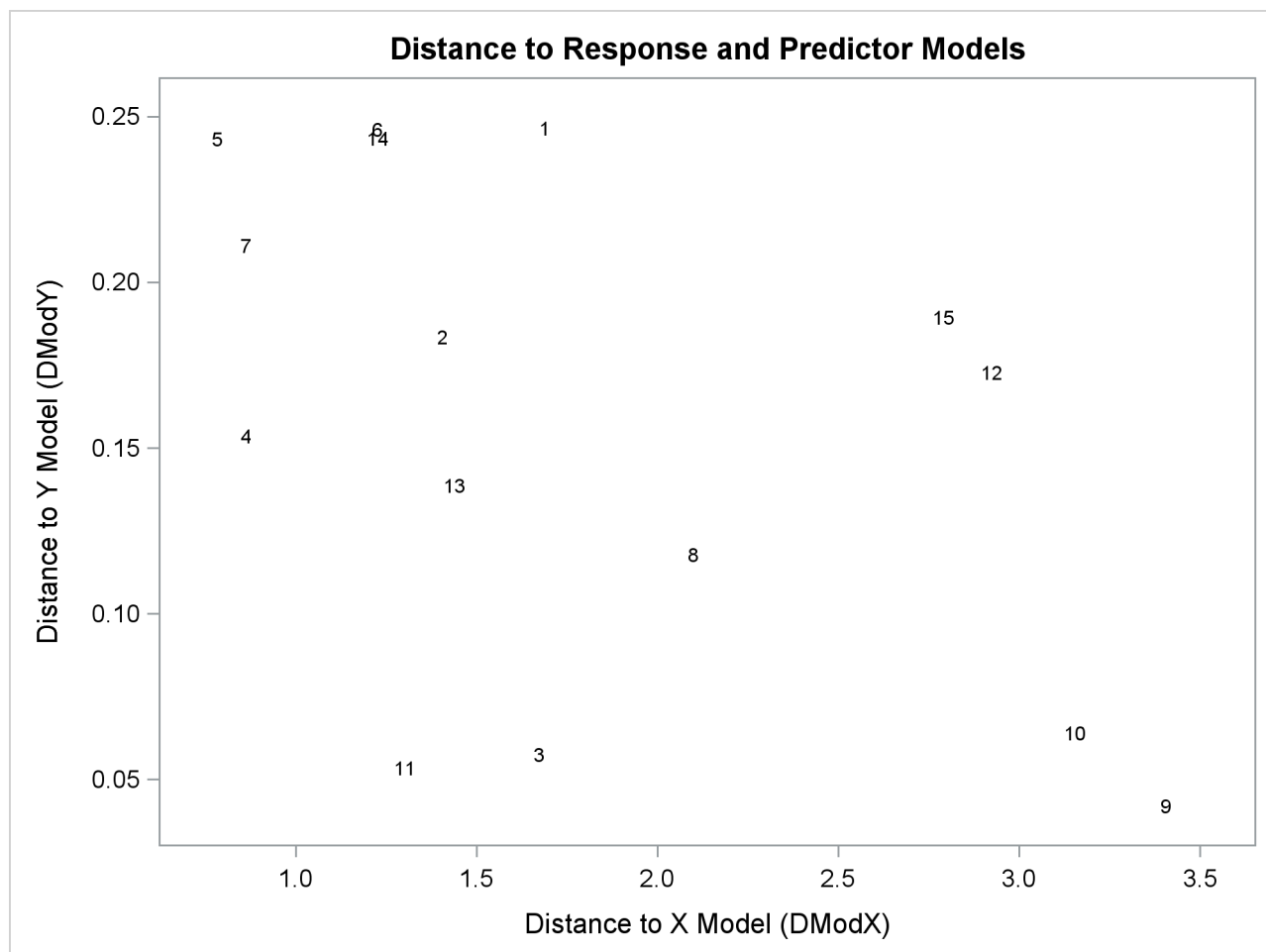
ods graphics off;
```

The plots are shown in [Output 70.2.1](#) and [Output 70.2.2](#).

**Output 70.2.1** Model Fit Diagnostics



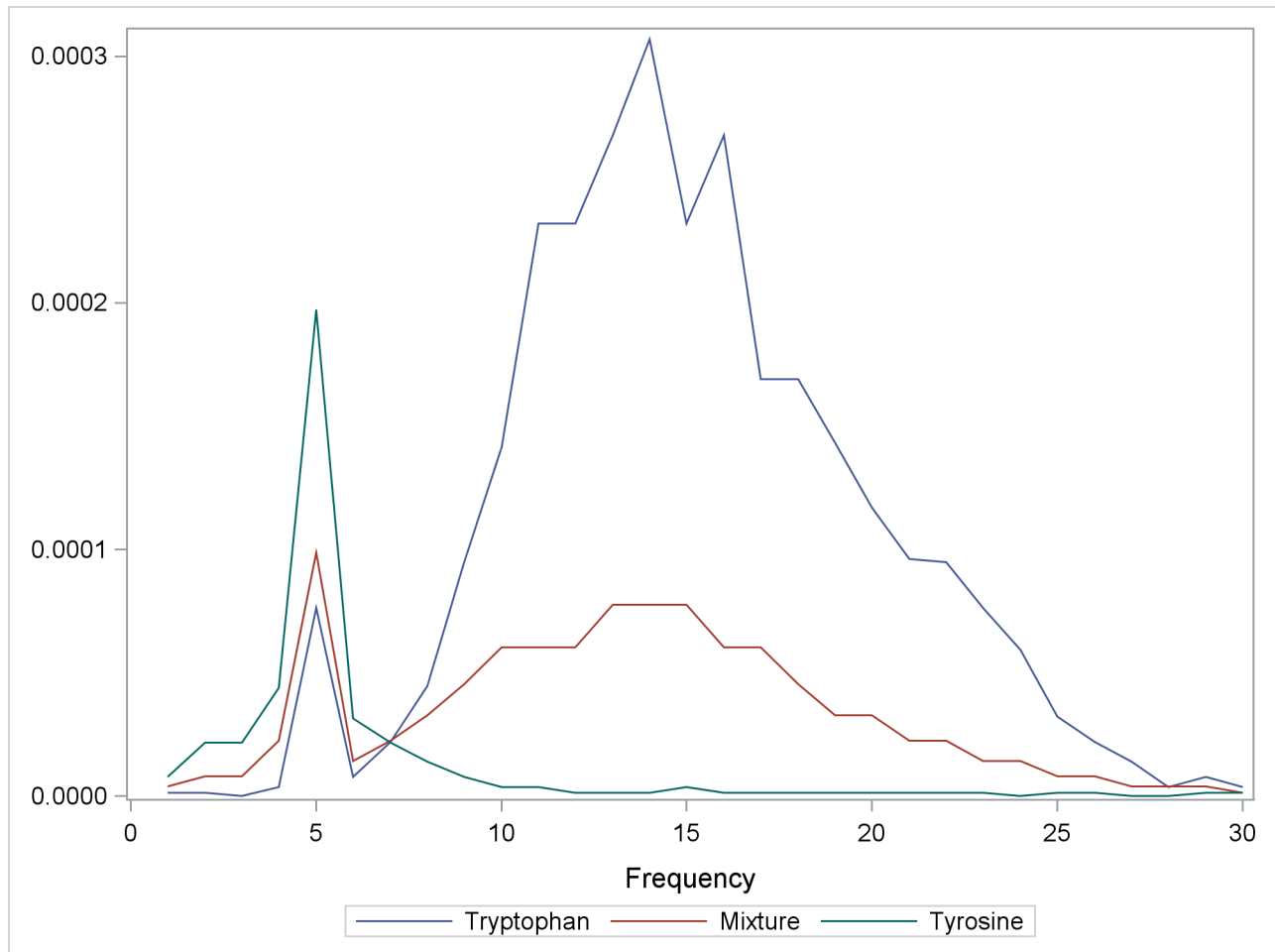


**Output 70.2.2** Predictor versus Response Distances to the Model

There appear to be no profound outliers in either the predictor space or the response space.

### Example 70.3: Choosing a PLS Model by Test Set Validation

This example demonstrates issues in spectrometric calibration. The data (Umetrics 1995) consist of spectrographic readings on 33 samples containing known concentrations of two amino acids, tyrosine and tryptophan. The spectra are measured at 30 frequencies across the overall range of frequencies. For example, Figure 70.3.1 shows the observed spectra for three samples, one with only tryptophan, one with only tyrosine, and one with a mixture of the two, all at a total concentration of  $10^{-6}$ .

**Output 70.3.1** Spectra for Three Samples of Tyrosine and Tryptophan

Of the 33 samples, 18 are used as a training set and 15 as a test set. The data originally appear in McAvoy et al. (1989).

These data were created in a lab, with the concentrations fixed in order to provide a wide range of applicability for the model. You want to use a linear function of the logarithms of the spectra to predict the logarithms of tyrosine and tryptophan concentration, as well as the logarithm of the total concentration. Actually, because of the possibility of zeros in both the responses and the predictors, slightly different transformations are used. The following statements create SAS data sets containing the training and test data, named `ftrain` and `ftest`, respectively.

```

data ftrain;
 input obsnam $ tot tyr f1-f30 @@;
 try = tot - tyr;
 if (tyr) then tyr_log = log10(tyr); else tyr_log = -8;
 if (try) then try_log = log10(try); else try_log = -8;
 tot_log = log10(tot);
 datalines;
17mix35 0.00003 0
-6.215 -5.809 -5.114 -3.963 -2.897 -2.269 -1.675 -1.235
-0.900 -0.659 -0.497 -0.395 -0.335 -0.315 -0.333 -0.377
-0.453 -0.549 -0.658 -0.797 -0.878 -0.954 -1.060 -1.266
-1.520 -1.804 -2.044 -2.269 -2.496 -2.714
19mix35 0.00003 3E-7
-5.516 -5.294 -4.823 -3.858 -2.827 -2.249 -1.683 -1.218
-0.907 -0.658 -0.501 -0.400 -0.345 -0.323 -0.342 -0.387
-0.461 -0.554 -0.665 -0.803 -0.887 -0.960 -1.072 -1.272
-1.541 -1.814 -2.058 -2.289 -2.496 -2.712
21mix35 0.00003 7.5E-7
-5.519 -5.294 -4.501 -3.863 -2.827 -2.280 -1.716 -1.262
-0.939 -0.694 -0.536 -0.444 -0.384 -0.369 -0.377 -0.421
-0.495 -0.596 -0.706 -0.824 -0.917 -0.988 -1.103 -1.294
-1.565 -1.841 -2.084 -2.320 -2.521 -2.729
23mix35 0.00003 1.5E-6

... more lines ...

mix6 0.0001 0.00009
-1.140 -0.757 -0.497 -0.362 -0.329 -0.412 -0.513 -0.647
-0.772 -0.877 -0.958 -1.040 -1.104 -1.162 -1.233 -1.317
-1.425 -1.543 -1.661 -1.804 -1.877 -1.959 -2.034 -2.249
-2.502 -2.732 -2.964 -3.142 -3.313 -3.576
;

data ftest;
 input obsnam $ tot tyr f1-f30 @@;
 try = tot - tyr;
 if (tyr) then tyr_log = log10(tyr); else tyr_log = -8;
 if (try) then try_log = log10(try); else try_log = -8;
 tot_log = log10(tot);
 datalines;
43trp6 1E-6 0
-5.915 -5.918 -6.908 -5.428 -4.117 -5.103 -4.660 -4.351
-4.023 -3.849 -3.634 -3.634 -3.572 -3.513 -3.634 -3.572
-3.772 -3.772 -3.844 -3.932 -4.017 -4.023 -4.117 -4.227
-4.492 -4.660 -4.855 -5.428 -5.103 -5.428
59mix6 1E-6 1E-7
-5.903 -5.903 -5.903 -5.082 -4.213 -5.083 -4.838 -4.639
-4.474 -4.213 -4.001 -4.098 -4.001 -4.001 -3.907 -4.001
-4.098 -4.098 -4.206 -4.098 -4.213 -4.213 -4.335 -4.474
-4.639 -4.838 -4.837 -5.085 -5.410 -5.410
51mix6 1E-6 2.5E-7
-5.907 -5.907 -5.415 -4.843 -4.213 -4.843 -4.843 -4.483
-4.343 -4.006 -4.006 -3.912 -3.830 -3.830 -3.755 -3.912

```

```

-4.006 -4.001 -4.213 -4.213 -4.335 -4.483 -4.483 -4.642
-4.841 -5.088 -5.088 -5.415 -5.415 -5.415
49mix6 1E-6 5E-7

... more lines ...

tyro2 0.0001 0.0001
-1.081 -0.710 -0.470 -0.337 -0.327 -0.433 -0.602 -0.841
-1.119 -1.423 -1.750 -2.121 -2.449 -2.818 -3.110 -3.467
-3.781 -4.029 -4.241 -4.366 -4.501 -4.366 -4.501 -4.501
-4.668 -4.668 -4.865 -4.865 -5.109 -5.111
;

```

The following statements fit a PLS model with 10 factors.

```

proc pls data=ftrain nfac=10;
 model tot_log tyr_log try_log = f1-f30;
run;

```

The table shown in [Output 70.3.2](#) indicates that only three or four factors are required to explain almost all of the variation in both the predictors and the responses.

**Output 70.3.2** Amount of Training Set Variation Explained

| The PLS Procedure                                                   |               |         |                     |         |  |
|---------------------------------------------------------------------|---------------|---------|---------------------|---------|--|
| Percent Variation Accounted for<br>by Partial Least Squares Factors |               |         |                     |         |  |
| Number of<br>Extracted<br>Factors                                   | Model Effects |         | Dependent Variables |         |  |
|                                                                     | Current       | Total   | Current             | Total   |  |
| 1                                                                   | 81.1654       | 81.1654 | 48.3385             | 48.3385 |  |
| 2                                                                   | 16.8113       | 97.9768 | 32.5465             | 80.8851 |  |
| 3                                                                   | 1.7639        | 99.7407 | 11.4438             | 92.3289 |  |
| 4                                                                   | 0.1951        | 99.9357 | 3.8363              | 96.1652 |  |
| 5                                                                   | 0.0276        | 99.9634 | 1.6880              | 97.8532 |  |
| 6                                                                   | 0.0132        | 99.9765 | 0.7247              | 98.5779 |  |
| 7                                                                   | 0.0052        | 99.9817 | 0.2926              | 98.8705 |  |
| 8                                                                   | 0.0053        | 99.9870 | 0.1252              | 98.9956 |  |
| 9                                                                   | 0.0049        | 99.9918 | 0.1067              | 99.1023 |  |
| 10                                                                  | 0.0034        | 99.9952 | 0.1684              | 99.2707 |  |

In order to choose the optimal number of PLS factors, you can explore how well models based on the training data with different numbers of factors fit the test data. To do so, use the `CV=TESTSET` option, with an argument pointing to the test data set `ftest`. The following statements also employ the ODS Graphics features in PROC PLS to display the cross validation results in a plot.

```

ods graphics on;

proc pls data=ftrain nfac=10 cv=testset(ftest)
 cvtest(stat=press seed=12345);

```

```

model tot_log tyr_log try_log = f1-f30;
run;

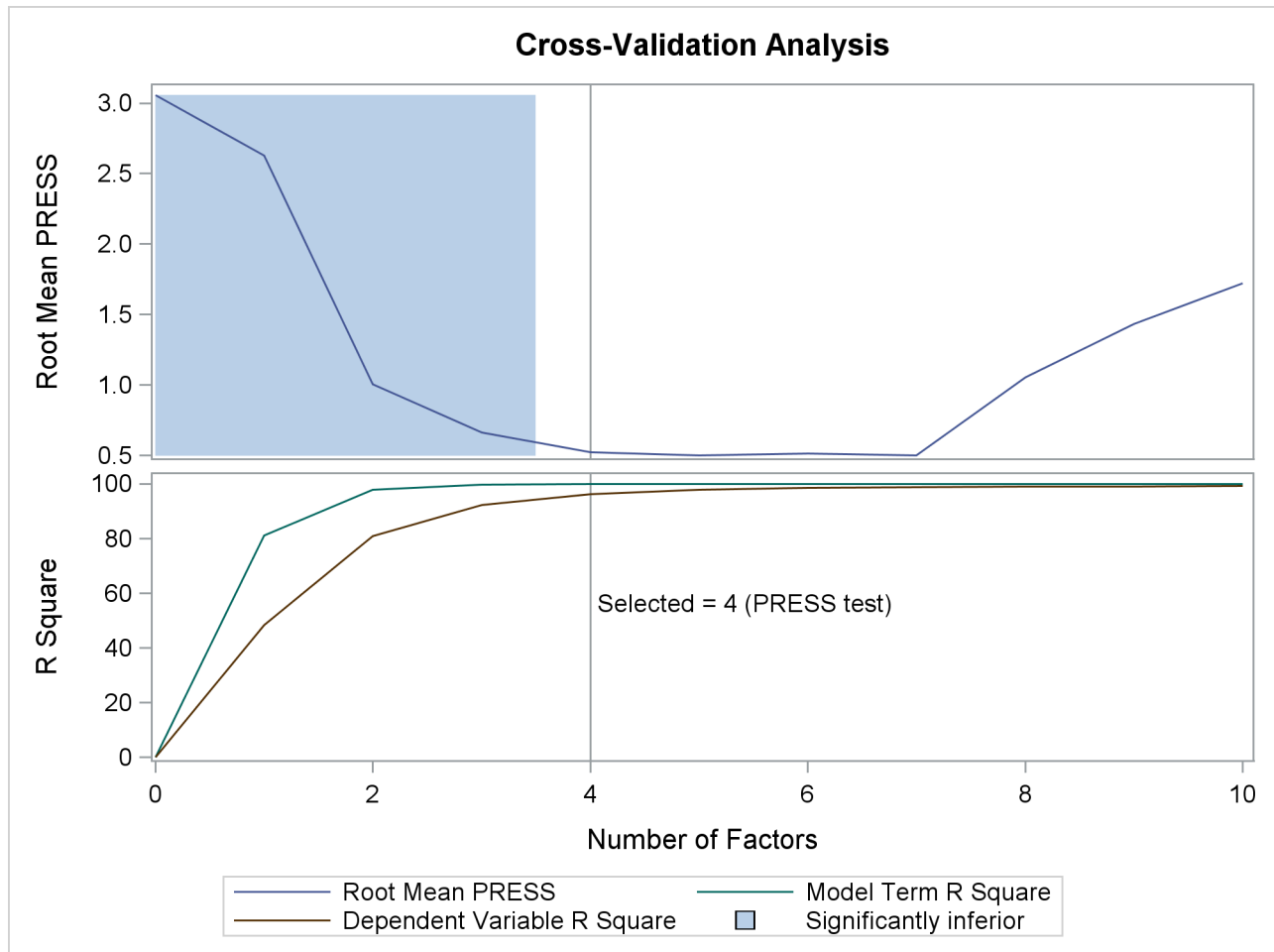
```

The tabular results of the test set validation are shown in [Output 70.3.3](#), and the graphical results are shown in [Output 70.3.4](#). They indicate that, although five PLS factors give the minimum predicted residual sum of squares, the residuals for four factors are insignificantly different from those for five. Thus, the smaller model is preferred.

**Output 70.3.3** Test Set Validation for the Number of PLS Factors

| The PLS Procedure                                                   |                       |                 |                     |         |
|---------------------------------------------------------------------|-----------------------|-----------------|---------------------|---------|
| Test Set Validation for the Number of Extracted Factors             |                       |                 |                     |         |
| Number of<br>Extracted<br>Factors                                   | Root<br>Mean<br>PRESS | Prob ><br>PRESS |                     |         |
| 0                                                                   | 3.056797              | <.0001          |                     |         |
| 1                                                                   | 2.630561              | <.0001          |                     |         |
| 2                                                                   | 1.00706               | 0.0070          |                     |         |
| 3                                                                   | 0.664603              | 0.0020          |                     |         |
| 4                                                                   | 0.521578              | 0.3800          |                     |         |
| 5                                                                   | 0.500034              | 1.0000          |                     |         |
| 6                                                                   | 0.513561              | 0.5100          |                     |         |
| 7                                                                   | 0.501431              | 0.6870          |                     |         |
| 8                                                                   | 1.055791              | 0.1530          |                     |         |
| 9                                                                   | 1.435085              | 0.1010          |                     |         |
| 10                                                                  | 1.720389              | 0.0320          |                     |         |
| Minimum root mean PRESS                                             |                       |                 | 0.5000              |         |
| Minimizing number of factors                                        |                       |                 | 5                   |         |
| Smallest number of factors with p > 0.1                             |                       |                 | 4                   |         |
| Percent Variation Accounted for<br>by Partial Least Squares Factors |                       |                 |                     |         |
| Number of<br>Extracted<br>Factors                                   | Model Effects         |                 | Dependent Variables |         |
|                                                                     | Current               | Total           | Current             | Total   |
| 1                                                                   | 81.1654               | 81.1654         | 48.3385             | 48.3385 |
| 2                                                                   | 16.8113               | 97.9768         | 32.5465             | 80.8851 |
| 3                                                                   | 1.7639                | 99.7407         | 11.4438             | 92.3289 |
| 4                                                                   | 0.1951                | 99.9357         | 3.8363              | 96.1652 |

**Output 70.3.4** Test Set Validation Plot

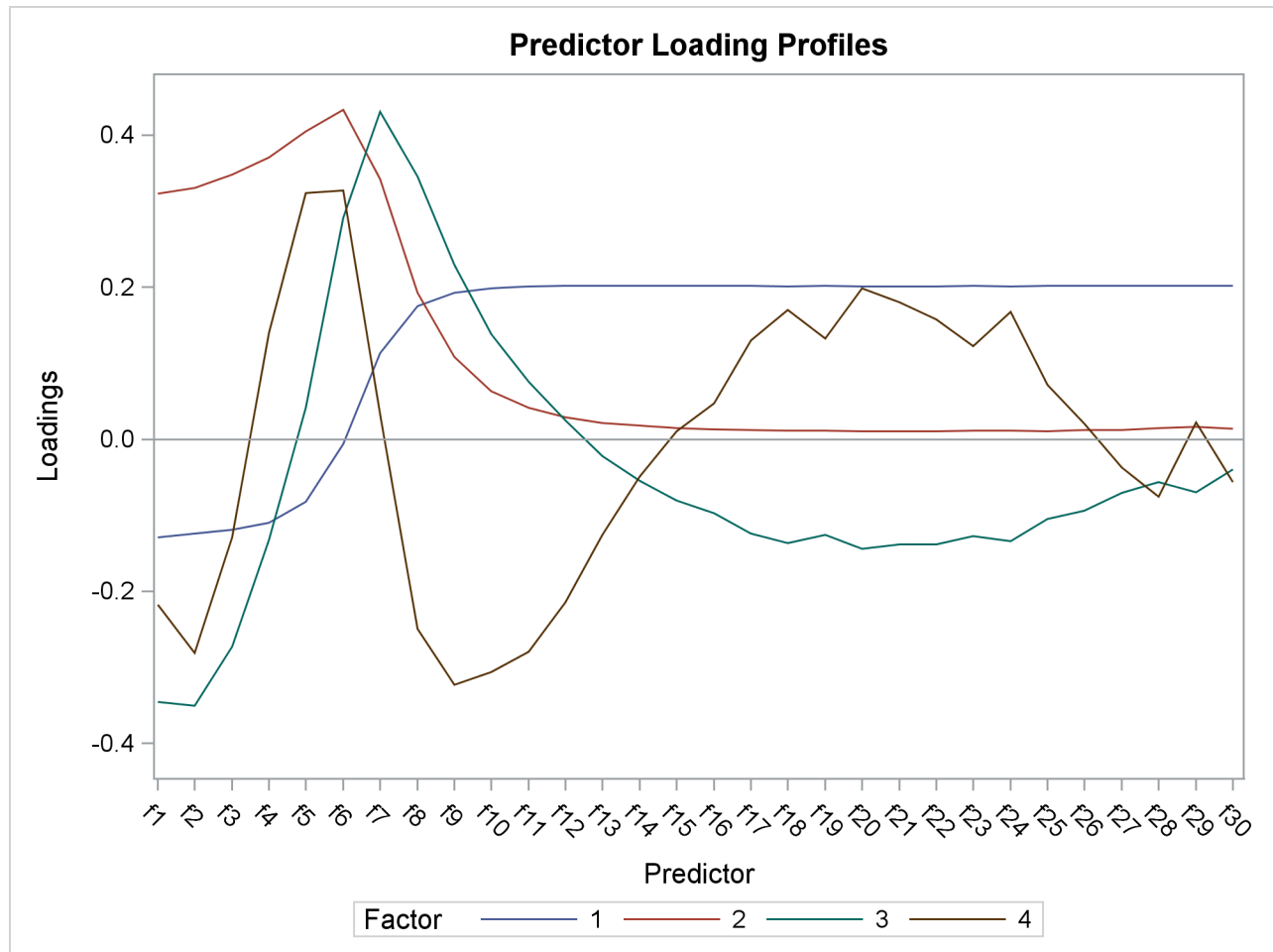


The factor loadings show how the PLS factors are constructed from the centered and scaled predictors. For spectral calibration, it is useful to plot the loadings against the frequency. In many cases, the physical meanings that can be attached to factor loadings help to validate the scientific interpretation of the PLS model. You can use ODS Graphics with PROC PLS to plot the loadings for the four PLS factors against frequency, as shown in the following statements.

```
proc pls data=ftrain nfac=4 plot=XLoadingProfiles;
 model tot_log tyr_log try_log = f1-f30;
run;

ods graphics off;
```

The resulting plot is shown in [Output 70.3.5](#).

**Output 70.3.5** Predictor Loadings across Frequencies

Notice that all four factors handle frequencies below and above about 7 or 8 differently. For example, the first factor is very nearly a simple contrast between the averages of the two sets of frequencies, and the second factor appears to be approximately a weighted sum of only the frequencies in the first set.

### Example 70.4: Partial Least Squares Spline Smoothing

The EFFECT statement makes it easy to construct a wide variety of linear models. In particular, you can use the spline effect to add smoothing terms to a model. A particular benefit of using spline effects in PROC PLS is that, when operating on spline basis functions, the partial least squares algorithm effectively chooses the amount of smoothing automatically, especially if you combine it with cross validation for the selecting the number of factors. This example employs the EFFECT statement to demonstrate partial least squares spline smoothing of agricultural data.

Weibe (1935) presents data from a study of uniformity of wheat yields over a certain rectangular plot of land. The following statements read these wheat yield measurements, indexed by row and column distances, into the SAS data set `Wheat`:

```

data Wheat;
 keep Row Column Yield;
 input Yield @@;
 iRow = int((_N-1)/12);
 iCol = mod(_N-1,12);
 Column = iCol*15 + 1; /* Column distance, in feet */
 Row = iRow* 1 + 1; /* Row distance, in feet */
 Row = 125 - Row + 1; /* Invert rows */
 datalines;
715 595 580 580 615 610 540 515 557 665 560 612
770 710 655 675 700 690 565 585 550 574 511 618
760 715 690 690 655 725 665 640 665 705 644 705
665 615 685 555 585 630 550 520 553 616 573 570
755 730 670 580 545 620 580 525 495 565 599 612
745 670 585 560 550 710 590 545 538 587 600 664
645 690 550 520 450 630 535 505 530 536 611 578
585 495 455 470 445 555 500 450 420 461 531 559

... more lines ...

570 585 635 765 550 675 765 620 608 705 677 660
505 500 580 655 470 565 570 555 537 585 589 619
465 430 510 680 460 600 670 615 620 594 616 784
;

```

The following statements use the PLS procedure to smooth these wheat yields using two spline effects, one for rows and another for columns, in addition to their crossproduct. Each spline effect has, by default, seven basis columns; thus their crossproduct has  $49 = 7^2$  columns, for a total of 63 parameters in the full linear model. However, the predictive PLS model does not actually need to have 63 degrees of freedom. Rather, the degree of smoothing is controlled by the number of PLS factors, which in this case is chosen automatically by random subset validation with the CV=RANDOM option.

```

ods graphics on;

proc pls data=Wheat cv=random(seed=1) cvtest(seed=12345)
 plot(only)=contourfit(obs=gradient);
 effect splCol = spline(Column);
 effect splRow = spline(Row);
 model Yield = splCol|splRow;
run;

ods graphics off;

```

These statements produce the output shown in [Output 70.4.1](#) through [Output 70.4.4](#).



**Output 70.4.1** Default Spline Basis: Model and Data Information

| The PLS Procedure              |                                  |
|--------------------------------|----------------------------------|
| Data Set                       | WORK.WHEAT                       |
| Factor Extraction Method       | Partial Least Squares            |
| PLS Algorithm                  | NIPALS                           |
| Number of Response Variables   | 1                                |
| Number of Predictor Parameters | 63                               |
| Missing Value Handling         | Exclude                          |
| Maximum Number of Factors      | 15                               |
| Validation Method              | 10-fold Random Subset Validation |
| Random Subset Seed             | 1                                |
| Validation Testing Criterion   | Prob T**2 > 0.1                  |
| Number of Random Permutations  | 1000                             |
| Random Permutation Seed        | 12345                            |
|                                |                                  |
| Number of Observations Read    | 1500                             |
| Number of Observations Used    | 1500                             |

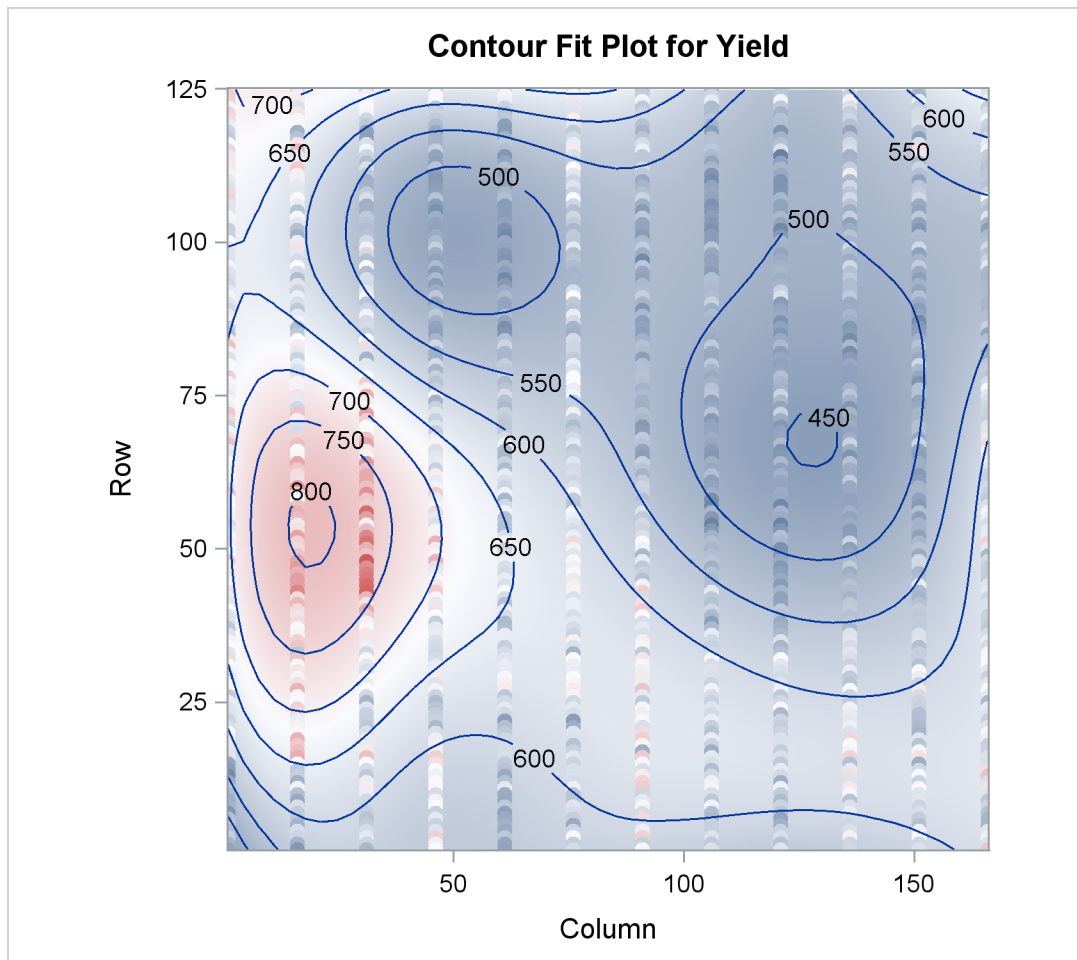
**Output 70.4.2** Default Spline Basis: Random Subset Validated PRESS Statistics for Number of Factors

| Random Subset Validation for the Number of Extracted Factors |                       |          |                |        |
|--------------------------------------------------------------|-----------------------|----------|----------------|--------|
| Number of<br>Extracted<br>Factors                            | Root<br>Mean<br>PRESS | T**2     | Prob ><br>T**2 |        |
| 0                                                            | 1.066355              | 251.8793 | <.0001         |        |
| 1                                                            | 0.826177              | 123.8161 | <.0001         |        |
| 2                                                            | 0.745877              | 61.6035  | <.0001         |        |
| 3                                                            | 0.725181              | 44.99644 | <.0001         |        |
| 4                                                            | 0.701464              | 23.20199 | <.0001         |        |
| 5                                                            | 0.687164              | 8.369711 | 0.0030         |        |
| 6                                                            | 0.683917              | 8.775847 | 0.0010         |        |
| 7                                                            | 0.677969              | 2.907019 | 0.0830         |        |
| 8                                                            | 0.676423              | 2.190871 | 0.1340         |        |
| 9                                                            | 0.676966              | 3.191284 | 0.0600         |        |
| 10                                                           | 0.675026              | 1.334638 | 0.2390         |        |
| 11                                                           | 0.673906              | 0.556455 | 0.4470         |        |
| 12                                                           | 0.673653              | 1.257292 | 0.2790         |        |
| 13                                                           | 0.672669              | 0        | 1.0000         |        |
| 14                                                           | 0.673596              | 2.386014 | 0.1190         |        |
| 15                                                           | 0.672828              | 0.02962  | 0.8820         |        |
| Minimum root mean PRESS                                      |                       |          |                | 0.6727 |
| Minimizing number of factors                                 |                       |          |                | 13     |
| Smallest number of factors with p > 0.1                      |                       |          |                | 8      |

**Output 70.4.3** Default Spline Basis: PLS Variation Summary for Split-Sample Validated Model

| Percent Variation Accounted for<br>by Partial Least Squares Factors |               |         |                     |         |
|---------------------------------------------------------------------|---------------|---------|---------------------|---------|
| Number of<br>Extracted<br>Factors                                   | Model Effects |         | Dependent Variables |         |
|                                                                     | Current       | Total   | Current             | Total   |
| 1                                                                   | 11.5269       | 11.5269 | 40.2471             | 40.2471 |
| 2                                                                   | 7.2314        | 18.7583 | 10.4908             | 50.7379 |
| 3                                                                   | 6.9147        | 25.6730 | 2.6523              | 53.3902 |
| 4                                                                   | 3.8433        | 29.5163 | 2.8806              | 56.2708 |
| 5                                                                   | 6.4795        | 35.9958 | 1.3197              | 57.5905 |
| 6                                                                   | 7.6201        | 43.6159 | 1.1700              | 58.7605 |
| 7                                                                   | 7.3214        | 50.9373 | 0.7186              | 59.4790 |
| 8                                                                   | 4.8363        | 55.7736 | 0.4548              | 59.9339 |

**Output 70.4.4** Default Spline Basis: Smoothed Yield



The cross validation results in [Output 70.4.2](#) point to a model with eight PLS factors; this is the smallest model whose predicted residual sum of squares (PRESS) is insignificantly different from the model with the absolute minimum PRESS. The variation summary in [Output 70.4.3](#) shows that this model accounts for about 60% of the variation in the Yield values. The OBS=GRADIENT suboption for the PLOT=CONTOURFIT option specifies that the observations in the resulting plot, [Output 70.4.4](#), be colored according to the same scheme as the surface of predicted yield. This coloration enables you to easily tell which observations are above the surface of predicted yield and which are below.

The surface of predicted yield is somewhat smoother than what Weibe (1935) settled on originally, with a predominance of simple, elliptically shaped contours. You can easily specify a potentially more granular model by increasing the number of knots in the spline bases. Even though the more granular model increases the number of predictor parameters, cross validation can still protect you from overfitting the data. The following statements are the same as those shown before, except that the spline effects now have twice as many basis functions:

```
ods graphics on;

proc pls data=Wheat cv=random(seed=1) cvtest(seed=12345)
 plot(only)=contourfit(obs=gradient);
 effect splCol = spline(Column / knotmethod=equal(14));
 effect splRow = spline(Row / knotmethod=equal(14));
 model Yield = splCol|splRow;
run;

ods graphics off;
```

The resulting output is shown in [Output 70.4.5](#) through [Output 70.4.8](#).

#### Output 70.4.5 More Granular Spline Basis: Model and Data Information

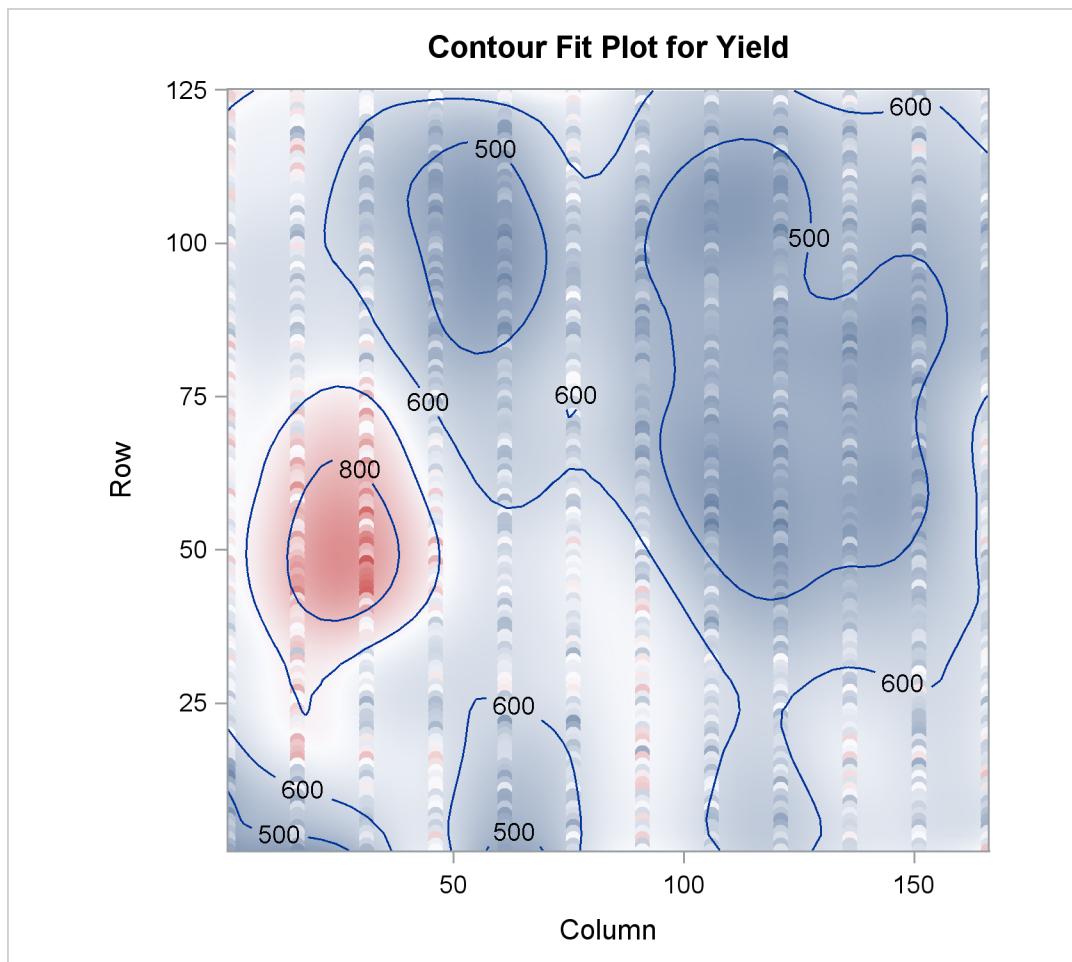
| The PLS Procedure              |                                  |
|--------------------------------|----------------------------------|
| Data Set                       | WORK.WHEAT                       |
| Factor Extraction Method       | Partial Least Squares            |
| PLS Algorithm                  | NIPALS                           |
| Number of Response Variables   | 1                                |
| Number of Predictor Parameters | 360                              |
| Missing Value Handling         | Exclude                          |
| Maximum Number of Factors      | 15                               |
| Validation Method              | 10-fold Random Subset Validation |
| Random Subset Seed             | 1                                |
| Validation Testing Criterion   | Prob T**2 > 0.1                  |
| Number of Random Permutations  | 1000                             |
| Random Permutation Seed        | 12345                            |
| Number of Observations Read    | 1500                             |
| Number of Observations Used    | 1500                             |

**Output 70.4.6** More Granular Spline Basis: Random Subset Validated PRESS Statistics for Number of Factors

| Random Subset Validation for the Number of Extracted Factors |                       |          |        |  |
|--------------------------------------------------------------|-----------------------|----------|--------|--|
| Number of<br>Extracted<br>Factors                            | Root<br>Mean<br>PRESS | T**2     | Prob > |  |
|                                                              |                       |          | T**2   |  |
| 0                                                            | 1.066355              | 247.9268 | <.0001 |  |
| 1                                                            | 0.652658              | 20.68858 | <.0001 |  |
| 2                                                            | 0.615087              | 0.074822 | 0.7740 |  |
| 3                                                            | 0.614128              | 0        | 1.0000 |  |
| 4                                                            | 0.615268              | 0.197678 | 0.6490 |  |
| 5                                                            | 0.618001              | 1.372038 | 0.2340 |  |
| 6                                                            | 0.622949              | 5.035504 | 0.0180 |  |
| 7                                                            | 0.626482              | 7.296797 | 0.0080 |  |
| 8                                                            | 0.633316              | 13.66045 | <.0001 |  |
| 9                                                            | 0.635239              | 16.16922 | <.0001 |  |
| 10                                                           | 0.636938              | 18.02295 | <.0001 |  |
| 11                                                           | 0.636494              | 16.9881  | <.0001 |  |
| 12                                                           | 0.63682               | 16.83341 | <.0001 |  |
| 13                                                           | 0.637719              | 16.74157 | <.0001 |  |
| 14                                                           | 0.637627              | 15.79342 | <.0001 |  |
| 15                                                           | 0.638431              | 16.12327 | <.0001 |  |
| Minimum root mean PRESS                                      |                       |          | 0.6141 |  |
| Minimizing number of factors                                 |                       |          | 3      |  |
| Smallest number of factors with p > 0.1                      |                       |          | 2      |  |

**Output 70.4.7** More Granular Spline Basis: PLS Variation Summary for Split-Sample Validated Model

| Number of<br>Extracted<br>Factors | Percent Variation Accounted for<br>by Partial Least Squares Factors |        |                     |         |
|-----------------------------------|---------------------------------------------------------------------|--------|---------------------|---------|
|                                   | Model Effects                                                       |        | Dependent Variables |         |
|                                   | Current                                                             | Total  | Current             | Total   |
| 1                                 | 1.7967                                                              | 1.7967 | 64.7792             | 64.7792 |
| 2                                 | 1.3719                                                              | 3.1687 | 6.3163              | 71.0955 |

**Output 70.4.8** More Granular Spline Basis: Smoothed Yield

Output 70.4.5 shows that the model now has 360 parameters, many more than before. In Output 70.4.6 you can see that with more granular spline effects, fewer PLS factors are required—only two, in fact. However, Output 70.4.7 shows that this model now accounts for over 70% of the variation in the Yield values, and the contours of predicted values in Output 70.4.8 are less inclined to be simple elliptical shapes.

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# Chapter 71

## The POWER Procedure

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## Overview: POWER Procedure

Power and sample size analysis optimizes the resource usage and design of a study, improving chances of conclusive results with maximum efficiency. The POWER procedure performs prospective power and sample size analyses for a variety of goals, such as the following:

- determining the sample size required to get a significant result with adequate probability (power)
- characterizing the power of a study to detect a meaningful effect
- conducting what-if analyses to assess sensitivity of the power or required sample size to other factors

Here *prospective* indicates that the analysis pertains to planning for a future study. This is in contrast to *retrospective* power analysis for a past study, which is not supported by the procedure.

A variety of statistical analyses are covered:

- *t* tests, equivalence tests, and confidence intervals for means
- tests, equivalence tests, and confidence intervals for binomial proportions
- multiple regression
- tests of correlation and partial correlation
- one-way analysis of variance
- rank tests for comparing two survival curves
- logistic regression with binary response
- Wilcoxon-Mann-Whitney (rank-sum) test

For more complex linear models, see Chapter 44, “[The GLMPOWER Procedure](#).”

Input for PROC POWER includes the components considered in study planning:

- design
- statistical model and test
- significance level (alpha)
- surmised effects and variability
- power
- sample size

You designate one of these components by a missing value in the input, in order to identify it as the result parameter. The procedure calculates this result value over one or more scenarios of input values for all other components. Power and sample size are the most common result values, but for some analyses the result can be something else. For example, you can solve for the sample size of a single group for a two-sample *t* test.

In addition to tabular results, PROC POWER produces graphs. You can produce the most common types of plots easily with default settings and use a variety of options for more customized graphics. For example, you can control the choice of axis variables, axis ranges, number of plotted points, mapping of graphical features (such as color, line style, symbol and panel) to analysis parameters, and legend appearance.

If ODS Graphics is enabled, then PROC POWER uses ODS Graphics to create graphs; otherwise, traditional graphs are produced.

For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS](#).”

For specific information about the statistical graphics and options available with the POWER procedure, see the `PLOT` statement and the section “[ODS Graphics](#)” on page 6081.

The POWER procedure is one of several tools available in SAS/STAT software for power and sample size analysis. PROC GLMPOWER supports more complex linear models. The Power and Sample Size application provides a user interface and implements many of the analyses supported in the procedures. See Chapter 44, “[The GLMPOWER Procedure](#),” and Chapter 72, “[The Power and Sample Size Application](#),” for details.

The following sections of this chapter describe how to use PROC POWER and discuss the underlying statistical methodology. The section “[Getting Started: POWER Procedure](#)” on page 5920 introduces PROC POWER with simple examples of power computation for a one-sample  $t$  test and sample size determination for a two-sample  $t$  test. The section “[Syntax: POWER Procedure](#)” on page 5927 describes the syntax of the procedure. The section “[Details: POWER Procedure](#)” on page 6018 summarizes the methods employed by PROC POWER and provides details on several special topics. The section “[Examples: POWER Procedure](#)” on page 6083 illustrates the use of the POWER procedure with several applications.

For an overview of methodology and SAS tools for power and sample size analysis, see Chapter 18, “[Introduction to Power and Sample Size Analysis](#).” For more discussion and examples, see O’Brien and Casteloe (2007); Casteloe (2000); Casteloe and O’Brien (2001); Muller and Benignus (1992); O’Brien and Muller (1993); Lenth (2001).

## Getting Started: POWER Procedure

### Computing Power for a One-Sample $t$ Test

Suppose you want to improve the accuracy of a machine used to print logos on sports jerseys. The logo placement has an inherently high variability, but the horizontal alignment of the machine can be adjusted. The operator agrees to pay for a costly adjustment if you can establish a nonzero mean horizontal displacement in either direction with high confidence. You have 150 jerseys at your disposal to measure, and you want to determine your chances of a significant result (power) by using a one-sample  $t$  test with a two-sided  $\alpha = 0.05$ .

You decide that 8 mm is the smallest displacement worth addressing. Hence, you will assume a true mean of 8 in the power computation. Experience indicates that the standard deviation is about 40.

Use the `ONESAMPLEMEANS` statement in the POWER procedure to compute the power. Indicate power as the result parameter by specifying the `POWER=` option with a missing value (.). Specify your conjectures for the mean and standard deviation by using the `MEAN=` and `STDDEV=` options and for the sample size by using the `NTOTAL=` option. The statements required to perform this analysis are as follows:

```

proc power;
 onesamplemeans
 mean = 8
 ntotal = 150
 stddev = 40
 power = .;
run;

```

Default values for the `TEST=`, `DIST=`, `ALPHA=`, `NULLMEAN=`, and `SIDES=` options specify a two-sided  $t$  test for a mean of 0, assuming a normal distribution with a significance level of  $\alpha = 0.05$ .

Figure 71.1 shows the output.

**Figure 71.1** Sample Size Analysis for One-Sample  $t$  Test

| The POWER Procedure        |        |
|----------------------------|--------|
| One-sample t Test for Mean |        |
| Fixed Scenario Elements    |        |
| Distribution               | Normal |
| Method                     | Exact  |
| Mean                       | 8      |
| Standard Deviation         | 40     |
| Total Sample Size          | 150    |
| Number of Sides            | 2      |
| Null Mean                  | 0      |
| Alpha                      | 0.05   |
| Computed Power             |        |
| Power                      | 0.682  |

The power is about 0.68. In other words, there is about a 2/3 chance that the  $t$  test will produce a significant result demonstrating the machine's average off-center displacement. This probability depends on the assumptions for the mean and standard deviation.

Now, suppose you want to account for some of your uncertainty in conjecturing the true mean and standard deviation by evaluating the power for four scenarios, using reasonable low and high values, 5 and 10 for the mean, and 30 and 50 for the standard deviation. Also, you might be able to measure more than 150 jerseys, and you would like to know under what circumstances you could get by with fewer. You want to plot power for sample sizes between 100 and 200 to visualize how sensitive the power is to changes in sample size for these four scenarios of means and standard deviations. The following statements perform this analysis:

```
ods listing style=htmlbluecml;
ods graphics on;

proc power;
 onesamplemeans
 mean = 5 10
 ntotal = 150
 stddev = 30 50
 power = .;
 plot x=n min=100 max=200;
run;

ods graphics off;
```

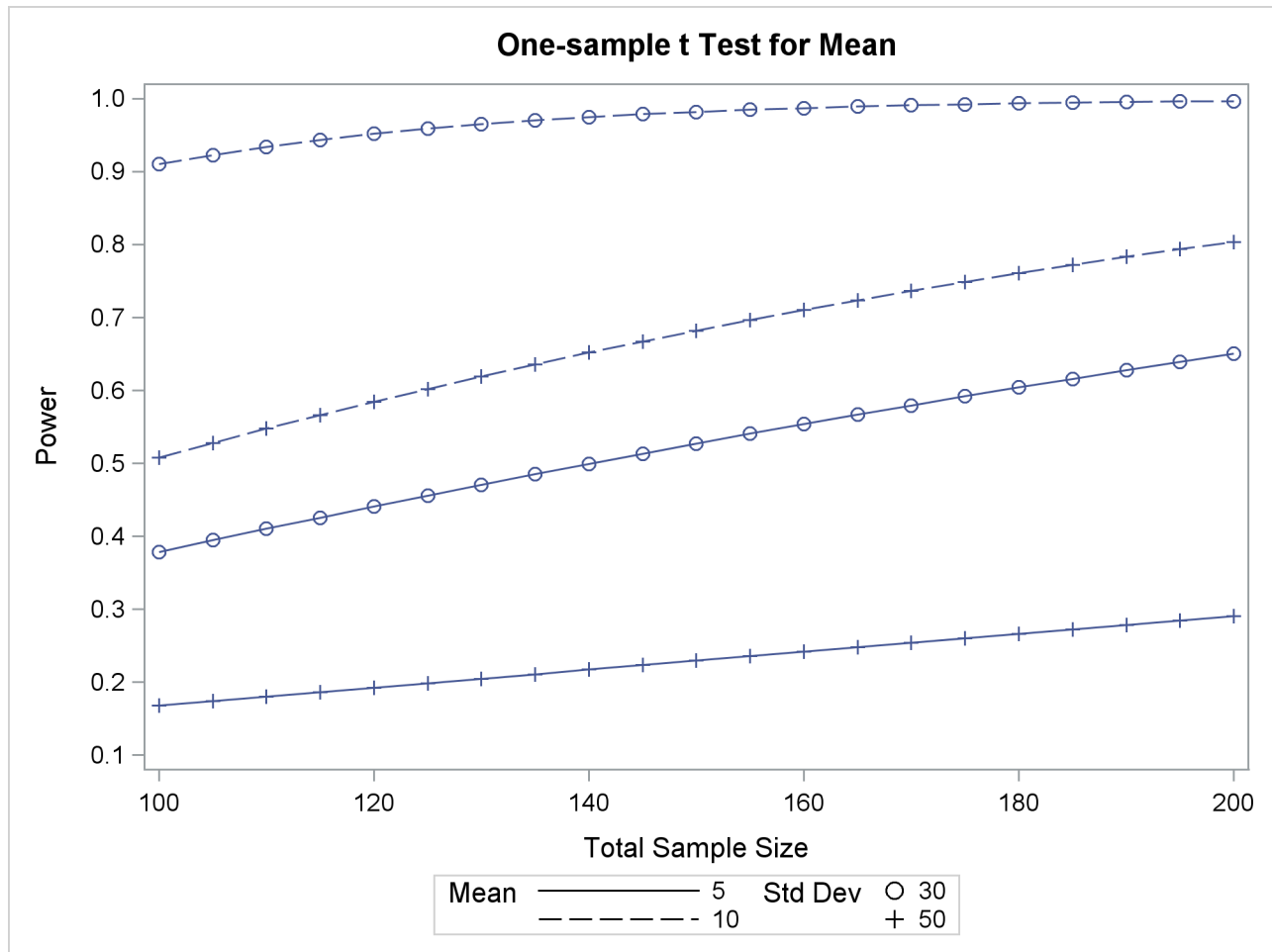
The new mean and standard deviation values are specified by using the **MEAN=** and **STDDEV=** options in the **ONESAMPLEMEANS** statement. The **PLOT** statement with **X=N** produces a plot with sample size on the X axis. (The result parameter, in this case the power, is always plotted on the other axis.) The **MIN=** and **MAX=** options in the **PLOT** statement determine the sample size range. The **ODS GRAPHICS ON** statement enables ODS Graphics. The **ODS LISTING STYLE=HTMLBLUECML** statement specifies the **HTMLBLUECML** style, which is suitable for use with **PROC POWER** because it allows both marker symbols and line styles to vary. See the section “**ODS Styles Suitable for Use with PROC POWER**” on page 6082 for more information.

Figure 71.2 shows the output, and Figure 71.3 shows the plot.

**Figure 71.2** Sample Size Analysis for One-Sample *t* Test with Input Ranges

| The POWER Procedure        |        |         |       |  |
|----------------------------|--------|---------|-------|--|
| One-sample t Test for Mean |        |         |       |  |
| Fixed Scenario Elements    |        |         |       |  |
| Distribution               | Normal |         |       |  |
| Method                     | Exact  |         |       |  |
| Total Sample Size          | 150    |         |       |  |
| Number of Sides            | 2      |         |       |  |
| Null Mean                  | 0      |         |       |  |
| Alpha                      | 0.05   |         |       |  |
| Computed Power             |        |         |       |  |
| Index                      | Mean   | Std Dev | Power |  |
| 1                          | 5      | 30      | 0.527 |  |
| 2                          | 5      | 50      | 0.229 |  |
| 3                          | 10     | 30      | 0.982 |  |
| 4                          | 10     | 50      | 0.682 |  |

**Figure 71.3** Plot of Power versus Sample Size for One-Sample  $t$  Test with Input Ranges



The power ranges from about 0.23 to 0.98 for a sample size of 150 depending on the mean and standard deviation. In Figure 71.3, the line style identifies the mean, and the plotting symbol identifies the standard deviation. The locations of plotting symbols indicate computed powers; the curves are linear interpolations of these points. The plot suggests sufficient power for a mean of 10 and standard deviation of 30 (for any of the sample sizes) but insufficient power for the other three scenarios.

### Determining Required Sample Size for a Two-Sample $t$ Test

In this example you want to compare two physical therapy treatments designed to increase muscle flexibility. You need to determine the number of patients required to achieve a power of at least 0.9 to detect a group mean difference in a two-sample  $t$  test. You will use  $\alpha = 0.05$  (two-tailed).

The mean flexibility with the standard treatment (as measured on a scale of 1 to 20) is well known to be about 13 and is thought to be between 14 and 15 with the new treatment. You conjecture three alternative scenarios for the means:

1.  $\mu_1 = 13, \mu_2 = 14$
2.  $\mu_1 = 13, \mu_2 = 14.5$
3.  $\mu_1 = 13, \mu_2 = 15$

You conjecture two scenarios for the common group standard deviation:

1.  $\sigma = 1.2$
2.  $\sigma = 1.7$

You also want to try three weighting schemes:

1. equal group sizes (balanced, or 1:1)
2. twice as many patients with the new treatment (1:2)
3. three times as many patients with the new treatment (1:3)

This makes  $3 \times 2 \times 3 = 18$  scenarios in all.

Use the **TWOSAMPLEMEANS** statement in the POWER procedure to determine the sample sizes required to give 90% power for each of these 18 scenarios. Indicate total sample size as the result parameter by specifying the **NTOTAL=** option with a missing value (.). Specify your conjectures for the means by using the **GROUPMEANS=** option. Using the “matched” notation (discussed in the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020), enclose the two group means for each scenario in parentheses. Use the **STDDEV=** option to specify scenarios for the common standard deviation. Specify the weighting schemes by using the **GROUPWEIGHTS=** option. You could again use the matched notation. But for illustrative purposes, specify the scenarios for each group weight separately by using the “crossed” notation, with scenarios for each group weight separated by a vertical bar (|). The statements that perform the analysis are as follows:

```
proc power;
 twosamplemeans
 groupmeans = (13 14) (13 14.5) (13 15)
 stddev = 1.2 1.7
 groupweights = 1 | 1 2 3
 power = 0.9
 ntotal = .;
run;
```

Default values for the **TEST=**, **DIST=**, **NULLDIFF=**, **ALPHA=**, and **SIDES=** options specify a two-sided  $t$  test of group mean difference equal to 0, assuming a normal distribution with a significance level of  $\alpha = 0.05$ . The results are shown in [Figure 71.4](#).

**Figure 71.4** Sample Size Analysis for Two-Sample *t* Test Using Group Means

| The POWER Procedure                          |        |       |         |         |              |         |
|----------------------------------------------|--------|-------|---------|---------|--------------|---------|
| Two-Sample <i>t</i> Test for Mean Difference |        |       |         |         |              |         |
| Fixed Scenario Elements                      |        |       |         |         |              |         |
| Distribution                                 | Normal |       |         |         |              |         |
| Method                                       | Exact  |       |         |         |              |         |
| Group 1 Weight                               | 1      |       |         |         |              |         |
| Nominal Power                                | 0.9    |       |         |         |              |         |
| Number of Sides                              | 2      |       |         |         |              |         |
| Null Difference                              | 0      |       |         |         |              |         |
| Alpha                                        | 0.05   |       |         |         |              |         |
| Computed N Total                             |        |       |         |         |              |         |
| Index                                        | Mean1  | Mean2 | Std Dev | Weight2 | Actual Power | N Total |
| 1                                            | 13     | 14.0  | 1.2     | 1       | 0.907        | 64      |
| 2                                            | 13     | 14.0  | 1.2     | 2       | 0.908        | 72      |
| 3                                            | 13     | 14.0  | 1.2     | 3       | 0.905        | 84      |
| 4                                            | 13     | 14.0  | 1.7     | 1       | 0.901        | 124     |
| 5                                            | 13     | 14.0  | 1.7     | 2       | 0.905        | 141     |
| 6                                            | 13     | 14.0  | 1.7     | 3       | 0.900        | 164     |
| 7                                            | 13     | 14.5  | 1.2     | 1       | 0.910        | 30      |
| 8                                            | 13     | 14.5  | 1.2     | 2       | 0.906        | 33      |
| 9                                            | 13     | 14.5  | 1.2     | 3       | 0.916        | 40      |
| 10                                           | 13     | 14.5  | 1.7     | 1       | 0.900        | 56      |
| 11                                           | 13     | 14.5  | 1.7     | 2       | 0.901        | 63      |
| 12                                           | 13     | 14.5  | 1.7     | 3       | 0.908        | 76      |
| 13                                           | 13     | 15.0  | 1.2     | 1       | 0.913        | 18      |
| 14                                           | 13     | 15.0  | 1.2     | 2       | 0.927        | 21      |
| 15                                           | 13     | 15.0  | 1.2     | 3       | 0.922        | 24      |
| 16                                           | 13     | 15.0  | 1.7     | 1       | 0.914        | 34      |
| 17                                           | 13     | 15.0  | 1.7     | 2       | 0.921        | 39      |
| 18                                           | 13     | 15.0  | 1.7     | 3       | 0.910        | 44      |

The interpretation is that in the best-case scenario (large mean difference of 2, small standard deviation of 1.2, and balanced design), a sample size of  $N = 18$  ( $n_1 = n_2 = 9$ ) patients is sufficient to achieve a power of at least 0.9. In the worst-case scenario (small mean difference of 1, large standard deviation of 1.7, and a 1:3 unbalanced design), a sample size of  $N = 164$  ( $n_1 = 41, n_2 = 123$ ) patients is necessary. The Nominal Power of 0.9 in the “Fixed Scenario Elements” table represents the input target power, and the Actual Power column in the “Computed N Total” table is the power at the sample size (N Total) adjusted to achieve the specified sample weighting exactly.



Note the following characteristics of the analysis, and ways you can modify them if you want:

- The total sample sizes are rounded up to multiples of the weight sums (2 for the 1:1 design, 3 for the 1:2 design, and 4 for the 1:3 design) to ensure that each group size is an integer. To request raw fractional sample size solutions, use the **NFRACTIONAL** option.
- Only the group weight that varies (the one for group 2) is displayed as an output column, while the weight for group 1 appears in the “Fixed Scenario Elements” table. To display the group weights together in output columns, use the matched version of the value list rather than the crossed version.
- If you can specify only differences between group means (instead of their individual values), or if you want to display the mean differences instead of the individual means, use the **MEANDIFF=** option instead of the **GROUPMEANS=** option.

The following statements implement all of these modifications:

```
proc power;
 twosamplemeans
 nfractional
 meandiff = 1 to 2 by 0.5
 stddev = 1.2 1.7
 groupweights = (1 1) (1 2) (1 3)
 power = 0.9
 ntotal = .;
run;
```

Figure 71.5 shows the new results.

**Figure 71.5** Sample Size Analysis for Two-Sample  $t$  Test Using Mean Differences

| The POWER Procedure                     |        |
|-----------------------------------------|--------|
| Two-Sample $t$ Test for Mean Difference |        |
| Fixed Scenario Elements                 |        |
| Distribution                            | Normal |
| Method                                  | Exact  |
| Nominal Power                           | 0.9    |
| Number of Sides                         | 2      |
| Null Difference                         | 0      |
| Alpha                                   | 0.05   |

Figure 71.5 continued

| Computed Ceiling N Total |           |         |         |         |                    |              |                 |
|--------------------------|-----------|---------|---------|---------|--------------------|--------------|-----------------|
| Index                    | Mean Diff | Std Dev | Weight1 | Weight2 | Fractional N Total | Actual Power | Ceiling N Total |
| 1                        | 1.0       | 1.2     | 1       | 1       | 62.507429          | 0.902        | 63              |
| 2                        | 1.0       | 1.2     | 1       | 2       | 70.065711          | 0.904        | 71              |
| 3                        | 1.0       | 1.2     | 1       | 3       | 82.665772          | 0.901        | 83              |
| 4                        | 1.0       | 1.7     | 1       | 1       | 123.418482         | 0.901        | 124             |
| 5                        | 1.0       | 1.7     | 1       | 2       | 138.598159         | 0.901        | 139             |
| 6                        | 1.0       | 1.7     | 1       | 3       | 163.899094         | 0.900        | 164             |
| 7                        | 1.5       | 1.2     | 1       | 1       | 28.961958          | 0.900        | 29              |
| 8                        | 1.5       | 1.2     | 1       | 2       | 32.308867          | 0.906        | 33              |
| 9                        | 1.5       | 1.2     | 1       | 3       | 37.893351          | 0.901        | 38              |
| 10                       | 1.5       | 1.7     | 1       | 1       | 55.977156          | 0.900        | 56              |
| 11                       | 1.5       | 1.7     | 1       | 2       | 62.717357          | 0.901        | 63              |
| 12                       | 1.5       | 1.7     | 1       | 3       | 73.954291          | 0.900        | 74              |
| 13                       | 2.0       | 1.2     | 1       | 1       | 17.298518          | 0.913        | 18              |
| 14                       | 2.0       | 1.2     | 1       | 2       | 19.163836          | 0.913        | 20              |
| 15                       | 2.0       | 1.2     | 1       | 3       | 22.282926          | 0.910        | 23              |
| 16                       | 2.0       | 1.7     | 1       | 1       | 32.413512          | 0.905        | 33              |
| 17                       | 2.0       | 1.7     | 1       | 2       | 36.195531          | 0.907        | 37              |
| 18                       | 2.0       | 1.7     | 1       | 3       | 42.504535          | 0.903        | 43              |

Note that the Nominal Power of 0.9 applies to the raw computed sample size (Fractional N Total), and the Actual Power column applies to the rounded sample size (Ceiling N Total). Some of the adjusted sample sizes in Figure 71.5 are lower than those in Figure 71.4 because underlying group sample sizes are allowed to be fractional (for example, the first Ceiling N Total of 63 corresponding to equal group sizes of 31.5).

## Syntax: POWER Procedure

The following statements are available in the POWER procedure:

```

PROC POWER < options > ;
 LOGISTIC < options > ;
 MULTREG < options > ;
 ONECORR < options > ;
 ONESAMPLEFREQ < options > ;
 ONESAMPLEMEANS < options > ;
 ONEWAYANOVA < options > ;
 PAIREDFREQ < options > ;
 PAIREDMEANS < options > ;
 PLOT < plot-options > < / graph-options > ;
 TWOSAMPLEFREQ < options > ;
 TWOSAMPLEMEANS < options > ;
 TWOSAMPLESURVIVAL < options > ;
 TWOSAMPLEWILCOXON < options > ;

```

The statements in the POWER procedure consist of the **PROC POWER** statement, a set of *analysis statements* (for requesting specific power and sample size analyses), and the **PLOT** statement (for producing graphs). The **PROC POWER** statement and at least one of the analysis statements are required. The analysis statements are **LOGISTIC**, **MULTREG**, **ONECORR**, **ONESAMPLEFREQ**, **ONESAMPLEMEANS**, **ONEWAYANOVA**, **PAIREFREQ**, **PAIREDMEANS**, **TWOSAMPLEFREQ**, **TWOSAMPLEMEANS**, **TWOSAMPLESURVIVAL**, and **TWOSAMPLEWILCOXON**.

You can use multiple analysis statements and multiple **PLOT** statements. Each analysis statement produces a separate sample size analysis. Each **PLOT** statement refers to the previous analysis statement and generates a separate graph (or set of graphs).

The name of an analysis statement describes the framework of the statistical analysis for which sample size calculations are desired. You use options in the analysis statements to identify the result parameter to compute, to specify the statistical test and computational options, and to provide one or more scenarios for the values of relevant analysis parameters.

Table 71.1 summarizes the basic functions of each statement in PROC POWER. The syntax of each statement in Table 71.1 is described in the following pages.

**Table 71.1** Statements in the POWER Procedure

| Statement                | Description                                                                                        |
|--------------------------|----------------------------------------------------------------------------------------------------|
| <b>PROC POWER</b>        | Invokes the procedure                                                                              |
| <b>LOGISTIC</b>          | Likelihood ratio chi-square test of a single predictor in logistic regression with binary response |
| <b>MULTREG</b>           | Tests of one or more coefficients in multiple linear regression                                    |
| <b>ONECORR</b>           | Fisher's $z$ test and $t$ test of (partial) correlation                                            |
| <b>ONESAMPLEFREQ</b>     | Tests, confidence interval precision, and equivalence tests of a single binomial proportion        |
| <b>ONESAMPLEMEANS</b>    | One-sample $t$ test, confidence interval precision, or equivalence test                            |
| <b>ONEWAYANOVA</b>       | One-way ANOVA including single-degree-of-freedom contrasts                                         |
| <b>PAIREFREQ</b>         | McNemar's test for paired proportions                                                              |
| <b>PAIREDMEANS</b>       | Paired $t$ test, confidence interval precision, or equivalence test                                |
| <b>PLOT</b>              | Displays plots for previous sample size analysis                                                   |
| <b>TWOSAMPLEFREQ</b>     | Chi-square, likelihood ratio, and Fisher's exact tests for two independent proportions             |
| <b>TWOSAMPLEMEANS</b>    | Two-sample $t$ test, confidence interval precision, or equivalence test                            |
| <b>TWOSAMPLESURVIVAL</b> | Log-rank, Gehan, and Tarone-Ware tests for comparing two survival curves                           |
| <b>TWOSAMPLEWILCOXON</b> | Wilcoxon-Mann-Whitney (rank-sum) test for 2 independent groups                                     |

See the section “Summary of Analyses” on page 6018 for a summary of the analyses available and the syntax required for them.

---

## PROC POWER Statement

**PROC POWER** < options > ;

The **PROC POWER** statement invokes the POWER procedure. You can specify the following option.

### **PLOTONLY**

specifies that only graphical results from the **PLOT** statement should be produced.

---

## LOGISTIC Statement

**LOGISTIC** < options > ;

The **LOGISTIC** statement performs power and sample size analyses for the likelihood ratio chi-square test of a single predictor in binary logistic regression, possibly in the presence of one or more covariates that might be correlated with the tested predictor.

## Summary of Options

Table 71.2 summarizes the options available in the **LOGISTIC** statement.

**Table 71.2** LOGISTIC Statement Options

| Option                              | Description                                                                 |
|-------------------------------------|-----------------------------------------------------------------------------|
| <b>Define analysis</b>              |                                                                             |
| <b>TEST=</b>                        | Specifies the statistical analysis                                          |
| <b>Specify analysis information</b> |                                                                             |
| <b>ALPHA=</b>                       | Specifies the significance level                                            |
| <b>COVARIATES=</b>                  | Specifies the distributions of predictor variables                          |
| <b>TESTPREDICTOR=</b>               | Specifies the distribution of the predictor variable being tested           |
| <b>VARDIST=</b>                     | Defines a distribution for a predictor variable                             |
| <b>Specify effects</b>              |                                                                             |
| <b>CORR=</b>                        | Specifies the multiple correlation between the predictor and the covariates |
| <b>COVODDSRATIOS=</b>               | Specifies the odds ratios for the covariates                                |
| <b>COVREGCOEFFS=</b>                | Specifies the regression coefficients for the covariates                    |
| <b>DEFAULTUNIT=</b>                 | Specifies the default change in the predictor variables                     |
| <b>INTERCEPT=</b>                   | Specifies the intercept                                                     |
| <b>RESPONSEPROB=</b>                | Specifies the response probability                                          |
| <b>TESTODDSRATIO=</b>               | Specifies the odds ratio being tested                                       |
| <b>TESTREGCOEFF=</b>                | Specifies the regression coefficient for the predictor variable             |
| <b>UNITS=</b>                       | Specifies the changes in the predictor variables                            |
| <b>Specify sample size</b>          |                                                                             |
| <b>NFRACTIONAL</b>                  | Enables fractional input and output for sample sizes                        |
| <b>NTOTAL=</b>                      | Specifies the sample size                                                   |
| <b>Specify power</b>                |                                                                             |
| <b>POWER=</b>                       | Specifies the desired power of the test                                     |

---

Table 71.2 *continued*

| Option                              | Description                                                            |
|-------------------------------------|------------------------------------------------------------------------|
| <b>Specify computational method</b> |                                                                        |
| DEFAULTNBINS=                       | Specifies the default number of categories for each predictor variable |
| NBINS=                              | Specifies the number of categories for predictor variables             |
| <b>Control ordering in output</b>   |                                                                        |
| OUTPUTORDER=                        | Controls the output order of parameters                                |

Table 71.3 summarizes the valid result parameters in the LOGISTIC statement.

Table 71.3 Summary of Result Parameters in the LOGISTIC Statement

| Analyses   | Solve For            | Syntax              |
|------------|----------------------|---------------------|
| TEST=LRCHI | Power<br>Sample size | POWER=.<br>NTOTAL=. |

## Dictionary of Options

### ALPHA=*number-list*

specifies the level of significance of the statistical test. The default is 0.05, corresponding to the usual  $0.05 \times 100\% = 5\%$  level of significance. See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *number-list*.

### CORR=*number-list*

specifies the multiple correlation ( $\rho$ ) between the tested predictor and the covariates. If you also specify the COVARIATES= option, then the sample size is either multiplied (if you are computing power) or divided (if you are computing sample size) by a factor of  $(1 - \rho^2)$ . See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *number-list*.

### COVARIATES=*grouped-name-list*

specifies the distributions of any predictor variables in the model but not being tested, using labels specified with the VARDIST= option. The distributions are assumed to be independent of each other and of the tested predictor. If this option is omitted, then the tested predictor specified by the TEST= option is assumed to be the only predictor in the model. See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *grouped-name-list*.

### COVODDSRATIOS=*grouped-number-list*

specifies the odds ratios for the covariates in the full model (including variables in the TESTPREDICTOR= and COVARIATES= options). The ordering of the values corresponds to the ordering in the COVARIATES= option. If the response variable is coded as  $Y = 1$  for success and  $Y = 0$  for failure, then the odds ratio for each covariate  $X$  is the odds of  $Y = 1$  when  $X = a$  divided by the odds of  $Y = 1$  when  $X = b$ , where  $a$  and  $b$  are determined from the DEFAULTUNIT= and UNITS= options. Values must be greater than zero. See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *grouped-number-list*.

**COVREGCOEFFS=***grouped-number-list*

specifies the regression coefficients for the covariates in the full model including the test predictor (as specified by the **TESTPREDICTOR=** option). The ordering of the values corresponds to the ordering in the **COVARIATES=** option. See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *grouped-number-list*.

**DEFAULTNBINS=***number*

specifies the default number of categories (or “bins”) into which the distribution for each predictor variable is divided in internal calculations. Higher values increase computational time and memory requirements but generally lead to more accurate results. Each test predictor or covariate that is absent from the **NBINS=** option derives its bin number from the **DEFAULTNBINS=** option. The default value is **DEFAULTNBINS=10**.

There are two variable distributions for which the number of bins can be overridden internally:

- For an ordinal distribution, the number of ordinal values is always used as the number of bins.
- For a binomial distribution, if the requested number of bins is larger than  $n + 1$ , where  $n$  is the sample size parameter of the binomial distribution, then exactly  $n + 1$  bins are used.

**DEFAULTUNIT=***change-spec*

specifies the default change in the predictor variables assumed for odds ratios specified with the **COVODDSRATIOS=** and **TESTODDSRATIO=** options. Each test predictor or covariate that is absent from the **UNITS=** option derives its change value from the **DEFAULTUNIT=** option. The value must be nonzero. The default value is **DEFAULTUNIT=1**. This option can be used only if at least one of the **COVODDSRATIOS=** and **TESTODDSRATIO=** options is used.

Valid specifications for *change-spec* are as follows:

*number* defines the odds ratio as the ratio of the response variable odds when  $X = a$  to the odds when  $X = a - \textit{number}$  for any constant  $a$ .

$\langle + | - \rangle \textit{SD}$  defines the odds ratio as the ratio of the odds when  $X = a$  to the odds when  $X = a - \sigma$  (or  $X = a + \sigma$ , if  $\textit{SD}$  is preceded by a minus sign (-)) for any constant  $a$ , where  $\sigma$  is the standard deviation of  $X$  (as determined from the **VARDIST=** option).

*multiple*\* $\textit{SD}$  defines the odds ratio as the ratio of the odds when  $X = a$  to the odds when  $X = a - \textit{multiple} * \sigma$  for any constant  $a$ , where  $\sigma$  is the standard deviation of  $X$  (as determined from the **VARDIST=** option).

**PERCENTILES**( $p1, p2$ ) defines the odds ratio as the ratio of the odds when  $X$  is equal to its  $p2 * 100$ th percentile to the odds when  $X$  is equal to its  $p1 * 100$ th percentile (where the percentiles are determined from the distribution specified in the **VARDIST=** option). Values for  $p1$  and  $p2$  must be strictly between 0 and 1.

**INTERCEPT=***number-list*

specifies the intercept in the full model (including variables in the **TESTPREDICTOR=** and **COVARIATES=** options). See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *number-list*.

**NBINS=**(*"name" = number <... "name" = number >*)

specifies the number of categories (or “bins”) into which the distribution for each predictor variable (identified by its *name* from the **VARDIST=** option) is divided in internal calculations. Higher values increase computational time and memory requirements but generally lead to more accurate results. Each predictor variable that is absent from the **NBINS=** option derives its bin number from the **DEFAULTNBINS=** option.

There are two variable distributions for which the **NBINS=** value can be overridden internally:

- For an ordinal distribution, the number of ordinal values is always used as the number of bins.
- For a binomial distribution, if the requested number of bins is larger than  $n + 1$ , where  $n$  is the sample size parameter of the binomial distribution, then exactly  $n + 1$  bins are used.

**NFRACTIONAL****NFRAC**

enables fractional input and output for sample sizes. See the section “Sample Size Adjustment Options” on page 6023 for information about the ramifications of the presence (and absence) of the **NFRACTIONAL** option.

**NTOTAL=***number-list*

specifies the sample size or requests a solution for the sample size with a missing value (**NTOTAL=.**). Values must be at least one. See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *number-list*.

**OUTPUTORDER=INTERNAL****OUTPUTORDER=REVERSE****OUTPUTORDER=SYNTAX**

controls how the input and default analysis parameters are ordered in the output. **OUTPUTORDER=INTERNAL** (the default) arranges the parameters in the output according to the following order of their corresponding options:

- **DEFAULTNBINS=**
- **NBINS=**
- **ALPHA=**
- **RESPONSEPROB=**
- **INTERCEPT=**
- **TESTPREDICTOR=**
- **TESTODDSRATIO=**
- **TESTREGCOEFF=**
- **COVARIATES=**
- **COVODDSRATIOS=**
- **COVREGCOEFFS=**
- **CORR=**
- **NTOTAL=**
- **POWER=**

The **OUTPUTORDER=SYNTAX** option arranges the parameters in the output in the same order in which their corresponding options are specified in the **LOGISTIC** statement. The **OUTPUTORDER=REVERSE** option arranges the parameters in the output in the reverse of the order in which their corresponding options are specified in the **LOGISTIC** statement.

**POWER=number-list**

specifies the desired power of the test or requests a solution for the power with a missing value (POWER=.). The power is expressed as a probability, a number between 0 and 1, rather than as a percentage. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**RESPONSEPROB=number-list**

specifies the response probability in the full model when all predictor variables (including variables in the [TESTPREDICTOR=](#) and [COVARIATES=](#) options) are equal to their means. The log odds of this probability are equal to the intercept in the full model where all predictor are centered at their means. If the response variable is coded as  $Y = 1$  for success and  $Y = 0$  for failure, then this probability is equal to the mean of  $Y$  in the full model when all  $X$ s are equal to their means. Values must be strictly between zero and one. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**TEST=LRCHI**

specifies the likelihood ratio chi-square test of a single model parameter in binary logistic regression. This is the default test option.

**TESTODDSRATIO=number-list**

specifies the odds ratio for the predictor variable being tested in the full model (including variables in the [TESTPREDICTOR=](#) and [COVARIATES=](#) options). If the response variable is coded as  $Y = 1$  for success and  $Y = 0$  for failure, then the odds ratio for the  $X$  being tested is the odds of  $Y = 1$  when  $X = a$  divided by the odds of  $Y = 1$  when  $X = b$ , where  $a$  and  $b$  are determined from the [DEFAULTUNIT=](#) and [UNITS=](#) options. Values must be greater than zero. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**TESTPREDICTOR=name-list**

specifies the distribution of the predictor variable being tested, using labels specified with the [VARDIST=](#) option. This distribution is assumed to be independent of the distributions of the covariates as defined in the [COVARIATES=](#) option. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *name-list*.

**TESTREGCOEFF=number-list**

specifies the regression coefficient for the predictor variable being tested in the full model including the covariates specified by the [COVARIATES=](#) option. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**UNITS=(“name” = change-spec <... “name” = change-spec >)**

specifies the changes in the predictor variables assumed for odds ratios specified with the [COVODDSRATIOS=](#) and [TESTODDSRATIO=](#) options. Each predictor variable whose *name* (from the [VARDIST=](#) option) is absent from the UNITS option derives its change value from the [DEFAULTUNIT=](#) option. This option can be used only if at least one of the [COVODDSRATIOS=](#) and [TESTODDSRATIO=](#) options is used.

Valid specifications for *change-spec* are as follows:

*number* defines the odds ratio as the ratio of the response variable odds when  $X = a$  to the odds when  $X = a - \textit{number}$  for any constant  $a$ .



**<+|->SD** defines the odds ratio as the ratio of the odds when  $X = a$  to the odds when  $X = a - \sigma$  (or  $X = a + \sigma$ , if SD is preceded by a minus sign (-)) for any constant  $a$ , where  $\sigma$  is the standard deviation of  $X$  (as determined from the **VARDIST=** option).

**multiple\*SD** defines the odds ratio as the ratio of the odds when  $X = a$  to the odds when  $X = a - multiple * \sigma$  for any constant  $a$ , where  $\sigma$  is the standard deviation of  $X$  (as determined from the **VARDIST=** option).

**PERCENTILES( $p1, p2$ )** defines the odds ratio as the ratio of the odds when  $X$  is equal to its  $p2 * 100$ th percentile to the odds when  $X$  is equal to its  $p1 * 100$ th percentile (where the percentiles are determined from the distribution specified in the **VARDIST=** option). Values for  $p1$  and  $p2$  must be strictly between 0 and 1.

Each unit value must be nonzero.

**VARDIST("label")=distribution (parameters)**  
defines a distribution for a predictor variable.

For the **VARDIST=** option,

|                     |                                                                                                                       |
|---------------------|-----------------------------------------------------------------------------------------------------------------------|
| <i>label</i>        | identifies the variable distribution in the output and with the <b>COVARIATES=</b> and <b>TESTPREDICTOR=</b> options. |
| <i>distribution</i> | specifies the distributional form of the variable.                                                                    |
| <i>parameters</i>   | specifies one or more parameters associated with the distribution.                                                    |

Choices for distributional forms and their parameters are as follows:

**ORDINAL ((*values*): (*probabilities*))** is an ordered categorical distribution. The *values* are any numbers separated by spaces. The *probabilities* are numbers between 0 and 1 (inclusive) separated by spaces. Their sum must be exactly 1. The number of *probabilities* must match the number of *values*.

**BETA ( $a, b <, l, r >$ )** is a beta distribution with shape parameters  $a$  and  $b$  and optional location parameters  $l$  and  $r$ . The values of  $a$  and  $b$  must be greater than 0, and  $l$  must be less than  $r$ . The default values for  $l$  and  $r$  are 0 and 1, respectively.

**BINOMIAL ( $p, n$ )** is a binomial distribution with probability of success  $p$  and number of independent Bernoulli trials  $n$ . The value of  $p$  must be greater than 0 and less than 1, and  $n$  must be an integer greater than 0. If  $n = 1$ , then the distribution is binary.

**EXPONENTIAL ( $\lambda$ )** is an exponential distribution with scale  $\lambda$ , which must be greater than 0.

**GAMMA ( $a, \lambda$ )** is a gamma distribution with shape  $a$  and scale  $\lambda$ . The values of  $a$  and  $\lambda$  must be greater than 0.

**LAPLACE ( $\theta, \lambda$ )** is a Laplace distribution with location  $\theta$  and scale  $\lambda$ . The value of  $\lambda$  must be greater than 0.

**LOGISTIC ( $\theta, \lambda$ )** is a logistic distribution with location  $\theta$  and scale  $\lambda$ . The value of  $\lambda$  must be greater than 0.

**LOGNORMAL ( $\theta, \lambda$ )** is a lognormal distribution with location  $\theta$  and scale  $\lambda$ . The value of  $\lambda$  must be greater than 0.

NORMAL ( $\theta, \lambda$ ) is a normal distribution with mean  $\theta$  and standard deviation  $\lambda$ . The value of  $\lambda$  must be greater than 0.

POISSON ( $m$ ) is a Poisson distribution with mean  $m$ . The value of  $m$  must be greater than 0.

UNIFORM ( $l, r$ ) is a uniform distribution on the interval  $[l, r]$ , where  $l < r$ .

## Restrictions on Option Combinations

To specify the intercept in the full model, choose one of the following two parameterizations:

- intercept (using the `INTERCEPT=` options)
- Prob( $Y = 1$ ) when all predictors are equal to their means (using the `RESPONSEPROB=` option)

To specify the effect associated with the predictor variable being tested, choose one of the following two parameterizations:

- odds ratio (using the `TESTODDSRATIO=` options)
- regression coefficient (using the `TESTREGCOEFFS=` option)

To describe the effects of the covariates in the full model, choose one of the following two parameterizations:

- odds ratios (using the `COVODDSRATIOS=` options)
- regression coefficients (using the `COVREGCOEFFS=` options)

## Option Groups for Common Analyses

This section summarizes the syntax for the common analyses supported in the `LOGISTIC` statement.

### Likelihood Ratio Chi-Square Test for One Predictor

You can express effects in terms of response probability and odds ratios, as in the following statements:

```
proc power;
 logistic
 vardist("x1a") = normal(0, 2)
 vardist("x1b") = normal(0, 3)
 vardist("x2") = poisson(7)
 vardist("x3a") = ordinal((-5 0 5) : (.3 .4 .3))
 vardist("x3b") = ordinal((-5 0 5) : (.4 .3 .3))
 testpredictor = "x1a" "x1b"
 covariates = "x2" | "x3a" "x3b"
 responseprob = 0.15
 testoddsratio = 1.75
 covoddsratios = (2.1 1.4)
 ntotal = 100
 power = .;
run;
```

The **VARDIST=** options define the distributions of the predictor variables. The **TESTPREDICTOR=** option specifies two scenarios for the test predictor distribution, Normal(10,2) and Normal(10,3). The **COVARIATES=** option specifies two covariates, the first with a Poisson(7) distribution. The second covariate has an ordinal distribution on the values -5, 0, and 5 with two scenarios for the associated probabilities: (.3, .4, .3) and (.4, .3, .3). The response probability in the full model with all variables equal to zero is specified by the **RESPONSEPROB=** option as 0.15. The odds ratio for a unit decrease in the tested predictor is specified by the **TESTODDSRATIO=** option to be 1.75. Corresponding odds ratios for the two covariates in the full model are specified by the **COVODDSRATIOS=** option to be 2.1 and 1.4. The **POWER=.** option requests a solution for the power at a sample size of 100 as specified by the **NTOTAL=** option.

Default values of the **TEST=** and **ALPHA=** options specify a likelihood ratio test of the first predictor with a significance level of 0.05. The default of **DEFAULTUNIT=1** specifies that all odds ratios are defined in terms of unit changes in predictors. The default of **DEFAULTNBINS=10** specifies that each of the three predictor variables is discretized into a distribution with 10 categories in internal calculations.

You can also express effects in terms of regression coefficients, as in the following statements:

```
proc power;
 logistic
 vardist("x1a") = normal(0, 2)
 vardist("x1b") = normal(0, 3)
 vardist("x2") = poisson(7)
 vardist("x3a") = ordinal((-5 0 5) : (.3 .4 .3))
 vardist("x3b") = ordinal((-5 0 5) : (.4 .3 .3))
 testpredictor = "x1a" "x1b"
 covariates = "x2" | "x3a" "x3b"
 intercept = -6.928162
 testregcoeff = 0.5596158
 covregcoeffs = (0.7419373 0.3364722)
 ntotal = 100
 power = .;
run;
```

The regression coefficients for the tested predictor (**TESTREGCOEFF=0.5596158**) and covariates (**COVREGCOEFFS=(0.7419373 0.3364722)**) are determined by taking the logarithm of the corresponding odds ratios. The intercept in the full model is specified as -6.928162 by the **INTERCEPT=** option. This number is calculated according to the formula at the end of “Analyses in the LOGISTIC Statement” on page 6029, which expresses the intercept in terms of the response probability, regression coefficients, and predictor means:

$$\text{Intercept} = \log\left(\frac{0.15}{1 - 0.15}\right) - (0.5596158(0) + 0.7419373(7) + 0.3364722(0))$$

---

## MULTREG Statement

**MULTREG** <options> ;

The **MULTREG** statement performs power and sample size analyses for Type III *F* tests of sets of predictors in multiple linear regression, assuming either fixed or normally distributed predictors.

## Summary of Options

Table 71.4 summarizes the options available in the MULTREG statement.

**Table 71.4** MULTREG Statement Options

| Option                              | Description                                             |
|-------------------------------------|---------------------------------------------------------|
| <b>Define analysis</b>              |                                                         |
| TEST=                               | Specifies the statistical analysis                      |
| <b>Specify analysis information</b> |                                                         |
| ALPHA=                              | Specifies the significance level                        |
| MODEL=                              | Specifies the assumed distribution of the predictors    |
| NFULLPREDICTORS=                    | Specifies the number of predictors in the full model    |
| NOINT                               | Specifies a no-intercept model                          |
| NREDUCEDPREDICTORS=                 | Specifies the number of predictors in the reduced model |
| NTESTPREDICTORS=                    | Specifies the number of predictors being tested         |
| <b>Specify effects</b>              |                                                         |
| PARTIALCORR=                        | Specifies the partial correlation                       |
| RSQUAREDIFF=                        | Specifies the difference in $R^2$                       |
| RSQUAREFULL=                        | Specifies the $R^2$ of the full model                   |
| RSQUAREREDUCED=                     | Specifies the $R^2$ of the reduced model                |
| <b>Specify sample size</b>          |                                                         |
| NFRACTIONAL                         | Enables fractional input and output for sample sizes    |
| NTOTAL=                             | Specifies the sample size                               |
| <b>Specify power</b>                |                                                         |
| POWER=                              | Specifies the desired power                             |
| <b>Control ordering in output</b>   |                                                         |
| OUTPUTORDER=                        | Controls the order of parameters                        |

Table 71.5 summarizes the valid result parameters in the MULTREG statement.

**Table 71.5** Summary of Result Parameters in the MULTREG Statement

| Analyses   | Solve For   | Syntax   |
|------------|-------------|----------|
| TEST=TYPE3 | Power       | POWER=.  |
|            | Sample size | NTOTAL=. |

## Dictionary of Options

### ALPHA=*number-list*

specifies the level of significance of the statistical test. The default is 0.05, corresponding to the usual  $0.05 \times 100\% = 5\%$  level of significance. See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *number-list*.

**MODEL=keyword-list**

specifies the assumed distribution of the tested predictors. **MODEL=FIXED** indicates a fixed predictor distribution. **MODEL=RANDOM** (the default) indicates a joint multivariate normal distribution for the response and tested predictors. You can use the aliases **CONDITIONAL** for **FIXED** and **UNCONDITIONAL** for **RANDOM**. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *keyword-list*.

**FIXED** fixed predictors

**RANDOM** random (multivariate normal) predictors

**NFRACTIONAL****NFRAC**

enables fractional input and output for sample sizes. See the section “[Sample Size Adjustment Options](#)” on page 6023 for information about the ramifications of the presence (and absence) of the **NFRACTIONAL** option.

**NFULLPREDICTORS=number-list****NFULLPRED=number-list**

specifies the number of predictors in the full model, not counting the intercept. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**NOINT**

specifies a no-intercept model (for both full and reduced models). By default, the intercept is included in the model. If you want to test the intercept, you can specify the **NOINT** option and simply consider the intercept to be one of the predictors being tested. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**NREDUCEDPREDICTORS=number-list****NREDUCEDPRED=number-list****NREDPRED=number-list**

specifies the number of predictors in the reduced model, not counting the intercept. This is the same as the difference between values of the **NFULLPREDICTORS=** and **NTESTPREDICTORS=** options. Note that supplying a value of 0 is the same as specifying an *F* test of a Pearson correlation. This option cannot be used at the same time as the **NTESTPREDICTORS=** option. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**NTESTPREDICTORS=number-list****NTESTPRED=number-list**

specifies the number of predictors being tested. This is the same as the difference between values of the **NFULLPREDICTORS=** and **NREDUCEDPREDICTORS=** options. Note that supplying identical values for the **NTESTPREDICTORS=** and **NFULLPREDICTORS=** options is the same as specifying an *F* test of a Pearson correlation. This option cannot be used at the same time as the **NREDUCEDPREDICTORS=** option. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**NTOTAL=number-list**

specifies the sample size or requests a solution for the sample size with a missing value (NTOTAL=.). The minimum acceptable value for the sample size depends on the MODEL=, NOINT, NFULLPREDICTORS=, NTESTPREDICTORS=, and NREDUCEDPREDICTORS= options. It ranges from  $p + 1$  to  $p + 3$ , where  $p$  is the value of the NFULLPREDICTORS option. See Table 71.30 for further information about minimum NTOTAL values, and see the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *number-list*.

**OUTPUTORDER=INTERNAL****OUTPUTORDER=REVERSE****OUTPUTORDER=SYNTAX**

controls how the input and default analysis parameters are ordered in the output. OUTPUTORDER=INTERNAL (the default) arranges the parameters in the output according to the following order of their corresponding options:

- MODEL=
- NFULLPREDICTORS=
- NTESTPREDICTORS=
- NREDUCEDPREDICTORS=
- ALPHA=
- PARTIALCORR=
- RSQUAREFULL=
- RSQUAREREDUCED=
- RSQUAREDIFF=
- NTOTAL=
- POWER=

The OUTPUTORDER=SYNTAX option arranges the parameters in the output in the same order in which their corresponding options are specified in the MULTREG statement. The OUTPUTORDER=REVERSE option arranges the parameters in the output in the reverse of the order in which their corresponding options are specified in the MULTREG statement.

**PARTIALCORR=number-list****PCORR=number-list**

specifies the partial correlation between the tested predictors and the response, adjusting for any other predictors in the model. See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *number-list*.

**POWER=number-list**

specifies the desired power of the test or requests a solution for the power with a missing value (POWER=.). The power is expressed as a probability, a number between 0 and 1, rather than as a percentage. See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *number-list*.

**RSQUAREDIFF=number-list****RSQDIFF=number-list**

specifies the difference in  $R^2$  between the full and reduced models. This is equivalent to the proportion of variation explained by the predictors you are testing. It is also equivalent to the squared semipartial correlation of the tested predictors with the response. See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *number-list*.

**RSQUAREFULL**=*number-list*

**RSQFULL**=*number-list*

specifies the  $R^2$  of the full model, where  $R^2$  is the proportion of variation explained by the model. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**RSQUAREREDUCED**=*number-list*

**RSQREDUCED**=*number-list*

**RSQRED**=*number-list*

specifies the  $R^2$  of the reduced model, where  $R^2$  is the proportion of variation explained by the model. If the reduced model is an empty or intercept-only model (in other words, if **NREDUCEDPREDICTORS**=0 or **NTESTPREDICTORS**=**NFULLPREDICTORS**), then **RSQUAREREDUCED**=0 is assumed. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**TEST**=**TYPE3**

specifies a Type III  $F$  test of a set of predictors adjusting for any other predictors in the model. This is the default test option.

## Restrictions on Option Combinations

To specify the number of predictors, use any two of these three options:

- the number of predictors in the full model (**NFULLPREDICTORS**=)
- the number of predictors in the reduced model (**NREDUCEDPREDICTORS**=)
- the number of predictors being tested (**NTESTPREDICTORS**=)

To specify the effect, choose one of the following parameterizations:

- partial correlation (by using the **PARTIALCORR**= option)
- $R^2$  for the full and reduced models (by using any two of **RSQUAREDIFF**=, **RSQUAREFULL**=, and **RSQUAREREDUCED**=)

## Option Groups for Common Analyses

This section summarizes the syntax for the common analyses supported in the **MULTREG** statement.

### **Type III F Test of a Set of Predictors**

You can express effects in terms of partial correlation, as in the following statements. Default values of the **TEST**=, **MODEL**=, and **ALPHA**= options specify a Type III  $F$  test with a significance level of 0.05, assuming normally distributed predictors.

```

proc power;
 multreg
 model = random
 nfullpredictors = 7
 ntestpredictors = 3
 partialcorr = 0.35
 ntotal = 100
 power = .;
run;

```

You can also express effects in terms of  $R^2$ :

```

proc power;
 multreg
 model = fixed
 nfullpredictors = 7
 ntestpredictors = 3
 rsquarefull = 0.9
 rsquarediff = 0.1
 ntotal = .
 power = 0.9;
run;

```

---

## ONECORR Statement

**ONECORR** <options> ;

The **ONECORR** statement performs power and sample size analyses for tests of simple and partial Pearson correlation between two variables. Both Fisher's  $z$  test and the  $t$  test are supported.

### Summary of Options

Table 71.6 summarizes the options available in the **ONECORR** statement.

**Table 71.6** ONECORR Statement Options

| Option                              | Description                                                             |
|-------------------------------------|-------------------------------------------------------------------------|
| <b>Define analysis</b>              |                                                                         |
| <b>DIST=</b>                        | Specifies the underlying distribution assumed for the test statistic    |
| <b>TEST=</b>                        | Specifies the statistical analysis                                      |
| <b>Specify analysis information</b> |                                                                         |
| <b>ALPHA=</b>                       | Specifies the significance level                                        |
| <b>MODEL=</b>                       | Specifies the assumed distribution of the variables                     |
| <b>NPARTIALVARS=</b>                | Specifies the number of variables adjusted for in the correlation       |
| <b>NULLCORR=</b>                    | Specifies the null value of the correlation                             |
| <b>SIDES=</b>                       | Specifies the number of sides and the direction of the statistical test |
| <b>Specify effects</b>              |                                                                         |
| <b>CORR=</b>                        | Specifies the correlation                                               |



Table 71.6 *continued*

| Option                            | Description                                          |
|-----------------------------------|------------------------------------------------------|
| <b>Specify sample size</b>        |                                                      |
| NFRACTIONAL                       | Enables fractional input and output for sample sizes |
| NTOTAL=                           | Specifies the sample size                            |
| <b>Specify power</b>              |                                                      |
| POWER=                            | Specifies the desired power of the test              |
| <b>Control ordering in output</b> |                                                      |
| OUTPUTORDER=                      | Controls the output order of parameters              |

Table 71.7 summarizes the valid result parameters in the `ONECORR` statement.

Table 71.7 Summary of Result Parameters in the `ONECORR` Statement

| Analyses     | Solve For            | Syntax              |
|--------------|----------------------|---------------------|
| TEST=PEARSON | Power<br>Sample size | POWER=.<br>NTOTAL=. |

## Dictionary of Options

### **ALPHA=***number-list*

specifies the level of significance of the statistical test. The default is 0.05, corresponding to the usual  $0.05 \times 100\% = 5\%$  level of significance. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

### **CORR=***number-list*

specifies the correlation between two variables, possibly adjusting for other variables as determined by the `NPARTIALVARS=` option. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

### **DIST=FISHERZ**

### **DIST=T**

specifies the underlying distribution assumed for the test statistic. FISHERZ corresponds to Fisher’s  $z$  normalizing transformation of the correlation coefficient. T corresponds to the  $t$  transformation of the correlation coefficient. Note that `DIST=T` is equivalent to analyses in the `MULTREG` statement with `NTESTPREDICTORS=1`. The default value is FISHERZ.

### **MODEL=***keyword-list*

specifies the assumed distribution of the first variable when `DIST=T`. The second variable is assumed to have a normal distribution. `MODEL=FIXED` indicates a fixed distribution. `MODEL=RANDOM` (the default) indicates a joint bivariate normal distribution with the second variable. You can use the aliases `CONDITIONAL` for `FIXED` and `UNCONDITIONAL` for `RANDOM`. This option can be used only for `DIST=T`. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *keyword-list*.

FIXED fixed variables

RANDOM random (bivariate normal) variables

## NFRACTIONAL

### NFRAC

enables fractional input and output for sample sizes. See the section “[Sample Size Adjustment Options](#)” on page 6023 for information about the ramifications of the presence (and absence) of the **NFRACTIONAL** option.

### NPARTIALVARS=*number-list*

### NPVARS=*number-list*

specifies the number of variables adjusted for in the correlation between the two primary variables. The default value is 0, corresponding to a simple correlation. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

### NTOTAL=*number-list*

specifies the sample size or requests a solution for the sample size with a missing value (**NTOTAL=.**). Values for the sample size must be at least  $p + 3$  when **DIST=T** and **MODEL=CONDITIONAL**, and at least  $p + 4$  when either **DIST=FISHER** or when **DIST=T** and **MODEL=UNCONDITIONAL**, where  $p$  is the value of the **NPARTIALVARS** option. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

### NULLCORR=*number-list*

### NULLC=*number-list*

specifies the null value of the correlation. The default value is 0. This option can be used only with the **DIST=FISHERZ** analysis. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

## OUTPUTORDER=INTERNAL

## OUTPUTORDER=REVERSE

## OUTPUTORDER=SYNTAX

controls how the input and default analysis parameters are ordered in the output. **OUTPUTORDER=INTERNAL** (the default) arranges the parameters in the output according to the following order of their corresponding options:

- **MODEL=**
- **SIDES=**
- **NULL=**
- **ALPHA=**
- **NPARTIALVARS=**
- **CORR=**
- **NTOTAL=**
- **POWER=**

The **OUTPUTORDER=SYNTAX** option arranges the parameters in the output in the same order in which their corresponding options are specified in the **ONECORR** statement. The **OUTPUTORDER=REVERSE** option arranges the parameters in the output in the reverse of the order in which their corresponding options are specified in the **ONECORR** statement.

**POWER=number-list**

specifies the desired power of the test or requests a solution for the power with a missing value (POWER=.). The power is expressed as a probability, a number between 0 and 1, rather than as a percentage. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**SIDES=keyword-list**

specifies the number of sides (or tails) and the direction of the statistical test. Valid keywords are

- 1 one-sided with alternative hypothesis in same direction as effect
- 2 two-sided
- U upper one-sided with alternative greater than null value
- L lower one-sided with alternative less than null value

The default value is 2.

**TEST=PEARSON**

specifies a test of the Pearson correlation coefficient between two variables, possibly adjusting for other variables. This is the default test option.

## Option Groups for Common Analyses

This section summarizes the syntax for the common analyses supported in the `ONECORR` statement.

### *Fisher's z Test for Pearson Correlation*

The following statements demonstrate a power computation for Fisher's z test for correlation. Default values of `TEST=PEARSON`, `ALPHA=0.05`, `SIDES=2`, and `NPARTIALVARS=0` are assumed.

```
proc power;
 onecorr dist=fisherz
 nullcorr = 0.15
 corr = 0.35
 ntotal = 180
 power = .;
run;
```

### *t Test for Pearson Correlation*

The following statements demonstrate a sample size computation for the *t* test for correlation. Default values of `TEST=PEARSON`, `MODEL=RANDOM`, `ALPHA=0.05`, and `SIDES=2` are assumed.

```
proc power;
 onecorr dist=t
 npartialvars = 4
 corr = 0.45
 ntotal = .
 power = 0.85;
run;
```

---

## ONESAMPLEFREQ Statement

**ONESAMPLEFREQ** < options > ;

The **ONESAMPLEFREQ** statement performs power and sample size analyses for exact and approximate tests (including equivalence, noninferiority, and superiority) and confidence interval precision for a single binomial proportion.

### Summary of Options

Table 71.8 summarizes the options available in the **ONESAMPLEFREQ** statement.

**Table 71.8** ONESAMPLEFREQ Statement Options

| Option                                         | Description                                                                                                                            |
|------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------|
| <b>Define analysis</b>                         |                                                                                                                                        |
| CI=                                            | Specifies an analysis of precision of a confidence interval                                                                            |
| TEST=                                          | Specifies the statistical analysis                                                                                                     |
| <b>Specify analysis information</b>            |                                                                                                                                        |
| ALPHA=                                         | Specifies the significance level                                                                                                       |
| EQUIVBOUNDS=                                   | Specifies the lower and upper equivalence bounds                                                                                       |
| LOWER=                                         | Specifies the lower equivalence bound                                                                                                  |
| MARGIN=                                        | Specifies the equivalence or noninferiority or superiority margin                                                                      |
| NULLPROPORTION=                                | Specifies the null proportion                                                                                                          |
| SIDES=                                         | Specifies the number of sides and the direction of the statistical test                                                                |
| UPPER=                                         | Specifies the upper equivalence bound                                                                                                  |
| <b>Specify effect</b>                          |                                                                                                                                        |
| HALFWIDTH=                                     | Specifies the desired confidence interval half-width                                                                                   |
| PROPORTION=                                    | Specifies the binomial proportion                                                                                                      |
| <b>Specify variance estimation</b>             |                                                                                                                                        |
| VAREST=                                        | Specifies how the variance is computed                                                                                                 |
| <b>Specify sample size</b>                     |                                                                                                                                        |
| NFRACTIONAL                                    | Enables fractional input and output for sample sizes                                                                                   |
| NTOTAL=                                        | Specifies the sample size                                                                                                              |
| <b>Specify power and related probabilities</b> |                                                                                                                                        |
| POWER=                                         | Specifies the desired power of the test                                                                                                |
| PROBWIDTH=                                     | Specifies the probability of obtaining a confidence interval half-width less than or equal to the value specified by <b>HALFWIDTH=</b> |
| <b>Choose computational method</b>             |                                                                                                                                        |
| METHOD=                                        | Specifies the computational method                                                                                                     |
| <b>Control ordering in output</b>              |                                                                                                                                        |
| OUTPUTORDER=                                   | Controls the output order of parameters                                                                                                |

---

Table 71.9 summarizes the valid result parameters for different analyses in the `ONESAMPLEFREQ` statement.

**Table 71.9** Summary of Result Parameters in the `ONESAMPLEFREQ` Statement

| Analyses                                   | Solve For            | Syntax                                        |
|--------------------------------------------|----------------------|-----------------------------------------------|
| <code>CI=WILSON</code>                     | Prob(width)          | <code>PROBWIDTH=.</code>                      |
| <code>CI=AGRESTICOULL</code>               | Prob(width)          | <code>PROBWIDTH=.</code>                      |
| <code>CI=JEFFREYS</code>                   | Prob(width)          | <code>PROBWIDTH=.</code>                      |
| <code>CI=EXACT</code>                      | Prob(width)          | <code>PROBWIDTH=.</code>                      |
| <code>CI=WALD</code>                       | Prob(width)          | <code>PROBWIDTH=.</code>                      |
| <code>CI=WALD_CORRECT</code>               | Prob(width)          | <code>PROBWIDTH=.</code>                      |
| <code>TEST=ADJZ METHOD=EXACT</code>        | Power                | <code>POWER=.</code>                          |
| <code>TEST=ADJZ METHOD=NORMAL</code>       | Power<br>Sample size | <code>POWER=.</code><br><code>NTOTAL=.</code> |
| <code>TEST=EQUIV_ADJZ METHOD=EXACT</code>  | Power                | <code>POWER=.</code>                          |
| <code>TEST=EQUIV_ADJZ METHOD=NORMAL</code> | Power<br>Sample size | <code>POWER=.</code><br><code>NTOTAL=.</code> |
| <code>TEST=EQUIV_EXACT</code>              | Power                | <code>POWER=.</code>                          |
| <code>TEST=EQUIV_Z METHOD=EXACT</code>     | Power                | <code>POWER=.</code>                          |
| <code>TEST=EQUIV_Z METHOD=NORMAL</code>    | Power<br>Sample size | <code>POWER=.</code><br><code>NTOTAL=.</code> |
| <code>TEST=EXACT</code>                    | Power                | <code>POWER=.</code>                          |
| <code>TEST=Z METHOD=EXACT</code>           | Power                | <code>POWER=.</code>                          |
| <code>TEST=Z METHOD=NORMAL</code>          | Power<br>Sample size | <code>POWER=.</code><br><code>NTOTAL=.</code> |

## Dictionary of Options

### **ALPHA=***number-list*

specifies the level of significance of the statistical test. The default is 0.05, corresponding to the usual  $0.05 \times 100\% = 5\%$  level of significance. If the `CI=` and `SIDES=1` options are used, then the value must be less than 0.5. See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *number-list*.

### **CI**

**CI=AGRESTICOULL** | **AC**

**CI=JEFFREYS**

**CI=EXACT** | **CLOPPERPEARSON** | **CP**

**CI=WALD**

**CI=WALD\_CORRECT**

**CI=WILSON** | **SCORE**

specifies an analysis of precision of a confidence interval for the sample binomial proportion.

The value of the **CI=** option specifies the type of confidence interval. The **CI=AGRESTICOULL** option is a generalization of the “Adjusted Wald / add 2 successes and 2 failures” interval of Agresti and Coull (1998) and is presented in Brown, Cai, and DasGupta (2001). It corresponds to the **TABLES / BINOMIAL (AGRESTICOULL)** option in PROC FREQ. The **CI=JEFFREYS** option specifies the equal-tailed Jeffreys prior Bayesian interval, corresponding to the **TABLES / BINOMIAL (JEFFREYS)** option in PROC FREQ. The **CI=EXACT** option specifies the exact Clopper-Pearson confidence interval based on enumeration, corresponding to the **TABLES / BINOMIAL (EXACT)** option in PROC FREQ. The **CI=WALD** option specifies the confidence interval based on the Wald test (also commonly called the  $z$  test or normal-approximation test), corresponding to the **TABLES / BINOMIAL (WALD)** option in PROC FREQ. The **CI=WALD\_CORRECT** option specifies the confidence interval based on the Wald test with continuity correction, corresponding to the **TABLES / BINOMIAL (CORRECT WALD)** option in PROC FREQ. The **CI=WILSON** option (the default) specifies the confidence interval based on the score statistic, corresponding to the **TABLES / BINOMIAL (WILSON)** option in PROC FREQ.

Instead of power, the relevant probability for this analysis is the probability of achieving a desired precision. Specifically, it is the probability that the half-width of the confidence interval will be at most the value specified by the **HALFWIDTH=** option.

**EQUIVBOUNDS=***grouped-number-list*

specifies the lower and upper equivalence bounds, representing the same information as the combination of the **LOWER=** and **UPPER=** options but grouping them together. The **EQUIVBOUNDS=** option can be used only with equivalence analyses (**TEST=EQUIV\_ADJZ | EQUIV\_EXACT | EQUIV\_Z**). Values must be strictly between 0 and 1. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *grouped-number-list*.

**HALFWIDTH=***number-list*

specifies the desired confidence interval half-width. The half-width for a two-sided interval is the length of the confidence interval divided by two. This option can be used only with the **CI=** analysis. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**LOWER=***number-list*

specifies the lower equivalence bound for the binomial proportion. The **LOWER=** option can be used only with equivalence analyses (**TEST=EQUIV\_ADJZ | EQUIV\_EXACT | EQUIV\_Z**). Values must be strictly between 0 and 1. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**MARGIN=***number-list*

specifies the equivalence or noninferiority or superiority margin, depending on the analysis.

The **MARGIN=** option can be used with one-sided analyses (**SIDES = 1 | U | L**), in which case it specifies the margin added to the null proportion value in the hypothesis test, resulting in a noninferiority or superiority test (depending on the agreement between the effect and hypothesis directions and the sign of the margin). A test with a null proportion  $p_0$  and a margin  $m$  is the same as a test with null proportion  $p_0 + m$  and no margin.

The **MARGIN=** option can also be used with equivalence analyses (**TEST=EQUIV\_ADJZ | EQUIV\_EXACT | EQUIV\_Z**) when the **NULLPROPORTION=** option is used, in which case it specifies the lower and upper equivalence bounds as  $p_0 - m$  and  $p_0 + m$ , where  $p_0$  is the value of the **NULLPROPORTION=** option and  $m$  is the value of the **MARGIN=** option.

The **MARGIN=** option cannot be used in conjunction with the **SIDES=2** option. (Instead, specify an equivalence analysis by using **TEST=EQUIV\_ADJZ** or **TEST=EQUIV\_EXACT** or **TEST=EQUIV\_Z**). Also, the **MARGIN=** option cannot be used with the **CI=** option.

Values must be strictly between  $-1$  and  $1$ . In addition, the sum of **NULLPROPORTION** and **MARGIN** must be strictly between  $0$  and  $1$  for one-sided analyses, and the derived lower equivalence bound ( $2 * \text{NULLPROPORTION} - \text{MARGIN}$ ) must be strictly between  $0$  and  $1$  for equivalence analyses.

See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

#### **METHOD=EXACT**

#### **METHOD=NORMAL**

specifies the computational method. **METHOD=EXACT** (the default) computes exact results by using the binomial distribution. **METHOD=NORMAL** computes approximate results by using the normal approximation to the binomial distribution.

#### **NFRACTIONAL**

#### **NFRAC**

enables fractional input and output for sample sizes. This option is invalid when the **METHOD=EXACT** option is specified. See the section “[Sample Size Adjustment Options](#)” on page 6023 for information about the ramifications of the presence (and absence) of the **NFRAC-TIONAL** option.

#### **NTOTAL=number-list**

specifies the sample size or requests a solution for the sample size with a missing value (**NTOTAL=.**). See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

#### **NULLPROPORTION=number-list**

#### **NULLP=number-list**

specifies the null proportion. A value of  $0.5$  corresponds to the sign test. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

#### **OUTPUTORDER=INTERNAL**

#### **OUTPUTORDER=REVERSE**

#### **OUTPUTORDER=SYNTAX**

controls how the input and default analysis parameters are ordered in the output. **OUTPUTORDER=INTERNAL** (the default) arranges the parameters in the output according to the following order of their corresponding options:

- **SIDES=**
- **NULLPROPORTION=**
- **ALPHA=**
- **PROPORTION=**
- **NTOTAL=**
- **POWER=**

The **OUTPUTORDER=SYNTAX** option arranges the parameters in the output in the same order in which their corresponding options are specified in the **ONESAMPLEFREQ** statement. The **OUTPUTORDER=REVERSE** option arranges the parameters in the output in the reverse of the order in which their corresponding options are specified in the **ONESAMPLEFREQ** statement.

**POWER=number-list**

specifies the desired power of the test or requests a solution for the power with a missing value (**POWER=.**). The power is expressed as a probability, a number between 0 and 1, rather than as a percentage. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**PROBWIDTH=number-list**

specifies the desired probability of obtaining a confidence interval half-width less than or equal to the value specified by the **HALFWIDTH=** option. A missing value (**PROBWIDTH=.**) requests a solution for this probability. Values are expressed as probabilities (for example, 0.9) rather than percentages. This option can be used only with the **CI=** analysis. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**PROPORTION=number-list**

**P=number-list**

specifies the binomial proportion—that is, the expected proportion of successes in the hypothetical binomial trial. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**SIDES=keyword-list**

specifies the number of sides (or tails) and the direction of the statistical test. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *keyword-list*. Valid keywords are as follows:

- 1 one-sided with alternative hypothesis in same direction as effect
- 2 two-sided
- U upper one-sided with alternative greater than null value
- L lower one-sided with alternative less than null value

If the effect size is zero, then **SIDES=1** is not permitted; instead, specify the direction of the test explicitly in this case with either **SIDES=L** or **SIDES=U**. The default value is 2.

**TEST**

**TEST= ADJZ**

**TEST= EQUIV\_ADJZ**

**TEST= EQUIV\_EXACT**

**TEST= EQUIV\_Z**

**TEST= EXACT**

**TEST= Z**

specifies the statistical analysis. **TEST=ADJZ** specifies a normal-approximate *z* test with continuity adjustment. **TEST=EQUIV\_ADJZ** specifies a normal-approximate two-sided equivalence test based on the *z* statistic with continuity adjustment and a TOST (two one-sided tests) procedure.



**TEST=EQUIV\_EXACT** specifies the exact binomial two-sided equivalence test based on a TOST (two one-sided tests) procedure. **TEST=EQUIV\_Z** specifies a normal-approximate two-sided equivalence test based on the  $z$  statistic without any continuity adjustment, which is the same as the chi-square statistic, and a TOST (two one-sided tests) procedure. **TEST** or **TEST=EXACT** (the default) specifies the exact binomial test. **TEST=Z** specifies a normal-approximate  $z$  test without any continuity adjustment, which is the same as the chi-square test when **SIDES=2**.

**UPPER=number-list**

specifies the upper equivalence bound for the binomial proportion. The **UPPER=** option can be used only with equivalence analyses (**TEST=EQUIV\_ADJZ** | **EQUIV\_EXACT** | **EQUIV\_Z**). Values must be strictly between 0 and 1. See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *number-list*.

**VAREST=keyword-list**

specifies how the variance is computed in the test statistic for the **TEST=Z**, **TEST=ADJZ**, **TEST=EQUIV\_Z**, and **TEST=EQUIV\_ADJZ** analyses. See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *keyword-list*. Valid keywords are as follows:

**NULL** (the default) estimates the variance by using the null proportion(s) (specified by some combination of the **NULLPROPORTION=**, **MARGIN=**, **LOWER=**, and **UPPER=** options). For **TEST=Z** and **TEST=ADJZ**, the null proportion is the value of the **NULLPROPORTION=** option plus the value of the **MARGIN=** option (if it is used). For **TEST=EQUIV\_Z** and **TEST=EQUIV\_ADJZ**, there are two null proportions, corresponding to the lower and upper equivalence bounds, one for each test in the TOST (two one-sided tests) procedure.

**SAMPLE** estimates the variance by using the observed sample proportion.

This option is ignored if the analysis is one other than **TEST=Z**, **TEST=ADJZ**, **TEST=EQUIV\_Z**, or **TEST=EQUIV\_ADJZ**.

## Option Groups for Common Analyses

This section summarizes the syntax for the common analyses supported in the **ONESAMPLEFREQ** statement.

### Exact Test of a Binomial Proportion

The following statements demonstrate a power computation for the exact test of a binomial proportion. Defaults for the **SIDES=** and **ALPHA=** options specify a two-sided test with a 0.05 significance level.

```
proc power;
 onesamplefreq test=exact
 nullproportion = 0.2
 proportion = 0.3
 ntotal = 100
 power = .;
run;
```

**z Test**

The following statements demonstrate a sample size computation for the  $z$  test of a binomial proportion. Defaults for the `SIDES=`, `ALPHA=`, and `VAREST=` options specify a two-sided test with a 0.05 significance level that uses the null variance estimate.

```
proc power;
 onesamplefreq test=z method=normal
 nullproportion = 0.8
 proportion = 0.85
 sides = u
 ntotal = .
 power = .9;
run;
```

**z Test with Continuity Adjustment**

The following statements demonstrate a sample size computation for the  $z$  test of a binomial proportion with a continuity adjustment. Defaults for the `SIDES=`, `ALPHA=`, and `VAREST=` options specify a two-sided test with a 0.05 significance level that uses the null variance estimate.

```
proc power;
 onesamplefreq test=adjz method=normal
 nullproportion = 0.15
 proportion = 0.1
 sides = l
 ntotal = .
 power = .9;
run;
```

**Exact Equivalence Test for a Binomial Proportion**

You can specify equivalence bounds by using the `EQUIVBOUNDS=` option, as in the following statements:

```
proc power;
 onesamplefreq test=equiv_exact
 proportion = 0.35
 equivbounds = (0.2 0.4)
 ntotal = 50
 power = .;
run;
```

You can also specify the combination of `NULLPROPORTION=` and `MARGIN=` options:

```
proc power;
 onesamplefreq test=equiv_exact
 proportion = 0.35
 nullproportion = 0.3
 margin = 0.1
 ntotal = 50
 power = .;
run;
```

Finally, you can specify the combination of LOWER= and UPPER= options:

```
proc power;
 onesamplefreq test=equiv_exact
 proportion = 0.35
 lower = 0.2
 upper = 0.4
 ntotal = 50
 power = .;
run;
```

Note that the three preceding analyses are identical.

### ***Exact Noninferiority Test for a Binomial Proportion***

A noninferiority test corresponds to an upper one-sided test with a negative-valued margin, as demonstrated in the following statements:

```
proc power;
 onesamplefreq test=exact
 sides = U
 proportion = 0.15
 nullproportion = 0.1
 margin = -0.02
 ntotal = 130
 power = .;
run;
```

### ***Exact Superiority Test for a Binomial Proportion***

A superiority test corresponds to an upper one-sided test with a positive-valued margin, as demonstrated in the following statements:

```
proc power;
 onesamplefreq test=exact
 sides = U
 proportion = 0.15
 nullproportion = 0.1
 margin = 0.02
 ntotal = 130
 power = .;
run;
```

### ***Confidence Interval Precision***

The following statements performs a confidence interval precision analysis for the Wilson score-based confidence interval for a binomial proportion. The default value of the ALPHA= option specifies a confidence level of 0.95.

```
proc power;
 onesamplefreq ci=wilson
 halfwidth = 0.1
 proportion = 0.3
 ntotal = 70
 probwidth = .;
run;
```

### Restrictions on Option Combinations

To specify the equivalence bounds for `TEST=EQUIV_ADJZ`, `TEST=EQUIV_EXACT`, and `TEST=EQUIV_Z`, use any of these three option sets:

- lower and upper equivalence bounds, using the `EQUIVBOUNDS=` option
- lower and upper equivalence bounds, using the `LOWER=` and `UPPER=` options
- null proportion (`NULLPROPORTION=`) and margin (`MARGIN=`)

## ONESAMPLEMEANS Statement

**ONESAMPLEMEANS** < options > ;

The `ONESAMPLEMEANS` statement performs power and sample size analyses for *t* tests, equivalence tests, and confidence interval precision involving one sample.

### Summary of Options

Table 71.10 summarizes the options available in the `ONESAMPLEMEANS` statement.

**Table 71.10** ONESAMPLEMEANS Statement Options

| Option                              | Description                                                                |
|-------------------------------------|----------------------------------------------------------------------------|
| <b>Define analysis</b>              |                                                                            |
| <code>CI=</code>                    | Specifies an analysis of precision of the confidence interval for the mean |
| <code>DIST=</code>                  | Specifies the underlying distribution assumed for the test statistic       |
| <code>TEST=</code>                  | Specifies the statistical analysis                                         |
| <b>Specify analysis information</b> |                                                                            |
| <code>ALPHA=</code>                 | Specifies the significance level                                           |
| <code>LOWER=</code>                 | Specifies the lower equivalence bound for the mean                         |
| <code>NULLMEAN=</code>              | Specifies the null mean                                                    |
| <code>SIDES=</code>                 | Specifies the number of sides and the direction of the statistical test    |
| <code>UPPER=</code>                 | Specifies the upper equivalence bound for the mean                         |
| <b>Specify effect</b>               |                                                                            |
| <code>HALFWIDTH=</code>             | Specifies the desired confidence interval half-width                       |
| <code>MEAN=</code>                  | Specifies the mean                                                         |
| <b>Specify variability</b>          |                                                                            |
| <code>CV=</code>                    | Specifies the coefficient of variation                                     |
| <code>STDDEV=</code>                | Specifies the standard deviation                                           |
| <b>Specify sample size</b>          |                                                                            |
| <code>NFRACTIONAL</code>            | Enables fractional input and output for sample sizes                       |
| <code>NTOTAL=</code>                | Specifies the sample size                                                  |

Table 71.10 *continued*

| Option                                         | Description                                                                                                                     |
|------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------|
| <b>Specify power and related probabilities</b> |                                                                                                                                 |
| POWER=                                         | Specifies the desired power of the test                                                                                         |
| PROBTYPE=                                      | Specifies the type of probability for the PROBWIDTH= option                                                                     |
| PROBWIDTH=                                     | Specifies the probability of obtaining a confidence interval half-width less than or equal to the value specified by HALFWIDTH= |
| <b>Control ordering in output</b>              |                                                                                                                                 |
| OUTPUTORDER=                                   | Controls the output order of parameters                                                                                         |

Table 71.11 summarizes the valid result parameters for different analyses in the ONESAMPLEMEANS statement.

Table 71.11 Summary of Result Parameters in the ONESAMPLEMEANS Statement

| Analyses              | Solve For          | Syntax      |
|-----------------------|--------------------|-------------|
| TEST=T DIST=NORMAL    | Power              | POWER=.     |
|                       | Sample size        | NTOTAL=.    |
|                       | Alpha              | ALPHA=.     |
|                       | Mean               | MEAN=.      |
|                       | Standard Deviation | STDDEV=.    |
| TEST=T DIST=LOGNORMAL | Power              | POWER=.     |
|                       | Sample size        | NTOTAL=.    |
| TEST=EQUIV            | Power              | POWER=.     |
|                       | Sample size        | NTOTAL=.    |
| CI=T                  | Prob(width)        | PROBWIDTH=. |
|                       | Sample size        | NTOTAL=.    |

## Dictionary of Options

### ALPHA=*number-list*

specifies the level of significance of the statistical test or requests a solution for alpha with a missing value (ALPHA=.). The default is 0.05, corresponding to the usual  $0.05 \times 100\% = 5\%$  level of significance. If the CI= and SIDES=1 options are used, then the value must be less than 0.5. See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *number-list*.

### CI

#### CI=T

specifies an analysis of precision of the confidence interval for the mean. Instead of power, the relevant probability for this analysis is the probability of achieving a desired precision. Specifically, it is the probability that the half-width of the confidence interval will be at most the value specified by the HALFWIDTH= option. If neither the CI= option nor the TEST= option is used, the default is TEST=T.

**CV=number-list**

specifies the coefficient of variation, defined as the ratio of the standard deviation to the mean. You can use this option only with **DIST=LOGNORMAL**. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**DIST=LOGNORMAL****DIST=NORMAL**

specifies the underlying distribution assumed for the test statistic. **NORMAL** corresponds to the normal distribution, and **LOGNORMAL** corresponds to the lognormal distribution. The default value is **NORMAL**.

**HALFWIDTH=number-list**

specifies the desired confidence interval half-width. The half-width is defined as the distance between the point estimate and a finite endpoint. This option can be used only with the **CI=T** analysis. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**LOWER=number-list**

specifies the lower equivalence bound for the mean. This option can be used only with the **TEST=EQUIV** analysis. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**MEAN=number-list**

specifies the mean, in the original scale, or requests a solution for the mean with a missing value (**MEAN=.**). The mean is arithmetic if **DIST=NORMAL** and geometric if **DIST=LOGNORMAL**. This option can be used only with the **TEST=T** and **TEST=EQUIV** analyses. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**NFRACTIONAL****NFRAC**

enables fractional input and output for sample sizes. See the section “[Sample Size Adjustment Options](#)” on page 6023 for information about the ramifications of the presence (and absence) of the **NFRACTIONAL** option.

**NTOTAL=number-list**

specifies the sample size or requests a solution for the sample size with a missing value (**NTOTAL=.**). See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**NULLMEAN=number-list****NULLM=number-list**

specifies the null mean, in the original scale (whether **DIST=NORMAL** or **DIST=LOGNORMAL**). The default value is 0 when **DIST=NORMAL** and 1 when **DIST=LOGNORMAL**. This option can be used only with the **TEST=T** analysis. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**OUTPUTORDER=INTERNAL****OUTPUTORDER=REVERSE****OUTPUTORDER=SYNTAX**

controls how the input and default analysis parameters are ordered in the output. **OUTPUTORDER=INTERNAL** (the default) arranges the parameters in the output according to the following order of their corresponding options:

- **SIDES=**
- **NULLMEAN=**
- **LOWER=**
- **UPPER=**
- **ALPHA=**
- **MEAN=**
- **HALFWIDTH=**
- **STDDEV=**
- **CV=**
- **NTOTAL=**
- **POWER=**
- **PROBTYPE=**
- **PROBWIDTH=**

The **OUTPUTORDER=SYNTAX** option arranges the parameters in the output in the same order in which their corresponding options are specified in the **ONESAMPLEMEANS** statement. The **OUTPUTORDER=REVERSE** option arranges the parameters in the output in the reverse of the order in which their corresponding options are specified in the **ONESAMPLEMEANS** statement.

**POWER=number-list**

specifies the desired power of the test or requests a solution for the power with a missing value (**POWER=.**). The power is expressed as a probability, a number between 0 and 1, rather than as a percentage. This option can be used only with the **TEST=T** and **TEST=EQUIV** analyses. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**PROBTYPE=keyword-list**

specifies the type of probability for the **PROBWIDTH=** option. A value of **CONDITIONAL** (the default) indicates the conditional probability that the confidence interval half-width is at most the value specified by the **HALFWIDTH=** option, given that the true mean is captured by the confidence interval. A value of **UNCONDITIONAL** indicates the unconditional probability that the confidence interval half-width is at most the value specified by the **HALFWIDTH=** option. You can use the alias **GIVENVALIDITY** for **CONDITIONAL**. The **PROBTYPE=** option can be used only with the **CI=T** analysis. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *keyword-list*.

**CONDITIONAL** width probability conditional on interval containing the mean

**UNCONDITIONAL** unconditional width probability

**PROBWIDTH=number-list**

specifies the desired probability of obtaining a confidence interval half-width less than or equal to the value specified by the **HALFWIDTH=** option. A missing value (**PROBWIDTH=.**) requests a solution for this probability. The type of probability is controlled with the **PROBTYPE=** option. Values are expressed as probabilities (for example, 0.9) rather than percentages. This option can be used only with the **CI=T** analysis. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**SIDES=keyword-list**

specifies the number of sides (or tails) and the direction of the statistical test or confidence interval. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *keyword-list*. Valid keywords and their interpretation for the **TEST=** analyses are as follows:

- 1 one-sided with alternative hypothesis in same direction as effect
- 2 two-sided
- U upper one-sided with alternative greater than null value
- L lower one-sided with alternative less than null value

For confidence intervals, **SIDES=U** refers to an interval between the lower confidence limit and infinity, and **SIDES=L** refers to an interval between minus infinity and the upper confidence limit. For both of these cases and **SIDES=1**, the confidence interval computations are equivalent. The **SIDES=** option can be used only with the **TEST=T** and **CI=T** analyses. The default value is 2.

**STDDEV=number-list****STD=number-list**

specifies the standard deviation, or requests a solution for the standard deviation with a missing value (**STDDEV=.**). You can use this option only with **DIST=NORMAL**. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**TEST****TEST=EQUIV****TEST=T**

specifies the statistical analysis. **TEST=EQUIV** specifies an equivalence test of the mean by using a two one-sided tests (TOST) analysis (Schuirmann 1987). **TEST** or **TEST=T** (the default) specifies a *t* test on the mean. If neither the **TEST=** option nor the **CI=** option is used, the default is **TEST=T**.

**UPPER=number-list**

specifies the upper equivalence bound for the mean, in the original scale (whether **DIST=NORMAL** or **DIST=LOGNORMAL**). This option can be used only with the **TEST=EQUIV** analysis. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.



## Restrictions on Option Combinations

To define the analysis, choose one of the following parameterizations:

- a statistical test (by using the `TEST=` option)
- confidence interval precision (by using the `CI=` option)

## Option Groups for Common Analyses

This section summarizes the syntax for the common analyses supported in the `ONESAMPLEMEANS` statement.

### One-Sample *t* Test

The following statements demonstrate a power computation for the one-sample *t* test. Default values for the `DIST=`, `SIDES=`, `NULLMEAN=`, and `ALPHA=` options specify a two-sided test for zero mean with a normal distribution and a significance level of 0.05.

```
proc power;
 onesamplemeans test=t
 mean = 7
 stddev = 3
 ntotal = 50
 power = .;
run;
```

### One-Sample *t* Test with Lognormal Data

The following statements demonstrate a sample size computation for the one-sample *t* test for lognormal data. Default values for the `SIDES=`, `NULLMEAN=`, and `ALPHA=` options specify a two-sided test for unit mean with a significance level of 0.05.

```
proc power;
 onesamplemeans test=t dist=lognormal
 mean = 7
 cv = 0.8
 ntotal = .
 power = 0.9;
run;
```

### Equivalence Test for Mean of Normal Data

The following statements demonstrate a power computation for the TOST equivalence test for a normal mean. Default values for the `DIST=` and `ALPHA=` options specify a normal distribution and a significance level of 0.05.

```
proc power;
 onesamplemeans test=equiv
 lower = 2
 upper = 7
 mean = 4
 stddev = 3
 ntotal = 100
 power = .;
run;
```

**Equivalence Test for Mean of Lognormal Data**

The following statements demonstrate a sample size computation for the TOST equivalence test for a log-normal mean. The default of `ALPHA=0.05` specifies a significance level of 0.05.

```
proc power;
 onesamplemeans test=equiv dist=lognormal
 lower = 1
 upper = 5
 mean = 3
 cv = 0.6
 ntotal = .
 power = 0.85;
run;
```

**Confidence Interval for Mean**

By default `CI=T` analyzes the conditional probability of obtaining the desired precision, given that the interval contains the true mean, as in the following statements. The defaults of `SIDES=2` and `ALPHA=0.05` specify a two-sided interval with a confidence level of 0.95.

```
proc power;
 onesamplemeans ci = t
 halfwidth = 14
 stddev = 8
 ntotal = 50
 probwidth = .;
run;
```

---

**ONEWAYANOVA Statement**

**ONEWAYANOVA** < options > ;

The **ONEWAYANOVA** statement performs power and sample size analyses for one-degree-of-freedom contrasts and the overall *F* test in one-way analysis of variance.

**Summary of Options**

Table 71.12 summarizes the options available in the **ONEWAYANOVA** statement.

**Table 71.12** ONEWAYANOVA Statement Options

| Option                              | Description                                                             |
|-------------------------------------|-------------------------------------------------------------------------|
| <b>Define analysis</b>              |                                                                         |
| <code>TEST=</code>                  | Specifies the statistical analysis                                      |
| <b>Specify analysis information</b> |                                                                         |
| <code>ALPHA=</code>                 | Specifies the significance level                                        |
| <code>CONTRAST=</code>              | Specifies coefficients for single-degree-of-freedom hypothesis tests    |
| <code>NULLCONTRAST=</code>          | Specifies the null value of the contrast                                |
| <code>SIDES=</code>                 | Specifies the number of sides and the direction of the statistical test |

Table 71.12 continued

| Option                                    | Description                                                 |
|-------------------------------------------|-------------------------------------------------------------|
| <b>Specify effect</b>                     |                                                             |
| GROUPMEANS=                               | Specifies the group means                                   |
| <b>Specify variability</b>                |                                                             |
| STDDEV=                                   | Specifies the error standard deviation                      |
| <b>Specify sample size and allocation</b> |                                                             |
| GROUPNS=                                  | Specifies the group sample sizes                            |
| GROUPWEIGHTS=                             | Specifies the sample size allocation weights for the groups |
| NFRACTIONAL                               | Enables fractional input and output for sample sizes        |
| NPERGROUP=                                | Specifies the common sample size per group                  |
| NTOTAL=                                   | Specifies the sample size                                   |
| <b>Specify power</b>                      |                                                             |
| POWER=                                    | Specifies the desired power of the test                     |
| <b>Control ordering in output</b>         |                                                             |
| OUTPUTORDER=                              | Controls the output order of parameters                     |

Table 71.13 summarizes the valid result parameters for different analyses in the `ONEWAYANOVA` statement.

Table 71.13 Summary of Result Parameters in the `ONEWAYANOVA` Statement

| Analyses      | Solve For   | Syntax                   |
|---------------|-------------|--------------------------|
| TEST=CONTRAST | Power       | POWER=.                  |
|               | Sample size | NTOTAL=.<br>NPERGROUP==. |
| TEST=OVERALL  | Power       | POWER=.                  |
|               | Sample size | NTOTAL=.<br>NPERGROUP==. |

## Dictionary of Options

### **ALPHA=***number-list*

specifies the level of significance of the statistical test. The default is 0.05, corresponding to the usual  $0.05 \times 100\% = 5\%$  level of significance. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

### **CONTRAST=** ( *values* ) < ( ... *values* ) >

specifies coefficients for single-degree-of-freedom hypothesis tests. You must provide a coefficient for every mean appearing in the `GROUPMEANS=` option. Specify multiple contrasts either with additional sets of coefficients or with additional `CONTRAST=` options. For example, you can specify two different contrasts of five means by using the following:

```
CONTRAST = (1 -1 0 0 0) (1 0 -1 0 0)
```

**GROUPMEANS**=*grouped-number-list*

**GMEANS**=*grouped-number-list*

specifies the group means. This option is used to implicitly set the number of groups. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *grouped-number-list*.

**GROUPNS**=*grouped-number-list*

**GNS**=*grouped-number-list*

specifies the group sample sizes. The number of groups represented must be the same as with the **GROUPMEANS**= option. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *grouped-number-list*.

**GROUPWEIGHTS**=*grouped-number-list*

**GWEIGHTS**=*grouped-number-list*

specifies the sample size allocation weights for the groups. This option controls how the total sample size is divided between the groups. Each set of values across all groups represents relative allocation weights. Additionally, if the **NFRACTIONAL** option is not used, the total sample size is restricted to be equal to a multiple of the sum of the group weights (so that the resulting design has an integer sample size for each group while adhering exactly to the group allocation weights). The number of groups represented must be the same as with the **GROUPMEANS**= option. Values must be integers unless the **NFRACTIONAL** option is used. The default value is 1 for each group, amounting to a balanced design. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *grouped-number-list*.

**NFRACTIONAL**

**NFRAC**

enables fractional input and output for sample sizes. See the section “[Sample Size Adjustment Options](#)” on page 6023 for information about the ramifications of the presence (and absence) of the **NFRACTIONAL** option.

**NPERGROUP**=*number-list*

**NPERG**=*number-list*

specifies the common sample size per group or requests a solution for the common sample size per group with a missing value (**NPERGROUP**=.). Use of this option implicitly specifies a balanced design. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**NTOTAL**=*number-list*

specifies the sample size or requests a solution for the sample size with a missing value (**NTOTAL**=.). See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**NULLCONTRAST**=*number-list*

**NULLC**=*number-list*

specifies the null value of the contrast. The default value is 0. This option can be used only with the **TEST=CONTRAST** analysis. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**OUTPUTORDER=INTERNAL****OUTPUTORDER=REVERSE****OUTPUTORDER=SYNTAX**

controls how the input and default analysis parameters are ordered in the output. **OUTPUTORDER=INTERNAL** (the default) arranges the parameters in the output according to the following order of their corresponding options:

- **CONTRAST=**
- **SIDES=**
- **NULLCONTRAST=**
- **ALPHA=**
- **GROUPMEANS=**
- **STDDEV=**
- **GROUPWEIGHTS=**
- **NTOTAL=**
- **NPERGROUP==**
- **GROUPNS=**
- **POWER=**

The **OUTPUTORDER=SYNTAX** option arranges the parameters in the output in the same order in which their corresponding options are specified in the **ONEWAYANOVA** statement. The **OUTPUTORDER=REVERSE** option arranges the parameters in the output in the reverse of the order in which their corresponding options are specified in the **ONEWAYANOVA** statement.

**POWER=number-list**

specifies the desired power of the test or requests a solution for the power with a missing value (**POWER=.**). The power is expressed as a probability, a number between 0 and 1, rather than as a percentage. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**SIDES=keyword-list**

specifies the number of sides (or tails) and the direction of the statistical test. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *keyword-list*. Valid keywords are as follows:

- |   |                                                                   |
|---|-------------------------------------------------------------------|
| 1 | one-sided with alternative hypothesis in same direction as effect |
| 2 | two-sided                                                         |
| U | upper one-sided with alternative greater than null value          |
| L | lower one-sided with alternative less than null value             |

This option can be used only with the **TEST=CONTRAST** analysis. The default value is 2.

**STDDEV=number-list****STD=number-list**

specifies the error standard deviation. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**TEST=CONTRAST****TEST=OVERALL**

specifies the statistical analysis. **TEST=CONTRAST** specifies a one-degree-of-freedom test of a contrast of means. The test is the usual  $F$  test for the two-sided case and the usual  $t$  test for the one-sided case. **TEST=OVERALL** specifies the overall  $F$  test of equality of all means. The default is **TEST=CONTRAST** if the **CONTRAST=** option is used, and **TEST=OVERALL** otherwise.

**Restrictions on Option Combinations**

To specify the sample size and allocation, choose one of the following parameterizations:

- sample size per group in a balanced design (by using the **NPERGROUP==** option)
- total sample size and allocation weights (by using the **NTOTAL=** and **GROUPWEIGHTS=** options)
- individual group sample sizes (by using the **GROUPNS=** option)

**Option Groups for Common Analyses**

This section summarizes the syntax for the common analyses supported in the **ONEWAYANOVA** statement.

**One-Degree-of-Freedom Contrast**

You can use the **NPERGROUP==** option in a balanced design, as in the following statements. Default values for the **SIDES=**, **NULLCONTRAST=**, and **ALPHA=** options specify a two-sided test for a contrast value of 0 with a significance level of 0.05.

```
proc power;
 onewayanova test=contrast
 contrast = (1 0 -1)
 groupmeans = 3 | 7 | 8
 stddev = 4
 npergroup = 50
 power = .;
run;
```

You can also specify an unbalanced design with the **NTOTAL=** and **GROUPWEIGHTS=** options:

```
proc power;
 onewayanova test=contrast
 contrast = (1 0 -1)
 groupmeans = 3 | 7 | 8
 stddev = 4
 groupweights = (1 2 2)
 ntotal = .
 power = 0.9;
run;
```

Another way to specify the sample sizes is with the `GROUPNS=` option:

```
proc power;
 onewayanova test=contrast
 contrast = (1 0 -1)
 groupmeans = 3 | 7 | 8
 stddev = 4
 groupns = (20 40 40)
 power = .;
run;
```

### Overall F Test

The following statements demonstrate a power computation for the overall F test in a one-way ANOVA. The default of `ALPHA=0.05` specifies a significance level of 0.05.

```
proc power;
 onewayanova test=overall
 groupmeans = 3 | 7 | 8
 stddev = 4
 npergroup = 50
 power = .;
run;
```

---

## PAIREDFREQ Statement

`PAIREDFREQ <options>;`

The `PAIREDFREQ` statement performs power and sample size analyses for McNemar's test for paired proportions.

### Summary of Options

Table 71.14 summarizes the options available in the `PAIREDFREQ` statement.

**Table 71.14** PAIREDFREQ Statement Options

| Option                              | Description                                                                                    |
|-------------------------------------|------------------------------------------------------------------------------------------------|
| <b>Define analysis</b>              |                                                                                                |
| <code>DIST=</code>                  | Specifies the underlying distribution assumed for the test statistic                           |
| <code>TEST=</code>                  | Specifies the statistical analysis                                                             |
| <b>Specify analysis information</b> |                                                                                                |
| <code>ALPHA=</code>                 | Specifies the significance level                                                               |
| <code>NULLDISCPRORATIO=</code>      | Specifies the null value of the ratio of discordant proportions                                |
| <code>SIDES=</code>                 | Specifies the number of sides and the direction of the statistical test or confidence interval |
| <b>Specify effects</b>              |                                                                                                |
| <code>CORR=</code>                  | Specifies the correlation $\phi$ between members of a pair                                     |
| <code>DISCPROPDIFF=</code>          | Specifies the discordant proportion difference $p_{01} - p_{10}$                               |
| <code>DISCPROPORTIONS=</code>       | Specifies the two discordant proportions, $p_{10}$ and $p_{01}$                                |

**Table 71.14** *continued*

| Option                             | Description                                                                                                   |
|------------------------------------|---------------------------------------------------------------------------------------------------------------|
| DISCPRORATIO=                      | Specifies the ratio $p_{01}/p_{10}$                                                                           |
| ODDSRATIO=                         | Specifies the odds ratio $[p_{\cdot 1}/(1 - p_{\cdot 1})] / [p_{1 \cdot}/(1 - p_{1 \cdot})]$                  |
| PAIREDPROPORTIONS=                 | Specifies the two paired proportions, $p_{1 \cdot}$ and $p_{\cdot 1}$                                         |
| PROPORTIONDIFF=                    | Specifies the proportion difference $p_{\cdot 1} - p_{1 \cdot}$ .                                             |
| REFPROPORTION=                     | Specifies either the reference first proportion $p_{1 \cdot}$ or the reference discordant proportion $p_{10}$ |
| RELATIVERISK=                      | Specifies the relative risk $p_{\cdot 1}/p_{1 \cdot}$ .                                                       |
| TOTALPROPDISC=                     | Specifies the discordant proportion sum, $p_{10} + p_{01}$                                                    |
| <b>Specify sample size</b>         |                                                                                                               |
| NFRACTIONAL                        | Enables fractional input and output for sample sizes                                                          |
| NPAIRS=                            | Specifies the total number of proportion pairs                                                                |
| <b>Specify power</b>               |                                                                                                               |
| POWER=                             | Specifies the desired power of the test                                                                       |
| <b>Choose computational method</b> |                                                                                                               |
| METHOD=                            | Specifies the computational method                                                                            |
| <b>Control ordering in output</b>  |                                                                                                               |
| OUTPUTORDER=                       | Controls the output order of parameters                                                                       |

Table 71.15 summarizes the valid result parameters in the PAIREFREQ statement.

**Table 71.15** Summary of Result Parameters in the PAIREFREQ Statement

| Analyses                      | Solve For            | Syntax              |
|-------------------------------|----------------------|---------------------|
| TEST=MCNEMAR METHOD=CONNOR    | Power<br>Sample size | POWER=.<br>NPAIRS=. |
| TEST=MCNEMAR METHOD=EXACT     | Power                | POWER=.             |
| TEST=MCNEMAR METHOD=MIETTINEN | Power<br>Sample size | POWER=.<br>NPAIRS=. |

## Dictionary of Options

**ALPHA=number-list**

specifies the level of significance of the statistical test. The default is 0.05, corresponding to the usual  $0.05 \times 100\% = 5\%$  level of significance. See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *number-list*.

**CORR=number-list**

specifies the correlation  $\phi$  between members of a pair. See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *number-list*.



**DISCPRORPORTIONS**=*grouped-number-list*

**DISCPS**=*grouped-number-list*

specifies the two discordant proportions,  $p_{10}$  and  $p_{01}$ . See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *grouped-number-list*.

**DISCPRPDIFF**=*number-list*

**DISCPDIFF**=*number-list*

specifies the difference  $p_{01} - p_{10}$  between discordant proportions. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**DISCPRPRATIO**=*number-list*

**DISCPRATIO**=*number-list*

specifies the ratio  $p_{01}/p_{10}$  of discordant proportions. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**DIST=EXACT\_COND**

**DIST=NORMAL**

specifies the underlying distribution assumed for the test statistic. **EXACT\_COND** corresponds to the exact conditional test, based on the exact binomial distribution of the two types of discordant pairs given the total number of discordant pairs. **NORMAL** corresponds to the conditional test based on the normal approximation to the binomial distribution of the two types of discordant pairs given the total number of discordant pairs. The default value is **EXACT\_COND**.

**METHOD=CONNOR**

**METHOD=EXACT**

**METHOD=MIETTINEN**

specifies the computational method. **METHOD=EXACT** (the default) uses the exact binomial distributions of the total number of discordant pairs and the two types of discordant pairs. **METHOD=CONNOR** uses an approximation from Connor (1987), and **METHOD=MIETTINEN** uses an approximation from Miettinen (1968). The **CONNOR** and **MIETTINEN** methods are valid only for **DIST=NORMAL**.

**NFRACTIONAL**

**NFRAC**

enables fractional input and output for sample sizes. See the section “[Sample Size Adjustment Options](#)” on page 6023 for information about the ramifications of the presence (and absence) of the **NFRACTIONAL** option. This option cannot be used with **METHOD=EXACT**.

**NPAIRS**=*number-list*

specifies the total number of proportion pairs (concordant and discordant) or requests a solution for the number of pairs with a missing value (**NPAIRS=.**). See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**NULLDISCPRORATIO=***number-list*

**NULLDISCRATIO=***number-list*

**NULLRATIO=***number-list*

**NULLR=***number-list*

specifies the null value of the ratio of discordant proportions. The default value is 1. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**ODDSRATIO=***number-list*

**OR=***number-list*

specifies the odds ratio  $[p_{.1}/(1 - p_{.1})] / [p_{1.}/(1 - p_{1.})]$ . See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**OUTPUTORDER=INTERNAL**

**OUTPUTORDER=REVERSE**

**OUTPUTORDER=SYNTAX**

controls how the input and default analysis parameters are ordered in the output. **OUTPUTORDER=INTERNAL** (the default) arranges the parameters in the output according to the following order of their corresponding options:

- **SIDES=**
- **NULLDISCPRORATIO=**
- **ALPHA=**
- **PAIREDPROPORTIONS=**
- **PROPORTIONDIFF=**
- **ODDSRATIO=**
- **RELATIVERISK=**
- **CORR=**
- **DISCPROPORTIONS=**
- **DISCPROPDIFF=**
- **TOTALPROPDISC=**
- **REFPROPORTION=**
- **DISCPRORATIO=**
- **NPAIRS=**
- **POWER=**

The **OUTPUTORDER=SYNTAX** option arranges the parameters in the output in the same order in which their corresponding options are specified in the **PAIREDFREQ** statement. The **OUTPUTORDER=REVERSE** option arranges the parameters in the output in the reverse of the order in which their corresponding options are specified in the **PAIREDFREQ** statement.

**PAIREDPROPORTIONS=***grouped-number-list*

**PPROPORTIONS=***grouped-number-list*

**PAIREDPS=***grouped-number-list*

**PPS=***grouped-number-list*

specifies the two paired proportions,  $p_{1.}$  and  $p_{.1}$ . See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *grouped-number-list*.

**POWER=***number-list*

specifies the desired power of the test or requests a solution for the power with a missing value (**POWER=.**). The power is expressed as a probability, a number between 0 and 1, rather than as a percentage. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**PROPORTIONDIFF=***number-list*

**PDIFF=***number-list*

specifies the proportion difference  $p_{.1} - p_{1.}$ . See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**REFPROPORTION=***number-list*

**REFP=***number-list*

specifies either the reference first proportion  $p_{1.}$  (when used in conjunction with the **PROPORTIONDIFF=**, **ODDSRATIO=**, or **RELATIVERISK=** option) or the reference discordant proportion  $p_{10}$  (when used in conjunction with the **DISCPROPDIFF=** or **DISCPROPRATIO=** option). See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**RELATIVERISK=***number-list*

**RR=***number-list*

specifies the relative risk  $p_{.1}/p_{1.}$ . See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**SIDES=***keyword-list*

specifies the number of sides (or tails) and the direction of the statistical test or confidence interval. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *keyword-list*. Valid keywords and their interpretation are as follows:

- 1 one-sided with alternative hypothesis in same direction as effect
- 2 two-sided
- U upper one-sided with alternative greater than null value
- L lower one-sided with alternative less than null value

If the effect size is zero, then **SIDES=1** is not permitted; instead, specify the direction of the test explicitly in this case with either **SIDES=L** or **SIDES=U**. The default value is 2.

**TEST=MCNEMAR**

specifies the McNemar test of paired proportions. This is the default test option.

**TOTALPROPDISC=***number-list*

**TOTALPDISC=***number-list*

**PDISC=***number-list*

specifies the sum of the two discordant proportions,  $p_{10} + p_{01}$ . See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *number-list*.

## Restrictions on Option Combinations

To specify the proportions, choose one of the following parameterizations:

- discordant proportions (using the **DISCPROPORTIONS=** option)
- difference and sum of discordant proportions (using the **DISCPROPDIFF=** and **TOTALPROPDISC=** options)
- difference of discordant proportions and reference discordant proportion (using the **DISCPROPDIFF=** and **REFPROPORTION=** options)
- ratio of discordant proportions and reference discordant proportion (using the **DISCPROPRATIO=** and **REFPROPORTION=** options)
- ratio and sum of discordant proportions (using the **DISCPROPRATIO=** and **TOTALPROPDISC=** options)
- paired proportions and correlation (using the **PAIREDPROPORTIONS=** and **CORR=** options)
- proportion difference, reference proportion, and correlation (using the **PROPORTIONDIFF=**, **REFPROPORTION=**, and **CORR=** options)
- odds ratio, reference proportion, and correlation (using the **ODDSRATIO=**, **REFPROPORTION=**, and **CORR=** options)
- relative risk, reference proportion, and correlation (using the **RELATIVERISK=**, **REFPROPORTION=**, and **CORR=** options)

## Option Groups for Common Analyses

This section summarizes the syntax for the common analyses supported in the **PAIREFREQ** statement.

### **McNemar Exact Conditional Test**

You can express effects in terms of the individual discordant proportions, as in the following statements. Default values for the **TEST=**, **SIDES=**, **ALPHA=**, and **NULLDISCPROPRATIO=** options specify a two-sided McNemar test for no effect with a significance level of 0.05.

```
proc power;
 pairedfreq dist=exact_cond
 discproportions = 0.15 | 0.45
 npairs = 80
 power = .;
run;
```

You can also express effects in terms of the difference and sum of discordant proportions:

```
proc power;
 pairedfreq dist=exact_cond
 discpropdiff = 0.3
 totalpropdisc = 0.6
 npairs = 80
 power = .;
run;
```

You can also express effects in terms of the difference of discordant proportions and the reference discordant proportion:

```
proc power;
 pairedfreq dist=exact_cond
 discpropdiff = 0.3
 refproportion = 0.15
 npairs = 80
 power = .;
run;
```

You can also express effects in terms of the ratio of discordant proportions and the denominator of the ratio:

```
proc power;
 pairedfreq dist=exact_cond
 discpropratio = 3
 refproportion = 0.15
 npairs = 80
 power = .;
run;
```

You can also express effects in terms of the ratio and sum of discordant proportions:

```
proc power;
 pairedfreq dist=exact_cond
 discpropratio = 3
 totalpropdisc = 0.6
 npairs = 80
 power = .;
run;
```

You can also express effects in terms of the paired proportions and correlation:

```
proc power;
 pairedfreq dist=exact_cond
 pairedproportions = 0.6 | 0.8
 corr = 0.4
 npairs = 45
 power = .;
run;
```

You can also express effects in terms of the proportion difference, reference proportion, and correlation:

```
proc power;
 pairedfreq dist=exact_cond
 proportiondiff = 0.2
 refproportion = 0.6
```

```

 corr = 0.4
 npairs = 45
 power = .;
run;

```

You can also express effects in terms of the odds ratio, reference proportion, and correlation:

```

proc power;
 pairedfreq dist=exact_cond
 oddsratio = 2.66667
 refproportion = 0.6
 corr = 0.4
 npairs = 45
 power = .;
run;

```

You can also express effects in terms of the relative risk, reference proportion, and correlation:

```

proc power;
 pairedfreq dist=exact_cond
 relativetrisk = 1.33333
 refproportion = 0.6
 corr = 0.4
 npairs = 45
 power = .;
run;

```

### ***McNemar Normal Approximation Test***

The following statements demonstrate a sample size computation for the normal-approximate McNemar test. The default value for the `METHOD=` option specifies an exact sample size computation. Default values for the `TEST=`, `SIDES=`, `ALPHA=`, and `NULLDISCPROPRATIO=` options specify a two-sided McNemar test for no effect with a significance level of 0.05.

```

proc power;
 pairedfreq dist=normal method=connor
 discproportions = 0.15 | 0.45
 npairs = .
 power = .9;
run;

```

---

## **PAIREDMEANS Statement**

**PAIREDMEANS** <options>;

The **PAIREDMEANS** statement performs power and sample size analyses for *t* tests, equivalence tests, and confidence interval precision involving paired samples.

## Summary of Options

Table 71.14 summarizes the options available in the PAIREDMEANS statement.

**Table 71.16** PAIREDMEANS Statement Options

| Option                                         | Description                                                                                                                         |
|------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------|
| <b>Define analysis</b>                         |                                                                                                                                     |
| CI=                                            | Specifies an analysis of precision of the confidence interval for the mean difference                                               |
| DIST=                                          | Specifies the underlying distribution assumed for the test statistic                                                                |
| TEST=                                          | Specifies the statistical analysis                                                                                                  |
| <b>Specify analysis information</b>            |                                                                                                                                     |
| ALPHA=                                         | Specifies the significance level                                                                                                    |
| LOWER=                                         | Specifies the lower equivalence bound                                                                                               |
| NULLDIFF=                                      | Specifies the null mean difference                                                                                                  |
| NULLRATIO=                                     | Specifies the null mean ratio                                                                                                       |
| SIDES=                                         | Specifies the number of sides and the direction of the statistical test or confidence interval                                      |
| UPPER=                                         | Specifies the upper equivalence bound                                                                                               |
| <b>Specify effects</b>                         |                                                                                                                                     |
| HALFWIDTH=                                     | Specifies the desired confidence interval half-width                                                                                |
| MEANDIFF=                                      | Specifies the mean difference                                                                                                       |
| MEANRATIO=                                     | Specifies the geometric mean ratio, $\gamma_2/\gamma_1$                                                                             |
| PAIREDMEANS=                                   | Specifies the two paired means                                                                                                      |
| <b>Specify variability</b>                     |                                                                                                                                     |
| CORR=                                          | Specifies the correlation between members of a pair                                                                                 |
| CV=                                            | Specifies the common coefficient of variation                                                                                       |
| PAIREDCVS=                                     | Specifies the coefficient of variation for each member of a pair                                                                    |
| PAIREDSTDDEVS=                                 | Specifies the standard deviation of each member of a pair                                                                           |
| STDDEV=                                        | Specifies the common standard deviation                                                                                             |
| <b>Specify sample size</b>                     |                                                                                                                                     |
| NFRACTIONAL                                    | Enables fractional input and output for sample sizes                                                                                |
| NPAIRS=                                        | Specifies the number of pairs                                                                                                       |
| <b>Specify power and related probabilities</b> |                                                                                                                                     |
| POWER=                                         | Specifies the desired power of the test                                                                                             |
| PROBTYPE=                                      | Specifies the type of probability for the PROBWIDTH= option                                                                         |
| PROBWIDTH=                                     | Specifies the probability of obtaining a confidence interval half-width less than or equal to the value specified by the HALFWIDTH= |
| <b>Control ordering in output</b>              |                                                                                                                                     |
| OUTPUTORDER=                                   | Controls the output order of parameters                                                                                             |

Table 71.17 summarizes the valid result parameters for different analyses in the PAIREDMEANS statement.

**Table 71.17** Summary of Result Parameters in the PAIREDMEANS Statement

| Analyses         | Solve For                  | Syntax                  |
|------------------|----------------------------|-------------------------|
| TEST=DIFF        | Power<br>Sample size       | POWER=.<br>NPAIRS=.     |
| TEST=RATIO       | Power<br>Sample size       | POWER=.<br>NPAIRS=.     |
| TEST=EQUIV_DIFF  | Power<br>Sample size       | POWER=.<br>NPAIRS=.     |
| TEST=EQUIV_RATIO | Power<br>Sample size       | POWER=.<br>NPAIRS=.     |
| CI=DIFF          | Prob(width)<br>Sample size | PROBWIDTH=.<br>NPAIRS=. |

## Dictionary of Options

### ALPHA=*number-list*

specifies the level of significance of the statistical test. The default is 0.05, corresponding to the usual  $0.05 \times 100\% = 5\%$  level of significance. If the CI= and SIDES=1 options are used, then the value must be less than 0.5. See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *number-list*.

### CI

#### CI=DIFF

specifies an analysis of precision of the confidence interval for the mean difference. Instead of power, the relevant probability for this analysis is the probability of achieving a desired precision. Specifically, it is the probability that the half-width of the observed confidence interval will be at most the value specified by the HALFWIDTH= option. If neither the CI= option nor the TEST= option is used, the default is TEST=DIFF.

### CORR=*number-list*

specifies the correlation between members of a pair. See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *number-list*.

### CV=*number-list*

specifies the coefficient of variation assumed to be common to both members of a pair. The coefficient of variation is defined as the ratio of the standard deviation to the mean. You can use this option only with DIST=LOGNORMAL. See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *number-list*.



**DIST=LOGNORMAL****DIST=NORMAL**

specifies the underlying distribution assumed for the test statistic. NORMAL corresponds to the normal distribution, and LOGNORMAL corresponds to the lognormal distribution. The default value (also the only acceptable value in each case) is NORMAL for **TEST=DIFF**, **TEST=EQUIV\_DIFF**, and **CI=DIFF**; and LOGNORMAL for **TEST=RATIO** and **TEST=EQUIV\_RATIO**.

**HALFWIDTH=number-list**

specifies the desired confidence interval half-width. The half-width is defined as the distance between the point estimate and a finite endpoint. This option can be used only with the **CI=DIFF** analysis. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**LOWER=number-list**

specifies the lower equivalence bound for the mean difference or mean ratio, in the original scale (whether **DIST=NORMAL** or **DIST=LOGNORMAL**). This option can be used only with the **TEST=EQUIV\_DIFF** and **TEST=EQUIV\_RATIO** analyses. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**MEANDIFF=number-list**

specifies the mean difference, defined as the mean of the difference between the second and first members of a pair,  $\mu_2 - \mu_1$ . This option can be used only with the **TEST=DIFF** and **TEST=EQUIV\_DIFF** analyses. When **TEST=EQUIV\_DIFF**, the mean difference is interpreted as the treatment mean minus the reference mean. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**MEANRATIO=number-list**

specifies the geometric mean ratio, defined as  $\gamma_2/\gamma_1$ . This option can be used only with the **TEST=RATIO** and **TEST=EQUIV\_RATIO** analyses. When **TEST=EQUIV\_RATIO**, the mean ratio is interpreted as the treatment mean divided by the reference mean. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**NFRACTIONAL****NFRAC**

enables fractional input and output for sample sizes. See the section “[Sample Size Adjustment Options](#)” on page 6023 for information about the ramifications of the presence (and absence) of the **NFRACTIONAL** option.

**NPAIRS=number-list**

specifies the number of pairs or requests a solution for the number of pairs with a missing value (**NPAIRS=.**). See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**NULLDIFF=number-list****NULLD=number-list**

specifies the null mean difference. The default value is 0. This option can be used only with the **TEST=DIFF** analysis. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**NULLRATIO=***number-list*

**NULLR=***number-list*

specifies the null mean ratio. The default value is 1. This option can be used only with the **TEST=RATIO** analysis. See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *number-list*.

**OUTPUTORDER=INTERNAL**

**OUTPUTORDER=REVERSE**

**OUTPUTORDER=SYNTAX**

controls how the input and default analysis parameters are ordered in the output. **OUTPUTORDER=INTERNAL** (the default) arranges the parameters in the output according to the following order of their corresponding options:

- **SIDES=**
- **NULLDIFF=**
- **NULLRATIO=**
- **LOWER=**
- **UPPER=**
- **ALPHA=**
- **PAIREDMEANS=**
- **MEANDIFF=**
- **MEANRATIO=**
- **HALFWIDTH=**
- **STDDEV=**
- **PAIREDSTDDEVS=**
- **CV=**
- **PAIREDCVS=**
- **CORR=**
- **NPAIRS=**
- **POWER=**
- **PROBTYPE=**
- **PROBWIDTH=**

The **OUTPUTORDER=SYNTAX** option arranges the parameters in the output in the same order in which their corresponding options are specified in the **PAIREDMEANS** statement. The **OUTPUTORDER=REVERSE** option arranges the parameters in the output in the reverse of the order in which their corresponding options are specified in the **PAIREDMEANS** statement.

**PAIREDCVS=***grouped-number-list*

specifies the coefficient of variation for each member of a pair. Unlike the **CV=** option, the **PAIREDCVS=** option supports different values for each member of a pair. Values must be nonnegative (unless both are equal to zero, which is permitted). This option can be used only with **DIST=LOGNORMAL**. See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *grouped-number-list*.

**PAIREDMEANS**=*grouped-number-list*

**PMEANS**=*grouped-number-list*

specifies the two paired means, in the original scale. The means are arithmetic if **DIST**=NORMAL and geometric if **DIST**=LOGNORMAL. This option cannot be used with the **CI**=DIFF analysis. When **TEST**=EQUIV\_DIFF, the means are interpreted as the reference mean (first) and the treatment mean (second). See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *grouped-number-list*.

**PAIREDSTDDEVS**=*grouped-number-list*

**PAIREDSTDS**=*grouped-number-list*

**PSTDDEVS**=*grouped-number-list*

**PSTDS**=*grouped-number-list*

specifies the standard deviation of each member of a pair. Unlike the **STDDEV**= option, the **PAIREDSTDDEVS**= option supports different values for each member of a pair. This option can be used only with **DIST**=NORMAL. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *grouped-number-list*.

**POWER**=*number-list*

specifies the desired power of the test or requests a solution for the power with a missing value (**POWER**=.). The power is expressed as a probability, a number between 0 and 1, rather than as a percentage. This option cannot be used with the **CI**=DIFF analysis. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**PROBTYPE**=*keyword-list*

specifies the type of probability for the **PROBWIDTH**= option. A value of CONDITIONAL (the default) indicates the conditional probability that the confidence interval half-width is at most the value specified by the **HALFWIDTH**= option, given that the true mean difference is captured by the confidence interval. A value of UNCONDITIONAL indicates the unconditional probability that the confidence interval half-width is at most the value specified by the **HALFWIDTH**= option. you can use the alias GIVENVALIDITY for CONDITIONAL. The **PROBTYPE**= option can be used only with the **CI**=DIFF analysis. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *keyword-list*.

CONDITIONAL width probability conditional on interval containing the mean

UNCONDITIONAL unconditional width probability

**PROBWIDTH**=*number-list*

specifies the desired probability of obtaining a confidence interval half-width less than or equal to the value specified by the **HALFWIDTH**= option. A missing value (**PROBWIDTH**=.) requests a solution for this probability. The type of probability is controlled with the **PROBTYPE**= option. Values are expressed as probabilities (for example, 0.9) rather than percentages. This option can be used only with the **CI**=DIFF analysis. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**SIDES**=*keyword-list*

specifies the number of sides (or tails) and the direction of the statistical test or confidence interval. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *keyword-list*. Valid keywords and their interpretation for the **TEST**= analyses are as follows:

- 1 one-sided with alternative hypothesis in same direction as effect
- 2 two-sided
- U upper one-sided with alternative greater than null value
- L lower one-sided with alternative less than null value

For confidence intervals, **SIDES=U** refers to an interval between the lower confidence limit and infinity, and **SIDES=L** refers to an interval between minus infinity and the upper confidence limit. For both of these cases and **SIDES=1**, the confidence interval computations are equivalent. The **SIDES=** option cannot be used with the **TEST=EQUIV\_DIFF** and **TEST=EQUIV\_RATIO** analyses. The default value is 2.

**STDDEV=number-list**

**STD=number-list**

specifies the standard deviation assumed to be common to both members of a pair. This option can be used only with **DIST=NORMAL**. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**TEST**

**TEST=DIFF**

**TEST=EQUIV\_DIFF**

**TEST=EQUIV\_RATIO**

**TEST=RATIO**

specifies the statistical analysis. **TEST** or **TEST=DIFF** (the default) specifies a paired *t* test on the mean difference. **TEST=EQUIV\_DIFF** specifies an additive equivalence test of the mean difference by using a two one-sided tests (TOST) analysis (Schuirmann 1987). **TEST=EQUIV\_RATIO** specifies a multiplicative equivalence test of the mean ratio by using a TOST analysis. **TEST=RATIO** specifies a paired *t* test on the geometric mean ratio. If neither the **TEST=** option nor the **CI=** option is used, the default is **TEST=DIFF**.

**UPPER=number-list**

specifies the upper equivalence bound for the mean difference or mean ratio, in the original scale (whether **DIST=NORMAL** or **DIST=LOGNORMAL**). This option can be used only with the **TEST=EQUIV\_DIFF** and **TEST=EQUIV\_RATIO** analyses. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

## Restrictions on Option Combinations

To define the analysis, choose one of the following parameterizations:

- a statistical test (by using the **TEST=** option)
- confidence interval precision (by using the **CI=** option)

To specify the means, choose one of the following parameterizations:

- individual means (by using the **PAIREDMEANS=** option)
- mean difference (by using the **MEANDIFF=** option)
- mean ratio (by using the **MEANRATIO=** option)

To specify the coefficient of variation, choose one of the following parameterizations:

- common coefficient of variation (by using the `CV=` option)
- individual coefficients of variation (by using the `PAIREDCVS=` option)

To specify the standard deviation, choose one of the following parameterizations:

- common standard deviation (by using the `STDDEV=` option)
- individual standard deviations (by using the `PAIREDSTDDEVS=` option)

## Option Groups for Common Analyses

This section summarizes the syntax for the common analyses supported in the `PAIREDMEANS` statement.

### *Paired t Test*

You can express effects in terms of the mean difference and variability in terms of a correlation and common standard deviation, as in the following statements. Default values for the `DIST=`, `SIDES=`, `NULLDIFF=`, and `ALPHA=` options specify a two-sided test for no difference with a normal distribution and a significance level of 0.05.

```
proc power;
 pairedmeans test=diff
 meandiff = 7
 corr = 0.4
 stddev = 12
 npairs = 50
 power = .;
run;
```

You can also express effects in terms of individual means and variability in terms of correlation and individual standard deviations:

```
proc power;
 pairedmeans test=diff
 pairedmeans = 8 | 15
 corr = 0.4
 pairedstddevs = (7 12)
 npairs = .
 power = 0.9;
run;
```

### *Paired t Test of Mean Ratio with Lognormal Data*

You can express variability in terms of correlation and a common coefficient of variation, as in the following statements. Defaults for the `DIST=`, `SIDES=`, `NULLRATIO=` and `ALPHA=` options specify a two-sided test of mean ratio = 1 assuming a lognormal distribution and a significance level of 0.05.

```

proc power;
 pairedmeans test=ratio
 meanratio = 7
 corr = 0.3
 cv = 1.2
 npairs = 30
 power = .;
run;

```

You can also express variability in terms of correlation and individual coefficients of variation:

```

proc power;
 pairedmeans test=ratio
 meanratio = 7
 corr = 0.3
 pairedcvs = 0.8 | 0.9
 npairs = 30
 power = .;
run;

```

#### ***Additive Equivalence Test for Mean Difference with Normal Data***

The following statements demonstrate a sample size computation for a TOST equivalence test for a normal mean difference. Default values for the `DIST=` and `ALPHA=` options specify a normal distribution and a significance level of 0.05.

```

proc power;
 pairedmeans test=equiv_diff
 lower = 2
 upper = 5
 meandiff = 4
 corr = 0.2
 stddev = 8
 npairs = .
 power = 0.9;
run;

```

#### ***Multiplicative Equivalence Test for Mean Ratio with Lognormal Data***

The following statements demonstrate a power computation for a TOST equivalence test for a lognormal mean ratio. Default values for the `DIST=` and `ALPHA=` options specify a lognormal distribution and a significance level of 0.05.

```

proc power;
 pairedmeans test=equiv_ratio
 lower = 3
 upper = 7
 meanratio = 5
 corr = 0.2
 cv = 1.1
 npairs = 50
 power = .;
run;

```

**Confidence Interval for Mean Difference**

By default CI=DIFF analyzes the conditional probability of obtaining the desired precision, given that the interval contains the true mean difference, as in the following statements. The defaults of SIDES=2 and ALPHA=0.05 specify a two-sided interval with a confidence level of 0.95.

```
proc power;
 pairedmeans ci = diff
 halfwidth = 4
 corr = 0.35
 stddev = 8
 npairs = 30
 probwidth = .;
run;
```

**PLOT Statement**

**PLOT** <plot-options> </graph-options> ;

The **PLOT** statement produces a graph or set of graphs for the sample size analysis defined by the previous analysis statement. The *plot-options* define the plot characteristics, and the *graph-options* are SAS/GRAPH-style options. If ODS Graphics is enabled, then the **PLOT** statement uses ODS Graphics to create graphs. For example:

```
ods listing style=htmlbluecml;
ods graphics on;

proc power;
 onesamplemeans
 mean = 5 10
 ntotal = 150
 stddev = 30 50
 power = .;
 plot x=n min=100 max=200;
run;

ods graphics off;
```

Otherwise, traditional graphics are produced. For example:

```
ods graphics off;

proc power;
 onesamplemeans
 mean = 5 10
 ntotal = 150
 stddev = 30 50
 power = .;
 plot x=n min=100 max=200;
run;
```

For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The ODS LISTING STYLE=HTMLBLUECML statement specifies the HTMLBLUECML style, which is suitable for use with PROC POWER because it allows both marker symbols and line styles to vary. See the section “ODS Styles Suitable for Use with PROC POWER” on page 6082 for more information.

## Options

You can specify the following *plot-options* in the PLOT statement.

### INTERPOL=JOIN | NONE

specifies the type of curve to draw through the computed points. The INTERPOL=JOIN option connects computed points by straight lines. The INTERPOL=NONE option leaves computed points unconnected.

### KEY=BYCURVE < ( *bycurve-options* ) >

### KEY=BYFEATURE < ( *byfeature-options* ) >

### KEY=ONCURVES

specifies the style of key (or “legend”) for the plot. The default is KEY=BYFEATURE, which specifies a key with a column of entries for each plot feature (line style, color, and/or symbol). Each entry shows the mapping between a value of the feature and the value(s) of the analysis parameter(s) linked to that feature. The KEY=BYCURVE option specifies a key with each row identifying a distinct curve in the plot. The KEY=ONCURVES option places a curve-specific label adjacent to each curve.

You can specify the following *byfeature-options* in parentheses after the KEY=BYCURVE option.

### NUMBERS=OFF | ON

specifies how the key should identify curves. If NUMBERS=OFF, then the key includes symbol, color, and line style samples to identify the curves. If NUMBERS=ON, then the key includes numbers matching numeric labels placed adjacent to the curves. The default is NUMBERS=ON.

### POS=BOTTOM | INSET

specifies the position of the key. The POS=BOTTOM option places the key below the X axis. The POS=INSET option places the key inside the plotting region and attempts to choose the least crowded corner. The default is POS=BOTTOM.

You can specify the following *byfeature-options* in parentheses after KEY=BYFEATURE option.

### POS=BOTTOM | INSET

specifies the position of the key. The POS=BOTTOM option places the key below the X axis. The POS=INSET option places the key inside the plotting region and attempts to choose the least crowded corner. The default is POS=BOTTOM.

### MARKERS=ANALYSIS | COMPUTED | NICE | NONE

specifies the locations for plotting symbols.

The MARKERS=ANALYSIS option places plotting symbols at locations corresponding to the values of the relevant input parameter from the analysis statement preceding the PLOT statement.

The MARKERS=COMPUTED option (the default) places plotting symbols at the locations of actual computed points from the sample size analysis.

The MARKERS=NICE option places plotting symbols at tick mark locations (corresponding to the argument axis).

The MARKERS=NONE option disables plotting symbols.



**MAX=number | DATAMAX**

specifies the maximum of the range of values for the parameter associated with the “argument” axis (the axis that is *not* representing the parameter being solved for). The default is DATAMAX, which specifies the maximum value that occurs for this parameter in the analysis statement that precedes the PLOT statement.

**MIN=number | DATAMIN**

specifies the minimum of the range of values for the parameter associated with the “argument” axis (the axis that is *not* representing the parameter being solved for). The default is DATAMIN, which specifies the minimum value that occurs for this parameter in the analysis statement that precedes the PLOT statement.

**NPOINTS=number****NPTS=number**

specifies the number of values for the parameter associated with the “argument” axis (the axis that is *not* representing the parameter being solved for). You cannot use the NPOINTS= and STEP= options simultaneously. The default value for typical situations is 20.

**STEP=number**

specifies the increment between values of the parameter associated with the “argument” axis (the axis that is *not* representing the parameter being solved for). You cannot use the STEP= and NPOINTS= options simultaneously. By default, the NPOINTS= option is used instead of the STEP= option.

**VARY ( feature < BY parameter-list > < , ... , feature < BY parameter-list > )**

specifies how plot features should be linked to varying analysis parameters. Available plot *features* are COLOR, LINESYLE, PANEL, and SYMBOL. A “panel” refers to a separate plot with a heading identifying the subset of values represented in the plot.

The *parameter-list* is a list of one or more names separated by spaces. Each name must match the name of an analysis option used in the analysis statement preceding the PLOT statement. Also, the name must be the *primary* name for the analysis option—that is, the one listed first in the syntax description.

If you omit the < BY *parameter-list* > portion for a feature, then one or more multivalued parameters from the analysis will be automatically selected for you.

**X=EFFECT N POWER**

specifies a plot with the requested type of parameter on the X axis and the parameter being solved for on the Y axis. When X=EFFECT, the parameter assigned to the X axis is the one most representative of “effect size.” When X=N, the parameter assigned to the X axis is the sample size. When X=POWER, the parameter assigned to the X axis is the one most representative of “power” (either power itself or a similar probability, such as Prob(Width) for confidence interval analyses). You cannot use the X= and Y= options simultaneously. The default is X=POWER, unless the result parameter is power or Prob(Width), in which case the default is X=N.

You can use the X=N option only when a scalar sample size parameter is used as input in the analysis. For example, X=N can be used with total sample size or sample size per group, or with two group sample sizes when one is being solved for.

Table 71.18 summarizes the parameters representing effect size in different analyses.

**Table 71.18** Effect Size Parameters for Different Analyses

| Analysis Statement and Options                                                                | Effect Size Parameters                              |
|-----------------------------------------------------------------------------------------------|-----------------------------------------------------|
| LOGISTIC                                                                                      | None                                                |
| MULTREG                                                                                       | Partial correlation or $R^2$ difference             |
| ONECORR                                                                                       | Correlation                                         |
| ONESAMPLEFREQ TEST                                                                            | Proportion                                          |
| ONESAMPLEFREQ CI                                                                              | CI half-width                                       |
| ONESAMPLEMEANS TEST=T,<br>ONESAMPLEMEANS TEST=EQUIV                                           | Mean                                                |
| ONESAMPLEMEANS CI=T                                                                           | CI half-width                                       |
| ONEWAYANOVA                                                                                   | None                                                |
| PAIREDFREQ                                                                                    | Discordant proportion difference or ratio           |
| PAIREDMEANS TEST=DIFF,<br>PAIREDMEANS TEST=EQUIV_DIFF                                         | Mean difference                                     |
| PAIREDMEANS TEST=RATIO,<br>PAIREDMEANS TEST=EQUIV_RATIO                                       | Mean ratio                                          |
| PAIREDMEANS CI=DIFF                                                                           | CI half-width                                       |
| TWOSAMPLEFREQ                                                                                 | Proportion difference, odds ratio, or relative risk |
| TWOSAMPLEMEANS TEST=DIFF,<br>TWOSAMPLEMEANS TEST=DIFF_SATT,<br>TWOSAMPLEMEANS TEST=EQUIV_DIFF | Mean difference                                     |
| TWOSAMPLEMEANS TEST=RATIO,<br>TWOSAMPLEMEANS TEST=EQUIV_RATIO                                 | Mean ratio                                          |
| TWOSAMPLEMEANS CI=DIFF                                                                        | CI half-width                                       |
| TWOSAMPLESURVIVAL                                                                             | Hazard ratio if used, else none                     |
| TWOSAMPLEWILCOXON                                                                             | None                                                |

**XOPTS=( *x-options* )**

specifies plot characteristics pertaining to the X axis.

You can specify the following *x-options* in parentheses.

**CROSSREF=NO | YES**

specifies whether the reference lines defined by the **REF=** *x-option* should be crossed with a reference line on the Y axis that indicates the solution point on the curve.

**REF=number-list**

specifies locations for reference lines extending from the X axis across the entire plotting region. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**Y=EFFECT N POWER**

specifies a plot with the requested type of parameter on the Y axis and the parameter being solved for on the X axis. When **Y=EFFECT**, the parameter assigned to the Y axis is the one most representative of “effect size.” When **Y=N**, the parameter assigned to the Y axis is the sample size. When **Y=POWER**, the parameter assigned to the Y axis is the one most representative of “power” (either power itself or a similar probability, such as Prob(Width) for confidence interval analyses). You cannot use the **Y=** and **X=** options simultaneously. By default, the **X=** option is used instead of the **Y=** option.

**YOPTS=( y-options )**

specifies plot characteristics pertaining to the Y axis.

You can specify the following *y-options* in parentheses.

**CROSSREF=NO | YES**

specifies whether the reference lines defined by the **REF= y-option** should be crossed with a reference line on the X axis that indicates the solution point on the curve.

**REF=number-list**

specifies locations for reference lines extending from the Y axis across the entire plotting region. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

You can specify the following *graph-options* in the **PLOT** statement after a slash (/).

**DESCRIPTION='string'**

specifies a descriptive string of up to 40 characters that appears in the “Description” field of the graphics catalog. The description does not appear on the plots. By default, PROC POWER assigns a description either of the form “Y versus X” (for a single-panel plot) or of the form “Y versus X (S),” where Y is the parameter on the Y axis, X is the parameter on the X axis, and S is a description of the subset represented on the current panel of a multipanel plot.

**NAME='string'**

specifies a name of up to eight characters for the catalog entry for the plot. The default name is PLOT*n*, where *n* is the number of the plot statement within the current invocation of PROC POWER. If the name duplicates the name of an existing entry, SAS/GRAPH software adds a number to the duplicate name to create a unique entry—for example, PLOT11 and PLOT12 for the second and third panels of a multipanel plot generated in the first **PLOT** statement in an invocation of PROC POWER.

## TWOSAMPLEFREQ Statement

**TWOSAMPLEFREQ** < options > ;

The **TWOSAMPLEFREQ** statement performs power and sample size analyses for tests of two independent proportions. Pearson’s chi-square, Fisher’s exact, and likelihood ratio chi-square tests are supported.

### Summary of Options

Table 71.19 summarizes the options available in the **TWOSAMPLEFREQ** statement.

**Table 71.19** TWOSAMPLEFREQ Statement Options

| Option                                    | Description                                                                                    |
|-------------------------------------------|------------------------------------------------------------------------------------------------|
| <b>Define analysis</b>                    |                                                                                                |
| TEST=                                     | Specifies the statistical analysis                                                             |
| <b>Specify analysis information</b>       |                                                                                                |
| ALPHA=                                    | Specifies the significance level                                                               |
| NULLODDSRATIO=                            | Specifies the null odds ratio                                                                  |
| NULLPROPORTIONDIFF=                       | Specifies the null proportion difference                                                       |
| NULLRELATIVERISK=                         | Specifies the null relative risk                                                               |
| SIDES=                                    | Specifies the number of sides and the direction of the statistical test or confidence interval |
| <b>Specify effects</b>                    |                                                                                                |
| GROUPPROPORTIONS=                         | Specifies the two independent proportions, $p_1$ and $p_2$                                     |
| ODDSRATIO=                                | Specifies the odds ratio $[p_2/(1 - p_2)] / [p_1/(1 - p_1)]$                                   |
| PROPORTIONDIFF=                           | Specifies the proportion difference $p_2 - p_1$                                                |
| REFPROPORTION=                            | Specifies the reference proportion $p_1$                                                       |
| RELATIVERISK=                             | Specifies the relative risk $p_2/p_1$                                                          |
| <b>Specify sample size and allocation</b> |                                                                                                |
| GROUPNS=                                  | Specifies the two group sample sizes                                                           |
| GROUPWEIGHTS=                             | Specifies the sample size allocation weights for the two groups                                |
| NFRACTIONAL                               | Enables fractional input and output for sample sizes                                           |
| NPERGROUP=                                | Specifies the common sample size per group                                                     |
| NTOTAL=                                   | Specifies the sample size                                                                      |
| <b>Specify power</b>                      |                                                                                                |
| POWER=                                    | Specifies the desired power of the test                                                        |
| <b>Control ordering in output</b>         |                                                                                                |
| OUTPUTORDER=                              | Controls the output order of parameters                                                        |

Table 71.20 summarizes the valid result parameters for different analyses in the `TWOSAMPLEFREQ` statement.

**Table 71.20** Summary of Result Parameters in the `TWOSAMPLEFREQ` Statement

| Analyses                 | Solve For   | Syntax                                            |
|--------------------------|-------------|---------------------------------------------------|
| <code>TEST=FISHER</code> | Power       | <code>POWER=.</code>                              |
|                          | Sample size | <code>NTOTAL=.</code><br><code>NPERGROUP=.</code> |
| <code>TEST=LRCHI</code>  | Power       | <code>POWER=.</code>                              |
|                          | Sample size | <code>NTOTAL=.</code><br><code>NPERGROUP=.</code> |
| <code>TEST=PCHI</code>   | Power       | <code>POWER=.</code>                              |
|                          | Sample size | <code>NTOTAL=.</code><br><code>NPERGROUP=.</code> |

## Dictionary of Options

### **ALPHA=***number-list*

specifies the level of significance of the statistical test. The default is 0.05, corresponding to the usual  $0.05 \times 100\% = 5\%$  level of significance. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

### **GROUPPROPORTIONS=***grouped-number-list*

### **GPROPORTIONS=***grouped-number-list*

### **GROUPPS=***grouped-number-list*

### **GPS=***grouped-number-list*

specifies the two independent proportions,  $p_1$  and  $p_2$ . See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *grouped-number-list*.

### **GROUPNS=***grouped-number-list*

### **GNS=***grouped-number-list*

specifies the two group sample sizes. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *grouped-number-list*.

### **GROUPWEIGHTS=***grouped-number-list*

### **GWEIGHTS=***grouped-number-list*

specifies the sample size allocation weights for the two groups. This option controls how the total sample size is divided between the two groups. Each pair of values for the two groups represents relative allocation weights. Additionally, if the `NFRACTIONAL` option is not used, the total sample size is restricted to be equal to a multiple of the sum of the two group weights (so that the resulting design has an integer sample size for each group while adhering exactly to the group allocation weights). Values must be integers unless the `NFRACTIONAL` option is used. The default value is (1 1), a balanced design with a weight of 1 for each group. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *grouped-number-list*.

**NFRACTIONAL****NFRAC**

enables fractional input and output for sample sizes. See the section “[Sample Size Adjustment Options](#)” on page 6023 for information about the ramifications of the presence (and absence) of the **NFRACTIONAL** option.

**NPERGROUP=number-list****NPERG=number-list**

specifies the common sample size per group or requests a solution for the common sample size per group with a missing value (**NPERGROUP=.**). Use of this option implicitly specifies a balanced design. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**NTOTAL=number-list**

specifies the sample size or requests a solution for the sample size with a missing value (**NTOTAL=.**). See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**NULLODDSRATIO=number-list****NULLOR=number-list**

specifies the null odds ratio. The default value is 1. This option can be used only with the **ODDSRATIO=** option in the **TEST=PCHI** analysis. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**NULLPROPORTIONDIFF=number-list****NULLPDIFF=number-list**

specifies the null proportion difference. The default value is 0. This option can be used only with the **GROUPPROPORTIONS=** or **PROPORTIONDIFF=** option in the **TEST=PCHI** analysis. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**NULLRELATIVERISK=number-list****NULLRR=number-list**

specifies the null relative risk. The default value is 1. This option can be used only with the **RELATIVERISK=** option in the **TEST=PCHI** analysis. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**ODDSRATIO=number-list****OR=number-list**

specifies the odds ratio  $[p_2/(1 - p_2)] / [p_1/(1 - p_1)]$ . See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**OUTPUTORDER=INTERNAL****OUTPUTORDER=REVERSE****OUTPUTORDER=SYNTAX**

controls how the input and default analysis parameters are ordered in the output. **OUTPUTORDER=INTERNAL** (the default) arranges the parameters in the output according to the following order of their corresponding options:

- SIDES=
- NULLPROPORTIONDIFF=
- NULLODDSRATIO=
- NULLRELATIVERISK=
- ALPHA=
- GROUPPROPORTIONS=
- REFPROPORTION=
- PROPORTIONDIFF=
- ODDSRATIO=
- RELATIVERISK=
- GROUPWEIGHTS=
- NTOTAL=
- NPERGROUP=
- GROUPNS=
- POWER=

The **OUTPUTORDER=SYNTAX** option arranges the parameters in the output in the same order in which their corresponding options are specified in the **TWOSAMPLEFREQ** statement. The **OUTPUTORDER=REVERSE** option arranges the parameters in the output in the reverse of the order in which their corresponding options are specified in the **TWOSAMPLEFREQ** statement.

**POWER=number-list**

specifies the desired power of the test or requests a solution for the power with a missing value (**POWER=.**). The power is expressed as a probability, a number between 0 and 1, rather than as a percentage. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**PROPORTIONDIFF=number-list**

**PDIFF=number-list**

specifies the proportion difference  $p_2 - p_1$ . See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**REFPROPORTION=number-list**

**REFP=number-list**

specifies the reference proportion  $p_1$ . See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**RELATIVERISK=number-list**

**RR=number-list**

specifies the relative risk  $p_2/p_1$ . See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**SIDES=keyword-list**

specifies the number of sides (or tails) and the direction of the statistical test or confidence interval. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *keyword-list*. Valid keywords and their interpretation are as follows:

- |   |                                                                   |
|---|-------------------------------------------------------------------|
| 1 | one-sided with alternative hypothesis in same direction as effect |
| 2 | two-sided                                                         |

- U upper one-sided with alternative greater than null value
- L lower one-sided with alternative less than null value

If the effect size is zero, then `SIDES=1` is not permitted; instead, specify the direction of the test explicitly in this case with either `SIDES=L` or `SIDES=U`. The default value is 2.

**TEST=FISHER**

**TEST=LRCHI**

**TEST=PCHI**

specifies the statistical analysis. `TEST=FISHER` specifies Fisher's exact test. `TEST=LRCHI` specifies the likelihood ratio chi-square test. `TEST=PCHI` (the default) specifies Pearson's chi-square test.

### Restrictions on Option Combinations

To specify the proportions, choose one of the following parameterizations:

- individual proportions (by using the `GROUPPROPORTIONS=` option)
- difference between proportions and reference proportion (by using the `PROPORTIONDIFF=` and `REFPROPORTION=` options)
- odds ratio and reference proportion (by using the `ODDSRATIO=` and `REFPROPORTION=` options)
- relative risk and reference proportion (by using the `RELATIVERISK=` and `REFPROPORTION=` options)

To specify the sample size and allocation, choose one of the following parameterizations:

- sample size per group in a balanced design (by using the `NPERGROUP=` option)
- total sample size and allocation weights (by using the `NTOTAL=` and `GROUPWEIGHTS=` options)
- individual group sample sizes (by using the `GROUPNS=` option)

### Option Groups for Common Analyses

This section summarizes the syntax for the common analyses supported in the `TWOSAMPLEFREQ` statement.

#### ***Pearson Chi-Square Test for Two Proportions***

You can use the `NPERGROUP=` option in a balanced design and express effects in terms of the individual proportions, as in the following statements. Default values for the `SIDES=` and `ALPHA=` options specify a two-sided test with a significance level of 0.05.



```

proc power;
 twosamplefreq test=pchi
 groupproportions = (.15 .25)
 nullproportiondiff = .03
 npergroup = 50
 power = .;
run;

```

You can also specify an unbalanced design by using the `NTOTAL=` and `GROUPWEIGHTS=` options and express effects in terms of the odds ratio. The default value of the `NULLODDSRATIO=` option specifies a test of no effect.

```

proc power;
 twosamplefreq test=pchi
 oddsratio = 2.5
 refproportion = 0.3
 groupweights = (1 2)
 ntotal = .
 power = 0.8;
run;

```

You can also specify sample sizes with the `GROUPNS=` option and express effects in terms of relative risks. The default value of the `NULLRELATIVERISK=` option specifies a test of no effect.

```

proc power;
 twosamplefreq test=pchi
 relativerisk = 1.5
 refproportion = 0.2
 groupns = 40 | 60
 power = .;
run;

```

You can also express effects in terms of the proportion difference. The default value of the `NULLPROPORTIONDIFF=` option specifies a test of no effect, and the default value of the `GROUPWEIGHTS=` option specifies a balanced design.

```

proc power;
 twosamplefreq test=pchi
 proportiondiff = 0.15
 refproportion = 0.4
 ntotal = 100
 power = .;
run;

```

### ***Fisher's Exact Conditional Test for Two Proportions***

The following statements demonstrate a power computation for Fisher's exact conditional test for two proportions. Default values for the `SIDES=` and `ALPHA=` options specify a two-sided test with a significance level of 0.05.

```

proc power;
 twosamplefreq test=fisher
 groupproportions = (.35 .15)
 npergroup = 50
 power = .;
run;

```

### Likelihood Ratio Chi-Square Test for Two Proportions

The following statements demonstrate a sample size computation for the likelihood ratio chi-square test for two proportions. Default values for the `SIDES=` and `ALPHA=` options specify a two-sided test with a significance level of 0.05.

```
proc power;
 twosamplefreq test=lrchi
 oddsratio = 2
 refproportion = 0.4
 npergroup = .
 power = 0.9;
run;
```

---

## TWOSAMPLEMEANS Statement

**TWOSAMPLEMEANS** <options> ;

The **TWOSAMPLEMEANS** statement performs power and sample size analyses for pooled and unpooled  $t$  tests, equivalence tests, and confidence interval precision involving two independent samples.

### Summary of Options

Table 71.21 summarizes the options available in the **TWOSAMPLEMEANS** statement.

**Table 71.21** TWOSAMPLEMEANS Statement Options

| Option                              | Description                                                                                    |
|-------------------------------------|------------------------------------------------------------------------------------------------|
| <b>Define analysis</b>              |                                                                                                |
| <code>CI=</code>                    | Specifies an analysis of precision of the confidence interval                                  |
| <code>DIST=</code>                  | Specifies the underlying distribution assumed for the test statistic                           |
| <code>TEST=</code>                  | Specifies the statistical analysis                                                             |
| <b>Specify analysis information</b> |                                                                                                |
| <code>ALPHA=</code>                 | Specifies the significance level                                                               |
| <code>LOWER=</code>                 | Specifies the lower equivalence bound                                                          |
| <code>NULLDIFF=</code>              | Specifies the null mean difference                                                             |
| <code>NULLRATIO=</code>             | Specifies the null mean ratio                                                                  |
| <code>SIDES=</code>                 | Specifies the number of sides and the direction of the statistical test or confidence interval |
| <code>UPPER=</code>                 | Specifies the upper equivalence bound                                                          |
| <b>Specify effects</b>              |                                                                                                |
| <code>HALFWIDTH=</code>             | Specifies the desired confidence interval half-width                                           |
| <code>GROUPMEANS=</code>            | Specifies the two group means                                                                  |
| <code>MEANDIFF=</code>              | Specifies the mean difference                                                                  |
| <code>MEANRATIO=</code>             | Specifies the geometric mean ratio, $\gamma_2/\gamma_1$                                        |
| <b>Specify variability</b>          |                                                                                                |
| <code>CV=</code>                    | Specifies the common coefficient of variation                                                  |

Table 71.21 *continued*

| Option                                         | Description                                                                                                               |
|------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------|
| GROUPSTDDEVS=                                  | Specifies the standard deviation of each group                                                                            |
| STDDEV=                                        | Specifies the common standard deviation                                                                                   |
| <b>Specify sample size and allocation</b>      |                                                                                                                           |
| GROUPNS=                                       | Specifies the two group sample sizes                                                                                      |
| GROUPWEIGHTS=                                  | Specifies the sample size allocation weights for the two groups                                                           |
| NFRACTIONAL                                    | Enables fractional input and output for sample sizes                                                                      |
| NPERGROUP=                                     | Specifies the common sample size per group                                                                                |
| NTOTAL=                                        | Specifies the sample size                                                                                                 |
| <b>Specify power and related probabilities</b> |                                                                                                                           |
| POWER=                                         | Specifies the desired power of the test                                                                                   |
| PROBTYPE=                                      | Specifies the type of probability for the <b>PROBWIDTH=</b> option                                                        |
| PROBWIDTH=                                     | Specifies the desired probability of obtaining a confidence interval half-width less than or equal to the value specified |
| <b>Control ordering in output</b>              |                                                                                                                           |
| OUTPUTORDER=                                   | Controls the output order of parameters                                                                                   |

Table 71.22 summarizes the valid result parameters for different analyses in the **TWOSAMPLEMEANS** statement.

Table 71.22 Summary of Result Parameters in the TWOSAMPLEMEANS Statement

| Analyses    | Solve For          | Syntax                                                                                                                        |
|-------------|--------------------|-------------------------------------------------------------------------------------------------------------------------------|
| TEST=DIFF   | Power              | POWER=.                                                                                                                       |
|             | Sample size        | NTOTAL=.                                                                                                                      |
|             |                    | NPERGROUP=.                                                                                                                   |
|             | Group sample size  | GROUPNS= <i>n1</i>   .<br>GROUPNS=.   <i>n2</i><br>GROUPNS= ( <i>n1</i> .)<br>GROUPNS= (. <i>n2</i> )                         |
|             | Group weight       | GROUPWEIGHTS= <i>w1</i>   .<br>GROUPWEIGHTS=.   <i>w2</i><br>GROUPWEIGHTS= ( <i>w1</i> .)<br>GROUPWEIGHTS= (. <i>w2</i> )     |
|             | Alpha              | ALPHA=.                                                                                                                       |
|             | Group mean         | GROUPMEANS= <i>mean1</i>   .<br>GROUPMEANS=.   <i>mean2</i><br>GROUPMEANS= ( <i>mean1</i> .)<br>GROUPMEANS= (. <i>mean2</i> ) |
|             | Mean difference    | MEANDIFF=.                                                                                                                    |
|             | Standard deviation | STDDEV=.                                                                                                                      |
|             | TEST=DIFF_SATT     | Power                                                                                                                         |
| Sample size |                    | NTOTAL=.                                                                                                                      |
|             |                    | NPERGROUP=.                                                                                                                   |

**Table 71.22** *continued*

| <b>Analyses</b>  | <b>Solve For</b>           | <b>Syntax</b>                          |
|------------------|----------------------------|----------------------------------------|
| TEST=RATIO       | Power<br>Sample size       | POWER=.<br>NTOTAL=.<br>NPERGROUP=.     |
| TEST=EQUIV_DIFF  | Power<br>Sample size       | POWER=.<br>NTOTAL=.<br>NPERGROUP=.     |
| TEST=EQUIV_RATIO | Power<br>Sample size       | POWER=.<br>NTOTAL=.<br>NPERGROUP=.     |
| CI=DIFF          | Prob(width)<br>Sample size | PROBWIDTH=.<br>NTOTAL=.<br>NPERGROUP=. |

## Dictionary of Options

### **ALPHA=number-list**

specifies the level of significance of the statistical test or requests a solution for alpha with a missing value (**ALPHA=.**). The default is 0.05, corresponding to the usual  $0.05 \times 100\% = 5\%$  level of significance. If the **CI=** and **SIDES=1** options are used, then the value must be less than 0.5. See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *number-list*.

### **CI**

#### **CI=DIFF**

specifies an analysis of precision of the confidence interval for the mean difference, assuming equal variances. Instead of power, the relevant probability for this analysis is the probability that the interval half-width is at most the value specified by the **HALFWIDTH=** option. If neither the **TEST=** option nor the **CI=** option is used, the default is **TEST=DIFF**.

### **CV=number-list**

specifies the coefficient of variation assumed to be common to both groups. The coefficient of variation is defined as the ratio of the standard deviation to the mean. You can use this option only with **DIST=LOGNORMAL**. See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *number-list*.

### **DIST=LOGNORMAL**

#### **DIST=NORMAL**

specifies the underlying distribution assumed for the test statistic. **NORMAL** corresponds to the normal distribution, and **LOGNORMAL** corresponds to the lognormal distribution. The default value (also the only acceptable value in each case) is **NORMAL** for **TEST=DIFF**, **TEST=DIFF\_SATT**, **TEST=EQUIV\_DIFF**, and **CI=DIFF**; and **LOGNORMAL** for **TEST=RATIO** and **TEST=EQUIV\_RATIO**.

**GROUPMEANS**=*grouped-number-list*

**GMEANS**=*grouped-number-list*

specifies the two group means or requests a solution for one group mean given the other. Means are in the original scale. They are arithmetic if **DIST=NORMAL** and geometric if **DIST=LOGNORMAL**. This option cannot be used with the **CI=DIFF** analysis. When **TEST=EQUIV\_DIFF**, the means are interpreted as the reference mean (first) and the treatment mean (second). See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *grouped-number-list*.

**GROUPNS**=*grouped-number-list*

**GNS**=*grouped-number-list*

specifies the two group sample sizes or requests a solution for one group sample size given the other. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *grouped-number-list*.

**GROUPSTDDEVS**=*grouped-number-list*

**GSTDDEVS**=*grouped-number-list*

**GROUPSTDS**=*grouped-number-list*

**GSTDS**=*grouped-number-list*

specifies the standard deviation of each group. Unlike the **STDDEV=** option, the **GROUPSTD-DEVS==** option supports different values for each group. It is valid only for the Satterthwaite *t* test (**TEST=DIFF\_SATT DIST=NORMAL**). See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *grouped-number-list*.

**GROUPWEIGHTS**=*grouped-number-list*

**GWEIGHTS**=*grouped-number-list*

specifies the sample size allocation weights for the two groups, or requests a solution for one group weight given the other. This option controls how the total sample size is divided between the two groups. Each pair of values for the two groups represents relative allocation weights. Additionally, if the **NFRACTIONAL** option is not used, the total sample size is restricted to be equal to a multiple of the sum of the two group weights (so that the resulting design has an integer sample size for each group while adhering exactly to the group allocation weights). Values must be integers unless the **NFRACTIONAL** option is used. The default value is (1 1), a balanced design with a weight of 1 for each group. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *grouped-number-list*.

**HALFWIDTH**=*number-list*

specifies the desired confidence interval half-width. The half-width is defined as the distance between the point estimate and a finite endpoint. This option can be used only with the **CI=DIFF** analysis. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**LOWER**=*number-list*

specifies the lower equivalence bound for the mean difference or mean ratio, in the original scale (whether **DIST=NORMAL** or **DIST=LOGNORMAL**). Values must be greater than 0 when **DIST=LOGNORMAL**. This option can be used only with the **TEST=EQUIV\_DIFF** and **TEST=EQUIV\_RATIO** analyses. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**MEANDIFF=number-list**

specifies the mean difference, defined as  $\mu_2 - \mu_1$ , or requests a solution for the mean difference with a missing value (MEANDIFF=.). This option can be used only with the TEST=DIFF, TEST=DIFF\_SATT, and TEST=EQUIV\_DIFF analyses. When TEST=EQUIV\_DIFF, the mean difference is interpreted as the treatment mean minus the reference mean. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**MEANRATIO=number-list**

specifies the geometric mean ratio, defined as  $\gamma_2/\gamma_1$ . This option can be used only with the TEST=RATIO and TEST=EQUIV\_RATIO analyses. When TEST=EQUIV\_RATIO, the mean ratio is interpreted as the treatment mean divided by the reference mean. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**NFRACTIONAL****NFRAC**

enables fractional input and output for sample sizes. See the section “[Sample Size Adjustment Options](#)” on page 6023 for information about the ramifications of the presence (and absence) of the NFRACTIONAL option.

**NPERGROUP=number-list****NPERG=number-list**

specifies the common sample size per group or requests a solution for the common sample size per group with a missing value (NPERGROUP=.). Use of this option implicitly specifies a balanced design. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**NTOTAL=number-list**

specifies the sample size or requests a solution for the sample size with a missing value (NTOTAL=.). See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**NULLDIFF=number-list****NULLD=number-list**

specifies the null mean difference. The default value is 0. This option can be used only with the TEST=DIFF and TEST=DIFF\_SATT analyses. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**NULLRATIO=number-list****NULLR=number-list**

specifies the null mean ratio. The default value is 1. This option can be used only with the TEST=RATIO analysis. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**OUTPUTORDER=INTERNAL****OUTPUTORDER=REVERSE****OUTPUTORDER=SYNTAX**

controls how the input and default analysis parameters are ordered in the output. OUTPUTORDER=INTERNAL (the default) arranges the parameters in the output according to the following order of their corresponding options:

- SIDES=
- NULLDIFF=
- NULLRATIO=
- LOWER=
- UPPER=
- ALPHA=
- GROUPMEANS=
- MEANDIFF=
- MEANRATIO=
- HALFWIDTH=
- STDDEV=
- GROUPSTDDEVS==
- CV=
- GROUPWEIGHTS=
- NTOTAL=
- NPERGROUP=
- GROUPNS=
- POWER=
- PROBTYP=
- PROBWIDTH=

The **OUTPUTORDER=SYNTAX** option arranges the parameters in the output in the same order in which their corresponding options are specified in the **TWOSAMPLEMEANS** statement. The **OUTPUTORDER=REVERSE** option arranges the parameters in the output in the reverse of the order in which their corresponding options are specified in the **TWOSAMPLEMEANS** statement.

**POWER=number-list**

specifies the desired power of the test or requests a solution for the power with a missing value (**POWER=.**). The power is expressed as a probability, a number between 0 and 1, rather than as a percentage. This option cannot be used with the **CI=DIFF** analysis. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**PROBTYP=keyword-list**

specifies the type of probability for the **PROBWIDTH=** option. A value of **CONDITIONAL** (the default) indicates the conditional probability that the confidence interval half-width is at most the value specified by the **HALFWIDTH=** option, given that the true mean difference is captured by the confidence interval. A value of **UNCONDITIONAL** indicates the unconditional probability that the confidence interval half-width is at most the value specified by the **HALFWIDTH=** option. you can use the alias **GIVENVALIDITY** for **CONDITIONAL**. The **PROBTYP=** option can be used only with the **CI=DIFF** analysis. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *keyword-list*.

**CONDITIONAL** width probability conditional on interval containing the mean

**UNCONDITIONAL** unconditional width probability

**PROBWIDTH=number-list**

specifies the desired probability of obtaining a confidence interval half-width less than or equal to the value specified by the **HALFWIDTH=** option. A missing value (**PROBWIDTH=.**) requests a solution for this probability. The type of probability is controlled with the **PROBTYPE=** option. Values are expressed as probabilities (for example, 0.9) rather than percentages. This option can be used only with the **CI=DIFF** analysis. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**SIDES=keyword-list**

specifies the number of sides (or tails) and the direction of the statistical test or confidence interval. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *keyword-list*. Valid keywords and their interpretation for the **TEST=** analyses are as follows:

- 1 one-sided with alternative hypothesis in same direction as effect
- 2 two-sided
- U upper one-sided with alternative greater than null value
- L lower one-sided with alternative less than null value

For confidence intervals, **SIDES=U** refers to an interval between the lower confidence limit and infinity, and **SIDES=L** refers to an interval between minus infinity and the upper confidence limit. For both of these cases and **SIDES=1**, the confidence interval computations are equivalent. The **SIDES=** option cannot be used with the **TEST=EQUIV\_DIFF** and **TEST=EQUIV\_RATIO** analyses. The default value is 2.

**STDDEV=number-list****STD=number-list**

specifies the standard deviation assumed to be common to both groups, or requests a solution for the common standard deviation with a missing value (**STDDEV=.**). This option can be used only with **DIST=NORMAL**. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**TEST****TEST=DIFF****TEST=DIFF\_SATT****TEST=EQUIV\_DIFF****TEST=EQUIV\_RATIO****TEST=RATIO**

specifies the statistical analysis. **TEST** or **TEST=DIFF** (the default) specifies a pooled *t* test on the mean difference, assuming equal variances. **TEST=DIFF\_SATT** specifies a Satterthwaite unpooled *t* test on the mean difference, assuming unequal variances. **TEST=EQUIV\_DIFF** specifies an additive equivalence test of the mean difference by using a two one-sided tests (TOST) analysis (Schuirmann 1987). **TEST=EQUIV\_RATIO** specifies a multiplicative equivalence test of the mean ratio by using a TOST analysis. **TEST=RATIO** specifies a pooled *t* test on the mean ratio, assuming equal coefficients of variation. If neither the **TEST=** option nor the **CI=** option is used, the default is **TEST=DIFF**.



**UPPER=number-list**

specifies the upper equivalence bound for the mean difference or mean ratio, in the original scale (whether `DIST=NORMAL` or `DIST=LOGNORMAL`). This option can be used only with the `TEST=EQUIV_DIFF` and `TEST=EQUIV_RATIO` analyses. See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *number-list*.

**Restrictions on Option Combinations**

To define the analysis, choose one of the following parameterizations:

- a statistical test (by using the `TEST=` option)
- confidence interval precision (by using the `CI=` option)

To specify the means, choose one of the following parameterizations:

- individual group means (by using the `GROUPMEANS=` option)
- mean difference (by using the `MEANDIFF=` option)
- mean ratio (by using the `MEANRATIO=` option)

To specify standard deviations in the Satterthwaite *t* test (`TEST=DIFF_SATT`), choose one of the following parameterizations:

- common standard deviation (by using the `STDDEV=` option)
- individual group standard deviations (by using the `GROUPSTDDEVS==` option)

To specify the sample sizes and allocation, choose one of the following parameterizations:

- sample size per group in a balanced design (by using the `NPERGROUP=` option)
- total sample size and allocation weights (by using the `NTOTAL=` and `GROUPWEIGHTS=` options)
- individual group sample sizes (by using the `GROUPNS=` option)

**Option Groups for Common Analyses**

This section summarizes the syntax for the common analyses supported in the `TWOSAMPLEMEANS` statement.

***Two-Sample t Test Assuming Equal Variances***

You can use the `NPERGROUP=` option in a balanced design and express effects in terms of the mean difference, as in the following statements. Default values for the `DIST=`, `SIDES=`, `NULLDIFF=`, and `ALPHA=` options specify a two-sided test for no difference with a normal distribution and a significance level of 0.05.

```

proc power;
 twosamplemeans test=diff
 meandiff = 7
 stddev = 12
 npergroup = 50
 power = .;
run;

```

You can also specify an unbalanced design by using the `NTOTAL=` and `GROUPWEIGHTS=` options and express effects in terms of individual group means:

```

proc power;
 twosamplemeans test=diff
 groupmeans = 8 | 15
 stddev = 4
 groupweights = (2 3)
 ntotal = .
 power = 0.9;
run;

```

Another way to specify the sample sizes is with the `GROUPNS=` option:

```

proc power;
 twosamplemeans test=diff
 groupmeans = 8 | 15
 stddev = 4
 groupns = (25 40)
 power = .;
run;

```

### ***Two-Sample Satterthwaite $t$ Test Assuming Unequal Variances***

The following statements demonstrate a power computation for the two-sample Satterthwaite  $t$  test allowing unequal variances. Default values for the `DIST=`, `SIDES=`, `NULLDIFF=`, and `ALPHA=` options specify a two-sided test for no difference with a normal distribution and a significance level of 0.05.

```

proc power;
 twosamplemeans test=diff_satt
 meandiff = 3
 groupstddevs = 5 | 8
 groupweights = (1 2)
 ntotal = 60
 power = .;
run;

```

### ***Two-Sample Pooled $t$ Test of Mean Ratio with Lognormal Data***

The following statements demonstrate a power computation for the pooled  $t$  test of a lognormal mean ratio. Default values for the `DIST=`, `SIDES=`, `NULLRATIO=`, and `ALPHA=` options specify a two-sided test of mean ratio = 1 assuming a lognormal distribution and a significance level of 0.05.

```

proc power;
 twosamplemeans test=ratio
 meanratio = 7
 cv = 0.8
 groupns = 50 | 70
 power = .;
run;

```

### **Additive Equivalence Test for Mean Difference with Normal Data**

The following statements demonstrate a sample size computation for the TOST equivalence test for a normal mean difference. A default value of `GROUPWEIGHTS=(1 1)` specifies a balanced design. Default values for the `DIST=` and `ALPHA=` options specify a significance level of 0.05 and an assumption of normally distributed data.

```

proc power;
 twosamplemeans test=equiv_diff
 lower = 2
 upper = 5
 meandiff = 4
 stddev = 8
 ntotal = .
 power = 0.9;
run;

```

### **Multiplicative Equivalence Test for Mean Ratio with Lognormal Data**

The following statements demonstrate a power computation for the TOST equivalence test for a lognormal mean ratio. Default values for the `DIST=` and `ALPHA=` options specify a significance level of 0.05 and an assumption of lognormally distributed data.

```

proc power;
 twosamplemeans test=equiv_ratio
 lower = 3
 upper = 7
 meanratio = 5
 cv = 0.75
 npergroup = 50
 power = .;
run;

```

### **Confidence Interval for Mean Difference**

By default `CI=DIFF` analyzes the conditional probability of obtaining the desired precision, given that the interval contains the true mean difference, as in the following statements. The defaults of `SIDES=2` and `ALPHA=0.05` specify a two-sided interval with a confidence level of 0.95.

```

proc power;
 twosamplemeans ci = diff
 halfwidth = 4
 stddev = 8
 groupns = (30 35)
 probwidth = .;
run;

```

## TWOSAMPLESURVIVAL Statement

**TWOSAMPLESURVIVAL** < options > ;

The **TWOSAMPLESURVIVAL** statement performs power and sample size analyses for comparing two survival curves. The log-rank, Gehan, and Tarone-Ware rank tests are supported.

### Summary of Options

Table 71.23 summarizes the options available in the **TWOSAMPLESURVIVAL** statement.

**Table 71.23** TWOSAMPLESURVIVAL Statement Options

| Option                                    | Description                                                                                    |
|-------------------------------------------|------------------------------------------------------------------------------------------------|
| <b>Define analysis</b>                    |                                                                                                |
| TEST=                                     | Specifies the statistical analysis                                                             |
| <b>Specify analysis information</b>       |                                                                                                |
| ACCRUALTIME=                              | Specifies the accrual time                                                                     |
| ALPHA=                                    | Specifies the significance level                                                               |
| FOLLOWUPTIME=                             | Specifies the follow-up time                                                                   |
| SIDES=                                    | Specifies the number of sides and the direction of the statistical test or confidence interval |
| TOTALTIME=                                | Specifies the total time                                                                       |
| <b>Specify effects</b>                    |                                                                                                |
| CURVE=                                    | Defines a survival curve                                                                       |
| GROUPMEDSURVTIMES=                        | Specifies the median survival times in each group                                              |
| GROUPSURVEXPHAZARDS=                      | Specifies exponential hazard rates of the survival curve for each group                        |
| GROUPSURVIVAL=                            | Specifies the survival curve for each group                                                    |
| HAZARDRATIO=                              | Specifies the hazard ratio                                                                     |
| REFSURVEXPHAZARD=                         | Specifies the exponential hazard rate of the survival curve for the reference group            |
| REFSURVIVAL=                              | Specifies the survival curve for the reference group                                           |
| <b>Specify loss information</b>           |                                                                                                |
| GROUPLOSS=                                | Specifies the exponential loss survival curve for each group                                   |
| GROUPLOSSEXPHAZARDS=                      | Specifies the exponential hazards of the loss in each group                                    |
| GROUPMEDLOSSTIMES=                        | Specifies the median times of the loss in each group                                           |
| <b>Specify sample size and allocation</b> |                                                                                                |
| ACCRUALRATEPERGROUP=                      | Specifies the common accrual rate per group                                                    |
| ACCRUALRATETOTAL=                         | Specifies the total accrual rate                                                               |
| EVENTSTOTAL=                              | Specifies the expected total number of events                                                  |
| GROUPACCRUALRATES=                        | Specifies the accrual rate for each group                                                      |
| GROUPNS=                                  | Specifies the two group sample sizes                                                           |
| GROUPWEIGHTS=                             | Specifies the sample size allocation weights for the two groups                                |
| NFRACTIONAL                               | Enables fractional input and output for sample sizes                                           |
| NPERGROUP=                                | Specifies the common sample size per group                                                     |
| NTOTAL=                                   | Specifies the sample size                                                                      |

**Table 71.23** *continued*

| Option                                               | Description                                        |
|------------------------------------------------------|----------------------------------------------------|
| <b>Specify power</b><br>POWER=                       | Specifies the desired power of the test            |
| <b>Specify computational method</b><br>NSUBINTERVAL= | Specifies the number of subintervals per unit time |
| <b>Control ordering in output</b><br>OUTPUTORDER=    | Controls the output order of parameters            |

Table 71.24 summarizes the valid result parameters for different analyses in the TWOSAMPLESURVIVAL statement.

**Table 71.24** Summary of Result Parameters in the TWOSAMPLESURVIVAL Statement

| Analyses        | Solve For            | Syntax                                                                                             |
|-----------------|----------------------|----------------------------------------------------------------------------------------------------|
| TEST=GEHAN      | Power<br>Sample size | POWER=.<br>NTOTAL=.<br>NPERGROUP=.<br>EVENTSTOTAL=.<br>ACCRUALRATETOTAL=.<br>ACCRUALRATEPERGROUP=. |
| TEST=LOGRANK    | Power<br>Sample size | POWER=.<br>NTOTAL=.<br>NPERGROUP=.<br>EVENTSTOTAL=.<br>ACCRUALRATETOTAL=.<br>ACCRUALRATEPERGROUP=. |
| TEST=TARONEWARE | Power<br>Sample size | POWER=.<br>NTOTAL=.<br>NPERGROUP=.<br>EVENTSTOTAL=.<br>ACCRUALRATETOTAL=.<br>ACCRUALRATEPERGROUP=. |

## Dictionary of Options

**ACCRUALRATEPERGROUP=***number-list*

**ACCRUALRATEPERG=***number-list*

**ARPERGROUP=***number-list*

**ARPERG=***number-list*

specifies the common accrual rate per group or requests a solution for the common accrual rate per group with a missing value (**ACCRUALRATEPERGROUP=.**). The accrual rate per group is the number of subjects in each group that enters the study per time unit during the accrual period. Use of this option implicitly specifies a balanced design. The **NFRACTIONAL** option is automatically

enabled when the `ACCRUALRATEPERGROUP=` option is used. See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *number-list*.

**ACCRUALRATETOTAL=number-list**

**ARTOTAL=number-list**

specifies the total accrual rate or requests a solution for the accrual rate with a missing value (`ACCRUALRATETOTAL=.`). The total accrual rate is the total number of subjects that enter the study per time unit during the accrual period. The `NFRACTIONAL` option is automatically enabled when the `ACCRUALRATETOTAL=` option is used. See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *number-list*.

**ACCRUALTIME=number-list | MAX**

**ACCTIME=number-list | MAX**

**ACCRUALT=number-list | MAX**

**ACCT=number-list | MAX**

specifies the accrual time. Accrual is assumed to occur uniformly from time 0 to the time specified by the `ACCRUALTIME=` option. If the `GROUPSURVIVAL=` or `REFSURVIVAL=` option is used, then the value of the total time (the sum of accrual and follow-up times) must be less than or equal to the largest time in *each* multipoint (piecewise linear) survival curve. If the `ACCRUALRATEPERGROUP=`, `ACCRUALRATETOTAL=`, or `GROUPACCRUALRATES=` option is used, then the accrual time must be greater than 0. See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *number-list*.

`ACCRUALTIME=MAX` can be used when each scenario in the analysis contains at least one piecewise linear survival curve (in the `GROUPSURVIVAL=` or `REFSURVIVAL=` option). It causes the accrual time to be automatically set, separately for each scenario, to the maximum possible time supported by the piecewise linear survival curve(s) in that scenario. It is not compatible with the `FOLLOWUPTIME=MAX` option or the `TOTALTIME=` option.

**ALPHA=number-list**

specifies the level of significance of the statistical test. The default is 0.05, corresponding to the usual  $0.05 \times 100\% = 5\%$  level of significance. See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *number-list*.

**CURVE("label")=points**

defines a survival curve.

For the `CURVE=` option,

*label* identifies the curve in the output and with the `GROUPLOSS=`, `GROUPSURVIVAL=`, and `REFSURVIVAL=` options.

*points* specifies one or more (time, survival) pairs on the curve, where the survival value denotes the probability of surviving until at least the specified time.

A single-point curve is interpreted as exponential, and a multipoint curve is interpreted as piecewise linear. Points can be expressed in either of two forms:

- a series of time:survival pairs separated by spaces. For example:

1:0.9 2:0.7 3:0.6

- a DOLIST of times enclosed in parentheses, followed by a colon (:), followed by a DOLIST of survival values enclosed in parentheses. For example:

(1 to 3 by 1) : (0.9 0.7 0.6)

The DOLIST format is the same as in the DATA step.

Points can also be expressed as combinations of the two forms. For example:

1:0.9 2:0.8 (3 to 6 by 1) : (0.7 0.65 0.6 0.55)

The points have the following restrictions:

- The time values must be nonnegative and strictly increasing.
- The survival values must be strictly decreasing.
- The survival value at a time of 0 must be equal to 1.
- If there is only one point, then the time must be greater than 0, and the survival value cannot be 0 or 1.

**EVENTSTOTAL=***number-list*

**EVENTTOTAL=***number-list*

**EETOTAL=***number-list*

specifies the expected total number of events—that is, deaths, whether observed or censored—during the entire study period, or requests a solution for this parameter with a missing value (**EVENTSTOTAL=.**). The **NFRACTIONAL** option is automatically enabled when the **EVENTSTOTAL=** option is used. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**FOLLOWUPTIME=***number-list* | **MAX**

**FUTIME=***number-list* | **MAX**

**FOLLOWUPT=***number-list* | **MAX**

**FUT=***number-list* | **MAX**

specifies the follow-up time, the amount of time in the study past the accrual time. If the **GROUPSURVIVAL=** or **REFSURVIVAL=** option is used, then the value of the total time (the sum of accrual and follow-up times) must be less than or equal to the largest time in *each* multipoint (piecewise linear) survival curve. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**FOLLOWUPTIME=MAX** can be used when each scenario in the analysis contains at least one piecewise linear survival curve (in the **GROUPSURVIVAL=** or **REFSURVIVAL=** option). It causes the follow-up time to be automatically set, separately for each scenario, to the maximum possible time supported by the piecewise linear survival curve(s) in that scenario. It is not compatible with the **ACCRUALTIME=MAX** option or the **TOTALTIME=** option.

**GROUPACCRUALRATES=***grouped-number-list*

**GACCRUALRATES=***grouped-number-list*

**GROUPARS=***grouped-number-list*

**GARS=***grouped-number-list*

specifies the accrual rate for each group. The groupwise accrual rates are the numbers of subjects in each group that enters the study per time unit during the accrual period. The **NFRACTIONAL** option is automatically enabled when the **GROUPACCRUALRATES=** option is used. See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *grouped-number-list*.

**GROUPLOSS=***grouped-name-list*

**GLOSS=***grouped-name-list*

specifies the exponential loss survival curve for each group, by using labels specified with the **CURVE=** option. Loss is assumed to follow an exponential curve, indicating the expected rate of censoring (in other words, loss to follow-up) over time. See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *grouped-name-list*.

**GROUPLOSSEXPHAZARDS=***grouped-number-list*

**GLOSSEXPHAZARDS=***grouped-number-list*

**GROUPLOSSEXPHS=***grouped-number-list*

**GLOSSEXPHS=***grouped-number-list*

specifies the exponential hazards of the loss in each group. Loss is assumed to follow an exponential curve, indicating the expected rate of censoring (in other words, loss to follow-up) over time. If none of the **GROUPLOSSEXPHAZARDS=**, **GROUPLOSS=**, and **GROUPMEDLOSSTIMES=** options are used, the default of **GROUPLOSSEXPHAZARDS=(0 0)** indicates no loss to follow-up. See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *grouped-number-list*.

**GROUPMEDLOSSTIMES=***grouped-number-list*

**GMEDLOSSTIMES=***grouped-number-list*

**GROUPMEDLOSSTS=***grouped-number-list*

**GMEDLOSSTS=***grouped-number-list*

specifies the median times of the loss in each group. Loss is assumed to follow an exponential curve, indicating the expected rate of censoring (in other words, loss to follow-up) over time. See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *grouped-number-list*.

**GROUPMEDSURVTIMES=***grouped-number-list*

**GMEDSURVTIMES=***grouped-number-list*

**GROUPMEDSURVTS=***grouped-number-list*

**GMEDSURVTS=***grouped-number-list*

specifies the median survival times in each group. When the **GROUPMEDSURVTIMES=** option is used, the survival curve in each group is assumed to be exponential. See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *grouped-number-list*.



**GROUPNS**=*grouped-number-list*

**GNS**=*grouped-number-list*

specifies the two group sample sizes. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *grouped-number-list*.

**GROUPSURVEXPHAZARDS**=*grouped-number-list*

**GSURVEXPHAZARDS**=*grouped-number-list*

**GROUPSURVEXPHS**=*grouped-number-list*

**GEXPHS**=*grouped-number-list*

specifies exponential hazard rates of the survival curve for each group. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *grouped-number-list*.

**GROUPSURVIVAL**=*grouped-name-list*

**GSURVIVAL**=*grouped-name-list*

**GROUPSURV**=*grouped-name-list*

**GSURV**=*grouped-name-list*

specifies the survival curve for each group, by using labels specified with the **CURVE=** option. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *grouped-name-list*.

**GROUPWEIGHTS**=*grouped-number-list*

**GWEIGHTS**=*grouped-number-list*

specifies the sample size allocation weights for the two groups. This option controls how the total sample size is divided between the two groups. Each pair of values for the two groups represents relative allocation weights. Additionally, if the **NFRACTIONAL** option is not used, the total sample size is restricted to be equal to a multiple of the sum of the two group weights (so that the resulting design has an integer sample size for each group while adhering exactly to the group allocation weights). Values must be integers unless the **NFRACTIONAL** option is used. The default value is (1 1), a balanced design with a weight of 1 for each group. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *grouped-number-list*.

**HAZARDRATIO**=*number-list*

**HR**=*number-list*

specifies the hazard ratio of the second group’s survival curve to the first group’s survival curve. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**NFRACTIONAL**

**NFRAC**

enables fractional input and output for sample sizes. This option is automatically enabled when any of the following options are used: **ACCRUALRATEPERGROUP=**, **ACCRUALRATETOTAL=**, **EVENTSTOTAL=**, and **GROUPACCRUALRATES=**. See the section “[Sample Size Adjustment Options](#)” on page 6023 for information about the ramifications of the presence (and absence) of the **NFRACTIONAL** option.

**NPERGROUP**=*number-list*

**NPERG**=*number-list*

specifies the common sample size per group or requests a solution for the common sample size per group with a missing value (**NPERGROUP**=.). Use of this option implicitly specifies a balanced design. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**NSUBINTERVAL**=*number-list*

**NSUBINTERVALS**=*number-list*

**NSUB**=*number-list*

**NSUBS**=*number-list*

specifies the number of subintervals per unit time to use in internal calculations. Higher values increase computational time and memory requirements but generally lead to more accurate results. The default value is 12. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**NTOTAL**=*number-list*

specifies the sample size or requests a solution for the sample size with a missing value (**NTOTAL**=.). See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**OUTPUTORDER**=INTERNAL

**OUTPUTORDER**=REVERSE

**OUTPUTORDER**=SYNTAX

controls how the input and default analysis parameters are ordered in the output. **OUTPUTORDER**=INTERNAL (the default) arranges the parameters in the output according to the following order of their corresponding options:

- **SIDES**=
- **ACCRUALTIME**=
- **FOLLOWUPTIME**=
- **TOTALTIME**=
- **NSUBINTERVAL**=
- **ALPHA**=
- **REFSURVIVAL**=
- **GROUPSURVIVAL**=
- **REFSURVEXPHAZARD**=
- **HAZARDRATIO**=
- **GROUPSURVEXPHAZARDS**=
- **GROUPMEDSURVTIMES**=
- **GROUPLOSSEXPHAZARDS**=
- **GROUPLOSS**=
- **GROUPMEDLOSSTIMES**=
- **GROUPWEIGHTS**=
- **NTOTAL**=
- **ACCRUALRATETOTAL**=
- **EVENTSTOTAL**=
- **NPERGROUP**=

- ACCRUALRATEPERGROUP=
- GROUPNS=
- GROUPACCRUALRATES=
- POWER=

The **OUTPUTORDER=SYNTAX** option arranges the parameters in the output in the same order in which their corresponding options are specified in the **TWOSAMPLESURVIVAL** statement. The **OUTPUTORDER=REVERSE** option arranges the parameters in the output in the reverse of the order in which their corresponding options are specified in the **TWOSAMPLESURVIVAL** statement.

**POWER=number-list**

specifies the desired power of the test or requests a solution for the power with a missing value (**POWER=.**). The power is expressed as a probability, a number between 0 and 1, rather than as a percentage. See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *number-list*.

**REFSURVEXPHAZARD=number-list**

**REFSURVEXPH=number-list**

specifies the exponential hazard rate of the survival curve for the first (reference) group. See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *number-list*.

**REFSURVIVAL=name-list**

**REFSURV=name-list**

specifies the survival curve for the first (reference) group, by using labels specified with the **CURVE=** option. See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *name-list*.

**SIDES=keyword-list**

specifies the number of sides (or tails) and the direction of the statistical test or confidence interval. See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *keyword-list*. Valid keywords and their interpretation are as follows:

- |   |                                                                                                         |
|---|---------------------------------------------------------------------------------------------------------|
| 1 | one-sided with alternative hypothesis in same direction as effect                                       |
| 2 | two-sided                                                                                               |
| U | upper one-sided with the alternative hypothesis favoring better survival in the second group            |
| L | lower one-sided with the alternative hypothesis favoring better survival in the first (reference) group |

The default value is 2.

**TEST=GEHAN**

**TEST=LOGRANK**

**TEST=TARONEWARE**

specifies the statistical analysis. **TEST=GEHAN** specifies the Gehan rank test. **TEST=LOGRANK** (the default) specifies the log-rank test. **TEST=TARONEWARE** specifies the Tarone-Ware rank test.

**TOTALTIME=***number-list* | **MAX**

**TOTALT=***number-list* | **MAX**

specifies the total time, which is equal to the sum of accrual and follow-up times. If the **GROUPSURVIVAL=** or **REFSURVIVAL=** option is used, then the value of the total time must be less than or equal to the largest time in *each* multipoint (piecewise linear) survival curve. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**TOTALTIME=MAX** can be used when each scenario in the analysis contains at least one piecewise linear survival curve (in the **GROUPSURVIVAL=** or **REFSURVIVAL=** option). It causes the total time to be automatically set, separately for each scenario, to the maximum possible time supported by the piecewise linear survival curve(s) in that scenario. It is not compatible with the **ACCRUALTIME=MAX** option or the **FOLLOWUPTIME=MAX** option.

## Restrictions on Option Combinations

To specify the survival curves, choose one of the following parameterizations:

- arbitrary piecewise linear or exponential curves (by using the **CURVE=** and **GROUPSURVIVAL=** options)
- curves with proportional hazards (by using the **CURVE=**, **REFSURVIVAL=**, and **HAZARDRATIO=** options)
- exponential curves, by using one of the following parameterizations:
  - median survival times (by using the **GROUPMEDSURVTIMES=** option)
  - the hazard ratio and the hazard of the reference curve (by using the **HAZARDRATIO=** and **REFSURVEXPHAZARD=** options)
  - the individual hazards (by using the **GROUPSURVEXPHAZARDS=** option)

To specify the study time, use any two of the following three options:

- accrual time (by using the **ACCRUALTIME=** option)
- follow-up time (by using the **FOLLOWUPTIME=** option)
- total time, the sum of accrual and follow-up times (by using the **TOTALTIME=** option)

To specify the sample size and allocation, choose one of the following parameterizations:

- sample size per group in a balanced design (by using the **NPERGROUP=** option)
- accrual rate per group in a balanced design (by using the **ACCRUALRATEPERGROUP=** option)
- total sample size and allocation weights (by using the **NTOTAL=** and **GROUPWEIGHTS=** options)
- total accrual rate and allocation weights (by using the **ACCRUALRATETOTAL=** and **GROUPWEIGHTS=** options)

- expected total number of events and allocation weights (by using the `EVENTSTOTAL=` and `GROUPWEIGHTS=` options)
- individual group sample sizes (by using the `GROUPNS=` option)
- individual group accrual rates (by using the `GROUPACCRUALRATES=` option)

The values of parameters that involve expected number of events or accrual rate are converted internally to the analogous sample size parameterization (that is, the `NPERGROUP=`, `NTOTAL=`, or `GROUPNS=` option) for the purpose of sample size adjustments according to the presence or absence of the `NFRAC-TIONAL` option.

To specify the exponential loss curves, choose one of the following parameterizations:

- a point on the loss curve of each group (by using the `CURVE=` and `GROUPLOSS=` options)
- median loss times (by using the `GROUPMEDLOSSTIMES=` option)
- the individual loss hazards (by using the `GROUPLOSSEXPHAZARDS=` option)

## Option Groups for Common Analyses

This section summarizes the syntax for the common analyses supported in the `TWOSAMPLESURVIVAL` statement.

### Log-Rank Test for Two Survival Curves

You can use the `NPERGROUP=` option in a balanced design and specify piecewise linear or exponential survival curves by using the `CURVE=` and `GROUPSURVIVAL=` options, as in the following statements. Default values for the `SIDES=`, `ALPHA=`, `NSUBINTERVAL=`, and `GROUPLOSSEXPHAZARDS=` options specify a two-sided test with a significance level of 0.05, an assumption of no loss to follow-up, and the use of 12 subintervals per unit time in computations.

```
proc power;
 twosamplesurvival test=logrank
 curve("Control") = (1 2 3):(0.8 0.7 0.6)
 curve("Treatment") = (5):(0.6)
 groupsurvival = "Control" | "Treatment"
 accrualtime = 2
 followuptime = 1
 npergroup = 50
 power = .;
run;
```

In the preceding example, the “Control” curve is piecewise linear (since it has more than one point), and the “Treatment” curve is exponential (since it has only one point).

You can also specify an unbalanced design by using the `NTOTAL=` and `GROUPWEIGHTS=` options and specify piecewise linear or exponential survival curves with proportional hazards by using the `CURVE=`, `REFSURVIVAL=`, and `HAZARDRATIO=` options:

```

proc power;
 twosamplesurvival test=logrank
 curve("Control") = (1 2 3):(0.8 0.7 0.6)
 refsurvival = "Control"
 hazardratio = 1.5
 accrualtime = 2
 followuptime = 1
 groupweights = (1 2)
 ntotal = .
 power = 0.8;
run;

```

Instead of computing sample size, you can compute the accrual rate by using the [ACCRUALRATETOTAL=](#) option:

```

proc power;
 twosamplesurvival test=logrank
 curve("Control") = (1 2 3):(0.8 0.7 0.6)
 refsurvival = "Control"
 hazardratio = 1.5
 accrualtime = 2
 followuptime = 1
 groupweights = (1 2)
 accrualratetotal = .
 power = 0.8;
run;

```

or the expected number of events by using the [EVENTSTOTAL=](#) option:

```

proc power;
 twosamplesurvival test=logrank
 curve("Control") = (1 2 3):(0.8 0.7 0.6)
 refsurvival = "Control"
 hazardratio = 1.5
 accrualtime = 2
 followuptime = 1
 groupweights = (1 2)
 eventstotal = .
 power = 0.8;
run;

```

You can also specify sample sizes with the [GROUPNS=](#) option and specify exponential survival curves in terms of median survival times:

```

proc power;
 twosamplesurvival test=logrank
 groupmedsurvtimes = (16 22)
 accrualtime = 6
 totaltime = 18
 groupns = 40 | 60
 power = .;
run;

```

You can also specify exponential survival curves in terms of the hazard ratio and reference hazard. The default value of the `GROUPWEIGHTS=` option specifies a balanced design.

```
proc power;
 twosamplesurvival test=logrank
 hazardratio = 1.2
 refsurvexpazard = 0.7
 accrualtime = 2
 totaltime = 4
 ntotal = 100
 power = .;
run;
```

You can also specify exponential survival curves in terms of the individual hazards, as in the following statements:

```
proc power;
 twosamplesurvival test=logrank
 groupsurvexpazards = 0.7 | 0.84
 accrualtime = 2
 totaltime = 4
 ntotal = .
 power = 0.9;
run;
```

### ***Gehan Rank Test for Two Survival Curves***

In addition to the log-rank test, you can also specify the Gehan tank test, as in the following statements. Default values for the `SIDES=`, `ALPHA=`, `NSUBINTERVAL=`, and `GROUPLOSSEXPHAZARDS=` options specify a two-sided test with a significance level of 0.05, an assumption of no loss to follow-up, and the use of 12 subintervals per unit time in computations.

```
proc power;
 twosamplesurvival test=gehan
 groupmedsurvtimes = 5 | 7
 accrualtime = 3
 totaltime = 6
 npergroup = .
 power = 0.8;
run;
```

### ***Tarone-Ware Rank Test for Two Survival Curves***

You can also specify the Tarone-Ware tank test, as in the following statements. Default values for the `SIDES=`, `ALPHA=`, `NSUBINTERVAL=`, and `GROUPLOSSEXPHAZARDS=` options specify a two-sided test with a significance level of 0.05, an assumption of no loss to follow-up, and the use of 12 subintervals per unit time in computations.

```

proc power;
 twosamplesurvival test=taroneware
 groupmedsurvtimes = 5 | 7
 accrualtime = 3
 totaltime = 6
 npergroup = 100
 power = .;
run;

```

## TWOSAMPLEWILCOXON Statement

**TWOSAMPLEWILCOXON** < options > ;

The **TWOSAMPLEWILCOXON** statement performs power and sample size analyses for the Wilcoxon-Mann-Whitney test (also called the Wilcoxon rank-sum test, Mann-Whitney-Wilcoxon test, or Mann-Whitney U test) for two independent groups.

Note that the O'Brien-Castelloe approach to computing power for the Wilcoxon test is approximate, based on asymptotic behavior as the total sample size gets large. The quality of the power approximation degrades for small sample sizes; conversely, the quality of the sample size approximation degrades if the two distributions are far apart, so that only a small sample is needed to detect a significant difference. But this degradation is rarely a problem in practical situations, in which experiments are usually performed for relatively close distributions.

### Summary of Options

Table 71.25 summarizes the options available in the **TWOSAMPLEWILCOXON** statement.

**Table 71.25** TWOSAMPLEWILCOXON Statement Options

| Option                                    | Description                                                             |
|-------------------------------------------|-------------------------------------------------------------------------|
| <b>Define analysis</b>                    |                                                                         |
| <b>TEST=</b>                              | Specifies the statistical analysis                                      |
| <b>Specify analysis information</b>       |                                                                         |
| <b>ALPHA=</b>                             | Specifies the significance level                                        |
| <b>SIDES=</b>                             | Specifies the number of sides and the direction of the statistical test |
| <b>Specify distributions</b>              |                                                                         |
| <b>VARDIST=</b>                           | Defines a distribution for a variable                                   |
| <b>VARIABLES=</b>                         | Specifies the distributions of two or more variables                    |
| <b>Specify sample size and allocation</b> |                                                                         |
| <b>GROUPNS=</b>                           | Specifies the two group sample sizes                                    |
| <b>GROUPWEIGHTS=</b>                      | Specifies the sample size allocation weights for the two groups         |
| <b>NFRACTIONAL</b>                        | Enables fractional input and output for sample sizes                    |
| <b>NPARGROUP=</b>                         | Specifies the common sample size per group                              |
| <b>NTOTAL=</b>                            | Specifies the sample size                                               |
| <b>Specify power</b>                      |                                                                         |
| <b>POWER=</b>                             | Specifies the desired power of the test                                 |



Table 71.25 *continued*

| Option                               | Description                                          |
|--------------------------------------|------------------------------------------------------|
| <b>Specify computational options</b> |                                                      |
| NBINS=                               | Specifies the number of categories for each variable |
| <b>Control ordering in output</b>    |                                                      |
| OUTPUTORDER=                         | Controls the output order of parameters              |

Table 71.26 summarizes the valid result parameters in the TWOSAMPLEWILCOXON statement.

Table 71.26 Summary of Result Parameters in the TWOSAMPLEWILCOXON Statement

| Analyses | Solve For            | Syntax                             |
|----------|----------------------|------------------------------------|
| TEST=WMW | Power<br>Sample size | POWER=.<br>NTOTAL=.<br>NPERGROUP=. |

## Dictionary of Options

### ALPHA=*number-list*

specifies the level of significance of the statistical test. The default is 0.05, corresponding to the usual  $0.05 \times 100\% = 5\%$  level of significance. See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *number-list*.

### GROUPNS=*grouped-number-list*

### GNS=*grouped-number-list*

specifies the two group sample sizes. See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *grouped-number-list*.

### GROUPWEIGHTS=*grouped-number-list*

### GWEIGHTS=*grouped-number-list*

specifies the sample size allocation weights for the two groups. This option controls how the total sample size is divided between the two groups. Each pair of values for the two groups represents relative allocation weights. Additionally, if the NFRAGMENTAL option is not used, the total sample size is restricted to be equal to a multiple of the sum of the two group weights (so that the resulting design has an integer sample size for each group while adhering exactly to the group allocation weights). Values must be integers unless the NFRAGMENTAL option is used. The default value is (1 1), a balanced design with a weight of 1 for each group. See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *grouped-number-list*.

### NBINS=*number-list*

specifies the number of categories (or “bins”) each variable’s distribution is divided into (unless it is ordinal, in which case the categories remain intact) in internal calculations. Higher values increase computational time and memory requirements but generally lead to more accurate results. However, if the value is too high, then numerical instability can occur. The default value is 1000. See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *number-list*.

**NFRACTIONAL****NFRAC**

enables fractional input and output for sample sizes. See the section “[Sample Size Adjustment Options](#)” on page 6023 for information about the ramifications of the presence (and absence) of the **NFRACTIONAL** option.

**NPERGROUP=number-list****NPERG=number-list**

specifies the common sample size per group or requests a solution for the common sample size per group with a missing value (**NPERGROUP=.**). Use of this option implicitly specifies a balanced design. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**NTOTAL=number-list**

specifies the sample size or requests a solution for the sample size with a missing value (**NTOTAL=.**). See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**OUTPUTORDER=INTERNAL****OUTPUTORDER=REVERSE****OUTPUTORDER=SYNTAX**

controls how the input and default analysis parameters are ordered in the output. **OUTPUTORDER=INTERNAL** (the default) arranges the parameters in the output according to the following order of their corresponding options:

- SIDES
- NBINS=
- ALPHA=
- VARIABLES=
- GROUPWEIGHTS=
- NTOTAL=
- NPERGROUP=
- GROUPNS=
- POWER=

The **OUTPUTORDER=SYNTAX** option arranges the parameters in the output in the same order in which their corresponding options are specified in the **TWOSAMPLEWILCOXON** statement. The **OUTPUTORDER=REVERSE** option arranges the parameters in the output in the reverse of the order in which their corresponding options are specified in the **TWOSAMPLEWILCOXON** statement.

**POWER=number-list**

specifies the desired power of the test or requests a solution for the power with a missing value (**POWER=.**). The power is expressed as a probability, a number between 0 and 1, rather than as a percentage. See the section “[Specifying Value Lists in Analysis Statements](#)” on page 6020 for information about specifying the *number-list*.

**SIDES=keyword-list**

specifies the number of sides (or tails) and the direction of the statistical test. Valid keywords are as follows:

- 1 one-sided with alternative hypothesis in same direction as effect
- 2 two-sided
- U upper one-sided with alternative greater than null value
- L lower one-sided with alternative less than null value

The default value is 2.

**TEST=WMW**

specifies the Wilcoxon-Mann-Whitney test for two independent groups. This is the default test option.

**VARDIST("label")=distribution (parameters)**

defines a distribution for a variable.

For the **VARDIST=** option,

- label* identifies the variable distribution in the output and with the **VARIABLES=** option.
- distribution* specifies the distributional form of the variable.
- parameters* specifies one or more parameters associated with the distribution.

Choices for distributional forms and their parameters are as follows:

**ORDINAL** (*(values)* : *(probabilities)*) is an ordered categorical distribution. The *values* are any numbers separated by spaces. The *probabilities* are numbers between 0 and 1 (inclusive) separated by spaces. Their sum must be exactly 1. The number of *probabilities* must match the number of *values*.

**BETA** (*a*, *b* <, *l*, *r* >) is a beta distribution with shape parameters *a* and *b* and optional location parameters *l* and *r*. The values of *a* and *b* must be greater than 0, and *l* must be less than *r*. The default values for *l* and *r* are 0 and 1, respectively.

**BINOMIAL** (*p*, *n*) is a binomial distribution with probability of success *p* and number of independent Bernoulli trials *n*. The value of *p* must be greater than 0 and less than 1, and *n* must be an integer greater than 0. If *n* = 1, then the distribution is binary.

**EXPONENTIAL** (*λ*) is an exponential distribution with scale *λ*, which must be greater than 0.

**GAMMA** (*a*, *λ*) is a gamma distribution with shape *a* and scale *λ*. The values of *a* and *λ* must be greater than 0.

**LAPLACE** (*θ*, *λ*) is a Laplace distribution with location *θ* and scale *λ*. The value of *λ* must be greater than 0.

**LOGISTIC** (*θ*, *λ*) is a logistic distribution with location *θ* and scale *λ*. The value of *λ* must be greater than 0.

**LOGNORMAL** (*θ*, *λ*) is a lognormal distribution with location *θ* and scale *λ*. The value of *λ* must be greater than 0.

**NORMAL** (*θ*, *λ*) is a normal distribution with mean *θ* and standard deviation *λ*. The value of *λ* must be greater than 0.

POISSON ( $m$ ) is a Poisson distribution with mean  $m$ . The value of  $m$  must be greater than 0.

UNIFORM ( $l, r$ ) is a uniform distribution on the interval  $[l, r]$ , where  $l < r$ .

**VARIABLES=***grouped-name-list*

**VAR=***grouped-name-list*

specifies the distributions of two or more variables, using labels specified with the **VARDIST=** option. See the section “Specifying Value Lists in Analysis Statements” on page 6020 for information about specifying the *grouped-name-list*.

## Restrictions on Option Combinations

To specify the sample size and allocation, choose one of the following parameterizations:

- sample size per group in a balanced design (using the **NPERGROUP=** option)
- total sample size and allocation weights (using the **NTOTAL=** and **GROUPWEIGHTS=** options)
- individual group sample sizes (using the **GROUPNS=** option)

## Option Groups for Common Analyses

This section summarizes the syntax for the common analyses supported in the **TWO SAMPLE WILCOXON** statement.

### *Wilcoxon-Mann-Whitney Test for Comparing Two Distributions*

The following statements perform a power analysis for Wilcoxon-Mann-Whitney tests comparing an ordinal variable with each other type of distribution. Default values for the **ALPHA=**, **NBINS=**, **SIDES=**, and **TEST=** options specify a two-sided test with a significance level of 0.05 and the use of 1000 categories per distribution when discretization is needed.

```
proc power;
 twosamplewilcoxon
 vardist("myordinal") = ordinal ((0 1 2) : (.2 .3 .5))
 vardist("mybeta1") = beta (1, 2)
 vardist("mybeta2") = beta (1, 2, 0, 2)
 vardist("mybinomial") = binomial (.3, 3)
 vardist("myexponential") = exponential (2)
 vardist("mygamma") = gamma (1.5, 2)
 vardist("mylaplace") = laplace (1, 2)
 vardist("mylogistic") = logistic (1, 2)
 vardist("mylognormal") = lognormal (1, 2)
 vardist("mynormal") = normal (3, 2)
 vardist("mypoisson") = poisson (2)
 vardist("myuniform") = uniform (0, 2)
 variables = "myordinal" | "mybeta1" "mybeta2" "mybinomial"
 "myexponential" "mygamma" "mylaplace"
 "mylogistic" "mylognormal" "mynormal"
 "mypoisson" "myuniform"

 ntotal = 40
 power = .;
run;
```

## Details: POWER Procedure

### Overview of Power Concepts

In statistical hypothesis testing, you typically express the belief that some effect exists in a population by specifying an alternative hypothesis  $H_1$ . You state a null hypothesis  $H_0$  as the assertion that the effect does *not* exist and attempt to gather evidence to reject  $H_0$  in favor of  $H_1$ . Evidence is gathered in the form of sample data, and a statistical test is used to assess  $H_0$ . If  $H_0$  is rejected but there really is *no* effect, this is called a *Type I error*. The probability of a Type I error is usually designated “alpha” or  $\alpha$ , and statistical tests are designed to ensure that  $\alpha$  is suitably small (for example, less than 0.05).

If there really is an effect in the population but  $H_0$  is *not* rejected in the statistical test, then a *Type II error* has been made. The probability of a Type II error is usually designated “beta” or  $\beta$ . The probability  $1 - \beta$  of avoiding a Type II error—that is, correctly rejecting  $H_0$  and achieving statistical significance—is called the *power*. (NOTE: Another more general definition of power is the probability of rejecting  $H_0$  for any given set of circumstances, even those corresponding to  $H_0$  being true. The POWER procedure uses this more general definition.)

An important goal in study planning is to ensure an acceptably high level of power. Sample size plays a prominent role in power computations because the focus is often on determining a sufficient sample size to achieve a certain power, or assessing the power for a range of different sample sizes.

Some of the analyses in the POWER procedure focus on *precision* rather than power. An analysis of confidence interval precision is analogous to a traditional power analysis, with “CI Half-Width” taking the place of effect size and “Prob(Width)” taking the place of power. The *CI Half-Width* is the margin of error associated with the confidence interval, the distance between the point estimate and an endpoint. The *Prob(Width)* is the probability of obtaining a confidence interval with *at most* a target half-width.

### Summary of Analyses

Table 71.27 gives a summary of the analyses supported in the POWER procedure. The name of the analysis statement reflects the type of data and design. The TEST=, CI=, and DIST= options specify the focus of the statistical hypothesis (in other words, the criterion on which the research question is based) and the test statistic to be used in data analysis.

**Table 71.27** Summary of Analyses

| Analysis                                                 | Statement     | Options      |
|----------------------------------------------------------|---------------|--------------|
| Logistic regression: likelihood ratio<br>chi-square test | LOGISTIC      |              |
| Multiple linear regression: Type III $F$ test            | MULTREG       |              |
| Correlation: Fisher’s $z$ test                           | ONECORR       | DIST=FISHERZ |
| Correlation: $t$ test                                    | ONECORR       | DIST=T       |
| Binomial proportion: exact test                          | ONESAMPLEFREQ | TEST=EXACT   |

Table 71.27 *continued*

| Analysis                                                            | Statement      | Options                                                                               |
|---------------------------------------------------------------------|----------------|---------------------------------------------------------------------------------------|
| Binomial proportion: $z$ test                                       | ONESAMPLEFREQ  | TEST=Z                                                                                |
| Binomial proportion: $z$ test with continuity adjustment            | ONESAMPLEFREQ  | TEST=ADJZ                                                                             |
| Binomial proportion: exact equivalence test                         | ONESAMPLEFREQ  | TEST=EQUIV_EXACT                                                                      |
| Binomial proportion: $z$ equivalence test                           | ONESAMPLEFREQ  | TEST=EQUIV_Z                                                                          |
| Binomial proportion: $z$ test with continuity adjustment            | ONESAMPLEFREQ  | TEST=EQUIV_ADJZ                                                                       |
| Binomial proportion: confidence interval                            | ONESAMPLEFREQ  | CI=AGRESTICOULL<br>CI=JEFFREYS<br>CI=EXACT<br>CI=WALD<br>CI=WALD_CORRECT<br>CI=WILSON |
| One-sample $t$ test                                                 | ONESAMPLEMEANS | TEST=T                                                                                |
| One-sample $t$ test with lognormal data                             | ONESAMPLEMEANS | TEST=T<br>DIST=LOGNORMAL                                                              |
| One-sample equivalence test for mean of normal data                 | ONESAMPLEMEANS | TEST=EQUIV                                                                            |
| One-sample equivalence test for mean of lognormal data              | ONESAMPLEMEANS | TEST=EQUIV<br>DIST=LOGNORMAL                                                          |
| Confidence interval for a mean                                      | ONESAMPLEMEANS | CI=T                                                                                  |
| One-way ANOVA: one-degree-of-freedom contrast                       | ONEWAYANOVA    | TEST=CONTRAST                                                                         |
| One-way ANOVA: overall $F$ test                                     | ONEWAYANOVA    | TEST=OVERALL                                                                          |
| McNemar exact conditional test                                      | PAIREFREQ      |                                                                                       |
| McNemar normal approximation test                                   | PAIREFREQ      | DIST=NORMAL                                                                           |
| Paired $t$ test                                                     | PAIREDMEANS    | TEST=DIFF                                                                             |
| Paired $t$ test of mean ratio with lognormal data                   | PAIREDMEANS    | TEST=RATIO                                                                            |
| Paired additive equivalence of mean difference with normal data     | PAIREDMEANS    | TEST=EQUIV_DIFF                                                                       |
| Paired multiplicative equivalence of mean ratio with lognormal data | PAIREDMEANS    | TEST=EQUIV_RATIO                                                                      |
| Confidence interval for mean of paired differences                  | PAIREDMEANS    | CI=DIFF                                                                               |
| Pearson chi-square test for two independent proportions             | TWOSAMPLEFREQ  | TEST=PCHI                                                                             |
| Fisher's exact test for two independent proportions                 | TWOSAMPLEFREQ  | TEST=FISHER                                                                           |

Table 71.27 continued

| Analysis                                                                | Statement         | Options          |
|-------------------------------------------------------------------------|-------------------|------------------|
| Likelihood ratio chi-square test for two independent proportions        | TWOSAMPLEFREQ     | TEST=LRCHI       |
| Two-sample <i>t</i> test assuming equal variances                       | TWOSAMPLEMEANS    | TEST=DIFF        |
| Two-sample Satterthwaite <i>t</i> test assuming unequal variances       | TWOSAMPLEMEANS    | TEST=DIFF_SATT   |
| Two-sample pooled <i>t</i> test of mean ratio with lognormal data       | TWOSAMPLEMEANS    | TEST=RATIO       |
| Two-sample additive equivalence of mean difference with normal data     | TWOSAMPLEMEANS    | TEST=EQUIV_DIFF  |
| Two-sample multiplicative equivalence of mean ratio with lognormal data | TWOSAMPLEMEANS    | TEST=EQUIV_RATIO |
| Two-sample confidence interval for mean difference                      | TWOSAMPLEMEANS    | CI=DIFF          |
| Log-rank test for comparing two survival curves                         | TWOSAMPLESURVIVAL | TEST=LOGRANK     |
| Gehan rank test for comparing two survival curves                       | TWOSAMPLESURVIVAL | TEST=GEHAN       |
| Tarone-Ware rank test for comparing two survival curves                 | TWOSAMPLESURVIVAL | TEST=TARONEWARE  |
| Wilcoxon-Mann-Whitney (rank-sum) test                                   | TWOSAMPLEWILCOXON |                  |

## Specifying Value Lists in Analysis Statements

To specify one or more scenarios for an analysis parameter (or set of parameters), you provide a list of values for the statement option that corresponds to the parameter(s). To identify the parameter you want to solve for, you place missing values in the appropriate list.

There are five basic types of such lists: *keyword-lists*, *number-lists*, *grouped-number-lists*, *name-lists*, and *grouped-name-lists*. Some parameters, such as the direction of a test, have values represented by one or more keywords in a *keyword-list*. Scenarios for scalar-valued parameters, such as power, are represented by a *number-list*. Scenarios for groups of scalar-valued parameters, such as group sample sizes in a multi-group design, are represented by a *grouped-number-list*. Scenarios for named parameters, such as reference survival curves, are represented by a *name-list*. Scenarios for groups of named parameters, such as group survival curves, are represented by a *grouped-name-list*.

The following subsections explain these five basic types of lists.

### Keyword-Lists

A *keyword-list* is a list of one or more keywords separated by spaces. For example, you can specify both two-sided and upper-tailed versions of a one-sample *t* test:

```
SIDES = 2 U
```

## Number-Lists

A *number-list* can be one of two things: a series of one or more numbers expressed in the form of one or more DOLISTS, or a missing value indicator (.).

The DOLIST format is the same as in the DATA step language. For example, for the one-sample  $t$  test you can specify four scenarios (30, 50, 70, and 100) for a total sample size in any of the following ways.

```
NTOTAL = 30 50 70 100
NTOTAL = 30 to 70 by 20 100
```

A missing value identifies a parameter as the result parameter; it is valid only with options representing parameters you can solve for in a given analysis. For example, you can request a solution for NTOTAL:

```
NTOTAL = .
```

## Grouped-Number-Lists

A *grouped-number-list* specifies multiple scenarios for numeric values in two or more groups, possibly including missing value indicators to solve for a specific group. The list can assume one of two general forms, a “crossed” version and a “matched” version.

### Crossed Grouped-Number-Lists

The crossed version of a grouped number list consists of a series of *number-lists* (see the section “[Number-Lists](#)” on page 6021), one representing each group, with groups separated by a vertical bar (|). The values for each group represent multiple scenarios for that group, and the scenarios for each individual group are crossed to produce the set of all scenarios for the analysis option. For example, you can specify the following six scenarios for the sizes ( $n_1, n_2$ ) of two groups

```
(20, 30)(20, 40)(20, 50)
(25, 30)(25, 40)(25, 50)
```

as follows:

```
GROUPNS = 20 25 | 30 40 50
```

If the analysis can solve for a value in one group given the other groups, then one of the *number-lists* in a *crossed grouped-number-list* can be a missing value indicator (.). For example, in a two-sample  $t$  test you can posit three scenarios for the group 2 sample size while solving for the group 1 sample size:

```
GROUPNS = . | 30 40 50
```

Some analyses can involve more than two groups. For example, you can specify  $2 \times 3 \times 1 = 6$  scenarios for the means of three groups in a one-way ANOVA as follows:

```
GROUPMEANS = 10 12 | 10 to 20 by 5 | 24
```



**Matched Grouped-Number-Lists**

The matched version of a grouped number list consists of a series of numeric lists, each enclosed in parentheses. Each list consists of a value for each group and represents a single scenario for the analysis option. Multiple scenarios for the analysis option are represented by multiple lists. For example, you can express the crossed grouped-number-list

```
GROUPNS = 20 25 | 30 40 50
```

alternatively in a matched format:

```
GROUPNS = (20 30) (20 40) (20 50) (25 30) (25 40) (25 50)
```

The matched version is particularly useful when you want to include only a subset of all combinations of individual group values. For example, you might want to pair 20 only with 50, and 25 only with 30 and 40:

```
GROUPNS = (20 50) (25 30) (25 40)
```

If the analysis can solve for a value in one group given the other groups, then you can replace the value for that group with a missing value indicator (.). If used, the missing value indicator must occur in the same group in every scenario. For example, you can solve for the group 1 sample size (as in the section “[Crossed Grouped-Number-Lists](#)” on page 6021) by using a matched format:

```
GROUPNS = (. 30) (. 40) (. 50)
```

Some analyses can involve more than two groups. For example, you can specify two scenarios for the means of three groups in a one-way ANOVA:

```
GROUPMEANS = (15 24 32) (12 25 36)
```

**Name-Lists**

A *name-list* is a list of one or more names in single or double quotes, separated by spaces. For example, you can specify two scenarios for the reference survival curve in a log-rank test:

```
REFSURVIVAL = "Curve A" "Curve B"
```

**Grouped-Name-Lists**

A *grouped-name-list* specifies multiple scenarios for names in two or more groups. The list can assume one of two general forms, a “crossed” version and a “matched” version.

**Crossed Grouped-Name-Lists**

The crossed version of a grouped name list consists of a series of *name-lists* (see the section “Name-Lists” on page 6022), one representing each group, with groups separated by a vertical bar (|). The values for each group represent multiple scenarios for that group, and the scenarios for each individual group are crossed to produce the set of all scenarios for the analysis option. For example, you can specify the following six scenarios for the survival curves ( $c_1, c_2$ ) of two groups

```
(“Curve A”, “Curve C”)(“Curve A”, “Curve D”)(“Curve A”, “Curve E”)
(“Curve B”, “Curve C”)(“Curve B”, “Curve D”)(“Curve B”, “Curve E”)
```

as follows:

```
GROUPSURVIVAL = "Curve A" "Curve B" | "Curve C" "Curve D"
 "Curve E"
```

**Matched Grouped-Name-Lists**

The matched version of a grouped name list consists of a series of name lists, each enclosed in parentheses. Each list consists of a name for each group and represents a single scenario for the analysis option. Multiple scenarios for the analysis option are represented by multiple lists. For example, you can express the crossed grouped-name-list

```
GROUPSURVIVAL = "Curve A" "Curve B" | "Curve C" "Curve D"
 "Curve E"
```

alternatively in a matched format:

```
GROUPSURVIVAL = ("Curve A" "Curve C")
 ("Curve A" "Curve D")
 ("Curve A" "Curve E")
 ("Curve B" "Curve C")
 ("Curve B" "Curve D")
 ("Curve B" "Curve E")
```

The matched version is particularly useful when you want to include only a subset of all combinations of individual group values. For example, you might want to pair “Curve A” only with “Curve C”, and “Curve B” only with “Curve D” and “Curve E”:

```
GROUPSURVIVAL = ("Curve A" "Curve C")
 ("Curve B" "Curve D")
 ("Curve B" "Curve E")
```

---

## Sample Size Adjustment Options

By default, PROC POWER rounds sample sizes conservatively (down in the input, up in the output) so that all total sizes (and individual group sample sizes, if a multigroup design) are integers. This is generally considered conservative because it selects the closest realistic design providing *at most* the power of the

(possibly fractional) input or mathematically optimized design. In addition, in a multigroup design, all group sizes are adjusted to be multiples of the corresponding group weights. For example, if GROUPWEIGHTS = (2 6), then all group 1 sample sizes become multiples of 2, and all group 2 sample sizes become multiples of 6 (and all total sample sizes become multiples of 8).

With the NFRACCTIONAL option, sample size input is not rounded, and sample size output (whether total or groupwise) are reported in two versions, a raw “fractional” version and a “ceiling” version rounded up to the nearest integer.

Whenever an input sample size is adjusted, both the original (“nominal”) and adjusted (“actual”) sample sizes are reported. Whenever computed output sample sizes are adjusted, both the original input (“nominal”) power and the achieved (“actual”) power at the adjusted sample size are reported.

---

## Error and Information Output

The Error column in the main output table provides reasons for missing results and flags numerical results that are bounds rather than exact answers. For example, consider the sample size analysis implemented by the following statements:

```
proc power;
 twosamplefreq test=pchi
 method=normal
 oddsratio= 1.0001
 refproportion=.4
 nulloddsratio=1
 power=.9
 ntotal=.;
run;
```

**Figure 71.6** Error Column

| The POWER Procedure                         |                      |
|---------------------------------------------|----------------------|
| Pearson Chi-square Test for Two Proportions |                      |
| Fixed Scenario Elements                     |                      |
| Distribution                                | Asymptotic normal    |
| Method                                      | Normal approximation |
| Null Odds Ratio                             | 1                    |
| Reference (Group 1) Proportion              | 0.4                  |
| Odds Ratio                                  | 1.0001               |
| Nominal Power                               | 0.9                  |
| Number of Sides                             | 2                    |
| Alpha                                       | 0.05                 |
| Group 1 Weight                              | 1                    |
| Group 2 Weight                              | 1                    |

Figure 71.6 *continued*

|              | Computed N Total |                           |
|--------------|------------------|---------------------------|
| Actual Power | N Total          | Error                     |
| 0.206        | 2.15E+09         | Solution is a lower bound |

The output in Figure 71.6 reveals that the sample size to achieve a power of 0.9 could not be computed, but that the sample size 2.15E+09 achieves a power of 0.206.

The Info column provides further details about Error column entries, warnings about any boundary conditions detected, and notes about any adjustments to input. Note that the Info column is hidden by default in the main output. You can view it by using the ODS OUTPUT statement to save the output as a data set and the PRINT procedure. For example, the following SAS statements print both the Error and Info columns for a power computation in a two-sample *t* test:

```
proc power;
 twosamplemeans
 meandiff= 0 7
 stddev=2
 ntotal=2 5
 power=.;
 ods output output=Power;
run;

proc print noobs data=Power;
 var MeanDiff NominalNTotal NTotal Power Error Info;
run;
```

The output is shown in Figure 71.7.

Figure 71.7 Error and Info Columns

| Mean Diff | Nominal NTotal | NTotal | Power | Error         | Info                         |
|-----------|----------------|--------|-------|---------------|------------------------------|
| 0         | 2              | 2      | .     | Invalid input | N too small / No effect      |
| 0         | 5              | 4      | 0.050 |               | Input N adjusted / No effect |
| 7         | 2              | 2      | .     | Invalid input | N too small                  |
| 7         | 5              | 4      | 0.477 |               | Input N adjusted             |

The mean difference of 0 specified with the MEANDIFF= option leads to a “No effect” message to appear in the Info column. The sample size of 2 specified with the NTOTAL= option leads to an “Invalid input” message in the Error column and an “NTotal too small” message in the Info column. The sample size of 5 leads to an “Input N adjusted” message in the Info column because it is rounded down to 4 to produce integer group sizes of 2 per group.

---

## Displayed Output

If you use the `PLOTONLY` option in the `PROC POWER` statement, the procedure displays only graphical output. Otherwise, the displayed output of the `POWER` procedure includes the following:

- the “Fixed Scenario Elements” table, which shows all applicable single-valued analysis parameters, in the following order: distribution, method, parameters input explicitly, and parameters supplied with defaults
- an output table showing the following when applicable (in order): the index of the scenario, all multivalued input, ancillary results, the primary computed result, and error descriptions
- plots (if requested)

For each input parameter, the order of the input values is preserved in the output.

Ancillary results include the following:

- Actual Power, the achieved power, if it differs from the input (Nominal) power value
- Actual Prob(Width), the achieved precision probability, if it differs from the input (Nominal) probability value
- Actual Alpha, the achieved significance level, if it differs from the input (Nominal) alpha value
- fractional sample size, if the `NFRACTIONAL` option is used in the analysis statement

If sample size is the result parameter and the `NFRACTIONAL` option is used in the analysis statement, then both “Fractional” and “Ceiling” sample size results are displayed. Fractional sample sizes correspond to the “Nominal” values of power or precision probability. Ceiling sample sizes are simply the fractional sample sizes rounded up to the nearest integer; they correspond to “Actual” values of power or precision probability.

---

## ODS Table Names

`PROC POWER` assigns a name to each table that it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in [Table 71.28](#). For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

**Table 71.28** ODS Tables Produced by PROC POWER

| ODS Table Name | Description                                                                                                                                                                             | Statement |
|----------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------|
| FixedElements  | Factoid with single-valued analysis parameters                                                                                                                                          | Default*  |
| Output         | All input and computed analysis parameters, error messages, and information messages for each scenario                                                                                  | Default   |
| PlotContent    | Data contained in plots, including analysis parameters and indices identifying plot features. ( <b>NOTE:</b> This table is saved as a data set and not displayed in PROC POWER output.) | PLOT      |

\*Depends on input.

## Computational Resources

### Memory

In the `TWOSAMPLESURVIVAL` statement, the amount of required memory is roughly proportional to the product of the number of subintervals (specified by the `NSUBINTERVAL=` option) and the total time of the study (specified by the `ACCRUALTIME=`, `FOLLOWUPTIME=`, and `TOTALTIME=` options). If you run out of memory, then you can try either specifying a smaller number of subintervals, changing the time scale to use a longer time unit (for example, years instead of months), or both.

### CPU Time

In the Satterthwaite  $t$  test analysis (`TWOSAMPLEMEANS TEST=DIFF_SATT`), the required CPU time grows as the mean difference decreases relative to the standard deviations. In the `PAIREDFREQ` statement, the required CPU time for the exact power computation (`METHOD=EXACT`) grows with the sample size.

## Computational Methods and Formulas

This section describes the approaches used in PROC POWER to compute power for each analysis. The first subsection defines some common notation. The following subsections describe the various power analyses, including discussions of the data, statistical test, and power formula for each analysis. Unless otherwise indicated, computed values for parameters besides power (for example, sample size) are obtained by solving power formulas for the desired parameters.

### Common Notation

Table 71.29 displays notation for some of the more common parameters across analyses. The Associated Syntax column shows examples of relevant analysis statement options, where applicable.

Table 71.29 Common Notation

| Symbol                     | Description                                                                                           | Associated Syntax                |
|----------------------------|-------------------------------------------------------------------------------------------------------|----------------------------------|
| $\alpha$                   | Significance level                                                                                    | ALPHA=                           |
| $N$                        | Total sample size                                                                                     | NTOTAL=, NPAIRS=                 |
| $n_i$                      | Sample size in $i$ th group                                                                           | NPERGROUP=,<br>GROUPNS=          |
| $w_i$                      | Allocation weight for $i$ th group (standardized to sum to 1)                                         | GROUPWEIGHTS=                    |
| $\mu$                      | (Arithmetic) mean                                                                                     | MEAN=                            |
| $\mu_i$                    | (Arithmetic) mean in $i$ th group                                                                     | GROUPMEANS=,<br>PAIREDMEANS=     |
| $\mu_{\text{diff}}$        | (Arithmetic) mean difference, $\mu_2 - \mu_1$ or $\mu_T - \mu_R$                                      | MEANDIFF=                        |
| $\mu_0$                    | Null mean or mean difference (arithmetic)                                                             | NULL=, NULLDIFF=                 |
| $\gamma$                   | Geometric mean                                                                                        | MEAN=                            |
| $\gamma_i$                 | Geometric mean in $i$ th group                                                                        | GROUPMEANS=,<br>PAIREDMEANS=     |
| $\gamma_0$                 | Null mean or mean ratio (geometric)                                                                   | NULL=, NULLRATIO=                |
| $\sigma$                   | Standard deviation (or common standard deviation per group)                                           | STDDEV=                          |
| $\sigma_i$                 | Standard deviation in $i$ th group                                                                    | GROUPSTDDEVS=,<br>PAIREDSTDDEVS= |
| $\sigma_{\text{diff}}$     | Standard deviation of differences                                                                     |                                  |
| CV                         | Coefficient of variation, defined as the ratio of the standard deviation to the (arithmetic) mean     | CV=, PAIREDCVS=                  |
| $\rho$                     | Correlation                                                                                           | CORR=                            |
| $\mu_T, \mu_R$             | Treatment and reference (arithmetic) means for equivalence test                                       | GROUPMEANS=,<br>PAIREDMEANS=     |
| $\gamma_T, \gamma_R$       | Treatment and reference geometric means for equivalence test                                          | GROUPMEANS=,<br>PAIREDMEANS=     |
| $\theta_L$                 | Lower equivalence bound                                                                               | LOWER=                           |
| $\theta_U$                 | Upper equivalence bound                                                                               | UPPER=                           |
| $t(\nu, \delta)$           | $t$ distribution with $df$ $\nu$ and noncentrality $\delta$                                           |                                  |
| $F(\nu_1, \nu_2, \lambda)$ | $F$ distribution with numerator $df$ $\nu_1$ , denominator $df$ $\nu_2$ , and noncentrality $\lambda$ |                                  |
| $t_{p;\nu}$                | $p$ th percentile of $t$ distribution with $df$ $\nu$                                                 |                                  |
| $F_{p;\nu_1,\nu_2}$        | $p$ th percentile of $F$ distribution with numerator $df$ $\nu_1$ and denominator $df$ $\nu_2$        |                                  |
| $\text{Bin}(N, p)$         | Binomial distribution with sample size $N$ and proportion $p$                                         |                                  |

A “lower one-sided” test is associated with SIDES=L (or SIDES=1 with the effect smaller than the null value), and an “upper one-sided” test is associated with SIDES=U (or SIDES=1 with the effect larger than the null value).

Owen (1965) defines a function, known as Owen's  $Q$ , that is convenient for representing terms in power formulas for confidence intervals and equivalence tests:

$$Q_\nu(t, \delta; a, b) = \frac{\sqrt{2\pi}}{\Gamma(\frac{\nu}{2})2^{\frac{\nu-2}{2}}} \int_a^b \Phi\left(\frac{tx}{\sqrt{\nu}} - \delta\right) x^{\nu-1} \phi(x) dx$$

where  $\phi(\cdot)$  and  $\Phi(\cdot)$  are the density and cumulative distribution function of the standard normal distribution, respectively.

## Analyses in the LOGISTIC Statement

### Likelihood Ratio Chi-Square Test for One Predictor (TEST=LRCHI)

The power computing formula is based on Shieh and O'Brien (1998); Shieh (2000); Self, Mauritsen, and Ohara (1992), and Hsieh (1989).

Define the following notation for a logistic regression analysis:

- $N$  = # subjects (NTOTAL)
- $K$  = # predictors (not counting intercept)
- $\mathbf{x} = (x_1, \dots, x_K)'$  = random variables for predictor vector
- $\mathbf{x}_{-1} = (x_2, \dots, x_K)'$
- $\boldsymbol{\mu} = (\mu_1, \dots, \mu_K)'$  =  $E\mathbf{x}$  = mean predictor vector
- $\mathbf{x}_i = (x_{i1}, \dots, x_{iK})'$  = predictor vector for subject  $i$  ( $i \in 1, \dots, N$ )
- $Y$  = random variable for response (0 or 1)
- $Y_i$  = response for subject  $i$  ( $i \in 1, \dots, N$ )
- $p_i = \text{Prob}(Y_i = 1 | \mathbf{x}_i)$  ( $i \in 1, \dots, N$ )
- $\phi = \text{Prob}(Y_i = 1 | \mathbf{x}_i = \boldsymbol{\mu})$  (RESPONSEPROB)
- $U_j$  = unit change for  $j$ th predictor (UNITS)
- $\text{OR}_j = \text{Odds}(Y_i = 1 | x_{ij} = c) / \text{Odds}(Y_i = 1 | x_{ij} = c - U_j)$  ( $c$  arbitrary,  $i \in 1, \dots, N$ ,  $j \in 1, \dots, K$ ) (TESTODDSRATIO if  $j = 1$ , COVODDSRATIOS if  $j > 1$ )
- $\Psi_0$  = intercept in full model (INTERCEPT)
- $\boldsymbol{\Psi} = (\Psi_1, \dots, \Psi_K)'$  = regression coefficients in full model  
( $\Psi_1 = \text{TESTREGCOEFF}$ , others = COVREGCOEFFS)
- $\rho = \text{Corr}(\mathbf{x}_{-1}, x_1)$  (CORR)
- $c_j = \#$  distinct possible values of  $x_{ij}$  ( $j \in 1, \dots, K$ ) (for any  $i$ ) (NBINS)
- $x_{gj}^*$  =  $g$ th possible value of  $x_{ij}$  ( $g \in 1, \dots, c_j$ ) ( $j \in 1, \dots, K$ )  
(for any  $i$ ) (VARDIST)
- $\pi_{gj} = \text{Prob}(x_{ij} = x_{gj}^*)$  ( $g \in 1, \dots, c_j$ ) ( $j \in 1, \dots, K$ )  
(for any  $i$ ) (VARDIST)
- $C = \prod_{j=1}^K c_j = \#$  possible values of  $\mathbf{x}_i$  (for any  $i$ )
- $\mathbf{x}_m^*$  =  $m$ th possible value of  $\mathbf{x}_i$  ( $m \in 1, \dots, C$ )
- $\pi_m = \text{Prob}(\mathbf{x}_i = \mathbf{x}_m^*)$  ( $m \in 1, \dots, C$ )



The logistic regression model is

$$\log\left(\frac{p_i}{1 - p_i}\right) = \Psi_0 + \Psi'x_i$$

The hypothesis test of the first predictor variable is

$$H_0: \Psi_1 = 0$$

$$H_1: \Psi_1 \neq 0$$

Assuming independence among all predictor variables,  $\pi_m$  is defined as follows:

$$\pi_m = \prod_{j=1}^K \pi_{h(m,j)j} \quad (m \in 1, \dots, C)$$

where  $h(m, j)$  is calculated according to the following algorithm:

```

z = m;
do j = K to 1;
 h(m, j) = mod(z - 1, c_j) + 1;
 z = floor((z - 1)/c_j) + 1;
end;

```

This algorithm causes the elements of the transposed vector  $\{h(m, 1), \dots, h(m, K)\}$  to vary fastest to slowest from right to left as  $m$  increases, as shown in the following table of  $h(m, j)$  values:

| $h(m, j)$ | $j$   |       |     |           |       |       |
|-----------|-------|-------|-----|-----------|-------|-------|
|           | 1     | 2     | ... | $K - 1$   | $K$   |       |
| 1         | 1     | 1     | ... | 1         | 1     |       |
| 1         | 1     | 1     | ... | 1         | 2     |       |
| ⋮         |       |       |     | ⋮         |       |       |
| ⋮         | 1     | 1     | ... | 1         | $c_K$ |       |
| ⋮         | 1     | 1     | ... | 2         | 1     |       |
| ⋮         | 1     | 1     | ... | 2         | 2     |       |
| ⋮         |       |       |     | ⋮         |       |       |
| $m$       | ⋮     | 1     | 1   | ...       | 2     | $c_K$ |
| ⋮         |       |       |     | ⋮         |       |       |
| ⋮         | $c_1$ | $c_2$ | ... | $c_{K-1}$ | 1     |       |
| ⋮         | $c_1$ | $c_2$ | ... | $c_{K-1}$ | 2     |       |
| ⋮         |       |       |     | ⋮         |       |       |
| $C$       | $c_1$ | $c_2$ | ... | $c_{K-1}$ | $c_K$ |       |

The  $x_m^*$  values are determined in a completely analogous manner.

The discretization is handled as follows (unless the distribution is ordinal, or binomial with sample size parameter at least as large as requested number of bins): for  $x_j$ , generate  $c_j$  quantiles at evenly spaced probability values such that each such quantile is at the midpoint of a bin with probability  $\frac{1}{c_j}$ . In other words,

$$x_{gj}^* = \left( \frac{g - 0.5}{c_j} \right) \text{th quantile of relevant distribution,}$$

$$(g \in 1, \dots, c_j)(j \in 1, \dots, K)$$

$$\pi_{gj} = \frac{1}{c_j} \quad (\text{same for all } g)$$

The primary noncentrality for the power computation is

$$\Delta^* = 2 \sum_{m=1}^C \pi_m [b'(\theta_m) (\theta_m - \theta_m^*) - (b(\theta_m) - b(\theta_m^*))]$$

where

$$b'(\theta) = \frac{\exp(\theta)}{1 + \exp(\theta)}$$

$$b(\theta) = \log(1 + \exp(\theta))$$

$$\theta_m = \Psi_0 + \Psi' \mathbf{x}_m^*$$

$$\theta_m^* = \Psi_0^* + \Psi^{*'} \mathbf{x}_m^*$$

where

$$\Psi_0^* = \Psi_0 + \Psi_1 \mu_1 = \text{intercept in reduced model, absorbing the tested predictor}$$

$$\Psi^* = (0, \Psi_2, \dots, \Psi_K)' = \text{coefficients in reduced model}$$

The power is

$$\text{power} = P(\chi^2(1, \Delta^* N(1 - \rho^2)) \geq \chi_{1-\alpha}^2(1))$$

The factor  $(1 - \rho^2)$  is the adjustment for correlation between the predictor that is being tested and other predictors, from Hsieh (1989).

Alternative input parameterizations are handled by the following transformations:

$$\Psi_0 = \log\left(\frac{\phi}{1 - \phi}\right) - \Psi' \boldsymbol{\mu}$$

$$\Psi_j = \frac{\log(\text{OR}_j)}{U_j} \quad (j \in 1, \dots, K)$$

## Analyses in the MULTREG Statement

### Type III F Test in Multiple Regression (TEST=TYPE3)

Maxwell (2000) discusses a number of different ways to represent effect sizes (and to compute exact power based on them) in multiple regression. PROC POWER supports two of these, multiple partial correlation and  $R^2$  in full and reduced models.

Let  $p$  denote the total number of predictors in the full model (excluding the intercept), and let  $Y$  denote the response variable. You are testing that the coefficients of  $p_1 \geq 1$  predictors in a set  $X_1$  are 0, controlling for all of the other predictors  $X_{-1}$ , which consists of  $p - p_1 \geq 0$  variables.

The hypotheses can be expressed in two different ways. The first is in terms of  $\rho_{YX_1|X_{-1}}$ , the multiple partial correlation between the predictors in  $X_1$  and the response  $Y$  adjusting for the predictors in  $X_{-1}$ :

$$H_0: \rho_{YX_1|X_{-1}}^2 = 0$$

$$H_1: \rho_{YX_1|X_{-1}}^2 > 0$$

The second is in terms of the multiple correlations in full ( $\rho_{Y|(X_1, X_{-1})}$ ) and reduced ( $\rho_{Y|X_{-1}}$ ) nested models:

$$H_0: \rho_{Y|(X_1, X_{-1})}^2 - \rho_{Y|X_{-1}}^2 = 0$$

$$H_1: \rho_{Y|(X_1, X_{-1})}^2 - \rho_{Y|X_{-1}}^2 > 0$$

Note that the squared values of  $\rho_{Y|(X_1, X_{-1})}$  and  $\rho_{Y|X_{-1}}$  are the population  $R^2$  values for full and reduced models.

The test statistic can be written in terms of the sample multiple partial correlation  $R_{YX_1|X_{-1}}$ ,

$$F = \begin{cases} (N - 1 - p) \frac{R_{YX_1|X_{-1}}^2}{1 - R_{YX_1|X_{-1}}^2}, & \text{intercept} \\ (N - p) \frac{R_{YX_1|X_{-1}}^2}{1 - R_{YX_1|X_{-1}}^2}, & \text{no intercept} \end{cases}$$

or the sample multiple correlations in full ( $R_{Y|(X_1, X_{-1})}$ ) and reduced ( $R_{Y|X_{-1}}$ ) models,

$$F = \begin{cases} (N - 1 - p) \frac{R_{Y|(X_1, X_{-1})}^2 - R_{Y|X_{-1}}^2}{1 - R_{Y|(X_1, X_{-1})}^2}, & \text{intercept} \\ (N - p) \frac{R_{Y|(X_1, X_{-1})}^2 - R_{Y|X_{-1}}^2}{1 - R_{Y|(X_1, X_{-1})}^2}, & \text{no intercept} \end{cases}$$

The test is the usual Type III  $F$  test in multiple regression:

$$\text{Reject } H_0 \text{ if } \begin{cases} F \geq F_{1-\alpha}(p_1, N - 1 - p), & \text{intercept} \\ F \geq F_{1-\alpha}(p_1, N - p), & \text{no intercept} \end{cases}$$

Although the test is invariant to whether the predictors are assumed to be random or fixed, the power is affected by this assumption. If the response and predictors are assumed to have a joint multivariate normal

distribution, then the exact power is given by the following formula:

$$\text{power} = \begin{cases} P \left[ \left( \frac{N-1-p}{p_1} \right) \left( \frac{R_{YX_1|X_{-1}}^2}{1-R_{YX_1|X_{-1}}^2} \right) \geq F_{1-\alpha}(p_1, N-1-p) \right], & \text{intercept} \\ P \left[ \left( \frac{N-p}{p_1} \right) \left( \frac{R_{YX_1|X_{-1}}^2}{1-R_{YX_1|X_{-1}}^2} \right) \geq F_{1-\alpha}(p_1, N-p) \right], & \text{no intercept} \end{cases}$$

$$= \begin{cases} P \left[ R_{YX_1|X_{-1}}^2 \geq \frac{F_{1-\alpha}(p_1, N-1-p)}{F_{1-\alpha}(p_1, N-1-p) + \frac{N-1-p}{p_1}} \right], & \text{intercept} \\ P \left[ R_{YX_1|X_{-1}}^2 \geq \frac{F_{1-\alpha}(p_1, N-p)}{F_{1-\alpha}(p_1, N-p) + \frac{N-p}{p_1}} \right], & \text{no intercept} \end{cases}$$

The distribution of  $R_{YX_1|X_{-1}}^2$  (for any  $\rho_{YX_1|X_{-1}}^2$ ) is given in Chapter 32 of Johnson, Kotz, and Balakrishnan (1995). Sample size tables are presented in Gatsonis and Sampson (1989).

If the predictors are assumed to have fixed values, then the exact power is given by the noncentral  $F$  distribution. The noncentrality parameter is

$$\lambda = N \frac{\rho_{YX_1|X_{-1}}^2}{1 - \rho_{YX_1|X_{-1}}^2}$$

or equivalently,

$$\lambda = N \frac{\rho_{Y|(X_1, X_{-1})}^2 - \rho_{Y|X_{-1}}^2}{1 - \rho_{Y|(X_1, X_{-1})}^2}$$

The power is

$$\text{power} = \begin{cases} P(F(p_1, N-1-p, \lambda) \geq F_{1-\alpha}(p_1, N-1-p)), & \text{intercept} \\ P(F(p_1, N-p, \lambda) \geq F_{1-\alpha}(p_1, N-p)), & \text{no intercept} \end{cases}$$

The minimum acceptable input value of  $N$  depends on several factors, as shown in Table 71.30.

**Table 71.30** Minimum Acceptable Sample Size Values in the MULTREG Statement

| Predictor Type | Intercept in Model? | $p_1 = 1?$ | Minimum $N$ |
|----------------|---------------------|------------|-------------|
| Random         | Yes                 | Yes        | $p + 3$     |
| Random         | Yes                 | No         | $p + 2$     |
| Random         | No                  | Yes        | $p + 2$     |
| Random         | No                  | No         | $p + 1$     |
| Fixed          | Yes                 | Yes or No  | $p + 2$     |
| Fixed          | No                  | Yes or No  | $p + 1$     |

## Analyses in the ONECORR Statement

### Fisher's z Test for Pearson Correlation (TEST=PEARSON DIST=FISHERZ)

Fisher's z transformation (Fisher 1921) of the sample correlation  $R_{Y|(X_1, X_{-1})}$  is defined as

$$z = \frac{1}{2} \log \left( \frac{1 + R_{Y|(X_1, X_{-1})}}{1 - R_{Y|(X_1, X_{-1})}} \right)$$

Fisher's z test assumes the approximate normal distribution  $N(\mu, \sigma^2)$  for z, where

$$\mu = \frac{1}{2} \log \left( \frac{1 + \rho_{Y|(X_1, X_{-1})}}{1 - \rho_{Y|(X_1, X_{-1})}} \right) + \frac{\rho_{Y|(X_1, X_{-1})}}{2(N - 1 - p^*)}$$

and

$$\sigma^2 = \frac{1}{N - 3 - p^*}$$

where  $p^*$  is the number of variables partialled out (Anderson 1984, pp. 132–133) and  $\rho_{Y|(X_1, X_{-1})}$  is the partial correlation between Y and  $X_1$  adjusting for the set of zero or more variables  $X_{-1}$ .

The test statistic

$$z^* = (N - 3 - p^*)^{\frac{1}{2}} \left[ z - \frac{1}{2} \log \left( \frac{1 + \rho_0}{1 - \rho_0} \right) - \frac{\rho_0}{2(N - 1 - p^*)} \right]$$

is assumed to have a normal distribution  $N(\delta, \nu)$ , where  $\rho_0$  is the null partial correlation and  $\delta$  and  $\nu$  are derived from Section 16.33 of Stuart and Ord (1994):

$$\begin{aligned} \delta &= (N - 3 - p^*)^{\frac{1}{2}} \left[ \frac{1}{2} \log \left( \frac{1 + \rho_{Y|(X_1, X_{-1})}}{1 - \rho_{Y|(X_1, X_{-1})}} \right) + \frac{\rho_{Y|(X_1, X_{-1})}}{2(N - 1 - p^*)} \left( 1 + \frac{5 + \rho_{Y|(X_1, X_{-1})}^2}{4(N - 1 - p^*)} \right) \right. \\ &\quad \left. + \frac{11 + 2\rho_{Y|(X_1, X_{-1})}^2 + 3\rho_{Y|(X_1, X_{-1})}^4}{8(N - 1 - p^*)^2} \right] - \frac{1}{2} \log \left( \frac{1 + \rho_0}{1 - \rho_0} \right) - \frac{\rho_0}{2(N - 1 - p^*)} \\ \nu &= \frac{N - 3 - p^*}{N - 1 - p^*} \left[ 1 + \frac{4 - \rho_{Y|(X_1, X_{-1})}^2}{2(N - 1 - p^*)} + \frac{22 - 6\rho_{Y|(X_1, X_{-1})}^2 - 3\rho_{Y|(X_1, X_{-1})}^4}{6(N - 1 - p^*)^2} \right] \end{aligned}$$

The approximate power is computed as

$$\text{power} = \begin{cases} \Phi \left( \frac{\delta - z_{1-\alpha}}{\nu^{\frac{1}{2}}} \right), & \text{upper one-sided} \\ \Phi \left( \frac{-\delta - z_{1-\alpha}}{\nu^{\frac{1}{2}}} \right), & \text{lower one-sided} \\ \Phi \left( \frac{\delta - z_{1-\frac{\alpha}{2}}}{\nu^{\frac{1}{2}}} \right) + \Phi \left( \frac{-\delta - z_{1-\frac{\alpha}{2}}}{\nu^{\frac{1}{2}}} \right), & \text{two-sided} \end{cases}$$

Because the test is biased, the achieved significance level might differ from the nominal significance level. The actual alpha is computed in the same way as the power except with the correlation  $\rho_{Y|(X_1, X_{-1})}$  replaced by the null correlation  $\rho_0$ .

***t* Test for Pearson Correlation (TEST=PEARSON DIST=T)**

The two-sided case is identical to multiple regression with an intercept and  $p_1 = 1$ , which is discussed in the section “Analyses in the MULTREG Statement” on page 6032.

Let  $p^*$  denote the number of variables partialled out. For the one-sided cases, the test statistic is

$$t = (N - 2 - p^*)^{\frac{1}{2}} \frac{R_{YX_1|X_{-1}}}{\left(1 - R_{YX_1|X_{-1}}^2\right)^{\frac{1}{2}}}$$

which is assumed to have a null distribution of  $t(N - 2 - p^*)$ .

If the  $X$  and  $Y$  variables are assumed to have a joint multivariate normal distribution, then the exact power is given by the following formula:

$$\begin{aligned} \text{power} &= \begin{cases} P \left[ (N - 2 - p^*)^{\frac{1}{2}} \frac{R_{YX_1|X_{-1}}}{\left(1 - R_{YX_1|X_{-1}}^2\right)^{\frac{1}{2}}} \geq t_{1-\alpha}(N - 2 - p^*) \right], & \text{upper one-sided} \\ P \left[ (N - 2 - p^*)^{\frac{1}{2}} \frac{R_{YX_1|X_{-1}}}{\left(1 - R_{YX_1|X_{-1}}^2\right)^{\frac{1}{2}}} \leq t_{\alpha}(N - 2 - p^*) \right], & \text{lower one-sided} \end{cases} \\ &= \begin{cases} P \left[ R_{Y|(X_1, X_{-1})} \geq \frac{t_{1-\alpha}(N-2-p^*)}{\left(t_{1-\alpha}^2(N-2-p^*) + N-2-p^*\right)^{\frac{1}{2}}} \right], & \text{upper one-sided} \\ P \left[ R_{Y|(X_1, X_{-1})} \leq \frac{t_{\alpha}(N-2-p^*)}{\left(t_{\alpha}^2(N-2-p^*) + N-2-p^*\right)^{\frac{1}{2}}} \right], & \text{lower one-sided} \end{cases} \end{aligned}$$

The distribution of  $R_{Y|(X_1, X_{-1})}$  (given the underlying true correlation  $\rho_{Y|(X_1, X_{-1})}$ ) is given in Chapter 32 of Johnson, Kotz, and Balakrishnan (1995).

If the  $X$  variables are assumed to have fixed values, then the exact power is given by the noncentral  $t$  distribution  $t(N - 2 - p^*, \delta)$ , where the noncentrality is

$$\delta = N^{\frac{1}{2}} \frac{\rho_{YX_1|X_{-1}}}{\left(1 - \rho_{YX_1|X_{-1}}^2\right)^{\frac{1}{2}}}$$

The power is

$$\text{power} = \begin{cases} P(t(N - 2 - p^*, \delta) \geq t_{1-\alpha}(N - 2 - p^*)), & \text{upper one-sided} \\ P(t(N - 2 - p^*, \delta) \leq t_{\alpha}(N - 2 - p^*)), & \text{lower one-sided} \end{cases}$$

## Analyses in the ONESAMPLEFREQ Statement

### Exact Test of a Binomial Proportion (TEST=EXACT)

Let  $X$  be distributed as  $\text{Bin}(N, p)$ . The hypotheses for the test of the proportion  $p$  are as follows:

$$H_0: p = p_0$$

$$H_1: \begin{cases} p \neq p_0, & \text{two-sided} \\ p > p_0, & \text{upper one-sided} \\ p < p_0, & \text{lower one-sided} \end{cases}$$

The exact test assumes binomially distributed data and requires  $N \geq 1$  and  $0 < p_0 < 1$ . The test statistic is

$$X = \text{number of successes} \sim \text{Bin}(N, p)$$

The significance probability  $\alpha$  is split symmetrically for two-sided tests, in the sense that each tail is filled with as much as possible up to  $\alpha/2$ .

Exact power computations are based on the binomial distribution and computing formulas such as the following from Johnson, Kotz, and Kemp (1992, equation 3.20):

$$P(X \geq C | N, p) = P\left(F_{v_1, v_2} \leq \frac{v_2 p}{v_1(1-p)}\right) \quad \text{where } v_1 = 2C \text{ and } v_2 = 2(N - C + 1)$$

Let  $C_L$  and  $C_U$  denote lower and upper critical values, respectively. Let  $\alpha_a$  denote the achieved (actual) significance level, which for two-sided tests is the sum of the favorable major tail ( $\alpha_M$ ) and the opposite minor tail ( $\alpha_m$ ).

For the upper one-sided case,

$$C_U = \min\{C : P(X \geq C | p_0) \leq \alpha\}$$

Reject  $H_0$  if  $X \geq C_U$

$$\alpha_a = P(X \geq C_U | p_0)$$

$$\text{power} = P(X \geq C_U | p)$$

For the lower one-sided case,

$$C_L = \max\{C : P(X \leq C | p_0) \leq \alpha\}$$

Reject  $H_0$  if  $X \leq C_L$

$$\alpha_a = P(X \leq C_L | p_0)$$

$$\text{power} = P(X \leq C_L | p)$$

For the two-sided case,

$$C_L = \max\{C : P(X \leq C | p_0) \leq \frac{\alpha}{2}\}$$

$$C_U = \min\{C : P(X \geq C | p_0) \leq \frac{\alpha}{2}\}$$

Reject  $H_0$  if  $X \leq C_L$  or  $X \geq C_U$

$$\alpha_a = P(X \leq C_L \text{ or } X \geq C_U | p_0)$$

$$\text{power} = P(X \leq C_L \text{ or } X \geq C_U | p)$$

***z Test for Binomial Proportion Using Null Variance (TEST=Z VAREST=NULL)***

For the normal approximation test, the test statistic is

$$Z(X) = \frac{X - Np_0}{[Np_0(1 - p_0)]^{\frac{1}{2}}}$$

For the METHOD=EXACT option, the computations are the same as described in the section “Exact Test of a Binomial Proportion (TEST=EXACT)” on page 6036 except for the definitions of the critical values.

For the upper one-sided case,

$$C_U = \min\{C : Z(C) \geq z_{1-\alpha}\}$$

For the lower one-sided case,

$$C_L = \max\{C : Z(C) \leq z_\alpha\}$$

For the two-sided case,

$$C_L = \max\{C : Z(C) \leq z_{\frac{\alpha}{2}}\}$$

$$C_U = \min\{C : Z(C) \geq z_{1-\frac{\alpha}{2}}\}$$

For the METHOD=NORMAL option, the test statistic  $Z(X)$  is assumed to have the normal distribution

$$N\left(\frac{N^{\frac{1}{2}}(p - p_0)}{[p_0(1 - p_0)]^{\frac{1}{2}}}, \frac{p(1 - p)}{p_0(1 - p_0)}\right)$$

The approximate power is computed as

$$\text{power} = \begin{cases} \Phi\left(\frac{z_\alpha + \sqrt{N} \frac{p - p_0}}{\sqrt{\frac{p(1-p)}{p_0(1-p_0)}}}\right), & \text{upper one-sided} \\ \Phi\left(\frac{z_\alpha - \sqrt{N} \frac{p - p_0}}{\sqrt{\frac{p(1-p)}{p_0(1-p_0)}}}\right), & \text{lower one-sided} \\ \Phi\left(\frac{z_{\frac{\alpha}{2}} + \sqrt{N} \frac{p - p_0}}{\sqrt{\frac{p(1-p)}{p_0(1-p_0)}}}\right) + \Phi\left(\frac{z_{\frac{\alpha}{2}} - \sqrt{N} \frac{p - p_0}}{\sqrt{\frac{p(1-p)}{p_0(1-p_0)}}}\right), & \text{two-sided} \end{cases}$$

The approximate sample size is computed in closed form for the one-sided cases by inverting the power equation,

$$N = \left(\frac{z_{\text{power}} \sqrt{p(1-p)} + z_{1-\alpha} \sqrt{p_0(1-p_0)}}{p - p_0}\right)^2$$

and by numerical inversion for the two-sided case.



***z Test for Binomial Proportion Using Sample Variance (TEST=Z VAREST=SAMPLE)***

For the normal approximation test using the sample variance, the test statistic is

$$Z_s(X) = \frac{X - Np_0}{[N\hat{p}(1 - \hat{p})]^{1/2}}$$

where  $\hat{p} = X/N$ .

For the METHOD=EXACT option, the computations are the same as described in the section “Exact Test of a Binomial Proportion (TEST=EXACT)” on page 6036 except for the definitions of the critical values.

For the upper one-sided case,

$$C_U = \min\{C : Z_s(C) \geq z_{1-\alpha}\}$$

For the lower one-sided case,

$$C_L = \max\{C : Z_s(C) \leq z_\alpha\}$$

For the two-sided case,

$$C_L = \max\{C : Z_s(C) \leq z_{\frac{\alpha}{2}}\}$$

$$C_U = \min\{C : Z_s(C) \geq z_{1-\frac{\alpha}{2}}\}$$

For the METHOD=NORMAL option, the test statistic  $Z_s(X)$  is assumed to have the normal distribution

$$N\left(\frac{N^{1/2}(p - p_0)}{[p(1 - p)]^{1/2}}, 1\right)$$

(see Chow, Shao, and Wang (2003, p. 82)).

The approximate power is computed as

$$\text{power} = \begin{cases} \Phi\left(z_\alpha + \sqrt{N} \frac{p - p_0}{\sqrt{p(1-p)}}\right), & \text{upper one-sided} \\ \Phi\left(z_\alpha - \sqrt{N} \frac{p - p_0}{\sqrt{p(1-p)}}\right), & \text{lower one-sided} \\ \Phi\left(z_{\frac{\alpha}{2}} + \sqrt{N} \frac{p - p_0}{\sqrt{p(1-p)}}\right) + \Phi\left(z_{\frac{\alpha}{2}} - \sqrt{N} \frac{p - p_0}{\sqrt{p(1-p)}}\right), & \text{two-sided} \end{cases}$$

The approximate sample size is computed in closed form for the one-sided cases by inverting the power equation,

$$N = p(1 - p) \left( \frac{z_{\text{power}} + z_{1-\alpha}}{p - p_0} \right)^2$$

and by numerical inversion for the two-sided case.

***z Test for Binomial Proportion with Continuity Adjustment Using Null Variance (TEST=ADJZ VAREST=NULL)***

For the normal approximation test with continuity adjustment, the test statistic is (Pagano and Gauvreau 1993, p. 295):

$$Z_c(X) = \frac{X - Np_0 + 0.5(1_{\{X < Np_0\}}) - 0.5(1_{\{X > Np_0\}})}{[Np_0(1 - p_0)]^{\frac{1}{2}}}$$

For the METHOD=EXACT option, the computations are the same as described in the section “Exact Test of a Binomial Proportion (TEST=EXACT)” on page 6036 except for the definitions of the critical values.

For the upper one-sided case,

$$C_U = \min\{C : Z_c(C) \geq z_{1-\alpha}\}$$

For the lower one-sided case,

$$C_L = \max\{C : Z_c(C) \leq z_\alpha\}$$

For the two-sided case,

$$C_L = \max\{C : Z_c(C) \leq z_{\frac{\alpha}{2}}\}$$

$$C_U = \min\{C : Z_c(C) \geq z_{1-\frac{\alpha}{2}}\}$$

For the METHOD=NORMAL option, the test statistic  $Z_c(X)$  is assumed to have the normal distribution  $N(\mu, \sigma^2)$ , where  $\mu$  and  $\sigma^2$  are derived as follows.

For convenience of notation, define

$$k = \frac{1}{2\sqrt{Np_0(1 - p_0)}}$$

Then

$$E[Z_c(X)] = 2kNp - 2kNp_0 + kP(X < Np_0) - kP(X > Np_0)$$

and

$$\begin{aligned} \text{Var}[Z_c(X)] &= 4k^2Np(1 - p) + k^2[1 - P(X = Np_0)] - k^2[P(X < Np_0) - P(X > Np_0)]^2 \\ &\quad + 4k^2[E(X1_{\{X < Np_0\}}) - E(X1_{\{X > Np_0\}})] - 4k^2Np[P(X < Np_0) - P(X > Np_0)] \end{aligned}$$

The probabilities  $P(X = Np_0)$ ,  $P(X < Np_0)$ , and  $P(X > Np_0)$  and the truncated expectations  $E(X1_{\{X < Np_0\}})$  and  $E(X1_{\{X > Np_0\}})$  are approximated by assuming the normal-approximate distribution of  $X$ ,  $N(Np, Np(1 - p))$ . Letting  $\phi(\cdot)$  and  $\Phi(\cdot)$  denote the standard normal PDF and CDF, respectively, and defining  $d$  as

$$d = \frac{Np_0 - Np}{[Np(1 - p)]^{\frac{1}{2}}}$$

the terms are computed as follows:

$$\begin{aligned}
 P(X = Np_0) &= 0 \\
 P(X < Np_0) &= \Phi(d) \\
 P(X > Np_0) &= 1 - \Phi(d) \\
 E(X1_{\{X < Np_0\}}) &= Np\Phi(d) - [Np(1-p)]^{\frac{1}{2}}\phi(d) \\
 E(X1_{\{X > Np_0\}}) &= Np[1 - \Phi(d)] + [Np(1-p)]^{\frac{1}{2}}\phi(d)
 \end{aligned}$$

The mean and variance of  $Z_c(X)$  are thus approximated by

$$\mu = k [2Np - 2Np_0 + 2\Phi(d) - 1]$$

and

$$\sigma^2 = 4k^2 \left[ Np(1-p) + \Phi(d)(1 - \Phi(d)) - 2(Np(1-p))^{\frac{1}{2}}\phi(d) \right]$$

The approximate power is computed as

$$\text{power} = \begin{cases} \Phi\left(\frac{z_\alpha + \mu}{\sigma}\right), & \text{upper one-sided} \\ \Phi\left(\frac{z_\alpha - \mu}{\sigma}\right), & \text{lower one-sided} \\ \Phi\left(\frac{z_{\frac{\alpha}{2}} + \mu}{\sigma}\right) + \Phi\left(\frac{z_{\frac{\alpha}{2}} - \mu}{\sigma}\right), & \text{two-sided} \end{cases}$$

The approximate sample size is computed by numerical inversion.

### ***z Test for Binomial Proportion with Continuity Adjustment Using Sample Variance (TEST=ADJZ VAREST=SAMPLE)***

For the normal approximation test with continuity adjustment using the sample variance, the test statistic is

$$Z_{cs}(X) = \frac{X - Np_0 + 0.5(1_{\{X < Np_0\}}) - 0.5(1_{\{X > Np_0\}})}{[N\hat{p}(1 - \hat{p})]^{\frac{1}{2}}}$$

where  $\hat{p} = X/N$ .

For the METHOD=EXACT option, the computations are the same as described in the section “[Exact Test of a Binomial Proportion \(TEST=EXACT\)](#)” on page 6036 except for the definitions of the critical values.

For the upper one-sided case,

$$C_U = \min\{C : Z_{cs}(C) \geq z_{1-\alpha}\}$$

For the lower one-sided case,

$$C_L = \max\{C : Z_{cs}(C) \leq z_\alpha\}$$

For the two-sided case,

$$C_L = \max\{C : Z_{cs}(C) \leq z_{\frac{\alpha}{2}}\}$$

$$C_U = \min\{C : Z_{cs}(C) \geq z_{1-\frac{\alpha}{2}}\}$$

For the METHOD=NORMAL option, the test statistic  $Z_{cs}(X)$  is assumed to have the normal distribution  $N(\mu, \sigma^2)$ , where  $\mu$  and  $\sigma^2$  are derived as follows.

For convenience of notation, define

$$k = \frac{1}{2\sqrt{Np(1-p)}}$$

Then

$$E[Z_{cs}(X)] \approx 2kNp - 2kNp_0 + kP(X < Np_0) - kP(X > Np_0)$$

and

$$\begin{aligned} \text{Var}[Z_{cs}(X)] \approx & 4k^2Np(1-p) + k^2[1 - P(X = Np_0)] - k^2[P(X < Np_0) - P(X > Np_0)]^2 \\ & + 4k^2[E(X1_{\{X < Np_0\}}) - E(X1_{\{X > Np_0\}})] - 4k^2Np[P(X < Np_0) - P(X > Np_0)] \end{aligned}$$

The probabilities  $P(X = Np_0)$ ,  $P(X < Np_0)$ , and  $P(X > Np_0)$  and the truncated expectations  $E(X1_{\{X < Np_0\}})$  and  $E(X1_{\{X > Np_0\}})$  are approximated by assuming the normal-approximate distribution of  $X$ ,  $N(Np, Np(1-p))$ . Letting  $\phi(\cdot)$  and  $\Phi(\cdot)$  denote the standard normal PDF and CDF, respectively, and defining  $d$  as

$$d = \frac{Np_0 - Np}{[Np(1-p)]^{\frac{1}{2}}}$$

the terms are computed as follows:

$$\begin{aligned} P(X = Np_0) &= 0 \\ P(X < Np_0) &= \Phi(d) \\ P(X > Np_0) &= 1 - \Phi(d) \\ E(X1_{\{X < Np_0\}}) &= Np\Phi(d) - [Np(1-p)]^{\frac{1}{2}}\phi(d) \\ E(X1_{\{X > Np_0\}}) &= Np[1 - \Phi(d)] + [Np(1-p)]^{\frac{1}{2}}\phi(d) \end{aligned}$$

The mean and variance of  $Z_{cs}(X)$  are thus approximated by

$$\mu = k[2Np - 2Np_0 + 2\Phi(d) - 1]$$

and

$$\sigma^2 = 4k^2 \left[ Np(1-p) + \Phi(d)(1 - \Phi(d)) - 2(Np(1-p))^{\frac{1}{2}}\phi(d) \right]$$

The approximate power is computed as

$$\text{power} = \begin{cases} \Phi\left(\frac{z_{\alpha} + \mu}{\sigma}\right), & \text{upper one-sided} \\ \Phi\left(\frac{z_{\alpha} - \mu}{\sigma}\right), & \text{lower one-sided} \\ \Phi\left(\frac{z_{\frac{\alpha}{2}} + \mu}{\sigma}\right) + \Phi\left(\frac{z_{\frac{\alpha}{2}} - \mu}{\sigma}\right), & \text{two-sided} \end{cases}$$

The approximate sample size is computed by numerical inversion.

### **Exact Equivalence Test of a Binomial Proportion (TEST=EQUIV\_EXACT)**

The hypotheses for the equivalence test are

$$H_0: p < \theta_L \quad \text{or} \quad p > \theta_U$$

$$H_1: \theta_L \leq p \leq \theta_U$$

where  $\theta_L$  and  $\theta_U$  are the lower and upper equivalence bounds, respectively.

The analysis is the two one-sided tests (TOST) procedure as described in Chow, Shao, and Wang (2003) on p. 84, but using exact critical values as on p. 116 instead of normal-based critical values.

Two different hypothesis tests are carried out:

$$H_{a0}: p < \theta_L$$

$$H_{a1}: p \geq \theta_L$$

and

$$H_{b0}: p > \theta_U$$

$$H_{b1}: p \leq \theta_U$$

If  $H_{a0}$  is rejected in favor of  $H_{a1}$  and  $H_{b0}$  is rejected in favor of  $H_{b1}$ , then  $H_0$  is rejected in favor of  $H_1$ .

The test statistic for each of the two tests ( $H_{a0}$  versus  $H_{a1}$  and  $H_{b0}$  versus  $H_{b1}$ ) is

$$X = \text{number of successes} \sim \text{Bin}(N, p)$$

Let  $C_U$  denote the critical value of the exact upper one-sided test of  $H_{a0}$  versus  $H_{a1}$ , and let  $C_L$  denote the critical value of the exact lower one-sided test of  $H_{b0}$  versus  $H_{b1}$ . These critical values are computed in the section “Exact Test of a Binomial Proportion (TEST=EXACT)” on page 6036. Both of these tests are rejected if and only if  $C_U \leq X \leq C_L$ . Thus, the exact power of the equivalence test is

$$\begin{aligned} \text{power} &= P(C_U \leq X \leq C_L) \\ &= P(X \geq C_U) - P(X \geq C_L + 1) \end{aligned}$$

The probabilities are computed using Johnson and Kotz (1970, equation 3.20).

**z Equivalence Test for Binomial Proportion Using Null Variance (TEST=EQUIV\_Z VAREST=NULL)**

The hypotheses for the equivalence test are

$$H_0: p < \theta_L \quad \text{or} \quad p > \theta_U$$

$$H_1: \theta_L \leq p \leq \theta_U$$

where  $\theta_L$  and  $\theta_U$  are the lower and upper equivalence bounds, respectively.

The analysis is the two one-sided tests (TOST) procedure as described in Chow, Shao, and Wang (2003) on p. 84, but using the null variance instead of the sample variance.

Two different hypothesis tests are carried out:

$$H_{a0}: p < \theta_L$$

$$H_{a1}: p \geq \theta_L$$

and

$$H_{b0}: p > \theta_U$$

$$H_{b1}: p \leq \theta_U$$

If  $H_{a0}$  is rejected in favor of  $H_{a1}$  and  $H_{b0}$  is rejected in favor of  $H_{b1}$ , then  $H_0$  is rejected in favor of  $H_1$ .

The test statistic for the test of  $H_{a0}$  versus  $H_{a1}$  is

$$Z_L(X) = \frac{X - N\theta_L}{[N\theta_L(1 - \theta_L)]^{\frac{1}{2}}}$$

The test statistic for the test of  $H_{b0}$  versus  $H_{b1}$  is

$$Z_U(X) = \frac{X - N\theta_U}{[N\theta_U(1 - \theta_U)]^{\frac{1}{2}}}$$

For the METHOD=EXACT option, let  $C_U$  denote the critical value of the exact upper one-sided test of  $H_{a0}$  versus  $H_{a1}$  using  $Z_L(X)$ . This critical value is computed in the section “z Test for Binomial Proportion Using Null Variance (TEST=Z VAREST=NULL)” on page 6037. Similarly, let  $C_L$  denote the critical value of the exact lower one-sided test of  $H_{b0}$  versus  $H_{b1}$  using  $Z_U(X)$ . Both of these tests are rejected if and only if  $C_U \leq X \leq C_L$ . Thus, the exact power of the equivalence test is

$$\begin{aligned} \text{power} &= P(C_U \leq X \leq C_L) \\ &= P(X \geq C_U) - P(X \geq C_L + 1) \end{aligned}$$

The probabilities are computed using Johnson and Kotz (1970, equation 3.20).

For the METHOD=NORMAL option, the test statistic  $Z_L(X)$  is assumed to have the normal distribution

$$N\left(\frac{N^{\frac{1}{2}}(p - \theta_L)}{[\theta_L(1 - \theta_L)]^{\frac{1}{2}}}, \frac{p(1 - p)}{\theta_L(1 - \theta_L)}\right)$$

and the test statistic  $Z_U(X)$  is assumed to have the normal distribution

$$N\left(\frac{N^{\frac{1}{2}}(p - \theta_U)}{[\theta_U(1 - \theta_U)]^{\frac{1}{2}}}, \frac{p(1 - p)}{\theta_U(1 - \theta_U)}\right)$$

(see Chow, Shao, and Wang (2003, p. 84)). The approximate power is computed as

$$\text{power} = \Phi\left(\frac{z_\alpha - \sqrt{N} \frac{p - \theta_U}{\sqrt{\theta_U(1 - \theta_U)}}}{\sqrt{\frac{p(1 - p)}{\theta_U(1 - \theta_U)}}}\right) + \Phi\left(\frac{z_\alpha + \sqrt{N} \frac{p - \theta_L}{\sqrt{\theta_L(1 - \theta_L)}}}{\sqrt{\frac{p(1 - p)}{\theta_L(1 - \theta_L)}}}\right) - 1$$

The approximate sample size is computed by numerically inverting the power formula, using the sample size estimate  $N_0$  of Chow, Shao, and Wang (2003, p. 85) as an initial guess:

$$N_0 = p(1 - p) \left( \frac{z_{1-\alpha} + z_{(1+\text{power})/2}}{0.5(\theta_U - \theta_L) - |p - 0.5(\theta_L + \theta_U)|} \right)^2$$

### ***z Equivalence Test for Binomial Proportion Using Sample Variance (TEST=EQUIV\_Z VAREST=SAMPLE)***

The hypotheses for the equivalence test are

$$H_0: p < \theta_L \quad \text{or} \quad p > \theta_U$$

$$H_1: \theta_L \leq p \leq \theta_U$$

where  $\theta_L$  and  $\theta_U$  are the lower and upper equivalence bounds, respectively.

The analysis is the two one-sided tests (TOST) procedure as described in Chow, Shao, and Wang (2003) on p. 84.

Two different hypothesis tests are carried out:

$$H_{a0}: p < \theta_L$$

$$H_{a1}: p \geq \theta_L$$

and

$$H_{b0}: p > \theta_U$$

$$H_{b1}: p \leq \theta_U$$

If  $H_{a0}$  is rejected in favor of  $H_{a1}$  and  $H_{b0}$  is rejected in favor of  $H_{b1}$ , then  $H_0$  is rejected in favor of  $H_1$ .

The test statistic for the test of  $H_{a0}$  versus  $H_{a1}$  is

$$Z_{sL}(X) = \frac{X - N\theta_L}{[N\hat{p}(1 - \hat{p})]^{\frac{1}{2}}}$$

where  $\hat{p} = X/N$ .

The test statistic for the test of  $H_{b0}$  versus  $H_{b1}$  is

$$Z_{sU}(X) = \frac{X - N\theta_U}{[N\hat{p}(1 - \hat{p})]^{\frac{1}{2}}}$$

For the METHOD=EXACT option, let  $C_U$  denote the critical value of the exact upper one-sided test of  $H_{a0}$  versus  $H_{a1}$  using  $Z_{sL}(X)$ . This critical value is computed in the section “z Test for Binomial Proportion Using Sample Variance (TEST=Z VAREST=SAMPLE)” on page 6038. Similarly, let  $C_L$  denote the critical value of the exact lower one-sided test of  $H_{b0}$  versus  $H_{b1}$  using  $Z_{sU}(X)$ . Both of these tests are rejected if and only if  $C_U \leq X \leq C_L$ . Thus, the exact power of the equivalence test is

$$\begin{aligned} \text{power} &= P(C_U \leq X \leq C_L) \\ &= P(X \geq C_U) - P(X \geq C_L + 1) \end{aligned}$$

The probabilities are computed using Johnson and Kotz (1970, equation 3.20).

For the METHOD=NORMAL option, the test statistic  $Z_{sL}(X)$  is assumed to have the normal distribution

$$N\left(\frac{N^{\frac{1}{2}}(p - \theta_L)}{[p(1-p)]^{\frac{1}{2}}}, 1\right)$$

and the test statistic  $Z_{sU}(X)$  is assumed to have the normal distribution

$$N\left(\frac{N^{\frac{1}{2}}(p - \theta_U)}{[p(1-p)]^{\frac{1}{2}}}, 1\right)$$

(see Chow, Shao, and Wang (2003), p. 84).

The approximate power is computed as

$$\text{power} = \Phi\left(z_\alpha - \sqrt{N} \frac{p - \theta_U}{\sqrt{p(1-p)}}\right) + \Phi\left(z_\alpha + \sqrt{N} \frac{p - \theta_L}{\sqrt{p(1-p)}}\right) - 1$$

The approximate sample size is computed by numerically inverting the power formula, using the sample size estimate  $N_0$  of Chow, Shao, and Wang (2003, p. 85) as an initial guess:

$$N_0 = p(1-p) \left( \frac{z_{1-\alpha} + z_{(1+\text{power})/2}}{0.5(\theta_U - \theta_L) - |p - 0.5(\theta_L + \theta_U)|} \right)^2$$

### ***z Equivalence Test for Binomial Proportion with Continuity Adjustment Using Null Variance (TEST=EQUIV\_ADJZ VAREST=NULL)***

The hypotheses for the equivalence test are

$$H_0: p < \theta_L \quad \text{or} \quad p > \theta_U$$

$$H_1: \theta_L \leq p \leq \theta_U$$

where  $\theta_L$  and  $\theta_U$  are the lower and upper equivalence bounds, respectively.

The analysis is the two one-sided tests (TOST) procedure as described in Chow, Shao, and Wang (2003) on p. 84, but using the null variance instead of the sample variance.

Two different hypothesis tests are carried out:

$$H_{a0}: p < \theta_L$$

$$H_{a1}: p \geq \theta_L$$



and

$$H_{b0}: p > \theta_U$$

$$H_{b1}: p \leq \theta_U$$

If  $H_{a0}$  is rejected in favor of  $H_{a1}$  and  $H_{b0}$  is rejected in favor of  $H_{b1}$ , then  $H_0$  is rejected in favor of  $H_1$ .

The test statistic for the test of  $H_{a0}$  versus  $H_{a1}$  is

$$Z_{cL}(X) = \frac{X - N\theta_L + 0.5(1_{\{X < N\theta_L\}}) - 0.5(1_{\{X > N\theta_L\}})}{\left[ N\hat{\theta}_L(1 - \hat{\theta}_L) \right]^{\frac{1}{2}}}$$

where  $\hat{p} = X/N$ .

The test statistic for the test of  $H_{b0}$  versus  $H_{b1}$  is

$$Z_{cU}(X) = \frac{X - N\theta_U + 0.5(1_{\{X < N\theta_U\}}) - 0.5(1_{\{X > N\theta_U\}})}{\left[ N\hat{\theta}_U(1 - \hat{\theta}_U) \right]^{\frac{1}{2}}}$$

For the METHOD=EXACT option, let  $C_U$  denote the critical value of the exact upper one-sided test of  $H_{a0}$  versus  $H_{a1}$  using  $Z_{cL}(X)$ . This critical value is computed in the section “z Test for Binomial Proportion with Continuity Adjustment Using Null Variance (TEST=ADJZ VAREST=NULL)” on page 6039. Similarly, let  $C_L$  denote the critical value of the exact lower one-sided test of  $H_{b0}$  versus  $H_{b1}$  using  $Z_{cU}(X)$ . Both of these tests are rejected if and only if  $C_U \leq X \leq C_L$ . Thus, the exact power of the equivalence test is

$$\begin{aligned} \text{power} &= P(C_U \leq X \leq C_L) \\ &= P(X \geq C_U) - P(X \geq C_L + 1) \end{aligned}$$

The probabilities are computed using Johnson and Kotz (1970, equation 3.20).

For the METHOD=NORMAL option, the test statistic  $Z_{cL}(X)$  is assumed to have the normal distribution  $N(\mu_L, \sigma_L^2)$ , and  $Z_{cU}(X)$  is assumed to have the normal distribution  $N(\mu_U, \sigma_U^2)$ , where  $\mu_L$ ,  $\mu_U$ ,  $\sigma_L^2$ , and  $\sigma_U^2$  are derived as follows.

For convenience of notation, define

$$k_L = \frac{1}{2\sqrt{N\theta_L(1 - \theta_L)}}$$

$$k_U = \frac{1}{2\sqrt{N\theta_U(1 - \theta_U)}}$$

Then

$$\begin{aligned} E[Z_{cL}(X)] &\approx 2k_L Np - 2k_L N\theta_L + k_L P(X < N\theta_L) - k_L P(X > N\theta_L) \\ E[Z_{cU}(X)] &\approx 2k_U Np - 2k_U N\theta_U + k_U P(X < N\theta_U) - k_U P(X > N\theta_U) \end{aligned}$$

and

$$\begin{aligned}\text{Var}[Z_{cL}(X)] &\approx 4k_L^2 Np(1-p) + k_L^2 [1 - P(X = N\theta_L)] - k_L^2 [P(X < N\theta_L) - P(X > N\theta_L)]^2 \\ &\quad + 4k_L^2 [E(X1_{\{X < N\theta_L\}}) - E(X1_{\{X > N\theta_L\}})] - 4k_L^2 Np [P(X < N\theta_L) - P(X > N\theta_L)] \\ \text{Var}[Z_{cU}(X)] &\approx 4k_U^2 Np(1-p) + k_U^2 [1 - P(X = N\theta_U)] - k_U^2 [P(X < N\theta_U) - P(X > N\theta_U)]^2 \\ &\quad + 4k_U^2 [E(X1_{\{X < N\theta_U\}}) - E(X1_{\{X > N\theta_U\}})] - 4k_U^2 Np [P(X < N\theta_U) - P(X > N\theta_U)]\end{aligned}$$

The probabilities  $P(X = N\theta_L)$ ,  $P(X < N\theta_L)$ ,  $P(X > N\theta_L)$ ,  $P(X = N\theta_U)$ ,  $P(X < N\theta_U)$ , and  $P(X > N\theta_U)$  and the truncated expectations  $E(X1_{\{X < N\theta_L\}})$ ,  $E(X1_{\{X > N\theta_L\}})$ ,  $E(X1_{\{X < N\theta_U\}})$ , and  $E(X1_{\{X > N\theta_U\}})$  are approximated by assuming the normal-approximate distribution of  $X$ ,  $N(Np, Np(1-p))$ . Letting  $\phi(\cdot)$  and  $\Phi(\cdot)$  denote the standard normal PDF and CDF, respectively, and defining  $d_L$  and  $d_U$  as

$$\begin{aligned}d_L &= \frac{N\theta_L - Np}{[Np(1-p)]^{\frac{1}{2}}} \\ d_U &= \frac{N\theta_U - Np}{[Np(1-p)]^{\frac{1}{2}}}\end{aligned}$$

the terms are computed as follows:

$$\begin{aligned}P(X = N\theta_L) &= 0 \\ P(X = N\theta_U) &= 0 \\ P(X < N\theta_L) &= \Phi(d_L) \\ P(X < N\theta_U) &= \Phi(d_U) \\ P(X > N\theta_L) &= 1 - \Phi(d_L) \\ P(X > N\theta_U) &= 1 - \Phi(d_U) \\ E(X1_{\{X < N\theta_L\}}) &= Np\Phi(d_L) - [Np(1-p)]^{\frac{1}{2}} \phi(d_L) \\ E(X1_{\{X < N\theta_U\}}) &= Np\Phi(d_U) - [Np(1-p)]^{\frac{1}{2}} \phi(d_U) \\ E(X1_{\{X > N\theta_L\}}) &= Np[1 - \Phi(d_L)] + [Np(1-p)]^{\frac{1}{2}} \phi(d_L) \\ E(X1_{\{X > N\theta_U\}}) &= Np[1 - \Phi(d_U)] + [Np(1-p)]^{\frac{1}{2}} \phi(d_U)\end{aligned}$$

The mean and variance of  $Z_{cL}(X)$  and  $Z_{cU}(X)$  are thus approximated by

$$\begin{aligned}\mu_L &= k_L [2Np - 2N\theta_L + 2\Phi(d_L) - 1] \\ \mu_U &= k_U [2Np - 2N\theta_U + 2\Phi(d_U) - 1]\end{aligned}$$

and

$$\begin{aligned}\sigma_L^2 &= 4k_L^2 [Np(1-p) + \Phi(d_L)(1 - \Phi(d_L)) - 2(Np(1-p))^{\frac{1}{2}} \phi(d_L)] \\ \sigma_U^2 &= 4k_U^2 [Np(1-p) + \Phi(d_U)(1 - \Phi(d_U)) - 2(Np(1-p))^{\frac{1}{2}} \phi(d_U)]\end{aligned}$$

The approximate power is computed as

$$\text{power} = \Phi\left(\frac{z_\alpha - \mu_U}{\sigma_U}\right) + \Phi\left(\frac{z_\alpha + \mu_L}{\sigma_L}\right) - 1$$

The approximate sample size is computed by numerically inverting the power formula.

***z Equivalence Test for Binomial Proportion with Continuity Adjustment Using Sample Variance (TEST=EQUIV\_ADJZ VAREST=SAMPLE)***

The hypotheses for the equivalence test are

$$H_0: p < \theta_L \quad \text{or} \quad p > \theta_U$$

$$H_1: \theta_L \leq p \leq \theta_U$$

where  $\theta_L$  and  $\theta_U$  are the lower and upper equivalence bounds, respectively.

The analysis is the two one-sided tests (TOST) procedure as described in Chow, Shao, and Wang (2003) on p. 84.

Two different hypothesis tests are carried out:

$$H_{a0}: p < \theta_L$$

$$H_{a1}: p \geq \theta_L$$

and

$$H_{b0}: p > \theta_U$$

$$H_{b1}: p \leq \theta_U$$

If  $H_{a0}$  is rejected in favor of  $H_{a1}$  and  $H_{b0}$  is rejected in favor of  $H_{b1}$ , then  $H_0$  is rejected in favor of  $H_1$ .

The test statistic for the test of  $H_{a0}$  versus  $H_{a1}$  is

$$Z_{csL}(X) = \frac{X - N\theta_L + 0.5(1_{\{X < N\theta_L\}}) - 0.5(1_{\{X > N\theta_L\}})}{[N\hat{p}(1 - \hat{p})]^{1/2}}$$

where  $\hat{p} = X/N$ .

The test statistic for the test of  $H_{b0}$  versus  $H_{b1}$  is

$$Z_{csU}(X) = \frac{X - N\theta_U + 0.5(1_{\{X < N\theta_U\}}) - 0.5(1_{\{X > N\theta_U\}})}{[N\hat{p}(1 - \hat{p})]^{1/2}}$$

For the METHOD=EXACT option, let  $C_U$  denote the critical value of the exact upper one-sided test of  $H_{a0}$  versus  $H_{a1}$  using  $Z_{csL}(X)$ . This critical value is computed in the section “z Test for Binomial Proportion with Continuity Adjustment Using Sample Variance (TEST=ADJZ VAREST=SAMPLE)” on page 6040. Similarly, let  $C_L$  denote the critical value of the exact lower one-sided test of  $H_{b0}$  versus  $H_{b1}$  using  $Z_{csU}(X)$ . Both of these tests are rejected if and only if  $C_U \leq X \leq C_L$ . Thus, the exact power of the equivalence test is

$$\begin{aligned} \text{power} &= P(C_U \leq X \leq C_L) \\ &= P(X \geq C_U) - P(X \geq C_L + 1) \end{aligned}$$

The probabilities are computed using Johnson and Kotz (1970, equation 3.20).

For the METHOD=NORMAL option, the test statistic  $Z_{csL}(X)$  is assumed to have the normal distribution  $N(\mu_L, \sigma_L^2)$ , and  $Z_{csU}(X)$  is assumed to have the normal distribution  $N(\mu_U, \sigma_U^2)$ , where  $\mu_L, \mu_U, \sigma_L^2$  and  $\sigma_U^2$  are derived as follows.

For convenience of notation, define

$$k = \frac{1}{2\sqrt{Np(1-p)}}$$

Then

$$E[Z_{csL}(X)] \approx 2kNp - 2kN\theta_L + kP(X < N\theta_L) - kP(X > N\theta_L)$$

$$E[Z_{csU}(X)] \approx 2kNp - 2kN\theta_U + kP(X < N\theta_U) - kP(X > N\theta_U)$$

and

$$\begin{aligned} \text{Var}[Z_{csL}(X)] \approx & 4k^2Np(1-p) + k^2[1 - P(X = N\theta_L)] - k^2[P(X < N\theta_L) - P(X > N\theta_L)]^2 \\ & + 4k^2[E(X1_{\{X < N\theta_L\}}) - E(X1_{\{X > N\theta_L\}})] - 4k^2Np[P(X < N\theta_L) - P(X > N\theta_L)] \end{aligned}$$

$$\begin{aligned} \text{Var}[Z_{csU}(X)] \approx & 4k^2Np(1-p) + k^2[1 - P(X = N\theta_U)] - k^2[P(X < N\theta_U) - P(X > N\theta_U)]^2 \\ & + 4k^2[E(X1_{\{X < N\theta_U\}}) - E(X1_{\{X > N\theta_U\}})] - 4k^2Np[P(X < N\theta_U) - P(X > N\theta_U)] \end{aligned}$$

The probabilities  $P(X = N\theta_L)$ ,  $P(X < N\theta_L)$ ,  $P(X > N\theta_L)$ ,  $P(X = N\theta_U)$ ,  $P(X < N\theta_U)$ , and  $P(X > N\theta_U)$  and the truncated expectations  $E(X1_{\{X < N\theta_L\}})$ ,  $E(X1_{\{X > N\theta_L\}})$ ,  $E(X1_{\{X < N\theta_U\}})$ , and  $E(X1_{\{X > N\theta_U\}})$  are approximated by assuming the normal-approximate distribution of  $X$ ,  $N(Np, Np(1-p))$ . Letting  $\phi(\cdot)$  and  $\Phi(\cdot)$  denote the standard normal PDF and CDF, respectively, and defining  $d_L$  and  $d_U$  as

$$d_L = \frac{N\theta_L - Np}{[Np(1-p)]^{\frac{1}{2}}}$$

$$d_U = \frac{N\theta_U - Np}{[Np(1-p)]^{\frac{1}{2}}}$$

the terms are computed as follows:

$$P(X = N\theta_L) = 0$$

$$P(X = N\theta_U) = 0$$

$$P(X < N\theta_L) = \Phi(d_L)$$

$$P(X < N\theta_U) = \Phi(d_U)$$

$$P(X > N\theta_L) = 1 - \Phi(d_L)$$

$$P(X > N\theta_U) = 1 - \Phi(d_U)$$

$$E(X1_{\{X < N\theta_L\}}) = Np\Phi(d_L) - [Np(1-p)]^{\frac{1}{2}}\phi(d_L)$$

$$E(X1_{\{X < N\theta_U\}}) = Np\Phi(d_U) - [Np(1-p)]^{\frac{1}{2}}\phi(d_U)$$

$$E(X1_{\{X > N\theta_L\}}) = Np[1 - \Phi(d_L)] + [Np(1-p)]^{\frac{1}{2}}\phi(d_L)$$

$$E(X1_{\{X > N\theta_U\}}) = Np[1 - \Phi(d_U)] + [Np(1-p)]^{\frac{1}{2}}\phi(d_U)$$

The mean and variance of  $Z_{csL}(X)$  and  $Z_{csU}(X)$  are thus approximated by

$$\begin{aligned}\mu_L &= k [2Np - 2N\theta_L + 2\Phi(d_L) - 1] \\ \mu_U &= k [2Np - 2N\theta_U + 2\Phi(d_U) - 1]\end{aligned}$$

and

$$\begin{aligned}\sigma_L^2 &= 4k^2 \left[ Np(1-p) + \Phi(d_L)(1-\Phi(d_L)) - 2(Np(1-p))^{\frac{1}{2}}\phi(d_L) \right] \\ \sigma_U^2 &= 4k^2 \left[ Np(1-p) + \Phi(d_U)(1-\Phi(d_U)) - 2(Np(1-p))^{\frac{1}{2}}\phi(d_U) \right]\end{aligned}$$

The approximate power is computed as

$$\text{power} = \Phi\left(\frac{z_\alpha - \mu_U}{\sigma_U}\right) + \Phi\left(\frac{z_\alpha + \mu_L}{\sigma_L}\right) - 1$$

The approximate sample size is computed by numerically inverting the power formula.

#### **Wilson Score Confidence Interval for Binomial Proportion (CI=WILSON)**

The two-sided  $100(1-\alpha)\%$  confidence interval for  $p$  is

$$\frac{X + \frac{z_{1-\alpha/2}^2}{2}}{N + z_{1-\alpha/2}^2} \pm \frac{z_{1-\alpha/2} N^{\frac{1}{2}}}{N + z_{1-\alpha/2}^2} \left( \hat{p}(1-\hat{p}) + \frac{z_{1-\alpha/2}^2}{4N} \right)^{\frac{1}{2}}$$

So the half-width for the two-sided  $100(1-\alpha)\%$  confidence interval is

$$\text{half-width} = \frac{z_{1-\alpha/2} N^{\frac{1}{2}}}{N + z_{1-\alpha/2}^2} \left( \hat{p}(1-\hat{p}) + \frac{z_{1-\alpha/2}^2}{4N} \right)^{\frac{1}{2}}$$

Prob(Width) is calculated exactly by adding up the probabilities of observing each  $X \in \{1, \dots, N\}$  that produces a confidence interval whose half-width is at most a target value  $h$ :

$$\text{Prob(Width)} = \sum_{i=0}^N P(X = i) 1_{\text{half-width} < h}$$

For references and more details about this and all other confidence intervals associated with the **CI=** option, see “[Binomial Proportion](#)” on page 2565 of Chapter 38, “[The FREQ Procedure](#).”

**Agresti-Coull “Add  $k$  Successes and Failures” Confidence Interval for Binomial Proportion (CI=AGRESTICOULL)**

The two-sided  $100(1 - \alpha)\%$  confidence interval for  $p$  is

$$\frac{X + \frac{z_{1-\alpha/2}^2}{2}}{N + z_{1-\alpha/2}^2} \pm z_{1-\alpha/2} \left( \frac{\frac{X + \frac{z_{1-\alpha/2}^2}{2}}{N + z_{1-\alpha/2}^2} \left( 1 - \frac{X + \frac{z_{1-\alpha/2}^2}{2}}{N + z_{1-\alpha/2}^2} \right)}{N + z_{1-\alpha/2}^2} \right)^{\frac{1}{2}}$$

So the half-width for the two-sided  $100(1 - \alpha)\%$  confidence interval is

$$\text{half-width} = z_{1-\alpha/2} \left( \frac{\frac{X + \frac{z_{1-\alpha/2}^2}{2}}{N + z_{1-\alpha/2}^2} \left( 1 - \frac{X + \frac{z_{1-\alpha/2}^2}{2}}{N + z_{1-\alpha/2}^2} \right)}{N + z_{1-\alpha/2}^2} \right)^{\frac{1}{2}}$$

Prob(Width) is calculated exactly by adding up the probabilities of observing each  $X \in \{1, \dots, N\}$  that produces a confidence interval whose half-width is at most a target value  $h$ :

$$\text{Prob(Width)} = \sum_{i=0}^N P(X = i) 1_{\text{half-width} < h}$$

**Jeffreys Confidence Interval for Binomial Proportion (CI=JEFFREYS)**

The two-sided  $100(1 - \alpha)\%$  confidence interval for  $p$  is

$$[L_J(X), U_J(X)]$$

where

$$L_J(X) = \begin{cases} 0, & X = 0 \\ \text{Beta}_{\alpha/2; X+1/2, N-X+1/2}, & X > 0 \end{cases}$$

and

$$U_J(X) = \begin{cases} \text{Beta}_{1-\alpha/2; X+1/2, N-X+1/2}, & X < N \\ 1, & X = N \end{cases}$$

The half-width of this two-sided  $100(1 - \alpha)\%$  confidence interval is defined as half the width of the full interval:

$$\text{half-width} = \frac{1}{2} (U_J(X) - L_J(X))$$

Prob(Width) is calculated exactly by adding up the probabilities of observing each  $X \in \{1, \dots, N\}$  that produces a confidence interval whose half-width is at most a target value  $h$ :

$$\text{Prob(Width)} = \sum_{i=0}^N P(X = i) 1_{\text{half-width} < h}$$

### **Exact Clopper-Pearson Confidence Interval for Binomial Proportion (CI=EXACT)**

The two-sided  $100(1 - \alpha)\%$  confidence interval for  $p$  is

$$[L_E(X), U_E(X)]$$

where

$$L_E(X) = \begin{cases} 0, & X = 0 \\ \text{Beta}_{\alpha/2; X, N-X+1}, & X > 0 \end{cases}$$

and

$$U_E(X) = \begin{cases} \text{Beta}_{1-\alpha/2; X+1, N-X}, & X < N \\ 1, & X = N \end{cases}$$

The half-width of this two-sided  $100(1 - \alpha)\%$  confidence interval is defined as half the width of the full interval:

$$\text{half-width} = \frac{1}{2} (U_E(X) - L_E(X))$$

Prob(Width) is calculated exactly by adding up the probabilities of observing each  $X \in \{1, \dots, N\}$  that produces a confidence interval whose half-width is at most a target value  $h$ :

$$\text{Prob(Width)} = \sum_{i=0}^N P(X = i) 1_{\text{half-width} < h}$$

**Wald Confidence Interval for Binomial Proportion (CI=WALD)**

The two-sided  $100(1 - \alpha)\%$  confidence interval for  $p$  is

$$\hat{p} \pm z_{1-\alpha/2} \left( \frac{\hat{p}(1 - \hat{p})}{N} \right)^{\frac{1}{2}}$$

So the half-width for the two-sided  $100(1 - \alpha)\%$  confidence interval is

$$\text{half-width} = z_{1-\alpha/2} \left( \frac{\hat{p}(1 - \hat{p})}{N} \right)^{\frac{1}{2}}$$

Prob(Width) is calculated exactly by adding up the probabilities of observing each  $X \in \{1, \dots, N\}$  that produces a confidence interval whose half-width is at most a target value  $h$ :

$$\text{Prob(Width)} = \sum_{i=0}^N P(X = i) 1_{\text{half-width} < h}$$

**Continuity-Corrected Wald Confidence Interval for Binomial Proportion (CI=WALD\_CORRECT)**

The two-sided  $100(1 - \alpha)\%$  confidence interval for  $p$  is

$$\hat{p} \pm \left[ z_{1-\alpha/2} \left( \frac{\hat{p}(1 - \hat{p})}{N} \right)^{\frac{1}{2}} + \frac{1}{2N} \right]$$

So the half-width for the two-sided  $100(1 - \alpha)\%$  confidence interval is

$$\text{half-width} = z_{1-\alpha/2} \left( \frac{\hat{p}(1 - \hat{p})}{N} \right)^{\frac{1}{2}} + \frac{1}{2N}$$

Prob(Width) is calculated exactly by adding up the probabilities of observing each  $X \in \{1, \dots, N\}$  that produces a confidence interval whose half-width is at most a target value  $h$ :

$$\text{Prob(Width)} = \sum_{i=0}^N P(X = i) 1_{\text{half-width} < h}$$



## Analyses in the ONESAMPLEMEANS Statement

### One-Sample $t$ Test (TEST=T)

The hypotheses for the one-sample  $t$  test are

$$H_0: \mu = \mu_0$$

$$H_1: \begin{cases} \mu \neq \mu_0, & \text{two-sided} \\ \mu > \mu_0, & \text{upper one-sided} \\ \mu < \mu_0, & \text{lower one-sided} \end{cases}$$

The test assumes normally distributed data and requires  $N \geq 2$ . The test statistics are

$$t = N^{\frac{1}{2}} \left( \frac{\bar{x} - \mu_0}{s} \right) \sim t(N - 1, \delta)$$

$$t^2 \sim F(1, N - 1, \delta^2)$$

where  $\bar{x}$  is the sample mean,  $s$  is the sample standard deviation, and

$$\delta = N^{\frac{1}{2}} \left( \frac{\mu - \mu_0}{\sigma} \right)$$

The test is

$$\text{Reject } H_0 \quad \text{if } \begin{cases} t^2 \geq F_{1-\alpha}(1, N - 1), & \text{two-sided} \\ t \geq t_{1-\alpha}(N - 1), & \text{upper one-sided} \\ t \leq t_{\alpha}(N - 1), & \text{lower one-sided} \end{cases}$$

Exact power computations for  $t$  tests are discussed in O'Brien and Muller (1993, Section 8.2), although not specifically for the one-sample case. The power is based on the noncentral  $t$  and  $F$  distributions:

$$\text{power} = \begin{cases} P(F(1, N - 1, \delta^2) \geq F_{1-\alpha}(1, N - 1)), & \text{two-sided} \\ P(t(N - 1, \delta) \geq t_{1-\alpha}(N - 1)), & \text{upper one-sided} \\ P(t(N - 1, \delta) \leq t_{\alpha}(N - 1)), & \text{lower one-sided} \end{cases}$$

Solutions for  $N$ ,  $\alpha$ , and  $\delta$  are obtained by numerically inverting the power equation. Closed-form solutions for other parameters, in terms of  $\delta$ , are as follows:

$$\mu = \delta \sigma N^{-\frac{1}{2}} + \mu_0$$

$$\sigma = \begin{cases} \delta^{-1} N^{\frac{1}{2}} (\mu - \mu_0), & |\delta| > 0 \\ \text{undefined}, & \text{otherwise} \end{cases}$$

### One-Sample $t$ Test with Lognormal Data (TEST=T DIST=LOGNORMAL)

The lognormal case is handled by reexpressing the analysis equivalently as a normality-based test on the log-transformed data, by using properties of the lognormal distribution as discussed in Johnson, Kotz, and Balakrishnan (1994, Chapter 14). The approaches in the section "One-Sample  $t$  Test (TEST=T)" on page 6054 then apply.

In contrast to the usual  $t$  test on normal data, the hypotheses with lognormal data are defined in terms of geometric means rather than arithmetic means. This is because the transformation of a null arithmetic mean of lognormal data to the normal scale depends on the unknown coefficient of variation, resulting in an ill-defined hypothesis on the log-transformed data. Geometric means transform cleanly and are more natural for lognormal data.

The hypotheses for the one-sample  $t$  test with lognormal data are

$$H_0: \frac{\gamma}{\gamma_0} = 1$$

$$H_1: \begin{cases} \frac{\gamma}{\gamma_0} \neq 1, & \text{two-sided} \\ \frac{\gamma}{\gamma_0} > 1, & \text{upper one-sided} \\ \frac{\gamma}{\gamma_0} < 1, & \text{lower one-sided} \end{cases}$$

Let  $\mu^*$  and  $\sigma^*$  be the (arithmetic) mean and standard deviation of the normal distribution of the log-transformed data. The hypotheses can be rewritten as follows:

$$H_0: \mu^* = \log(\gamma_0)$$

$$H_1: \begin{cases} \mu^* \neq \log(\gamma_0), & \text{two-sided} \\ \mu^* > \log(\gamma_0), & \text{upper one-sided} \\ \mu^* < \log(\gamma_0), & \text{lower one-sided} \end{cases}$$

where  $\mu^* = \log(\gamma)$ .

The test assumes lognormally distributed data and requires  $N \geq 2$ .

The power is

$$\text{power} = \begin{cases} P(F(1, N-1, \delta^2) \geq F_{1-\alpha}(1, N-1)), & \text{two-sided} \\ P(t(N-1, \delta) \geq t_{1-\alpha}(N-1)), & \text{upper one-sided} \\ P(t(N-1, \delta) \leq t_{\alpha}(N-1)), & \text{lower one-sided} \end{cases}$$

where

$$\delta = N^{\frac{1}{2}} \left( \frac{\mu^* - \log(\gamma_0)}{\sigma^*} \right)$$

$$\sigma^* = [\log(\text{CV}^2 + 1)]^{\frac{1}{2}}$$

### **Equivalence Test for Mean of Normal Data (TEST=EQUIV DIST=NORMAL)**

The hypotheses for the equivalence test are

$$H_0: \mu < \theta_L \quad \text{or} \quad \mu > \theta_U$$

$$H_1: \theta_L \leq \mu \leq \theta_U$$

The analysis is the two one-sided tests (TOST) procedure of Schuirmann (1987). The test assumes normally distributed data and requires  $N \geq 2$ . Phillips (1990) derives an expression for the exact power assuming a two-sample balanced design; the results are easily adapted to a one-sample design:

$$\text{power} = Q_{N-1} \left( (-t_{1-\alpha}(N-1)), \frac{\mu - \theta_U}{\sigma N^{-\frac{1}{2}}}; 0, \frac{(N-1)^{\frac{1}{2}}(\theta_U - \theta_L)}{2\sigma N^{-\frac{1}{2}}(t_{1-\alpha}(N-1))} \right) - \\ Q_{N-1} \left( (t_{1-\alpha}(N-1)), \frac{\mu - \theta_L}{\sigma N^{-\frac{1}{2}}}; 0, \frac{(N-1)^{\frac{1}{2}}(\theta_U - \theta_L)}{2\sigma N^{-\frac{1}{2}}(t_{1-\alpha}(N-1))} \right)$$

where  $Q(\cdot, \cdot; \cdot, \cdot)$  is Owen's Q function, defined in the section "Common Notation" on page 6027.

### **Equivalence Test for Mean of Lognormal Data (TEST=EQUIV DIST=LOGNORMAL)**

The lognormal case is handled by reexpressing the analysis equivalently as a normality-based test on the log-transformed data, by using properties of the lognormal distribution as discussed in Johnson, Kotz, and Balakrishnan (1994, Chapter 14). The approaches in the section "Equivalence Test for Mean of Normal Data (TEST=EQUIV DIST=NORMAL)" on page 6055 then apply.

In contrast to the additive equivalence test on normal data, the hypotheses with lognormal data are defined in terms of geometric means rather than arithmetic means. This is because the transformation of an arithmetic mean of lognormal data to the normal scale depends on the unknown coefficient of variation, resulting in an ill-defined hypothesis on the log-transformed data. Geometric means transform cleanly and are more natural for lognormal data.

The hypotheses for the equivalence test are

$$H_0: \gamma \leq \theta_L \quad \text{or} \quad \gamma \geq \theta_U$$

$$H_1: \theta_L < \gamma < \theta_U$$

$$\text{where } 0 < \theta_L < \theta_U$$

The analysis is the two one-sided tests (TOST) procedure of Schuirmann (1987) on the log-transformed data. The test assumes lognormally distributed data and requires  $N \geq 2$ . Diletti, Hauschke, and Steinijans (1991) derive an expression for the exact power assuming a crossover design; the results are easily adapted to a one-sample design:

$$\text{power} = Q_{N-1} \left( (-t_{1-\alpha}(N-1)), \frac{\log(\gamma) - \log(\theta_U)}{\sigma^* N^{-\frac{1}{2}}}; 0, \frac{(N-1)^{\frac{1}{2}}(\log(\theta_U) - \log(\theta_L))}{2\sigma^* N^{-\frac{1}{2}}(t_{1-\alpha}(N-1))} \right) - \\ Q_{N-1} \left( (t_{1-\alpha}(N-1)), \frac{\log(\gamma) - \log(\theta_L)}{\sigma^* N^{-\frac{1}{2}}}; 0, \frac{(N-1)^{\frac{1}{2}}(\log(\theta_U) - \log(\theta_L))}{2\sigma^* N^{-\frac{1}{2}}(t_{1-\alpha}(N-1))} \right)$$

where

$$\sigma^* = [\log(\text{CV}^2 + 1)]^{\frac{1}{2}}$$

is the standard deviation of the log-transformed data, and  $Q(\cdot, \cdot; \cdot, \cdot)$  is Owen's Q function, defined in the section "Common Notation" on page 6027.

### Confidence Interval for Mean (CI=T)

This analysis of precision applies to the standard  $t$ -based confidence interval:

$$\begin{cases} \left[ \bar{x} - t_{1-\frac{\alpha}{2}}(N-1)\frac{s}{\sqrt{N}}, \bar{x} + t_{1-\frac{\alpha}{2}}(N-1)\frac{s}{\sqrt{N}} \right], & \text{two-sided} \\ \left[ \bar{x} - t_{1-\alpha}(N-1)\frac{s}{\sqrt{N}}, \infty \right), & \text{upper one-sided} \\ \left( -\infty, \bar{x} + t_{1-\alpha}(N-1)\frac{s}{\sqrt{N}} \right], & \text{lower one-sided} \end{cases}$$

where  $\bar{x}$  is the sample mean and  $s$  is the sample standard deviation. The “half-width” is defined as the distance from the point estimate  $\bar{x}$  to a finite endpoint,

$$\text{half-width} = \begin{cases} t_{1-\frac{\alpha}{2}}(N-1)\frac{s}{\sqrt{N}}, & \text{two-sided} \\ t_{1-\alpha}(N-1)\frac{s}{\sqrt{N}}, & \text{one-sided} \end{cases}$$

A “valid” confidence interval captures the true mean. The exact probability of obtaining at most the target confidence interval half-width  $h$ , unconditional or conditional on validity, is given by Beal (1989):

$$\begin{aligned} \Pr(\text{half-width} \leq h) &= \begin{cases} P\left(\chi^2(N-1) \leq \frac{h^2 N(N-1)}{\sigma^2(t_{1-\frac{\alpha}{2}}^2(N-1))}\right), & \text{two-sided} \\ P\left(\chi^2(N-1) \leq \frac{h^2 N(N-1)}{\sigma^2(t_{1-\alpha}^2(N-1))}\right), & \text{one-sided} \end{cases} \\ \Pr(\text{half-width} \leq h \mid \text{validity}) &= \begin{cases} \left(\frac{1}{1-\alpha}\right) 2 \left[ Q_{N-1}\left((t_{1-\frac{\alpha}{2}}(N-1)), 0; 0, b_1\right) - Q_{N-1}(0, 0; 0, b_1) \right], & \text{two-sided} \\ \left(\frac{1}{1-\alpha}\right) Q_{N-1}\left((t_{1-\alpha}(N-1)), 0; 0, b_1\right), & \text{one-sided} \end{cases} \end{aligned}$$

where

$$b_1 = \frac{h(N-1)^{\frac{1}{2}}}{\sigma(t_{1-\frac{\alpha}{2}}(N-1))N^{-\frac{1}{2}}}$$

$c$  = number of sides

and  $Q(\cdot, \cdot; \cdot, \cdot)$  is Owen’s Q function, defined in the section “Common Notation” on page 6027.

A “quality” confidence interval is both sufficiently narrow (half-width  $\leq h$ ) and valid:

$$\begin{aligned} \Pr(\text{quality}) &= \Pr(\text{half-width} \leq h \text{ and validity}) \\ &= \Pr(\text{half-width} \leq h \mid \text{validity})(1 - \alpha) \end{aligned}$$

## Analyses in the ONEWAYANOVA Statement

### One-Degree-of-Freedom Contrast (TEST=CONTRAST)

The hypotheses are

$$\begin{aligned} H_0: c_1\mu_1 + \cdots + c_G\mu_G &= c_0 \\ H_1: \begin{cases} c_1\mu_1 + \cdots + c_G\mu_G \neq c_0, & \text{two-sided} \\ c_1\mu_1 + \cdots + c_G\mu_G > c_0, & \text{upper one-sided} \\ c_1\mu_1 + \cdots + c_G\mu_G < c_0, & \text{lower one-sided} \end{cases} \end{aligned}$$

where  $G$  is the number of groups,  $\{c_1, \dots, c_G\}$  are the contrast coefficients, and  $c_0$  is the null contrast value.

The test is the usual  $F$  test for a contrast in one-way ANOVA. It assumes normal data with common group variances and requires  $N \geq G + 1$  and  $n_i \geq 1$ .

O'Brien and Muller (1993, Section 8.2.3.2) give the exact power as

$$\text{power} = \begin{cases} P(F(1, N - G, \delta^2) \geq F_{1-\alpha}(1, N - G)), & \text{two-sided} \\ P(t(N - G, \delta) \geq t_{1-\alpha}(N - G)), & \text{upper one-sided} \\ P(t(N - G, \delta) \leq t_{\alpha}(N - G)), & \text{lower one-sided} \end{cases}$$

where

$$\delta = N^{\frac{1}{2}} \left( \frac{\sum_{i=1}^G c_i \mu_i - c_0}{\sigma \left( \sum_{i=1}^G \frac{c_i^2}{w_i} \right)^{\frac{1}{2}}} \right)$$

### Overall F Test (TEST=OVERALL)

The hypotheses are

$$H_0: \mu_1 = \mu_2 = \dots = \mu_G$$

$$H_1: \mu_i \neq \mu_j \text{ for some } i, j$$

where  $G$  is the number of groups.

The test is the usual overall  $F$  test for equality of means in one-way ANOVA. It assumes normal data with common group variances and requires  $N \geq G + 1$  and  $n_i \geq 1$ .

O'Brien and Muller (1993, Section 8.2.3.1) give the exact power as

$$\text{power} = P(F(G - 1, N - G, \lambda) \geq F_{1-\alpha}(G - 1, N - G))$$

where the noncentrality is

$$\lambda = N \left( \frac{\sum_{i=1}^G w_i (\mu_i - \bar{\mu})^2}{\sigma^2} \right)$$

and

$$\bar{\mu} = \sum_{i=1}^G w_i \mu_i$$

## Analyses in the PAIREDFREQ Statement

### Overview of Conditional McNemar tests

Notation:

|         |         | Case          |               |              |
|---------|---------|---------------|---------------|--------------|
|         |         | Failure       | Success       |              |
| Control | Failure | $n_{00}$      | $n_{01}$      | $n_{0\cdot}$ |
|         | Success | $n_{10}$      | $n_{11}$      | $n_{1\cdot}$ |
|         |         | $n_{\cdot 0}$ | $n_{\cdot 1}$ | $N$          |

$$n_{00} = \#\{\text{control=failure, case=failure}\}$$

$$n_{01} = \#\{\text{control=failure, case=success}\}$$

$$n_{10} = \#\{\text{control=success, case=failure}\}$$

$$n_{11} = \#\{\text{control=success, case=success}\}$$

$$N = n_{00} + n_{01} + n_{10} + n_{11}$$

$$n_D = n_{01} + n_{10} \equiv \# \text{ discordant pairs}$$

$$\hat{\pi}_{ij} = \frac{n_{ij}}{N}$$

$$\pi_{ij} = \text{theoretical population value of } \hat{\pi}_{ij}$$

$$\pi_{1\cdot} = \pi_{10} + \pi_{11}$$

$$\pi_{\cdot 1} = \pi_{01} + \pi_{11}$$

$$\phi = \text{Corr}(\text{control observation, case observation}) \quad (\text{within a pair})$$

$$\text{DPR} = \text{“discordant proportion ratio”} = \frac{\pi_{01}}{\pi_{10}}$$

$$\text{DPR}_0 = \text{null DPR}$$

Power formulas are given here in terms of the discordant proportions  $\pi_{10}$  and  $\pi_{01}$ . If the input is specified in terms of  $\{\pi_{1\cdot}, \pi_{\cdot 1}, \phi\}$ , then it can be converted into values for  $\{\pi_{10}, \pi_{01}\}$  as follows:

$$\pi_{01} = \pi_{\cdot 1}(1 - \pi_{1\cdot}) - \phi((1 - \pi_{1\cdot})\pi_{\cdot 1}(1 - \pi_{\cdot 1})\pi_{1\cdot})^{\frac{1}{2}}$$

$$\pi_{10} = \pi_{01} + \pi_{1\cdot} - \pi_{\cdot 1}$$

All McNemar tests covered in PROC POWER are *conditional*, meaning that  $n_D$  is assumed fixed at its observed value.

For the usual  $\text{DPR}_0 = 1$ , the hypotheses are

$$H_0: \pi_{\cdot 1} = \pi_{1\cdot}$$

$$H_1: \begin{cases} \pi_{\cdot 1} \neq \pi_{1\cdot}, & \text{two-sided} \\ \pi_{\cdot 1} > \pi_{1\cdot}, & \text{upper one-sided} \\ \pi_{\cdot 1} < \pi_{1\cdot}, & \text{lower one-sided} \end{cases}$$

The test statistic for both tests covered in PROC POWER (DIST=EXACT\_COND and DIST=NORMAL) is the McNemar statistic  $Q_M$ , which has the following form when  $DPR_0 = 1$ :

$$Q_{M_0} = \frac{(n_{01} - n_{10})^2}{n_{01} + n_{10}}$$

For the conditional McNemar tests, this is equivalent to the square of the  $Z(X)$  statistic for the test of a single proportion (normal approximation to binomial), where the proportion is  $\frac{\pi_{01}}{\pi_{01} + \pi_{10}}$ , the null is 0.5, and “ $N$ ” is  $n_D$  (see, for example, Schork and Williams 1980):

$$\begin{aligned} Z(X) &= \frac{n_{01} - n_D(0.5)}{[n_D 0.5(1 - 0.5)]^{\frac{1}{2}}} \sim N\left(\frac{n_D^{\frac{1}{2}}\left(\frac{\pi_{01}}{\pi_{01} + \pi_{10}} - 0.5\right)}{[0.5(1 - 0.5)]^{\frac{1}{2}}}, \frac{\frac{\pi_{01}}{\pi_{01} + \pi_{10}}\left(1 - \frac{\pi_{01}}{\pi_{01} + \pi_{10}}\right)}{0.5(1 - 0.5)}\right) \\ &= \frac{n_{01} - (n_{01} + n_{10})(0.5)}{[(n_{01} + n_{10})0.5(1 - 0.5)]^{\frac{1}{2}}} \\ &= \frac{n_{01} - n_{10}}{[n_{01} + n_{10}]^{\frac{1}{2}}} \\ &= \sqrt{Q_{M_0}} \end{aligned}$$

This can be generalized to a custom null for  $\frac{\pi_{01}}{\pi_{01} + \pi_{10}}$ , which is equivalent to specifying a custom null DPR:

$$\left[\frac{\pi_{01}}{\pi_{01} + \pi_{10}}\right]_0 \equiv \left[\frac{1}{1 + \frac{1}{\frac{\pi_{01}}{\pi_{10}}}}\right]_0 \equiv \frac{1}{1 + \frac{1}{DPR_0}}$$

So, a conditional McNemar test (asymptotic or exact) with a custom null is equivalent to the test of a single proportion  $p_1 \equiv \frac{\pi_{01}}{\pi_{01} + \pi_{10}}$  with a null value  $p_0 \equiv \frac{1}{1 + \frac{1}{DPR_0}}$ , with a sample size of  $n_D$ :

$$H_0: p_1 = p_0$$

$$H_1: \begin{cases} p_1 \neq p_0, & \text{two-sided} \\ p_1 > p_0, & \text{one-sided U} \\ p_1 < p_0, & \text{one-sided L} \end{cases}$$

which is equivalent to

$$H_0: DPR = DPR_0$$

$$H_1: \begin{cases} DPR \neq DPR_0, & \text{two-sided} \\ DPR > DPR_0, & \text{one-sided U} \\ DPR < DPR_0, & \text{one-sided L} \end{cases}$$

The general form of the test statistic is thus

$$Q_M = \frac{(n_{01} - n_D p_0)^2}{n_D p_0 (1 - p_0)}$$

The two most common conditional McNemar tests assume either the exact conditional distribution of  $Q_M$  (covered by the DIST=EXACT\_COND analysis) or a standard normal distribution for  $Q_M$  (covered by the DIST=NORMAL analysis).

**McNemar Exact Conditional Test (TEST=MCNEMAR DIST=EXACT\_COND)**

For DIST=EXACT\_COND, the power is calculated assuming that the test is conducted by using the exact conditional distribution of  $Q_M$  (conditional on  $n_D$ ). The power is calculated by first computing the conditional power for each possible  $n_D$ . The unconditional power is computed as a weighted average over all possible outcomes of  $n_D$ :

$$\text{power} = \sum_{n_D=0}^N P(n_D)P(\text{Reject } p_1 = p_0 | n_D)$$

where  $n_D \sim \text{Bin}(\pi_{01} + \pi_{10}, N)$ , and  $P(\text{Reject } p_1 = p_0 | n_D)$  is calculated by using the exact method in the section “Exact Test of a Binomial Proportion (TEST=EXACT)” on page 6036.

The achieved significance level, reported as “Actual Alpha” in the analysis, is computed in the same way except by using the actual alpha of the one-sample test in place of its power:

$$\text{actual alpha} = \sum_{n_D=0}^N P(n_D)\alpha^*(p_1, p_0 | n_D)$$

where  $\alpha^*(p_1, p_0 | n_D)$  is the actual alpha calculated by using the exact method in the section “Exact Test of a Binomial Proportion (TEST=EXACT)” on page 6036 with proportion  $p_1$ , null  $p_0$ , and sample size  $n_D$ .

**McNemar Normal Approximation Test (TEST=MCNEMAR DIST=NORMAL)**

For DIST=NORMAL, power is calculated assuming the test is conducted by using the normal-approximate distribution of  $Q_M$  (conditional on  $n_D$ ).

For the METHOD=EXACT option, the power is calculated in the same way as described in the section “McNemar Exact Conditional Test (TEST=MCNEMAR DIST=EXACT\_COND)” on page 6061, except that  $P(\text{Reject } p_1 = p_0 | n_D)$  is calculated by using the exact method in the section “z Test for Binomial Proportion Using Null Variance (TEST=Z VAREST=NULL)” on page 6037. The achieved significance level is calculated in the same way as described at the end of the section “McNemar Exact Conditional Test (TEST=MCNEMAR DIST=EXACT\_COND)” on page 6061.

For the METHOD=MIETTINEN option, approximate sample size for the one-sided cases is computed according to equation (5.6) in Miettinen (1968):

$$N = \frac{\left\{ z_{1-\alpha}(p_{10} + p_{01}) + z_{power} \left[ (p_{10} + p_{01})^2 - \frac{1}{4}(p_{01} - p_{10})^2(3 + p_{10} + p_{01}) \right]^{\frac{1}{2}} \right\}^2}{(p_{10} + p_{01})(p_{01} - p_{10})^2}$$

Approximate power for the one-sided cases is computed by solving the sample size equation for power, and approximate power for the two-sided case follows easily by summing the one-sided powers each at  $\alpha/2$ :

$$\text{power} = \begin{cases} \Phi \left( \frac{(p_{01} - p_{10})[N(p_{10} + p_{01})]^{\frac{1}{2}} - z_{1-\alpha}(p_{10} + p_{01})}{[(p_{10} + p_{01})^2 - \frac{1}{4}(p_{01} - p_{10})^2(3 + p_{10} + p_{01})]^{\frac{1}{2}}} \right), & \text{upper one-sided} \\ \Phi \left( \frac{-(p_{01} - p_{10})[N(p_{10} + p_{01})]^{\frac{1}{2}} - z_{1-\alpha}(p_{10} + p_{01})}{[(p_{10} + p_{01})^2 - \frac{1}{4}(p_{01} - p_{10})^2(3 + p_{10} + p_{01})]^{\frac{1}{2}}} \right), & \text{lower one-sided} \\ \Phi \left( \frac{(p_{01} - p_{10})[N(p_{10} + p_{01})]^{\frac{1}{2}} - z_{1-\frac{\alpha}{2}}(p_{10} + p_{01})}{[(p_{10} + p_{01})^2 - \frac{1}{4}(p_{01} - p_{10})^2(3 + p_{10} + p_{01})]^{\frac{1}{2}}} \right) + \\ \Phi \left( \frac{-(p_{01} - p_{10})[N(p_{10} + p_{01})]^{\frac{1}{2}} - z_{1-\frac{\alpha}{2}}(p_{10} + p_{01})}{[(p_{10} + p_{01})^2 - \frac{1}{4}(p_{01} - p_{10})^2(3 + p_{10} + p_{01})]^{\frac{1}{2}}} \right), & \text{two-sided} \end{cases}$$



The two-sided solution for  $N$  is obtained by numerically inverting the power equation.

In general, compared to METHOD=CONNOR, the METHOD=MIETTINEN approximation tends to be slightly more accurate but can be slightly anticonservative in the sense of underestimating sample size and overestimating power (Lachin 1992, p. 1250).

For the METHOD=CONNOR option, approximate sample size for the one-sided cases is computed according to equation (3) in Connor (1987):

$$N = \frac{\left\{ z_{1-\alpha}(p_{10} + p_{01})^{\frac{1}{2}} + z_{power} [p_{10} + p_{01} - (p_{01} - p_{10})^2]^{\frac{1}{2}} \right\}^2}{(p_{01} - p_{10})^2}$$

Approximate power for the one-sided cases is computed by solving the sample size equation for power, and approximate power for the two-sided case follows easily by summing the one-sided powers each at  $\alpha/2$ :

$$\text{power} = \begin{cases} \Phi \left( \frac{(p_{01} - p_{10})N^{\frac{1}{2}} - z_{1-\alpha}(p_{10} + p_{01})^{\frac{1}{2}}}{[p_{10} + p_{01} - (p_{01} - p_{10})^2]^{\frac{1}{2}}} \right), & \text{upper one-sided} \\ \Phi \left( \frac{-(p_{01} - p_{10})N^{\frac{1}{2}} - z_{1-\alpha}(p_{10} + p_{01})^{\frac{1}{2}}}{[p_{10} + p_{01} - (p_{01} - p_{10})^2]^{\frac{1}{2}}} \right), & \text{lower one-sided} \\ \Phi \left( \frac{(p_{01} - p_{10})N^{\frac{1}{2}} - z_{1-\frac{\alpha}{2}}(p_{10} + p_{01})^{\frac{1}{2}}}{[p_{10} + p_{01} - (p_{01} - p_{10})^2]^{\frac{1}{2}}} \right) + \\ \Phi \left( \frac{-(p_{01} - p_{10})N^{\frac{1}{2}} - z_{1-\frac{\alpha}{2}}(p_{10} + p_{01})^{\frac{1}{2}}}{[p_{10} + p_{01} - (p_{01} - p_{10})^2]^{\frac{1}{2}}} \right), & \text{two-sided} \end{cases}$$

The two-sided solution for  $N$  is obtained by numerically inverting the power equation.

In general, compared to METHOD=MIETTINEN, the METHOD=CONNOR approximation tends to be slightly less accurate but slightly conservative in the sense of overestimating sample size and underestimating power (Lachin 1992, p. 1250).

## Analyses in the PAIREDMEANS Statement

### Paired $t$ Test (TEST=DIFF)

The hypotheses for the paired  $t$  test are

$$H_0: \mu_{\text{diff}} = \mu_0$$

$$H_1: \begin{cases} \mu_{\text{diff}} \neq \mu_0, & \text{two-sided} \\ \mu_{\text{diff}} > \mu_0, & \text{upper one-sided} \\ \mu_{\text{diff}} < \mu_0, & \text{lower one-sided} \end{cases}$$

The test assumes normally distributed data and requires  $N \geq 2$ . The test statistics are

$$t = N^{\frac{1}{2}} \left( \frac{\bar{d} - \mu_0}{s_d} \right) \sim t(N - 1, \delta)$$

$$t^2 \sim F(1, N - 1, \delta^2)$$

where  $\bar{d}$  and  $s_d$  are the sample mean and standard deviation of the differences and

$$\delta = N^{\frac{1}{2}} \left( \frac{\mu_{\text{diff}} - \mu_0}{\sigma_{\text{diff}}} \right)$$

and

$$\sigma_{\text{diff}} = (\sigma_1^2 + \sigma_2^2 - 2\rho\sigma_1\sigma_2)^{\frac{1}{2}}$$

The test is

$$\text{Reject } H_0 \quad \text{if } \begin{cases} t^2 \geq F_{1-\alpha}(1, N-1), & \text{two-sided} \\ t \geq t_{1-\alpha}(N-1), & \text{upper one-sided} \\ t \leq t_{\alpha}(N-1), & \text{lower one-sided} \end{cases}$$

Exact power computations for  $t$  tests are given in O'Brien and Muller (1993, Section 8.2.2):

$$\text{power} = \begin{cases} P(F(1, N-1, \delta^2) \geq F_{1-\alpha}(1, N-1)), & \text{two-sided} \\ P(t(N-1, \delta) \geq t_{1-\alpha}(N-1)), & \text{upper one-sided} \\ P(t(N-1, \delta) \leq t_{\alpha}(N-1)), & \text{lower one-sided} \end{cases}$$

### **Paired $t$ Test for Mean Ratio with Lognormal Data (TEST=RATIO)**

The lognormal case is handled by reexpressing the analysis equivalently as a normality-based test on the log-transformed data, by using properties of the lognormal distribution as discussed in Johnson, Kotz, and Balakrishnan (1994, Chapter 14). The approaches in the section “Paired  $t$  Test (TEST=DIFF)” on page 6062 then apply.

In contrast to the usual  $t$  test on normal data, the hypotheses with lognormal data are defined in terms of geometric means rather than arithmetic means.

The hypotheses for the paired  $t$  test with lognormal pairs  $\{Y_1, Y_2\}$  are

$$H_0: \frac{\gamma_2}{\gamma_1} = \gamma_0$$

$$H_1: \begin{cases} \frac{\gamma_2}{\gamma_1} \neq \gamma_0, & \text{two-sided} \\ \frac{\gamma_2}{\gamma_1} > \gamma_0, & \text{upper one-sided} \\ \frac{\gamma_2}{\gamma_1} < \gamma_0, & \text{lower one-sided} \end{cases}$$

Let  $\mu_1^*$ ,  $\mu_2^*$ ,  $\sigma_1^*$ ,  $\sigma_2^*$ , and  $\rho^*$  be the (arithmetic) means, standard deviations, and correlation of the bivariate normal distribution of the log-transformed data  $\{\log Y_1, \log Y_2\}$ . The hypotheses can be rewritten as follows:

$$H_0: \mu_2^* - \mu_1^* = \log(\gamma_0)$$

$$H_1: \begin{cases} \mu_2^* - \mu_1^* \neq \log(\gamma_0), & \text{two-sided} \\ \mu_2^* - \mu_1^* > \log(\gamma_0), & \text{upper one-sided} \\ \mu_2^* - \mu_1^* < \log(\gamma_0), & \text{lower one-sided} \end{cases}$$

where

$$\begin{aligned}\mu_1^* &= \log \gamma_1 \\ \mu_2^* &= \log \gamma_2 \\ \sigma_1^* &= [\log(\text{CV}_1^2 + 1)]^{\frac{1}{2}} \\ \sigma_2^* &= [\log(\text{CV}_2^2 + 1)]^{\frac{1}{2}} \\ \rho^* &= \frac{\log \{\rho \text{CV}_1 \text{CV}_2 + 1\}}{\sigma_1^* \sigma_2^*}\end{aligned}$$

and  $\text{CV}_1$ ,  $\text{CV}_2$ , and  $\rho$  are the coefficients of variation and the correlation of the original untransformed pairs  $\{Y_1, Y_2\}$ . The conversion from  $\rho$  to  $\rho^*$  is shown in Jones and Miller (1966).

The test assumes lognormally distributed data and requires  $N \geq 2$ . The power is

$$\text{power} = \begin{cases} P(F(1, N-1, \delta^2) \geq F_{1-\alpha}(1, N-1)), & \text{two-sided} \\ P(t(N-1, \delta) \geq t_{1-\alpha}(N-1)), & \text{upper one-sided} \\ P(t(N-1, \delta) \leq t_{\alpha}(N-1)), & \text{lower one-sided} \end{cases}$$

where

$$\delta = N^{\frac{1}{2}} \left( \frac{\mu_1^* - \mu_2^* - \log(\gamma_0)}{\sigma^*} \right)$$

and

$$\sigma^* = (\sigma_1^{*2} + \sigma_2^{*2} - 2\rho^* \sigma_1^* \sigma_2^*)^{\frac{1}{2}}$$

### **Additive Equivalence Test for Mean Difference with Normal Data (TEST=EQUIV\_DIFF)**

The hypotheses for the equivalence test are

$$H_0: \mu_{\text{diff}} < \theta_L \quad \text{or} \quad \mu_{\text{diff}} > \theta_U$$

$$H_1: \theta_L \leq \mu_{\text{diff}} \leq \theta_U$$

The analysis is the two one-sided tests (TOST) procedure of Schuirmann (1987). The test assumes normally distributed data and requires  $N \geq 2$ . Phillips (1990) derives an expression for the exact power assuming a two-sample balanced design; the results are easily adapted to a paired design:

$$\begin{aligned}\text{power} &= Q_{N-1} \left( (-t_{1-\alpha}(N-1)), \frac{\mu_{\text{diff}} - \theta_U}{\sigma_{\text{diff}} N^{-\frac{1}{2}}}; 0, \frac{(N-1)^{\frac{1}{2}}(\theta_U - \theta_L)}{2\sigma_{\text{diff}} N^{-\frac{1}{2}}(t_{1-\alpha}(N-1))} \right) - \\ &Q_{N-1} \left( (t_{1-\alpha}(N-1)), \frac{\mu_{\text{diff}} - \theta_L}{\sigma_{\text{diff}} N^{-\frac{1}{2}}}; 0, \frac{(N-1)^{\frac{1}{2}}(\theta_U - \theta_L)}{2\sigma_{\text{diff}} N^{-\frac{1}{2}}(t_{1-\alpha}(N-1))} \right)\end{aligned}$$

where

$$\sigma_{\text{diff}} = (\sigma_1^2 + \sigma_2^2 - 2\rho\sigma_1\sigma_2)^{\frac{1}{2}}$$

and  $Q(\cdot, \cdot; \cdot, \cdot)$  is Owen's Q function, defined in the section "Common Notation" on page 6027.

**Multiplicative Equivalence Test for Mean Ratio with Lognormal Data (TEST=EQUIV\_RATIO)**

The lognormal case is handled by reexpressing the analysis equivalently as a normality-based test on the log-transformed data, by using properties of the lognormal distribution as discussed in Johnson, Kotz, and Balakrishnan (1994, Chapter 14). The approaches in the section “Additive Equivalence Test for Mean Difference with Normal Data (TEST=EQUIV\_DIFF)” on page 6064 then apply.

In contrast to the additive equivalence test on normal data, the hypotheses with lognormal data are defined in terms of geometric means rather than arithmetic means.

The hypotheses for the equivalence test are

$$H_0: \frac{\gamma_T}{\gamma_R} \leq \theta_L \quad \text{or} \quad \frac{\gamma_T}{\gamma_R} \geq \theta_U$$

$$H_1: \theta_L < \frac{\gamma_T}{\gamma_R} < \theta_U$$

where  $0 < \theta_L < \theta_U$

The analysis is the two one-sided tests (TOST) procedure of Schuirmann (1987) on the log-transformed data. The test assumes lognormally distributed data and requires  $N \geq 2$ . Diletti, Hauschke, and Steinijans (1991) derive an expression for the exact power assuming a crossover design; the results are easily adapted to a paired design:

$$\text{power} = Q_{N-1} \left( (-t_{1-\alpha}(N-1)), \frac{\log\left(\frac{\gamma_T}{\gamma_R}\right) - \log(\theta_U)}{\sigma^* N^{-\frac{1}{2}}}; 0, \frac{(N-1)^{\frac{1}{2}}(\log(\theta_U) - \log(\theta_L))}{2\sigma^* N^{-\frac{1}{2}}(t_{1-\alpha}(N-1))} \right) -$$

$$Q_{N-1} \left( (t_{1-\alpha}(N-1)), \frac{\log\left(\frac{\gamma_T}{\gamma_R}\right) - \log(\theta_L)}{\sigma^* N^{-\frac{1}{2}}}; 0, \frac{(N-1)^{\frac{1}{2}}(\log(\theta_U) - \log(\theta_L))}{2\sigma^* N^{-\frac{1}{2}}(t_{1-\alpha}(N-1))} \right)$$

where  $\sigma^*$  is the standard deviation of the differences between the log-transformed pairs (in other words, the standard deviation of  $\log(Y_T) - \log(Y_R)$ , where  $Y_T$  and  $Y_R$  are observations from the treatment and reference, respectively), computed as

$$\sigma^* = (\sigma_R^{*2} + \sigma_T^{*2} - 2\rho^* \sigma_R^* \sigma_T^*)^{\frac{1}{2}}$$

$$\sigma_R^* = [\log(\text{CV}_R^2 + 1)]^{\frac{1}{2}}$$

$$\sigma_T^* = [\log(\text{CV}_T^2 + 1)]^{\frac{1}{2}}$$

$$\rho^* = \frac{\log\{\rho \text{CV}_R \text{CV}_T + 1\}}{\sigma_R^* \sigma_T^*}$$

where  $\text{CV}_R$ ,  $\text{CV}_T$ , and  $\rho$  are the coefficients of variation and the correlation of the original untransformed pairs  $\{Y_T, Y_R\}$ , and  $Q(\cdot, \cdot; \cdot, \cdot)$  is Owen’s Q function. The conversion from  $\rho$  to  $\rho^*$  is shown in Jones and Miller (1966), and Owen’s Q function is defined in the section “Common Notation” on page 6027.

**Confidence Interval for Mean Difference (CI=DIFF)**

This analysis of precision applies to the standard  $t$ -based confidence interval:

$$\left[ \bar{d} - t_{1-\frac{\alpha}{2}}(N-1) \frac{s_d}{\sqrt{N}}, \quad \bar{d} + t_{1-\frac{\alpha}{2}}(N-1) \frac{s_d}{\sqrt{N}} \right], \quad \text{two-sided}$$

$$\left[ \bar{d} - t_{1-\alpha}(N-1) \frac{s_d}{\sqrt{N}}, \quad \infty \right), \quad \text{upper one-sided}$$

$$\left( -\infty, \quad \bar{d} + t_{1-\alpha}(N-1) \frac{s_d}{\sqrt{N}} \right], \quad \text{lower one-sided}$$

where  $\bar{d}$  and  $s_d$  are the sample mean and standard deviation of the differences. The “half-width” is defined as the distance from the point estimate  $\bar{d}$  to a finite endpoint,

$$\text{half-width} = \begin{cases} t_{1-\frac{\alpha}{2}}(N-1) \frac{s_d}{\sqrt{N}}, & \text{two-sided} \\ t_{1-\alpha}(N-1) \frac{s_d}{\sqrt{N}}, & \text{one-sided} \end{cases}$$

A “valid” confidence interval captures the true mean difference. The exact probability of obtaining at most the target confidence interval half-width  $h$ , unconditional or conditional on validity, is given by Beal (1989):

$$\Pr(\text{half-width} \leq h) = \begin{cases} P \left( \chi^2(N-1) \leq \frac{h^2 N(N-1)}{\sigma_{\text{diff}}^2 (t_{1-\frac{\alpha}{2}}^2(N-1))} \right), & \text{two-sided} \\ P \left( \chi^2(N-1) \leq \frac{h^2 N(N-1)}{\sigma_{\text{diff}}^2 (t_{1-\alpha}^2(N-1))} \right), & \text{one-sided} \end{cases}$$

$$\Pr(\text{half-width} \leq h \mid \text{validity}) = \begin{cases} \left(\frac{1}{1-\alpha}\right) 2 \left[ Q_{N-1} \left( (t_{1-\frac{\alpha}{2}}(N-1)), 0; 0, b_1 \right) - Q_{N-1}(0, 0; 0, b_1) \right], & \text{two-sided} \\ \left(\frac{1}{1-\alpha}\right) Q_{N-1} \left( (t_{1-\alpha}(N-1)), 0; 0, b_1 \right), & \text{one-sided} \end{cases}$$

where

$$\sigma_{\text{diff}} = (\sigma_1^2 + \sigma_2^2 - 2\rho\sigma_1\sigma_2)^{\frac{1}{2}}$$

$$b_1 = \frac{h(N-1)^{\frac{1}{2}}}{\sigma_{\text{diff}}(t_{1-\frac{\alpha}{c}}(N-1))N^{-\frac{1}{2}}}$$

$c$  = number of sides

and  $Q(\cdot, \cdot; \cdot, \cdot)$  is Owen’s Q function, defined in the section “Common Notation” on page 6027.

A “quality” confidence interval is both sufficiently narrow (half-width  $\leq h$ ) and valid:

$$\begin{aligned} \Pr(\text{quality}) &= \Pr(\text{half-width} \leq h \text{ and validity}) \\ &= \Pr(\text{half-width} \leq h \mid \text{validity})(1 - \alpha) \end{aligned}$$

## Analyses in the TWOSAMPLEFREQ Statement

### Overview of the $2 \times 2$ Table

Notation:

|       |   | Outcome     |         |       |
|-------|---|-------------|---------|-------|
|       |   | Failure     | Success |       |
| Group | 1 | $n_1 - x_1$ | $x_1$   | $n_1$ |
|       | 2 | $n_2 - x_2$ | $x_2$   | $n_2$ |
|       |   | $N - m$     | $m$     | $N$   |

$$\begin{aligned}
x_1 &= \# \text{ successes in group 1} \\
x_2 &= \# \text{ successes in group 2} \\
m &= x_1 + x_2 = \text{total \# successes} \\
\hat{p}_1 &= \frac{x_1}{n_1} \\
\hat{p}_2 &= \frac{x_2}{n_2} \\
\hat{p} &= \frac{m}{N} = w_1 \hat{p}_1 + w_2 \hat{p}_2
\end{aligned}$$

The hypotheses are

$$\begin{aligned}
H_0: p_2 - p_1 &= p_0 \\
H_1: \begin{cases} p_2 - p_1 \neq p_0, & \text{two-sided} \\ p_2 - p_1 > p_0, & \text{upper one-sided} \\ p_2 - p_1 < p_0, & \text{lower one-sided} \end{cases}
\end{aligned}$$

where  $p_0$  is constrained to be 0 for all but the unconditional Pearson chi-square test.

Internal calculations are performed in terms of  $p_1$ ,  $p_2$ , and  $p_0$ . An input set consisting of OR,  $p_1$ , and  $OR_0$  is transformed as follows:

$$\begin{aligned}
p_2 &= \frac{(OR)p_1}{1 - p_1 + (OR)p_1} \\
p_{10} &= p_1 \\
p_{20} &= \frac{OR_0 p_{10}}{1 - p_{10} + (OR_0)p_{10}} \\
p_0 &= p_{20} - p_{10}
\end{aligned}$$

An input set consisting of RR,  $p_1$ , and  $RR_0$  is transformed as follows:

$$\begin{aligned}
p_2 &= (RR)p_1 \\
p_{10} &= p_1 \\
p_{20} &= (RR_0)p_{10} \\
p_0 &= p_{20} - p_{10}
\end{aligned}$$

Note that the transformation of either  $OR_0$  or  $RR_0$  to  $p_0$  is not unique. The chosen parameterization fixes the null value  $p_{10}$  at the input value of  $p_1$ .

### **Pearson Chi-Square Test for Two Proportions (TEST=PCHI)**

The usual Pearson chi-square test is unconditional. The test statistic

$$z_P = \frac{\hat{p}_2 - \hat{p}_1 - p_0}{\left[ \hat{p}(1 - \hat{p}) \left( \frac{1}{n_1} + \frac{1}{n_2} \right) \right]^{\frac{1}{2}}} = [Nw_1w_2]^{\frac{1}{2}} \frac{\hat{p}_2 - \hat{p}_1 - p_0}{\hat{p}(1 - \hat{p})}$$

is assumed to have a null distribution of  $N(0, 1)$ .

Sample size for the one-sided cases is given by equation (4) in Fleiss, Tytun, and Ury (1980). One-sided power is computed as suggested by Diegert and Diegert (1981) by inverting the sample size formula. Power for the two-sided case is computed by adding the lower-sided and upper-sided powers each with  $\alpha/2$ , and sample size for the two-sided case is obtained by numerically inverting the power formula. A custom null value  $p_0$  for the proportion difference  $p_2 - p_1$  is also supported.

$$\text{power} = \begin{cases} \Phi \left( \frac{(p_2 - p_1 - p_0)(N w_1 w_2)^{\frac{1}{2}} - z_{1-\alpha} [(w_1 p_1 + w_2 p_2)(1 - w_1 p_1 - w_2 p_2)]^{\frac{1}{2}}}{[w_2 p_1 (1 - p_1) + w_1 p_2 (1 - p_2)]^{\frac{1}{2}}} \right), & \text{upper one-sided} \\ \Phi \left( \frac{-(p_2 - p_1 - p_0)(N w_1 w_2)^{\frac{1}{2}} - z_{1-\alpha} [(w_1 p_1 + w_2 p_2)(1 - w_1 p_1 - w_2 p_2)]^{\frac{1}{2}}}{[w_2 p_1 (1 - p_1) + w_1 p_2 (1 - p_2)]^{\frac{1}{2}}} \right), & \text{lower one-sided} \\ \Phi \left( \frac{(p_2 - p_1 - p_0)(N w_1 w_2)^{\frac{1}{2}} - z_{1-\frac{\alpha}{2}} [(w_1 p_1 + w_2 p_2)(1 - w_1 p_1 - w_2 p_2)]^{\frac{1}{2}}}{[w_2 p_1 (1 - p_1) + w_1 p_2 (1 - p_2)]^{\frac{1}{2}}} \right) + \\ \Phi \left( \frac{-(p_2 - p_1 - p_0)(N w_1 w_2)^{\frac{1}{2}} - z_{1-\frac{\alpha}{2}} [(w_1 p_1 + w_2 p_2)(1 - w_1 p_1 - w_2 p_2)]^{\frac{1}{2}}}{[w_2 p_1 (1 - p_1) + w_1 p_2 (1 - p_2)]^{\frac{1}{2}}} \right), & \text{two-sided} \end{cases}$$

For the one-sided cases, a closed-form inversion of the power equation yield an approximate total sample size

$$N = \frac{\left[ z_{1-\alpha} \{ (w_1 p_1 + w_2 p_2)(1 - w_1 p_1 - w_2 p_2) \}^{\frac{1}{2}} + z_{\text{power}} \{ w_2 p_1 (1 - p_1) + w_1 p_2 (1 - p_2) \}^{\frac{1}{2}} \right]^2}{w_1 w_2 (p_2 - p_1 - p_0)^2}$$

For the two-sided case, the solution for  $N$  is obtained by numerically inverting the power equation.

### Likelihood Ratio Chi-Square Test for Two Proportions (TEST=LRCHI)

The usual likelihood ratio chi-square test is unconditional. The test statistic

$$z_{\text{LR}} = (-1_{\{p_2 < p_1\}}) \sqrt{2N \sum_{i=1}^2 \left[ w_i \hat{p}_i \log \left( \frac{\hat{p}_i}{\hat{p}} \right) + w_i (1 - \hat{p}_i) \log \left( \frac{1 - \hat{p}_i}{1 - \hat{p}} \right) \right]}$$

is assumed to have a null distribution of  $N(0, 1)$  and an alternative distribution of  $N(\delta, 1)$ , where

$$\delta = N^{\frac{1}{2}} (-1_{\{p_2 < p_1\}}) \sqrt{2 \sum_{i=1}^2 \left[ w_i p_i \log \left( \frac{p_i}{w_1 p_1 + w_2 p_2} \right) + w_i (1 - p_i) \log \left( \frac{1 - p_i}{1 - (w_1 p_1 + w_2 p_2)} \right) \right]}$$

The approximate power is

$$\text{power} = \begin{cases} \Phi(\delta - z_{1-\alpha}), & \text{upper one-sided} \\ \Phi(-\delta - z_{1-\alpha}), & \text{lower one-sided} \\ \Phi\left(\delta - z_{1-\frac{\alpha}{2}}\right) + \Phi\left(-\delta - z_{1-\frac{\alpha}{2}}\right), & \text{two-sided} \end{cases}$$

For the one-sided cases, a closed-form inversion of the power equation yield an approximate total sample size

$$N = \left( \frac{z_{\text{power}} + z_{1-\alpha}}{\delta} \right)^2$$

For the two-sided case, the solution for  $N$  is obtained by numerically inverting the power equation.

### Fisher's Exact Conditional Test for Two Proportions (Test=FISHER)

Fisher's exact test is conditional on the observed total number of successes  $m$ . Power and sample size computations are based on a test with similar power properties, the continuity-adjusted arcsine test. The test statistic

$$z_A = (4Nw_1w_2)^{\frac{1}{2}} \left[ \arcsin \left( \left[ \hat{p}_2 + \frac{1}{2Nw_2} (1_{\{\hat{p}_2 < \hat{p}_1\}} - 1_{\{\hat{p}_2 > \hat{p}_1\}}) \right]^{\frac{1}{2}} \right) - \arcsin \left( \left[ \hat{p}_1 + \frac{1}{2Nw_1} (1_{\{\hat{p}_1 < \hat{p}_2\}} - 1_{\{\hat{p}_1 > \hat{p}_2\}}) \right]^{\frac{1}{2}} \right) \right]$$

is assumed to have a null distribution of  $N(0, 1)$  and an alternative distribution of  $N(\delta, 1)$ , where

$$\delta = (4Nw_1w_2)^{\frac{1}{2}} \left[ \arcsin \left( \left[ p_2 + \frac{1}{2Nw_2} (1_{\{p_2 < p_1\}} - 1_{\{p_2 > p_1\}}) \right]^{\frac{1}{2}} \right) - \arcsin \left( \left[ p_1 + \frac{1}{2Nw_1} (1_{\{p_1 < p_2\}} - 1_{\{p_1 > p_2\}}) \right]^{\frac{1}{2}} \right) \right]$$

The approximate power for the one-sided balanced case is given by Walters (1979) and is easily extended to the unbalanced and two-sided cases:

$$\text{power} = \begin{cases} \Phi(\delta - z_{1-\alpha}), & \text{upper one-sided} \\ \Phi(-\delta - z_{1-\alpha}), & \text{lower one-sided} \\ \Phi(\delta - z_{1-\frac{\alpha}{2}}) + \Phi(-\delta - z_{1-\frac{\alpha}{2}}), & \text{two-sided} \end{cases}$$

### Analyses in the TWOSAMPLEMEANS Statement

#### Two-Sample $t$ Test Assuming Equal Variances (TEST=DIFF)

The hypotheses for the two-sample  $t$  test are

$$H_0: \mu_{\text{diff}} = \mu_0$$

$$H_1: \begin{cases} \mu_{\text{diff}} \neq \mu_0, & \text{two-sided} \\ \mu_{\text{diff}} > \mu_0, & \text{upper one-sided} \\ \mu_{\text{diff}} < \mu_0, & \text{lower one-sided} \end{cases}$$

The test assumes normally distributed data and common standard deviation per group, and it requires  $N \geq 3$ ,  $n_1 \geq 1$ , and  $n_2 \geq 1$ . The test statistics are

$$t = N^{\frac{1}{2}}(w_1w_2)^{\frac{1}{2}} \left( \frac{\bar{x}_2 - \bar{x}_1 - \mu_0}{s_p} \right) \sim t(N - 2, \delta)$$

$$t^2 \sim F(1, N - 2, \delta^2)$$

where  $\bar{x}_1$  and  $\bar{x}_2$  are the sample means and  $s_p$  is the pooled standard deviation, and

$$\delta = N^{\frac{1}{2}}(w_1w_2)^{\frac{1}{2}} \left( \frac{\mu_{\text{diff}} - \mu_0}{\sigma} \right)$$



The test is

$$\text{Reject } H_0 \quad \text{if } \begin{cases} t^2 \geq F_{1-\alpha}(1, N-2), & \text{two-sided} \\ t \geq t_{1-\alpha}(N-2), & \text{upper one-sided} \\ t \leq t_{\alpha}(N-2), & \text{lower one-sided} \end{cases}$$

Exact power computations for  $t$  tests are given in O'Brien and Muller (1993, Section 8.2.1):

$$\text{power} = \begin{cases} P(F(1, N-2, \delta^2) \geq F_{1-\alpha}(1, N-2)), & \text{two-sided} \\ P(t(N-2, \delta) \geq t_{1-\alpha}(N-2)), & \text{upper one-sided} \\ P(t(N-2, \delta) \leq t_{\alpha}(N-2)), & \text{lower one-sided} \end{cases}$$

Solutions for  $N$ ,  $n_1$ ,  $n_2$ ,  $\alpha$ , and  $\delta$  are obtained by numerically inverting the power equation. Closed-form solutions for other parameters, in terms of  $\delta$ , are as follows:

$$\begin{aligned} \mu_{\text{diff}} &= \delta\sigma(Nw_1w_2)^{-\frac{1}{2}} + \mu_0 \\ \mu_1 &= \delta\sigma(Nw_1w_2)^{-\frac{1}{2}} + \mu_0 - \mu_2 \\ \mu_2 &= \delta\sigma(Nw_1w_2)^{-\frac{1}{2}} + \mu_0 - \mu_1 \\ \sigma &= \begin{cases} \delta^{-1}(Nw_1w_2)^{\frac{1}{2}}(\mu_{\text{diff}} - \mu_0), & |\delta| > 0 \\ \text{undefined}, & \text{otherwise} \end{cases} \\ w_1 &= \begin{cases} \frac{1}{2} \pm \frac{1}{2} \left[ 1 - \frac{4\delta^2\sigma^2}{N(\mu_{\text{diff}} - \mu_0)^2} \right]^{\frac{1}{2}}, & 0 < |\delta| \leq \frac{1}{2}N^{\frac{1}{2}} \frac{|\mu_{\text{diff}} - \mu_0|}{\sigma} \\ \text{undefined}, & \text{otherwise} \end{cases} \\ w_2 &= \begin{cases} \frac{1}{2} \pm \frac{1}{2} \left[ 1 - \frac{4\delta^2\sigma^2}{N(\mu_{\text{diff}} - \mu_0)^2} \right]^{\frac{1}{2}}, & 0 < |\delta| \leq \frac{1}{2}N^{\frac{1}{2}} \frac{|\mu_{\text{diff}} - \mu_0|}{\sigma} \\ \text{undefined}, & \text{otherwise} \end{cases} \end{aligned}$$

Finally, here is a derivation of the solution for  $w_1$ :

Solve the  $\delta$  equation for  $w_1$  (which requires the quadratic formula). Then determine the range of  $\delta$  given  $w_1$ :

$$\begin{aligned} \min_{w_1}(\delta) &= \begin{cases} 0, & \text{when } w_1 = 0 \text{ or } 1, \text{ if } (\mu_{\text{diff}} - \mu_0) \geq 0 \\ \frac{1}{2}N^{\frac{1}{2}} \frac{(\mu_{\text{diff}} - \mu_0)}{\sigma}, & \text{when } w_1 = \frac{1}{2}, \text{ if } (\mu_{\text{diff}} - \mu_0) < 0 \end{cases} \\ \max_{w_1}(\delta) &= \begin{cases} 0, & \text{when } w_1 = 0 \text{ or } 1, \text{ if } (\mu_{\text{diff}} - \mu_0) < 0 \\ \frac{1}{2}N^{\frac{1}{2}} \frac{(\mu_{\text{diff}} - \mu_0)}{\sigma}, & \text{when } w_1 = \frac{1}{2}, \text{ if } (\mu_{\text{diff}} - \mu_0) \geq 0 \end{cases} \end{aligned}$$

This implies

$$|\delta| \leq \frac{1}{2}N^{\frac{1}{2}} \frac{|\mu_{\text{diff}} - \mu_0|}{\sigma}$$

**Two-Sample Satterthwaite  $t$  Test Assuming Unequal Variances (TEST=DIFF\_SATT)**

The hypotheses for the two-sample Satterthwaite  $t$  test are

$$H_0: \mu_{\text{diff}} = \mu_0$$

$$H_1: \begin{cases} \mu_{\text{diff}} \neq \mu_0, & \text{two-sided} \\ \mu_{\text{diff}} > \mu_0, & \text{upper one-sided} \\ \mu_{\text{diff}} < \mu_0, & \text{lower one-sided} \end{cases}$$

The test assumes normally distributed data and requires  $N \geq 3$ ,  $n_1 \geq 1$ , and  $n_2 \geq 1$ . The test statistics are

$$t = \frac{\bar{x}_2 - \bar{x}_1 - \mu_0}{\left[ \frac{s_1^2}{n_1} + \frac{s_2^2}{n_2} \right]^{\frac{1}{2}}} = N^{\frac{1}{2}} \frac{\bar{x}_2 - \bar{x}_1 - \mu_0}{\left[ \frac{s_1^2}{w_1} + \frac{s_2^2}{w_2} \right]^{\frac{1}{2}}}$$

$$F = t^2$$

where  $\bar{x}_1$  and  $\bar{x}_2$  are the sample means and  $s_1$  and  $s_2$  are the sample standard deviations.

DiSantostefano and Muller (1995, p. 585) state, the test is based on assuming that under  $H_0$ ,  $F$  is distributed as  $F(1, \nu)$ , where  $\nu$  is given by Satterthwaite's approximation (Satterthwaite 1946),

$$\nu = \frac{\left[ \frac{\sigma_1^2}{n_1} + \frac{\sigma_2^2}{n_2} \right]^2}{\frac{\left[ \frac{\sigma_1^2}{n_1} \right]^2}{n_1-1} + \frac{\left[ \frac{\sigma_2^2}{n_2} \right]^2}{n_2-1}} = \frac{\left[ \frac{\sigma_1^2}{w_1} + \frac{\sigma_2^2}{w_2} \right]^2}{\frac{\left[ \frac{\sigma_1^2}{w_1} \right]^2}{Nw_1-1} + \frac{\left[ \frac{\sigma_2^2}{w_2} \right]^2}{Nw_2-1}}$$

Since  $\nu$  is unknown, in practice it must be replaced by an estimate

$$\hat{\nu} = \frac{\left[ \frac{s_1^2}{n_1} + \frac{s_2^2}{n_2} \right]^2}{\frac{\left[ \frac{s_1^2}{n_1} \right]^2}{n_1-1} + \frac{\left[ \frac{s_2^2}{n_2} \right]^2}{n_2-1}} = \frac{\left[ \frac{s_1^2}{w_1} + \frac{s_2^2}{w_2} \right]^2}{\frac{\left[ \frac{s_1^2}{w_1} \right]^2}{Nw_1-1} + \frac{\left[ \frac{s_2^2}{w_2} \right]^2}{Nw_2-1}}$$

So the test is

$$\text{Reject } H_0 \text{ if } \begin{cases} F \geq F_{1-\alpha}(1, \hat{\nu}), & \text{two-sided} \\ t \geq t_{1-\alpha}(\hat{\nu}), & \text{upper one-sided} \\ t \leq t_{\alpha}(\hat{\nu}), & \text{lower one-sided} \end{cases}$$

Exact solutions for power for the two-sided and upper one-sided cases are given in Moser, Stevens, and Watts (1989). The lower one-sided case follows easily by using symmetry. The equations are as follows:

$$\text{power} = \begin{cases} \int_0^\infty P(F(1, N-2, \lambda) > h(u)F_{1-\alpha}(1, v(u))|u) f(u)du, & \text{two-sided} \\ \int_0^\infty P(t(N-2, \lambda^{\frac{1}{2}}) > [h(u)]^{\frac{1}{2}} t_{1-\alpha}(v(u))|u) f(u)du, & \text{upper one-sided} \\ \int_0^\infty P(t(N-2, \lambda^{\frac{1}{2}}) < [h(u)]^{\frac{1}{2}} t_\alpha(v(u))|u) f(u)du, & \text{lower one-sided} \end{cases}$$

where

$$h(u) = \frac{\left(\frac{1}{n_1} + \frac{u}{n_2}\right)(n_1 + n_2 - 2)}{\left[(n_1 - 1) + (n_2 - 1)\frac{u\sigma_1^2}{\sigma_2^2}\right]\left(\frac{1}{n_1} + \frac{\sigma_2^2}{\sigma_1^2 n_2}\right)}$$

$$v(u) = \frac{\left(\frac{1}{n_1} + \frac{u}{n_2}\right)^2}{\frac{1}{n_1^2(n_1-1)} + \frac{u^2}{n_2^2(n_2-1)}}$$

$$\lambda = \frac{(\mu_{\text{diff}} - \mu_0)^2}{\frac{\sigma_1^2}{n_1} + \frac{\sigma_2^2}{n_2}}$$

$$f(u) = \frac{\Gamma\left(\frac{n_1+n_2-2}{2}\right)}{\Gamma\left(\frac{n_1-1}{2}\right)\Gamma\left(\frac{n_2-1}{2}\right)} \left[\frac{\sigma_1^2(n_2-1)}{\sigma_2^2(n_1-1)}\right]^{\frac{n_2-1}{2}} u^{\frac{n_2-3}{2}} \left[1 + \left(\frac{n_2-1}{n_1-1}\right)\frac{u\sigma_1^2}{\sigma_2^2}\right]^{-\left(\frac{n_1+n_2-2}{2}\right)}$$

The density  $f(u)$  is obtained from the fact that

$$\frac{u\sigma_1^2}{\sigma_2^2} \sim F(n_2 - 1, n_1 - 1)$$

### **Two-Sample Pooled $t$ Test of Mean Ratio with Lognormal Data (TEST=RATIO)**

The lognormal case is handled by reexpressing the analysis equivalently as a normality-based test on the log-transformed data, by using properties of the lognormal distribution as discussed in Johnson, Kotz, and Balakrishnan (1994, Chapter 14). The approaches in the section “Two-Sample  $t$  Test Assuming Equal Variances (TEST=DIFF)” on page 6069 then apply.

In contrast to the usual  $t$  test on normal data, the hypotheses with lognormal data are defined in terms of geometric means rather than arithmetic means. The test assumes equal coefficients of variation in the two groups.

The hypotheses for the two-sample  $t$  test with lognormal data are

$$H_0: \frac{\gamma_2}{\gamma_1} = \gamma_0$$

$$H_1: \begin{cases} \frac{\gamma_2}{\gamma_1} \neq \gamma_0, & \text{two-sided} \\ \frac{\gamma_2}{\gamma_1} > \gamma_0, & \text{upper one-sided} \\ \frac{\gamma_2}{\gamma_1} < \gamma_0, & \text{lower one-sided} \end{cases}$$

Let  $\mu_1^*$ ,  $\mu_2^*$ , and  $\sigma^*$  be the (arithmetic) means and common standard deviation of the corresponding normal distributions of the log-transformed data. The hypotheses can be rewritten as follows:

$$H_0: \mu_2^* - \mu_1^* = \log(\gamma_0)$$

$$H_1: \begin{cases} \mu_2^* - \mu_1^* \neq \log(\gamma_0), & \text{two-sided} \\ \mu_2^* - \mu_1^* > \log(\gamma_0), & \text{upper one-sided} \\ \mu_2^* - \mu_1^* < \log(\gamma_0), & \text{lower one-sided} \end{cases}$$

where

$$\mu_1^* = \log \gamma_1$$

$$\mu_2^* = \log \gamma_2$$

The test assumes lognormally distributed data and requires  $N \geq 3$ ,  $n_1 \geq 1$ , and  $n_2 \geq 1$ .

The power is

$$\text{power} = \begin{cases} P(F(1, N-2, \delta^2) \geq F_{1-\alpha}(1, N-2)), & \text{two-sided} \\ P(t(N-2, \delta) \geq t_{1-\alpha}(N-2)), & \text{upper one-sided} \\ P(t(N-2, \delta) \leq t_{\alpha}(N-2)), & \text{lower one-sided} \end{cases}$$

where

$$\delta = N^{\frac{1}{2}}(w_1 w_2)^{\frac{1}{2}} \left( \frac{\mu_2^* - \mu_1^* - \log(\gamma_0)}{\sigma^*} \right)$$

$$\sigma^* = [\log(\text{CV}^2 + 1)]^{\frac{1}{2}}$$

### **Additive Equivalence Test for Mean Difference with Normal Data (TEST=EQUIV\_DIFF)**

The hypotheses for the equivalence test are

$$H_0: \mu_{\text{diff}} < \theta_L \quad \text{or} \quad \mu_{\text{diff}} > \theta_U$$

$$H_1: \theta_L \leq \mu_{\text{diff}} \leq \theta_U$$

The analysis is the two one-sided tests (TOST) procedure of Schuirmann (1987). The test assumes normally distributed data and requires  $N \geq 3$ ,  $n_1 \geq 1$ , and  $n_2 \geq 1$ . Phillips (1990) derives an expression for the exact power assuming a balanced design; the results are easily adapted to an unbalanced design:

$$\text{power} = Q_{N-2} \left( (-t_{1-\alpha}(N-2)), \frac{\mu_{\text{diff}} - \theta_U}{\sigma N^{-\frac{1}{2}}(w_1 w_2)^{-\frac{1}{2}}}; 0, \frac{(N-2)^{\frac{1}{2}}(\theta_U - \theta_L)}{2\sigma N^{-\frac{1}{2}}(w_1 w_2)^{-\frac{1}{2}}(t_{1-\alpha}(N-2))} \right) -$$

$$Q_{N-2} \left( (t_{1-\alpha}(N-2)), \frac{\mu_{\text{diff}} - \theta_L}{\sigma N^{-\frac{1}{2}}(w_1 w_2)^{-\frac{1}{2}}}; 0, \frac{(N-2)^{\frac{1}{2}}(\theta_U - \theta_L)}{2\sigma N^{-\frac{1}{2}}(w_1 w_2)^{-\frac{1}{2}}(t_{1-\alpha}(N-2))} \right)$$

where  $Q(\cdot, \cdot; \cdot, \cdot)$  is Owen's Q function, defined in the section "Common Notation" on page 6027.

**Multiplicative Equivalence Test for Mean Ratio with Lognormal Data (TEST=EQUIV\_RATIO)**

The lognormal case is handled by reexpressing the analysis equivalently as a normality-based test on the log-transformed data, by using properties of the lognormal distribution as discussed in Johnson, Kotz, and Balakrishnan (1994, Chapter 14). The approaches in the section “Additive Equivalence Test for Mean Difference with Normal Data (TEST=EQUIV\_DIFF)” on page 6073 then apply.

In contrast to the additive equivalence test on normal data, the hypotheses with lognormal data are defined in terms of geometric means rather than arithmetic means.

The hypotheses for the equivalence test are

$$H_0: \frac{\gamma_T}{\gamma_R} \leq \theta_L \quad \text{or} \quad \frac{\gamma_T}{\gamma_R} \geq \theta_U$$

$$H_1: \theta_L < \frac{\gamma_T}{\gamma_R} < \theta_U$$

$$\text{where } 0 < \theta_L < \theta_U$$

The analysis is the two one-sided tests (TOST) procedure of Schuirmann (1987) on the log-transformed data. The test assumes lognormally distributed data and requires  $N \geq 3$ ,  $n_1 \geq 1$ , and  $n_2 \geq 1$ . Diletti, Hauschke, and Steinijans (1991) derive an expression for the exact power assuming a crossover design; the results are easily adapted to an unbalanced two-sample design:

$$\text{power} = Q_{N-2} \left( (-t_{1-\alpha}(N-2)), \frac{\log\left(\frac{\gamma_T}{\gamma_R}\right) - \log(\theta_U)}{\sigma^* N^{-\frac{1}{2}}(w_1 w_2)^{-\frac{1}{2}}}; 0, \frac{(N-2)^{\frac{1}{2}}(\log(\theta_U) - \log(\theta_L))}{2\sigma^* N^{-\frac{1}{2}}(w_1 w_2)^{-\frac{1}{2}}(t_{1-\alpha}(N-2))} \right) -$$

$$Q_{N-2} \left( (t_{1-\alpha}(N-2)), \frac{\log\left(\frac{\gamma_T}{\gamma_R}\right) - \log(\theta_L)}{\sigma^* N^{-\frac{1}{2}}(w_1 w_2)^{-\frac{1}{2}}}; 0, \frac{(N-2)^{\frac{1}{2}}(\log(\theta_U) - \log(\theta_L))}{2\sigma^* N^{-\frac{1}{2}}(w_1 w_2)^{-\frac{1}{2}}(t_{1-\alpha}(N-2))} \right)$$

where

$$\sigma^* = [\log(\text{CV}^2 + 1)]^{\frac{1}{2}}$$

is the (assumed common) standard deviation of the normal distribution of the log-transformed data, and  $Q(\cdot, \cdot; \cdot, \cdot)$  is Owen's Q function, defined in the section “Common Notation” on page 6027.

**Confidence Interval for Mean Difference (CI=DIFF)**

This analysis of precision applies to the standard  $t$ -based confidence interval:

$$\left[ (\bar{x}_2 - \bar{x}_1) - t_{1-\frac{\alpha}{2}}(N-2) \frac{s_p}{\sqrt{N w_1 w_2}}, \right. \\ \left. (\bar{x}_2 - \bar{x}_1) + t_{1-\frac{\alpha}{2}}(N-2) \frac{s_p}{\sqrt{N w_1 w_2}} \right], \quad \text{two-sided}$$

$$\left[ (\bar{x}_2 - \bar{x}_1) - t_{1-\alpha}(N-2) \frac{s_p}{\sqrt{N w_1 w_2}}, \infty \right), \quad \text{upper one-sided}$$

$$\left( -\infty, (\bar{x}_2 - \bar{x}_1) + t_{1-\alpha}(N-2) \frac{s_p}{\sqrt{N w_1 w_2}} \right], \quad \text{lower one-sided}$$

where  $\bar{x}_1$  and  $\bar{x}_2$  are the sample means and  $s_p$  is the pooled standard deviation. The “half-width” is defined as the distance from the point estimate  $\bar{x}_2 - \bar{x}_1$  to a finite endpoint,

$$\text{half-width} = \begin{cases} t_{1-\frac{\alpha}{2}}(N-2) \frac{s_p}{\sqrt{Nw_1w_2}}, & \text{two-sided} \\ t_{1-\alpha}(N-2) \frac{s_p}{\sqrt{Nw_1w_2}}, & \text{one-sided} \end{cases}$$

A “valid” confidence interval captures the true mean. The exact probability of obtaining at most the target confidence interval half-width  $h$ , unconditional or conditional on validity, is given by Beal (1989):

$$\Pr(\text{half-width} \leq h) = \begin{cases} P \left( \chi^2(N-2) \leq \frac{h^2 N(N-2)(w_1w_2)}{\sigma^2(t_{1-\frac{\alpha}{2}}^2(N-2))} \right), & \text{two-sided} \\ P \left( \chi^2(N-2) \leq \frac{h^2 N(N-2)(w_1w_2)}{\sigma^2(t_{1-\alpha}^2(N-2))} \right), & \text{one-sided} \end{cases}$$

$$\Pr(\text{half-width} \leq h \mid \text{validity}) = \begin{cases} \left(\frac{1}{1-\alpha}\right) 2 \left[ Q_{N-2} \left( (t_{1-\frac{\alpha}{2}}(N-2)), 0; 0, b_2 \right) - Q_{N-2}(0, 0; 0, b_2) \right], & \text{two-sided} \\ \left(\frac{1}{1-\alpha}\right) Q_{N-2} \left( (t_{1-\alpha}(N-2)), 0; 0, b_2 \right), & \text{one-sided} \end{cases}$$

where

$$b_2 = \frac{h(N-2)^{\frac{1}{2}}}{\sigma(t_{1-\frac{\alpha}{2}}(N-2))N^{-\frac{1}{2}}(w_1w_2)^{-\frac{1}{2}}}$$

$c$  = number of sides

and  $Q(\cdot, \cdot; \cdot, \cdot)$  is Owen’s Q function, defined in the section “Common Notation” on page 6027.

A “quality” confidence interval is both sufficiently narrow (half-width  $\leq h$ ) and valid:

$$\begin{aligned} \Pr(\text{quality}) &= \Pr(\text{half-width} \leq h \text{ and validity}) \\ &= \Pr(\text{half-width} \leq h \mid \text{validity})(1 - \alpha) \end{aligned}$$

### Analyses in the TWOSAMPLESURVIVAL Statement

#### Rank Tests for Two Survival Curves (TEST=LOGRANK, TEST=GEHAN, TEST=TARONEWARE)

The method is from Lakatos (1988) and Cantor (1997, pp. 83–92).

Define the following notation:

- $X_j(i)$  =  $i$ th input time point on survival curve for group  $j$
- $S_j(i)$  = input survivor function value corresponding to  $X_j(i)$
- $h_j(t)$  = hazard rate for group  $j$  at time  $t$
- $\Psi_j(t)$  = loss hazard rate for group  $j$  at time  $t$
- $\lambda_j$  = exponential hazard rate for group  $j$
- $R$  = hazard ratio of group 2 to group 1  $\equiv$  (assumed constant) value of  $\frac{h_2(t)}{h_1(t)}$
- $m_j$  = median survival time for group  $j$
- $b$  = number of subintervals per time unit
- $T$  = accrual time
- $\tau$  = follow-up time after accrual
- $L_j$  = exponential loss rate for group  $j$
- $XL_j$  = input time point on loss curve for group  $j$
- $SL_j$  = input survivor function value corresponding to  $XL_j$
- $mL_j$  = median survival time for group  $j$
- $r_i$  = rank for  $i$ th time point

Each survival curve can be specified in one of several ways.

- For exponential curves:
  - a single point  $(X_j(1), S_j(1))$  on the curve
  - median survival time
  - hazard rate
  - hazard ratio (for curve 2, with respect to curve 1)
- For piecewise linear curves with proportional hazards:
  - a set of points  $\{(X_1(1), S_1(1)), (X_1(2), S_1(2)), \dots\}$  (for curve 1)
  - hazard ratio (for curve 2, with respect to curve 1)
- For arbitrary piecewise linear curves:
  - a set of points  $\{(X_j(1), S_j(1)), (X_j(2), S_j(2)), \dots\}$

A total of  $M + 1$  evenly spaced time points  $\{t_0 = 0, t_1, t_2, \dots, t_M = T + \tau\}$  are used in calculations, where

$$M = \text{floor}((T + \tau)b)$$

The hazard function is calculated for each survival curve at each time point. For an exponential curve, the (constant) hazard is given by one of the following, depending on the input parameterization:

$$h_j(t) = \begin{cases} \lambda_j \\ \lambda_1 R \\ \frac{-\log(\frac{1}{2})}{m_j} \\ \frac{-\log(S_j(1))}{X_j(1)} \\ \frac{-\log(S_1(1))}{X_1(1)} R \end{cases}$$

For a piecewise linear curve, define the following additional notation:

$$\begin{aligned} t_i^- &= \text{largest input time } X \text{ such that } X \leq t_i \\ t_i^+ &= \text{smallest input time } X \text{ such that } X > t_i \end{aligned}$$

The hazard is computed by using linear interpolation as follows:

$$h_j(t_i) = \frac{S_j(t_i^-) - S_j(t_i^+)}{[S_j(t_i^+) - S_j(t_i^-)][t_i - t_i^-] + S_j(t_i^-)[t_i^+ - t_i^-]}$$

With proportional hazards, the hazard rate of group 2's curve in terms of the hazard rate of group 1's curve is

$$h_2(t) = h_1(t)R$$

Hazard function values  $\{\Psi_j(t_i)\}$  for the loss curves are computed in an analogous way from  $\{L_j, XL_j, SL_j, mL_j\}$ .

The expected number at risk  $N_j(i)$  at time  $i$  in group  $j$  is calculated for each group and time points 0 through  $M - 1$ , as follows:

$$\begin{aligned} N_j(0) &= Nw_j \\ N_j(i + 1) &= N_j(i) \left[ 1 - h_j(t_i) \left( \frac{1}{b} \right) - \Psi_j(t_i) \left( \frac{1}{b} \right) - \left( \frac{1}{b(T + \tau - t_i)} \right) 1_{\{t_i > \tau\}} \right] \end{aligned}$$

Define  $\theta_i$  as the ratio of hazards and  $\phi_i$  as the ratio of expected numbers at risk for time  $t_i$ :

$$\begin{aligned} \theta_i &= \frac{h_2(t_i)}{h_1(t_i)} \\ \phi_i &= \frac{N_2(i)}{N_1(i)} \end{aligned}$$

The expected number of deaths in each subinterval is calculated as follows:

$$D_i = [h_1(t_i)N_1(i) + h_2(t_i)N_2(i)] \left( \frac{1}{b} \right)$$



The rank values are calculated as follows according to which test statistic is used:

$$r_i = \begin{cases} 1, & \text{log-rank} \\ N_1(i) + N_2(i), & \text{Gehan} \\ \sqrt{N_1(i) + N_2(i)}, & \text{Tarone-Ware} \end{cases}$$

The distribution of the test statistic is approximated by  $N(E, 1)$  where

$$E = \frac{\sum_{i=0}^{M-1} D_i r_i \left[ \frac{\phi_i \theta_i}{1 + \phi_i \theta_i} - \frac{\phi_i}{1 + \phi_i} \right]}{\sqrt{\sum_{i=0}^{M-1} D_i r_i^2 \frac{\phi_i}{(1 + \phi_i)^2}}}$$

Note that  $N^{\frac{1}{2}}$  can be factored out of the mean  $E$ , and so it can be expressed equivalently as

$$E = N^{\frac{1}{2}} E^* = N^{\frac{1}{2}} \left[ \frac{\sum_{i=0}^{M-1} D_i^* r_i^* \left[ \frac{\phi_i \theta_i}{1 + \phi_i \theta_i} - \frac{\phi_i}{1 + \phi_i} \right]}{\sqrt{\sum_{i=0}^{M-1} D_i^* r_i^{*2} \frac{\phi_i}{(1 + \phi_i)^2}}} \right]$$

where  $E^*$  is free of  $N$  and

$$D_i^* = [h_1(t_i)N_1^*(i) + h_2(t_i)N_2^*(i)] \left( \frac{1}{b} \right)$$

$$r_i^* = \begin{cases} 1, & \text{log-rank} \\ N_1^*(i) + N_2^*(i), & \text{Gehan} \\ \sqrt{N_1^*(i) + N_2^*(i)}, & \text{Tarone-Ware} \end{cases}$$

$$N_j^*(0) = w_j$$

$$N_j^*(i + 1) = N_j^*(i) \left[ 1 - h_j(t_i) \left( \frac{1}{b} \right) - \Psi_j(t_i) \left( \frac{1}{b} \right) - \left( \frac{1}{b(T + \tau - t_i)} \right) 1_{\{t_i > \tau\}} \right]$$

The approximate power is

$$\text{power} = \begin{cases} \Phi \left( -N^{\frac{1}{2}} E^* - z_{1-\alpha} \right), & \text{upper one-sided} \\ \Phi \left( N^{\frac{1}{2}} E^* - z_{1-\alpha} \right), & \text{lower one-sided} \\ \Phi \left( -N^{\frac{1}{2}} E^* - z_{1-\frac{\alpha}{2}} \right) + \Phi \left( N^{\frac{1}{2}} E^* - z_{1-\frac{\alpha}{2}} \right), & \text{two-sided} \end{cases}$$

Note that the upper and lower one-sided cases are expressed differently than in other analyses. This is because  $E^* > 0$  corresponds to a higher survival curve in group 1 and thus, by the convention used in PROC power for two-group analyses, the lower side.

For the one-sided cases, a closed-form inversion of the power equation yield an approximate total sample size

$$N = \left( \frac{z_{\text{power}} + z_{1-\alpha}}{E^*} \right)^2$$

For the two-sided case, the solution for  $N$  is obtained by numerically inverting the power equation.

Accrual rates are converted to and from sample sizes according to the equation  $a_j = n_j/T$ , where  $a_j$  is the accrual rate for group  $j$ .

Expected numbers of events—that is, deaths, whether observed or censored—are converted to and from sample sizes according to the equation

$$e_j = \begin{cases} n_j [1 - S_j(\tau)], & T = 0 \\ n_j \left[ 1 - \frac{1}{T} \int_0^T S_j(T + \tau - t) dt \right], & T > 0 \end{cases}$$

where  $e_j$  is the expected number of events in group  $j$ . For an exponential curve, the equation simplifies to

$$e_j = \begin{cases} n_j [1 - \exp(-\lambda_j \tau)], & T = 0 \\ n_j \left[ 1 - \frac{1}{\lambda_j T} (\exp(-\lambda_j \tau) - \exp(-\lambda_j (T + \tau))) \right], & T > 0 \end{cases}$$

For a piecewise linear curve, first define  $K_j$  as the number of time points in the following collection:  $\tau$ ,  $T + \tau$ , and input time points for group  $j$  strictly between  $\tau$  and  $T + \tau$ . Denote the ordered set of these points as  $\{u_{j1}, \dots, u_{jK_j}\}$ . The survival function values  $S_j(\tau)$  and  $S_j(T + \tau)$  are calculated by linear interpolation between adjacent input time points if they do not coincide with any input time points. Then the equation for a piecewise linear curve simplifies to

$$e_j = \begin{cases} n_j [1 - S_j(\tau)], & T = 0 \\ n_j \left[ 1 - \frac{1}{2T} \sum_{i=1}^{K_j-1} (u_{j,i+1} - u_{ji}) (S_j(u_{ji}) + S_j(u_{j,i+1})) \right], & T > 0 \end{cases}$$

### Analyses in the TWOSAMPLEWILCOXON Statement

#### **Wilcoxon-Mann-Whitney Test for Comparing Two Distributions (TEST=WMW)**

The power approximation in this section is applicable to the Wilcoxon-Mann-Whitney (WMW) test as invoked with the WILCOXON option in the PROC NPAR1WAY statement of the NPAR1WAY procedure. The approximation is based on O'Brien and Casteloe (2006) and an estimator called  $\widehat{WMW}_{\text{odds}}$ . See O'Brien and Casteloe (2006) for a definition of  $\widehat{WMW}_{\text{odds}}$ , which need not be derived in detail here for purposes of explaining the power formula.

Let  $Y_1$  and  $Y_2$  be independent observations from any two distributions that you want to compare using the WMW test. For purposes of deriving the asymptotic distribution of  $\widehat{WMW}_{\text{odds}}$  (and consequently the power computation as well), these distributions must be formulated as ordered categorical (“ordinal”) distributions.

If a distribution is continuous, it can be discretized using a large number of categories with negligible loss of accuracy. Each nonordinal distribution is divided into  $b$  categories, where  $b$  is the value of the NBINS parameter, with breakpoints evenly spaced on the probability scale. That is, each bin contains an equal probability  $1/b$  for that distribution. Then the breakpoints across both distributions are pooled to form a collection of  $C$  bins (heretofore called “categories”), and the probabilities of bin membership for each distribution are recalculated. The motivation for this method of binning is to avoid degenerate representations of the distributions—that is, small handfuls of large probabilities among mostly empty bins—as can be caused by something like an evenly spaced grid across raw values rather than probabilities.

After the discretization process just mentioned, there are now two ordinal distributions, each with a set of probabilities across a common set of  $C$  ordered categories. For simplicity of notation, assume (without loss of generality) the response values to be  $1, \dots, C$ . Represent the conditional probabilities as

$$\tilde{p}_{ij} = \text{Prob}(Y_i = j \mid \text{group} = i), i \in \{1, 2\} \quad \text{and} \quad j \in \{1, \dots, C\}$$

and the group allocation weights as

$$w_i = \frac{n_i}{N} = \text{Prob}(\text{group} = i), \quad i \in \{1, 2\}$$

The joint probabilities can then be calculated simply as

$$p_{ij} = \text{Prob}(\text{group} = i, Y_i = j) = w_i \tilde{p}_{ij}, i \in \{1, 2\} \quad \text{and} \quad j \in \{1, \dots, C\}$$

The next step in the power computation is to compute the probabilities that a randomly chosen pair of observations from the two groups is concordant, discordant, or tied. It is useful to define these probabilities as functions of the terms  $Rs_{ij}$  and  $Rd_{ij}$ , defined as follows, where  $Y$  is a random observation drawn from the joint distribution across groups and categories:

$$\begin{aligned} Rs_{ij} &= \text{Prob}(Y \text{ is concordant with cell}(i, j)) + \frac{1}{2}\text{Prob}(Y \text{ is tied with cell}(i, j)) \\ &= \text{Prob}((\text{group} < i \text{ and } Y < j) \text{ or } (\text{group} > i \text{ and } Y > j)) + \\ &\quad \frac{1}{2}\text{Prob}(\text{group} \neq i \text{ and } Y = j) \\ &= \sum_{g=1}^2 \sum_{c=1}^C w_g \tilde{p}_{gc} \left[ I_{(g-i)(c-j) > 0} + \frac{1}{2} I_{g \neq i, c=j} \right] \end{aligned}$$

and

$$\begin{aligned} Rd_{ij} &= \text{Prob}(Y \text{ is discordant with cell}(i, j)) + \frac{1}{2}\text{Prob}(Y \text{ is tied with cell}(i, j)) \\ &= \text{Prob}((\text{group} < i \text{ and } Y > j) \text{ or } (\text{group} > i \text{ and } Y < j)) + \\ &\quad \frac{1}{2}\text{Prob}(\text{group} \neq i \text{ and } Y = j) \\ &= \sum_{g=1}^2 \sum_{c=1}^C w_g \tilde{p}_{gc} \left[ I_{(g-i)(c-j) < 0} + \frac{1}{2} I_{g \neq i, c=j} \right] \end{aligned}$$

For an independent random draw  $Y_1, Y_2$  from the two distributions,

$$\begin{aligned} P_c &= \text{Prob}(Y_1, Y_2 \text{ concordant}) + \frac{1}{2}\text{Prob}(Y_1, Y_2 \text{ tied}) \\ &= \sum_{i=1}^2 \sum_{j=1}^C w_i \tilde{p}_{ij} Rs_{ij} \end{aligned}$$

and

$$\begin{aligned} P_d &= \text{Prob}(Y_1, Y_2 \text{ discordant}) + \frac{1}{2}\text{Prob}(Y_1, Y_2 \text{ tied}) \\ &= \sum_{i=1}^2 \sum_{j=1}^C w_i \tilde{p}_{ij} Rd_{ij} \end{aligned}$$

Then

$$\text{WMW}_{\text{odds}} = \frac{P_c}{P_d}$$

Proceeding to compute the theoretical standard error associated with  $WMW_{odds}$  (that is, the population analogue to the sample standard error),

$$SE(WMW_{odds}) = \frac{2}{P_d} \left[ \sum_{i=1}^2 \sum_{j=1}^C w_i \tilde{p}_{ij} (WMW_{odds} R_{dij} - R_{s_{ij}})^2 / N \right]^{\frac{1}{2}}$$

Converting to the natural log scale and using the delta method,

$$SE(\log(WMW_{odds})) = \frac{SE(WMW_{odds})}{WMW_{odds}}$$

The next step is to produce a “smoothed” version of the  $2 \times C$  cell probabilities that conforms to the null hypothesis of the Wilcoxon-Mann-Whitney test (in other words, independence in the  $2 \times C$  contingency table of probabilities). Let  $SE_{H_0}(\log(WMW_{odds}))$  denote the theoretical standard error of  $\log(WMW_{odds})$  assuming  $H_0$ .

Finally we have all of the terms needed to compute the power, using the noncentral chi-square and normal distributions:

$$\text{power} = \begin{cases} P \left( Z \geq \frac{SE_{H_0}(\log(WMW_{odds}))}{SE(\log(WMW_{odds}))} z_{1-\alpha} - \delta^* N^{\frac{1}{2}} \right), & \text{upper one-sided} \\ P \left( Z \leq \frac{SE_{H_0}(\log(WMW_{odds}))}{SE(\log(WMW_{odds}))} z_{\alpha} - \delta^* N^{\frac{1}{2}} \right), & \text{lower one-sided} \\ P \left( \chi^2(1, (\delta^*)^2 N) \geq \left[ \frac{SE_{H_0}(\log(WMW_{odds}))}{SE(\log(WMW_{odds}))} \right]^2 \chi^2_{1-\alpha}(1) \right), & \text{two-sided} \end{cases}$$

where

$$\delta^* = \frac{\log(WMW_{odds})}{N^{\frac{1}{2}} SE(\log(WMW_{odds}))}$$

is the primary noncentrality—that is, the “effect size” that quantifies how much the two conjectured distributions differ.  $Z$  is a standard normal random variable,  $\chi^2(df, nc)$  is a noncentral  $\chi^2$  random variable with degrees of freedom  $df$  and noncentrality  $nc$ , and  $N$  is the total sample size.

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “[Statistical Graphics Using ODS](#).”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS](#).”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “[A Primer on ODS Statistical Graphics](#)” on page 599 in Chapter 21, “[Statistical Graphics Using ODS](#).”

If ODS Graphics is not enabled, then PROC POWER creates traditional graphics.

You can reference every graph produced through ODS Graphics with a name. The names of the graphs that PROC POWER generates are listed in [Table 71.31](#), along with the required statements and options.

**Table 71.31** Graphs Produced by PROC POWER

| ODS Graph Name | Plot Description                                                                                         | Option |
|----------------|----------------------------------------------------------------------------------------------------------|--------|
| PowerPlot      | Plot with two of the following three parameters on the X and Y axes: power, sample size, and effect size | PLOT   |
| PowerAbort     | Empty plot that shows an error message when a plot could not be produced                                 | PLOT   |

## ODS Styles Suitable for Use with PROC POWER

ODS styles control the appearance of graphs produced by PROC POWER. ODS provides over 50 styles, but most are not suitable for use in PROC POWER. PROC POWER requires a style that distinguishes curves based on a combination of color, line style, and symbol marker. Styles that are well-suited for use in PROC POWER include: STATISTICAL, ANALYSIS, DEFAULT, LISTING, and HTMLBLUECML. The HTMLBLUE and PLATEAU styles are commonly used, but they are not well-suited for use with PROC POWER because they rely primarily on color to distinguish curves rather than a combination of color, line style, and symbol marker.

In this chapter, a style is explicitly specified at the start of each example that uses ODS Graphics to remind you to use one of the suitable styles. Styles are specified in an ODS destination statement. Destinations include LISTING, HTML, RTF, PDF, and many others. You can set the style and the destination as follows:

```
ods html style=htmlbluecml;
ods graphics on;

proc power;
 onesamplemeans
 mean = 5 10
 ntotal = 150
 stddev = 30 50
 power = .;
 plot x=n min=100 max=200;
run;

ods graphics off;
ods html close;
```

For more information about ODS and ODS destinations, see Chapter 20, “Using the Output Delivery System.” For more information ODS styles, see Chapter 21, “Statistical Graphics Using ODS.”

## Examples: POWER Procedure

### Example 71.1: One-Way ANOVA

This example deals with the same situation as in Example 44.1 of Chapter 44, “The GLMPOWER Procedure.”

Hocking (1985, p. 109) describes a study of the effectiveness of electrolytes in reducing lactic acid buildup for long-distance runners. You are planning a similar study in which you will allocate five different fluids to runners on a 10-mile course and measure lactic acid buildup immediately after the run. The fluids consist of water and two commercial electrolyte drinks, EZDure and LactoZap, each prepared at two concentrations, low (EZD1 and LZ1) and high (EZD2 and LZ2).

You conjecture that the standard deviation of lactic acid measurements given any particular fluid is about 3.75, and that the expected lactic acid values will correspond roughly to those in Table 71.32. You are least familiar with the LZ1 drink and hence decide to consider a range of reasonable values for that mean.

**Table 71.32** Mean Lactic Acid Buildup by Fluid

| Water | EZD1 | EZD2 | LZ1      | LZ2  |
|-------|------|------|----------|------|
| 35.6  | 33.7 | 30.2 | 29 or 28 | 25.9 |

You are interested in four different comparisons, shown in Table 71.33 with appropriate contrast coefficients.

**Table 71.33** Planned Comparisons

| Comparison                | Contrast Coefficients |      |      |     |     |
|---------------------------|-----------------------|------|------|-----|-----|
|                           | Water                 | EZD1 | EZD2 | LZ1 | LZ2 |
| Water versus electrolytes | 4                     | -1   | -1   | -1  | -1  |
| EZD versus LZ             | 0                     | 1    | 1    | -1  | -1  |
| EZD1 versus EZD2          | 0                     | 1    | -1   | 0   | 0   |
| LZ1 versus LZ2            | 0                     | 0    | 0    | 1   | -1  |

For each of these contrasts you want to determine the sample size required to achieve a power of 0.9 for detecting an effect with magnitude in accord with Table 71.32. You are not yet attempting to choose a single sample size for the study, but rather checking the range of sample sizes needed for individual contrasts. You plan to test each contrast at  $\alpha = 0.025$ . In the interests of reducing costs, you will provide twice as many runners with water as with any of the electrolytes; in other words, you will use a sample size weighting scheme of 2:1:1:1:1. Use the `ONEWAYANOVA` statement in the POWER procedure to compute the sample sizes.

The statements required to perform this analysis are as follows:

```
proc power;
 onewayanova
 groupmeans = 35.6 | 33.7 | 30.2 | 29 28 | 25.9
 stddev = 3.75
 groupweights = (2 1 1 1 1)
 alpha = 0.025
 ntotal = .
 power = 0.9
 contrast = (4 -1 -1 -1 -1) (0 1 1 -1 -1)
 (0 1 -1 0 0) (0 0 0 1 -1);
run;
```

The `NTOTAL=` option with a missing value (.) indicates total sample size as the result parameter. The `GROUPMEANS=` option with values from Table 71.32 specifies your conjectures for the means. With only one mean varying (the LZ1 mean), the “crossed” notation is simpler, showing scenarios for each group mean, separated by vertical bars (|). See the section “Specifying Value Lists in Analysis Statements” on page 6020 for more details on crossed and matched notations for grouped values. The contrasts in Table 71.33 are specified with the `CONTRAST=` option, by using the “matched” notation with each contrast enclosed in parentheses. The `STDDEV=`, `ALPHA=`, and `POWER=` options specify the error standard deviation, significance level, and power. The `GROUPWEIGHTS=` option specifies the weighting schemes. Default values for the `NULLCONTRAST=` and `SIDES=` options specify a two-sided *t* test of the contrast equal to 0. See Output 71.1.1 for the results.

**Output 71.1.1** Sample Sizes for One-Way ANOVA Contrasts

| The POWER Procedure                 |                    |           |    |    |    |                 |      |      |    |      |              |         |
|-------------------------------------|--------------------|-----------|----|----|----|-----------------|------|------|----|------|--------------|---------|
| Single DF Contrast in One-Way ANOVA |                    |           |    |    |    |                 |      |      |    |      |              |         |
| Fixed Scenario Elements             |                    |           |    |    |    |                 |      |      |    |      |              |         |
| Method                              |                    | Exact     |    |    |    |                 |      |      |    |      |              |         |
| Alpha                               |                    | 0.025     |    |    |    |                 |      |      |    |      |              |         |
| Standard Deviation                  |                    | 3.75      |    |    |    |                 |      |      |    |      |              |         |
| Group Weights                       |                    | 2 1 1 1 1 |    |    |    |                 |      |      |    |      |              |         |
| Nominal Power                       |                    | 0.9       |    |    |    |                 |      |      |    |      |              |         |
| Number of Sides                     |                    | 2         |    |    |    |                 |      |      |    |      |              |         |
| Null Contrast Value                 |                    | 0         |    |    |    |                 |      |      |    |      |              |         |
| Computed N Total                    |                    |           |    |    |    |                 |      |      |    |      |              |         |
| Index                               | -----Contrast----- |           |    |    |    | -----Means----- |      |      |    |      | Actual Power | N Total |
| 1                                   | 4                  | -1        | -1 | -1 | -1 | 35.6            | 33.7 | 30.2 | 29 | 25.9 | 0.947        | 30      |
| 2                                   | 4                  | -1        | -1 | -1 | -1 | 35.6            | 33.7 | 30.2 | 28 | 25.9 | 0.901        | 24      |
| 3                                   | 0                  | 1         | 1  | -1 | -1 | 35.6            | 33.7 | 30.2 | 29 | 25.9 | 0.929        | 60      |
| 4                                   | 0                  | 1         | 1  | -1 | -1 | 35.6            | 33.7 | 30.2 | 28 | 25.9 | 0.922        | 48      |
| 5                                   | 0                  | 1         | -1 | 0  | 0  | 35.6            | 33.7 | 30.2 | 29 | 25.9 | 0.901        | 174     |
| 6                                   | 0                  | 1         | -1 | 0  | 0  | 35.6            | 33.7 | 30.2 | 28 | 25.9 | 0.901        | 174     |
| 7                                   | 0                  | 0         | 0  | 1  | -1 | 35.6            | 33.7 | 30.2 | 29 | 25.9 | 0.902        | 222     |
| 8                                   | 0                  | 0         | 0  | 1  | -1 | 35.6            | 33.7 | 30.2 | 28 | 25.9 | 0.902        | 480     |

The sample sizes in [Output 71.1.1](#) range from 24 for the comparison of water versus electrolytes to 480 for the comparison of LZ1 versus LZ2, both assuming the smaller LZ1 mean. The sample size for the latter comparison is relatively large because the small mean difference of  $28 - 25.9 = 2.1$  is hard to detect.

The Nominal Power of 0.9 in the “Fixed Scenario Elements” table in [Output 71.1.1](#) represents the input target power, and the Actual Power column in the “Computed N Total” table is the power at the sample size (N Total) adjusted to achieve the specified sample weighting. Note that all of the sample sizes are rounded up to multiples of 6 to preserve integer group sizes (since the group weights add up to 6). You can use the `NFRACTIONAL` option in the `ONEWAYANOVA` statement to compute raw fractional sample sizes.

Suppose you want to plot the required sample size for the range of power values from 0.5 to 0.95. First, define the analysis by specifying the same statements as before, but add the `PLOTONLY` option to the `PROC POWER` statement to disable the nongraphical results. Next, specify the `PLOT` statement with `X=POWER` to request a plot with power on the X axis. (The result parameter, here sample size, is always plotted on the other axis.) Use the `MIN=` and `MAX=` options in the `PLOT` statement to specify the power range. The following statements produce the plot shown in [Output 71.1.2](#).

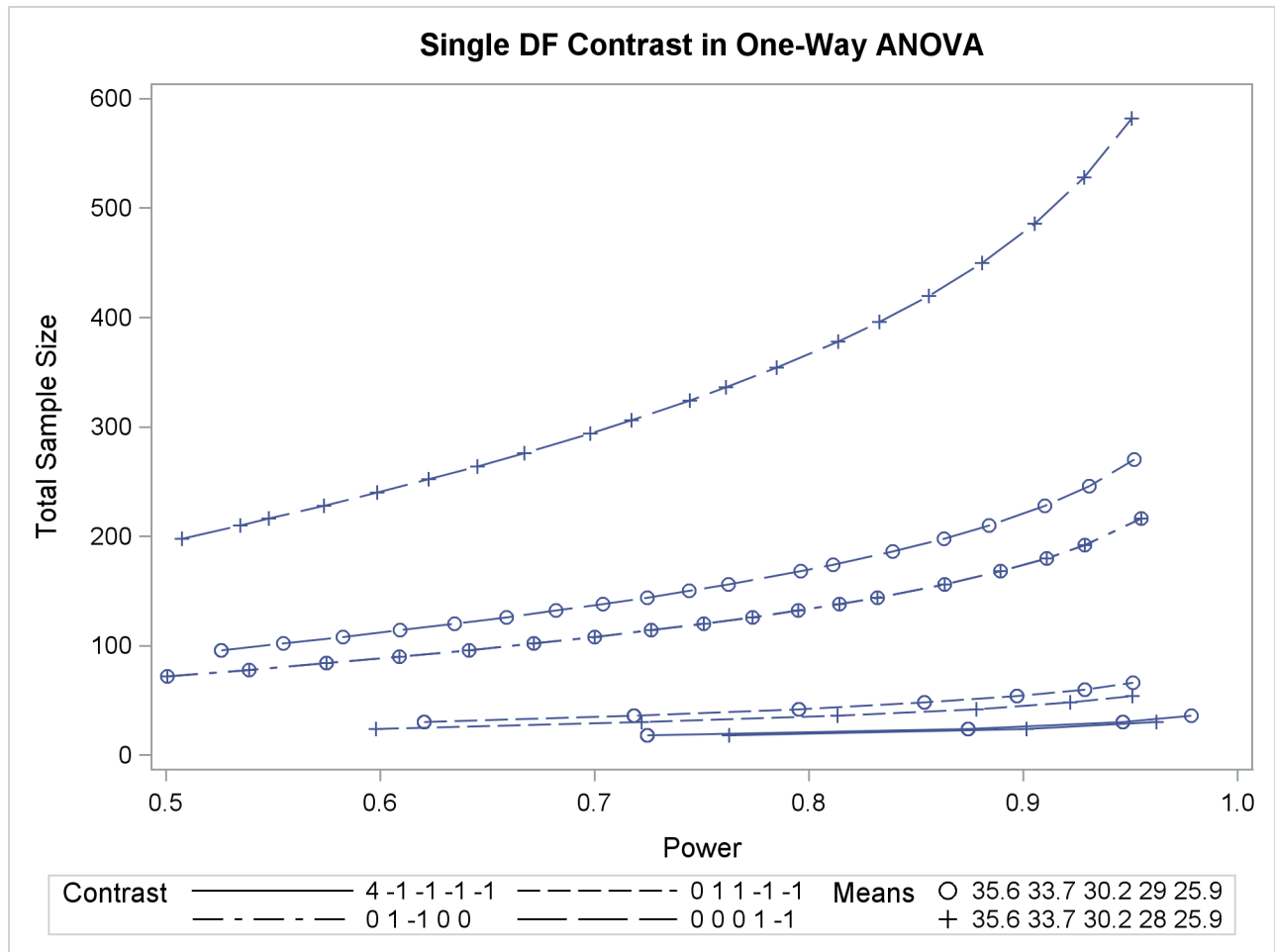
```
ods listing style=htmlbluecml;
ods graphics on;

proc power plotonly;
 onewayanova
 groupmeans = 35.6 | 33.7 | 30.2 | 29 28 | 25.9
 stddev = 3.75
 groupweights = (2 1 1 1 1)
 alpha = 0.025
 ntotal = .
 power = 0.9
 contrast = (4 -1 -1 -1 -1) (0 1 1 -1 -1)
 (0 1 -1 0 0) (0 0 0 1 -1);
 plot x=power min=.5 max=.95;
run;
```

The `ODS LISTING STYLE=HTMLBLUECML` statement specifies the `HTMLBLUECML` style, which is suitable for use with `PROC POWER` because it allows both marker symbols and line styles to vary. See the section “[ODS Styles Suitable for Use with PROC POWER](#)” on page 6082 for more information.



**Output 71.1.2** Plot of Sample Size versus Power for One-Way ANOVA Contrasts



In **Output 71.1.2**, the line style identifies the contrast, and the plotting symbol identifies the group means scenario. The plot shows that the required sample size is highest for the (0 0 0 1 -1) contrast, corresponding to the test of LZ1 versus LZ2 that was previously found to require the most resources, in either cell means scenario.

Note that some of the plotted points in [Output 71.1.2](#) are unevenly spaced. This is because the plotted points are the *rounded* sample size results at their corresponding *actual* power levels. The range specified with the `MIN=` and `MAX=` values in the `PLOT` statement corresponds to *nominal* power levels. In some cases, actual power is substantially higher than nominal power. To obtain plots with evenly spaced points (but with *fractional* sample sizes at the computed points), you can use the `NFRACTIONAL` option in the analysis statement preceding the `PLOT` statement.

Finally, suppose you want to plot the power for the range of sample sizes you will likely consider for the study (the range of 24 to 480 that achieves 0.9 power for different comparisons). In the `ONEWAYANOVA` statement, identify power as the result (`POWER=.`), and specify `NTOTAL=24`. The following statements produce the plot:

```
proc power plotonly;
 onewayanova
 groupmeans = 35.6 | 33.7 | 30.2 | 29 28 | 25.9
 stddev = 3.75
 groupweights = (2 1 1 1 1)
 alpha = 0.025
 ntotal = 24
 power = .
 contrast = (4 -1 -1 -1 -1) (0 1 1 -1 -1)
 (0 1 -1 0 0) (0 0 0 1 -1);
 plot x=n min=24 max=480;
run;

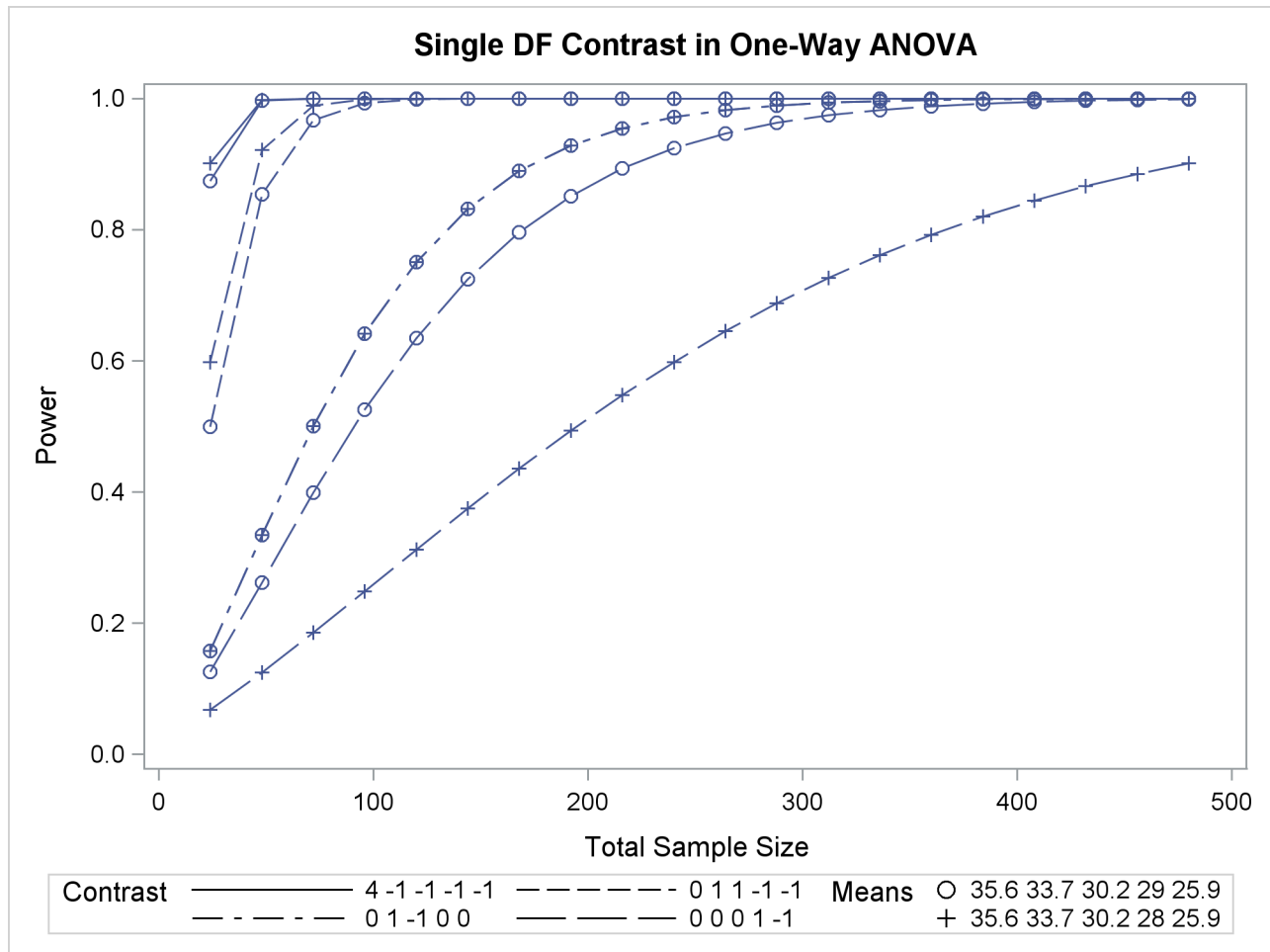
ods graphics off;
```

The `X=N` option in the `PLOT` statement requests a plot with sample size on the X axis.

Note that the value specified with the `NTOTAL=24` option is not used. It is overridden in the plot by the `MIN=` and `MAX=` options in the `PLOT` statement, and the `PLOTONLY` option in the `PROC POWER` statement disables nongraphical results. But the `NTOTAL=` option (along with a value) is still needed in the `ONEWAYANOVA` statement as a placeholder, to identify the desired parameterization for sample size.

Output 71.1.3 shows the resulting plot.

**Output 71.1.3** Plot of Power versus Sample Size for One-Way ANOVA Contrasts



Although Output 71.1.2 and Output 71.1.3 surface essentially the same computations for practical power ranges, they each provide a different quick visual assessment. Output 71.1.2 reveals the range of required sample sizes for powers of interest, and Output 71.1.3 reveals the range of achieved powers for sample sizes of interest.

### Example 71.2: The Sawtooth Power Function in Proportion Analyses

For many common statistical analyses, the power curve is monotonically increasing: the more samples you take, the more power you achieve. However, in statistical analyses of discrete data, such as tests of proportions, the power curve is often nonmonotonic. A small increase in sample size can result in a *decrease* in power, a decrease that is sometimes substantial. The explanation is that the actual significance level (in other words, the achieved Type I error rate) for discrete tests strays below the target level and varies with sample size. The power loss from a decrease in the Type I error rate can outweigh the power gain from an increase in sample size. The example discussed here demonstrates this “sawtooth” phenomenon. For additional discussion on the topic, see Chernick and Liu (2002).

Suppose you have a new scheduling system for an airline, and you want to determine how many flights you must observe to have at least an 80% chance of establishing an improvement in the proportion of late arrivals on a specific travel route. You will use a one-sided exact binomial proportion test with a null proportion of 30%, the frequency of late arrivals under the previous scheduling system, and a nominal significance level of  $\alpha = 0.05$ . Well-supported predictions estimate the new late arrival rate to be about 20%, and you will base your sample size determination on this assumption.

The POWER procedure does not currently compute exact sample size directly for the exact binomial test. But you can get an initial estimate by computing the approximate sample size required for a  $z$  test. Use the `ONESAMPLEFREQ` statement in the POWER procedure with `TEST=Z` and `METHOD=NORMAL` to compute the approximate sample size to achieve a power of 0.8 by using the  $z$  test. The following statements perform the analysis:

```
proc power;
 onesamplefreq test=z method=normal
 sides = 1
 alpha = 0.05
 nullproportion = 0.3
 proportion = 0.2
 ntotal = .
 power = 0.8;
run;
```

The `NTOTAL=` option with a missing value (.) indicates sample size as the result parameter. The `SIDES=1` option specifies a one-sided test. The `ALPHA=`, `NULLPROPORTION=`, and `POWER=` options specify the significance level of 0.05, null value of 0.3, and target power of 0.8, respectively. The `PROPORTION=` option specifies your conjecture of 0.3 for the true proportion.

**Output 71.2.1** Approximate Sample Size for  $z$  Test of a Proportion

| The POWER Procedure            |                      |      |
|--------------------------------|----------------------|------|
| Z Test for Binomial Proportion |                      |      |
| Fixed Scenario Elements        |                      |      |
| Method                         | Normal approximation |      |
| Number of Sides                |                      | 1    |
| Null Proportion                |                      | 0.3  |
| Alpha                          |                      | 0.05 |
| Binomial Proportion            |                      | 0.2  |
| Nominal Power                  |                      | 0.8  |
| Variance Estimate              | Null Variance        |      |
| Computed N Total               |                      |      |
| Actual                         | N                    |      |
| Power                          | Total                |      |
| 0.800                          | 119                  |      |

The results, shown in [Output 71.2.1](#), indicate that you need to observe about  $N = 119$  flights to have an 80% chance of rejecting the hypothesis of a late arrival proportion of 30% or higher, if the true proportion is 20%,

by using the  $z$  test. A similar analysis (Output 71.2.2) reveals an approximate sample size of  $N = 129$  for the  $z$  test with continuity correction, which is performed by using `TEST=ADJZ`:

```
proc power;
 onesamplefreq test=adjz method=normal
 sides = 1
 alpha = 0.05
 nullproportion = 0.3
 proportion = 0.2
 ntotal = .
 power = 0.8;
run;
```

**Output 71.2.2** Approximate Sample Size for  $z$  Test with Continuity Correction

| The POWER Procedure                                       |                      |       |
|-----------------------------------------------------------|----------------------|-------|
| Z Test for Binomial Proportion with Continuity Adjustment |                      |       |
| Fixed Scenario Elements                                   |                      |       |
| Method                                                    | Normal approximation |       |
| Number of Sides                                           |                      | 1     |
| Null Proportion                                           |                      | 0.3   |
| Alpha                                                     |                      | 0.05  |
| Binomial Proportion                                       |                      | 0.2   |
| Nominal Power                                             |                      | 0.8   |
| Variance Estimate                                         | Null Variance        |       |
| Computed N Total                                          |                      |       |
|                                                           | Actual               | N     |
|                                                           | Power                | Total |
|                                                           | 0.801                | 129   |

Based on the approximate sample size results, you decide to explore the power of the exact binomial test for sample sizes between 110 and 140. The following statements produce the plot:

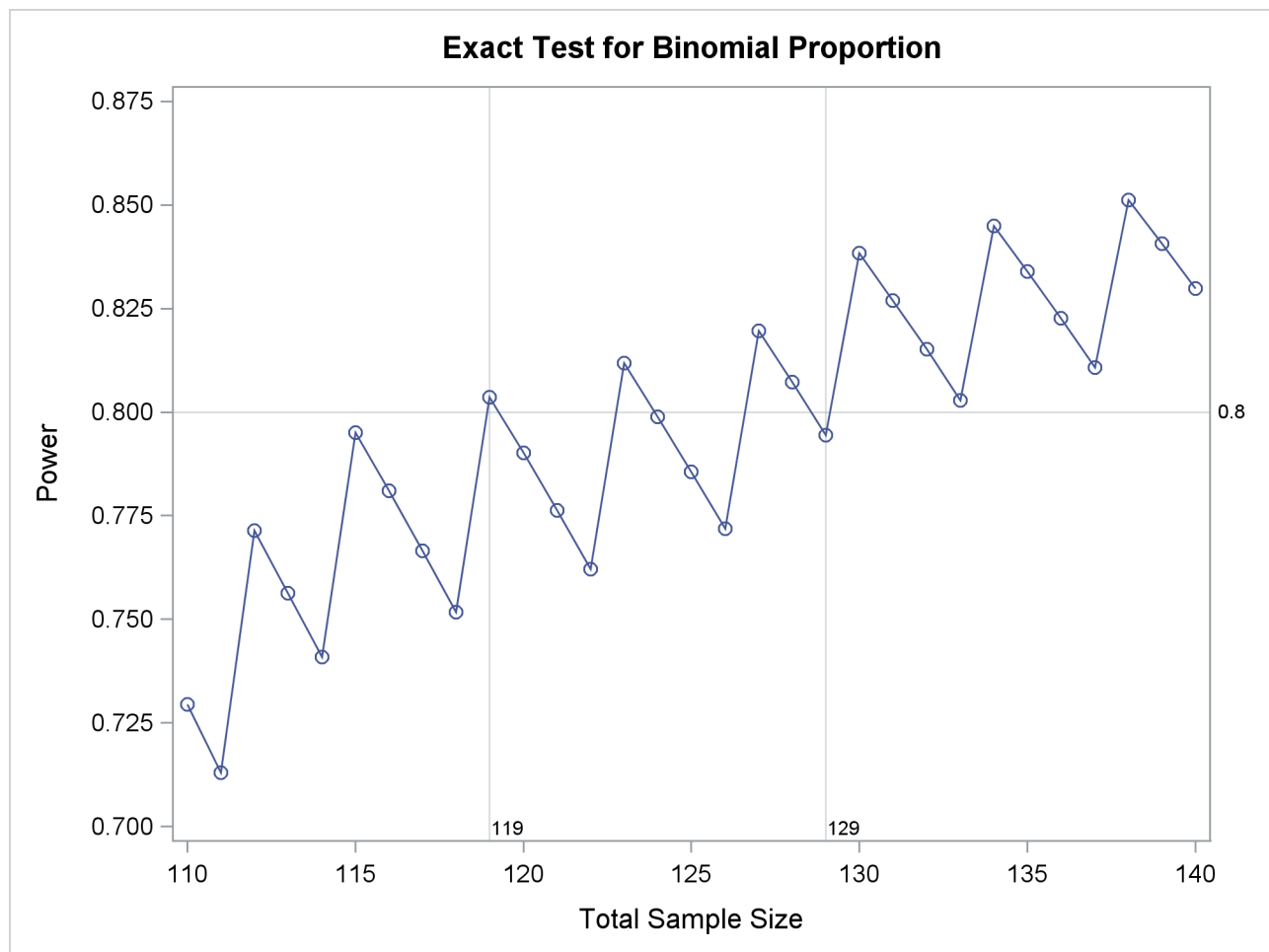
```
ods listing style=htmlbluecml;
ods graphics on;

proc power plotonly;
 onesamplefreq test=exact
 sides = 1
 alpha = 0.05
 nullproportion = 0.3
 proportion = 0.2
 ntotal = 119
 power = .;
 plot x=n min=110 max=140 step=1
 yopts=(ref=.8) xopts=(ref=119 129);
run;
```

The ODS LISTING STYLE=HTMLBLUECML statement specifies the HTMLBLUECML style, which is suitable for use with PROC POWER because it allows both marker symbols and line styles to vary. See the section “ODS Styles Suitable for Use with PROC POWER” on page 6082 for more information.

The TEST=EXACT option in the ONESAMPLEFREQ statement specifies the exact binomial test, and the missing value (.) for the POWER= option indicates power as the result parameter. The PLOTONLY option in the PROC POWER statement disables nongraphical output. The PLOT statement with X=N requests a plot with sample size on the X axis. The MIN= and MAX= options in the PLOT statement specify the sample size range. The YOPTS=(REF=) and XOPTS=(REF=) options add reference lines to highlight the approximate sample size results. The STEP=1 option produces a point at each integer sample size. The sample size value specified with the NTOTAL= option in the ONESAMPLEFREQ statement is overridden by the MIN= and MAX= options in the PLOT statement. Output 71.2.3 shows the resulting plot.

**Output 71.2.3** Plot of Power versus Sample Size for Exact Binomial Test



Note the sawtooth pattern in Output 71.2.3. Although the power surpasses the target level of 0.8 at  $N = 119$ , it decreases to 0.79 with  $N = 120$  and further to 0.76 with  $N = 122$  before rising again to 0.81 with  $N = 123$ . Not until  $N = 130$  does the power stay above the 0.8 target. Thus, a more conservative sample size recommendation of 130 might be appropriate, depending on the precise goals of the sample size determination.

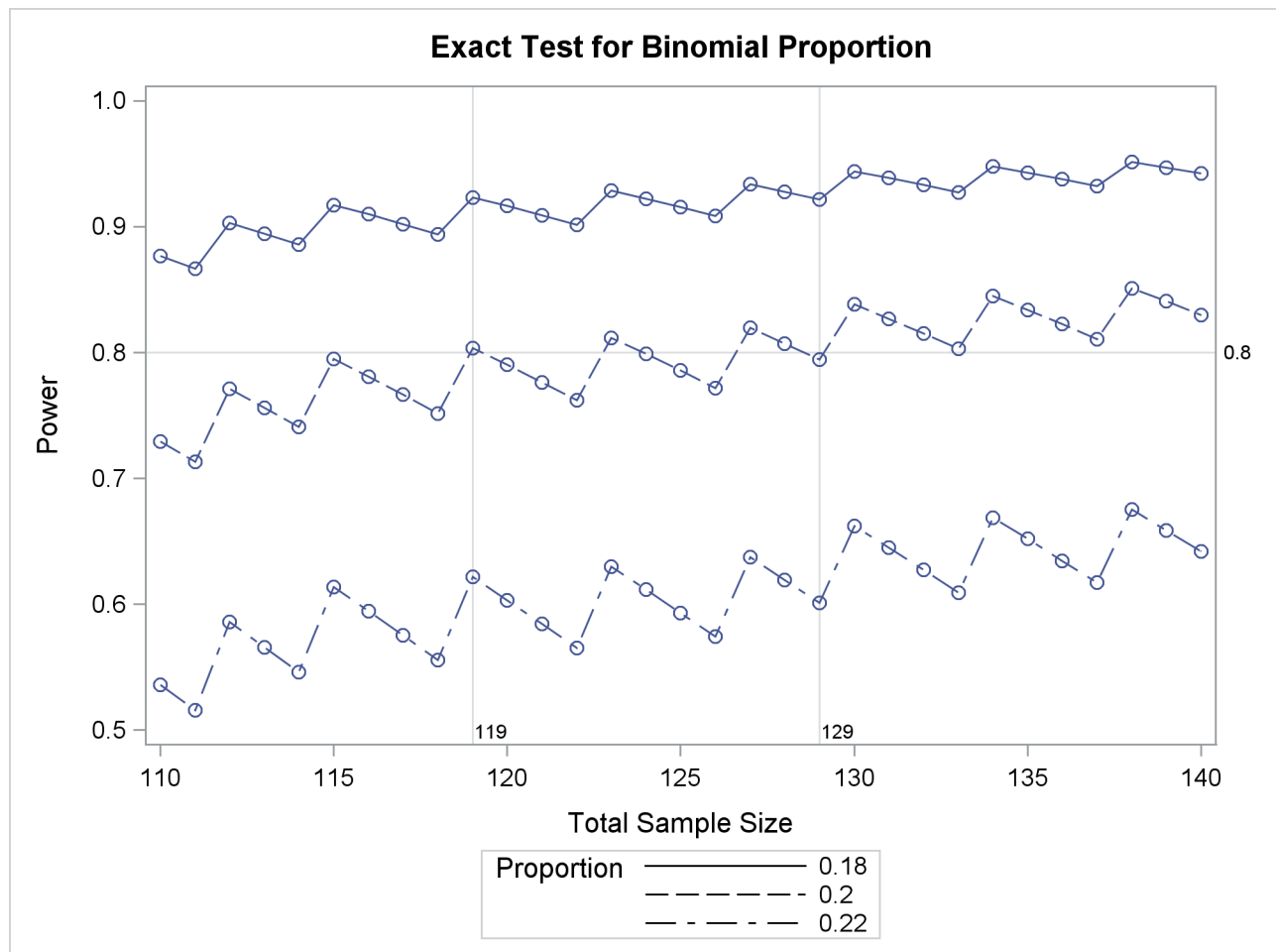
In addition to considering alternative sample sizes, you might also want to assess the sensitivity of the power to inaccuracies in assumptions about the true proportion. The following statements produce a plot including true proportion values of 0.18 and 0.22. They are identical to the previous statements except for

the additional true proportion values specified with the `PROPORTION=` option in the `ONESAMPLEFREQ` statement.

```
proc power plotonly;
 onesamplefreq test=exact
 sides = 1
 alpha = 0.05
 nullproportion = 0.3
 proportion = 0.18 0.2 0.22
 ntotal = 119
 power = .;
 plot x=n min=110 max=140 step=1
 yopts=(ref=.8) xopts=(ref=119 129);
run;
```

Output 71.2.4 shows the resulting plot.

**Output 71.2.4** Plot for Assessing Sensitivity to True Proportion Value



The plot reveals a dramatic sensitivity to the true proportion value. For  $N=119$ , the power is about 0.92 if the true proportion is 0.18, and as low as 0.62 if the proportion is 0.22. Note also that the power jumps occur at the same sample sizes in all three curves; the curves are only shifted and stretched vertically. This is because spikes and valleys in power curves are invariant to the true proportion value; they are due to changes in the critical value of the test.

A closer look at some ancillary output from the analysis sheds light on this property of the sawtooth pattern. You can add an ODS OUTPUT statement to save the plot content corresponding to [Output 71.2.3](#) to a data set:

```
proc power plotonly;
 ods output plotcontent=PlotData;
 onesamplefreq test=exact
 sides = 1
 alpha = 0.05
 nullproportion = 0.3
 proportion = 0.2
 ntotal = 119
 power = .;
 plot x=n min=110 max=140 step=1
 yopts=(ref=.8) xopts=(ref=119 129);
run;
```

The PlotData data set contains parameter values for each point in the plot. The parameters include underlying characteristics of the putative test. The following statements print the critical value and actual significance level along with sample size and power:

```
proc print data=PlotData;
 var NTotal LowerCritVal Alpha Power;
run;
```



Output 71.2.5 shows the plot data.

**Output 71.2.5** Numerical Content of Plot

| Obs | NTotal | Lower<br>CritVal | Alpha  | Power |
|-----|--------|------------------|--------|-------|
| 1   | 110    | 24               | 0.0356 | 0.729 |
| 2   | 111    | 24               | 0.0313 | 0.713 |
| 3   | 112    | 25               | 0.0446 | 0.771 |
| 4   | 113    | 25               | 0.0395 | 0.756 |
| 5   | 114    | 25               | 0.0349 | 0.741 |
| 6   | 115    | 26               | 0.0490 | 0.795 |
| 7   | 116    | 26               | 0.0435 | 0.781 |
| 8   | 117    | 26               | 0.0386 | 0.767 |
| 9   | 118    | 26               | 0.0341 | 0.752 |
| 10  | 119    | 27               | 0.0478 | 0.804 |
| 11  | 120    | 27               | 0.0425 | 0.790 |
| 12  | 121    | 27               | 0.0377 | 0.776 |
| 13  | 122    | 27               | 0.0334 | 0.762 |
| 14  | 123    | 28               | 0.0465 | 0.812 |
| 15  | 124    | 28               | 0.0414 | 0.799 |
| 16  | 125    | 28               | 0.0368 | 0.786 |
| 17  | 126    | 28               | 0.0327 | 0.772 |
| 18  | 127    | 29               | 0.0453 | 0.820 |
| 19  | 128    | 29               | 0.0404 | 0.807 |
| 20  | 129    | 29               | 0.0359 | 0.794 |
| 21  | 130    | 30               | 0.0493 | 0.838 |
| 22  | 131    | 30               | 0.0441 | 0.827 |
| 23  | 132    | 30               | 0.0394 | 0.815 |
| 24  | 133    | 30               | 0.0351 | 0.803 |
| 25  | 134    | 31               | 0.0480 | 0.845 |
| 26  | 135    | 31               | 0.0429 | 0.834 |
| 27  | 136    | 31               | 0.0384 | 0.823 |
| 28  | 137    | 31               | 0.0342 | 0.811 |
| 29  | 138    | 32               | 0.0466 | 0.851 |
| 30  | 139    | 32               | 0.0418 | 0.841 |
| 31  | 140    | 32               | 0.0374 | 0.830 |

Note that whenever the critical value changes, the actual  $\alpha$  jumps up to a value close to the nominal  $\alpha=0.05$ , and the power also jumps up. Then while the critical value stays constant, the actual  $\alpha$  and power slowly decrease. The critical value is independent of the true proportion value. So you can achieve a locally maximal power by choosing a sample size corresponding to a spike on the sawtooth curve, and this choice is locally optimal *regardless* of the unknown value of the true proportion. Locally optimal sample sizes in this case include 115, 119, 123, 127, 130, and 134.

As a point of interest, the power does not always jump sharply and decrease gradually. The shape of the sawtooth depends on the direction of the test and the location of the null proportion relative to 0.5. For example, if the direction of the hypothesis in this example is reversed (by switching true and null proportion values) so that the rejection region is in the upper tail, then the power curve exhibits sharp decreases and gradual increases. The following statements are similar to those producing the plot in [Output 71.2.3](#) but with values of the `PROPORTION=` and `NULLPROPORTION=` options switched:

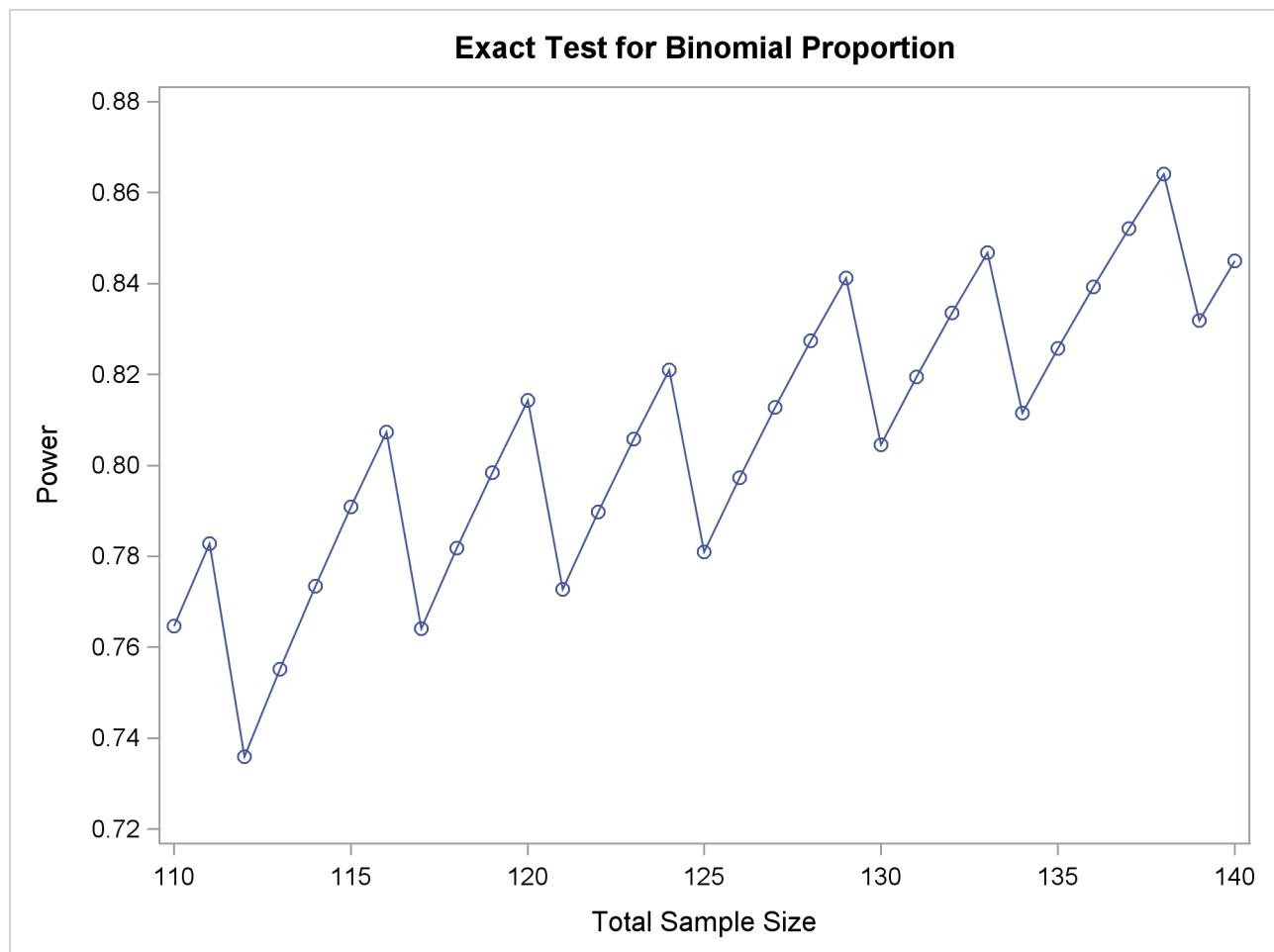
```

proc power plotonly;
 onesamplefreq test=exact
 sides = 1
 alpha = 0.05
 nullproportion = 0.2
 proportion = 0.3
 ntotal = 119
 power = .;
 plot x=n min=110 max=140 step=1;
run;

```

The resulting plot is shown in [Output 71.2.6](#).

**Output 71.2.6** Plot of Power versus Sample Size for Another One-sided Test



Finally, two-sided tests can lead to even more irregular power curve shapes, since changes in lower and upper critical values affect the power in different ways. The following statements produce a plot of power versus sample size for the scenario of a two-sided test with high alpha and a true proportion close to the null value:

```

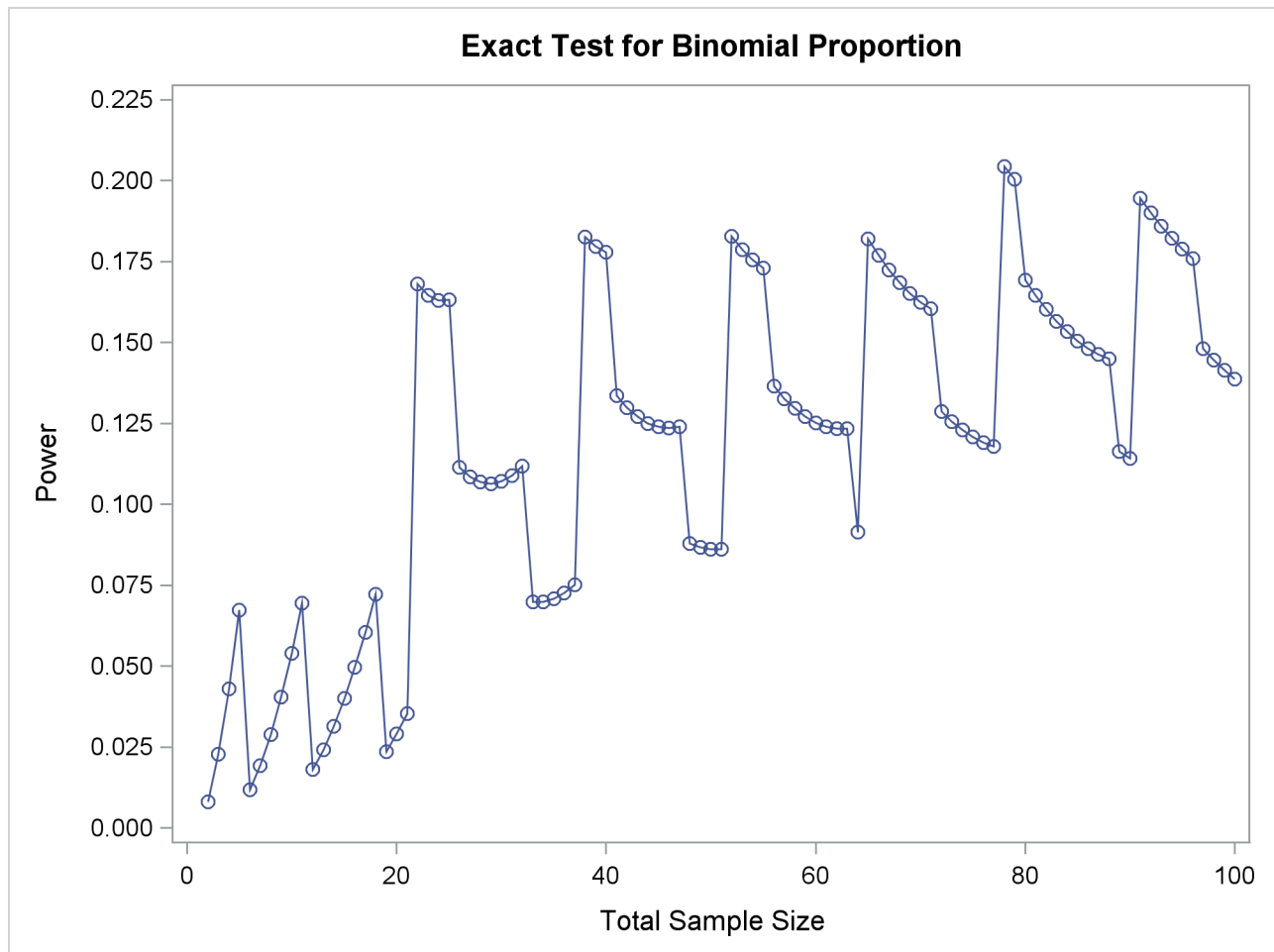
proc power plotonly;
 onesamplefreq test=exact
 sides = 2
 alpha = 0.2
 nullproportion = 0.1
 proportion = 0.09
 ntotal = 10
 power = .;
 plot x=n min=2 max=100 step=1;
run;

ods graphics off;

```

Output 71.2.7 shows the resulting plot.

**Output 71.2.7** Plot of Power versus Sample Size for a Two-Sided Test



Due to the irregular shapes of power curves for proportion tests, the question “Which sample size should I use?” is often insufficient. A sample size solution produced directly in PROC POWER reveals the smallest possible sample size to achieve your target power. But as the examples in this section demonstrate, it is helpful to consult graphs for answers to questions such as the following:

- Which sample size will guarantee that all higher sample sizes also achieve my target power?
- Given a candidate sample size, can I increase it slightly to achieve locally maximal power, or perhaps even decrease it and get higher power?

---

### Example 71.3: Simple AB/BA Crossover Designs

Crossover trials are experiments in which each subject is given a sequence of different treatments. They are especially common in clinical trials for medical studies. The reduction in variability from taking multiple measurements on a subject allows for more precise treatment comparisons. The simplest such design is the AB/BA crossover, in which each subject receives each of two treatments in a randomized order.

Under certain simplifying assumptions, you can test the treatment difference in an AB/BA crossover trial by using either a paired or two-sample  $t$  test (or equivalence test, depending on the hypothesis). This example will demonstrate when and how you can use the `PAIREDMEANS` statement in PROC POWER to perform power analyses for AB/BA crossover designs.

Senn (1993, Chapter 3) discusses a study comparing the effects of two bronchodilator medications in treatment of asthma, by using an AB/BA crossover design. Suppose you want to plan a similar study comparing two new medications, “Xilodol” and “Brantium.” Half of the patients would be assigned to sequence AB, getting a dose of Xilodol in the first treatment period, a wash-out period of one week, and then a dose of Brantium in the second treatment period. The other half would be assigned to sequence BA, following the same schedule but with the drugs reversed. In each treatment period you would administer the drugs in the morning and then measure peak expiratory flow (PEF) at the end of the day, with higher PEF representing better lung function.

You conjecture that the mean and standard deviation of PEF are about  $\mu_A = 330$  and  $\sigma_A = 40$  for Xilodol and  $\mu_B = 310$  and  $\sigma_B = 55$  for Brantium, and that each pair of measurements on the same subject will have a correlation of about 0.3. You want to compute the power of both one-sided and two-sided tests of mean difference, with a significance level of  $\alpha = 0.01$ , for a sample size of 100 patients and also plot the power for a range of 50 to 200 patients. Note that the allocation ratio of patients to the two sequences is irrelevant in this analysis.

The choice of statistical test depends on which assumptions are reasonable. One possibility is a  $t$  test. A paired or two-sample  $t$  test is valid when there is no carryover effect and no interactions between patients, treatments, and periods. See Senn (1993, Chapter 3) for more details. The choice between a paired or a two-sample test depends on what you assume about the period effect. If you assume no period effect, then a paired  $t$  test is the appropriate analysis for the design, with the first member of each pair being the Xilodol measurement (regardless of which sequence the patient belongs to). Otherwise, the two-sample  $t$  test approach is called for, since this analysis adjusts for the period effect by using an extra degree of freedom.

Suppose you assume no period effect. Then you can use the `PAIREDMEANS` statement in PROC POWER with the `TEST=DIFF` option to perform a sample size analysis for the paired  $t$  test. Indicate power as the result parameter by specifying the `POWER=` option with a missing value (.). Specify the conjectured means and standard deviations for each drug by using the `PAIREDMEANS=` and `PAIREDSTDDEVS=` options and the correlation by using the `CORR=` option. Specify both one- and two-sided tests by using the `SIDES=` option, the significance level by using the `ALPHA=` option, and the sample size (in terms of number of pairs) by using the `NPAIRS=` option. Generate a plot of power versus sample size by specifying the `PLOT`

statement with `X=N` to request a plot with sample size on the X axis. (The result parameter, here power, is always plotted on the other axis.) Use the `MIN=` and `MAX=` options in the `PLOT` statement to specify the sample size range (as numbers of pairs).

The following statements perform the sample size analysis:

```
ods listing style=htmlbluecml;
ods graphics on;

proc power;
 pairedmeans test=diff
 pairedmeans = (330 310)
 pairedstddevs = (40 55)
 corr = 0.3
 sides = 1 2
 alpha = 0.01
 npairs = 100
 power = .;
 plot x=n min=50 max=200;
run;

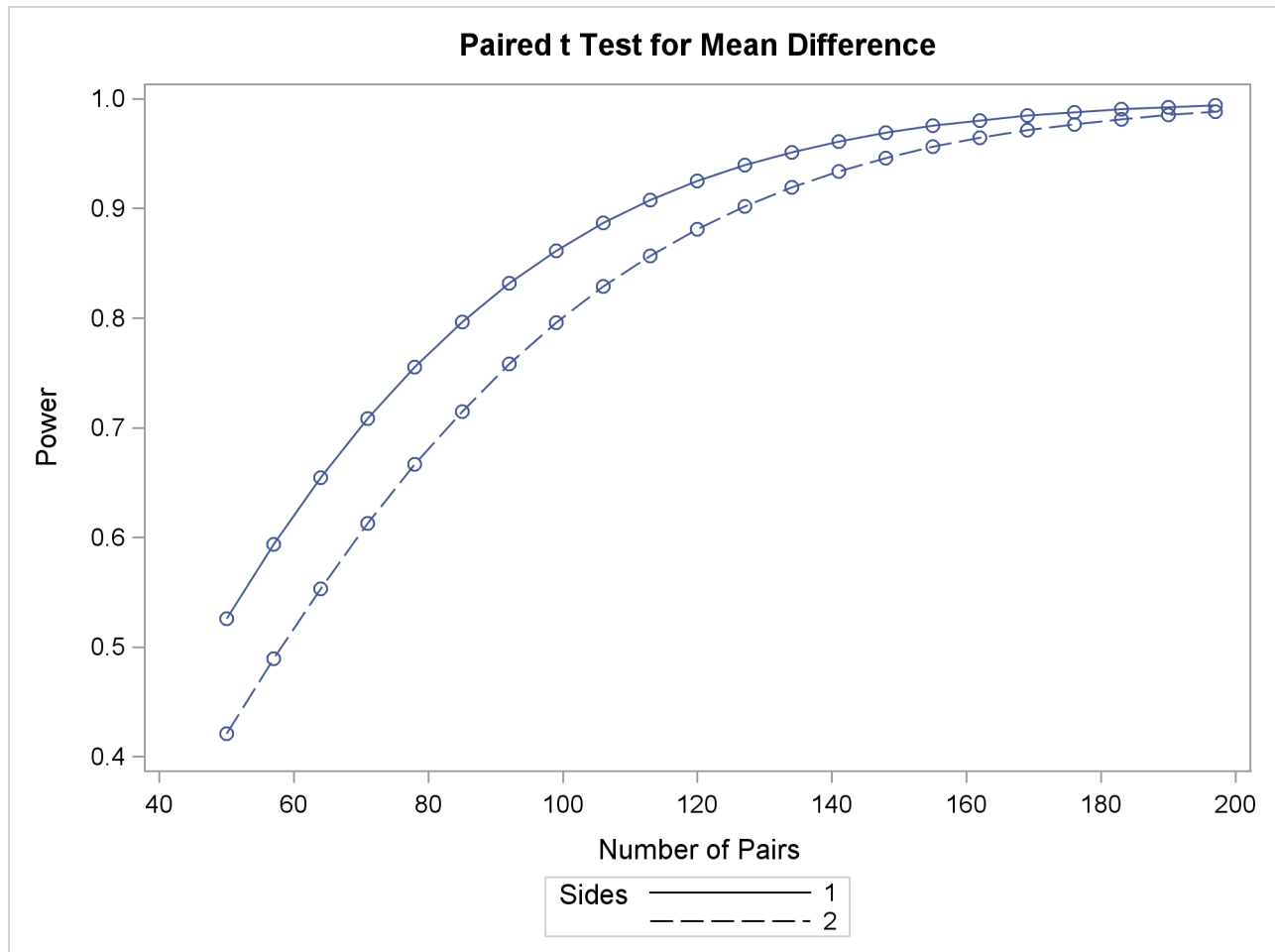
ods graphics off;
```

The `ODS LISTING STYLE=HTMLBLUECML` statement specifies the `HTMLBLUECML` style, which is suitable for use with `PROC POWER` because it allows both marker symbols and line styles to vary. See the section “[ODS Styles Suitable for Use with PROC POWER](#)” on page 6082 for more information.

Default values for the `NULLDIFF=` and `DIST=` options specify a null mean difference of 0 and the assumption of normally distributed data. The output is shown in [Output 71.3.1](#) and [Output 71.3.2](#).

**Output 71.3.1** Power for Paired *t* Analysis of Crossover Design

| The POWER Procedure               |       |        |
|-----------------------------------|-------|--------|
| Paired t Test for Mean Difference |       |        |
| Fixed Scenario Elements           |       |        |
| Distribution                      |       | Normal |
| Method                            |       | Exact  |
| Alpha                             |       | 0.01   |
| Mean 1                            |       | 330    |
| Mean 2                            |       | 310    |
| Standard Deviation 1              |       | 40     |
| Standard Deviation 2              |       | 55     |
| Correlation                       |       | 0.3    |
| Number of Pairs                   |       | 100    |
| Null Difference                   |       | 0      |
| Computed Power                    |       |        |
| Index                             | Sides | Power  |
| 1                                 | 1     | 0.865  |
| 2                                 | 2     | 0.801  |

**Output 71.3.2** Plot of Power versus Sample Size for Paired  $t$  Analysis of Crossover Design

The “Computed Power” table in [Output 71.3.1](#) shows that the power with 100 patients is about 0.8 for the two-sided test and 0.87 for the one-sided test with the alternative of larger Brantium mean. In [Output 71.3.2](#), the line style identifies the number of sides of the test. The plotting symbols identify locations of actual computed powers; the curves are linear interpolations of these points. The plot demonstrates how much higher the power is in the one-sided test than in the two-sided test for the range of sample sizes.

Suppose now that instead of detecting a difference between Xilodol and Brantium, you want to establish that they are similar—in particular, that the absolute mean PEF difference is at most 35. You might consider this goal if, for example, one of the drugs has fewer side effects and if a difference of no more than 35 is considered clinically small. Instead of a standard  $t$  test, you would conduct an *equivalence test* of the treatment mean difference for the two drugs. You would test the hypothesis that the true difference is less than  $-35$  or more than  $35$  against the alternative that the mean difference is between  $-35$  and  $35$ , by using an additive model and a two one-sided tests (“TOST”) analysis.

Assuming no period effect, you can use the `PAIREDMEANS` statement with the `TEST=EQUIV_DIFF` option to perform a sample size analysis for the paired equivalence test. Indicate power as the result parameter by specifying the `POWER=` option with a missing value (.). Use the `LOWER=` and `UPPER=` options to specify the equivalence bounds of  $-35$  and  $35$ . Use the `PAIREDMEANS=`, `PAIREDSTDDEVS=`, `CORR=`, and `ALPHA=` options in the same way as in the  $t$  test at the beginning of this example to specify the remaining parameters.

The following statements perform the sample size analysis:

```
proc power;
 pairedmeans test=equiv_add
 lower = -35
 upper = 35
 pairedmeans = (330 310)
 pairedstddevs = (40 55)
 corr = 0.3
 alpha = 0.01
 npairs = 100
 power = .;
run;
```

The default option `DIST=NORMAL` specifies an assumption of normally distributed data. The output is shown in [Output 71.3.3](#).

**Output 71.3.3** Power for Paired Equivalence Test for Crossover Design

| The POWER Procedure                         |        |
|---------------------------------------------|--------|
| Equivalence Test for Paired Mean Difference |        |
| Fixed Scenario Elements                     |        |
| Distribution                                | Normal |
| Method                                      | Exact  |
| Lower Equivalence Bound                     | -35    |
| Upper Equivalence Bound                     | 35     |
| Alpha                                       | 0.01   |
| Reference Mean                              | 330    |
| Treatment Mean                              | 310    |
| Standard Deviation 1                        | 40     |
| Standard Deviation 2                        | 55     |
| Correlation                                 | 0.3    |
| Number of Pairs                             | 100    |
| Computed Power                              |        |
| Power                                       | 0.598  |

The power for the paired equivalence test with 100 patients is about 0.6.

---

## Example 71.4: Noninferiority Test with Lognormal Data

The typical goal in noninferiority testing is to conclude that a new treatment or process or product is not appreciably worse than some standard. This is accomplished by convincingly rejecting a one-sided null hypothesis that the new treatment is appreciably worse than the standard. When designing such studies, investigators must define precisely what constitutes “appreciably worse.”

You can use the POWER procedure for sample size analyses for a variety of noninferiority tests, by specifying custom, one-sided null hypotheses for common tests. This example illustrates the strategy (often called Blackwelder's scheme; Blackwelder 1982) by comparing the means of two independent lognormal samples. The logic applies to one-sample, two-sample, and paired-sample problems involving normally distributed measures and proportions.

Suppose you are designing a study hoping to show that a new (less expensive) manufacturing process does not produce appreciably more pollution than the current process. Quantifying “appreciably worse” as 10%, you seek to show that the mean pollutant level from the new process is less than 110% of that from the current process. In standard hypothesis testing notation, you seek to reject

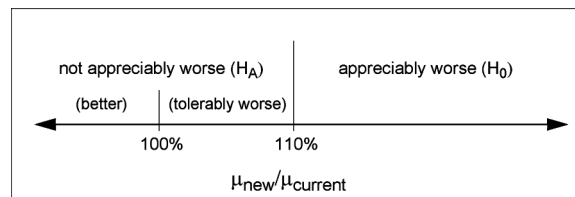
$$H_0: \frac{\mu_{\text{new}}}{\mu_{\text{current}}} \geq 1.10$$

in favor of

$$H_A: \frac{\mu_{\text{new}}}{\mu_{\text{current}}} < 1.10$$

This is described graphically in Figure 71.8. Mean ratios below 100% are better levels for the new process; a ratio of 100% indicates absolute equivalence; ratios of 100–110% are “tolerably” worse; and ratios exceeding 110% are appreciably worse.

**Figure 71.8** Hypotheses for the Pollutant Study



An appropriate test for this situation is the common two-group  $t$  test on log-transformed data. The hypotheses become

$$H_0: \log(\mu_{\text{new}}) - \log(\mu_{\text{current}}) \geq \log(1.10)$$

$$H_A: \log(\mu_{\text{new}}) - \log(\mu_{\text{current}}) < \log(1.10)$$

Measurements of the pollutant level will be taken by using laboratory models of the two processes and will be treated as independent lognormal observations with a coefficient of variation ( $\sigma/\mu$ ) between 0.5 and 0.6 for both processes. You will end up with 300 measurements for the current process and 180 for the new one. It is important to avoid a Type I error here, so you set the Type I error rate to 0.01. Your theoretical work suggests that the new process will actually reduce the pollutant by about 10% (to 90% of current), but you need to compute and graph the power of the study if the new levels are actually between 70% and 120% of current levels.

Implement the sample size analysis by using the `TWOSAMPLEMEANS` statement in PROC POWER with the `TEST=RATIO` option. Indicate power as the result parameter by specifying the `POWER=` option with a missing value (.). Specify a series of scenarios for the mean ratio between 0.7 and 1.2 by using the `MEANRATIO=` option. Use the `NULLRATIO=` option to specify the null mean ratio of 1.10. Specify `SIDES=L` to indicate a one-sided test with the alternative hypothesis stating that the mean ratio is *lower* than the null value. Specify the significance level, scenarios for the coefficient of variation, and the group



sample sizes by using the `ALPHA=`, `CV=`, and `GROUPNS=` options. Generate a plot of power versus mean ratio by specifying the `PLOT` statement with the `X=EFFECT` option to request a plot with mean ratio on the X axis. (The result parameter, here power, is always plotted on the other axis.) Use the `STEP=` option in the `PLOT` statement to specify an interval of 0.05 between computed points in the plot.

The following statements perform the desired analysis:

```
ods listing style=htmlbluecml;
ods graphics on;

proc power;
 twosamplemeans test=ratio
 meanratio = 0.7 to 1.2 by 0.1
 nullratio = 1.10
 sides = L
 alpha = 0.01
 cv = 0.5 0.6
 groupns = (300 180)
 power = .;
 plot x=effect step=0.05;
run;

ods graphics off;
```

The `ODS LISTING STYLE=HTMLBLUECML` statement specifies the `HTMLBLUECML` style, which is suitable for use with `PROC POWER` because it allows both marker symbols and line styles to vary. See the section “[ODS Styles Suitable for Use with PROC POWER](#)” on page 6082 for more information.

Note the use of `SIDES=L`, which forces computations for cases that need a rejection region that is opposite to the one providing the most one-tailed power; in this case, it is the lower tail. Such cases will show power that is less than the prescribed Type I error rate. The default option `DIST=LOGNORMAL` specifies the assumption of lognormally distributed data. The default `MIN=` and `MAX=` options in the plot statement specify an X axis range identical to the effect size range in the `TWOSAMPLEMEANS` statement (mean ratios between 0.7 and 1.2).

Output 71.4.1 and Output 71.4.2 show the results.

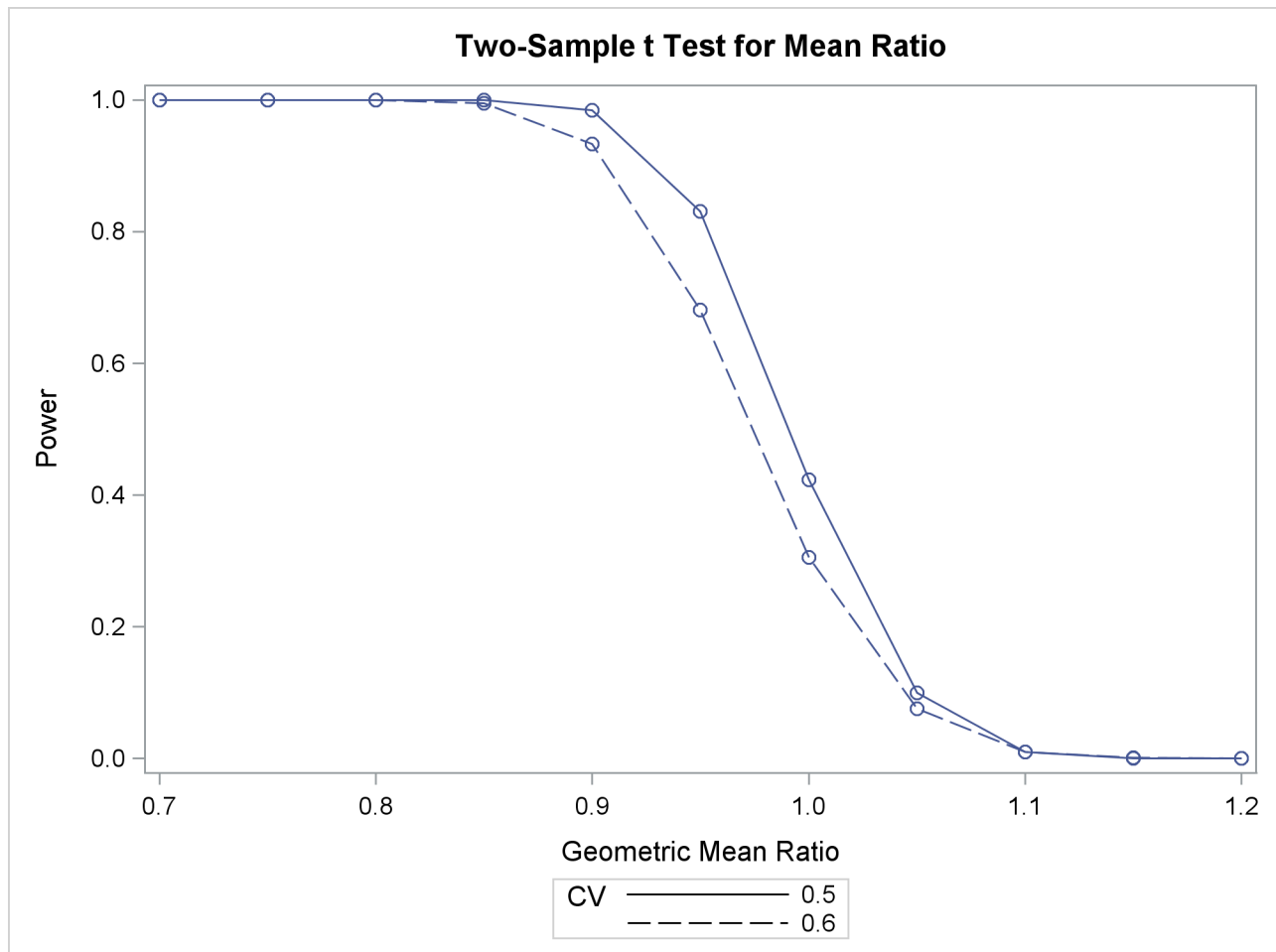
#### Output 71.4.1 Power for Noninferiority Test of Ratio

| The POWER Procedure              |           |
|----------------------------------|-----------|
| Two-Sample t Test for Mean Ratio |           |
| Fixed Scenario Elements          |           |
| Distribution                     | Lognormal |
| Method                           | Exact     |
| Number of Sides                  | L         |
| Null Geometric Mean Ratio        | 1.1       |
| Alpha                            | 0.01      |
| Group 1 Sample Size              | 300       |
| Group 2 Sample Size              | 180       |

**Output 71.4.1** continued

| Computed Power |                |     |       |
|----------------|----------------|-----|-------|
| Index          | Geo Mean Ratio | CV  | Power |
| 1              | 0.7            | 0.5 | >.999 |
| 2              | 0.7            | 0.6 | >.999 |
| 3              | 0.8            | 0.5 | >.999 |
| 4              | 0.8            | 0.6 | >.999 |
| 5              | 0.9            | 0.5 | 0.985 |
| 6              | 0.9            | 0.6 | 0.933 |
| 7              | 1.0            | 0.5 | 0.424 |
| 8              | 1.0            | 0.6 | 0.306 |
| 9              | 1.1            | 0.5 | 0.010 |
| 10             | 1.1            | 0.6 | 0.010 |
| 11             | 1.2            | 0.5 | <.001 |
| 12             | 1.2            | 0.6 | <.001 |

**Output 71.4.2** Plot of Power versus Mean Ratio for Noninferiority Test



The “Computed Power” table in [Output 71.4.1](#) shows that power exceeds 0.90 if the true mean ratio is 90% or less, as surmised. But power is unacceptably low (0.31–0.42) if the processes happen to be truly equivalent. Note that the power is identical to the alpha level (0.01) if the true mean ratio is 1.10 and below 0.01 if the true mean ratio is appreciably worse (>110%). In [Output 71.4.2](#), the line style identifies the coefficient of variation. The plotting symbols identify locations of actual computed powers; the curves are linear interpolations of these points.

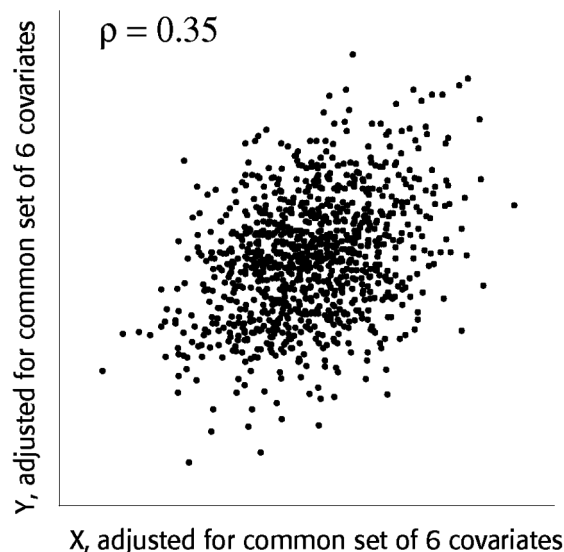
## Example 71.5: Multiple Regression and Correlation

You are working with a team of preventive cardiologists investigating whether elevated serum homocysteine levels are linked to atherosclerosis (plaque buildup) in coronary arteries. The planned analysis is an ordinary least squares regression to assess the relationship between total homocysteine level (tHcy) and a plaque burden index (PBI), adjusting for six other variables: age, gender, plasma levels of folate, vitamin B<sub>6</sub>, vitamin B<sub>12</sub>, and a serum cholesterol index. You will regress PBI on tHcy and the six other predictors (plus the intercept) and use a Type III *F* test to assess whether tHcy is a significant predictor after adjusting for the others. You wonder whether 100 subjects will provide adequate statistical power.

This is a correlational study at a single time. Subjects will be screened so that about half will have had a heart problem. All eight variables will be measured during one visit. Most clinicians are familiar with simple correlations between two variables, so you decide to pose the statistical problem in terms of estimating and testing the partial correlation between  $X_1 = \text{tHcy}$  and  $Y = \text{PBI}$ , controlling for the six other predictor variables ( $R_{YX_1|X_{-1}}$ ). This greatly simplifies matters, especially the elicitation of the conjectured effect.

You use partial regression plots like that shown in [Figure 71.9](#) to teach the team that the partial correlation between PBI and tHcy is the correlation of two sets of residuals obtained from ordinary regression models, one from regressing PBI on the six covariates and the other from regressing tHcy on the same covariates. Thus each subject has “expected” tHcy and PBI values based on the six covariates. The cardiologists believe that subjects whose tHcy is relatively higher than expected will also have a PBI that is relatively higher than expected. The partial correlation quantifies that adjusted association just as a standard simple correlation does with the unadjusted linear association between two variables.

**Figure 71.9** Partial Regression Plot



Based on previously published studies of various coronary risk factors and after viewing a set of scatterplots showing various correlations, the team surmises that the true partial correlation is likely to be at least 0.35.

You want to compute the statistical power for a sample size of  $N = 100$  by using  $\alpha = 0.05$ . You also want to plot power for sample sizes between 50 and 150. Use the **MULTREG** statement to compute the power and the **PLOT** statement to produce the graph. Since the predictors are observed rather than fixed in advanced, and a joint multivariate normal assumption seems tenable, use **MODEL=RANDOM**. The following statements perform the power analysis:

```
ods listing style=htmlbluecml;
ods graphics on;

proc power;
 multreg
 model = random
 nfullpredictors = 7
 ntestpredictors = 1
 partialcorr = 0.35
 ntotal = 100
 power = .;
 plot x=n min=50 max=150;
run;

ods graphics off;
```

The **ODS LISTING STYLE=HTMLBLUECML** statement specifies the **HTMLBLUECML** style, which is suitable for use with **PROC POWER** because it allows both marker symbols and line styles to vary. See the section “**ODS Styles Suitable for Use with PROC POWER**” on page 6082 for more information.

The **POWER=.** option identifies power as the parameter to compute. The **NFULLPREDICTORS=** option specifies seven total predictors (not including the intercept), and the **NTESTPREDICTORS=** option indicates that one of those predictors is being tested. The **PARTIALCORR=** and **NTOTAL=** options specify the partial correlation and sample size, respectively. The default value for the **ALPHA=** option sets the significance level to 0.05. The **X=N** option in the plot statement requests a plot of sample size on the X axis, and the **MIN=** and **MAX=** options specify the sample size range.

Output 71.5.1 shows the output, and Output 71.5.2 shows the plot.

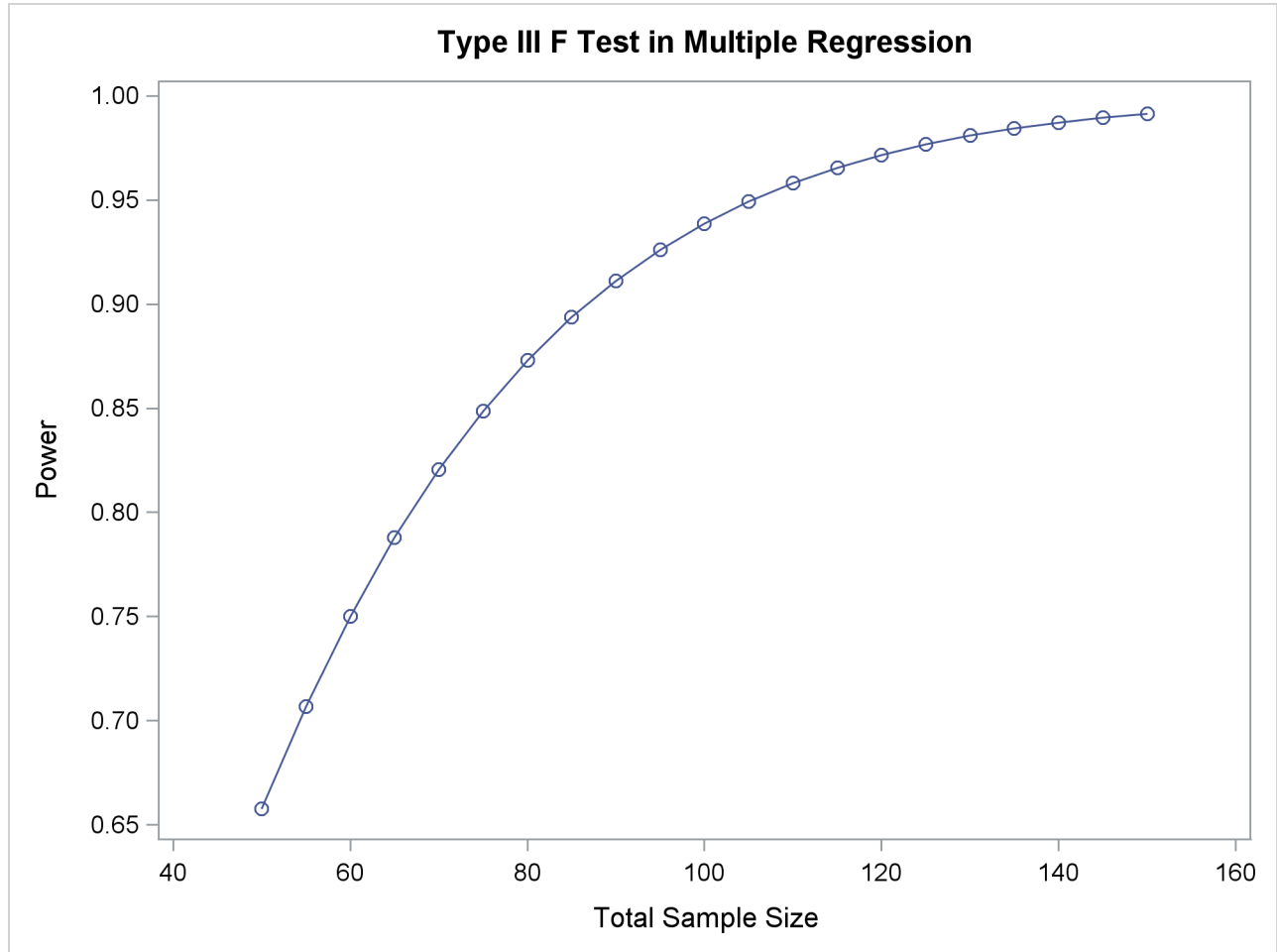
### Output 71.5.1 Power Analysis for Multiple Regression

| The POWER Procedure                    |          |
|----------------------------------------|----------|
| Type III F Test in Multiple Regression |          |
| Fixed Scenario Elements                |          |
| Method                                 | Exact    |
| Model                                  | Random X |
| Number of Predictors in Full Model     | 7        |
| Number of Test Predictors              | 1        |
| Partial Correlation                    | 0.35     |
| Total Sample Size                      | 100      |
| Alpha                                  | 0.05     |

**Output 71.5.1** *continued*

|                       |
|-----------------------|
| <b>Computed Power</b> |
| <b>Power</b>          |
| 0.939                 |

**Output 71.5.2** Plot of Power versus Sample Size for Multiple Regression



For the sample size  $N = 100$ , the study is almost balanced with respect to Type I and Type II error rates, with  $\alpha = 0.05$  and  $\beta = 1 - 0.937 = 0.063$ . The study thus seems well designed at this sample size.

Now suppose that in a follow-up meeting with the cardiologists, you discover that their specific intent is to demonstrate that the (partial) correlation between PBI and tHcy is greater than 0.2. You suggest changing the planned data analysis to a one-sided Fisher’s  $z$  test with a null correlation of 0.2. The following statements perform a power analysis for this test:

```

proc power;
 onecorr dist=fisherz
 npvars = 6
 corr = 0.35
 nullcorr = 0.2
 sides = 1
 ntotal = 100
 power = .;
run;

```

The **DIST=FISHERZ** option in the **ONECORR** statement specifies Fisher's  $z$  test. The **NPARTIALVARS=** option specifies that six additional variables are adjusted for in the partial correlation. The **CORR=** option specifies the conjectured correlation of 0.35, and the **NULLCORR=** option indicates the null value of 0.2. The **SIDES=** option specifies a one-sided test.

Output 71.5.3 shows the output.

**Output 71.5.3** Power Analysis for Fisher's  $z$  Test

| The POWER Procedure                       |                                    |  |
|-------------------------------------------|------------------------------------|--|
| Fisher's $z$ Test for Pearson Correlation |                                    |  |
| Fixed Scenario Elements                   |                                    |  |
| Distribution                              | Fisher's $z$ transformation of $r$ |  |
| Method                                    | Normal approximation               |  |
| Number of Sides                           | 1                                  |  |
| Null Correlation                          | 0.2                                |  |
| Number of Variables Partialled Out        | 6                                  |  |
| Correlation                               | 0.35                               |  |
| Total Sample Size                         | 100                                |  |
| Nominal Alpha                             | 0.05                               |  |
| Computed Power                            |                                    |  |
| Actual                                    |                                    |  |
| Alpha                                     | Power                              |  |
| 0.05                                      | 0.466                              |  |

The power for Fisher's  $z$  test is less than 50%, the decrease being mostly due to the smaller effect size (relative to the null value). When asked for a recommendation for a new sample size goal, you compute the required sample size to achieve a power of 0.95 (to balance Type I and Type II errors) and 0.85 (a threshold deemed to be minimally acceptable to the team). The following statements perform the sample size determination:

```

proc power;
 onecorr dist=fisherz
 npvars = 6
 corr = 0.35
 nullcorr = 0.2
 sides = 1
 ntotal = .
 power = 0.85 0.95;
run;

```

The `NTOTAL=.` option identifies sample size as the parameter to compute, and the `POWER=` option specifies the target powers.

#### Output 71.5.4 Sample Size Determination for Fisher's $z$ Test

| The POWER Procedure                       |               |              |                                    |         |
|-------------------------------------------|---------------|--------------|------------------------------------|---------|
| Fisher's $z$ Test for Pearson Correlation |               |              |                                    |         |
| Fixed Scenario Elements                   |               |              |                                    |         |
| Distribution                              |               |              | Fisher's $z$ transformation of $r$ |         |
| Method                                    |               |              | Normal approximation               |         |
| Number of Sides                           |               |              |                                    | 1       |
| Null Correlation                          |               |              |                                    | 0.2     |
| Number of Variables Partialled Out        |               |              |                                    | 6       |
| Correlation                               |               |              |                                    | 0.35    |
| Nominal Alpha                             |               |              |                                    | 0.05    |
| Computed N Total                          |               |              |                                    |         |
| Index                                     | Nominal Power | Actual Alpha | Actual Power                       | N Total |
| 1                                         | 0.85          | 0.05         | 0.850                              | 280     |
| 2                                         | 0.95          | 0.05         | 0.950                              | 417     |

The results in [Output 71.5.4](#) reveal a required sample size of 417 to achieve a power of 0.95 and a required sample size of 280 to achieve a power of 0.85.

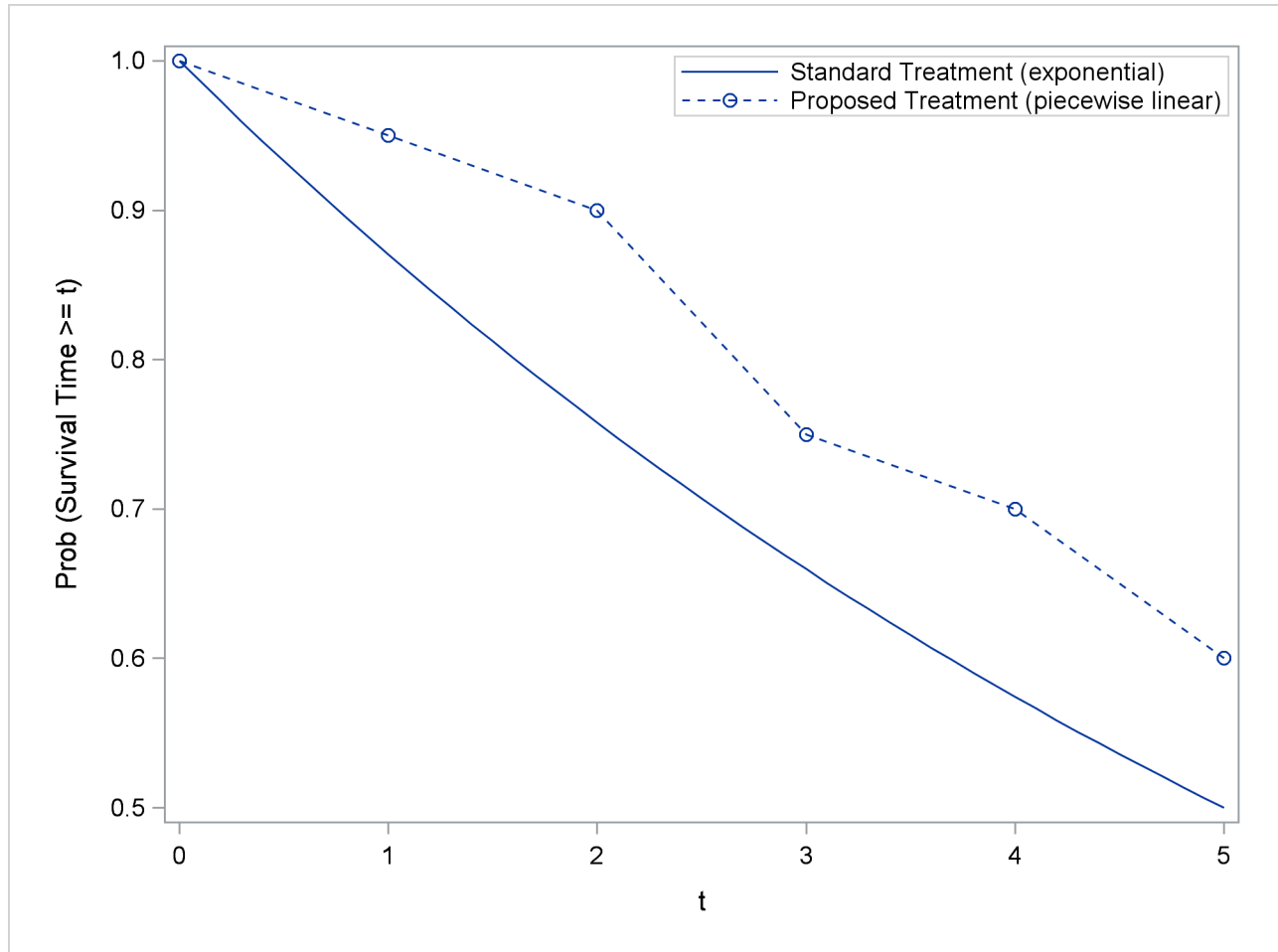
### Example 71.6: Comparing Two Survival Curves

You are consulting for a clinical research group planning a trial to compare survival rates for proposed and standard cancer treatments. The planned data analysis is a log-rank test to nonparametrically compare the overall survival curves for the two treatments. Your goal is to determine an appropriate sample size to achieve a power of 0.8 for a two-sided test with  $\alpha = 0.05$  by using a balanced design.

The survival curve for patients on the standard treatment is well known to be approximately exponential with a median survival time of five years. The research group conjectures that the new proposed treatment will yield a (nonexponential) survival curve similar to the dashed line in [Figure 71.6.1](#).

Patients will be accrued uniformly over two years and then followed for an additional three years past the accrual period. Some loss to follow-up is expected, with roughly exponential rates that would result in about 50% loss with the standard treatment within 10 years. The loss to follow-up with the proposed treatment is more difficult to predict, but 50% loss would be expected to occur sometime between years 5 and 20.

**Output 71.6.1** Survival Curves



Use the `TWOSAMPLESURVIVAL` statement with the `TEST=LOGRANK` option to compute the required sample size for the log-rank test. The following statements perform the analysis:

```
proc power;
 twosamplesurvival test=logrank
 curve("Standard") = 5 : 0.5
 curve("Proposed") = (1 to 5 by 1) : (0.95 0.9 0.75 0.7 0.6)
 groupsurvival = "Standard" | "Proposed"
 accrualtime = 2
 followuptime = 3
 groupmedlosstimes = 10 | 20 5
 power = 0.8
 npergroup = .;
run;
```



The **CURVE=** option defines the two survival curves. The “Standard” curve has only one point, specifying an exponential form with a survival probability of 0.5 at year 5. The “Proposed” curve is a piecewise linear curve defined by the five points shown in Figure 71.6.1. The **GROUPSURVIVAL=** option assigns the survival curves to the two groups, and the **ACCRUALTIME=** and **FOLLOWUPTIME=** options specify the accrual and follow-up times. The **GROUPMEDLOSSTIMES=** option specifies the years at which 50% loss is expected to occur. The **POWER=** option specifies the target power, and the **NPERGROUP=** option identifies sample size per group as the parameter to compute. Default values for the **SIDES=** and **ALPHA=** options specify a two-sided test with  $\alpha = 0.05$ .

Output 71.6.2 shows the results.

**Output 71.6.2** Sample Size Determination for Log-Rank Test

| The POWER Procedure                   |                              |              |             |  |
|---------------------------------------|------------------------------|--------------|-------------|--|
| Log-Rank Test for Two Survival Curves |                              |              |             |  |
| Fixed Scenario Elements               |                              |              |             |  |
| Method                                | Lakatos normal approximation |              |             |  |
| Accrual Time                          | 2                            |              |             |  |
| Follow-up Time                        | 3                            |              |             |  |
| Group 1 Survival Curve                | Standard                     |              |             |  |
| Form of Survival Curve 1              | Exponential                  |              |             |  |
| Group 2 Survival Curve                | Proposed                     |              |             |  |
| Form of Survival Curve 2              | Piecewise Linear             |              |             |  |
| Group 1 Median Loss Time              | 10                           |              |             |  |
| Nominal Power                         | 0.8                          |              |             |  |
| Number of Sides                       | 2                            |              |             |  |
| Number of Time Sub-Intervals          | 12                           |              |             |  |
| Alpha                                 | 0.05                         |              |             |  |
| Computed N Per Group                  |                              |              |             |  |
| Index                                 | Median Loss Time             | Actual Power | N Per Group |  |
| 1                                     | 20                           | 0.800        | 228         |  |
| 2                                     | 5                            | 0.801        | 234         |  |

The required sample size per group to achieve a power of 0.8 is 228 if the median loss time is 20 years for the proposed treatment. Only six more patients are required in each group if the median loss time is as short as five years.

## Example 71.7: Confidence Interval Precision

An investment firm has hired you to help plan a study to estimate the success of a new investment strategy called “IntuiVest.” The study involves complex simulations of market conditions over time, and it tracks the balance of a hypothetical brokerage account starting with \$50,000. Each simulation is very expensive in terms of computing time. You are asked to determine an appropriate number of simulations to estimate

the average change in the account balance at the end of three years. The goal is to have a 95% chance of obtaining a 90% confidence interval whose half-width is at most \$1,000. That is, the firm wants to have a 95% chance of being able to correctly claim at the end of the study that “Our research shows with 90% confidence that IntuiVest yields a profit of \$X +/- \$1,000 at the end of three years on an initial investment of \$50,000 (under simulated market conditions).”

The probability of achieving the desired precision (that is, a small interval width) can be calculated either unconditionally or conditionally given that the true mean is captured by the interval. You decide to use the conditional form, considering two of its advantages:

- The conditional probability is usually lower than the unconditional probability for the same sample size, meaning that the conditional form is generally conservative.
- The overall probability of achieving the desired precision *and* capturing the true mean is easily computed as the product of the half-width probability and the confidence level. In this case, the overall probability is  $0.95 \times 0.9 = 0.855$ .

Based on some initial simulations, you expect a standard deviation between \$25,000 and \$45,000 for the ending account balance. You will consider both of these values in the sample size analysis.

As mentioned in the section “[Overview of Power Concepts](#)” on page 6018, an analysis of confidence interval precision is analogous to a traditional power analysis, with “CI Half-Width” taking the place of effect size and “Prob(Width)” taking the place of power. In this example, the target CI Half-Width is 1000, and the desired Prob(Width) is 0.95.

In addition to computing sample sizes for a half-width of \$1,000, you are asked to plot the required number of simulations for a range of half-widths between \$500 and \$2,000. Use the [ONESAMPLEMEANS](#) statement with the [CI=T](#) option to implement the sample size determination. The following statements perform the analysis:

```
ods listing style=htmlbluecml;
ods graphics on;

proc power;
 onesamplemeans ci=t
 alpha = 0.1
 halfwidth = 1000
 stddev = 25000 45000
 probwidth = 0.95
 ntotal = .;
 plot x=effect min=500 max=2000;
run;

ods graphics off;
```

The ODS LISTING STYLE=HTMLBLUECML statement specifies the HTMLBLUECML style, which is suitable for use with PROC POWER because it allows both marker symbols and line styles to vary. See the section “[ODS Styles Suitable for Use with PROC POWER](#)” on page 6082 for more information.

The [NTOTAL=](#) option identifies sample size as the parameter to compute. The [ALPHA=0.1](#) option specifies a confidence level of  $1 - \alpha = 0.9$ . The [HALFWIDTH=](#) option specifies the target half-width, and the [STDDEV=](#) option specifies the conjectured standard deviation values. The [PROBWIDTH=](#) option specifies

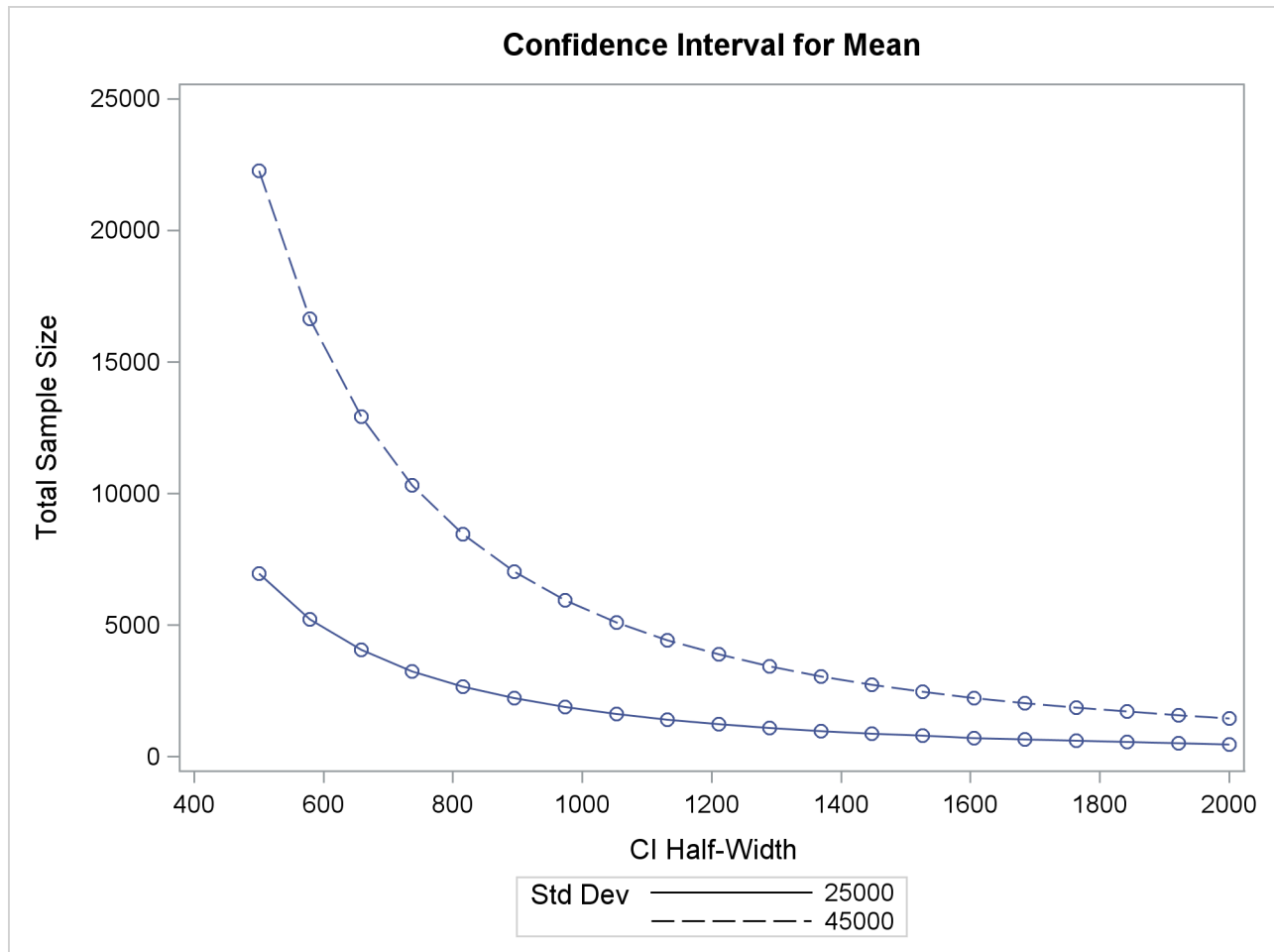
the desired probability of achieving the target precision. The default value `PROBTYPE=CONDITIONAL` specifies that this probability is conditional on the true mean being captured by the interval. The default of `SIDES=2` indicates a two-sided interval.

Output 71.7.1 shows the output, and Output 71.7.2 shows the plot.

#### Output 71.7.1 Sample Size Determination for Confidence Interval Precision

| The POWER Procedure          |         |                     |         |
|------------------------------|---------|---------------------|---------|
| Confidence Interval for Mean |         |                     |         |
| Fixed Scenario Elements      |         |                     |         |
| Distribution                 |         | Normal              |         |
| Method                       |         | Exact               |         |
| Alpha                        |         | 0.1                 |         |
| CI Half-Width                |         | 1000                |         |
| Nominal Prob (Width)         |         | 0.95                |         |
| Number of Sides              |         | 2                   |         |
| Prob Type                    |         | Conditional         |         |
| Computed N Total             |         |                     |         |
| Index                        | Std Dev | Actual Prob (Width) | N Total |
| 1                            | 25000   | 0.951               | 1788    |
| 2                            | 45000   | 0.950               | 5652    |

**Output 71.7.2** Plot of Sample Size versus Confidence Interval Half-Width



The number of simulations required in order to have a 95% chance of obtaining a half-width of at most 1000 is between 1788 and 5652, depending on the standard deviation. The plot reveals that more than 20,000 simulations would be required for a half-width of 500, assuming the higher standard deviation.

---

## Example 71.8: Customizing Plots

This example demonstrates various ways you can modify and enhance plots:

- assigning analysis parameters to axes
- fine-tuning a sample size axis
- adding reference lines
- linking plot features to analysis parameters
- choosing key (legend) styles
- modifying symbol locations

The example plots are all based on a sample size analysis for a two-sample  $t$  test of group mean difference. You start by computing the sample size required to achieve a power of 0.9 by using a two-sided test with  $\alpha = 0.05$ , assuming the first mean is 12, the second mean is either 15 or 18, and the standard deviation is either 7 or 9.

Use the `TWOSAMPLEMEANS` statement with the `TEST=DIFF` option to compute the required sample sizes. Indicate total sample size as the result parameter by supplying a missing value (.) with the `NTOTAL=` option. Use the `GROUPMEANS=`, `STDDEV=`, and `POWER=` options to specify values of the other parameters. The following statements perform the sample size computations:

```
proc power;
 twosamplemeans test=diff
 groupmeans = 12 | 15 18
 stddev = 7 9
 power = 0.9
 ntotal = .;
run;
```

Default values for the `NULLDIFF=`, `SIDES=`, `GROUPWEIGHTS=`, and `DIST=` options specify a null mean difference of 0, two-sided test, balanced design, and assumption of normally distributed data, respectively.

[Output 71.8.1](#) shows that the required sample size ranges from 60 to 382, depending on the unknown standard deviation and second mean.

**Output 71.8.1** Computed Sample Sizes

| The POWER Procedure                   |       |         |              |         |  |
|---------------------------------------|-------|---------|--------------|---------|--|
| Two-Sample t Test for Mean Difference |       |         |              |         |  |
| Fixed Scenario Elements               |       |         |              |         |  |
| Distribution                          |       |         |              | Normal  |  |
| Method                                |       |         |              | Exact   |  |
| Group 1 Mean                          |       |         |              | 12      |  |
| Nominal Power                         |       |         |              | 0.9     |  |
| Number of Sides                       |       |         |              | 2       |  |
| Null Difference                       |       |         |              | 0       |  |
| Alpha                                 |       |         |              | 0.05    |  |
| Group 1 Weight                        |       |         |              | 1       |  |
| Group 2 Weight                        |       |         |              | 1       |  |
| Computed N Total                      |       |         |              |         |  |
| Index                                 | Mean2 | Std Dev | Actual Power | N Total |  |
| 1                                     | 15    | 7       | 0.902        | 232     |  |
| 2                                     | 15    | 9       | 0.901        | 382     |  |
| 3                                     | 18    | 7       | 0.904        | 60      |  |
| 4                                     | 18    | 9       | 0.904        | 98      |  |

**Assigning Analysis Parameters to Axes**

Use the `PLOT` statement to produce plots for all power and sample size analyses in PROC POWER. For the sample size analysis described at the beginning of this example, suppose you want to plot the required sample size on the Y axis against a range of powers between 0.5 and 0.95 on the X axis. The `X=` and `Y=` options specify which parameter to plot against the result and which axis to assign to this parameter. You can use either the `X=` or the `Y=` option, but not both. Use the `X=POWER` option in the `PLOT` statement to request a plot with power on the X axis. The result parameter, here total sample size, is always plotted on the other axis. Use the `MIN=` and `MAX=` options to specify the range of the axis indicated with either the `X=` or the `Y=` option. Here, specify `MIN=0.5` and `MAX=0.95` to specify the power range. The following statements produce the plot:

```
ods listing style=htmlbluecml;
ods graphics on;

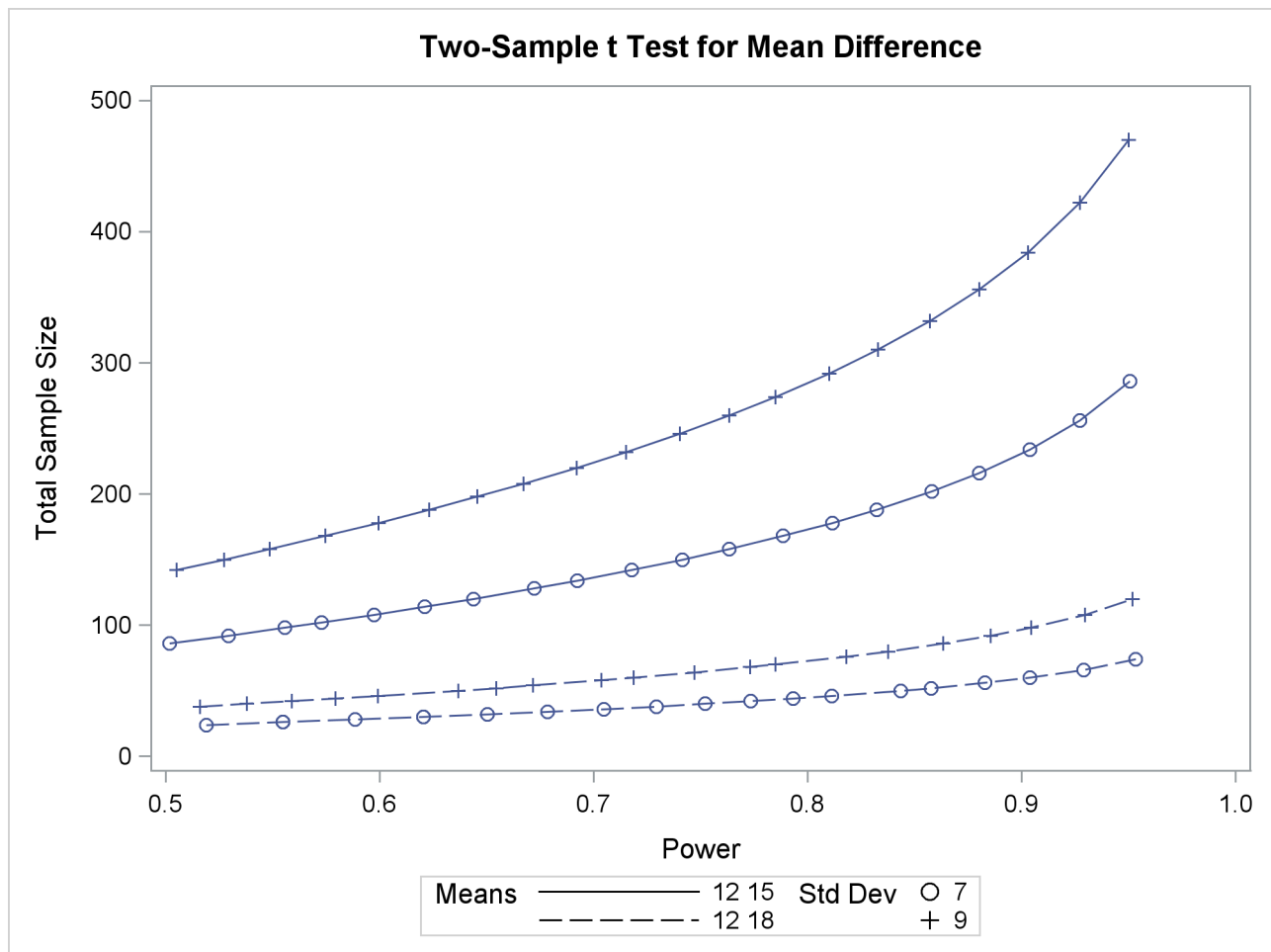
proc power plotonly;
 twosamplemeans test=diff
 groupmeans = 12 | 15 18
 stddev = 7 9
 power = 0.9
 ntotal = .;
 plot x=power min=0.5 max=0.95;
run;
```

The ODS LISTING STYLE=HTMLBLUECML statement specifies the HTMLBLUECML style, which is suitable for use with PROC POWER because it allows both marker symbols and line styles to vary. See the section “ODS Styles Suitable for Use with PROC POWER” on page 6082 for more information.

Note that the value (0.9) of the POWER= option in the TWOSAMPLEMEANS statement is only a placeholder when the PLOTONLY option is used and both the MIN= and MAX= options are used, because the values of the MIN= and MAX= options override the value of 0.9. But the POWER= option itself is still required in the TWOSAMPLEMEANS statement, to provide a complete specification of the sample size analysis.

The resulting plot is shown in Output 71.8.2.

**Output 71.8.2** Plot of Sample Size versus Power

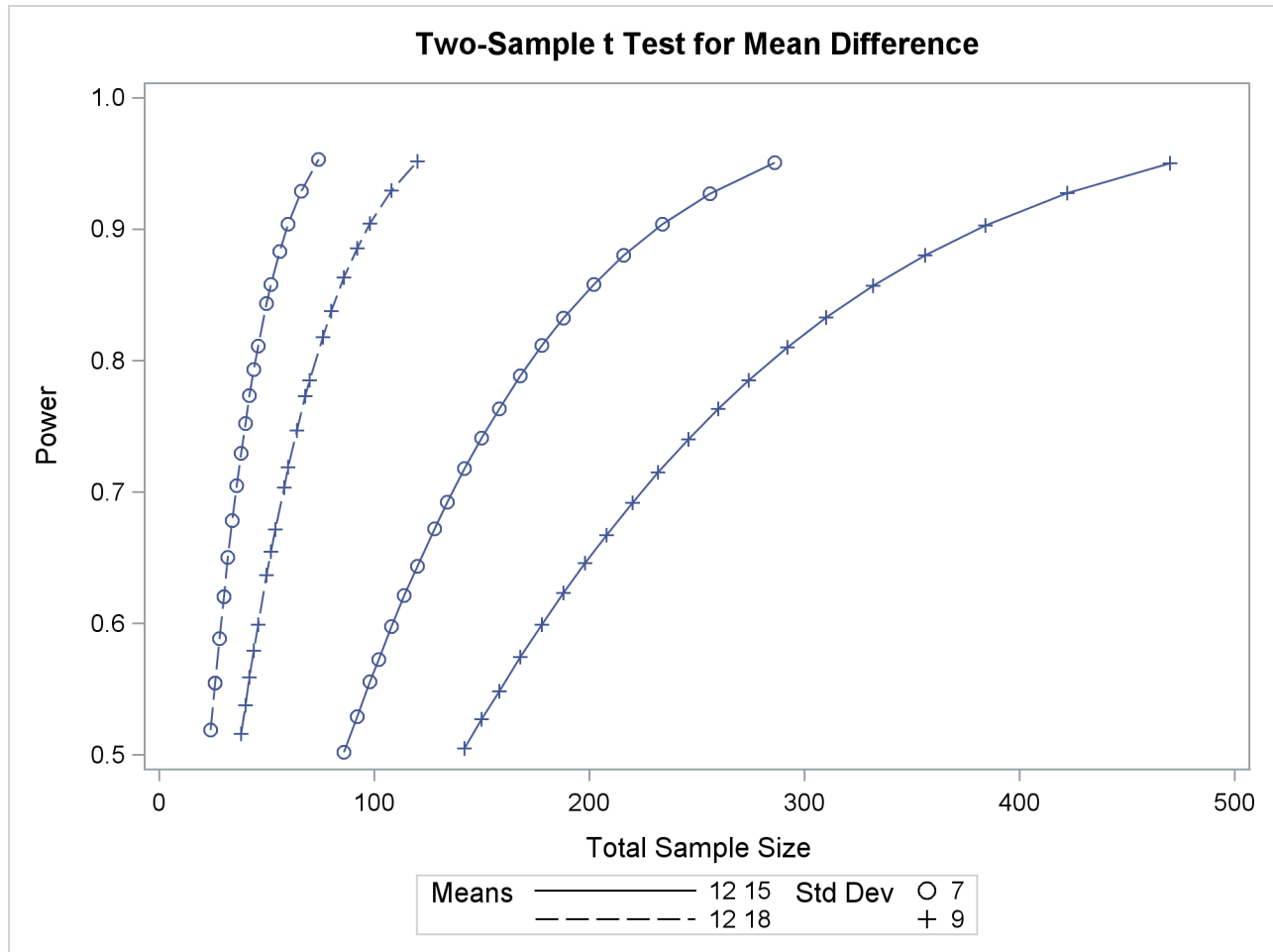


The line style identifies the group means scenario, and the plotting symbol identifies the standard deviation scenario. The locations of plotting symbols indicate computed sample sizes; the curves are linear interpolations of these points. By default, each curve consists of approximately 20 computed points (sometimes slightly more or less, depending on the analysis).

If you would rather plot power on the Y axis versus sample size on the X axis, you have two general strategies to choose from. One strategy is to use the Y= option instead of the X= option in the PLOT statement:

```
plot y=power min=0.5 max=0.95;
```

**Output 71.8.3** Plot of Power versus Sample Size using First Strategy



Note that the resulting plot (Output 71.8.3) is essentially a mirror image of Output 71.8.2. The axis ranges are set such that each curve in Output 71.8.3 contains similar values of Y instead of X. Each plotted point represents the computed value of the X axis at the input value of the Y axis.

A second strategy for plotting power versus sample size (when originally solving for sample size) is to invert the analysis and base the plot on computed power for a given range of sample sizes. This strategy works well for monotonic power curves (as is the case for the *t* test and most other continuous analyses). It is advantageous in the sense of preserving the traditional role of the Y axis as the computed parameter. A common way to implement this strategy is as follows:

- Determine the range of sample sizes sufficient to cover at the desired power range for all curves (where each “curve” represents a scenario for standard deviation and second group mean).
- Use this range for the X axis of a plot.

To determine the required sample sizes for target powers of 0.5 and 0.95, change the values in the **POWER=** option as follows to reflect this range:



```

proc power;
 twosamplemeans test=diff
 groupmeans = 12 | 15 18
 stddev = 7 9
 power = 0.5 0.95
 ntotal = .;
run;

```

Output 71.8.4 reveals that a sample size range of 24 to 470 is approximately sufficient to cover the desired power range of 0.5 to 0.95 for all curves (“approximately” because the actual power at the rounded sample size of 24 is slightly higher than the nominal power of 0.5).

**Output 71.8.4** Computed Sample Sizes

| The POWER Procedure                   |        |         |               |              |         |  |
|---------------------------------------|--------|---------|---------------|--------------|---------|--|
| Two-Sample t Test for Mean Difference |        |         |               |              |         |  |
| Fixed Scenario Elements               |        |         |               |              |         |  |
| Distribution                          | Normal |         |               |              |         |  |
| Method                                | Exact  |         |               |              |         |  |
| Group 1 Mean                          | 12     |         |               |              |         |  |
| Number of Sides                       | 2      |         |               |              |         |  |
| Null Difference                       | 0      |         |               |              |         |  |
| Alpha                                 | 0.05   |         |               |              |         |  |
| Group 1 Weight                        | 1      |         |               |              |         |  |
| Group 2 Weight                        | 1      |         |               |              |         |  |
| Computed N Total                      |        |         |               |              |         |  |
| Index                                 | Mean2  | Std Dev | Nominal Power | Actual Power | N Total |  |
| 1                                     | 15     | 7       | 0.50          | 0.502        | 86      |  |
| 2                                     | 15     | 7       | 0.95          | 0.951        | 286     |  |
| 3                                     | 15     | 9       | 0.50          | 0.505        | 142     |  |
| 4                                     | 15     | 9       | 0.95          | 0.950        | 470     |  |
| 5                                     | 18     | 7       | 0.50          | 0.519        | 24      |  |
| 6                                     | 18     | 7       | 0.95          | 0.953        | 74      |  |
| 7                                     | 18     | 9       | 0.50          | 0.516        | 38      |  |
| 8                                     | 18     | 9       | 0.95          | 0.952        | 120     |  |

To plot power on the Y axis for sample sizes between 20 and 500, use the `X=N` option in the `PLOT` statement with `MIN=20` and `MAX=500`:

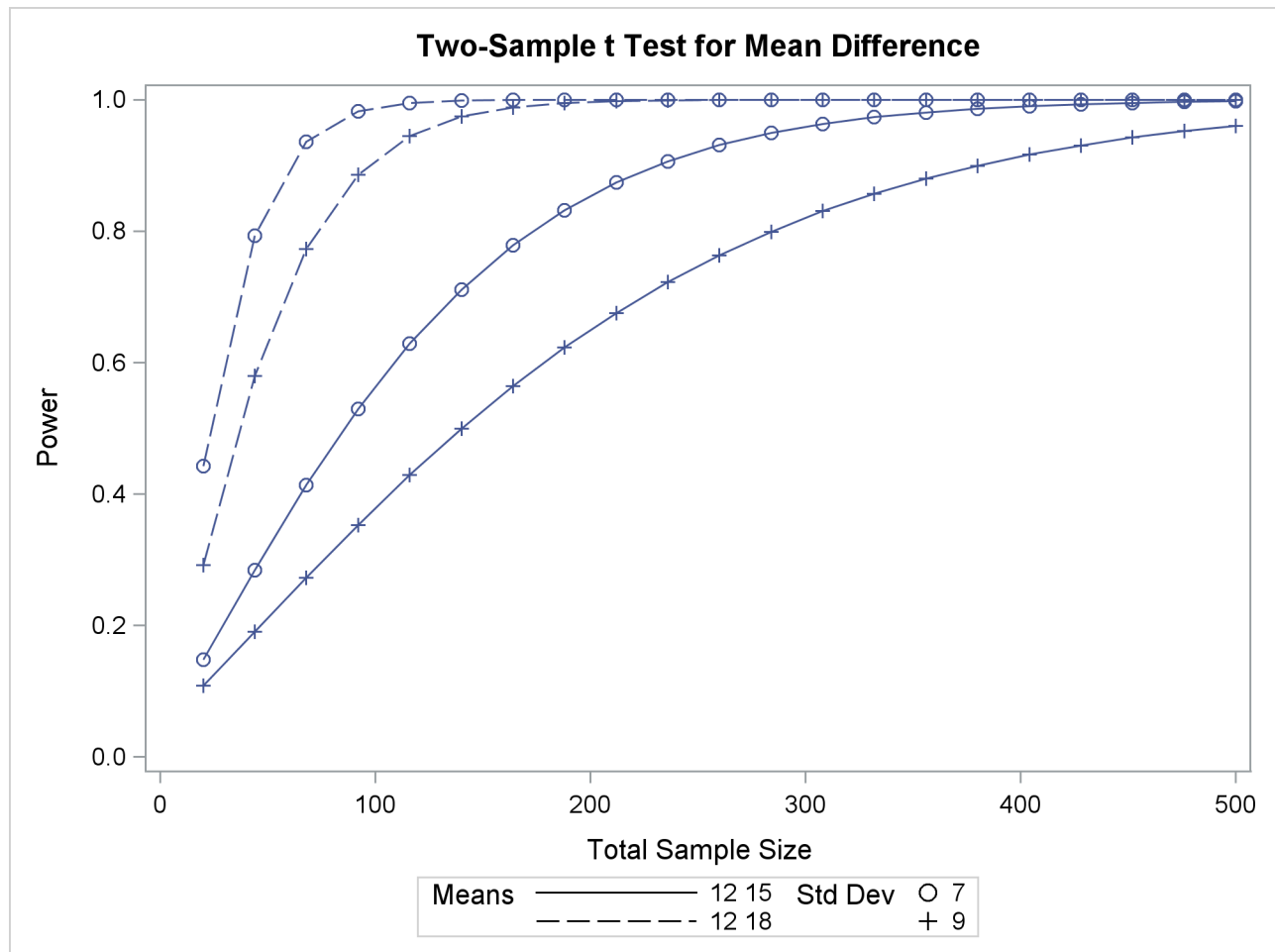
```

proc power plotonly;
 twosamplemeans test=diff
 groupmeans = 12 | 15 18
 stddev = 7 9
 power = .
 ntotal = 200;
 plot x=n min=20 max=500;
run;

```

Each curve in the resulting plot in [Output 71.8.5](#) covers at least a power range of 0.5 to 0.95.

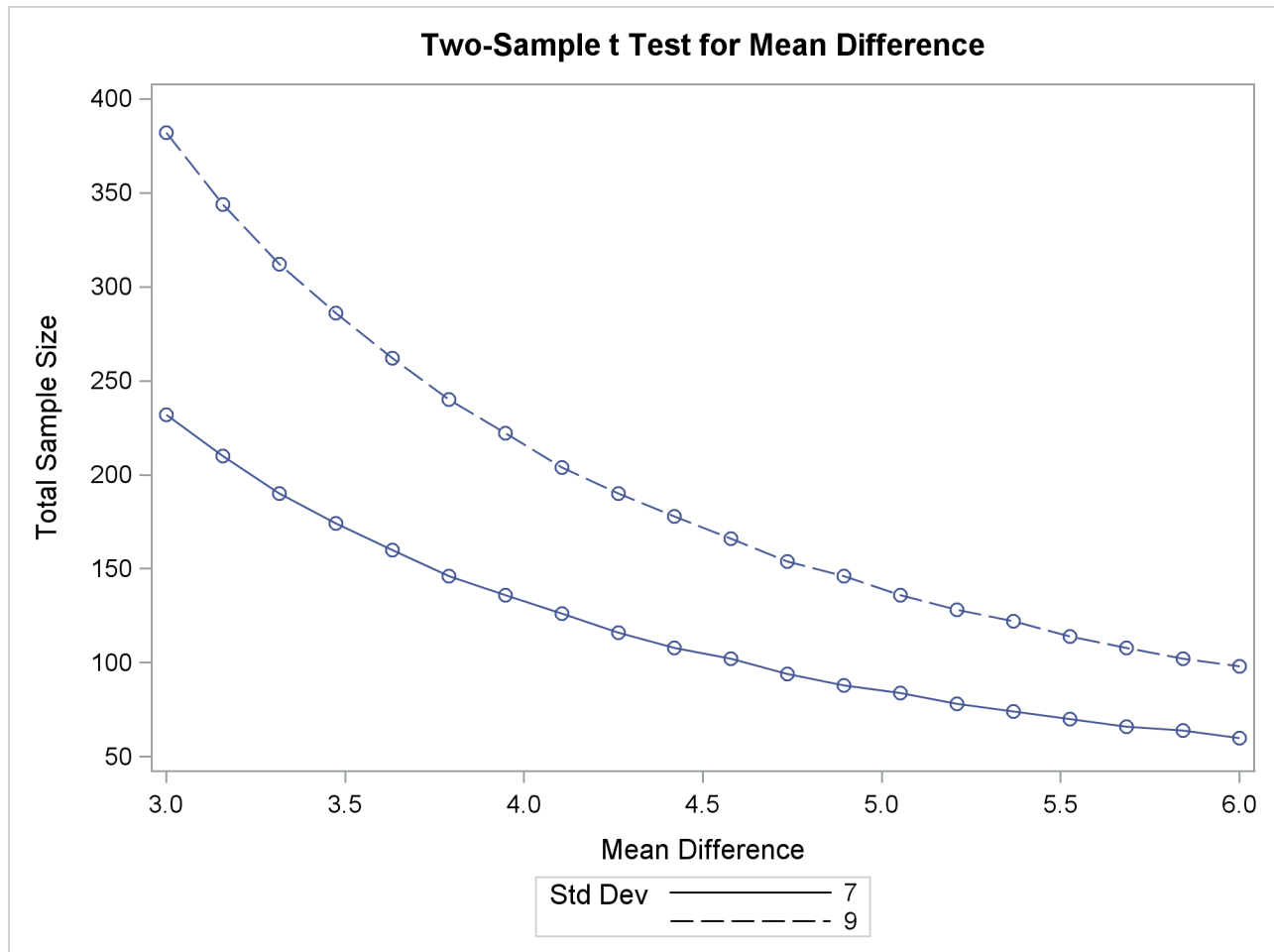
**Output 71.8.5** Plot of Power versus Sample Size Using Second Strategy



Finally, suppose you want to produce a plot of sample size versus effect size for a power of 0.9. In this case, the “effect size” is defined to be the mean difference. You need to reparameterize the analysis by using the `MEANDIFF=` option instead of the `GROUPMEANS=` option to produce a plot, since each plot axis must be represented by a scalar parameter. Use the `X=EFFECT` option in the `PLOT` statement to assign the mean difference to the X axis. The following statements produce a plot of required sample size to detect mean differences between 3 and 6:

```
proc power plotonly;
 twosamplemeans test=diff
 meandiff = 3 6
 stddev = 7 9
 power = 0.9
 ntotal = .;
 plot x=effect min=3 max=6;
run;
```

The resulting plot [Output 71.8.6](#) shows how the required sample size decreases with increasing mean difference.

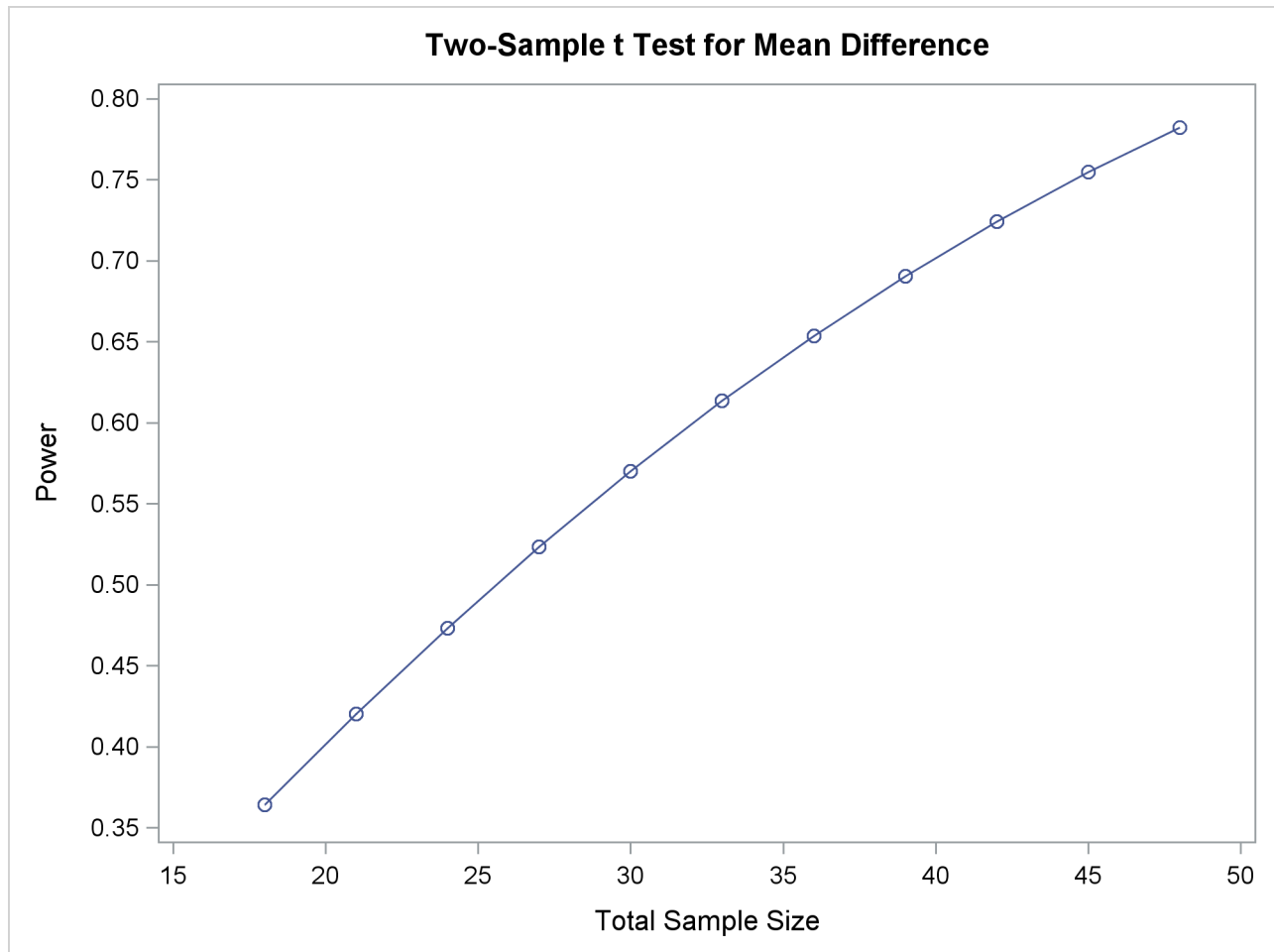
**Output 71.8.6** Plot of Sample Size versus Mean Difference

### Fine-Tuning a Sample Size Axis

Consider the following plot request for a sample size analysis similar to the one in [Output 71.8.1](#) but with only a single scenario, and with unbalanced sample size allocation of 2:1:

```
proc power plotonly;
 ods output plotcontent=PlotData;
 twosamplemeans test=diff
 groupmeans = 12 | 18
 stddev = 7
 groupweights = 2 | 1
 power = .
 ntotal = 20;
 plot x=n min=20 max=50 npoints=20;
run;
```

The `MIN=`, `MAX=`, and `NPOINTS=` options in the `PLOT` statement request a plot with 20 points between 20 and 50. But the resulting plot ([Output 71.8.7](#)) appears to have only 11 points, and they range from 18 to 48.

**Output 71.8.7** Plot with Overlapping Points

The reason that this plot has fewer points than usual is due to the rounding of sample sizes. If you do not use the **NFRACTIONAL** option in the analysis statement (here, the **TWOSAMPLEMEANS** statement), then the set of sample size points determined by the **MIN=**, **MAX=**, **NPOINTS=**, and **STEP=** options in the **PLOT** statement can be rounded to satisfy the allocation weights. In this case, they are rounded down to the nearest multiples of 3 (the sum of the weights), and many of the points overlap. To see the overlap, you can print the **NominalNTotal** (unadjusted) and **NTotal** (rounded) variables in the **PlotContent** ODS object (here saved to a data set called **PlotData**):

```
proc print data=PlotData;
 var NominalNTotal NTotal;
run;
```

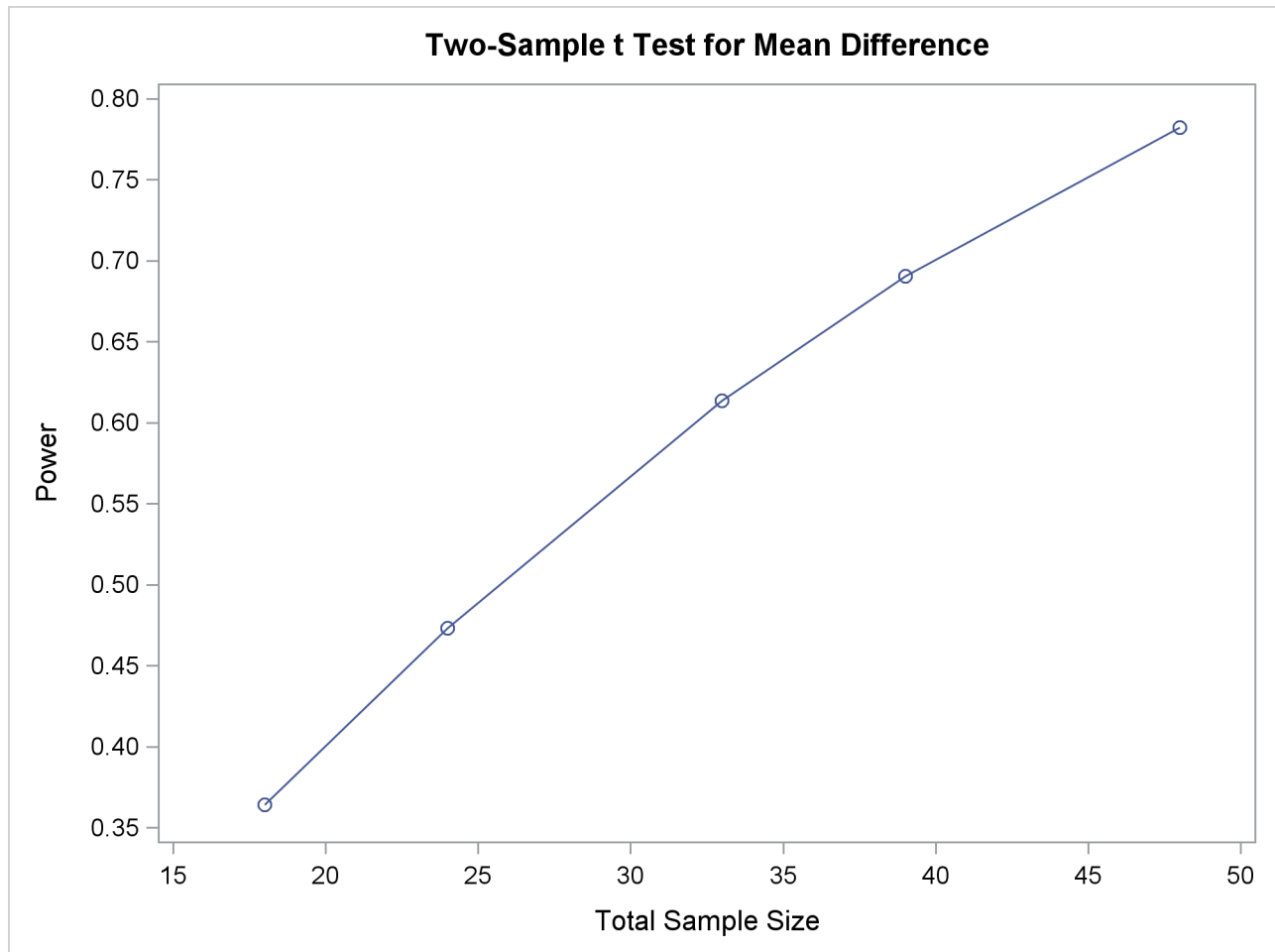
The output is shown in [Output 71.8.8](#).

**Output 71.8.8** Sample Sizes

| Obs | Nominal<br>NTotal | NTotal |
|-----|-------------------|--------|
| 1   | 18.0              | 18     |
| 2   | 19.6              | 18     |
| 3   | 21.2              | 21     |
| 4   | 22.7              | 21     |
| 5   | 24.3              | 24     |
| 6   | 25.9              | 24     |
| 7   | 27.5              | 27     |
| 8   | 29.1              | 27     |
| 9   | 30.6              | 30     |
| 10  | 32.2              | 30     |
| 11  | 33.8              | 33     |
| 12  | 35.4              | 33     |
| 13  | 36.9              | 36     |
| 14  | 38.5              | 36     |
| 15  | 40.1              | 39     |
| 16  | 41.7              | 39     |
| 17  | 43.3              | 42     |
| 18  | 44.8              | 42     |
| 19  | 46.4              | 45     |
| 20  | 48.0              | 48     |

Besides overlapping of sample size points, another peculiarity that might occur without the `NFRAC-``TIONAL` option is unequal spacing—for example, in the plot in [Output 71.8.9](#), created with the following statements:

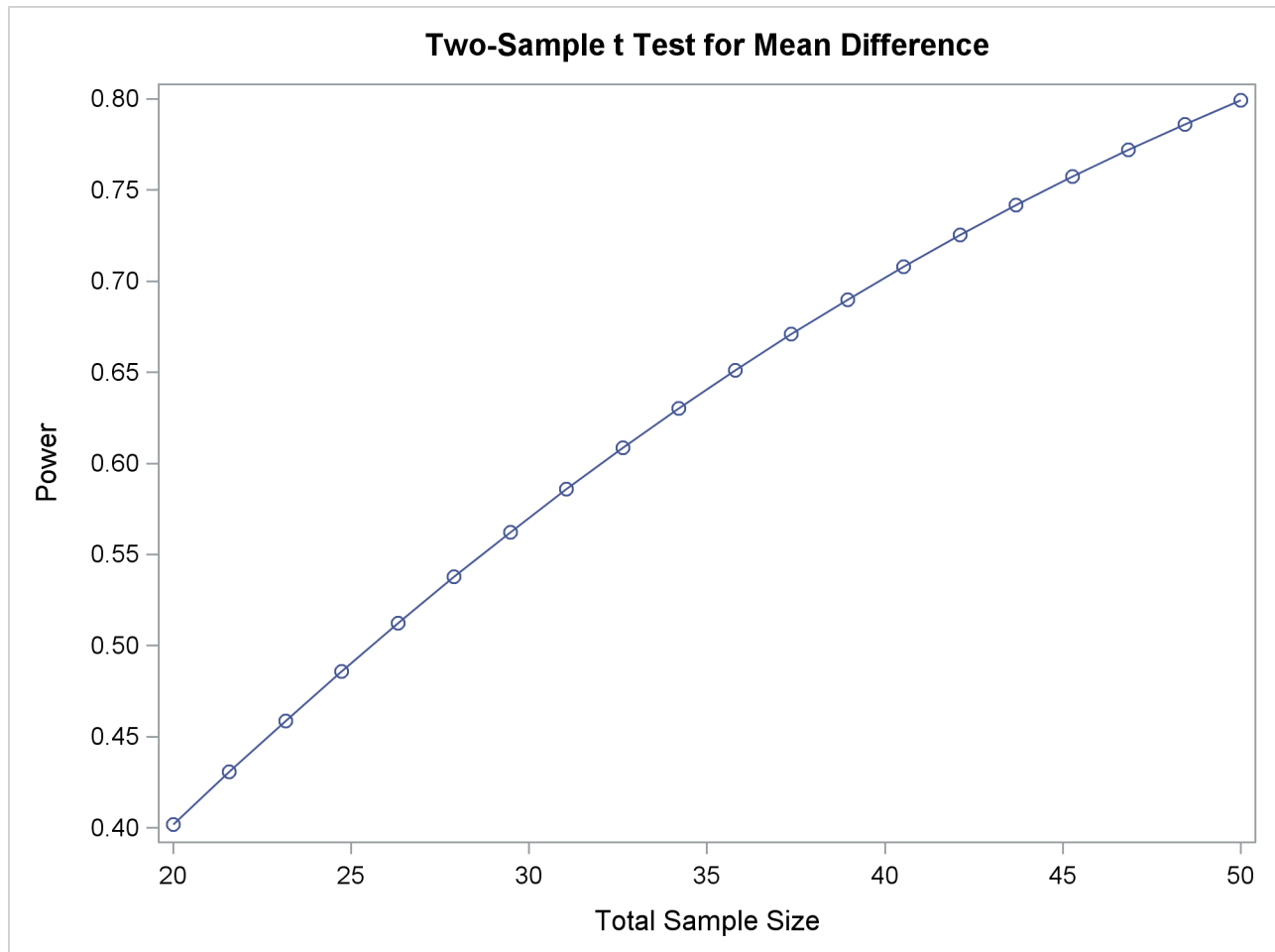
```
proc power plotonly;
 twosamplemeans test=diff
 groupmeans = 12 | 18
 stddev = 7
 groupweights = 2 | 1
 power = .
 ntotal = 20;
 plot x=n min=20 max=50 npoints=5;
run;
```

**Output 71.8.9** Plot with Unequally Spaced Points

If you want to guarantee evenly spaced, nonoverlapping sample size points in your plots, you can either (1) use the **NFRACTIONAL** option in the analysis statement preceding the **PLOT** statement or (2) use the **STEP=** option and provide values for the **MIN=**, **MAX=**, and **STEP=** options in the **PLOT** statement that are multiples of the sum of the allocation weights. Note that this sum is simply 1 for one-sample and paired designs and 2 for balanced two-sample designs. So any integer step value works well for one-sample and paired designs, and any even step value works well for balanced two-sample designs. Both of these strategies will avoid rounding adjustments.

The following statements implement the first strategy to create the plot in [Output 71.8.10](#), by using the **NFRACTIONAL** option in the **TWOSAMPLEMEANS** statement:

```
proc power plotonly;
 twosamplemeans test=diff
 nfractional
 groupmeans = 12 | 18
 stddev = 7
 groupweights = 2 | 1
 power = .
 ntotal = 20;
 plot x=n min=20 max=50 npoints=20;
run;
```

**Output 71.8.10** Plot with Fractional Sample Sizes

To implement the second strategy, use multiples of 3 for the `STEP=`, `MIN=`, and `MAX=` options in the `PLOT` statement (because the sum of the allocation weights is  $2 + 1 = 3$ ). The following statements use `STEP=3`, `MIN=18`, and `MAX=48` to create a plot that looks identical to the plot in [Output 71.8.7](#) but suffers no overlapping of points:

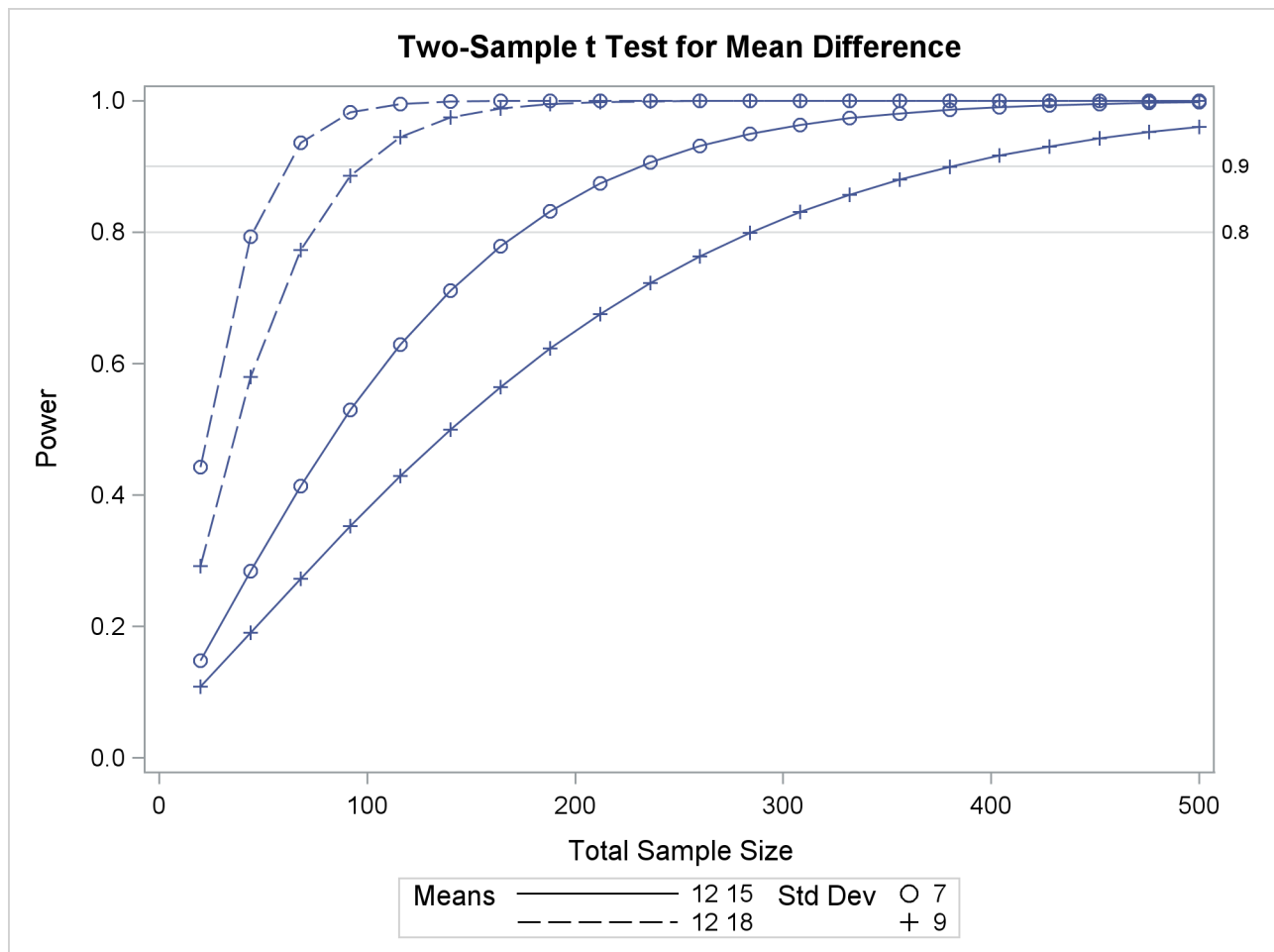
```
proc power plotonly;
 twosamplemeans test=diff
 groupmeans = 12 | 18
 stddev = 7
 groupweights = 2 | 1
 power = .
 ntotal = 20;
 plot x=n min=18 max=48 step=3;
run;
```

## Adding Reference Lines

Suppose you want to add reference lines to highlight  $\text{power}=0.8$  and  $\text{power}=0.9$  on the plot in [Output 71.8.5](#). You can add simple reference lines by using the `YOPTS=` option and `REF=` suboption in the `PLOT` statement to produce [Output 71.8.11](#), with the following statements:

```
proc power plotonly;
 twosamplemeans test=diff
 groupmeans = 12 | 15 18
 stddev = 7 9
 power = .
 ntotal = 100;
 plot x=n min=20 max=500
 yopts=(ref=0.8 0.9);
run;
```

**Output 71.8.11** Plot with Simple Reference Lines on Y Axis



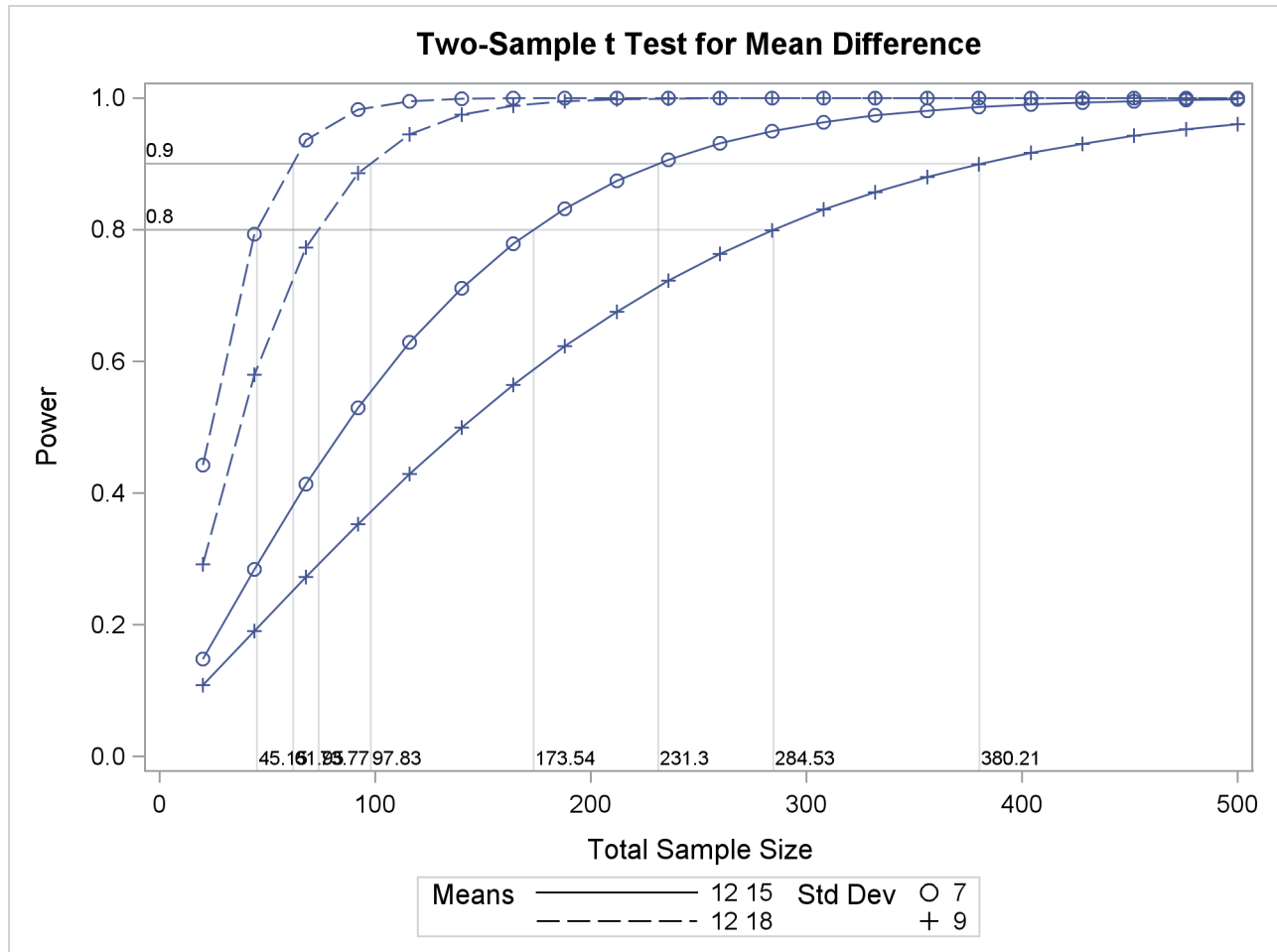
Or you can specify `CROSSREF=YES` to add reference lines that intersect each curve and cross over to the other axis:



```
plot x=n min=20 max=500
 yopts=(ref=0.8 0.9 crossref=yes);
```

The resulting plot is shown in [Output 71.8.12](#).

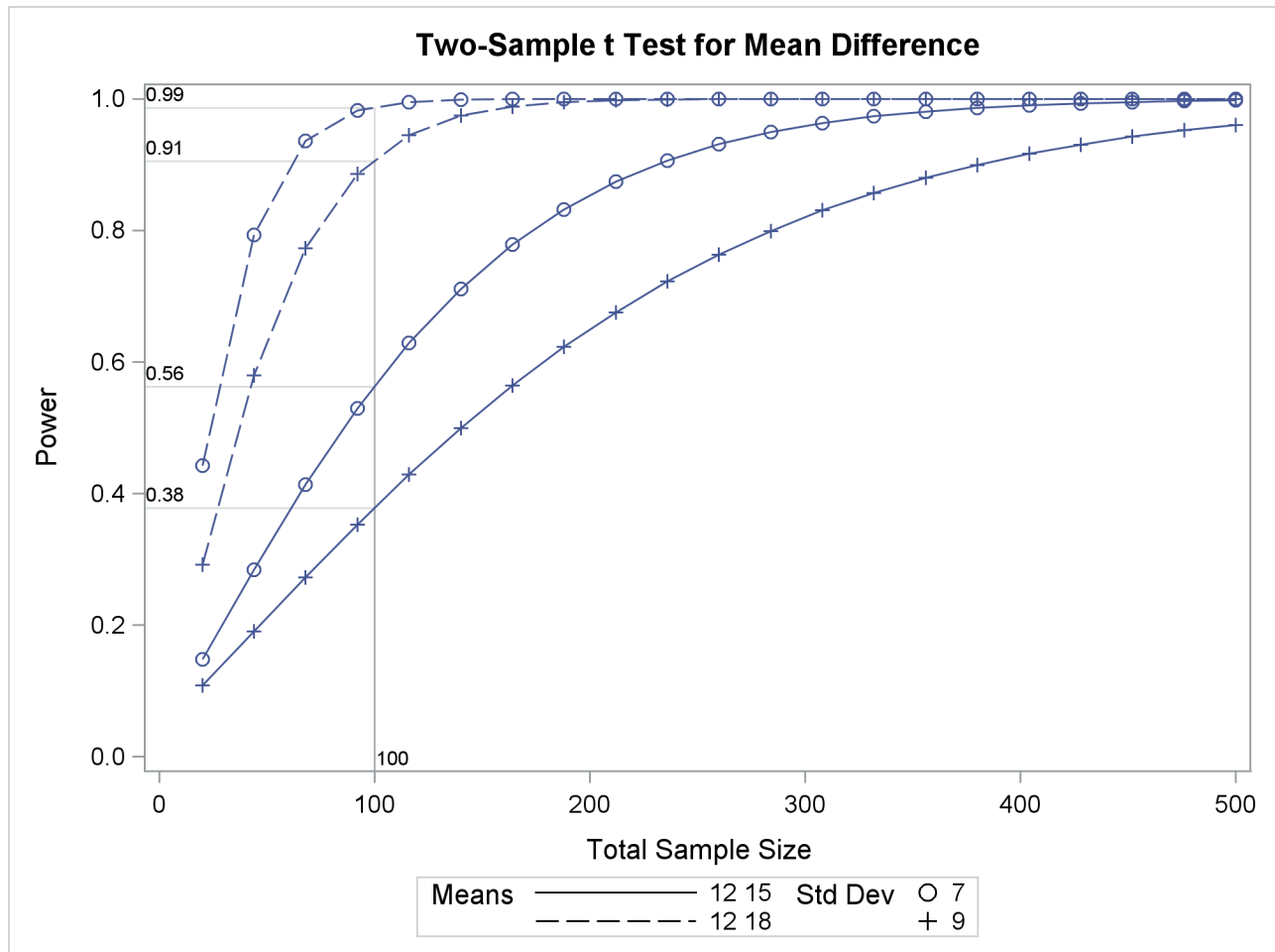
**Output 71.8.12** Plot with CROSSREF=YES Style Reference Lines from Y Axis



You can also add reference lines for the X axis by using the `XOPTS=` option instead of the `YOPTS=` option. For example, the following `PLOT` statement produces [Output 71.8.13](#), which has crossing reference lines highlighting the sample size of 100:

```
plot x=n min=20 max=500
 xopts=(ref=100 crossref=yes);
```

Note that the values that label the reference lines at the X axis in [Output 71.8.12](#) and at the Y axis in [Output 71.8.13](#) are linearly interpolated from two neighboring points on the curves. Thus they might not exactly match corresponding values that are computed directly from the methods in the section “[Computational Methods and Formulas](#)” on page 6027—that is, computed by PROC POWER in the absence of a PLOT statement. The two ways of computing these values generally differ by a negligible amount.

**Output 71.8.13** Plot with CROSSREF=YES Style Reference Lines from X Axis

### Linking Plot Features to Analysis Parameters

You can use the **VARY** option in the **PLOT** statement to specify which of the following features you want to associate with analysis parameters.

- line style
- plotting symbol
- color
- panel

You can specify mappings between each of these features and one or more analysis parameters, or you can simply choose a subset of these features to use (and rely on default settings to associate these features with multiple-valued analysis parameters).

Suppose you supplement the sample size analysis in **Output 71.8.5** to include three values of alpha, by using the following statements:

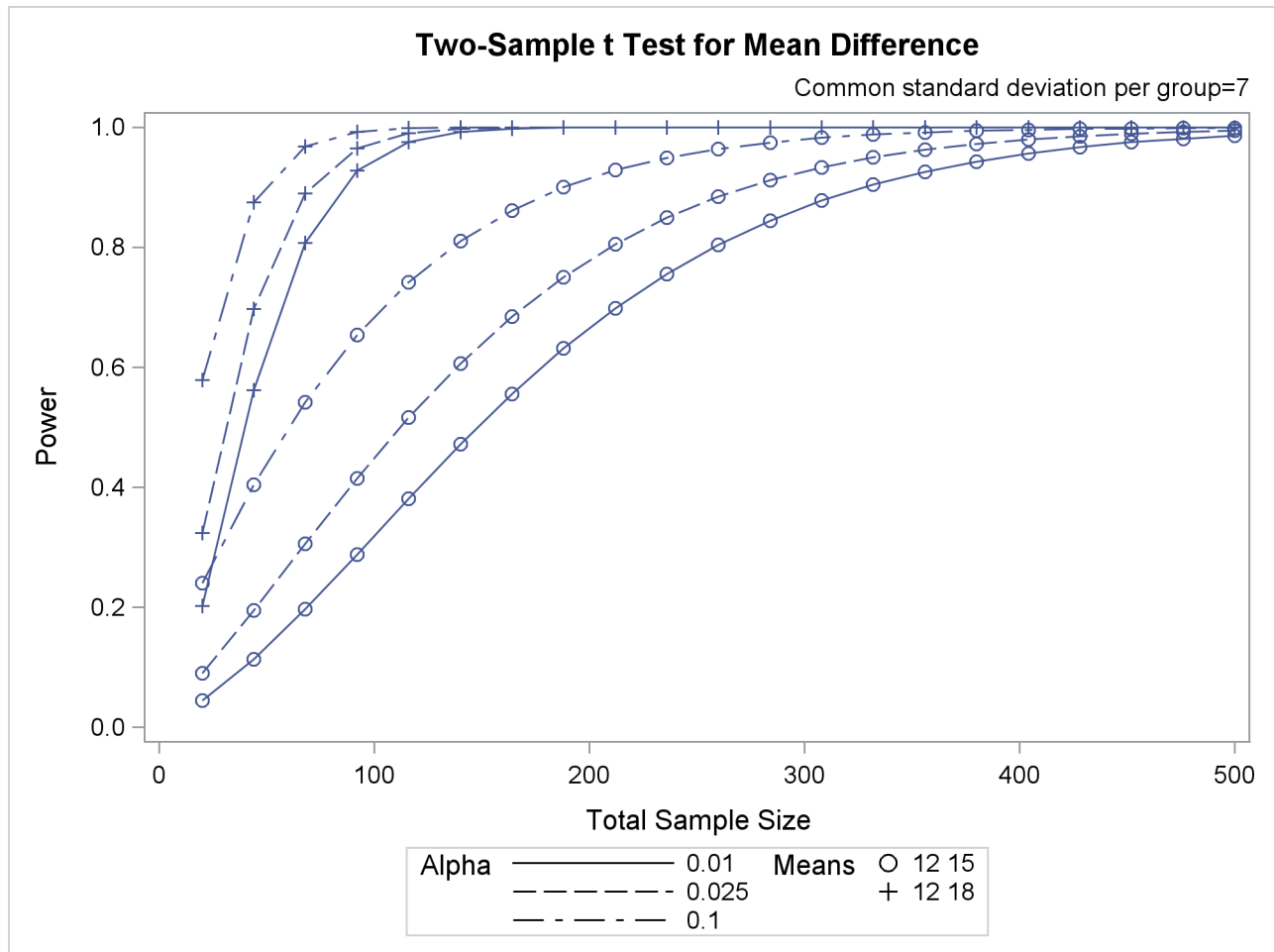
```

proc power plotonly;
 twosamplemeans test=diff
 groupmeans = 12 | 15 18
 stddev = 7 9
 alpha = 0.01 0.025 0.1
 power = .
 ntotal = 100;
 plot x=n min=20 max=500;
run;

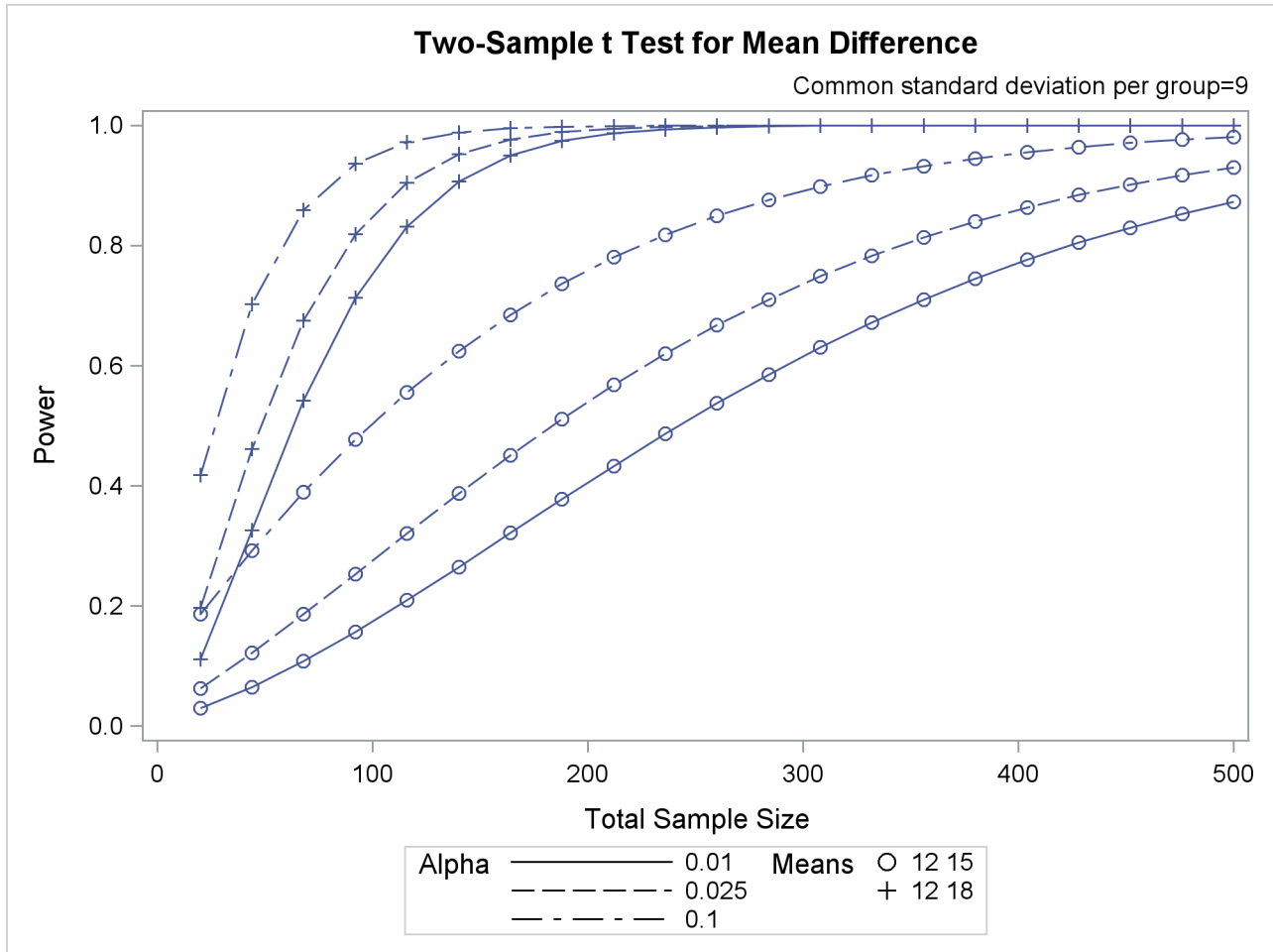
```

The defaults for the **VARY** option in the **PLOT** statement specify line style varying by the **ALPHA=** parameter, plotting symbol varying by the **GROUPMEANS=** parameter, panel varying by the **STDDEV=** parameter, and color remaining constant. The resulting plot, consisting of two panels, is shown in [Output 71.8.14](#).

**Output 71.8.14** Plot with Default VARY Settings



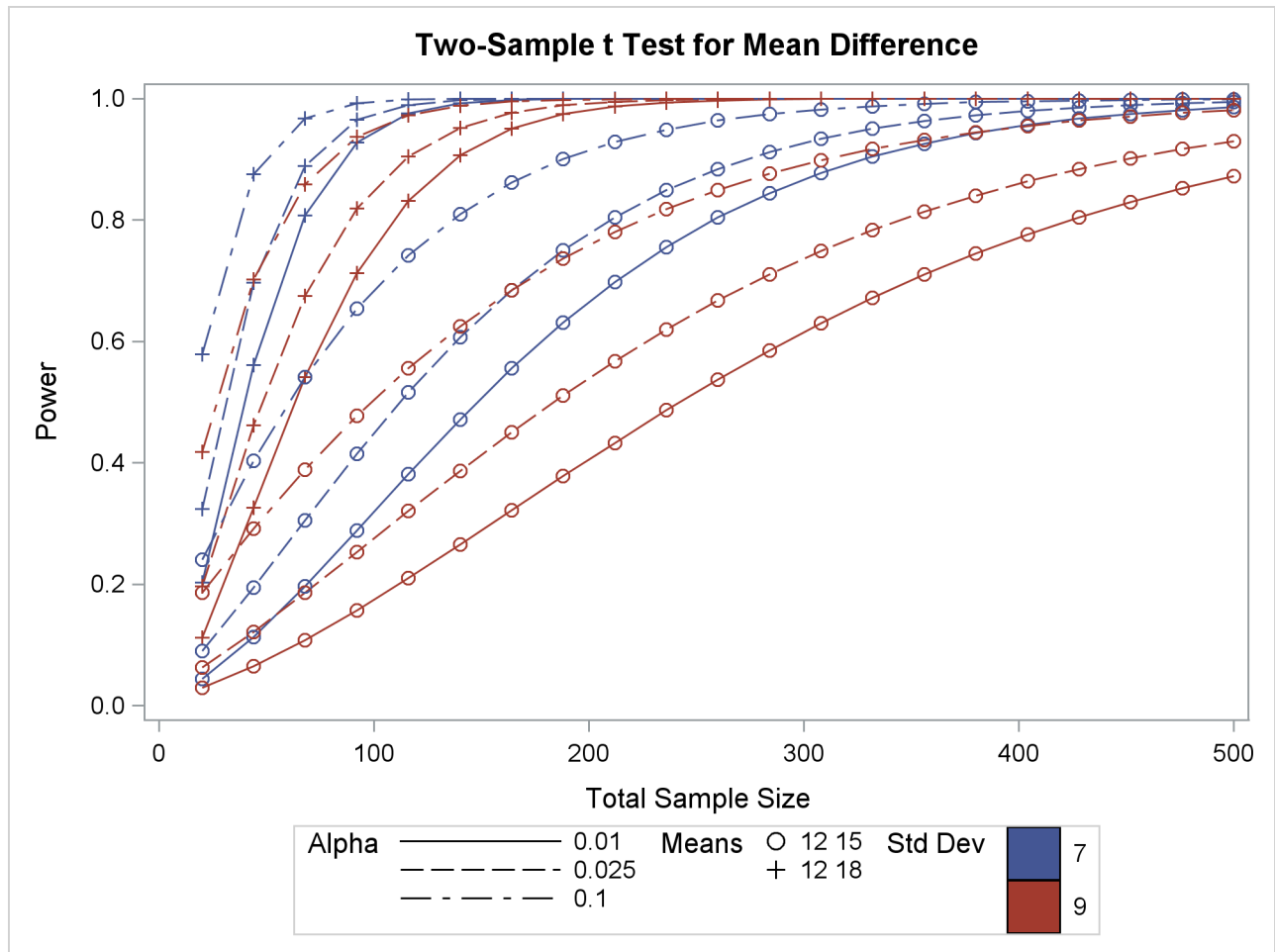
Output 71.8.14 continued



Suppose you want to produce a plot with only one panel that varies color in addition to line style and plotting symbol. Include the `LINESTYLE`, `SYMBOL`, and `COLOR` keywords in the `VARY` option in the `PLOT` statement, as follows, to produce the plot in Output 71.8.15:

```
plot x=n min=20 max=500
 vary (linestyle, symbol, color);
```

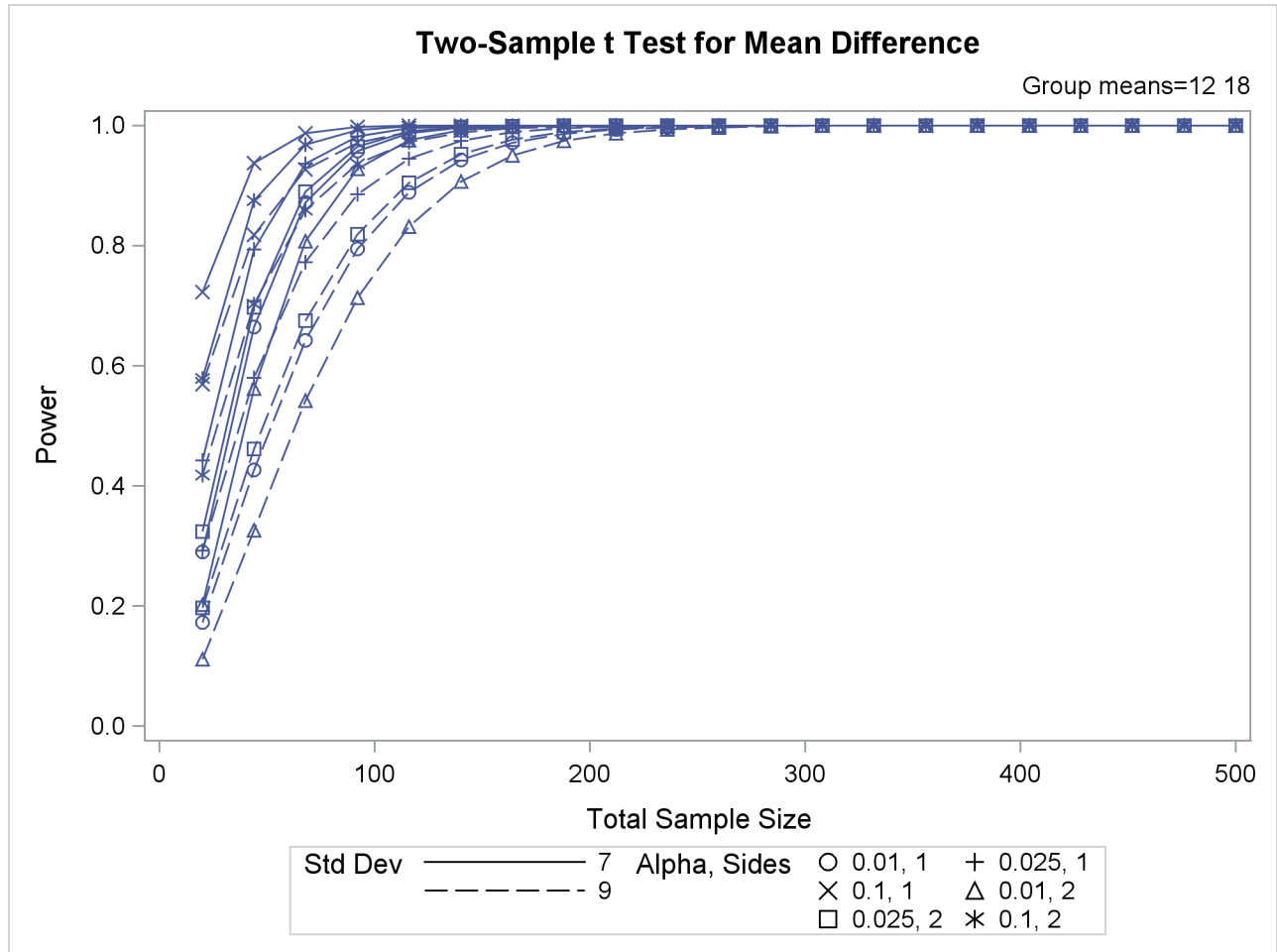
Output 71.8.15 Plot with Varying Color Instead of Panel



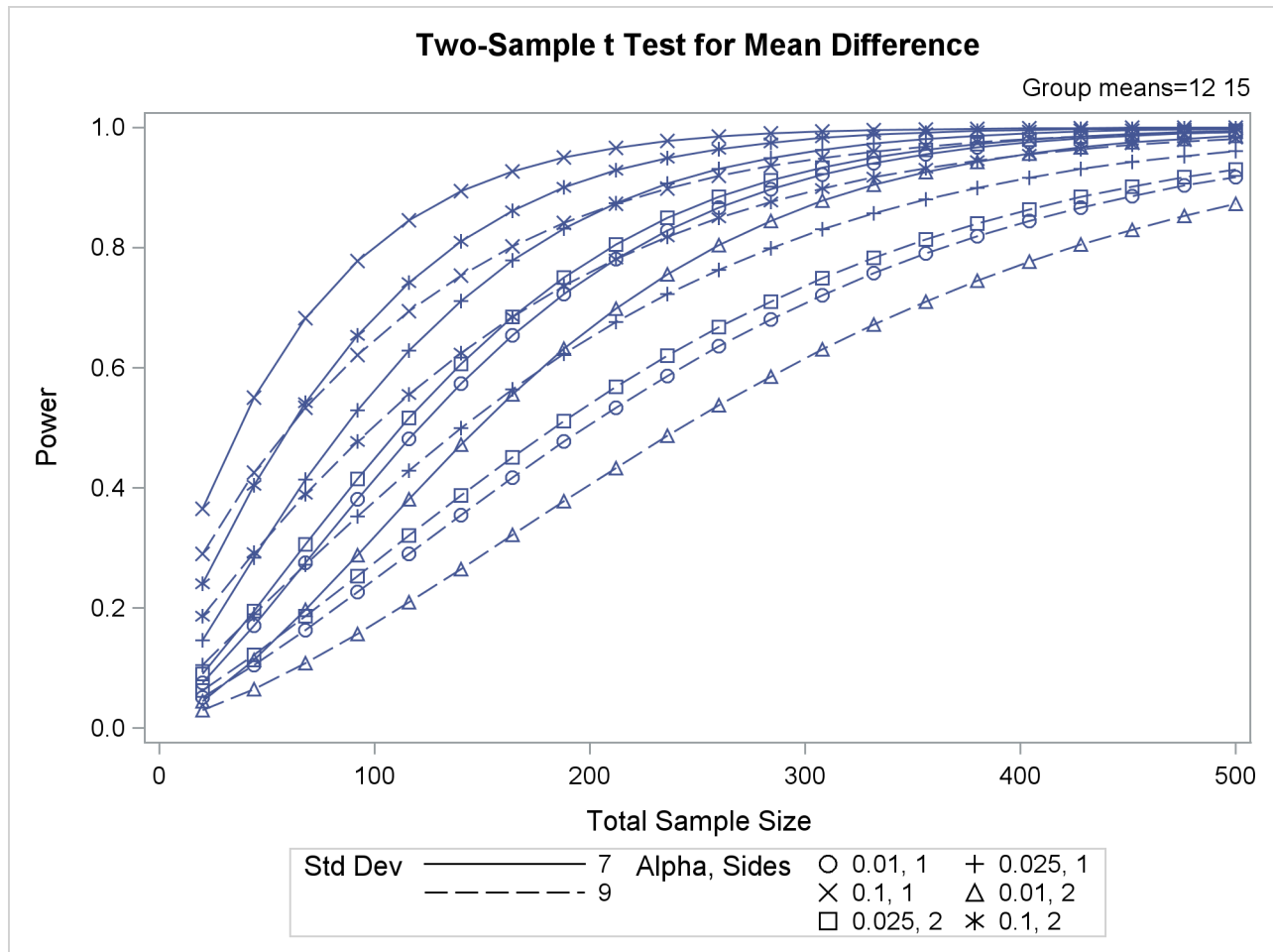
Finally, suppose you want to specify which features are used *and* which analysis parameters they are linked to. The following PLOT statement produces a two-panel plot (shown in Output 71.8.16) in which line style varies by standard deviation, plotting symbol varies by both alpha and sides, and panel varies by means:

```
plot x=n min=20 max=500
 vary (linestyle by stddev,
 symbol by alpha sides,
 panel by groupmeans);
```

**Output 71.8.16** Plot with Features Explicitly Linked to Parameters



Output 71.8.16 continued

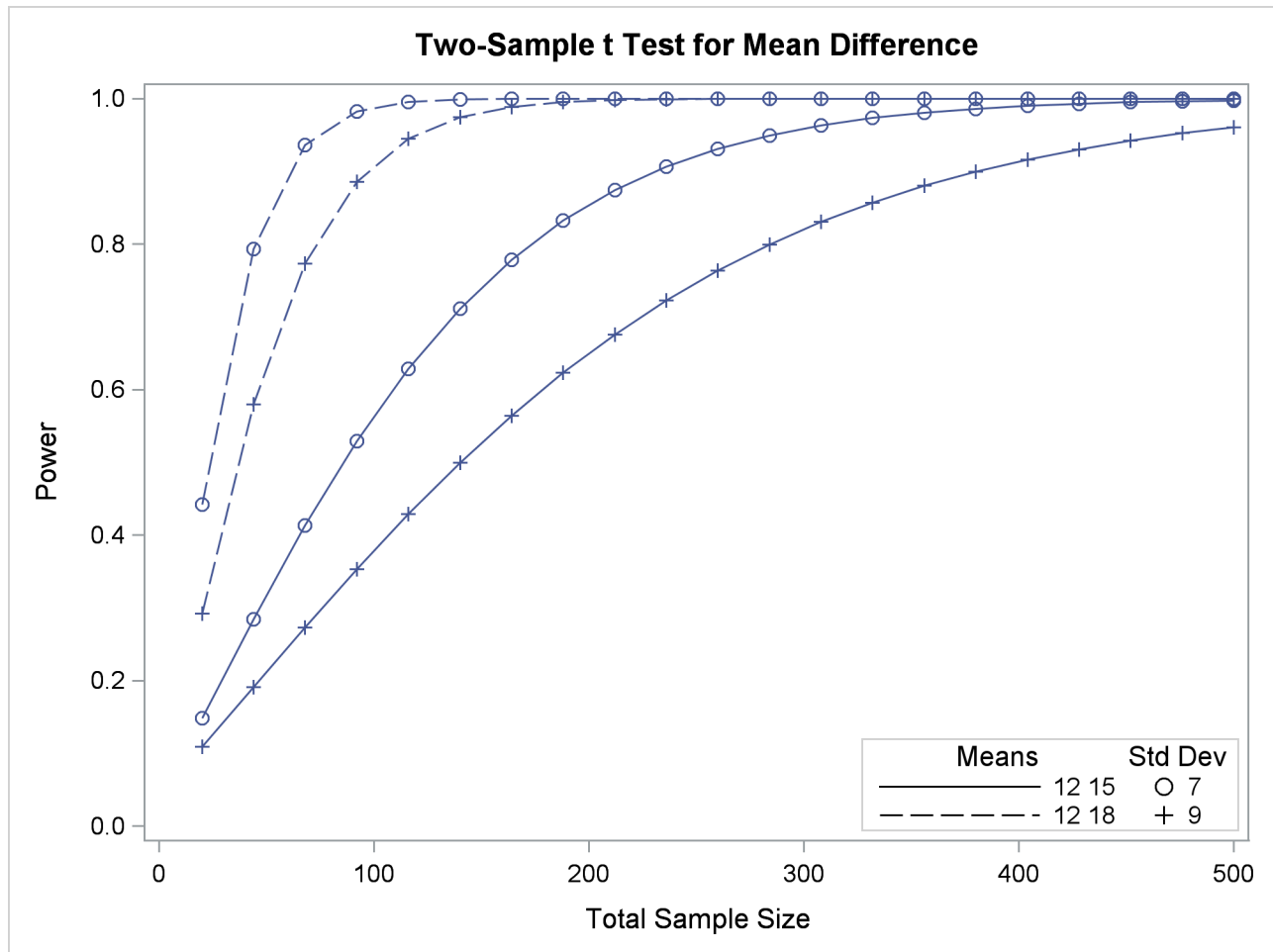


### Choosing Key (Legend) Styles

The default style for the key (or “legend”) is one that displays the association between levels of features and levels of analysis parameters, located below the X axis. For example, [Output 71.8.5](#) demonstrates this style of key.

You can reproduce [Output 71.8.5](#) with the same key but a different location, inside the plotting region, by using the `POS=INSET` option within the `KEY=BYFEATURE` option in the `PLOT` statement. The following statements product the plot in [Output 71.8.17](#):

```
proc power plotonly;
 twosamplemeans test=diff
 groupmeans = 12 | 15 18
 stddev = 7 9
 power = .
 ntotal = 200;
 plot x=n min=20 max=500
 key = byfeature(pos=inset);
run;
```

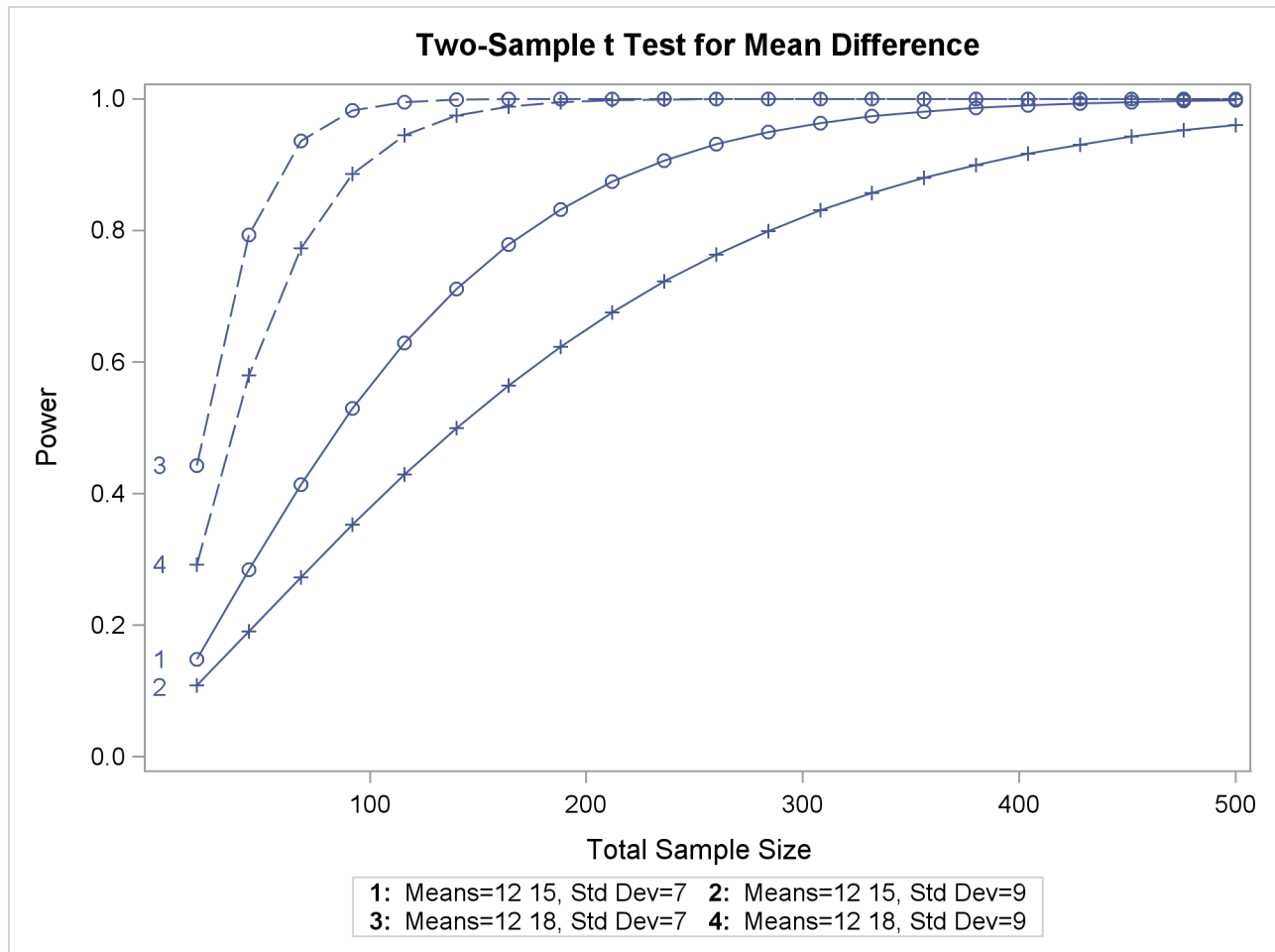
**Output 71.8.17** Plot with a By-Feature Key inside the Plotting Region

Alternatively, you can specify a key that identifies each individual curve separately by number by using the `KEY=BYCURVE` option in the `PLOT` statement:

```
plot x=n min=20 max=500
 key = bycurve;
```

The resulting plot is shown in [Output 71.8.18](#).



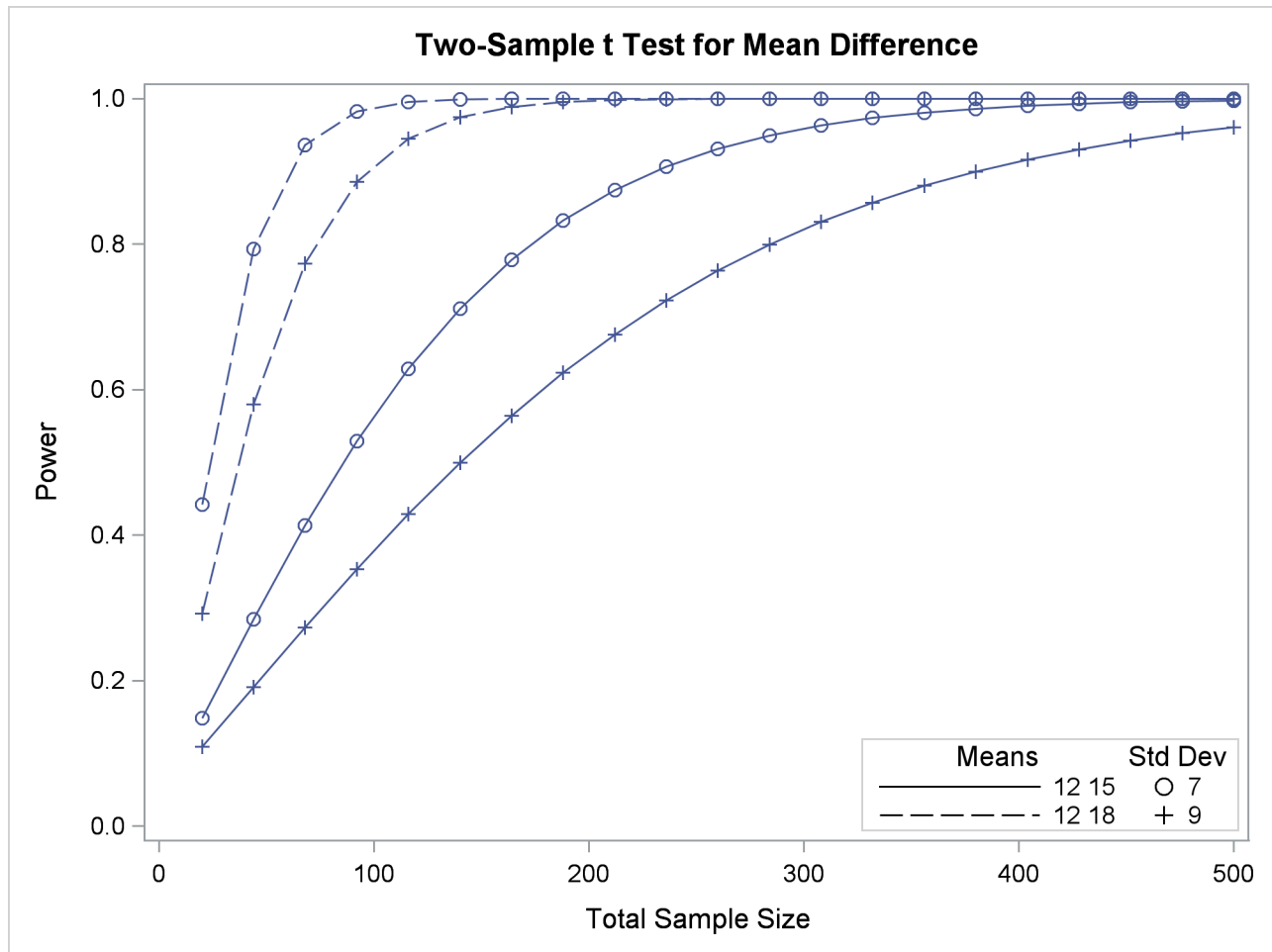
**Output 71.8.18** Plot with a Numbered By-Curve Key

Use the `NUMBERS=OFF` option within the `KEY=BYCURVE` option to specify a nonnumbered key that identifies curves with samples of line styles, symbols, and colors:

```
plot x=n min=20 max=500
 key = bycurve(numbers=off pos=inset);
```

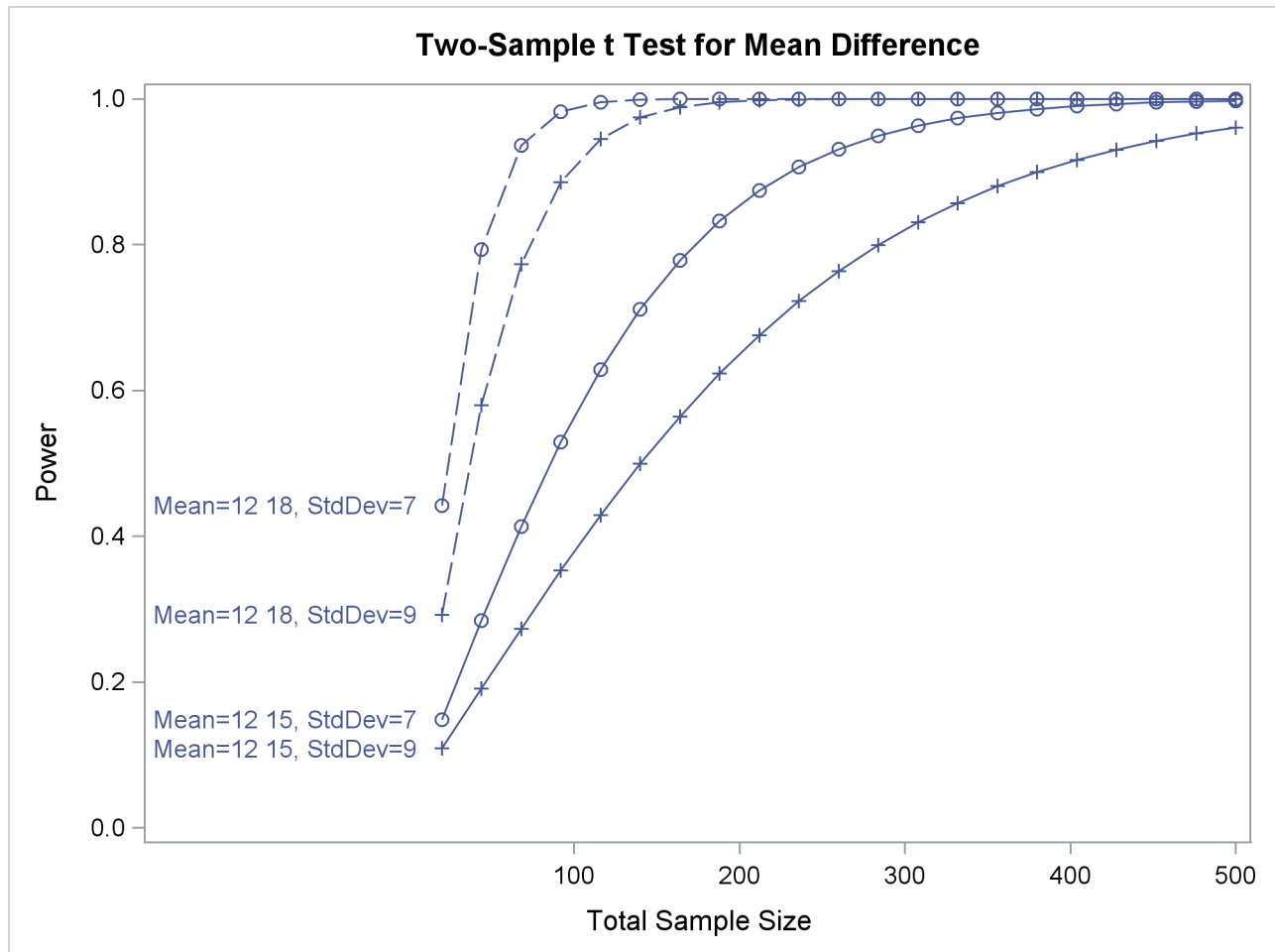
The `POS=INSET` suboption places the key within the plotting region. The resulting plot is shown in [Output 71.8.19](#).

**Output 71.8.19** Plot with a Nonnumbered By-Curve Key



Finally, you can attach labels directly to curves with the `KEY=ONCURVES` option. The following `PLOT` statement produces [Output 71.8.20](#):

```
plot x=n min=20 max=500
 key = oncurves;
```

**Output 71.8.20** Plot with Directly Labeled Curves

### Modifying Symbol Locations

The default locations for plotting symbols are the points computed directly from the power and sample size algorithms. For example, [Output 71.8.5](#) shows plotting symbols corresponding to computed points. The curves connecting these points are interpolated (as indicated by the `INTERPOL=` option in the `PLOT` statement).

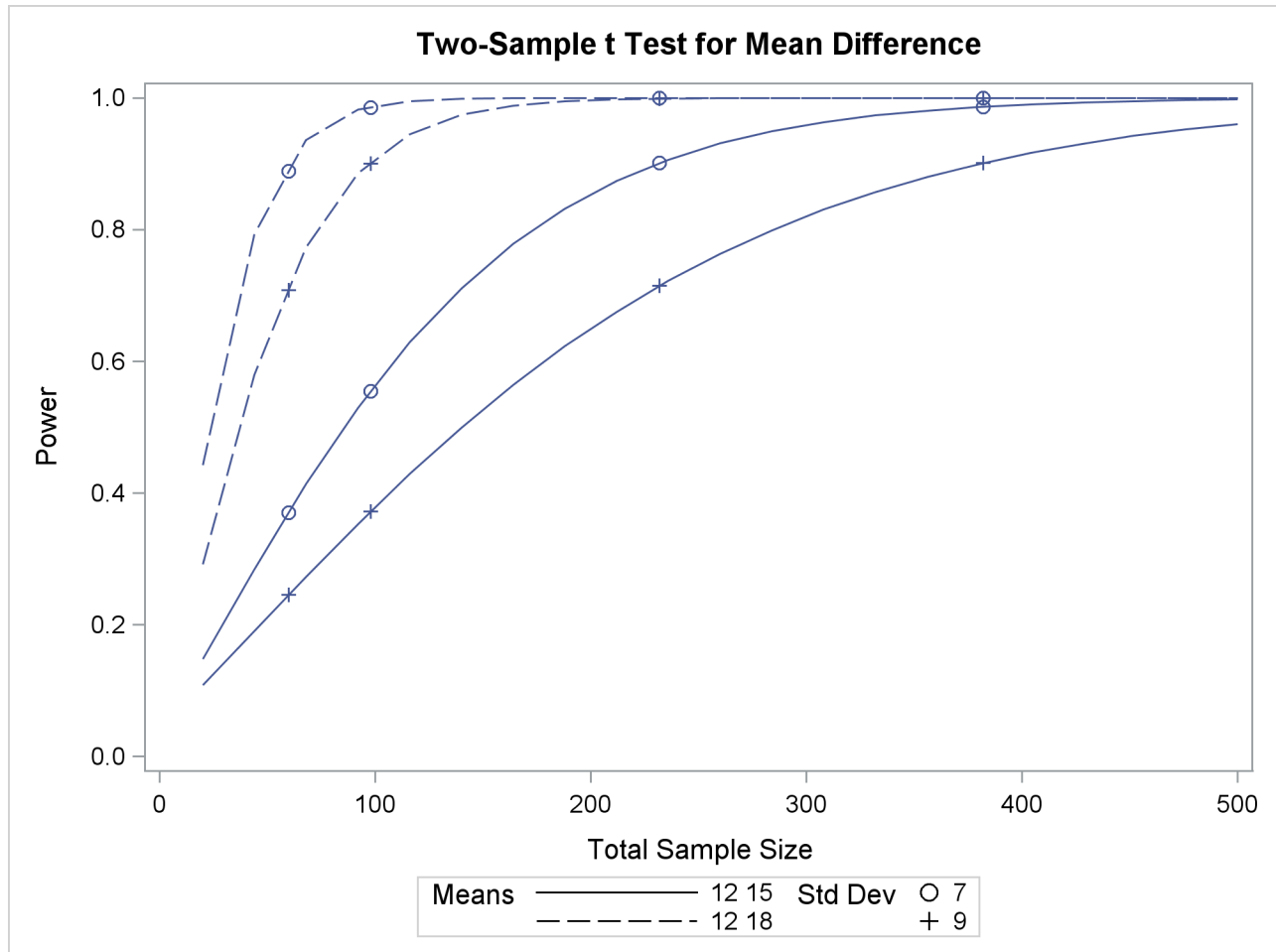
You can modify the locations of plotting symbols by using the `MARKERS=` option in the `PLOT` statement. The `MARKERS=ANALYSIS` option places plotting symbols at locations corresponding to the input specified in the analysis statement preceding the `PLOT` statement. You might prefer this as an alternative to using reference lines to highlight specific points. For example, you can reproduce [Output 71.8.5](#), but with the plotting symbols located at the sample sizes shown in [Output 71.8.1](#), by using the following statements:

```
proc power plotonly;
 twosamplemeans test=diff
 groupmeans = 12 | 15 18
 stddev = 7 9
 power = .
 ntotal = 232 382 60 98;
```

```
plot x=n min=20 max=500
 markers=analysis;
run;
```

The analysis statement here is the **TWOSAMPLEMEANS** statement. The **MARKERS=ANALYSIS** option in the **PLOT** statement causes the plotting symbols to occur at sample sizes specified by the **NTOTAL=** option in the **TWOSAMPLEMEANS** statement: 232, 382, 60, and 98. The resulting plot is shown in **Output 71.8.21**.

**Output 71.8.21** Plot with **MARKERS=ANALYSIS**

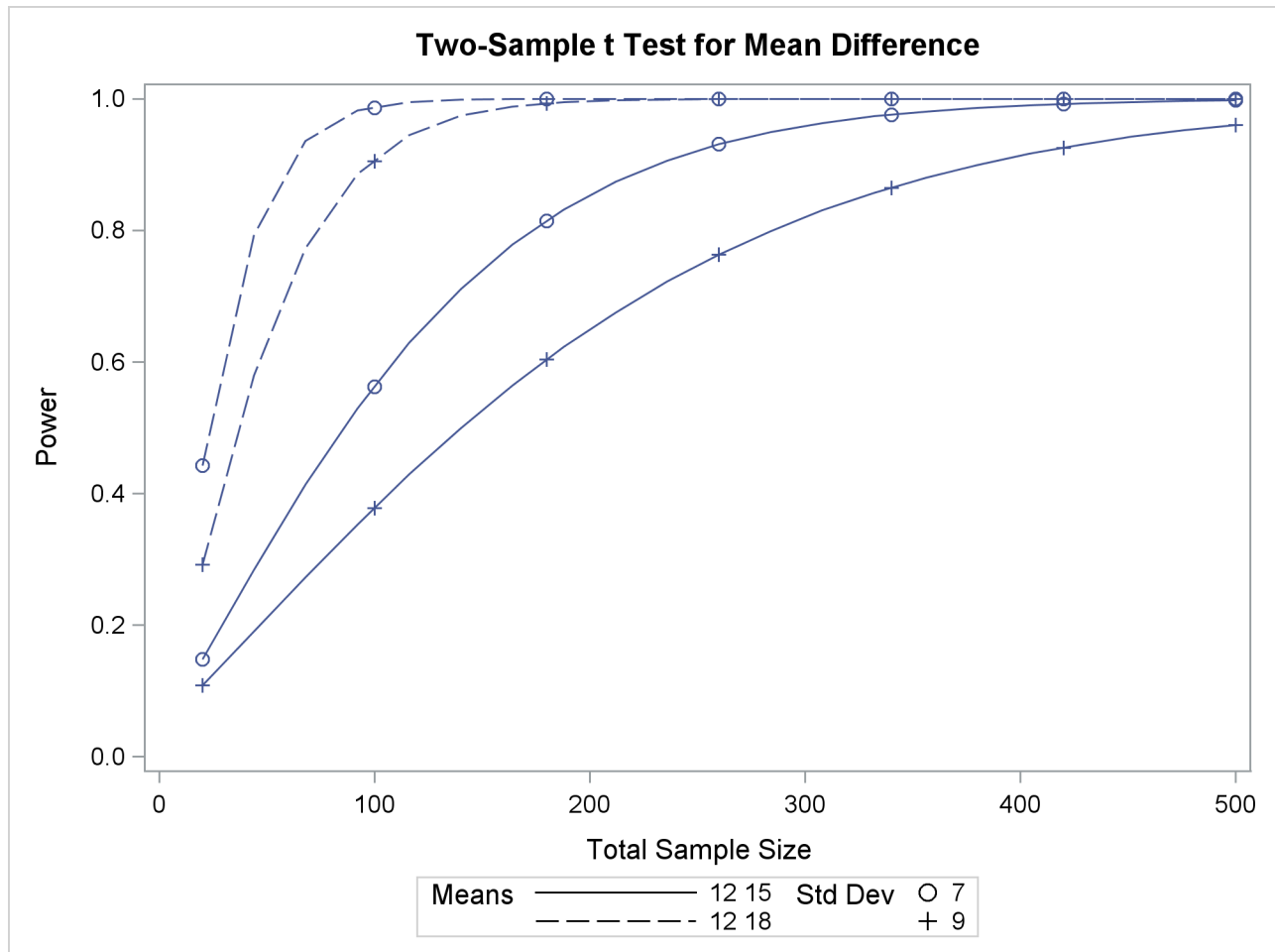


You can also use the **MARKERS=NICE** option to align symbols with the tick marks on one of the axes (the X axis when the **X=** option is used, or the Y axis when the **Y=** option is used):

```
plot x=n min=20 max=500
 markers=nice;
```

The plot created by this **PLOT** statement is shown in **Output 71.8.22**.

Output 71.8.22 Plot with MARKERS=NICE



Note that the plotting symbols are aligned with the tick marks on the X axis because the `X=` option is specified.

### Example 71.9: Binary Logistic Regression with Independent Predictors

Suppose you are planning an industrial experiment similar to the analysis in “Getting Started: LOGISTIC Procedure” on page 4166 of Chapter 54, “The LOGISTIC Procedure,” but for a different type of ingot. The primary test of interest is the likelihood ratio chi-square test of the effect of heating time on the readiness of the ingots for rolling. Ingot will be randomized independently into one of four different heating times (5, 10, 15, and 20 minutes) with allocation ratios 2:3:3:2 and three different soaking times (2, 4, and 6 minutes) with allocation ratios 2:2:1. The mass of each ingot will be measured as a covariate.

You want to know how many ingots you must sample to have a 90% chance of detecting an odds ratio as small as 1.2 for a five-minute heating time increase. The odds ratio is defined here as the odds of the ingot not being ready given a heating time of  $h$  minutes divided by the odds given a heating time of  $h - 5$  minutes, for any time  $h$ . You will use a significance level of  $\alpha = 0.1$  to balance Type I and Type II errors since you consider their importance to be roughly equal.

The distributions of heating time and soaking time are determined by the design, but you must conjecture the distribution of ingot mass. Suppose you expect its distribution to be approximately normal with mean 4 kg and standard deviation between 1 kg and 2 kg.

You are powering the study for an odds ratio of 1.2 for the heating time, but you must also conjecture odds ratios for soaking time and mass. You suspect that the odds ratio for a unit increase in soaking time is about 1.4, and the odds ratio for a unit increase in mass is between 1 and 1.3.

Finally, you must provide a guess for the average probability of an ingot not being ready for rolling, averaged across all possible design profiles. Existing data suggest that this probability lies between 0.15 and 0.25.

You decide to evaluate sample size at the two extremes of each parameter for which you conjectured a range. Use the following statements to perform the sample size determination:

```
proc power;
 logistic
 vardist("Heat") = ordinal((5 10 15 20) : (0.2 0.3 0.3 0.2))
 vardist("Soak") = ordinal((2 4 6) : (0.4 0.4 0.2))
 vardist("Mass1") = normal(4, 1)
 vardist("Mass2") = normal(4, 2)
 testpredictor = "Heat"
 covariates = "Soak" | "Mass1" "Mass2"
 responseprob = 0.15 0.25
 testoddsratio = 1.2
 units= ("Heat" = 5)
 covoddsratios = 1.4 | 1 1.3
 alpha = 0.1
 power = 0.9
 ntotal = .;
run;
```

The **VARDIST=** option is used to define the distributions of the predictor variables. The distributions of heating and soaking times are defined by the experimental design, with ordinal probabilities derived from the allocation ratios. The two conjectured standard deviations for the ingot mass are represented in the Mass1 and Mass2 distributions. The **TESTPREDICTOR=** option identifies the predictor being tested, and the **COVARIATES=** option specifies the scenarios for the remaining predictors in the model (soaking time and mass). The **RESPONSEPROB=** option specifies the overall response probability, and the **TESTODDSRATIO=** and **UNITS=** options indicate the odds ratio and increment for heating time. The **COVODDSRATIOS=** option specifies the scenarios for the odds ratios of soaking time and mass. The default **DEFAULTUNIT=1** option specifies a unit change for both of these odds ratios. The **ALPHA=** option sets the significance level, and the **POWER=** option defines the target power. Finally, the **NTOTAL=** option with a missing value (.) identifies the parameter to solve for.

Output 71.9.1 shows the results.

**Output 71.9.1** Sample Sizes for Test of Heating Time in Logistic Regression

| The POWER Procedure                                |          |                             |              |            |             |       |       |          |         |      |
|----------------------------------------------------|----------|-----------------------------|--------------|------------|-------------|-------|-------|----------|---------|------|
| Likelihood Ratio Chi-Square Test for One Predictor |          |                             |              |            |             |       |       |          |         |      |
| Fixed Scenario Elements                            |          |                             |              |            |             |       |       |          |         |      |
| Method                                             |          | Shieh-O'Brien approximation |              |            |             |       |       |          |         |      |
| Alpha                                              |          | 0.1                         |              |            |             |       |       |          |         |      |
| Test Predictor                                     |          | Heat                        |              |            |             |       |       |          |         |      |
| Odds Ratio for Test Predictor                      |          | 1.2                         |              |            |             |       |       |          |         |      |
| Unit for Test Pred Odds Ratio                      |          | 5                           |              |            |             |       |       |          |         |      |
| Nominal Power                                      |          | 0.9                         |              |            |             |       |       |          |         |      |
| Computed N Total                                   |          |                             |              |            |             |       |       |          |         |      |
| Index                                              | Response |                             | -Covariates- | --Cov ORs- | -Cov Units- | Total |       | N Actual | N Total |      |
|                                                    | Prob     |                             |              |            |             | Bins  | Power |          |         |      |
| 1                                                  | 0.15     | Soak                        | Mass1        | 1.4        | 1.0         | 1     | 1     | 120      | 0.900   | 1878 |
| 2                                                  | 0.15     | Soak                        | Mass1        | 1.4        | 1.3         | 1     | 1     | 120      | 0.900   | 1872 |
| 3                                                  | 0.15     | Soak                        | Mass2        | 1.4        | 1.0         | 1     | 1     | 120      | 0.900   | 1878 |
| 4                                                  | 0.15     | Soak                        | Mass2        | 1.4        | 1.3         | 1     | 1     | 120      | 0.900   | 1857 |
| 5                                                  | 0.25     | Soak                        | Mass1        | 1.4        | 1.0         | 1     | 1     | 120      | 0.900   | 1342 |
| 6                                                  | 0.25     | Soak                        | Mass1        | 1.4        | 1.3         | 1     | 1     | 120      | 0.900   | 1348 |
| 7                                                  | 0.25     | Soak                        | Mass2        | 1.4        | 1.0         | 1     | 1     | 120      | 0.900   | 1342 |
| 8                                                  | 0.25     | Soak                        | Mass2        | 1.4        | 1.3         | 1     | 1     | 120      | 0.900   | 1369 |

The required sample size ranges from 1342 to 1878, depending on the unknown true values of the overall response probability, mass standard deviation, and soaking time odds ratio. The overall response probability clearly has the largest influence among these parameters, with a sample size increase of almost 40% going from 0.25 to 0.15.

**Example 71.10: Wilcoxon-Mann-Whitney Test**

Consider a hypothetical clinical trial to treat interstitial cystitis (IC), a painful, chronic inflammatory condition of the bladder with no known cause that most commonly affects women. Two treatments will be compared: lidocaine alone (“lidocaine”) versus lidocaine plus a fictitious experimental drug called Mironel (“Mir+lido”). The design is balanced, randomized, double-blind, and female-only. The primary outcome is a measure of overall improvement at week 4 of the study, measured on a seven-point Likert scale as shown in Table 71.34.

**Table 71.34** Self-Report Improvement Scale

| Compared to when I started<br>this study, my condition is: |    |
|------------------------------------------------------------|----|
| Much worse                                                 | -3 |
| Worse                                                      | -2 |
| Slightly worse                                             | -1 |
| The same                                                   | 0  |
| Slightly better                                            | +1 |
| Better                                                     | +2 |
| Much better                                                | +3 |

The planned data analysis is a one-sided Wilcoxon-Mann-Whitney test with  $\alpha = 0.05$  where the alternative hypothesis represents greater improvement for “Mir+lido.”

You are asked to graphically assess the power of the planned trial for sample sizes between 100 and 250, assuming that the conditional outcome probabilities given treatment are equal to the values in [Table 71.35](#).

**Table 71.35** Conjectured Conditional Probabilities

| Treatment | Response |      |      |      |      |      |      |
|-----------|----------|------|------|------|------|------|------|
|           | -3       | -2   | -1   | 0    | +1   | +2   | +3   |
| Lidocaine | 0.01     | 0.04 | 0.20 | 0.50 | 0.20 | 0.04 | 0.01 |
| Mir+lido  | 0.01     | 0.03 | 0.15 | 0.35 | 0.30 | 0.10 | 0.06 |

Use the following statements to compute the power at sample sizes of 100 and 250 and generate a power curve:

```
ods listing style=htmlbluecml;
ods graphics on;

proc power;
 twosamplewilcoxon
 vardist("lidocaine") = ordinal ((-3 -2 -1 0 1 2 3) :
 (.01 .04 .20 .50 .20 .04 .01))
 vardist("Mir+lido") = ordinal ((-3 -2 -1 0 1 2 3) :
 (.01 .03 .15 .35 .30 .10 .06))
 variables = "lidocaine" | "Mir+lido"
 sides = u
 ntotal = 100 250
 power = .;
 plot step=10;
run;

ods graphics off;
```

The ODS LISTING STYLE=HTMLBLUECML statement specifies the HTMLBLUECML style, which is suitable for use with PROC POWER because it allows both marker symbols and line styles to vary. See the section “[ODS Styles Suitable for Use with PROC POWER](#)” on page 6082 for more information.



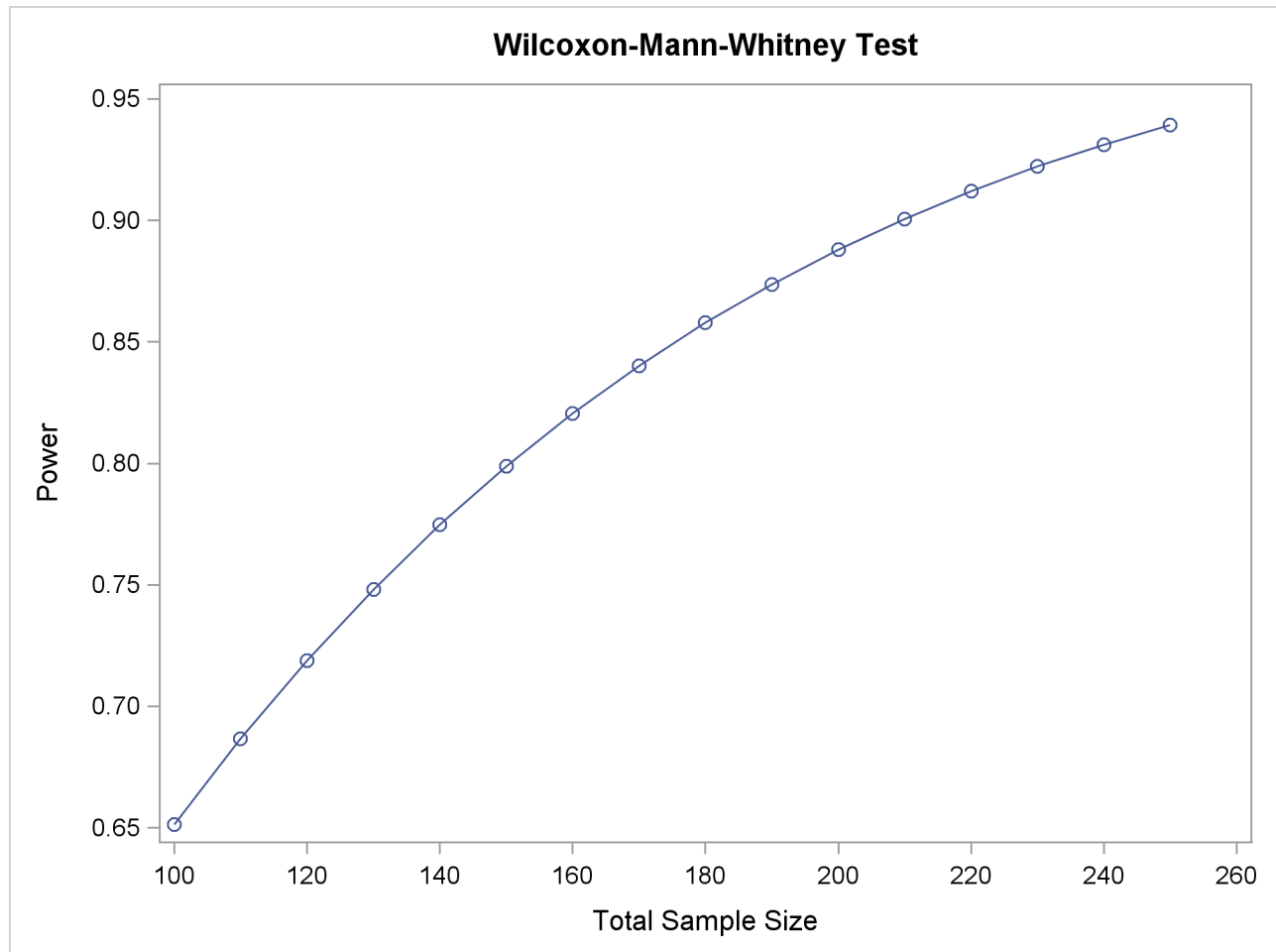
The **VARDIST=** option is used to define the distribution for each treatment, and the **VARIABLES=** option specifies the distributions to compare. The **SIDES=U** option corresponds to the alternative hypothesis that the second distribution ("Mir+lido") is more favorable. The **NTOTAL=** option specifies the total sample sizes of interest, and the **POWER=** option with a missing value (.) identifies the parameter to solve for. The default **GROUPWEIGHTS=** and **ALPHA=** options specify a balanced design and significance level  $\alpha = 0.05$ .

The **STEP=10** option in the **PLOT** statement requests a point for each sample size increment of 10. The default values for the **X=**, **MIN=**, and **MAX=** plot options specify a sample size range of 100 to 250 (the same as in the analysis) for the X axis.

The tabular and graphical results are shown in [Output 71.10.1](#) and [Output 71.10.2](#), respectively.

**Output 71.10.1** Power Values for Wilcoxon-Mann-Whitney Test

| The POWER Procedure        |                                 |       |
|----------------------------|---------------------------------|-------|
| Wilcoxon-Mann-Whitney Test |                                 |       |
| Fixed Scenario Elements    |                                 |       |
| Method                     | O'Brien-Castelloe approximation |       |
| Number of Sides            | U                               |       |
| Group 1 Variable           | lidocaine                       |       |
| Group 2 Variable           | Mir+lido                        |       |
| Pooled Number of Bins      | 7                               |       |
| Alpha                      | 0.05                            |       |
| Group 1 Weight             | 1                               |       |
| Group 2 Weight             | 1                               |       |
| NBins Per Group            | 1000                            |       |
| Computed Power             |                                 |       |
| Index                      | N                               |       |
|                            | Total                           | Power |
| 1                          | 100                             | 0.651 |
| 2                          | 250                             | 0.939 |

**Output 71.10.2** Plot of Power versus Sample Size for Wilcoxon Power Analysis

The achieved power ranges from 0.651 to 0.939, increasing with sample size.

---

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## Chapter 72

# The Power and Sample Size Application

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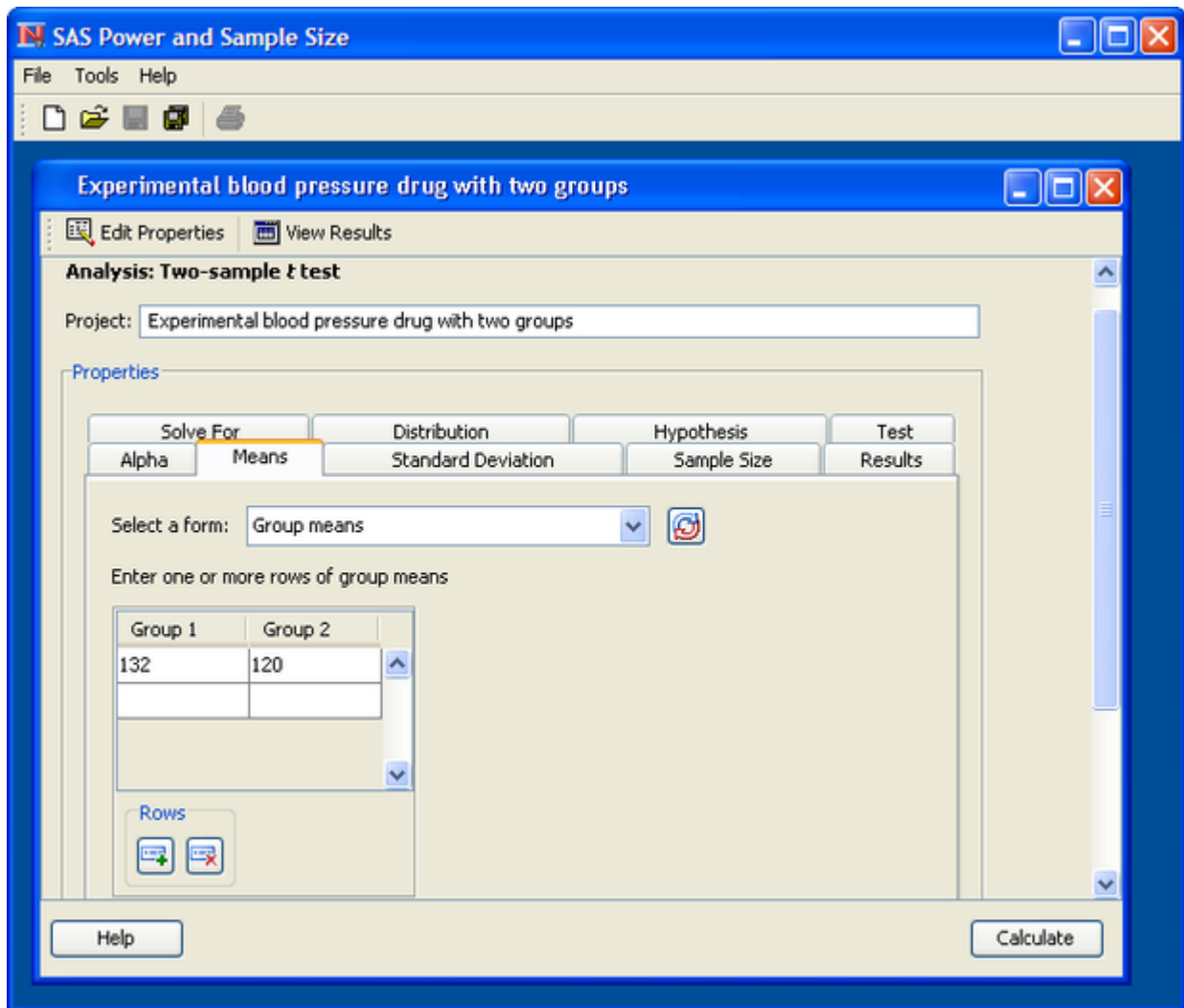
## Overview: PSS Application

### SAS Power and Sample Size

The SAS Power and Sample Size application (PSS) is a desktop application that provides easy access to power analysis and sample size determination techniques. The application is intended for students and researchers as well as experienced SAS users and statisticians.

Figure 72.1 shows the graphical user interface. PSS relies on the SAS/STAT procedures POWER and GLMPOWER for its computations.

Figure 72.1 PSS Application



This section describes the statistical tasks that are available with the application as well as its principal features.

## Analyses

PSS provides power and sample size computations for a variety of statistical analyses. Included are  $t$  tests for means; equivalence tests and confidence intervals for means and proportions; exact binomial, chi-square, Fisher's exact, and McNemar tests for proportions; correlation and regression (multiple and logistic); one-way analysis of variance; linear models; tests of distribution; and rank tests for comparing survival curves.

Table 72.1 lists the analyses that are available.

**Table 72.1** Available Analyses

| Category                               | Analysis                                         |
|----------------------------------------|--------------------------------------------------|
| Means                                  | One-sample $t$ test                              |
|                                        | Paired $t$ test                                  |
|                                        | Two-sample $t$ test                              |
| Confidence intervals                   | One proportion                                   |
|                                        | One-sample means                                 |
|                                        | Paired means                                     |
|                                        | Two-sample means                                 |
| Equivalence tests                      | One proportion                                   |
|                                        | One-sample means                                 |
|                                        | Paired means                                     |
|                                        | Two-sample means                                 |
| Proportions                            | One proportion                                   |
|                                        | Two correlated proportions                       |
|                                        | Two independent proportions                      |
| Correlation and regression             | Pearson correlation coefficient                  |
|                                        | Logistic regression with a binary response       |
|                                        | Multiple regression                              |
| Analysis of variance and linear models | One-way ANOVA                                    |
|                                        | General linear univariate models                 |
| Survival analysis                      | Two-sample survival rank tests                   |
| Distribution tests                     | Wilcoxon Mann-Whitney test for two distributions |

## Features

PSS provides multiple input parameter options, stores the results in a project format, displays power curves, and produces narratives for the results. Narratives are descriptions of the input parameters and include a statement about the computed power or sample size. The SAS log and SAS code are also available.

All analyses offer computation of power or sample size. Some analyses offer computation of sample size per group as well as total sample size.



Where appropriate, several alternate ways of entering values for certain parameters are offered. For example, in the two-sample  $t$  test analysis, means can be entered for individual groups or as a difference. The null mean difference can be specified as a default of zero or can be explicitly entered.

Information about existing analyses is stored in a project format. You can access each project to review the results or to edit your input parameters and produce another analysis.

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## Getting Started: PSS Application

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### Overview

This section is intended to get you off to a quick start with PSS. More detailed information about using the application is found in “How to Use: PSS Application” on page 6166 and in the example sections.

To start the application on a PC using the Windows operating system, select **Start►Programs►SAS►SAS Power and Sample Size 3.1** (or the latest release).

When you first use the application for a release, you are asked some configuration questions. For more information see the section “Configuration” on page 6182.

As an initial step, you also must define a SAS connection. If you have Foundation SAS software installed on the PC that you are using for PSS, this step can be done for you automatically. To define a connection or to determine whether one has already been defined, see the section “SAS Connections” on page 6166.

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### The Basic Steps

Here are the basic steps that you follow to use PSS.

1. Start a new project by selecting **File►New** on the menu bar or clicking the **New** icon on the toolbar.
2. In the New window, select the desired analysis type and click **OK**.  
A project window for the analysis type appears with the Edit Properties page displayed. (The tabs on the Edit Properties page and their content vary according to the analysis type.)
3. Click each tab to enter the relevant data for the analysis. (For more information about the types of data to enter, see the example sections.)
4. After you have entered all the data, click the **Calculate** button.
5. After PSS calculates the results, the project window displays the View Results page with the Summary Table tab displayed by default.
6. To view other results or to review the SAS code or the SAS log, click any of the tabs on the left side of the View Results page.
7. To print any results page, select **File►Print** on the menu bar.

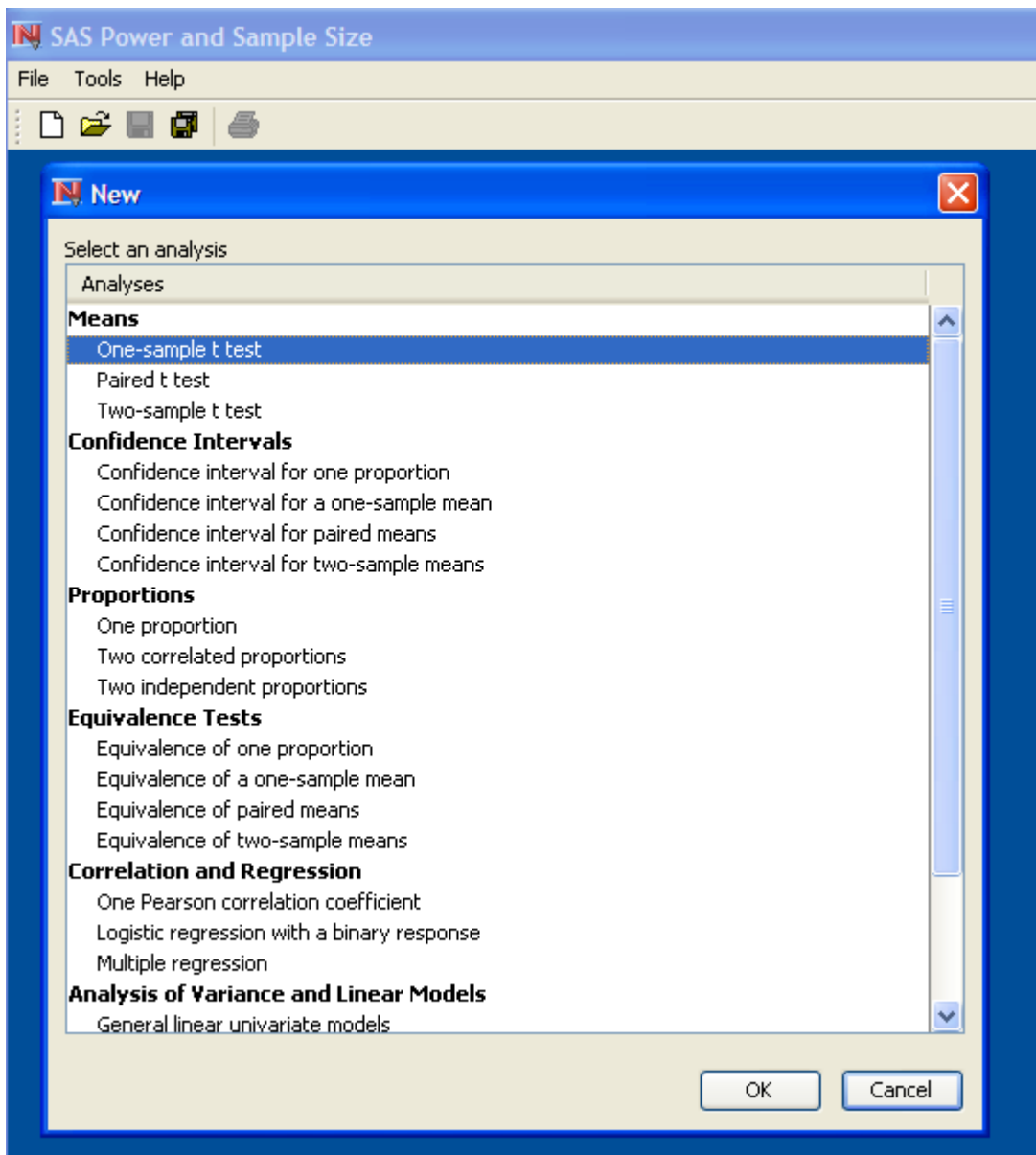
The remainder of this section takes you through a simple example.

## A Simple Example

Suppose you want to determine the power for a new marketing study. You want to compare car sales in the southeastern region to the national average of 1.0 car per salesperson per day. You believe that the actual average for the region is 1.6 cars per salesperson per day. You want to test if the mean for a single group is larger than a specific value, so the one-sample  $t$  test is the appropriate analysis. The conjectured mean is 1.6 and the null mean is 1.0. You intend to use a significance level of 0.05 for the one-sided test. You want to calculate power for two standard deviations, 0.5 and 0.75, and two sample sizes, 10 and 20 dealerships.

First, open a new project by selecting **File►New** on the menu bar or clicking the **New** icon on the toolbar. The New window appears. Then, select the appropriate analysis.

**Figure 72.2** New Window



For this example, the selected analysis is the **One-sample t test** in the **Means** section, as shown at the top of [Figure 72.2](#). Select the analysis from the list and click **OK**. The **One-sample t test** project window appears with the Edit Properties page displayed, as shown in [Figure 72.3](#).

**Figure 72.3** Edit Properties Page

**Regional car sales versus the national average**

Edit Properties | View Results

**Analysis: One-sample t Test**

Project:

Properties

Standard Deviation | Sample Size | Results

Solve For | Distribution | Hypothesis | Alpha | Means

Select a quantity to solve for

Power

Sample size

◀ Previous tab | Next tab ▶

Enter a descriptive label of the project in the **Project:** field. For the example, change the description to *Regional car sales versus the national average*. The description is used to identify the project when you reopen it from the Open window.

Select **File►Save** to save the description change. Note in [Figure 72.3](#) that the title bar of the window contains your project description after you have saved the change.

Properties of the project are displayed on several tabs. You can change from tab to tab by clicking a tab or by clicking the **Next tab** or **Previous tab** buttons. To display help about the properties for a tab, click the **Help** button at the bottom of the Edit Properties page.

## Entering Parameter Values

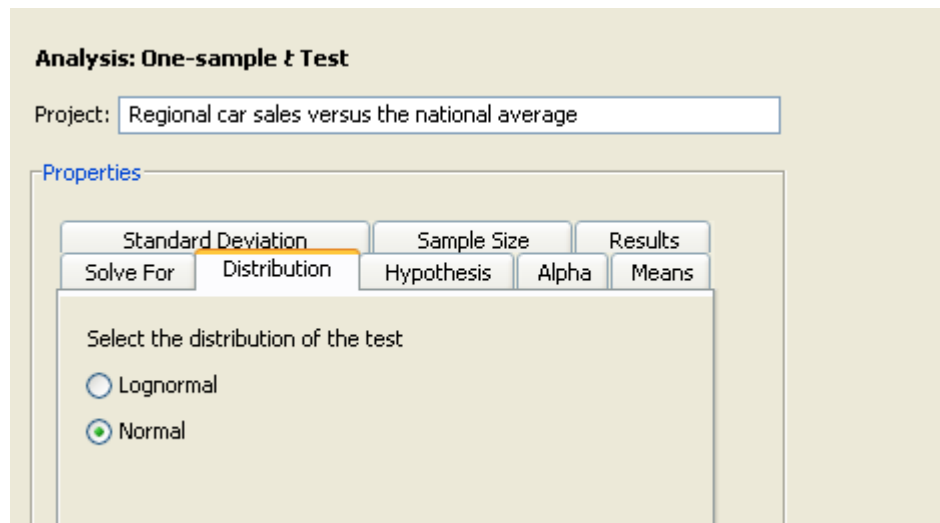
First, click the **Solve For** tab and choose to calculate power or sample size. For this example, select the **Power** option, as shown in [Figure 72.3](#).

Next, you must provide values for two analysis options and four parameters. These parameters are set in separate tabs on the Edit Properties page and are labeled **Distribution**, **Hypothesis**, **Alpha**, **Mean**, **Standard Deviation**, and **Sample Size**.

### *Distribution*

Click the **Distribution** tab to select a **Normal** or **Lognormal** distribution. For the example, you are using means rather than mean ratios, so select **Normal**, as shown in [Figure 72.4](#).

**Figure 72.4** Distribution Tab



### *Hypothesis*

Click the **Hypothesis** tab to select a one- or two-sided test. Because you are interested only in whether the southeastern region produces higher daily car sales than the national average, select **One-sided test**, as shown in [Figure 72.5](#).

Figure 72.5 Hypothesis Tab

**Analysis: One-sample  $t$  Test**

Project:

Properties

|                    |             |         |
|--------------------|-------------|---------|
| Standard Deviation | Sample Size | Results |
| Solve For          | Hypothesis  | Alpha   |
| Distribution       |             | Means   |

Select a one or two-sided hypothesis test

One-sided test       Lower one-sided test  
 Two-sided test       Upper one-sided test

There are three one-sided test options: **One-sided test**, **Upper one-sided test**, and **Lower one-sided test**. The **Upper one-sided test** option would also be appropriate for this example.

### Alpha

Click the **Alpha** tab to specify one or more significance levels. Enter 0.05, as shown in Figure 72.6.

Figure 72.6 Alpha Tab

Properties

|                    |             |         |
|--------------------|-------------|---------|
| Standard Deviation | Sample Size | Results |
| Solve For          | Hypothesis  | Alpha   |
| Distribution       |             | Means   |

Specify one or more significance levels

Alpha

Rows



This value will be the default unless the default has been changed in the Preferences window. To set preferences, select **Tools►Preferences** on the menu bar. For more information about setting preferences, see the section “[Setting Preferences](#)” on page 6169.

### Mean

Click the **Means** tab to enter one or more means and null means. For the example, enter 1.6 in the Mean table and 1.0 in the Null Mean table. [Figure 72.7](#) shows the entered values.

**Figure 72.7** Means Tab

The screenshot shows a software window titled "Properties" with a "Means" tab selected. The window contains two input tables. The first table, labeled "Mean", has a single row with the value "1.6". The second table, labeled "Null Mean", has a single row with the value "1.0". Below each table are "Rows" buttons with "+" and "-" icons. The window also has several other tabs: "Standard Deviation", "Sample Size", "Results", "Solve For", "Distribution", "Hypothesis", and "Alpha".

Note that additional input rows are available if you want to enter additional sets of parameters. You can also append and delete rows using the  and  buttons beneath the table. In addition, by selecting a row and right-clicking, you can choose to insert and delete rows in the body of the table from a pop-up menu.

### Standard Deviation

Click the **Standard Deviation** tab to enter standard deviations. You are interested in two standard deviations, 0.5 and 0.75. Enter them in the table, as shown in [Figure 72.8](#).

**Figure 72.8** Standard Deviation Tab

The screenshot shows a software window titled "Properties" with several tabs: "Solve For", "Distribution", "Hypothesis", "Alpha", and "Means". The "Standard Deviation" tab is selected and highlighted in orange. Below the tabs, there are sub-tabs: "Standard Deviation", "Sample Size", and "Results". The "Standard Deviation" sub-tab is active. The main area contains the text "Enter one or more standard deviations". Below this is a list box labeled "Std. Dev." containing the values "0.5" and "0.75". At the bottom of the list box are two buttons: a green plus sign and a red minus sign, with the label "Rows" above them.

**Sample Size**

You want to be able to sample between 10 and 20 dealerships. Click the **Sample Size** tab and enter these two values, as shown in Figure 72.9.

**Figure 72.9** Sample Size Tab

The screenshot shows the same software window as Figure 72.8, but with the "Sample Size" sub-tab selected and highlighted in orange. The main area contains the text "Enter one or more values for total sample size". Below this is a list box labeled "Total N" containing the values "10" and "20". At the bottom of the list box are two buttons: a green plus sign and a red minus sign, with the label "Rows" above them. Below the list box is a section titled "Fractional Sample Sizes" with a checkbox labeled "Allow fractional sample sizes", which is currently unchecked.

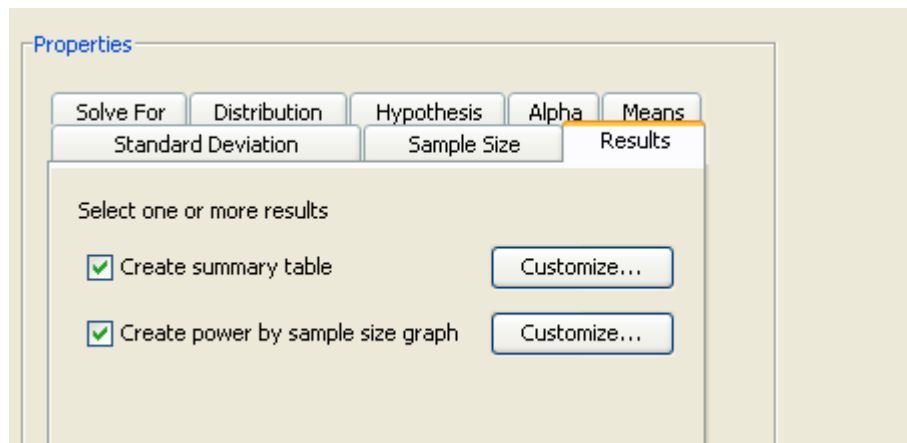
### Scenarios

The input values are combined into one or more scenarios. In this case, each of the two standard deviations is combined with each of the two sample sizes for a total of four scenarios. Then power is computed for each scenario. In this example, only a single value or setting is present for the mean, null mean, and alpha level, so they are common to all scenarios.

### Results Options

Click the **Results** tab to select results options including a Summary Table and a Power by Sample Size graph.

**Figure 72.10** Results Tab

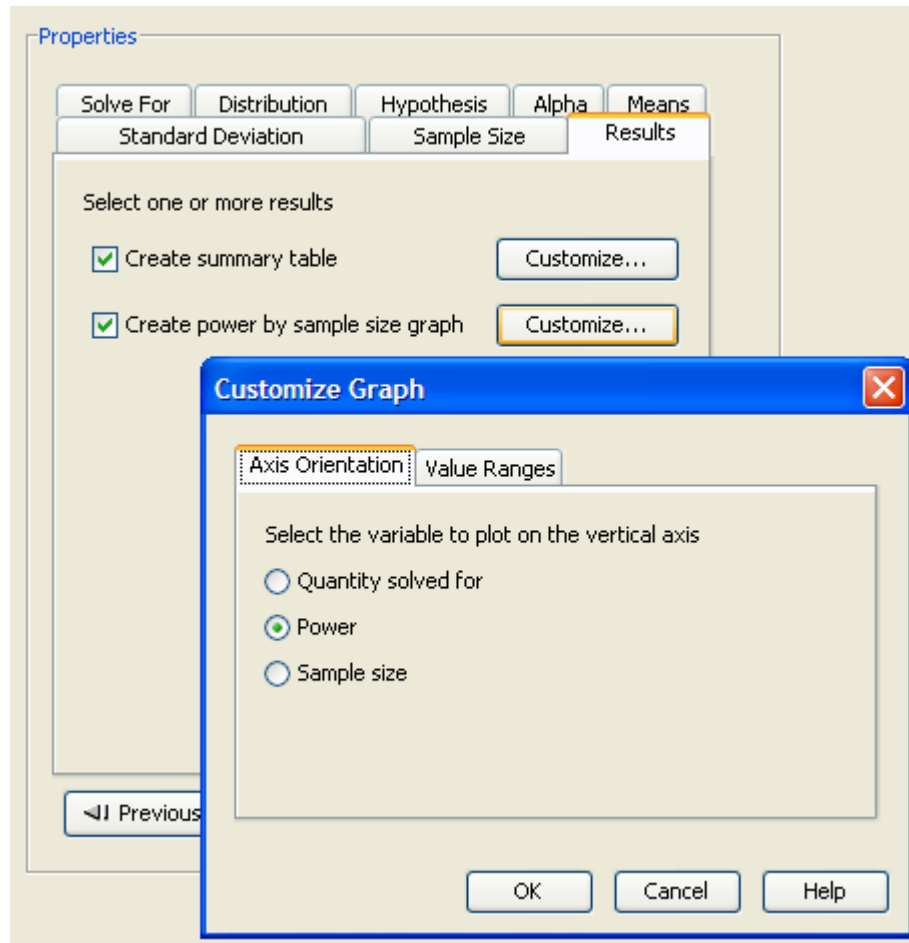


For this example, select both results check boxes: **Create summary table** and **Create power by sample size graph**, as shown in Figure 72.10. These selections can also be set as preferences; see the section “Setting Preferences” on page 6169.

### Customizing the Power by Sample Size Graph

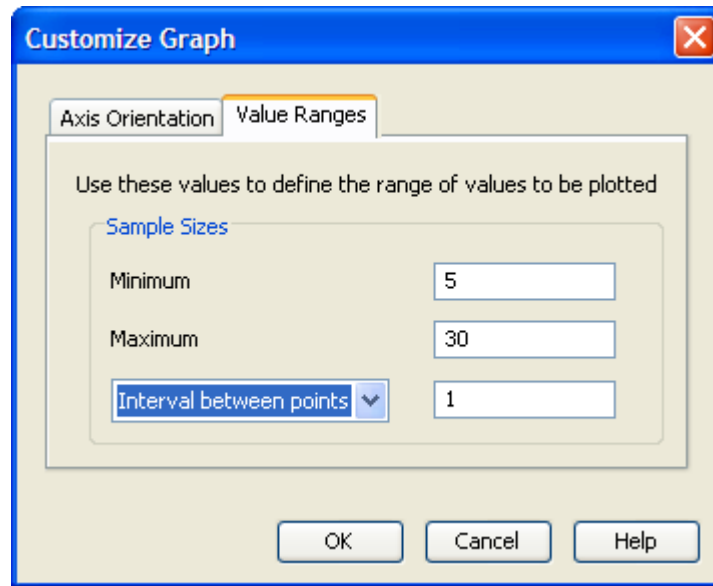
Click the **Customize** button beside the **Create power by sample size graph** check box to customize the graph. The Customize Graph window contains two tabs: **Axis Orientation** and **Value Ranges**, as shown in Figure 72.11.



**Figure 72.11** Customize Graph Window with Axis Orientation Tab

Click the **Axis Orientation** tab to select which quantity you would like to plot on the vertical axis. You can choose to display the quantity solved for (either power or sample size) on the vertical axis or you can choose to display power or sample size on the vertical axis with the other quantity appearing on the horizontal axis. The default is **Quantity solved for** (or power) on the vertical axis, which is appropriate for this graph.

The summary table is created using the two sample sizes specified in the Sample Size table, 10 and 20. If you want to create a graph that contains more than these two sample sizes, you can do so by customizing the value ranges for the graph. Click the **Value Ranges** tab to set the axis range for sample sizes, as shown in Figure 72.12.

**Figure 72.12** Customize Graph Window with Value Ranges Tab

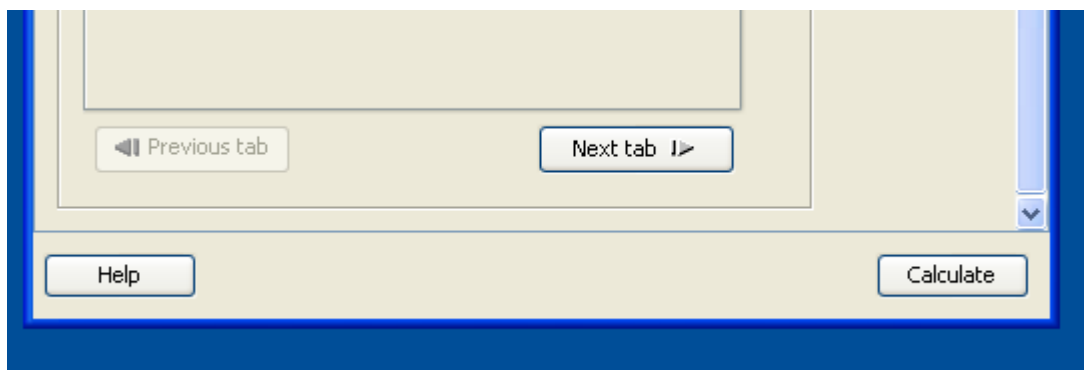
Enter 5 for the minimum and 30 for the maximum. Also, select **Interval between points** in the drop-down list and enter a value of 1. These values set the sample size axis to range from 5 to 30 in increments of 1. The completed Value Ranges section of the window is shown in [Figure 72.12](#).

When you solve for power, you can set a range for sample size values, but not for the powers; and vice versa when you solve for sample size. That is, you cannot set the range of axis values for the quantity that you are solving for.

Click **OK** to save the values that you have entered and return to the Edit Properties page.

## Performing the Analysis

You have now specified all of the necessary input values. Click **Calculate** to perform the analysis, as shown in [Figure 72.13](#).

**Figure 72.13** Calculate Button on the Edit Properties Page

Alternatively, you could choose to save the information that you have entered by selecting **File►Save** from the menu bar or clicking the **Save** toolbar icon, and perform the analysis at another time. No error checking is done when you save the project.

You can close the project by selecting **File►Close** on the menu bar or clicking the window close **X** in the upper right corner of the project window. You can reopen a project by selecting **File►Open** on the menu bar or clicking the **Open** toolbar icon.

For this example, click **Calculate**.

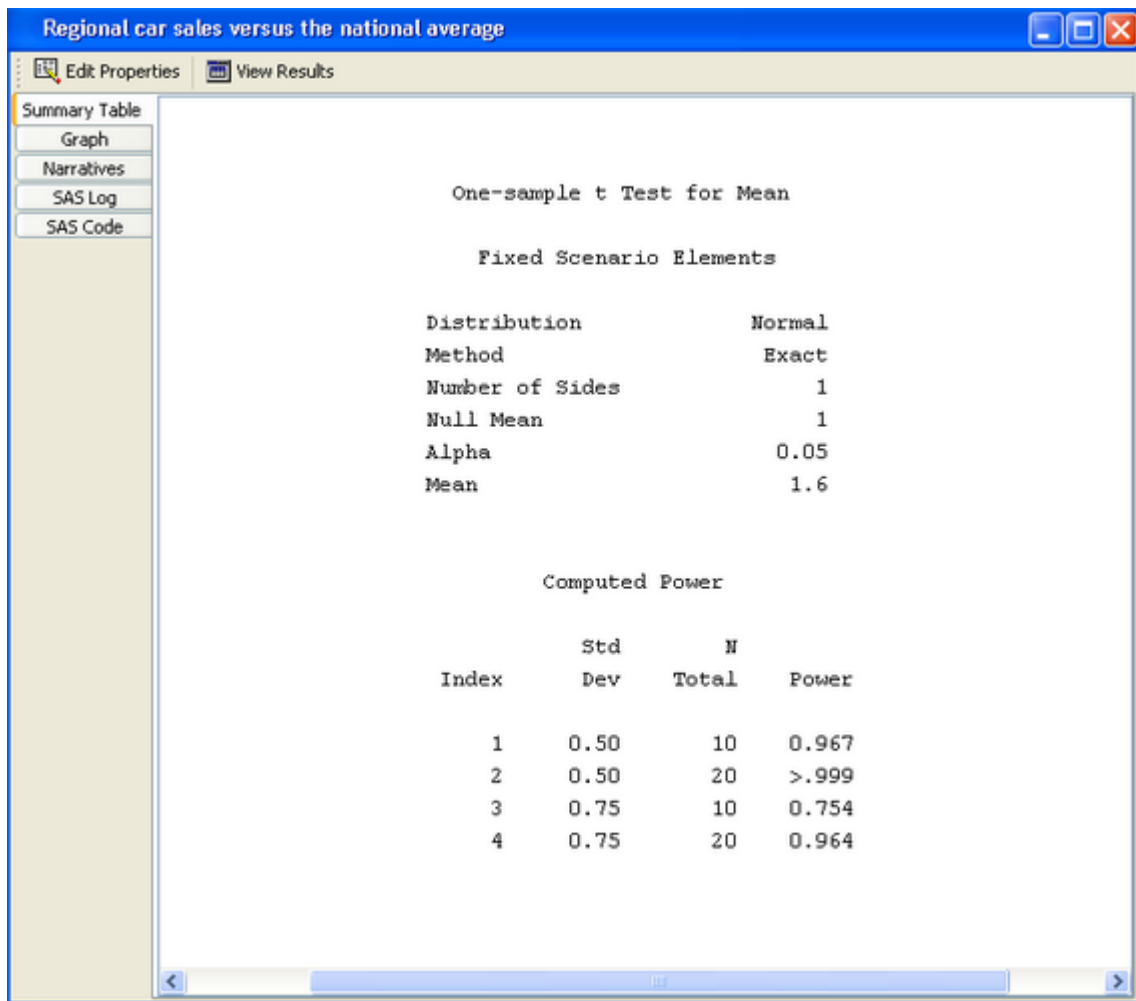
## Viewing the Results

Results appear on the View Results page and are viewable in separate tabs. The tabs include **Summary Table**, **Graph**, **Narratives**, **SAS Log**, and **SAS Code** (located on the left side of the View Results page). The **Summary Table** and **Graph** tabs appear if you selected those options on the **Results** tab of the Edit Properties page. The other tabs always appear.

### Summary Table

Click the **Summary Table** tab to view the summary table.

**Figure 72.14** Summary Table Tab with Fixed Scenario Elements and Computed Power Tables



The Summary table consists of two subtables, as shown in Figure 72.14. The Fixed Scenario Elements table includes the parameters or options that have a single value for the analysis. The Computed Power table contains the input parameters that have been given more than one value, and it shows the computed quantity, power.

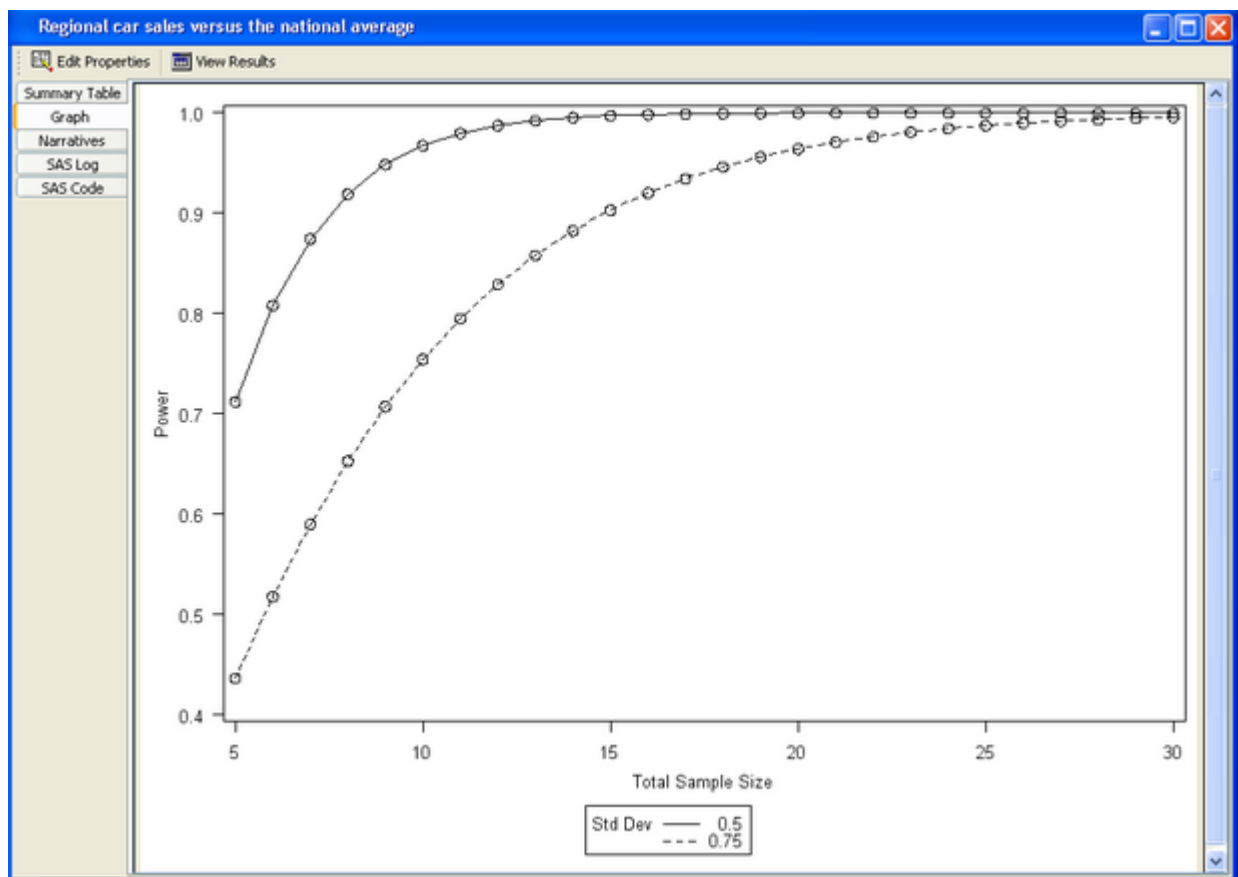
Thus, the Computed Power table contains four rows for the four combinations of standard deviation and sample size. From the table you can see that all four powers are high. The smallest value of power, 0.754, is associated with the largest standard deviation and the smallest sample size. In other words, the probability of rejecting the null hypothesis is greater than 75% in all four scenarios.

### Power by Sample Size Graph

Click the **Graph** tab to view the power by sample size graph.

The power by sample size graph in Figure 72.15 contains one curve for each standard deviation. For a standard deviation of 0.5 (the upper curve), increasing sample size above 10 does not lead to much increase in power. If you are satisfied with a power of 0.75 or greater, 10 samples would be adequate for standard deviations between 0.5 and 0.75.

**Figure 72.15** Graph Tab with Power by Sample Size Graph



### Narratives

Click the **Narratives** tab to display a facility for creating narratives.

Narratives are descriptions of the values that compose each scenario and include a statement about the computed power or sample size.

To create narratives, choose one or more scenarios in the table at the bottom of the tab. A narrative for each selected scenario is displayed in the top portion of the tab. See Figure 72.16.

**Figure 72.16** Narrative Tab

The screenshot shows the SAS software interface for the 'Regional car sales versus the national average' analysis. The 'Narratives' tab is selected in the left sidebar. The main window displays a narrative for a one-sample t test. Below the narrative is a 'Create Narratives' section with a table of scenarios and a 'Clear all selections' button.

**Narratives**

For a one-sample t test of a normal mean with a one-sided significance level of 0.05 and null mean 1, assuming a standard deviation of 0.5, a sample size of 10 has a power of 0.967 to detect a mean of 1.6.

**Create Narratives**

Select one or more scenarios

| Select                              | Index | Sides | NullMean | Alpha | Mean | StdDev | NTotal | Power      | Error | Info |
|-------------------------------------|-------|-------|----------|-------|------|--------|--------|------------|-------|------|
| <input checked="" type="checkbox"/> | 1     | 1     | 1        | 0.05  | 1.6  | 0.50   | 10     | 0.96747525 |       |      |
| <input type="checkbox"/>            | 2     | 1     | 1        | 0.05  | 1.6  | 0.50   | 20     | 0.99978391 |       |      |
| <input type="checkbox"/>            | 3     | 1     | 1        | 0.05  | 1.6  | 0.75   | 10     | 0.75442476 |       |      |
| <input type="checkbox"/>            | 4     | 1     | 1        | 0.05  | 1.6  | 0.75   | 20     | 0.9641728  |       |      |

Hide columns with constant input values

Clear all selections

For the example, select the first row in the table. The following narrative is displayed for the scenario with a standard deviation of 0.5 and a sample size of 10:

For a one-sample  $t$  test of a normal mean with a one-sided significance level of 0.05 and null mean 1, assuming a standard deviation of 0.5, a sample size of 10 has a power of 0.967 to detect a mean of 1.6.

You can select several rows in the table. As you select each one, a corresponding narrative is created and displayed in the top portion of the table. Selecting a second scenario (the third row) produces the following output, where the narrative for the first row is followed by the narrative for the third row:

For a one-sample  $t$  test of a normal mean with a one-sided significance level of 0.05 and null mean 1, assuming a standard deviation of 0.5, a sample size of 10 has a power of 0.967 to detect a mean of 1.6.

For a one-sample  $t$  test of a normal mean with a one-sided significance level of 0.05 and null mean 1, assuming a standard deviation of 0.75, a sample size of 10 has a power of 0.754 to detect a mean of 1.6.

### **Other Results**

Other results include the SAS log and the SAS code.

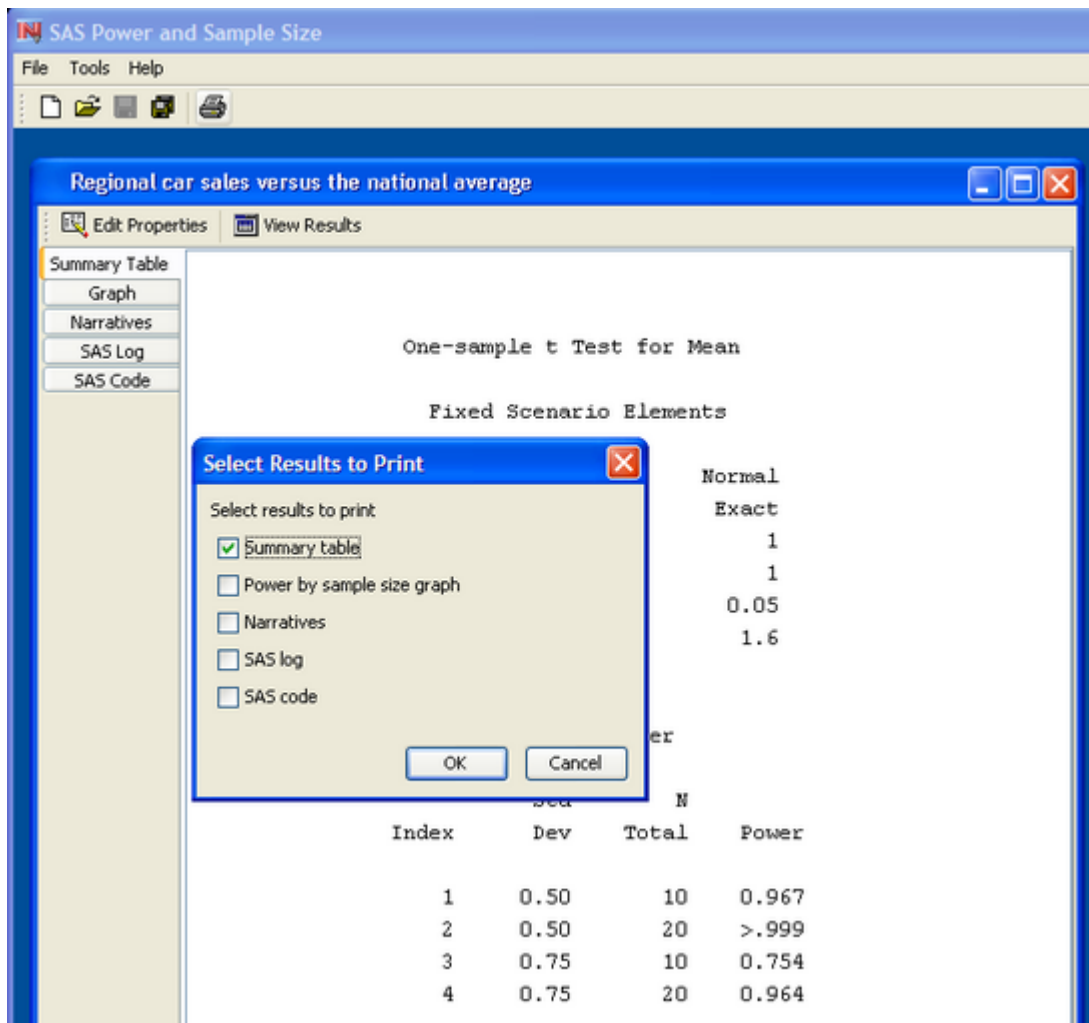
The SAS log that was produced when the **Calculate** button was last clicked appears on the **SAS Log** tab.

The SAS statements that produced the results appear on the **SAS Code** tab.

### **Printing Results**

To print one or more results, select **File►Print** from the menu bar or click the **Print** toolbar icon. A window is displayed that lists all available results, as shown in [Figure 72.17](#). Select the results that you want to print and click **OK**.

Figure 72.17 Print Selection Window



## Changing Properties

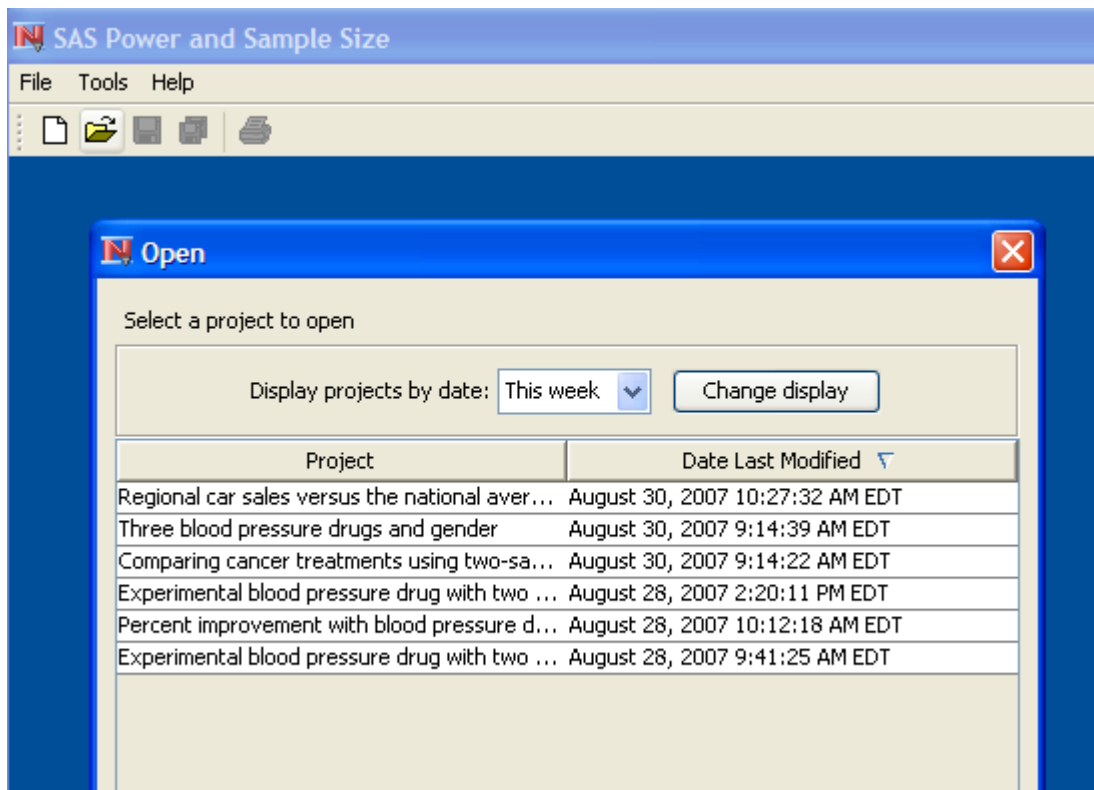
If you want to change some values of the properties and rerun the analysis, change to the Edit Properties page and continue. The icons for selecting the Edit Properties and View Results pages are in the command bar just below the project window title.

## Closing the Project

When you are finished working with a project, close it by clicking the **X** in the upper right corner of the project window or selecting **File►Close** on the menu bar. If you have not saved the project, you will be asked if you want to save it before closing.

## Opening a Project

You can reopen existing projects using the Open window. Select **File►Open** on the menu bar or click the **Open** toolbar icon.

**Figure 72.18** Open Window Containing the Analysis Created in the Example

As shown in Figure 72.18, the analysis that you just completed is listed in the table. The label that you assigned to it, `Regional car sales versus the national average`, appears in the **Project** column of the table. The table also contains the date that the analysis was last modified. If you do not see the project that you are looking for, change the value of the **Display projects by date** box to `All` by selecting `All` from the drop-down list, and click the **Change display** button.

You can sort the projects in the table by clicking the header of the desired column. The sort direction is indicated by arrows displayed in the column header.

Select the project that you want to open and click **OK**. You can also double-click the project entry to open it.

### Changing Values and Rerunning the Analysis

After viewing the graph, you might want to re-create the graph with a different range for sample sizes. On the **Results** tab of the Edit Properties page, click the **Customize** button for the power by sample size graph. The **Customize Graph** window is displayed.

On the **Value Ranges** tab of the window, change the Maximum value in the Sample Size table from 30 to 20. Click **OK**.

Rerun the analysis by clicking **Calculate**. The View Results page is displayed again and the graph now has the new maximum value for the sample size axis.



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## How to Use: PSS Application

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### Overview

The PSS application is an application that resides on your desktop. It requires a connection to SAS software either on your desktop machine or a remote machine. You can set default values for several parameters and options as preferences. More detail on creating and editing projects is provided. Projects can be imported and exported.

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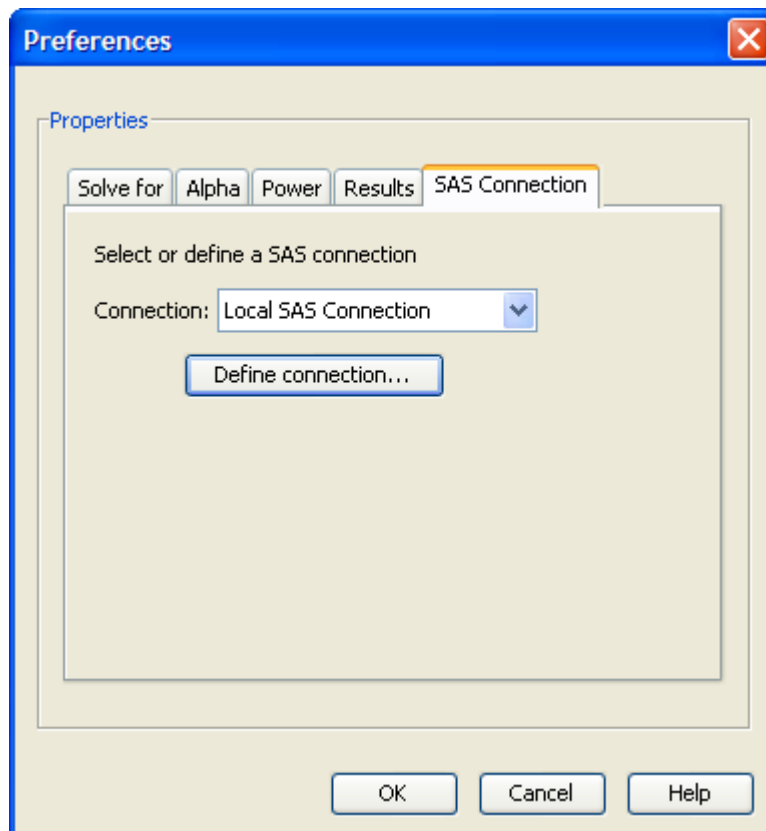
### SAS Connections

Connections to SAS servers are defined in the Preferences window. To access the Preferences window, select **Tools►Preferences** on the menu bar.

Click the **SAS Connection** tab to select or define a connection to a SAS server. A connection to a SAS server is required in order to calculate results. The server can be on your local (desktop) machine or on a remote machine.

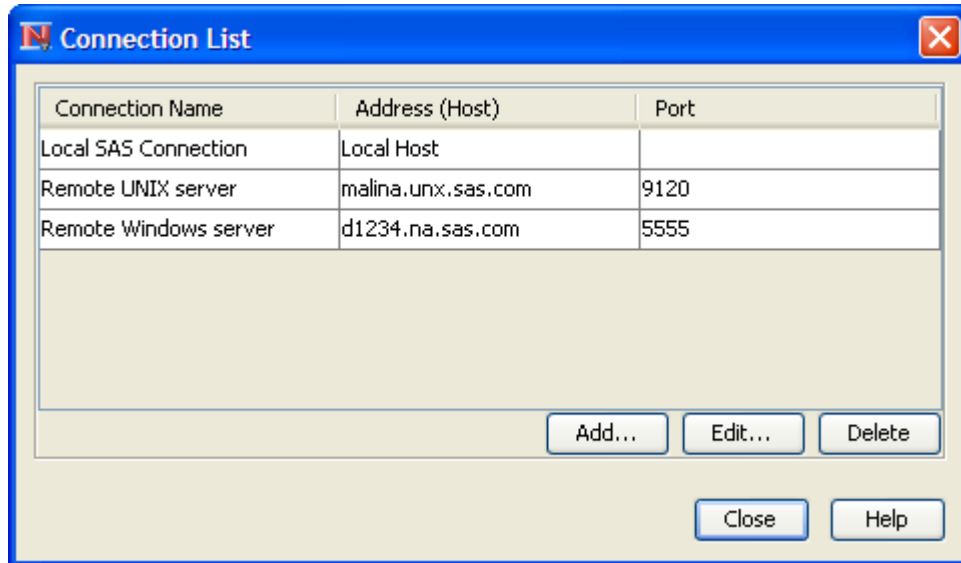
You can define several SAS connections and choose the one you want to use. To select a previously defined connection, choose it from the **Connection** list on the **SAS Connection** tab; see [Figure 72.19](#).

**Figure 72.19** SAS Connection Tab



To define a SAS connection, click the **Define connection** button. The Connection List window appears, as shown in Figure 72.20. To create a new connection, click **Add**. To edit an existing connection, select it in the Connection List and click **Edit**.

Figure 72.20 Connection List



### Defining a SAS Connection

After you click the **Add** or **Edit** button, the Define SAS Connection window appears, as shown in Figure 72.21. If you clicked **Edit**, the previously defined information is available for editing.

Figure 72.21 Define Connection Window

**Define SAS Connection**

Connection Label

Label:

SAS Connection Configuration

Are the SAS server and SAS Power and Sample Size running on the same machine?

Yes  No

Local Server Properties

Enter the full pathname of the SAS command

Pathname:

Remote Server Properties

Platform

UNIX  Windows

Connection Product

SAS/Connect

SAS Server Properties

Name:  Port:

User id and password are required

Enter a descriptive label for the connection. The label is used to distinguish among the connections in the connections list.

Then, select **Yes** or **No** to specify whether the SAS connection is to the local machine (that is, the one on which PSS is running) or to a remote machine, respectively.

### ***Defining a Local Connection***

To define a connection to the local machine, enter the full path name of (or browse for) the SAS executable file (*sas.exe* on Microsoft Windows).

Test the SAS connection by clicking the **Test SAS Connection** button.

### Defining a Remote Connection

To define a connection to a remote machine, select either the **UNIX** or **Windows** option to indicate that the remote SAS server is on a machine running the UNIX or Microsoft Windows operating systems, respectively. Then, specify the machine name and port number that the SAS/Connect spawner is using on the remote machine. Contact the SAS server administrator for this information.

If the remote machine is running Microsoft Windows, select the **User id and password are required** if authentication is required to access the SAS server (that is, if the SAS **-security** option is used). By default, authentication is required for SAS servers running on UNIX operating systems.

Test the SAS connection by clicking the **Test SAS Connection** button.

### Additional Settings

Click the **Settings** button on the Define SAS Connection window to access some additional settings for a remote connection to a SAS server. For the most part these settings are prompts that PSS expects to receive from the SAS/CONNECT spawner on the remote machine, as shown in [Figure 72.22](#).

If the remote SAS server is on a UNIX machine, you must specify the full pathname of the SAS command. Contact the SAS server administrator for this information.

**Figure 72.22** Connection Settings Window

The screenshot shows a dialog box titled "Settings" with a close button in the top right corner. The dialog is divided into two sections: "UNIX" and "Windows".

**UNIX Section:**

- Command prompt: Hello>
- User ID prompt: Username:
- Password prompt: Password:
- SAS command: (empty field)
- SAS options: -dmr -noterminal -comamid tcp

**Windows Section:**

- User ID prompt: Username:
- Password prompt: Password:

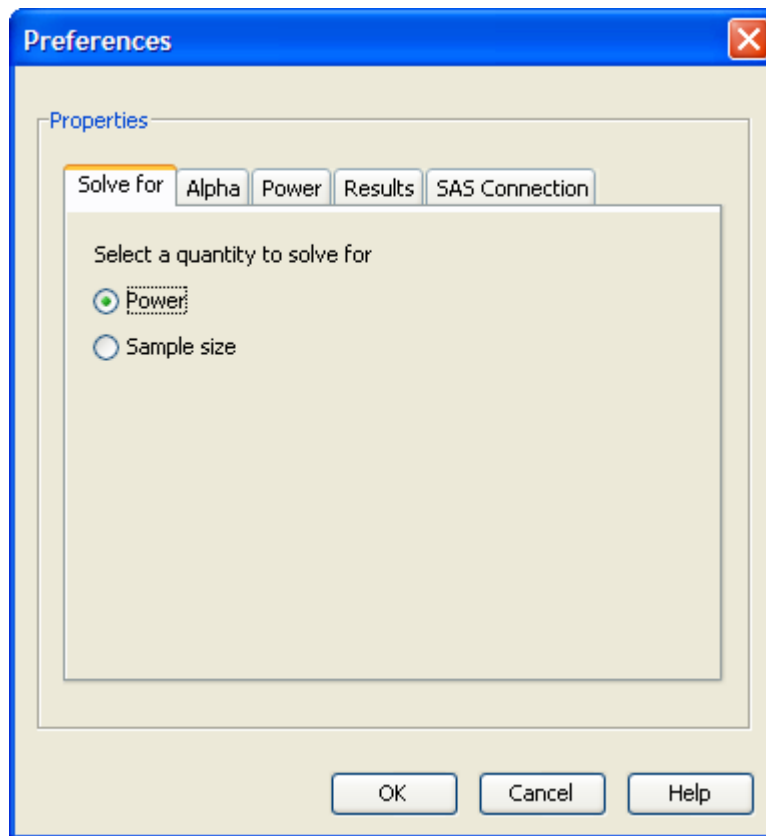
At the bottom of the dialog are three buttons: "OK", "Cancel", and "Reset".

## Setting Preferences

In the Preferences window you can set default values for options that are used by all analyses.

To access the Preferences window, select **Tools►Preferences** on the menu bar. [Figure 72.23](#) shows the Preferences window.

Figure 72.23 Preferences Window



Preference values are used as the defaults for each newly opened project (that is, those that are opened from the New window). For a specific project, each of these default values can be overridden on the Edit Properties page.

Changes in preferences do not change the state of an existing analysis (that is, one that is accessed from the Open window).

### Selecting the Quantity to Solve For

Click the **Solve For** tab to select **Power** or **Sample Size** as the default value to be solved for; see Figure 72.23. For confidence interval analyses, selecting **Power** is equivalent to selecting **Prob(Width)**.

For analyses that offer both **Sample size per group** and **Total sample size**, the **Sample size** option on this page corresponds to total sample size.

## Setting Alphas

Click the **Alpha** tab to enter one or more values for alpha. Alpha is the significance level (false positive probability). For confidence interval analyses, alpha values are transformed into confidence levels by  $(1 - \alpha)$ . For example, an alpha of 0.05 would represent a confidence level of 0.95.


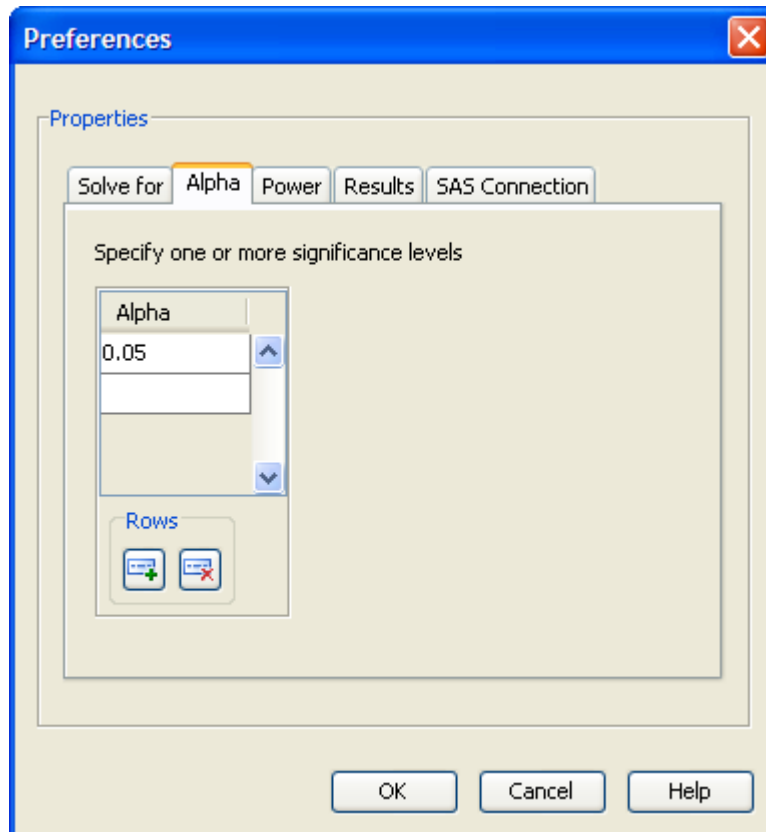
To set default values of alpha, enter one or more values in the **Alpha** data entry table. See Figure 72.24. It is not necessary to have any default values for alpha. Add more rows to the table as needed using the  button at the bottom of the table.

Figure 72.24 Alpha Preference Tab

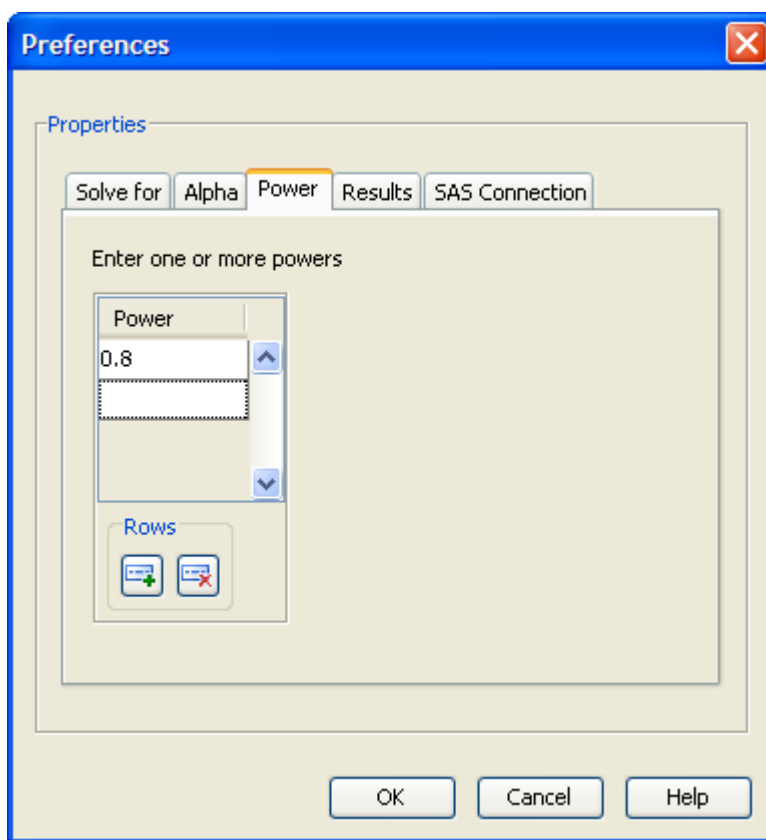


## Setting Powers

Click the **Power** tab to enter one or more values for power. It is not necessary to have any default values for power. For confidence interval analyses, power values are treated as `prob(width)` values.

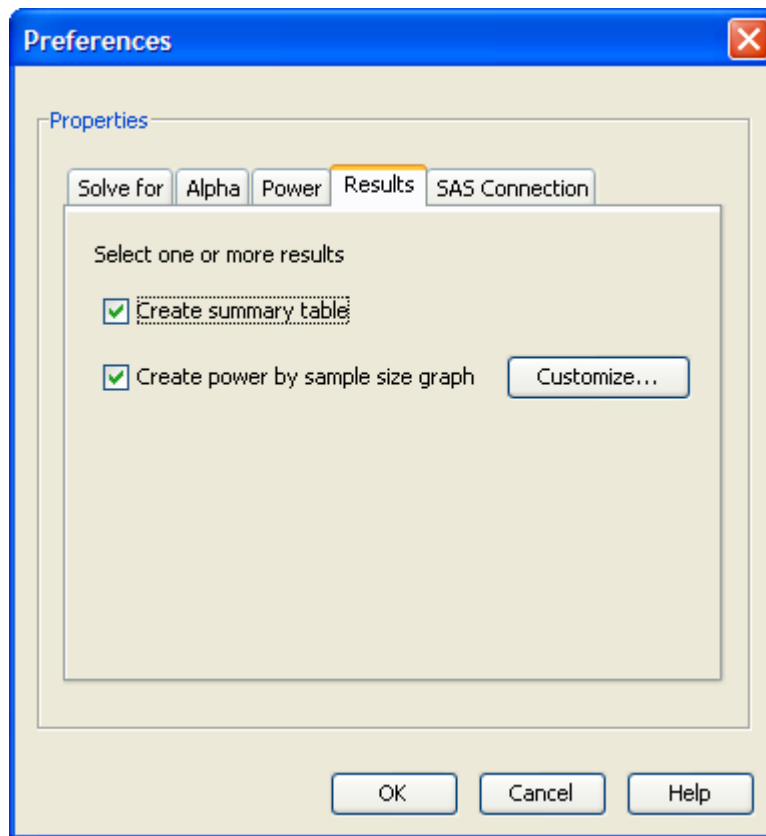
To set default values of power, enter one or more values in the **Power** data entry table; see Figure 72.25.

Figure 72.25 Power Preference Tab



### Setting Results Options

Click the **Results** tab to make default selections for the summary table and the power by sample size graph options; see Figure 72.26.

**Figure 72.26** Results Options Preferences Tab

The summary table consists of the input parameter values and the calculated quantity (power or sample size). Select the **Create summary table** check box to create the table by default.

To request that an analysis create a power by sample size graph by default, select the **Create power by sample size graph** check box.

---

## Creating and Editing PSS Projects

A PSS project is an instance of an analysis. The first decision in using PSS is to choose the appropriate test or design. Select the **File►New** on the menu bar or click the **New** icon on the toolbar. The New window appears with a list of the available analyses. Select the type of analysis that you want from the list and click **OK**.

When the project is first opened, the Edit Properties page is displayed. It is described in the section “[Editing Properties](#)” on page 6174.

After the properties have been specified and the analysis is performed, the View Results page is displayed. See the section “[Viewing the Results](#)” on page 6178.

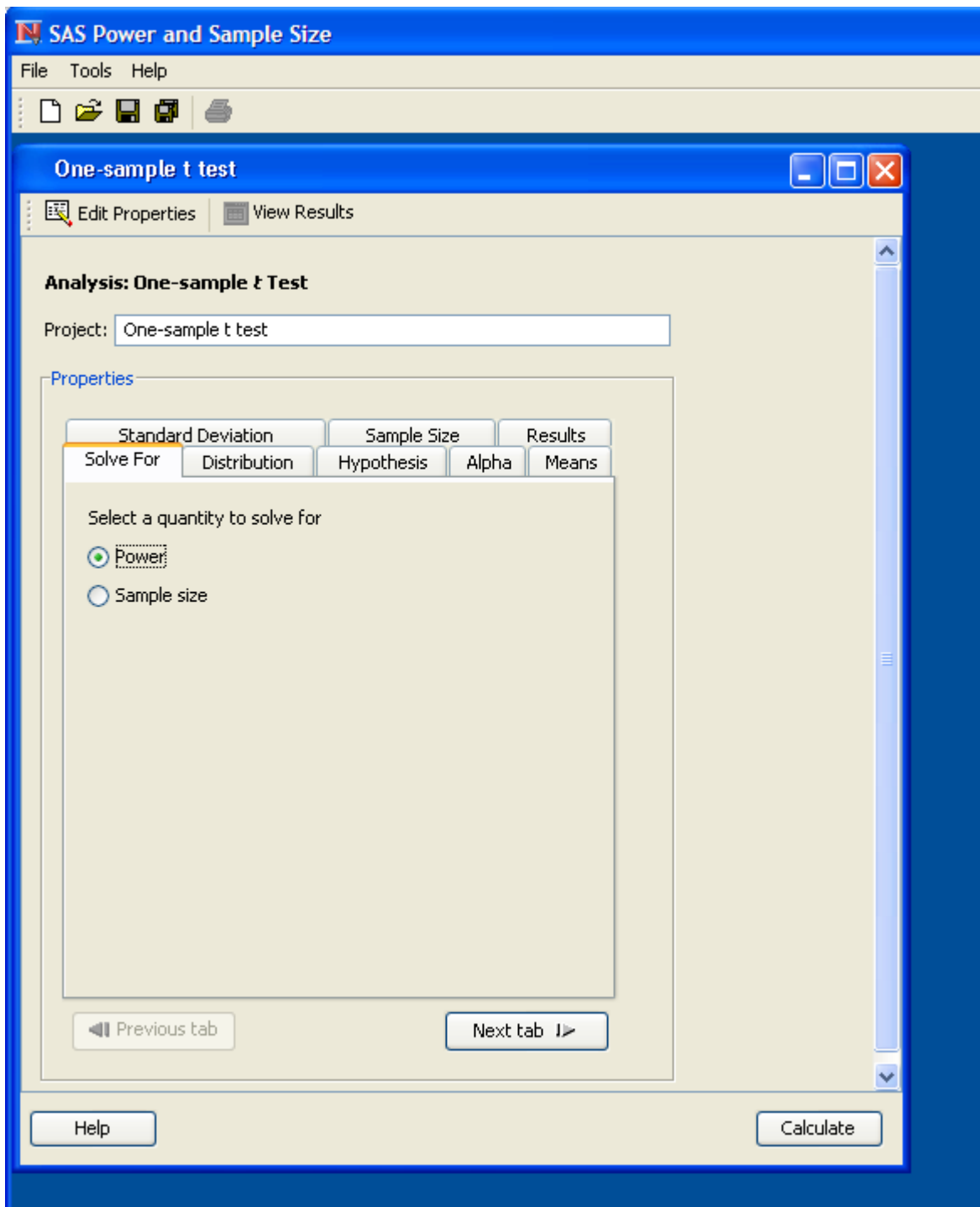
A project that has been saved and closed can be reopened from the Open window. Select **File►Open** on the menu bar or click the **Open** icon on the toolbar.



## Editing Properties

The Edit Properties page consists of several analysis options and input parameters that are relevant to the particular analysis. These options and parameters are organized on several tabs, as shown in Figure 72.27.

Figure 72.27 Edit Properties Page

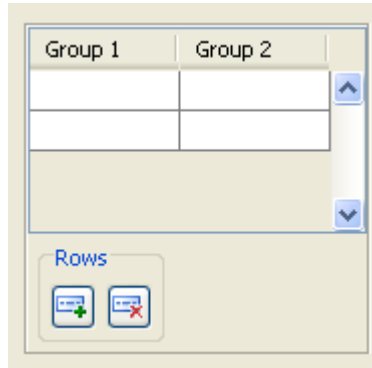


The Edit Properties page contains various controls by which you can enter values or select choices. In addition to the usual data entry controls such as text fields and check boxes, several specialized controls are present: data entry tables and the Alternate Forms control. More detailed descriptions follow.



### Using Data Tables

Data entry tables are composed of data entry fields for one or more rows and columns. [Figure 72.28](#) shows a two-row, two-column table.

**Figure 72.28** Two-Column Data Entry Table with Controls






Type an appropriate value in each field. It is not necessary to type data in all rows or to delete empty rows. However, if a table has more than one column, the cells of a row must be completely filled or completely blank. Rows with values in some but not all cells are not allowed.

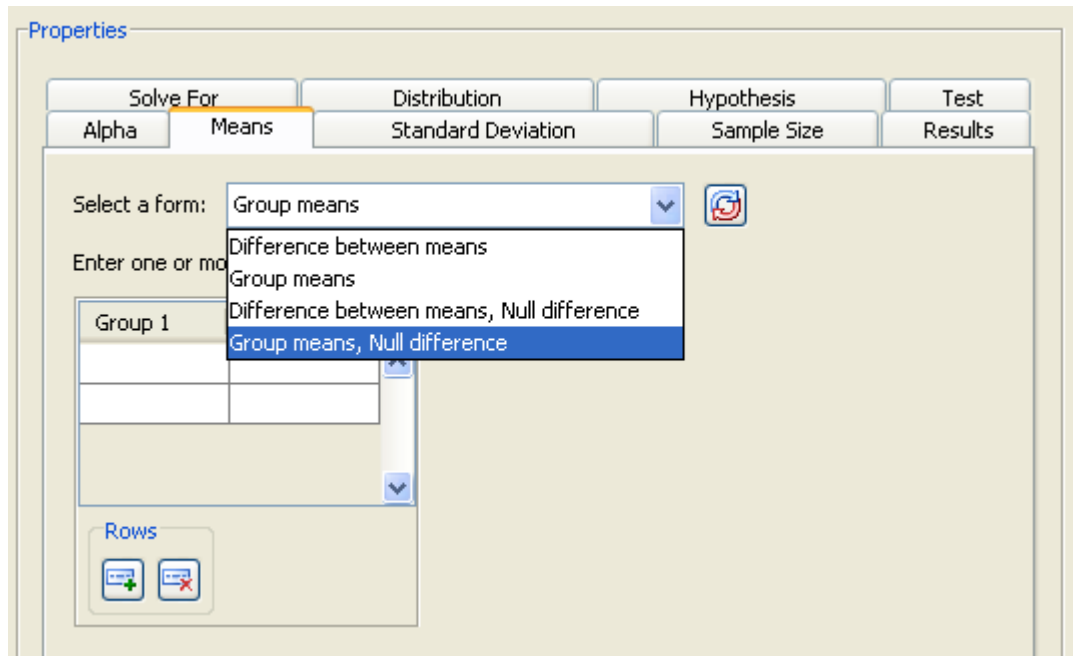
To append more rows, click the  button beneath the table. To delete the last row of the table, click the  button.

Also, you can display a pop-up menu to perform additional actions such as inserting and deleting rows. First, select the row to insert before or delete, then right-click to display the pop-menu and select the desired action.

### Using Alternate Forms

For some input parameters, there are several ways in which data may be entered. For example, in the two-sample  $t$  test analysis, group means can be entered as either individual means or a difference between means.

The alternate forms are displayed in a drop-down list with an adjacent  button, as shown in [Figure 72.29](#). The  button enables you to cycle through the alternatives, displaying each one in turn. To see what forms are available, you can open the drop-down list and select the one you want or you can click the  button until the form that you want is displayed.

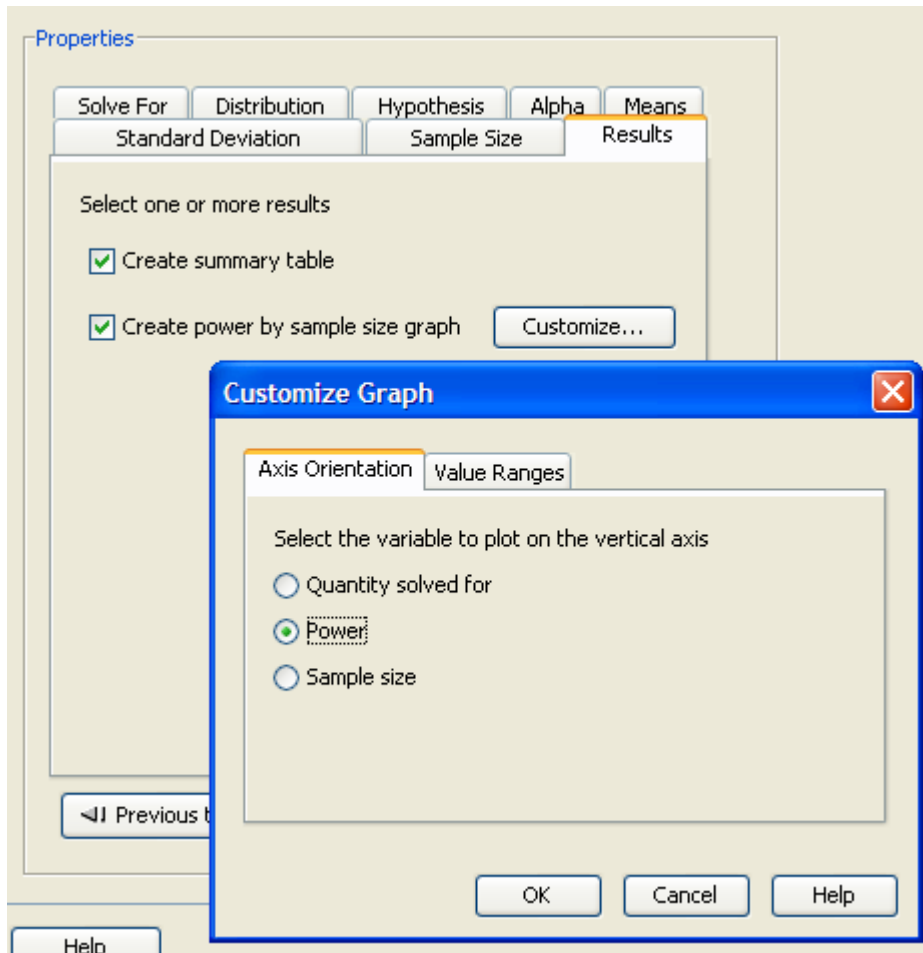
**Figure 72.29** Select a form Drop-Down List and Button

The alternate form last used for an analysis is saved and displayed as the default when a new instance of the analysis is opened.

### **Customizing Graphs**

The Edit Properties page for all analyses contains a **Results** tab. You can choose to create a graph, and you can optionally choose to customize the graph by clicking the **Customize** button that is beside the **Create power and sample size graph** choice.

As shown in Figure 72.30, the Customize Graph window consists of an **Axis Orientation** tab and a **Value Ranges** tab. Use the **Axis Orientation** options to specify which axes you want used for power and for sample size. Use the **Value Ranges** settings to specify the axis range for the non-target quantity (that is, the power axis if you are solving for sample size or the sample size axis if you are solving for power).

**Figure 72.30** Customize Graph Window

When specifying a value range, you can specify a minimum value and a maximum value. Also, you can select either the *Number of points* or the *Interval between points* choice for the axis and specify a value. All of these values are optional; specify only the ones you want.

### **Scenarios**

A scenario is one instance of a complete set of values for an analysis. For example, if two alpha values and two total sample size values are specified with all other input parameters taking only a single value, there would be four scenarios—the four combinations of two alphas and two sample sizes.

### **Performing the Analysis**

To perform the analysis, click **Calculate** at the lower right of the Edit Properties page. The input parameters are checked for validity, and the analysis is performed. The View Results page is then displayed.

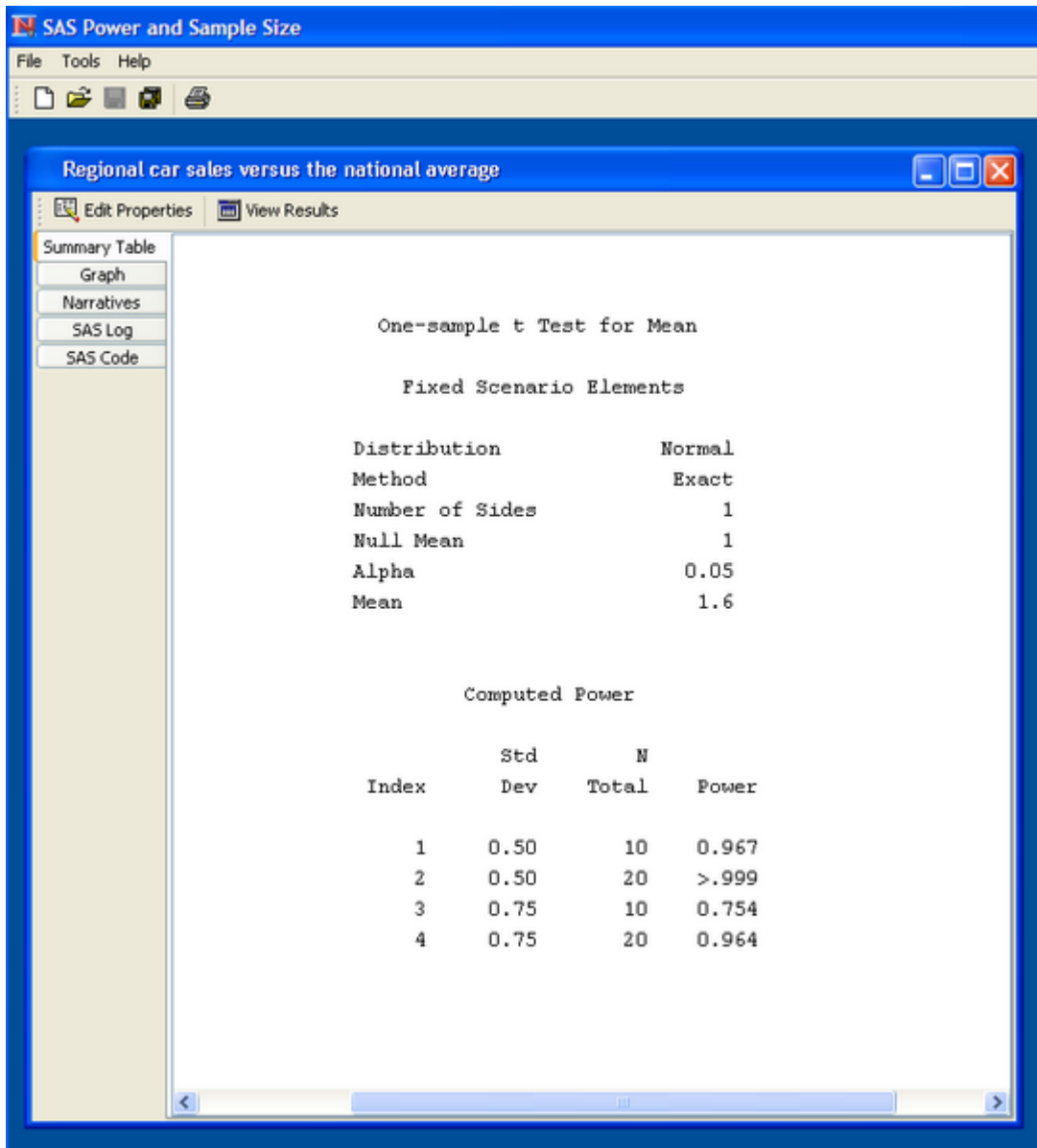
## Viewing the Results

The results appear in separate tabs on the View Results Page. These tabs include **Summary Table**, **Graph**, **Narratives**, **SAS Log**, and **SAS Code**.

### Viewing the Summary Table

Click the **Summary Table** tab to view the summary table. It consists of two subtables, as shown in Figure 72.31. The `Fixed Scenario Elements` table includes the options and parameter values that are constant for the analysis. The `Computed Power` table includes the calculated power or sample size values and the values for input parameters that have multiple values specified for the analysis.

**Figure 72.31** View Results Page with Summary Table

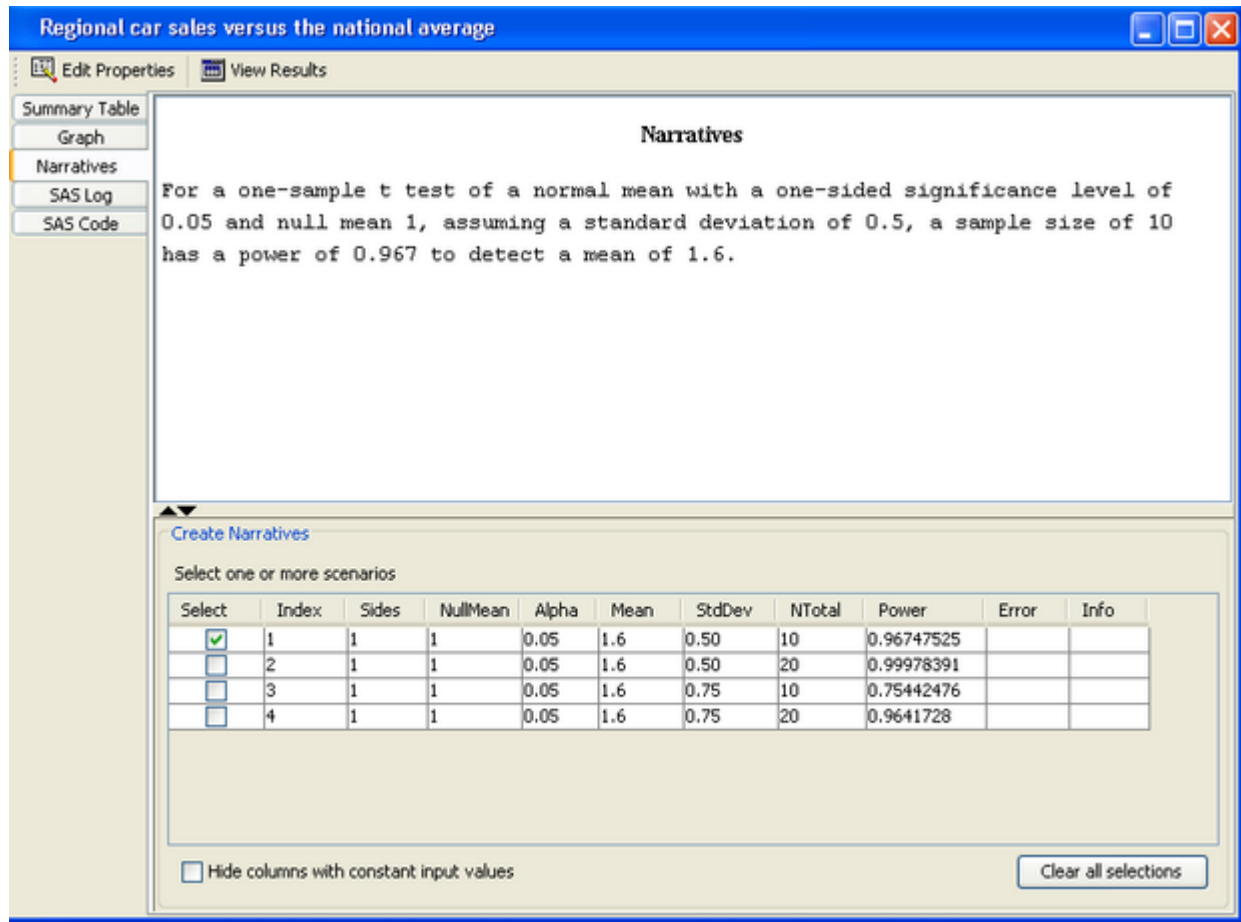


### Creating Narratives

Click the **Narratives** tab to display a facility to create narratives. Narratives are descriptions of the input parameter values and calculated quantities in sentence or paragraph form. Each narrative corresponds to one calculated quantity value.

The **Narratives** tab is divided into a narrative selector panel and a narrative display panel. To create a narrative, select the row in the narrative selector panel that corresponds to it. You can select as many rows as you want. See Figure 72.32.

**Figure 72.32** Narrative Selector and Display



The narrative selector table often contains columns whose values do not vary. For example, in Figure 72.32, the Sides, NullMean, Alpha, and Mean columns contain values that do not vary. You can hide these columns by selecting the **Hide columns with constant input values** check box.

### Viewing the SAS Log and Code

Click the **SAS Code** tab to view the SAS statements that are used to generate the analysis results. Click the **SAS Log** tab to view the SAS log that corresponds to the analysis.

The SAS code differs slightly from the statements in the SAS log. Statements that are used to place the results in the location maintained by the application are not included. This is done to prevent you from overwriting the results stored by the application if you run the SAS code outside of the application.

### **Printing Results**

To print one or more results, click the **Print** icon on the toolbar or select **File►Print** on the menu bar. The Select Results to Print window is displayed. You can choose to print one or more of the results by selecting the corresponding options here.

### **Saving the Project**

To save a project, click the **Save** toolbar icon or select **File►Save** from the menu bar. Projects can be saved even if some of the information is invalid. Error checking is performed when the **Calculate** button is clicked.

### **Closing the Project**

To close a project, click the **X** in the upper right corner of the project window or select **File►Close** from the menu bar.

---

## **Importing and Exporting Projects**

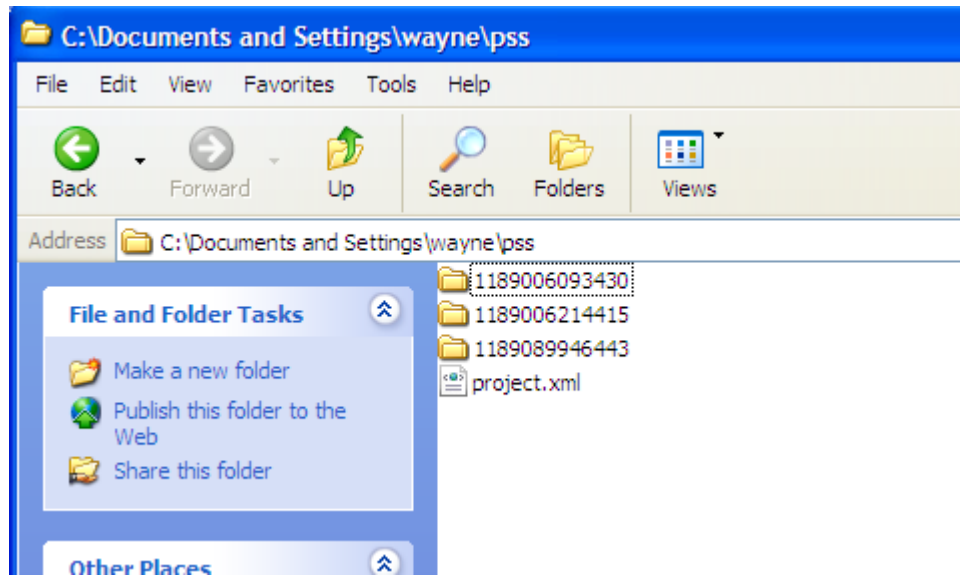
PSS projects can be imported from the same machine or a different machine. Also, the active project (the project that is open and on top of any other open projects) can be exported.

### **Importing Projects**

A PSS project that was created on another machine or by another user can be imported and used. Also, importing projects is the recommended way of moving existing PSS projects that were created with PSS release 2.0 (a Web application) to PSS release 3.1 (a desktop application).

PSS files are stored in a folder entitled *pss*. The *pss* folder contains a *project.xml* file and individual folders for each project. See [Figure 72.33](#).

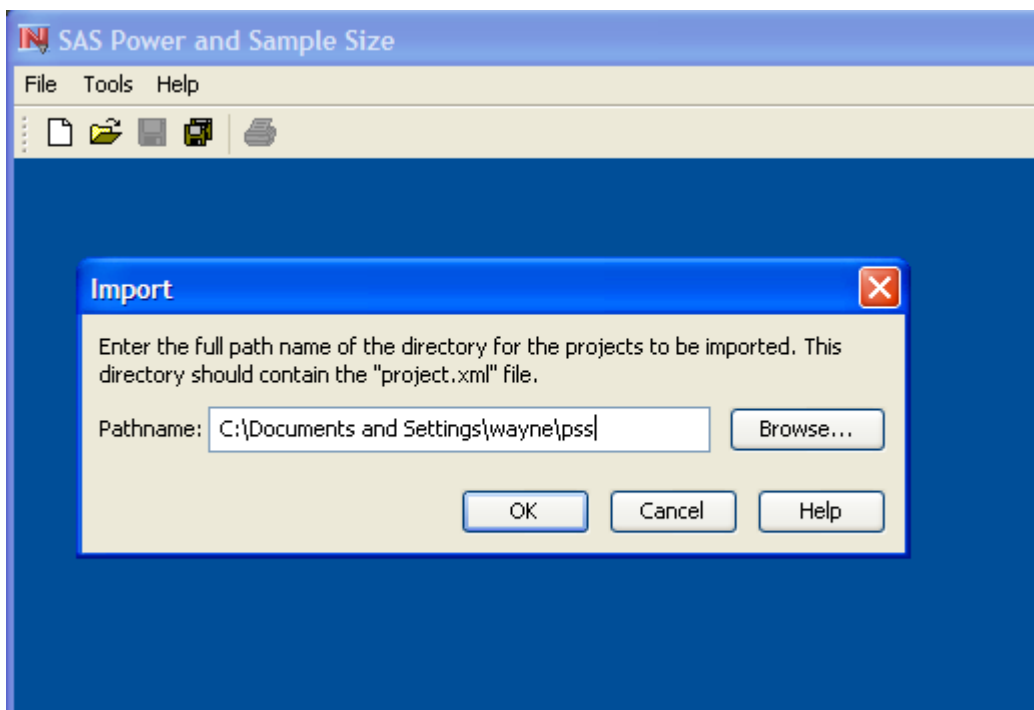
Figure 72.33 PSS Directory Structure



If PSS files are on another machine, they must first be copied to a temporary location on the desktop machine that is running PSS. The entire *pss* folder should be copied.

To import projects, select **File►Import** from the menu bar. Then, specify the full pathname of the *pss* folder.

Figure 72.34 Import Projects Window





To import PSS 2.0 files, you need to find the *pss* folder. The easiest way to do this is to search for the *project.xml* file. If you find several files with this name, you need to decide which one or more to import.

## Exporting the Active Project

If you want to send a PSS project to someone, you can export the active project. The active project is the one that is open and that has focus (is displayed on top of any other open projects). Select **File►Export active project** and specify a temporary directory to hold the exported project.

The recipient must import the project using PSS.

---

## Details: PSS Application

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### Software Requirements

PSS is available in SAS 9.2 or later for the following platforms: Microsoft Windows 7, Vista, and XP.

Two configurations are available for SAS connections: local and remote. With the local configuration, PSS and SAS must reside on the same machine. With the remote configuration, PSS and SAS can reside on different machines. SAS connections are defined and selected on the **SAS Connection** tab on the Preferences window. More information about SAS connections is found in the section “[SAS Connections](#)” on page 6166.

For both configurations, Base SAS and SAS/STAT software must be installed and SAS/GRAPH software is recommended.

For the remote configuration, SAS/CONNECT and SAS/IntrNet software must also be installed. For more information about configuring the remote SAS server, click **Help►Contents** on the menu bar and then click **Configuring a Remote SAS Server** under **Special Topics** in the table of contents.

---

### Installation

SAS Power and Sample Size is installed separately from the SAS/STAT product. Contact your SAS site representative to have the application installed.

SAS Power and Sample Size is installed using the SAS Software Deployment Wizard. It is listed as an available product with, but separate from, Foundation SAS which contains the SAS/STAT and SAS/GRAPH products that are required for using the application.

---

### Configuration

When you first run SAS Power and Sample Size 3.1 (PSS), you are asked to provide configuration information.

First, you are asked for the name of a directory to contain the your power and sample size projects. A folder named *pss* is created in the specified directory, and projects are stored in the *pss* folder. This directory cannot be the same as the one used by PSS 2.0. If it is, PSS requires that another folder name be provided.

Then, if the appropriate release of the SAS System is available on the desktop machine, you are asked whether a connection should be automatically created to it. If you respond **NO**, then PSS informs you that a connection to the SAS server is necessary and asks if you want to select one now or later. A connection to a SAS server is not necessary to use the application until the **Calculate** button on the Edit Properties page of a project is clicked. More information about connections is available in the section “[Setting Preferences](#)” on page 6169.

Then, PSS displays a wizard to help you import existing PSS projects from either a previous release (PSS 2.0) or the current one (PSS 3.1). More information is available in the section “[Importing Projects](#)” on page 6180.

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## Example: Two-Sample $t$ Test

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### Overview

The one-sample  $t$  test compares the mean of a sample to a given value. The two-sample  $t$  test compares the means of two samples. The paired  $t$  test compares the mean of the differences in the observations to a given number. PSS provides power and sample size computations for all of these types of  $t$  tests. For more information about power and sample size analysis for  $t$  tests, see Chapter 71, “[The POWER Procedure](#).”

The two-sample  $t$  test tests for differences or ratios between means for two groups. The groups are assumed to be independent. This example describes three examples using the two-sample  $t$  test: for equal variances, for unequal variances, and for mean ratios.

---

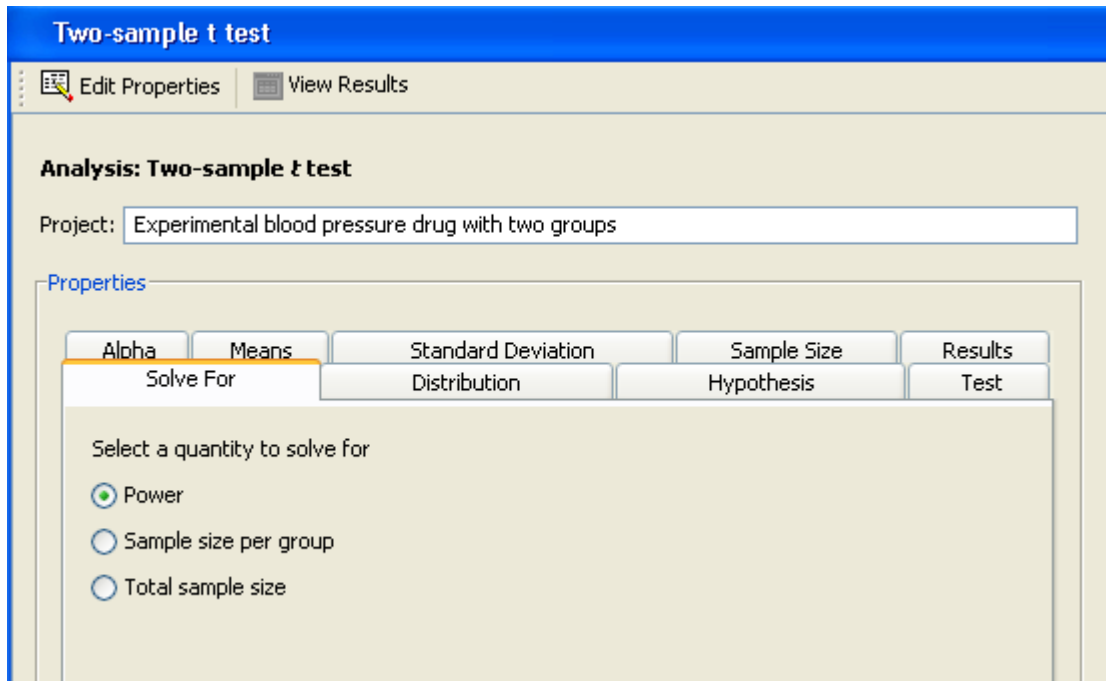
### Test of Two Independent Means for Equal Variances

Suppose you are interested in testing whether an experimental drug produces a lower systolic blood pressure than a placebo does. Will 25 subjects per treatment group yield a satisfactory power for this test? From previous work, you expect that the blood pressure is 132 for the control group and 120 for the drug treatment group and that the standard deviation is 15 for both groups. You want to use a one-sided test with a significance level of 0.05. Because there are two independent groups and you are assuming that blood pressure is normally distributed, the two-sample  $t$  test is an appropriate analysis.

Start by creating a new project. Select **File**►**New**. In the New window, select **Two-sample t test** from the list. The Two-Sample  $t$  test project window appears, with the Edit Properties page displayed.

### Editing Properties

On this page enter a name to describe the project and enter project properties. Click each tab on the Edit Properties page to enter the desired properties. You can also change tabs by clicking the **Next tab** or **Previous tab** buttons. See [Figure 72.3](#).

Figure 72.35 Two-Sample  $t$  Test

### Project Description

The description is used to identify this particular project in the Open and Delete windows. Type a description for your project in the **Project:** text box.

For this example, change the description to `Experimental blood pressure drug with two groups`, as shown in Figure 72.35.

### Solve For

For the two-sample  $t$  test analysis, you can choose to solve for power, sample size per group, or total sample size. Specify the desired quantity type on the **Solve For** tab.

Click the **Solve For** tab and select the **Power** option as shown in Figure 72.35. For information about solving for sample size, see the section “Solving for Sample Size” on page 6204.

### Distribution

Click the **Distribution** tab to select a distribution option that specifies the underlying distribution for the test statistic, as shown in Figure 72.36.

Figure 72.36 Distribution Tab

**Analysis: Two-sample  $t$  test**

Project:

Properties

|           |              |                    |             |         |
|-----------|--------------|--------------------|-------------|---------|
| Alpha     | Means        | Standard Deviation | Sample Size | Results |
| Solve For | Distribution | Hypothesis         | Test        |         |

Select the distribution of the test

Lognormal

Normal

For this example, you are interested in means rather than mean ratios, so select the **Normal** option.

### Hypothesis

Click the **Hypothesis** tab to select the type of test; see Figure 72.37.

Figure 72.37 Hypothesis Tab

**Analysis: Two-sample  $t$  test**

Project:

Properties

|           |              |                    |             |         |
|-----------|--------------|--------------------|-------------|---------|
| Alpha     | Means        | Standard Deviation | Sample Size | Results |
| Solve For | Distribution | Hypothesis         | Test        |         |

Select a one or two-sided hypothesis test

One-sided test       Lower one-sided test

Two-sided test       Upper one-sided test

You can choose either a one- or two-sided test. If you do not know the direction of the effect (that is, whether it is positive or negative), the two-sided test is appropriate. If you know the effect's direction, the one-sided test is appropriate. For the one-sided test, the alternative hypothesis is assumed to be in the same direction as the effect. If you specify a one-sided test and the effect is in the unexpected direction, the results of the analysis are invalid.

The **One-sided test** option assumes that you know the correct direction of the test. Select the **Lower one-sided test** and **Upper one-sided test** options to explicitly indicate the direction of the one-sided test.

Because you are interested only in whether the experimental drug lowers blood pressure, select the **One-sided test** option on the **Hypothesis** tab.

### Test

Click the **Test** tab to select either the pooled  $t$  test or the Satterthwaite  $t$  test.

**Figure 72.38** Test Tab

**Analysis: Two-sample  $t$  test**

Project: Experimental blood pressure drug with two groups

Properties

|           |              |                    |             |         |
|-----------|--------------|--------------------|-------------|---------|
| Alpha     | Means        | Standard Deviation | Sample Size | Results |
| Solve For | Distribution | Hypothesis         | Test        |         |

Select a test

Pooled  $t$  test

Satterthwaite  $t$  test

With the independent variances that the example uses, select **Pooled  $t$  test** option. The Satterthwaite  $t$  test is used with unequal variances; it is available only with the normal distribution.

### Alpha

Click the **Alpha** tab to specify one or more significance levels, as shown in [Figure 72.39](#).

Figure 72.39 Alpha Tab

**Analysis: Two-sample *t* test**

Project:

Properties

| Solve For | Distribution       | Hypothesis  | Test    |
|-----------|--------------------|-------------|---------|
| Alpha     | Standard Deviation | Sample Size | Results |

Specify one or more significance levels

| Alpha |
|-------|
| 0.05  |
|       |

Rows

Alpha is the significance level (that is, the probability of falsely rejecting the null hypothesis). If you frequently use the same values for alpha, set them as defaults in the Preferences window. See the section “Setting Preferences” on page 6169 for more information about setting preferences.

Type the desired significance level of 0.05 in the first cell of the Alpha table (if it is not already the default value).

### **Means**

Click the **Means** tab to select one of four possible ways to enter the means and the null mean difference, as shown in Figure 72.40.

Figure 72.40 Means Tab

Properties

Solve For: Means | Distribution: Standard Deviation | Hypothesis: Power | Test: Sample Size | Alpha: Results

Select a form: Group means

Enter one or more rows of group means

| Group 1 | Group 2 |
|---------|---------|
| 132     | 120     |
|         |         |

Rows

Select one of the following forms from the **Select A Form** list. The four available forms are:

**Difference between means**

Enter the difference between the group means. The null mean difference is assumed to be 0.

**Group means**

Enter the means for each group. The null mean difference is assumed to be 0. The difference is formed by subtracting the mean for group 1 from the mean for group 2.

**Difference between means, Null difference**

Enter the difference between the group means and a null mean difference.

**Group means, Null difference**

Enter the means for each group and a null mean difference. The difference is formed by subtracting the mean for group 1 from the mean for group 2.

For this analysis, you can enter the means for the two groups either individually or as a difference. If your null mean difference is not zero, enter that value in the Null Mean table. (The Null Mean table is displayed only for the **Group means, Null Difference** and **Difference between means, Null difference** forms.)

For this example, a null mean difference of 0 is reasonable, so select the **Group means** form from the list, as shown in Figure 72.40. Enter the control mean of 132 in the first row of the first column and the experimental mean of 120 in the first row of the second column.

**Standard Deviation**

Click the **Standard Deviation** tab to enter the standard deviation for the two groups. It is assumed to be equal for both groups.

For the example, enter a single value of 15, as shown in [Figure 72.41](#).

**Figure 72.41** Standard Deviation Tab

The screenshot shows a software interface with a 'Properties' window. The 'Distribution' tab is selected, and the 'Standard Deviation' sub-tab is active. The 'Std. Dev.' input field contains the value '15'. Below the input field are 'Rows' controls with '+' and '-' buttons.

**Sample Size**

Click the **Sample Size** tab to select one of three possible ways to enter the sample sizes, as shown in [Figure 72.40](#).

Select one of the following forms from the **Select A Form** list:

**Sample size per group**

Enter the sample size for one of the two groups. The group sizes are assumed to be equal.

**Group sample sizes**

Enter the sample size for each of the two groups. The group sizes can be equal or unequal.

**Total N, Group weights**

Enter the total sample size for the two groups and the relative sample sizes for each group. For more information about using relative sample sizes, see the section [“Using Unequal Group Sizes”](#) on page 6205.

Examine the alternatives by clicking the **Select a form** down arrow. For this example, select the **Sample size per group** form. You want to examine a curve of powers in the power by sample size graph, so enter the values 20, 25, and 30 in the Sample Size table, as shown in [Figure 72.42](#). If you need to add more rows to the table, add them by clicking the button beneath the table.



**Figure 72.42** Sample Size Tab

The screenshot shows a software interface for calculating sample size. The 'Properties' window has several tabs: 'Solve For', 'Distribution', 'Hypothesis', and 'Test'. Under 'Solve For', 'Alpha' is 0.05 and 'Means' is 132, 120. Under 'Distribution', 'Standard Deviation' is 15. Under 'Hypothesis', 'Sample Size' is selected. Under 'Test', 'Results' is selected. The 'Sample size per group' form is selected, and the 'N Per Group' list box contains 20, 25, and 30. There are also 'Rows' controls with '+' and '-' buttons.

**Summary of Properties**

Table 72.2 contains the values of the input parameters for the example.

**Table 72.2** Summary of Input Properties

| Parameter          | Value                 |
|--------------------|-----------------------|
| Solve for          | Power                 |
| Distribution       | Normal                |
| Hypothesis         | One-sided test        |
| Test               | Pooled t test         |
| Alpha              | 0.05                  |
| Means form         | Group means           |
| Means              | 132, 120              |
| Standard deviation | 15                    |
| Sample size form   | Sample size per group |
| Sample size        | 20, 25, 30            |

**Results**

Click the **Results** tab to request desired results. Summary table and power by sample size graph options are available.

For the example, select the **Create summary table** and **Create power by sample size graph** check boxes.

Click **Calculate** to perform the analysis. If there are no errors in the input values, the View Results page appears. If there are errors in the input parameter values, you are prompted to correct them.

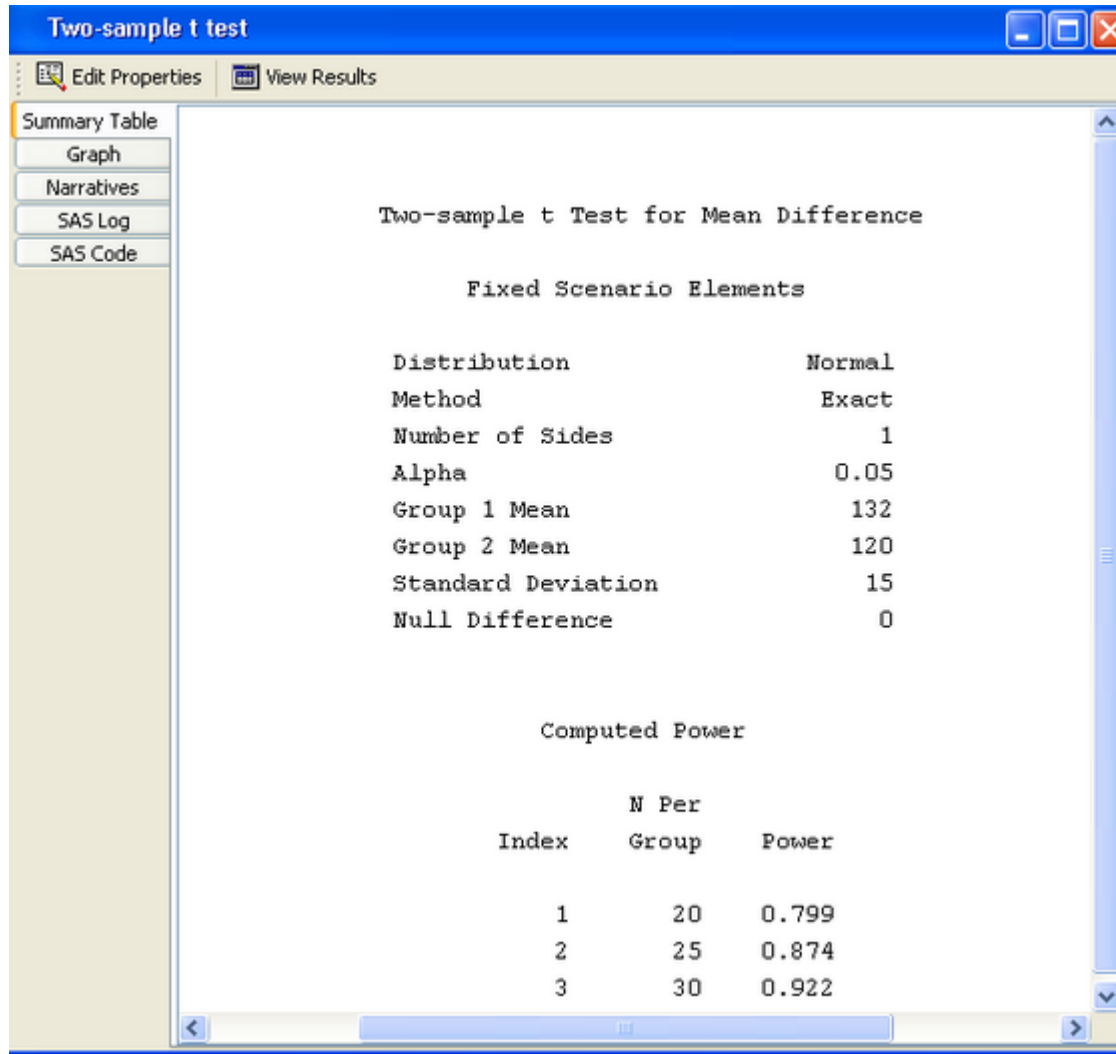
## Viewing Results

The results are listed on separate tabs on the View Results page. Click the tab of each result that you want to view.

### Summary Table

Click the **Summary Table** tab to view a table that includes the values of the input parameters and the computed quantity (in this example, power). See Figure 72.43.

Figure 72.43 Results Page with Summary Table

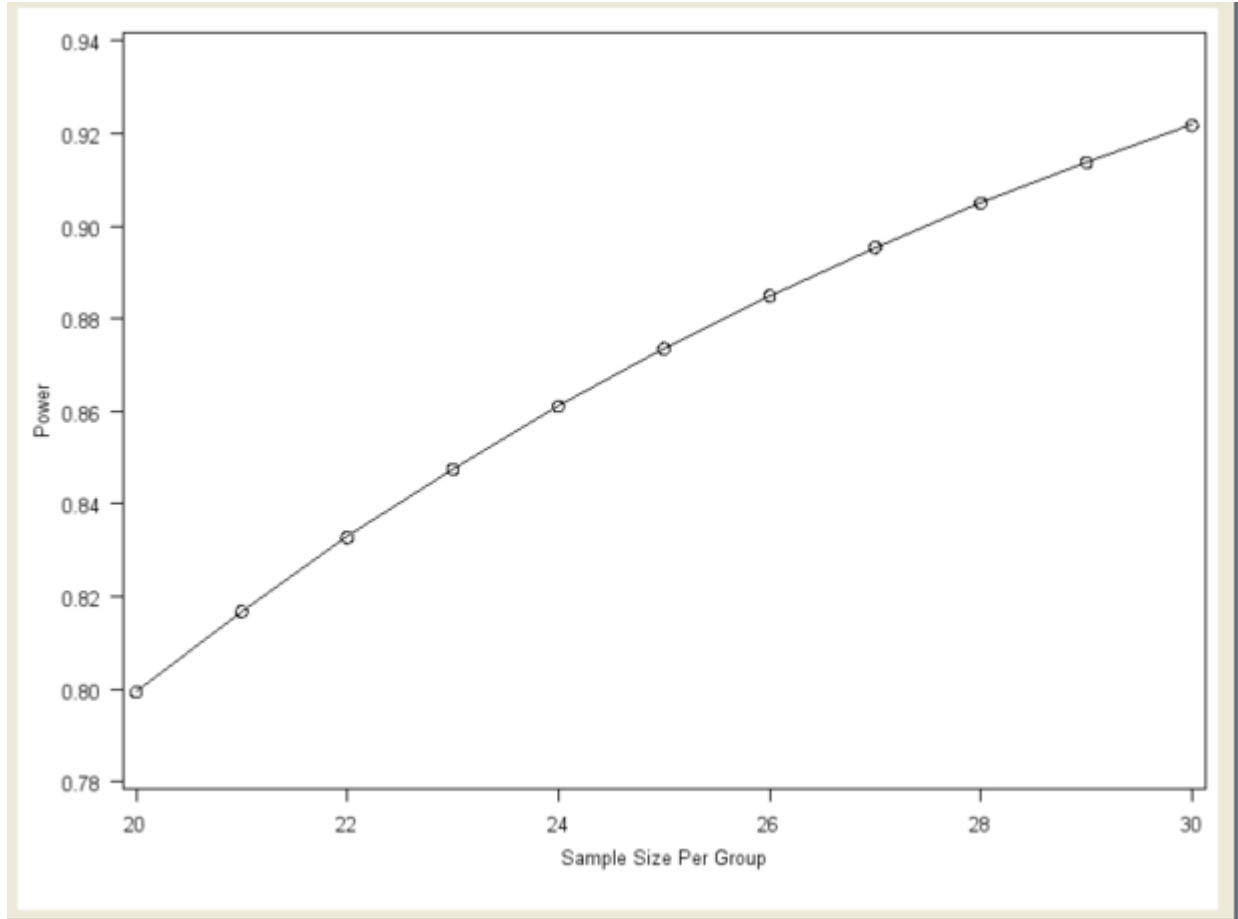


The table consists of two subtables: the `Fixed Scenario Elements` table that contains the input parameters that have only one value for the analysis, and the `Computed Power` table that contains the input parameters that have more than one value for the analysis and the corresponding power. Only the N per group parameter appears in the `Computed Power` table; all of the other input parameters have a single value. The computed power for a sample size per group of 25 is 0.874. Thus, you have a probability of 0.87 that the study will find the expected result if the assumptions and conjectured values are correct.

**Power by Sample Size Graph**

Click the **Graph** tab to view a power by sample size graph that displays power on the vertical axis and sample size per group on the horizontal axis. See [Figure 72.44](#).

**Figure 72.44** Power by Sample Size Graph



The range of values for the horizontal axis is 20 to 30, which were the smallest and largest values, respectively, that you entered on the **Sample Size** tab. You can customize the graph by specifying the values for the sample size axis (see the section “[Customizing Graphs](#)” on page 6176).

**Narratives**

Click the **Narratives** tab to create and display a sentence- or paragraph-length text summary of the input parameter values and the computed quantity for combinations of the input parameter values; see [Figure 72.45](#).

Figure 72.45 Narrative Selector and Display

**Narratives**

For a two-sample pooled t test of a normal mean difference with a one-sided significance level of 0.05, assuming a common standard deviation of 15, a sample size of 20 per group has a power of 0.799 to detect a difference between the means 132 and 120.

---

**Create Narratives**

Select one or more scenarios

| Select                              | Index | Sides | Alpha | Mean1 | Mean2 | StdDev | NPerGroup | NullDiff | Power      | Error | Info |
|-------------------------------------|-------|-------|-------|-------|-------|--------|-----------|----------|------------|-------|------|
| <input checked="" type="checkbox"/> | 1     | 1     | 0.05  | 132   | 120   | 15     | 20        | 0        | 0.79940818 |       |      |
| <input type="checkbox"/>            | 2     | 1     | 0.05  | 132   | 120   | 15     | 25        | 0        | 0.87355245 |       |      |
| <input type="checkbox"/>            | 3     | 1     | 0.05  | 132   | 120   | 15     | 30        | 0        | 0.92176938 |       |      |

To create a narrative, selected the desired scenario (row) in the narrative selector table at the bottom of the **Narratives** tab.

In this example, select the narrative for the sample size per group of 20, which yields a power of 0.799. The following text summary is displayed:

For a two-sample pooled t test of a normal mean difference with a one-sided significance level of 0.05, assuming a common standard deviation of 15, a sample size of 20 per group has a power of 0.799 to detect a difference between the means 132 and 120.

To create other narratives, select the desired rows in the narrative selector table. If you also select the second row for the sample size of 25, another text summary is displayed below the first one:

For a two-sample pooled t test of a normal mean difference with a one-sided significance level of 0.05, assuming a common standard deviation of 15, a sample size of 20 per group has a power of 0.799 to detect a difference between the means 132 and 120.

For a two-sample pooled  $t$  test of a normal mean difference with a one-sided significance level of 0.05, assuming a common standard deviation of 15, a sample size of 25 per group has a power of 0.874 to detect a difference between the means 132 and 120.

To change some values of the analysis and rerun it, select the Edit Properties page, change the desired properties, and click the **Calculate** button again.

## Test of Two Independent Means for Unequal Variances

In the preceding example, you assumed that the population standard deviations were equal. If you believe that the population standard deviations are not equal, use the same two-sample  $t$  test analysis as with the preceding example, but change the test option and enter group standard deviations.

You can use the previous example to demonstrate this test. If the project is not already open, open it by selecting **File►Open** on the menu bar, and then selecting the project that you have been using.

Make a copy of the project by selecting **File►Save As**. Enter a different project description, Experimental blood pressure drug with two groups for unequal variances. Click **OK**.

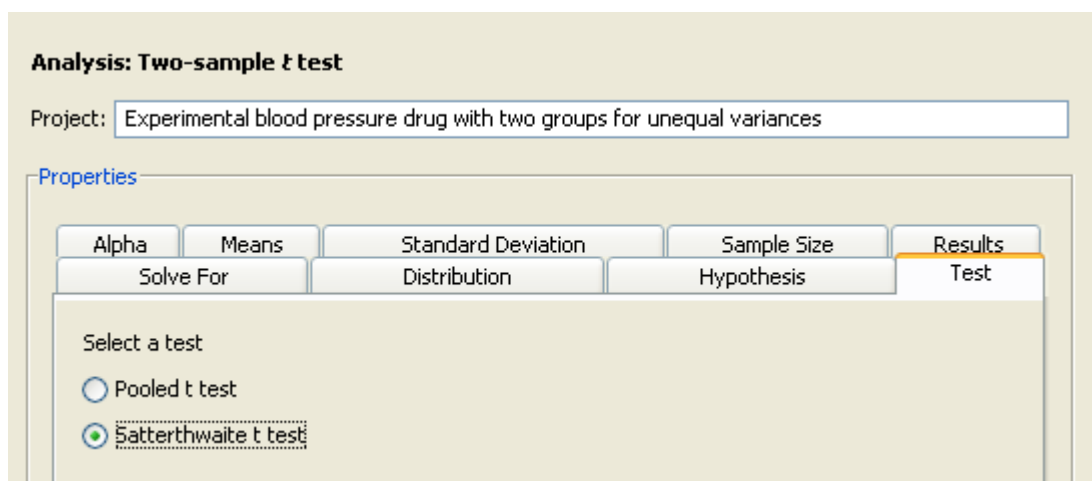
The copy of the project is opened, and the current project is closed.

### Editing Properties

#### Test

On the **Test** tab of the copied project, change the test to **Satterthwaite  $t$  test**, as shown in Figure 72.46.

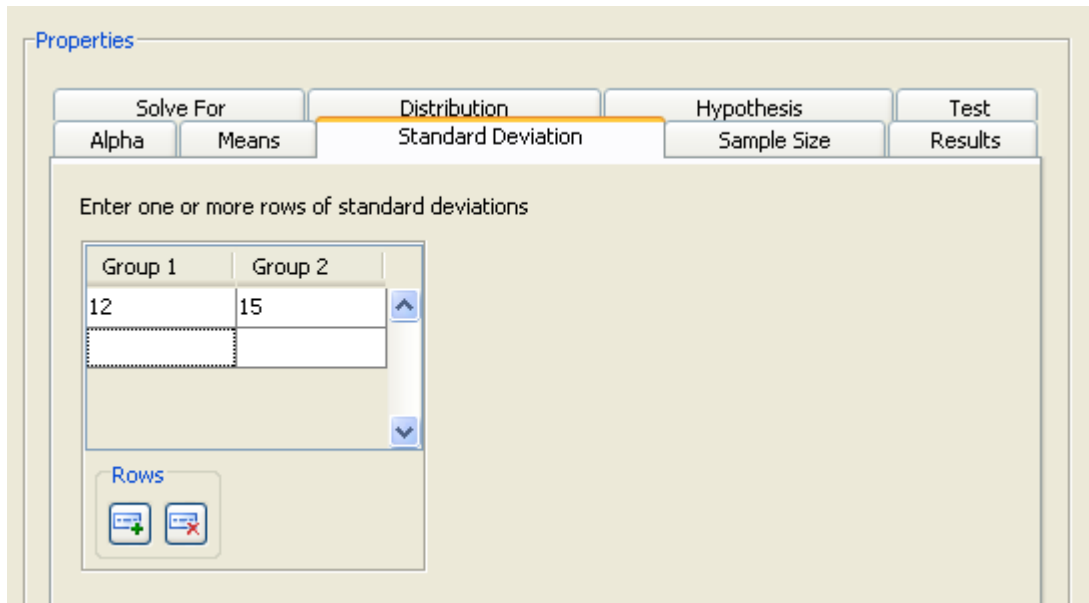
Figure 72.46 Satterthwaite  $t$  Test Option



#### Specifying Group Standard Deviations

Click the **Standard Deviation** tab and enter the group standard deviations of 12 and 15 on a single row, as shown in Figure 72.47.

**Figure 72.47** Group Standard Deviations



**Summary of Input Parameters**

Table 72.3 contains the values of the input parameters for the example.

**Table 72.3** Summary of Input Parameters

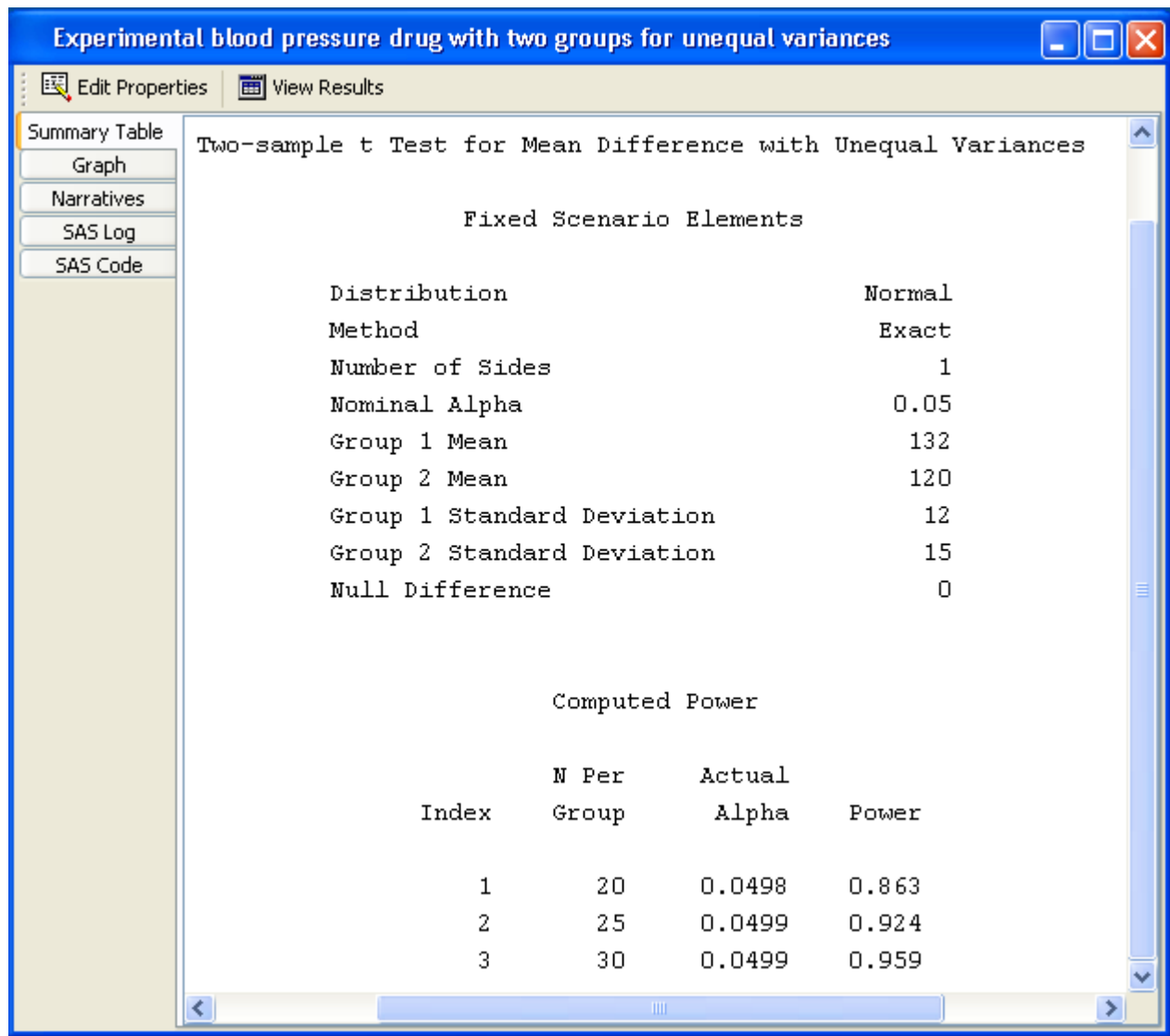
| Parameter          | Value                 |
|--------------------|-----------------------|
| Distribution       | Normal                |
| Hypothesis         | One-sided test        |
| Test               | Satterthwaite t test  |
| Alpha              | 0.05                  |
| Means form         | Group means           |
| Means              | 132, 120              |
| Standard deviation | 12, 15                |
| Sample size form   | Sample size per group |
| Sample size        | 20, 25, 30            |

Click **Calculate** to run the analysis.

**Viewing Results**

The power for a sample size per group of 25 is 0.924, as shown in Figure 72.48. Notice that the actual alpha is 0.0499. This is because the Satterthwaite *t* test is (slightly) biased.

Figure 72.48 Satterthwaite Test Results



If you modified the previous example, when you select the **Narratives** tab, the following message is displayed:

Previously selected narratives have been cleared because one or more input parameter values have changed.

In the previous analysis, you created narratives for two scenarios. Because this analysis uses group standard deviations, those selected narratives were cleared. The message would also have appeared if you had changed the number of scenarios.

Use the narrative selector table to create other narratives.

---

## Test of Mean Ratios

Instead of comparing means for a control and drug treatment group, you might want to investigate whether the blood pressure of the treatment group is lowered by a given percentage of the control group, say 10 percent. That is, you expect the ratio of the treatment group to the control group to be 90% or less.

PSS provides a two-sample  $t$  test of a mean ratio when the data are lognormally distributed.

For mean ratios, the coefficient of variation (CV) is used instead of standard deviation. In this example, you can expect the CV to be between 0.5 and 0.6. You also want to compare an equally weighted sampling of groups with an overweighted sampling in which the control group contains twice as many subjects as the treatment group: 50 and 25, respectively.

Make a copy of the project by selecting **File►Save As**. Enter a different project description, `Percent improvement with blood pressure drug`.

The copy of the project is opened.

## Editing Properties

Several of the input parameters for the test of mean ratios differ from the ones described in the section “[Test of Two Independent Means for Equal Variances](#)” on page 6183. Mean ratios and coefficients of variation are used instead of mean differences and standard deviations. These two parameters are discussed in detail in this section. For the input parameters and options that have been discussed previously in this example, only the values for this example are given.

### **Solve For Tab**

Click the **Solve For** tab to select the **Power** option as the quantity to be solved for, as shown in [Figure 72.49](#).



Figure 72.49 Project Description, Solve for Tab

The screenshot shows a software window titled "Percent improvement with blood pressure drug". At the top, there are two buttons: "Edit Properties" and "View Results". Below this, the analysis is identified as a "Two-sample t test". The "Project:" field contains the text "Percent improvement with blood pressure drug". A "Properties" section contains a grid of tabs: "Alpha", "Means", "Standard Deviation", "Sample Size", and "Results". The "Solve For" sub-tab is active, showing options: "Power" (selected with a radio button), "Sample size per group", and "Total sample size".

**Distribution**

You are interested in mean ratios rather than means, so select the **Lognormal** option on the **Distribution** tab, as shown in Figure 72.50.

Figure 72.50 Distribution Tab with Lognormal Option

The screenshot shows the "Properties" section of the software window. The "Distribution" sub-tab is active, showing options: "Lognormal" (selected with a radio button) and "Normal". The tabs above are "Means", "Coefficient of Variation", "Sample Size", and "Results". The sub-tabs below are "Solve For", "Distribution", "Hypothesis", "Test", and "Alpha".

**Hypothesis and Alpha**

Click the **Hypothesis** tab and select the **One-sided test** option.

Click the **Alpha** tab and type 0.05 as the significance level in the first cell of the table, if it is not already there.

## Means

Click the **Means** tab to select the input form for entering mean ratios. There are four alternate forms for entering means or mean ratios:

### Mean ratio

Enter the ratio of the two group means—that is, the treatment mean divided by the reference mean. The null ratio is assumed to be 1.

### Group means

Enter the means for each group. The ratio of the means is formed by dividing the mean for group 2 by the mean for group 1. The null ratio is assumed to be 1.

### Mean ratio, Null ratio

Enter the ratio of the two group means—that is, the treatment mean divided by the reference mean. Enter the null ratio.

### Group means, Null ratio

Enter the means for each group. The ratio of the means is formed by dividing the mean for group 2 by the mean for group 1. Enter the null ratio.

As shown in [Figure 72.51](#), select the **Mean ratio** form which uses a default null ratio of 1. Enter a single mean ratio value of 0.9.

**Figure 72.51** Means Tab with Mean Ration Form and Values

The screenshot shows a software interface with a 'Properties' window. At the top, there are several tabs: 'Solve For', 'Distribution', 'Hypothesis', 'Test', and 'Alpha'. Below these are sub-tabs: 'Means', 'Coefficient of Variation', 'Sample Size', and 'Results'. The 'Solve For' tab is selected, and its dropdown menu is open, showing 'Mean ratio' as the selected option. Below the dropdown, there is a text input field labeled 'Enter one or more mean ratios' which contains the value '0.9'. To the right of this field is a small icon. Below the input field is a 'Rows' section with two buttons: a plus sign and a minus sign.

**Coefficient of Variation**

On the **Coefficient of Variation** tab, enter the coefficients of variation. They are assumed to be equal for the two groups.

For this example, enter 0.5 and 0.6, as shown in Figure 72.52.

**Figure 72.52** Coefficient of Variation Tab

Properties

Solve For: Means | Distribution: Coefficient of Variation | Hypothesis: Sample Size | Test: Results | Alpha: Results

Enter one or more coefficients of variation

| CV  |
|-----|
| 0.5 |
| 0.6 |

Rows

Buttons: +, -

**Sample Size**

On the **Sample Size** tab, select the **Group sample sizes** form and enter two sets of values: 25 and 25 in the first row and 25 and 50 in the second row, as shown in Figure 72.53.

**Figure 72.53** Sample Sizes

Properties

Solve For: Means | Distribution: Coefficient of Variation | Hypothesis: Sample Size | Test: Results | Alpha: Results

Select a form: Group sample sizes

Enter one or more rows of group sample sizes

| Group 1 | Group 2 |
|---------|---------|
| 25      | 25      |
| 25      | 50      |

Rows

Buttons: +, -

### Summary of Input Parameters

Table 72.4 contains the values of the input parameters for the example.

**Table 72.4** Summary of Input Parameters

| Parameter                 | Value              |
|---------------------------|--------------------|
| Hypothesis                | One-sided test     |
| Distribution              | Lognormal          |
| Alpha                     | 0.05               |
| Means form                | Mean ratio         |
| Mean ratio                | 0.9                |
| Coefficients of variation | 0.5, 0.6           |
| Sample size form          | Group sample sizes |
| Sample Size               | (25, 25), (25, 50) |

### Results

On the **Results** tab, select the **Create summary table** and **Create power by sample size graph** check boxes.

Click **Calculate** to perform the analysis.

In this case, the following message is displayed:

The power by sample size graph is not available when specifying sample sizes for two groups.

If you want a power by sample size graph, you can choose to plot total sample size instead by using the **Total N, Group weights** sample size form on the **Sample Size** tab. For more information about using this input form, see the section “Using Unequal Group Sizes” on page 6205.

### Viewing Results

The first thing that you notice from the summary table in [Figure 72.54](#) is that the calculated powers are quite low—they range from 0.163 to 0.229. You have less than a 25% probability of detecting the difference that you are looking for. Clearly, this set of parameter values leads to insufficient power. To increase power, you might choose a larger sample size or a larger alpha.

Figure 72.54 Summary Table

Percent improvement with blood pressure drug

Edit Properties View Results

Summary Table  
Narratives  
SAS Log  
SAS Code

Two-sample t Test for Mean Ratio

Fixed Scenario Elements

|                           |           |
|---------------------------|-----------|
| Distribution              | Lognormal |
| Method                    | Exact     |
| Number of Sides           | 1         |
| Alpha                     | 0.05      |
| Geometric Mean Ratio      | 0.9       |
| Null Geometric Mean Ratio | 1         |

Computed Power

| Index | CV  | N1 | N2 | Power |
|-------|-----|----|----|-------|
| 1     | 0.5 | 25 | 25 | 0.193 |
| 2     | 0.5 | 25 | 50 | 0.229 |
| 3     | 0.6 | 25 | 25 | 0.163 |
| 4     | 0.6 | 25 | 50 | 0.190 |

You can also see that oversampling the control group improves power slightly, 0.229 versus 0.193 for the coefficient of variation of 0.5. However, this is a marginal increase that is probably not worth the added expense.

For the example, use larger sample sizes with equal cell sizes. Return to the Edit Properties page by clicking the **Edit Properties** icon near the top of the window.

Then, on the **Sample size** tab, change to the **Sample size per group** form. Specify sample sizes of 50, 100, 150, and 200, as shown in Figure 72.55.

**Figure 72.55** Modified Sample Size Values

Properties

Solve For: Means | Distribution: Coefficient of Variation | Hypothesis: | Test: Sample Size | Alpha: Results

Select a form: Sample size per group

Enter one or more values for sample size per group

N Per Group

50  
100  
150  
200

Rows

+ -

Table 72.5 contains the modified values of the input parameters for the example.

**Table 72.5** Modified Summary of Input Parameters

| Parameter        | Value                 |
|------------------|-----------------------|
| Sample size form | Sample size per group |
| Sample size      | 50, 100, 150, 200     |

Rerun the analysis by clicking **Calculate**.

Figure 72.56 displays the summary table. The largest sample size of 200 (per group) yields a power of 0.72 for a coefficient of variation of 0.5, and 0.599 for one of 0.6. With a total of 400 subjects, you still have a 30% to 40% probability of not detecting the effect even if it exists.

Figure 72.56 Summary Table for Modified Sample Sizes

The screenshot shows a SAS window titled "Percent improvement with blood pressure drug". On the left, there is a navigation pane with options: "Summary Table" (selected), "Narratives", "SAS Log", and "SAS Code". The main area displays the following information:

**Fixed Scenario Elements**

|                           |           |
|---------------------------|-----------|
| Distribution              | Lognormal |
| Method                    | Exact     |
| Number of Sides           | 1         |
| Alpha                     | 0.05      |
| Geometric Mean Ratio      | 0.9       |
| Null Geometric Mean Ratio | 1         |

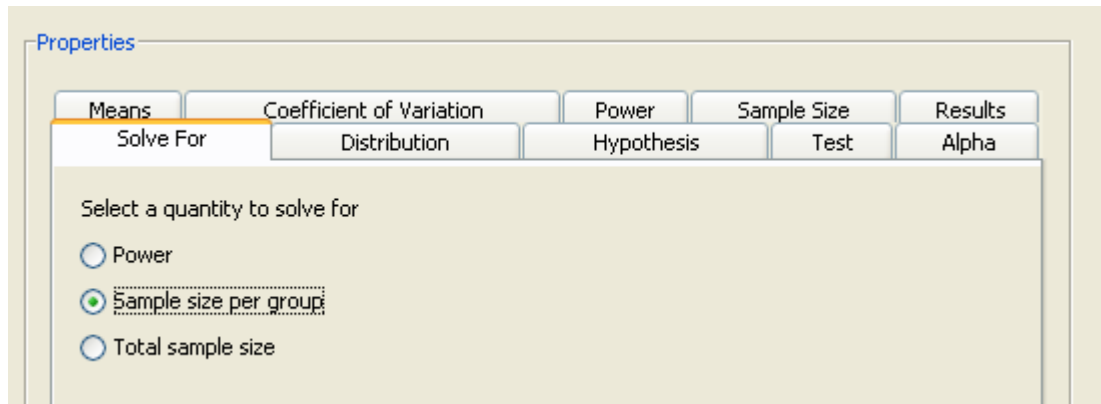
**Computed Power**

| Index | CV  | N Per Group | Power |
|-------|-----|-------------|-------|
| 1     | 0.5 | 50          | 0.296 |
| 2     | 0.5 | 100         | 0.471 |
| 3     | 0.5 | 150         | 0.611 |
| 4     | 0.5 | 200         | 0.720 |
| 5     | 0.6 | 50          | 0.242 |
| 6     | 0.6 | 100         | 0.380 |
| 7     | 0.6 | 150         | 0.499 |
| 8     | 0.6 | 200         | 0.599 |

## Additional Topics

### Solving for Sample Size

Several types of analysis enable you to solve for either total sample size or sample size per group. The sample size per group choice assumes equal group sizes. When solving for total sample size, the group sizes can be equal or unequal. Select the desired quantity on the **Solve For** tab. An example of these options is shown in Figure 72.57.

**Figure 72.57** Solve For Tab with Sample Size Selected

For either of the two sample size options, you must specify one or more values for power on the **Power** tab. If you frequently use the same values for power, set them as the default in the Preferences window, which is accessed by **Tools►Preferences**. Changing preferences affects only projects that you create after the change; existing projects are not affected.

If you select total sample size, you must specify whether the group sizes are equal or unequal. Select the appropriate option on the **Sample Size** tab. For unequal group sizes, you must specify the relative sample sizes for the two groups. For information about providing relative sample sizes, see the section “Using Unequal Group Sizes” on page 6205.

### Using Unequal Group Sizes

When solving for either power or total sample size, you might have unequal group sizes. If so, you must provide relative sample sizes for the groups. Weights must be greater than 0 but do not have to sum to 1.

Select the **Total N, Group weights** form on the **Sample Size** tab. Enter total sample sizes of 30 and 60 in the **Total N** table. Select the **Unequal group sizes** option and click **Enter Relative Sample Sizes**, as seen in Figure 72.58.



**Figure 72.58** Sample Size Tab with Group Weights Form

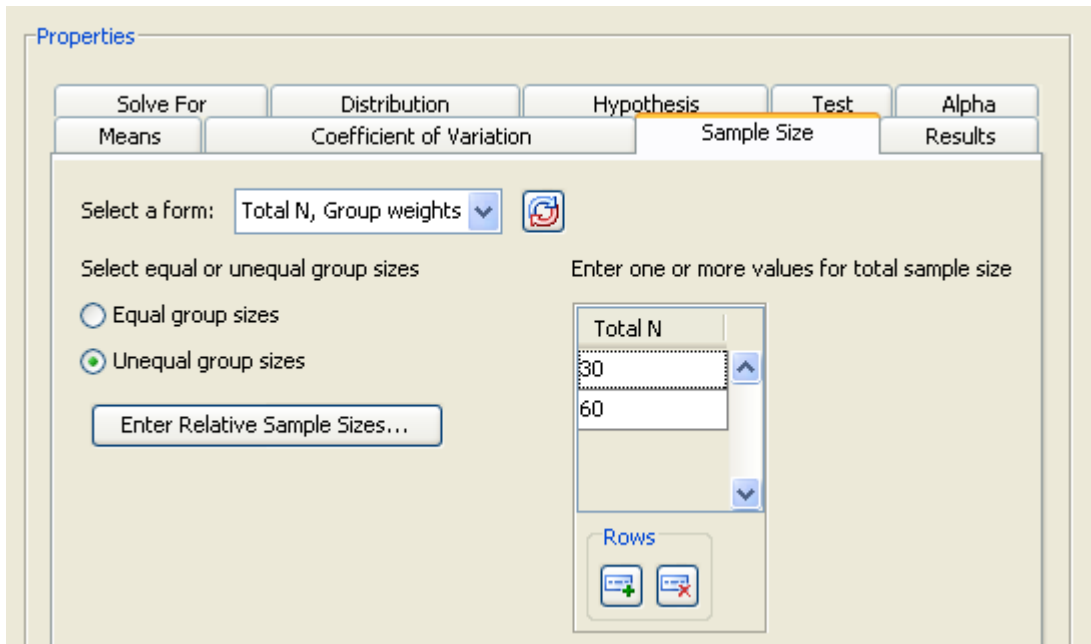
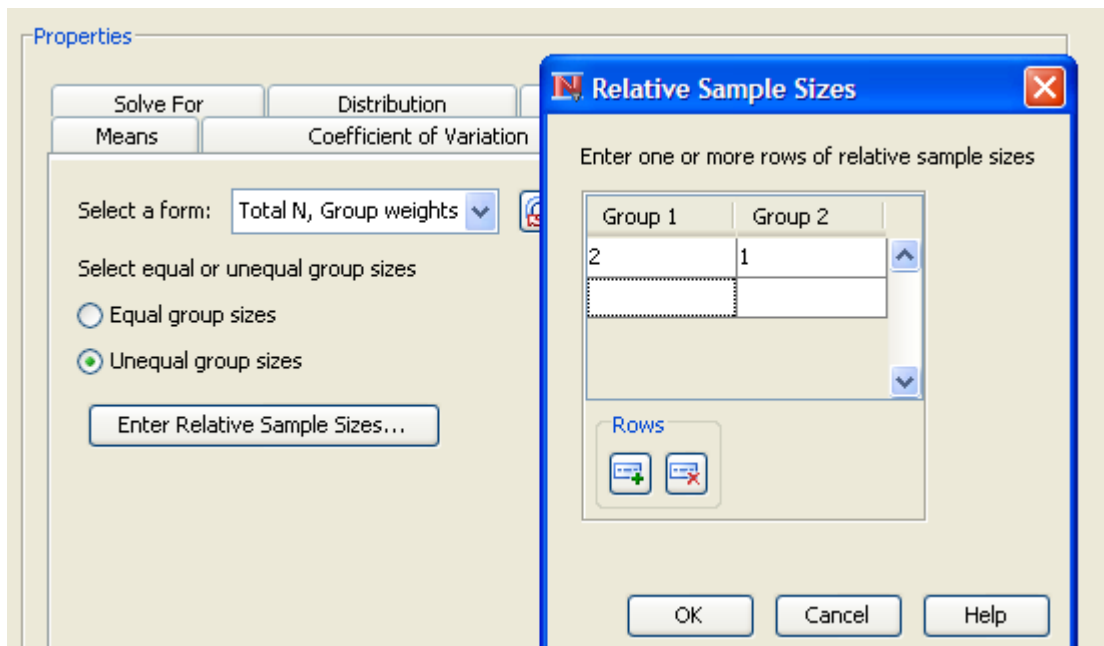


Figure 72.59 displays the window in which you can enter relative sample sizes. As an example, enter 2 for the first group and 1 for the second. In this case, you are sampling the drug treatment group twice as often as the control group.

**Figure 72.59** Relative Sample Sizes Window



The weights control how the total sample size is divided between the two groups. In the example, the sample size for groups 1 and 2 is 20 and 10, respectively, for a total sample size of 30.

Click **OK** to save the values and return to the Edit Properties page.

---

## Example: Analysis of Variance

---

### Overview

PSS offers power and sample size calculations for analysis of variance in two tasks: one-way ANOVA and general linear univariate models. Optional contrasts are available in both tasks.

In the one-way ANOVA task, you can solve for sample size per group as well as total sample size. The contrast facility for the one-way ANOVA task enables you to select orthogonal polynomials as well as to specify contrast coefficients. For more information about power and sample size analysis for one-way ANOVA, see Chapter 71, “[The POWER Procedure](#).”

In the general linear univariate models task, you specify linear models for a single dependent variable. Type III tests and contrasts of fixed effects are included, and the model can include covariates. For more information about power and sample size analysis for linear univariate models, see Chapter 44, “[The GLMPOWER Procedure](#).”

---

### The Example

Suppose you are interested in testing how two experimental drugs affect systolic blood pressure relative to a standard drug. You want to include both men and women in the study. You have a two-factor design: a drug factor with three levels and a gender factor with two levels. You choose a main-effects-only model because you do not expect a drug by gender interaction. You want to calculate the sample size that will produce a power of 0.9 using a significance level of 0.05. You believe that the error standard deviation is between 5 and 7 mm pressure. This is a two-way analysis of variance, so the general linear univariate models task is the appropriate one.

### Editing Properties

Start by opening the New window (**File►New**). In the **Analysis of Variance and Linear models** section of the New window, select **General linear univariate models**. The **General univariate linear models** project appears, with the Edit Properties page displayed.

#### **Project Description**

For the example, change the project description to Three blood pressure drugs and gender.

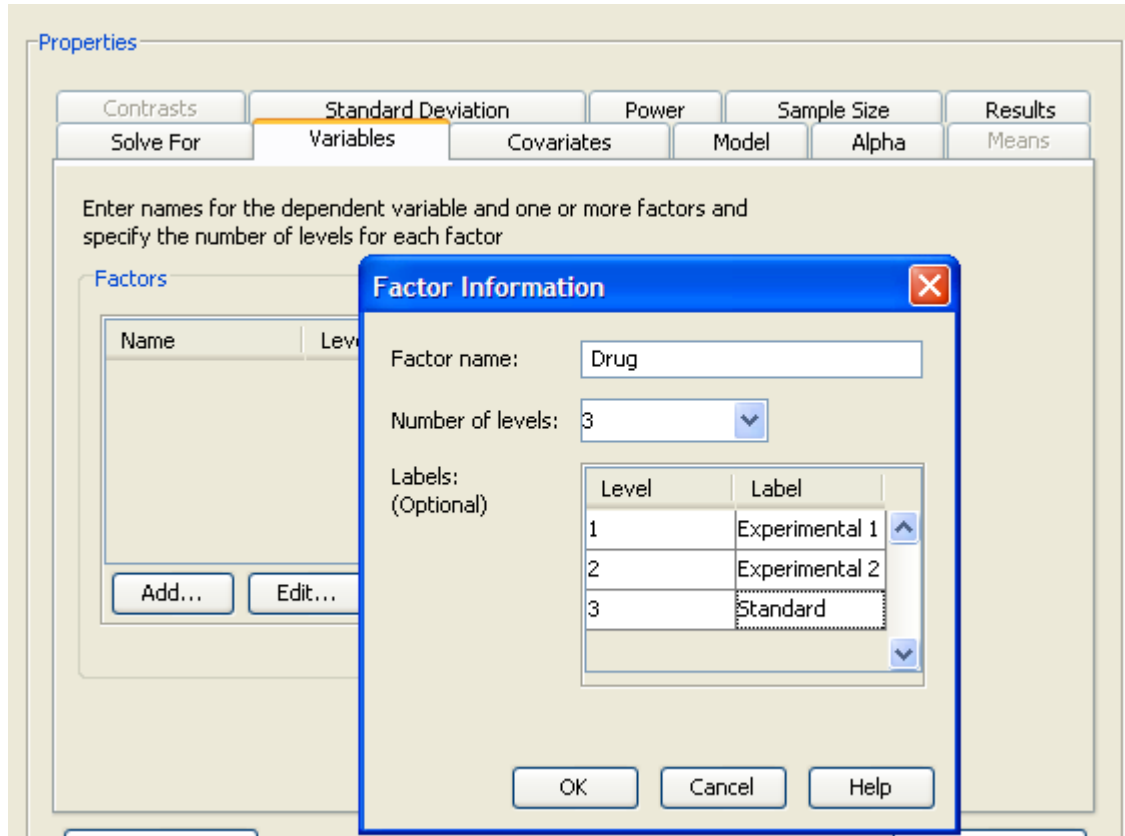
#### **Solve For**

Click the **Solve For** tab and select the **Sample size** option.

### Variables

Click the **Variables** tab to enter the names of the factors in the design. Click the **Add** button. The Factor Definition window appears, as shown in Figure 72.60.

**Figure 72.60** Factor Definition Window



Enter the name for the first factor, *Drug*, and enter the number of factor levels in the **Number of levels:** list box. There are three levels for this factor. Optionally, you can provide a label for each factor level. This label is used to identify factor levels on other tabs of the Edit Properties page. For this example enter the labels *Experimental 1*, *Experimental 2*, and *Standard* for the three levels of the *Drug* factor. Click **OK** when you are finished.

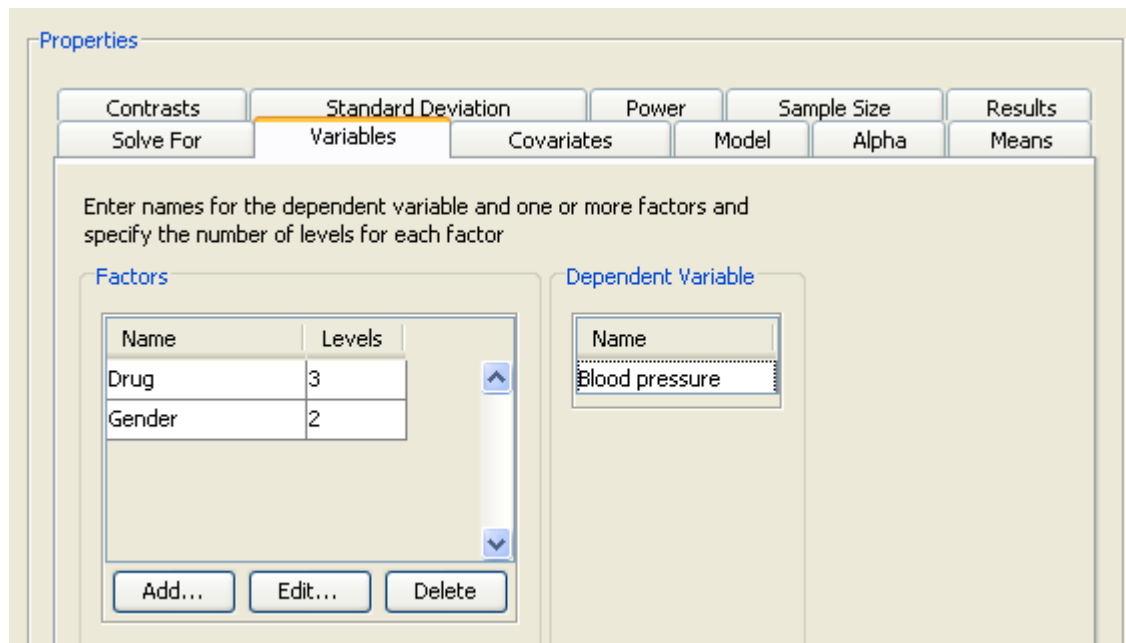
Click the **Add** button again and repeat the process for the second factor, *Gender* with two levels and labels *Female* and *Male*.

Factors can contain blanks and other special characters. Do not use an asterisk (\*) because a factor name with an asterisk might be confused with an interaction effect. Factor names can be any length, but they must be distinct from one another in the first 32 characters.

On the **Variables** tab, you can also specify the name of the dependent variable; in this example, *Blood pressure* is used.

The completed **Variables** tab is shown in [Figure 72.61](#).

**Figure 72.61** Variables Tab with Factors and Number of Levels



### **Model**

Click the **Model** tab, then choose from three model options:

#### **Main effects**

Only the main effects are included in the model.

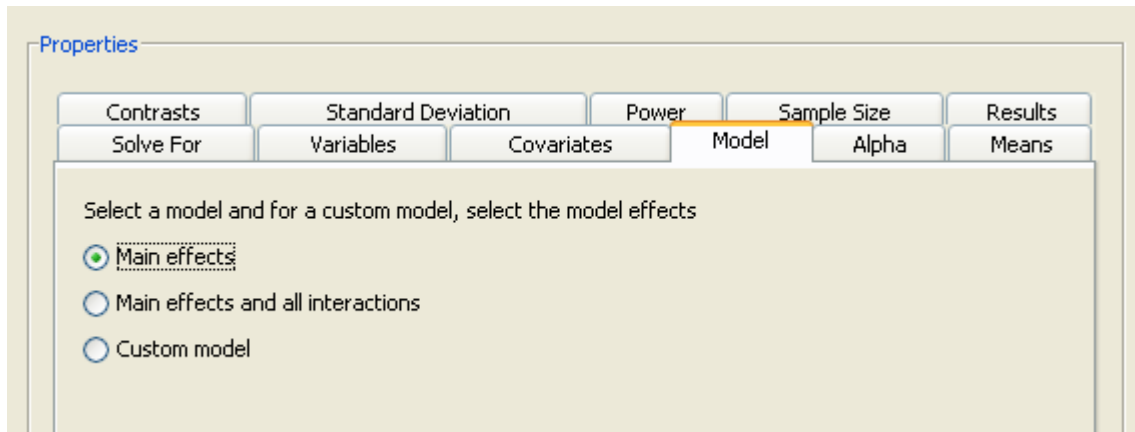
#### **Main effects and all interactions**

The main effects and all possible interactions are included in the model.

#### **Custom model**

Selected effects are included in the model. The effects are selected in a model builder that is displayed when this model is selected. For more information about specifying a custom model, see the section “[Specifying a Custom Model](#)” on page 6220.

For this example, choose the default **Main effects** model, as shown in [Figure 72.62](#).

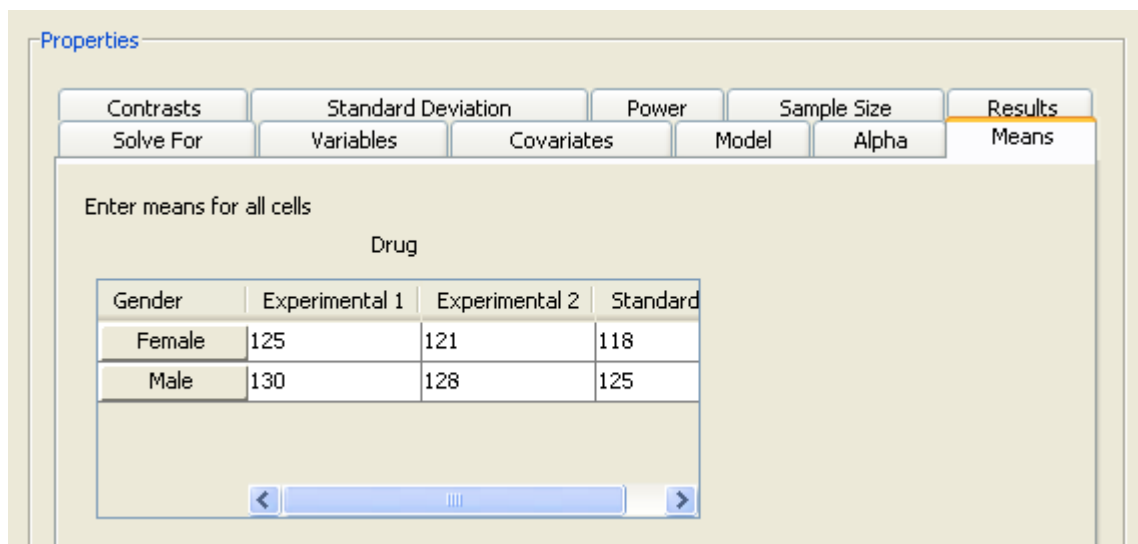
**Figure 72.62** Model Tab with Main Effects Selected**Alpha**

Click the **Alpha** tab to specify one or more significance levels. For the example, specify a single significance level of 0.05.

Alpha is the significance level (that is, the probability of falsely rejecting the null hypothesis). If you frequently use the same values for alpha, set them as the defaults in the Preferences window (**Tools►Preferences**).

**Means**

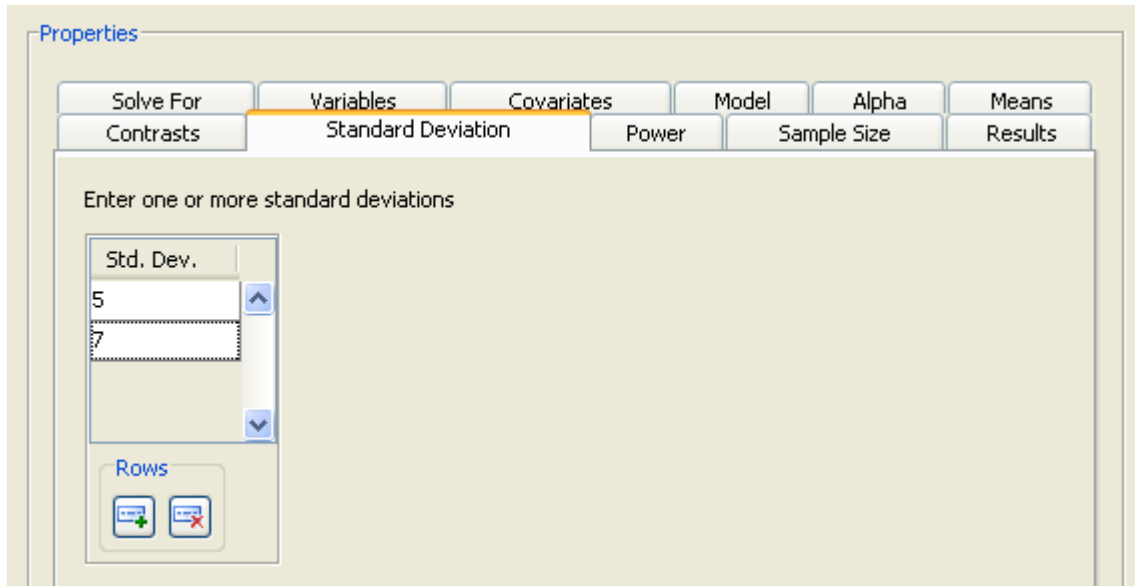
Click the **Means** tab to enter projected cell means for each cell of the design. The completed means for the example are shown in Figure 72.63.

**Figure 72.63** Means Tab with Cell Means

### Standard Deviation

Click the **Standard Deviation** tab to specify one or more conjectured error standard deviations. The standard deviation is the same as the root mean squared error. For this example, enter two standard deviations, 5 and 7, as shown in Figure 72.64.

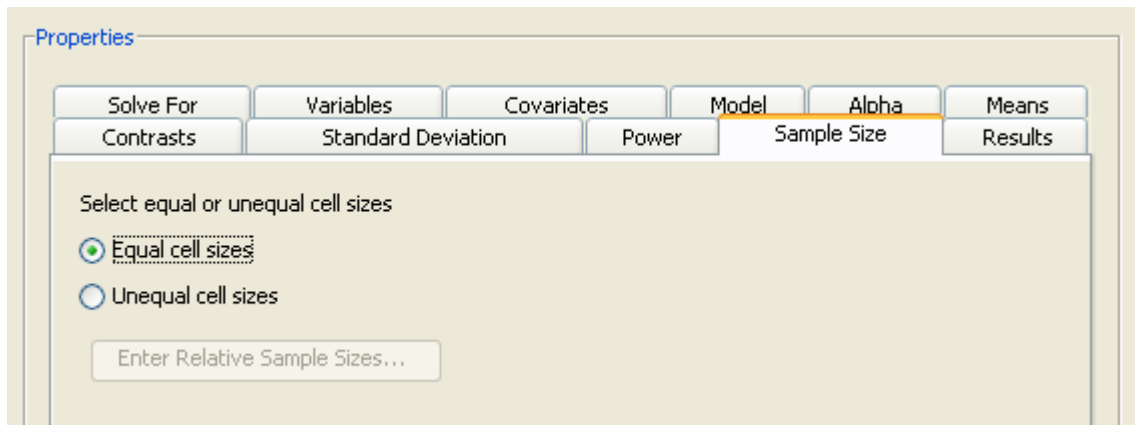
**Figure 72.64** Standard Deviations Tab



### Relative Sample Size

Click the **Sample Size** tab to select whether cell sample sizes are equal or unequal.

**Figure 72.65** Sample Size Tab with Equal Cell Sample Sizes



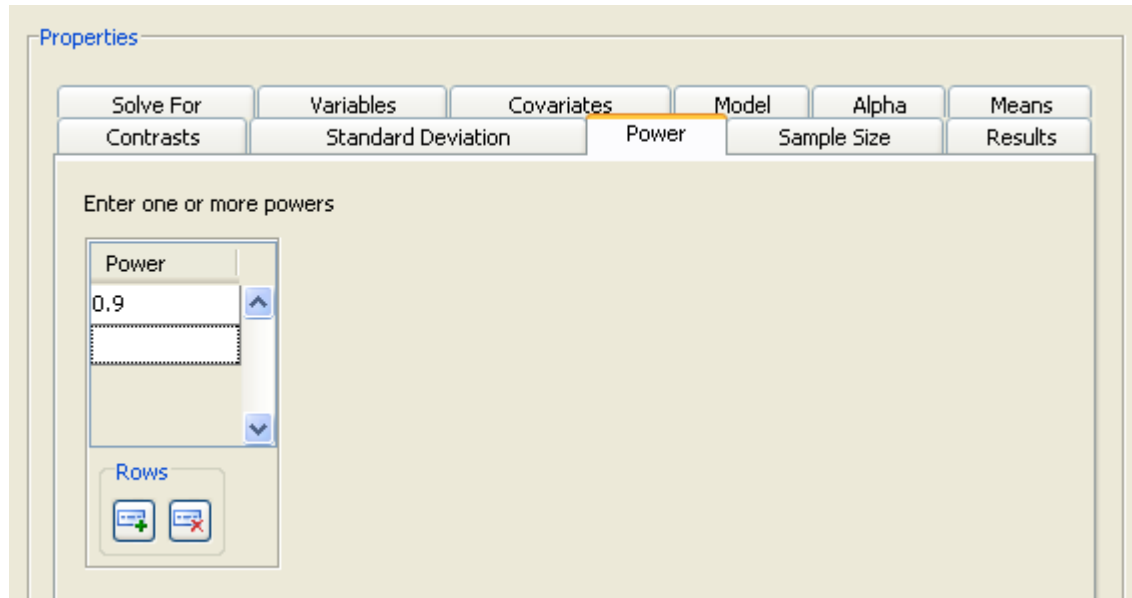
For the example, select the **Equal cell sizes** option, as shown in Figure 72.65.

When solving for sample size, it is necessary to specify whether the cell sample sizes are equal or unequal. If cell sizes are unequal, relative sample size weights must also be specified. For more information about providing sample size weights, see the section “Using Unequal Cell Sizes” on page 6217.

### Power

Click the **Power** tab to specify one or more powers. For this example, enter a single power of 0.9, as shown in Figure 72.66.

**Figure 72.66** Power Tab



### Summary of Input Parameters

Table 72.6 contains the values of the input parameters for the example.

**Table 72.6** Summary of Input Parameters

| Parameter             | Value            |
|-----------------------|------------------|
| Model                 | Main effects     |
| Alpha                 | 0.05             |
| Means                 | See Table 72.7   |
| Standard deviation    | 5, 7             |
| Relative sample sizes | Equal cell sizes |
| Power                 | 0.9              |

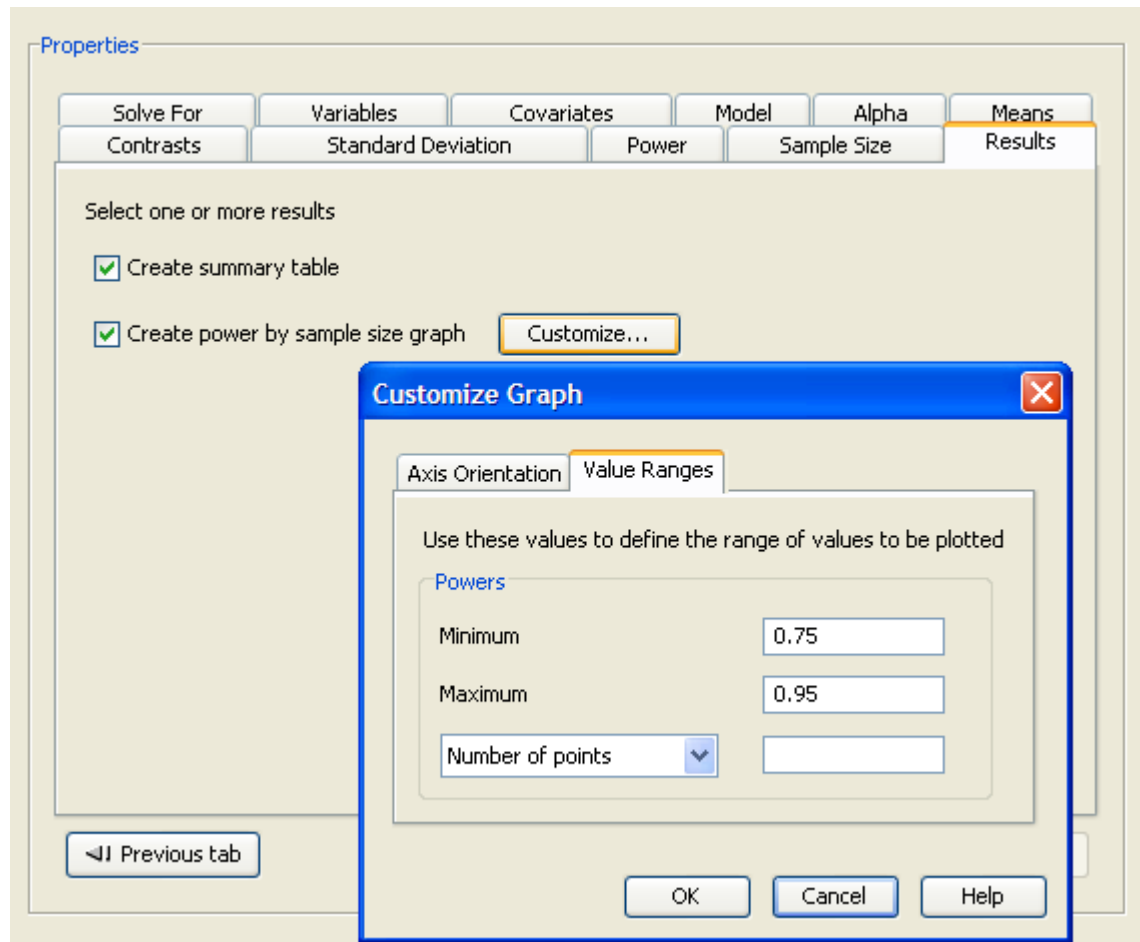
**Table 72.7** Cell Means

| Gender | Drug           |                |          |
|--------|----------------|----------------|----------|
|        | Experimental 1 | Experimental 2 | Standard |
| Female | 125            | 121            | 118      |
| Male   | 130            | 128            | 125      |

### Results Options

Click the **Results** tab to select desired results. For the example, select both the **Create summary table** and **Create power by sample size graph** check boxes.

The graph consists of four points, one for each of the four scenarios that were created by combining the two factor main effects with the two standard deviations. This graph is not very informative, so specify a range of powers for the horizontal power axis. To change the power axis of the graph, click the **Customize** button beside the **Create power by sample size graph** check box to open the Customize Graph window.

**Figure 72.67** Value Ranges on Customize Graph Window



Click the **Value Ranges** tab and enter a minimum power of 0.75 and a maximum power of 0.95, as shown in Figure 72.67. Click **OK** to close the window.

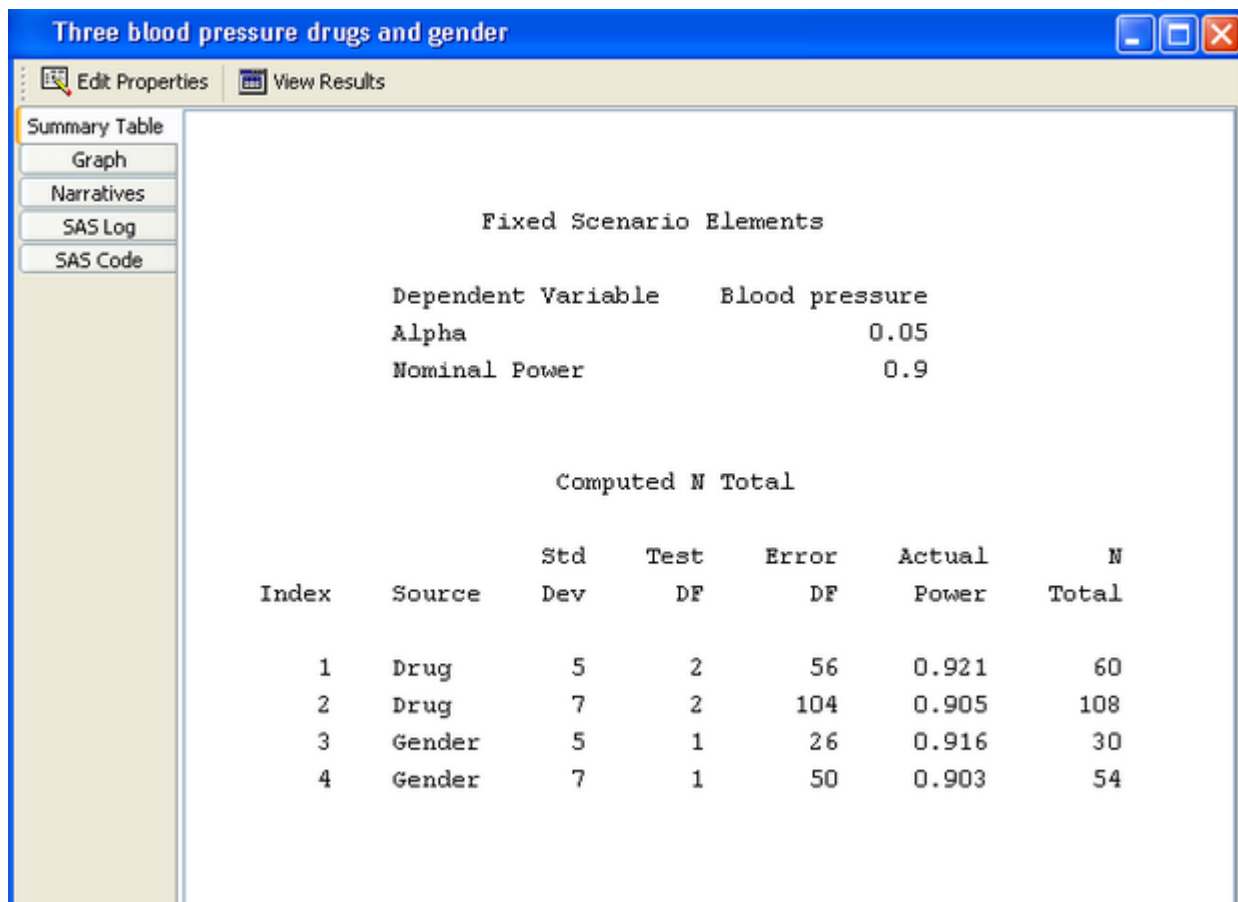
Now, click **Calculate** to perform the analysis.

## Viewing Results

The results are displayed in separate tabs on the View Results page.

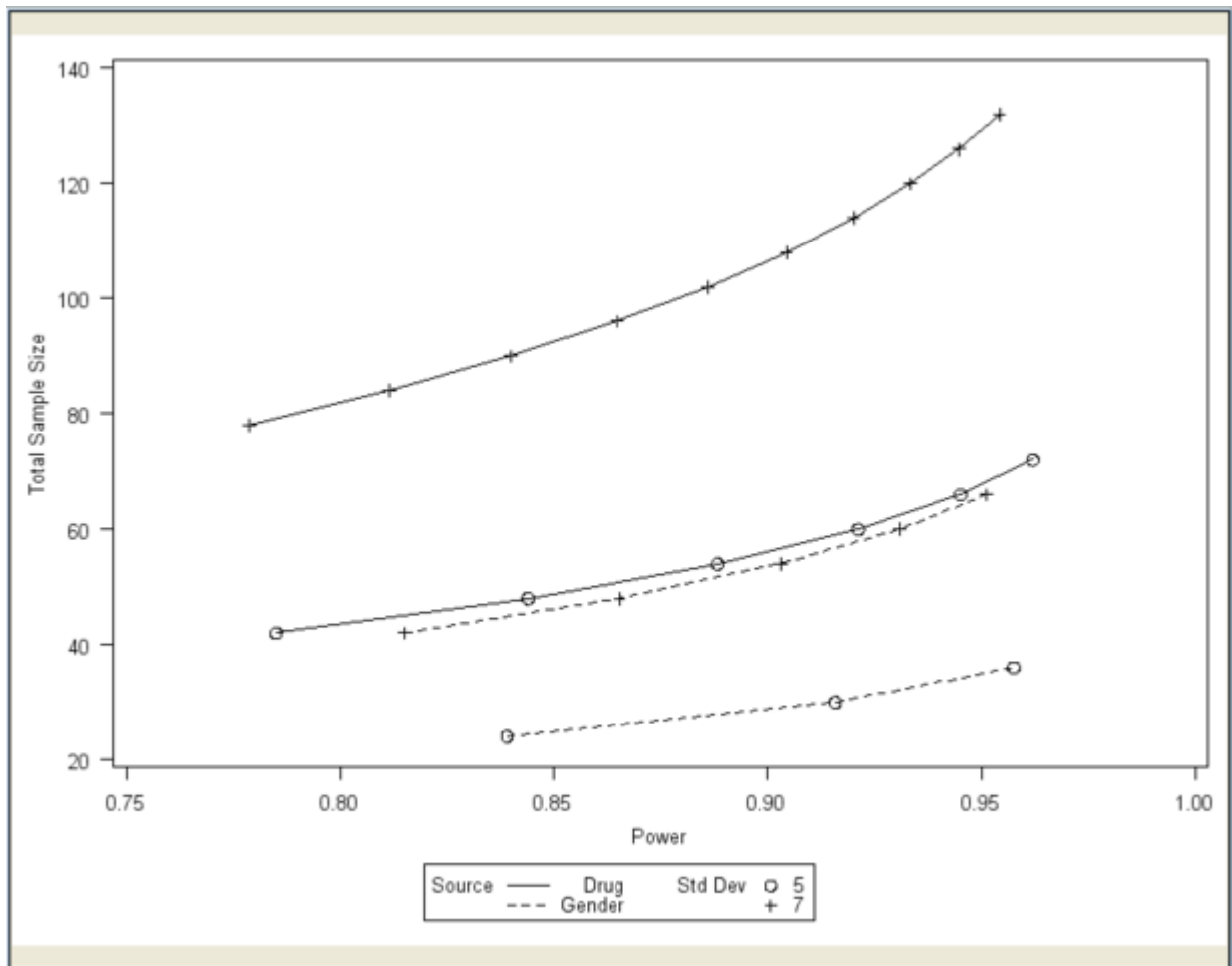
Click the **Summary Table** tab to view the summary table. In the `Computed N Total` table, sample sizes are listed for each combination of factor and standard deviation (Figure 72.68). You need a total sample size between 60 and 108 to yield a power of 0.9 for the `Drug` effect if the standard deviation is between 5 and 7. You need a sample size of half that for the `Gender` effect.

Figure 72.68 Summary Table



Click the **Graph** tab to view the power by sample size graph, as shown in Figure 72.69. One approximately linear curve is displayed for each standard deviation and factor combination.

Figure 72.69 Power by Sample Size Graph



Click the **Narratives** tab to create narratives of one or more scenarios. Select the first scenario, the Drug effect with the standard deviation of 5, in the narrative selector table. Note that the cell means are not included in the following narrative description:

For the usual F test of the Drug effect in the general linear univariate model with fixed class effects [Blood pressure = Drug Gender] using a significance level of 0.05, assuming the specified cell means and an error standard deviation of 5, a total sample size of 60 assuming a balanced design is required to obtain a power of at least 0.9. The actual power is 0.921.

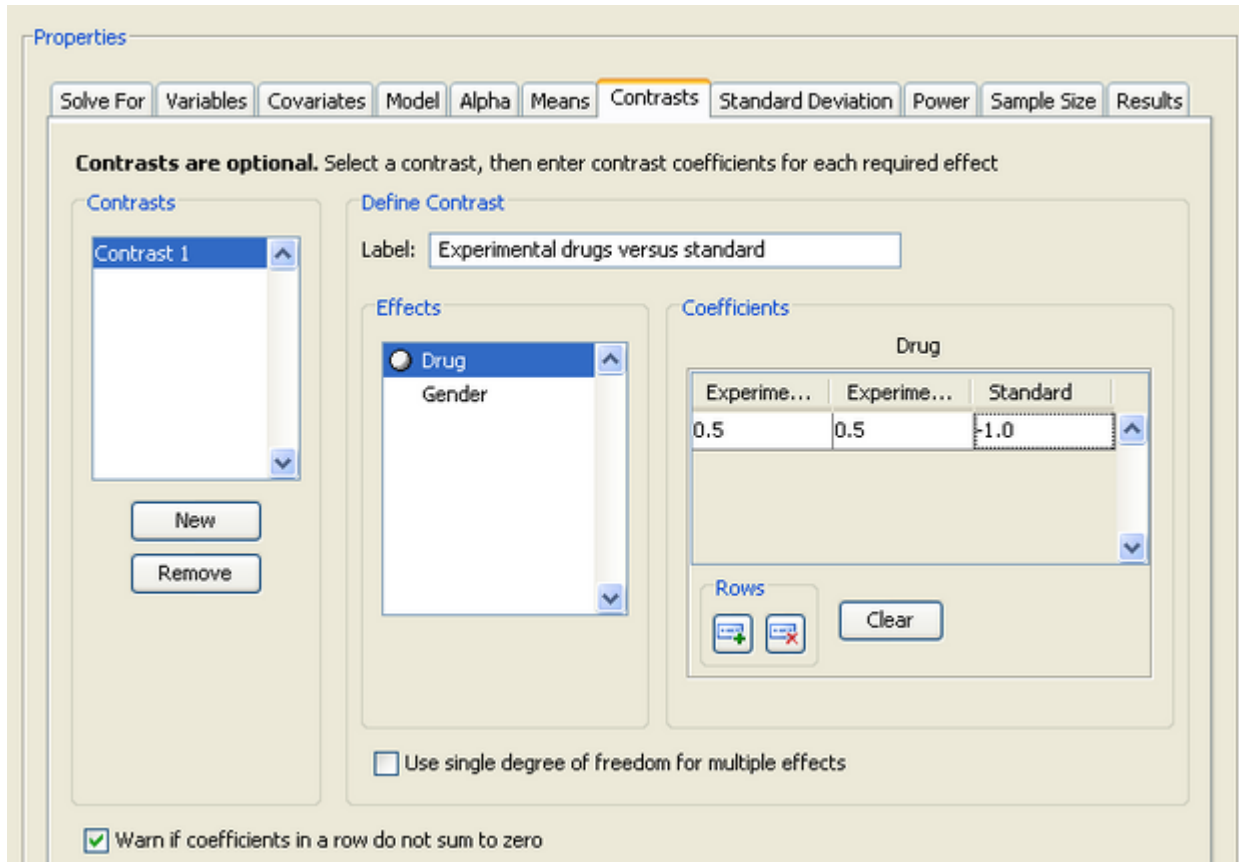
For more information about using the narrative facility, see the section “[Creating Narratives](#)” on page 6179.

## Additional Topics

### Adding Contrasts

Click the **Contrasts** tab to define one or more contrasts. Contrasts are optional. PSS allows contrasts to be added when using either a main effects model or a main effects and interactions model. At least two factors must have been specified in order to be able to enter contrasts. The contrast tab appears in [Figure 72.70](#).

**Figure 72.70** Contrast Tab with Coefficients



To create a contrast, click the **New** button. Then, select the newly created contrast (Contrast 1) from the list.

Specify a label for the contrast in the **Label** field. The label should be different from all of the factor names and all interactions in the model, as well as other contrast labels.

Then, for each term you want to include in the contrast, select the term in the **Effects** list and enter at least two coefficients per term. It is not necessary to enter zeros; blanks are considered to be zeros.

To clear all of the contrast coefficients for a term, click the **Clear** button. To remove a previously defined contrast, select it from the **Contrasts** list and click the **Remove** button.

In this example, you are interested in comparing the two experimental drugs to the standard drug. As shown in [Figure 72.70](#), the contrast coefficients are 0.5, 0.5, and  $-1$  for the three levels of the Drug effect.

Figure 72.71 shows the two scenarios for the contrast at the bottom of the Computed N Total table. The two scenarios also appear in the graph but the graph is not shown here.

**Figure 72.71** Computed N Total Table for the Contrast

| Fixed Scenario Elements |          |                                    |                |         |          |              |         |  |
|-------------------------|----------|------------------------------------|----------------|---------|----------|--------------|---------|--|
| Dependent Variable      |          |                                    | Blood pressure |         |          |              |         |  |
| Alpha                   |          |                                    | 0.05           |         |          |              |         |  |
| Nominal Power           |          |                                    | 0.9            |         |          |              |         |  |
| Computed N Total        |          |                                    |                |         |          |              |         |  |
| Index                   | Type     | Source                             | Std Dev        | Test DF | Error DF | Actual Power | N Total |  |
| 1                       | Effect   | Drug                               | 5              | 2       | 56       | 0.921        | 60      |  |
| 2                       | Effect   | Drug                               | 7              | 2       | 104      | 0.905        | 108     |  |
| 3                       | Effect   | Gender                             | 5              | 1       | 26       | 0.916        | 30      |  |
| 4                       | Effect   | Gender                             | 7              | 1       | 50       | 0.903        | 54      |  |
| 5                       | Contrast | Experimental drugs versus standard | 5              | 1       | 62       | 0.924        | 66      |  |
| 6                       | Contrast | Experimental drugs versus standard | 7              | 1       | 116      | 0.909        | 120     |  |

## Using Unequal Cell Sizes

Click the **Sample Size** tab to select the equal or unequal cell sizes option.

**Figure 72.72** Sample Size Tab

Properties

Solve For    Variables    Covariates    Model    **Alpha**    Means

Contrasts    Standard Deviation    Power    **Sample Size**    Results

Select equal or unequal cell sizes

Equal cell sizes

Unequal cell sizes

Enter Relative Sample Sizes...

For the example, select the **Unequal cell sizes** option, as seen in Figure 72.72, and then click the **Enter Relative Sample Sizes** button.

Figure 72.73 shows the window in which you can enter relative sample sizes. As an example, enter the sample size weights from Table 72.8.

**Table 72.8** Sample Size Weights

| Gender         | Drug           |                |          |
|----------------|----------------|----------------|----------|
|                | Experimental 1 | Experimental 2 | Standard |
| <b>Males</b>   | 1              | 1              | 2        |
| <b>Females</b> | 1              | 1              | 2        |

If you have unequal cell sizes, you must enter relative sample size weights for the cells. Weights do not have to sum to 1 across the cells. Some weights can be zero, but enough weights must be greater than zero so that the effects and contrasts are estimable.

In this case, you want the sample size of the standard group to be twice that of each of the two experimental groups. Click **OK** to save the values and return to the Edit Properties page.

**Figure 72.73** Relative Sample Sizes Window

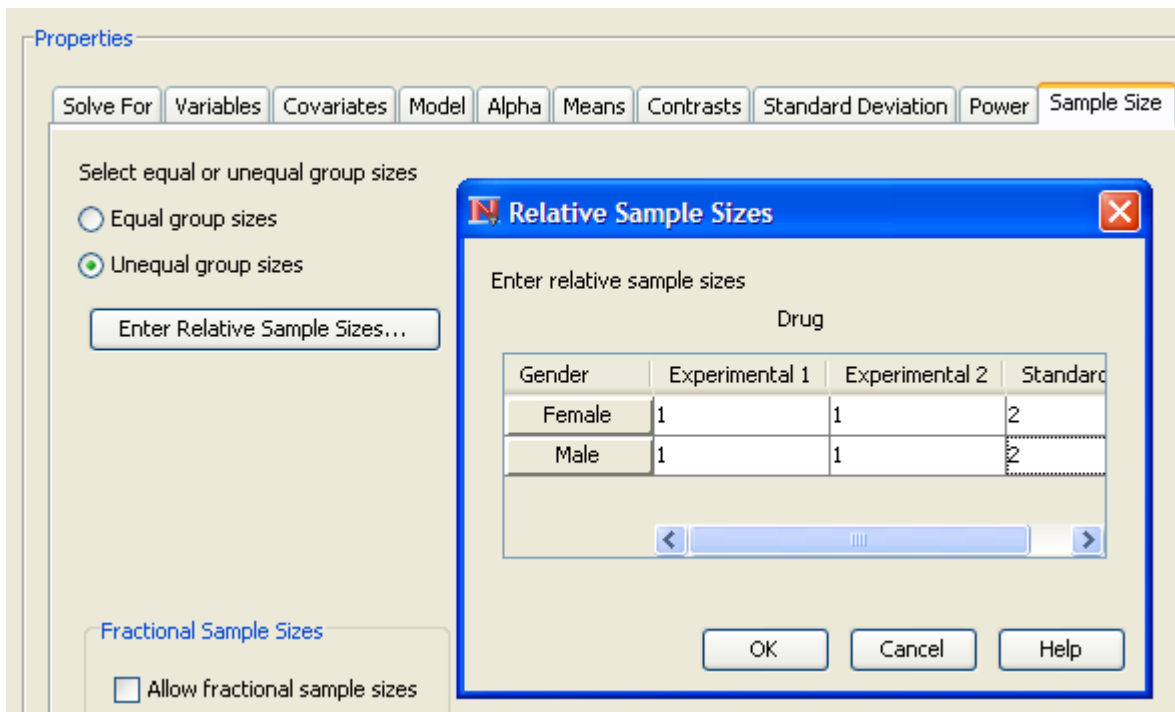


Figure 72.74 shows the summary table for the Drug by Gender example.

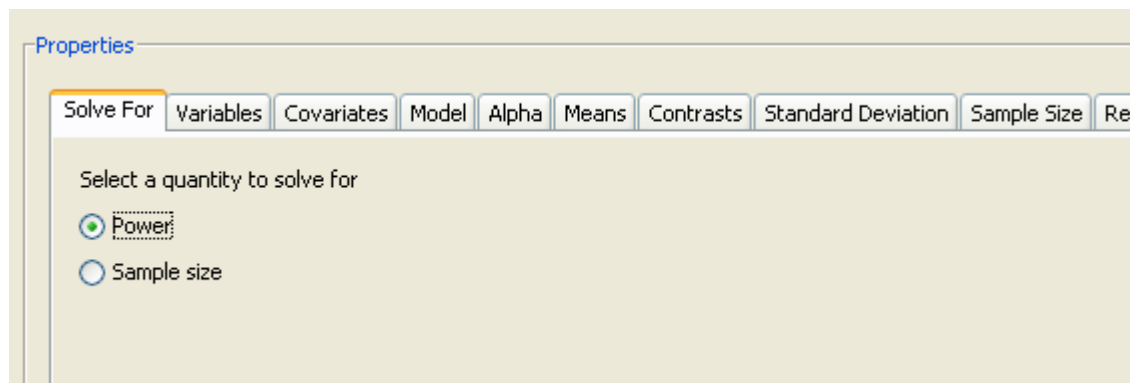
**Figure 72.74** Summary Table for Unbalanced Design Example

| Fixed Scenario Elements |          |                                    |         |         |          |              |         |  |
|-------------------------|----------|------------------------------------|---------|---------|----------|--------------|---------|--|
| Dependent Variable      |          | Blood pressure                     |         |         |          |              |         |  |
| Weight Variable         |          | _Weight_                           |         |         |          |              |         |  |
| Alpha                   |          | 0.05                               |         |         |          |              |         |  |
| Nominal Power           |          | 0.9                                |         |         |          |              |         |  |
| Computed N Total        |          |                                    |         |         |          |              |         |  |
| Index                   | Type     | Source                             | Std Dev | Test DF | Error DF | Actual Power | N Total |  |
| 1                       | Effect   | Drug                               | 5       | 2       | 52       | 0.910        | 56      |  |
| 2                       | Effect   | Drug                               | 7       | 2       | 100      | 0.902        | 104     |  |
| 3                       | Effect   | Gender                             | 5       | 1       | 28       | 0.944        | 32      |  |
| 4                       | Effect   | Gender                             | 7       | 1       | 52       | 0.926        | 56      |  |
| 5                       | Contrast | Experimental drugs versus standard | 5       | 1       | 52       | 0.911        | 56      |  |
| 6                       | Contrast | Experimental drugs versus standard | 7       | 1       | 100      | 0.901        | 104     |  |

## Solving for Power

In addition to solving for sample size, you can also solve for power. Figure 72.75 shows the two options. Click the **Solve For** tab to select the **Power** option.

**Figure 72.75** Solve For Tab with Power Option Selected



When solving for power, you must provide sample size information. For the general linear univariate model analysis, you provide this information by using one of two alternate forms. To choose the desired alternate form, select the desired form from the **Select a form** list box on the **Sample Size** tab. The alternate forms are:

**Sample size per cell**

Enter the sample size for a cell. Cell sizes are assumed to be equal. Sample size is reported in the summary table as total sample size.

**Total N, Cell weights**

Enter the total sample size and specify whether cell sizes are to be equal or unequal. Select the **Equal cell sizes** or **Unequal cell sizes** option. For unequal cell sizes, you also enter cell weights. Click the **Enter Relative Sample Sizes** button to display a window that is used to enter the data. For more information about using unequal cell sizes, see the section “[Using Unequal Cell Sizes](#)” on page 6217.

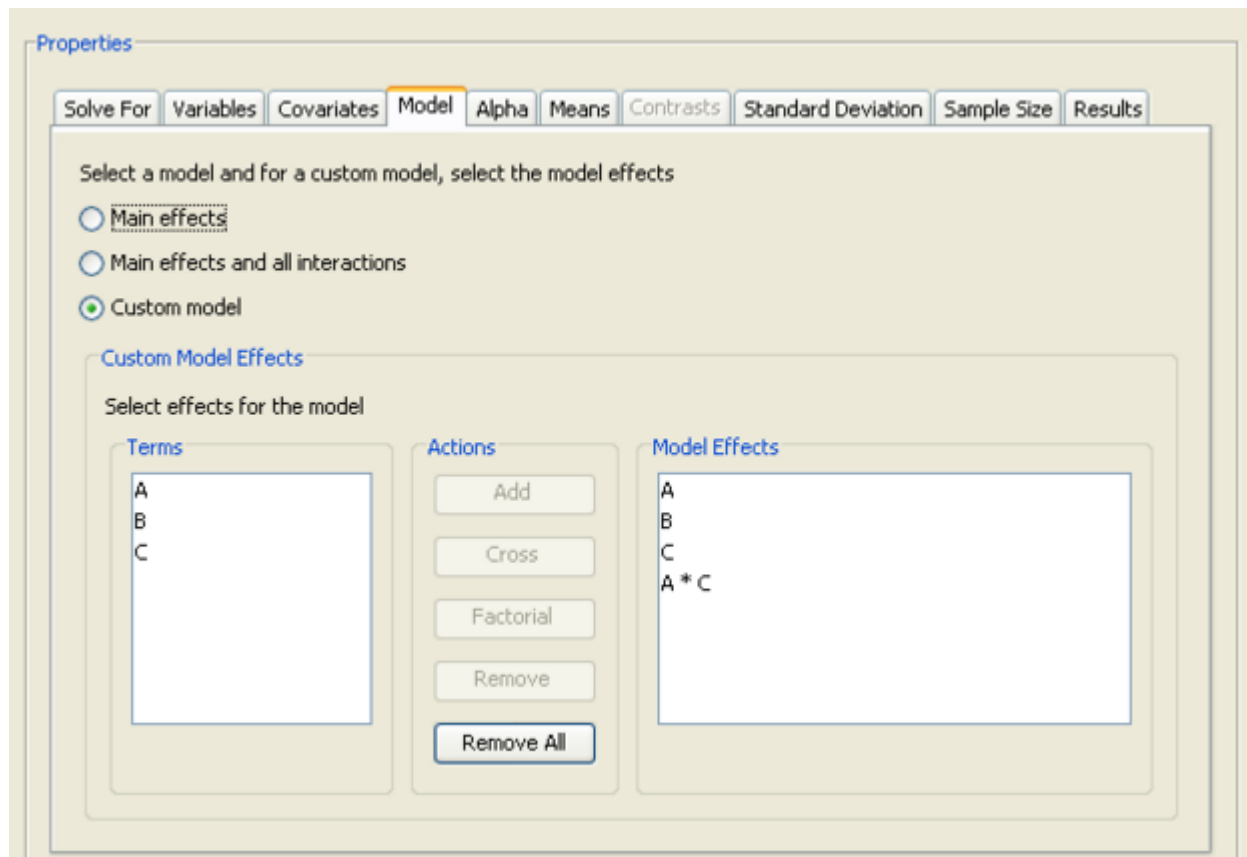
**Specifying a Custom Model**

Click the **Model** tab to select from three types of models: a **Main effects** model, a **Main effects and all interactions** model, and a **Custom model**.

To specify a custom model, select the **Custom model** option; then a model building facility is displayed.

The facility displays a list of the factors on the left. Construct the desired model using the **Add**, **Cross**, and **Factorial** buttons. The example shown in [Figure 72.76](#) has the three main effects and one of the four possible interactions.

Figure 72.76 Model Tab with Custom Model Builder Displayed



Add the three main effects (A, B, C) by selecting them in the **Terms** list and clicking the **Add** button. Add the  $A \times B$  interaction by selecting the A and B factors in the **Terms** list and clicking the **Cross** button.

To create the complete factorial design of several factors, select the factors in the **Terms** list, then click the **Factorial** button. All possible main effects and interactions are added to the **Model Effects** list.

To remove effects, select them in the **Model Effects** list and click the **Remove** button. Clicking the **Remove All** button removes all effects in the model.



## Including Covariates

Click the **Covariates** tab to enter covariate information.

**Figure 72.77** Covariates Tab with Proportional Reduction in Variance Form

The screenshot shows a software window titled "Properties" with several tabs: "Contrasts", "Standard Deviation", "Power", "Sample Size", and "Results". Below these are sub-tabs: "Solve For", "Variables", "Covariates", "Model", "Alpha", and "Means". The "Covariates" sub-tab is active. The main area contains the following text and controls:

- Covariates are optional.** Select the number of covariates
- Number of covariates: 4 (dropdown menu)
- Select a form: Proportional reduction in variance (dropdown menu) [Icon]
- Enter one or more proportional reduction in variance values
- A list box labeled "Reduction" containing the value 0.3, with up and down arrow buttons.
- Below the list box are two buttons labeled "Rows": one with a plus sign and one with a minus sign.

Figure 72.77 illustrates four covariates and a proportional reduction in variation of 0.3. The results for the analysis are not shown.

Covariates are optional. If you have covariates, include the total number of degrees of freedom for all covariates. To do this, add the number of continuous covariates and the sum of the degrees of freedom of the classification covariates, and enter this total in the **Number of Covariates** list box. For example, with two continuous covariates and a single classification covariate factor with three levels, the total would be  $2 + (3 - 1) = 4$ .

Also, you must enter the correlation between the dependent variable and the set of covariates. Two alternate forms are available: **Multiple correlation** and **Proportional reduction in variance**. Select the desired form and enter one or more values.

The multiple correlation is between the set of covariates and the dependent variable. Proportional reduction in variation is how much the variance of the dependent variable is reduced by the inclusion of the covariates, expressed as a proportion between 0 and 1.

---

## Example: Two-Sample Survival Rank Tests

---

### Overview

Survival analysis often involves the comparison of survival curves. PSS provides sample size and power calculations for two-sample survival rank analyses. Several rank tests are available: Gehan, log-rank, and Tarone-Ware. There are also several ways to specify the survival functions. For more information about power and sample size analysis for survival rank tests, see Chapter 71, “The POWER Procedure.”

---

### The Example

Suppose you want to compare survival rates for an existing cancer treatment and a new treatment. You intend to use a log-rank test to compare the overall survival curves for the two treatments. You want to determine a sample size to achieve a power of 0.8 for a two-sided test using a balanced design, with a significance level of 0.05.

The survival curve of patients for the existing treatment is known to be approximately exponential with a median survival time of five years. You think that the proposed treatment will yield a survival curve described by the times and probabilities listed in Table 72.9. Patients are to be accrued uniformly over two years and followed for three years.

**Table 72.9** Survival Probabilities for Proposed Treatment

| Time | Probability |
|------|-------------|
| 1    | 0.95        |
| 2    | 0.90        |
| 3    | 0.75        |
| 4    | 0.70        |
| 5    | 0.60        |

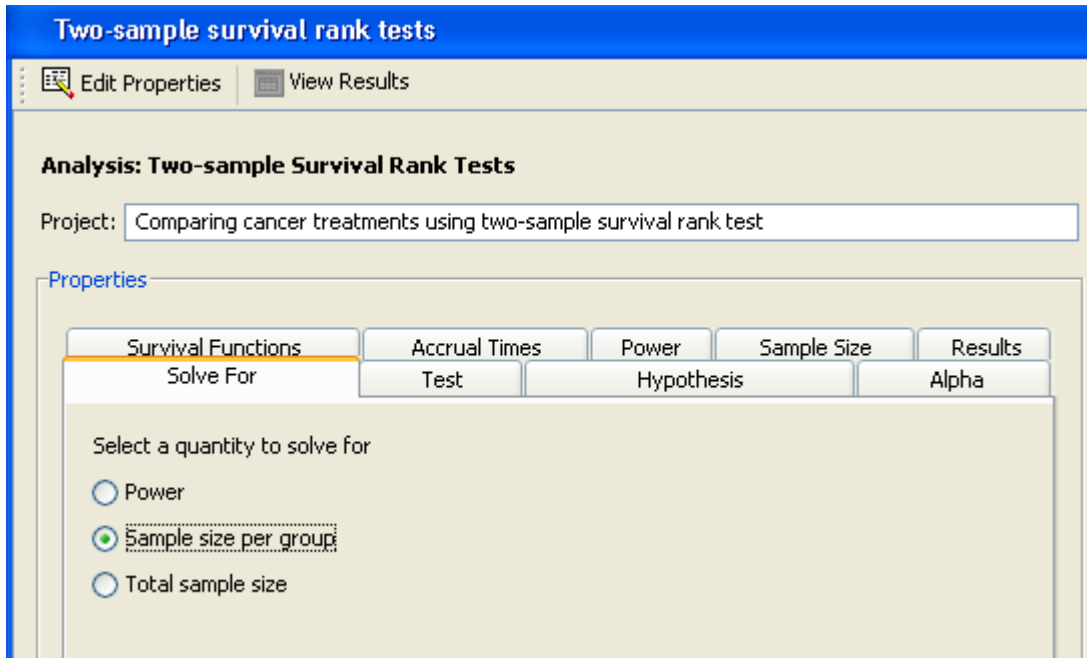
To create a new survival analysis project, select **File►New**. Then, under the **Survival Analysis** section, select **Two-sample survival rank tests** and click **OK**. The **Two-sample survival rank tests** project appears with the Edit Properties page displayed.

## Editing Properties

### Project Description

For the example, change the project description to `Comparing cancer treatments using two-sample survival rank test`.

**Figure 72.78** Project Description and Solve For Tab



### Solve For

Click the **Solve For** tab to select the quantity to solve for. For this example, select the **Sample size per group** option, as shown in Figure 72.78. For information about calculating total sample size, see the section “Solving for Sample Size” on page 6204.

In this analysis you can solve for power, sample size per group, or total sample size.

### Test

Click the **Test** tab to select a rank test. For this example, select the **Log-rank** option, as shown in Figure 72.79.

Figure 72.79 Test Tab

**Analysis: Two-sample Survival Rank Tests**

Project:

Properties

|                    |               |            |             |         |
|--------------------|---------------|------------|-------------|---------|
| Survival Functions | Accrual Times | Power      | Sample Size | Results |
| Solve For          | Test          | Hypothesis |             | Alpha   |

Select a test

Gehan rank

Log-rank

Tarone-Ware rank

Several rank tests are available: Gehan, log-rank, and Tarone-Ware. The Gehan test is most sensitive to survival differences near the beginning of the study period, the log-rank test is uniformly sensitive throughout the study period, and the Tarone-Ware test is somewhere in between.

### Hypothesis

Click the **Hypothesis** tab to select a one- or two-sided test. For the example, select the **Two-sided test** option, as shown in Figure 72.80.

Figure 72.80 Hypothesis Tab

**Analysis: Two-sample Survival Rank Tests**

Project:

Properties

|                    |               |            |             |         |
|--------------------|---------------|------------|-------------|---------|
| Survival Functions | Accrual Times | Power      | Sample Size | Results |
| Solve For          | Test          | Hypothesis |             | Alpha   |

Select a one or two-sided hypothesis test

One-sided test       Lower one-sided test

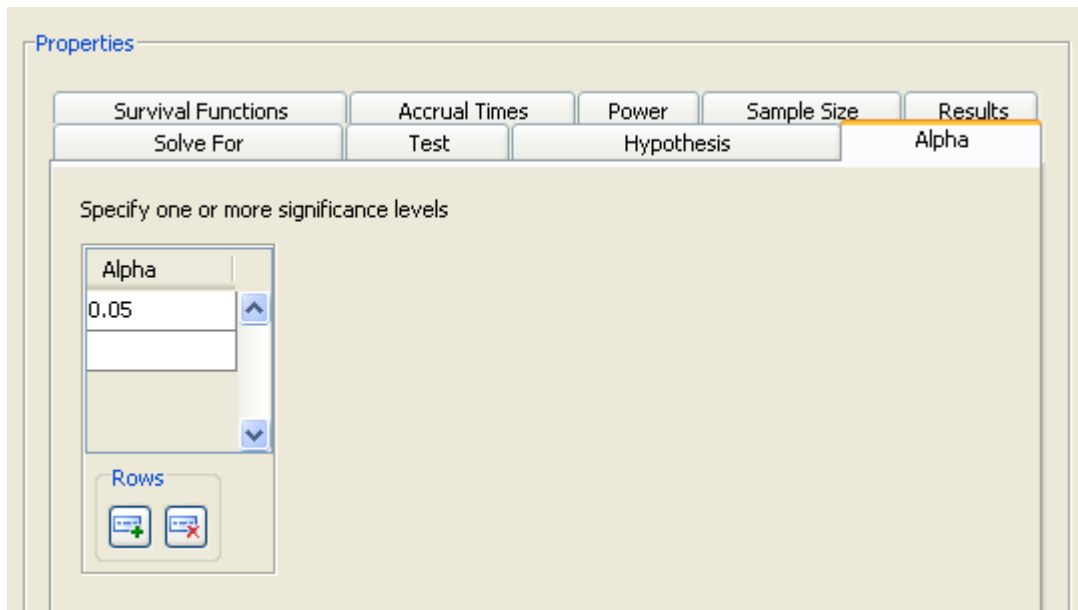
Two-sided test       Upper one-sided test

You can choose either a one- or two-sided test. For the one-sided test, the alternative hypothesis is assumed to be in the same direction as the effect. If you do not know the direction of the effect (that is, whether it is positive or negative), the two-sided test is appropriate. If you know the effect's direction, the one-sided test is appropriate. If you specify a one-sided test and the effect is in the unexpected direction, the results of the analysis are invalid.

### Alpha

Click the **Alpha** tab to enter one or more values for the significance level. For the example, enter the desired significance level of 0.05 in the first cell of the Alpha table, as shown in [Figure 72.81](#), if it is not already the default value.

**Figure 72.81** Alpha Tab



The significance level is the probability of falsely rejecting the null hypothesis. If you frequently use the same values for alpha, set them as the defaults in the Preferences window.

### Survival Functions

Click the **Survival Functions** tab to select the input form for the survival functions.

**Figure 72.82** Survival Functions Tab with Number of Curves

The screenshot shows the 'Properties' dialog box with the 'Survival Functions' tab selected. At the top, there are four tabs: 'Solve For', 'Test', 'Hypothesis', and 'Alpha'. Under 'Solve For', 'Survival Functions' is selected. Below this, there are four sub-tabs: 'Accrual Times', 'Power', 'Sample Size', and 'Results'. The main area contains a 'Select a form:' dropdown set to 'Survival curves' and a 'Select the number of curves; specify times and probabilities for each curve' instruction. On the left, under 'Curves', 'Number of survival curves:' is set to 2, and a list shows 'Function 1' and 'Function 2'. On the right, under 'Define Curve', 'Label:' is 'Function 1' and 'Group:' has radio buttons for 1 (selected) and 2. Below this is a table with columns 'Time' and 'Probability' and two empty rows. At the bottom right, there are 'Rows' controls with '+' and '-' buttons.

Examine the input alternatives available in the **Select a form** list. There are four alternate forms for entering survival functions. The first three apply only to exponential curves; the fourth applies to both piecewise linear and exponential curves.

#### **Group median survival times**

Enter median survival times for the two groups.

#### **Group hazards**

Enter hazards for the two groups.

#### **Hazards, Hazard ratios**

Enter hazards for the reference group and hazard ratios.

#### **Survival curves**

Enter survival probabilities and their associated times for each of several curves. Select or enter the number of curves from the drop-down list; at least two curves are required. Then, for each curve, select it in the left-hand list, select the Group 1 or Group 2 option, and then define the survival curve by entering pairs of times and probabilities. Enter a time and probability pair only if the probability is less than that of the previous pair.

For information about using the other forms, see the section “[Using the Other Survival Curve Forms](#)” on page 6236.

For each survival curve, select the curve in the left-hand list. Then, enter a descriptive label and select which group it is for. The labels should be unique. Finally, enter pairs of survival times and probabilities.

When you enter probabilities, enter a time and probability pair only when the probability for a survival curve changes. For example, if the probability for curve 1 at time 1 and 2 is 0.9 and at time 3 is 0.8, enter 0.9 for time 1 and 0.8 for time 3.

To specify an exponential survival curve, enter a single time and probability pair. In the example, the exponential curve for the existing treatment is defined by a probability of 0.5 at time 5.

The units of time for the survival curves must correspond to the units for the accrual, follow-up, and total times, which are described in the section “[Accrual Times](#)” on page 6229.

You can also compare several survival curves. For example, if you have two scenarios, A and B, for group 1’s curve and two scenarios, C and D, for group 2’s curve, then specify probabilities for the four curves and assign A and B to group 1 and C and D to group 2.

For the example, select the **Survival curves** form, as shown in [Figure 72.82](#). Enter the value, 2, in the **Number of survival curves** list box.

For the example enter the following values:

- For the first survival curve, enter a label of `Existing treatment` and select the **Group 1** option. For the first curve, enter a time of 5 and a probability of 0.5. [Figure 72.83](#) shows the resulting values.

**Figure 72.83** Survival Times and Probabilities for Curve 1

The screenshot shows the 'Properties' dialog box with the following configuration:

- Solve For:** Survival Functions
- Test:** Accrual Times
- Hypothesis:** Power
- Alpha:** Sample Size
- Results:** Results
- Select a form:** Survival curves
- Select the number of curves; specify times and probabilities for each curve:**
  - Curves:** Number of survival curves: 2
  - Define Curve:**
    - Label:** Existing treatment
    - Group:** 1 (selected)
    - Table:**

| Time | Probability |
|------|-------------|
| 5    | 0.5         |
|      |             |
|      |             |

- For the second curve select `Function 2` in the selection list on the left side of the tab. Enter a label of `Proposed treatment` and select the **Group 2** option. Then, enter time values of 1 through 5 and


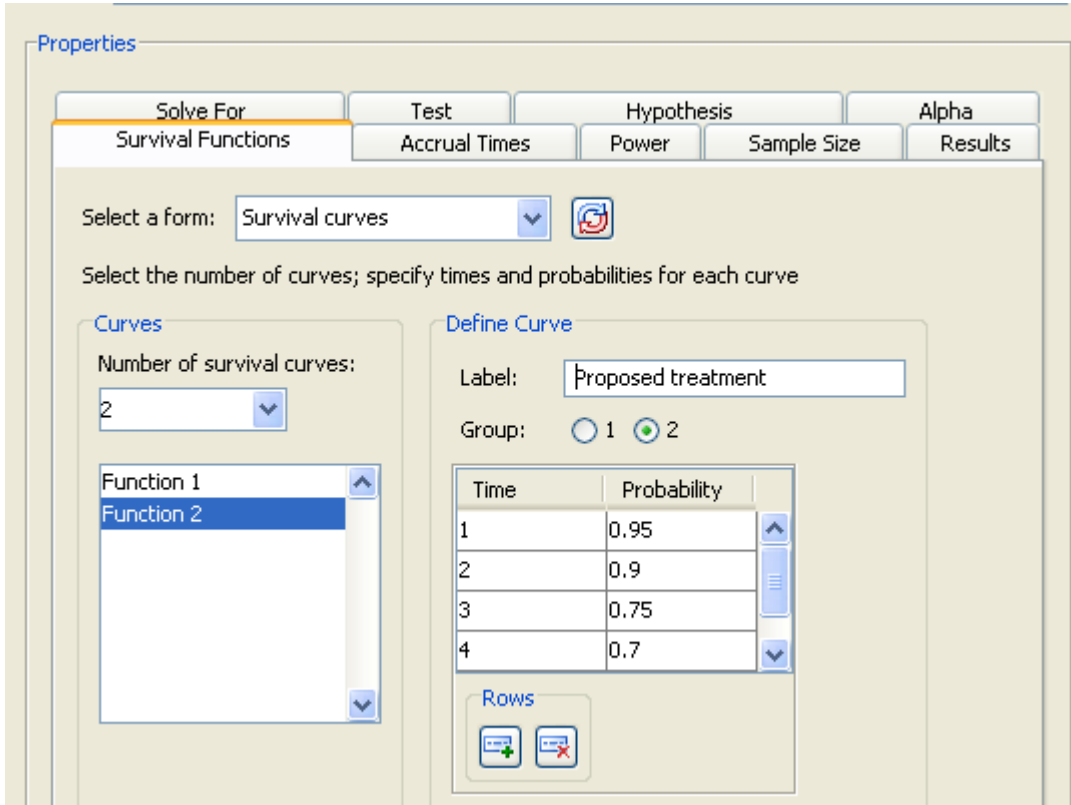
the corresponding probabilities of 0.95, 0.9, 0.75, 0.7, and 0.6. To add rows to the table, click the  button beneath the table.


Figure 72.84 shows these values; the last row of the time and probability table is not displayed.

**Figure 72.84** Survival Times and Probabilities for Curve 2



Properties

Solve For: Survival Functions | Test: Accrual Times | Hypothesis: Power | Alpha: Sample Size | Results

Select a form: Survival curves 

Select the number of curves; specify times and probabilities for each curve

**Curves**

Number of survival curves: 2



Function 1  
Function 2

**Define Curve**

Label: Proposed treatment

Group:  1  2

| Time | Probability |
|------|-------------|
| 1    | 0.95        |
| 2    | 0.9         |
| 3    | 0.75        |
| 4    | 0.7         |

Rows  

### **Accrual Times**

Click the **Accrual times** tab to select an input form for accrual times and to enter the times.



Figure 72.85 Accrual Times Tab

Examine the alternatives available in the **Select a form** list.

Accrual time is the period during which subjects are brought into the study. Follow-up time is the period during which subjects are observed after all subjects have been included in the study. Total time is the sum of accrual and follow-up time. The units of time for the accrual, follow-up, and total times must correspond to the units you used specified for the survival curves.

When you enter survival curves, the sum of the accrual and follow-up times must be less than the largest time for each survival curve. This does not apply to survival curves represented by a single time, which represent exponential curves.

On the **Accrual Times** tab, there are three alternate forms for entering accrual and follow-up times:

**Accrual times, Follow-up times**

Enter accrual and follow-up times.

**Accrual times, Total times**

Enter accrual and total times.

**Follow-up times, Total times**

Enter follow-up and total times.

For the example, select the **Accrual times, Follow-up times** form. Then enter a single value of 2 in the Accrual table and a value of 3 in the Follow-up table, as shown in Figure 72.85.

**Power**

Click the **Power** tab to enter one or more power values. For the example, enter a single value of 0.8.

When you calculate sample size, it is necessary to specify one or more powers.

**Summary of Input Parameters**

Table 72.10 contains the values of the input parameters for the example.

**Table 72.10** Summary of Input Parameters

| Parameter                        | Value                           |
|----------------------------------|---------------------------------|
| Solve for                        | Sample size per group           |
| Test                             | Log-rank                        |
| Hypothesis                       | Two-sided test                  |
| Alpha                            | 0.05                            |
| Survival function form           | Survival curves                 |
| Survival curves                  | See Table 72.11 and Table 72.12 |
| Accrual and follow-up times form | Accrual time, Follow-up times   |
| Accrual times                    | 2                               |
| Follow-up times                  | 3                               |
| Power                            | 0.8                             |

Table 72.11 and Table 72.12 contain times and probabilities for the two survival curves, respectively.

**Table 72.11** Survival Times and Probabilities for Existing Treatment (Survival Curve 1)

| Time | Probability |
|------|-------------|
| 5    | 0.5         |

**Table 72.12** Survival Times and Probabilities for Proposed Treatment (Survival Curve 2)

| Time | Probability |
|------|-------------|
| 1    | 0.95        |
| 2    | 0.90        |
| 3    | 0.75        |
| 4    | 0.70        |
| 5    | 0.60        |

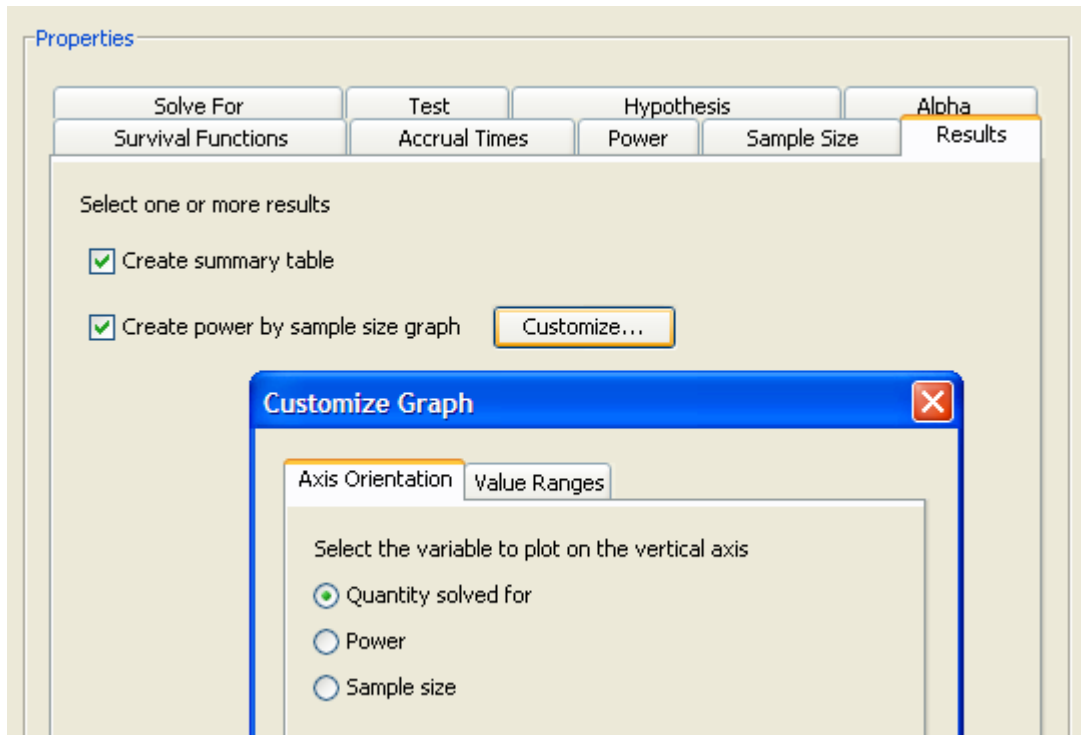
**Result Options**

Click the **Results** tab to specify the desired result options. For the example, request both results by selecting both the **Create summary table** and **Create power by sample size graph** check boxes.

Specifying only one power (as in this example) produces a graph with a single point. You might be interested in a plot of sample sizes for a range of powers—say, between 0.75 and 0.85. You can customize the graph by specifying the values for the power axis. Also, you might want to change the appearance of the graph to have sample size (per group) on the vertical axis and power on the horizontal axis.

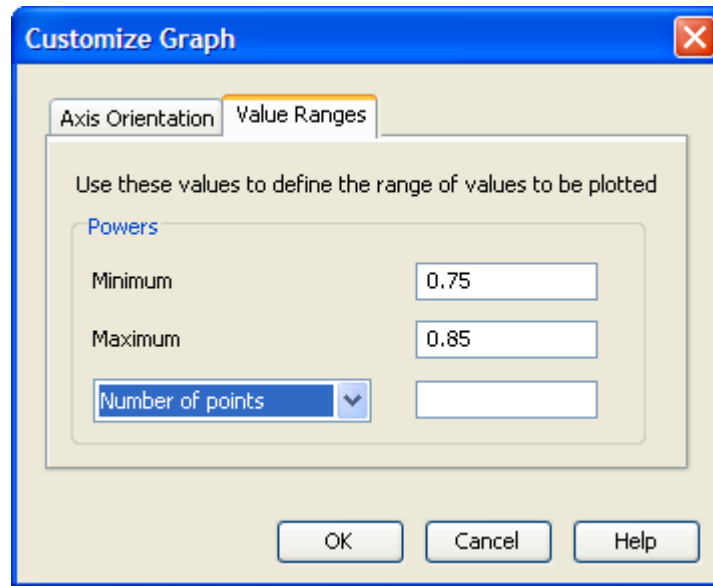
Click the **Customize** button beside the **Create power by sample size graph** check box to customize the graph. The Customize Graph window is displayed, as shown in [Figure 72.86](#).

**Figure 72.86** Customize Graph Window with Axis Orientation Tab



Click the **Axis Orientation** tab to select which variable to plot on the vertical axis. For the example, select the **Quantity solved for** option, as shown in [Figure 72.86](#). This option plots sample size on the vertical axis and power on the horizontal axis. You could also have chosen the **Sample size** option.

Click the **Value Ranges** tab to enter minimum and maximum values for a plot axis. For the example, enter a minimum of 0.75 and a maximum of 0.85 in the Powers text boxes. This sets the range of values on the axis for powers. The completed Value Ranges tab of the window is displayed in [Figure 72.87](#). You can set the axis values only for the quantity that is not being solved for.

**Figure 72.87** Customize Graph Window with Value Ranges Tab

Click **OK** to save the values that you have entered and return to the Edit Properties page.

Then, click **Calculate** to perform the analysis. If there are no errors in the input parameter values, the View Results page appears. If there are errors in the input parameter values, you are prompted to correct them.

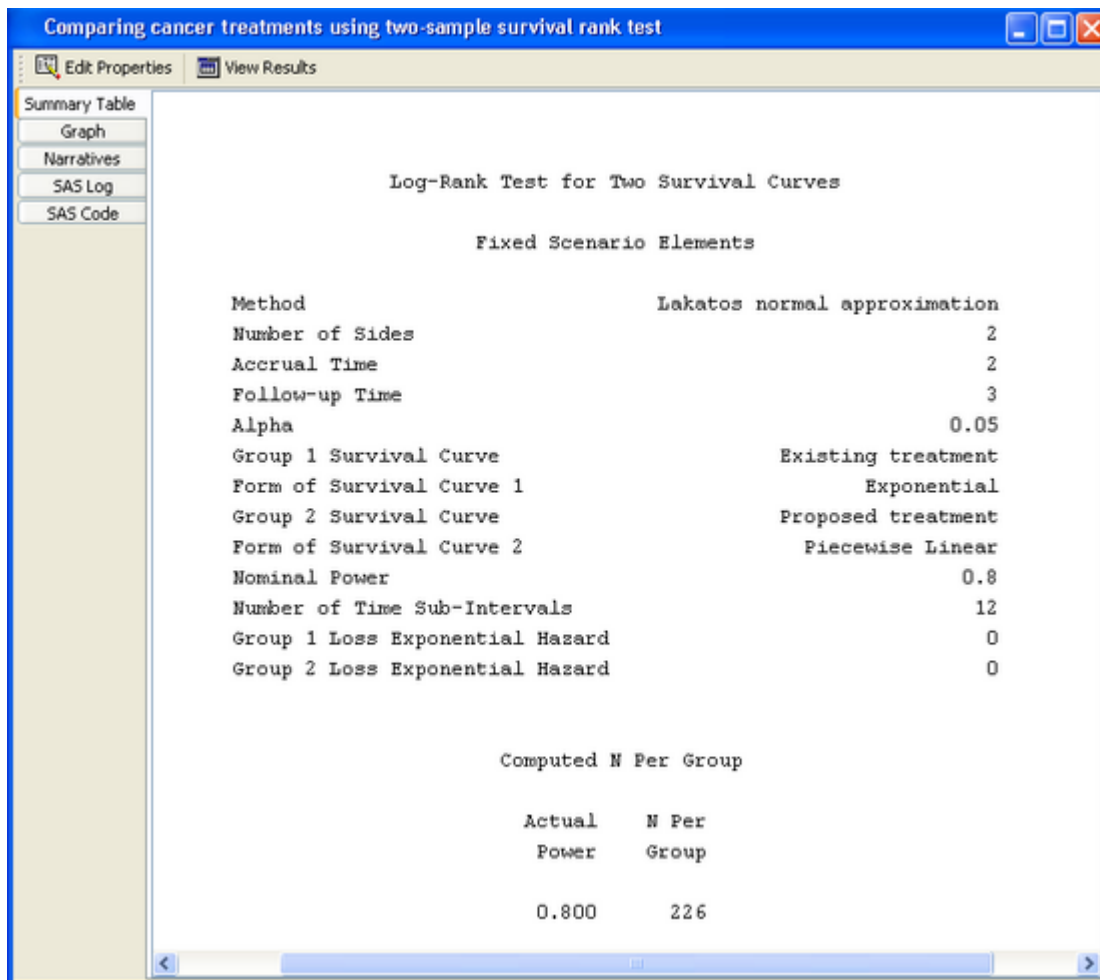
## Viewing Results

The results appear in separate tabs on the View Results page of the project. Select the tab of each result that you want to view.

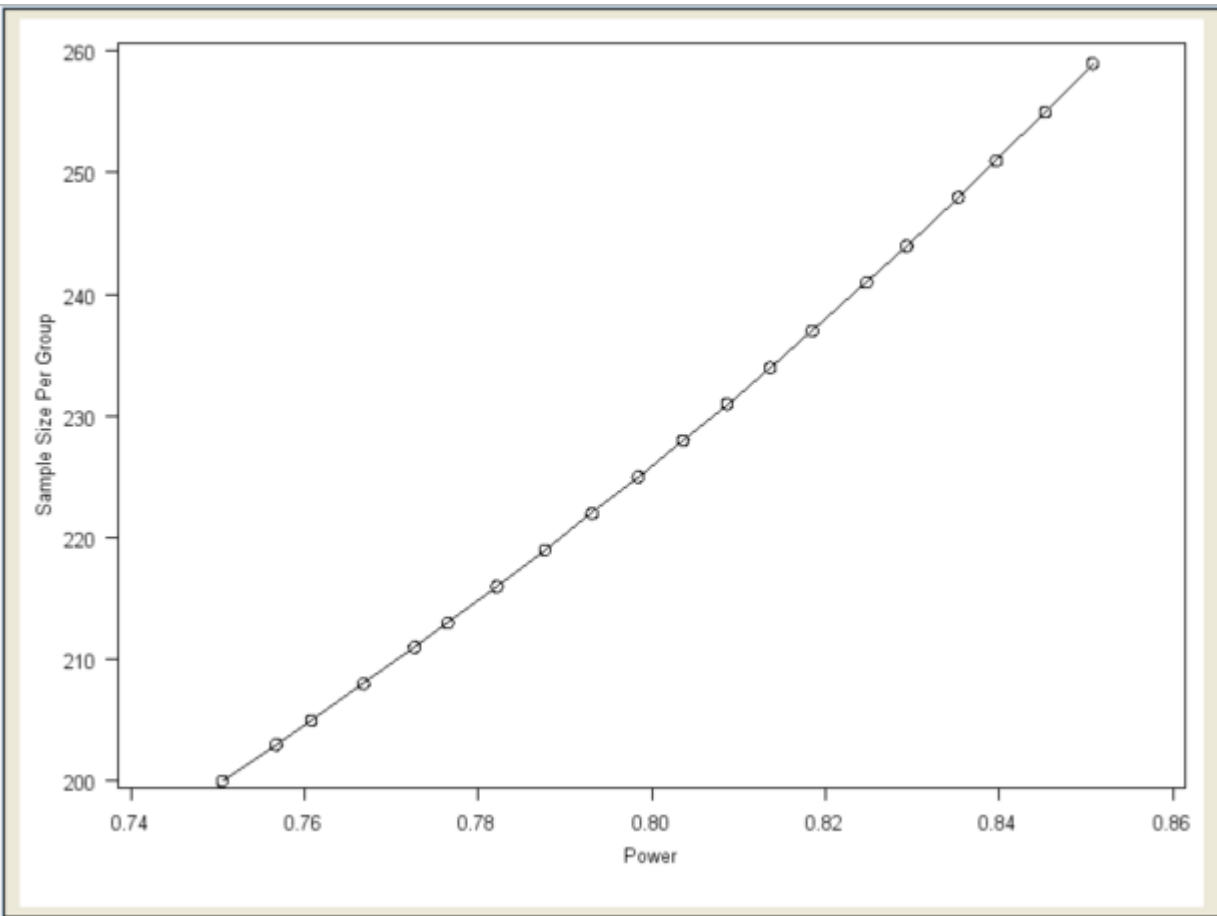
### **Summary Table**

Click the **Summary Table** tab to view the summary table. It is composed of two subtables. As shown in [Figure 72.88](#), the *Fixed Scenario Elements* and *Computed N Per Group* tables include the values of the input parameters and the computed quantity (in this case, sample size per group, *N per group*). The sample size per group for the single requested scenario is 226.

Figure 72.88 Summary Table

**Power by Sample Size Graph**

Click the **Graph** tab to view the power by sample size graph.

**Figure 72.89** Power by Sample Size Graph

As you can see in [Figure 72.89](#), the graph is curved slightly upward with larger powers associated with larger sample sizes. Sample size is plotted on the vertical axis as requested in the Customize Graph window.

### **Narratives**

Click the **Narratives** tab to create one or more narratives. To generate a narrative, select the single scenario in the narrative selector table at the bottom of the tab. The narrative for this task does not include the survival times and probabilities for the survival curves:

For a log-rank test comparing two survival curves with a two-sided significance level of 0.05, assuming uniform accrual with an accrual time of 2 and a follow-up time of 3, a sample size of 226 per group is required to obtain a power of at least 0.8 for the exponential curve, “Existing treatment,” and the piecewise linear curve, “Proposed treatment.” The actual power is 0.800.

For information about selecting additional narratives when multiple scenarios are present, see the section “[Creating Narratives](#)” on page 6179.

## Additional Topics

### Using the Other Survival Curve Forms

Survival functions can be specified as median survival times, hazards, or a combination of hazards for one group and hazard ratios. These all assume exponential curves.

Suppose you are interested in comparing the proposed and existing treatments using their median survival times. The survival times are five years and four years for the two groups, respectively.

**Figure 72.90** Median Survival Times and List of Alternate Forms

The screenshot shows a software interface with a 'Properties' window. At the top, there are several tabs: 'Solve For', 'Test', 'Hypothesis', and 'Alpha'. Under 'Solve For', there are sub-tabs: 'Survival Functions', 'Accrual Times', 'Power', 'Sample Size', and 'Results'. The 'Survival Functions' tab is active. Below the tabs, there is a 'Select a form:' dropdown menu with 'Group median survival times' selected. To the right of the dropdown is a circular icon with a red 'X'. Below this, the text 'Enter one or more rows of median survival times' is displayed. A table with two columns, 'Group 1' and 'Group 2', is shown. The first row contains the values '5' and '4'. Below the table, there is a 'Rows' section with two icons: a green plus sign and a red minus sign.

| Group 1 | Group 2 |
|---------|---------|
| 5       | 4       |
|         |         |

Click the **Survival Functions** tab and examine the list of alternate forms available in the **Select a form:** list. For this example, select the **Group median survival times** option.

For the example, enter 5 and 4 in the first row of the table. The completed table is shown in [Figure 72.90](#).

You can enter one or more sets of two median survival times. The results of the analysis are not shown.

# Chapter 73

## The PRINCOMP Procedure

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## Overview: PRINCOMP Procedure

The PRINCOMP procedure performs principal component analysis. As input you can use raw data, a correlation matrix, a covariance matrix, or a sum-of-squares-and-crossproducts (SSCP) matrix. You can create output data sets containing eigenvalues, eigenvectors, and standardized or unstandardized principal component scores.

Principal component analysis is a multivariate technique for examining relationships among several quantitative variables. The choice between using factor analysis and using principal component analysis depends in part on your research objectives. You should use the PRINCOMP procedure if you are interested in summarizing data and detecting linear relationships. You can use principal components to reduce the number of



variables in regression, clustering, and so on. See Chapter 9, “Introduction to Multivariate Procedures,” for a detailed comparison of the PRINCOMP and FACTOR procedures.

You can use ODS Graphics to display the scree plot, component pattern plot, component pattern profile plot, matrix plot of component scores, and component score plots. These plots are especially valuable tools in exploratory data analysis.

Principal component analysis was originated by Pearson (1901) and later developed by Hotelling (1933). The application of principal components is discussed by Rao (1964); Cooley and Lohnes (1971); Gnanadesikan (1977). Excellent statistical treatments of principal components are found in Kshirsagar (1972); Morrison (1976); Mardia, Kent, and Bibby (1979).

Given a data set with  $p$  numeric variables, you can compute  $p$  principal components. Each principal component is a linear combination of the original variables, with coefficients equal to the eigenvectors of the correlation or covariance matrix. The eigenvectors are customarily taken with unit length. The principal components are sorted by descending order of the eigenvalues, which are equal to the variances of the components.

Principal components have a variety of useful properties (Rao 1964; Kshirsagar 1972):

- The eigenvectors are orthogonal, so the principal components represent jointly perpendicular directions through the space of the original variables.
- The principal component scores are jointly uncorrelated. Note that this property is quite distinct from the previous one.
- The first principal component has the largest variance of any unit-length linear combination of the observed variables. The  $j$ th principal component has the largest variance of any unit-length linear combination orthogonal to the first  $j - 1$  principal components. The last principal component has the smallest variance of any linear combination of the original variables.
- The scores on the first  $j$  principal components have the highest possible generalized variance of any set of unit-length linear combinations of the original variables.
- The first  $j$  principal components provide a least squares solution to the model

$$\mathbf{Y} = \mathbf{XB} + \mathbf{E}$$

where  $\mathbf{Y}$  is an  $n \times p$  matrix of the centered observed variables;  $\mathbf{X}$  is the  $n \times j$  matrix of scores on the first  $j$  principal components;  $\mathbf{B}$  is the  $j \times p$  matrix of eigenvectors;  $\mathbf{E}$  is an  $n \times p$  matrix of residuals; and you want to minimize  $\text{trace}(\mathbf{E}'\mathbf{E})$ , the sum of all the squared elements in  $\mathbf{E}$ . In other words, the first  $j$  principal components are the best linear predictors of the original variables among all possible sets of  $j$  variables, although any nonsingular linear transformation of the first  $j$  principal components would provide equally good prediction. The same result is obtained if you want to minimize the determinant or the Euclidean (Schur, Frobenius) norm of  $\mathbf{E}'\mathbf{E}$  rather than the trace.

- In geometric terms, the  $j$ -dimensional linear subspace spanned by the first  $j$  principal components provides the best possible fit to the data points as measured by the sum of squared perpendicular distances from each data point to the subspace. This is in contrast to the geometric interpretation of least squares regression, which minimizes the sum of squared vertical distances. For example, suppose you have two variables. Then, the first principal component minimizes the sum of squared perpendicular distances from the points to the first principal axis. This is in contrast to least squares, which would minimize the sum of squared vertical distances from the points to the fitted line.

Principal component analysis can also be used for exploring polynomial relationships and for multivariate outlier detection (Gnanadesikan 1977), and it is related to factor analysis, correspondence analysis, allometry, and biased regression techniques (Mardia, Kent, and Bibby 1979).

## Getting Started: PRINCOMP Procedure

The following data provide crime rates per 100,000 people in seven categories for each of the 50 states in 1977. Since there are seven numeric variables, it is impossible to plot all the variables simultaneously. Principal components can be used to summarize the data in two or three dimensions, and they help to visualize the data. The following statements produce [Figure 73.1](#) through [Figure 73.5](#).

```

title 'Crime Rates per 100,000 Population by State';

data Crime;
 input State $1-15 Murder Rape Robbery Assault
 Burglary Larceny Auto_Theft;
 datalines;
Alabama 14.2 25.2 96.8 278.3 1135.5 1881.9 280.7
Alaska 10.8 51.6 96.8 284.0 1331.7 3369.8 753.3
Arizona 9.5 34.2 138.2 312.3 2346.1 4467.4 439.5
Arkansas 8.8 27.6 83.2 203.4 972.6 1862.1 183.4
California 11.5 49.4 287.0 358.0 2139.4 3499.8 663.5
Colorado 6.3 42.0 170.7 292.9 1935.2 3903.2 477.1
Connecticut 4.2 16.8 129.5 131.8 1346.0 2620.7 593.2
Delaware 6.0 24.9 157.0 194.2 1682.6 3678.4 467.0
Florida 10.2 39.6 187.9 449.1 1859.9 3840.5 351.4
Georgia 11.7 31.1 140.5 256.5 1351.1 2170.2 297.9
Hawaii 7.2 25.5 128.0 64.1 1911.5 3920.4 489.4
Idaho 5.5 19.4 39.6 172.5 1050.8 2599.6 237.6
Illinois 9.9 21.8 211.3 209.0 1085.0 2828.5 528.6
Indiana 7.4 26.5 123.2 153.5 1086.2 2498.7 377.4
Iowa 2.3 10.6 41.2 89.8 812.5 2685.1 219.9
Kansas 6.6 22.0 100.7 180.5 1270.4 2739.3 244.3
Kentucky 10.1 19.1 81.1 123.3 872.2 1662.1 245.4
Louisiana 15.5 30.9 142.9 335.5 1165.5 2469.9 337.7
Maine 2.4 13.5 38.7 170.0 1253.1 2350.7 246.9
Maryland 8.0 34.8 292.1 358.9 1400.0 3177.7 428.5
Massachusetts 3.1 20.8 169.1 231.6 1532.2 2311.3 1140.1
Michigan 9.3 38.9 261.9 274.6 1522.7 3159.0 545.5
Minnesota 2.7 19.5 85.9 85.8 1134.7 2559.3 343.1
Mississippi 14.3 19.6 65.7 189.1 915.6 1239.9 144.4
Missouri 9.6 28.3 189.0 233.5 1318.3 2424.2 378.4
Montana 5.4 16.7 39.2 156.8 804.9 2773.2 309.2
Nebraska 3.9 18.1 64.7 112.7 760.0 2316.1 249.1
Nevada 15.8 49.1 323.1 355.0 2453.1 4212.6 559.2
New Hampshire 3.2 10.7 23.2 76.0 1041.7 2343.9 293.4
New Jersey 5.6 21.0 180.4 185.1 1435.8 2774.5 511.5
New Mexico 8.8 39.1 109.6 343.4 1418.7 3008.6 259.5
New York 10.7 29.4 472.6 319.1 1728.0 2782.0 745.8
North Carolina 10.6 17.0 61.3 318.3 1154.1 2037.8 192.1

```

```

North Dakota 0.9 9.0 13.3 43.8 446.1 1843.0 144.7
Ohio 7.8 27.3 190.5 181.1 1216.0 2696.8 400.4
Oklahoma 8.6 29.2 73.8 205.0 1288.2 2228.1 326.8
Oregon 4.9 39.9 124.1 286.9 1636.4 3506.1 388.9
Pennsylvania 5.6 19.0 130.3 128.0 877.5 1624.1 333.2
Rhode Island 3.6 10.5 86.5 201.0 1489.5 2844.1 791.4
South Carolina 11.9 33.0 105.9 485.3 1613.6 2342.4 245.1
South Dakota 2.0 13.5 17.9 155.7 570.5 1704.4 147.5
Tennessee 10.1 29.7 145.8 203.9 1259.7 1776.5 314.0
Texas 13.3 33.8 152.4 208.2 1603.1 2988.7 397.6
Utah 3.5 20.3 68.8 147.3 1171.6 3004.6 334.5
Vermont 1.4 15.9 30.8 101.2 1348.2 2201.0 265.2
Virginia 9.0 23.3 92.1 165.7 986.2 2521.2 226.7
Washington 4.3 39.6 106.2 224.8 1605.6 3386.9 360.3
West Virginia 6.0 13.2 42.2 90.9 597.4 1341.7 163.3
Wisconsin 2.8 12.9 52.2 63.7 846.9 2614.2 220.7
Wyoming 5.4 21.9 39.7 173.9 811.6 2772.2 282.0
;

```

```
ods graphics on;
```

```
proc princomp out=Crime_Components plots= score(ellipse ncomp=3);
 id State;
run;
```

Figure 73.1 displays the PROC PRINCOMP output, beginning with simple statistics followed by the correlation matrix. The PROC PRINCOMP statement requests by default principal components computed from the correlation matrix, so the total variance is equal to the number of variables, 7.

**Figure 73.1** Number of Observations and Simple Statistics from the PRINCOMP Procedure

| Crime Rates per 100,000 Population by State |              |              |             |             |
|---------------------------------------------|--------------|--------------|-------------|-------------|
| The PRINCOMP Procedure                      |              |              |             |             |
|                                             | Observations | 50           |             |             |
|                                             | Variables    | 7            |             |             |
| Simple Statistics                           |              |              |             |             |
|                                             | Murder       | Rape         | Robbery     | Assault     |
| Mean                                        | 7.444000000  | 25.734000000 | 124.0920000 | 211.3000000 |
| StD                                         | 3.866768941  | 10.75962995  | 88.3485672  | 100.2530492 |
| Simple Statistics                           |              |              |             |             |
|                                             | Burglary     | Larceny      | Auto_Theft  |             |
| Mean                                        | 1291.904000  | 2671.288000  | 377.5260000 |             |
| StD                                         | 432.455711   | 725.908707   | 193.3944175 |             |

Figure 73.1 continued

| Correlation Matrix |        |        |         |         |          |         |            |
|--------------------|--------|--------|---------|---------|----------|---------|------------|
|                    | Murder | Rape   | Robbery | Assault | Burglary | Larceny | Auto_Theft |
| Murder             | 1.0000 | 0.6012 | 0.4837  | 0.6486  | 0.3858   | 0.1019  | 0.0688     |
| Rape               | 0.6012 | 1.0000 | 0.5919  | 0.7403  | 0.7121   | 0.6140  | 0.3489     |
| Robbery            | 0.4837 | 0.5919 | 1.0000  | 0.5571  | 0.6372   | 0.4467  | 0.5907     |
| Assault            | 0.6486 | 0.7403 | 0.5571  | 1.0000  | 0.6229   | 0.4044  | 0.2758     |
| Burglary           | 0.3858 | 0.7121 | 0.6372  | 0.6229  | 1.0000   | 0.7921  | 0.5580     |
| Larceny            | 0.1019 | 0.6140 | 0.4467  | 0.4044  | 0.7921   | 1.0000  | 0.4442     |
| Auto_Theft         | 0.0688 | 0.3489 | 0.5907  | 0.2758  | 0.5580   | 0.4442  | 1.0000     |

Figure 73.2 displays the eigenvalues. The first principal component explains about 58.8% of the total variance, the second principal component explains about 17.7%, and the third principal component explains about 10.4%. Note that the eigenvalues sum to the total variance.

The eigenvalues indicate that two or three components provide a good summary of the data, two components accounting for 76% of the total variance and three components explaining 87%. Subsequent components contribute less than 5% each.

Figure 73.2 Results of Principal Component Analysis: PROC PRINCOMP

| Eigenvalues of the Correlation Matrix |            |            |            |            |
|---------------------------------------|------------|------------|------------|------------|
|                                       | Eigenvalue | Difference | Proportion | Cumulative |
| 1                                     | 4.11495951 | 2.87623768 | 0.5879     | 0.5879     |
| 2                                     | 1.23872183 | 0.51290521 | 0.1770     | 0.7648     |
| 3                                     | 0.72581663 | 0.40938458 | 0.1037     | 0.8685     |
| 4                                     | 0.31643205 | 0.05845759 | 0.0452     | 0.9137     |
| 5                                     | 0.25797446 | 0.03593499 | 0.0369     | 0.9506     |
| 6                                     | 0.22203947 | 0.09798342 | 0.0317     | 0.9823     |
| 7                                     | 0.12405606 |            | 0.0177     | 1.0000     |

Figure 73.3 displays the eigenvectors. From the eigenvectors matrix, you can represent the first principal component Prin1 as a linear combination of the original variables:

$$\begin{aligned}
 \text{Prin1} &= 0.300279 \times (\text{Murder}) \\
 &+ 0.431759 \times (\text{Rape}) \\
 &+ 0.396875 \times (\text{Robbery}) \\
 &\cdot \\
 &\cdot \\
 &\cdot \\
 &+ 0.295177 \times (\text{Auto_Theft})
 \end{aligned}$$

Similarly, the second principal component Prin2 is

$$\begin{aligned} \text{Prin2} = & -0.629174 \times (\text{Murder}) \\ & - 0.169435 \times (\text{Rape}) \\ & + 0.042247 \times (\text{Robbery}) \\ & \cdot \\ & \cdot \\ & \cdot \\ & - 0.502421 \times (\text{Auto_Theft}) \end{aligned}$$

where the variables are standardized.

**Figure 73.3** Results of Principal Component Analysis: PROC PRINCOMP

|                   | Eigenvectors |          |          |          |          |          |          |
|-------------------|--------------|----------|----------|----------|----------|----------|----------|
|                   | Prin1        | Prin2    | Prin3    | Prin4    | Prin5    | Prin6    | Prin7    |
| <b>Murder</b>     | 0.300279     | -.629174 | 0.178245 | -.232114 | 0.538123 | 0.259117 | 0.267593 |
| <b>Rape</b>       | 0.431759     | -.169435 | -.244198 | 0.062216 | 0.188471 | -.773271 | -.296485 |
| <b>Robbery</b>    | 0.396875     | 0.042247 | 0.495861 | -.557989 | -.519977 | -.114385 | -.003903 |
| <b>Assault</b>    | 0.396652     | -.343528 | -.069510 | 0.629804 | -.506651 | 0.172363 | 0.191745 |
| <b>Burglary</b>   | 0.440157     | 0.203341 | -.209895 | -.057555 | 0.101033 | 0.535987 | -.648117 |
| <b>Larceny</b>    | 0.357360     | 0.402319 | -.539231 | -.234890 | 0.030099 | 0.039406 | 0.601690 |
| <b>Auto_Theft</b> | 0.295177     | 0.502421 | 0.568384 | 0.419238 | 0.369753 | -.057298 | 0.147046 |

The first component is a measure of the overall crime rate since the first eigenvector shows approximately equal loadings on all variables. The second eigenvector has high positive loadings on variables Auto\_Theft and Larceny and high negative loadings on variables Murder and Assault. There is also a small positive loading on Burglary and a small negative loading on Rape. This component seems to measure the preponderance of property crime over violent crime. The interpretation of the third component is not obvious.

The ODS GRAPHICS statement enables the PRINCOMP procedure to produce statistical graphs by using ODS Graphics. See Chapter 21, “Statistical Graphics Using ODS,” for more information. PLOTS=SCORE(ELLIPSE NCOMP=3) in the PROC PRINCOMP statement requests the pairwise component score plots for the first three components with a 95% prediction ellipse overlaid on each of the scatter plot. Figure 73.4 shows the plot of the first two components. It is possible to identify regional trends on the plot of the first two components. Nevada and California are at the extreme right, with high overall crime rates but an average ratio of property crime to violent crime. North and South Dakota are at the extreme left, with low overall crime rates. Southeastern states tend to be at the bottom of the plot, with a higher-than-average ratio of violent crime to property crime. New England states tend to be in the upper part of the plot, with a higher-than-average ratio of property crime to violent crime. Assuming the first two components are from a bivariate normal distribution, the ellipse identifies Nevada as a possible outlier.

**Figure 73.4** Plot of the First Two Component Scores

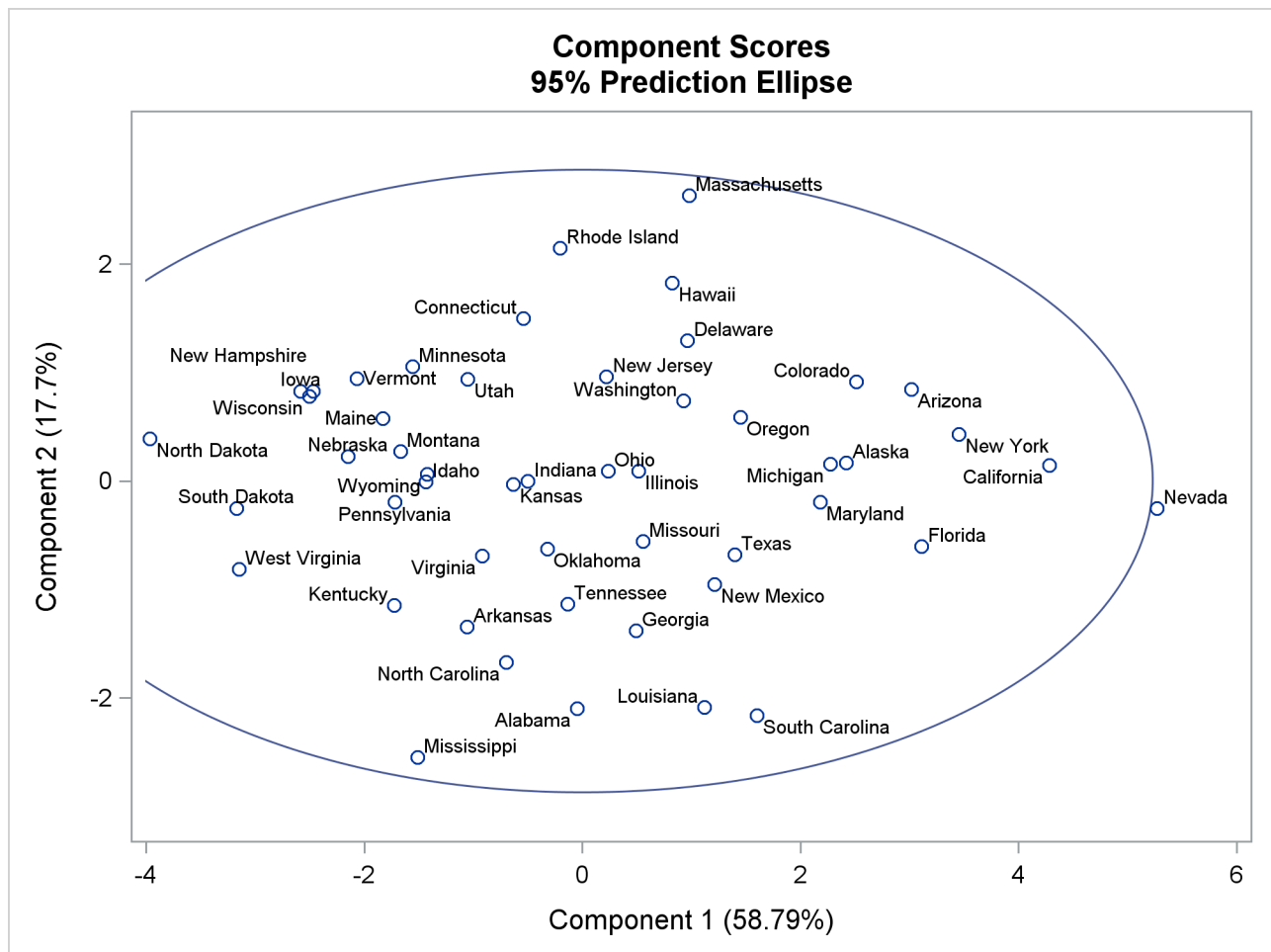
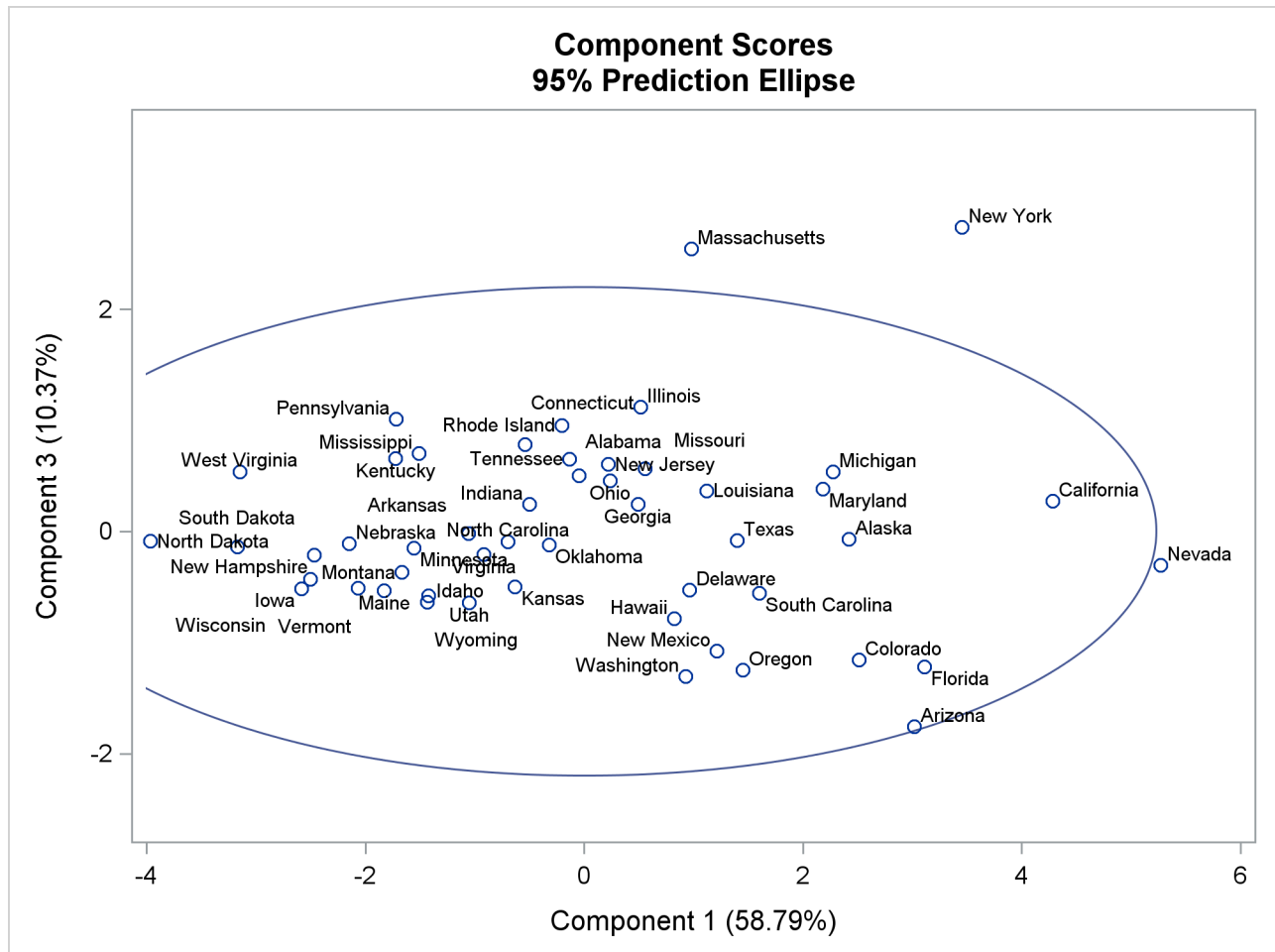


Figure 73.5 shows the plot of the first and third components. Assuming the first and the third components are from a bivariate normal distribution, the ellipse identifies Nevada, Massachusetts, and New York as possible outliers.

Figure 73.5 Plot of the First and Third Component Scores



The most striking feature of the plot of the first and third principal components is that Massachusetts and New York are outliers on the third component.

## Syntax: PRINCOMP Procedure

The following statements are available in the PRINCOMP procedure:

```

PROC PRINCOMP < options > ;
 BY variables ;
 FREQ variable ;
 ID variables ;
 PARTIAL variables ;
 VAR variables ;
 WEIGHT variable ;

```

Usually only the VAR statement is used in addition to the PROC PRINCOMP statement. The rest of this section provides detailed syntax information for each of the preceding statements, beginning with the PROC PRINCOMP statement. The remaining statements are described in alphabetical order.

---

## PROC PRINCOMP Statement

**PROC PRINCOMP** < options > ;

The PROC PRINCOMP statement invokes the PRINCOMP procedure. Optionally, it also identifies input and output data sets, specifies the analyses performed, and controls displayed output. [Table 73.1](#) summarizes the options available in the PROC PRINCOMP statement.

**Table 73.1** Summary of PROC PRINCOMP Statement Options

| Option                                | Description                                                                 |
|---------------------------------------|-----------------------------------------------------------------------------|
| <b>Specify data sets</b>              |                                                                             |
| DATA=                                 | Specifies input data set name                                               |
| OUT=                                  | Specifies output data set name                                              |
| OUTSTAT=                              | Specifies output data set name containing various statistics                |
| <b>Specify details of analysis</b>    |                                                                             |
| COV                                   | Computes the principal components from the covariance matrix                |
| N=                                    | Specifies the number of principal components to be computed                 |
| NOINT                                 | Omits the intercept from the model                                          |
| PREFIX=                               | Specifies a prefix for naming the principal components                      |
| PARPREFIX=                            | Specifies a prefix for naming the residual variables                        |
| SINGULAR=                             | Specifies the singularity criterion                                         |
| STD                                   | Standardizes the principal component scores                                 |
| VARDEF=                               | Specifies the divisor used in calculating variances and standard deviations |
| <b>Suppress the display of output</b> |                                                                             |
| NOPRINT                               | Suppresses the display of all output                                        |
| <b>Specify ODS Graphics details</b>   |                                                                             |
| PLOTS=                                | Specifies options that control the details of the plots                     |

The following list provides details about these options.

### COVARIANCE

#### COV

computes the principal components from the covariance matrix. If you omit the COV option, the correlation matrix is analyzed. Use of the COV option causes variables with large variances to be more strongly associated with components with large eigenvalues and causes variables with small variances to be more strongly associated with components with small eigenvalues. You should not specify the COV option unless the units in which the variables are measured are comparable or the variables are standardized in some way.



**DATA=SAS-data-set**

specifies the SAS data set to be analyzed. The data set can be an ordinary SAS data set or a TYPE=ACE, TYPE=CORR, TYPE=COV, TYPE=FACTOR, TYPE=SSCP, TYPE=UCORR, or TYPE=UCOV data set (see Appendix A, “[Special SAS Data Sets](#)”). Also, the PRINCOMP procedure can read the \_TYPE\_='COVB' matrix from a TYPE=EST data set. If you omit the DATA= option, the procedure uses the most recently created SAS data set.

**N=number**

specifies the number of principal components to be computed. The default is the number of variables. The value of the N= option must be an integer greater than or equal to zero.

**NOINT**

omits the intercept from the model. In other words, the NOINT option requests that the covariance or correlation matrix not be corrected for the mean. When you use the PRINCOMP procedure with the NOINT option, the covariance matrix and, hence, the standard deviations are not corrected for the mean. If you are interested in the standard deviations corrected for the mean, you can get them by using a procedure such as the MEANS procedure.

If you use a TYPE=SSCP data set as input to the PRINCOMP procedure and list the variable Intercept in the VAR statement, the procedure acts as if you had also specified the NOINT option. If you use NOINT and also create an OUTSTAT= data set, the data set is TYPE=UCORR or TYPE=UCOV rather than TYPE=CORR or TYPE=COV.

**NOPRINT**

suppresses the display of all output. Note that this option temporarily disables the Output Delivery System (ODS). For more information, see Chapter 20, “[Using the Output Delivery System](#).”

**OUT=SAS-data-set**

creates an output SAS data set that contains all the original data as well as the principal component scores.

If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*. For details about OUT= data sets, see the section “[Output Data Sets](#)” on page 6253.

**OUTSTAT=SAS-data-set**

creates an output SAS data set that contains means, standard deviations, number of observations, correlations or covariances, eigenvalues, and eigenvectors. If you specify the COV option, the data set is TYPE=COV or TYPE=UCOV, depending on the NOINT option, and it contains covariances; otherwise, the data set is TYPE=CORR or TYPE=UCORR, depending on the NOINT option, and it contains correlations. If you specify the PARTIAL statement, the OUTSTAT= data set contains R squares as well.

If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*. For details about OUTSTAT= data sets, see the section “[Output Data Sets](#)” on page 6253.

**PLOTS** <(global-plot-options)> <= plot-request <(options)>>

**PLOTS** <(global-plot-options)> <= (plot-request <(options)> <... plot-request <(options)>>>

controls the plots produced through ODS Graphics. When you specify only one plot request, you can omit the parentheses around the plot request. Here are some examples:

```
plots=none
plots=(scatter pattern)
plots(unpack)=scree
plots(ncomp=3 flip)=(pattern(circles=0.5 1.0) score)
```

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;
proc princomp plots=all;
 var x1--x10;
run;
ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS](#).”

If ODS Graphics is enabled, but do not specify the PLOTS= option, PROC PRINCOMP produces the scree plot by default.

The global plot options include the following:

#### **FLIP**

flips or interchanges the X-axis and Y-axis dimension for the component score plots and the component pattern plots. For example, if there are three components, the default plots ( $y * x$ ) are Component 2 \* Component 1, Component 3 \* Component 1, and Component 3 \* Component 2. When you specify PLOTS(FLIP), the plots are Component 1 \* Component 2, Component 1 \* Component 3, and Component 2 \* Component 3.

#### **NCOMP= $n$**

specifies the number of components  $n$  ( $\geq 2$ ) to be plotted for the component pattern plots and the component score plots. If the NCOMP= option is again specified in an individual plot, such as PLOTS=SCORE(NCOMP=  $m$ ), the value  $m$  will determine the number of components to be plotted in the component score plots. Be aware that the number of plots ( $n \times (n - 1) / 2$ ) produced grows quadratically when  $n$  increases. The default is 5 or the total number of components  $m$  ( $\geq 2$ ), whichever is smaller. If  $n > m$ , NCOMP=  $m$  will be used.

#### **ONLY**

suppresses the default plots. Only plots specifically requested are displayed.

#### **UNPACKPANEL**

##### **UNPACK**

suppresses paneling in the scree plot. By default, multiple plots can appear in an output panel. Specify UNPACKPANEL to get each plot in a separate panel. You can specify PLOTS(UNPACKPANEL) to unpack the default plots. You can also specify UNPACKPANEL as a suboption with SCREE (such as PLOTS=SCREE(UNPACKPANEL)).

The plot requests include the following:

**ALL**

produces all appropriate plots. You can specify other options with ALL; for example, to request all plots and unpack only the scree plot, specify PLOTS=(ALL SCREE(UNPACKPANEL)).

**EIGEN | EIGENVALUE | SCREE < ( UNPACKPANEL ) >**

produces the scree plot of eigenvalues and proportion variance explained. By default, both plots are output in a panel. Specify PLOTS= SCREE(UNPACKPANEL) to get each plot in a separate panel.

**MATRIX**

produces the matrix plot of principal component scores.

**NONE**

suppresses the display of all graphics output.

**PATTERN < ( pattern-options ) >**

produces the pairwise component pattern plots. Each variable is plotted as an observation whose coordinates are correlations between the variable and the two corresponding components on the plot. Use the NCOMP= option (for instance, PLOTS=PATTERN(NCOMP=3)) described in the following to control the number of plots to be displayed.

The available *pattern-options* are as follows:

**CIRCLES < = number list >**

plots the variance percentage circles. Each number in the list must be greater than 0. If the number is greater than or equal to 1, it is interpreted as a percentage and divided by 100; CIRCLES=0.05 and CIRCLES=5 are equivalent. For each number (*c*) specified, a ( $c \times 100\%$ ) variance circle is created.

By default, there is no circle for the scatter pattern plot (PLOTS=PATTERN) and a unit circle with a 100% variance circle is plotted for the vector pattern plot (PLOTS=PATTERN (VECTOR)). You can display multiple circles by specifying PLOTS=PATTERN(CIRCLES= ). For example, specifying PLOTS=PATTERN(CIRCLES=.3 .6 1.0) will display the 30%, 60%, and 100% variance circles in the pattern plots.

**FLIP**

flips or interchanges the X-axis and Y-axis dimensions for the component pattern plots. Specify PLOTS=PATTERN(FLIP) to flip the X-axis and Y-axis dimensions.

**NCOMP=*n***

specifies the number of components  $n (\geq 2)$  to be plotted. The default is 5 or the total number of components  $m (\geq 2)$ , whichever is smaller. If  $n > m$ , NCOMP= *m* will be used. Be aware that the number of plots ( $n \times (n - 1)/2$ ) produced grows quadratically when *n* increases.

**VECTOR**

plots pattern in a vector form.

**PATTERNPROFILE | PROFILE**

produces the pattern profile plot. There is a profile for each component. The Y-axis value represents the correlation between the variable (corresponding to the X-axis value) and the profiled principal component.

**SCORE < ( score-options ) >**

produces the pairwise component score plots. Use the NCOMP= option (for instance, PLOTS=SCORE(NCOMP=3)) described in the following to control the number of plots to be displayed.

The available *score-options* are as follows:

**ALPHA=number list**

specifies a list of numbers for the prediction ellipses to be displayed in the score plots. Each value ( $\alpha$ ) in the list must be greater than 0. If  $\alpha$  is greater than or equal to 1, it is interpreted as a percentage and divided by 100; ALPHA=0.05 and ALPHA=5 are equivalent.

**ELLIPSE**

requests prediction ellipses for the principal component scores of a new observation to be created in the principal component score plots. See the section “Confidence and Prediction Ellipses” in “The CORR Procedure” (*Base SAS Procedures Guide: Statistical Procedures*), for details about the computation of a prediction ellipse.

**FLIP**

flips or interchanges the X-axis and Y-axis dimensions for the component score plots. Specify PLOTS=SCORE(FLIP) to flip the X-axis and Y-axis dimensions.

**NCOMP=n**

specifies the number of components  $n$  ( $\geq 2$ ) to be plotted. The default is 5 or the total number of components  $m$  ( $\geq 2$ ), whichever is smaller. If  $n > m$ , NCOMP=  $m$  will be used. Be aware that the number of plots ( $n \times (n - 1)/2$ ) produced grows quadratically when  $n$  increases.

**PAINT <=position>**

creates plots of component  $i$  versus component  $j$ , painted by component  $k$ . When there are at least three components, the PLOTS=SCORE option is specified, and the PAINT option is not specified, a painted score plot for component 3 versus component 2, painted by component 1 is produced. Use the PAINT option when you want to create painted score plots involving other triples of components.

PLOTS=SCORE(PAINT), PLOTS=SCORE(PAINT=F), and PLOTS=SCORE(PAINT=FIRST) are all equivalent and create painted plots of  $i \times j$ , painted by  $k$  for triples  $(i, j, k)$  where  $k < j < i$ .

PLOTS=SCORE(PAINT=L) and PLOTS=SCORE(PAINT=LAST) are equivalent and create painted plots of  $i \times j$ , painted by  $k$  for triples  $(i, j, k)$  where  $j < i < k$ .

PLOTS=SCORE(PAINT=M) and PLOTS=SCORE(PAINT=MIDDLE) are equivalent and create painted plots of  $i \times j$ , painted by  $k$  for triples  $(i, j, k)$  where  $j < k < i$ .

**PREFIX=name**

specifies a prefix for naming the principal components. By default, the names are Prin1, Prin2, . . . , Prin*n*. If you specify PREFIX=ABC, the components are named ABC1, ABC2, ABC3, and so on. The number of characters in the prefix plus the number of digits required to designate the variables should not exceed the current name length defined by the VALIDVARNAME= system option.

**PARPREFIX=name****PPREFIX=name****RPREFIX=name**

specifies a prefix for naming the residual variables in the OUT= data set and the OUTSTAT= data set. By default, the prefix is R\_. The number of characters in the prefix plus the maximum length of the variable names should not exceed the current name length defined by the VALIDVARNAME= system option.

**SINGULAR=p****SING=p**

specifies the singularity criterion, where  $0 < p < 1$ . If a variable in a PARTIAL statement has an R square as large as  $1 - p$  when predicted from the variables listed before it in the statement, the variable is assigned a standardized coefficient of 0. By default, SINGULAR=1E-8.

**STANDARD****STD**

standardizes the principal component scores in the OUT= data set to unit variance. If you omit the STANDARD option, the scores have variance equal to the corresponding eigenvalue. Note that STANDARD has no effect on the eigenvalues themselves.

**VARDEF=DF | N | WDF | WEIGHT | WGT**

specifies the divisor used in calculating variances and standard deviations. By default, VARDEF=DF. The following table displays the values and associated divisors.

| Value        | Divisor                  | Formula                                                    |
|--------------|--------------------------|------------------------------------------------------------|
| DF           | error degrees of freedom | $n - i$ (before partialing)                                |
|              |                          | $n - p - i$ (after partialing)                             |
| N            | number of observations   | $n$                                                        |
| WEIGHT   WGT | sum of weights           | $\sum_{j=1}^n w_j$                                         |
| WDF          | sum of weights minus one | $\left(\sum_{j=1}^n w_j\right) - i$ (before partialing)    |
|              |                          | $\left(\sum_{j=1}^n w_j\right) - p - i$ (after partialing) |

In the formulas for VARDEF=DF and VARDEF=WDF,  $p$  is the number of degrees of freedom of the variables in the PARTIAL statement, and  $i$  is 0 if the NOINT option is specified and 1 otherwise.

---

## BY Statement

**BY variables ;**

You can specify a BY statement with PROC PRINCOMP to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the PRINCOMP procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

---

## FREQ Statement

**FREQ variable ;**

The FREQ statement specifies a variable that provides frequencies for each observation in the DATA= data set. Specifically, if  $n$  is the value of the FREQ variable for a given observation, then that observation is used  $n$  times.

The analysis produced using a FREQ statement reflects the expanded number of observations. The total number of observations is considered equal to the sum of the FREQ variable. You could produce the same analysis (without the FREQ statement) by first creating a new data set that contains the expanded number of observations. For example, if the value of the FREQ variable is 5 for the first observation, the first 5 observations in the new data set would be identical. Each observation in the old data set would be replicated  $n_j$  times in the new data set, where  $n_j$  is the value of the FREQ variable for that observation.

If the value of the FREQ variable is missing or is less than one, the observation is not used in the analysis. If the value is not an integer, only the integer portion is used.

---

## ID Statement

**ID variables ;**

The ID statement labels observations with values from the first ID variable in the principal component score plot. If one or more ID variables are specified, their values are displayed in tooltips of the component score plot and the matrix plot of component scores.

---

## PARTIAL Statement

**PARTIAL** *variables* ;

If you want to analyze a partial correlation or covariance matrix, specify the names of the numeric variables to be partialled out in the PARTIAL statement. The PRINCOMP procedure computes the principal components of the residuals from the prediction of the VAR variables by the PARTIAL variables. If you request an OUT= or OUTSTAT= data set, the residual variables are named by prefixing the characters R\_ by default or the string specified in the PARPREFIX= option to the VAR variables.

---

## VAR Statement

**VAR** *variables* ;

The VAR statement lists the numeric variables to be analyzed. If you omit the VAR statement, all numeric variables not specified in other statements are analyzed. If, however, the DATA= data set is TYPE=SSCP, the default set of variables used as VAR variables does not include Intercept so that the correlation or covariance matrix is constructed correctly. If you want to analyze Intercept as a separate variable, you should specify it in the VAR statement.

---

## WEIGHT Statement

**WEIGHT** *variable* ;

If you want to use relative weights for each observation in the input data set, place the weights in a variable in the data set and specify the name in a WEIGHT statement. This is often done when the variance associated with each observation is different and the values of the weight variable are proportional to the reciprocals of the variances.

The observation is used in the analysis only if the value of the WEIGHT statement variable is nonmissing and is greater than zero.

---

## Details: PRINCOMP Procedure

---

### Missing Values

Observations with missing values for any variable in the VAR, PARTIAL, FREQ, or WEIGHT statement are omitted from the analysis and are given missing values for principal component scores in the OUT= data set. If a correlation, covariance, or SSCP matrix is read, it can contain missing values as long as every pair of variables has at least one nonmissing entry.

## Output Data Sets

### OUT= Data Set

The OUT= data set contains all the variables in the original data set plus new variables containing the principal component scores. The N= option determines the number of new variables. The names of the new variables are formed by concatenating the value given by the PREFIX= option (or Prin if PREFIX= is omitted) and the numbers 1, 2, 3, and so on. The new variables have mean 0 and variance equal to the corresponding eigenvalue, unless you specify the STANDARD option to standardize the scores to unit variance. Also, if you specify the COV option, the procedure computes the principal component scores from the corrected or the uncorrected (if the NOINT option is specified) variables rather than the standardized variables.

If you use a PARTIAL statement, the OUT= data set also contains the residuals from predicting the VAR variables from the PARTIAL variables.

An OUT= data set cannot be created if the DATA= data set is TYPE=ACE, TYPE=CORR, TYPE=COV, TYPE=EST, TYPE=FACTOR, TYPE=SSCP, TYPE=UCORR, or TYPE=UCOV.

### OUTSTAT= Data Set

The OUTSTAT= data set is similar to the TYPE=CORR data set produced by the CORR procedure. The following table relates the TYPE= value for the OUTSTAT= data set to the options specified in the PROC PRINCOMP statement.

| Options   | TYPE= |
|-----------|-------|
| (default) | CORR  |
| COV       | COV   |
| NOINT     | UCORR |
| COV NOINT | UCOV  |

Note that the default (neither the COV nor NOINT option) produces a TYPE=CORR data set.

The new data set contains the following variables:

- the BY variables, if any
- two new variables, \_TYPE\_ and \_NAME\_, both character variables
- the variables analyzed (that is, those in the VAR statement); or, if there is no VAR statement, all numeric variables not listed in any other statement; or, if there is a PARTIAL statement, the residual variables as described under the OUT= data set

Each observation in the new data set contains some type of statistic as indicated by the \_TYPE\_ variable. The values of the \_TYPE\_ variable are as follows:

MEAN            mean of each variable. If you specify the PARTIAL statement, this observation is omitted.



|          |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
|----------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| STD      | standard deviations. If you specify the COV option, this observation is omitted, so the SCORE procedure does not standardize the variables before computing scores. If you use the PARTIAL statement, the standard deviation of a variable is computed as its root mean squared error as predicted from the PARTIAL variables.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
| USTD     | uncorrected standard deviations. When you specify the NOINT option in the PROC PRINCOMP statement, the OUTSTAT= data set contains standard deviations not corrected for the mean. However, if you also specify the COV option in the PROC PRINCOMP statement, this observation is omitted.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
| N        | number of observations on which the analysis is based. This value is the same for each variable. If you specify the PARTIAL statement and the value of the VARDEF= option is DF or unspecified, then the number of observations is decremented by the degrees of freedom for the PARTIAL variables.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
| SUMWGT   | the sum of the weights of the observations. This value is the same for each variable. If you specify the PARTIAL statement and VARDEF=WDF, then the sum of the weights is decremented by the degrees of freedom for the PARTIAL variables. This observation is output only if the value is different from that in the observation with _TYPE_='N'.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |
| CORR     | correlations between each variable and the variable specified by the _NAME_ variable. The number of observations with _TYPE_='CORR' is equal to the number of variables being analyzed. If you specify the COV option, no _TYPE_='CORR' observations are produced. If you use the PARTIAL statement, the partial correlations, not the raw correlations, are output.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
| UCORR    | uncorrected correlation matrix. When you specify the NOINT option without the COV option in the PROC PRINCOMP statement, the OUTSTAT= data set contains a matrix of correlations not corrected for the means. However, if you also specify the COV option in the PROC PRINCOMP statement, this observation is omitted.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |
| COV      | covariances between each variable and the variable specified by the _NAME_ variable. _TYPE_='COV' observations are produced only if you specify the COV option. If you use the PARTIAL statement, the partial covariances, not the raw covariances, are output.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
| UCOV     | uncorrected covariance matrix. When you specify the NOINT and COV options in the PROC PRINCOMP statement, the OUTSTAT= data set contains a matrix of covariances not corrected for the means.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
| EIGENVAL | eigenvalues. If the N= option requested fewer than the maximum number of principal components, only the specified number of eigenvalues are produced, with missing values filling out the observation.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |
| SCORE    | eigenvectors. The _NAME_ variable contains the name of the corresponding principal component as constructed from the PREFIX= option. The number of observations with _TYPE_='SCORE' equals the number of principal components computed. The eigenvectors have unit length unless you specify the STD option, in which case the unit-length eigenvectors are divided by the square roots of the eigenvalues to produce scores with unit standard deviations.<br><br>To obtain the principal component scores, if the COV option is not specified, these coefficients should be multiplied by the standardized data. With the COV option, these coefficients should be multiplied by the centered data. Means obtained from the observation with _TYPE_='MEAN' and standard deviations obtained from the observation with _TYPE_='STD' should be used for centering and standardizing the data. |

|          |                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
|----------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| USCORE   | scoring coefficients to be applied without subtracting the mean from the raw variables. <code>_TYPE_='USCORE'</code> observations are produced when you specify the <code>NOINT</code> option in the <code>PROC PRINCOMP</code> statement.<br><br>To obtain the principal component scores, these coefficients should be multiplied by the data that are standardized by the uncorrected standard deviations obtained from the observation with <code>_TYPE_='USTD'</code> . |
| RSQUARED | R squares for each VAR variable as predicted by the PARTIAL variables                                                                                                                                                                                                                                                                                                                                                                                                        |
| B        | regression coefficients for each VAR variable as predicted by the PARTIAL variables. This observation is produced only if you specify the <code>COV</code> option.                                                                                                                                                                                                                                                                                                           |
| STB      | standardized regression coefficients for each VAR variable as predicted by the PARTIAL variables. If you specify the <code>COV</code> option, this observation is omitted.                                                                                                                                                                                                                                                                                                   |

The data set can be used with the `SCORE` procedure to compute principal component scores, or it can be used as input to the `FACTOR` procedure specifying `METHOD=SCORE` to rotate the components. If you use the `PARTIAL` statement, the scoring coefficients should be applied to the residuals, not the original variables.

---

## Computational Resources

Let

- $n$  = number of observations
- $v$  = number of VAR variables
- $p$  = number of PARTIAL variables
- $c$  = number of components

- The minimum allocated memory required (in bytes) is

$$232v + 120p + 48c + \max(8cv, 8vp + 4(v + p)(v + p + 1))$$

- The time required to compute the correlation matrix is roughly proportional to

$$n(v + p)^2 + \frac{p}{2}(v + p)(v + p + 1)$$

- The time required to compute eigenvalues is roughly proportional to  $v^3$ .
- The time required to compute eigenvectors is roughly proportional to  $cv^2$ .

---

## Displayed Output

The PRINCOMP procedure displays the following items if the DATA= data set is not TYPE=CORR, TYPE=COV, TYPE=SSCP, TYPE=UCORR, or TYPE=UCOV:

- simple statistics, including the mean and std (standard deviation) for each variable. If you specify the NOINT option, the uncorrected standard deviation (ustd) is displayed.
- the correlation or, if you specify the COV option, the covariance matrix

The PRINCOMP procedure displays the following items if you use the PARTIAL statement:

- regression statistics, giving the R square and RMSE (root mean squared error) for each VAR variable as predicted by the PARTIAL variables (not shown)
- standardized regression coefficients or, if you specify the COV option, regression coefficients for predicting the VAR variables from the PARTIAL variables (not shown)
- the partial correlation matrix or, if you specify the COV option, the partial covariance matrix (not shown)

The PRINCOMP procedure displays the following item if you specify the COV option:

- the total variance

The PRINCOMP procedure displays the following items unless you specify the NOPRINT option:

- eigenvalues of the correlation or covariance matrix, as well as the difference between successive eigenvalues, the proportion of variance explained by each eigenvalue, and the cumulative proportion of variance explained
- the eigenvectors

---

## ODS Table Names

PROC PRINCOMP assigns a name to each table it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in [Table 73.2](#). For more information about ODS, see Chapter 20, “[Using the Output Delivery System.](#)”

All of the tables are created with the specification of the PROC PRINCOMP statement; a few tables need an additional PARTIAL statement.

**Table 73.2** ODS Tables Produced by PROC PRINCOMP

| ODS Table Name | Description        | Statement / Option |
|----------------|--------------------|--------------------|
| Corr           | Correlation matrix | default            |

**Table 73.2** *Continued*

| ODS Table Name   | Description                                              | Statement and Option      |
|------------------|----------------------------------------------------------|---------------------------|
| Cov              | Covariance matrix                                        | COV                       |
| Eigenvalues      | Eigenvalues                                              | default                   |
| Eigenvectors     | Eigenvectors                                             | default                   |
| NObsNVar         | Number of observations, variables, and partial variables | default                   |
| ParCorr          | Partial correlation matrix                               | PARTIAL statement         |
| ParCov           | Uncorrected partial covariance matrix                    | PARTIAL statement and COV |
| RegCoef          | Regression coefficients                                  | PARTIAL statement and COV |
| RSquareRMSE      | Regression statistics: R squares and RMSEs               | PARTIAL statement         |
| SimpleStatistics | Simple statistics                                        | default                   |
| StdRegCoef       | Standardized regression coefficients                     | PARTIAL statement         |
| TotalVariance    | Total variance                                           | COV                       |

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “[Statistical Graphics Using ODS.](#)”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS.](#)”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “[A Primer on ODS Statistical Graphics](#)” on page 599 in Chapter 21, “[Statistical Graphics Using ODS.](#)”

Some graphs are produced by default; other graphs are produced by using statements and options. You can reference every graph produced through ODS Graphics with a name. The names of the graphs that PROC PRINCOMP generates are listed in [Table 73.3](#), along with the required statements and options.

**Table 73.3** Graphs Produced by PROC PRINCOMP

| ODS Graph Name     | Plot Description                                                            | Statement and Option                          |
|--------------------|-----------------------------------------------------------------------------|-----------------------------------------------|
| PaintedScorePlot   | Score plot of component $i$ versus component $j$ , painted by component $k$ | PLOTS=SCORE when number of variables $\geq 3$ |
| PatternPlot        | Component pattern plot                                                      | PLOTS=PATTERN                                 |
| PatternProfilePlot | Component pattern profile plot                                              | PLOTS=PATTERNPROFILE                          |
| ScoreMatrixPlot    | Matrix plot of component scores                                             | PLOTS=MATRIX                                  |
| ScorePlot          | Component score plot                                                        | PLOTS=SCORE                                   |
| ScreePlot          | Scree and variance plots                                                    | default and PLOTS=SCREE                       |
| VariancePlot       | Variance proportion explained plot                                          | PLOTS=SCREE(UNPACKPANEL)                      |

---

## Examples: PRINCOMP Procedure

---

### Example 73.1: Temperatures

This example analyzes mean daily temperatures in selected cities in January and July. Both the raw data and the principal components are plotted to illustrate how principal components are orthogonal rotations of the original variables.

The following statements create the Temperature data set.

```
data Temperature;
 length Cityid $ 2;
 title 'Mean Temperature in January and July for Selected Cities ';
 input City $1-15 January July;
 Cityid = substr(City,1,2);
 datalines;
Mobile 51.2 81.6
Phoenix 51.2 91.2
Little Rock 39.5 81.4
Sacramento 45.1 75.2
Denver 29.9 73.0

 ... more lines ...

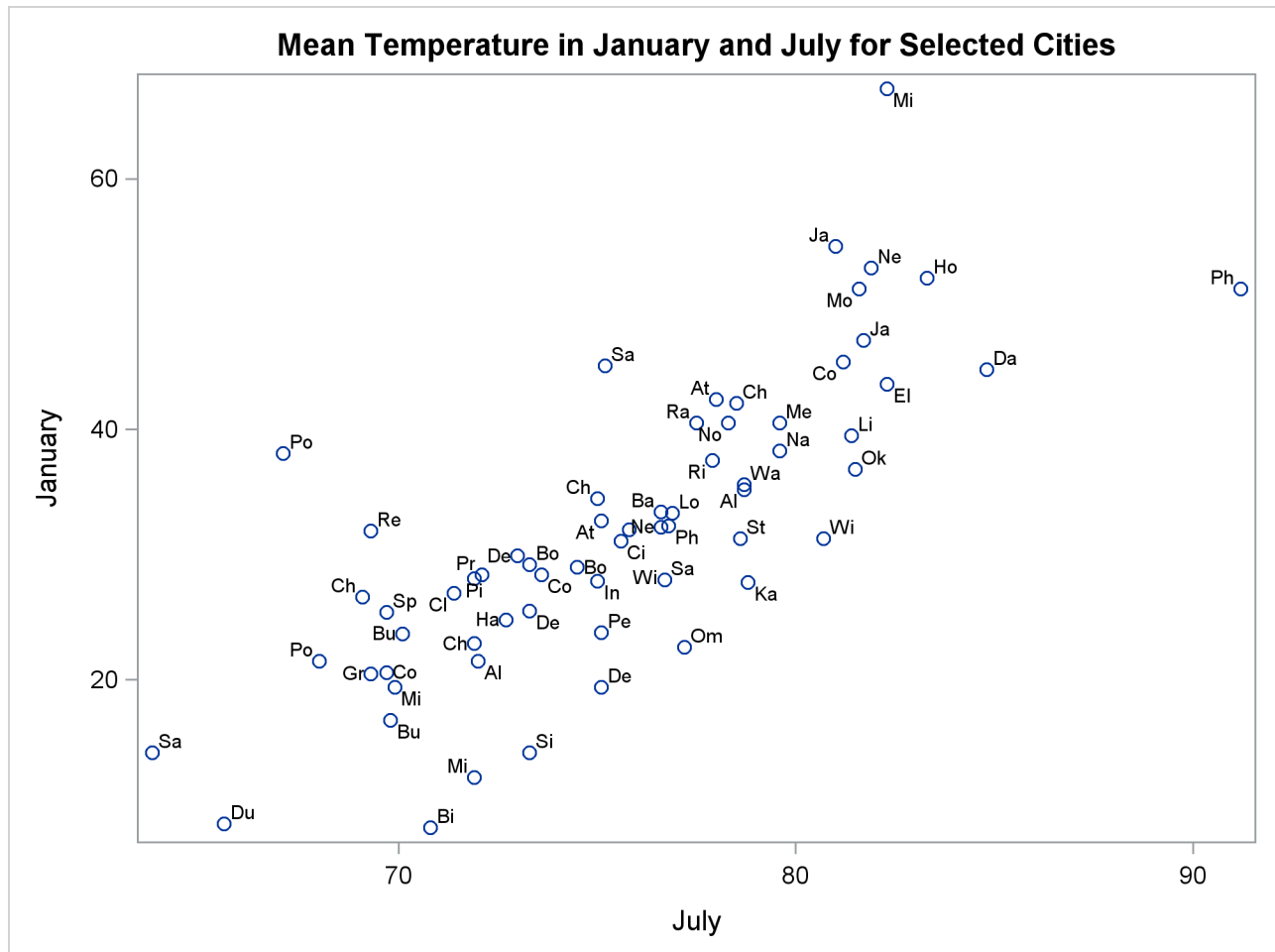
Cheyenne 26.6 69.1
;
```

The following statements plot the temperature data set. The Cityid variable instead of City is used as a data label in the scatter plot for possible label clashing.

```
title 'Mean Temperature in January and July for Selected Cities';
proc sgplot data=Temperature;
 scatter x=July y=January / datalabel=Cityid;
run;
```

The results are displayed in [Output 73.1.1](#), which shows a scatter diagram of the 64 pairs of data points with July temperatures plotted against January temperatures.

Output 73.1.1 Plot of Raw Data



The following step requests a principal component analysis on the Temperature data set:

```
ods graphics on;

title 'Mean Temperature in January and July for Selected Cities';
proc princomp data=Temperature cov plots=score(ellipse);
 var July January;
 id Cityid;
run;
```

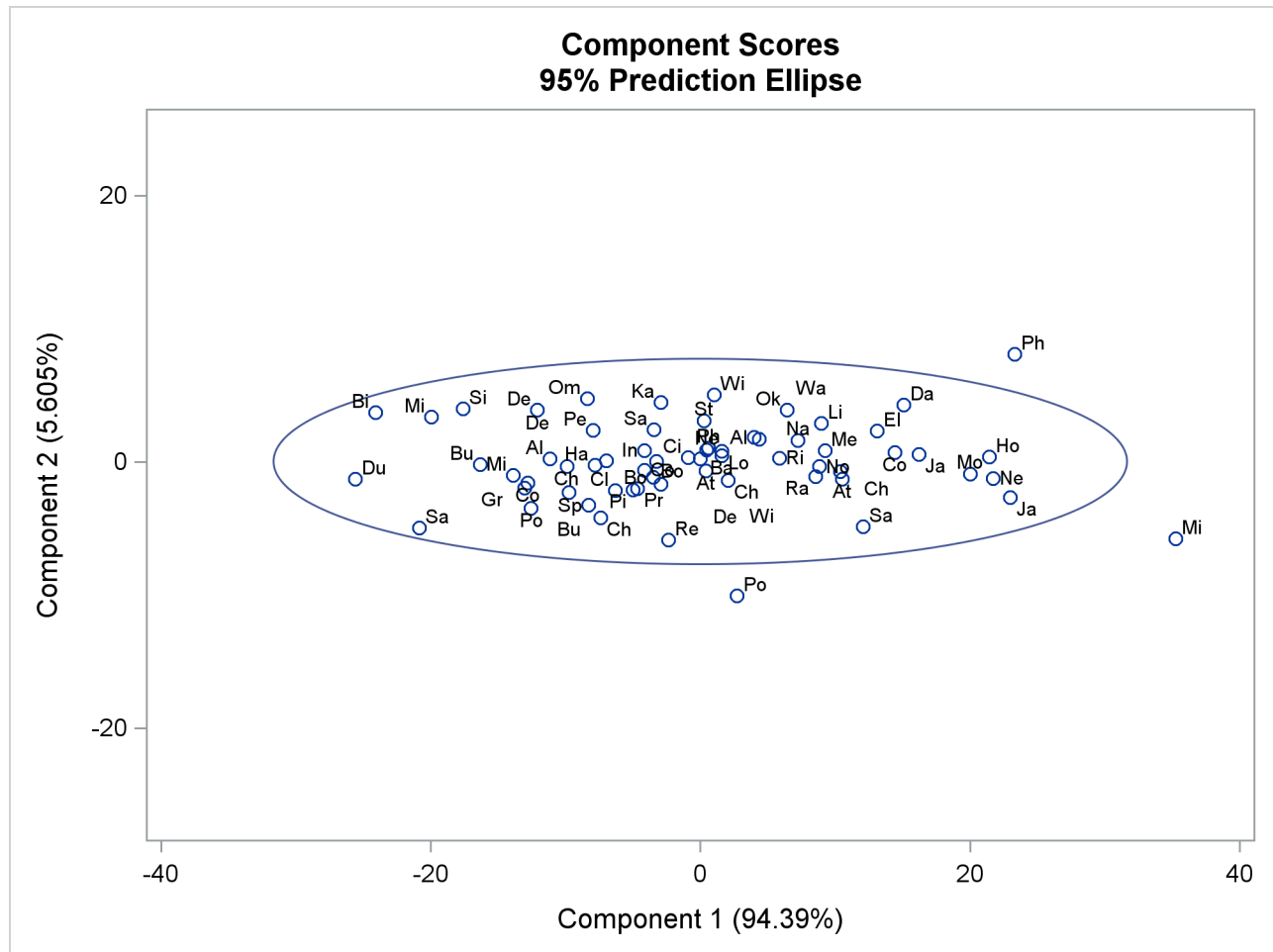
Output 73.1.2 displays the PROC PRINCOMP output. The standard deviation of January (11.712) is higher than the standard deviation of July (5.128). The COV option in the PROC PRINCOMP statement requests the principal components to be computed from the covariance matrix. The total variance is 163.474. The first principal component explains about 94% of the total variance, and the second principal component explains only about 6%. The eigenvalues sum to the total variance.

Note that January receives a higher loading on Prin1 because it has a higher standard deviation than July, and the PRINCOMP procedure calculates the scores by using the centered variables rather than the standardized variables.

**Output 73.1.2** Results of Principal Component Analysis

| Mean Temperature in January and July for Selected Cities |                |              |             |            |
|----------------------------------------------------------|----------------|--------------|-------------|------------|
| The PRINCOMP Procedure                                   |                |              |             |            |
|                                                          | Observations   | 64           |             |            |
|                                                          | Variables      | 2            |             |            |
| Simple Statistics                                        |                |              |             |            |
|                                                          |                | July         | January     |            |
|                                                          | Mean           | 75.60781250  | 32.09531250 |            |
|                                                          | StD            | 5.12761910   | 11.71243309 |            |
| Covariance Matrix                                        |                |              |             |            |
|                                                          |                | July         | January     |            |
|                                                          | July           | 26.2924777   | 46.8282912  |            |
|                                                          | January        | 46.8282912   | 137.1810888 |            |
|                                                          | Total Variance | 163.47356647 |             |            |
| Eigenvalues of the Covariance Matrix                     |                |              |             |            |
|                                                          | Eigenvalue     | Difference   | Proportion  | Cumulative |
| 1                                                        | 154.310607     | 145.147647   | 0.9439      | 0.9439     |
| 2                                                        | 9.162960       |              | 0.0561      | 1.0000     |
| Eigenvectors                                             |                |              |             |            |
|                                                          |                | Prin1        | Prin2       |            |
|                                                          | July           | 0.343532     | 0.939141    |            |
|                                                          | January        | 0.939141     | -.343532    |            |

PLOTS=SCORE in the PROC PRINCOMP statement requests a plot of the second principal component against the first principal component as shown in [Output 73.1.3](#). It is clear from this plot that the principal components are orthogonal rotations of the original variables and that the first principal component has a larger variance than the second principal component. In fact, the first component has a larger variance than either of the original variables July and January. The ellipse indicates that Miami, Phoenix, and Portland are possible outliers.

**Output 73.1.3** Plot of Component 2 by Component 1

## Example 73.2: Basketball Data

The data in this example are rankings of 35 college basketball teams. The rankings were made before the start of the 1985–86 season by 10 news services.

The purpose of the principal component analysis is to compute a single variable that best summarizes all 10 of the preseason rankings.

Note that the various news services rank different numbers of teams, varying from 20 through 30 (there is a missing rank in one of the variables, *WashPost*). And, of course, not all services rank the same teams, so there are missing values in these data. Each of the 35 teams is ranked by at least one news service.

The PRINCOMP procedure omits observations with missing values. To obtain principal component scores for all of the teams, it is necessary to replace the missing values. Since it is the best teams that are ranked, it is not appropriate to replace missing values with the mean of the nonmissing values. Instead, an ad hoc method is used that replaces missing values with the mean of the unassigned ranks. For example, if 20 teams are ranked by a news service, then ranks 21 through 35 are unassigned. The mean of ranks 21 through 35 is 28, so missing values for that variable are replaced by the value 28. To prevent the method of missing-value replacement from having an undue effect on the analysis, each observation is weighted according to the



number of nonmissing values it has. See [Example 74.2](#) in Chapter 74, “The PRINQUAL Procedure,” for an alternative analysis of these data.

Since the first principal component accounts for 78% of the variance, there is substantial agreement among the rankings. The eigenvector shows that all the news services are about equally weighted; this is also suggested by the nearly horizontal line of the pattern profile plot in [Output 73.2.3](#). So a simple average would work almost as well as the first principal component. The following statements produce [Output 73.2.1](#).

```

/*-----*/
/*
/* Pre-season 1985 College Basketball Rankings
/* (rankings of 35 teams by 10 news services)
/*
/* Note: (a) news services rank varying numbers of teams;
/* (b) not all teams are ranked by all news services;
/* (c) each team is ranked by at least one service;
/* (d) rank 20 is missing for UPI.
/*
/*-----*/

```

```

data HoopsRanks;
 input School $13. CSN DurSun DurHer WashPost USAToday
 Sport InSports UPI AP SI;
 label CSN = 'Community Sports News (Chapel Hill, NC)'
 DurSun = 'Durham Sun'
 DurHer = 'Durham Morning Herald'
 WashPost = 'Washington Post'
 USAToday = 'USA Today'
 Sport = 'Sport Magazine'
 InSports = 'Inside Sports'
 UPI = 'United Press International'
 AP = 'Associated Press'
 SI = 'Sports Illustrated'
 ;
 format CSN--SI 5.1;
 datalines;
Louisville 1 8 1 9 8 9 6 10 9 9
Georgia Tech 2 2 4 3 1 1 1 2 1 1
Kansas 3 4 5 1 5 11 8 4 5 7
Michigan 4 5 9 4 2 5 3 1 3 2
Duke 5 6 7 5 4 10 4 5 6 5
UNC 6 1 2 2 3 4 2 3 2 3
Syracuse 7 10 6 11 6 6 5 6 4 10
Notre Dame 8 14 15 13 11 20 18 13 12 .
Kentucky 9 15 16 14 14 19 11 12 11 13
LSU 10 9 13 . 13 15 16 9 14 8
DePaul 11 . 21 15 20 . 19 . . 19
Georgetown 12 7 8 6 9 2 9 8 8 4
Navy 13 20 23 10 18 13 15 . 20 .
Illinois 14 3 3 7 7 3 10 7 7 6
Iowa 15 16 . . 23 . . 14 . 20
Arkansas 16 . . . 25 16
Memphis State 17 . 11 . 16 8 20 . 15 12
Washington 18 17 . .

```

```

UAB 19 13 10 . 12 17 . 16 16 15
UNLV 20 18 18 19 22 . 14 18 18 .
NC State 21 17 14 16 15 . 12 15 17 18
Maryland 22 . . . 19 . . . 19 14
Pittsburgh 23
Oklahoma 24 19 17 17 17 12 17 . 13 17
Indiana 25 12 20 18 21
Virginia 26 . 22 . . 18
Old Dominion 27
Auburn 28 11 12 8 10 7 7 11 10 11
St. Johns 29 14
UCLA 30 19 . .
St. Joseph's . . 19
Tennessee . . 24 . . 16
Montana . . . 20
Houston 24
Virginia Tech 13 . . .
;

/* PROC MEANS is used to output a data set containing the */
/* maximum value of each of the newspaper and magazine */
/* rankings. The output data set, maxrank, is then used */
/* to set the missing values to the next highest rank plus */
/* thirty-six, divided by two (that is, the mean of the */
/* missing ranks). This ad hoc method of replacing missing */
/* values is based more on intuition than on rigorous */
/* statistical theory. Observations are weighted by the */
/* number of nonmissing values. */
/* */

title 'Pre-Season 1985 College Basketball Rankings';
proc means data=HoopsRanks;
 output out=MaxRank
 max=CSNMax DurSunMax DurHerMax
 WashPostMax USATodayMax SportMax
 InSportsMax UPIMax APMax SIMax;
run;

```

**Output 73.2.1** Summary Statistics for Basketball Rankings Using PROC MEANS

| Pre-Season 1985 College Basketball Rankings |                                         |    |            |
|---------------------------------------------|-----------------------------------------|----|------------|
| The MEANS Procedure                         |                                         |    |            |
| Variable                                    | Label                                   | N  | Mean       |
| CSN                                         | Community Sports News (Chapel Hill, NC) | 30 | 15.500000  |
| DurSun                                      | Durham Sun                              | 20 | 10.500000  |
| DurHer                                      | Durham Morning Herald                   | 24 | 12.500000  |
| WashPost                                    | Washington Post                         | 19 | 10.4210526 |
| USAToday                                    | USA Today                               | 25 | 13.000000  |
| Sport                                       | Sport Magazine                          | 20 | 10.500000  |
| InSports                                    | Inside Sports                           | 20 | 10.500000  |
| UPI                                         | United Press International              | 19 | 10.000000  |
| AP                                          | Associated Press                        | 20 | 10.500000  |
| SI                                          | Sports Illustrated                      | 20 | 10.500000  |

| Variable | Label                                   | Std Dev   | Minimum  |
|----------|-----------------------------------------|-----------|----------|
| CSN      | Community Sports News (Chapel Hill, NC) | 8.8034084 | 1.000000 |
| DurSun   | Durham Sun                              | 5.9160798 | 1.000000 |
| DurHer   | Durham Morning Herald                   | 7.0710678 | 1.000000 |
| WashPost | Washington Post                         | 6.0673607 | 1.000000 |
| USAToday | USA Today                               | 7.3598007 | 1.000000 |
| Sport    | Sport Magazine                          | 5.9160798 | 1.000000 |
| InSports | Inside Sports                           | 5.9160798 | 1.000000 |
| UPI      | United Press International              | 5.6273143 | 1.000000 |
| AP       | Associated Press                        | 5.9160798 | 1.000000 |
| SI       | Sports Illustrated                      | 5.9160798 | 1.000000 |

| Variable | Label                                   | Maximum   |
|----------|-----------------------------------------|-----------|
| CSN      | Community Sports News (Chapel Hill, NC) | 30.000000 |
| DurSun   | Durham Sun                              | 20.000000 |
| DurHer   | Durham Morning Herald                   | 24.000000 |
| WashPost | Washington Post                         | 20.000000 |
| USAToday | USA Today                               | 25.000000 |
| Sport    | Sport Magazine                          | 20.000000 |
| InSports | Inside Sports                           | 20.000000 |
| UPI      | United Press International              | 19.000000 |
| AP       | Associated Press                        | 20.000000 |
| SI       | Sports Illustrated                      | 20.000000 |

The following statements produce [Output 73.2.2](#) and [Output 73.2.3](#):

```

data Basketball;
 set HoopsRanks;
 if _n_=1 then set MaxRank;
 array Services{10} CSN--SI;
 array MaxRanks{10} CSNMax--SIMax;
 keep School CSN--SI Weight;
 Weight=0;
 do i=1 to 10;
 if Services{i}=. then Services{i}=(MaxRanks{i}+36)/2;
 else Weight=Weight+1;
 end;
run;

ods graphics on;

proc princomp data=Basketball n=1 out=PCBasketball standard
 plots=patternprofile;
 var CSN--SI;
 weight Weight;
run;

```

### Output 73.2.2 Principal Components Analysis of Basketball Rankings Using PROC PRINCOMP

| Pre-Season 1985 College Basketball Rankings |              |             |             |             |             |
|---------------------------------------------|--------------|-------------|-------------|-------------|-------------|
| The PRINCOMP Procedure                      |              |             |             |             |             |
|                                             | Observations | 35          |             |             |             |
|                                             | Variables    | 10          |             |             |             |
| Simple Statistics                           |              |             |             |             |             |
|                                             | CSN          | DurSun      | DurHer      | WashPost    | USAToday    |
| Mean                                        | 13.33640553  | 13.06451613 | 12.88018433 | 13.83410138 | 12.55760369 |
| StD                                         | 22.08036285  | 21.66394183 | 21.38091837 | 23.47841791 | 20.48207965 |
| Simple Statistics                           |              |             |             |             |             |
|                                             | Sport        | InSports    | UPI         | AP          | SI          |
| Mean                                        | 13.83870968  | 13.24423963 | 13.59216590 | 12.83410138 | 13.52534562 |
| StD                                         | 23.37756267  | 22.20231526 | 23.25602811 | 21.40782406 | 22.93219584 |

## Output 73.2.2 continued

| Correlation Matrix |                                         | CSN    | DurSun | DurHer |
|--------------------|-----------------------------------------|--------|--------|--------|
| CSN                | Community Sports News (Chapel Hill, NC) | 1.0000 | 0.6505 | 0.6415 |
| DurSun             | Durham Sun                              | 0.6505 | 1.0000 | 0.8341 |
| DurHer             | Durham Morning Herald                   | 0.6415 | 0.8341 | 1.0000 |
| WashPost           | Washington Post                         | 0.6121 | 0.7667 | 0.7035 |
| USAToday           | USA Today                               | 0.7456 | 0.8860 | 0.8877 |
| Sport              | Sport Magazine                          | 0.4806 | 0.6940 | 0.7788 |
| InSports           | Inside Sports                           | 0.6558 | 0.7702 | 0.7900 |
| UPI                | United Press International              | 0.7007 | 0.9015 | 0.7676 |
| AP                 | Associated Press                        | 0.6779 | 0.8437 | 0.8788 |
| SI                 | Sports Illustrated                      | 0.6135 | 0.7518 | 0.7761 |

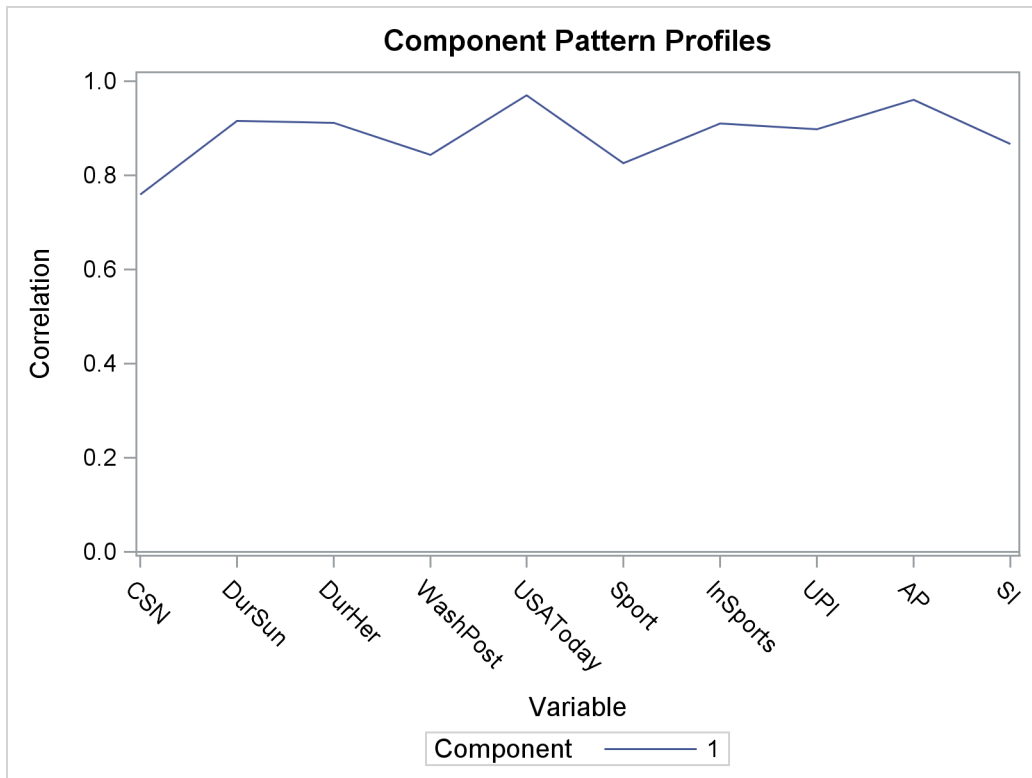
| Correlation Matrix |           |          |        |           |        |        |        |
|--------------------|-----------|----------|--------|-----------|--------|--------|--------|
|                    | Wash Post | USAToday | Sport  | In Sports | UPI    | AP     | SI     |
| CSN                | 0.6121    | 0.7456   | 0.4806 | 0.6558    | 0.7007 | 0.6779 | 0.6135 |
| DurSun             | 0.7667    | 0.8860   | 0.6940 | 0.7702    | 0.9015 | 0.8437 | 0.7518 |
| DurHer             | 0.7035    | 0.8877   | 0.7788 | 0.7900    | 0.7676 | 0.8788 | 0.7761 |
| WashPost           | 1.0000    | 0.7984   | 0.6598 | 0.8717    | 0.6953 | 0.7809 | 0.5952 |
| USAToday           | 0.7984    | 1.0000   | 0.7716 | 0.8475    | 0.8539 | 0.9479 | 0.8426 |
| Sport              | 0.6598    | 0.7716   | 1.0000 | 0.7176    | 0.6220 | 0.8217 | 0.7701 |
| InSports           | 0.8717    | 0.8475   | 0.7176 | 1.0000    | 0.7920 | 0.8830 | 0.7332 |
| UPI                | 0.6953    | 0.8539   | 0.6220 | 0.7920    | 1.0000 | 0.8436 | 0.7738 |
| AP                 | 0.7809    | 0.9479   | 0.8217 | 0.8830    | 0.8436 | 1.0000 | 0.8212 |
| SI                 | 0.5952    | 0.8426   | 0.7701 | 0.7332    | 0.7738 | 0.8212 | 1.0000 |

| Eigenvalues of the Correlation Matrix |            |            |            |            |
|---------------------------------------|------------|------------|------------|------------|
|                                       | Eigenvalue | Difference | Proportion | Cumulative |
| 1                                     | 7.88601647 |            | 0.7886     | 0.7886     |

| Eigenvectors |                                         |          |
|--------------|-----------------------------------------|----------|
|              |                                         | Prin1    |
| CSN          | Community Sports News (Chapel Hill, NC) | 0.270205 |
| DurSun       | Durham Sun                              | 0.326048 |
| DurHer       | Durham Morning Herald                   | 0.324392 |
| WashPost     | Washington Post                         | 0.300449 |
| USAToday     | USA Today                               | 0.345200 |
| Sport        | Sport Magazine                          | 0.293881 |
| InSports     | Inside Sports                           | 0.324088 |
| UPI          | United Press International              | 0.319902 |
| AP           | Associated Press                        | 0.342151 |
| SI           | Sports Illustrated                      | 0.308570 |

**Output 73.2.3** Pattern Profile Plot

The following statements produce [Output 73.2.4](#):

```
proc sort data=PCBasketball;
 by Prin1;
run;

proc print;
 var School Prin1;
 title 'Pre-Season 1985 College Basketball Rankings';
 title2 'College Teams as Ordered by PROC PRINCOMP';
run;
```

**Output 73.2.4** Basketball Rankings Using PROC PRINCOMP

Pre-Season 1985 College Basketball Rankings  
College Teams as Ordered by PROC PRINCOMP

| Obs | School        | Prin1    |
|-----|---------------|----------|
| 1   | Georgia Tech  | -0.58068 |
| 2   | UNC           | -0.53317 |
| 3   | Michigan      | -0.47874 |
| 4   | Kansas        | -0.40285 |
| 5   | Duke          | -0.38464 |
| 6   | Illinois      | -0.33586 |
| 7   | Syracuse      | -0.31578 |
| 8   | Louisville    | -0.31489 |
| 9   | Georgetown    | -0.29735 |
| 10  | Auburn        | -0.09785 |
| 11  | Kentucky      | 0.00843  |
| 12  | LSU           | 0.00872  |
| 13  | Notre Dame    | 0.09407  |
| 14  | NC State      | 0.19404  |
| 15  | UAB           | 0.19771  |
| 16  | Oklahoma      | 0.23864  |
| 17  | Memphis State | 0.25319  |
| 18  | Navy          | 0.28921  |
| 19  | UNLV          | 0.35103  |
| 20  | DePaul        | 0.43770  |
| 21  | Iowa          | 0.50213  |
| 22  | Indiana       | 0.51713  |
| 23  | Maryland      | 0.55910  |
| 24  | Arkansas      | 0.62977  |
| 25  | Virginia      | 0.67586  |
| 26  | Washington    | 0.67756  |
| 27  | Tennessee     | 0.70822  |
| 28  | St. Johns     | 0.71425  |
| 29  | Virginia Tech | 0.71638  |
| 30  | St. Joseph's  | 0.73492  |
| 31  | UCLA          | 0.73965  |
| 32  | Pittsburgh    | 0.75078  |
| 33  | Houston       | 0.75534  |
| 34  | Montana       | 0.75790  |
| 35  | Old Dominion  | 0.76821  |

## Example 73.3: Job Ratings

This example uses the PRINCOMP procedure to analyze job performance. Police officers were rated by their supervisors in 14 categories as part of standard police departmental administrative procedure.

The following statements create the Jobratings data set:

```
options validvarname=any;
data Jobratings;
 input 'Communication Skills'n 'Problem Solving'n
 'Learning Ability'n 'Judgment Under Pressure'n
 'Observational Skills'n 'Willingness to Confront Problems'n
 'Interest in People'n 'Interpersonal Sensitivity'n
 'Desire for Self-Improvement'n 'Appearance'n
 'Dependability'n 'Physical Ability'n
 'Integrity'n 'Overall Rating'n;
 datalines;
2 6 8 3 8 8 5 3 8 7 9 8 6 7 7 4 7 5 8 8 7 6 8 5 7 6 6 7 5 6 7 5 7 8 6 3 7 7 5
8 7 5 6 7 8 6 9 7 7 7 9 8 8 9 9 7 9 9 9 9 7 7 9 8 8 7 8 8 8 8 8 9 8 9 7 8 9 9
8 8 8 7 9 9 8 9 9 9 9 8 8 9 8 9 9 7 9 8 8 7 7 9 4 7 9 8 4 6 8 8 8 6 3 5 6 5 2
... more lines ...
7 8 9 9 7 9 9 7 9 9 9 9 8 9 9 8 9 9 8 9 9 8 9 9 7 6 6 5 6 3 9 9 5 6 7 4 8 6
;
```

The data set Jobratings contains 14 variables. Each variable contains the job ratings, using a scale measurement from 1 to 10 (1=fail to comply, 10=exceptional). The last variable Overall Rating contains a score as an overall index on how each officer performs.

The following statements request a principal component analysis on the Jobratings data set, output the scores to the Scores data set (OUT= Scores), and produce default plots. Note that variable Overall Rating is excluded from the analysis.

```
ods graphics on;

proc princomp data=Jobratings(drop='Overall Rating'n);
run;
```

Figure 73.3.1 and Figure 73.3.2 display the PROC PRINCOMP output, beginning with simple statistics followed by the correlation matrix. By default, the PROC PRINCOMP statement requests principal components computed from the correlation matrix, so the total variance is equal to the number of variables, 13. In this example, it would also be reasonable to use the COV option, which would cause variables with a high variance (such as Dependability) to have more influence on the results than variables with a low variance (such as Learning Ability). If you used the COV option, scores would be computed from centered rather than standardized variables.



**Output 73.3.1** Simple Statistics and Correlation Matrix from the PRINCOMP Procedure

| The PRINCOMP Procedure |                                  |                    |                           |                             |                      |
|------------------------|----------------------------------|--------------------|---------------------------|-----------------------------|----------------------|
|                        | Observations                     | 37                 |                           |                             |                      |
|                        | Variables                        | 13                 |                           |                             |                      |
| Simple Statistics      |                                  |                    |                           |                             |                      |
|                        | Communication Skills             | Problem Solving    | Learning Ability          | Judgment Under Pressure     | Observational Skills |
| Mean                   | 6.567567568                      | 6.675675676        | 6.891891892               | 6.378378378                 | 7.081081081          |
| StD                    | 1.878837414                      | 1.748873511        | 1.696135866               | 2.252792728                 | 1.816259563          |
| Simple Statistics      |                                  |                    |                           |                             |                      |
|                        | Willingness to Confront Problems | Interest in People | Interpersonal Sensitivity | Desire for Self-Improvement | Appearance           |
| Mean                   | 6.756756757                      | 6.675675676        | 6.540540541               | 7.027027027                 | 7.135135135          |
| StD                    | 2.126622327                      | 1.871631108        | 2.218540494               | 1.707605316                 | 1.436859271          |
| Simple Statistics      |                                  |                    |                           |                             |                      |
|                        | Dependability                    | Physical Ability   | Integrity                 |                             |                      |
| Mean                   | 7.027027027                      | 7.162162162        | 7.081081081               |                             |                      |
| StD                    | 1.499749729                      | 1.343988953        | 1.460182226               |                             |                      |

Output 73.3.1 continued

| Correlation Matrix               |                      |                 |                  |                         |
|----------------------------------|----------------------|-----------------|------------------|-------------------------|
|                                  | Communication Skills | Problem Solving | Learning Ability | Judgment Under Pressure |
| Communication Skills             | 1.0000               | 0.7254          | 0.3685           | 0.6107                  |
| Problem Solving                  | 0.7254               | 1.0000          | 0.6715           | 0.6877                  |
| Learning Ability                 | 0.3685               | 0.6715          | 1.0000           | 0.5126                  |
| Judgment Under Pressure          | 0.6107               | 0.6877          | 0.5126           | 1.0000                  |
| Observational Skills             | 0.4338               | 0.6207          | 0.7603           | 0.5761                  |
| Willingness to Confront Problems | 0.5708               | 0.6504          | 0.3545           | 0.6227                  |
| Interest in People               | 0.4646               | 0.3828          | 0.1024           | 0.5635                  |
| Interpersonal Sensitivity        | 0.2975               | 0.3113          | 0.3112           | 0.4915                  |
| Desire for Self-Improvement      | 0.0211               | 0.1890          | 0.3079           | 0.1489                  |
| Appearance                       | -.0086               | 0.1064          | 0.1885           | 0.1382                  |
| Dependability                    | -.2619               | -.0389          | 0.0121           | -.1347                  |
| Physical Ability                 | -.1145               | -.0361          | 0.0932           | -.1217                  |
| Integrity                        | -.2096               | -.1852          | -.1085           | -.1025                  |

| Correlation Matrix               |                      |                                  |                    |
|----------------------------------|----------------------|----------------------------------|--------------------|
|                                  | Observational Skills | Willingness to Confront Problems | Interest in People |
| Communication Skills             | 0.4338               | 0.5708                           | 0.4646             |
| Problem Solving                  | 0.6207               | 0.6504                           | 0.3828             |
| Learning Ability                 | 0.7603               | 0.3545                           | 0.1024             |
| Judgment Under Pressure          | 0.5761               | 0.6227                           | 0.5635             |
| Observational Skills             | 1.0000               | 0.4655                           | 0.2449             |
| Willingness to Confront Problems | 0.4655               | 1.0000                           | 0.4751             |
| Interest in People               | 0.2449               | 0.4751                           | 1.0000             |
| Interpersonal Sensitivity        | 0.4921               | 0.2170                           | 0.5652             |
| Desire for Self-Improvement      | 0.4113               | 0.1931                           | 0.3765             |
| Appearance                       | 0.0915               | 0.1111                           | 0.2750             |
| Dependability                    | -.1640               | 0.2286                           | 0.1220             |
| Physical Ability                 | 0.0741               | 0.1114                           | 0.0215             |
| Integrity                        | -.0549               | -.1813                           | 0.1115             |

| Correlation Matrix      |                           |                             |            |
|-------------------------|---------------------------|-----------------------------|------------|
|                         | Interpersonal Sensitivity | Desire for Self-Improvement | Appearance |
| Communication Skills    | 0.2975                    | 0.0211                      | -.0086     |
| Problem Solving         | 0.3113                    | 0.1890                      | 0.1064     |
| Learning Ability        | 0.3112                    | 0.3079                      | 0.1885     |
| Judgment Under Pressure | 0.4915                    | 0.1489                      | 0.1382     |

Output 73.3.1 continued

| Correlation Matrix               |                              |                                |            |
|----------------------------------|------------------------------|--------------------------------|------------|
|                                  | Interpersonal<br>Sensitivity | Desire for<br>Self-Improvement | Appearance |
| Observational Skills             | 0.4921                       | 0.4113                         | 0.0915     |
| Willingness to Confront Problems | 0.2170                       | 0.1931                         | 0.1111     |
| Interest in People               | 0.5652                       | 0.3765                         | 0.2750     |
| Interpersonal Sensitivity        | 1.0000                       | 0.5460                         | 0.4121     |
| Desire for Self-Improvement      | 0.5460                       | 1.0000                         | 0.5645     |
| Appearance                       | 0.4121                       | 0.5645                         | 1.0000     |
| Dependability                    | 0.0790                       | 0.2166                         | 0.5525     |
| Physical Ability                 | 0.1747                       | 0.3248                         | 0.3479     |
| Integrity                        | 0.1747                       | 0.3667                         | 0.4183     |

| Correlation Matrix               |               |                     |           |
|----------------------------------|---------------|---------------------|-----------|
|                                  | Dependability | Physical<br>Ability | Integrity |
| Communication Skills             | -.2619        | -.1145              | -.2096    |
| Problem Solving                  | -.0389        | -.0361              | -.1852    |
| Learning Ability                 | 0.0121        | 0.0932              | -.1085    |
| Judgment Under Pressure          | -.1347        | -.1217              | -.1025    |
| Observational Skills             | -.1640        | 0.0741              | -.0549    |
| Willingness to Confront Problems | 0.2286        | 0.1114              | -.1813    |
| Interest in People               | 0.1220        | 0.0215              | 0.1115    |
| Interpersonal Sensitivity        | 0.0790        | 0.1747              | 0.1747    |
| Desire for Self-Improvement      | 0.2166        | 0.3248              | 0.3667    |
| Appearance                       | 0.5525        | 0.3479              | 0.4183    |
| Dependability                    | 1.0000        | 0.5628              | 0.3415    |
| Physical Ability                 | 0.5628        | 1.0000              | 0.5027    |
| Integrity                        | 0.3415        | 0.5027              | 1.0000    |

Figure 73.3.2 displays the eigenvalues. The first principal component explains about 50% of the total variance, the second principal component explains about 13.6%, and the third principal component explains about 7.7%. Note that the eigenvalues sum to the total variance. The eigenvalues indicate that three to five components provide a good summary of the data, with three components accounting for about 71.7% of the total variance and five components explaining about 82.7%. Subsequent components contribute less than 5% each.

**Output 73.3.2** Eigenvalues and Eigenvectors from the PRINCOMP Procedure

| Eigenvalues of the Correlation Matrix |            |            |            |            |
|---------------------------------------|------------|------------|------------|------------|
|                                       | Eigenvalue | Difference | Proportion | Cumulative |
| 1                                     | 4.69468687 | 1.81899683 | 0.3611     | 0.3611     |
| 2                                     | 2.87569003 | 1.67100277 | 0.2212     | 0.5823     |
| 3                                     | 1.20468727 | 0.03118935 | 0.0927     | 0.6750     |
| 4                                     | 1.17349791 | 0.45846322 | 0.0903     | 0.7653     |
| 5                                     | 0.71503470 | 0.15713583 | 0.0550     | 0.8203     |
| 6                                     | 0.55789887 | 0.09269082 | 0.0429     | 0.8632     |
| 7                                     | 0.46520805 | 0.04118763 | 0.0358     | 0.8990     |
| 8                                     | 0.42402041 | 0.13454552 | 0.0326     | 0.9316     |
| 9                                     | 0.28947489 | 0.06869311 | 0.0223     | 0.9539     |
| 10                                    | 0.22078178 | 0.03221769 | 0.0170     | 0.9708     |
| 11                                    | 0.18856410 | 0.06620108 | 0.0145     | 0.9853     |
| 12                                    | 0.12236302 | 0.05427092 | 0.0094     | 0.9948     |
| 13                                    | 0.06809210 |            | 0.0052     | 1.0000     |

## Output 73.3.2 continued

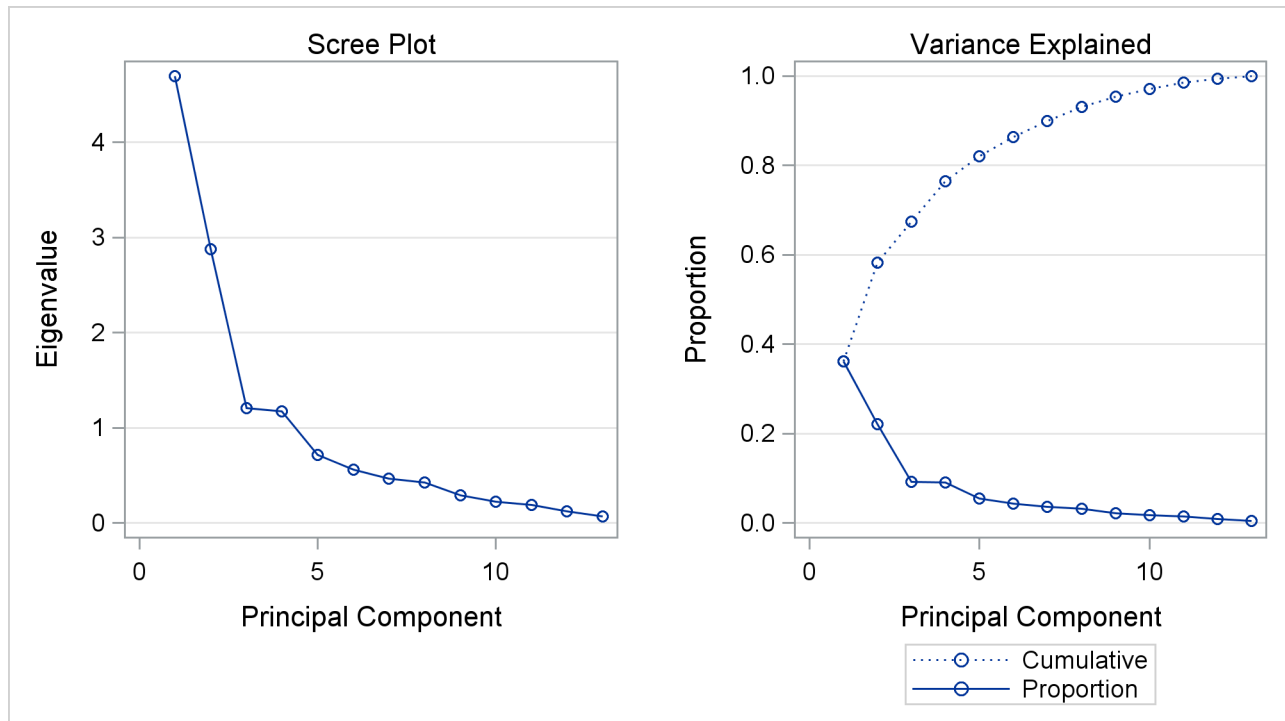
| Eigenvectors                     |          |          |          |          |
|----------------------------------|----------|----------|----------|----------|
|                                  | Prin1    | Prin2    | Prin3    | Prin4    |
| Communication Skills             | 0.323548 | -.236730 | 0.206727 | 0.092655 |
| Problem Solving                  | 0.383857 | -.160898 | -.091224 | 0.212751 |
| Learning Ability                 | 0.322899 | -.050464 | -.553565 | 0.056656 |
| Judgment Under Pressure          | 0.379958 | -.142821 | 0.155157 | -.025467 |
| Observational Skills             | 0.359246 | -.067434 | -.424397 | -.148191 |
| Willingness to Confront Problems | 0.333754 | -.064285 | 0.183338 | 0.459764 |
| Interest in People               | 0.296160 | 0.082187 | 0.575827 | -.140226 |
| Interpersonal Sensitivity        | 0.302693 | 0.180810 | 0.119231 | -.432281 |
| Desire for Self-Improvement      | 0.225795 | 0.344251 | -.123236 | -.333516 |
| Appearance                       | 0.158341 | 0.425329 | 0.052469 | -.022665 |
| Dependability                    | 0.025597 | 0.427337 | 0.079019 | 0.520679 |
| Physical Ability                 | 0.052980 | 0.418985 | -.185687 | 0.312555 |
| Integrity                        | -.006172 | 0.435225 | 0.015874 | -.147905 |
| Eigenvectors                     |          |          |          |          |
|                                  | Prin5    | Prin6    | Prin7    | Prin8    |
| Communication Skills             | 0.293138 | 0.260352 | -.215988 | -.550645 |
| Problem Solving                  | 0.025258 | 0.252518 | -.140816 | -.104392 |
| Learning Ability                 | -.138393 | 0.168405 | 0.150062 | 0.055518 |
| Judgment Under Pressure          | 0.043612 | 0.175269 | 0.361045 | 0.391055 |
| Observational Skills             | 0.093417 | -.221005 | 0.022944 | 0.177808 |
| Willingness to Confront Problems | -.024447 | -.304704 | -.247094 | 0.259896 |
| Interest in People               | 0.023973 | -.159653 | -.015476 | 0.131682 |
| Interpersonal Sensitivity        | -.047507 | -.238610 | 0.501550 | -.303435 |
| Desire for Self-Improvement      | -.174557 | -.266896 | -.621875 | 0.020842 |
| Appearance                       | -.441729 | 0.494677 | -.051864 | -.204081 |
| Dependability                    | -.289013 | -.044047 | 0.221520 | 0.079762 |
| Physical Ability                 | 0.486621 | -.299641 | 0.145579 | -.340453 |
| Integrity                        | 0.578186 | 0.421421 | -.087126 | 0.396179 |
| Eigenvectors                     |          |          |          |          |
|                                  | Prin9    | Prin10   | Prin11   | Prin12   |
| Communication Skills             | -.050648 | 0.107002 | 0.262509 | 0.341232 |
| Problem Solving                  | 0.283104 | 0.221940 | -.548010 | -.492803 |
| Learning Ability                 | 0.391053 | -.223399 | 0.132338 | 0.442471 |
| Judgment Under Pressure          | -.315796 | -.392714 | -.286021 | 0.111225 |
| Observational Skills             | -.141401 | 0.225326 | 0.502509 | -.416669 |
| Willingness to Confront Problems | -.387665 | 0.158552 | 0.047611 | 0.168464 |
| Interest in People               | 0.540942 | -.277206 | 0.299254 | -.197252 |
| Interpersonal Sensitivity        | -.097727 | 0.393688 | -.196906 | 0.137833 |
| Desire for Self-Improvement      | 0.018350 | -.105222 | -.293349 | 0.219662 |
| Appearance                       | -.350816 | -.186793 | 0.226289 | -.256802 |

Output 73.3.2 *continued*

| Eigenvectors                     |          |          |          |          |
|----------------------------------|----------|----------|----------|----------|
|                                  | Prin9    | Prin10   | Prin11   | Prin12   |
| Dependability                    | 0.250326 | 0.336689 | 0.049300 | 0.146711 |
| Physical Ability                 | -.072184 | -.432711 | -.090520 | -.154868 |
| Integrity                        | 0.030130 | 0.284351 | 0.021483 | 0.113790 |
| Eigenvectors                     |          |          |          |          |
|                                  | Prin13   |          |          |          |
| Communication Skills             | 0.291574 |          |          |          |
| Problem Solving                  | -.073999 |          |          |          |
| Learning Ability                 | -.307096 |          |          |          |
| Judgment Under Pressure          | 0.382730 |          |          |          |
| Observational Skills             | 0.278776 |          |          |          |
| Willingness to Confront Problems | -.459746 |          |          |          |
| Interest in People               | -.112818 |          |          |          |
| Interpersonal Sensitivity        | -.222427 |          |          |          |
| Desire for Self-Improvement      | 0.263644 |          |          |          |
| Appearance                       | -.177399 |          |          |          |
| Dependability                    | 0.445532 |          |          |          |
| Physical Ability                 | -.034075 |          |          |          |
| Integrity                        | -.129601 |          |          |          |

PROC PRINCOMP produces the scree plot as shown in [Figure 73.3.3](#) by default when ODS Graphics is enabled. You can obtain more plots by specifying the PLOTS= option in the PROC PRINCOMP statement.

The “Scree Plot” on the left shows that the eigenvalue of the first component is approximately 6.5 and the eigenvalue of the second component is largely decreased to under 2.0. The “Variance Explained” plot on the right shows that you can explain a near 80% of total variance with the first four principal components.

**Output 73.3.3** Scree Plot from the PRINCOMP Procedure

The first component reflects overall performance since the first eigenvector shows approximately equal loadings on all variables. The second eigenvector has high positive loadings on the variables Observational Skills and Willingness to Confront Problems but even higher negative loadings on the variables Interest in People and Interpersonal Sensitivity. This component seems to reflect the ability to take action, but it also reflects a lack of interpersonal skills. The third eigenvector has a very high positive loading on the variable Physical Ability and high negative loadings on the variables Problem Solving and Learning Ability. This component seems to reflect physical strength, but also shows poor learning and problem-solving skills.

In short, the three components represent the following:

First Component: overall performance  
 Second Component: smart, tough, and introverted  
 Third Component: superior strength and average intellect

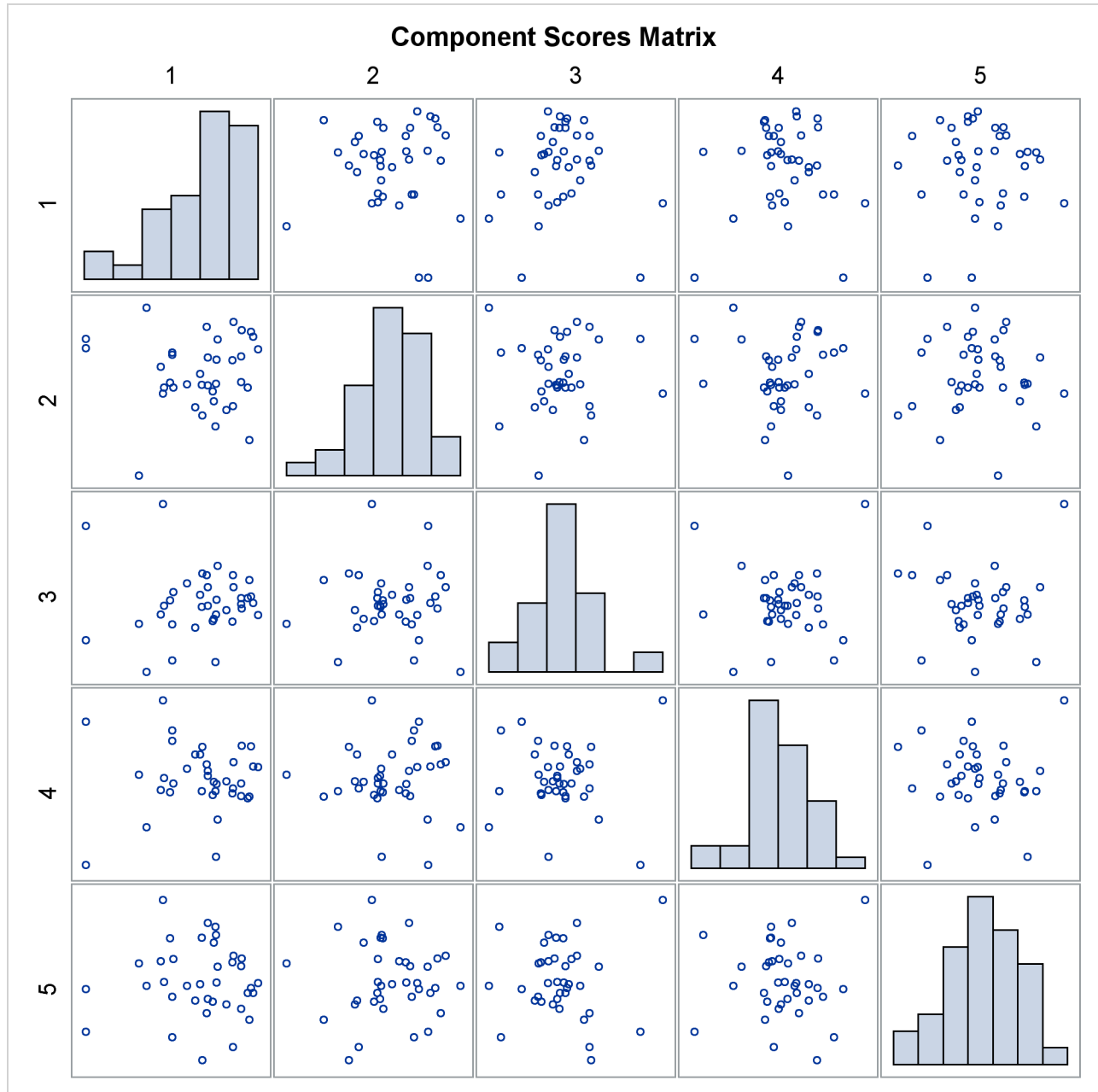
PROC PRINCOMP also produces other plots besides the scree plot, which are helpful while interpreting the results. The following statements request plots from the PRINCOMP procedure:

```
proc princomp data=Jobratings (drop='Overall Rating'n)
 plots (ncomp=3)=all n=5;
run;
```

PLOTS=ALL(NCOMP=3) in the PROC PRINCOMP statement requests all plots to be produced but limits the number of components to be plotted in the component pattern plots and the component score plots to three. The N=5 option sets the number of principal components to be computed to five. Besides a scree plot similar to the one shown before, the rest of plots are displayed in the following context.

Output 73.3.4 shows a matrix plot of component scores between the first five principal components. The histogram of each component is displayed in the diagonal element of the matrix. The histograms indicate that the first principal component is skewed to the left and the second principal component is slightly skewed to the right.

**Output 73.3.4** Matrix Plot of Component Scores

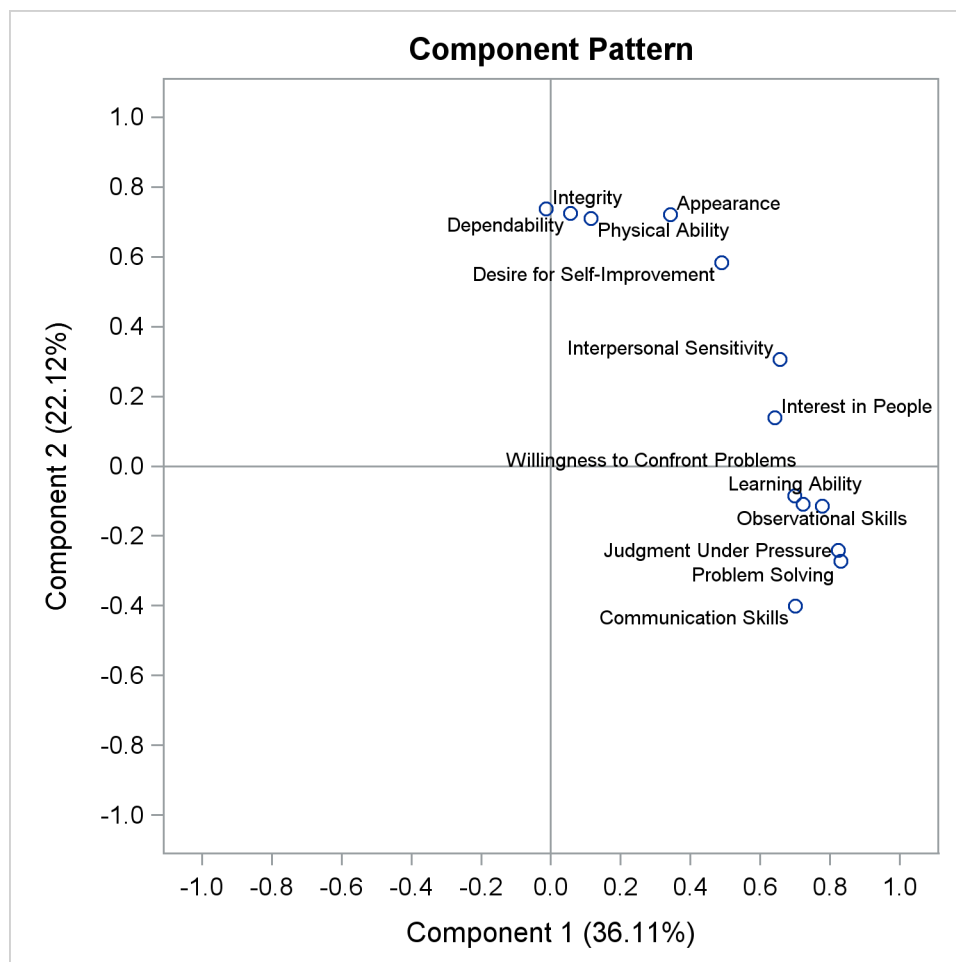




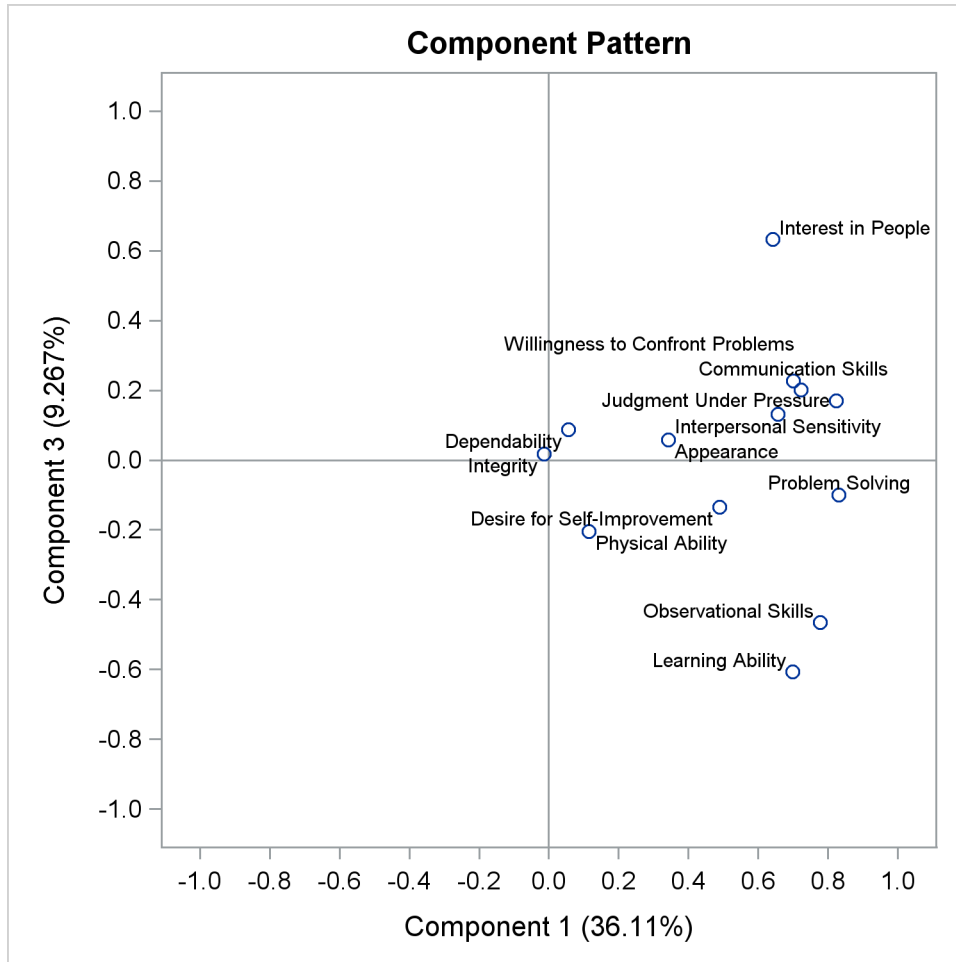
The pairwise component pattern plots are shown in [Output 73.3.5](#) to [Output 73.3.7](#). The pattern plots show the following:

- All variables positively and evenly correlate with the first principal component ([Output 73.3.5](#) and [Output 73.3.6](#)).
- The variables Observational Skills and Willingness to Confront Problems correlate highly with the second component, and the variables Interest in People and Interpersonal Sensitivity correlate highly but negatively with the second component ([Output 73.3.5](#)).
- The variable Physical Ability correlates highly with the third component, and the variables Problem Solving and Learning Ability correlate highly but negatively with the third component ([Output 73.3.6](#)).
- The variable Observational Skills, Willingness to Confront Problems, Interest in People, and Interpersonal Sensitivity correlate highly (either positively or negatively) with the second component, but all have very low correlations with the third component; the variables Physical Ability and Problem Solving correlate highly (either positively or negatively) with the third component, but both have very low correlations with the second component ([Output 73.3.7](#)).

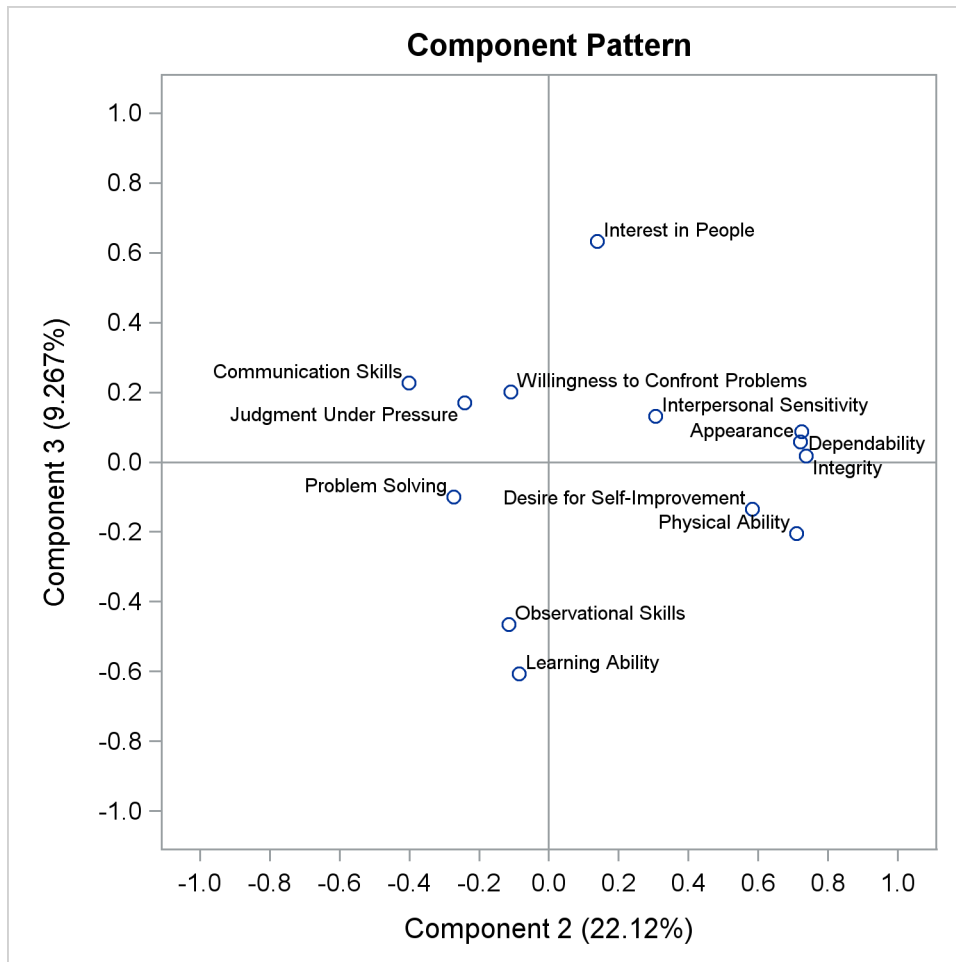
**Output 73.3.5** Pattern Plot of Component 2 by Component 1



**Output 73.3.6** Pattern Plot of Component 3 by Component 1

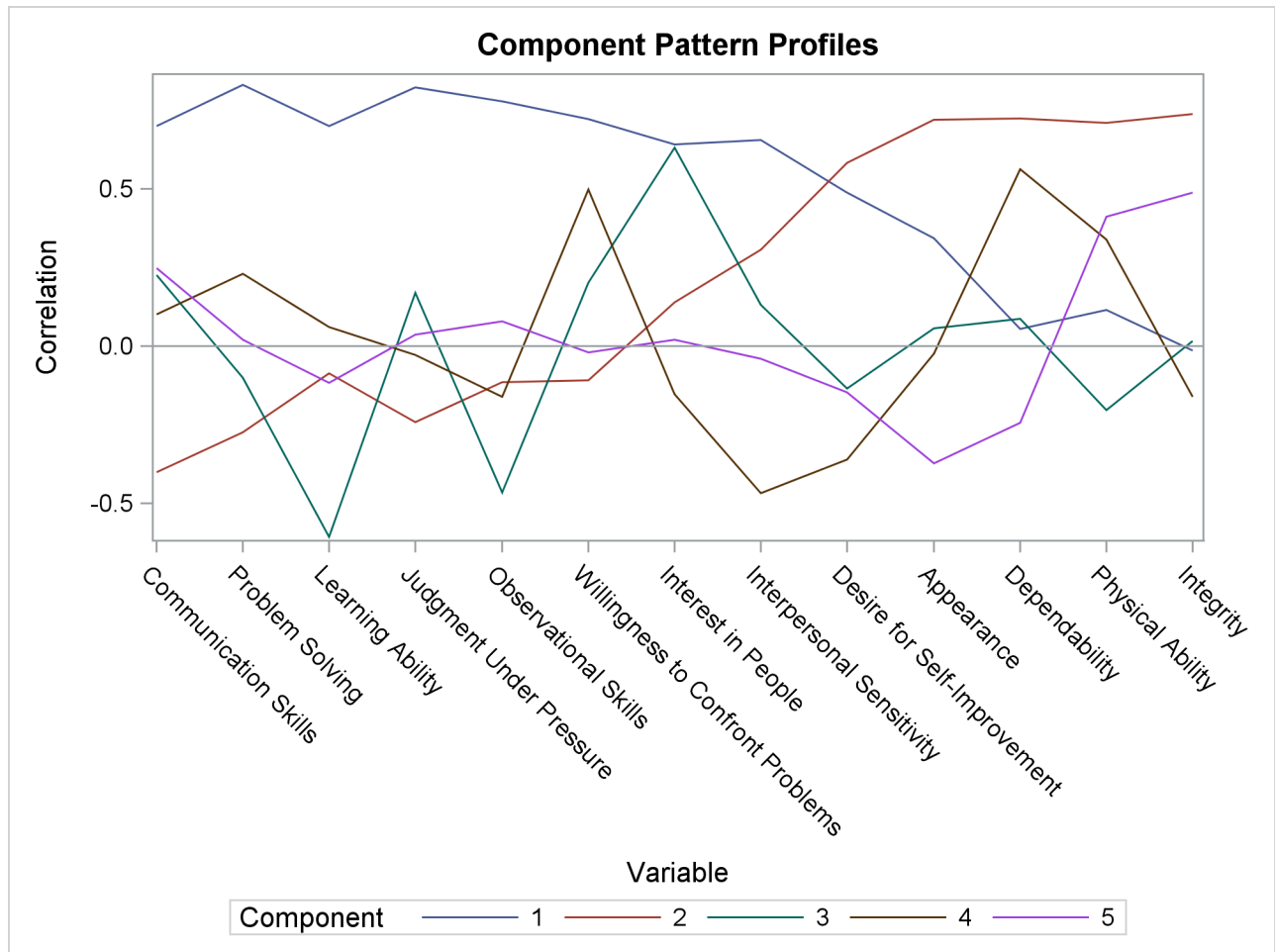


**Output 73.3.7** Pattern Plot of Component 3 by Component 2



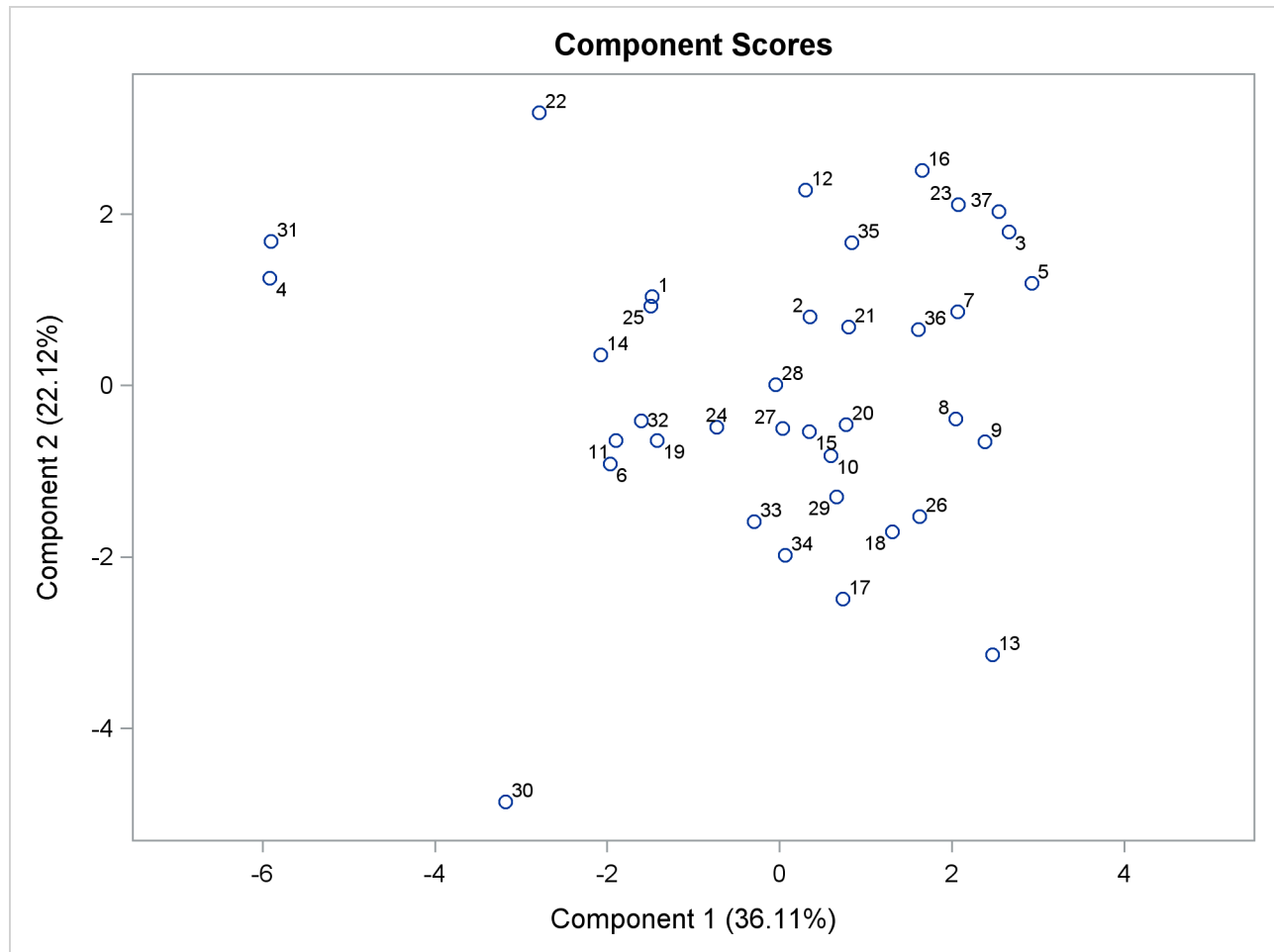
Output 73.3.8 shows a component pattern profile. As it was shown in the pattern plots, the nearly horizontal profile from the first component indicates that the first component is mostly correlated evenly across all variables.

**Output 73.3.8** Component Pattern Profile Plot from the PRINCOMP Procedure



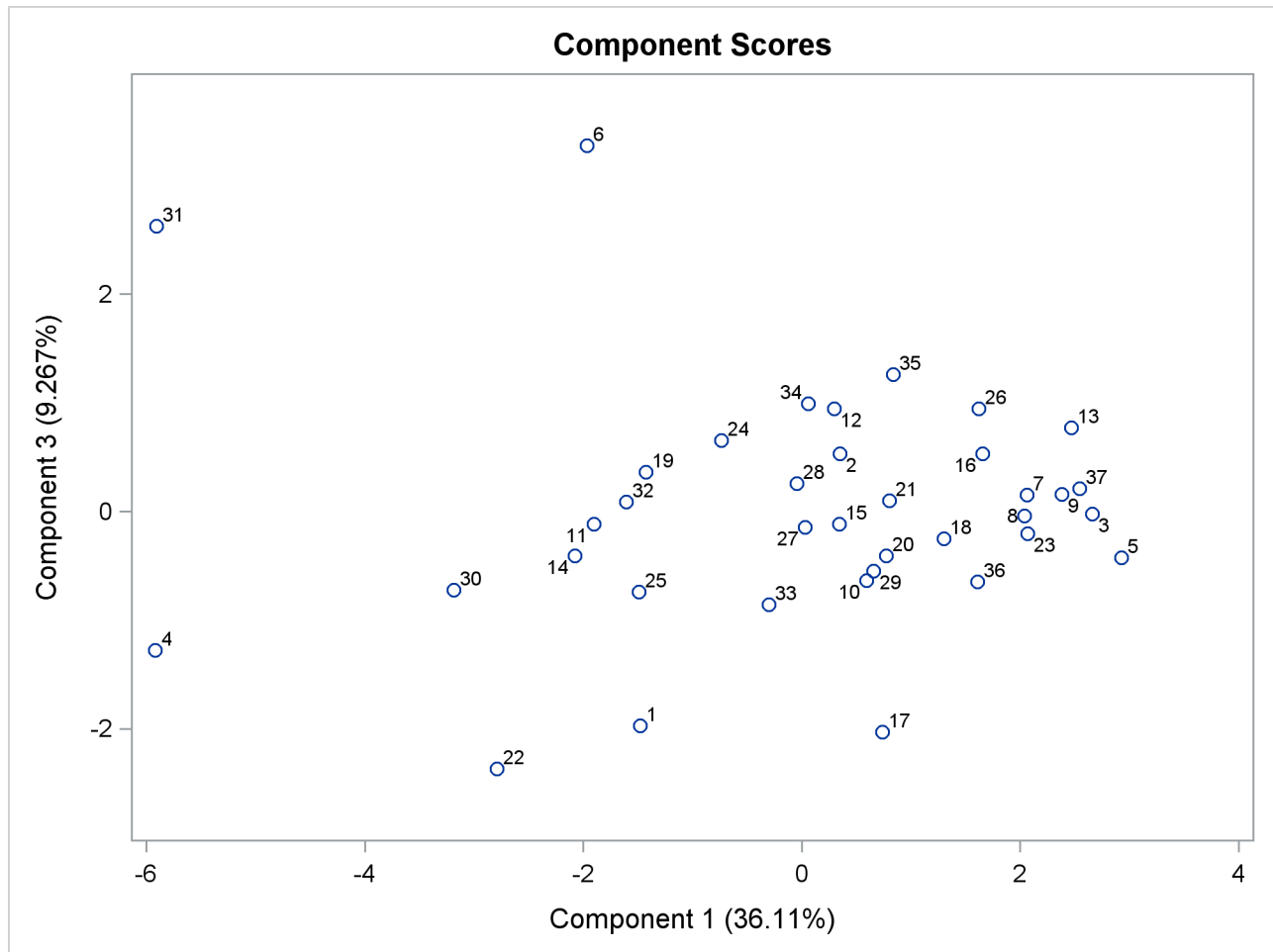
Output 73.3.9 through Output 73.3.11 display the pairwise component score plots. Observation numbers are used as the plotting symbol.

Output 73.3.9 shows a scatter plot of the first and third components. Observations 82, 9, and 84 seem like outliers on the first component; Observations 16 and 59 can be potential outliers on the second component.

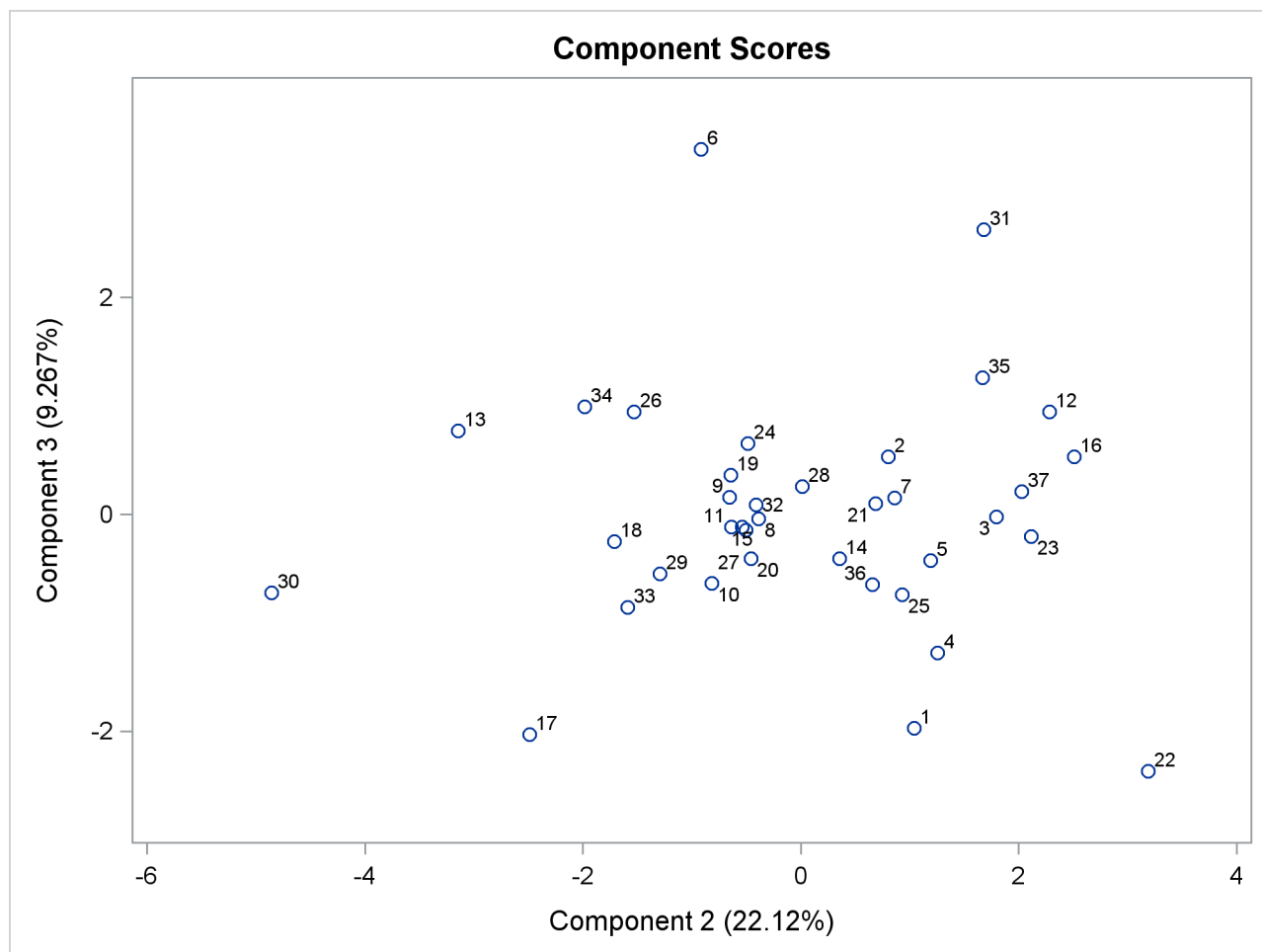
**Output 73.3.9** Component 2 versus Component 1

Output 73.3.10 shows a scatter plot of the first and third components. Observations 82, 9, and 84 seem like outliers on the first component.

**Output 73.3.10** Component 3 versus Component 1

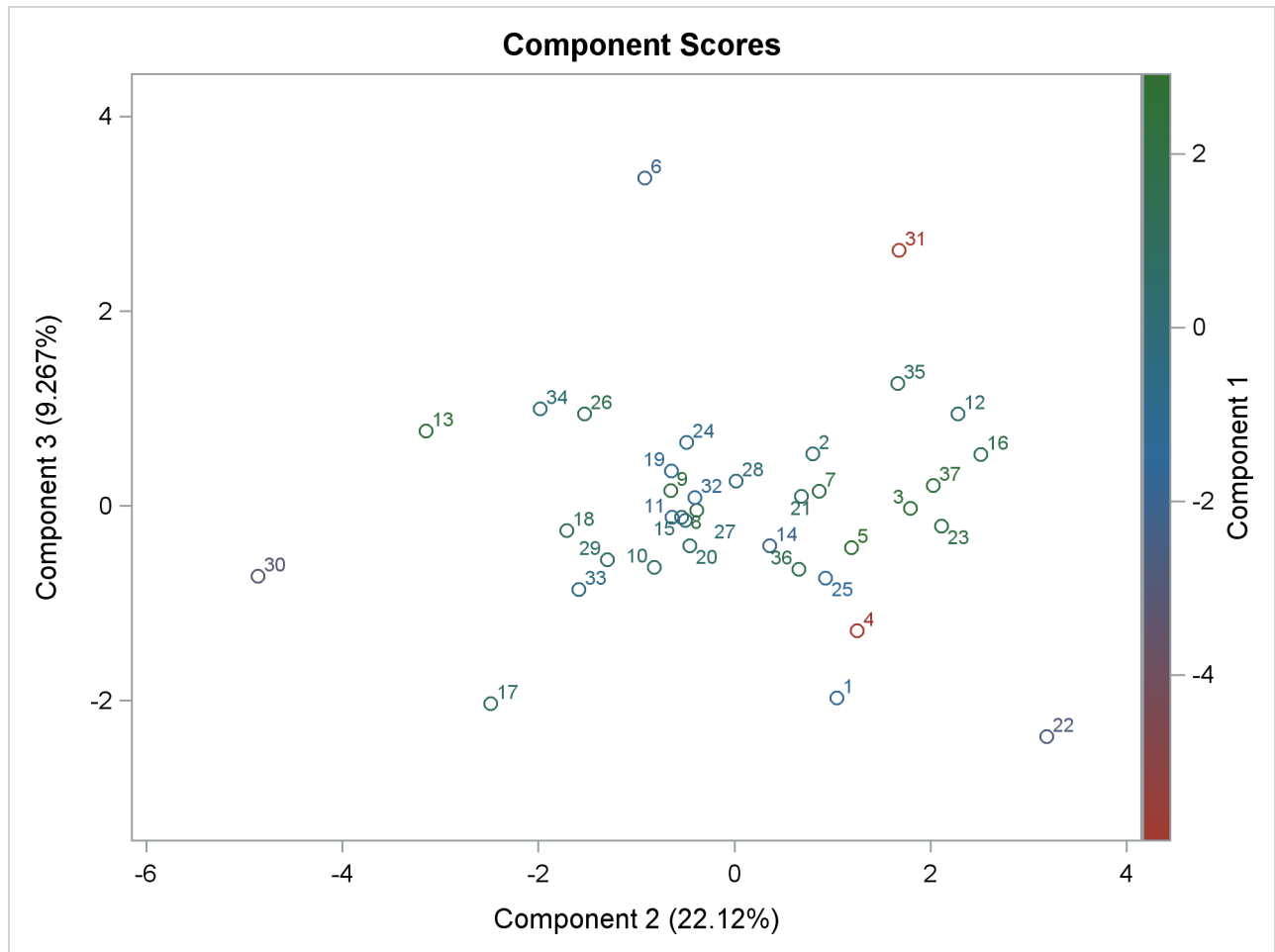


Output 73.3.11 shows a scatter plot of the second and third components. Observations 95, 15, 16, and 59 can be potential outliers on the second component.

**Output 73.3.11** Component 3 versus Component 2

Output 73.3.12 shows a scatter plot of the second and third components, displaying the first component with color. Color interpolation in the HTMLBLUE style ranges from red (minimum) to blue (middle) and to green (maximum).

**Output 73.3.12** Component 3 versus Component 2, Painted by Component 1





---

## References

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# Chapter 74

## The PRINQUAL Procedure

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## Overview: PRINQUAL Procedure

The PRINQUAL procedure performs principal component analysis (PCA) of qualitative, quantitative, or mixed data. PROC PRINQUAL is based on the work of Kruskal and Shepard (1974); Young, Takane, and de Leeuw (1978); Young (1981); Winsberg and Ramsay (1983). PROC PRINQUAL finds linear and non-linear transformations of variables, using the method of alternating least squares, that optimize properties of the transformed variables' correlation or covariance matrix. Nonoptimal transformations such as logarithm and rank are also available. You can use ODS Graphics to display the results. You can use PROC PRINQUAL to do the following:

- fit metric and nonmetric principal component analyses
- perform metric and nonmetric multidimensional preference (MDPREF) analyses (Carroll 1972)
- transform data prior to their use in other analyses
- reduce the number of variables for subsequent use in regression analyses, cluster analyses, and other analyses
- detect nonlinear relationships

PROC PRINQUAL provides three methods, each of which seeks to optimize a different property of the transformed variables' covariance or correlation matrix. These methods are as follows:

- maximum total variance, or MTV
- minimum generalized variance, or MGV
- maximum average correlation, or MAC

The MTV method is based on a PCA model, and it is the most commonly used method. All three methods attempt to find transformations that decrease the rank of the covariance matrix computed from the transformed variables. Transforming the variables to maximize the total variance accounted for by a few linear combinations locates the observations in a space with a dimensionality that approximates the stated number of linear combinations as much as possible, given the transformation constraints. Transforming the variables to minimize their generalized variance or maximize the average correlations also reduces the dimensionality, but without a stated target for the final dimensionality. See the section [“The Three Methods of Variable Transformation”](#) on page 6311 for more information about all three methods.

The data can contain variables measured on nominal, ordinal, interval, and ratio scales of measurement (Siegel 1956). Any mix is allowed with all methods. PROC PRINQUAL can do the following:

- transform nominal variables by optimally scoring the categories (Fisher 1938)
- transform ordinal variables monotonically by scoring the ordered categories so that order is weakly preserved (adjacent categories can be merged) and the covariance matrix is optimized. You can undo ties optimally or leave them tied (Kruskal 1964). You can also transform ordinal variables to ranks.
- transform interval and ratio scale of measurement variables linearly, or transform them nonlinearly with spline transformations (de Boor 1978; van Rijckevorsel 1982) or monotone spline transformations (Winsberg and Ramsay 1983). In addition, nonoptimal transformations for logarithm, rank, exponential, power, logit, and inverse trigonometric sine are available.
- estimate missing data without constraint, with category constraints (missing values within the same group get the same value), and with order constraints (missing value estimates in adjacent groups can be tied to preserve a specified ordering). See Gifi (1990) and Young (1981).

The transformed qualitative (nominal and ordinal) variables can be thought of as being quantified by the analysis, with the quantification done in the context set by the algorithm. The data are quantified so that the proportion of variance accounted for by a stated number of principal components is locally maximized, the generalized variance of the variables is locally minimized, or the average of the correlations is locally maximized.

The PROC PRINQUAL iterations produce a set of transformed variables. Each variable's new scoring satisfies a set of constraints based on the original scoring of the variable and the specified transformation type. First, all variables are required to satisfy standardization constraints; that is, all variables have a fixed mean and variance. The other constraints include linear constraints, weak order constraints, category constraints, and smoothness constraints. The new set of scores is selected from the sets of possible scorings that do not violate the constraints so that the method criterion is locally optimized.

## Getting Started: PRINQUAL Procedure

PROC PRINQUAL can be used to fit a principal component model with nonlinear transformations of the variables and graphically display the results. This example finds monotonic transformations of ratings of automobiles.

```

title 'Ratings for Automobiles Manufactured in 1980';

data cars;
 input Origin $ 1-8 Make $ 10-19 Model $ 21-36
 (MPG Reliability Acceleration Braking Handling Ride
 Visibility Comfort Quiet Cargo) (1.);
 datalines;
GMC Buick Century 3334444544
GMC Buick Electra 2434453555
GMC Buick Lesabre 2354353545
GMC Buick Regal 3244443424

... more lines ...

GMC Pontiac Sunbird 3134533234
;

ods graphics on;

proc prinqual data=cars plots=all maxiter=100;
 transform monotone(mpg -- cargo);
 id model;
run;

```

The PROC PRINQUAL statement names the input data set Cars. The ODS GRAPHICS statement, along with the PLOTS=ALL option, requests all graphical displays. The MDPREF option requests the PCA plot with the scores (automobiles) represented as points and the structure (variables) represented as vectors. By default, the vector lengths are increased by a factor of 2.5 to produce a better graphical display. If instead you were to specify MDPREF=1, you would get the actual vectors, and they would all be short and would end near the origin where there are a lot of points. It is often the case that increasing the vector lengths by a factor of 2 or 3 makes a better graphical display, so by default the vector lengths are increased by a factor of 2.5. Up to 100 iterations are requested with the MAXITER= option. All of the numeric variable are specified with a MONOTONE transformation, so their original values, 1 to 5, are optimally rescored to maximize fit to a two-component model while preserving the original order. The Model variable provides the labels for the row points in the plot.

The iteration history table is shown in [Figure 74.1](#). The monotonic transformations allow the PCA to account for 5% more variance in two principal components than the ordinary PCA model applied to the untransformed data.

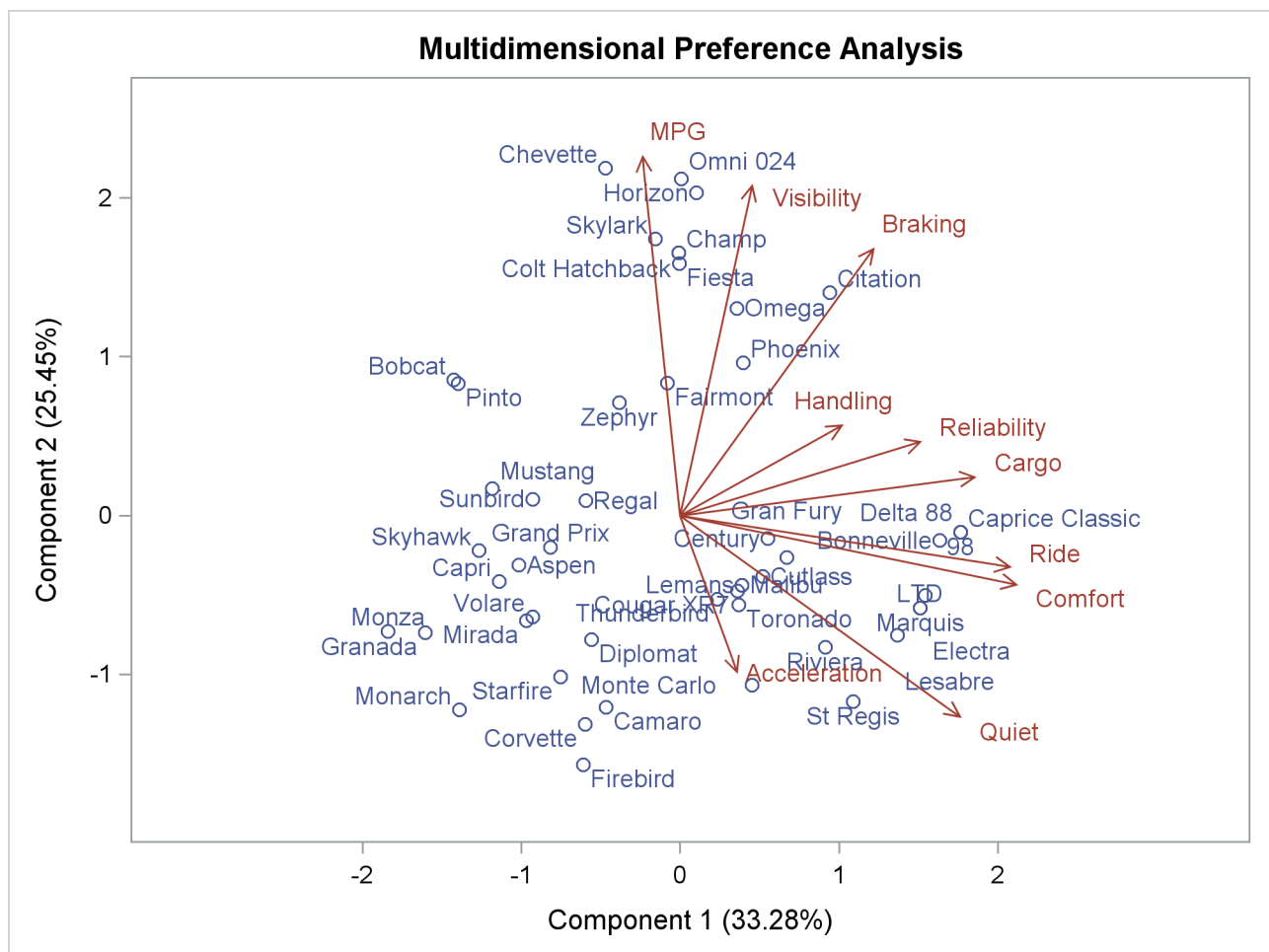
Figure 74.1 Automobile Ratings Iteration History

| Ratings for Automobiles Manufactured in 1980 |                   |                   |                           |                     |           |
|----------------------------------------------|-------------------|-------------------|---------------------------|---------------------|-----------|
| The PRINQUAL Procedure                       |                   |                   |                           |                     |           |
| PRINQUAL MTV Algorithm Iteration History     |                   |                   |                           |                     |           |
| Iteration<br>Number                          | Average<br>Change | Maximum<br>Change | Proportion<br>of Variance | Criterion<br>Change | Note      |
| 1                                            | 0.18087           | 1.24219           | 0.53742                   |                     |           |
| 2                                            | 0.06916           | 0.77503           | 0.57244                   | 0.03502             |           |
| 3                                            | 0.04653           | 0.38237           | 0.57978                   | 0.00734             |           |
| 4                                            | 0.03387           | 0.18682           | 0.58300                   | 0.00321             |           |
| 5                                            | 0.02661           | 0.13506           | 0.58484                   | 0.00185             |           |
| 6                                            | 0.01730           | 0.09213           | 0.58600                   | 0.00115             |           |
| 7                                            | 0.00969           | 0.07107           | 0.58660                   | 0.00061             |           |
| 8                                            | 0.00705           | 0.04798           | 0.58685                   | 0.00025             |           |
| 9                                            | 0.00544           | 0.03482           | 0.58699                   | 0.00014             |           |
| 10                                           | 0.00442           | 0.02641           | 0.58708                   | 0.00009             |           |
| 11                                           | 0.00363           | 0.02062           | 0.58714                   | 0.00006             |           |
| 12                                           | 0.00298           | 0.01643           | 0.58717                   | 0.00004             |           |
| 13                                           | 0.00245           | 0.01325           | 0.58720                   | 0.00002             |           |
| 14                                           | 0.00201           | 0.01077           | 0.58721                   | 0.00002             |           |
| 15                                           | 0.00165           | 0.00880           | 0.58723                   | 0.00001             |           |
| 16                                           | 0.00136           | 0.00721           | 0.58723                   | 0.00001             |           |
| 17                                           | 0.00112           | 0.00591           | 0.58724                   | 0.00001             |           |
| 18                                           | 0.00092           | 0.00485           | 0.58724                   | 0.00000             |           |
| 19                                           | 0.00075           | 0.00399           | 0.58724                   | 0.00000             |           |
| 20                                           | 0.00062           | 0.00328           | 0.58725                   | 0.00000             |           |
| 21                                           | 0.00051           | 0.00269           | 0.58725                   | 0.00000             |           |
| 22                                           | 0.00042           | 0.00221           | 0.58725                   | 0.00000             |           |
| 23                                           | 0.00035           | 0.00182           | 0.58725                   | 0.00000             |           |
| 24                                           | 0.00028           | 0.00149           | 0.58725                   | 0.00000             |           |
| 25                                           | 0.00023           | 0.00123           | 0.58725                   | 0.00000             |           |
| 26                                           | 0.00019           | 0.00101           | 0.58725                   | 0.00000             |           |
| 27                                           | 0.00016           | 0.00083           | 0.58725                   | 0.00000             |           |
| 28                                           | 0.00013           | 0.00068           | 0.58725                   | 0.00000             |           |
| 29                                           | 0.00011           | 0.00056           | 0.58725                   | 0.00000             |           |
| 30                                           | 0.00009           | 0.00046           | 0.58725                   | 0.00000             |           |
| 31                                           | 0.00007           | 0.00038           | 0.58725                   | 0.00000             |           |
| 32                                           | 0.00006           | 0.00031           | 0.58725                   | 0.00000             |           |
| 33                                           | 0.00005           | 0.00025           | 0.58725                   | 0.00000             |           |
| 34                                           | 0.00004           | 0.00021           | 0.58725                   | 0.00000             |           |
| 35                                           | 0.00003           | 0.00017           | 0.58725                   | 0.00000             |           |
| 36                                           | 0.00003           | 0.00014           | 0.58725                   | 0.00000             |           |
| 37                                           | 0.00002           | 0.00012           | 0.58725                   | 0.00000             |           |
| 38                                           | 0.00002           | 0.00010           | 0.58725                   | 0.00000             |           |
| 39                                           | 0.00001           | 0.00008           | 0.58725                   | 0.00000             |           |
| 40                                           | 0.00001           | 0.00006           | 0.58725                   | 0.00000             |           |
| 41                                           | 0.00001           | 0.00005           | 0.58725                   | 0.00000             |           |
| 42                                           | 0.00001           | 0.00004           | 0.58725                   | 0.00000             | Converged |

Algorithm converged.

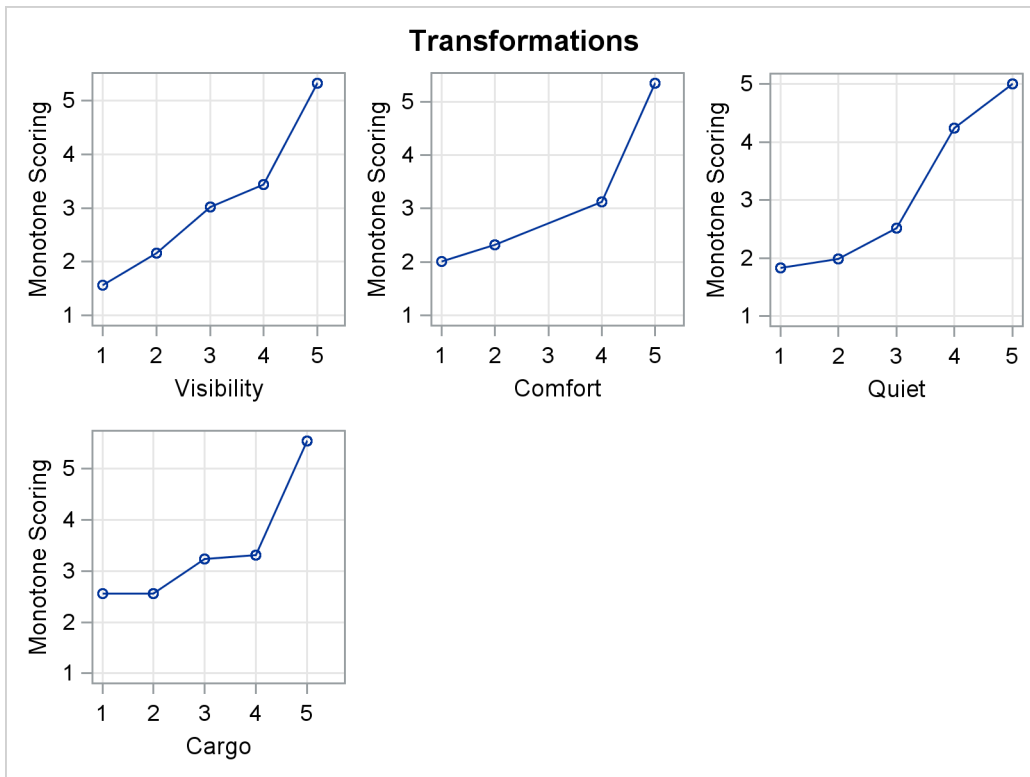
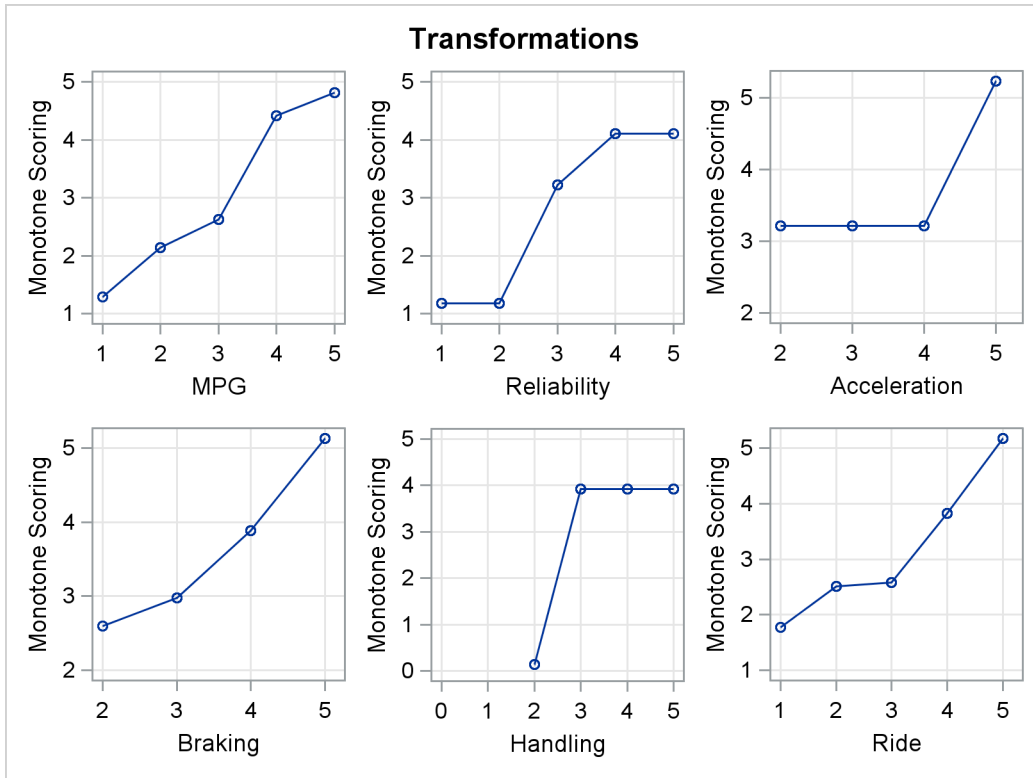
The PCA biplot in Figure 74.2 shows the transformed automobile ratings projected into the two-dimensional plane of the analysis. The automobiles on the left tend to be smaller than the autos on the right, and the autos at the top tend to be cheaper than the autos at the bottom. The vectors can help you interpret the plot of the scores. Longer vectors show the variables that better fit the two-dimensional model. In contrast, shorter vectors show the variables that do not fit the two-dimensional model as well. They tend to be located less in the plot and more away from the plot; hence their projection into the plot is shorter. To envision this, lay a pencil on your desk directly under a light, and slowly rotate it up to form a 90-degree angle with your desk. As you do so, the shadow or projection of the pencil onto your desk will get progressively shorter. The results show, for example, that the Chevette would be expected to do well on gas mileage but not well on quiet and acceleration. In contrast, the Corvette and the Firebird have the opposite pattern.

**Figure 74.2** Automobile Ratings PCA Biplot



There are many patterns shown in the transformations in Figure 74.3. The transformation of Braking, for example, is not very different from the original scoring. The optimal scoring for other variables, such as Acceleration and Handling, is binary. Automobiles are differentiated by high versus everything else or low versus everything else.

**Figure 74.3** Automobile Ratings Transformations





---

## Syntax: PRINQUAL Procedure

The following statements are available in the PRINQUAL procedure:

```

PROC PRINQUAL < options > ;
 TRANSFORM transform(variables < / t-options >)
 < transform(variables < / t-options >)... > ;
 ID variables ;
 FREQ variable ;
 WEIGHT variable ;
 BY variables ;

```

To use PROC PRINQUAL, you need the PROC PRINQUAL and TRANSFORM statements. You can abbreviate all *options* and *t-options* to their first three letters. This is a special feature of PROC PRINQUAL and is not generally true of other SAS/STAT procedures.

The rest of this section provides detailed syntax information about each of the preceding statements, beginning with the PROC PRINQUAL statement. The remaining statements are described in alphabetical order.

---

## PROC PRINQUAL Statement

```

PROC PRINQUAL < options > ;

```

The PROC PRINQUAL statement invokes the PRINQUAL procedure. Optionally, this statement identifies an input data set, creates an output data set, specifies the algorithm and other computational details, and controls displayed output. Table 74.1 summarizes the options available in the PROC PRINQUAL statement.

**Table 74.1** Summary of PROC PRINQUAL Statement Options

| Option                         | Description                                         |
|--------------------------------|-----------------------------------------------------|
| <b>Input Data Set Options</b>  |                                                     |
| DATA=                          | Specifies input SAS data set                        |
| <b>Output Data Set Details</b> |                                                     |
| APPROXIMATIONS                 | Outputs approximations to transformed variables     |
| APREFIX=                       | Specifies prefix for approximation variables        |
| CORRELATIONS                   | Outputs correlations and component structure matrix |
| MDPREF=                        | Specifies a multidimensional preference analysis    |
| OUT=                           | Specifies output data set                           |
| PREFIX=                        | Specifies prefix for principal component scores     |
| REPLACE                        | Replaces raw data with transformed data             |
| SCORES                         | Outputs principal component scores                  |
| STANDARD                       | Standardizes principal component scores             |
| TPREFIX=                       | Specifies prefix for transformed variables          |
| TSTANDARD=                     | Specifies transformation standardization            |

---

Table 74.1 *continued*

| Option                          | Description                                         |
|---------------------------------|-----------------------------------------------------|
| <b>Method and Iterations</b>    |                                                     |
| CCONVERGE=                      | Specifies minimum criterion change                  |
| CHANGE=                         | Specifies number of first iteration to be displayed |
| CONVERGE=                       | Specifies minimum data change                       |
| COVARIANCE                      | Analyzes covariances                                |
| DUMMY                           | Initializes using dummy variables                   |
| INITITER=                       | Specifies number of MAC initialization iterations   |
| MAXITER=                        | Specifies maximum number of iterations              |
| METHOD=                         | Specifies iterative algorithm                       |
| NOCHECK                         | Suppresses numerical error checking                 |
| N                               | Specifies number of principal components            |
| REFRESH=                        | Specifies number of MGCV models before refreshing   |
| REITERATE                       | Restarts iterations                                 |
| SINGULAR=                       | Specifies singularity criterion                     |
| TYPE=                           | Specifies input observation type                    |
| <b>Missing Data Handling</b>    |                                                     |
| MONOTONE=                       | Includes monotone special missing values            |
| NOMISS                          | Excludes observations with missing values           |
| UNTIE=                          | Unties special missing values                       |
| <b>Control Displayed Output</b> |                                                     |
| NOPRINT                         | Suppresses displayed output                         |
| PLOTS=                          | Specifies ODS Graphics details                      |

The following list describes these options in alphabetical order.

**APREFIX=***name*

**APR=***name*

specifies a prefix for naming the approximation variables. By default, APREFIX=A. Specifying the APREFIX= option also implies the APPROXIMATIONS option.

**APPROXIMATIONS**

**APPROX**

**APP**

includes principal component approximations to the transformed variables (Eckart and Young 1936) in the output data set. Variable names are constructed from the value of the APREFIX= option and the input variable names. If you specify the APREFIX= option, then approximations are automatically included. If you specify the APPROXIMATIONS option and not the APREFIX= option, then the APPROXIMATIONS option uses the default, APREFIX=A, to construct the variable names.

**CCONVERGE=*n*****CCO=*n***

specifies the minimum change in the criterion being optimized that is required to continue iterating. By default, CCONVERGE=0.0. The CCONVERGE= option is ignored for METHOD=MAC. For the MGV method, specify CCONVERGE=-2 to ensure data convergence.

**CHANGE=*n*****CHA=*n***

specifies the number of the first iteration to be displayed in the iteration history table. The default is CHANGE=1. When you specify a larger value for *n*, the first *n* - 1 iterations are not displayed, thus speeding up the analysis. The CHANGE= option is most useful with the MGV method, which is much slower than the other methods.

**CONVERGE=*n*****CON=*n***

specifies the minimum average absolute change in standardized variable scores that is required to continue iterating. By default, CONVERGE=0.00001. Average change is computed over only those variables that can be transformed by the iterations—that is, all LINEAR, OPSCORE, MONOTONE, UNTIE, SPLINE, MSPLINE, and SSPLINE variables and nonoptimal transformation variables with missing values. For more information, see the section “[Optimal Transformations](#)” on page 6306.

**COVARIANCE****COV**

computes the principal components from the covariance matrix. The variables are always centered to mean zero. If you do not specify the COVARIANCE option, the variables are also standardized to variance one, which means the analysis is based on the correlation matrix.

**CORRELATIONS****COR**

includes correlations and the component structure matrix in the output data set. By default, this information is not included.

**DATA=*SAS-data-set***

specifies the SAS data set to be analyzed. The data set must be an ordinary SAS data set; it cannot be a TYPE=CORR or TYPE=COV data set. If you omit the DATA= option, PROC PRINQUAL uses the most recently created SAS data set.

**DUMMY****DUM**

expands variables specified for OPSCORE optimal transformations to dummy variables for the initialization (Tenenhaus and Vachette 1977). By default, the initial values of OPSCORE variables are the actual data values. The dummy variable nominal initialization requires considerable time and memory, so it might not be possible to use the DUMMY option with large data sets. No separate report of the initialization is produced. Initialization results are incorporated into the first iteration displayed in the iteration history table. For details, see the section “[Optimal Transformations](#)” on page 6306.

**INITITER=*n*****INI=*n***

specifies the number of MAC iterations required to initialize the data before starting MTV or MGW iterations. By default, INITITER=0. The INITITER= option is ignored if METHOD=MAC.

**MAXITER=*n*****MAX=*n***

specifies the maximum number of iterations. By default, MAXITER=30.

**MDPREF<=*n*>****MDP<=*n*>**

specifies a multidimensional preference analysis by implying the STANDARD, SCORES, and CORRELATIONS options. This option also suppresses warnings when there are more variables than observations.

When ODS Graphics is enabled, an MDPREF plot is produced with points for each row and vectors for each column. Often, the vectors are short, and a better graphical display is produced when the vectors are stretched. The absolute lengths of each vector can optionally be changed by specifying MDPREF=*n*. Then the vector coordinates are all multiplied by *n*. Usually, *n* will be a value such as 2, 2.5, or 3. The default is 2.5. Specify MDPREF=1 to see the vectors without any stretching. The relative lengths of the different vectors is important and interpretable, and these are preserved by the stretching.

**METHOD=MAC | MGW | MTV****MET=MAC | MGW | MTV**

specifies the optimization method. By default, METHOD=MTV. Values of the METHOD= option are MTV, for maximum total variance; MGW, for minimum generalized variance; and MAC, for maximum average correlation. You can use the MAC method when all variables are positively correlated or when no monotonicity constraints are placed on any transformations. See the section “[The Three Methods of Variable Transformation](#)” on page 6311 for more information.

**MONOTONE=*two-letters*****MON=*two-letters***

specifies the first and last special missing value in the list of those special missing values to be estimated using within-variable order and category constraints. By default, there are no order constraints on missing value estimates. The *two-letters* value must consist of two letters in alphabetical order. For example, MONOTONE=DF means that the estimate of .D must be less than or equal to the estimate of .E, which must be less than or equal to the estimate of .F; no order constraints are placed on estimates of .\_, .A through .C, and .G through .Z. For details, see the sections “[Missing Values](#)” on page 6316 and “[Optimal Scaling](#)” on page 8298 in Chapter 97, “[The TRANSREG Procedure](#).”

**N=*n***

specifies the number of principal components to be computed. By default, N=2.

**NOCHECK****NOC**

turns off computationally intensive numerical error checking for the MGW method. If you do not specify the NOCHECK option, the procedure computes R square from the squared length of the predicted values vector and compares this value to the R square computed from the error sum of squares that is a byproduct of the sweep algorithm (Goodnight 1978). If the two values of R square differ by more than the square root of the value of the SINGULAR= option, a warning is displayed, the value of the REFRESH= option is halved, and the model is refit after refreshing. Specifying the NOCHECK option slightly speeds up the algorithm. Note that other less computationally intensive error checking is always performed.

**NOMISS****NOM**

excludes all observations with missing values from the analysis, but does not exclude them from the OUT= data set. If you omit the NOMISS option, PROC PRINQUAL simultaneously computes the optimal transformations of the nonmissing values and estimates the missing values that minimize squared error.

Casewise deletion of observations with missing values occurs when you specify the NOMISS option, when there are missing values in IDENTITY variables, when there are weights less than or equal to 0, or when there are frequencies less than 1. Excluded observations are output with a blank value for the \_TYPE\_ variable, and they have a weight of 0. They do not contribute to the analysis but are scored and transformed as *supplementary* or passive observations. See the sections “[Passive Observations](#)” on page 6322 and “[Missing Values](#)” on page 6316 for more information about excluded observations and missing data.

**NOPRINT****NOP**

suppresses the display of all output. This option disables the Output Delivery System (ODS), including ODS Graphics, for the duration of the procedure. For more information, see Chapter 20, “[Using the Output Delivery System](#).”

**OUT=SAS-data-set**

specifies an output SAS data set that contains results of the analysis. If you omit the OUT= option, PROC PRINQUAL still creates an output data set and names it by using the DATA $n$  convention. If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*. You can use the REPLACE, APPROXIMATIONS, SCORES, and CORRELATIONS options to control what information is included in the output data set. For details, see the section “[Output Data Set](#)” on page 6318.

**PLOTS** <(global-plot-options)> <= plot-request <(options)>>

**PLOTS** <(global-plot-options)> <= (plot-request <(options)> <... plot-request <(options)>>>

controls the plots produced through ODS Graphics. When you specify only one plot request, you can omit the parentheses from around the plot request. Here are some examples:

```
plots=none
plots=transformation
plots(unpack)=transformation
```

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;

proc prinqual plots=all;
 transformation spline(x1-x10);
run;

ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

If ODS Graphics is enabled, but do not specify the PLOTS= option, then PROC PRINQUAL produces an MDPREF plot when the MDPREF option is specified.

The global plot options include the following:

#### **FLIP**

##### **FLI**

flips or interchanges the X-axis and Y-axis dimensions for MDPREF plots. The FLIP option can be specified either as a global plot option (for example, PLOTS(FLIP)) or with the MDPREF option (for example, PLOTS=MDPREF(FLIP)).

#### **INTERPOLATE**

##### **INT**

uses observations that are excluded from the analysis for interpolation in the fit and transformation plots. By default, observations with zero weight are excluded from all plots. These include observations with a zero, negative, or missing weight or frequency and observations excluded due to missing and invalid values. You can specify PLOTS(INTERPOLATE)=(*plot-requests*) to include some of these observations in the plots. You can use this option, for example, with sparse data sets to show smoother functions over the range of the data (see the section “The PLOTS(INTERPOLATE) Option” on page 8340 in Chapter 97, “The TRANSREG Procedure”).

#### **ONLY**

##### **ONL**

suppresses the default plots. Only plots specifically requested are displayed.

**UNPACKPANEL****UNPACK****UNP**

suppresses paneling. By default, multiple plots can appear in some output panels. Specify UNPACKPANEL to get each plot in a separate panel.

The plot requests include the following:

**ALL**

produces all appropriate plots.

**TRANSFORMATION****TRA****TRANSFORMATION(UNPACK)****TRA(UNP)**

plots the variable transformations. By default, multiple plots can appear in some output panels. Specify UNPACKPANEL to display each plot in a separate panel.

**MDPREF****MDP**

plots multidimensional preference analysis results. The MDPREF plot can also be requested by specifying the [MDPREF](#) option in the PROC PRINQUAL statement outside the PLOTS= option.

**NONE**

suppresses all plots.

**PREFIX=*name*****PRE=*name***

specifies a prefix for naming the principal components. By default, PREFIX=Prin. As a result, the principal component default names are Prin1, Prin2, . . . , Prin*n*.

**REFRESH=*n*****REF=*n***

specifies the number of variables to scale in the MGCV method before computing a new inverse. By default, REFRESH=5. PROC PRINQUAL uses the REFRESH= option in the sweep algorithm of the MGCV method. Large values for the REFRESH= option make the method run faster but with more numerical error. Small values make the method run more slowly but with more numerical accuracy.

**REITERATE****REI**

enables PROC PRINQUAL to use previous transformations as starting points. The REITERATE option affects only variables that are iteratively transformed (specified as LINEAR, SPLINE, MSPLINE, SSPLINE, UNTIE, OPSCORE, and MONOTONE). For iterative transformations, the REITERATE option requests a search in the input data set for a variable that consists of the value of the TPREFIX= option followed by the original variable name. If such a variable is found, it is used to provide the initial values for the first iteration. The final transformation is a member of the transformation family defined by the original variable, not the transformation family defined by the initialization variable. See the section “[REITERATE Option Usage](#)” on page 6321.

**REPLACE****REP**

replaces the original data with the transformed data in the output data set. The names of the transformed variables in the output data set correspond to the names of the original variables in the input data set. If you do not specify the REPLACE option, both original variables and transformed variables (with names constructed from the TPREFIX= option and the original variable names) are included in the output data set.

**SCORES****SCO**

includes principal component scores in the output data set. By default, scores are not included.

**SINGULAR=*n*****SIN=*n***

specifies the largest value within rounding error of zero. By default, SINGULAR=1E-8. PROC PRINQUAL uses the value of the SINGULAR= option for checking  $(1 - R^2)$  when constructing full-rank matrices of predictor variables, checking denominators before dividing, and so on.

**STANDARD****STD**

standardizes the principal component scores in the output data set to mean zero and variance one instead of the default mean zero and variance equal to the corresponding eigenvalue. See the SCORES option.

**TPREFIX=*name*****TPR=*name***

specifies a prefix for naming the transformed variables. By default, TPREFIX=T. The TPREFIX= option is ignored if you specify the REPLACE option.

**TSTANDARD=CENTER | NOMISS | ORIGINAL | Z****TST=CEN | NOM | ORI | Z**

specifies the standardization of the transformed variables in the OUT= data set. By default, TSTANDARD=ORIGINAL. When you specify the TSTANDARD= option in the PROC PRINQUAL statement, it is the default standardization for all variables. When you specify TSTANDARD= as a *t-option*, it overrides the default standardization just for selected variables.

**CENTER** centers the output variables to mean zero, but the variances are the same as the variances of the input variables.

**NOMISS** sets the means and variances of the transformed variables in the OUT= data set, computed over all output values that correspond to nonmissing values in the input data set, to the means and variances computed from the nonmissing observations of the original variables. The TSTANDARD=NOMISS specification is useful with missing data. When a variable is linearly transformed, the final variable contains the original nonmissing values and the missing value estimates. In other words, the nonmissing values are unchanged. If your data have no missing values, TSTANDARD=NOMISS and TSTANDARD=ORIGINAL produce the same results.

**ORIGINAL** sets the means and variances of the transformed variables to the means and variances of the original variables. This is the default.

**Z** standardizes the variables to mean zero, variance one.



For nonoptimal variable transformations, the means and variances of the original variables are actually the means and variances of the nonlinearly transformed variables, unless you specify the ORIGINAL nonoptimal *t-option* in the TRANSFORM statement. For example, if a variable X with no missing values is specified as LOG, then, by default, the final transformation of X is simply LOG(X), not LOG(X) standardized to the mean of X and variance of X.

**TYPE=**'text '|name

**TYP=**'text '|name

specifies the valid value for the `_TYPE_` variable in the input data set. If PROC PRINQUAL finds an input `_TYPE_` variable, it uses only observations with a `_TYPE_` value that matches the TYPE= value. This enables a PROC PRINQUAL OUT= data set containing correlations to be used as input to PROC PRINQUAL without requiring a WHERE statement to exclude the correlations. If a `_TYPE_` variable is not in the data set, all observations are used. The default is TYPE='SCORE', so if you do not specify the TYPE= option, only observations with `_TYPE_ = 'SCORE'` are used.

PROC PRINQUAL displays a note when it reads observations with blank values of `_TYPE_`, but it does not automatically exclude those observations. Data sets created by the TRANSREG and PRINQUAL procedures have blank `_TYPE_` values for those observations that were excluded from the analysis due to nonpositive weights, nonpositive frequencies, or missing data. When these observations are read again, they are excluded for the same reason that they were excluded from their original analysis, not because their `_TYPE_` value is blank.

**UNTIE=**two-letters

**UNT=**two-letters

specifies the first and last special missing values in the list of those special missing values that are to be estimated with within-variable order constraints but no category constraints. The *two-letters* value must consist of two letters in alphabetical order. By default, there are category constraints but no order constraints on special missing value estimates. For details, see the section “Missing Values” on page 6316. Also, see the section “Optimal Scaling” on page 8298 in Chapter 97, “The TRANSREG Procedure.”

---

## BY Statement

**BY** variables ;

You can specify a BY statement with PROC PRINQUAL to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the PRINQUAL procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are

arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.

- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

## FREQ Statement

**FREQ** *variable* ;

If one variable in the input data set represents the frequency of occurrence for other values in the observation, list the variable's name in a FREQ statement. PROC PRINQUAL then treats the data set as if each observation appeared  $n$  times, where  $n$  is the value of the FREQ variable for the observation. Noninteger values of the FREQ variable are truncated to the largest integer less than the FREQ value. The observation is used in the analysis only if the value of the FREQ statement variable is greater than or equal to 1.

## ID Statement

**ID** *variables* ;

The ID statement includes additional character or numeric variables in the output data set. The variables must be contained in the input data set.

## TRANSFORM Statement

**TRANSFORM** *transform(variables </ t-options>)< transform(variables </ t-options>)... >* ;

The TRANSFORM statement lists the variables to be analyzed (*variables*) and specifies the transformation (*transform*) to apply to each variable listed. You must specify a transformation for each variable list in the TRANSFORM statement. The variables are variables in the data set. The *t-options* are transformation options that provide details for the transformation; these depend on the *transform* chosen. The *t-options* are listed after a slash in the parentheses that enclose the variables.

For example, the following statements find a quadratic polynomial transformation of all variables in the data set:

```
proc prinqual;
 transform spline(_all_ / degree=2);
run;
```

Or, if N1 through N10 are nominal variables and M1 through M10 are ordinal variables, you can use the following statements:

```
proc prinqual;
 transform opscore (N1-N10) monotone (M1-M10) ;
run;
```

The following sections describe the transformations available (specified with *transform*) and the options available for some of the transformations (specified with *t-options*).

## Families of Transformations

There are three types of transformation families: nonoptimal, optimal, and other. The families are described as follows:

|                            |                                                                                                                                                                                                                                                                             |
|----------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Nonoptimal transformations | preprocess the specified variables, replacing each one with a single new nonoptimal, nonlinear transformation.                                                                                                                                                              |
| Optimal transformations    | replace the specified variables with new, iteratively derived optimal transformation variables that fit the specified model better than the original variable (except in contrived cases where the transformation fits the model exactly as well as the original variable). |
| Other transformations      | are the IDENTITY and SSPLINE transformations. These do not fit into either of the preceding categories.                                                                                                                                                                     |

Table 74.2 summarizes the transformations in each family.

**Table 74.2** Transformation Families

| Transformation                    | Description                         |
|-----------------------------------|-------------------------------------|
| <b>Nonoptimal Transformations</b> |                                     |
| ARSIN                             | Inverse trigonometric sine          |
| EXP                               | Exponential                         |
| LOG                               | Logarithm                           |
| LOGIT                             | Logit                               |
| POWER                             | Raises variables to specified power |
| RANK                              | Transforms to ranks                 |
| <b>Optimal Transformations</b>    |                                     |
| LINEAR                            | Linear                              |
| MONOTONE                          | Monotonic, ties preserved           |
| MSPLINE                           | Monotonic B-spline                  |
| OPSCORE                           | Optimal scoring                     |
| SPLINE                            | B-spline                            |
| UNTIE                             | Monotonic, ties not preserved       |
| <b>Other Transformations</b>      |                                     |
| IDENTITY                          | Identity, no transformation         |
| SSPLINE                           | Iterative smoothing spline          |

The *transform* is followed by a variable (or list of variables) enclosed in parentheses. Optionally, depending on the *transform*, the parentheses can also contain *t-options*, which follow the variables and a slash. For

example, the following statement computes the LOG transformation of X and Y:

```
transform log(X Y);
```

A more complex example follows:

```
transform spline(Y / nknots=2) log(X1 X2 X3);
```

The preceding statement uses the SPLINE transformation of the variable Y and the LOG transformation of the variables X1, X2, and X3. In addition, it uses the NKNOTS= option with the SPLINE transformation and specifies two knots.

The rest of this section provides syntax details for members of the three families of transformations. The *t-options* are discussed in the section “Transformation Options (t-options)” on page 6307.

### **Nonoptimal Transformations**

Nonoptimal transformations are computed before the iterative algorithm begins. Nonoptimal transformations create a single new transformed variable that replaces the original variable. The new variable is not transformed by the subsequent iterative algorithms (except for a possible linear transformation and missing value estimation).

The following list provides syntax and details for nonoptimal variable transformations.

#### **ARSIN**

##### **ARS**

finds an inverse trigonometric sine transformation. Variables specified in the ARSIN *transform* must be numeric and in the interval  $(-1.0 \leq x \leq 1.0)$ , and they are typically continuous.

#### **EXP**

exponentiates variables ( $x$  is transformed to  $a^x$ ). To specify the value of  $a$ , use the **PARAMETER=** *t-option*. By default,  $a$  is the mathematical constant  $e = 2.718\dots$ . Variables specified with the EXP *transform* must be numeric, and they are typically continuous.

#### **LOG**

transforms variables to logarithms ( $x$  is transformed to  $\log_a(x)$ ). To specify the base of the logarithm, use the **PARAMETER=** *t-option*. The default is a natural logarithm with base  $e = 2.718\dots$ . Variables specified with the LOG *transform* must be numeric and positive, and they are typically continuous.

#### **LOGIT**

finds a logit transformation on the variables. The logit of  $x$  is  $\log(x/(1-x))$ . Unlike other transformations, LOGIT does not have a three-letter abbreviation. Variables specified with the LOGIT *transform* must be numeric and in the interval  $(0.0 < x < 1.0)$ , and they are typically continuous.

#### **POWER**

##### **POW**

raises variables to a specified power ( $x$  is transformed to  $x^a$ ). You must specify the power parameter  $a$  by specifying the **PARAMETER=** *t-option* following the variables.

```
power(variable / parameter=number)
```

You can use POWER for squaring variables (PARAMETER=2), reciprocal transformations (PARAMETER=-1), square roots (PARAMETER=0.5), and so on. Variables specified with the POWER *transform* must be numeric, and they are typically continuous.

**RANK****RAN**

transforms variables to ranks. Ranks are averaged within ties. The smallest input value is assigned the smallest rank. Variables specified with the RANK *transform* must be numeric.

**Optimal Transformations**

Optimal transformations are iteratively derived. Missing values for these types of variables can be optimally estimated (see the section “Missing Values” on page 6316). See the sections “OPSCORE, MONOTONE, UNTIE, and LINEAR Transformations” on page 8298 and “SPLINE and MSPLINE Transformations” on page 8300 in Chapter 97, “The TRANSREG Procedure,” for more information about the optimal transformations.

The following list provides syntax and details for optimal transformations.

**LINEAR****LIN**

finds an optimal linear transformation of each variable. For variables with no missing values, the transformed variable is the same as the original variable. For variables with missing values, the transformed nonmissing values have a different scale and origin than the original values. Variables specified with the LINEAR *transform* must be numeric.

**MONOTONE****MON**

finds a monotonic transformation of each variable, with the restriction that ties are preserved. The Kruskal (1964) secondary least squares monotonic transformation is used. This transformation weakly preserves order and category membership (ties). Variables specified with the MONOTONE *transform* must be numeric, and they are typically discrete.

**MSPLINE****MSP**

finds a monotonically increasing B-spline transformation with monotonic coefficients (de Boor 1978; de Leeuw 1986) of each variable. You can specify the DEGREE=, KNOTS=, NKNOTS=, and EVENLY= *t-options* with MSPLINE. By default, PROC PRINQUAL uses a quadratic spline. Variables specified with the MSPLINE *transform* must be numeric, and they are typically continuous.

**OPSCORE****OPS**

finds an optimal scoring of each variable. The OPSCORE transformation assigns scores to each class (level) of the variable. The Fisher (1938) optimal scoring method is used. Variables specified with the OPSCORE *transform* can be either character or numeric; numeric variables should be discrete.

**SPLINE****SPL**

finds a B-spline transformation (de Boor 1978) of each variable. By default, PROC PRINQUAL uses a cubic polynomial transformation. You can specify the DEGREE=, KNOTS=, NKNOTS=, and EVENLY *t-options* with SPLINE. Variables specified with the SPLINE *transform* must be numeric, and they are typically continuous.

**UNTIE****UNT**

finds a monotonic transformation of each variable without the restriction that ties are preserved. PROC PRINQUAL uses the Kruskal (1964) primary least squares monotonic transformation method. This transformation weakly preserves order but not category membership (it might untie some previously tied values). Variables specified with the UNTIE *transform* must be numeric, and they are typically discrete.

**Other Transformations****IDENTITY****IDE**

specifies variables that are not changed by the iterations. The IDENTITY transformation is used for variables when no transformation and no missing data estimation are desired. However, the REFLECT, ADDITIVE, TSTANDARD=Z, and TSTANDARD=CENTER options can linearly transform all variables, including IDENTITY variables, after the iterations. Observations with missing values in IDENTITY variables are excluded from the analysis, and no optimal scores are computed for missing values in IDENTITY variables. Variables specified with the IDENTITY *transform* must be numeric.

**SSPLINE****SSP**

finds an iterative smoothing spline transformation of each variable. The SSPLINE transformation does not generally minimize squared error. You can specify the smoothing parameter with either the SM= *t-option* or the PARAMETER= *t-option*. The default smoothing parameter is SM=0. Variables specified with the SSPLINE *transform* must be numeric, and they are typically continuous.

**Transformation Options (t-options)**

If you use a nonoptimal, optimal, or other transformation, you can use *t-options*, which specify additional details of the transformation. The *t-options* are specified within the parentheses that enclose variables and are listed after a slash. For example:

```
proc prinqual;
 transform spline(X Y / nknots=3);
run;
```

The preceding statements find an optimal variable transformation (SPLINE) of the variables X and Y and use a *t-option* to specify the number of knots (NKNOTS=). The following is a more complex example:

```
proc prinqual;
 transform spline(Y / nknots=3) spline(X1 X2 / nknots=6);
run;
```

These statements use the SPLINE transformation for all three variables and use *t-options* as well; the NKNOTS= option specifies the number of knots for the spline.

The following sections discuss the *t-options* available for nonoptimal, optimal, and other transformations.

Table 74.3 summarizes the *t-options*.

**Table 74.3** Transformation Options

| Option                           | Description                                  |
|----------------------------------|----------------------------------------------|
| <b>Nonoptimal Transformation</b> |                                              |
| ORIGINAL                         | Uses original mean and variance              |
| <b>Parameter Specification</b>   |                                              |
| PARAMETER=                       | Specifies miscellaneous parameters           |
| SM                               | Specifies smoothing parameter                |
| <b>Spline</b>                    |                                              |
| DEGREE=                          | Specifies the degree of the spline           |
| EVENLY                           | Spaces the knots evenly                      |
| KNOTS=                           | Specifies the interior knots or break points |
| NKNOTS=                          | Creates $n$ knots                            |
| <b>Other t-options</b>           |                                              |
| NAME=                            | Renames variables                            |
| REFLECT                          | Reflects the variable around the mean        |
| TSTANDARD=                       | Specifies transformation standardization     |

**Nonoptimal Transformation t-options****ORIGINAL****ORI**

matches the variable's final mean and variance to the mean and variance of the original variable. By default, the mean and variance are based on the transformed values. The ORIGINAL *t-option* is available for all of the nonoptimal transformations.

**Parameter t-options****PARAMETER=number****PAR=number**

specifies the transformation parameter. The PARAMETER= *t-option* is available for the EXP, LOG, POWER, SMOOTH, and SSPLINE transformations. For EXP, the parameter is the value to be exponentiated; for LOG, the parameter is the base value; and for POWER, the parameter is the power. For SMOOTH and SSPLINE, the parameter is the raw smoothing parameter. (See the SM= option for an alternative way to specify the smoothing parameter.) The default for the PARAMETER= *t-option* for the LOG and EXP transformations is  $e = 2.718 \dots$ . The default parameter for SSPLINE is computed from SM=0. For the POWER transformation, you must specify the PARAMETER= *t-option*; there is no default.

**SM= $n$** 

specifies a smoothing parameter in the range 0 to 100, just like PROC GPLOT uses. For example, SM=50 in PROC PRINQUAL is equivalent to I=SM50 on the SYMBOL statement with PROC GPLOT. You can specify the SM= *t-option* only with the SSPLINE transformation. The smoothness of the function increases as the value of the smoothing parameter increases. By default, SM=0.

**Spline *t*-options**

The following *t*-options are available with the SPLINE and MSPLINE optimal transformations.

**DEGREE=*n*****DEG=*n***

specifies the degree of the B-spline transformation. The degree must be a nonnegative integer. The defaults are DEGREE=3 for SPLINE variables and DEGREE=2 for MSPLINE variables.

The polynomial degree should be a small integer, usually 0, 1, 2, or 3. Larger values are rarely useful. If you have any doubt as to what degree to specify, use the default.

**EVENLY<=*n*>****EVE<=*n*>**

is used with the NKNOTS= *t*-option to space the knots evenly. The differences between adjacent knots are constant. If you specify NKNOTS=*k*, *k* knots are created at

$$\text{minimum} + i((\text{maximum} - \text{minimum})/(k + 1))$$

for  $i = 1, \dots, k$ . For example, if you specify

```
spline(X / knots=2 evenly)
```

and the variable *X* has a minimum of 4 and a maximum of 10, then the two interior knots are 6 and 8. Without the EVENLY *t*-option, the NKNOTS= *t*-option places knots at percentiles, so the knots are not evenly spaced.

By default for the SPLINE and MSPLINE transformations, the smaller exterior knots are all the same and just a little smaller than the minimum. Similarly, by default, the larger exterior knots are all the same and just a little larger than the maximum. However, if you specify EVENLY=*n*, then the *n* exterior knots are evenly spaced as well. The number of exterior knots must be greater than or equal to the degree. You can specify values larger than the degree when you want to interpolate slightly beyond the range or your data. The exterior knots must be less than the minimum or greater than the maximum, and hence the knots across all sets are not precisely equally spaced. For example, with data ranging from 0 to 10, and with EVENLY=3 and NKNOTS=4, the first exterior knots are -4.000000000001, -2.000000000001, and -0.000000000001, the interior knots are 2, 4, 6, and 8, and the second exterior knots are 10.000000000001, 12.000000000001, and 14.000000000001.

**KNOTS=*number-list* | *n* TO *m* BY *p*****KNO=*number-list* | *n* TO *m* BY *p***

specifies the interior knots or break points. By default, there are no knots. The first time you specify a value in the knot list, it indicates a discontinuity in the *n*th (from DEGREE=*n*) derivative of the transformation function at the value of the knot. The second mention of a value indicates a discontinuity in the (*n* - 1) derivative of the transformation function at the value of the knot. Knots can be repeated any number of times to decrease the smoothness at the break points, but the values in the knot list can never decrease.

You cannot use the KNOTS= *t*-option with the NKNOTS= *t*-option. You should keep the number of knots small. (See the section “Specifying the Number of Knots” on page 8301 in Chapter 97, “The TRANSREG Procedure.”)



**NKNOTS=*n*****NKN=*n***

creates *n* knots, the first at the 100/(*n* + 1) percentile, the second at the 200/(*n* + 1) percentile, and so on. Knots are always placed at data values; there is no interpolation. For example, if NKNOTS=3, knots are placed at the 25th percentile, the median, and the 75th percentile. By default, NKNOTS=0. The NKNOTS= *t-option* must be ≥ 0.

You cannot use the NKNOTS= *t-option* with the KNOTS= *t-option*. You should keep the number of knots small. (See the section “Specifying the Number of Knots” on page 8301 in Chapter 97, “The TRANSREG Procedure.”)

**Other *t-options***

The following *t-options* are available for all transformations.

**NAME=(*variable-list*)****NAM=(*variable-list*)**

renames variables as they are used in the TRANSFORM statement. This option allows a variable to be used more than once. For example, if the variable X is a character variable, then the following step stores both the original character variable X and a numeric variable XC that contains category numbers in the output data set.

```
proc prinqual data=A n=1 out=B;
 transform linear(Y) opscore(X / name=(XC));
 id X;
run;
```

**REFLECT****REF**

reflects the transformation

$$y = -(y - \bar{y}) + \bar{y}$$

after the iterations are completed and before the final standardization and results calculations.

**TSTANDARD=CENTER | NOMISS | ORIGINAL | Z****TST=CEN | NOM | ORI | Z**

specifies the standardization of the transformed variables in the OUT= data set. By default, TSTANDARD=ORIGINAL. When the TSTANDARD= option is specified in the PROC PRINQUAL statement, it specifies the default standardization for all variables. When you specify TSTANDARD= as a *t-option*, it overrides the default standardization only for selected variables.

**WEIGHT Statement****WEIGHT *variable* ;**

When you use a WEIGHT statement, a weighted residual sum of squares is minimized. The WEIGHT statement has no effect on degrees of freedom or number of observations, but the weights affect most other calculations. The observation is used in the analysis only if the value of the WEIGHT statement variable is greater than 0.

---

## Details: PRINQUAL Procedure

---

### The Three Methods of Variable Transformation

The three methods of variable transformation provided by PROC PRINQUAL are discussed in the following sections.

#### The Maximum Total Variance (MTV) Method

The MTV method (Young, Takane, and de Leeuw 1978) is based on the principal component model, and it attempts to maximize the sum of the first  $r$  eigenvalues of the covariance matrix. This method transforms variables to be (in a least squares sense) as similar to linear combinations of  $r$  principal component score variables as possible, where  $r$  can be much smaller than the number of variables. This maximizes the total variance of the first  $r$  components (the trace of the covariance matrix of the first  $r$  principal components). See *SAS Technical Report R-108*.

On each iteration, the MTV algorithm alternates classical principal component analysis (Hotelling 1933) with optimal scaling (Young 1981). When all variables are ordinal preference ratings, this corresponds to MDPREF analysis (Carroll 1972). You can request the dummy variable initialization method suggested by Tenenhaus and Vachette (1977), who independently propose the same iterative algorithm for nominal and interval scale-of-measurement variables.

#### The Minimum Generalized Variance (MGV) Method

The MGV method (Sarle 1984) uses an iterated multiple regression algorithm in an attempt to minimize the determinant of the covariance matrix of the transformed variables. This method transforms each variable to be (in a least squares sense) as similar to linear combinations of the remaining variables as possible. This locally minimizes the generalized variance of the transformed variables, the determinant of the covariance matrix, the volume of the parallelepiped defined by the transformed variables, and the sphericity (the extent to which a quadratic form in the optimized covariance matrix defines a sphere). See *SAS Technical Report R-108*.

On each iteration for each variable, the MGV algorithm alternates multiple regression with optimal scaling. The multiple regression involves predicting the selected variable from all other variables. You can request a dummy variable initialization by using a modification of the Tenenhaus and Vachette (1977) method that is appropriate with a regression algorithm. This method can be viewed as a way of investigating the nature of the linear and nonlinear dependencies in, and the rank of, a data matrix containing variables that can be nonlinearly transformed. This method tries to create a less-than-full-rank data matrix. The matrix contains the transformation of each variable that is most similar to what the other transformed variables predict.

#### The Maximum Average Correlation (MAC) Method

The MAC method (de Leeuw 1985) uses an iterated constrained multiple regression algorithm in an attempt to maximize the average of the elements of the correlation matrix. This method transforms each variable to be (in a least squares sense) as similar to the average of the remaining variables as possible.

On each iteration for each variable, the MAC algorithm alternates computing an equally weighted average of the other variables with optimal scaling. The MAC method is similar to the MGV method in that each

variable is scaled to be as similar to a linear combination of the other variables as possible, given the constraints on the transformation. However, optimal weights are not computed. You can use the MAC method when all variables are positively correlated or when no monotonicity constraints are placed on any transformations. Do not use this method with negatively correlated variables when some optimal transformations are constrained to be increasing because the signs of the correlations are not taken into account. The MAC method is useful as an initialization method for the MTV and MGW methods.

---

## Understanding How PROC PRINQUAL Works

In the following example, PROC PRINQUAL uses the MTV method to linearize a curved scatter plot. Let

$$\begin{aligned} X_1 &= -1 \text{ to } 1 \text{ by } 0.02 \\ X_2 &= X_1^3 + \epsilon \\ X_3 &= X_2^5 + \epsilon \end{aligned}$$

where  $\epsilon$  is normal error.

These three variables define a curved swarm of points in three-dimensional space. First, the SGSCATTER procedure is used to display two-dimensional views of these data. Next, PROC PRINQUAL is used to straighten the scatter plot, making it more one-dimensional by finding a smooth transformation of each variable. The N=1 option in the PROC PRINQUAL statement requests one principal component. The TRANSFORM statement requests a cubic spline transformation with nine knots. *Splines* are curves, which are usually required to be continuous and smooth. See the section “[Splines](#)” on page 6315 for more information about splines. See Smith (1979) for an excellent introduction to splines.

PROC PRINQUAL transforms each variable to be as much as possible like the first principal component (or more generally, to be close to the space defined by the first N= principal components). One component accounts for 92 percent of the variance of the untransformed data and over 99 percent of the variance of the transformed data (see [Figure 74.5](#)). Note that the results did not converge in the default 50 iterations, so more iterations were requested using the MAXITER= option. The transformations are requested by specifying PLOTS=TRANSFORMATION and are displayed in [Figure 74.6](#).

PROC PRINQUAL creates an output data set that contains both the original and transformed variables. The original variables are named X1, X2, and X3, and the transformed variables are named TX1, TX2, and TX3. The transformed variables are displayed using the SGSCATTER procedure in [Figure 74.7](#).

The following statements produce [Figure 74.4](#) through [Figure 74.7](#):

```
ods graphics on;

* Generate Three-Dimensional Data;
data X;
 do X1 = -1 to 1 by 0.02;
 X2 = X1 ** 3 + 0.05 * normal(7);
 X3 = X1 ** 5 + 0.05 * normal(7);
 output;
 end;
run;
```

```

proc sgscatter data=x;
 plot x1*x2 x1*x3 x3*x2;
run;

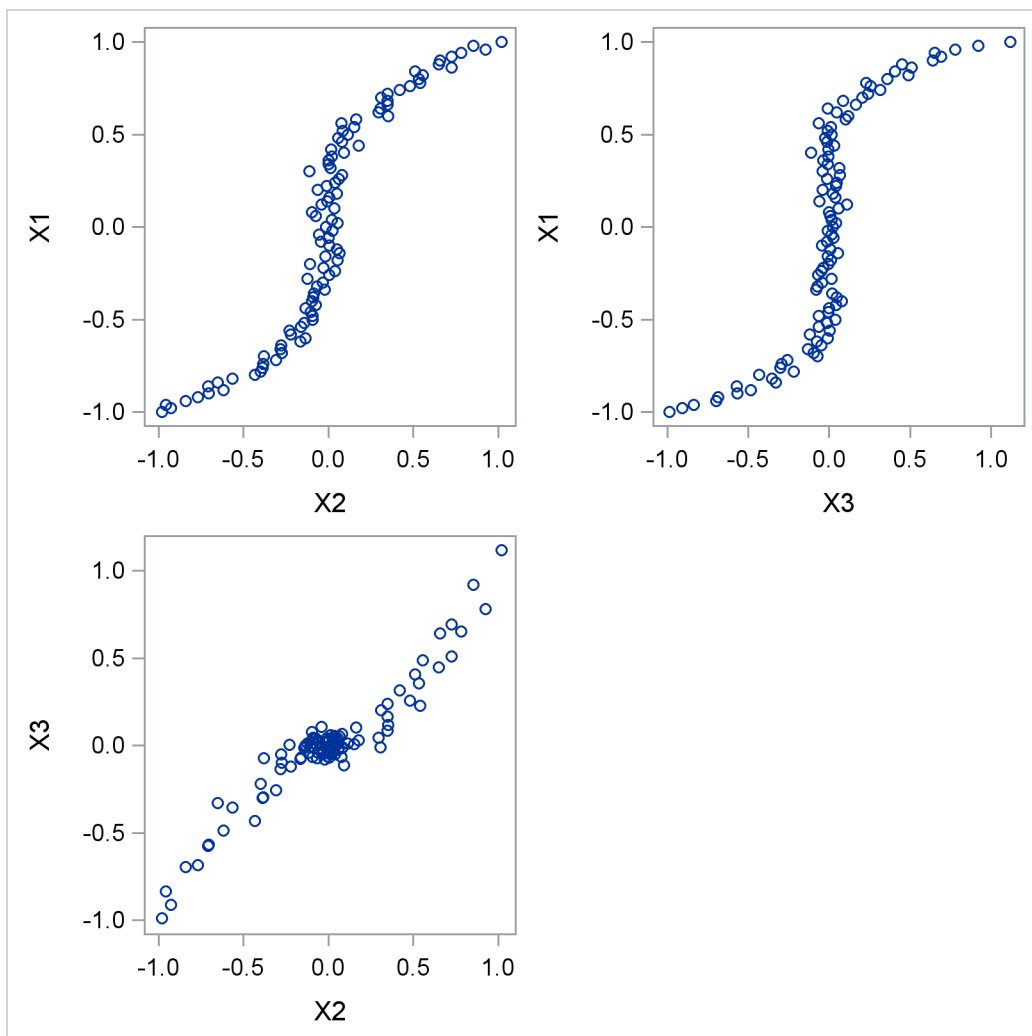
* Try to Straighten the Scatter Plot;
proc prinqual data=X n=1 maxiter=2000 plots=transformation out=results;
 title 'Linearize the Scatter Plot';
 transform spline(X1-X3 / nknots=9);
run;

* Plot the Linearized Scatter Plot;
proc sgscatter data=results;
 plot tx1*tx2 tx1*tx3 tx3*tx2;
run;

```

The three-dimensional data in Figure 74.4 and Figure 74.7 are displayed in three two-dimensional plots, arrayed as if they were three faces of a cube that was flattened as you might flatten a box.

**Figure 74.4** Three-Dimensional Scatter Plot



**Figure 74.5** PRINQUAL Iteration History

Linearize the Scatter Plot

The PRINQUAL Procedure

PRINQUAL MTV Algorithm Iteration History

| Iteration Number | Average Change | Maximum Change | Proportion of Variance | Criterion Change | Note      |
|------------------|----------------|----------------|------------------------|------------------|-----------|
| 1                | 0.15125        | 0.93453        | 0.92376                |                  |           |
| 2                | 0.04589        | 0.14682        | 0.98030                | 0.05653          |           |
| 3                | 0.03154        | 0.10125        | 0.98626                | 0.00596          |           |
| 4                | 0.02258        | 0.06890        | 0.98890                | 0.00265          |           |
| 5                | 0.01682        | 0.04777        | 0.99028                | 0.00137          |           |
| 6                | 0.01297        | 0.03782        | 0.99106                | 0.00078          |           |
| 7                | 0.01032        | 0.03029        | 0.99154                | 0.00048          |           |
| .                |                |                |                        |                  |           |
| .                |                |                |                        |                  |           |
| .                |                |                |                        |                  |           |
| 1670             | 0.00001        | 0.00005        | 0.99371                | 0.00000          |           |
| 1671             | 0.00001        | 0.00005        | 0.99371                | 0.00000          |           |
| 1672             | 0.00001        | 0.00005        | 0.99371                | 0.00000          | Converged |

Algorithm converged.

**Figure 74.6** Transformations

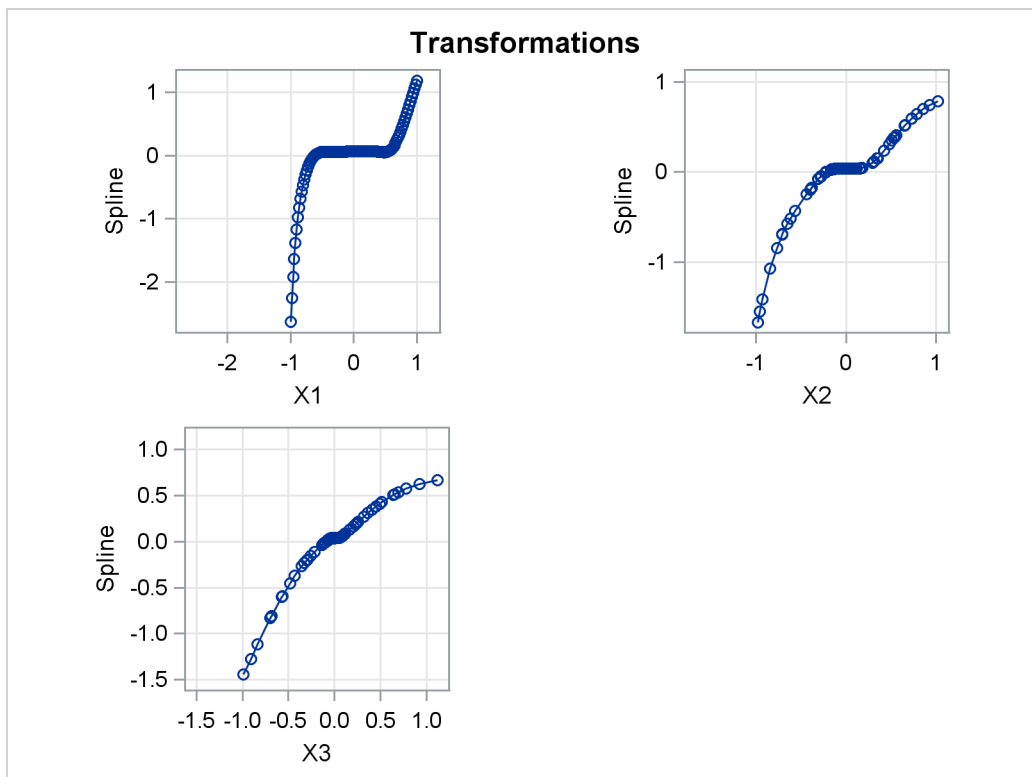
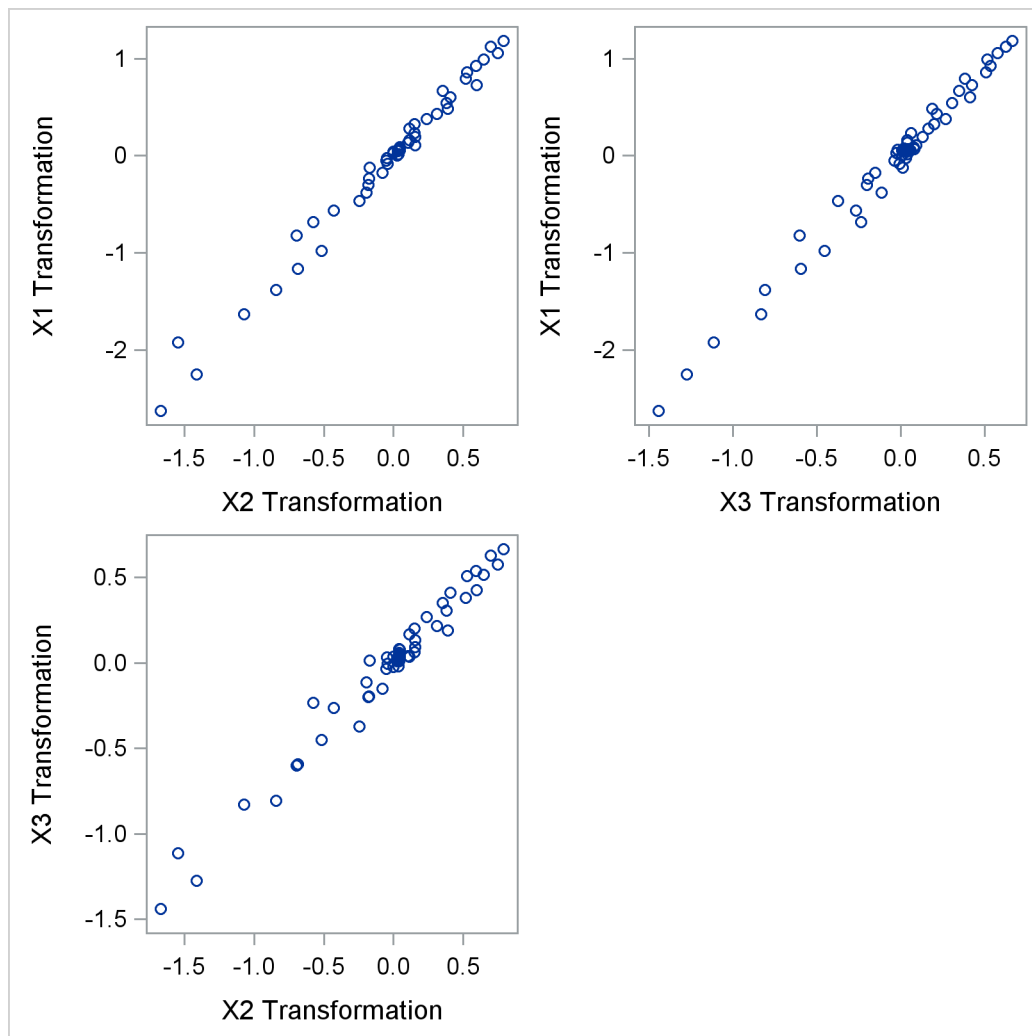


Figure 74.7 Linearized Scatter Plot



## Splines

Splines are curves, and they are usually required to be continuous and smooth. Splines are usually defined as piecewise polynomials of degree  $n$  with function values and first  $n - 1$  derivatives that agree at the points where they join. The abscissa values of the join points are called *knots*. The term “spline” is also used for polynomials (splines with no knots) and piecewise polynomials with more than one discontinuous derivative. Splines with no knots are generally smoother than splines with knots, which are generally smoother than splines with multiple discontinuous derivatives. Splines with few knots are generally smoother than splines with many knots; however, increasing the number of knots usually increases the fit of the spline function to the data. Knots give the curve freedom to bend to follow the data more closely. See Smith (1979) for an excellent introduction to splines. There are many examples and detailed discussions of splines in Chapter 97, “The TRANSREG Procedure.” See the sections “Linear and Nonlinear Regression Functions” on page 8250, “Smoothing Splines” on page 8263, “SPLINE and MSPLINE Transformations” on page 8300, “Specifying the Number of Knots” on page 8301, “SPLINE, BSPLINE, and PSPLINE Comparisons” on page 8302, “Linear and Nonlinear Regression Functions” on page 8250, “Simultaneously Fitting

Two Regression Functions” on page 8254, and examples “Using Splines and Knots” on page 8233 and Example 97.1.

---

## Missing Values

PROC PRINQUAL can estimate missing values, subject to optional constraints, so that the covariance matrix is optimized. The procedure provides several approaches for handling missing data. When you specify the NOMISS option in the PROC PRINQUAL statement, observations with missing values are excluded from the analysis. Otherwise, missing data are estimated, using variable means as initial estimates. Missing values for OPSCORE character variables are treated the same as any other category during the initialization. See the section “Missing Values” on page 8289 in Chapter 97, “The TRANSREG Procedure,” for more information about missing data estimation.

---

## Controlling the Number of Iterations

Several options in the PROC PRINQUAL statement control the number of iterations performed. Iteration terminates when any one of the following conditions is satisfied:

- The number of iterations equals the value of the MAXITER= option.
- The average absolute change in variable scores from one iteration to the next is less than the value of the CONVERGE= option.
- The criterion change is less than the value of the CCONVERGE= option.

With the MTV method, the change in the proportion of variance criterion can become negative when the data have converged so that it is numerically impossible, within machine precision, to increase the criterion. Because the MTV algorithm is convergent, a negative criterion change is the result of very small amounts of rounding error. The MGV method displays the average squared multiple correlation (which is not the criterion being optimized), so the criterion change can become negative well before convergence. The MAC method criterion (average correlation) is never computed, so the CCONVERGE= option is ignored for METHOD=MAC. You can specify a negative value for either convergence option if you want to define convergence only in terms of the other convergence option.

With the MGV method, iterations minimize the generalized variance (determinant), but the generalized variance is not reported for two reasons. First, in most data sets, the generalized variance is almost always near zero (or will be after one or two iterations), which is its minimum. This does not mean that iteration is complete; it simply means that at least one multiple correlation is at or near one. The algorithm continues minimizing the determinant in  $(m - 1)$ ,  $(m - 2)$  dimensions, and so on. Because the generalized variance is almost always near zero, it does not provide a good indication of how the iterations are progressing. The mean R square provides a better indication of convergence. The second reason for not reporting the generalized variance is that almost no additional time is required to compute R square values for each step. This is because the error sum of squares is a byproduct of the algorithm at each step. Computing the determinant at the end of each iteration adds more computations to an already computationally intensive algorithm.

You can increase the number of iterations to ensure convergence by increasing the value of the MAXITER= option and decreasing the value of the CONVERGE= option. Because the average absolute change in standardized variable scores seldom decreases below  $1E-11$ , you typically do not specify a value for the CONVERGE= option less than  $1E-8$  or  $1E-10$ . Most of the data changes occur during the first few iterations, but the data can still change after 50 or even 100 iterations. You can try different combinations of values for the CONVERGE= and MAXITER= options to ensure convergence without extreme overiteration. If the data do not converge with the default specifications, specify the REITERATE option, or try CONVERGE= $1E-8$  and MAXITER=50, or CONVERGE= $1E-10$  and MAXITER=200.

---

## Performing a Principal Component Analysis of Transformed Data

PROC PRINQUAL produces an iteration history table that displays (for each iteration) the iteration number, the maximum and average absolute change in standardized variable scores computed over the iteratively transformed variables, the criterion being optimized, and the criterion change. In order to examine the results of the analysis in more detail, you can analyze the information in the output data set by using other SAS procedures.

Specifically, use the PRINCOMP procedure to perform a principal components analysis on the transformed data. PROC PRINCOMP accepts the raw data from PROC PRINQUAL but issues a warning, because the PROC PRINQUAL output data set has `_NAME_` and `_TYPE_` variables but is not a TYPE=CORR data set. You can ignore this warning.

If the output data set contains both scores and correlations, you must subset it for analysis with PROC PRINCOMP. Otherwise, the correlation observations are treated as ordinary observations and the PROC PRINCOMP results are incorrect. For example, consider the following statements:

```
proc prinqual data=a out=b correlations replace;
 transform spline(var1-var50 / nknots=3);
run;

proc princomp data=b;
 where _TYPE_='SCORE';
run;
```

Also note that the proportion of variance accounted for, as reported by PROC PRINCOMP, can exceed the proportion of variance accounted for in the last PROC PRINQUAL iteration. This is because PROC PRINQUAL reports the variance accounted for by the components analysis that generated the current scaling of the data, not a components analysis of the current scaling of the data.

---

## Using the MAC Method

You can use the MAC algorithm alone by specifying METHOD=MAC, or you can use it as an initialization algorithm for METHOD=MTV and METHOD=MGV analyses by specifying the iteration option INITITER= . If any variables are negatively correlated, do not use the MAC algorithm with monotonic transformations (MONOTONE, UNTIE, and MSPLINE) because the signs of the correlations among the variables are not used when computing variable approximations. If an approximation is negatively correlated with the original variable, monotone constraints would make the optimally scaled variable a constant, which is not allowed (see the section “Avoiding Constant Transformations” on page 6321). When used



with other transformations, the MAC algorithm can reverse the scoring of the variables. So, for example, if variable  $X$  is designated  $\text{LOG}(X)$  with  $\text{METHOD}=\text{MAC}$  and  $\text{TSTANDARD}=\text{ORIGINAL}$ , the final transformation (for example,  $\text{TX}$ ) might not be  $\text{LOG}(X)$ . If  $\text{TX}$  is not  $\text{LOG}(X)$ , it has the same mean as  $\text{LOG}(X)$  and the same variance as  $\text{LOG}(X)$ , and it is perfectly negatively correlated with  $\text{LOG}(X)$ . PROC PRINQUAL displays a note for every variable that is reversed in this manner.

You can use the  $\text{METHOD}=\text{MAC}$  algorithm to reverse the scorings of some rating variables before a factor analysis. The correlations among bipolar ratings such as 'like - dislike', 'hot - cold', and 'fragile - monumental' are typically both positive and negative. If some items are reversed to say 'dislike - like', 'cold - hot', and 'monumental - fragile', some of the negative signs can be eliminated, and the factor pattern matrix would be cleaner. You can use PROC PRINQUAL with  $\text{METHOD}=\text{MAC}$  and  $\text{LINEAR}$  transformations to reverse some items, maximizing the average of the intercorrelations.

---

## Output Data Set

PROC PRINQUAL produces an output data set by default. By specifying the  $\text{OUT}=\text{, APPROXIMATIONS, SCORES, REPLACE,}$  and  $\text{CORRELATIONS}$  options in the PROC PRINQUAL statement, you can name this data set and control its contents.

By default, the procedure creates an output data set that contains variables with  $\text{\_TYPE\_}=\text{'SCORE'}$ . These observations contain original variables, transformed variables, components, or data approximations. If you specify the  $\text{CORRELATIONS}$  option in the PROC PRINQUAL statement, the data set also contains observations with  $\text{\_TYPE\_}=\text{'CORR'}$ ; these observations contain correlations or component structure information.

## Structure and Content

The output data set can have 16 different forms, depending on the specified combinations of the  $\text{REPLACE, SCORES, APPROXIMATIONS,}$  and  $\text{CORRELATIONS}$  options. You can specify any combination of these options. To illustrate, assume that the data matrix consists of  $N$  observations and  $m$  variables, and  $n$  components are computed. Then define the following:

- D** the  $N \times m$  matrix of original data with variable names that correspond to the names of the variables in the input data set. However, when you use the  $\text{OPSCORE}$  transformation on character variables, those variables are replaced by numeric variables that contain category numbers.
- T** the  $N \times m$  matrix of transformed data with variable names constructed from the value of the  $\text{TPREFIX=}$  option (if you do not specify the  $\text{REPLACE}$  option) and the names of the variables in the input data set
- S** the  $N \times n$  matrix of component scores with variable names constructed from the value of the  $\text{PREFIX=}$  option and integers
- A** the  $N \times m$  matrix of data approximations with variable names constructed from the value of the  $\text{APREFIX=}$  option and the names of the variables in the input data set
- R<sub>TD</sub>** the  $m \times m$  matrix of correlations between the transformed variables and the original variables with variable names that correspond to the names of the variables in the input data set. When missing values exist, casewise deletion is used to compute the correlations.
- R<sub>TT</sub>** the  $m \times m$  matrix of correlations among the transformed variables with the variable names constructed from the value of the  $\text{TPREFIX=}$  option (if you do not specify the  $\text{REPLACE}$  option) and the names of the variables in the input data set

- R<sub>TS</sub>** the  $m \times n$  matrix of correlations between the transformed variables and the principal component scores (component structure matrix) with variable names constructed from the value of the PREFIX= option and integers
- R<sub>TA</sub>** the  $m \times m$  matrix of correlations between the transformed variables and the variable approximations with variable names constructed from the value of the APREFIX= option and the names of the variables in the input data set

To create a data set Work.A that contains all information, specify the following options in the PROC PRINQUAL statement:

```
proc prinqual scores approximations correlations out=a;
```

Also use a TRANSFORM statement appropriate for your data. Then the Work.A data set contains the following:

```

D T S A
RTD RTT RTS RTA
```

To eliminate the bottom partitions that contain the correlations and component structure, do not specify the CORRELATIONS option. For example, use the following PROC PRINQUAL statement with an appropriate TRANSFORM statement:

```
proc prinqual scores approximations out=a;
```

Then the Work.A data set contains the following:

```
D T S A
```

Suppose you use the following PROC PRINQUAL statement (with an appropriate TRANSFORM statement):

```
proc prinqual out=a;
```

This creates a data set Work.A of the following form:

```
D T
```

To output transformed data and component scores only, specify the following options in the PROC PRINQUAL statement:

```
proc prinqual replace scores out=a;
```

Then the Work.A data set contains the following:

```
T S
```

## **`_TYPE_` and `_NAME_` Variables**

In addition to the preceding information, the output data set contains two character variables, the variable `_TYPE_` (length 8) and the variable `_NAME_` (length 32).

The `_TYPE_` variable has the value 'SCORE' if the observation contains variables, transformed variables, components, or data approximations; the `_TYPE_` variable has the value 'CORR' if the observation contains correlations or component structure.

By default, the `_NAME_` variable has values 'ROW1', 'ROW2', and so on, for the observations with `_TYPE_='SCORE'`. If you use an ID statement, the variable `_NAME_` contains the formatted ID variable for SCORES observations. The values of the variable `_NAME_` for observations with `_TYPE_='CORR'` are the names of the transformed variables.

Certain procedures, such as PROC PRINCOMP, which can use the PROC PRINQUAL output data set, issue a warning that the PROC PRINQUAL data set contains `_NAME_` and `_TYPE_` variables but is not a TYPE=CORR data set. You can ignore this warning.

## **Variable Names**

The TPREFIX=, APREFIX=, and PREFIX= options specify prefixes for the transformed and approximation variable names and for principal component score variables, respectively. PROC PRINQUAL constructs transformed and approximation variable names from a prefix and the first characters of the original variable name. The number of characters in the prefix plus the number of characters in the original variable name (including the final digits, if any) required to uniquely designate the new variables should not exceed 32. For example, if the APREFIX= parameter that you specify is one character, PROC PRINQUAL adds the first 31 characters of the original variable name; if your prefix is four characters, only the first 28 characters of the original variable name are added.

## **Effect of the TSTANDARD= and COVARIANCE Options**

The values in the output data set are affected by the TSTANDARD= and COVARIANCE options. If you specify TSTANDARD=NOMISS, the NOMISS standardization is performed on the transformed data after the iterations have been completed, but before the output data set is created. The new means and variances are used in creating the output data set. Then, if you do not specify the COVARIANCE option, the data are transformed to mean zero and variance one. The principal component scores and data approximations are computed from the resulting matrix. The data are then linearly transformed to have the mean and variance specified by the TSTANDARD= option. The data approximations are transformed so that the means within each pair of a transformed variable and its approximation are the same. The ratio of the variance of a variable approximation to the variance of the corresponding transformed variable equals the proportion of the variance of the variable that is accounted for by the components model.

If you specify the COVARIANCE option and do not specify TSTANDARD=Z, you can input the transformed data to PROC PRINCOMP, again specifying the COVARIANCE option, to perform a components analysis of the results of PROC PRINQUAL. Similarly, if you do not specify the COVARIANCE option with PROC PRINQUAL and you input the transformed data to PROC PRINCOMP without the COVARIANCE option, you receive the same report. However, some combinations of PROC PRINQUAL options, such as COVARIANCE and TSTANDARD=Z, while valid, produce approximations and scores that cannot be reproduced by PROC PRINCOMP.

The component scores in the output data set are computed from the correlations among the transformed variables, or from the covariances if you specified the COVARIANCE option. The component scores are

computed after the TSTANDARD=NOMISS transformation, if specified. The means of the component scores in the output data set are always zero. The variances equal the corresponding eigenvalues, unless you specify the STANDARD option; then the variances are set to one.

---

## Avoiding Constant Transformations

There are times when the optimal scaling produces a constant transformed variable. This can happen with the MONOTONE, UNTIE, and MSPLINE transformations when the target is negatively correlated with the original input variable. It can happen with all transformations when the target is uncorrelated with the original input variable. When this happens, the procedure modifies the target to avoid a constant transformation. This strategy avoids certain nonoptimal solutions.

If the transformation is monotonic and a constant transformed variable results, the procedure multiplies the target by  $-1$  and tries the optimal scaling again. If the transformation is not monotonic or if the multiplication by  $-1$  did not help, the procedure tries using a random target. If the transformation is still constant, the previous nonconstant transformation is retained. When a constant transformation is avoided by any strategy, this message is displayed: “A constant transformation was avoided for *name*.”

---

## Constant Variables

Constant and almost constant variables are zeroed and ignored.

---

## Character OPSCORE Variables

Character OPSCORE variables are replaced by a numeric variable containing category numbers before the iterations, and the character values are discarded. Only the first eight characters are considered in determining category membership. If you want the original character variable in the output data set, give it a different name in the OPSCORE specification (OPSCORE(x / name=(x2)) and name the original variable in the ID statement (ID x;).

---

## REITERATE Option Usage

You can use the REITERATE option to perform additional iterations when PROC PRINQUAL stops before the data have adequately converged. For example, suppose you execute the following code:

```
proc prinqual data=A cor out=B;
 transform mspline (X1-X5);
run;
```

If the transformations do not converge in the default 30 iterations, you can perform more iterations without repeating the first 30 iterations, as follows:

```
proc prinqual data=B reiterate cor out=B;
 transform mspline(X1-X5);
run;
```

Note that a WHERE statement is not necessary to exclude the correlation observations. They are automatically excluded because their `_TYPE_` variable value is not 'SCORE'.

You can also use the REITERATE option to specify starting values other than the original values for the transformations. Providing alternate starting points might avoid local optima. Here are two examples.

```
proc prinqual data=A out=B;
 transform rank(X1-X5);
run;

proc prinqual data=B reiterate out=C;
 /* Use ranks as the starting point. */
 transform monotone(X1-X5);
run;

data B;
 set A;
 array TXS[5] TX1-TX5;
 do j = 1 to 5;
 TXS[j] = normal(0);
 end;
run;

proc prinqual data=B reiterate out=C;
 /* Use a random starting point. */
 transform monotone(X1-X5);
run;
```

Note that divergence with the REITERATE option, particularly in the second iteration, is not an error since the initial transformation is not required to be a valid member of the transformation family. When you specify the REITERATE option, the iteration does not terminate when the criterion change is negative during the first 10 iterations.

---

## Passive Observations

Observations can be excluded from the analysis for several reasons, including zero weight, zero frequency, missing values in variables designated as IDENTITY, or missing values with the NOMISS option specified. These observations are passive in that they do not contribute to determining transformations, R square, total variance, and so on. However, some information can be computed for them, such as approximations, principal component scores, and transformed values. Passive observations in the output data set have a blank value for the variable `_TYPE_`.

Missing value estimates for passive observations might converge slowly with METHOD=MTV. In the following example, the missing value estimates should be 2, 5, and 8. Since the nonpassive observations do not change, the procedure converges in one iteration but the missing value estimates do not converge. The extra iterations produced by specifying CONVERGE=-1 and CCONVERGE=-1, as shown in the second PROC PRINQUAL step that follows, generate the expected results.

```

data A;
 input X Y;
 datalines;
1 1
2 .
3 3
4 4
5 .
6 6
7 7
8 .
9 9
;

proc prinqual nomiss data=A nomiss n=1 out=B method=mtv;
 transform lin(X Y);
run;

proc print;
run;

proc prinqual nomiss data=A nomiss n=1 out=B method=mtv converge=-1 cconverge=-1;
 transform lin(X Y);
run;

proc print;
run;

```

---

## Computational Resources

This section provides information about the computational resources required to run PROC PRINQUAL.

Let

- $N$  = number of observations
- $m$  = number of variables
- $n$  = number of principal components
- $k$  = maximum spline degree
- $p$  = maximum number of knots

- For the MTV algorithm, more than

$$56m + 8Nm + 8(6N + (p + k + 2)(p + k + 11))$$

bytes of array space are required.

- For the MGV and MAC algorithms, more than  $56m$  plus the maximum of the data matrix size and the optimal scaling work space bytes of array space are required. The data matrix size is  $8Nm$  bytes. The optimal scaling work space requires less than  $8(6N + (p + k + 2)(p + k + 1))$  bytes.
- For the MTV and MGV algorithms, more than  $56m + 4m(m + 1)$  bytes of array space are required.
- PROC PRINQUAL tries to store the original and transformed data in memory. If there is not enough memory, a utility data set is used, potentially resulting in a large increase in execution time. The amount of memory for the preceding data formulas is an underestimate of the amount of memory needed to handle most problems. These formulas give an absolute minimum amount of memory required. If a utility data set is used, and if memory could be used with perfect efficiency, then roughly the amount of memory stated previously would be needed. In reality, most problems require at least two or three times the minimum.
- PROC PRINQUAL sorts the data once. The sort time is roughly proportional to  $mN^{3/2}$ .
- For the MTV algorithm, the time required to compute the variable approximations is roughly proportional to  $2Nm^2 + 5m^3 + nm^2$ .
- For the MGV algorithm, one regression analysis per iteration is required to compute model parameter estimates. The time required to accumulate the crossproduct matrix is roughly proportional to  $Nm^2$ . The time required to compute the regression coefficients is roughly proportional to  $m^3$ . For each variable for each iteration, the swept crossproduct matrix is updated with time roughly proportional to  $m(N+m)$ . The swept crossproduct matrix is updated for each variable with time roughly proportional to  $m^2$ , until computations are refreshed, requiring all sweeps to be performed again.
- The only computationally intensive part of the MAC algorithm is the optimal scaling, since variable approximations are simple averages.
- Each optimal scaling is a multiple regression problem, although some transformations are handled with faster special-case algorithms. The number of regressors for the optimal scaling problems depends on the original values of the variable and the type of transformation. For each monotone spline transformation, an unknown number of multiple regressions is required to find a set of coefficients that satisfies the constraints. The B-spline basis is generated twice for each SPLINE and MSPLINE transformation for each iteration. The time required to generate the B-spline basis is roughly proportional to  $Nk^2$ .

---

## Displayed Output

The main output from PROC PRINQUAL is the output data set. However, the procedure does produce displayed output in the form of an iteration history table that includes the following:

- iteration number
- the criterion being optimized
- criterion change
- maximum and average absolute change in standardized variable scores computed over variables that can be iteratively transformed
- notes
- final convergence status

## ODS Table Names

PROC PRINQUAL assigns a name to each table it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in Table 74.4 along with the PROC PRINQUAL statement options needed to produce the table. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

**Table 74.4** ODS Tables Produced by PROC PRINQUAL

| ODS Table Name    | Description                 | Option      |
|-------------------|-----------------------------|-------------|
| ConvergenceStatus | Convergence Status          | default     |
| Footnotes         | Iteration History Footnotes | default     |
| MAC               | MAC Iteration History       | METHOD=MAC  |
| MGV               | MGV Iteration History       | METHOD=MGV  |
| MTV               | MTV Iteration History       | METHOD=MTV  |
| PctVar            | Percentage of Variance      | nonprinting |

The nonprinting “PctVar” table is not displayed and does not appear in the ODS trace output unless you specify it in an ODS OUTPUT statement, as in the following example:

```
ods output pctvar=pvardataset;
```

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “Statistical Graphics Using ODS.”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “A Primer on ODS Statistical Graphics” on page 599 in Chapter 21, “Statistical Graphics Using ODS.”

The plots are produced only when you specify the options shown in the table. You can reference every graph produced through ODS Graphics with a name. The names of the graphs that PROC PRINQUAL generates are listed in Table 74.5, along with the required statements and options.

**Table 74.5** Graphs Produced by PROC PRINQUAL

| ODS Graph Name     | Plot Description                     | Option               |
|--------------------|--------------------------------------|----------------------|
| MDPrefPlot         | Multidimensional preference analysis | MDPREF               |
| TransformationPlot | Variable transformation              | PLOTS=TRANSFORMATION |



## Examples: PRINQUAL Procedure

### Example 74.1: Multidimensional Preference Analysis of Automobile Data

This example uses PROC PRINQUAL to perform a nonmetric multidimensional preference (MDPREF) analysis (Carroll 1972). MDPREF analysis is a principal component analysis of a data matrix with columns that correspond to people and rows that correspond to objects. The data are ratings or rankings of each person's preference for each object. The data are the transpose of the usual multivariate data matrix. (In other words, the columns are people; in the more typical matrix the rows represent people.) The final result of an MDPREF analysis is a biplot (Gabriel 1981) of the resulting preference space. A biplot displays the judges and objects in a single plot by projecting them onto the plane in the transformed variable space that accounts for the most variance.

In 1980, 25 judges gave their preferences for each of 17 new automobiles. The ratings were made on a 0 to 9 scale, with 0 meaning very weak preference and 9 meaning very strong preference for the automobile. The following statements create a SAS data set with the manufacturer and model of each automobile along with the ratings:

```

title 'Preference Ratings for Automobiles Manufactured in 1980';

options validvarname=any;

data CarPref;
 input Make $ 1-10 Model $ 12-22 @25 ('1'n-'25'n) (1.);
 datalines;
Cadillac Eldorado 8007990491240508971093809
Chevrolet Chevette 0051200423451043003515698
Chevrolet Citation 4053305814161643544747795
Chevrolet Malibu 6027400723121345545668658
Ford Fairmont 2024006715021443530648655
Ford Mustang 5007197705021101850657555
Ford Pinto 0021000303030201500514078
Honda Accord 5956897609699952998975078
Honda Civic 4836709507488852567765075
Lincoln Continental 7008990592230409962091909
Plymouth Gran Fury 7006000434101107333458708
Plymouth Horizon 3005005635461302444675655
Plymouth Volare 4005003614021602754476555
Pontiac Firebird 0107895613201206958265907
Volkswagen Dasher 4858696508877795377895000
Volkswagen Rabbit 4858509709695795487885000
Volvo DL 9989998909999987989919000
;

```

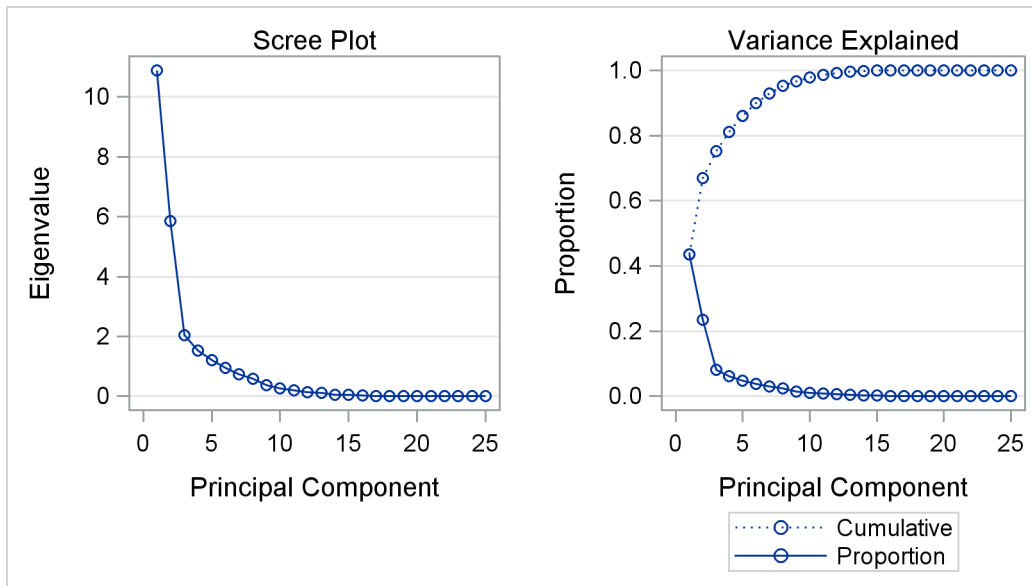
The following statements run PROC PRINCOMP and create a scree plot. The results of this step are shown in [Output 74.1.1](#).

```

ods graphics on;
* Principal Component Analysis of the Original Data;
proc princomp data=CarPref;
 ods select ScreePlot;
 var '1'n-'25'n;
run;

```

Output 74.1.1 Eigenvalue Plot



The scree or eigenvalue plot in [Output 74.1.1](#) shows that two principal components should be retained. There is a clear separation between the first two components and the remaining components. There are eight eigenvalues that are precisely zero because there are eight fewer observations than variables in the data matrix. One additional eigenvalue is zero, for a total of nine zero eigenvalues, since the correlation matrix is based on centered data. The following statements create the data set and perform a principal component analysis of the original data.

PROC PRINQUAL fits the nonmetric MDPREF model. PROC PRINQUAL monotonically transforms the raw judgments to maximize the proportion of variance accounted for by the first two principal components. The MONOTONE option is specified in the TRANSFORM statement to request a nonmetric MDPREF analysis; alternatively, you can instead specify the IDENTITY option for a metric analysis. Several options are used in the PROC PRINQUAL statement. The option DATA=CarPref specifies the input data set, OUT=Results creates an output data set, and N=2 and the default METHOD=MTV transform the data to better fit a two-component model. The REPLACE option replaces the original data with the monotonically transformed data in the OUT= data set. The MDPREF option standardizes the component scores to variance one so that the geometry of the biplot is correct, and it creates two variables in the OUT= data set named Prin1 and Prin2. These variables contain the standardized principal component scores and structure matrix, which are used to make the biplot. If the variables in data matrix  $\mathbf{X}$  are standardized to mean zero and variance one, and  $n$  is the number of rows in  $\mathbf{X}$ , then  $\mathbf{X} = \mathbf{V}\mathbf{\Lambda}^{1/2}\mathbf{W}'$  is the principal component model, where  $\mathbf{X}'\mathbf{X}/(n-1) = \mathbf{W}\mathbf{\Lambda}\mathbf{W}'$ . The  $\mathbf{W}$  and  $\mathbf{\Lambda}$  contain the eigenvectors and eigenvalues of the correlation matrix of  $\mathbf{X}$ . The first two columns of  $\mathbf{V}$ , the standardized component scores, and  $\mathbf{W}\mathbf{\Lambda}^{1/2}$ , which is the structure matrix, are output. The advantage of creating a biplot based on principal components is that coordinates do not depend on the sample size. The following statements transform the data and produce [Output 74.1.2](#).

```
* Transform the Data to Better Fit a Two Component Model;
proc prinqual data=CarPref out=Results n=2 replace mdpref;
 title2 'Multidimensional Preference (MDPREF) Analysis';
 title3 'Optimal Monotonic Transformation of Preference Data';
 id model;
 transform monotone('1'n-'25'n);
run;
```

## Output 74.1.2 PRINQUAL Iteration History

| Preference Ratings for Automobiles Manufactured in 1980 |                   |                   |                           |                     |               |
|---------------------------------------------------------|-------------------|-------------------|---------------------------|---------------------|---------------|
| Multidimensional Preference (MDPREF) Analysis           |                   |                   |                           |                     |               |
| Optimal Monotonic Transformation of Preference Data     |                   |                   |                           |                     |               |
| The PRINQUAL Procedure                                  |                   |                   |                           |                     |               |
| PRINQUAL MTV Algorithm Iteration History                |                   |                   |                           |                     |               |
| Iteration<br>Number                                     | Average<br>Change | Maximum<br>Change | Proportion<br>of Variance | Criterion<br>Change | Note          |
| 1                                                       | 0.24994           | 1.28017           | 0.66946                   |                     |               |
| 2                                                       | 0.07223           | 0.36958           | 0.80194                   | 0.13249             |               |
| 3                                                       | 0.04522           | 0.29026           | 0.81598                   | 0.01404             |               |
| 4                                                       | 0.03096           | 0.25213           | 0.82178                   | 0.00580             |               |
| 5                                                       | 0.02182           | 0.23045           | 0.82493                   | 0.00315             |               |
| 6                                                       | 0.01602           | 0.19017           | 0.82680                   | 0.00187             |               |
| 7                                                       | 0.01219           | 0.14748           | 0.82793                   | 0.00113             |               |
| 8                                                       | 0.00953           | 0.11031           | 0.82861                   | 0.00068             |               |
| 9                                                       | 0.00737           | 0.06461           | 0.82904                   | 0.00043             |               |
| 10                                                      | 0.00556           | 0.04469           | 0.82930                   | 0.00026             |               |
| 11                                                      | 0.00445           | 0.04087           | 0.82944                   | 0.00014             |               |
| 12                                                      | 0.00381           | 0.03706           | 0.82955                   | 0.00011             |               |
| 13                                                      | 0.00319           | 0.03348           | 0.82965                   | 0.00009             |               |
| 14                                                      | 0.00255           | 0.02999           | 0.82971                   | 0.00006             |               |
| 15                                                      | 0.00213           | 0.02824           | 0.82976                   | 0.00005             |               |
| 16                                                      | 0.00183           | 0.02646           | 0.82980                   | 0.00004             |               |
| 17                                                      | 0.00159           | 0.02472           | 0.82983                   | 0.00003             |               |
| 18                                                      | 0.00139           | 0.02305           | 0.82985                   | 0.00003             |               |
| 19                                                      | 0.00123           | 0.02145           | 0.82988                   | 0.00002             |               |
| 20                                                      | 0.00109           | 0.01993           | 0.82989                   | 0.00002             |               |
| 21                                                      | 0.00096           | 0.01850           | 0.82991                   | 0.00001             |               |
| 22                                                      | 0.00086           | 0.01715           | 0.82992                   | 0.00001             |               |
| 23                                                      | 0.00076           | 0.01588           | 0.82993                   | 0.00001             |               |
| 24                                                      | 0.00067           | 0.01440           | 0.82994                   | 0.00001             |               |
| 25                                                      | 0.00059           | 0.00871           | 0.82994                   | 0.00001             |               |
| 26                                                      | 0.00050           | 0.00720           | 0.82995                   | 0.00000             |               |
| 27                                                      | 0.00043           | 0.00642           | 0.82995                   | 0.00000             |               |
| 28                                                      | 0.00037           | 0.00573           | 0.82995                   | 0.00000             |               |
| 29                                                      | 0.00031           | 0.00510           | 0.82995                   | 0.00000             |               |
| 30                                                      | 0.00027           | 0.00454           | 0.82995                   | 0.00000             | Not Converged |

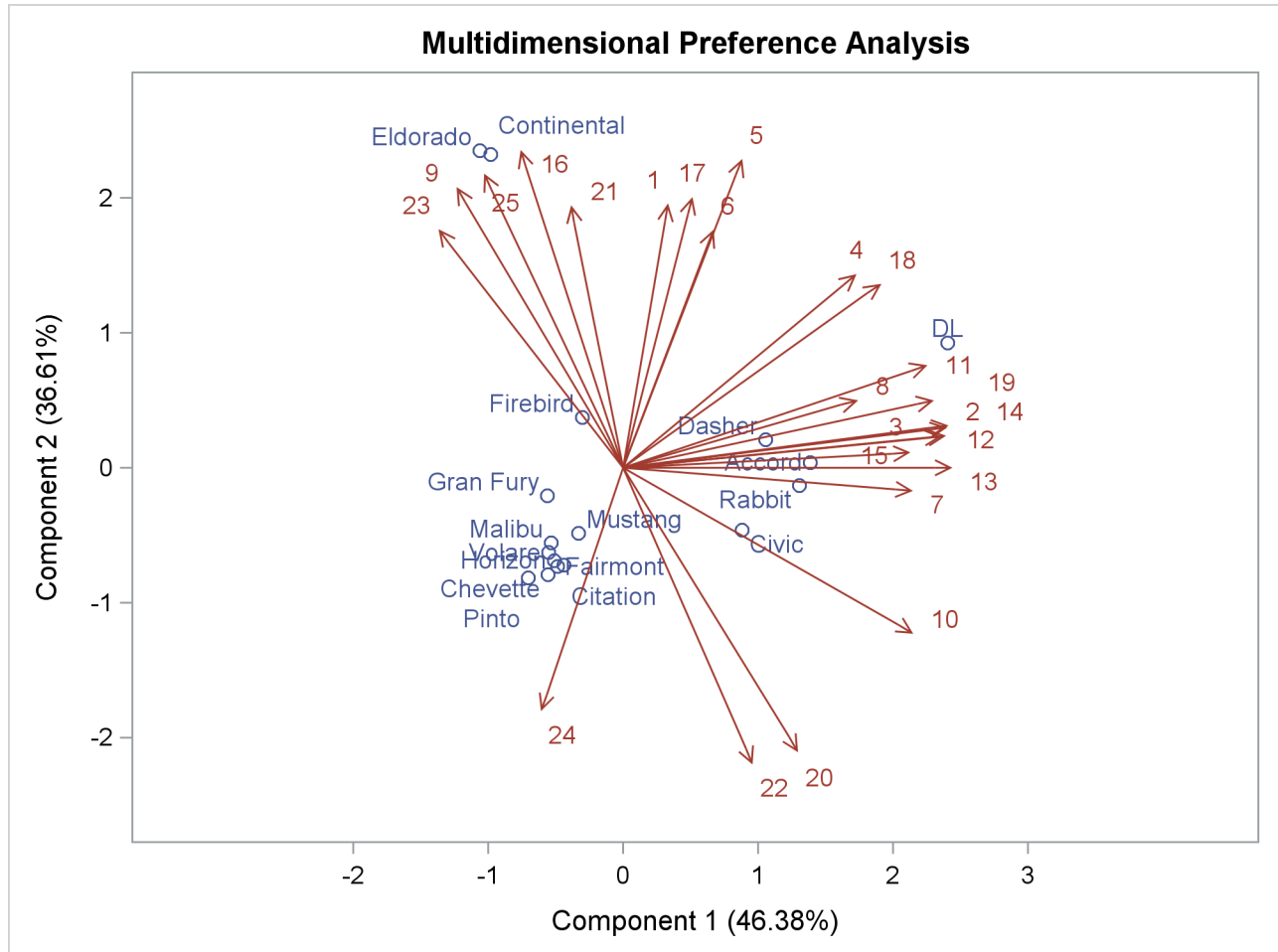
**WARNING:** Failed to converge, however criterion change is less than 0.0001.

The iteration history displayed by PROC PRINQUAL indicates that the proportion of variance is increased from an initial 0.66946 to 0.82995. The proportion of variance accounted for by PROC PRINQUAL on the first iteration equals the cumulative proportion of variance shown by PROC PRINCOMP for the first two principal components. PROC PRINQUAL's initial iteration performs a standard principal component analysis of the raw data. The columns labeled Average Change, Maximum Change, and Criterion Change contain values that always decrease, indicating that PROC PRINQUAL is improving the transformations at a monotonically decreasing rate over the iterations. This does not always happen, and when it does not, it suggests that the analysis might be converging to a degenerate solution. See [Example 74.2](#) for a discussion

of a degenerate solution. The algorithm does not converge in 30 iterations. However, the criterion change is small, indicating that more iterations are unlikely to have much effect on the results.

The biplot, shown in [Output 74.1.3](#), is automatically displayed by PROC PRINQUAL when ODS Graphics is enabled and the MDPREF option is specified.

**Output 74.1.3** Biplot Made with PRINQUAL



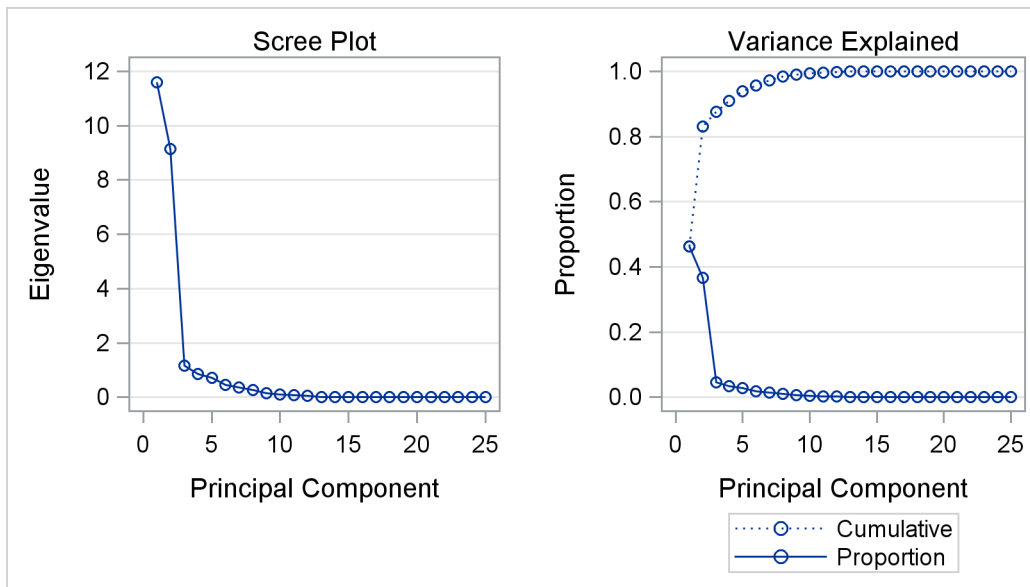
The second PROC PRINCOMP analysis is performed on the transformed data. The WHERE statement is used to retain only the monotonically transformed judgments. The scree plot shows that the first two eigenvalues are now much larger than the remaining smaller eigenvalues. The second eigenvalue has increased markedly at the expense of the next several eigenvalues. Two principal components seem to be necessary and sufficient to adequately describe these judges' preferences for these automobiles. The cumulative proportion of variance displayed by PROC PRINCOMP for the first two principal components is 0.83. The following statements perform the analysis and produce [Output 74.1.4](#):

```

* Final Principal Component Analysis;
proc princomp data=Results;
 ods select ScreePlot;
 var '1'n-'25'n;
 where _TYPE_='SCORE';
run;

```

Output 74.1.4 Transformed Data Eigenvalue Plot



The remainder of the example discusses the MDPREF biplot. A biplot is a plot that displays the relation between the row points and the columns of a data matrix. The rows of  $\mathbf{V}$ , the standardized component scores, and  $\mathbf{W}\mathbf{\Lambda}^{1/2}$ , the structure matrix, contain enough information to reproduce  $\mathbf{X}$ . The  $(i, j)$  element of  $\mathbf{X}$  is the product of row  $i$  of  $\mathbf{V}$  and row  $j$  of  $\mathbf{W}\mathbf{\Lambda}^{1/2}$ . If all but the first two columns of  $\mathbf{V}$  and  $\mathbf{W}\mathbf{\Lambda}^{1/2}$  are discarded, the  $(i, j)$  element of  $\mathbf{X}$  is approximated by the product of row  $i$  of  $\mathbf{V}$  and row  $j$  of  $\mathbf{W}\mathbf{\Lambda}^{1/2}$ .

Since the MDPREF analysis is based on a principal component model, the dimensions of the MDPREF biplot are the first two principal components. The first principal component is the longest dimension through the MDPREF biplot. The first principal component is overall preference, which is the most salient dimension in the preference judgments. One end points in the direction that is on the average preferred most by the judges, and the other end points in the least preferred direction. The second principal component is orthogonal to the first principal component, and it is the orthogonal direction that is the second most salient. The interpretation of the second dimension varies from example to example.

With an MDPREF biplot, it is geometrically appropriate to represent each automobile (object) by a point and each judge by a vector. The automobile points have coordinates that are the scores of the automobile on the first two principal components. The judge vectors emanate from the origin of the space and go through a point whose coordinates are the coefficients of the judge (variable) on the first two principal components.

The absolute length of a vector is arbitrary. However, the relative lengths of the vectors indicate fit, with the squared lengths being proportional to the communalities that you can get in PROC FACTOR output. The direction of the vector indicates the direction that is most preferred by the individual judge, with preference increasing as the vector moves from the origin. Let  $\mathbf{v}'$  be row  $i$  of  $\mathbf{V}$ ,  $\mathbf{u}'$  be row  $j$  of  $\mathbf{U} = \mathbf{W}\mathbf{\Lambda}^{1/2}$ ,  $\|\mathbf{v}\|$

be the length of  $\mathbf{v}$ ,  $\|\mathbf{u}\|$  be the length of  $\mathbf{u}$ , and  $\theta$  be the angle between  $\mathbf{v}$  and  $\mathbf{u}$ . The predicted degree of preference that an individual judge has for an automobile is  $\mathbf{u}'\mathbf{v} = \|\mathbf{u}\| \|\mathbf{v}\| \cos \theta$ . Each automobile point can be orthogonally projected onto the vector. The projection of automobile  $i$  on vector  $j$  is  $\mathbf{u}((\mathbf{u}'\mathbf{v})/(\mathbf{u}'\mathbf{u}))$ , and the length of this projection is  $\|\mathbf{v}\| \cos \theta$ . The automobile that projects farthest along a vector in the direction it points is that judge's most preferred automobile, since the length of this projection,  $\|\mathbf{v}\| \cos \theta$ , differs from the predicted preference,  $\|\mathbf{u}\| \|\mathbf{v}\| \cos \theta$ , only by  $\|\mathbf{u}\|$ , which is constant for each judge.

To interpret the biplot, look for directions through the plot that show a continuous change in some attribute of the automobiles, or look for regions in the plot that contain clusters of automobile points and determine what attributes the automobiles have in common. Points that are tightly clustered in a region of the plot represent automobiles that have the same preference patterns across the judges. Vectors that point in roughly the same direction represent judges who have similar preference patterns.

In the biplot, American automobiles are located at the left of the space, while European and Japanese automobiles are located at the right. At the top of the space are expensive American automobiles (Cadillac Eldorado, Lincoln Continental), while at the bottom are inexpensive ones (Ford Pinto, Chevrolet Chevette). The first principal component differentiates American from imported automobiles, and the second arranges automobiles by price and other associated characteristics.

The two expensive American automobiles form a cluster, the sporty automobile (Pontiac Firebird) is by itself, the Volvo DL is by itself, and the remaining imported autos form a cluster, as do the remaining American autos. It seems there are 5 prototypical automobiles in this set of 17, in terms of preference patterns among the 25 judges.

Most of the judges prefer the imported automobiles, especially the Volvo. There is also a fairly large minority that prefer the expensive autos, whether or not they are American (those with vectors that point toward one o'clock), or simply prefer expensive American automobiles (vectors that point toward eleven o'clock). There are two judges who prefer anything except expensive American autos (five o'clock vectors), and one who prefers inexpensive American autos (seven o'clock vector).

Several vectors point toward the upper-right corner of the plot, toward a region with no automobiles. This is the region between the European and Japanese autos at the right and the luxury autos at the top. This suggests that there is a market for luxury Japanese and European automobiles.

The next part of this example modifies the graph template for the MDPREF plot to display group information (the make of the automobile) in the MDPREF plot. First you need to run the PROC PRINQUAL step with ODS trace output enabled to find the name of the graph template for the MDPREF plot:

```
ods trace on;
proc prinqual data=CarPref out=Results n=2 replace mdpref;
 title2 'Multidimensional Preference (MDPREF) Analysis';
 title3 'Optimal Monotonic Transformation of Preference Data';
 id model;
 transform monotone('1'n-'25'n);
run;
```

The results are as follows:

Output Added:

```

Name: MDPrefPlot
Label: 2 by 1
Template: Stat.Prinqual.Graphics.MDPref
Path: Prinqual.MDPREF.MDPrefPlot

```

The following step displays the template:

```
proc template;
 source Stat.Prinqual.Graphics.MDPref;
run;
```

The following template is displayed:

```
define statgraph Stat.Prinqual.Graphics.MDPref;
 notes "Multidimensional Preference Analysis Plot";
 dynamic xVar yVar xVec yVec ylab xlab yshortlab xshortlab xOri yOri
 stretch;
 begingraph;
 entrytitle "Multidimensional Preference Analysis";
 layout overlayequated / equatetype=fit xaxisopts=(label=XLAB shortlabel
 =XSHORTLAB offsetmin=0.1 offsetmax=0.1) yaxisopts=(label=YLAB
 shortlabel=YSHORTLAB offsetmin=0.1 offsetmax=0.1);
 scatterplot y=YVAR x=XVAR / datalabel=IDLAB1 rolename=(_tip1=
 OBSNUMVAR _id2=IDLAB2 _id3=IDLAB3 _id4=IDLAB4 _id5=IDLAB5 _id6=
 IDLAB6 _id7=IDLAB7 _id8=IDLAB8 _id9=IDLAB9 _id10=IDLAB10 _id11=
 IDLAB11 _id12=IDLAB12 _id13=IDLAB13 _id14=IDLAB14 _id15=IDLAB15
 _id16=IDLAB16 _id17=IDLAB17 _id18=IDLAB18 _id19=IDLAB19 _id20=
 IDLAB20) tip=(y x datalabel _tip1 _id2 _id3 _id4 _id5 _id6 _id7
 _id8 _id9 _id10 _id11 _id12 _id13 _id14 _id15 _id16 _id17 _id18
 _id19 _id20) datalabelattrs=GRAPHVALUETEXT (color=
 GraphData1:ContrastColor) markerattrs=GRAPHDATA1;
 vectorplot y=YVEC x=XVEC xorigin=0 yorigin=0 / datalabel=LABEL2VAR
 shaftprotected=false rolename=(_tip1=VNAME _tip2=VLABEL _tip3=
 YORI _tip4=XORI _tip5=LENGTH _tip6=LENGTH2) tip=(y x datalabel
 _tip1 _tip2 _tip3 _tip4 _tip5 _tip6) datalabelattrs=
 GRAPHVALUETEXT (color=GraphData2:ContrastColor) lineattrs=
 GRAPHDATA2 (pattern=solid) primary=true;
 if (0)
 entry "Vector Stretch = " STRETCH / autoalign=(topright topleft
 bottomright bottomleft right left top bottom);
 endif;
 endlayout;
endgraph;
end;
```

The following step adds a PROC PRINQUAL statement and a RUN statement, removes attribute options from the SCATTERPLOT statement, adds a GROUP=IDLAB2 option to use the second ID variable as a group variable, and adds a NAME='s' option along with a DISCRETELEGEND statement to display the groups in a legend:

```

proc template;
 define statgraph Stat.Prinqual.Graphics.MDPref;
 notes "Multidimensional Preference Analysis Plot";
 dynamic xVar yVar xVec yVec ylab xlab yshortlab xshortlab xOri yOri
 stretch;
 begingraph;
 entrytitle "Multidimensional Preference Analysis";
 layout overlayequated / equatetype=fit xaxisopts=(label=XLAB shortlabel
 =XSHORTLAB offsetmin=0.1 offsetmax=0.1) yaxisopts=(label=YLAB
 shortlabel=YSHORTLAB offsetmin=0.1 offsetmax=0.1);
 scatterplot y=YVAR x=XVAR / datalabel=IDLAB1 rolename=(_tip1=
 OBSNUMVAR _id2=IDLAB2 _id3=IDLAB3 _id4=IDLAB4 _id5=IDLAB5 _id6=
 IDLAB6 _id7=IDLAB7 _id8=IDLAB8 _id9=IDLAB9 _id10=IDLAB10 _id11=
 IDLAB11 _id12=IDLAB12 _id13=IDLAB13 _id14=IDLAB14 _id15=IDLAB15
 _id16=IDLAB16 _id17=IDLAB17 _id18=IDLAB18 _id19=IDLAB19 _id20=
 IDLAB20) tip=(y x datalabel _tip1 _id2 _id3 _id4 _id5 _id6 _id7
 _id8 _id9 _id10 _id11 _id12 _id13 _id14 _id15 _id16 _id17 _id18
 _id19 _id20)

 group=idlab2 name='s'; *<==== add the group variable ====<<<<;

 vectorplot y=YVEC x=XVEC xorigin=0 yorigin=0 / datalabel=LABEL2VAR
 shaftprotected=false rolename=(_tip1=VNAME _tip2=VLABEL _tip3=
 YORI _tip4=XORI _tip5=LENGTH _tip6=LENGTH2) tip=(y x datalabel
 _tip1 _tip2 _tip3 _tip4 _tip5 _tip6) datalabelattrs=
 GRAPHVALUETEXT (color=GraphData2:ContrastColor) lineattrs=
 GRAPHDATA2 (pattern=solid) primary=true;

 discretelegend 's'; *<==== add a legend ====<<<<;

 if (0)
 entry "Vector Stretch = " STRETCH / autoalign=(topright topleft
 bottomright bottomleft right left top bottom);
 endif;
 endlayout;
 endgraph;
end;
run;

```

The following step creates the MDPREF plot with the make of the automobile added as a second ID variable and displayed in the graph as a group variable:

```

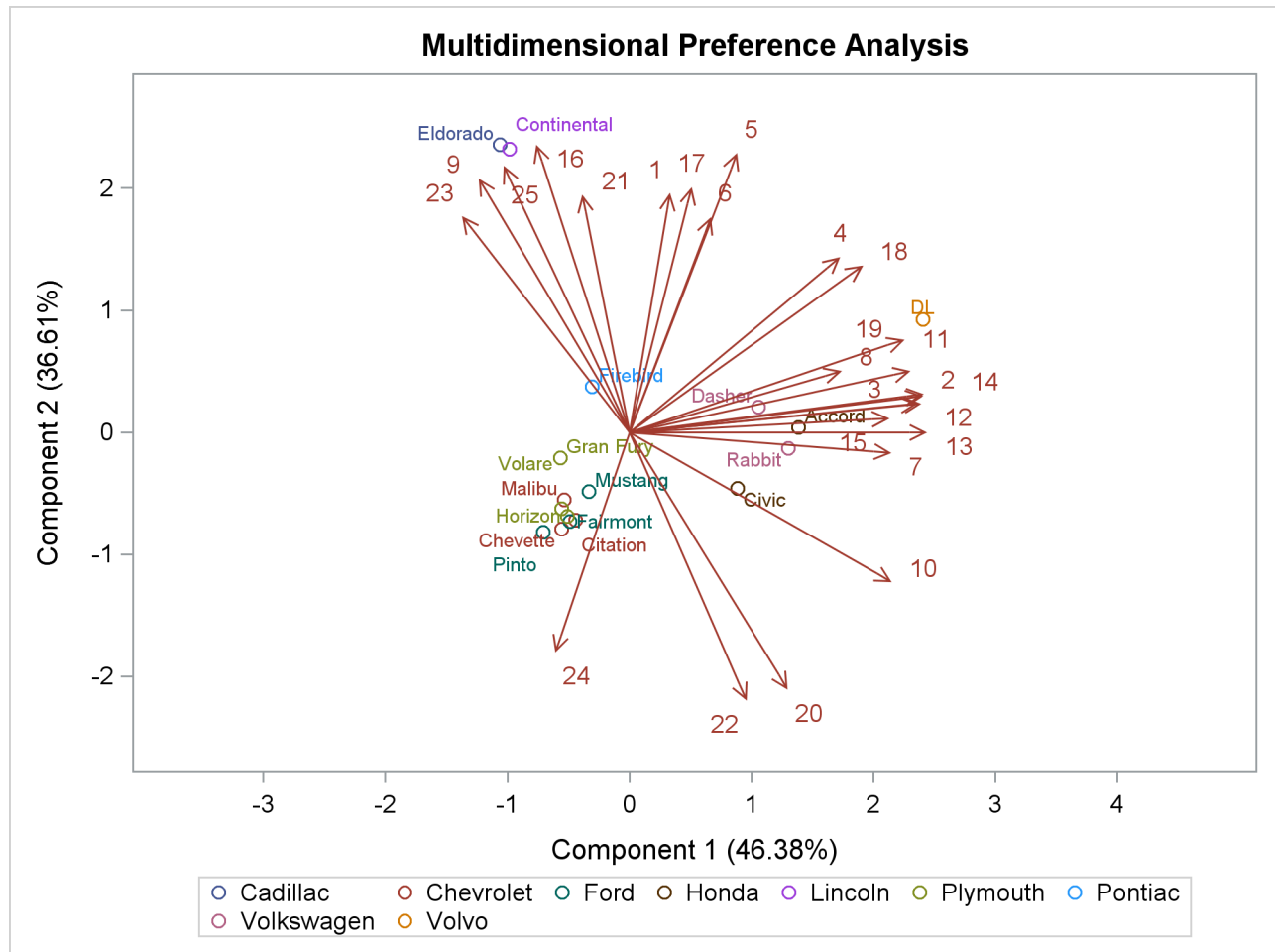
proc prinqual data=CarPref out=Results n=2 replace mdpref;
 title2 'Multidimensional Preference (MDPREF) Analysis';
 title3 'Optimal Monotonic Transformation of Preference Data';
 id model make;
 transform monotone('1'n-'25'n);
run;

```

The results are displayed in [Output 74.1.5](#).



Output 74.1.5 Biplot with a Group Variable



The following step restores the default template:

```
proc template;
 delete Stat.Prinqual.Graphics.MDPref / store=sasuser.templat;
run;
```

## Example 74.2: Principal Components of Basketball Rankings

The data in this example are 1985–1986 preseason rankings of 35 U.S. college basketball teams by 10 different news services. The services do not all rank the same teams or the same number of teams, so there are missing values in these data. Each of the 35 teams in the data set is ranked by at least one news service. One way of summarizing these data is with a principal component analysis, since the rankings should all be related to a single underlying variable, the first principal component.

You can use PROC PRINQUAL to estimate the missing ranks and compute scores for all observations. You can formulate a PROC PRINQUAL analysis that assumes that the observed ranks are ordinal variables and replaces the ranks with new numbers that are monotonic with the ranks and better fit the one prin-

principal component model. The missing rank estimates need to be constrained since a news service would have positioned the unranked teams below the teams it ranked. PROC PRINQUAL should impose order constraints within the nonmissing values and between the missing and nonmissing values, but not within the missing values. PROC PRINQUAL has sophisticated missing data handling facilities; however, these facilities cannot directly handle this problem. The solution requires reformulating the problem.

By performing some preliminary data manipulations, specifying the N=1 option in the PROC PRINQUAL statement, and specifying the UNTIE transformation in the TRANSFORM statement, you can make the missing value estimates conform to the requirements. The PROC MEANS step finds the largest rank for each variable. The next DATA step replaces missing values with a value that is one larger than the largest observed rank. The PROC PRINQUAL N=1 option specifies that the variables should be transformed to make them as one-dimensional as possible. The UNTIE transformation in the TRANSFORM statement monotonically transforms the ranks, untying any ties in an optimal way. Because the only ties are for the values that replace the missing values, and because these values are larger than the observed values, the rescaling of the data satisfies the preceding requirements.

The following statements create the data set and perform the transformations discussed previously. These statements produce [Output 74.2.1](#) and [Output 74.2.2](#).

```

* Preseason 1985 College Basketball Rankings
* (rankings of 35 teams by 10 news services)
*
* Note: (a) Various news services rank varying numbers of teams.
* (b) Not all 35 teams are ranked by all news services.
* (c) Each team is ranked by at least one service.
* (d) Rank 20 is missing for UPI.;

title1 '1985 Preseason College Basketball Rankings';

data bballm;
 input School $13. CSN DurhamSun DurhamHerald WashingtonPost
 USA_Today SportMagazine InsideSports UPI AP SportsIllustrated;
 label CSN = 'Community Sports News (Chapel Hill, NC)'
 DurhamSun = 'Durham Sun'
 DurhamHerald = 'Durham Morning Herald'
 WashingtonPost = 'Washington Post'
 USA_Today = 'USA Today'
 SportMagazine = 'Sport Magazine'
 InsideSports = 'Inside Sports'
 UPI = 'United Press International'
 AP = 'Associated Press'
 SportsIllustrated = 'Sports Illustrated'
 ;
 format CSN--SportsIllustrated 5.1;
 datalines;
Louisville 1 8 1 9 8 9 6 10 9 9
Georgia Tech 2 2 4 3 1 1 1 2 1 1
Kansas 3 4 5 1 5 11 8 4 5 7
Michigan 4 5 9 4 2 5 3 1 3 2
Duke 5 6 7 5 4 10 4 5 6 5
UNC 6 1 2 2 3 4 2 3 2 3
Syracuse 7 10 6 11 6 6 5 6 4 10
Notre Dame 8 14 15 13 11 20 18 13 12 .

```

```

Kentucky 9 15 16 14 14 19 11 12 11 13
LSU 10 9 13 . 13 15 16 9 14 8
DePaul 11 . 21 15 20 . 19 . . 19
Georgetown 12 7 8 6 9 2 9 8 8 4
Navy 13 20 23 10 18 13 15 . 20 .
Illinois 14 3 3 7 7 3 10 7 7 6
Iowa 15 16 . . 23 . . 14 . 20
Arkansas 16 . . . 25 16
Memphis State 17 . 11 . 16 8 20 . 15 12
Washington 18 17 . .
UAB 19 13 10 . 12 17 . 16 16 15
UNLV 20 18 18 19 22 . 14 18 18 .
NC State 21 17 14 16 15 . 12 15 17 18
Maryland 22 . . . 19 . . . 19 14
Pittsburgh 23
Oklahoma 24 19 17 17 17 12 17 . 13 17
Indiana 25 12 20 18 21
Virginia 26 . 22 . . 18
Old Dominion 27
Auburn 28 11 12 8 10 7 7 11 10 11
St. Johns 29 14
UCLA 30 19 . .
St. Joseph's . . 19
Tennessee . . 24 . . 16
Montana . . . 20
Houston 24
Virginia Tech 13 . . .
;

```

```

* Find maximum rank for each news service and replace
* each missing value with the next highest rank.;

```

```

proc means data=bballm noprint;
 output out=maxrank
 max=mcsn mdurs mdurh mwas musa mspom mins mupi map mspoi;
run;

```

```

data bball;
 set bballm;
 if _n_=1 then set maxrank;
 array services[10] CSN--SportsIllustrated;
 array maxranks[10] mcsn--mspoi;
 keep School CSN--SportsIllustrated;
 do i=1 to 10;
 if services[i]=. then services[i]=maxranks[i]+1;
 end;
run;

```

```

* Assume that the ranks are ordinal and that unranked teams would have
* been ranked lower than ranked teams. Monotonically transform all ranked
* teams while estimating the unranked teams. Enforce the constraint that
* the missing ranks are estimated to be less than the observed ranks.
* Order the unranked teams optimally within this constraint. Do this so
* as to maximize the variance accounted for by one linear combination.
* This makes the data as nearly rank one as possible, given the constraints.
*

```

\* NOTE: The UNTIE transformation should be used with caution.  
 \* It frequently produces degenerate results.;

ods graphics on;

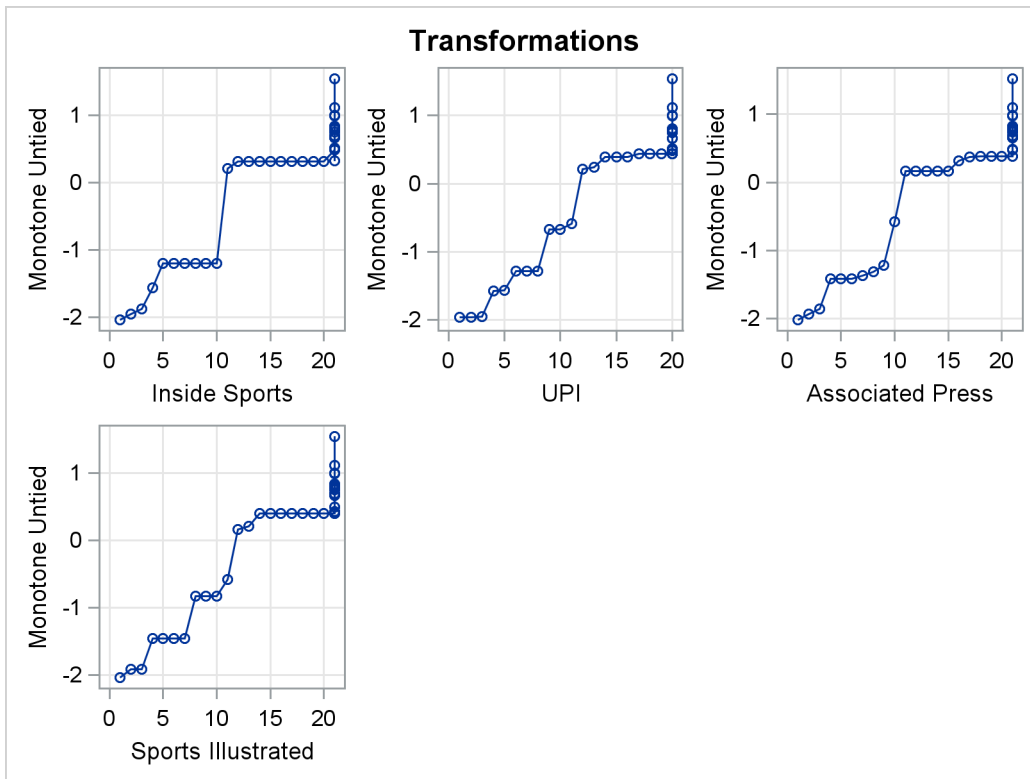
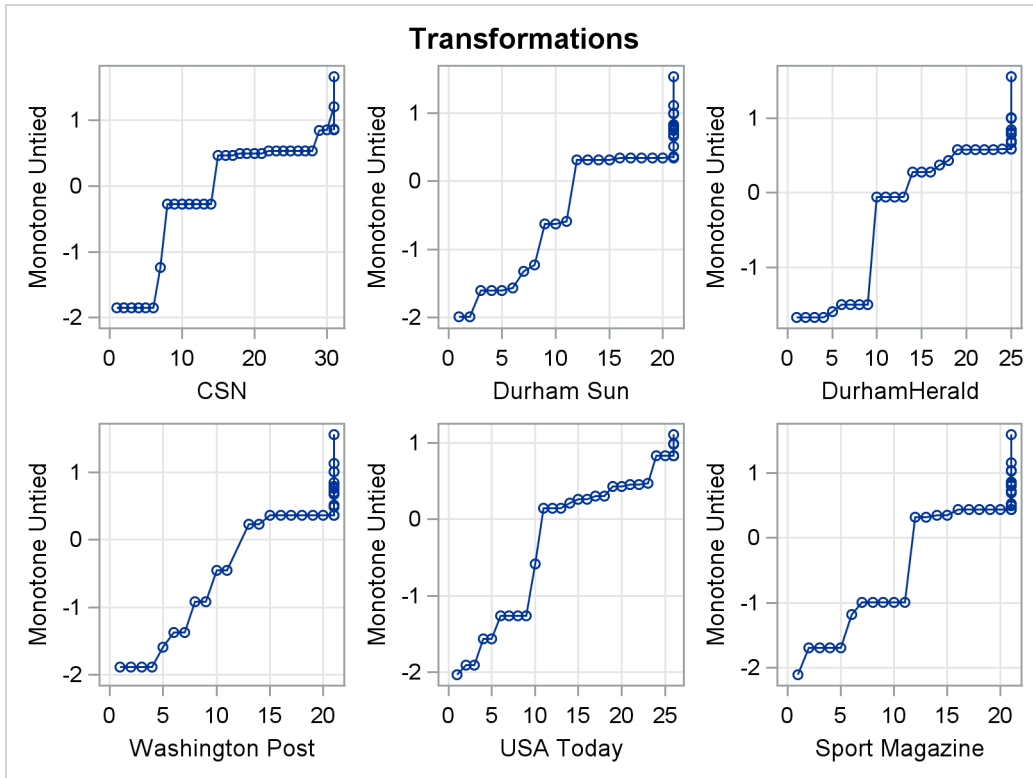
```
proc prinqual data=bball out=tbball scores n=1 tstandard=z
 plots=transformations;
 title2 'Optimal Monotonic Transformation of Ranked Teams';
 title3 'with Constrained Estimation of Unranked Teams';
 transform untie(CSN -- SportsIllustrated);
 id School;
run;
```

**Output 74.2.1 PRINQUAL Iteration History**

| 1985 Preseason College Basketball Rankings<br>Optimal Monotonic Transformation of Ranked Teams<br>with Constrained Estimation of Unranked Teams |                   |                   |                           |                     |               |
|-------------------------------------------------------------------------------------------------------------------------------------------------|-------------------|-------------------|---------------------------|---------------------|---------------|
| The PRINQUAL Procedure                                                                                                                          |                   |                   |                           |                     |               |
| PRINQUAL MTV Algorithm Iteration History                                                                                                        |                   |                   |                           |                     |               |
| Iteration<br>Number                                                                                                                             | Average<br>Change | Maximum<br>Change | Proportion<br>of Variance | Criterion<br>Change | Note          |
| 1                                                                                                                                               | 0.18563           | 0.76531           | 0.85850                   |                     |               |
| 2                                                                                                                                               | 0.03225           | 0.14627           | 0.94362                   | 0.08512             |               |
| 3                                                                                                                                               | 0.02126           | 0.10530           | 0.94669                   | 0.00307             |               |
| 4                                                                                                                                               | 0.01467           | 0.07526           | 0.94801                   | 0.00132             |               |
| 5                                                                                                                                               | 0.01067           | 0.05282           | 0.94865                   | 0.00064             |               |
| 6                                                                                                                                               | 0.00800           | 0.03669           | 0.94899                   | 0.00034             |               |
| 7                                                                                                                                               | 0.00617           | 0.02862           | 0.94919                   | 0.00020             |               |
| 8                                                                                                                                               | 0.00486           | 0.02636           | 0.94932                   | 0.00013             |               |
| 9                                                                                                                                               | 0.00395           | 0.02453           | 0.94941                   | 0.00009             |               |
| 10                                                                                                                                              | 0.00327           | 0.02300           | 0.94947                   | 0.00006             |               |
| 11                                                                                                                                              | 0.00275           | 0.02166           | 0.94952                   | 0.00005             |               |
| 12                                                                                                                                              | 0.00236           | 0.02041           | 0.94956                   | 0.00004             |               |
| 13                                                                                                                                              | 0.00205           | 0.01927           | 0.94959                   | 0.00003             |               |
| 14                                                                                                                                              | 0.00181           | 0.01818           | 0.94962                   | 0.00003             |               |
| 15                                                                                                                                              | 0.00162           | 0.01719           | 0.94964                   | 0.00002             |               |
| 16                                                                                                                                              | 0.00147           | 0.01629           | 0.94966                   | 0.00002             |               |
| 17                                                                                                                                              | 0.00136           | 0.01546           | 0.94968                   | 0.00002             |               |
| 18                                                                                                                                              | 0.00128           | 0.01469           | 0.94970                   | 0.00002             |               |
| 19                                                                                                                                              | 0.00121           | 0.01398           | 0.94971                   | 0.00001             |               |
| 20                                                                                                                                              | 0.00115           | 0.01332           | 0.94973                   | 0.00001             |               |
| 21                                                                                                                                              | 0.00111           | 0.01271           | 0.94974                   | 0.00001             |               |
| 22                                                                                                                                              | 0.00105           | 0.01213           | 0.94975                   | 0.00001             |               |
| 23                                                                                                                                              | 0.00099           | 0.01155           | 0.94976                   | 0.00001             |               |
| 24                                                                                                                                              | 0.00095           | 0.01095           | 0.94977                   | 0.00001             |               |
| 25                                                                                                                                              | 0.00091           | 0.01038           | 0.94978                   | 0.00001             |               |
| 26                                                                                                                                              | 0.00088           | 0.00986           | 0.94978                   | 0.00001             |               |
| 27                                                                                                                                              | 0.00084           | 0.00936           | 0.94979                   | 0.00001             |               |
| 28                                                                                                                                              | 0.00081           | 0.00889           | 0.94980                   | 0.00001             |               |
| 29                                                                                                                                              | 0.00077           | 0.00846           | 0.94980                   | 0.00000             |               |
| 30                                                                                                                                              | 0.00073           | 0.00805           | 0.94980                   | 0.00000             | Not Converged |

WARNING: Failed to converge, however criterion change is less than 0.0001.

Output 74.2.2 Transformations



An alternative approach is to use the pairwise deletion option of the CORR procedure to compute the correlation matrix and then use PROC PRINCOMP or PROC FACTOR to perform the principal component analysis. This approach has several disadvantages. The correlation matrix might not be positive semidefinite (PSD), an assumption required for principal component analysis. PROC PRINQUAL always produces a PSD correlation matrix. Even with pairwise deletion, PROC CORR removes the six observations that have only a single nonmissing value from this data set. Finally, it is still not possible to calculate scores on the principal components for those teams that have missing values.

You can compute the composite ranking by using PROC PRINCOMP and some preliminary data manipulations, similar to those discussed previously.

Chapter 73, “[The PRINCOMP Procedure](#),” contains an example where the average of the unused ranks in each poll is substituted for the missing values, and each observation is weighted by the number of nonmissing values. This method has much to recommend it. It is much faster and simpler than using PROC PRINQUAL. It is also much less prone to degeneracies and capitalization on chance. However, PROC PRINCOMP does not allow the nonmissing ranks to be monotonically transformed and the missing values untied to optimize fit.

PROC PRINQUAL monotonically transforms the observed ranks and estimates the missing ranks (within the constraints given previously) to account for almost 95 percent of the variance of the transformed data by just one dimension. PROC FACTOR is then used to report details of the principal component analysis of the transformed data. As shown by the Factor Pattern values in [Output 74.2.3](#), nine of the ten news services have a correlation of 0.95 or larger with the scores on the first principal component after the data are optimally transformed. The scores are sorted and the composite ranking is displayed following the PROC FACTOR output. More confidence can be placed in the stability of the scores for teams that are ranked by the majority of the news services than in scores for teams that are seldom ranked.

The monotonic transformations are plotted for each of the ten news services. See [Output 74.2.2](#). These plots show the values of the raw ranks (with the missing ranks replaced by the maximum rank plus one) versus the rescored (transformed) ranks. The transformations are the step functions that maximize the fit of the data to the principal component model. Smoother transformations could be found by using MSPLINE transformations, but MSPLINE transformations would not correctly handle the missing data problem.

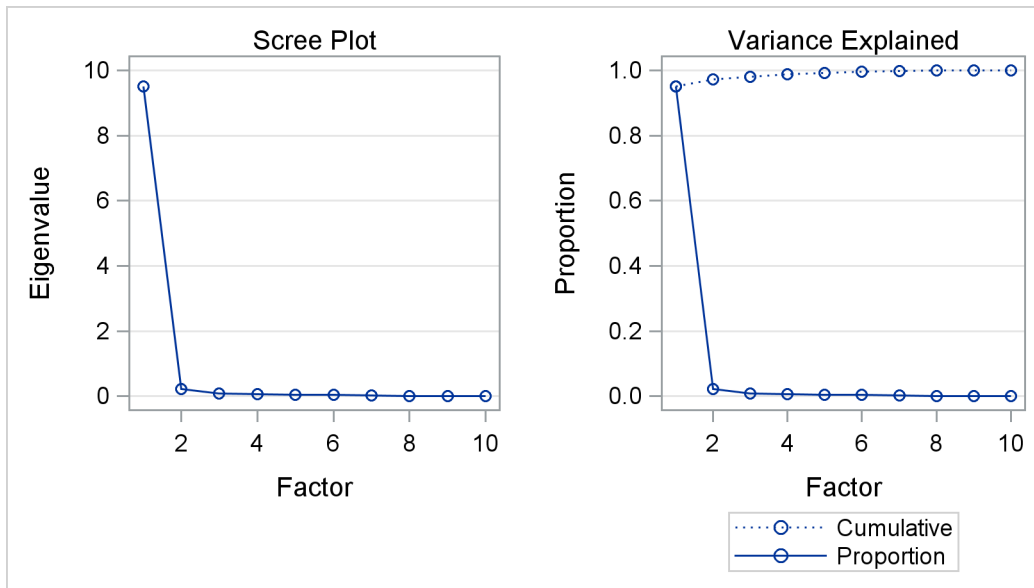
The following statements perform the final analysis and produce [Output 74.2.3](#):

```
* Perform the Final Principal Component Analysis;
proc factor nfact=1 plots=scree;
 title4 'Principal Component Analysis';
 ods select factorpattern screeplot;
 var TCSN -- TSportsIllustrated;
run;

proc sort;
 by Prin1;
run;

* Display Scores on the First Principal Component;
proc print;
 title4 'Teams Ordered by Scores on First Principal Component';
 var School Prin1;
run;
```

**Output 74.2.3** Principal Components of College Basketball Rankings



**Output 74.2.3** *continued*

| Factor Pattern     |                                  |         |
|--------------------|----------------------------------|---------|
|                    |                                  | Factor1 |
| TCSN               | CSN Transformation               | 0.91136 |
| TDurhamSun         | DurhamSun Transformation         | 0.98887 |
| TDurhamHerald      | DurhamHerald Transformation      | 0.97402 |
| TWashingtonPost    | WashingtonPost Transformation    | 0.97408 |
| TUSA_Today         | USA_Today Transformation         | 0.98867 |
| TSportMagazine     | SportMagazine Transformation     | 0.95331 |
| TInsideSports      | InsideSports Transformation      | 0.98521 |
| TUPI               | UPI Transformation               | 0.98534 |
| TAP                | AP Transformation                | 0.99590 |
| TSportsIllustrated | SportsIllustrated Transformation | 0.98615 |

**Output 74.2.3** *continued*

1985 Preseason College Basketball Rankings  
 Optimal Monotonic Transformation of Ranked Teams  
 with Constrained Estimation of Unranked Teams  
 Teams Ordered by Scores on First Principal Component

| Obs | School        | Prin1    |
|-----|---------------|----------|
| 1   | Georgia Tech  | -6.20315 |
| 2   | UNC           | -5.93314 |
| 3   | Michigan      | -5.71034 |
| 4   | Kansas        | -4.78699 |
| 5   | Duke          | -4.75896 |
| 6   | Illinois      | -4.19220 |
| 7   | Georgetown    | -4.02861 |
| 8   | Louisville    | -3.73087 |
| 9   | Syracuse      | -3.47497 |
| 10  | Auburn        | -1.78429 |
| 11  | LSU           | -0.35928 |
| 12  | Memphis State | 0.46737  |
| 13  | Kentucky      | 0.63661  |
| 14  | Notre Dame    | 0.71919  |
| 15  | Navy          | 0.76187  |
| 16  | UAB           | 0.98316  |
| 17  | DePaul        | 1.09891  |
| 18  | Oklahoma      | 1.12012  |
| 19  | NC State      | 1.15144  |
| 20  | UNLV          | 1.28766  |
| 21  | Iowa          | 1.45260  |
| 22  | Indiana       | 1.48123  |
| 23  | Maryland      | 1.54935  |
| 24  | Virginia      | 2.01385  |
| 25  | Arkansas      | 2.02718  |
| 26  | Washington    | 2.10878  |
| 27  | Tennessee     | 2.27770  |
| 28  | Virginia Tech | 2.36103  |
| 29  | St. Johns     | 2.37387  |
| 30  | Montana       | 2.43502  |
| 31  | UCLA          | 2.52481  |
| 32  | Pittsburgh    | 3.00907  |
| 33  | Old Dominion  | 3.03324  |
| 34  | St. Joseph's  | 3.39259  |
| 35  | Houston       | 4.69614  |

The ordinary PROC PRINQUAL missing data handling facilities do not work for these data because they do not constrain the missing data estimates properly. If you code the missing ranks as missing and specify linear transformations, then you can compute least squares estimates of the missing values without transforming the observed values. The first principal component then accounts for 92 percent of the variance after 20 iterations. However, Virginia Tech is ranked number 11 by its score even though it appeared in only one poll (Inside Sports ranked it number 13, anchoring it firmly in the middle). Specifying monotone transformations is also inappropriate since they too allow unranked teams to move in between ranked teams.

With these data, the combination of monotone transformations and the freedom to score the missing ranks without constraint leads to degenerate transformations. PROC PRINQUAL tries to merge the 35 points



into two points, producing a perfect fit in one dimension. There is evidence for this after 20 iterations when the Average Change, Maximum Change, and Criterion Change values are all increasing, instead of the more stable decreasing change rate seen in the analysis shown. The change rates all stop increasing after 41 iterations, and it is clear by 70 or 80 iterations that one component will account for 100 percent of the transformed variables variance after sufficient iteration. While this might seem desirable (after all, it is a perfect fit), you should, in fact, be on guard when this happens. Whenever convergence is slow, the rates of change increase, or the final data perfectly fit the model, the solution is probably degenerating because of too few constraints on the scorings.

PROC PRINQUAL can account for 100 percent of the variance by scoring Montana and UCLA with one positive value on all variables and scoring all the other teams with one negative value on all variables. This inappropriate analysis suggests that all ranked teams are equally good except for two teams that are less good. Both of these two teams are ranked by only one news service, and their only nonmissing rank is last in the poll. This accounts for the degeneracy.

---

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# Chapter 75

## The PROBIT Procedure

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## Overview: PROBIT Procedure

The PROBIT procedure calculates maximum likelihood estimates of regression parameters and the natural (or threshold) response rate for quantal response data from biological assays or other discrete event data. This includes probit, logit, ordinal logistic, and extreme value (or gompit) regression models.

Probit analysis developed from the need to analyze qualitative (dichotomous or polytomous) dependent variables within the regression framework. Many response variables are binary by nature (yes/no), while others are measured ordinally rather than continuously (degree of severity). Researchers have shown ordinary least squares (OLS) regression to be inadequate when the dependent variable is discrete (Collett 2003; Agresti 2002). Probit or logit analyses are more appropriate in this case.

The PROBIT procedure computes maximum likelihood estimates of the parameters  $\beta$  and  $C$  of the probit equation by using a modified Newton-Raphson algorithm. When the response  $Y$  is binary, with values 0 and 1, the probit equation is

$$p = \Pr(Y = 0) = C + (1 - C)F(\mathbf{x}'\beta)$$

where

- $\beta$  is a vector of parameter estimates
- $F$  is a cumulative distribution function (normal, logistic, or extreme value)
- $\mathbf{x}$  is a vector of explanatory variables
- $p$  is the probability of a response
- $C$  is the natural (threshold) response rate

Notice that PROC PROBIT, by default, models the probability of the *lower* response levels. The choice of the distribution function  $F$  (normal for the probit model, logistic for the logit model, and extreme value or Gompertz for the gompit model) determines the type of analysis. For most problems, there is relatively little difference between the normal and logistic specifications of the model. Both distributions are symmetric about the value zero. The extreme value (or Gompertz) distribution, however, is not symmetric, approaching 0 on the left more slowly than it approaches 1 on the right. You can use the extreme value distribution where such asymmetry is appropriate.

For ordinal response models, the response,  $Y$ , of an individual or an experimental unit can be restricted to one of a (usually small) number,  $k + 1$  ( $k \geq 1$ ), of ordinal values, denoted for convenience by  $1, \dots, k, k + 1$ . For example, the severity of coronary disease can be classified into three response categories as 1=no disease, 2=angina pectoris, and 3=myocardial infraction. The PROBIT procedure fits a common slopes cumulative model, which is a parallel-lines regression model based on the cumulative probabilities of the response categories rather than on their individual probabilities. The cumulative model has the form

$$\Pr(Y \leq 1 | \mathbf{x}) = F(\mathbf{x}'\boldsymbol{\beta})$$

$$\Pr(Y \leq i | \mathbf{x}) = F(\alpha_i + \mathbf{x}'\boldsymbol{\beta}), \quad 2 \leq i \leq k$$

where  $\alpha_2, \dots, \alpha_k$  are  $k - 1$  intercept parameters. By default, the covariate vector  $\mathbf{x}$  contains an overall intercept term.

You can set or estimate the natural (threshold) response rate  $C$ . Estimation of  $C$  can begin either from an initial value that you specify or from the rate observed in a control group. By default, the natural response rate is fixed at zero.

An observation in the data set analyzed by the PROBIT procedure might contain the response and explanatory values for one subject. Alternatively, it might provide the number of observed events from a number of subjects at a particular setting of the explanatory variables. In this case, PROC PROBIT models the probability of an event.

The PROBIT procedure uses ODS Graphics to create graphs as part of its output. For general information about ODS Graphics, see Chapter 21, “[Statistical Graphics Using ODS](#).” For specific information about the graphics available in the PROBIT procedure, see the section “[ODS Graphics](#)” on page 6415.

## Getting Started: PROBIT Procedure

The following example illustrates how you can use the PROBIT procedure to compute the threshold response rate and regression parameter estimates for quantal response data.

### Estimating the Natural Response Threshold Parameter

Suppose you want to test the effect of a drug at 12 dosage levels. You randomly divide 180 subjects into 12 groups of 15—one group for each dosage level. You then conduct the experiment and, for each subject, record the presence or absence of a positive response to the drug. You summarize the data by counting the number of subjects responding positively in each dose group. Your data set is as follows:

```
data study;
 input Dose Respond @@;
 Number = 15;
 datalines;
0 3 1.1 4 1.3 4 2.0 3 2.2 5 2.8 4
3.7 5 3.9 9 4.4 8 4.8 11 5.9 12 6.8 13
;
```

The variable `dose` represents the amount of drug administered. The first group, receiving a dose level of 0, is the control group. The variable `number` represents the number of subjects in each group. All groups are equal in size; hence, `number` has the value 15 for all observations. The variable `respond` represents the number of subjects responding to the associated drug dosage.

You can model the probability of positive response as a function of dosage by using the following statements:

```
ods graphics on;

proc probit data=study log10 optc plots=(predpplot ippplot);
 model respond/number=dose;
 output out=new p=p_hat;
run;
```

The `DATA=` option specifies that PROC PROBIT analyze the SAS data set `study`. The `LOG10` option replaces the first continuous independent variable (`dose`) with its common logarithm. The `OPTC` option estimates the natural response rate. When you use the `LOG10` option with the `OPTC` option, any observations with a dose value less than or equal to zero are used in the estimation as a control group.

The `PLOTS=` option in the PROC PROBIT statement, together with the ODS GRAPHICS statement, requests two plots for the estimated probability values and dosage levels. For general information about ODS Graphics, see Chapter 21, “Statistical Graphics Using ODS.” For specific information about the graphics available in the PROBIT procedure, see the section “ODS Graphics” on page 6415.

The MODEL statement specifies a proportional response by using the variables `respond` and `number` in *events/trials* syntax. The variable `dose` is the stimulus or explanatory variable.

The OUTPUT statement creates a new data set, `new`, that contains all the variables in the original data set, and a new variable, `p_hat`, that represents the predicted probabilities.

The results from this analysis are displayed in the following figures.

Figure 75.1 displays background information about the model fit. Included are the name of the input data set, the response variables used, and the number of observations, events, and trials. The last line in Figure 75.1 shows the final value of the log-likelihood function.

Figure 75.2 displays the table of parameter estimates for the model. The parameter  $C$ , which is the natural response threshold or the proportion of individuals responding at zero dose, is estimated to be 0.2409. Since both the intercept and the slope coefficient have significant  $p$ -values (0.0020, 0.0010), you can write the model for

$$\text{Pr}(\text{response}) = C + (1 - C)F(\mathbf{x}'\beta)$$

as

$$\text{Pr}(\text{response}) = 0.2409 + 0.7591(\Phi(-4.1439 + 6.2308 \times \log_{10}(\text{dose})))$$

where  $\Phi$  is the normal cumulative distribution function.

Finally, PROC PROBIT specifies the resulting tolerance distribution by providing the mean MU and scale parameter SIGMA as well as the covariance matrix of the distribution parameters in Figure 75.3.

**Figure 75.1** Model Fitting Information for the PROBIT Procedure

| The Probit Procedure              |              |
|-----------------------------------|--------------|
| Model Information                 |              |
| Data Set                          | WORK.STUDY   |
| Events Variable                   | Respond      |
| Trials Variable                   | Number       |
| Number of Observations            | 12           |
| Number of Events                  | 81           |
| Number of Trials                  | 180          |
| Number of Events In Control Group | 3            |
| Number of Trials In Control Group | 15           |
| Name of Distribution              | Normal       |
| Log Likelihood                    | -104.3945783 |

**Figure 75.2** Model Parameter Estimates for the PROBIT Procedure

| Analysis of Maximum Likelihood Parameter Estimates |    |          |                |                       |         |            |            |
|----------------------------------------------------|----|----------|----------------|-----------------------|---------|------------|------------|
| Parameter                                          | DF | Estimate | Standard Error | 95% Confidence Limits |         | Chi-Square | Pr > ChiSq |
| Intercept                                          | 1  | -4.1438  | 1.3415         | -6.7731               | -1.5146 | 9.54       | 0.0020     |
| Log10 (Dose)                                       | 1  | 6.2308   | 1.8996         | 2.5076                | 9.9539  | 10.76      | 0.0010     |
| _C_                                                | 1  | 0.2409   | 0.0523         | 0.1385                | 0.3433  |            |            |

**Figure 75.3** Tolerance Distribution Estimates for the PROBIT Procedure

| Estimated Covariance Matrix for Tolerance Parameters |           |           |           |
|------------------------------------------------------|-----------|-----------|-----------|
|                                                      | MU        | SIGMA     | _C_       |
| MU                                                   | 0.001158  | -0.000493 | 0.000954  |
| SIGMA                                                | -0.000493 | 0.002394  | -0.000999 |
| _C_                                                  | 0.000954  | -0.000999 | 0.002731  |

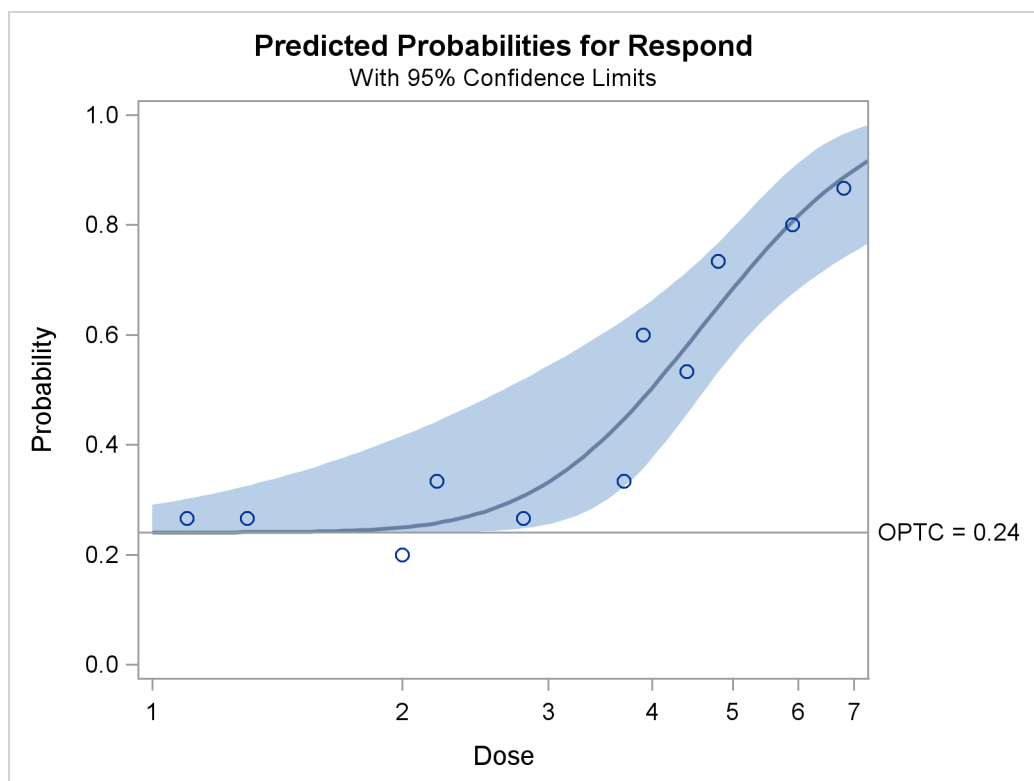
The PLOT=PREDPLOT option creates the plot in Figure 75.4, showing the relationship between dosage level, observed response proportions, and estimated probability values. The dashed lines represent pointwise confidence bands for the fitted probabilities, and a reference line is plotted at the estimated threshold value of 0.24.

The PLOT=IPPPLOT option creates the plot in Figure 75.5, showing the inverse relationship between dosage level and observed response proportions/estimated probability values. The dashed lines represent pointwise fiducial limits for the predicted values of the dose variable, and a reference line is also plotted at the estimated threshold value of 0.24.

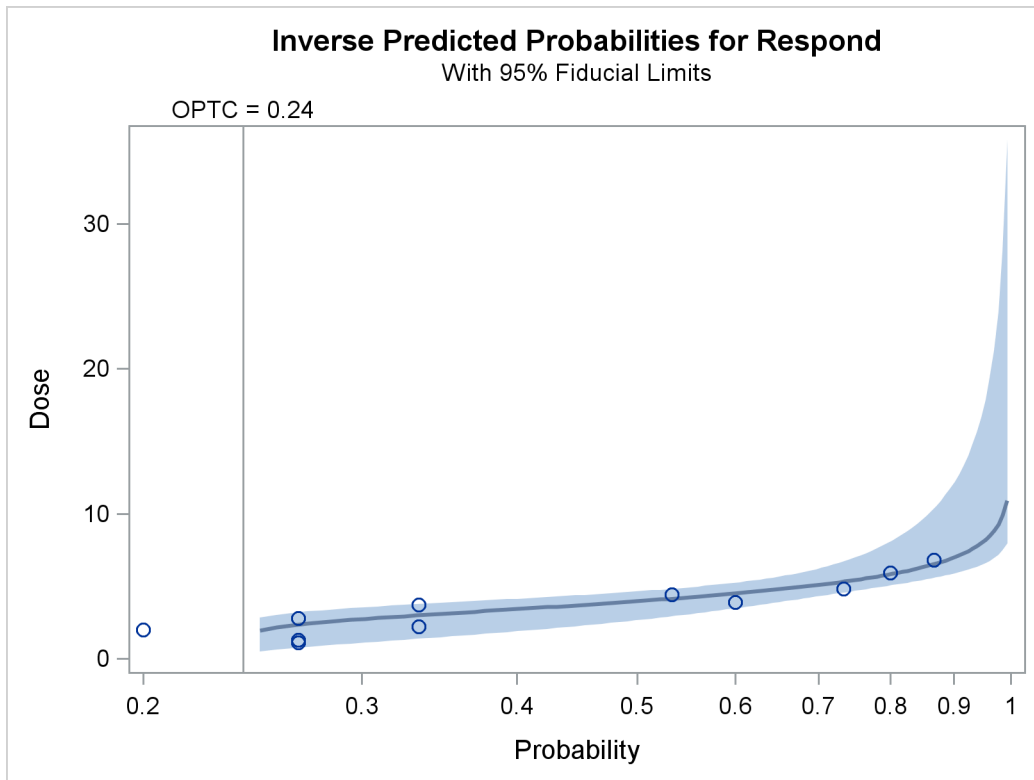


The two plot options can be put together with the PLOTS= option, as shown in the PROC PROBIT statement.

**Figure 75.4** Plot of Observed and Fitted Probabilities versus Dose Level



**Figure 75.5** Inverse Predicted Probability Plot with Fiducial Limits



---

## Syntax: PROBIT Procedure

The following statements are available in the PROBIT procedure:

```

PROC PROBIT < options > ;
 BY variables ;
 CDFPLOT < VAR=variable > < options > ;
 CLASS variables ;
 ESTIMATE < 'label' > estimate-specification < (divisor=n) >
 < , ... < 'label' > estimate-specification < (divisor=n) > > < / options > ;
 EFFECTPLOT < plot-type < (plot-definition-options) > > < / options > ;
 INSET < keyword-list > < / options > ;
 IPPPLOT < VAR=variable > < options > ;
 LPREDPLOT < VAR=variable > < options > ;
 LSMEANS < model-effects > < / options > ;
 LSMESTIMATE model-effect < 'label' > values < (divisor=n) >
 < , ... < 'label' > values < (divisor=n) > > < / options > ;
 MODEL response = independents < / options > ;
 OUTPUT < OUT=SAS-data-set > < options > ;
 PREDPPLOT < VAR=variable > < options > ;
 SLICE model-effect < / options > ;
 STORE < OUT= > item-store-name < / LABEL='label' > ;
 TEST < model-effects > < / options > ;
 WEIGHT variable ;

```

A MODEL statement is required. Only a single MODEL statement can be used with one invocation of the PROBIT procedure. If multiple MODEL statements are present, only the last one is used. Main effects and higher-order terms can be specified in the MODEL statement, as in the GLM procedure. If a CLASS statement is used, it must precede the MODEL statement.

The CDFPLOT, INSET, IPPPLOT, LPREDPLOT, and PREDPPLOT statements are used to produce graphical output. You can use any appropriate combination of the graphical statements after the MODEL statement.

The ESTIMATE, EFFECTPLOT, LSMEANS, LSMESTIMATE, SLICE, STORE, and TEST statements are common to many procedures. Summary descriptions of functionality and syntax for these statements are also given after the PROC PROBIT statement in alphabetical order, and full documentation about them is available in Chapter 19, “Shared Concepts and Topics.”

---

## PROC PROBIT Statement

```

PROC PROBIT < options > ;

```

The PROC PROBIT statement invokes the PROBIT procedure. Table 75.1 summarizes the options available in the PROC PROBIT statement.

Table 75.1 PROC PROBIT Statement Options

| Option       | Description                                                                            |
|--------------|----------------------------------------------------------------------------------------|
| COVOUT       | Writes the parameter estimate covariance matrix to the OUTEST= data set                |
| C=           | Controls how the natural response is handled                                           |
| DATA=        | Specifies the SAS data set to be used                                                  |
| GOUT=        | Specifies a graphics catalog in which to save graphics output                          |
| HPROB=       | Specifies a minimum probability level for the Pearson's chi-square                     |
| INEST=       | Specifies an input SAS data set that contains initial estimates                        |
| INVERSECL    | Computes confidence limits                                                             |
| LACKFIT      | Performs two goodness-of-fit tests                                                     |
| LOG          | Replaces the first continuous independent variable with its natural logarithm          |
| LOG10        | Replaces the first continuous independent variable with log to the base 10             |
| NAMELEN=     | Specifies the length of effect names to be <i>n</i> characters                         |
| NOPRINT      | Suppresses the display of all output including graphics                                |
| OPTC         | Controls how the natural response is handled                                           |
| ORDER=       | Specifies the sort order for the levels of the classification variables                |
| OUTEST=      | Specifies a SAS data set to contain the parameter estimates                            |
| PLOT   PLOTS | Controls the plots produced through ODS Graphics                                       |
| XDATA=       | Specifies an input SAS data set that contains values for all the independent variables |

You can specify the following *options* in the PROC PROBIT statement.

### COVOUT

writes the parameter estimate covariance matrix to the OUTEST= data set.

### C=*rate*

### OPTC

controls how the natural response is handled. Specify the OPTC option to request that the natural response rate *C* be estimated. Specify the C=*rate* option to set the natural response rate or to provide the initial estimate of the natural response rate. The natural response rate value must be a number between 0 and 1.

- If you specify neither the OPTC nor the C= option, a natural response rate of zero is assumed.
- If you specify both the OPTC and the C= option, the C= option should be a reasonable initial estimate of the natural response rate. For example, you could use the ratio of the number of responses to the number of subjects in a control group.
- If you specify the C= option but not the OPTC option, the natural response rate is set to the specified value and not estimated.
- If you specify the OPTC option but not the C= option, PROC PROBIT's action depends on the response variable, as follows:
  - If you specify either the LN or LOG10 option and some subjects have the first independent variable (dose) values less than or equal to zero, these subjects are treated as a control group. The initial estimate of *C* is then the ratio of the number of responses to the number of subjects in this group.

- If you do not specify the LN or LOG10 option or if there is no control group, then one of the following occurs:
  - If all responses are greater than zero, the initial estimate of the natural response rate is the minimal response rate (the ratio of the number of responses to the number of subjects in a dose group) across all dose levels.
  - If one or more of the responses is zero (making the response rate zero in that dose group), the initial estimate of the natural rate is the reciprocal of twice the largest number of subjects in any dose group in the experiment.

**DATA=SAS-data-set**

specifies the SAS data set to be used by PROC PROBIT. By default, the procedure uses the most recently created SAS data set.

**GOUT=graphics-catalog**

specifies a graphics catalog in which to save graphics output.

**HPROB=*p***

specifies a minimum probability level for the Pearson's chi-square to indicate a good fit. The default value is 0.10. The LACKFIT option must also be specified for this option to have any effect. For Pearson's goodness-of-fit chi-square values with probability greater than the HPROB= value, the fiducial limits, if requested with the INVERSECL option, are computed by using a critical value of 1.96. For chi-square values with probability less than the value of the HPROB= option, the critical value is a 0.95 two-sided quantile value taken from the *t* distribution with degrees of freedom equal to  $(k - 1) \times m - q$ , where *k* is the number of levels for the response variable, *m* is the number of different sets of independent variable values, and *q* is the number of parameters fit in the model. Note that the HPROB= option can also appear in the MODEL statement.

**INEST=SAS-data-set**

specifies an input SAS data set that contains initial estimates for all the parameters in the model. See the section “[INEST= SAS-data-set](#)” on page 6407 for a detailed description of the contents of the INEST= data set.

**INVERSECL<(PROB=rates)>**

computes confidence limits for the values of the first continuous independent variable (such as dose) that yield selected response rates. You can optionally specify a list of response rates as *rates*. The response rates must be between zero and one, and can be a list separated by blanks, commas, or in the form of a DO list.

For example,

```
PROB = .1 TO .9 by .1
PROB = .1 .2 .3 .4
PROB = .01, .25, .75, .9
```

are valid lists of response rates.

If the algorithm fails to converge (this can happen when *C* is nonzero), missing values are reported for the confidence limits. See the section “[Inverse Confidence Limits](#)” on page 6410 for details. Note that the INVERSECL option can also appear in the MODEL statement.

**LACKFIT**

performs two goodness-of-fit tests (a Pearson's chi-square test and a log-likelihood ratio chi-square test) for the fitted model.

To compute the test statistics, proper grouping of the observations into subpopulations is needed. You can use the AGGREGATE or AGGREGATE= option for this end. See the entry for the AGGREGATE and AGGREGATE= options under the MODEL statement. If neither AGGREGATE nor AGGREGATE= is specified, PROC PROBIT assumes each observation is from a separate subpopulation and computes the goodness-of-fit test statistics only for the *events/trials* syntax.

**NOTE:** This test is not appropriate if the data are very sparse, with only a few values at each set of the independent variable values.

If the Pearson's chi-square test statistic is significant, then the covariance estimates and standard error estimates are adjusted. See the section "[Lack-of-Fit Tests](#)" on page 6408 for a description of the tests. Note that the LACKFIT option can also appear in the MODEL statement.

**LOG****LN**

analyzes the data by replacing the first continuous independent variable with its natural logarithm. This variable is usually the level of some treatment such as dosage. In addition to the usual output given by the INVERSECL option, the estimated dose values and 95% fiducial limits for dose are also displayed. If you specify the OPTC option, any observations with a dose value less than or equal to zero are used in the estimation as a control group. If you do not specify the OPTC option with the LOG or LN option, then any observations with the first continuous independent variable values less than or equal to zero are ignored.

**LOG10**

specifies an analysis like that of the LN or LOG option, except that the common logarithm (log to the base 10) of the dose value is used rather than the natural logarithm.

**NAMELEN=*n***

specifies the length of effect names in tables and output data sets to be *n* characters, where *n* is a value between 20 and 200. The default length is 20 characters.

**NOPRINT**

suppresses the display of all output including graphics. Note that this option temporarily disables the Output Delivery System (ODS). For more information, see Chapter 20, "[Using the Output Delivery System.](#)"

**OPTC**

controls how the natural response is handled. See the description of the **C=** option on page 6353 for details.

**ORDER=DATA | FORMATTED | FREQ | INTERNAL**

specifies the sort order for the levels of the classification variables (which are specified in the **CLASS** statement). This option applies to the levels for all classification variables, except when you use the (default) ORDER=FORMATTED option with numeric classification variables that have no explicit format. With this option, the levels of such variables are ordered by their internal value.

The ORDER= option can take the following values:

| Value of ORDER=  | Levels Sorted By                                                                                                                       |
|------------------|----------------------------------------------------------------------------------------------------------------------------------------|
| <b>DATA</b>      | Order of appearance in the input data set                                                                                              |
| <b>FORMATTED</b> | External formatted value, except for numeric variables with no explicit format, which are sorted by their unformatted (internal) value |
| <b>FREQ</b>      | Descending frequency count; levels with the most observations come first in the order                                                  |
| <b>INTERNAL</b>  | Unformatted value                                                                                                                      |

By default, ORDER=FORMATTED. For ORDER=FORMATTED and ORDER=INTERNAL, the sort order is machine-dependent.

This order also applies to the levels of the response variable. Response level ordering is important because PROC PROBIT always models the probability of response levels at the beginning of the ordering. See the section “[Response Level Ordering](#)” on page 6404 for further details.

For more information about sort order, see the chapter on the SORT procedure in the *Base SAS Procedures Guide* and the discussion of BY-group processing in *SAS Language Reference: Concepts*.

#### **OUTEST=SAS-data-set**

specifies a SAS data set to contain the parameter estimates and, if the COVOUT option is specified, their estimated covariances. If you omit this option, the output data set is not created. The contents of the data set are described in the section “[OUTEST= SAS-data-set](#)” on page 6411.

#### **PLOT | PLOTS <=plot-request >**

#### **PLOT | PLOTS <=(plot-request < ...plot-request > )>**

specifies options that control details of the plots created by ODS Graphics. These plots are related to a dose variable, which is identified as the first single continuous independent variable in the MODEL statement. If there are interaction terms with this variable in the model, the PROBIT procedure will not produce any plot.

You can specify more than one plot request within the parentheses after PLOTS=. For a single plot request, you can omit the parentheses.

ODS Graphics must be enabled before plots can be requested. For example:

```
proc probit plots=predplot;
 model r/n = dose;
run;
```

For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS](#).”

The following plot requests are available.

**ALL**

creates all appropriate plots.

**CDFPLOT**<(LEVEL=(*character-list*))>

requests the plot of predicted cumulative distribution function (CDF) of the multinomial response variable as a function of a single continuous independent variable (dose variable). This single continuous independent variable must be the first single continuous independent variable listed in the MODEL statement. You can request this plot only with a multinomial model.

The LEVEL= suboption specifies the levels of the multinomial response variable for which the CDF curves are requested. There are  $k - 1$  curves for a  $k$ -level multinomial response variable (for the highest level, it is the constant line 1). You can specify any of them to be plotted by the LEVEL= suboption.

**IPPLOT**

requests the inverse plot of the predicted probability against the first single continuous variable (dose variable) in the MODEL statement for the binomial model. You can request this plot only with a binomial model. The confidence limits for the predicted values of the dose variable are the computed fiducial limits, not the inverse of the confidence limits of the predicted probabilities. See the section “[Inverse Confidence Limits](#)” on page 6410 for more details.

**LPREDPLOT**<(LEVEL=(*character-list*))>

requests the plot of the linear predictor  $x'b$  against the first single continuous variable (dose variable) in the MODEL statement for either the binomial model or the multinomial model. The confidence limits for the predicted values are available only for the binomial model.

For the multinomial model, you can use the LEVEL= suboption to specify the levels for which the linear predictor lines are plotted.

**NONE**

suppresses all plots.

**PREDPLOT**<(LEVEL=(*character-list*))>

requests the plot of the predicted probability against the first single continuous variable (dose variable) in the MODEL statement for both the binomial model and the multinomial model. Confidence limits are available only for the binomial model.

For the multinomial model, you can use the LEVEL= suboption to specify the levels for which the linear predictor lines are plotted.

**XDATA=SAS-data-set**

specifies an input SAS data set that contains values for all the independent variables in the MODEL statement and variables in the CLASS statement. If there are covariates specified in a MODEL statement, you specify fixed values for the effects in the MODEL statement by the XDATA= data set when predicted values and/or fiducial limits for a single continuous variable (dose variable) are required. These specified values for the effects in the MODEL statement are also used for generating plots. See the section “[XDATA= SAS-data-set](#)” on page 6411 for a detailed description of the contents of the XDATA= data set.



---

## BY Statement

**BY** *variables* ;

You can specify a BY statement with PROC PROBIT to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the PROBIT procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

---

## CDFPLOT Statement

**CDFPLOT** < **VAR=***variable* > < *options* > ;

The CDFPLOT statement plots the predicted cumulative distribution function (CDF) of the multinomial response variable as a function of a single continuous independent variable (dose variable). You can use this statement only after a multinomial model statement.

**VAR=***variable*

specifies a single continuous variable (dose variable) in the independent variable list of the MODEL statement. If a VAR= *variable* is not specified, the first single continuous variable in the independent variable list of the MODEL statement is used. If such a variable does not exist in the independent variable list of the MODEL statement, an error is reported.

The predicted cumulative distribution function is defined as

$$\hat{F}_j(\mathbf{x}) = C + (1 - C)F(\hat{a}_j + \mathbf{x}'\hat{\mathbf{b}})$$

where  $j = 1, \dots, k$  are the indexes of the  $k$  levels of the multinomial response variable,  $F$  is the CDF of the distribution used to model the cumulative probabilities,  $\hat{\mathbf{b}}$  is the vector of estimated parameters,  $\mathbf{x}$  is the covariate vector,  $\hat{a}_j$  are estimated ordinal intercepts with  $\hat{a}_1 = 0$ , and  $C$  is the threshold parameter, either known or estimated from the model. Let  $x_1$  be the covariate corresponding to the dose variable and  $\mathbf{x}_{-1}$  be the vector of the rest of the covariates. Let the corresponding estimated parameters be  $\hat{b}_1$  and  $\hat{\mathbf{b}}_{-1}$ . Then

$$\hat{F}_j(\mathbf{x}) = C + (1 - C)F(\hat{a}_j + x_1\hat{b}_1 + \mathbf{x}'_{-1}\hat{\mathbf{b}}_{-1})$$

To plot  $\hat{F}_j$  as a function of  $x_1$ ,  $\mathbf{x}_{-1}$  must be specified. You can use the XDATA= option to provide the values of  $\mathbf{x}_{-1}$  (see the XDATA= option in the PROC PROBIT statement for details), or use the default values that follow the rules:

- If the effect contains a continuous variable (or variables), the overall mean of this effect is used.
- If the effect is a single classification variable, the highest level of the variable is used.

### options

specify the levels of the multinomial response variable for which the CDF curves are requested, and add features to the plot. There are  $k - 1$  curves for a  $k$ -level multinomial response variable (for the highest level, it is the constant line 1). You can specify any of them to be plotted by the LEVEL= option in the CDFPLOT statement. See the LEVEL= option for how to specify the levels.

An attached box on the right side of the plot is used to label these curves with the names of their levels. You can specify the color of this box by using the CLABBOX= option.

You can use options in the CDFPLOT statement to do the following:

- superimpose specification limits
- specify the levels for which the CDF curves are requested
- specify graphical enhancements (such as color or text height)

## Summary of Options

Table 75.2 through Table 75.8 summarize the *options* available in the CDFPLOT statement. The “Dictionary of Options” on page 6362 describes each option in detail.

### CDF Options

**Table 75.2** Options for CDFPLOT

|                                 |                                                                          |
|---------------------------------|--------------------------------------------------------------------------|
| LEVEL=( <i>character-list</i> ) | Specifies the names of the levels for which the CDF curves are requested |
| NOTHRESH                        | Suppresses the threshold line                                            |
| THRESHLABPOS= <i>value</i>      | Specifies the position for the label of the threshold line               |

**General Options****Table 75.3** Color Options

|                               |                                   |
|-------------------------------|-----------------------------------|
| <i>C</i> AXIS= <i>color</i>   | Specifies color for axis          |
| <i>C</i> FIT= <i>color</i>    | Specifies color for fitted curves |
| <i>C</i> FRAME= <i>color</i>  | Specifies color for frame         |
| <i>C</i> GRID= <i>color</i>   | Specifies color for grid lines    |
| <i>C</i> HREF= <i>color</i>   | Specifies color for HREF= lines   |
| <i>C</i> LABBOX= <i>color</i> | Specifies color for label box     |
| <i>C</i> TEXT= <i>color</i>   | Specifies color for text          |
| <i>C</i> VREF= <i>color</i>   | Specifies color for VREF= lines   |

**Table 75.4** Options to Enhance Plots Produced on Graphics Devices

|                                          |                                                      |
|------------------------------------------|------------------------------------------------------|
| <i>AN</i> NOTATE=<br><i>SAS-data-set</i> | Specifies an Annotate data set                       |
| <i>IN</i> BORDER                         | Requests a border around plot                        |
| <i>L</i> FIT= <i>linetype</i>            | Specifies line style for fitted curves               |
| <i>L</i> GRID= <i>linetype</i>           | Specifies line style for grid lines                  |
| <i>NO</i> FRAME                          | Suppresses the frame around plotting areas           |
| <i>NO</i> GRID                           | Suppresses grid lines                                |
| <i>NO</i> FIT                            | Suppresses CDF curves                                |
| <i>NO</i> HLABEL                         | Suppresses horizontal labels                         |
| <i>NO</i> HTICK                          | Suppresses horizontal ticks                          |
| <i>NO</i> VTICK                          | Suppresses vertical ticks                            |
| <i>TURN</i> VLABELS                      | Vertically strings out characters in vertical labels |
| <i>W</i> FIT= <i>n</i>                   | Specifies thickness for fitted curves                |
| <i>W</i> GRID= <i>n</i>                  | Specifies thickness for grids                        |
| <i>W</i> REFL= <i>n</i>                  | Specifies thickness for reference lines              |

**Table 75.5** Axis Options

|                                                        |                                                |
|--------------------------------------------------------|------------------------------------------------|
| HAXIS= <i>value1 to value2</i><br>< by <i>value3</i> > | Specifies tick mark values for horizontal axis |
| HOFFSET= <i>value</i>                                  | Specifies offset for horizontal axis           |
| HLOWER= <i>value</i>                                   | Specifies lower limit on horizontal axis scale |
| HUPPER= <i>value</i>                                   | Specifies upper limit on horizontal axis scale |
| NHTICK= <i>n</i>                                       | Specifies number of ticks for horizontal axis  |
| NVTICK= <i>n</i>                                       | Specifies number of ticks for vertical axis    |
| VAXIS= <i>value1 to value2</i><br>< by <i>value3</i> > | Specifies tick mark values for vertical axis   |
| VAXISLABEL= <i>'label'</i>                             | Specifies label for vertical axis              |
| VOFFSET= <i>value</i>                                  | Specifies offset for vertical axis             |
| VLOWER= <i>value</i>                                   | Specifies lower limit on vertical axis scale   |
| VUPPER= <i>value</i>                                   | Specifies upper limit on vertical axis scale   |
| WAXIS= <i>n</i>                                        | Specifies thickness for axis                   |

**Table 75.6** Graphics Catalog Options

|                              |                                                   |
|------------------------------|---------------------------------------------------|
| DESCRIPTION= <i>'string'</i> | Specifies description for graphics catalog member |
| NAME= <i>'string'</i>        | Specifies name for plot in graphics catalog       |

**Table 75.7** Options for Text Enhancement

|                        |                                               |
|------------------------|-----------------------------------------------|
| FONT= <i>font</i>      | Specifies software font for text              |
| HEIGHT= <i>value</i>   | Specifies height of text outside framed areas |
| INHEIGHT= <i>value</i> | Specifies height of text inside framed areas  |

**Table 75.8** Options for Reference Lines

|                                                |                                                         |
|------------------------------------------------|---------------------------------------------------------|
| <b>HREF</b> < (INTERSECT) ><br>=value-list     | Requests horizontal reference line                      |
| <b>HREFLABELS</b> =<br>(‘label1’,...,‘labeln’) | Specifies labels for HREF= lines                        |
| <b>HREFLABPOS</b> = <i>n</i>                   | Specifies vertical position of labels for HREF= lines   |
| <b>LHREF</b> = <i>linetype</i>                 | Specifies line style for HREF= lines                    |
| <b>LVREF</b> = <i>linetype</i>                 | Specifies line style for VREF= lines                    |
| <b>VREF</b> < (INTERSECT) ><br>=value-list     | Requests vertical reference line                        |
| <b>VREFLABELS</b> =<br>(‘label1’,...,‘labeln’) | Specifies labels for VREF= lines                        |
| <b>VREFLABPOS</b> = <i>n</i>                   | Specifies horizontal position of labels for VREF= lines |

## Dictionary of Options

The following entries provide detailed descriptions of the *options* in the CDFPLOT statement.

**ANNOTATE**=*SAS-data-set*

**ANNO**=*SAS-data-set*

specifies an Annotate data set, as described in *SAS/GRAPH: Reference*, that enables you to add features to the CDF plot. The ANNOTATE= data set you specify in the CDFPLOT statement is used for all plots created by the statement.

**CAXIS**=*color*

**CAXES**=*color*

specifies the color used for the axes and tick marks. This option overrides any COLOR= specifications in an AXIS statement. The default is the first color in the device color list.

**CFIT**=*color*

specifies the color for the fitted CDF curves. The default is the first color in the device color list.

**CFRAME**=*color*

**CFR**=*color*

specifies the color for the area enclosed by the axes and frame. This area is not shaded by default.

**CGRID**=*color*

specifies the color for grid lines. The default is the first color in the device color list.

**CLABBOX**=*color*

specifies the color for the area enclosed by the label box for CDF curves. This area is not shaded by default.

**CHREF=***color*

**CH=***color*

specifies the color for lines requested by the HREF= option. The default is the first color in the device color list.

**CTEXT=***color*

specifies the color for tick mark values and axis labels. The default is the color specified for the CTEXT= option in the most recent GOPTIONS statement.

**CVREF=***color*

**CV=***color*

specifies the color for lines requested by the VREF= option. The default is the first color in the device color list.

**DESCRIPTION=**"*string*"

**DES=**"*string*"

specifies a description, up to 40 characters, that appears in the PROC GREPLAY master menu. The default is the variable name.

**FONT=***font*

specifies a software font for reference line and axis labels. You can also specify fonts for axis labels in an AXIS statement. The FONT= font takes precedence over the FTEXT= font specified in the most recent GOPTIONS statement. Hardware characters are used by default.

**HAXIS=***value1 to value2 < by value3 >*

specifies tick mark values for the horizontal axis; *value1*, *value2*, and *value3* must be numeric, and *value1* must be less than *value2*. The lower tick mark is *value1*. Tick marks are drawn at increments of *value3*. The last tick mark is the greatest value that does not exceed *value2*. If *value3* is omitted, a value of 1 is used.

Examples of HAXIS= lists follow:

```
haxis = 0 to 10
haxis = 2 to 10 by 2
haxis = 0 to 200 by 10
```

**HEIGHT=***value*

specifies the height of text used outside framed areas. The default value is 3.846 (in percentage).

**HLOWER=***value*

specifies the lower limit on the horizontal axis scale. The HLOWER= option specifies *value* as the lower horizontal axis tick mark. The tick mark interval and the upper axis limit are determined automatically. This option has no effect if the HAXIS= option is used.

**HOFFSET=***value*

specifies offset for horizontal axis. The default value is 1.

**HUPPER=*value***

specifies *value* as the upper horizontal axis tick mark. The tick mark interval and the lower axis limit are determined automatically. This option has no effect if the HAXIS= option is used.

**HREF < (INTERSECT) > =*value-list***

requests reference lines perpendicular to the horizontal axis. If (INTERSECT) is specified, a second reference line perpendicular to the vertical axis is drawn that intersects the fit line at the same point as the horizontal axis reference line. If a horizontal axis reference line label is specified, the intersecting vertical axis reference line is labeled with the vertical axis value. See also the CHREF=, HREFLABELS=, and LHREF= options.

**HREFLABELS='label1',..., 'labeln'****HREFLABEL='label1',..., 'labeln'****HREFLAB='label1',..., 'labeln'**

specifies labels for the lines requested by the HREF= option. The number of labels must equal the number of lines. Enclose each label in quotes. Labels can be up to 16 characters.

**HREFLABPOS=*n***

specifies the vertical position of labels for HREF= lines. The following table shows valid values for *n* and the corresponding label placements.

| <i>n</i> | Label Placement         |
|----------|-------------------------|
| 1        | Top                     |
| 2        | Staggered from top      |
| 3        | Bottom                  |
| 4        | Staggered from bottom   |
| 5        | Alternating from top    |
| 6        | Alternating from bottom |

**INBORDER**

requests a border around CDF plots.

**INHEIGHT=*value***

Specifies height of text inside framed areas.

**LEVEL=(*character-list*)****ORDINAL=(*character-list*)**

specifies the names of the levels for which CDF curves are requested. Names should be quoted and separated by space. If there is no correct name provided, no CDF curve is plotted.

**LFIT=*linetype***

specifies a line style for fitted curves. By default, fitted curves are drawn by connecting solid lines (*linetype* = 1).

**LGRID=*linetype***

specifies a line style for all grid lines. *linetype* is between 1 and 46. The default is 35.

**LHREF=***linetype*

**LH=***linetype*

specifies the line type for lines requested by the HREF= option. The default is 2, which produces a dashed line.

**LVREF=***linetype*

**LV=***linetype*

specifies the line type for lines requested by the VREF= option. The default is 2, which produces a dashed line.

**NAME=**'string'

specifies a name for the plot, up to eight characters, that appears in the PROC GREPLAY master menu. The default is 'PROBIT'.

**NHTICK=***n*

Specifies number of ticks for horizontal axis.

**NVTICK=***n*

Specifies number of ticks for vertical axis.

**NOFIT**

suppresses the fitted CDF curves.

**NOFRAME**

suppresses the frame around plotting areas.

**NOGRID**

suppresses grid lines.

**NOHLABEL**

suppresses horizontal labels.

**NOHTICK**

suppresses horizontal tick marks.

**NOTHRESH**

suppresses the threshold line.

**NOVLABEL**

suppresses vertical labels.

**TURNVLABELS**

vertically strings out characters in vertical labels.

**NOVTICK**

suppresses vertical tick marks.

**THRESLABPOS=***n*

specifies the horizontal position of labels for the threshold line. The following table shows valid values for *n* and the corresponding label placements.



| <i>n</i> | <b>Label Placement</b> |
|----------|------------------------|
| 1        | Left                   |
| 2        | Right                  |

**VAXIS=***value1 to value2 < by value3 >*

specifies tick mark values for the vertical axis; *value1*, *value2*, and *value3* must be numeric, and *value1* must be less than *value2*. The lower tick mark is *value1*. Tick marks are drawn at increments of *value3*. The last tick mark is the greatest value that does not exceed *value2*. This method of specification of tick marks is not valid for logarithmic axes. If *value3* is omitted, a value of 1 is used.

Examples of VAXIS= lists follow:

```
vaxis = 0 to 10
vaxis = 0 to 2 by .1
```

**VAXISLABEL=***'string'*

specifies a label for the vertical axis.

**VLOWER=***value*

specifies the lower limit on the vertical axis scale. The VLOWER= option specifies *value* as the lower vertical axis tick mark. The tick mark interval and the upper axis limit are determined automatically. This option has no effect if the VAXIS= option is used.

**VOFFSET=***value*

specifies the offset for the vertical axis.

**VREF=***value-list*

requests reference lines perpendicular to the vertical axis. If (INTERSECT) is specified, a second reference line perpendicular to the horizontal axis is drawn that intersects the fit line at the same point as the vertical axis reference line. If a vertical axis reference line label is specified, the intersecting horizontal axis reference line is labeled with the horizontal axis value. See also the CVREF=, LVREF=, and VREFLABELS= options.

**VREFLABELS=***'label1',...,'labeln'***VREFLABEL=***'label1',...,'labeln'***VREFLAB=***'label1',...,'labeln'*

specifies labels for the lines requested by the VREF= option. The number of labels must equal the number of lines. Enclose each label in quotes. Labels can be up to 16 characters.

**VREFLABPOS=***n*

specifies the horizontal position of labels for VREF= lines. The following table shows valid values for *n* and the corresponding label placements.

| <i>n</i> | <b>Label Placement</b> |
|----------|------------------------|
| 1        | Left                   |
| 2        | Right                  |

**VUPPER=***value*

specifies the upper limit on the vertical axis scale. The VUPPER= option specifies *value* as the upper vertical axis tick mark. The tick mark interval and the lower axis limit are determined automatically. This option has no effect if the VAXIS= option is used.

**WAXIS=***n*

specifies line thickness for axes and frame. The default value is 1.

**WFIT=***n*

specifies line thickness for fitted curves. The default value is 1.

**WGRID=***n*

specifies line thickness for grids. The default value is 1.

**WREFL=***n*

specifies line thickness for reference lines. The default value is 1.

## CLASS Statement

**CLASS** *variables* < / **TRUNCATE** > ;

The CLASS statement names the classification variables to be used in the model. Typical classification variables are Treatment, Sex, Race, Group, and Replication. If you use the CLASS statement, it must appear before the MODEL statement.

Classification variables can be either character or numeric. By default, class levels are determined from the entire set of formatted values of the CLASS variables.

**NOTE:** Prior to SAS 9, class levels were determined by using no more than the first 16 characters of the formatted values. To revert to this previous behavior, you can use the TRUNCATE option in the CLASS statement.

In any case, you can use formats to group values into levels. See the discussion of the FORMAT procedure in the *Base SAS Procedures Guide* and the discussions of the FORMAT statement and SAS formats in *SAS Formats and Informats: Reference*. You can adjust the order of CLASS variable levels with the ORDER= option in the PROC PROBIT statement. You can specify the following option in the CLASS statement after a slash (/):

**TRUNCATE**

specifies that class levels should be determined by using only up to the first 16 characters of the formatted values of CLASS variables. When formatted values are longer than 16 characters, you can use this option to revert to the levels as determined in releases prior to SAS 9.

## EFFECTPLOT Statement

**EFFECTPLOT** < *plot-type* < (*plot-definition-options*) > > < / *options* > ;

The EFFECTPLOT statement produces a display of the fitted model and provides options for changing and enhancing the displays. Table 75.9 describes the available *plot-types* and their *plot-definition-options*.

**Table 75.9** Plot-Types and Plot-Definition-Options

| Plot-Type and Description                                                                                                                                                                                                                    | Plot-Definition-Options                                                                                                              |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------|
| <p><b>BOX</b></p> <p>Displays a box plot of continuous response data at each level of a CLASS effect, with predicted values superimposed and connected by a line. This is an alternative to the <b>INTERACTION</b> plot-type.</p>            | <p><b>PLOTBY=</b> variable or CLASS effect<br/> <b>X=</b> CLASS variable or effect</p>                                               |
| <p><b>CONTOUR</b></p> <p>Displays a contour plot of predicted values against two continuous covariates.</p>                                                                                                                                  | <p><b>PLOTBY=</b> variable or CLASS effect<br/> <b>X=</b> continuous variable<br/> <b>Y=</b> continuous variable</p>                 |
| <p><b>FIT</b></p> <p>Displays a curve of predicted values versus a continuous variable.</p>                                                                                                                                                  | <p><b>PLOTBY=</b> variable or CLASS effect<br/> <b>X=</b> continuous variable</p>                                                    |
| <p><b>INTERACTION</b></p> <p>Displays a plot of predicted values (possibly with error bars) versus the levels of a CLASS effect. The predicted values are connected with lines and can be grouped by the levels of another CLASS effect.</p> | <p><b>PLOTBY=</b> variable or CLASS effect<br/> <b>SLICEBY=</b> variable or CLASS effect<br/> <b>X=</b> CLASS variable or effect</p> |
| <p><b>SLICEFIT</b></p> <p>Displays a curve of predicted values versus a continuous variable grouped by the levels of a CLASS effect.</p>                                                                                                     | <p><b>PLOTBY=</b> variable or CLASS effect<br/> <b>SLICEBY=</b> variable or CLASS effect<br/> <b>X=</b> continuous variable</p>      |

For full details about the syntax and options of the EFFECTPLOT statement, see the section “EFFECTPLOT Statement” on page 411 in Chapter 19, “Shared Concepts and Topics.”

## ESTIMATE Statement

```
ESTIMATE <'label'> estimate-specification <(divisor=n)>
 < , ... <'label'> estimate-specification <(divisor=n)> >
 </options>;
```

The ESTIMATE statement provides a mechanism for obtaining custom hypothesis tests. Estimates are formed as linear estimable functions of the form  $L\beta$ . You can perform hypothesis tests for the estimable functions, construct confidence limits, and obtain specific nonlinear transformations.

Table 75.10 summarizes the options available in the ESTIMATE statement.

**Table 75.10** ESTIMATE Statement Options

| Option                                                     | Description                                                               |
|------------------------------------------------------------|---------------------------------------------------------------------------|
| <b>Construction and Computation of Estimable Functions</b> |                                                                           |
| DIVISOR=                                                   | Specifies a list of values to divide the coefficients                     |
| NOFILL                                                     | Suppresses the automatic fill-in of coefficients for higher-order effects |
| SINGULAR=                                                  | Tunes the estimability checking difference                                |
| <b>Degrees of Freedom and <math>p</math>-values</b>        |                                                                           |
| ADJUST=                                                    | Determines the method for multiple comparison adjustment of estimates     |
| ALPHA= $\alpha$                                            | Determines the confidence level ( $1 - \alpha$ )                          |
| LOWER                                                      | Performs one-sided, lower-tailed inference                                |
| STEPDOWN                                                   | Adjusts multiplicity-corrected $p$ -values further in a step-down fashion |
| TESTVALUE=                                                 | Specifies values under the null hypothesis for tests                      |
| UPPER                                                      | Performs one-sided, upper-tailed inference                                |
| <b>Statistical Output</b>                                  |                                                                           |
| CL                                                         | Constructs confidence limits                                              |
| CORR                                                       | Displays the correlation matrix of estimates                              |
| COV                                                        | Displays the covariance matrix of estimates                               |
| E                                                          | Prints the L matrix                                                       |
| JOINT                                                      | Produces a joint $F$ or chi-square test for the estimable functions       |
| SEED=                                                      | Specifies the seed for computations that depend on random numbers         |

For details about the syntax of the ESTIMATE statement, see the section “ESTIMATE Statement” on page 437 in Chapter 19, “Shared Concepts and Topics.”

## INSET Statement

```
INSET < keyword-list > < / options > ;
```

The box or table of summary information produced on plots made with the CDFPLOT, IPPLOT, LPREDPLOT, or PREDPLOT statement is called an *inset*. You can use the INSET statement to customize both the information that is printed in the inset box and the appearance of the inset box. To supply the information that is displayed in the inset box, you specify *keywords* corresponding to the information you want shown. For example, the following statements produce a predicted probability plot with the number of trials, the number of events, the name of the distribution, and the estimated optimum natural threshold in the inset.

```
proc probit data=epidemic;
 model r/n = dose;
 predpplot;
 inset nobs ntrials nevents dist optc;
run;
```

By default, inset entries are identified with appropriate labels. However, you can provide a customized label by specifying the *keyword* for that entry followed by the equal sign (=) and the label in quotes. For example, the following INSET statement produces an inset containing the number of observations and the name of the distribution, labeled “Sample Size” and “Distribution” in the inset.

```
inset nobs='Sample Size' dist='Distribution';
```

If you specify a keyword that does not apply to the plot you are creating, then the keyword is ignored.

The *options* control the appearance of the box.

If you specify more than one INSET statement, only the first one is used.

### Keywords Used in the INSET Statement

Table 75.11 and Table 75.12 list keywords available in the INSET statement to display summary statistics, distribution parameters, and distribution fitting information.

**Table 75.11** Summary Statistics

|          |                                           |
|----------|-------------------------------------------|
| NOBS     | Number of observations                    |
| NTRIALS  | Number of trials                          |
| NEVENTS  | Number of events                          |
| C        | User-input threshold                      |
| OPTC     | Estimated natural threshold               |
| NRESPLEV | Number of levels of the response variable |

**Table 75.12** General Information

|            |                                                     |
|------------|-----------------------------------------------------|
| CONFIDENCE | Confidence coefficient for all confidence intervals |
| DIST       | Name of the distribution                            |

### Options Used in the INSET Statement

Table 75.13 and Table 75.14 list the options available in the INSET statement.

**Table 75.13** Color and Pattern Options

|                       |                                        |
|-----------------------|----------------------------------------|
| CFILL= <i>color</i>   | Specifies color for filling box        |
| CFILLH= <i>color</i>  | Specifies color for filling box header |
| CFRAME= <i>color</i>  | Specifies color for frame              |
| CHEADER= <i>color</i> | Specifies color for text in header     |
| CTEXT= <i>color</i>   | Specifies color for text               |

**Table 75.14** General Appearance Options

|                                        |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
|----------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| FONT= <i>font</i>                      | Specifies software font for text                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |
| HEIGHT= <i>value</i>                   | Specifies height of text                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
| HEADER= <i>'quoted string'</i>         | Specifies text for header or box title                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |
| NOFRAME                                | Omits frame around box                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |
| POS= <i>value</i><br><DATA   PERCENT > | Determines the position of the inset. The <i>value</i> can be a compass point (N, NE, E, SE, S, SW, W, NW) or a pair of coordinates (x, y) enclosed in parentheses. The coordinates can be specified in axis percentage units or axis data units.                                                                                                                                                                                                                                                                           |
| REFPOINT= <i>name</i>                  | Specifies the reference point for an inset that is positioned by a pair of coordinates with the POS= option. You use the REFPOINT= option in conjunction with the POS= coordinates. The REFPOINT= option specifies which corner of the inset frame you have specified with coordinates (x, y), and it can take the value of BR (bottom right), BL (bottom left), TR (top right), or TL (top left). The default is REFPOINT=BL. If the inset position is specified as a compass point, then the REFPOINT= option is ignored. |

## IPPLOT Statement

**IPPLOT** < *variable* > < *options* > ;

The IPPLOT statement plots the inverse of the predicted probability (IPP) against a single continuous variable (dose variable) in the MODEL statement for the binomial model. You can only use this statement after a binomial model statement. The confidence limits for the predicted values of the dose variable are the computed fiducial limits, not the inverse of the confidence limits of the predicted probabilities. See the section “Inverse Confidence Limits” on page 6410 for more details.

**VAR=** *variable*

specifies a single continuous variable (dose variable) in the independent variable list of the MODEL statement. If a VAR= variable is not specified, the first single continuous variable in the independent variable list of the MODEL statement is used. If such a variable does not exist in the independent variable list of the MODEL statement, an error is reported.

For the binomial model, the response variable is a probability. An estimate of the dose level  $\hat{x}_1$  needed for a response of  $p$  is given by

$$\hat{x}_1 = (F^{-1}(p) - \mathbf{x}'_{-1} \hat{\mathbf{b}}_{-1}) / \hat{b}_1$$

where  $F$  is the cumulative distribution function used to model the probability,  $\mathbf{x}_{-1}$  is the vector of the rest of the covariates,  $\hat{\mathbf{b}}_{-1}$  is the vector of the estimated parameters corresponding to  $\mathbf{x}_{-1}$ , and  $\hat{b}_1$  is the estimated parameter for the dose variable of interest.

To plot  $\hat{x}_1$  as a function of  $p$ ,  $x_{-1}$  must be specified. You can use the XDATA= option to provide the values of  $x_{-1}$  (see the XDATA= option in the PROC PROBIT statement for details), or use the default values that follow the rules:

- If the effect contains a continuous variable (or variables), the overall mean of this effect is used.
- If the effect is a single classification variable, the highest level of the variable is used.

#### options

add features to the plot.

You can use options in the IPPLOT statement to do the following:

- superimpose specification limits
- suppress or add the observed data points on the plot
- suppress or add the fiducial limits on the plot
- specify graphical enhancements (such as color or text height)

### Summary of Options

Table 75.15 through Table 75.21 summarize the *options* available in the IPPLOT statement. The “Dictionary of Options” on page 6374 describes each option in detail.

#### IPP Options

**Table 75.15** Plot Layout Options for IPPLOT

|                            |                                                            |
|----------------------------|------------------------------------------------------------|
| NOCONF                     | Suppresses fiducial limits                                 |
| NODATA                     | Suppresses observed data points on the plot                |
| NOTHRESH                   | Suppresses the threshold line                              |
| THRESHLABPOS= <i>value</i> | Specifies the position for the label of the threshold line |

#### General Options

**Table 75.16** Color Options

|                      |                                   |
|----------------------|-----------------------------------|
| CAXIS= <i>color</i>  | Specifies color for axis          |
| CFIT= <i>color</i>   | Specifies color for fitted curves |
| CFRAME= <i>color</i> | Specifies color for frame         |
| CGRID= <i>color</i>  | Specifies color for grid lines    |
| CHREF= <i>color</i>  | Specifies color for HREF= lines   |
| CTEXT= <i>color</i>  | Specifies color for text          |
| CVREF= <i>color</i>  | Specifies color for VREF= lines   |

**Table 75.17** Options to Enhance Plots Produced on Graphics Devices

|                                  |                                                              |
|----------------------------------|--------------------------------------------------------------|
| ANNOTATE=<br><i>SAS-data-set</i> | Specifies an Annotate data set                               |
| INBORDER                         | Requests a border around plot                                |
| LFIT= <i>linetype</i>            | Specifies line style for fitted curves and confidence limits |
| LGRID= <i>linetype</i>           | Specifies line style for grid lines                          |
| NOFRAME                          | Suppresses the frame around plotting areas                   |
| NOGRID                           | Suppresses grid lines                                        |
| NOFIT                            | Suppresses fitted curves                                     |
| NOHLABEL                         | Suppresses horizontal labels                                 |
| NOHTICK                          | Suppresses horizontal ticks                                  |
| NOVTICK                          | Suppresses vertical ticks                                    |
| TURNVLABELS                      | Vertically strings out characters in vertical labels         |
| WFIT= <i>n</i>                   | Specifies thickness for fitted curves                        |
| WGRID= <i>n</i>                  | Specifies thickness for grids                                |
| WREFL= <i>n</i>                  | Specifies thickness for reference lines                      |

**Table 75.18** Axis Options

|                                                        |                                                |
|--------------------------------------------------------|------------------------------------------------|
| HAXIS= <i>value1 to value2</i><br>< <i>by value3</i> > | Specifies tick mark values for horizontal axis |
| HOFFSET= <i>value</i>                                  | Specifies offset for horizontal axis           |
| HLOWER= <i>value</i>                                   | Specifies lower limit on horizontal axis scale |
| HUPPER= <i>value</i>                                   | Specifies upper limit on horizontal axis scale |
| NHTICK= <i>n</i>                                       | Specifies number of ticks for horizontal axis  |
| NVTICK= <i>n</i>                                       | Specifies number of ticks for vertical axis    |
| VAXIS= <i>value1 to value2</i><br>< <i>by value3</i> > | Specifies tick mark values for vertical axis   |
| VAXISLABEL= <i>'label'</i>                             | Specifies label for vertical axis              |
| VOFFSET= <i>value</i>                                  | Specifies offset for vertical axis             |
| VLOWER= <i>value</i>                                   | Specifies lower limit on vertical axis scale   |
| VUPPER= <i>value</i>                                   | Specifies upper limit on vertical axis scale   |
| WAXIS= <i>n</i>                                        | Specifies thickness for axis                   |



**Table 75.19** Options for Reference Lines

|                                        |                                                         |
|----------------------------------------|---------------------------------------------------------|
| HREF<(INTERSECT)><br>=value-list       | Requests horizontal reference line                      |
| HREFLABELS=<br>(‘label1’,...,‘labeln’) | Specifies labels for HREF= lines                        |
| HREFLABPOS= <i>n</i>                   | Specifies vertical position of labels for HREF= lines   |
| LHREF= <i>linetype</i>                 | Specifies line style for HREF= lines                    |
| LVREF= <i>linetype</i>                 | Specifies line style for VREF= lines                    |
| VREF<(INTERSECT)><br>=value-list       | Requests vertical reference line                        |
| VREFLABELS=<br>(‘label1’,...,‘labeln’) | Specifies labels for VREF= lines                        |
| VREFLABPOS= <i>n</i>                   | Specifies horizontal position of labels for VREF= lines |

**Table 75.20** Graphics Catalog Options

|                              |                                                   |
|------------------------------|---------------------------------------------------|
| DESCRIPTION= <i>‘string’</i> | Specifies description for graphics catalog member |
| NAME= <i>‘string’</i>        | Specifies name for plot in graphics catalog       |

**Table 75.21** Options for Text Enhancement

|                        |                                                    |
|------------------------|----------------------------------------------------|
| FONT= <i>font</i>      | Specifies software font for text                   |
| HEIGHT= <i>value</i>   | Specifies height of text used outside framed areas |
| INHEIGHT= <i>value</i> | Specifies height of text inside framed areas       |

## Dictionary of Options

The following entries provide detailed descriptions of the *options* in the IPPLOT statement.

**ANNOTATE**=*SAS-data-set*

**ANNO**=*SAS-data-set*

specifies an Annotate data set, as described in *SAS/GRAPH: Reference*, that enables you to add features to the IPP plot. The ANNOTATE= data set you specify in the IPPLOT statement is used for all plots created by the statement.

**CAXIS**=*color*

**CAXES**=*color*

specifies the color used for the axes and tick marks. This option overrides any COLOR= specifications in an AXIS statement. The default is the first color in the device color list.

**CFIT=***color*

specifies the color for the fitted IPP curves. The default is the first color in the device color list.

**CFRAME=***color***CFR=***color*

specifies the color for the area enclosed by the axes and frame. This area is not shaded by default.

**CGRID=***color*

specifies the color for grid lines. The default is the first color in the device color list.

**CHREF=***color***CH=***color*

specifies the color for lines requested by the HREF= option. The default is the first color in the device color list.

**CTEXT=***color*

specifies the color for tick mark values and axis labels. The default is the color specified for the CTEXT= option in the most recent GOPTIONS statement.

**CVREF=***color***CV=***color*

specifies the color for lines requested by the VREF= option. The default is the first color in the device color list.

**DESCRIPTION=**'*string*'**DES=**'*string*'

specifies a description, up to 40 characters, that appears in the PROC GREPLAY master menu. The default is the variable name.

**FONT=***font*

specifies a software font for reference line and axis labels. You can also specify fonts for axis labels in an AXIS statement. The FONT= font takes precedence over the FTEXT= font specified in the most recent GOPTIONS statement. Hardware characters are used by default.

**HAXIS=***value1 to value2 < by value3 >*

specifies tick mark values for the horizontal axis; *value1*, *value2*, and *value3* must be numeric, and *value1* must be less than *value2*. The lower tick mark is *value1*. Tick marks are drawn at increments of *value3*. The last tick mark is the greatest value that does not exceed *value2*. If *value3* is omitted, a value of 1 is used.

Examples of HAXIS= lists follow:

```

haxis = 0 to 10
haxis = 2 to 10 by 2
haxis = 0 to 200 by 10

```

**HEIGHT=***value*

specifies the height of text used outside framed areas. The default value is 3.846 (in percentage).

**HLOWER=***value*

specifies the lower limit on the horizontal axis scale. The HLOWER= option specifies *value* as the lower horizontal axis tick mark. The tick mark interval and the upper axis limit are determined automatically. This option has no effect if the HAXIS= option is used.

**HOFFSET=***value*

specifies offset for horizontal axis. The default value is 1.

**HUPPER=***value*

specifies *value* as the upper horizontal axis tick mark. The tick mark interval and the lower axis limit are determined automatically. This option has no effect if the HAXIS= option is used.

**HREF < (INTERSECT) > =***value-list*

requests reference lines perpendicular to the horizontal axis. If (INTERSECT) is specified, a second reference line perpendicular to the vertical axis is drawn that intersects the fit line at the same point as the horizontal axis reference line. If a horizontal axis reference line label is specified, the intersecting vertical axis reference line is labeled with the vertical axis value. See also the CHREF=, HREFLABELS=, and LHREF= options.

**HREFLABELS=**'*label1*',...,'*labeln*'**HREFLABEL=**'*label1*',...,'*labeln*'**HREFLAB=**'*label1*',...,'*labeln*'

specifies labels for the lines requested by the HREF= option. The number of labels must equal the number of lines. Enclose each label in quotes. Labels can be up to 16 characters.

**HREFLABPOS=***n*

specifies the vertical position of labels for HREF= lines. The following table shows valid values for *n* and the corresponding label placements.

| <i>n</i> | Label Placement         |
|----------|-------------------------|
| 1        | Top                     |
| 2        | Staggered from top      |
| 3        | Bottom                  |
| 4        | Staggered from bottom   |
| 5        | Alternating from top    |
| 6        | Alternating from bottom |

**INBORDER**

requests a border around IPP plots.

**INHEIGHT=***value*

Specifies height of text inside framed areas.

**LFIT=***linetype*

specifies a line style for fitted curves and confidence limits. By default, fitted curves are drawn by connecting solid lines (*linetype* = 1) and confidence limits are drawn by connecting dashed lines (*linetype* = 3).

**LGRID=***linetype*

specifies a line style for all grid lines. The value for *linetype* must be between 1 and 46. The default is 35.

**LHREF=***linetype***LH=***linetype*

specifies the line type for lines requested by the HREF= option. The default is 2, which produces a dashed line.

**LVREF=***linetype***LV=***linetype*

specifies the line type for lines requested by the VREF= option. The default is 2, which produces a dashed line.

**NAME=**'string'

specifies a name for the plot, up to eight characters, that appears in the PROC GREPLAY master menu. The default is 'PROBIT'.

**NHTICK=***n*

Specifies number of ticks for horizontal axis.

**NVTICK=***n*

Specifies number of ticks for vertical axis.

**NOCONF**

suppresses fiducial limits from the plot.

**NODATA**

suppresses observed data points from the plot.

**NOFIT**

suppresses the fitted IPP curves.

**NOFRAME**

suppresses the frame around plotting areas.

**NOGRID**

suppresses grid lines.

**NOHLABEL**

suppresses horizontal labels.

**NOHTICK**

suppresses horizontal tick marks.

**NOTHRESH**

suppresses the threshold line.

**NOVLABEL**

suppresses vertical labels.

**TURNVLABELS**

vertically strings out characters in vertical labels.

**NOVTICK**

suppresses vertical tick marks.

**THRESHLABPOS=*n***

specifies the vertical position of labels for the threshold line. The following table shows valid values for *n* and the corresponding label placements.

| <i>n</i> | Label Placement |
|----------|-----------------|
| 1        | Top             |
| 2        | Bottom          |

**VAXIS=*value1 to value2 < by value3 >***

specifies tick mark values for the vertical axis; *value1*, *value2*, and *value3* must be numeric, and *value1* must be less than *value2*. The lower tick mark is *value1*. Tick marks are drawn at increments of *value3*. The last tick mark is the greatest value that does not exceed *value2*. This method of specification of tick marks is not valid for logarithmic axes. If *value3* is omitted, a value of 1 is used.

Examples of VAXIS= lists follow:

```
vaxis = 0 to 10
vaxis = 0 to 2 by .1
```

**VAXISLABEL=*'string'***

specifies a label for the vertical axis.

**VLOWER=*value***

specifies the lower limit on the vertical axis scale. The VLOWER= option specifies *value* as the lower vertical axis tick mark. The tick mark interval and the upper axis limit are determined automatically. This option has no effect if the VAXIS= option is used.

**VOFFSET=*value***

specifies the offset for the vertical axis.

**VREF=*value-list***

requests reference lines perpendicular to the vertical axis. If (INTERSECT) is specified, a second reference line perpendicular to the horizontal axis is drawn that intersects the fit line at the same point as the vertical axis reference line. If a vertical axis reference line label is specified, the intersecting horizontal axis reference line is labeled with the horizontal axis value. See also the CVREF=, LVREF=, and VREFLABELS= options.

**VREFLABELS=*'label1', ..., 'labeln'*****VREFLABEL=*'label1', ..., 'labeln'*****VREFLAB=*'label1', ..., 'labeln'***

specifies labels for the lines requested by the VREF= option. The number of labels must equal the number of lines. Enclose each label in quotes. Labels can be up to 16 characters.

**VREFLABPOS=*n***

specifies the horizontal position of labels for VREF= lines. The following table shows valid values for *n* and the corresponding label placements.

| <i>n</i> | Label Placement |
|----------|-----------------|
| 1        | Left            |
| 2        | Right           |

**VUPPER=*value***

specifies the upper limit on the vertical axis scale. The VUPPER= option specifies *value* as the upper vertical axis tick mark. The tick mark interval and the lower axis limit are determined automatically. This option has no effect if the VAXIS= option is used.

**WAXIS=*n***

specifies line thickness for axes and frame. The default value is 1.

**WFIT=*n***

specifies line thickness for fitted curves. The default value is 1.

**WGRID=*n***

specifies line thickness for grids. The default value is 1.

**WREFL=*n***

specifies line thickness for reference lines. The default value is 1.

---

## LPREDPLOT Statement

**LPREDPLOT** < VAR=*variable* > < options > ;

The LPREDPLOT statement plots the linear predictor (LPRED)  $\mathbf{x}'\mathbf{b}$  against a single continuous variable (dose variable) in the MODEL statement for either the binomial model or the multinomial model. The confidence limits for the predicted values are available only for the binomial model.

**VAR= *variable***

specifies a single continuous variable (dose variable) in the independent variable list of the MODEL statement for which the linear predictor plot is plotted. If a VAR= variable is not specified, the first single continuous variable in the independent variable list of the MODEL statement is used. If such a variable does not exist in the independent variable list of the MODEL statement, an error is reported.

Let  $x_1$  be the covariate of the dose variable,  $\mathbf{x}_{-1}$  be the vector of the rest of the covariates,  $\hat{\mathbf{b}}_{-1}$  be the vector of estimated parameters corresponding to  $\mathbf{x}_{-1}$ , and  $\hat{b}_1$  be the estimated parameter for the dose variable of interest.

To plot  $\hat{\mathbf{x}}'\mathbf{b}$  as a function of  $x_1$ ,  $\mathbf{x}_{-1}$  must be specified. You can use the XDATA= option to provide the values of  $\mathbf{x}_{-1}$  (see the XDATA= option in the PROC PROBIT statement for details), or use the default values that follow these rules:

- If the effect contains a continuous variable (or variables), the overall mean of this effect is used.
- If the effect is a single classification variable, the highest level of the variable is used.

*options*

add features to the plot.

For the multinomial model, you can use the LEVEL= option to specify the levels for which the linear predictor lines are plotted. The lines are labeled by the names of their levels in the middle.

You can use options in the LPREDPLOT statement to do the following:

- superimpose specification limits
- suppress or add the observed data points on the plot for the binomial model
- suppress or add the confidence limits for the binomial model
- specify the levels for which the linear predictor lines are requested for the multinomial model
- specify graphical enhancements (such as color or text height)

**Summary of Options**

Table 75.22 through Table 75.28 list all *options* by function. The “[Dictionary of Options](#)” on page 6382 describes each option in detail.

***LPRED Options*****Table 75.22** Plot Layout Options for LPREDPLOT

|                                 |                                                                                                                        |
|---------------------------------|------------------------------------------------------------------------------------------------------------------------|
| LEVEL=( <i>character-list</i> ) | Specifies the names of the levels for which the linear predictor lines are requested (only for the multinomial model ) |
| NOCONF                          | Suppresses fiducial limits (only for the binomial model)                                                               |
| NODATA                          | Suppresses observed data points on the plot (only for the binomial model)                                              |
| NOTHRESH                        | Suppresses the threshold line                                                                                          |
| THRESHLABPOS= <i>value</i>      | Specifies the position for the label of the threshold line                                                             |

***General Options*****Table 75.23** Color Options

|                      |                                   |
|----------------------|-----------------------------------|
| CAXIS= <i>color</i>  | Specifies color for axis          |
| CFIT= <i>color</i>   | Specifies color for fitted curves |
| CFRAME= <i>color</i> | Specifies color for frame         |
| CGRID= <i>color</i>  | Specifies color for grid lines    |
| CHREF= <i>color</i>  | Specifies color for HREF= lines   |
| CTEXT= <i>color</i>  | Specifies color for text          |
| CVREF= <i>color</i>  | Specifies color for VREF= lines   |

**Table 75.24** Options to Enhance Plots Produced on Graphics Devices

|                                  |                                                              |
|----------------------------------|--------------------------------------------------------------|
| ANNOTATE=<br><i>SAS-data-set</i> | Specifies an Annotate data set                               |
| INBORDER                         | Requests a border around plot                                |
| LFIT= <i>linetype</i>            | Specifies line style for fitted curves and confidence limits |
| LGRID= <i>linetype</i>           | Specifies line style for grid lines                          |
| NOFRAME                          | Suppresses the frame around plotting areas                   |
| NOGRID                           | Suppresses grid lines                                        |
| NOFIT                            | Suppresses fitted curves                                     |
| NOHLABEL                         | Suppresses horizontal labels                                 |
| NOHTICK                          | Suppresses horizontal ticks                                  |
| NOVTICK                          | Suppresses vertical ticks                                    |
| TURNVLABELS                      | Vertically strings out characters in vertical labels         |
| WFIT= <i>n</i>                   | Specifies thickness for fitted curves                        |
| WGRID= <i>n</i>                  | Specifies thickness for grids                                |
| WREFL= <i>n</i>                  | Specifies thickness for reference lines                      |

**Table 75.25** Axis Options

|                                                        |                                                |
|--------------------------------------------------------|------------------------------------------------|
| HAXIS= <i>value1 to value2</i><br>< by <i>value3</i> > | Specifies tick mark values for horizontal axis |
| HOFFSET= <i>value</i>                                  | Specifies offset for horizontal axis           |
| HLOWER= <i>value</i>                                   | Specifies lower limit on horizontal axis scale |
| HUPPER= <i>value</i>                                   | Specifies upper limit on horizontal axis scale |
| NHTICK= <i>n</i>                                       | Specifies number of ticks for horizontal axis  |
| NVTICK= <i>n</i>                                       | Specifies number of ticks for vertical axis    |
| VAXIS= <i>value1 to value2</i><br>< by <i>value3</i> > | Specifies tick mark values for vertical axis   |
| VAXISLABEL= <i>'label'</i>                             | Specifies label for vertical axis              |
| VOFFSET= <i>value</i>                                  | Specifies offset for vertical axis             |
| VLOWER= <i>value</i>                                   | Specifies lower limit on vertical axis scale   |
| VUPPER= <i>value</i>                                   | Specifies upper limit on vertical axis scale   |
| WAXIS= <i>n</i>                                        | Specifies thickness for axis                   |

**Table 75.26** Graphics Catalog Options

|                              |                                                   |
|------------------------------|---------------------------------------------------|
| DESCRIPTION= <i>'string'</i> | Specifies description for graphics catalog member |
| NAME= <i>'string'</i>        | Specifies name for plot in graphics catalog       |



**Table 75.27** Options for Text Enhancement

|                                    |                                                    |
|------------------------------------|----------------------------------------------------|
| <code>FONT=<i>font</i></code>      | Specifies software font for text                   |
| <code>HEIGHT=<i>value</i></code>   | Specifies height of text used outside framed areas |
| <code>INHEIGHT=<i>value</i></code> | Specifies height of text inside framed areas       |

**Table 75.28** Options for Reference Lines

|                                                                  |                                                         |
|------------------------------------------------------------------|---------------------------------------------------------|
| <code>HREF&lt;(INTERSECT)&gt;<br/>=<i>value-list</i></code>      | Requests horizontal reference line                      |
| <code>HREFLABELS=<br/>(<i>label1</i>, ..., <i>labeln</i>)</code> | Specifies labels for HREF= lines                        |
| <code>HREFLABPOS=<i>n</i></code>                                 | Specifies vertical position of labels for HREF= lines   |
| <code>LHREF=<i>linetype</i></code>                               | Specifies line style for HREF= lines                    |
| <code>LVREF=<i>linetype</i></code>                               | Specifies line style for VREF= lines                    |
| <code>VREF&lt;(INTERSECT)&gt;<br/>=<i>value-list</i></code>      | Requests vertical reference line                        |
| <code>VREFLABELS=<br/>(<i>label1</i>, ..., <i>labeln</i>)</code> | Specifies labels for VREF= lines                        |
| <code>VREFLABPOS=<i>n</i></code>                                 | Specifies horizontal position of labels for VREF= lines |

## Dictionary of Options

The following entries provide detailed descriptions of the *options* in the LPREDPLOT statement.

**ANNOTATE=*SAS-data-set***

**ANNO=*SAS-data-set***

specifies an Annotate data set, as described in *SAS/GRAPH: Reference*, that enables you to add features to the LPRED plot. The ANNOTATE= data set you specify in the LPREDPLOT statement is used for all plots created by the statement.

**CAXIS=*color***

**CAXES=*color***

specifies the color used for the axes and tick marks. This option overrides any COLOR= specifications in an AXIS statement. The default is the first color in the device color list.

**CFIT=*color***

specifies the color for the fitted LPRED lines. The default is the first color in the device color list.

**CFRAME=*color***

**CFR=*color***

specifies the color for the area enclosed by the axes and frame. This area is not shaded by default.

**CGRID=***color*

specifies the color for grid lines. The default is the first color in the device color list.

**CHREF=***color***CH=***color*

specifies the color for lines requested by the HREF= option. The default is the first color in the device color list.

**CTEXT=***color*

specifies the color for tick mark values and axis labels. The default is the color specified for the CTEXT= option in the most recent GOPTIONS statement.

**CVREF=***color***CV=***color*

specifies the color for lines requested by the VREF= option. The default is the first color in the device color list.

**DESCRIPTION=**'*string*'**DES=**'*string*'

specifies a description, up to 40 characters, that appears in the PROC GREPLAY master menu. The default is the variable name.

**FONT=***font*

specifies a software font for reference line and axis labels. You can also specify fonts for axis labels in an AXIS statement. The FONT= font takes precedence over the FTEXT= font specified in the most recent GOPTIONS statement. Hardware characters are used by default.

**HAXIS=***value1 to value2 < by value3 >*

specifies tick mark values for the horizontal axis; *value1*, *value2*, and *value3* must be numeric, and *value1* must be less than *value2*. The lower tick mark is *value1*. Tick marks are drawn at increments of *value3*. The last tick mark is the greatest value that does not exceed *value2*. If *value3* is omitted, a value of 1 is used.

Examples of HAXIS= lists follow:

```
haxis = 0 to 10
haxis = 2 to 10 by 2
haxis = 0 to 200 by 10
```

**HEIGHT=***value*

specifies the height of text used outside framed areas. The default value is 3.846 (in percentage).

**HLOWER=***value*

specifies the lower limit on the horizontal axis scale. The HLOWER= option specifies *value* as the lower horizontal axis tick mark. The tick mark interval and the upper axis limit are determined automatically. This option has no effect if the HAXIS= option is used.

**HOFFSET=*value***

specifies offset for horizontal axis. The default value is 1.

**HUPPER=*value***

specifies *value* as the upper horizontal axis tick mark. The tick mark interval and the lower axis limit are determined automatically. This option has no effect if the HAXIS= option is used.

**HREF < (INTERSECT) > =*value-list***

requests reference lines perpendicular to the horizontal axis. If (INTERSECT) is specified, a second reference line perpendicular to the vertical axis is drawn that intersects the fit line at the same point as the horizontal axis reference line. If a horizontal axis reference line label is specified, the intersecting vertical axis reference line is labeled with the vertical axis value. See also the CHREF=, HREFLABELS=, and LHREF= options.

**HREFLABELS='label1',..., 'labeln'****HREFLABEL='label1',..., 'labeln'****HREFLAB='label1',..., 'labeln'**

specifies labels for the lines requested by the HREF= option. The number of labels must equal the number of lines. Enclose each label in quotes. Labels can be up to 16 characters.

**HREFLABPOS=*n***

specifies the vertical position of labels for HREF= lines. The following table shows valid values for *n* and the corresponding label placements.

| <i>n</i> | Label Placement         |
|----------|-------------------------|
| 1        | Top                     |
| 2        | Staggered from top      |
| 3        | Bottom                  |
| 4        | Staggered from bottom   |
| 5        | Alternating from top    |
| 6        | Alternating from bottom |

**INBORDER**

requests a border around LPRED plots.

**INHEIGHT=*value***

Specifies height of text inside framed areas.

**LEVEL=(*character-list*)****ORDINAL=(*character-list*)**

specifies the names of the levels for which linear predictor lines are requested. Names should be quoted and separated by space. If there is no correct name provided, no LPRED line is plotted.

**LFIT=*linetype***

specifies a line style for fitted curves and confidence limits. By default, fitted curves are drawn by connecting solid lines (*linetype* = 1) and confidence limits are drawn by connecting dashed lines (*linetype* = 3).

**LGRID=***linetype*

specifies a line style for all grid lines. The value for *linetype* is between 1 and 46. The default is 35.

**LHREF=***linetype***LH=***linetype*

specifies the line type for lines requested by the HREF= option. The default is 2, which produces a dashed line.

**LVREF=***linetype***LV=***linetype*

specifies the line type for lines requested by the VREF= option. The default is 2, which produces a dashed line.

**NAME=**'string'

specifies a name for the plot, up to eight characters, that appears in the PROC GREPLAY master menu. The default is 'PROBIT'.

**NHTICK=***n*

Specifies number of ticks for horizontal axis.

**NVTICK=***n*

Specifies number of ticks for vertical axis.

**NOCONF**

suppresses confidence limits from the plot. This works only for the binomial model. Confidence limits are not plotted for the multinomial model.

**NODATA**

suppresses observed data points from the plot. This works only for the binomial model. Data points are not plotted for the multinomial model.

**NOFIT**

suppresses the fitted LPRED lines.

**NOFRAME**

suppresses the frame around plotting areas.

**NOGRID**

suppresses grid lines.

**NOHLABEL**

suppresses horizontal labels.

**NOHTICK**

suppresses horizontal tick marks.

**NOTHRESH**

suppresses the threshold line.

**NOVLABEL**

suppresses vertical labels.

**NOVTICK**

suppresses vertical tick marks.

**TURNVLABELS**

vertically strings out characters in vertical labels.

**THRESHLABPOS=*n***

specifies the horizontal position of labels for the threshold line. The following table shows valid values for *n* and the corresponding label placements.

| <i>n</i> | Label Placement |
|----------|-----------------|
| 1        | Left            |
| 2        | Right           |

**VAXIS=*value1 to value2 < by value3 >***

specifies tick mark values for the vertical axis; *value1*, *value2*, and *value3* must be numeric, and *value1* must be less than *value2*. The lower tick mark is *value1*. Tick marks are drawn at increments of *value3*. The last tick mark is the greatest value that does not exceed *value2*. This method of specification of tick marks is not valid for logarithmic axes. If *value3* is omitted, a value of 1 is used.

Examples of VAXIS= lists follow:

```
vaxis = 0 to 10
vaxis = 0 to 2 by .1
```

**VAXISLABEL=*'string'***

specifies a label for the vertical axis.

**VLOWER=*value***

specifies the lower limit on the vertical axis scale. The VLOWER= option specifies *value* as the lower vertical axis tick mark. The tick mark interval and the upper axis limit are determined automatically. This option has no effect if the VAXIS= option is used.

**VOFFSET=*value***

specifies the offset for the vertical axis.

**VREF=*value-list***

requests reference lines perpendicular to the vertical axis. If (INTERSECT) is specified, a second reference line perpendicular to the horizontal axis is drawn that intersects the fit line at the same point as the vertical axis reference line. If a vertical axis reference line label is specified, the intersecting horizontal axis reference line is labeled with the horizontal axis value. See also the CVREF=, LVREF=, and VREFLABELS= options.

**VREFLABELS=**'label1',...,'labeln'

**VREFLABEL=**'label1',...,'labeln'

**VREFLAB=**'label1',...,'labeln'

specifies labels for the lines requested by the VREF= option. The number of labels must equal the number of lines. Enclose each label in quotes. Labels can be up to 16 characters.

**VREFLABPOS=***n*

specifies the horizontal position of labels for VREF= lines. The following table shows valid values for *n* and the corresponding label placements.

| <i>n</i> | Label Placement |
|----------|-----------------|
| 1        | Left            |
| 2        | Right           |

**VUPPER=***number*

specifies the upper limit on the vertical axis scale. The VUPPER= option specifies *number* as the upper vertical axis tick mark. The tick mark interval and the lower axis limit are determined automatically. This option has no effect if the VAXIS= option is used.

**WAXIS=***n*

specifies line thickness for axes and frame. The default value is 1.

**WFIT=***n*

specifies line thickness for fitted lines. The default value is 1.

**WGRID=***n*

specifies line thickness for grids. The default value is 1.

**WREFL=***n*

specifies line thickness for reference lines. The default value is 1.

---

## LSMEANS Statement

**LSMEANS** < *model-effects* > < / *options* > ;

The LSMEANS statement computes and compares least squares means (LS-means) of fixed effects. LS-means are *predicted population margins*—that is, they estimate the marginal means over a balanced population. In a sense, LS-means are to unbalanced designs as class and subclass arithmetic means are to balanced designs.

Table 75.29 summarizes the options available in the LSMEANS statement.

**Table 75.29** LSMEANS Statement Options

| Option                                              | Description                                                                                 |
|-----------------------------------------------------|---------------------------------------------------------------------------------------------|
| <b>Construction and Computation of LS-Means</b>     |                                                                                             |
| AT                                                  | Modifies the covariate value in computing LS-means                                          |
| BYLEVEL                                             | Computes separate margins                                                                   |
| DIFF                                                | Requests differences of LS-means                                                            |
| OM=                                                 | Specifies the weighting scheme for LS-means computation as determined by the input data set |
| SINGULAR=                                           | Tunes estimability checking                                                                 |
| <b>Degrees of Freedom and <math>p</math>-values</b> |                                                                                             |
| ADJUST=                                             | Determines the method for multiple-comparison adjustment of LS-means differences            |
| ALPHA= $\alpha$                                     | Determines the confidence level $(1 - \alpha)$                                              |
| STEPDOWN                                            | Adjusts multiple-comparison $p$ -values further in a step-down fashion                      |
| <b>Statistical Output</b>                           |                                                                                             |
| CL                                                  | Constructs confidence limits for means and mean differences                                 |
| CORR                                                | Displays the correlation matrix of LS-means                                                 |
| COV                                                 | Displays the covariance matrix of LS-means                                                  |
| E                                                   | Prints the L matrix                                                                         |
| LINES                                               | Produces a “Lines” display for pairwise LS-means differences                                |
| MEANS                                               | Prints the LS-means                                                                         |
| PLOTS=                                              | Requests graphs of means and mean comparisons                                               |
| SEED=                                               | Specifies the seed for computations that depend on random numbers                           |

For details about the syntax of the LSMEANS statement, see the section “LSMEANS Statement” on page 453 in Chapter 19, “Shared Concepts and Topics.”

## LSMESTIMATE Statement

```
LSMESTIMATE model-effect < 'label' > values < divisor=n >
 < , ... < 'label' > values < divisor=n > >
 < / options > ;
```

The LSMESTIMATE statement provides a mechanism for obtaining custom hypothesis tests among least squares means.

Table 75.30 summarizes the options available in the LSMESTIMATE statement.

**Table 75.30** LSMESTIMATE Statement Options

| Option                                              | Description                                                                         |
|-----------------------------------------------------|-------------------------------------------------------------------------------------|
| <b>Construction and Computation of LS-Means</b>     |                                                                                     |
| AT                                                  | Modifies covariate values in computing LS-means                                     |
| BYLEVEL                                             | Computes separate margins                                                           |
| DIVISOR=                                            | Specifies a list of values to divide the coefficients                               |
| OM=                                                 | Specifies the weighting scheme for LS-means computation as determined by a data set |
| SINGULAR=                                           | Tunes estimability checking                                                         |
| <b>Degrees of Freedom and <math>p</math>-values</b> |                                                                                     |
| ADJUST=                                             | Determines the method for multiple-comparison adjustment of LS-means differences    |
| ALPHA= $\alpha$                                     | Determines the confidence level ( $1 - \alpha$ )                                    |
| LOWER                                               | Performs one-sided, lower-tailed inference                                          |
| STEPDOWN                                            | Adjusts multiple-comparison $p$ -values further in a step-down fashion              |
| TESTVALUE=                                          | Specifies values under the null hypothesis for tests                                |
| UPPER                                               | Performs one-sided, upper-tailed inference                                          |
| <b>Statistical Output</b>                           |                                                                                     |
| CL                                                  | Constructs confidence limits for means and mean differences                         |
| CORR                                                | Displays the correlation matrix of LS-means                                         |
| COV                                                 | Displays the covariance matrix of LS-means                                          |
| E                                                   | Prints the <b>L</b> matrix                                                          |
| ELSM                                                | Prints the <b>K</b> matrix                                                          |
| JOINT                                               | Produces a joint $F$ or chi-square test for the LS-means and LS-means differences   |
| SEED=                                               | Specifies the seed for computations that depend on random numbers                   |

For details about the syntax of the LSMESTIMATE statement, see the section “LSMESTIMATE Statement” on page 470 in Chapter 19, “Shared Concepts and Topics.”

## MODEL Statement

*< label >* **MODEL** *response = effects < / options >* ;

*< label >* **MODEL** *events/trials = effects < / options >* ;

The MODEL statement names the variables used as the response and the independent variables. Additionally, you can specify the distribution used to model the response, as well as other options. Only a single MODEL statement can be used with one invocation of the PROBIT procedure. If multiple MODEL statements are present, only the last is used. Main effects and interaction terms can be specified in the MODEL statement, as in the GLM procedure.



The optional *label*, which must be a valid SAS name, is used to label output from the matching MODEL statement.

The *response* can be a single variable with a value that is used to indicate the level of the observed response. For example, the response might be a variable called *Symptoms* that takes on the values ‘None,’ ‘Mild,’ or ‘Severe.’ Note that, for dichotomous response variables, the probability of the lower sorted value is modeled by default (see the section “[Details: PROBIT Procedure](#)” on page 6404). Because the model fit by the PROBIT procedure requires ordered response levels, you might need to use either the ORDER=DATA option in the PROC PROBIT statement or a numeric coding of the response to get the desired ordering of levels.

Alternatively, the response can be specified as a pair of variable names separated by a slash (/). The value of the first variable, *events*, is the number of positive responses (or events). The value of the second variable, *trials*, is the number of trials. Both variables must be numeric and nonnegative, and the ratio of the first variable value to the second variable value must be between 0 and 1, inclusive. For example, the variables might be *hits*, a variable containing the number of hits for a baseball player, and *AtBats*, a variable containing the number of times at bat. A model for hitting proportion (batting average) as a function of age could be specified as

```
model hits/AtBats=age;
```

The *effects* following the equal sign are the covariates in the model. Higher-order effects, such as interactions and nested terms, are allowed in the list, as in the GLM procedure. Variable names and combinations of variable names representing higher-order terms are allowed to appear in this list. Classification variables can be used as effects, and indicator variables are generated for the class levels. If you do not specify any covariates following the equal sign, an intercept-only model is fit.

Table 75.31 summarizes the options available in the MODEL statement.

**Table 75.31** MODEL Statement Options

| Option        | Description                                                                                            |
|---------------|--------------------------------------------------------------------------------------------------------|
| AGGREGATE     | Specifies the subpopulations                                                                           |
| ALPHA=        | Sets the significance level                                                                            |
| CONVERGE=     | Specifies the convergence criterion                                                                    |
| CORRB         | Displays the estimated correlation matrix                                                              |
| COVB          | Displays the estimated covariance matrix                                                               |
| DISTRIBUTION= | Specifies the cumulative distribution function                                                         |
| HPROB=        | Specifies a minimum probability level                                                                  |
| INITIAL=      | Sets initial values for the parameters                                                                 |
| INTERCEPT=    | Initializes the intercept parameter                                                                    |
| INVERSECL     | Computes confidence limits                                                                             |
| ITPRINT       | Displays the iteration history, the final evaluation of the gradient, and the second derivative matrix |
| LACKFIT       | Performs two goodness-of-fit tests                                                                     |
| MAXITER=      | Specifies the maximum number of iterations                                                             |
| NOINT         | Fits a model with no intercept parameter                                                               |
| SCALE=        | Specifies the method for estimating the dispersion parameter                                           |
| SINGULAR=     | Specifies the singularity criterion                                                                    |

The following options are available in the MODEL statement.

## AGGREGATE

### AGGREGATE=*variable-list*

specifies the subpopulations on which the Pearson's chi-square test statistic and the log-likelihood ratio chi-square test statistic (deviance) are calculated if the LACKFIT option is specified. See the section "[Rescaling the Covariance Matrix](#)" on page 6409 for details of Pearson's chi-square and deviance calculations.

Observations with common values in the given list of variables are regarded as coming from the same subpopulation. Variables in the list can be any variables in the input data set. Specifying the AGGREGATE option is equivalent to specifying the AGGREGATE= option with a variable list that includes all independent variables in the MODEL statement. The PROBIT procedure sorts the input data set according to the variables specified in this list. Information for the sorted data set is reported in the "Response-Covariate Profile" table.

The deviance and Pearson's goodness-of-fit statistics are calculated if the LACKFIT option is specified in the MODEL statement. The calculated results are reported in the "Goodness-of-Fit" table. If the Pearson's chi-square test is significant with the test level specified by the HPROB= option, the fiducial limits, if required with the INVERSECL option in the MODEL statement, are modified (see the section "[Inverse Confidence Limits](#)" on page 6410 for details). Also, the covariance matrix is rescaled by the dispersion parameter when the SCALE= option is specified.

### ALPHA=*value*

sets the significance level for the confidence intervals for regression parameters, fiducial limits for the predicted values, and confidence intervals for the predicted probabilities. The value must be between 0 and 1. The default value is ALPHA=0.05.

### CONVERGE=*value*

specifies the convergence criterion. Convergence is declared when the maximum change in the parameter estimates between Newton-Raphson steps is less than the value specified. The change is a relative change if the parameter is greater than 0.01 in absolute value; otherwise, it is an absolute change.

By default, CONVERGE=1.0E-8.

## CORRB

displays the estimated correlation matrix of the parameter estimates.

## COVB

displays the estimated covariance matrix of the parameter estimates.

### DISTRIBUTION=*distribution-type*

### DIST=*distribution-type*

### D=*distribution-type*

specifies the cumulative distribution function used to model the response probabilities. The distributions are described in the section "[Details: PROBIT Procedure](#)" on page 6404. Valid values for *distribution-type* are as follows:

NORMAL      the normal distribution for the probit model  
 LOGISTIC    the logistic distribution for the logit model  
 EXTREMEVALUE | EXTREME | GOMPERTZ    the extreme value, or Gompertz distribution for the gompit model

By default, DISTRIBUTION=NORMAL.

**HPROB=*p***

specifies a minimum probability level for the Pearson's chi-square to indicate a good fit. The default value is 0.10. The LACKFIT option must also be specified for this option to have any effect. For Pearson's goodness-of-fit chi-square values with probability greater than the HPROB= value, the fiducial limits, if requested with the INVERSECL option, are computed by using a critical value of 1.96. For chi-square values with probability less than the value of the HPROB= option, the critical value is a 0.95 two-sided quantile value taken from the *t* distribution with degrees of freedom equal to  $(k - 1) \times m - q$ , where *k* is the number of levels for the response variable, *m* is the number of different sets of independent variable values, and *q* is the number of parameters fit in the model. If you specify the HPROB= option in both the PROC PROBIT and MODEL statements, the MODEL statement option takes precedence.

**INITIAL=*values***

sets initial values for the parameters in the model other than the intercept. The values must be given in the order in which the variables are listed in the MODEL statement. If some of the independent variables listed in the MODEL statement are classification variables, then there must be as many values given for that variable as there are classification levels minus 1. The INITIAL option can be specified as follows.

| Type of List             | Specification              |
|--------------------------|----------------------------|
| List separated by blanks | <code>initial=3 4 5</code> |
| List separated by commas | <code>initial=3,4,5</code> |

By default, all parameters have initial estimates of zero.

**NOTE:** The INITIAL= option is overwritten by the INEST= option in the PROC PROBIT statement.

**INTERCEPT=*value***

initializes the intercept parameter to *value*. By default, INTERCEPT=0.

**INVERSECL<(PROB=*rates*)>**

computes confidence limits for the values of the first continuous independent variable (such as dose) that yield selected response rates. You can optionally specify a list of response rates as *rates*. The response rates must be between zero and one; they can be a list separated by blanks, commas, or in the form of a DO list. For example, the following expressions are all valid lists of response rates:

```
PROB = .1 TO .9 by .1
PROB = .1 .2 .3 .4
PROB = .01, .25, .75, .9
```

If the algorithm fails to converge (this can happen when *C* is nonzero), missing values are reported for the confidence limits. See the section “Inverse Confidence Limits” on page 6410 for details.

**ITPRINT**

displays the iteration history, the final evaluation of the gradient, and the second derivative matrix (Hessian).

**LACKFIT**

performs two goodness-of-fit tests (a Pearson's chi-square test and a log-likelihood ratio chi-square test) for the fitted model.

To compute the test statistics, proper grouping of the observations into subpopulations is needed. You can use the AGGREGATE or AGGREGATE= option for this purpose. See the entry for the AGGREGATE and AGGREGATE= options under the MODEL statement. If neither AGGREGATE nor AGGREGATE= is specified, PROC PROBIT assumes each observation is from a separate subpopulation and computes the goodness-of-fit test statistics only for the *events/trials* syntax.

**NOTE:** This test is not appropriate if the data are very sparse, with only a few values at each set of the independent variable values.

If the Pearson's chi-square test statistic is significant, then the covariance estimates and standard error estimates are adjusted. See the section "Lack-of-Fit Tests" on page 6408 for a description of the tests. Note that the LACKFIT option can also appear in the PROC PROBIT statement. See the section "PROC PROBIT Statement" on page 6352 for details.

**MAXITER=***value***MAXIT=***value*

specifies the maximum number of iterations to be performed in estimating the parameters. By default, MAXITER=50.

**NOINT**

fits a model with no intercept parameter. If the INTERCEPT= option is also specified, the intercept is fixed at the specified value; otherwise, it is set to zero. This is most useful when the response is binary. When the response has  $k$  levels, then  $k - 1$  intercept parameters are fit. The NOINT option sets the intercept parameter corresponding to the lowest response level equal to zero. A Lagrange multiplier, or score, test for the restricted model is computed when the NOINT option is specified.

**SCALE=***scale*

enables you to specify the method for estimating the dispersion parameter. To correct for overdispersion or underdispersion, the covariance matrix is multiplied by the estimate of the dispersion parameter. Valid values for *scale* are as follows:

- |              |                                                                                                                                                                                                          |
|--------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| D   DEVIANCE | specifies that the dispersion parameter be estimated by the deviance divided by its degrees of freedom.                                                                                                  |
| P   PEARSON  | specifies that the dispersion parameter be estimated by the Pearson's chi-square statistic divided by its degrees of freedom. This is set as the default method for estimating the dispersion parameter. |

You can use the AGGREGATE= option to define the subpopulations for calculating the Pearson's chi-square statistic and the deviance.

The "Goodness-of-Fit" table includes the Pearson's chi-square statistic, the deviance, their degrees of freedom, the ratio of each statistic divided by its degrees of freedom, and the corresponding  $p$ -value.

**SINGULAR=value**

specifies the singularity criterion for determining linear dependencies in the set of independent variables. The sum of squares and crossproducts matrix of the independent variables is formed and swept. If the relative size of a pivot becomes less than the value specified, then the variable corresponding to the pivot is considered to be linearly dependent on the previous set of variables considered. By default, *value*=1E-12.

---

## OUTPUT Statement

**OUTPUT** < **OUT=SAS-data-set** *keyword=name* ... *keyword=name* > ;

The OUTPUT statement creates a new SAS data set containing all variables in the input data set and, optionally, the fitted probabilities, the estimate of  $\mathbf{x}'\boldsymbol{\beta}$ , and the estimate of its standard error. Estimates of the probabilities,  $\mathbf{x}'\boldsymbol{\beta}$ , and the standard errors are computed for observations with missing response values as long as the values of all the explanatory variables are nonmissing. This enables you to compute these statistics for additional settings of the explanatory variables that are of interest but for which responses are not observed.

You can specify multiple OUTPUT statements. Each OUTPUT statement creates a new data set and applies only to the preceding MODEL statement. If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*.

Details on the specifications in the OUTPUT statement are as follows:

*keyword=name* specifies the statistics to include in the output data set and assigns names to the new variables that contain the statistics. Specify a keyword for each desired statistic (see the following list of keywords), an equal sign, and the variable to contain the statistic.

The keywords allowed and the statistics they represent are as follows:

PROB | P cumulative probability estimates

$$p = C + (1 - C)F(a_j + \mathbf{x}'\boldsymbol{\beta})$$

STD standard error estimates of  $a_j + \mathbf{x}'\mathbf{b}$

XBETA estimates of  $a_j + \mathbf{x}'\boldsymbol{\beta}$

**OUT=SAS-data-set** names the output data set. By default, the new data set is named by using the *DATA**n* convention.

When the *single variable response* syntax is used, the `_LEVEL_` variable is added to the output data set, and there are  $k - 1$  output observations for each input observation, where  $k$  is the number of response levels. There is no observation output corresponding to the highest response level. For each of the  $k - 1$  observations, the PROB variable contains the fitted probability of obtaining a response level up to the level indicated by the `_LEVEL_` variable, the XBETA variable contains  $a_j + \mathbf{x}'\mathbf{b}$ , where  $j$  references the levels ( $a_1 = 0$ ), and the STD variable contains the standard error estimate of the XBETA variable. See the section “[Details: PROBIT Procedure](#)” on page 6404 for the formulas for the parameterizations.

## PREDPLOT Statement

**PREDPLOT** < VAR=*variable* > < *options* > ;

The PREDPLOT statement plots the predicted probability against a single continuous variable (dose variable) in the MODEL statement for both the binomial model and the multinomial model. Confidence limits are available only for the binomial model. An attached box on the right side of the plot is used to label predicted probability curves with the names of their levels for the multinomial model. You can specify the color of this box by using the CLABBOX= option.

### VAR=*variable*

specifies a single continuous variable (dose variable) in the independent variable list of the MODEL statement. If a VAR= variable is not specified, the first single continuous variable in the independent variable list of the MODEL statement is used. If such a variable does not exist in the independent variable list of the MODEL statement, an error is reported.

The predicted probability is

$$\hat{p} = C + (1 - C)F(\mathbf{x}'\hat{\mathbf{b}})$$

for the binomial model and

$$\begin{aligned} \hat{p}_1 &= C + (1 - C)F(\mathbf{x}'\hat{\mathbf{b}}) \\ \hat{p}_j &= (1 - C)(F(\hat{a}_j + \mathbf{x}'\hat{\mathbf{b}}) - F(\hat{a}_{j-1} + \mathbf{x}'\hat{\mathbf{b}})) \quad j = 2, \dots, k - 1 \\ \hat{p}_k &= (1 - C)(1 - F(\hat{a}_{k-1} + \mathbf{x}'\hat{\mathbf{b}})) \end{aligned}$$

for the multinomial model with  $k$  response levels, where  $F$  is the cumulative distribution function used to model the probability,  $\mathbf{x}'$  is the vector of the covariates,  $\hat{a}_j$  are the estimated ordinal intercepts with  $\hat{a}_1 = 0$ ,  $C$  is the threshold parameter, either known or estimated from the model, and  $\hat{\mathbf{b}}'$  is the vector of estimated parameters.

To plot  $\hat{p}$  (or  $\hat{p}_j$ ) as a function of a continuous variable  $x_1$ , the remaining covariates  $\mathbf{x}_{-1}$  must be specified. You can use the XDATA= option to provide the values of  $\mathbf{x}_{-1}$  (see the XDATA= option in the PROC PROBIT statement for details), or use the default values that follow these rules:

- If the effect contains a continuous variable (or variables), the overall mean of this effect is used.
- If the effect is a single classification variable, the highest level of the variable is used.

### *options*

enable you to plot the observed data and add features to the plot.

You can use options in the PREDPLOT statement to do the following:

- superimpose specification limits
- suppress or add observed data points for the binomial model
- suppress or add confidence limits for the binomial model
- specify the levels for which predicted probability curves are requested for the multinomial model
- specify graphical enhancements (such as color or text height)

## Summary of Options

Table 75.32 through Table 75.38 list all *options* by function. The “Dictionary of Options” on page 6398 describes each option in detail.

### **PREDPLOT Options**

**Table 75.32** Plot Layout Options for PREDPLOT

|                                 |                                                                                                                             |
|---------------------------------|-----------------------------------------------------------------------------------------------------------------------------|
| LEVEL=( <i>character-list</i> ) | Specifies the names of the levels for which the predicted probability curves are requested (only for the multinomial model) |
| NOCONF                          | Suppresses confidence limits                                                                                                |
| NODATA                          | Suppresses observed data points on the plot                                                                                 |
| NOTHRESH                        | Suppresses the threshold line                                                                                               |
| THRESHLABPOS= <i>value</i>      | Specifies the position for the label of the threshold line                                                                  |

### **General Options**

**Table 75.33** Color Options

|                       |                                   |
|-----------------------|-----------------------------------|
| CAXIS= <i>color</i>   | Specifies color for the axes      |
| CFIT= <i>color</i>    | Specifies color for fitted curves |
| CFRAME= <i>color</i>  | Specifies color for frame         |
| CGRID= <i>color</i>   | Specifies color for grid lines    |
| CHREF= <i>color</i>   | Specifies color for HREF= lines   |
| CLABBOX= <i>color</i> | Specifies color for label box     |
| CTEXT= <i>color</i>   | Specifies color for text          |
| CVREF= <i>color</i>   | Specifies color for VREF= lines   |

**Table 75.34** Options to Enhance Plots Produced on Graphics Devices

|                                  |                                                              |
|----------------------------------|--------------------------------------------------------------|
| ANNOTATE=<br><i>SAS-data-set</i> | Specifies an Annotate data set                               |
| INBORDER                         | Requests a border around plot                                |
| LFIT= <i>linetype</i>            | Specifies line style for fitted curves and confidence limits |
| LGRID= <i>linetype</i>           | Specifies line style for grid lines                          |
| NOFRAME                          | Suppresses the frame around plotting areas                   |
| NOGRID                           | Suppresses grid lines                                        |
| NOFIT                            | Suppresses fitted curves                                     |
| NOHLABEL                         | Suppresses horizontal labels                                 |
| NOHTICK                          | Suppresses horizontal ticks                                  |
| NOVTICK                          | Suppresses vertical ticks                                    |
| TURNVLABELS                      | Vertically strings out characters in vertical labels         |
| WFIT= <i>n</i>                   | Specifies thickness for fitted curves                        |
| WGRID= <i>n</i>                  | Specifies thickness for grids                                |
| WREFL= <i>n</i>                  | Specifies thickness for reference lines                      |

**Table 75.35** Axis Options

|                                                        |                                                |
|--------------------------------------------------------|------------------------------------------------|
| HAXIS= <i>value1 to value2</i><br>< by <i>value3</i> > | Specifies tick mark values for horizontal axis |
| HOFFSET= <i>value</i>                                  | Specifies offset for horizontal axis           |
| HLOWER= <i>value</i>                                   | Specifies lower limit on horizontal axis scale |
| HUPPER= <i>value</i>                                   | Specifies upper limit on horizontal axis scale |
| NHTICK= <i>n</i>                                       | Specifies number of ticks for horizontal axis  |
| NVTICK= <i>n</i>                                       | Specifies number of ticks for vertical axis    |
| VAXIS= <i>value1 to value2</i><br>< by <i>value3</i> > | Specifies tick mark values for vertical axis   |
| VAXISLABEL= <i>'label'</i>                             | Specifies label for vertical axis              |
| VOFFSET= <i>value</i>                                  | Specifies offset for vertical axis             |
| VLOWER= <i>value</i>                                   | Specifies lower limit on vertical axis scale   |
| VUPPER= <i>value</i>                                   | Specifies upper limit on vertical axis scale   |
| WAXIS= <i>n</i>                                        | Specifies thickness for axis                   |

**Table 75.36** Graphics Catalog Options

|                              |                                                   |
|------------------------------|---------------------------------------------------|
| DESCRIPTION= <i>'string'</i> | Specifies description for graphics catalog member |
| NAME= <i>'string'</i>        | Specifies name for plot in graphics catalog       |



**Table 75.37** Options for Text Enhancement

|                             |                                                    |
|-----------------------------|----------------------------------------------------|
| <code>FONT=font</code>      | Specifies software font for text                   |
| <code>HEIGHT=value</code>   | Specifies height of text used outside framed areas |
| <code>INHEIGHT=value</code> | Specifies height of text inside framed areas       |

**Table 75.38** Options for Reference Lines

|                                                       |                                                         |
|-------------------------------------------------------|---------------------------------------------------------|
| <code>HREF&lt;(INTERSECT)&gt;<br/>=value-list</code>  | Requests horizontal reference line                      |
| <code>HREFLABELS=<br/>(label1', ..., 'labeln')</code> | Specifies labels for HREF= lines                        |
| <code>HREFLABPOS=n</code>                             | Specifies vertical position of labels for HREF= lines   |
| <code>LHREF=linetype</code>                           | Specifies line style for HREF= lines                    |
| <code>LVREF=linetype</code>                           | Specifies line style for VREF= lines                    |
| <code>VREF&lt;(INTERSECT)&gt;<br/>=value-list</code>  | Requests vertical reference line                        |
| <code>VREFLABELS=<br/>(label1', ..., 'labeln')</code> | Specifies labels for VREF= lines                        |
| <code>VREFLABPOS=n</code>                             | Specifies horizontal position of labels for VREF= lines |

## Dictionary of Options

The following entries provide detailed descriptions of the *options* in the PREDPPLOT statement.

**ANNOTATE=SAS-data-set**

**ANNO=SAS-data-set**

specifies an Annotate data set, as described in *SAS/GRAPH: Reference*, that enables you to add features to the predicted probability plot. The ANNOTATE= data set you specify in the PREDPPLOT statement is used for all plots created by the statement.

**CAXIS=color**

**CAXES=color**

specifies the color used for the axes and tick marks. This option overrides any COLOR= specifications in an AXIS statement. The default is the first color in the device color list.

**CFIT=color**

specifies the color for the fitted predicted probability curves. The default is the first color in the device color list.

**CFRAME=color**

**CFR=color**

specifies the color for the area enclosed by the axes and frame. This area is not shaded by default.

**CGRID=***color*

specifies the color for grid lines. The default is the first color in the device color list.

**CHREF=***color***CH=***color*

specifies the color for lines requested by the HREF= option. The default is the first color in the device color list.

**CTEXT=***color*

specifies the color for tick mark values and axis labels. The default is the color specified for the CTEXT= option in the most recent GOPTIONS statement.

**CVREF=***color***CV=***color*

specifies the color for lines requested by the VREF= option. The default is the first color in the device color list.

**DESCRIPTION=**'*string*'**DES=**'*string*'

specifies a description, up to 40 characters, that appears in the PROC GREPLAY master menu. The default is the variable name.

**FONT=***font*

specifies a software font for reference line and axis labels. You can also specify fonts for axis labels in an AXIS statement. The FONT= font takes precedence over the FTEXT= font specified in the most recent GOPTIONS statement. Hardware characters are used by default.

**HAXIS=***value1 to value2 < by value3 >*

specifies tick mark values for the horizontal axis; *value1*, *value2*, and *value3* must be numeric, and *value1* must be less than *value2*. The lower tick mark is *value1*. Tick marks are drawn at increments of *value3*. The last tick mark is the greatest value that does not exceed *value2*. If *value3* is omitted, a value of 1 is used.

Examples of HAXIS= lists follow:

```
haxis = 0 to 10
haxis = 2 to 10 by 2
haxis = 0 to 200 by 10
```

**HEIGHT=***value*

specifies the height of text used outside framed areas.

**HLOWER=***value*

specifies the lower limit on the horizontal axis scale. The HLOWER= option specifies *value* as the lower horizontal axis tick mark. The tick mark interval and the upper axis limit are determined automatically. This option has no effect if the HAXIS= option is used.

**HOFFSET=***value*

specifies the offset for the horizontal axis. The default value is 1.

**HUPPER=***value*

specifies *value* as the upper horizontal axis tick mark. The tick mark interval and the lower axis limit are determined automatically. This option has no effect if the HAXIS= option is used.

**HREF <(INTERSECT)> =***value-list*

requests reference lines perpendicular to the horizontal axis. If (INTERSECT) is specified, a second reference line perpendicular to the vertical axis is drawn that intersects the fit line at the same point as the horizontal axis reference line. If a horizontal axis reference line label is specified, the intersecting vertical axis reference line is labeled with the vertical axis value. See also the CHREF=, HREFLABELS=, and LHREF= options.

**HREFLABELS=**'*label1*',...,'*labeln*'**HREFLABEL=**'*label1*',...,'*labeln*'**HREFLAB=**'*label1*',...,'*labeln*'

specifies labels for the lines requested by the HREF= option. The number of labels must equal the number of lines. Enclose each label in quotes. Labels can be up to 16 characters.

**HREFLABPOS=***n*

specifies the vertical position of labels for HREF= lines. The following table shows valid values for *n* and the corresponding label placements.

| <i>n</i> | Label Placement         |
|----------|-------------------------|
| 1        | Top                     |
| 2        | Staggered from top      |
| 3        | Bottom                  |
| 4        | Staggered from bottom   |
| 5        | Alternating from top    |
| 6        | Alternating from bottom |

**INBORDER**

requests a border around predicted probability plots.

**INHEIGHT=***value*

Specifies height of text inside framed areas.

**LEVEL=**(*character-list*)**ORDINAL=** (*character-list*)

specifies the names of the levels for which predicted probability curves are requested. Names should be quoted and separated by space. If there is no correct name provided, no fitted probability curve is plotted.

**LFIT=***linetype*

specifies a line style for fitted curves and confidence limits. By default, fitted curves are drawn by connecting solid lines (*linetype* = 1) and confidence limits are drawn by connecting dashed lines (*linetype* = 3).

**LGRID=***linetype*

specifies a line style for all grid lines. The value for *linetype* is between 1 and 46. The default is 35.

**LHREF=***linetype***LH=***linetype*

specifies the line type for lines requested by the HREF= option. The default is 2, which produces a dashed line.

**LVREF=***linetype***LV=***linetype*

specifies the line type for lines requested by the VREF= option. The default is 2, which produces a dashed line.

**NAME=**'string'

specifies a name for the plot, up to eight characters, that appears in the PROC GREPLAY master menu. The default is 'PROBIT'.

**NHTICK=***n*

Specifies number of ticks for horizontal axis.

**NVTICK=***n*

Specifies number of ticks for vertical axis.

**NOCONF**

suppresses confidence limits from the plot. This works only for the binomial model. Confidence limits are not plotted for the multinomial model.

**NODATA**

suppresses observed data points from the plot. This works only for the binomial model. The data points are not plotted for the multinomial model.

**NOFIT**

suppresses the fitted predicted probability curves.

**NOFRAME**

suppresses the frame around plotting areas.

**NOGRID**

suppresses grid lines.

**NOHLABEL**

suppresses horizontal labels.

**NOHTICK**

suppresses horizontal tick marks.

**NOTHRESH**

suppresses the threshold line.

**NOVLABEL**

suppresses vertical labels.

**NOVTICK**

suppresses vertical tick marks.

**TURNVLABELS**

vertically strings out characters in vertical labels.

**THRESHLABPOS=*n***

specifies the horizontal position of labels for the threshold line. The following table shows valid values for *n* and the corresponding label placements.

| <i>n</i> | Label Placement |
|----------|-----------------|
| 1        | Left            |
| 2        | Right           |

**VAXIS=*value1 to value2 < by value3 >***

specifies tick mark values for the vertical axis; *value1*, *value2*, and *value3* must be numeric, and *value1* must be less than *value2*. The lower tick mark is *value1*. Tick marks are drawn at increments of *value3*. The last tick mark is the greatest value that does not exceed *value2*. This method of specification of tick marks is not valid for logarithmic axes. If *value3* is omitted, a value of 1 is used.

Examples of VAXIS= lists follow:

```
vaxis = 0 to 10
vaxis = 0 to 2 by .1
```

**VAXISLABEL=*'string'***

specifies a label for the vertical axis.

**VLOWER=*value***

specifies the lower limit on the vertical axis scale. The VLOWER= option specifies *value* as the lower vertical axis tick mark. The tick mark interval and the upper axis limit are determined automatically. This option has no effect if the VAXIS= option is used.

**VOFFSET=*value***

specifies the offset for the vertical axis.

**VREF=*value-list***

requests reference lines perpendicular to the vertical axis. If (INTERSECT) is specified, a second reference line perpendicular to the horizontal axis is drawn that intersects the fit line at the same point as the vertical axis reference line. If a vertical axis reference line label is specified, the intersecting horizontal axis reference line is labeled with the horizontal axis value. See also the CVREF=, LVREF=, and VREFLABELS= options.

**VREFLABELS=*'label1', ..., 'labeln'*****VREFLABEL=*'label1', ..., 'labeln'*****VREFLAB=*'label1', ..., 'labeln'***

specifies labels for the lines requested by the VREF= option. The number of labels must equal the number of lines. Enclose each label in quotes. Labels can be up to 16 characters.

**VREFLABPOS=*n***

specifies the horizontal position of labels for VREF= lines. The following table shows valid values for *n* and the corresponding label placements.

| <i>n</i> | Label Placement |
|----------|-----------------|
| 1        | Left            |
| 2        | Right           |

**VUPPER=*value***

specifies the upper limit on the vertical axis scale. The VUPPER= option specifies *value* as the upper vertical axis tick mark. The tick mark interval and the lower axis limit are determined automatically. This option has no effect if the VAXIS= option is used.

**WAXIS=*n***

specifies line thickness for axes and frame. The default value is 1.

**WFIT=*n***

specifies line thickness for fitted curves. The default value is 1.

**WGRID=*n***

specifies line thickness for grids. The default value is 1.

**WREFL=*n***

specifies line thickness for reference lines. The default value is 1.

---

## SLICE Statement

**SLICE** *model-effect* < / options > ;

The SLICE statement provides a general mechanism for performing a partitioned analysis of the LS-means for an interaction. This analysis is also known as an analysis of simple effects.

The SLICE statement uses the same options as the LSMEANS statement, which are summarized in Table 19.21. For details about the syntax of the SLICE statement, see the section “SLICE Statement” on page 498 in Chapter 19, “Shared Concepts and Topics.”

---

## STORE Statement

**STORE** < OUT= > *item-store-name* < / LABEL='label' > ;

The STORE statement requests that the procedure save the context and results of the statistical analysis. The resulting item store has a binary file format that cannot be modified. The contents of the item store can be processed with the PLM procedure.

For details about the syntax of the STORE statement, see the section “STORE Statement” on page 501 in Chapter 19, “Shared Concepts and Topics.”

---

## TEST Statement

**TEST** < model-effects > < / options > ;

The TEST statement enables you to perform chi-square tests for model effects that test Type I, Type II, or Type III hypotheses. By default, the Type III tests are performed. For more information, see Chapter 19, “Shared Concepts and Topics.”

---

## WEIGHT Statement

**WEIGHT** variable ;

A WEIGHT statement can be used with PROC PROBIT to weight each observation by the value of the variable specified. The contribution of each observation to the likelihood function is multiplied by the value of the weight variable. Observations with zero, negative, or missing weights are not used in model estimation.

---

## Details: PROBIT Procedure

---

### Missing Values

PROC PROBIT does not use any observations having missing values for any of the independent variables, the response variables, or the weight variable. If only the response variables are missing, statistics requested in the OUTPUT statement are computed.

---

### Response Level Ordering

For binary response data, PROC PROBIT fits the following model by default:

$$\Phi^{-1} \left( \frac{p - C}{1 - C} \right) = \mathbf{x}'\boldsymbol{\beta}$$

where  $p$  is the probability of the response level identified as the first level in the “Response Profile” table in the output and  $\Phi$  is the normal cumulative distribution function. By default, the covariate vector  $\mathbf{x}$  contains an intercept term. This is sometimes called Abbot’s formula.

Because of the symmetry of the normal (and logistic) distribution, the effect of reversing the order of the two response values is to change the signs of  $\boldsymbol{\beta}$  in the preceding equation.

By default, response levels appear in ascending, sorted order (that is, the lowest level appears first, and then the next lowest, and so on). There are a number of ways that you can control the sort order of the response categories and, therefore, which level is assigned the first ordered level. One of the most common sets of response levels is  $\{0,1\}$ , with 1 representing the event with the probability that is to be modeled.

Consider the example where  $Y$  takes the values 1 and 0 for event and nonevent, respectively, and EXPOSURE is the explanatory variable. By default, PROC PROBIT assigns the first ordered level to response level 0, causing the probability of the nonevent to be modeled. There are several ways to change this.

Besides recoding the variable  $Y$ , you can do the following:

- assign a format to  $Y$  such that the first formatted value (when the formatted values are put in sorted order) corresponds to the event. For the following example,  $Y=0$  could be assigned formatted value 'nonevent' and  $Y=1$  could be assigned formatted value 'event.' Since ORDER=FORMATTED by default,  $Y=1$  becomes the first ordered level. See [Example 75.3](#) for an illustration of this method.

```
proc format;
 value disease 1='event' 0='nonevent';
run;
proc probit;
 model y=exposure;
 format y disease.;
run;
```

- arrange the input data set so that  $Y=1$  appears first and use the ORDER=DATA option in the PROC PROBIT statement. Since ORDER=DATA sorts levels in order of their appearance in the data set,  $Y=1$  becomes the first ordered level. Note that this option causes classification variables to be sorted by their order of appearance in the data set, also.

---

## Computational Method

The log-likelihood function is maximized by means of a ridge-stabilized Newton-Raphson algorithm. Initial regression parameter estimates are set to zero. The INITIAL= and INTERCEPT= options in the MODEL statement can be used to give nonzero initial estimates.

The log-likelihood function,  $L$ , is computed as

$$L = \sum_i w_i \ln(p_i)$$

where the sum is over the observations in the data set,  $w_i$  is the weight for the  $i$ th observation, and  $p_i$  is the modeled probability of the observed response. In the case of the events/trials syntax in the MODEL statement, each observation contributes two terms corresponding to the probability of the event and the probability of its complement:

$$L = \sum_i w_i [r_i \ln(p_i) + (n_i - r_i) \ln(1 - p_i)]$$

where  $r_i$  is the number of events and  $n_i$  is the number of trials for observation  $i$ . This log-likelihood function differs from the log-likelihood function for a binomial or multinomial distribution by additive terms consisting of the log of binomial or multinomial coefficients. These terms are parameter-independent and do not affect the model estimation or the standard errors and tests.



The estimated covariance matrix,  $V$ , of the parameter estimates is computed as the negative inverse of the information matrix of second derivatives of  $L$  with respect to the parameters evaluated at the final parameter estimates. Thus, the estimated covariance matrix is derived from the observed information matrix rather than the expected information matrix (these are generally not the same). The standard error estimates for the parameter estimates are taken as the square roots of the corresponding diagonal elements of  $V$ .

If convergence of the maximum likelihood estimates is attained, a Type III chi-square test statistic is computed for each effect, testing whether there is any contribution from any of the levels of the effect. This statistic is computed as a quadratic form in the appropriate parameter estimates by using the corresponding submatrix of the asymptotic covariance matrix estimate. See Chapter 42, “The GLM Procedure,” and Chapter 15, “The Four Types of Estimable Functions,” for more information about Type III estimable functions.

The asymptotic covariance matrix is computed as the inverse of the observed information matrix. Note that if the NOINT option is specified and classification variables are used, the first classification variable contains a contribution from an intercept term. The results are displayed in an ODS table named “Type3Analysis”.

Chi-square tests for individual parameters are Wald tests based on the observed information matrix and the parameter estimates. If an effect has a single degree of freedom in the parameter estimates table, the chi-square test for this parameter is equivalent to the Type III test for this effect.

Prior to SAS 8.2, a multiple-degrees-of-freedom statistic was computed for each effect to test for contribution from any level of the effect. In general, the Type III test statistic in a main-effect-only model (no interaction terms) will be equal to the previously computed effect statistic, unless there are collinearities among the effects. If there are collinearities, the Type III statistic will adjust for them, and the value of the Type III statistic and the number of degrees of freedom might not be equal to those of the previous effect statistic.

The theory behind these tests assumes large samples. If the samples are not large, it might be better to base the tests on log-likelihood ratios. These changes in log likelihood can be obtained by fitting the model twice, once with all the parameters of interest and once leaving out the parameters to be tested. See Cox and Oakes (1984) for a discussion of the merits of some possible test methods.

If some of the independent variables are perfectly correlated with the response pattern, then the theoretical parameter estimates can be infinite. Although fitted probabilities of 0 and 1 are not especially pathological, infinite parameter estimates are required to yield these probabilities. Due to the finite precision of computer arithmetic, the actual parameter estimates are not infinite. Indeed, since the tails of the distributions allowed in the PROBIT procedure become small rapidly, an argument to the cumulative distribution function of around 20 becomes effectively infinite. In the case of such parameter estimates, the standard error estimates and the corresponding chi-square tests are not trustworthy.

---

## Distributions

The distributions,  $F(x)$ , allowed in the PROBIT procedure are specified with the DISTRIBUTION= option in the MODEL statement. The cumulative distribution functions for the available distributions are

| Cumulative Distribution Function                                            | Distribution              |
|-----------------------------------------------------------------------------|---------------------------|
| $\int_{-\infty}^x \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{z^2}{2}\right) dz$ | Normal                    |
| $\frac{1}{1+e^{-x}}$                                                        | Logistic                  |
| $1 - e^{-e^x}$                                                              | Extreme value or Gompertz |

The variances of these three distributions are not all equal to 1, and their means are not all equal to zero. Their means and variances are shown in the following table, where  $\gamma$  is the Euler constant.

| Distribution              | Mean      | Variance  |
|---------------------------|-----------|-----------|
| Normal                    | 0         | 1         |
| Logistic                  | 0         | $\pi^2/3$ |
| Extreme value or Gompertz | $-\gamma$ | $\pi^2/6$ |

When comparing parameter estimates by using different distributions, you need to take into account the different scalings and, for the extreme value (or Gompertz) distribution, a possible shift in location. For example, if the fitted probabilities are in the neighborhood of 0.1 to 0.9, then the parameter estimates from the logistic model should be about  $\pi/\sqrt{3}$  larger than the estimates from the probit model.

---

## INEST= SAS-data-set

The INEST= data set names a SAS data set that specifies initial estimates for all the parameters in the model.

The INEST= data set must contain the intercept variables (named Intercept for binary response model and Intercept, Intercept2, Intercept3, and so forth, for multinomial response models) and all independent variables in the MODEL statement.

If BY processing is used, the INEST= data set should also include the BY variables, and there must be at least one observation for each BY group. If there is more than one observation in a BY group, the first one read is used for that BY group.

If the INEST= data set also contains the \_TYPE\_ variable, only observations with the \_TYPE\_ value “PARMS” are used as starting values. Combining the INEST= data set and the option MAXIT= in the MODEL statement, partial scoring can be done, such as predicting on a validation data set by using the model built from a training data set.

You can specify starting values for the iterative algorithm in the INEST= data set. This data set overwrites the INITIAL= option in the MODEL statement, which is a little difficult to use for models with multilevel interaction effects. The INEST= data set has the same structure as the “OUTEST= SAS-data-set” on page 6411, but it is not required to have all the variables or observations that appear in the OUTEST= data set. One simple use of the INEST= option is passing the previous OUTEST= data set directly to the next model as an INEST= data set, assuming that the two models have the same parameterization.

---

## Model Specification

For a two-level response, the probability that the lesser response occurs is modeled by the probit equation as

$$p = C + (1 - C)F(\mathbf{x}'\mathbf{b})$$

The probability of the other (complementary) event is  $1 - p$ .

For a multilevel response with outcomes labeled  $l_i$  for  $i = 1, 2, \dots, k$ , the probability,  $p_j$ , of observing level  $l_j$  is as follows:

$$\begin{aligned}
 p_1 &= C + (1 - C)F(\mathbf{x}'\mathbf{b}) \\
 p_2 &= (1 - C)(F(a_2 + \mathbf{x}'\mathbf{b}) - F(\mathbf{x}'\mathbf{b})) \\
 &\vdots \\
 p_j &= (1 - C)(F(a_j + \mathbf{x}'\mathbf{b}) - F(a_{j-1} + \mathbf{x}'\mathbf{b})) \\
 &\vdots \\
 p_k &= (1 - C)(1 - F(a_{k-1} + \mathbf{x}'\mathbf{b}))
 \end{aligned}$$

Thus, for a  $k$ -level response, there are  $k - 2$  additional parameters,  $a_2, a_3, \dots, a_{k-1}$ , estimated. These parameters are denoted by `Interceptj`,  $j = 2, 3, \dots, k - 1$ , in the output.

An intercept parameter is always added to the set of independent variables as the first term in the model unless the `NOINT` option is specified in the `MODEL` statement. If a classification variable taking on  $k$  levels is used as one of the independent variables, a set of  $k$  indicator variables is generated to model the effect of this variable. Because of the presence of the intercept term, there are at most  $k - 1$  degrees of freedom for this effect in the model.

---

## Lack-of-Fit Tests

Two goodness-of-fit tests can be requested from the PROBIT procedure: a Pearson's chi-square test and a log-likelihood ratio chi-square test.

To compute the test statistics, you can use the `AGGREGATE` or `AGGREGATE=` option grouping the observations into subpopulations. If neither `AGGREGATE` nor `AGGREGATE=` is specified, `PROC PROBIT` assumes that each observation is from a separate subpopulation and computes the goodness-of-fit test statistics only for the *events/trials* syntax.

If the Pearson's goodness-of-fit chi-square test is requested and the  $p$ -value for the test is too small, variances and covariances are adjusted by a heterogeneity factor (the goodness-of-fit chi-square divided by its degrees of freedom) and a critical value from the  $t$  distribution is used to compute the fiducial limits. The Pearson's chi-square test statistic is computed as

$$\chi_P^2 = \sum_{i=1}^m \sum_{j=1}^k \frac{(r_{ij} - n_i \hat{p}_{ij})^2}{n_i \hat{p}_{ij}}$$

where the sum on  $i$  is over grouping, the sum on  $j$  is over levels of response,  $r_{ij}$  is the frequency of response level  $j$  for the  $i$ th grouping,  $n_i$  is the total frequency for the  $i$ th grouping, and  $\hat{p}_{ij}$  is the fitted probability for the  $j$ th level at the  $i$ th grouping.

The likelihood ratio chi-square test statistic is computed as

$$\chi_D^2 = 2 \sum_{i=1}^m \sum_{j=1}^k r_{ij} \ln \left( \frac{r_{ij}}{n_i \hat{p}_{ij}} \right)$$

This quantity is sometimes called the deviance. If the modeled probabilities fit the data, these statistics should be approximately distributed as chi-square with degrees of freedom equal to  $(k - 1) \times m - q$ , where  $k$  is the number of levels of the multinomial or binomial response,  $m$  is the number of sets of independent variable values (covariate patterns), and  $q$  is the number of parameters fit in the model.

In order for the Pearson's statistic and the deviance to be distributed as chi-square, there must be sufficient replication within the groupings. When this is not true, the data are sparse, and the  $p$ -values for these statistics are not valid and should be ignored. Similarly, these statistics, divided by their degrees of freedom, cannot serve as indicators of overdispersion. A large difference between the Pearson's statistic and the deviance provides some evidence that the data are too sparse to use either statistic.

---

## Rescaling the Covariance Matrix

One way of correcting overdispersion is to multiply the covariance matrix by a dispersion parameter. You can supply the value of the dispersion parameter directly, or you can estimate the dispersion parameter based on either the Pearson's chi-square statistic or the deviance for the fitted model.

The Pearson's chi-square statistic  $\chi_P^2$  and the deviance  $\chi_D^2$  are defined in the section "Lack-of-Fit Tests" on page 6408. If the SCALE= option is specified in the MODEL statement, the dispersion parameter is estimated by

$$\hat{\sigma}^2 = \begin{cases} \chi_P^2 / (m(k - 1) - q) & \text{SCALE=PEARSON} \\ \chi_D^2 / (m(k - 1) - q) & \text{SCALE=DEVIANC} \\ (\text{constant})^2 & \text{SCALE=constant} \end{cases}$$

In order for the Pearson's statistic and the deviance to be distributed as chi-square, there must be sufficient replication within the subpopulations. When this is not true, the data are sparse, and the  $p$ -values for these statistics are not valid and should be ignored. Similarly, these statistics, divided by their degrees of freedom, cannot serve as indicators of overdispersion. A large difference between the Pearson's statistic and the deviance provides some evidence that the data are too sparse to use either statistic.

You can use the AGGREGATE (or AGGREGATE=) option to define the subpopulation profiles. If you do not specify this option, each observation is regarded as coming from a separate subpopulation. For *events/trials* syntax, each observation represents  $n$  Bernoulli trials, where  $n$  is the value of the *trials* variable; for *single-trial* syntax, each observation represents a single trial. Without the AGGREGATE (or AGGREGATE=) option, the Pearson's chi-square statistic and the deviance are calculated only for *events/trials* syntax.

Note that the parameter estimates are not changed by this method. However, their standard errors are adjusted for overdispersion, affecting their significance tests.

---

## Tolerance Distribution

For a single independent variable, such as a dosage level, the models for the probabilities can be justified on the basis of a population with mean  $\mu$  and scale parameter  $\sigma$  of tolerances for the subjects. Then, given a dose  $x$ , the probability,  $P$ , of observing a response in a particular subject is the probability that the subject's tolerance is less than the dose or

$$P = F\left(\frac{x - \mu}{\sigma}\right)$$

Thus, in this case, the intercept parameter,  $b_0$ , and the regression parameter,  $b_1$ , are related to  $\mu$  and  $\sigma$  by

$$b_0 = -\frac{\mu}{\sigma}, \quad b_1 = \frac{1}{\sigma}$$

**NOTE:** The parameter  $\sigma$  is not equal to the standard deviation of the population of tolerances for the logistic and extreme value distributions.

---

## Inverse Confidence Limits

In bioassay problems, estimates of the values of the independent variables that yield a desired response are often needed. For instance, the value yielding a 50% response rate (called the ED50 or LD50) is often used. The INVERSECL option requests that confidence limits be computed for the value of the independent variable that yields a specified response. These limits are computed only for the first continuous variable effect in the model. The other variables are set either at their mean values if they are continuous or at the reference (last) level if they are discrete variables. For a discussion of inverse confidence limits, see Hubert, Bohidar, and Peace (1988).

For the PROBIT procedure, the response variable is a probability. An estimate of the first continuous variable value needed to achieve a response of  $p$  is given by

$$\hat{x}_1 = \frac{1}{b_1} (F^{-1}(p) - \mathbf{x}^* \mathbf{b}^*)$$

where  $F$  is the cumulative distribution function used to model the probability,  $\mathbf{x}^*$  is the vector of independent variables excluding the first one, which can be specified by the XDATA= option described in the section “XDATA= SAS-data-set” on page 6411,  $\mathbf{b}^*$  is the vector of parameter estimates excluding the first one, and  $b_1$  is the estimated regression coefficient for the independent variable of interest. This estimate assumes that there is no natural response rate ( $C = 0$ ). When  $C$  is nonzero, the quantiles and confidence limits for the independent variable correspond to the adjusted probability  $C + (1 - C)p$ , rather than to  $p$ . As a result, an estimate of the value yielding response rate  $p$  is associated with the  $(p - C)/(1 - C)$  quantile. For example, if  $C = 0.1$  then an estimate of the LD50 is found corresponding to the 0.44 quantile. This value can be thought of as yielding 50% of the variable’s effect, but a 44% response rate. For both binary and ordinal models, the INVERSECL option provides estimates of the value of  $x_1$ , which yields  $\Pr(\text{first response level}) = p$ , for various values of  $p$ .

This estimator is given as a ratio of random variables, such as  $r = a/b$ . Confidence limits for this ratio can be computed by using Fieller’s theorem. A brief description of this theorem follows. See Finney (1971) for a more complete description of Fieller’s theorem.

If the random variables  $a$  and  $b$  are thought to be distributed as jointly normal, then for any fixed value  $r$  the following probability statement holds if  $z$  is an  $\alpha/2$  quantile from the standard normal distribution and  $\mathbf{V}$  is the variance-covariance matrix of  $a$  and  $b$ :

$$\Pr((a - rb)^2 > z^2(V_{aa} - 2rV_{ab} + r^2V_{bb})) = \alpha$$

Usually the inequality can be solved for  $r$  to yield a confidence interval. The PROBIT procedure uses a value of 1.96 for  $z$ , corresponding to an  $\alpha$  value of 0.05, unless the goodness-of-fit  $p$ -value is less than the specified value of the HPROB= option. When this happens, the covariance matrix is scaled by the heterogeneity factor, and a  $t$  distribution quantile is used for  $z$ .

It is possible for the roots of the equation for  $r$  to be imaginary or for the confidence interval to be all points outside of an interval. In these cases, the limits are set to missing by the PROBIT procedure.

Although the normal and logistic distribution give comparable fitted values of  $p$  if the empirically observed proportions are not too extreme, they can give appreciably different values when extrapolated into the tails. Correspondingly, the estimates of the confidence limits and dose values can be different for the two distributions even when they agree quite well in the body of the data. Extrapolation outside of the range of the actual data is often sensitive to model assumptions, and caution is advised if extrapolation is necessary.

---

## OUTEST= SAS-data-set

The OUTEST= data set contains parameter estimates and the log likelihood for the model. You can specify a label in the MODEL statement to distinguish between the estimates for different models used by the PROBIT procedure. If you specify the COVOUT option, the OUTEST= data set also contains the estimated covariance matrix of the parameter estimates.

The OUTEST= data set contains each variable used as a dependent or independent variable in any MODEL statement. One observation consists of parameter values for the model with the dependent variable having the value -1. If you specify the COVOUT option, there are additional observations containing the rows of the estimated covariance matrix. For these observations, the dependent variable contains the parameter estimate for the corresponding row variable. The following variables are also added to the data set:

|                        |                                                                                                                                                                        |
|------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>_MODEL_</code>   | a character variable containing the label of the MODEL statement, if present, or blank otherwise                                                                       |
| <code>_NAME_</code>    | a character variable containing the name of the dependent variable for the parameter estimates observations or the name of the row for the covariance matrix estimates |
| <code>_TYPE_</code>    | a character variable containing the type of the observation, either PARMS for parameter estimates or COV for covariance estimates                                      |
| <code>_DIST_</code>    | a character variable containing the name of the distribution modeled                                                                                                   |
| <code>_LNLIKE_</code>  | a numeric variable containing the last computed value of the log likelihood                                                                                            |
| <code>_C_</code>       | a numeric variable containing the estimated threshold parameter                                                                                                        |
| <code>INTERCEPT</code> | a numeric variable containing the intercept parameter estimates and covariances                                                                                        |

Any BY variables specified are also added to the OUTEST= data set.

---

## XDATA= SAS-data-set

The XDATA= data set is used for specifying values for the effects in the MODEL statement when predicted values and/or fiducial limits for a single continuous variable (dose variable) are required. It is also used for plots specified by the CDFPLOT, IPPLOT, LPREDPLOT, and PREDPLOT statement.

The XDATA= data names a SAS data set that contains user input values for all the independent variables in the MODEL statement and the variables in the CLASS statement. The XDATA= data set has the same structure as the DATA= data set but is not required to have all the variables or observations that appear in the DATA= data set.

The XDATA= data set must contain all the independent variables in the MODEL statement and variables in the CLASS statement. Even though variables in the CLASS statement are not used in the MODEL statement, valid values are required for these variables in the XDATA= data set. Missing values are not allowed. For independent variables in the MODEL statement, although the dose variable's value is not used in the computing of predicted values and/or fiducial limits for the dose variable, missing values are not allowed in the XDATA= data set for any of the independent variables. Missing values are allowed for the dependent variables and other variables if they are included in the XDATA= data set and not listed in the CLASS statement.

If BY processing is used, the XDATA= data set should also include the BY variables, and there must be at least one valid observation for each BY group. If there is more than one valid observation in one BY group, the last one read is used for that BY group.

If there is no XDATA= data set in the PROC PROBIT statement, by default, the PROBIT procedure will use overall mean for effects containing continuous variable (or variables) and the highest level of a single classification variable as reference level. The rules are summarized as follows:

- If the effect contains a continuous variable (or variables), the overall mean of this effect is used.
- If the effect is a single classification variable, the highest level of the variable is used.

---

## Traditional High-Resolution Graphics

This section provides examples of using syntax available with the traditional high-resolution plots. A more modern alternative is to use ODS Graphics. See the section “ODS Graphics” on page 6415 for details.

There are four plot statements that you can use to request traditional high-resolution plots: CDFPLOT, IPPPLOT, LPREDPLOT, and PREDPLOT. Some of these statements apply only to either the binomial model or the multinomial model. Table 75.39 shows the availability of these statements for different models.

**Table 75.39** Plot Statement Availability

| Statement | Binomial | Multinomial |
|-----------|----------|-------------|
| CDFPLOT   | No       | Yes         |
| IPPPLOT   | Yes      | No          |
| LPREDPLOT | Yes      | Yes         |
| PREDPLOT  | Yes      | Yes         |

The following example uses the data set study in the section “Estimating the Natural Response Threshold Parameter” on page 6347 to illustrate how to create high-resolution plots for the binomial model:

```
proc probit data=study log10 optc;
 model respond/number=dose;
 predpplot var=dose cfit=blue; inset;
 lpredplot var=dose cfit=blue; inset;
 ippplot var=dose cfit=blue; inset/pos=se;
run;
```



All plot statements must follow the MODEL statement. The VAR= option specifies a continuous independent variable (dose variable) against which the predicted probability or the linear predictor is plotted. The INSET statement requests the inset box with summary information. See the section “[INSET Statement](#)” on page 6369 for more details.

The PREDPLOT statement creates a plot that shows the relationship between dosage level, observed response proportions, and estimated probability values. See the section “[PREDPLOT Statement](#)” on page 6395 for more details. The IPPLOT statement creates a similar plot. See the section “[IPPLOT Statement](#)” on page 6371 for details about this plot. The LPREDPLOT statement creates a linear predictor plot, which is described in the section “[LPREDPLOT Statement](#)” on page 6379.

The following example uses the data set multi from [Example 75.2](#) to illustrate how to create high-resolution plots for the multinomial model:

```
proc probit data=multi order=data;
 class prep symptoms;
 model symptoms=prep ldose;
 cdfplot var=ldose level=("None" "Mild" "Severe")
 cfit=blue cframe=ligr noconf;
 lpredplot var=ldose level=("None" "Mild" "Severe")
 cfit=blue cframe=ligr;
 predpplot var=ldose level=("None" "Mild" "Severe")
 cfit=blue cframe=ligr;
 weight n;
run;
```

The CDFPLOT statement creates a plot that shows the relationship between the cumulative response probabilities and the dose levels. The multinomial model plots are similar to those with the binomial model.

---

## Displayed Output

If you request the iteration history (ITPRINT), PROC PROBIT displays the following:

- the current value of the log likelihood
- the ridging parameter for the modified Newton-Raphson optimization process
- the current estimate of the parameters
- the current estimate of the parameter  $C$  for a natural (threshold) model
- the values of the gradient and the Hessian on the last iteration

If you include classification variables, PROC PROBIT displays the following:

- the numbers of levels for each classification variable
- the (ordered) values of the levels
- the number of observations used



After the model is fit, PROC PROBIT displays the following:

- the name of the input data set
- the name of the dependent variables
- the number of observations used
- the number of events and the number of trials
- the final value of the log-likelihood function
- the parameter estimates
- the standard error estimates of the parameter estimates
- approximate chi-square test statistics for the test

If you specify the COVB or CORRB options, PROC PROBIT displays the following:

- the estimated covariance matrix for the parameter estimates
- the estimated correlation matrix for the parameter estimates

If you specify the LACKFIT option, PROC PROBIT displays the following:

- a count of the number of levels of the response and the number of distinct sets of independent variables
- a goodness-of-fit test based on the Pearson's chi-square
- a goodness-of-fit test based on the likelihood-ratio chi-square

If you specify only one independent variable, the normal distribution is used to model the probabilities, and the response is binary, then PROC PROBIT displays the following:

- the mean MU of the stimulus tolerance
- the scale parameter SIGMA of the stimulus tolerance
- the covariance matrix for MU, SIGMA, and the natural response parameter C

If you specify the INVERSECL options, PROC PROBIT also displays the following:

- the estimated dose along with the 95% fiducial limits for probability levels 0.01 to 0.10, 0.15 to 0.85 by 0.05, and 0.90 to 0.99

## ODS Table Names

PROC PROBIT assigns a name to each table it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in the following table. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

**Table 75.40** ODS Tables Produced by PROC PROBIT

| ODS Table Name     | Description                              | Statement | Option    |
|--------------------|------------------------------------------|-----------|-----------|
| ClassLevels        | Classification variable levels           | CLASS     | Default   |
| ConvergenceStatus  | Convergence status                       | MODEL     | Default   |
| CorrB              | Parameter estimate correlation matrix    | MODEL     | CORRB     |
| CovB               | Parameter estimate covariance matrix     | MODEL     | COVB      |
| CovTolerance       | Covariance matrix for location and scale | MODEL     | Default   |
| GoodnessOfFit      | Goodness-of-fit tests                    | MODEL     | LACKFIT   |
| Heterogeneity      | Heterogeneity correction                 | MODEL     | LACKFIT   |
| IterHistory        | Iteration history                        | MODEL     | ITPRINT   |
| LagrangeStatistics | Lagrange statistics                      | MODEL     | NOINT     |
| LastGrad           | Last evaluation of the gradient          | MODEL     | ITPRINT   |
| LastHess           | Last evaluation of the Hessian           | MODEL     | ITPRINT   |
| LogProbitAnalysis  | Probit analysis for log dose             | MODEL     | INVERSECL |
| ModelInfo          | Model information                        | MODEL     | Default   |
| MuSigma            | Location and scale                       | MODEL     | Default   |
| NObs               | Observations summary                     | PROC      | Default   |
| ParameterEstimates | Parameter estimates                      | MODEL     | Default   |
| ParmInfo           | Parameter indices                        | MODEL     | Default   |
| ProbitAnalysis     | Probit analysis for linear dose          | MODEL     | INVERSECL |
| ResponseLevels     | Response-covariate profile               | MODEL     | LACKFIT   |
| ResponseProfiles   | Counts for ordinal data                  | MODEL     | Default   |
| Type3Analysis      | Type III tests                           | MODEL     | Default   |

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “Statistical Graphics Using ODS.”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “A Primer on ODS Statistical Graphics” on page 599 in Chapter 21, “Statistical Graphics Using ODS.”

These ODS graphs are controlled by the PLOTS= option in the PROC PROBIT statement. You can specify more than one graph request with the PLOTS= option. Table 75.41 summarizes these requests.

**Table 75.41** Options for Plots

| Option    | Plot                             |
|-----------|----------------------------------|
| ALL       | All appropriate plots            |
| CDFPLOT   | Estimated cumulative probability |
| IPPPLOT   | Inverse predicted probability    |
| LPREDPLOT | Linear predictor                 |
| NONE      | No plot                          |
| PREDPPLOT | Predicted probability            |

The following subsections provide information about these graphs.

### ODS Graph Names

PROC PROBIT assigns a name to each graph it creates using ODS. You can use these names to reference the graphs when using ODS. The names are listed in Table 75.42.

**Table 75.42** Graphs Produced by PROC PROBIT

| ODS Graph Name | Plot Description                 | Statement | PLOTS= Option |
|----------------|----------------------------------|-----------|---------------|
| CDFPlot        | Estimated cumulative probability | PROC      | CDFPLOT       |
| IPPPlot        | Inverse predicted probability    | PROC      | IPPPLOT       |
| LPredPlot      | Linear predictor                 | PROC      | LPREDPLOT     |
| PredPPlot      | Predicted probability            | PROC      | PREDPPLOT     |

### CDF Plot

For a multinomial model, the predicted cumulative distribution function is defined as

$$\hat{F}_j(\mathbf{x}) = C + (1 - C)F(\hat{a}_j + \mathbf{x}'\hat{\mathbf{b}})$$

where  $j = 1, \dots, k$  are the indexes of the  $k$  levels of the multinomial response variable,  $F$  is the CDF of the distribution used to model the cumulative probabilities,  $\hat{\mathbf{b}}$  is the vector of estimated parameters,  $\mathbf{x}$  is the covariate vector,  $\hat{a}_j$  are estimated ordinal intercepts with  $\hat{a}_1 = 0$ , and  $C$  is the threshold parameter, either known or estimated from the model. Let  $x_1$  be the covariate corresponding to the dose variable and  $\mathbf{x}_{-1}$  be the vector of the rest of the covariates. Let the corresponding estimated parameters be  $\hat{b}_1$  and  $\hat{\mathbf{b}}_{-1}$ . Then

$$\hat{F}_j(\mathbf{x}) = C + (1 - C)F(\hat{a}_j + x_1\hat{b}_1 + \mathbf{x}'_{-1}\hat{\mathbf{b}}_{-1})$$

To plot  $\hat{F}_j$  as a function of  $x_1$ ,  $\mathbf{x}_{-1}$  must be specified. You can use the XDATA= option to provide the values of  $\mathbf{x}_{-1}$  (see the XDATA= option in the PROC PROBIT statement for details), or use the default values that follow these rules:

- If the effect contains a continuous variable (or variables), the overall mean of this effect is used.
- If the effect is a single classification variable, the highest level of the variable is used.

The LEVEL= suboption specify the levels of the multinomial response variable for which the CDF curves are requested. There are  $k - 1$  curves for a  $k$ -level multinomial response variable (for the highest level, it is the constant line 1). You can specify any of them to be plotted by the LEVEL= suboption. See the plot in [Output 75.2.6](#) for an example.

### Inverse Predicted Probability Plot

For the binomial model, the response variable is a probability. An estimate of the dose level  $\hat{x}_1$  needed for a response of  $p$  is given by

$$\hat{x}_1 = (F^{-1}(p) - \mathbf{x}'_{-1}\hat{\mathbf{b}}_{-1})/\hat{b}_1$$

where  $F$  is the cumulative distribution function used to model the probability,  $\mathbf{x}_{-1}$  is the vector of the rest of the covariates,  $\hat{\mathbf{b}}_{-1}$  is the vector of the estimated parameters corresponding to  $\mathbf{x}_{-1}$ , and  $\hat{b}_1$  is the estimated parameter for the dose variable of interest.

To plot  $\hat{x}_1$  as a function of  $p$ ,  $\mathbf{x}_{-1}$  must be specified. You can use the XDATA= option to provide the values of  $\mathbf{x}_{-1}$  (see the XDATA= option in the PROC PROBIT statement for details), or use the default values that follow these rules:

- If the effect contains a continuous variable (or variables), the overall mean of this effect is used.
- If the effect is a single classification variable, the highest level of the variable is used.

[Output 75.4.12](#) in [Example 75.4](#) shows an inverse predicted probability plot.

### Linear Predictor Plot

For both binomial models and multinomial models, the linear predictor  $\mathbf{x}'\mathbf{b}$  can be plotted against the first single continuous variable (dose variable) in the MODEL statement.

Let  $x_1$  be the covariate of the dose variable,  $\mathbf{x}_{-1}$  be the vector of the rest of the covariates,  $\hat{\mathbf{b}}_{-1}$  be the vector of estimated parameters corresponding to  $\mathbf{x}_{-1}$ , and  $\hat{b}_1$  be the estimated parameter for the dose variable of interest.

To plot  $\hat{\mathbf{x}}'\mathbf{b}$  as a function of  $x_1$ ,  $\mathbf{x}_{-1}$  must be specified. You can use the XDATA= option to provide the values of  $\mathbf{x}_{-1}$  (see the XDATA= option in the PROC PROBIT statement for details), or use the default values that follow these rules:

- If the effect contains a continuous variable (or variables), the overall mean of this effect is used.
- If the effect is a single classification variable, the highest level of the variable is used.

For the multinomial model, you can use the LEVEL= suboption to specify the levels for which the linear predictor lines are plotted.

The confidence limits for the predicted values are only available for the binomial model. [Output 75.4.13](#) in [Example 75.4](#) shows a linear predictor plot for a binomial model.

## Predicted Probability Plot

The predicted probability is

$$\hat{p} = C + (1 - C)F(\mathbf{x}'\hat{\mathbf{b}})$$

for the binomial model and

$$\begin{aligned}\hat{p}_1 &= C + (1 - C)F(\mathbf{x}'\hat{\mathbf{b}}) \\ \hat{p}_j &= (1 - C)(F(\hat{a}_j + \mathbf{x}'\hat{\mathbf{b}}) - F(\hat{a}_{j-1} + \mathbf{x}'\hat{\mathbf{b}})), \quad j = 2, \dots, k - 1 \\ \hat{p}_k &= (1 - C)(1 - F(\hat{a}_{k-1} + \mathbf{x}'\hat{\mathbf{b}}))\end{aligned}$$

for the multinomial model with  $k$  response levels, where  $F$  is the cumulative distribution function used to model the probability,  $\mathbf{x}'$  is the vector of the covariates,  $\hat{a}_j$  are the estimated ordinal intercepts with  $\hat{a}_1 = 0$ ,  $C$  is the threshold parameter, either known or estimated from the model, and  $\hat{\mathbf{b}}'$  is the vector of estimated parameters.

To plot  $\hat{p}$  (or  $\hat{p}_j$ ) as a function of a continuous variable  $x_1$ , the remaining covariates  $\mathbf{x}_{-1}$  must be specified. You can use the XDATA= option to provide the values of  $\mathbf{x}_{-1}$  (see the XDATA= option in the PROC PROBIT statement for details), or use the default values that follow these rules:

- If the effect contains a continuous variable (or variables), the overall mean of this effect is used.
- If the effect is a single classification variable, the highest level of the variable is used.

For the multinomial model, you can use the LEVEL= suboption to specify the levels for which the linear predictor lines are plotted.

Confidence limits are plotted only for the binomial model. [Output 75.1.7](#) in [Example 75.1](#) shows a predicted probability plot for a binomial model; and [Output 75.2.3](#) in [Example 75.2](#) shows a predicted probability plot for a multinomial model.

## Examples: PROBIT Procedure

### Example 75.1: Dosage Levels

In this example, Dose is a variable representing the level of a stimulus, N represents the number of subjects tested at each level of the stimulus, and Response is the number of subjects responding to that level of the stimulus. Both probit and logit response models are fit to the data. The LOG10 option in the PROC PROBIT statement requests that the log base 10 of Dose is used as the independent variable. Specifically, for a given level of Dose, the probability  $p$  of a positive response is modeled as

$$p = \Pr(\text{Response}) = F(b_0 + b_1 \times \log_{10}(\text{Dose}))$$

The probabilities are estimated first by using the normal distribution function (the default) and then by using the logistic distribution function. Note that, in this model specification, the natural rate is assumed to be zero.

The LACKFIT option specifies lack-of-fit tests and the INVERSECL option specifies inverse confidence limits.

In the DATA step that reads the data, a number of observations are generated that have a missing value for the response. Although the PROBIT procedure does not use the observations with the missing values to fit the model, it does give predicted values for all nonmissing sets of independent variables. These data points fill in the plot of fitted and observed values in the logistic model displayed in [Output 75.1.7](#). The plot, requested with the PLOT=PREDPLOT option, displays the estimated logistic cumulative distribution function and the observed response rates.

The following statements produce [Output 75.1.1](#):

```
data a;
 infile cards eof=eof;
 input Dose N Response @@;
 Observed= Response/N;
 output;
 return;
eof: do Dose=0.5 to 7.5 by 0.25;
 output;
 end;
 datalines;
1 10 1 2 12 2 3 10 4 4 10 5
5 12 8 6 10 8 7 10 10
;

ods graphics on;

proc probit log10;
 model Response/N=Dose / lackfit inversecl itprint;
 output out=B p=Prob std=std xbeta=xbeta;
run;
```

**Output 75.1.1** Probit Analysis with Normal Distribution

| The Probit Procedure                      |       |               |              |              |
|-------------------------------------------|-------|---------------|--------------|--------------|
| Iteration History for Parameter Estimates |       |               |              |              |
| Iter                                      | Ridge | Loglikelihood | Intercept    | Log10 (Dose) |
| 0                                         | 0     | -51.292891    | 0            | 0            |
| 1                                         | 0     | -37.881166    | -1.355817008 | 2.635206083  |
| 2                                         | 0     | -37.286169    | -1.764939171 | 3.3408954936 |
| 3                                         | 0     | -37.280389    | -1.812147863 | 3.4172391614 |
| 4                                         | 0     | -37.280388    | -1.812704962 | 3.418117919  |
| 5                                         | 0     | -37.280388    | -1.812704962 | 3.418117919  |

Output 75.1.1 *continued*

| Model Information                                  |                            |              |                |                       |            |            |
|----------------------------------------------------|----------------------------|--------------|----------------|-----------------------|------------|------------|
| Data Set                                           |                            |              |                | WORK.A                |            |            |
| Events Variable                                    |                            |              |                | Response              |            |            |
| Trials Variable                                    |                            |              |                | N                     |            |            |
| Number of Observations                             |                            |              |                | 7                     |            |            |
| Number of Events                                   |                            |              |                | 38                    |            |            |
| Number of Trials                                   |                            |              |                | 74                    |            |            |
| Name of Distribution                               |                            |              |                | Normal                |            |            |
| Log Likelihood                                     |                            |              |                | -37.28038802          |            |            |
| Last Evaluation of the Negative of the Gradient    |                            |              |                |                       |            |            |
|                                                    | Intercept                  |              | Log10 (Dose)   |                       |            |            |
|                                                    | 3.4349069E-7               |              | -2.09809E-8    |                       |            |            |
| Last Evaluation of the Negative of the Hessian     |                            |              |                |                       |            |            |
|                                                    |                            | Intercept    | Log10 (Dose)   |                       |            |            |
|                                                    | Intercept                  | 36.005280383 | 20.152675982   |                       |            |            |
|                                                    | Log10 (Dose)               | 20.152675982 | 13.078826305   |                       |            |            |
| Goodness-of-Fit Tests                              |                            |              |                |                       |            |            |
| Statistic                                          |                            | Value        | DF             | Value/DF              | Pr > ChiSq |            |
| Pearson Chi-Square                                 |                            | 3.6497       | 5              | 0.7299                | 0.6009     |            |
| L.R. Chi-Square                                    |                            | 4.6381       | 5              | 0.9276                | 0.4616     |            |
| Response-Covariate Profile                         |                            |              |                |                       |            |            |
|                                                    | Response Levels            |              | 2              |                       |            |            |
|                                                    | Number of Covariate Values |              | 7              |                       |            |            |
| Analysis of Maximum Likelihood Parameter Estimates |                            |              |                |                       |            |            |
| Parameter                                          | DF                         | Estimate     | Standard Error | 95% Confidence Limits | Chi-Square | Pr > ChiSq |
| Intercept                                          | 1                          | -1.8127      | 0.4493         | -2.6934 -0.9320       | 16.27      | <.0001     |
| Log10 (Dose)                                       | 1                          | 3.4181       | 0.7455         | 1.9569 4.8794         | 21.02      | <.0001     |
| Probit Model in Terms of Tolerance Distribution    |                            |              |                |                       |            |            |
|                                                    |                            | MU           |                | SIGMA                 |            |            |
|                                                    |                            | 0.53032254   |                | 0.29255866            |            |            |

**Output 75.1.1** *continued*

| Estimated Covariance Matrix<br>for Tolerance Parameters |           |           |
|---------------------------------------------------------|-----------|-----------|
|                                                         | MU        | SIGMA     |
| MU                                                      | 0.002418  | -0.000409 |
| SIGMA                                                   | -0.000409 | 0.004072  |

The  $p$ -values in the goodness-of-fit table of 0.6009 for the Pearson's chi-square and 0.4616 for the likelihood ratio chi-square indicate an adequate fit for the model fit with the normal distribution.

Tolerance distribution parameter estimates for the normal distribution indicate a mean tolerance for the population of 0.5303.

**Output 75.1.2** displays probit analysis with the logarithm of dose levels. The LD50 (ED50 for log dose) is 0.5303, the dose corresponding to a probability of 0.5. This is the same as the mean tolerance for the normal distribution.



**Output 75.1.2** Probit Analysis with Normal Distribution

| The Probit Procedure           |             |                     |         |
|--------------------------------|-------------|---------------------|---------|
| Probit Analysis on Log10(Dose) |             |                     |         |
| Probability                    | Log10(Dose) | 95% Fiducial Limits |         |
| 0.01                           | -0.15027    | -0.69518            | 0.07710 |
| 0.02                           | -0.07052    | -0.55766            | 0.13475 |
| 0.03                           | -0.01992    | -0.47064            | 0.17156 |
| 0.04                           | 0.01814     | -0.40534            | 0.19941 |
| 0.05                           | 0.04911     | -0.35233            | 0.22218 |
| 0.06                           | 0.07546     | -0.30731            | 0.24165 |
| 0.07                           | 0.09857     | -0.26793            | 0.25881 |
| 0.08                           | 0.11926     | -0.23273            | 0.27425 |
| 0.09                           | 0.13807     | -0.20080            | 0.28837 |
| 0.10                           | 0.15539     | -0.17147            | 0.30142 |
| 0.15                           | 0.22710     | -0.05086            | 0.35631 |
| 0.20                           | 0.28410     | 0.04369             | 0.40124 |
| 0.25                           | 0.33299     | 0.12343             | 0.44116 |
| 0.30                           | 0.37690     | 0.19348             | 0.47857 |
| 0.35                           | 0.41759     | 0.25658             | 0.51504 |
| 0.40                           | 0.45620     | 0.31429             | 0.55182 |
| 0.45                           | 0.49356     | 0.36754             | 0.58999 |
| 0.50                           | 0.53032     | 0.41693             | 0.63057 |
| 0.55                           | 0.56709     | 0.46296             | 0.67451 |
| 0.60                           | 0.60444     | 0.50618             | 0.72271 |
| 0.65                           | 0.64305     | 0.54734             | 0.77603 |
| 0.70                           | 0.68374     | 0.58745             | 0.83550 |
| 0.75                           | 0.72765     | 0.62776             | 0.90265 |
| 0.80                           | 0.77655     | 0.66999             | 0.98008 |
| 0.85                           | 0.83354     | 0.71675             | 1.07279 |
| 0.90                           | 0.90525     | 0.77313             | 1.19191 |
| 0.91                           | 0.92257     | 0.78646             | 1.22098 |
| 0.92                           | 0.94139     | 0.80083             | 1.25265 |
| 0.93                           | 0.96208     | 0.81653             | 1.28759 |
| 0.94                           | 0.98519     | 0.83394             | 1.32672 |
| 0.95                           | 1.01154     | 0.85367             | 1.37149 |
| 0.96                           | 1.04250     | 0.87669             | 1.42424 |
| 0.97                           | 1.08056     | 0.90480             | 1.48928 |
| 0.98                           | 1.13116     | 0.94189             | 1.57602 |
| 0.99                           | 1.21092     | 0.99987             | 1.71321 |

Output 75.1.3 displays probit analysis with dose levels. The ED50 for dose is 3.39 with a 95% confidence interval of (2.61, 4.27).

**Output 75.1.3** Probit Analysis with Normal Distribution

| The Probit Procedure    |          |                     |          |
|-------------------------|----------|---------------------|----------|
| Probit Analysis on Dose |          |                     |          |
| Probability             | Dose     | 95% Fiducial Limits |          |
| 0.01                    | 0.70750  | 0.20175             | 1.19427  |
| 0.02                    | 0.85012  | 0.27691             | 1.36380  |
| 0.03                    | 0.95517  | 0.33834             | 1.48444  |
| 0.04                    | 1.04266  | 0.39324             | 1.58274  |
| 0.05                    | 1.11971  | 0.44429             | 1.66793  |
| 0.06                    | 1.18976  | 0.49282             | 1.74443  |
| 0.07                    | 1.25478  | 0.53960             | 1.81473  |
| 0.08                    | 1.31600  | 0.58515             | 1.88042  |
| 0.09                    | 1.37427  | 0.62980             | 1.94252  |
| 0.10                    | 1.43019  | 0.67380             | 2.00181  |
| 0.15                    | 1.68696  | 0.88950             | 2.27147  |
| 0.20                    | 1.92353  | 1.10584             | 2.51906  |
| 0.25                    | 2.15276  | 1.32870             | 2.76161  |
| 0.30                    | 2.38180  | 1.56128             | 3.01000  |
| 0.35                    | 2.61573  | 1.80543             | 3.27374  |
| 0.40                    | 2.85893  | 2.06200             | 3.56306  |
| 0.45                    | 3.11573  | 2.33098             | 3.89038  |
| 0.50                    | 3.39096  | 2.61175             | 4.27138  |
| 0.55                    | 3.69051  | 2.90374             | 4.72619  |
| 0.60                    | 4.02199  | 3.20759             | 5.28090  |
| 0.65                    | 4.39594  | 3.52651             | 5.97077  |
| 0.70                    | 4.82770  | 3.86765             | 6.84706  |
| 0.75                    | 5.34134  | 4.24385             | 7.99189  |
| 0.80                    | 5.97787  | 4.67724             | 9.55169  |
| 0.85                    | 6.81617  | 5.20900             | 11.82480 |
| 0.90                    | 8.03992  | 5.93105             | 15.55653 |
| 0.91                    | 8.36704  | 6.11584             | 16.63320 |
| 0.92                    | 8.73752  | 6.32165             | 17.89163 |
| 0.93                    | 9.16385  | 6.55431             | 19.39034 |
| 0.94                    | 9.66463  | 6.82245             | 21.21881 |
| 0.95                    | 10.26925 | 7.13949             | 23.52275 |
| 0.96                    | 11.02811 | 7.52816             | 26.56066 |
| 0.97                    | 12.03830 | 8.03149             | 30.85201 |
| 0.98                    | 13.52585 | 8.74763             | 37.67206 |
| 0.99                    | 16.25233 | 9.99709             | 51.66627 |

The following statements request probit analysis of dosage levels with the logistic distribution:

```
proc probit log10 plot=predpplot;
 model Response/N=Dose / d=logistic inversecl;
 output out=B p=Prob std=std xbeta=xbeta;
run;
```

The regression parameter estimates in [Output 75.1.4](#) for the logistic model of  $-3.22$  and  $5.97$  are approximately  $\pi/\sqrt{3}$  times as large as those for the normal model.

**Output 75.1.4** Probit Analysis with Logistic Distribution

| The Probit Procedure                               |              |          |                |                       |         |            |            |
|----------------------------------------------------|--------------|----------|----------------|-----------------------|---------|------------|------------|
| Model Information                                  |              |          |                |                       |         |            |            |
| Data Set                                           | WORK.B       |          |                |                       |         |            |            |
| Events Variable                                    | Response     |          |                |                       |         |            |            |
| Trials Variable                                    | N            |          |                |                       |         |            |            |
| Number of Observations                             | 7            |          |                |                       |         |            |            |
| Number of Events                                   | 38           |          |                |                       |         |            |            |
| Number of Trials                                   | 74           |          |                |                       |         |            |            |
| Name of Distribution                               | Logistic     |          |                |                       |         |            |            |
| Log Likelihood                                     | -37.11065336 |          |                |                       |         |            |            |
| Analysis of Maximum Likelihood Parameter Estimates |              |          |                |                       |         |            |            |
| Parameter                                          | DF           | Estimate | Standard Error | 95% Confidence Limits |         | Chi-Square | Pr > ChiSq |
| Intercept                                          | 1            | -3.2246  | 0.8861         | -4.9613               | -1.4880 | 13.24      | 0.0003     |
| Log10(Dose)                                        | 1            | 5.9702   | 1.4492         | 3.1299                | 8.8105  | 16.97      | <.0001     |

Output 75.1.5 and Output 75.1.6 show that both the ED50 and the LD50 are similar to those for the normal model.

**Output 75.1.5** Probit Analysis with Logistic Distribution

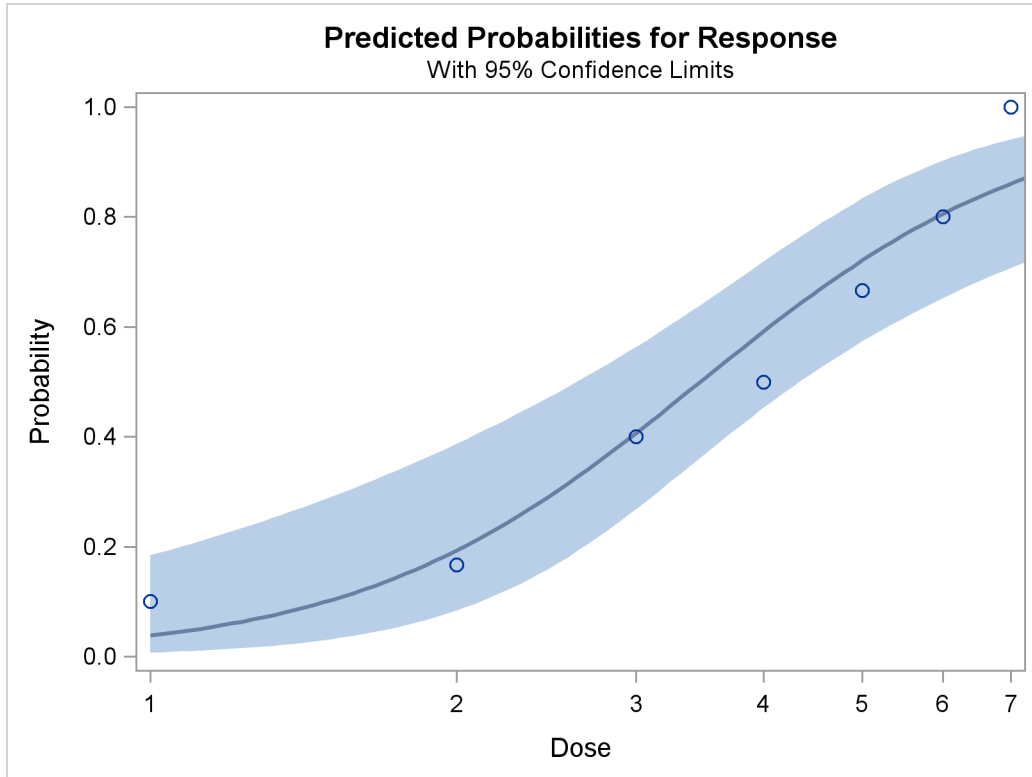
| The Probit Procedure           |             |                     |         |
|--------------------------------|-------------|---------------------|---------|
| Probit Analysis on Log10(Dose) |             |                     |         |
| Probability                    | Log10(Dose) | 95% Fiducial Limits |         |
| 0.01                           | -0.22955    | -0.97441            | 0.04234 |
| 0.02                           | -0.11175    | -0.75158            | 0.12404 |
| 0.03                           | -0.04212    | -0.62018            | 0.17265 |
| 0.04                           | 0.00780     | -0.52618            | 0.20771 |
| 0.05                           | 0.04693     | -0.45265            | 0.23533 |
| 0.06                           | 0.07925     | -0.39205            | 0.25826 |
| 0.07                           | 0.10686     | -0.34037            | 0.27796 |
| 0.08                           | 0.13103     | -0.29521            | 0.29530 |
| 0.09                           | 0.15259     | -0.25502            | 0.31085 |
| 0.10                           | 0.17209     | -0.21875            | 0.32498 |
| 0.15                           | 0.24958     | -0.07552            | 0.38207 |
| 0.20                           | 0.30792     | 0.03092             | 0.42645 |
| 0.25                           | 0.35611     | 0.11742             | 0.46451 |
| 0.30                           | 0.39820     | 0.19143             | 0.49932 |
| 0.35                           | 0.43644     | 0.25684             | 0.53275 |
| 0.40                           | 0.47221     | 0.31588             | 0.56619 |
| 0.45                           | 0.50651     | 0.36986             | 0.60089 |
| 0.50                           | 0.54013     | 0.41957             | 0.63807 |
| 0.55                           | 0.57374     | 0.46559             | 0.67894 |
| 0.60                           | 0.60804     | 0.50846             | 0.72474 |
| 0.65                           | 0.64381     | 0.54896             | 0.77673 |
| 0.70                           | 0.68205     | 0.58815             | 0.83637 |
| 0.75                           | 0.72414     | 0.62752             | 0.90582 |
| 0.80                           | 0.77233     | 0.66915             | 0.98876 |
| 0.85                           | 0.83067     | 0.71631             | 1.09242 |
| 0.90                           | 0.90816     | 0.77562             | 1.23343 |
| 0.91                           | 0.92766     | 0.79014             | 1.26931 |
| 0.92                           | 0.94922     | 0.80607             | 1.30912 |
| 0.93                           | 0.97339     | 0.82378             | 1.35391 |
| 0.94                           | 1.00100     | 0.84384             | 1.40523 |
| 0.95                           | 1.03332     | 0.86713             | 1.46546 |
| 0.96                           | 1.07245     | 0.89511             | 1.53864 |
| 0.97                           | 1.12237     | 0.93053             | 1.63228 |
| 0.98                           | 1.19200     | 0.97952             | 1.76329 |
| 0.99                           | 1.30980     | 1.06166             | 1.98569 |

**Output 75.1.6** Probit Analysis with Logistic Distribution

| The Probit Procedure    |          |                     |          |
|-------------------------|----------|---------------------|----------|
| Probit Analysis on Dose |          |                     |          |
| Probability             | Dose     | 95% Fiducial Limits |          |
| 0.01                    | 0.58945  | 0.10607             | 1.10241  |
| 0.02                    | 0.77312  | 0.17718             | 1.33058  |
| 0.03                    | 0.90757  | 0.23978             | 1.48817  |
| 0.04                    | 1.01813  | 0.29773             | 1.61327  |
| 0.05                    | 1.11413  | 0.35266             | 1.71922  |
| 0.06                    | 1.20018  | 0.40546             | 1.81244  |
| 0.07                    | 1.27896  | 0.45670             | 1.89654  |
| 0.08                    | 1.35218  | 0.50675             | 1.97379  |
| 0.09                    | 1.42100  | 0.55588             | 2.04572  |
| 0.10                    | 1.48625  | 0.60430             | 2.11339  |
| 0.15                    | 1.77656  | 0.84038             | 2.41030  |
| 0.20                    | 2.03199  | 1.07379             | 2.66961  |
| 0.25                    | 2.27043  | 1.31046             | 2.91416  |
| 0.30                    | 2.50152  | 1.55393             | 3.15736  |
| 0.35                    | 2.73172  | 1.80652             | 3.40996  |
| 0.40                    | 2.96627  | 2.06957             | 3.68292  |
| 0.45                    | 3.21006  | 2.34345             | 3.98927  |
| 0.50                    | 3.46837  | 2.62768             | 4.34578  |
| 0.55                    | 3.74746  | 2.92138             | 4.77466  |
| 0.60                    | 4.05546  | 3.22451             | 5.30573  |
| 0.65                    | 4.40366  | 3.53961             | 5.98041  |
| 0.70                    | 4.80891  | 3.87391             | 6.86079  |
| 0.75                    | 5.29836  | 4.24155             | 8.05044  |
| 0.80                    | 5.92009  | 4.66820             | 9.74455  |
| 0.85                    | 6.77126  | 5.20365             | 12.37149 |
| 0.90                    | 8.09391  | 5.96508             | 17.11715 |
| 0.91                    | 8.46559  | 6.16800             | 18.59129 |
| 0.92                    | 8.89644  | 6.39837             | 20.37592 |
| 0.93                    | 9.40575  | 6.66469             | 22.58957 |
| 0.94                    | 10.02317 | 6.97977             | 25.42292 |
| 0.95                    | 10.79732 | 7.36428             | 29.20549 |
| 0.96                    | 11.81534 | 7.85438             | 34.56521 |
| 0.97                    | 13.25466 | 8.52173             | 42.88232 |
| 0.98                    | 15.55972 | 9.53941             | 57.98207 |
| 0.99                    | 20.40815 | 11.52549            | 96.75820 |

The PLOT=PREDPLOT option together with the ODS GRAPHICS statement creates the plot of observed and fitted probabilities in [Output 75.1.7](#). The dashed line represent pointwise confidence bands for the probabilities.

**Output 75.1.7** Plot of Observed and Fitted Probabilities



## Example 75.2: Multilevel Response

In this example, two preparations, a standard preparation and a test preparation, are each given at several dose levels to groups of insects. The symptoms are recorded for each insect within each group, and two multilevel probit models are fit. Because the natural sort order of the three levels is not the same as the response order, the ORDER=DATA option is specified in the PROC PROBIT statement to get the desired order. The following statements fit two models:

```

data multi;
 input Prep $ Dose Symptoms $ N;
 LDose=log10(Dose);
 if Prep='test' then PrepDose=LDose;
 else PrepDose=0;
 datalines;
stand 10 None 33
stand 10 Mild 7
stand 10 Severe 10
stand 20 None 17
stand 20 Mild 13
stand 20 Severe 17
stand 30 None 14
stand 30 Mild 3
stand 30 Severe 28
stand 40 None 9
stand 40 Mild 8
stand 40 Severe 32
test 10 None 44
test 10 Mild 6
test 10 Severe 0
test 20 None 32
test 20 Mild 10
test 20 Severe 12
test 30 None 23
test 30 Mild 7
test 30 Severe 21
test 40 None 16
test 40 Mild 6
test 40 Severe 19
;

proc probit order=data data=multi;
 class Prep Symptoms;
 nonpara: model Symptoms=Prep LDose PrepDose / lackfit;
 weight N;
run;

proc probit order=data data=multi;
 class Prep Symptoms;
 parallel: model Symptoms=Prep LDose / lackfit;
 weight N;
run;

```

Results of these two models are shown in [Output 75.2.1](#) and [Output 75.2.2](#). The first model allows for nonparallelism between the dose response curves for the two preparations by inclusion of an interaction between Prep and LDose. The interaction term is labeled PrepDose in the “Analysis of Parameter Estimates” table. The results of this first model indicate that the parameter for the interaction term is not significant, having a Wald chi-square of 0.73. Also, since the first model is a generalization of the second, a likelihood ratio test statistic for this same parameter can be obtained by multiplying the difference in log likelihoods between the two models by 2. The value obtained,  $2 \times (-345.94 - (-346.31))$ , is 0.73. This is in close agreement with the Wald chi-square from the first model. The lack-of-fit test statistics for the two models do not indicate a problem with either fit.

**Output 75.2.1** Multilevel Response: Nonparallel Analysis

| The Probit Procedure                               |              |                  |                |                       |         |            |            |
|----------------------------------------------------|--------------|------------------|----------------|-----------------------|---------|------------|------------|
| Model Information                                  |              |                  |                |                       |         |            |            |
| Data Set                                           | WORK.MULTI   |                  |                |                       |         |            |            |
| Dependent Variable                                 | Symptoms     |                  |                |                       |         |            |            |
| Weight Variable                                    | N            |                  |                |                       |         |            |            |
| Number of Observations                             | 23           |                  |                |                       |         |            |            |
| Name of Distribution                               | Normal       |                  |                |                       |         |            |            |
| Log Likelihood                                     | -345.9401767 |                  |                |                       |         |            |            |
| Class Level Information                            |              |                  |                |                       |         |            |            |
| Name                                               | Levels       | Values           |                |                       |         |            |            |
| Prep                                               | 2            | stand test       |                |                       |         |            |            |
| Symptoms                                           | 3            | None Mild Severe |                |                       |         |            |            |
| Analysis of Maximum Likelihood Parameter Estimates |              |                  |                |                       |         |            |            |
| Parameter                                          | DF           | Estimate         | Standard Error | 95% Confidence Limits |         | Chi-Square | Pr > ChiSq |
| Intercept                                          | 1            | 3.8080           | 0.6252         | 2.5827                | 5.0333  | 37.10      | <.0001     |
| Intercept2                                         | 1            | 0.4684           | 0.0559         | 0.3589                | 0.5780  | 70.19      | <.0001     |
| Prep stand                                         | 1            | -1.2573          | 0.8190         | -2.8624               | 0.3479  | 2.36       | 0.1247     |
| Prep test                                          | 0            | 0.0000           | .              | .                     | .       | .          | .          |
| LDose                                              | 1            | -2.1512          | 0.3909         | -2.9173               | -1.3851 | 30.29      | <.0001     |
| PrepDose                                           | 1            | -0.5072          | 0.5945         | -1.6724               | 0.6580  | 0.73       | 0.3935     |



**Output 75.2.2** Multilevel Response: Parallel Analysis

| The Probit Procedure                               |             |                  |                |                       |         |            |            |
|----------------------------------------------------|-------------|------------------|----------------|-----------------------|---------|------------|------------|
| Model Information                                  |             |                  |                |                       |         |            |            |
| Data Set                                           | WORK.MULTI  |                  |                |                       |         |            |            |
| Dependent Variable                                 | Symptoms    |                  |                |                       |         |            |            |
| Weight Variable                                    | N           |                  |                |                       |         |            |            |
| Number of Observations                             | 23          |                  |                |                       |         |            |            |
| Name of Distribution                               | Normal      |                  |                |                       |         |            |            |
| Log Likelihood                                     | -346.306141 |                  |                |                       |         |            |            |
| Class Level Information                            |             |                  |                |                       |         |            |            |
| Name                                               | Levels      | Values           |                |                       |         |            |            |
| Prep                                               | 2           | stand test       |                |                       |         |            |            |
| Symptoms                                           | 3           | None Mild Severe |                |                       |         |            |            |
| Analysis of Maximum Likelihood Parameter Estimates |             |                  |                |                       |         |            |            |
| Parameter                                          | DF          | Estimate         | Standard Error | 95% Confidence Limits |         | Chi-Square | Pr > ChiSq |
| Intercept                                          | 1           | 3.4148           | 0.4126         | 2.6061                | 4.2235  | 68.50      | <.0001     |
| Intercept2                                         | 1           | 0.4678           | 0.0558         | 0.3584                | 0.5772  | 70.19      | <.0001     |
| Prep stand                                         | 1           | -0.5675          | 0.1259         | -0.8142               | -0.3208 | 20.33      | <.0001     |
| Prep test                                          | 0           | 0.0000           | .              | .                     | .       | .          | .          |
| LDose                                              | 1           | -2.3721          | 0.2949         | -2.9502               | -1.7940 | 64.68      | <.0001     |

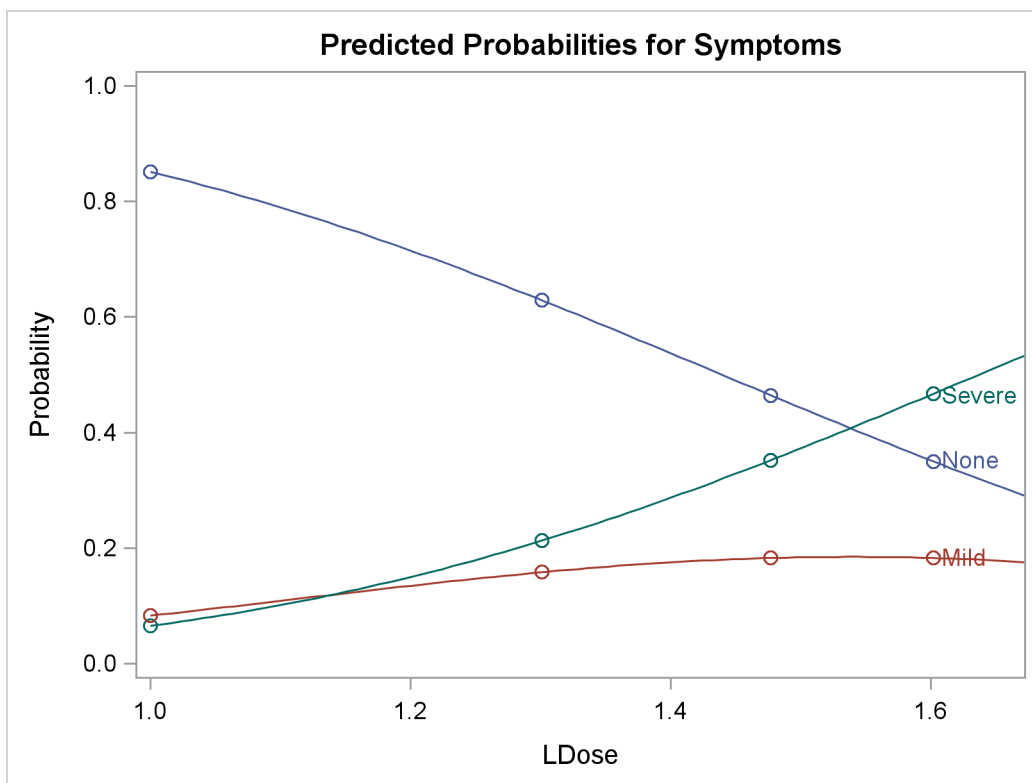
The negative coefficient associated with LDose indicates that the probability of having no symptoms (Symptoms='None') or no or mild symptoms (Symptoms='None' or Symptoms='Mild') decreases as LDose increases; that is, the probability of a severe symptom increases with LDose. This association is apparent for both treatment groups.

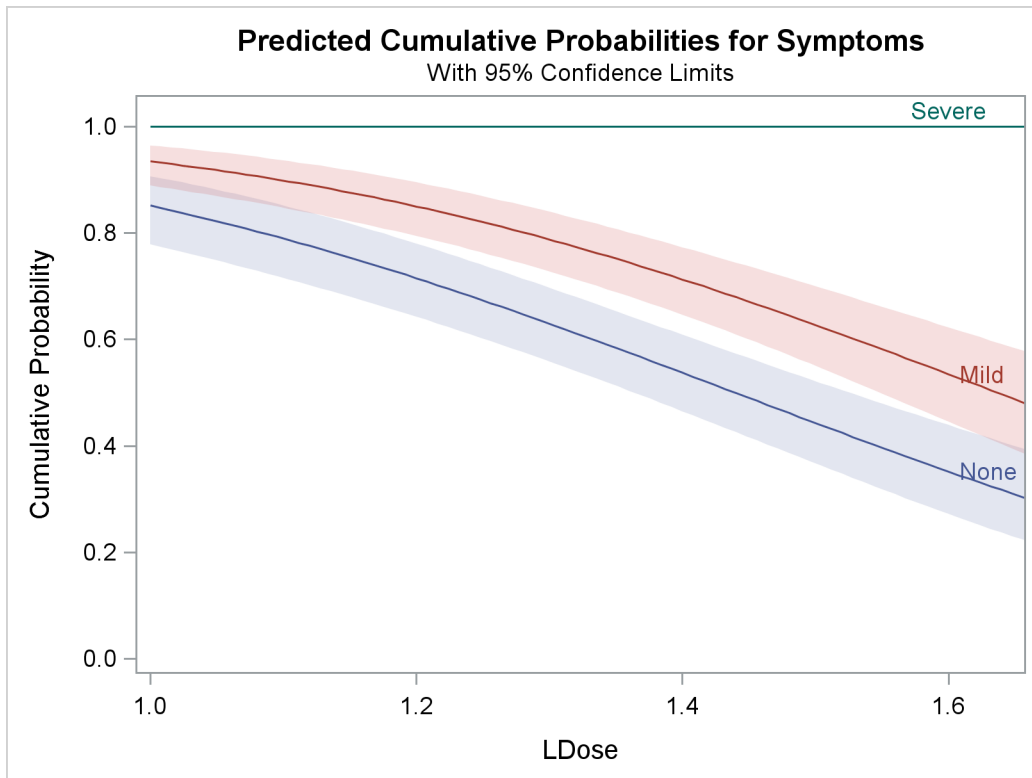
The negative coefficient associated with the standard treatment group (Prep = stand) indicates that the standard treatment is associated with more severe symptoms across all LDose values.

The following statements use the PLOTS= option to create the plot shown in [Output 75.2.3](#) and [Output 75.2.4](#). [Output 75.2.3](#) is the plot of the probabilities of the response taking on individual levels as a function of LDose. Since there are two covariates, LDose and Prep, the value of the classification variable Prep is fixed at the highest level, test. Instead of individual response level probabilities, the CDFPLOT option creates the plot of the cumulative response probabilities with confidence limits shown in [Output 75.2.4](#).

```
proc probit data=multi order=data
 plots=(predpplot(level=("None" "Mild" "Severe"))
 cdfplot(level=("None" "Mild" "Severe")));
class Prep Symptoms;
parallel: model Symptoms=Prep LDose / lackfit;
weight N;
run;
```

**Output 75.2.3** Plot of Predicted Probabilities for the Test Preparation Group



**Output 75.2.4** Plot of Predicted Cumulative Probabilities for the Test Preparation Group

The following statements use the XDATA= data set to create plots of predicted probabilities and cumulative probabilities with Prep set to the stand level. The resulting plots are shown in [Output 75.2.5](#) and [Output 75.2.6](#).

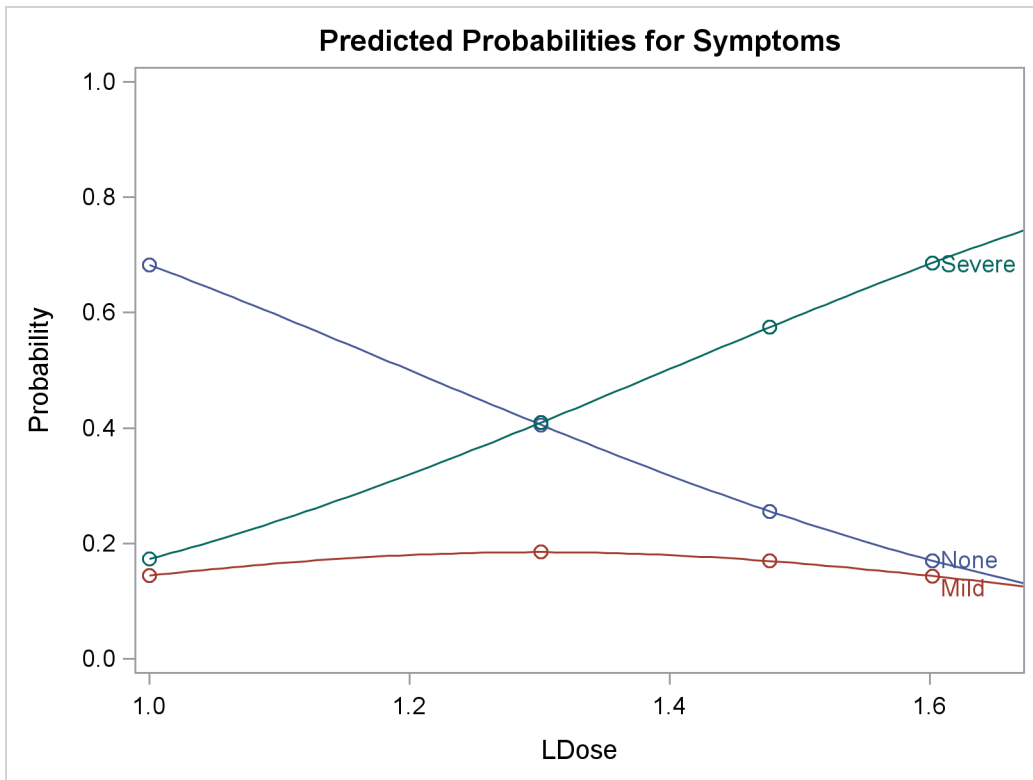
```

data xrow;
 input Prep $ Dose Symptoms $ N;
 LDose=log10(Dose);
 datalines;
stand 40 Severe 32
run;

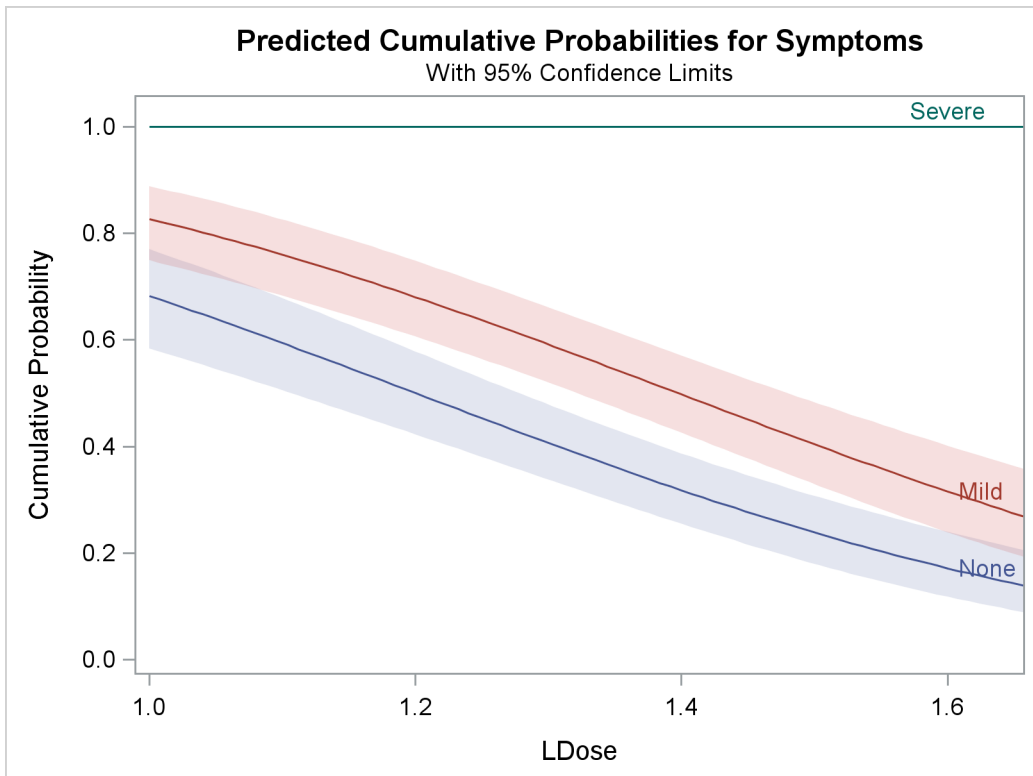
proc probit data=multi order=data xdata=xrow
 plots=(predpplot(level=("None" "Mild" "Severe"))
 cdfplot(level=("None" "Mild" "Severe")));
 class Prep Symptoms;
 parallel: model Symptoms=Prep LDose / lackfit;
 weight N;
run;

```

**Output 75.2.5** Plot of Predicted Probabilities for the Standard Preparation Group



**Output 75.2.6** Plot of Predicted Cumulative Probabilities for the Standard Preparation Group



### Example 75.3: Logistic Regression

In this example, a series of people are asked whether or not they would subscribe to a new newspaper. For each person, the variables `sex` (Female, Male), `age`, and `subs` (1=yes,0=no) are recorded. The PROBIT procedure is used to fit a logistic regression model to the probability of a positive response (subscribing) as a function of the variables `sex` and `age`. Specifically, the probability of subscribing is modeled as

$$p = \Pr(\text{subs} = 1) = F(b_0 + b_1 \times \text{sex} + b_2 \times \text{age})$$

where  $F$  is the cumulative logistic distribution function.

By default, the PROBIT procedure models the probability of the lower response level for binary data. One way to model  $\Pr(\text{subs} = 1)$  is to format the response variable so that the formatted value corresponding to `subs=1` is the lower level. The following statements format the values of `subs` as 1 = 'accept' and 0 = 'reject', so that PROBIT models  $\Pr(\text{accept}) = \Pr(\text{subs} = 1)$ . They produce [Output 75.3.1](#).

```
data news;
 input sex $ age subs @@;
 datalines;
Female 35 0 Male 44 0
Male 45 1 Female 47 1
Female 51 0 Female 47 0
Male 54 1 Male 47 1
Female 35 0 Female 34 0
Female 48 0 Female 56 1
Male 46 1 Female 59 1
Female 46 1 Male 59 1
Male 38 1 Female 39 0
Male 49 1 Male 42 1
Male 50 1 Female 45 0
Female 47 0 Female 30 1
Female 39 0 Female 51 0
Female 45 0 Female 43 1
Male 39 1 Male 31 0
Female 39 0 Male 34 0
Female 52 1 Female 46 0
Male 58 1 Female 50 1
Female 32 0 Female 52 1
Female 35 0 Female 51 0
;

proc format;
 value subscrib 1 = 'accept' 0 = 'reject';
run;

proc probit data=news;
 class subs sex;
 model subs=sex age / d=logistic itprint;
 format subs subscrib.;
run;
```

**Output 75.3.1** Logistic Regression of Subscription Status

| The Probit Procedure                      |       |               |              |              |              |
|-------------------------------------------|-------|---------------|--------------|--------------|--------------|
| Iteration History for Parameter Estimates |       |               |              |              |              |
| Iter                                      | Ridge | Loglikelihood | Intercept    | sexFemale    | age          |
| 0                                         | 0     | -27.725887    | 0            | 0            | 0            |
| 1                                         | 0     | -20.142659    | -3.634567629 | -1.648455751 | 0.1051634384 |
| 2                                         | 0     | -19.52245     | -5.254865196 | -2.234724956 | 0.1506493473 |
| 3                                         | 0     | -19.490439    | -5.728485385 | -2.409827238 | 0.1639621828 |
| 4                                         | 0     | -19.490303    | -5.76187293  | -2.422349862 | 0.1649007124 |
| 5                                         | 0     | -19.490303    | -5.7620267   | -2.422407743 | 0.1649050312 |
| 6                                         | 0     | -19.490303    | -5.7620267   | -2.422407743 | 0.1649050312 |

| Model Information      |              |
|------------------------|--------------|
| Data Set               | WORK.NEWS    |
| Dependent Variable     | subs         |
| Number of Observations | 40           |
| Name of Distribution   | Logistic     |
| Log Likelihood         | -19.49030281 |

| Class Level Information |        |               |
|-------------------------|--------|---------------|
| Name                    | Levels | Values        |
| subs                    | 2      | accept reject |
| sex                     | 2      | Female Male   |

| Last Evaluation of the Negative of the Gradient |              |              |            |
|-------------------------------------------------|--------------|--------------|------------|
|                                                 | Intercept    | sexFemale    | age        |
|                                                 | -5.95557E-12 | 8.768324E-10 | -1.6367E-8 |

| Last Evaluation of the Negative of the Hessian |              |              |              |
|------------------------------------------------|--------------|--------------|--------------|
|                                                | Intercept    | sexFemale    | age          |
| Intercept                                      | 6.4597397447 | 4.6042218284 | 292.04051848 |
| sexFemale                                      | 4.6042218284 | 4.6042218284 | 216.20829515 |
| age                                            | 292.04051848 | 216.20829515 | 13487.329973 |

Output 75.3.1 continued

| Analysis of Maximum Likelihood Parameter Estimates |        |          |                |                       |         |            |            |        |
|----------------------------------------------------|--------|----------|----------------|-----------------------|---------|------------|------------|--------|
| Parameter                                          | DF     | Estimate | Standard Error | 95% Confidence Limits |         | Chi-Square | Pr > ChiSq |        |
| Intercept                                          | 1      | -5.7620  | 2.7635         | -11.1783              | -0.3458 | 4.35       | 0.0371     |        |
| sex                                                | Female | 1        | -2.4224        | 0.9559                | -4.2959 | -0.5489    | 6.42       | 0.0113 |
| sex                                                | Male   | 0        | 0.0000         | .                     | .       | .          | .          | .      |
| age                                                | 1      | 0.1649   | 0.0652         | 0.0371                | 0.2927  | 6.40       | 0.0114     |        |

Output 75.3.1 shows that there appears to be an effect due to both the variables sex and age. The positive coefficient for age indicates that older people are more likely to subscribe than younger people. The negative coefficient for sex indicates that females are less likely to subscribe than males.

## Example 75.4: An Epidemiology Study

The data in this example, which are from an epidemiology study, consist of five variables: the number,  $r$ , of individuals surviving after an epidemic, out of  $n$  treated, for combinations of medicine dosage (dose), treatment (treat = A, B), and sex (sex = 0(Female), 1(Male)).

To see whether the two treatments have different effects on male and female individual survival rates, the interaction term between the two variables treat and sex is included in the model.

The following invocation of PROC PROBIT fits the binary probit model to the grouped data:

```
data epidemic;
 input treat$ dose n r sex @@;
 label dose = Dose;
 datalines;
A 2.17 142 142 0 A .57 132 47 1
A 1.68 128 105 1 A 1.08 126 100 0
A 1.79 125 118 0 B 1.66 117 115 1
B 1.49 127 114 0 B 1.17 51 44 1
B 2.00 127 126 0 B .80 129 100 1
;

data xval;
 input treat $ dose sex;
 datalines;
B 2. 1
;
```

```

proc probit optc lackfit covout data=epidemic
 outest = out1 xdata = xval
 Plots=(predpplot ippplot lpredplot);
 class treat sex;
 model r/n = dose treat sex sex*treat/corrb covb inversecl;
 output out = out2 p =p;
run;

```

The results of this analysis are shown in the outputs that follow.

Output 75.4.1 displays the table of level information for *all* classification variables in the CLASS statement.

**Output 75.4.1** Class Level Information

| The Probit Procedure    |        |        |
|-------------------------|--------|--------|
| Class Level Information |        |        |
| Name                    | Levels | Values |
| treat                   | 2      | A B    |
| sex                     | 2      | 0 1    |



Output 75.4.2 displays the table of parameter information for the effects in the MODEL statement.

**Output 75.4.2** Parameter Information

| Parameter Information |           |       |     |
|-----------------------|-----------|-------|-----|
| Parameter             | Effect    | treat | sex |
| Intercept             | Intercept |       |     |
| dose                  | dose      |       |     |
| treatA                | treat     | A     |     |
| treatB                | treat     | B     |     |
| sex0                  | sex       |       | 0   |
| sex1                  | sex       |       | 1   |
| treatAsex0            | treat*sex | A     | 0   |
| treatAsex1            | treat*sex | A     | 1   |
| treatBsex0            | treat*sex | B     | 0   |
| treatBsex1            | treat*sex | B     | 1   |

Output 75.4.3 displays background information about the model fit. Included are the name of the input data set, the response variables used, the numbers of observations, events, and trials, the type of distribution, and the final value of the log-likelihood function.

**Output 75.4.3** Model Information

| The Probit Procedure   |               |
|------------------------|---------------|
| Model Information      |               |
| Data Set               | WORK.EPIDEMIC |
| Events Variable        | r             |
| Trials Variable        | n             |
| Number of Observations | 10            |
| Number of Events       | 1011          |
| Number of Trials       | 1204          |
| Name of Distribution   | Normal        |
| Log Likelihood         | -387.2467391  |

Output 75.4.4 displays the table of goodness-of-fit tests requested with the LACKFIT option in the PROC PROBIT statement. Two goodness-of-fit statistics, the Pearson's chi-square statistic and the likelihood ratio chi-square statistic, are computed. The grouping method for computing these statistics can be specified by the AGGREGATE= option. The details can be found in the AGGREGATE= option, and an example can be found in the second part of this example. By default, the PROBIT procedure uses the covariates in the MODEL statement to do grouping. Observations with the same values of the covariates in the MODEL statement are grouped into cells and the two statistics are computed according to these cells. The total number of cells and the number of levels for the response variable are reported next in the "Response-Covariate Profile."

In this example, neither the Pearson's chi-square nor the log-likelihood ratio chi-square tests are significant at the 0.1 level, which is the default test level used by the PROBIT procedure. That means that the model, which includes the interaction of treat and sex, is suitable for this epidemiology data set. (Further investigation shows that models without the interaction of treat and sex are not acceptable by either test.)

#### Output 75.4.4 Goodness-of-Fit Tests and Response-Covariate Profile

| Goodness-of-Fit Tests |        |    |          |            |
|-----------------------|--------|----|----------|------------|
| Statistic             | Value  | DF | Value/DF | Pr > ChiSq |
| Pearson Chi-Square    | 4.9317 | 4  | 1.2329   | 0.2944     |
| L.R. Chi-Square       | 5.7079 | 4  | 1.4270   | 0.2220     |

| Response-Covariate Profile |    |
|----------------------------|----|
| Response Levels            | 2  |
| Number of Covariate Values | 10 |

Output 75.4.5 displays the Type III test results for all effects specified in the MODEL statement, which include the degrees of freedom for the effect, the Wald Chi-Square test statistic, and the *p*-value.

#### Output 75.4.5 Type III Tests

| Type III Analysis of Effects |    |                 |            |
|------------------------------|----|-----------------|------------|
| Effect                       | DF | Wald Chi-Square | Pr > ChiSq |
| dose                         | 1  | 42.1691         | <.0001     |
| treat                        | 1  | 16.1421         | <.0001     |
| sex                          | 1  | 1.7710          | 0.1833     |
| treat*sex                    | 1  | 13.9343         | 0.0002     |

Output 75.4.6 displays the table of parameter estimates for the model. The PROBIT procedure displays information for all the parameters of an effect. Degenerate parameters are indicated by 0 degree of freedom. Confidence intervals are computed for all parameters with nonzero degrees of freedom, including the natural threshold C if the OPTC option is specified in the PROC PROBIT statement. The confidence level can be specified by the ALPHA= option in the MODEL statement. The default confidence level is 95%.

**Output 75.4.6** Analysis of Parameter Estimates

| Analysis of Maximum Likelihood Parameter Estimates |     |          |                |                       |         |            |            |        |
|----------------------------------------------------|-----|----------|----------------|-----------------------|---------|------------|------------|--------|
| Parameter                                          | DF  | Estimate | Standard Error | 95% Confidence Limits |         | Chi-Square | Pr > ChiSq |        |
| Intercept                                          | 1   | -0.8871  | 0.3632         | -1.5991               | -0.1752 | 5.96       | 0.0146     |        |
| dose                                               | 1   | 1.6774   | 0.2583         | 1.1711                | 2.1837  | 42.17      | <.0001     |        |
| treat                                              | A   | 1        | -1.2537        | 0.2616                | -1.7664 | -0.7410    | 22.97      | <.0001 |
| treat                                              | B   | 0        | 0.0000         | .                     | .       | .          | .          |        |
| sex                                                | 0   | 1        | -0.4633        | 0.2289                | -0.9119 | -0.0147    | 4.10       | 0.0429 |
| sex                                                | 1   | 0        | 0.0000         | .                     | .       | .          | .          |        |
| treat*sex                                          | A 0 | 1        | 1.2899         | 0.3456                | 0.6126  | 1.9672     | 13.93      | 0.0002 |
| treat*sex                                          | A 1 | 0        | 0.0000         | .                     | .       | .          | .          |        |
| treat*sex                                          | B 0 | 0        | 0.0000         | .                     | .       | .          | .          |        |
| treat*sex                                          | B 1 | 0        | 0.0000         | .                     | .       | .          | .          |        |
| _C_                                                | 1   | 0.2735   | 0.0946         | 0.0881                | 0.4589  | .          | .          |        |

From [Table 75.4.6](#), you can see the following results:

- The variable dose has a significant positive effect on the survival rate.
- Individuals under treatment A have a lower survival rate.
- Male individuals have a higher survival rate.
- Female individuals under treatment A have a higher survival rate.

[Output 75.4.7](#) and [Output 75.4.8](#) display tables of estimated covariance matrix and estimated correlation matrix for estimated parameters with a nonzero degree of freedom, respectively. They are computed by the inverse of the Hessian matrix of the estimated parameters.

**Output 75.4.7** Estimated Covariance Matrix

| Estimated Covariance Matrix |           |           |           |           |            |
|-----------------------------|-----------|-----------|-----------|-----------|------------|
|                             | Intercept | dose      | treatA    | sex0      | treatAsex0 |
| Intercept                   | 0.131944  | -0.087353 | 0.053551  | 0.030285  | -0.067056  |
| dose                        | -0.087353 | 0.066723  | -0.047506 | -0.034081 | 0.058620   |
| treatA                      | 0.053551  | -0.047506 | 0.068425  | 0.036063  | -0.075323  |
| sex0                        | 0.030285  | -0.034081 | 0.036063  | 0.052383  | -0.063599  |
| treatAsex0                  | -0.067056 | 0.058620  | -0.075323 | -0.063599 | 0.119408   |
| _C_                         | -0.028073 | 0.018196  | -0.017084 | -0.008088 | 0.019134   |

| Estimated Covariance Matrix |           |
|-----------------------------|-----------|
|                             | _C_       |
| Intercept                   | -0.028073 |
| dose                        | 0.018196  |
| treatA                      | -0.017084 |
| sex0                        | -0.008088 |
| treatAsex0                  | 0.019134  |
| _C_                         | 0.008948  |

**Output 75.4.8** Estimated Correlation Matrix

| Estimated Correlation Matrix |           |           |           |           |            |
|------------------------------|-----------|-----------|-----------|-----------|------------|
|                              | Intercept | dose      | treatA    | sex0      | treatAsex0 |
| Intercept                    | 1.000000  | -0.930998 | 0.563595  | 0.364284  | -0.534227  |
| dose                         | -0.930998 | 1.000000  | -0.703083 | -0.576477 | 0.656744   |
| treatA                       | 0.563595  | -0.703083 | 1.000000  | 0.602359  | -0.833299  |
| sex0                         | 0.364284  | -0.576477 | 0.602359  | 1.000000  | -0.804154  |
| treatAsex0                   | -0.534227 | 0.656744  | -0.833299 | -0.804154 | 1.000000   |
| _C_                          | -0.817027 | 0.744699  | -0.690420 | -0.373565 | 0.585364   |

| Estimated Correlation Matrix |           |
|------------------------------|-----------|
|                              | _C_       |
| Intercept                    | -0.817027 |
| dose                         | 0.744699  |
| treatA                       | -0.690420 |
| sex0                         | -0.373565 |
| treatAsex0                   | 0.585364  |
| _C_                          | 1.000000  |

Output 75.4.9 displays the computed values and fiducial limits for the first single continuous variable dose in the MODEL statement, given the probability levels, without the effect of the natural threshold, and when the option INVERSECL in the MODEL statement is specified. If there is no single continuous variable in the MODEL specification but the INVERSECL option is specified, an error is reported.

**Output 75.4.9** Probit Analysis on Dose

| The Probit Procedure    |          |                     |          |
|-------------------------|----------|---------------------|----------|
| Probit Analysis on dose |          |                     |          |
| Probability             | dose     | 95% Fiducial Limits |          |
| 0.01                    | -0.85801 | -1.81301            | -0.33743 |
| 0.02                    | -0.69549 | -1.58167            | -0.21116 |
| 0.03                    | -0.59238 | -1.43501            | -0.13093 |
| 0.04                    | -0.51482 | -1.32476            | -0.07050 |
| 0.05                    | -0.45172 | -1.23513            | -0.02130 |
| 0.06                    | -0.39802 | -1.15888            | 0.02063  |
| 0.07                    | -0.35093 | -1.09206            | 0.05742  |
| 0.08                    | -0.30877 | -1.03226            | 0.09039  |
| 0.09                    | -0.27043 | -0.97790            | 0.12040  |
| 0.10                    | -0.23513 | -0.92788            | 0.14805  |
| 0.15                    | -0.08900 | -0.72107            | 0.26278  |
| 0.20                    | 0.02714  | -0.55706            | 0.35434  |
| 0.25                    | 0.12678  | -0.41669            | 0.43322  |
| 0.30                    | 0.21625  | -0.29095            | 0.50437  |
| 0.35                    | 0.29917  | -0.17477            | 0.57064  |
| 0.40                    | 0.37785  | -0.06487            | 0.63387  |
| 0.45                    | 0.45397  | 0.04104             | 0.69546  |
| 0.50                    | 0.52888  | 0.14481             | 0.75654  |
| 0.55                    | 0.60380  | 0.24800             | 0.81819  |
| 0.60                    | 0.67992  | 0.35213             | 0.88157  |
| 0.65                    | 0.75860  | 0.45879             | 0.94803  |
| 0.70                    | 0.84151  | 0.56985             | 1.01942  |
| 0.75                    | 0.93099  | 0.68770             | 1.09847  |
| 0.80                    | 1.03063  | 0.81571             | 1.18970  |
| 0.85                    | 1.14677  | 0.95926             | 1.30171  |
| 0.90                    | 1.29290  | 1.12867             | 1.45386  |
| 0.91                    | 1.32819  | 1.16747             | 1.49273  |
| 0.92                    | 1.36654  | 1.20867             | 1.53590  |
| 0.93                    | 1.40870  | 1.25284             | 1.58450  |
| 0.94                    | 1.45579  | 1.30084             | 1.64012  |
| 0.95                    | 1.50949  | 1.35397             | 1.70515  |
| 0.96                    | 1.57258  | 1.41443             | 1.78353  |
| 0.97                    | 1.65015  | 1.48626             | 1.88238  |
| 0.98                    | 1.75326  | 1.57833             | 2.01720  |
| 0.99                    | 1.91577  | 1.71776             | 2.23537  |

If the XDATA= option is used to input a data set for the independent variables in the MODEL statement, the PROBIT procedure uses these values for the independent variables other than the single continuous variable. Missing values are not permitted in the XDATA= data set for the independent variables, although the value for the single continuous variable is not used in the computing of the fiducial limits. A suitable valid value should be given. In the data set xval created by the SAS statements on page 6436, dose = 2.

Only one observation from the XDATA= data set is used to produce a probit analysis table for a combination of classification variable levels. If more than one observation is present in the XDATA= data set, only the last observation is used.

See the section “XDATA= SAS-data-set” on page 6411 for the default values for those effects other than the single continuous variable, for which the fiducial limits are computed.

In this example, there are two classification variables, treat and sex. Fiducial limits for the dose variable are computed for the highest level of the classification variables, treat = B and sex = 1, which is the default specification. Since these are the default values, you would get the same values and fiducial limits if you did not specify the XDATA= option in this example. The confidence level for the fiducial limits can be specified by the ALPHA= option in the MODEL statement. The default level is 95%.

If a LOG10 or LOG option is used in the PROC PROBIT statement, the values and the fiducial limits are computed for both the single continuous variable and its logarithm.

Output 75.4.10 displays the OUTEST= data set. All parameters for an effect are included. The name of a parameter is generated by combining the variable names and levels in the effect. The maximum length of a parameter name is 32.

**Output 75.4.10** Outest Data Set for Epidemiology Study

| Obs | MODEL      | NAME | TYPE  | DIST   | STATUS | LNLIKE    | r        | Intercept |          |
|-----|------------|------|-------|--------|--------|-----------|----------|-----------|----------|
| 1   | r          |      | PARMS | Normal | 0      | Converged | -387.247 | -1.00000  | -0.88714 |
| 2   | Intercept  |      | COV   | Normal | 0      | Converged | -387.247 | -0.88714  | 0.13194  |
| 3   | dose       |      | COV   | Normal | 0      | Converged | -387.247 | 1.67739   | -0.08735 |
| 4   | treatA     |      | COV   | Normal | 0      | Converged | -387.247 | -1.25367  | 0.05355  |
| 5   | treatB     |      | COV   | Normal | 0      | Converged | -387.247 | 0.00000   | 0.00000  |
| 6   | sex0       |      | COV   | Normal | 0      | Converged | -387.247 | -0.46329  | 0.03029  |
| 7   | sex1       |      | COV   | Normal | 0      | Converged | -387.247 | 0.00000   | 0.00000  |
| 8   | treatAsex0 |      | COV   | Normal | 0      | Converged | -387.247 | 1.28991   | -0.06706 |
| 9   | treatAsex1 |      | COV   | Normal | 0      | Converged | -387.247 | 0.00000   | 0.00000  |
| 10  | treatBsex0 |      | COV   | Normal | 0      | Converged | -387.247 | 0.00000   | 0.00000  |
| 11  | treatBsex1 |      | COV   | Normal | 0      | Converged | -387.247 | 0.00000   | 0.00000  |
| 12  | _C_        |      | COV   | Normal | 0      | Converged | -387.247 | 0.27347   | -0.02807 |

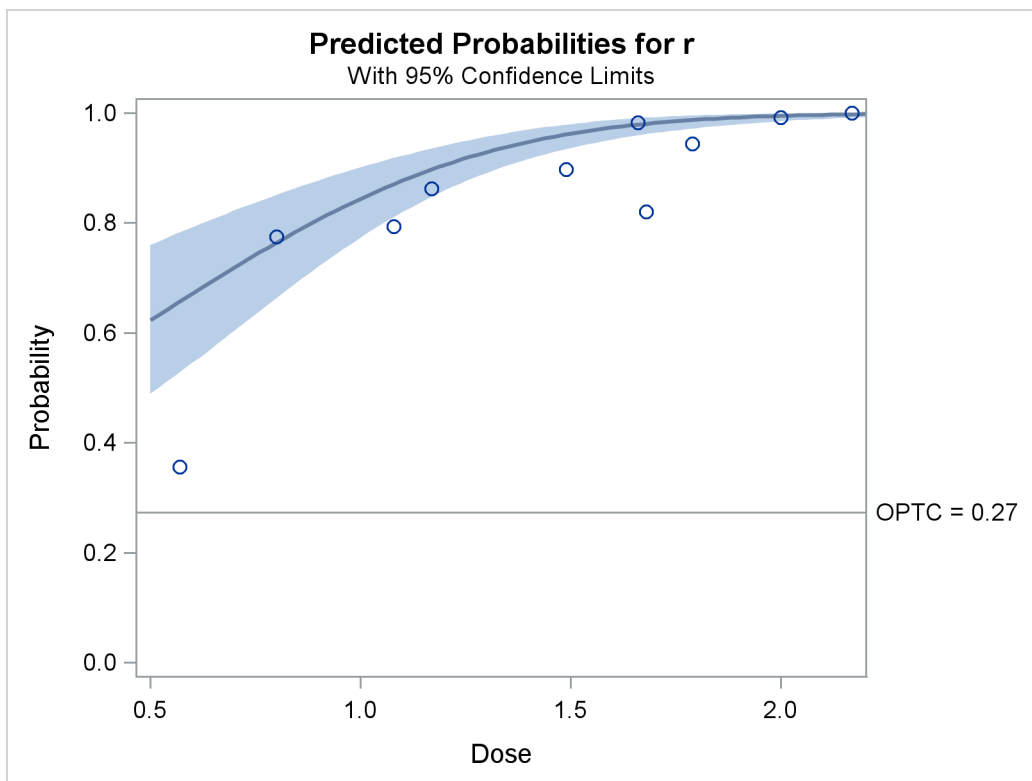
  

| Obs | treat    |          |   |          | treat |          |       |       | _C_ |          |
|-----|----------|----------|---|----------|-------|----------|-------|-------|-----|----------|
|     | dose     | treatA   | B | sex0     | sex1  | Asex0    | Asex1 | Bsex0 |     | Bsex1    |
| 1   | 1.67739  | -1.25367 | 0 | -0.46329 | 0     | 1.28991  | 0     | 0     | 0   | 0.27347  |
| 2   | -0.08735 | 0.05355  | 0 | 0.03029  | 0     | -0.06706 | 0     | 0     | 0   | -0.02807 |
| 3   | 0.06672  | -0.04751 | 0 | -0.03408 | 0     | 0.05862  | 0     | 0     | 0   | 0.01820  |
| 4   | -0.04751 | 0.06843  | 0 | 0.03606  | 0     | -0.07532 | 0     | 0     | 0   | -0.01708 |
| 5   | 0.00000  | 0.00000  | 0 | 0.00000  | 0     | 0.00000  | 0     | 0     | 0   | 0.00000  |
| 6   | -0.03408 | 0.03606  | 0 | 0.05238  | 0     | -0.06360 | 0     | 0     | 0   | -0.00809 |
| 7   | 0.00000  | 0.00000  | 0 | 0.00000  | 0     | 0.00000  | 0     | 0     | 0   | 0.00000  |
| 8   | 0.05862  | -0.07532 | 0 | -0.06360 | 0     | 0.11941  | 0     | 0     | 0   | 0.01913  |
| 9   | 0.00000  | 0.00000  | 0 | 0.00000  | 0     | 0.00000  | 0     | 0     | 0   | 0.00000  |
| 10  | 0.00000  | 0.00000  | 0 | 0.00000  | 0     | 0.00000  | 0     | 0     | 0   | 0.00000  |
| 11  | 0.00000  | 0.00000  | 0 | 0.00000  | 0     | 0.00000  | 0     | 0     | 0   | 0.00000  |
| 12  | 0.01820  | -0.01708 | 0 | -0.00809 | 0     | 0.01913  | 0     | 0     | 0   | 0.00895  |

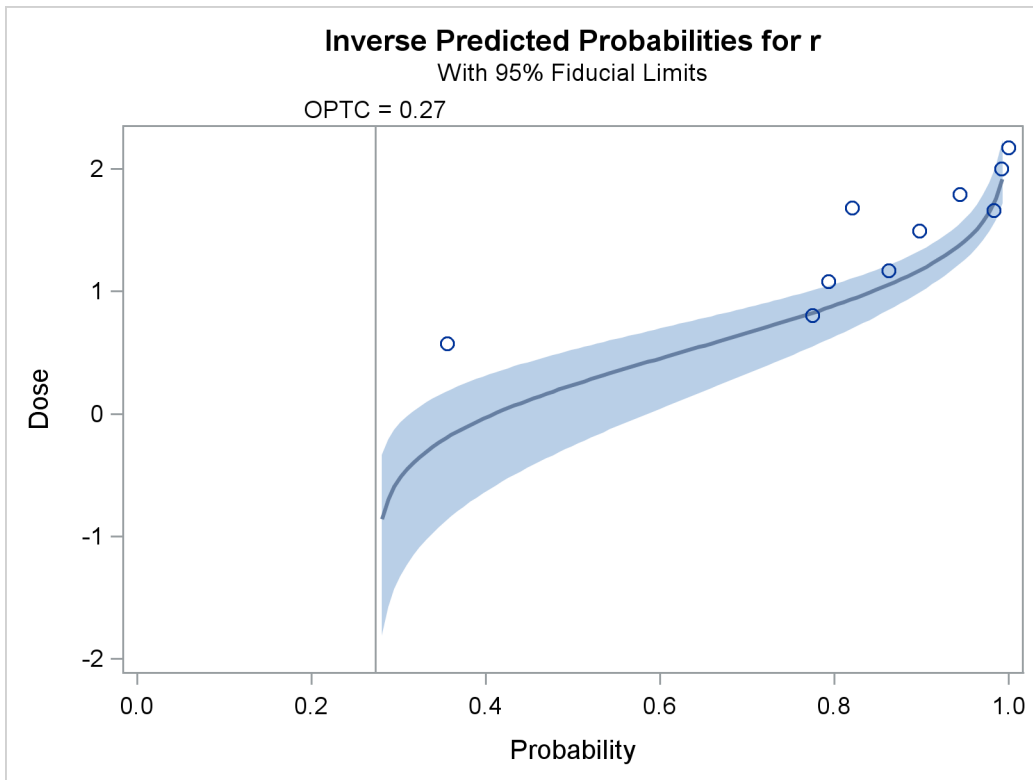
The plots in the following three outputs, [Output 75.4.11](#), [Output 75.4.12](#), and [Output 75.4.13](#), are generated by the PLOTS= option. The first plot, specified with the PREDPLOT option, is the plot of the predicted probability against the first single continuous variable dose in the MODEL statement. You can specify values of other independent variables in the MODEL statement by using an XDATA= data set or by using the default values.

The second plot, specified with the IPPPLOT option, is the inverse of the predicted probability plot with the fiducial limits. It should be pointed out that the fiducial limits are *not* just the inverse of the confidence limits in the predicted probability plot; see the section “[Inverse Confidence Limits](#)” on page 6410 for the computation of these limits. The third plot, specified with the LPREDPLOT option, is the plot of the linear predictor  $x'$ , against the first single continuous variable with the Wald confidence intervals.

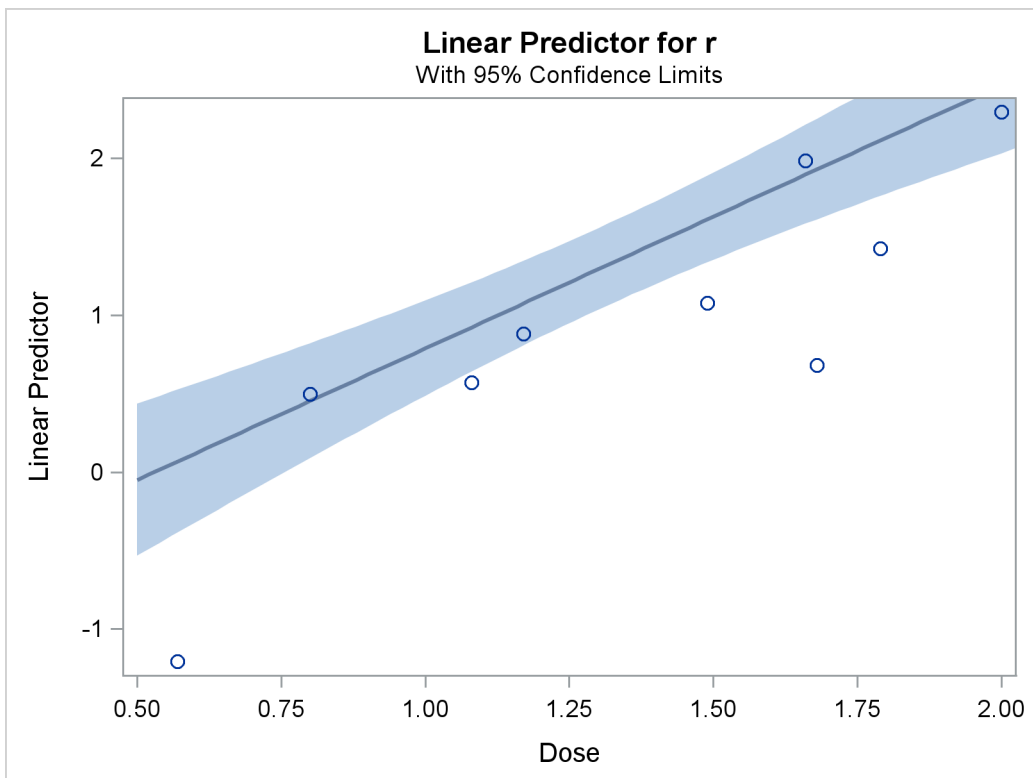
**Output 75.4.11** Predicted Probability Plot



**Output 75.4.12** Inverse Predicted Probability Plot



**Output 75.4.13** Linear Predictor Plot





When you combine the INEST= data set and the MAXIT= option in the MODEL statement, the PROBIT procedure can do prediction, if the parameterizations for the models used for the training data and the validation data are exactly the same. The following SAS statements show an example:

```

data validate;
 input treat $ dose sex n r group @@;
 datalines;
B 2.0 0 44 43 1 B 2.0 1 54 52 2
B 1.5 1 36 32 3 B 1.5 0 45 40 4
A 2.0 0 66 64 5 A 2.0 1 89 89 6
A 1.5 1 45 39 7 A 1.5 0 66 60 8
B 2.0 0 44 44 1 B 2.0 1 54 54 2
B 1.5 1 36 30 3 B 1.5 0 45 41 4
A 2.0 0 66 65 5 A 2.0 1 89 88 6
A 1.5 1 45 38 7 A 1.5 0 66 59 8
;

proc probit optc data=validate inest=out1;
 class treat sex;
 model r/n = dose treat sex sex*treat / maxit = 0;
 output out = out3 p =p;
run;

proc probit optc lackfit data=validate inest=out1;
 class treat sex;
 model r/n = dose treat sex sex*treat / aggregate = group;
 output out = out4 p =p;
run;

```

After the first invocation of PROC PROBIT, you have the estimated parameters and their covariance matrix in the data set OUTEST = Out1, and the fitted probabilities for the training data set epidemic in the data set OUTPUT = Out2. See [Output 75.4.10](#) for the data set Out1 and [Output 75.4.14](#) for the data set Out2.

The validation data are collected in data set validate. The second invocation of PROC PROBIT simply passes the estimated parameters from the training data set epidemic to the validation data set validate for prediction. The predicted probabilities are stored in the data set OUTPUT = Out3 (see [Output 75.4.15](#)). The third invocation of PROC PROBIT passes the estimated parameters as initial values for a new fit of the validation data set with the same model. Predicted probabilities are stored in the data set OUTPUT = Out4 (see [Output 75.4.16](#)). Goodness-of-fit tests are computed based on the cells grouped by the AGGREGATE= group variable. Results are shown in [Output 75.4.17](#).

**Output 75.4.14** Out2

| Obs | treat | dose | n   | r   | sex | p       |
|-----|-------|------|-----|-----|-----|---------|
| 1   | A     | 2.17 | 142 | 142 | 0   | 0.99272 |
| 2   | A     | 0.57 | 132 | 47  | 1   | 0.35925 |
| 3   | A     | 1.68 | 128 | 105 | 1   | 0.81899 |
| 4   | A     | 1.08 | 126 | 100 | 0   | 0.77517 |
| 5   | A     | 1.79 | 125 | 118 | 0   | 0.96682 |
| 6   | B     | 1.66 | 117 | 115 | 1   | 0.97901 |
| 7   | B     | 1.49 | 127 | 114 | 0   | 0.90896 |
| 8   | B     | 1.17 | 51  | 44  | 1   | 0.89749 |
| 9   | B     | 2.00 | 127 | 126 | 0   | 0.98364 |
| 10  | B     | 0.80 | 129 | 100 | 1   | 0.76414 |

**Output 75.4.15** Out3

| Obs | treat | dose | sex | n  | r  | group | p       |
|-----|-------|------|-----|----|----|-------|---------|
| 1   | B     | 2.0  | 0   | 44 | 43 | 1     | 0.98364 |
| 2   | B     | 2.0  | 1   | 54 | 52 | 2     | 0.99506 |
| 3   | B     | 1.5  | 1   | 36 | 32 | 3     | 0.96247 |
| 4   | B     | 1.5  | 0   | 45 | 40 | 4     | 0.91145 |
| 5   | A     | 2.0  | 0   | 66 | 64 | 5     | 0.98500 |
| 6   | A     | 2.0  | 1   | 89 | 89 | 6     | 0.91835 |
| 7   | A     | 1.5  | 1   | 45 | 39 | 7     | 0.74300 |
| 8   | A     | 1.5  | 0   | 66 | 60 | 8     | 0.91666 |
| 9   | B     | 2.0  | 0   | 44 | 44 | 1     | 0.98364 |
| 10  | B     | 2.0  | 1   | 54 | 54 | 2     | 0.99506 |
| 11  | B     | 1.5  | 1   | 36 | 30 | 3     | 0.96247 |
| 12  | B     | 1.5  | 0   | 45 | 41 | 4     | 0.91145 |
| 13  | A     | 2.0  | 0   | 66 | 65 | 5     | 0.98500 |
| 14  | A     | 2.0  | 1   | 89 | 88 | 6     | 0.91835 |
| 15  | A     | 1.5  | 1   | 45 | 38 | 7     | 0.74300 |
| 16  | A     | 1.5  | 0   | 66 | 59 | 8     | 0.91666 |

Output 75.4.16 Out4

| Obs | treat | dose | sex | n  | r  | group | p       |
|-----|-------|------|-----|----|----|-------|---------|
| 1   | B     | 2.0  | 0   | 44 | 43 | 1     | 0.98954 |
| 2   | B     | 2.0  | 1   | 54 | 52 | 2     | 0.98262 |
| 3   | B     | 1.5  | 1   | 36 | 32 | 3     | 0.86187 |
| 4   | B     | 1.5  | 0   | 45 | 40 | 4     | 0.90095 |
| 5   | A     | 2.0  | 0   | 66 | 64 | 5     | 0.98768 |
| 6   | A     | 2.0  | 1   | 89 | 89 | 6     | 0.98614 |
| 7   | A     | 1.5  | 1   | 45 | 39 | 7     | 0.88075 |
| 8   | A     | 1.5  | 0   | 66 | 60 | 8     | 0.88964 |
| 9   | B     | 2.0  | 0   | 44 | 44 | 1     | 0.98954 |
| 10  | B     | 2.0  | 1   | 54 | 54 | 2     | 0.98262 |
| 11  | B     | 1.5  | 1   | 36 | 30 | 3     | 0.86187 |
| 12  | B     | 1.5  | 0   | 45 | 41 | 4     | 0.90095 |
| 13  | A     | 2.0  | 0   | 66 | 65 | 5     | 0.98768 |
| 14  | A     | 2.0  | 1   | 89 | 88 | 6     | 0.98614 |
| 15  | A     | 1.5  | 1   | 45 | 38 | 7     | 0.88075 |
| 16  | A     | 1.5  | 0   | 66 | 59 | 8     | 0.88964 |

Output 75.4.17 Goodness-of-Fit Table

| The Probit Procedure  |  |        |    |          |            |
|-----------------------|--|--------|----|----------|------------|
| Goodness-of-Fit Tests |  |        |    |          |            |
| Statistic             |  | Value  | DF | Value/DF | Pr > ChiSq |
| Pearson Chi-Square    |  | 2.8101 | 2  | 1.4050   | 0.2454     |
| L.R. Chi-Square       |  | 2.8080 | 2  | 1.4040   | 0.2456     |

## Example 75.5: Model Postfitting Analysis

Recall the previous example of an epidemic study, in which the `treat*sex` interaction is statistically significant. Suppose you want to know whether such an effect is the same at different levels of the two categorical variables.

The following SAS statements fit a probit model and use the `SLICE` statement to request analysis of the two-way interaction term `treat*sex`:

```
proc probit data=epidemic;
 class treat sex;
 model r/n = dose treat sex treat*sex;
 slice treat*sex / diff;
 effectplot;
run;
```

Output 75.5.1 displays the test results for the interaction effect. As you can see, the difference between the two treatments is not significant among females.

**Output 75.5.1** Tests Conditional on treat\*sex

| The Probit Procedure          |           |            |            |
|-------------------------------|-----------|------------|------------|
| Chi-Square Test for treat*sex |           |            |            |
| Least Squares Means Slice     |           |            |            |
| Slice                         | Num<br>DF | Chi-Square | Pr > ChiSq |
| treat A                       | 1         | 18.52      | <.0001     |

| Chi-Square Test for treat*sex |           |            |            |
|-------------------------------|-----------|------------|------------|
| Least Squares Means Slice     |           |            |            |
| Slice                         | Num<br>DF | Chi-Square | Pr > ChiSq |
| treat B                       | 1         | 2.65       | 0.1035     |

| Chi-Square Test for treat*sex |           |            |            |
|-------------------------------|-----------|------------|------------|
| Least Squares Means Slice     |           |            |            |
| Slice                         | Num<br>DF | Chi-Square | Pr > ChiSq |
| sex 0                         | 1         | 0.00       | 0.9579     |

| Chi-Square Test for treat*sex |           |            |            |
|-------------------------------|-----------|------------|------------|
| Least Squares Means Slice     |           |            |            |
| Slice                         | Num<br>DF | Chi-Square | Pr > ChiSq |
| sex 1                         | 1         | 47.43      | <.0001     |

The DIFF option computes effect differences between groups within the same slice. Results are displayed in [Output 75.5.2](#).

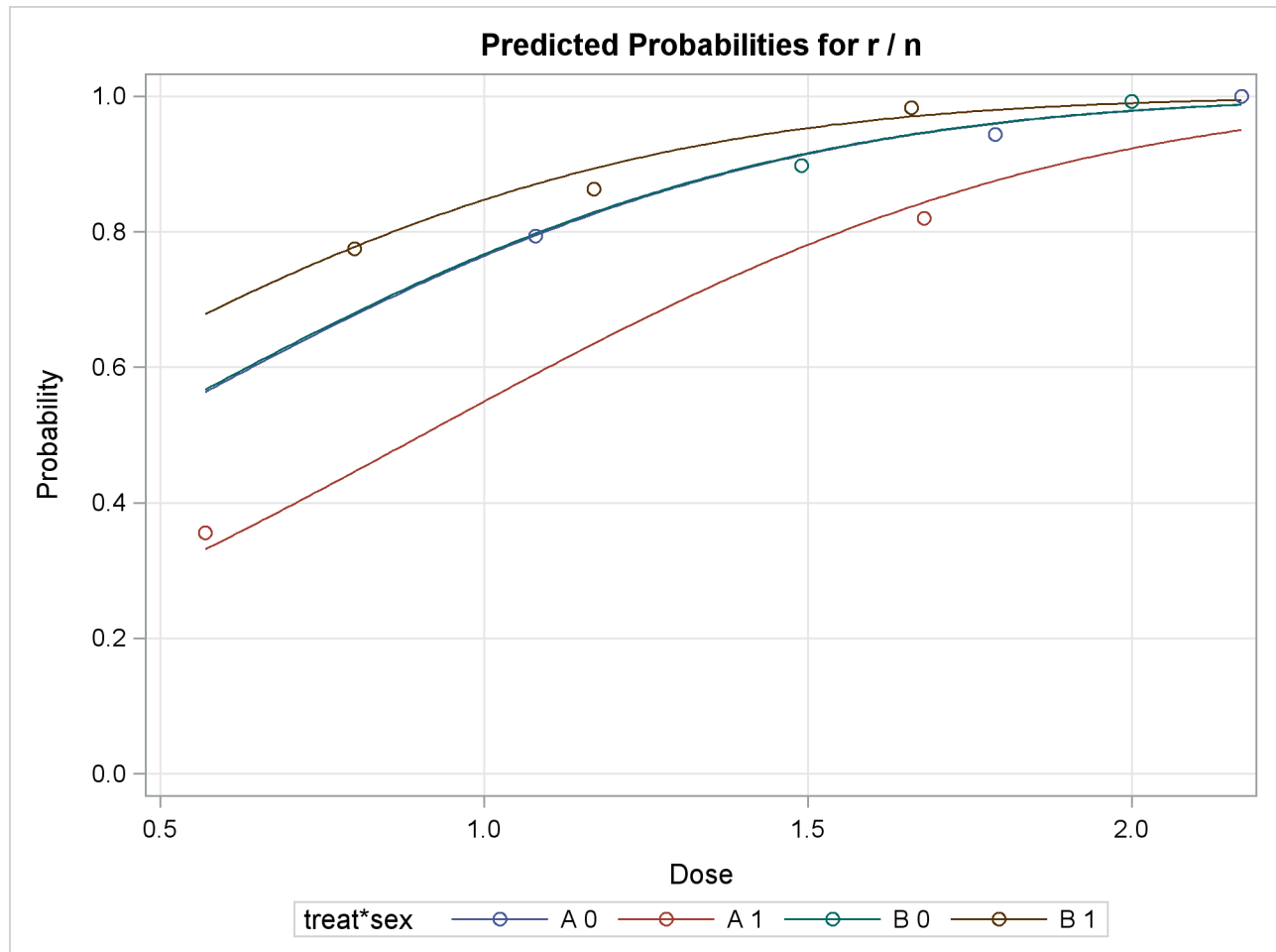
**Output 75.5.2** Effect Differences Conditional on treat\*sex

| Simple Differences of treat*sex Least Squares Means |     |      |          |                   |         |         |
|-----------------------------------------------------|-----|------|----------|-------------------|---------|---------|
| Slice                                               | sex | _sex | Estimate | Standard<br>Error | z Value | Pr >  z |
| treat A                                             | 0   | 1    | 0.5957   | 0.1384            | 4.30    | <.0001  |

Output 75.5.2 *continued*

| Simple Differences of treat*sex Least Squares Means |       |        |          |                |         |         |
|-----------------------------------------------------|-------|--------|----------|----------------|---------|---------|
| Slice                                               | sex   | _sex   | Estimate | Standard Error | z Value | Pr >  z |
| treat B                                             | 0     | 1      | -0.2956  | 0.1816         | -1.63   | 0.1035  |
| Simple Differences of treat*sex Least Squares Means |       |        |          |                |         |         |
| Slice                                               | treat | _treat | Estimate | Standard Error | z Value | Pr >  z |
| sex 0                                               | A     | B      | -0.00899 | 0.1702         | -0.05   | 0.9579  |
| Simple Differences of treat*sex Least Squares Means |       |        |          |                |         |         |
| Slice                                               | treat | _treat | Estimate | Standard Error | z Value | Pr >  z |
| sex 1                                               | A     | B      | -0.9003  | 0.1307         | -6.89   | <.0001  |

The EFFECTPLOT statement produces a predicted probability plot for dose by the four groups that are formed by the treat\*sex interaction. The plot is displayed in [Output 75.5.3](#). The two overlapping curves represent the two treatment groups for females, suggesting no treatment effect. It appears that males tend to respond to the two treatments differently: those on treatment B have a better survival rate, and those on treatment A have a worse chance of survival.

**Output 75.5.3** Predicted Probability versus Dose Level by treat\*sex

## References

- Agresti, A. (2002), *Categorical Data Analysis*, Second Edition, New York: John Wiley & Sons.
- Collett, D. (2003), *Modelling Binary Data*, Second Edition, London: Chapman & Hall.
- Cox, D. R. and Oakes, D. (1984), *Analysis of Survival Data*, London: Chapman & Hall.
- Finney, D. J. (1971), *Probit Analysis*, Third Edition, Cambridge: Cambridge University Press.
- Hubert, J. J., Bohidar, N. R., and Peace, K. E. (1988), "Assessment of Pharmacological Activity," *Biopharmaceutical Statistics for Drug Development*.



## Chapter 76

# The QUANTLIFE Procedure (Experimental)

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---

---

## Overview: QUANTLIFE Procedure

The QUANTLIFE procedure performs quantile regression analysis for survival data, where observations are not always directly observed.

Quantile regression (Koenker and Bassett 1978) is a type of regression analysis that explores how the conditional quantile of a response variable depends on its covariates. By estimating a set of conditional quantiles, you can gain more insight about the conditional distribution of the response given its covariates.



Quantile regression provides a flexible way to capture heterogeneous effects in the sense that the tails and the central location of the conditional distributions can vary differently with the covariates. Thus, quantile regression offers a powerful tool in survival analysis, where the lifetimes are skewed, and extreme survival times can be of special interest (Koenker and Geling 2001; Huang 2010).

When the observations are fully observed, you can use the QUANTREG procedure to fit a standard quantile regression model. See Chapter 77, “The QUANTREG Procedure,” for an introduction to the basic concepts of quantile regression analysis.

However, lifetime data often contain incomplete observations because of censoring (Klein and Moeschberger 2003; Hosmer, Lemeshow, and May 2008). When censoring occurs, the usual standard quantile regression approach can lead to biased estimates. Thus, special approaches have been developed that account for censoring and provide valid estimates. Portnoy (2003) proposed a method to estimate conditional quantile functions by generalizing the idea of the Kaplan-Meier estimator of the survival function. Peng and Huang (2008) developed a different quantile regression approach that is motivated by the Nelson-Aalen estimator of the cumulative hazard function. Both methods can be implemented with linear programming algorithms and both are available in the QUANTLIFE procedure. Like the standard quantile regression method for uncensored data, these two methods are distribution-free and apply to heteroscedastic data.

---

## Features

The QUANTLIFE procedure provides the following features:

- quantile regression methods for censored data that are based on generalizations of the Kaplan-Meier and the Nelson-Aalen estimator
- the interior point algorithm for parameter estimation, which uses parallel computing when multiple processors are available
- hypothesis tests for the regression parameter
- semiparametric quantile regression that uses spline effects
- survival plots, conditional quantile plots, and quantile process plots

---

## Quantile Regression

Suppose a data set contains observations  $(Y_i, x_i)$ , where  $Y_i$  is a dependent variable of interest (such as the survival time or some monotone transformation of the survival time) and  $x_i$  is a  $p \times 1$  vector of covariates.

You can use regression analysis to explore the relationship between a response  $Y_i$  and its predictor  $x_i$ . Classical linear regression estimates the conditional mean function  $E(Y_i|x_i)$  with a linear predictor  $x_i'\beta$ ; a linear quantile regression estimates the  $\tau$ th conditional quantile function  $Q_\tau(Y_i|x_i)$  with a different linear predictor  $x_i'\beta(\tau)$ , where the quantile level  $\tau$  ranges between 0 and 1. For example,  $x_i'\beta(0.95)$  is the linear predictor for the 0.95th quantile (commonly referred to as the 95th percentile).

The quantile regression coefficient  $\beta(\tau)$  can be estimated by minimizing the following objective function over  $b$ :

$$r(b) = \sum_{i=1}^n \rho_{\tau}(Y_i - x_i' b),$$

The loss function  $\rho_{\tau}(u)$  is defined as  $u(\tau - I(u < 0))$ , in contrast to the square loss function for classical linear regression.

When  $\tau = 0.5$ , the coefficient  $\beta(0.5)$  minimizes the sum of absolute residuals, which corresponds to median regression (or  $L_1$  regression).

The following set of regression quantiles is referred to as the *quantile process*, and it completely describes the conditional distribution of  $Y_i$  given the predictor  $x_i$ :

$$\{\beta(\tau) : \tau \in (0, 1)\}$$

When all the observations are observed, you can use the QUANTREG procedure to estimate the quantile function  $Q(\tau|X = x)$  and draw statistical inference about the regression parameters  $\beta(\tau)$ . See Chapter 77, “The QUANTREG Procedure,” for details.

However, when the observations are incomplete, as is the case with censored data in survival analysis, the classical quantile regression method is not appropriate. The QUANTLIFE procedure implements appropriate quantile regression methods to model the relationship between the response  $Y_i$  and the predictor  $x_i$ .

## Getting Started: QUANTLIFE Procedure

This example uses the human immunodeficiency virus (HIV) study data from Hosmer and Lemeshow (1999) to illustrate the basic features of PROC QUANTLIFE.

In this study, subjects were followed after a confirmed diagnosis of HIV. The primary goal was to evaluate the effect of various factors on the survival time. Two covariates for each subject were collected: age and history of prior intravenous drug use.

The following DATA step creates the data set HIV, which contains the variable Time (the follow-up time in days), the variable Status (with value 0 if Time was censored and 1 otherwise), the variable Drug (with value 1 for prior intravenous drug use and 0 otherwise), and the variable Age (the patient’s age in years at the beginning of the follow-up).

```
data HIV;
 input Time Age Drug Status;
 datalines;
 5 46 0 1
 6 35 1 0
 8 30 1 1
 3 30 1 1
 22 36 0 1
 1 32 1 0
 ... more lines ...
 1 34 1 1
;
```

You can use PROC QUANTLIFE to explore the relationship between the survival time and the two covariates at different quantiles.

Suppose you are interested in the median survivors and in the longer and shorter survivors. The following statements fit a linear model for the 25th, 50th, and 75th percentiles:

```
ods graphics on;
proc quantlife data=hiv log plots=quantplot seed=1268;
 class Drug;
 model Time*Status(0) = Drug Age / quantile=(0.25 0.5 0.75);
 Drug_Effect: test Drug;
run;
```

The LOG option fits a quantile regression model for the log of Time, as is done by an accelerated failure time (AFT) model in standard survival analysis. The SEED= option is specified to maintain reproducibility of the resampling method that is used for statistical inference.

The MODEL statement specifies the response variable, Time, and the censoring variable, Censor. The value that indicates censoring is enclosed in parentheses. The values of Time are considered to be censored if the value of Censor is 0; otherwise, they are considered to be event times. The QUANTILE= option requests a fit of the conditional quantile function  $Q(\tau|X = x)$  at the quantile levels 0.25, 0.5, and 0.75.

The TEST statement requests a test for the hypothesis that there is no Drug effect at each of the quantile levels.

Figure 76.1 displays basic model information. For example, you can see from Figure 76.1 that the response is log(Time), and the censoring rate is 20%.

**Figure 76.1** Model Fitting Information

| The QUANTLIFE Procedure          |        |              |
|----------------------------------|--------|--------------|
| Model Information                |        |              |
| Data Set                         |        | WORK.HIV     |
| Dependent Variable               |        | Log(Time)    |
| Censoring Variable               |        | Status       |
| Censoring Value(s)               |        | 0            |
| Number of Observations           |        | 100          |
| Method                           |        | Kaplan-Meier |
| Replications                     |        | 200          |
| Seed for Random Number Generator |        | 1268         |
| Class Level Information          |        |              |
| Name                             | Levels | Values       |
| Drug                             | 2      | 0 1          |

Figure 76.1 continued

| Summary of the Number of Event and Censored Values |       |          |                  |
|----------------------------------------------------|-------|----------|------------------|
| Total                                              | Event | Censored | Percent Censored |
| 100                                                | 80    | 20       | 20.00            |

Figure 76.2 displays the parameter estimates, which are computed using the default Kaplan-Meier-type estimator. See the section “Kaplan-Meier-Type Estimator for Censored Quantile Regression” on page 6468 for details. In addition, Figure 76.2 displays standard errors, 95% confidence limits,  $t$  values, and  $p$ -values that are computed by the default resampling method, exponentially weighted resampling. See the section “Exponentially Weighted Method” on page 6470.

A different quantile regression model is fitted for each quantile, and the first column (Quantile) in Figure 76.2 identifies the model for the parameter estimates. Age has a negative effect on survival time. You can use the parameter estimates to predict the survival time at the quantiles of interests. For example, the 75th percentile survival time for a person with no previous IV drug use at age 45 is

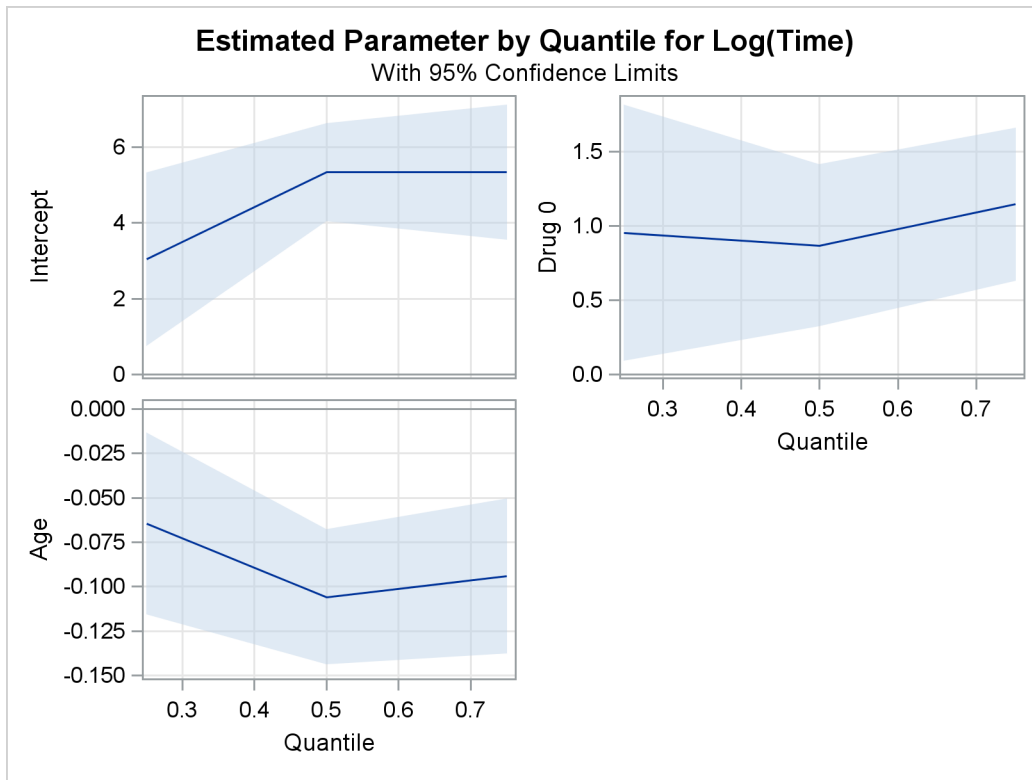
$$\exp(5.3351 + 1.1451 - 0.0941 \times 36) = 9.4 \text{ years}$$

Figure 76.2 Parameter Estimates

| Parameter Estimates |           |    |          |                |                       |         |         |         |        |
|---------------------|-----------|----|----------|----------------|-----------------------|---------|---------|---------|--------|
| Quantile            | Parameter | DF | Estimate | Standard Error | 95% Confidence Limits |         | t Value | Pr >  t |        |
| 0.2500              | Intercept | 1  | 3.0373   | 1.1680         | 0.7482                | 5.3265  | 2.60    | 0.0108  |        |
|                     | Drug      | 0  | 1        | 0.9516         | 0.4403                | 0.0887  | 1.8146  | 2.16    | 0.0331 |
|                     | Drug      | 1  | 0        | 0              | 0                     | 0       | 0       | .       | .      |
|                     | Age       | 1  | -0.0646  | 0.0261         | -0.1158               | -0.0135 | -2.48   | 0.0150  |        |
| 0.5000              | Intercept | 1  | 5.3351   | 0.6605         | 4.0406                | 6.6296  | 8.08    | <.0001  |        |
|                     | Drug      | 0  | 1        | 0.8681         | 0.2786                | 0.3219  | 1.4142  | 3.12    | 0.0024 |
|                     | Drug      | 1  | 0        | 0              | 0                     | 0       | 0       | .       | .      |
|                     | Age       | 1  | -0.1059  | 0.0194         | -0.1439               | -0.0679 | -5.46   | <.0001  |        |
| 0.7500              | Intercept | 1  | 5.3351   | 0.9091         | 3.5532                | 7.1170  | 5.87    | <.0001  |        |
|                     | Drug      | 0  | 1        | 1.1451         | 0.2625                | 0.6307  | 1.6596  | 4.36    | <.0001 |
|                     | Drug      | 1  | 0        | 0              | 0                     | 0       | 0       | .       | .      |
|                     | Age       | 1  | -0.0941  | 0.0223         | -0.1378               | -0.0505 | -4.23   | <.0001  |        |

The PLOTS=QUANTPLOT option in the PROC QUANTLIFE statement requests the quantile process plots, which are shown in Figure 76.3. The quantile process plot is a scatter plot of an estimated regression. Figure 76.3 shows that the estimated coefficients for the two covariates does not change much across quantiles.

**Figure 76.3** Estimated Parameters



The tests that are requested by the TEST statement are shown in Figure 76.4.

**Figure 76.4** Tests of Significance

| Test Drug_Effect Results |    |            |        |       |
|--------------------------|----|------------|--------|-------|
| Quantile                 | DF | Chi-Square | Pr >   | ChiSq |
| 0.2500                   | 1  | 4.67       | 0.0307 |       |
| 0.5000                   | 1  | 9.70       | 0.0018 |       |
| 0.7500                   | 1  | 19.03      | <.0001 |       |

The tests indicate that the coefficient of Drug is significantly different from 0 at the 25th, 50th, and 75th percentiles.

## Syntax: QUANTLIFE Procedure

The following statements are available in the QUANTLIFE procedure:

```

PROC QUANTLIFE < options > ;
 BASELINE < options > ;
 BY variables ;
 CLASS variables ;
 EFFECT name = effect-type (variables < / options >) ;
 MODEL response < * censor(list) > = < effects > < / options > ;
 OUTPUT < OUT=SAS-data-set > < keyword=name ... keyword=name > ;
 TEST effects < / options > ;
 WEIGHT variable ;

```

The PROC QUANTLIFE and MODEL statements are required. The PROC QUANTLIFE statement invokes the procedure. The CLASS statement specifies which explanatory variables are treated as categorical. The MODEL statement specifies the variables to be used in the regression. You can specify main effects and interaction terms in the MODEL statement, as you can in the GLM procedure (Chapter 42, “The GLM Procedure.”) The OUTPUT statement creates an output data set to contain predicted values, residuals, and estimated standard errors. The TEST statement requests linear tests for the model parameters. The WEIGHT statement identifies a variable in the input data set whose values are used to weight the observations. In one invocation of PROC QUANTLIFE, multiple OUTPUT and TEST statements are allowed.

The rest of this section provides detailed syntax information for each statement, beginning with the PROC QUANTLIFE statement. The remaining statements are covered in alphabetical order.

## PROC QUANTLIFE Statement

```

PROC QUANTLIFE < options > ;

```

The PROC QUANTLIFE statement invokes the QUANTLIFE procedure. Table 76.1 summarizes the options available in this statement.

**Table 76.1** Options Available in the PROC QUANTLIFE Statement

| Option                  | Description                                                                         |
|-------------------------|-------------------------------------------------------------------------------------|
| <b>Data Set Options</b> |                                                                                     |
| DATA=                   | Specifies the input SAS data set                                                    |
| OUTBOOTEST=             | Creates an output SAS data set for parameter estimates from resampled data sets     |
| <b>Basic Options</b>    |                                                                                     |
| ALPHA=                  | Specifies the confidence level                                                      |
| CI=                     | Specifies a resampling method for computing confidence interval and test statistics |
| LOG                     | Requests log transformation of the response                                         |
| METHOD=                 | Specifies a method to fit quantile regression                                       |
| NAMELEN=                | Specifies the length of effect names                                                |
| NREP=                   | Specifies the number of replications                                                |
| SEED=                   | Specifies the seed for the random number generator                                  |

Table 76.1 continued

| Option                       | Description                                                                 |
|------------------------------|-----------------------------------------------------------------------------|
| PLOTS=                       | Specifies the plots to be produced with ODS graphics                        |
| <b>Computational Options</b> |                                                                             |
| GRIDSIZE=                    | Specifies a step size for the grid for computing regression quantiles       |
| INITTAU=                     | Specifies the first quantile level for computing regression quantiles       |
| KAPPA=                       | Specifies the step-length parameter for the interior point algorithm        |
| MAXIT=                       | Specifies the maximum number of iterations for the interior point algorithm |
| TOLERANCE=                   | Specifies the convergence criterion of the interior point algorithm         |

You can specify the following *options* in the PROC QUANTLIFE statement.

**ALPHA=***value*

specifies the confidence level for the regression parameters. The *value* must be between 0 and 1. The default is ALPHA=0.05, which corresponds to a 95% confidence interval.

**CI=** EW | PW | NONE

specifies the method used to compute confidence intervals for regression parameters. In addition to confidence intervals, the QUANTLIFE procedure also computes standard errors, *t* values, and *p*-values for regression parameters. You can suppress these computations by specifying CI=NONE. The QUANTLIFE procedure provides two resampling methods for computing confidence intervals, the exponentially weighted (EW) method and the pairwise (PW) resampling method. See the section “Confidence Interval” on page 6470 methods for details. The default is CI=EW, which requests the exponentially weighted method.

**DATA=***SAS-data-set*

specifies the input SAS data set that the QUANTLIFE procedure uses. By default, the most recently created SAS data set is used.

**GRIDSIZE=***value*

specifies the step size for computing regression quantiles. The *value* must be between 0 and 1. See the section “Details: QUANTLIFE Procedure” on page 6468 for details.

**INITTAU=***value*

specifies the first quantile level for computing regression quantiles. The *value* must be between 0 and 1. See the section “Details: QUANTLIFE Procedure” on page 6468 for details.

**KAPPA=***value*

specifies the step-length parameter for the interior point algorithm. The *value* must be between 0 and 1. The interior point method used by the QUANTLIFE is identical to the interior point method used by the QUANTREG procedure. See the section Chapter 77.13, “Interior Point Algorithm,” for details. The default is KAPPA=0.99995.

**LOG**

requests that a log transformation of the response variable be performed before the model is fitted.

**MAXIT=*n***

specifies the maximum number of iterations for the interior point algorithm. The default is MAXIT=1000.

**METHOD= KM | NA**

specifies the method used to estimate the regression parameters. KM specifies the Kaplan-Meier-type method (see the section “[Kaplan-Meier-Type Estimator for Censored Quantile Regression](#)” on page 6468) and NA specifies the Nelson-Aalen-type method (see the section “[Nelson-Aalen-Type Estimator for Censored Quantile Regression](#)” on page 6469). The default is METHOD=KM.

**NAMELEN=*n***

specifies the length of effect names in tables and output data sets to be *n* characters, where *n* is a value between 20 and 200. The default is NAMELEN=20.

**NREP=*n***

specifies the number of replications to draw in the resampling method. The default is NREP=200.

**OUTBOOTEST=*SAS-data-set***

creates a data set to contain the parameter estimates from the resampled data sets.

See the section “[OUTBOOTEST= Output Data Set](#)” on page 6471 for a detailed description of the contents of the OUTBOOTEST= data set.

**PLOTS =(*plot-request* < ...*plot-request* >)**

requests various plots.

When you specify one *plot-request*, you can omit the parentheses around the plot request.

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;

proc quantlife plots=survival;
 model y=x1;
run;

ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS](#).”

You can specify one or more of the following *plot-requests*:

**ALL**

creates all appropriate plots.

**NONE**

suppresses all the plots in the procedure. Specifying this option is equivalent to disabling ODS Graphics for the entire procedure.



**QUANTILE**

plots the estimated quantile function for each combination of covariate values in the COVARIATES= data set specified in the BASELINE statement. If the COVARIATES= data set is not specified, the estimated quantile function is plotted for the reference set of covariate values that consists of reference levels for the CLASS variables and average values for the continuous variables. When the estimated quantile function is not monotonic, the quantile function (Chernozhukov, Fernandez-Val, and Galichon 2009) is rearranged to make it monotonic and then plotted.

**QUANTPLOT </ UNPACK >**

plots the regression quantile process. The estimated coefficient of each specified covariate effect is plotted as a function of the quantile level. You can use the UNPACK option to create individual process plots.

**SURVIVAL**

plots the estimated survival function for each combination of covariate values in the COVARIATES= data set specified in the BASELINE statement. If the COVARIATES= data set is not specified, the estimated survival function is plotted for the reference set of covariate values that consists of reference levels for the CLASS variables and average values for the continuous variables.

**SEED=number**

specifies a positive integer to start the pseudorandom number generator. The default is a value that is generated from reading the time of day from the computer's clock. However, to duplicate the results under identical situations, you must specify the same seed in subsequent runs of the QUANTLIFE procedure. The seed information is displayed in the "Model Information" table.

**TOLERANCE=value**

specifies the tolerance for the convergence criterion of the interior point algorithm. Both the QUANTLIFE procedure and the QUANTREG procedure use the duality gap as the convergence criterion. See Chapter 77.13, "Interior Point Algorithm," for details. The default is TOLERANCE=1E-8.

---

## BASELINE Statement

```
BASELINE < OUT=SAS-data-set> < COVARIATES=SAS-data-set> < keyword=name ... keyword=name>
;
```

The BASELINE statement creates an output data set to contain the survival function estimates or the conditional quantile function estimates for every set of covariates (x) in the COVARIATES= data set. If the COVARIATES= data set is not specified, PROC QUANTLIFE uses a reference set of covariates that consists of the reference levels for the CLASS variables and the average values for the continuous variables.

The following options are available in the BASELINE statement.

**OUT=SAS-data-set**

names the output data set. If you omit the OUT= option, the data set is created and given a default name by using the DATA*n* convention. See the section "OUT= Output Data Set in the BASELINE Statement" on page 6471 for more information.

**COVARIATES=*SAS-data-set***

names the SAS data set that contains the sets of explanatory variable values for which the quantities of interest are estimated. All variables in the COVARIATES= data set are copied to the OUT= data set. Thus, the variables in the COVARIATES= data set can be used to identify the covariate sets in the OUT= data set.

***keyword =name***

specifies the statistics to be included in the OUT= data set and assigns names to the variables that contain these statistics. Specify a *keyword* for each desired statistic, an equal sign, and the name of the variable for the statistic.

You can specify the following *keywords*:

**SURVIVAL**

specifies the estimated survival function.

**QUANTILE**

specifies the estimated quantile function.

**TAU**

specifies the quantile level, which is the complement of the survival function.

---

## BY Statement

**BY variables ;**

You can specify a BY statement with PROC QUANTLIFE to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the QUANTLIFE procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

---

## CLASS Statement

**CLASS** *variables* </ **TRUNCATE** > ;

The CLASS statement names the classification variables to be used in the model. Typical classification variables are Treatment, Sex, Race, Group, and Replication. If you use the CLASS statement, it must appear before the MODEL statement.

Classification variables can be either character or numeric. By default, class levels are determined from the entire set of formatted values of the CLASS variables.

In any case, you can use formats to group values into levels. See the discussion of the FORMAT procedure in the *Base SAS Procedures Guide* and the discussions of the FORMAT statement and SAS formats in *SAS Formats and Informats: Reference*.

You can specify the following option in the CLASS statement after a slash (/):

### TRUNCATE

specifies that class levels should be determined by using only up to the first 16 characters of the formatted values of CLASS variables.

---

## EFFECT Statement

**EFFECT** *name=effect-type* (*variables* </ *options* > ) ;

The EFFECT statement enables you to construct special collections of columns for design matrices. These collections are referred to as *constructed effects* to distinguish them from the usual model effects that are formed from continuous or classification variables, as discussed in the section “GLM Parameterization of Classification Variables and Effects” on page 383 in Chapter 19, “Shared Concepts and Topics.”

You can specify the following *effect-types*:

|                          |                                                                                                                                                                                                           |
|--------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>COLLECTION</b>        | is a collection effect that defines one or more variables as a single effect with multiple degrees of freedom. The variables in a collection are considered as a unit for estimation and inference.       |
| <b>LAG</b>               | is a classification effect in which the level that is used for a given period corresponds to the level in the preceding period.                                                                           |
| <b>MULTIMEMBER   MM</b>  | is a multimember classification effect whose levels are determined by one or more variables that appear in a CLASS statement.                                                                             |
| <b>POLYNOMIAL   POLY</b> | is a multivariate polynomial effect in the specified numeric variables.                                                                                                                                   |
| <b>SPLINE</b>            | is a regression spline effect whose columns are univariate spline expansions of one or more variables. A spline expansion replaces the original variable with an expanded or larger set of new variables. |

Table 76.2 summarizes the *options* available in the EFFECT statement.

**Table 76.2** EFFECT Statement Options

| Option                             | Description                                                                                                                                           |
|------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Collection Effects Options</b>  |                                                                                                                                                       |
| DETAILS                            | Displays the constituents of the collection effect                                                                                                    |
| <b>Lag Effects Options</b>         |                                                                                                                                                       |
| DESIGNROLE=                        | Names a variable that controls to which lag design an observation is assigned                                                                         |
| DETAILS                            | Displays the lag design of the lag effect                                                                                                             |
| NLAG=                              | Specifies the number of periods in the lag                                                                                                            |
| PERIOD=                            | Names the variable that defines the period                                                                                                            |
| WITHIN=                            | Names the variable or variables that define the group within which each period is defined                                                             |
| <b>Multimember Effects Options</b> |                                                                                                                                                       |
| NOEFFECT                           | Specifies that observations with all missing levels for the multi-member variables should have zero values in the corresponding design matrix columns |
| WEIGHT=                            | Specifies the weight variable for the contributions of each of the classification effects                                                             |
| <b>Polynomial Effects Options</b>  |                                                                                                                                                       |
| DEGREE=                            | Specifies the degree of the polynomial                                                                                                                |
| MDEGREE=                           | Specifies the maximum degree of any variable in a term of the polynomial                                                                              |
| STANDARDIZE=                       | Specifies centering and scaling suboptions for the variables that define the polynomial                                                               |
| <b>Spline Effects Options</b>      |                                                                                                                                                       |
| BASIS=                             | Specifies the type of basis (B-spline basis or truncated power function basis) for the spline expansion                                               |
| DEGREE=                            | Specifies the degree of the spline transformation                                                                                                     |
| KNOTMETHOD=                        | Specifies how to construct the knots for spline effects                                                                                               |

For more information about the syntax of these *effect-types* and how columns of constructed effects are computed, see the section “EFFECT Statement” on page 393 in Chapter 19, “Shared Concepts and Topics.”

---

## MODEL Statement

```
MODEL response < * censor(list) > = < effects > < / options > ;
```

The MODEL statement identifies the response variable, the optional censoring variable, and the explanatory effects, including covariates, main effects, interactions, and nested effects; see the section “Specification of Effects” on page 3324 of Chapter 42, “The GLM Procedure,” for more information. In the MODEL

statement, the response variable precedes the equal sign. This name can optionally be followed by an asterisk, the name of the censoring variable, and a list of censoring values (separated by blanks or commas if you list more than one value) enclosed in parentheses. If the censoring variable takes on one of these values, the corresponding failure time is considered to be censored. Following the equal sign are the explanatory effects (sometimes called independent variables or covariates) for the model.

The censoring variable must be numeric.

## Options

You can specify the following *options* after a slash (/).

### NOINT

specifies no intercept regression.

### QUANTILE=*number-list* | PROCESS

specifies the quantile levels of interest for quantile regression analysis. You can specify any number of quantile levels in the interval (0, 1). You can also compute the entire quantile process by specifying the PROCESS option.

If you do not specify the QUANTILE= option, the QUANTLIFE procedure fits a median regression, which corresponds to QUANTILE=0.5.

---

## OUTPUT Statement

**OUTPUT** < **OUT**=*SAS-data-set* > *keyword=name* < . . . *keyword=name* > ;

The OUTPUT statement creates a SAS data set to contain statistics that are calculated after fitting models for all quantiles specified by the QUANTILE= option in the MODEL statement. At least one specification of the form *keyword=name* is required.

All variables in the original data set are included in the new data set, along with the variables that are created. These new variables contain fitted values and estimated quantiles. If you want to create a permanent SAS data set, you must specify a two-level name (see the section “SAS Files” in *SAS Language Reference: Concepts* for more information about permanent SAS data sets).

The following specifications can appear in the OUTPUT statement:

**OUT**=*SAS-data-set* specifies the new data set. By default, the procedure uses the *DATA**n* convention to name the new data set. See the section “**OUT= Output Data Set in the OUTPUT Statement**” on page 6471 for more information.

*keyword=name* specifies the statistics to include in the output data set and gives names to the new variables. Specify a keyword for each desired statistic (see the following list of keywords), an equal sign, and the variable to contain the statistic.

You can specify the following *keywords*, which represent the indicated statistics:

- PREDICTED | P** specifies a variable to contain the predicted response.
- RESIDUAL | RES** specifies a variable to contain the residuals,  $y_i - x_i' \hat{\beta}(\tau)$ .
- SAMPLEWEIGHT | SW** specifies variables for sample weights from the bootstrap samples. For the  $i$ th sample, a column that contains the weights that are used for that sample is added. The name of this column is formed by appending an index  $i$  to the name that you specify. If you do not specify a name, then the default prefix is *sw*.
- STDP** specifies a variable to contain the estimates of the standard errors of the estimated response.

---

## TEST Statement

*<label:> TEST effects </options> ;*

In quantile regression analysis, you might be interested in testing whether a covariate effect is statistically significant for a given quantile. You can use the TEST statement to obtain a test for the canonical linear hypothesis concerning the parameters of the tested *effects*,

$$\beta_j = 0, \quad j = i_1, \dots, i_q$$

where  $q$  is the total number of parameters of the tested effects. The tested *effects* can be any set of effects in the MODEL statement.

You can include multiple TEST statements, provided that they appear after the MODEL statement. The optional *label*, which must be a valid SAS name, is used to identify output from the corresponding TEST statement. See the section “Testing Effects of Covariates” on page 6470 for more information about these tests.

---

## WEIGHT Statement

**WEIGHT** *variable* ;

The WEIGHT statement specifies a weight variable in the input data set.

To request weighted quantile regression, place the weights in a variable and specify the name in the WEIGHT statement. The values of the WEIGHT variable can be nonintegral and are not truncated. Observations with nonpositive or missing values for the weight variable do not contribute to the fit of the model. See the section Chapter 77.13, “Details: QUANTREG Procedure,” for more information about weighted quantile regression.

---

## Details: QUANTLIFE Procedure

---

### Notation for Censored Quantile Regression

Let  $T$  be a dependent variable, such as a survival time, and let  $x$  be a  $p \times 1$  covariate vector. Quantile regression methods focus on modeling the conditional quantile function,  $Q_\tau(T|x)$ , which is defined as

$$Q_\tau(T|x) = \inf\{t : P(T \leq t|x) = \tau\}, 0 < \tau < 1$$

For example,  $Q_{0.5}(T|x)$  is the conditional median quantile, and  $Q_{0.95}(T|x)$  is the conditional quantile function that corresponds to the 95th percentile.

A linear quantile regression model for  $Q_\tau(T|x)$  has the form  $x'\beta(\tau)$ . One of the advantages of quantile regression analysis is that the covariate effect  $\beta(\tau)$  can change with  $\tau$ . Unlike ordinary least squares regression, which estimates the conditional expectation function  $E(T|x)$ , quantile regression offers the flexibility to model the entire conditional distribution.

Given observations  $(T_i, x_i), i = 1, \dots, n$ , standard quantile regression estimates the regression coefficients  $\beta(\tau)$  by minimizing the following objective function over  $b$ :

$$r(b) = \sum_{i=1}^n \rho_\tau(T_i - x_i' b)$$

where  $\rho_\tau(u) = u(\tau - I(u < 0))$ .

However, in many applications, the responses  $T_i$  are subject to censoring. For example, in a biomedical study, censoring occurs when patients withdraw from the study or die from a cause that is unrelated to the disease being studied.

Let  $C_i$  denote the censoring variable. In the case of right-censoring, the triples  $(x_i, Y_i, \Delta_i)$  are observed, where  $Y_i = \min(T_i, C_i)$  and  $\Delta_i = I(T_i \leq C_i)$  are the observed response variable and the censoring indicator, respectively. Standard quantile regression leads to a biased estimator of the regression parameters  $\beta(\tau)$ .

The following sections describe two methods for estimating the quantile coefficient  $\beta(\tau)$  in the presence of right-censoring.

---

### Kaplan-Meier-Type Estimator for Censored Quantile Regression

Portnoy (2003) proposes the use of weighted quantile regression to sequentially estimate  $\beta(\tau_k)$  along the equally spaced grid  $0 < \tau_1 < \dots < \tau_M < 1$ . You can request this method by specifying the METHOD=KM option in the PROC QUANTLIFE statement. The grid points  $0 < \tau_1 < \dots < \tau_M < 1$  are equally spaced with  $\tau_1$  specified by the INITTAU= option and the step between adjacent grid points specified by the GRIDSIZE=option.

This method uses a weight function  $w_i(\tau)$  for each censored observation. The weight function is constructed as follows: Let  $\hat{\tau}_i$  be the first grid point at which  $x_i'\hat{\beta}(\tau_i) \geq C_i$  and  $x_i'\hat{\beta}(\tau_{i+1}) < C_i$ ; otherwise let  $\hat{\tau}_i = 1$ . When computing the  $\tau$ th quantile, assign weight  $w_i(\tau) = \frac{\tau - \hat{\tau}_i}{1 - \hat{\tau}_i}$  to the censored observation  $Y_i$  if  $\tau > \hat{\tau}_i$ ; otherwise assign  $w_i(\tau) = 1$ . The algorithm for computing  $\hat{\beta}(\tau_k), k = 1, \dots, M$  is as follows:

1. Compute  $\hat{\beta}(\tau_1)$  by using the standard quantile regression method.
2. For  $k = 2, \dots, M$ , obtain  $\hat{\beta}(\tau_k)$  sequentially by minimizing the following weighted quantile regression objective function:

$$r_w(b) = \sum_{\Delta_i=1} \rho_{\tau_k}(Y_i - x_i'b) + \sum_{\Delta_i=0} \{w_i(\tau_k) \rho_{\tau_k}(Y_i - x_i'b) + (1 - w_i(\tau_k)) \rho_{\tau_k}(Y^* - x_i'b)\}$$

where  $w_i(\tau_k)$  is the weight for the right-censored observation  $Y_i$  at computing  $\hat{\beta}(\tau_k)$ , and the complementary weight  $1 - w_i(\tau_k)$  are for  $Y^*$ , a large constant that is greater than all  $x_i'\hat{\beta}(\tau)$ .

The weighted quantile regression method is similar to Efron’s redistribution-of-mass idea (Efron 1967) for the Kaplan-Meier estimator.

Note that if all observations are uncensored,  $\hat{\beta}(\tau_k)$  is the same as the standard quantile regression estimator.

## Nelson-Aalen-Type Estimator for Censored Quantile Regression

Peng and Huang (2008) propose a method for censored quantile regression that is based on the Nelson-Aalen estimator of the cumulative hazard function. Let  $F_i(t|x) = P(T_i \leq t|x)$ ,  $\Lambda(t|x_i) = -\log(1 - F_i(t|x_i))$ , and  $N_i(t) = I\{\{T_i \leq t\} \text{ and } \{\Delta_i = 1\}\}$ . Then the following equation is a martingale process that is associated with the counting process  $N_i(t)$  (Fleming and Harrington 1991):

$$M_i(t) = N_i(t) - \Lambda(t \wedge Y_i|x)$$

Based on the martingale process, Peng and Huang (2008) derive the following estimating equation:

$$n^{-1/2} \sum_{i=1}^n x_i [N_i(\exp(x_i'\beta(\tau))) - \int_0^\tau I(Y_i \geq \exp(x_i'\beta(\tau))) dH(u)] = 0$$

where  $H(u) = -\log(1 - u)$  and  $u \in [0, 1)$ . By approximating the integral in the estimating equation on a grid  $0 = \tau_0 < \tau_1 < \dots < \tau_M < 1$ , the regression quantiles  $\beta(\tau_k)$ ,  $k = 1, \dots, M$ , can be estimated sequentially by solving the following linear programming problem:

$$\min \{\alpha(\tau_k)'u + (\Delta - \alpha(\tau_k))'v \mid z = Xb + u - v, u \geq 0, v \geq 0\}$$

where

$$\alpha(\tau_k) = \sum_{j=1}^{k-1} I(Y_i \geq \exp(x_i'\hat{\beta}(\tau_j))) H((u_{j+1}) - H(u_j))$$

See Koenker (2008) for details. You can request this method by specifying the METHOD=NA option. The grid points  $0 = \tau_0 < \tau_1 < \dots < \tau_M < 1$  are equally spaced with  $\tau_1$  specified by the INITTAU=option and the grid step between two adjacent grid points specified by the GRIDSIZE=option.



## Confidence Interval

Direct computation of the covariance of the parameter estimators involves a complicated density estimation. Instead, the QUANTLIFE procedure computes confidence intervals for the quantile regression parameters  $\beta(\tau)$  by using resampling methods. The QUANTLIFE procedure implements two different methods, the exponentially weighted method and the pairwise resampling method.

### Exponentially Weighted Method

This method samples weights  $w_i, i = 1, \dots, n$ , from a standard exponential distribution with mean 1 and variance 1. Then it computes the censored quantile regression estimators  $\hat{\beta}(\tau)$  based on the observed data  $(x_i, Y_i, \Delta_i)$  with the weights  $w_i$ . These steps are repeated B times (where B is the value of the NREP= option in the PROC QUANTLIFE statement). The confidence intervals can be obtained from these B estimates. You can specify this method with the CI=EW option in the PROC QUANTLIFE statement.

### Pairwise Method

This method samples  $(x_i, Y_i, \Delta_i)$  with replacement and computes the quantile regression estimators  $\hat{\beta}(\tau)$  based on the resampled data. These steps are repeated B times (where B is the value of the NREP= option in the PROC QUANTLIFE statement). The confidence intervals can be obtained from these B estimates. You can specify this method with the CI=PW option in the PROC QUANTLIFE statement.

## Testing Effects of Covariates

Consider the linear model

$$y_i = \mathbf{x}'_{1i}\boldsymbol{\beta}_1 + \mathbf{x}'_{2i}\boldsymbol{\beta}_2 + \epsilon_i$$

where  $\boldsymbol{\beta}_1$  and  $\boldsymbol{\beta}_2$  are  $p$ -dimensional and  $q$ -dimensional parameters, respectively, and  $\epsilon_i, i = 1, \dots, n$ , are errors. Denote  $\mathbf{x}'_i = (\mathbf{x}'_{1i}, \mathbf{x}'_{2i})$ , and let  $\hat{\boldsymbol{\beta}}_1(\tau)$  and  $\hat{\boldsymbol{\beta}}_2(\tau)$  be the parameter estimates for  $\boldsymbol{\beta}_1$  and  $\boldsymbol{\beta}_2$ , respectively, at the  $\tau$ th quantile.

The QUANTLIFE procedure implements the Wald test for the hypothesis:

$$H_0 : \boldsymbol{\beta}_2(\tau) = \mathbf{0}$$

The Wald test statistic, which is based on the estimated coefficients  $\hat{\boldsymbol{\beta}}_2$  from the unrestricted fitted model, is given by

$$T_W(\tau) = \hat{\boldsymbol{\beta}}'_2(\tau) \hat{\boldsymbol{\Sigma}}(\tau)^{-1} \hat{\boldsymbol{\beta}}_2(\tau)$$

where  $\hat{\boldsymbol{\Sigma}}(\tau)$  is an estimator of the covariance of  $\hat{\boldsymbol{\beta}}_2(\tau)$ , which is obtained by using resampling methods.

---

## Output Data Sets

### OUTBOOTEST= Output Data Set

The OUTBOOTEST= data set contains parameter estimates for the specified model from resampled data sets. A set of observations is created for each quantile level and for each resampled data set.

If the QUANTLIFE procedure does not produce valid solutions, the parameter estimates are set to missing in the OUTBOOTEST= data set.

If created, this data set contains all variables that are specified in the MODEL statement. Each observation contains parameter estimates for a specified quantile level.

The following variables are also included in the data set:

- any specified BY variables
- `_STATUS_`, a character variable of length 12 that contains the status of the model fit: either NORMAL, NOUNIQUE, or NOVALID
- Intercept, a numeric variable that contains the intercept parameter estimates
- `_TAU_`, a numeric variable that contains the specified quantile levels

For continuous explanatory variables, the names of the parameters are the same as they are for the corresponding variables. For CLASS variables, the parameter names are obtained by concatenating the corresponding CLASS variable name with the CLASS category. For interaction and nested effects, the parameter names are created by concatenating the names of each component effect.

### OUT= Output Data Set in the OUTPUT Statement

The OUT= data set that is specified in the OUTPUT statement contains all the variables in the input data set, along with statistics you request by specifying *keyword=name* options. The additional variables are calculated for each observation in the input data set.

### OUT= Output Data Set in the BASELINE Statement

The OUT= data set that is specified in the BASELINE statement contains all the variables in the COVARIATES= data set, along with statistics you request by specifying *keyword=name* options.

---

## ODS Table Names

Table 76.3 lists the names that the QUANTLIFE procedure assigns to each table it creates. You can specify these names when you use the Output Delivery System (ODS) to select tables and create output data sets.

**Table 76.3** ODS Tables Produced in PROCQUANTLIFE

| ODS Table Name     | Description                                | Statement | Option  |
|--------------------|--------------------------------------------|-----------|---------|
| ClassLevels        | Classification variable levels             | CLASS     | Default |
| ModelInfo          | Model information                          | MODEL     | Default |
| NObs               | Number of observations                     | PROC      | Default |
| ParameterEstimates | Parameter estimates                        | MODEL     | Default |
| CensoredSummary    | Summary of event and censored observations | PROC      | Dfault  |
| Tests              | Results for tests                          | TEST      | Default |

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “Statistical Graphics Using ODS.”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “A Primer on ODS Statistical Graphics” on page 599 in Chapter 21, “Statistical Graphics Using ODS.”

The QUANTLIFE procedure assigns a name to each graph it creates. You can use these names to refer to the graphs when you use ODS. The names along with the required statements and options are listed in Table 76.4.

**Table 76.4** Graphs Produced by PROC QUANTLIFE

| ODS Graph Name | Plot Description                                             | PLOTS= Option      |
|----------------|--------------------------------------------------------------|--------------------|
| QuantilePlot   | Quantile function plot                                       | QUANTILE           |
| QuantPanel     | Panel of quantile plots with confidence limits               | QUANTPLOT          |
| QuantPlot      | Scatter plot for regression quantiles with confidence limits | QUANTPLOT / UNPACK |
| SurvivalPlot   | Survivor function plot                                       | SURVIVAL           |

---

## Examples: QUANTLIFE Procedure

---

### Example 76.1: Primary Biliary Cirrhosis Study

This example illustrates how to detect varying covariate effects on survival time with quantile regression analysis. Consider a study of primary biliary cirrhosis, a rare but fatal chronic liver disease discussed by Fleming and Harrington (1991). Researchers followed 418 patients with this disease, of whom 161 died during the study.

The data set contains the following variables:

- Time, follow-up time, in years
- Status, event indicator with value 1 for death time and value 0 for censored time
- Age, age in years from birth to study registration
- Albumin, serum albumin level, in gm/dl
- Bilirubin, serum bilirubin level, in mg/dl
- Edema, edema presence
- Prottime, prothrombin time, in seconds

The following statements create the data set PBC that is used in this example:

```
data pbc;
 input Time Status Age Albumin Bilirubin Edema Prottime @@;
 label Time="Follow-up Time in Days";
 logAlbumin = log(Albumin);
 logBilirubin = log(Bilirubin);
 logProttime = log(Prottime);
 datalines;
 400 1 58.7652 2.60 14.5 1.0 12.2 4500 0 56.4463 4.14 1.1 0.0 10.6
 1012 1 70.0726 3.48 1.4 0.5 12.0 1925 1 54.7406 2.54 1.8 0.5 10.3
 1504 0 38.1054 3.53 3.4 0.0 10.9 2503 1 66.2587 3.98 0.8 0.0 11.0
 1832 0 55.5346 4.09 1.0 0.0 9.7 2466 1 53.0568 4.00 0.3 0.0 11.0
 2400 1 42.5079 3.08 3.2 0.0 11.0 51 1 70.5599 2.74 12.6 1.0 11.5
 3762 1 53.7139 4.16 1.4 0.0 12.0 304 1 59.1376 3.52 3.6 0.0 13.6

 ... more lines ...

 989 0 35.0000 3.23 0.7 0.0 10.8 681 1 67.0000 2.96 1.2 0.0 10.9
 1103 0 39.0000 3.83 0.9 0.0 11.2 1055 0 57.0000 3.42 1.6 0.0 9.9
 691 0 58.0000 3.75 0.8 0.0 10.4 976 0 53.0000 3.29 0.7 0.0 10.6
;
```

The next statements fit a linear model for the log of survival time of the PBC patients with the covariates logBilirubin, logProttime, logAlbumin, Age, and Edema.

```
ods graphics on;
proc quantlife data=pbcc log method=na plot=(quantplot survival) seed=1268;
 model Time*Status(0)=logBilirubin logProttime logAlbumin Age Edema
 /quantile=(.1 .2 .3 .4 .5 .6 .75);
run;
```

You use the QUANTILE= option to specify a set of quantiles of interest for comparing quantile-specific covariate effects. The METHOD= option specifies the Nelson-Aalen method for estimating the regression parameters.

The QUANTLIFE procedure provides resampling methods for computing confidence limits for the parameters; see the section “Confidence Interval” on page 6470 for details. By default, the repetition number is 200. You can request a different number of repetitions with the NREP= option. You can also use the SEED= option to specify the seed for generating random numbers so that you can later reproduce the results.

Figure 76.1.1 displays model information and information about censoring in the data. Out of 418 observations, 257 are censored.

**Output 76.1.1** Model Information

| The QUANTLIFE Procedure                            |              |          |                  |
|----------------------------------------------------|--------------|----------|------------------|
| Model Information                                  |              |          |                  |
| Data Set                                           | WORK.PBC     |          |                  |
| Dependent Variable                                 | Log(Time)    |          |                  |
| Censoring Variable                                 | Status       |          |                  |
| Censoring Value(s)                                 | 0            |          |                  |
| Number of Observations                             | 418          |          |                  |
| Method                                             | Nelson-Aalen |          |                  |
| Replications                                       | 200          |          |                  |
| Seed for Random Number Generator                   | 1268         |          |                  |
| Summary of the Number of Event and Censored Values |              |          |                  |
| Total                                              | Event        | Censored | Percent Censored |
| 418                                                | 161          | 257      | 61.48            |

Figure 76.1.2 provides the parameter estimates. Each quantile level has a set of parameter estimates and confidence limits.

**Output 76.1.2** Parameter Estimates at Different Quantiles

| Parameter Estimates |              |    |          |                |                       |          |         |         |
|---------------------|--------------|----|----------|----------------|-----------------------|----------|---------|---------|
| Quantile            | Parameter    | DF | Estimate | Standard Error | 95% Confidence Limits |          | t Value | Pr >  t |
| 0.1000              | Intercept    | 1  | 14.8030  | 4.0967         | 6.7736                | 22.8325  | 3.61    | 0.0003  |
|                     | logBilirubin | 1  | -0.4488  | 0.1485         | -0.7398               | -0.1578  | -3.02   | 0.0027  |
|                     | logProtime   | 1  | -3.6378  | 1.4560         | -6.4915               | -0.7841  | -2.50   | 0.0129  |
|                     | logAlbumin   | 1  | 1.9286   | 0.9756         | 0.0165                | 3.8408   | 1.98    | 0.0487  |
|                     | Age          | 1  | -0.0244  | 0.0107         | -0.0455               | -0.00334 | -2.27   | 0.0237  |
|                     | Edema        | 1  | -1.0712  | 0.6688         | -2.3820               | 0.2396   | -1.60   | 0.1100  |
| 0.2000              | Intercept    | 1  | 15.1800  | 2.6664         | 9.9540                | 20.4060  | 5.69    | <.0001  |
|                     | logBilirubin | 1  | -0.6532  | 0.0886         | -0.8268               | -0.4796  | -7.37   | <.0001  |
|                     | logProtime   | 1  | -3.3273  | 0.9401         | -5.1699               | -1.4847  | -3.54   | 0.0004  |
|                     | logAlbumin   | 1  | 1.6842   | 0.6888         | 0.3343                | 3.0342   | 2.45    | 0.0149  |
|                     | Age          | 1  | -0.0291  | 0.00687        | -0.0425               | -0.0156  | -4.23   | <.0001  |
|                     | Edema        | 1  | -0.7265  | 0.3179         | -1.3497               | -0.1034  | -2.29   | 0.0228  |
| 0.3000              | Intercept    | 1  | 13.2382  | 2.5296         | 8.2804                | 18.1961  | 5.23    | <.0001  |
|                     | logBilirubin | 1  | -0.6013  | 0.0762         | -0.7506               | -0.4521  | -7.90   | <.0001  |
|                     | logProtime   | 1  | -2.5816  | 0.8907         | -4.3273               | -0.8359  | -2.90   | 0.0039  |
|                     | logAlbumin   | 1  | 1.7246   | 0.7142         | 0.3248                | 3.1245   | 2.41    | 0.0162  |
|                     | Age          | 1  | -0.0244  | 0.00716        | -0.0385               | -0.0104  | -3.41   | 0.0007  |
|                     | Edema        | 1  | -0.8577  | 0.2763         | -1.3992               | -0.3163  | -3.10   | 0.0020  |
| 0.4000              | Intercept    | 1  | 13.4716  | 3.0874         | 7.4204                | 19.5228  | 4.36    | <.0001  |
|                     | logBilirubin | 1  | -0.6047  | 0.0846         | -0.7705               | -0.4389  | -7.15   | <.0001  |
|                     | logProtime   | 1  | -2.1632  | 1.1726         | -4.4615               | 0.1351   | -1.84   | 0.0658  |
|                     | logAlbumin   | 1  | 0.9819   | 0.7191         | -0.4274               | 2.3912   | 1.37    | 0.1728  |
|                     | Age          | 1  | -0.0255  | 0.00681        | -0.0389               | -0.0122  | -3.74   | 0.0002  |
|                     | Edema        | 1  | -1.0589  | 0.3104         | -1.6672               | -0.4506  | -3.41   | 0.0007  |
| 0.5000              | Intercept    | 1  | 10.9205  | 2.8047         | 5.4235                | 16.4175  | 3.89    | 0.0001  |
|                     | logBilirubin | 1  | -0.5315  | 0.0904         | -0.7087               | -0.3543  | -5.88   | <.0001  |
|                     | logProtime   | 1  | -1.2222  | 1.2142         | -3.6020               | 1.1577   | -1.01   | 0.3148  |
|                     | logAlbumin   | 1  | 1.5700   | 0.6284         | 0.3383                | 2.8016   | 2.50    | 0.0129  |
|                     | Age          | 1  | -0.0318  | 0.00883        | -0.0491               | -0.0145  | -3.60   | 0.0004  |
|                     | Edema        | 1  | -0.7316  | 0.3743         | -1.4653               | 0.00202  | -1.95   | 0.0513  |
| 0.6000              | Intercept    | 1  | 11.2381  | 2.6294         | 6.0846                | 16.3917  | 4.27    | <.0001  |
|                     | logBilirubin | 1  | -0.5701  | 0.0852         | -0.7370               | -0.4031  | -6.69   | <.0001  |
|                     | logProtime   | 1  | -1.3508  | 1.1402         | -3.5856               | 0.8840   | -1.18   | 0.2368  |
|                     | logAlbumin   | 1  | 1.3704   | 0.5091         | 0.3726                | 2.3682   | 2.69    | 0.0074  |
|                     | Age          | 1  | -0.0226  | 0.0109         | -0.0440               | -0.00111 | -2.06   | 0.0399  |
|                     | Edema        | 1  | -0.5141  | 0.3088         | -1.1193               | 0.0912   | -1.66   | 0.0968  |
| 0.7500              | Intercept    | 1  | 10.0954  | 3.1893         | 3.8445                | 16.3463  | 3.17    | 0.0017  |
|                     | logBilirubin | 1  | -0.6366  | 0.1071         | -0.8466               | -0.4267  | -5.94   | <.0001  |
|                     | logProtime   | 1  | -0.9670  | 1.2343         | -3.3862               | 1.4521   | -0.78   | 0.4338  |
|                     | logAlbumin   | 1  | 1.8148   | 0.5883         | 0.6618                | 2.9678   | 3.08    | 0.0022  |
|                     | Age          | 1  | -0.0203  | 0.0156         | -0.0509               | 0.0102   | -1.30   | 0.1931  |
|                     | Edema        | 1  | -0.3529  | 0.3120         | -0.9644               | 0.2586   | -1.13   | 0.2587  |

For comparison, the following statements use the LIFEREG procedure to fit a Weibull distribution to the data. The LIFEREG procedure fits an accelerated failure time model, which assumes that the effect of independent variables is multiplicative on the event time.

```
proc lifereg data=pb;
 model Time*Status(0)=logBilirubin logProttime logAlbumin Age Edema;
run;
```

Figure 76.1.3 provides the parameter estimates that are computed by PROC LIFEREG.

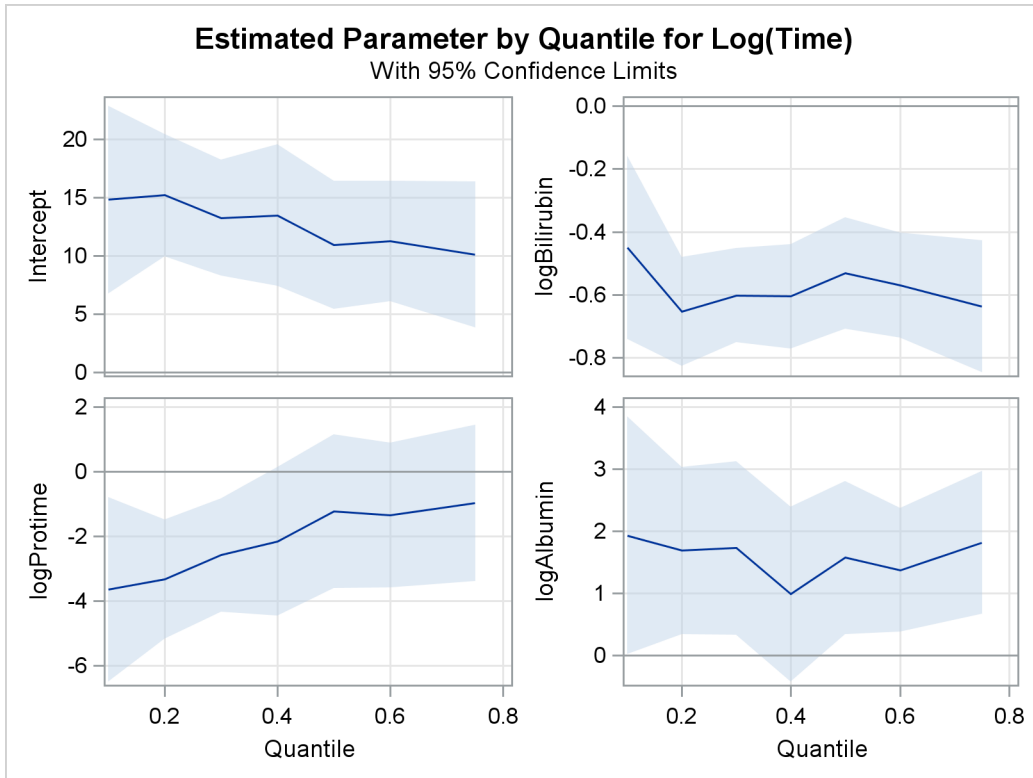
**Output 76.1.3** Parameter Estimates From PROC LIFEREG

| The LIFEREG Procedure                              |    |          |                |                       |         |            |            |
|----------------------------------------------------|----|----------|----------------|-----------------------|---------|------------|------------|
| Analysis of Maximum Likelihood Parameter Estimates |    |          |                |                       |         |            |            |
| Parameter                                          | DF | Estimate | Standard Error | 95% Confidence Limits |         | Chi-Square | Pr > ChiSq |
| Intercept                                          | 1  | 12.2155  | 1.4539         | 9.3658                | 15.0651 | 70.59      | <.0001     |
| logBilirubin                                       | 1  | -0.5770  | 0.0556         | -0.6861               | -0.4680 | 107.55     | <.0001     |
| logProttime                                        | 1  | -1.7565  | 0.5248         | -2.7850               | -0.7280 | 11.20      | 0.0008     |
| logAlbumin                                         | 1  | 1.6694   | 0.4276         | 0.8313                | 2.5074  | 15.24      | <.0001     |
| Age                                                | 1  | -0.0265  | 0.0053         | -0.0368               | -0.0162 | 25.35      | <.0001     |
| Edema                                              | 1  | -0.6303  | 0.1805         | -0.9842               | -0.2764 | 12.19      | 0.0005     |
| Scale                                              | 1  | 0.6807   | 0.0430         | 0.6014                | 0.7704  |            |            |
| Weibull Shape                                      | 1  | 1.4691   | 0.0928         | 1.2980                | 1.6628  |            |            |

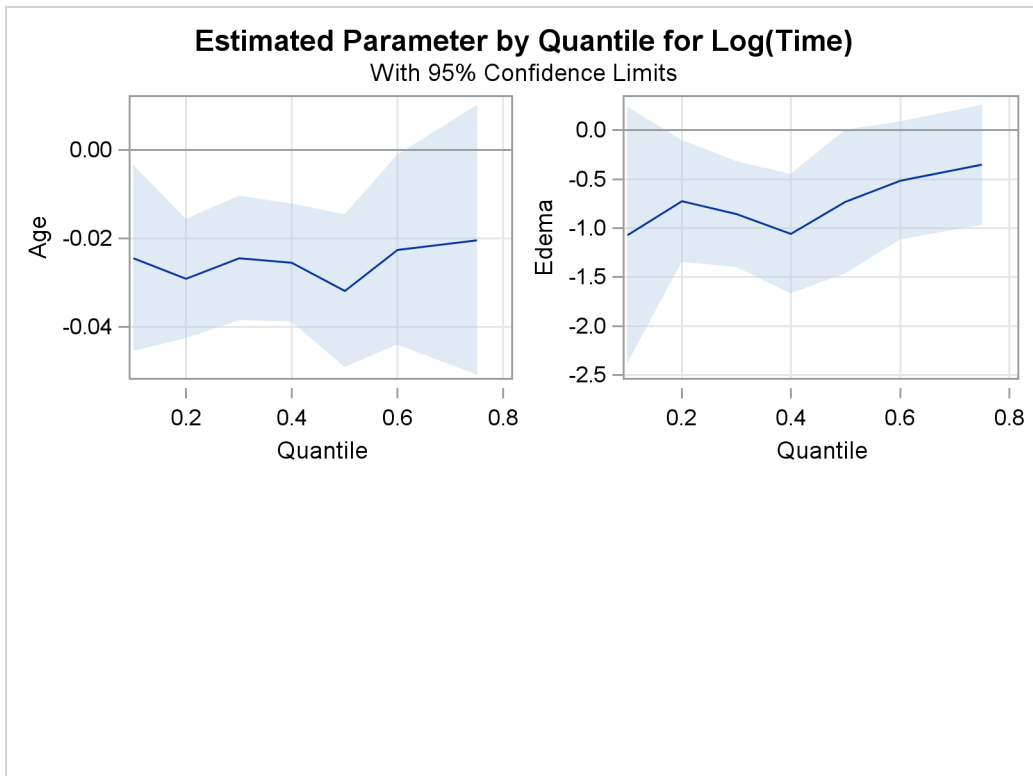
The  $p$ -value for logProttime is very small. For this same variable, the  $p$ -values that result from the quantile regression analysis are 0.3148 for the 0.5th quantile and 0.4338 for the 0.75th quantile, and the  $p$ -values are much smaller for the lower quantiles. Apparently, the effect of this covariate depends on which side of the response distribution is being modeled.

The PLOT=QUANTPLOT option in the PROC QUANTLIFE statement requests the quantile process plots in Figure 76.1.4 and Figure 76.1.5. These displays plot the estimated regression parameter against the quantile level. You can use these plots to compare quantile-specific covariate effects. If the curve is not constant, it can indicate heterogeneity in the data. The interpretation of the regression coefficients at a given quantile is similar to classical regression analysis. That is, the coefficient from a given covariate indicates the effect on  $\log(\text{Time})$  of a unit change in that covariate, assuming that the other covariates are fixed.

**Output 76.1.4** Quantile Processes with 95% Confidence Bands



**Output 76.1.5** Quantile Processes with 95% Confidence Bands





In the first panel, you can see that the effect of logProtime has a negative effect over the lower quantiles, which diminishes in magnitude at the median and upper quantiles. This insight would be missed with the accelerated failure model.

## Example 76.2: Drug Abuse Study

This example reproduces analysis done by Portnoy (2003), which demonstrates how to use quantile regression to analyze survival times. The example uses drug abuse data provided by Hosmer and Lemeshow (1999). The goal of this study is to compare treatment effects on reducing drug abuse.

The data set contains the following variables:

- Time, time to return to drug use in days
- Status, event indicator with value 1 for return to drug use and value 0 for censored time
- Age, age in years at enrollment
- Treatment, with value 1 for six-month treatment and value 0 for three-month treatment
- Beck, Beck Depression Inventory score at admission to the program
- IV3, indicator of the recent IV drug use
- NDT, number of prior drug treatments.
- RACE, race indicator with value 1 for white and value 0 for nonwhite
- SITE, treatment sites (A and B)
- LOT, length (days) of treatment.

The following statements create the data set:

```
data uis;
 input ID Age Becktota Hercoc Ivhx Ndrugtx Race Treat Site Lot Time
 Censor;
 Iv3 = (Ivhx = 3);
 Nd1 = 1/((Ndrugtx+1)/10);
 Nd2 = (1/((Ndrugtx+1)/10))*log((Ndrugtx+1)/10);
 if (Treat =1) then Frac = Lot/180;
 else Frac = Lot/90;
 datalines;
 1 39 9.0000 4 3 1 0 1 0 123 188 1
 2 33 34.0000 4 2 8 0 1 0 25 26 1
 3 33 10.0000 2 3 3 0 1 0 7 207 1
 4 32 20.0000 4 3 1 0 0 0 66 144 1

 ... more lines ...

 626 28 10.0 4 2 3 0 1 1 21 35 1
 627 35 17.0 1 3 2 0 0 1 184 379 1
 628 46 31.5 1 3 15 1 1 1 9 377 1
;
```

The following statements replicate the analysis of Portnoy (2003):

```
ods graphics on;
proc quantlife data=uis log seed=999 plots=(quantplot survival);
 class Race Site Treat;
 model Time*Censor(0)=Nd1 Nd2 Iv3 Becktota
 Treat Frac Race Age|Site
 / quantile=0.05 to 0.85 by 0.05 ;
 baseline out=Predsurvf survival=survf quantile=Time;

run;
```

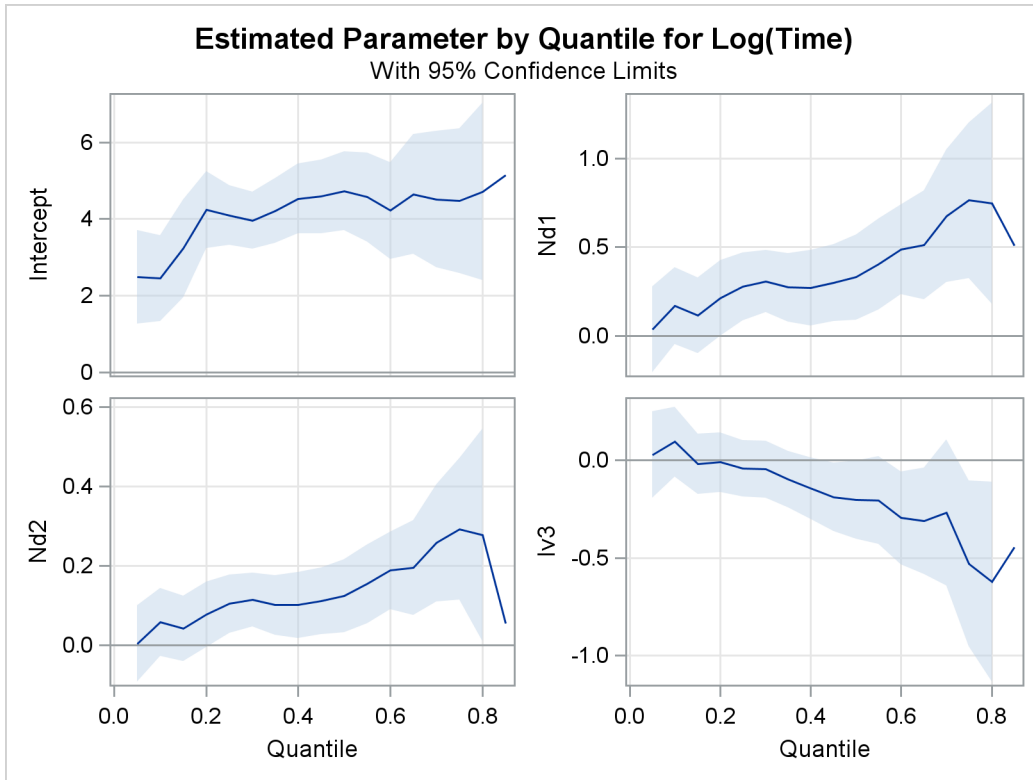
Figure 76.2.1 displays the model information. Out of 628 subjects, 53 contain missing values and are not included in the analysis. The censoring rate is 20.87%.

### Output 76.2.1 Model Information

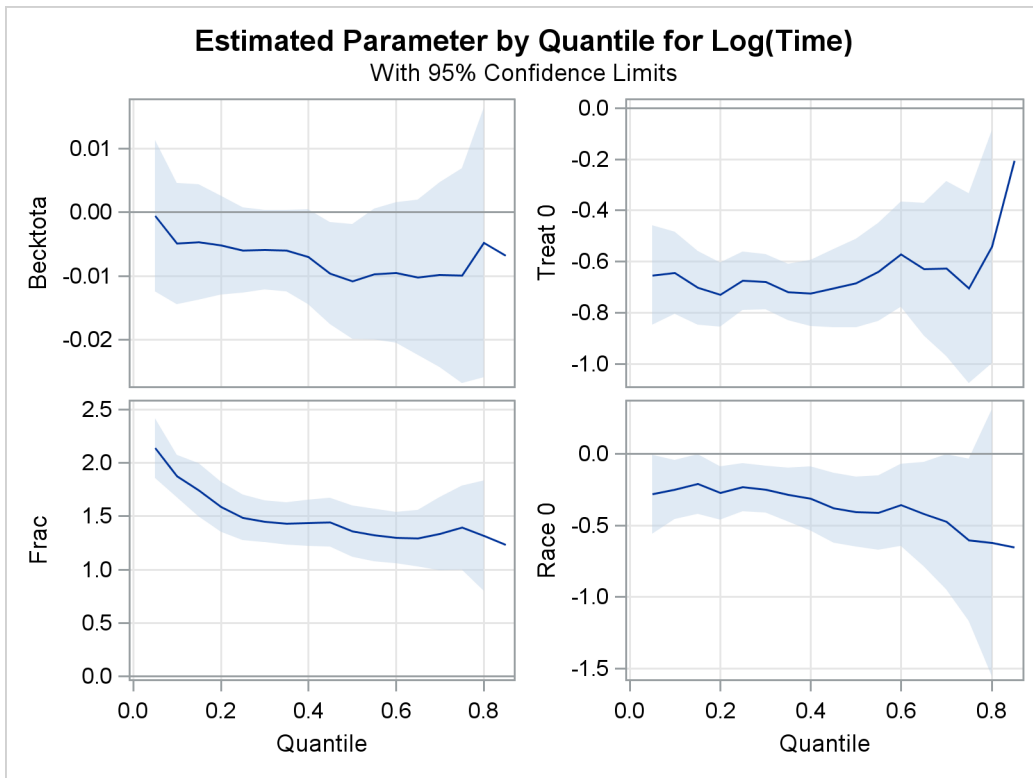
| The QUANTLIFE Procedure                            |              |          |                  |
|----------------------------------------------------|--------------|----------|------------------|
| Model Information                                  |              |          |                  |
| Data Set                                           | WORK.UIS     |          |                  |
| Dependent Variable                                 | Log(Time)    |          |                  |
| Censoring Variable                                 | Censor       |          |                  |
| Censoring Value(s)                                 | 0            |          |                  |
| Number of Observations                             | 575          |          |                  |
| Method                                             | Kaplan-Meier |          |                  |
| Replications                                       | 200          |          |                  |
| Seed for Random Number Generator                   | 999          |          |                  |
| Class Level Information                            |              |          |                  |
| Name                                               | Levels       | Values   |                  |
| Race                                               | 2            | 0 1      |                  |
| Site                                               | 2            | 0 1      |                  |
| Treat                                              | 2            | 0 1      |                  |
| Summary of the Number of Event and Censored Values |              |          |                  |
| Total                                              | Event        | Censored | Percent Censored |
| 575                                                | 464          | 111      | 19.30            |

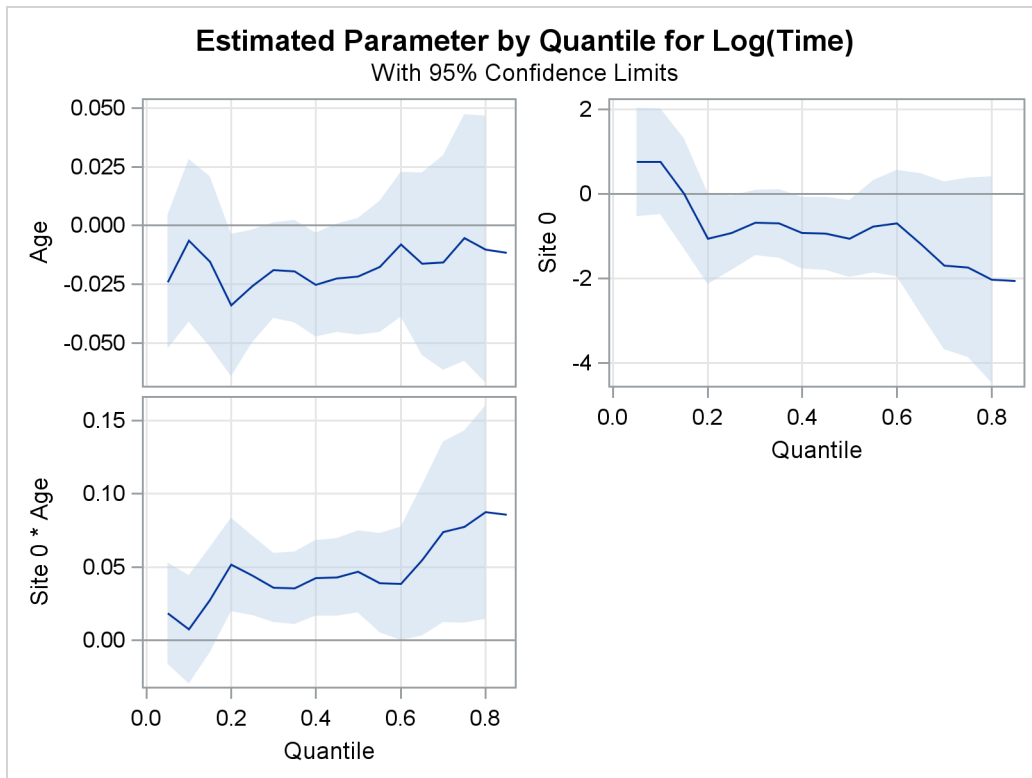
Figure 76.2.2, Figure 76.2.3, and Figure 76.2.4 display regression quantile process plots for each covariate.

**Output 76.2.2** Quantile Processes with 95% Confidence Bands



**Output 76.2.3** Quantile Processes with 95% Confidence Bands



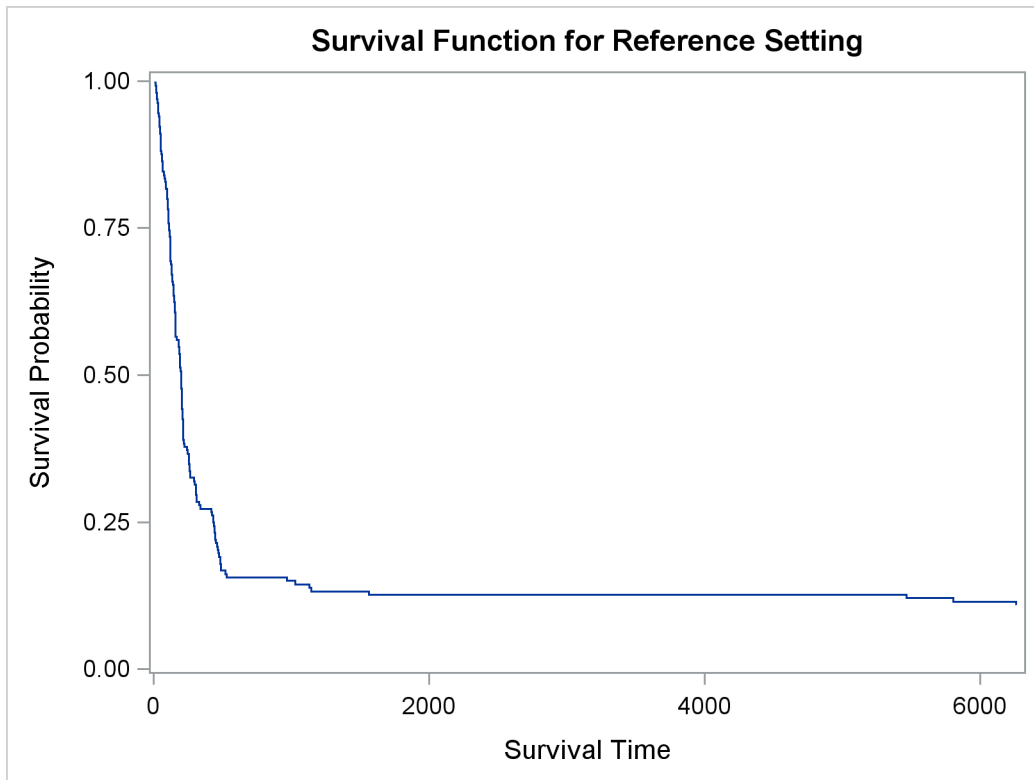
**Output 76.2.4** Quantile Processes with 95% Confidence Bands

You can see the varying effects for Nd and Frac, while the treatment effect is fairly constant. See Portnoy (2003) for more details about the covariate effects that can be discovered with quantile regression.

In survival analysis, a plot of the estimated survival function is often of interest. There is a one-to-one relationship between the quantile function and the survival function. When you specify the PLOTS= SURVIVAL option, the QUANTLIFE procedure estimates the survival function by fitting a quantile regression model for a grid of equally spaced quantile levels. You can specify the grid points with the INITTAU=option and the step between adjacent grid points with the GRIDSIZE=option. See the section “Kaplan-Meier-Type Estimator for Censored Quantile Regression” on page 6468 for more information.

Figure 76.4 shows the estimated survival function at the reference set of covariate values that consist of reference levels for the CLASS variables and average values for the continuous variables. You can output the predicted survival function by specifying the SURVIVAL= option in the BASELINE statement.

**Output 76.2.5** Survival Function



---

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# Chapter 77

## The QUANTREG Procedure

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## Overview: QUANTREG Procedure

The QUANTREG procedure models the effects of covariates on the conditional quantiles of a response variable by means of quantile regression.

Ordinary least squares (OLS) regression models the relationship between one or more covariates  $X$  and the *conditional mean* of the response variable  $Y$  given  $X = x$ . Quantile regression, which was introduced by Koenker and Bassett (1978), extends the regression model to *conditional quantiles* of the response variable, such as the median or the 90th percentile. Quantile regression is particularly useful when the rate of change in the conditional quantile, expressed by the regression coefficients, depends on the quantile.

**Figure 77.1** Trout Density in Streams

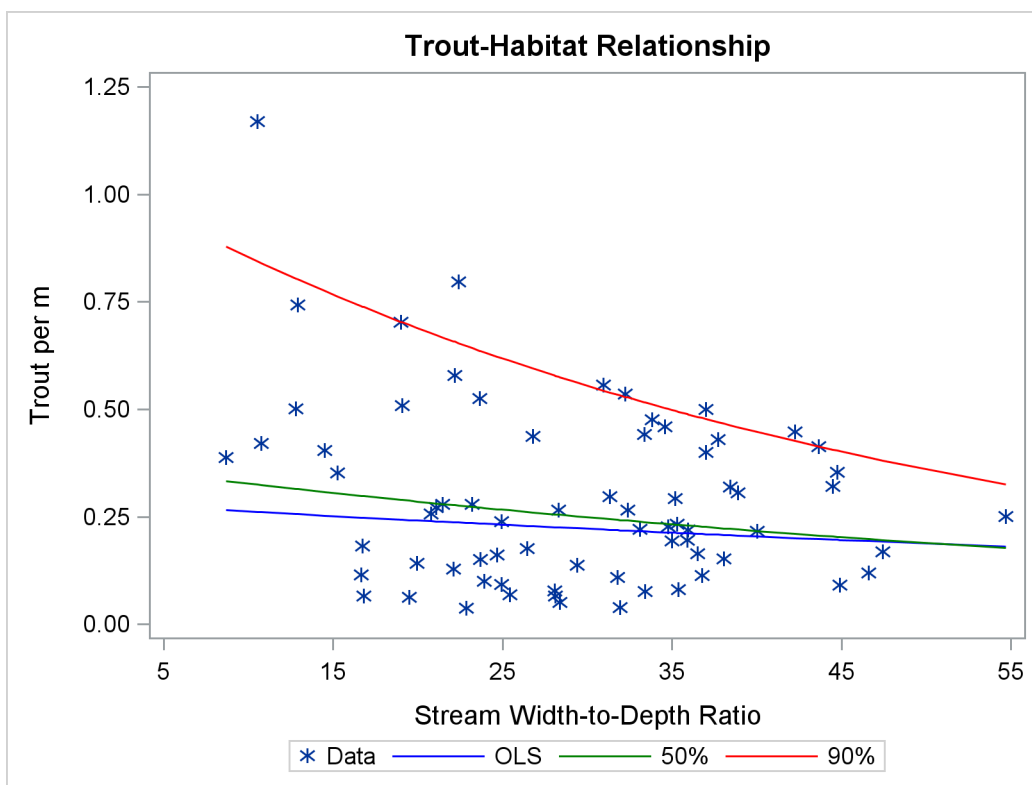


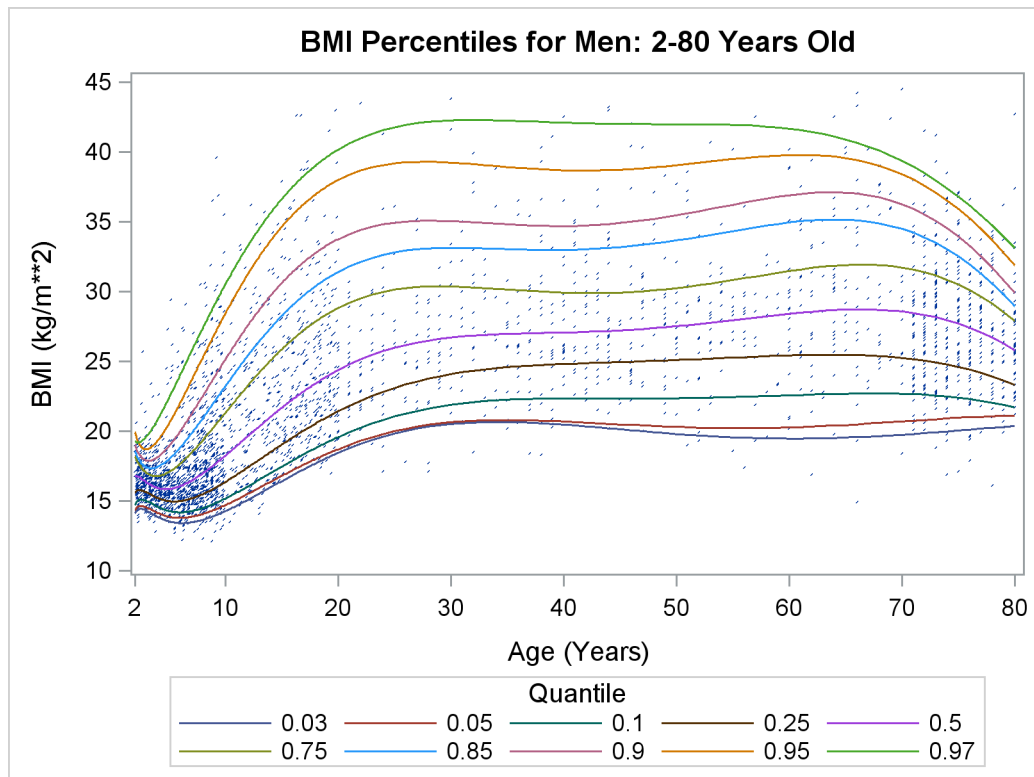
Figure 77.1 illustrates an ecological study in which it is revealing to model upper conditional quantiles. The points represent measurements of trout density and stream width-to-depth ratio taken at 13 streams over seven years.

As analyzed by Dunham, Cade, and Terrell (2002), in addition to the ratio, trout density depends on a number of unmeasured limiting factors related to the integrity of stream habitat. The interaction of these factors results in unequal variances for the conditional distributions of density given the ratio. When the ratio is the “active” limiting effect, changes in the upper conditional percentiles of density provide a better estimate of this effect than changes in the conditional mean.

The red and green curves represent the conditional 90th and 50th percentiles of density as determined with the QUANTREG procedure. The analysis was done by using a simple linear regression model for the logarithm of density. (The curves in Figure 77.1 were obtained by transforming the fitted lines back to the

original scale. For more details, see the section “Analysis of Fish-Habitat Relationships” on page 6490.) The slope parameter for the 90th percentile has an estimated value of  $-0.0215$  and is significant with a  $p$ -value less than 0.01. On the other hand, the slope parameter for the 50th percentile is not significantly different from zero. Similarly, the slope parameter for the mean, obtained with OLS regression, is not significantly different from zero.

**Figure 77.2** Quantiles for Body Mass Index



Quantile regression is especially useful with data that are heterogeneous in the sense that the tails and the central location of the conditional distributions vary differently with the covariates. An even more pronounced example of heterogeneity is shown in Figure 77.2, which plots the body mass index of 8,250 men versus their age.

Here, both upper (overweight) and lower (underweight) conditional quantiles are important because they provide the basis for developing growth charts and establishing health standards. The curves in Figure 77.2 were determined with the QUANTREG procedure by using polynomial quantile regression; details are provided in the section “Growth Charts for Body Mass Index” on page 6495. Clearly, the rate of change with age (as expressed by the regression coefficients), particularly for ages less than 20, is different for each conditional quantile.

Heterogeneous data occur in many fields, including biomedicine, econometrics, survival analysis, and ecology. Quantile regression, which includes median regression as a special case, provides a complete picture of the covariate effect when a set of percentiles is modeled, and so it offers the capability to capture important features of the data that might be missed by models that average over the conditional distribution.

Because it makes no distributional assumption about the error term in the model, quantile regression offers considerable model robustness. The assumption of normality, which is often made with OLS regression

in order to compute conditional quantiles as offsets from the mean, forces a common set of regression coefficients for all the quantiles. Obviously, quantiles with common slopes would be inappropriate in the preceding examples.

Quantile regression is also flexible in the sense that it does not involve a link function that relates the variance and the mean of the response variable. Generalized linear models, which you can fit with the GENMOD procedure, require both a link function and a distributional assumption such as the normal or Poisson distribution. The goal of generalized linear models is inference about the regression parameters in the linear predictor for the mean of the population. In contrast, the goal of quantile regression is inference on regression coefficients for the conditional quantiles of a response variable that is usually assumed to be continuous.

Quantile regression also offers a degree of data robustness. Unlike OLS regression, it is robust to extreme points in the response direction (outliers). However, it is not robust to extreme points in the covariate space (leverage points). When both types of robustness are of concern, you should consider using the ROBUSTREG procedure (Chapter 80, “The ROBUSTREG Procedure.”)

Also, unlike OLS regression, quantile regression is equivariant to monotone transformations of the response variable. For instance, as illustrated in the trout example, the logarithm of the 90th conditional percentile of trout density is the 90th conditional percentile of the logarithm of density.

Note that quantile regression cannot be carried out simply by segmenting the unconditional distribution of the response variable and then obtaining least squares fits for the subsets. This approach leads to disastrous results when, for example, the data include outliers. In contrast, quantile regression uses *all* of the data for fitting quantiles, even the extreme quantiles.

---

## Features

The main features of the QUANTREG procedure are as follows:

- offers simplex, interior point, and smoothing algorithms for estimation
- provides sparsity, rank, and resampling methods for confidence intervals
- provides asymptotic and bootstrap methods for covariance and correlation matrices of the estimated parameters
- provides the Wald, likelihood ratio, and rank tests for the regression parameter estimates and the Wald test for heteroscedasticity
- provides outlier and leverage-point diagnostics
- enables parallel computing when multiple processors are available
- provides row-wise or column-wise output data sets with multiple quantiles
- provides regression quantile spline fits
- produces fit plots, diagnostic plots, and quantile process plots by using ODS Graphics

The next section provides notation and a formal definition for quantile regression.

## Quantile Regression

Quantile regression generalizes the concept of a univariate quantile to a conditional quantile given one or more covariates. Recall that a student's score on a test is at the  $\tau$  quantile if his or her score is better than that of  $100\tau\%$  of the students who took the test. The score is also said to be at the  $100\tau$  percentile.

For a random variable  $Y$  with probability distribution function

$$F(y) = \text{Prob}(Y \leq y)$$

the  $\tau$  quantile of  $Y$  is defined as the inverse function

$$Q(\tau) = \inf \{y : F(y) \geq \tau\}$$

where  $0 < \tau < 1$ . In particular, the median is  $Q(1/2)$ .

For a random sample  $\{y_1, \dots, y_n\}$  of  $Y$ , it is well known that the sample median minimizes the sum of absolute deviations

$$\text{median} = \arg \min_{\xi \in \mathbf{R}} \sum_{i=1}^n |y_i - \xi|$$

Likewise, the general  $\tau$  sample quantile  $\xi(\tau)$ , which is the analog of  $Q(\tau)$ , is formulated as the minimizer

$$\xi(\tau) = \arg \min_{\xi \in \mathbf{R}} \sum_{i=1}^n \rho_\tau(y_i - \xi)$$

where  $\rho_\tau(z) = z(\tau - I(z < 0))$ ,  $0 < \tau < 1$ , and where  $I(\cdot)$  denotes the indicator function. The loss function  $\rho_\tau$  assigns a weight of  $\tau$  to positive residuals  $y_i - \xi$  and a weight of  $1 - \tau$  to negative residuals.

Using this loss function, the linear conditional quantile function extends the  $\tau$  sample quantile  $\xi(\tau)$  to the regression setting in the same way that the linear conditional mean function extends the sample mean. Recall that OLS regression estimates the linear conditional mean function  $E(Y|X = x) = \mathbf{x}'\boldsymbol{\beta}$  by solving for

$$\hat{\boldsymbol{\beta}} = \arg \min_{\boldsymbol{\beta} \in \mathbf{R}^p} \sum_{i=1}^n (y_i - \mathbf{x}'_i \boldsymbol{\beta})^2$$

The estimated parameter  $\hat{\boldsymbol{\beta}}$  minimizes the sum of squared residuals in the same way that the sample mean  $\hat{\mu}$  minimizes the sum of squares:

$$\hat{\mu} = \arg \min_{\mu \in \mathbf{R}} \sum_{i=1}^n (y_i - \mu)^2$$

Likewise, quantile regression estimates the linear conditional quantile function,  $Q(\tau|X = x) = \mathbf{x}'\boldsymbol{\beta}(\tau)$ , by solving

$$\hat{\boldsymbol{\beta}}(\tau) = \arg \min_{\boldsymbol{\beta} \in \mathbf{R}^p} \sum_{i=1}^n \rho_{\tau}(y_i - \mathbf{x}_i' \boldsymbol{\beta})$$

for  $\tau \in (0, 1)$ . The quantity  $\hat{\boldsymbol{\beta}}(\tau)$  is called the  $\tau$  regression quantile. The case  $\tau = 0.5$ , which minimizes the sum of absolute residuals, corresponds to median regression, which is also known as  $L_1$  regression.

The set of regression quantiles

$$\{\boldsymbol{\beta}(\tau) : \tau \in (0, 1)\}$$

is referred to as the *quantile process*.

The QUANTREG procedure computes the quantile function  $Q(\tau|X = x)$  and conducts statistical inference on the estimated parameters  $\hat{\boldsymbol{\beta}}(\tau)$ .

## Getting Started: QUANTREG Procedure

The following examples demonstrate how you can use the QUANTREG procedure to fit linear models for selected quantiles or for the entire quantile process. The first example explains the use of the procedure in the fish-habitat example, and the second example explains the use of the procedure to construct growth charts for body mass index.

### Analysis of Fish-Habitat Relationships

Quantile regression is used extensively in ecological studies (Cade and Noon 2003). Recently, Dunham, Cade, and Terrell (2002) applied quantile regression to analyze fish-habitat relationships for Lahontan cutthroat trout in 13 streams of the eastern Lahontan basin, which covers most of northern Nevada and parts of southern Oregon. The density of trout (number of trout per meter) was measured by sampling stream sites from 1993 to 1999. The width-to-depth ratio of the stream site was determined as a measure of stream habitat.

The goal of this study was to explore the relationship between the conditional quantiles of trout density and the width-to-depth ratio. The scatter plot of the data in [Figure 77.1](#) indicates a nonlinear relationship, and so it is reasonable to fit regression models for the conditional quantiles of the log of density. Since regression quantiles are equivariant under any monotonic (linear or nonlinear) transformation (Koenker and Hallock 2001), the exponential transformation converts the conditional quantiles to the original density scale.

The data set trout, which follows, includes the average numbers of Lahontan cutthroat trout per meter of stream (Density), the logarithm of Density (LnDensity), and the width-to-depth ratios (WDRatio) for 71 samples.

```
data trout;
 input Density WDRatio LnDensity @@;
 datalines;
0.38732 8.6819 -0.94850 1.16956 10.5102 0.15662
0.42025 10.7636 -0.86690 0.50059 12.7884 -0.69197
0.74235 12.9266 -0.29793 0.40385 14.4884 -0.90672
0.35245 15.2476 -1.04284 0.11499 16.6495 -2.16289
0.18290 16.7188 -1.69881 0.06619 16.7859 -2.71523
0.70330 19.0141 -0.35197 0.50845 19.0548 -0.67639

... more lines ...

0.25125 54.6916 -1.38129
;
```

The following statements use the QUANTREG procedure to fit a simple linear model for the 50th and 90th percentiles of LnDensity:

```
ods graphics on;

proc quantreg data=trout alpha=0.1 ci=resampling;
 model LnDensity = WDRatio / quantile=0.5 0.9
 CovB seed=1268;
 test WDRatio / wald lr;
run;
```

The MODEL statement specifies a simple linear regression model with LnDensity as the response variable  $Y$  and WDRatio as the covariate  $X$ . The QUANTILE= option requests that the regression quantile function  $Q(\tau|X = x) = \mathbf{x}'\boldsymbol{\beta}(\tau)$  be estimated by solving

$$\hat{\boldsymbol{\beta}}(\tau) = \arg \min_{\boldsymbol{\beta} \in \mathbb{R}^2} \sum_{i=1}^n \rho_{\tau}(y_i - \mathbf{x}'_i \boldsymbol{\beta})$$

where  $\tau = (0.5, 0.9)$ .

By default, the regression coefficients  $\hat{\boldsymbol{\beta}}(\tau)$  are estimated with the simplex algorithm, which is explained in the section “[Simplex Algorithm](#)” on page 6516. The ALPHA= option requests 90% confidence limits for the regression parameters, and the option CI=RESAMPLING specifies that the intervals are to be computed with the MCMB resampling method of He and Hu (2002). By specifying the CI=RESAMPLING option, the QUANTREG procedure also computes standard errors,  $t$  values, and  $p$ -values of regression parameters with the MCMB resampling method. The SEED= option specifies a seed for the resampling method. The COVB option requests covariance matrices for the estimated regression coefficients, and the TEST statement requests tests for the hypothesis that the slope parameter (the coefficient of WDRatio) is zero.

Figure 77.3 displays model information and summary statistics for the variables in the model. The summary statistics include the median and the standardized median absolute deviation (MAD), which are robust measures of univariate location and scale, respectively. See Huber (1981, p. 108) for more details about the standardized MAD.

**Figure 77.3** Model Fitting Information and Summary Statistics

| The QUANTREG Procedure          |            |         |         |         |                    |         |
|---------------------------------|------------|---------|---------|---------|--------------------|---------|
| Model Information               |            |         |         |         |                    |         |
| Data Set                        | WORK.TROUT |         |         |         |                    |         |
| Dependent Variable              | LnDensity  |         |         |         |                    |         |
| Number of Independent Variables | 1          |         |         |         |                    |         |
| Number of Observations          | 71         |         |         |         |                    |         |
| Optimization Algorithm          | Simplex    |         |         |         |                    |         |
| Method for Confidence Limits    | Resampling |         |         |         |                    |         |
| Summary Statistics              |            |         |         |         |                    |         |
| Variable                        | Q1         | Median  | Q3      | Mean    | Standard Deviation | MAD     |
| WDRatio                         | 22.0917    | 29.4083 | 35.9382 | 29.1752 | 9.9859             | 10.4970 |
| LnDensity                       | -2.0511    | -1.3813 | -0.8669 | -1.4973 | 0.7682             | 0.8214  |

Figure 77.4 and Figure 77.5 display the parameter estimates, standard errors, 95% confidence limits, *t* values, and *p*-values that are computed by the resampling method.

**Figure 77.4** Parameter Estimates at QUANTILE=0.5

| Parameter Estimates |    |          |                |                       |         |         |         |
|---------------------|----|----------|----------------|-----------------------|---------|---------|---------|
| Parameter           | DF | Estimate | Standard Error | 90% Confidence Limits |         | t Value | Pr >  t |
| Intercept           | 1  | -0.9811  | 0.3952         | -1.6400               | -0.3222 | -2.48   | 0.0155  |
| WDRatio             | 1  | -0.0136  | 0.0123         | -0.0341               | 0.0068  | -1.11   | 0.2705  |

**Figure 77.5** Parameter Estimates at QUANTILE=0.9

| Parameter Estimates |    |          |                |                       |         |         |         |
|---------------------|----|----------|----------------|-----------------------|---------|---------|---------|
| Parameter           | DF | Estimate | Standard Error | 90% Confidence Limits |         | t Value | Pr >  t |
| Intercept           | 1  | 0.0576   | 0.2606         | -0.3769               | 0.4921  | 0.22    | 0.8257  |
| WDRatio             | 1  | -0.0215  | 0.0075         | -0.0340               | -0.0091 | -2.88   | 0.0053  |

The 90th percentile of trout density can be predicted from the width-to-depth ratio as follows:

$$y_{90} = \exp(0.0576 - 0.0215x)$$

This is the upper dashed curve plotted in Figure 77.1. The lower dashed curve for the median can be obtained in a similar fashion.

The covariance matrices for the estimated parameters are shown in Figure 77.6. The resampling method used for the confidence intervals is used to compute these matrices.

**Figure 77.6** Covariance Matrices of the Estimated Parameters

| Estimated Covariance Matrix for Quantile = 0.5 |           |          |
|------------------------------------------------|-----------|----------|
|                                                | Intercept | WDRatio  |
| Intercept                                      | 0.156191  | -.004653 |
| WDRatio                                        | -.004653  | 0.000151 |

| Estimated Covariance Matrix for Quantile = 0.9 |           |          |
|------------------------------------------------|-----------|----------|
|                                                | Intercept | WDRatio  |
| Intercept                                      | 0.067914  | -.001877 |
| WDRatio                                        | -.001877  | 0.000056 |

The tests requested with the TEST statement are shown in Figure 77.7. Both the Wald test and the likelihood ratio test indicate that the coefficient of width-to-depth ratio is significantly different from zero at the 90th percentile, but the deference is not significant at the median.

**Figure 77.7** Tests of Significance

| Test Results |                  |           |        |            |
|--------------|------------------|-----------|--------|------------|
| Quantile     | Test             | Test      | Chi-   |            |
|              |                  | Statistic | Square | Pr > ChiSq |
| 0.5          | Wald             | 1.2339    | 1      | 0.2666     |
| 0.5          | Likelihood Ratio | 1.1467    | 1      | 0.2842     |
| 0.9          | Wald             | 8.3031    | 1      | 0.0040     |
| 0.9          | Likelihood Ratio | 9.0529    | 1      | 0.0026     |

In many quantile regression problems it is useful to examine how the estimated regression parameters for each covariate change as a function of  $\tau$  in the interval  $(0, 1)$ . The following statements use the QUANTREG procedure to request the estimated quantile processes  $\hat{\beta}(\tau)$  for the slope and intercept parameters:

```
proc quantreg data=trout alpha=0.1 ci=resampling;
 model LnDensity = WDRatio / quantile=process seed=1268
 plot=quantplot;
run;
```

The QUANTILE=PROCESS option requests an estimate of the quantile process for each regression parameter. The options ALPHA=0.1 and CI=RESAMPLING specify that 90% confidence bands for the quantile processes are to be computed with the resampling method.

Figure 77.8 displays a portion of the objective function table for the entire quantile process. The objective function is evaluated at 77 values of  $\tau$  in the interval  $(0, 1)$ . The table also provides predicted values of the



conditional quantile function  $Q(\tau)$  at the mean for WDRatio, which can be used to estimate the conditional density function.

**Figure 77.8** Objective Function

| Objective Function for Quantile Process |          |                    |                   |
|-----------------------------------------|----------|--------------------|-------------------|
| Label                                   | Quantile | Objective Function | Predicted at Mean |
| t0                                      | 0.005634 | 0.7044             | -3.2582           |
| t1                                      | 0.020260 | 2.5331             | -3.0331           |
| t2                                      | 0.031348 | 3.7421             | -2.9376           |
| t3                                      | 0.046131 | 5.2538             | -2.7013           |
| .                                       | .        | .                  | .                 |
| .                                       | .        | .                  | .                 |
| .                                       | .        | .                  | .                 |
| t73                                     | 0.945705 | 4.1433             | -0.4361           |
| t74                                     | 0.966377 | 2.5858             | -0.4287           |
| t75                                     | 0.976060 | 1.8512             | -0.4082           |
| t76                                     | 0.994366 | 0.4356             | -0.4082           |

Figure 77.9 displays a portion of the table of the quantile processes for the estimated parameters and confidence limits.

**Figure 77.9** Objective Function

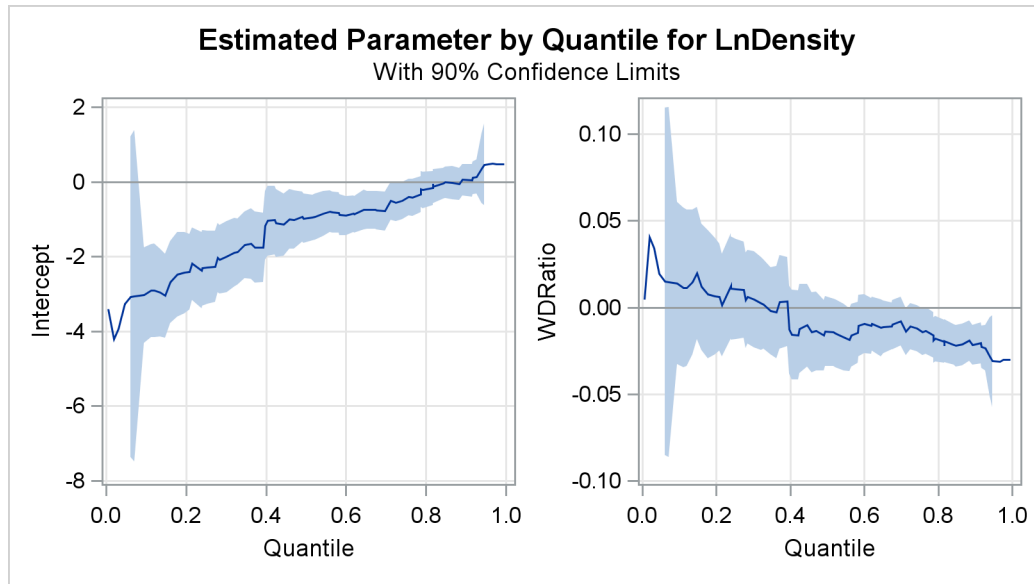
| Parameter Estimates for Quantile Process |          |           |          |
|------------------------------------------|----------|-----------|----------|
| Label                                    | Quantile | Intercept | WDRatio  |
| .                                        | .        | .         | .        |
| .                                        | .        | .         | .        |
| .                                        | .        | .         | .        |
| t57                                      | 0.765705 | -0.42205  | -0.01335 |
| lower90                                  | 0.765705 | -0.91952  | -0.02682 |
| upper90                                  | 0.765705 | 0.07541   | 0.00012  |
| t58                                      | 0.786206 | -0.32688  | -0.01592 |
| lower90                                  | 0.786206 | -0.80883  | -0.02895 |
| upper90                                  | 0.786206 | 0.15507   | -0.00289 |
| .                                        | .        | .         | .        |
| .                                        | .        | .         | .        |
| .                                        | .        | .         | .        |

The PLOT=QUANTPLOT option in the MODEL statement, together with ODS Graphics, requests a plot of the estimated quantile processes. The left side of Figure 77.10 displays the process for the intercept, and the right side displays the process for the coefficient of WDRatio.

The process plot for WDRatio shows that the slope parameter changes from positive to negative as the quantile increases, and it changes sign with a sharp drop at the 40th percentile. The 90% confidence bands show that the relationship between LnDensity and WDRatio (expressed by the slope) is not significant below

the 78th percentile. This situation can also be seen in Figure 77.9, which shows that 0 falls between the lower and upper confidence limits of the slope parameter for quantiles below 0.78. Since the confidence intervals for the extreme quantiles are not stable due to insufficient data, the confidence band is not displayed outside the interval (0.05, 0.95).

**Figure 77.10** Quantile Processes for Intercept and Slope



## Growth Charts for Body Mass Index

Body mass index (BMI) is defined as the ratio of weight (kg) to squared height ( $m^2$ ) and is a widely used measure for categorizing individuals as overweight or underweight. The percentiles of BMI for specified ages are of particular interest. As age increases, these percentiles provide growth patterns of BMI not only for the majority of the population, but also for underweight or overweight extremes of the population. In addition, the percentiles of BMI for a specified age provide a reference for individuals at that age with respect to the population.

Smooth quantile curves have been widely used for reference charts in medical diagnosis to identify unusual subjects, whose measurements lie in the tails of the reference distribution. This example explains how to use the QUANTREG procedure to create growth charts for BMI.

A SAS data set named `bmimen` was created by merging and cleaning the 1999–2000 and 2001–2002 survey results for men published by the National Center for Health Statistics. This data set contains the variables Weight (kg), Height (m), BMI ( $kg/m^2$ ), Age (year), and `SeQN` (respondent sequence number) for 8,250 men. More details can be found in Chen (2005).

The data set used in this example is a subset of the original data set of Chen (2005). It contains the two variables BMI and Age with 3264 observations.

```
data bmimen;
 input BMI Age @@;
 SqrtAge = sqrt(Age);
 InveAge = 1/Age;
```

```

LogBMI = log(BMI);
datalines;
18.6 2.0 17.1 2.0 19.0 2.0 16.8 2.0 19.0 2.1 15.5 2.1
16.7 2.1 16.1 2.1 18.0 2.1 17.8 2.1 18.3 2.1 16.9 2.1
15.9 2.1 20.6 2.1 16.7 2.1 15.4 2.1 15.9 2.1 17.7 2.1

... more lines ...

29.0 80.0 24.1 80.0 26.6 80.0 24.2 80.0 22.7 80.0 28.4 80.0
26.3 80.0 25.6 80.0 24.8 80.0 28.6 80.0 25.7 80.0 25.8 80.0
22.5 80.0 25.1 80.0 27.0 80.0 27.9 80.0 28.5 80.0 21.7 80.0
33.5 80.0 26.1 80.0 28.4 80.0 22.7 80.0 28.0 80.0 42.7 80.0
;

```

The logarithm of BMI is used as the response (although this does not improve the quantile regression fit, it helps with statistical inference.) A preliminary median regression is fitted with a parametric model, which involves six powers of Age.

The following statements invoke the QUANTREG procedure:

```

proc quantreg data=bmimen algorithm=interior(tolerance=1e-5) ci=resampling;
 model logbmi = inveage sqrtage age sqrtage*age
 age*age age*age*age
 / diagnostics cutoff=4.5 quantile=.5 seed=1268;
 id age bmi;
 test_age_cubic: test age*age*age / wald lr rankscore(tau);
run;

```

The MODEL statement provides the model, and the option QUANTILE=0.5 requests median regression, which computes  $\hat{\beta}(\frac{1}{2})$  by using the interior point algorithm as requested with the ALGORITHM= option. See the section “Interior Point Algorithm” on page 6517 for details about this algorithm.

Figure 77.11 displays the estimated parameters, standard errors, 95% confidence intervals,  $t$  values, and  $p$ -values that are computed by the resampling method as requested by the CI= option. All of the parameters are considered significant since the  $p$ -values are smaller than 0.001.

**Figure 77.11** Parameter Estimates with Median Regression: Men

| The QUANTREG Procedure |    |          |                |                       |         |                 |
|------------------------|----|----------|----------------|-----------------------|---------|-----------------|
| Parameter Estimates    |    |          |                |                       |         |                 |
| Parameter              | DF | Estimate | Standard Error | 95% Confidence Limits |         | t Value Pr >  t |
| Intercept              | 1  | 7.8909   | 0.8168         | 6.2895                | 9.4924  | 9.66 <.0001     |
| InveAge                | 1  | -1.8354  | 0.4350         | -2.6884               | -0.9824 | -4.22 <.0001    |
| SqrtAge                | 1  | -5.1247  | 0.7135         | -6.5237               | -3.7257 | -7.18 <.0001    |
| Age                    | 1  | 1.9759   | 0.2537         | 1.4785                | 2.4733  | 7.79 <.0001     |
| SqrtAge*Age            | 1  | -0.3347  | 0.0424         | -0.4179               | -0.2515 | -7.89 <.0001    |
| Age*Age                | 1  | 0.0227   | 0.0029         | 0.0170                | 0.0284  | 7.77 <.0001     |
| Age*Age*Age            | 1  | -0.0000  | 0.0000         | -0.0001               | -0.0000 | -7.40 <.0001    |

The TEST statement requests Wald, likelihood ratio, and rank tests for the significance of the cubic term in Age. The test results, shown in Figure 77.12, indicate that this term is significant. Higher-order terms are not significant.

**Figure 77.12** Test of Significance for Cubic Term

| Test test_age_cubic Results |                   |    |                |            |
|-----------------------------|-------------------|----|----------------|------------|
| Test                        | Test<br>Statistic | DF | Chi-<br>Square | Pr > ChiSq |
| Wald                        | 54.7417           | 1  | 54.74          | <.0001     |
| Likelihood Ratio            | 56.9473           | 1  | 56.95          | <.0001     |
| Rank_Tau                    | 42.5731           | 1  | 42.57          | <.0001     |

Median regression and, more generally, quantile regression are robust to extremes of the response variable. The DIAGNOSTICS option in the MODEL statement requests a diagnostic table of outliers, shown in Figure 77.13, which uses a cutoff value specified with the CUTOFF= option. The variables specified in the ID statement are included in the table.

With CUTOFF=4.5, 14 men are identified as outliers. All of these men have large positive standardized residuals, which indicates that they are overweight for their age. The cutoff value 4.5 is ad hoc; it corresponds to a probability less than  $0.5E-5$  if normality is assumed, but the standardized residuals for median regression usually do not meet this assumption.

In order to construct the chart shown in Figure 77.2, the same model used for median regression is used for other quantiles. Note that the QUANTREG procedure can compute fitted values for multiple quantiles.

**Figure 77.13** Diagnostics with Median Regression

| Diagnostics |           |           |                          |         |
|-------------|-----------|-----------|--------------------------|---------|
| Obs         | Age       | BMI       | Standardized<br>Residual | Outlier |
| 1337        | 8.900000  | 36.500000 | 5.3575                   | *       |
| 1376        | 9.200000  | 39.600000 | 5.8723                   | *       |
| 1428        | 9.400000  | 36.900000 | 5.3036                   | *       |
| 1505        | 9.900000  | 35.500000 | 4.8862                   | *       |
| 1764        | 14.900000 | 46.800000 | 5.6403                   | *       |
| 1838        | 16.200000 | 50.400000 | 5.9138                   | *       |
| 1845        | 16.300000 | 42.600000 | 4.6683                   | *       |
| 1870        | 16.700000 | 42.600000 | 4.5930                   | *       |
| 1957        | 18.100000 | 49.900000 | 5.5053                   | *       |
| 2002        | 18.700000 | 52.700000 | 5.8106                   | *       |
| 2016        | 18.900000 | 48.400000 | 5.1603                   | *       |
| 2264        | 32.000000 | 55.600000 | 5.3085                   | *       |
| 2291        | 35.000000 | 60.900000 | 5.9406                   | *       |
| 2732        | 66.000000 | 14.900000 | -4.7849                  | *       |

The following statements request fitted values for 10 quantile levels ranging from 0.03 to 0.97:

```
proc quantreg data=bmimen algorithm=interior(tolerance=1e-5) ci=none;
 model logbmi = inveage sqrtage age sqrtage*age
 age*age age*age*age
 / quantile=0.03,0.05,0.1,0.25,0.5,0.75,
 0.85,0.90,0.95,0.97;
 output out=outp pred=p/columnwise;
run;

data outbmi;
 set outp;
 pbmi = exp(p);
run;

proc sgplot data=outbmi;
 title 'BMI Percentiles for Men: 2-80 Years Old';
 yaxis label='BMI (kg/m**2)' min=10 max=45 values=(10 15 20 25 30 35 40 45);
 xaxis label='Age (Years)' min=2 max=80 values=(2 10 20 30 40 50 60 70 80);

 scatter x=age y=bmi /markerattrs=(size=1);
 series x=age y=pbmi/group=QUANTILE;
run;
```

The fitted values are stored in the OUTPUT data set outp. The COLUMNWISE option arranges these fitted values for all quantiles in the single variable p by groups of the quantiles. After the exponential transformation, the fitted BMI values together with the original BMI values are plotted against age to create the display shown in [Figure 77.2](#).

The fitted quantile curves reveal important information. During the quick growth period (ages 2 to 20), the dispersion of BMI increases dramatically; it becomes stable during middle age, and then it contracts after age 60. This pattern suggests that effective population weight control should start in childhood.

Compared to the 97th percentile in reference growth charts published by CDC in 2000 (Kuczmarski, Ogden, and Guo 2002), the 97th percentile for 10-year-old boys in [Figure 77.2](#) is 6.4 BMI units higher (an increase of 27%). This can be interpreted as a warning of overweight or obesity. See Chen (2005) for a detailed analysis.

## Syntax: QUANTREG Procedure

The following statements are available in the QUANTREG procedure:

```

PROC QUANTREG < options > ;
 BY variables ;
 CLASS variables ;
 EFFECT name = effect-type (variables < / options >) ;
 ESTIMATE < 'label' > estimate-specification < / options > ;
 ID variables ;
 MODEL response = independents < / options > ;
 OUTPUT < OUT= SAS-data-set > < options > ;
 PERFORMANCE < options > ;
 TEST effects < / options > ;
 WEIGHT variable ;

```

The PROC QUANTREG statement invokes the QUANTREG procedure. The CLASS statement specifies which explanatory variables are treated as categorical. The ID statement names variables to identify observations in the outlier diagnostics tables. The MODEL statement is required and specifies the variables used in the regression. Main effects and interaction terms can be specified in the MODEL statement, as in the GLM procedure (Chapter 42, “The GLM Procedure.”) The OUTPUT statement creates an output data set containing predicted values, residuals, and estimated standard errors. The PERFORMANCE statement tunes the performance of PROC QUANTREG by using single or multiple processors available in the hardware. The TEST statement requests linear tests for the model parameters. The WEIGHT statement identifies a variable in the input data set whose values are used to weight the observations. In one invocation of PROC QUANTREG, multiple OUTPUT and TEST statements are allowed.

The EFFECT and ESTIMATE statements are also available in other procedures. Summary descriptions of functionality and syntax for these statements are provided in this chapter, and you can find full documentation about them in Chapter 19, “Shared Concepts and Topics.”

## PROC QUANTREG Statement

```

PROC QUANTREG < options > ;

```

The PROC QUANTREG statement invokes the QUANTREG procedure. [Table 77.1](#) summarizes the options available in the PROC QUANTREG statement.

**Table 77.1** PROC QUANTREG Statement Options

| Option     | Description                                                     |
|------------|-----------------------------------------------------------------|
| ALGORITHM= | Specifies an algorithm to estimate the regression parameters    |
| CI=        | Specifies a method to compute confidence intervals              |
| DATA=      | Specifies the input SAS data set                                |
| INEST=     | Specifies an input SAS data set that contains initial estimates |
| NAMELEN=   | Specifies the length of effect names                            |
| ORDER=     | Specifies the order in which to sort classification variables   |

Table 77.1 continued

| Option  | Description                                                         |
|---------|---------------------------------------------------------------------|
| OUTEST= | Specifies an output SAS data set containing the parameter estimates |
| PLOT    | Specifies options that control details of the plots                 |

You can specify the following options in the PROC QUANTREG statement.

**ALGORITHM=***algorithm* < (*suboptions*) >

specifies an algorithm to estimate the regression parameters. Three algorithms are available: simplex (SIMPLEX), interior point (INTERIOR), and smoothing (SMOOTH).

The default algorithm depends on the number of the observations ( $n$ ) and the number of the covariates ( $p$ ) in the model estimation. See Table 77.2 for the relevant defaults.

Table 77.2 The Default Estimation Algorithm

|               | $p \leq 100$   | $p > 100$ |
|---------------|----------------|-----------|
| $n \leq 5000$ | Simplex        | Smoothing |
| $n > 5000$    | Interior point | Smoothing |

Table 77.3 summarizes the options available for each of these methods.

Table 77.3 Options for Estimation Algorithms

| ALGORITHM= Value | Algorithm      | Suboptions               |
|------------------|----------------|--------------------------|
| SIMPLEX          | Simplex        | MAXSTATIONARY=           |
| INTERIOR         | Interior point | KAPPA= MAXIT= TOLERANCE= |
| SMOOTH           | Smoothing      | RRATIO=                  |

With ALGORITHM=SIMPLEX you can specify the following *suboption*:

- MAXSTATIONARY= $m$  specifies that if the objective function has not improved for  $m$  consecutive iterations, the algorithm terminates. By default,  $m = 1000$ .

With ALGORITHM=INTERIOR you can specify the following *suboptions*:

- KAPPA=*value* specifies the step length parameter for the interior point algorithm. This parameter should be between 0 and 1. The larger the parameter, the faster the algorithm. However, numeric instability can occur as the parameter approaches 1. By default, KAPPA=0.99995. See the section “Interior Point Algorithm” on page 6517 for details.
- MAXIT= $m$  sets the maximum number of iterations for the interior point algorithm. By default,  $m = 1000$ .
- TOLERANCE=*value* specifies the tolerance for the convergence criterion of the interior point algorithm. The default *value* is  $1E-8$ . The QUANTREG procedure uses the duality gap as the convergence criterion. See the section “Interior Point Algorithm” on page 6517 for details.

With the interior point algorithm, you can use the PERFORMANCE statement to enable parallel computing when multiple processors are available in the hardware.

With ALGORITHM=SMOOTH you can specify the following *suboption*:

- RRATIO=*value* specifies the reduction ratio for the smoothing algorithm. This ratio is used for reducing the threshold of the smoothing algorithm. The *value* should be between 0 and 1. In theory, the smaller the reduction ration, the faster the smoothing algorithm. However, the optimal ratio is quite data dependent in practice. See the section “Smoothing Algorithm” on page 6520 for details.

**ALPHA=*value***

sets the confidence level for the confidence intervals for regression parameters. The *value* must be between 0 and 1. The default is ALPHA=0.05, corresponding to a 0.95 confidence interval.

**CI=NONE | RANK | SPARSITY<(BF | HS)></IID> | RESAMPLING<(NREP=*n*)>**

specifies a method to compute confidence intervals for regression parameters. When you specify CI=SPARSITY or CI=RESAMPLING, the QUANTREG procedure also computes standard errors, *t* values, and *p*-values for regression parameters.

The following table summarizes these methods.

**Table 77.4** Options for Confidence Intervals

| Value of CI= | Method                           | Additional Options |
|--------------|----------------------------------|--------------------|
| NONE         | No confidence intervals computed |                    |
| RANK         | By inverting rank-score tests    |                    |
| SPARSITY     | By estimating sparsity function  | HS BF IID          |
| RESAMPLING   | By resampling                    | NREP               |

By default, when there are fewer than 5,000 observations, fewer than 20 variables in the data set, and the algorithm is simplex, the QUANTREG procedure computes confidence intervals by using the inverting rank-score test method; otherwise, the resampling method is used.

By default, confidence intervals are not computed for the quantile process, which is estimated when you specify the QUANTILE=PROCESS option in the MODEL statement. Confidence intervals for the quantile process are computed with the sparsity or resampling methods when you specify CI=SPARSITY or CI=RESAMPLING, respectively. The rank method for confidence intervals is not available with quantile processes because it is computationally prohibitive.

With the SPARSITY option, there are two suboptions for estimating the sparsity function. If you specify the IID suboption, the sparsity function is estimated by assuming that the errors in the linear model are independent and identically distributed (iid). By default, the sparsity function is estimated by assuming that the conditional quantile function is locally linear. See the section “Sparsity” on page 6523 for details. With both methods two bandwidth selection methods are available. You can specify the Bofinger method with the BF suboption or the Hall-Sheather method with the HS suboption. By default, the Hall-Sheather method is used.

With the RESAMPLING option, you can specify the number of repeats with the NREP=*n* suboption. By default, NREP=200. The value of *n* must be greater than 50.



**DATA=SAS-data-set**

specifies the input SAS data set used by the QUANTREG procedure. By default, the most recently created SAS data set is used.

**INEST=SAS-data-set**

specifies an input SAS data set that contains initial estimates for all the parameters in the model. The interior point algorithm and the smoothing algorithm use these estimates as a start. See the section “[INEST= Data Set](#)” on page 6529 for a detailed description of the contents of the INEST= data set.

**NAMELEN=*n***

specifies the length of effect names in tables and output data sets to be *n* characters, where *n* is a value between 20 and 200. The default length is 20 characters.

**ORDER=DATA | FORMATTED | FREQ | INTERNAL**

specifies the sort order for the levels of the classification variables (which are specified in the **CLASS** statement). This option applies to the levels for all classification variables, except when you use the (default) ORDER=FORMATTED option with numeric classification variables that have no explicit format. With this option, the levels of such variables are ordered by their internal value.

The ORDER= option can take the following values:

| Value of ORDER=  | Levels Sorted By                                                                                                                       |
|------------------|----------------------------------------------------------------------------------------------------------------------------------------|
| <b>DATA</b>      | Order of appearance in the input data set                                                                                              |
| <b>FORMATTED</b> | External formatted value, except for numeric variables with no explicit format, which are sorted by their unformatted (internal) value |
| <b>FREQ</b>      | Descending frequency count; levels with the most observations come first in the order                                                  |
| <b>INTERNAL</b>  | Unformatted value                                                                                                                      |

By default, ORDER=FORMATTED. For ORDER=FORMATTED and ORDER=INTERNAL, the sort order is machine-dependent. For more information about sort order, see the chapter on the SORT procedure in the *Base SAS Procedures Guide* and the discussion of BY-group processing in *SAS Language Reference: Concepts*.

**OUTEST=SAS-data-set**

specifies an output SAS data set containing the parameter estimates for all quantiles. See the section “[OUTEST= Data Set](#)” on page 6529 for a detailed description of the contents of the OUTEST= data set.

**PLOT | PLOTS**< (*global-plot-options*) > <=*plot-request* >

**PLOT | PLOTS**< (*global-plot-options*) > <=*(plot-request* < ... *plot-request* > ) >

specifies options that control details of the plots. These plots fall into two categories, diagnostic plots and fit plots. If you do not specify the PLOTS= option, PROC QUANTREG produces the quantile fit plot by default when a single continuous variable is specified in the model. You can use the PLOTS= option in the PROC QUANTREG statement to request various diagnostic plots. In addition

to these two categories of plots, you can use the **PLOT=** option in the MODEL statement to request the quantile process plot for any effects specified in the model.

When you specify one *plot-request*, you can omit the parentheses around the plot request. Here are some examples:

```
plots=ddplot
plots=(ddplot rdplot)
```

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;

proc quantreg plots=fitplot;
 model y=x1;
run;

ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS](#).”

The *global-plot-options* apply to all plots generated by the QUANTREG procedure. The following global plot option is available:

**MAXPOINTS=NONE** | *number*

specifies that plots with elements that require processing more than *number* points be suppressed. The default is MAXPOINTS=5000. This cutoff is ignored if you specify MAXPOINTS=NONE.

**ONLY**

suppresses the default quantile fit plot. Only plots specifically requested are displayed.

You can specify more than one plot request within the parentheses after PLOTS=. For a single plot request, you can omit the parentheses. The following plot requests are available.

**ALL**

creates all appropriate plots.

**DDPLOT<(LABEL=ALL | LEVERAGE | NONE | OUTLIER)>**

creates a plot of robust distance against Mahalanobis distance. See the section “[Leverage Point and Outlier Detection](#)” on page 6528 for details about robust distance. The LABEL= option specifies how the points on this plot are to be labeled, as summarized by the following table.

**Table 77.5** Options for Label

| Value of LABEL= | Label Method          |
|-----------------|-----------------------|
| ALL             | Label all points      |
| LEVERAGE        | Label leverage points |
| NONE            | No labels             |
| OUTLIERS        | Label outliers        |

By default, the QUANTREG procedure labels both outliers and leverage points.

If you specify ID variables in the ID statement, the values of the first ID variable are used as labels; otherwise, observation numbers are used as labels.

**FITPLOT<(NOLIMITS | SHOWLIMITS | NODATA)>**

creates a plot of fitted conditional quantiles against the single continuous variable that is specified in the model. This plot is produced only when the response is modeled as a function of a single continuous variable. Multiple lines or curves are drawn on this plot if you specify several quantiles with the QUANTILE= option in the MODEL statement. By default, confidence limits are added to the plot when a single quantile is requested, and the confidence limits are not shown on the plot when multiple quantiles are requested. The NOLIMITS option suppresses these limits. The SHOWLIMITS option adds these limits when multiple quantiles are requested. The NODATA option suppresses the observed data, which are superimposed on the plot by default.

**HISTOGRAM**

creates a histogram for the standardized residuals based on the quantile regression estimates. The histogram is superimposed with a normal density curve and a kernel density curve.

**NONE**

suppresses all plots.

**QQPLOT**

creates the normal quantile-quantile plot for the standardized residuals based on the quantile regression estimates.

**RDPLOT<(LABEL=ALL | LEVERAGE | NONE | OUTLIER)>**

creates the plot of standardized residual against robust distance. See the section “[Leverage Point and Outlier Detection](#)” on page 6528 for details about robust distance. The LABEL= option specifies a label method for points on this plot. These label methods are described in [Table 77.5](#).

By default, the QUANTREG procedure labels both outliers and leverage points.

If you specify ID variables in the ID statement, the values of the first ID variable are used as labels; otherwise, observation numbers are used as labels.

**PP**

requests preprocessing to speed up the interior point algorithm or the smoothing algorithm. The preprocessing uses a subsampling algorithm to reduce the original problem to a smaller one iteratively. It assumes that the data set is evenly distributed. Preprocessing should be used only for very large data sets, such as data sets with more than 100,000 observations. See Portnoy and Koenker (1997) for details.

---

## BY Statement

**BY variables ;**

You can specify a BY statement with PROC QUANTREG to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input

data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the QUANTREG procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

---

## CLASS Statement

**CLASS** *variables* < / **TRUNCATE** > ;

The CLASS statement names the classification variables to be used in the model. Typical classification variables are Treatment, Sex, Race, Group, and Replication. If you use the CLASS statement, it must appear before the MODEL statement.

Classification variables can be either character or numeric. By default, class levels are determined from the entire set of formatted values of the CLASS variables.

**NOTE:** Prior to SAS 9, class levels were determined by using no more than the first 16 characters of the formatted values. To revert to this previous behavior, you can use the TRUNCATE option in the CLASS statement.

In any case, you can use formats to group values into levels. See the discussion of the FORMAT procedure in the *Base SAS Procedures Guide* and the discussions of the FORMAT statement and SAS formats in *SAS Formats and Informats: Reference*. You can adjust the order of CLASS variable levels with the ORDER= option in the PROC QUANTREG statement. You can specify the following option in the CLASS statement after a slash (/):

### TRUNCATE

specifies that class levels should be determined by using only up to the first 16 characters of the formatted values of CLASS variables. When formatted values are longer than 16 characters, you can use this option to revert to the levels as determined in releases prior to SAS 9.

---

## EFFECT Statement

**EFFECT** *name=effect-type (variables < / options >)* ;

The EFFECT statement enables you to construct special collections of columns for design matrices. These collections are referred to as *constructed effects* to distinguish them from the usual model effects that are formed from continuous or classification variables, as discussed in the section “GLM Parameterization of Classification Variables and Effects” on page 383 in Chapter 19, “Shared Concepts and Topics.”

You can specify the following *effect-types*:

|                          |                                                                                                                                                                                                           |
|--------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>COLLECTION</b>        | is a collection effect that defines one or more variables as a single effect with multiple degrees of freedom. The variables in a collection are considered as a unit for estimation and inference.       |
| <b>LAG</b>               | is a classification effect in which the level that is used for a given period corresponds to the level in the preceding period.                                                                           |
| <b>MULTIMEMBER   MM</b>  | is a multimember classification effect whose levels are determined by one or more variables that appear in a CLASS statement.                                                                             |
| <b>POLYNOMIAL   POLY</b> | is a multivariate polynomial effect in the specified numeric variables.                                                                                                                                   |
| <b>SPLINE</b>            | is a regression spline effect whose columns are univariate spline expansions of one or more variables. A spline expansion replaces the original variable with an expanded or larger set of new variables. |

Table 77.6 summarizes the *options* available in the EFFECT statement.

**Table 77.6** EFFECT Statement Options

| Option                             | Description                                                                                                                                          |
|------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Collection Effects Options</b>  |                                                                                                                                                      |
| DETAILS                            | Displays the constituents of the collection effect                                                                                                   |
| <b>Lag Effects Options</b>         |                                                                                                                                                      |
| DESIGNROLE=                        | Names a variable that controls to which lag design an observation is assigned                                                                        |
| DETAILS                            | Displays the lag design of the lag effect                                                                                                            |
| NLAG=                              | Specifies the number of periods in the lag                                                                                                           |
| PERIOD=                            | Names the variable that defines the period                                                                                                           |
| WITHIN=                            | Names the variable or variables that define the group within which each period is defined                                                            |
| <b>Multimember Effects Options</b> |                                                                                                                                                      |
| NOEFFECT                           | Specifies that observations with all missing levels for the multimember variables should have zero values in the corresponding design matrix columns |
| WEIGHT=                            | Specifies the weight variable for the contributions of each of the classification effects                                                            |

Table 77.6 *continued*

| Option                            | Description                                                                                             |
|-----------------------------------|---------------------------------------------------------------------------------------------------------|
| <b>Polynomial Effects Options</b> |                                                                                                         |
| DEGREE=                           | Specifies the degree of the polynomial                                                                  |
| MDEGREE=                          | Specifies the maximum degree of any variable in a term of the polynomial                                |
| STANDARDIZE=                      | Specifies centering and scaling suboptions for the variables that define the polynomial                 |
| <b>Spline Effects Options</b>     |                                                                                                         |
| BASIS=                            | Specifies the type of basis (B-spline basis or truncated power function basis) for the spline expansion |
| DEGREE=                           | Specifies the degree of the spline transformation                                                       |
| KNOTMETHOD=                       | Specifies how to construct the knots for spline effects                                                 |

For more information about the syntax of these *effect-types* and how columns of constructed effects are computed, see the section “EFFECT Statement” on page 393 in Chapter 19, “Shared Concepts and Topics.”

## ESTIMATE Statement

```
ESTIMATE <'label'> estimate-specification <(divisor=n)>
 < , ... <'label'> estimate-specification <(divisor=n)> >
 </ options > ;
```

The ESTIMATE statement provides a mechanism for obtaining custom hypothesis tests. Estimates are formed as linear estimable functions of the form  $L\beta$ . You can perform hypothesis tests for the estimable functions, construct confidence limits, and obtain specific nonlinear transformations.

Table 77.7 summarizes the options available in the ESTIMATE statement.

Table 77.7 ESTIMATE Statement Options

| Option                                                     | Description                                                               |
|------------------------------------------------------------|---------------------------------------------------------------------------|
| <b>Construction and Computation of Estimable Functions</b> |                                                                           |
| DIVISOR=                                                   | Specifies a list of values to divide the coefficients                     |
| NOFILL                                                     | Suppresses the automatic fill-in of coefficients for higher-order effects |
| SINGULAR=                                                  | Tunes the estimability checking difference                                |

Table 77.7 continued

| Option                                              | Description                                                               |
|-----------------------------------------------------|---------------------------------------------------------------------------|
| <b>Degrees of Freedom and <math>p</math>-values</b> |                                                                           |
| ADJUST=                                             | Determines the method for multiple comparison adjustment of estimates     |
| ALPHA= $\alpha$                                     | Determines the confidence level ( $1 - \alpha$ )                          |
| LOWER                                               | Performs one-sided, lower-tailed inference                                |
| STEPDOWN                                            | Adjusts multiplicity-corrected $p$ -values further in a step-down fashion |
| TESTVALUE=                                          | Specifies values under the null hypothesis for tests                      |
| UPPER                                               | Performs one-sided, upper-tailed inference                                |
| <b>Statistical Output</b>                           |                                                                           |
| CL                                                  | Constructs confidence limits                                              |
| CORR                                                | Displays the correlation matrix of estimates                              |
| COV                                                 | Displays the covariance matrix of estimates                               |
| E                                                   | Prints the $L$ matrix                                                     |
| JOINT                                               | Produces a joint $F$ or chi-square test for the estimable functions       |
| SEED=                                               | Specifies the seed for computations that depend on random numbers         |

For details about the syntax of the ESTIMATE statement, see the section “ESTIMATE Statement” on page 437 in Chapter 19, “Shared Concepts and Topics.”

## ID Statement

**ID** *variables* ;

When the diagnostics table is requested with the DIAGNOSTICS option in the MODEL statement, the variables listed in the ID statement are displayed in addition to the observation number. These values are useful for identifying observations. If the ID statement is omitted, only the observation number is displayed.

## MODEL Statement

**<label>** MODEL *response* = *<effects>* *</options>* ;

Main effects and interaction terms can be specified in the MODEL statement, as in the GLM procedure (Chapter 42, “The GLM Procedure.”) Classification variables in the MODEL statement must be specified in the CLASS statement.

The optional *label*, which must be a valid SAS name, is used to label output from the matching MODEL statement.

## Options

Table 77.8 summarizes the options available in the MODEL statement.

**Table 77.8** MODEL Statement Options

| Option      | Description                                                          |
|-------------|----------------------------------------------------------------------|
| CORRB       | Produces the estimated correlation matrix                            |
| COVB        | Produces the estimated covariance matrix                             |
| CUTOFF=     | Specifies the multiplier of the cutoff value for outlier detection   |
| DIAGNOSTICS | Requests the outlier diagnostics                                     |
| ITPRINT     | Displays the iteration history                                       |
| LEVERAGE    | Requests an analysis of leverage points                              |
| NODIAG      | Suppresses the computation for outlier diagnostics                   |
| NOINT       | Specifies no-intercept regression                                    |
| NOSUMMARY   | Suppresses the computation for summary statistics                    |
| PLOT=       | Requests plots                                                       |
| QUANTILE=   | Specifies the quantile levels                                        |
| SCALE=      | Specifies the scale value used to compute the standardized residuals |
| SEED=       | Specifies the seed for the random number generator                   |
| SINGULAR=   | Specifies the tolerance for testing singularity                      |

You can specify the following options for the model fit.

### CORRB

produces the estimated correlation matrix of the parameter estimates. When the resampling method is used to compute the confidence intervals, the QUANTREG procedure computes the bootstrap correlation. When the sparsity method is used to compute the confidence intervals, the procedure computes the asymptotic correlation based on an estimator of the sparsity function. The rank method for confidence intervals does not provide a correlation estimate.

### COVB

produces the estimated covariance matrix of the parameter estimates. When the resampling method is used to compute the confidence intervals, the QUANTREG procedure computes the bootstrap covariance. When the sparsity method is used to compute the confidence intervals, the procedure computes the asymptotic covariance based on an estimator of the sparsity function. The rank method for confidence intervals does not provide a covariance estimate.

### CUTOFF=*value*

specifies the multiplier of the cutoff value for outlier detection. The default *value* is 3.

### DIAGNOSTICS<(ALL)>

requests the outlier diagnostics. By default, only observations identified as outliers or leverage points are displayed. To request that all observations be displayed, specify the ALL option.

### ITPRINT

displays the iteration history of the interior point algorithm or the smoothing algorithm.



**LEVERAGE<(CUTOFF=*value* | CUTOFFALPHA=*value* | H=*n*)>**

requests an analysis of leverage points for the continuous covariates. The results are added to the diagnostics table, which you can request with the DIAGNOSTICS option in the MODEL statement. You can specify the cutoff value for leverage-point detection with the CUTOFF= option. The default cutoff value is  $\sqrt{\chi_{p;1-\alpha}^2}$ , where  $\alpha$  can be specified with the CUTOFFALPHA= option. By default,  $\alpha = 0.025$ . You can use the H= option to specify the number of points to be minimized for the MCD algorithm used for the leverage-point analysis. By default,  $H = [(3n + p + 1)/4]$ , where  $n$  is the number of observations and  $p$  is the number of independent variables. The LEVERAGE option is ignored if the model includes classification variables as covariates.

**NODIAG**

suppresses the computation for outlier diagnostics. If you specify the NODIAG option, the diagnostics summary table will not be provided.

**NOINT**

specifies no intercept regression.

**NOSUMMARY**

suppresses the computation for summary statistics. If you specify the NOSUMMARY option, the summary statistics table will not be provided.

**PLOT=*plot-option*****PLOTS=(*plot-options*)**

You can use the PLOTS= option in the MODEL statement together with ODS Graphics to request the quantile process plot in addition to all plots available with the PLOT= option in the PROC QUANTREG statement. The plot options in the PROC QUANTREG statement overwrite the plot options in the MODEL statement if you specify the same options in both statements.

You can specify the following plot option only in the MODEL statement:

**QUANTPLOT<(EFFECTS) </ <NOLIMITS> <EXTENDCI> <UNPACK> <OLS> > >**

plots the regression quantile process. The estimated coefficient of each specified covariate effect is plotted as a function of the quantile. If you do not specify a covariate effect, quantile processes are plotted for all covariate effects in the MODEL statement. You can use the NOLIMITS option to suppress confidence bands for the quantile processes. By default, confidence bands are plotted, and process plots are displayed in panels, each of which can hold up to four plots. By default, the confidence limits are plotted for quantiles in the range between 0.05 and 0.95. You can use the EXTENDCI option to plot the confidence limits even for quantiles outside this range. You can use the UNPACK option to create individual process plots. For an individual process plot, you can superimpose the ordinary least squares estimate and its confidence limits by specifying the OLS option. The confidence level of the ordinary least squares estimate is specified with the ALPHA= option in the PROC QUANTREG statement.

Again, ODS Graphics must be enabled before requesting plots.

For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

**QUANTILE=number-list | PROCESS**

specifies the quantile levels for the quantile regression. You can specify any number of quantile levels in (0, 1). You can also compute the entire quantile process by specifying the PROCESS option. Only the simplex algorithm is available for computing the quantile process.

If you do not specify the QUANTILE= option, the QUANTREG procedure fits a median regression, which corresponds to QUANTILE=0.5.

**SCALE=number**

specifies the scale value used to compute the standardized residuals. By default, the scale is computed as the corrected median of absolute residuals. See the section “[Leverage Point and Outlier Detection](#)” on page 6528 for details.

**SEED=number**

specifies the seed for the random number generator used to compute the MCMB confidence intervals. This seed is also used to randomly select the subgroups for preprocessing when you specify the PP option in the PROC QUANTREG statement. If you do not specify a seed, or if you specify a value less than or equal to zero, the seed is generated from reading the time of day from the computer clock.

By default or if you specify zero, the QUANTREG procedure generates a seed between one and one billion.

**SINGULAR=value**

sets the tolerance for testing singularity of the information matrix and the crossproducts matrix for the initial least squares estimates. Roughly, the test requires that a pivot be at least this value times the original diagonal value. By default, SINGULAR=1E-12.

---

## OUTPUT Statement

**OUTPUT** < **OUT=SAS-data-set** > *keyword=name* < . . . *keyword=name* > < / **COLUMNWISE** > ;

The OUTPUT statement creates a SAS data set containing statistics calculated after fitting models for all specified quantiles with the QUANTILE= option in the MODEL statement. At least one specification of the form *keyword=name* is required.

All variables in the original data set are included in the new data set, along with the variables created as options to the OUTPUT statement. These new variables contain fitted values and estimated quantiles. If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*.

If you specify multiple quantiles in the MODEL statement, the COLUMNWISE option arranges the created OUTPUT data set in column-wise form. This arrangement repeats the input data for each quantile. By default, the OUTPUT data set is created in row-wise form. For each appropriate keyword specified in the OUTPUT statement, one variable for each specified quantile is generated. These variables appear in the sorted order of the specified quantiles.

The following specifications can appear in the OUTPUT statement:

- `OUT=SAS-data-set` specifies the new data set. By default, the procedure uses the `DATAn` convention to name the new data set.
- `keyword=name` specifies the statistics to include in the output data set and gives names to the new variables. Specify a keyword for each desired statistic (see the following list of keywords), an equal sign, and the variable to contain the statistic.

The keywords allowed and the statistics they represent are as follows:

- `LEVERAGE` specifies a variable to indicate leverage points. To include this variable in the OUTPUT data set, you must specify the `LEVERAGE` option in the MODEL statement. See the section “[Leverage Point and Outlier Detection](#)” on page 6528 for how to define `LEVERAGE`.
- `MAHADIST | MD` specifies a variable to contain the Mahalanobis distance. To include this variable in the OUTPUT data set, you must specify the `LEVERAGE` option in the MODEL statement.
- `OUTLIER` specifies a variable to indicate outliers. See the section “[Leverage Point and Outlier Detection](#)” on page 6528 for how to define `OUTLIER`.
- `PREDICTED | P` specifies a variable to contain the estimated response.
- `QUANTILE | Q` specifies a variable to contain the quantile for which the quantile regression is fitted. If you specify the `COLUMNWISE` option, this variable is created by default. If multiple quantiles are specified in the MODEL statement and the `COLUMNWISE` option is not specified, this variable is not created.
- `RESIDUAL | RES` specifies a variable to contain the residuals (unstandardized)
- $$y_i - \mathbf{x}'_i \hat{\boldsymbol{\beta}}$$
- `ROBDIST | RD` specifies a variable to contain the robust MCD distance. To include this variable in the OUTPUT data set, you must specify the `LEVERAGE` option in the MODEL statement.
- `SPLINE | SP` specifies a variable to contain the estimated spline effect, which includes all spline effects in the model and their interactions.
- `SRESIDUAL | SR` specifies a variable to contain the standardized residuals
- $$\frac{y_i - \mathbf{x}'_i \hat{\boldsymbol{\beta}}}{\hat{\sigma}}$$
- See the section “[Leverage Point and Outlier Detection](#)” on page 6528 for how to compute  $\sigma$ .
- `STDP` specifies a variable to contain the estimates of the standard errors of the estimated response.

---

## PERFORMANCE Statement

The PERFORMANCE statement is used to change default options that affect the performance of PROC QUANTREG and to request tables that show the performance options in effect and timing details.

**PERFORMANCE** < options > ;

The following options are available:

### CPUCOUNT=1-1024

#### CPUCOUNT=ACTUAL

specifies the number of processors to use in the computation of the interior point algorithm. CPU-COUNT=ACTUAL sets CPUCOUNT to be the number of physical processors available. Note that this can be less than the physical number of CPUs if the SAS process has been restricted by system administration tools. Setting CPUCOUNT= to a number greater than the actual number of available CPUs might result in reduced performance. This option overrides the SAS system option CPU-COUNT=. If CPUCOUNT=1, then NOTHREADS is in effect, and PROC QUANTREG uses singly threaded code.

#### DETAILS

requests the “PerfSettings” table that shows the performance settings in effect and the “Timing” table that provides a broad timing breakdown of the PROC QUANTREG step.

#### THREADS

enables multithreaded computation for the interior point algorithm. This option overrides the SAS system option THREADS | NOTHREADS. If you do not specify the ALGORITHM=INTERIOR option, then PROC QUANTREG ignores this option and uses singly threaded code.

#### NOTHREADS

disables multithreaded computation for the interior point algorithm. This option overrides the SAS system option THREADS | NOTHREADS.

---

## TEST Statement

< label: > **TEST** effects < / options > ;

In quantile regression analysis, you might be interested in testing whether a covariate effect is statistically significant for a given quantile. In other situations, you might be interested in testing whether the coefficients of a covariate are the same across a set of quantiles. You can use the TEST Statement to perform these tests.

### Testing Effects of Covariates

You can use TEST statement to obtain a test for the canonical linear hypothesis concerning the parameters of the tested effects

$$\beta_j = 0, \quad j = i_1, \dots, i_q$$

where  $q$  is the total number of parameters of the tested effects. The tested *effects* can be any set of effects in the MODEL statement. Three types of tests (Wald, likelihood ratio, and rank methods) are available for testing effects of covariates by the following *options* in the TEST statement after a slash (/):

**WALD**

requests Wald tests.

**LR**

requests likelihood ratio tests.

**RANKSCORE < (NORMAL | WILCOXON | SIGN | TAU) >**

requests rank tests. The NORMAL, WILCOXON, and SIGN functions are implemented and suitable for iid error models, and the TAU score function is implemented and appropriate for non-iid error models. By default, the TAU score function is used. See Koenker (2005) for more information about the score functions.

**Testing for Heteroscedasticity**

You can test whether there is any difference among the estimated coefficients across quantiles if several quantiles are specified in the MODEL statement. The test for such heteroscedasticity can be requested by the option QINTERACT after a slash (/) in the TEST statement. See [Example 77.5](#).

You can submit multiple TEST statements, provided that they appear after the MODEL statement. The optional *label*, which must be a valid SAS name, is used to identify output from the corresponding TEST statement. See the section “[Linear Test](#)” on page 6526 for details about these tests.

**WEIGHT Statement**

**WEIGHT** *variable* ;

The WEIGHT statement specifies a weight variable in the input data set.

To request weighted quantile regression, place the weights in a variable and specify the name in the WEIGHT statement. The values of the WEIGHT variable can be nonintegral and are not truncated. Observations with nonpositive or missing values for the weight variable do not contribute to the fit of the model. See the section “[Details: QUANTREG Procedure](#)” on page 6514 for more information about weighted quantile regression.

**Details: QUANTREG Procedure****Quantile Regression as an Optimization Problem**

The model for linear quantile regression is

$$y = \mathbf{A}'\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

where  $\mathbf{y} = (y_1, \dots, y_n)'$  is the  $(n \times 1)$  vector of responses,  $\mathbf{A}' = (\mathbf{x}_1, \dots, \mathbf{x}_n)'$  is the  $(n \times p)$  regressor matrix,  $\boldsymbol{\beta} = (\beta_1, \dots, \beta_p)'$  is the  $(p \times 1)$  vector of unknown parameters, and  $\boldsymbol{\epsilon} = (\epsilon_1, \dots, \epsilon_n)'$  is the  $(n \times 1)$  vector of unknown errors.

$L_1$  regression, also known as median regression, is a natural extension of the sample median when the response is conditioned on the covariates. In  $L_1$  regression, the least absolute residuals estimate  $\hat{\beta}_{LAR}$ , referred to as the  $L_1$ -norm estimate, is obtained as the solution of the minimization problem

$$\min_{\beta \in \mathbf{R}^p} \sum_{i=1}^n |y_i - \mathbf{x}'_i \beta|$$

More generally, for quantile regression Koenker and Bassett (1978) defined the  $\tau$  regression quantile,  $0 < \tau < 1$ , as any solution to the minimization problem

$$\min_{\beta \in \mathbf{R}^p} \left[ \sum_{i \in \{i: y_i \geq \mathbf{x}'_i \beta\}} \tau |y_i - \mathbf{x}'_i \beta| + \sum_{i \in \{i: y_i < \mathbf{x}'_i \beta\}} (1 - \tau) |y_i - \mathbf{x}'_i \beta| \right]$$

The solution is denoted as  $\hat{\beta}(\tau)$ , and the  $L_1$ -norm estimate corresponds to  $\hat{\beta}(1/2)$ . The  $\tau$  regression quantile is an extension of the  $\tau$  sample quantile  $\hat{\xi}(\tau)$ , which can be formulated as the solution of

$$\min_{\xi \in \mathbf{R}} \left[ \sum_{i \in \{i: y_i \geq \xi\}} \tau |y_i - \xi| + \sum_{i \in \{i: y_i < \xi\}} (1 - \tau) |y_i - \xi| \right]$$

If you specify weights  $w_i, i = 1, \dots, n$ , with the WEIGHT statement, weighted quantile regression is carried out by solving

$$\min_{\beta_w \in \mathbf{R}^p} \left[ \sum_{i \in \{i: y_i \geq \mathbf{x}'_i \beta_w\}} w_i \tau |y_i - \mathbf{x}'_i \beta_w| + \sum_{i \in \{i: y_i < \mathbf{x}'_i \beta_w\}} w_i (1 - \tau) |y_i - \mathbf{x}'_i \beta_w| \right]$$

Weighted regression quantiles  $\beta_w$  can be used for L-estimation; see Koenker and Zhao (1994).

---

## Optimization Algorithms

The optimization problem for median regression has been formulated and solved as a linear programming (LP) problem since the 1950s. Variations of the simplex algorithm, especially the method of Barrodale and Roberts (1973), have been widely used to solve this problem. The simplex algorithm is computationally demanding in large statistical applications, and in theory the number of iterations can increase exponentially with the sample size. This algorithm is often useful with data containing no more than tens of thousands of observations.

Several alternatives have been developed to handle  $L_1$  regression for larger data sets. The interior point approach of Karmarkar (1984) solves a sequence of quadratic problems in which the relevant interior of the constraint set is approximated by an ellipsoid. The worst-case performance of the interior point algorithm has been proved to be better than that of the simplex algorithm. More important, experience has shown that the interior point algorithm is advantageous for larger problems.

Like  $L_1$  regression, general quantile regression fits nicely into the standard primal-dual formulations of linear programming.

In addition to the interior point method, various heuristic approaches are available for computing  $L_1$ -type solutions. Among these, the finite smoothing algorithm of Madsen and Nielsen (1993) is the most useful. It approximates the  $L_1$ -type objective function with a smoothing function, so that the Newton-Raphson algorithm can be used iteratively to obtain a solution after a finite number of iterations. The smoothing algorithm extends naturally to general quantile regression.

The QUANTREG procedure implements the simplex, interior point, and smoothing algorithms. The remainder of this section describes these algorithms in more detail.

### Simplex Algorithm

Let  $\boldsymbol{\mu} = [y - \mathbf{A}'\boldsymbol{\beta}]_+$ ,  $\boldsymbol{\nu} = [\mathbf{A}'\boldsymbol{\beta} - y]_+$ ,  $\boldsymbol{\phi} = [\boldsymbol{\beta}]_+$ , and  $\boldsymbol{\varphi} = [-\boldsymbol{\beta}]_+$ , where  $[z]_+$  is the nonnegative part of  $z$ .

Let  $D_{LAR}(\boldsymbol{\beta}) = \sum_{i=1}^n |y_i - \mathbf{x}'_i \boldsymbol{\beta}|$ . For the  $L_1$  problem, the simplex approach solves  $\min_{\boldsymbol{\beta}} D_{LAR}(\boldsymbol{\beta})$  by reformulating it as the constrained minimization problem

$$\min_{\boldsymbol{\beta}} \{ \mathbf{e}'\boldsymbol{\mu} + \mathbf{e}'\boldsymbol{\nu} \mid \mathbf{y} = \mathbf{A}'\boldsymbol{\beta} + \boldsymbol{\mu} - \boldsymbol{\nu}, \{\boldsymbol{\mu}, \boldsymbol{\nu}\} \in \mathbf{R}_+^n \}$$

where  $\mathbf{e}$  denotes an  $(n \times 1)$  vector of ones.

Let  $\mathbf{B} = [\mathbf{A}' \quad -\mathbf{A}' \quad \mathbf{I} \quad -\mathbf{I}]$ ,  $\boldsymbol{\theta} = (\boldsymbol{\phi}' \quad \boldsymbol{\varphi}' \quad \boldsymbol{\mu}' \quad \boldsymbol{\nu}')$ , and  $\mathbf{d} = (\mathbf{0}' \quad \mathbf{0}' \quad \mathbf{e}' \quad \mathbf{e}')$ , where  $\mathbf{0}' = (0 \ 0 \ \dots \ 0)_p$ . The reformulation presents a standard LP problem:

$$\begin{aligned} (P) \quad & \min_{\boldsymbol{\theta}} \mathbf{d}'\boldsymbol{\theta} \\ & \text{subject to} \quad \mathbf{B}\boldsymbol{\theta} = \mathbf{y} \\ & \quad \boldsymbol{\theta} \geq \mathbf{0} \end{aligned}$$

This problem has the dual formulation

$$\begin{aligned} (D) \quad & \max_{\mathbf{z}} \mathbf{y}'\mathbf{z} \\ & \text{subject to} \quad \mathbf{B}'\mathbf{z} \leq \mathbf{d} \end{aligned}$$

which can be simplified as

$$\max_{\mathbf{z}} \mathbf{y}'\mathbf{z}; \quad \text{subject to} \quad \mathbf{A}\mathbf{z} = \mathbf{0}, \mathbf{z} \in [-1, 1]^n$$

By setting  $\boldsymbol{\eta} = \frac{1}{2} + \frac{1}{2}\mathbf{e}$ ,  $\mathbf{b} = \frac{1}{2}\mathbf{A}\mathbf{e}$ , the problem becomes

$$\max_{\boldsymbol{\eta}} \mathbf{y}'\boldsymbol{\eta}; \quad \text{subject to} \quad \mathbf{A}\boldsymbol{\eta} = \mathbf{b}, \boldsymbol{\eta} \in [0, 1]^n$$

For quantile regression, the minimization problem is  $\min_{\boldsymbol{\beta}} \sum \rho_{\tau}(y_i - \mathbf{x}'_i \boldsymbol{\beta})$ , and a similar set of steps leads to the dual formulation

$$\max_{\mathbf{z}} \mathbf{y}'\mathbf{z}; \quad \text{subject to} \quad \mathbf{A}\mathbf{z} = (1 - \tau)\mathbf{A}\mathbf{e}, \mathbf{z} \in [0, 1]^n$$

The QUANTREG procedure solves this LP problem by using the simplex algorithm of Barrodale and Roberts (1973). This algorithm solves the primary LP problem (P) by two stages, which exploit the special structure of the coefficient matrix  $\mathbf{B}$ . The first stage picks the columns in  $\mathbf{A}'$  or  $-\mathbf{A}'$  as pivotal columns. The

second stage interchanges the columns in  $\mathbf{I}$  or  $-\mathbf{I}$  as basis or nonbasis columns, respectively. The algorithm obtains an optimal solution by executing these two stages interactively. Moreover, because of the special structure of  $\mathbf{B}$ , only the main data matrix  $\mathbf{A}$  is stored in the current memory.

Although this special version of the simplex algorithm was introduced for median regression, it extends naturally to quantile regression for any given quantile and even to the entire quantile process (Koenker and d'Orey 1994). It greatly reduces the computing time required by the general simplex algorithm, and it is suitable for data sets with fewer than 5,000 observations and 50 variables.

## Interior Point Algorithm

There are many variations of interior point algorithms. The QUANTREG procedure uses the primal-dual predictor-corrector algorithm implemented by Lustig, Marsten, and Shanno (1992). The text by Roos, Terlaky, and Vial (1997) provides more information about this particular algorithm. The following brief introduction of this algorithm uses the notation in the first reference.

To be consistent with the conventional LP setting, let  $\mathbf{c} = -\mathbf{y}$ ,  $\mathbf{b} = (1 - \tau)\mathbf{A}\mathbf{e}$ , and let  $\mathbf{u}$  be the general upper bound. The linear program to be solved is

$$\begin{array}{ll} & \min\{\mathbf{c}'\mathbf{z}\} \\ \text{subject to} & \mathbf{Az} = \mathbf{b} \\ & \mathbf{0} \leq \mathbf{z} \leq \mathbf{u} \end{array}$$

To simplify the computation, this is treated as the *primal* problem. The problem has  $n$  variables. The index  $i$  denotes a variable number, and  $k$  denotes an iteration number. If  $k$  is used as a subscript or superscript, it denotes “of iteration  $k$ .”

Let  $\mathbf{v}$  be the primal slack so that  $\mathbf{z} + \mathbf{v} = \mathbf{u}$ . Associate dual variables  $\mathbf{w}$  with these constraints. The interior point algorithm solves the system of equations to satisfy the Karush-Kuhn-Tucker (KKT) conditions for optimality:

$$\begin{array}{l} \mathbf{Az} = \mathbf{b} \\ \mathbf{z} + \mathbf{v} = \mathbf{u} \\ \mathbf{A}'\mathbf{t} + \mathbf{s} - \mathbf{w} = \mathbf{c} \\ \mathbf{ZSe} = \mathbf{0} \\ \mathbf{VWe} = \mathbf{0} \\ \mathbf{z}, \mathbf{s}, \mathbf{v}, \mathbf{w} \geq \mathbf{0} \\ \text{where} \\ \mathbf{W} = \text{diag}(\mathbf{w}) \text{ (that is, } W_{i,j} = w_i \text{ if } i = j, W_{i,j} = 0 \text{ otherwise)} \\ \mathbf{V} = \text{diag}(\mathbf{v}), \mathbf{Z} = \text{diag}(\mathbf{z}), \mathbf{S} = \text{diag}(\mathbf{s}) \end{array}$$

These are the conditions for feasibility, with the addition of *complementarity* conditions  $\mathbf{ZSe} = \mathbf{0}$  and  $\mathbf{VWe} = \mathbf{0}$ .  $\mathbf{c}'\mathbf{z} = \mathbf{b}'\mathbf{t} - \mathbf{u}'\mathbf{w}$  must occur at the optimum. Complementarity forces the optimal objectives of the primal and dual to be equal,  $\mathbf{c}'\mathbf{z}_{opt} = \mathbf{b}'\mathbf{t}_{opt} - \mathbf{u}'\mathbf{w}_{opt}$ , as



$$\begin{aligned}
0 &= \mathbf{v}'_{opt} \mathbf{w}_{opt} = (\mathbf{u} - \mathbf{z}_{opt})' \mathbf{w}_{opt} = \mathbf{u}' \mathbf{w}_{opt} - \mathbf{z}'_{opt} \mathbf{w}_{opt} \\
0 &= \mathbf{z}'_{opt} \mathbf{s}_{opt} = \mathbf{s}'_{opt} \mathbf{z}_{opt} = (\mathbf{c} - \mathbf{A}' \mathbf{t}_{opt} + \mathbf{w}_{opt})' \mathbf{z}_{opt} \\
&= \mathbf{c}' \mathbf{z}_{opt} - \mathbf{t}'_{opt} (\mathbf{A} \mathbf{z}_{opt}) + \mathbf{w}'_{opt} \mathbf{z}_{opt} = \mathbf{c}' \mathbf{z}_{opt} - \mathbf{b}' \mathbf{t}_{opt} + \mathbf{u}' \mathbf{w}_{opt}
\end{aligned}$$

Therefore

$$0 = \mathbf{c}' \mathbf{z}_{opt} - \mathbf{b}' \mathbf{t}_{opt} + \mathbf{u}' \mathbf{w}_{opt}$$

The *duality gap*,  $\mathbf{c}' \mathbf{z} - \mathbf{b}' \mathbf{t} + \mathbf{u}' \mathbf{w}$ , is used to measure the convergence of the algorithm. You can specify a tolerance for this convergence criterion with the TOLERANCE= option in the PROC QUANTREG statement.

Before the optimum is reached, it is possible for a solution  $(\mathbf{z}, \mathbf{t}, \mathbf{s}, \mathbf{v}, \mathbf{w})$  to violate the KKT conditions in one of several ways:

- Primal bound constraints can be broken,  $\delta_b = \mathbf{u} - \mathbf{z} - \mathbf{v} \neq \mathbf{0}$ .
- Primal constraints can be broken,  $\delta_c = \mathbf{b} - \mathbf{A} \mathbf{z} \neq \mathbf{0}$ .
- Dual constraints can be broken,  $\delta_d \mathbf{s} = \mathbf{c} - \mathbf{A}' \mathbf{t} - \mathbf{s} + \mathbf{w} \neq \mathbf{0}$ .
- Complementarity conditions are unsatisfied,  $\mathbf{z}' \mathbf{s} \neq 0$  and  $\mathbf{v}' \mathbf{w} \neq 0$ .

The interior point algorithm works by using Newton's method to find a direction  $(\Delta z^k, \Delta t^k, \Delta s^k, \Delta v^k, \Delta w^k)$  to move from the current solution  $(\mathbf{z}^k, \mathbf{t}^k, \mathbf{s}^k, \mathbf{v}^k, \mathbf{w}^k)$  toward a better solution:

$$(\mathbf{z}^{k+1}, \mathbf{t}^{k+1}, \mathbf{s}^{k+1}, \mathbf{v}^{k+1}, \mathbf{w}^{k+1}) = (\mathbf{z}^k, \mathbf{t}^k, \mathbf{s}^k, \mathbf{v}^k, \mathbf{w}^k) + \kappa (\Delta z^k, \Delta t^k, \Delta s^k, \Delta v^k, \Delta w^k)$$

$\kappa$  is the *step length* and is assigned a value as large as possible, but not so large that a  $\mathbf{z}_i^{k+1}$  or  $\mathbf{s}_i^{k+1}$  is "too close" to zero. You can control the step length with the KAPPA= option in the PROC QUANTREG statement.

The QUANTREG procedure implements a predictor-corrector variant of the primal-dual interior point algorithm. First, Newton's method is used to find a direction  $(\Delta z_{aff}^k, \Delta t_{aff}^k, \Delta s_{aff}^k, \Delta v_{aff}^k, \Delta w_{aff}^k)$  in which to move. This is known as the *affine* step.

In iteration  $k$ , the *affine* step system that must be solved is

$$\begin{aligned}
\Delta z_{aff} + \Delta v_{aff} &= \delta_b \\
\mathbf{A} \Delta z_{aff} &= \delta_c \\
\mathbf{A}' \Delta t_{aff} + \Delta s_{aff} - \Delta w_{aff} &= \delta_d \\
\mathbf{S} \Delta z_{aff} + \mathbf{Z} \Delta s_{aff} &= -\mathbf{Z} \mathbf{S} \mathbf{e} \\
\mathbf{V} \Delta w_{aff} + \mathbf{W} \Delta z_{aff} &= -\mathbf{V} \mathbf{W} \mathbf{e}
\end{aligned}$$

Therefore, the computations involved in solving the affine step are

$$\begin{aligned}
 \Theta &= \mathbf{SZ}^{-1} + \mathbf{WV}^{-1} \\
 \rho &= \Theta^{-1}(\delta_d + (\mathbf{S} - \mathbf{W})\mathbf{e} - \mathbf{V}^{-1}\mathbf{W}\delta_b) \\
 \Delta t_{aff} &= (\mathbf{A}\Theta^{-1}\mathbf{A}')^{-1}(\delta_c + \mathbf{A}\rho) \\
 \Delta z_{aff} &= \Theta^{-1}\mathbf{A}'\Delta t_{aff} - \rho \\
 \Delta v_{aff} &= \delta_b - \Delta z_{aff} \\
 \Delta w_{aff} &= -\mathbf{W}\mathbf{e} - \mathbf{V}^{-1}\mathbf{W}\Delta z_{aff} \\
 \Delta s_{aff} &= -\mathbf{S}\mathbf{e} - \mathbf{Z}^{-1}\mathbf{S}\Delta z_{aff} \\
 (\mathbf{z}_{aff}, \mathbf{t}_{aff}, \mathbf{s}_{aff}, \mathbf{v}_{aff}, \mathbf{w}_{aff}) &= (\mathbf{z}, \mathbf{t}, \mathbf{s}, \mathbf{v}, \mathbf{w}) + \kappa(\Delta z_{aff}, \Delta t_{aff}, \Delta s_{aff}, \Delta v_{aff}, \Delta w_{aff})
 \end{aligned}$$

where  $\kappa$  is the *step length* as before.

The success of the affine step is gauged by calculating the complementarity of  $\mathbf{z}'\mathbf{s}$  and  $\mathbf{v}'\mathbf{w}$  at  $(\mathbf{z}_{aff}^k, \mathbf{t}_{aff}^k, \mathbf{s}_{aff}^k, \mathbf{v}_{aff}^k, \mathbf{w}_{aff}^k)$  and comparing it with the complementarity at the starting point  $(\mathbf{z}^k, \mathbf{t}^k, \mathbf{s}^k, \mathbf{v}^k, \mathbf{w}^k)$ . If the affine step was successful in reducing the complementarity by a substantial amount, the need for centering is not great, and a value close to zero is assigned to  $\sigma$  in a second linear system (see following), which is used to determine a centering vector. If, however, the affine step was unsuccessful, then centering is deemed beneficial, and a value close to 1.0 is assigned to  $\sigma$ . In other words, the value of  $\sigma$  is adaptively altered depending on progress made toward the optimum.

The following linear system is solved to determine a centering vector  $(\Delta z_c, \Delta t_c, \Delta s_c, \Delta v_c, \Delta w_c)$  from  $(\mathbf{z}_{aff}, \mathbf{t}_{aff}, \mathbf{s}_{aff}, \mathbf{v}_{aff}, \mathbf{w}_{aff})$ :

$$\begin{aligned}
 \Delta z_c + \Delta v_c &= \mathbf{0} \\
 \mathbf{A}\Delta z_c &= \mathbf{0} \\
 \mathbf{A}'\Delta t_c + \Delta s_c - \Delta w_c &= \mathbf{0} \\
 \mathbf{S}\Delta z_c + \mathbf{Z}\Delta s_c &= -\mathbf{Z}_{aff}\mathbf{S}_{aff}\mathbf{e} + \sigma\mu\mathbf{e} \\
 \mathbf{V}\Delta w_c + \mathbf{W}\Delta v_c &= -\mathbf{V}_{aff}\mathbf{W}_{aff}\mathbf{e} + \sigma\mu\mathbf{e}
 \end{aligned}$$

where  $\zeta_{start} = \mathbf{z}'\mathbf{s} + \mathbf{v}'\mathbf{w}$ , complementarity at the start of the iteration  
 $\zeta_{aff} = \mathbf{z}'_{aff}\mathbf{s}_{aff} + \mathbf{v}'_{aff}\mathbf{w}_{aff}$ , the affine complementarity  
 $\mu = \zeta_{aff}/2n$ , the average complementarity  
 $\sigma = (\zeta_{aff}/\zeta_{start})^3$

Therefore, the computations involved in solving the centering step are

$$\begin{aligned}
 \rho &= \Theta^{-1}(\sigma\mu(\mathbf{Z}^{-1} - \mathbf{V}^{-1})\mathbf{e} - \mathbf{Z}^{-1}\mathbf{Z}_{aff}\mathbf{S}_{aff}\mathbf{e} + \mathbf{V}^{-1}\mathbf{V}_{aff}\mathbf{W}_{aff}\mathbf{e}) \\
 \Delta t_c &= (\mathbf{A}\Theta^{-1}\mathbf{A}')^{-1}\mathbf{A}\rho \\
 \Delta z_c &= \Theta^{-1}\mathbf{A}'\Delta t_c - \rho \\
 \Delta v_c &= -\Delta z_c \\
 \Delta w_c &= \sigma\mu\mathbf{V}^{-1}\mathbf{e} - \mathbf{V}^{-1}\mathbf{V}_{aff}\mathbf{W}_{aff}\mathbf{e} - \mathbf{V}^{-1}\mathbf{W}_{aff}\Delta v_c \\
 \Delta s_c &= \sigma\mu\mathbf{Z}^{-1}\mathbf{e} - \mathbf{Z}^{-1}\mathbf{Z}_{aff}\mathbf{S}_{aff}\mathbf{e} - \mathbf{Z}^{-1}\mathbf{S}_{aff}\Delta z_c
 \end{aligned}$$

Then

$$\begin{aligned}(\Delta z, \Delta t, \Delta s, \Delta v, \Delta w) &= (\Delta z_{aff}, \Delta t_{aff}, \Delta s_{aff}, \Delta v_{aff}, \Delta w_{aff}) + (\Delta z_c, \Delta t_c, \Delta s_c, \Delta v_c, \Delta w_c) \\(z^{k+1}, t^{k+1}, s^{k+1}, v^{k+1}, w^{k+1}) &= (z^k, t^k, s^k, v^k, w^k) + \kappa(\Delta z, \Delta t, \Delta s, \Delta v, \Delta w)\end{aligned}$$

where, as before,  $\kappa$  is the *step length* assigned a value as large as possible, but not so large that a  $z_i^{k+1}$ ,  $s_i^{k+1}$ ,  $v_i^{k+1}$ , or  $w_i^{k+1}$  is “too close” to zero.

Although the predictor-corrector variant entails solving two linear systems instead of one, fewer iterations are usually required to reach the optimum. The additional overhead of the second linear system is small because the matrix  $(\mathbf{A}\Theta^{-1}\mathbf{A}')$  has already been factorized in order to solve the first linear system.

You can specify the starting point with the INEST= option in the PROC statement. By default, the starting point is set to be the least squares estimate.

### Smoothing Algorithm

To minimize the sum of the absolute residuals  $D_{LAR}(\boldsymbol{\beta})$ , the smoothing algorithm approximates the non-differentiable function  $D_{LAR}$  by the following smooth function, which is referred to as the Huber function:

$$D_\gamma(\boldsymbol{\beta}) = \sum_{i=1}^n H_\gamma(r_i(\boldsymbol{\beta}))$$

where

$$H_\gamma(t) = \begin{cases} t^2/(2\gamma) & \text{if } |t| \leq \gamma \\ |t| - \gamma/2 & \text{if } |t| > \gamma \end{cases}$$

Here  $r_i(\boldsymbol{\beta}) = y_i - \mathbf{x}_i'\boldsymbol{\beta}$ , and the *threshold*  $\gamma$  is a positive real number. The function  $D_\gamma$  is continuously differentiable and a minimizer  $\beta_\gamma$  of  $D_\gamma$  is close to a minimizer  $\hat{\boldsymbol{\beta}}_{LAR}$  of  $D_{LAR}(\boldsymbol{\beta})$  when  $\gamma$  is close to zero.

The advantage of the smoothing algorithm as described in Madsen and Nielsen (1993) is that the  $L_1$  solution  $\hat{\boldsymbol{\beta}}_{LAR}$  can be detected when  $\gamma > 0$  is small. In other words, it is not necessary to let  $\gamma$  converge to zero in order to find a minimizer of  $D_{LAR}(\boldsymbol{\beta})$ . The algorithm terminates before going through the entire sequence of values of  $\gamma$  that are generated by the algorithm. Convergence is indicated by no change of the status of residuals  $r_i(\boldsymbol{\beta})$  as  $\gamma$  goes through this sequence.

The smoothing algorithm extends naturally from  $L_1$  regression to general quantile regression; see Chen (2007). The function

$$D_{\rho_\tau}(\boldsymbol{\beta}) = \sum_{i=1}^n \rho_\tau(y_i - \mathbf{x}_i'\boldsymbol{\beta})$$

can be approximated by the smooth function

$$D_{\gamma,\tau}(\boldsymbol{\beta}) = \sum_{i=1}^n H_{\gamma,\tau}(r_i(\boldsymbol{\beta}))$$

where

$$H_{\gamma,\tau}(t) = \begin{cases} t(\tau - 1) - \frac{1}{2}(\tau - 1)^2\gamma & \text{if } t \leq (\tau - 1)\gamma \\ \frac{t^2}{2\gamma} & \text{if } (\tau - 1)\gamma \leq t \leq \tau\gamma \\ t\tau - \frac{1}{2}\tau^2\gamma & \text{if } t \geq \tau\gamma \end{cases}$$

The function  $H_{\gamma,\tau}$  is determined by whether  $r_i(\boldsymbol{\beta}) \leq (\tau - 1)\gamma$ ,  $r_i(\boldsymbol{\beta}) \geq \tau\gamma$ , or  $(\tau - 1)\gamma \leq r_i(\boldsymbol{\beta}) \leq \tau\gamma$ . These inequalities divide  $\mathbf{R}^p$  into subregions separated by the parallel hyperplanes  $r_i(\boldsymbol{\beta}) = (\tau - 1)\gamma$  and  $r_i(\boldsymbol{\beta}) = \tau\gamma$ . The set of all such hyperplanes is denoted by  $B_{\gamma,\tau}$ :

$$B_{\gamma,\tau} = \{\boldsymbol{\beta} \in \mathbf{R}^p \mid \exists i : r_i(\boldsymbol{\beta}) = (\tau - 1)\gamma \text{ or } r_i(\boldsymbol{\beta}) = \tau\gamma\}$$

Define the sign vector  $\mathbf{s}_\gamma(\boldsymbol{\beta}) = (s_1(\boldsymbol{\beta}), \dots, s_n(\boldsymbol{\beta}))'$  as

$$s_i = s_i(\boldsymbol{\beta}) = \begin{cases} -1 & \text{if } r_i(\boldsymbol{\beta}) \leq (\tau - 1)\gamma \\ 0 & \text{if } (\tau - 1)\gamma \leq r_i(\boldsymbol{\beta}) \leq \tau\gamma \\ 1 & \text{if } r_i(\boldsymbol{\beta}) \geq \tau\gamma \end{cases}$$

and introduce

$$w_i = w_i(\boldsymbol{\beta}) = 1 - s_i^2(\boldsymbol{\beta})$$

Therefore,

$$\begin{aligned} H_{\gamma,\tau}(r_i(\boldsymbol{\beta})) &= \frac{1}{2\gamma} w_i r_i^2(\boldsymbol{\beta}) \\ &+ s_i \left[ \frac{1}{2} r_i(\boldsymbol{\beta}) + \frac{1}{4} (1 - 2\tau)\gamma + s_i (r_i(\boldsymbol{\beta}) (\tau - \frac{1}{2}) - \frac{1}{4} (1 - 2\tau + 2\tau^2)\gamma) \right] \end{aligned}$$

yielding

$$D_{\gamma,\tau}(\boldsymbol{\beta}) = \frac{1}{2\gamma} \mathbf{r}' \mathbf{W}_{\gamma,\tau} \mathbf{r} + \mathbf{v}'(s) \mathbf{r} + c(s)$$

where  $\mathbf{W}_{\gamma,\tau}$  is the diagonal  $n \times n$  matrix with diagonal elements  $w_i(\boldsymbol{\beta})$ ,  $\mathbf{v}'(s) = (s_1((2\tau - 1)s_1 + 1)/2, \dots, s_n((2\tau - 1)s_n + 1)/2)$ ,  $c(s) = \sum [\frac{1}{4}(1 - 2\tau)\gamma s_i - \frac{1}{4}s_i^2(1 - 2\tau + 2\tau^2)\gamma]$ , and  $\mathbf{r}(\boldsymbol{\beta}) = (r_1(\boldsymbol{\beta}), \dots, r_n(\boldsymbol{\beta}))'$ .

The gradient of  $D_{\gamma,\tau}$  is given by

$$D_{\gamma,\tau}^{(1)}(\boldsymbol{\beta}) = -\mathbf{A} \left[ \frac{1}{\gamma} \mathbf{W}_{\gamma,\tau}(\boldsymbol{\beta}) \mathbf{r}(\boldsymbol{\beta}) + \mathbf{v}(s) \right]$$

and for  $\boldsymbol{\beta} \in \mathbf{R}^p \setminus B_{\gamma,\tau}$  the Hessian exists and is given by

$$D_{\gamma,\tau}^{(2)}(\boldsymbol{\beta}) = \frac{1}{\gamma} \mathbf{A} \mathbf{W}_{\gamma,\tau}(\boldsymbol{\beta}) \mathbf{A}'$$

The gradient is a continuous function in  $\mathbf{R}^p$ , whereas the Hessian is piecewise constant.

Following Madsen and Nielsen (1993), the vector  $\mathbf{s}$  is referred to as a  $\gamma$ -feasible sign vector if there exists  $\boldsymbol{\beta} \in \mathbf{R}^p \setminus B_{\gamma, \tau}$  with  $\mathbf{s}_{\gamma}(\boldsymbol{\beta}) = \mathbf{s}$ . If  $\mathbf{s}$  is  $\gamma$ -feasible, then  $Q_s$  is defined as the quadratic function  $Q_s(\boldsymbol{\alpha})$  that is derived from  $D_{\gamma, \tau}(\boldsymbol{\beta})$  by substituting  $\mathbf{s}$  for  $\mathbf{s}_{\gamma}$ . Thus, for any  $\boldsymbol{\beta}$  with  $\mathbf{s}_{\gamma} = \mathbf{s}$ ,

$$Q_s(\boldsymbol{\alpha}) = \frac{1}{2}(\boldsymbol{\alpha} - \boldsymbol{\beta})' D_{\gamma, \tau}^{(2)}(\boldsymbol{\beta})(\boldsymbol{\alpha} - \boldsymbol{\beta}) + D_{\gamma, \tau}^{(1)}(\boldsymbol{\beta})(\boldsymbol{\alpha} - \boldsymbol{\beta}) + D_{\gamma, \tau}(\boldsymbol{\beta})$$

In the domain  $C_s = \{\boldsymbol{\alpha} | \mathbf{s}_{\gamma}(\boldsymbol{\alpha}) = \mathbf{s}\}$

$$D_{\gamma, \tau}(\boldsymbol{\alpha}) = Q_s(\boldsymbol{\alpha})$$

For each  $\gamma > 0$  and  $\theta \in \mathbf{R}^p$ , there can be one or several corresponding quadratics  $Q_s$ . If  $\theta \notin B_{\gamma, \tau}$  then  $Q_s$  is characterized by  $\theta$  and  $\gamma$ , but for  $\theta \in B_{\gamma, \tau}$  the quadratic is not unique. Therefore, a *reference*

$$(\gamma, \theta, \mathbf{s})$$

determines the quadratic.

Again following Madsen and Nielsen (1993), let

$(\gamma, \theta, \mathbf{s})$  be a *feasible reference* if  $\mathbf{s}$  is a  $\gamma$ -feasible sign vector with  $\theta \in C_s$ , and

$(\gamma, \theta, \mathbf{s})$  be a *solution reference* if it is feasible and  $\theta$  minimizes  $D_{\gamma, \tau}$ .

The smoothing algorithm for minimizing  $D_{\rho, \tau}$  is based on minimizing  $D_{\gamma, \tau}$  for a set of decreasing  $\gamma$ . For each new value of  $\gamma$ , information from the previous solution is used. Finally, when  $\gamma$  is small enough, a solution can be found by the modified Newton-Raphson algorithm as stated by Madsen and Nielsen (1993):

```

find an initial solution reference $(\gamma, \boldsymbol{\beta}_{\gamma}, \mathbf{s})$
repeat
 decrease γ
 find a solution reference $(\gamma, \boldsymbol{\beta}_{\gamma}, \mathbf{s})$
until $\gamma = 0$
 $\boldsymbol{\beta}_0$ is the solution.

```

By default, the initial solution reference is found by letting  $\boldsymbol{\beta}_{\gamma}$  be the least squares solution. Alternatively, you can specify the initial solution reference with the INEST= option in the PROC QUANTREG statement. Then  $\gamma$  and  $\mathbf{s}$  are chosen according to these initial values.

There are several approaches for determining a decreasing sequence of values of  $\gamma$ . The QUANTREG procedure uses a strategy by Madsen and Nielsen (1993). The computation involved is not significant comparing with the Newton-Raphson step. You can control the ratio of consecutive decreasing values of  $\gamma$  with the RRATIO= suboption of the ALGORITHM= option in the PROC QUANTREG statement. By default,

$$\text{RRATIO} = \begin{cases} 0.1 & \text{if } n \geq 10000 \text{ and } p \leq 20 \\ 0.9 & \text{if } \frac{p}{n} \geq 0.1 \text{ or } \{n \leq 5000 \text{ and } p \geq 300\} \\ 0.5 & \text{otherwise} \end{cases}$$

For the  $L_1$  and quantile regression, it turns out that the smoothing algorithm is very efficient and competitive, especially for a *fat* data set—namely, when  $\frac{p}{n} > 0.05$  and  $\mathbf{A}\mathbf{A}'$  is dense. See Chen (2007) for a complete smoothing algorithm and details.

## Confidence Interval

The QUANTREG procedure provides three methods to compute confidence intervals for the regression quantile parameter  $\beta(\tau)$ : sparsity, rank, and resampling. The sparsity method is the most direct and the fastest, but it involves estimation of the sparsity function, which is not robust for data that are not independently and identically distributed. To deal with this problem, the QUANTREG procedure computes a Huber sandwich estimate by using a local estimate of the sparsity function. The rank method, which computes confidence intervals by inverting the rank score test, does not suffer from this problem, but it uses the simplex algorithm and is computationally expensive with large data sets. The resampling method, which uses the bootstrap approach, addresses these problems, but at a computation cost.

Based on these properties, the QUANTREG uses a combination of the resampling and rank methods as the default. For data sets with more than either 5,000 observations or 20 variables, the QUANTREG procedure uses the MCMB resampling method; otherwise it uses the rank method. You can request a particular method by using the CI= option in the PROC QUANTREG statement.

### Sparsity

Consider the linear model

$$y_i = \mathbf{x}_i' \boldsymbol{\beta} + \epsilon_i$$

and assume that  $\{\epsilon_i\}$ ,  $i = 1, \dots, n$ , are iid with a distribution  $F$  and a density  $f = F'$ , where  $f(F^{-1}(\tau)) > 0$  in a neighborhood of  $\tau$ . Under some mild conditions

$$\sqrt{n}(\hat{\boldsymbol{\beta}}(\tau) - \boldsymbol{\beta}(\tau)) \rightarrow N(0, \omega^2(\tau, F)\boldsymbol{\Omega}^{-1})$$

where  $\omega^2(\tau, F) = \tau(1-\tau)/f^2(F^{-1}(\tau))$  and  $\boldsymbol{\Omega} = \lim_{n \rightarrow \infty} n^{-1} \sum \mathbf{x}_i \mathbf{x}_i'$ . See Koenker and Bassett (1982b).

This asymptotic distribution for the regression quantile  $\hat{\boldsymbol{\beta}}(\tau)$  can be used to construct confidence intervals. However, the reciprocal of the density function

$$s(\tau) = [f(F^{-1}(\tau))]^{-1}$$

which is called the *sparsity function*, must first be estimated.

Since

$$s(t) = \frac{d}{dt} F^{-1}(t)$$

$s(t)$  can be estimated by the difference quotient of the empirical quantile function—that is,

$$\hat{s}_n(t) = [\hat{F}_n^{-1}(t + h_n) - \hat{F}_n^{-1}(t - h_n)]/2h_n$$

where  $\hat{F}_n$  is an estimate of  $F^{-1}$  and  $h_n$  is a bandwidth that tends to zero as  $n \rightarrow \infty$ .

The QUANTREG procedure provides two bandwidth methods. The Bofinger bandwidth

$$h_n = n^{-1/5} \left( \frac{4.5s^2(t)}{(s^{(2)}(t))^2} \right)^{1/5}$$

is an optimizer of mean squared error for standard density estimation, and the Hall-Sheather bandwidth

$$h_n = n^{-1/3} z_\alpha^{2/3} \left( \frac{1.5s(t)}{s^{(2)}(t)} \right)^{1/3}$$

is based on Edgeworth expansions for studentized quantiles, where  $s^{(2)}(t)$  is the second derivative of  $s(t)$  and  $z_\alpha$  satisfies  $\Phi(z_\alpha) = 1 - \alpha/2$  for the construction of  $1 - \alpha$  confidence intervals. The quantity

$$\frac{s(t)}{s^{(2)}(t)} = \frac{f^2}{2(f^{(1)}/f)^2 + [(f^{(1)}/f)^2 - f^{(2)}/f]}$$

is not sensitive to  $f$  and can be estimated by assuming  $f$  is Gaussian.

$\hat{F}^{-1}$  can be estimated by the empirical quantile function of the residuals from the quantile regression fit,

$$\hat{F}^{-1}(t) = r_{(i)}, \text{ for } t \in [(i-1)/n, i/n),$$

or the empirical quantile function of regression proposed by Bassett and Koenker (1982),

$$\hat{F}^{-1}(t) = \bar{\mathbf{x}}' \hat{\boldsymbol{\beta}}(t)$$

The QUANTREG procedure interpolates the first empirical quantile function and gets the piecewise linear version

$$\hat{F}^{-1}(t) = \begin{cases} r_{(1)} & \text{if } t \in [0, 1/2n) \\ \lambda r_{(i+1)} + (1-\lambda)r_{(i)} & \text{if } t \in [(2j-1)/2n, (2i+1)/2n) \\ r_{(n)} & \text{if } t \in [(2n-1), 1] \end{cases}$$

$\hat{F}^{-1}$  is set to a constant if  $t \pm h_n$  falls outside  $[0, 1]$ .

This estimator of the sparsity function is sensitive to the iid assumption. Alternately, Koenker and Machado (1999) considered the non-iid case. By assuming local linearity of the conditional quantile function  $Q(\tau|x)$  in  $x$ , they proposed a local estimator of the density function by using the difference quotient. A Huber sandwich estimate of the covariance and standard error is computed and used to construct the confidence intervals. One difficulty with this method is the selection of the bandwidth when using the difference quotient. With a small sample size, either the Bofinger or the Hall-Sheather bandwidth tends to be too large to assure local linearity of the conditional quantile function. The QUANTREG procedure uses a heuristic bandwidth selection in these cases.

By default, the QUANTREG procedure computes non-iid confidence intervals. You can request iid confidence intervals with the IID option in the PROC statement.

## Inversion of Rank Tests

The classical theory of rank tests can be extended to test the hypothesis  $H_0: \beta_2 = \eta$  in the linear regression model  $\mathbf{y} = \mathbf{X}_1\beta_1 + \mathbf{X}_2\beta_2 + \boldsymbol{\epsilon}$ . Here  $(\mathbf{X}_1, \mathbf{X}_2) = \mathbf{A}'$ . See Gutenbrunner and Jureckova (1992) for more details. By inverting this test, confidence intervals can be computed for the regression quantiles that correspond to  $\beta_2$ .

The rank score function  $\hat{a}_n(t) = (\hat{a}_{n1}(t), \dots, \hat{a}_{nn}(t))$  can be obtained by solving the dual problem

$$\max_a \{(\mathbf{y} - \mathbf{X}_2\boldsymbol{\eta})'a \mid \mathbf{X}_1'a = (1-t)\mathbf{X}_1'e, a \in [0, 1]^n\}$$

For a fixed quantile  $\tau$ , integrating  $\hat{a}_{ni}(t)$  with respect to the  $\tau$ -quantile score function

$$\varphi_\tau(t) = \tau - I(t < \tau)$$

yields the  $\tau$ -quantile scores

$$\hat{b}_{ni} = - \int_0^1 \varphi_\tau(t) d\hat{a}_{ni}(t) = \hat{a}_{ni}(\tau) - (1 - \tau)$$

Under the null hypothesis  $H_0: \beta_2 = \eta$

$$S_n(\eta) = n^{-1/2} \mathbf{X}'_2 \hat{b}_n(\eta) \rightarrow N(0, \tau(1 - \tau) \mathbf{\Omega}_n)$$

for large  $n$ , where  $\mathbf{\Omega}_n = n^{-1} \mathbf{X}'_2 (\mathbf{I} - \mathbf{X}_1 (\mathbf{X}'_1 \mathbf{X}_1)^{-1} \mathbf{X}'_1) \mathbf{X}_2$ .

Let

$$T_n(\eta) = \frac{1}{\sqrt{\tau(1 - \tau)}} S_n(\eta) \mathbf{\Omega}_n^{-1/2}$$

Then  $T_n(\hat{\beta}_2(\tau)) = 0$  from the constraint  $\mathbf{A}\hat{\mathbf{a}} = (1 - \tau)\mathbf{A}\mathbf{e}$  in the full model. In order to obtain confidence intervals for  $\beta_2$ , a critical value can be specified for  $T_n$ . The dual vector  $\hat{a}_n(\eta)$  is a piecewise constant in  $\eta$ , and  $\eta$  can be altered without compromising the optimality of  $\hat{a}_n(\eta)$  as long as the signs of the residuals in the primal quantile regression problem do not change. When  $\eta$  gets to such a boundary, the solution does change, but can be restored by taking one simplex pivot. The process can continue in this way until  $T_n(\eta)$  exceeds the specified critical value. Since  $T_n(\eta)$  is piecewise constant, interpolation can be used to obtain the desired level of confidence interval; see Koenker and d'Orey (1994).

## Resampling

The bootstrap can be implemented to compute confidence intervals for regression quantile estimates. As in other regression applications, both the residual bootstrap and the  $xy$ -pair bootstrap can be used. The former assumes iid random errors and resamples from the residuals, while the later resamples  $xy$  pairs and accommodates some forms of heteroscedasticity. Koenker (1994) considered a more interesting resampling mechanism, resampling directly from the full regression quantile process, which he called the Heqf bootstrap.

In contrast with these bootstrap methods, Parzen, Wei, and Ying (1994) observed that

$$S(\boldsymbol{\beta}) = n^{-1/2} \sum_{i=1}^n \mathbf{x}_i (\tau - I(y_i \leq \mathbf{x}'_i \boldsymbol{\beta}))$$

which is the estimating equation for the  $\tau$  regression quantile, is a pivotal quantity for the  $\tau$  quantile regression parameter  $\beta_\tau$ . In other words, the distribution of  $\mathbf{S}(\boldsymbol{\beta})$  can be generated exactly by a random vector  $\mathbf{U}$ , which is a weighted sum of independent, re-centered Bernoulli variables. They further showed that for large  $n$ , the distribution of  $\hat{\boldsymbol{\beta}}(\tau) - \beta_\tau$  can be approximated by the conditional distribution of  $\hat{\boldsymbol{\beta}}_U - \hat{\boldsymbol{\beta}}_n(\tau)$ , where  $\hat{\boldsymbol{\beta}}_U$  solves an augmented quantile regression problem with  $n + 1$  observations with  $\mathbf{x}_{n+1} = -n^{-1/2} \mathbf{u} / \tau$  and  $y_{n+1}$  sufficiently large for a given realization of  $u$ . By exploiting the asymptotically pivotal role of the quantile regression “gradient condition,” this approach also achieves some robustness to certain heteroscedasticity.

Although the bootstrap method by Parzen, Wei, and Ying (1994) is much simpler, it is too time-consuming for relatively large data sets, especially for high-dimensional data sets. The QUANTREG procedure implements a new, general resampling method developed by He and Hu (2002), which is referred to as the



Markov chain marginal bootstrap (MCMB). For quantile regression, the MCMB method has the advantage that it solves  $p$  one-dimensional equations instead of  $p$ -dimensional equations, as do the previous bootstrap methods. This greatly improves the feasibility of the resampling method in computing confidence intervals for regression quantiles.

---

## Covariance-Correlation

You can specify the COVB and CORRB options in the MODEL statement to request covariance and correlation matrices for the estimated parameters.

The QUANTREG procedure provides two methods for computing the covariance and correlation matrices of the estimated parameters: an asymptotic method and a bootstrap method. Bootstrap covariance and correlation matrices are computed when resampling confidence intervals are computed. Asymptotic covariance and correlation matrices are computed when asymptotic confidence intervals are computed. The rank method for confidence intervals does not provide a covariance-correlation estimate.

## Asymptotic Covariance-Correlation

This method corresponds to the sparsity method for the confidence intervals. For the sparsity function in the computation of the asymptotic covariance and correlation, the QUANTREG procedure provides both iid and non-iid estimates. By default, the QUANTREG procedure computes non-iid estimates.

## Bootstrap Covariance-Correlation

This method corresponds to the resampling method for the confidence intervals. The Markov chain marginal bootstrap (MCMB) method is used.

---

## Linear Test

Consider the linear model

$$y_i = \mathbf{x}'_{1i}\boldsymbol{\beta}_1 + \mathbf{x}'_{2i}\boldsymbol{\beta}_2 + \epsilon_i$$

where  $\boldsymbol{\beta}_1$  and  $\boldsymbol{\beta}_2$  are  $p$ - and  $q$ -dimensional unknown parameters, and  $\{\epsilon_i\}$ ,  $i = 1, \dots, n$ , are errors with unknown density function  $f_i$ . Let  $\mathbf{x}'_i = (\mathbf{x}'_{1i}, \mathbf{x}'_{2i})$ ;  $\hat{\boldsymbol{\beta}}_1(\tau)$  and  $\hat{\boldsymbol{\beta}}_2(\tau)$  be the parameter estimates for  $\boldsymbol{\beta}_1$  and  $\boldsymbol{\beta}_2$  respectively at the  $\tau$  quantile. The covariance matrix  $\boldsymbol{\Omega}$  for the parameter estimates is partitioned correspondingly as  $\boldsymbol{\Omega}_{ij}$  with  $i = 1, 2$ ;  $j = 1, 2$ ; and  $\boldsymbol{\Omega}^{22} = (\boldsymbol{\Omega}_{22} - \boldsymbol{\Omega}_{21}\boldsymbol{\Omega}_{11}^{-1}\boldsymbol{\Omega}_{12})^{-1}$ .

## Testing Effects of Covariates

Three tests are available in the QUANTREG procedure for the linear null hypothesis  $H_0 : \boldsymbol{\beta}_2 = 0$  at the  $\tau$  quantile.

The Wald test statistic, which is based on the estimated coefficients for the unrestricted model, is given by

$$T_W(\tau) = \hat{\boldsymbol{\beta}}'_2(\tau)\hat{\boldsymbol{\Sigma}}(\tau)^{-1}\hat{\boldsymbol{\beta}}_2(\tau)$$

where  $\hat{\boldsymbol{\Sigma}}(\tau)$  is an estimator of the covariance of  $\hat{\boldsymbol{\beta}}_2(\tau)$ . The QUANTREG procedure provides two estimators for the covariance, as described in the previous section. The estimator based on the asymptotic covariance is

$$\hat{\Sigma}(\tau) = \frac{1}{n} \hat{\omega}(\tau)^2 \Omega^{22}$$

where  $\hat{\omega}(\tau) = \sqrt{\tau(1-\tau)}\hat{s}(\tau)$  and  $\hat{s}(\tau)$  is the estimated sparsity function. The estimator based on the bootstrap covariance is the empirical covariance of the MCMB samples.

The likelihood ratio test is based on the difference between the objective function values in the restricted and unrestricted models. Let  $D_0(\tau) = \sum \rho_\tau(y_i - \mathbf{x}_i \hat{\beta}(\tau))$  and  $D_1(\tau) = \sum \rho_\tau(y_i - \mathbf{x}_{1i} \hat{\beta}_1(\tau))$ , and set

$$T_{LR}(\tau) = 2(\tau(1-\tau)\hat{s}(\tau))^{-1}(D_1(\tau) - D_0(\tau))$$

where  $\hat{s}(\tau)$  is the estimated sparsity function.

The rank test statistic is given by

$$T_R(\tau) = \mathbf{S}'_n \mathbf{M}_n^{-1} \mathbf{S}_n / A^2(\varphi)$$

where

$$\mathbf{S}_n = n^{-1/2}(\mathbf{X}_2 - \hat{\mathbf{X}}_2)' \hat{\mathbf{b}}_n$$

$$\Psi = \text{diag}(f_i(Q_{y_i}(\tau|\mathbf{x}_{1i}, \mathbf{x}_{2i})))$$

$$\hat{\mathbf{X}}_2 = \mathbf{X}_1(\mathbf{X}'_1 \Psi \mathbf{X}_1)^{-1} \mathbf{X}'_1 \mathbf{X}_2$$

$$\mathbf{M}_n = (\mathbf{X}_2 - \hat{\mathbf{X}}_2)(\mathbf{X}_2 - \hat{\mathbf{X}}_2)' / n$$

$$\hat{\mathbf{b}}_{ni} = \int_0^1 \hat{\mathbf{a}}_{ni}(t) d\varphi(t)$$

$$\hat{\mathbf{a}}(t) = \max_{\mathbf{a}} \{\mathbf{y}' \mathbf{a} | \mathbf{X}'_1 \mathbf{a} = (1-t)\mathbf{X}'_1 \mathbf{e}, \mathbf{a} \in [0, 1]^n\}$$

$$A^2(\varphi) = \int_0^1 (\varphi(t) - \bar{\varphi}(t))^2 dt$$

$$\bar{\varphi}(t) = \int_0^1 \varphi(t) dt$$

and  $\varphi(t)$  is a score function.

The following score functions are available in the QUANTREG procedure:

**Wilcoxon scores:**  $\phi(t) = t - 1/2$

**Normal scores:**  $\phi(t) = \Phi^{-1}(t)$ , where  $\Phi$  is the normal distribution function

**Sign scores:**  $\phi(t) = 1/2 \text{ sign}(t - 1/2)$

**Tau scores:**  $\phi_\tau(t) = \tau - I(t < \tau)$ .

The rank test statistic  $T_R(\tau)$ , unlike Wald tests or likelihood ratio tests, requires no estimation of the nuisance parameter  $f_i$  under iid error models (Gutenbrunner et al. 1993).

Koenker and Machado (1999) prove that the three test statistics ( $T_W(\tau)$ ,  $T_{LR}(\tau)$ , and  $T_R(\tau)$ ) are asymptotically equivalent and that their distributions converge to  $\chi^2_q$  under the null hypothesis, where  $q$  is the dimension of  $\beta_2$ .

## Testing for Heteroscedasticity

After you obtain the parameter estimates for several quantiles specified in the MODEL statement, you can test whether there are significant difference for the estimates for the same covariates across the quantiles. For example, if you want to test whether the parameters  $\beta_2$  are the same across quantiles, the null hypothesis  $H_0$  can be written as:  $\beta_2(\tau_1) = \dots = \beta_2(\tau_k)$ , where  $\tau_j, j = 1, \dots, k$ , are the quantiles specified in the MODEL statement. See Koenker and Bassett (1982a) for details.

---

## Leverage Point and Outlier Detection

The QUANTREG procedure uses robust multivariate location and scale estimates for leverage-point detection.

Mahalanobis distance is defined as

$$\text{MD}(\mathbf{x}_i) = [(\mathbf{x}_i - \bar{\mathbf{x}})' \bar{\mathbf{C}}(\mathbf{A})^{-1} (\mathbf{x}_i - \bar{\mathbf{x}})]^{1/2}$$

where  $\bar{\mathbf{x}} = \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i$  and  $\bar{\mathbf{C}}(\mathbf{A}) = \frac{1}{n-1} \sum_{i=1}^n (\mathbf{x}_i - \bar{\mathbf{x}})' (\mathbf{x}_i - \bar{\mathbf{x}})$  are the empirical multivariate location and scale. Here,  $\mathbf{x}_i = (\mathbf{x}_{i1}, \dots, \mathbf{x}_{i(p-1)})'$  does not include the intercept variable. The relationship between the Mahalanobis distance  $\text{MD}(\mathbf{x}_i)$  and the matrix  $\mathbf{H} = (h_{ij}) = \mathbf{A}'(\mathbf{A}\mathbf{A}')^{-1}\mathbf{A}$  is

$$h_{ii} = \frac{1}{n-1} \text{MD}_i^2 + \frac{1}{n}$$

Robust distance is defined as

$$\text{RD}(\mathbf{x}_i) = [(\mathbf{x}_i - \mathbf{T}(\mathbf{A}))' \mathbf{C}(\mathbf{A})^{-1} (\mathbf{x}_i - \mathbf{T}(\mathbf{A}))]^{1/2}$$

where  $\mathbf{T}(\mathbf{A})$  and  $\mathbf{C}(\mathbf{A})$  are robust multivariate location and scale estimates computed with the minimum covariance determinant (MCD) method of Rousseeuw and Van Driessen (1999).

These distances are used to detect leverage points. You can use the DIAGNOSTICS and LEVERAGE options in the MODEL statement to request leverage-point and outlier diagnostics. Two new variables, Leverage and Outlier, are created and saved in an output data set specified in the OUTPUT statement.

Let  $C(p) = \sqrt{\chi_{p;1-\alpha}^2}$  be the cutoff value. The variable LEVERAGE is defined as

$$\text{LEVERAGE} = \begin{cases} 0 & \text{if } \text{RD}(\mathbf{x}_i) \leq C(p) \\ 1 & \text{otherwise} \end{cases}$$

You can specify a cutoff value with the LEVERAGE option in the MODEL statement.

Residuals  $r_i, i = 1, \dots, n$ , based on quantile regression estimates are used to detect vertical outliers. The variable OUTLIER is defined as

$$\text{OUTLIER} = \begin{cases} 0 & \text{if } |r_i| \leq k\sigma \\ 1 & \text{otherwise} \end{cases}$$

You can specify the multiplier  $k$  of the cutoff value with the CUTOFF= option in the MODEL statement. You can specify the scale  $\sigma$  with the SCALE= option in the MODEL statement. By default,  $k = 3$  and the scale  $\sigma$  is computed as the corrected median of the absolute residuals  $\sigma = \text{median}\{|r_i|/\beta_0, i = 1, \dots, n\}$ , where  $\beta_0 = \Phi^{-1}(0.75)$  is an adjustment constant for consistency with the normal distribution.

An ODS table called DIAGNOSTICS contains these two variables.

---

## INEST= Data Set

The INEST= data set specifies initial estimates for all the parameters in the model. The INEST= data set must contain the intercept variable (named Intercept) and all independent variables in the MODEL statement.

If BY processing is used, the INEST= data set should also include the BY variables, and there must be at least one observation for each BY group. If there is more than one observation in one BY group, the first one read is used for that BY group.

If the INEST= data set also contains the `_TYPE_` variable, only observations with the `_TYPE_` value 'PARMS' are used as starting values.

You can specify starting values for the interior point algorithm or the smoothing algorithm in the INEST= data set. The INEST= data set has the same structure as the OUTEST= data set but is not required to have all the variables or observations that appear in the OUTEST= data set. One simple use of the INEST= option is passing the previous OUTEST= data set directly to the next model as an INEST= data set, assuming that the two models have the same parameterization. If you specify more than one quantile in the MODEL statement, the same initial values are used for all quantiles.

---

## OUTEST= Data Set

The OUTEST= data set contains parameter estimates for the specified model with all quantiles. A set of observations is created for each quantile specified. You can also specify a label in the MODEL statement to distinguish between the estimates for different models used by the QUANTREG procedure.

Note that, if the QUANTREG procedure does not produce valid solutions, the parameter estimates are set to missing in the OUTEST data set.

If created, this data set contains all variables specified in the MODEL statement and the BY statement. Each observation consists of parameter values for a specified quantile with the dependent variable having the value `-1`.

The following variables are also added to the data set:

|                          |                                                                                                                                                              |
|--------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>_MODEL_</code>     | a character variable of length 8 containing the label of the MODEL statement, if present. Otherwise, the variable's value is blank.                          |
| <code>_ALGORITHM_</code> | a character variable of length 8 containing the name of the algorithm used for computing the parameter estimates, either SIMPLEX, INTERIOR, or SMOOTH        |
| <code>_TYPE_</code>      | a character variable of length 8 containing the type of the observation. it is fixed as PARMS to indicate that the observation includes parameter estimates. |
| <code>_STATUS_</code>    | a character variable of length 12 containing the status of model fitting, either NORMAL, NOUNIQUE, or NOVALID                                                |
| Intercept                | a numeric variable containing the intercept parameter estimates                                                                                              |
| <code>_QUANTILE_</code>  | a numeric variable containing the specified quantile levels                                                                                                  |

Any BY variables specified are also added to the OUTEST= data set.

## Computational Resources

The various algorithms need different amounts of memory for working space. Let  $p$  be the number of parameters estimated and  $n$  be the number of observations used in the model estimation.

For the simplex algorithm, the minimum working space (in bytes) needed is

$$2np + 6n + 10p$$

for the interior point algorithm,

$$np + p^2 + 13n + 4p$$

and for the smoothing algorithm,

$$np + p^2 + 6n + 4p$$

For the last two algorithms, if you want to use preprocessing, an extra amount

$$np + 6n + 2p$$

is needed.

If sufficient space is available, the input data set is kept in memory; otherwise, the input data set is reread as necessary, and the execution time of the procedure increases substantially.

## ODS Table Names

The QUANTREG procedure assigns a name to each table it creates. You can specify these names when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in the following table.

**Table 77.9** ODS Tables Produced in PROC QUANTREG

| ODS Table Name     | Description                             | Statement   | Option      |
|--------------------|-----------------------------------------|-------------|-------------|
| ClassLevels        | Classification variable levels          | CLASS       | default     |
| CorrB              | Parameter estimate correlation matrix   | MODEL       | CORRB       |
| CovB               | Parameter estimate covariance matrix    | MODEL       | COVB        |
| Diagnostics        | Outlier diagnostics                     | MODEL       | DIAGNOSTICS |
| DiagSummary        | Summary of the outlier diagnostics      | MODEL       | DIAGNOSTICS |
| IPIterHistory      | Iteration history (Interior Point)      | MODEL       | ITPRINT     |
| ModelInfo          | Model information                       | MODEL       | default     |
| NObs               | Number of observations                  | PROC        | default     |
| ObjFunction        | Objective function                      | MODEL       | default     |
| ParameterEstimates | Parameter estimates                     | MODEL       | default     |
| ParmInfo           | Parameter indices                       | MODEL       | default     |
| PerfSettings       | Performance settings                    | PERFORMANCE | DETAILS     |
| ProcessEst         | Quantile process estimates              | MODEL       | QUANTILE=   |
| ProcessObj         | Objective function for quantile process | MODEL       | QUANTILE=   |
| SMIterHistory      | Iteration history (Smoothing)           | MODEL       | ITPRINT     |
| SummaryStatistics  | Summary statistics for model variables  | MODEL       | default     |
| Tests              | Results for tests                       | TEST        | default     |
| ScalableTiming     | Timing details                          | PERFORMANCE | DETAILS     |

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “[Statistical Graphics Using ODS.](#)”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS.](#)”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “[A Primer on ODS Statistical Graphics](#)” on page 599 in Chapter 21, “[Statistical Graphics Using ODS.](#)”

For a single quantile, two plots are particularly useful in revealing outliers and leverage points. The first is a scatter plot of the standardized residuals for the specified quantile against the robust distances. The second is a scatter plot of the robust distances against the classical Mahalanobis distances. You can request these two plots by using the PLOT=RDPLOT and PLOT=DDPLOT options.

You can also request a normal quantile-quantile plot and a histogram of the standardized residuals for the specified quantile with the PLOT=QQPLOT and PLOT=HISTOGRAM options, respectively.

You can request a plot of fitted conditional quantiles by the single continuous variable specified in the model with the PLOT=FITPLOT option.

All these plots can be requested by specifying corresponding plot options in either the PROC QUANTREG statement or the MODEL statement. If you specify same plot options in both statements, options in the PROC QUANTREG statement override options in the MODEL statement.

You can specify the PLOT=QUANTPLOT option in only the MODEL statement to request a quantile process plot with confidence bands.

The plot options in the PROC QUANTREG statement and the MODEL statement are summarized in [Table 77.10](#). See the PLOT= option in the PROC QUANTREG statement and the PLOT= option in the MODEL statement for details.

**Table 77.10** Options for Plots

| Keyword   | Plot                                              |
|-----------|---------------------------------------------------|
| ALL       | All appropriate plots                             |
| DDPLOT    | Robust distance vs. Mahalanobis distance          |
| FITPLOT   | Conditional quantile fit vs. independent variable |
| HISTOGRAM | Histogram of standardized robust residuals        |
| NONE      | No plot                                           |
| QUANTPLOT | Scatter plot of regression quantile               |
| QQPLOT    | Q-Q plot of standardized robust residuals         |
| RDPLOT    | Standardized robust residual vs. robust distance  |

The following subsections provide information about these graphs.

## ODS Graph Names

The QUANTREG procedure assigns a name to each graph it creates. You can use these names to reference the graphs when using ODS. The names along with the required statements and options are listed in Table 77.11.

**Table 77.11** Graphs Produced by PROC QUANTREG

| ODS Graph Name | Plot Description                                             | Statement  | Option              |
|----------------|--------------------------------------------------------------|------------|---------------------|
| DDPlot         | Robust distance versus Mahalanobis distance                  | PROC MODEL | DDPLOT              |
| FitPlot        | Quantile fit versus independent variable                     | PROC MODEL | FITPLOT             |
| Histogram      | Histogram of standardized robust residuals                   | PROC MODEL | HISTOGRAM           |
| QQPlot         | Q-Q plot of standardized robust residuals                    | PROC MODEL | QQPLOT              |
| QuantPanel     | Panel of quantile plots with confidence limits               | MODEL      | QUANTPLOT           |
| QuantPlot      | Scatter plot for regression quantiles with confidence limits | MODEL      | QUANTPLOT<br>UNPACK |
| RDPlot         | Standardized robust residual versus robust distance          | PROC MODEL | RDPLOT              |

## Fit Plot

When the model has a single independent continuous variable (with or without the intercept), the QUANTREG procedure automatically creates a plot of fitted conditional quantiles against this independent variable for one or more quantiles specified in the MODEL statement.

The following example reuses the trout data set in the section “[Analysis of Fish-Habitat Relationships](#)” on page 6490 to show the fit plot for one or several quantiles.

```
ods graphics on;

proc quantreg data=trout ci=resampling;
 model LnDensity = WDRatio / quantile=0.9 seed=1268;
run;

proc quantreg data=trout ci=resampling;
 model LnDensity = WDRatio / quantile=0.5 0.75 0.9 seed=1268;
run;
```

For a single quantile, the confidence limits for the fitted conditional quantiles are also plotted if you specify the CI=RESAMPLING or CI=SPARSITY option. (See [Figure 77.14](#).) For multiple quantiles, confidence limits are not plotted by default. (See [Figure 77.15](#).) You can add the confidence limits on the plot by specifying the option PLOT=FITPLOT(SHOWLIMITS).

The QUANTREG procedure also provides fit plots for quantile regression splines and polynomials if they are based on a single continuous variable. See [Example 77.4](#) and [Example 77.5](#) for some examples.

Figure 77.14 Fit Plot with Confidence Limits

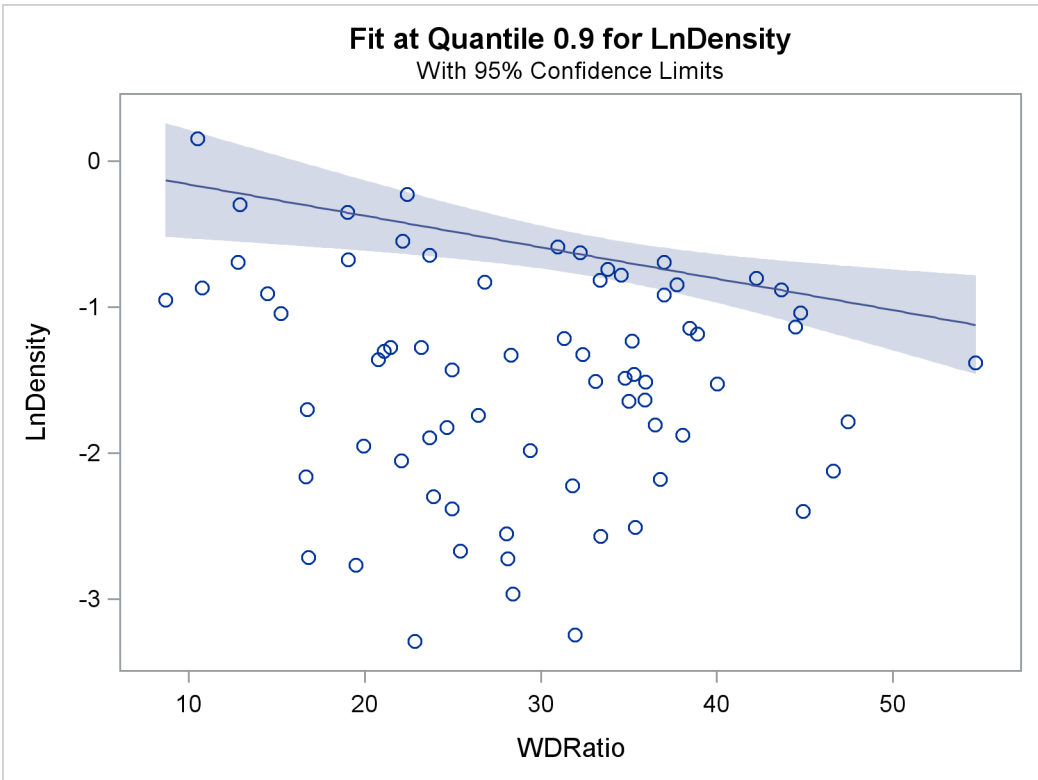
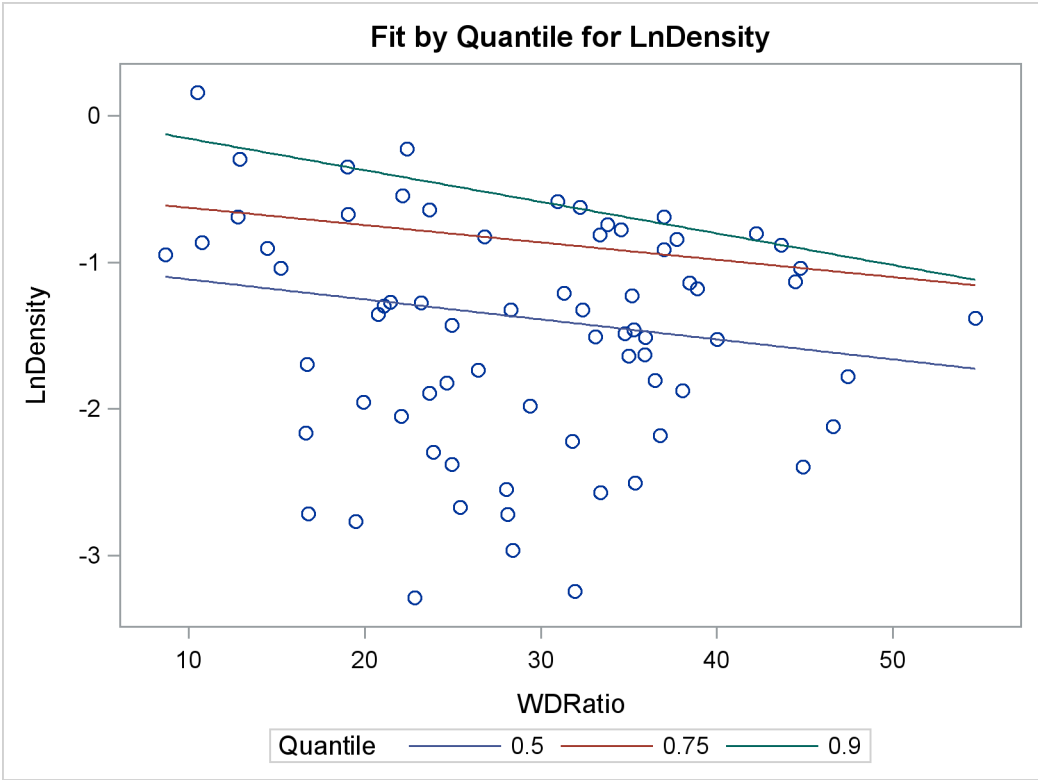


Figure 77.15 Fit Plot for Multiple Quantiles





## Quantile Process Plot

A quantile process plot is a scatter plot of an estimated regression parameter against quantile. You can request this plot with the PLOT=QUANTPLOT option in the MODEL statement when multiple regression quantiles or the entire quantile process is computed. Quantile process plots are often used to check model variations at different quantiles, which is usually called model heterogeneity.

By default, panels are used to hold multiple process plots (up to four in each panel). You can use the UNPACK option to request individual process plots. Figure 77.10 in the section “Analysis of Fish-Habitat Relationships” on page 6490 shows a panel with two quantile process plots. Output 77.2.9 in Example 77.2 shows a single quantile process plot. Example 77.3 demonstrates more quantile process plots and their usage.

## Distance-Distance Plot

The distance-distance plot (DDPLOT) is mainly used for leverage-point diagnostics. It is a scatter plot of the robust distances against the classical Mahalanobis distances for the continuous independent variables. See the section “Leverage Point and Outlier Detection” on page 6528 for details about the robust distance. If there is a classification variable specified in the model, this plot is not created.

You can use the PLOT=DDPLOT option to request this plot. The following statements use the growth data set in Example 77.2 to create a single plot, shown in Output 77.2.4 in Example 77.2:

```
ods graphics on;

proc quantreg data=growth ci=resampling plot=ddplot;
 model GDP = lgdp2 mse2 fse2 fhe2 mhe2 lexp2
 lintr2 gedy2 Iy2 gcony2 lblakp2 pol2 ttrad2
 / quantile=.5 diagnostics leverage(cutoff=8) seed=1268;
 id Country;
run;
```

The reference lines represent the cutoff values. The diagonal line is also drawn to show the distribution of the distances. By default, all outliers and leverage points are labeled with observation numbers. To change the default, you can use the LABEL= option as described in Table 77.5.

## Residual-Distance Plot

The residual-distance plot (RDPLOT) is used for both outlier and leverage-point diagnostics. It is a scatter plot of the standardized residuals against the robust distances. See the section “Leverage Point and Outlier Detection” on page 6528 for details about the robust distance. If a classification variable is specified in the model, this plot is not created.

You can use the PLOT=RDPLOT option to request this plot. The following statements use the growth data set in Example 77.2 to create a single plot, shown in Output 77.2.3 in Example 77.2:

```
ods graphics on;

proc quantreg data=growth ci=resampling plot=rdplot;
 model GDP = lgdp2 mse2 fse2 fhe2 mhe2 lexp2
 lintr2 gedy2 Iy2 gcony2 lblakp2 pol2 ttrad2
 / quantile=.5 diagnostics leverage(cutoff=8) seed=1268;
 id Country;
run;
```

The reference lines represent the cutoff values. By default, all outliers and leverage points are labeled with observation numbers. To change the default, you can use the LABEL= option as described in [Table 77.5](#).

If you specify ID variables in the ID statement, instead of observation numbers, the values of the first ID variable are used as labels.

## Histogram and Q-Q Plot

PROC QUANTREG produces a histogram and a Q-Q plot for the standardized residuals. The histogram is superimposed with a normal density curve and a kernel density curve. Using the growth data set in [Example 77.2](#), the following statements create the plot shown in [Output 77.2.5](#) in [Example 77.2](#):

```
ods graphics on;

proc quantreg data=growth ci=resampling plot=histogram;
 model GDP = lgdp2 mse2 fse2 fhe2 mhe2 lexp2
 lintr2 gedy2 Iy2 gcony2 lblakp2 pol2 ttrad2
 / quantile=.5 diagnostics leverage(cutoff=8) seed=1268;
 id Country;
run;
```

---

## Examples: QUANTREG Procedure

---

### Example 77.1: Comparison of Algorithms

This example illustrates and compares the three algorithms for regression estimation available in the QUANTREG procedure. The simplex algorithm is the default because of its stability. Although this algorithm is slower than the interior point and smoothing algorithms for large data sets, the difference is not as significant for data sets with fewer than 5,000 observations and 50 variables. The simplex algorithm can also compute the entire quantile process, which is shown in [Example 77.2](#).

The following statements generate 1,000 random observations. The first 950 observations are from a linear model, and the last 50 observations are significantly biased in the y-direction. In other words, 5% of the observations are contaminated with outliers.

```
data a (drop=i);
 do i=1 to 1000;
 x1=rannor(1234);
 x2=rannor(1234);
 e=rannor(1234);
 if i > 950 then y=100 + 10*e;
 else y=10 + 5*x1 + 3*x2 + 0.5 * e;
 output;
 end;
run;
```

The following statements invoke the QUANTREG procedure to fit a median regression model with the default simplex algorithm. They produce the results in [Output 77.1.1](#) through [Output 77.1.3](#).

```
proc quantreg data=a;
 model y = x1 x2;
run;
```

[Output 77.1.1](#) displays model information and summary statistics for variables in the model. It indicates that the simplex algorithm is used to compute the optimal solution and the rank method is used to compute confidence intervals of the parameters.

By default, the QUANTREG procedure fits a median regression model. This is indicated by the quantile value 0.5 in [Output 77.1.2](#), which also displays the objective function value and the predicted value of the response at the means of the covariates.

[Output 77.1.3](#) displays parameter estimates and confidence limits. These estimates are reasonable, which indicates that median regression is robust to the 50 outliers.

**Output 77.1.1** Model Fit Information and Summary Statistics with Simplex Algorithm

| BMI Percentiles for Men: 2-80 Years Old |          |         |         |         |                    |        |
|-----------------------------------------|----------|---------|---------|---------|--------------------|--------|
| The QUANTREG Procedure                  |          |         |         |         |                    |        |
| Model Information                       |          |         |         |         |                    |        |
| Data Set                                | WORK.A   |         |         |         |                    |        |
| Dependent Variable                      | y        |         |         |         |                    |        |
| Number of Independent Variables         | 2        |         |         |         |                    |        |
| Number of Observations                  | 1000     |         |         |         |                    |        |
| Optimization Algorithm                  | Simplex  |         |         |         |                    |        |
| Method for Confidence Limits            | Inv_Rank |         |         |         |                    |        |
| Summary Statistics                      |          |         |         |         |                    |        |
| Variable                                | Q1       | Median  | Q3      | Mean    | Standard Deviation | MAD    |
| x1                                      | -0.6546  | 0.0230  | 0.7099  | 0.0222  | 0.9933             | 1.0085 |
| x2                                      | -0.7891  | -0.0747 | 0.6839  | -0.0401 | 1.0394             | 1.0857 |
| y                                       | 6.1045   | 10.6936 | 14.9569 | 14.4864 | 20.4087            | 6.5696 |

**Output 77.1.2** Quantile and Objective Function with Simplex Algorithm

| Quantile and Objective Function |           |
|---------------------------------|-----------|
| Quantile                        | 0.5       |
| Objective Function              | 2441.1927 |
| Predicted Value at Mean         | 10.0259   |

**Output 77.1.3** Parameter Estimates with Simplex Algorithm

| Parameter Estimates |    |          |                       |         |
|---------------------|----|----------|-----------------------|---------|
| Parameter           | DF | Estimate | 95% Confidence Limits |         |
| Intercept           | 1  | 10.0364  | 9.9959                | 10.0756 |
| x1                  | 1  | 5.0106   | 4.9602                | 5.0388  |
| x2                  | 1  | 3.0294   | 2.9944                | 3.0630  |

The following statements refit the model by using the interior point algorithm:

```
proc quantreg algorithm=interior(tolerance=1e-6)
 ci=none data=a;
 model y = x1 x2 / itprint nosummary;
run;
```

The TOLERANCE= option specifies the stopping criterion for convergence of the interior point algorithm, which is controlled by the duality gap. Although the default criterion is 1E-8, the value 1E-6 is often sufficient. The ITPRINT option requests the iteration history for the algorithm. The option CI=NONE suppresses the computation of confidence limits, and the option NOSUMMARY suppresses the table of summary statistics.

Output 77.1.4 displays model fit information.

**Output 77.1.4** Model Fit Information with Interior Point Algorithm

| BMI Percentiles for Men: 2-80 Years Old |          |
|-----------------------------------------|----------|
| The QUANTREG Procedure                  |          |
| Model Information                       |          |
| Data Set                                | WORK.A   |
| Dependent Variable                      | y        |
| Number of Independent Variables         | 2        |
| Number of Observations                  | 1000     |
| Optimization Algorithm                  | Interior |

Output 77.1.5 displays the iteration history of the interior point algorithm. Note that the duality gap is less than  $1\text{E-}6$  in the final iteration. The table also provides the number of iterations, the number of corrections, the primal step length, the dual step length, and the objective function value at each iteration.

**Output 77.1.5** Iteration History for the Interior Point Algorithm

| Iteration History of Interior Point Algorithm |      |            |             |           |                    |  |
|-----------------------------------------------|------|------------|-------------|-----------|--------------------|--|
| Duality Gap                                   | Iter | Correction | Primal Step | Dual Step | Objective Function |  |
| 2623                                          | 1    | 1          | 0.3113      | 0.4910    | 3303.4688          |  |
| 3215                                          | 2    | 2          | 0.0427      | 1.0000    | 2461.3774          |  |
| 1127                                          | 3    | 3          | 0.9882      | 0.3653    | 2451.1337          |  |
| 760.88658                                     | 4    | 4          | 0.3381      | 1.0000    | 2442.8104          |  |
| 77.10290                                      | 5    | 5          | 1.0000      | 0.8916    | 2441.2627          |  |
| 8.43666                                       | 6    | 6          | 0.9370      | 0.8381    | 2441.2085          |  |
| 1.82868                                       | 7    | 7          | 0.8375      | 0.7674    | 2441.1985          |  |
| 0.40584                                       | 8    | 8          | 0.6980      | 0.8636    | 2441.1948          |  |
| 0.09550                                       | 9    | 9          | 0.9438      | 0.5955    | 2441.1930          |  |
| 0.00665                                       | 10   | 10         | 0.9818      | 0.9304    | 2441.1927          |  |
| 0.0002248                                     | 11   | 11         | 0.9179      | 0.9994    | 2441.1927          |  |
| 5.44651E-8                                    | 12   | 12         | 1.0000      | 1.0000    | 2441.1927          |  |

Output 77.1.6 displays the parameter estimates obtained with the interior point algorithm, which are identical to those obtained with the simplex algorithm.

**Output 77.1.6** Parameter Estimates with Interior Point Algorithm

| Parameter Estimates |    |          |
|---------------------|----|----------|
| Parameter           | DF | Estimate |
| Intercept           | 1  | 10.0364  |
| x1                  | 1  | 5.0106   |
| x2                  | 1  | 3.0294   |

The following statements refit the model by using the smoothing algorithm. They produce the results in Output 77.1.7 through Output 77.1.9.

```
proc quantreg algorithm=smooth(rratio=.5) ci=none data=a;
 model y = x1 x2 / itprint nosummary;
run;
```

The RRATIO= option controls the reduction speed of the threshold. Output 77.1.7 displays the model fit information.

**Output 77.1.7** Model Fit Information with Smoothing Algorithm

| BMI Percentiles for Men: 2-80 Years Old |        |
|-----------------------------------------|--------|
| The QUANTREG Procedure                  |        |
| Model Information                       |        |
| Data Set                                | WORK.A |
| Dependent Variable                      | y      |
| Number of Independent Variables         | 2      |
| Number of Observations                  | 1000   |
| Optimization Algorithm                  | Smooth |

Output 77.1.8 displays the iteration history of the smoothing algorithm. The threshold controls the convergence. Note that the thresholds decrease by a factor of at least 0.5, the value specified with the RRATIO= option. The table also provides the number of iterations, the number of factorizations, the number of full updates, the number of partial updates, and the objective function value in each iteration. For details concerning the smoothing algorithm, see Chen (2007).

**Output 77.1.8** Iteration History for the Smoothing Algorithm

| Iteration History of Smoothing Algorithm |      |       |             |                |                    |
|------------------------------------------|------|-------|-------------|----------------|--------------------|
| Threshold                                | Iter | Refac | Full Update | Partial Update | Objective Function |
| 227.24557                                | 1    | 1     | 1000        | 0              | 4267.0988          |
| 116.94090                                | 15   | 4     | 1480        | 2420           | 3631.9653          |
| 1.44064                                  | 17   | 4     | 1480        | 2583           | 2441.4719          |
| 0.72032                                  | 20   | 5     | 1980        | 2598           | 2441.3315          |
| 0.36016                                  | 22   | 6     | 2248        | 2607           | 2441.2369          |
| 0.18008                                  | 24   | 7     | 2376        | 2608           | 2441.2056          |
| 0.09004                                  | 26   | 8     | 2446        | 2613           | 2441.1997          |
| 0.04502                                  | 28   | 9     | 2481        | 2617           | 2441.1971          |
| 0.02251                                  | 30   | 10    | 2497        | 2618           | 2441.1956          |
| 0.01126                                  | 32   | 11    | 2505        | 2620           | 2441.1946          |
| 0.00563                                  | 34   | 12    | 2510        | 2621           | 2441.1933          |
| 0.00281                                  | 35   | 13    | 2514        | 2621           | 2441.1930          |
| 0.0000846                                | 36   | 14    | 2517        | 2621           | 2441.1927          |
| 1E-12                                    | 37   | 14    | 2517        | 2621           | 2441.1927          |

Output 77.1.9 displays the parameter estimates obtained with the smoothing algorithm, which are identical to those obtained with the simplex and interior point algorithms. All three algorithms should have the same parameter estimates unless the problem does not have a unique solution.

**Output 77.1.9** Parameter Estimates with Smoothing Algorithm

| Parameter Estimates |    |          |
|---------------------|----|----------|
| Parameter           | DF | Estimate |
| Intercept           | 1  | 10.0364  |
| x1                  | 1  | 5.0106   |
| x2                  | 1  | 3.0294   |

The interior point algorithm and the smoothing algorithm offer better performance than the simplex algorithm for large data sets. See Chen (2004) for more details on choosing an appropriate algorithm on the basis of data set size. All three algorithms should have the same parameter estimates, unless the optimization problem has multiple solutions.

---

**Example 77.2: Quantile Regression for Econometric Growth Data**

This example uses a SAS data set named *Growth*, which contains economic growth rates for countries during two time periods, 1965–1975 and 1975–1985. The data come from a study by Barro and Lee (1994) and have also been analyzed by Koenker and Machado (1999).

There are 161 observations and 15 variables in the data set. The variables, which are listed in the following table, include the national growth rates (GDP) for the two periods, 13 covariates, and a name variable (Country) for identifying the countries in one of the two periods.

| Variable | Description                  |
|----------|------------------------------|
| Country  | Country's name and period    |
| GDP      | Annual change per capita GDP |
| lgdp2    | Initial per capita GDP       |
| mse2     | Male secondary education     |
| fse2     | Female secondary education   |
| fhe2     | Female higher education      |
| mhe2     | Male higher education        |
| lexp2    | Life expectancy              |
| lintr2   | Human capital                |
| gedy2    | Education/GDP                |
| ly2      | Investment/GDP               |
| gcony2   | Public consumption/GDP       |
| lblakp2  | Black market premium         |
| pol2     | Political instability        |
| ttrad2   | Growth rate terms trade      |

The goal is to study the effect of the covariates on GDP. The following statements request median regression for a preliminary exploration. They produce the results in [Output 77.2.1](#) through [Output 77.2.6](#).

```

data growth;
 length Country$ 22;
 input Country GDP lgdp2 mse2 fse2 fhe2 mhe2 lexp2 lintr2 gedy2
 Iy2 gcony2 lblakp2 pol2 ttrad2 @@;
 datalines;
Algeria75 .0415 7.330 .1320 .0670 .0050 .0220 3.880 .1138 .0382
 .1898 .0601 .3823 .0833 .1001
Algeria85 .0244 7.745 .2760 .0740 .0070 .0370 3.978 -.107 .0437
 .3057 .0850 .9386 .0000 .0657
Argentina75 .0187 8.220 .7850 .6200 .0740 .1660 4.181 .4060 .0221
 .1505 .0596 .1924 .3575 -.011
Argentina85 -.014 8.407 .9360 .9020 .1320 .2030 4.211 .1914 .0243
 .1467 .0314 .3085 .7010 -.052
Australia75 .0259 9.101 2.541 2.353 .0880 .2070 4.263 6.937 .0348
 .3272 .0257 .0000 .0080 -.016

... more lines ...

Zambia75 .0120 6.989 .3760 .1190 .0130 .0420 3.757 .4388 .0339
 .3688 .2513 .3945 .0000 -.032
Zambia85 -.046 7.109 .4200 .2740 .0110 .0270 3.854 .8812 .0477
 .1632 .2637 .6467 .0000 -.033
Zimbabwe75 .0320 6.860 .1450 .0170 .0080 .0450 3.833 .7156 .0337
 .2276 .0246 .1997 .0000 -.040
Zimbabwe85 -.011 7.180 .2200 .0650 .0060 .0400 3.944 .9296 .0520
 .1559 .0518 .7862 .7161 -.024

;

ods graphics on;

proc quantreg data=growth ci=resampling
 plots=(rdplot ddplot reshistogram);
 model GDP = lgdp2 mse2 fse2 fhe2 mhe2 lexp2
 lintr2 gedy2 Iy2 gcony2 lblakp2 pol2 ttrad2
 / quantile=.5 diagnostics leverage(cutoff=8) seed=1268;
 id Country;
 test_lgdp2: test lgdp2 / lr wald;
run;

```

The QUANTREG procedure employs the default simplex algorithm to estimate the parameters. The MCMB resampling method is used to compute confidence limits.

Output 77.2.1 displays model information and summary statistics for the variables in the model. Six summary statistics are computed, including the median and the median absolute deviation (MAD), which are robust measures of univariate location and scale, respectively. For the variable `lintr2` (Human Capital), both the mean and standard deviation are much larger than the corresponding robust measures, median and MAD. This indicates that this variable might have outliers.



**Output 77.2.1** Model Information and Summary Statistics

| BMI Percentiles for Men: 2-80 Years Old |             |         |         |          |                    |        |
|-----------------------------------------|-------------|---------|---------|----------|--------------------|--------|
| The QUANTREG Procedure                  |             |         |         |          |                    |        |
| Model Information                       |             |         |         |          |                    |        |
| Data Set                                | WORK.GROWTH |         |         |          |                    |        |
| Dependent Variable                      | GDP         |         |         |          |                    |        |
| Number of Independent Variables         | 13          |         |         |          |                    |        |
| Number of Observations                  | 161         |         |         |          |                    |        |
| Optimization Algorithm                  | Simplex     |         |         |          |                    |        |
| Method for Confidence Limits            | Resampling  |         |         |          |                    |        |
| Summary Statistics                      |             |         |         |          |                    |        |
| Variable                                | Q1          | Median  | Q3      | Mean     | Standard Deviation | MAD    |
| lgdp2                                   | 6.9890      | 7.7450  | 8.6080  | 7.7905   | 0.9543             | 1.1579 |
| mse2                                    | 0.3160      | 0.7230  | 1.2675  | 0.9666   | 0.8574             | 0.6835 |
| fse2                                    | 0.1270      | 0.4230  | 0.9835  | 0.7117   | 0.8331             | 0.5011 |
| fhe2                                    | 0.0110      | 0.0350  | 0.0890  | 0.0792   | 0.1216             | 0.0400 |
| mhe2                                    | 0.0400      | 0.1060  | 0.2060  | 0.1584   | 0.1752             | 0.1127 |
| lexp2                                   | 3.8670      | 4.0640  | 4.2430  | 4.0440   | 0.2028             | 0.2728 |
| lintr2                                  | 0.00160     | 0.5604  | 1.8805  | 1.4625   | 2.5491             | 1.0058 |
| gedy2                                   | 0.0248      | 0.0343  | 0.0466  | 0.0360   | 0.0141             | 0.0151 |
| Iy2                                     | 0.1396      | 0.1955  | 0.2671  | 0.2010   | 0.0877             | 0.0981 |
| gcony2                                  | 0.0480      | 0.0767  | 0.1276  | 0.0914   | 0.0617             | 0.0566 |
| lblakp2                                 | 0           | 0.0696  | 0.2407  | 0.1916   | 0.3070             | 0.1032 |
| pol2                                    | 0           | 0.0500  | 0.2429  | 0.1683   | 0.2409             | 0.0741 |
| ttrad2                                  | -0.0240     | -0.0100 | 0.00730 | -0.00570 | 0.0375             | 0.0239 |
| GDP                                     | 0.00290     | 0.0196  | 0.0351  | 0.0191   | 0.0248             | 0.0237 |

Output 77.2.2 displays parameter estimates and 95% confidence limits computed with the rank method.

### Output 77.2.2 Parameter Estimates

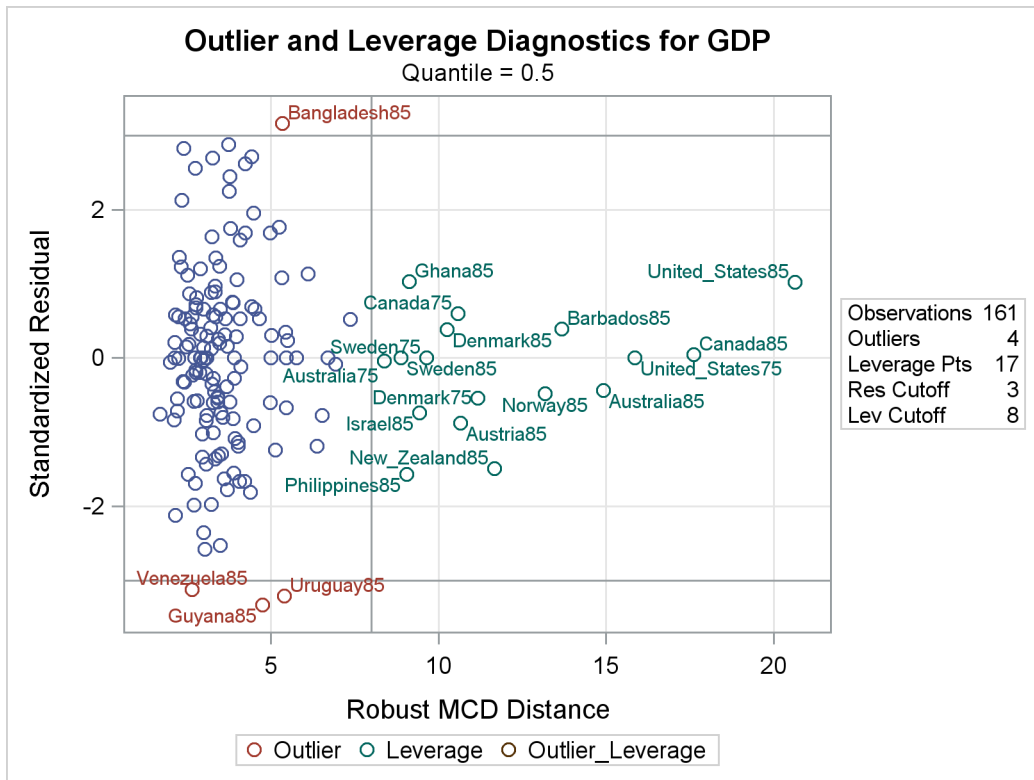
| Parameter Estimates |    |          |                |                       |         |         |         |
|---------------------|----|----------|----------------|-----------------------|---------|---------|---------|
| Parameter           | DF | Estimate | Standard Error | 95% Confidence Limits |         | t Value | Pr >  t |
| Intercept           | 1  | -0.0488  | 0.0733         | -0.1937               | 0.0961  | -0.67   | 0.5065  |
| lgdp2               | 1  | -0.0269  | 0.0041         | -0.0350               | -0.0188 | -6.58   | <.0001  |
| mse2                | 1  | 0.0110   | 0.0080         | -0.0048               | 0.0269  | 1.38    | 0.1710  |
| fse2                | 1  | -0.0011  | 0.0088         | -0.0185               | 0.0162  | -0.13   | 0.8960  |
| fhe2                | 1  | 0.0148   | 0.0321         | -0.0485               | 0.0782  | 0.46    | 0.6441  |
| mhe2                | 1  | 0.0043   | 0.0268         | -0.0487               | 0.0573  | 0.16    | 0.8735  |
| lexp2               | 1  | 0.0683   | 0.0229         | 0.0232                | 0.1135  | 2.99    | 0.0033  |
| lintr2              | 1  | -0.0022  | 0.0015         | -0.0052               | 0.0008  | -1.44   | 0.1513  |
| gedy2               | 1  | -0.0508  | 0.1654         | -0.3777               | 0.2760  | -0.31   | 0.7589  |
| Iy2                 | 1  | 0.0723   | 0.0248         | 0.0233                | 0.1213  | 2.92    | 0.0041  |
| gcony2              | 1  | -0.0935  | 0.0382         | -0.1690               | -0.0181 | -2.45   | 0.0154  |
| lblakp2             | 1  | -0.0269  | 0.0084         | -0.0435               | -0.0104 | -3.22   | 0.0016  |
| pol2                | 1  | -0.0301  | 0.0093         | -0.0485               | -0.0117 | -3.23   | 0.0015  |
| ttrad2              | 1  | 0.1613   | 0.0740         | 0.0149                | 0.3076  | 2.18    | 0.0310  |

Diagnostics for the median regression fit are displayed in [Output 77.2.3](#) and [Output 77.2.4](#), which are requested with the PLOTS= option. [Output 77.2.3](#) plots the standardized residuals from median regression against the robust MCD distance. This display is used to diagnose both vertical outliers and horizontal leverage points. [Output 77.2.4](#) plots the robust MCD distance against the Mahalanobis distance. This display is used to diagnose leverage points.

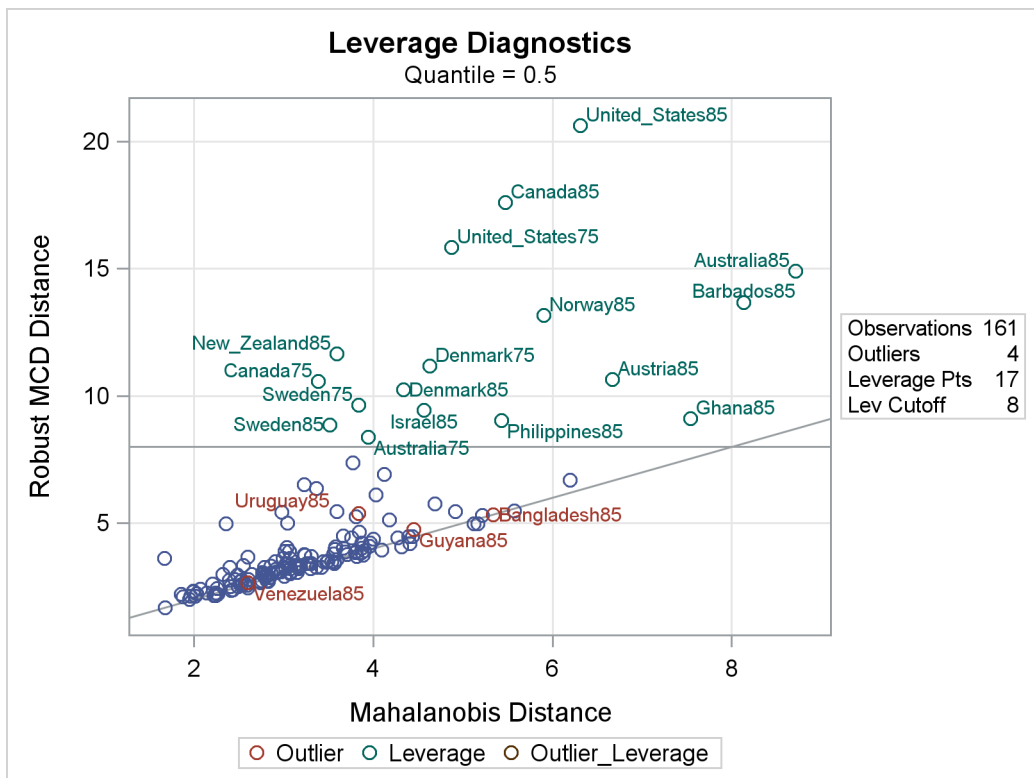
The cutoff value 8 specified with the LEVERAGE option is close to the maximum of the Mahalanobis distance. Eighteen points are diagnosed as high leverage points, and almost all are countries with high human capital, which is the major contributor to the high leverage as observed from the summary statistics. Four points are diagnosed as outliers by using the default cutoff value of 3. However, these are not extreme outliers.

A histogram of the standardized residuals and two fitted density curves are displayed in [Output 77.2.5](#). This shows that median regression fits the data well.

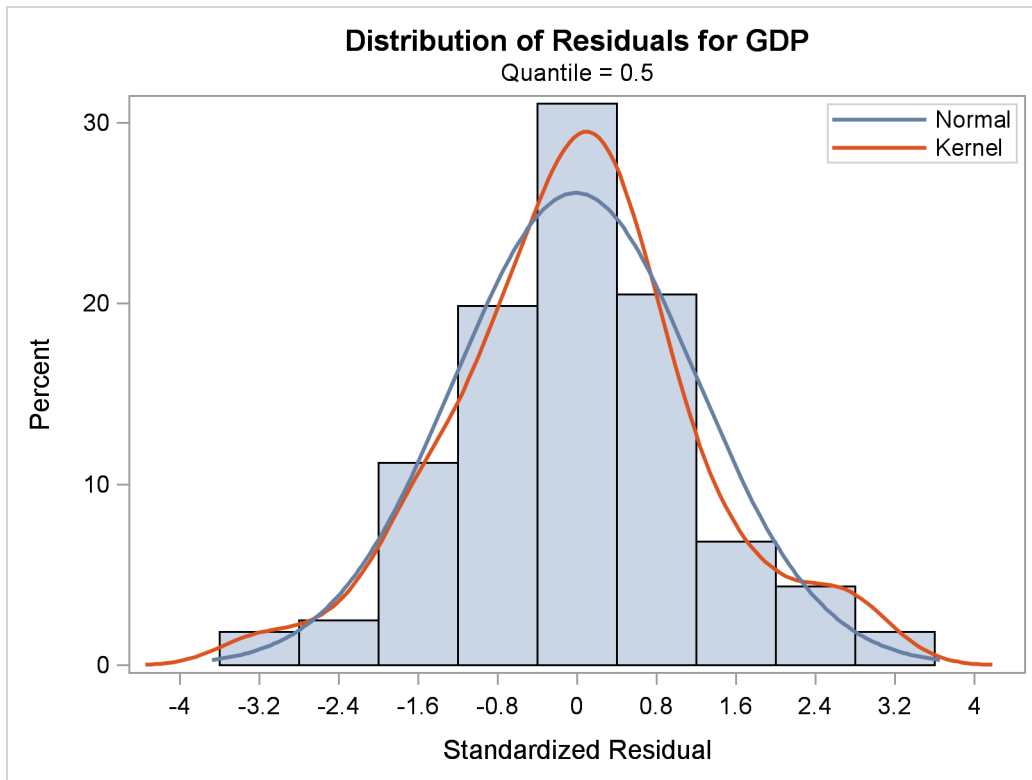
**Output 77.2.3** Residual-Robust Distance Plot



**Output 77.2.4** Robust Distance-Mahalanobis Distance Plot



**Output 77.2.5** Histogram for Residuals



Tests of significance for the initial per-capita GDP (LGDP2) are shown in [Output 77.2.6](#).

**Output 77.2.6** Tests for Regression Coefficient

| Test test_lgdp2 Results |                |        |        |            |
|-------------------------|----------------|--------|--------|------------|
| Test                    | Test Statistic | Chi-DF | Square | Pr > ChiSq |
| Wald                    | 43.2684        | 1      | 43.27  | <.0001     |
| Likelihood Ratio        | 36.3047        | 1      | 36.30  | <.0001     |

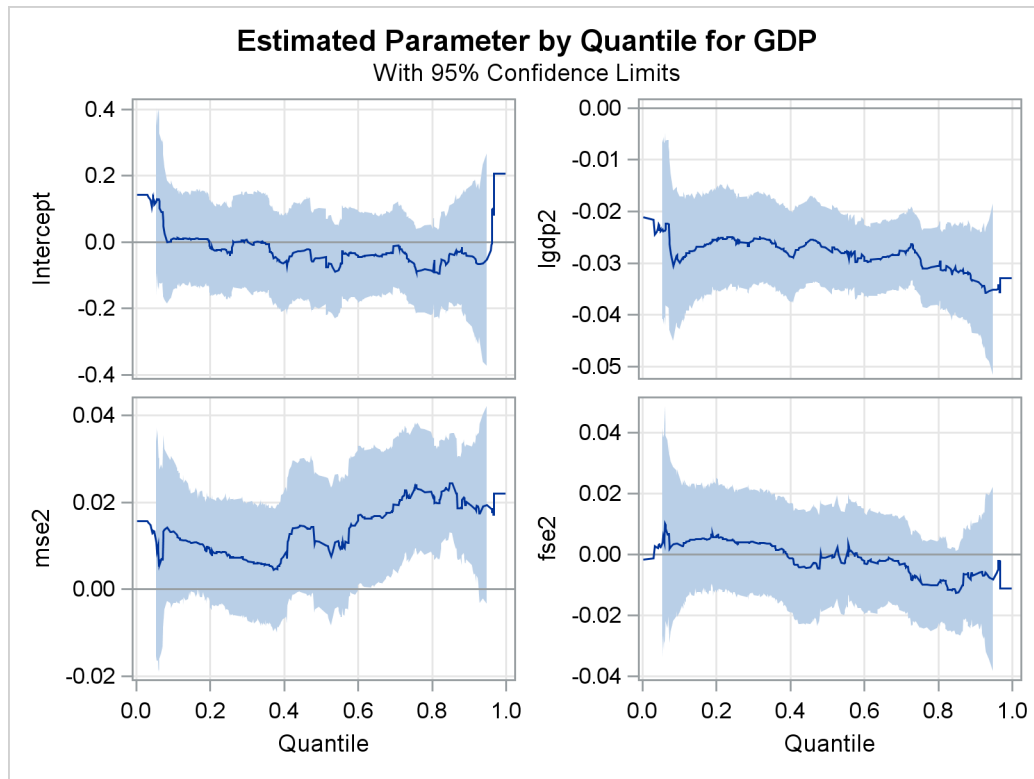
The QUANTREG procedure computes entire quantile processes for covariates when you specify QUANTILE=PROCESS in the MODEL statement, as follows:

```
proc quantreg data=growth ci=resampling;
 model GDP = lgdp2 mse2 fse2 fhe2 mhe2 lexp2 lintr2
 gedy2 Iy2 gcony2 lblackp2 pol2 ttrad2
 / quantile=process plot=quantplot seed=1268;
run;
```

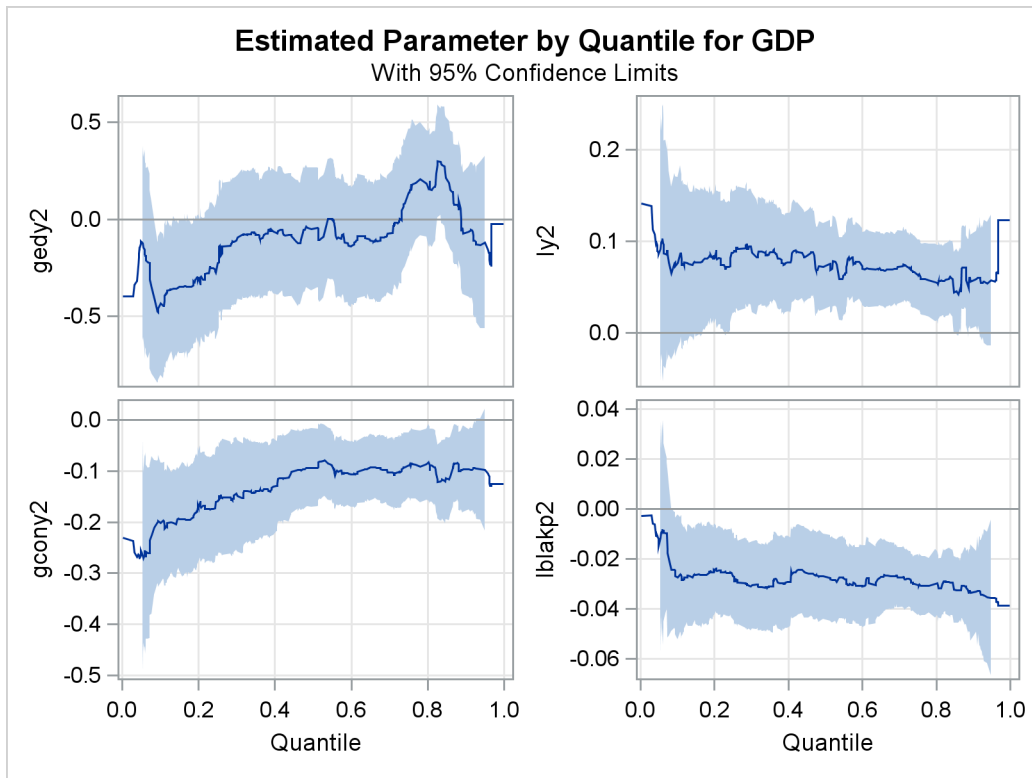
Confidence limits for quantile processes can be computed with the sparsity or resampling methods, but not the rank method, because the computation would be prohibitively expensive.

A total of 14 quantile process plots are produced. [Output 77.2.7](#) and [Output 77.2.8](#) display two panels of eight selected process plots. The 95% confidence bands are shaded.

**Output 77.2.7** Quantile Processes with 95% Confidence Bands



**Output 77.2.8** Quantile Processes with 95% Confidence Bands

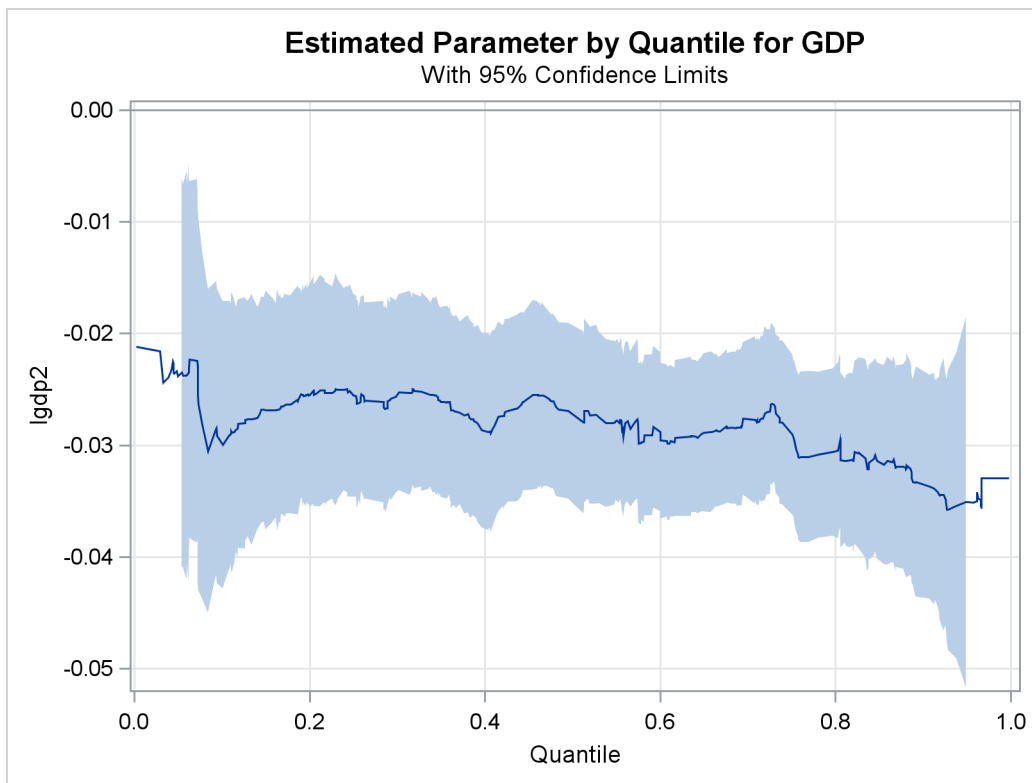


As pointed out by Koenker and Machado (1999), previous studies of the Barro growth data have focused on the effect of the initial per-capita GDP on the growth of this variable (annual change per-capita GDP). A single process plot for this effect can be requested with the following statements:

```
proc quantreg data=growth ci=resampling;
 model GDP = lgdp2 mse2 fse2 fhe2 mhe2 lexp2 lintr2
 gedy2 ly2 gcony2 lblakp2 pol2 ttrad2
 / quantile=process plot=quantplot(lgdp2) seed=1268;
run;
```

The plot is shown in [Output 77.2.9](#).

**Output 77.2.9** Quantile Process Plot for LGDP2



The confidence bands here are computed with the MCMB resampling method, unlike in Koenker and Machado (1999), where the rank method was used to compute confidence limits for a few selected points. [Output 77.2.9](#) suggests that the effect of the initial level of GDP is relatively constant over the entire distribution, with a slightly stronger effect in the upper tail.

The effects of other covariates are quite varied. An interesting covariate is public consumption/GDP (`gcony2`) (first plot in second panel), which has a constant effect over the upper half of the distribution and a larger effect in the lower tail. For an analysis of the effects of the other covariates, see Koenker and Machado (1999).

---

### Example 77.3: Quantile Regression Analysis of Birth-Weight Data

This example is patterned after a quantile regression analysis of covariates associated with birth weight that was carried out by Koenker and Hallock (2001). Their study used a subset of the June 1997 Detailed Natality Data published by the National Center for Health Statistics and demonstrated that conditional quantile functions provide more complete information about the covariate effects than ordinary least squares regression.

This example is based on Koenker and Hallock (2001); Abreveya (2001); it uses data for live, singleton births to mothers in the United States who were recorded as black or white, and who were between the ages

of 18 and 45. For convenience, this example uses 50,000 observations, which were randomly selected from the qualified observations. Observations with missing data for any of the variables were deleted.

The following table describes the variables in the data.

| Variable | Description                                                                                                               |
|----------|---------------------------------------------------------------------------------------------------------------------------|
| Weight   | Infant's birth weight                                                                                                     |
| Black    | Indicator of black mother                                                                                                 |
| Married  | Indicator of married mother                                                                                               |
| Boy      | Indicator of boy                                                                                                          |
| Visit    | Prenatal visit: 0 = no visit, 1 = visit in second trimester,<br>2 = visit in last trimester, 3 = visit in first trimester |
| Ed       | Mother's education level: 0 = high school, 1 = some college,<br>2 = college, 3 = less than high school                    |
| Smoke    | Indicator of smoking mother                                                                                               |
| CigsPer  | Number of cigarettes smoked per day                                                                                       |
| Mom_Age  | Mother's age                                                                                                              |
| M_WtGain | Mother's weight gain during pregnancy                                                                                     |

There are four levels of education of the mother. By default, the QUANTREG procedure treats the highest level (3 - less than high school) as a reference level. The regression coefficients of other levels measure the effect relative to this level. Likewise, there are four levels of prenatal medical care of the mother, and a first visit in the first trimester serves as the reference level. These two variables are treated as classification variables in the model.

The following statements fit a regression model for 19 quantiles of birth weight, which are evenly spaced in the interval (0, 1). The model includes linear and quadratic effects for the age of the mother and for weight gain during pregnancy.

```
ods graphics on;

proc quantreg ci=sparsity/iid algorithm=interior(tolerance=5.e-4)
 data=sashelp.bweight;
 class visit ed;
 model weight = black married boy visit ed smoke
 cigspers mom_age mom_age*mom_age
 m_wtgain m_wtgain*m_wtgain /
 quantile= 0.05 to 0.95 by 0.05
 plot=quantplot;
run;
```



**Output 77.3.1** Model Information and Summary Statistics

| BMI Percentiles for Men: 2-80 Years Old    |                 |         |         |         |                    |         |
|--------------------------------------------|-----------------|---------|---------|---------|--------------------|---------|
| The QUANTREG Procedure                     |                 |         |         |         |                    |         |
| Model Information                          |                 |         |         |         |                    |         |
| Data Set                                   | SASHELP.BWEIGHT |         |         |         |                    |         |
| Dependent Variable                         | weight          |         |         |         |                    |         |
| Number of Independent Variables            | 9               |         |         |         |                    |         |
| Number of Continuous Independent Variables | 7               |         |         |         |                    |         |
| Number of Class Independent Variables      | 2               |         |         |         |                    |         |
| Number of Observations                     | 50000           |         |         |         |                    |         |
| Optimization Algorithm                     | Interior        |         |         |         |                    |         |
| Method for Confidence Limits               | Sparsity        |         |         |         |                    |         |
| Summary Statistics                         |                 |         |         |         |                    |         |
| Variable                                   | Q1              | Median  | Q3      | Mean    | Standard Deviation | MAD     |
| black                                      | 0               | 0       | 0       | 0.1628  | 0.3692             | 0       |
| married                                    | 0               | 1.0000  | 1.0000  | 0.7126  | 0.4525             | 0       |
| boy                                        | 0               | 1.0000  | 1.0000  | 0.5158  | 0.4998             | 0       |
| smoke                                      | 0               | 0       | 0       | 0.1307  | 0.3370             | 0       |
| cigsper                                    | 0               | 0       | 0       | 1.4766  | 4.6541             | 0       |
| mom_age                                    | -4.0000         | 0       | 5.0000  | 0.4161  | 5.7285             | 5.9304  |
| mom_age*mom_age                            | 4.0000          | 16.0000 | 49.0000 | 32.9877 | 39.2861            | 22.2390 |
| m_wtgain                                   | -8.0000         | 0       | 9.0000  | 0.7092  | 12.8761            | 11.8608 |
| m_wtgain*m_wtgain                          | 16.0000         | 64.0000 | 196.0   | 166.3   | 298.8              | 88.9561 |
| weight                                     | 3062.0          | 3402.0  | 3720.0  | 3370.8  | 566.4              | 504.1   |

Output 77.3.1 displays the model information and summary statistics for the variables in the model.

Among the 11 independent variables, Black, Married, Boy, and Smoke are binary variables. For these variables, the mean represents the proportion in the category. The two continuous variables, Mom\_Age and M\_WtGain, are centered at their medians, which are 27 and 30, respectively.

The quantile plots for the intercept and the other 15 factors with nonzero degree of freedom are shown in the following four panels. In each plot, the regression coefficient at a given quantile indicates the effect on birth weight of a unit change in that factor, assuming that the other factors are fixed. The bands represent 95% confidence intervals.

Although the data set used here is a subset of the Natality data set, the results are quite similar to those of Koenker and Hallock (2001) for the full data set.

In [Output 77.3.2](#), the first plot is for the intercept. As explained by Koenker and Hallock (2001), the intercept “may be interpreted as the estimated conditional quantile function of the birth-weight distribution of a girl born to an unmarried, white mother with less than a high school education, who is 27 years old and had a weight gain of 30 pounds, didn’t smoke, and had her first prenatal visit in the first trimester of the pregnancy.”

The second plot shows that infants born to black mothers weigh less than infants born to white mothers, especially in the lower tail of the birth-weight distribution. The third plot shows that marital status has a large positive effect on birth weight, especially in the lower tail. The fourth plot shows that boys weigh more than girls for any chosen quantile; this difference is smaller in the lower quantiles of the distribution.

In [Output 77.3.3](#), the first three plots deal with prenatal care. Compared with babies born to mothers who had a prenatal visit in the first trimester, babies born to mothers who received no prenatal care weigh less, especially in the lower quantiles of the birth-weight distributions. As noted by Koenker and Hallock (2001), “babies born to mothers who delayed prenatal visits until the second or third trimester have substantially *higher* birthweights in the lower tail than mothers who had a prenatal visit in the first trimester. This might be interpreted as the self-selection effect of mothers confident about favorable outcomes.”

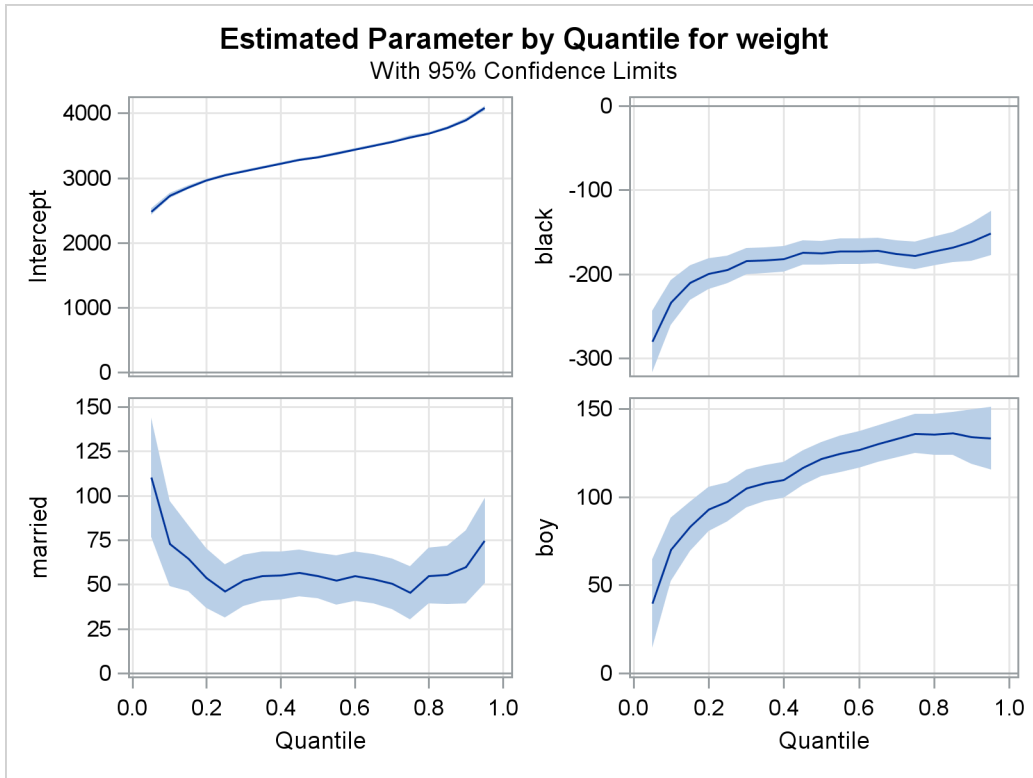
The fourth plot in [Output 77.3.3](#) and the first two plots in [Output 77.3.4](#) are for variables related to education. Education beyond high school is associated with a positive effect on birth weight. The effect of high school education is uniformly around 15 grams across the entire birth-weight distribution (this is a pure location shift effect), while the effect of some college and college education is more positive in the lower quantiles than the upper quantiles.

The remaining two plots in [Output 77.3.4](#) show that smoking is associated with a large negative effect on birth weight.

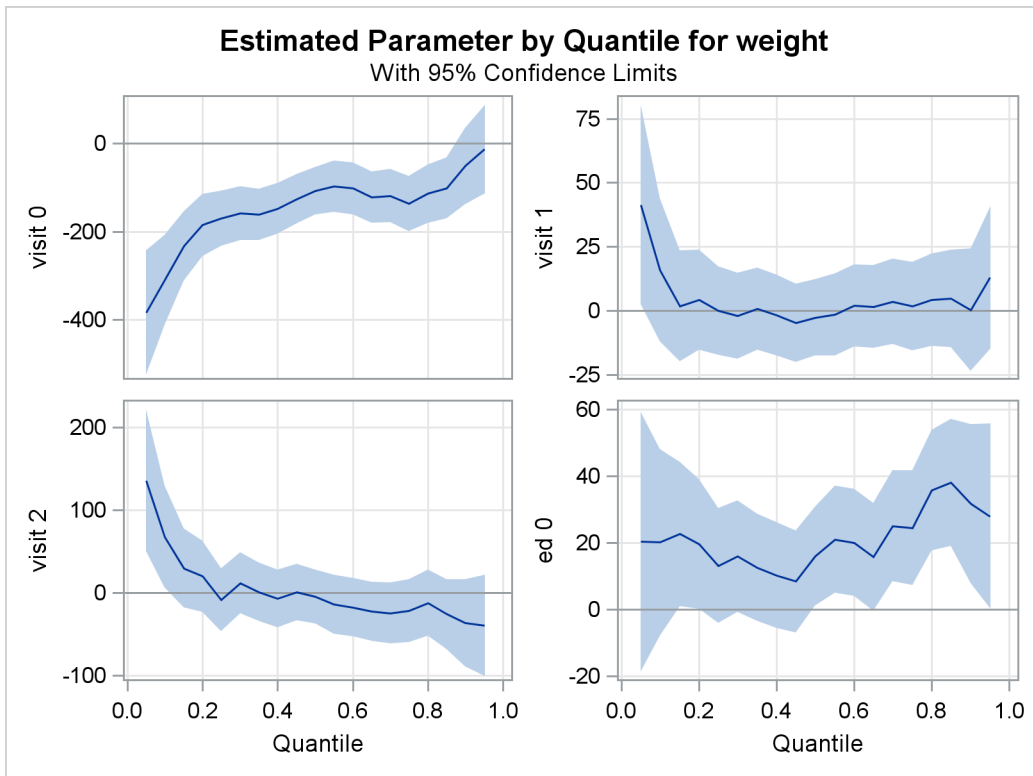
The linear and quadratic effects for the two continuous variables are shown in [Output 77.3.5](#). Both of these variables are centered at their median. At the lower quantiles, the quadratic effect of the mother’s age is more concave. The optimal age at the first quantile is about 33, and the optimal age at the third quantile is about 38. The effect of the mother’s weight gain is clearly positive, as indicated by the narrow confidence bands for both linear and quadratic coefficients.

See Koenker and Hallock (2001) for more details about the covariate effects discovered with quantile regression.

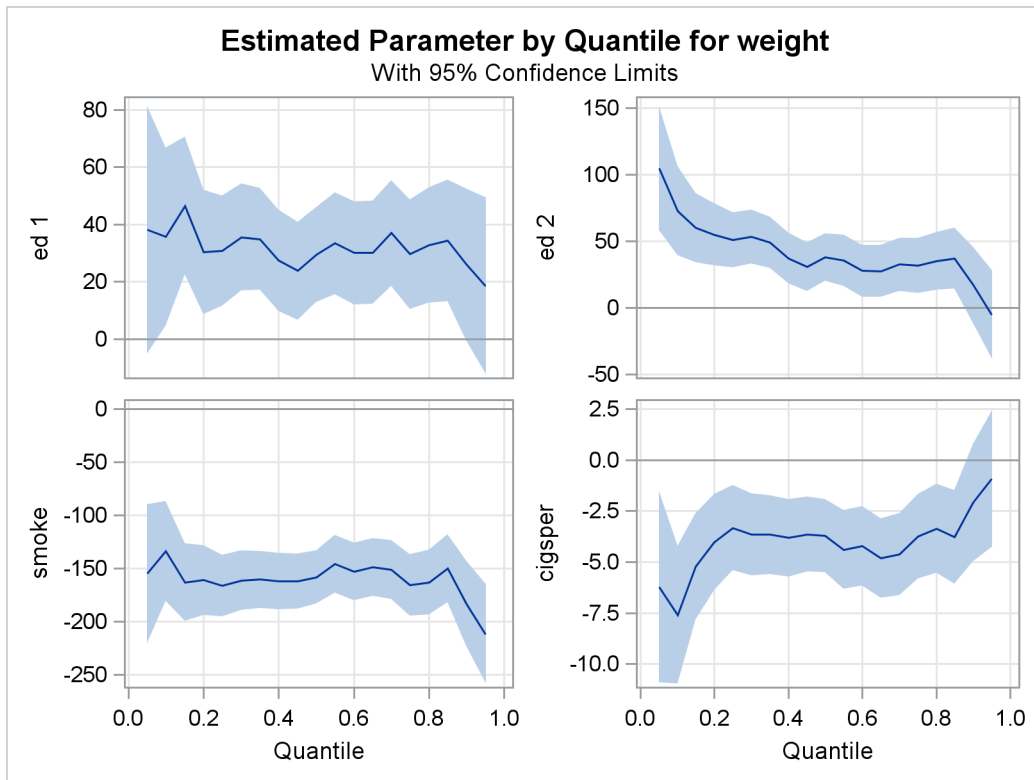
**Output 77.3.2** Quantile Processes with 95% Confidence Bands



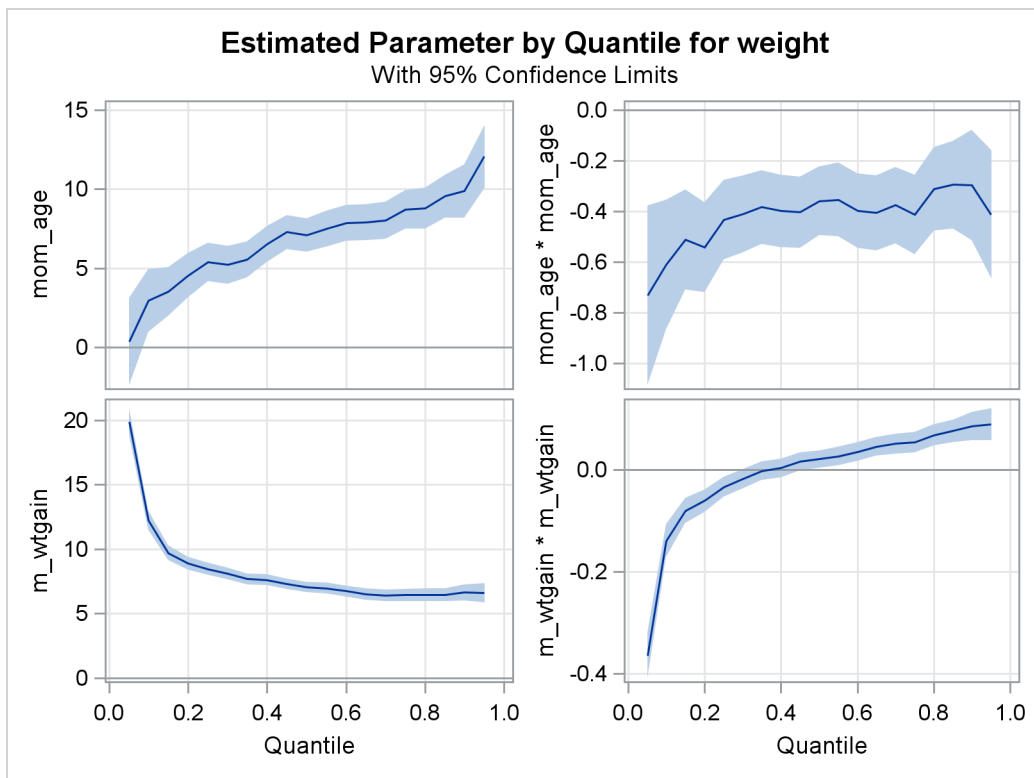
**Output 77.3.3** Quantile Processes with 95% Confidence Bands



**Output 77.3.4** Quantile Processes with 95% Confidence Bands



**Output 77.3.5** Quantile Processes with 95% Confidence Bands



## Example 77.4: Nonparametric Quantile Regression for Ozone Levels

Tracing seasonal trends in the level of tropospheric ozone is essential for predicting high-level periods, observing long-term trends, and discovering potential changes in pollution. Traditional methods for modeling seasonal effects are based on the conditional mean of ozone concentration; however, the upper conditional quantiles are more critical from a public health perspective. In this example, the QUANTREG procedure fits conditional quantile curves for seasonal effects by using nonparametric quantile regression with cubic B-splines.

The data used here are from Chock, Winkler, and Chen (2000), who studied the association between daily mortality and ambient air pollutant concentrations in Pittsburgh, Pennsylvania. The data set ozone contains the following two variables: Ozone (daily-maximum one-hour ozone concentration (ppm)) and Days (index of 1,095 days (3 years)).

```
data ozone;
 days = _n_;
 input ozone @@;
 datalines;
0.0060 0.0060 0.0320 0.0320 0.0320 0.0150 0.0150 0.0150 0.0200 0.0200
0.0160 0.0070 0.0270 0.0160 0.0150 0.0240 0.0220 0.0220 0.0220 0.0185
0.0150 0.0150 0.0110 0.0070 0.0070 0.0240 0.0380 0.0240 0.0265 0.0290
0.0310 0.0460 0.0360 0.0260 0.0300 0.0250 0.0280 0.0310 0.0370 0.0325

... more lines ...

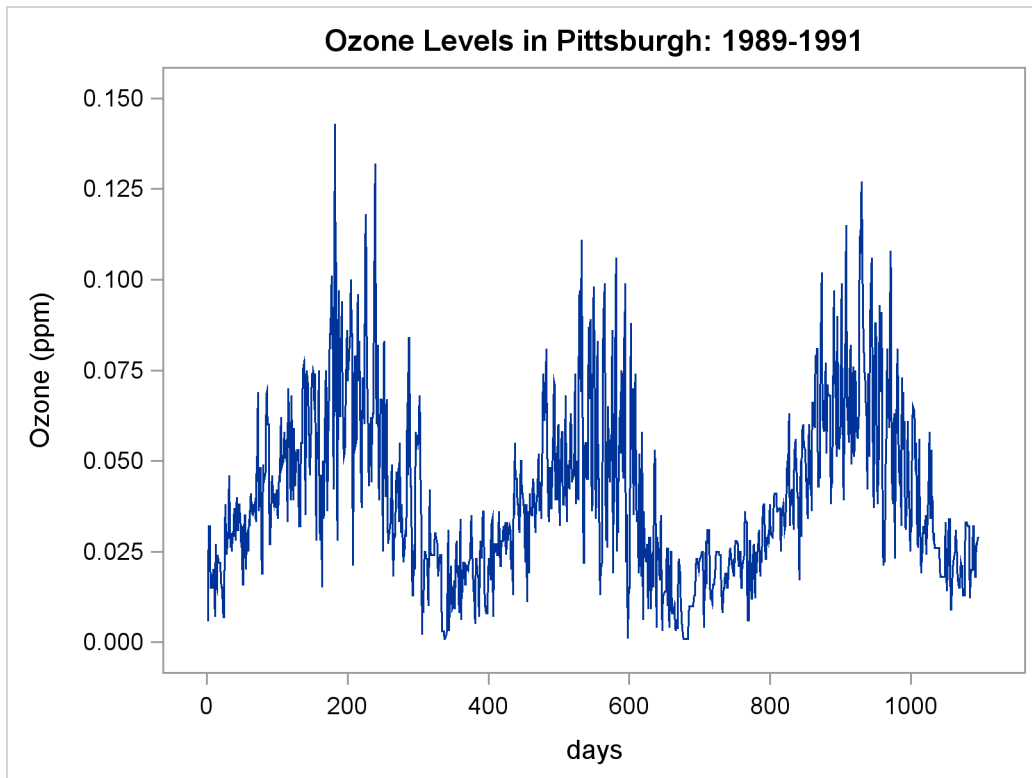
0.0220 0.0210 0.0210 0.0130 0.0130 0.0130 0.0330 0.0330 0.0330 0.0325
0.0320 0.0320 0.0320 0.0120 0.0200 0.0200 0.0200 0.0320 0.0320 0.0250
0.0180 0.0180 0.0270 0.0270 0.0290
;
```

Output 77.4.1, which displays the time series plot of ozone concentration for the three years, shows a clear seasonal pattern.

In this example, cubic B-splines are used to fit the seasonal effect. These splines are generated with 11 knots, which split the 3 years into 12 seasons. The following statements create the spline basis and fit multiple quantile regression spline curves:

```
ods graphics on;

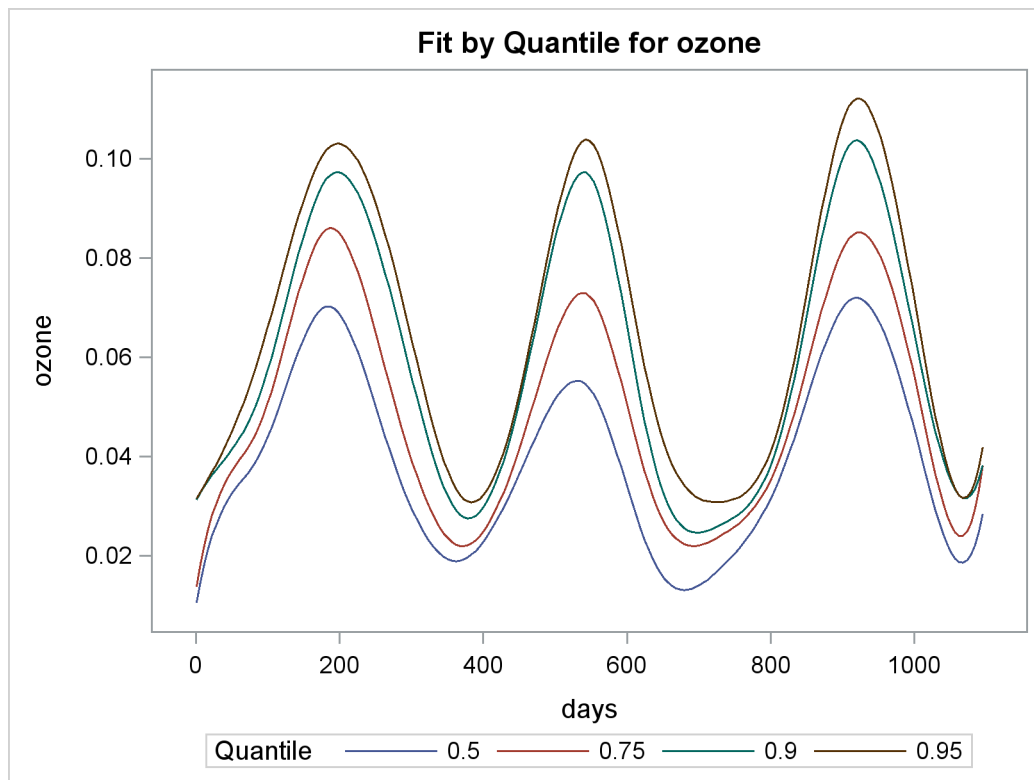
proc quantreg data=ozone algorithm=smooth ci=none plot=fitplot(nodata);
 effect sp = spline(days / knotmethod = list
 (90 182 272 365 455 547 637 730 820 912 1002));
 model ozone = sp / quantile = 0.5 0.75 0.90 0.95 seed=1268;
run;
```

**Output 77.4.1** Time Series of Ozone Levels in Pittsburgh, Pennsylvania

The EFFECT statement creates spline bases for the variable Days. The KNOTMETHOD=LIST option provides all internal knots for these bases. Cubic spline bases are generated by default. These bases are treated as components of the spline effect  $sp$ , which is used in the MODEL statement. Spline fits for four quantiles are requested with the QUANTILE= option.

When ODS Graphics is enabled, the QUANTREG procedure automatically generates a fit plot, which includes all fitted curves.

Output 77.4.2 displays these curves obtained with the QUANTREG procedure. The curves show that peak ozone levels occur in the summer. For the three years (1989–1991), the median curve (labeled 50%) does not cross the 0.08 ppm line, which is the 1997 EPA 8-hour standard. The median curve and the 75% curve show a drop for the ozone concentration levels in 1990. However, with the 90% and 95% curves, peak ozone levels tend to increase. This indicates that there might have been more days with low ozone concentration in 1990, but the top 10% and 5% tend to have higher ozone concentration levels.

**Output 77.4.2** Quantiles of Ozone Levels in Pittsburgh, Pennsylvania

The quantile curves also show that high ozone concentration in 1989 had a longer duration than in 1990 and 1991. This is indicated by the wider spread of the quantile curves in 1989.

---

### Example 77.5: Quantile Polynomial Regression for Salary Data

This example uses the data set from a university union survey of salaries of professors in 1991. The survey covered departments in U.S. colleges and universities that list programs in statistics. The goal here is to examine the relationship between faculty salaries and years of service.

The data include salaries and years of service for 459 professors. The scatter plot in [Output 77.5.1](#) shows that the relationship is not linear, and a quadratic or cubic regression curve is appropriate. [Output 77.5.1](#) shows a cubic curve.

The curve in [Output 77.5.1](#) does not adequately describe the conditional salary distributions and how they change with length of service. [Output 77.5.2](#) shows the 25th, 50th, and 75th percentiles for each number of years, which gives a better picture of the conditional distributions.

```

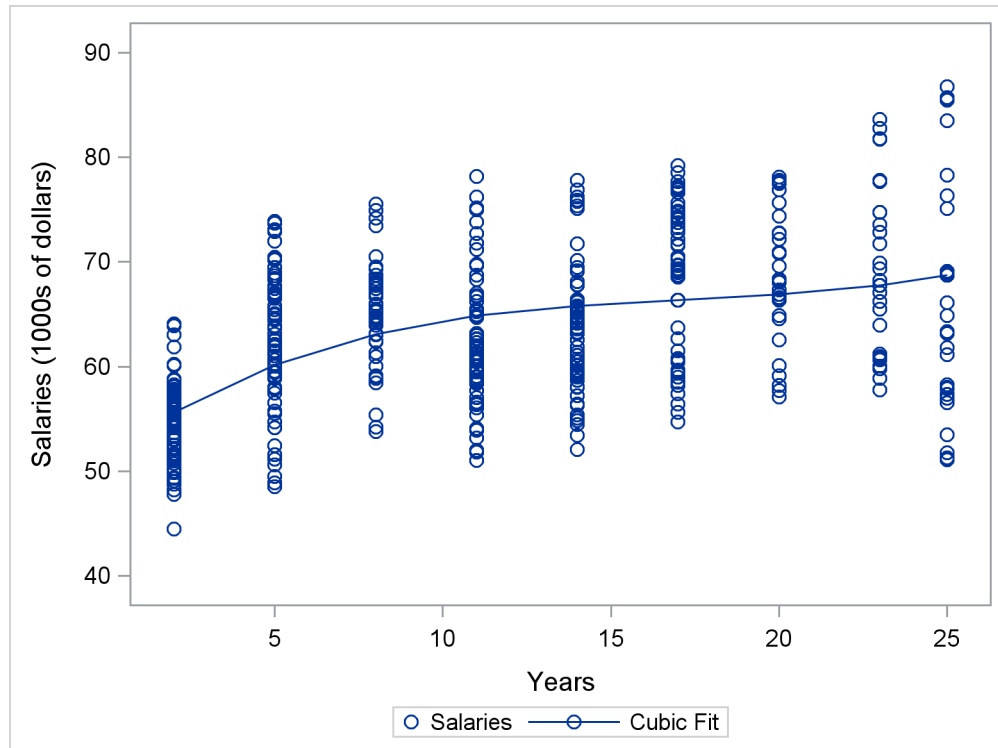
data salary;
 input Salaries Years @@;
 label Salaries='Salaries (1000s of dollars)';
 datalines;
54.94 2 58.24 2 58.11 2 52.23 2 52.98 2 57.62 2
44.48 2 57.22 2 54.24 2 54.79 2 56.42 2 61.90 2
63.90 2 64.10 2 47.77 2 54.86 2 49.31 2 53.37 2
51.69 2 53.66 2 58.77 2 56.77 2 53.06 2 54.86 2
50.96 2 56.46 2 51.67 2 49.37 2 56.86 2 49.85 2

... more lines ...

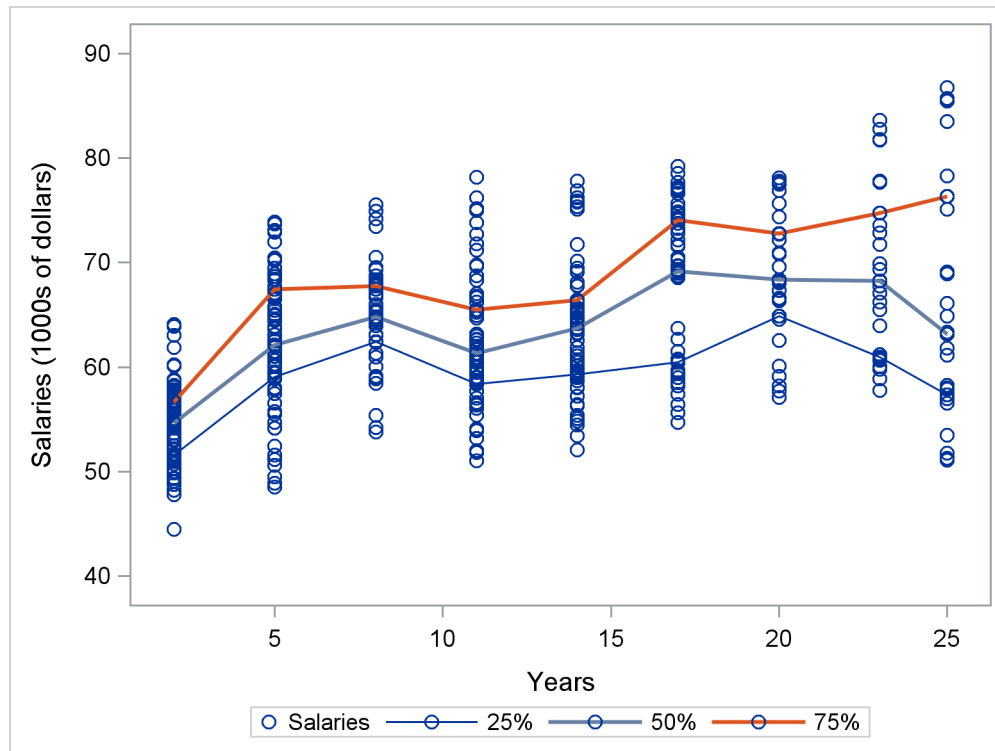
85.72 25 64.87 25 51.76 25 51.11 25 51.31 25 78.28 25
57.91 25 86.78 25 58.27 25 56.56 25 76.33 25 61.83 25
69.13 25 63.15 25 66.13 25
;

```

**Output 77.5.1** Salary with Years as Professor: Cubic Fit





**Output 77.5.2** Salary with Years as Professor: Sample Quantiles

These descriptive percentiles do not clearly show trends with length of service. The following statements use the QUANTREG procedure to obtain a smooth version by using polynomial quantile regression. The results are shown in [Output 77.5.3](#) and [Output 77.5.5](#).

```
ods graphics on;

proc quantreg data=salary ci=sparsity;
 model salaries = years years*years years*years*years
 /quantile=0.25 0.5 0.75
 plot=fitplot(showlimits);

 test years/QINTERACT;

run;
```

[Output 77.5.3](#) displays the regression coefficients for the three quantiles, from which you can see that there is a difference among the estimated parameters of the variable *years* across the three quantiles. To test whether the difference is significant, you can specify the option QINTERACT in the TEST statement. [Output 77.5.4](#) indicates that the difference is not significant with the *p*-value greater than 0.05.

**Output 77.5.3** Regression Coefficients

| BMI Percentiles for Men: 2-80 Years Old |    |          |                |                       |         |         |         |
|-----------------------------------------|----|----------|----------------|-----------------------|---------|---------|---------|
| The QUANTREG Procedure                  |    |          |                |                       |         |         |         |
| Parameter Estimates                     |    |          |                |                       |         |         |         |
| Parameter                               | DF | Estimate | Standard Error | 95% Confidence Limits |         | t Value | Pr >  t |
| Intercept                               | 1  | 48.2509  | 1.3484         | 45.6011               | 50.9007 | 35.78   | <.0001  |
| Years                                   | 1  | 2.2234   | 0.5455         | 1.1514                | 3.2953  | 4.08    | <.0001  |
| Years*Years                             | 1  | -0.1292  | 0.0500         | -0.2275               | -0.0308 | -2.58   | 0.0101  |
| Years*Years*Years                       | 1  | 0.0024   | 0.0013         | -0.0001               | 0.0049  | 1.86    | 0.0634  |

| Parameter Estimates |    |          |                |                       |         |         |         |
|---------------------|----|----------|----------------|-----------------------|---------|---------|---------|
| Parameter           | DF | Estimate | Standard Error | 95% Confidence Limits |         | t Value | Pr >  t |
| Intercept           | 1  | 50.2512  | 1.2812         | 47.7334               | 52.7690 | 39.22   | <.0001  |
| Years               | 1  | 2.7173   | 0.5947         | 1.5485                | 3.8860  | 4.57    | <.0001  |
| Years*Years         | 1  | -0.1632  | 0.0632         | -0.2873               | -0.0390 | -2.58   | 0.0101  |
| Years*Years*Years   | 1  | 0.0034   | 0.0018         | -0.0002               | 0.0070  | 1.85    | 0.0647  |

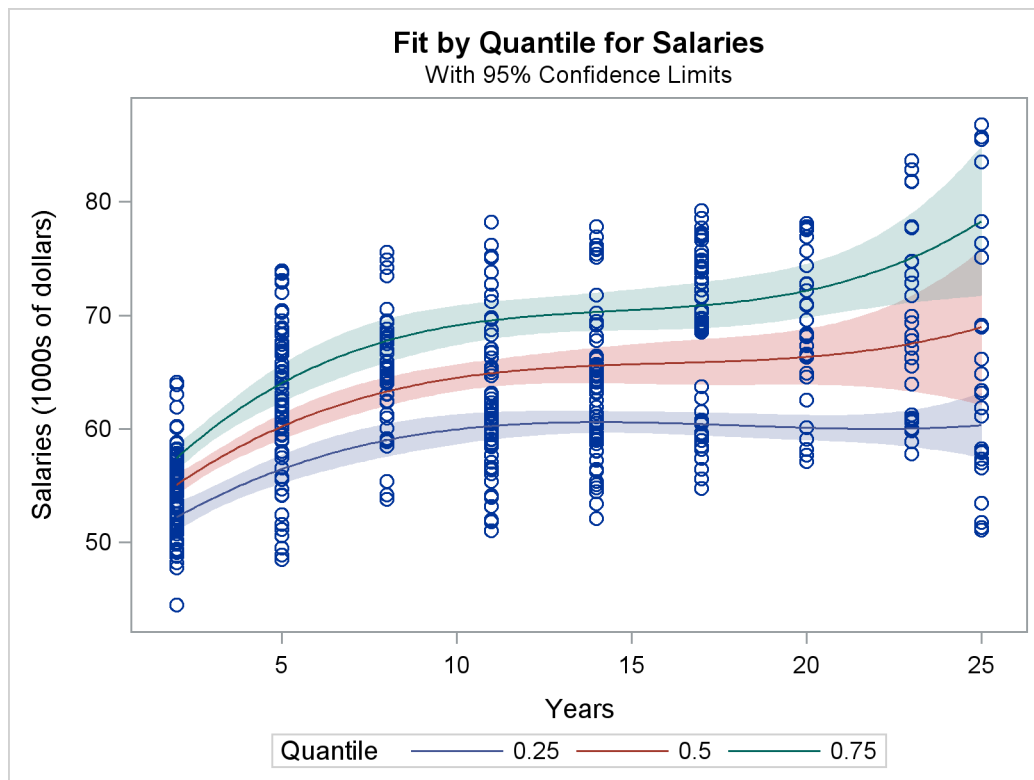
  

| Parameter Estimates |    |          |                |                       |         |         |         |
|---------------------|----|----------|----------------|-----------------------|---------|---------|---------|
| Parameter           | DF | Estimate | Standard Error | 95% Confidence Limits |         | t Value | Pr >  t |
| Intercept           | 1  | 51.0298  | 1.5886         | 47.9078               | 54.1517 | 32.12   | <.0001  |
| Years               | 1  | 3.6513   | 0.7594         | 2.1590                | 5.1436  | 4.81    | <.0001  |
| Years*Years         | 1  | -0.2390  | 0.0764         | -0.3892               | -0.0888 | -3.13   | 0.0019  |
| Years*Years*Years   | 1  | 0.0055   | 0.0021         | 0.0013                | 0.0096  | 2.60    | 0.0098  |

**Output 77.5.4** Tests for Heteroscedasticity

| Test Results Equal Coefficients Across Quantiles |    |        |       |
|--------------------------------------------------|----|--------|-------|
| Chi-Square                                       | DF | Pr >   | ChiSq |
| 3.4026                                           | 2  | 0.1825 |       |

The three fitted quantile curves with 95% confidence limits in the [Output 77.5.5](#) clearly show that salary dispersion increases gradually with length of service. After 15 years, a salary over \$70,000 is relatively high, while a salary less than \$60,000 is relatively low. Percentile curves of this type are useful in medical science as reference curves; see Yu, Lu, and Stabder (2003).

**Output 77.5.5** Salary with Years as Professor: Regression Quantiles

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# Chapter 78

## The QUANTSELECT Procedure

### (Experimental)

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## Overview: QUANTSELECT Procedure

Quantile regression, which was introduced by Koenker and Bassett (1978), is a modern method that models the effects of covariates on the conditional quantiles of a response variable. The QUANTSELECT procedure performs effect selection in the framework of quantile regression. A variety of effect selection methods are available, including greedy methods and penalty methods. The QUANTSELECT procedure offers extensive capabilities for customizing the effect selection processes with a variety of candidate selecting, effect-selection stopping, and final-model choosing criteria. PROC QUANTSELECT also provides graphical summaries for the effect selection processes.

The QUANTSELECT procedure compares most closely to the GLMSELECT and QUANTREG procedures. PROC GLMSELECT performs effect selection in the framework of general linear models. PROC QUANTREG supports a variety of estimation and inference methods for quantile regression but does not directly provide effect selection facilities. The QUANTSELECT procedure, as a counterpart of PROC GLMSELECT for quantile regression, fills this gap.

The QUANTSELECT procedure focuses on linear quantile models for univariate responses and offers great flexibility for and insight into the effect selection algorithm. The QUANTSELECT procedure inherits most of its syntax from PROC GLMSELECT and PROC QUANTREG. The QUANTSELECT procedure provides results that are similar to those of PROC GLMSELECT and PROC QUANTREG. These results (displayed tables, output data sets, and macro variables) make it easy to explore the selected models in PROC QUANTREG.

---

## Features

The main features of the QUANTSELECT procedure are as follows:

- supports the following model specifications:
  - interaction (crossed) effects and nested effects
  - constructed effects such as regression splines
  - hierarchy among effects
  - partitioning of data into training, validation, and testing roles
- provides the following selection controls:
  - multiple methods for effect selection
  - selection for quantile process and single quantile levels
  - selection of individual or grouped effects
  - selection based on a variety of selection criteria
  - stopping rules based on a variety of model evaluation criteria
- produces the following display and output:
  - graphical representation of the selection process
  - output data sets that contain predicted values and residuals
  - an output data set that contains the design matrix
  - macro variables that contain selected effects

The QUANTSELECT procedure supports the following effect selection methods. These methods are explained in detail in the section “[Effect Selection Methods](#)” on page 6597.

- Forward selection starts with no effects or with forced-in effects in the model and adds more effects.
- Backward elimination starts with all effects in the model and deletes effects.
- Stepwise regression is similar to the forward selection method except that effects already in the model do not necessarily stay there.
- LASSO regression adds and deletes effects based on a constrained version of estimated check risk where the L1-norm of regression coefficients is penalized (Tibshirani 1996; Belloni and Chernozhukov 2011). Adaptive LASSO (Zou 2006; Wu and Liu 2009) is implemented as a special case of LASSO methods where the L1-norm of certain weighted regression coefficients is penalized. See the discussion in the section “[LASSO Method \(LASSO\)](#)” on page 6598 for additional details. The QUANTSELECT procedure uses LASSO methods only to determine the adding and dropping covariate effects at a step; a post-penalized model that is associated with the step is refitted without penalty, and the selection criteria and the parameter estimates are from the post-penalized model.

The QUANTSELECT procedure is intended primarily as an effect selection procedure and does not include regression diagnostics and hypothesis testing. The intention is that you use the QUANTSELECT procedure to select a model or a set of models, where each model contains a set of selected effects, and then you can further investigate these models by using PROC QUANTREG or other analytic tools.

---

## Getting Started: QUANTSELECT Procedure

This example demonstrates how you can use the QUANTSELECT procedure to select covariate effects for quantile regression. The data set under investigation contains salary and performance information for Major League Baseball (MLB) players, excluding pitchers, who played at least one game in both the 1986 and 1987 seasons. The salaries (Time Inc. 1987) are for the 1987 season, and the performance measures are from 1986 (Reichler 1987).

```
data baseball;
 length team $ 12;
 input name $ 1-18 nAtBat nHits nHome nRuns nRBI nBB
 yrMajor crAtBat crHits crHome crRuns crRbi crBB
 League $ Division $ Team $ Position $ nOuts nAssts
 nError Salary;
 label name="Player's Name"
 nAtBat="Times at Bat in 1986"
 nHits="Hits in 1986"
 nHome="Home Runs in 1986"
 nRuns="Runs in 1986"
 nRBI="RBIs in 1986"
 nBB="Walks in 1986"
 yrMajor="Years in the Major Leagues"
 crAtBat="Career times at bat"
 crHits="Career Hits"
```



```

crHome="Career Home Runs"
crRuns="Career Runs"
crRbi="Career RBIs"
crBB="Career Walks"
League="League at the end of 1986"
Division="Division at the end of 1986"
Team="Team at the end of 1986"
Position="Position(s) in 1986"
nOuts="Put Outs in 1986"
nAssts="Assists in 1986"
nError="Errors in 1986"
Salary="1987 Salary in $ Thousands";
if League='American' and Division='East' then Div='AE';
if League='American' and Division='West' then Div='AW';
if League='National' and Division='East' then Div='NE';
if League='National' and Division='West' then Div='NW';
logSalary = log(Salary);
datalines;
Allanson, Andy 293 66 1 30 29 14
 1 293 66 1 30 29 14
 American East Cleveland C 446 33 20 .
Ashby, Alan 315 81 7 24 38 39
... more lines ...

Wilson, Willie 631 170 9 77 44 31
 11 4908 1457 30 775 357 249
 American West KansasCity CF 408 4 3 1000
;

```

Suppose you want to investigate how the MLB players' salaries for the 1987 season depend on performance measures for the players' previous season and MLB careers. As a starting point for such an analysis, you can use the following statements to obtain a parsimonious conditional median model at  $\tau = 0.5$ :

```

proc quantselect data=baseball;
 class Div;
 model Salary = nAtBat nHits nHome nRuns nRBI nBB yrMajor crAtBat
 crHits crHome crRuns crRbi crBB nAssts nError nOuts
 Div
 / selection=lasso(adaptive stop=aic choose=sbc sh=7);
run;

```

The `SELECTION=LASSO(ADAPTIVE)` option in the `MODEL` statement specifies the adaptive LASSO method (Zou 2006), which controls the effect selection process. The `STOP=AIC` option specifies that Akaike's information criterion (AIC) be used to determine the stopping condition. The `CHOOSE=SBC` option specifies that the Schwarz Bayesian information criterion (SBC) be used to determine the final selected model. The `SH=` option specifies the number of stop horizons, which requests that the selection process be stopped whenever the `STOP=` criterion values at step  $s + 1, \dots, s + SH$  are worse than those for step  $s$  for some  $s \in \{0, 1, \dots\}$ .

Figure 78.1 shows the "Model Information" table, which indicates the effect selection settings. You can see that the default quantile type is single level, so this effect selection is effective only for  $\tau = 0.5$ .

**Figure 78.1** Model Information

| The QUANTSELECT Procedure |                |
|---------------------------|----------------|
| Model Information         |                |
| Data Set                  | WORK.BASEBALL  |
| Dependent Variable        | Salary         |
| Selection Method          | Adaptive LASSO |
| Quantile Type             | Single Level   |
| Stop Criterion            | AIC            |
| Choose Criterion          | SBC            |

Figure 78.2 summarizes the effect selection process, which starts with an intercept-only model at step 0. At step 1, the effect that corresponds to the career runs is added to the model that reduced the AIC value from 2691.6511 to 2510.7297. You can see that step 10 has the minimum AIC and that step 7 has the minimum SBC. Common sense also tells you that the SBC favors a smaller model than the AIC.

**Figure 78.2** Selection Summary

| The QUANTSELECT Procedure |                |                   |            |            |
|---------------------------|----------------|-------------------|------------|------------|
| Quantile = 0.5            |                |                   |            |            |
| Selection Summary         |                |                   |            |            |
| Step                      | Effect Entered | Number Effects In | AIC        | SBC        |
| 0                         | Intercept      | 1                 | 2691.6511  | 2695.2232  |
| -----                     |                |                   |            |            |
| 1                         | crRuns         | 2                 | 2510.7297  | 2517.8740  |
| 2                         | nHits          | 3                 | 2470.4807  | 2481.1971  |
| 3                         | crHome         | 4                 | 2463.5953  | 2477.8839  |
| 4                         | nBB            | 5                 | 2463.7806  | 2481.6414  |
| 5                         | nOuts          | 6                 | 2455.6212  | 2477.0541  |
| 6                         | Div AW         | 7                 | 2451.4609  | 2476.4660  |
| 7                         | nAtBat         | 8                 | 2445.0446  | 2473.6218* |
| 8                         | crBB           | 9                 | 2445.5432  | 2477.6926  |
| 9                         | nHome          | 10                | 2443.4818  | 2479.2033  |
| 10                        | nRuns          | 11                | 2442.6036* | 2481.8973  |
| 11                        | crAtBat        | 12                | 2442.8387  | 2485.7046  |
| 12                        | yrMajor        | 13                | 2443.5374  | 2489.9754  |
| 13                        | nError         | 14                | 2445.2085  | 2495.2187  |
| 14                        | Div NE         | 15                | 2446.4042  | 2499.9865  |
| 15                        | nRBI           | 16                | 2448.2003  | 2505.3547  |
| 16                        | nAssts         | 17                | 2449.9731  | 2510.6997  |

\* Optimal Value Of Criterion

Figure 78.3 shows that the selection process stopped at a local minimum of the STOP= criterion, which is step 10. According to the SH=7 option, the effect selection process is stopped at step 10 because all the AIC values for step 11 through step 17 are no less than the AIC at step 10. Step 17 is ignored in the selection summary table because it is the last step.

**Figure 78.3** Stop Reason

```
Selection stopped at a local minimum of the AIC criterion.
```

Figure 78.4 shows how the final selected model is determined. CHOOSE=SBC is specified in this example, so the model at step 7 is chosen as the final selected model.

**Figure 78.4** Selection Reason

```
The model at step 7 is selected where SBC is 2473.62.
```

Figure 78.5 shows the final selected effects and Figure 78.6 shows the parameter estimates for the final selected model.

**Figure 78.5** Selected Effects

```
The QUANTSELECT Procedure

Quantile = 0.5

Selected Effects: Intercept nAtBat nHits nBB crHome crRuns nOuts Div AW
```

Figure 78.6 Parameter Estimates

| Parameter Estimates |    |            |                       |
|---------------------|----|------------|-----------------------|
| Parameter           | DF | Estimate   | Standardized Estimate |
| Intercept           | 1  | -18.187539 | 0                     |
| nAtBat              | 1  | -1.582714  | -0.500417             |
| nHits               | 1  | 7.044354   | 0.686968              |
| nBB                 | 1  | 2.053726   | 0.097911              |
| crHome              | 1  | 1.429926   | 0.272726              |
| crRuns              | 1  | 0.425955   | 0.316167              |
| nOuts               | 1  | 0.282803   | 0.175489              |
| Div AW              | 1  | -57.671778 | -0.056862             |

Quantile regression can fit a conditional quantile model at any quantile level  $\tau \in (0, 1)$ , so it can describe the entire distribution of a response variable conditional on covariate effects. To further investigate the effects that might affect the MLB players' salaries, you can also conduct effect selection at  $\tau = 0.1$  and  $\tau = 0.9$ , which correspond to low-end salaries and high-end salaries respectively. The following statements use the same selection settings that are used in the previous program:

```
proc quantselect data=baseball;
 class Div;
 model Salary = nAtBat nHits nHome nRuns nRBI nBB yrMajor crAtBat
 crHits crHome crRuns crRbi crBB nAssts nError nOuts
 Div
 / quantiles=0.1 0.9 selection=lasso(adaptive stop=aic choose=sbc sh=7);
run;
```

Figure 78.7 shows the effect selection summary with  $\tau = 0.1$ .

**Figure 78.7** Selection Summary:  $\tau = 0.1$

| The QUANTSELECT Procedure |                |                |                   |            |            |  |
|---------------------------|----------------|----------------|-------------------|------------|------------|--|
| Quantile = 0.1            |                |                |                   |            |            |  |
| Selection Summary         |                |                |                   |            |            |  |
| Step                      | Effect Entered | Effect Removed | Number Effects In | AIC        | SBC        |  |
| 0                         | Intercept      |                | 1                 | 2008.3489  | 2011.9211  |  |
| -----                     |                |                |                   |            |            |  |
| 1                         | crRuns         |                | 2                 | 1918.7675  | 1925.9118  |  |
| 2                         | nHits          |                | 3                 | 1897.2425  | 1907.9590* |  |
| 3                         | yrMajor        |                | 4                 | 1897.2476  | 1911.5362  |  |
| 4                         | crBB           |                | 5                 | 1896.1765  | 1914.0373  |  |
| 5                         | nBB            |                | 6                 | 1894.1257  | 1915.5587  |  |
| 6                         | Div AW         |                | 7                 | 1891.0577  | 1916.0628  |  |
| 7                         | crHome         |                | 8                 | 1892.2575  | 1920.8348  |  |
| 8                         |                | crHome         | 7                 | 1891.0577  | 1916.0628  |  |
| 9                         | nAtBat         |                | 8                 | 1889.6365* | 1918.2137  |  |
| 10                        | nHome          |                | 9                 | 1891.2595  | 1923.4089  |  |
| 11                        | crHome         |                | 10                | 1890.7463  | 1926.4679  |  |
| 12                        | nRBI           |                | 11                | 1892.7421  | 1932.0358  |  |
| 13                        | Div NW         |                | 12                | 1892.9745  | 1935.8404  |  |
| 14                        |                | nRBI           | 11                | 1891.3217  | 1930.6154  |  |
| 15                        | crAtBat        |                | 12                | 1891.8810  | 1934.7468  |  |

\* Optimal Value Of Criterion

Figure 78.8 shows the parameter estimates for the final selected model with  $\tau = 0.1$ . You can see from Figure 78.8 that low-end salaries for MLB players depend mainly on career runs and hits in 1986.

**Figure 78.8** Parameter Estimates:  $\tau = 0.1$

| The QUANTSELECT Procedure |    |           |                       |  |
|---------------------------|----|-----------|-----------------------|--|
| Quantile = 0.1            |    |           |                       |  |
| Parameter Estimates       |    |           |                       |  |
| Parameter                 | DF | Estimate  | Standardized Estimate |  |
| Intercept                 | 1  | -4.397043 | 0                     |  |
| nHits                     | 1  | 0.878564  | 0.085678              |  |
| crRuns                    | 1  | 0.327350  | 0.242977              |  |

Figure 78.9 shows the effect selection summary with  $\tau = 0.9$ .

**Figure 78.9** Selection Summary:  $\tau = 0.9$

| The QUANTSELECT Procedure |                |                |                   |            |            |  |
|---------------------------|----------------|----------------|-------------------|------------|------------|--|
| Quantile = 0.9            |                |                |                   |            |            |  |
| Selection Summary         |                |                |                   |            |            |  |
| Step                      | Effect Entered | Effect Removed | Number Effects In | AIC        | SBC        |  |
| 0                         | Intercept      |                | 1                 | 2436.7289  | 2440.3011  |  |
| -----                     |                |                |                   |            |            |  |
| 1                         | crHits         |                | 2                 | 2197.4349  | 2204.5792  |  |
| 2                         | crRbi          |                | 3                 | 2183.6148  | 2194.3313  |  |
| 3                         | nHits          |                | 4                 | 2113.2757  | 2127.5643  |  |
| 4                         |                | crRbi          | 3                 | 2127.8632  | 2138.5797  |  |
| 5                         | crRbi          |                | 4                 | 2113.2757  | 2127.5643  |  |
| 6                         |                | crRbi          | 3                 | 2127.8632  | 2138.5797  |  |
| 7                         | crRbi          |                | 4                 | 2113.2757  | 2127.5643  |  |
| 8                         | crHome         |                | 5                 | 2099.2203  | 2117.0811  |  |
| 9                         |                | crRbi          | 4                 | 2099.3891  | 2113.6777  |  |
| 10                        | crRbi          |                | 5                 | 2099.2203  | 2117.0811  |  |
| 11                        |                | crRbi          | 4                 | 2099.3891  | 2113.6777  |  |
| 12                        | nOuts          |                | 5                 | 2067.1926  | 2085.0533  |  |
| 13                        | Div AW         |                | 6                 | 2048.2393  | 2069.6723  |  |
| 14                        | crRuns         |                | 7                 | 2028.8040  | 2053.8090  |  |
| 15                        | nAtBat         |                | 8                 | 2012.8195  | 2041.3968  |  |
| 16                        |                | crHits         | 7                 | 2017.0290  | 2042.0341  |  |
| 17                        | crRbi          |                | 8                 | 2009.3551  | 2037.9324  |  |
| 18                        | crAtBat        |                | 9                 | 2011.2415  | 2043.3908  |  |
| 19                        |                | crRbi          | 8                 | 2011.4053  | 2039.9825  |  |
| 20                        | crRbi          |                | 9                 | 2011.2415  | 2043.3908  |  |
| 21                        |                | crAtBat        | 8                 | 2009.3551  | 2037.9324  |  |
| 22                        | crAtBat        |                | 9                 | 2011.2415  | 2043.3908  |  |
| 23                        | nBB            |                | 10                | 2004.5033  | 2040.2249  |  |
| 24                        |                | crAtBat        | 9                 | 2003.1023  | 2035.2517* |  |
| 25                        | crAtBat        |                | 10                | 2004.5033  | 2040.2249  |  |
| 26                        |                | crAtBat        | 9                 | 2003.1023  | 2035.2517  |  |
| 27                        | crAtBat        |                | 10                | 2004.5033  | 2040.2249  |  |
| 28                        | nError         |                | 11                | 2004.2230  | 2043.5167  |  |
| 29                        | crHits         |                | 12                | 2003.0544  | 2045.9203  |  |
| 30                        | Div NE         |                | 13                | 2001.9603  | 2048.3983  |  |
| 31                        | Div AE         |                | 14                | 2001.8349* | 2051.8451  |  |
| 32                        | nRuns          |                | 15                | 2003.5961  | 2057.1784  |  |
| 33                        | nHome          |                | 16                | 2004.2721  | 2061.4266  |  |
| 34                        | nRBI           |                | 17                | 2006.0023  | 2066.7289  |  |
| 35                        | yrMajor        |                | 18                | 2007.9975  | 2072.2963  |  |
| 36                        | crBB           |                | 19                | 2009.9514  | 2077.8223  |  |

\* Optimal Value Of Criterion

Figure 78.9 continued

| The QUANTSELECT Procedure    |                |                |            |           |           |
|------------------------------|----------------|----------------|------------|-----------|-----------|
| Quantile = 0.9               |                |                |            |           |           |
| Selection Summary            |                |                |            |           |           |
| Step                         | Effect Entered | Effect Removed | Number     | AIC       | SBC       |
|                              |                |                | Effects In |           |           |
| 37                           | nAssts         |                | 20         | 2011.9095 | 2083.3525 |
| * Optimal Value Of Criterion |                |                |            |           |           |

Figure 78.10 shows the parameter estimates for the final selected model with  $\tau = 0.9$ .

Figure 78.10 Parameter Estimates:  $\tau = 0.9$ 

| Parameter Estimates |    |             |                       |  |
|---------------------|----|-------------|-----------------------|--|
| Parameter           | DF | Estimate    | Standardized Estimate |  |
| Intercept           | 1  | 92.893875   | 0                     |  |
| nAtBat              | 1  | -1.858170   | -0.587509             |  |
| nHits               | 1  | 8.155573    | 0.795335              |  |
| nBB                 | 1  | 3.392794    | 0.161751              |  |
| crHome              | 1  | 3.191472    | 0.608700              |  |
| crRuns              | 1  | 1.394317    | 1.034939              |  |
| crRbi               | 1  | -0.913371   | -0.664951             |  |
| nOuts               | 1  | 0.437241    | 0.271323              |  |
| Div AW              | 1  | -167.110005 | -0.164764             |  |

To visually illustrate how the model evolves through the selection process, the QUANTSELECT procedure provides the coefficient plot, the average check loss plot, and several criterion plots in either packed or unpacked forms. You can request these plots by using the PLOTS= option. The following statements request all the plots for the baseball data at  $\tau = 0.1$ ; they also use the STOP=AIC criterion, the CHOOSE=SBC criterion, and the SH=7 option:

```
ods graphics on;
proc quantselect data=baseball plot=all;
 class Div;
 model Salary = nAtBat nHits nHome nRuns nRBI nBB yrMajor crAtBat
 crHits crHome crRuns crRbi crBB nAssts nError nOuts
 Div
 / quantiles=0.1 selection=lasso(adaptive stop=aic choose=sbc sh=7);
run;
```

Figure 78.11 shows the progression of the parameter estimates as the selection process proceeds.

**Figure 78.11** Coefficient Panel:  $\tau = 0.1$

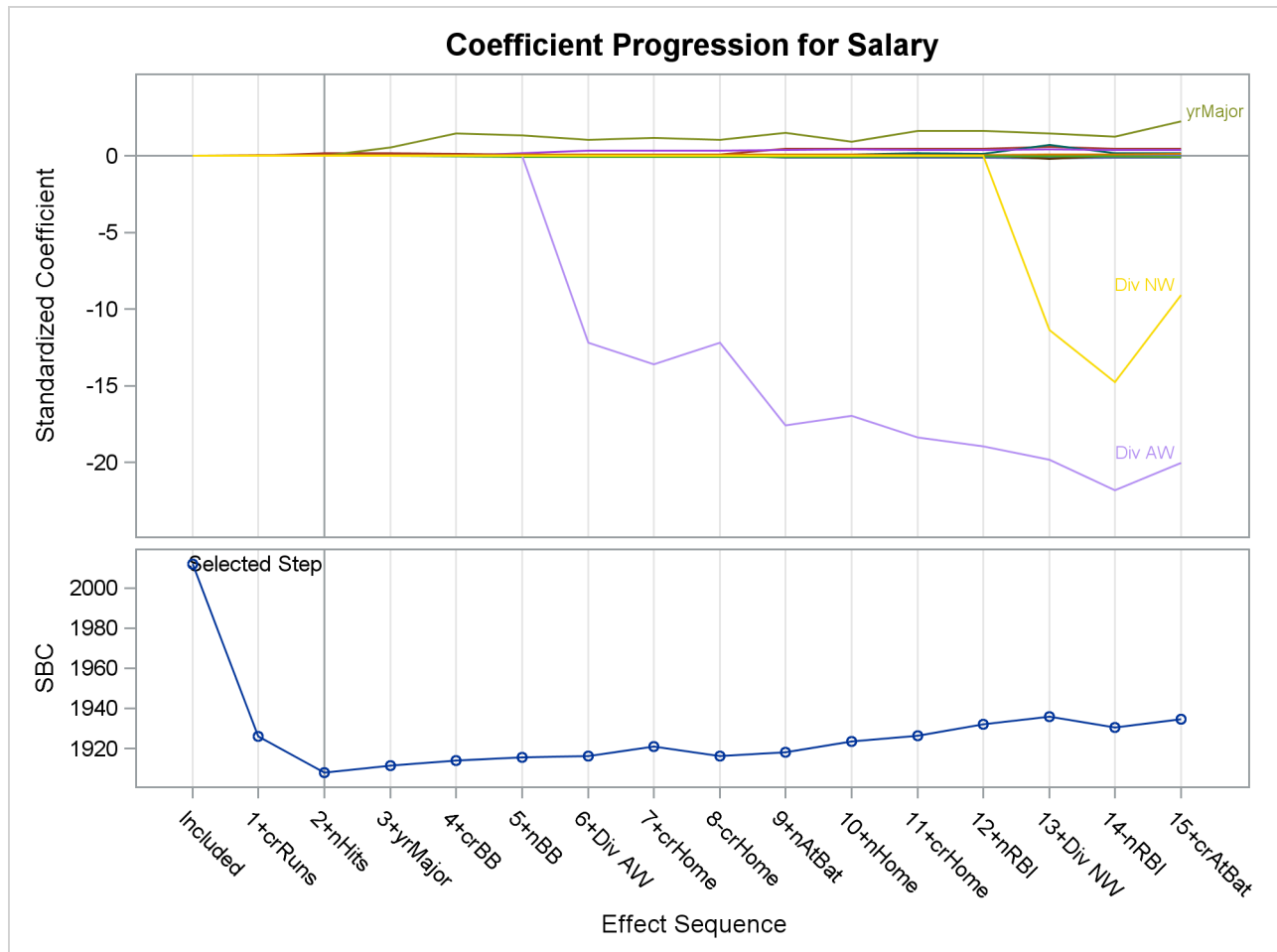




Figure 78.12 shows the progression of the average check losses as the selection process proceeds.

**Figure 78.12** Average Check Loss Plot:  $\tau = 0.1$

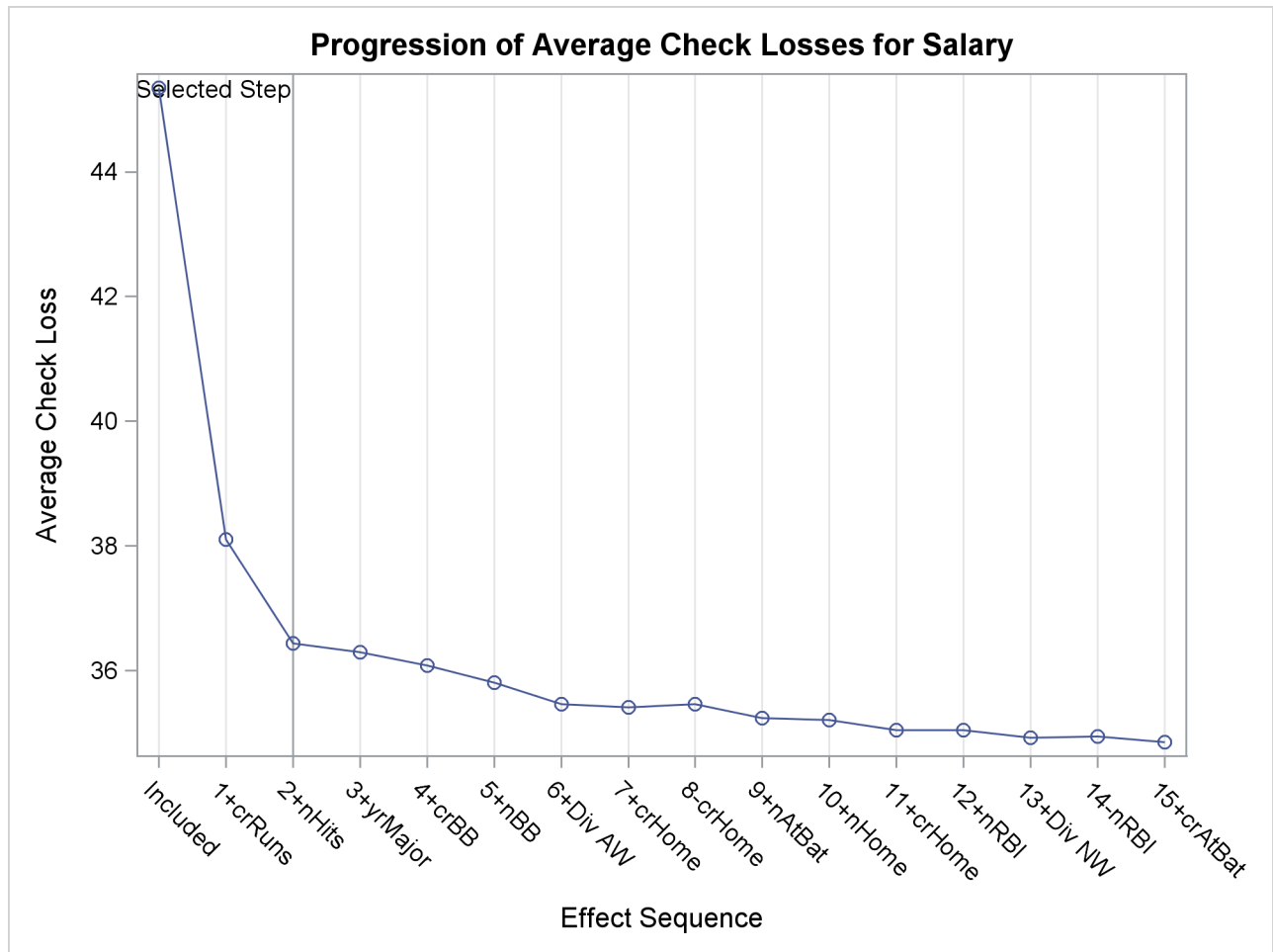
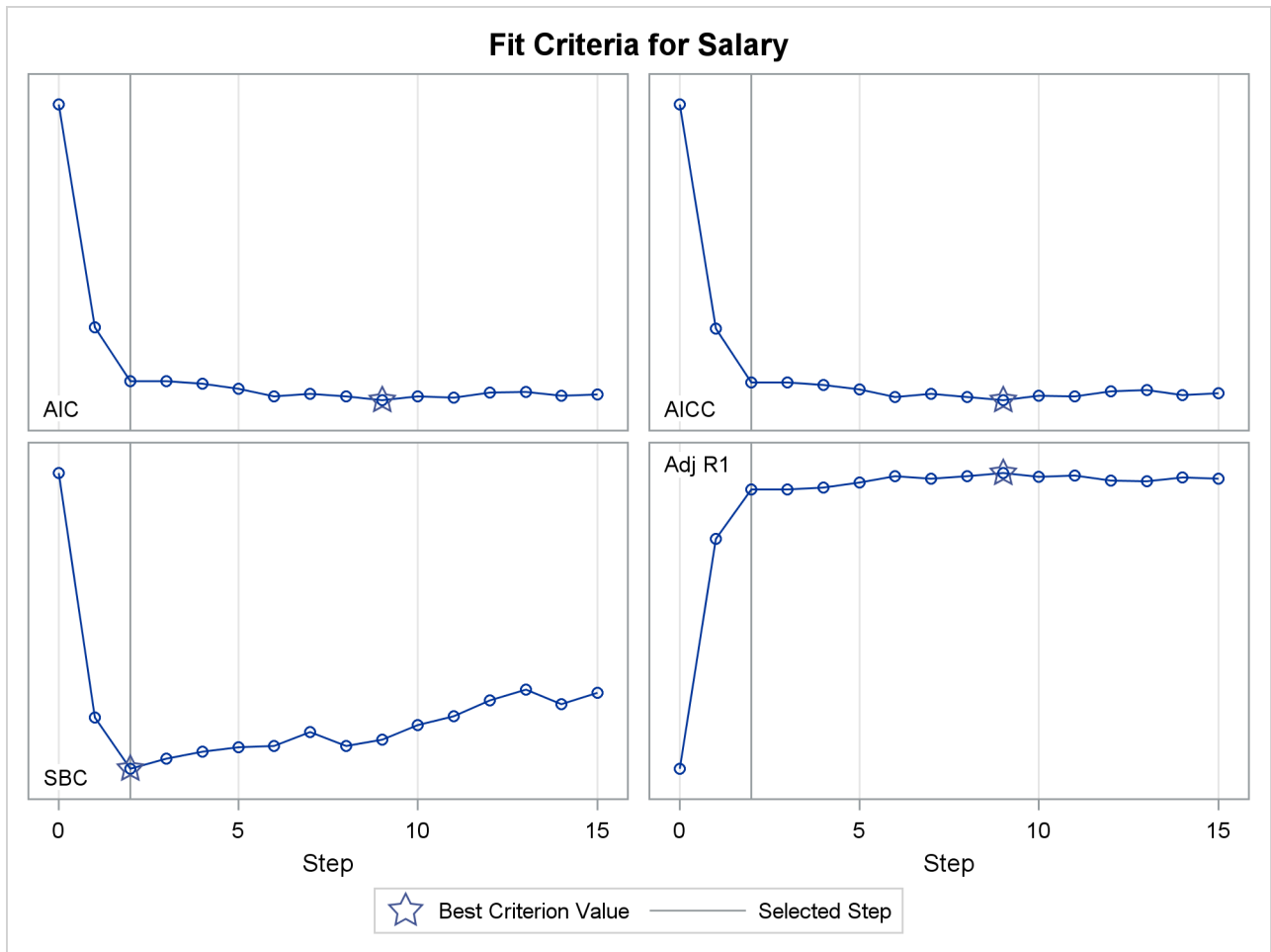


Figure 78.13 shows the progression of four effect selection criteria as the selection process proceeds.

**Figure 78.13** Criterion Panel:  $\tau = 0.1$



---

## Syntax: QUANTSELECT Procedure

The following statements are available in PROC QUANTSELECT:

```

PROC QUANTSELECT < options > ;
 BY variables ;
 CLASS variable < (v-options) > < variable < (v-options ...) > > < / v-options > < options > ;
 EFFECT name = effect-type (variables < / options >) ;
 MODEL variable = < effects > < / options > ;
 OUTPUT < OUT=SAS-data-set > < keyword < =name > > < ... keyword < =name > > ;
 PARTITION < options > ;
 WEIGHT variable ;

```

The PROC QUANTSELECT statement invokes the procedure. All statements other than the **MODEL** statement are optional. **CLASS** and **EFFECT** statements, if present, must precede the **MODEL** statement.

---

## PROC QUANTSELECT Statement

```

PROC QUANTSELECT < options > ;

```

Table 78.1 lists the *options* available in the PROC QUANTSELECT statement.

**Table 78.1** PROC QUANTSELECT Statement Options

| <i>option</i>               | Description                                           |
|-----------------------------|-------------------------------------------------------|
| <b>Data Set Options</b>     |                                                       |
| <b>DATA=</b>                | Names a data set to use for the regression            |
| <b>MAXMACRO=</b>            | Sets the maximum number of macro variables to produce |
| <b>TESTDATA=</b>            | Names a data set that contains test data              |
| <b>VALDATA=</b>             | Names a data set that contains validation data        |
| <b>ODS Graphics Options</b> |                                                       |
| <b>PLOTS=</b>               | Produces ODS Graphics displays                        |
| <b>Other Options</b>        |                                                       |
| <b>OUTDESIGN=</b>           | Names a data set that contains the design matrix      |
| <b>NOPRINT</b>              | Suppresses displayed output (including plots)         |
| <b>SEED=</b>                | Sets the seed used for pseudorandom number generation |

You can specify the following *options* (shown in alphabetical order) in the PROC QUANTSELECT statement.

**DATA=SAS-data-set**

names the SAS data set to be used by PROC QUANTSELECT. If the DATA= option is not specified, PROC QUANTSELECT uses the most recently created SAS data set. If the data set contains a variable named `_ROLE_`, then this variable is used to assign observations for training, validation, and testing roles. See the section “Using Validation and Test Data” on page 6602 for more information about using the `_ROLE_` variable.

**MAXMACRO=n**

specifies the maximum number of macro variables with selected effects to create. By default, MAXMACRO=100.

PROC QUANTSELECT saves the list of selected effects in a macro variable, `&_QRSIND`. For example, suppose your input effect list consists of `x1–x10`. Then `&_QRSIND` would be set to `x1 x3 x4 x10` if the first, third, fourth, and tenth effects were selected for the model. This list can be used in the MODEL statement of a subsequent procedure.

If you specify the OUTDESIGN= option in the PROC QUANTSELECT statement, then PROC QUANTSELECT saves the list of columns in the design matrix in a macro variable named `&_QRSMOD`.

With multiple quantile levels and BY processing, one macro variable is created for each combination of quantile level and BY group, and the macro variables are indexed by the BY-group number and the quantile level index. You can use the MAXMACRO= option to either limit or increase the number of these macro variables when you are processing data sets with many combinations of quantile level and BY group.

With a single quantile level and no BY-group processing, PROC QUANTSELECT creates the macro variables shown in Table 78.2.

**Table 78.2** Macro Variables Created for a Single Quantile Level and No BY Processing

| Macro Variable Name     | Contains                       |
|-------------------------|--------------------------------|
| <code>_QRSIND</code>    | Selected effects               |
| <code>_QRSIND1</code>   | Selected effects               |
| <code>_QRSINDT1</code>  | Selected effects               |
| <code>_QRSIND1T1</code> | Selected effects               |
| <code>_QRSMOD</code>    | Selected design matrix columns |
| <code>_QRSMOD1</code>   | Selected design matrix columns |
| <code>_QRSMODT1</code>  | Selected design matrix columns |
| <code>_QRSMOD1T1</code> | Selected design matrix columns |

With multiple quantile levels and BY-group processing, PROC QUANTSELECT creates the macro variables shown in Table 78.3.

**Table 78.3** Macro Variables Created for a Multiple Quantile Levels and BY-Group Processing

| Macro Variable Name | Contains                                           |
|---------------------|----------------------------------------------------|
| _QRSIND             | Selected effects for quantile 1 and BY group 1     |
| _QRSINDT1           | Selected effects for quantile 1 and BY group 1     |
| _QRSINDT2           | Selected effects for quantile 2 and BY group 1     |
| .                   |                                                    |
| .                   |                                                    |
| .                   |                                                    |
| _QRSIND1            | Selected effects for quantile 1 and BY group 1     |
| _QRSIND1T1          | Selected effects for quantile 1 and BY group 1     |
| _QRSIND1T2          | Selected effects for quantile 2 and BY group 1     |
| .                   |                                                    |
| .                   |                                                    |
| .                   |                                                    |
| _QRSIND2            | Selected effects for quantile 1 and BY group 2     |
| _QRSIND2T1          | Selected effects for quantile 1 and BY group 2     |
| _QRSIND2T2          | Selected effects for quantile 2 and BY group 2     |
| .                   |                                                    |
| .                   |                                                    |
| .                   |                                                    |
| _QRSIND $mTn$       | Selected effects for quantile $n$ and BY group $m$ |

If you specify the OUTDESIGN= option, PROC QUANTSELECT also creates the macro variables shown in Table 78.4.

**Table 78.4** Macro Variables Created When the OUTDESIGN= Option Is Specified

| Macro Variable Name | Contains                                                         |
|---------------------|------------------------------------------------------------------|
| _QRSMOD             | Selected design matrix columns for BY group 1                    |
| _QRSMOD1            | Selected design matrix columns for BY group 1                    |
| _QRSMOD2            | Selected design matrix columns for BY group 2                    |
| .                   |                                                                  |
| .                   |                                                                  |
| .                   |                                                                  |
| _QRSMOD $mTn$       | Selected design matrix columns for quantile $n$ and BY group $m$ |

The macros variables in [Table 78.5](#) show the number of quantiles and BY groups:

**Table 78.5** Macro Variables Showing the Number of Quantiles and BY Groups

| Macro Variable Name | Contains                                                                                                                                                                                          |
|---------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| _QRSNUMBYS          | The number of BY groups                                                                                                                                                                           |
| _QRSNUMTAUS         | The number of quantiles                                                                                                                                                                           |
| _QRSBY1NUMTAUS      | The number of <code>_QRS1INDj</code> macro variables actually made                                                                                                                                |
| _QRSBY2NUMTAUS      | The number of <code>_QRS2INDj</code> macro variables actually made                                                                                                                                |
| .                   | .                                                                                                                                                                                                 |
| .                   | .                                                                                                                                                                                                 |
| .                   | .                                                                                                                                                                                                 |
| _QRSNUMBYTAUS       | The number of <code>_QRSiINDj</code> macro variables actually made. This value can be less than <code>_QRSNUMBYS × _QRSNUMTAUS</code> , and it is less than or equal to <code>MAXMACRO=n</code> . |

See the section “[Macro Variables That Contain Selected Models](#)” on page 6600 for more information.

#### **NOPRINT**

suppresses all displayed output (including plots).

#### **OUTDESIGN**< (*options*)= >< SAS-data-set >

creates a data set that contains the design matrix. By default, the QUANTSELECT procedure includes in the OUTDESIGN data set the X matrix that corresponds to all the effects in the selected models. Two schemes for naming the columns of the design matrix are available:

- In the first scheme, names of the parameters are constructed from the parameter labels that appear in the parameter estimates table. This naming scheme is the default when you do not request BY processing; it is not available when you do use BY processing.
- In the second scheme, the design matrix column names consist of a prefix followed by an index. The default name prefix is `_X`. This scheme is used when you specify the `PREFIX=` option or a BY statement; otherwise the first scheme is used.

You can specify the following *options* in parentheses to control the contents of the OUTDESIGN= data set:

#### **ADDINPUTVARS**

includes all the input data set variables in the OUTDESIGN= data set.

#### **ADDVALDATA**

includes all the VALDATA= data set variables in the OUTDESIGN= data set. This option is ignored if the VALDATA= data set is not specified.

#### **ADDTTESTDATA**

includes all the TESTDATA= data set variables in the OUTDESIGN= data set. This option is ignored if TESTDATA= data set is not specified.

**FULLMODEL**

includes in the OUTDESIGN= data set parameters that correspond to all effects that are specified in the MODEL statement. By default, only parameters that correspond to the selected model are included.

**NAMES**

produces a table that associates columns in the OUTDESIGN= data set with the labels of the parameters they represent.

**PREFIX**<=*prefix*>

creates the design matrix column names from a prefix followed by an index. The default *prefix* is *\_X*.

**PLOTS** <(global-plot-options)> <=*plot-request* <(options)>>

**PLOTS** <(global-plot-options)> <=*(plot-request* <(options)> <... *plot-request* <(options)>>>

controls the plots that are produced through ODS Graphics. When you specify only one *plot-request*, you can omit the parentheses around it. Here are some examples:

```
plots=all
plots=coefficients(unpack)
plots(unpack)=(coef acl crit)
```

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;
proc quantselect plots=all;
 class temp sex / split;
 model depVar = sex sex*temp;
run;
```

For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS](#).”

You can specify the following *global-plot-options*, which apply to all plots generated by the QUANTSELECT procedure, unless they are altered by specific plot *options*.

**ENDSTEP**=*n*

specifies that the step ranges shown on the horizontal axes of plots terminate at the specified step. By default, the step range shown terminates at the final step of the selection process. If you specify the ENDSTEP= option as both a *global-plot-option* and as an *option* for a specific *plot-request*, then PROC QUANTSELECT uses the ENDSTEP=*n* *option* for the specific *plot-request*.

**LOGP** | **LOGPVALUE**

displays the natural logarithm of the entry and removal significance levels when the **SELECT=SL** option is specified in the MODEL statement.

**MAXSTEPLABEL**=*n*

specifies the maximum number of characters beyond which labels of effects on plots are truncated. The default is MAXSTEPLABEL=256.

**MAXPARMLABEL=*n***

specifies the maximum number of characters beyond which parameter labels on plots are truncated. The default is MAXPARMLABEL=256.

**STARTSTEP=*n***

specifies that the step ranges shown on the horizontal axes of plots start at the specified step. By default, the step range shown starts at the initial step of the selection process. If you specify the STATSTEP= option as both a *global-plot-option* and as an *option* for a specific *plot-request*, then PROC QUANTSELECT uses the STARTSTEP=*n* *option* for the specific *plot-request*. The default is STARTSTEP=0.

**STEPAXIS=EFFECT | NORMB | NUMBER**

specifies the method for labeling the horizontal plot axis. This axis represents the sequence of entering or departing effects. The default is STEPAXIS=EFFECT.

**STEPAXIS=EFFECT**

labels each step by a prefix followed by the name of the effect that enters or leaves at that step. The prefix consists of the step number followed by a “+” sign or a “-” sign, depending on whether the effect enters or leaves at that step.

**STEPAXIS=NORMB**

labels the horizontal axis value at step *i* with the penalty on the parameter estimates at step *i*, normalized by the penalty on the parameter estimates at the final step. This option is valid only with regularization selection methods.

**STEPAXIS=NUMBER**

labels each step with the step number.

**UNPACK**

displays each graph separately. (By default, some graphs can appear together in a single panel.) You can also specify UNPACK as a suboption with CRITERIA and COEFFICIENTS options for specific *plot-requests*.

The following list describes the specific *plot-requests* and their *options*.

**ALL**

displays all appropriate graphs.

**ACL | ACLPLOT < (*aclplot-option*) >**

plots the progression of the average check losses on the training data, and on the test and validation data when these data are provided with the TESTDATA= or VALDATA= options or are produced by using a PARTITION statement. When the PROC QUANTSELECT procedure is applied on multiple quantile levels, the ACL option and its suboptions apply to the ACL plots for each of the quantile levels.

You can specify the following *aclplot-option*:

**STEPAXIS=EFFECT | NORMB | NUMBER**

specifies the method for labeling the horizontal plot axis. See the STEPAXIS= option in the *global-plot-options* for more information.



**COEF | COEFFICIENTS | COEFFICIENTPANEL** < (*coefficient-panel-options*) >

displays a panel of two plots for each quantile level. The upper plot shows the progression of the parameter values as the selection process proceeds. The lower plot shows the progression of the **CHOOSE=** criterion. If no **CHOOSE=** criterion is in effect, then the AICC criterion is displayed. You can specify the following *coefficient-panel-options*:

**LABELGAP=percentage**

specifies the percentage of the vertical axis range that forms the minimum gap between successive parameter labels at the final step of the coefficient progression plot. If the values of more than one parameter at the final step are closer than this gap, then the labels on all but one of these parameters are suppressed. The default is LABELGAP=5.

**LOGP | LOGPVALUE**

displays the natural logarithm of the entry and removal significance levels when the **SELECT=SL** option is specified in the MODEL statement.

**STEPAXIS=EFFECT | NORMB | NUMBER**

specifies the horizontal axis to be used. See the **STEPAXIS=** option in the *global-options* for more information.

**UNPACK | UNPACKPANEL**

displays the coefficient progression and the **CHOOSE=** criterion progression in separate plots.

**CRIT | CRITERIA | CRITERIONPANEL** < (*criterion-panel-options*) >

plots a panel of model fit criteria. If multiple quantile levels apply, the CRITERIA option plots a panel of model fit criteria for each quantile level. The criteria that are displayed are AIC, AICC, and SBC, in addition to any other criteria that are named in the **CHOOSE=**, **SELECT=**, **STOP=**, and **STATS=** options in the MODEL statement. You can specify the following *criterion-panel-options*:

**STEPAXIS=EFFECT | NORMB | NUMBER**

specifies the horizontal axis to be used. See the **STEPAXIS=** option in the *global-options* for more information.

**UNPACK | UNPACKPANEL**

displays each criterion progression on a separate plot.

**NONE**

suppresses all plots.

**SEED=number**

specifies an integer that is used to start the pseudorandom number generator for random partitioning of data for training, testing, and validation. If you do not specify a seed or if you specify a value less than or equal to 0, the seed is generated by reading the time of day from the computer's clock.

**TESTDATA=SAS-data-set**

names a SAS data set that contains test data. This data set must contain all the effects that are specified in the MODEL statement. Furthermore, when you also specify a BY statement and the TESTDATA= data set contains any of the BY variables, then the TESTDATA= data set must also contain all the

BY variables sorted in the order of the BY variables. In this case, only the test data for a specific BY group are used with the corresponding BY group in the analysis data. If the TESTDATA= data set contains none of the BY variables, then the entire TESTDATA= data set is used with each BY group of the analysis data.

If you specify both a TESTDATA= data set and the **PARTITION** statement, then the testing observations from the DATA= data set are merged with the TESTDATA= data set for testing purposes.

#### **VALDATA=SAS-data-set**

names a SAS data set that contains validation data. This data set must contain all the effects that are specified in the **MODEL** statement. Furthermore, when a BY statement is used and the VALDATA= data set contains any of the BY variables, then the VALDATA= data set must also contain all the BY variables sorted in the order of the BY variables. In this case, only the validation data for a specific BY group are used with the corresponding BY group in the analysis data. If the VALDATA= data set contains none of the BY variables, then the entire VALDATA= data set is used with each BY group of the analysis data.

If you specify both a VALDATA= data set and the **PARTITION** statement, then the validation observations from the DATA= data set are merged with the VALDATA= data set for validation purposes.

---

## BY Statement

**BY variables ;**

You can specify a BY statement with PROC QUANTSELECT to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the QUANTSELECT procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

## CLASS Statement

**CLASS** *variable* < (*v-options*) > < *variable* < (*v-options* . . . ) > > < / *v-options* > < *options* > ;

The CLASS statement names the classification variables to be used in the analysis. The CLASS statement must precede the MODEL statement.

Table 78.6 summarizes the *options* and *v-options* available in the CLASS statement.

**Table 78.6** CLASS Statement Options

| <i>option or v-option</i> | Description                                     |
|---------------------------|-------------------------------------------------|
| DELIMITER=                | Specifies the delimiter                         |
| DESCENDING                | Reverses the sort order                         |
| MISSING                   | Allows for missing values                       |
| ORDER=                    | Specifies the sort order                        |
| PARAM=                    | Specifies the parameterization method           |
| REF=                      | Specifies the reference level                   |
| SHOW                      | Requests a table for each CLASS variable        |
| SPLIT                     | Splits CLASS variables into independent effects |

You can specify the following *options* after a slash (/):

### DELIMITER='c'

specifies the delimiter character, 'c', to be used between levels of classification variables when parameter names and lists of class level values are built. The default delimiter is a space. This option is useful if the levels of a classification variable contain embedded blanks.

### SHOW | SHOWCODING

requests a table that shows the coding used for each classification variable.

You can specify various *v-options* for each variable by enclosing them in parentheses after the variable name; these are called individual *v-options*. You can also specify global *v-options* by placing them after a slash (/) at the end of the CLASS statement. Global *v-options* are applied to all the variables specified in the CLASS statement. If you specify more than one CLASS statement, the global *v-options* specified in any one CLASS statement apply to all CLASS statements. However, individual CLASS variable *v-options* override the global *v-options*.

You can specify the following *v-options*:

### DESCENDING

#### DESC

reverses the sort order of the classification variable.

### MISSING

allows missing values, such as ' .' for a numeric variable or a blank for a character variable, as valid values for the CLASS variable.

**ORDER=DATA | FORMATTED | FREQ | INTERNAL**

specifies the sort order for the levels of classification variables. If ORDER=FORMATTED for numeric variables for which you have supplied no explicit format, the levels are ordered by their internal values. The following table shows how PROC QUANTSELECT interprets values of the ORDER= option.

| Value of ORDER=  | Levels Sorted By                                                                                                                       |
|------------------|----------------------------------------------------------------------------------------------------------------------------------------|
| <b>DATA</b>      | Order of appearance in the input data set                                                                                              |
| <b>FORMATTED</b> | External formatted value, except for numeric variables with no explicit format, which are sorted by their unformatted (internal) value |
| <b>FREQ</b>      | Descending frequency count; levels with the most observations come first in the order                                                  |
| <b>INTERNAL</b>  | Unformatted value                                                                                                                      |

By default, ORDER=FORMATTED. For FORMATTED and INTERNAL, the sort order is machine dependent.

For more information about sort order, see the chapter on the SORT procedure in the Bookrefprocguide and the discussion of BY-group processing in *SAS Language Reference: Concepts*.

**PARAM=keyword**

specifies the parameterization method for the classification variable or variables. Design matrix columns are created from CLASS variables according to the following coding schemes. The default is PARAM=GLM. If PARAM=ORTHOPOLY or PARAM=POLY, and the CLASS levels are numeric, then the ORDER= option in the CLASS statement is ignored, and the internal, unformatted values are used. See the section “CLASS Variable Parameterization and the SPLIT Option” on page 3570 in Chapter 45, “The GLMSELECT Procedure,” for more information.

|                                 |                                                                                                                                          |
|---------------------------------|------------------------------------------------------------------------------------------------------------------------------------------|
| <b>EFFECT</b>                   | specifies effect coding.                                                                                                                 |
| <b>GLM</b>                      | specifies less-than-full-rank coding. This option can be used only as a global <i>v-option</i> (after the slash in the CLASS statement). |
| <b>ORDINAL   THERMOMETER</b>    | specifies the cumulative parameterization for an ordinal CLASS variable.                                                                 |
| <b>POLYNOMIAL   POLY</b>        | specifies polynomial coding.                                                                                                             |
| <b>REFERENCE   REF</b>          | specifies reference-cell coding.                                                                                                         |
| <b>ORTHEFFECT</b>               | orthogonalizes PARAM=EFFECT.                                                                                                             |
| <b>ORTHORDINAL   ORTHOTHERM</b> | orthogonalizes PARAM=ORDINAL.                                                                                                            |
| <b>ORTHOPOLY</b>                | orthogonalizes PARAM=POLYNOMIAL.                                                                                                         |
| <b>ORTHREF</b>                  | orthogonalizes PARAM=REFERENCE.                                                                                                          |

The EFFECT, POLYNOMIAL, REFERENCE, and ORDINAL coding schemes and their orthogonal parameterizations are full rank. The REF= option in the CLASS statement determines the reference level for the EFFECT and REFERENCE schemes and their orthogonal parameterizations.

**REF= 'level' | FIRST | LAST**

specifies the reference level for PARAM=EFFECT, PARAM=REFERENCE, and their orthogonalizations. For an individual (but not a global) REF= *v-option*, you can specify the *level* of the variable to use as the reference level. For a global or individual REF= *v-option*, you can specify REF=FIRST (which designates the first-ordered level as reference) or REF=LAST (which designates the last-ordered level as reference). The default is REF=LAST.

**SPLIT**

enables the columns of the design matrix that correspond to any effect that contains a split classification variable to be selected to enter or leave a model independently of the other design columns of that effect. For example, suppose a variable named `temp` has three levels with values 'hot', 'warm', and 'cold', and a variable named `sex` has two levels with values 'M' and 'F'. The following statements include SPLIT as a global *v-option*:

```
proc quantselect;
 class temp sex / split;
 model depVar = sex sex*temp;
run;
```

Because both the classification variables are split, the two effects named in the **MODEL** statement are split into eight effects. The effect 'sex' is split into two effects labeled 'sex\_M' and 'sex\_F'. The effect 'sex\*temp' is split into six effects labeled 'sex\_M\*temp\_hot', 'sex\_F\*temp\_hot', 'sex\_M\*temp\_warm', 'sex\_F\*temp\_warm', 'sex\_M\*temp\_cold', and 'sex\_F\*temp\_cold'. The previous PROC QUANTSELECT statements are equivalent to the following statements for the split version of the DATA= data set:

```
proc quantselect;
 model depVar = sex_M sex_F sex_M*temp_hot sex_F*temp_hot
 sex_M*temp_warm sex_F*temp_warm
 sex_M*temp_cold sex_F*temp_cold;
run;
```

You can specify the SPLIT option for individual classification variables. For example, consider the following PROC QUANTSELECT statements:

```
proc quantselect;
 class temp(split) sex;
 model depVar = sex sex*temp;
run;
```

In this case, the effect 'sex' is not split, and the effect 'sex\*temp' is split into three effects labeled 'sex\*temp\_hot', 'sex\*temp\_warm', and 'sex\*temp\_cold'. Furthermore each of these three split effects now has two parameters that correspond to the two levels of 'sex,' and the previous PROC QUANTSELECT statements are equivalent to the following statements for the split version of the DATA= data set:

```
proc quantselect;
 class sex;
 model depVar = sex sex*temp_hot sex*temp_warm sex*temp_cold;
run;
```

## EFFECT Statement

**EFFECT** *name=effect-type (variables < / options>)* ;

The EFFECT statement enables you to construct special collections of columns for design matrices. These collections are referred to as *constructed effects* to distinguish them from the usual model effects that are formed from continuous or classification variables, as discussed in the section “GLM Parameterization of Classification Variables and Effects” on page 383 in Chapter 19, “Shared Concepts and Topics.”

You can specify the following *effect-types*:

|                          |                                                                                                                                                                                                           |
|--------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>COLLECTION</b>        | is a collection effect that defines one or more variables as a single effect with multiple degrees of freedom. The variables in a collection are considered as a unit for estimation and inference.       |
| <b>LAG</b>               | is a classification effect in which the level that is used for a given period corresponds to the level in the preceding period.                                                                           |
| <b>MULTIMEMBER   MM</b>  | is a multimember classification effect whose levels are determined by one or more variables that appear in a CLASS statement.                                                                             |
| <b>POLYNOMIAL   POLY</b> | is a multivariate polynomial effect in the specified numeric variables.                                                                                                                                   |
| <b>SPLINE</b>            | is a regression spline effect whose columns are univariate spline expansions of one or more variables. A spline expansion replaces the original variable with an expanded or larger set of new variables. |

Table 78.7 summarizes the *options* available in the EFFECT statement.

**Table 78.7** EFFECT Statement Options

| Option                             | Description                                                                                                                                          |
|------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Collection Effects Options</b>  |                                                                                                                                                      |
| DETAILS                            | Displays the constituents of the collection effect                                                                                                   |
| <b>Lag Effects Options</b>         |                                                                                                                                                      |
| DESIGNROLE=                        | Names a variable that controls to which lag design an observation is assigned                                                                        |
| DETAILS                            | Displays the lag design of the lag effect                                                                                                            |
| NLAG=                              | Specifies the number of periods in the lag                                                                                                           |
| PERIOD=                            | Names the variable that defines the period                                                                                                           |
| WITHIN=                            | Names the variable or variables that define the group within which each period is defined                                                            |
| <b>Multimember Effects Options</b> |                                                                                                                                                      |
| NOEFFECT                           | Specifies that observations with all missing levels for the multimember variables should have zero values in the corresponding design matrix columns |
| WEIGHT=                            | Specifies the weight variable for the contributions of each of the classification effects                                                            |

Table 78.7 continued

| Option                            | Description                                                                                             |
|-----------------------------------|---------------------------------------------------------------------------------------------------------|
| <b>Polynomial Effects Options</b> |                                                                                                         |
| DEGREE=                           | Specifies the degree of the polynomial                                                                  |
| MDEGREE=                          | Specifies the maximum degree of any variable in a term of the polynomial                                |
| STANDARDIZE=                      | Specifies centering and scaling suboptions for the variables that define the polynomial                 |
| <b>Spline Effects Options</b>     |                                                                                                         |
| BASIS=                            | Specifies the type of basis (B-spline basis or truncated power function basis) for the spline expansion |
| DEGREE=                           | Specifies the degree of the spline transformation                                                       |
| KNOTMETHOD=                       | Specifies how to construct the knots for spline effects                                                 |

For more information about the syntax of these *effect-types* and how columns of constructed effects are computed, see the section “EFFECT Statement” on page 393 in Chapter 19, “Shared Concepts and Topics.”

## MODEL Statement

**MODEL** *dependent* = < effects > / < options > ;

The MODEL statement names the dependent variable and the covariate effects, including covariates, main effects, constructed effects, interactions, and nested effects; see the section “Specification of Effects” on page 3324 in Chapter 42, “The GLM Procedure,” for more information. If you omit the explanatory effects, PROC QUANTSELECT fits an intercept-only model.

After the keyword MODEL, specify the dependent (response) variable, followed by an equal sign, followed by the explanatory effects.

Table 78.8 summarizes the *options* available in the MODEL statement.

Table 78.8 MODEL Statement Options

| Option     | Description                                               |
|------------|-----------------------------------------------------------|
| DETAILS=   | Specifies the level of effect selection detail to display |
| HIERARCHY= | Specifies hierarchy of effects to impose                  |
| NOINT      | Specifies models without an explicit intercept            |
| QUANTILES= | Specifies quantile levels to be applied                   |
| SELECTION= | Specifies effect selection method                         |
| STATS=     | Specifies additional statistics to be displayed           |
| TEST=      | Specifies the test type for computing significance levels |

The following list provides details about the *options* that you can specify in the MODEL statement after a slash (/):

**DETAILS=ALL | SUMMARY**

specifies the level of effect selection detail that is displayed. The DETAILS=SUMMARY option produces only the selection summary table. The DETAILS=ALL option produces the following:

- entry and removal statistics for each variable that is selected in the model building process
- average check loss and parameter estimates
- entry and removal statistics for the top five candidates for inclusion or exclusion at each step
- a selection summary table

The default is DETAILS=SUMMARY.

**HIERARCHY=keyword****HIER=keyword**

specifies whether and how the model hierarchy requirement is applied. This option also controls whether a single effect or multiple effects are allowed to enter or leave the model in one step. You can specify that only CLASS effects, or both CLASS and continuous effects, be subject to the hierarchy requirement. This option is ignored unless you also specify one of the following options: SELECTION=FORWARD, SELECTION=BACKWARD, or SELECTION=STEPWISE.

Model hierarchy refers to the requirement that for any term to be in the model, all model effects contained in the term must be present in the model. For example, in order for the interaction A\*B to enter the model, the main effects A and B must be in the model. Likewise, neither effect A nor effect B can leave the model while the interaction A\*B is in the model.

You can specify the following *keywords*:

**NONE**

specifies that model hierarchy not be maintained. Any single effect can enter or leave the model at any given step of the selection process.

**SINGLE**

specifies that only one effect enter or leave the model at one time, subject to the model hierarchy requirement. For example, suppose that the model contains the main effects A and B and the interaction A\*B. In the first step of the selection process, either A or B can enter the model. In the second step, the other main effect can enter the model. The interaction effect can enter the model only when both main effects have already entered. Also, before A or B can be removed from the model, the A\*B interaction must first be removed. All effects (CLASS and interval) are subject to the hierarchy requirement.

**SINGLECLASS**

is the same as HIERARCHY=SINGLE except that only CLASS effects are subject to the hierarchy requirement.

The default is HIERARCHY=NONE.

**NOINT**

suppresses the intercept term that is otherwise included in the model.



**QUANTILES**=< *number-list* | **PROCESS** < (*option*) > >

**QUANTILE**=< *number-list* | **PROCESS** < (*option*) > >

specifies the quantile levels for the quantile regression. You can specify any number of quantile levels in (0, 1). If you do not specify this option, the QUANTSELECT procedure performs median regression effect selection that corresponds to QUANTILES=0.5.

If you specify the QUANTILES=PROCESS option, the QUANTSELECT procedure performs effect selection for quantile process regression. The QUANTILES=PROCESS option cannot be used with LASSO selection methods. You can specify the following *option* in parentheses after QUANTILES=PROCESS.

**NTAU**=*n* | **ALL**

specifies how many quantile levels that you expect to cover for the quantile process. If you specify NTAU=ALL, the QUANTSELECT procedure performs effect selection for accurate quantile process regression. If you specify NTAU=*n*, the QUANTSELECT procedure performs effect selection for approximate quantile process regression. The approximate quantile process is computed at *n* equally spaced quantile levels:  $\{\frac{1}{n+1}, \dots, \frac{n}{n+1}\}$ .

**SELECTION**=*method* < (*method-options*) >

specifies the *method* used to select the model, optionally followed by parentheses that enclose *method-options* that apply to the specified method. The default is SELECTION=STEPWISE.

You can specify the following *methods*, which are explained in detail in the section “Effect Selection Methods” on page 6597.

|                 |                                                                                                                                                                                                                                                                                                                                                                                                               |
|-----------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>NONE</b>     | specifies full model fitting without effect selection.                                                                                                                                                                                                                                                                                                                                                        |
| <b>FORWARD</b>  | specifies forward selection. This method starts with no effects in the model and adds effects.                                                                                                                                                                                                                                                                                                                |
| <b>BACKWARD</b> | specifies backward elimination. This method starts with all effects in the model and deletes effects.                                                                                                                                                                                                                                                                                                         |
| <b>STEPWISE</b> | specifies stepwise regression. This is similar to the FORWARD method except that effects already in the model do not necessarily stay there.                                                                                                                                                                                                                                                                  |
| <b>LASSO</b>    | specifies a method that adds and deletes parameters based on a version of estimated check risk where the weighted L1-norm of certain weighted regression coefficients is penalized. For more information, see the section “LASSO Method (LASSO)” on page 6598. If the model contains CLASS variables or constructed effects, these CLASS variables or constructed effects are split into separate covariates. |

Table 78.9 lists the applicable *method-options* for each *method*.

**Table 78.9** Applicable *method-options* for Each *method*

| <i>method-option</i> | FORWARD | BACKWARD | STEPWISE | LASSO |
|----------------------|---------|----------|----------|-------|
| ADAPTIVE             |         |          |          | X     |
| CHOOSE=              | X       | X        | X        | X     |
| INCLUDE=             | X       | X        | X        | X     |
| MAXSTEP=             | X       | X        | X        | X     |
| SELECT=              | X       | X        | X        |       |
| SLENTRY=             | X       |          | X        |       |
| SLSTAY=              |         | X        | X        |       |
| STOP=                | X       | X        | X        | X     |
| STOPHORIZON=         | X       | X        | X        | X     |

You can specify the following *method-option* in parentheses after the *method*. As described in [Table 78.9](#), not all *method-options* apply to every SELECTION= method.

**ADAPTIVE****ADAPT**

specifies the adaptive LASSO selection method. The ADAPTIVE option can be used only with the SELECTION=LASSO option.

**CHOOSE=***criterion*

chooses from the list of models (with one model at each step of the selection process) the model that yields the best value of the specified *criterion* as the final selected model. If the optimal value of the specified *criterion* occurs for more than one model, then the model with the smallest number of parameters is chosen. If you do not specify the CHOOSE= option, then the model selected is the model at the final step in the selection process for the SELECT=SL criterion, or the STOP= option is applied as the CHOOSE= option for all the other cases.

You can specify the following values for *criterion* in the CHOOSE= option. See the section “[Criteria Used in Model Selection Methods](#)” on page 6598 for more information about these criteria.

**ADJR1** chooses the model with the largest adjusted quantile regression R statistic.

**AIC** chooses the model with the smallest Akaike’s information criterion.

**AICC** chooses the model with the smallest corrected Akaike’s information criterion.

**SBC** chooses the model with the smallest Schwarz Bayesian information criterion.

**VALIDATE** chooses the model with the smallest average check loss for the validation data. You can specify CHOOSE=VALIDATE only if you have specified a [VALDATA=](#) data set in the PROC QUANTSELECT statement or if you have reserved part of the input data for validation by using either a [PARTITION](#) statement or a [\\_ROLE\\_](#) variable in the input data.

**INCLUDE=***n*

forces the first *n* effects listed in the MODEL statement to be included in all models. The selection methods are performed on the other effects in the MODEL statement. The INCLUDE= option is available only with SELECTION=FORWARD, SELECTION=STEPWISE, and SELECTION=BACKWARD.

**MAXSTEP=*n***

specifies the maximum number of selection steps. The default value of *n* is the number of effects in the MODEL statement when SELECTION=FORWARD or SELECTION=BACKWARD and is three times the number of effects when SELECTION=STEPWISE or SELECTION=LASSO.

**SELECT=*criterion***

specifies the criterion that PROC QUANTSELECT uses to determine the order in which effects enter or leave at each step of the specified selection method. This option is not valid when SELECTION=LASSO. You can specify the following values for *criterion*: ADJR1, AIC, AICC, SBC, SL, and VALIDATE. See the section “Criteria Used in Model Selection Methods” on page 6598 for more information about these criteria.

When SELECT=SL, the effect selection depends on the selection method and is described in the relevant subsection of the section “Effect Selection Methods” on page 6597. Otherwise, the effect that is selected to enter or leave at a step of the selection process is the effect whose addition to or removal from the current model produces the maximum improvement in the specified criterion.

If validation data exist, the default is SELECT=VALIDATE; otherwise, the default is SELECT=SBC.

**SLENTRY=*value*****SLE=*value***

specifies the significance level for entry, used when the STOP=SL or SELECT=SL option is in effect. The defaults are 0.50 when SELECTION=FORWARD and 0.15 when SELECTION=STEPWISE.

**SLSTAY=*value*****SLS=*value***

specifies the significance level for staying in the model, used when the STOP=SL or SELECT=SL option is in effect. The defaults are 0.10 when SELECTION=BACKWARD and 0.15 when SELECTION=STEPWISE.

**STOP=*criterion***

specifies the *criterion* for stopping the selection process. If the maximum number of steps is specified in the MAXSTEP= option and the *criterion* does not stop the selection process before the maximum number of steps for the selection method, then the selection process terminates at the maximum number of steps.

You can specify the following values for *criterion*. See the section “Criteria Used in Model Selection Methods” on page 6598 for more detailed descriptions of these criteria.

- |              |                                                                                                                                                                               |
|--------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>NONE</b>  | enables the model selection process to go through all possible steps.                                                                                                         |
| <b>ADJR1</b> | stops selection at the step where the next SH= steps (or all remaining steps) would yield models with smaller values of the adjusted quantile regression R (ADJR1) statistic. |
| <b>AIC</b>   | stops selection at the step where the next SH= steps (or all remaining steps) would yield models with larger values of Akaike’s information criterion.                        |

|                 |                                                                                                                                                                                                                                                                                                                                                                                                                                   |
|-----------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>AICC</b>     | stops selection at the step where the next SH= steps (or all remaining steps) would yield models with larger values of the corrected Akaike's information criterion.                                                                                                                                                                                                                                                              |
| <b>SBC</b>      | stops selection at the step where the next SH= steps (or all remaining steps) would yield models with larger values of the Schwarz Bayesian information criterion.                                                                                                                                                                                                                                                                |
| <b>VALIDATE</b> | stops selection at the step where the next SH= steps (or all remaining steps) would yield models with larger values of the average check loss for the validation data. You can specify STOP=VALIDATE only if you have specified a VALDATA= data set in the PROC QUANTSELECT statement or if you have reserved part of the input data for validation by using either a PARTITION statement or a _ROLE_ variable in the input data. |

The default value of this option depends on other options as follows:

- If you specify SELECT=SL and you also specify the SLE= *method-option* or the SLS= *method-option*, the STOP option is ignored.
- If do not specify both SELECT=SL and one or both of the SLE= or SLS= *method-options* and validation data exist, the default is STOP=VALIDATE.
- If do not specify both SELECT=SL and one or both of the SLE= or SLS= *method-options* and validation data do not exist, the default is one of the following:
  - When you specify SELECTION=LASSO, the default is STOP=SBC.
  - When you specify SELECTION=NONE, FORWARD, BACKWARD, or STEPWISE, the default is the criterion specified in the SELECT= *method-option*.

#### **STOPHORIZON=*n***

##### **SH=*n***

looks ahead for the specified number of steps to decide whether an extremum of the stop criterion is achieved. This option applies only to the STOP= criterion. The default is STOPHORIZON=1.

For example, suppose that the stop criterion values at steps 1 through 5 are 4, 3, 5, 6, and 2, respectively. If you specify STOPHORIZON=1, then the selection process terminates after looking at the model at step 3, and the final selected model is the model at step 2. If you specify STOPHORIZON=2, the selection process stops after looking at the model at step 4, and the final selected model is the model at step 2. However, if you specify STOPHORIZON=3 or higher, then the local minimum in the stop value sequence at step 2 cannot stop the selection process because a lower value is achieved at step 5, which is within 3 steps beyond this local minimum step.

##### **STAT=*name* | (*names*)**

##### **STATS=*name* | (*names*)**

specifies which model fit statistics to display in the selection summary table. To specify multiple model fit statistics, specify a list of *names* in parentheses. If you omit this option, the default set of statistics that are displayed in these tables includes all the criteria that are specified in any of the CHOOSE=, SELECT=, and STOP= *method-options*.

You can specify the following values for *name*:

|              |                                                                                                                                                                                                                                                                                                                                                                                                                                             |
|--------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>ADJR1</b> | displays the adjusted quantile regression R statistic.                                                                                                                                                                                                                                                                                                                                                                                      |
| <b>AIC</b>   | displays the Akaike's information criterion.                                                                                                                                                                                                                                                                                                                                                                                                |
| <b>AICC</b>  | displays the corrected Akaike's information criterion.                                                                                                                                                                                                                                                                                                                                                                                      |
| <b>ACL</b>   | displays the average check losses for the training, test, and validation data. The ACL statistics for the test and validation data are reported only if you have specified the <b>TESTDATA=</b> option or the <b>VALDATA=</b> option in the PROC QUANTSELECT statement or if you have reserved part of the input data for testing or validation by using either a <b>PARTITION</b> statement or a <b>_ROLE_</b> variable in the input data. |
| <b>R1</b>    | displays the quantile regression R statistic.                                                                                                                                                                                                                                                                                                                                                                                               |
| <b>SBC</b>   | displays the Schwarz Bayesian information criterion.                                                                                                                                                                                                                                                                                                                                                                                        |

The statistics ADJR1, AIC, AICC, and SBC can be computed with little computation cost. However, computing ACL for test and validation data when these are not used in any of the **CHOOSE=**, **SELECT=**, and **STOP=** *method-options* can hurt performance.

**TEST=***name*

specifies the test type for computing significance levels.

You can specify the following values for *name*:

**LR1** specifies the likelihood ratio test Type I. The LR1 test score is defined as

$$\frac{2(D_1(\tau) - D_2(\tau))}{\tau(1 - \tau)\hat{s}}$$

where  $D_1(\tau) = \sum \rho_\tau(y_i - \mathbf{x}_i \hat{\boldsymbol{\beta}}_1(\tau))$  is the sum of check losses for the reduced model,  $D_2(\tau) = \sum \rho_\tau(y_i - \mathbf{x}_i \hat{\boldsymbol{\beta}}(\tau))$  is the sum of check losses for the extended model, and  $\hat{s}$  is the estimated sparsity function. For more information about the sparsity function, see the section “Sparsity” on page 6523 of Chapter 77, “The QUANTREG Procedure.”

**LR2** specifies the likelihood ratio test Type II. The LR2 test score is defined as

$$\frac{2D_2(\tau) (\log(D_1(\tau)) - \log(D_2(\tau)))}{\tau(1 - \tau)\hat{s}}$$

where  $\hat{s}$  is computed on the reduced model for testing the entry effect and on the extended model for testing the removal effect.

## OUTPUT Statement

**OUTPUT** < **OUT**=SAS-data-set > < keyword < =name > > ... < keyword < =name > > ;

The OUTPUT statement creates a new SAS data set that saves diagnostic measures that are calculated for the selected model. If you do not specify a *keyword*, then the only diagnostic included is the predicted response.

All the variables in the original data set are included in the new data set, along with variables that are created by the *keyword* options in the OUTPUT statement. These new variables contain the values of a variety of statistics and diagnostic measures that are calculated for each observation in the data set.

The OUTPUT data set is created in row-wise form, and the variable `_QUANTILE_` is optional. For each appropriate keyword specified in the OUTPUT statement, one variable for each specified quantile level is generated. These variables appear in the sorted order of the specified quantile levels.

If you specify a BY statement, then a variable `_BY_` that indexes the BY groups is included. For each observation, the value of `_BY_` is the index of the BY group to which this observation belongs. This variable is useful for matching BY groups with macro variables that PROC QUANTSELECT creates. See the section “[Macro Variables That Contain Selected Models](#)” on page 6600 for more information.

If you have partitioned the input data with a `PARTITION` statement, then a character variable `_ROLE_` is included in the output data set. The following table shows the value of `_ROLE_` for each observation:

| <code>_ROLE_ Value</code> | Observation Role |
|---------------------------|------------------|
| TEST                      | Testing          |
| TRAIN                     | Training         |
| VALIDATE                  | Validation       |

If you want to create a permanent SAS data set, you must specify a two-level name. For more information about permanent SAS data sets, see the discussion in *SAS Language Reference: Concepts*.

You can specify the following arguments in the OUTPUT statement:

*keyword* < =name >

specifies the statistics to include in the output data set and optionally names the new variables that contain the statistics. Specify one of the following *keywords* for each desired statistic, followed optionally by an equal sign, and the *name* of a variable to contain the statistic. If you specify *keyword*=*name*, the new variable that contains the requested statistic has the specified name. If you omit the optional =*name* after a *keyword*, then the new variable name is formed by using a prefix of one or more characters that identify the statistic, followed by an underscore (`_`), followed by the dependent variable name.

**PREDICTED** | **PRED** | **P** includes predicted values in the output data set. The prefix for the default name is p.

**RESIDUAL** | **RESID** | **R** includes residuals, calculated as `ACTUAL – PREDICTED`, in the output data set. The prefix for the default name is r.

**OUT=SAS-data-set**

names the output data set. By default, PROC QUANTSELECT uses the *DATA*n** convention to name the new data set.

## PARTITION Statement

**PARTITION** < *option* > ;

The PARTITION statement specifies how observations in the input data set are logically partitioned into disjoint subsets for model training, validation, and testing. Either you can designate a variable in the input data set and a set of formatted values of that variable to determine the role of each observation, or you can specify proportions to use for random assignment of observations for each role.

An alternative to using a PARTITION statement is to provide a variable named `_ROLE_` in the input data set to define roles of observations in the input data. If you specify a PARTITION statement, then any `_ROLE_` variable in the input data set is ignored. If you do not use a PARTITION statement and the input data do not contain a variable named `_ROLE_`, then all observations in the input data set are assigned to model training.

You can specify either (but not both) of the following *options*:

**ROLEVAR=variable** (< **TEST=***value*> < **TRAIN=***value*> < **VALIDATE=***value*>)

**ROLE=variable** (< **TEST=***value*> < **TRAIN=***value*> < **VALIDATE=***value*>)

names the variable in the input data set whose values are used to assign roles to each observation. The **TEST=**, **TRAIN=**, and **VALIDATE=** suboptions specify the formatted values of this variable that are used to assign observations roles. If you do not specify the **TRAIN=** suboption, then all observations whose role is not determined by the **TEST=** or **VALIDATE=** suboptions are assigned to training. If you specify a **TESTDATA=** data set in the PROC QUANTSELECT statement, then you cannot also specify the **TEST=** suboption in the PARTITION statement. If you specify a **VALDATA=** data set in the PROC QUANTSELECT statement, then you cannot also specify the **VALIDATE=** suboption in the PARTITION statement.

**FRACTION**(< **TEST=***fraction*> < **VALIDATE=***fraction*>)

requests that specified proportions of the observations in the input data set be randomly assigned training and validation roles. You specify the proportions for testing and validation by using the **TEST=** and **VALIDATE=** suboptions. If you specify both the **TEST=** and the **VALIDATE=** suboptions, then the sum of the specified fractions must be less than 1 and the remaining fraction of the observations are assigned to the training role. If you specify a **TESTDATA=** data set in the PROC QUANTSELECT statement, then you cannot also specify the **TEST=** suboption in the PARTITION statement. If you specify a **VALDATA=** data set in the PROC QUANTSELECT statement, then you cannot also specify the **VALIDATE=** suboption in the PARTITION statement.

## WEIGHT Statement

**WEIGHT** *variable* ;

A WEIGHT statement names a variable in the input data set with values that are relative weights for a weighted quantile regression fit.



Values of the weight variable must be nonnegative. If an observation's weight is 0, the observation is deleted from the analysis. If a weight is negative or missing, it is set to 0, and the observation is excluded from the analysis.

---

## Details: QUANTSELECT Procedure

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### Effect Selection Methods

The effect selection methods implemented in PROC QUANTSELECT are specified with the **SELECTION=** option in the **MODEL** statement.

#### Full Model Fitted (NONE)

The complete model specified in the **MODEL** statement is used to fit the model, and no effect selection is done. You request this method by specifying **SELECTION=NONE** in the **MODEL** statement.

#### Forward Selection (FORWARD)

The forward selection technique begins with just the forced-in covariates and then sequentially adds the effect that most improves the fit. The process terminates when no significant improvement can be obtained by adding any effect. You request this method by specifying **SELECTION=FORWARD** in the **MODEL** statement.

If you specify the **SELECT=SL method-option**, you can use the **TEST= method-option** to specify a test statistic for gauging improvement in fit. For example, if **TEST=LR1**, at each step the effect that yields the most significant likelihood ratio statistic is added and the process continues until all effects that are not in the model have LR1 statistics that are not significant at the entry significance level (which is specified in the **SLE=** option). Because effects can contribute different degrees of freedom to the model, it is necessary to compare the *p*-values that correspond to these statistics.

#### Backward Elimination (BACKWARD)

The backward elimination technique starts from the full model, which includes all independent effects. Then effects are deleted one by one until a stopping condition is satisfied. At each step, the effect that shows the smallest contribution to the model is deleted. You request this method by specifying **SELECTION=BACKWARD** in the **MODEL** statement.

Suppose you specify the **SELECT=SL method-option** and the **TEST=LR1 method-option** to gauge improvement in quantile regression fit. At any step, the predictor that produces the least significant LR1 statistic is dropped and the process continues until all effects that remain in the model have LR1 statistics that are significant at the stay significance level (which is specified in the **SLS=** option).

#### Stepwise Selection (STEPWISE)

The stepwise method is a modification of the forward selection technique in which effects already in the model do not necessarily stay there. You request this method by specifying **SELECTION=STEPWISE** in the **MODEL** statement.



In the implementation of the stepwise selection method, the same entry and removal approaches for the forward selection and backward elimination methods are used to assess contributions of effects as they are added to or removed from a model. Suppose you specify `SELECT=SL`. If, at a step of the stepwise method, any effect in the model is not significant at the level specified by the `SLSTAY= method-option`, then the least significant of these effects is removed from the model and the algorithm proceeds to the next step. This ensures that no effect can be added to a model while some effect currently in the model is not deemed significant. Only after all necessary deletions have been accomplished can another effect be added to the model. In this case, the effect whose addition yields the most significant statistic value is added to the model and the algorithm proceeds to the next step. The stepwise process ends when none of the effects outside the model is significant at the level specified by the `SLENTY= method-option` and every effect in the model is significant at the level specified by the `SLSTAY= method-option`. In some cases, neither of these two conditions for stopping is met and the sequence of models cycles. In this case, the stepwise method terminates at the end of the second cycle.

Just as with forward selection and backward elimination, you can use the `SELECT= method-option` to change the criterion used to assess effect contributions. You can also use the `STOP= method-option` to specify a stopping criterion and use the `CHOOSE= method-option` to specify a criterion used to select among the sequence of models produced.

## LASSO Method (LASSO)

The standard LASSO method uses a standardized design matrix that orthogonalizes selectable covariates against forced-in covariates, and then scales the orthogonalized selectable covariates so that they all have the same sum of squares. See the information about the standard parameter estimate in the section “[Parameter Estimates](#)” on page 6606 for more information about design matrix orthogonalization. The LASSO method initializes all the selectable coefficients into 0 at step 0. The predictor that reduces the average check loss the fastest relative to the L1-norm of the selectable coefficient increment is determined, and a step is taken in the direction of this predictor.

The difference between adaptive LASSO and standard LASSO methods is in the prescaling of the selectable coefficients. After orthogonalization against forced-in covariates, the adaptive LASSO method first fits a full model without penalty, and then scales the orthogonalized selectable covariates with the corresponding coefficients from the full model. This adaptive scaling can be equivalently substituted by using a weighted L1-norm penalty, where the weights are the reciprocals of the corresponding coefficients from the full model.

The length of this step determines the coefficient of this predictor and is chosen when some residual changes its sign or some predictor that is not used in the model can reduce the average check loss more efficiently. This process continues until all predictors are in the model.

As with other selection methods, the issue of when to stop the selection process is crucial. You can use the `CHOOSE= method-option` to specify a criterion for choosing among the models at each step. You can also use the `STOP= method-option` to specify a stopping criterion. See the section “[Criteria Used in Model Selection Methods](#)” on page 6598 for more information and [Table 78.10](#) for the formulas for evaluating these criteria.

---

## Criteria Used in Model Selection Methods

PROC QUANTSELECT supports a variety of fit statistics that you can specify as criteria for the `CHOOSE=`, `SELECT=`, and `STOP= method-options` in the `MODEL` statement.

## Single Quantile Effect Section

The following fit statistics are available for single quantile effect selection:

|                              |                                                                                                                                                                                                                                                                                  |
|------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>AIC</b>                   | applies the Akaike's information criterion (Akaike 1981; Darlington 1968; Judge et al. 1985).                                                                                                                                                                                    |
| <b>AICC</b>                  | applies the corrected Akaike's information criterion (Hurvich and Tsai 1989).                                                                                                                                                                                                    |
| <b>SBC</b>                   | applies the Schwarz Bayesian information criterion (Schwarz 1978; Judge et al. 1985).                                                                                                                                                                                            |
| <b>SL&lt;(LR1   LR2)&gt;</b> | specifies the significance level of a statistic used to assess an effect's contribution to the fit when it is added to or removed from a model. LR1 specifies likelihood ratio Type I, and LR2 specifies the likelihood ratio Type II. By default, the LR1 statistic is applied. |
| <b>ADJR1</b>                 | applies the adjusted quantile regression R statistic.                                                                                                                                                                                                                            |
| <b>VALIDATE</b>              | applies the average check loss for the validation data.                                                                                                                                                                                                                          |

Table 78.10 provides formulas and definitions for these fit statistics.

**Table 78.10** Formulas and Definitions for Model Fit Summary Statistics for Single Quantile Effect Section

| Statistic     | Definition or Formula                                                                                             |
|---------------|-------------------------------------------------------------------------------------------------------------------|
| $n$           | Number of observations                                                                                            |
| $p$           | Number of parameters including the intercept                                                                      |
| $r_i(\tau)$   | Residual for the $i$ th observation; $r_i(\tau) = y_i - \mathbf{x}_i \boldsymbol{\beta}(\tau)$                    |
| $D(\tau)$     | Total sum of check losses; $D(\tau) = \sum_{i=1}^n \rho_{\tau}(r_i)$                                              |
| $D_0(\tau)$   | Total sum of check losses for intercept-only model if intercept is a forced-in effect, otherwise for empty-model. |
| $ACL(\tau)$   | Average check loss; $ACL(\tau) = \frac{D(\tau)}{n}$                                                               |
| $R1(\tau)$    | Counterpart of linear regression R-square for quantile regression; $1 - \frac{D(\tau)}{D_0(\tau)}$                |
| $ADJR1(\tau)$ | Adjusted R1; $(\tau) = 1 - \frac{(n-1)D(\tau)}{(n-p)D_0(\tau)}$                                                   |
| $AIC(\tau)$   | $2n \ln(ACL(\tau)) + 2p$                                                                                          |
| $AICC(\tau)$  | $2n \ln(ACL(\tau)) + \frac{2pn}{n-p-1}$                                                                           |
| $SBC(\tau)$   | $2n \ln(ACL(\tau)) + p \ln(n)$                                                                                    |

## Quantile Process Effect Section

The following statistics are available for quantile process effect selection:

|              |                                                                                             |
|--------------|---------------------------------------------------------------------------------------------|
| <b>AIC</b>   | specifies Akaike's information criterion (Akaike 1981; Darlington 1968; Judge et al. 1985). |
| <b>AICC</b>  | specifies the corrected Akaike's information criterion (Hurvich and Tsai 1989).             |
| <b>SBC</b>   | specifies Schwarz Bayesian information criterion (Schwarz 1978; Judge et al. 1985).         |
| <b>ADJR1</b> | specifies the adjusted quantile regression R statistic.                                     |

**VALIDATE** specifies average check loss for the validation data.

Table 78.11 provides formulas and definitions for the fit statistics.

**Table 78.11** Formulas and Definitions for Model Fit Summary Statistics for Quantile Process Effect Section

| Statistic | Definition or Formula                                                                                                                      |
|-----------|--------------------------------------------------------------------------------------------------------------------------------------------|
| $D$       | Integral of total sum of check losses; $D = \int_0^1 D(\tau)d\tau$                                                                         |
| $D_0$     | Integral of total sum of check losses for intercept-only model or empty-model if the NOINT option is used; $D_0 = \int_0^1 D_0(\tau)d\tau$ |
| ACL       | Integral of average check loss; $ACL = \frac{D}{n}$                                                                                        |
| R1        | $1 - \frac{D}{D_0}$                                                                                                                        |
| ADJR1     | Adjusted R1; $1 - \frac{(n-1)D}{(n-p)D_0}$                                                                                                 |
| AIC       | $\int_0^1 AIC(\tau)d\tau$                                                                                                                  |
| AICC      | $\int_0^1 AICC(\tau)d\tau$                                                                                                                 |
| SBC       | $\int_0^1 SBC(\tau)d\tau$                                                                                                                  |

## Macro Variables That Contain Selected Models

PROC QUANTSELECT saves the list of selected effects in a macro variable so that you can use other SAS procedures to perform post-selection analyses. This list does not explicitly include the intercept so that you can use it in the **MODEL** statement of other SAS/STAT regression procedures.

Table 78.12 describes the macro variables that PROC QUANTSELECT creates. When multiple quantile levels or BY processing are used, one macro variable, indexed by the quantile level order and the BY group number, is created for each quantile level and BY group combination.

**Table 78.12** Macro Variables Created for Subsequent Processing

| Macro Variable                                       | Description                                                 |
|------------------------------------------------------|-------------------------------------------------------------|
| <b>Single Quantile Level and No BY processing</b>    |                                                             |
| _QRSIND                                              | Selected model                                              |
| <b>Multiple Quantile Levels and No BY Processing</b> |                                                             |
| _QRSNUMTAUS                                          | Number of quantile levels                                   |
| _QRSINDT1                                            | Selected model for the first quantile level                 |
| _QRSINDT2                                            | Selected model for the second quantile level                |
| ...                                                  |                                                             |
| <b>Single Quantile Level and BY Processing</b>       |                                                             |
| _QRSNUMBYS                                           | Number of BY groups                                         |
| _QRSIND1                                             | Selected model for BY group 1                               |
| _QRSIND2                                             | Selected model for BY group 2                               |
| ...                                                  |                                                             |
| <b>Multiple Quantile Levels and BY Processing</b>    |                                                             |
| _QRSNUMTAUS                                          | Number of quantile levels                                   |
| _QRSNUMBYS                                           | Number of BY groups                                         |
| _QRSIND1T1                                           | Selected model for the first quantile level and BY group 1  |
| _QRSIND1T2                                           | Selected model for the second quantile level and BY group 1 |
| ...                                                  |                                                             |
| _QRSIND2T1                                           | Selected model for the first quantile level and BY group 2  |
| _QRSIND2T2                                           | Selected model for the second quantile level and BY group 2 |
| ...                                                  |                                                             |

The macro variables \_QRSIND, \_QRSINDT1, \_QRSIND1, and \_QRSIND1T1 are all synonyms. If you do not specify multiple quantile levels or BY processing, the macro variables \_QRSNUMTAUS and \_QRSNUMBYS are both set to 1.

PROC QUANTSELECT creates two output data set variables, \_BY\_ and \_QUANTILE\_, to aid in associating macro variables with output data set observations when multiple quantile levels or BY processing are used. The values of these two variables are integers that match the  $i,j$  components of the macro variable names  $\_QRSIND_{i}T_{j}$ .

## Using Validation and Test Data

When you have sufficient data, you can subdivide your data into three parts: training, validation, and test data. During the selection process, models are fit on the training data, and the prediction error for the models so obtained is found by using the validation data. This prediction error on the validation data can be used to decide when to terminate the selection process or to decide which effects to include as the selection process proceeds. Finally, after a selected model has been obtained, the test set can be used to assess how the selected model generalizes on data that played no role in selecting the model.

In some cases you might want to use only training and test data. For example, you might decide to use an information criterion to decide which effects to include and when to terminate the selection process. In this case no validation data are required, but test data can still be useful in assessing the predictive performance of the selected model. In other cases you might decide to use validation data during the selection process but forgo assessing the selected model on test data. Hastie, Tibshirani, and Friedman (2001) note that it is difficult to give a general rule for how many observations you should assign to each role. They note that a typical split might be 50% for training and 25% each for validation and testing.

PROC QUANTSELECT provides several methods for partitioning data into training, validation, and test data. You can provide data for each role in separate data sets that you specify with the `DATA=`, `TESTDATA=`, and `VALDATA=` options in the PROC QUANTSELECT procedure. An alternative method is to use a `PARTITION` statement to logically subdivide the `DATA=` data set into separate roles. You can name the fractions of the data that you want to reserve as test data and validation data. The following statements randomly subdivide the `inData` data set to use 25% of the data for validation and 25% for testing, leaving 50% of the data for training:

```
proc quantselect data=inData;
 partition fraction(test=0.25 validate=0.25);
 ...
run;
```

If you need to exercise more control over the partitioning of the input data set, you can name a variable in the input data set and a formatted value of that variable to correspond to each role. The following statements assign roles to observations in the `inData` data set based on the value of the variable named `group` in that data set:

```
proc quantselect data=inData;
 partition roleVar=group(test='group 1' train='group 2');
 ...
run;
```

Observations whose value of the variable `group` is `'group 1'` are assigned for testing, and those whose value is `'group 2'` are assigned to training. All other observations are ignored.

You can also combine the use of the `PARTITION` statement with named data sets for specifying data roles. For example, the following statements reserve 40% of the `inData` data set for validation, leaving the remaining 60% for training:

```
proc quantselect data=inData testData=inTest;
 partition fraction(validate=0.4);
 ...
run;
```

Data for testing are supplied in the `inTest` data set. Because a `TESTDATA=` data set is specified, additional observations for testing cannot be reserved by specifying a `PARTITION` statement.

When you use a `PARTITION` statement, the output data set that is created by an `OUTPUT` statement contains a character variable `_ROLE_` whose values 'TRAIN', 'TEST', and 'VALIDATE' indicate the role of each observation. `_ROLE_` is blank for observations that were not assigned to any of these three roles. When the input data set specified in the `DATA=` option in the `PROC QUANTSELECT` statement contains an `_ROLE_` variable, no `PARTITION` statement is used, and the `TESTDATA=` and `VALDATA=` options are not specified, then the `_ROLE_` variable is used to define the roles of each observation. This is useful when you want to rerun `PROC QUANTSELECT` but use the same data partitioning as you used in a previous `PROC QUANTSELECT` step. For example, the following statements use the same data for testing and training in both `PROC QUANTSELECT` steps:

```
proc quantselect data=inData;
 partition fraction(test=0.5);
 model y=x1-x10 / selection=forward;
 output out=outDataForward;
run;

proc quantselect data=outDataForward;
 model y=x1-x10 / selection=backward;
run;
```

When you have reserved observations for training, validation, and testing, a model that is fit on the training data is scored on the validation and test data, and the average check loss, denoted by ACL, is computed separately for each of these subsets. The ACL for each data role is the sum of check losses for observations in that role divided by the number of observations in that role.

### Using the Validation ACL as the STOP= Criterion

If you have provided observations for validation, then you can use the `STOP=VALIDATE` *method-option* to specify the validation ACL as the `STOP=` criterion in the `SELECTION=` option in the `MODEL` statement. At step  $k$  of the selection process, the best candidate effect to enter or leave the current model is determined. The “best candidate” means the effect that gives the best value of the `SELECT=` criterion that does not need to be based on the validation data. The validation ACL for the model with this candidate effect added is computed. If this validation ACL is greater than the validation ACL for the model at step  $k$ , then the selection process terminates at step  $k$ .

### Using the Validation ACL as the CHOOSE= Criterion

When you specify the `CHOOSE=VALIDATE` *method-option* in the `SELECTION=` option in the `MODEL` statement, the validation ACL is computed for the models at each step of the selection process. The model that yields the smallest validation ACL and contains the fewest effects is selected.

### Using the Validation ACL as the SELECT= Criterion

You request the validation ACL as the selection criterion by specifying the `SELECT=VALIDATE` *method-option* in the `SELECTION=` option in the `MODEL` statement. At step  $k$  of the selection process, the validation ACL is computed for each model where a candidate for entry is added or candidate for removal is dropped. The selected candidate for entry or removal is the one that yields a model with the minimal validation ACL.

---

## Displayed Output

The following sections describe the output that is displayed by PROC QUANTSELECT. The output is organized into various tables, which are discussed in the order of appearance. The contents of a table might change depending on the options you specify.

### Model Information

The “Model Information” table displays basic information about the data sets and the settings used to control effect selection. These settings include the following:

- the selection method
- the criteria used to select effects, stop the selection, and choose the selected model
- the effect hierarchy enforced

The ODS name of the “Model Information” table is ModelInfo.

### Number of Observations

The “Number of Observations” table displays the number of observations read from the input data set and the number of observations used in the analysis. If you use a **PARTITION** statement, the table also displays the number of observations used for each data role. If you specify **TESTDATA=** or **VALDATA=** data sets in the PROC QUANTSELECT statement, then “Number of Observations” tables are also produced for these data sets. The ODS name of the “Number of Observations” table is NObs.

### Class Level Information

The “Class Level Information” table lists the levels of every variable specified in the **CLASS** statement. The ODS name of the “Class Level Information” table is ClassLevelInfo.

### Class Level Coding

The “Class Level Coding” table shows the coding used for every variable specified in the **CLASS** statement. The ODS name of the “Class Level Coding” table is ClassLevelCoding.

### Candidates

The “Candidates” table displays the effect name and value of the criterion used to select entering or departing effects at each step of the selection process. The effects are displayed in sorted order from best to worst of the selection criterion. You request this table with the **DETAILS=** option in the **MODEL** statement. The ODS name of the “Candidates” table is either EntryCandidates for addition candidates or RemovalCandidates for removal candidates.

## Selection Summary

The “Selection Summary” table displays details about the sequence of steps of the selection process. For each step, the effect that entered or dropped out is displayed along with the statistics used to select the effect, stop the selection, and choose the selected model. You can request that additional statistics be displayed with the `STATS=` option in the `MODEL` statement. For all criteria that you can use for effect selection, the steps at which the optimal values of these criteria occur are also indicated. The ODS name of the “Selection Summary” table is `SelectionSummary`.

## Stop Reason

The “Stop Reason” table displays the reason why the selection stopped. [Table 78.13](#) shows the possible stop reasons.

**Table 78.13** Reasons for Stopping

| Stop Reason | Description                                                                                                      |
|-------------|------------------------------------------------------------------------------------------------------------------|
| 1           | The selected model is a perfect fit.                                                                             |
| 2           | The specified maximum number of steps has been reached.                                                          |
| 3           | The specified maximum number of effects are in the model.                                                        |
| 4           | The specified minimum number of effects are in the model.                                                        |
| 5           | The stopping criterion found a local optimum.                                                                    |
| 6           | No suitable add or drop candidate is available.                                                                  |
| 7           | All effects are in the model.                                                                                    |
| 8           | All effects have been dropped.                                                                                   |
| 9           | The sequence of effect additions and removals is cycling.                                                        |
| 10          | Adding or dropping any effect does not improve the <code>SELECT=</code> criterion.                               |
| 11          | No effect is significant at the specified significance level for entry or significance level for staying levels. |
| 12          | All remaining effects are required.                                                                              |

The ODS name of the “Stop Reason” table is `StopReason`.

## Selection Reason

The “Selection Reason” table displays how the final selected model is determined. [Table 78.14](#) shows the possible selection reasons:

**Table 78.14** Selection Reasons

| Selection Reason | Description                                                                                                        |
|------------------|--------------------------------------------------------------------------------------------------------------------|
| 1                | The last valid model that occurs in the selection process is the final model.                                      |
| 2                | The first model with the minimum <code>CHOOSE=</code> criterion value in the selection process is the final model. |

The ODS name of the “Selection Reason” table is `SelectionReason`.



## Selected Effects

The “Selected Effects” table displays a string that contains the list of effects in the selected model. The ODS name of the “Selected Effects” table is SelectedEffects.

## Parameter Estimates

The “Parameter Estimates” table displays the parameters in the selected model and their estimates. The following information is displayed for each parameter in the selected model:

- the parameter label that includes the effect name and level information for effects that contain classification variables
- the degrees of freedom (DF) for the parameter. There is one degree of freedom unless the model is not full rank.
- the parameter estimate
- the standard parameter estimate, which is computed on a standardized design matrix. Let  $\mathbf{X} = (\mathbf{X}_1, \mathbf{X}_2)$  denote the original design matrix, where  $\mathbf{X}_1$  is the submatrix for all the forced-in effects, and  $\mathbf{X}_2$  is the submatrix for the rest of the effects that are subject to selection. Let

$$\mathbf{X}_2^* = [\mathbf{I} - \mathbf{X}_1(\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{X}_1']\mathbf{X}_2 \text{ and } \mathbf{X}_2^{**} = (s_Y \sqrt{n - p_1})^{-1} [\text{diag}(\mathbf{X}_2^{**'}\mathbf{X}_2^{**})]^{-\frac{1}{2}} \mathbf{X}_2^*$$

where  $p_1$  is the rank of  $\mathbf{X}_1$  and  $s_Y = \sqrt{\frac{\mathbf{Y}^*\mathbf{Y}^*}{n - p_1}}$  with  $\mathbf{Y}^* = [\mathbf{I} - \mathbf{X}_1(\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{X}_1']\mathbf{Y}$ .

Then standard parameter estimates are defined as  $(\mathbf{0}, \boldsymbol{\beta}_2^{**})$ , where  $(\boldsymbol{\beta}_1, \boldsymbol{\beta}_2^{**})$  are the parameter estimates computed on the standardized design matrix  $(\mathbf{X}_1, \mathbf{X}_2^{**})$ .

You can also use the `DETAILS=` option in the `MODEL` statement to request “Parameter Estimates” tables for the models at each step of the selection process. The ODS name of the “Parameter Estimates” table is “ParameterEstimates.”

## ODS Table Names

PROC QUANTSELECT assigns a name to each table it creates. You can use these names to refer to the table when you use the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in Table 78.15.

For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

**Table 78.15** ODS Tables Produced by PROC QUANTSELECT

| ODS Table Name    | Description            | Statement | Option   |
|-------------------|------------------------|-----------|----------|
| BSplineDetails    | B-spline basis details | EFFECT    | DETAILS  |
| EntryCandidates   | Entry effect ranking   | MODEL     | DETAILS= |
| RemovalCandidates | Removal effect ranking | MODEL     | DETAILS= |

**Table 78.15** *continued*

| ODS Table Name      | Description                                  | Statement | Option           |
|---------------------|----------------------------------------------|-----------|------------------|
| ClassLevelCoding    | Classification variable coding               | CLASS     | SHOWCODING       |
| ClassLevelInfo      | Classification variable levels               | CLASS     | Default          |
| CollectionLevelInfo | Levels of collection effects                 | EFFECT    | DETAILS          |
| MMLevelInfo         | Levels of multimember effects                | EFFECT    | DETAILS          |
| ModelInfo           | Model information                            | MODEL     | Default          |
| NObs                | Number of observations                       | MODEL     | Default          |
| ParameterNames      | Labels for column names in the design matrix | PROC      | OUTDESIGN(names) |
| ParameterEstimates  | Selected model parameter estimates           | MODEL     | Default          |
| PolynomialDetails   | Polynomial details                           | EFFECT    | DETAILS          |
| PolynomialScaling   | Polynomial scaling                           | EFFECT    | DETAILS          |
| SelectedEffects     | List of selected effects                     | MODEL     | Default          |
| SelectionSummary    | Selection summary                            | MODEL     | Default          |
| StopDetails         | Stopping criterion details                   | MODEL     | Default          |
| StopReason          | Reason why selection stopped                 | MODEL     | Default          |
| TPFSplineDetails    | Thin-plate spline basis details              | EFFECT    | DETAILS          |

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “Statistical Graphics Using ODS.”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “A Primer on ODS Statistical Graphics” on page 599 in Chapter 21, “Statistical Graphics Using ODS.”

PROC QUANTSELECT assigns a name to each graph it creates using ODS. You can use these names to refer to the graphs when using ODS. The names are listed in Table 78.16.

**Table 78.16** ODS Graphics Produced by PROC QUANTSELECT

| ODS Graph Name      | Plot Description                                 | PLOTS Option         |
|---------------------|--------------------------------------------------|----------------------|
| ACLPlot             | Average check loss by step                       | ACL                  |
| AICCPLOT            | Corrected Akaike’s information criterion by step | CRITERIA(UNPACK)     |
| AICPlot             | Akaike’s information criterion by step           | CRITERIA(UNPACK)     |
| AdjR1Plot           | Adjusted quantile regression R by step           | CRITERIA(UNPACK)     |
| ChooseCriterionPlot | CHOOSE= criterion by step                        | COEFFICIENTS(UNPACK) |

Table 78.16 continued

| ODS Graph Name   | Plot Description                                | PLOTS= Option        |
|------------------|-------------------------------------------------|----------------------|
| CoefficientPanel | Coefficients and CHOOSE= criterion by step      | COEFFICIENTS         |
| CoefficientPlot  | Coefficients by step                            | COEFFICIENTS(UNPACK) |
| CriterionPanel   | Fit criteria by step                            | CRITERIA             |
| SBCPlot          | Schwarz Bayesian information criterion by step  | CRITERIA(UNPACK)     |
| ValidateACLPlot  | Average square error on validation data by step | CRITERIA(UNPACK)     |

## Example: QUANTSELECT Procedure

### Example 78.1: Simulated Data Example

This simulation study exemplifies the unity of motive and effect for the PROC QUANTSELECT procedure. The following statements generate a data set that is based on a naive instrumental model (Chernozhukov and Hansen 2008):

```

%let seed=321;
%let p=20;
%let n=3000;

data analysisData;
 array x{&p} x1-x&p;
 do i=1 to &n;
 U = ranuni(&seed);
 x1 = ranuni(&seed);
 x2 = ranexp(&seed);
 x3 = abs(rannor(&seed));
 y = x1*(U-0.1) + x2*(U*U-0.25) + x3*(exp(U)-exp(0.9));
 do j=4 to &p;
 x{j} = ranuni(&seed);
 end;
 output;
 end;
run;

```

Variable  $U$  of the data set indicates the true quantile level of the response  $y$  conditional on  $\mathbf{x} = (x_1, \dots, x_p)$ .

Let  $Q_y(\tau|\mathbf{x}) = \mathbf{x}\boldsymbol{\beta}(\tau)$  denote the underlying quantile regression model, where  $\boldsymbol{\beta}(\tau) = (\beta_1(\tau), \dots, \beta_p(\tau))'$ . Then, the true parameter functions are

$$\begin{aligned}
 \beta_1(\tau) &= \tau - 0.1 \\
 \beta_2(\tau) &= \tau^2 - 0.25 \\
 \beta_3(\tau) &= \exp(\tau) - \exp(0.9) \\
 \beta_4(\tau) &= \dots = \beta_p(\tau) = 0
 \end{aligned}$$

It is easy to see that, at  $\tau = 0.1$ , only  $\beta_2(0.1) = -0.24$  and  $\beta_3(0.1) = \exp(0.1) - \exp(0.9) \approx -1.354432$  are nonzero parameters. Therefore, an effective effect selection method should select  $x_2$  and  $x_3$  and drop all the other effects in this data set at  $\tau = 0.1$ . By the same rationale,  $x_1$  and  $x_3$  should be selected at  $\tau = 0.5$  with  $\beta_1(0.5) = 0.4$  and  $\beta_3(0.5) \approx -0.810882$ , and  $x_1$  and  $x_2$  should be selected at  $\tau = 0.9$  with  $\beta_1(0.9) = 0.8$  and  $\beta_2(0.9) = 0.56$ .

The following statements use PROC QUANTSELECT with the adaptive LASSO method:

```
proc quantselect data=analysisData;
 model y= x1-x&p / quantile=0.1 0.5 0.9
 selection=lasso(adaptive);
run;
```

The selected effects and the relevant estimates are shown in [Output 78.1.1](#) for  $\tau = 0.1$ , [Output 78.1.2](#) for  $\tau = 0.5$ , and [Output 78.1.3](#) for  $\tau = 0.9$ . You can see that the adaptive LASSO method correctly selects active effects for all three quantile levels.

**Output 78.1.1** Parameter Estimates at  $\tau = 0.1$

| The QUANTSELECT Procedure         |    |           |                       |
|-----------------------------------|----|-----------|-----------------------|
| Quantile = 0.1                    |    |           |                       |
| Selected Effects: Intercept x2 x3 |    |           |                       |
| Parameter Estimates               |    |           |                       |
| Parameter                         | DF | Estimate  | Standardized Estimate |
| Intercept                         | 1  | 0.011793  | 0                     |
| x2                                | 1  | -0.228709 | -0.218287             |
| x3                                | 1  | -1.379907 | -0.784520             |

**Output 78.1.2** Parameter Estimates at  $\tau = 0.5$

| The QUANTSELECT Procedure         |    |           |                       |
|-----------------------------------|----|-----------|-----------------------|
| Quantile = 0.5                    |    |           |                       |
| Selected Effects: Intercept x1 x3 |    |           |                       |
| Parameter Estimates               |    |           |                       |
| Parameter                         | DF | Estimate  | Standardized Estimate |
| Intercept                         | 1  | 0.011778  | 0                     |
| x1                                | 1  | 0.425843  | 0.118792              |
| x3                                | 1  | -0.863316 | -0.490822             |

**Output 78.1.3** Parameter Estimates at  $\tau = 0.9$ 

| The QUANTSELECT Procedure         |    |           |                       |
|-----------------------------------|----|-----------|-----------------------|
| Quantile = 0.9                    |    |           |                       |
| Selected Effects: Intercept x1 x2 |    |           |                       |
| Parameter Estimates               |    |           |                       |
| Parameter                         | DF | Estimate  | Standardized Estimate |
| Intercept                         | 1  | -0.007738 | 0                     |
| x1                                | 1  | 0.782942  | 0.218407              |
| x2                                | 1  | 0.576445  | 0.550177              |

The QUANTSELECT procedure can perform effect selection not only at a single quantile level but also for the entire quantile process. You can specify the QUANTILE=PROCESS option to do effect selection for the entire quantile process. With the QUANTILE=PROCESS option specified, the ParameterEstimates table produced by the QUANTSELECT procedure actually shows the mean prediction model of  $y$  conditional on  $x$ . In this simulation study, the true mean model is

$$E(y|x) = x\beta$$

where

$$\begin{aligned}\beta_1 &= E(U) - 0.1 = 0.4 \\ \beta_2 &= E(U^2) - 0.25 \approx 0.083333 \\ \beta_3 &= E(\exp(U)) - \exp(0.9) \approx -0.741321 \\ \beta_4 &= \dots = \beta_p = 0\end{aligned}$$

The following statements perform effect selection for the quantile process with the forward selection method.

```
proc quantselect data=analysisData;
 model y= x1-x&p / quantile=process(ntau=all)
 selection=forward;
run;
```

Output 78.1.4 shows that, by default, the SELECT= and STOP= options are both set to SBC. The selected effects and the relevant estimates for the conditional mean model are shown in Output 78.1.5.

**Output 78.1.4** Model Information

| The QUANTSELECT Procedure |                   |
|---------------------------|-------------------|
| Model Information         |                   |
| Data Set                  | WORK.ANALYSISDATA |
| Dependent Variable        | Y                 |
| Selection Method          | Forward           |
| Quantile Type             | Process           |
| Select Criterion          | SBC               |
| Stop Criterion            | SBC               |
| Choose Criterion          | SBC               |

**Output 78.1.5** Parameter Estimates

| Parameter Estimates |    |           |                       |
|---------------------|----|-----------|-----------------------|
| Parameter           | DF | Estimate  | Standardized Estimate |
| Intercept           | 1  | 0.007833  | 0                     |
| x1                  | 1  | 0.418825  | 0.116834              |
| x2                  | 1  | 0.094791  | 0.090472              |
| x3                  | 1  | -0.785686 | -0.446687             |

Linear regression is the most popular method for estimating conditional means. The following statements show how to select effects with the GLMSELECT procedure, and [Output 78.1.6](#) shows the resulting selected effects and their estimates. You can see that the mean estimates from the QUANTSELECT procedure are similar to those from the GLMSELECT procedure. However, quantile regression can provide detailed distribution information, which is not available from linear regression.

```
proc glmselect data=analysisData;
 model y= x1-x3 / selection=forward(select=sbc stop=sbc choose=sbc);
run;
```

**Output 78.1.6** Parameter Estimates

| The GLMSELECT Procedure |    |           |                |         |
|-------------------------|----|-----------|----------------|---------|
| Selected Model          |    |           |                |         |
| Parameter Estimates     |    |           |                |         |
| Parameter               | DF | Estimate  | Standard Error | t Value |
| Intercept               | 1  | -0.010143 | 0.043129       | -0.24   |
| x1                      | 1  | 0.434553  | 0.057385       | 7.57    |
| x2                      | 1  | 0.114183  | 0.016771       | 6.81    |
| x3                      | 1  | -0.797194 | 0.028156       | -28.31  |

---

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# Chapter 79

## The REG Procedure

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---

## Overview: REG Procedure

The REG procedure is one of many regression procedures in the SAS System. It is a general-purpose procedure for regression, while other SAS regression procedures provide more specialized applications.

Other SAS/STAT procedures that perform at least one type of regression analysis are the CATMOD, GENMOD, GLM, LOGISTIC, MIXED, NLIN, ORTHOREG, PROBIT, RSREG, and TRANSREG procedures. SAS/ETS procedures are specialized for applications in time series or simultaneous systems. These other SAS/STAT regression procedures are summarized in Chapter 4, “[Introduction to Regression Procedures](#),” which also contains an overview of regression techniques and defines many of the statistics computed by PROC REG and other regression procedures.

PROC REG provides the following capabilities:

- multiple MODEL statements

- nine model-selection methods
- interactive changes both in the model and the data used to fit the model
- linear equality restrictions on parameters
- tests of linear hypotheses and multivariate hypotheses
- collinearity diagnostics
- predicted values, residuals, studentized residuals, confidence limits, and influence statistics
- correlation or crossproduct input
- requested statistics available for output through output data sets
- ODS Graphics. For more information, see the section “[ODS Graphics](#)” on page 6745.

Nine model-selection methods are available in PROC REG. In the simplest method, PROC REG fits the complete model that you specify. The other eight methods involve various ways of including or excluding variables from the model. You specify these methods with the `SELECTION=` option in the `MODEL` statement.

The methods are identified in the following list and are explained in detail in the section “[Model-Selection Methods](#)” on page 6701.

|          |                                                                                                                                                     |
|----------|-----------------------------------------------------------------------------------------------------------------------------------------------------|
| NONE     | no model selection. This is the default. The complete model specified in the <code>MODEL</code> statement is fit to the data.                       |
| FORWARD  | forward selection. This method starts with no variables in the model and adds variables.                                                            |
| BACKWARD | backward elimination. This method starts with all variables in the model and deletes variables.                                                     |
| STEPWISE | stepwise regression. This is similar to the FORWARD method except that variables already in the model do not necessarily stay there.                |
| MAXR     | forward selection to fit the best one-variable model, the best two-variable model, and so on. Variables are switched so that R square is maximized. |
| MINR     | similar to the MAXR method, except that variables are switched so that the increase in R square from adding a variable to the model is minimized.   |
| RSQUARE  | finds a specified number of models with the highest R square in a range of model sizes.                                                             |
| ADJRSQ   | finds a specified number of models with the highest adjusted R square in a range of model sizes.                                                    |
| CP       | finds a specified number of models with the lowest $C_p$ in a range of model sizes.                                                                 |

---

## Getting Started: REG Procedure

---

### Simple Linear Regression

Suppose that a response variable  $Y$  can be predicted by a linear function of a regressor variable  $X$ . You can estimate  $\beta_0$ , the intercept, and  $\beta_1$ , the slope, in

$$Y_i = \beta_0 + \beta_1 X_i + \epsilon_i$$

for the observations  $i = 1, 2, \dots, n$ . Fitting this model with the REG procedure requires only the following MODEL statement, where  $y$  is the outcome variable and  $x$  is the regressor variable.

```
proc reg;
 model y=x;
run;
```

For example, you might use regression analysis to find out how well you can predict a child's weight if you know that child's height. The CLASS data set used in this example is available in the Sashelp library.

The equation of interest is

$$\text{Weight} = \beta_0 + \beta_1 \text{Height} + \epsilon$$

The variable Weight is the response or dependent variable in this equation, and  $\beta_0$  and  $\beta_1$  are the unknown parameters to be estimated. The variable Height is the regressor or independent variable, and  $\epsilon$  is the unknown error. The following commands invoke the REG procedure and fit this model to the data.

```
ods graphics on;

proc reg data=sashelp.class;
 model Weight = Height;
run;

ods graphics off;
```

Figure 79.1 includes some information concerning model fit.

The  $F$  statistic for the overall model is highly significant ( $F = 57.076$ ,  $p < 0.0001$ ), indicating that the model explains a significant portion of the variation in the data.

The degrees of freedom can be used in checking accuracy of the data and model. The model degrees of freedom are one less than the number of parameters to be estimated. This model estimates two parameters,  $\beta_0$  and  $\beta_1$ ; thus, the degrees of freedom should be  $2 - 1 = 1$ . The corrected total degrees of freedom are always one less than the total number of observations in the data set, in this case  $19 - 1 = 18$ .

Several simple statistics follow the ANOVA table. The Root MSE is an estimate of the standard deviation of the error term. The coefficient of variation, or Coeff Var, is a unitless expression of the variation in the data. The R-square and Adj R-square are two statistics used in assessing the fit of the model; values close to 1 indicate a better fit. The R-square of 0.77 indicates that Height accounts for 77% of the variation in Weight.

**Figure 79.1** ANOVA Table

| The REG Procedure          |                |                |             |         |        |
|----------------------------|----------------|----------------|-------------|---------|--------|
| Model: MODEL1              |                |                |             |         |        |
| Dependent Variable: Weight |                |                |             |         |        |
| Analysis of Variance       |                |                |             |         |        |
| Source                     | DF             | Sum of Squares | Mean Square | F Value | Pr > F |
| Model                      | 1              | 7193.24912     | 7193.24912  | 57.08   | <.0001 |
| Error                      | 17             | 2142.48772     | 126.02869   |         |        |
| Corrected Total            | 18             | 9335.73684     |             |         |        |
|                            | Root MSE       | 11.22625       | R-Square    | 0.7705  |        |
|                            | Dependent Mean | 100.02632      | Adj R-Sq    | 0.7570  |        |
|                            | Coeff Var      | 11.22330       |             |         |        |

The “Parameter Estimates” table in [Figure 79.2](#) contains the estimates of  $\beta_0$  and  $\beta_1$ . The table also contains the  $t$  statistics and the corresponding  $p$ -values for testing whether each parameter is significantly different from zero. The  $p$ -values ( $t = -4.43$ ,  $p = 0.0004$  and  $t = 7.55$ ,  $p < 0.0001$ ) indicate that the intercept and Height parameter estimates, respectively, are highly significant.

From the parameter estimates, the fitted model is

$$\text{Weight} = -143.0 + 3.9 \times \text{Height}$$

**Figure 79.2** Parameter Estimates

| Parameter Estimates |    |                    |                |         |         |
|---------------------|----|--------------------|----------------|---------|---------|
| Variable            | DF | Parameter Estimate | Standard Error | t Value | Pr >  t |
| Intercept           | 1  | -143.02692         | 32.27459       | -4.43   | 0.0004  |
| Height              | 1  | 3.89903            | 0.51609        | 7.55    | <.0001  |

If ODS Graphics is enabled, then PROC REG produces a variety of plots. [Figure 79.3](#) shows a plot of the residuals versus the regressor and [Figure 79.4](#) shows a panel of diagnostic plots.

**Figure 79.3** Residuals vs. Regressor

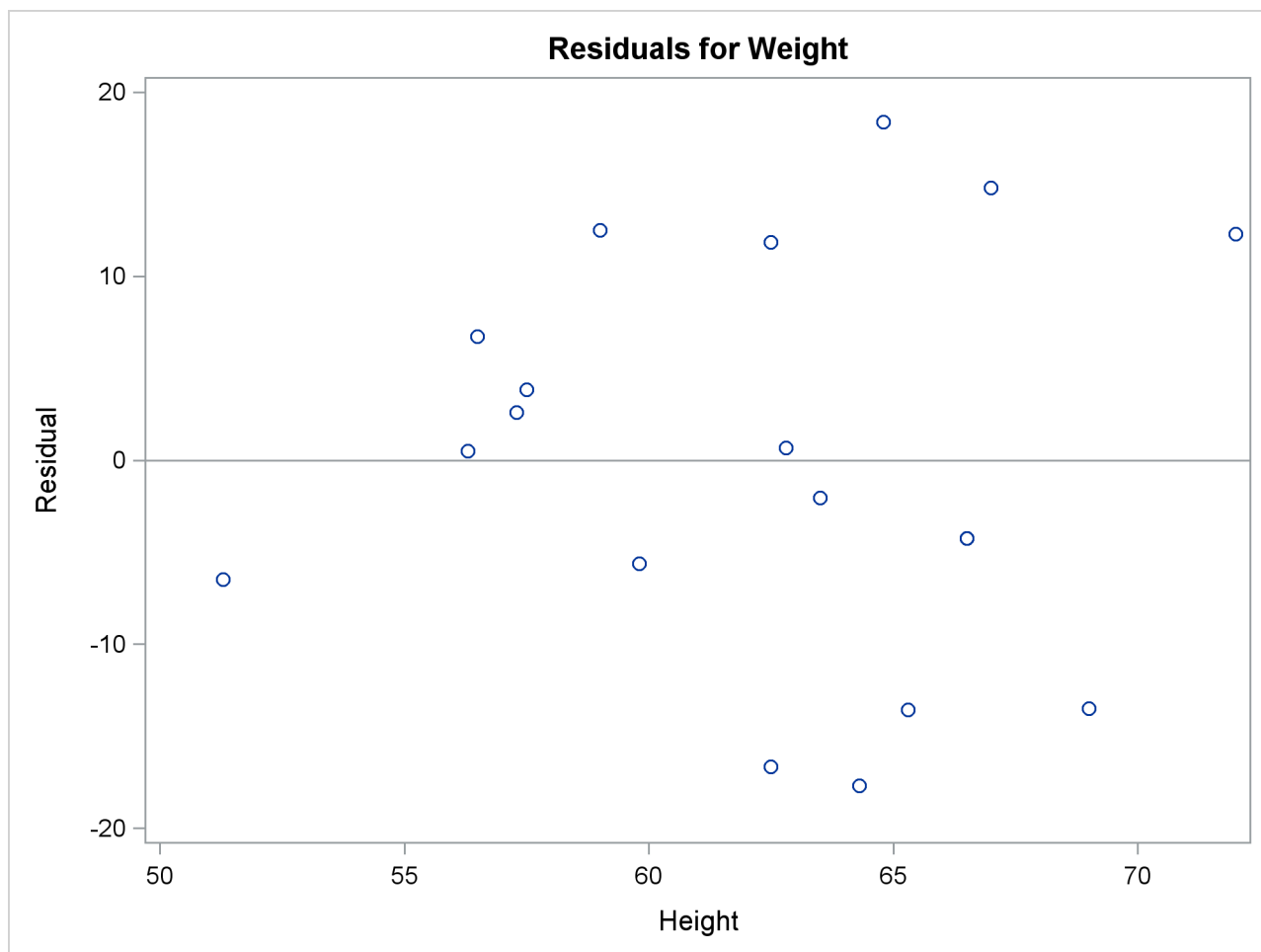
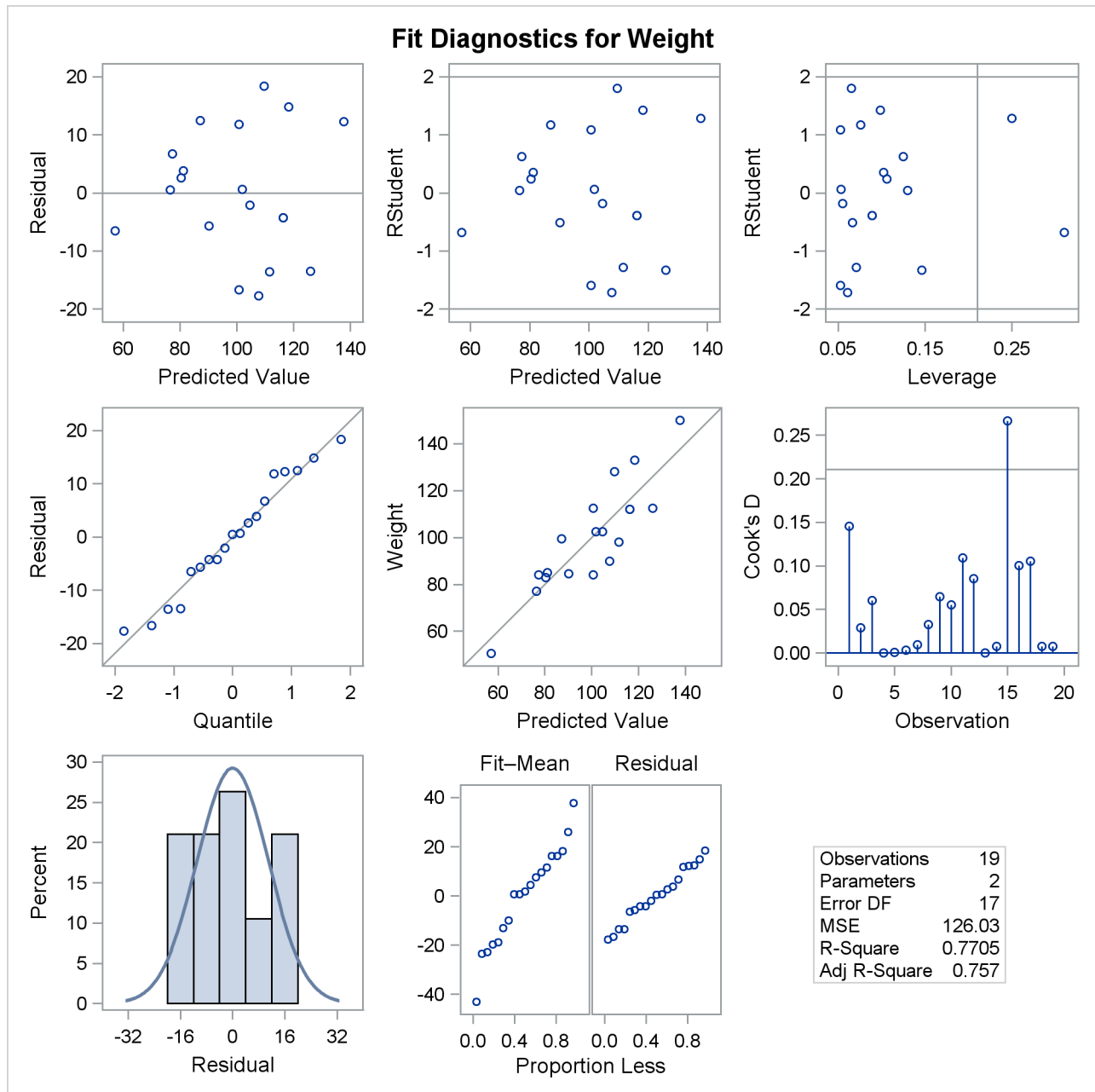


Figure 79.4 Fit Diagnostics



A trend in the residuals would indicate nonconstant variance in the data. The plot of residuals by predicted values in the upper-left corner of the diagnostics panel in Figure 79.4 might indicate a slight trend in the residuals; they appear to increase slightly as the predicted values increase. A fan-shaped trend might indicate the need for a variance-stabilizing transformation. A curved trend (such as a semicircle) might indicate the need for a quadratic term in the model. Since these residuals have no apparent trend, the analysis is considered to be acceptable.

## Polynomial Regression

Consider a response variable  $Y$  that can be predicted by a polynomial function of a regressor variable  $X$ . You can estimate  $\beta_0$ , the intercept;  $\beta_1$ , the slope due to  $X$ ; and  $\beta_2$ , the slope due to  $X^2$ , in

$$Y_i = \beta_0 + \beta_1 X_i + \beta_2 X_i^2 + \epsilon_i$$

for the observations  $i = 1, 2, \dots, n$ .

Consider the following example on population growth trends. The population of the United States from 1790 to 2000 is fit to linear and quadratic functions of time. Note that the quadratic term, `YearSq`, is created in the `DATA` step; this is done since polynomial effects such as `Year*Year` cannot be specified in the `MODEL` statement in `PROC REG`. The data are as follows:

```
data USPopulation;
 input Population @@;
 retain Year 1780;
 Year = Year+10;
 YearSq = Year*Year;
 Population = Population/1000;
 datalines;
3929 5308 7239 9638 12866 17069 23191 31443 39818 50155
62947 75994 91972 105710 122775 131669 151325 179323 203211
226542 248710 281422
;

ods graphics on;

proc reg data=USPopulation plots=ResidualByPredicted;
 var YearSq;
 model Population=Year / r clm cli;
run;
```

The `DATA` option ensures that the procedure uses the intended data set. Any variable that you might add to the model but that is not included in the first `MODEL` statement must appear in the `VAR` statement.

The “Analysis of Variance” and “Parameter Estimates” tables are displayed in [Figure 79.5](#).

Figure 79.5 ANOVA Table and Parameter Estimates

| The REG Procedure              |                |                    |                |         |         |
|--------------------------------|----------------|--------------------|----------------|---------|---------|
| Model: MODEL1                  |                |                    |                |         |         |
| Dependent Variable: Population |                |                    |                |         |         |
| Analysis of Variance           |                |                    |                |         |         |
| Source                         | DF             | Sum of Squares     | Mean Square    | F Value | Pr > F  |
| Model                          | 1              | 146869             | 146869         | 228.92  | <.0001  |
| Error                          | 20             | 12832              | 641.58160      |         |         |
| Corrected Total                | 21             | 159700             |                |         |         |
|                                | Root MSE       | 25.32946           | R-Square       | 0.9197  |         |
|                                | Dependent Mean | 94.64800           | Adj R-Sq       | 0.9156  |         |
|                                | Coeff Var      | 26.76175           |                |         |         |
| Parameter Estimates            |                |                    |                |         |         |
| Variable                       | DF             | Parameter Estimate | Standard Error | t Value | Pr >  t |
| Intercept                      | 1              | -2345.85498        | 161.39279      | -14.54  | <.0001  |
| Year                           | 1              | 1.28786            | 0.08512        | 15.13   | <.0001  |

The Model  $F$  statistic is significant ( $F = 228.92$ ,  $p < 0.0001$ ), indicating that the model accounts for a significant portion of variation in the data. The R-square indicates that the model accounts for 92% of the variation in population growth. The fitted equation for this model is

$$\text{Population} = -2345.85 + 1.29 \times \text{Year}$$

In the MODEL statement, three options are specified: R requests a residual analysis to be performed, CLI requests 95% confidence limits for an individual value, and CLM requests these limits for the expected value of the dependent variable. You can request specific  $100(1 - \alpha)\%$  limits with the ALPHA= option in the PROC REG or MODEL statement.

Figure 79.6 shows the “Output Statistics” table. The residual, its standard error, and the studentized residuals are displayed for each observation. The studentized residual is the residual divided by its standard error. The magnitude of each studentized residual is shown in a print plot. Studentized residuals follow a  $t$  distribution and can be used to identify outlying or extreme observations. Asterisks (\*) extending beyond the dashed lines indicate that the residual is more than three standard errors from zero. Many observations having absolute studentized residuals greater than two might indicate an inadequate model. Cook’s  $D$  is a measure of the change in the predicted values upon deletion of that observation from the data set; hence, it measures the influence of the observation on the estimated regression coefficients.



Figure 79.6 Output Statistics

| The REG Procedure              |                    |                 |                        |             |          |                |          |          |
|--------------------------------|--------------------|-----------------|------------------------|-------------|----------|----------------|----------|----------|
| Model: MODEL1                  |                    |                 |                        |             |          |                |          |          |
| Dependent Variable: Population |                    |                 |                        |             |          |                |          |          |
| Output Statistics              |                    |                 |                        |             |          |                |          |          |
| Obs                            | Dependent Variable | Predicted Value | Std Error Mean Predict | 95% CL Mean |          | 95% CL Predict |          | Residual |
| 1                              | 3.9290             | -40.5778        | 10.4424                | -62.3602    | -18.7953 | -97.7280       | 16.5725  | 44.5068  |
| 2                              | 5.3080             | -27.6991        | 9.7238                 | -47.9826    | -7.4156  | -84.2950       | 28.8968  | 33.0071  |
| 3                              | 7.2390             | -14.8205        | 9.0283                 | -33.6533    | 4.0123   | -70.9128       | 41.2719  | 22.0595  |
| 4                              | 9.6380             | -1.9418         | 8.3617                 | -19.3841    | 15.5004  | -57.5827       | 53.6991  | 11.5798  |
| 5                              | 12.8660            | 10.9368         | 7.7314                 | -5.1906     | 27.0643  | -44.3060       | 66.1797  | 1.9292   |
| 6                              | 17.0690            | 23.8155         | 7.1470                 | 8.9070      | 38.7239  | -31.0839       | 78.7148  | -6.7465  |
| 7                              | 23.1910            | 36.6941         | 6.6208                 | 22.8834     | 50.5048  | -17.9174       | 91.3056  | -13.5031 |
| 8                              | 31.4430            | 49.5727         | 6.1675                 | 36.7075     | 62.4380  | -4.8073        | 103.9528 | -18.1297 |
| 9                              | 39.8180            | 62.4514         | 5.8044                 | 50.3436     | 74.5592  | 8.2455         | 116.6573 | -22.6334 |
| 10                             | 50.1550            | 75.3300         | 5.5491                 | 63.7547     | 86.9053  | 21.2406        | 129.4195 | -25.1750 |
| 11                             | 62.9470            | 88.2087         | 5.4170                 | 76.9090     | 99.5084  | 34.1776        | 142.2398 | -25.2617 |
| 12                             | 75.9940            | 101.0873        | 5.4170                 | 89.7876     | 112.3870 | 47.0562        | 155.1184 | -25.0933 |
| 13                             | 91.9720            | 113.9660        | 5.5491                 | 102.3907    | 125.5413 | 59.8765        | 168.0554 | -21.9940 |
| 14                             | 105.7100           | 126.8446        | 5.8044                 | 114.7368    | 138.9524 | 72.6387        | 181.0505 | -21.1346 |
| 15                             | 122.7750           | 139.7233        | 6.1675                 | 126.8580    | 152.5885 | 85.3432        | 194.1033 | -16.9483 |
| 16                             | 131.6690           | 152.6019        | 6.6208                 | 138.7912    | 166.4126 | 97.9904        | 207.2134 | -20.9329 |
| 17                             | 151.3250           | 165.4805        | 7.1470                 | 150.5721    | 180.3890 | 110.5812       | 220.3799 | -14.1555 |
| 18                             | 179.3230           | 178.3592        | 7.7314                 | 162.2317    | 194.4866 | 123.1163       | 233.6020 | 0.9638   |
| 19                             | 203.2110           | 191.2378        | 8.3617                 | 173.7956    | 208.6801 | 135.5969       | 246.8787 | 11.9732  |
| 20                             | 226.5420           | 204.1165        | 9.0283                 | 185.2837    | 222.9493 | 148.0241       | 260.2088 | 22.4255  |
| 21                             | 248.7100           | 216.9951        | 9.7238                 | 196.7116    | 237.2786 | 160.3992       | 273.5910 | 31.7149  |
| 22                             | 281.4220           | 229.8738        | 10.4424                | 208.0913    | 251.6562 | 172.7235       | 287.0240 | 51.5482  |

| Output Statistics |                    |                  |             |      |  |          |
|-------------------|--------------------|------------------|-------------|------|--|----------|
| Obs               | Std Error Residual | Student Residual | -2 -1 0 1 2 |      |  | Cook's D |
| 1                 | 23.077             | 1.929            |             | ***  |  | 0.381    |
| 2                 | 23.389             | 1.411            |             | **   |  | 0.172    |
| 3                 | 23.666             | 0.932            |             | *    |  | 0.063    |
| 4                 | 23.909             | 0.484            |             |      |  | 0.014    |
| 5                 | 24.121             | 0.0800           |             |      |  | 0.000    |
| 6                 | 24.300             | -0.278           |             |      |  | 0.003    |
| 7                 | 24.449             | -0.552           |             | *    |  | 0.011    |
| 8                 | 24.567             | -0.738           |             | *    |  | 0.017    |
| 9                 | 24.655             | -0.918           |             | *    |  | 0.023    |
| 10                | 24.714             | -1.019           |             | **   |  | 0.026    |
| 11                | 24.743             | -1.021           |             | **   |  | 0.025    |
| 12                | 24.743             | -1.014           |             | **   |  | 0.025    |
| 13                | 24.714             | -0.890           |             | *    |  | 0.020    |
| 14                | 24.655             | -0.857           |             | *    |  | 0.020    |
| 15                | 24.567             | -0.690           |             | *    |  | 0.015    |
| 16                | 24.449             | -0.856           |             | *    |  | 0.027    |
| 17                | 24.300             | -0.583           |             | *    |  | 0.015    |
| 18                | 24.121             | 0.0400           |             |      |  | 0.000    |
| 19                | 23.909             | 0.501            |             | *    |  | 0.015    |
| 20                | 23.666             | 0.948            |             | *    |  | 0.065    |
| 21                | 23.389             | 1.356            |             | **   |  | 0.159    |
| 22                | 23.077             | 2.234            |             | **** |  | 0.511    |

Figure 79.7 shows the residual statistics table. A fairly close agreement between the PRESS statistic (see Table 79.9) and the Sum of Squared Residuals indicates that the MSE is a reasonable measure of the predictive accuracy of the fitted model (Neter, Wasserman, and Kutner 1990).

**Figure 79.7** Residual Statistics

|                               |       |
|-------------------------------|-------|
| Sum of Residuals              | 0     |
| Sum of Squared Residuals      | 12832 |
| Predicted Residual SS (PRESS) | 16662 |

Graphical representations are very helpful in interpreting the information in the “Output Statistics” table. When ODS Graphics is enabled, the REG procedure produces a default set of diagnostic plots that are appropriate for the requested analysis.

Figure 79.8 displays a panel of diagnostics plots. These diagnostics indicate an inadequate model:

- The plots of residual and studentized residual versus predicted value show a clear quadratic pattern.
- The plot of studentized residual versus leverage seems to indicate that there are two outlying data points. However, the plot of Cook’s  $D$  distance versus observation number reveals that these two points are just the data points for the endpoint years 1790 and 2000. These points show up as apparent outliers because the departure of the linear model from the underlying quadratic behavior in the data shows up most strongly at these endpoints.
- The normal quantile plot of the residuals and the residual histogram are not consistent with the assumption of Gaussian errors. This occurs as the residuals themselves still contain the quadratic behavior that is not captured by the linear model.
- The plot of the dependent variable versus the predicted value exhibits a quadratic form around the 45-degree line that represents a perfect fit.
- The “Residual-Fit” (or RF) plot consisting of side-by-side quantile plots of the centered fit and the residuals shows that the spread in the residuals is no greater than the spread in the centered fit. For inappropriate models, the spread of the residuals in such a plot is often greater than the spread of the centered fit. In this case, the RF plot shows that the linear model does indeed capture the increasing trend in the data, and hence accounts for much of the variation in the response.

Figure 79.8 Diagnostics Panel

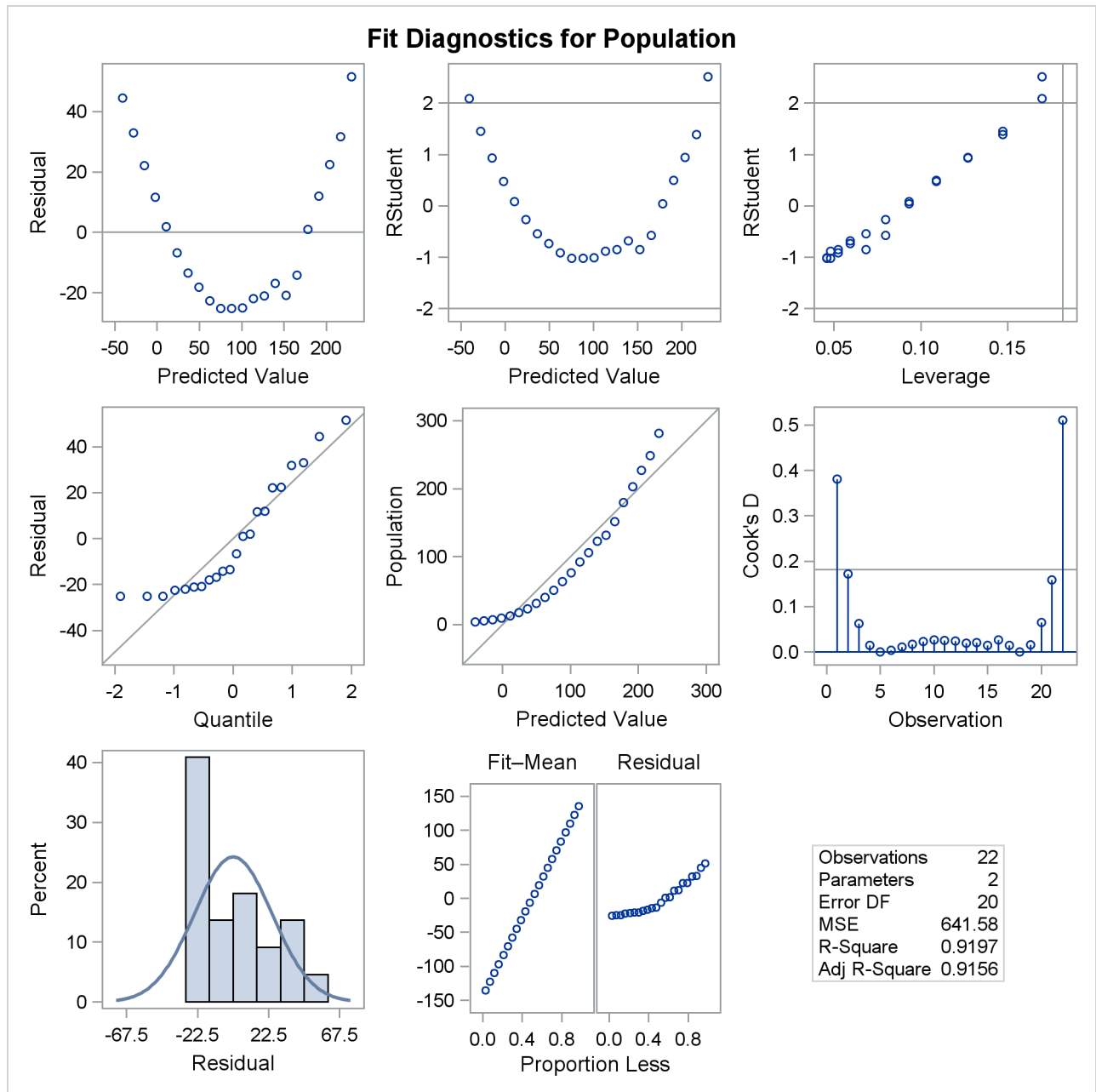


Figure 79.9 shows a plot of residuals versus Year. Again you can see the quadratic pattern that strongly indicates that a quadratic term should be added to the model.

**Figure 79.9** Residual Plot

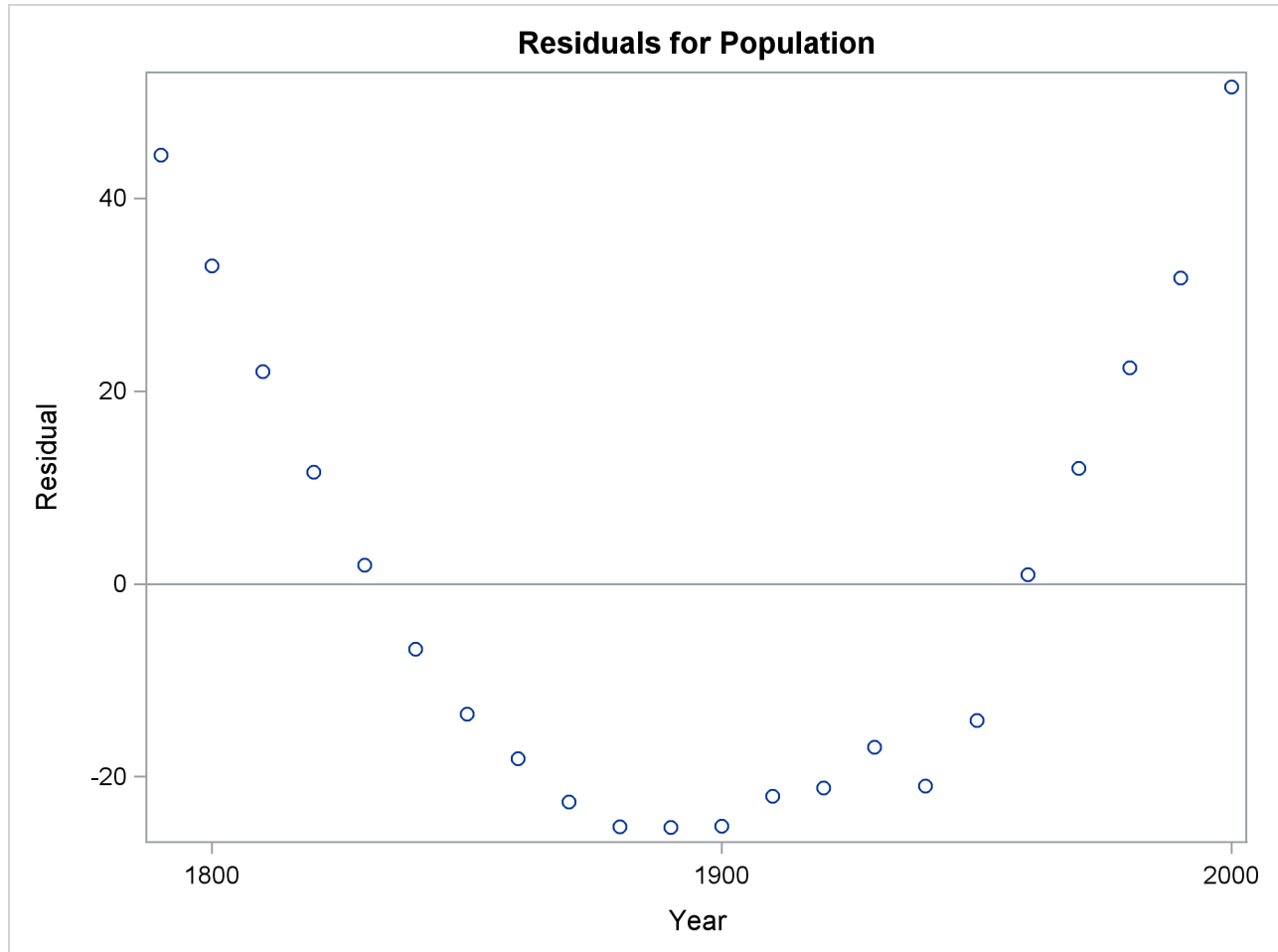
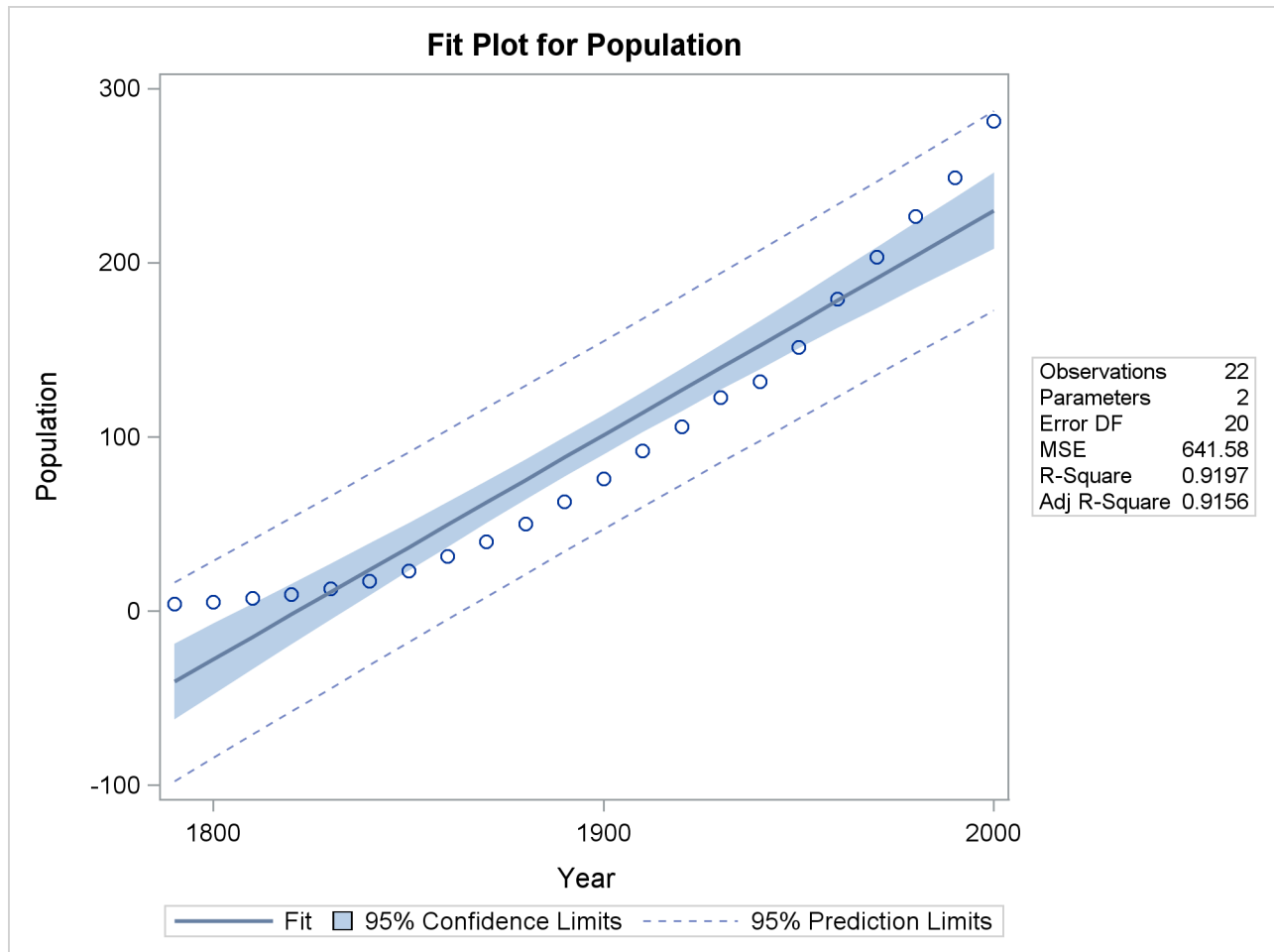


Figure 79.10 shows the “FitPlot” consisting of a scatter plot of the data overlaid with the regression line, and 95% confidence and prediction limits. Note that this plot also indicates that the model fails to capture the quadratic nature of the data. This plot is produced for models containing a single regressor. You can use the ALPHA= option in the model statement to change the significance level of the confidence band and prediction limits.

Figure 79.10 Fit Plot



These default plots provide strong evidence that the `Yearsq` needs to be added to the model. You can use the interactive feature of PROC REG to do this by specifying the following statements:

```
add Yearsq;
print;
run;
```

The ADD statement requests that `Yearsq` be added to the model, and the PRINT command causes the model to be refit and displays the ANOVA and parameter estimates for the new model. The print statement also produces updated ODS graphical displays.

Figure 79.11 displays the ANOVA table and parameter estimates for the new model.

Figure 79.11 ANOVA Table and Parameter Estimates

| Analysis of Variance |                |                    |                |         |         |
|----------------------|----------------|--------------------|----------------|---------|---------|
| Source               | DF             | Sum of Squares     | Mean Square    | F Value | Pr > F  |
| Model                | 2              | 159529             | 79765          | 8864.19 | <.0001  |
| Error                | 19             | 170.97193          | 8.99852        |         |         |
| Corrected Total      | 21             | 159700             |                |         |         |
|                      | Root MSE       | 2.99975            | R-Square       | 0.9989  |         |
|                      | Dependent Mean | 94.64800           | Adj R-Sq       | 0.9988  |         |
|                      | Coeff Var      | 3.16938            |                |         |         |
| Parameter Estimates  |                |                    |                |         |         |
| Variable             | DF             | Parameter Estimate | Standard Error | t Value | Pr >  t |
| Intercept            | 1              | 21631              | 639.50181      | 33.82   | <.0001  |
| Year                 | 1              | -24.04581          | 0.67547        | -35.60  | <.0001  |
| YearSq               | 1              | 0.00668            | 0.00017820     | 37.51   | <.0001  |

The overall  $F$  statistic is still significant ( $F = 8864.19$ ,  $p < 0.0001$ ). The R-square has increased from 0.9197 to 0.9989, indicating that the model now accounts for 99.9% of the variation in Population. All effects are significant with  $p < 0.0001$  for each effect in the model.

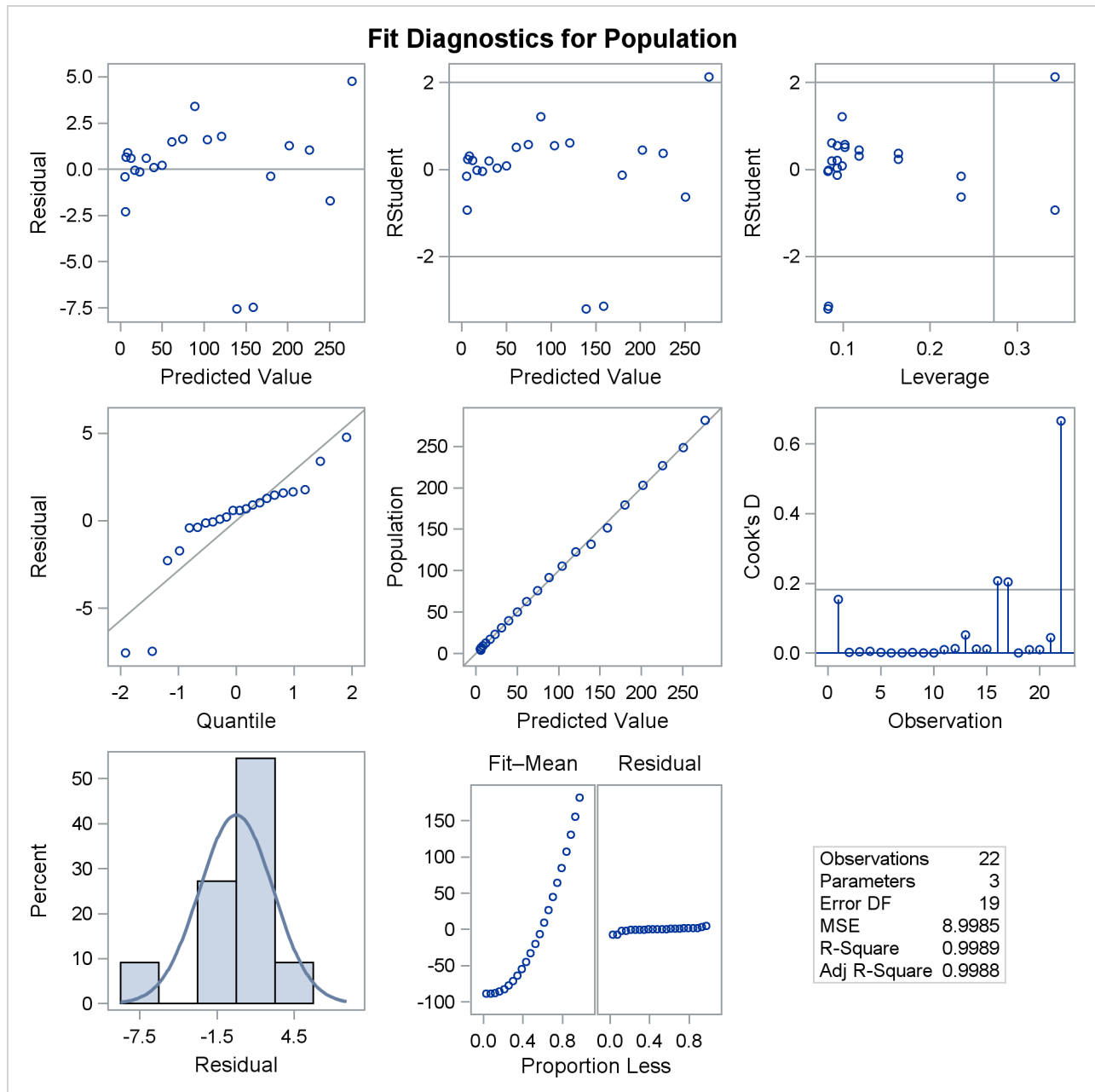
The fitted equation is now

$$\text{Population} = 21631 - 24.046 \times \text{Year} + 0.0067 \times \text{Yearsq}$$

Figure 79.12 show the panel of diagnostics for this quadratic polynomial model. These diagnostics indicate that this model is considerably more successful than the corresponding linear model:

- The plots of residuals and studentized residuals versus predicted values exhibit no obvious patterns.
- The points on the plot of the dependent variable versus the predicted values lie along a 45-degree line, indicating that the model successfully predicts the behavior of the dependent variable.
- The plot of studentized residual versus leverage shows that the years 1790 and 2000 are leverage points with 2000 showing up as an outlier. This is confirmed by the plot of Cook's  $D$  distance versus observation number. This suggests that while the quadratic model fits the current data well, the model might not be quite so successful over a wider range of data. You might want to investigate whether the population trend over the last couple of decades is growing slightly faster than quadratically.

Figure 79.12 Diagnostics Panel



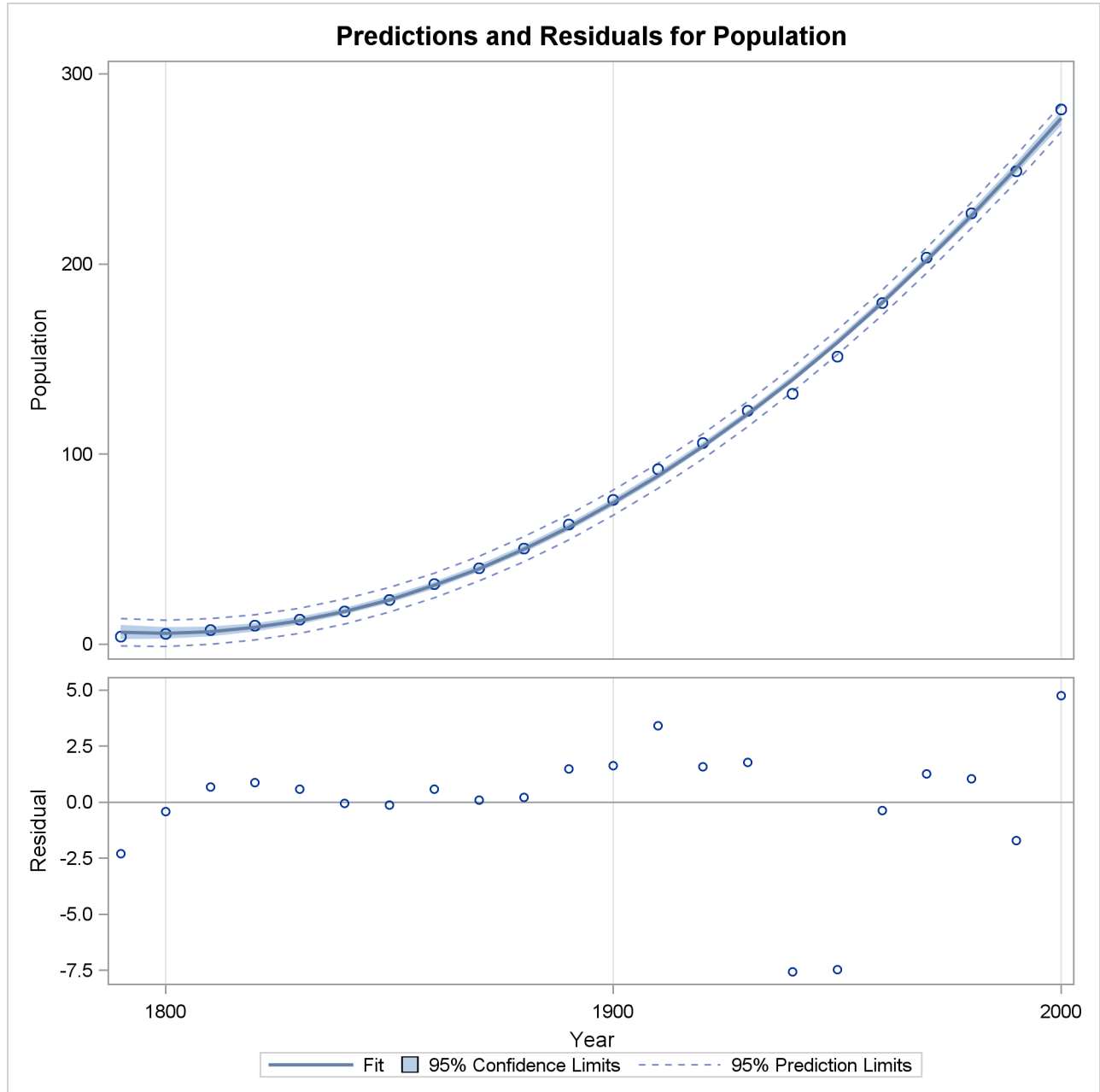
When a model contains more than one regressor, PROC REG does not produce a fit plot. However, when all the regressors in the model are functions of a single variable, it is appropriate to plot predictions and residuals as a function of that variable. You request such plots by using the PLOTS=PREDICTIONS option in the PROC REG statement, as the following code illustrates:

```
proc reg data=USPopulation plots=predictions(X=Year);
 model Population=Year Yearsq;
quit;

ods graphics off;
```

Figure 79.13 shows the data, predictions, and residuals by Year. These plots confirm that the quadratic polynomial model successfully model the growth in U.S. population between the years 1780 and 2000.

**Figure 79.13** Predictions and Residuals by Year



To complete an analysis of these data, you might want to examine influence statistics and, since the data are essentially time series data, examine the Durbin-Watson statistic.



---

## Using PROC REG Interactively

The REG procedure can be used interactively. After you specify a model with a MODEL statement and run PROC REG with a RUN statement, a variety of statements can be executed without reinvoking PROC REG.

The section “[Interactive Analysis](#)” on page 6697 describes which statements can be used interactively. These interactive statements can be executed singly or in groups by following the single statement or group of statements with a RUN statement. Note that the MODEL statement can be repeated. This is an important difference from the GLM procedure, which supports only one MODEL statement.

If you use PROC REG interactively, you can end the REG procedure with a DATA step, another PROC step, an ENDSAS statement, or a QUIT statement. The syntax of the QUIT statement is

```
quit;
```

When you are using PROC REG interactively, additional RUN statements do not end PROC REG but tell the procedure to execute additional statements.

When a BY statement is used with PROC REG, interactive processing is not possible; that is, once the first RUN statement is encountered, processing proceeds for each BY group in the data set, and no further statements are accepted by the procedure.

When you use PROC REG interactively, you can fit a model, perform diagnostics, and then refit the model and perform diagnostics on the refitted model. Most of the interactive statements implicitly refit the model; for example, if you use the ADD statement to add a variable to the model, the regression equation is automatically recomputed. The two exceptions to this automatic recomputing are the PAINT and REWEIGHT statements. These two statements do not cause the model to be refitted. To refit the model, you can follow these statements either with a REFIT statement, which causes the model to be explicitly recomputed, or with another interactive statement that causes the model to be implicitly recomputed.

## Syntax: REG Procedure

The following statements are available in the REG procedure:

```

PROC REG < options > ;
 < label: > MODEL dependents = < regressors > < / options > ;
 BY variables ;
 FREQ variable ;
 ID variables ;
 VAR variables ;
 WEIGHT variable ;
 ADD variables ;
 CODE < options > ;
 DELETE variables ;
 < label: > MTEST < equation, ..., equation > < / options > ;
 OUTPUT < OUT=SAS-data-set > < keyword=names > < ... keyword=names > ;
 PAINT < condition | ALLOBS > < / options > | < STATUS | UNDO > ;
 PLOT < yvariable* xvariable > < =symbol > < ... yvariable* xvariable > < =symbol > < / options > ;
 PRINT < options > < ANOVA > < MODELDATA > ;
 REFIT ;
 RESTRICT equation, ..., equation ;
 REWEIGHT < condition | ALLOBS > < / options > | < STATUS | UNDO > ;
 STORE < options > ;
 < label: > TEST equation, < , ..., equation > < / option > ;

```

Although there are numerous statements and options available in PROC REG, many analyses use only a few of them. Often you can find the features you need by looking at an example or by scanning this section.

In the preceding list, brackets denote optional specifications, and vertical bars denote a choice of one of the specifications separated by the vertical bars. In all cases, *label* is optional.

The PROC REG statement is required. To fit a model to the data, you must specify the MODEL statement. If you want to use only the options available in the PROC REG statement, you do not need a MODEL statement, but you must use a VAR statement. (See the example in the section “OUTSSCP= Data Sets” on page 6696.) Several MODEL statements can be used. In addition, several MTEST, OUTPUT, PAINT, PLOT, PRINT, RESTRICT, and TEST statements can follow each MODEL statement.

The ADD, DELETE, and REWEIGHT statements are used interactively to change the regression model and the data used in fitting the model. The ADD, DELETE, MTEST, OUTPUT, PLOT, PRINT, RESTRICT, and TEST statements implicitly refit the model; changes made to the model are reflected in the results from these statements. The REFIT statement is used to refit the model explicitly and is most helpful when it follows PAINT and REWEIGHT statements, which do not refit the model.

The **BY**, **FREQ**, **ID**, **VAR**, and **WEIGHT** statements are optionally specified once for the entire PROC step, and they must appear before the first RUN statement.

When a **TYPE=**CORR, **TYPE=**COV, or **TYPE=**SSCP data set is used as an input data set to **PROC REG**, statements and options that require the original data are not available. Specifically, the **OUTPUT**, **PAINT**, **PLOT**, and **REWEIGHT** statements and the **MODEL** and **PRINT** statement options **P**, **R**, **CLM**, **CLI**, **DW**, **DWPROB**, **INFLUENCE**, **PARTIAL**, and **PARTIALDATA** are disabled.

You can specify the following statements with the REG procedure in addition to the **PROC REG** statement:

|                 |                                                                                                                                                                                                                           |
|-----------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>ADD</b>      | adds independent variables to the regression model.                                                                                                                                                                       |
| <b>BY</b>       | specifies variables to define subgroups for the analysis.                                                                                                                                                                 |
| <b>CODE</b>     | requests that the procedure write SAS DATA step code to a file or catalog entry for computing predicted values according to the fitted model.                                                                             |
| <b>DELETE</b>   | deletes independent variables from the regression model.                                                                                                                                                                  |
| <b>FREQ</b>     | specifies a frequency variable.                                                                                                                                                                                           |
| <b>ID</b>       | names a variable to identify observations in the tables.                                                                                                                                                                  |
| <b>MODEL</b>    | specifies the dependent and independent variables in the regression model, requests a model selection method, displays predicted values, and provides details on the estimates (according to which options are selected). |
| <b>MTEST</b>    | performs multivariate tests across multiple dependent variables.                                                                                                                                                          |
| <b>OUTPUT</b>   | creates an output data set and names the variables to contain predicted values, residuals, and other diagnostic statistics.                                                                                               |
| <b>PAINT</b>    | paints points in scatter plots.                                                                                                                                                                                           |
| <b>PLOT</b>     | generates scatter plots.                                                                                                                                                                                                  |
| <b>PRINT</b>    | displays information about the model and can reset options.                                                                                                                                                               |
| <b>REFIT</b>    | refits the model.                                                                                                                                                                                                         |
| <b>RESTRICT</b> | places linear equality restrictions on the parameter estimates.                                                                                                                                                           |
| <b>REWEIGHT</b> | excludes specific observations from analysis or changes the weights of observations used.                                                                                                                                 |
| <b>STORE</b>    | requests that the procedure save the estimated parameters of the fitted model.                                                                                                                                            |
| <b>TEST</b>     | performs an <i>F</i> test on linear functions of the parameters.                                                                                                                                                          |
| <b>VAR</b>      | lists variables for which crossproducts are to be computed, variables that can be interactively added to the model, or variables to be used in scatter plots.                                                             |
| <b>WEIGHT</b>   | declares a variable to weight observations.                                                                                                                                                                               |

The **CODE** and **STORE** statements are also used by many other procedures. A summary description of functionality and syntax for these statements is also shown after the **PROC REG** statement in alphabetical order, but you can find full documentation about them in the section “**STORE Statement**” on page 501 of Chapter 19, “**Shared Concepts and Topics**.”

## PROC REG Statement

**PROC REG** < options > ;

The PROC REG statement invokes the REG procedure. The PROC REG statement is required. If you want to fit a model to the data, you must also use a **MODEL** statement. If you want to use only the PROC REG options, you do not need a **MODEL** statement, but you must use a **VAR** statement. If you do not use a **MODEL** statement, then the COVOUT and OUTEST= options are not available.

Table 79.1 summarizes the options available in the PROC REG statement. Note that any option specified in the PROC REG statement applies to all **MODEL** statements.

**Table 79.1** PROC REG Statement Options

| Option                              | Description                                                                                                                   |
|-------------------------------------|-------------------------------------------------------------------------------------------------------------------------------|
| <b>Data Set Options</b>             |                                                                                                                               |
| DATA=                               | Names a data set to use for the regression                                                                                    |
| OUTEST=                             | Outputs a data set that contains parameter estimates and other model fit summary statistics                                   |
| OUTSSCP=                            | Outputs a data set that contains sums of squares and crossproducts                                                            |
| COVOUT                              | Outputs the covariance matrix for parameter estimates to the OUTEST= data set                                                 |
| EDF                                 | Outputs the number of regressors, the error degrees of freedom, and the model R square to the OUTEST= data set                |
| OUTSEB                              | Outputs standard errors of the parameter estimates to the OUTEST= data set                                                    |
| OUTSTB                              | Outputs standardized parameter estimates to the OUTEST= data set. Use only with the RIDGE= or PCOMIT= option.                 |
| OUTVIF                              | Outputs the variance inflation factors to the OUTEST= data set. Use only with the RIDGE= or PCOMIT= option.                   |
| PCOMIT=                             | Performs incomplete principal component analysis and outputs estimates to the OUTEST= data set                                |
| PRESS                               | Outputs the PRESS statistic to the OUTEST= data set                                                                           |
| RIDGE=                              | Performs ridge regression analysis and outputs estimates to the OUTEST= data set                                              |
| RSQUARE                             | Same effect as the EDF option                                                                                                 |
| TABLEOUT                            | Outputs standard errors, confidence limits, and associated test statistics of the parameter estimates to the OUTEST= data set |
| <b>ODS Graphics Options</b>         |                                                                                                                               |
| PLOTS=                              | Produces ODS graphical displays                                                                                               |
| <b>Traditional Graphics Options</b> |                                                                                                                               |
| ANNOTATE=                           | Specifies an annotation data set                                                                                              |
| GOUT=                               | Specifies the graphics catalog in which graphics output is saved                                                              |
| <b>Display Options</b>              |                                                                                                                               |
| CORR                                | Displays correlation matrix for variables listed in <b>MODEL</b> and <b>VAR</b> statements                                    |

Table 79.1 *continued*

| Option               | Description                                                                                   |
|----------------------|-----------------------------------------------------------------------------------------------|
| <b>SIMPLE</b>        | Displays simple statistics for each variable listed in <b>MODEL</b> and <b>VAR</b> statements |
| <b>USSCP</b>         | Displays uncorrected sums of squares and crossproducts matrix                                 |
| <b>ALL</b>           | Displays all statistics ( <b>CORR</b> , <b>SIMPLE</b> , and <b>USSCP</b> )                    |
| <b>NOPRINT</b>       | Suppresses output                                                                             |
| <b>LINEPRINTER</b>   | Creates printer plots                                                                         |
| <b>Other Options</b> |                                                                                               |
| <b>ALPHA=</b>        | Sets significance value for confidence and prediction intervals and tests                     |
| <b>SINGULAR=</b>     | Sets criterion for checking for singularity                                                   |

Following are explanations of the options that you can specify in the **PROC REG** statement (in alphabetical order).

Note that any option specified in the **PROC REG** statement applies to all **MODEL** statements.

#### **ALL**

requests the display of many tables. Using the **ALL** option in the **PROC REG** statement is equivalent to specifying **ALL** in every **MODEL** statement. The **ALL** option also implies the **CORR**, **SIMPLE**, and **USSCP** options.

#### **ALPHA=number**

sets the significance level used for the construction of confidence intervals. The value must be between 0 and 1; the default value of 0.05 results in 95% intervals. This option affects the **PROC REG** option **TABLEOUT**; the **MODEL** options **CLB**, **CLI**, and **CLM**; the **OUTPUT** statement keywords **LCL**, **LCLM**, **UCL**, and **UCLM**; the **PLOT** statement keywords **LCL.**, **LCLM.**, **UCL.**, and **UCLM.**; and the **PLOT** statement options **CONF** and **PRED**.

#### **ANNOTATE=SAS-data-set**

#### **ANNO=SAS-data-set**

specifies an input data set containing annotate variables, as described in *SAS/GRAPH: Reference*. You can use this data set to add features to the traditional graphics that you request with the **PLOT** statement. Features provided in this data set are applied to all plots produced in the current run of **PROC REG**. To add features to individual plots, use the **ANNOTATE=** option in the **PLOT** statement. This option cannot be used if the **LINEPRINTER** option is specified.

#### **CORR**

displays the correlation matrix for all variables listed in the **MODEL** or **VAR** statement.

#### **COVOUT**

outputs the covariance matrices for the parameter estimates to the **OUTEST=** data set. This option is valid only if the **OUTEST=** option is also specified. See the section “**OUTEST= Data Set**” on page 6690.

**DATA=SAS-data-set**

names the SAS data set to be used by PROC REG. The data set can be an ordinary SAS data set or a TYPE=CORR, TYPE=COV, or TYPE=SSCP data set. If one of these special TYPE= data sets is used, the **OUTPUT**, **PAINT**, **PLOT**, and **REWEIGHT** statements, ODS Graphics, and some options in the **MODEL** and **PRINT** statements are not available. See Appendix A, “Special SAS Data Sets,” for more information about TYPE= data sets. If the DATA= option is not specified, PROC REG uses the most recently created SAS data set.

**EDF**

outputs the number of regressors in the model excluding and including the intercept, the error degrees of freedom, and the model R square to the OUTEST= data set.

**GOUT=graphics-catalog**

specifies the graphics catalog in which traditional graphics output is saved. The default *graphics-catalog* is WORK.GSEG. The GOUT= option cannot be used if the **LINEPRINTER** option is specified.

**LINEPRINTER | LP**

creates printer plots. If you do not specify this option, requested plots are created on a high-resolution graphics device. See the **PLOTS=** option for information about using ODS graphics to create modern statistical graphics.

**NOPRINT**

suppresses the normal display of results. Note that this option temporarily disables the Output Delivery System (ODS); see Chapter 20, “Using the Output Delivery System,” for more information.

**OUTEST=SAS-data-set**

requests that parameter estimates and optional model fit summary statistics be output to this data set. See the section “**OUTEST= Data Set**” on page 6690 for details. If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*.

**OUTSEB**

outputs the standard errors of the parameter estimates to the OUTEST= data set. The value SEB for the variable `_TYPE_` identifies the standard errors. If the **RIDGE=** or **PCOMIT=** option is specified, additional observations are included and identified by the values **RIDGESEB** and **IPCSEB**, respectively, for the variable `_TYPE_`. The standard errors for ridge regression estimates and IPC estimates are limited in their usefulness because these estimates are biased. This option is available for all model selection methods except **RSQUARE**, **ADJRSQ**, and **CP**.

**OUTSSCP=SAS-data-set**

requests that the sums of squares and crossproducts matrix be output to this TYPE=SSCP data set. See the section “**OUTSSCP= Data Sets**” on page 6696 for details. If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*.

**OUTSTB**

outputs the standardized parameter estimates as well as the usual estimates to the OUTEST= data set when the **RIDGE=** or **PCOMIT=** option is specified. The values **RIDGESTB** and **IPCSTB** for the variable `_TYPE_` identify ridge regression estimates and IPC estimates, respectively.

**OUTVIF**

outputs the variance inflation factors (VIF) to the OUTEST= data set when the RIDGE= or PCOMIT= option is specified. The factors are the diagonal elements of the inverse of the correlation matrix of regressors as adjusted by ridge regression or IPC analysis. These observations are identified in the output data set by the values RIDGEVIF and IPCVIF for the variable `_TYPE_`.

**PCOMIT=*list***

requests an incomplete principal component (IPC) analysis for each value *m* in the list. The procedure computes parameter estimates by using all but the last *m* principal components. Each value of *m* produces a set of IPC estimates, which are output to the OUTEST= data set. The values of *m* are saved by the variable `_PCOMIT_`, and the value of the variable `_TYPE_` is set to IPC to identify the estimates. Only nonnegative integers can be specified with the PCOMIT= option.

If you specify the PCOMIT= option, **RESTRICT** statements are ignored.

**PLOTS** <(global-plot-options)> <= plot-request <(options)>>

**PLOTS** <(global-plot-options)> <= (plot-request <(options)> <... plot-request <(options)>>>

controls the plots produced through ODS Graphics. When you specify only one plot request, you can omit the parentheses around the plot request. Here are some examples:

```
plots = none
plots = diagnostics (unpack)
plots = (all fit (stats)=none)
plots (label) = (rstudentbyleverage cooks)
plots (only) = (diagnostics (stats=all) fit (nocli stats=(aic sbc)))
```

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;

proc reg;
 model y = x1-x10;
run;

proc reg plots=diagnostics(stats=(default aic sbc));
 model y = x1-x10;
run;

ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

If ODS Graphics is enabled but you do not specify the PLOTS= option, then PROC REG produces a default set of plots. Table 79.2 lists the default set of plots produced.

**Table 79.2** Default Graphs Produced

| Plot             | Conditional On                                         |
|------------------|--------------------------------------------------------|
| DiagnosticsPanel | Unconditional                                          |
| ResidualPlot     | Unconditional                                          |
| FitPlot          | Model with one regressor (excluding intercept)         |
| PartialPlot      | PARTIAL option specified in MODEL statement            |
| RidgePanel       | RIDGE= option specified in PROC REG or MODEL statement |

For models with multiple dependent variables, separate plots are produced for each dependent variable. For jobs with more than one MODEL statement, plots are produced for each model statement.

The *global-options* apply to all plots generated by the REG procedure, unless it is altered by a *specific-plot-option*. The following global plot options are available:

**LABEL**

specifies that the LABEL option be applied to each plot that supports a LABEL option. See the descriptions of the specific plots for details.

**MAXPOINTS=NONE** | *max* < *heat-max* >

suppresses most plots that require processing more than *max* points. When the number of points exceeds *max* but does not exceed *heat-max* divided by the number of independent variables, heat maps are displayed instead of scatter plots for the fit and residual plots. All other plots are suppressed when the number of points exceeds *max*. The default is MAXPOINTS=5000 150000. These cutoffs are ignored if you specify MAXPOINTS=NONE.

**NOTE:** Heat maps are experimental in this release.

**MODELLABEL**

requests that the model label be displayed in the upper-left corner of all plots. This option is useful when you use more than one MODEL statement.

**ONLY**

suppress the default plots. Only plots specifically requested are displayed.

**STATS=ALL** | **DEFAULT** | **NONE** | (*plot-statistics*)

requests statistics that are included on the fit plot and diagnostics panel. Table 79.3 lists the statistics that you can request. STATS=ALL requests all these statistics; STATS=NONE suppresses them.

**Table 79.3** Statistics Available on Plots

| Keyword  | Default | Description                           |
|----------|---------|---------------------------------------|
| ADJRSQ   | x       | adjusted R-square                     |
| AIC      |         | Akaike's information criterion        |
| BIC      |         | Sawa's Bayesian information criterion |
| CP       |         | Mallows' $C_p$ statistic              |
| COEFFVAR |         | coefficient of variation              |
| DEPMEAN  |         | mean of dependent                     |



Table 79.3 *continued*

| Keyword | Default | Description                                                  |
|---------|---------|--------------------------------------------------------------|
| DEFAULT |         | all default statistics                                       |
| EDF     | x       | error degrees of freedom                                     |
| GMSEP   |         | estimated MSE of prediction, assuming multivariate normality |
| JP      |         | final prediction error                                       |
| MSE     | x       | mean squared error                                           |
| NOBS    | x       | number of observations used                                  |
| NPARM   | x       | number of parameters in the model (including the intercept)  |
| PC      |         | Amemiya's prediction criterion                               |
| RSQUARE | x       | R-square                                                     |
| SBC     |         | SBC statistic                                                |
| SP      |         | SP statistic                                                 |
| SSE     |         | error sum of squares                                         |

You request statistics in addition to the default set by including the keyword `DEFAULT` in the *plot-statistics* list.

**UNPACK**

suppresses paneling.

**USEALL**

specifies that predicted values at data points with missing dependent variable(s) be included on appropriate plots. By default, only points used in constructing the SSCP matrix appear on plots.

The following specific plots are available:

**ADJRSQ** <(adjrsq-options)>

displays the adjusted R-square values for the models examined when you request variable selection with the `SELECTION=` option in the `MODEL` statement.

The following *adjrsq-options* are available for models where you request the `RSQUARE`, `ADJRSQ`, or `CP` selection method:

**LABEL**

requests that the model number corresponding to the one displayed in the “Subset Selection Summary” table be used to label the model with the largest adjusted R-square statistic at each value of the number of parameters.

**LABELVARS**

requests that the list (excluding the intercept) of the regressors in the relevant model be used to label the model with the largest adjusted R-square statistic at each value of the number of parameters.

**AIC** <(aic-options)>

displays Akaike's information criterion (AIC) for the models examined when you request variable selection with the SELECTION= option in the **MODEL** statement.

The following *aic-options* are available for models where you request the RSQUARE, ADJRSQ, or CP selection method:

**LABEL**

requests that the model number corresponding to the one displayed in the "Subset Selection Summary" table be used to label the model with the smallest AIC statistic at each value of the number of parameters.

**LABELVARS**

requests that the list (excluding the intercept) of the regressors in the relevant model be used to label the model with the smallest AIC statistic at each value of the number of parameters.

**ALL**

produces all appropriate plots.

**BIC** <(bic-options)>

displays Sawa's Bayesian information criterion (BIC) for the models examined when you request variable selection with the SELECTION= option in the **MODEL** statement.

The following *bic-options* are available for models where you request the RSQUARE, ADJRSQ, or CP selection method:

**LABEL**

requests that the model number corresponding to the one displayed in the "Subset Selection Summary" table be used to label the model with the smallest BIC statistic at each value of the number of parameters.

**LABELVARS**

requests that the list (excluding the intercept) of the regressors in the relevant model be used to label the model with the smallest BIC statistic at each value of the number of parameters.

**COOKSD** <(LABEL)>

plots Cook's  $D$  statistic by observation number. Observations whose Cook's  $D$  statistic lies above the horizontal reference line at value  $4/n$ , where  $n$  is the number of observations used, are deemed to be influential (Rawlings, Pantula, and Dickey 1998). If you specify the LABEL option, then points deemed as influential are labeled. If you do not specify an ID variable, the observation number within the current BY group is used as the label. If you specify one or more ID variables in one or more ID statements, then the first ID variable you specify is used for the labeling.

**CP** <(cp-options)>

displays Mallows'  $C_p$  statistic for the models examined when you request variable selection with the SELECTION= option in the **MODEL** statement. For models where you request the RSQUARE, ADJRSQ, or CP selection, reference lines corresponding to the equations  $C_p = p$  and  $C_p = 2p - p_{full}$ , where  $p_{full}$  is the number of parameters in the full model (excluding the intercept) and  $p$  is the number of parameters in the subset model (including the intercept), are displayed on the plot of  $C_p$  versus  $p$ . For the purpose of parameter estimation, Hocking (1976)

suggests selecting a model where  $C_p \leq 2p - p_{full}$ . For the purpose of prediction, Hocking suggests the criterion  $C_p \leq p$ . Mallows (1973) suggests that all subset models with  $C_p$  small and near  $p$  be considered for further study.

The following *cp-options* are available for models where you request the RSQUARE, ADJRSQ, or CP selection method:

#### **LABEL**

requests that the model number corresponding to the one displayed in the “Subset Selection Summary” table be used to label the model with the smallest  $C_p$  statistic at each value of the number of parameters.

#### **LABELVARS**

requests that the list (excluding the intercept) of the regressors in the relevant model be used to label the model with the smallest  $C_p$  statistic at each value of the number of parameters.

#### **CRITERIA | CRITERIONPANEL <(criteria-options)>**

produces a panel of fit criteria for the models examined when you request variable selection with the SELECTION= option in the MODEL statement. The fit criteria displayed are R-square, adjusted R-square, Mallows’  $C_p$ , Akaike’s information criterion (AIC), Sawa’s Bayesian information criterion (BIC), and Schwarz’s Bayesian information criterion (SBC). For SELECTION=RSQUARE, SELECTION=ADJRSQ, or SELECTION=CP, scatter plots of these statistics versus the number of parameters (including the intercept) are displayed. For other selection methods, line plots of these statistics as function of the selection step number are displayed.

The following *criteria-options* are available:

#### **LABEL**

requests that the model number corresponding to the one displayed in the “Subset Selection Summary” table be used to label the best model at each value of the number of parameters. This option applies only to the RSQUARE, ADJRSQ, and CP selection methods.

#### **LABELVARS**

requests that the list (excluding the intercept) of the regressors in the relevant model be used to label the best model at each value of the number of parameters. Since these labels are typically long, LABELVARS is supported only when the panel is unpacked. This option applies only to the RSQUARE, ADJRSQ, and CP selection methods.

#### **UNPACK**

suppresses paneling. Separate plots are produced for each of the six fit statistics. For models where you request the RSQUARE, ADJRSQ, or CP selection, two reference lines corresponding to the equations  $C_p = p$  and  $C_p = 2p - p_{full}$ , where  $p_{full}$  is the number of parameters in the full model (excluding the intercept) and  $p$  is the number of parameters in the subset model (including the intercept), are displayed on the plot of  $C_p$  versus  $p$ . For the purpose of parameter estimation, Hocking (1976) suggests selecting a model where  $C_p \leq 2p - p_{full}$ . For the purpose of prediction, Hocking suggests the criterion  $C_p \leq p$ . Mallows (1973) suggests that all subset models with  $C_p$  small and near  $p$  be considered for further study.

**DFBETAS** <(DFBETAS-options)>

produces panels of DFBETAS by observation number for the regressors in the model. Note that each panel contains at most six plots, and multiple panels are used in the case where there are more than six regressors (including the intercept) in the model. Observations whose DFBETAS' statistics for a regressor are greater in magnitude than  $2/\sqrt{n}$ , where  $n$  is the number of observations used, are deemed to be influential for that regressor (Rawlings, Pantula, and Dickey 1998).

The following *DFBETAS-options* are available:

**COMMONAXES**

specifies that the same DFBETAS axis be used in all panels when multiple panels are needed. By default, the DFBETAS axis is chosen independently for each panel. If you also specify the UNPACK option, then the same DFBETAS axis is used for each regressor.

**LABEL**

specifies that observations whose magnitude are greater than  $2/\sqrt{n}$  be labeled. If you do not specify an ID variable, the observation number within the current BY group is used as the label. If you specify one or more ID variables on one or more ID statements, then the first ID variable you specify is used for the labeling.

**UNPACK**

suppresses paneling. The DFBETAS statistics for each regressor are displayed on separate plots.

**DFFITS** <(LABEL)>

plots the DFFITS statistic by observation number. Observations whose DFFITS' statistic is greater in magnitude than  $2\sqrt{p/n}$ , where  $n$  is the number of observations used and  $p$  is the number of regressors, are deemed to be influential (Rawlings, Pantula, and Dickey 1998). If you specify the LABEL option, then these influential observations are labeled. If you do not specify an ID variable, the observation number within the current BY group is used as the label. If you specify one or more ID variables in one or more ID statements, then the first ID variable you specify is used for the labeling.

**DIAGNOSTICS** <(diagnostics-options)>

produces a summary panel of fit diagnostics:

- residuals versus the predicted values
- studentized residuals versus the predicted values
- studentized residuals versus the leverage
- normal quantile plot of the residuals
- dependent variable values versus the predicted values
- Cook's  $D$  versus observation number
- histogram of the residuals
- "Residual-Fit" (or RF) plot consisting of side-by-side quantile plots of the centered fit and the residuals
- box plot of the residuals if you specify the STATS=NONE suboption

You can specify the following *diagnostics-options*:

**STATS=stats-options**

determines which model fit statistics are included in the panel. See the global STATS= suboption for details. The PLOTS= suboption of the DIAGNOSTICSPANEL option overrides the global PLOTS= suboption.

**UNPACK**

produces the eight plots in the panel as individual plots. Note that you can also request individual plots in the panel by name without having to unpack the panel.

**FITPLOT | FIT <(fit-options)>**

produces a scatter plot of the data overlaid with the regression line, confidence band, and prediction band for models that depend on at most one regressor excluding the intercept. When the number of points exceeds the MAXPOINTS=*max* value, a heat map is displayed instead of a scatter plot. By default, heat maps are not displayed if the number of observations times the number of independent variables is greater than 150,000. See the MAXPOINTS= option.

You can specify the following *fit-options*:

**NOCLI**

suppresses the prediction limits.

**NOCLM**

suppresses the confidence limits.

**NOLIMITS**

suppresses the confidence and prediction limits.

**STATS=stats-options**

determines which model fit statistics are included in the panel. See the global STATS= suboption for details. The PLOTS= suboption of the FITPLOT option overrides the global PLOTS= suboption.

**OBSERVEDBYPREDICTED <(LABEL)>**

plots dependent variable values by the predicted values. If you specify the LABEL option, then points deemed as outliers or influential (see the RSTUDENTBYLEVERAGE option for details) are labeled.

**NONE**

suppresses all plots.

**PARTIAL <(UNPACK)>**

produces panels of partial regression plots for each regressor with at most six regressors per panel. If you specify the UNPACK option, then all partial plot panels are unpacked.

**PREDICTIONS (X=numeric-variable <prediction-options>)**

produces a panel of two plots whose horizontal axis is the variable you specify in the required X= suboption. The upper plot in the panel is a scatter plot of the residuals. The lower plot shows the data overlaid with the regression line, confidence band, and prediction band. This plot is appropriate for models where all regressors are known to be functions of the single variable that you specify in the X= suboption.

You can specify the following *prediction-options*:

**NOCLI**

suppresses the prediction limits.

**NOCLM**

suppresses the confidence limits

**NOLIMITS**

suppresses the confidence and prediction limits

**SMOOTH**

requests a nonparametric smoothing of the residuals as a function of the variable you specify in the X= suboption. This nonparametric fit is a loess fit that uses local linear polynomials, linear interpolation, and a smoothing parameter that is selected to yield a local minimum of the corrected Akaike's information criterion (AICC). See Chapter 53, "The LOESS Procedure," for details. The SMOOTH option is not supported when a **FREQ** statement is used.

**UNPACK**

suppresses paneling.

**QQPLOT | QQ**

produces a normal quantile plot of the residuals.

**RESIDUALBOXPLOT | BOXPLOT <(LABEL)>**

produces a box plot consisting of the residuals. If you specify label option, points deemed far-outliers are labeled. If you do not specify an ID variable, the observation number within the current BY group is used as the label. If you specify one or more ID variables in one or more ID statements, then the first ID variable you specify is used for the labeling.

**RESIDUALBYPREDICTED <(LABEL)>**

plots residuals by predicted values. If you specify the LABEL option, then points deemed as outliers or influential (see the RSTUDENTBYLEVERAGE option for details) are labeled.

**RESIDUALS <(residual-options)>**

produces panels of the residuals versus the regressors in the model. Each panel contains at most six plots, and multiple panels are used when the model contains more than six regressors (including the intercept). When the number of points exceeds the **MAXPOINTS=max** value, a heat map is displayed instead of a scatter plot. By default, heat maps are not displayed if the number of observations times the number of independent variables is greater than 150,000. See the **MAXPOINTS=** option. You can specify the following *residual-options*:

**SMOOTH**

requests a nonparametric smoothing of the residuals for each regressor. Each nonparametric fit is a loess fit that uses local linear polynomials, linear interpolation, and a smoothing parameter that is selected to yield a local minimum of the corrected Akaike's information criterion (AICC). See Chapter 53, "The LOESS Procedure," for details. The SMOOTH option is not supported when a **FREQ** statement is used.

**UNPACK**

suppresses paneling.

**RESIDUALHISTOGRAM**

produces a histogram of the residuals.

**RFPLOT | RF**

produces a “Residual-Fit” (or RF) plot consisting of side-by-side quantile plots of the centered fit and the residuals. This plot “shows how much variation in the data is explained by the fit and how much remains in the residuals” (Cleveland 1993).

**RIDGE | RIDGEPANEL | RIDGEPLOT** <(ridge-options)>

creates panels of VIF values and standardized ridge estimates by ridge values for each coefficient. The VIF values for each coefficient are connected by lines and are displayed in the upper plot in each panel. The points corresponding to the standardized estimates of each coefficient are connected by lines and are displayed in the lower plot in each panel. By default, at most 10 coefficients are represented in a panel and multiple panels are produced for models with more than 10 regressors. For ridge estimates to be computed and plotted, the OUTEST= option must be specified in the PROC REG statement, and the RIDGE= list must be specified in either the PROC REG or the MODEL statement. (See Example 79.5.)

The following *ridge-options* are available:

**COMMONAXES**

specifies that the same VIF axis and the same standardized estimate axis are used in all panels when multiple panels are needed. By default, these axes are chosen independently for the regressors shown in each panel.

**RIDGEAXIS=LINEAR | LOG**

specifies the axis type used to display the ridge parameters. The default is RIDGEAXIS=LINEAR. Note that the point with the ridge parameter equal to zero is not displayed if you specify RIDGEAXIS=LOG.

**UNPACK**

suppresses paneling. The traces of the VIF statistics and standardized estimates are shown in separate plots.

**VARSPERPLOT=ALL****VARSPERPLOT=number**

specifies the maximum number of regressors displayed in each panel or in each plot if you additionally specify the UNPACK option. If you specify VARSPERPLOT=ALL, then the VIF values and ridge traces for all regressors are displayed in a single panel.

**VIFAXIS=LINEAR | LOG**

specifies the axis type used to display the VIF statistics. The default is VIFAXIS=LINEAR.

**RSQUARE** <(rsquare-options)>

displays the R-square values for the models examined when you request variable selection with the SELECTION= option in the MODEL statement.

The following *rsquare-options* are available for models where you request the RSQUARE, ADJRSQ, or CP selection method:

**LABEL**

requests that the model number corresponding to the one displayed in the “Subset Selection Summary” table be used to label the model with the largest R-square statistic at each value of the number of parameters.

**LABELVARS**

requests that the list (excluding the intercept) of the regressors in the relevant model be used to label the model with the largest R-square statistic at each value of the number of parameters.

**RSTUDENTBYLEVERAGE <(LABEL)>**

plots studentized residuals by leverage. Observations whose studentized residuals lie outside the band between the reference lines  $RSTUDENT = \pm 2$  are deemed outliers. Observations whose leverage values are greater than the vertical reference  $LEVERAGE = 2p/n$ , where  $p$  is the number of parameters including the intercept and  $n$  is the number of observations used, are deemed influential (Rawlings, Pantula, and Dickey 1998). If you specify the LABEL option, then points deemed as outliers or influential are labeled. If you do not specify an ID variable, the observation number within the current BY group is used as the label. If you specify one or more ID variables in one or more ID statements, then the first ID variable you specify is used for the labeling.

**RSTUDENTBYPREDICTED <(LABEL)>**

plots studentized residuals by predicted values. If you specify the LABEL option, then points deemed as outliers or influential (see the RSTUDENTBYLEVERAGE option for details) are labeled.

**SBC <(sbc-options)>**

displays Schwarz’s Bayesian information criterion (SBC) for the models examined when you request variable selection with the SELECTION= option in the MODEL statement.

The following *sbc-options* are available for models where you request the RSQUARE, ADJRSQ, or CP selection method:

**LABEL**

requests that the model number corresponding to the one displayed in the “Subset Selection Summary” table be used to label the model with the smallest SBC statistic at each value of the number of parameters.

**LABELVARS**

requests that the list (excluding the intercept) of the regressors in the relevant model be used to label the model with the smallest SBC statistic at each value of the number of parameters.

**PRESS**

outputs the PRESS statistic to the OUTEST= data set. The values of this statistic are saved in the variable `_PRESS_`. This option is available for all model selection methods except RSQUARE, ADJRSQ, and CP.

**RIDGE=*list***

requests a ridge regression analysis and specifies the values of the ridge constant  $k$  (see the section “Computations for Ridge Regression and IPC Analysis” on page 6739). Each value of  $k$  produces



a set of ridge regression estimates that are placed in the OUTEST= data set. The values of  $k$  are saved by the variable `_RIDGE_`, and the value of the variable `_TYPE_` is set to RIDGE to identify the estimates.

Only nonnegative numbers can be specified with the RIDGE= option. [Example 79.5](#) illustrates this option.

If ODS Graphics is enabled (see the section “[ODS Graphics](#)” on page 6745), then ridge regression plots are automatically produced. These plots consist of panels containing ridge traces for the regressors, with at most eight ridge traces per panel.

If you specify the RIDGE= option, `RESTRICT` statements are ignored.

### RSQUARE

has the same effect as the `EDF` option.

### SIMPLE

displays the sum, mean, variance, standard deviation, and uncorrected sum of squares for each variable used in PROC REG.

### SINGULAR= $n$

tunes the mechanism used to check for singularities. The default value is machine dependent but is approximately  $1E-7$  on most machines. This option is rarely needed.

Singularity checking is described in the section “[Computational Methods](#)” on page 6740.

### TABLEOUT

outputs the standard errors and  $100(1 - \alpha)\%$  confidence limits for the parameter estimates, the  $t$  statistics for testing if the estimates are zero, and the associated  $p$ -values to the OUTEST= data set. The `_TYPE_` variable values `STDERR`, `LnB`, `UnB`, `T`, and `PVALUE`, where  $n = 100(1 - \alpha)$ , identify these rows in the OUTEST= data set. The  $\alpha$  level can be set with the ALPHA= option in the `PROC REG` or `MODEL` statement. The OUTEST= option must be specified in the `PROC REG` statement for this option to take effect.

### USSCP

displays the uncorrected sums-of-squares and crossproducts matrix for all variables used in the procedure.

---

## ADD Statement

**ADD** *variables* ;

The ADD statement adds independent variables to the regression model. Only variables used in the `VAR` statement or used in `MODEL` statements before the first RUN statement can be added to the model. You can use the ADD statement interactively to add variables to the model or to include a variable that was previously deleted with a `DELETE` statement. Each use of the ADD statement modifies the `MODEL` label.

See the section “[Interactive Analysis](#)” on page 6697 for an example.

---

## BY Statement

**BY variables ;**

You can specify a BY statement with PROC REG to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the REG procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

When a BY statement is used with PROC REG, interactive processing is not possible; that is, once the first RUN statement is encountered, processing proceeds for each BY group in the data set, and no further statements are accepted by the procedure. A BY statement that appears after the first RUN statement is ignored.

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

---

## CODE Statement

**CODE < options > ;**

The CODE statement enables you to write SAS DATA step code for computing predicted values of the fitted model either to a file or to a catalog entry. This code can then be included in a DATA step to score new data.

Table 79.4 summarizes the *options* available in the CODE statement.

**Table 79.4** CODE Statement Options

| Option   | Description                                                                  |
|----------|------------------------------------------------------------------------------|
| CATALOG= | Names the catalog entry where the generated code is saved                    |
| DUMMIES  | Retains the dummy variables in the data set                                  |
| ERROR    | Computes the error function                                                  |
| FILE=    | Names the file where the generated code is saved                             |
| FORMAT=  | Specifies the numeric format for the regression coefficients                 |
| GROUP=   | Specifies the group identifier for array names and statement labels          |
| IMPUTE   | Imputes predicted values for observations with missing or invalid covariates |

Table 79.4 *continued*

| Option    | Description                                         |
|-----------|-----------------------------------------------------|
| LINESIZE= | Specifies the line size of the generated code       |
| LOOKUP=   | Specifies the algorithm for looking up CLASS levels |
| RESIDUAL  | Computes residuals                                  |

For details about the syntax of the CODE statement, see the section “CODE Statement” on page 390 in Chapter 19, “Shared Concepts and Topics.”

---

## DELETE Statement

**DELETE** *variables* ;

The DELETE statement deletes independent variables from the regression model. The DELETE statement performs the opposite function of the ADD statement and is used in a similar manner. Each use of the DELETE statement modifies the MODEL label.

For an example of how the ADD statement is used (and how the DELETE statement can be used), see the section “Interactive Analysis” on page 6697.

---

## FREQ Statement

**FREQ** *variable* ;

When a FREQ statement appears, each observation in the input data set is assumed to represent  $n$  observations, where  $n$  is the value of the FREQ variable. The analysis produced when you use a FREQ statement is the same as an analysis produced by using a data set that contains  $n$  observations in place of each observation in the input data set. When the procedure determines degrees of freedom for significance tests, the total number of observations is considered to be equal to the sum of the values of the FREQ variable.

If the value of the FREQ variable is missing or is less than 1, the observation is not used in the analysis. If the value is not an integer, only the integer portion is used.

The FREQ statement must appear before the first RUN statement, or it is ignored.

---

## ID Statement

**ID** *variables* ;

When one of the MODEL statement options CLI, CLM, P, R, and INFLUENCE is requested, the variables listed in the ID statement are displayed beside each observation. These variables can be used to identify each observation. If the ID statement is omitted, the observation number is used to identify the observations.

Although there are no restrictions on the length of ID variables, PROC REG might truncate ID values to 16 characters for display purposes.

## MODEL Statement

`< label: > MODEL dependents = < regressors > < / options > ;`

After the keyword MODEL, the dependent (response) variables are specified, followed by an equal sign and the regressor variables. Variables specified in the MODEL statement must be numeric variables in the data set being analyzed. For example, if you want to specify a quadratic term for variable X1 in the model, you cannot use X1\*X1 in the MODEL statement but must create a new variable (for example, X1SQUARE=X1\*X1) in a DATA step and use this new variable in the MODEL statement. The label in the MODEL statement is optional.

Table 79.5 summarizes the options available in the MODEL statement. Equations for the statistics available are given in the section “Model Fit and Diagnostic Statistics” on page 6715.

**Table 79.5** MODEL Statement Options

| Option                                          | Description                                                                                    |
|-------------------------------------------------|------------------------------------------------------------------------------------------------|
| <b>Model Selection and Details of Selection</b> |                                                                                                |
| SELECTION=                                      | Specifies model selection method                                                               |
| BEST=                                           | Specifies maximum number of subset models displayed or output to the OUTEST= data set          |
| DETAILS                                         | Produces summary statistics at each step                                                       |
| DETAILS=                                        | Specifies the display details for FORWARD, BACKWARD, and STEPWISE methods                      |
| GROUPNAMES=                                     | Provides names for groups of variables                                                         |
| INCLUDE=                                        | Includes first $n$ variables in the model                                                      |
| MAXSTEP=                                        | Specifies maximum number of steps that might be performed                                      |
| NOINT                                           | Fits a model without the intercept term                                                        |
| PCOMIT=                                         | Performs incomplete principal component analysis and outputs estimates to the OUTEST= data set |
| RIDGE=                                          | Performs ridge regression analysis and outputs estimates to the OUTEST= data set               |
| SLE=                                            | Sets criterion for entry into model                                                            |
| SLS=                                            | Sets criterion for staying in model                                                            |
| START=                                          | Specifies number of variables in model to begin the comparing and switching process            |
| STOP=                                           | Stops selection criterion                                                                      |
| <b>Statistics</b>                               |                                                                                                |
| ADJRSQ                                          | Computes adjusted R square                                                                     |
| AIC                                             | Computes Akaike's information criterion                                                        |
| B                                               | Computes parameter estimates for each model                                                    |
| BIC                                             | Computes Sawa's Bayesian information criterion                                                 |
| CP                                              | Computes Mallows' $C_p$ statistic                                                              |
| GMSEP                                           | Computes estimated MSE of prediction assuming multivariate normality                           |
| JP                                              | Computes $J_p$ , the final prediction error                                                    |
| MSE                                             | Computes MSE for each model                                                                    |
| PC                                              | Computes Amemiya's prediction criterion                                                        |

Table 79.5 *continued*

| Option                         | Description                                                                                                              |
|--------------------------------|--------------------------------------------------------------------------------------------------------------------------|
| RMSE                           | Displays root MSE for each model                                                                                         |
| SBC                            | Computes the SBC statistic                                                                                               |
| SP                             | Computes $S_p$ statistic for each model                                                                                  |
| SSE                            | Computes error sum of squares for each model                                                                             |
| <b>Data Set Options</b>        |                                                                                                                          |
| EDF                            | Outputs the number of regressors, the error degrees of freedom, and the model R square to the OUTEST= data set           |
| OUTSEB                         | Outputs standard errors of the parameter estimates to the OUTEST= data set                                               |
| OUTSTB                         | Outputs standardized parameter estimates to the OUTEST= data set. Use only with the RIDGE= or PCOMIT= option.            |
| OUTVIF                         | Outputs the variance inflation factors to the OUTEST= data set. Use only with the RIDGE= or PCOMIT= option.              |
| PRESS                          | Outputs the PRESS statistic to the OUTEST= data set                                                                      |
| RSQUARE                        | Has same effect as the EDF option                                                                                        |
| <b>Regression Calculations</b> |                                                                                                                          |
| I                              | Displays inverse of sums of squares and crossproducts                                                                    |
| XPX                            | Displays sums-of-squares and crossproducts matrix                                                                        |
| <b>Details on Estimates</b>    |                                                                                                                          |
| ACOV                           | Displays heteroscedasticity- consistent covariance matrix of estimates and heteroscedasticity-consistent standard errors |
| ACOVMETHOD=                    | Specifies method for computing the asymptotic heteroscedasticity-consistent covariance matrix                            |
| COLLIN                         | Produces collinearity analysis                                                                                           |
| COLLINOINT                     | Produces collinearity analysis with intercept adjusted out                                                               |
| CORRB                          | Displays correlation matrix of estimates                                                                                 |
| COVB                           | Displays covariance matrix of estimates                                                                                  |
| HCC                            | Displays heteroscedasticity-consistent standard errors                                                                   |
| HCCMETHOD=                     | Specifies method for computing the asymptotic heteroscedasticity-consistent covariance matrix                            |
| LACKFIT                        | Performs lack-of-fit test                                                                                                |
| PARTIALR2                      | Displays squared semipartial correlation coefficients computed using Type I sums of squares                              |
| PCORR1                         | Displays squared partial correlation coefficients computed using Type I sums of squares                                  |
| PCORR2                         | Displays squared partial correlation coefficients computed using Type II sums of squares                                 |
| SCORR1                         | Displays squared semipartial correlation coefficients computed using Type I sums of squares                              |
| SCORR2                         | Displays squared semipartial correlation coefficients computed using Type II sums of squares                             |
| SEQB                           | Displays a sequence of parameter estimates during selection process                                                      |

Table 79.5 *continued*

| Option                                   | Description                                                                                                                                                       |
|------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| SPEC                                     | Tests that first and second moments of model are correctly specified                                                                                              |
| SS1                                      | Displays the sequential sums of squares                                                                                                                           |
| SS2                                      | Displays the partial sums of squares                                                                                                                              |
| STB                                      | Displays standardized parameter estimates                                                                                                                         |
| TOL                                      | Displays tolerance values for parameter estimates                                                                                                                 |
| WHITE                                    | Displays heteroscedasticity-consistent standard errors                                                                                                            |
| VIF                                      | Computes variance-inflation factors                                                                                                                               |
| <b>Predicted and Residual Values</b>     |                                                                                                                                                                   |
| CLB                                      | Computes $100(1 - \alpha)\%$ confidence limits for the parameter estimates                                                                                        |
| CLI                                      | Computes $100(1 - \alpha)\%$ confidence limits for an individual predicted value                                                                                  |
| CLM                                      | Computes $100(1 - \alpha)\%$ confidence limits for the expected value of the dependent variable                                                                   |
| DW                                       | Computes a Durbin-Watson statistic                                                                                                                                |
| DWPROB                                   | Computes a Durbin-Watson statistic and $p$ -value                                                                                                                 |
| INFLUENCE                                | Computes influence statistics                                                                                                                                     |
| P                                        | Computes predicted values                                                                                                                                         |
| PARTIAL                                  | Displays partial regression plots for each regressor                                                                                                              |
| PARTIALDATA                              | Displays partial regression data                                                                                                                                  |
| R                                        | Produces analysis of residuals                                                                                                                                    |
| <b>Display Options and Other Options</b> |                                                                                                                                                                   |
| ALL                                      | Requests the following options:<br>ACOV, CLB, CLI, CLM, CORRB, COVB, HCC, I, P,<br>PCORR1, PCORR2, R, SCORR1, SCORR2, SEQB, SPEC,<br>SS1, SS2, STB, TOL, VIF, XPX |
| ALPHA=                                   | Sets significance value for confidence and prediction intervals and tests                                                                                         |
| NOPRINT                                  | Suppresses display of results                                                                                                                                     |
| SIGMA=                                   | Specifies the true standard deviation of error term for computing CP and BIC                                                                                      |
| SINGULAR=                                | Sets criterion for checking for singularity                                                                                                                       |

You can specify the following options in the **MODEL** statement after a slash (/).

### ACOV

displays the estimated asymptotic covariance matrix of the estimates under the hypothesis of heteroscedasticity and heteroscedasticity-consistent standard errors of parameter estimates. See the **HCCMETHOD=** option and the **HCC** option and the section “Testing for Heteroscedasticity” on page 6732 for more information.

**ACOVMETHOD=0,1,2, or 3**

See the **HCCMETHOD=** option.

**ADJRSQ**

computes R square adjusted for degrees of freedom for each model selected (Darlington 1968; Judge et al. 1980).

**AIC**

outputs Akaike's information criterion for each model selected (Akaike 1969; Judge et al. 1980) to the OUTEST= data set. If **SELECTION=ADJRSQ**, **SELECTION=RSQUARE**, or **SELECTION=CP** is specified, then the AIC statistic is also added to the SubsetSelSummary table.

**ALL**

requests all these options: **ACOV**, **CLB**, **CLI**, **CLM**, **CORRB**, **COVB**, **HCC**, **I**, **P**, **PCORR1**, **PCORR2**, **R**, **SCORR1**, **SCORR2**, **SEQB**, **SPEC**, **SS1**, **SS2**, **STB**, **TOL**, **VIF**, and **XPX**.

**ALPHA=number**

sets the significance level used for the construction of confidence intervals for the current **MODEL** statement. The value must be between 0 and 1; the default value of 0.05 results in 95% intervals. This option affects the **MODEL** options **CLB**, **CLI**, and **CLM**; the **OUTPUT** statement keywords **LCL**, **LCLM**, **UCL**, and **UCLM**; the **PLOT** statement keywords **LCL.**, **LCLM.**, **UCL.**, and **UCLM.**; and the **PLOT** statement options **CONF** and **PRED**. If you specify this option in the **MODEL** statement, it takes precedence over the **ALPHA=** option in the **PROC REG** statement.

**B**

is used with the **RSQUARE**, **ADJRSQ**, and **CP** model-selection methods to compute estimated regression coefficients for each model selected.

**BEST=n**

is used with the **RSQUARE**, **ADJRSQ**, and **CP** model-selection methods. If **SELECTION=CP** or **SELECTION=ADJRSQ** is specified, the **BEST=** option specifies the maximum number of subset models to be displayed or output to the OUTEST= data set. For **SELECTION=RSQUARE**, the **BEST=** option requests the maximum number of subset models for each size.

If the **BEST=** option is used without the **B** option (displaying estimated regression coefficients), the variables in each **MODEL** are listed in order of inclusion instead of the order in which they appear in the **MODEL** statement.

If the **BEST=** option is omitted and the number of regressors is less than 11, all possible subsets are evaluated. If the **BEST=** option is omitted and the number of regressors is greater than 10, the number of subsets selected is, at most, equal to the number of regressors. A small value of the **BEST=** option greatly reduces the CPU time required for large problems.

**BIC**

outputs Sawa's Bayesian information criterion for each model selected (Sawa 1978; Judge et al. 1980) to the OUTEST= data set. If **SELECTION=ADJRSQ**, **SELECTION=RSQUARE**, or **SELECTION=CP** is specified, then the BIC statistic is also added to the SubsetSelSummary table.

**CLB**

requests the  $100(1 - \alpha)\%$  upper and lower confidence limits for the parameter estimates. By default, the 95% limits are computed; the **ALPHA=** option in the **PROC REG** or **MODEL** statement can be

used to change the  $\alpha$  level. If any of the **MODEL** statement options **ACOV**, **HCC**, or **WHITE** are in effect, then the **CLB** option also produces heteroscedasticity-consistent  $100(1 - \alpha)\%$  upper and lower confidence limits for the parameter estimates.

**CLI**

requests the  $100(1 - \alpha)\%$  upper and lower confidence limits for an individual predicted value. By default, the 95% limits are computed; the **ALPHA=** option in the **PROC REG** or **MODEL** statement can be used to change the  $\alpha$  level. The confidence limits reflect variation in the error, as well as variation in the parameter estimates. See the section “[Predicted and Residual Values](#)” on page 6708 and Chapter 4, “[Introduction to Regression Procedures](#),” for more information.

**CLM**

displays the  $100(1 - \alpha)\%$  upper and lower confidence limits for the expected value of the dependent variable (mean) for each observation. By default, the 95% limits are computed; the **ALPHA=** in the **PROC REG** or **MODEL** statement can be used to change the  $\alpha$  level. This is not a prediction interval (see the **CLI** option) because it takes into account only the variation in the parameter estimates, not the variation in the error term. See the section “[Predicted and Residual Values](#)” on page 6708 and Chapter 4, “[Introduction to Regression Procedures](#),” for more information.

**COLLIN**

requests a detailed analysis of collinearity among the regressors. This includes eigenvalues, condition indices, and decomposition of the variances of the estimates with respect to each eigenvalue. See the section “[Collinearity Diagnostics](#)” on page 6713.

**COLLINOINT**

requests the same analysis as the **COLLIN** option with the intercept variable adjusted out rather than included in the diagnostics. See the section “[Collinearity Diagnostics](#)” on page 6713.

**CORRB**

displays the correlation matrix of the estimates. This is the  $(\mathbf{X}'\mathbf{X})^{-1}$  matrix scaled to unit diagonals.

**COVB**

displays the estimated covariance matrix of the estimates. This matrix is  $(\mathbf{X}'\mathbf{X})^{-1}s^2$ , where  $s^2$  is the estimated mean squared error.

**CP**

outputs Mallows’  $C_p$  statistic for each model selected (Mallows 1973; Hocking 1976) to the **OUTEST=** data set. See the section “[Criteria Used in Model-Selection Methods](#)” on page 6704 for a discussion of the use of  $C_p$ . If **SELECTION=ADJRSQ**, **SELECTION=RSQUARE**, or **SELECTION=CP** is specified, then the  $C_p$  statistic is also added to the **SubsetSelSummary** table.

**DETAILS****DETAILS=name**

specifies the level of detail produced when the **BACKWARD**, **FORWARD**, or **STEPWISE** method is used, where *name* can be **ALL**, **STEPS**, or **SUMMARY**. The **DETAILS** or **DETAILS=ALL** option produces entry and removal statistics for each variable in the model building process, ANOVA and parameter estimates at each step, and a selection summary table. The option **DETAILS=STEPS** provides the step information and summary table. The option **DETAILS=SUMMARY** produces only the summary table. The default if the **DETAILS** option is omitted is **DETAILS=STEPS**.



**DW**

calculates a Durbin-Watson statistic to test whether or not the errors have first-order autocorrelation. (This test is appropriate only for time series data.) Note that your data should be sorted by the date/time ID variable before you use this option. The sample autocorrelation of the residuals is also produced. See the section “[Autocorrelation in Time Series Data](#)” on page 6738.

**DWPROB**

calculates a Durbin-Watson statistic and a  $p$ -value to test whether or not the errors have first-order autocorrelation. Note that it is not necessary to specify the DW option if the DWPROB option is specified. (This test is appropriate only for time series data.) Note that your data should be sorted by the date/time ID variable before you use this option. The sample autocorrelation of the residuals is also produced. See the section “[Autocorrelation in Time Series Data](#)” on page 6738.

**EDF**

outputs the number of regressors in the model excluding and including the intercept, the error degrees of freedom, and the model R square to the OUTEST= data set.

**GMSEP**

outputs the estimated mean square error of prediction assuming that both independent and dependent variables are multivariate normal (Stein 1960; Darlington 1968) to the OUTEST= data set. (Note that Hocking’s formula (1976, eq. 4.20) contains a misprint: “ $n - 1$ ” should read “ $n - 2$ .”) If SELECTION=ADJRSQL, SELECTION=RSQUARE, or SELECTION=CP is specified, then the GMSEP statistic is also added to the SubsetSelSummary table.

**GROUPNAMES=***'name1' 'name2' ...*

provides names for variable groups. This option is available only in the BACKWARD, FORWARD, and STEPWISE methods. The group name can be up to 32 characters. Subsets of independent variables listed in the **MODEL** statement can be designated as variable groups. This is done by enclosing the appropriate variables in braces. Variables in the same group are entered into or removed from the regression model at the same time. However, if the tolerance of any variable (see the **TOL** option on page 6659) in a group is less than the setting of the **SINGULAR=** option, then the variable is not entered into the model with the rest of its group. If the **GROUPNAMES=** option is not used, then the names GROUP1, GROUP2, ..., GROUP $n$  are assigned to groups encountered in the **MODEL** statement. Variables not enclosed by braces are used as groups of a single variable.

For example:

```
model y={x1 x2} x3 / selection=stepwise
 groupnames='x1 x2' 'x3';
```

Another example:

```
model y={ht wgt age} bodyfat / selection=forward
 groupnames='htwgtage' 'bodyfat';
```

**HCC**

requests heteroscedasticity-consistent standard errors of the parameter estimates. You can use the **HCCMETHOD=** option to specify the method used to compute the heteroscedasticity-consistent covariance matrix.

**HCCMETHOD=0,1,2, or 3**

specifies the method used to obtain a heteroscedasticity-consistent covariance matrix for use with the **ACOV**, **HCC**, or **WHITE** option in the **MODEL** statement and for heteroscedasticity-consistent tests with the **TEST** statement. The default is **HCCMETHOD=0**. See the section “[Testing for Heteroscedasticity](#)” on page 6732 for details.

**I**

displays the  $(\mathbf{X}'\mathbf{X})^{-1}$  matrix. The inverse of the crossproducts matrix is bordered by the parameter estimates and SSE matrices.

**INCLUDE=*n***

forces the first *n* independent variables listed in the **MODEL** statement to be included in all models. The selection methods are performed on the other variables in the **MODEL** statement. The **INCLUDE=** option is not available with **SELECTION=NONE**.

**INFLUENCE**

requests a detailed analysis of the influence of each observation on the estimates and the predicted values. See the section “[Influence Statistics](#)” on page 6717 for details.

**JP**

outputs  $J_p$ , the estimated mean square error of prediction for each model selected assuming that the values of the regressors are fixed and that the model is correct to the **OUTEST=** data set. The  $J_p$  statistic is also called the final prediction error (FPE) by Akaike (Nicholson 1948; Lord 1950; Mallows 1967; Darlington 1968; Rothman 1968; Akaike 1969; Hocking 1976; Judge et al. 1980) If **SELECTION=ADJRSQ**, **SELECTION=RSQUARE**, or **SELECTION=CP** is specified, then the  $J_p$  statistic is also added to the SubsetSelSummary table.

**LACKFIT**

performs a lack-of-fit test. See the section “[Testing for Lack of Fit](#)” on page 6733 for more information. See Draper and Smith (1981) for a discussion of lack-of-fit tests.

**MSE**

computes the mean square error for each model selected (Darlington 1968).

**MAXSTEP=*n***

specifies the maximum number of steps that are done when **SELECTION=FORWARD**, **SELECTION=BACKWARD**, or **SELECTION=STEPWISE** is used. The default value is the number of independent variables in the model for the **FORWARD** and **BACKWARD** methods and three times this number for the stepwise method.

**NOINT**

suppresses the intercept term that is otherwise included in the model.

**NOPRINT**

suppresses the normal display of regression results. Note that this option temporarily disables the Output Delivery System (ODS); see Chapter 20, “[Using the Output Delivery System](#),” for more information.

**OUTSEB**

outputs the standard errors of the parameter estimates to the OUTEST= data set. The value SEB for the variable `_TYPE_` identifies the standard errors. If the RIDGE= or PCOMIT= option is specified, additional observations are included and identified by the values RIDGESEB and IPCSEB, respectively, for the variable `_TYPE_`. The standard errors for ridge regression estimates and incomplete principal components (IPC) estimates are limited in their usefulness because these estimates are biased. This option is available for all model-selection methods except RSQUARE, ADJRSQ, and CP.

**OUTSTB**

outputs the standardized parameter estimates as well as the usual estimates to the OUTEST= data set when the RIDGE= or PCOMIT= option is specified. The values RIDGESTB and IPCSTB for the variable `_TYPE_` identify ridge regression estimates and IPC estimates, respectively.

**OUTVIF**

outputs the variance inflation factors (VIF) to the OUTEST= data set when the RIDGE= or PCOMIT= option is specified. The factors are the diagonal elements of the inverse of the correlation matrix of regressors as adjusted by ridge regression or IPC analysis. These observations are identified in the output data set by the values RIDGEVIF and IPCVIF for the variable `_TYPE_`.

**P**

calculates predicted values from the input data and the estimated model. The display includes the observation number, the ID variable (if one is specified), the actual and predicted values, and the residual. If the CLI, CLM, or R option is specified, the P option is unnecessary. See the section “[Predicted and Residual Values](#)” on page 6708 for more information.

**PARTIAL**

requests partial regression leverage plots for each regressor. You can use the [PARTIALDATA](#) option to obtain a tabular display of the partial regression leverage data. If ODS Graphics is enabled (see the section “[ODS Graphics](#)” on page 6745), then these partial plots are produced in panels with up to six plots per panel. See the section “[Influence Statistics](#)” on page 6717 for more information.

**PARTIALDATA**

requests partial regression leverage data for each regressor. You can request partial regression leverage plots of these data with the [PARTIAL](#) option. See the section “[Influence Statistics](#)” on page 6717 for more information.

**PARTIALR2 <( < TESTS > < SEQTESTS > ) >**

See the [SCORR1](#) option.

**PC**

outputs Amemiya’s prediction criterion for each model selected (Amemiya 1976; Judge et al. 1980) to the OUTEST= data set. If SELECTION=ADJRSQ, SELECTION=RSQUARE, or SELECTION=CP is specified, then the PC statistic is also added to the SubsetSelSummary table.

**PCOMIT=*list***

requests an IPC analysis for each value *m* in the list. The procedure computes parameter estimates by using all but the last *m* principal components. Each value of *m* produces a set of IPC estimates, which is output to the OUTEST= data set. The values of *m* are saved by the variable `_PCOMIT_`, and the value of the variable `_TYPE_` is set to IPC to identify the estimates. Only nonnegative integers can be specified with the PCOMIT= option.

If you specify the PCOMIT= option, **RESTRICT** statements are ignored. The PCOMIT= option is ignored if you use the SELECTION= option in the **MODEL** statement.

### **PCORR1**

displays the squared partial correlation coefficients computed using Type I sum of squares (SS). This is calculated as  $SS/(SS+SSE)$ , where SSE is the error sum of squares.

### **PCORR2**

displays the squared partial correlation coefficients computed using Type II sums of squares. These are calculated the same way as with the PCORR1 option, except that Type II SS are used instead of Type I SS.

### **PRESS**

outputs the PRESS statistic to the OUTEST= data set. The values of this statistic are saved in the variable `_PRESS_`. This option is available for all model-selection methods except RSQUARE, ADJRSQ, and CP.

### **R**

requests an analysis of the residuals. The results include everything requested by the **P** option plus the standard errors of the mean predicted and residual values, the studentized residual, and Cook's *D* statistic to measure the influence of each observation on the parameter estimates. See the section “[Predicted and Residual Values](#)” on page 6708 for more information.

### **RIDGE=list**

requests a ridge regression analysis and specifies the values of the ridge constant  $k$  (see the section “[Computations for Ridge Regression and IPC Analysis](#)” on page 6739). Each value of  $k$  produces a set of ridge regression estimates that are placed in the OUTEST= data set. The values of  $k$  are saved by the variable `_RIDGE_`, and the value of the variable `_TYPE_` is set to RIDGE to identify the estimates.

Only nonnegative numbers can be specified with the RIDGE= option. [Example 79.5](#) illustrates this option.

If you specify the RIDGE= option, **RESTRICT** statements are ignored. The RIDGE= option is ignored if you use the SELECTION= option in the **MODEL** statement.

### **RMSE**

displays the root mean square error for each model selected.

### **RSQUARE**

has the same effect as the **EDF** option.

### **SBC**

outputs the SBC statistic for each model selected (Schwarz 1978; Judge et al. 1980) to the OUTEST= data set. If SELECTION=ADJRSQ, SELECTION=RSQUARE, or SELECTION=CP is specified, then the SBC statistic is also added to the SubsetSelSummary table.

### **SCORR1 <( < TESTS > < SEQTESTS > ) >**

displays the squared semipartial correlation coefficients computed using Type I sums of squares. This is calculated as  $SS/SST$ , where SST is the corrected total SS. If the **NOINT** option is used, the uncorrected total SS is used in the denominator. The optional arguments TESTS and SEQTESTS request are sequentially added to a model. The *F*-test values are computed as the Type I sum of squares

for the variable in question divided by a mean square error. If you specify the TESTS option, the denominator MSE is the residual mean square for the full model specified in the MODEL statement. If you specify the SEQTESTS option, the denominator MSE is the residual mean square for the model containing all the independent variables that have been added to the model up to and including the variable in question. The TESTS and SEQTESTS options are not supported if you specify model selection methods or the RIDGE or PCOMIT options. Note that the [PARTIALR2](#) option is a synonym for the SCORR1 option.

### SCORR2 < ( TESTS ) >

displays the squared semipartial correlation coefficients computed using Type II sums of squares. These are calculated the same way as with the SCORR1 option, except that Type II SS are used instead of Type I SS. The optional TEST argument requests  $F$  tests and  $p$ -values as variables are sequentially added to a model. The  $F$ -test values are computed as the Type II sum of squares for the variable in question divided by the residual mean square for the full model specified in the MODEL statement. The TESTS option is not supported if you specify model selection methods or the RIDGE or PCOMIT options.

### SELECTION=*name*

specifies the method used to select the model, where *name* can be FORWARD (or F), BACKWARD (or B), STEPWISE, MAXR, MINR, RSQUARE, ADJRSQ, CP, or NONE (use the full model). The default method is NONE. See the section “[Model-Selection Methods](#)” on page 6701 for a description of each method.

### SEQB

produces a sequence of parameter estimates as each variable is entered into the model. This is displayed as a matrix where each row is a set of parameter estimates.

### SIGMA=*n*

specifies the true standard deviation of the error term to be used in computing the CP and BIC statistics. If the SIGMA= option is not specified, an estimate from the full model is used. This option is available in the RSQUARE, ADJRSQ, and CP model-selection methods only.

### SINGULAR=*n*

tunes the mechanism used to check for singularities. If you specify this option in the MODEL statement, it takes precedence over the SINGULAR= option in the PROC REG statement. The default value is machine dependent but is approximately  $1E-7$  on most machines. This option is rarely needed. Singularity checking is described in the section “[Computational Methods](#)” on page 6740.

### SLENTY=*value*

### SLE=*value*

specifies the significance level for entry into the model used in the FORWARD and STEPWISE methods. The defaults are 0.50 for FORWARD and 0.15 for STEPWISE.

### SLSTAY=*value*

### SLS=*value*

specifies the significance level for staying in the model for the BACKWARD and STEPWISE methods. The defaults are 0.10 for BACKWARD and 0.15 for STEPWISE.

**SP**

outputs the  $S_p$  statistic for each model selected (Hocking 1976) to the OUTEST= data set. If SELECTION=ADJRSQ, SELECTION=RSQUARE, or SELECTION=CP is specified, then the SP statistic is also added to the SubsetSelSummary table.

**SPEC**

performs a test that the first and second moments of the model are correctly specified. See the section “Testing for Heteroscedasticity” on page 6732 for more information.

**SS1**

displays the sequential sums of squares (Type I SS) along with the parameter estimates for each term in the model. See Chapter 15, “The Four Types of Estimable Functions,” for more information about the different types of sums of squares.

**SS2**

displays the partial sums of squares (Type II SS) along with the parameter estimates for each term in the model. See the SS1 option also.

**SSE**

computes the error sum of squares for each model selected.

**START=*s***

is used to begin the comparing-and-switching process in the MAXR, MINR, and STEPWISE methods for a model containing the first *s* independent variables in the MODEL statement, where *s* is the START value. For these methods, the default is START=0.

For the RSQUARE, ADJRSQ, and CP methods, START=*s* specifies the smallest number of regressors to be reported in a subset model. For these methods, the default is START=1.

The START= option cannot be used with model-selection methods other than the six described here.

**STB**

produces standardized regression coefficients. A standardized regression coefficient is computed by dividing a parameter estimate by the ratio of the sample standard deviation of the dependent variable to the sample standard deviation of the regressor.

**STOP=*s***

causes PROC REG to stop when it has found the “best” *s*-variable model, where *s* is the STOP value. For the RSQUARE, ADJRSQ, and CP methods, STOP=*s* specifies the largest number of regressors to be reported in a subset model. For the MAXR and MINR methods, STOP=*s* specifies the largest number of regressors to be included in the model.

The default setting for the STOP= option is the number of variables in the MODEL statement. This option can be used only with the MAXR, MINR, RSQUARE, ADJRSQ, and CP methods.

**TOL**

produces tolerance values for the estimates. Tolerance for a variable is defined as  $1 - R^2$ , where  $R^2$  is obtained from the regression of the variable on all other regressors in the model. See the section “Collinearity Diagnostics” on page 6713 for more details.

**VIF**

produces variance inflation factors with the parameter estimates. Variance inflation is the reciprocal of tolerance. See the section “[Collinearity Diagnostics](#)” on page 6713 for more detail.

**WHITE**

See the [HCC](#) option.

**XPX**

displays the  $X'X$  crossproducts matrix for the model. The crossproducts matrix is bordered by the  $X'Y$  and  $Y'Y$  matrices.

**MTEST Statement**

```
<label:> MTEST <equation <, ..., equation>> </options>;
```

where each *equation* is a linear function composed of coefficients and variable names. The *label* is optional.

The MTEST statement is used to test hypotheses in multivariate regression models where there are several dependent variables fit to the same regressors. If no equations or options are specified, the MTEST statement tests the hypothesis that all estimated parameters except the intercept are zero.

The hypotheses that can be tested with the MTEST statement are of the form

$$(\mathbf{L}\boldsymbol{\beta} - \mathbf{c})\mathbf{M} = 0$$

where  $\mathbf{L}$  is a linear function on the regressor side,  $\boldsymbol{\beta}$  is a matrix of parameters,  $\mathbf{c}$  is a column vector of constants,  $\mathbf{j}$  is a row vector of ones, and  $\mathbf{M}$  is a linear function on the dependent side. The special case where the constants are zero is

$$\mathbf{L}\boldsymbol{\beta}\mathbf{M} = 0$$

See the section “[Multivariate Tests](#)” on page 6734 for more details.

Each linear function extends across either the regressor variables or the dependent variables. If the equation is across the dependent variables, then the constant term, if specified, must be zero. The equations for the regressor variables form the  $\mathbf{L}$  matrix and  $\mathbf{c}$  vector in the preceding formula; the equations for dependent variables form the  $\mathbf{M}$  matrix. If no equations for the dependent variables are given, PROC REG uses an identity matrix for  $\mathbf{M}$ , testing the same hypothesis across all dependent variables. If no equations for the regressor variables are given, PROC REG forms a linear function corresponding to a test that all the nonintercept parameters are zero.

As an example, consider the following statements:

```
model y1 y2 y3=x1 x2 x3;
mtest x1,x2;
mtest y1-y2, y2 -y3, x1;
mtest y1-y2;
```



The first MTEST statement tests the hypothesis that the X1 and X2 parameters are zero for Y1, Y2, and Y3. In addition, the second MTEST statement tests the hypothesis that the X1 parameter is the same for all three dependent variables. For the same model, the third MTEST statement tests the hypothesis that all parameters except the intercept are the same for dependent variables Y1 and Y2.

You can specify the following options in the MTEST statement:

#### **CANPRINT**

displays the canonical correlations for the hypothesis combinations and the dependent variable combinations. If you specify

```
mtest / canprint;
```

the canonical correlations between the regressors and the dependent variables are displayed.

#### **DETAILS**

displays the **M** matrix and various intermediate calculations.

#### **MSTAT=FAPPROX**

#### **MSTAT=EXACT**

specifies the method of evaluating the multivariate test statistics. The default is MSTAT=FAPPROX, which specifies that the multivariate tests are evaluated by using the usual approximations based on the *F* distribution, as discussed in the “Multivariate Tests” section in Chapter 4, “[Introduction to Regression Procedures](#).” Alternatively, you can specify MSTAT=EXACT to compute exact *p*-values for three of the four tests (Wilks’ lambda, the Hotelling-Lawley trace, and Roy’s greatest root) and an improved *F* approximation for the fourth (Pillai’s trace). While MSTAT=EXACT provides better control of the significance probability for the tests, especially for Roy’s greatest root, computations for the exact *p*-values can be appreciably more demanding, and are in fact infeasible for large problems (many dependent variables). Thus, although MSTAT=EXACT is more accurate for most data, it is not the default method.

#### **PRINT**

displays the **H** and **E** matrices.

## **OUTPUT Statement**

```
OUTPUT < OUT=SAS-data-set > < keyword=names > < ... keyword=names > ;
```

The OUTPUT statement creates a new SAS data set that saves diagnostic measures calculated after fitting the model. The OUTPUT statement refers to the most recent **MODEL** statement. At least one *keyword=names* specification is required.

All the variables in the original data set are included in the new data set, along with variables created in the OUTPUT statement. These new variables contain the values of a variety of statistics and diagnostic measures that are calculated for each observation in the data set. If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*.

The OUTPUT statement cannot be used when a TYPE=CORR, TYPE=COV, or TYPE=SSCP data set is used as the input data set for PROC REG. See the section “[Input Data Sets](#)” on page 6686 for more details.



The statistics created in the OUTPUT statement are described in this section. More details are given in the section “[Predicted and Residual Values](#)” on page 6708 and the section “[Influence Statistics](#)” on page 6717. Also see Chapter 4, “[Introduction to Regression Procedures](#),” for definitions of the statistics available from the REG procedure.

You can specify the following options in the OUTPUT statement:

**OUT=SAS data set**

gives the name of the new data set. By default, the procedure uses the *DATA*n** convention to name the new data set.

*keyword=names*

specifies the statistics to include in the output data set and names the new variables that contain the statistics. Specify a keyword for each desired statistic (see the following list of keywords), an equal sign, and the variable or variables to contain the statistic.

In the output data set, the first variable listed after a keyword in the OUTPUT statement contains that statistic for the first dependent variable listed in the MODEL statement; the second variable contains the statistic for the second dependent variable in the MODEL statement, and so on. The list of variables following the equal sign can be shorter than the list of dependent variables in the MODEL statement. In this case, the procedure creates the new names in order of the dependent variables in the MODEL statement.

For example, the following SAS statements create an output data set named b:

```
proc reg data=a;
 model y z=x1 x2;
 output out=b
 p=yhat zhat
 r=yresid zresid;
run;
```

In addition to the variables in the input data set, b contains the following variables:

- yhat, with values that are predicted values of the dependent variable y
- zhat, with values that are predicted values of the dependent variable z
- yresid, with values that are the residual values of y
- zresid, with values that are the residual values of z

You can specify the following keywords in the OUTPUT statement. See the section “[Model Fit and Diagnostic Statistics](#)” on page 6715 for computational formulas.

**Table 79.6** Keywords for OUTPUT Statement

| Keyword                | Description                                                                                                                                 |
|------------------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| COOKD= <i>names</i>    | Cook’s <i>D</i> influence statistic                                                                                                         |
| COVRATIO= <i>names</i> | standard influence of observation on covariance of betas, as discussed in the section “ <a href="#">Influence Statistics</a> ” on page 6717 |
| DFFITS= <i>names</i>   | standard influence of observation on predicted value                                                                                        |
| H= <i>names</i>        | leverage, $\mathbf{x}_i (\mathbf{X}'\mathbf{X})^{-1} \mathbf{x}_i'$                                                                         |

Table 79.6 *continued*

| Keyword                     | Description                                                                                                                                                                         |
|-----------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| LCL= <i>names</i>           | lower bound of a $100(1 - \alpha)\%$ confidence interval for an individual prediction. This includes the variance of the error, as well as the variance of the parameter estimates. |
| LCLM= <i>names</i>          | lower bound of a $100(1 - \alpha)\%$ confidence interval for the expected value (mean) of the dependent variable                                                                    |
| PREDICTED   P= <i>names</i> | predicted values                                                                                                                                                                    |
| PRESS= <i>names</i>         | <i>i</i> th residual divided by $(1 - h)$ , where <i>h</i> is the leverage, and where the model has been refit without the <i>i</i> th observation                                  |
| RESIDUAL   R= <i>names</i>  | residuals, calculated as ACTUAL minus PREDICTED                                                                                                                                     |
| RSTUDENT= <i>names</i>      | a studentized residual with the current observation deleted                                                                                                                         |
| STDI= <i>names</i>          | standard error of the individual predicted value                                                                                                                                    |
| STDP= <i>names</i>          | standard error of the mean predicted value                                                                                                                                          |
| STDR= <i>names</i>          | standard error of the residual                                                                                                                                                      |
| STUDENT= <i>names</i>       | studentized residuals, which are the residuals divided by their standard errors                                                                                                     |
| UCL= <i>names</i>           | upper bound of a $100(1 - \alpha)\%$ confidence interval for an individual prediction                                                                                               |
| UCLM= <i>names</i>          | upper bound of a $100(1 - \alpha)\%$ confidence interval for the expected value (mean) of the dependent variable                                                                    |

## PAINT Statement

**PAINT** < *condition* | **ALLOBS** > < / *options* > ;

**PAINT** < **STATUS** | **UNDO** > ;

The PAINT statement is used with line printer plots. See the **PLOTS=** option for information about using ODS graphics to create modern statistical graphics.

The PAINT statement selects observations to be *painted* or highlighted in a scatter plot on line printer output; the PAINT statement is ignored if the **LINEPRINTER** option is not specified in the **PROC REG** statement.

All observations that satisfy *condition* are painted using some specific symbol. The PAINT statement does not generate a scatter plot and must be followed by a **PLOT** statement, which does generate a scatter plot. Several PAINT statements can be used before a **PLOT** statement, and all prior PAINT statement requests are applied to all later **PLOT** statements.

The PAINT statement lists the observation numbers of the observations selected, the total number of observations selected, and the plotting symbol used to paint the points.

On a plot, paint symbols take precedence over all other symbols. If any position contains more than one painted point, the paint symbol for the observation plotted last is used.

The PAINT statement cannot be used when a **TYPE=CORR**, **TYPE=COV**, or **TYPE=SSCP** data set is used as the input data set for **PROC REG**. Also, the PAINT statement cannot be used for models with more than

one dependent variable. Note that the syntax for the PAIN<sub>T</sub> statement is the same as the syntax for the REWEIGHT statement.

## Specifying Condition

*Condition* is used to select observations to be painted. The syntax of *condition* is

*variable compare value*

or

*variable compare value* *logical* *variable compare value*

where

*variable* is one of the following:

- a variable name in the input data set
- OBS., which is the observation number
- *keyword.*, where *keyword* is a keyword for a statistic requested in the OUTPUT statement

*compare* is an operator that compares *variable* to *value*. *Compare* can be any one of the following: <, <=, >, >=, =, ^ =. The operators LT, LE, GT, GE, EQ, and NE, respectively, can be used instead of the preceding symbols. See the “Expressions” section in *SAS Language Reference: Concepts* for more information about comparison operators.

*value* gives an unformatted value of *variable*. Observations are selected to be painted if they satisfy the condition created by *variable compare value*. *Value* can be a number or a character string. If *value* is a character string, it must be eight characters or less and must be enclosed in quotes. In addition, *value* is case-sensitive. In other words, the statements

```
paint name='henry';
```

and

```
paint name='Henry';
```

are not the same.

*logical* is one of two logical operators. Either AND or OR can be used. To specify AND, use AND or the symbol &. To specify OR, use OR or the symbol |.

Here are some examples of the *variable compare value* form:

```
paint name='Henry';
paint residual.>=20;
paint obs.=99;
```

Here are some examples of the *variable compare value* *logical* *variable compare value* form:

```

paint name='Henry'|name='Mary';
paint residual.>=20 or residual.<=10;
paint obs.>=11 and residual.<=20;

```

## Using ALLOBS

Instead of specifying *condition*, the ALLOBS option can be used to select all observations. This is most useful when you want to unpaint all observations. For example,

```

paint allobs / reset;

```

resets the symbols for all observations.

## Options in the PAINT Statement

The following options can be used when either a condition is specified, the ALLOBS option is specified, or nothing is specified before the slash. If only an option is listed, the option applies to the observations selected in the previous PAINT statement, *not* to the observations selected by reapplying the condition from the previous PAINT statement. For example, in the statements

```

paint r.>0 / symbol='a';
reweight r.>0;
refit;
paint / symbol='b';

```

the second PAINT statement paints only those observations selected in the first PAINT statement. No additional observations are painted even if, after refitting the model, there are new observations that meet the condition in the first PAINT statement.

**NOTE:** Options are not available when either the UNDO or STATUS option is used.

You can specify the following options after a slash (/).

### NOLIST

suppresses the display of the selected observation numbers. If the NOLIST option is not specified, a list of observations selected is written to the log. The list includes the observation numbers and painting symbol used to paint the points. The total number of observations selected to be painted is also shown.

### RESET

changes the painting symbol to the current default symbol, effectively unpainting the observations selected. If you set the default symbol by using the SYMBOL= option in the PLOT statement, the RESET option in the PAINT statement changes the painting symbol to the symbol you specified. Otherwise, the default symbol of '1' is used.

### SYMBOL='character'

specifies a painting symbol. If the SYMBOL= option is omitted, the painting symbol is either the one used in the most recent PAINT statement or, if there are no previous PAINT statements, the symbol '@'. For example,

```
paint / symbol='#';
```

changes the painting symbol for the observations selected by the most recent PAIN statement to '#'. As another example,

```
paint temp lt 22 / symbol='c';
```

changes the painting symbol to 'c' for all observations with TEMP<22. In general, the numbers 1, 2, ..., 9 and the asterisk are not recommended as painting symbols. These symbols are used as default symbols in the PLOT statement, where they represent the number of replicates at a point. If SYMBOL="" is used, no painting is done in the current plot. If SYMBOL=' ' is used, observations are painted with a blank and are no longer seen on the plot.

## STATUS and UNDO

Instead of specifying *condition* or the ALLOBS option, you can use the STATUS or UNDO option as follows:

### STATUS

lists (in the log) the observation number and plotting symbol of all currently painted observations.

### UNDO

undoes changes made by the most recent PAIN statement. Observations might be, but are not necessarily, unpainted. For example:

```
paint obs. <=10 / symbol='a';
...other interactive statements
paint obs.=1 / symbol='b';
...other interactive statements
paint undo;
```

The last PAIN statement changes the plotting symbol used for observation 1 back to 'a'. If the statement

```
paint / reset;
```

is used instead, observation 1 is unpainted.

---

## PLOT Statement

```
PLOT <yvariable* xvariable> <=symbol> <...yvariable* xvariable> <=symbol> </ options> ;
```

The PLOT statement is used with line printer and traditional graphics. See the PLOTS= option for information about using ODS graphics to create modern statistical graphics.

The PLOT statement in PROC REG displays scatter plots with *yvariable* on the vertical axis and *xvariable* on the horizontal axis. Line printer plots are generated if the LINEPRINTER option is specified in the PROC

REG statement; otherwise, the traditional graphics are created. Points in line printer plots can be marked with *symbols*, while global graphics statements such as GOPTIONS and SYMBOL are used to enhance the traditional graphics. Note that the plots you request by using the PLOT statement are independent of the ODS graphical displays (see the section “ODS Graphics” on page 6745) that are available in PROC REG.

As with most other interactive statements, the PLOT statement implicitly refits the model. For example, if a PLOT statement is preceded by a REWEIGHT statement, the model is recomputed, and the plot reflects the new model.

If there are multiple MODEL statements preceding a PLOT statement, then the PLOT statement refers to the latest MODEL statement.

The PLOT statement cannot be used when a TYPE=CORR, TYPE=COV, or TYPE=SSCP data set is used as input to PROC REG.

You can specify several PLOT statements for each MODEL statement, and you can specify more than one plot in each PLOT statement.

### Specifying Yvariables, Xvariables, and Symbol

More than one *yvariable*\**xvariable* pair can be specified to request multiple plots. The *yvariables* and *xvariables* can be as follows:

- any variables specified in the VAR or MODEL statement before the first RUN statement
- *keyword.*, where *keyword* is a regression diagnostic statistic available in the OUTPUT statement (see Table 79.7). For example,

```
plot predicted.*residual.;
```

generates one plot of the predicted values by the residuals for each dependent variable in the MODEL statement. These statistics can also be plotted against any of the variables in the VAR or MODEL statements.

- the keyword OBS. (the observation number), which can be plotted against any of the preceding variables
- the keyword NPP. or NQQ., which can be used with any of the preceding variables to construct normal P-P or Q-Q plots, respectively (see the section “Construction of Q-Q and P-P Plots” on page 6739 for more information)
- keywords for model fit summary statistics available in the OUTEST= data set with \_TYPE\_= PARMS (see Table 79.7). A SELECTION= method (other than NONE) must be requested in the MODEL statement for these variables to be plotted. If one member of a *yvariable*\**xvariable* pair is from the OUTEST= data set, the other member must also be from the OUTEST= data set.

The OUTPUT statement and the OUTEST= option are not required when their keywords are specified in the PLOT statement.

The *yvariable* and *xvariable* specifications can be replaced by a set of variables and statistics enclosed in parentheses. When this occurs, all possible combinations of *yvariable* and *xvariable* are generated. For example, the following two statements are equivalent:

```
plot (y1 y2)*(x1 x2);
plot y1*x1 y1*x2 y2*x1 y2*x2;
```

The statement

```
plot;
```

is equivalent to respecifying the most recent PLOT statement without any options. However, the line printer options COLLECT, HPLOTS=, SYMBOL=, and VPLOTS=, described in the section “Line Printer Plots” on page 6675, apply across PLOT statements and remain in effect if they have been previously specified.

Options used for the traditional graphics are described in the following section; see “Line Printer Plots” on page 6675 for more information.

## Traditional Graphics

The display of traditional graphics is described in the following paragraphs, the options are summarized in Table 79.7 and described in the section “Dictionary of PLOT Statement Options” on page 6671.

Several line printer statements and options are not supported for the traditional graphics. In particular the PAINT statement is disabled, as are the PLOT statement options CLEAR, COLLECT, HPLOTS=, NOCOLLECT, SYMBOL=, and VPLOTS=. To display more than one plot per page or to collect plots from multiple PLOT statements, use the PROC GREPLAY statement (see *SAS/GRAPH: Reference*). Also note that traditional graphics options are not recognized for line printer plots.

The fitted model equation and a label are displayed in the top margin of the plot; this display can be suppressed with the NOMODEL option. If the label is requested but cannot fit on one line, it is not displayed. The equation and label are displayed on one line when possible; if more lines are required, the label is displayed in the first line with the model equation in successive lines. If displaying the entire equation causes the plot to be unacceptably small, the equation is truncated. Table 79.8 lists options to control the display of the equation.

Four statistics are displayed by default in the right margin: the number of observations, R square, the adjusted R square, and the root mean square error. The display of these statistics can be suppressed with the NOSTAT option. You can specify other options to request the display of various statistics in the right margin; see Table 79.8.

A default reference line at zero is displayed if residuals are plotted. If the dependent variable is plotted against the independent variable in a simple linear regression model, the fitted regression line is displayed by default. Default reference lines can be suppressed with the NOLINE option; the lines are not displayed if the OVERLAY option is specified.

Specialized plots are requested with special options. For each coefficient, the RIDGEPLOT option plots the ridge estimates against the ridge values  $k$ ; see the description of the RIDGEPLOT option in the section “Dictionary of PLOT Statement Options” on page 6671 for more details. The CONF option plots  $100(1 - \alpha)\%$  confidence intervals for the mean while the PRED option plots  $100(1 - \alpha)\%$  prediction intervals; see the description of these options in the section “Dictionary of PLOT Statement Options” on page 6671 for more details.

If a SELECTION= method is requested, the fitted model equation and the statistics displayed in the margin correspond to the selected model. For the ADJRSQ and CP methods, the selected model is treated as a submodel of the full model. If a CP.\*NP. plot is requested, the CHOCKING= and CMALLOWS= options display model selection reference lines; see the descriptions of these options in the section “Dictionary of PLOT Statement Options” on page 6671 for more details.

**PLOT Statement variable Keywords**

The following table lists the keywords available as PLOT statement *xvariables* and *yvariables*. All keywords have a trailing dot; for example, “*COOKD.*” requests Cook’s *D* statistic. Neither the **OUTPUT** statement nor the **OUTEST=** option needs to be specified.

**Table 79.7** Keywords for PLOT Statement *xvariables*

| Keyword                                               | Description                                                                                    |
|-------------------------------------------------------|------------------------------------------------------------------------------------------------|
| <b>Diagnostic Statistics</b>                          |                                                                                                |
| COOKD.                                                | Cook’s <i>D</i> influence statistics                                                           |
| COVRATIO.                                             | standard influence of observation on covariance of betas                                       |
| DFFITS.                                               | standard influence of observation on predicted value                                           |
| H.                                                    | leverage                                                                                       |
| LCL.                                                  | lower bound of $100(1 - \alpha)\%$ confidence interval for individual prediction               |
| LCLM.                                                 | lower bound of $100(1 - \alpha)\%$ confidence interval for the mean of the dependent variable  |
| PREDICTED.<br>  PRED.   P.                            | predicted values                                                                               |
| PRESS.                                                | residuals from refitting the model with current observation deleted                            |
| RESIDUAL.   R.                                        | residuals                                                                                      |
| RSTUDENT.                                             | studentized residuals with the current observation deleted                                     |
| STDI.                                                 | standard error of the individual predicted value                                               |
| STDP.                                                 | standard error of the mean predicted value                                                     |
| STDR.                                                 | standard error of the residual                                                                 |
| STUDENT.                                              | residuals divided by their standard errors                                                     |
| UCL.                                                  | upper bound of $100(1 - \alpha)\%$ confidence interval for individual prediction               |
| UCLM.                                                 | upper bound of $100(1 - \alpha)\%$ confidence interval for the mean of the dependent variables |
| <b>Other Keywords Used with Diagnostic Statistics</b> |                                                                                                |
| NPP.                                                  | normal probability-probability plot                                                            |
| NQQ.                                                  | normal quantile-quantile plot                                                                  |
| OBS.                                                  | observation number (cannot plot against <b>OUTEST=</b> statistics)                             |
| <b>Model Fit Summary Statistics</b>                   |                                                                                                |
| ADJRSQ.                                               | adjusted R-square                                                                              |
| AIC.                                                  | Akaike’s information criterion                                                                 |
| BIC.                                                  | Sawa’s Bayesian information criterion                                                          |
| CP.                                                   | Mallows’ $C_p$ statistic                                                                       |
| EDF.                                                  | error degrees of freedom                                                                       |
| GMSEP.                                                | estimated MSE of prediction, assuming multivariate normality                                   |
| IN.                                                   | number of regressors in the model not including the intercept                                  |
| JP.                                                   | final prediction error                                                                         |
| MSE.                                                  | mean squared error                                                                             |
| NP.                                                   | number of parameters in the model (including the intercept)                                    |
| PC.                                                   | Amemiya’s prediction criterion                                                                 |
| RMSE.                                                 | root MSE                                                                                       |



Table 79.7 continued

| Keyword | Description          |
|---------|----------------------|
| RSQ.    | R-square             |
| SBC.    | SBC statistic        |
| SP.     | SP statistic         |
| SSE.    | error sum of squares |

### Summary of PLOT Statement Graphics Options

Table 79.8 summarizes the *options* available in the PLOT statement. These *options* are available unless the LINEPRINTER option is specified in the PROC REG statement. For complete descriptions, see the section “Dictionary of PLOT Statement Options” on page 6671.

Table 79.8 Traditional Graphics Options

| Option                            | Description                                                                         |
|-----------------------------------|-------------------------------------------------------------------------------------|
| <b>General Graphics Options</b>   |                                                                                     |
| ANNOTATE=<br><i>SAS-data-set</i>  | Specifies the annotate data set                                                     |
| CHOCKING= <i>color</i>            | Requests a reference line for $C_p$ model selection criteria                        |
| CMALLOWS= <i>color</i>            | Requests a reference line for the $C_p$ model selection criterion                   |
| CONF                              | Requests plots of $100(1 - \alpha)\%$ confidence intervals for the mean             |
| DESCRIPTION=<br>' <i>string</i> ' | Specifies a description for graphics catalog member                                 |
| NAME='' <i>string</i> '           | Names the plot in the graphics catalog                                              |
| OVERLAY                           | Overlays plots from the same model                                                  |
| PRED                              | Requests plots of $100(1 - \alpha)\%$ prediction intervals for individual responses |
| RIDGEPLOT                         | Requests the ridge trace for ridge regression                                       |
| <b>Axis and Legend Options</b>    |                                                                                     |
| LEGEND= <i>LEGENDn</i>            | Specifies LEGEND statement to be used                                               |
| NOLEGEND                          | Suppresses display of the legend                                                    |
| HAXIS= <i>values</i>              | Specifies tick mark values for horizontal axis                                      |
| VAXIS= <i>values</i>              | Specifies tick mark values for vertical axis                                        |
| <b>Reference Line Options</b>     |                                                                                     |
| HREF= <i>values</i>               | Specifies reference lines perpendicular to horizontal axis                          |
| LHREF= <i>linetype</i>            | Specifies line style for HREF= lines                                                |
| LLINE= <i>linetype</i>            | Specifies line style for lines displayed by default                                 |
| LVREF= <i>linetype</i>            | Specifies line style for VREF= lines                                                |
| NOLINE                            | Suppresses display of any default reference line                                    |
| VREF= <i>values</i>               | Specifies reference lines perpendicular to vertical axis                            |
| <b>Color Options</b>              |                                                                                     |
| CAXIS= <i>color</i>               | Specifies color for axis line and tick marks                                        |
| CFRAME= <i>color</i>              | Specifies color for frame                                                           |
| CHREF= <i>color</i>               | Specifies color for HREF= lines                                                     |
| CLINE= <i>color</i>               | Specifies color for lines displayed by default                                      |
| CTEXT= <i>color</i>               | Specifies color for text                                                            |

Table 79.8 *continued*

| Option                                                      | Description                                                                                                                       |
|-------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------|
| CVREF= <i>color</i>                                         | Specifies color for VREF= lines                                                                                                   |
| <b>Options for Displaying the Fitted Model Equation</b>     |                                                                                                                                   |
| MODELFONT= <i>font</i>                                      | Specifies font of model equation and model label                                                                                  |
| MODELHT= <i>value</i>                                       | Specifies text height of model equation and model label                                                                           |
| MODELLAB= <i>'label'</i>                                    | Specifies model label                                                                                                             |
| NOMODEL                                                     | Suppresses display of the fitted model and the label                                                                              |
| <b>Options for Displaying Statistics in the Plot Margin</b> |                                                                                                                                   |
| AIC                                                         | Displays Akaike's information criterion                                                                                           |
| BIC                                                         | Displays Sawa's Bayesian information criterion                                                                                    |
| CP                                                          | Displays Mallows' $C_p$ statistic                                                                                                 |
| EDF                                                         | Displays the error degrees of freedom                                                                                             |
| GMSEP                                                       | Displays the estimated MSE of prediction assuming multivariate normality                                                          |
| IN                                                          | Displays the number of regressors in the model not including the intercept                                                        |
| JP                                                          | Displays the $J_p$ statistic                                                                                                      |
| MSE                                                         | Displays the mean squared error                                                                                                   |
| NOSTAT                                                      | Suppresses display of the default statistics: the number of observations, R-square, adjusted R-square, and root mean square error |
| NP                                                          | Displays the number of parameters in the model including the intercept, if any                                                    |
| PC                                                          | Displays the PC statistic                                                                                                         |
| SBC                                                         | Displays the SBC statistic                                                                                                        |
| SP                                                          | Displays the $S_p$ statistic                                                                                                      |
| SSE                                                         | Displays the error sum of squares                                                                                                 |
| STATFONT= <i>font</i>                                       | Specifies font of text displayed in the margin                                                                                    |
| STATHT= <i>value</i>                                        | Specifies height of text displayed in the margin                                                                                  |

**Dictionary of PLOT Statement Options**

The following entries describe the PLOT statement *options* in detail. Note that these *options* are available unless you specify the LINEPRINTER option in the PROC REG statement.

**AIC**

displays Akaike's information criterion in the plot margin.

**ANNOTATE=SAS-data-set****ANNO=SAS-data-set**

specifies an input data set that contains appropriate variables for annotation. This applies only to displays created with the current PLOT statement. See *SAS/GRAPH: Reference* for more information.

**BIC**

displays Sawa's Bayesian information criterion in the plot margin.

**CAXIS=***color*

**CAXES=***color*

**CA=***color*

specifies the color for the axes, frame, and tick marks.

**CFRAME=***color*

**CFR=***color*

specifies the color for filling the area enclosed by the axes and the frame.

**CHOCKING=***color*

requests reference lines corresponding to the equations  $C_p = p$  and  $C_p = 2p - p_{full}$ , where  $p_{full}$  is the number of parameters in the full model (excluding the intercept) and  $p$  is the number of parameters in the subset model (including the intercept). The *color* must be specified; the  $C_p = p$  line is solid and the  $C_p = 2p - p_{full}$  line is dashed. Only PLOT statements of the form PLOT CP.\*NP. produce these lines.

For the purpose of parameter estimation, Hocking (1976) suggests selecting a model where  $C_p \leq 2p - p_{full}$ . For the purpose of prediction, Hocking suggests the criterion  $C_p \leq p$ . You can request the single reference line  $C_p = p$  with the CMALLOWS= option. If, for example, you specify both CHOCKING=RED and CMALLOWS=BLUE, then the  $C_p = 2p - p_{full}$  line is red and the  $C_p = p$  line is blue.

**CHREF=***color*

**CH=***color*

specifies the color for lines requested with the HREF= option.

**CLINE=***color*

**CL=***color*

specifies the color for lines displayed by default. See the [NOLINE](#) option for details.

**CMALLOWS=***color*

requests a  $C_p = p$  reference line, where  $p$  is the number of parameters (including the intercept) in the subset model. The *color* must be specified; the line is solid. Only PLOT statements of the form PLOT CP.\*NP. produce this line.

Mallows (1973) suggests that all subset models with  $C_p$  small and near  $p$  be considered for further study. See the [CHOCKING=](#) option for related model-selection criteria.

**CONF**

is a keyword used as a shorthand option to request plots that include  $(100 - \alpha)\%$  confidence intervals for the mean response. The ALPHA= option in the [PROC REG](#) or [MODEL](#) statement selects the significance level  $\alpha$ , which is 0.05 by default. The CONF option is valid for simple regression models only, and is ignored for plots where confidence intervals are inappropriate. The CONF option replaces the CONF95 option; however, the CONF95 option is still supported when the ALPHA= option is not specified. The OVERLAY option is ignored when the CONF option is specified.

**CP**

displays Mallows'  $C_p$  statistic in the plot margin.

**CTEXT=***color***CT=***color*

specifies the color for text including tick mark labels, axis labels, the fitted model label and equation, the statistics displayed in the margin, and legends.

**CVREF=***color***CV=***color*

specifies the color for lines requested with the VREF= option.

**DESCRIPTION=**'*string*'**DESC=**'*string*'

specifies a descriptive string, up to 40 characters, that appears in the description field of the PROC GREPLAY master menu.

**EDF**

displays the error degrees of freedom in the plot margin.

**GMSEP**

displays the estimated mean square error of prediction in the plot margin. Note that the estimate is calculated under the assumption that both independent and dependent variables have a multivariate normal distribution.

**HAXIS=***values***HA=***values*

specifies tick mark values for the horizontal axis.

**HREF=***values*

specifies where reference lines perpendicular to the horizontal axis are to appear.

**IN**

displays the number of regressors in the model (not including the intercept) in the plot margin.

**JP**

displays the  $J_p$  statistic in the plot margin.

**LEGEND=**LEGEND*n*

specifies the LEGEND*n* statement to be used. The LEGEND*n* statement is a global graphics statement; see *SAS/GRAPH: Reference* for more information.

**LHREF=***linetype***LH=***linetype*

specifies the line style for lines requested with the HREF= option. The default *linetype* is 2. Note that LHREF=1 requests a solid line. See *SAS/GRAPH: Reference* for a table of available line types.

**LLINE=***linetype***LL=***linetype*

specifies the line style for reference lines displayed by default; see the NOLINE option for details. The default *linetype* is 2. Note that LLINE=1 requests a solid line.

**LVREF=***linetype*

**LV=***linetype*

specifies the line style for lines requested with the VREF= option. The default *linetype* is 2. Note that LVREF=1 requests a solid line.

**MODELFONT=***font*

specifies the font used for displaying the fitted model label and the fitted model equation. See *SAS/GRAPH: Reference* for tables of software fonts.

**MODELHT=***height*

specifies the text height for the fitted model label and the fitted model equation.

**MODELLAB=**'*label*'

specifies the label to be displayed with the fitted model equation. By default, no label is displayed. If the label does not fit on one line, it is not displayed. See the section “Traditional Graphics” on page 6668 for more information.

**MSE**

displays the mean squared error in the plot margin.

**NAME=**'*string*'

specifies a descriptive string, up to eight characters, that appears in the name field of the PROC GREPLAY master menu. The default *string* is REG.

**NOLEGEND**

suppresses the display of the legend.

**NOLINE**

suppresses the display of default reference lines. A default reference line at zero is displayed if residuals are plotted. If the dependent variable is plotted against the independent variable in a simple regression model, then the fitted regression line is displayed by default. Default reference lines are not displayed if the OVERLAY option is specified.

**NOMODEL**

suppresses the display of the fitted model equation.

**NOSTAT**

suppresses the display of statistics in the plot margin. By default, the number of observations, R-square, adjusted R-square, and root MSE are displayed.

**NP**

displays the number of regressors in the model including the intercept, if any, in the plot margin.

**OVERLAY**

overlays all plots specified in the PLOT statement from the same model on one set of axes. The variables for the first plot label the axes. The procedure automatically scales the axes to fit all of the variables unless the HAXIS= or VAXIS= option is used. Default reference lines are not displayed. A default legend is produced; the LEGEND= option can be used to customize the legend.

**PC**

displays the PC statistic in the plot margin.

**PRED**

is a keyword used as a shorthand option to request plots that include  $(100 - \alpha)\%$  prediction intervals for individual responses. The ALPHA= option in the PROC REG or MODEL statement selects the significance level  $\alpha$ , which is 0.05 by default. The PRED option is valid for simple regression models only, and is ignored for plots where prediction intervals are inappropriate. The PRED option replaces the PRED95 option; however, the PRED95 option is still supported when the ALPHA= option is not specified. The OVERLAY option is ignored when the PRED option is specified.

**RIDGEPLOT**

creates overlaid plots of ridge estimates against ridge values for each coefficient. The points corresponding to the estimates of each coefficient in the plot are connected by lines. For ridge estimates to be computed and plotted, the OUTEST= option must be specified in the PROC REG statement, and the RIDGE=list must be specified in either the PROC REG or MODEL statement.

**SBC**

displays the SBC statistic in the plot margin.

**SP**

displays the  $S_p$  statistic in the plot margin.

**SSE**

displays the error sum of squares in the plot margin.

**STATFONT=font**

specifies the font used for displaying the statistics that appear in the plot margin. See *SAS/GRAPH: Reference* for tables of software fonts.

**STATHT=height**

specifies the text height of the statistics that appear in the plot margin.

**USEALL**

specifies that predicted values at data points with missing dependent variable(s) be included on appropriate plots. By default, only points used in constructing the SSCP matrix appear on plots.

**VAXIS=values****VA=values**

specifies tick mark values for the vertical axis.

**VREF=values**

specifies where reference lines perpendicular to the vertical axis are to appear.

**Line Printer Plots**

Line printer plots are requested with the LINEPRINTER option in the PROC REG statement. Points in line printer plots can be marked with *symbols*, which can be specified as a single character enclosed in quotes or the name of any variable in the input data set.

If a character variable is used for the symbol, the first (leftmost) nonblank character in the formatted value of the variable is used as the plotting symbol. If a character in quotes is specified, that character becomes

the plotting symbol. If a character is used as the plotting symbol, and if there are different plotting symbols needed at the same point, the symbol '?' is used at that point.

If an unformatted numeric variable is used for the symbol, the symbols '1', '2', ..., '9' are used for variable values 1, 2, ..., 9. For noninteger values, only the integer portion is used as the plotting symbol. For values of 10 or greater, the symbol '\*' is used. For negative values, a '?' is used. If a numeric variable is used, and if there is more than one plotting symbol needed at the same point, the sum of the variable values is used at that point. If the sum exceeds 9, the symbol '\*' is used.

If a symbol is not specified, the number of replicates at the point is displayed. The symbol '\*' is used if there are 10 or more replicates.

If the LINEPRINTER option is used, you can specify the following options in the PLOT statement after a slash (/):

#### **CLEAR**

clears any collected scatter plots before plotting begins but does not turn off the COLLECT option. Use this option when you want to begin a new collection with the plots in the current PLOT statement. For more information about collecting plots, see the COLLECT and NOCOLLECT options in this section.

#### **COLLECT**

specifies that plots begin to be collected from one PLOT statement to the next and that subsequent plots show an overlay of all collected plots. This option enables you to overlay plots before and after changes to the model or to the data used to fit the model. Plots collected before changes are unaffected by the changes and can be overlaid on later plots. You can request more than one plot with this option, and you do not need to request the same number of plots in subsequent PLOT statements. If you specify an unequal number of plots, plots in corresponding positions are overlaid. For example, the statements

```
plot residual.*predicted. y*x / collect;
run;
```

produce two plots. If these statements are then followed by

```
plot residual.*x;
run;
```

two plots are again produced. The first plot shows residual against X values overlaid on residual against predicted values. The second plot is the same as that produced by the first PLOT statement.

Axes are scaled for the first plot or plots collected. The axes are not rescaled as more plots are collected.

Once specified, the COLLECT option remains in effect until the NOCOLLECT option is specified.

#### **HLOTS=*number***

sets the number of scatter plots that can be displayed across the page. The procedure begins with one plot per page. The value of the HLOTS= option remains in effect until you change it in a later PLOT statement. See the VPLOTS= option for an example.

**NOCOLLECT**

specifies that the collection of scatter plots ends after adding the plots in the current PLOT statement. PROC REG starts with the NOCOLLECT option in effect. After you specify the NOCOLLECT option, any following PLOT statement produces a new plot that contains only the plots requested by that PLOT statement.

For more information, see the [COLLECT](#) option.

**OVERLAY**

enables requested scatter plots to be superimposed. The axes are scaled so that points on all plots are shown. If the HPLOTS= or VPLOTS= option is set to more than one, the overlaid plot occupies the first position on the page. The OVERLAY option is similar to the COLLECT option in that both options produce superimposed plots. However, OVERLAY superimposes only the plots in the associated PLOT statement; COLLECT superimposes plots across PLOT statements. The OVERLAY option can be used when the COLLECT option is in effect.

**SYMBOL='character'**

changes the default plotting symbol used for all scatter plots produced in the current and in subsequent PLOT statements. Both SYMBOL="" and SYMBOL=' ' are allowed.

If the SYMBOL= option has not been specified, the default symbol is '1' for positions with one observation, '2' for positions with two observations, and so on. For positions with more than 9 observations, '\*' is used. The SYMBOL= option (or a plotting symbol) is needed to avoid any confusion caused by this default convention. Specifying a particular symbol is especially important when either the OVERLAY or COLLECT option is being used.

If you specify the SYMBOL= option and use a number for *character*, that number is used for all points in the plot. For example, the statement

```
plot y** / symbol='1';
```

produces a plot with the symbol '1' used for all points.

If you specify a plotting symbol and the SYMBOL= option, the plotting symbol overrides the SYMBOL= option. For example, in the statements

```
plot y** y*v='.' / symbol='*';
```

the symbol used for the plot of Y against X is '\*', and a '.' is used for the plot of Y against V.

If a paint symbol is defined with a [PAINT](#) statement, the paint symbol takes precedence over both the SYMBOL= option and the default plotting symbol for the PLOT statement.

**VPLOTS=number**

sets the number of scatter plots that can be displayed down the page. The procedure begins with one plot per page. The value of the VPLOTS= option remains in effect until you change it in a later PLOT statement.

For example, to specify a total of six plots per page, with two rows of three plots, use the HPLOTS= and VPLOTS= options as follows:



```
plot y1*x1 y1*x2 y1*x3 y2*x1 y2*x2 y2*x3 /
 hplots=3 vplots=2;
run;
```

---

## PRINT Statement

**PRINT** <options> <ANOVA> <MODELDATA> ;

The PRINT statement enables you to interactively display the results of **MODEL** statement options, produce an ANOVA table, display the data for variables used in the current model, or redisplay the options specified in a **MODEL** or a previous PRINT statement. In addition, like most other interactive statements in PROC REG, the PRINT statement implicitly refits the model; thus, effects of **REWEIGHT** statements are seen in the resulting tables. If ODS Graphics is enabled (see the section “**ODS Graphics**” on page 6745), the PRINT statement also requests the use of the ODS graphical displays associated with the current model.

The following specifications can appear in the PRINT statement:

### options

interactively displays the results of **MODEL** statement options, where *options* is one or more of the following: ACOV, ALL, CLI, CLM, COLLIN, COLLINOINT, CORRB, COVB, DW, I, INFLUENCE, P, PARTIAL, PCORR1, PCORR2, R, SCORR1, SCORR2, SEQB, SPEC, SS1, SS2, STB, TOL, VIF, or XPX. See the section “**MODEL Statement**” on page 6649 for a description of these options.

### ANOVA

produces the ANOVA table associated with the current model. This is either the model specified in the last **MODEL** statement or the model that incorporates changes made by **ADD**, **DELETE**, or **REWEIGHT** statements after the last **MODEL** statement.

### MODELDATA

displays the data for variables used in the current model.

Use the statement

```
print;
```

to reprint options in the most recently specified PRINT or **MODEL** statement.

Options that require original data values, such as R or INFLUENCE, cannot be used when a TYPE=CORR, TYPE=COV, or TYPE=SSCP data set is used as the input data set to PROC REG. See the section “**Input Data Sets**” on page 6686 for more detail.

---

## REFIT Statement

**REFIT** ;

The REFIT statement causes the current model and corresponding statistics to be recomputed immediately. No output is generated by this statement. The REFIT statement is needed after one or more **REWEIGHT**

statements to cause them to take effect before subsequent **PAINT** or **REWEIGHT** statements. This is sometimes necessary when you are using statistical conditions in **REWEIGHT** statements. For example, consider the following statements:

```
paint student.>2;
plot student.*p.;
reweight student.>2;
refit;
paint student.>2;
plot student.*p.;
```

The second **PAINT** statement paints any additional observations that meet the condition after deleting observations and refitting the model. The **REFIT** statement is used because the **REWEIGHT** statement does not cause the model to be recomputed. In this particular example, the same effect could be achieved by replacing the **REFIT** statement with a **PLOT** statement.

Most interactive statements can be used to implicitly refit the model; any plots or statistics produced by these statements reflect changes made to the model and changes made to the data used to compute the model. The two exceptions are the **PAINT** and **REWEIGHT** statements, which do not cause the model to be recomputed.

---

## RESTRICT Statement

**RESTRICT** *equation* <, ..., *equation* > ;

A **RESTRICT** statement is used to place restrictions on the parameter estimates in the **MODEL** preceding it. More than one **RESTRICT** statement can follow each **MODEL** statement. Each **RESTRICT** statement replaces any previous **RESTRICT** statement. To lift all restrictions on a model, submit a new **MODEL** statement. If there are several restrictions, separate them with commas. The statement

```
restrict equation1=equation2=equation3;
```

is equivalent to imposing the two restrictions

```
restrict equation1=equation2;
restrict equation2=equation3;
```

Each restriction is written as a linear equation and can be written as

*equation*

or

*equation* = *equation*

The form of each *equation* is

$$c_1 \times \text{variable}_1 \pm c_2 \times \text{variable}_2 \pm \cdots \pm c_n \times \text{variable}_n$$

where the  $c_j$ 's are constants and the *variable<sub>j</sub>*'s are any regressor variables.

When no equal sign appears, the linear combination is set equal to zero. Each variable name mentioned must be a variable in the `MODEL` statement to which the `RESTRICT` statement refers. The keyword `INTERCEPT` can also be used as a variable name, and it refers to the intercept parameter in the regression model.

Note that the parameters associated with the variables are restricted, not the variables themselves. Restrictions should be consistent and not redundant.

Examples of valid `RESTRICT` statements include the following:

```
restrict x1;
restrict a+b=1;
restrict a=b=c;
restrict a=b, b=c;
restrict 2*f=g+h, intercept+f=0;
restrict f=g=h=intercept;
```

The third and fourth statements in this list produce identical restrictions. You cannot specify

```
restrict f-g=0,
 f-intercept=0,
 g-intercept=1;
```

because the three restrictions are not consistent. If these restrictions are included in a `RESTRICT` statement, one of the restrict parameters is set to zero and has zero degrees of freedom, indicating that PROC REG is unable to apply a restriction.

The restrictions usually operate even if the model is not of full rank. Check to ensure that  $DF = -1$  for each restriction. In addition, the model  $DF$  should decrease by 1 for each restriction.

The parameter estimates are those that minimize the quadratic criterion (SSE) subject to the restrictions. If a restriction cannot be applied, its parameter value and degrees of freedom are listed as zero.

The method used for restricting the parameter estimates is to introduce a Lagrangian parameter for each restriction (Pringle and Rayner 1971). The estimates of these parameters are displayed with test statistics. Note that the  $t$  statistic reported for the Lagrangian parameters does not follow a Student's  $t$  distribution, but its square follows a beta distribution (LaMotte 1994). The  $p$ -value for these parameters is computed using the beta distribution.

The Lagrangian parameter  $\gamma$  measures the sensitivity of the SSE to the restriction constant. If the restriction constant is changed by a small amount  $\epsilon$ , the SSE is changed by  $2\gamma\epsilon$ . The  $t$  ratio tests the significance of the restrictions. If  $\gamma$  is zero, the restricted estimates are the same as the unrestricted estimates, and a change in the restriction constant in either direction increases the SSE.

`RESTRICT` statements are ignored if the `PCOMIT=` or `RIDGE=` option is specified in the `PROC REG` statement.

---

## REWEIGHT Statement

```
REWEIGHT < condition | ALLOBS > < / options > ;
REWEIGHT < STATUS | UNDO > ;
```

The REWEIGHT statement interactively changes the weights of observations that are used in computing the regression equation. The REWEIGHT statement can change observation weights, or set them to zero, which causes selected observations to be excluded from the analysis. When a REWEIGHT statement sets observation weights to zero, the observations are not deleted from the data set. More than one REWEIGHT statement can be used. The requests from all REWEIGHT statements are applied to the subsequent statements. Each use of the REWEIGHT statement modifies the MODEL label.

The model and corresponding statistics are not recomputed after a REWEIGHT statement. For example, consider the following statements:

```
reweight r.>0;
reweight r.>0;
```

The second REWEIGHT statement does not exclude any additional observations since the model is not recomputed after the first REWEIGHT statement. Either use a [REFIT](#) statement to explicitly refit the model, or implicitly refit the model by following the REWEIGHT statement with any other interactive statement except a [PAINT](#) statement or another REWEIGHT statement.

The REWEIGHT statement cannot be used if a TYPE=CORR, TYPE=COV, or TYPE=SSCP data set is used as an input data set to PROC REG. Note that the syntax used in the REWEIGHT statement is the same as the syntax in the [PAINT](#) statement.

The syntax of the REWEIGHT statement is described in the following sections.

For detailed examples of using this statement, see the section “[Reweight Observations in an Analysis](#)” on page 6726.

## Specifying Condition

*Condition* is used to find observations to be reweighted. The syntax of *condition* is

*variable compare value*

or

*variable compare value logical variable compare value*

where

*variable* is one of the following:

- a variable name in the input data set
- OBS., which is the observation number
- *keyword.*, where *keyword* is a keyword for a statistic requested in the [OUTPUT](#) statement. The keyword specification is applied to all dependent variables in the model.

*compare* is an operator that compares *variable* to *value*. *Compare* can be any one of the following: <, <=, >, >=, =, ^ =. The operators LT, LE, GT, GE, EQ, and NE, respectively, can be used instead of the preceding symbols. See the “Expressions” chapter in *SAS Language Reference: Concepts* for more information about comparison operators.

*value* gives an unformatted value of *variable*. Observations are selected to be reweighted if they satisfy the condition created by *variable compare value*. *Value* can be a number or a character string. If *value* is a character string, it must be eight characters or less and must be enclosed in quotes. In addition, *value* is case-sensitive. In other words, the following two statements are not the same:

```
reweight name='steve';
```

```
reweight name='Steve';
```

*logical* is one of two logical operators. Either AND or OR can be used. To specify AND, use AND or the symbol &. To specify OR, use OR or the symbol |.

Here are some examples of the *variable compare value* form:

```
reweight obs. le 10;
reweight temp=55;
reweight type='new';
```

Here are some example of the *variable compare value logical variable compare value* form:

```
reweight obs.<=10 and residual.<2;
reweight student.<-2 or student.>2;
reweight name='Mary' | name='Susan';
```

## Using ALLOBS

Instead of specifying *condition*, you can use the ALLOBS option to select all observations. This is most useful when you want to restore the original weights of all observations. For example,

```
reweight allobs / reset;
```

resets weights for all observations and uses all observations in the subsequent analysis. Note that

```
reweight allobs;
```

specifies that all observations be excluded from analysis. Consequently, using ALLOBS is useful only if you also use one of the options discussed in the following section.

## Options in the REWEIGHT Statement

The following options can be used when either a condition, ALLOBS, or nothing is specified before the slash. If only an option is listed, the option applies to the observations selected in the previous REWEIGHT statement, not to the observations selected by reapplying the condition from the previous REWEIGHT statement. For example, consider the following statements:

```
reweight r.>0 / weight=0.1;
refit;
reweight;
```

The second **REWEIGHT** statement excludes from the analysis only those observations selected in the first **REWEIGHT** statement. No additional observations are excluded even if there are new observations that meet the condition in the first **REWEIGHT** statement.

**NOTE:** Options are not available when either the **UNDO** or **STATUS** option is used.

### **NOLIST**

suppresses the display of the selected observation numbers. If you omit the **NOLIST** option, a list of observations selected is written to the log.

### **RESET**

resets the observation weights to their original values as defined by the **WEIGHT** statement or to **WEIGHT=1** if no **WEIGHT** statement is specified. For example,

```
reweight / reset;
```

resets observation weights to the original weights in the data set. If previous **REWEIGHT** statements have been submitted, this **REWEIGHT** statement applies only to the observations selected by the previous **REWEIGHT** statement. Note that, although the **RESET** option does reset observation weights to their original values, it does not cause the model and corresponding statistics to be recomputed.

### **WEIGHT=value**

changes observation weights to the specified nonnegative real number. If you omit the **WEIGHT=** option, the observation weights are set to zero, and observations are excluded from the analysis. For example:

```
reweight name='Alan';
...other interactive statements
reweight / weight=0.5;
```

The first **REWEIGHT** statement changes weights to zero for all observations with **name='Alan'**, effectively deleting these observations. The subsequent analysis does not include these observations. The second **REWEIGHT** statement applies only to those observations selected by the previous **REWEIGHT** statement, and it changes the weights to 0.5 for all the observations with **NAME='Alan'**. Thus, the next analysis includes all original observations; however, those observations with **NAME='Alan'** have their weights set to 0.5.

## **STATUS and UNDO**

If you omit *condition* and the **ALLOBS** options, you can specify one of the following options.

### **STATUS**

writes to the log the observation's number and the weight of all reweighted observations. If an observation's weight has been set to zero, it is reported as deleted. However, the observation is not deleted from the data set, only from the analysis.

### **UNDO**

undoes the changes made by the most recent **REWEIGHT** statement. Weights might be, but are not necessarily, reset. For example, consider the following statements:

```
reweight student.>2 / weight=0.1;
reweight;
reweight undo;
```

The first **REWEIGHT** statement sets the weights of observations that satisfy the condition to 0.1. The second **REWEIGHT** statement sets the weights of the same observations to zero. The third **REWEIGHT** statement undoes the second, changing the weights back to 0.1.

## STORE Statement

```
STORE < OUT= > item-store-name < / LABEL= 'label' > ;
```

The **STORE** statement requests that the procedure save the estimated parameters of the fitted model. The resulting item store is a binary file format that cannot be modified. The contents of the item store can be processed with the **PLM** procedure.

For details about the syntax of the **STORE** statement, see the section “**STORE Statement**” on page 501 of Chapter 19, “**Shared Concepts and Topics**.”

**NOTE:** The information stored by the **STORE** statement in **PROC REG** is a subset of what is usually stored by other procedures that implement this statement. In particular, **PROC REG** stores only the estimated parameters of the model, so that you can later use the **CODE** statement in **PROC PLM** to write **SAS DATA** step code for prediction to a file or catalog entry. With only this subset of information, many other postprocessing features of **PROC PLM** are not available for item stores that are created by **PROC REG**.

## TEST Statement

```
< label: > TEST equation, < , . . . , equation > < / option > ;
```

The **TEST** statement tests hypotheses about the parameters estimated in the preceding **MODEL** statement. It has the same syntax as the **RESTRICT** statement except that it supports an option. Each equation specifies a linear hypothesis to be tested. The rows of the hypothesis are separated by commas.

Variable names must correspond to regressors, and each variable name represents the coefficient of the corresponding variable in the model. An optional label is useful to identify each test with a name. The keyword **INTERCEPT** can be used instead of a variable name to refer to the model’s intercept.

The **REG** procedure performs an *F* test for the joint hypotheses specified in a single **TEST** statement. More than one **TEST** statement can accompany a **MODEL** statement. The numerator is the usual quadratic form of the estimates; the denominator is the mean squared error. If hypotheses can be represented by

$$\mathbf{L}\boldsymbol{\beta} = \mathbf{c}$$

then the numerator of the *F* test is

$$\mathbf{Q} = (\mathbf{L}\mathbf{b} - \mathbf{c})'(\mathbf{L}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{L}')^{-1}(\mathbf{L}\mathbf{b} - \mathbf{c})$$

divided by degrees of freedom, where  $\mathbf{b}$  is the estimate of  $\beta$ . For example:

```
model y=a1 a2 b1 b2;
aplustest a1+a2=1;
b1: test b1=0, b2=0;
b2: test b1, b2;
```

The last two statements are equivalent; since no constant is specified, zero is assumed.

Note that, when the **ACOV**, **HCC**, or **WHITE** option is specified in the **MODEL** statement, tests are recomputed using the heteroscedasticity-consistent covariance matrix specified with the **HCCMETHOD=** option in the **MODEL** statement (see the section “Testing for Heteroscedasticity” on page 6732).

One option can be specified in the **TEST** statement after a slash (/):

#### **PRINT**

displays intermediate calculations. This includes  $\mathbf{L}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{L}'$  bordered by  $\mathbf{Lb}-\mathbf{c}$ , and  $(\mathbf{L}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{L}')^{-1}$  bordered by  $(\mathbf{L}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{L}')^{-1}(\mathbf{Lb}-\mathbf{c})$ .

## **VAR Statement**

**VAR** *variables* ;

The **VAR** statement is used to include numeric variables in the crossproducts matrix that are not specified in the first **MODEL** statement.

Variables not listed in **MODEL** statements before the first **RUN** statement must be listed in the **VAR** statement if you want the ability to add them interactively to the model with an **ADD** statement, to include them in a new **MODEL** statement, or to plot them in a scatter plot with the **PLOT** statement.

In addition, if you want to use options in the **PROC REG** statement and do not want to fit a model to the data (with a **MODEL** statement), you must use a **VAR** statement.

## **WEIGHT Statement**

**WEIGHT** *variable* ;

A **WEIGHT** statement names a variable in the input data set with values that are relative weights for a weighted least squares fit. If the weight value is proportional to the reciprocal of the variance for each observation, then the weighted estimates are the best linear unbiased estimates (BLUE).

Values of the weight variable must be nonnegative. If an observation's weight is zero, the observation is deleted from the analysis. If a weight is negative or missing, it is set to zero, and the observation is excluded from the analysis. A more complete description of the **WEIGHT** statement can be found in Chapter 42, “The GLM Procedure.”

Observation weights can be changed interactively with the **REWEIGHT** statement.



---

## Details: REG Procedure

---

### Missing Values

PROC REG constructs only one crossproducts matrix for the variables in all regressions. If any variable needed for any regression is missing, the observation is excluded from all estimates. If you include variables with missing values in the `VAR` statement, the corresponding observations are excluded from all analyses, even if you never include the variables in a model. PROC REG assumes that you might want to include these variables after the first `RUN` statement and deletes observations with missing values.

---

### Input Data Sets

PROC REG does not compute new regressors. For example, if you want a quadratic term in your model, you should create a new variable when you prepare the input data. For example, the statement

```
model y=x1 x1*x1;
```

is not valid. Note that this `MODEL` statement is valid in the GLM procedure.

The input data set for most applications of PROC REG contains standard rectangular data, but special `TYPE=CORR`, `TYPE=COV`, and `TYPE=SSCP` data sets can also be used. `TYPE=CORR` and `TYPE=COV` data sets created by the CORR procedure contain means and standard deviations. In addition, `TYPE=CORR` data sets contain correlations and `TYPE=COV` data sets contain covariances. `TYPE=SSCP` data sets created in previous runs of PROC REG that used the `OUTSSCP=` option contain the sums of squares and crossproducts of the variables.

See Appendix A, “Special SAS Data Sets,” and the “SAS Files” section in *SAS Language Reference: Concepts* for more information about special SAS data sets.

These summary files save CPU time. It takes  $nk^2$  operations (where  $n$  = number of observations and  $k$  = number of variables) to calculate crossproducts; the regressions are of the order  $k^3$ . When  $n$  is in the thousands and  $k$  is less than 10, you can save 99% of the CPU time by reusing the SSCP matrix rather than recomputing it.

When you want to use a special SAS data set as input, PROC REG must determine the `TYPE` for the data set. PROC CORR and PROC REG automatically set the type for their output data sets. However, if you create the data set by some other means (such as a `DATA` step), you must specify its type with the `TYPE=` data set option. If the `TYPE` for the data set is not specified when the data set is created, you can specify `TYPE=` as a data set option in the `DATA=` option in the `PROC REG` statement. For example:

```
proc reg data=a(type=corr);
```

When a TYPE=CORR, TYPE=COV, or TYPE=SSCP data set is used with PROC REG, statements and options that require the original data values have no effect. The **OUTPUT**, **PAINT**, **PLOT**, and **REWEIGHT** statements and the **MODEL** and **PRINT** statement options **P**, **R**, **CLM**, **CLI**, **DW**, **INFLUENCE**, and **PARTIAL** are disabled since the original observations needed to calculate predicted and residual values are not present.

### Example Using TYPE=CORR Data Set

The following statements use PROC CORR to produce an input data set for PROC REG. The fitness data for this analysis can be found in [Example 79.2](#).

```
proc corr data=fitness outp=r noprint;
 var Oxygen RunTime Age Weight RunPulse MaxPulse RestPulse;
run;
proc print data=r;
run;
proc reg data=r;
 model Oxygen=RunTime Age Weight;
run;
```

Since the OUTP= data set from PROC CORR is automatically set to TYPE=CORR, the TYPE= data set option is not required in this example. The data set containing the correlation matrix is displayed by the PRINT procedure as shown in [Figure 79.14](#). [Figure 79.15](#) shows results from the regression that uses the TYPE=CORR data as an input data set.

**Figure 79.14** TYPE=CORR Data Set Created by PROC CORR

|    |                | O       | R       | W       | R       | M       | R       |         |
|----|----------------|---------|---------|---------|---------|---------|---------|---------|
|    |                | x       | u       | e       | u       | a       | e       |         |
|    |                | y       | n       | i       | u       | p       | s       |         |
| O  | P              | g       | i       | A       | l       | l       | l       |         |
| b  | E              | e       | m       | g       | h       | s       | s       |         |
| s  | —              | n       | e       | e       | t       | e       | e       |         |
| 1  | MEAN           | 47.3758 | 10.5861 | 47.6774 | 77.4445 | 169.645 | 173.774 | 53.4516 |
| 2  | STD            | 5.3272  | 1.3874  | 5.2114  | 8.3286  | 10.252  | 9.164   | 7.6194  |
| 3  | N              | 31.0000 | 31.0000 | 31.0000 | 31.0000 | 31.000  | 31.000  | 31.0000 |
| 4  | CORR Oxygen    | 1.0000  | -0.8622 | -0.3046 | -0.1628 | -0.398  | -0.237  | -0.3994 |
| 5  | CORR RunTime   | -0.8622 | 1.0000  | 0.1887  | 0.1435  | 0.314   | 0.226   | 0.4504  |
| 6  | CORR Age       | -0.3046 | 0.1887  | 1.0000  | -0.2335 | -0.338  | -0.433  | -0.1641 |
| 7  | CORR Weight    | -0.1628 | 0.1435  | -0.2335 | 1.0000  | 0.182   | 0.249   | 0.0440  |
| 8  | CORR RunPulse  | -0.3980 | 0.3136  | -0.3379 | 0.1815  | 1.000   | 0.930   | 0.3525  |
| 9  | CORR MaxPulse  | -0.2367 | 0.2261  | -0.4329 | 0.2494  | 0.930   | 1.000   | 0.3051  |
| 10 | CORR RestPulse | -0.3994 | 0.4504  | -0.1641 | 0.0440  | 0.352   | 0.305   | 1.0000  |

Figure 79.15 Regression on TYPE=CORR Data Set

| The REG Procedure          |    |                    |                |         |         |
|----------------------------|----|--------------------|----------------|---------|---------|
| Model: MODEL1              |    |                    |                |         |         |
| Dependent Variable: Oxygen |    |                    |                |         |         |
| Analysis of Variance       |    |                    |                |         |         |
| Source                     | DF | Sum of Squares     | Mean Square    | F Value | Pr > F  |
| Model                      | 3  | 656.27095          | 218.75698      | 30.27   | <.0001  |
| Error                      | 27 | 195.11060          | 7.22632        |         |         |
| Corrected Total            | 30 | 851.38154          |                |         |         |
| Root MSE                   |    | 2.68818            | R-Square       | 0.7708  |         |
| Dependent Mean             |    | 47.37581           | Adj R-Sq       | 0.7454  |         |
| Coeff Var                  |    | 5.67416            |                |         |         |
| Parameter Estimates        |    |                    |                |         |         |
| Variable                   | DF | Parameter Estimate | Standard Error | t Value | Pr >  t |
| Intercept                  | 1  | 93.12615           | 7.55916        | 12.32   | <.0001  |
| RunTime                    | 1  | -3.14039           | 0.36738        | -8.55   | <.0001  |
| Age                        | 1  | -0.17388           | 0.09955        | -1.75   | 0.0921  |
| Weight                     | 1  | -0.05444           | 0.06181        | -0.88   | 0.3862  |

The following example uses the saved crossproducts matrix:

```
proc reg data=fitness outsscp=sscp noprint;
 model Oxygen=RunTime Age Weight RunPulse MaxPulse RestPulse;
run;
proc print data=sscp;
run;
proc reg data=sscp;
 model Oxygen=RunTime Age Weight;
run;
```

First, all variables are used to fit the data and create the SSCP data set. [Figure 79.16](#) shows the PROC PRINT display of the SSCP data set. The SSCP data set is then used as the input data set for PROC REG, and a reduced model is fit to the data.

**Figure 79.16** TYPE=SSCP Data Set Created by PROC REG

| Obs | _TYPE_ | _NAME_    | Intercept | RunTime  | Age       | Weight    |
|-----|--------|-----------|-----------|----------|-----------|-----------|
| 1   | SSCP   | Intercept | 31.00     | 328.17   | 1478.00   | 2400.78   |
| 2   | SSCP   | RunTime   | 328.17    | 3531.80  | 15687.24  | 25464.71  |
| 3   | SSCP   | Age       | 1478.00   | 15687.24 | 71282.00  | 114158.90 |
| 4   | SSCP   | Weight    | 2400.78   | 25464.71 | 114158.90 | 188008.20 |
| 5   | SSCP   | RunPulse  | 5259.00   | 55806.29 | 250194.00 | 407745.67 |
| 6   | SSCP   | MaxPulse  | 5387.00   | 57113.72 | 256218.00 | 417764.62 |
| 7   | SSCP   | RestPulse | 1657.00   | 17684.05 | 78806.00  | 128409.28 |
| 8   | SSCP   | Oxygen    | 1468.65   | 15356.14 | 69767.75  | 113522.26 |
| 9   | N      |           | 31.00     | 31.00    | 31.00     | 31.00     |

| Obs | RunPulse  | MaxPulse  | RestPulse | Oxygen    |
|-----|-----------|-----------|-----------|-----------|
| 1   | 5259.00   | 5387.00   | 1657.00   | 1468.65   |
| 2   | 55806.29  | 57113.72  | 17684.05  | 15356.14  |
| 3   | 250194.00 | 256218.00 | 78806.00  | 69767.75  |
| 4   | 407745.67 | 417764.62 | 128409.28 | 113522.26 |
| 5   | 895317.00 | 916499.00 | 281928.00 | 248497.31 |
| 6   | 916499.00 | 938641.00 | 288583.00 | 254866.75 |
| 7   | 281928.00 | 288583.00 | 90311.00  | 78015.41  |
| 8   | 248497.31 | 254866.75 | 78015.41  | 70429.86  |
| 9   | 31.00     | 31.00     | 31.00     | 31.00     |

[Figure 79.17](#) also shows the PROC REG results for the reduced model. (For the PROC REG results for the full model, see [Figure 79.29](#).)

**Figure 79.17** Regression on TYPE=SSCP Data Set

| The REG Procedure          |    |                    |                |         |         |
|----------------------------|----|--------------------|----------------|---------|---------|
| Model: MODEL1              |    |                    |                |         |         |
| Dependent Variable: Oxygen |    |                    |                |         |         |
| Analysis of Variance       |    |                    |                |         |         |
| Source                     | DF | Sum of Squares     | Mean Square    | F Value | Pr > F  |
| Model                      | 3  | 656.27095          | 218.75698      | 30.27   | <.0001  |
| Error                      | 27 | 195.11060          | 7.22632        |         |         |
| Corrected Total            | 30 | 851.38154          |                |         |         |
| Root MSE                   |    | 2.68818            | R-Square       | 0.7708  |         |
| Dependent Mean             |    | 47.37581           | Adj R-Sq       | 0.7454  |         |
| Coeff Var                  |    | 5.67416            |                |         |         |
| Parameter Estimates        |    |                    |                |         |         |
| Variable                   | DF | Parameter Estimate | Standard Error | t Value | Pr >  t |
| Intercept                  | 1  | 93.12615           | 7.55916        | 12.32   | <.0001  |
| RunTime                    | 1  | -3.14039           | 0.36738        | -8.55   | <.0001  |
| Age                        | 1  | -0.17388           | 0.09955        | -1.75   | 0.0921  |
| Weight                     | 1  | -0.05444           | 0.06181        | -0.88   | 0.3862  |

In the preceding example, the TYPE= data set option is not required since PROC REG sets the OUTSSCP= data set to TYPE=SSCP.

## Output Data Sets

### OUTEST= Data Set

The OUTEST= specification produces a TYPE=EST output SAS data set containing estimates and optional statistics from the regression models. For each BY group on each dependent variable occurring in each MODEL statement, PROC REG outputs an observation to the OUTEST= data set. The variables output to the data set are as follows:

- the BY variables, if any
- `_MODEL_`, a character variable containing the label of the corresponding MODEL statement, or `MODEL $n$`  if no label is specified, where  $n$  is 1 for the first MODEL statement, 2 for the second model statement, and so on
- `_TYPE_`, a character variable with the value 'PARMS' for every observation

- `_DEPVAR_`, the name of the dependent variable
- `_RMSE_`, the root mean squared error or the estimate of the standard deviation of the error term
- Intercept, the estimated intercept, unless the NOINT option is specified
- all the variables listed in any `MODEL` or `VAR` statement. Values of these variables are the estimated regression coefficients for the model. A variable that does not appear in the model corresponding to a given observation has a missing value in that observation. The dependent variable in each model is given a value of  $-1$ .

If you specify the COVOUT option, the covariance matrix of the estimates is output after the estimates; the `_TYPE_` variable is set to the value 'COV' and the names of the rows are identified by the character variable, `_NAME_`.

If you specify the TABLEOUT option, the following statistics listed by `_TYPE_` are added after the estimates:

- STDERR, the standard error of the estimate
- T, the  $t$  statistic for testing if the estimate is zero
- PVALUE, the associated  $p$ -value
- $L_nB$ , the  $100(1-\alpha)$  lower confidence limit for the estimate, where  $n$  is the nearest integer to  $100(1-\alpha)$  and  $\alpha$  defaults to 0.05 or is set by using the ALPHA= option in the `PROC REG` or `MODEL` statement
- $U_nB$ , the  $100(1-\alpha)$  upper confidence limit for the estimate

Specifying the option ADJRSQ, AIC, BIC, CP, EDF, GMSEP, JP, MSE, PC, RSQUARE, SBC, SP, or SSE in the `PROC REG` or `MODEL` statement automatically outputs these statistics and the model  $R^2$  for each model selected, regardless of the model selection method. Additional variables, in order of occurrence, are as follows:

- `_IN_`, the number of regressors in the model not including the intercept
- `_P_`, the number of parameters in the model including the intercept, if any
- `_EDF_`, the error degrees of freedom
- `_SSE_`, the error sum of squares, if the SSE option is specified
- `_MSE_`, the mean squared error, if the MSE option is specified
- `_RSQ_`, the R square statistic
- `_ADJRSQ_`, the adjusted R square, if the ADJRSQ option is specified
- `_CP_`, the  $C_p$  statistic, if the CP option is specified
- `_SP_`, the  $S_p$  statistic, if the SP option is specified
- `_JP_`, the  $J_p$  statistic, if the JP option is specified

- `_PC_`, the PC statistic, if the PC option is specified
- `_GMSEP_`, the GMSEP statistic, if the GMSEP option is specified
- `_AIC_`, the AIC statistic, if the AIC option is specified
- `_BIC_`, the BIC statistic, if the BIC option is specified
- `_SBC_`, the SBC statistic, if the SBC option is specified

The following statements produce and display the OUTEST= data set. This example uses the population data given in the section “Polynomial Regression” on page 6620. Figure 79.18 through Figure 79.20 show the regression equations and the resulting OUTEST= data set.

```
proc reg data=USPopulation outest=est;
 m1: model Population=Year;
 m2: model Population=Year YearSq;
run;
proc print data=est;
run;
```

**Figure 79.18** Regression Output for Model M1

| The REG Procedure              |    |                    |                |          |         |
|--------------------------------|----|--------------------|----------------|----------|---------|
| Model: m1                      |    |                    |                |          |         |
| Dependent Variable: Population |    |                    |                |          |         |
| Analysis of Variance           |    |                    |                |          |         |
| Source                         | DF | Sum of Squares     | Mean Square    | F Value  | Pr > F  |
| Model                          | 1  | 146869             | 146869         | 228.92   | <.0001  |
| Error                          | 20 | 12832              | 641.58160      |          |         |
| Corrected Total                | 21 | 159700             |                |          |         |
|                                |    | Root MSE           | 25.32946       | R-Square | 0.9197  |
|                                |    | Dependent Mean     | 94.64800       | Adj R-Sq | 0.9156  |
|                                |    | Coeff Var          | 26.76175       |          |         |
| Parameter Estimates            |    |                    |                |          |         |
| Variable                       | DF | Parameter Estimate | Standard Error | t Value  | Pr >  t |
| Intercept                      | 1  | -2345.85498        | 161.39279      | -14.54   | <.0001  |
| Year                           | 1  | 1.28786            | 0.08512        | 15.13    | <.0001  |

**Figure 79.19** Regression Output for Model M2

| Analysis of Variance |    |                    |                |         |         |
|----------------------|----|--------------------|----------------|---------|---------|
| Source               | DF | Sum of Squares     | Mean Square    | F Value | Pr > F  |
| Model                | 2  | 159529             | 79765          | 8864.19 | <.0001  |
| Error                | 19 | 170.97193          | 8.99852        |         |         |
| Corrected Total      | 21 | 159700             |                |         |         |
| Root MSE             |    | 2.99975            | R-Square       | 0.9989  |         |
| Dependent Mean       |    | 94.64800           | Adj R-Sq       | 0.9988  |         |
| Coeff Var            |    | 3.16938            |                |         |         |
| Parameter Estimates  |    |                    |                |         |         |
| Variable             | DF | Parameter Estimate | Standard Error | t Value | Pr >  t |
| Intercept            | 1  | 21631              | 639.50181      | 33.82   | <.0001  |
| Year                 | 1  | -24.04581          | 0.67547        | -35.60  | <.0001  |
| YearSq               | 1  | 0.00668            | 0.00017820     | 37.51   | <.0001  |

**Figure 79.20** OUTEST= Data Set

| Obs | _MODEL_ | _TYPE_ | _DEPVAR_   | _RMSE_  | Intercept | Year     | Population | YearSq     |
|-----|---------|--------|------------|---------|-----------|----------|------------|------------|
| 1   | m1      | PARMS  | Population | 25.3295 | -2345.85  | 1.2879   | -1         | .          |
| 2   | m2      | PARMS  | Population | 2.9998  | 21630.89  | -24.0458 | -1         | .006684346 |

The following modification of the previous example uses the TABLEOUT and ALPHA= options to obtain additional information in the OUTEST= data set:

```
proc reg data=USPopulation outest=est tableout alpha=0.1;
 m1: model Population=Year/noprint;
 m2: model Population=Year YearSq/noprint;
run;
proc print data=est;
run;
```

Notice that the TABLEOUT option causes standard errors, *t* statistics, *p*-values, and confidence limits for the estimates to be added to the OUTEST= data set. Also note that the ALPHA= option is used to set the confidence level at 90%. The OUTEST= data set is shown in [Figure 79.21](#).



**Figure 79.21** The OUTEST= Data Set When TABLEOUT Is Specified

| Obs | MODEL | TYPE   | DEPVAR     | RMSE    | Intercept | Year     | Population | YearSq  |
|-----|-------|--------|------------|---------|-----------|----------|------------|---------|
| 1   | m1    | PARMS  | Population | 25.3295 | -2345.85  | 1.2879   | -1         | .       |
| 2   | m1    | STDERR | Population | 25.3295 | 161.39    | 0.0851   | .          | .       |
| 3   | m1    | T      | Population | 25.3295 | -14.54    | 15.1300  | .          | .       |
| 4   | m1    | PVALUE | Population | 25.3295 | 0.00      | 0.0000   | .          | .       |
| 5   | m1    | L90B   | Population | 25.3295 | -2624.21  | 1.1411   | .          | .       |
| 6   | m1    | U90B   | Population | 25.3295 | -2067.50  | 1.4347   | .          | .       |
| 7   | m2    | PARMS  | Population | 2.9998  | 21630.89  | -24.0458 | -1         | 0.0067  |
| 8   | m2    | STDERR | Population | 2.9998  | 639.50    | 0.6755   | .          | 0.0002  |
| 9   | m2    | T      | Population | 2.9998  | 33.82     | -35.5988 | .          | 37.5096 |
| 10  | m2    | PVALUE | Population | 2.9998  | 0.00      | 0.0000   | .          | 0.0000  |
| 11  | m2    | L90B   | Population | 2.9998  | 20525.11  | -25.2138 | .          | 0.0064  |
| 12  | m2    | U90B   | Population | 2.9998  | 22736.68  | -22.8778 | .          | 0.0070  |

A slightly different OUTEST= data set is created when you use the RSQUARE selection method. The following statements request only the “best” model for each subset size but ask for a variety of model selection statistics, as well as the estimated regression coefficients. An OUTEST= data set is created and displayed. See [Figure 79.22](#) and [Figure 79.23](#) for the results.

```
proc reg data=fitness outest=est;
 model Oxygen=Age Weight RunTime RunPulse RestPulse MaxPulse
 / selection=rsquare mse jp gmsep cp aic bic sbc b best=1;
run;
proc print data=est;
run;
```

Figure 79.22 PROC REG Output for Physical Fitness Data: Best Models

| The REG Procedure          |          |         |         |         |                             |        |         |
|----------------------------|----------|---------|---------|---------|-----------------------------|--------|---------|
| Model: MODEL1              |          |         |         |         |                             |        |         |
| Dependent Variable: Oxygen |          |         |         |         |                             |        |         |
| R-Square Selection Method  |          |         |         |         |                             |        |         |
| Number in Model            | R-Square | C(p)    | AIC     | BIC     | Estimated MSE of Prediction | J(p)   | MSE     |
| 1                          | 0.7434   | 13.6988 | 64.5341 | 65.4673 | 8.0546                      | 8.0199 | 7.53384 |
| 2                          | 0.7642   | 12.3894 | 63.9050 | 64.8212 | 7.9478                      | 7.8621 | 7.16842 |
| 3                          | 0.8111   | 6.9596  | 59.0373 | 61.3127 | 6.8583                      | 6.7253 | 5.95669 |
| 4                          | 0.8368   | 4.8800  | 56.4995 | 60.3996 | 6.3984                      | 6.2053 | 5.34346 |
| 5                          | 0.8480   | 5.1063  | 56.2986 | 61.5667 | 6.4565                      | 6.1782 | 5.17634 |
| 6                          | 0.8487   | 7.0000  | 58.1616 | 64.0748 | 6.9870                      | 6.5804 | 5.36825 |

| Number in Model | R-Square | SBC      | Intercept | Age      | Weight   | RunTime  |
|-----------------|----------|----------|-----------|----------|----------|----------|
| 1               | 0.7434   | 67.40210 | 82.42177  | .        | .        | -3.31056 |
| 2               | 0.7642   | 68.20695 | 88.46229  | -0.15037 | .        | -3.20395 |
| 3               | 0.8111   | 64.77326 | 111.71806 | -0.25640 | .        | -2.82538 |
| 4               | 0.8368   | 63.66941 | 98.14789  | -0.19773 | .        | -2.76758 |
| 5               | 0.8480   | 64.90250 | 102.20428 | -0.21962 | -0.07230 | -2.68252 |
| 6               | 0.8487   | 68.19952 | 102.93448 | -0.22697 | -0.07418 | -2.62865 |

| Number in Model | R-Square | RunPulse | RestPulse | MaxPulse |
|-----------------|----------|----------|-----------|----------|
| 1               | 0.7434   | .        | .         | .        |
| 2               | 0.7642   | .        | .         | .        |
| 3               | 0.8111   | -0.13091 | .         | .        |
| 4               | 0.8368   | -0.34811 | .         | 0.27051  |
| 5               | 0.8480   | -0.37340 | .         | 0.30491  |
| 6               | 0.8487   | -0.36963 | -0.02153  | 0.30322  |

**Figure 79.23** PROC PRINT Output for Physical Fitness Data: OUTEST= Data Set

| Obs | MODEL  | TYPE  | DEPVAR | RMSE    | Intercept | Age      | Weight    |
|-----|--------|-------|--------|---------|-----------|----------|-----------|
| 1   | MODEL1 | PARMS | Oxygen | 2.74478 | 82.422    | .        | .         |
| 2   | MODEL1 | PARMS | Oxygen | 2.67739 | 88.462    | -0.15037 | .         |
| 3   | MODEL1 | PARMS | Oxygen | 2.44063 | 111.718   | -0.25640 | .         |
| 4   | MODEL1 | PARMS | Oxygen | 2.31159 | 98.148    | -0.19773 | .         |
| 5   | MODEL1 | PARMS | Oxygen | 2.27516 | 102.204   | -0.21962 | -0.072302 |
| 6   | MODEL1 | PARMS | Oxygen | 2.31695 | 102.934   | -0.22697 | -0.074177 |

| Obs | RunTime  | RunPulse | RestPulse | Max<br>Pulse | Oxygen | _IN_ | _P_ | _EDF_ | _MSE_   |
|-----|----------|----------|-----------|--------------|--------|------|-----|-------|---------|
| 1   | -3.31056 | .        | .         | .            | -1     | 1    | 2   | 29    | 7.53384 |
| 2   | -3.20395 | .        | .         | .            | -1     | 2    | 3   | 28    | 7.16842 |
| 3   | -2.82538 | -0.13091 | .         | .            | -1     | 3    | 4   | 27    | 5.95669 |
| 4   | -2.76758 | -0.34811 | .         | 0.27051      | -1     | 4    | 5   | 26    | 5.34346 |
| 5   | -2.68252 | -0.37340 | .         | 0.30491      | -1     | 5    | 6   | 25    | 5.17634 |
| 6   | -2.62865 | -0.36963 | -0.021534 | 0.30322      | -1     | 6    | 7   | 24    | 5.36825 |

| Obs | RSQ     | CP      | JP      | GMSEP   | AIC     | BIC     | SBC     |
|-----|---------|---------|---------|---------|---------|---------|---------|
| 1   | 0.74338 | 13.6988 | 8.01990 | 8.05462 | 64.5341 | 65.4673 | 67.4021 |
| 2   | 0.76425 | 12.3894 | 7.86214 | 7.94778 | 63.9050 | 64.8212 | 68.2069 |
| 3   | 0.81109 | 6.9596  | 6.72530 | 6.85833 | 59.0373 | 61.3127 | 64.7733 |
| 4   | 0.83682 | 4.8800  | 6.20531 | 6.39837 | 56.4995 | 60.3996 | 63.6694 |
| 5   | 0.84800 | 5.1063  | 6.17821 | 6.45651 | 56.2986 | 61.5667 | 64.9025 |
| 6   | 0.84867 | 7.0000  | 6.58043 | 6.98700 | 58.1616 | 64.0748 | 68.1995 |

## OUTSSCP= Data Sets

The OUTSSCP= option produces a TYPE=SSCP output SAS data set containing sums of squares and crossproducts. A special row (observation) and column (variable) of the matrix called Intercept contain the number of observations and sums. Observations are identified by the character variable `_NAME_`. The data set contains all variables used in `MODEL` statements. You can specify additional variables that you want included in the crossproducts matrix with a `VAR` statement.

The SSCP data set is used when a large number of observations are explored in many different runs. The SSCP data set can be saved and used for subsequent runs, which are much less expensive since PROC REG never reads the original data again. If you run PROC REG once to create only a SSCP data set, you should list all the variables that you might need in a `VAR` statement or include all the variables that you might need in a `MODEL` statement.

The following statements use the fitness data from [Example 79.2](#) to produce an output data set with the OUTSSCP= option. The resulting output is shown in [Figure 79.24](#).

```
proc reg data=fitness outsscp=sscp;
 var Oxygen RunTime Age Weight RestPulse RunPulse MaxPulse;
run;
proc print data=sscp;
run;
```

Since a model is not fit to the data and since the only request is to create the SSCP data set, a **MODEL** statement is not required in this example. However, since the **MODEL** statement is not used, the **VAR** statement is required.

**Figure 79.24** SSCP Data Set Created with OUTSSCP= Option: REG Procedure

| Obs | _TYPE_ | _NAME_    | Intercept | Oxygen    | RunTime  | Age       |
|-----|--------|-----------|-----------|-----------|----------|-----------|
| 1   | SSCP   | Intercept | 31.00     | 1468.65   | 328.17   | 1478.00   |
| 2   | SSCP   | Oxygen    | 1468.65   | 70429.86  | 15356.14 | 69767.75  |
| 3   | SSCP   | RunTime   | 328.17    | 15356.14  | 3531.80  | 15687.24  |
| 4   | SSCP   | Age       | 1478.00   | 69767.75  | 15687.24 | 71282.00  |
| 5   | SSCP   | Weight    | 2400.78   | 113522.26 | 25464.71 | 114158.90 |
| 6   | SSCP   | RestPulse | 1657.00   | 78015.41  | 17684.05 | 78806.00  |
| 7   | SSCP   | RunPulse  | 5259.00   | 248497.31 | 55806.29 | 250194.00 |
| 8   | SSCP   | MaxPulse  | 5387.00   | 254866.75 | 57113.72 | 256218.00 |
| 9   | N      |           | 31.00     | 31.00     | 31.00    | 31.00     |

| Obs | Weight    | RestPulse | RunPulse  | MaxPulse  |
|-----|-----------|-----------|-----------|-----------|
| 1   | 2400.78   | 1657.00   | 5259.00   | 5387.00   |
| 2   | 113522.26 | 78015.41  | 248497.31 | 254866.75 |
| 3   | 25464.71  | 17684.05  | 55806.29  | 57113.72  |
| 4   | 114158.90 | 78806.00  | 250194.00 | 256218.00 |
| 5   | 188008.20 | 128409.28 | 407745.67 | 417764.62 |
| 6   | 128409.28 | 90311.00  | 281928.00 | 288583.00 |
| 7   | 407745.67 | 281928.00 | 895317.00 | 916499.00 |
| 8   | 417764.62 | 288583.00 | 916499.00 | 938641.00 |
| 9   | 31.00     | 31.00     | 31.00     | 31.00     |

## Interactive Analysis

PROC REG enables you to change interactively both the model and the data used to compute the model, and to produce and highlight scatter plots. See the section “Using PROC REG Interactively” on page 6630 for an overview of interactive analysis that uses PROC REG. The following statements can be used interactively (without reinvoking PROC REG): **ADD**, **DELETE**, **MODEL**, **MTEST**, **OUTPUT**, **PAINT**, **PLOT**, **PRINT**, **REFIT**, **RESTRICT**, **REWEIGHT**, and **TEST**. All interactive features are disabled if there is a **BY** statement.

The **ADD**, **DELETE**, and **REWEIGHT** statements can be used to modify the current **MODEL**. Every use of an **ADD**, **DELETE**, or **REWEIGHT** statement causes the model label to be modified by attaching an additional number to it. This number is the cumulative total of the number of **ADD**, **DELETE**, or **REWEIGHT** statements following the current **MODEL** statement.

A more detailed explanation of changing the data used to compute the model is given in the section “Reweightings Observations in an Analysis” on page 6726.

The following statements illustrate the usefulness of the interactive features. First, the full regression model is fit to the Sashelp.Class data, and Figure 79.25 is produced.

```
ods graphics on;

proc reg data=sashelp.Class plots(modelLabel only)=ResidualByPredicted;
 model Weight=Age Height;
run;
```

Figure 79.25 Interactive Analysis: Full Model

| The REG Procedure          |    |                    |                |         |         |
|----------------------------|----|--------------------|----------------|---------|---------|
| Model: MODEL1              |    |                    |                |         |         |
| Dependent Variable: Weight |    |                    |                |         |         |
| Analysis of Variance       |    |                    |                |         |         |
| Source                     | DF | Sum of Squares     | Mean Square    | F Value | Pr > F  |
| Model                      | 2  | 7215.63710         | 3607.81855     | 27.23   | <.0001  |
| Error                      | 16 | 2120.09974         | 132.50623      |         |         |
| Corrected Total            | 18 | 9335.73684         |                |         |         |
| Root MSE                   |    | 11.51114           | R-Square       | 0.7729  |         |
| Dependent Mean             |    | 100.02632          | Adj R-Sq       | 0.7445  |         |
| Coeff Var                  |    | 11.50811           |                |         |         |
| Parameter Estimates        |    |                    |                |         |         |
| Variable                   | DF | Parameter Estimate | Standard Error | t Value | Pr >  t |
| Intercept                  | 1  | -141.22376         | 33.38309       | -4.23   | 0.0006  |
| Age                        | 1  | 1.27839            | 3.11010        | 0.41    | 0.6865  |
| Height                     | 1  | 3.59703            | 0.90546        | 3.97    | 0.0011  |

Next, the regression model is reduced by the following statements, and Figure 79.26 is produced.

```
delete age;
print;
run;
```

**Figure 79.26** Interactive Analysis: Reduced Model

| Analysis of Variance |                |                    |                |         |         |
|----------------------|----------------|--------------------|----------------|---------|---------|
| Source               | DF             | Sum of Squares     | Mean Square    | F Value | Pr > F  |
| Model                | 1              | 7193.24912         | 7193.24912     | 57.08   | <.0001  |
| Error                | 17             | 2142.48772         | 126.02869      |         |         |
| Corrected Total      | 18             | 9335.73684         |                |         |         |
|                      | Root MSE       | 11.22625           | R-Square       | 0.7705  |         |
|                      | Dependent Mean | 100.02632          | Adj R-Sq       | 0.7570  |         |
|                      | Coeff Var      | 11.22330           |                |         |         |
| Parameter Estimates  |                |                    |                |         |         |
| Variable             | DF             | Parameter Estimate | Standard Error | t Value | Pr >  t |
| Intercept            | 1              | -143.02692         | 32.27459       | -4.43   | 0.0004  |
| Height               | 1              | 3.89903            | 0.51609        | 7.55    | <.0001  |

Note that the MODEL label has been changed from MODEL1 to MODEL1.1, since the original MODEL has been changed by the delete statement.

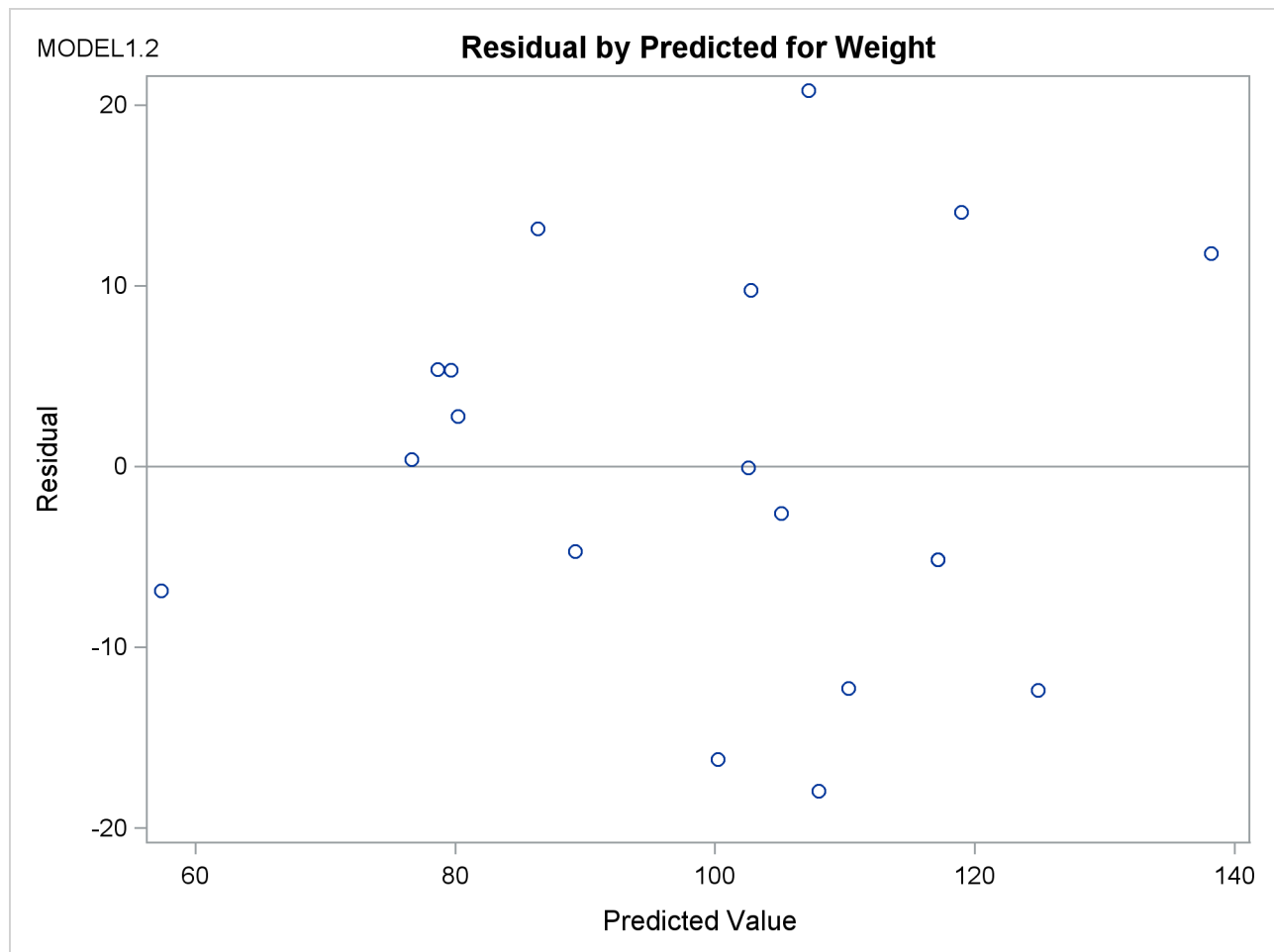
When ODS Graphics is enabled, updated plots are produced whenever a **PRINT** statement is used. The option

```
plots(modelLabel only)=ResidualByPredicted
```

in the PROC REG statement specifies that the only plot produced is a scatter plot of residuals by predicted values. The MODEL LABEL option specifies that the current model label is added to the plot.

The following statements generate a scatter plot of the residuals against the predicted values from the full model. [Figure 79.27](#) is produced, and the scatter plot shows a possible outlier.

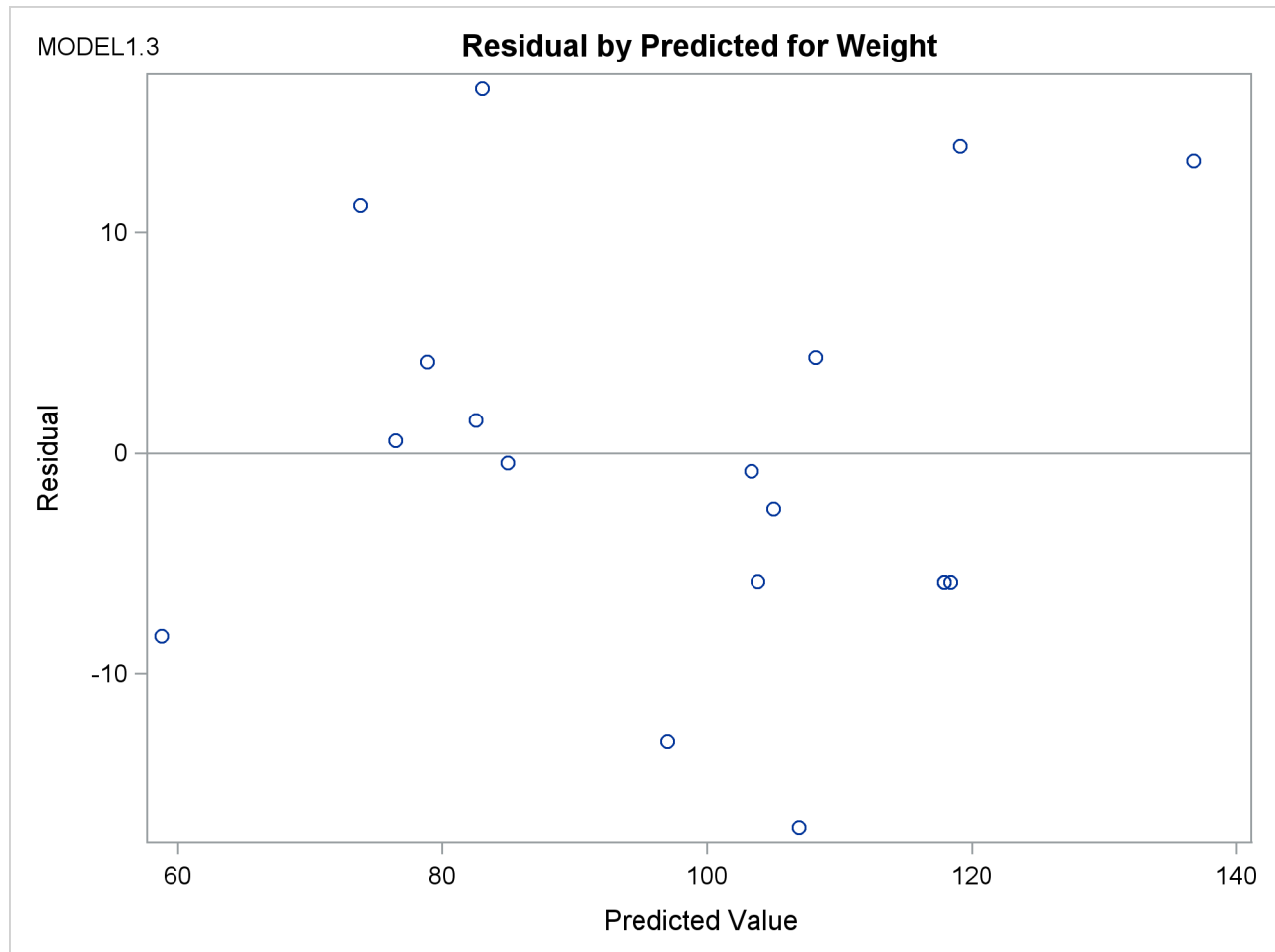
```
add age;
print;
run;
```

**Figure 79.27** Interactive Analysis: Scatter Plot

The following statements delete the observation with the largest residual, refit the regression model, and produce a scatter plot of residuals against predicted values for the refitted model. [Figure 79.28](#) shows the new scatter plot.

```
reweight r.>20;
print;
run;

ods graphics off;
```

**Figure 79.28** Interactive Analysis: Scatter Plot

## Model-Selection Methods

The nine methods of model selection implemented in PROC REG are specified with the `SELECTION=` option in the `MODEL` statement. Each method is discussed in this section.

### Full Model Fitted (NONE)

This method is the default and provides no model selection capability. The complete model specified in the `MODEL` statement is used to fit the model. For many regression analyses, this might be the only method you need.

### Forward Selection (FORWARD)

The forward-selection technique begins with no variables in the model. For each of the independent variables, the FORWARD method calculates  $F$  statistics that reflect the variable's contribution to the model if it is included. The  $p$ -values for these  $F$  statistics are compared to the `SLENTRY=` value that is specified in the `MODEL` statement (or to 0.50 if the `SLENTRY=` option is omitted). If no  $F$  statistic has a significance level



greater than the `SLENTRY=` value, the FORWARD selection stops. Otherwise, the FORWARD method adds the variable that has the largest  $F$  statistic to the model. The FORWARD method then calculates  $F$  statistics again for the variables still remaining outside the model, and the evaluation process is repeated. Thus, variables are added one by one to the model until no remaining variable produces a significant  $F$  statistic. Once a variable is in the model, it stays.

### Backward Elimination (BACKWARD)

The backward elimination technique begins by calculating  $F$  statistics for a model which includes all of the independent variables. Then the variables are deleted from the model one by one until all the variables remaining in the model produce  $F$  statistics significant at the `SLSTAY=` level specified in the `MODEL` statement (or at the 0.10 level if the `SLSTAY=` option is omitted). At each step, the variable showing the smallest contribution to the model is deleted.

### Stepwise (STEPWISE)

The stepwise method is a modification of the forward-selection technique and differs in that variables already in the model do not necessarily stay there. As in the forward-selection method, variables are added one by one to the model, and the  $F$  statistic for a variable to be added must be significant at the `SLENTRY=` level. After a variable is added, however, the stepwise method looks at all the variables already included in the model and deletes any variable that does not produce an  $F$  statistic significant at the `SLSTAY=` level. Only after this check is made and the necessary deletions are accomplished can another variable be added to the model. The stepwise process ends when none of the variables outside the model has an  $F$  statistic significant at the `SLENTRY=` level and every variable in the model is significant at the `SLSTAY=` level, or when the variable to be added to the model is the one just deleted from it.

### Maximum R<sup>2</sup> Improvement (MAXR)

The maximum R square improvement technique does not settle on a single model. Instead, it tries to find the “best” one-variable model, the “best” two-variable model, and so forth, although it is not guaranteed to find the model with the largest R square for each size.

The MAXR method begins by finding the one-variable model producing the highest R square. Then another variable, the one that yields the greatest increase in R square, is added. Once the two-variable model is obtained, each of the variables in the model is compared to each variable not in the model. For each comparison, the MAXR method determines if removing one variable and replacing it with the other variable increases R square. After comparing all possible switches, the MAXR method makes the switch that produces the largest increase in R square. Comparisons begin again, and the process continues until the MAXR method finds that no switch could increase R square. Thus, the two-variable model achieved is considered the “best” two-variable model the technique can find. Another variable is then added to the model, and the comparing-and-switching process is repeated to find the “best” three-variable model, and so forth.

The difference between the STEPWISE method and the MAXR method is that all switches are evaluated before any switch is made in the MAXR method. In the STEPWISE method, the “worst” variable might be removed without considering what adding the “best” remaining variable might accomplish. The MAXR method might require much more computer time than the STEPWISE method.

## Minimum R<sup>2</sup> (MINR) Improvement

The MINR method closely resembles the MAXR method, but the switch chosen is the one that produces the smallest increase in R square. For a given number of variables in the model, the MAXR and MINR methods usually produce the same “best” model, but the MINR method considers more models of each size.

## R<sup>2</sup> Selection (RSQUARE)

The RSQUARE method finds subsets of independent variables that best predict a dependent variable by linear regression in the given sample. You can specify the largest and smallest number of independent variables to appear in a subset and the number of subsets of each size to be selected. The RSQUARE method can efficiently perform all possible subset regressions and display the models in decreasing order of R square magnitude within each subset size. Other statistics are available for comparing subsets of different sizes. These statistics, as well as estimated regression coefficients, can be displayed or output to a SAS data set.

The subset models selected by the RSQUARE method are optimal in terms of R square for the given sample, but they are not necessarily optimal for the population from which the sample is drawn or for any other sample for which you might want to make predictions. If a subset model is selected on the basis of a large R square value or any other criterion commonly used for model selection, then all regression statistics computed for that model under the assumption that the model is given a priori, including all statistics computed by PROC REG, are biased.

While the RSQUARE method is a useful tool for exploratory model building, no statistical method can be relied on to identify the “true” model. Effective model building requires substantive theory to suggest relevant predictors and plausible functional forms for the model.

The RSQUARE method differs from the other selection methods in that RSQUARE always identifies the model with the largest R square for each number of variables considered. The other selection methods are not guaranteed to find the model with the largest R square. The RSQUARE method requires much more computer time than the other selection methods, so a different selection method such as the STEPWISE method is a good choice when there are many independent variables to consider.

## Adjusted R<sup>2</sup> Selection (ADJRSQ)

This method is similar to the RSQUARE method, except that the adjusted R square statistic is used as the criterion for selecting models, and the method finds the models with the highest adjusted R square within the range of sizes.

## Mallows' C<sub>p</sub> Selection (CP)

This method is similar to the ADJRSQ method, except that Mallows'  $C_p$  statistic is used as the criterion for model selection. Models are listed in ascending order of  $C_p$ .

## Additional Information about Model-Selection Methods

If the RSQUARE or STEPWISE procedure (as documented in *SAS User's Guide: Statistics, Version 5 Edition*) is requested, PROC REG with the appropriate model-selection method is actually used.

Reviews of model-selection methods by Hocking (1976) and Judge et al. (1980) describe these and other variable-selection methods.

---

## Criteria Used in Model-Selection Methods

When many significance tests are performed, each at a level of, for example, 5%, the overall probability of rejecting at least one true null hypothesis is much larger than 5%. If you want to guard against including any variables that do not contribute to the predictive power of the model in the population, you should specify a very small SLE= significance level for the FORWARD and STEPWISE methods and a very small SLS= significance level for the BACKWARD and STEPWISE methods.

In most applications, many of the variables considered have some predictive power, however small. If you want to choose the model that provides the best prediction computed using the sample estimates, you need only to guard against estimating more parameters than can be reliably estimated with the given sample size, so you should use a moderate significance level, perhaps in the range of 10% to 25%.

In addition to R square, the  $C_p$  statistic is displayed for each model generated in the model-selection methods. The  $C_p$  statistic is proposed by Mallows (1973) as a criterion for selecting a model. It is a measure of total squared error defined as

$$C_p = \frac{SSE_p}{s^2} - (N - 2p)$$

where  $s^2$  is the MSE for the full model, and  $SSE_p$  is the sum-of-squares error for a model with  $p$  parameters including the intercept, if any. If  $C_p$  is plotted against  $p$ , Mallows recommends the model where  $C_p$  first approaches  $p$ . When the right model is chosen, the parameter estimates are unbiased, and this is reflected in  $C_p$  near  $p$ . For further discussion, see Daniel and Wood (1980).

The adjusted R square statistic is an alternative to R square that is adjusted for the number of parameters in the model. The adjusted R square statistic is calculated as

$$ADJRSQ = 1 - \frac{(n - i)(1 - R^2)}{n - p}$$

where  $n$  is the number of observations used in fitting the model, and  $i$  is an indicator variable that is 1 if the model includes an intercept, and 0 otherwise.

---

## Limitations in Model-Selection Methods

The use of model-selection methods can be time-consuming in some cases because there is no built-in limit on the number of independent variables, and the calculations for a large number of independent variables can be lengthy. The recommended limit on the number of independent variables for the MINR method is  $20 + i$ , where  $i$  is the value of the INCLUDE= option.

For the RSQUARE, ADJRSQ, or CP method, with a large value of the BEST= option, adding one more variable to the list from which regressors are selected might significantly increase the CPU time. Also, the time required for the analysis is highly dependent on the data and on the values of the BEST=, START=, and STOP= options.

## Parameter Estimates and Associated Statistics

The following example uses the fitness data from [Example 79.2](#). [Figure 79.30](#) shows the parameter estimates and the tables from the SS1, SS2, STB, CLB, COVB, and CORRB options:

```
proc reg data=fitness;
 model Oxygen=RunTime Age Weight RunPulse MaxPulse RestPulse
 / ss1 ss2 stb clb covb corrb;
run;
```

The procedure first displays an analysis of variance table ([Figure 79.29](#)). The  $F$  statistic for the overall model is significant, indicating that the model explains a significant portion of the variation in the data.

**Figure 79.29** ANOVA Table

| The REG Procedure          |    |                |             |         |        |
|----------------------------|----|----------------|-------------|---------|--------|
| Model: MODEL1              |    |                |             |         |        |
| Dependent Variable: Oxygen |    |                |             |         |        |
| Analysis of Variance       |    |                |             |         |        |
| Source                     | DF | Sum of Squares | Mean Square | F Value | Pr > F |
| Model                      | 6  | 722.54361      | 120.42393   | 22.43   | <.0001 |
| Error                      | 24 | 128.83794      | 5.36825     |         |        |
| Corrected Total            | 30 | 851.38154      |             |         |        |
| Root MSE                   |    | 2.31695        | R-Square    | 0.8487  |        |
| Dependent Mean             |    | 47.37581       | Adj R-Sq    | 0.8108  |        |
| Coeff Var                  |    | 4.89057        |             |         |        |

The procedure next displays parameter estimates and some associated statistics ([Figure 79.30](#)). First, the estimates are shown, followed by their standard errors. The next two columns of the table contain the  $t$  statistics and the corresponding probabilities for testing the null hypothesis that the parameter is not significantly different from zero. These probabilities are usually referred to as  $p$ -values. For example, the Intercept term in the model is estimated to be 102.9 and is significantly different from zero. The next two columns of the table are the result of requesting the SS1 and SS2 options, and they show sequential and partial sums of squares (SS) associated with each variable. The standardized estimates (produced by the STB option) are the parameter estimates that result when all variables are standardized to a mean of 0 and a variance of 1. These estimates are computed by multiplying the original estimates by the standard deviation of the regressor (independent) variable and then dividing by the standard deviation of the dependent variable. The CLB option adds the upper and lower 95% confidence limits for the parameter estimates; the  $\alpha$  level can be changed by specifying the ALPHA= option in the [PROC REG](#) or [MODEL](#) statement.

**Figure 79.30** SS1, SS2, STB, CLB, COVB, and CORRB Options: Parameter Estimates

| Parameter Estimates |    |                    |                |         |         |           |
|---------------------|----|--------------------|----------------|---------|---------|-----------|
| Variable            | DF | Parameter Estimate | Standard Error | t Value | Pr >  t | Type I SS |
| Intercept           | 1  | 102.93448          | 12.40326       | 8.30    | <.0001  | 69578     |
| RunTime             | 1  | -2.62865           | 0.38456        | -6.84   | <.0001  | 632.90010 |
| Age                 | 1  | -0.22697           | 0.09984        | -2.27   | 0.0322  | 17.76563  |
| Weight              | 1  | -0.07418           | 0.05459        | -1.36   | 0.1869  | 5.60522   |
| RunPulse            | 1  | -0.36963           | 0.11985        | -3.08   | 0.0051  | 38.87574  |
| MaxPulse            | 1  | 0.30322            | 0.13650        | 2.22    | 0.0360  | 26.82640  |
| RestPulse           | 1  | -0.02153           | 0.06605        | -0.33   | 0.7473  | 0.57051   |

| Parameter Estimates |    |            |                       |                       |           |
|---------------------|----|------------|-----------------------|-----------------------|-----------|
| Variable            | DF | Type II SS | Standardized Estimate | 95% Confidence Limits |           |
| Intercept           | 1  | 369.72831  | 0                     | 77.33541              | 128.53355 |
| RunTime             | 1  | 250.82210  | -0.68460              | -3.42235              | -1.83496  |
| Age                 | 1  | 27.74577   | -0.22204              | -0.43303              | -0.02092  |
| Weight              | 1  | 9.91059    | -0.11597              | -0.18685              | 0.03850   |
| RunPulse            | 1  | 51.05806   | -0.71133              | -0.61699              | -0.12226  |
| MaxPulse            | 1  | 26.49142   | 0.52161               | 0.02150               | 0.58493   |
| RestPulse           | 1  | 0.57051    | -0.03080              | -0.15786              | 0.11480   |

The final two tables are produced as a result of requesting the COVB and CORRB options (Figure 79.31). These tables show the estimated covariance matrix of the parameter estimates, and the estimated correlation matrix of the estimates.

**Figure 79.31** SS1, SS2, STB, CLB, COVB, and CORRB Options: Covariances and Correlations

| Covariance of Estimates |              |              |              |              |
|-------------------------|--------------|--------------|--------------|--------------|
| Variable                | Intercept    | RunTime      | Age          | Weight       |
| Intercept               | 153.84081152 | 0.7678373769 | -0.902049478 | -0.178237818 |
| RunTime                 | 0.7678373769 | 0.1478880839 | -0.014191688 | -0.004417672 |
| Age                     | -0.902049478 | -0.014191688 | 0.009967521  | 0.0010219105 |
| Weight                  | -0.178237818 | -0.004417672 | 0.0010219105 | 0.0029804131 |
| RunPulse                | 0.280796516  | -0.009047784 | -0.001203914 | 0.0009644683 |
| MaxPulse                | -0.832761667 | 0.0046249498 | 0.0035823843 | -0.001372241 |
| RestPulse               | -0.147954715 | -0.010915224 | 0.0014897532 | 0.0003799295 |

| Covariance of Estimates |              |              |              |
|-------------------------|--------------|--------------|--------------|
| Variable                | RunPulse     | MaxPulse     | RestPulse    |
| Intercept               | 0.280796516  | -0.832761667 | -0.147954715 |
| RunTime                 | -0.009047784 | 0.0046249498 | -0.010915224 |
| Age                     | -0.001203914 | 0.0035823843 | 0.0014897532 |
| Weight                  | 0.0009644683 | -0.001372241 | 0.0003799295 |
| RunPulse                | 0.0143647273 | -0.014952457 | -0.000764507 |
| MaxPulse                | -0.014952457 | 0.0186309364 | 0.0003425724 |
| RestPulse               | -0.000764507 | 0.0003425724 | 0.0043631674 |

| Correlation of Estimates |           |         |         |         |
|--------------------------|-----------|---------|---------|---------|
| Variable                 | Intercept | RunTime | Age     | Weight  |
| Intercept                | 1.0000    | 0.1610  | -0.7285 | -0.2632 |
| RunTime                  | 0.1610    | 1.0000  | -0.3696 | -0.2104 |
| Age                      | -0.7285   | -0.3696 | 1.0000  | 0.1875  |
| Weight                   | -0.2632   | -0.2104 | 0.1875  | 1.0000  |
| RunPulse                 | 0.1889    | -0.1963 | -0.1006 | 0.1474  |
| MaxPulse                 | -0.4919   | 0.0881  | 0.2629  | -0.1842 |
| RestPulse                | -0.1806   | -0.4297 | 0.2259  | 0.1054  |

| Correlation of Estimates |          |          |           |
|--------------------------|----------|----------|-----------|
| Variable                 | RunPulse | MaxPulse | RestPulse |
| Intercept                | 0.1889   | -0.4919  | -0.1806   |
| RunTime                  | -0.1963  | 0.0881   | -0.4297   |
| Age                      | -0.1006  | 0.2629   | 0.2259    |
| Weight                   | 0.1474   | -0.1842  | 0.1054    |
| RunPulse                 | 1.0000   | -0.9140  | -0.0966   |
| MaxPulse                 | -0.9140  | 1.0000   | 0.0380    |
| RestPulse                | -0.0966  | 0.0380   | 1.0000    |

For further discussion of the parameters and statistics, see the section “Displayed Output” on page 6740, and Chapter 4, “Introduction to Regression Procedures.”

## Predicted and Residual Values

The display of the predicted values and residuals is controlled by the P, R, CLM, and CLI options in the **MODEL** statement. The P option causes PROC REG to display the observation number, the ID value (if an ID statement is used), the actual value, the predicted value, and the residual. The R, CLI, and CLM options also produce the items under the P option. Thus, P is unnecessary if you use one of the other options.

The R option requests more detail, especially about the residuals. The standard errors of the mean predicted value and the residual are displayed. The studentized residual, which is the residual divided by its standard error, is both displayed and plotted. A measure of influence, Cook's  $D$ , is displayed. Cook's  $D$  measures the change to the estimates that results from deleting each observation (Cook 1977, 1979). This statistic is very similar to DFFITS.

The CLM option requests that PROC REG display the  $100(1 - \alpha)\%$  lower and upper confidence limits for the mean predicted values. This accounts for the variation due to estimating the parameters only. If you want a  $100(1 - \alpha)\%$  confidence interval for observed values, then you can use the CLI option, which adds in the variability of the error term. The  $\alpha$  level can be specified with the ALPHA= option in the **PROC REG** or **MODEL** statement.

You can use these statistics in **PLOT** and **PAINT** statements. This is useful in performing a variety of regression diagnostics. For definitions of the statistics produced by these options, see Chapter 4, “Introduction to Regression Procedures.”

The following statements use the U.S. population data found in the section “Polynomial Regression” on page 6620. The results are shown in Figure 79.32 and Figure 79.33.

```
data USPop2;
 input Year @@;
 YearSq=Year*Year;
 datalines;
2010 2020 2030
;
data USPop2;
 set USPopulation USPop2;
run;

proc reg data=USPop2;
 id Year;
 model Population=Year YearSq / r cli clm;
run;
```

**Figure 79.32** Regression Using the R, CLI, and CLM Options

| The REG Procedure              |    |                    |                |         |         |
|--------------------------------|----|--------------------|----------------|---------|---------|
| Model: MODEL1                  |    |                    |                |         |         |
| Dependent Variable: Population |    |                    |                |         |         |
| Analysis of Variance           |    |                    |                |         |         |
| Source                         | DF | Sum of Squares     | Mean Square    | F Value | Pr > F  |
| Model                          | 2  | 159529             | 79765          | 8864.19 | <.0001  |
| Error                          | 19 | 170.97193          | 8.99852        |         |         |
| Corrected Total                | 21 | 159700             |                |         |         |
| Root MSE                       |    | 2.99975            | R-Square       | 0.9989  |         |
| Dependent Mean                 |    | 94.64800           | Adj R-Sq       | 0.9988  |         |
| Coeff Var                      |    | 3.16938            |                |         |         |
| Parameter Estimates            |    |                    |                |         |         |
| Variable                       | DF | Parameter Estimate | Standard Error | t Value | Pr >  t |
| Intercept                      | 1  | 21631              | 639.50181      | 33.82   | <.0001  |
| Year                           | 1  | -24.04581          | 0.67547        | -35.60  | <.0001  |
| YearSq                         | 1  | 0.00668            | 0.00017820     | 37.51   | <.0001  |



**Figure 79.33** Regression Using the R, CLI, and CLM Options

| The REG Procedure              |      |                    |                 |                        |             |          |                |          |
|--------------------------------|------|--------------------|-----------------|------------------------|-------------|----------|----------------|----------|
| Model: MODEL1                  |      |                    |                 |                        |             |          |                |          |
| Dependent Variable: Population |      |                    |                 |                        |             |          |                |          |
| Output Statistics              |      |                    |                 |                        |             |          |                |          |
| Obs                            | Year | Dependent Variable | Predicted Value | Std Error Mean Predict | 95% CL Mean |          | 95% CL Predict |          |
| 1                              | 1790 | 3.9290             | 6.2127          | 1.7565                 | 2.5362      | 9.8892   | -1.0631        | 13.4884  |
| 2                              | 1800 | 5.3080             | 5.7226          | 1.4560                 | 2.6751      | 8.7701   | -1.2565        | 12.7017  |
| 3                              | 1810 | 7.2390             | 6.5694          | 1.2118                 | 4.0331      | 9.1057   | -0.2021        | 13.3409  |
| 4                              | 1820 | 9.6380             | 8.7531          | 1.0305                 | 6.5963      | 10.9100  | 2.1144         | 15.3918  |
| 5                              | 1830 | 12.8660            | 12.2737         | 0.9163                 | 10.3558     | 14.1916  | 5.7087         | 18.8386  |
| 6                              | 1840 | 17.0690            | 17.1311         | 0.8650                 | 15.3207     | 18.9415  | 10.5968        | 23.6655  |
| 7                              | 1850 | 23.1910            | 23.3254         | 0.8613                 | 21.5227     | 25.1281  | 16.7932        | 29.8576  |
| 8                              | 1860 | 31.4430            | 30.8566         | 0.8846                 | 29.0051     | 32.7080  | 24.3107        | 37.4024  |
| 9                              | 1870 | 39.8180            | 39.7246         | 0.9163                 | 37.8067     | 41.6425  | 33.1597        | 46.2896  |
| 10                             | 1880 | 50.1550            | 49.9295         | 0.9436                 | 47.9545     | 51.9046  | 43.3476        | 56.5114  |
| 11                             | 1890 | 62.9470            | 61.4713         | 0.9590                 | 59.4641     | 63.4785  | 54.8797        | 68.0629  |
| 12                             | 1900 | 75.9940            | 74.3499         | 0.9590                 | 72.3427     | 76.3571  | 67.7583        | 80.9415  |
| 13                             | 1910 | 91.9720            | 88.5655         | 0.9436                 | 86.5904     | 90.5405  | 81.9836        | 95.1473  |
| 14                             | 1920 | 105.7100           | 104.1178        | 0.9163                 | 102.2000    | 106.0357 | 97.5529        | 110.6828 |
| 15                             | 1930 | 122.7750           | 121.0071        | 0.8846                 | 119.1556    | 122.8585 | 114.4612       | 127.5529 |
| 16                             | 1940 | 131.6690           | 139.2332        | 0.8613                 | 137.4305    | 141.0359 | 132.7010       | 145.7654 |
| 17                             | 1950 | 151.3250           | 158.7962        | 0.8650                 | 156.9858    | 160.6066 | 152.2618       | 165.3306 |
| 18                             | 1960 | 179.3230           | 179.6961        | 0.9163                 | 177.7782    | 181.6139 | 173.1311       | 186.2610 |
| 19                             | 1970 | 203.2110           | 201.9328        | 1.0305                 | 199.7759    | 204.0896 | 195.2941       | 208.5715 |
| 20                             | 1980 | 226.5420           | 225.5064        | 1.2118                 | 222.9701    | 228.0427 | 218.7349       | 232.2779 |
| 21                             | 1990 | 248.7100           | 250.4168        | 1.4560                 | 247.3693    | 253.4644 | 243.4378       | 257.3959 |
| 22                             | 2000 | 281.4220           | 276.6642        | 1.7565                 | 272.9877    | 280.3407 | 269.3884       | 283.9400 |
| 23                             | 2010 | .                  | 304.2484        | 2.1073                 | 299.8377    | 308.6591 | 296.5754       | 311.9214 |
| 24                             | 2020 | .                  | 333.1695        | 2.5040                 | 327.9285    | 338.4104 | 324.9910       | 341.3479 |
| 25                             | 2030 | .                  | 363.4274        | 2.9435                 | 357.2665    | 369.5883 | 354.6310       | 372.2238 |

| Output Statistics |      |          |                    |                  |             |   |  |          |
|-------------------|------|----------|--------------------|------------------|-------------|---|--|----------|
| Obs               | Year | Residual | Std Error Residual | Student Residual | -2 -1 0 1 2 |   |  | Cook's D |
| 1                 | 1790 | -2.2837  | 2.432              | -0.939           |             | * |  | 0.153    |
| 2                 | 1800 | -0.4146  | 2.623              | -0.158           |             |   |  | 0.003    |
| 3                 | 1810 | 0.6696   | 2.744              | 0.244            |             |   |  | 0.004    |
| 4                 | 1820 | 0.8849   | 2.817              | 0.314            |             |   |  | 0.004    |
| 5                 | 1830 | 0.5923   | 2.856              | 0.207            |             |   |  | 0.001    |
| 6                 | 1840 | -0.0621  | 2.872              | -0.0216          |             |   |  | 0.000    |
| 7                 | 1850 | -0.1344  | 2.873              | -0.0468          |             |   |  | 0.000    |
| 8                 | 1860 | 0.5864   | 2.866              | 0.205            |             |   |  | 0.001    |
| 9                 | 1870 | 0.0934   | 2.856              | 0.0327           |             |   |  | 0.000    |
| 10                | 1880 | 0.2255   | 2.847              | 0.0792           |             |   |  | 0.000    |

Figure 79.33 continued

| The REG Procedure              |      |          |                       |                     |             |       |  |             |
|--------------------------------|------|----------|-----------------------|---------------------|-------------|-------|--|-------------|
| Model: MODEL1                  |      |          |                       |                     |             |       |  |             |
| Dependent Variable: Population |      |          |                       |                     |             |       |  |             |
| Output Statistics              |      |          |                       |                     |             |       |  |             |
| Obs                            | Year | Residual | Std Error<br>Residual | Student<br>Residual | -2 -1 0 1 2 |       |  | Cook's<br>D |
| 11                             | 1890 | 1.4757   | 2.842                 | 0.519               |             | *     |  | 0.010       |
| 12                             | 1900 | 1.6441   | 2.842                 | 0.578               |             | *     |  | 0.013       |
| 13                             | 1910 | 3.4065   | 2.847                 | 1.196               |             | **    |  | 0.052       |
| 14                             | 1920 | 1.5922   | 2.856                 | 0.557               |             | *     |  | 0.011       |
| 15                             | 1930 | 1.7679   | 2.866                 | 0.617               |             | *     |  | 0.012       |
| 16                             | 1940 | -7.5642  | 2.873                 | -2.632              |             | ***** |  | 0.208       |
| 17                             | 1950 | -7.4712  | 2.872                 | -2.601              |             | ***** |  | 0.205       |
| 18                             | 1960 | -0.3731  | 2.856                 | -0.131              |             |       |  | 0.001       |
| 19                             | 1970 | 1.2782   | 2.817                 | 0.454               |             |       |  | 0.009       |
| 20                             | 1980 | 1.0356   | 2.744                 | 0.377               |             |       |  | 0.009       |
| 21                             | 1990 | -1.7068  | 2.623                 | -0.651              |             | *     |  | 0.044       |
| 22                             | 2000 | 4.7578   | 2.432                 | 1.957               |             | ***   |  | 0.666       |
| 23                             | 2010 | .        | .                     | .                   |             |       |  | .           |
| 24                             | 2020 | .        | .                     | .                   |             |       |  | .           |
| 25                             | 2030 | .        | .                     | .                   |             |       |  | .           |

After producing the usual analysis of variance and parameter estimates tables (Figure 79.32), the procedure displays the results of requesting the options for predicted and residual values (Figure 79.33). For each observation, the requested information is shown. Note that the ID variable is used to identify each observation. Also note that, for observations with missing dependent variables, the predicted value, standard error of the predicted value, and confidence intervals for the predicted value are still available.

The columnar print plot of studentized residuals and Cook's  $D$  statistics are displayed as a result of requesting the R option. In the plot of studentized residuals, the large number of observations with absolute values greater than two indicates an inadequate model. You can use ODS Graphics to obtain plots of studentized residuals by predicted values or leverage; see Example 79.1 for a similar example.

## Models of Less Than Full Rank

If the model is not full rank, there are an infinite number of least squares solutions for the estimates. PROC REG chooses a nonzero solution for all variables that are linearly independent of previous variables and a zero solution for other variables. This solution corresponds to using a generalized inverse in the normal equations, and the expected values of the estimates are the Hermite normal form of  $\mathbf{X}$  multiplied by the true parameters:

$$E(\mathbf{b}) = (\mathbf{X}'\mathbf{X})^{-}(\mathbf{X}'\mathbf{X})\boldsymbol{\beta}$$

Degrees of freedom for the zeroed estimates are reported as zero. The hypotheses that are not testable have  $t$  tests reported as missing. The message that the model is not full rank includes a display of the relations that exist in the matrix.

The following statements use the fitness data from [Example 79.2](#). The variable `Dif=RunPulse-RestPulse` is created. When this variable is included in the model along with `RunPulse` and `RestPulse`, there is a linear dependency (or exact collinearity) between the independent variables. [Figure 79.34](#) shows how this problem is diagnosed.

```
data fit2;
 set fitness;
 Dif=RunPulse-RestPulse;
run;
proc reg data=fit2;
 model Oxygen=RunTime Age Weight RunPulse MaxPulse RestPulse Dif;
run;
```

**Figure 79.34** Model That Is Not Full Rank: REG Procedure

| The REG Procedure          |    |                    |                |         |         |
|----------------------------|----|--------------------|----------------|---------|---------|
| Model: MODEL1              |    |                    |                |         |         |
| Dependent Variable: Oxygen |    |                    |                |         |         |
| Analysis of Variance       |    |                    |                |         |         |
| Source                     | DF | Sum of Squares     | Mean Square    | F Value | Pr > F  |
| Model                      | 6  | 722.54361          | 120.42393      | 22.43   | <.0001  |
| Error                      | 24 | 128.83794          | 5.36825        |         |         |
| Corrected Total            | 30 | 851.38154          |                |         |         |
| Root MSE                   |    | 2.31695            | R-Square       | 0.8487  |         |
| Dependent Mean             |    | 47.37581           | Adj R-Sq       | 0.8108  |         |
| Coeff Var                  |    | 4.89057            |                |         |         |
| Parameter Estimates        |    |                    |                |         |         |
| Variable                   | DF | Parameter Estimate | Standard Error | t Value | Pr >  t |
| Intercept                  | 1  | 102.93448          | 12.40326       | 8.30    | <.0001  |
| RunTime                    | 1  | -2.62865           | 0.38456        | -6.84   | <.0001  |
| Age                        | 1  | -0.22697           | 0.09984        | -2.27   | 0.0322  |
| Weight                     | 1  | -0.07418           | 0.05459        | -1.36   | 0.1869  |
| RunPulse                   | B  | -0.36963           | 0.11985        | -3.08   | 0.0051  |
| MaxPulse                   | 1  | 0.30322            | 0.13650        | 2.22    | 0.0360  |
| RestPulse                  | B  | -0.02153           | 0.06605        | -0.33   | 0.7473  |
| Dif                        | 0  | 0                  | .              | .       | .       |

PROC REG produces a message informing you that the model is less than full rank. Parameters with DF=0 are not estimated, and parameters with DF=B are biased. In addition, the form of the linear dependency among the regressors is displayed.

---

## Collinearity Diagnostics

When a regressor is nearly a linear combination of other regressors in the model, the affected estimates are unstable and have high standard errors. This problem is called *collinearity* or *multicollinearity*. It is a good idea to find out which variables are nearly collinear with which other variables. The approach in PROC REG follows that of Belsley, Kuh, and Welsch (1980). PROC REG provides several methods for detecting collinearity with the COLLIN, COLLINOINT, TOL, and VIF options.

The COLLIN option in the MODEL statement requests that a collinearity analysis be performed. First,  $X'X$  is scaled to have 1s on the diagonal. If you specify the COLLINOINT option, the intercept variable is adjusted out first. Then the eigenvalues and eigenvectors are extracted. The analysis in PROC REG is reported with eigenvalues of  $X'X$  rather than singular values of  $X$ . The eigenvalues of  $X'X$  are the squares of the singular values of  $X$ .

The condition indices are the square roots of the ratio of the largest eigenvalue to each individual eigenvalue. The largest condition index is the condition number of the scaled  $X$  matrix. Belsley, Kuh, and Welsch (1980) suggest that, when this number is around 10, weak dependencies might be starting to affect the regression estimates. When this number is larger than 100, the estimates might have a fair amount of numerical error (although the statistical standard error almost always is much greater than the numerical error).

For each variable, PROC REG produces the proportion of the variance of the estimate accounted for by each principal component. A collinearity problem occurs when a component associated with a high condition index contributes strongly (variance proportion greater than about 0.5) to the variance of two or more variables.

The VIF option in the MODEL statement provides the variance inflation factors (VIF). These factors measure the inflation in the variances of the parameter estimates due to collinearities that exist among the regressor (independent) variables. There are no formal criteria for deciding if a VIF is large enough to affect the predicted values.

The TOL option requests the tolerance values for the parameter estimates. The tolerance is defined as  $1 / \text{VIF}$ .

For a complete discussion of the preceding methods, see Belsley, Kuh, and Welsch (1980). For a more detailed explanation of using the methods with PROC REG, see Freund and Littell (1986).

This example uses the COLLIN option on the fitness data found in [Example 79.2](#). The following statements produce [Figure 79.35](#).

```
proc reg data=fitness;
 model Oxygen=RunTime Age Weight RunPulse MaxPulse RestPulse
 / tol vif collin;
run;
```

Figure 79.35 Regression Using the TOL, VIF, and COLLIN Options

| The REG Procedure          |    |                    |                |         |         |           |
|----------------------------|----|--------------------|----------------|---------|---------|-----------|
| Model: MODEL1              |    |                    |                |         |         |           |
| Dependent Variable: Oxygen |    |                    |                |         |         |           |
| Analysis of Variance       |    |                    |                |         |         |           |
| Source                     | DF | Sum of Squares     | Mean Square    | F Value | Pr > F  |           |
| Model                      | 6  | 722.54361          | 120.42393      | 22.43   | <.0001  |           |
| Error                      | 24 | 128.83794          | 5.36825        |         |         |           |
| Corrected Total            | 30 | 851.38154          |                |         |         |           |
| Root MSE                   |    | 2.31695            | R-Square       | 0.8487  |         |           |
| Dependent Mean             |    | 47.37581           | Adj R-Sq       | 0.8108  |         |           |
| Coeff Var                  |    | 4.89057            |                |         |         |           |
| Parameter Estimates        |    |                    |                |         |         |           |
| Variable                   | DF | Parameter Estimate | Standard Error | t Value | Pr >  t | Tolerance |
| Intercept                  | 1  | 102.93448          | 12.40326       | 8.30    | <.0001  | .         |
| RunTime                    | 1  | -2.62865           | 0.38456        | -6.84   | <.0001  | 0.62859   |
| Age                        | 1  | -0.22697           | 0.09984        | -2.27   | 0.0322  | 0.66101   |
| Weight                     | 1  | -0.07418           | 0.05459        | -1.36   | 0.1869  | 0.86555   |
| RunPulse                   | 1  | -0.36963           | 0.11985        | -3.08   | 0.0051  | 0.11852   |
| MaxPulse                   | 1  | 0.30322            | 0.13650        | 2.22    | 0.0360  | 0.11437   |
| RestPulse                  | 1  | -0.02153           | 0.06605        | -0.33   | 0.7473  | 0.70642   |
| Parameter Estimates        |    |                    |                |         |         |           |
| Variable                   | DF | Variance Inflation |                |         |         |           |
| Intercept                  | 1  | 0                  |                |         |         |           |
| RunTime                    | 1  | 1.59087            |                |         |         |           |
| Age                        | 1  | 1.51284            |                |         |         |           |
| Weight                     | 1  | 1.15533            |                |         |         |           |
| RunPulse                   | 1  | 8.43727            |                |         |         |           |
| MaxPulse                   | 1  | 8.74385            |                |         |         |           |
| RestPulse                  | 1  | 1.41559            |                |         |         |           |

Figure 79.35 continued

| Collinearity Diagnostics |            |                 |                                   |            |            |
|--------------------------|------------|-----------------|-----------------------------------|------------|------------|
| Number                   | Eigenvalue | Condition Index | -----Proportion of Variation----- |            |            |
|                          |            |                 | Intercept                         | RunTime    | Age        |
| 1                        | 6.94991    | 1.00000         | 0.00002326                        | 0.00021086 | 0.00015451 |
| 2                        | 0.01868    | 19.29087        | 0.00218                           | 0.02522    | 0.14632    |
| 3                        | 0.01503    | 21.50072        | 0.00061541                        | 0.12858    | 0.15013    |
| 4                        | 0.00911    | 27.62115        | 0.00638                           | 0.60897    | 0.03186    |
| 5                        | 0.00607    | 33.82918        | 0.00133                           | 0.12501    | 0.11284    |
| 6                        | 0.00102    | 82.63757        | 0.79966                           | 0.09746    | 0.49660    |
| 7                        | 0.00017947 | 196.78560       | 0.18981                           | 0.01455    | 0.06210    |

| Collinearity Diagnostics |            |                                   |            |            |
|--------------------------|------------|-----------------------------------|------------|------------|
| Number                   | Weight     | -----Proportion of Variation----- |            |            |
|                          |            | RunPulse                          | MaxPulse   | RestPulse  |
| 1                        | 0.00019651 | 0.00000862                        | 0.00000634 | 0.00027850 |
| 2                        | 0.01042    | 0.00000244                        | 0.00000743 | 0.39064    |
| 3                        | 0.23571    | 0.00119                           | 0.00125    | 0.02809    |
| 4                        | 0.18313    | 0.00149                           | 0.00123    | 0.19030    |
| 5                        | 0.44442    | 0.01506                           | 0.00833    | 0.36475    |
| 6                        | 0.10330    | 0.06948                           | 0.00561    | 0.02026    |
| 7                        | 0.02283    | 0.91277                           | 0.98357    | 0.00568    |

## Model Fit and Diagnostic Statistics

This section gathers the formulas for the statistics available in the **MODEL**, **PLOT**, and **OUTPUT** statements. The model to be fit is  $Y = X\beta + \epsilon$ , and the parameter estimate is denoted by  $b = (X'X)^{-1}X'Y$ . The subscript  $i$  denotes values for the  $i$ th observation, the parenthetical subscript ( $i$ ) means that the statistic is computed by using all observations except the  $i$ th observation, and the subscript  $jj$  indicates the  $j$ th diagonal matrix entry. The ALPHA= option in the **PROC REG** or **MODEL** statement is used to set the  $\alpha$  value for the  $t$  statistics.

Table 79.9 contains the summary statistics for assessing the fit of the model.

Table 79.9 Formulas and Definitions for Model Fit Summary Statistics

| Model Option or Statistic | Definition or Formula                                                                     |
|---------------------------|-------------------------------------------------------------------------------------------|
| $n$                       | the number of observations                                                                |
| $p$                       | the number of parameters including the intercept                                          |
| $i$                       | 1 if there is an intercept, 0 otherwise                                                   |
| $\hat{\sigma}^2$          | the estimate of pure error variance from the SIGMA= option or from fitting the full model |
| $SST_0$                   | the uncorrected total sum of squares for the dependent variable                           |

Table 79.9 continued

| Model Option or Statistic | Definition or Formula                                                                           |
|---------------------------|-------------------------------------------------------------------------------------------------|
| SST <sub>1</sub>          | the total sum of squares corrected for the mean for the dependent variable                      |
| SSE                       | the error sum of squares                                                                        |
| MSE                       | $\frac{SSE}{n - p}$                                                                             |
| R <sup>2</sup>            | $1 - \frac{SSE}{SST_i}$                                                                         |
| ADJRSQ                    | $1 - \frac{(n - i)(1 - R^2)}{n - p}$                                                            |
| AIC                       | $n \ln \left( \frac{SSE}{n} \right) + 2p$                                                       |
| BIC                       | $n \ln \left( \frac{SSE}{n} \right) + 2(p + 2)q - 2q^2$ where $q = \frac{n\hat{\sigma}^2}{SSE}$ |
| CP (C <sub>p</sub> )      | $\frac{SSE}{\hat{\sigma}^2} + 2p - n$                                                           |
| GMSEP                     | $\frac{MSE(n + 1)(n - 2)}{n(n - p - 1)} = \frac{1}{n} S_p(n + 1)(n - 2)$                        |
| JP (J <sub>p</sub> )      | $\frac{n + p}{n} MSE$                                                                           |
| PC                        | $\frac{n + p}{n - p} (1 - R^2) = J_p \left( \frac{n}{SST_i} \right)$                            |
| PRESS                     | the sum of squares of pred <sub>r<sub>i</sub></sub> (see Table 79.10)                           |
| RMSE                      | $\sqrt{MSE}$                                                                                    |
| SBC                       | $n \ln \left( \frac{SSE}{n} \right) + p \ln(n)$                                                 |
| SP (S <sub>p</sub> )      | $\frac{MSE}{n - p - 1}$                                                                         |

Table 79.10 contains the diagnostic statistics and their formulas; these formulas and further information can be found in Chapter 4, “Introduction to Regression Procedures,” and in the section “Influence Statistics” on page 6717. Each statistic is computed for each observation.

Table 79.10 Formulas and Definitions for Diagnostic Statistics

| MODEL Option or Statistic | Formula                                                   |
|---------------------------|-----------------------------------------------------------|
| PRED ( $\hat{Y}_i$ )      | $X_i \mathbf{b}$                                          |
| RES ( $r_i$ )             | $Y_i - \hat{Y}_i$                                         |
| H ( $h_i$ )               | $\mathbf{x}_i (\mathbf{X}'\mathbf{X})^{-1} \mathbf{x}_i'$ |
| STDP                      | $\sqrt{h_i \hat{\sigma}^2}$                               |
| STDI                      | $\sqrt{(1 + h_i) \hat{\sigma}^2}$                         |
| STDR                      | $\sqrt{(1 - h_i) \hat{\sigma}^2}$                         |

Table 79.10 continued

| MODEL Option or Statistic  | Formula                                                                                                                          |
|----------------------------|----------------------------------------------------------------------------------------------------------------------------------|
| LCL                        | $\hat{Y}_i - t_{\frac{\alpha}{2}} \text{STDI}$                                                                                   |
| LCLM                       | $\hat{Y}_i - t_{\frac{\alpha}{2}} \text{STDP}$                                                                                   |
| UCL                        | $\hat{Y}_i + t_{\frac{\alpha}{2}} \text{STDI}$                                                                                   |
| UCLM                       | $\hat{Y}_i + t_{\frac{\alpha}{2}} \text{STDP}$                                                                                   |
| STUDENT                    | $\frac{r_i}{\text{STDR}_i}$                                                                                                      |
| RSTUDENT                   | $\frac{r_i}{\hat{\sigma}_{(i)} \sqrt{1 - h_i}}$                                                                                  |
| COOKD                      | $\frac{1}{p} \text{STUDENT}^2 \frac{\text{STDP}^2}{\text{STDR}^2}$                                                               |
| COVRATIO                   | $\frac{\det(\hat{\sigma}_{(i)}^2 (\mathbf{x}'_{(i)} \mathbf{x}_{(i)})^{-1})}{\det(\hat{\sigma}^2 (\mathbf{X}'\mathbf{X})^{-1})}$ |
| DFFITs                     | $\frac{(\hat{Y}_i - \hat{Y}_{(i)})}{(\hat{\sigma}_{(i)} \sqrt{h_i})}$                                                            |
| DFBETAS <sub>j</sub>       | $\frac{\mathbf{b}_j - \mathbf{b}_{(i)j}}{\hat{\sigma}_{(i)} \sqrt{(\mathbf{X}'\mathbf{X})_{jj}}}$                                |
| PRESS(predr <sub>i</sub> ) | $\frac{r_i}{1 - h_i}$                                                                                                            |

## Influence Statistics

This section discusses the INFLUENCE option, which produces several influence statistics, and the PARTIAL option, which produces partial regression leverage plots.

### The INFLUENCE Option

The INFLUENCE option (in the MODEL statement) requests the statistics proposed by Belsley, Kuh, and Welsch (1980) to measure the influence of each observation on the estimates. Influential observations are those that, according to various criteria, appear to have a large influence on the parameter estimates.

Let  $\mathbf{b}(i)$  be the parameter estimates after deleting the  $i$ th observation; let  $s(i)^2$  be the variance estimate after deleting the  $i$ th observation; let  $\mathbf{X}(i)$  be the  $\mathbf{X}$  matrix without the  $i$ th observation; let  $\hat{y}(i)$  be the  $i$ th value predicted without using the  $i$ th observation; let  $r_i = y_i - \hat{y}_i$  be the  $i$ th residual; and let  $h_i$  be the  $i$ th diagonal of the projection matrix for the predictor space, also called the *hat matrix*:

$$h_i = \mathbf{x}_i (\mathbf{X}'\mathbf{X})^{-1} \mathbf{x}_i'$$

Belsley, Kuh, and Welsch (1980) propose a cutoff of  $2p/n$ , where  $n$  is the number of observations used to fit the model and  $p$  is the number of parameters in the model. Observations with  $h_i$  values above this cutoff should be investigated.



For each observation, PROC REG first displays the residual, the studentized residual (RSTUDENT), and the  $h_i$ . The studentized residual RSTUDENT differs slightly from STUDENT since the error variance is estimated by  $s_{(i)}^2$  without the  $i$ th observation, not by  $s^2$ . For example,

$$\text{RSTUDENT} = \frac{r_i}{s_{(i)} \sqrt{(1 - h_i)}}$$

Observations with RSTUDENT larger than 2 in absolute value might need some attention.

The COVRATIO statistic measures the change in the determinant of the covariance matrix of the estimates by deleting the  $i$ th observation:

$$\text{COVRATIO} = \frac{\det \left( s_{(i)}^2 (\mathbf{X}'_{(i)} \mathbf{X}_{(i)})^{-1} \right)}{\det \left( s^2 (\mathbf{X}' \mathbf{X})^{-1} \right)}$$

Belsley, Kuh, and Welsch (1980) suggest that observations with

$$|\text{COVRATIO} - 1| \geq \frac{3p}{n}$$

where  $p$  is the number of parameters in the model and  $n$  is the number of observations used to fit the model, are worth investigation.

The DFFITS statistic is a scaled measure of the change in the predicted value for the  $i$ th observation and is calculated by deleting the  $i$ th observation. A large value indicates that the observation is very influential in its neighborhood of the  $\mathbf{X}$  space.

$$\text{DFFITS} = \frac{\hat{y}_i - \hat{y}_{(i)}}{s_{(i)} \sqrt{h_{(i)}}}$$

Large values of DFFITS indicate influential observations. A general cutoff to consider is 2; a size-adjusted cutoff recommended by Belsley, Kuh, and Welsch (1980) is  $2\sqrt{p/n}$ , where  $n$  and  $p$  are as defined previously.

The DFFITS statistic is very similar to Cook's  $D$ , defined in the section "Predicted and Residual Values" on page 6708.

The DFBETAS statistics are the scaled measures of the change in each parameter estimate and are calculated by deleting the  $i$ th observation:

$$\text{DFBETAS}_j = \frac{b_j - b_{(i)j}}{s_{(i)} \sqrt{(\mathbf{X}' \mathbf{X})_{jj}^{-1}}}$$

where  $(\mathbf{X}' \mathbf{X})_{jj}$  is the  $(j, j)$  element of  $(\mathbf{X}' \mathbf{X})^{-1}$ .

In general, large values of DFBETAS indicate observations that are influential in estimating a given parameter. Belsley, Kuh, and Welsch (1980) recommend 2 as a general cutoff value to indicate influential observations and  $2/\sqrt{n}$  as a size-adjusted cutoff.

The following statements use the population example in the section “Polynomial Regression” on page 6620. See Figure 79.32 for the fitted regression equation. The INFLUENCE option produces the tables shown in Figure 79.36 and Figure 79.37.

```
proc reg data=USPopulation;
 model Population=Year YearSq / influence;
run;
```

**Figure 79.36** Regression Using the INFLUENCE Option

| The REG Procedure              |          |          |        |        |        |                   |         |           |         |
|--------------------------------|----------|----------|--------|--------|--------|-------------------|---------|-----------|---------|
| Model: MODEL1                  |          |          |        |        |        |                   |         |           |         |
| Dependent Variable: Population |          |          |        |        |        |                   |         |           |         |
| Output Statistics              |          |          |        |        |        |                   |         |           |         |
| Obs                            | Residual | RStudent | Hat    | Diag   | Cov    | -----DFBETAS----- |         |           |         |
|                                |          |          | H      | H      |        | Ratio             | DFFITs  | Intercept | Year    |
| 1                              | -2.2837  | -0.9361  | 0.3429 | 0.3429 | 1.5519 | -0.6762           | -0.4924 | 0.4862    | -0.4802 |
| 2                              | -0.4146  | -0.1540  | 0.2356 | 0.2356 | 1.5325 | -0.0855           | -0.0540 | 0.0531    | -0.0523 |
| 3                              | 0.6696   | 0.2379   | 0.1632 | 0.1632 | 1.3923 | 0.1050            | 0.0517  | -0.0505   | 0.0494  |
| 4                              | 0.8849   | 0.3065   | 0.1180 | 0.1180 | 1.3128 | 0.1121            | 0.0335  | -0.0322   | 0.0310  |
| 5                              | 0.5923   | 0.2021   | 0.0933 | 0.0933 | 1.2883 | 0.0648            | 0.0040  | -0.0032   | 0.0025  |
| 6                              | -0.0621  | -0.0210  | 0.0831 | 0.0831 | 1.2827 | -0.0063           | 0.0012  | -0.0012   | 0.0013  |
| 7                              | -0.1344  | -0.0455  | 0.0824 | 0.0824 | 1.2813 | -0.0136           | 0.0054  | -0.0055   | 0.0056  |
| 8                              | 0.5864   | 0.1994   | 0.0870 | 0.0870 | 1.2796 | 0.0615            | -0.0339 | 0.0343    | -0.0347 |
| 9                              | 0.0934   | 0.0318   | 0.0933 | 0.0933 | 1.2969 | 0.0102            | -0.0067 | 0.0067    | -0.0068 |
| 10                             | 0.2255   | 0.0771   | 0.0990 | 0.0990 | 1.3040 | 0.0255            | -0.0182 | 0.0183    | -0.0183 |
| 11                             | 1.4757   | 0.5090   | 0.1022 | 0.1022 | 1.2550 | 0.1717            | -0.1272 | 0.1275    | -0.1276 |
| 12                             | 1.6441   | 0.5680   | 0.1022 | 0.1022 | 1.2420 | 0.1916            | -0.1426 | 0.1426    | -0.1424 |
| 13                             | 3.4065   | 1.2109   | 0.0990 | 0.0990 | 1.0320 | 0.4013            | -0.2895 | 0.2889    | -0.2880 |
| 14                             | 1.5922   | 0.5470   | 0.0933 | 0.0933 | 1.2345 | 0.1755            | -0.1173 | 0.1167    | -0.1160 |
| 15                             | 1.7679   | 0.6064   | 0.0870 | 0.0870 | 1.2123 | 0.1871            | -0.1076 | 0.1067    | -0.1056 |
| 16                             | -7.5642  | -3.2147  | 0.0824 | 0.0824 | 0.3286 | -0.9636           | 0.4130  | -0.4063   | 0.3987  |
| 17                             | -7.4712  | -3.1550  | 0.0831 | 0.0831 | 0.3425 | -0.9501           | 0.2131  | -0.2048   | 0.1957  |
| 18                             | -0.3731  | -0.1272  | 0.0933 | 0.0933 | 1.2936 | -0.0408           | -0.0007 | 0.0012    | -0.0016 |
| 19                             | 1.2782   | 0.4440   | 0.1180 | 0.1180 | 1.2906 | 0.1624            | 0.0415  | -0.0432   | 0.0449  |
| 20                             | 1.0356   | 0.3687   | 0.1632 | 0.1632 | 1.3741 | 0.1628            | 0.0732  | -0.0749   | 0.0766  |
| 21                             | -1.7068  | -0.6406  | 0.2356 | 0.2356 | 1.4380 | -0.3557           | -0.2107 | 0.2141    | -0.2176 |
| 22                             | 4.7578   | 2.1312   | 0.3429 | 0.3429 | 0.9113 | 1.5395            | 1.0656  | -1.0793   | 1.0933  |

**Figure 79.37** Residual Statistics

|                               |             |
|-------------------------------|-------------|
| Sum of Residuals              | -4.7569E-11 |
| Sum of Squared Residuals      | 170.97193   |
| Predicted Residual SS (PRESS) | 237.71229   |

In [Figure 79.36](#), observations 16, 17, and 19 exceed the cutoff value of 2 for RSTUDENT. None of the observations exceeds the general cutoff of 2 for DFFITS or the DFBETAS, but observations 16, 17, and 19 exceed at least one of the size-adjusted cutoffs for these statistics. Observations 1 and 19 exceed the cutoff for the hat diagonals, and observations 1, 2, 16, 17, and 18 exceed the cutoffs for COVRATIO. Taken together, these statistics indicate that you should look first at observations 16, 17, and 19 and then perhaps investigate the other observations that exceeded a cutoff.

When ODS Graphics is enabled, you can request influence diagnostic plots by using the PLOTS= option in the PROC REG statement as shown in the following statements:

```
ods graphics on;

proc reg data=USPopulation
 plots(label)=(Cooksd RStudentByLeverage DFFITS DFBETAS);
 id Year;
 model Population=Year YearSq;
run;

ods graphics off;
```

The LABEL suboption specified in the PLOTS(LABEL)= option requests that observations that exceed the relevant cutoffs for the statistics being plotted are labeled. Since Year has been named in an ID statement, the value of Year is used for the labels. The requested plots are shown in [Figure 79.38](#).

Figure 79.38 Influence Diagnostics

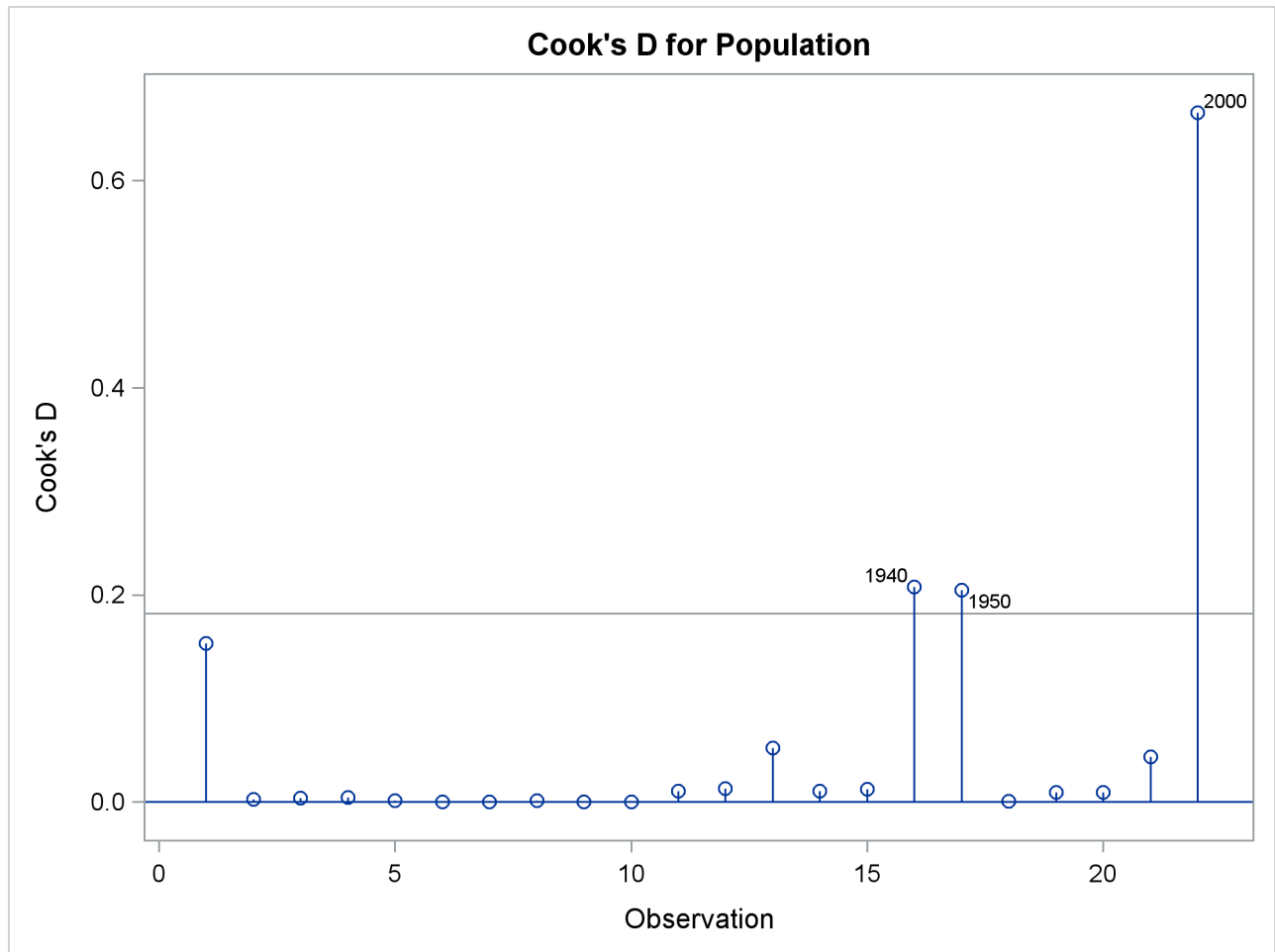


Figure 79.38 continued

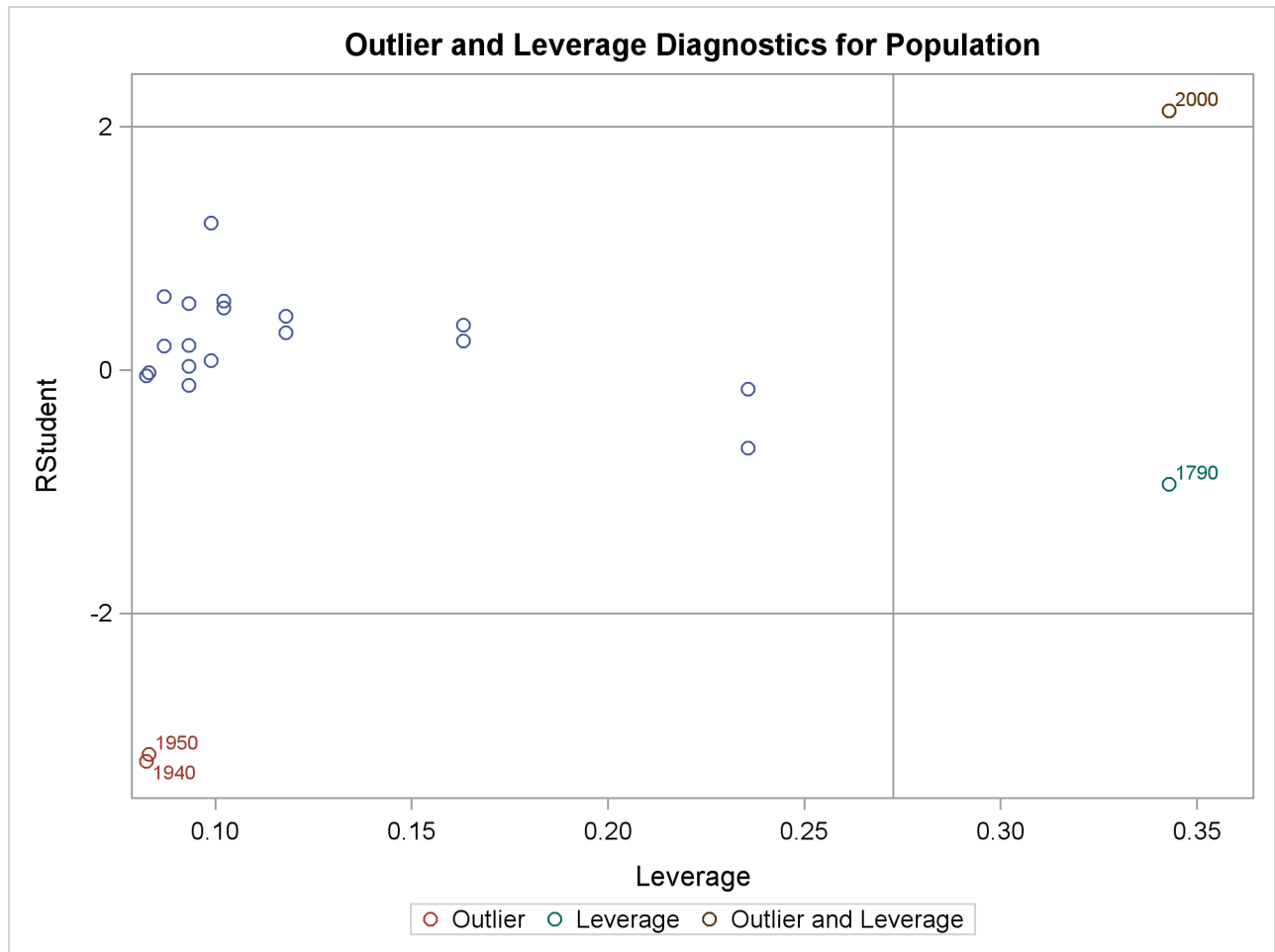


Figure 79.38 continued

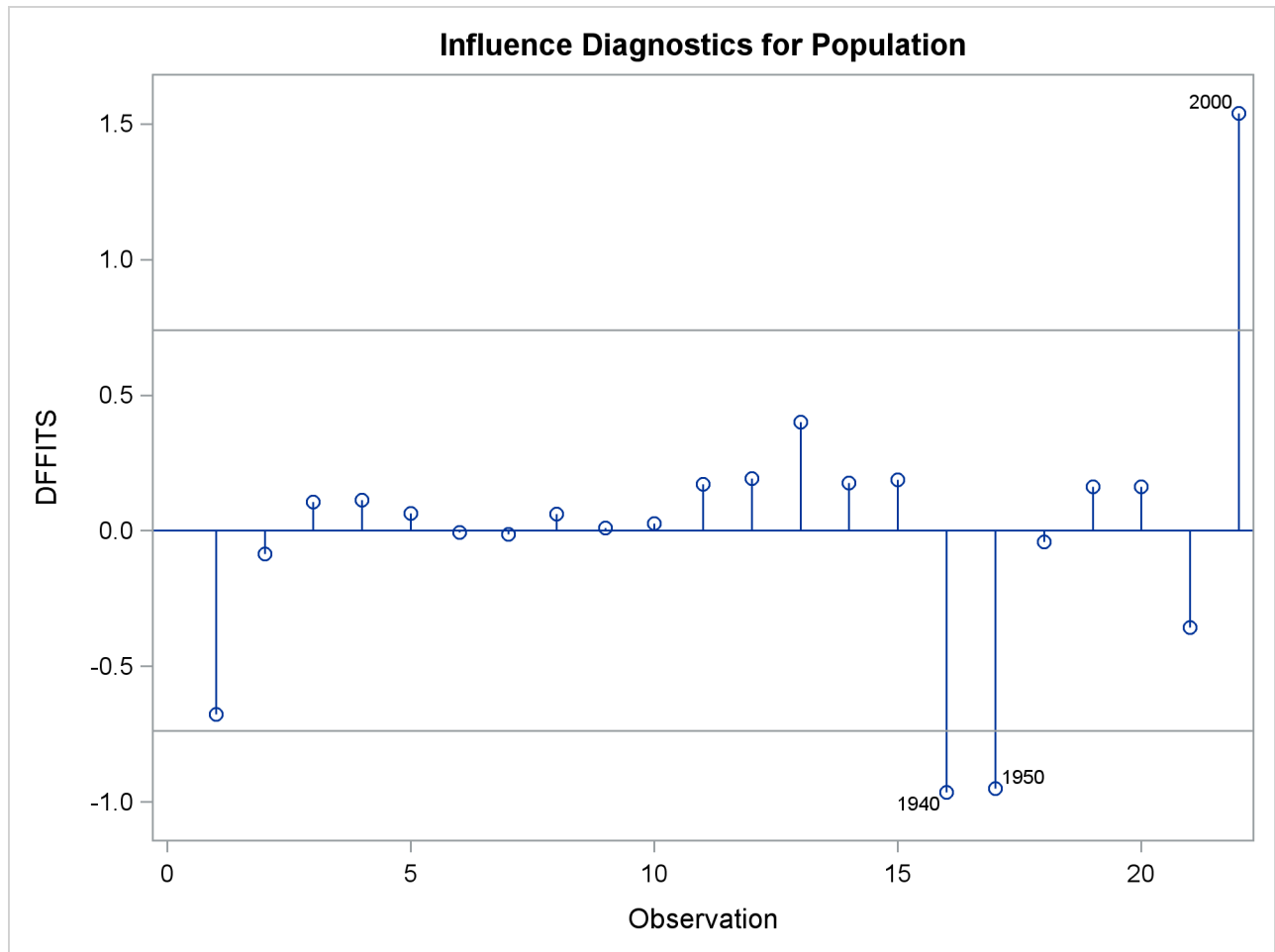
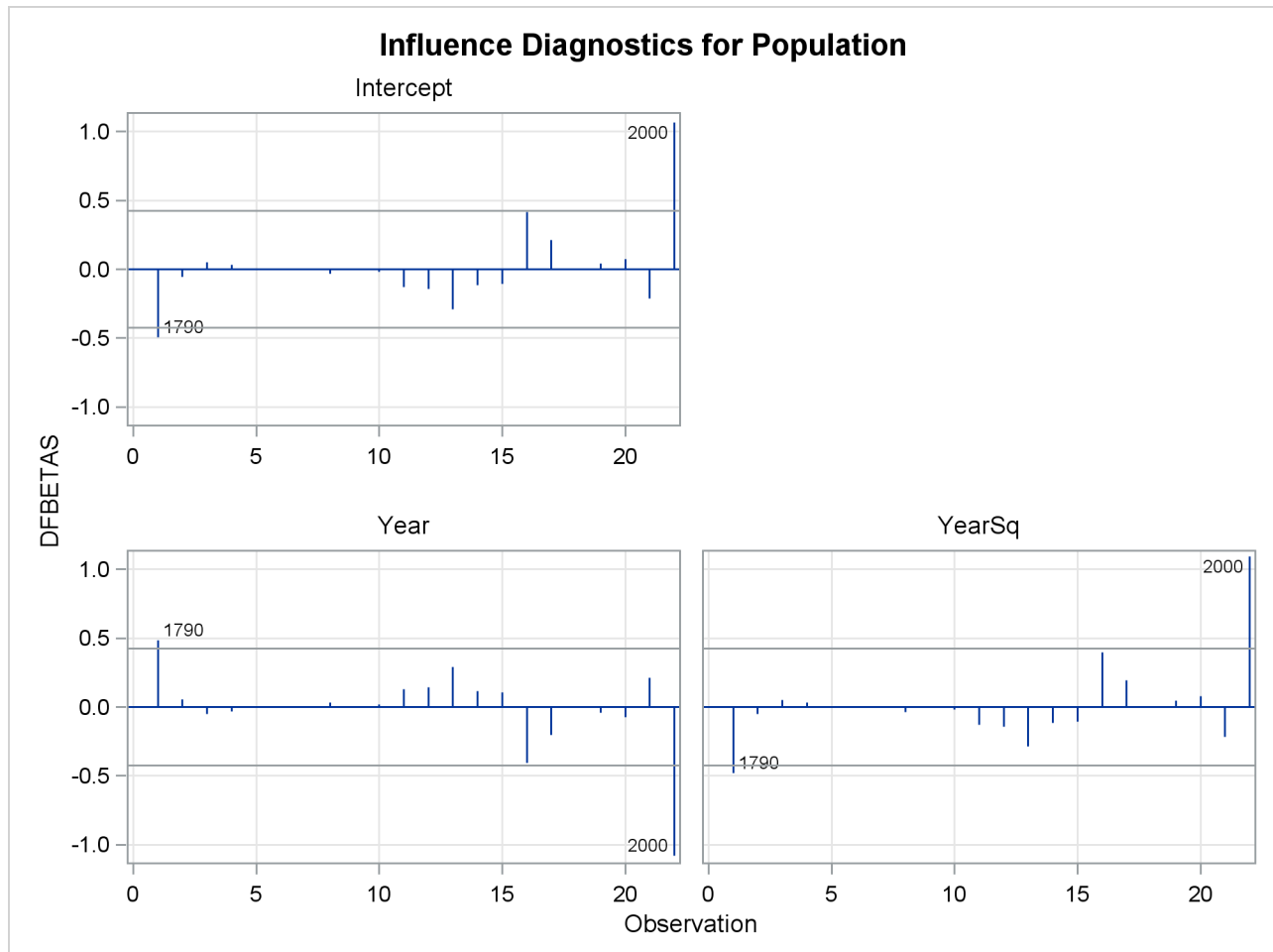


Figure 79.38 continued



### The PARTIAL and PARTIALDATA Options

The PARTIAL option in the MODEL statement produces partial regression leverage plots. If ODS Graphics is not enabled, this option requires the use of the LINEPRINTER option in the PROC REG statement. One plot is created for each regressor in the current full model. For example, plots are produced for regressors included by using ADD statements; plots are not produced for interim models in the various model-selection methods but only for the full model. If you use a model-selection method and the final model contains only a subset of the original regressors, the PARTIAL option still produces plots for all regressors in the full model. If ODS Graphics is enabled, these plots are produced as high-resolution graphics, in panels with a maximum of six partial regression leverage plots per panel. Multiple panels are displayed for models with more than six regressors.

For a given regressor, the partial regression leverage plot is the plot of the dependent variable and the regressor after they have been made orthogonal to the other regressors in the model. These can be obtained by plotting the residuals for the dependent variable against the residuals for the selected regressor, where the residuals for the dependent variable are calculated with the selected regressor omitted, and the residuals for the selected regressor are calculated from a model where the selected regressor is regressed on the remaining regressors. A line fit to the points has a slope equal to the parameter estimate in the full model.

When ODS Graphics is not enabled, points in the plot are marked by the number of replicates appearing at one position. The symbol '\*' is used if there are 10 or more replicates. If an ID statement is specified, the leftmost nonblank character in the value of the ID variable is used as the plotting symbol.

The PARTIALDATA option in the MODEL statement produces a table that contains the partial regression data that are displayed in the partial regression leverage plots. You can request partial regression data even if you do not request plots with the PARTIAL option.

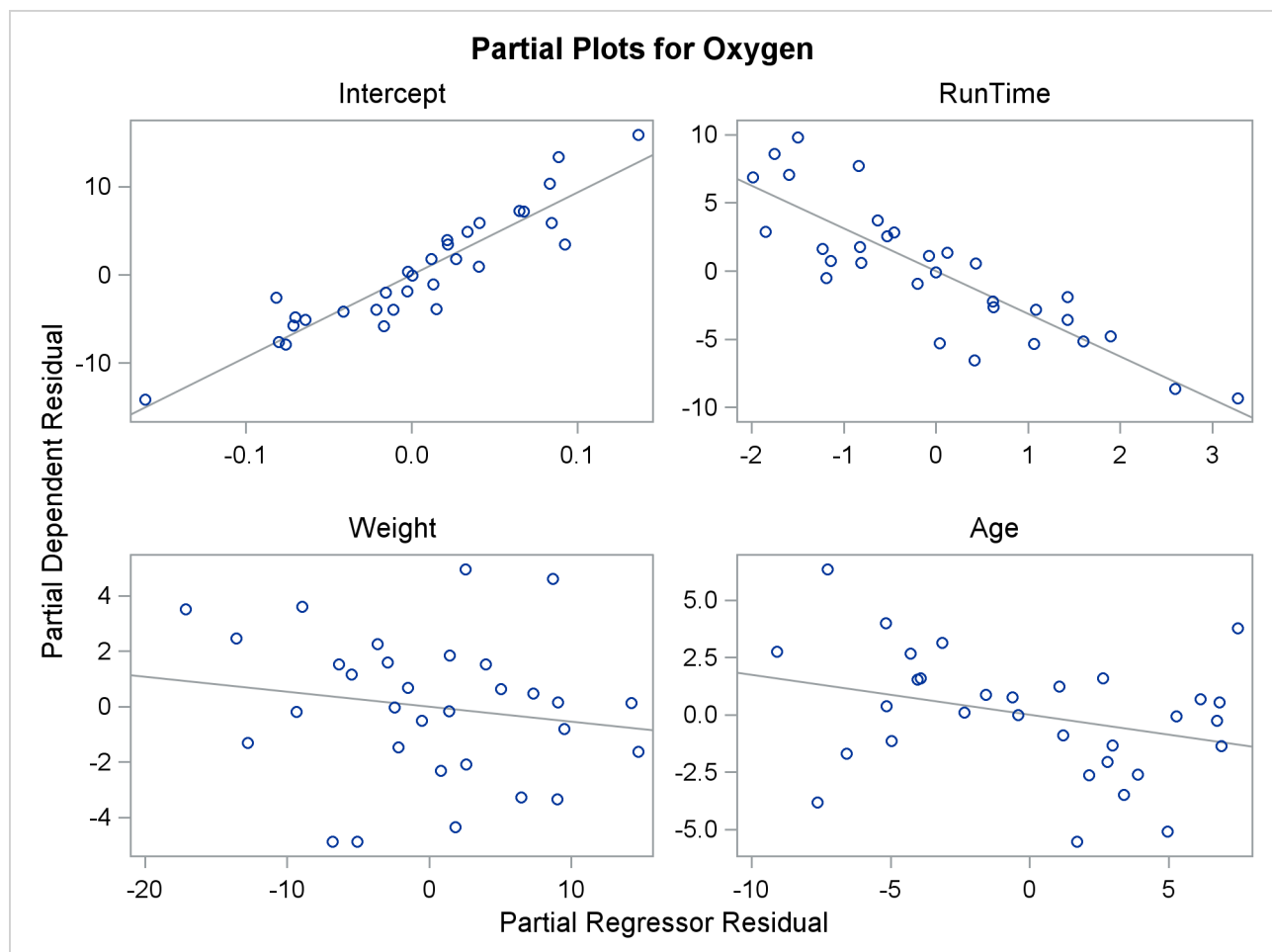
The following statements use the fitness data in Example 79.2 with the PARTIAL option and ODS Graphics to produce the partial regression leverage plots. The plots are shown in Figure 79.39.

```
ods graphics on;

proc reg data=fitness;
 model Oxygen=RunTime Weight Age / partial;
run;

ods graphics off;
```

**Figure 79.39** Partial Regression Leverage Plots





## Reweighting Observations in an Analysis

Reweighting observations is an interactive feature of PROC REG that enables you to change the weights of observations used in computing the regression equation. Observations can also be deleted from the analysis (not from the data set) by changing their weights to zero. In the following statements, the Sashelp.Class data are used to illustrate some of the features of the REWEIGHT statement. First, the full model is fit, and the residuals are displayed in Figure 79.40.

```
proc reg data=sashelp.Class;
 model Weight=Age Height / p;
 id Name;
run;
```

**Figure 79.40** Full Model for Sashelp.Class Data, Residuals Shown

| The REG Procedure             |         |                    |                 |          |
|-------------------------------|---------|--------------------|-----------------|----------|
| Model: MODEL1                 |         |                    |                 |          |
| Dependent Variable: Weight    |         |                    |                 |          |
| Output Statistics             |         |                    |                 |          |
| Obs                           | Name    | Dependent Variable | Predicted Value | Residual |
| 1                             | Alfred  | 112.5000           | 124.8686        | -12.3686 |
| 2                             | Alice   | 84.0000            | 78.6273         | 5.3727   |
| 3                             | Barbara | 98.0000            | 110.2812        | -12.2812 |
| 4                             | Carol   | 102.5000           | 102.5670        | -0.0670  |
| 5                             | Henry   | 102.5000           | 105.0849        | -2.5849  |
| 6                             | James   | 83.0000            | 80.2266         | 2.7734   |
| 7                             | Jane    | 84.5000            | 89.2191         | -4.7191  |
| 8                             | Janet   | 112.5000           | 102.7663        | 9.7337   |
| 9                             | Jeffrey | 84.0000            | 100.2095        | -16.2095 |
| 10                            | John    | 99.5000            | 86.3415         | 13.1585  |
| 11                            | Joyce   | 50.5000            | 57.3660         | -6.8660  |
| 12                            | Judy    | 90.0000            | 107.9625        | -17.9625 |
| 13                            | Louise  | 77.0000            | 76.6295         | 0.3705   |
| 14                            | Mary    | 112.0000           | 117.1544        | -5.1544  |
| 15                            | Philip  | 150.0000           | 138.2164        | 11.7836  |
| 16                            | Robert  | 128.0000           | 107.2043        | 20.7957  |
| 17                            | Ronald  | 133.0000           | 118.9529        | 14.0471  |
| 18                            | Thomas  | 85.0000            | 79.6676         | 5.3324   |
| 19                            | William | 112.0000           | 117.1544        | -5.1544  |
| Sum of Residuals              |         |                    |                 | 0        |
| Sum of Squared Residuals      |         |                    | 2120.09974      |          |
| Predicted Residual SS (PRESS) |         |                    | 3272.72186      |          |

Upon examining the data and residuals, you realize that observation 17 (Ronald) was mistakenly included in the analysis. Also, you would like to examine the effect of reweighting to 0.5 those observations with residuals that have absolute values greater than or equal to 17. The following statements show how you request this reweighting:

```
reweight obs.=17;
reweight r. le -17 or r. ge 17 / weight=0.5;
print p;
run;
```

At this point, a message appears (in the log) that tells you which observations have been reweighted and what the new weights are. Figure 79.41 is produced.

**Figure 79.41** Model with Reweighted Observations

| The REG Procedure             |         |                 |                    |                 |          |
|-------------------------------|---------|-----------------|--------------------|-----------------|----------|
| Model: MODEL1.2               |         |                 |                    |                 |          |
| Dependent Variable: Weight    |         |                 |                    |                 |          |
| Output Statistics             |         |                 |                    |                 |          |
| Obs                           | Name    | Weight Variable | Dependent Variable | Predicted Value | Residual |
| 1                             | Alfred  | 1.0000          | 112.5000           | 121.6250        | -9.1250  |
| 2                             | Alice   | 1.0000          | 84.0000            | 79.9296         | 4.0704   |
| 3                             | Barbara | 1.0000          | 98.0000            | 107.5484        | -9.5484  |
| 4                             | Carol   | 1.0000          | 102.5000           | 102.1663        | 0.3337   |
| 5                             | Henry   | 1.0000          | 102.5000           | 104.3632        | -1.8632  |
| 6                             | James   | 1.0000          | 83.0000            | 79.9762         | 3.0238   |
| 7                             | Jane    | 1.0000          | 84.5000            | 87.8225         | -3.3225  |
| 8                             | Janet   | 1.0000          | 112.5000           | 103.6889        | 8.8111   |
| 9                             | Jeffrey | 1.0000          | 84.0000            | 98.7606         | -14.7606 |
| 10                            | John    | 1.0000          | 99.5000            | 85.3117         | 14.1883  |
| 11                            | Joyce   | 1.0000          | 50.5000            | 58.6811         | -8.1811  |
| 12                            | Judy    | 0.5000          | 90.0000            | 106.8740        | -16.8740 |
| 13                            | Louise  | 1.0000          | 77.0000            | 76.8377         | 0.1623   |
| 14                            | Mary    | 1.0000          | 112.0000           | 116.2429        | -4.2429  |
| 15                            | Philip  | 1.0000          | 150.0000           | 135.9688        | 14.0312  |
| 16                            | Robert  | 0.5000          | 128.0000           | 103.5150        | 24.4850  |
| 17                            | Ronald  | 0               | 133.0000           | 117.8121        | 15.1879  |
| 18                            | Thomas  | 1.0000          | 85.0000            | 78.1398         | 6.8602   |
| 19                            | William | 1.0000          | 112.0000           | 116.2429        | -4.2429  |
| Sum of Residuals              |         |                 |                    | 0               |          |
| Sum of Squared Residuals      |         |                 |                    | 1500.61194      |          |
| Predicted Residual SS (PRESS) |         |                 |                    | 2287.57621      |          |

The first REWEIGHT statement excludes observation 17, and the second REWEIGHT statement reweights observations 12 and 16 to 0.5. An important feature to note from this example is that the model is not refit until after the PRINT statement. REWEIGHT statements do not cause the model to be refit. This is so that multiple REWEIGHT statements can be applied to a subsequent model.

In this example, since the intent is to reweight observations with large residuals, the observation that was mistakenly included in the analysis should be deleted; then the model should be fit for those remaining observations, and the observations with large residuals should be reweighted. To accomplish this, use the `REFIT` statement. Note that the model label has been changed from `MODEL1` to `MODEL1.2` since two `REWEIGHT` statements have been used. The following statements produce Figure 79.42:

```
reweight allobs / weight=1.0;
reweight obs.=17;
refit;
reweight r. le -17 or r. ge 17 / weight=.5;
print;
run;
```

**Figure 79.42** Observations Excluded from Analysis, Model Refitted, and Observations Reweighted

| The REG Procedure             |         |                 |                    |                 |          |
|-------------------------------|---------|-----------------|--------------------|-----------------|----------|
| Model: MODEL1.5               |         |                 |                    |                 |          |
| Dependent Variable: Weight    |         |                 |                    |                 |          |
| Output Statistics             |         |                 |                    |                 |          |
| Obs                           | Name    | Weight Variable | Dependent Variable | Predicted Value | Residual |
| 1                             | Alfred  | 1.0000          | 112.5000           | 120.9716        | -8.4716  |
| 2                             | Alice   | 1.0000          | 84.0000            | 79.5342         | 4.4658   |
| 3                             | Barbara | 1.0000          | 98.0000            | 107.0746        | -9.0746  |
| 4                             | Carol   | 1.0000          | 102.5000           | 101.5681        | 0.9319   |
| 5                             | Henry   | 1.0000          | 102.5000           | 103.7588        | -1.2588  |
| 6                             | James   | 1.0000          | 83.0000            | 79.7204         | 3.2796   |
| 7                             | Jane    | 1.0000          | 84.5000            | 87.5443         | -3.0443  |
| 8                             | Janet   | 1.0000          | 112.5000           | 102.9467        | 9.5533   |
| 9                             | Jeffrey | 1.0000          | 84.0000            | 98.3117         | -14.3117 |
| 10                            | John    | 1.0000          | 99.5000            | 85.0407         | 14.4593  |
| 11                            | Joyce   | 1.0000          | 50.5000            | 58.6253         | -8.1253  |
| 12                            | Judy    | 1.0000          | 90.0000            | 106.2625        | -16.2625 |
| 13                            | Louise  | 1.0000          | 77.0000            | 76.5908         | 0.4092   |
| 14                            | Mary    | 1.0000          | 112.0000           | 115.4651        | -3.4651  |
| 15                            | Philip  | 1.0000          | 150.0000           | 134.9953        | 15.0047  |
| 16                            | Robert  | 0.5000          | 128.0000           | 103.1923        | 24.8077  |
| 17                            | Ronald  | 0               | 133.0000           | 117.0299        | 15.9701  |
| 18                            | Thomas  | 1.0000          | 85.0000            | 78.0288         | 6.9712   |
| 19                            | William | 1.0000          | 112.0000           | 115.4651        | -3.4651  |
| Sum of Residuals              |         |                 |                    | 0               |          |
| Sum of Squared Residuals      |         |                 |                    | 1637.81879      |          |
| Predicted Residual SS (PRESS) |         |                 |                    | 2473.87984      |          |

Notice that this results in a slightly different model than the previous set of statements: only observation 16 is reweighted to 0.5. Also note that the model label is now `MODEL1.5` since five `REWEIGHT` statements have been used for this model.

Another important feature of the **REWEIGHT** statement is the ability to nullify the effect of a previous or all **REWEIGHT** statements. First, assume that you have several **REWEIGHT** statements in effect and you want to restore the original weights of all the observations. The following **REWEIGHT** statement accomplishes this and produces Figure 79.43:

```
reweight allobs / reset;
print;
run;
```

**Figure 79.43** Restoring Weights of All Observations

| The REG Procedure             |         |                    |                 |          |
|-------------------------------|---------|--------------------|-----------------|----------|
| Model: MODEL1.6               |         |                    |                 |          |
| Dependent Variable: Weight    |         |                    |                 |          |
| Output Statistics             |         |                    |                 |          |
| Obs                           | Name    | Dependent Variable | Predicted Value | Residual |
| 1                             | Alfred  | 112.5000           | 124.8686        | -12.3686 |
| 2                             | Alice   | 84.0000            | 78.6273         | 5.3727   |
| 3                             | Barbara | 98.0000            | 110.2812        | -12.2812 |
| 4                             | Carol   | 102.5000           | 102.5670        | -0.0670  |
| 5                             | Henry   | 102.5000           | 105.0849        | -2.5849  |
| 6                             | James   | 83.0000            | 80.2266         | 2.7734   |
| 7                             | Jane    | 84.5000            | 89.2191         | -4.7191  |
| 8                             | Janet   | 112.5000           | 102.7663        | 9.7337   |
| 9                             | Jeffrey | 84.0000            | 100.2095        | -16.2095 |
| 10                            | John    | 99.5000            | 86.3415         | 13.1585  |
| 11                            | Joyce   | 50.5000            | 57.3660         | -6.8660  |
| 12                            | Judy    | 90.0000            | 107.9625        | -17.9625 |
| 13                            | Louise  | 77.0000            | 76.6295         | 0.3705   |
| 14                            | Mary    | 112.0000           | 117.1544        | -5.1544  |
| 15                            | Philip  | 150.0000           | 138.2164        | 11.7836  |
| 16                            | Robert  | 128.0000           | 107.2043        | 20.7957  |
| 17                            | Ronald  | 133.0000           | 118.9529        | 14.0471  |
| 18                            | Thomas  | 85.0000            | 79.6676         | 5.3324   |
| 19                            | William | 112.0000           | 117.1544        | -5.1544  |
| Sum of Residuals              |         |                    |                 | 0        |
| Sum of Squared Residuals      |         |                    | 2120.09974      |          |
| Predicted Residual SS (PRESS) |         |                    | 3272.72186      |          |

The resulting model is identical to the original model specified at the beginning of this section. Notice that the model label is now MODEL1.6. Note that the Weight column does not appear, since all observations have been reweighted to have weight=1.

Now suppose you want only to undo the changes made by the most recent **REWEIGHT** statement. Use **REWEIGHT UNDO** for this. The following statements produce Figure 79.44:

```

reweight r. le -12 or r. ge 12 / weight=.75;
reweight r. le -17 or r. ge 17 / weight=.5;
reweight undo;
print;
run;

```

**Figure 79.44** Example of UNDO in REWEIGHT Statement

| The REG Procedure             |         |                 |                    |                 |          |
|-------------------------------|---------|-----------------|--------------------|-----------------|----------|
| Model: MODEL1.9               |         |                 |                    |                 |          |
| Dependent Variable: Weight    |         |                 |                    |                 |          |
| Output Statistics             |         |                 |                    |                 |          |
| Obs                           | Name    | Weight Variable | Dependent Variable | Predicted Value | Residual |
| 1                             | Alfred  | 0.7500          | 112.5000           | 125.1152        | -12.6152 |
| 2                             | Alice   | 1.0000          | 84.0000            | 78.7691         | 5.2309   |
| 3                             | Barbara | 0.7500          | 98.0000            | 110.3236        | -12.3236 |
| 4                             | Carol   | 1.0000          | 102.5000           | 102.8836        | -0.3836  |
| 5                             | Henry   | 1.0000          | 102.5000           | 105.3936        | -2.8936  |
| 6                             | James   | 1.0000          | 83.0000            | 80.1133         | 2.8867   |
| 7                             | Jane    | 1.0000          | 84.5000            | 89.0776         | -4.5776  |
| 8                             | Janet   | 1.0000          | 112.5000           | 103.3322        | 9.1678   |
| 9                             | Jeffrey | 0.7500          | 84.0000            | 100.2835        | -16.2835 |
| 10                            | John    | 0.7500          | 99.5000            | 86.2090         | 13.2910  |
| 11                            | Joyce   | 1.0000          | 50.5000            | 57.0745         | -6.5745  |
| 12                            | Judy    | 0.7500          | 90.0000            | 108.2622        | -18.2622 |
| 13                            | Louise  | 1.0000          | 77.0000            | 76.5275         | 0.4725   |
| 14                            | Mary    | 1.0000          | 112.0000           | 117.6752        | -5.6752  |
| 15                            | Philip  | 1.0000          | 150.0000           | 138.9211        | 11.0789  |
| 16                            | Robert  | 0.7500          | 128.0000           | 107.0063        | 20.9937  |
| 17                            | Ronald  | 0.7500          | 133.0000           | 119.4681        | 13.5319  |
| 18                            | Thomas  | 1.0000          | 85.0000            | 79.3061         | 5.6939   |
| 19                            | William | 1.0000          | 112.0000           | 117.6752        | -5.6752  |
| Sum of Residuals              |         |                 |                    | 0               |          |
| Sum of Squared Residuals      |         |                 |                    | 1694.87114      |          |
| Predicted Residual SS (PRESS) |         |                 |                    | 2547.22751      |          |

The resulting model reflects changes made only by the first **REWEIGHT** statement since the third **REWEIGHT** statement negates the effect of the second **REWEIGHT** statement. Observations 1, 3, 9, 10, 12, 16, and 17 have their weights changed to 0.75. Note that the label MODEL1.9 reflects the use of nine **REWEIGHT** statements for the current model.

Now suppose you want to reset the observations selected by the most recent **REWEIGHT** statement to their original weights. Use the **REWEIGHT** statement with the **RESET** option to do this. The following statements produce [Figure 79.45](#):

```

reweight r. le -12 or r. ge 12 / weight=.75;
reweight r. le -17 or r. ge 17 / weight=.5;
reweight / reset;
print;
run;

```

**Figure 79.45** REWEIGHT Statement with RESET option

| The REG Procedure             |         |                 |                    |                 |          |
|-------------------------------|---------|-----------------|--------------------|-----------------|----------|
| Model: MODEL1.12              |         |                 |                    |                 |          |
| Dependent Variable: Weight    |         |                 |                    |                 |          |
| Output Statistics             |         |                 |                    |                 |          |
| Obs                           | Name    | Weight Variable | Dependent Variable | Predicted Value | Residual |
| 1                             | Alfred  | 0.7500          | 112.5000           | 126.0076        | -13.5076 |
| 2                             | Alice   | 1.0000          | 84.0000            | 77.8727         | 6.1273   |
| 3                             | Barbara | 0.7500          | 98.0000            | 111.2805        | -13.2805 |
| 4                             | Carol   | 1.0000          | 102.5000           | 102.4703        | 0.0297   |
| 5                             | Henry   | 1.0000          | 102.5000           | 105.1278        | -2.6278  |
| 6                             | James   | 1.0000          | 83.0000            | 80.2290         | 2.7710   |
| 7                             | Jane    | 1.0000          | 84.5000            | 89.7199         | -5.2199  |
| 8                             | Janet   | 1.0000          | 112.5000           | 102.0122        | 10.4878  |
| 9                             | Jeffrey | 0.7500          | 84.0000            | 100.6507        | -16.6507 |
| 10                            | John    | 0.7500          | 99.5000            | 86.6828         | 12.8172  |
| 11                            | Joyce   | 1.0000          | 50.5000            | 56.7703         | -6.2703  |
| 12                            | Judy    | 1.0000          | 90.0000            | 108.1649        | -18.1649 |
| 13                            | Louise  | 1.0000          | 77.0000            | 76.4327         | 0.5673   |
| 14                            | Mary    | 1.0000          | 112.0000           | 117.1975        | -5.1975  |
| 15                            | Philip  | 1.0000          | 150.0000           | 138.7581        | 11.2419  |
| 16                            | Robert  | 1.0000          | 128.0000           | 108.7016        | 19.2984  |
| 17                            | Ronald  | 0.7500          | 133.0000           | 119.0957        | 13.9043  |
| 18                            | Thomas  | 1.0000          | 85.0000            | 80.3076         | 4.6924   |
| 19                            | William | 1.0000          | 112.0000           | 117.1975        | -5.1975  |
| Sum of Residuals              |         |                 |                    | 0               |          |
| Sum of Squared Residuals      |         |                 |                    | 1879.08980      |          |
| Predicted Residual SS (PRESS) |         |                 |                    | 2959.57279      |          |

Note that observations that meet the condition of the second REWEIGHT statement (residuals with an absolute value greater than or equal to 17) now have weights reset to their original value of 1. Observations 1, 3, 9, 10, and 17 have weights of 0.75, but observations 12 and 16 (which meet the condition of the second REWEIGHT statement) have their weights reset to 1.

Notice how the last three examples show three ways to change weights back to a previous value. In the first example, ALLOBS and the RESET option are used to change weights for all observations back to their original values. In the second example, the UNDO option is used to negate the effect of a previous REWEIGHT statement, thus changing weights for observations selected in the previous REWEIGHT statement to the weights specified in still another REWEIGHT statement. In the third example, the RESET option is used to change weights for observations selected in a previous REWEIGHT statement back to their original values.

Finally, note that the label MODEL1.12 indicates that 12 REWEIGHT statements have been applied to the original model.

## Testing for Heteroscedasticity

The regression model is specified as  $y_i = \mathbf{x}_i \boldsymbol{\beta} + \epsilon_i$ , where the  $\epsilon_i$ 's are identically and independently distributed:  $E(\boldsymbol{\epsilon}) = 0$  and  $E(\boldsymbol{\epsilon}'\boldsymbol{\epsilon}) = \sigma^2 \mathbf{I}$ . If the  $\epsilon_i$ 's are not independent or their variances are not constant, the parameter estimates are unbiased, but the estimate of the covariance matrix is inconsistent.

In the case of heteroscedasticity, if the regression data are from a simple random sample, then White (1980), showed that matrix

$$\text{HC}_0 = (\mathbf{X}'\mathbf{X})^{-1} (\mathbf{X}' \text{diag}(e_i^2) \mathbf{X}) (\mathbf{X}'\mathbf{X})^{-1}$$

where

$$e_i = y_i - \mathbf{x}_i \mathbf{b}$$

is an asymptotically consistent estimate of the covariance matrix. MacKinnon and White (1985) introduced three alternative heteroscedasticity-consistent covariance matrix estimators that are all asymptotically equivalent to the estimator  $\text{HC}_0$  but that typically have better small sample behavior. These estimators labeled  $\text{HC}_1$ ,  $\text{HC}_2$ , and  $\text{HC}_3$  are defined as follows:

$$\text{HC}_1 = \frac{n}{n-p} \text{HC}_0$$

where  $n$  is the number of observations and  $p$  is the number of regressors including the intercept.

$$\text{HC}_2 = (\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}' \text{diag}\left(\frac{e_i^2}{1-h_{ii}}\right) \mathbf{X} (\mathbf{X}'\mathbf{X})^{-1}$$

where

$$h_{ii} = \mathbf{x}_i (\mathbf{X}'\mathbf{X})^{-1} \mathbf{x}_i'$$

is the leverage of the  $i$ th observation.

$$\text{HC}_3 = (\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}' \text{diag}\left(\frac{e_i^2}{(1-h_{ii})^2}\right) \mathbf{X} (\mathbf{X}'\mathbf{X})^{-1}$$

Long and Ervin (2000) studied the performance of these estimators and recommend using the  $\text{HC}_3$  estimator if the sample size is less than 250.

You can use the `HCCMETHOD=0,1,2, or 3` in the `MODEL` statement to select a heteroscedasticity-consistent covariance matrix estimator, with `HC0` being the default. The `ACOV` option in the `MODEL` statement displays the heteroscedasticity-consistent covariance matrix estimator in effect and adds heteroscedasticity-consistent standard errors, also known as White standard errors, to the parameter estimates table. If you specify the `HCC` or `WHITE` option in the `MODEL` statement, but do not also specify the `ACOV` option, then the heteroscedasticity-consistent standard errors are added to the parameter estimates table but the heteroscedasticity-consistent covariance matrix is not displayed.

The `SPEC` option performs a model specification test. The null hypothesis for this test maintains that the errors are homoscedastic and independent of the regressors and that several technical assumptions about the model specification are valid. For details, see theorem 2 and assumptions 1–7 of White (1980). When the model is correctly specified and the errors are independent of the regressors, the rejection of this null hypothesis is evidence of heteroscedasticity. In implementing this test, an estimator of the average covariance matrix (White 1980, p. 822) is constructed and inverted. The nonsingularity of this matrix is one of the assumptions in the null hypothesis about the model specification. When PROC REG determines this matrix to be numerically singular, a generalized inverse is used and a note to this effect is written to the log. In such cases, care should be taken in interpreting the results of this test.

When you specify the `SPEC`, `ACOV`, `HCC`, or `WHITE` option in the `MODEL` statement, tests listed in the `TEST` statement are performed with both the usual covariance matrix and the heteroscedasticity-consistent covariance matrix requested with the `HCCMETHOD=` option. Tests performed with the consistent covariance matrix are asymptotic. For more information, see White (1980).

Both the `ACOV` and `SPEC` options can be specified in a `MODEL` or `PRINT` statement.

---

## Testing for Lack of Fit

The test for lack of fit compares the variation around the model with “pure” variation within replicated observations. This measures the adequacy of the specified model. In particular, if there are  $n_i$  replicated observations  $Y_{i1}, \dots, Y_{in_i}$  of the response all at the same values  $\mathbf{x}_i$  of the regressors, then you can predict the true response at  $\mathbf{x}_i$  either by using the predicted value  $\hat{Y}_i$  based on the model or by using the mean  $\bar{Y}_i$  of the replicated values. The test for lack of fit decomposes the residual error into a component due to the variation of the replications around their mean value (the “pure” error) and a component due to the variation of the mean values around the model prediction (the “bias” error):

$$\sum_i \sum_{j=1}^{n_i} (Y_{ij} - \hat{Y}_i)^2 = \sum_i \sum_{j=1}^{n_i} (Y_{ij} - \bar{Y}_i)^2 + \sum_i n_i (\bar{Y}_i - \hat{Y}_i)^2$$

If the model is adequate, then both components estimate the nominal level of error; however, if the bias component of error is much larger than the pure error, then this constitutes evidence that there is significant lack of fit.

If some observations in your design are replicated, you can test for lack of fit by specifying the `LACKFIT` option in the `MODEL` statement (see Example 79.6). Note that, since all other tests use total error rather than pure error, you might want to hand-calculate the tests with respect to pure error if the lack of fit is significant. On the other hand, significant lack of fit indicates that the specified model is inadequate, so if this is a problem you can also try to refine the model.



## Multivariate Tests

The MTEST statement described in the section “MTEST Statement” on page 6660 can test hypotheses involving several dependent variables in the form

$$(\mathbf{L}\boldsymbol{\beta} - \mathbf{c})\mathbf{M} = 0$$

where  $\mathbf{L}$  is a linear function on the regressor side,  $\boldsymbol{\beta}$  is a matrix of parameters,  $\mathbf{c}$  is a column vector of constants,  $\mathbf{j}$  is a row vector of ones, and  $\mathbf{M}$  is a linear function on the dependent side. The special case where the constants are zero is

$$\mathbf{L}\boldsymbol{\beta}\mathbf{M} = 0$$

To test this hypothesis, PROC REG constructs two matrices called  $\mathbf{H}$  and  $\mathbf{E}$  that correspond to the numerator and denominator of a univariate  $F$  test:

$$\mathbf{H} = \mathbf{M}'(\mathbf{L}\mathbf{B} - \mathbf{c}\mathbf{j})'(\mathbf{L}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{L}')^{-1}(\mathbf{L}\mathbf{B} - \mathbf{c}\mathbf{j})\mathbf{M}$$

$$\mathbf{E} = \mathbf{M}'(\mathbf{Y}'\mathbf{Y} - \mathbf{B}'(\mathbf{X}'\mathbf{X})\mathbf{B})\mathbf{M}$$

These matrices are displayed for each MTEST statement if the PRINT option is specified.

Four test statistics based on the eigenvalues of  $\mathbf{E}^{-1}\mathbf{H}$  or  $(\mathbf{E} + \mathbf{H})^{-1}\mathbf{H}$  are formed. These are Wilks' lambda, Pillai's trace, the Hotelling-Lawley trace, and Roy's greatest root. These test statistics are discussed in Chapter 4, “Introduction to Regression Procedures.”

The following code creates MANOVA data from Morrison (1976):

```
* Manova Data from Morrison (1976, 190);
data a;
 input sex $ drug $ @;
 do rep=1 to 4;
 input y1 y2 @;
 sexcode=(sex='m')-(sex='f');
 drug1=(drug='a')-(drug='c');
 drug2=(drug='b')-(drug='c');
 sexdrug1=sexcode*drug1;
 sexdrug2=sexcode*drug2;
 output;
end;
datalines;
m a 5 6 5 4 9 9 7 6
m b 7 6 7 7 9 12 6 8
m c 21 15 14 11 17 12 12 10
```

```
f a 7 10 6 6 9 7 8 10
f b 10 13 8 7 7 6 6 9
f c 16 12 14 9 14 8 10 5
;
```

The following statements perform a multivariate analysis of variance and produce Figure 79.46 through Figure 79.49:

```
proc reg;
 model y1 y2=sexcode drug1 drug2 sexdrug1 sexdrug2;
 y1y2drug: mtest y1=y2, drug1,drug2;
 drugshow: mtest drug1, drug2 / print canprint;
run;
```

**Figure 79.46** Multivariate Analysis of Variance: REG Procedure

| The REG Procedure      |                |                    |                |         |         |
|------------------------|----------------|--------------------|----------------|---------|---------|
| Model: MODEL1          |                |                    |                |         |         |
| Dependent Variable: y1 |                |                    |                |         |         |
| Analysis of Variance   |                |                    |                |         |         |
| Source                 | DF             | Sum of Squares     | Mean Square    | F Value | Pr > F  |
| Model                  | 5              | 316.00000          | 63.20000       | 12.04   | <.0001  |
| Error                  | 18             | 94.50000           | 5.25000        |         |         |
| Corrected Total        | 23             | 410.50000          |                |         |         |
|                        | Root MSE       | 2.29129            | R-Square       | 0.7698  |         |
|                        | Dependent Mean | 9.75000            | Adj R-Sq       | 0.7058  |         |
|                        | Coeff Var      | 23.50039           |                |         |         |
| Parameter Estimates    |                |                    |                |         |         |
| Variable               | DF             | Parameter Estimate | Standard Error | t Value | Pr >  t |
| Intercept              | 1              | 9.75000            | 0.46771        | 20.85   | <.0001  |
| sexcode                | 1              | 0.16667            | 0.46771        | 0.36    | 0.7257  |
| drug1                  | 1              | -2.75000           | 0.66144        | -4.16   | 0.0006  |
| drug2                  | 1              | -2.25000           | 0.66144        | -3.40   | 0.0032  |
| sexdrug1               | 1              | -0.66667           | 0.66144        | -1.01   | 0.3269  |
| sexdrug2               | 1              | -0.41667           | 0.66144        | -0.63   | 0.5366  |

Figure 79.47 Multivariate Analysis of Variance: REG Procedure

| Analysis of Variance |    |                    |                |         |         |
|----------------------|----|--------------------|----------------|---------|---------|
| Source               | DF | Sum of Squares     | Mean Square    | F Value | Pr > F  |
| Model                | 5  | 69.33333           | 13.86667       | 2.19    | 0.1008  |
| Error                | 18 | 114.00000          | 6.33333        |         |         |
| Corrected Total      | 23 | 183.33333          |                |         |         |
| Root MSE             |    | 2.51661            | R-Square       | 0.3782  |         |
| Dependent Mean       |    | 8.66667            | Adj R-Sq       | 0.2055  |         |
| Coeff Var            |    | 29.03782           |                |         |         |
| Parameter Estimates  |    |                    |                |         |         |
| Variable             | DF | Parameter Estimate | Standard Error | t Value | Pr >  t |
| Intercept            | 1  | 8.66667            | 0.51370        | 16.87   | <.0001  |
| sexcode              | 1  | 0.16667            | 0.51370        | 0.32    | 0.7493  |
| drug1                | 1  | -1.41667           | 0.72648        | -1.95   | 0.0669  |
| drug2                | 1  | -0.16667           | 0.72648        | -0.23   | 0.8211  |
| sexdrug1             | 1  | -1.16667           | 0.72648        | -1.61   | 0.1257  |
| sexdrug2             | 1  | -0.41667           | 0.72648        | -0.57   | 0.5734  |

Figure 79.48 Multivariate Analysis of Variance: First Test

| The REG Procedure                              |            |         |        |        |        |
|------------------------------------------------|------------|---------|--------|--------|--------|
| Model: MODEL1                                  |            |         |        |        |        |
| Multivariate Test: y1y2drug                    |            |         |        |        |        |
| Multivariate Statistics and Exact F Statistics |            |         |        |        |        |
|                                                | S=1        | M=0     | N=8    |        |        |
| Statistic                                      | Value      | F Value | Num DF | Den DF | Pr > F |
| Wilks' Lambda                                  | 0.28053917 | 23.08   | 2      | 18     | <.0001 |
| Pillai's Trace                                 | 0.71946083 | 23.08   | 2      | 18     | <.0001 |
| Hotelling-Lawley Trace                         | 2.56456456 | 23.08   | 2      | 18     | <.0001 |
| Roy's Greatest Root                            | 2.56456456 | 23.08   | 2      | 18     | <.0001 |

The four multivariate test statistics are all highly significant, giving strong evidence that the coefficients of drug1 and drug2 are not the same across dependent variables y1 and y2.

**Figure 79.49** Multivariate Analysis of Variance: Second Test

| The REG Procedure                                                                      |                       |                                |                            |                               |        |
|----------------------------------------------------------------------------------------|-----------------------|--------------------------------|----------------------------|-------------------------------|--------|
| Model: MODEL1                                                                          |                       |                                |                            |                               |        |
| Multivariate Test: drugshow                                                            |                       |                                |                            |                               |        |
| Error Matrix (E)                                                                       |                       |                                |                            |                               |        |
|                                                                                        | 94.5                  |                                | 76.5                       |                               |        |
|                                                                                        | 76.5                  |                                | 114                        |                               |        |
| Hypothesis Matrix (H)                                                                  |                       |                                |                            |                               |        |
|                                                                                        | 301                   |                                | 97.5                       |                               |        |
|                                                                                        | 97.5                  |                                | 36.33333333                |                               |        |
|                                                                                        | Canonical Correlation | Adjusted Canonical Correlation | Approximate Standard Error | Squared Canonical Correlation |        |
| 1                                                                                      | 0.905903              | 0.899927                       | 0.040101                   | 0.820661                      |        |
| 2                                                                                      | 0.244371              | .                              | 0.210254                   | 0.059717                      |        |
| Eigenvalues of Inv(E)*H<br>= CanRsq/(1-CanRsq)                                         |                       |                                |                            |                               |        |
|                                                                                        | Eigenvalue            | Difference                     | Proportion                 | Cumulative                    |        |
| 1                                                                                      | 4.5760                | 4.5125                         | 0.9863                     | 0.9863                        |        |
| 2                                                                                      | 0.0635                |                                | 0.0137                     | 1.0000                        |        |
| Test of H0: The canonical correlations in the current row and all that follow are zero |                       |                                |                            |                               |        |
|                                                                                        | Likelihood Ratio      | Approximate F Value            | Num DF                     | Den DF                        | Pr > F |
| 1                                                                                      | 0.16862952            | 12.20                          | 4                          | 34                            | <.0001 |
| 2                                                                                      | 0.94028273            | 1.14                           | 1                          | 18                            | 0.2991 |
| Multivariate Statistics and F Approximations                                           |                       |                                |                            |                               |        |
|                                                                                        | S=2                   | M=-0.5                         | N=7.5                      |                               |        |
| Statistic                                                                              | Value                 | F Value                        | Num DF                     | Den DF                        | Pr > F |
| Wilks' Lambda                                                                          | 0.16862952            | 12.20                          | 4                          | 34                            | <.0001 |
| Pillai's Trace                                                                         | 0.88037810            | 7.08                           | 4                          | 36                            | 0.0003 |
| Hotelling-Lawley Trace                                                                 | 4.63953666            | 19.40                          | 4                          | 19.407                        | <.0001 |
| Roy's Greatest Root                                                                    | 4.57602675            | 41.18                          | 2                          | 18                            | <.0001 |
| NOTE: F Statistic for Roy's Greatest Root is an upper bound.                           |                       |                                |                            |                               |        |
| NOTE: F Statistic for Wilks' Lambda is exact.                                          |                       |                                |                            |                               |        |

The four multivariate test statistics are all highly significant, giving strong evidence that the coefficients of drug1 and drug2 are not zero for both dependent variables.

---

## Autocorrelation in Time Series Data

When regression is performed on time series data, the errors might not be independent. Often errors are autocorrelated; that is, each error is correlated with the error immediately before it. Autocorrelation is also a symptom of systematic lack of fit. The DW option provides the Durbin-Watson  $d$  statistic to test that the autocorrelation is zero:

$$d = \frac{\sum_{i=2}^n (e_i - e_{i-1})^2}{\sum_{i=1}^n e_i^2}$$

The value of  $d$  is close to 2 if the errors are uncorrelated. The distribution of  $d$  is reported by Durbin and Watson (1951). Tables of the distribution are found in most econometrics textbooks, such as Johnston (1972) and Pindyck and Rubinfeld (1981).

The sample autocorrelation estimate is displayed after the Durbin-Watson statistic. The sample is computed as

$$r = \frac{\sum_{i=2}^n e_i e_{i-1}}{\sum_{i=1}^n e_i^2}$$

This autocorrelation of the residuals might not be a very good estimate of the autocorrelation of the true errors, especially if there are few observations and the independent variables have certain patterns. If there are missing observations in the regression, these measures are computed as though the missing observations did not exist.

Positive autocorrelation of the errors generally tends to make the estimate of the error variance too small, so confidence intervals are too narrow and true null hypotheses are rejected with a higher probability than the stated significance level. Negative autocorrelation of the errors generally tends to make the estimate of the error variance too large, so confidence intervals are too wide and the power of significance tests is reduced. With either positive or negative autocorrelation, least squares parameter estimates are usually not as efficient as generalized least squares parameter estimates. For more details, see Judge et al. (1985, Chapter 8) and the *SAS/ETS User's Guide*.

The following SAS statements request the DWPROB option for the U.S. population data (see [Figure 79.50](#)). If you use the DW option instead of the DWPROB option, then  $p$ -values are not produced.

```
proc reg data=USPopulation;
 model Population=Year YearSq / dwProb;
run;
```

**Figure 79.50** Regression Using DW Option

| The REG Procedure              |        |
|--------------------------------|--------|
| Model: MODEL1                  |        |
| Dependent Variable: Population |        |
| Durbin-Watson D                | 1.191  |
| Pr < DW                        | 0.0050 |
| Pr > DW                        | 0.9950 |
| Number of Observations         | 22     |
| 1st Order Autocorrelation      | 0.323  |

## Computations for Ridge Regression and IPC Analysis

In ridge regression analysis, the crossproduct matrix for the independent variables is centered (the NOINT option is ignored if it is specified) and scaled to one on the diagonal elements. The ridge constant  $k$  (specified with the RIDGE= option) is then added to each diagonal element of the crossproduct matrix. The ridge regression estimates are the least squares estimates obtained by using the new crossproduct matrix.

Let  $\mathbf{X}$  be an  $n \times p$  matrix of the independent variables after centering the data, and let  $\mathbf{Y}$  be an  $n \times 1$  vector corresponding to the dependent variable. Let  $\mathbf{D}$  be a  $p \times p$  diagonal matrix with diagonal elements as in  $\mathbf{X}'\mathbf{X}$ . The ridge regression estimate corresponding to the ridge constant  $k$  can be computed as

$$\mathbf{D}^{-\frac{1}{2}}(\mathbf{Z}'\mathbf{Z} + k\mathbf{I}_p)^{-1}\mathbf{Z}'\mathbf{Y}$$

where  $\mathbf{Z} = \mathbf{X}\mathbf{D}^{-\frac{1}{2}}$  and  $\mathbf{I}_p$  is a  $p \times p$  identity matrix.

For IPC analysis, the smallest  $m$  eigenvalues of  $\mathbf{Z}'\mathbf{Z}$  (where  $m$  is specified with the PCOMIT= option) are omitted to form the estimates.

For information about ridge regression and IPC standardized parameter estimates, parameter estimate standard errors, and variance inflation factors, see Rawlings, Pantula, and Dickey (1998); Neter, Wasserman, and Kutner (1990); Marquardt and Snee (1975). Unlike Rawlings, Pantula, and Dickey (1998), the REG procedure uses the mean squared errors of the submodels instead of the full model MSE to compute the standard errors of the parameter estimates.

## Construction of Q-Q and P-P Plots

If a normal probability-probability or quantile-quantile plot for the variable  $x$  is requested, the  $n$  nonmissing values of  $x$  are first ordered from smallest to largest:

$$x_{(1)} \leq x_{(2)} \leq \cdots \leq x_{(n)}$$

If a Q-Q plot is requested (with a PLOT statement of the form PLOT *yvariable*\*NQQ.), the  $i$ th-ordered value  $x_{(i)}$  is represented by a point with  $y$ -coordinate  $x_{(i)}$  and  $x$ -coordinate  $\Phi^{-1}\left(\frac{i-0.375}{n+0.25}\right)$ , where  $\Phi(\cdot)$  is the standard normal distribution.

If a P-P plot is requested (with a **PLOT** statement of the form **PLOT yvariable\*NPP.**), the  $i$ th-ordered value  $x_{(i)}$  is represented by a point with y-coordinate  $\frac{i}{n}$  and x-coordinate  $\Phi\left(\frac{x_{(i)}-\mu}{\sigma}\right)$ , where  $\mu$  is the mean of the nonmissing  $x$ -values and  $\sigma$  is the standard deviation. If an  $x$ -value has multiplicity  $k$  (that is,  $x_{(i)} = \dots = x_{(i+k-1)}$ ), then only the point  $\left(\Phi\left(\frac{x_{(i)}-\mu}{\sigma}\right), \frac{i+k-1}{n}\right)$  is displayed.

---

## Computational Methods

The REG procedure first composes a crossproducts matrix. The matrix can be calculated from input data, reformed from an input correlation matrix, or read in from an SSCP data set. For each model, the procedure selects the appropriate crossproducts from the main matrix. The normal equations formed from the crossproducts are solved by using a sweep algorithm (Goodnight 1979). The method is accurate for data that are reasonably scaled and not too collinear.

The mechanism that PROC REG uses to check for singularity involves the diagonal (pivot) elements of  $X'X$  as it is being swept. If a pivot is less than **SINGULAR\*CSS**, then a singularity is declared and the pivot is not swept (where **CSS** is the corrected sum of squares for the regressor and **SINGULAR** is machine dependent but is approximately  $1E-7$  on most machines or reset in the **PROC REG** statement).

The sweep algorithm is also used in many places in the model-selection methods. The **RSQUARE** method uses the leaps-and-bounds algorithm by Furnival and Wilson (1974).

---

## Computer Resources in Regression Analysis

The REG procedure is efficient for ordinary regression; however, requests for optional features can greatly increase the amount of time required.

The major computational expense in the regression analysis is the collection of the crossproducts matrix. For  $p$  variables and  $n$  observations, the time required is proportional to  $np^2$ . For each model run, PROC REG needs time roughly proportional to  $k^3$ , where  $k$  is the number of regressors in the model. Include an additional  $nk^2$  for the **R**, **CLM**, or **CLI** option and another  $nk^2$  for the **INFLUENCE** option.

Most of the memory that PROC REG needs to solve large problems is used for crossproducts matrices. PROC REG requires  $4p^2$  bytes for the main crossproducts matrix plus  $4k^2$  bytes for the largest model. If several output data sets are requested, memory is also needed for buffers.

See the section “**Input Data Sets**” on page 6686 for information about how to use **TYPE=SSCP** data sets to reduce computing time.

---

## Displayed Output

Many of the more specialized tables are described in detail in previous sections. Most of the formulas for the statistics are in Chapter 4, “**Introduction to Regression Procedures**,” while other formulas can be found in the section “**Model Fit and Diagnostic Statistics**” on page 6715 and the section “**Influence Statistics**” on page 6717.

The analysis-of-variance table includes the following:

- the Source of the variation, Model for the fitted regression, Error for the residual error, and C Total for the total variation after correcting for the mean. The Uncorrected Total Variation is produced when the NOINT option is used.
- the degrees of freedom (DF) associated with the source
- the Sum of Squares for the term
- the Mean Square, the sum of squares divided by the degrees of freedom
- the F Value for testing the hypothesis that all parameters are zero except for the intercept. This is formed by dividing the mean square for Model by the mean square for Error.
- the Prob>F, the probability of getting a greater  $F$  statistic than that observed if the hypothesis is true. This is the significance probability.

Other statistics displayed include the following:

- Root MSE is an estimate of the standard deviation of the error term. It is calculated as the square root of the mean square error.
- Dep Mean is the sample mean of the dependent variable.
- C.V. is the coefficient of variation, computed as 100 times Root MSE divided by Dep Mean. This expresses the variation in unitless values.
- R-square is a measure between 0 and 1 that indicates the portion of the (corrected) total variation that is attributed to the fit rather than left to residual error. It is calculated as SS(Model) divided by SS(Total). It is also called the *coefficient of determination*. It is the square of the multiple correlation—in other words, the square of the correlation between the dependent variable and the predicted values.
- Adj R-square, the adjusted R square, is a version of R square that has been adjusted for degrees of freedom. It is calculated as

$$\bar{R}^2 = 1 - \frac{(n - i)(1 - R^2)}{n - p}$$

where  $i$  is equal to 1 if there is an intercept and 0 otherwise,  $n$  is the number of observations used to fit the model, and  $p$  is the number of parameters in the model.

The parameter estimates and associated statistics are then displayed, and they include the following:

- the Variable used as the regressor, including the name Intercept to represent the estimate of the intercept parameter
- the degrees of freedom (DF) for the variable. There is one degree of freedom unless the model is not full rank.
- the Parameter Estimate



- the Standard Error, the estimate of the standard deviation of the parameter estimate
- T for H0: Parameter=0, the  $t$  test that the parameter is zero. This is computed as the Parameter Estimate divided by the Standard Error.
- the Prob > |T|, the probability that a  $t$  statistic would obtain a greater absolute value than that observed given that the true parameter is zero. This is the two-tailed significance probability.

If model-selection methods other than NONE, RSQUARE, ADJRSQ, and CP are used, the analysis-of-variance table and the parameter estimates with associated statistics are produced at each step. Also displayed are the following:

- C(p), which is Mallows'  $C_p$  statistic
- bounds on the condition number of the correlation matrix for the variables in the model (Berk 1977)

After statistics for the final model are produced, the following is displayed when the method chosen is FORWARD, BACKWARD, or STEPWISE:

- a Summary table listing Step number, Variable Entered or Removed, Partial and Model R-square, and C(p) and F statistics

The RSQUARE method displays its results beginning with the model containing the fewest independent variables and producing the largest R square. Results for other models with the same number of variables are then shown in order of decreasing R square, and so on, for models with larger numbers of variables. The ADJRSQ and CP methods group models of all sizes together and display results beginning with the model having the optimal value of adjusted R square and  $C_p$ , respectively.

For each model considered, the RSQUARE, ADJRSQ, and CP methods display the following:

- Number in Model or IN, the number of independent variables used in each model
- R-square or RSQ, the squared multiple correlation coefficient

If the B option is specified, the RSQUARE, ADJRSQ, and CP methods produce the following:

- Parameter Estimates, the estimated regression coefficients

If the B option is not specified, the RSQUARE, ADJRSQ, and CP methods display the following:

- Variables in Model, the names of the independent variables included in the model

## ODS Table Names

PROC REG assigns a name to each table it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in the following table. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

**Table 79.11** ODS Tables Produced by PROC REG

| ODS Table Name      | Description                                                                                                      | Statement | Option                                                              |
|---------------------|------------------------------------------------------------------------------------------------------------------|-----------|---------------------------------------------------------------------|
| ACovEst             | Consistent covariance of estimates matrix                                                                        | MODEL     | ALL, ACOV                                                           |
| ACovTestANOVA       | Test ANOVA using ACOV estimates                                                                                  | TEST      | ACOV (MODEL statement)                                              |
| ANOVA               | Model ANOVA table                                                                                                | MODEL     | Default                                                             |
| CanCorr             | Canonical correlations for hypothesis combinations                                                               | MTEST     | CANPRINT                                                            |
| CollinDiag          | Collinearity Diagnostics table                                                                                   | MODEL     | COLLIN                                                              |
| CollinDiagNoInt     | Collinearity Diagnostics for no intercept model                                                                  | MODEL     | COLLINOINT                                                          |
| ConditionBounds     | Bounds on condition number                                                                                       | MODEL     | (SELECTION=BACKWARD   FORWARD   STEPWISE   MAXR   MINR) and DETAILS |
| Corr                | Correlation matrix for analysis variables                                                                        | PROC      | ALL, CORR                                                           |
| CorrB               | Correlation of estimates                                                                                         | MODEL     | CORRB                                                               |
| CovB                | Covariance of estimates                                                                                          | MODEL     | COVB                                                                |
| CrossProducts       | Bordered model $\mathbf{X}'\mathbf{X}$ matrix                                                                    | MODEL     | ALL, XPX                                                            |
| DWStatistic         | Durbin-Watson statistic                                                                                          | MODEL     | ALL, DW                                                             |
| DependenceEquations | Linear dependence equations                                                                                      | MODEL     | Default if needed                                                   |
| Eigenvalues         | MTest eigenvalues                                                                                                | MTEST     | CANPRINT                                                            |
| Eigenvectors        | MTest eigenvectors                                                                                               | MTEST     | CANPRINT                                                            |
| EntryStatistics     | Entry statistics for selection methods                                                                           | MODEL     | (SELECTION=BACKWARD   FORWARD   STEPWISE   MAXR   MINR) and DETAILS |
| ErrorPlusHypothesis | MTest error plus hypothesis matrix $\mathbf{H}+\mathbf{E}$                                                       | MTEST     | PRINT                                                               |
| ErrorSSCP           | MTest error matrix $\mathbf{E}$                                                                                  | MTEST     | PRINT                                                               |
| FitStatistics       | Model fit statistics                                                                                             | MODEL     | Default                                                             |
| HypothesisSSCP      | MTest hypothesis matrix                                                                                          | MTEST     | PRINT                                                               |
| InvMTestCov         | $\text{Inv}(\mathbf{L} \text{Ginv}(\mathbf{X}'\mathbf{X}) \mathbf{L}')$ and $\text{Inv}(\mathbf{Lb}-\mathbf{c})$ | MTEST     | DETAILS                                                             |

Table 79.11 continued

| ODS Table Name     | Description                                                                                      | Statement | Option                                                          |
|--------------------|--------------------------------------------------------------------------------------------------|-----------|-----------------------------------------------------------------|
| InvTestCov         | Inv( $\mathbf{L} \text{Ginv}(\mathbf{X}'\mathbf{X}) \mathbf{L}'$ ) and<br>Inv( $\mathbf{Lb-c}$ ) | TEST      | PRINT                                                           |
| InvXPX             | Bordered $\mathbf{X}'\mathbf{X}$ inverse matrix                                                  | MODEL     | I                                                               |
| MTestCov           | $\mathbf{L} \text{Ginv}(\mathbf{X}'\mathbf{X}) \mathbf{L}'$ and $\mathbf{Lb-c}$                  | MTEST     | DETAILS                                                         |
| MTransform         | MTest matrix $\mathbf{M}$ , across<br>dependents                                                 | MTEST     | DETAILS                                                         |
| MultStat           | Multivariate test statistics                                                                     | MTEST     | Default                                                         |
| NObs               | Number of observations                                                                           |           | Default                                                         |
| OutputStatistics   | Output statistics table                                                                          | MODEL     | ALL, CLI, CLM,<br>INFLUENCE, P, R                               |
| PartialData        | Partial regression leverage<br>data                                                              | MODEL     | PARTIALDATA                                                     |
| ParameterEstimates | Model parameter estimates                                                                        | MODEL     | Default if SELECTION= is<br>not specified                       |
| RemovalStatistics  | Removal statistics for<br>selection methods                                                      | MODEL     | (SELECTION=BACKWARD<br>  STEPWISE   MAXR  <br>MINR) and DETAILS |
| ResidualStatistics | Residual statistics and<br>PRESS statistic                                                       | MODEL     | ALL, CLI, CLM,<br>INFLUENCE, P, R                               |
| SelParmEst         | Parameter estimates for<br>selection methods                                                     | MODEL     | SELECTION=BACKWARD<br>  FORWARD   STEPWISE  <br>MAXR   MINR     |
| SelectionSummary   | Selection summary for<br>FORWARD, BACKWARD,<br>and STEPWISE methods                              | MODEL     | SELECTION=BACKWARD<br>  FORWARD   STEPWISE                      |
| SeqParmEst         | Sequential parameter<br>estimates                                                                | MODEL     | SEQB                                                            |
| SimpleStatistics   | Simple statistics for analysis<br>variables                                                      | PROC      | ALL, SIMPLE                                                     |
| SpecTest           | White's heteroscedasticity<br>test                                                               | MODEL     | ALL, SPEC                                                       |
| SubsetSelSummary   | Selection summary for<br>R-square, Adj-RSq, and<br>Cp methods                                    | MODEL     | SELECTION=RSQUARE  <br>ADJRSQ   CP                              |
| TestANOVA          | Test ANOVA table                                                                                 | TEST      | Default                                                         |
| TestCov            | $\mathbf{L} \text{Ginv}(\mathbf{X}'\mathbf{X}) \mathbf{L}'$ and $\mathbf{Lb-c}$                  | TEST      | PRINT                                                           |
| USSCP              | Uncorrected SSCP matrix<br>for analysis variables                                                | PROC      | ALL, USSCP                                                      |

---

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “[Statistical Graphics Using ODS](#).”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS](#).”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “[A Primer on ODS Statistical Graphics](#)” on page 599 in Chapter 21, “[Statistical Graphics Using ODS](#).”

The following sections describe the ODS graphical displays produced by PROC REG.

### Diagnostics Panel

The “Diagnostics Panel” provides a display that you can use to get an overall assessment of your model. See [Figure 79.8](#) for an example.

The panel contains the following plots:

- residuals versus the predicted values
- externally studentized residuals (RSTUDENT) versus the predicted values
- externally studentized residuals versus the leverage
- normal quantile-quantile plot (Q-Q plot) of the residuals
- dependent variable values versus the predicted values
- Cook’s  $D$  versus observation number
- histogram of the residuals
- “Residual-Fit” (or RF) plot consisting of side-by-side quantile plots of the centered fit and the residuals
- box plot of the residuals if you specify the STATS=NONE suboption

Patterns in the plots of residuals or studentized residuals versus the predicted values, or spread of the residuals being greater than the spread of the centered fit in the RF plot, are indications of an inadequate model. Patterns in the spread about the 45-degree reference line in the plot of the dependent variable values versus the predicted values are also indications of an inadequate model.

The Q-Q plot, residual histogram, and box plot of the residuals are useful for diagnosing violations of the normality and homoscedasticity assumptions. If the data in a Q-Q plot come from a normal distribution, the points will cluster tightly around the reference line. A normal density is overlaid on the residual histogram to help in detecting departures from normality.

Following Rawlings, Pantula, and Dickey (1998), reference lines are shown on the relevant plots to identify observations deemed outliers or influential. Observations whose externally studentized residual magnitudes exceed 2 are deemed outliers. Observations whose leverage value exceeds  $2p/n$  or whose Cook’s

$D$  value exceeds  $4/n$  are deemed influential ( $p$  is the number of regressors including the intercept, and  $n$  is the number of observations used in the analysis). If you specify the LABEL suboption of the PLOTS=DIAGNOSTICS option, then the points deemed outliers or influential are labeled on the appropriate plots.

Fit statistics are shown in the lower right of the plot and can be customized or suppressed by using the STATS= suboption of the PLOTS=DIAGNOSTICS option.

### Residuals by Regressor Plots

Panels of plots of the residuals versus each of the regressors in the model are produced by default. Patterns in these plots are indications of an inadequate model. To help in detecting patterns, you can use the SMOOTH= suboption of the PLOTS=RESIDUALS option to add loess fits to these residual plots. See Figure 79.1.6 for an example.

### Fit and Prediction Plots

A fit plot consisting of a scatter plot of the data overlaid with the regression line, as well as confidence and prediction limits, is produced for models depending on a single regressor. Fit statistics are shown to the right of the plot and can be customized or suppressed by using the STATS= suboption of the PLOTS=FIT option.

When a model contains more than one regressor, a fit plot is not appropriate. However, if all the regressors in the model are transformations of a single variable in the input data set, then you can request a scatter plot of the dependent variable overlaid with a fit line and confidence and prediction limits versus this variable. You can also plot residuals versus this variable. You request these plots, shown in a panel, with the PLOTS=PREDICTION option. See Figure 79.13 for an example.

### Influence Plots

In addition to the “Cook’s D Plot” and the “RStudent By Leverage Plot,” you can request plots of the DFBETAS and DFFITS statistics versus observation number by using the PLOTS=DFBETAS and PLOTS=DFFITS options. You can also obtain partial regression leverage plots by using the PLOTS=PARTIAL option. See the section “Influence Statistics” on page 6717 for examples of these plots and details about their interpretation.

### Ridge and VIF Plots

When you use ridge regression, you can request plots of the variance inflation factor (VIF) values and standardized ridge estimates by ridge values for each coefficient with the PLOTS=RIDGE option. See Example 79.5 for examples.

## Variable Selection Plots

When you request variable selection by using the `SELECTION=` option in the `MODEL` statement, you can request plots of fit criteria for the models examined by using the `PLOTS=CRITERIA` option. The fit criteria are displayed versus the step number for the `FORWARD`, `BACKWARD`, and `STEPWISE` selection methods and the step at which the optimal value of each criterion is obtained is indicated using a “Star” marker. For the all-subset-based selection methods (`SELECTION=RSQUARE|ADJRSQ|CP`), the fit criteria are displayed versus the number of observations in the model.

The criteria are shown in a panel, but you can use the `UNPACK` suboption of the `PLOTS=CRITERIA` option to obtain separate plots for each criterion. You can also use the `LABEL` suboption of the `PLOTS=CRITERIA` option to request that optimal models be labeled on the plots. [Example 79.2](#) provides several examples.

## Heat Maps (Experimental)

`PROC REG` can produce either fit and residual scatter plots for smaller data sets or heat maps for larger data sets. The global plot option `MAXPOINTS=max heat-max` controls which of these are produced. When the number of points exceeds the value of `max` but does not exceed the value of `heat-max` divided by the number of independent variables, heat maps are displayed instead of scatter plots for the fit and residual plots. All other graphs are suppressed when the number of points exceeds `max`. The default is `MAXPOINTS=5000 150000`. These cutoffs are ignored if you specify `MAXPOINTS=NONE`. The following statements create both scatter plots and heat maps with artificial data:

```
data x;
 do i = 1 to 25000;
 x = 2 * normal(104);
 y = x + sin(x * 2) + 3 * normal(104);
 output;
 end;
run;

ods graphics on;

proc reg data=x plots(maxpoints=30000);
 model y = x;
run; quit;

proc reg data=x;
 model y = x;
run; quit;
```

Scatter plots are displayed in [Output 79.51](#), and heat maps are displayed in [Output 79.52](#).

Figure 79.51 Scatter Plot

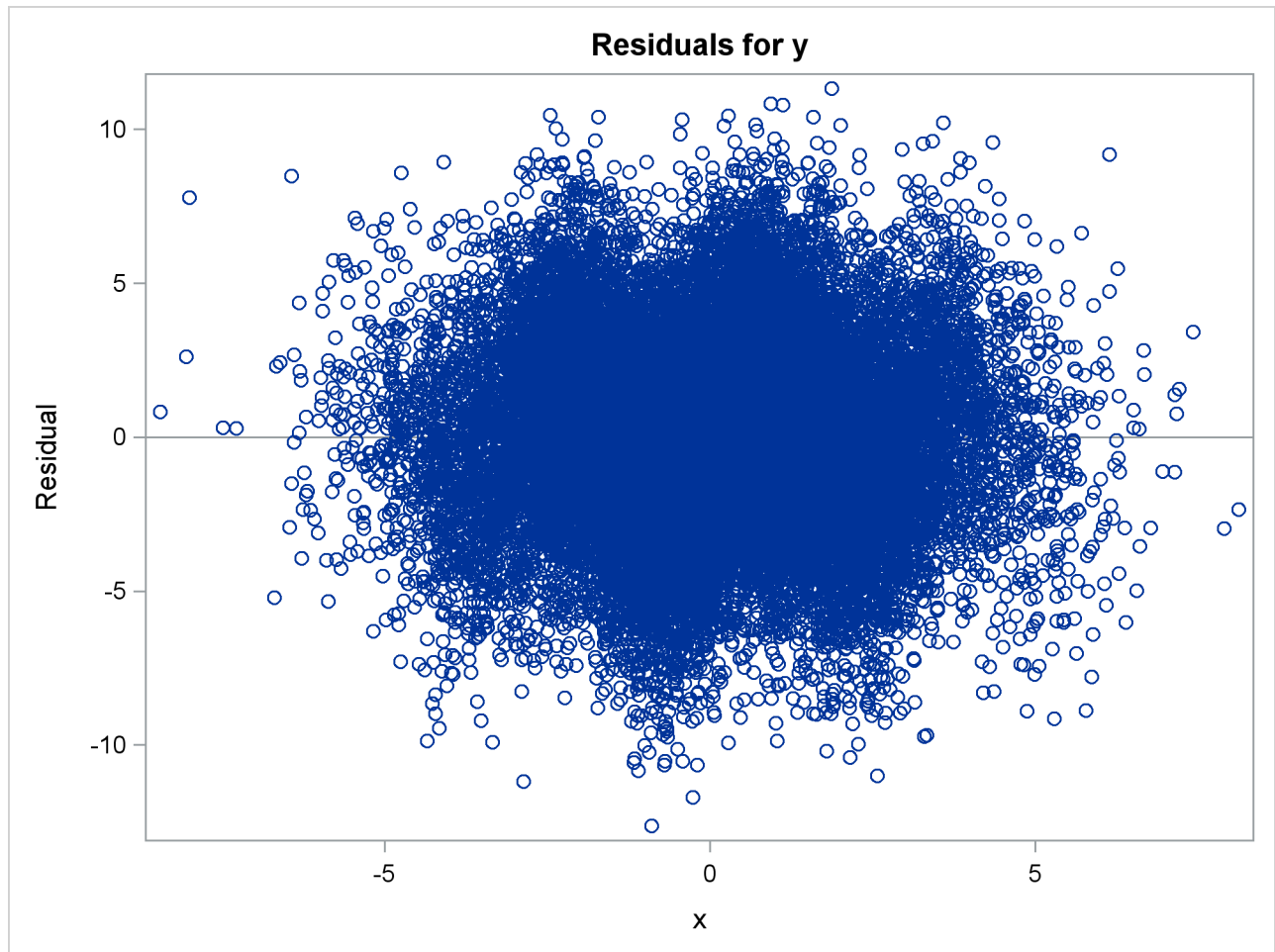


Figure 79.51 continued

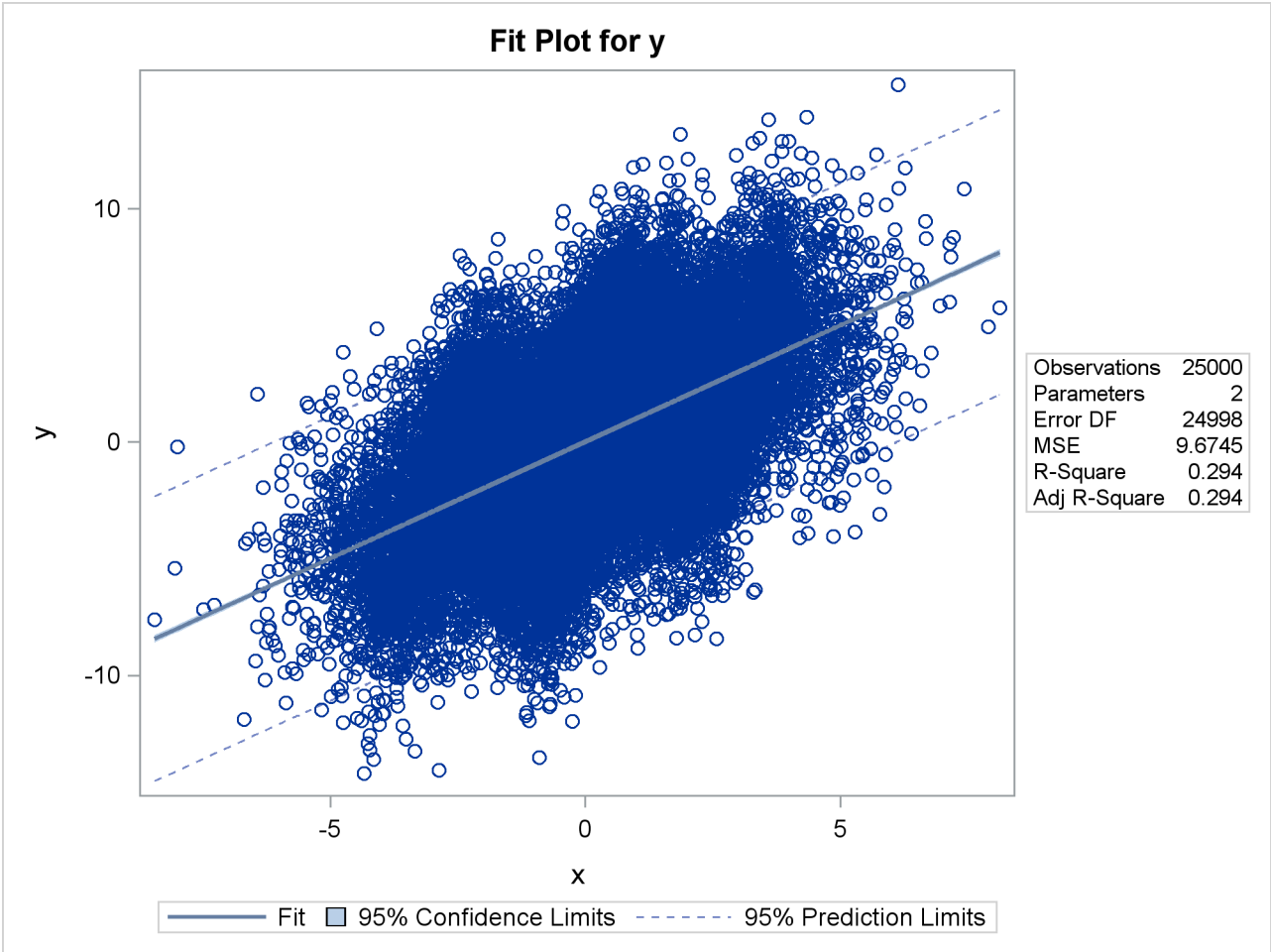




Figure 79.52 Heat Map

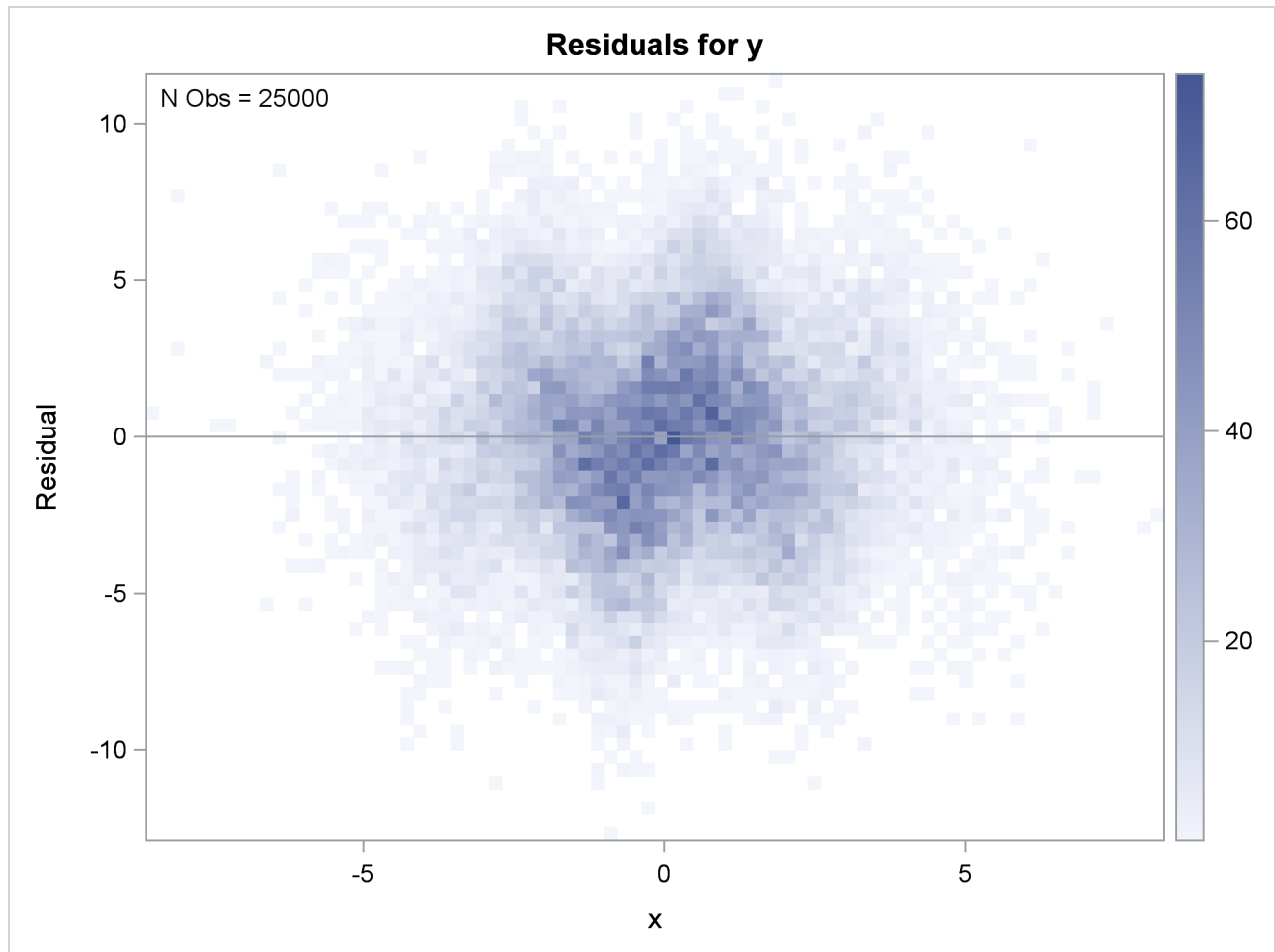
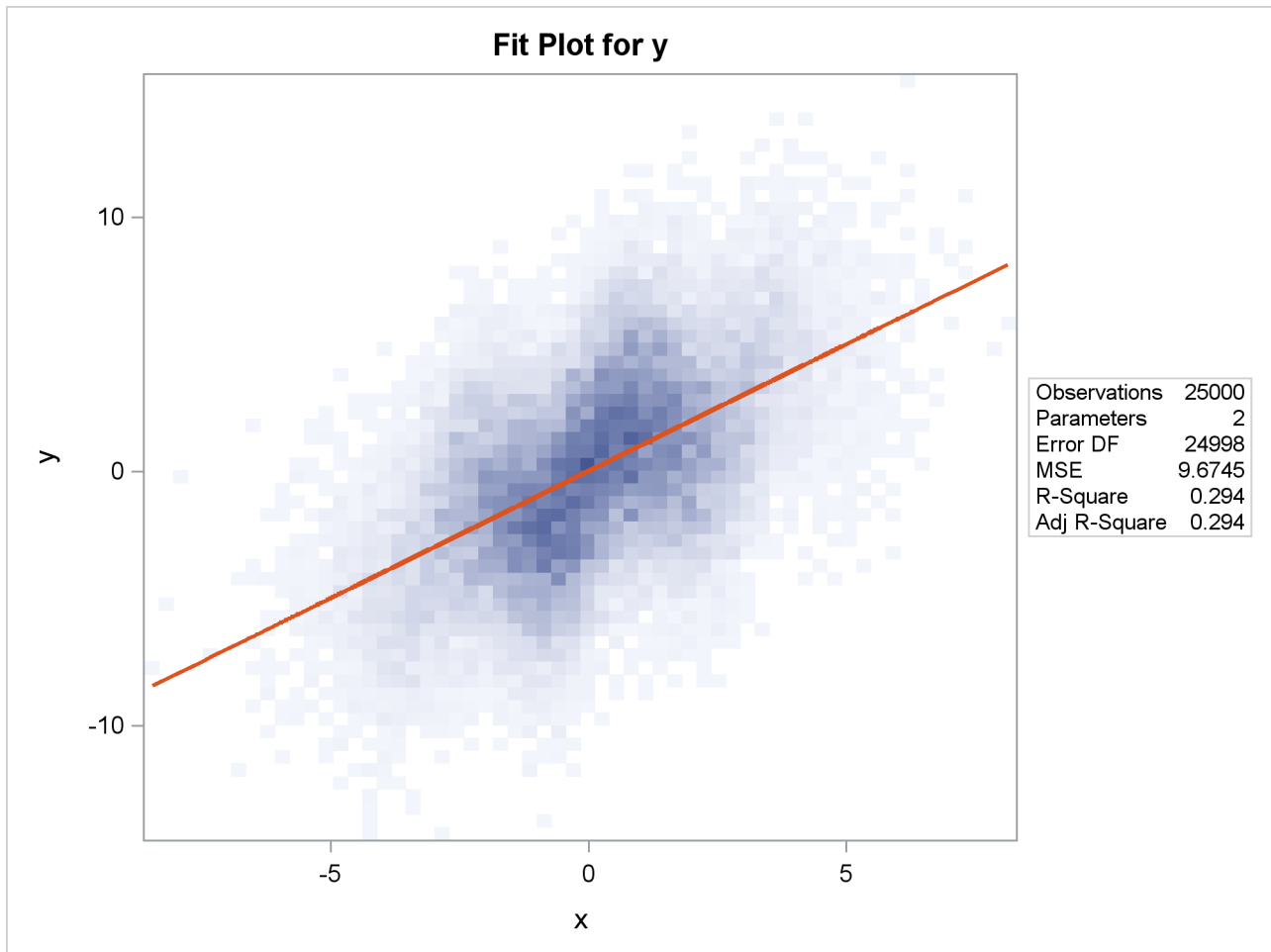


Figure 79.52 continued



The heat maps show more clearly that the sine function is not fit well by the linear fit function.

## ODS Graph Names

PROC REG assigns a name to each graph it creates using ODS. You can use these names to reference the graphs when using ODS. The names are listed in Table 79.12.

**Table 79.12** ODS Graphical Displays Produced by PROC REG

| ODS Graph Name         | Plot Description                                                                                 | PLOTS Option                                       |
|------------------------|--------------------------------------------------------------------------------------------------|----------------------------------------------------|
| AdjrsqPlot             | Adjusted R-square statistic for models examined doing variable selection                         | ADJRSQ                                             |
| AICPlot                | AIC statistic for models examined doing variable selection                                       | AIC                                                |
| BICPlot                | BIC statistic for models examined doing variable selection                                       | BIC                                                |
| CooksDPlot             | Cook's $D$ statistic versus observation number                                                   | COOKSD                                             |
| CPPlot                 | $C_p$ statistic for models examined doing variable selection                                     | CP                                                 |
| DFFITSPlot             | DFFITS statistics versus observation number                                                      | DFFITS                                             |
| DFBETASPanel           | Panel of DFBETAS statistics versus observation number                                            | DFBETAS                                            |
| DFBETASPlot            | DFBETAS statistics versus observation number                                                     | DFBETAS(UNPACK)                                    |
| DiagnosticsPanel       | Panel of fit diagnostics                                                                         | DIAGNOSTICS                                        |
| FitPlot                | Regression line, confidence limits, and prediction limits overlaid on a scatter plot of the data | FIT, <code>MAXPOINTS=max</code> not exceeded       |
| FitPlot                | Regression line overlaid on a heat map of the data                                               | FIT, <code>MAXPOINTS=max</code> exceeded           |
| ObservedByPredicted    | Dependent variable versus predicted values                                                       | OBSERVEDBYPREDICTED                                |
| PartialPlot            | Partial regression plot                                                                          | PARTIAL                                            |
| PredictionPanel        | Panel of residuals and fit versus specified variable                                             | PREDICTIONS                                        |
| PredictionPlot         | Regression line, confidence limits, and prediction limits versus specified variable              | PREDICTIONS(UNPACK)                                |
| PredictionResidualPlot | Residuals versus specified variable                                                              | PREDICTIONS(UNPACK)                                |
| QQPlot                 | Normal quantile plot of residuals                                                                | QQ                                                 |
| ResidualBoxPlot        | Box plot of residuals                                                                            | BOXPLOT                                            |
| ResidualByPredicted    | Residuals versus predicted values                                                                | RESIDUALBYPREDICTED                                |
| ResidualHistogram      | Histogram of fit residuals                                                                       | RESIDUALHISTOGRAM                                  |
| ResidualPlot           | Scatter plot of residuals versus regressor                                                       | RESIDUALS, <code>MAXPOINTS=max</code> not exceeded |
| ResidualPlot           | Heat map of residuals versus regressor                                                           | RESIDUALS, <code>MAXPOINTS=max</code> exceeded     |

Table 79.12 continued

| ODS Graph Name          | Plot Description                                                     | PLOTS Option        |
|-------------------------|----------------------------------------------------------------------|---------------------|
| RFPlot                  | Side-by-side plots of quantiles of centered fit and residuals        | RF                  |
| RidgePanel              | Plot of VIF and ridge traces                                         | RIDGE               |
| RidgePlot               | Plot of ridge traces                                                 | RIDGE(UNPACK)       |
| RSquarePlot             | R-square statistic for models examined doing variable selection      | RSQUARE             |
| RStudentByLeverage      | Studentized residuals versus leverage                                | RSTUDENTBYLEVERAGE  |
| RStudentByPredicted     | Studentized residuals versus predicted values                        | RSTUDENTBYPREDICTED |
| SBCPlot                 | SBC statistic for models examined doing variable selection           | SBC                 |
| SelectionCriterionPanel | Panel of fit statistics for models examined doing variable selection | CRITERIA            |
| VIFPlot                 | Plot of VIF traces                                                   | RIDGE(UNPACK)       |

## Examples: REG Procedure

### Example 79.1: Modeling Salaries of Major League Baseball Players

This example features the use of ODS Graphics in the process of building models by using the REG procedure and highlights the use of fit and influence diagnostics.

The following data set contains salary and performance information for Major League Baseball players who played at least one game in both the 1986 and 1987 seasons, excluding pitchers. The salaries (*Sports Illustrated*, April 20, 1987) are for the 1987 season and the performance measures are from 1986 (Collier Books, *The 1987 Baseball Encyclopedia Update*).

```

data baseball;
 length name $ 18;
 length team $ 12;
 input name $ 1-18 no_atbat no_hits no_home no_runs no_rbi no_bb yr_major
 cr_atbat cr_hits cr_home cr_runs cr_rbi cr_bb league $
 division $ team $ position $ no_outs no_assts no_error salary;
 logSalary = log10(salary);
 label name="Player's Name"
 no_hits="Hits in 1986"
 no_runs="Runs in 1986"
 no_rbi="RBIs in 1986"
 no_bb="Walks in 1986"
 yr_major="Years in MLB"
 cr_hits="Career Hits"
 salary="1987 Salary in $ Thousands"
 logSalary = "log10(Salary)";

```

```

datalines;
Allanson, Andy 293 66 1 30 29 14
 1 293 66 1 30 29 14
 American East Cleveland C 446 33 20 .
Ashby, Alan 315 81 7 24 38 39
 14 3449 835 69 321 414 375
 National West Houston C 632 43 10 475
Davis, Alan 479 130 18 66 72 76
 3 1624 457 63 224 266 263
 American West Seattle 1B 880 82 14 480
Dawson, Andre 496 141 20 65 78 37
 11 5628 1575 225 828 838 354
 National East Montreal RF 200 11 3 500
Galarraga, Andres 321 87 10 39 42 30
 2 396 101 12 48 46 33
 National East Montreal 1B 805 40 4 91.5
Griffin, Alfredo 594 169 4 74 51 35
 11 4408 1133 19 501 336 194
 American West Oakland SS 282 421 25 750

... more lines ...

Wilson, Willie 631 170 9 77 44 31
 11 4908 1457 30 775 357 249
 American West KansasCity CF 408 4 3 1000
;

```

Suppose you want to investigate whether you can model the players' salaries for the 1987 season based on batting statistics for the previous season and lifetime batting performance. Since the variation in salaries is much greater for higher salaries, it is appropriate to apply a log transformation for this analysis. The following statements begin the analysis:

```

ods graphics on;

proc reg data=baseball;
 id name team league;
 model logSalary = no_hits no_runs no_rbi no_bb yr_major cr_hits;
run;

```

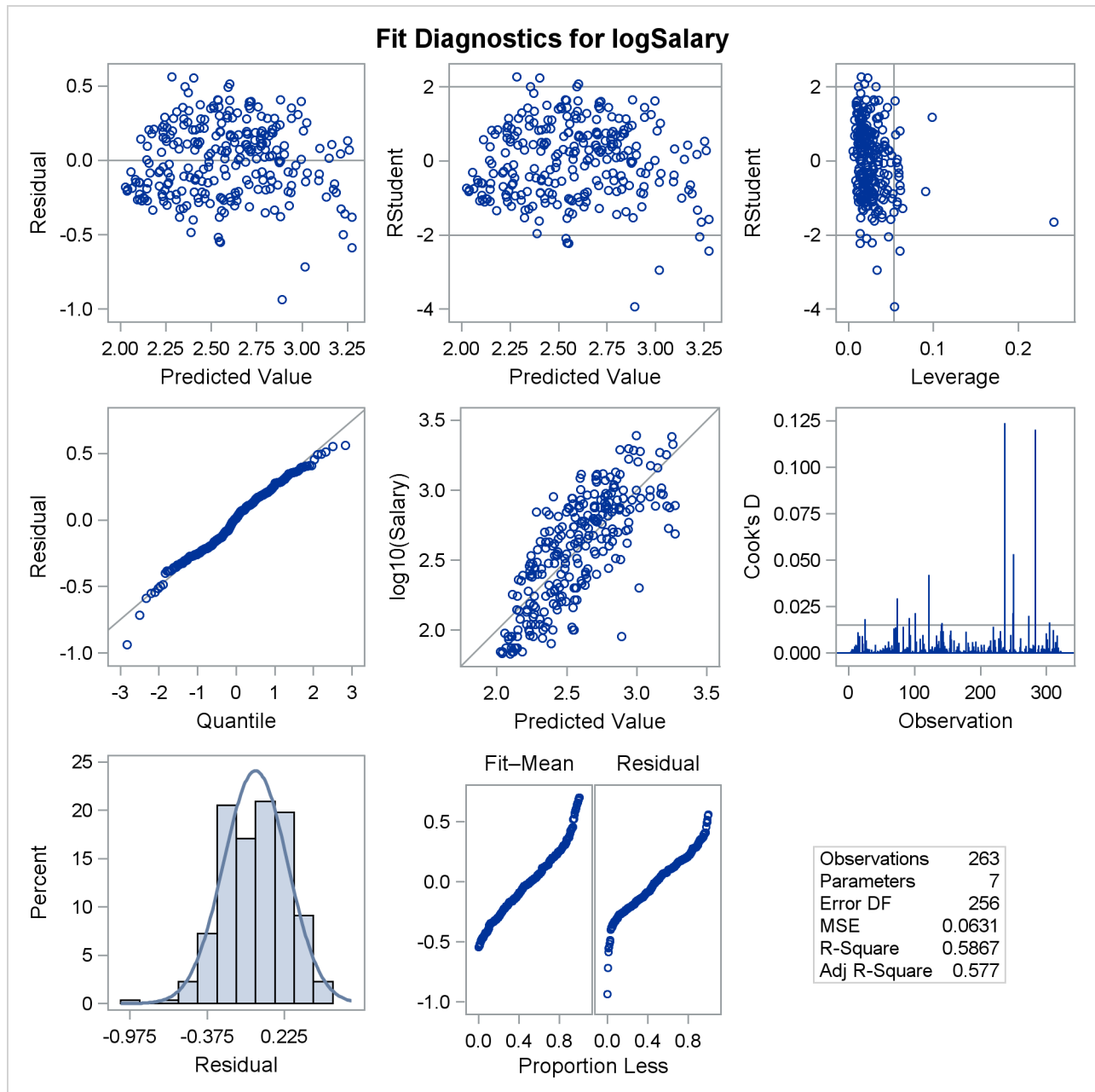
Output 79.1.1 shows the default output produced by PROC REG. The number of observations table shows that 59 observations are excluded because they have missing values for at least one of the variables used in the analysis. The analysis of variance and parameter estimates tables provide details about the fitted model.

**Output 79.1.1** Default Output from PROC REG

| The REG Procedure                           |               |                |                    |                |         |         |
|---------------------------------------------|---------------|----------------|--------------------|----------------|---------|---------|
| Model: MODEL1                               |               |                |                    |                |         |         |
| Dependent Variable: logSalary log10(Salary) |               |                |                    |                |         |         |
| Number of Observations Read                 |               |                |                    |                |         | 322     |
| Number of Observations Used                 |               |                |                    |                |         | 263     |
| Number of Observations with Missing Values  |               |                |                    |                |         | 59      |
| Analysis of Variance                        |               |                |                    |                |         |         |
| Source                                      | DF            | Sum of Squares | Mean Square        | F Value        | Pr > F  |         |
| Model                                       | 6             | 22.92208       | 3.82035            | 60.56          | <.0001  |         |
| Error                                       | 256           | 16.14954       | 0.06308            |                |         |         |
| Corrected Total                             | 262           | 39.07162       |                    |                |         |         |
| Root MSE                                    |               | 0.25117        | R-Square           | 0.5867         |         |         |
| Dependent Mean                              |               | 2.57416        | Adj R-Sq           | 0.5770         |         |         |
| Coeff Var                                   |               | 9.75719        |                    |                |         |         |
| Parameter Estimates                         |               |                |                    |                |         |         |
| Variable                                    | Label         | DF             | Parameter Estimate | Standard Error | t Value | Pr >  t |
| Intercept                                   | Intercept     | 1              | 1.80065            | 0.05912        | 30.46   | <.0001  |
| no_hits                                     | Hits in 1986  | 1              | 0.00288            | 0.00091244     | 3.15    | 0.0018  |
| no_runs                                     | Runs in 1986  | 1              | 0.00008638         | 0.00173        | 0.05    | 0.9602  |
| no_rbi                                      | RBI's in 1986 | 1              | 0.00054382         | 0.00102        | 0.53    | 0.5947  |
| no_bb                                       | Walks in 1986 | 1              | 0.00292            | 0.00104        | 2.81    | 0.0054  |
| yr_major                                    | Years in MLB  | 1              | 0.03087            | 0.00836        | 3.69    | 0.0003  |
| cr_hits                                     | Career Hits   | 1              | 0.00010384         | 0.00006328     | 1.64    | 0.1020  |

Before you accept a regression model, it is important to examine influence and fit diagnostics to see whether the model might be unduly influenced by a few observations and whether the data support the assumptions that underlie the linear regression. To facilitate such investigations, you can obtain diagnostic plots by enabling ODS Graphics.

Output 79.1.2 Fit Diagnostics

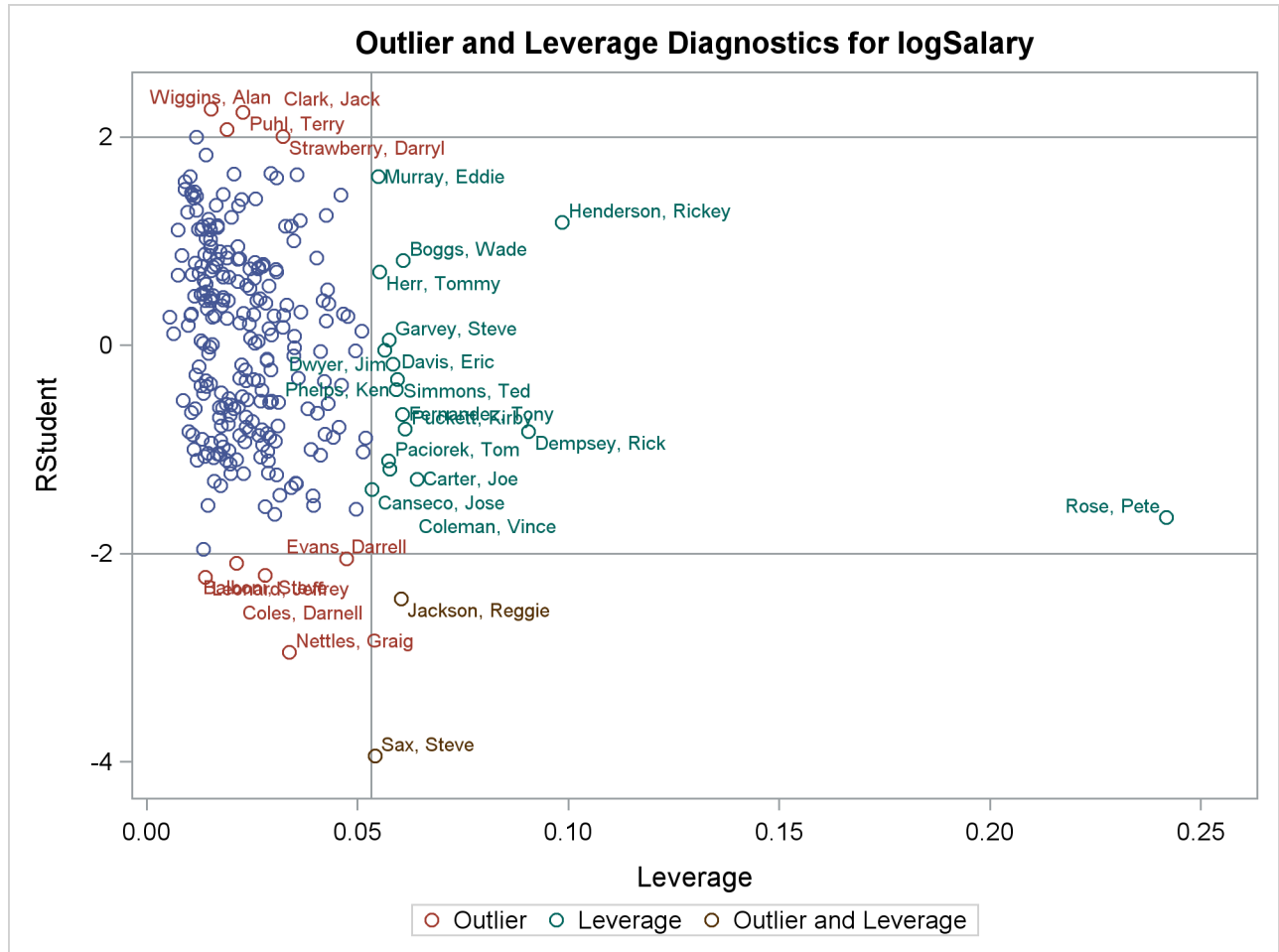


Output 79.1.2 shows a panel of diagnostic plots. The plot of externally studentized residuals (RStudent) by leverage values reveals that there is one observation with very high leverage that might be overly influencing the fit produced. The plot of Cook's  $D$  by observation also indicates two highly influential observations. To investigate further, you can use the PLOTS= option in the PROC REG statement as follows to produce labeled versions of these plots:

```
proc reg data=baseball
 plots(only label)=(RStudentByLeverage CooksD);
 id name team league;
 model logSalary = no_hits no_runs no_rbi no_bb yr_major cr_hits;
run;
```

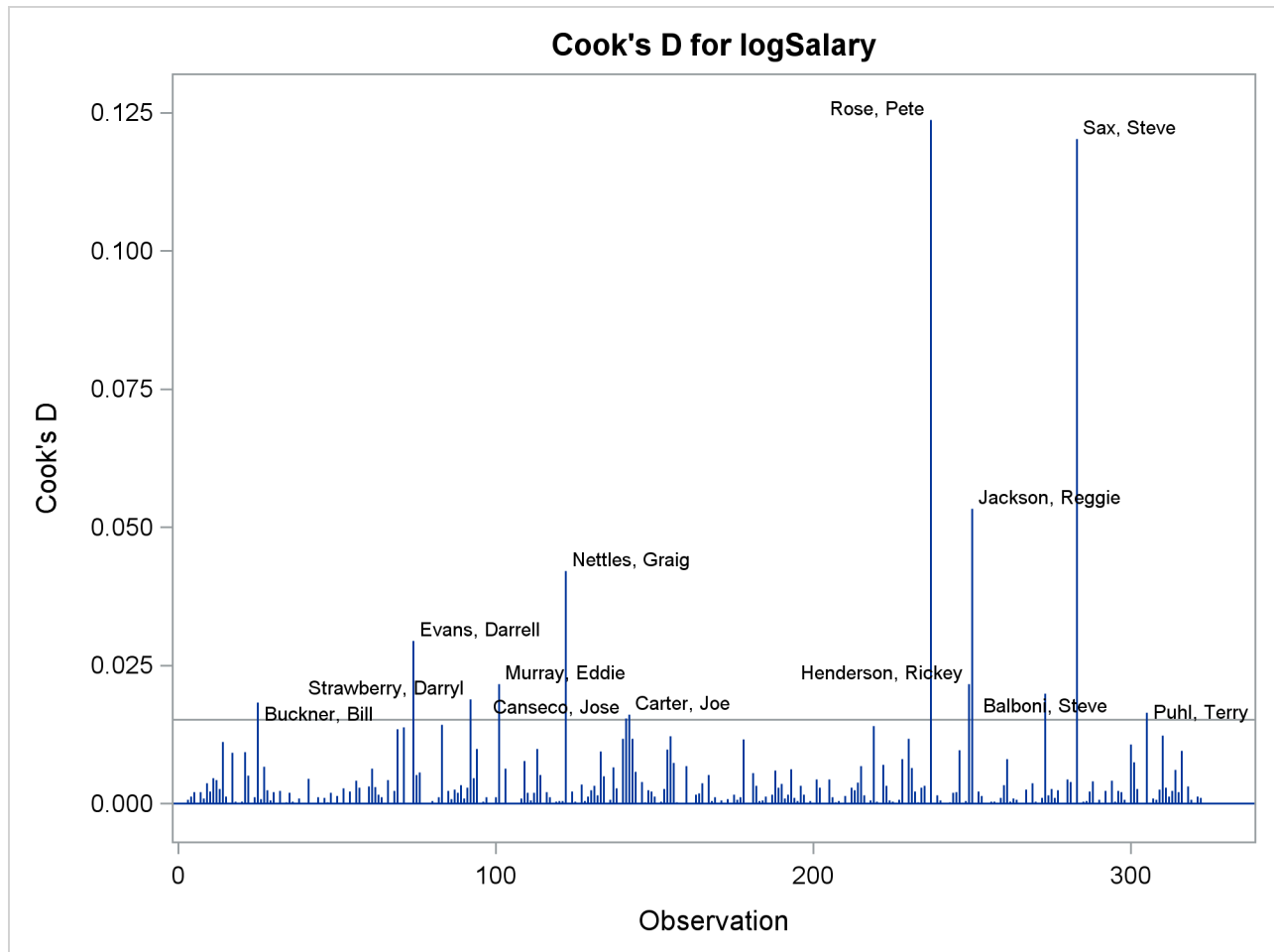
Output 79.1.3 and Output 79.1.4 reveal that Pete Rose is the highly influential observation. You might obtain a better fit to the remaining data if you omit his statistics when building the model.

**Output 79.1.3** Outlier and Leverage Diagnostics





Output 79.1.4 Cook's D

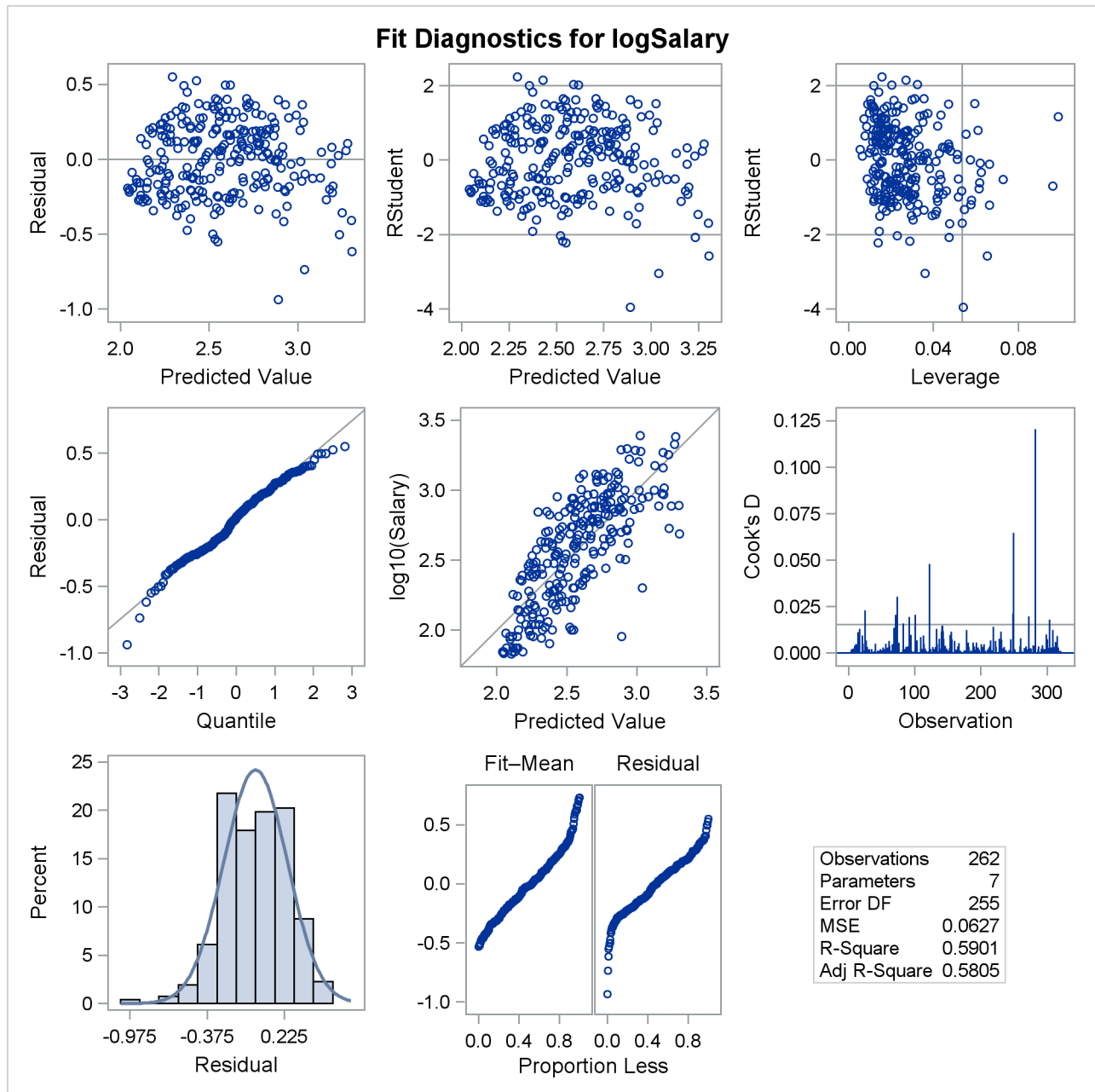


The following statements use a WHERE statement to omit Pete Rose's statistics when building the model. An alternative way to do this within PROC REG is to use a **REWEIGHT** statement. See "Reweight Observations in an Analysis" on page 6726 for details about reweighting.

```
proc reg data=baseball
 plots=(RStudentByLeverage(label) residuals(smooth));
 where name^="Rose, Pete";
 id name team league;
 model logSalary = no_hits no_runs no_rbi no_bb yr_major cr_hits;
run;
```

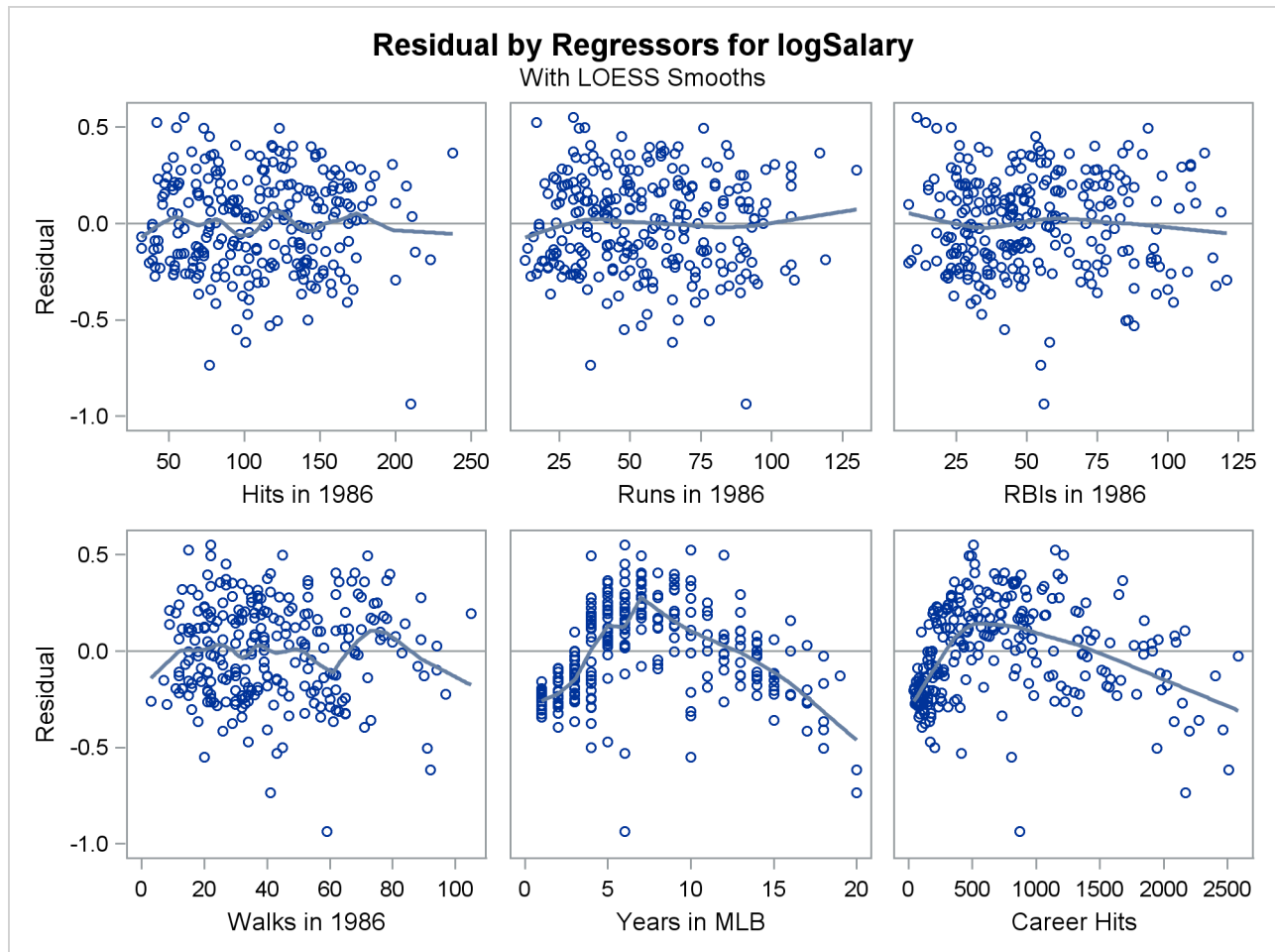
Output 79.1.5 shows the new fit diagnostics panel. You can see that there are still several influential and outlying observations. One possible reason for observing outliers is that the linear model specified is not appropriate to capture the variation in this data. You can often see evidence of an inappropriate model by observing patterns in plots of residuals.

Output 79.1.5 Fit Diagnostics



Output 79.1.6 shows plots of the residuals by the regressors in the model. When you specify the RESIDUALS(SMOOTH) suboption of the PLOTS option in the PROC REG statement, a loess fit is overlaid on each of these plots. You can see the same clear pattern in the residual plots for yr\_major and cr\_hits. Players near the start of their careers and players near the end of their careers get paid less than the model predicts.

Output 79.1.6 Residuals by Regressors



You can address this lack of fit by using polynomials of degree 2 for these two variables as shown in the following statements:

```
data baseball;
 set baseball(where=(name^="Rose, Pete"));
 yr_major2 = yr_major*yr_major;
 cr_hits2 = cr_hits*cr_hits;
run;

proc reg data=baseball
 plots=(diagnostics(stats=none) RStudentByLeverage(label)
 CooksD(label) Residuals(smooth)
 DFFITS(label) DFBETAS ObservedByPredicted(label));
 id name team league;
 model logSalary = no_hits no_runs no_rbi no_bb yr_major cr_hits
 yr_major2 cr_hits2;
run;
ods graphics off;
```

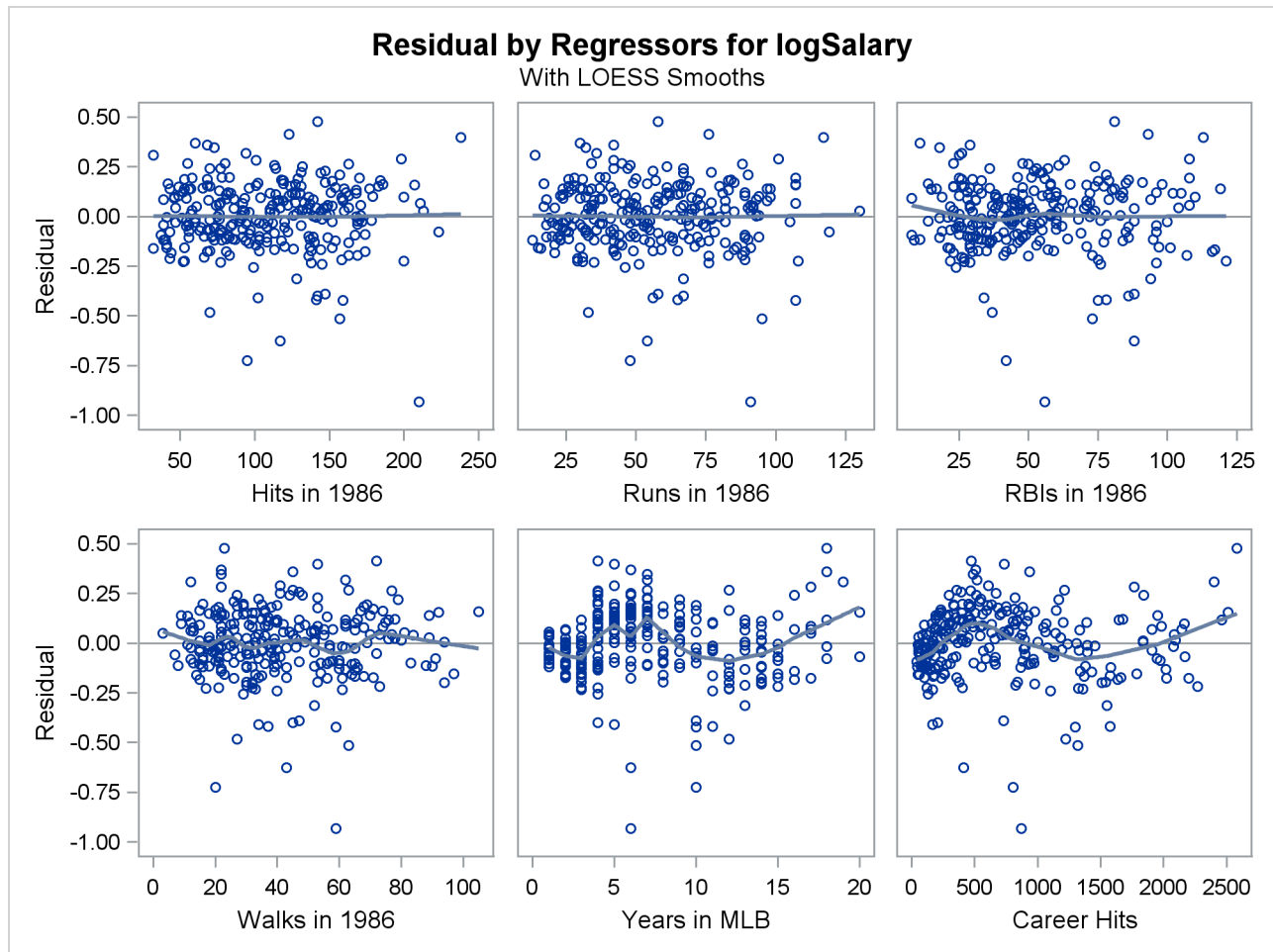
Output 79.1.7 shows the analysis of variance and parameter estimates for this model. Note that the R-square value of 0.787 for this model is considerably larger than the R-square value of 0.587 for the initial model shown in Output 79.1.1.

**Output 79.1.7** Output from PROC REG

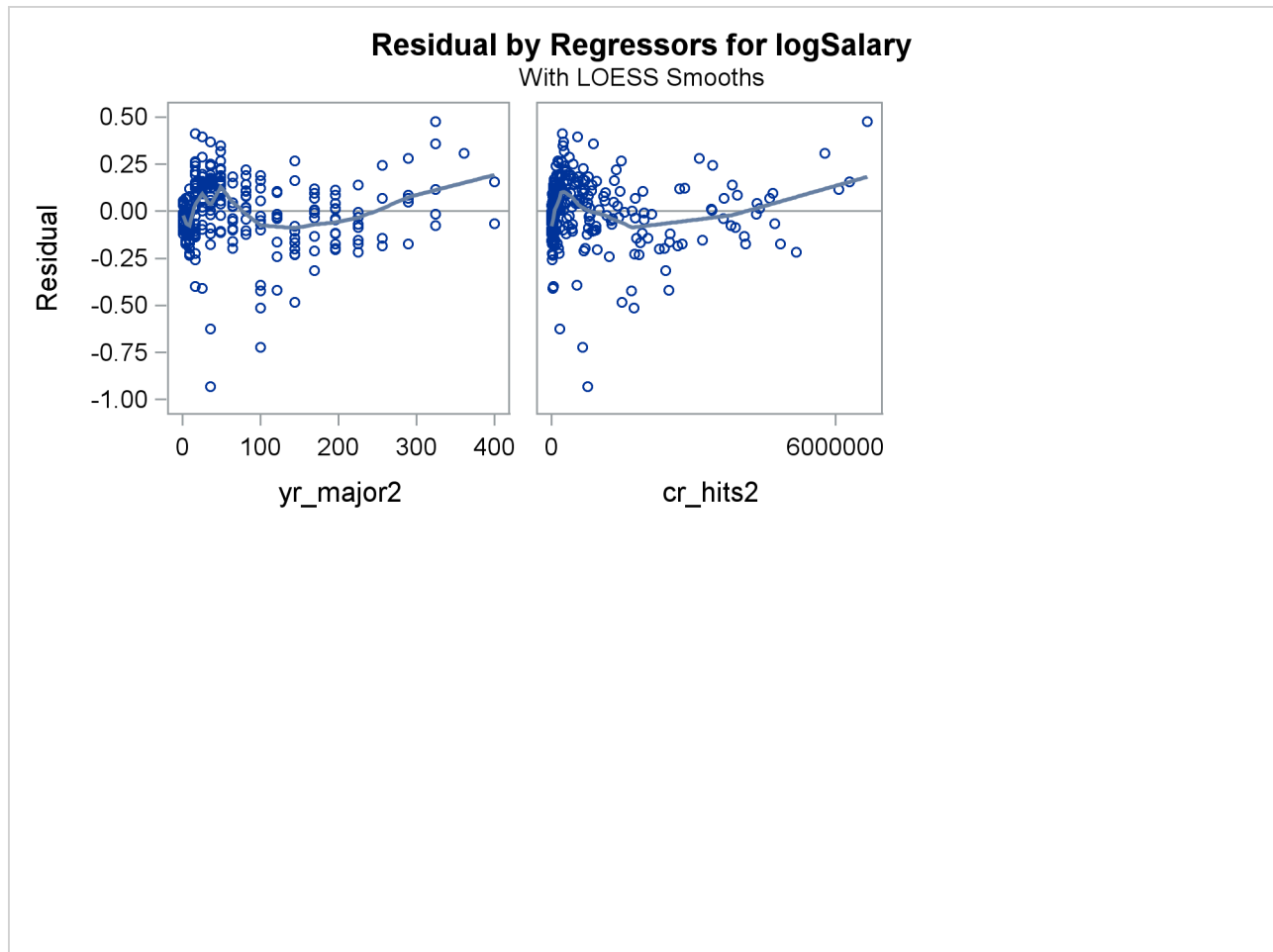
| The REG Procedure                           |                |                |                    |                |         |         |
|---------------------------------------------|----------------|----------------|--------------------|----------------|---------|---------|
| Model: MODEL1                               |                |                |                    |                |         |         |
| Dependent Variable: logSalary log10(Salary) |                |                |                    |                |         |         |
| Analysis of Variance                        |                |                |                    |                |         |         |
| Source                                      | DF             | Sum of Squares | Mean Square        | F Value        | Pr > F  |         |
| Model                                       | 8              | 30.69367       | 3.83671            | 117.13         | <.0001  |         |
| Error                                       | 253            | 8.28706        | 0.03276            |                |         |         |
| Corrected Total                             | 261            | 38.98073       |                    |                |         |         |
|                                             | Root MSE       | 0.18098        | R-Square           | 0.7874         |         |         |
|                                             | Dependent Mean | 2.57301        | Adj R-Sq           | 0.7807         |         |         |
|                                             | Coeff Var      | 7.03393        |                    |                |         |         |
| Parameter Estimates                         |                |                |                    |                |         |         |
| Variable                                    | Label          | DF             | Parameter Estimate | Standard Error | t Value | Pr >  t |
| Intercept                                   | Intercept      | 1              | 1.64564            | 0.05030        | 32.72   | <.0001  |
| no_hits                                     | Hits in 1986   | 1              | -0.00005539        | 0.00069200     | -0.08   | 0.9363  |
| no_runs                                     | Runs in 1986   | 1              | 0.00093586         | 0.00125        | 0.75    | 0.4549  |
| no_rbi                                      | RBI's in 1986  | 1              | 0.00187            | 0.00074649     | 2.51    | 0.0127  |
| no_bb                                       | Walks in 1986  | 1              | 0.00218            | 0.00075057     | 2.90    | 0.0040  |
| yr_major                                    | Years in MLB   | 1              | 0.10383            | 0.01495        | 6.94    | <.0001  |
| cr_hits                                     | Career Hits    | 1              | 0.00073955         | 0.00011970     | 6.18    | <.0001  |
| yr_major2                                   |                | 1              | -0.00625           | 0.00071687     | -8.73   | <.0001  |
| cr_hits2                                    |                | 1              | -1.44072E-7        | 4.348471E-8    | -3.31   | 0.0011  |

The plots of residuals by regressors in Output 79.1.8 and Output 79.1.9 show that the strong pattern in the plots for cr\_majors and cr\_hits has been reduced, although there is still some indication of a pattern remaining in these residuals. This suggests that a quadratic function might be insufficient to capture dependence of salary on these regressors.

Output 79.1.8 Residuals by Regressors

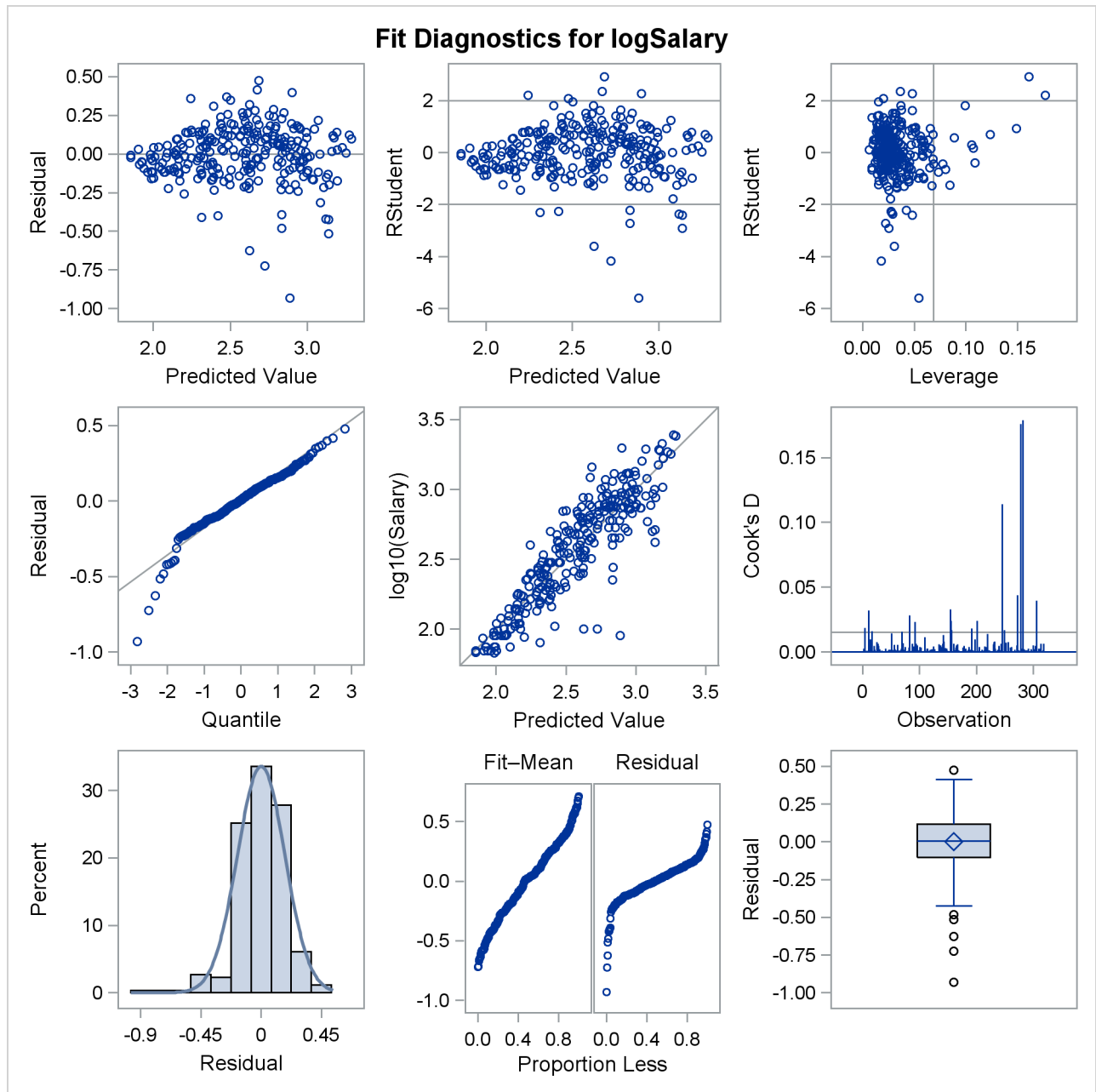


**Output 79.1.9** Residuals by Regressors

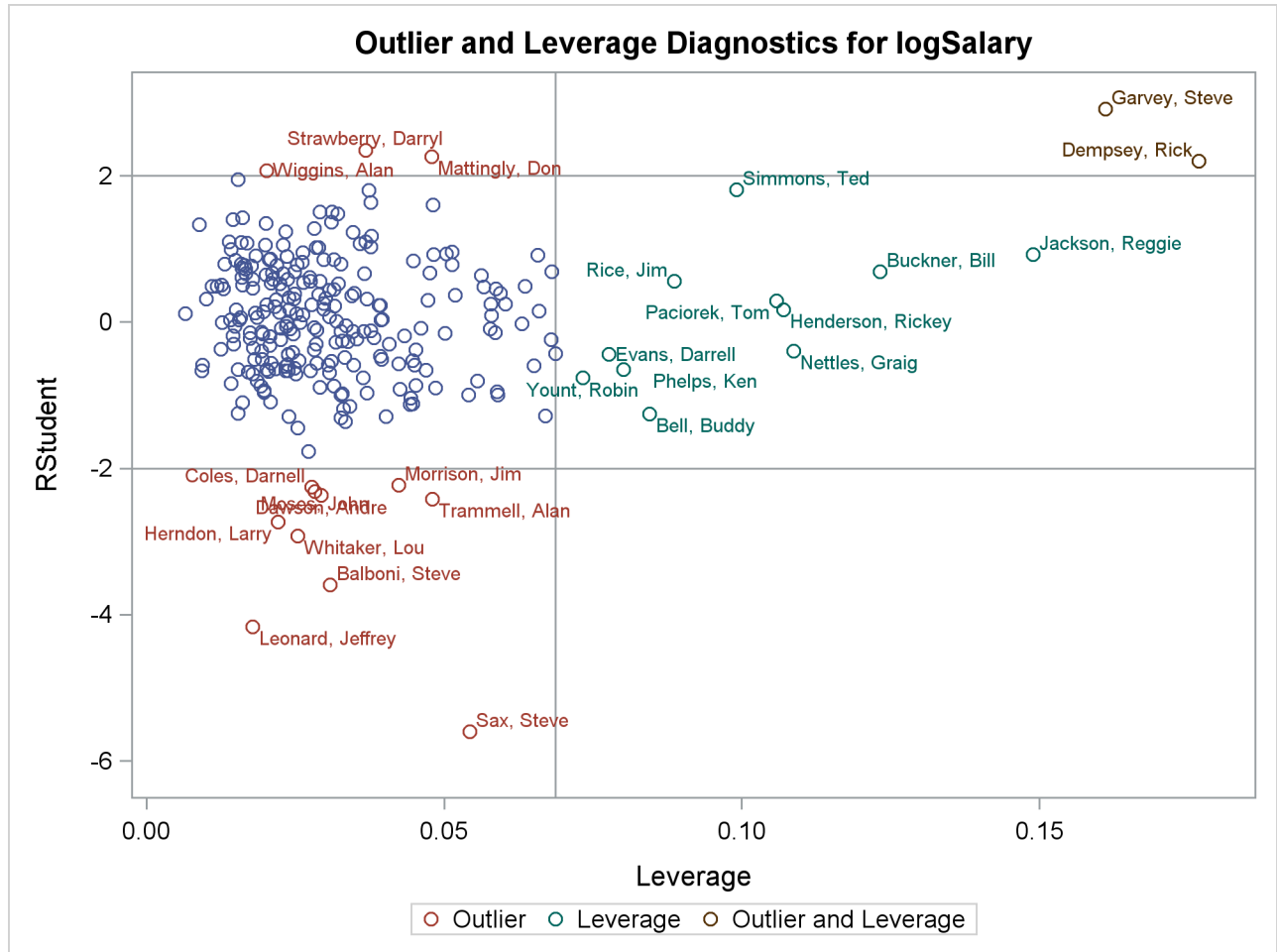


Output 79.1.10 show the diagnostics plots; three of the plots, with points of interest labeled, are shown individually in Output 79.1.11, Output 79.1.12, and Output 79.1.13. The `STATS=NONE` suboption specified in the `PLOTS=DIAGNOSTICS` option replaces the inset of statistics with a box plot of the residuals in the fit diagnostics panel. The observed by predicted value plot reveals a reasonably successful model for explaining the variation in salary for most of the players. However, the model tends to overpredict the salaries of several players near the lower end of the salary range. This bias can also be seen in the distribution of the residuals that you can see in the histogram, Q-Q plot, and box plot in Output 79.1.10.

Output 79.1.10 Fit Diagnostics

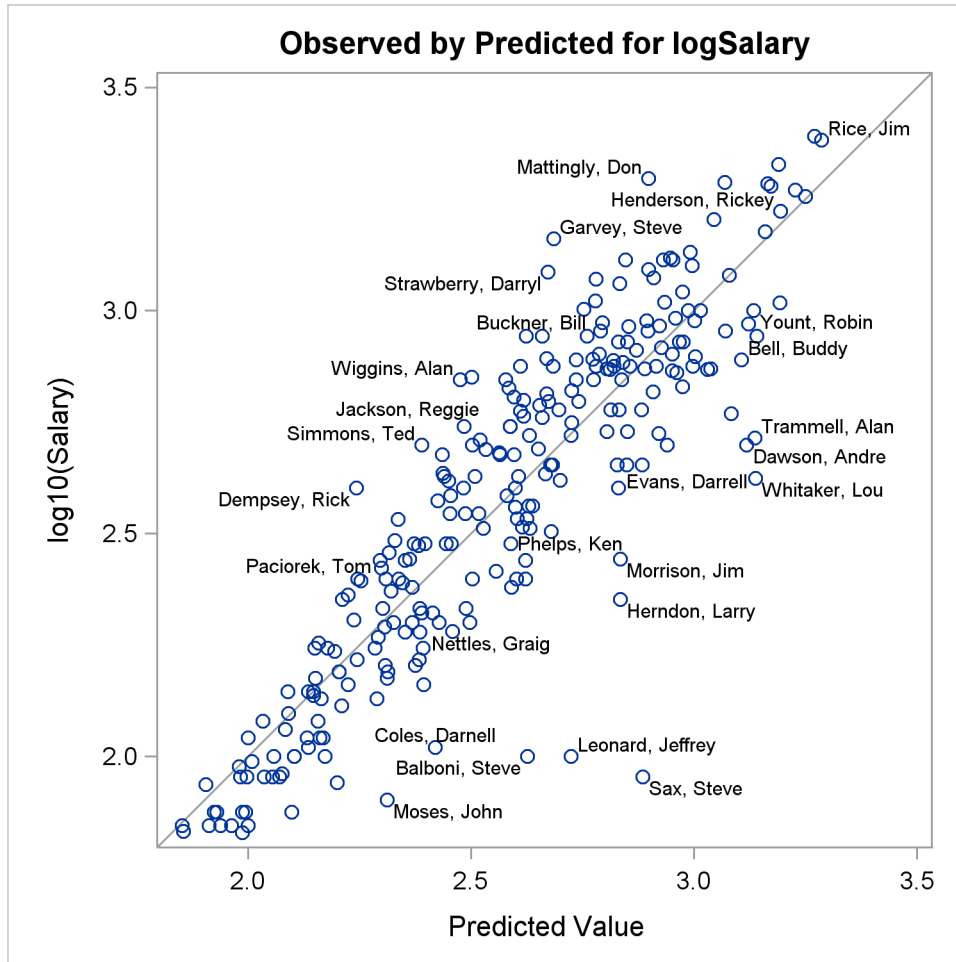


Output 79.1.11 Outlier and Leverage Diagnostics

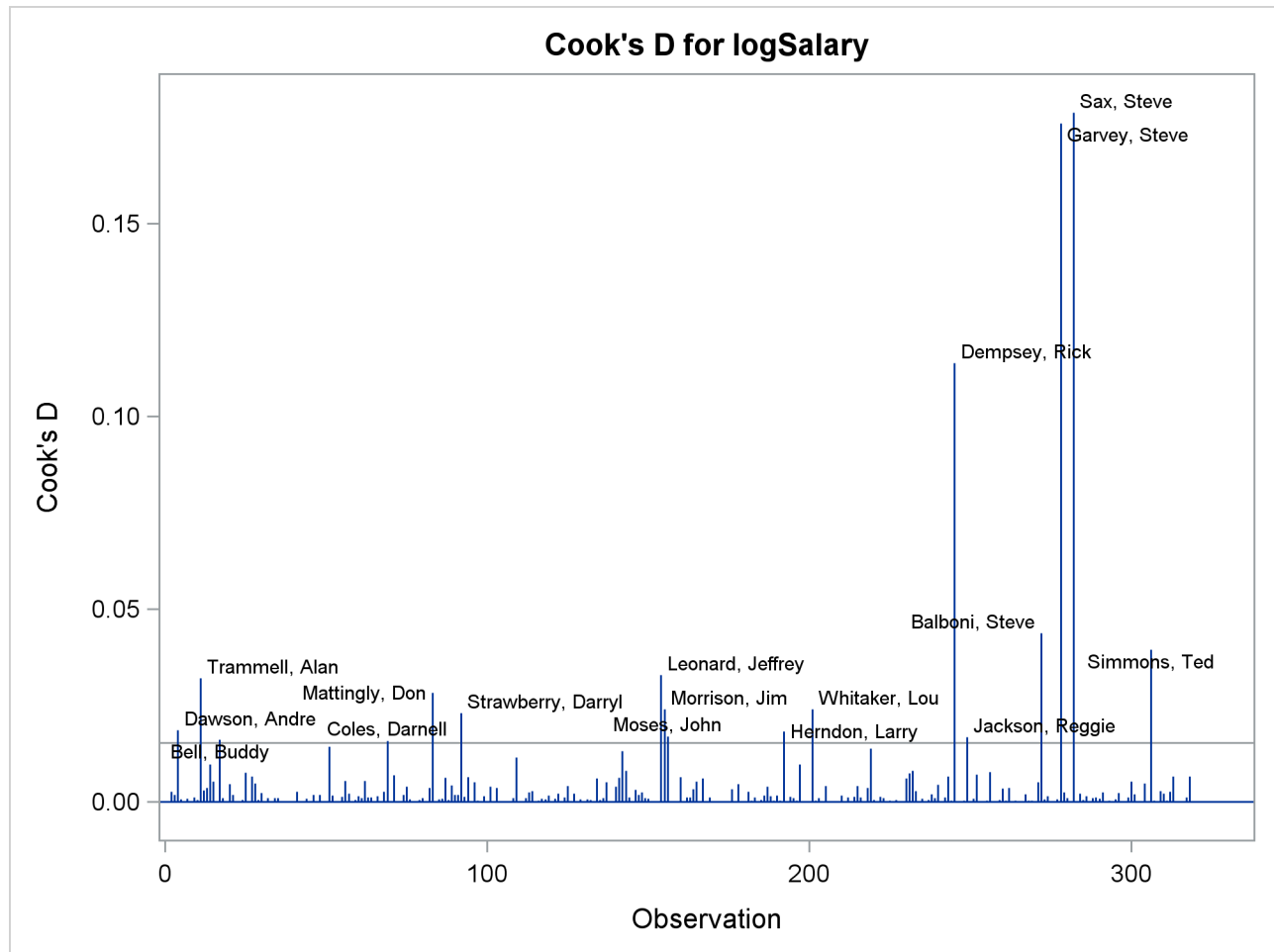




Output 79.1.12 Observed by Predicted Values

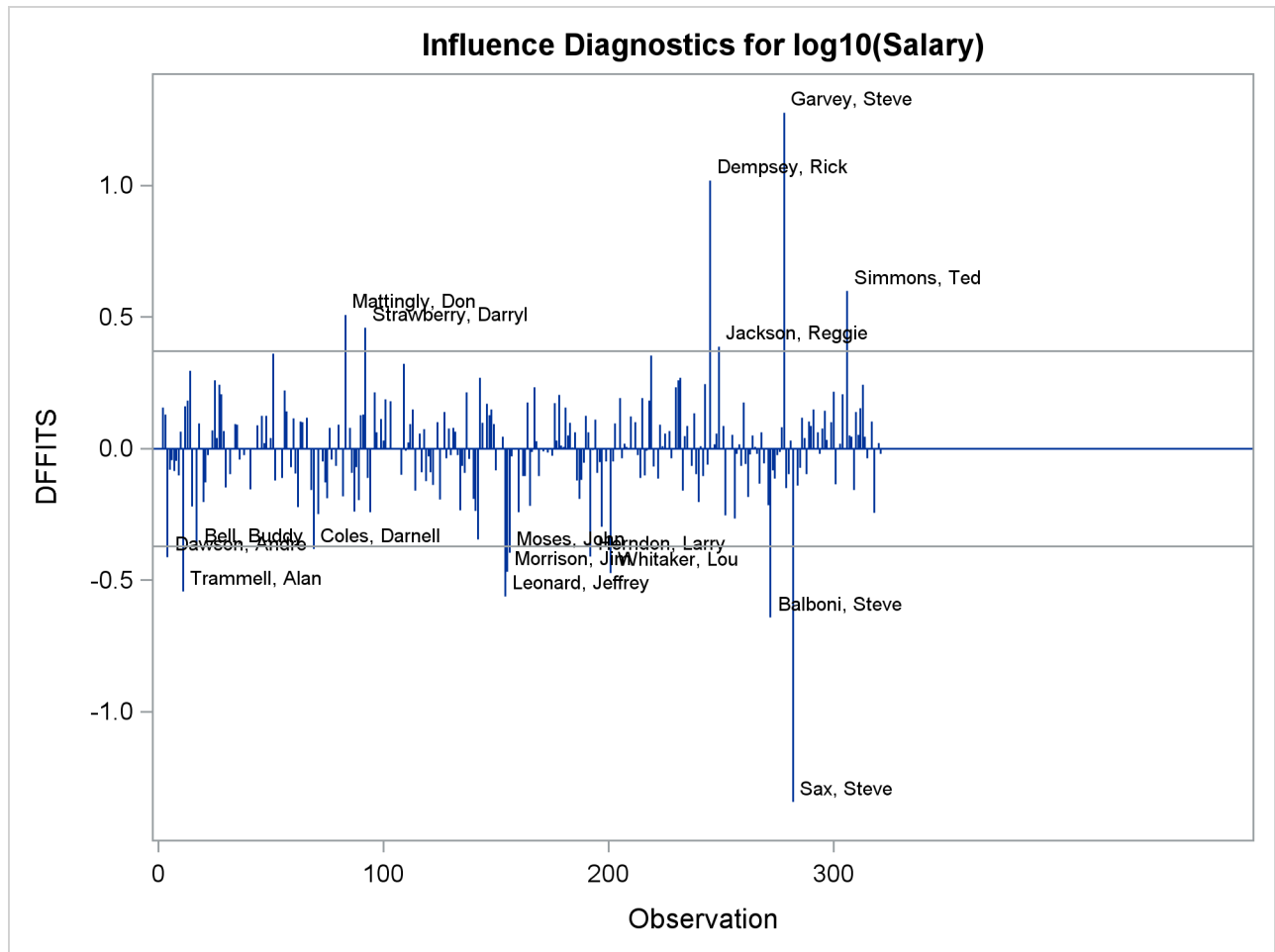


Output 79.1.13 Cook's D

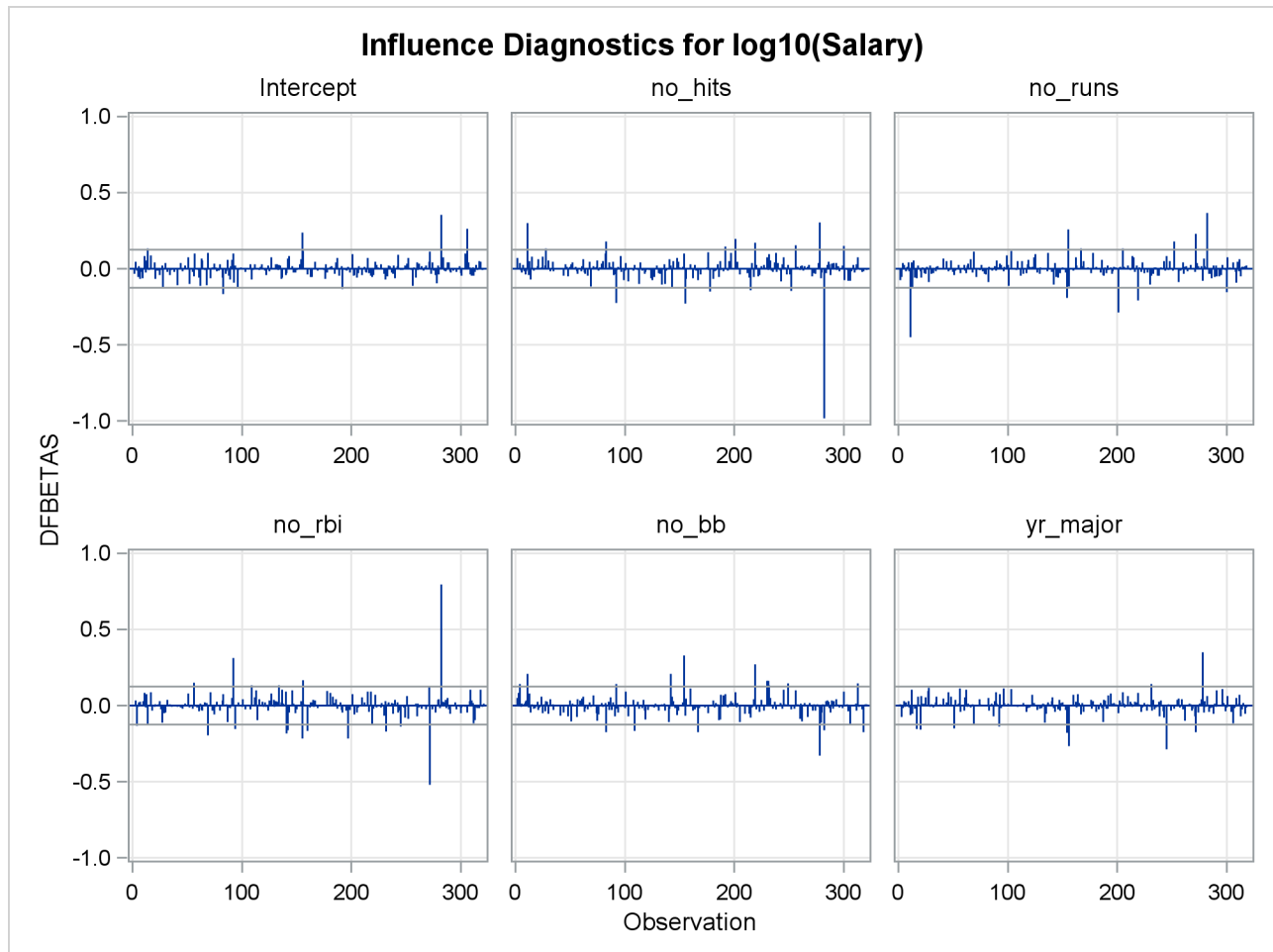


The RStudent by leverage plot in [Output 79.1.11](#) and the Cook's  $D$  plot in [Output 79.1.13](#) show that there are still a number of influential observations. By specifying the DFFITS and DFBETAS suboptions of the PLOTS= option, you obtain additional influence diagnostics plots shown in [Output 79.1.14](#) and [Output 79.1.15](#). See "Influence Statistics" on page 6717 for details about the interpretation DFFITS and DFBETAS statistics.

Output 79.1.14 DFFITS



Output 79.1.15 DFBETAS



You can continue this analysis by investigating how the influential observations identified in the various influence plots affect the fit. You can also use PROC ROBUSTREG to obtain a fit that is resistant to the presence of high leverage points and outliers.

## Example 79.2: Aerobic Fitness Prediction

Aerobic fitness (measured by the ability to consume oxygen) is fit to some simple exercise tests. The goal is to develop an equation to predict fitness based on the exercise tests rather than on expensive and cumbersome oxygen consumption measurements. Three model-selection methods are used: forward selection, backward selection, and MAXR selection. Here are the data:

```
-----Data on Physical Fitness-----
| These measurements were made on men involved in a physical |
| fitness course at N.C.State Univ. The variables are Age |
| (years), Weight (kg), Oxygen intake rate (ml per kg body |
| weight per minute), time to run 1.5 miles (minutes), heart |
| rate while resting, heart rate while running (same time |
| Oxygen rate measured), and maximum heart rate recorded while |
| running. |
| ***Certain values of MaxPulse were changed for this analysis. |

data fitness;
 input Age Weight Oxygen RunTime RestPulse RunPulse MaxPulse @@;
 datalines;
44 89.47 44.609 11.37 62 178 182 40 75.07 45.313 10.07 62 185 185
44 85.84 54.297 8.65 45 156 168 42 68.15 59.571 8.17 40 166 172
38 89.02 49.874 9.22 55 178 180 47 77.45 44.811 11.63 58 176 176
40 75.98 45.681 11.95 70 176 180 43 81.19 49.091 10.85 64 162 170
44 81.42 39.442 13.08 63 174 176 38 81.87 60.055 8.63 48 170 186
44 73.03 50.541 10.13 45 168 168 45 87.66 37.388 14.03 56 186 192
45 66.45 44.754 11.12 51 176 176 47 79.15 47.273 10.60 47 162 164
54 83.12 51.855 10.33 50 166 170 49 81.42 49.156 8.95 44 180 185
51 69.63 40.836 10.95 57 168 172 51 77.91 46.672 10.00 48 162 168
48 91.63 46.774 10.25 48 162 164 49 73.37 50.388 10.08 67 168 168
57 73.37 39.407 12.63 58 174 176 54 79.38 46.080 11.17 62 156 165
52 76.32 45.441 9.63 48 164 166 50 70.87 54.625 8.92 48 146 155
51 67.25 45.118 11.08 48 172 172 54 91.63 39.203 12.88 44 168 172
51 73.71 45.790 10.47 59 186 188 57 59.08 50.545 9.93 49 148 155
49 76.32 48.673 9.40 56 186 188 48 61.24 47.920 11.50 52 170 176
52 82.78 47.467 10.50 53 170 172
;
```

The following statements demonstrate the FORWARD, BACKWARD, and MAXR model selection methods:

```
proc reg data=fitness;
 model Oxygen=Age Weight RunTime RunPulse RestPulse MaxPulse
 / selection=forward;
 model Oxygen=Age Weight RunTime RunPulse RestPulse MaxPulse
 / selection=backward;
 model Oxygen=Age Weight RunTime RunPulse RestPulse MaxPulse
 / selection=maxr;
run;
```

Output 79.2.1 shows the sequence of models produced by the FORWARD model-selection method.

**Output 79.2.1** Forward Selection Method: PROC REG

| The REG Procedure                                              |                    |                |             |         |        |  |
|----------------------------------------------------------------|--------------------|----------------|-------------|---------|--------|--|
| Model: MODEL1                                                  |                    |                |             |         |        |  |
| Dependent Variable: Oxygen                                     |                    |                |             |         |        |  |
| Forward Selection: Step 1                                      |                    |                |             |         |        |  |
| Variable RunTime Entered: R-Square = 0.7434 and C(p) = 13.6988 |                    |                |             |         |        |  |
| Analysis of Variance                                           |                    |                |             |         |        |  |
| Source                                                         | DF                 | Sum of Squares | Mean Square | F Value | Pr > F |  |
| Model                                                          | 1                  | 632.90010      | 632.90010   | 84.01   | <.0001 |  |
| Error                                                          | 29                 | 218.48144      | 7.53384     |         |        |  |
| Corrected Total                                                | 30                 | 851.38154      |             |         |        |  |
| Variable                                                       | Parameter Estimate | Standard Error | Type II SS  | F Value | Pr > F |  |
| Intercept                                                      | 82.42177           | 3.85530        | 3443.36654  | 457.05  | <.0001 |  |
| RunTime                                                        | -3.31056           | 0.36119        | 632.90010   | 84.01   | <.0001 |  |
| Bounds on condition number: 1, 1                               |                    |                |             |         |        |  |
| Forward Selection: Step 2                                      |                    |                |             |         |        |  |
| Variable Age Entered: R-Square = 0.7642 and C(p) = 12.3894     |                    |                |             |         |        |  |
| Analysis of Variance                                           |                    |                |             |         |        |  |
| Source                                                         | DF                 | Sum of Squares | Mean Square | F Value | Pr > F |  |
| Model                                                          | 2                  | 650.66573      | 325.33287   | 45.38   | <.0001 |  |
| Error                                                          | 28                 | 200.71581      | 7.16842     |         |        |  |
| Corrected Total                                                | 30                 | 851.38154      |             |         |        |  |
| Variable                                                       | Parameter Estimate | Standard Error | Type II SS  | F Value | Pr > F |  |
| Intercept                                                      | 88.46229           | 5.37264        | 1943.41071  | 271.11  | <.0001 |  |
| Age                                                            | -0.15037           | 0.09551        | 17.76563    | 2.48    | 0.1267 |  |
| RunTime                                                        | -3.20395           | 0.35877        | 571.67751   | 79.75   | <.0001 |  |

Output 79.2.1 *continued*

Bounds on condition number: 1.0369, 4.1478

---

Forward Selection: Step 3

Variable RunPulse Entered: R-Square = 0.8111 and C(p) = 6.9596

## Analysis of Variance

| Source          | DF | Sum of Squares | Mean Square | F Value | Pr > F |
|-----------------|----|----------------|-------------|---------|--------|
| Model           | 3  | 690.55086      | 230.18362   | 38.64   | <.0001 |
| Error           | 27 | 160.83069      | 5.95669     |         |        |
| Corrected Total | 30 | 851.38154      |             |         |        |

| Variable  | Parameter Estimate | Standard Error | Type II SS | F Value | Pr > F |
|-----------|--------------------|----------------|------------|---------|--------|
| Intercept | 111.71806          | 10.23509       | 709.69014  | 119.14  | <.0001 |
| Age       | -0.25640           | 0.09623        | 42.28867   | 7.10    | 0.0129 |
| RunTime   | -2.82538           | 0.35828        | 370.43529  | 62.19   | <.0001 |
| RunPulse  | -0.13091           | 0.05059        | 39.88512   | 6.70    | 0.0154 |

Bounds on condition number: 1.3548, 11.597

---

Forward Selection: Step 4

Variable MaxPulse Entered: R-Square = 0.8368 and C(p) = 4.8800

## Analysis of Variance

| Source          | DF | Sum of Squares | Mean Square | F Value | Pr > F |
|-----------------|----|----------------|-------------|---------|--------|
| Model           | 4  | 712.45153      | 178.11288   | 33.33   | <.0001 |
| Error           | 26 | 138.93002      | 5.34346     |         |        |
| Corrected Total | 30 | 851.38154      |             |         |        |

| Variable  | Parameter Estimate | Standard Error | Type II SS | F Value | Pr > F |
|-----------|--------------------|----------------|------------|---------|--------|
| Intercept | 98.14789           | 11.78569       | 370.57373  | 69.35   | <.0001 |
| Age       | -0.19773           | 0.09564        | 22.84231   | 4.27    | 0.0488 |
| RunTime   | -2.76758           | 0.34054        | 352.93570  | 66.05   | <.0001 |
| RunPulse  | -0.34811           | 0.11750        | 46.90089   | 8.78    | 0.0064 |
| MaxPulse  | 0.27051            | 0.13362        | 21.90067   | 4.10    | 0.0533 |

Output 79.2.1 *continued*

| Bounds on condition number: 8.4182, 76.851                   |                    |                |             |         |        |
|--------------------------------------------------------------|--------------------|----------------|-------------|---------|--------|
| -----                                                        |                    |                |             |         |        |
| Forward Selection: Step 5                                    |                    |                |             |         |        |
| Variable Weight Entered: R-Square = 0.8480 and C(p) = 5.1063 |                    |                |             |         |        |
| Analysis of Variance                                         |                    |                |             |         |        |
| Source                                                       | DF                 | Sum of Squares | Mean Square | F Value | Pr > F |
| Model                                                        | 5                  | 721.97309      | 144.39462   | 27.90   | <.0001 |
| Error                                                        | 25                 | 129.40845      | 5.17634     |         |        |
| Corrected Total                                              | 30                 | 851.38154      |             |         |        |
| Variable                                                     | Parameter Estimate | Standard Error | Type II SS  | F Value | Pr > F |
| Intercept                                                    | 102.20428          | 11.97929       | 376.78935   | 72.79   | <.0001 |
| Age                                                          | -0.21962           | 0.09550        | 27.37429    | 5.29    | 0.0301 |
| Weight                                                       | -0.07230           | 0.05331        | 9.52157     | 1.84    | 0.1871 |
| RunTime                                                      | -2.68252           | 0.34099        | 320.35968   | 61.89   | <.0001 |
| RunPulse                                                     | -0.37340           | 0.11714        | 52.59624    | 10.16   | 0.0038 |
| MaxPulse                                                     | 0.30491            | 0.13394        | 26.82640    | 5.18    | 0.0316 |
| Bounds on condition number: 8.7312, 104.83                   |                    |                |             |         |        |

The final variable available to add to the model, RestPulse, is not added since it does not meet the 50% (the default value of the SLE option is 0.5 for FORWARD selection) significance-level criterion for entry into the model.

The BACKWARD model-selection method begins with the full model. Output 79.2.2 shows the steps of the BACKWARD method. RestPulse is the first variable deleted, followed by Weight. No other variables are deleted from the model since the variables remaining (Age, RunTime, RunPulse, and MaxPulse) are all significant at the 10% (the default value of the SLS option is 0.1 for the BACKWARD elimination method) significance level.



**Output 79.2.2** Backward Selection Method: PROC REG

| Backward Elimination: Step 0                                    |                    |                |             |         |        |
|-----------------------------------------------------------------|--------------------|----------------|-------------|---------|--------|
| All Variables Entered: R-Square = 0.8487 and C(p) = 7.0000      |                    |                |             |         |        |
| Analysis of Variance                                            |                    |                |             |         |        |
| Source                                                          | DF                 | Sum of Squares | Mean Square | F Value | Pr > F |
| Model                                                           | 6                  | 722.54361      | 120.42393   | 22.43   | <.0001 |
| Error                                                           | 24                 | 128.83794      | 5.36825     |         |        |
| Corrected Total                                                 | 30                 | 851.38154      |             |         |        |
| Variable                                                        | Parameter Estimate | Standard Error | Type II SS  | F Value | Pr > F |
| Intercept                                                       | 102.93448          | 12.40326       | 369.72831   | 68.87   | <.0001 |
| Age                                                             | -0.22697           | 0.09984        | 27.74577    | 5.17    | 0.0322 |
| Weight                                                          | -0.07418           | 0.05459        | 9.91059     | 1.85    | 0.1869 |
| RunTime                                                         | -2.62865           | 0.38456        | 250.82210   | 46.72   | <.0001 |
| RunPulse                                                        | -0.36963           | 0.11985        | 51.05806    | 9.51    | 0.0051 |
| RestPulse                                                       | -0.02153           | 0.06605        | 0.57051     | 0.11    | 0.7473 |
| MaxPulse                                                        | 0.30322            | 0.13650        | 26.49142    | 4.93    | 0.0360 |
| Bounds on condition number: 8.7438, 137.13                      |                    |                |             |         |        |
| Backward Elimination: Step 1                                    |                    |                |             |         |        |
| Variable RestPulse Removed: R-Square = 0.8480 and C(p) = 5.1063 |                    |                |             |         |        |
| Analysis of Variance                                            |                    |                |             |         |        |
| Source                                                          | DF                 | Sum of Squares | Mean Square | F Value | Pr > F |
| Model                                                           | 5                  | 721.97309      | 144.39462   | 27.90   | <.0001 |
| Error                                                           | 25                 | 129.40845      | 5.17634     |         |        |
| Corrected Total                                                 | 30                 | 851.38154      |             |         |        |

**Output 79.2.2** *continued*

| Variable  | Parameter Estimate | Standard Error | Type II SS | F Value | Pr > F |
|-----------|--------------------|----------------|------------|---------|--------|
| Intercept | 102.20428          | 11.97929       | 376.78935  | 72.79   | <.0001 |
| Age       | -0.21962           | 0.09550        | 27.37429   | 5.29    | 0.0301 |
| Weight    | -0.07230           | 0.05331        | 9.52157    | 1.84    | 0.1871 |
| RunTime   | -2.68252           | 0.34099        | 320.35968  | 61.89   | <.0001 |
| RunPulse  | -0.37340           | 0.11714        | 52.59624   | 10.16   | 0.0038 |
| MaxPulse  | 0.30491            | 0.13394        | 26.82640   | 5.18    | 0.0316 |

Bounds on condition number: 8.7312, 104.83

---

Backward Elimination: Step 2

Variable Weight Removed: R-Square = 0.8368 and C(p) = 4.8800

Analysis of Variance

| Source          | DF | Sum of Squares | Mean Square | F Value | Pr > F |
|-----------------|----|----------------|-------------|---------|--------|
| Model           | 4  | 712.45153      | 178.11288   | 33.33   | <.0001 |
| Error           | 26 | 138.93002      | 5.34346     |         |        |
| Corrected Total | 30 | 851.38154      |             |         |        |

| Variable  | Parameter Estimate | Standard Error | Type II SS | F Value | Pr > F |
|-----------|--------------------|----------------|------------|---------|--------|
| Intercept | 98.14789           | 11.78569       | 370.57373  | 69.35   | <.0001 |
| Age       | -0.19773           | 0.09564        | 22.84231   | 4.27    | 0.0488 |
| RunTime   | -2.76758           | 0.34054        | 352.93570  | 66.05   | <.0001 |
| RunPulse  | -0.34811           | 0.11750        | 46.90089   | 8.78    | 0.0064 |
| MaxPulse  | 0.27051            | 0.13362        | 21.90067   | 4.10    | 0.0533 |

Bounds on condition number: 8.4182, 76.851

The MAXR method tries to find the “best” one-variable model, the “best” two-variable model, and so on. [Output 79.2.3](#) shows that the one-variable model contains RunTime; the two-variable model contains RunTime and Age; the three-variable model contains RunTime, Age, and RunPulse; the four-variable model contains Age, RunTime, RunPulse, and MaxPulse; the five-variable model contains Age, Weight, RunTime, RunPulse, and MaxPulse; and finally, the six-variable model contains all the variables in the `MODEL` statement.

**Output 79.2.3** Maximum R-Square Improvement Selection Method: PROC REG

| Maximum R-Square Improvement: Step 1                           |                    |                |             |         |        |
|----------------------------------------------------------------|--------------------|----------------|-------------|---------|--------|
| Variable RunTime Entered: R-Square = 0.7434 and C(p) = 13.6988 |                    |                |             |         |        |
| Analysis of Variance                                           |                    |                |             |         |        |
| Source                                                         | DF                 | Sum of Squares | Mean Square | F Value | Pr > F |
| Model                                                          | 1                  | 632.90010      | 632.90010   | 84.01   | <.0001 |
| Error                                                          | 29                 | 218.48144      | 7.53384     |         |        |
| Corrected Total                                                | 30                 | 851.38154      |             |         |        |
| Variable                                                       | Parameter Estimate | Standard Error | Type II SS  | F Value | Pr > F |
| Intercept                                                      | 82.42177           | 3.85530        | 3443.36654  | 457.05  | <.0001 |
| RunTime                                                        | -3.31056           | 0.36119        | 632.90010   | 84.01   | <.0001 |
| -----                                                          |                    |                |             |         |        |
| Bounds on condition number: 1, 1                               |                    |                |             |         |        |
| The above model is the best 1-variable model found.            |                    |                |             |         |        |
| Maximum R-Square Improvement: Step 2                           |                    |                |             |         |        |
| Variable Age Entered: R-Square = 0.7642 and C(p) = 12.3894     |                    |                |             |         |        |
| Analysis of Variance                                           |                    |                |             |         |        |
| Source                                                         | DF                 | Sum of Squares | Mean Square | F Value | Pr > F |
| Model                                                          | 2                  | 650.66573      | 325.33287   | 45.38   | <.0001 |
| Error                                                          | 28                 | 200.71581      | 7.16842     |         |        |
| Corrected Total                                                | 30                 | 851.38154      |             |         |        |
| Variable                                                       | Parameter Estimate | Standard Error | Type II SS  | F Value | Pr > F |
| Intercept                                                      | 88.46229           | 5.37264        | 1943.41071  | 271.11  | <.0001 |
| Age                                                            | -0.15037           | 0.09551        | 17.76563    | 2.48    | 0.1267 |
| RunTime                                                        | -3.20395           | 0.35877        | 571.67751   | 79.75   | <.0001 |

**Output 79.2.3** *continued*

Bounds on condition number: 1.0369, 4.1478

---

The above model is the best 2-variable model found.

Maximum R-Square Improvement: Step 3

Variable RunPulse Entered: R-Square = 0.8111 and C(p) = 6.9596

Analysis of Variance

| Source          | DF | Sum of Squares | Mean Square | F Value | Pr > F |
|-----------------|----|----------------|-------------|---------|--------|
| Model           | 3  | 690.55086      | 230.18362   | 38.64   | <.0001 |
| Error           | 27 | 160.83069      | 5.95669     |         |        |
| Corrected Total | 30 | 851.38154      |             |         |        |

| Variable  | Parameter Estimate | Standard Error | Type II SS | F Value | Pr > F |
|-----------|--------------------|----------------|------------|---------|--------|
| Intercept | 111.71806          | 10.23509       | 709.69014  | 119.14  | <.0001 |
| Age       | -0.25640           | 0.09623        | 42.28867   | 7.10    | 0.0129 |
| RunTime   | -2.82538           | 0.35828        | 370.43529  | 62.19   | <.0001 |
| RunPulse  | -0.13091           | 0.05059        | 39.88512   | 6.70    | 0.0154 |

Bounds on condition number: 1.3548, 11.597

---

The above model is the best 3-variable model found.

Maximum R-Square Improvement: Step 4

Variable MaxPulse Entered: R-Square = 0.8368 and C(p) = 4.8800

Analysis of Variance

| Source          | DF | Sum of Squares | Mean Square | F Value | Pr > F |
|-----------------|----|----------------|-------------|---------|--------|
| Model           | 4  | 712.45153      | 178.11288   | 33.33   | <.0001 |
| Error           | 26 | 138.93002      | 5.34346     |         |        |
| Corrected Total | 30 | 851.38154      |             |         |        |

## Output 79.2.3 continued

| Variable  | Parameter Estimate | Standard Error | Type II SS | F Value | Pr > F |
|-----------|--------------------|----------------|------------|---------|--------|
| Intercept | 98.14789           | 11.78569       | 370.57373  | 69.35   | <.0001 |
| Age       | -0.19773           | 0.09564        | 22.84231   | 4.27    | 0.0488 |
| RunTime   | -2.76758           | 0.34054        | 352.93570  | 66.05   | <.0001 |
| RunPulse  | -0.34811           | 0.11750        | 46.90089   | 8.78    | 0.0064 |
| MaxPulse  | 0.27051            | 0.13362        | 21.90067   | 4.10    | 0.0533 |

Bounds on condition number: 8.4182, 76.851

The above model is the best 4-variable model found.

Maximum R-Square Improvement: Step 5

Variable Weight Entered: R-Square = 0.8480 and C(p) = 5.1063

## Analysis of Variance

| Source          | DF | Sum of Squares | Mean Square | F Value | Pr > F |
|-----------------|----|----------------|-------------|---------|--------|
| Model           | 5  | 721.97309      | 144.39462   | 27.90   | <.0001 |
| Error           | 25 | 129.40845      | 5.17634     |         |        |
| Corrected Total | 30 | 851.38154      |             |         |        |

| Variable  | Parameter Estimate | Standard Error | Type II SS | F Value | Pr > F |
|-----------|--------------------|----------------|------------|---------|--------|
| Intercept | 102.20428          | 11.97929       | 376.78935  | 72.79   | <.0001 |
| Age       | -0.21962           | 0.09550        | 27.37429   | 5.29    | 0.0301 |
| Weight    | -0.07230           | 0.05331        | 9.52157    | 1.84    | 0.1871 |
| RunTime   | -2.68252           | 0.34099        | 320.35968  | 61.89   | <.0001 |
| RunPulse  | -0.37340           | 0.11714        | 52.59624   | 10.16   | 0.0038 |
| MaxPulse  | 0.30491            | 0.13394        | 26.82640   | 5.18    | 0.0316 |

Output 79.2.3 *continued*

| Bounds on condition number: 8.7312, 104.83                      |                    |                |             |         |        |
|-----------------------------------------------------------------|--------------------|----------------|-------------|---------|--------|
| -----                                                           |                    |                |             |         |        |
| The above model is the best 5-variable model found.             |                    |                |             |         |        |
| Maximum R-Square Improvement: Step 6                            |                    |                |             |         |        |
| Variable RestPulse Entered: R-Square = 0.8487 and C(p) = 7.0000 |                    |                |             |         |        |
| Analysis of Variance                                            |                    |                |             |         |        |
| Source                                                          | DF                 | Sum of Squares | Mean Square | F Value | Pr > F |
| Model                                                           | 6                  | 722.54361      | 120.42393   | 22.43   | <.0001 |
| Error                                                           | 24                 | 128.83794      | 5.36825     |         |        |
| Corrected Total                                                 | 30                 | 851.38154      |             |         |        |
| Variable                                                        | Parameter Estimate | Standard Error | Type III SS | F Value | Pr > F |
| Intercept                                                       | 102.93448          | 12.40326       | 369.72831   | 68.87   | <.0001 |
| Age                                                             | -0.22697           | 0.09984        | 27.74577    | 5.17    | 0.0322 |
| Weight                                                          | -0.07418           | 0.05459        | 9.91059     | 1.85    | 0.1869 |
| RunTime                                                         | -2.62865           | 0.38456        | 250.82210   | 46.72   | <.0001 |
| RunPulse                                                        | -0.36963           | 0.11985        | 51.05806    | 9.51    | 0.0051 |
| RestPulse                                                       | -0.02153           | 0.06605        | 0.57051     | 0.11    | 0.7473 |
| MaxPulse                                                        | 0.30322            | 0.13650        | 26.49142    | 4.93    | 0.0360 |
| Bounds on condition number: 8.7438, 137.13                      |                    |                |             |         |        |

Note that for all three of these methods, RestPulse contributes least to the model. In the case of forward selection, it is not added to the model. In the case of backward selection, it is the first variable to be removed from the model. In the case of MAXR selection, RestPulse is included only for the full model.

For the STEPWISE, BACKWARD, and FORWARD selection methods, you can control the amount of detail displayed by using the DETAILS option, and you can use ODS Graphics to produce plots that show how selection criteria progress as the selection proceeds. For example, the following statements display only the selection summary table for the FORWARD selection method (Output 79.2.4) and produce the plots shown in Output 79.2.5 and Output 79.2.6.

```
ods graphics on;

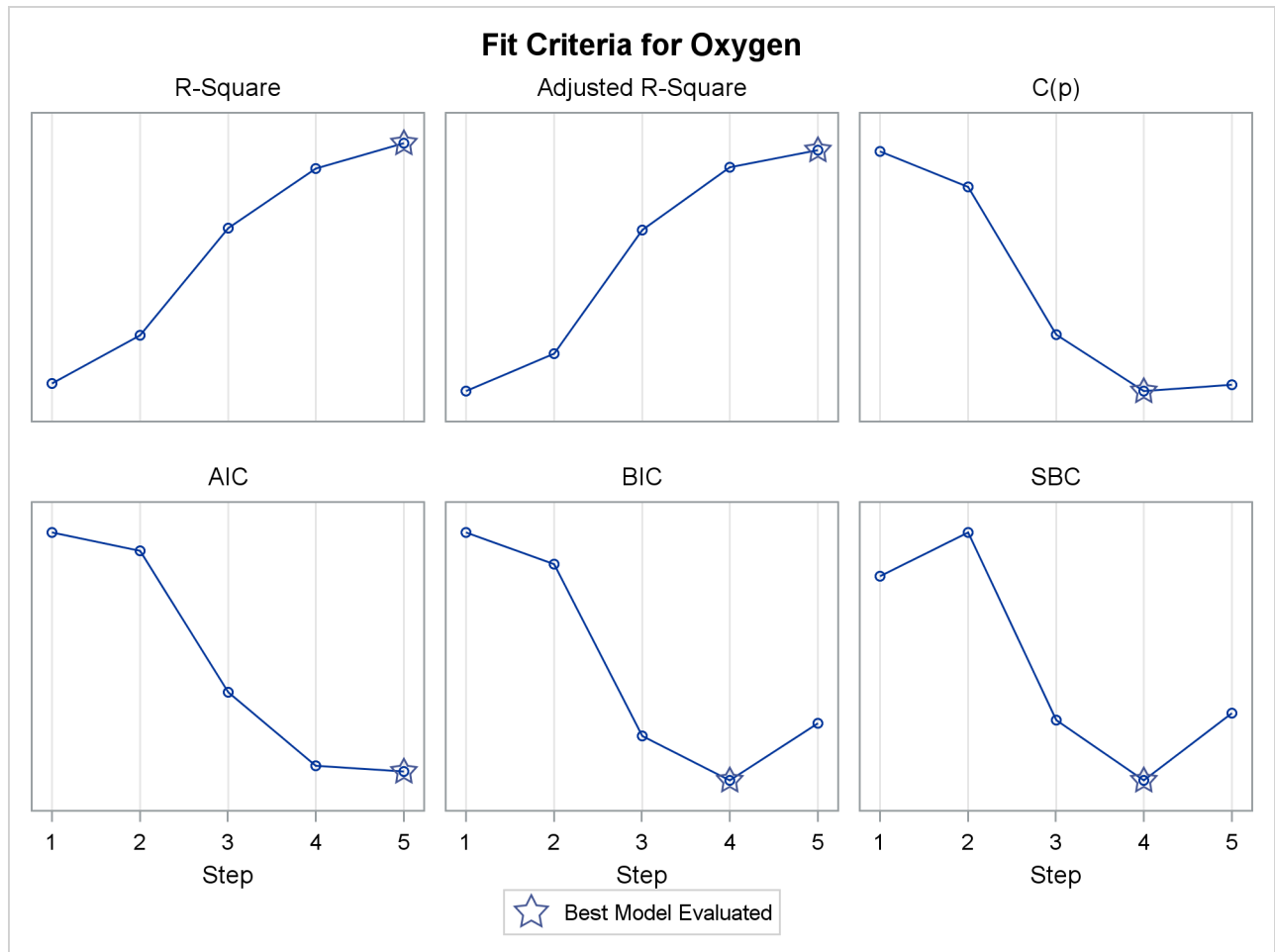
proc reg data=fitness plots=(criteria sbc);
 model Oxygen=Age Weight RunTime RunPulse RestPulse MaxPulse
 / selection=forward details=summary;
run;
```

**Output 79.2.4** Forward Selection Summary

| The REG Procedure            |                  |                |                  |                |         |         |        |
|------------------------------|------------------|----------------|------------------|----------------|---------|---------|--------|
| Model: MODEL1                |                  |                |                  |                |         |         |        |
| Dependent Variable: Oxygen   |                  |                |                  |                |         |         |        |
| Summary of Forward Selection |                  |                |                  |                |         |         |        |
| Step                         | Variable Entered | Number Vars In | Partial R-Square | Model R-Square | C(p)    | F Value | Pr > F |
| 1                            | RunTime          | 1              | 0.7434           | 0.7434         | 13.6988 | 84.01   | <.0001 |
| 2                            | Age              | 2              | 0.0209           | 0.7642         | 12.3894 | 2.48    | 0.1267 |
| 3                            | RunPulse         | 3              | 0.0468           | 0.8111         | 6.9596  | 6.70    | 0.0154 |
| 4                            | MaxPulse         | 4              | 0.0257           | 0.8368         | 4.8800  | 4.10    | 0.0533 |
| 5                            | Weight           | 5              | 0.0112           | 0.8480         | 5.1063  | 1.84    | 0.1871 |

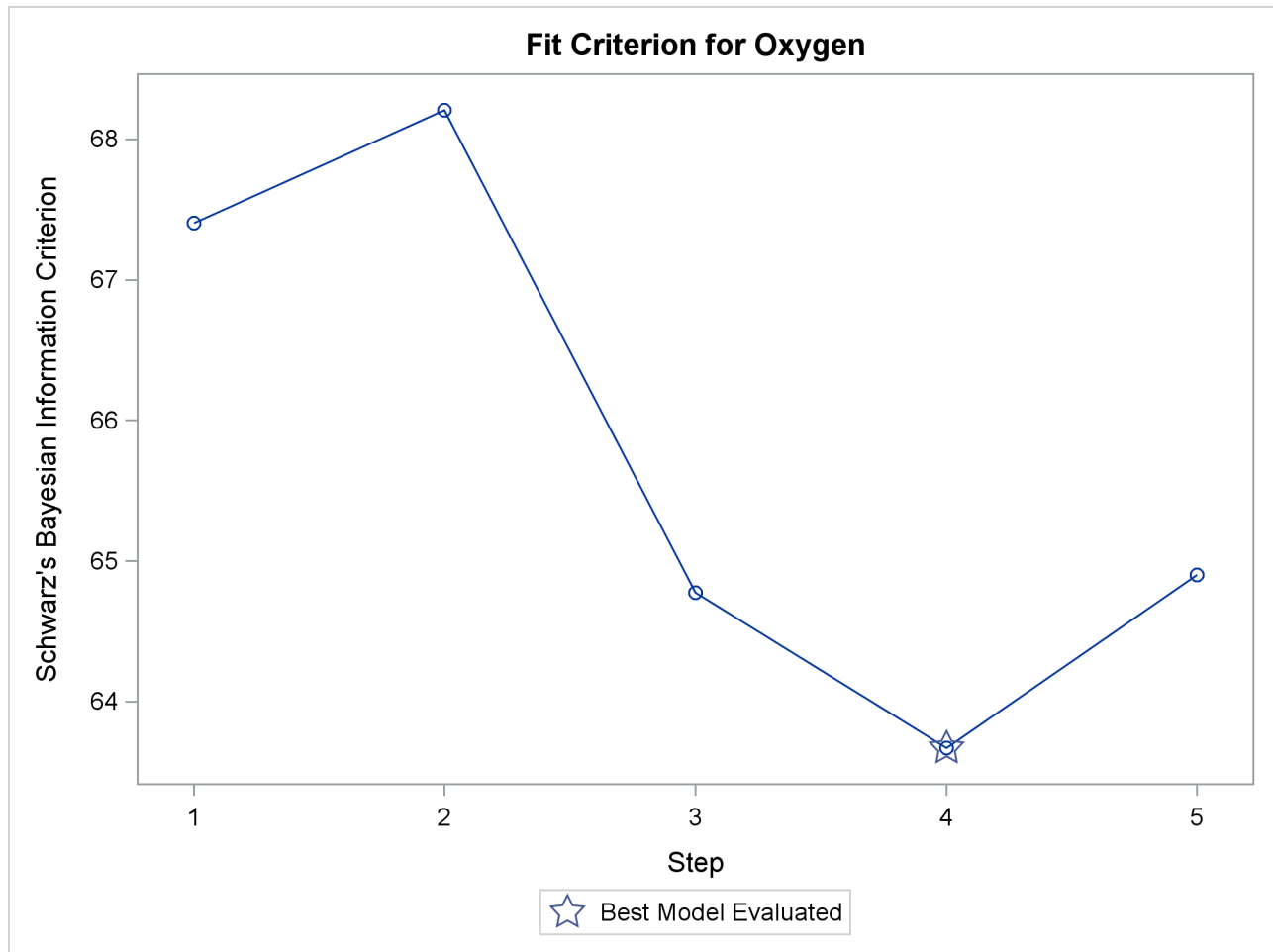
**Output 79.2.5** show how six fit criteria progress as the forward selection proceeds. The step at which each criterion achieves its best value is indicated. For example, the BIC criterion achieves its minimum value for the model at step 4. Note that this does not mean that the model at step 4 achieves the smallest BIC criterion among all possible models that use a subset of the regressors; the model at step 4 yields the smallest BIC statistic among the models at each step of the forward selection. **Output 79.2.6** show the progression of the SBC statistic in its own plot. If you want to see six of the selection criteria in individual plots, you can specify the UNPACK suboption of the PLOTS=CRITERIA option in the **PROC REG** statement.

**Output 79.2.5** Fit Criteria





Output 79.2.6 SBC Criterion



Next, the RSQUARE model-selection method is used to request R square and  $C_p$  statistics for all possible combinations of the six independent variables. The following statements produce [Output 79.2.7](#):

```
proc reg data=fitness plots=(criteria(label) cp);
 model Oxygen=Age Weight RunTime RunPulse RestPulse MaxPulse
 / selection=rsquare cp;
 title 'Physical fitness data: all models';
run;
```

**Output 79.2.7** All Models by the RSQUARE Method: PROC REG

```

Physical fitness data: all models

The REG Procedure
Model: MODEL1
Dependent Variable: Oxygen

R-Square Selection Method

```

| Model Index | Number in Model | R-Square | C(p)     | Variables in Model          |
|-------------|-----------------|----------|----------|-----------------------------|
| 1           | 1               | 0.7434   | 13.6988  | RunTime                     |
| 2           | 1               | 0.1595   | 106.3021 | RestPulse                   |
| 3           | 1               | 0.1584   | 106.4769 | RunPulse                    |
| 4           | 1               | 0.0928   | 116.8818 | Age                         |
| 5           | 1               | 0.0560   | 122.7072 | MaxPulse                    |
| 6           | 1               | 0.0265   | 127.3948 | Weight                      |
| -----       |                 |          |          |                             |
| 7           | 2               | 0.7642   | 12.3894  | Age RunTime                 |
| 8           | 2               | 0.7614   | 12.8372  | RunTime RunPulse            |
| 9           | 2               | 0.7452   | 15.4069  | RunTime MaxPulse            |
| 10          | 2               | 0.7449   | 15.4523  | Weight RunTime              |
| 11          | 2               | 0.7435   | 15.6746  | RunTime RestPulse           |
| 12          | 2               | 0.3760   | 73.9645  | Age RunPulse                |
| 13          | 2               | 0.3003   | 85.9742  | Age RestPulse               |
| 14          | 2               | 0.2894   | 87.6951  | RunPulse MaxPulse           |
| 15          | 2               | 0.2600   | 92.3638  | Age MaxPulse                |
| 16          | 2               | 0.2350   | 96.3209  | RunPulse RestPulse          |
| 17          | 2               | 0.1806   | 104.9523 | Weight RestPulse            |
| 18          | 2               | 0.1740   | 105.9939 | RestPulse MaxPulse          |
| 19          | 2               | 0.1669   | 107.1332 | Weight RunPulse             |
| 20          | 2               | 0.1506   | 109.7057 | Age Weight                  |
| 21          | 2               | 0.0675   | 122.8881 | Weight MaxPulse             |
| -----       |                 |          |          |                             |
| 22          | 3               | 0.8111   | 6.9596   | Age RunTime RunPulse        |
| 23          | 3               | 0.8100   | 7.1350   | RunTime RunPulse MaxPulse   |
| 24          | 3               | 0.7817   | 11.6167  | Age RunTime MaxPulse        |
| 25          | 3               | 0.7708   | 13.3453  | Age Weight RunTime          |
| 26          | 3               | 0.7673   | 13.8974  | Age RunTime RestPulse       |
| 27          | 3               | 0.7619   | 14.7619  | RunTime RunPulse RestPulse  |
| 28          | 3               | 0.7618   | 14.7729  | Weight RunTime RunPulse     |
| 29          | 3               | 0.7462   | 17.2588  | Weight RunTime MaxPulse     |
| 30          | 3               | 0.7452   | 17.4060  | RunTime RestPulse MaxPulse  |
| 31          | 3               | 0.7451   | 17.4243  | Weight RunTime RestPulse    |
| 32          | 3               | 0.4666   | 61.5873  | Age RunPulse RestPulse      |
| 33          | 3               | 0.4223   | 68.6250  | Age RunPulse MaxPulse       |
| 34          | 3               | 0.4091   | 70.7102  | Age Weight RunPulse         |
| 35          | 3               | 0.3900   | 73.7424  | Age RestPulse MaxPulse      |
| 36          | 3               | 0.3568   | 79.0013  | Age Weight RestPulse        |
| 37          | 3               | 0.3538   | 79.4891  | RunPulse RestPulse MaxPulse |

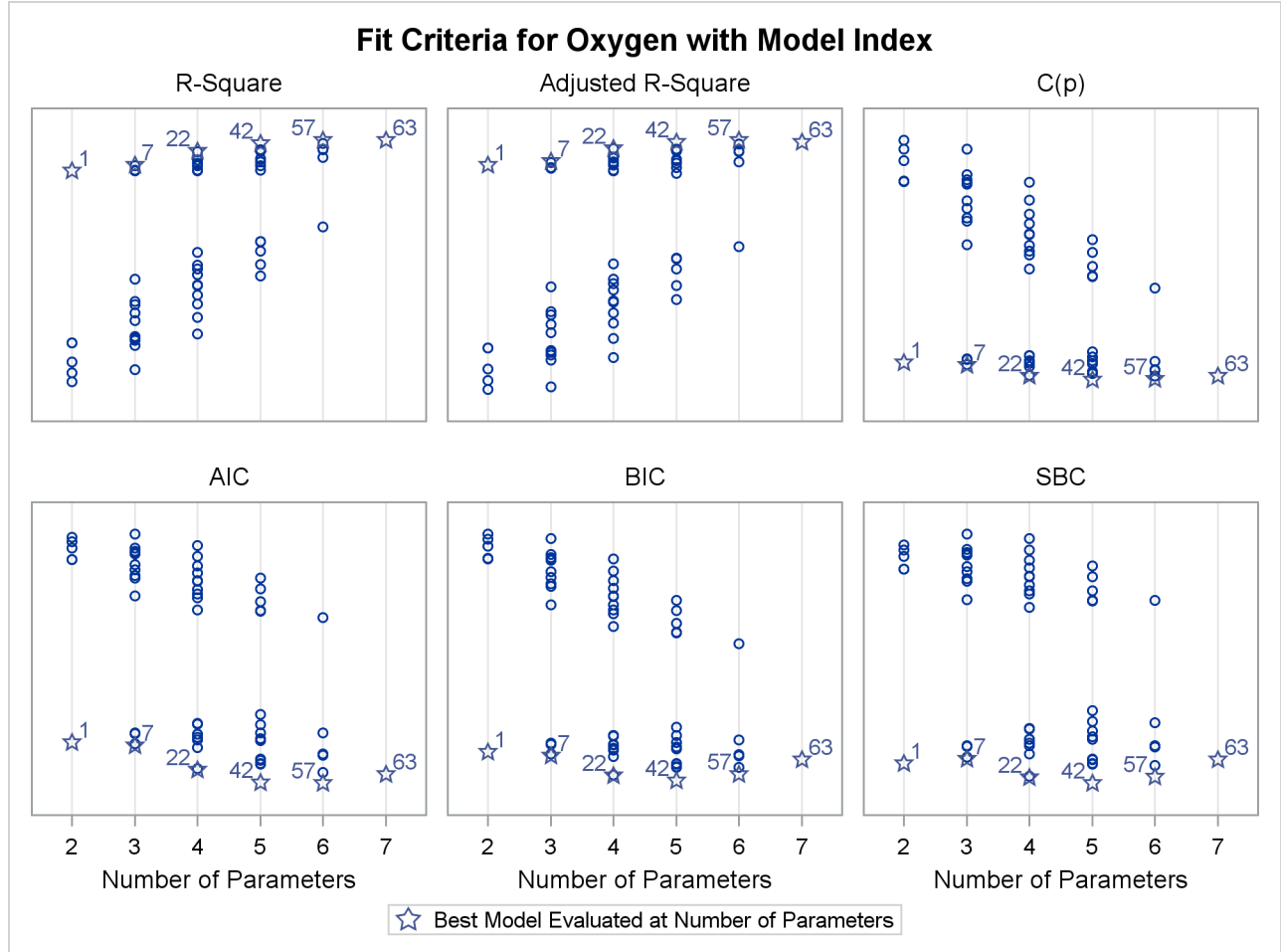
## Output 79.2.7 continued

| Physical fitness data: all models |                 |          |          |                                                   |
|-----------------------------------|-----------------|----------|----------|---------------------------------------------------|
| The REG Procedure                 |                 |          |          |                                                   |
| Model: MODEL1                     |                 |          |          |                                                   |
| Dependent Variable: Oxygen        |                 |          |          |                                                   |
| R-Square Selection Method         |                 |          |          |                                                   |
| Model Index                       | Number in Model | R-Square | C(p)     | Variables in Model                                |
| 38                                | 3               | 0.3208   | 84.7216  | Weight RunPulse MaxPulse                          |
| 39                                | 3               | 0.2902   | 89.5693  | Age Weight MaxPulse                               |
| 40                                | 3               | 0.2447   | 96.7952  | Weight RunPulse RestPulse                         |
| 41                                | 3               | 0.1882   | 105.7430 | Weight RestPulse MaxPulse                         |
| -----                             |                 |          |          |                                                   |
| 42                                | 4               | 0.8368   | 4.8800   | Age RunTime RunPulse MaxPulse                     |
| 43                                | 4               | 0.8165   | 8.1035   | Age Weight RunTime RunPulse                       |
| 44                                | 4               | 0.8158   | 8.2056   | Weight RunTime RunPulse MaxPulse                  |
| 45                                | 4               | 0.8117   | 8.8683   | Age RunTime RunPulse RestPulse                    |
| 46                                | 4               | 0.8104   | 9.0697   | RunTime RunPulse RestPulse MaxPulse               |
| 47                                | 4               | 0.7862   | 12.9039  | Age Weight RunTime MaxPulse                       |
| 48                                | 4               | 0.7834   | 13.3468  | Age RunTime RestPulse MaxPulse                    |
| 49                                | 4               | 0.7750   | 14.6788  | Age Weight RunTime RestPulse                      |
| 50                                | 4               | 0.7623   | 16.7058  | Weight RunTime RunPulse RestPulse                 |
| 51                                | 4               | 0.7462   | 19.2550  | Weight RunTime RestPulse MaxPulse                 |
| 52                                | 4               | 0.5034   | 57.7590  | Age Weight RunPulse RestPulse                     |
| 53                                | 4               | 0.5025   | 57.9092  | Age RunPulse RestPulse MaxPulse                   |
| 54                                | 4               | 0.4717   | 62.7830  | Age Weight RunPulse MaxPulse                      |
| 55                                | 4               | 0.4256   | 70.0963  | Age Weight RestPulse MaxPulse                     |
| 56                                | 4               | 0.3858   | 76.4100  | Weight RunPulse RestPulse MaxPulse                |
| -----                             |                 |          |          |                                                   |
| 57                                | 5               | 0.8480   | 5.1063   | Age Weight RunTime RunPulse MaxPulse              |
| 58                                | 5               | 0.8370   | 6.8461   | Age RunTime RunPulse RestPulse MaxPulse           |
| 59                                | 5               | 0.8176   | 9.9348   | Age Weight RunTime RunPulse RestPulse             |
| 60                                | 5               | 0.8161   | 10.1685  | Weight RunTime RunPulse RestPulse<br>MaxPulse     |
| 61                                | 5               | 0.7887   | 14.5111  | Age Weight RunTime RestPulse MaxPulse             |
| 62                                | 5               | 0.5541   | 51.7233  | Age Weight RunPulse RestPulse MaxPulse            |
| -----                             |                 |          |          |                                                   |
| 63                                | 6               | 0.8487   | 7.0000   | Age Weight RunTime RunPulse RestPulse<br>MaxPulse |

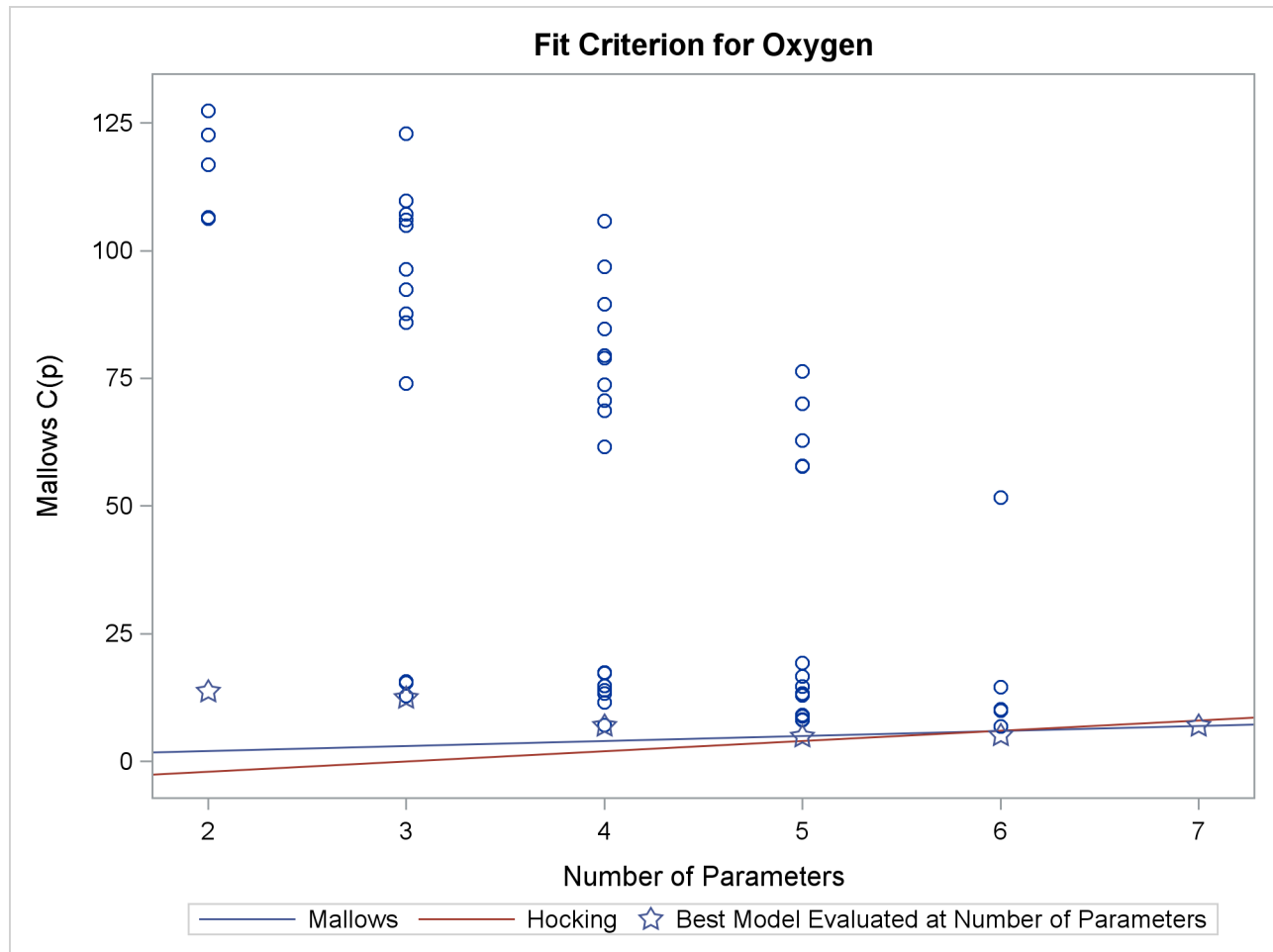
The models in [Output 79.2.7](#) are arranged first by the number of variables in the model and then by the magnitude of R square for the model.

Output 79.2.8 shows the panel of fit criteria for the RSQUARE selection method. The best models (based on the R-square statistic) for each subset size are indicated on the plots. The LABEL suboption specifies that these models are labeled by the model number that appears in the summary table shown in Output 79.2.7.

Output 79.2.8 Fit Criteria



Output 79.2.9 shows the plot of the  $C_p$  criterion by number of regressors in the model. Useful reference lines suggested by Mallows (1973) and Hocking (1976) are included on the plot. However, because all possible subset models are included on this plot, the better models are all compressed near the bottom of the plot.

Output 79.2.9  $C_p$  Criterion

The following statements use the BEST=20 option in the model statement and SELECTION=CP to restrict attention to the models that yield the 20 smallest values of the  $C_p$  statistic:

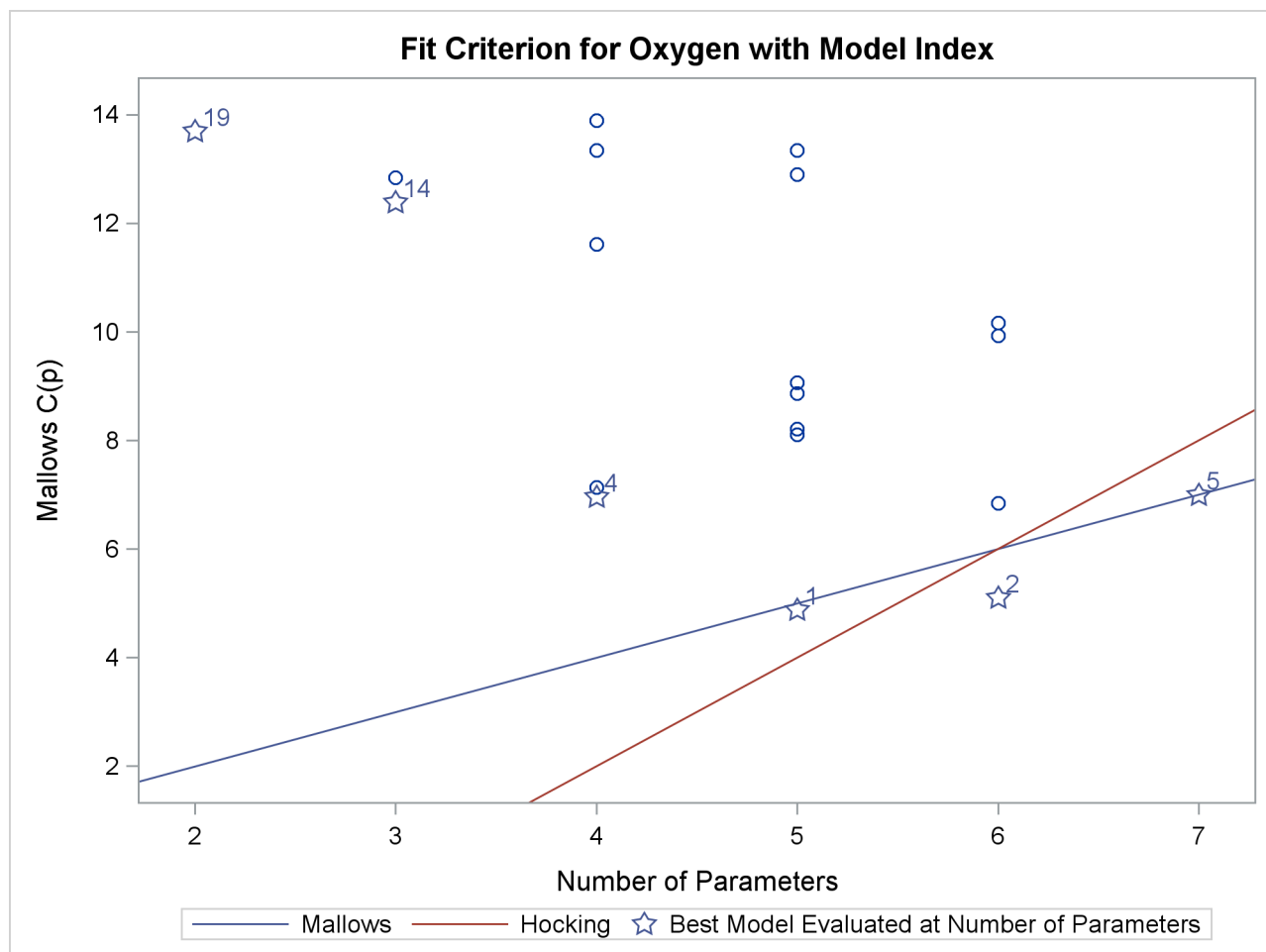
```
proc reg data=fitness plots(only)=cp(label);
 model Oxygen=Age Weight RunTime RunPulse RestPulse MaxPulse
 / selection=cp best=20;
run;

ods graphics off;
```

Output 79.2.10 shows the summary table listing the regressors in the 20 models that yield the smallest  $C_p$  values, and Output 79.2.11 presents the results graphically. Reference lines  $C_p = 2p - p_{full}$  and  $C_p = p$  are shown on this plot. See the PLOTS=CP option on page 6639 for interpretations of these lines. For the Fitness data, these lines indicate that a six-variable model is a reasonable choice for doing parameter estimation, while a five-variable model might be suitable for doing prediction.

**Output 79.2.10**  $C_p$  Selection Summary: PROC REG

| The REG Procedure          |                 |         |          |                                                |  |
|----------------------------|-----------------|---------|----------|------------------------------------------------|--|
| Model: MODEL1              |                 |         |          |                                                |  |
| Dependent Variable: Oxygen |                 |         |          |                                                |  |
| C(p) Selection Method      |                 |         |          |                                                |  |
| Model Index                | Number in Model | C(p)    | R-Square | Variables in Model                             |  |
| 1                          | 4               | 4.8800  | 0.8368   | Age RunTime RunPulse MaxPulse                  |  |
| 2                          | 5               | 5.1063  | 0.8480   | Age Weight RunTime RunPulse MaxPulse           |  |
| 3                          | 5               | 6.8461  | 0.8370   | Age RunTime RunPulse RestPulse MaxPulse        |  |
| 4                          | 3               | 6.9596  | 0.8111   | Age RunTime RunPulse                           |  |
| 5                          | 6               | 7.0000  | 0.8487   | Age Weight RunTime RunPulse RestPulse MaxPulse |  |
| 6                          | 3               | 7.1350  | 0.8100   | RunTime RunPulse MaxPulse                      |  |
| 7                          | 4               | 8.1035  | 0.8165   | Age Weight RunTime RunPulse                    |  |
| 8                          | 4               | 8.2056  | 0.8158   | Weight RunTime RunPulse MaxPulse               |  |
| 9                          | 4               | 8.8683  | 0.8117   | Age RunTime RunPulse RestPulse                 |  |
| 10                         | 4               | 9.0697  | 0.8104   | RunTime RunPulse RestPulse MaxPulse            |  |
| 11                         | 5               | 9.9348  | 0.8176   | Age Weight RunTime RunPulse RestPulse          |  |
| 12                         | 5               | 10.1685 | 0.8161   | Weight RunTime RunPulse RestPulse MaxPulse     |  |
| 13                         | 3               | 11.6167 | 0.7817   | Age RunTime MaxPulse                           |  |
| 14                         | 2               | 12.3894 | 0.7642   | Age RunTime                                    |  |
| 15                         | 2               | 12.8372 | 0.7614   | RunTime RunPulse                               |  |
| 16                         | 4               | 12.9039 | 0.7862   | Age Weight RunTime MaxPulse                    |  |
| 17                         | 3               | 13.3453 | 0.7708   | Age Weight RunTime                             |  |
| 18                         | 4               | 13.3468 | 0.7834   | Age RunTime RestPulse MaxPulse                 |  |
| 19                         | 1               | 13.6988 | 0.7434   | RunTime                                        |  |
| 20                         | 3               | 13.8974 | 0.7673   | Age RunTime RestPulse                          |  |

Output 79.2.11  $C_p$  Criterion

Before making a final decision about which model to use, you would want to perform collinearity diagnostics. Note that, since many different models have been fit and the choice of a final model is based on  $R$  square, the statistics are biased and the  $p$ -values for the parameter estimates are not valid.

## Example 79.3: Predicting Weight by Height and Age

In this example, the weights of schoolchildren are modeled as a function of their heights and ages. The example shows the use of a BY statement with PROC REG, multiple MODEL statements, and the OUTEST= and OUTSSCP= options, which create data sets. Here are the data:

```
-----Data on Age, Weight, and Height of Children-----
| Age (months), height (inches), and weight (pounds) were |
| recorded for a group of school children. |
| From Lewis and Taylor (1967). |

data htwt;
 input sex $ age :3.1 height weight @@;
 datalines;
f 143 56.3 85.0 f 155 62.3 105.0 f 153 63.3 108.0 f 161 59.0 92.0
f 191 62.5 112.5 f 171 62.5 112.0 f 185 59.0 104.0 f 142 56.5 69.0
f 160 62.0 94.5 f 140 53.8 68.5 f 139 61.5 104.0 f 178 61.5 103.5
f 157 64.5 123.5 f 149 58.3 93.0 f 143 51.3 50.5 f 145 58.8 89.0
f 191 65.3 107.0 f 150 59.5 78.5 f 147 61.3 115.0 f 180 63.3 114.0

 ... more lines ...

m 164 66.5 112.0 m 189 65.0 114.0 m 164 61.5 140.0 m 167 62.0 107.5
m 151 59.3 87.0
;
```

Modeling is performed separately for boys and girls. Since the BY statement is used, interactive processing is not possible in this example; no statements can appear after the first RUN statement.

The following statements produce [Output 79.3.1](#) through [Output 79.3.4](#):

```
proc reg outest=est1 outsscp=sscp1 rsquare;
 by sex;
 eq1: model weight=height;
 eq2: model weight=height age;
run;

proc print data=sscp1;
 title2 'SSCP type data set';
run;

proc print data=est1;
 title2 'EST type data set';
run;
```



**Output 79.3.1** Height and Weight Data: Submodel for Female Children

```

----- sex=f -----
 The REG Procedure
 Model: eq1
 Dependent Variable: weight

 Analysis of Variance

```

| Source          | DF  | Sum of Squares | Mean Square | F Value | Pr > F |
|-----------------|-----|----------------|-------------|---------|--------|
| Model           | 1   | 21507          | 21507       | 141.09  | <.0001 |
| Error           | 109 | 16615          | 152.42739   |         |        |
| Corrected Total | 110 | 38121          |             |         |        |

|                |          |          |        |
|----------------|----------|----------|--------|
| Root MSE       | 12.34615 | R-Square | 0.5642 |
| Dependent Mean | 98.87838 | Adj R-Sq | 0.5602 |
| Coeff Var      | 12.48620 |          |        |

```

 Parameter Estimates

```

| Variable  | DF | Parameter Estimate | Standard Error | t Value | Pr >  t |
|-----------|----|--------------------|----------------|---------|---------|
| Intercept | 1  | -153.12891         | 21.24814       | -7.21   | <.0001  |
| height    | 1  | 4.16361            | 0.35052        | 11.88   | <.0001  |

**Output 79.3.2** Height and Weight Data: Full Model for Female Children

```

----- sex=f -----

 The REG Procedure
 Model: eq2
 Dependent Variable: weight

 Analysis of Variance

Source DF Sum of Mean
 DF Squares Square F Value Pr > F

Model 2 22432 11216 77.21 <.0001
Error 108 15689 145.26700
Corrected Total 110 38121

 Root MSE 12.05268 R-Square 0.5884
 Dependent Mean 98.87838 Adj R-Sq 0.5808
 Coeff Var 12.18939

 Parameter Estimates

Variable DF Parameter Standard
 DF Estimate Error t Value Pr > |t|

Intercept 1 -150.59698 20.76730 -7.25 <.0001
height 1 3.60378 0.40777 8.84 <.0001
age 1 1.90703 0.75543 2.52 0.0130

```

**Output 79.3.3** Height and Weight Data: Submodel for Male Children

```

----- sex=m -----

 The REG Procedure
 Model: eq1
 Dependent Variable: weight

 Analysis of Variance

Source DF Sum of Mean
 DF Squares Square F Value Pr > F

Model 1 31126 31126 206.24 <.0001
Error 124 18714 150.92222
Corrected Total 125 49840

 Root MSE 12.28504 R-Square 0.6245
 Dependent Mean 103.44841 Adj R-Sq 0.6215
 Coeff Var 11.87552

 Parameter Estimates

Variable DF Parameter Standard
 DF Estimate Error t Value Pr > |t|

Intercept 1 -125.69807 15.99362 -7.86 <.0001
height 1 3.68977 0.25693 14.36 <.0001

```

**Output 79.3.4** Height and Weight Data: Full Model for Male Children

```

----- sex=m -----

 The REG Procedure
 Model: eq2
 Dependent Variable: weight

 Analysis of Variance

Source DF Sum of Mean
 DF Squares Square F Value Pr > F

Model 2 32975 16487 120.24 <.0001
Error 123 16866 137.11922
Corrected Total 125 49840

 Root MSE 11.70979 R-Square 0.6616
 Dependent Mean 103.44841 Adj R-Sq 0.6561
 Coeff Var 11.31945

 Parameter Estimates

Variable DF Parameter Standard
 DF Estimate Error t Value Pr > |t|

Intercept 1 -113.71346 15.59021 -7.29 <.0001
height 1 2.68075 0.36809 7.28 <.0001
age 1 3.08167 0.83927 3.67 0.0004

```

For both female and male children, the overall  $F$  statistics for both models are significant, indicating that the model explains a significant portion of the variation in the data. For females, the full model is

$$\text{weight} = -150.57 + 3.60 \times \text{height} + 1.91 \times \text{age}$$

and for males, the full model is

$$\text{weight} = -113.71 + 2.68 \times \text{height} + 3.08 \times \text{age}$$

The OUTSSCP= data set is shown in [Output 79.3.5](#). Note how the BY groups are separated. Observations with `_TYPE_='N'` contain the number of observations in the associated BY group. Observations with `_TYPE_='SSCP'` contain the rows of the uncorrected sums of squares and crossproducts matrix. The observations with `_NAME_='Intercept'` contain crossproducts for the intercept.

**Output 79.3.5** SSCP Matrix

| SSCP type data set |     |        |           |           |           |            |           |
|--------------------|-----|--------|-----------|-----------|-----------|------------|-----------|
| Obs                | sex | _TYPE_ | _NAME_    | Intercept | height    | weight     | age       |
| 1                  | f   | SSCP   | Intercept | 111.0     | 6718.40   | 10975.50   | 1824.90   |
| 2                  | f   | SSCP   | height    | 6718.4    | 407879.32 | 669469.85  | 110818.32 |
| 3                  | f   | SSCP   | weight    | 10975.5   | 669469.85 | 1123360.75 | 182444.95 |
| 4                  | f   | SSCP   | age       | 1824.9    | 110818.32 | 182444.95  | 30363.81  |
| 5                  | f   | N      |           | 111.0     | 111.00    | 111.00     | 111.00    |
| 6                  | m   | SSCP   | Intercept | 126.0     | 7825.00   | 13034.50   | 2072.10   |
| 7                  | m   | SSCP   | height    | 7825.0    | 488243.60 | 817919.60  | 129432.57 |
| 8                  | m   | SSCP   | weight    | 13034.5   | 817919.60 | 1398238.75 | 217717.45 |
| 9                  | m   | SSCP   | age       | 2072.1    | 129432.57 | 217717.45  | 34515.95  |
| 10                 | m   | N      |           | 126.0     | 126.00    | 126.00     | 126.00    |

The OUTEST= data set is displayed in [Output 79.3.6](#); again, the BY groups are separated. The `_MODEL_` column contains the labels for models from the `MODEL` statements. If no labels are specified, the defaults `MODEL1` and `MODEL2` would appear as values for `_MODEL_`. Note that `_TYPE_='PARMS'` for all observations, indicating that all observations contain parameter estimates. The `_DEPVAR_` column displays the dependent variable, and the `_RMSE_` column gives the root mean square error for the associated model. The Intercept column gives the estimate for the intercept for the associated model, and variables with the same name as variables in the original data set (height, age) give parameter estimates for those variables. The dependent variable, weight, is shown with a value of -1. The `_IN_` column contains the number of regressors in the model not including the intercept; `_P_` contains the number of parameters in the model; `_EDF_` contains the error degrees of freedom; and `_RSQ_` contains the R square statistic. Finally, note that the `_IN_`, `_P_`, `_EDF_`, and `_RSQ_` columns appear in the OUTEST= data set since the `RSQUARE` option is specified in the `PROC REG` statement.

**Output 79.3.6** OUTEST Data Set

| EST type data set |     |     |       |        |           |          |         |     |         |   |     |     |         |
|-------------------|-----|-----|-------|--------|-----------|----------|---------|-----|---------|---|-----|-----|---------|
| Obs               | sex | Eq  | Model | DepVar | Intercept | height   | weight  | age | IN      | P | EDF | RSQ |         |
| 1                 | f   | eq1 | PARMS | weight | 12.3461   | -153.129 | 4.16361 | -1  | .       | 1 | 2   | 109 | 0.56416 |
| 2                 | f   | eq2 | PARMS | weight | 12.0527   | -150.597 | 3.60378 | -1  | 1.90703 | 2 | 3   | 108 | 0.58845 |
| 3                 | m   | eq1 | PARMS | weight | 12.2850   | -125.698 | 3.68977 | -1  | .       | 1 | 2   | 124 | 0.62451 |
| 4                 | m   | eq2 | PARMS | weight | 11.7098   | -113.713 | 2.68075 | -1  | 3.08167 | 2 | 3   | 123 | 0.66161 |

## Example 79.4: Regression with Quantitative and Qualitative Variables

At times it is desirable to have independent variables in the model that are qualitative rather than quantitative. This is easily handled in a regression framework. Regression uses qualitative variables to distinguish between populations. There are two main advantages of fitting both populations in one model. You gain the ability to test for different slopes or intercepts in the populations, and more degrees of freedom are available for the analysis.

Regression with qualitative variables is different from analysis of variance and analysis of covariance. Analysis of variance uses qualitative independent variables only. Analysis of covariance uses quantitative variables in addition to the qualitative variables in order to account for correlation in the data and reduce MSE; however, the quantitative variables are not of primary interest and merely improve the precision of the analysis.

Consider the case where  $Y_i$  is the dependent variable,  $X1_i$  is a quantitative variable,  $X2_i$  is a qualitative variable taking on values 0 or 1, and  $X1_i X2_i$  is the interaction. The variable  $X2_i$  is called a dummy, binary, or indicator variable. With values 0 or 1, it distinguishes between two populations. The model is of the form

$$Y_i = \beta_0 + \beta_1 X1_i + \beta_2 X2_i + \beta_3 X1_i X2_i + \epsilon_i$$

for the observations  $i = 1, 2, \dots, n$ . The parameters to be estimated are  $\beta_0$ ,  $\beta_1$ ,  $\beta_2$ , and  $\beta_3$ . The number of dummy variables used is one less than the number of qualitative levels. This yields a nonsingular  $X'X$  matrix. See Chapter 10 of Neter, Wasserman, and Kutner (1990) for more details.

An example from Neter, Wasserman, and Kutner (1990) follows. An economist is investigating the relationship between the size of an insurance firm and the speed at which it implements new insurance innovations. He believes that the type of firm might affect this relationship and suspects that there might be some interaction between the size and type of firm. The dummy variable in the model enables the two firms to have different intercepts. The interaction term enables the firms to have different slopes as well.

In this study,  $Y_i$  is the number of months from the time the first firm implemented the innovation to the time it was implemented by the  $i$ th firm. The variable  $X1_i$  is the size of the firm, measured in total assets of the firm. The variable  $X2_i$  denotes the firm type; it is 0 if the firm is a mutual fund company and 1 if the firm is a stock company. The dummy variable enables each firm type to have a different intercept and slope.

The previous model can be broken down into a model for each firm type by plugging in the values for  $X2_i$ . If  $X2_i = 0$ , the model is

$$Y_i = \beta_0 + \beta_1 X1_i + \epsilon_i$$

This is the model for a mutual company. If  $X2_i = 1$ , the model for a stock firm is

$$Y_i = (\beta_0 + \beta_2) + (\beta_1 + \beta_3) X1_i + \epsilon_i$$

This model has intercept  $\beta_0 + \beta_2$  and slope  $\beta_1 + \beta_3$ .

The data<sup>1</sup> follow. Note that the interaction term is created in the DATA step since polynomial effects such as size\*type are not allowed in the MODEL statement in the REG procedure.

```

title 'Regression with Quantitative and Qualitative Variables';
data insurance;
 input time size type @@;
 sizetype=size*type;
 datalines;
17 151 0 26 92 0 21 175 0 30 31 0 22 104 0 0 277 0 12 210 0
19 120 0 4 290 0 16 238 0 28 164 1 15 272 1 11 295 1 38 68 1
31 85 1 21 224 1 20 166 1 13 305 1 30 124 1 14 246 1
;

```

The following statements begin the analysis and produce the ANOVA table in [Output 79.4.1](#):

```

proc reg data=insurance;
 model time = size type sizetype;
run;

```

**Output 79.4.1** ANOVA Table and Parameter Estimates

| Regression with Quantitative and Qualitative Variables |    |                    |                |         |         |
|--------------------------------------------------------|----|--------------------|----------------|---------|---------|
| The REG Procedure                                      |    |                    |                |         |         |
| Model: MODEL1                                          |    |                    |                |         |         |
| Dependent Variable: time                               |    |                    |                |         |         |
| Analysis of Variance                                   |    |                    |                |         |         |
| Source                                                 | DF | Sum of Squares     | Mean Square    | F Value | Pr > F  |
| Model                                                  | 3  | 1504.41904         | 501.47301      | 45.49   | <.0001  |
| Error                                                  | 16 | 176.38096          | 11.02381       |         |         |
| Corrected Total                                        | 19 | 1680.80000         |                |         |         |
| Root MSE                                               |    | 3.32021            | R-Square       | 0.8951  |         |
| Dependent Mean                                         |    | 19.40000           | Adj R-Sq       | 0.8754  |         |
| Coeff Var                                              |    | 17.11450           |                |         |         |
| Parameter Estimates                                    |    |                    |                |         |         |
| Variable                                               | DF | Parameter Estimate | Standard Error | t Value | Pr >  t |
| Intercept                                              | 1  | 33.83837           | 2.44065        | 13.86   | <.0001  |
| size                                                   | 1  | -0.10153           | 0.01305        | -7.78   | <.0001  |
| type                                                   | 1  | 8.13125            | 3.65405        | 2.23    | 0.0408  |
| sizetype                                               | 1  | -0.00041714        | 0.01833        | -0.02   | 0.9821  |

<sup>1</sup>From Neter, J., et al., *Applied Linear Statistical Models*, Third Edition, Copyright (c) 1990, Richard D. Irwin. Reprinted with permission of The McGraw-Hill Companies.

The overall  $F$  statistic is significant ( $F = 45.490, p < 0.0001$ ). The interaction term is not significant ( $t = -0.023, p = 0.9821$ ). Hence, this term should be removed and the model refitted, as shown in the following statements:

```
delete sizetype;
print;
run;
```

The **DELETE** statement removes the interaction term (sizetype) from the model. The new ANOVA and parameter estimates tables are shown in **Output 79.4.2**.

**Output 79.4.2** ANOVA Table and Parameter Estimates

| Analysis of Variance |                |                    |                |         |         |
|----------------------|----------------|--------------------|----------------|---------|---------|
| Source               | DF             | Sum of Squares     | Mean Square    | F Value | Pr > F  |
| Model                | 2              | 1504.41333         | 752.20667      | 72.50   | <.0001  |
| Error                | 17             | 176.38667          | 10.37569       |         |         |
| Corrected Total      | 19             | 1680.80000         |                |         |         |
|                      | Root MSE       | 3.22113            | R-Square       | 0.8951  |         |
|                      | Dependent Mean | 19.40000           | Adj R-Sq       | 0.8827  |         |
|                      | Coeff Var      | 16.60377           |                |         |         |
| Parameter Estimates  |                |                    |                |         |         |
| Variable             | DF             | Parameter Estimate | Standard Error | t Value | Pr >  t |
| Intercept            | 1              | 33.87407           | 1.81386        | 18.68   | <.0001  |
| size                 | 1              | -0.10174           | 0.00889        | -11.44  | <.0001  |
| type                 | 1              | 8.05547            | 1.45911        | 5.52    | <.0001  |

The overall  $F$  statistic is still significant ( $F = 72.497, p < 0.0001$ ). The intercept and the coefficients associated with size and type are significantly different from zero ( $t = 18.675, p < 0.0001$ ;  $t = -11.443, p < 0.0001$ ;  $t = 5.521, p < 0.0001$ , respectively). Notice that the R square did not change with the omission of the interaction term.

The fitted model is

$$\text{time} = 33.87 - 0.102 \times \text{size} + 8.055 \times \text{type}$$

The fitted model for a mutual fund company ( $X_{2i} = 0$ ) is

$$\text{time} = 33.87 - 0.102 \times \text{size}$$



and the fitted model for a stock company ( $X_{2i} = 1$ ) is

$$\text{time} = (33.87 + 8.055) - 0.102 \times \text{size}$$

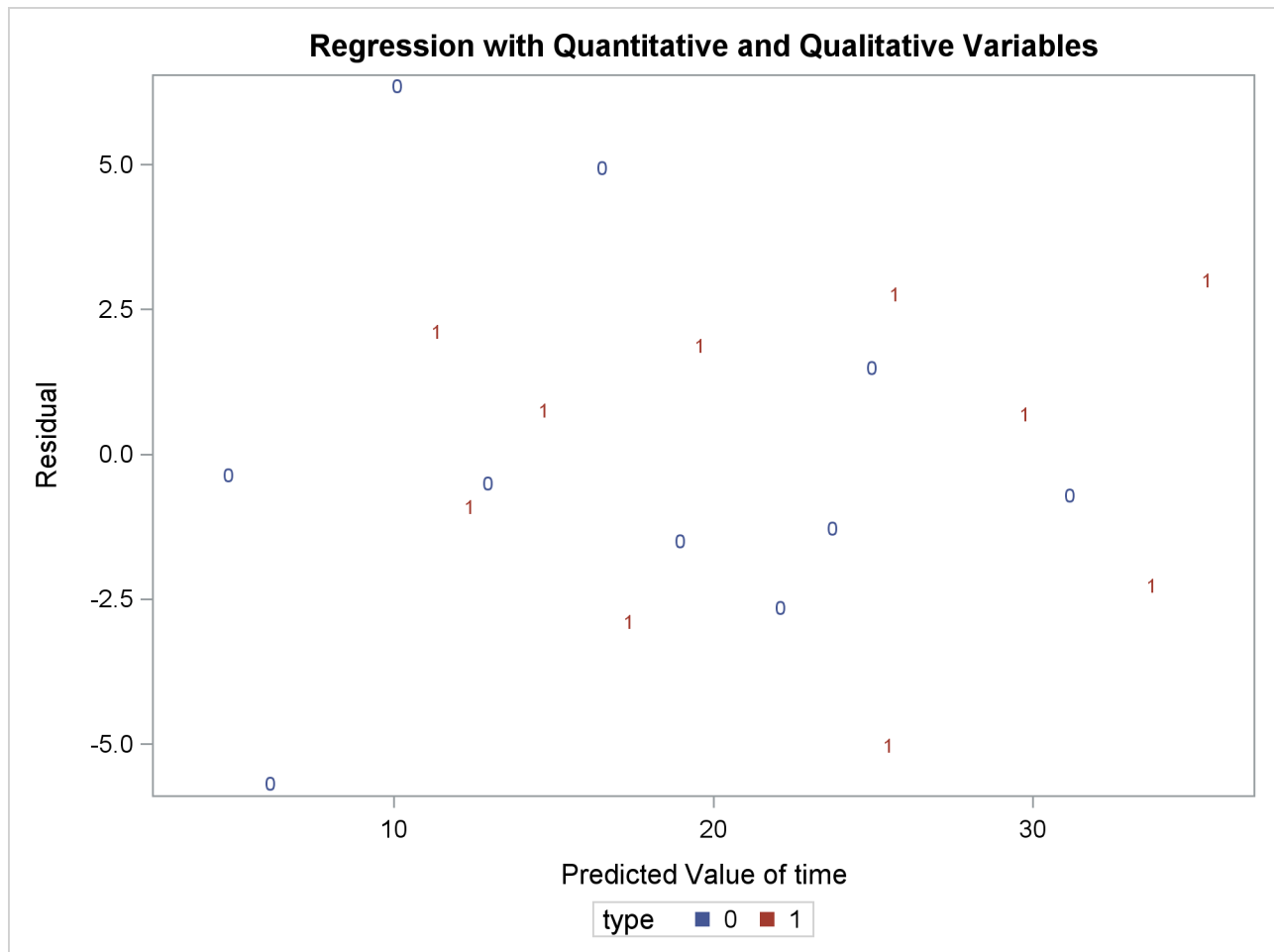
So the two models have different intercepts but the same slope.

The following statements first use an **OUTPUT** statement to save the residuals and predicted values from the new model in the OUT= data set. Next PROC SGPLOT is used to produce **Output 79.4.3**, which plots residuals versus predicted values. The firm type is used as the plot symbol; this can be useful in determining if the firm types have different residual patterns.

```
output out=out r=r p=p;
run;

proc sgplot data=out;
 scatter x=p y=r / markerchar=type group=type;
run;
```

**Output 79.4.3** Plot of Residual vs. Predicted Values

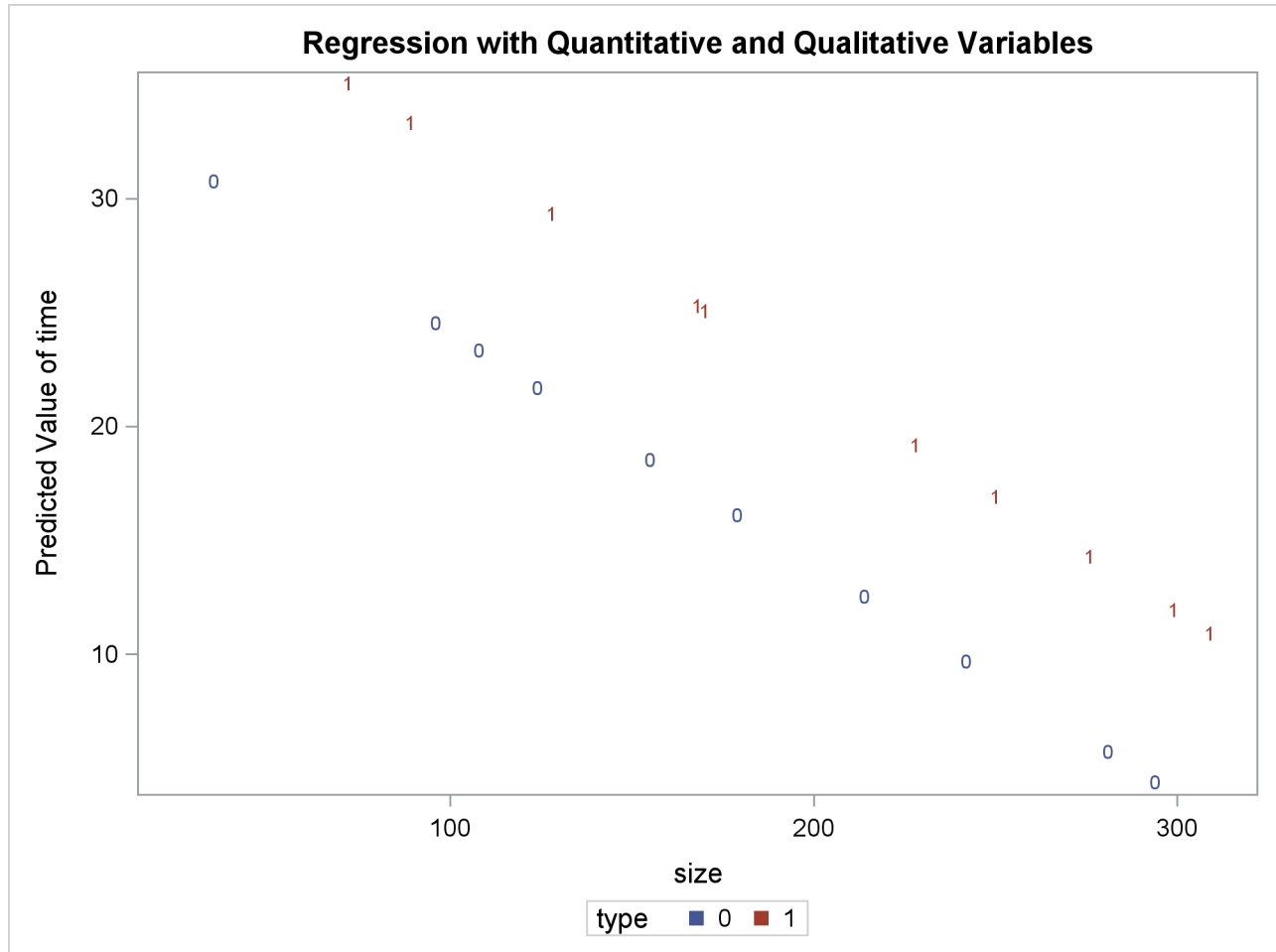


The residuals show no major trend. Neither firm type by itself shows a trend either. This indicates that the model is satisfactory.

The following statements produce the plot of the predicted values versus size that appears in [Output 79.4.4](#), where the firm type is again used as the plotting symbol:

```
proc sgplot data=out;
 scatter x=size y=p / markerchar=type group=type;
run;
```

**Output 79.4.4** Plot of Predicted vs. Size



The different intercepts are very evident in this plot.

## Example 79.5: Ridge Regression for Acetylene Data

This example uses the acetylene data in Marquardt and Snee (1975) to illustrate the RIDGEPLOT and OUTVIF options. Here are the data:

```

data acetyl;
 input x1-x4 @@;
 x1x2 = x1 * x2;
 x1x1 = x1 * x1;
 label x1 = 'reactor temperature(celsius)'
 x2 = 'h2 to n-heptone ratio'
 x3 = 'contact time(sec)'
 x4 = 'conversion percentage'
 x1x2= 'temperature-ratio interaction'
 x1x1= 'squared temperature';
 datalines;
1300 7.5 .012 49 1300 9 .012 50.2 1300 11 .0115 50.5
1300 13.5 .013 48.5 1300 17 .0135 47.5 1300 23 .012 44.5
1200 5.3 .04 28 1200 7.5 .038 31.5 1200 11 .032 34.5
1200 13.5 .026 35 1200 17 .034 38 1200 23 .041 38.5
1100 5.3 .084 15 1100 7.5 .098 17 1100 11 .092 20.5
1100 17 .086 29.5
;

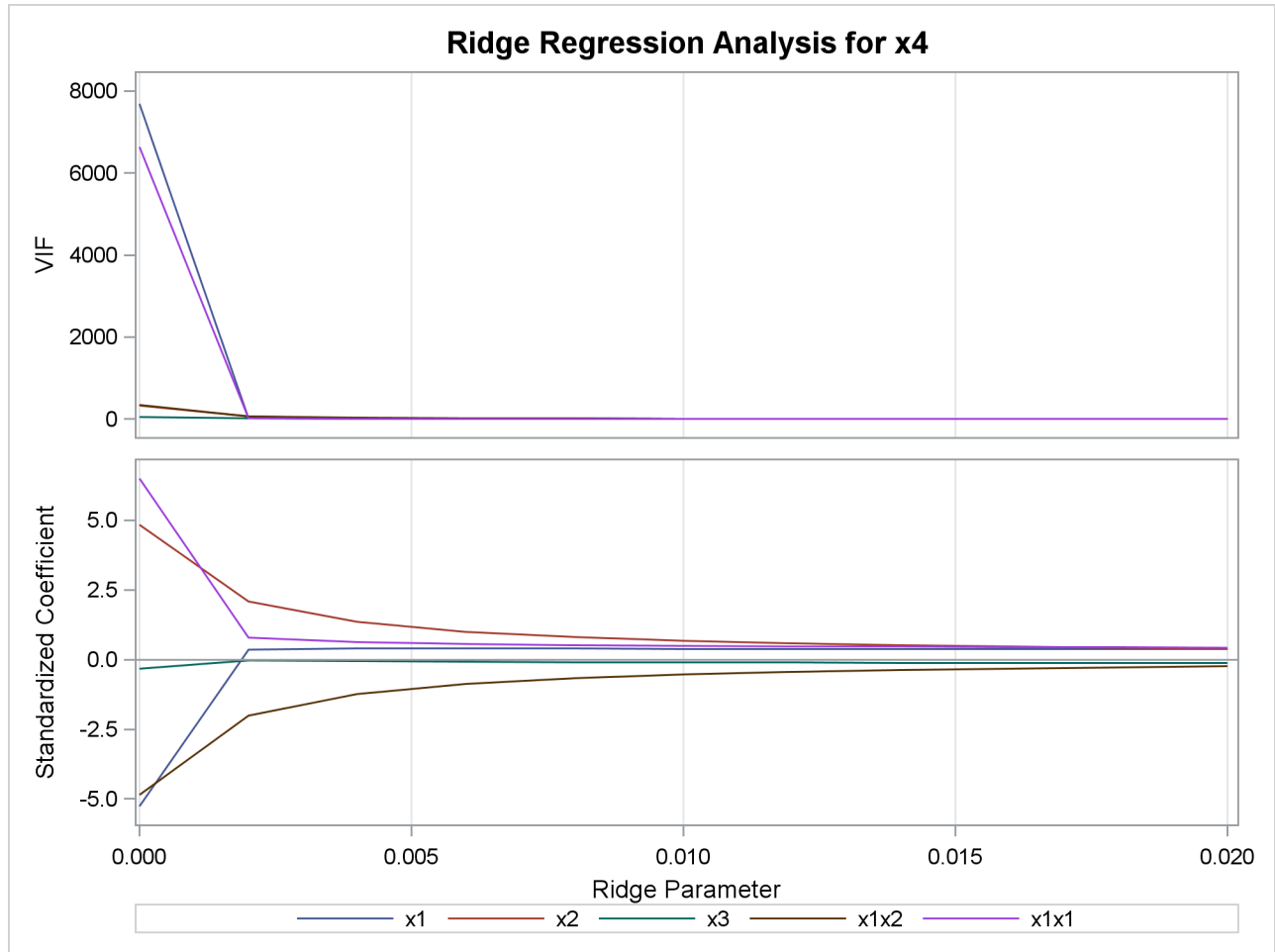
ods graphics on;

proc reg data=acetyl outvif
 outest=b ridge=0 to 0.02 by .002;
 model x4=x1 x2 x3 x1x2 x1x1;
run;
proc print data=b;
run;

```

When ODS Graphics is enabled and you request ridge regression by using the RIDGE= option in the PROC REG statement, PROC REG produces a panel showing variance inflation factors (VIF) in the upper plot in the panel and ridge traces in the lower plot. This panel is shown in [Output 79.5.1](#).

**Output 79.5.1** Ridge Regression and VIF Traces



The OUTVIF option outputs the variance inflation factors to the OUTEST= data set that is shown in [Output 79.5.2](#).

Output 79.5.2 OUTEST Data Set Showing VIF Values

| Obs | MODEL  | TYPE     | DEPVAR | RIDGE | PCOMIT | RMSE    | Intercept |
|-----|--------|----------|--------|-------|--------|---------|-----------|
| 1   | MODEL1 | PARMS    | x4     | .     | .      | 1.15596 | 390.538   |
| 2   | MODEL1 | RIDGEVIF | x4     | 0.000 | .      | .       | .         |
| 3   | MODEL1 | RIDGE    | x4     | 0.000 | .      | 1.15596 | 390.538   |
| 4   | MODEL1 | RIDGEVIF | x4     | 0.002 | .      | .       | .         |
| 5   | MODEL1 | RIDGE    | x4     | 0.002 | .      | 2.69721 | -103.388  |
| 6   | MODEL1 | RIDGEVIF | x4     | 0.004 | .      | .       | .         |
| 7   | MODEL1 | RIDGE    | x4     | 0.004 | .      | 3.22340 | -93.797   |
| 8   | MODEL1 | RIDGEVIF | x4     | 0.006 | .      | .       | .         |
| 9   | MODEL1 | RIDGE    | x4     | 0.006 | .      | 3.47752 | -87.687   |
| 10  | MODEL1 | RIDGEVIF | x4     | 0.008 | .      | .       | .         |
| 11  | MODEL1 | RIDGE    | x4     | 0.008 | .      | 3.62677 | -83.593   |
| 12  | MODEL1 | RIDGEVIF | x4     | 0.010 | .      | .       | .         |
| 13  | MODEL1 | RIDGE    | x4     | 0.010 | .      | 3.72505 | -80.603   |
| 14  | MODEL1 | RIDGEVIF | x4     | 0.012 | .      | .       | .         |
| 15  | MODEL1 | RIDGE    | x4     | 0.012 | .      | 3.79477 | -78.276   |
| 16  | MODEL1 | RIDGEVIF | x4     | 0.014 | .      | .       | .         |
| 17  | MODEL1 | RIDGE    | x4     | 0.014 | .      | 3.84693 | -76.381   |
| 18  | MODEL1 | RIDGEVIF | x4     | 0.016 | .      | .       | .         |
| 19  | MODEL1 | RIDGE    | x4     | 0.016 | .      | 3.88750 | -74.785   |
| 20  | MODEL1 | RIDGEVIF | x4     | 0.018 | .      | .       | .         |
| 21  | MODEL1 | RIDGE    | x4     | 0.018 | .      | 3.92004 | -73.407   |
| 22  | MODEL1 | RIDGEVIF | x4     | 0.020 | .      | .       | .         |
| 23  | MODEL1 | RIDGE    | x4     | 0.020 | .      | 3.94679 | -72.193   |

| Obs | x1      | x2      | x3       | x1x2    | x1x1    | x4 |
|-----|---------|---------|----------|---------|---------|----|
| 1   | -0.78   | 10.174  | -121.626 | -0.008  | 0.00    | -1 |
| 2   | 7682.37 | 320.022 | 53.525   | 344.545 | 6643.32 | -1 |
| 3   | -0.78   | 10.174  | -121.626 | -0.008  | 0.00    | -1 |
| 4   | 11.18   | 58.731  | 10.744   | 63.208  | 11.22   | -1 |
| 5   | 0.05    | 4.404   | -9.065   | -0.003  | 0.00    | -1 |
| 6   | 4.36    | 23.939  | 9.996    | 25.744  | 5.15    | -1 |
| 7   | 0.06    | 2.839   | -21.338  | -0.002  | 0.00    | -1 |
| 8   | 2.93    | 13.011  | 9.383    | 13.976  | 3.81    | -1 |
| 9   | 0.06    | 2.110   | -28.447  | -0.001  | 0.00    | -1 |
| 10  | 2.36    | 8.224   | 8.838    | 8.821   | 3.23    | -1 |
| 11  | 0.06    | 1.689   | -33.377  | -0.001  | 0.00    | -1 |
| 12  | 2.04    | 5.709   | 8.343    | 6.112   | 2.89    | -1 |
| 13  | 0.06    | 1.414   | -37.177  | -0.001  | 0.00    | -1 |
| 14  | 1.84    | 4.226   | 7.891    | 4.514   | 2.65    | -1 |
| 15  | 0.06    | 1.221   | -40.297  | -0.001  | 0.00    | -1 |
| 16  | 1.69    | 3.279   | 7.476    | 3.493   | 2.46    | -1 |
| 17  | 0.06    | 1.078   | -42.965  | -0.001  | 0.00    | -1 |
| 18  | 1.57    | 2.637   | 7.094    | 2.801   | 2.31    | -1 |
| 19  | 0.06    | 0.968   | -45.309  | -0.001  | 0.00    | -1 |
| 20  | 1.47    | 2.182   | 6.741    | 2.310   | 2.18    | -1 |
| 21  | 0.06    | 0.880   | -47.407  | -0.000  | 0.00    | -1 |
| 22  | 1.39    | 1.847   | 6.415    | 1.949   | 2.06    | -1 |
| 23  | 0.06    | 0.809   | -49.310  | -0.000  | 0.00    | -1 |

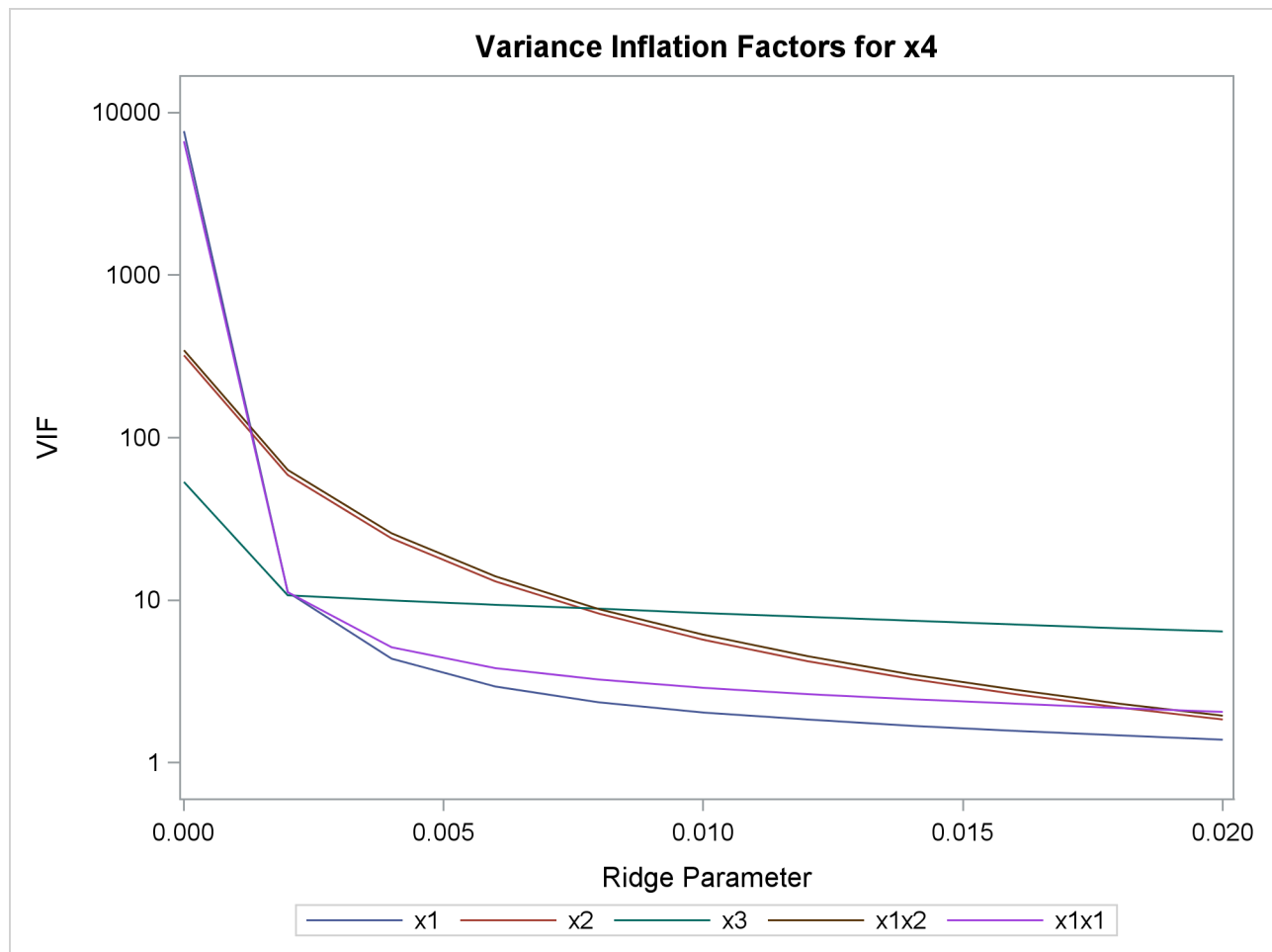
If you want to obtain separate plots containing the ridge traces and VIF traces, you can specify the UNPACK suboption in the PLOTS=RIDGE option. You can also request that one or both of the VIF axis and ridge parameter axis be displayed on a logarithmic scale. You can see in [Output 79.5.1](#) that the VIF traces for several of the parameters are nearly indistinguishable when displayed on a linear scale. The following code illustrates how you obtain separate VIF and ridge traces with the VIF values displayed on a logarithmic scale. Note that you can obtain plots of VIF values even though you do not specify the OUTVIF option in the PROC REG statement.

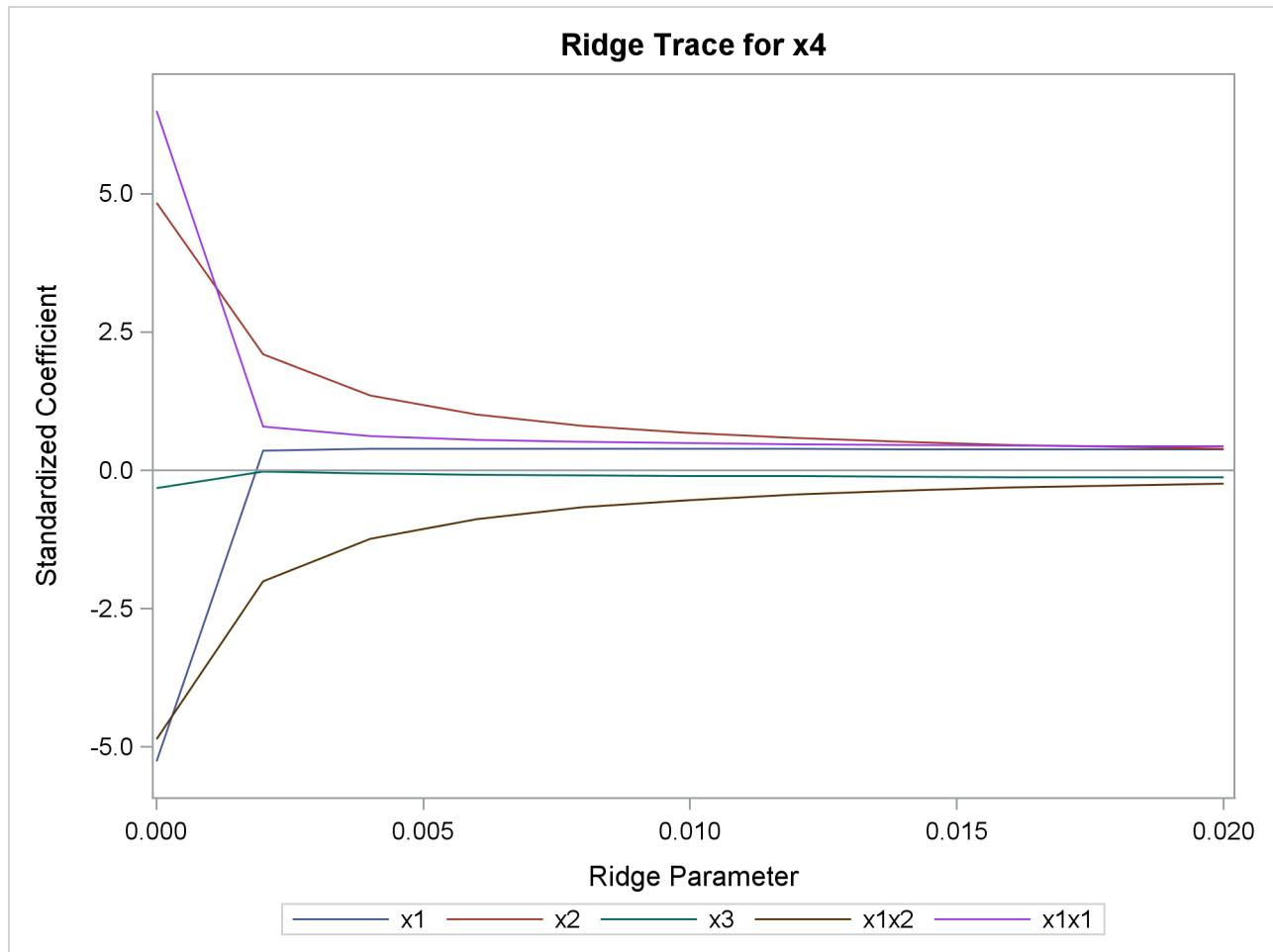
```
proc reg data=acetyl plots(only)=ridge(unpack VIFaxis=log)
 outest=b ridge=0 to 0.02 by .002;
 model x4=x1 x2 x3 x1x2 x1x1;
run;

ods graphics off;
```

The requested plots are shown in [Output 79.5.3](#) and [Output 79.5.4](#).

**Output 79.5.3** VIF Traces



**Output 79.5.4** Ridge Traces

### Example 79.6: Chemical Reaction Response

This example shows how you can use lack-of-fit tests with the REG procedure. See the section “[Testing for Lack of Fit](#)” on page 6733 for details about lack-of-fit tests.

In a study of the percentage of raw material that responds in a reaction, researchers identified the following five factors:

- the feed rate of the chemicals (FeedRate), ranging from 10 to 15 liters per minute
- the percentage of the catalyst (Catalyst), ranging from 1% to 2%
- the agitation rate of the reactor (AgitRate), ranging from 100 to 120 revolutions per minute
- the temperature (Temperature), ranging from 140 to 180 degrees Celsius
- the concentration (Concentration), ranging from 3% to 6%

The following data set contains the results of an experiment designed to estimate main effects for all factors:

```

data reaction;
 input FeedRate Catalyst AgitRate Temperature
 Concentration ReactionPercentage;
 datalines;
10.0 1.0 100 140 6.0 37.5
10.0 1.0 120 180 3.0 28.5
10.0 2.0 100 180 3.0 40.4
10.0 2.0 120 140 6.0 48.2
15.0 1.0 100 180 6.0 50.7
15.0 1.0 120 140 3.0 28.9
15.0 2.0 100 140 3.0 43.5
15.0 2.0 120 180 6.0 64.5
12.5 1.5 110 160 4.5 39.0
12.5 1.5 110 160 4.5 40.3
12.5 1.5 110 160 4.5 38.7
12.5 1.5 110 160 4.5 39.7
;

```

The first eight runs of this experiment enable orthogonal estimation of the main effects for all factors. The last four comprise four replicates of the centerpoint.

The following statements fit a linear model. Because this experiment includes replications, you can test for lack of fit by using the LACKFIT option in the MODEL statement.

```

proc reg data=reaction;
 model ReactionPercentage=FeedRate Catalyst AgitRate
 Temperature Concentration / lackfit;
run;

```

Output 79.6.1 shows that the lack of fit for the linear model is significant, indicating that a more complex model is required. Models that include interactions should be investigated. In this case, this will require additional experimentation to obtain appropriate data for estimating the effects.

**Output 79.6.1** Analysis of Variance

| The REG Procedure                      |    |                |             |         |        |
|----------------------------------------|----|----------------|-------------|---------|--------|
| Model: MODEL1                          |    |                |             |         |        |
| Dependent Variable: ReactionPercentage |    |                |             |         |        |
| Analysis of Variance                   |    |                |             |         |        |
| Source                                 | DF | Sum of Squares | Mean Square | F Value | Pr > F |
| Model                                  | 5  | 990.27000      | 198.05400   | 33.29   | 0.0003 |
| Error                                  | 6  | 35.69917       | 5.94986     |         |        |
| Lack of Fit                            | 3  | 34.15167       | 11.38389    | 22.07   | 0.0151 |
| Pure Error                             | 3  | 1.54750        | 0.51583     |         |        |
| Corrected Total                        | 11 | 1025.96917     |             |         |        |
| Root MSE                               |    | 2.43923        | R-Square    | 0.9652  |        |
| Dependent Mean                         |    | 41.65833       | Adj R-Sq    | 0.9362  |        |
| Coeff Var                              |    | 5.85533        |             |         |        |



---

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# Chapter 80

## The ROBUSTREG Procedure

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## Overview: ROBUSTREG Procedure

The main purpose of robust regression is to detect outliers and provide resistant (stable) results in the presence of outliers. In order to achieve this stability, robust regression limits the influence of outliers. Historically, three classes of problems have been addressed with robust regression techniques:

- problems with outliers in the  $y$ -direction (response direction)
- problems with multivariate outliers in the  $x$ -space (that is, outliers in the covariate space, which are also referred to as leverage points)
- problems with outliers in both the  $y$ -direction and the  $x$ -space

Many methods have been developed in response to these problems. However, in statistical applications of outlier detection and robust regression, the methods most commonly used today are Huber M estimation, high breakdown value estimation, and combinations of these two methods. The ROBUSTREG procedure provides four such methods: M estimation, LTS estimation, S estimation, and MM estimation.

- M estimation was introduced by Huber (1973), and it is the simplest approach both computationally and theoretically. Although it is not robust with respect to leverage points, it is still used extensively in data analysis when contamination can be assumed to be mainly in the response direction.
- Least trimmed squares (LTS) estimation is a high breakdown value method introduced by Rousseeuw (1984). The breakdown value is a measure of the proportion of contamination that an estimation method can withstand and still maintain its robustness. The performance of this method was improved by the FAST-LTS algorithm of Rousseeuw and Van Driessen (2000).
- S estimation is a high breakdown value method introduced by Rousseeuw and Yohai (1984). With the same breakdown value, it has a higher statistical efficiency than LTS estimation.
- MM estimation, introduced by Yohai (1987), combines high breakdown value estimation and M estimation. It has both the high breakdown property and a higher statistical efficiency than S estimation.

---

## Features

The main features of the ROBUSTREG procedure are as follows:

- offers four estimation methods: M, LTS, S, and MM
- provides 10 weight functions for M estimation
- provides robust R-square and deviance for all estimates
- provides asymptotic covariance and confidence intervals for regression parameter with the M, S, and MM methods

- provides robust Wald and F tests for regression parameters with the M and MM methods
- provides Mahalanobis distance and robust Mahalanobis distance with generalized minimum covariance determinant (MCD) algorithm
- provides outlier and leverage-point diagnostics
- supports parallel computing for S and LTS estimates
- supports constructed effects including spline and multimember effects
- produces fit plots and diagnostic plots by using ODS Graphics

---

## Getting Started: ROBUSTREG Procedure

The following examples demonstrate how you can use the ROBUSTREG procedure to fit a linear regression model and obtain outlier and leverage-point diagnostics.

---

### M Estimation

This example shows how you can use the ROBUSTREG procedure to do M estimation, which is a commonly used method for outlier detection and robust regression when contamination is mainly in the response direction.

```

data stack;
 input x1 x2 x3 y exp $ @@;
 datalines;
80 27 89 42 e1 80 27 88 37 e2
75 25 90 37 e3 62 24 87 28 e4
62 22 87 18 e5 62 23 87 18 e6
62 24 93 19 e7 62 24 93 20 e8
58 23 87 15 e9 58 18 80 14 e10
58 18 89 14 e11 58 17 88 13 e12
58 18 82 11 e13 58 19 93 12 e14
50 18 89 8 e15 50 18 86 7 e16
50 19 72 8 e17 50 19 79 8 e18
50 20 80 9 e19 56 20 82 15 e20
70 20 91 15 e21
;

```

The data set `stack` is the well-known stack-loss data set presented by Brownlee (1965). The data describe the operation of a plant for the oxidation of ammonia to nitric acid and consist of 21 four-dimensional observations. The explanatory variables for the response stack-loss ( $y$ ) are the rate of operation ( $x_1$ ), the cooling water inlet temperature ( $x_2$ ), and the acid concentration ( $x_3$ ).

The following ROBUSTREG statements analyze the data:

```
proc robustreg data=stack;
 model y = x1 x2 x3 / diagnostics leverage;
 id exp;
 test x3;
run;
```

By default, the procedure does M estimation with the bisquare weight function, and it uses the median method for estimating the scale parameter. The MODEL statement specifies the covariate effects. The DIAGNOSTICS option requests a table for outlier diagnostics, and the LEVERAGE option adds leverage-point diagnostic results to this table for continuous covariate effects. The ID statement specifies that the variable `exp` is used to identify each observation (experiment) in this table. If the ID statement is omitted, the observation number is used to identify the observations. The TEST statement requests a test of significance for the covariate effects specified. The results of this analysis are displayed in the following figures.

**Figure 80.1** Model Fitting Information and Summary Statistics

| The ROBUSTREG Procedure         |              |         |         |         |                    |        |
|---------------------------------|--------------|---------|---------|---------|--------------------|--------|
| Model Information               |              |         |         |         |                    |        |
| Data Set                        | WORK.STACK   |         |         |         |                    |        |
| Dependent Variable              | y            |         |         |         |                    |        |
| Number of Independent Variables | 3            |         |         |         |                    |        |
| Number of Observations          | 21           |         |         |         |                    |        |
| Method                          | M Estimation |         |         |         |                    |        |
| Summary Statistics              |              |         |         |         |                    |        |
| Variable                        | Q1           | Median  | Q3      | Mean    | Standard Deviation | MAD    |
| x1                              | 53.0000      | 58.0000 | 62.0000 | 60.4286 | 9.1683             | 5.9304 |
| x2                              | 18.0000      | 20.0000 | 24.0000 | 21.0952 | 3.1608             | 2.9652 |
| x3                              | 82.0000      | 87.0000 | 89.5000 | 86.2857 | 5.3586             | 4.4478 |
| y                               | 10.0000      | 15.0000 | 19.5000 | 17.5238 | 10.1716            | 5.9304 |

Figure 80.1 displays the model fitting information and summary statistics for the response variable and the continuous covariates. The columns labeled Q1, Median, and Q3 provide the lower quantile, median, and upper quantile, respectively. The column labeled MAD provides a robust estimate of the univariate scale, which is computed as the standardized median absolute deviation (MAD). See Huber (1981, p. 108) for more details about the standardized MAD. The columns labeled Mean and Standard Deviation provide the usual mean and standard deviation. A large difference between the standard deviation and the MAD for a variable indicates some extreme values for this variable. In the stack-loss data, the stack-loss (response `y`) has the biggest difference between the standard deviation and the MAD.

**Figure 80.2** Model Parameter Estimates

| Parameter Estimates |    |          |                |                       |          |            |            |
|---------------------|----|----------|----------------|-----------------------|----------|------------|------------|
| Parameter           | DF | Estimate | Standard Error | 95% Confidence Limits |          | Chi-Square | Pr > ChiSq |
| Intercept           | 1  | -42.2854 | 9.5045         | -60.9138              | -23.6569 | 19.79      | <.0001     |
| x1                  | 1  | 0.9276   | 0.1077         | 0.7164                | 1.1387   | 74.11      | <.0001     |
| x2                  | 1  | 0.6507   | 0.2940         | 0.0744                | 1.2270   | 4.90       | 0.0269     |
| x3                  | 1  | -0.1123  | 0.1249         | -0.3571               | 0.1324   | 0.81       | 0.3683     |
| Scale               | 1  | 2.2819   |                |                       |          |            |            |

Figure 80.2 displays the table of robust parameter estimates, standard errors, and confidence limits. The row labeled Scale provides a point estimate of the scale parameter in the linear regression model, which is obtained by the median method. See the section “M Estimation” on page 6838 for more information about scale estimation methods. For the stack-loss data, M estimation yields the fitted linear model:

$$\hat{y} = -42.2845 + 0.9276x_1 + 0.6507x_2 - 0.1123x_3$$

**Figure 80.3** Diagnostics

| Diagnostics |     |                      |                     |          |                              |         |
|-------------|-----|----------------------|---------------------|----------|------------------------------|---------|
| Obs         | exp | Mahalanobis Distance | Robust MCD Distance | Leverage | Standardized Robust Residual | Outlier |
| 1           | e1  | 2.2536               | 5.5284              | *        | 1.0995                       |         |
| 2           | e2  | 2.3247               | 5.6374              | *        | -1.1409                      |         |
| 3           | e3  | 1.5937               | 4.1972              | *        | 1.5604                       |         |
| 4           | e4  | 1.2719               | 1.5887              |          | 3.0381                       | *       |
| 21          | e21 | 2.1768               | 3.6573              | *        | -4.5733                      | *       |

Figure 80.3 displays outlier and leverage-point diagnostics. Standardized robust residuals are computed based on the estimated parameters. Both the Mahalanobis distance and the robust MCD distance are displayed. Outliers and leverage points, identified with asterisks, are defined by the standardized robust residuals and robust MCD distances that exceed the corresponding cutoff values displayed in the diagnostics summary. Observations 4 and 21 are outliers because their standardized robust residuals exceed the cutoff value in absolute value. The procedure detects four observations with high leverage. Leverage points (points with high leverage) with smaller standardized robust residuals than the cutoff value in absolute value are called good leverage points; others are called bad leverage points. Observation 21 is a bad leverage point.

Two particularly useful plots for revealing outliers and leverage points are a scatter plot of the standardized robust residuals against the robust distances (RD PLOT) and a scatter plot of the robust distances against the classical Mahalanobis distances (DD PLOT).



For the stack-loss data, the following statements produce the RDPLLOT in Figure 80.4 and the DDPLLOT in Figure 80.5. The histogram and the normal quantile-quantile plots (shown in Figure 80.6 and Figure 80.7, respectively) for the standardized robust residuals are also created with the HISTOGRAM and QQPLOT suboptions of the PLOTS= option.

```
ods graphics on;

proc robustreg data=stack plots=(rdplot ddplot histogram qqplot);
 model y = x1 x2 x3;
run;

ods graphics off;
```

These plots are helpful in identifying outliers in addition to good and bad high leverage points.

These plots are requested when ODS Graphics is enabled by specifying the PLOTS= option in the PROC ROBUSTREG statement. For general information about ODS Graphics, see Chapter 21, “Statistical Graphics Using ODS.” For specific information about the graphics available in the ROBUSTREG procedure, see the section “ODS Graphics” on page 6865.

**Figure 80.4** RDPLLOT for Stackloss Data

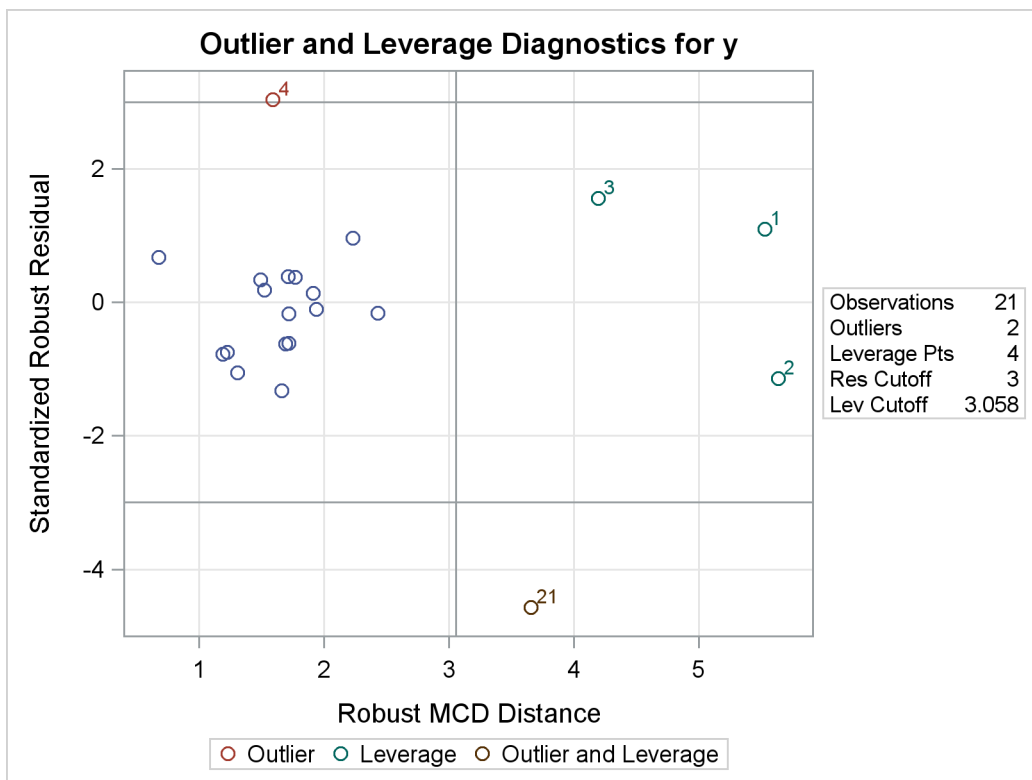


Figure 80.5 DDPLOT for Stackloss Data

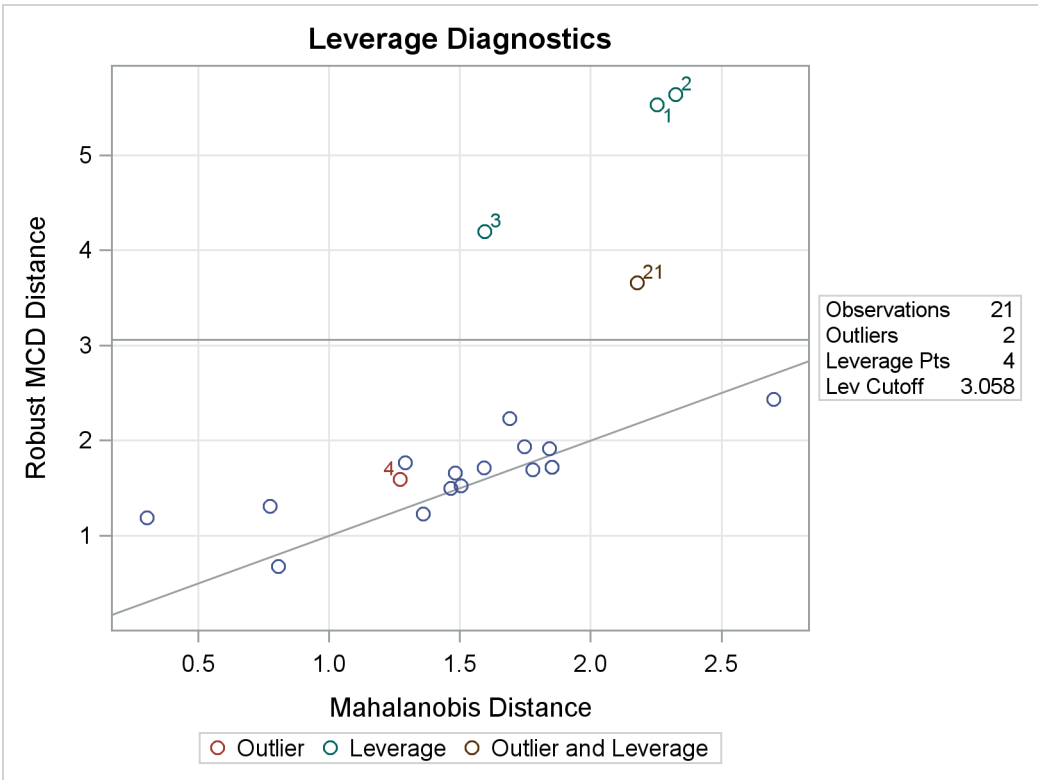


Figure 80.6 Histogram

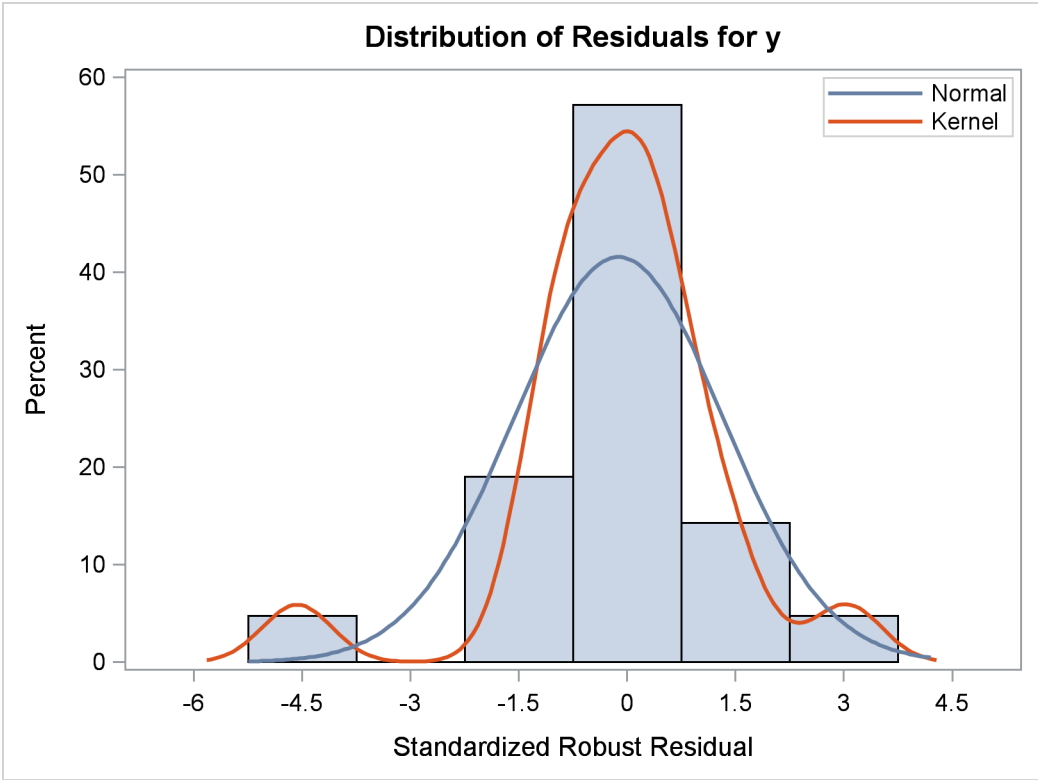


Figure 80.7 Q-Q Plot

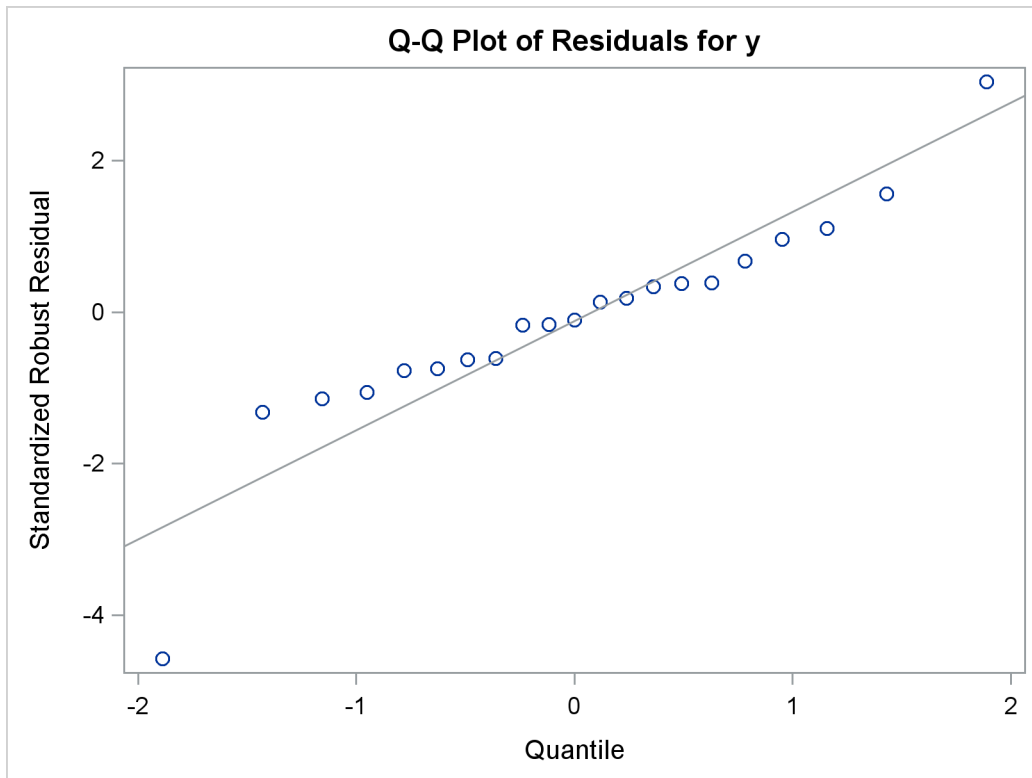


Figure 80.8 displays robust versions of goodness-of-fit statistics for the model. You can use the robust information criteria, AICR and BICR, for model selection and comparison. For both AICR and BICR, the lower the value, the more desirable the model.

Figure 80.8 Goodness-of-Fit Statistics

| Goodness-of-Fit |          |
|-----------------|----------|
| Statistic       | Value    |
| R-Square        | 0.6659   |
| AICR            | 29.5231  |
| BICR            | 36.3361  |
| Deviance        | 125.7905 |

Figure 80.9 displays the test results requested by the TEST statement. The ROBUSTREG procedure conducts two robust linear tests, the  $\rho$  test and the  $R_n^2$  test. See the section “Linear Tests” on page 6844 for information about how the procedure computes test statistics and the correction factor lambda. Due to the large  $p$ -values for both tests, you can conclude that the effect x3 is not significant at the 5% level.

**Figure 80.9** Test of Significance

| Robust Linear Test |                   |        |    |                |            |
|--------------------|-------------------|--------|----|----------------|------------|
| Test               | Test<br>Statistic | Lambda | DF | Chi-<br>Square | Pr > ChiSq |
| Rho                | 0.9378            | 0.7977 | 1  | 1.18           | 0.2782     |
| Rn2                | 0.8092            |        | 1  | 0.81           | 0.3683     |

For the bisquare weight function, the default tuning constant,  $c = 4.685$ , is chosen to yield a 95% asymptotic efficiency of the M estimates with the Gaussian distribution. See the section “M Estimation” on page 6838 for details. The smaller the constant  $c$ , the lower the asymptotic efficiency but the sharper the M estimate as an outlier detector. For the stack-loss data set, you could consider using a sharper outlier detector.

In the following PROC ROBUSTREG step, a smaller constant,  $c = 3.5$ , is used. This tuning constant corresponds to an efficiency close to 85%. See Chen and Yin (2002) for the relationship between the tuning constant and asymptotic efficiency of M estimates.

```
proc robustreg method=m(wf=bisquare(c=3.5)) data=stack;
 model y = x1 x2 x3 / diagnostics leverage;
 id exp;
 test x3;
run;
```

Figure 80.10 displays the table of robust parameter estimates, standard errors, and confidence limits with the constant  $c = 3.5$ .

The refitted linear model is

$$\hat{y} = -37.1076 + 0.8191x_1 + 0.5173x_2 - 0.0728x_3$$

**Figure 80.10** Model Parameter Estimates

| The ROBUSTREG Procedure |    |          |                   |                          |          |                |            |
|-------------------------|----|----------|-------------------|--------------------------|----------|----------------|------------|
| Parameter Estimates     |    |          |                   |                          |          |                |            |
| Parameter               | DF | Estimate | Standard<br>Error | 95% Confidence<br>Limits |          | Chi-<br>Square | Pr > ChiSq |
| Intercept               | 1  | -37.1076 | 5.4731            | -47.8346                 | -26.3805 | 45.97          | <.0001     |
| x1                      | 1  | 0.8191   | 0.0620            | 0.6975                   | 0.9407   | 174.28         | <.0001     |
| x2                      | 1  | 0.5173   | 0.1693            | 0.1855                   | 0.8492   | 9.33           | 0.0022     |
| x3                      | 1  | -0.0728  | 0.0719            | -0.2138                  | 0.0681   | 1.03           | 0.3111     |
| Scale                   | 1  | 1.4265   |                   |                          |          |                |            |

Figure 80.11 displays outlier and leverage-point diagnostics with the constant  $c = 3.5$ . Besides observations 4 and 21, observations 1 and 3 are also detected as outliers.

Figure 80.11 Diagnostics

| Diagnostics |     |                         |                           |          |                                    |         |
|-------------|-----|-------------------------|---------------------------|----------|------------------------------------|---------|
| Obs         | exp | Mahalanobis<br>Distance | Robust<br>MCD<br>Distance | Leverage | Standardized<br>Robust<br>Residual | Outlier |
| 1           | e1  | 2.2536                  | 5.5284                    | *        | 4.2719                             | *       |
| 2           | e2  | 2.3247                  | 5.6374                    | *        | 0.7158                             |         |
| 3           | e3  | 1.5937                  | 4.1972                    | *        | 4.4142                             | *       |
| 4           | e4  | 1.2719                  | 1.5887                    |          | 5.7792                             | *       |
| 21          | e21 | 2.1768                  | 3.6573                    | *        | -6.2727                            | *       |

## LTS Estimation

If the data are contaminated in the  $x$ -space, M estimation does not do well. The following example shows how you can use LTS estimation to deal with this situation.

```
data hbk;
 input index $ x1 x2 x3 y @@;
 datalines;
 1 10.1 19.6 28.3 9.7 2 9.5 20.5 28.9 10.1
 3 10.7 20.2 31.0 10.3 4 9.9 21.5 31.7 9.5
 5 10.3 21.1 31.1 10.0 6 10.8 20.4 29.2 10.0
 7 10.5 20.9 29.1 10.8 8 9.9 19.6 28.8 10.3
 9 9.7 20.7 31.0 9.6 10 9.3 19.7 30.3 9.9
 11 11.0 24.0 35.0 -0.2 12 12.0 23.0 37.0 -0.4
 13 12.0 26.0 34.0 0.7 14 11.0 34.0 34.0 0.1
 15 3.4 2.9 2.1 -0.4 16 3.1 2.2 0.3 0.6
 17 0.0 1.6 0.2 -0.2 18 2.3 1.6 2.0 0.0
 19 0.8 2.9 1.6 0.1 20 3.1 3.4 2.2 0.4
 21 2.6 2.2 1.9 0.9 22 0.4 3.2 1.9 0.3
 23 2.0 2.3 0.8 -0.8 24 1.3 2.3 0.5 0.7
 25 1.0 0.0 0.4 -0.3 26 0.9 3.3 2.5 -0.8
 27 3.3 2.5 2.9 -0.7 28 1.8 0.8 2.0 0.3
 29 1.2 0.9 0.8 0.3 30 1.2 0.7 3.4 -0.3
 31 3.1 1.4 1.0 0.0 32 0.5 2.4 0.3 -0.4
 33 1.5 3.1 1.5 -0.6 34 0.4 0.0 0.7 -0.7
 35 3.1 2.4 3.0 0.3 36 1.1 2.2 2.7 -1.0
 37 0.1 3.0 2.6 -0.6 38 1.5 1.2 0.2 0.9
 39 2.1 0.0 1.2 -0.7 40 0.5 2.0 1.2 -0.5
 41 3.4 1.6 2.9 -0.1 42 0.3 1.0 2.7 -0.7
 43 0.1 3.3 0.9 0.6 44 1.8 0.5 3.2 -0.7
 45 1.9 0.1 0.6 -0.5 46 1.8 0.5 3.0 -0.4
 47 3.0 0.1 0.8 -0.9 48 3.1 1.6 3.0 0.1
 49 3.1 2.5 1.9 0.9 50 2.1 2.8 2.9 -0.4
```

|    |     |     |     |      |    |     |     |     |      |
|----|-----|-----|-----|------|----|-----|-----|-----|------|
| 51 | 2.3 | 1.5 | 0.4 | 0.7  | 52 | 3.3 | 0.6 | 1.2 | -0.5 |
| 53 | 0.3 | 0.4 | 3.3 | 0.7  | 54 | 1.1 | 3.0 | 0.3 | 0.7  |
| 55 | 0.5 | 2.4 | 0.9 | 0.0  | 56 | 1.8 | 3.2 | 0.9 | 0.1  |
| 57 | 1.8 | 0.7 | 0.7 | 0.7  | 58 | 2.4 | 3.4 | 1.5 | -0.1 |
| 59 | 1.6 | 2.1 | 3.0 | -0.3 | 60 | 0.3 | 1.5 | 3.3 | -0.9 |
| 61 | 0.4 | 3.4 | 3.0 | -0.3 | 62 | 0.9 | 0.1 | 0.3 | 0.6  |
| 63 | 1.1 | 2.7 | 0.2 | -0.3 | 64 | 2.8 | 3.0 | 2.9 | -0.5 |
| 65 | 2.0 | 0.7 | 2.7 | 0.6  | 66 | 0.2 | 1.8 | 0.8 | -0.9 |
| 67 | 1.6 | 2.0 | 1.2 | -0.7 | 68 | 0.1 | 0.0 | 1.1 | 0.6  |
| 69 | 2.0 | 0.6 | 0.3 | 0.2  | 70 | 1.0 | 2.2 | 2.9 | 0.7  |
| 71 | 2.2 | 2.5 | 2.3 | 0.2  | 72 | 0.6 | 2.0 | 1.5 | -0.2 |
| 73 | 0.3 | 1.7 | 2.2 | 0.4  | 74 | 0.0 | 2.2 | 1.6 | -0.9 |
| 75 | 0.3 | 0.4 | 2.6 | 0.2  |    |     |     |     |      |

;

The data set hbk is an artificial data set generated by Hawkins, Bradu, and Kass (1984). Both ordinary least squares (OLS) estimation and M estimation (not shown here) suggest that observations 11 to 14 are outliers. However, these four observations were generated from the underlying model, whereas observations 1 to 10 were contaminated. The reason that OLS estimation and M estimation do not pick up the contaminated observations is that they cannot distinguish good leverage points (observations 11 to 14) from bad leverage points (observations 1 to 10). In such cases, the LTS method identifies the true outliers.

The following statements invoke the ROBUSTREG procedure with the LTS estimation method:

```
proc robustreg data=hbk fwls method=lts;
 model y = x1 x2 x3 / diagnostics leverage;
 id index;
run;
```

Figure 80.12 displays the model fitting information and summary statistics for the response variable and independent covariates.

**Figure 80.12** Model Fitting Information and Summary Statistics

| The ROBUSTREG Procedure         |                |        |        |        |                    |        |
|---------------------------------|----------------|--------|--------|--------|--------------------|--------|
| Model Information               |                |        |        |        |                    |        |
| Data Set                        | WORK.HBK       |        |        |        |                    |        |
| Dependent Variable              | y              |        |        |        |                    |        |
| Number of Independent Variables | 3              |        |        |        |                    |        |
| Number of Observations          | 75             |        |        |        |                    |        |
| Method                          | LTS Estimation |        |        |        |                    |        |
| Summary Statistics              |                |        |        |        |                    |        |
| Variable                        | Q1             | Median | Q3     | Mean   | Standard Deviation | MAD    |
| x1                              | 0.8000         | 1.8000 | 3.1000 | 3.2067 | 3.6526             | 1.9274 |
| x2                              | 1.0000         | 2.2000 | 3.3000 | 5.5973 | 8.2391             | 1.6309 |
| x3                              | 0.9000         | 2.1000 | 3.0000 | 7.2307 | 11.7403            | 1.7791 |
| y                               | -0.5000        | 0.1000 | 0.7000 | 1.2787 | 3.4928             | 0.8896 |

Figure 80.13 displays information about the LTS fit, which includes the breakdown value of the LTS estimate. The breakdown value is a measure of the proportion of contamination that an estimation method can withstand and still maintain its robustness. In this example the LTS estimate minimizes the sum of 57 smallest squares of residuals. It can still estimate the true underlying model if the remaining 18 observations are contaminated. This corresponds to the breakdown value around 0.25, which is set as the default.

**Figure 80.13** LTS Profile

| LTS Profile                      |        |
|----------------------------------|--------|
| Total Number of Observations     | 75     |
| Number of Squares Minimized      | 57     |
| Number of Coefficients           | 4      |
| Highest Possible Breakdown Value | 0.2533 |

Figure 80.14 displays parameter estimates for covariates and scale. Two robust estimates of the scale parameter are displayed. See the section “Final Weighted Scale Estimator” on page 6847 for how these estimates are computed. The weighted scale estimator (Wscale) is a more efficient estimator of the scale parameter.

**Figure 80.14** LTS Parameter Estimates

| LTS Parameter Estimates |    |          |
|-------------------------|----|----------|
| Parameter               | DF | Estimate |
| Intercept               | 1  | -0.3431  |
| x1                      | 1  | 0.0901   |
| x2                      | 1  | 0.0703   |
| x3                      | 1  | -0.0731  |
| Scale (sLTS)            | 0  | 0.7451   |
| Scale (Wscale)          | 0  | 0.5749   |

Figure 80.15 displays outlier and leverage-point diagnostics. The ID variable index is used to identify the observations. If you do not specify this ID variable, the observation number is used to identify the observations. However, the observation number depends on how the data are read. The first 10 observations are identified as outliers, and observations 11 to 14 are identified as good leverage points.

**Figure 80.15** Diagnostics

| Diagnostics |       |                         |                 |          |                                    |         |
|-------------|-------|-------------------------|-----------------|----------|------------------------------------|---------|
| Obs         | index | Mahalanobis<br>Distance | Robust          |          | Standardized<br>Robust<br>Residual | Outlier |
|             |       |                         | MCD<br>Distance | Leverage |                                    |         |
| 1           | 1     | 1.9168                  | 29.4424         | *        | 17.0868                            | *       |
| 2           | 2     | 1.8558                  | 30.2054         | *        | 17.8428                            | *       |
| 3           | 3     | 2.3137                  | 31.8909         | *        | 18.3063                            | *       |
| 4           | 4     | 2.2297                  | 32.8621         | *        | 16.9702                            | *       |
| 5           | 5     | 2.1001                  | 32.2778         | *        | 17.7498                            | *       |
| 6           | 6     | 2.1462                  | 30.5892         | *        | 17.5155                            | *       |
| 7           | 7     | 2.0105                  | 30.6807         | *        | 18.8801                            | *       |
| 8           | 8     | 1.9193                  | 29.7994         | *        | 18.2253                            | *       |
| 9           | 9     | 2.2212                  | 31.9537         | *        | 17.1843                            | *       |
| 10          | 10    | 2.3335                  | 30.9429         | *        | 17.8021                            | *       |
| 11          | 11    | 2.4465                  | 36.6384         | *        | 0.0406                             |         |
| 12          | 12    | 3.1083                  | 37.9552         | *        | -0.0874                            |         |
| 13          | 13    | 2.6624                  | 36.9175         | *        | 1.0776                             |         |
| 14          | 14    | 6.3816                  | 41.0914         | *        | -0.7875                            |         |

Figure 80.16 displays the final weighted least squares estimates. These estimates are least squares estimates computed after deleting the detected outliers.

**Figure 80.16** Final Weighted LS Estimates

| Parameter Estimates for Final Weighted Least Squares Fit |    |          |                   |                          |        |                     |        |
|----------------------------------------------------------|----|----------|-------------------|--------------------------|--------|---------------------|--------|
| Parameter                                                | DF | Estimate | Standard<br>Error | 95% Confidence<br>Limits |        | Chi-<br>Square Pr > | ChiSq  |
| Intercept                                                | 1  | -0.1805  | 0.1044            | -0.3852                  | 0.0242 | 2.99                | 0.0840 |
| x1                                                       | 1  | 0.0814   | 0.0667            | -0.0493                  | 0.2120 | 1.49                | 0.2222 |
| x2                                                       | 1  | 0.0399   | 0.0405            | -0.0394                  | 0.1192 | 0.97                | 0.3242 |
| x3                                                       | 1  | -0.0517  | 0.0354            | -0.1210                  | 0.0177 | 2.13                | 0.1441 |
| Scale                                                    | 0  | 0.5572   |                   |                          |        |                     |        |



## Syntax: ROBUSTREG Procedure

The following statements are available in the ROBUSTREG procedure:

```

PROC ROBUSTREG < options > ;
 BY variables ;
 CLASS variables ;
 EFFECT name=effect-type(variables < / options >) ;
 ID variables ;
 MODEL response = < effects > < / options > ;
 OUTPUT < OUT=SAS-data-set > keyword=name < . . . keyword=name > ;
 PERFORMANCE < options > ;
 TEST effects ;
 WEIGHT variable ;

```

The PROC ROBUSTREG statement invokes the procedure. The METHOD= option in the PROC ROBUSTREG statement selects one of the four estimation methods, M, LTS, S, and MM. By default, Huber M estimation is used. The MODEL statement is required and specifies the variables used in the regression. Main effects and interaction terms can be specified in the MODEL statement, as in the GLM procedure (Chapter 42, “The GLM Procedure.”) The CLASS statement specifies which explanatory variables are treated as categorical. The ID statement names variables to identify observations in the outlier diagnostics tables. The WEIGHT statement identifies a variable in the input data set whose values are used to weight the observations. The OUTPUT statement creates an output data set that contains final weights, predicted values, and residuals. The TEST statement requests robust linear tests for the model parameters. The PERFORMANCE statement tunes the performance of the procedure by using single or multiple processors available on the hardware. Multiple OUTPUT and TEST statements are permitted.

## PROC ROBUSTREG Statement

```

PROC ROBUSTREG < options > ;

```

The PROC ROBUSTREG statement invokes the ROBUSTREG procedure. Table 80.1 summarizes the options available in the PROC ROBUSTREG statement.

**Table 80.1** PROC ROBUSTREG Statement Options

| Option   | Description                                                                           |
|----------|---------------------------------------------------------------------------------------|
| COVOUT   | Saves the estimated covariance matrix                                                 |
| DATA=    | Specifies the input SAS data set                                                      |
| FWLS     | Computes the final weighted least squares estimates                                   |
| INEST=   | Specifies an input SAS data set that contains initial estimates                       |
| ITPRINT  | Displays the iteration history for the iteratively reweighted least squares algorithm |
| METHOD=  | Specifies the estimation method                                                       |
| NAMELEN= | Specifies the length of effect names                                                  |
| ORDER=   | Specifies the order in which to sort classification variables                         |
| OUTEST=  | Specifies an output SAS data set that contains the parameter estimates                |

Table 80.1 *continued*

| Option | Description                                         |
|--------|-----------------------------------------------------|
| PLOT   | Specifies options that control details of the plots |
| SEED=  | Specifies the seed for the random number generator  |

You can specify the following *options* in the PROC ROBUSTREG statement.

**COVOUT**

saves the estimated covariance matrix in the OUTEST= data set. This option is not supported for LTS estimation.

**DATA=SAS-data-set**

specifies the input SAS data set used by PROC ROBUSTREG. By default, the most recently created SAS data set is used.

**FWLS**

computes the final weighted least squares estimates. These estimates are equivalent to the least squares estimates after the detected outliers are deleted.

**INEST=SAS-data-set**

specifies an input SAS data set that contains initial estimates for all the parameters in the model. See the section “[INEST= Data Set](#)” on page 6861 for a detailed description of the contents of the INEST= data set.

**ITPRINT**

displays the iteration history for the iteratively reweighted least squares algorithm used by M and MM estimation. You can also use this option in the MODEL statement.

**NAMELEN=*n***

specifies the length of effect names in tables and output data sets to be *n* characters, where *n* is a value between 20 and 200. The default length is 20 characters.

**ORDER=DATA | FORMATTED | FREQ | INTERNAL**

specifies the sort order for the levels of the classification variables (which are specified in the CLASS statement). This option applies to the levels for all classification variables, except when you use the (default) ORDER=FORMATTED option with numeric classification variables that have no explicit format. With this option, the levels of such variables are ordered by their internal value.

The ORDER= option can take the following values:

| Value of ORDER= | Levels Sorted By                                                                                                                       |
|-----------------|----------------------------------------------------------------------------------------------------------------------------------------|
| DATA            | Order of appearance in the input data set                                                                                              |
| FORMATTED       | External formatted value, except for numeric variables with no explicit format, which are sorted by their unformatted (internal) value |
| FREQ            | Descending frequency count; levels with the most observations come first in the order                                                  |
| INTERNAL        | Unformatted value                                                                                                                      |

By default, ORDER=FORMATTED. For ORDER=FORMATTED and ORDER=INTERNAL, the sort order is machine-dependent. For more information about sort order, see the chapter on the SORT procedure in the *Base SAS Procedures Guide* and the discussion of BY-group processing in *SAS Language Reference: Concepts*.

**OUTEST=SAS-data-set**

specifies an output SAS data set that contains the parameter estimates, and, if the COVOUT option is specified, the estimated covariance matrix. See the section “OUTEST= Data Set” on page 6862 for a detailed description of the contents of the OUTEST= data set.

**PLOT | PLOTS** <(global-plot-options)> <=plot-request >

**PLOT | PLOTS** <(global-plot-options)> <=(plot-request < ...plot-request > )>

specifies options that control details of the plots. If ODS Graphics is enabled but you do not specify the PLOTS= option, then PROC ROBUSTREG produces the robust fit plot by default when the model includes a single continuous independent variable.

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;
proc robustreg data=stack plots=all;
 model y = x1 x2 x3;
run;
ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The *global-plot-options* apply to all plots generated by the ROBUSTREG procedure. The following *global-plot-option* is available:

**ONLY**

suppresses the default robust fit plot. Only plots specifically requested are displayed.

You can specify more than one *plot-request* within the parentheses after PLOTS=. For a single plot request, you can omit the parentheses. The following *plot-requests* are available.

**ALL**

creates all appropriate plots.

**DDPLOT** <(LABEL=ALL | LEVERAGE | NONE | OUTLIER)>

creates a plot of robust distance against Mahalanobis distance. See the section “Leverage Point and Outlier Detection” on page 6860 for details about robust distance. The LABEL= option specifies how the points on this plot are to be labeled, as summarized by the following table.

**Table 80.2** Options for Label

| Value of LABEL= | Label Method          |
|-----------------|-----------------------|
| ALL             | Label all points      |
| LEVERAGE        | Label leverage points |
| NONE            | No labels             |
| OUTLIERS        | Label outliers        |

By default, the ROBUSTREG procedure labels both outliers and leverage points.

If you specify ID variables in the ID statement, the values of the first ID variable are used as labels; otherwise, observation numbers are used as labels.

**FITPLOT <(NOLIMITS)>**

creates a plot of robust fit against the single independent continuous variable specified in the model. You can request this plot when only a single independent continuous variable is specified in the model. Confidence limits are added on the plot by default. The NOLIMITS option suppresses these limits.

**HISTOGRAM**

creates a histogram for the standardized robust residuals. The histogram is superimposed with a normal density curve and a kernel density curve.

**NONE**

suppresses all plots.

**QQPLOT**

creates the normal quantile-quantile plot for the standardized robust residuals.

**RD PLOT <(LABEL=ALL | LEVERAGE | NONE | OUTLIER)>**

creates the plot of standardized robust residual against robust distance. See the section “[Leverage Point and Outlier Detection](#)” on page 6860 for details about robust distance. The LABEL= option specifies a label method for points on this plot. These label methods are described in [Table 80.2](#).

If you specify ID variables in the ID statement, the values of the first ID variable are used as labels; otherwise, observation numbers are used as labels.

**SEED=number**

specifies the seed for the random number generator used to randomly select the subgroups and subsets for LTS and S estimation. By default or if you specify zero, the ROBUSTREG procedure generates a random seed.

**METHOD=method-type <(options)>**

specifies the estimation method and some additional *options* for the estimation method. PROC ROBUSTREG provides four estimation methods: M estimation, LTS estimation, S estimation, and MM estimation. The default method is M estimation.

**NOTE:** Since the LTS and S methods use subsampling algorithms, these methods are not suitable in an analysis with variables that have only a few unequal values or a few unequal values within one BY group. For example, indicator variables that correspond to a classification variable often fall into this type. The same issue also applies to the initial LTS and S estimates in the MM method. In case of a model that includes classification independent variables or continuous independent variables with a few unequal values, the M method is recommended.

## Options with METHOD=M

With METHOD=M <(options)>, you can specify the following *options*:

### ASYMPCOV=H1 | H2 | H3

specifies the type of asymptotic covariance computed for the M estimate. The three types are described in the section “Asymptotic Covariance and Confidence Intervals” on page 6843. By default, ASYMPCOV= H1.

### CONVERGENCE=criterion <(EPS=value)>

specifies a convergence criterion for the M estimate. The three criteria listed in the following table are available.

**Table 80.3** Options to Specify Convergence Criteria

| Type        | Option             |
|-------------|--------------------|
| Coefficient | CONVERGENCE=COEF   |
| Residual    | CONVERGENCE=RESID  |
| Weight      | CONVERGENCE=WEIGHT |

By default, CONVERGENCE=COEF. You can specify the precision of the convergence criterion with the EPS= option. By default, EPS=1E-8.

### MAXITER=*n*

sets the maximum number of iterations during the parameter estimation. By default, MAXITER=1000.

### SCALE=scale-type | value

specifies the scale parameter or a method for estimating the scale parameter. These methods and options are summarized in the following table.

**Table 80.4** Options to Specify Scale

| Scale           | Option              | Default <i>d</i> |
|-----------------|---------------------|------------------|
| Fixed constant  | SCALE=value         |                  |
| Huber estimate  | SCALE=HUBER <(D=d)> | 2.5              |
| Median estimate | SCALE=MED           |                  |
| Tukey estimate  | SCALE=TUKEY <(D=d)> | 2.5              |

By default, SCALE=MED.

### WEIGHTFUNCTION=function-type

#### WF=function-type

specifies the weight function used for the M estimate. The ROBUSTREG procedure provides 10 weight functions, which are listed in the following table. You can specify the parameters in these functions with the A=, B=, and C= options. These functions are described in the section “M Estimation” on page 6838. The default weight function is bisquare.

**Table 80.5** Options to Specify Weight Functions

| Weight Function | Option                          | Default <i>a, b, c</i> |
|-----------------|---------------------------------|------------------------|
| Andrews         | WF=ANDREWS <(C=c)>              | 1.339                  |
| Bisquare        | WF=BISQUARE <(C=c)>             | 4.685                  |
| Cauchy          | WF=CAUCHY <(C=c)>               | 2.385                  |
| Fair            | WF=FAIR <(C=c)>                 | 1.4                    |
| Hampel          | WF=HAMPEL <(<A=a> <B=b> <C=c>)> | 2, 4, 8                |
| Huber           | WF=HUBER <(C=c)>                | 1.345                  |
| Logistic        | WF=LOGISTIC <(C=c)>             | 1.205                  |
| Median          | WF=MEDIAN <(C=c)>               | 0.01                   |
| Talworth        | WF=TALWORTH <(C=c)>             | 2.795                  |
| Welsch          | WF=WELSCH <(C=c)>               | 2.985                  |

### Options with METHOD=LTS

With METHOD=LTS <(options)>, you can specify the following options:

#### **CSTEP=n**

specifies the number of concentration steps (C-steps) for the LTS estimate. See the section “LTS Estimate” on page 6845 for information about how the default value is determined.

#### **H=n**

specifies the quantile for the LTS estimate. See the section “LTS Estimate” on page 6845 for information about how the default value is determined.

#### **IADJUST=ALL | NONE**

requests (IADJUST=ALL) or suppresses (IADJUST=NONE) the intercept adjustment for all estimates in the LTS algorithm. By default, the intercept adjustment is used for data sets with fewer than 10,000 observations. See the section “Algorithm” on page 6845 for details.

#### **NBEST=n**

specifies the number of best solutions kept for each subgroup during the computation of the LTS estimate. The default number is 10, which is the maximum number allowed.

#### **NREP=n**

specifies the number of times to repeat least squares fit in subgroups during the computation of the LTS estimate. See the section “LTS Estimate” on page 6845 for information about how the default number is determined.

#### **SUBANALYSIS**

requests a display of the subgrouping information and parameter estimates within subgroups. This option generates the ODS tables shown in Table 80.6.

**Table 80.6** ODS Tables Available with SUBANALYSIS Option

| ODS Table Name   | Description                      |
|------------------|----------------------------------|
| BestEstimates    | Best final estimates for LTS     |
| BestSubEstimates | Best estimates for each subgroup |
| CStep            | C-step information for LTS       |
| Groups           | Grouping information for LTS     |

**SUBGROUPSIZE=*n***

specifies the data set size of the subgroups in the computation of the LTS estimate. The default number is 300.

**Options with METHOD=S**

With METHOD=S <(options)>, you can specify the following options:

**ASYMPCOV=H1 | H2 | H3 | H4**

specifies the type of asymptotic covariance computed for the S estimate. The four types are described in the section “Asymptotic Covariance and Confidence Intervals” on page 6849. By default, ASYMPCOV=H4.

**CHIF= TUKEY | YOHAI**

specifies the  $\chi$  function for the S estimate. PROC ROBUSTREG provides two  $\chi$  functions, Tukey’s bisquare function and Yohai’s optimal function, which you can request with CHIF=TUKEY and CHIF=YOHAJ, respectively. The default is Tukey’s bisquare function.

**EFF=*value***

specifies the efficiency (as a fraction) for the S estimate. The parameter  $k_0$  in the  $\chi$  function is determined by this efficiency. The default efficiency is determined such that the consistent S estimate has the breakdown value of 25%. This option is overwritten by the K0= option if both of them are used.

**K0=*value***

specifies the  $k_0$  parameter in the  $\chi$  function of the S estimate. For CHIF=TUKEY, the default is 1.548. For CHIF=YOHAJ, the default is 0.66. These default values correspond to a 50% breakdown value of the consistent S estimate.

**MAXITER=*n***

sets the maximum number of iterations for computing the scale parameter of the S estimate. By default, MAXITER=1000.

**NREP=*n***

specifies the number of repeats of subsampling in the computation of the S estimate. See the section “[Algorithm](#)” on page 6848 for information about how the default number of repeats is determined.

**NOREFINE**

suppresses the refinement for the S estimate. See the section “[Algorithm](#)” on page 6848 for details.

**SUBSETSIZE=*n***

specifies the size of the subset for the S estimate. See the section “[Algorithm](#)” on page 6848 for information about how the default value is determined.

**TOLERANCE=*value***

specifies the tolerance for the S estimate of the scale. The default value is 0.001.

**Options with METHOD=MM**

With METHOD=MM <(options)>, you can specify the following options:

**ASYMPCOV=H1 | H2 | H3 | H4**

specifies the type of asymptotic covariance computed for the MM estimate. The four types are described in the section “[Details: ROBUSTREG Procedure](#)” on page 6838. By default, ASYMPCOV=H4.

**BIATEST <(ALPHA=*number*)>**

requests the bias test for the final MM estimate. See the section “[Bias Test](#)” on page 6852 for details about this test.

**CHIF= TUKEY | YOHAI**

selects the  $\chi$  function for the MM estimate. PROC ROBUSTREG provides two  $\chi$  functions: Tukey’s bisquare function and Yohai’s optimal function, which you can request with CHIF=TUKEY and CHIF=YOHAJ, respectively. The default is Tukey’s bisquare function. This  $\chi$  function is also used by the initial S estimate if you specify the INITEST=S option.

**CONVERGENCE=*criterion* <(EPS=*number*)>**

specifies a convergence criterion for the MM estimate. The three criteria listed in [Table 80.7](#) are available.

**Table 80.7** Options to Specify Convergence Criteria

| Type        | Option             |
|-------------|--------------------|
| Coefficient | CONVERGENCE=COEF   |
| Residual    | CONVERGENCE=RESID  |
| Weight      | CONVERGENCE=WEIGHT |

By default, CONVERGENCE=COEF. You can specify the precision of the convergence criterion with the EPS= option. By default, EPS=1E–8.



**EFF=value**

specifies the efficiency (as a fraction) for the MM estimate. The parameter  $k_1$  in the  $\chi$  function is determined by this efficiency. The default efficiency is set to 0.85, which corresponds to  $k_1 = 3.440$  for CHIF=TUKEY or  $k_1 = 0.868$  for CHIF=YOHAI.

**INITH=h**

specifies the integer  $h$  for the initial LTS estimate used by the MM estimator. See the section “Algorithm” on page 6851 for how to specify  $h$  and how the default is determined.

**INITEST=LTS | S**

specifies the initial estimator for the MM estimator. By default, the LTS estimator with its default settings is used as the initial estimator for the MM estimator.

**K0=number**

specifies the parameter  $k_0$  in the  $\chi$  function for the MM estimate. For CHIF=TUKEY, the default is  $k_0 = 2.9366$ . For CHIF=YOHAI, the default is  $k_0 = 0.7405$ . These default values correspond to the 25% breakdown value of the MM estimator.

**MAXITER=n**

sets the maximum number of iterations during the parameter estimation. By default, MAXITER=1000.

---

## BY Statement

**BY variables ;**

You can specify a BY statement with PROC ROBUSTREG to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the ROBUSTREG procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

---

## CLASS Statement

**CLASS** *variables* < / **TRUNCATE** > ;

The CLASS statement names the classification variables to be used in the model. Typical classification variables are Treatment, Sex, Race, Group, and Replication. If you use the CLASS statement, it must appear before the MODEL statement.

Classification variables can be either character or numeric. By default, class levels are determined from the entire set of formatted values of the CLASS variables.

**NOTE:** Prior to SAS 9, class levels were determined by using no more than the first 16 characters of the formatted values. To revert to this previous behavior, you can use the TRUNCATE option in the CLASS statement.

In any case, you can use formats to group values into levels. See the discussion of the FORMAT procedure in the *Base SAS Procedures Guide* and the discussions of the FORMAT statement and SAS formats in *SAS Formats and Informats: Reference*. You can adjust the order of CLASS variable levels with the ORDER= option in the PROC ROBUSTREG statement. You can specify the following option in the CLASS statement after a slash (/):

### TRUNCATE

specifies that class levels should be determined by using only up to the first 16 characters of the formatted values of CLASS variables. When formatted values are longer than 16 characters, you can use this option to revert to the levels as determined in releases prior to SAS 9.

---

## EFFECT Statement

**EFFECT** *name=effect-type* (*variables* < / *options* > ) ;

The EFFECT statement enables you to construct special collections of columns for design matrices. These collections are referred to as *constructed effects* to distinguish them from the usual model effects that are formed from continuous or classification variables, as discussed in the section “GLM Parameterization of Classification Variables and Effects” on page 383 in Chapter 19, “Shared Concepts and Topics.”

You can specify the following *effect-types*:

|                          |                                                                                                                                                                                                           |
|--------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>COLLECTION</b>        | is a collection effect that defines one or more variables as a single effect with multiple degrees of freedom. The variables in a collection are considered as a unit for estimation and inference.       |
| <b>LAG</b>               | is a classification effect in which the level that is used for a given period corresponds to the level in the preceding period.                                                                           |
| <b>MULTIMEMBER   MM</b>  | is a multimember classification effect whose levels are determined by one or more variables that appear in a CLASS statement.                                                                             |
| <b>POLYNOMIAL   POLY</b> | is a multivariate polynomial effect in the specified numeric variables.                                                                                                                                   |
| <b>SPLINE</b>            | is a regression spline effect whose columns are univariate spline expansions of one or more variables. A spline expansion replaces the original variable with an expanded or larger set of new variables. |

Table 80.8 summarizes the *options* available in the EFFECT statement.

**Table 80.8** EFFECT Statement Options

| Option                             | Description                                                                                                                                           |
|------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Collection Effects Options</b>  |                                                                                                                                                       |
| DETAILS                            | Displays the constituents of the collection effect                                                                                                    |
| <b>Lag Effects Options</b>         |                                                                                                                                                       |
| DESIGNROLE=                        | Names a variable that controls to which lag design an observation is assigned                                                                         |
| DETAILS                            | Displays the lag design of the lag effect                                                                                                             |
| NLAG=                              | Specifies the number of periods in the lag                                                                                                            |
| PERIOD=                            | Names the variable that defines the period                                                                                                            |
| WITHIN=                            | Names the variable or variables that define the group within which each period is defined                                                             |
| <b>Multimember Effects Options</b> |                                                                                                                                                       |
| NOEFFECT                           | Specifies that observations with all missing levels for the multi-member variables should have zero values in the corresponding design matrix columns |
| WEIGHT=                            | Specifies the weight variable for the contributions of each of the classification effects                                                             |
| <b>Polynomial Effects Options</b>  |                                                                                                                                                       |
| DEGREE=                            | Specifies the degree of the polynomial                                                                                                                |
| MDEGREE=                           | Specifies the maximum degree of any variable in a term of the polynomial                                                                              |
| STANDARDIZE=                       | Specifies centering and scaling suboptions for the variables that define the polynomial                                                               |
| <b>Spline Effects Options</b>      |                                                                                                                                                       |
| BASIS=                             | Specifies the type of basis (B-spline basis or truncated power function basis) for the spline expansion                                               |
| DEGREE=                            | Specifies the degree of the spline transformation                                                                                                     |
| KNOTMETHOD=                        | Specifies how to construct the knots for spline effects                                                                                               |

For more information about the syntax of these *effect-types* and how columns of constructed effects are computed, see the section “EFFECT Statement” on page 393 in Chapter 19, “Shared Concepts and Topics.”

## ID Statement

**ID** *variables* ;

When the diagnostics table is requested with the DIAGNOSTICS option in the MODEL statement, the variables listed in the ID statement are displayed in addition to the observation number. These variables

can be used to identify each observation. If the ID statement is omitted, the observation number is used to identify the observations.

## MODEL Statement

*< label: >* **MODEL** *response = < effects > < / options >* ;

Main effects and interaction terms can be specified in the MODEL statement, as in the GLM procedure (Chapter 42, “The GLM Procedure.”)

The optional *label*, which must be a valid SAS name, is used to label the model in the OUTEST data set.

Table 80.9 summarizes the options available in the MODEL statement.

**Table 80.9** MODEL Statement Options

| Option      | Description                                                        |
|-------------|--------------------------------------------------------------------|
| ALPHA=      | Specifies the significance level                                   |
| CORRB       | Produces the estimated correlation matrix                          |
| COVB        | Produces the estimated covariance matrix                           |
| CUTOFF=     | Specifies the multiplier of the cutoff value for outlier detection |
| DIAGNOSTICS | Requests the outlier diagnostics                                   |
| FAILRATIO=  | Specifies the failure-ratio threshold                              |
| ITPRINT     | Displays the iteration history                                     |
| LEVERAGE    | Requests an analysis of leverage points                            |
| NOGOODFIT   | Suppresses the computation of goodness-of-fit statistics           |
| NOINT       | Specifies no-intercept regression                                  |
| SINGULAR=   | Specifies the tolerance for testing singularity                    |

You can specify the following *options* for the model fit.

### **ALPHA=***value*

specifies the significance level for the confidence intervals for regression parameters. The value must be between 0 and 1. By default, ALPHA=0.05.

### **CORRB**

produces the estimated correlation matrix of the parameter estimates.

### **COVB**

produces the estimated covariance matrix of the parameter estimates.

### **CUTOFF=***value*

specifies the multiplier of the cutoff value for outlier detection. By default, CUTOFF=3.

### **DIAGNOSTICS** *< (ALL) >*

requests the outlier diagnostics. By default, only observations identified as outliers or leverage points are displayed. Specify the ALL option to display all observations.

**FAILRATIO=***value*

specifies the failure-ratio threshold for the subsampling algorithm of an LTS or S estimate. It also applies to the initial LTS or S step in an MM estimate. The threshold must be between 0 and 1. Its default value is 0.99. See the section “[LTS Estimate](#)” on page 6845 or “[S Estimate](#)” on page 6847 for details.

**ITPRINT**

displays the iteration history for the iteratively reweighted least squares algorithm used by M and MM estimation. You can also use this option in the PROC ROBUSTREG statement.

**LEVERAGE** < (*leverage-options*) >

requests an analysis of leverage points for the covariates. The results are added to the diagnostics table, which you can request with the DIAGNOSTICS option in the MODEL statement.

The following *leverage-options* are available:

**CUTOFF=***value*

specifies the leverage cutoff value for leverage-point detection. See the section “[Leverage Point and Outlier Detection](#)” on page 6860 for details. The cutoff value can also be specified with the leverage cutoff  $\alpha$  value by using the CUTOFFALPHA= option.

**CUTOFFALPHA=***value*

specifies the leverage cutoff  $\alpha$  value for leverage-point detection. The respective leverage cutoff value equals  $\sqrt{\chi_{p;1-\alpha}^2}$  (or  $\sqrt{\chi_{q;1-\alpha}^2}$  if projection is applied in the generalized MCD algorithm). By default,  $\alpha = 0.025$ .

**H=***n***QUANTILE=***n*

specifies the quantile to be minimized for the MCD algorithm that is used for the leverage-point analysis. By default,  $H = [(3n + p + 1)/4]$ , where  $n$  is the number of observations and  $p$  is the number of independent variables excluding the intercept.

**MCDALPHA=***value*

specifies the MCD cutoff  $\alpha$  value for the final MCD reweighting step. The respective MCD cutoff value equals  $\sqrt{\chi_{p;1-\alpha}^2}$  (or  $\sqrt{\chi_{q;1-\alpha}^2}$  if projection is applied in the generalized MCD algorithm). By default,  $\alpha = 0.025$ .

**MCDCUTOFF=***value***MDCDUT=***value*

specifies the MCD cutoff value for the final MCD reweighting step. See the section “[Mahalanobis Distance versus Robust Distance](#)” on page 6853 and Rousseeuw and Van Driessen (1999) for details. The cutoff value can also be specified with the MCD cutoff  $\alpha$  value by using the MCDALPHA= option.

**MCDINFO**

requests that detailed information about the MCD covariance estimate be displayed, including the low-dimensional structure, the breakdown value, the MCD center, and the MCD covariance itself. The option outputs the ODS tables of the MCD profile, MCD center, MCD covariance, and MCD correlation.

**OPC | OFFPLANECOEF**

requests the ODS table of the coefficients for MCD-dropped components, when projection is applied in the generalized MCD algorithm. The OFFPLANECOEF option is ignored for the regular MCD algorithm.

**PROJECTIONALPHA=value****PALPHA=value**

specifies the projection cutoff  $\alpha$  value to be used to judge whether an observation is on or off the low-dimensional hyperplane identified by the generalized MCD algorithm. The respective projection cutoff value equals  $\sqrt{\chi^2_{1;1-\alpha}}$ . By default,  $\alpha = 0.001$ .

**PROJECTIONCUTOFF=value****PCUTOFF=value**

specifies the projection cutoff value to be used to judge whether an observation is on or off the low-dimensional hyperplane identified by the projected MCD algorithm. See the section “Mahalanobis Distance versus Robust Distance” on page 6853 and Rousseeuw and Van Driessen (1999) for details. The projection cutoff value can also be specified with the projection cutoff  $\alpha$  value by using the PALPHA= option.

**PROJECTIONTOLERANCE=value****PTOL=value**

specifies the projection tolerance value for the low-dimensional structure detection. See the section “Leverage Point and Outlier Detection” on page 6860 for details.

**NOGOODFIT**

suppresses the computation of goodness-of-fit statistics.

**NOINT**

specifies no-intercept regression.

**SINGULAR=value**

specifies the tolerance for testing singularity of the information matrix and the crossproducts matrix for the initial least squares estimates. Roughly, the test requires that a pivot be at least *value* times the original diagonal value. By default, SINGULAR=1E-12.

---

## OUTPUT Statement

**OUTPUT** < **OUT=SAS-data-set** > *keyword=name* < . . . *keyword=name* > ;

The OUTPUT statement creates an output SAS data set that contains statistics calculated after fitting the model. At least one specification of the form *keyword=name* is required.

All variables in the original data set are included in the new data set, along with the variables that are created with *keyword* options in the OUTPUT statement. These new variables contain fitted values and estimated quantiles. If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*.

The following specifications can appear in the OUTPUT statement:

- OUT=SAS-data-set** specifies the new data set. By default, the procedure uses the  $DATA_n$  convention to name the new data set.
- keyword=name** specifies the statistics to include in the output data set and gives names to the new variables. Specify a keyword for each desired statistic (see the following list), an equal sign, and the variable to contain the statistic.

The keywords allowed and the statistics they represent are as follows:

- LEVERAGE** specifies a variable to indicate leverage points. To include this variable in the OUTPUT data set, you must specify the LEVERAGE option in the MODEL statement. See the section “[Leverage Point and Outlier Detection](#)” on page 6860 for how to define LEVERAGE.
- MD** specifies a variable to contain the Mahalanobis distances. See the section “[Robust Distance](#)” on page 6853 for the definition of Mahalanobis distance.
- OUTLIER** specifies a variable to indicate outliers. See the section “[Leverage Point and Outlier Detection](#)” on page 6860 for information about how to define OUTLIER.
- PMD** specifies a variable to contain the projected Mahalanobis distances. See the section “[Robust Distance](#)” on page 6853 for the definition of projected Mahalanobis distance.
- POD** specifies a variable to contain the projected off-plane distances. See the section “[Robust Distance](#)” on page 6853 for the definition of off-plane distance.
- PRD** specifies a variable to contain the projected robust MCD Mahalanobis distances. See the section “[Robust Distance](#)” on page 6853 for the definition of projected robust distance.
- PREDICTED | P** specifies a variable to contain the estimated responses
- $$\hat{y}_i = \mathbf{x}'_i \hat{\boldsymbol{\theta}}$$
- RD** specifies a variable to contain the robust MCD Mahalanobis distances. See the section “[Robust Distance](#)” on page 6853 for the definition of robust distance.
- RESIDUAL | R** specifies a variable to contain the unstandardized residuals
- $$y_i - \hat{y}_i \text{ or } y_i - \mathbf{x}'_i \hat{\boldsymbol{\theta}}$$
- SRESIDUAL | SR** specifies a variable to contain the standardized residuals
- $$\frac{y_i - \hat{y}_i}{\hat{\sigma}} \text{ or } \frac{y_i - \mathbf{x}'_i \hat{\boldsymbol{\theta}}}{\hat{\sigma}}.$$
- By default, the LTS method uses Wscale as  $\hat{\sigma}$  for computing the standardized residuals.
- STDP** specifies a variable to contain the estimates of the standard errors of the estimated mean responses

$$\sqrt{\mathbf{x}'_i \boldsymbol{\Sigma} \mathbf{x}_i}$$

where  $\boldsymbol{\Sigma}$  denotes the covariance matrix of the parameter estimates. You can request the ODS table of this covariance matrix by using the COVB option of the MODEL statement. The STDP= option is applied to M, S, and MM estimation, but not to LTS estimation.

STDI specifies a variable to contain the estimates of the standard errors of the individual predicted values

$$\sqrt{\mathbf{x}'_i \boldsymbol{\Sigma} \mathbf{x}_i + \hat{\sigma}^2}.$$

The STDI= option is applied to M, S, and MM estimation, but not to LTS estimation.

WEIGHT specifies a variable to contain the computed final weights.

## PERFORMANCE Statement

The PERFORMANCE statement is used to specify options that affect the performance of PROC ROBUSTREG and to request tables that show the performance options in effect and timing details. See Chen (2002) for some empirical results.

**PERFORMANCE** < options > ;

The following *options* are available:

### CPUCOUNT=*n* | ACTUAL

specifies the number of processors to use for forming crossproduct matrices. You can specify any integer in the range 1–1024 for *n*. CPUCOUNT=ACTUAL sets CPUCOUNT to be the number of physical processors available. Note that this can be less than the physical number of CPUs if the SAS process has been restricted by system administration tools. Setting CPUCOUNT= to a number greater than the actual number of available CPUs might result in reduced performance. This option overrides the SAS system option CPUCOUNT=. If CPUCOUNT=1, then NOTHREADS is in effect, and PROC ROBUSTREG uses singly threaded code.

### DETAILS

requests the PerfSettings table that shows the performance settings in effect and the “Timing” table that provides a broad timing breakdown of the PROC ROBUSTREG step.

### THREADS

enables multithreaded computation. This option overrides the SAS system option NOTHREADS.

### NOTHREADS

disables multithreaded computation. This option overrides the SAS system option THREADS.

## TEST Statement

< label: > **TEST** effects ;

With M estimation and MM estimation, the TEST statement provides a means of obtaining a test for the canonical linear hypothesis concerning the parameters of the tested effects

$$\theta_j = 0, \quad j = i_1, \dots, i_q$$

where *q* is the total number of parameters of the tested effects.



PROC ROBUSTREG provides two kinds of robust tests: the  $\rho$  test and the  $R_n^2$  test. They are described in the section “[Details: ROBUSTREG Procedure](#)” on page 6838. No test is available for LTS and S estimation.

The optional *label*, which must be a valid SAS name, is used to label output from the corresponding TEST statement.

## WEIGHT Statement

**WEIGHT** *variable* ;

The WEIGHT statement specifies a weight variable in the input data set.

If you want to use fixed weights for each observation in the input data set, place the weights in a variable in the data set and specify the name in a WEIGHT statement. The values of the WEIGHT variable can be nonintegral and are not truncated. Observations with nonpositive or missing values for the weight variable do not contribute to the fit of the model.

## Details: ROBUSTREG Procedure

This section describes the statistical and computational aspects of the ROBUSTREG procedure. The following notation is used throughout this section.

Let  $\mathbf{X} = (x_{ij})$  denote an  $n \times p$  matrix,  $\mathbf{y} = (y_1, \dots, y_n)'$  denote a given  $n$ -vector of responses, and  $\boldsymbol{\theta} = (\theta_1, \dots, \theta_p)'$  denote an unknown  $p$ -vector of parameters or coefficients whose components are to be estimated. The matrix  $\mathbf{X}$  is called the design matrix. Consider the usual linear model

$$\mathbf{y} = \mathbf{X}\boldsymbol{\theta} + \mathbf{e}$$

where  $\mathbf{e} = (e_1, \dots, e_n)'$  is an  $n$ -vector of unknown errors. It is assumed that (for a given  $\mathbf{X}$ ) the components  $e_i$  of  $\mathbf{e}$  are independent and identically distributed according to a distribution  $L(\cdot/\sigma)$ , where  $\sigma$  is a scale parameter (usually unknown). Often  $L(\cdot) \approx \Phi(\cdot)$ , the standard normal distribution function. The vector of residuals for a given value of  $\hat{\boldsymbol{\theta}}$  is denoted by  $\mathbf{r} = (r_1, \dots, r_n)'$  and the  $i$ th row of the matrix  $\mathbf{X}$  is denoted by  $\mathbf{x}_i'$ .

## M Estimation

M estimation in the context of regression was first introduced by Huber (1973) as a result of making the least squares approach robust. Although M estimators are not robust with respect to leverage points, they are popular in applications where leverage points are not an issue.

Instead of minimizing a sum of squares of the residuals, a Huber-type M estimator  $\hat{\boldsymbol{\theta}}_M$  of  $\boldsymbol{\theta}$  minimizes a sum of less rapidly increasing functions of the residuals:

$$Q(\boldsymbol{\theta}) = \sum_{i=1}^n \rho\left(\frac{r_i}{\sigma}\right)$$

where  $\mathbf{r} = \mathbf{y} - \mathbf{X}\boldsymbol{\theta}$ . For the ordinary least squares estimation,  $\rho$  is the square function,  $\rho(z) = z^2$ .

If  $\sigma$  is known, then by taking derivatives with respect to  $\boldsymbol{\theta}$ ,  $\hat{\boldsymbol{\theta}}_M$  is also a solution of the system of  $p$  equations:

$$\sum_{i=1}^n \psi\left(\frac{r_i}{\sigma}\right) x_{ij} = 0, \quad j = 1, \dots, p$$

where  $\psi = \frac{\partial \rho}{\partial z}$ . If  $\rho$  is convex,  $\hat{\boldsymbol{\theta}}_M$  is the unique solution.

The ROBUSTREG procedure solves this system by using iteratively reweighted least squares (IRLS). The weight function  $w(x)$  is defined as

$$w(z) = \frac{\psi(z)}{z}$$

The ROBUSTREG procedure provides 10 kinds of weight functions through the WEIGHTFUNCTION= option in the MODEL statement. Each weight function corresponds to a  $\rho$  function. See the section “Weight Functions” on page 6840 for a complete discussion. You can specify the scale parameter  $\sigma$  with the SCALE= option in the PROC ROBUSTREG statement.

If  $\sigma$  is unknown, both  $\boldsymbol{\theta}$  and  $\sigma$  are estimated by minimizing the function

$$Q(\boldsymbol{\theta}, \sigma) = \sum_{i=1}^n \left[ \rho\left(\frac{r_i}{\sigma}\right) + a \right] \sigma, \quad a > 0$$

The algorithm proceeds by alternately improving  $\hat{\boldsymbol{\theta}}$  in a location step and  $\hat{\sigma}$  in a scale step.

For the scale step, three methods are available to estimate  $\sigma$ , which you can select with the SCALE= option.

1. (SCALE=HUBER <(D=d)>) Compute  $\hat{\sigma}$  by the iteration

$$\left(\hat{\sigma}^{(m+1)}\right)^2 = \frac{1}{nh} \sum_{i=1}^n \chi_d\left(\frac{r_i}{\hat{\sigma}^{(m)}}\right) \left(\hat{\sigma}^{(m)}\right)^2$$

where

$$\chi_d(x) = \begin{cases} x^2/2 & \text{if } |x| < d \\ d^2/2 & \text{otherwise} \end{cases}$$

is the Huber function and  $h = \frac{n-p}{n} \left( d^2 + (1-d^2)\Phi(d) - 0.5 - d\sqrt{2\pi}e^{-\frac{1}{2}d^2} \right)$  is the Huber constant (Huber 1981, p. 179). You can specify  $d$  with the D=d option. By default, D=2.5.

2. (SCALE=TUKEY <(D=d)>) Compute  $\hat{\sigma}$  by solving the supplementary equation

$$\frac{1}{n-p} \sum_{i=1}^n \chi_d \left( \frac{r_i}{\sigma} \right) = \beta$$

where

$$\chi_d(x) = \begin{cases} \frac{3x^2}{d^2} - \frac{3x^4}{d^4} + \frac{x^6}{d^6} & \text{if } |x| < d \\ 1 & \text{otherwise} \end{cases}$$

Here  $\psi = \frac{1}{6}\chi_1'$  is Tukey's bisquare function, and  $\beta = \int \chi_d(s)d\Phi(s)$  is the constant such that the solution  $\hat{\sigma}$  is asymptotically consistent when  $L(\cdot/\sigma) = \Phi(\cdot)$  (Hampel et al. 1986, p. 149). You can specify  $d$  with the D=d option. By default, D=2.5.

3. (SCALE=MED) Compute  $\hat{\sigma}$  by the iteration

$$\hat{\sigma}^{(m+1)} = \text{median} \left\{ |y_i - \mathbf{x}_i' \hat{\boldsymbol{\theta}}^{(m)}| / \beta_0, i = 1, \dots, n \right\}$$

where  $\beta_0 = \Phi^{-1}(.75)$  is the constant such that the solution  $\hat{\sigma}$  is asymptotically consistent when  $L(\cdot/\sigma) = \Phi(\cdot)$  (Hampel et al. 1986, p. 312).

SCALE=MED is the default.

## Algorithm

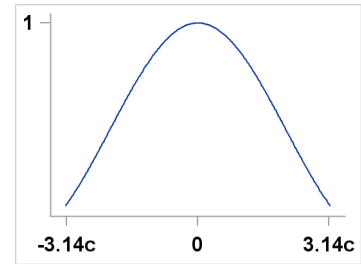
The basic algorithm for computing M estimates for regression is iteratively reweighted least squares (IRLS). As the name suggests, a weighted least squares fit is carried out inside an iteration loop. For each iteration, a set of weights for the observations is used in the least squares fit. The weights are constructed by applying a weight function to the current residuals. Initial weights are based on residuals from an initial fit. The ROBUSTREG procedure uses the unweighted least squares fit as a default initial fit. The iteration terminates when a convergence criterion is satisfied. The maximum number of iterations is set to 1,000. You can specify the weight function and the convergence criteria.

## Weight Functions

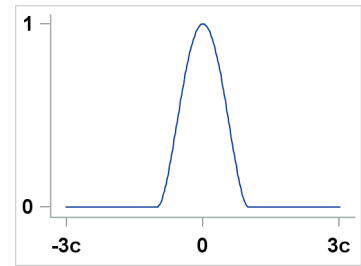
You can specify the weight function for M estimation with the WEIGHTFUNCTION= option. The ROBUSTREG procedure provides 10 weight functions. By default, the procedure uses the bisquare weight function. In most cases, M estimates are more sensitive to the parameters of these weight functions than to the type of the weight function. The median weight function is not stable and is seldom recommended in data analysis; it is included in the procedure for completeness. You can specify the parameters for these weight functions. Except for the Hampel and median weight functions, default values for these parameters are defined such that the corresponding M estimates have 95% asymptotic efficiency in the location model with the Gaussian distribution (Holland and Welsch 1977).

The following list shows the weight functions available. See Table 80.5 for the default values of the constants in these weight functions.

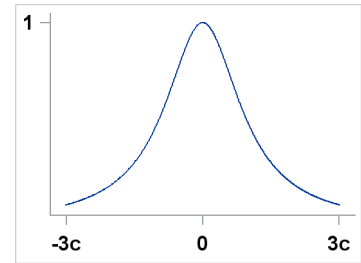
Andrews 
$$W(x, c) = \begin{cases} \frac{\sin(x/c)}{x/c} & \text{if } |x| \leq \pi c \\ 0 & \text{otherwise} \end{cases}$$



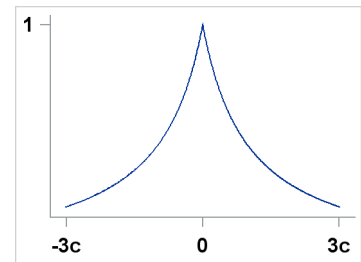
Bisquare 
$$W(x, c) = \begin{cases} (1 - (x/c)^2)^2 & \text{if } |x| < c \\ 0 & \text{otherwise} \end{cases}$$



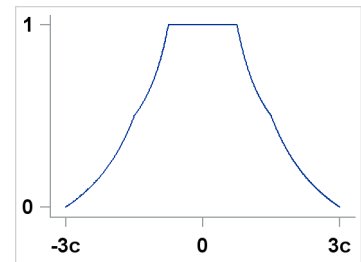
Cauchy 
$$W(x, c) = \frac{1}{1 + (|x|/c)^2}$$



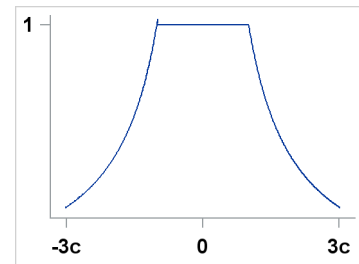
Fair 
$$W(x, c) = \frac{1}{(1 + |x|/c)}$$



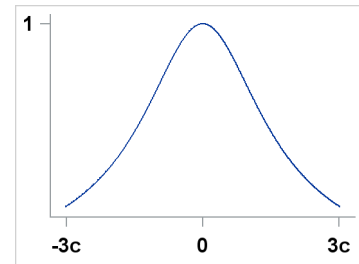
Hampel 
$$W(x, a, b, c) = \begin{cases} 1 & |x| < a \\ \frac{a}{|x|} & a < |x| \leq b \\ \frac{a}{|x|} \frac{c-|x|}{c-b} & b < |x| \leq c \\ 0 & \text{otherwise} \end{cases}$$



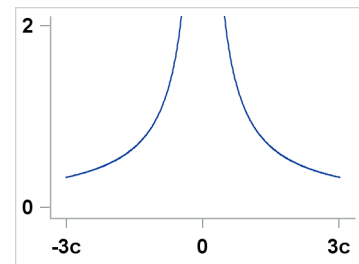
Huber  $W(x, c) = \begin{cases} 1 & \text{if } |x| < c \\ \frac{c}{|x|} & \text{otherwise} \end{cases}$



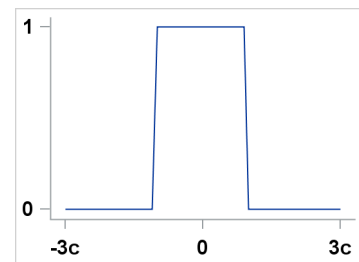
Logistic  $W(x, c) = \frac{\tanh(x/c)}{x/c}$



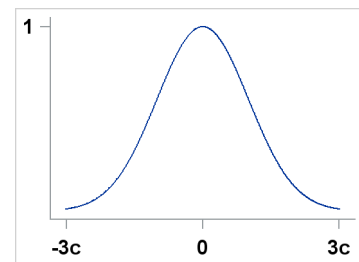
Median  $W(x, c) = \begin{cases} \frac{1}{c} & \text{if } x = 0 \\ \frac{1}{|x|} & \text{otherwise} \end{cases}$



Talworth  $W(x, c) = \begin{cases} 1 & \text{if } |x| < c \\ 0 & \text{otherwise} \end{cases}$



Welsch  $W(x, c) = \exp\left(-\frac{(x/c)^2}{2}\right)$



## Convergence Criteria

The following convergence criteria are available in PROC ROBUSTREG:

- relative change in the coefficients (CONVERGENCE= COEF)

- relative change in the scaled residuals (CONVERGENCE= RESID)
- relative change in weights (CONVERGENCE= WEIGHT)

You can specify the criteria with the CONVERGENCE= option in the PROC ROBUSTREG statement. The default is CONVERGENCE= COEF.

You can specify the precision of the convergence criterion with the EPS= suboption. The default is EPS=1E-8.

In addition to these convergence criteria, a convergence criterion based on scale-independent measure of the gradient is always checked. See Coleman et al. (1980) for more details. A warning is issued if this criterion is not satisfied.

### Asymptotic Covariance and Confidence Intervals

The following three estimators of the asymptotic covariance of the robust estimator are available in PROC ROBUSTREG:

$$\text{H1: } K^2 \frac{[1/(n-p)] \sum (\psi(r_i))^2}{[(1/n) \sum (\psi'(r_i))]^2} (\mathbf{X}'\mathbf{X})^{-1}$$

$$\text{H2: } K \frac{[1/(n-p)] \sum (\psi(r_i))^2}{[(1/n) \sum (\psi'(r_i))]} \mathbf{W}^{-1}$$

$$\text{H3: } K^{-1} \frac{1}{(n-p)} \sum (\psi(r_i))^2 \mathbf{W}^{-1} (\mathbf{X}'\mathbf{X}) \mathbf{W}^{-1}$$

where  $K = 1 + \frac{p}{n} \frac{\text{Var}(\psi')}{(E\psi')^2}$  is a correction factor and  $W_{jk} = \sum \psi'(r_i) x_{ij} x_{ik}$ . See Huber (1981, p. 173) for more details.

You can specify the asymptotic covariance estimate with the option ASYMPCOV= option. The ROBUSTREG procedure uses H1 as the default because of its simplicity and stability. Confidence intervals are computed from the diagonal elements of the estimated asymptotic covariance matrix.

### R Square and Deviance

The robust version of R-square is defined as

$$R^2 = \frac{\sum \rho \left( \frac{y_i - \hat{\mu}}{\hat{s}} \right) - \sum \rho \left( \frac{y_i - \mathbf{x}'_i \hat{\boldsymbol{\theta}}}{\hat{s}} \right)}{\sum \rho \left( \frac{y_i - \hat{\mu}}{\hat{s}} \right)}$$

and the robust deviance is defined as the optimal value of the objective function on the  $\sigma^2$  scale

$$D = 2\hat{s}^2 \sum \rho \left( \frac{y_i - \mathbf{x}'_i \hat{\boldsymbol{\theta}}}{\hat{s}} \right)$$

where  $\rho' = \psi$ ,  $\hat{\boldsymbol{\theta}}$  is the M estimator of  $\boldsymbol{\theta}$ ,  $\hat{\mu}$  is the M estimator of location, and  $\hat{s}$  is the M estimator of the scale parameter in the full model.

## Linear Tests

Two tests are available in PROC ROBUSTREG for the canonical linear hypothesis

$$H_0 : \theta_j = 0, \quad j = i_1, \dots, i_q$$

where  $q$  is the total number of parameters of the tested effects. The first test is a robust version of the  $F$  test, which is referred to as the  $\rho$  test. Denote the M estimators in the full and reduced models as  $\hat{\boldsymbol{\theta}}(0) \in \Omega_0$  and  $\hat{\boldsymbol{\theta}}(1) \in \Omega_1$ , respectively. Let

$$\begin{aligned} Q_0 &= Q(\hat{\boldsymbol{\theta}}(0)) = \min\{Q(\boldsymbol{\theta}) \mid \boldsymbol{\theta} \in \Omega_0\} \\ Q_1 &= Q(\hat{\boldsymbol{\theta}}(1)) = \min\{Q(\boldsymbol{\theta}) \mid \boldsymbol{\theta} \in \Omega_1\} \end{aligned}$$

with

$$Q = \sum_{i=1}^n \rho\left(\frac{r_i}{\sigma}\right)$$

The robust  $F$  test is based on the test statistic

$$S_n^2 = \frac{2}{q}[Q_1 - Q_0]$$

Asymptotically  $S_n^2 \sim \lambda \chi_q^2$  under  $H_0$ , where the standardization factor is  $\lambda = \int \psi^2(s) d\Phi(s) / \int \psi'(s) d\Phi(s)$  and  $\Phi$  is the cumulative distribution function of the standard normal distribution. Large values of  $S_n^2$  are significant. This test is a special case of the general  $\tau$  test of Hampel et al. (1986, Section 7.2).

The second test is a robust version of the Wald test, which is referred to as  $R_n^2$  test. The test uses a test statistic

$$R_n^2 = n(\hat{\theta}_{i_1}, \dots, \hat{\theta}_{i_q}) \mathbf{H}_{22}^{-1}(\hat{\theta}_{i_1}, \dots, \hat{\theta}_{i_q})'$$

where  $\frac{1}{n} \mathbf{H}_{22}$  is the  $q \times q$  block (corresponding to  $\theta_{i_1}, \dots, \theta_{i_q}$ ) of the asymptotic covariance matrix of the M estimate  $\hat{\boldsymbol{\theta}}_M$  of  $\boldsymbol{\theta}$  in a  $p$ -parameter linear model.

Under  $H_0$ , the statistic  $R_n^2$  has an asymptotic  $\chi^2$  distribution with  $q$  degrees of freedom. Large values of  $R_n^2$  are significant. See Hampel et al. (1986, Chapter 7) for more details.

## Model Selection

When M estimation is used, two criteria are available in PROC ROBUSTREG for model selection. The first criterion is a counterpart of the Akaike (1974) information criterion for robust regression (AICR); it is defined as

$$\text{AICR} = 2 \sum_{i=1}^n \rho(r_{i:p}) + \alpha p$$

where  $r_{i:p} = (y_i - \mathbf{x}_i' \hat{\boldsymbol{\theta}}) / \hat{\sigma}$ ,  $\hat{\sigma}$  is a robust estimate of  $\sigma$  and  $\hat{\boldsymbol{\theta}}$  is the M estimator with  $p$ -dimensional design matrix.

As with AIC,  $\alpha$  is the weight of the penalty for dimensions. The ROBUSTREG procedure uses  $\alpha = 2E\psi^2/E\psi'$  (Ronchetti 1985) and estimates it by using the final robust residuals.

The second criterion is a robust version of the Schwarz information criteria (BICR); it is defined as

$$\text{BICR} = 2 \sum_{i=1}^n \rho(r_{i;p}) + p \log(n)$$

## High-Breakdown-Value Estimation

The *breakdown value* of an estimator is defined as the smallest fraction of contamination that can cause the estimator to take on values that are arbitrarily far from its value on the uncontaminated data. The breakdown value of an estimator can be used as a measure of the robustness of the estimator. Rousseeuw and Leroy (1987) and others introduced the following high-breakdown-value estimators for linear regression.

### LTS Estimate

The least trimmed squares (LTS) estimate proposed by Rousseeuw (1984) is defined as the  $p$ -vector

$$\hat{\theta}_{LTS} = \arg \min_{\theta} Q_{LTS}(\theta) \text{ with } Q_{LTS}(\theta) = \sum_{i=1}^h r_i^2$$

where  $r_{(1)}^2 \leq r_{(2)}^2 \leq \dots \leq r_{(n)}^2$  are the ordered squared residuals  $r_i^2 = (y_i - \mathbf{x}_i' \theta)^2$ ,  $i = 1, \dots, n$ , and  $h$  is defined in the range  $\frac{n}{2} + 1 \leq h \leq \frac{3n+p+1}{4}$ .

You can specify the parameter  $h$  with the H= option in the PROC ROBUSTREG statement. By default,  $h = \lceil \frac{3n+p+1}{4} \rceil$ . The breakdown value is  $\frac{n-h}{n}$  for the LTS estimate.

The ROBUSTREG procedure computes LTS estimates by using the FAST-LTS algorithm of Rousseeuw and Van Driessen (2000). The estimates are often used to detect outliers in the data, which are then down-weighted in the resulting weighted LS regression.

### Algorithm

Least trimmed squares (LTS) regression is based on the subset of  $h$  observations (out of a total of  $n$  observations) whose least squares fit possesses the smallest sum of squared residuals. The coverage  $h$  can be set between  $\frac{n}{2}$  and  $n$ . The LTS method was proposed by Rousseeuw (1984, p. 876) as a highly robust regression estimator with breakdown value  $\frac{n-h}{n}$ . The ROBUSTREG procedure uses the FAST-LTS algorithm given by Rousseeuw and Van Driessen (2000). The intercept adjustment technique is also used in this implementation. However, because this adjustment is expensive to compute, it is optional. You can use the IADJUST= option in the PROC ROBUSTREG statement to request or suppress the intercept adjustment. By default, PROC ROBUSTREG does intercept adjustment for data sets with fewer than 10,000 observations. The steps of the algorithm are described briefly as follows. See Rousseeuw and Van Driessen (2000) for details.

1. The default  $h$  is  $\lceil \frac{3n+p+1}{4} \rceil$ , where  $p$  is the number of independent variables. You can specify any integer  $h$  with  $\lceil \frac{n}{2} \rceil + 1 \leq h \leq \lceil \frac{3n+p+1}{4} \rceil$  with the H= option in the MODEL statement. The breakdown value for LTS,  $\frac{n-h}{n}$ , is reported. The default  $h$  is a good compromise between breakdown value and statistical efficiency.
2. If  $p = 1$  (single regressor), the procedure uses the exact algorithm of Rousseeuw and Leroy (1987, p. 172).



3. If  $p \geq 2$ , PROC ROBUSTREG uses the following algorithm. If  $n < 2 \textit{ssubs}$ , where  $\textit{ssubs}$  is the size of the subgroups (you can specify  $\textit{ssubs}$  by using the SUBGROUPSIZE= option in the PROC ROBUSTREG statement; by default,  $\textit{ssubs} = 300$ ), PROC ROBUSTREG draws a random  $p$ -subset and computes the regression coefficients by using these  $p$  points (if the regression is degenerate, another  $p$ -subset is drawn). The absolute residuals for all observations in the data set are computed, and the first  $h$  points with smallest absolute residuals are selected. From this selected  $h$ -subset, PROC ROBUSTREG carries out  $\textit{nsteps}$  C-steps (concentration steps; see Rousseeuw and Van Driessen (2000) for details). You can specify  $\textit{nsteps}$  with the CSTEP= option in the PROC ROBUSTREG statement; by default,  $\textit{nsteps} = 2$ . PROC ROBUSTREG redraws  $p$ -subsets and repeats the preceding computation  $\textit{nrep}$  times, and then finds the  $\textit{nbsol}$  (at most) solutions with the lowest sums of  $h$  squared residuals. You can specify  $\textit{nrep}$  with the NREP= option in the PROC ROBUSTREG statement; by default,  $\textit{NREP} = \min\{500, \binom{n}{p}\}$ . For small  $n$  and  $p$ , all  $\binom{n}{p}$  subsets are used and the NREP= option is ignored (Rousseeuw and Hubert 1996). You can specify  $\textit{nbsol}$  with the NBEST= option in the PROC ROBUSTREG statement; by default,  $\textit{NBEST} = 10$ . For each of these  $\textit{nbsol}$  best solutions, C-steps are taken until convergence and the best final solution is found.
4. If  $n \geq 5\textit{ssubs}$ , construct five disjoint random subgroups with size  $\textit{ssubs}$ . If  $2\textit{ssubs} < n < 5\textit{ssubs}$ , the data are split into at most four subgroups with  $\textit{ssubs}$  or more observations in each subgroup, so that each observation belongs to a subgroup and the subgroups have roughly the same size. Let  $\textit{nsubs}$  denote the number of subgroups. Inside each subgroup, PROC ROBUSTREG repeats the step 3 algorithm  $\textit{nrep} / \textit{nsubs}$  times, keeps the  $\textit{nbsol}$  best solutions, and pools the subgroups, yielding the merged set of size  $\textit{nmerged}$ . In the merged set, for each of the  $\textit{nsubs} \times \textit{nbsol}$  best solutions,  $\textit{nsteps}$  C-steps are carried out by using  $\textit{nmerged}$  and  $\textit{hmerged} = \lceil \textit{nmerged} \frac{h}{n} \rceil$  and the  $\textit{nbsol}$  best solutions are kept. In the full data set, for each of these  $\textit{nbsol}$  best solutions, C-steps are taken by using  $n$  and  $h$  until convergence and the best final solution is found.

**NOTE:** At step 3 in the algorithm, a randomly selected  $p$ -subset might be degenerate (that is, its design matrix might be singular). If the total number of  $p$ -subsets from any subgroup is more than 4,000 and the ratio of degenerate  $p$ -subsets is more than the threshold specified in FAILRATIO= option, the algorithm is terminated with an error message.

### R-Square

The robust version of R-square for the LTS estimate is defined as

$$R_{LTS}^2 = 1 - \frac{s_{LTS}^2(\mathbf{X}, \mathbf{y})}{s_{LTS}^2(\mathbf{1}, \mathbf{y})}$$

for models with the intercept term and as

$$R_{LTS}^2 = 1 - \frac{s_{LTS}^2(\mathbf{X}, \mathbf{y})}{s_{LTS}^2(\mathbf{0}, \mathbf{y})}$$

for models without the intercept term, where

$$s_{LTS}(\mathbf{X}, \mathbf{y}) = d_{h,n} \sqrt{\frac{1}{h} \sum_{i=1}^h r_{(i)}^2}$$

Note that  $s_{LTS}$  is a preliminary estimate of the parameter  $\sigma$  in the distribution function  $L(\cdot/\sigma)$ .

Here  $d_{h,n}$  is chosen to make  $s_{LTS}$  consistent, assuming a Gaussian model. Specifically,

$$d_{h,n} = 1/\sqrt{1 - \frac{2n}{hc_{h,n}}\phi(1/c_{h,n})}$$

$$c_{h,n} = 1/\Phi^{-1}\left(\frac{h+n}{2n}\right)$$

with  $\Phi$  and  $\phi$  being the distribution function and the density function of the standard normal distribution, respectively.

### Final Weighted Scale Estimator

The ROBUSTREG procedure displays two scale estimators,  $s_{LTS}$  and Wscale. The estimator Wscale is a more efficient scale estimator based on the preliminary estimate  $s_{LTS}$ ; it is defined as

$$\text{Wscale} = \sqrt{\frac{\sum_i w_i r_i^2}{\sum_i w_i - p}}$$

where

$$w_i = \begin{cases} 0 & \text{if } |r_i|/s_{LTS} > k \\ 1 & \text{otherwise} \end{cases}$$

You can specify  $k$  with the CUTOFF= option in the MODEL statement. By default,  $k = 3$ .

## S Estimate

The S estimate proposed by Rousseeuw and Yohai (1984) is defined as the  $p$ -vector

$$\hat{\theta}_S = \arg \min_{\theta} S(\theta)$$

where the dispersion  $S(\theta)$  is the solution of

$$\frac{1}{n-p} \sum_{i=1}^n \chi\left(\frac{y_i - \mathbf{x}_i' \theta}{S}\right) = \beta$$

Here  $\beta$  is set to  $\int \chi(s) d\Phi(s)$  such that  $\hat{\theta}_S$  and  $S(\hat{\theta}_S)$  are asymptotically consistent estimates of  $\theta$  and  $\sigma$  for the Gaussian regression model. The breakdown value of the S estimate is

$$\frac{\beta}{\max_s \chi(s)}$$

The ROBUSTREG procedure provides two choices for  $\chi$ : Tukey's bisquare function and Yohai's optimal function.

Tukey's bisquare function, which you can specify with the option CHIF=TUKEY, is

$$\chi_{k_0}(s) = \begin{cases} 3\left(\frac{s}{k_0}\right)^2 - 3\left(\frac{s}{k_0}\right)^4 + \left(\frac{s}{k_0}\right)^6, & \text{if } |s| \leq k_0 \\ 1 & \text{otherwise} \end{cases}$$

The constant  $k_0$  controls the breakdown value and efficiency of the S estimate. If you specify the efficiency by using the EFF= option, you can determine the corresponding  $k_0$ . The default  $k_0$  is 2.9366 such that the breakdown value of the S estimate is 0.25 with a corresponding asymptotic efficiency for the Gaussian model of 75.9%.

The Yohai function, which you can specify with the option CHIF=YOHAI, is

$$\chi_{k_0}(s) = \begin{cases} \frac{s^2}{2} & \text{if } |s| \leq 2k_0 \\ k_0^2 [b_0 + b_1(\frac{s}{k_0})^2 + b_2(\frac{s}{k_0})^4 + b_3(\frac{s}{k_0})^6 + b_4(\frac{s}{k_0})^8] & \text{if } 2k_0 < |s| \leq 3k_0 \\ 3.25k_0^2 & \text{if } |s| > 3k_0 \end{cases}$$

where  $b_0 = 1.792$ ,  $b_1 = -0.972$ ,  $b_2 = 0.432$ ,  $b_3 = -0.052$ , and  $b_4 = 0.002$ . If you specify the efficiency by using the EFF= option, you can determine the corresponding  $k_0$ . By default,  $k_0$  is set to 0.7405 such that the breakdown value of the S estimate is 0.25 with a corresponding asymptotic efficiency for the Gaussian model of 72.7%.

### Algorithm

The ROBUSTREG procedure implements the algorithm by Marazzi (1993) for the S estimate, which is a refined version of the algorithm proposed by Ruppert (1992). The refined algorithm is briefly described as follows.

Initialize  $iter = 1$ .

1. Draw a random  $q$ -subset of the total  $n$  observations and compute the regression coefficients by using these  $q$  observations (if the regression is degenerate, draw another  $q$ -subset), where  $q \geq p$  can be specified with the SUBSIZE= option. By default,  $q = p$ .
2. Compute the residuals:  $r_i = y_i - \sum_{j=1}^p x_{ij}\theta_j$  for  $i = 1, \dots, n$ . If  $iter = 1$ , set  $s^* = 2\text{median}\{|r_i|, i = 1, \dots, n\}$ ; if  $s^* = 0$ , set  $s^* = \min\{|r_i|, i = 1, \dots, n\}$ ; else while  $\sum_{i=1}^n \chi(r_i/s^*) > (n-p)\beta$ , set  $s^* = 1.5s^*$ ; go to step 3. If  $iter > 1$  and  $\sum_{i=1}^n \chi(r_i/s^*) \leq (n-p)\beta$ , go to step 3; otherwise, go to step 5.

3. Solve for  $s$  the equation

$$\frac{1}{n-p} \sum_{i=1}^n \chi(r_i/s) = \beta$$

using an iterative algorithm.

4. If  $iter > 1$  and  $s > s^*$ , go to step 5. Otherwise, set  $s^* = s$  and  $\theta^* = \theta$ . If  $s^* < \text{TOLS}$ , return  $s^*$  and  $\theta^*$ ; otherwise, go to step 5.
5. If  $iter < \text{NREP}$ , set  $iter = iter + 1$  and return to step 1; otherwise, return  $s^*$  and  $\theta^*$ .

The ROBUSTREG procedure does the following refinement step by default. You can request that this refinement not be done by using the NOREFINE option in the PROC ROBUSTREG statement.

6. Let  $\psi = \chi'$ . Using the values  $s^*$  and  $\theta^*$  from the previous steps, compute M estimates  $\theta_M$  and  $\sigma_M$  of  $\theta$  and  $\sigma$  with the setup for M estimation that is described in the section “M Estimation” on page 6838. If  $\sigma_M > s^*$ , give a warning and return  $s^*$  and  $\theta^*$ ; otherwise, return  $\sigma_M$  and  $\theta_M$ .

You can specify TOLS with the TOLERANCE= option; by default, TOLERANCE=0.001. Alternately, you can specify NREP with the NREP= option. You can also use the options NREP=NREP0 or NREP=NREP1 to determine NREP according to the following table. NREP=NREP0 is set as the default.

**Table 80.11** Default NREP

| <b>P</b> | <b>NREP0</b> | <b>NREP1</b> |
|----------|--------------|--------------|
| 1        | 150          | 500          |
| 2        | 300          | 1000         |
| 3        | 400          | 1500         |
| 4        | 500          | 2000         |
| 5        | 600          | 2500         |
| 6        | 700          | 3000         |
| 7        | 850          | 3000         |
| 8        | 1250         | 3000         |
| 9        | 1500         | 3000         |
| >9       | 1500         | 3000         |

**NOTE:** At step 1 in the algorithm, a randomly selected  $q$ -subset might be degenerate. If the total number of  $q$ -subsets from any subgroup is more than 4,000 and the ratio of degenerate  $q$ -subsets is more than the threshold specified in FAILRATIO= option, the algorithm is terminated with an error message.

### ***R-Square and Deviance***

The robust version of R-square for the S estimate is defined as

$$R_S^2 = 1 - \frac{(n-p)S_p^2}{(n-1)S_\mu^2}$$

for the model with the intercept term and

$$R_S^2 = 1 - \frac{(n-p)S_p^2}{nS_0^2}$$

for the model without the intercept term, where  $S_p$  is the S estimate of the scale in the full model,  $S_\mu$  is the S estimate of the scale in the regression model with only the intercept term, and  $S_0$  is the S estimate of the scale without any regressor. The deviance  $D$  is defined as the optimal value of the objective function on the  $\sigma^2$  scale:

$$D = S_p^2$$

### ***Asymptotic Covariance and Confidence Intervals***

Since the S estimate satisfies the first-order necessary conditions as the M estimate, it has the same asymptotic covariance as that of the M estimate. All three estimators of the asymptotic covariance for the M estimate in the section “Asymptotic Covariance and Confidence Intervals” on page 6843 can be used for the S estimate. Besides, the weighted covariance estimator H4 described in the section “Asymptotic Covariance and Confidence Intervals” on page 6852 is also available and is set as the default. Confidence intervals for estimated parameters are computed from the diagonal elements of the estimated asymptotic covariance matrix.

## MM Estimation

MM estimation is a combination of high-breakdown-value estimation and efficient estimation, which was introduced by Yohai (1987). It has the following three steps:

1. Compute an initial (consistent) high-breakdown-value estimate  $\hat{\theta}'$ . The ROBUSTREG procedure provides two kinds of estimates as the initial estimate: the LTS estimate and the S estimate. By default, the LTS estimate is used because of its speed and high breakdown value. The breakdown value of the final MM estimate is decided by the breakdown value of the initial LTS estimate and the constant  $k_0$  in the  $\chi$  function. To use the S estimate as the initial estimate, you specify the INITEST=S option in the PROC ROBUSTREG statement. In this case, the breakdown value of the final MM estimate is decided only by the constant  $k_0$ . Instead of computing the LTS estimate or the S estimate as the initial estimate, you can also specify the initial estimate explicitly by using the INEST= option in the PROC ROBUSTREG statement. See the section “[INEST= Data Set](#)” on page 6861 for details.

2. Find  $\hat{\sigma}'$  such that

$$\frac{1}{n-p} \sum_{i=1}^n \chi \left( \frac{y_i - \mathbf{x}'_i \hat{\theta}'}{\hat{\sigma}'} \right) = \beta$$

where  $\beta = \int \chi(s) d\Phi(s)$ .

The ROBUSTREG procedure provides two choices for  $\chi$ : Tukey’s bisquare function and Yohai’s optimal function.

Tukey’s bisquare function, which you can specify with the option CHIF=TUKEY, is

$$\chi_{k_0}(s) = \begin{cases} 3\left(\frac{s}{k_0}\right)^2 - 3\left(\frac{s}{k_0}\right)^4 + \left(\frac{s}{k_0}\right)^6 & \text{if } |s| \leq k_0 \\ 1 & \text{otherwise} \end{cases}$$

where  $k_0$  can be specified with the K0= option. The default  $k_0$  is 2.9366 such that the asymptotically consistent scale estimate  $\hat{\sigma}'$  has the breakdown value of 25%.

Yohai’s optimal function, which you can specify with the option CHIF=YOHAI, is

$$\chi_{k_0}(s) = \begin{cases} \frac{s^2}{2} & \text{if } |s| \leq 2k_0 \\ k_0^2 [b_0 + b_1 \left(\frac{s}{k_0}\right)^2 + b_2 \left(\frac{s}{k_0}\right)^4 + b_3 \left(\frac{s}{k_0}\right)^6 + b_4 \left(\frac{s}{k_0}\right)^8] & \text{if } 2k_0 < |s| \leq 3k_0 \\ 3.25k_0^2 & \text{if } |s| > 3k_0 \end{cases}$$

where  $b_0 = 1.792$ ,  $b_1 = -0.972$ ,  $b_2 = 0.432$ ,  $b_3 = -0.052$ , and  $b_4 = 0.002$ . You can specify  $k_0$  with the K0= option. The default  $k_0$  is 0.7405 such that the asymptotically consistent scale estimate  $\hat{\sigma}'$  has the breakdown value of 25%.

3. Find a local minimum  $\hat{\theta}_{MM}$  of

$$Q_{MM} = \sum_{i=1}^n \rho \left( \frac{y_i - \mathbf{x}'_i \theta}{\hat{\sigma}'} \right)$$

such that  $Q_{MM}(\hat{\theta}_{MM}) \leq Q_{MM}(\hat{\theta}')$ . The algorithm for M estimation is used here.

The ROBUSTREG procedure provides two choices for  $\rho$ : Tukey's bisquare function and Yohai's optimal function.

Tukey's bisquare function, which you can specify with the option CHIF=DUKEY, is

$$\rho(s) = \chi_{k_1}(s) = \begin{cases} 3\left(\frac{s}{k_1}\right)^2 - 3\left(\frac{s}{k_1}\right)^4 + \left(\frac{s}{k_1}\right)^6 & \text{if } |s| \leq k_1 \\ 1 & \text{otherwise} \end{cases}$$

where  $k_1$  can be specified with the K1= option. The default  $k_1$  is 3.440 such that the MM estimate has 85% asymptotic efficiency with the Gaussian distribution.

Yohai's optimal function, which you can specify with the option CHIF=YOHA, is

$$\rho(s) = \chi_{k_1}(s) = \begin{cases} \frac{s^2}{2} & \text{if } |s| \leq 2k_1 \\ k_1^2 [b_0 + b_1\left(\frac{s}{k_1}\right)^2 + b_2\left(\frac{s}{k_1}\right)^4 + b_3\left(\frac{s}{k_1}\right)^6 + b_4\left(\frac{s}{k_1}\right)^8] & \text{if } 2k_1 < |s| \leq 3k_1 \\ 3.25k_1^2 & \text{if } |s| > 3k_1 \end{cases}$$

where  $k_1$  can be specified with the K1= option. The default  $k_1$  is 0.868 such that the MM estimate has 85% asymptotic efficiency with the Gaussian distribution.

## Algorithm

The initial LTS estimate is computed using the algorithm described in the section "LTS Estimate" on page 6845. You can control the quantile of the LTS estimate with the option INITH= $h$ , where  $h$  is an integer between  $\lfloor \frac{n}{2} \rfloor + 1$  and  $\lfloor \frac{3n+p+1}{4} \rfloor$ . By default,  $h = \lfloor \frac{3n+p+1}{4} \rfloor$ , which corresponds to a breakdown value of around 25%.

The initial S estimate is computed using the algorithm described in the section "S Estimate" on page 6847. You can control the breakdown value and efficiency of this initial S estimate by the constant  $k_0$ , which can be specified with the K0 option.

The scale parameter  $\sigma$  is solved by an iterative algorithm

$$(\sigma^{(m+1)})^2 = \frac{1}{(n-p)\beta} \sum_{i=1}^n \chi_{k_0} \left( \frac{r_i}{\sigma^{(m)}} \right) (\sigma^{(m)})^2$$

where  $\beta = \int \chi_{k_0}(s) d\Phi(s)$ .

Once the scale parameter is computed, the iteratively reweighted least squares (IRLS) algorithm with fixed scale parameter is used to compute the final MM estimate.

## Convergence Criteria

In the iterative algorithm for the scale parameter, the relative change of the scale parameter controls the convergence.

In the iteratively reweighted least squares algorithm, the same convergence criteria for the M estimate used before are used here.

## Bias Test

Although the final MM estimate inherits the high-breakdown-value property, its bias due to the distortion of the outliers can be high. Yohai, Stahel, and Zamar (1991) introduced a bias test. The ROBUSTREG procedure implements this test when you specify the BIASTEST= option in the PROC ROBUSTREG statement. This test is based on the initial scale estimate  $\hat{\sigma}'$  and the final scale estimate  $\hat{\sigma}'_1$ , which is the solution of

$$\frac{1}{n-p} \sum_{i=1}^n \chi \left( \frac{y_i - \mathbf{x}'_i \hat{\boldsymbol{\theta}}_{MM}}{\hat{\sigma}'_1} \right) = \beta$$

Let  $\psi_{k_0}(z) = \frac{\partial \chi_{k_0}(z)}{\partial z}$  and  $\psi_{k_1}(z) = \frac{\partial \chi_{k_1}(z)}{\partial z}$ . Compute

$$\tilde{r}_i = (y_i - \mathbf{x}'_i \hat{\boldsymbol{\theta}}') / \hat{\sigma}' \quad \text{for } i = 1, \dots, n$$

$$v_0 = \frac{(1/n) \sum \psi'_{k_0}(\tilde{r}_i)}{(\hat{\sigma}'_1/n) \sum \psi_{k_0}(\tilde{r}_i) \tilde{r}_i}$$

$$p_i^{(0)} = \frac{\psi_{k_0}(\tilde{r}_i)}{(1/n) \sum \psi'_{k_0}(\tilde{r}_i)} \quad \text{for } i = 1, \dots, n$$

$$p_i^{(1)} = \frac{\psi_{k_1}(\tilde{r}_i)}{(1/n) \sum \psi'_{k_1}(\tilde{r}_i)} \quad \text{for } i = 1, \dots, n$$

$$d^2 = \frac{1}{n} \sum (p_i^{(1)} - p_i^{(0)})^2$$

Let

$$T = \frac{2n(\hat{\sigma}'_1 - \hat{\sigma}')}{v_0 d^2 (\hat{\sigma}')^2}$$

Standard asymptotic theory shows that  $T$  approximately follows a  $\chi^2$  distribution with  $p$  degrees of freedom. If  $T$  exceeds the  $\alpha$  quantile  $\chi^2_\alpha$  of the  $\chi^2$  distribution with  $p$  degrees of freedom, then the ROBUSTREG procedure gives a warning and recommends that you use other methods. Otherwise, the final MM estimate and the initial scale estimate are reported. You can specify  $\alpha$  with the ALPHA= option following the BIASTEST= option. By default, ALPHA=0.99.

## Asymptotic Covariance and Confidence Intervals

Since the MM estimate is computed as a M estimate with a known scale in the last step, the asymptotic covariance for the M estimate can be used here for the asymptotic covariance of the MM estimate. Besides the three estimators H1, H2, and H3 as described in the section “Asymptotic Covariance and Confidence Intervals” on page 6843, a weighted covariance estimator H4 is available. H4 is calculated as

$$K^2 \frac{[1/(n-p)] \sum (\psi(r_i))^2}{[(1/n) \sum (\psi'(r_i))]^2} \mathbf{W}^{-1}$$

where  $K = 1 + \frac{p}{n} \frac{\text{Var}(\psi')}{(E\psi')^2}$  is the correction factor and  $W_{jk} = \frac{1}{\bar{w}} \sum w_i x_{ij} x_{ik}$ ,  $\bar{w} = \frac{1}{n} \sum w_i$ .

You can specify these estimators with the option ASYMPCOV= [H1 | H2 | H3 | H4]. The ROBUSTREG procedure uses H4 as the default. Confidence intervals for estimated parameters are computed from the diagonal elements of the estimated asymptotic covariance matrix.

## R Square and Deviance

The robust version of R-square for the MM estimate is defined as

$$R^2 = \frac{\sum \rho\left(\frac{y_i - \hat{\mu}}{\hat{s}}\right) - \sum \rho\left(\frac{y_i - \mathbf{x}'_i \hat{\boldsymbol{\theta}}}{\hat{s}}\right)}{\sum \rho\left(\frac{y_i - \hat{\mu}}{\hat{s}}\right)}$$

and the robust deviance is defined as the optimal value of the objective function on the  $\sigma^2$  scale,

$$D = 2\hat{s}^2 \sum \rho\left(\frac{y_i - \mathbf{x}'_i \hat{\boldsymbol{\theta}}}{\hat{s}}\right)$$

where  $\rho' = \psi$ ,  $\hat{\boldsymbol{\theta}}$  is the MM estimator of  $\boldsymbol{\theta}$ ,  $\hat{\mu}$  is the MM estimator of location, and  $\hat{s}$  is the MM estimator of the scale parameter in the full model.

## Linear Tests

For MM estimation, the same  $\rho$  test and  $R_n^2$  test used for M estimation can be used. See the section “Linear Tests” on page 6844 for details.

## Model Selection

For MM estimation, the same two model selection methods used for M estimation can be used. See the section “Model Selection” on page 6844 for details.

## Robust Distance

The ROBUSTREG procedure uses the robust multivariate location and scatter estimates for leverage-point detection. The procedure computes a robust version of the Mahalanobis distance by using a generalized minimum covariance determinant (MCD) method. The original MCD method was proposed by Rousseeuw (1984).

## Algorithm

PROC ROBUSTREG implements a generalized MCD algorithm based on the fast-MCD algorithm formulated by Rousseeuw and Van Driessen (1999), which is similar to the algorithm for least trimmed squares (LTS).

## Mahalanobis Distance versus Robust Distance

The canonical Mahalanobis distance is defined as

$$\text{MD}(\mathbf{x}_i) = [(\mathbf{x}_i - \bar{\mathbf{x}})' \bar{\mathbf{C}}(\mathbf{X})^{-1} (\mathbf{x}_i - \bar{\mathbf{x}})]^{1/2}$$

where  $\bar{\mathbf{x}} = \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i$  and  $\bar{\mathbf{C}}(\mathbf{X}) = \frac{1}{n-1} \sum_{i=1}^n (\mathbf{x}_i - \bar{\mathbf{x}})' (\mathbf{x}_i - \bar{\mathbf{x}})$  are the empirical multivariate location and scatter, respectively. Here  $\mathbf{x}_i = (x_{i1}, \dots, x_{ip})'$  excludes the intercept. The relation between the Mahalanobis distance  $\text{MD}(\mathbf{x}_i)$  and the hat matrix  $\mathbf{H} = (h_{ij}) = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'$  is

$$h_{ii} = \frac{1}{n-1} \text{MD}_i^2 + \frac{1}{n}$$



The canonical robust distance is defined as

$$RD(\mathbf{x}_i) = [(\mathbf{x}_i - \mathbf{T}(\mathbf{X}))' \mathbf{C}(\mathbf{X})^{-1} (\mathbf{x}_i - \mathbf{T}(\mathbf{X}))]^{1/2}$$

where  $\mathbf{T}(\mathbf{X})$  and  $\mathbf{C}(\mathbf{X})$  are the robust multivariate location and scatter, respectively, obtained by MCD.

To achieve robustness, the MCD algorithm estimates the covariance of a multivariate data set mainly through an MCD  $h$ -point subset of the data set. This subset has the smallest sample-covariance determinant among all the possible  $h$ -subsets. Accordingly, the breakdown value for the MCD algorithm equals  $\frac{(n-h)}{n}$ . This means the MCD estimate is reliable, even if up to  $\frac{100(n-h)}{n}\%$  observations in the data set are contaminated.

## Low-Dimensional Structure

It is possible that the original data are in  $p$  dimensional space, but the  $h$ -point subset that yields the minimum covariance determinant lies in a lower-dimensional hyperplane. Applying the canonical MCD algorithm to such a data set would result in a singular covariance problem (called exact fit in Rousseeuw and Van Driessen (1999)), so that the relevant robust distances cannot be computed. To deal with the singularity problem and provide further leverage point analysis, PROC ROBUSTREG implements a generalized MCD algorithm. See the section “Generalized MCD Algorithm” on page 6857 for details. The algorithm distinguishes in-(hyper)plane points from off-(hyper)plane points, and performs MCD leverage point analysis in the dimension-reduced space by projecting all points onto the hyperplane.

Low-dimensional structure is often induced by classification covariates. Suppose, in a study with 25 female subjects and 5 male subjects, that *gender* is the only classification effect. If the breakdown setting is larger than  $\frac{5}{(25+5)}$ , the canonical MCD algorithm fails, and so does the relevant leverage point analysis. In this case, the MCD  $h$ -subset would contain only female observations and the constant gender in the  $h$ -subset would cause the relevant MCD estimate to be singular. The generalized MCD algorithm solves that problem by identifying all male observations as off-plane leverage points, and then carries out the leverage point analysis with all the other covariates being centered separately for female and male groups against their group means.

In general, low-dimensional structure is not necessarily due to classification covariates. Imagine that 80 children are supposed to play on a straight trail (denoted by  $y = x$ ), but some adventurous children go off the trail. The following statements generate the children data and the relevant scatter plot.

```
data children;
 do i=1 to 80;
 off_trail=ranuni(321)>.9;
 x=rannor(111)*ranuni(321);
 trail_x=(i-40)/80*3;
 trail_y=trail_x;
 if off_trail=1 then y=x-1+rannor(321);
 else y=x;
 output;
 end;
run;

proc sgplot data=children;
 series x=trail_x y=trail_y/lineattrs=(color="red" pattern=4);
 scatter x=x y=y/group=off_trail;
 ellipse x=x y=y/alpha=.05 lineattrs=(color="green" pattern=34);
run;
```

Figure 80.17 shows the positions of all the 80 children, the trail (as a red dashed line), and a contour curve of regular Mahalanobis distance centered at the mean position (as a green dotted ellipse). In terms of regular Mahalanobis distance, the associated covariance estimate is not singular, but its relevant leverage point analysis completely ignores the trail (which is the entity of the low-dimensional structure). The children outside of the ellipse are defined as leverage points, but the children off the trail would not be viewed as leverage points unless they have large Mahalanobis distances. As mentioned in Rousseeuw and Van Driessen (1999), the canonical MCD method can find the low-dimensional structure, but it does not provide further robust covariance estimation because the MCD covariance estimate is singular. As an improved version of the canonical MCD method, the generalized MCD method can find the trail, identify the children off the trail as off-plane leverage points, and further execute in-plane leverage analysis. The following statements apply the generalized MCD algorithm on the children data set.

```
ods graphics on;
proc robustreg data=children plots=ddplot(label=none);
 model i = x y/leverage(mcdinfo opc);
run;
ods graphics off;
```

**Figure 80.17** Scatter Plot for Children Data

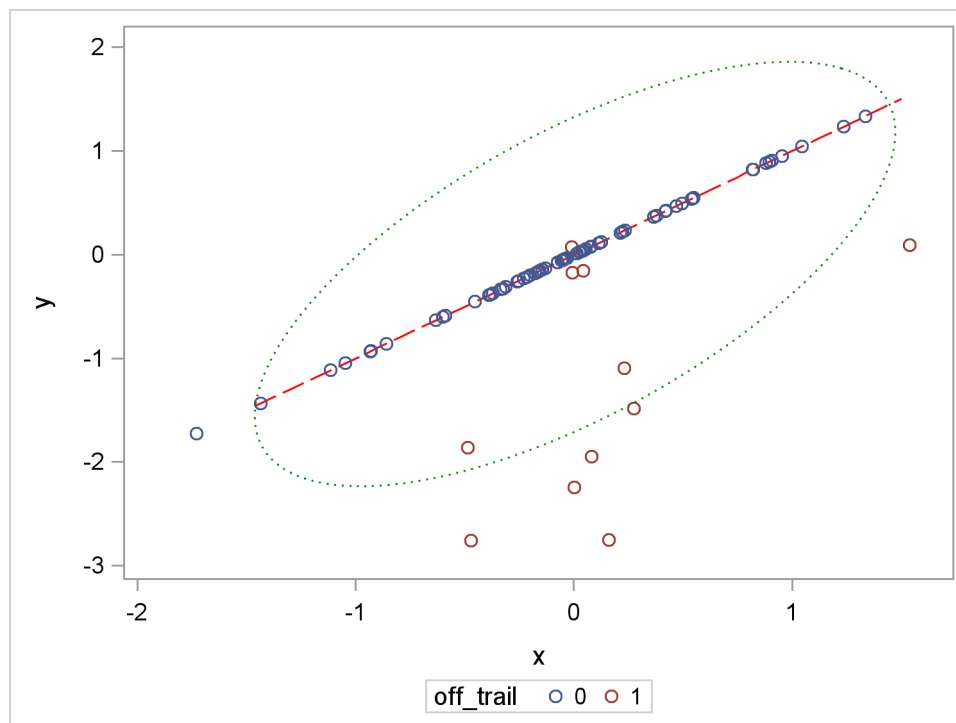


Figure 80.18 exactly identifies the equation underlying the trail. The analysis projects off-plane points onto the trail and computes their projected robust distances and projected Mahalanobis distances the same way as is done for the in-plane points.

**Figure 80.18** Robust Dependence Equations

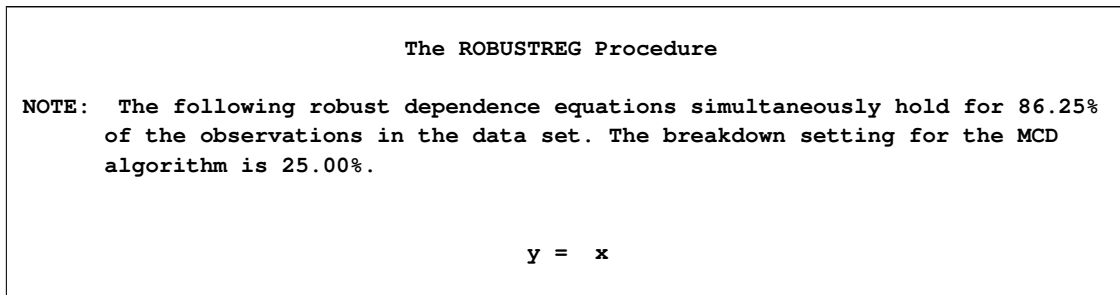
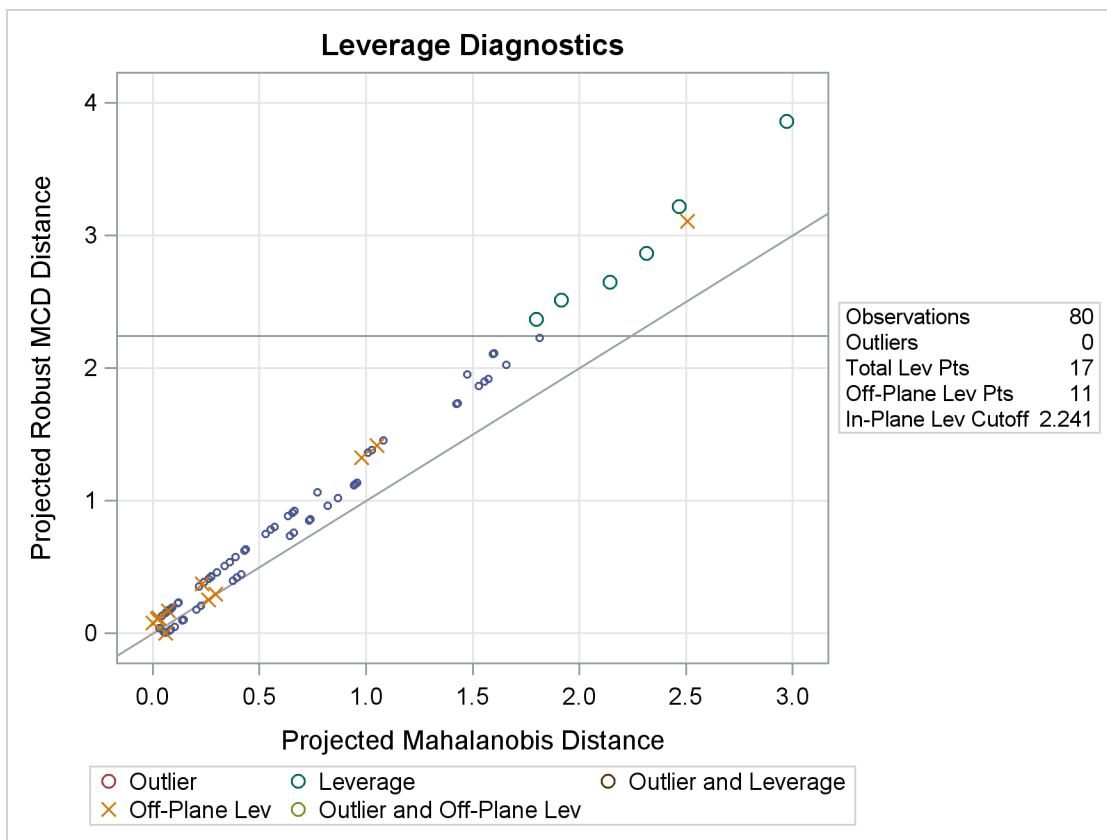


Figure 80.19 shows the relevant distance-distance plot. Robust distance is typically larger than Mahalanobis distance because the sample covariance can be strongly influenced by unusual points that cause the sample covariance to be larger than the MCD covariance.

**Figure 80.19** DDPlot for Children Data



**NOTE:** The PROC ROBUSTREG step in this example is used to obtain the leverage diagnostics; the response is not relevant for this analysis.

Through the off-plane and in-plane symbols and the horizontal cutoff line in Figure 80.19, you can separate all the children into four groups:

- on-trail and close to the MCD center

- on-trail but far away from the MCD center
- off-trail but close to the MCD center
- off-trail and far away from the MCD center

The children in the latter three groups are defined as leverage points in PROC ROBUSTREG.

### Generalized MCD Algorithm

The generalized MCD algorithm follows the same resampling strategy as the canonical MCD algorithm by Rousseeuw and Van Driessen (1999) but with modifications in the following aspects.

1. Data are orthonormalized before further processing. The orthonormalized covariates,  $\mathbf{x}_i^*$ , are defined by  $\mathbf{x}_i^* = (\mathbf{x}_i - \bar{\mathbf{x}})\mathbf{P}\mathbf{\Lambda}^{-1/2}$ , where  $\mathbf{P}$  and  $\mathbf{\Lambda}$  are the eigenvector and eigenvalue matrices of  $\bar{\mathbf{C}}(\mathbf{X})$  (that is,  $\bar{\mathbf{C}}(\mathbf{X}) = \mathbf{P}\mathbf{\Lambda}\mathbf{P}'$ ).
2. Let

$$S_h(\mathbf{X}^*) = \frac{1}{h-1} \sum_{j=1}^h (\mathbf{x}_{i_j}^* - \bar{\mathbf{x}}^*)' (\mathbf{x}_{i_j}^* - \bar{\mathbf{x}}^*) = \sum_{j=1}^{p-1} \lambda_j \mathbf{p}_j \mathbf{p}_j'$$

denote the covariance and eigendecomposition for a low-dimensional  $h$ -subset  $\{\mathbf{x}_{i_1}^*, \dots, \mathbf{x}_{i_h}^*\}$ , where  $\bar{\mathbf{x}}^* = \frac{1}{h} \sum_{j=1}^h \mathbf{x}_{i_j}^*$  and the eigenvalues satisfy

$$\lambda_1 \geq \dots \geq \lambda_q > 0 = \lambda_{q+1} = \dots = \lambda_p$$

Then, the rank of  $S_h(\mathbf{X}^*)$  equals  $q$ , and the pseudo-determinant of  $S_h(\mathbf{X}^*)$  is defined as  $\prod_{j=1}^q \lambda_j$ .

In finite precision arithmetic,  $q$  is defined as the number of  $\lambda$ 's with  $\frac{\lambda_i}{\lambda_1}$  being larger than a certain tolerance value. You can specify this tolerance with the PTOL suboption of the LEVERAGE option.

3. Given  $S_h(\mathbf{X}^*)$  and  $\bar{\mathbf{x}}^*$  as the covariance and center estimates, the projected Mahalanobis distance for  $\mathbf{x}_i$  is defined as

$$\left[ \sum_{j=1}^q \frac{((\mathbf{x}_i^* - \bar{\mathbf{x}}^*)\mathbf{p}_j)^2}{\lambda_j} \right]^{1/2}$$

The generalized algorithm also computes off-plane distance for each  $\mathbf{x}_i$  as

$$\left[ \sum_{j=q+1}^p ((\mathbf{x}_i^* - \bar{\mathbf{x}}^*)\mathbf{p}_j)^2 \right]^{1/2}$$

In finite precision arithmetic,  $((\mathbf{x}_i^* - \bar{\mathbf{x}}^*)\mathbf{p}_j)^2$  in the previous off-plane formula are truncated to zero if they satisfy

$$\frac{((\mathbf{x}_i^* - \bar{\mathbf{x}}^*)\mathbf{p}_j)^2}{\lambda_j} \leq \text{cutoff}$$

You can tune this cutoff by using either the PCUTOFF or the PALPHA suboption of the LEVERAGE option. The points with zero off-plane distances are called in-plane points; otherwise, they are called off-plane points. Analogous to ordering all points in terms of their canonical Mahalanobis distances, with the generalized MCD algorithm the points are first sorted by their off-plane distances, and the points with the same off-plane distance values are further sorted by their projected Mahalanobis distances.

4. Instead of comparing the determinants of  $h$ -subset covariance matrices, the generalized algorithm compares both the ranks and pseudo-determinants of the  $h$ -subset covariance matrices. If the ranks of two matrices are different, the matrix with smaller rank is treated as if its determinant were smaller. If two matrices are of the same rank, they are compared in terms of their pseudo-determinants.
5. Suppose that the  $S_h(\mathbf{X}^*)$  of the minimum determinant is singular. Then the relevant low-dimensional structure or hyperplane can be identified by using the eigendecomposition of  $S_h(\mathbf{X}^*)$ . The eigenvectors that correspond to the nonzero eigenvalues form a basis for the low-dimensional hyperplane. The projected off-plane distance (POD) for  $\mathbf{x}_i$  is defined as the off-plane distance associated with the  $S_h(\mathbf{X}^*)$ . To provide further leverage analysis on the low-dimensional hyperplane, every  $\mathbf{x}_i^*$  is transformed into  $(\mathbf{x}_i^* \mathbf{p}_1, \dots, \mathbf{x}_i^* \mathbf{p}_q)$ , where  $\mathbf{p}_j$  are the eigenvectors of the  $S_h(\mathbf{X}^*)$ . The projected robust distance (PRD) is then computed as the reweighted Mahalanobis distance on all the transformed in-plane points. The off-plane points are assigned zero weights at the reweighting stage, because they are leverage points by definition. The in-plane points are classified into two groups, the normal group and the in-plane leverage group. This classification is made by comparing their projected robust distances with a leverage cutoff value. See the section “Leverage Point and Outlier Detection” on page 6860 for details. This reweighting process mirrors the one proposed by Rousseeuw and Van Driessen (1999). However, the degrees of freedom  $p$  for the reweighting critical  $\chi^2$  value is replaced by  $q$ . You can control the  $\chi^2$  critical value with the MDCUTOFF= or the MCDALPHA= option.

If the data set under investigation has a low-dimensional structure, you can use two ODS objects, DependenceEquations and MCDDependenceEquations, to identify the regressors that are linear combinations of other regressors plus certain constants. The equations in DependenceEquations hold for the entire data set, while the equations in MCDDependenceEquations apply only to the majority of the observations.

By using the OPC suboption of the LEVERAGE option, you can request an ODS table called DroppedComponents. Figure 80.20 shows the DroppedComponents table for the children data example. This table contains a set of coefficient vectors for regressors, which form a basis of the complementary space for the relevant low-dimensional structure.

**Figure 80.20** MCD Dropped Components

| Coefficients for<br>MCD-Dropped<br>Components |                 |
|-----------------------------------------------|-----------------|
| Parameter                                     | Robust<br>Drop1 |
| x                                             | -1.000          |
| y                                             | 1.0000          |

By using the MCDINFO suboption of the LEVERAGE option, you can request that detailed information about the MCD covariance estimate be displayed in four ODS tables: MCDProfile, MCDCenter, MCD Cov, and MCDCorr. Figure 80.21 shows an example of the MCD information tables for the children data. The number of dimensions in the table MCDProfile equals the number of nonintercept regressors minus the number of design dropped components. The specified value of H is the same as  $h$  for the  $h$ -subset that you can specify with the QUANTILE= suboption of the LEVERAGE option in the MODEL statement, and the reweighted H is the number of observations that are actually used to compute the MCD center and MCD covariance after the reweighting step of the MCD algorithm.

**Figure 80.21** MCD Information

| MCD Profile                         |  |  |        |
|-------------------------------------|--|--|--------|
| Number of Dimensions                |  |  | 2      |
| Number of Robust Dropped Components |  |  | 1      |
| Number of Observations              |  |  | 80     |
| Number of Off-Plane Observations    |  |  | 11     |
| Specified Value of H                |  |  | 60     |
| Reweighted Value of H               |  |  | 63     |
| Breakdown Value                     |  |  | 0.2500 |

| MCD Center     |           |        |  |
|----------------|-----------|--------|--|
| Parameter Name | Parameter | Center |  |
| x              | x         | 0.0307 |  |
| y              | y         | 0.0307 |  |

| MCD Covariance |  |          |          |
|----------------|--|----------|----------|
|                |  | x        | y        |
| x              |  | 0.207713 | 0.207713 |
| y              |  | 0.207713 | 0.207713 |

| MCD Correlation |  |   |   |
|-----------------|--|---|---|
|                 |  | x | y |
| x               |  | 1 | 1 |
| y               |  | 1 | 1 |

## Leverage Point and Outlier Detection

The regular variable LEVERAGE is defined as

$$\text{LEVERAGE} = \begin{cases} 0 & \text{if } \text{RD}(\mathbf{x}_i) \leq C(p) \\ 1 & \text{otherwise} \end{cases}$$

where  $C(p) = \sqrt{\chi_{p;1-\alpha}^2}$  is the cutoff value.  $C(p)$  can be set with the leverage CUTOFF= option, and  $\alpha$  can be set with the leverage CUTOFFALPHA= option.

If projected robust distances are computed for a data set that has a low-dimensional structure, the default cutoff value is  $C(q) = \sqrt{\chi_{q;1-\alpha}^2}$  where  $q$  is the dimensionality of the low-dimensional space. The LEVERAGE is then defined as

$$\text{LEVERAGE} = \begin{cases} 0 & \text{if } \text{POD}(\mathbf{x}_i) = 0 \text{ and } \text{PRD}(\mathbf{x}_i) \leq C(q) \\ 1 & \text{if } \text{POD}(\mathbf{x}_i) = 0 \text{ and } \text{PRD}(\mathbf{x}_i) > C(q) \text{ (called in-plane leverage)} \\ 1 & \text{if } \text{POD}(\mathbf{x}_i) > 0 \text{ (called off-plane leverage)} \end{cases}$$

where POD is the projected off-plane distance and PRD denotes the projected robust distance. You can specify a cutoff value with the CUTOFF or the CUTOFFALPHA suboptions of the LEVERAGE option in the MODEL statement.

Residuals  $r_i, i = 1, \dots, n$ , based on robust regression estimates are used to detect vertical outliers. The variable OUTLIER is defined as

$$\text{OUTLIER} = \begin{cases} 0 & \text{if } |r_i| \leq k\hat{\sigma} \\ 1 & \text{otherwise} \end{cases}$$

where  $\hat{\sigma}$  is the estimated scale in the model and the multiplier  $k$  of the cutoff value is specified by the CUTOFF= option in the MODEL statement. By default,  $k = 3$ .

An ODS table called Diagnostics contains the LEVERAGE and OUTLIER variables.

## Implementation of the WEIGHT Statement

You can use the WEIGHT statement to specify a weight variable in the input data set. See the section “WEIGHT Statement” on page 6838 for more information. This section describes how PROC ROBUSTREG implements the WEIGHT statement for each of the estimation methods and for leverage detection.

### M Estimation

If you use M estimation with a known scale, instead of minimizing  $Q(\boldsymbol{\theta}) = \sum_{i=1}^n \rho\left(\frac{r_i}{\sigma}\right)$ , the weighted M estimation minimizes the weighted Huber-type objective function

$$Q(\boldsymbol{\theta}) = \sum_{i=1}^n v_i \rho\left(\frac{r_i}{\sigma}\right),$$

where  $v$  is the weight variable specified by the WEIGHT statement. If you use M estimation with an unknown scale, the weight variable is used in the location steps but not in the scale steps. See the section “M Estimation” on page 6838 and the SCALE= option for more details. For estimating the covariance of the weighted M estimation,  $\psi(r_i)$  and  $\psi'(r_i)$  are obtained from the final iteration of the weighted M estimation, and  $\mathbf{X}'\mathbf{X}$  and  $\mathbf{W}$  are respectively replaced by  $\mathbf{X}'\mathbf{V}\mathbf{X}$  and  $W_{jk} = \sum v_i \psi'(r_i) x_{ij} x_{ik}$ , where  $\mathbf{V}$  is a diagonal matrix with its diagonal elements being  $v_i$ 's. See the section “Asymptotic Covariance and Confidence Intervals” on page 6843 for more information. The weight variable does not affect the model degrees of freedom  $p$  and the error degrees of freedom  $n - p$ .

## LTS Estimation

LTS estimation ignores the weight variable.

## S Estimation

S estimation applies the weight variable only in its M-refinement step. Except for the initial estimates, the M-refinement step of S estimation is the same as the weighted M estimation with unknown scale. If you use the NOREFINE suboption, S estimation ignores the weight variable along with the M-refinement step.

## MM Estimation

By default, the initial step of MM estimation is the initial LTS estimation. Unlike the regular LTS estimation, the initial LTS estimation is applied on the weighted data  $(y_i^*, \mathbf{x}_i^*)$ 's, where  $y_i^* = \sqrt{v_i} y_i$  and  $\mathbf{x}_i^* = \sqrt{v_i} \mathbf{x}_i$ . After the initial LTS estimation, the weight variable is ignored for the subsequent scale adjustment.

You can use INITEST=S to specify the initial S estimation as the initial step of the MM estimation. Similarly to the regular S estimation, the weight variable is used only in the M-refinement step of the initial S estimation. There is no subsequent scale adjustment step if the initial S estimation is applied.

Except for the initial estimates, the final M estimation of the MM estimation is the same as the weighted M estimation with known scale.

## Final Weighted Least Squares Estimation

Final weighted least squares estimation is always applied on the weighted data  $(y_i^*, \mathbf{x}_i^*)$  no matter how the weight variable is applied in the preceding estimation. For example, if the option METHOD=LTS is specified along with the option FWLS, although the outliers identified by LTS estimation do not depend on the weight variable, final weighted least squares estimation applies the weight variable on all the points that are not outliers.

## Robust Distances and Leverage Detection

Robust distance computation ignores the weight variable. Because leverage detection depends on robust distance, it also ignores the weight variable.

---

## INEST= Data Set

When you use M or MM estimation, you can use the INEST= data set to specify initial estimates for all the parameters in the model. The INEST= option is ignored if you specify LTS or S estimation by using the



METHOD=LTS or METHOD=S option or if you specify the INITEST= option after the METHOD=MM option in the PROC ROBUSTREG statement. The INEST= data set must contain the intercept variable (named Intercept) and all independent variables in the MODEL statement.

If BY processing is used, the INEST= data set should also include the BY variables, and there must be at least one observation for each BY group. If there is more than one observation in a BY group, the first one read is used for that BY group.

If the INEST= data set also contains the \_TYPE\_ variable, only observations with \_TYPE\_ value “PARMS” are used as starting values.

You can specify starting values for the iteratively reweighted least squares algorithm in the INEST= data set. The INEST= data set has the same structure as the OUTEST= data set but is not required to have all the variables or observations that appear in the OUTEST= data set. One simple use of the INEST= option is passing the previous OUTEST= data set directly to the next model as an INEST= data set, assuming that the two models have the same parameterization.

## OUTEST= Data Set

The OUTEST= data set contains parameter estimates for the model. You can specify a label in the MODEL statement to distinguish between the estimates for different models used by the ROBUSTREG procedure. If the COVOUT option is specified, the OUTEST= data set also contains the estimated covariance matrix of the parameter estimates. If the ROBUSTREG procedure does not converge, the parameter estimates are set to missing in the OUTEST data set.

The OUTEST= data set contains all variables specified in the MODEL statement and the BY statement. One observation consists of parameter values for the model with the dependent variable having the value  $-1$ . If the COVOUT option is specified, there are additional observations that contain the rows of the estimated covariance matrix. For these observations, the dependent variable contains the parameter estimate for the corresponding row variable. The following variables are also added to the data set:

|                        |                                                                                                                                                                  |
|------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>_MODEL_</code>   | is a character variable that contains the label of the MODEL statement, if present. Otherwise, the variable's value is blank.                                    |
| <code>_NAME_</code>    | is a character variable that contains the name of the dependent variable for the parameter estimates or the name of the row for the covariance matrix estimates. |
| <code>_TYPE_</code>    | is a character variable that contains the type of the observation, either PARMS for parameter estimates or COV for covariance estimates.                         |
| <code>_METHOD_</code>  | is a character variable that contains the type of estimation method: either M estimation, LTS estimation, S estimation, or MM estimation.                        |
| <code>_STATUS_</code>  | is a character variable that contains the status of model fitting: either Converged, Warning, or Failed.                                                         |
| <code>INTERCEPT</code> | is a numeric variable that contains the intercept parameter estimates and covariances.                                                                           |
| <code>_SCALE_</code>   | is a numeric variable that contains the scale parameter estimates.                                                                                               |

Any BY variables specified are also added to the OUTEST= data set.

## Computational Resources

The algorithms for the various estimation methods need a different amount of memory for working space. Let  $p$  be the number of parameters estimated and  $n$  be the number of observations used in the model estimation.

For M estimation, the minimum working space (in bytes) needed is

$$3n + 2p^2 + 30p$$

If sufficient space is available, the input data set is also kept in memory; otherwise, the input data set is read again for computing the iteratively reweighted least squares estimates and the execution time of the procedure increases substantially. For each reweighted least squares,  $O(np^2 + p^3)$  multiplications and additions are required for computing the crossproduct matrix and its inverse. The  $O(v)$  notation means that, for large values of the argument,  $v$ ,  $O(v)$  is approximately a constant times  $v$ .

Since the iteratively reweighted least squares algorithm converges very quickly (normally within fewer than 20 iterations), the computation of M estimates is fast.

LTS estimation is more expensive in computation. The minimum working space (in bytes) needed is

$$np + 12n + 4p^2 + 60p$$

The memory is mainly used to store the current data used by LTS for modeling. The LTS algorithm uses subsampling and spends much of its computing time on resampling and computing estimates for subsamples. Since it resamples if singularity is detected, it might take more time if the data set has serious singularities.

The MCD algorithm for leverage-point diagnostics is similar to the LTS algorithm.

## ODS Table Names

The ROBUSTREG procedure assigns a name to each table it creates. You can specify these names when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in the following table.

**Table 80.12** ODS Tables Produced by PROC ROBUSTREG

| ODS Table Name      | Description                           | Statement | Option      |
|---------------------|---------------------------------------|-----------|-------------|
| BestEstimates       | Best final estimates for LTS          | PROC      | SUBANALYSIS |
| BestSubEstimates    | Best estimates for each subgroup      | PROC      | SUBANALYSIS |
| BiasTest            | Bias test for MM estimation           | PROC      | BIATEST     |
| ClassLevels         | Classification variable levels        | CLASS     | Default     |
| CorrB               | Parameter estimate correlation matrix | MODEL     | CORRB       |
| CovB                | Parameter estimate covariance matrix  | MODEL     | COVB        |
| CStep               | C-step for LTS fitting                | PROC      | SUBANALYSIS |
| DependenceEquations | Design dependence equations           | MODEL     | LEVERAGE    |
| Diagnostics         | Outlier diagnostics                   | MODEL     | DIAGNOSTICS |

Table 80.12 (continued)

| ODS Table Name         | Description                             | Statement | Option             |
|------------------------|-----------------------------------------|-----------|--------------------|
| DiagSummary            | Summary of the outlier diagnostics      | MODEL     | Default            |
| DroppedComponents      | Coefficients for MCD-dropped components | MODEL     | LEVERAGE (OPC)     |
| GoodFit                | R square, deviance, AIC, and BIC        | MODEL     | METHOD             |
| InitLTSPROFILE         | Profile for initial LTS estimate        | PROC      | METHOD             |
| InitSProfile           | Profile for initial S estimate          | PROC      | METHOD             |
| IterHistory            | Iteration history                       | PROC      | ITPRINT            |
| LTSEstimates           | LTS parameter estimates                 | PROC      | METHOD             |
| LTSLocationScale       | Location and scale for LTS              | PROC      | METHOD             |
| LTSProfile             | Profile for LTS estimator               | PROC      | METHOD             |
| LTSRsquare             | R square for LTS estimate               | PROC      | METHOD             |
| MCDDependenceEquations | Robust dependence equations             | MODEL     | LEVERAGE           |
| MCDProfile             | MCD profile                             | MODEL     | LEVERAGE (MCDINFO) |
| MCDCenter              | MCD center estimate                     | MODEL     | LEVERAGE (MCDINFO) |
| MCDcov                 | MCD covariance estimate                 | MODEL     | LEVERAGE (MCDINFO) |
| MCDcorr                | MCD correlation estimate                | MODEL     | LEVERAGE (MCDINFO) |
| MMProfile              | Profile for MM estimator                | PROC      | METHOD             |
| ModelInfo              | Model information                       | MODEL     | Default            |
| NObs                   | Observations summary                    | PROC      | Default            |
| ParameterEstimates     | Parameter estimates                     | MODEL     | Default            |
| ParameterEstimatesF    | Final weighted LS estimates             | PROC      | FWLS               |
| ParameterEstimatesR    | Reduced parameter estimates             | TEST      | Default            |
| ParmInfo               | Parameter indices                       | MODEL     | Default            |
| SProfile               | Profile for S estimator                 | PROC      | METHOD             |
| Groups                 | Groups for LTS fitting                  | PROC      | SUBANALYSIS        |
| SummaryStatistics      | Summary statistics for model variables  | MODEL     | Default            |
| Tests                  | Results for tests                       | TEST      | Default            |

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “[Statistical Graphics Using ODS.](#)”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS.](#)”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “[A Primer on ODS Statistical Graphics](#)” on page 599 in Chapter 21, “[Statistical Graphics Using ODS.](#)”

If the model includes a single continuous independent variable, a plot of robust fit against this variable (FITPLOT) is provided by default. Two plots are particularly useful in revealing outliers and leverage points. The first is a scatter plot of the standardized robust residuals against the robust distances (RDPLOT). The second is a scatter plot of the robust distances against the classical Mahalanobis distances (DDPLOT). In addition to these two plots, a histogram and a quantile-quantile plot of the standardized robust residuals are also helpful.

PROC ROBUSTREG assigns a name to each graph it creates using ODS. You can use these names to refer to the graphs when using ODS. The names and PLOTS= options are listed in [Table 80.13](#).

**Table 80.13** Graphs Produced by PROC ROBUSTREG

| ODS Graph Name | Plot Description                                                                                                 | Statement | PLOTS= Option |
|----------------|------------------------------------------------------------------------------------------------------------------|-----------|---------------|
| DDPlot         | Robust distance versus Mahalanobis distance (or projected robust distance versus Projected Mahalanobis distance) | PROC      | DDPLOT        |
| FitPlot        | Robust fit versus independent variable                                                                           | PROC      | FITPLOT       |
| Histogram      | Histogram of standardized robust residuals                                                                       | PROC      | HISTOGRAM     |
| QQPlot         | Q-Q plot of standardized robust residuals                                                                        | PROC      | QQPLOT        |
| RDPlot         | Standardized robust residual versus robust distance (or projected robust distance)                               | PROC      | RDPLOT        |

## Fit Plot

When the model has a single independent continuous variable (with or without the intercept), the ROBUSTREG procedure automatically creates a plot of robust fit against this independent variable.

The following simple example shows the fit plot. The data, from Rousseeuw and Leroy (1987, Table 3), include the logarithm of surface temperature and the logarithm of light intensity for 47 stars in the direction of the constellation Cygnus.

```
data star;
 input index x y @@;
 label x = 'Log Temperature'
 y = 'Log Light Intensity';
 datalines;
 1 4.37 5.23 2 4.56 5.74 3 4.26 4.93 4 4.56 5.74
 5 4.30 5.19 6 4.46 5.46 7 3.84 4.65 8 4.57 5.27
 9 4.26 5.57 10 4.37 5.12 11 3.49 5.73 12 4.43 5.45
 13 4.48 5.42 14 4.01 4.05 15 4.29 4.26 16 4.42 4.58
 17 4.23 3.94 18 4.42 4.18 19 4.23 4.18 20 3.49 5.89
 21 4.29 4.38 22 4.29 4.22 23 4.42 4.42 24 4.49 4.85
 25 4.38 5.02 26 4.42 4.66 27 4.29 4.66 28 4.38 4.90
 29 4.22 4.39 30 3.48 6.05 31 4.38 4.42 32 4.56 5.10
 33 4.45 5.22 34 3.49 6.29 35 4.23 4.34 36 4.62 5.62
 37 4.53 5.10 38 4.45 5.22 39 4.53 5.18 40 4.43 5.57
 41 4.38 4.62 42 4.45 5.06 43 4.50 5.34 44 4.45 5.34
 45 4.55 5.54 46 4.45 4.98 47 4.42 4.50
 ;
```

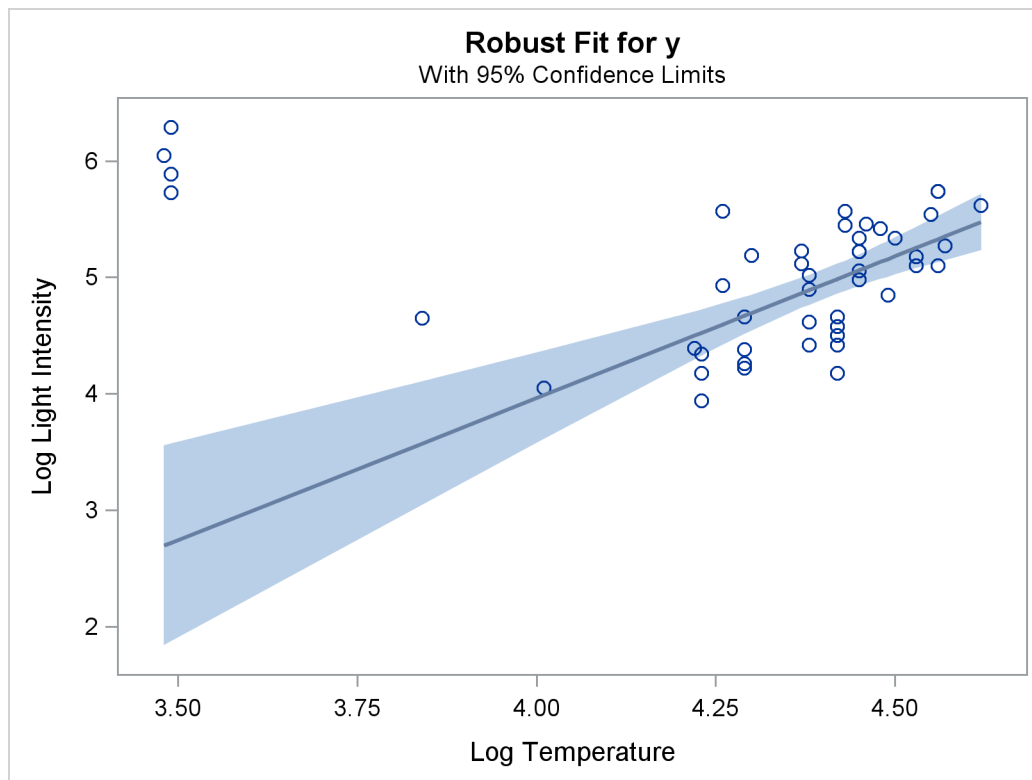
The following statements plot the robust fit of the logarithm of light intensity with the MM method against the logarithm of the surface temperature.

```
ods graphics on;

proc robustreg data=star method=mm;
 model y = x;
run;
```

Figure 80.22 shows the fit plot. Confidence limits are added on the plot by default.

Figure 80.22 Robust Fit



You can suppress the confidence limits with the NOLIMITS option, as shown in the following statements:

```
proc robustreg data=star method=mm plot=fitplot(nolimits);
 model y = x;
run;
```

### Distance-Distance Plot

The distance-distance plot (DDPLOT) is mainly used for leverage-point diagnostics. It is a scatter plot of the robust distances (or projected robust distances) against the classical Mahalanobis distances (or projected classical Mahalanobis distances) for the independent variables. See the section “[Leverage Point and Outlier Detection](#)” on page 6860 for details about the robust distance.

You can use the PLOT=DDPLOT option to request this plot. The following statements use the stack data set in the section “[M Estimation](#)” on page 6811 to create the single plot shown in [Figure 80.5](#).

```
proc robustreg data=stack plot=ddplot;
 model y = x1 x2 x3;
run;
```

The reference lines represent the cutoff values. The diagonal line is also drawn to show the distribution of the distances. By default, all outliers and leverage points are labeled with observation numbers. To change the default, you can use the LABEL= option as described in [Table 80.2](#).

If you specify ID variables in the ID statement, the values of the first ID variable instead of observation numbers are used as labels.

## Residual-Distance Plot

The residual-distance plot (RDPLOT) is used for both outlier and leverage-point diagnostics. It is a scatter plot of the standardized robust residuals against the robust distances. See the section “[Leverage Point and Outlier Detection](#)” on page 6860 for details about the robust distance.

You can use the PLOT=RDPLOT option to request this plot. The following statements use the stack data set in the section “[M Estimation](#)” on page 6811 to create the plot shown in [Figure 80.4](#).

```
proc robustreg data=stack plot=rdplot;
 model y = x1 x2 x3;
run;
```

The reference lines represent the cutoff values. By default, all outliers and leverage points are labeled with observation numbers. To change the default, you can use the LABEL= option as described in [Table 80.2](#).

If you specify ID variables in the ID statement, the values of the first ID variable instead of observation numbers are used as labels.

## Histogram and Q-Q Plot

PROC ROBUSTREG produces a histogram and a Q-Q plot for the standardized robust residuals. The histogram is superimposed with a normal density curve and a kernel density curve. Using the stack data set in the section “[M Estimation](#)” on page 6811, the following statements create the plots in [Figure 80.6](#) and [Figure 80.7](#).

```
proc robustreg data=stack plots=(histogram qqplot);
 model y = x1 x2 x3;
run;
```

---

## Examples: ROBUSTREG Procedure

---

### Example 80.1: Comparison of Robust Estimates

This example contrasts several of the robust methods available in the ROBUSTREG procedure.

The following statements generate 1,000 random observations. The first 900 observations are from a linear model, and the last 100 observations are significantly biased in the  $y$ -direction. In other words, 10% of the observations are contaminated with outliers.

```
data a (drop=i);
 do i=1 to 1000;
 x1=rannor(1234);
 x2=rannor(1234);
 e=rannor(1234);
 if i > 900 then y=100 + e;
 else y=10 + 5*x1 + 3*x2 + .5 * e;
 output;
 end;
run;
```

The following statements invoke PROC REG and PROC ROBUSTREG with the data set a.

```
proc reg data=a;
 model y = x1 x2;
run;

proc robustreg data=a method=m;
 model y = x1 x2;
run;

proc robustreg data=a method=mm seed=100;
 model y = x1 x2;
run;

proc robustreg data=a method=s seed=100;
 model y = x1 x2;
run;

proc robustreg data=a method=lts seed=100;
 model y = x1 x2;
run;
```

The tables of parameter estimates generated by using M estimation, MM estimation, S estimation, and LTS estimation in the ROBUSTREG procedure are shown in [Output 80.1.2](#), [Output 80.1.3](#), [Output 80.1.4](#), and [Output 80.1.5](#), respectively. For comparison, the ordinary least squares (OLS) estimates produced by the REG procedure (Chapter 79, “The REG Procedure”) are shown in [Output 80.1.1](#). The four robust methods, M, MM, S, and LTS, correctly estimate the regression coefficients for the underlying model (10, 5, and 3), but the OLS estimate does not.

**Output 80.1.1** OLS Estimates for Data with 10% Contamination

| The REG Procedure     |    |                    |                |         |         |
|-----------------------|----|--------------------|----------------|---------|---------|
| Model: MODEL1         |    |                    |                |         |         |
| Dependent Variable: y |    |                    |                |         |         |
| Parameter Estimates   |    |                    |                |         |         |
| Variable              | DF | Parameter Estimate | Standard Error | t Value | Pr >  t |
| Intercept             | 1  | 19.06712           | 0.86322        | 22.09   | <.0001  |
| x1                    | 1  | 3.55485            | 0.86892        | 4.09    | <.0001  |
| x2                    | 1  | 2.12341            | 0.83039        | 2.56    | 0.0107  |



**Output 80.1.2** M Estimates for Data with 10% Contamination

| The ROBUSTREG Procedure         |              |          |                |                       |         |            |            |
|---------------------------------|--------------|----------|----------------|-----------------------|---------|------------|------------|
| Model Information               |              |          |                |                       |         |            |            |
| Data Set                        | WORK.A       |          |                |                       |         |            |            |
| Dependent Variable              | Y            |          |                |                       |         |            |            |
| Number of Independent Variables | 2            |          |                |                       |         |            |            |
| Number of Observations          | 1000         |          |                |                       |         |            |            |
| Method                          | M Estimation |          |                |                       |         |            |            |
| Parameter Estimates             |              |          |                |                       |         |            |            |
| Parameter                       | DF           | Estimate | Standard Error | 95% Confidence Limits |         | Chi-Square | Pr > ChiSq |
| Intercept                       | 1            | 10.0024  | 0.0174         | 9.9683                | 10.0364 | 331908     | <.0001     |
| x1                              | 1            | 5.0077   | 0.0175         | 4.9735                | 5.0420  | 82106.9    | <.0001     |
| x2                              | 1            | 3.0161   | 0.0167         | 2.9834                | 3.0488  | 32612.5    | <.0001     |
| Scale                           | 1            | 0.5780   |                |                       |         |            |            |

**Output 80.1.3** MM Estimates for Data with 10% Contamination

| The ROBUSTREG Procedure         |               |          |                |                       |         |            |            |
|---------------------------------|---------------|----------|----------------|-----------------------|---------|------------|------------|
| Model Information               |               |          |                |                       |         |            |            |
| Data Set                        | WORK.A        |          |                |                       |         |            |            |
| Dependent Variable              | Y             |          |                |                       |         |            |            |
| Number of Independent Variables | 2             |          |                |                       |         |            |            |
| Number of Observations          | 1000          |          |                |                       |         |            |            |
| Method                          | MM Estimation |          |                |                       |         |            |            |
| Parameter Estimates             |               |          |                |                       |         |            |            |
| Parameter                       | DF            | Estimate | Standard Error | 95% Confidence Limits |         | Chi-Square | Pr > ChiSq |
| Intercept                       | 1             | 10.0035  | 0.0176         | 9.9690                | 10.0379 | 323947     | <.0001     |
| x1                              | 1             | 5.0085   | 0.0178         | 4.9737                | 5.0433  | 79600.6    | <.0001     |
| x2                              | 1             | 3.0181   | 0.0168         | 2.9851                | 3.0511  | 32165.0    | <.0001     |
| Scale                           | 0             | 0.6733   |                |                       |         |            |            |

**Output 80.1.4** S Estimates for Data with 10% Contamination

```

The ROBUSTREG Procedure

Model Information

Data Set WORK.A
Dependent Variable Y
Number of Independent Variables 2
Number of Observations 1000
Method S Estimation

Parameter Estimates

Parameter DF Estimate Standard Error 95% Confidence Limits Chi-Square Pr > ChiSq

Intercept 1 10.0055 0.0180 9.9703 10.0408 309917 <.0001
x1 1 5.0096 0.0182 4.9740 5.0452 76045.2 <.0001
x2 1 3.0210 0.0172 2.9873 3.0547 30841.3 <.0001
Scale 0 0.6721

```

**Output 80.1.5** LTS Estimates for Data with 10% Contamination

```

The ROBUSTREG Procedure

Model Information

Data Set WORK.A
Dependent Variable Y
Number of Independent Variables 2
Number of Observations 1000
Method LTS Estimation

LTS Parameter Estimates

Parameter DF Estimate

Intercept 1 10.0083
x1 1 5.0316
x2 1 3.0396
Scale (sLTS) 0 0.5880
Scale (Wscale) 0 0.5113

```

The next statements demonstrate that if the percentage of contamination is increased to 40%, the M method and the MM method with default options fail to estimate the underlying model. [Output 80.1.6](#) and [Output 80.1.7](#) display these estimates. However, by tuning the constant  $c$  for the M method and the constants INITH and K0 for the MM method, you can increase the breakdown values of the estimates and capture the right model. [Output 80.1.8](#) and [Output 80.1.9](#) display these estimates. Similarly, you can tune the constant EFF for the S method and the constant H for the LTS method and correctly estimate the underlying model with these methods. Results are not presented.

```

data b (drop=i);
 do i=1 to 1000;
 x1=rannor(1234);
 x2=rannor(1234);
 e=rannor(1234);
 if i > 600 then y=100 + e;
 else y=10 + 5*x1 + 3*x2 + .5 * e;
 output;
 end;
run;

proc robustreg data=b method=m;
 model y = x1 x2;
run;

proc robustreg data=b method=mm;
 model y = x1 x2;
run;

proc robustreg data=b method=m(wf=bisquare(c=2));
 model y = x1 x2;
run;

proc robustreg data=b method=mm(inith=502 k0=1.8);
 model y = x1 x2;
run;

```

### Output 80.1.6 M Estimates (Default Setting) for Data with 40% Contamination

| The ROBUSTREG Procedure         |              |          |                |                       |         |            |            |
|---------------------------------|--------------|----------|----------------|-----------------------|---------|------------|------------|
| Model Information               |              |          |                |                       |         |            |            |
| Data Set                        | WORK.B       |          |                |                       |         |            |            |
| Dependent Variable              | y            |          |                |                       |         |            |            |
| Number of Independent Variables | 2            |          |                |                       |         |            |            |
| Number of Observations          | 1000         |          |                |                       |         |            |            |
| Method                          | M Estimation |          |                |                       |         |            |            |
| Parameter Estimates             |              |          |                |                       |         |            |            |
| Parameter                       | DF           | Estimate | Standard Error | 95% Confidence Limits |         | Chi-Square | Pr > ChiSq |
| Intercept                       | 1            | 44.8991  | 1.5609         | 41.8399               | 47.9584 | 827.46     | <.0001     |
| x1                              | 1            | 2.4309   | 1.5712         | -0.6485               | 5.5104  | 2.39       | 0.1218     |
| x2                              | 1            | 1.3742   | 1.5015         | -1.5687               | 4.3171  | 0.84       | 0.3601     |
| Scale                           | 1            | 56.6342  |                |                       |         |            |            |

**Output 80.1.7** MM Estimates (Default Setting) for Data with 40% Contamination

```

The ROBUSTREG Procedure

Model Information

Data Set WORK.B
Dependent Variable Y
Number of Independent Variables 2
Number of Observations 1000
Method MM Estimation

Parameter Estimates

Parameter DF Estimate Standard Error 95% Confidence Limits Chi-Square Pr > ChiSq

Intercept 1 43.0607 1.7978 39.5370 46.5844 573.67 <.0001
x1 1 2.7369 1.8140 -0.8185 6.2924 2.28 0.1314
x2 1 1.5211 1.7265 -1.8628 4.9049 0.78 0.3783
Scale 0 52.8496

```

**Output 80.1.8** M Estimates (Tuned) for Data with 40% Contamination

```

The ROBUSTREG Procedure

Model Information

Data Set WORK.B
Dependent Variable Y
Number of Independent Variables 2
Number of Observations 1000
Method M Estimation

Parameter Estimates

Parameter DF Estimate Standard Error 95% Confidence Limits Chi-Square Pr > ChiSq

Intercept 1 10.0137 0.0219 9.9708 10.0565 209688 <.0001
x1 1 4.9905 0.0220 4.9473 5.0336 51399.1 <.0001
x2 1 3.0399 0.0210 2.9987 3.0811 20882.4 <.0001
Scale 1 1.0531

```

**Output 80.1.9** MM Estimates (Tuned) for Data with 40% Contamination

| The ROBUSTREG Procedure         |               |          |                |                       |         |            |            |
|---------------------------------|---------------|----------|----------------|-----------------------|---------|------------|------------|
| Model Information               |               |          |                |                       |         |            |            |
| Data Set                        | WORK.B        |          |                |                       |         |            |            |
| Dependent Variable              | Y             |          |                |                       |         |            |            |
| Number of Independent Variables | 2             |          |                |                       |         |            |            |
| Number of Observations          | 1000          |          |                |                       |         |            |            |
| Method                          | MM Estimation |          |                |                       |         |            |            |
| Parameter Estimates             |               |          |                |                       |         |            |            |
| Parameter                       | DF            | Estimate | Standard Error | 95% Confidence Limits |         | Chi-Square | Pr > ChiSq |
| Intercept                       | 1             | 10.0103  | 0.0213         | 9.9686                | 10.0520 | 221639     | <.0001     |
| x1                              | 1             | 4.9890   | 0.0218         | 4.9463                | 5.0316  | 52535.9    | <.0001     |
| x2                              | 1             | 3.0363   | 0.0201         | 2.9970                | 3.0756  | 22895.5    | <.0001     |
| Scale                           | 0             | 1.8992   |                |                       |         |            |            |

When there are bad leverage points, the M method fails to estimate the underlying model no matter what constant  $c$  you use. In this case, other methods (LTS, S, and MM) in PROC ROBUSTREG, which are robust to bad leverage points, correctly estimate the underlying model.

The following statements generate and analyze 1,000 observations with 1% bad high leverage points.

```
data c (drop=i);
 do i=1 to 1000;
 x1=rannor(1234);
 x2=rannor(1234);
 e=rannor(1234);
 if i > 600 then y=100 + e;
 else y=10 + 5*x1 + 3*x2 + .5 * e;
 if i < 11 then x1=200 * rannor(1234);
 if i < 11 then x2=200 * rannor(1234);
 if i < 11 then y= 100*e;
 output;
 end;
run;

proc robustreg data=c method=mm(inith=502 k0=1.8) seed=100;
 model y = x1 x2;
run;

proc robustreg data=c method=s(k0=1.8) seed=100;
 model y = x1 x2;
run;
```

```
proc robustreg data=c method=lts(h=502) seed=100;
 model y = x1 x2;
run;
```

Output 80.1.10 displays the MM estimates with initial LTS estimates, Output 80.1.11 displays the S estimates, and Output 80.1.12 displays the LTS estimates.

**Output 80.1.10** MM Estimates for Data with 1% Leverage Points

| The ROBUSTREG Procedure         |               |          |                |                       |         |            |            |
|---------------------------------|---------------|----------|----------------|-----------------------|---------|------------|------------|
| Model Information               |               |          |                |                       |         |            |            |
| Data Set                        | WORK.C        |          |                |                       |         |            |            |
| Dependent Variable              | Y             |          |                |                       |         |            |            |
| Number of Independent Variables | 2             |          |                |                       |         |            |            |
| Number of Observations          | 1000          |          |                |                       |         |            |            |
| Method                          | MM Estimation |          |                |                       |         |            |            |
| Parameter Estimates             |               |          |                |                       |         |            |            |
| Parameter                       | DF            | Estimate | Standard Error | 95% Confidence Limits |         | Chi-Square | Pr > ChiSq |
| Intercept                       | 1             | 9.9820   | 0.0215         | 9.9398                | 10.0241 | 215369     | <.0001     |
| x1                              | 1             | 5.0303   | 0.0206         | 4.9898                | 5.0707  | 59469.1    | <.0001     |
| x2                              | 1             | 3.0222   | 0.0221         | 2.9789                | 3.0655  | 18744.9    | <.0001     |
| Scale                           | 0             | 2.2134   |                |                       |         |            |            |

**Output 80.1.11** S Estimates for Data with 1% Leverage Points

| The ROBUSTREG Procedure         |              |          |                |                       |         |            |            |
|---------------------------------|--------------|----------|----------------|-----------------------|---------|------------|------------|
| Model Information               |              |          |                |                       |         |            |            |
| Data Set                        | WORK.C       |          |                |                       |         |            |            |
| Dependent Variable              | Y            |          |                |                       |         |            |            |
| Number of Independent Variables | 2            |          |                |                       |         |            |            |
| Number of Observations          | 1000         |          |                |                       |         |            |            |
| Method                          | S Estimation |          |                |                       |         |            |            |
| Parameter Estimates             |              |          |                |                       |         |            |            |
| Parameter                       | DF           | Estimate | Standard Error | 95% Confidence Limits |         | Chi-Square | Pr > ChiSq |
| Intercept                       | 1            | 9.9808   | 0.0216         | 9.9383                | 10.0232 | 212532     | <.0001     |
| x1                              | 1            | 5.0303   | 0.0208         | 4.9896                | 5.0710  | 58656.3    | <.0001     |
| x2                              | 1            | 3.0217   | 0.0222         | 2.9782                | 3.0652  | 18555.7    | <.0001     |
| Scale                           | 0            | 2.2094   |                |                       |         |            |            |

**Output 80.1.12** LTS Estimates for Data with 1% Leverage Points

| The ROBUSTREG Procedure         |    |                |
|---------------------------------|----|----------------|
| Model Information               |    |                |
| Data Set                        |    | WORK.C         |
| Dependent Variable              |    | Y              |
| Number of Independent Variables |    | 2              |
| Number of Observations          |    | 1000           |
| Method                          |    | LTS Estimation |
| LTS Parameter Estimates         |    |                |
| Parameter                       | DF | Estimate       |
| Intercept                       | 1  | 9.9742         |
| x1                              | 1  | 5.0010         |
| x2                              | 1  | 3.0219         |
| Scale (sLTS)                    | 0  | 0.9952         |
| Scale (Wscale)                  | 0  | 0.5216         |

**Example 80.2: Robust ANOVA**

The classical analysis of variance (ANOVA) technique based on least squares assumes that the underlying experimental errors are normally distributed. However, data often contain outliers due to recording or other errors. In other cases, extreme responses occur when control variables in the experiments are set to extremes. It is important to distinguish these extreme points and determine whether they are outliers or important extreme cases. You can use the ROBUSTREG procedure for robust analysis of variance based on M estimation. Typically, there are no high leverage points in a well-designed experiment, so M estimation is appropriate.

The following example shows how to use the ROBUSTREG procedure for robust ANOVA.

An experiment was carried out to study the effects of two successive treatments (T1, T2) on the recovery time of mice with certain diseases. Sixteen mice were randomly assigned into four groups for the four different combinations of the treatments. The recovery times (time) were recorded (in hours) as shown in the following data set recover.

```
data recover;
 input T1 $ T2 $ time @@;
 datalines;
0 0 20.2 0 0 23.9 0 0 21.9 0 0 42.4
1 0 27.2 1 0 34.0 1 0 27.4 1 0 28.5
0 1 25.9 0 1 34.5 0 1 25.1 0 1 34.2
1 1 35.0 1 1 33.9 1 1 38.3 1 1 39.9
;
```

The following statements invoke the GLM procedure (Chapter 42, “The GLM Procedure”) for a standard ANOVA:

```
proc glm data=recover;
 class T1 T2;
 model time = T1 T2 T1*T2;
run;
```

**Output 80.2.1** Overall ANOVA

| The GLM Procedure        |          |                |             |           |        |
|--------------------------|----------|----------------|-------------|-----------|--------|
| Dependent Variable: time |          |                |             |           |        |
| Source                   | DF       | Sum of Squares | Mean Square | F Value   | Pr > F |
| Model                    | 3        | 209.9118750    | 69.9706250  | 1.86      | 0.1905 |
| Error                    | 12       | 451.9225000    | 37.6602083  |           |        |
| Corrected Total          | 15       | 661.8343750    |             |           |        |
|                          | R-Square | Coeff Var      | Root MSE    | time Mean |        |
|                          | 0.317167 | 19.94488       | 6.136791    | 30.76875  |        |

**Output 80.2.2** Model ANOVA

| Source | DF | Type I SS   | Mean Square | F Value | Pr > F |
|--------|----|-------------|-------------|---------|--------|
| T1     | 1  | 81.4506250  | 81.4506250  | 2.16    | 0.1671 |
| T2     | 1  | 106.6056250 | 106.6056250 | 2.83    | 0.1183 |
| T1*T2  | 1  | 21.8556250  | 21.8556250  | 0.58    | 0.4609 |

Output 80.2.1 indicates that the overall model effect is not significant at the 10% level, and Output 80.2.2 indicates that neither treatment is significant at the 10% level.

The following statements invoke the ROBUSTREG procedure with the same model:

```
proc robustreg data=recover;
 class T1 T2;
 model time = T1 T2 T1*T2 / diagnostics;
 T1_T2: test T1*T2;
 output out=robout r=resid sr=stdres;
run;
```

Output 80.2.3 shows some basic information about the model and the response variable time.



**Output 80.2.3** Model Fitting Information and Summary Statistics

| The ROBUSTREG Procedure                    |              |         |         |         |                    |        |
|--------------------------------------------|--------------|---------|---------|---------|--------------------|--------|
| Model Information                          |              |         |         |         |                    |        |
| Data Set                                   | WORK.RECOVER |         |         |         |                    |        |
| Dependent Variable                         | time         |         |         |         |                    |        |
| Number of Independent Variables            | 2            |         |         |         |                    |        |
| Number of Continuous Independent Variables | 0            |         |         |         |                    |        |
| Number of Class Independent Variables      | 2            |         |         |         |                    |        |
| Number of Observations                     | 16           |         |         |         |                    |        |
| Method                                     | M Estimation |         |         |         |                    |        |
| Summary Statistics                         |              |         |         |         |                    |        |
| Variable                                   | Q1           | Median  | Q3      | Mean    | Standard Deviation | MAD    |
| time                                       | 25.5000      | 31.2000 | 34.7500 | 30.7688 | 6.6425             | 6.8941 |

The “Parameter Estimates” table in [Output 80.2.4](#) indicates that the main effects of both treatments are significant at the 5% level.

**Output 80.2.4** Model Parameter Estimates

| Parameter Estimates |     |          |                |                       |         |            |            |
|---------------------|-----|----------|----------------|-----------------------|---------|------------|------------|
| Parameter           | DF  | Estimate | Standard Error | 95% Confidence Limits |         | Chi-Square | Pr > ChiSq |
| Intercept           | 1   | 36.7655  | 2.0489         | 32.7497               | 40.7814 | 321.98     | <.0001     |
| T1                  | 0   | -6.8307  | 2.8976         | -12.5100              | -1.1514 | 5.56       | 0.0184     |
| T1                  | 1   | 0.0000   | .              | .                     | .       | .          | .          |
| T2                  | 0   | -7.6755  | 2.8976         | -13.3548              | -1.9962 | 7.02       | 0.0081     |
| T2                  | 1   | 0.0000   | .              | .                     | .       | .          | .          |
| T1*T2               | 0 0 | -0.2619  | 4.0979         | -8.2936               | 7.7698  | 0.00       | 0.9490     |
| T1*T2               | 0 1 | 0.0000   | .              | .                     | .       | .          | .          |
| T1*T2               | 1 0 | 0.0000   | .              | .                     | .       | .          | .          |
| T1*T2               | 1 1 | 0.0000   | .              | .                     | .       | .          | .          |
| Scale               | 1   | 3.5346   |                |                       |         |            |            |

The reason for the difference between the traditional ANOVA and the robust ANOVA is explained by [Output 80.2.5](#), which shows that the fourth observation is an outlier. Further investigation shows that the original value of 24.4 for the fourth observation was recorded incorrectly.

[Output 80.2.6](#) displays the robust test results. The interaction between the two treatments is not significant. [Output 80.2.7](#) displays the robust residuals and standardized robust residuals.

**Output 80.2.5** Diagnostics

| Diagnostics |                 |         |
|-------------|-----------------|---------|
|             | Standardized    |         |
| Obs         | Robust Residual | Outlier |
| 4           | 5.7722          | *       |

**Output 80.2.6** Test of Significance

| Robust Linear Test T1_T2 |                |        |    |               |         |
|--------------------------|----------------|--------|----|---------------|---------|
| Test                     | Test Statistic | Lambda | DF | Chi-Square Pr | > ChiSq |
| Rho                      | 0.0041         | 0.7977 | 1  | 0.01          | 0.9431  |
| Rn2                      | 0.0041         |        | 1  | 0.00          | 0.9490  |

**Output 80.2.7** ROBUSTREG Output

| Obs | T1 | T2 | time | resid   | stdres   |
|-----|----|----|------|---------|----------|
| 1   | 0  | 0  | 20.2 | -1.7974 | -0.50851 |
| 2   | 0  | 0  | 23.9 | 1.9026  | 0.53827  |
| 3   | 0  | 0  | 21.9 | -0.0974 | -0.02756 |
| 4   | 0  | 0  | 42.4 | 20.4026 | 5.77222  |
| 5   | 1  | 0  | 27.2 | -1.8900 | -0.53472 |
| 6   | 1  | 0  | 34.0 | 4.9100  | 1.38911  |
| 7   | 1  | 0  | 27.4 | -1.6900 | -0.47813 |
| 8   | 1  | 0  | 28.5 | -0.5900 | -0.16693 |
| 9   | 0  | 1  | 25.9 | -4.0348 | -1.14152 |
| 10  | 0  | 1  | 34.5 | 4.5652  | 1.29156  |
| 11  | 0  | 1  | 25.1 | -4.8348 | -1.36785 |
| 12  | 0  | 1  | 34.2 | 4.2652  | 1.20668  |
| 13  | 1  | 1  | 35.0 | -1.7655 | -0.49950 |
| 14  | 1  | 1  | 33.9 | -2.8655 | -0.81070 |
| 15  | 1  | 1  | 38.3 | 1.5345  | 0.43413  |
| 16  | 1  | 1  | 39.9 | 3.1345  | 0.88679  |

**Example 80.3: Growth Study of De Long and Summers**

Robust regression and outlier detection techniques have considerable applications to econometrics. The following example from Zaman, Rousseeuw, and Orhan (2001) shows how these techniques substantially improve the ordinary least squares (OLS) results for the growth study of De Long and Summers.

De Long and Summers (1991) studied the national growth of 61 countries from 1960 to 1985 by using OLS with the following data set growth.

```
data growth;
 input country $ GDP LFG EQP NEQ GAP @@;
 datalines;
Argentin 0.0089 0.0118 0.0214 0.2286 0.6079
Austria 0.0332 0.0014 0.0991 0.1349 0.5809
Belgium 0.0256 0.0061 0.0684 0.1653 0.4109
Bolivia 0.0124 0.0209 0.0167 0.1133 0.8634
Botswana 0.0676 0.0239 0.1310 0.1490 0.9474

... more lines ...

Venezuel 0.0120 0.0378 0.0340 0.0760 0.4974
Zambia -0.0110 0.0275 0.0702 0.2012 0.8695
Zimbabwe 0.0110 0.0309 0.0843 0.1257 0.8875
;
```

The regression equation they used is

$$\text{GDP} = \beta_0 + \beta_1\text{LFG} + \beta_2\text{GAP} + \beta_3\text{EQP} + \beta_4\text{NEQ} + \epsilon$$

where the response variable is the growth in gross domestic product per worker (GDP) and the regressors are labor force growth (LFG), relative GDP gap (GAP), equipment investment (EQP), and nonequipment investment (NEQ).

The following statements invoke the REG procedure (Chapter 79, “The REG Procedure”) for the OLS analysis:

```
proc reg data=growth;
 model GDP = LFG GAP EQP NEQ;
run;
```

The OLS analysis shown in [Output 80.3.1](#) indicates that GAP and EQP have a significant influence on GDP at the 5% level.

**Output 80.3.1** OLS Estimates

| The REG Procedure       |    |                    |                |         |         |
|-------------------------|----|--------------------|----------------|---------|---------|
| Model: MODEL1           |    |                    |                |         |         |
| Dependent Variable: GDP |    |                    |                |         |         |
| Parameter Estimates     |    |                    |                |         |         |
| Variable                | DF | Parameter Estimate | Standard Error | t Value | Pr >  t |
| Intercept               | 1  | -0.01430           | 0.01028        | -1.39   | 0.1697  |
| LFG                     | 1  | -0.02981           | 0.19838        | -0.15   | 0.8811  |
| GAP                     | 1  | 0.02026            | 0.00917        | 2.21    | 0.0313  |
| EQP                     | 1  | 0.26538            | 0.06529        | 4.06    | 0.0002  |
| NEQ                     | 1  | 0.06236            | 0.03482        | 1.79    | 0.0787  |

The following statements invoke the ROBUSTREG procedure with the default M estimation.

```
ods graphics on;

proc robustreg data=growth plots=all;
 model GDP = LFG GAP EQP NEQ / diagnostics leverage;
 id country;
run;

ods graphics off;
```

Output 80.3.2 displays model information and summary statistics for variables in the model.

**Output 80.3.2** Model Fitting Information and Summary Statistics

| The ROBUSTREG Procedure         |        |        |        |              |                    |         |
|---------------------------------|--------|--------|--------|--------------|--------------------|---------|
| Model Information               |        |        |        |              |                    |         |
| Data Set                        |        |        |        | WORK.GROWTH  |                    |         |
| Dependent Variable              |        |        |        | GDP          |                    |         |
| Number of Independent Variables |        |        |        | 4            |                    |         |
| Number of Observations          |        |        |        | 61           |                    |         |
| Method                          |        |        |        | M Estimation |                    |         |
| Summary Statistics              |        |        |        |              |                    |         |
| Variable                        | Q1     | Median | Q3     | Mean         | Standard Deviation | MAD     |
| LFG                             | 0.0118 | 0.0239 | 0.0281 | 0.0211       | 0.00979            | 0.00949 |
| GAP                             | 0.5796 | 0.8015 | 0.8863 | 0.7258       | 0.2181             | 0.1778  |
| EQP                             | 0.0265 | 0.0433 | 0.0720 | 0.0523       | 0.0296             | 0.0325  |
| NEQ                             | 0.0956 | 0.1356 | 0.1812 | 0.1399       | 0.0570             | 0.0624  |
| GDP                             | 0.0121 | 0.0231 | 0.0310 | 0.0224       | 0.0155             | 0.0150  |

Output 80.3.3 displays the M estimates. Besides GAP and EQP, the robust analysis also indicates that NEQ is significant. This new finding is explained by Output 80.3.4, which shows that Zambia, the 60th country in the data, is an outlier. Output 80.3.4 also identifies leverage points based on the robust MCD distances; however, there are no serious high-leverage points in this data set.

**Output 80.3.3** M Estimates

| Parameter Estimates |    |          |                |                       |         |            |            |
|---------------------|----|----------|----------------|-----------------------|---------|------------|------------|
| Parameter           | DF | Estimate | Standard Error | 95% Confidence Limits |         | Chi-Square | Pr > ChiSq |
| Intercept           | 1  | -0.0247  | 0.0097         | -0.0437               | -0.0058 | 6.53       | 0.0106     |
| LFG                 | 1  | 0.1040   | 0.1867         | -0.2619               | 0.4699  | 0.31       | 0.5775     |
| GAP                 | 1  | 0.0250   | 0.0086         | 0.0080                | 0.0419  | 8.36       | 0.0038     |
| EQP                 | 1  | 0.2968   | 0.0614         | 0.1764                | 0.4172  | 23.33      | <.0001     |
| NEQ                 | 1  | 0.0885   | 0.0328         | 0.0242                | 0.1527  | 7.29       | 0.0069     |
| Scale               | 1  | 0.0099   |                |                       |         |            |            |

**Output 80.3.4** Diagnostics

| Diagnostics |           |                      |                     |          |                              |         |
|-------------|-----------|----------------------|---------------------|----------|------------------------------|---------|
| Obs         | country   | Mahalanobis Distance | Robust MCD Distance | Leverage | Standardized Robust Residual | Outlier |
| 1           | Argentina | 2.6083               | 4.0639              | *        | -0.9424                      |         |
| 5           | Botswana  | 3.4351               | 6.7391              | *        | 1.4200                       |         |
| 8           | Canada    | 3.1876               | 4.6843              | *        | -0.1972                      |         |
| 9           | Chile     | 3.6752               | 5.0599              | *        | -1.8784                      |         |
| 17          | Finland   | 2.6024               | 3.8186              | *        | -1.7971                      |         |
| 23          | HongKong  | 2.1225               | 3.8238              | *        | 1.7161                       |         |
| 27          | Israel    | 2.6461               | 5.0336              | *        | 0.0909                       |         |
| 31          | Japan     | 2.9179               | 4.7140              | *        | 0.0216                       |         |
| 53          | Tanzania  | 2.2600               | 4.3193              | *        | -1.8082                      |         |
| 57          | U.S.      | 3.8701               | 5.4874              | *        | 0.1448                       |         |
| 58          | Uruguay   | 2.5953               | 3.9671              | *        | -0.0978                      |         |
| 59          | Venezuel  | 2.9239               | 4.1663              | *        | 0.3573                       |         |
| 60          | Zambia    | 1.8562               | 2.7135              |          | -4.9798                      | *       |
| 61          | Zimbabwe  | 1.9634               | 3.9128              | *        | -2.5959                      |         |

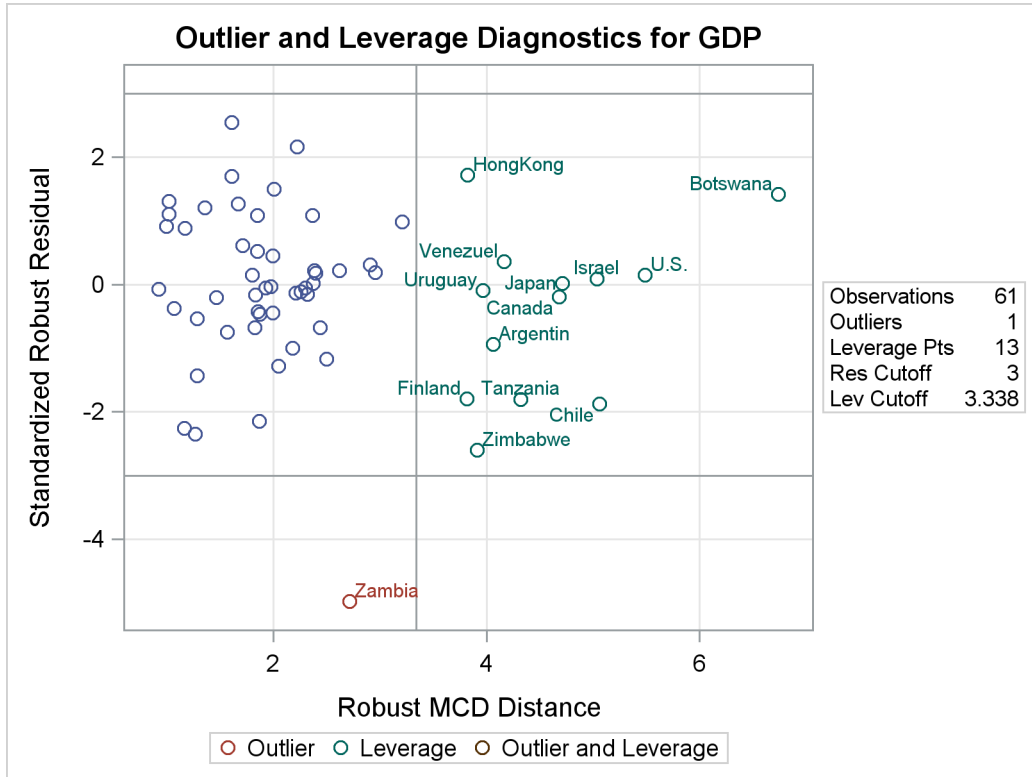
Output 80.3.5 displays robust versions of goodness-of-fit statistics for the model.

**Output 80.3.5** Goodness-of-Fit Statistics

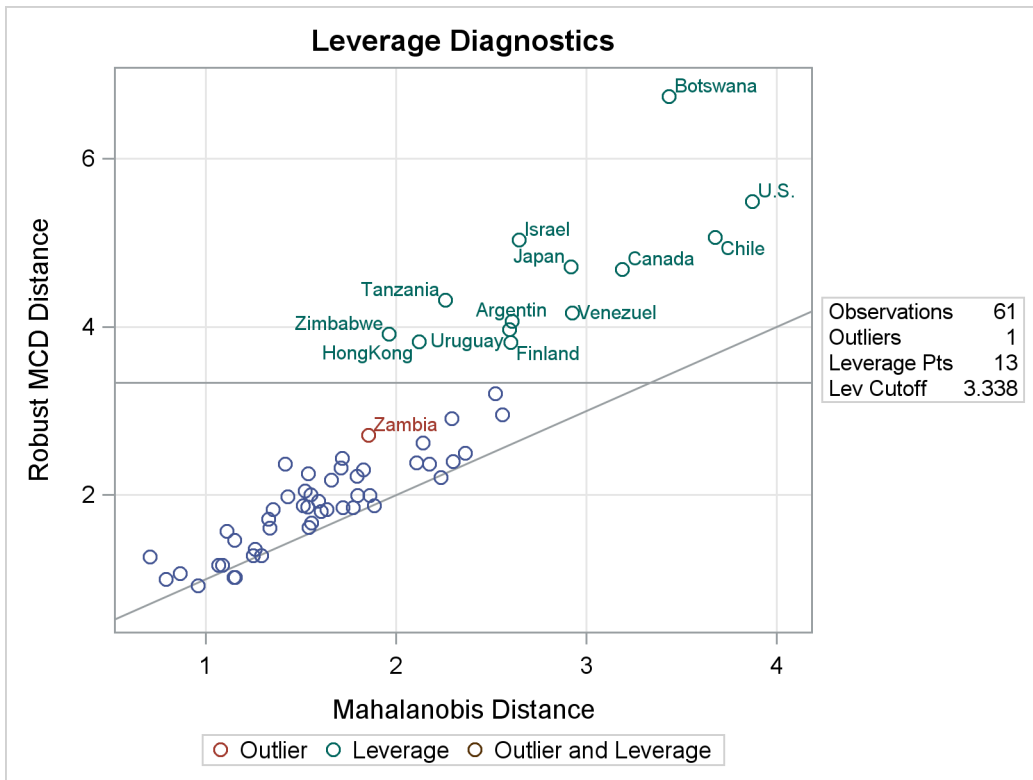
| Goodness-of-Fit |         |
|-----------------|---------|
| Statistic       | Value   |
| R-Square        | 0.3178  |
| AICR            | 80.2134 |
| BICR            | 91.5095 |
| Deviance        | 0.0070  |

The PLOTS=ALL option generates four diagnostic plots. Output 80.3.6 and Output 80.3.7 are for outlier and leverage-point diagnostics. Output 80.3.8 and Output 80.3.9 are a histogram and a Q-Q plot of the standardized robust residuals, respectively.

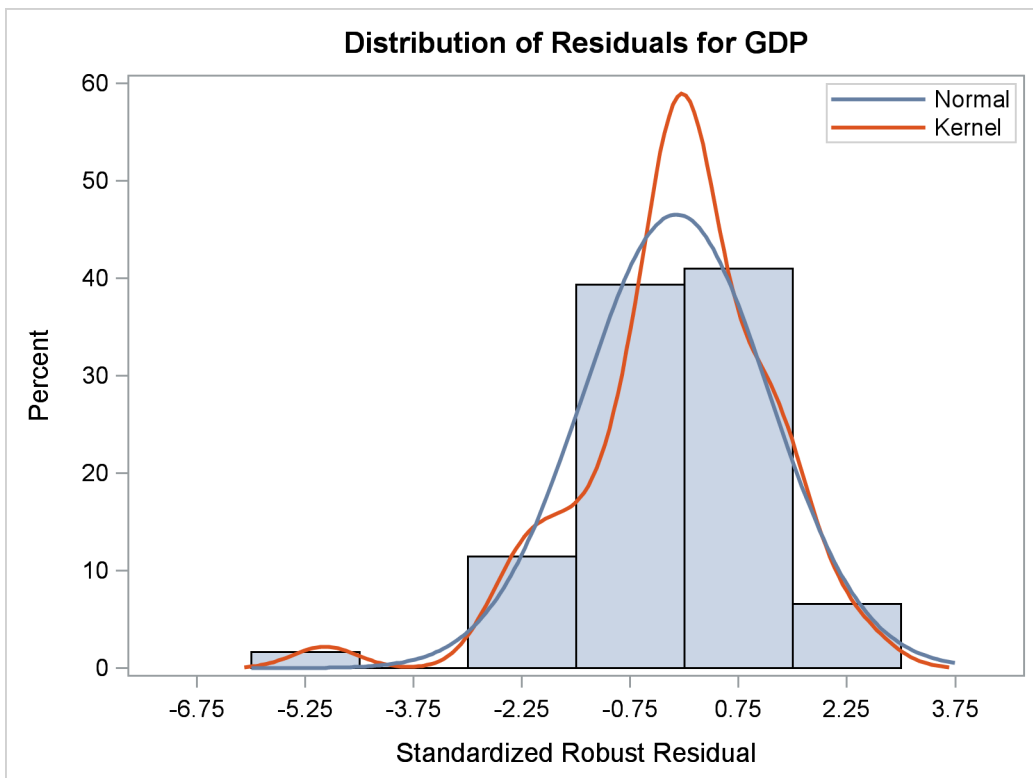
**Output 80.3.6** RDPLLOT for growth Data



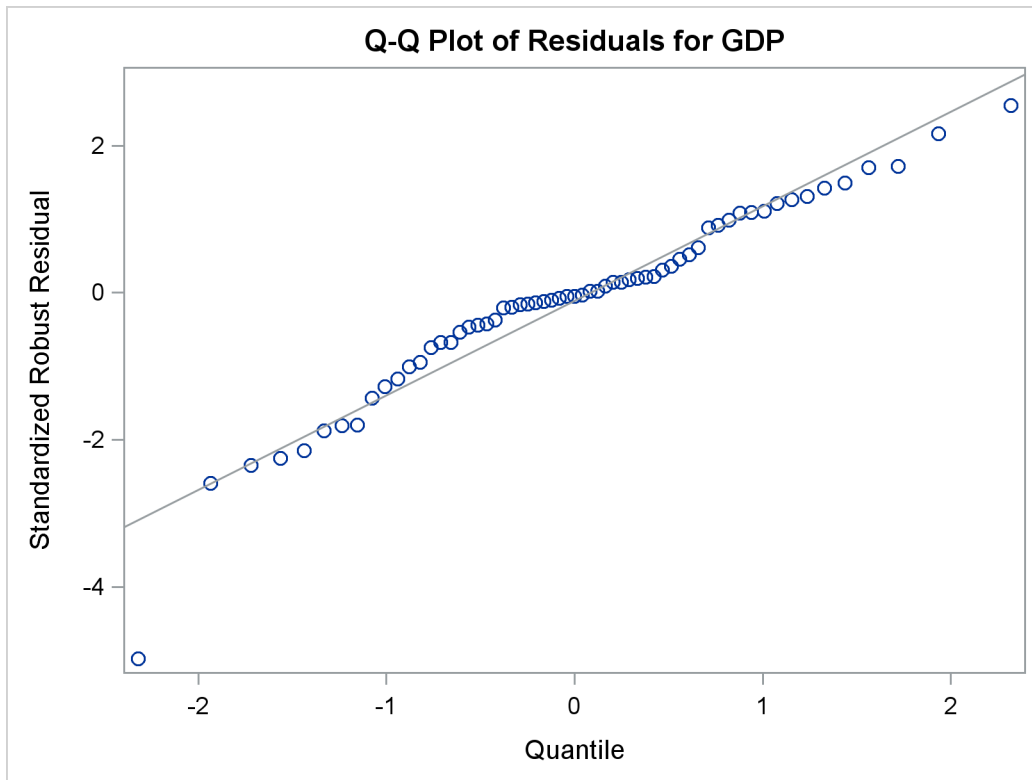
**Output 80.3.7** DDLOT for growth Data



**Output 80.3.8** Histogram



**Output 80.3.9** Q-Q Plot



The following statements invoke the ROBUSTREG procedure with LTS estimation, which was used by Zaman, Rousseeuw, and Orhan (2001). The results are consistent with those of M estimation.

```
proc robustreg method=lts(h=33) fwls data=growth seed=100;
 model GDP = LFG GAP EQP NEQ / diagnostics leverage;
 id country;
run;
```

**Output 80.3.10** LTS Estimates and LTS R Square

| The ROBUSTREG Procedure |    |          |
|-------------------------|----|----------|
| LTS Parameter Estimates |    |          |
| Parameter               | DF | Estimate |
| Intercept               | 1  | -0.0249  |
| LFG                     | 1  | 0.1123   |
| GAP                     | 1  | 0.0214   |
| EQP                     | 1  | 0.2669   |
| NEQ                     | 1  | 0.1110   |
| Scale (sLTS)            | 0  | 0.0076   |
| Scale (Wscale)          | 0  | 0.0109   |



**Output 80.3.10** *continued*

| R-Square for LTS<br>Estimation |        |
|--------------------------------|--------|
| R-Square                       | 0.7418 |

Output 80.3.10 displays the LTS estimates and the LTS R Square.

**Output 80.3.11** Diagnostics

| Diagnostics |           |                         |                           |          |                                    |         |
|-------------|-----------|-------------------------|---------------------------|----------|------------------------------------|---------|
| Obs         | country   | Mahalanobis<br>Distance | Robust<br>MCD<br>Distance | Leverage | Standardized<br>Robust<br>Residual | Outlier |
| 1           | Argentina | 2.6083                  | 4.0639                    | *        | -1.0715                            |         |
| 5           | Botswana  | 3.4351                  | 6.7391                    | *        | 1.6574                             |         |
| 8           | Canada    | 3.1876                  | 4.6843                    | *        | -0.2324                            |         |
| 9           | Chile     | 3.6752                  | 5.0599                    | *        | -2.0896                            |         |
| 17          | Finland   | 2.6024                  | 3.8186                    | *        | -1.6367                            |         |
| 23          | HongKong  | 2.1225                  | 3.8238                    | *        | 1.7570                             |         |
| 27          | Israel    | 2.6461                  | 5.0336                    | *        | 0.2334                             |         |
| 31          | Japan     | 2.9179                  | 4.7140                    | *        | 0.0971                             |         |
| 53          | Tanzania  | 2.2600                  | 4.3193                    | *        | -1.2978                            |         |
| 57          | U.S.      | 3.8701                  | 5.4874                    | *        | 0.0605                             |         |
| 58          | Uruguay   | 2.5953                  | 3.9671                    | *        | -0.0857                            |         |
| 59          | Venezuel  | 2.9239                  | 4.1663                    | *        | 0.4113                             |         |
| 60          | Zambia    | 1.8562                  | 2.7135                    |          | -4.4984                            | *       |
| 61          | Zimbabwe  | 1.9634                  | 3.9128                    | *        | -2.1201                            |         |

Output 80.3.11 displays outlier and leverage-point diagnostics based on the LTS estimates and the robust MCD distances.

**Output 80.3.12** Final Weighted LS Estimates

| Parameter Estimates for Final Weighted Least Squares Fit |    |          |                   |                          |         |                |            |
|----------------------------------------------------------|----|----------|-------------------|--------------------------|---------|----------------|------------|
| Parameter                                                | DF | Estimate | Standard<br>Error | 95% Confidence<br>Limits |         | Chi-<br>Square | Pr > ChiSq |
| Intercept                                                | 1  | -0.0222  | 0.0093            | -0.0405                  | -0.0039 | 5.65           | 0.0175     |
| LFG                                                      | 1  | 0.0446   | 0.1771            | -0.3026                  | 0.3917  | 0.06           | 0.8013     |
| GAP                                                      | 1  | 0.0245   | 0.0082            | 0.0084                   | 0.0406  | 8.89           | 0.0029     |
| EQP                                                      | 1  | 0.2824   | 0.0581            | 0.1685                   | 0.3964  | 23.60          | <.0001     |
| NEQ                                                      | 1  | 0.0849   | 0.0314            | 0.0233                   | 0.1465  | 7.30           | 0.0069     |
| Scale                                                    | 0  | 0.0116   |                   |                          |         |                |            |

Output 80.3.12 displays the final weighted least squares estimates, which are identical to those reported in Zaman, Rousseeuw, and Orhan (2001).

## Example 80.4: Constructed Effects

The algorithms of PROC ROBUSTREG assume that a response variable is linearly dependent on the regressors. However, in practice, a response often depends on some factors in a nonlinear manner. This example demonstrates how a nonlinear response-factor relationship can be modeled by using constructed effects. (See the section “EFFECT Statement” on page 393 of Chapter 19, “Shared Concepts and Topics,” for details.)

The following data set contains 526 female observations and 474 male observations sampled from 2003 National Health and Nutrition Examination Survey (NHANES). Each observation is composed of three values: BMI (body mass index), Age, and Gender, measured for subjects whose ages are between 20 and 60.

```
data BMI;
 input BMI Age Gender $ @@;
 datalines;
46.16 30.33 F 20.67 31.83 F 30.98 51.33 F 30.71 31.42 F
29.81 30.50 M 19.94 25.08 F 29.97 41.67 F 24.48 26.92 F
34.34 51.25 F 20.24 53.67 F 27.72 60.25 F 32.85 41.67 M
22.75 47.50 F 32.78 22.42 F 43.07 29.50 F 38.34 58.50 F
40.03 39.92 F 21.78 56.42 M 28.77 39.83 F 28.77 28.75 F
29.73 54.25 M 33.75 35.67 M 28.48 35.83 M 22.12 29.58 F

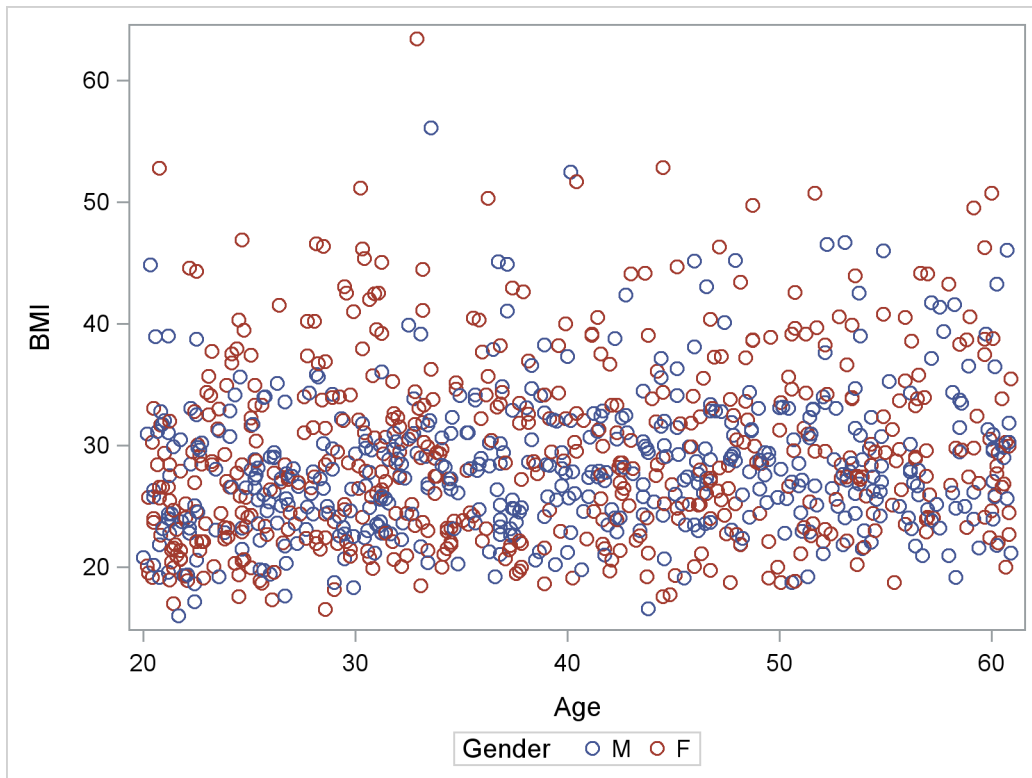
... more lines ...

26.98 42.50 F 29.44 39.75 M 25.60 52.67 F 19.30 22.00 F
26.53 27.92 F 23.77 29.00 F 29.86 60.58 M 25.41 44.08 M
26.53 24.83 M 33.33 42.08 F 30.52 32.50 F 31.89 38.17 F
32.20 35.92 F 21.73 26.67 M 32.10 39.33 M 25.13 51.75 M
;
```

The goal of this analysis is to evaluate whether the BMI by Age curves are different between women and men at a 5% significance level. In order to provide sufficient flexibility to model the effect of Age on BMI, you can use regression splines that you define with an EFFECT statement. In this example, a regression spline of degree 2 with three knots is used for variable Age. The knots are placed at the 25, 50, and 75 percentiles of Age. This analysis assume that there is no interaction between Gender and Age, so that the BMI by Age curves for women and men are the same up to a constant. The following statements produce the BMI by Age scatter plot shown in Output 80.4.1:

```
proc sort data=bmi;
 by age;
run;

ods graphics on;
proc sgplot data=bmi;
 scatter x=age y=bmi/group=gender;
run;
```

**Output 80.4.1** Scatter Plot for BMI Data

The observations with large BMI values (for example, BMI > 40) are outliers that can substantially influence an ordinary least squares (OLS) analysis. [Output 80.4.1](#) shows that the distributions of BMI conditional on Age are skewed toward the side of large BMI, and there are more observations with large BMI values (outliers) in the female group. Hence you can expect a significant Gender difference in the BMI by Age OLS regression analysis. This expectation is confirmed by the OLS Gender  $p$ -value = 0.0059 in [Output 80.4.2](#), which is produced by the following statements:

```
proc glmselect data=bmi;
 class gender;
 effect Age_Sp=spl(age/degree=2 knotmethod=percentiles(3));
 model bmi = gender age_sp /selection=none showpvalues;
 output out=out_ols P=pred R=res;
run;
```

## Output 80.4.2 OLS Estimates

| The GLMSELECT Procedure            |    |           |                |         |         |
|------------------------------------|----|-----------|----------------|---------|---------|
| Least Squares Model (No Selection) |    |           |                |         |         |
| Parameter Estimates                |    |           |                |         |         |
| Parameter                          | DF | Estimate  | Standard Error | t Value | Pr >  t |
| Intercept                          | 1  | 29.890089 | 1.022825       | 29.22   | <.0001  |
| Gender F                           | 1  | 1.167332  | 0.422565       | 2.76    | 0.0058  |
| Gender M                           | 0  | 0         | .              | .       | .       |
| Age_Sp 1                           | 1  | -4.404487 | 1.473761       | -2.99   | 0.0029  |
| Age_Sp 2                           | 1  | -3.329537 | 1.374096       | -2.42   | 0.0156  |
| Age_Sp 3                           | 1  | -0.966875 | 1.314964       | -0.74   | 0.4623  |
| Age_Sp 4                           | 1  | -1.611621 | 1.123854       | -1.43   | 0.1519  |
| Age_Sp 5                           | 1  | -0.484787 | 1.701281       | -0.28   | 0.7757  |
| Age_Sp 6                           | 0  | 0         | .              | .       | .       |

A robust regression method can reduce the outlier influence by automatically assigning smaller or even zero weights to outliers. For the BMI data, a robust regression method is likely to set less weight on observations with large BMI, so more female observations would receive smaller weights than male observations. The following statements invoke PROC ROBUSTREG with the BMI data set:

```
proc robustreg data=bmi method=s seed=100;
 class gender;
 effect Age_Sp=spl(age/degree=2 knotmethod=percentiles(3));
 model bmi = gender age_sp;
 output out=out_s P=pred R=res;
run;
```

Output 80.4.3 shows the parameter estimates and the diagnostics summary produced by PROC ROBUSTREG with the S method. In contrast to OLS, the robust  $p$ -value=0.5573 of the Gender coefficient indicates that the Gender effect is not significant. The outlier diagnostics based on the S estimates find 19 outliers that are assigned lower weights by the S method than by the OLS method.

## Output 80.4.3 S Estimates and S Diagnostics Summary

| The ROBUSTREG Procedure |     |          |                |                       |         |            |            |
|-------------------------|-----|----------|----------------|-----------------------|---------|------------|------------|
| Parameter Estimates     |     |          |                |                       |         |            |            |
| Parameter               | DF  | Estimate | Standard Error | 95% Confidence Limits |         | Chi-Square | Pr > ChiSq |
| Intercept               | 1   | 28.2858  | 1.0081         | 26.3100               | 30.2616 | 787.33     | <.0001     |
| Gender                  | F 1 | 0.2409   | 0.4114         | -0.5654               | 1.0473  | 0.34       | 0.5581     |
| Gender                  | M 0 | 0.0000   | .              | .                     | .       | .          | .          |
| Age_Sp                  | 1 1 | -3.8956  | 1.4376         | -6.7133               | -1.0779 | 7.34       | 0.0067     |
| Age_Sp                  | 2 1 | -1.8692  | 1.3430         | -4.5014               | 0.7630  | 1.94       | 0.1640     |
| Age_Sp                  | 3 1 | -0.8336  | 1.2877         | -3.3574               | 1.6903  | 0.42       | 0.5174     |
| Age_Sp                  | 4 1 | -0.2329  | 1.1055         | -2.3997               | 1.9338  | 0.04       | 0.8331     |
| Age_Sp                  | 5 1 | 0.0055   | 1.6632         | -3.2543               | 3.2652  | 0.00       | 0.9974     |
| Age_Sp                  | 6 0 | 0.0000   | .              | .                     | .       | .          | .          |
| Scale                   | 0   | 6.1715   |                |                       |         |            |            |

| Diagnostics Summary |            |        |
|---------------------|------------|--------|
| Observation Type    | Proportion | Cutoff |
| Outlier             | 0.0190     | 3.0000 |

To further compare the OLS and S outputs, the following statements plot the BMI predictions in variable Age for both methods in the same graph, which is shown in [Output 80.4.4](#):

```

data out2_s;
 set out_s;
 if gender="F" then label="F, S ";
 if gender="M" then label="M, S ";
run;

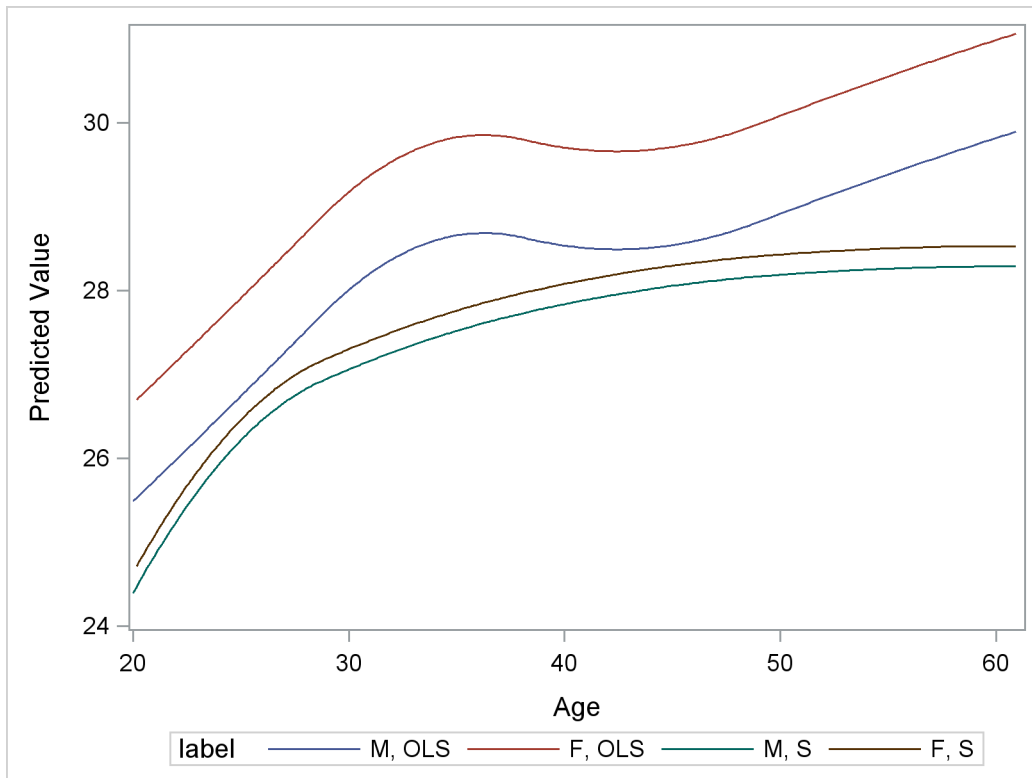
data out2_ols;
 merge bmi out_ols;
 if gender='F' then label='F, OLS';
 if gender='M' then label='M, OLS';
 keep pred bmi gender age label;
run;

data out2;
 set out2_ols out2_s;
run;

proc sgplot data=out2;
 series x=age y=pred/group=label;
run;

```

Output 80.4.4 OLS and S Predictions



You can observe the following differences between the OLS and S predictions:

- The OLS prediction is larger
- The OLS curves have a local maximum near Age = 35

Then, a question remains: is the significance of the Gender effect for the OLS regression due solely to the outlying observations? To tentatively answer this question, the following statements drop the observations with the top 10% of BMI values from the original data set and reapply OLS and S methods on the reduced data set:

```
data three;
 set bmi;
 where bmi<38.315;
run;

proc robustreg data=three method=s seed=100;
 class gender;
 effect Age_Sp=spl(age/degree=2 knotmethod=percentiles(3));
 model bmi = gender age_sp;
 output out=out_s P=pred R=res;
run;
```

```

data out2_s;
 set out_s;
 if gender="F" then label="F, S ";
 if gender="M" then label="M, S ";
run;

proc glmselect data=three outdesign=four;
 class gender;
 effect Age_Sp=spl(age/degree=2 knotmethod=percentiles(3));
 model bmi = gender age_sp /selection=none showpvalues;
 output out=out_ols P=pred R=res;
run;

data out2_ols;
 merge three out_ols;
 if gender='F' then label='F, OLS';
 if gender='M' then label='M, OLS';
 keep pred bmi gender age label;
run;

data out2;
 set out2_ols out2_s;
run;

proc sgplot data=out2;
 series x=age y=pred/group=label;
run;
ods graphics off;

```

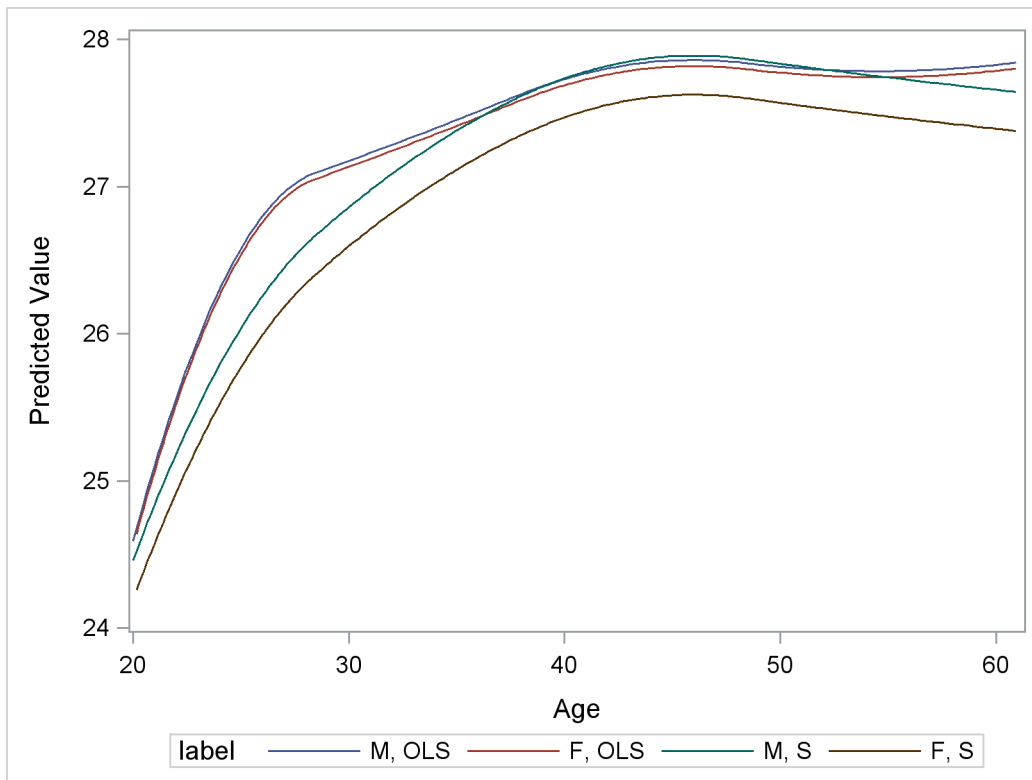
### Output 80.4.5 S Estimates

| The ROBUSTREG Procedure |     |          |                |                       |         |            |            |
|-------------------------|-----|----------|----------------|-----------------------|---------|------------|------------|
| Parameter Estimates     |     |          |                |                       |         |            |            |
| Parameter               | DF  | Estimate | Standard Error | 95% Confidence Limits |         | Chi-Square | Pr > ChiSq |
| Intercept               | 1   | 27.6427  | 0.9741         | 25.7334               | 29.5520 | 805.23     | <.0001     |
| Gender                  | F 1 | -0.2650  | 0.4023         | -1.0535               | 0.5234  | 0.43       | 0.5100     |
| Gender                  | M 0 | 0.0000   | .              | .                     | .       | .          | .          |
| Age_Sp                  | 1 1 | -3.1859  | 1.4032         | -5.9361               | -0.4356 | 5.15       | 0.0232     |
| Age_Sp                  | 2 1 | -1.5354  | 1.3051         | -4.0934               | 1.0226  | 1.38       | 0.2394     |
| Age_Sp                  | 3 1 | -0.3776  | 1.2499         | -2.8273               | 2.0721  | 0.09       | 0.7626     |
| Age_Sp                  | 4 1 | 0.3299   | 1.0668         | -1.7610               | 2.4208  | 0.10       | 0.7572     |
| Age_Sp                  | 5 1 | 0.0949   | 1.6221         | -3.0845               | 3.2742  | 0.00       | 0.9534     |
| Age_Sp                  | 6 0 | 0.0000   | .              | .                     | .       | .          | .          |
| Scale                   | 0   | 4.9440   |                |                       |         |            |            |

**Output 80.4.6** OLS Estimates

| The GLMSELECT Procedure            |    |           |                |         |         |
|------------------------------------|----|-----------|----------------|---------|---------|
| Least Squares Model (No Selection) |    |           |                |         |         |
| Parameter Estimates                |    |           |                |         |         |
| Parameter                          | DF | Estimate  | Standard Error | t Value | Pr >  t |
| Intercept                          | 1  | 27.841568 | 0.780817       | 35.66   | <.0001  |
| Gender F                           | 1  | -0.040924 | 0.317749       | -0.13   | 0.8976  |
| Gender M                           | 0  | 0         | .              | .       | .       |
| Age_Sp 1                           | 1  | -3.253964 | 1.121292       | -2.90   | 0.0038  |
| Age_Sp 2                           | 1  | -0.975273 | 1.034172       | -0.94   | 0.3459  |
| Age_Sp 3                           | 1  | -0.508979 | 0.999609       | -0.51   | 0.6108  |
| Age_Sp 4                           | 1  | 0.089393  | 0.852774       | 0.10    | 0.9165  |
| Age_Sp 5                           | 1  | -0.113706 | 1.298157       | -0.09   | 0.9302  |
| Age_Sp 6                           | 0  | 0         | .              | .       | .       |

**Output 80.4.7** OLS and S Predictions on the Reduced Data Set



In the reduced data set, 71 female observations and 29 male observations are dropped. [Output 80.4.5](#) and [Output 80.4.6](#) respectively show the refitted S and OLS parameter estimates, and [Output 80.4.7](#) displays the fitted curves on the reduced data set. You can see that Gender is no longer significant for the OLS model, and the OLS turning pattern has also disappeared, but the new S curves do not change much from the previous ones. The OLS BMI by Age curves in [Output 80.4.7](#) are closer to the S curves than to the OLS curves in [Output 80.4.4](#). This suggests that indeed the difference between the OLS and S estimate results are due solely to the influence of the outlying observations.



## Example 80.5: Robust Diagnostics

This example models the selling price of a house as a function of several covariates. One of these covariates is a classification variable that indicates whether a house is located on a corner lot (called a corner house in this example). Because corner houses are relatively rare, the inclusion of this classification effect in the model introduces a low-dimensional structure (that is, the majority of the observations are located in a lower dimensional hyperplane defined by being non-corner houses) into the design matrix. As discussed in “Robust Distance” on page 6853, the presence of this low dimensional structure causes difficulties in the traditional computation of robust distances. This example illustrates how you can use the projected robust distance to address those difficulties and to obtain meaningful leverage diagnostics. It also shows how you can use the RD PLOT= and DD PLOT= options to illustrate the outlier-leverage relationship.

The following house price data set contains 66 home resale records on seven variables from February 15 to April 30, 1993 (Data and Story Library 2005). The records are randomly selected from the database maintained by the Albuquerque Board of Realtors.

```
data house;
 input price sqft age feats ne cor tax @@;
 label price = "Selling price"
 sqft = "Square feet of living space"
 age = "Age of home in year"
 feats = "Number out of 11 features (dishwasher, refrigerator,
 microwave, disposer, washer, intercom, skylight(s),
 compactor, dryer, handicap fit, cable TV access)"
 ne = "Located in northeast sector of city (1) or not (0)"
 cor = "Corner location (1) or not (0)"
 tax = "Annual taxes";
 sum = sqft+age+feats+ne+cor+tax;
 id = _N_;
 datalines;
2050 2650 13 7 1 0 1639
2150 2664 6 5 1 0 1193
2150 2921 3 6 1 0 1635
1999 2580 4 4 1 0 1732

... more lines ...

870 1273 4 4 0 0 638
869 1165 7 4 0 0 694
766 1200 7 4 0 1 634
739 970 4 4 0 1 541
;
```

To illustrate the dependence detection ability of the generalized MCD algorithm, an extra variable `sum` is created such that all the observations satisfy  $\text{sum} = \text{sqft} + \text{age} + \text{feats} + \text{ne} + \text{cor} + \text{tax}$ . Adding `sum` does not change the rank of the original design matrix, so that `sum` is expected to be ignored in the model and also in the diagnostics. The next statements apply the MM method and the generalized MCD algorithm to the house price data.

```
ods graphics on;
proc robustreg data=house method=MM plots=all;
 model price = sqft age feats ne cor tax sum /
 leverage(opc mcdinfo) diagnostics;
run;
```

As shown in [Output 80.5.1](#) and [Output 80.5.2](#), PROC ROBUSTREG finds the design dependence equation and forces the parameter estimate of variable sum to be zero.

**Output 80.5.1** MM Estimates

| The ROBUSTREG Procedure |    |          |                |                       |          |            |            |
|-------------------------|----|----------|----------------|-----------------------|----------|------------|------------|
| Parameter Estimates     |    |          |                |                       |          |            |            |
| Parameter               | DF | Estimate | Standard Error | 95% Confidence Limits |          | Chi-Square | Pr > ChiSq |
| Intercept               | 1  | 46.4062  | 79.1714        | -108.767              | 201.5792 | 0.34       | 0.5578     |
| sqft                    | 1  | 0.3809   | 0.0756         | 0.2327                | 0.5291   | 25.37      | <.0001     |
| age                     | 1  | -2.6067  | 1.7610         | -6.0582               | 0.8449   | 2.19       | 0.1388     |
| feats                   | 1  | 8.3627   | 14.7107        | -20.4697              | 37.1951  | 0.32       | 0.5697     |
| ne                      | 1  | 65.0081  | 40.1329        | -13.6508              | 143.6671 | 2.62       | 0.1053     |
| cor                     | 1  | -19.2997 | 38.1907        | -94.1520              | 55.5526  | 0.26       | 0.6133     |
| tax                     | 1  | 0.4699   | 0.1260         | 0.2229                | 0.7170   | 13.90      | 0.0002     |
| sum                     | 0  | 0.0000   | .              | .                     | .        | .          | .          |
| Scale                   | 0  | 157.5593 |                |                       |          |            |            |

**Output 80.5.2** Design Dependence Equations

NOTE: The following variables have been ignored in the MCD computation because of linear dependence.

$$\text{sum} = \text{sqft} + \text{age} + \text{feats} + \text{ne} + \text{cor} + \text{tax}$$

Moreover, PROC ROBUSTREG also identifies a robust dependence equation on cor in [Output 80.5.3](#), which holds for 77.27% of the observations but not for the entire data set.

**Output 80.5.3** Robust Dependence Equations

NOTE: The following robust dependence equations simultaneously hold for 77.27% of the observations in the data set. The breakdown setting for the MCD algorithm is 22.73%.

$$\text{cor} = 0$$

Another way to represent the low-dimensional structure is to specify the coefficients of the MCD-dropped components on the data (see [Output 80.5.4](#)), which form a basis of the complementary space to the relevant low-dimensional hyperplane.

**Output 80.5.4** Coefficients for MCD-Dropped Components

| Coefficients for MCD-Dropped Components |              |              |
|-----------------------------------------|--------------|--------------|
| Parameter                               | Design Drop0 | Robust Drop1 |
| sqft                                    | 0            | 0            |
| age                                     | 0            | 0            |
| feats                                   | 0            | 0            |
| ne                                      | 0            | 0            |
| cor                                     | 0            | 1.0000       |
| tax                                     | 0            | 0            |
| sum                                     | 1.0000       | 0            |

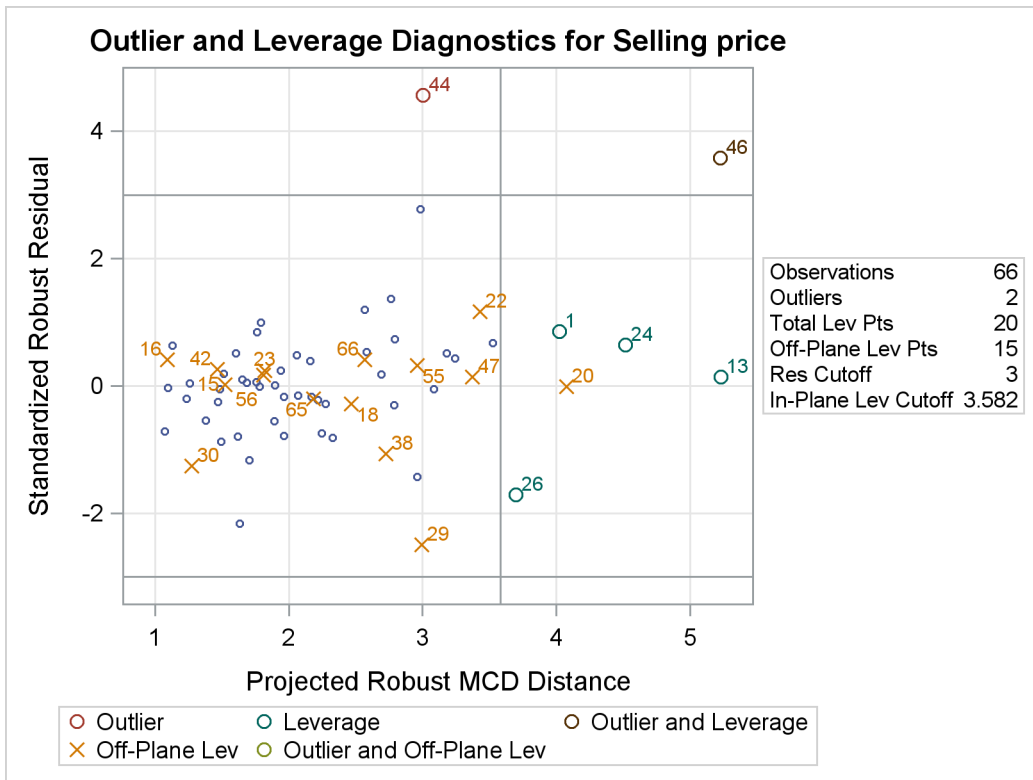
By the definitions of projected robust distance and leverage point, an observation is called an off-plane leverage point if at least one of the robust or design dependence equations does not apply to the observation. In this example, the observations with  $cor = 1$  are all off-plane leverage points. [Output 80.5.5](#) lists the leverage points and outliers along with the relevant distance measurements and standardized residuals.

**Output 80.5.5** Diagnostics

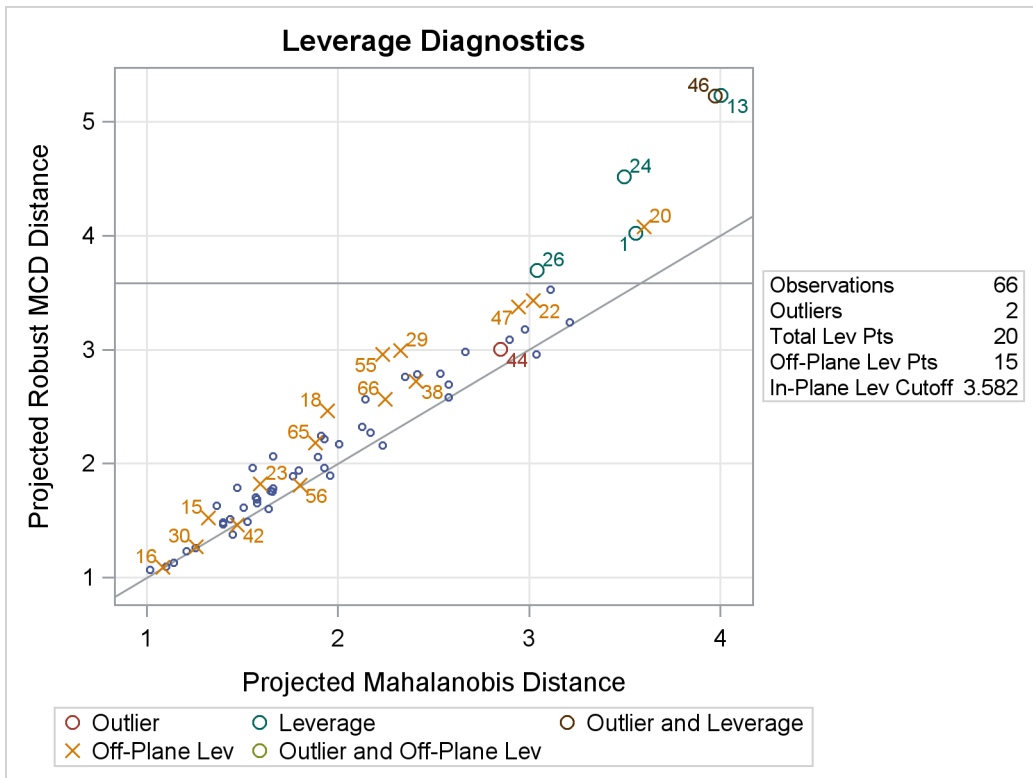
| Diagnostics |                                             |        |           |          |                                    |         |
|-------------|---------------------------------------------|--------|-----------|----------|------------------------------------|---------|
| Obs         | -----Projected Distance-----<br>Mahalanobis | Robust | Off-Plane | Leverage | Standardized<br>Robust<br>Residual | Outlier |
| 1           | 3.5567                                      | 4.0211 | 0.0000    | *        | 0.8522                             |         |
| 13          | 4.0034                                      | 5.2310 | 0.0000    | *        | 0.1411                             |         |
| 15          | 1.3221                                      | 1.5219 | 2.3681    | *        | 0.0226                             |         |
| 16          | 1.0839                                      | 1.0905 | 2.3681    | *        | 0.4148                             |         |
| 18          | 1.9452                                      | 2.4655 | 2.3681    | *        | -0.2789                            |         |
| 20          | 3.6006                                      | 4.0771 | 2.3681    | *        | -0.0150                            |         |
| 22          | 3.0210                                      | 3.4307 | 2.3681    | *        | 1.1664                             |         |
| 23          | 1.5920                                      | 1.8197 | 2.3681    | *        | 0.2422                             |         |
| 24          | 3.4967                                      | 4.5154 | 0.0000    | *        | 0.6464                             |         |
| 26          | 3.0420                                      | 3.6975 | 0.0000    | *        | -1.7068                            |         |
| 29          | 2.3264                                      | 2.9925 | 2.3681    | *        | -2.4980                            |         |
| 30          | 1.2587                                      | 1.2714 | 2.3681    | *        | -1.2558                            |         |
| 38          | 2.4064                                      | 2.7249 | 2.3681    | *        | -1.0620                            |         |
| 42          | 1.4722                                      | 1.4645 | 2.3681    | *        | 0.2584                             |         |
| 44          | 2.8491                                      | 3.0019 | 0.0000    |          | 4.5665                             | *       |
| 46          | 3.9725                                      | 5.2271 | 0.0000    | *        | 3.5835                             | *       |
| 47          | 2.9431                                      | 3.3728 | 2.3681    | *        | 0.1365                             |         |
| 55          | 2.2325                                      | 2.9590 | 2.3681    | *        | 0.3217                             |         |
| 56          | 1.7999                                      | 1.8119 | 2.3681    | *        | 0.1715                             |         |
| 65          | 1.8831                                      | 2.1822 | 2.3681    | *        | -0.1990                            |         |
| 66          | 2.2483                                      | 2.5673 | 2.3681    | *        | 0.4134                             |         |

From [Output 80.5.6](#) and [Output 80.5.7](#), you can see that there is no apparent corner-related difference for the houses in terms of standardized robust residual and projected MD versus projected RD, although all the corner houses are defined as off-plane leverage points.

Output 80.5.6 Projected RDPLLOT



Output 80.5.7 Projected DDPLLOT



Output 80.5.8 shows more details of the robust diagnostics. The number of dimensions indicates that six regressors are used in the MCD analysis. Since sum is excluded in model fitting, it is ignored in the MCD analysis. The number of robust dropped components equals 1 due to cor. The number of off-plane points implies the 15 corner-house observations. The reweighted value of H is the number of observations that are finally used to estimate the MCD covariance.

**Output 80.5.8** MCD Information

| MCD Profile                         |  |  |  |  |  |  |        |
|-------------------------------------|--|--|--|--|--|--|--------|
| Number of Dimensions                |  |  |  |  |  |  | 6      |
| Number of Robust Dropped Components |  |  |  |  |  |  | 1      |
| Number of Observations              |  |  |  |  |  |  | 66     |
| Number of Off-Plane Observations    |  |  |  |  |  |  | 15     |
| Specified Value of H                |  |  |  |  |  |  | 51     |
| Reweighted Value of H               |  |  |  |  |  |  | 47     |
| Breakdown Value                     |  |  |  |  |  |  | 0.2273 |

| MCD Center     |           |        |  |
|----------------|-----------|--------|--|
| Parameter Name | Parameter | Center |  |
| sqft           | sqft      | 1752.7 |  |
| age            | age       | 12.809 |  |
| feats          | feats     | 4.0426 |  |
| ne             | ne        | 0.6170 |  |
| cor            | cor       | -2E-16 |  |
| tax            | tax       | 895.40 |  |
| sum            | sum       | 2665.6 |  |

| MCD Covariance |          |          |          |          |     |          |          |
|----------------|----------|----------|----------|----------|-----|----------|----------|
|                | sqft     | age      | feats    | ne       | cor | tax      | sum      |
| sqft           | 248870.3 | -853.232 | 147.0347 | 88.60083 | 0   | 148494.5 | 396747.3 |
| age            | -853.232 | 126.2886 | -1.18733 | 1.229417 | 0   | -1251.44 | -1978.34 |
| feats          | 147.0347 | -1.18733 | 0.99815  | 0.234043 | 0   | 87.0259  | 361.5814 |
| ne             | 88.60083 | 1.229417 | 0.234043 | 0.241443 | 0   | 45.76688 | 134.42   |
| cor            | 0        | 0        | 0        | 0        | 0   | 0        | 0        |
| tax            | 148494.5 | -1251.44 | 87.0259  | 45.76688 | 0   | 106652.5 | 255147   |
| sum            | 396747.3 | -1978.34 | 361.5814 | 134.42   | 0   | 255147   | 650413.7 |

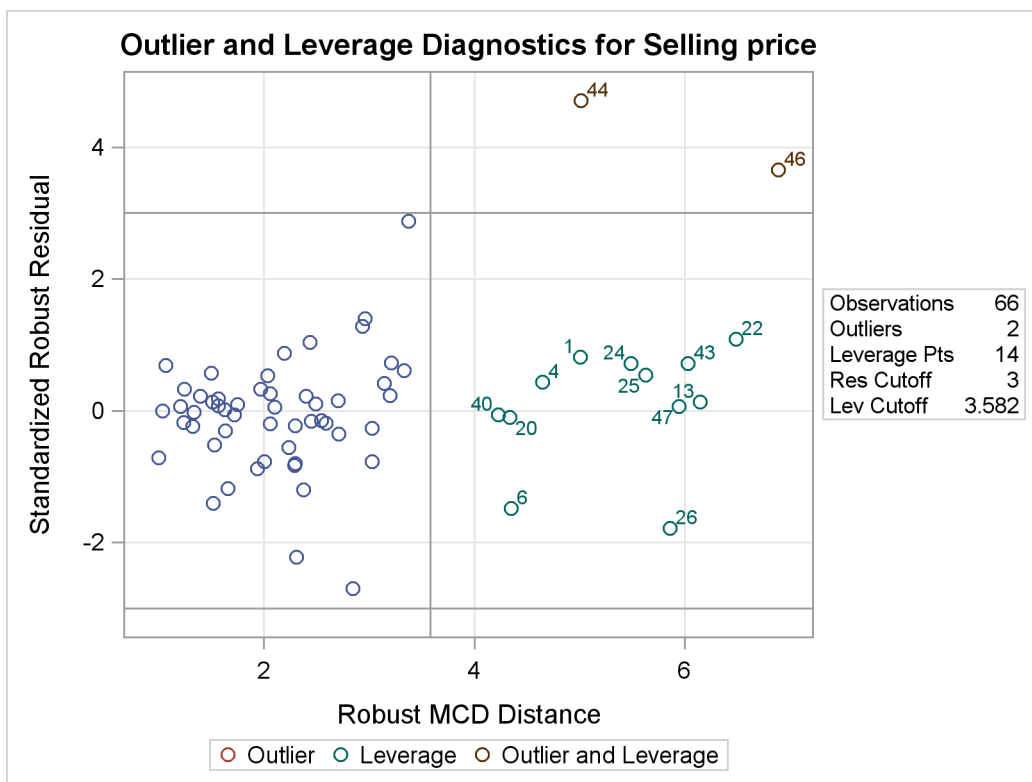
  

| MCD Correlation |          |          |          |          |     |          |          |
|-----------------|----------|----------|----------|----------|-----|----------|----------|
|                 | sqft     | age      | feats    | ne       | cor | tax      | sum      |
| sqft            | 1        | -0.15219 | 0.295009 | 0.361446 | 0   | 0.911462 | 0.986126 |
| age             | -0.15219 | 1        | -0.10575 | 0.222643 | 0   | -0.34099 | -0.21829 |
| feats           | 0.295009 | -0.10575 | 1        | 0.476749 | 0   | 0.266726 | 0.448759 |
| ne              | 0.361446 | 0.222643 | 0.476749 | 1        | 0   | 0.285206 | 0.339204 |
| cor             | 0        | 0        | 0        | 0        | 0   | 0        | 0        |
| tax             | 0.911462 | -0.34099 | 0.266726 | 0.285206 | 0   | 1        | 0.968747 |
| sum             | 0.986126 | -0.21829 | 0.448759 | 0.339204 | 0   | 0.968747 | 1        |

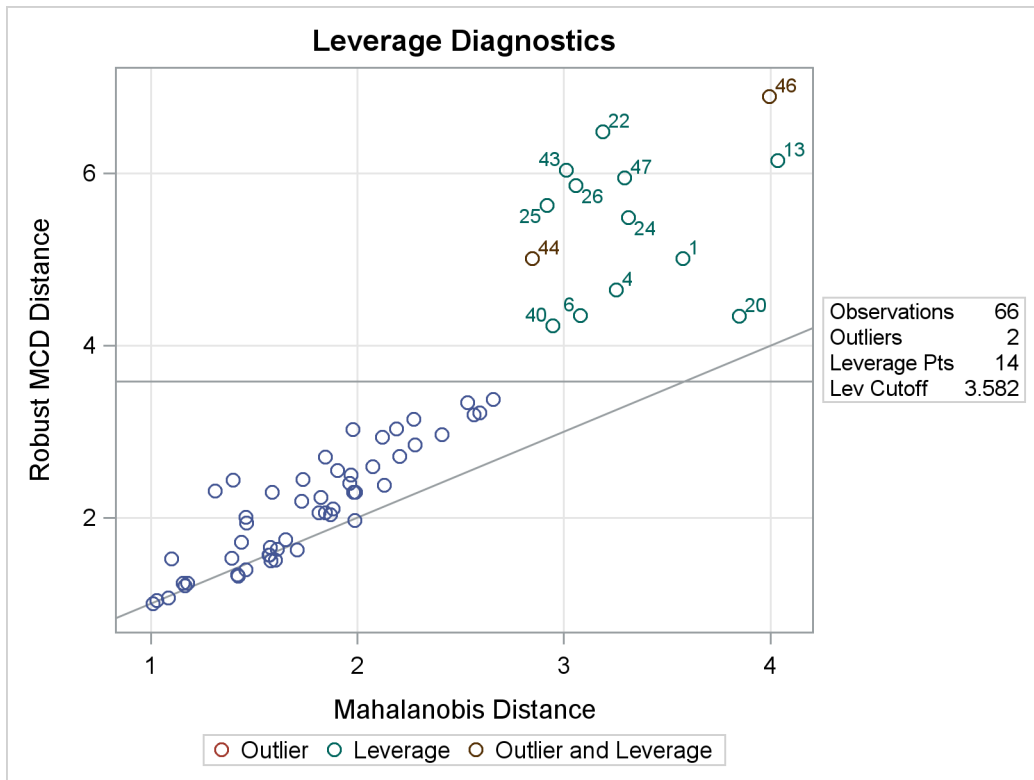
You might speculate that the projected MD and projected RD are equal to the regular MD and RD on the same data set without the variable `cor`. In fact, this is not true. (See [Output 80.5.9](#) and [Output 80.5.10](#) for the RD PLOT and DD PLOT on the data set without `cor`.) When included in the MODEL, `cor` is dropped in the distance calculation, but it is still used for the initial orthonormalization step and the  $h$ -subset searching. In this example, inclusion of `cor` causes all the other covariates to be centered separately for corner houses and non-corner houses. However, without `cor`, the centering process does not distinguish corner houses from non-corner houses, so that the MCD algorithm can still be influenced by `cor` through the correlation between `cor` and other covariates. The following statements drop the variable `cor` and produce the RD PLOT and DD PLOT for the reduced model, which are shown in [Output 80.5.9](#) and [Output 80.5.10](#):

```
proc robustreg data=house method=MM plots=all;
 model price = sqft age feats ne tax/leverage(mcdinfo) diagnostics;
run;
ods graphics off;
```

**Output 80.5.9** RD PLOT for the Reduced Model



**Output 80.5.10** DDPLLOT for the Reduced Model



Compared with [Output 80.5.8](#), [Output 80.5.11](#) shows the changes of the MCD information by removing *cor* from the model. You can see that the corner houses are no longer identified as off-plane points and the reweighted value of *H* is increased from 47 to 52. The breakdown value is intact because it depends only on the specified value of *H* and the total number of observations.

**Output 80.5.11** MCD Information for the Reduced Model

| MCD Profile                         |        |
|-------------------------------------|--------|
| Number of Dimensions                | 5      |
| Number of Robust Dropped Components | 0      |
| Number of Observations              | 66     |
| Number of Off-Plane Observations    | 0      |
| Specified Value of <i>H</i>         | 51     |
| Reweighted Value of <i>H</i>        | 52     |
| Breakdown Value                     | 0.2273 |



## Output 80.5.11 continued

| MCD Center |           |           |        |  |  |
|------------|-----------|-----------|--------|--|--|
| Parameter  |           |           |        |  |  |
|            | Parameter | Parameter | Center |  |  |
|            | sqft      | sqft      | 1710.9 |  |  |
|            | age       | age       | 11.173 |  |  |
|            | feats     | feats     | 3.9423 |  |  |
|            | ne        | ne        | 0.5962 |  |  |
|            | tax       | tax       | 858.10 |  |  |

| MCD Covariance |          |          |          |          |          |
|----------------|----------|----------|----------|----------|----------|
|                | sqft     | age      | feats    | ne       | tax      |
| sqft           | 216974.7 | 681.2327 | 199.2492 | 103.0388 | 107503.1 |
| age            | 681.2327 | 64.49887 | -0.9506  | 1.855581 | -187.135 |
| feats          | 199.2492 | -0.9506  | 0.878959 | 0.152715 | 114.9076 |
| ne             | 103.0388 | 1.855581 | 0.152715 | 0.245475 | 49.98077 |
| tax            | 107503.1 | -187.135 | 114.9076 | 49.98077 | 66558.68 |

| MCD Correlation |          |          |          |          |          |
|-----------------|----------|----------|----------|----------|----------|
|                 | sqft     | age      | feats    | ne       | tax      |
| sqft            | 1        | 0.182102 | 0.456255 | 0.44647  | 0.89457  |
| age             | 0.182102 | 1        | -0.12625 | 0.466337 | -0.09032 |
| feats           | 0.456255 | -0.12625 | 1        | 0.328771 | 0.475075 |
| ne              | 0.44647  | 0.466337 | 0.328771 | 1        | 0.391018 |
| tax             | 0.89457  | -0.09032 | 0.475075 | 0.391018 | 1        |

---

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# Chapter 81

## The RSREG Procedure

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### Overview: RSREG Procedure

The RSREG procedure uses the method of least squares to fit quadratic response surface regression models. Response surface models are a kind of general linear model in which attention focuses on characteristics of the fit response function and in particular, where optimum estimated response values occur.

In addition to fitting a quadratic function, you can use the RSREG procedure to do the following:

- test for lack of fit
- test for the significance of individual factors
- analyze the canonical structure of the estimated response surface
- compute the ridge of optimum response
- predict new values of the response

The RSREG procedure uses ODS Graphics to display the response surfaces, residuals, fit diagnostics, and ridges of optimum response. For general information about ODS Graphics, see Chapter 21, “Statistical Graphics Using ODS.”

---

## Comparison to Other SAS Software

Other SAS/STAT procedures can be used to fit the response surface, but the RSREG procedure is more specialized. PROC RSREG uses a much more compact model syntax than other procedures; for example, the following statements model a three-factor response surface in the REG, GLM, and RSREG procedures:

```
proc reg;
 model y=x1 x1*x1
 x2 x1*x2 x2*x2
 x3 x1*x3 x2*x3 x3*x3;
run;

proc glm;
 model y=x1|x2|x3@2;
run;

proc rsreg;
 model y=x1 x2 x3;
run;
```

Additionally, PROC RSREG includes specialized methodology for analyzing the fitted response surface, such as canonical analysis and optimum response ridges.

Note that the ADX Interface in SAS/QC software provides an *interactive* environment for constructing and analyzing many different kinds of experiments, including response surface experiments. The ADX Interface is the preferred interactive SAS System tool for analyzing experiments, since it includes facilities for checking underlying assumptions and graphically optimizing the response surface; see *Getting Started with the SAS ADX Interface for Design of Experiments* for more information. The RSREG procedure is appropriate for analyzing experiments in a batch environment.

---

## Terminology

Variables are referred to according to the following conventions:

|                        |                                                                                                                                                                                                                                                                                               |
|------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| factor variables       | independent variables used to construct the quadratic response surface. To estimate the necessary parameters, each variable must have at least three distinct values in the data. Independent variables must be numeric.                                                                      |
| response variables     | the dependent variables to which the quadratic response surfaces are fit. Dependent variables must be numeric.                                                                                                                                                                                |
| covariates             | additional independent variables for use in the regression but not in the formation of the quadratic response surface. Covariates must be numeric.                                                                                                                                            |
| <b>WEIGHT</b> variable | a variable for weighting the observations in the regression. The <b>WEIGHT</b> variable must be numeric.                                                                                                                                                                                      |
| <b>ID</b> variables    | variables not previously described that are transferred to an output data set containing statistics for each observation in the input data set. This data set is created by using the <b>OUT=</b> option in the PROC RSREG statement. <b>ID</b> variables can be either character or numeric. |
| <b>BY</b> variables    | variables for grouping observations. Separate analyses are obtained for each <b>BY</b> group. <b>BY</b> variables can be either character or numeric.                                                                                                                                         |

---

## Getting Started: RSREG Procedure

### A Response Surface with a Simple Optimum

This example uses the three-factor quadratic model discussed in John (1971). Settings of the temperature, gas–liquid ratio, and packing height are controlled factors in the production of a certain chemical; Schneider and Stockett (1963) performed an experiment in order to determine the values of these three factors that minimize the unpleasant odor of the chemical. The following statements input the SAS data set `smell`; the variable `Odor` is the response, while the variables `T`, `R`, and `H` are the independent factors.

```

title 'Response Surface with a Simple Optimum';
data smell;
 input Odor T R H @@;
 label
 T = "Temperature"
 R = "Gas-Liquid Ratio"
 H = "Packing Height";
 datalines;
66 40 .3 4 39 120 .3 4 43 40 .7 4 49 120 .7 4
58 40 .5 2 17 120 .5 2 -5 40 .5 6 -40 120 .5 6
65 80 .3 2 7 80 .7 2 43 80 .3 6 -22 80 .7 6
-31 80 .5 4 -35 80 .5 4 -26 80 .5 4
;

```

The following statements invoke PROC RSREG on the data set `smell`. Figure 81.1 through Figure 81.3 display the results of the analysis, including a lack-of-fit test requested with the `LACKFIT` option.

```
proc rsreg data=smell;
 model Odor = T R H / lackfit;
run;
```

Figure 81.1 displays the coding coefficients for the transformation of the independent variables to lie between  $-1$  and  $1$ , simple statistics for the response variable, hypothesis tests for linear, quadratic, and crossproduct terms, and the lack-of-fit test. The hypothesis tests can be used to gain a rough idea of importance of the effects; here the crossproduct terms are not significant. However, the lack of fit for the model is significant, so more complicated modeling or further experimentation with additional variables should be performed before firm conclusions are made concerning the underlying process.

**Figure 81.1** Summary Statistics and Analysis of Variance

| Response Surface with a Simple Optimum            |                |                       |             |         |        |
|---------------------------------------------------|----------------|-----------------------|-------------|---------|--------|
| The RSREG Procedure                               |                |                       |             |         |        |
| Coding Coefficients for the Independent Variables |                |                       |             |         |        |
| Factor                                            | Subtracted off | Divided by            |             |         |        |
| T                                                 | 80.000000      | 40.000000             |             |         |        |
| R                                                 | 0.500000       | 0.200000              |             |         |        |
| H                                                 | 4.000000       | 2.000000              |             |         |        |
| Response Surface for Variable Odor                |                |                       |             |         |        |
| Response Mean                                     | 15.200000      |                       |             |         |        |
| Root MSE                                          | 22.478508      |                       |             |         |        |
| R-Square                                          | 0.8820         |                       |             |         |        |
| Coefficient of Variation                          | 147.8849       |                       |             |         |        |
| Regression                                        | DF             | Type I Sum of Squares | R-Square    | F Value | Pr > F |
| Linear                                            | 3              | 7143.250000           | 0.3337      | 4.71    | 0.0641 |
| Quadratic                                         | 3              | 11445                 | 0.5346      | 7.55    | 0.0264 |
| Crossproduct                                      | 3              | 293.500000            | 0.0137      | 0.19    | 0.8965 |
| Total Model                                       | 9              | 18882                 | 0.8820      | 4.15    | 0.0657 |
| Residual                                          | DF             | Sum of Squares        | Mean Square | F Value | Pr > F |
| Lack of Fit                                       | 3              | 2485.750000           | 828.583333  | 40.75   | 0.0240 |
| Pure Error                                        | 2              | 40.666667             | 20.333333   |         |        |
| Total Error                                       | 5              | 2526.416667           | 505.283333  |         |        |

Parameter estimates and the factor ANOVA are shown in Figure 81.2. Looking at the parameter estimates, you can see that the crossproduct terms are not significantly different from zero, as noted previously. The Estimate column contains estimates based on the raw data, and the Parameter Estimate from Coded Data column contains estimates based on the coded data. The factor ANOVA table displays tests for all four parameters corresponding to each factor—the parameters corresponding to the linear effect, the quadratic effect, and the effects of the crossproducts with each of the other two factors. The only factor with a significant overall effect is R, indicating that the level of noise left unexplained by the model is still too high to estimate the effects of T and H accurately. This might be due to the lack of fit.

**Figure 81.2** Parameter Estimates and Hypothesis Tests

| Parameter | DF | Estimate     | Standard Error | t Value | Pr >  t | Parameter Estimate from Coded Data |
|-----------|----|--------------|----------------|---------|---------|------------------------------------|
| Intercept | 1  | 568.958333   | 134.609816     | 4.23    | 0.0083  | -30.666667                         |
| T         | 1  | -4.102083    | 1.489024       | -2.75   | 0.0401  | -12.125000                         |
| R         | 1  | -1345.833333 | 335.220685     | -4.01   | 0.0102  | -17.000000                         |
| H         | 1  | -22.166667   | 29.780489      | -0.74   | 0.4902  | -21.375000                         |
| T*T       | 1  | 0.020052     | 0.007311       | 2.74    | 0.0407  | 32.083333                          |
| R*T       | 1  | 1.031250     | 1.404907       | 0.73    | 0.4959  | 8.250000                           |
| R*R       | 1  | 1195.833333  | 292.454665     | 4.09    | 0.0095  | 47.833333                          |
| H*T       | 1  | 0.018750     | 0.140491       | 0.13    | 0.8990  | 1.500000                           |
| H*R       | 1  | -4.375000    | 28.098135      | -0.16   | 0.8824  | -1.750000                          |
| H*H       | 1  | 1.520833     | 2.924547       | 0.52    | 0.6252  | 6.083333                           |

| Factor | DF | Sum of Squares | Mean Square | F Value | Pr > F | Label            |
|--------|----|----------------|-------------|---------|--------|------------------|
| T      | 4  | 5258.016026    | 1314.504006 | 2.60    | 0.1613 | Temperature      |
| R      | 4  | 11045          | 2761.150641 | 5.46    | 0.0454 | Gas-Liquid Ratio |
| H      | 4  | 3813.016026    | 953.254006  | 1.89    | 0.2510 | Packing Height   |

Figure 81.3 displays the canonical analysis and eigenvectors. The canonical analysis indicates that the directions of principal orientation for the predicted response surface are along the axes associated with the three factors, confirming the small interaction effect in the regression ANOVA (Figure 81.1). The largest eigenvalue (48.8588) corresponds to the eigenvector (0.238091, 0.971116, -0.015690), the largest component of which (0.971116) is associated with R; similarly, the second-largest eigenvalue (31.1035) is associated with T. The third eigenvalue (6.0377), associated with H, is quite a bit smaller than the other two, indicating that the response surface is relatively insensitive to changes in this factor. The coded form of the canonical analysis indicates that the estimated response surface is at a minimum when T and R are both near the middle of their respective ranges (that is, the coded critical values for T and R are both near 0) and H is relatively high; in uncoded terms, the model predicts that the unpleasant odor is minimized when  $T = 84.876502$ ,  $R = 0.539915$ , and  $H = 7.541050$ .



Figure 81.3 Canonical Analysis and Eigenvectors

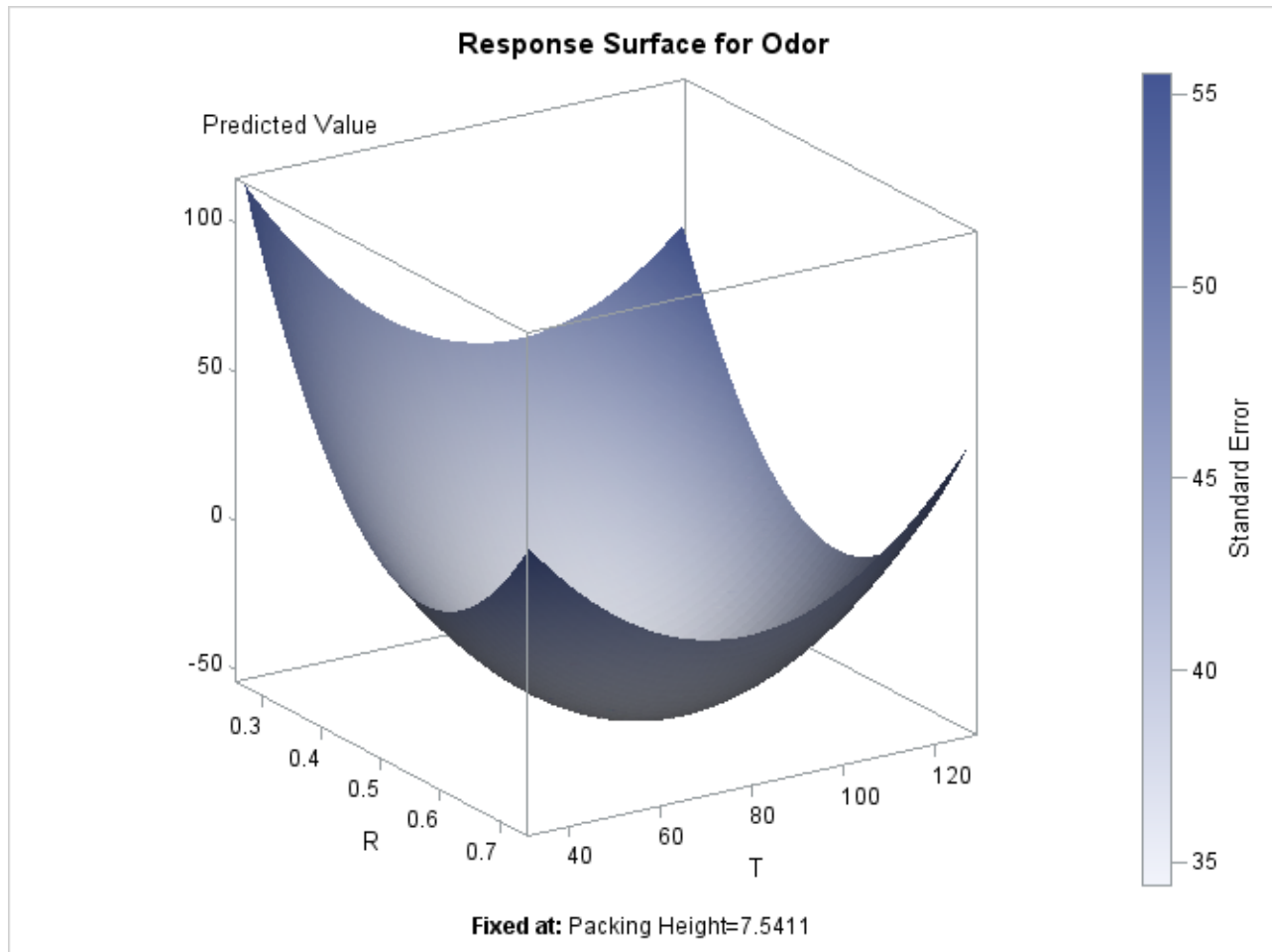
| Factor                                          | Critical Value |           | Label            |
|-------------------------------------------------|----------------|-----------|------------------|
|                                                 | Coded          | Uncoded   |                  |
| T                                               | 0.121913       | 84.876502 | Temperature      |
| R                                               | 0.199575       | 0.539915  | Gas-Liquid Ratio |
| H                                               | 1.770525       | 7.541050  | Packing Height   |
| Predicted value at stationary point: -52.024631 |                |           |                  |
| Eigenvalues                                     | Eigenvectors   |           |                  |
|                                                 | T              | R         | H                |
| 48.858807                                       | 0.238091       | 0.971116  | -0.015690        |
| 31.103461                                       | 0.970696       | -0.237384 | 0.037399         |
| 6.037732                                        | -0.032594      | 0.024135  | 0.999177         |
| Stationary point is a minimum.                  |                |           |                  |

To plot the response surface with respect to two of the factor variables, fix H, the least significant factor variable, at its estimated optimum value. The following statements use ODS Graphics to display the surface:

```
ods graphics on;
proc rsreg data=smell
 plots(unpack)=surface(3d at (H=7.541050));
 model Odor = T R H;
 ods select 'T * R = Pred';
run;
ods graphics off;
```

Note that the ODS SELECT statement is specified to select the plot of interest.

Figure 81.4 The Response Surface at the Optimum H



Alternatively, the following statements produce an output data set containing the surface information, which you can then use for plotting surfaces or searching for optima. The first DATA step fixes H, the least significant factor variable, at its estimated optimum value (7.541), and generates a grid of points for T and R. To ensure that the grid data do not affect parameter estimates, the response variable (Odor) is set to missing. (See the section “Missing Values” on page 6924.) The second DATA step concatenates these grid points to the original data. Then PROC RSREG computes predictions for the combined data. The last DATA step subsets the predicted values over just the grid points, which excludes the predictions at the original data.

```

data grid;
 do;
 Odor = . ;
 H = 7.541;
 do T = 20 to 140 by 5;
 do R = .1 to .9 by .05;
 output;
 end;
 end;
 end;
run;
data grid;

```

```

 set smell grid;
run;

proc rsreg data=grid out=predict noprint;
 model Odor = T R H / predict;
run;

data grid;
 set predict;
 if H = 7.541;
run;

```

---

## Syntax: RSREG Procedure

The following statements are available in the RSREG procedure.

```

PROC RSREG < options > ;
 MODEL responses = independents < / options > ;
 RIDGE < options > ;
 WEIGHT variable ;
 ID variables ;
 BY variables ;

```

The PROC RSREG and MODEL statements are required.

The BY, ID, MODEL, RIDGE, and WEIGHT statements are described after the PROC RSREG statement, and they can appear in any order.

---

## PROC RSREG Statement

```

PROC RSREG < options > ;

```

The PROC RSREG statement invokes the RSREG procedure. [Table 81.1](#) summarizes the options available in the PROC RSREG statement.

**Table 81.1** PROC RSREG Statement Options

| Option  | Description                                      |
|---------|--------------------------------------------------|
| DATA=   | Names the input SAS data set                     |
| NOPRINT | Suppresses the normal display of results         |
| OUT=    | Creates the output SAS data set                  |
| PLOTS   | Controls the plots produced through ODS Graphics |

The following list describes these options.

**DATA=SAS-data-set**

specifies the input SAS data set that contains the data to be analyzed. By default, PROC RSREG uses the most recently created SAS data set.

**NOPRINT**

suppresses the normal display of results when only the output data set is required.

For more information, see the description of the NOPRINT option in the [MODEL](#) and [RIDGE](#) statements.

Note that this option temporarily disables the Output Delivery System (ODS); see Chapter 20, “[Using the Output Delivery System](#),” for more information.

**OUT=SAS-data-set**

creates an output SAS data set that contains statistics for each observation in the input data set. In particular, this data set contains the [BY](#) variables, the [ID](#) variables, the [WEIGHT](#) variable, the variables in the [MODEL](#) statement, and the [output options](#) requested in the [MODEL](#) statement. You must specify [output statistic options](#) in the [MODEL](#) statement; otherwise, the output data set is created but contains no observations. If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*. For more details, see the section “[OUT=SAS-data-set](#)” on page 6928.

**PLOTS** < (*global-plot-option*) >=*plot-request*< (*options*)>**PLOTS** < (*global-plot-option*) >=*(plot-request*< (*options*)>< . . . *plot-request*< (*options*)> >

controls the plots produced through ODS Graphics. When you specify only one *plot-request*, you can omit the parentheses from around the *plot-request*. For example:

```
plots = all
plots = (diagnostics ridge surface(unpack))
plots(unpack) = surface(overlaypairs)
```

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;
proc rsreg plots=all;
 model y=x;
run;
ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS](#).”

By default, no graphs are created; you must specify the PLOTS= option to make graphs. See [Figure 81.4](#), [Output 81.1.5](#), [Output 81.1.6](#), [Output 81.2.3](#), and [Output 81.2.4](#) for examples of the ODS graphical displays.

The following *global-plot-option* is available.

**UNPACKPANELS | UNPACK**

suppresses paneling. By default, multiple plots can appear in some output *panels*. Specify the UNPACK option to display each plot separately.

The following *plot-requests* are available.

**ALL**

produces all appropriate plots. You can specify other options with ALL; for example, to display all plots and unpack the SURFACE contours you can specify `plots=(all surface(unpack))`.

**DIAGNOSTICS <(LABEL | UNPACK)>**

displays a panel of summary fit diagnostic plots. The plots produced and their usage are discussed in Table 81.2.

**Table 81.2** Diagnostic Plots

| Diagnostic Plot                                                           | Usage                                                                                                                                                                                                                                  |
|---------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Cook's <i>D</i> statistic versus observation number                       | Evaluate influence of an observation on the entire parameter estimate vector                                                                                                                                                           |
| Dependent variable values versus predicted values                         | Evaluate adequacy of fit and detect influential observations                                                                                                                                                                           |
| Externally studentized residuals (RStudent) versus leverage               | Detect outliers and influential (high-leverage) observations                                                                                                                                                                           |
| Externally studentized residuals versus predicted values                  | Evaluate adequacy of fit and detect outliers                                                                                                                                                                                           |
| Histogram of residuals                                                    | Confirm normality of error terms                                                                                                                                                                                                       |
| Normal quantile plot of residuals                                         | Confirm normality and homogeneity of error terms, and detect outliers                                                                                                                                                                  |
| Residuals versus predicted values<br><i>Residual-fit</i> (RF) spread plot | Evaluate adequacy of fit and detect outliers<br>side-by-side quantile plots of the centered fit and the residuals show "how much variation in the data is explained by the fit and how much remains in the residuals" (Cleveland 1993) |

Observations satisfying  $RStudent > 2$  or  $RStudent < -2$  are called *outliers*, and observations with leverage  $> 2p/n$  are called *influential*, where  $n$  is the number of observations used in fitting the model and  $p$  is the number of parameters used in the model (Rawlings, Pantula, and Dickey 1998). Specifying the LABEL option labels the influential and outlying observations—the label is the first ID variable if the ID statement is specified; otherwise, it is the observation number. Note in the Cook's *D* plot that only observations with *D* exceeding  $4/n$  are labeled; these are also called influential observations. The UNPACK option displays each diagnostic plot separately. See Output 81.2.3 for an example of the diagnostics panel.

**FIT** <(GRIDSIZE=*number*)>

plots the predicted values against a single predictor when you have only one factor or only one covariate in the model. The GRIDSIZE= option specifies the number of points at which the fitted values are computed; by default, GRIDSIZE=200.

**NONE**

suppresses all plots.

**RESIDUALS** <(UNPACK | SMOOTH)>

displays plots of residuals against each factor and covariate. The UNPACK option displays each residual plot separately. The SMOOTH option overlays a loess smooth on each residual plot; see Chapter 53, “The LOESS Procedure,” for more information. See [Output 81.1.5](#) for an example of this plot.

**RIDGE** <(UNPACK)>

displays the maximum and/or minimum ridge plots. This option is available only when a **MAXIMUM** or **MINIMUM** option is specified in the RIDGE statement. The UNPACK option displays the estimated response and factor level ridge plots separately. See [Output 81.1.5](#) for an example of this plot.

**SURFACE** <(surface-options)>

displays the response surface for each response variable and each pair of factors with all other factors and covariates fixed at their means. By default a panel of contour plots is produced; see [Output 81.1.6](#) for an example of this plot. The following *surface-options* can be specified:

**3D**

displays three-dimensional surface plots instead of contour plots. See [Figure 81.4](#) for an example of this plot.

**AT** <keyword><(variable=value-list | keyword <...variable=value-list | keyword>)>

specifies fixed values for factors and covariates. You can specify one or more numbers in the *value-list* or one of the following *keywords*:

|          |                                                                  |
|----------|------------------------------------------------------------------|
| MIN      | sets the variable to its minimum value.                          |
| MEAN     | sets the variable to its mean value.                             |
| MIDRANGE | sets the variable to the middle value: $\frac{\max + \min}{2}$ . |
| MAX      | sets the variable to its maximum value.                          |

Specifying a keyword immediately after AT sets the default value of all variables; for example, **AT MIN** sets all variables not displayed on an axis to their minimum values. By default, continuous variables are set to their means (**AT MEAN**) when they are not used on an axis. For example, if your model contains variables X1, X2, and X3, then specifying **AT (X1=7 9)** produces a contour plot of X2 versus X3 fixing X1 = 7 and then another contour plot with X1 = 9, along with contour plots of X1 versus X2 fixing X3 at its mean, and X1 versus X3 fixing X2 at its mean.

**EXTEND**=*value*

extends the surface *value*-times the range of each factor in each direction, which enables you to see more of the fitted surface. For example, if factor A has range [0, 10], then specifying **EXTEND=0.1** will compute and display the surface for A in [-1, 11]. You can specify *value* ≥ 0; by default, *value* = 0.1.

**FILL=PRED | SE | NONE**

produces a filled contour plot for either the predicted values or the standard errors. FILL=SE is the default. If the 3D option is also specified, then the contour plot is projected onto the surface.

**GRIDSIZE=*n***

creates an  $n \times n$  grid of points at which the estimated values for the surface and standard errors are computed, for  $n \geq 1$ . By default,  $n = 50$ .

**LINE=<PRED | SE | NONE>**

produces a contour line plot for either the predicted values or the standard errors. LINE=PRED is the default. If the 3D option is also specified, then specifying LINE displays a grid on the surface, and the other LINE= specifications are ignored.

**NODESIGN**

suppresses the display of the design points on the contour surface plots and the overlaid contour-line plots.

**OVERLAYPAIRS**

produces overlaid contour line plots for all pairs of response variables in addition to the contour surface plots. See Figure 81.6 for an example of this plot.

**ROTATE=*angle***

rotates the 3-D surface plots *angle* degrees,  $-180 < angle < 180$ . By default, *angle* = 57.

**TILT=*angle***

tilts the 3-D surface plots *angle* degrees,  $-180 < angle < 180$ . By default, *angle* = 20.

**UNPACKPANELS | UNPACK**

suppresses paneling, and displays each surface plot separately.

## BY Statement

**BY** *variables* ;

You can specify a BY statement with PROC RSREG to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the RSREG procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

---

## ID Statement

**ID** *variables* ;

The ID statement names variables that are to be transferred to the data set created by the **OUT=** option in the PROC RSREG statement.

---

## MODEL Statement

**MODEL** *responses = independents* </ *options* > ;

In the MODEL statement, you specify the response (dependent) variables followed by an equal sign and then the independent variables, some of which can be covariates.

Table 81.3 summarizes the *options* available in the MODEL statement. The *statistic options* specify which statistics are output to the **OUT=** data set. If none of the *statistic options* are selected, the data set is created but contains no observations. The *statistic option* keywords become values of the special variable **\_TYPE\_** in the output data set.

**Table 81.3** MODEL Statement Options

| Option                           | Description                                                                                            |
|----------------------------------|--------------------------------------------------------------------------------------------------------|
| BYOUT                            | Uses only the first BY group to estimate the model                                                     |
| COVAR=                           | Declares variables to be simple linear regressors                                                      |
| LACKFIT                          | Performs a lack-of-fit test                                                                            |
| NOCODE                           | Performs the canonical and ridge analyses using original values                                        |
| PRESS                            | Displays the predicted residual sum of squares (PRESS) statistic                                       |
| <b>Suppress Displayed Output</b> |                                                                                                        |
| NOANOVA                          | Suppresses the analysis of variance and parameter estimates                                            |
| NOOPTIMAL                        | Suppresses the canonical analysis                                                                      |
| NOPRINT                          | Suppresses both the analysis of variance and the canonical analysis                                    |
| <b>Output Statistics</b>         |                                                                                                        |
| ACTUAL                           | Includes observed response values                                                                      |
| PREDICT                          | Includes values predicted by the model                                                                 |
| RESIDUAL                         | Includes the residuals                                                                                 |
| L95                              | Includes the lower bound of a 95% confidence interval for an individual predicted value                |
| U95                              | Includes the upper bound of a 95% confidence interval for an individual predicted value                |
| L95M                             | Includes the lower bound of a 95% confidence interval for the expected value of the dependent variable |
| U95M                             | Includes the upper bound of a 95% confidence interval for the expected value of the dependent variable |
| D                                | Includes Cook's <i>D</i> influence statistic                                                           |



The following list describes these options in alphabetical order.

**ACTUAL**

specifies that the observed response values from the input data set be written to the output data set.

**BYOUT**

uses only the first BY group to estimate the model. Subsequent BY groups have scoring statistics computed in the output data set only. The BYOUT option is used only when a BY statement is specified.

**COVAR=*n***

declares that the first *n* variables on the right side of the model are simple linear regressors (covariates) and not factors in the quadratic response surface. By default, PROC RSREG forms quadratic and crossproduct effects for all regressor variables in the MODEL statement.

See the section “[Handling Covariates](#)” on page 6926 for more details and [Example 81.2](#) for an example that uses covariates.

**D**

specifies that Cook’s *D* influence statistic be written to the output data set.

See Chapter 4, “[Introduction to Regression Procedures](#),” for details and formulas.

**LACKFIT**

performs a lack-of-fit test.

See Draper and Smith (1981) for a discussion of lack-of-fit tests.

**L95**

specifies that the lower bound of a 95% confidence interval for an individual predicted value be written to the output data set. The variance used in calculating this bound is a function of both the mean square error and the variance of the parameter estimates.

See Chapter 4, “[Introduction to Regression Procedures](#),” for details and formulas.

**L95M**

specifies that the lower bound of a 95% confidence interval for the expected value of the dependent variable be written to the output data set. The variance used in calculating this bound is a function of the variance of the parameter estimates.

See Chapter 4, “[Introduction to Regression Procedures](#),” for details and formulas.

**NOANOVA****NOAOV**

suppresses the display of the analysis of variance and parameter estimates from the model fit.

**NOCODE**

performs the canonical and ridge analyses with the parameter estimates derived from fitting the response to the original values of the factor variables, rather than their coded values (see the section “[Coding the Factor Variables](#)” on page 6923 for more details). Use this option if the data are already stored in a coded form.

**NOOPTIMAL****NOOPT**

suppresses the display of the canonical analysis for the quadratic response surface.

**NOPRINT**

suppresses the display of both the analysis of variance and the canonical analysis.

**PREDICT**

specifies that the values predicted by the model be written to the output data set.

**PRESS**

computes and displays the predicted residual sum of squares (PRESS) statistic for each dependent variable in the model. The PRESS statistic is added to the summary information at the beginning of the analysis of variance, so if the **NOANOVA** or **NOPRINT** option is specified, then the PRESS option has no effect.

See Chapter 4, “[Introduction to Regression Procedures](#),” for details and formulas.

**RESIDUAL**

specifies that the residuals, calculated as **ACTUAL – PREDICTED**, be written to the output data set.

**U95**

specifies that the upper bound of a 95% confidence interval for an individual predicted value be written to the output data set. The variance used in calculating this bound is a function of both the mean square error and the variance of the parameter estimates.

See Chapter 4, “[Introduction to Regression Procedures](#),” for details and formulas.

**U95M**

specifies that the upper bound of a 95% confidence interval for the expected value of the dependent variable be written to the output data set. The variance used in calculating this bound is a function of the variance of the parameter estimates.

See Chapter 4, “[Introduction to Regression Procedures](#),” for details and formulas.

**RIDGE Statement**

**RIDGE** < options > ;

A RIDGE statement computes the ridge of optimum response. The ridge starts at a given point  $x_0$ , and the point on the ridge at radius  $r$  from  $x_0$  is the collection of factor settings that optimizes the predicted response at this radius. You can think of the ridge as climbing or falling as fast as possible on the surface of predicted response. Thus, the ridge analysis can be used as a tool to help interpret an existing response surface or to indicate the direction in which further experimentation should be performed.

The default starting point,  $x_0$ , has each coordinate equal to the point midway between the highest and lowest values of the factor in the design. The default radii at which the ridge is computed are 0, 0.1, . . . , 0.9, 1. If the ridge analysis is based on the response surface fit to coded values for the factor variables (see the section “[Coding the Factor Variables](#)” on page 6923 for details), then this results in a ridge that starts at the point with a coded zero value for each coordinate and extends toward, but not beyond, the edge of the range of

experimentation. Alternatively, both the center point of the ridge and the radii at which it is to be computed can be specified.

You can specify the following options in the RIDGE statement:

**CENTER**=*uncoded-factor-values*

gives the coordinates of the point  $x_0$  from which to begin the ridge. The coordinates should be given in the original (uncoded) factor variable values and should be separated by commas. There must be as many coordinates specified as there are factors in the model, and the order of the coordinates must be the same as that used in the **MODEL** statement. This starting point should be well inside the range of experimentation. The default sets each coordinate equal to the value midway between the highest and lowest values for the associated factor.

**MAXIMUM**

**MAX**

computes the ridge of maximum response. Both the **MIN** and **MAX** options can be specified; at least one must be specified.

**MINIMUM**

**MIN**

computes the ridge of minimum response. Both the **MIN** and **MAX** options can be specified; at least one must be specified.

**NOPRINT**

suppresses the display of the ridge analysis when only an output data set is required.

**OUTR**=*SAS-data-set*

creates an output SAS data set containing the computed optimum ridge.

For details, see the section “**OUTR**=*SAS-data-set*” on page 6929.

**RADIUS**=*coded-radii*

gives the distances from the ridge starting point at which to compute the optima. The values in the list represent distances between coded points. The list can take any of the following forms or can be composed of mixtures of them:

$m_1, m_2, \dots, m_n$  specifies several values.

$m$  TO  $n$  specifies a sequence where  $m$  equals the starting value,  $n$  equals the ending value, and the increment equals 1.

$m$  TO  $n$  BY  $i$  specifies a sequence where  $m$  equals the starting value,  $n$  equals the ending value, and  $i$  equals the increment.

Mixtures of the preceding forms should be separated by commas. The default list runs from 0 to 1 by increments of 0.1. The following are examples of valid lists.

```
radius=0 to 5 by .5;
radius=0, .2, .25, .3, .5 to 1.0 by .1;
```

---

## WEIGHT Statement

**WEIGHT** variable ;

When a WEIGHT statement is specified, a weighted residual sum of squares

$$\sum_i w_i (y_i - \hat{y}_i)^2$$

is minimized, where  $w_i$  is the value of the variable specified in the WEIGHT statement,  $y_i$  is the observed value of the response variable, and  $\hat{y}_i$  is the predicted value of the response variable.

The observation is used in the analysis only if the value of the WEIGHT statement variable is greater than zero. The WEIGHT statement has no effect on degrees of freedom or number of observations. If the weights for the observations are proportional to the reciprocals of the error variances, then the weighted least squares estimates are best linear unbiased estimators (BLUE).

---

## Details: RSREG Procedure

---

### Introduction to Response Surface Experiments

Many industrial experiments are conducted to discover which values of given factor variables optimize a response. If each factor is measured at three or more values, a quadratic response surface can be estimated by least squares regression. The predicted optimal value can be found from the estimated surface if the surface is shaped like a simple hill or valley. If the estimated surface is more complicated, or if the predicted optimum is far from the region of experimentation, then the shape of the surface can be analyzed to indicate the directions in which new experiments should be performed.

Suppose that a response variable  $y$  is measured at combinations of values of two factor variables,  $x_1$  and  $x_2$ . The quadratic response surface model for this variable is written as

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1^2 + \beta_4 x_2^2 + \beta_5 x_1 x_2 + \epsilon$$

The steps in the analysis for such data are as follows:

1. [model fitting and analysis of variance](#), including [lack-of-fit testing](#), to estimate parameters
2. [canonical analysis](#) to investigate the shape of the predicted response surface
3. [ridge analysis](#) to search for the region of optimum response

### Model Fitting and Analysis of Variance

The first task in analyzing the response surface is to estimate the parameters of the model by least squares regression and to obtain information about the fit in the form of an analysis of variance. The estimated surface is typically curved: a *hill* with the peak occurring at the unique estimated point of maximum response, a *valley*, or a *saddle surface* with no unique minimum or maximum. Use the results of this phase of the analysis to answer the following questions:

- What is the contribution of each type of effect—linear, quadratic, and crossproduct—to the statistical fit? The ANOVA table with sources labeled “Regression” addresses this question.
- What part of the residual error is due to lack of fit? Does the quadratic response model adequately represent the true response surface? If you specify the **LACKFIT** option in the MODEL statement, then the ANOVA table with sources labeled “Residual” addresses this question. See the section “**Lack-of-Fit Test**” on page 6922 for details.
- What is the contribution of each factor variable to the statistical fit? Can the response be predicted accurately if the variable is removed? The ANOVA table with sources labeled “Factor” addresses this question.
- What are the predicted responses for a grid of factor values? (See the section “**Plotting the Surface**” on page 6924 and the section “**Searching for Multiple Response Conditions**” on page 6924.)

### Lack-of-Fit Test

The lack-of-fit test compares the variation around the model with *pure* variation within replicated observations. This measures the adequacy of the quadratic response surface model. In particular, if there are  $n_i$  replicated observations  $Y_{i1}, \dots, Y_{in_i}$  of the response all at the same values  $\mathbf{x}_i$  of the factors, then you can predict the true response at  $\mathbf{x}_i$  either by using the predicted value  $\hat{Y}_i$  based on the model or by using the mean  $\bar{Y}_i$  of the replicated values. The lack-of-fit test decomposes the residual error into a component due to the variation of the replications around their mean value (the *pure* error) and a component due to the variation of the mean values around the model prediction (the *bias* error):

$$\sum_i \sum_{j=1}^{n_i} (Y_{ij} - \hat{Y}_i)^2 = \sum_i \sum_{j=1}^{n_i} (Y_{ij} - \bar{Y}_i)^2 + \sum_i n_i (\bar{Y}_i - \hat{Y}_i)^2$$

If the model is adequate, then both components estimate the nominal level of error; however, if the bias component of error is much larger than the pure error, then this constitutes evidence that there is significant lack of fit.

If some observations in your design are replicated, you can test for lack of fit by specifying the **LACKFIT** option in the MODEL statement. Note that, since all other tests use total error rather than pure error, you might want to hand-calculate the tests with respect to pure error if the lack of fit is significant. On the other hand, significant lack of fit indicates that the quadratic model is inadequate, so if this is a problem you can also try to refine the model, possibly by using PROC GLM for general polynomial modeling; see Chapter 42, “**The GLM Procedure**,” for more information. **Example 81.1** illustrates the use of the **LACKFIT** option.

### Canonical Analysis

The second task in analyzing the response surface is to examine the overall shape of the curve and determine whether the estimated stationary point is a maximum, a minimum, or a saddle point. The canonical analysis can be used to answer the following questions:

- Is the surface shaped like a hill, a valley, or a saddle, or is it flat?
- If there is a unique optimum combination of factor values, where is it?

- To which factor or factors are the predicted responses most sensitive?

The eigenvalues and eigenvectors in the matrix of second-order parameters characterize the shape of the response surface. The eigenvectors point in the directions of principal orientation for the surface, and the signs and magnitudes of the associated eigenvalues give the shape of the surface in these directions. Positive eigenvalues indicate directions of upward curvature, and negative eigenvalues indicate directions of downward curvature. The larger an eigenvalue is in absolute value, the more pronounced is the curvature of the response surface in the associated direction. Often, all the coefficients of an eigenvector except for one are relatively small, indicating that the vector points roughly along the axis associated with the factor corresponding to the single large coefficient. In this case, the canonical analysis can be used to determine the relative sensitivity of the predicted response surface to variations in that factor. (See the section “Getting Started: RSREG Procedure” on page 6907 for an example.)

## Ridge Analysis

If the estimated surface is found to have a simple optimum well within the range of experimentation, the analysis performed by the preceding two steps might be sufficient. In more complicated situations, further search for the region of optimum response is required. The method of ridge analysis computes the estimated ridge of optimum response for increasing radii from the center of the original design. The ridge analysis answers the following question:

- If there is not a unique optimum of the response surface within the range of experimentation, in which direction should further searching be done in order to locate the optimum?

You can use the `RIDGE` statement to compute the ridge of maximum or minimum response.

---

## Coding the Factor Variables

For the results of the canonical and ridge analyses to be interpretable, the values of different factor variables should be comparable. This is because the canonical and ridge analyses of the response surface are not invariant with respect to differences in scale and location of the factor variables. The analysis of variance is not affected by these changes. Although the actual predicted surface does not change, its parameterization does. The usual solution to this problem is to code each factor variable so that its minimum in the experiment is  $-1$  and its maximum is  $1$  and to carry through the analysis with the coded values instead of the original ones. This practice has the added benefit of making  $1$  a reasonable boundary radius for the ridge analysis since  $1$  represents approximately the edge of the experimental region. By default, PROC RSREG computes the linear transformation to perform this coding as the data are initially read in, and the canonical and ridge analyses are performed on the model fit to the coded data. The actual form of the coding operation for each value of a variable is

$$\text{coded value} = (\text{original value} - M)/S$$

where  $M$  is the average of the highest and lowest values for the variable in the design and  $S$  is half their difference.

---

## Missing Values

If an observation has missing data for any of the variables used by the procedure, then that observation is not used in the estimation process. If one or more response variables are missing, but no factor or covariate variables are missing, then predicted values and confidence limits are computed for the output data set, but the residual and Cook's  $D$  statistic are missing.

---

## Plotting the Surface

Specifying the `PLOTS=SURFACE` option in the PROC RSREG statement displays contour plots for all pairs of factors in the model (see Example 81.1), while specifying the `PLOTS=SURFACE(3D)` option displays a three-dimensional surface as shown in Figure 81.4.

You can also generate predicted values for a grid of points with the `PREDICT` option (see the section “Getting Started: RSREG Procedure” on page 6907 for an example) and then use these values to create a contour plot or a three-dimensional plot of the response surface over a two-dimensional grid. Any two factor variables can be chosen to form the grid for the plot. Several plots can be generated by using different pairs of factor variables.

---

## Searching for Multiple Response Conditions

Suppose you have the following data with two factors and three responses, and you want to find the factor setting that produces responses in a certain region:

```
data a;
 input x1 x2 y1 y2 y3;
 datalines;
-1 -1 1.8 1.940 3.6398
-1 1 2.6 1.843 4.9123
 1 -1 5.4 1.063 6.0128
 1 1 0.7 1.639 2.3629
 0 0 8.5 0.134 9.0910
 0 0 3.0 0.545 3.7349
 0 0 9.8 0.453 10.4412
 0 0 4.1 1.117 5.0042
 0 0 4.8 1.690 6.6245
 0 0 5.9 1.165 6.9420
 0 0 7.3 1.013 8.7442
 0 0 9.3 1.179 10.2762
 1.4142 0 3.9 0.945 5.0245
-1.4142 0 1.7 0.333 2.4041
 0 1.4142 3.0 1.869 5.2695
 0 -1.4142 5.7 0.099 5.4346
;
```

You want to find the values of  $x_1$  and  $x_2$  that maximize  $y_1$  subject to  $y_2 < 2$  and  $y_3 < y_2 + y_1$ . The exact answer is not easy to obtain analytically, but you can obtain a practically feasible solution by checking conditions

across a grid of values in the range of interest. First, append a grid of factor values to the observed data, with missing values for the responses:

```
data b;
 set a end=eof;
 output;
 if eof then do;
 y1=.;
 y2=.;
 y3=.;
 do x1=-2 to 2 by .1;
 do x2=-2 to 2 by .1;
 output;
 end;
 end;
 end;
run;
```

Next, use PROC RSREG to fit a response surface model to the data and to compute predicted values for both the observed data and the grid, putting the predicted values in a data set c:

```
proc rsreg data=b out=c;
 model y1 y2 y3=x1 x2 / predict;
run;
```

Finally, find the subset of predicted values that satisfy the constraints, sort by the unconstrained variable, and display the top five predictions:

```
data d;
 set c;
 if y2<2;
 if y3<y2+y1;

proc sort data=d;
 by descending y1;
run;

data d; set d;
 if (_n_ <= 5);
proc print;
run;
```

The results are displayed in [Figure 81.5](#). They indicate that optimal values of the factors are around 0.3 for  $x_1$  and around  $-0.5$  for  $x_2$ .

**Figure 81.5** Top Five Predictions

| Obs | x1  | x2   | _TYPE_  | y1      | y2      | y3      |
|-----|-----|------|---------|---------|---------|---------|
| 1   | 0.3 | -0.5 | PREDICT | 6.92570 | 0.75784 | 7.60471 |
| 2   | 0.3 | -0.6 | PREDICT | 6.91424 | 0.74174 | 7.54194 |
| 3   | 0.3 | -0.4 | PREDICT | 6.91003 | 0.77870 | 7.64341 |
| 4   | 0.4 | -0.6 | PREDICT | 6.90769 | 0.73357 | 7.51836 |
| 5   | 0.4 | -0.5 | PREDICT | 6.90540 | 0.75135 | 7.56883 |

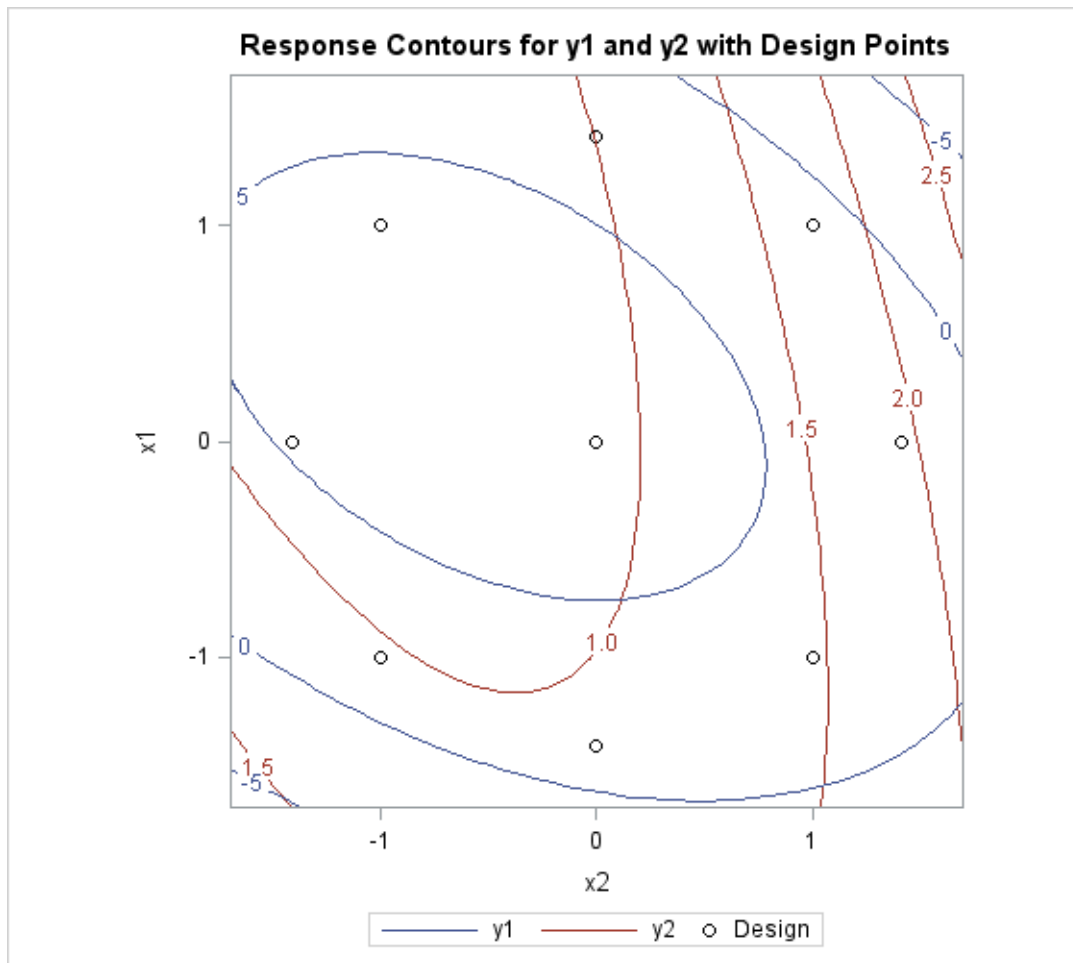


If you are also interested in simultaneously optimizing  $y_1$  and  $y_2$ , you can specify the following statements to make a visual comparison of the two response surfaces by overlaying their contour plots:

```
ods graphics on;
proc rsreg data=a plots=surface(overlaypairs);
 model y1 y2=x1 x2;
run;
ods graphics off;
```

Figure 81.6 shows that you have to make some compromises in any attempt to maximize both  $y_1$  and  $y_2$ ; however, you might be able to maximize  $y_1$  while minimizing  $y_2$ .

**Figure 81.6** Overlaid Line Contours of Predicted Responses



## Handling Covariates

Covariate regressors are added to a response surface model because they are believed to account for a sizable yet relatively uninteresting portion of the variation in the data. What the experimenter is really interested in is the response corrected for the effect of the covariates. A common example is the block effect in a block design. In the canonical and ridge analyses of a response surface, which estimate responses at hypothetical

levels of the factor variables, the actual value of the predicted response is computed by using the average values of the covariates. The estimated response values do optimize the estimated surface of the response corrected for covariates, but true prediction of the response requires actual values for the covariates. You can use the `COVAR=` option in the `MODEL` statement to include covariates in the response surface model. Example 81.2 illustrates the use of this option.

---

## Computational Method

### Canonical Analysis

For each response variable, the model can be written in the form

$$y_i = \mathbf{x}_i' \mathbf{A} \mathbf{x}_i + \mathbf{b}' \mathbf{x}_i + \mathbf{c}' \mathbf{z}_i + \epsilon_i$$

where

$y_i$  is the  $i$ th observation of the response variable.

$\mathbf{x}_i = (x_{i1}, x_{i2}, \dots, x_{ik})'$  are the  $k$  factor variables for the  $i$ th observation.

$\mathbf{z}_i = (z_{i1}, z_{i2}, \dots, z_{iL})'$  are the  $L$  covariates, including the intercept term.

$\mathbf{A}$  is the  $k \times k$  symmetrized matrix of quadratic parameters, with diagonal elements equal to the coefficients of the pure quadratic terms in the model and off-diagonal elements equal to half the coefficient of the corresponding crossproduct.

$\mathbf{b}$  is the  $k \times 1$  vector of linear parameters.

$\mathbf{c}$  is the  $L \times 1$  vector of covariate parameters, one of which is the intercept.

$\epsilon_i$  is the error associated with the  $i$ th observation. Tests performed by PROC RSREG assume that errors are independently and normally distributed with mean zero and variance  $\sigma^2$ .

The parameters in  $\mathbf{A}$ ,  $\mathbf{b}$ , and  $\mathbf{c}$  are estimated by least squares. To optimize  $y$  with respect to  $\mathbf{x}$ , take partial derivatives, set them to zero, and solve:

$$\frac{\partial y}{\partial \mathbf{x}} = 2\mathbf{x}'\mathbf{A} + \mathbf{b}' = \mathbf{0} \implies \mathbf{x} = -\frac{1}{2}\mathbf{A}^{-1}\mathbf{b}$$

You can determine if the solution is a maximum or minimum by looking at the eigenvalues of  $\mathbf{A}$ :

| <b>If the eigenvalues...</b> | <b>then the solution is...</b> |
|------------------------------|--------------------------------|
| are all negative             | a maximum                      |
| are all positive             | a minimum                      |
| have mixed signs             | a saddle point                 |
| contain zeros                | in a flat area                 |

## Ridge Analysis

If the largest eigenvalue is positive, its eigenvector gives the direction of steepest ascent from the stationary point; if the largest eigenvalue is negative, its eigenvector gives the direction of steepest descent. The eigenvectors corresponding to small or zero eigenvalues point in directions of relative flatness.

The point on the optimum response ridge at a given radius  $R$  from the ridge origin is found by optimizing

$$(\mathbf{x}_0 + \mathbf{d})' \mathbf{A}(\mathbf{x}_0 + \mathbf{d}) + \mathbf{b}'(\mathbf{x}_0 + \mathbf{d})$$

over  $\mathbf{d}$  satisfying  $\mathbf{d}'\mathbf{d} = R^2$ , where  $\mathbf{x}_0$  is the  $k \times 1$  vector containing the ridge origin and  $\mathbf{A}$  and  $\mathbf{b}$  are as previously discussed. By the method of Lagrange multipliers, the optimal  $\mathbf{d}$  has the form

$$\mathbf{d} = -(\mathbf{A} - \mu\mathbf{I})^{-1}(\mathbf{A}\mathbf{x}_0 + 0.5\mathbf{b})$$

where  $\mathbf{I}$  is the  $k \times k$  identity matrix and  $\mu$  is chosen so that  $\mathbf{d}'\mathbf{d} = R^2$ . There can be several values of  $\mu$  that satisfy this constraint; the correct one depends on which sort of response ridge is of interest. If you are searching for the ridge of maximum response, then the appropriate  $\mu$  is the unique one that satisfies the constraint and is greater than all the eigenvalues of  $\mathbf{A}$ . Similarly, the appropriate  $\mu$  for the ridge of minimum response satisfies the constraint and is less than all the eigenvalues of  $\mathbf{A}$ . (See Myers and Montgomery (1995) for details.)

---

## Output Data Sets

### OUT=SAS-data-set

An output data set containing statistics requested with options in the MODEL statement for each observation in the input data set is created whenever the OUT= option is specified in the PROC RSREG statement. The data set contains the following variables:

- the BY variables
- the ID variables
- the WEIGHT variable
- the independent variables in the MODEL statement
- the variable \_TYPE\_, which identifies the observation type in the output data set. \_TYPE\_ is a character variable with a length of eight, and it takes on the values 'ACTUAL', 'PREDICT', 'RESIDUAL', 'U95M', 'L95M', 'U95', 'L95', and 'D', corresponding to the options specified.
- the response variables containing special output values identified by the \_TYPE\_ variable

All confidence limits use the two-tailed Student's  $t$  value.

## OUTR=SAS-data-set

An output data set containing the optimum response ridge is created when the **OUTR=** option is specified in the **RIDGE** statement. The data set contains the following variables:

- the current values of the **BY** variables
- a character variable **\_DEPVAR\_** containing the name of the dependent variable
- a character variable **\_TYPE\_** identifying the type of ridge being computed, **MINIMUM** or **MAXIMUM**. If both **MAXIMUM** and **MINIMUM** are specified, the data set contains observations for the minimum ridge followed by observations for the maximum ridge.
- a numeric variable **\_RADIUS\_** giving the distance from the ridge starting point
- the values of the model factors at the estimated optimum point at distance **\_RADIUS\_** from the ridge starting point
- a numeric variable **\_PRED\_**, which is the estimated expected value of the dependent variable at the optimum
- a numeric variable **\_STDERR\_**, which is the standard error of the estimated expected value

---

## Displayed Output

All estimates and hypothesis tests assume that the model is correctly specified and the errors are distributed according to classical statistical assumptions.

The output displayed by PROC RSREG includes the following.

### Estimation and Analysis of Variance

- The actual form of the coding operation for each value of a variable is

$$\text{coded value} = \frac{1}{S}(\text{original value} - M)$$

where  $M$  is the average of the highest and lowest values for the variable in the design and  $S$  is half their difference. The **Subtracted off** column contains the  $M$  values for this formula for each factor variable, and  $S$  is found in the **Divided by** column.

- The summary table for the response variable contains the following information.
  - “Response Mean” is the mean of the response variable in the sample. When a **WEIGHT** statement is specified, the mean  $\bar{y}$  is calculated by

$$\bar{y} = \frac{\sum_i w_i y_i}{\sum_i w_i}$$

- “Root MSE” estimates the standard deviation of the response variable and is calculated as the square root of the “Total Error” mean square.

- The “R-Square” value is  $R^2$ , or the coefficient of determination.  $R^2$  measures the proportion of the variation in the response that is attributed to the model rather than to random error.
- The “Coefficient of Variation” is 100 times the ratio of the “Root MSE” to the “Response Mean.”
- A table analyzing the significance of the terms of the regression is displayed. Terms are brought into the regression in four steps: (1) the “Intercept” and any covariates in the model, (2) “Linear” terms like  $X_1$  and  $X_2$ , (3) pure “Quadratic” terms like  $X_1*X_1$  or  $X_2*X_2$ , and (4) “Crossproduct” terms like  $X_1*X_2$ . The table displays the following information:
  - the degrees of freedom in the DF column, which should be the same as the number of corresponding parameters unless one or more of the parameters are not estimable
  - Type I Sum of Squares, also called the sequential sums of squares, which measures the reduction in the error sum of squares as sets of terms (Linear, Quadratic, and so forth) are added to the model
  - R-Square, which measures the portion of total  $R^2$  contributed as each set of terms (Linear, Quadratic, and so forth) is added to the model
  - F Value, which tests the null hypothesis that all parameters in the term are zero by using the Total Error mean square as the denominator. This is a test of a Type I hypothesis, containing the usual  $F$  test numerator, conditional on the effects of subsequent variables not being in the model.
  - $\text{Pr} > F$ , which is the significance value or probability of obtaining at least as great an  $F$  ratio given that the null hypothesis is true.
- The Sum of Squares column partitions the “Total Error” into “Lack of Fit” and “Pure Error.” When “Lack of Fit” is significant, there is variation around the model other than random error (such as cubic effects of the factor variables).
  - The “Total Error” Mean Square estimates  $\sigma^2$ , the variance.
  - F Value tests the null hypothesis that the variation is adequately described by random error.
- A table containing the parameter estimates from the model is displayed.
  - The Estimate column contains the parameter estimates based on the *uncoded* values of the factor variables. If an effect is a linear combination of previous effects, the parameter for the effect is not estimable. When this happens, the degrees of freedom are zero, the parameter estimate is set to zero, and estimates and tests on other parameters are conditional on this parameter being zero.
  - The Standard Error column contains the estimated standard deviations of the parameter estimates based on *uncoded* data.
  - The t Value column contains  $t$  values of a test of the null hypothesis that the true parameter is zero when the *uncoded* values of the factor variables are used.
  - The  $\text{Pr} > |T|$  column gives the significance value or probability of a greater absolute  $t$  ratio given that the true parameter is zero.
  - The Parameter Estimate from Coded Data column contains the parameter estimates based on the *coded* values of the factor variables. These are the estimates used in the subsequent canonical and ridge analyses.

- The sum of squares are partitioned by the factors in the model, and an analysis table is displayed. The test on a factor is a joint test on all the parameters involving that factor. For example, the test for the factor X1 tests the null hypothesis that the true parameters for X1, X1\*X1, and X1\*X2 are all zero.

## Canonical Analysis

- The Critical Value columns contain the values of the factor variables that correspond to the stationary point of the fitted response surface. The critical values can be at a minimum, maximum, or saddle point.
- The eigenvalues and eigenvectors are from the matrix of quadratic parameter estimates based on the coded data. They characterize the shape of the response surface.

## Ridge Analysis

- The Coded Radius column contains the distance from the coded version of the associated point to the coded version of the origin of the ridge. The origin is given by the point at radius zero.
- The Estimated Response column contains the estimated value of the response variable at the associated point. The standard error of this estimate is also given. This quantity is useful for assessing the relative credibility of the prediction at a given radius. Typically, this standard error increases rapidly as the ridge moves up to and beyond the design perimeter, reflecting the inherent difficulty of making predictions beyond the range of experimentation.
- The Uncoded Factor Values columns contain the values of the uncoded factor variables that give the optimum response at this radius from the ridge origin.

---

## ODS Table Names

PROC RSREG assigns a name to each table it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in Table 81.4. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

**Table 81.4** ODS Tables Produced by PROC RSREG

| ODS Table Name     | Description                                       | Statement |
|--------------------|---------------------------------------------------|-----------|
| Coding             | Coding coefficients for the independent variables | default   |
| ErrorANOVA         | Error analysis of variance                        | default   |
| FactorANOVA        | Factor analysis of variance                       | default   |
| FitStatistics      | Overall statistics for fit                        | default   |
| ModelANOVA         | Model analysis of variance                        | default   |
| ParameterEstimates | Estimated linear parameters                       | default   |
| Ridge              | Ridge analysis for optimum response               | RIDGE     |
| Spectral           | Spectral analysis                                 | default   |
| StationaryPoint    | Stationary point of response surface              | default   |

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “Statistical Graphics Using ODS.”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “A Primer on ODS Statistical Graphics” on page 599 in Chapter 21, “Statistical Graphics Using ODS.”

PROC RSREG assigns a name to each graph it creates using ODS. The names are listed in Table 81.5. You can use these names to reference the graphs when using ODS. You must also specify the PLOTS= option and any other options indicated in Table 81.5.

**Table 81.5** Graphs Produced by PROC RSREG

| ODS Graph Name      | Plot Description                     | PLOTS= Option                |
|---------------------|--------------------------------------|------------------------------|
| FitPlot             | Fit plot for 1 predictor             | FIT                          |
| DiagnosticsPanel    | Panel of fit diagnostics             | DIAGNOSTICS                  |
| CooksDPlot          | Cook’s <i>D</i> plot                 | DIAGNOSTICS(UNPACK)          |
| ObservedByPredicted | Observed by predicted                | DIAGNOSTICS(UNPACK)          |
| QQPlot              | Residual Q-Q plot                    | DIAGNOSTICS(UNPACK)          |
| ResidualByPredicted | Residual by predicted values         | DIAGNOSTICS(UNPACK)          |
| ResidualHistogram   | Residual histogram                   | DIAGNOSTICS(UNPACK)          |
| RFPlot              | RF plot                              | DIAGNOSTICS(UNPACK)          |
| RStudentByPredicted | Studentized residuals by predicted   | DIAGNOSTICS(UNPACK)          |
| RStudentByLeverage  | RStudent by hat diagonals            | DIAGNOSTICS(UNPACK)          |
| ResidualPlots       | Panel of residuals by predictors     | RESIDUALS                    |
|                     | Residuals by predictors              | RESIDUALS(UNPACK)            |
| RidgePlots          | Panel of ridge plot and factors      | RIDGE                        |
|                     |                                      | (with RIDGE MAX or MIN)      |
|                     | Ridge plot                           | RIDGE(UNPACK)                |
|                     |                                      | (with RIDGE MAX or MIN)      |
|                     | Ridge factors                        | RIDGE(UNPACK)                |
|                     |                                      | (with RIDGE MAX or MIN)      |
| Contour             | Panel of contour plots               | SURFACE                      |
|                     | Contour plots                        | SURFACE(UNPACK)              |
| Surface             | Panel of 3-D surface plots           | SURFACE(3D)                  |
|                     | 3-D surface plots                    | SURFACE(3D UNPACK)           |
| ContourOverlay      | Panel of overlaid line-contour plots | SURFACE(OVERLAYPAIRS)        |
|                     | Overlaid line-contour plots          | SURFACE(OVERLAYPAIRS UNPACK) |

---

## Examples: RSREG Procedure

---

### Example 81.1: A Saddle Surface Response Using Ridge Analysis

Myers (1976) analyzes an experiment reported by Frankel (1961) aimed at maximizing the yield of mercaptobenzothiazole (MBT) by varying processing time and temperature. Myers (1976) uses a two-factor model in which the estimated surface does not have a unique optimum. A ridge analysis is used to determine the region in which the optimum lies. The objective is to find the settings of time and temperature in the processing of a chemical that maximize the yield. The following statements produce [Output 81.1.1](#) through [Output 81.1.6](#):

```
data d;
 input Time Temp MBT;
 label Time = "Reaction Time (Hours)"
 Temp = "Temperature (Degrees Centigrade)"
 MBT = "Percent Yield Mercaptobenzothiazole";
 datalines;
 4.0 250 83.8
 20.0 250 81.7
 12.0 250 82.4
 12.0 250 82.9
 12.0 220 84.7
 12.0 280 57.9
 12.0 250 81.2
 6.3 229 81.3
 6.3 271 83.1
 17.7 229 85.3
 17.7 271 72.7
 4.0 250 82.0
 ;

ods graphics on;
proc rsreg data=d plots=(ridge surface);
 model MBT=Time Temp / lackfit;
 ridge max;
run;
ods graphics off;
```

[Output 81.1.1](#) displays the coding coefficients for the transformation of the independent variables to lie between  $-1$  and  $1$  and some simple statistics for the response variable.



**Output 81.1.1** Coding and Response Variable Information

| The RSREG Procedure                               |                |            |
|---------------------------------------------------|----------------|------------|
| Coding Coefficients for the Independent Variables |                |            |
| Factor                                            | Subtracted off | Divided by |
| Time                                              | 12.000000      | 8.000000   |
| Temp                                              | 250.000000     | 30.000000  |

| Response Surface for Variable MBT: Percent Yield Mercaptobenzothiazole |           |
|------------------------------------------------------------------------|-----------|
| Response Mean                                                          | 79.916667 |
| Root MSE                                                               | 4.615964  |
| R-Square                                                               | 0.8003    |
| Coefficient of Variation                                               | 5.7760    |

**Output 81.1.2** shows that the lack of fit for the model is highly significant. Since the quadratic model does not fit the data very well, firm statements about the underlying process should not be based only on the current analysis. Note from the analysis of variance for the model that the test for the time factor is not significant. If further experimentation is undertaken, it might be best to fix Time at a moderate to high value and to concentrate on the effect of temperature. In the actual experiment discussed here, extra runs were made that confirmed the results of the following analysis.

**Output 81.1.2** Analyses of Variance

| Regression   | DF | Type I Sum<br>of Squares | R-Square | F Value | Pr > F |
|--------------|----|--------------------------|----------|---------|--------|
| Linear       | 2  | 313.585803               | 0.4899   | 7.36    | 0.0243 |
| Quadratic    | 2  | 146.768144               | 0.2293   | 3.44    | 0.1009 |
| Crossproduct | 1  | 51.840000                | 0.0810   | 2.43    | 0.1698 |
| Total Model  | 5  | 512.193947               | 0.8003   | 4.81    | 0.0410 |

| Residual    | DF | Sum of<br>Squares | Mean Square | F Value | Pr > F |
|-------------|----|-------------------|-------------|---------|--------|
| Lack of Fit | 3  | 124.696053        | 41.565351   | 39.63   | 0.0065 |
| Pure Error  | 3  | 3.146667          | 1.048889    |         |        |
| Total Error | 6  | 127.842720        | 21.307120   |         |        |

**Output 81.1.2** *continued*

| Parameter | DF | Estimate    | Standard Error | t Value | Pr >  t | Parameter Estimate from Coded Data |
|-----------|----|-------------|----------------|---------|---------|------------------------------------|
| Intercept | 1  | -545.867976 | 277.145373     | -1.97   | 0.0964  | 82.173110                          |
| Time      | 1  | 6.872863    | 5.004928       | 1.37    | 0.2188  | -1.014287                          |
| Temp      | 1  | 4.989743    | 2.165839       | 2.30    | 0.0608  | -8.676768                          |
| Time*Time | 1  | 0.021631    | 0.056784       | 0.38    | 0.7164  | 1.384394                           |
| Temp*Time | 1  | -0.030075   | 0.019281       | -1.56   | 0.1698  | -7.218045                          |
| Temp*Temp | 1  | -0.009836   | 0.004304       | -2.29   | 0.0623  | -8.852519                          |

| Factor | DF | Sum of Squares | Mean Square | F Value | Pr > F |
|--------|----|----------------|-------------|---------|--------|
| Time   | 3  | 61.290957      | 20.430319   | 0.96    | 0.4704 |
| Temp   | 3  | 461.250925     | 153.750308  | 7.22    | 0.0205 |

| Factor | Label                            |
|--------|----------------------------------|
| Time   | Reaction Time (Hours)            |
| Temp   | Temperature (Degrees Centigrade) |

The canonical analysis (Output 81.1.3) indicates that the predicted response surface is shaped like a saddle. The eigenvalue of 2.5 shows that the valley orientation of the saddle is less curved than the hill orientation, with an eigenvalue of -9.99. The coefficients of the associated eigenvectors show that the valley is more aligned with Time and the hill with Temp. Because the canonical analysis resulted in a saddle point, the estimated surface does not have a unique optimum.

**Output 81.1.3** Canonical Analysis

| Factor | Critical Value |            | Label                            |
|--------|----------------|------------|----------------------------------|
|        | Coded          | Uncoded    |                                  |
| Time   | -0.441758      | 8.465935   | Reaction Time (Hours)            |
| Temp   | -0.309976      | 240.700718 | Temperature (Degrees Centigrade) |

Predicted value at stationary point: 83.741940

| Eigenvalues | Eigenvectors |           |
|-------------|--------------|-----------|
|             | Time         | Temp      |
| 2.528816    | 0.953223     | -0.302267 |
| -9.996940   | 0.302267     | 0.953223  |

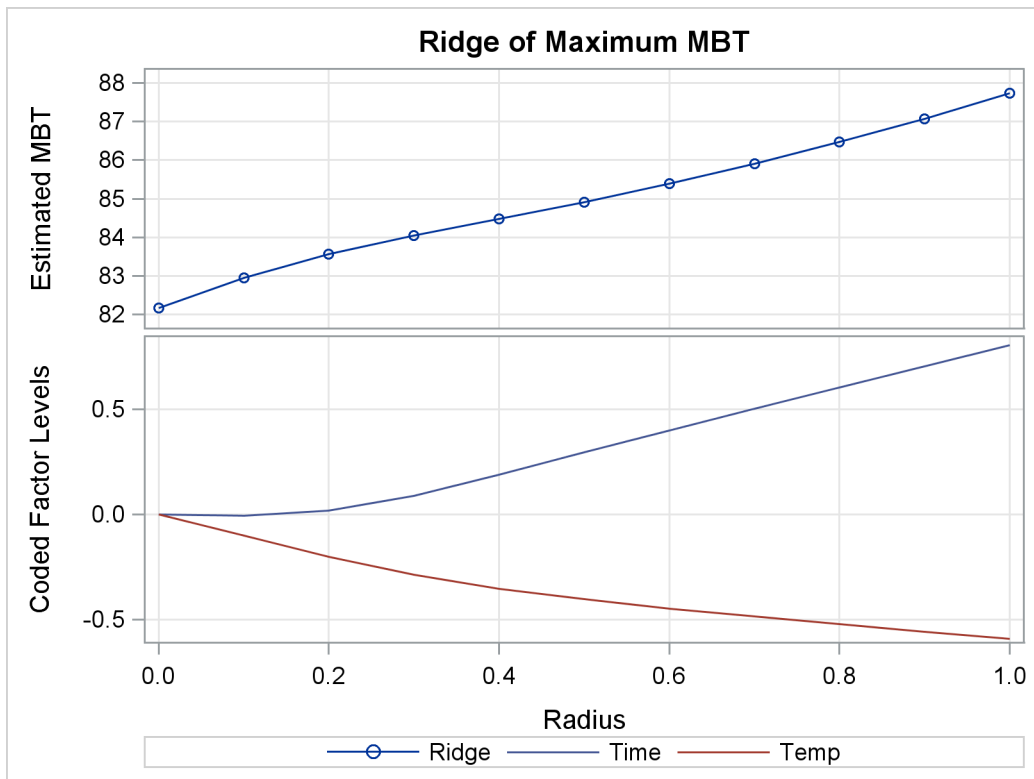
Stationary point is a saddle point.

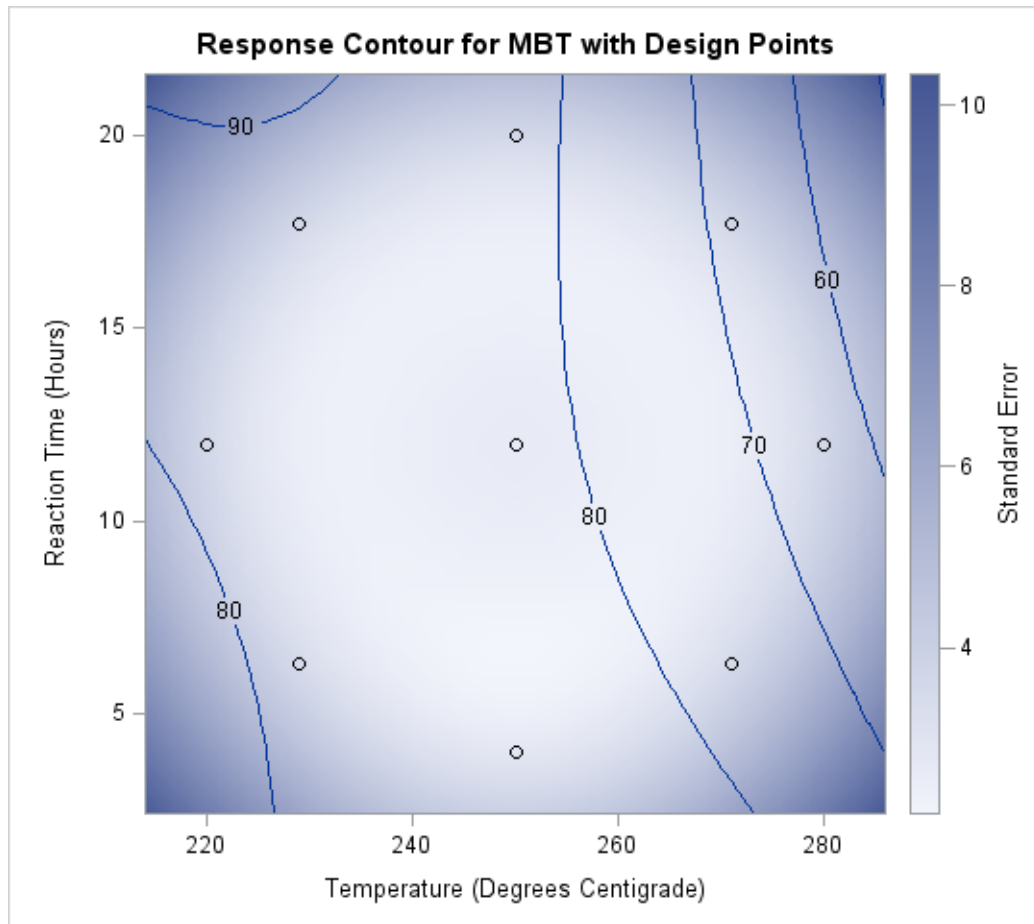
However, the ridge analysis in Output 81.1.4 and the ridge plot in Output 81.1.5 indicate that maximum yields result from relatively high reaction times and low temperatures. A contour plot of the predicted response surface, shown in Output 81.1.6, confirms this conclusion.

**Output 81.1.4** Ridge Analysis

| Estimated Ridge of Maximum Response for Variable<br>MBT: Percent Yield Mercaptobenzothiazole |                       |                   |                       |            |
|----------------------------------------------------------------------------------------------|-----------------------|-------------------|-----------------------|------------|
| Coded<br>Radius                                                                              | Estimated<br>Response | Standard<br>Error | Uncoded Factor Values |            |
|                                                                                              |                       |                   | Time                  | Temp       |
| 0.0                                                                                          | 82.173110             | 2.665023          | 12.000000             | 250.000000 |
| 0.1                                                                                          | 82.952909             | 2.648671          | 11.964493             | 247.002956 |
| 0.2                                                                                          | 83.558260             | 2.602270          | 12.142790             | 244.023941 |
| 0.3                                                                                          | 84.037098             | 2.533296          | 12.704153             | 241.396084 |
| 0.4                                                                                          | 84.470454             | 2.457836          | 13.517555             | 239.435227 |
| 0.5                                                                                          | 84.914099             | 2.404616          | 14.370977             | 237.919138 |
| 0.6                                                                                          | 85.390012             | 2.410981          | 15.212247             | 236.624811 |
| 0.7                                                                                          | 85.906767             | 2.516619          | 16.037822             | 235.449230 |
| 0.8                                                                                          | 86.468277             | 2.752355          | 16.850813             | 234.344204 |
| 0.9                                                                                          | 87.076587             | 3.130961          | 17.654321             | 233.284652 |
| 1.0                                                                                          | 87.732874             | 3.648568          | 18.450682             | 232.256238 |

**Output 81.1.5** Ridge Plot of Predicted Response Surface



**Output 81.1.6** Contour Plot of Predicted Response Surface

## Example 81.2: Response Surface Analysis with Covariates

One way of viewing covariates is as extra sources of variation in the dependent variable that can mask the variation due to primary factors. This example demonstrates the use of the `COVAR=` option in PROC RSREG to fit a response surface model to the dependent variables corrected for the covariates.

You have a chemical process with a yield that you hypothesize to be dependent on three factors: reaction time, reaction temperature, and reaction pressure. You perform an experiment to measure this dependence. You are willing to include up to 20 runs in your experiment, but you can perform no more than 8 runs on the same day, so the design for the experiment is composed of three blocks. Additionally, you know that the grade of raw material for the reaction has a significant impact on the yield. You have no control over this, but you keep track of it. The following statements create a SAS data set containing the results of the experiment:

```
data Experiment;
 input Day Grade Time Temp Pressure Yield;
 datalines;
1 67 -1 -1 -1 32.98
1 68 -1 1 1 47.04
1 70 1 -1 1 67.11
```

```

1 66 1 1 -1 26.94
1 74 0 0 0 103.22
1 68 0 0 0 42.94
2 75 -1 -1 1 122.93
2 69 -1 1 -1 62.97
2 70 1 -1 -1 72.96
2 71 1 1 1 94.93
2 72 0 0 0 93.11
2 74 0 0 0 112.97
3 69 1.633 0 0 78.88
3 67 -1.633 0 0 52.53
3 68 0 1.633 0 68.96
3 71 0 -1.633 0 92.56
3 70 0 0 1.633 88.99
3 72 0 0 -1.633 102.50
3 70 0 0 0 82.84
3 72 0 0 0 103.12
;

```

Your first analysis neglects to take the covariates into account. The following statements use PROC RSREG to fit a response surface to the observed yield, but note that Day and Grade are omitted:

```

proc rsreg data=Experiment;
 model Yield = Time Temp Pressure;
run;

```

The ANOVA results shown in [Output 81.2.1](#) indicate that *no* process variable effects are significantly larger than the background noise.

**Output 81.2.1** Analysis of Variance Ignoring Covariates

| The RSREG Procedure |    |                          |                   |             |        |
|---------------------|----|--------------------------|-------------------|-------------|--------|
| Regression          | DF | Type I Sum<br>of Squares | R-Square          | F Value     | Pr > F |
| Linear              | 3  | 1880.842426              | 0.1353            | 0.67        | 0.5915 |
| Quadratic           | 3  | 2370.438681              | 0.1706            | 0.84        | 0.5023 |
| Crossproduct        | 3  | 241.873250               | 0.0174            | 0.09        | 0.9663 |
| Total Model         | 9  | 4493.154356              | 0.3233            | 0.53        | 0.8226 |
|                     |    |                          |                   |             |        |
|                     |    |                          | Sum of<br>Squares | Mean Square |        |
| Residual            | DF |                          |                   |             |        |
| Total Error         | 10 | 9405.129724              |                   | 940.512972  |        |

However, when the yields are adjusted for covariate effects of day and grade of raw material, very strong process variable effects are revealed. The following statements produce the ANOVA results in [Output 81.2.2](#). Note that in order to include the effects of the classification factor Day as covariates, you need to create dummy variables indicating each day separately.

```

data Experiment;
 set Experiment;
 d1 = (Day = 1);
 d2 = (Day = 2);
 d3 = (Day = 3);

ods graphics on;
proc rsreg data=Experiment plots=all;
 model Yield = d1-d3 Grade Time Temp Pressure / covar=4;
run;
ods graphics off;

```

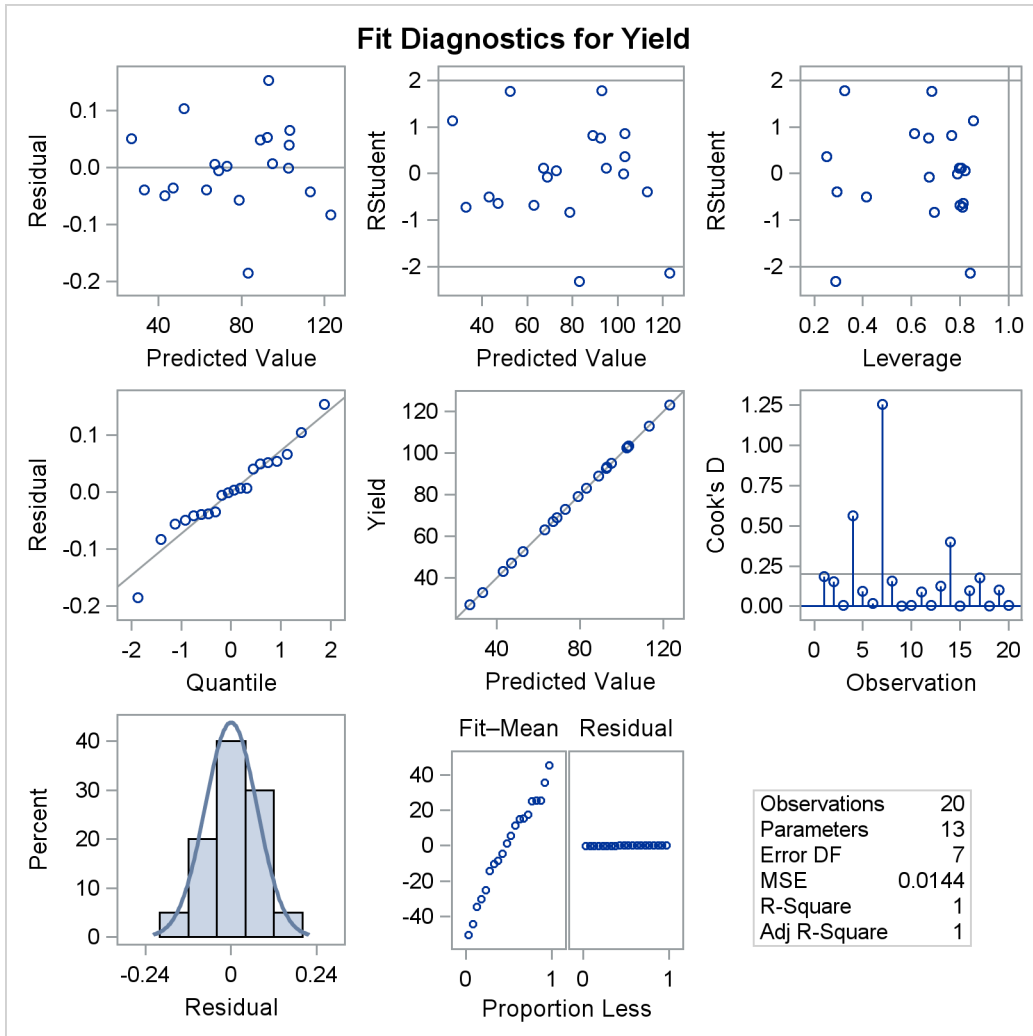
The results show very strong effects due to both the covariates and the process variables.

### Output 81.2.2 Analysis of Variance Including Covariates

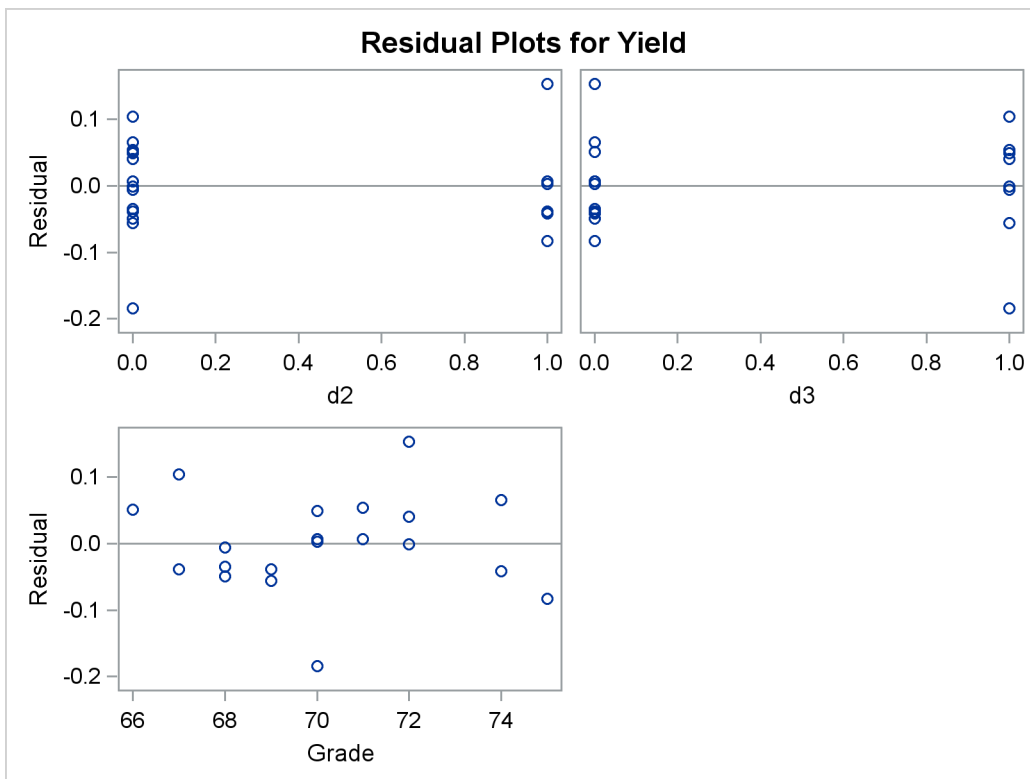
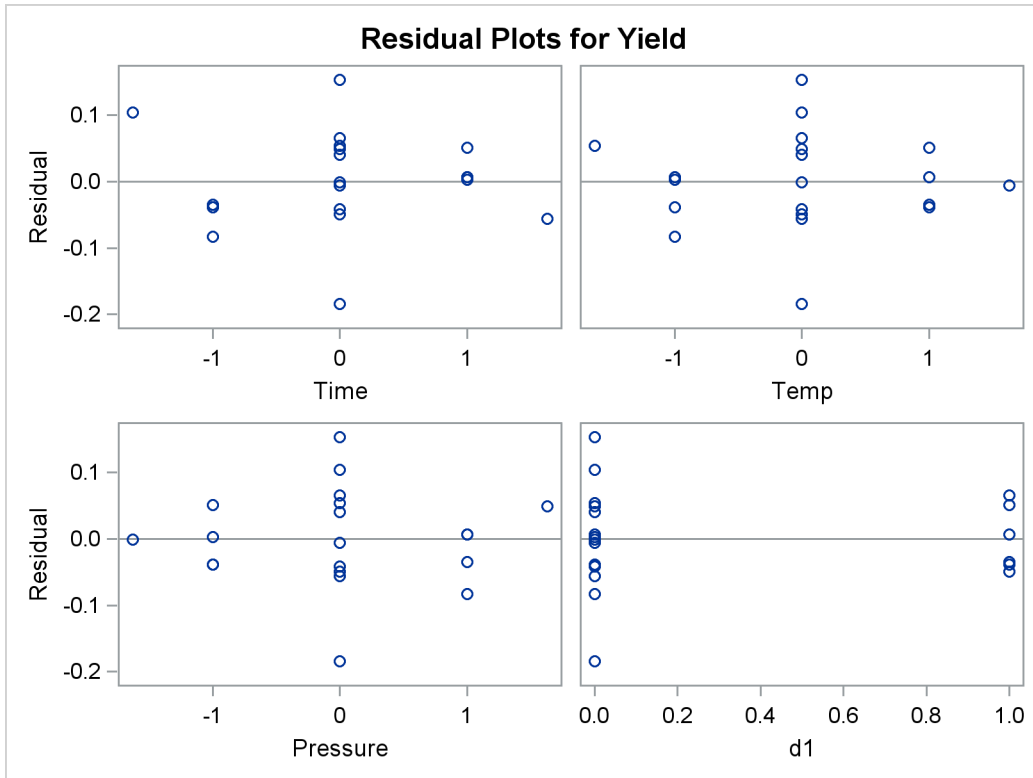
| The RSREG Procedure |    |                          |             |         |        |
|---------------------|----|--------------------------|-------------|---------|--------|
| Regression          | DF | Type I Sum<br>of Squares | R-Square    | F Value | Pr > F |
| Covariates          | 3  | 13695                    | 0.9854      | 316957  | <.0001 |
| Linear              | 3  | 156.524497               | 0.0113      | 3622.53 | <.0001 |
| Quadratic           | 3  | 22.989775                | 0.0017      | 532.06  | <.0001 |
| Crossproduct        | 3  | 23.403614                | 0.0017      | 541.64  | <.0001 |
| Total Model         | 12 | 13898                    | 1.0000      | 80413.2 | <.0001 |
| Residual            | DF | Sum of<br>Squares        | Mean Square |         |        |
| Total Error         | 7  | 0.100820                 | 0.014403    |         |        |

The number of observations in the data set might be too small for the diagnostic plots in [Output 81.2.3](#) to dependably identify problems; however, some outliers are indicated. The residual plots in [Output 81.2.4](#) do not display any obvious structure.

**Output 81.2.3** Fit Diagnostics



Output 81.2.4 Residual Plots





---

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# Chapter 82

## The SCORE Procedure

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---

### Overview: SCORE Procedure

The SCORE procedure multiplies values from two SAS data sets, one containing coefficients (for example, factor-scoring coefficients or regression coefficients) and the other containing raw data to be scored using the coefficients from the first data set. The result of this multiplication is a SAS data set containing linear combinations of the coefficients and the raw data values.

Many statistical procedures output coefficients that PROC SCORE can apply to raw data to produce scores. The new score variable is formed as a linear combination of raw data and scoring coefficients. For each observation in the raw data set, PROC SCORE multiplies the value of a variable in the raw data set by the matching scoring coefficient from the data set of scoring coefficients. This multiplication process is repeated for each variable in the VAR statement. The resulting products are then summed to produce the value of the new score variable. This entire process is repeated for each observation in the raw data set. In other words, PROC SCORE cross multiplies part of one data set with another.

---

## Raw Data Set

The raw data set can contain the original data used to calculate the scoring coefficients, or it can contain an entirely different data set. The raw data set must contain all the variables needed to produce scores. In addition, the scoring coefficients and the variables in the raw data set that are used in scoring must have the same names. See the section “Getting Started: SCORE Procedure” on page 6947 for more information.

---

## Scoring Coefficients Data Set

The data set containing scoring coefficients must contain two special variables: the `_TYPE_` variable and the `_NAME_` or `_MODEL_` variable.

- The `_TYPE_` variable identifies the observations that contain scoring coefficients.
- The `_NAME_` or `_MODEL_` variable provides a SAS name for the new score variable.

PROC SCORE first looks for a `_NAME_` variable in the SCORE= input data set. If there is such a variable, the variable's value is what SCORE uses to name the new score variable. If the SCORE= data set does not have a `_NAME_` variable, then PROC SCORE looks for a `_MODEL_` variable.

For example, PROC FACTOR produces an output data set that contains factor-scoring coefficients. In this output data set, the scoring coefficients are identified by `_TYPE_='SCORE'`. For `_TYPE_='SCORE'`, the `_NAME_` variable has values of 'Factor1', 'Factor2', and so forth. PROC SCORE gives the new score variables the names Factor1, Factor2, and so forth.

As another example, the REG procedure produces an output data set that contains parameter estimates. In this output data set, the parameter estimates are identified by `_TYPE_='PARMS'`. The `_MODEL_` variable contains the label used in the MODEL statement in PROC REG, or it uses `MODEL $n$`  if no label is specified. This label is the name PROC SCORE gives to the new score variable.

---

## Standardization of Raw Data

PROC SCORE automatically standardizes or centers the DATA= variables for you, based on information from the original variables and analysis from the SCORE= data set.

If the SCORE= scoring coefficients data set contains observations with `_TYPE_='MEAN'` and `_TYPE_='STD'`, then PROC SCORE standardizes the raw data before scoring. For example, this type of SCORE= data set can come from PROC PRINCOMP without the COV option.

If the SCORE= scoring coefficients data set contains observations with `_TYPE_='MEAN'` but `_TYPE_='STD'` is absent, then PROC SCORE centers the raw data (the means are subtracted) before scoring. For example, this type of SCORE= data set can come from PROC PRINCOMP with the COV option.

If the SCORE= scoring coefficients data set does not contain observations with `_TYPE_='MEAN'` and `_TYPE_='STD'`, or if you use the NOSTD option, then PROC SCORE does not center or standardize the raw data.

If the SCORE= scoring coefficients are obtained from observations with `_TYPE_='USCORE'`, then PROC SCORE “standardizes” the raw data by using the uncorrected standard deviations identified by `_TYPE_='USTD'`, and the means are not subtracted from the raw data. For example, this type of SCORE= data set can come from PROC PRINCOMP with the NOINT option. For more information about `_TYPE_='USCORE'` scoring coefficients in TYPE=UCORR or TYPE=UCOV output data sets, see Appendix A, “Special SAS Data Sets.”

You can use PROC SCORE to score the data that were also used to generate the scoring coefficients, although more typically, scoring results are directly obtained from the OUT= data set in a procedure that computes scoring coefficients. When scoring new data, it is important to realize that PROC SCORE assumes that the new data have approximately the same scales as the original data. For example, if you specify the COV option with PROC PRINCOMP for the original analysis, the scoring coefficients in the PROC PRINCOMP OUTSTAT= data set are not appropriate for standardized data. With the COV option, PROC PRINCOMP will not output `_TYPE_='STD'` observations to the OUTSTAT= data set, and PROC SCORE will only subtract the means of the original (not new) variables from the new variables before multiplying. Without the COV option in PROC PRINCOMP, both the original variable means and standard deviations will be in the OUTSTAT= data set, and PROC SCORE will subtract the original variable means from the new variables and divide them by the original variable standard deviations before multiplying.

In general, procedures that output scoring coefficients in their OUTSTAT= data sets provide the necessary information for PROC SCORE to determine the appropriate standardization. However, if you use PROC SCORE with a scoring coefficients data set that you constructed without `_TYPE_='MEAN'` and `_TYPE_='STD'` observations, you might have to do the relevant centering or standardization of the new data first. If you do this, you must use the means and standard deviations of the original variables—that is, the variables that were used to generate the coefficients—not the means and standard deviations of the variables to be scored.

See the section “Getting Started: SCORE Procedure” on page 6947 for further illustration.

---

## Getting Started: SCORE Procedure

The SCORE procedure multiplies the values from two SAS data sets and creates a new data set to contain the results of the multiplication. The variables in the new data set are linear combinations of the variables in the two input data sets. Typically, one of these data sets contains raw data that you want to score, and the other data set contains scoring coefficients.

The following example demonstrates how to use the SCORE procedure to multiply values from two SAS data sets, one containing factor-scoring coefficients and the other containing raw data to be scored using the scoring coefficients.

Suppose you are interested in the performance of three different types of schools: private schools, state-run urban schools, and state-run rural schools. You want to compare the schools’ performances as measured by student grades on standard tests in English, mathematics, and biology. You administer these tests and record the scores for each of the three types of schools.

The following DATA step creates the SAS data set Schools. The data are provided by Chaseling (1996).

```

data Schools;
 input Type $ English Math Biology @@;
 datalines;
p 52 55 45 p 42 49 40 p 63 64 54
p 47 50 51 p 64 69 47 p 63 67 54
p 59 63 42 p 56 61 41 p 41 44 72
p 39 42 45 p 56 63 44 p 63 73 42

 ... more lines ...

r 50 47 49 r 55 48 46 r 38 36 51
;

```

The data set `Schools` contains the character variable `Type`, which represents the type of school. Valid values are `p` (private schools), `r` (state-run rural schools), and `u` (state-run urban schools).

The three numeric variables in the data set are `English`, `Math`, and `Biology`, which represent the student scores for English, mathematics, and biology, respectively. The double trailing at sign (`@@`) in the `INPUT` statement specifies that observations are input from each line until all values are read.

The following statements invoke the `FACTOR` procedure to compute the data set of factor scoring coefficients. The statements perform a principal components factor analysis that uses all three numeric variables in the SAS data set `Schools`. The `OUTSTAT=` option requests that `PROC FACTOR` output the factor scores to the data set `Scores`. The `NOPRINT` option suppresses display of the output.

```

proc factor data=Schools score outstat=Scores noprint;
 var english math biology;
run;

proc score data=schools score=Scores out=New;
 var english math biology;
 id type;
run;

```

The SCORE procedure is then invoked using Schools as the raw data set to be scored and Scores as the scoring data set. The OUT= option creates the SAS data set New to contain the linear combinations.

The VAR statement specifies that the variables English, Math, and Biology are used in computing scores. The ID statement copies the variable Type from the Schools data set to the output data set New.

The following statements print the SAS output data set Scores, the first two observations from the original data set Schools, and the first two observations of the resulting data set New.

```

title 'OUTSTAT= Data Set from PROC FACTOR';
proc print data=Scores;
run;

title 'First Two Observations of the DATA= Data Set from PROC SCORE';
proc print data=Schools(obs=2);
run;

title 'First Two Observations of the OUT= Data Set from PROC SCORE';
proc print data=New(obs=2);
run;

```

Figure 82.1 displays the output data set Scores produced by the FACTOR procedure. The last observation (number 11) contains the scoring coefficients (`_TYPE_='SCORE'`). Only one factor has been retained.

**Figure 82.1** Listing of the Data Set Created by PROC FACTOR

| OUTSTAT= Data Set from PROC FACTOR |          |         |         |         |         |
|------------------------------------|----------|---------|---------|---------|---------|
| Obs                                | _TYPE_   | _NAME_  | English | Math    | Biology |
| 1                                  | MEAN     |         | 55.525  | 52.325  | 50.350  |
| 2                                  | STD      |         | 12.949  | 12.356  | 12.239  |
| 3                                  | N        |         | 120.000 | 120.000 | 120.000 |
| 4                                  | CORR     | English | 1.000   | 0.833   | 0.672   |
| 5                                  | CORR     | Math    | 0.833   | 1.000   | 0.594   |
| 6                                  | CORR     | Biology | 0.672   | 0.594   | 1.000   |
| 7                                  | COMMUNAL |         | 0.881   | 0.827   | 0.696   |
| 8                                  | PRIORS   |         | 1.000   | 1.000   | 1.000   |
| 9                                  | EIGENVAL |         | 2.405   | 0.437   | 0.159   |
| 10                                 | PATTERN  | Factor1 | 0.939   | 0.910   | 0.834   |
| 11                                 | SCORE    | Factor1 | 0.390   | 0.378   | 0.347   |

Figure 82.2 lists the first two observations of the original SAS data set (Schools).



**Figure 82.2** First Two Observations of the Schools Data Set

| First Two Observations of the DATA= Data Set from PROC SCORE |      |         |      |         |
|--------------------------------------------------------------|------|---------|------|---------|
| Obs                                                          | Type | English | Math | Biology |
| 1                                                            | p    | 52      | 55   | 45      |
| 2                                                            | p    | 42      | 49   | 40      |

Figure 82.3 lists the first two observations of the output data set New created by PROC SCORE.

**Figure 82.3** Listing of the New Data Set

| First Two Observations of the OUT= Data Set from PROC SCORE |      |          |
|-------------------------------------------------------------|------|----------|
| Obs                                                         | Type | Factor1  |
| 1                                                           | p    | -0.17604 |
| 2                                                           | p    | -0.80294 |

The score variable Factor1 in the New data set is named according to the value of the `_NAME_` variable in the Scores data set. The values of the variable Factor1 are computed as follows: the DATA= data set variables are standardized using the same means and standard deviations that PROC FACTOR used when extracting the factors because the Scores data set contains observations with `_TYPE_='MEAN'` and `_TYPE_='STD'`.

Note that in order to correctly use standardized scoring coefficients created by other procedures such as PROC FACTOR in this example, the data to be scored must be standardized in the same way that the data were standardized when the scoring coefficients were computed. Otherwise, the resulting scores might be incorrect. PROC SCORE does this automatically if the SCORE= data set is the original OUTSTAT= data set output from the procedure creating the scoring coefficients.

These standardized variables are then multiplied by their respective standardized scoring coefficients from the data set Scores. These products are summed over all three variables, and the sum is the value of the new variable Factor1. The first two values of the scored variable Factor1 are obtained as follows:

$$\left( \frac{(52 - 55.525)}{12.949} \times 0.390 \right) + \left( \frac{(55 - 52.325)}{12.356} \times 0.378 \right) + \left( \frac{(45 - 50.350)}{12.239} \times 0.347 \right) = -0.17604$$

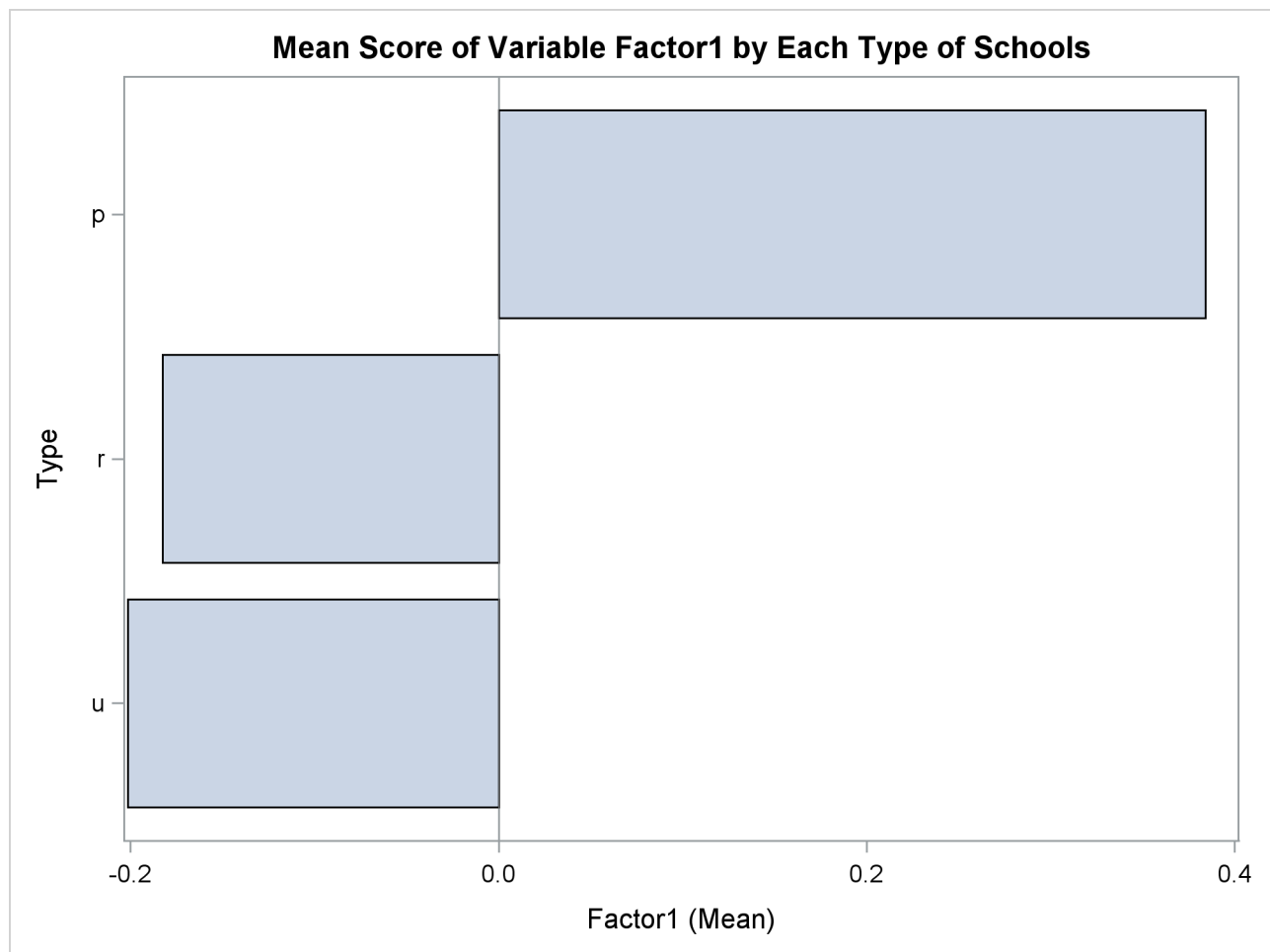
$$\left( \frac{(42 - 55.525)}{12.949} \times 0.390 \right) + \left( \frac{(49 - 52.325)}{12.356} \times 0.378 \right) + \left( \frac{(40 - 50.350)}{12.239} \times 0.347 \right) = -0.80294$$

The following statements request that the SGPLOT procedure produce a horizontal bar chart of the variable `Type`. The length of each bar represents the mean of the variable `Factor1`.

```
title 'Mean Score of Variable Factor1 by Each Type of Schools';
proc sgplot data=New;
 hbar type / stat = mean response=Factor1;
run;
```

Figure 82.4 displays the mean score of the variable `Factor1` for each of the three school types. For private schools (`Type=p`), the average value of the variable `Factor1` is 0.384, while for state-run schools the average values are much lower. The state-run urban schools (`Type=u`) have the lowest mean value of  $-0.202$ , and the state-run rural schools (`Type=r`) have a mean value of  $-0.183$ .

**Figure 82.4** Bar Chart of School Type



## Syntax: SCORE Procedure

The following statements are available in the SCORE procedure:

```
PROC SCORE DATA=SAS-data-set < options > ;
 BY variables ;
 ID variables ;
 VAR variables ;
```

The only required statement is the PROC SCORE statement. The BY, ID, and VAR statements are described following the PROC SCORE statement.

## PROC SCORE Statement

```
PROC SCORE DATA=SAS-data-set < options > ;
```

The PROC SCORE statement invokes the SCORE procedure. Table 82.1 summarizes the options available in the PROC SCORE statement.

**Table 82.1** PROC SCORE Statement Options

| Option          | Description                                                   |
|-----------------|---------------------------------------------------------------|
| <b>DATA=</b>    | Names the input SAS data set containing the raw data to score |
| <b>NOSTD</b>    | Suppresses centering and scaling of the raw data              |
| <b>OUT=</b>     | Specifies the name of the SAS data set                        |
| <b>PREDICT</b>  | Treats coefficients of $-1$ as $0$                            |
| <b>RESIDUAL</b> | Reverses the sign of each score                               |
| <b>SCORE=</b>   | Names the data set containing the scoring coefficients        |
| <b>TYPE=</b>    | Specifies the observations that contain scoring coefficients  |

You can specify the following options in the PROC SCORE statement.

### **DATA=SAS-data-set**

names the input SAS data set containing the raw data to score. This option is required.

### **NOSTD**

suppresses centering and scaling of the raw data. Ordinarily, if PROC SCORE finds `_TYPE_='MEAN'`, `_TYPE_='USCORE'`, `_TYPE_='USTD'`, or `_TYPE_='STD'` observations in the SCORE= data set, the procedure uses these to standardize the raw data before scoring.

### **OUT=SAS-data-set**

specifies the name of the SAS data set created by PROC SCORE. If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*. If the OUT= option is omitted, PROC SCORE still creates an output data set and automatically names it according to the DATA $n$  convention, as if you omitted a data set name in a DATA statement.

**PREDICT**

specifies that PROC SCORE should treat coefficients of  $-1$  in the SCORE= data set as 0. In regression applications, the dependent variable is coded with a coefficient of  $-1$ . Applied directly to regression results, PROC SCORE produces negative residuals (see the description of the RESIDUAL option, which follows); the PREDICT option produces predicted values instead.

**RESIDUAL**

reverses the sign of each score. Applied directly to regression results, PROC SCORE produces negative residuals (PREDICT–ACTUAL); the RESIDUAL option produces positive residuals (ACTUAL–PREDICT) instead.

**SCORE=SAS-data-set**

names the data set containing the scoring coefficients. If you omit the SCORE= option, the most recently created SAS data set is used. This data set must have two special variables: `_TYPE_` and either `_NAME_` or `_MODEL_`.

**TYPE=name or 'string'**

specifies the observations in the SCORE= data set that contain scoring coefficients. The TYPE= procedure option is unrelated to the data set option that has the same name. PROC SCORE examines the values of the special variable `_TYPE_` in the SCORE= data set. When the value of `_TYPE_` matches `TYPE=name`, the observation in the SCORE= data set is used to score the raw data in the DATA= data set.

If you omit the TYPE= option, scoring coefficients are read from observations with either `_TYPE_='SCORE'` or `_TYPE_='USCORE'`. Because the default for PROC SCORE is `TYPE=SCORE`, you need not specify the TYPE= option for factor scoring or for computing scores from OUTSTAT= data sets from the CANCELL, CANDISC, PRINCOMP, or VARCLUS procedure. When you use regression coefficients from PROC REG, specify `TYPE=PARMS`.

The maximum length of the argument specified in the TYPE= option depends on the length defined by the VALIDVARIABLE= SAS system option. For additional information, see *SAS System Options: Reference*.

Note that the TYPE= option setting is not case sensitive. For example, the two option settings `TYPE='MyScore'` and `TYPE='myscore'` are equivalent.

---

## BY Statement

**BY variables ;**

You can specify a BY statement with PROC SCORE to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.

- Specify the `NOTSORTED` or `DESCENDING` option in the `BY` statement for the `SCORE` procedure. The `NOTSORTED` option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the `BY` variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the `BY` variables by using the `DATASETS` procedure (in Base SAS software).

For more information about `BY`-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the `DATASETS` procedure, see the discussion in the *Base SAS Procedures Guide*.

You can specify a `BY` statement to apply separate groups of scoring coefficients to the entire `DATA=` data set.

If the `DATA=` data set does not contain any of the `BY` variables, the entire `DATA=` data set is scored by each `BY` group of scoring coefficients in the `SCORE=` data set.

If the `DATA=` data set contains some but not all of the `BY` variables, or if some `BY` variables do not have the same type or length in the `DATA=` data set as in the `SCORE=` data set, then `PROC SCORE` prints an error message and stops.

If all the `BY` variables appear in the `DATA=` data set with the same type and length as in the `SCORE=` data set, then each `BY` group in the `DATA=` data set is scored using scoring coefficients from the corresponding `BY` group in the `SCORE=` data set. The `BY` groups in the `DATA=` data set must be in the same order as in the `SCORE=` data set. All `BY` groups in the `DATA=` data set must also appear in the `SCORE=` data set. If you do not specify the `NOTSORTED` option, some `BY` groups can appear in the `SCORE=` data set but not in the `DATA=` data set; such `BY` groups are not used in computing scores.

---

## ID Statement

**ID** *variables* ;

The `ID` statement identifies variables from the `DATA=` data set to be included in the `OUT=` data set. If there is no `ID` statement, all variables from the `DATA=` data set are included in the `OUT=` data set. The `ID` variables can be character or numeric.

---

## VAR Statement

**VAR** *variables* ;

The `VAR` statement specifies the variables to be used in computing scores. These variables must be in both the `DATA=` and `SCORE=` input data sets and must be numeric. If you do not specify a `VAR` statement, the procedure uses all numeric variables in the `SCORE=` data set. You should almost always specify a `VAR` statement with `PROC SCORE` because you would rarely use all the numeric variables in your data set to compute scores.

---

## Details: SCORE Procedure

---

### Missing Values

If one of the scoring variables in the DATA= data set has a missing value for an observation, all the scores have missing values for that observation. The exception to this criterion is that if the PREDICT option is specified, the variable with a coefficient of  $-1$  can tolerate a missing value and still produce a prediction score. Also, a variable with a coefficient of  $0$  can tolerate a missing value.

If a scoring coefficient in the SCORE= data set has a missing value for an observation, the coefficient is not used in creating the new score variable for the observation. In other words, missing values of scoring coefficients are treated as zeros. This treatment affects only the observation in which the missing value occurs.

---

### Regression Parameter Estimates from PROC REG

If the SCORE= data set is an OUTEST= data set produced by PROC REG and if you specify TYPE=PARMS, the interpretation of the new score variables depends on the PROC SCORE options chosen and the variables listed in the VAR statement. If the VAR statement contains only the independent variables used in a model in PROC REG, the new score variables give the predicted values. If the VAR statement contains the dependent variables and the independent variables used in a model in PROC REG, the interpretation of the new score variables depends on the PROC SCORE options chosen. If you omit both the PREDICT and the RESIDUAL options, the new score variables give negative residuals (PREDICT–ACTUAL). If you specify the RESIDUAL option, the new score variables give positive residuals (ACTUAL–PREDICT). If you specify the PREDICT option, the new score variables give predicted values.

Unless you specify the NOINT option for PROC REG, the OUTEST= data set contains the variable Intercept. The SCORE procedure uses the intercept value in computing the scores.

---

### Output Data Set

PROC SCORE produces an output data set but displays no output. The output OUT= data set contains the following variables:

- the ID variables, if any
- all variables from the DATA= data set, if no ID variables are specified
- the BY variables, if any
- the new score variables, named from the `_NAME_` or `_MODEL_` values in the SCORE= data set

---

## Computational Resources

Let

- $v$  = number of variables used in computing scores
- $s$  = number of new score variables
- $b$  = maximum number of new score variables in a BY group
- $n$  = original input value

### Memory

The array storage required is approximately  $8(4v + (3 + v)b + s)$  bytes. When you do not use BY processing, the array storage required is approximately  $8(4v + (4 + v)s)$  bytes.

### Time

The time required to construct the scoring matrix is roughly proportional to  $vs$ , and the time needed to compute the scores is roughly proportional to  $nvs$ .

---

## Examples: SCORE Procedure

The following three examples use a subset of the Fitness data set. The complete data set is given in Chapter 79, “The REG Procedure.”

---

### Example 82.1: Factor Scoring Coefficients

This example shows how to use PROC SCORE with factor scoring coefficients. First, the FACTOR procedure produces an output data set containing scoring coefficients in observations identified by `_TYPE_='SCORE'`. These data, together with the original data set Fitness, are supplied to PROC SCORE, resulting in a data set containing scores Factor1 and Factor2. The following statements produce Output 82.1.1 through Output 82.1.3:

```

/* This data set contains only the first 12 observations */
/* from the full data set used in the chapter on PROC REG. */
data Fitness;
 input Age Weight Oxygen RunTime RestPulse RunPulse @@;
 datalines;
44 89.47 44.609 11.37 62 178 40 75.07 45.313 10.07 62 185
44 85.84 54.297 8.65 45 156 42 68.15 59.571 8.17 40 166
38 89.02 49.874 9.22 55 178 47 77.45 44.811 11.63 58 176
40 75.98 45.681 11.95 70 176 43 81.19 49.091 10.85 64 162
44 81.42 39.442 13.08 63 174 38 81.87 60.055 8.63 48 170
44 73.03 50.541 10.13 45 168 45 87.66 37.388 14.03 56 186
;

```

```

proc factor data=Fitness outstat=FactOut
 method=prin rotate=varimax score;
 var Age Weight RunTime RunPulse RestPulse;
 title 'Factor Scoring Example';
run;

proc print data=FactOut;
 title2 'Data Set from PROC FACTOR';
run;

proc score data=Fitness score=FactOut out=FScore;
 var Age Weight RunTime RunPulse RestPulse;
run;

proc print data=FScore;
 title2 'Data Set from PROC SCORE';
run;

```

Output 82.1.1 shows the PROC FACTOR output. The scoring coefficients for the two factors are shown at the end of the PROC FACTOR output.

**Output 82.1.1** Creating an OUTSTAT= Data Set with PROC FACTOR

|                                                              |                          |            |            |            |
|--------------------------------------------------------------|--------------------------|------------|------------|------------|
| Factor Scoring Example                                       |                          |            |            |            |
| The FACTOR Procedure                                         |                          |            |            |            |
|                                                              | Input Data Type          |            | Raw Data   |            |
|                                                              | Number of Records Read   |            | 12         |            |
|                                                              | Number of Records Used   |            | 12         |            |
|                                                              | N for Significance Tests |            | 12         |            |
| Factor Scoring Example                                       |                          |            |            |            |
| The FACTOR Procedure                                         |                          |            |            |            |
| Initial Factor Method: Principal Components                  |                          |            |            |            |
| Prior Communality Estimates: ONE                             |                          |            |            |            |
| Eigenvalues of the Correlation Matrix: Total = 5 Average = 1 |                          |            |            |            |
|                                                              | Eigenvalue               | Difference | Proportion | Cumulative |
| 1                                                            | 2.30930638               | 1.11710686 | 0.4619     | 0.4619     |
| 2                                                            | 1.19219952               | 0.30997249 | 0.2384     | 0.7003     |
| 3                                                            | 0.88222702               | 0.37965990 | 0.1764     | 0.8767     |
| 4                                                            | 0.50256713               | 0.38886717 | 0.1005     | 0.9773     |
| 5                                                            | 0.11369996               |            | 0.0227     | 1.0000     |



Output 82.1.1 *continued*

2 factors will be retained by the MINEIGEN criterion.

## Factor Pattern

|           | Factor1 | Factor2  |
|-----------|---------|----------|
| Age       | 0.29795 | 0.93675  |
| Weight    | 0.43282 | -0.17750 |
| RunTime   | 0.91983 | 0.28782  |
| RunPulse  | 0.72671 | -0.38191 |
| RestPulse | 0.81179 | -0.23344 |

## Variance Explained by Each Factor

| Factor1   | Factor2   |
|-----------|-----------|
| 2.3093064 | 1.1921995 |

Final Communality Estimates: Total = 3.501506

| Age        | Weight     | RunTime    | RunPulse   | RestPulse  |
|------------|------------|------------|------------|------------|
| 0.96628351 | 0.21883401 | 0.92893333 | 0.67396207 | 0.71349297 |

## Factor Scoring Example

The FACTOR Procedure  
Rotation Method: Varimax

## Orthogonal Transformation Matrix

|   | 1        | 2       |
|---|----------|---------|
| 1 | 0.92536  | 0.37908 |
| 2 | -0.37908 | 0.92536 |

## Rotated Factor Pattern

|           | Factor1  | Factor2  |
|-----------|----------|----------|
| Age       | -0.07939 | 0.97979  |
| Weight    | 0.46780  | -0.00018 |
| RunTime   | 0.74207  | 0.61503  |
| RunPulse  | 0.81725  | -0.07792 |
| RestPulse | 0.83969  | 0.09172  |

**Output 82.1.1** *continued*

| Variance Explained by Each Factor                               |            |            |            |            |
|-----------------------------------------------------------------|------------|------------|------------|------------|
|                                                                 | Factor1    | Factor2    |            |            |
|                                                                 | 2.1487753  | 1.3527306  |            |            |
| Final Communality Estimates: Total = 3.501506                   |            |            |            |            |
| Age                                                             | Weight     | RunTime    | RunPulse   | RestPulse  |
| 0.96628351                                                      | 0.21883401 | 0.92893333 | 0.67396207 | 0.71349297 |
| Factor Scoring Example                                          |            |            |            |            |
| The FACTOR Procedure                                            |            |            |            |            |
| Rotation Method: Varimax                                        |            |            |            |            |
| Scoring Coefficients Estimated by Regression                    |            |            |            |            |
| Squared Multiple Correlations of the Variables with Each Factor |            |            |            |            |
|                                                                 | Factor1    | Factor2    |            |            |
|                                                                 | 1.0000000  | 1.0000000  |            |            |
| Standardized Scoring Coefficients                               |            |            |            |            |
|                                                                 | Factor1    | Factor2    |            |            |
| Age                                                             | -0.17846   | 0.77600    |            |            |
| Weight                                                          | 0.22987    | -0.06672   |            |            |
| RunTime                                                         | 0.27707    | 0.37440    |            |            |
| RunPulse                                                        | 0.41263    | -0.17714   |            |            |
| RestPulse                                                       | 0.39952    | -0.04793   |            |            |

Output 82.1.2 lists the OUTSTAT= data set from PROC FACTOR. Note that observations 18 and 19 have `_TYPE_='SCORE'`. Observations 1 and 2 have `_TYPE_='MEAN'` and `_TYPE_='STD'`, respectively. These four observations are used by PROC SCORE.

**Output 82.1.2** OUTSTAT= Data Set from PROC FACTOR Reproduced with PROC PRINT

| Factor Scoring Example<br>Data Set from PROC FACTOR |          |           |         |         |         |          |               |
|-----------------------------------------------------|----------|-----------|---------|---------|---------|----------|---------------|
| Obs                                                 | _TYPE_   | _NAME_    | Age     | Weight  | RunTime | RunPulse | Rest<br>Pulse |
| 1                                                   | MEAN     |           | 42.4167 | 80.5125 | 10.6483 | 172.917  | 55.6667       |
| 2                                                   | STD      |           | 2.8431  | 6.7660  | 1.8444  | 8.918    | 9.2769        |
| 3                                                   | N        |           | 12.0000 | 12.0000 | 12.0000 | 12.000   | 12.0000       |
| 4                                                   | CORR     | Age       | 1.0000  | 0.0128  | 0.5005  | -0.095   | -0.0080       |
| 5                                                   | CORR     | Weight    | 0.0128  | 1.0000  | 0.2637  | 0.173    | 0.2396        |
| 6                                                   | CORR     | RunTime   | 0.5005  | 0.2637  | 1.0000  | 0.556    | 0.6620        |
| 7                                                   | CORR     | RunPulse  | -0.0953 | 0.1731  | 0.5555  | 1.000    | 0.4853        |
| 8                                                   | CORR     | RestPulse | -0.0080 | 0.2396  | 0.6620  | 0.485    | 1.0000        |
| 9                                                   | COMMUNAL |           | 0.9663  | 0.2188  | 0.9289  | 0.674    | 0.7135        |
| 10                                                  | PRIORS   |           | 1.0000  | 1.0000  | 1.0000  | 1.000    | 1.0000        |
| 11                                                  | EIGENVAL |           | 2.3093  | 1.1922  | 0.8822  | 0.503    | 0.1137        |
| 12                                                  | UNROTATE | Factor1   | 0.2980  | 0.4328  | 0.9198  | 0.727    | 0.8118        |
| 13                                                  | UNROTATE | Factor2   | 0.9368  | -0.1775 | 0.2878  | -0.382   | -0.2334       |
| 14                                                  | TRANSFOR | Factor1   | 0.9254  | -0.3791 | .       | .        | .             |
| 15                                                  | TRANSFOR | Factor2   | 0.3791  | 0.9254  | .       | .        | .             |
| 16                                                  | PATTERN  | Factor1   | -0.0794 | 0.4678  | 0.7421  | 0.817    | 0.8397        |
| 17                                                  | PATTERN  | Factor2   | 0.9798  | -0.0002 | 0.6150  | -0.078   | 0.0917        |
| 18                                                  | SCORE    | Factor1   | -0.1785 | 0.2299  | 0.2771  | 0.413    | 0.3995        |
| 19                                                  | SCORE    | Factor2   | 0.7760  | -0.0667 | 0.3744  | -0.177   | -0.0479       |

Since the PROC SCORE statement does not contain the NOSTD option, the data in the Fitness data set are standardized before scoring. For each variable specified in the VAR statement, the mean and standard deviation are obtained from the FactOut data set. For each observation in the Fitness data set, the variables are then standardized. For example, for observation 1 in the Fitness data set, the variable Age is standardized to  $0.5569 = [(44 - 42.4167)/2.8431]$ .

After the data in the Fitness data set are standardized, the standardized values of the variables in the VAR statement are multiplied by the matching coefficients in the FactOut data set, and the resulting products are summed. This sum is output as a value of the new score variable.

Output 82.1.3 displays the FScore data set produced by PROC SCORE. This data set contains the variables Age, Weight, Oxygen, RunTime, RestPulse, and RunPulse from the Fitness data set. It also contains Factor1 and Factor2, the two new score variables.

**Output 82.1.3** OUT= Data Set from PROC SCORE Reproduced with PROC PRINT

| Factor Scoring Example<br>Data Set from PROC SCORE |     |        |        |             |               |              |          |          |
|----------------------------------------------------|-----|--------|--------|-------------|---------------|--------------|----------|----------|
| Obs                                                | Age | Weight | Oxygen | Run<br>Time | Rest<br>Pulse | Run<br>Pulse | Factor1  | Factor2  |
| 1                                                  | 44  | 89.47  | 44.609 | 11.37       | 62            | 178          | 0.82129  | 0.35663  |
| 2                                                  | 40  | 75.07  | 45.313 | 10.07       | 62            | 185          | 0.71173  | -0.99605 |
| 3                                                  | 44  | 85.84  | 54.297 | 8.65        | 45            | 156          | -1.46064 | 0.36508  |
| 4                                                  | 42  | 68.15  | 59.571 | 8.17        | 40            | 166          | -1.76087 | -0.27657 |
| 5                                                  | 38  | 89.02  | 49.874 | 9.22        | 55            | 178          | 0.55819  | -1.67684 |
| 6                                                  | 47  | 77.45  | 44.811 | 11.63       | 58            | 176          | -0.00113 | 1.40715  |
| 7                                                  | 40  | 75.98  | 45.681 | 11.95       | 70            | 176          | 0.95318  | -0.48598 |
| 8                                                  | 43  | 81.19  | 49.091 | 10.85       | 64            | 162          | -0.12951 | 0.36724  |
| 9                                                  | 44  | 81.42  | 39.442 | 13.08       | 63            | 174          | 0.66267  | 0.85740  |
| 10                                                 | 38  | 81.87  | 60.055 | 8.63        | 48            | 170          | -0.44496 | -1.53103 |
| 11                                                 | 44  | 73.03  | 50.541 | 10.13       | 45            | 168          | -1.11832 | 0.55349  |
| 12                                                 | 45  | 87.66  | 37.388 | 14.03       | 56            | 186          | 1.20836  | 1.05948  |

**Example 82.2: Regression Parameter Estimates**

In this example, PROC REG computes regression parameter estimates for the Fitness data. (See [Example 82.1](#) to for more information about how to create the Fitness data set.) The parameter estimates are output to a data set and used as scoring coefficients. For the first part of this example, PROC SCORE is used to score the Fitness data, which are the same data used in the regression.

In the second part of this example, PROC SCORE is used to score a new data set, Fitness2. For PROC SCORE, the TYPE= specification is PARMS, and the names of the score variables are found in the variable `_MODEL_`, which gets its values from the model label. The following code produces [Output 82.2.1](#) through [Output 82.2.3](#):

```
proc reg data=Fitness outest=RegOut;
 OxyHat: model Oxygen=Age Weight RunTime RunPulse RestPulse;
 title 'Regression Scoring Example';
run;

proc print data=RegOut;
 title2 'OUTEST= Data Set from PROC REG';
run;

proc score data=Fitness score=RegOut out=RScoreP type=parms;
 var Age Weight RunTime RunPulse RestPulse;
run;
```

```

proc print data=RScoreP;
 title2 'Predicted Scores for Regression';
run;

proc score data=Fitness score=RegOut out=RScoreR type=parms;
 var Oxygen Age Weight RunTime RunPulse RestPulse;
run;

proc print data=RScoreR;
 title2 'Negative Residual Scores for Regression';
run;

```

Output 82.2.1 shows the PROC REG output. The column labeled “Parameter Estimates” lists the parameter estimates. These estimates are output to the RegOut data set.

**Output 82.2.1** Creating an OUTEST= Data Set with PROC REG

| Regression Scoring Example  |    |                    |                |         |         |
|-----------------------------|----|--------------------|----------------|---------|---------|
| The REG Procedure           |    |                    |                |         |         |
| Model: OxyHat               |    |                    |                |         |         |
| Dependent Variable: Oxygen  |    |                    |                |         |         |
| Number of Observations Read |    |                    |                | 12      |         |
| Number of Observations Used |    |                    |                | 12      |         |
| Analysis of Variance        |    |                    |                |         |         |
| Source                      | DF | Sum of Squares     | Mean Square    | F Value | Pr > F  |
| Model                       | 5  | 509.62201          | 101.92440      | 15.80   | 0.0021  |
| Error                       | 6  | 38.70060           | 6.45010        |         |         |
| Corrected Total             | 11 | 548.32261          |                |         |         |
| Root MSE                    |    | 2.53970            | R-Square       | 0.9294  |         |
| Dependent Mean              |    | 48.38942           | Adj R-Sq       | 0.8706  |         |
| Coeff Var                   |    | 5.24847            |                |         |         |
| Parameter Estimates         |    |                    |                |         |         |
| Variable                    | DF | Parameter Estimate | Standard Error | t Value | Pr >  t |
| Intercept                   | 1  | 151.91550          | 31.04738       | 4.89    | 0.0027  |
| Age                         | 1  | -0.63045           | 0.42503        | -1.48   | 0.1885  |
| Weight                      | 1  | -0.10586           | 0.11869        | -0.89   | 0.4068  |
| RunTime                     | 1  | -1.75698           | 0.93844        | -1.87   | 0.1103  |
| RunPulse                    | 1  | -0.22891           | 0.12169        | -1.88   | 0.1090  |
| RestPulse                   | 1  | -0.17910           | 0.13005        | -1.38   | 0.2176  |

Output 82.2.2 lists the RegOut data set. Note that `_TYPE_='PARMS'` and `_MODEL_='OXYHAT'`, which are from the label in the MODEL statement in PROC REG.

**Output 82.2.2** OUTEST= Data Set from PROC REG Reproduced with PROC PRINT

| Regression Scoring Example     |          |          |          |               |           |          |
|--------------------------------|----------|----------|----------|---------------|-----------|----------|
| OUTEST= Data Set from PROC REG |          |          |          |               |           |          |
| Obs                            | _MODEL_  | _TYPE_   | _DEPVAR_ | _RMSE_        | Intercept | Age      |
| 1                              | OxyHat   | PARMS    | Oxygen   | 2.53970       | 151.916   | -0.63045 |
| Obs                            | Weight   | RunTime  | RunPulse | Rest<br>Pulse | Oxygen    |          |
| 1                              | -0.10586 | -1.75698 | -0.22891 | -0.17910      | -1        |          |

Output 82.2.3 lists the data sets created by PROC SCORE. Since the SCORE= data set does not contain observations with `_TYPE_='MEAN'` or `_TYPE_='STD'`, the data in the Fitness data set are not standardized before scoring. The SCORE= data set contains the variable Intercept, so this intercept value is used in computing the score. To produce the RScoreP data set, the VAR statement in PROC SCORE includes only the independent variables from the model in PROC REG. As a result, the OxyHat variable contains predicted values. To produce the RScoreR data set, the VAR statement in PROC SCORE includes both the dependent variables and the independent variables from the model in PROC REG. As a result, the OxyHat variable contains negative residuals (PREDICT-ACTUAL) as shown in Output 82.2.4. If the RESIDUAL option is specified, the variable OxyHat contains positive residuals (ACTUAL-PREDICT). If the PREDICT option is specified, the OxyHat variable contains predicted values.

**Output 82.2.3** Predicted Scores from the OUT= Data Set Created by PROC SCORE

| Regression Scoring Example      |     |        |        |             |               |              |         |
|---------------------------------|-----|--------|--------|-------------|---------------|--------------|---------|
| Predicted Scores for Regression |     |        |        |             |               |              |         |
| Obs                             | Age | Weight | Oxygen | Run<br>Time | Rest<br>Pulse | Run<br>Pulse | OxyHat  |
| 1                               | 44  | 89.47  | 44.609 | 11.37       | 62            | 178          | 42.8771 |
| 2                               | 40  | 75.07  | 45.313 | 10.07       | 62            | 185          | 47.6050 |
| 3                               | 44  | 85.84  | 54.297 | 8.65        | 45            | 156          | 56.1211 |
| 4                               | 42  | 68.15  | 59.571 | 8.17        | 40            | 166          | 58.7044 |
| 5                               | 38  | 89.02  | 49.874 | 9.22        | 55            | 178          | 51.7386 |
| 6                               | 47  | 77.45  | 44.811 | 11.63       | 58            | 176          | 42.9756 |
| 7                               | 40  | 75.98  | 45.681 | 11.95       | 70            | 176          | 44.8329 |
| 8                               | 43  | 81.19  | 49.091 | 10.85       | 64            | 162          | 48.6020 |
| 9                               | 44  | 81.42  | 39.442 | 13.08       | 63            | 174          | 41.4613 |
| 10                              | 38  | 81.87  | 60.055 | 8.63        | 48            | 170          | 56.6171 |
| 11                              | 44  | 73.03  | 50.541 | 10.13       | 45            | 168          | 52.1299 |
| 12                              | 45  | 87.66  | 37.388 | 14.03       | 56            | 186          | 37.0080 |

**Output 82.2.4** Residual Scores from the OUT= Data Set Created by PROC SCORE

| Regression Scoring Example              |     |        |        |          |            |           |          |
|-----------------------------------------|-----|--------|--------|----------|------------|-----------|----------|
| Negative Residual Scores for Regression |     |        |        |          |            |           |          |
| Obs                                     | Age | Weight | Oxygen | Run Time | Rest Pulse | Run Pulse | OxyHat   |
| 1                                       | 44  | 89.47  | 44.609 | 11.37    | 62         | 178       | -1.73195 |
| 2                                       | 40  | 75.07  | 45.313 | 10.07    | 62         | 185       | 2.29197  |
| 3                                       | 44  | 85.84  | 54.297 | 8.65     | 45         | 156       | 1.82407  |
| 4                                       | 42  | 68.15  | 59.571 | 8.17     | 40         | 166       | -0.86657 |
| 5                                       | 38  | 89.02  | 49.874 | 9.22     | 55         | 178       | 1.86460  |
| 6                                       | 47  | 77.45  | 44.811 | 11.63    | 58         | 176       | -1.83542 |
| 7                                       | 40  | 75.98  | 45.681 | 11.95    | 70         | 176       | -0.84811 |
| 8                                       | 43  | 81.19  | 49.091 | 10.85    | 64         | 162       | -0.48897 |
| 9                                       | 44  | 81.42  | 39.442 | 13.08    | 63         | 174       | 2.01935  |
| 10                                      | 38  | 81.87  | 60.055 | 8.63     | 48         | 170       | -3.43787 |
| 11                                      | 44  | 73.03  | 50.541 | 10.13    | 45         | 168       | 1.58892  |
| 12                                      | 45  | 87.66  | 37.388 | 14.03    | 56         | 186       | -0.38002 |

The second part of this example uses the parameter estimates to score a new data set. The following statements produce [Output 82.2.5](#) and [Output 82.2.6](#):

```

/* The FITNESS2 data set contains observations 13-16 from */
/* the FITNESS data set used in EXAMPLE 2 in the PROC REG */
/* chapter. */
data Fitness2;
 input Age Weight Oxygen RunTime RestPulse RunPulse;
 datalines;
45 66.45 44.754 11.12 51 176
47 79.15 47.273 10.60 47 162
54 83.12 51.855 10.33 50 166
49 81.42 49.156 8.95 44 180
;
proc print data=Fitness2;
 title 'Regression Scoring Example';
 title2 'New Raw Data Set to be Scored';
run;

proc score data=Fitness2 score=RegOut out=NewPred type=parms
 nostd predict;
 var Oxygen Age Weight RunTime RunPulse RestPulse;
run;

proc print data=NewPred;
 title2 'Predicted Scores for Regression';
 title3 'for Additional Data from FITNESS2';
run;

```

Output 82.2.5 lists the Fitness2 data set.

**Output 82.2.5** Listing of the Fitness2 Data Set

| Regression Scoring Example<br>New Raw Data Set to be Scored |     |        |        |             |               |              |
|-------------------------------------------------------------|-----|--------|--------|-------------|---------------|--------------|
| Obs                                                         | Age | Weight | Oxygen | Run<br>Time | Rest<br>Pulse | Run<br>Pulse |
| 1                                                           | 45  | 66.45  | 44.754 | 11.12       | 51            | 176          |
| 2                                                           | 47  | 79.15  | 47.273 | 10.60       | 47            | 162          |
| 3                                                           | 54  | 83.12  | 51.855 | 10.33       | 50            | 166          |
| 4                                                           | 49  | 81.42  | 49.156 | 8.95        | 44            | 180          |

PROC SCORE scores the Fitness2 data set by using the parameter estimates in the RegOut data set. These parameter estimates result from fitting a regression equation to the Fitness data set. The NOSTD option is specified, so the raw data are not standardized before scoring. (However, the NOSTD option is not necessary here. The SCORE= data set does not contain observations with `_TYPE_='MEAN'` or `_TYPE_='STD'`, so standardization is not performed.) The VAR statement contains the dependent variables and the independent variables used in PROC REG. In addition, the PREDICT option is specified. This combination gives predicted values for the new score variable. The name of the new score variable is OxyHat, from the value of the `_MODEL_` variable in the SCORE= data set. [Output 82.2.6](#) shows the data set produced by PROC SCORE.

**Output 82.2.6** Predicted Scores from the OUT= Data Set Created by PROC SCORE and Reproduced Using PROC PRINT

| Regression Scoring Example<br>Predicted Scores for Regression<br>for Additional Data from FITNESS2 |     |        |        |             |               |              |         |
|----------------------------------------------------------------------------------------------------|-----|--------|--------|-------------|---------------|--------------|---------|
| Obs                                                                                                | Age | Weight | Oxygen | Run<br>Time | Rest<br>Pulse | Run<br>Pulse | OxyHat  |
| 1                                                                                                  | 45  | 66.45  | 44.754 | 11.12       | 51            | 176          | 47.5507 |
| 2                                                                                                  | 47  | 79.15  | 47.273 | 10.60       | 47            | 162          | 49.7802 |
| 3                                                                                                  | 54  | 83.12  | 51.855 | 10.33       | 50            | 166          | 43.9682 |
| 4                                                                                                  | 49  | 81.42  | 49.156 | 8.95        | 44            | 180          | 47.5949 |



### Example 82.3: Custom Scoring Coefficients

This example uses a specially created custom scoring data set and produces [Output 82.3.1](#) and [Output 82.3.2](#). The first scoring coefficient creates a variable that is Age–Weight; the second scoring coefficient evaluates the variable RunPulse–RstPulse; and the third scoring coefficient totals all six variables. Since the scoring coefficients data set (data set A) does not contain any observations with `_TYPE_='MEAN'` or `_TYPE_='STD'`, the data in the Fitness data set (see [Example 82.1](#)) are not standardized before scoring.

The following statements produce [Output 82.3.1](#) and [Output 82.3.2](#):

```
data A;
 input _type_ $ _name_ $
 Age Weight RunTime RunPulse RestPulse;
 datalines;
SCORE AGE_WGT 1 -1 0 0 0
SCORE RUN_RST 0 0 0 1 -1
SCORE TOTAL 1 1 1 1 1
;
proc print data=A;
 title 'Constructed Scoring Example';
 title2 'Scoring Coefficients';
run;

proc score data=Fitness score=A out=B;
 var Age Weight RunTime RunPulse RestPulse;
run;

proc print data=B;
 title2 'Scored Data';
run;
```

**Output 82.3.1** Custom Scoring Data Set and Scored Fitness Data: PROC PRINT

| Constructed Scoring Example<br>Scoring Coefficients |        |         |     |        |             |              |               |
|-----------------------------------------------------|--------|---------|-----|--------|-------------|--------------|---------------|
| Obs                                                 | _type_ | _name_  | Age | Weight | Run<br>Time | Run<br>Pulse | Rest<br>Pulse |
| 1                                                   | SCORE  | AGE_WGT | 1   | -1     | 0           | 0            | 0             |
| 2                                                   | SCORE  | RUN_RST | 0   | 0      | 0           | 1            | -1            |
| 3                                                   | SCORE  | TOTAL   | 1   | 1      | 1           | 1            | 1             |

**Output 82.3.2** Custom Scored Fitness Data: PROC PRINT

| Constructed Scoring Example<br>Scored Data |     |        |        |             |               |              |         |         |        |
|--------------------------------------------|-----|--------|--------|-------------|---------------|--------------|---------|---------|--------|
| Obs                                        | Age | Weight | Oxygen | Run<br>Time | Rest<br>Pulse | Run<br>Pulse | AGE_WGT | RUN_RST | TOTAL  |
| 1                                          | 44  | 89.47  | 44.609 | 11.37       | 62            | 178          | -45.47  | 116     | 384.84 |
| 2                                          | 40  | 75.07  | 45.313 | 10.07       | 62            | 185          | -35.07  | 123     | 372.14 |
| 3                                          | 44  | 85.84  | 54.297 | 8.65        | 45            | 156          | -41.84  | 111     | 339.49 |
| 4                                          | 42  | 68.15  | 59.571 | 8.17        | 40            | 166          | -26.15  | 126     | 324.32 |
| 5                                          | 38  | 89.02  | 49.874 | 9.22        | 55            | 178          | -51.02  | 123     | 369.24 |
| 6                                          | 47  | 77.45  | 44.811 | 11.63       | 58            | 176          | -30.45  | 118     | 370.08 |
| 7                                          | 40  | 75.98  | 45.681 | 11.95       | 70            | 176          | -35.98  | 106     | 373.93 |
| 8                                          | 43  | 81.19  | 49.091 | 10.85       | 64            | 162          | -38.19  | 98      | 361.04 |
| 9                                          | 44  | 81.42  | 39.442 | 13.08       | 63            | 174          | -37.42  | 111     | 375.50 |
| 10                                         | 38  | 81.87  | 60.055 | 8.63        | 48            | 170          | -43.87  | 122     | 346.50 |
| 11                                         | 44  | 73.03  | 50.541 | 10.13       | 45            | 168          | -29.03  | 123     | 340.16 |
| 12                                         | 45  | 87.66  | 37.388 | 14.03       | 56            | 186          | -42.66  | 130     | 388.69 |

---

## References

Chaseling, J. (1996), "Standard Test Results of Students at Three Types of Schools," Sample data, Faculty of Environmental Sciences, Griffith University, Queensland, Australia.



# Chapter 83

## The SEQDESIGN Procedure

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## Overview: SEQDESIGN Procedure

The purpose of the SEQDESIGN procedure is to design interim analyses for clinical trials. Clinical trials are experiments on human subjects to demonstrate the efficacy and safety of new drugs or treatments. A simple example is a trial to test the effectiveness of a new drug in humans by comparing the outcomes in a group of patients who receive the new drug with the outcomes in a comparable group of patients who receive a placebo.

A clinical trial is conducted according to a plan called a *protocol*. A protocol details the objectives of the trial, the data collection process, and the analysis. The protocol specifies the null hypothesis and an alternative hypothesis, a test statistic, the probability  $\alpha$  of a Type I error, the probability  $\beta$  of a Type II error, the sample size needed to attain a specified power of  $1 - \beta$  at an alternative reference, and critical values that are associated with the test statistic.

In a fixed-sample trial, data about all individuals are first collected and then examined at the end of the study. Most major trials have committees that periodically monitor safety and efficacy data during the trial and recommend that a trial be stopped for safety concerns such as an unacceptable toxicity level. In certain situations, the committee might recommend that a trial be stopped for efficacy. In contrast to a fixed-sample trial, a group sequential trial provides for interim analyses before the completion of the trial while maintaining the specified overall Type I and Type II error probabilities.

A group sequential trial is most useful in situations where it is important to monitor the trial to prevent unnecessary exposure of patients to an unsafe new drug, or alternatively to a placebo treatment if the new drug shows significant improvement. In most cases, if a group sequential trial stops early for safety concerns,

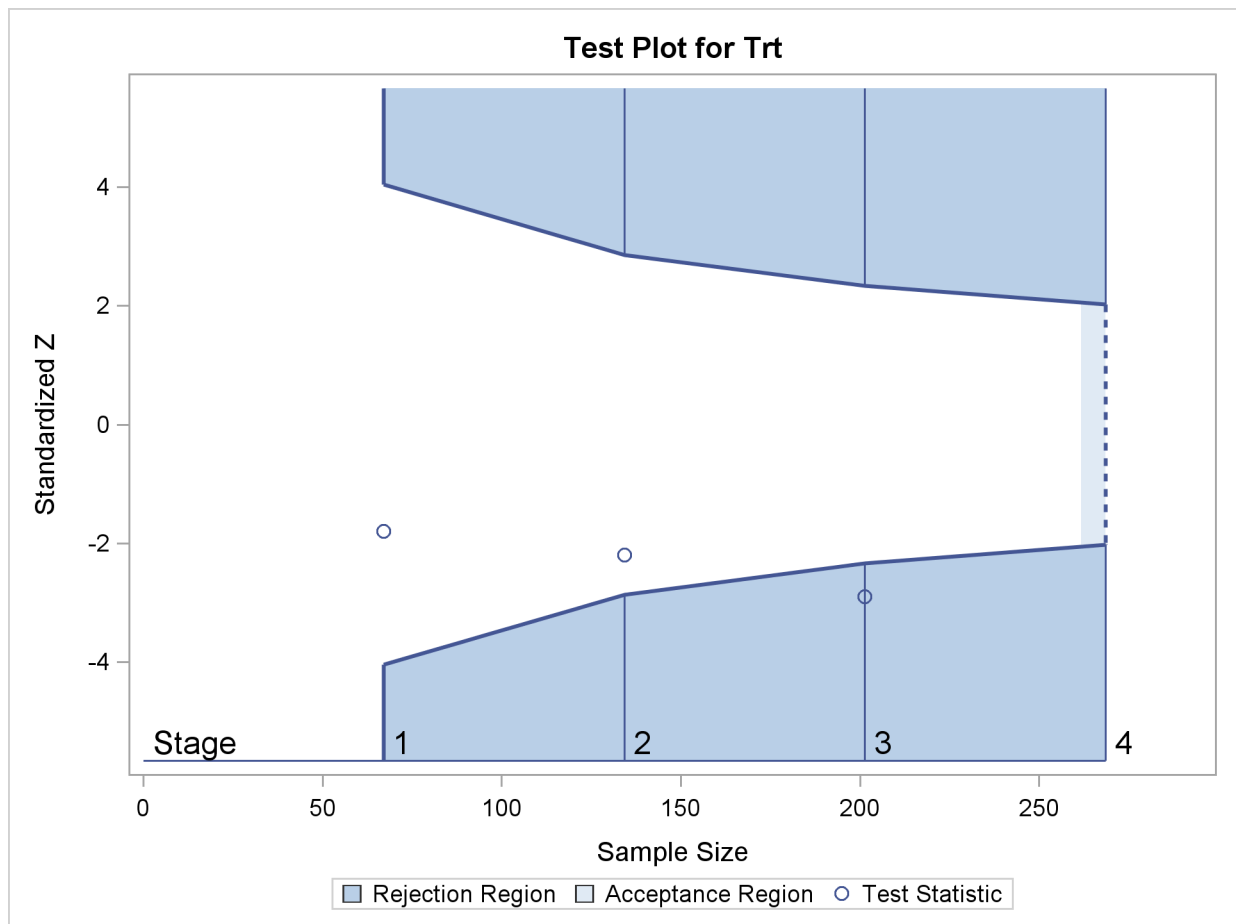
fewer patients are exposed to the new treatment than in the fixed-sample trial. If a trial stops early for efficacy reasons, the new treatment is available sooner than it would be in a fixed-sample trial. Early stopping can also save time and resources.

A group sequential design provides detailed specifications for a group sequential trial. In addition to the usual specification for a fixed-sample design, it provides the total number of stages (the number of interim stages plus a final stage) and a stopping criterion to reject, to accept, or to either reject or accept the null hypothesis at each interim stage. It also provides critical values and the sample size at each stage for the trial.

At each interim stage, the data collected at the current stage in addition to the data collected at previous stages are analyzed, and statistics such as a maximum likelihood test statistic and its associated standard error are computed. The test statistic is then compared with critical values that are generated from the sequential design, and the trial is stopped or continued. If a trial continues to the final stage, the null hypothesis is either rejected or accepted. The critical values for each stage are chosen in such a way that the overall  $\alpha$  and  $\beta$  are maintained at the specified levels.

Figure 83.1 shows a two-sided symmetric group sequential trial that stops early to reject the null hypothesis that the parameter  $\text{Trt}$  is zero.

**Figure 83.1** Sequential Plot for Two-Sided Test



The trial has four stages, which are indicated by the vertical lines labeled 1, 2, 3, and 4. With early stopping to reject the null hypothesis, the lower rejection boundary is constructed by connecting the lower critical values for the stages. Similarly, the upper rejection boundary is constructed by connecting the upper critical values for the stages. The horizontal axis indicates the sample size for the group sequential trial, and the vertical axis indicates the values of the test statistic on the standardized  $Z$  scale.

At each interim stage, if the test statistic falls into a rejection region (the darker shaded areas in [Figure 83.1](#)), the trial stops and the null hypothesis is rejected. Otherwise, the trial continues to the next stage. At the final stage (stage 4), the null hypothesis is rejected if  $Z$  falls into a rejection region. Otherwise, the null hypothesis is not rejected. In [Figure 83.1](#), the test statistic does not fall into the rejection regions for stages 1 and 2, and so the trial continues to stage 3. At stage 3, the test statistic falls into the rejection region, and the null hypothesis is rejected.

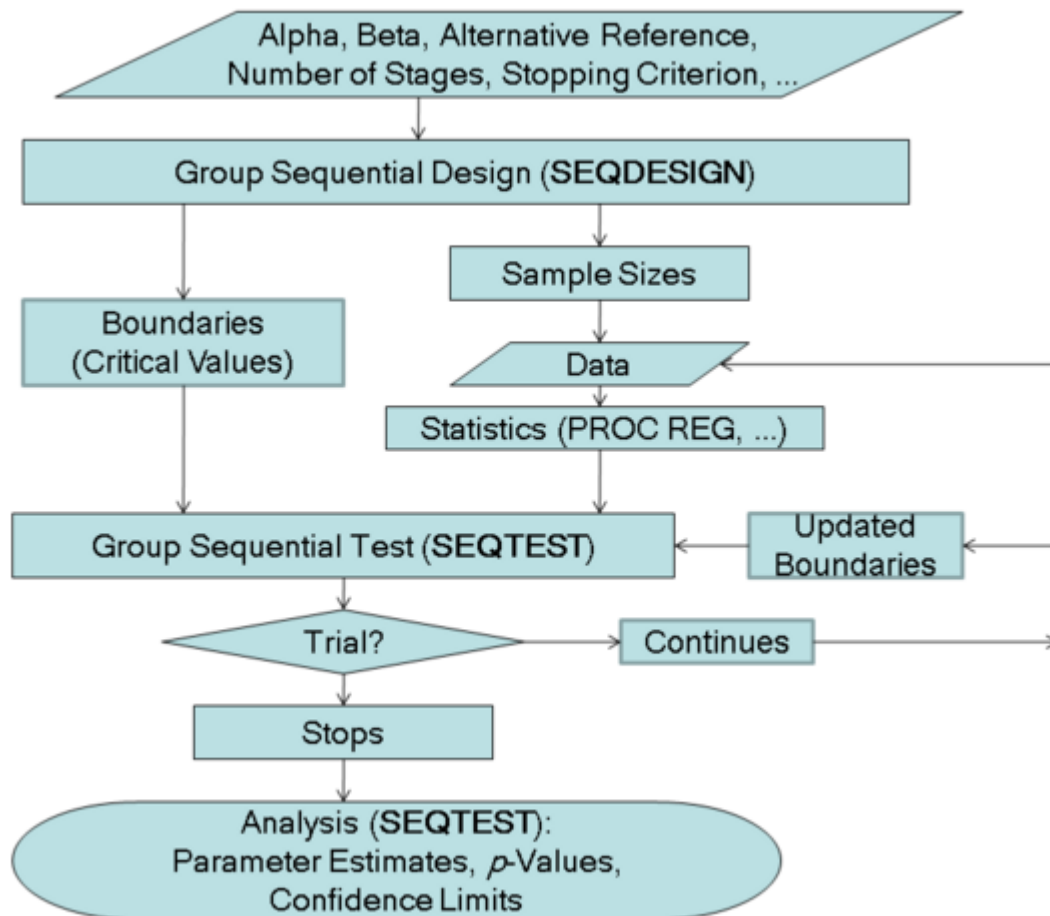
A group sequential trial usually involves six steps:

1. You specify the statistical details of the design, including the null and alternative hypotheses, a test statistic for the hypothesis test, the Type I and II error probabilities, a stopping criterion, the total number of stages, and the relative information level at each stage.
2. You compute the boundary values for the trial based on the specifications in Step 1. You also compute the sample size required at each stage for the specified hypothesis test.
3. At each stage, you collect additional data with the required sample sizes. The data available at each stage include the data collected at previous stages in addition to the data collected at the current stage.
4. At each stage, you analyze the available data with a procedure such as the REG procedure, and you compute the test statistic.
5. At each stage, you compare the test statistic with the corresponding boundary values. You stop the trial to reject or accept the hypothesis, or you continue the trial to the next stage. If you continue the trial to the final stage, you either accept or reject the hypothesis.
6. After the trial stops, you compute parameter estimates, confidence limits for the parameter, and a  $p$ -value for the hypothesis test.

You use the SEQDESIGN procedure at Step 2 to compute the initial boundary values and required sample sizes for the trial. You use the companion SEQTEST procedure at Step 5 to compare the test statistic with its boundary values. At stage 1, the boundary values are derived by using the boundary information tables created by the SEQDESIGN procedure. These boundary information tables are structured for input to the SEQTEST procedure. At each subsequent stage, the boundary values are derived by using the test information tables created by the SEQTEST procedure at the previous stage. These test information tables are also structured for input to the SEQTEST procedure. You also use the SEQTEST procedure at Step 6 to compute parameter estimates, confidence limits, and  $p$ -values after the trial stops.

The flowchart in [Figure 83.2](#) summarizes the steps in a typical group sequential trial and the relevant SAS procedures.

Figure 83.2 Group Sequential Trial



## Features of the SEQDESIGN Procedure

The SEQDESIGN procedure assumes that the standardized  $Z$  test statistics for the null hypothesis  $H_0 : \theta = 0$  at the stages have the joint canonical distribution with the information levels at the stages for the parameter  $\theta$ . This implies that these test statistics are normally distributed. If the test statistic is not normally distributed, then it is assumed that the test statistic is computed from a large sample such that the statistic has an approximately normal distribution. See the section “Statistical Assumptions for Group Sequential Designs” on page 7015 for a detailed description of the joint canonical distribution.

You can use the SEQDESIGN procedure to compute required sample sizes for commonly used hypothesis tests. Note that for a fixed-sample design, you should use the POWER and GLMPOWER procedures to compute sample sizes.

The applicable tests include tests for binomial proportions and the log-rank test for two survival distributions. See the section “Applicable One-Sample Tests and Sample Size Computation” on page 7050, the section “Applicable Two-Sample Tests and Sample Size Computation” on page 7052, and the section “Applicable Regression Parameter Tests and Sample Size Computation” on page 7061 for examples of applicable tests in group sequential trials.



At each stage, the data are analyzed with a statistical procedure such as the REG procedure, and a test statistic and its associated information level are computed. The information level is the amount of information available about the unknown parameter. For a maximum likelihood statistic, the information level is the inverse of its variance.

At each stage, you use the SEQTEST procedure to derive the boundary values that correspond to the information level associated with the test statistic. You then use the SEQTEST procedure to compare the test statistic with these boundary values. When a trial is stopped at an interim stage or at the final stage, the SEQTEST procedure also derives parameter estimates, confidence limits for the parameter, and a  $p$ -value for hypothesis testing.

---

## Output from the SEQDESIGN Procedure

In addition to computing the boundary values for a group sequential design, the SEQDESIGN procedure computes the following quantities:

- maximum sample size (as a percentage of the corresponding fixed-sample size) if the trial does not stop at an interim stage
- average sample numbers (as percentages of the corresponding fixed-sample sizes for nonsurvival data or fixed-sample numbers of events for survival data) under various hypothetical references, including the null and alternative references
- stopping probabilities at each stage under various hypothetical references to indicate how likely it is that the trial will stop at that stage
- sample sizes required at each stage for the specified hypothesis test
- numbers of events required at each stage for the specified hypothesis test with survival data

You can create more than one design with multiple DESIGN statements in the SEQDESIGN procedure and then choose the design with the most desirable features. The next two subsections introduce some basic aspects of group sequential designs that are useful for getting started with the SEQDESIGN procedure.

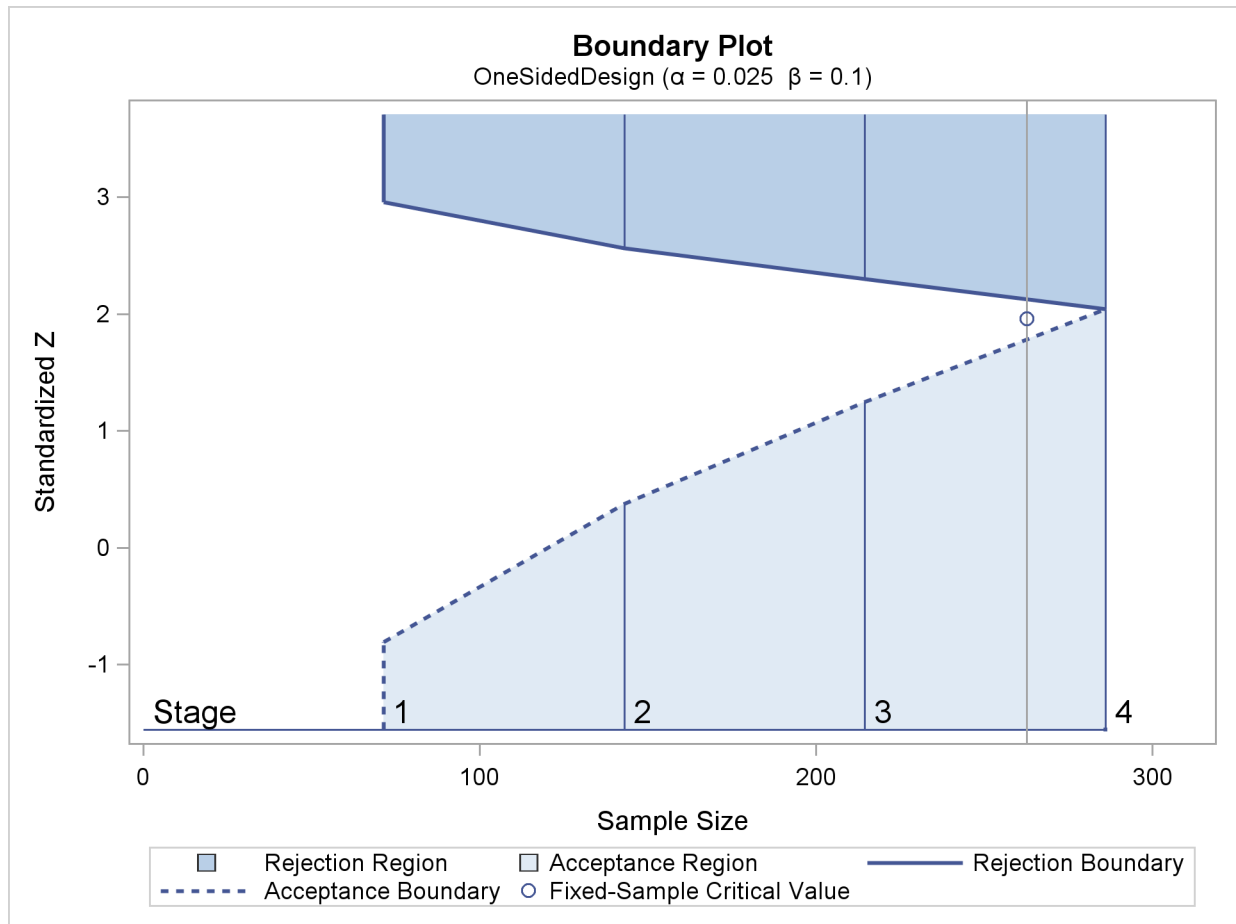
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## Boundaries for Group Sequential Designs

A one-sided test is a test of a hypothesis with either a lower alternative ( $H_1 : \theta < 0$ ) or an upper alternative ( $H_1 : \theta > 0$ ), and a two-sided test is a test with a two-sided alternative ( $H_1 : \theta \neq 0$ ). The number of critical values for a test depends on whether the alternative is one-sided or two-sided, and it also depends on whether the trial is conducted with a fixed-sample design or a group sequential design.

For a fixed-sample trial, a one-sided test has one critical value and a two-sided test has two critical values. These critical values are computed with the specified Type I error probability  $\alpha$ . In contrast, at each interim stage of a group sequential trial, a one-sided test has up to two critical values and a two-sided group sequential test has up to four critical values. Thus, there are two or four possible boundaries for a group sequential design, and each boundary is a set of critical values, one from each stage.

Figure 83.3 illustrates the boundaries for a one-sided test with an upper alternative that allows for early stopping to either reject or accept the null hypothesis.

**Figure 83.3** Boundary Plot for One-Sided Design

With an upper alternative, as in this example, the design has the following two boundaries: an upper  $\alpha$  (rejection) boundary for the rejection region that consists of upper rejection critical values and an upper  $\beta$  (acceptance) boundary for the acceptance region that consists of upper acceptance critical values. The stages are indicated by vertical lines with accompanying stage numbers. In Figure 83.3, the horizontal axis indicates the cumulative sample size for the group sequential trial. The vertical axis indicates the critical values at each stage on the standardized Z scale. Other scales can be used for the vertical axis, including the MLE scale, score statistic scale, and  $p$ -value scale.

At each interim stage, if the test statistic is in the rejection region (darker shaded area in Figure 83.3), the trial stops and the null hypothesis is rejected. If the test statistic is in the acceptance region (lightly shaded area in Figure 83.3), the trial stops and the hypothesis is accepted. Otherwise, the trial continues to the next stage. If the trial proceeds to the final stage (stage 4), the upper  $\alpha$  and upper  $\beta$  critical values are identical, and the trial stops to either reject or accept the null hypothesis.

If you do not want to stop a trial when a test statistic falls in the acceptance region at an interim stage, you can derive a design with a nonbinding acceptance boundary to allow the trial to continue while maintaining the Type I error level. You need to increase the sample size for a design with this nonbinding feature. See the section “Acceptance ( $\beta$ ) Boundary” on page 7035 for a description of the nonbinding acceptance boundary.

---

## Group Sequential Methods

For a group sequential design, there are two possible boundaries for a one-sided test and four possible boundaries for a two-sided test. Each boundary consists of one boundary value (critical value) for each stage. The SEQDESIGN procedure provides various methods for computing the boundary values.

The boundary value for a fixed-sample test cannot be applied to each stage of sequential design because, as shown by Armitage, McPherson, and Rowe (1969), repeated significance tests at a fixed level on accumulating data increase the probability of a Type I error. For example, with a fixed-sample two-sided test, the critical values  $\pm 1.96$  for a standardized  $Z$  statistic produce a Type I error probability level  $\alpha = 0.05$ . But for a two-sided group sequential test with two equally spaced stages, if the same critical values  $\pm 1.96$  are used to reject the null hypothesis at these two stages, the Type I error probability level is  $\alpha = 0.083$ , larger than the fixed-sample  $\alpha$ .

Numerous methods are available for deriving the critical values for each boundary in a sequential design. Pocock (1977) applies repeated significance tests to group sequential trials with equal-size groups and derives a constant critical value on the standardized normal  $Z$  scale across all stages that maintains the specified Type I error probability level. O'Brien and Fleming (1979) propose a sequential procedure that has boundary values (in absolute value) decrease over the stages on the standardized normal  $Z$  scale.

The SEQDESIGN procedure provides the following three types of methods:

- fixed boundary shape methods, which derive boundaries with specified boundary shapes
- Whitehead methods, which adjust boundaries derived for continuous monitoring so that they apply to discrete monitoring
- error spending methods

Each type of methods uses a distinct approach to derive the boundary values for a group sequential trial. Whitehead methods require much less computation with resulting Type I error probability and power that are close but differ slightly from the specified values due to the approximations used in deriving the tests (Jennison and Turnbull 2000, p. 106). Fixed boundary shape methods derive boundary values by estimating a fixed number of parameters and require more computation. Error spending methods derive boundary values at each stage sequentially and require much more computation than other types of methods for group sequential trials with a large number of stages.

Within each type of methods, you can choose methods that creating boundary values range from conservative stopping boundary values at early stages to liberal stopping boundary values at very early stages.

You can use the SEQDESIGN procedure to specify methods from the same type for each design. A different method can be specified for each boundary separately, but all methods in a design must be of the same type.

### Fixed Boundary Shape Methods

The fixed boundary shape methods include the unified family methods and the Haybittle-Peto method. The unified family methods (Kittelson and Emerson 1999) derive boundaries from specified boundary shapes. These methods include Pocock's method (Pocock 1977) and the O'Brien-Fleming method (O'Brien and Fleming 1979) as special cases.

The Haybittle-Peto method (Haybittle 1971; Peto et al. 1976) uses a value of 3 for the critical values in interim stages, so the critical value at the final stage is close to the critical value for the fixed-sample design. In the SEQDESIGN procedure, the Haybittle-Peto method has been generalized to allow for different boundary values at interim stages.

## Whitehead Methods

Whitehead and Stratton (1983) and Whitehead (1997, 2001) develop triangular and straight-line boundaries by adapting tests constructed for continuous monitoring to discrete monitoring of group sequential tests. With continuous monitoring, the values for each boundary fall in a straight line when plotted on the score statistic scale. The discrete boundary is derived by subtracting the expected overshoot from the continuous boundary to obtain the desired Type I and Type II error probabilities. For a design with early stopping to either reject or accept the null hypothesis, the boundaries form a triangle when plotted on the score statistic scale. See the section “Score Statistic” on page 7005 for a detailed description of the score statistic.

## Error Spending Methods

For every sequential design, the  $\alpha$  and  $\beta$  errors at each stage can be computed from the boundary values. On the other hand, you can derive the boundary values from specified  $\alpha$  and  $\beta$  errors for each stage. The error spending function approach (Lan and DeMets 1983) uses an error spending function to specify the errors at each stage for each boundary and then derives the boundary values.

---

## Getting Started: SEQDESIGN Procedure

This section illustrates a clinical study design that uses a two-sided O’Brien-Fleming design (O’Brien and Fleming 1979) to stop the trial early for ethical concerns about possible harm or for unexpectedly strong efficacy of the new drug.

Suppose that a pharmaceutical company is conducting a clinical trial to test the efficacy of a new cholesterol-lowering drug. The primary focus is low-density lipoprotein (LDL), the so-called bad cholesterol, which is a risk factor for coronary heart disease. LDL is measured in *mg / dL*, milligrams per deciliter of blood.

The trial consists of two groups of equally allocated patients with elevated LDL levels: an experimental group given the new drug and a placebo control group. Suppose the changes in LDL level after the treatment for individuals in the experimental and control groups are normally distributed with means  $\mu_e$  and  $\mu_c$ , respectively, and have a common variance  $\sigma^2$ . Then the null hypothesis of no effect for the new drug is  $H_0 : \theta = 0$ , where  $\theta = \mu_e - \mu_c$ .

For a fixed-sample design with a total sample size  $N$ , the MLE for  $\theta$  is computed as  $\hat{\theta} = \hat{\mu}_e - \hat{\mu}_c$ , where  $\hat{\mu}_e$  and  $\hat{\mu}_c$  are the sample means of the decreases in LDL level in the experimental and control groups, respectively.

Following the derivation in the section “Test for the Difference between Two Normal Means” on page 7053, the statistic  $\hat{\theta}$  has a normal distribution

$$\hat{\theta} \sim N\left(\theta, \frac{4\sigma^2}{N}\right)$$

Thus, under the null hypothesis  $H_0 : \theta = 0$ , the standardized statistic

$$Z = \frac{\hat{\theta}}{\sqrt{\frac{4\sigma^2}{N}}} \sim N(0, 1)$$

The  $Z$  statistic can be used to test the null hypothesis  $H_0$ . If the variance  $\sigma^2$  is unknown, the sample variance can be used to compute the test statistic if it is assumed that the sample variance is computed from a large sample such that the  $Z$  statistic has an approximately standard normal distribution.

With a Type I error probability  $\alpha = 0.05$ , the critical values for the  $Z$  statistic are given by  $\Phi^{-1}(\alpha/2) = -1.96$  and  $\Phi^{-1}(1 - \alpha/2) = 1.96$ , where  $\Phi$  is the cumulative standard normal distribution function. At the end of study, if  $Z \geq 1.96$ , the null hypothesis is rejected for harmful drug effect, and if  $Z \leq -1.96$ , the null hypothesis is rejected for efficacy of the new drug. Otherwise, the null hypothesis is not rejected and the drug effect is not significant.

Also suppose that for the trial, the alternative reference  $\theta = -10$  is the clinically meaningful difference that the trial should detect with a high probability (power). Further suppose that a good estimate of the standard deviation for the changes in LDL level is  $\hat{\sigma} = 20$ . The following statements invoke the SEQDESIGN procedure and request a four-stage O'Brien-Fleming design for standardized normal test statistics:

```
ods graphics on;
proc seqdesign altref=-10
 plots=boundary(hscale=samplesize)
 ;
 TwoSidedOBrienFleming: design nstages=4
 method=obf
 ;
 samplesize model=twosamplemean(stddev=20);
ods output Boundary=Bnd_LDL;
run;
ods graphics off;
```

The ALTREF= option specifies the alternative reference, and the actual maximum information is derived in the SEQDESIGN procedure. With ODS Graphics enabled, the PLOTS=BOUNDARY option displays a boundary plot with the rejection and acceptance regions.

In the DESIGN statement, the label **TwoSidedOBrienFleming** identifies the design in the output tables. By default (or equivalently if you specify ALT=TWOSIDED and STOP=REJECT in the DESIGN statement), the design has a two-sided alternative hypothesis in which early stopping in the interim stages occurs to reject the null hypothesis. That is, at each interim stage, the trial either is stopped to reject the null hypothesis or continues to the next stage.

The NSTAGES=4 option in the DESIGN statement specifies the total number of stages in the group sequential trial, including three interim stages and a final stage. In the SEQDESIGN procedure, the null hypothesis for the design is  $H_0 : \theta = 0$ . By default (or equivalently if you specify ALPHA=0.05 and BETA=0.10 in the DESIGN statement), the design has a Type I error probability  $\alpha = 0.05$ , and a Type II error probability  $\beta = 0.10$ ; the latter corresponds to a power of  $1 - \beta = 0.90$  at the alternative reference  $H_1 : \theta = -10$ .

For a two-sided design with early stopping to reject the null hypothesis, there are two boundaries for the design: an upper  $\alpha$  boundary that consists of upper rejection critical values and a lower  $\alpha$  boundary that consists of lower rejection critical values. Each boundary is a set of critical values, one from each stage.

With the METHOD=OBF option in the DESIGN statement, the O'Brien-Fleming method is used for the two boundaries for the design; see [Figure 83.7](#).

A property of the boundaries constructed with the O'Brien-Fleming design is that the null hypothesis is more difficult to reject in the early stages than in the later stages. That is, the trial is rejected in the early stages only with overwhelming evidence, because in these stages there might not be a sufficient number of responses for a reliable estimate of the treatment effect.

The SAMPLESIZE statement with the MODEL=TWOSAMPLEMEAN option uses the derived maximum information to compute required sample sizes for a two-sample test for mean difference. The ODS OUTPUT statement with the BOUNDARY=BND\_LDL option creates an output data set named BND\_LDL which contains the resulting boundary information.

In a clinical trial, the amount of information about an unknown parameter available from the data can be measured by the Fisher information. For a maximum likelihood statistic, the information level is the inverse of its variance. See the section “[Maximum Likelihood Estimator](#)” on page 7004 for a detailed description of Fisher information. At each stage of the trial, data are collected and analyzed with a statistical procedure, and a test statistic and its corresponding information level are computed.

In this example, you can use the REG procedure to compute the maximum likelihood estimate  $\hat{\theta}$  for the drug effect and the corresponding standard error for  $\hat{\theta}$ . At stage 1, you can use the SEQTEST procedure to compare the test statistic with adjusted boundaries derived from the boundary information stored in the BOUND\_LDL data set. At each subsequent stage, you can use the SEQTEST procedure to compare the test statistic with adjusted boundaries derived from the boundary information stored in the test information table created by the SEQTEST procedure at the previous stage. The test information tables are structured for input to the SEQTEST procedure.

At each interim stage, the trial will either be stopped to reject the null hypothesis or continue to the next stage. At the final stage, the null hypothesis is either rejected or accepted.

By default (or equivalently if you specify INFO=EQUAL in the DESIGN statement), the SEQDESIGN procedure derives boundary values with equally spaced information levels for all stages—that is, the same information increment between successive stages. The “Design Information,” “Method Information,” and “Boundary Information” tables are displayed by default, as shown in [Figure 83.4](#), [Figure 83.5](#), and [Figure 83.6](#), respectively.

The “Design Information” table in [Figure 83.4](#) displays design specifications and four derived statistics: the actual maximum information, the maximum information, the average sample number under the null hypothesis (Null Ref ASN), and the average sample number under the alternative hypothesis (Alt Ref ASN). Except for the actual maximum information, each statistic is expressed as a percentage of the identical statistic for the corresponding fixed-sample information. The average sample number is the expected sample size (for nonsurvival data) or expected number of events (for survival data). Note that for a symmetric two-sided design, the ALTREF=-10 option implies a lower alternative reference of -10 and an upper alternative reference of 10.

**Figure 83.4** O'Brien-Fleming Design Information

| The SEQDESIGN Procedure                   |                 |
|-------------------------------------------|-----------------|
| Design: TwoSidedOBrienFleming             |                 |
| Design Information                        |                 |
| Statistic Distribution                    | Normal          |
| Boundary Scale                            | Standardized Z  |
| Alternative Hypothesis                    | Two-Sided       |
| Early Stop                                | Reject Null     |
| Method                                    | O'Brien-Fleming |
| Boundary Key                              | Both            |
| Alternative Reference                     | -10             |
| Number of Stages                          | 4               |
| Alpha                                     | 0.05            |
| Beta                                      | 0.1             |
| Power                                     | 0.9             |
| Max Information (Percent of Fixed Sample) | 102.2163        |
| Max Information                           | 0.107403        |
| Null Ref ASN (Percent of Fixed Sample)    | 101.5728        |
| Alt Ref ASN (Percent of Fixed Sample)     | 76.7397         |

The maximum information is the information level at the final stage of the group sequential trial. The Max Information (Percent Fixed-Sample) is the maximum information for the sequential design expressed as a percentage of the information for the corresponding fixed-sample design. In Figure 83.4, the Max Information (Percent Fixed-Sample) is 102.22%, which means that the information needed for the group sequential trial is 2.22% more than that of the corresponding fixed-sample design if the trial does not stop at any interim stage.

The Null Ref ASN (Percent Fixed-Sample) is the average sample number (expected sample size) required under the null hypothesis for the group sequential design expressed as a percentage of the sample size for the corresponding fixed-sample design. In Figure 83.4, the Null Ref ASN is 101.57%, which means that the expected sample size for the group sequential trial is 1.57% greater than the corresponding fixed-sample size.

Similarly, the Alt Ref ASN (Percent Fixed-Sample) is the average sample number (expected sample size) required under the alternative hypothesis for the group sequential design expressed as a percentage of the sample size for the corresponding fixed-sample design. In Figure 83.4, the Alt Ref ASN is 76.74%, which means that the expected sample size for the group sequential trial is 76.74% of the corresponding fixed-sample size. That is, if the alternative hypothesis is true, then on average, only 76.74% of the fixed-sample size is needed for the group sequential trial.

In this example, the O'Brien-Fleming design requires only a slight increase in sample size if the trial proceeds to the final stage. On the other hand, if the alternative hypothesis is correct, this design provides a substantial saving in sample size on average.

The “Method Information” table in [Figure 83.5](#) displays the computed Type I and Type II error probabilities  $\alpha$  and  $\beta$ , and the derived drift parameter for the design. For a two-sided test with early stopping to reject the null hypothesis, both lower and upper  $\alpha$  boundaries are created. With the specified ALTREF= option, the alternative references are also included.

With the zero null reference, the drift parameter is the standardized alternative reference at the final stage  $\theta_1 \sqrt{I_X}$ , where  $\theta_1$  is the alternative reference and  $I_X$  is the maximum information. See the section “[Specified and Derived Parameters](#)” on page 7039 for a detailed description of the drift parameter. The drift parameters for the design are derived in the SEQDESIGN procedure even if the alternative reference is not specified or derived in the procedure.

**Figure 83.5** Method Information

| Method Information |                 |         |         |                          |     |         |
|--------------------|-----------------|---------|---------|--------------------------|-----|---------|
| Boundary           | Method          | Alpha   | Beta    | -----Unified Family----- |     |         |
|                    |                 |         |         | Rho                      | Tau | C       |
| Upper Alpha        | O'Brien-Fleming | 0.02500 | 0.10000 | 0.5                      | 0   | 2.02429 |
| Lower Alpha        | O'Brien-Fleming | 0.02500 | 0.10000 | 0.5                      | 0   | 2.02429 |

| Method Information |                       |          |
|--------------------|-----------------------|----------|
| Boundary           | Alternative Reference | Drift    |
| Upper Alpha        | 10                    | 3.277238 |
| Lower Alpha        | -10                   | -3.27724 |

The O'Brien-Fleming method belongs to the unified family of designs, which is parameterized by two parameters,  $\rho$  and  $\tau$ , as implemented in the SEQDESIGN procedure. See [Table 83.3](#) for parameter values of commonly used methods in the unified family. The “Method Information” table in [Figure 83.5](#) displays the values of  $\rho = 0.5$  and  $\tau = 0$ , which are the parameters for the O'Brien-Fleming method. The table also displays the derived parameter  $C_\alpha = 2.0243$ , which is used in the construction of symmetric lower and upper  $\alpha$  boundaries; see the section “[Unified Family Methods](#)” on page 7025.

The “Boundary Information” table in [Figure 83.6](#) displays the information level, including the proportion, actual level, and corresponding sample size (N) at each stage. The table also displays the lower and upper alternative references, and the lower and upper boundary values at each stage.



Figure 83.6 Boundary Information

| Boundary Information (Standardized Z Scale) |                             |          |          |                       |         |
|---------------------------------------------|-----------------------------|----------|----------|-----------------------|---------|
| Null Reference = 0                          |                             |          |          |                       |         |
| _Stage_                                     | -----Information Level----- |          |          | -----Alternative----- |         |
|                                             | Proportion                  | Actual   | N        | Lower                 | Upper   |
| 1                                           | 0.2500                      | 0.026851 | 42.96116 | -1.63862              | 1.63862 |
| 2                                           | 0.5000                      | 0.053701 | 85.92233 | -2.31736              | 2.31736 |
| 3                                           | 0.7500                      | 0.080552 | 128.8835 | -2.83817              | 2.83817 |
| 4                                           | 1.0000                      | 0.107403 | 171.8447 | -3.27724              | 3.27724 |

| Boundary Information (Standardized Z Scale) |                           |             |  |
|---------------------------------------------|---------------------------|-------------|--|
| Null Reference = 0                          |                           |             |  |
| _Stage_                                     | -----Boundary Values----- |             |  |
|                                             | ---Lower---               | ---Upper--- |  |
|                                             | Alpha                     | Alpha       |  |
| 1                                           | -4.04859                  | 4.04859     |  |
| 2                                           | -2.86278                  | 2.86278     |  |
| 3                                           | -2.33745                  | 2.33745     |  |
| 4                                           | -2.02429                  | 2.02429     |  |

The information proportion is the proportion of maximum information available at each stage and N is the corresponding sample size. By default (or equivalently if you specify BOUNDARYSCALE=STDZ), the procedure displays boundary values with the standardized Z scale in the boundary information table and the boundary plot. The alternative reference on the standardized Z scale at stage  $k$  is given by  $\theta_1 \sqrt{I_k}$ , where  $\theta_1$  is the alternative reference and  $I_k$  is the information available at stage  $k$ ,  $k = 1, 2, 3, 4$ . These standardized alternative references for the design are derived in the SEQDESIGN procedure even if the alternative reference is not specified or derived in the procedure.

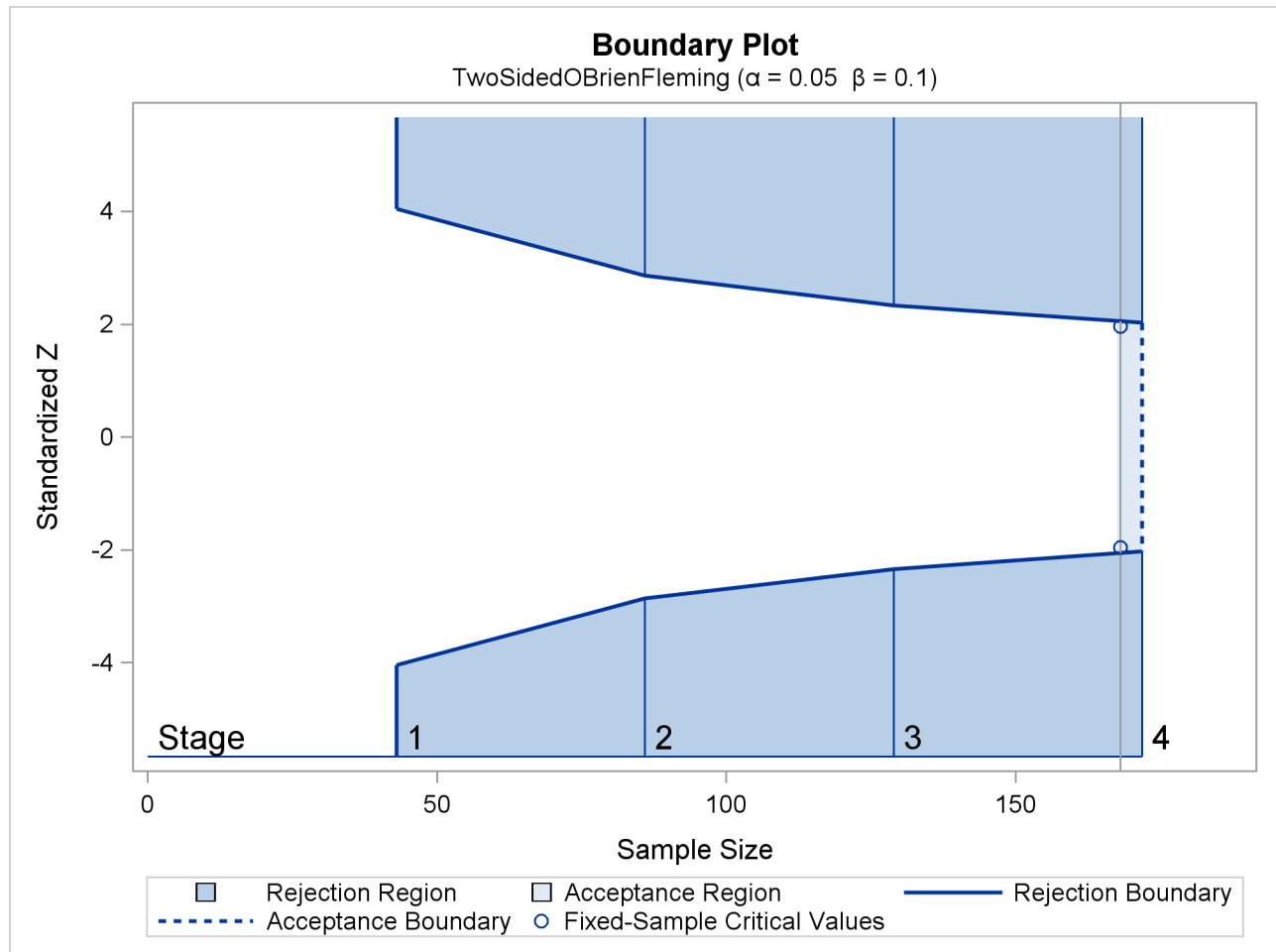
In this example, a standardized Z statistic is computed by standardizing the parameter estimate of the effect in LDL level. A lower Z test statistic indicates a beneficial effect. Consequently, at each interim stage, if the standardized Z test statistic is less than or equal to the corresponding lower  $\alpha$  boundary value, the hypothesis  $H_0 : \theta = 0$  is rejected for efficacy. If the test statistic is greater than or equal to the corresponding upper  $\alpha$  boundary value, the hypothesis  $H_0$  is rejected for harmful effect. Otherwise, the process continues to the next stage. At the final stage (stage 4), the hypothesis  $H_0$  is rejected for efficacy if the Z statistic is less than or equal to the corresponding lower  $\alpha$  boundary value  $-2.0243$ , and the hypothesis  $H_0$  is rejected for harmful effect if the Z statistic is greater than or equal to the corresponding upper  $\alpha$  boundary value  $2.0243$ . Otherwise, the hypothesis of no significant difference is accepted.

Note that in a typical trial, the actual information levels do not match the information levels specified in the design. The SEQTEST procedure modifies the boundary values stored in the BOUND\_LDL data set to adjust for these new information levels.

With ODS Graphics enabled, a detailed boundary plot with the rejection and acceptance regions is displayed, as shown in Figure 83.7. This plot displays the boundary values in the “Boundary Information” table in Figure 83.6. The stages are indicated by vertical lines with accompanying stage numbers. The horizontal axis indicates the sample sizes for the stages. Note that comparing with a fixed-sample design, only a small increase in sample size is needed for the O’Brien-Fleming design, as shown in Figure 83.7.

If a test statistic at an interim stage is in the rejection region (shaded area), the trial stops and the null hypothesis is rejected. If the statistic is not in any rejection region, the trial continues to the next stage.

**Figure 83.7** Boundary Plot



The boundary plot also displays critical values for the corresponding fixed-sample design. The symbol “o” identifies the fixed-sample critical values of  $-1.96$  and  $1.96$ , and the accompanying vertical line indicates the required sample size for the fixed-sample design at the horizontal axis. Note that the boundary values  $\pm 2.0243$  at the final stage are close to the fixed-sample critical values  $\pm 1.96$ .

When you specify the `SAMPLESIZE` statement, the maximum information (either explicitly specified or derived in the `SEQDESIGN` procedure) is used to compute the required sample sizes for the study. The `MODEL=TWOSAMPLEMEAN(STDDEV=20)` option specifies the test for the difference between two normal means. See the section “[Test for the Difference between Two Normal Means](#)” on page 7053 for a detailed derivation of these required sample sizes.

The “Sample Size Summary” table in Figure 83.8 displays the parameters for the sample size computation and the resulting maximum and expected sample sizes.

**Figure 83.8** Sample Size Summary

| Sample Size Summary             |                  |
|---------------------------------|------------------|
| Test                            | Two-Sample Means |
| Mean Difference                 | -10              |
| Standard Deviation              | 20               |
| Max Sample Size                 | 171.8447         |
| Expected Sample Size (Null Ref) | 170.7627         |
| Expected Sample Size (Alt Ref)  | 129.0137         |

The “Sample Sizes (N)” table in Figure 83.9 displays the required sample sizes at each stage for the trial, in both fractional and integer numbers. The derived fractional sample sizes are displayed under the heading “Fractional N.” These sample sizes are rounded up to integers under the heading “Ceiling N.” By default (or equivalently if you specify WEIGHT=1 in the MODEL=TWOSAMPLEMEAN option), the sample sizes for the two groups are equal for the two-sample test.

**Figure 83.9** Derived Sample Sizes

| Sample Sizes (N)                      |        |          |          |             |
|---------------------------------------|--------|----------|----------|-------------|
| Two-Sample Z Test for Mean Difference |        |          |          |             |
| -----Fractional N-----                |        |          |          |             |
| _Stage_                               | N      | N(Grp 1) | N(Grp 2) | Information |
| 1                                     | 42.96  | 21.48    | 21.48    | 0.0269      |
| 2                                     | 85.92  | 42.96    | 42.96    | 0.0537      |
| 3                                     | 128.88 | 64.44    | 64.44    | 0.0806      |
| 4                                     | 171.84 | 85.92    | 85.92    | 0.1074      |
| Sample Sizes (N)                      |        |          |          |             |
| Two-Sample Z Test for Mean Difference |        |          |          |             |
| -----Ceiling N-----                   |        |          |          |             |
| _Stage_                               | N      | N(Grp 1) | N(Grp 2) | Information |
| 1                                     | 44     | 22       | 22       | 0.0275      |
| 2                                     | 86     | 43       | 43       | 0.0538      |
| 3                                     | 130    | 65       | 65       | 0.0812      |
| 4                                     | 172    | 86       | 86       | 0.1075      |

In practice, integer sample sizes are used in the trial, and the resulting information levels increase slightly. Thus, 22, 43, 65, and 86 individuals are needed in each of the two groups for the four stages, respectively.

## Syntax: SEQDESIGN Procedure

The following statements are available in the SEQDESIGN procedure:

```
PROC SEQDESIGN < options > ;
 < label: > DESIGN options ;
 SAMPLESIZE < MODEL= option > ;
```

The PROC SEQDESIGN statement and the DESIGN statement are required for the SEQDESIGN procedure. Each DESIGN statement requests a new group sequential design, and multiple DESIGN statements can be used to create more than one design for comparison of features. The label, which must be a valid SAS name, is used to identify the design in the output tables and graphics. The SAMPLESIZE statement computes the required sample sizes for the design specified in each DESIGN statement. With a selected design, the SAMPLESIZE statement computes the required sample sizes for the trial.

## PROC SEQDESIGN Statement

```
PROC SEQDESIGN < options > ;
```

The PROC SEQDESIGN statement invokes the SEQDESIGN procedure. [Table 83.1](#) summarizes the options available in the PROC SEQDESIGN statement.

**Table 83.1** Summary of PROC SEQDESIGN Options

| Option                   | Description                                          |
|--------------------------|------------------------------------------------------|
| <b>Design Parameters</b> |                                                      |
| ALTREF=                  | Specifies the alternative reference                  |
| BOUNDARYSCALE=           | Specifies the statistic scale for the boundary       |
| MAXINFO=                 | Specifies the maximum information level              |
| <b>Table Output</b>      |                                                      |
| ERRSPEND                 | Displays the cumulative error spending at each stage |
| PSS                      | Displays powers and expected sample sizes            |
| STOPPROB                 | Displays expected cumulative stopping probabilities  |
| <b>Graphics Output</b>   |                                                      |
| PLOTS=ASN                | Displays the expected sample numbers plot            |
| PLOTS=BOUNDARY           | Displays the detailed boundary plot                  |
| PLOTS=COMBINEDBOUNDARY   | Displays the combined boundary plot                  |
| PLOTS=ERRSPEND           | Displays the error spending plot                     |
| PLOTS=POWER              | Displays the powers plot                             |

By default, the SEQDESIGN procedure displays tables of design information, method information, and boundary information for each specified design. If ODS Graphics is enabled, it also displays a detailed boundary plot.

In addition, you can use output options to display output tables such as expected cumulative stopping probability at each stage under various hypothetical references. If ODS Graphics is enabled, you can also use output options to display plots such as powers and expected sample sizes under various hypothetical references.

The following options can be used in the PROC SEQDESIGN statement to derive boundary values for all sequential designs in the procedure. They are listed in alphabetical order.

**ALTREF= $\theta_1$  < (< LOWER= $\theta_{1l}$  > < UPPER= $\theta_{1u}$  > ) >**

specifies the alternative reference—that is, the hypothetical reference under the alternative hypothesis at which the power is computed. The LOWER= and UPPER= options are applicable only for a two-sided design with different lower and upper alternative references.

For a one-sided design,  $\theta_{1l} = -|\theta_1|$  is the lower alternative reference and  $\theta_{1u} = |\theta_1|$  is the upper alternative reference. For a two-sided design, the specified  $\theta_{1l}$  and  $\theta_{1u}$  are the lower and upper alternative references, respectively. If the LOWER= option is not specified,  $\theta_{1l} = -|\theta_1|$ , and if the UPPER= option is not specified,  $\theta_{1u} = |\theta_1|$ .

The specification of the ALTREF= option depends on the hypothesis used in the clinical trial. For example, suppose the null hypothesis  $H_0 : \theta = 0$  with an alternative hypothesis  $H_1 : \theta = \theta_1$  is used to compare two binomial populations,  $p_a = p_b$ . Then  $\theta_1$  is the proportion difference under  $H_1$  if  $\theta = p_a - p_b$ , and  $\theta_1$  is the log odds ratio under  $H_1$  if  $\theta = \log\left(\frac{p_a(1-p_b)}{p_b(1-p_a)}\right)$ .

If the ALTREF= option is not specified, the alternative reference  $\theta_1$  can also be specified or derived in the SAMPLESIZE statement. If  $\theta_1$  is specified or derived in the SAMPLESIZE statement,  $\theta_{1l} = -|\theta_1|$  and  $\theta_{1u} = |\theta_1|$  are the lower and upper alternative references, respectively.

Note that if the SAMPLESIZE statement is specified with a two-sided design, the sample sizes derived by using the lower and upper alternatives might be different. If  $\theta_1$  is specified or derived in the SAMPLESIZE statement, it is used to compute the sample sizes. Otherwise, the  $\theta_1$  specified in the ALTREF= option is used.

**BOUNDARYSCALE=MLE | SCORE | STDZ | PVALUE**

**BSCALE=MLE | SCORE | STDZ | PVALUE**

specifies the scale for the statistic that is displayed in the boundary table and boundary plots. The keywords MLE, SCORE, STDZ, and PVALUE correspond to the boundary with the maximum likelihood estimate scale, the score statistic scale, the standardized normal Z scale, and the  $p$ -value scale, respectively. The default is BOUNDARYSCALE=STDZ.

With the BOUNDARYSCALE=MLE or BOUNDARYSCALE=SCORE option, the maximum information must be either explicitly specified with the MAXINFO= option or derived in the SEQDESIGN procedure to provide the necessary information level at each stage to compute the boundary values. See the section “Boundary Scales” on page 7017 for a detailed description of the statistic scale for the boundary values.

Note that for a two-sided design, the  $p$ -value scale displays the one-sided fixed-sample  $p$ -value under the null hypothesis with a lower alternative hypothesis.

**MAXINFO=number**

specifies the maximum information level for the design. If the MAXINFO=option is specified and the alternative reference is either specified explicitly with the ALTREF= option or derived from the SAMPLESIZE statement, then the Type I and Type II error probability levels cannot be met simultaneously. In this case, the ALPHA= option in the DESIGN statement is applicable only with the BOUNDARYKEY=ALPHA option (which is the default) in the DESIGN statement, and the Type II error probability  $\beta$  is derived. The BETA= option in the DESIGN statement is applicable only with the BOUNDARYKEY=BETA option in the DESIGN statement, and the Type I error probability  $\alpha$  is derived.

**Table Output Options**

The following options can be used in the PROC SEQDESIGN statement to display addition table output. They are listed in alphabetical order.

**ERRSPEND**

displays the error spending at each stage for each boundary in the design.

**PSS <( CREF=  $c_1 < c_2 \dots >$  )>**

displays powers and expected sample sizes under various hypothetical references, where the numbers  $c_i \geq 0$ .

For a one-sided design, the power and expected sample sizes under hypotheses  $\theta = c_i \theta_1$  are displayed, where  $\theta_1$  is the alternative reference and  $c_i$  are the values specified in the CREF= option.

For a two-sided design, the power and expected sample sizes under hypotheses  $\theta = c_i \theta_{1l}$  and  $\theta = c_i \theta_{1u}$  are displayed, where  $\theta_{1l}$  and  $\theta_{1u}$  are the lower and upper alternative references, respectively. The default is CREF= 0 0.5 1.0 1.5.

Note that for a symmetric two-sided design, only the power and expected sample sizes under hypotheses  $\theta = c_i \theta_{1u}$  are derived. See the section “Type I and Type II Errors” on page 7022 for a detailed description of the power computation. See the section “Powers and Expected Sample Sizes” on page 7069 for a detailed description of the expected sample size computation.

**STOPPROB <( CREF=  $c_1 < c_2 \dots >$  )>**

displays expected cumulative stopping probabilities under various hypothetical references, where the numbers  $c_i \geq 0$ .

For a one-sided design, expected cumulative stopping probabilities at each stage under hypotheses  $\theta = c_i \theta_1$  are displayed, where  $\theta_1$  is the alternative reference and  $c_i$  are the values specified in the CREF= option.

For a two-sided design, expected cumulative stopping probabilities at each stage under hypotheses  $\theta = c_i \theta_{1l}$  and  $\theta = c_i \theta_{1u}$  are displayed, where  $\theta_{1l}$  and  $\theta_{1u}$  are the lower and upper alternative references, respectively. Note that for a symmetric two-sided design, only expected cumulative stopping probabilities under hypotheses  $\theta = c_i \theta_{1u}$  are derived. The default is CREF= 0 0.5 1.0 1.5.

## Graphics Output Options

This section describes the options for using ODS Graphics with the SEQDESIGN procedure to create plots.

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;
proc seqdesign altref=-10 plots=boundary(hscale=samplesize);
 TwoSidedOBrienFleming: design nstages=4 method=obf;
 samplesize model=twosamplemean(stddev=20);
run;
ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The following options can be used in the PROC SEQDESIGN statement to display graphs with ODS Graphics. They are listed in alphabetical order.

**PLOTS** < ( **ONLY** ) > < = *plot-request* >

**PLOTS** < ( **ONLY** ) > < = ( *plot-request* < ... *plot-request* > ) >

specifies options that control the details of the plots. The default is PLOTS=BOUNDARY. The global plot option ONLY suppresses the default plots and displays only plots specifically requested.

The plot request options are as follows.

### ALL

produces all appropriate plots.

**ASN** < ( **CREF=**  $c_1 < c_2 \dots >$  ) >

displays a plot of the average sample numbers (expected sample sizes for nonsurvival data or expected numbers of events for survival data) under various hypothetical references, where the numbers  $c_i \geq 0$ . These average sample numbers are displayed as percentages of the average sample numbers for the corresponding fixed-sample design.

For a one-sided design, expected sample numbers under hypotheses  $\theta = c_i \theta_1$  are displayed, where  $\theta_1$  is the alternative reference and  $c_i$  are the values specified in the CREF= option.

For a two-sided design, expected sample numbers under hypotheses  $\theta = c_i \theta_{1l}$  and  $\theta = c_i \theta_{1u}$  are displayed, where  $\theta_{1l}$  and  $\theta_{1u}$  are the lower and upper alternative references, respectively. Note that for a symmetric two-sided design, only the average sample numbers under hypotheses  $\theta = c_i \theta_{1u}$  are derived. The default is CREF= 0 to 1.5 by 0.01.

**BOUNDARY** < ( **HSCALE=INFO** | **SAMPLESIZE** ) >

displays a plot of the resulting sequential boundaries with the acceptance and rejection regions for each design. Either the information level (HSCALE=INFO) or the sample size (HSCALE=SAMPLESIZE) is displayed on the horizontal axis. If the maximum information is not available for the design, the information in percentage of its corresponding fixed-sample design are used in the plot. The stage number for each stage is displayed inside the plot. The default is HSCALE=INFO.

If the HSCALE=SAMPLESIZE option is specified, the SAMPLESIZE statement must also be specified. The options MODEL=INPUTNEVENTS, MODEL=TWOSAMPLESURVIVAL, and MODEL=PHREG in the SAMPLESIZE statement indicate survival data. For a sample that

does not contain survival data, the sample size at each stage is displayed on the horizontal axis. For survival data, the number of events is displayed on the horizontal axis at each stage. The critical values for the corresponding fixed-sample design are also displayed in the plot.

**COMBINEDBOUNDARY** < ( **HSCALE=INFO** | **SAMPLESIZE** | **STAGE** ) >

displays a plot of the resulting sequential boundaries for all designs simultaneously. You can display the information level (**HSCALE=INFO**), the sample size (**HSCALE=SAMPLESIZE**), or the stage number (**HSCALE=STAGE**) on the horizontal axis. The default is **HSCALE=INFO**. With **HSCALE=INFO**, if the maximum information is not available for the design, then the information in percentage of its corresponding fixed-sample design is used in the plot.

If the **HSCALE=SAMPLESIZE** option is specified, the **SAMPLESIZE** statement must also be specified. The options **MODEL=INPUTNEVENTS**, **MODEL=TWOSAMPLESURVIVAL**, and **MODEL=PHREG** in the **SAMPLESIZE** statement indicate survival data. For a sample that does not contain survival data, the sample size at each stage is displayed on the horizontal axis. For survival data, the number of events is displayed on the horizontal axis at each stage.

**ERRSPEND** < ( **HSCALE=INFO** | **STAGE** ) >

displays a plot of the error spending for all sequential boundaries in the designs simultaneously. You can display the information level (**HSCALE=INFO**) or the stage number (**HSCALE=STAGE**) on the horizontal axis. With **HSCALE=INFO**, the information fractions are used in the plot. The default is **HSCALE=STAGE**.

**NONE**

suppresses all plots.

**POWER** < ( **CREF=**  $c_1 < c_2 \dots$  ) >

displays a plot of the power curves under various hypothetical references, where the numbers  $c_i \geq 0$ .

For a one-sided design, powers under hypotheses  $\theta = c_i \theta_1$  are displayed, where  $\theta_1$  is the alternative reference and  $c_i$  are the values specified in the **CREF=** option.

For a two-sided design, powers under hypotheses  $\theta = c_i \theta_{1l}$  and  $\theta = c_i \theta_{1u}$  are displayed, where  $\theta_{1l}$  and  $\theta_{1u}$  are the lower and upper alternative references, respectively. Note that for a symmetric two-sided design, only powers under hypotheses  $\theta = c_i \theta_{1u}$  are derived. The default is **CREF=** 0 to 1.5 by 0.01.

---

## DESIGN Statement

< label: > **DESIGN** < options > ;

The **DESIGN** statement requests a new group sequential design. You can use multiple **DESIGN** statements, and each **DESIGN** statement corresponds to a separate group sequential design.



Table 83.2 summarizes the options available in the DESIGN statement.

**Table 83.2** Design Statement Options

| Option                   | Description                                                                                                        |
|--------------------------|--------------------------------------------------------------------------------------------------------------------|
| <b>Design Parameters</b> |                                                                                                                    |
| ALPHA=                   | Specifies the Type I error probability level $\alpha$                                                              |
| ALT=                     | Specifies the type of alternative hypothesis                                                                       |
| BETA=                    | Specifies the Type II error probability level $\beta$                                                              |
| BETAOVERLAP=             | Checks for overlapping of the lower and upper $\beta$ boundaries in a two-sided design with error spending methods |
| BOUNDARYKEY=             | Specifies the type of error probability to maintain                                                                |
| INFO=                    | Specifies the information levels                                                                                   |
| NSTAGES=                 | Specifies the number of stages                                                                                     |
| STOP=                    | Specifies the condition for early stopping                                                                         |
| <b>Boundary Methods</b>  |                                                                                                                    |
| METHOD=                  | Specifies methods for boundary values                                                                              |

The required NSTAGES= option specifies the number of stages. The METHOD= option is required if the number of stages specified in the NSTAGES= option is greater than one. The following options can be used in the DESIGN statement. They are listed in alphabetical order.

**ALPHA= $\alpha$  < (< LOWER= $\alpha_l$  > < UPPER= $\alpha_u$  > ) >**

specifies the Type I error probability  $\alpha$ . The default is  $\alpha = 0.05$ . The LOWER= and UPPER= options are applicable only for the two-sided design. The LOWER= option specifies the lower Type I error probability  $\alpha_l$ , and the upper Type I error probability is computed as  $\alpha_u = \alpha - \alpha_l$ . The UPPER= option specifies the upper Type I error probability  $\alpha_u$ , and the lower Type I error probability is computed as  $\alpha_l = \alpha - \alpha_u$ . If both LOWER= and UPPER= options are not specified,  $\alpha_l = \alpha_u = \alpha/2$ .

If both the MAXINFO= and ALTREF= options are specified, then the Type I and Type II error probability levels cannot be met simultaneously. In this case, the ALPHA= option is applicable only with the BOUNDARYKEY=ALPHA option (which is the default), and the Type II error probability  $\beta$  is derived.

**ALT=LOWER | UPPER | TWOSIDED**

specifies the type of alternative hypothesis in the design. For a test of  $H_0 : \theta = 0$ , the keywords LOWER, UPPER, and TWOSIDED correspond to the alternatives of  $\theta < 0$ ,  $\theta > 0$ , and  $\theta \neq 0$ , respectively. The default is ALT=TWOSIDED.

**BETA= $\beta$  < (< LOWER= $\beta_l$  > < UPPER= $\beta_u$  > ) >**

specifies the Type II error probability level  $\beta$ . The default is  $\beta = 0.10$ . The LOWER= and UPPER= options are applicable only for the two-sided design. The LOWER= option specifies the lower Type II error probability level  $\beta_l$ , and the UPPER= option specifies the upper Type II error probability level  $\beta_u$ . If the LOWER= or UPPER= option is not specified,  $\beta$  is used.

If both the MAXINFO= and ALTREF= options are specified, then the Type I and Type II error probability levels cannot be met simultaneously. In this case, the BETA= option is applicable only with the BOUNDARYKEY=BETA option, and the Type I error probability  $\alpha$  is derived.

**BETAOVERLAP=ADJUST | NOADJUST****OVERLAP=ADJUST | NOADJUST**

specifies whether to check for overlapping of the lower and upper  $\beta$  boundaries for the two corresponding one-sided tests. This option applies to two-sided designs with STOP=ACCEPT or STOP=BOTH that are constructed with error spending methods, and this type of overlapping might result from a small  $\beta$  spending at an interim stage. When you specify BETAOVERLAP=ADJUST, the procedure checks for this type of overlapping. If such overlapping is found, the  $\beta$  boundaries for the two-sided design at that stage are set to missing, and the  $\beta$  spending values at subsequent stages are adjusted, as described in the section “[Boundary Adjustments for Overlapping Lower and Upper  \$\beta\$  Boundaries](#)” on page 7039”.

You can specify BETAOVERLAP=NOADJUST to request that no adjustment be made. The default is BETAOVERLAP=ADJUST.

**BOUNDARYKEY=ALPHA | BETA | BOTH | NONE**

specifies types of errors to be maintained in the resulting boundary. The default is BOUNDARYKEY=ALPHA if both ALTREF= and MAXINFO= options are specified. Otherwise, the default is BOUNDARYKEY=NONE for Whitehead methods with the STOP=BOTH option, and it is BOUNDARYKEY=BOTH for others.

See the section “[Applicable Boundary Keys](#)” on page 7041 for a detailed description of applicable boundary keys.

**INFO=EQUAL****INFO=CUM( numbers )**

specifies relative information levels for all stages in the design. The INFO=EQUAL option specifies equally spaced information levels, and the INFO=CUM option specifies cumulative relative information levels. The default is INFO=EQUAL.

If the number of information levels specified in the INFO=CUM option is less than the number of stages specified in the NSTAGES= option, the last available information increment is used as the information increment for each subsequent stage.

**METHOD=WHITEHEAD < ( TAU= $\tau$  < ( < LOWER= $\tau_l$  > < UPPER= $\tau_u$  > ) > ) >****METHOD=method****METHOD(boundary) = method**

specifies the methods for the boundaries in the design, where  $0 \leq \tau < 0.5$ .

For a one-sided design, an  $\alpha$  boundary is created with the STOP=REJECT or STOP=BOTH option, and a  $\beta$  boundary is created with the STOP=ACCEPT or STOP=BOTH option. For a two-sided design, lower and upper  $\alpha$  boundaries are created with the STOP=REJECT or STOP=BOTH option, and lower and upper  $\beta$  boundaries are created with the STOP=ACCEPT or STOP=BOTH option.

There are three types of methods available in the SEQDESIGN procedure. The unified family methods and Haybittle-Peto methods derive boundary values with fixed boundary shape; the Whitehead methods derive boundary values by adjusting the boundary values generated from continuous monitoring; and the error spending methods derive the boundary values from the specified errors used at each stage. You can specify different methods for the same design, but all methods must be from the same group.

For a design with early stopping to reject or accept the null hypothesis, the METHOD=WHITEHEAD option uses Whitehead’s triangular design and double-triangular design for a one-sided design and

two-sided design, respectively (Whitehead and Stratton 1983; Whitehead 1997, 2001). For a design with early stopping only to reject the null hypothesis or only to accept the null hypothesis, you can specify the slope of the boundary line in the score statistic scale with the TAU=  $\tau$  option. The default is TAU=0.25. See the section “[Whitehead Methods](#)” on page 7030 for a detailed description of the Whitehead methods.

The following options specify available error spending methods for the boundary. Each of these methods can be specified with the METHOD= option for all boundaries, or with the METHOD(*boundary*) = option for an individual boundary. See the section “[Error Spending Methods](#)” on page 7034 for a detailed description of these error spending methods.

**ERRFUNCGAMMA < ( GAMMA=  $\gamma$  ) >**

specifies a gamma cumulative error spending function for the boundary (Hwang, Shih, and DeCani 1990). The GAMMA= option specifies the gamma parameter  $\gamma$  in the function, where  $\gamma \leq 3$ . The boundaries created with  $\gamma = 1$  are similar to the boundaries from the Pocock method, and the boundaries created with  $\gamma = -4$  or  $\gamma = -5$  are similar to the boundaries from the O’Brien-Fleming method. The default is GAMMA=-2, which is the average of  $\gamma = 1$  and  $\gamma = -5$ .

**ERRFUNCOBF**

specifies the O’Brien-Fleming-type cumulative error spending function for the boundary (Lan and DeMets 1983).

**ERRFUNCPOC**

specifies the Pocock-type cumulative error spending function for the boundary (Lan and DeMets 1983).

**ERRFUNCPW < ( RHO= $\rho$  ) >**

specifies a power cumulative error spending function for the boundary (Jennison and Turnbull 2000, p. 148). The RHO= option specifies the power parameter  $\rho$  in the function, where  $\rho \geq 0.25$ . The boundaries created with  $\rho = 1$  are similar to the boundaries from the Pocock method, and the boundaries created with  $\rho = 3$  are similar to the boundaries from the O’Brien-Fleming method. The default is RHO=2, which is the average of  $\rho = 1$  and  $\rho = 3$ .

**ERRSPEND ( *numbers* )**

specifies the relative cumulative error spending at each stage.

With a fixed boundary shape, you can use the following available Haybittle-Peto methods and unified family methods to derive the boundary. You can specify each of these methods in the METHOD= option for all boundaries, or in the METHOD(*boundary*) = option for an individual boundary. See the section “[Haybittle-Peto Method](#)” on page 7029 for a detailed description of the Haybittle-Peto methods, and see the section “[Unified Family Methods](#)” on page 7025 for a detailed description of unified family methods.

**HP | HAYBITTLE | PETO < ( Z= *numbers* | PVALUE= *numbers* ) >**

specifies the Haybittle-Peto method (Haybittle 1971; Peto et al. 1976). The values specified are used to create the boundary values. The boundary value at the final stage can be derived in the procedure to maintain the Type I and Type II error probability levels. The default is Z=3.

**OBF | OBRIENFLEMING**

specifies the O'Brien-Fleming method (O'Brien and Fleming 1979). The O'Brien-Fleming method is equivalent to a power family method with  $RHO=0.5$ .

**POC | POCOCK**

specifies the Pocock method (Pocock 1977). The Pocock method is equivalent to a power family method with  $RHO=0$ .

**POW | POWER < ( RHO= $\rho$  ) >**

specifies a power family method (Wang and Tsiatis 1987; Emerson and Fleming 1989; Pampallona and Tsiatis 1994). The  $RHO=$  option specifies the power parameter  $\rho$  in the power family method, where  $\rho \geq -0.25$ . The power family method with  $\rho = 0$  corresponds to the Pocock method, and the power family method with  $\rho = 0.5$  corresponds to the O'Brien-Fleming method. The default is  $RHO=0.25$ , a value halfway between the Pocock and O'Brien-Fleming methods. A power family method is equivalent to a unified family method with  $RHO=\rho$  and  $TAU=0$ .

**TRI | TRIANGULAR < ( TAU= $\tau$  ) >**

specifies a unified family triangular method (Kittelson and Emerson 1999), where  $0 \leq \tau \leq 1$ . The default is  $TAU=1.0$ . The triangular method is identical to the unified family method with  $RHO=0.5$  and  $TAU=\tau$ . Note that this unified family triangular method is different from Whitehead's triangular method.

**UNI | UNIFIED < ( < TAU= $\tau$  > < RHO= $\rho$  > ) >**

specifies a unified family method (Kittelson and Emerson 1999). The  $TAU=$  and  $RHO=$  options specify the  $\tau$  and  $\rho$  parameters in a unified family method, respectively, where  $\rho \geq 0$  and  $0 \leq \tau \leq 2\rho$ . The defaults are  $TAU=0$  and  $RHO=0.25$ . See the section "Unified Family Methods" on page 7025 for a detailed description of the unified family methods.

The O'Brien-Fleming, Pocock, power family, and triangular methods are all special cases of the unified family methods. Table 83.3 summarizes the corresponding parameters in the unified family for these methods.

**Table 83.3** Parameters in the Unified Family for Various Methods

| Method          | Option             | Unified Family |        |
|-----------------|--------------------|----------------|--------|
|                 |                    | Rho            | Tau    |
| Pocock          | POC                | 0              | 0      |
| O'Brien-Fleming | OBF                | 0.5            | 0      |
| Power family    | POW (RHO= $\rho$ ) | $\rho$         | 0      |
| Triangular      | TRI (TAU= $\tau$ ) | 0.5            | $\tau$ |

Note that the power parameter  $\rho = 1/2 - \Delta = \rho^* - 1/2$ , where  $\Delta$  is the power parameter used in Jennison and Turnbull (2000) and Wang and Tsiatis (1987) and  $\rho^*$  is the power parameter used in Kittelson and Emerson (1999).

If a method with specified parameters is used for all boundaries in the design, you can use the `METHOD=` option to specify the method. Otherwise, you can use the following `METHOD(boundary)=` options to specify different methods from the same group for the boundaries.

**METHOD(ALPHA)=method**

**METHOD(REJECT)=method**

specifies the method for the  $\alpha$  boundary of a one-sided design or the lower and upper  $\alpha$  boundaries for a two-sided design.

**METHOD(LOWERALPHA)=method**

**METHOD(LOWERREJECT)=method**

specifies the method for the lower  $\alpha$  boundary of a two-sided design.

**METHOD(UPPERALPHA)=method**

**METHOD(UPPERREJECT)=method**

specifies the method for the upper  $\alpha$  boundary of a two-sided design.

**METHOD(BETA)=method**

**METHOD(ACCEPT)=method**

specifies the method for the  $\beta$  boundary of a one-sided design or the lower and upper  $\beta$  boundaries for a two-sided design.

**METHOD(LOWERBETA)=method**

**METHOD(LOWERACCEPT)=method**

specifies the method for the lower  $\beta$  boundary of a two-sided design.

**METHOD(UPPERBETA)=method**

**METHOD(UPPERACCEPT)=method**

specifies the method for the upper  $\beta$  boundary of a two-sided design.

**NSTAGES=number**

specifies the number of stages for the design. This option is required in the `DESIGN` statement, and the maximum allowed number of stages is 25.

**STOP=ACCEPT**

**STOP=REJECT**

**STOP=BOTH < ( BETABOUNDARY=BINDING | NONBINDING ) >**

specifies the early stopping criterion for the design. The keywords `ACCEPT`, `REJECT`, and `BOTH` correspond to early stopping only to accept, only to reject, and either to accept or reject the null hypothesis  $H_0$ , respectively. The default is `STOP=REJECT`. With `STOP=BOTH`, the `BETABOUNDARY=BINDING` suboption computes the Type I error probability with the acceptance boundary, and the `BETABOUNDARY=NONBINDING` suboption computes the Type I error probability without the acceptance boundary. The default is `BETABOUNDARY=BINDING`. The `BETABOUNDARY=NONBINDING` option is not applicable with `METHOD=WHITEHEAD`.

## SAMPLESIZE Statement

**SAMPLESIZE** < **MODEL=** *option* > ;

If each observation in the data set provides one unit of information in a hypothesis testing such as a one-sample test for the mean, the SAMPLESIZE statement computes the required sample sizes for the sequential design specified in each DESIGN statement. However, for a survival analysis, an individual in the survival time data might provide only partial information because of censoring. For this hypothesis, the SAMPLESIZE statement computes the required numbers of events. With additional accrual information in a survival analysis, the sample sizes can also be computed.

Only one SAMPLESIZE statement can be specified. For each specified group sequential design, the SAMPLESIZE statement computes the required sample sizes or numbers of events. The SAMPLESIZE statement is not required if the SEQDESIGN procedure is used only to compare features among different designs. Table 83.4 summarizes the options available in the SAMPLESIZE statement.

**Table 83.4** SAMPLESIZE Statement Options

| Option                     | Description                                                        |
|----------------------------|--------------------------------------------------------------------|
| <b>Fixed-Sample Models</b> |                                                                    |
| INPUTNOBS                  | Specifies the sample size for fixed-sample design                  |
| INPUTNEVENTS               | Specifies the number of events for fixed-sample design             |
| <b>One-Sample Models</b>   |                                                                    |
| ONESAMPLEMEAN              | Specifies the one-sample Z test for mean                           |
| ONESAMPLEFREQ              | Specifies the one-sample test for binomial proportion              |
| <b>Two-Sample Models</b>   |                                                                    |
| TWOSAMPLEMEAN              | Specifies the two-sample Z test for mean difference                |
| TWOSAMPLEFREQ              | Specifies the two-sample test for binomial proportions             |
| TWOSAMPLESURVIVAL          | Specifies the log-rank test for two survival distributions         |
| <b>Regression Models</b>   |                                                                    |
| REG                        | Specifies the test for a regression parameter                      |
| LOGISTIC                   | Specifies the test for a logistic regression parameter             |
| PHREG                      | Specifies the test for a proportional hazards regression parameter |

The MODEL= option specifies the input sample size or number of events from a fixed-sample study, or it specifies a statistical model to compute the required sample size. The MODEL=INPUTNOBS option specifies the input sample size from a fixed-sample study of nonsurvival data, and the MODEL=INPUTNEVENTS option specifies the number of events from a fixed-sample study of survival data. The remaining MODEL= options specify the statistical models used to compute the required sample size. The default is MODEL=TWOSAMPLEMEAN, the two-sample Z test for the mean difference.

With the MODEL=INPUTNOBS or MODEL=INPUTNEVENTS option, the required sample size or number of events for the group sequential trial is computed by multiplying the input sample size or number of events by the ratio between the design information level and its corresponding fixed-sample information level. This ratio can be obtained by dividing the Max Information (Percent Fixed-Sample) in the “Design Information” table by 100. See the section “Design Information” on page 7068 for a description of the “Design Information” table.

## Fixed-Sample Models

The following two options compute the required sample size or number of events for a group sequential trial by using the sample size or number of events for the fixed-sample design.

### MODEL=INPUTNOBS ( options )

specifies the sample size information for a fixed-sample design. The available options are as follows:

- N=  $n$
- SAMPLE= ONE | TWO
- WEIGHT=  $w_a < w_b >$
- MATCHNOBS= YES | NO

The required N= $n$  option specifies the sample size  $n$  for the fixed-sample design. The SAMPLE=ONE option specifies a one-sample test, and the SAMPLE=TWO option specifies a two-sample test. The default is SAMPLE=ONE.

With a two-sample test, the WEIGHT= option specifies the sample size allocation weights for the two groups. If  $w_b$  is not specified,  $w_b = 1$  is used. The default is WEIGHT=1, equal allocation for the two groups. The derived fractional sample sizes are rounded up to integers, and the MATCHNOBS=YES option requests these integer sample sizes to match the sample size allocation.

See the section “[Input Sample Size for Fixed-Sample Design](#)” on page 7044 for a detailed description of the input sample size for the fixed-sample design in sample size computation.

### MODEL=INPUTNEVENTS ( D= $d$ < options > )

specifies the sample size information for a fixed-sample survival test. The required D= $d$  option specifies the fixed-sample number of events  $d$ . To derive the sample size, you need to specify additional options from the following list:

- ACCNOBS=  $n_a$
- ACCRATE=  $r_a$
- ACCRUAL= UNIFORM | EXP(PARM= $\gamma_0$ )
- ACCTIME=  $T_a$
- FOLTIME=  $T_f$
- HAZARD=  $h_a < h_b >$
- LOSS= NONE | EXP( HAZARD= $\tau$  | MEDLOSSTIME= $t_\tau$  )
- MEDSURVTIME=  $t_a < t_b >$
- SAMPLE= ONE | TWO
- TOTALTIME=  $T$
- WEIGHT=  $w_a < w_b >$

The SAMPLE=ONE option specifies a one-sample test, and the SAMPLE=TWO option specifies a two-sample test. The default is SAMPLE=ONE. With a two-sample test, the WEIGHT= option specifies the sample size allocation weights for the two groups. If  $w_b$  is not specified,  $w_b=1$  is used. The default is WEIGHT=1.



For a one-sample test, the HAZARD=  $h_a$  option specifies the hazard rate  $h_a$  explicitly, and the MEDSURVTIME= $t_a$  option specifies the hazard rate implicitly through the median survival time  $t_a$ . Similarly, for a two-sample test, the HAZARD=  $h_a h_b$  option specifies the hazard rates  $h_a$  and  $h_b$  for groups A and B explicitly, and the MEDSURVTIME= $t_a t_b$  option specifies hazard rates for groups A and B implicitly through the median survival times  $t_a$  and  $t_b$ . Also, for a two-sample test,  $h_b = h_a$  if  $h_b$  is not specified and  $t_b = t_a$  if  $t_b$  is not specified.

The ACCRUAL= option specifies the method for individual accrual. The default ACCRUAL=UNIFORM option specifies that the individual accrual is uniform in the accrual time  $T_a$  with a constant accrual rate  $r_a$ , and the ACCRUAL=EXP(PARM= $\gamma_0$ ) option specifies that the individual accrual is truncated exponential with a scaled power parameter  $\gamma_0$ , where  $\gamma_0 \geq -10$  and  $\gamma_0 \neq 0$ . With a scaled parameter  $\gamma_0$ , the power parameter for the truncated exponential with the accrual time  $T_a$  is given by  $\gamma = \gamma_0/T_a$ .

The ACCTIME= and FOLTIME= options specify the accrual time  $T_a$  and follow-up time  $T_f$ , respectively. The TOTALTIME= option specifies the total study time,  $T = T_a + T_f$ .

The ACCRATE= option specifies the constant accrual rate  $r_a$ . If you specify the ACCRATE= option, then you must also specify one of the ACCTIME=, FOLTIME=, and TOTALTIME= options for the sample size computation. Otherwise, you must specify two of the ACCTIME=, FOLTIME=, and TOTALTIME= options to compute the accrual rate and sample size.

The ACCNOBS= option specifies the total number of individuals in the study. If you specify the ACCNOBS= option, then you must also specify one of the ACCTIME=, FOLTIME=, and TOTALTIME= options for the sample size computation. Otherwise, you must specify two of the ACCTIME=, FOLTIME=, and TOTALTIME= options to compute the accrual rate and sample size.

The LOSS= option specifies the individual loss to follow up in the sample size computation. The default LOSS=NONE option specifies no loss to follow up, and the LOSS=EXP option specifies exponential loss function. The HAZARD= $\tau$  suboption specifies the exponential loss hazard rate  $\tau$ , and the MEDLOSSTIME= $t_\tau$  suboption specifies the exponential loss hazard rate through the median loss times  $t_\tau$ .

See the section “[Input Number of Events for Fixed-Sample Design](#)” on page 7044 for a detailed description of the input number of events for the fixed-sample design in sample size computation.

## One-Sample Models

The following two options compute the required sample size for a one-sample group sequential test:

**MODEL=ONESAMPLEMEAN** < ( options ) >

specifies the one-sample  $Z$  test for mean. The available options are as follows:

- MEAN=  $\mu_1$
- STDDEV=  $\sigma$

The MEAN= option specifies the alternative reference  $\mu_1$  and is required if the alternative reference is not specified or derived in the procedure. If the MEAN=option is not specified, the specified or derived alternative reference is used.

The STDDEV= option specifies the standard deviation  $\sigma$ . The default is STDDEV=1. See the section “[Test for a Normal Mean](#)” on page 7050 for a detailed description of the one-sample  $Z$  test for mean.



Note that the one-sample  $Z$  test for mean also includes the paired difference in two-treatment comparison (Jennison and Turnbull 2000, pp. 51–52), where  $\mu_1$  is the mean of differences within pairs under the alternative hypothesis and  $\sigma$  is the standard deviation for the mean of differences within pairs.

**MODEL=ONESAMPLEFREQ** < ( options ) >

specifies the one-sample test for binomial proportion with the null hypothesis  $H_0 : \theta = 0$  and the alternative hypothesis  $H_1 : \theta = \theta_1$ , where  $\theta = p - p_0$  and  $\theta_1 = p_1 - p_0$ . The available options are as follows:

- NULLPROP=  $p_0$
- PROP=  $p_1$
- REF= NULLPROP | PROP

The NULLPROP= and PROP= options specify the proportions under the null and alternative hypotheses, respectively. The default for the null reference is NULLPROP=0.5. The PROP= option is required if the alternative reference is not specified or derived in the procedure. If the PROP= option is not specified, the specified or derived alternative reference  $\theta_1$  is used to compute the alternative reference  $p_1 = p_0 + \theta_1$ .

The REF= option specifies the hypothesis under which the proportion is used in the sample size computation. The REF=NULLPROP option uses the null hypothesis, and the REF=PROP option uses the alternative hypothesis to compute the sample size. The default is REF=PROP. See the section “[Test for a Binomial Proportion](#)” on page 7051 for a detailed description of the one-sample tests for proportion.

## Two-Sample Models

The following three options compute the required sample size or number of events for a two-sample group sequential trial.

**MODEL=TWOSAMPLEMEAN** < ( options ) >

specifies the two-sample  $Z$  test for mean difference. The available options are as follows:

- MEANDIFF=  $\theta_1$
- STDDEV=  $\sigma_a$  <  $\sigma_b$  >
- WEIGHT=  $w_a$  <  $w_b$  >
- MATCHNOBS= YES | NO

The MEANDIFF= option specifies the alternative reference  $\theta_1$  and is required if the alternative reference is not specified or derived in the procedure. If the MEANDIFF= option is not specified, the specified or derived alternative reference is used.

The STDDEV= option specifies the standard deviations  $\sigma_a$  and  $\sigma_b$ . If  $\sigma_b$  is not specified,  $\sigma_b = \sigma_a$ . The default is STDDEV=1.

The WEIGHT= option specifies the sample size allocation weights for the two groups. If  $w_b$  is not specified,  $w_b = 1$  is used. The default is WEIGHT=1, equal sample size for the two groups. The derived fractional sample sizes are rounded up to integers, and the MATCHNOBS=YES option requests these integer sample sizes to match the sample size allocation. The default is MATCHNOBS=NO.

See the section “[Test for the Difference between Two Normal Means](#)” on page 7053 for a detailed description of the two-sample  $Z$  test for mean difference.

**MODEL=TWOSAMPLEFREQ** < ( options ) >

specifies the two-sample test for binomial proportions. The available options are as follows:

- NULLPROP=  $p_{0a} < p_{0b} >$
- PROP=  $p_{1a}$
- TEST= PROP | LOGOR | LOGRR
- REF= NULLPROP | PROP | AVGNULLPROP | AVGPROP
- WEIGHT=  $w_a < w_b >$
- MATCHNOBS= YES | NO

The NULLPROP= option specifies proportions  $p_a = p_{0a}$  and  $p_b = p_{0b}$  in groups A and B, respectively, under the null hypothesis. If  $p_{0b}$  is not specified,  $p_{0b} = p_{0a}$ . The default is NULLPROP=0.5.

The PROP= option specifies proportion  $p_a = p_{1a}$  in group A under the alternative hypothesis. The proportion  $p_{1b}$  in group B under the alternative hypothesis is given by  $p_{1b} = p_{0b}$ . The PROP= option is required if the alternative reference is not specified or derived in the procedure. If the PROP= option is not specified, the specified or derived alternative reference is used to compute  $p_{1a}$ , the proportion in group A under the alternative hypothesis.

The TEST= option specifies the null hypothesis  $H_0 : \theta = 0$  in the test. The TEST=PROP option uses the difference in proportions  $\theta = (p_a - p_b) - (p_{0a} - p_{0b})$ , the TEST=LOGOR option uses the log odds-ratio test  $\theta = \delta - \delta_0$ , where

$$\delta = \log \left( \frac{p_a(1 - p_b)}{p_b(1 - p_a)} \right) \quad \delta_0 = \log \left( \frac{p_{0a}(1 - p_{0b})}{p_{0b}(1 - p_{0a})} \right)$$

and the TEST=LOGRR option uses the log relative risk test with  $\theta = \delta - \delta_0$ , where

$$\delta = \log \left( \frac{p_a}{p_b} \right) \quad \delta_0 = \log \left( \frac{p_{0a}}{p_{0b}} \right)$$

The default is TEST=LOGOR.

The REF= option specifies the hypothesis under which the proportions are used in the sample size computation. The REF=NULLPROP option uses the null proportions  $p_{0a}$  and  $p_{0b}$ , the REF=PROP option uses the alternative proportions  $p_{1a}$  and  $p_{1b}$ , the REF=AVGNULLPROP option uses the average null proportion, and the REF=AVGPROP option uses the average alternative proportion. The default is REF=PROP.

The WEIGHT= option specifies the sample size allocation weights for the two groups. If  $w_b$  is not specified,  $w_b = 1$  is used. The default is WEIGHT=1, equal sample size for the two groups. The derived fractional sample sizes are also rounded up to integers, and the MATCHNOBS=YES option requests that these integer sample sizes match the sample size allocation.

See the section “Test for the Difference between Two Binomial Proportions” on page 7054, the section “Test for Two Binomial Proportions with a Log Odds Ratio Statistic” on page 7056, and the section “Test for Two Binomial Proportions with a Log Relative Risk Statistic” on page 7057 for a detailed description of the two-sample tests for proportions.

**MODEL=TWOSAMPLESURVIVAL** < ( options ) >

**MODEL=TWOSAMPLESURV** < ( options ) >

specifies the log-rank test for two survival distributions with the null hypothesis  $H_0 : \theta = \delta - \delta_0 = 0$ , where the parameter  $\delta = -\log(h_a/h_b)$ ,  $\delta_0$  is the value of  $\delta$  under the null hypothesis and the values  $h_a$  and  $h_b$  are the constant hazard rates for groups A and B, respectively.

The available options for the number of events are as follows:

- NULLHAZARD=  $h_{0a} < h_{0b} >$
- NULLMEDSURVTIME=  $t_{0a} < t_{0b} >$
- HAZARD=  $h_{1a}$
- HAZARDRATIO=  $\lambda_1$
- MEDSURVTIME=  $t_{1a}$

The NULLHAZARD= option specifies hazard rates  $h_a = h_{0a}$  and  $h_b = h_{0b}$  for groups A and B, respectively, under the null hypothesis. If  $h_{0b}$  is not specified,  $h_{0b} = h_{0a}$ . The NULLMEDSURVTIME= option specifies the median survival times  $t_a = t_{0a}$  and  $t_b = t_{0b}$  under the null hypothesis. If  $t_{0b}$  is not specified,  $t_{0b} = t_{0a}$ . If both NULLHAZARD= and NULLMEDSURVTIME= option are not specified, NULLHAZARD=0.06931, which corresponds to NULLMEDSURVTIME=10, is used.

The hazard rate for group B under the alternative hypothesis,  $h_{1b}$ , is identical to the hazard rate under the null hypothesis,  $h_{0b}$ . The HAZARD=, MEDSURVTIME=, and HAZARDRATIO= options specify the group A hazard rate  $h_{1a}$ , the group A median survival time  $t_{1a}$ , and the hazard ratio  $\lambda_1 = h_{1a}/h_{1b}$ , respectively, under the alternative hypothesis. The HAZARD=, MEDSURVTIME=, or HAZARDRATIO= option is required if the alternative reference is not specified or derived in the procedure. If these three options are not specified, the specified or derived alternative reference  $\theta_1$  is used to compute  $h_{1a}$  from the equation:

$$\theta_1 = -\log\left(\frac{h_{1a}}{h_{1b}}\right) - \left(-\log\left(\frac{h_{0a}}{h_{0b}}\right)\right) = -\log\left(\frac{h_{1a}}{h_{0a}}\right)$$

To derive the sample size, you need to specify additional *options* from the following list:

- ACCNOBS=  $n_a$
- ACCRATE=  $r_a$
- ACCRUAL= UNIFORM | EXP(PARM= $\gamma_0$ )
- ACCTIME=  $T_a$
- FOLTIME=  $T_f$
- LOSS= NONE | EXP( HAZARD= $\tau$  | MEDLOSSTIME= $t_\tau$  )
- REF= NULLHAZARD | HAZARD
- TOTALTIME=  $T$
- WEIGHT=  $w_a < w_b >$

The REF= option specifies the hypothesis under which the hazard is used in the sample size computation. The REF=NULLHAZARD option uses the null hypothesis, and the REF=HAZARD option uses the alternative hypothesis. The default is REF=HAZARD.

The WEIGHT= option specifies the sample size allocation weights for the two groups. If  $w_b$  is not specified,  $w_b = 1$  is used. The default is WEIGHT=1, equal sample size for the two groups.

The ACCRUAL= option specifies the method for individual accrual. The default ACCRUAL=UNIFORM option specifies that the individual accrual is uniform in the accrual time  $T_a$  with a constant accrual rate  $r_a$ , and the ACCRUAL=EXP(PARM= $\gamma_0$ ) option specifies that the individual accrual is truncated exponential with a scaled power parameter  $\gamma_0$ , where  $\gamma_0 \geq -10$  and  $\gamma_0 \neq 0$ . With a scaled parameter  $\gamma_0$ , the power parameter for the truncated exponential with the accrual time  $T_a$  is given by  $\gamma = \gamma_0/T_a$ .

The ACCTIME= and FOLTIME= options specify the accrual time  $T_a$  and follow-up time  $T_f$ , respectively. The TOTALTIME= option specifies the total study time,  $T = T_a + T_f$ .

The ACCRATE= option specifies the constant accrual rate  $r_a$ . If you specify the ACCRATE= option, then you must also specify one of the ACCTIME=, FOLTIME=, and TOTALTIME= options for the sample size computation. Otherwise, you must specify two of the ACCTIME=, FOLTIME=, and TOTALTIME= options to compute the accrual rate and sample size.

The ACCNOBS= option specifies the total number of individuals in the study. If you specify the ACCNOBS= option, then you must also specify one of the ACCTIME=, FOLTIME=, and TOTALTIME= options for the sample size computation. Otherwise, you must specify two of the ACCTIME=, FOLTIME=, and TOTALTIME= options to compute the accrual rate and sample size.

The LOSS= option specifies the individual loss to follow up in the sample size computation. The default LOSS=NONE option specifies no loss to follow up, and the LOSS=EXP option specifies exponential loss function. The HAZARD= $\tau$  suboption specifies the exponential loss hazard rate  $\tau$ , and the MEDLOSSTIME= $t_\tau$  suboption specifies the exponential loss hazard rate through the median loss times  $t_\tau$ .

See the section “[Test for Two Survival Distributions with a Log-Rank Test](#)” on page 7059 for a detailed description of the two-sample log-rank test for survival data.

## Regression Models

The following three options compute the required sample size or number of events for group sequential tests on a regression parameter.

**MODEL=REG** < ( options ) >

specifies the Z test for a normal regression parameter. The available options are as follows:

- BETA=  $\beta_1$
- VARIANCE=  $\sigma_y^2$
- XVARIANCE=  $\sigma_x^2$
- XRSQUARE=  $r_x^2$

The BETA= option specifies the alternative reference  $\beta_1$  and is required if the alternative reference is not specified or derived in the procedure. If the BETA= option is not specified,  $\beta_1 = \theta_1$ , the specified or derived alternative reference.

The VARIANCE= and XVARIANCE= options specify the variances for the response variable Y and covariate X, respectively. The defaults are VARIANCE=1 and XVARIANCE=1. For a model with

more than one covariate, the XRSQUARE= option can be used to derive the variance of X after adjusting for other covariates. The default is XRSQUARE=0.

See the section “[Test for a Parameter in the Regression Model](#)” on page 7061 for a detailed description of the Z test for the regression parameter.

**MODEL=LOGISTIC** < ( options ) >

specifies the Z test for a logistic regression parameter. The available options are as follows:

- BETA=  $\beta_1$
- PROP=  $p$
- XVARIANCE=  $\sigma_x^2$
- XRSQUARE=  $r_x^2$

The BETA= option specifies the alternative reference  $\beta_1$  and is required if the alternative reference is not specified or derived in the procedure. If the BETA= option is not specified,  $\beta_1 = \theta_1$ , the specified or derived alternative reference.

The PROP= option specifies the proportion of the binary response variable Y. The default is PROP=0.5. The XVARIANCE= option specifies the variance of the covariate X. The default is XVARIANCE=1. For a model with more than one covariate, the XRSQUARE= option can be used to derive the variance of X after adjusting for other covariates. The default is XRSQUARE=0.

See the section “[Test for a Parameter in the Logistic Regression Model](#)” on page 7062 for a detailed description of the Z test for the logistic regression parameter.

**MODEL=PHREG** < ( options ) >

specifies the Z test for a proportional hazards regression parameter. The available options for the number of events are as follows:

- BETA=  $\beta_1$
- XVARIANCE=  $\sigma_x^2$
- XRSQUARE=  $r_x^2$

The BETA= option specifies the alternative reference  $\beta_1$  and is required if the alternative reference is not specified or derived in the procedure. If the BETA= option is not specified,  $\beta_1 = \theta_1$ , the specified or derived alternative reference.

The XVARIANCE= option specifies the variance of the covariate X. The default is XVARIANCE=1. For a model with more than one covariate, the XRSQUARE= option can be used to derive the variance of X after adjusting for other covariates. The default is XRSQUARE=0.

To derive the sample size, you need to specify additional *options* from the following list:

- ACCNOBS=  $n_a$
- ACCRATE=  $r_a$
- ACCRUAL= UNIFORM | EXP(PARM= $\gamma_0$ )
- ACCTIME=  $T_a$
- FOLTIME=  $T_f$

- HAZARD=  $h_a$
- LOSS= NONE | EXP( HAZARD= $\tau$  | MEDLOSSTIME= $t_\tau$  )
- MEDSURVTIME=  $t_a$
- TOTALTIME=  $T$

The hazard rate is required for the sample size computation. The HAZARD=  $h_a$  option specifies the hazard rate  $h_a$  explicitly, and the MEDSURVTIME= $t_a$  option specifies the hazard rate implicitly through the median survival time  $t_a$ .

The ACCRUAL= option specifies the method for individual accrual. The default ACCRUAL=UNIFORM option specifies that the individual accrual is uniform in the accrual time  $T_a$  with a constant accrual rate  $r_a$ , and the ACCRUAL=EXP(PARM= $\gamma_0$ ) option specifies that the individual accrual is truncated exponential with a scaled power parameter  $\gamma_0$ , where  $\gamma_0 \geq -10$  and  $\gamma_0 \neq 0$ . With a scaled parameter  $\gamma_0$ , the power parameter for the truncated exponential with the accrual time  $T_a$  is given by  $\gamma = \gamma_0/T_a$ .

The ACCTIME= and FOLTIME= options specify the accrual time  $T_a$  and follow-up time  $T_f$ , respectively. The TOTALTIME= option specifies the total study time,  $T = T_a + T_f$ .

The ACCRATE= option specifies the constant accrual rate  $r_a$ . If you specify the ACCRATE= option, then you must also specify one of the ACCTIME=, FOLTIME=, and TOTALTIME= options for the sample size computation. Otherwise, you must specify two of the ACCTIME=, FOLTIME=, and TOTALTIME= options to compute the accrual rate and sample size.

The ACCNOBS= option specifies the total number of individuals in the study. If you specify the ACCNOBS= option, then you must also specify one of the ACCTIME=, FOLTIME=, and TOTALTIME= options for the sample size computation. Otherwise, you must specify two of the ACCTIME=, FOLTIME=, and TOTALTIME= options to compute the accrual rate and sample size.

The LOSS= option specifies the individual loss to follow up in the sample size computation. The default LOSS=NONE option specifies no loss to follow up, and the LOSS=EXP option specifies exponential loss function. The HAZARD= $\tau$  suboption specifies the exponential loss hazard rate  $\tau$ , and the MEDLOSSTIME= $t_\tau$  suboption specifies the exponential loss hazard rate through the median loss times  $t_\tau$ .

See the section “Test for a Parameter in the Proportional Hazards Regression Model” on page 7063 for a detailed description of the  $Z$  test for the proportional hazards regression parameter.

## Details: SEQDESIGN Procedure

### Fixed-Sample Clinical Trials

A clinical trial is a research study in consenting human beings to answer specific health questions. One type of trial is a treatment trial, which tests the effectiveness of an experimental treatment. An example is a planned experiment designed to assess the efficacy of a treatment in humans by comparing the outcomes in a group of patients who receive the test treatment with the outcomes in a comparable group of patients who

receive a placebo control treatment, where patients in both groups are enrolled, treated, and followed over the same time period.

A clinical trial is conducted according to a plan called a protocol. The protocol provides detailed description of the study. For a fixed-sample trial, the study protocol contains detailed information such as the null hypothesis, the one-sided or two-sided test, and the Type I and II error probability levels. It also includes the test statistic and its associated critical values in the hypothesis testing.

Generally, the efficacy of a new treatment is demonstrated by testing a hypothesis  $H_0 : \theta = 0$  in a clinical trial, where  $\theta$  is the parameter of interest. For example, to test whether a population mean  $\mu$  is greater than a specified value  $\mu_0$ ,  $\theta = \mu - \mu_0$  can be used with an alternative  $\theta > 0$ .

A one-sided test is a test of the hypothesis with either an upper (greater) or a lower (lesser) alternative, and a two-sided test is a test of the hypothesis with a two-sided alternative. The drug industry often prefers to use a one-sided test to demonstrate clinical superiority based on the argument that a study should not be run if the test drug would be worse (Chow, Shao, and Wang 2003, p. 28). But in practice, two-sided tests are commonly performed in drug development (Senn 1997, p. 161). For a fixed Type I error probability  $\alpha$ , the sample sizes required by one-sided and two-sided tests are different. See Senn (1997, pp. 161–167) for a detailed description of issues involving one-sided and two-sided tests.

For independent and identically distributed observations  $y_1, y_2, \dots, y_n$  of a random variable, the likelihood function for  $\theta$  is

$$L(\theta) = \prod_{j=1}^n L_j(\theta)$$

where  $\theta$  is the population parameter and  $L_j(\theta)$  is the probability or probability density of  $y_j$ . Using the likelihood function, two statistics can be derived that are useful for inference: the maximum likelihood estimator and the score statistic.

### Maximum Likelihood Estimator

The maximum likelihood estimate (MLE) of  $\theta$  is the value  $\hat{\theta}$  that maximizes the likelihood function for  $\theta$ . Under mild regularity conditions,  $\hat{\theta}$  is an asymptotically unbiased estimate of  $\theta$  with variance  $1/E_\theta(I(\theta))$ , where  $I(\theta)$  is the Fisher information

$$I(\theta) = -\frac{\partial^2 \log(L(\theta))}{\partial \theta^2}$$

and  $E_\theta(I(\theta))$  is the expected Fisher information (Diggle et al. 2002, p. 340)

$$E_\theta(I(\theta)) = -E_\theta \left( \frac{\partial^2 \log(L(\theta))}{\partial \theta^2} \right)$$

The score function for  $\theta$  is defined as

$$S(\theta) = \frac{\partial \log(L(\theta))}{\partial \theta}$$

and usually, the MLE can be derived by solving the likelihood equation  $S(\theta) = 0$ . Asymptotically, the MLE is normally distributed (Lindgren 1976, p. 272):

$$\hat{\theta} \sim N \left( \theta, \frac{1}{E_\theta(I(\theta))} \right)$$

If the Fisher information  $I(\theta)$  does not depend on  $\theta$ , then  $I(\theta)$  is known. Otherwise, either the expected information evaluated at the MLE  $\hat{\theta}$  ( $E_{\theta=\hat{\theta}}(I(\theta))$ ) or the observed information  $I(\hat{\theta})$  can be used for the Fisher information (Cox and Hinkley 1974, p. 302; Efron and Hinkley 1978, p. 458), where the observed Fisher information

$$I(\hat{\theta}) = - \left( \frac{\partial^2 \log(L(\theta))}{\partial \theta^2} \Big|_{\theta = \hat{\theta}} \right)$$

If the Fisher information  $I(\theta)$  does depend on  $\theta$ , the observed Fisher information is recommended for the variance of the maximum likelihood estimator (Efron and Hinkley 1978, p. 457).

Thus, asymptotically, for large  $n$ ,

$$\hat{\theta} \sim N \left( \theta, \frac{1}{I} \right)$$

where  $I$  is the information, either the expected Fisher information  $E_{\theta=0}(I(\theta))$  or the observed Fisher information  $I(\hat{\theta})$ .

So to test  $H_0 : \theta = 0$  versus  $H_1 : \theta \neq 0$ , you can use the standardized  $Z$  test statistic

$$Z = \frac{\hat{\theta}}{\sqrt{\text{Var}(\hat{\theta})}} = \hat{\theta} \sqrt{I} \sim N(0, 1)$$

and the two-sided  $p$ -value is given by

$$\text{Prob}(|Z| > |z_0|) = 1 - 2\Phi(|z_0|)$$

where  $\Phi$  is the cumulative standard normal distribution function and  $z_0$  is the observed  $Z$  statistic.

If the BOUNDARYSCALE=SCORE is specified in the SEQDESIGN procedure, the boundary values for the test statistic are displayed in the score statistic scale. With the standardized  $Z$  statistic, the score statistic  $S = Z\sqrt{I} = \hat{\theta}I$  and

$$S \sim N(0, I)$$

## Score Statistic

The score statistic is based on the score function for  $\theta$ ,

$$S(\theta) = \frac{\partial \log(L(\theta))}{\partial \theta}$$

Under the null hypothesis  $H_0 : \theta = 0$ , the score statistic  $S(0)$  is the first derivative of the log likelihood evaluated at the null reference 0:

$$S(0) = \frac{\partial \log(L(\theta))}{\partial \theta} \Big|_{\theta = 0}$$

Under regularity conditions,  $S(0)$  is asymptotically normally distributed with mean zero and variance  $E_{\theta=0}(I(\theta))$ , the expected Fisher information evaluated at the null hypothesis  $\theta = 0$  (Kalbfleisch and Prentice 1980, p. 45), where  $I(\theta)$  is the Fisher information

$$I(\theta) = -E \left( \frac{\partial^2 \log(L(\theta))}{\partial \theta^2} \right)$$



That is, for large  $n$ ,

$$S(0) \sim N(0, E_{\theta=0}(I(\theta)))$$

Asymptotically, the variance of the score statistic  $S(0)$ ,  $E_{\theta=0}(I(\theta))$ , can also be replaced by the expected Fisher information evaluated at the MLE  $\theta = \hat{\theta}$  ( $E_{\theta=\hat{\theta}}(I(\theta))$ ), the observed Fisher information evaluated at the null hypothesis  $\theta = 0$  ( $I(0)$ ), or the observed Fisher information evaluated at the MLE  $\theta = \hat{\theta}$  ( $I(\hat{\theta})$ ) (Kalbfleisch and Prentice 1980, p. 46), where

$$I(0) = - \left( \frac{\partial^2 \log(L(\theta))}{\partial \theta^2} \Big|_{\theta=0} \right)$$

$$I(\hat{\theta}) = - \left( \frac{\partial^2 \log(L(\theta))}{\partial \theta^2} \Big|_{\theta=\hat{\theta}} \right)$$

Thus, asymptotically, for large  $n$ ,

$$S(0) \sim N(0, I)$$

where  $I$  is the information, either an expected Fisher information ( $E_{\theta=0}(I(\theta))$  or  $E_{\theta=\hat{\theta}}(I(\theta))$ ) or a observed Fisher information ( $I(0)$  or  $I(\hat{\theta})$ ).

So to test  $H_0 : \theta = 0$  versus  $H_1 : \theta \neq 0$ , you can use the standardized  $Z$  test statistic

$$Z = \frac{S(0)}{\sqrt{I}}$$

If the BOUNDARYSCALE=MLE is specified in the SEQDESIGN procedure, the boundary values for the test statistic are displayed in the MLE scale. With the standardized  $Z$  statistic, the MLE statistic  $\hat{\theta} = Z/\sqrt{I} = U(0)/I$  and

$$\hat{\theta} \sim N\left(0, \frac{1}{I}\right)$$

## One-Sample Test for Mean

The following one-sample test for mean is used to demonstrate fixed-sample clinical trials in the section “One-Sided Fixed-Sample Tests in Clinical Trials” on page 7007 and the section “Two-Sided Fixed-Sample Tests in Clinical Trials” on page 7010.

Suppose  $y_1, y_2, \dots, y_n$  are  $n$  observations of a response variable  $Y$  from a normal distribution

$$y_i \sim N(\theta, \sigma^2)$$

where  $\theta$  is the unknown mean and  $\sigma^2$  is the known variance.

Then the log likelihood function for  $\theta$  is

$$\log(L(\theta)) = \sum_{j=1}^n -\frac{1}{2} \frac{(y_j - \theta)^2}{\sigma^2} + c$$

where  $c$  is a constant. The first derivative is

$$\frac{\partial \log(L(\theta))}{\partial \theta} = \frac{1}{\sigma^2} \sum_{j=1}^n (y_j - \theta) = \frac{n}{\sigma^2} (\bar{y} - \theta)$$

where  $\bar{y}$  is the sample mean.

Setting the first derivative to zero, the MLE of  $\theta$  is  $\hat{\theta} = \bar{y}$ , the sample mean. The variance for  $\hat{\theta}$  can be derived from the Fisher information

$$I(\theta) = -\frac{\partial^2 \log(L(\theta))}{\partial \theta^2} = \frac{n}{\sigma^2}$$

Since the Fisher information  $I_0 = I(\theta)$  does not depend on  $\theta$  in this case,  $1/I_0$  is used as the variance for  $\hat{\theta}$ . Thus the sample mean  $\bar{y}$  has a normal distribution with mean  $\theta$  and variance  $\sigma^2/n$ :

$$\hat{\theta} = \bar{y} \sim N\left(\theta, \frac{1}{I_0}\right) = N\left(\theta, \frac{\sigma^2}{n}\right)$$

Under the null hypothesis  $H_0 : \theta = 0$ , the score statistic

$$S(0) = \frac{\partial \log(L(\theta))}{\partial \theta} \Big|_{\theta=0} = \frac{n}{\sigma^2} \bar{y}$$

has a mean zero and variance

$$I(\theta) = -\frac{\partial^2 \log(L(\theta))}{\partial \theta^2} = \frac{n}{\sigma^2}$$

With the MLE  $\hat{\theta}$ , the corresponding standardized statistic is computed as  $Z = \hat{\theta} \sqrt{I_0} = \bar{y}/(\sigma/\sqrt{n})$ , which has a normal distribution with variance 1:

$$Z \sim N\left(\theta \sqrt{I_0}, 1\right) = N\left(\frac{\theta}{\sigma/\sqrt{n}}, 1\right)$$

Also, the corresponding score statistic is computed as  $S = \hat{\theta} I_0 = n\bar{y}/\sigma^2$  and

$$S \sim N\left(\theta I_0, I_0\right) = N\left(\frac{n\theta}{\sigma^2}, \frac{n}{\sigma^2}\right)$$

which is identical to  $S(0)$  computed under the null hypothesis  $H_0 : \theta = 0$ .

Note that if the variable  $Y$  does not have a normal distribution, then it is assumed that the sample size  $n$  is large such that the sample mean has an approximately normal distribution.

## One-Sided Fixed-Sample Tests in Clinical Trials

A one-sided test has either an upper (greater) or a lower (lesser) alternative. This section describes one-sided tests with upper alternatives only. Corresponding results for one-sided tests with lower alternatives can be derived similarly.

For a one-sided test of  $H_0 : \delta \leq \delta_0$  with an upper alternative  $H_1 : \delta > \delta_0$ , an equivalent null hypothesis is  $H_0 : \theta \leq 0$  with an upper alternative  $H_1 : \theta > 0$ , where  $\theta = \delta - \delta_0$ . A fixed-sample test rejects  $H_0$  if the

standardized test statistic  $Z_0 = \hat{\theta} \sqrt{I_0} \geq C_\alpha$ , where  $\hat{\theta}$  is the sample estimate of  $\theta$  and  $C_\alpha = \Phi^{-1}(1 - \alpha)$  is the critical value.

The  $p$ -value of the test is given by  $1 - \Phi(Z_0)$ , and the hypothesis  $H_0$  is rejected if the  $p$ -value is less than  $\alpha$ . An upper  $(1 - \alpha)$  confidence interval has the lower limit

$$\theta_l = \hat{\theta} - \frac{\Phi^{-1}(1 - \alpha)}{\sqrt{I_0}} = \frac{Z_0 - \Phi^{-1}(1 - \alpha)}{\sqrt{I_0}}$$

The hypothesis  $H_0$  is rejected if the confidence interval for the parameter  $\theta$  does not contain zero—that is, if the lower limit  $\theta_l$  is greater than 0.

With an alternative reference  $\theta = \theta_1$ ,  $\theta_1 > 0$ , a Type II error probability is defined as

$$\beta = P_{\theta=\theta_1}(Z_0 < C_\alpha)$$

which is equivalent to

$$\beta = P_{\theta=\theta_1}(Z_0 - \theta_1 \sqrt{I_0} < C_\alpha - \theta_1 \sqrt{I_0}) = \Phi(C_\alpha - \theta_1 \sqrt{I_0})$$

Thus,  $\Phi^{-1}(\beta) = C_\alpha - \theta_1 \sqrt{I_0}$ . Then, with  $C_\alpha = \Phi^{-1}(1 - \alpha)$ ,

$$\theta_1 \sqrt{I_0} = \Phi^{-1}(1 - \alpha) + \Phi^{-1}(1 - \beta)$$

The drift parameter  $\theta_1 \sqrt{I_0}$  can be computed for specified  $\alpha$  and  $\beta$  and the maximum information is given by

$$I_0 = \left( \frac{\Phi^{-1}(1 - \alpha) + \Phi^{-1}(1 - \beta)}{\theta_1} \right)^2$$

If the maximum information is available, then the required sample size can be derived. For example, in a one-sample test for the mean with a specific standard deviation  $\sigma$ , the sample size  $n$  required for the test is

$$n = \sigma^2 I_0 = \sigma^2 \left( \frac{\Phi^{-1}(1 - \alpha) + \Phi^{-1}(1 - \beta)}{\theta_1} \right)^2$$

On the other hand, if the alternative reference  $\theta_1$ , standard deviation  $\sigma$ , and sample size  $n$  are all specified, then  $\alpha$  can be derived for a given  $\beta$  and, similarly,  $\beta$  can be derived for a given  $\alpha$ .

With an alternative reference  $\theta = \theta_1$ ,  $\theta_1 > 0$ , the power  $1 - \beta$  is the probability of correctly rejecting the null hypothesis  $H_0$  at  $\theta_1$ :

$$1 - \beta = 1 - P_{\theta=\theta_1}(Z_0 < C_\alpha) = \Phi(\theta_1 \sqrt{I_0} - C_\alpha)$$

## Superiority Trials

A superiority trial that tests the response to a new drug is clinically superior to a comparative placebo control or active control therapy. If a positive value indicates a beneficial effect, a test for superiority has

$$H_0 : \theta \leq 0 \quad H_1 : \theta > 0$$

where  $H_0$  is the hypothesis of nonsuperiority and  $H_1$  is the alternative hypothesis of superiority.

The superiority test rejects the hypothesis  $H_0$  and declares superiority if the standardized statistic  $Z_0 = \hat{\theta}\sqrt{T_0} \geq C_\alpha$ , where the critical value  $C_\alpha = \Phi^{-1}(1 - \alpha)$ .

For example, if  $\theta$  is the response difference between the treatment and placebo control groups, then a superiority trial can be

$$H_0 : \theta \leq 0 \quad H_1 : \theta = 6$$

with a Type I error probability level  $\alpha = 0.025$  and a power  $1 - \beta = 0.90$  at  $\theta_1 = 6$ .

## Noninferiority Trials

A noninferiority trial does not compare the response to a new treatment with the response to a placebo. Instead, it demonstrates the effectiveness of a new treatment compared with that of a nonexisting placebo by showing that the response of a new treatment is not clinically inferior to the response of a standard therapy with an established effect. That is, this type of trial attempts to demonstrate that the new treatment effect is not worse than the standard therapy effect by an acceptable margin. These trials are often performed when there is an existing effective therapy for a serious disease, and therefore a placebo control group cannot be ethically included.

It can be difficult to specify an appropriate noninferiority margin. One practice is to choose with reference to the effect of the active control in historical placebo-controlled trials (Snapinn 2000, p. 20). With this practice, there is some basis to imply that the new treatment is better than the placebo for a positive noninferiority trial.

If a positive value indicates a beneficial effect, a test for noninferiority has a null hypothesis  $\delta \leq -\delta_0$  and an alternative hypothesis  $\delta = \delta_1 > -\delta_0$ , where  $\delta_0 > 0$  is the specified noninferiority margin.

An equivalent test has

$$H_0 : \theta \leq 0 \quad H_1 : \theta = \theta_1 > 0$$

where the parameter  $\theta = \delta + \delta_0$ ,  $H_0$  is the null hypothesis of inferiority, and  $H_1$  is the alternative hypothesis of noninferiority,

The noninferiority test rejects the hypothesis  $H_0$  and declares noninferiority if the standardized statistic  $Z_0 = \hat{\theta}\sqrt{T_0} = (\hat{\delta} + \delta_0)\sqrt{T_0} \geq C_\alpha$ , where the critical value  $C_\alpha = \Phi^{-1}(1 - \alpha)$ .

For example, if  $\delta$  is the response difference between the treatment and active control groups and  $\delta_0 = 2$  is the noninferiority margin, then a noninferiority trial with a power  $1 - \beta = 0.90$  at  $\delta_1 = 1$  might be

$$H_0 : \theta \leq 0 \quad H_1 : \theta = 3$$

where  $\theta = \delta + \delta_0 = \delta + 2$ .

## Two-Sided Fixed-Sample Tests in Clinical Trials

A two-sided test is a test of a hypothesis with a two-sided alternative. Two-sided tests include simple symmetric tests and more complicated asymmetric tests that might have distinct lower and upper alternative references.

### Symmetric Two-Sided Tests for Equality

For a symmetric two-sided test with the null hypothesis  $\delta = \delta_0$  against the alternative  $\delta \neq \delta_0$ , an equivalent null hypothesis is  $H_0 : \theta = 0$  with a two-sided alternative  $H_1 : \theta \neq 0$ , where  $\theta = \delta - \delta_0$ . A fixed-sample test rejects  $H_0$  if  $|\hat{\theta}\sqrt{I_0}| \geq C_{\alpha/2}$ , where  $\hat{\theta}$  is a sample estimate of  $\theta$  and  $C_{\alpha/2} = \Phi^{-1}(1 - \alpha/2)$  is the critical value.

A common two-sided test is the test for the response difference between a treatment group and a control group. The null and alternative hypotheses are  $H_0 : \theta = 0$  and  $H_1 : \theta \neq 0$ , respectively, where  $\theta$  is the response difference between the two groups. If a greater value indicates a beneficial effect, then there are three possible results:

- The test rejects the hypothesis  $H_0$  of equality and indicates that the treatment is significantly better if the standardized statistic  $Z_0 = \hat{\theta}\sqrt{I_0} \geq C_{\alpha/2}$ .
- The test rejects the hypothesis  $H_0$  and indicates the treatment is significantly worse if the standardized statistic  $Z_0 = \hat{\theta}\sqrt{I_0} \leq -C_{\alpha/2}$ .
- The test indicates no significant difference between the two responses if  $-C_{\alpha/2} < \hat{\theta}\sqrt{I_0} < C_{\alpha/2}$ .

The  $p$ -value of the test is  $2(1 - \Phi(Z_0))$  if  $Z_0 > 0$  and  $2\Phi(Z_0)$  if  $Z_0 \leq 0$ . The hypothesis  $H_0$  is rejected if the  $p$ -value of the test is less than  $\alpha$ —that is, if  $1 - \Phi(Z_0) < \alpha/2$  or  $\Phi(Z_0) < \alpha/2$ . A symmetric  $(1 - \alpha)$  confidence interval for  $\theta$  has lower and upper limits

$$\left( \hat{\theta} - \frac{C_{\alpha/2}}{\sqrt{I_0}}, \hat{\theta} + \frac{C_{\alpha/2}}{\sqrt{I_0}} \right)$$

which is

$$\left( \frac{1}{\sqrt{I_0}} (Z_0 - C_{\alpha/2}), \frac{1}{\sqrt{I_0}} (Z_0 + C_{\alpha/2}) \right)$$

The hypothesis  $H_0$  is rejected if the confidence interval for the parameter  $\theta$  does not contain zero. That is, the lower limit is greater than zero or the upper limit is less than zero.

With an alternative reference  $\theta = \theta_1 > 0$ , a Type II error probability is defined as

$$\beta = P_{\theta=\theta_1}(-C_{\alpha/2} < Z_0 < C_{\alpha/2})$$

which is

$$\beta = P_{\theta=\theta_1} \left( (-C_{\alpha/2} - \theta_1\sqrt{I_0}) < (Z_0 - \theta_1\sqrt{I_0}) < (C_{\alpha/2} - \theta_1\sqrt{I_0}) \right)$$

Thus

$$\beta = \Phi\left(C_{\alpha/2} - \theta_1 \sqrt{I_0}\right) - \Phi\left(-C_{\alpha/2} - \theta_1 \sqrt{I_0}\right)$$

The resulting power  $1 - \beta$  is the probability of correctly rejecting the null hypothesis, which includes the probability for the lower alternative and the probability for the upper alternative. The SEQDESIGN procedure uses only the probability of correctly rejecting the null hypothesis for the correct alternative in the power computation.

Thus, under the upper alternative hypothesis, the power in the SEQDESIGN procedure is computed as the probability of rejecting the null hypothesis for the upper alternative,  $1 - \Phi\left(C_{\alpha/2} - \theta_1 \sqrt{I_0}\right) = \Phi\left(\theta_1 \sqrt{I_0} - C_{\alpha/2}\right)$ , and a very small probability of rejecting the null hypothesis for the lower alternative,  $\Phi\left(-C_{\alpha/2} - \theta_1 \sqrt{I_0}\right)$ , is ignored. This power computation is more rational than the power based on the probability of correctly rejecting the null hypothesis (Whitehead 1997, p. 75).

That is,

$$\beta = P_{\theta=\theta_1}\left((Z_0 - \theta_1 \sqrt{I_0}) < (C_{\alpha/2} - \theta_1 \sqrt{I_0})\right) = \Phi\left(C_{\alpha/2} - \theta_1 \sqrt{I_0}\right)$$

Then with  $\Phi^{-1}(\beta) = C_{\alpha/2} - \theta_1 \sqrt{I_0}$ ,

$$\theta_1 \sqrt{I_0} = C_{\alpha/2} - \Phi^{-1}(\beta) = \Phi^{-1}(1 - \alpha/2) + \Phi^{-1}(1 - \beta)$$

The drift parameter  $\theta_1 \sqrt{I_0}$  can be derived for specified  $\alpha$  and  $\beta$ , and the maximum information is given by

$$I_0 = \left(\frac{\Phi^{-1}(1 - \alpha/2) + \Phi^{-1}(1 - \beta)}{\theta_1}\right)^2$$

If the maximum information is available, then the required sample size can be derived. For example, in a one-sample test for mean, if the standard deviation  $\sigma$  is known, the sample size  $n$  required for the test is

$$n = \sigma^2 I_0 = \sigma^2 \left(\frac{\Phi^{-1}(1 - \alpha/2) + \Phi^{-1}(1 - \beta)}{\theta_1}\right)^2$$

On the other hand, if the alternative reference  $\theta_1$ , standard deviation  $\sigma$ , and sample size  $n$  are all known, then  $\alpha$  can be derived with a given  $\beta$  and, similarly,  $\beta$  can be derived with a given  $\alpha$ .

### Generalized Two-Sided Tests for Equality

For a generalized two-sided test with the null hypothesis  $\delta = \delta_0$  against the alternative  $\delta \neq \delta_0$ , an equivalent null hypothesis is  $H_0 : \theta \leq 0$  with a two-sided alternative  $H_1 : \theta \neq 0$ , where  $\theta = \delta - \delta_0$ . A fixed-sample test rejects  $H_0$  if the standardized statistic  $Z_0 = \hat{\theta} \sqrt{I_0} < -C_{\alpha_l}$  or  $Z_0 = \hat{\theta} \sqrt{I_0} > C_{\alpha_u}$ , where the critical values  $C_{\alpha_l} = \Phi^{-1}(1 - \alpha_l)$  and  $C_{\alpha_u} = \Phi^{-1}(1 - \alpha_u)$ .

With the lower alternative reference  $\theta_{1l} < 0$ , a lower Type II error probability is defined as

$$\beta_l = P_{\theta=\theta_{1l}}\left(-C_{\alpha_l} \leq Z_{0l} \sqrt{I_0}\right) = P_{\theta=\theta_{1l}}\left(-C_{\alpha_l} - \theta_{1l} \sqrt{I_0} \leq Z_{0l} \sqrt{I_0} - \theta_{1l} \sqrt{I_0}\right)$$

This implies

$$\beta_l = 1 - \Phi(-C_{\alpha_l} - \theta_{1l} \sqrt{I_0})$$

and the power is the probability of correctly rejecting the null hypothesis for the lower alternative,

$$1 - \beta_l = \Phi(-C_{\alpha_l} - \theta_{1l} \sqrt{I_0})$$

The lower drift parameter is derived as

$$\theta_{1l} \sqrt{I_0} = -(\Phi^{-1}(1 - \alpha_l) + \Phi^{-1}(1 - \beta_l))$$

Then, with specified  $\alpha_l$  and  $\beta_l$ , if the maximum information is known, the lower alternative reference  $\theta_{1l}$  can be derived. If the maximum information is unknown, then with the specified lower alternative reference  $\theta_{1l}$ , the maximum information required is

$$I_{0l} = \left( \frac{\Phi^{-1}(1 - \alpha_l) + \Phi^{-1}(1 - \beta_l)}{-\theta_{1l}} \right)^2$$

Similarly, the upper drift parameter is derived as

$$\theta_{1u} \sqrt{I_0} = \Phi^{-1}(1 - \alpha_u) + \Phi^{-1}(1 - \beta_u)$$

For a given  $\alpha_u$ ,  $\beta_u$ , and the upper alternative reference  $\theta_{1u}$ , the maximum information required is

$$I_{0u} = \left( \frac{\Phi^{-1}(1 - \alpha_u) + \Phi^{-1}(1 - \beta_u)}{\theta_{1u}} \right)^2$$

Thus, the maximum information required for the design is given by

$$I_0 = \max(I_{0l}, I_{0u})$$

Note that with the maximum information level  $I_0$ , if  $I_{0l} < I_0$ , then the derived power from the lower alternative is larger than the specified  $1 - \beta_l$ . Similarly, if  $I_{0u} < I_0$ , then the derived power from the upper alternative is larger than the specified  $1 - \beta_u$ .

If maximum information is available, the required sample size can be derived. For example, in a one-sample test for mean, if the standard deviation  $\sigma$  is known, the sample size  $n$  required for the test is  $n = \sigma^2 I_0$ .

On the other hand, if the alternative references, Type I error probabilities  $\alpha_l$  and  $\alpha_u$ , standard deviation  $\sigma$ , and sample size  $n$  are all specified, then the Type II error probabilities  $\beta_l$  and  $\beta_u$  and the corresponding powers can be derived.

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## Group Sequential Methods

A group sequential design provides interim analyses before the formal completion of a trial. The monitoring process provides possible early stopping for either positive or negative results and thus reduces the time to complete the trial. With a specified number of stages, the design creates critical values such that at each

interim analysis, a hypothesis can be rejected, accepted, or continued to the next time point. At the final stage, a hypothesis is either rejected or accepted. Usually, the critical values are derived such that the specified overall Type I and Type II error probability levels are maintained in the design.

For example, to test a null hypothesis  $H_0$  with an upper alternative in a fixed-sample design, a critical value  $c_\alpha$  is created. The null hypothesis  $H_0$  is rejected if the test statistic is greater than or equal to the critical value  $c_\alpha$ . Otherwise,  $H_0$  is accepted. But, for a group sequential design with early stopping to reject or accept the null hypothesis  $H_0$ , there are two critical values created at each interim analysis: an  $\alpha$  critical value  $c_{\alpha k}$  to reject the null hypothesis and a  $\beta$  critical value  $c_{\beta k}$  to accept the null hypothesis. The null hypothesis  $H_0$  is rejected if the test statistic is greater than or equal to the  $\alpha$  critical value  $c_{\alpha k}$ , and  $H_0$  is accepted if the test statistic is less than the  $\beta$  critical value  $c_{\beta k}$ . If the test statistic is between these two critical values, the process continues to the next stage. At the final stage, the two critical values are equal, and the hypothesis is either rejected or accepted.

Armitage, McPherson, and Rowe (1969) showed that repeated significance tests at a fixed level on accumulating data increase the probability of obtaining a significant result under the null hypothesis. For example, with a significance level 0.05 in a two-sided fixed-sample test, the critical value is 1.96. If this value is used in a five-stage group sequential trial with early stopping to reject the null hypothesis, then the probability of rejecting the null hypothesis at or before the fifth stage is 0.14169, much larger than the nominal value 0.05 (Armitage, McPherson, and Rowe 1969, p. 239).

Pocock (1977) applied these repeated significance tests to group sequential trials with equally spaced information levels and derives a constant critical value on the standardized normal  $Z$  scale across all stages that maintains the Type I error probability level. For example, with a significance level 0.05 in a two-sided test, the derived critical value at each stage is 2.413 on the standardized normal  $Z$  scale, larger than the fixed-sample critical value 1.96. The corresponding nominal  $p$ -value is 0.0158, which is smaller than the fixed-sample  $p$ -value 0.025 (Pocock 1977, p. 193).

O'Brien and Fleming (1979) proposed a sequential procedure that has boundary values decrease over the stages on the standardized normal  $Z$  scale to make the early stop less likely. The procedure has conservative stopping boundary values at very early stages, and boundary values at the final stage are close to the fixed-sample design. For example, with a significance level 0.05 in a two-sided test, the derived critical values at these five stages on the standardized normal  $Z$  scale are 4.562, 3.226, 2.634, 2.281, and 2.040.

The following references: Wang and Tsiatis (1987); Emerson and Fleming (1989); Pampallona and Tsiatis (1994) generalized the Pocock and O'Brien-Fleming methods to the power family, where a power parameter is used to allow a continuous set of designs between the Pocock and O'Brien-Fleming methods.

Kittelson and Emerson (1999) extended the methods in the power family even further to the unified family, which also includes the exact triangular method. The shape and location of each of the four boundaries can be independently specified in the unified family methods.

Whitehead and Stratton (1983) and Whitehead (1997, 2001) developed triangular methods by adapting tests for continuous monitoring to discrete monitoring. With early stopping to reject or accept the null hypothesis in a one-sided test, the derived continuation region has a triangular shape for the score-scaled boundaries. Only elementary calculations are needed to derive the boundary values for Whitehead's triangular methods.

For a sequential design, you can derive the  $\alpha$  and  $\beta$  error probabilities at each stage from the boundaries. On the other hand, you can derive the boundaries from specified  $\alpha$  and  $\beta$  error probabilities at each stage. The error spending function approach (Lan and DeMets 1983) uses the error spending function to specify the error probabilities at each stage and then uses these probabilities to derive the boundaries. You can specify  $\alpha$  and  $\beta$  explicitly or implicitly with an error spending function for the cumulative probabilities.



See Jennison and Turnbull (2000, pp. 5–11) for a more detailed history of group sequential methods.

The following three types of methods are available in the SEQDESIGN procedure to derive boundaries in a sequential design:

- fixed boundary shape methods, which derive boundaries with specified boundary shapes. These include the unified family method and Haybittle-Peto method.
- Whitehead methods, which adjust the boundaries from continuous monitoring for discrete monitoring
- error spending methods

You can use the SEQDESIGN procedure to specify methods from the same group for each design. A different method can be specified for each boundary separately, but all methods in a design must be from the same group.

### Fixed Boundary Shape Methods

The fixed boundary shape methods include the unified family method (Kittelson and Emerson 1999) and the Haybittle-Peto method (Haybittle 1971; Peto et al. 1976). The unified family methods derive the boundary values with the specified boundary shape. The unified family methods include the Pocock method (Pocock 1977), the O'Brien-Fleming method (O'Brien and Fleming 1979), the power family method (Wang and Tsiatis 1987; Emerson and Fleming 1989; Pampallona and Tsiatis 1994), and the triangular method (Kittelson and Emerson 1999). See the section “[Unified Family Methods](#)” on page 7025 for a detailed description of the methods that use the unified family approach.

The Haybittle-Peto method uses a value of 3 for the critical values in interim stages, so that the critical value at the final stage is close to the original design without interim monitoring. In the SEQDESIGN procedure, the Haybittle-Peto method has been generalized to allow for different boundary values at different stages. See the section “[Haybittle-Peto Method](#)” on page 7029 for a detailed description of the Haybittle-Peto method.

### Whitehead Methods

The Whitehead methods (Whitehead and Stratton 1983; Whitehead 1997, 2001) derive the boundary values by adapting the continuous monitoring tests to the discrete monitoring of group sequential tests. The Type I error probability and power corresponding to the resulting boundaries are extremely close but differ slightly from the specified values because of the approximations used in deriving the tests (Jennison and Turnbull 2000, p. 106). The SEQDESIGN procedure provides the BOUNDARYKEY= option to adjust the boundary value at the final stage for the exact Type I or Type II error probability level. See the section “[Whitehead Methods](#)” on page 7030 for a detailed description of Whitehead's methods.

### Error Spending Methods

An error spending method (Lan and DeMets 1983) uses the error spending function to specify the error spending at each stage and then uses these error probabilities to derive the boundary values. You can specify these errors explicitly or with an error spending function for these cumulative errors. See the section “[Error Spending Methods](#)” on page 7034 for a detailed description of the error spending methods.

Error spending methods derive boundary values at each stage sequentially and require much more computation than other types of methods for group sequential trials with a large number of stages, especially for a two-sided asymmetric design with early stopping to accept  $H_0$ , or to reject or accept  $H_0$ .

The sample size requirement for some applicable tests can also be computed in the procedure. After the actual data from a clinical trial are collected, you can then use the boundary information created in the SEQDESIGN procedure to perform a group sequential test in the SEQTEST procedure.

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## Statistical Assumptions for Group Sequential Designs

The SEQDESIGN procedure assumes that with a total number of stages  $K$ , the sequence of the standardized test statistics  $\{Z_1, Z_2, \dots, Z_K\}$  has the canonical joint distribution with information levels  $\{I_1, I_2, \dots, I_K\}$  for the parameter  $\theta$  (Jennison and Turnbull 2000, p. 49):

- $(Z_1, Z_2, \dots, Z_K)$  is multivariate normal
- $Z_k \sim N(\theta\sqrt{I_k}, 1)$ ,  $k = 1, 2, \dots, K$
- $\text{Cov}(Z_{k_1}, Z_{k_2}) = \sqrt{(I_{k_1}/I_{k_2})}$ ,  $1 \leq k_1 \leq k_2 \leq K$

In terms of the maximum likelihood estimator,  $\hat{\theta}_k = Z_k/\sqrt{I_k}$ ,  $k = 1, 2, \dots, K$ , the canonical joint distribution can be expressed as follows:

- $(\hat{\theta}_1, \hat{\theta}_2, \dots, \hat{\theta}_K)$  is multivariate normal
- $\hat{\theta}_k \sim N(\theta, 1/I_k)$ ,  $k = 1, 2, \dots, K$
- $\text{Cov}(\hat{\theta}_{k_1}, \hat{\theta}_{k_2}) = 1/I_{k_2}$ ,  $1 \leq k_1 \leq k_2 \leq K$

Furthermore, in terms of the score statistics  $S_k = Z_k\sqrt{I_k}$ ,  $k = 1, 2, \dots, K$ , the canonical joint distribution can be expressed as follows:

- $(S_1, S_2, \dots, S_K)$  is multivariate normal
- $S_k \sim N(\theta I_k, I_k)$ ,  $k = 1, 2, \dots, K$
- $\text{Cov}(S_{k_1}, S_{k_2}) = \text{Var}(S_{k_1}) = I_{k_1}$ ,  $1 \leq k_1 \leq k_2 \leq K$

That is, the increments  $S_1, S_2 - S_1, \dots$ , and  $S_K - S_{(K-1)}$  are independently distributed.

If the test statistic is computed from the data that are not from a normal distribution, such as a binomial distribution, then it is assumed that the test statistic is computed from a large sample such that the statistic has an approximately normal distribution.

If the increments  $S_1, S_2 - S_1, \dots$ , and  $S_K - S_{(K-1)}$  are not independently distributed, then it is inappropriate to use group sequential methods in the SEQDESIGN procedure. One such example is the Gehan statistic, which is a weighted log-rank statistic for censored data. See Jennison and Turnbull (2000, pp.

232–233, 276–277) and Proschan, Lan, and Wittes (2006, pp. 150–151) for a description of statistics with nonindependent increments.

If a trial stops at an early interim stage with only a small number of responses observed, it can lead to a distrust of the statistical findings, which rely on the assumption that the sample is large (Whitehead 1997, p. 167). A group sequential design can be specified such that at the first interim analysis, there are a sufficient number of responses to ensure that the analysis to be conducted is both reliable and persuasive (Whitehead 1997, p. 167).

Alternatively, a method such as the O'Brien-Fleming method can be used to derive conservative stopping boundary values at very early stages to make the early stop less likely. That is, the trial is stopped in early stages only with overwhelming evidence.

A simple example of the group sequential tests is the test for a normal mean,  $\mu = \mu_0$ . Suppose  $y_1, y_2, \dots, y_n$  are  $n$  observations of a response variable  $Y$  in a data set from a normal distribution with an unknown mean  $\mu$  and a known variance  $\sigma^2$ . Then the maximum likelihood estimate of  $\mu$  is the sample mean

$$\bar{y} = \frac{1}{n} \sum_{j=1}^n y_j$$

The sample mean has a normal distribution with mean  $\mu$  and variance  $\sigma^2/n$ :

$$\bar{y} \sim N\left(\mu, \frac{\sigma^2}{n}\right)$$

An equivalent hypothesis for  $\mu = \mu_0$  is  $H_0 : \theta = 0$ , where  $\theta = \mu - \mu_0$ . The MLE statistic for  $\theta$ ,

$$\hat{\theta} = \bar{y} - \mu_0 \sim N(\theta, I_0^{-1})$$

where the information  $I_0 = n/\sigma^2$ .

For a group sequential test with  $K$  stages, there are  $N_1, N_2, \dots, N_K$  observations available at these stages. At stage  $k$ , the sample mean is computed as

$$\bar{y}_k = \frac{1}{N_k} \sum_{j=1}^{N_k} y_{kj}$$

where  $y_{kj}$  is the value of the  $j$ th observation available at the  $k$ th stage and  $N_k$  is the cumulative sample size at stage  $k$ , which includes the  $N_{k-1}$  observations collected at previous stages and the  $N_k - N_{k-1}$  observations collected at the current stage.

The maximum likelihood estimate

$$\hat{\theta}_k = \bar{y}_k - \mu_0 \sim N(\theta, I_k^{-1})$$

where the information

$$I_k = \frac{1}{\text{Var}(\bar{y}_k)} = \frac{N_k}{\sigma^2}$$

is the inverse of the variance.

Thus, the standardized statistic

$$Z_k = \hat{\theta}_k \sqrt{I_k} = (\bar{y}_k - \mu_0) \sqrt{I_k} \sim N(\theta \sqrt{I_k}, 1)$$

The covariance of  $Z_{k_1}$  and  $Z_{k_2}$ ,  $1 \leq k_1 \leq k_2 \leq K$  can be expressed as

$$\text{Cov}(Z_{k_1}, Z_{k_2}) = \frac{1}{\sqrt{(I_{k_1} I_{k_2})}} \text{Cov}(S_{k_1}, S_{k_2})$$

where  $S_{k_1} = Z_{k_1} \sqrt{I_{k_1}}$  and  $S_{k_2} = Z_{k_2} \sqrt{I_{k_2}}$ .

Since  $S_{k_2} - S_{k_1}$  is independent of  $S_{k_1}$ ,  $\text{Cov}(S_{k_1}, S_{k_2}) = \text{Var}(S_{k_1}) = I_{k_1}$  and

$$\text{Cov}(Z_{k_1}, Z_{k_2}) = \frac{1}{\sqrt{(I_{k_1} I_{k_2})}} I_{k_1} = \sqrt{I_{k_1}/I_{k_2}}$$

Thus the statistics  $\{Z_1, Z_2, \dots, Z_K\}$  has the canonical joint distribution with information levels  $\{I_1, I_2, \dots, I_K\}$  for the parameter  $\mu$ . See the section “[Applicable One-Sample Tests and Sample Size Computation](#)” on page 7050, the section “[Applicable Two-Sample Tests and Sample Size Computation](#)” on page 7052, and the section “[Applicable Regression Parameter Tests and Sample Size Computation](#)” on page 7061 for more examples of applicable tests in group sequential trials.

## Boundary Scales

The boundaries computed by the SEQDESIGN procedure are applied to test statistics computed during the analysis, and so generally, the scale you select for the boundaries is determined by the scale of the statistics that you will be using.

The following scales are available in the SEQDESIGN procedure:

- MLE, maximum likelihood estimate
- standardized Z
- score statistic  $S$
- $p$ -value

These scales are all equivalent for a given set of boundary values—that is, there exists a unique transformation between any two of these scales. If you know the boundary values in terms of statistics from one scale, you can uniquely derive the boundary values of statistics for other scales. You can specify the scale with the BOUNDARYSCALE= option; the default is BOUNDARYSCALE=STDZ, the standardized Z scale.

You can also select the boundary scale to better examine the features of an individual group sequential design or to compare features among multiple designs. For example, with the standardized Z scale, the boundary values for the Pocock design are identical across all stages, and the O’Brien-Fleming design has boundary values (in absolute value) that decrease over the stages.

The remaining section demonstrates the transformations from one scale to the other scales. If the maximum likelihood estimate  $\hat{\theta}$  is computed by the analysis, then

$$\hat{\theta} \sim N\left(\theta, \frac{1}{I}\right)$$

where  $I$  is the Fisher information if it does not depend on  $\theta$ . Otherwise,  $I$  is either the expected Fisher information evaluated at  $\hat{\theta}$  or the observed Fisher information. See the section “[Maximum Likelihood Estimator](#)” on page 7004 for a detailed description of these statistics.

With the MLE statistic  $\hat{\theta}$ , the corresponding standardized  $Z$  statistic is computed as

$$Z = \hat{\theta} \sqrt{I} \sim N\left(\theta \sqrt{I}, 1\right)$$

and the corresponding score statistic is computed as

$$S = \hat{\theta} I \sim N(\theta I, I)$$

Similarly, if a score statistic  $S$  is computed by the analysis, then with

$$S \sim N(\theta I, I)$$

where  $I$  is the information, either an expected Fisher information ( $E_{\theta=0}(I(\theta))$  or  $E_{\theta=\hat{\theta}}(I(\theta))$ ) or an observed Fisher information ( $I(0)$  or  $I(\hat{\theta})$ ).

The corresponding standardized  $Z$  statistic is computed as

$$Z = \frac{S}{\sqrt{I}} \sim N\left(\theta \sqrt{I}, 1\right)$$

and the corresponding MLE-scaled statistic is computed as

$$\hat{\theta} = \frac{S}{I} \sim N\left(\theta, \frac{1}{I}\right)$$

With a standardized normal  $Z$  statistic, the corresponding fixed-sample nominal  $p$ -value depends on the type of alternative hypothesis. With an upper alternative, the nominal  $p$ -value is defined as the one-sided  $p$ -value under the null hypothesis  $H_0 : \theta = 0$  with an upper alternative:

$$p_k = 1 - \Phi(Z)$$

With a lower alternative or a two-sided alternative, the nominal  $p$ -value is defined as the one-sided  $p$ -value under the null hypothesis  $H_0 : \theta = 0$  with a lower alternative:

$$p_k = \Phi(Z)$$

which is an increasing function of the standardized  $Z$  statistic (Emerson, Kittelson, and Gillen 2005, p. 12).

The BOUNDARYSCALE= MLE, STDZ, SCORE, and PVALUE options display the boundary values in the MLE, standardize  $Z$ , score, and  $p$ -value scales, respectively. For example, suppose  $y_{k1}, y_{k2}, \dots, y_{kn_k}$

are  $n_k$  observations of a response variable  $Y$  in a data set from a normal distribution with an unknown mean  $\mu$  and a known variance  $\sigma^2$ . Then

$$y_{kj} \sim N(\mu, \sigma^2)$$

for  $k = 1, 2, \dots, K$ , where  $K$  is the number of groups and  $n_k$  is the number of observations at group  $k$ .

If  $N_k$  is the cumulative number of observations for the first  $k$  groups, then the sample mean from these  $N_k$  observations

$$\bar{y}_k = \frac{1}{N_k} \sum_{j=1}^{N_k} y_{kj}$$

has a normal distribution with mean  $\theta$  and variance  $\sigma^2/N_k$ :

$$\bar{y}_k \sim N\left(\theta, \frac{\sigma^2}{N_k}\right)$$

To test the null hypothesis  $\mu = \mu_0$ ,  $H_0 : \theta = 0$ , where  $\theta = \mu - \mu_0$  can be used. The MLE of  $\theta$  is  $\hat{\theta}_k = \bar{y}_k - \mu_0$  and

$$\hat{\theta}_k \sim N\left(\theta, \frac{1}{I_k}\right)$$

where the information is the inverse of the variance of  $\bar{y}_k$ ,

$$I_k = \frac{N_k}{\sigma^2}$$

The corresponding standardized  $Z$  statistic is

$$Z_k = \hat{\theta}_k I_k^{\frac{1}{2}} \sim N\left(\theta I_k^{\frac{1}{2}}, 1\right)$$

The score statistic in the SEQDESIGN procedure is then given by

$$S_k = \hat{\theta}_k I_k = Z_k I_k^{\frac{1}{2}} \sim N(\theta I_k, I_k)$$

For a null hypothesis  $H_0 : \theta = 0$  with an upper alternative, the nominal  $p$ -value of the standardized  $Z$  statistic is  $p_k = 1 - \Phi(Z_k)$ . For a null hypothesis  $H_0 : \theta = 0$  with a lower alternative or a two-sided alternative, the nominal  $p$ -value of the standardized  $Z$  statistic is  $p_k = \Phi(Z_k)$ .

## Boundary Variables

The boundaries created in group sequential trials depend on the type of the alternative hypothesis and the early stopping criterion. Table 83.5 shows the boundaries created with various design specifications.

**Table 83.5** Boundary Variables

| Alternative Hypothesis | Specifications<br>Early Stopping | Boundary Variables |      |       |       |
|------------------------|----------------------------------|--------------------|------|-------|-------|
|                        |                                  | Lower              |      | Upper |       |
|                        |                                  | Alpha              | Beta | Beta  | Alpha |
| Lower                  | Accept $H_0$                     |                    | X    |       |       |
|                        | Reject $H_0$                     | X                  |      |       |       |
|                        | Accept/Reject $H_0$              | X                  | X    |       |       |
| Upper                  | Accept $H_0$                     |                    |      | X     |       |
|                        | Reject $H_0$                     |                    |      |       | X     |
|                        | Accept/Reject $H_0$              |                    |      | X     | X     |
| Two-sided              | Accept $H_0$                     |                    | X    | X     |       |
|                        | Reject $H_0$                     | X                  |      |       | X     |
|                        | Accept/Reject $H_0$              | X                  | X    | X     | X     |

Up to four boundaries can be generated in a group sequential design:

- the upper  $\alpha$  boundary, to reject the null hypothesis for the upper alternative
- the upper  $\beta$  boundary, to accept the null hypothesis with an upper alternative
- the lower  $\beta$  boundary, to accept the null hypothesis with a lower alternative
- the lower  $\alpha$  boundary, to reject the null hypothesis for the lower alternative

For a two-sided design, the null hypothesis is accepted only if both the hypothesis is accepted with an upper alternative and the hypothesis is accepted with a lower alternative.

For a one-sided design with a lower alternative, only the lower boundaries are created. Similarly, for a one-sided design with an upper alternative, only the upper boundaries are created. For example, Figure 83.10 shows the boundary plot for a one-sided test with an upper alternative.

Figure 83.10 Boundary Plot for One-Sided Test

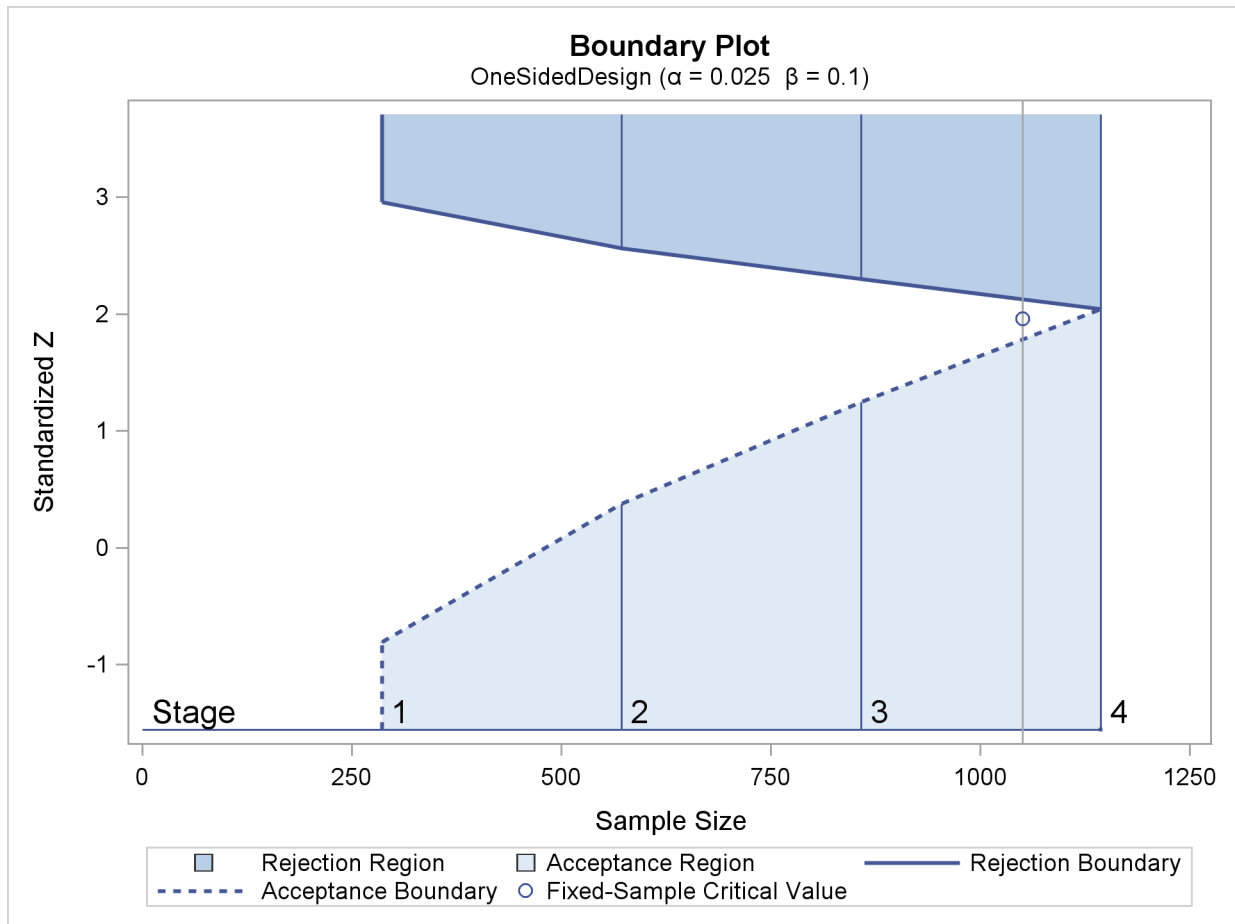


Figure 83.10 corresponds to a one-sided sequential design with early stopping to reject or accept the null hypothesis. For a sequential test with early stopping only to reject the null hypothesis, there are no acceptance boundary values at interim stages. The acceptance boundary value and its associated acceptance region are displayed only at the final stage. Similarly, for a sequential test with early stopping only to accept the null hypothesis, there are no rejection boundary values at interim stages. The rejection boundary value and its associated rejection region are displayed only at the final stage.

For a two-sided design, both the lower and upper boundaries are created. For a design with early stopping to reject the null hypothesis,  $\alpha$  boundaries are created. Similarly, for a design with early stopping to accept the null hypothesis,  $\beta$  boundaries are created. For a design with early stopping to accept or reject the null hypothesis, both the  $\alpha$  and  $\beta$  boundaries are created.



For example, Figure 83.11 shows the boundary plot for a two-sided test.

**Figure 83.11** Boundary Plot for Two-Sided Test

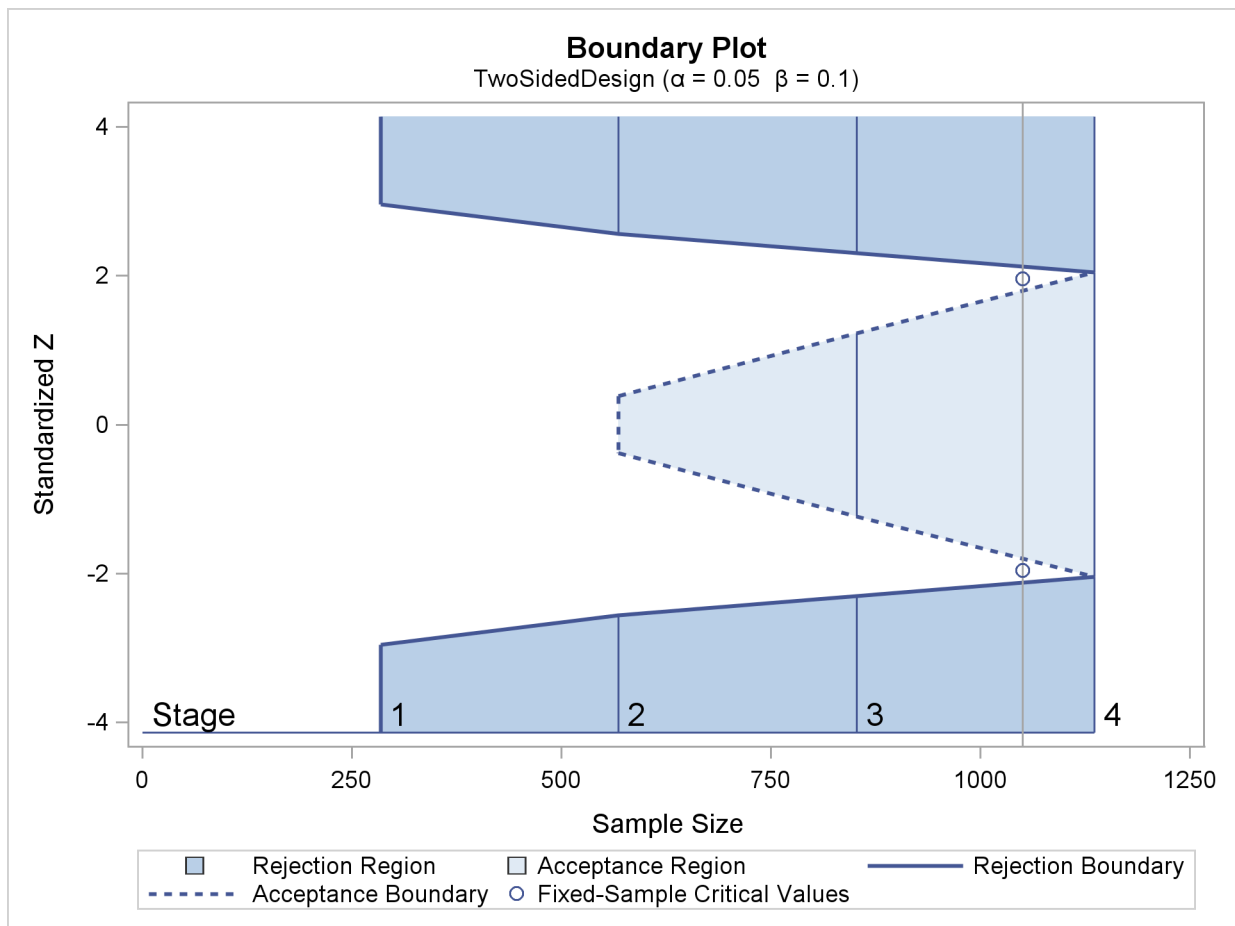


Figure 83.11 corresponds to a two-sided sequential design with early stopping to reject or accept the null hypothesis. For a sequential test with early stopping only to reject the null hypothesis, there are no acceptance boundary values at interim stages. The acceptance boundary value and its associated acceptance region are displayed only at the final stage. Similarly, for a sequential test with early stopping only to accept the null hypothesis, there are no rejection boundary values at interim stages. The rejection boundary value and its associated rejection region are displayed only at the final stage.

## Type I and Type II Errors

The Type I error is the error of rejecting the null hypothesis when the null hypothesis is correct, and the Type II error is the error of not rejecting the null hypothesis when the null hypothesis is incorrect. The level of significance  $\alpha$  is the probability of making a Type I error. The Type II error depends on the hypothetical reference of the alternative hypothesis, and the Type II error probability  $\beta$  is defined as the probability of not rejecting the null hypothesis when a specific alternative reference is true. The power  $1 - \beta$  is then defined as the probability of rejecting the null hypothesis at the alternative reference.

In a sequential design, if the maximum information and alternative reference are not both specified, the critical values are created such that both the specified Type I and the specified Type II error probability

levels are maintained in the design. Otherwise, the critical values are created such that either the specified Type I error probability or the specified Type II error probability is maintained.

### One-Sided Tests

For a  $K$ -stage group sequential design with an upper alternative hypothesis  $H_1 : \theta = \theta_1$  and early stopping to reject or accept the null hypothesis  $H_0 : \theta = 0$ , the boundaries contain the upper  $\alpha$  critical values  $a_k$  and upper  $\beta$  critical values  $b_k$ ,  $k = 1, 2, \dots, K$ . At each interim stage,  $b_k < a_k$ , the null hypothesis  $H_0$  is rejected if the observed statistic  $z_k \geq a_k$ ,  $H_0$  is accepted if  $z_k < b_k$ , or the process is continued to the next stage if  $b_k \leq z_k < a_k$ . At the final stage  $b_K = a_K$ , the hypothesis is either rejected or accepted.

The overall Type I error probability  $\alpha$  is given by

$$\alpha = \sum_{k=1}^K \alpha_k$$

where  $\alpha_k$  is the  $\alpha$  spending at stage  $k$ . That is, at stage 1,

$$\alpha_1 = P_{\theta=0}(z_1 \geq a_1)$$

At a subsequent stage  $k$ ,

$$\alpha_k = P_{\theta=0}(b_j \leq z_j < a_j, j = 1, 2, \dots, k-1, z_k \geq a_k)$$

Similarly, the Type II error probability

$$\beta = \sum_{k=1}^K \beta_k$$

where  $\beta_k$  is the  $\beta$  spending at stage  $k$ . That is, at stage 1,

$$\beta_1 = P_{\theta=\theta_1}(z_1 < b_1)$$

At a subsequent stage  $k$ ,

$$\beta_k = P_{\theta=\theta_1}(b_j \leq z_j < a_j, j = 1, 2, \dots, k-1, z_k < b_k)$$

With an upper alternative hypothesis  $H_1 : \theta = \theta_1 > 0$ , the power  $1 - \beta$  is the probability of rejecting the null hypothesis for the upper alternative.

$$1 - \beta = 1 - \sum_{k=1}^K \beta_k = \sum_{k=1}^K P_{\theta=\theta_1}(b_j \leq z_j < a_j, j = 1, 2, \dots, k-1, z_k \geq a_k)$$

For a design with early stopping to reject  $H_0$  only, the interim upper  $\beta$  critical values are set to  $-\infty$ ,  $b_k = -\infty$ ,  $k = 1, 2, \dots, K-1$ , and  $\beta = \beta_K$ . For a design with early stopping to accept  $H_0$  only, the interim upper  $\alpha$  critical values are set to  $\infty$ ,  $a_k = \infty$ ,  $k = 1, 2, \dots, K-1$ , and  $\alpha = \alpha_K$ .

Similarly, the Type I and Type II error probabilities for a  $K$ -stage design with a lower alternative hypothesis  $H_0 : \theta = -\theta_1$  can also be derived.

## Two-Sided Tests

For a  $K$ -stage group sequential design with two-sided alternative hypotheses  $H_{1u} : \theta = \theta_{1u}$  and  $H_{1l} : \theta = \theta_{1l}$ , and early stopping to reject or accept the null hypothesis  $H_0 : \theta = 0$ , the boundaries contain the upper  $\alpha$  critical values  $a_k$ , upper  $\beta$  critical values  $b_k$ , lower  $\beta$  critical values  ${}_b b_k$ , and lower  $\alpha$  critical values  ${}_a a_k$ ,  $k = 1, 2, \dots, K$ . At each interim stage,  ${}_a a_k < {}_b b_k \leq b_k < a_k$ , the null hypothesis  $H_0$  is rejected if the observed statistic  $z_k \geq a_k$  or  $z_k \leq {}_a a_k$ ,  $H_0$  is accepted if  ${}_b b_k < z_k < b_k$ , or the process is continued to the next stage if  $b_k \leq z_k < a_k$  or  ${}_a a_k < z_k \leq {}_b b_k$ . At the final stage  $b_K = a_K$  and  ${}_b b_K = {}_a a_K$ , the hypothesis is either rejected or accepted.

The overall upper Type I error probability  $\alpha_u$  is given by

$$\alpha_u = \sum_{k=1}^K \alpha_{uk}$$

where  $\alpha_{uk}$  is the  $\alpha$  spending at stage  $k$  for the upper alternative. That is, at stage 1,

$$\alpha_{u1} = P_{\theta=0}(z_1 \geq a_1)$$

At a subsequent stage  $k$ ,

$$\alpha_{uk} = P_{\theta=0}({}_a a_j < z_j \leq {}_b b_j \text{ or } b_j \leq z_j < a_j, j = 1, 2, \dots, k-1, z_k \geq a_k)$$

Similarly, the overall lower Type I error probability  $\alpha_l$  can also be derived, and the overall Type I error probability  $\alpha = \alpha_l + \alpha_u$ .

The overall upper Type II error probability  $\beta_u$  is given by

$$\beta_u = \sum_{k=1}^K \beta_{uk}$$

where  $\beta_{uk}$  is the upper  $\beta$  spending at stage  $k$ . That is, at stage 1,

$$\beta_{u1} = P_{\theta=\theta_{1u}}(z_1 < {}_a a_1 \text{ or } {}_b b_1 < z_1 < b_1)$$

At a subsequent stage  $k$ ,

$$\beta_{uk} = P_{\theta=\theta_{1u}}({}_a a_j < z_j \leq {}_b b_j \text{ or } b_j \leq z_j < a_j, j = 1, 2, \dots, k-1, z_k < {}_a a_k \text{ or } {}_b b_k < z_k < b_k)$$

With an upper alternative hypothesis  $H_1 : \theta = \theta_{1u} > 0$ , the power  $1 - \beta_u$  is the probability of rejecting the null hypothesis for the upper alternative:

$$1 - \beta_u = 1 - \sum_{k=1}^K \beta_{uk}$$

which is

$$P_{\theta=\theta_{1u}}({}_a a_j < z_j \leq {}_b b_j \text{ or } b_j \leq z_j < a_j, j = 1, 2, \dots, k-1, z_k \geq a_k)$$

The overall lower Type II error probability  $\beta_l$  and power  $1 - \beta_l$  can be similarly derived.

For a design with early stopping only to reject  $H_0$ , both the interim lower and upper  $\beta$  critical values are set to missing,  $k = 1, 2, \dots, K - 1$ , and  $\beta_{lK} = \beta_l$ ,  $\beta_{uK} = \beta_u$ . For a design with early stopping only to accept  $H_0$ , the interim upper  $\alpha$  critical values are set to  $\infty$ ,  $\alpha_{uk} = \infty$ , and the interim lower  $\alpha$  critical values are set to  $-\infty$ ,  $\alpha_{lk} = -\infty$ ,  $k = 1, 2, \dots, K - 1$ , and  $\alpha_{uK} = \alpha_u$ ,  $\alpha_{lK} = \alpha_l$ .

## Unified Family Methods

Unified family methods (Kittelsohn and Emerson 1999) derive boundary values with a specified boundary shape. For example, Pocock's method (Pocock 1977) derives equal boundary values for all stages in the standardized  $Z$  scale. In addition to Pocock's method, the unified family methods include the O'Brien-Fleming, power family, and unified family triangular methods.

The boundary values at each stage depend on the information fractions

$$\Pi_k = \frac{I_k}{I_X}$$

where  $I_k$  is the information available at stage  $k$  and  $I_X$  is the maximum information, the information available at the end of the trial if the trial does not stop early.

### Boundary Values in Standardized $Z$ Scale

With the unified family method, the boundary values for the upper  $\alpha$  boundary  $Z_{\alpha u}$ , upper  $\beta$  boundary  $Z_{\beta u}$ , lower  $\beta$  boundary  $Z_{\beta l}$ , and lower  $\alpha$  boundary  $Z_{\alpha l}$ , using the standardized normal scale, are given by the following:

- $Z_{\alpha u}(\Pi_k) = f_{\alpha u}(\Pi_k) C_{\alpha u}$
- $Z_{\beta u}(\Pi_k) = \theta_{1u} I_k^{\frac{1}{2}} - f_{\beta u}(\Pi_k) C_{\beta u}$
- $Z_{\beta l}(\Pi_k) = \theta_{1l} I_k^{\frac{1}{2}} + f_{\beta l}(\Pi_k) C_{\beta l}$
- $Z_{\alpha l}(\Pi_k) = -f_{\alpha l}(\Pi_k) C_{\alpha l}$

where  $\theta_{1l} (< 0)$  and  $\theta_{1u} (> 0)$  are the lower and upper alternative references,  $f_{\alpha l}(\Pi_k)$ ,  $f_{\beta l}(\Pi_k)$ ,  $f_{\beta u}(\Pi_k)$ , and  $f_{\alpha u}(\Pi_k)$  are the specified shape functions, and  $C_{\alpha l}$ ,  $C_{\beta l}$ ,  $C_{\beta u}$ , and  $C_{\alpha u}$  are the critical values derived to achieve the specified  $\alpha$  and  $\beta$  levels.

If a derived lower  $\beta$  boundary value  $Z_{\beta l}(\Pi_k)$  is greater than its corresponding upper  $\beta$  boundary value  $Z_{\beta u}(\Pi_k)$ , then both values are set to missing.

Note that the drift parameters  $d_l = \theta_{1l} \sqrt{I_X}$  and  $d_u = \theta_{1u} \sqrt{I_X}$  are derived in the SEQDESIGN procedure. The boundary values in standardized  $Z$  scale can be derived without specifying the maximum information and alternative reference.

## Shape Parameters

The shape function in the SEQDESIGN procedure is given by

$$f(\Pi_k) = f(\Pi_k; \tau, \rho) = \tau \Pi_k^{\frac{1}{2}} + \Pi_k^{-\rho} = \Pi_k^{\frac{1}{2}} (\tau + \Pi_k^{-(\rho+\frac{1}{2})})$$

where the parameters  $\rho \geq 0$  and  $0 \leq \tau \leq 2\rho$  can be specified for each boundary separately.

The parameters  $\tau$  and  $\rho$  determine the shape of the boundaries. Special cases of the unified family methods also include power family methods and triangular methods. Table 83.6 summarizes the corresponding parameter values in the unified family for these methods.

**Table 83.6** Parameters in the Unified Family for Various Methods

| Method          | Option             | Unified Family |        |
|-----------------|--------------------|----------------|--------|
|                 |                    | Rho            | Tau    |
| Pocock          | POC                | 0              | 0      |
| O'Brien-Fleming | OFB                | 0.5            | 0      |
| Power family    | POW (RHO= $\rho$ ) | $\rho$         | 0      |
| Triangular      | TRI (TAU= $\tau$ ) | 0.5            | $\tau$ |

Note that the power parameter  $\rho = 1/2 - \Delta = \rho^* - 1/2$ , where  $\Delta$  is the power parameter used in Jennison and Turnbull (2000) and Wang and Tsiatis (1987) and  $\rho^*$  is the power parameter used in Kittelson and Emerson (1999).

Also note that instead of the three parameters used in the unified family methods by Kittelson and Emerson (1999), only two parameters are used in the SEQDESIGN procedure. The other parameter is fixed at zero.

## Boundary Values in MLE Scale

If the maximum information is available, the boundary values derived from a unified family method can also be displayed in the MLE scale:

- $\theta_{\alpha u}(\Pi_k) = I_k^{-\frac{1}{2}} f_{\alpha u}(\Pi_k) C_{\alpha u}$
- $\theta_{\beta u}(\Pi_k) = \theta_{1u} - I_k^{-\frac{1}{2}} f_{\beta u}(\Pi_k) C_{\beta u}$
- $\theta_{\beta l}(\Pi_k) = \theta_{1l} + I_k^{-\frac{1}{2}} f_{\beta l}(\Pi_k) C_{\beta l}$
- $\theta_{\alpha l}(\Pi_k) = -I_k^{-\frac{1}{2}} f_{\alpha l}(\Pi_k) C_{\alpha l}$

These MLE scale boundary values are computed by multiplying  $I_k^{-\frac{1}{2}}$  by the standardized  $Z$  scale boundary values at stage  $k$ .

### Boundary Values in Score Scale

If the maximum information is available, the boundary values derived from a unified family method can also be displayed in the score scale:

- $S_{\alpha u}(\Pi_k) = I_k^{\frac{1}{2}} f_{\alpha u}(\Pi_k) C_{\alpha u}$
- $S_{\beta u}(\Pi_k) = \theta_{1u} I_k - I_k^{\frac{1}{2}} f_{\beta u}(\Pi_k) C_{\beta u}$
- $S_{\beta l}(\Pi_k) = \theta_{1l} I_k + I_k^{\frac{1}{2}} f_{\beta l}(\Pi_k) C_{\beta l}$
- $S_{\alpha l}(\Pi_k) = -I_k^{\frac{1}{2}} f_{\alpha l}(\Pi_k) C_{\alpha l}$

These MLE scale boundary values are computed by multiplying  $I_k^{\frac{1}{2}}$  by the standardized  $Z$  scale boundary values at stage  $k$ .

### Boundary Values in $p$ -Value Scale

For a design with a lower alternative or a two-sided alternative, the  $p$ -value scale boundary values are the cumulative normal distribution function values of the standardized  $Z$  boundary values:

- $P_{\alpha u}(\Pi_k) = \Phi(Z_{\alpha u}(\Pi_k))$
- $P_{\beta u}(\Pi_k) = \Phi(Z_{\beta u}(\Pi_k))$
- $P_{\beta l}(\Pi_k) = \Phi(Z_{\beta l}(\Pi_k))$
- $P_{\alpha l}(\Pi_k) = \Phi(Z_{\alpha l}(\Pi_k))$

These nominal  $p$ -values are the one-sided fixed-sample  $p$ -values under the null hypothesis with a lower alternative.

For a one-sided design with an upper alternative, the  $p$ -value scale boundary values are the one-sided fixed-sample  $p$ -values under the null hypothesis with an upper alternative:

- $P_{\alpha u}(\Pi_k) = 1 - \Phi(Z_{\alpha u}(\Pi_k))$
- $P_{\beta u}(\Pi_k) = 1 - \Phi(Z_{\beta u}(\Pi_k))$

### Pocock's Method

The shape function for Pocock's method (Pocock 1977) is given by

$$f(\Pi_k) = 1$$

The resulting boundary values for a two-sided design with an early stopping to reject the null hypothesis  $H_0 : \theta = 0$  are as follows:

- $Z_{\alpha u}(\Pi_k) = C_{\alpha u}$
- $Z_{\alpha l}(\Pi_k) = -C_{\alpha l}$

That is, the rejection boundary values are constant over all stages of different information levels in the standardized  $Z$  scale.

Note that compared with other designs, Pocock's design tends to stop the trials early with a larger  $p$ -value. For a new treatment, Pocock's design to stop a trial early with a large  $p$ -value might not be persuasive enough to make a new treatment widely accepted (Pocock and White 1999). A Pocock design is illustrated in Example 83.3.

### O'Brien-Fleming Method

The shape function for the O'Brien-Fleming method (O'Brien and Fleming 1979) is given by

$$f(\Pi_k) = \Pi_k^{-\frac{1}{2}}$$

The resulting boundary values for a two-sided design with early stopping to reject the null hypothesis  $H_0 : \theta = 0$  are as follows:

- $Z_{\alpha u}(\Pi_k) = \Pi_k^{-\frac{1}{2}} C_{\alpha u}$
- $Z_{\alpha l}(\Pi_k) = -\Pi_k^{-\frac{1}{2}} C_{\alpha l}$

That is, the rejection boundaries are inversely proportional to the square root of the information levels in the standardized  $Z$  scale.

In the score scale, these boundaries can be displayed as follows:

- $S_{\alpha u}(\Pi_k) = C_{\alpha u} I_X^{\frac{1}{2}}$
- $S_{\alpha l}(\Pi_k) = -C_{\alpha l} I_X^{\frac{1}{2}}$

which are constants over all stages in the score scale. An O'Brien-Fleming design is illustrated in Example 83.2.

### Power Family Method

The shape function for a power family method (Wang and Tsatis 1987; Emerson and Fleming 1989; Pampallona and Tsatis 1994) is given by

$$f(\Pi_k) = \Pi_k^{-\rho}$$

The resulting boundary values for a two-sided design with early stopping to reject the null hypothesis  $H_0 : \theta = 0$  are as follows:

- $Z_{\alpha u}(\Pi_k) = \Pi_k^{-\rho} C_{\alpha u}$
- $Z_{\alpha l}(\Pi_k) = -\Pi_k^{-\rho} C_{\alpha l}$

The rejection boundaries depend on the power parameter  $\rho$ . The power family includes the Pocock and O'Brien-Fleming methods, and the power parameter is used to allow continuous movement between these two methods.

### Triangular Method

The shape function for a triangular method (Kittelson and Emerson 1999) in the unified family is given by

$$f(\Pi_k) = \Pi_k^{-\frac{1}{2}} + \tau \Pi_k^{\frac{1}{2}}$$

The resulting boundary values for a two-sided design with early stopping to reject the null hypothesis  $H_0 : \theta = 0$  are as follows:

- $Z_{\alpha u}(\Pi_k) = (\Pi_k^{-\frac{1}{2}} + \tau \Pi_k^{\frac{1}{2}}) C_{\alpha u} = C_{\alpha u} \Pi_k^{-\frac{1}{2}} (1 + \tau \Pi_k)$
- $Z_{\alpha l}(\Pi_k) = -(\Pi_k^{-\frac{1}{2}} + \tau \Pi_k^{\frac{1}{2}}) C_{\alpha l} = -C_{\alpha l} \Pi_k^{-\frac{1}{2}} (1 + \tau \Pi_k)$

In the score scale, these boundaries are as follows:

- $S_{\alpha u}(\Pi_k) = C_{\alpha u} I_X^{\frac{1}{2}} (1 + \tau \Pi_k) = C_{\alpha u} I_X^{\frac{1}{2}} + C_{\alpha u} \tau I_X^{-\frac{1}{2}} I_k$
- $S_{\alpha l}(\Pi_k) = -C_{\alpha l} I_X^{\frac{1}{2}} (1 + \tau \Pi_k) = -C_{\alpha l} I_X^{\frac{1}{2}} - C_{\alpha l} \tau I_X^{-\frac{1}{2}} I_k$

Thus, in the score scale, the boundary function is a linear function of the information  $I_k$ . With these straight-line boundaries, a triangular method for a one-sided trial with early stopping to reject or accept the null hypothesis produces a triangular continuation region. Similarly, for a two-sided design, the continuation region is a union of two separate triangular regions. A triangular method is illustrated in [Example 83.6](#).

---

### Haybittle-Peto Method

The Haybittle-Peto method (Haybittle 1971; Peto et al. 1976) uses a value of 3 for the critical values in interim stages, so that the critical value at the final stage is close to the original design without interim monitoring.

In the SEQDESIGN procedure, the Haybittle-Peto method has been generalized to allow for different boundary values at different stages. That is, with the standardized normal scale, the boundary values are given by the following:

- $Z_{\alpha u}(\Pi_k) = z_{\alpha u k}$
- $Z_{\beta u}(\Pi_k) = \theta_{1u} I_k^{\frac{1}{2}} - z_{\beta u k}$



- $Z_{\beta l}(\Pi_k) = \theta_{1l} I_k^{\frac{1}{2}} + z_{\beta lk}$
- $Z_{\alpha l}(\Pi_k) = -z_{\alpha lk}$

where  $\theta_{1l}$  and  $\theta_{1u}$  are the lower and upper alternative references and the boundary values  $z_{\alpha uk}$ ,  $z_{\beta uk}$ ,  $z_{\beta lk}$ , and  $z_{\alpha lk}$  are specified either explicitly with the HP( *Z= numbers*) option or implicitly with the HP( *PVALUE= numbers*) option. The HP( *PVALUE= numbers*) option specifies the nominal  $p$ -values  $p_k$  for the corresponding boundary values  $z_k$ :

$$z_k = \Phi^{-1}(1 - p_k)$$

The Haybittle-Peto method is illustrated in [Example 83.5](#).

## Whitehead Methods

The Whitehead methods (Whitehead and Stratton 1983; Whitehead 1997, 2001) derive boundary values by adjusting the boundary values generated from continuous monitoring. With continuous monitoring, the boundary values are on a straight line in the score scale for each boundary. For a group sequential design, the boundary values at an interim stage  $k$  depend on the information fractions

$$\Pi_k = \frac{I_k}{I_X}$$

where  $I_k$  is the information available at stage  $k$  and  $I_X$  is the maximum information, the information available at the end of the trial if the trial does not stop early.

## One-Sided Symmetric Designs

A one-sided symmetric design is a one-sided design with identical Type I and Type II error probabilities. For a one-sided symmetric design with an upper alternative,  $\alpha_u = \beta_u$ , the boundary values in the score scale from continuous monitoring are as follows:

- $S_{\alpha u}(\Pi_k) = C_u \theta_u^{-1} + \tau_u \theta_u I_k$
- $S_{\beta u}(\Pi_k) = \theta_u I_k - (C_u \theta_u^{-1} - \tau_u \theta_u I_k)$

where  $\theta_u$  is the upper alternative reference,  $\tau_u$  is a specified constant for the slope,  $0 \leq \tau_u < \frac{1}{2}$ , and  $C_u$  is a constant, fixed for STOP=BOTH and derived for STOP=ACCEPT and STOP=REJECT.

The upper  $\beta$  boundary value can also be expressed as

- $S_{\beta u}(\Pi_k) = -C_u \theta_u^{-1} + (1 - \tau_u) \theta_u I_k$

Thus, these straight-line boundaries form a triangle in the score statistic scale.

To adjust for the nature of discrete monitoring, the group sequential boundary values are given by the following:

- $S_{\alpha u}(\Pi_k) = C_u \theta_u^{-1} + \tau_u \theta_u I_k - g_k$
- $S_{\beta u}(\Pi_k) = -C_u \theta_u^{-1} + (1 - \tau_u) \theta_u I_k + g_k$

where  $g_1 = 0.583\sqrt{I_1}$  and  $g_k = 0.583\sqrt{I_k - I_{(k-1)}}$ ,  $k > 1$  are the adjustments.

Note that with the adjustment  $g_k$ , the resulting boundaries form a Christmas tree shape within the original triangle and are referred to as the Christmas tree boundaries (Whitehead 1997, p. 73).

### One-Sided Asymmetric Designs

For a one-sided asymmetric design with an upper alternative,  $\alpha_u \neq \beta_u$ , the boundary values computed using the score scale, are given by the following:

- $S_{\alpha u}(\Pi_k) = C_u \tilde{\theta}_u^{-1} + \tau_u \tilde{\theta}_u I_k - g_k$
- $S_{\beta u}(\Pi_k) = -C_u \tilde{\theta}_u^{-1} + (1 - \tau_u) \tilde{\theta}_u I_k + g_k$

where  $\tilde{\theta}_u$  is the modified alternative reference

$$\tilde{\theta}_u = \frac{2\Phi^{-1}(1 - \alpha_u)}{\Phi^{-1}(1 - \alpha_u) + \Phi^{-1}(1 - \beta_u)} \theta_u$$

The modified alternative reference  $\tilde{\theta}_u = \theta_u$  if  $\alpha_u = \beta_u$ .

For a design with early stopping to reject or accept the null hypothesis,  $S_{\alpha u}(1) = S_{\beta u}(1)$ , the boundary values at the final stage are equal. The modified drift parameter  $\tilde{d}_u$  is given by

$$\tilde{d}_u = \tilde{\theta}_u \sqrt{I_X} = \frac{1}{1 - 2\tau_u} \left( \sqrt{h_K^2 + 2C_u(1 - 2\tau_u)} - h_K \right)$$

where  $h_K = g_K I_X^{-\frac{1}{2}} = 0.583\sqrt{1 - \Pi_{(K-1)}}$ .

A one-sided Whitehead design with early stopping to reject or accept the null hypothesis is illustrated in Example 83.7.

### Two-Sided Designs

The boundary values for a two-sided design are generated by combining boundary values from two one-sided designs. With the STOP=BOTH option, this produces a double triangular design (Whitehead 1997, p. 98).

The boundary values for a two-sided design, using the score scale, are then given by the following:

- $S_{\alpha u}(\Pi_k) = C_u \tilde{\theta}_u^{-1} + \tau_u \tilde{\theta}_u I_k - g_k$
- $S_{\beta u}(\Pi_k) = -C_u \tilde{\theta}_u^{-1} + (1 - \tau_u) \tilde{\theta}_u I_k + g_k$
- $S_{\beta l}(\Pi_k) = -C_l \tilde{\theta}_l^{-1} + (1 - \tau_l) \tilde{\theta}_l I_k - g_k$
- $S_{\alpha l}(\Pi_k) = C_l \tilde{\theta}_l^{-1} + \tau_l \tilde{\theta}_l I_k + g_k$

where the modified alternative references are

$$\tilde{\theta}_u = \frac{2\Phi^{-1}(1 - \alpha_u)}{\Phi^{-1}(1 - \alpha_u) + \Phi^{-1}(1 - \beta_u)} \theta_u$$

$$\tilde{\theta}_l = \frac{2\Phi^{-1}(1 - \alpha_l)}{\Phi^{-1}(1 - \alpha_l) + \Phi^{-1}(1 - \beta_l)} \theta_l$$

The modified alternative reference  $\tilde{\theta}_u = \theta_u$  if  $\alpha_u = \beta_u$  and  $\tilde{\theta}_l = \theta_l$  if  $\alpha_l = \beta_l$ .

For a design with early stopping to reject or accept the null hypothesis, the two upper boundary values at the final stage are identical and the two lower boundary values at the final stage are identical. That is,  $S_{\alpha l}(1) = S_{\beta l}(1)$  and  $S_{\alpha u}(1) = S_{\beta u}(1)$ . These modified drift parameters are then given by

$$\tilde{d}_l = \tilde{\theta}_l \sqrt{I_X} = \frac{1}{1 - 2\tau_l} \left( \sqrt{h_K^2 + 2C_l(1 - 2\tau_l)} - h_K \right)$$

$$\tilde{d}_u = \tilde{\theta}_u \sqrt{I_X} = \frac{1}{1 - 2\tau_u} \left( \sqrt{h_K^2 + 2C_u(1 - 2\tau_u)} - h_K \right)$$

where  $h_K = g_K I_X^{-\frac{1}{2}} = 0.583 \sqrt{1 - \Pi_{(K-1)}}$ .

For a design with early stopping to reject the null hypothesis, or a design with early stopping to accept the null hypothesis, you can specify the slope parameters  $\tau_u$  and  $\tau_l$  in the TAU= option, and then the intercept parameters  $C_u$  and  $C_l$ , and the resulting boundary values are derived. If both the maximum information and alternative references are specified, the procedure derives  $C_u$  and  $C_l$  by maintaining either the overall  $\alpha$  levels (BOUNDARYKEY=ALPHA) or the overall  $\beta$  levels (BOUNDARYKEY=BETA). If the maximum information and alternative reference are not both specified, the procedure derives the boundary values  $C_u$  and  $C_l$  by maintaining both the overall  $\alpha$  and overall  $\beta$  levels.

For a design with early stopping to reject or accept the null hypothesis (STOP=BOTH), Whitehead's triangular test uses  $\tau_u = \tau_l = 0.25$  and compute  $C_u = -2 \log(2\alpha_u)$  and  $C_l = -2 \log(2\alpha_l)$  for the boundary values. If the maximum information and alternative reference are both specified, the BOUNDARYKEY=ALPHA option uses the specified  $\alpha$  values to compute the  $\beta$  values and boundary values. The final-stage boundary values are modified to maintain the overall  $\alpha$  levels if they exist. Similarly, the BOUNDARYKEY=BETA option uses the specified  $\beta$  values to compute the  $\alpha$  values and boundary values. The final-stage boundary values are modified to maintain the overall  $\beta$  levels if they exist.

If the maximum information and alternative reference are not both specified, the specified  $\alpha$  and  $\beta$  values are used to derive boundary values. The BOUNDARYKEY=NONE option uses these boundary values without adjustment. The BOUNDARYKEY=ALPHA option modifies the final-stage boundary values to maintain the overall  $\alpha$  levels if they exist. Similarly, the BOUNDARYKEY=BETA option modifies the final-stage boundary values to maintain the overall  $\beta$  levels if they exist.

## Applicable Boundary Keys

Table 83.7 lists applicable boundary keys for a design that uses Whitehead methods.

**Table 83.7** Applicable Boundary Keys for Whitehead Methods

| Early Stopping      | Specified Parameters |      | Boundary Keys |      |      |      |
|---------------------|----------------------|------|---------------|------|------|------|
|                     | (Alt Ref – Max Info) | Tau  | Alpha         | Beta | None | Both |
| Reject $H_0$        | X                    | X    | X             | X    |      |      |
| Accept $H_0$        | X                    | X    | X             | X    |      |      |
| Reject/Accept $H_0$ | X                    | 0.25 | X             | X    |      |      |
| Reject $H_0$        |                      | X    |               |      |      | X    |
| Accept $H_0$        |                      | X    |               |      |      | X    |
| Reject/Accept $H_0$ |                      | 0.25 | X             | X    | X    |      |

Note that the symbol “X” under “(Alt Ref – Max Info)” indicates that both alternative reference and maximum information are specified.

For a design with early stopping to reject the null hypothesis, or a design with early stopping to accept the null hypothesis, you can specify the slope parameter  $\tau_u$  in the TAU= option, and then the intercept parameter  $C_u$  and the resulting boundary values are derived. If both the maximum information and alternative reference are specified, the procedure derives  $C_u$  by maintaining either the overall  $\alpha$  levels (BOUNDARYKEY=ALPHA) or the overall  $\beta$  levels (BOUNDARYKEY=BETA). If the maximum information and alternative reference are not both specified, the procedure derives the boundary values and  $C_u$  by maintaining both the overall  $\alpha$  and overall  $\beta$  levels.

For a design with early stopping to reject or accept the null hypothesis (STOP=BOTH), Whitehead’s triangular test uses  $\tau_u = 0.25$  and solves  $C_u = 2 \log\left(\frac{1}{2\alpha_u}\right)$  for the boundary values. If the maximum information and alternative reference are both specified, the BOUNDARYKEY=ALPHA option uses the specified  $\alpha$  value to compute the  $\beta$  value and boundary values. The final-stage boundary value is modified to maintain the overall  $\alpha$  level if it exists. Similarly, the BOUNDARYKEY=BETA option uses the specified  $\beta$  value to compute the  $\alpha$  value and boundary values. The final-stage boundary value is modified to maintain the overall  $\beta$  level if it exists.

If the maximum information and alternative reference are not both specified, the specified  $\alpha$  and  $\beta$  values are used to derive boundary values. The BOUNDARYKEY=NONE option uses these boundary values without adjustment. The BOUNDARYKEY=ALPHA option modifies the final-stage boundary value to maintain the overall  $\alpha$  level if it exists. Similarly, the BOUNDARYKEY=BETA option modifies the final-stage boundary value to maintain the overall  $\beta$  level if it exists.

## Error Spending Methods

For each sequential design, the  $\alpha$  and  $\beta$  errors spent at each stage can be computed from the boundary values. For example, for a  $K$ -stage design with an upper alternative hypothesis  $H_1 : \theta = \theta_1$  and early stopping to reject the null hypothesis  $H_0 : \theta = 0$ , the boundary values in a standardized  $Z$  scale are the upper  $\alpha$  critical values  $a_k, k = 1, 2, \dots, K$ . At each interim stage, the null hypothesis  $H_0$  is rejected if the observed standardized  $Z$  statistic  $z_k \geq a_k$ . Otherwise, the process continues to the next stage. At the final stage, the hypothesis is rejected if  $z_K \geq a_K$ . Otherwise, the null hypothesis is accepted.

The boundary values  $a_k$  are derived such that the overall Type I error probability

$$\alpha = \sum_{k=1}^K \alpha_k$$

where  $\alpha_k$  is the  $\alpha$  spending at stage  $k$ . That is, at stage 1,

$$\alpha_1 = P_{\theta=0}(z_1 \geq a_1)$$

At a subsequent stage  $k$ ,

$$\alpha_k = P_{\theta=0}(z_j < a_j, j = 1, 2, \dots, k-1, z_k \geq a_k)$$

Since each design can be uniquely identified by the  $\alpha$  and  $\beta$  errors spent at each stage, a design can then be derived by specifying the  $\alpha$  and  $\beta$  errors to be used at each stage. The error spending method (Lan and DeMets 1983) distributes the error to be used at each stage and then derives the boundary values. Numerous forms of the error spending function are available. Kim and DeMets (1987) examine the functions  $f(t) = t$ ,  $f(t) = t^{\frac{3}{2}}$ , and  $f(t) = t^2$ , where  $t$  is the information fraction. Jennison and Turnbull (2000, p. 148) generalize these functions to the power functions  $f(t; \rho) = t^\rho, \rho > 0$ .

The ERRFUNCPOC option uses the cumulative error spending function (Lan and DeMets 1983)

$$E(t) = \begin{cases} 1 & \text{if } t \geq 1 \\ \log(1 + (e-1)t) & \text{if } 0 < t < 1 \\ 0 & \text{otherwise} \end{cases}$$

With a specified error of  $\alpha$  or  $\beta$ , the cumulative error spending at stage  $k$  is  $\alpha E(\Pi_k)$  or  $\beta E(\Pi_k)$ , where  $\Pi_k = I_k/I_X$  is the information fraction at stage  $k$ . The method produces boundaries similar to those produced with Pocock's method.

The ERRFUNCOBF option uses the cumulative error spending function (Lan and DeMets 1983)

$$E(t; a) = \begin{cases} 1 & \text{if } t \geq 1 \\ \frac{1}{a} 2(1 - \Phi(\frac{z(1-a/2)}{\sqrt{t}})) & \text{if } 0 < t < 1 \\ 0 & \text{otherwise} \end{cases}$$

where  $a$  is either  $\alpha$  for the  $\alpha$  spending function or  $\beta$  for the  $\beta$  spending function. That is, with a specified error of  $\alpha$  or  $\beta$ , the cumulative error spending at stage  $k$  is  $\alpha E(\Pi_k; \alpha)$  or  $\beta E(\Pi_k; \beta)$ . The method produces boundaries similar to those produced with the O'Brien-Fleming method.

The ERRFUNCGAMMA option uses the gamma cumulative error spending function (Hwang, Shih, and DeCani 1990)

$$E(t; \gamma) = \begin{cases} 1 & \text{if } t \geq 1 \\ \frac{1-e^{-\gamma t}}{1-e^{-\gamma}} & \text{if } 0 < t < 1, \gamma \neq 0 \\ t & \text{if } 0 < t < 1, \gamma = 0 \\ 0 & \text{otherwise} \end{cases}$$

where  $\gamma$  is the parameter  $\gamma$  specified in the GAMMA= option. That is, with a specified error of  $\alpha$  or  $\beta$ , the cumulative error spending at stage  $k$  is  $\alpha E(\Pi_k; \gamma)$  or  $\beta E(\Pi_k; \gamma)$ .

The ERRFUNCPOW option uses the cumulative error spending function (Jennison and Turnbull 2000, p. 148)

$$E(t; \rho) = \begin{cases} 1 & \text{if } t \geq 1 \\ t^\rho & \text{if } 0 < t < 1 \\ 0 & \text{otherwise} \end{cases}$$

where  $\rho$  is the power parameter specified in the RHO= option. That is, with a specified error of  $\alpha$  or  $\beta$ , the cumulative error spending at stage  $k$  is  $\alpha E(\Pi_k; \rho)$  or  $\beta E(\Pi_k; \rho)$ .

Error spending methods derive boundary values at each stage sequentially and require much more computation than other types of methods for group sequential trials with a large number of stages, especially for a two-sided asymmetric design with early stopping to accept  $H_0$ , or to reject or accept  $H_0$ .

Note that for a two-sided design with the STOP=BOTH or STOP=ACCEPT option, at each interim stage, the SEQDESIGN procedure first produces the lower and upper  $\beta$  boundary values based on the one-sided  $\beta$  spending. If the lower  $\beta$  boundary value is greater than or equal to its corresponding upper  $\beta$  boundary value, there is no early stopping to accept the null hypothesis at this stage, and the corresponding  $\beta$  spending is distributed proportionally to the remaining stages.

For the error spending functions not available in the SEQDESIGN procedure, you can first compute the corresponding error spending at each stage explicitly, then use the SEQDESIGN procedure with the ERRSPEND= option to specify these errors directly.

For example, if the information levels are equally spaced in a five-stage design, the option ERRFUNCPOW (RHO=2) produces relative cumulative errors of  $(1/5)^2$ ,  $(2/5)^2$ ,  $(3/5)^2$ ,  $(4/5)^2$ , and 1. This is equivalent to using the option ERRSPEND (1 4 9 16 25).

A one-sided error spending design is illustrated in [Example 83.8](#) and a two-sided asymmetric error spending design is illustrated in [Example 83.11](#).

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## Acceptance ( $\beta$ ) Boundary

In a group sequential trial, the rejection boundary is derived under the null hypothesis  $H_0$  and is used to stop the trial early to reject  $H_0$ . Similarly, the acceptance boundary is derived under the alternative hypothesis and is used to stop the trial early to accept  $H_0$ . But, for a trial with early stopping either to reject or to accept the null hypothesis, dependency exists between these two boundaries. This section describes the effects of the acceptance boundary on the derivation of the rejection boundary in a group sequential trial.

The following statements create a one-sided four-stage group sequential design with early stopping either to reject or to accept  $H_0$ :

```
ods graphics on;
proc seqdesign altref=10;
 ErrSpendPower_2: design nstages=4
 method=errfuncpow(rho=2)
 alt=upper stop=both
 alpha=0.025 beta=0.10;
run;
ods graphics off;
```

The ALTREF=10 option specifies the alternative reference 10. The METHOD=ERRFUNCPOW(RHO=2) option uses a  $\rho = 2$  power family error spending method to generate the rejection boundary. The ALPHA=0.025 and BETA=0.10 options specify the Type I error level 0.025 and Type II error level 0.10, respectively.

The power parameter  $\rho = 2$  used in the design lies between  $\rho = 1$  and  $\rho = 3$ , where the boundaries created with the  $\rho = 1$  power family error spending method are similar to the boundaries created from the Pocock method, and the boundaries created with  $\rho = 3$  are similar to the boundaries created from the O'Brien-Fleming method.

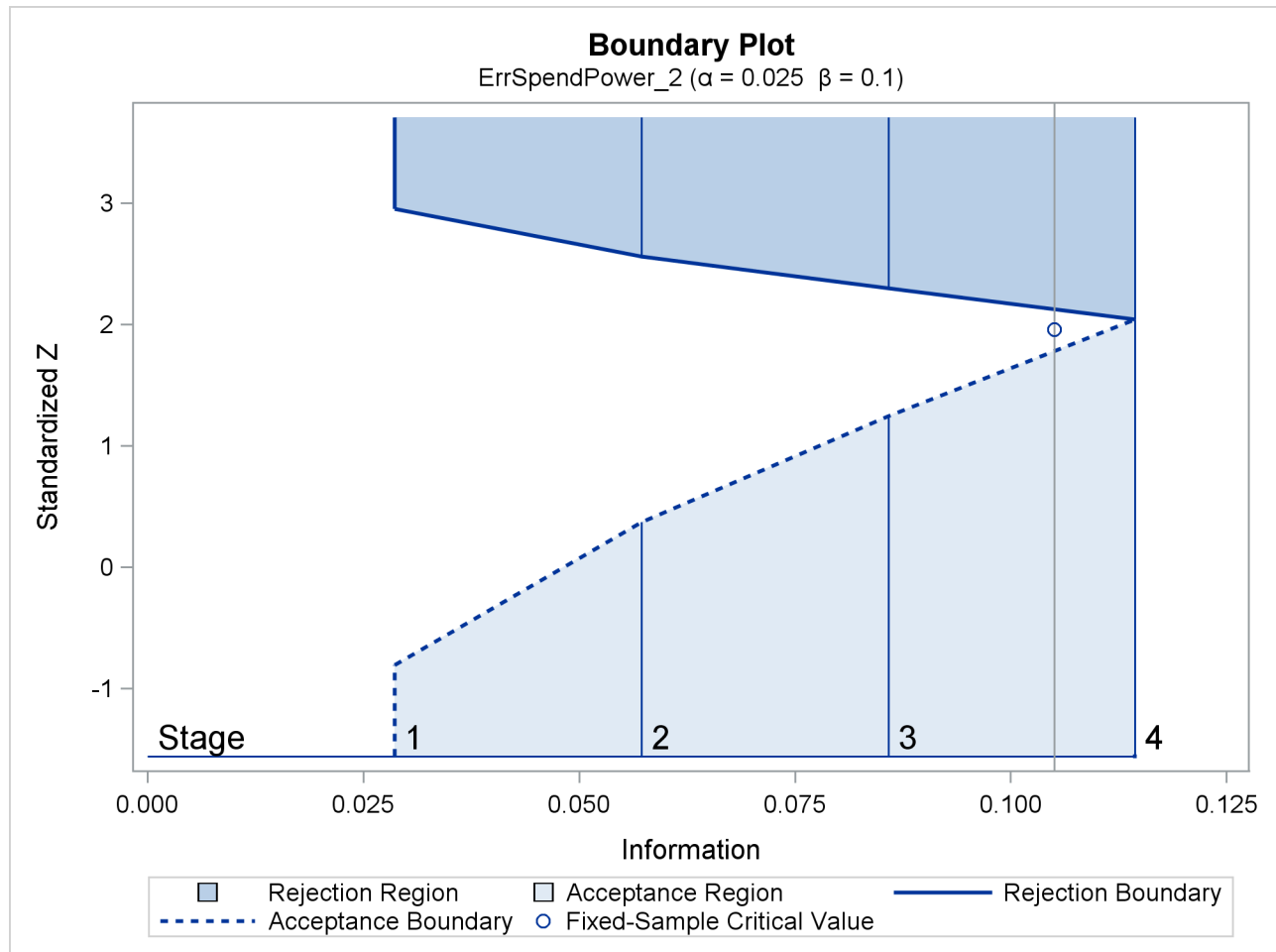
The “Boundary Information” table in Figure 83.12 shows the rejection and acceptance boundary values at the stages. With an error spending function method, the boundary values are derived sequentially. In particular, the rejection boundary value at a stage is derived conditionally on both rejection and acceptance boundary values at the previous stage. See the section “Error Spending Methods” on page 7034 for a detailed description of the error spending methods.

**Figure 83.12** Boundary Information

| The SEQDESIGN Procedure                     |                         |          |                        |                           |         |
|---------------------------------------------|-------------------------|----------|------------------------|---------------------------|---------|
| Design: ErrSpendPower_2                     |                         |          |                        |                           |         |
| Boundary Information (Standardized Z Scale) |                         |          |                        |                           |         |
| Null Reference = 0                          |                         |          |                        |                           |         |
| _Stage_                                     | ---Information Level--- |          | -Alternative-          | -----Boundary Values----- |         |
|                                             | Proportion              | Actual   | --Reference--<br>Upper | Beta                      | Alpha   |
| 1                                           | 0.2500                  | 0.028605 | 1.69130                | -0.80640                  | 2.95517 |
| 2                                           | 0.5000                  | 0.05721  | 2.39186                | 0.37356                   | 2.55934 |
| 3                                           | 0.7500                  | 0.085815 | 2.92942                | 1.24940                   | 2.29904 |
| 4                                           | 1.0000                  | 0.11442  | 3.38261                | 2.04182                   | 2.04182 |

With ODS Graphics enabled, the “Boundary Plot” is displayed by default, as shown in Figure 83.13. The continuation region is affected by the acceptance boundary, and the rejection boundary is thus adjusted for this acceptance boundary to maintain the Type I error level.

Figure 83.13 Boundary Plot



For a design with early stopping either to accept or to reject  $H_0$ , the shapes of boundaries affect the critical value at the final stage. For the acceptance boundary, a liberal method at early stages, such as a  $\rho = 1$  power family error spending method, lowers the critical value at the final stage. For the rejection boundary, a conservative method at early stages, such as a  $\rho = 3$  power family error spending method, also lowers the critical value at the final stage. In addition, a larger Type II error level also lowers the critical value at the final stage. The resulting critical value at the final stage might even be less than the critical value for the corresponding fixed-sample design.

To illustrate how this can occur, the following statements use a  $\rho = 1$  power family error spending method for the acceptance boundary and a  $\rho = 3$  power family error spending method for the rejection boundary to create a group sequential design:

```
proc seqdesign altref=10;
 ErrSpendPower_3_1: design nstages=4
 method(alpha)=errfuncpow(rho=3)
 method(beta)= errfuncpow(rho=1)
 alt=upper stop=both
 alpha=0.025 beta=0.10;
run;
```



The resulting “Boundary Information” table in Figure 83.14 shows that the boundary value at the final stage 1.9267 is less than 1.96, the critical value of the corresponding fixed-sample design.

**Figure 83.14** Boundary Information

| The SEQDESIGN Procedure                     |                         |          |                        |                           |         |
|---------------------------------------------|-------------------------|----------|------------------------|---------------------------|---------|
| Design: ErrSpendPower_3_1                   |                         |          |                        |                           |         |
| Boundary Information (Standardized Z Scale) |                         |          |                        |                           |         |
| Null Reference = 0                          |                         |          |                        |                           |         |
| _Stage_                                     | ---Information Level--- |          | -Alternative-          | -----Boundary Values----- |         |
|                                             | Proportion              | Actual   | --Reference--<br>Upper | -----Upper-----<br>Beta   | Alpha   |
| 1                                           | 0.2500                  | 0.029725 | 1.72410                | -0.23587                  | 3.35935 |
| 2                                           | 0.5000                  | 0.05945  | 2.43824                | 0.63117                   | 2.76024 |
| 3                                           | 0.7500                  | 0.089175 | 2.98622                | 1.31554                   | 2.35119 |
| 4                                           | 1.0000                  | 0.1189   | 3.44819                | 1.92672                   | 1.92672 |

That is,  $H_0$  can be rejected even if the test statistic at the final stage is less than the critical value for the corresponding fixed-sample design, which is not desirable. Therefore, for a design with an acceptance boundary, the design should be used with care.

Another reason why the rejection boundary should not be affected by the acceptance boundary is that a Data and Safety Monitoring Board (DSMB) might not strictly adhere to this acceptance boundary, and thus the Type I error level might not be maintained. Therefore, it might not be desirable for the rejection boundary to be affected by the acceptance boundary (Lan and DeMets 2009, p. 103).

To use a design whose rejection boundary is not affected by the acceptance boundary and that can still stop the trial early to accept  $H_0$ , you can use one of the following strategies:

- You can use the conditional power approach for a design that stops early only to reject  $H_0$ . For this design, the conditional power at an interim stage  $k$  can be defined as the total probability of rejecting  $H_0$  at any future stages under a specified hypothetical reference, given the observed statistic at stage  $k$ . A small conditional power indicates a small probability of success (rejecting  $H_0$ ) given the current data, and the trial can be stopped early to accept  $H_0$  (Lan, Simon, and Halperin 1982; Lan and DeMets 2009, p. 101). For a detailed description of conditional power, see the section “Stochastic Curtailment” in Chapter 84, “The SEQTEST Procedure.”
- You can use a design with a nonbinding acceptance boundary (Zhu, Ni, and Yao 2011, pp. 132–133). For this design, the rejection boundary is created by ignoring the acceptance boundary. Thus, the Type I error level is maintained even when a trial is allowed to continue for a test statistic that falls in the acceptance region, and the rejection boundary values (with the standardized Z statistic scale) are identical to the boundary values that are derived in the corresponding design that stops early only to reject  $H_0$ .

## Boundary Adjustments for Overlapping Lower and Upper $\beta$ Boundaries

For the fixed boundary shape methods and Whitehead methods, the boundary values for all stages are derived simultaneously for each boundary. For a two-sided design with STOP=ACCEPT or STOP=BOTH, simultaneous derivation might result in overlapping of the lower and upper  $\beta$  boundaries. That is, at an interim stage  $k$ , the lower  $\beta$  boundary value might be greater than its corresponding upper  $\beta$  boundary value. In this case, these two  $\beta$  boundary values are set to missing and the design does not stop at stage  $k$  to accept the null hypothesis (Jennison and Turnbull 2000, p. 113).

For the error spending methods, the boundary values are derived sequentially for the stages. For a two-sided design with STOP=ACCEPT or STOP=BOTH, a small  $\beta$  spending at an interim stage might result in overlapping of the lower and upper  $\beta$  boundaries for the two corresponding one-sided tests. Specifically, this form of overlapping occurs at an interim stage  $k$  if the upper  $\beta$  boundary value derived from the one-sided test for the upper alternative is less than the lower  $\beta$  boundary value derived from the one-sided test for the lower alternative (Kittelson and Emerson 1999, pp. 881–882; Rudser and Emerson 2007, p. 6). You can use the BETAOVERLAP= option to specify how this type of overlapping is to be handled.

If BETAOVERLAP=ADJUST (which is the default) is specified, the procedure derives the boundary values for the two-sided design and then checks for overlapping of the two one-sided  $\beta$  boundaries at interim stages. If overlapping occurs at a particular stage, the  $\beta$  boundary values for the two-sided design are set to missing (so the trial does not stop to accept the null hypothesis at this stage), and the  $\beta$  spending values at subsequent stages are adjusted proportionally as follows.

If the  $\beta$  boundary values are set to missing at stage  $k$  in a  $K$ -stage trial, the adjusted  $\beta$  spending value at stage  $k$ ,  $e'_k$ , is updated for these missing  $\beta$  boundary values, and then the  $\beta$  spending values at subsequent stages are adjusted proportionally by

$$e'_j = e'_k + \frac{e_j - e_k}{e_K - e_k} (e_K - e'_k)$$

for  $j = k + 1, \dots, K$ , where  $e_j$  and  $e'_j$  are the cumulative  $\beta$  spending values at stage  $j$  before and after the adjustment, respectively.

After all these adjusted  $\beta$  spending values are computed, the boundary values are then further modified for these adjusted  $\beta$  spending values.

If you specify BETAOVERLAP=NOADJUST, no adjustment is made when overlapping of one-sided  $\beta$  boundaries occurs. The BETAOVERLAP= option is illustrated in [Example 83.10](#).

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## Specified and Derived Parameters

In the SEQDESIGN procedure, the type of alternative hypothesis (ALT= option) and the condition for early stopping (STOP= option) must be specified for each sequential design. The drift parameters are derived for each design specified. Other parameters, such as Type I error probability  $\alpha$ , Type II error probability  $\beta$ , the alternative reference  $\theta_1$ , and maximum information are either specified or derived in the SEQDESIGN procedure.

Table 83.8 summarizes the available combinations for the specified and derived parameters in the SEQDESIGN procedure.

**Table 83.8** Specified and Derived Parameters in the SEQDESIGN Procedure

| Specified Parameters |          |       |      | Derived Parameters |          |       |      |       |
|----------------------|----------|-------|------|--------------------|----------|-------|------|-------|
| Alt Ref              | Max Info | Alpha | Beta | Alt Ref            | Max Info | Alpha | Beta | Drift |
| Z                    | X        | X     |      |                    |          |       | X    | X     |
| Z                    | X        |       | X    |                    |          | X     |      | X     |
| Z                    | X        |       |      |                    |          | X     | X    | X     |
| Z                    |          | X     | X    |                    | X        |       |      | X     |
|                      | X        | X     | X    | X                  |          |       |      | X     |
|                      |          | X     | X    |                    |          |       |      | X     |

The symbol “X” indicates that the parameter is either specified or derived in the design and the symbol “Z” indicates that the alternative reference is either specified explicitly with the ALTREF= option or derived from the SAMPLESIZE statement. The drift parameter is always derived in the SEQDESIGN procedure.

For example, if the ALTREF= option is specified without the MAXINFO= option being specified, then the maximum information is derived in the SEQDESIGN procedure with the specified  $\alpha$  and  $\beta$ , as illustrated in Example 83.5.

The drift parameter is the standardized reference difference at the final stage. For a design, the drift parameter is

$$d_l = \theta_{1l} \sqrt{I_X}$$

if it has a lower alternative, and

$$d_u = \theta_{1u} \sqrt{I_X}$$

if it has an upper alternative, where  $I_X$  is the maximum information and  $\theta_{1l}$  and  $\theta_{1u}$  are the lower and upper alternative references, respectively.

If the alternative reference and the maximum information are not both specified, then the specified  $\alpha$  and  $\beta$  are used to derive the drift parameter. Then if either the alternative reference or the maximum information is specified, the other is derived from the drift parameter.

If both the alternative reference and the maximum information are specified, then either the  $\alpha$  error or the  $\beta$  error is derived in the procedure. However, for a Haybittle-Peto method with the BOUNDARYKEY=NONE option, both  $\alpha$  and  $\beta$  errors are derived from the completely specified boundary values.

For a nonsymmetric two-sided design with different lower and upper specifications (such as different lower and upper  $\alpha$  errors,  $\beta$  errors, or alternative references in absolute values), the derived lower and upper boundaries are not symmetric. If the alternative references  $\theta_{1l}$  and  $\theta_{1u}$  are not both specified, then the SEQDESIGN procedure assumes symmetric alternative references,  $\theta_1 = \theta_{1u} = -\theta_{1l}$ , for the computation of the boundary values.

## Applicable Boundary Keys

In the SEQDESIGN procedure, the BOUNDARYKEY= option in the DESIGN statement specifies the types of errors to be maintained for the design. Table 83.9 lists applicable boundary keys for designs that use unified family and Haybittle-Peto methods, designs that use error spending methods, and designs that use the Haybittle-Peto method only.

**Table 83.9** Applicable Boundary Keys for Designs without Whitehead Methods

| Method                 | Specified Parameters<br>(Alt Ref – Max Info) | Boundary Keys |      |      |      |
|------------------------|----------------------------------------------|---------------|------|------|------|
|                        |                                              | Alpha         | Beta | None | Both |
| Unified                | X                                            | X             | X    |      |      |
| Unified/Haybittle-Peto | X                                            | X             | X    |      |      |
| Error spending         | X                                            | X             | X    |      |      |
| Haybittle-Peto         | X                                            | X             | X    | X    |      |
| Unified/Haybittle-Peto |                                              |               |      |      | X    |
| Error spending         |                                              |               |      |      | X    |
| Haybittle-Peto         |                                              |               |      |      | X    |

Note that the symbol “X” under “(Alt Ref – Max Info)” indicates that both the alternative reference and maximum information are specified, and the method “Unified/Haybittle-Peto” indicates that both the unified method and the Haybittle-Peto method are used in the same design.

If the ALTREF= and MAXINFO= options are both specified, then Type I and Type II error probability levels cannot be met simultaneously if both error probabilities are specified. The BOUNDARYKEY=ALPHA option maintains the Type I error probability level  $\alpha$  and derives Type II error probability  $\beta$ . The BOUNDARYKEY=BETA option maintains the Type II error probability level  $\beta$  and derives Type I error probability  $\alpha$ .

If the Haybittle-Peto method is used for all boundaries, the BOUNDARYKEY=NONE option uses the specified  $\alpha$  boundary value (STOP=REJECT or STOP=BOTH) and the specified  $\beta$  boundary value (STOP=ACCEPT) at the final stage for the design.

If the ALTREF= and MAXINFO= options are not both specified, the BOUNDARYKEY=BOTH option derives boundary values that maintain both Type I and Type II error probability levels.

Table 83.10 lists applicable boundary keys for a design that uses Whitehead methods.

**Table 83.10** Applicable Boundary Keys for Whitehead Methods

| Early Stopping      | Specified Parameters |      | Boundary Keys |      |      |      |
|---------------------|----------------------|------|---------------|------|------|------|
|                     | (Alt Ref – Max Info) | Tau  | Alpha         | Beta | None | Both |
| Reject $H_0$        | X                    | X    | X             | X    |      |      |
| Accept $H_0$        | X                    | X    | X             | X    |      |      |
| Reject/Accept $H_0$ | X                    | 0.25 | X             | X    |      |      |
| Reject $H_0$        |                      | X    |               |      |      | X    |
| Accept $H_0$        |                      | X    |               |      |      | X    |
| Reject/Accept $H_0$ |                      | 0.25 | X             | X    | X    |      |

Note that the symbol “X” under “(Alt Ref – Max Info)” indicates that both alternative reference and maximum information are specified.

If the ALTREF= and MAXINFO= options are both specified, then Type I and Type II error probability levels cannot be achieved simultaneously if both are specified. the BOUNDARYKEY=ALPHA option maintains the Type I error probability level  $\alpha$  and derives Type II error probability  $\beta$ . The BOUNDARYKEY=BETA option maintains the Type II error probability level  $\beta$  and derives the Type I error probability  $\alpha$ .

If the ALTREF= and MAXINFO= options are not both specified, then for a design with the STOP=REJECT or STOP=ACCEPT option, the BOUNDARYKEY=BOTH option derives boundary values that maintain both Type I and Type II error probability levels. If the STOP=BOTH option is specified, Whitehead’s triangular method produces boundaries with approximate Type I and Type II error probabilities. The BOUNDARYKEY=NONE option specifies no adjustment to these boundaries. The BOUNDARYKEY=ALPHA and BOUNDARYKEY=BETA options maintain the Type I error probability level  $\alpha$  and Type II error probability level  $\beta$ , respectively, by adjusting boundary values at the final stage.

## Sample Size Computation

The SEQDESIGN procedure assumes that the data are from a multivariate normal distribution and the sequence of the standardized test statistics  $\{Z_1, Z_2, \dots, Z_K\}$  has the following canonical joint distribution:

- $(Z_1, Z_2, \dots, Z_K)$  is multivariate normal
- $Z_k \sim N(\theta\sqrt{I_k}, 1)$
- $\text{Cov}(Z_{k_1}, Z_{k_2}) = \sqrt{I_{k_1}/I_{k_2}}$ ,  $1 \leq k_1 \leq k_2 \leq K$

where  $K$  is the total number of stages and  $I_k$  is the information available at stage  $k$ .

If the test statistic is computed from the data that are not from a normal distribution, such as a binomial distribution, then it is assumed that the test statistic is computed from a large sample such that the statistic has an approximately normal distribution.

In a typical clinical trial, the sample size required depends on the Type I error probability level  $\alpha$ , alternative reference  $\theta_1$ , power  $1 - \beta$ , and variance of the response variable. Given a one-sided null hypothesis  $H_0 : \theta = 0$  with an upper alternative hypothesis  $H_1 : \theta = \theta_1$ , the information required for a fixed-sample test is given by

$$I_0 = \frac{(\Phi^{-1}(1 - \alpha) + \Phi^{-1}(1 - \beta))^2}{\theta_1^2}$$

The parameter  $\theta$  and the subsequent alternative reference  $\theta_1$  depend on the test specified in the clinical trial. For example, suppose you are comparing two binomial populations  $p_a = p_b$ ; then  $\theta = p_a - p_b$  is the difference between two proportions if the proportion difference statistic is used, and  $\theta = \log\left(\frac{p_a(1-p_b)}{p_b(1-p_a)}\right)$ , the log odds ratio for the two proportions if the log odds ratio statistic is used.

If the maximum likelihood estimate  $\hat{\theta}$  from the likelihood function can be derived, then the asymptotic variance for  $\hat{\theta}$  is  $\text{Var}(\hat{\theta}) = 1/I$ , where  $I$  is Fisher information for  $\theta$ . The resulting statistic  $\hat{\theta}$  corresponds to the MLE statistic scale as specified in the BOUNDARYSCALE=MLE option in the PROC SEQDESIGN statement,  $\hat{\theta}\sqrt{I}$  corresponds to the standardized Z scale (BOUNDARYSCALE=STDZ), and  $\hat{\theta} I$  corresponds to the score statistic scale (BOUNDARYSCALE=SCORE).

Alternatively, if the score statistic  $S$  is derived in a statistical procedure, it can be used as the test statistic and its asymptotic variance is given by Fisher information,  $I$ . In this case,  $S/\sqrt{I}$  corresponds to the standardized Z scale and  $S/I$  corresponds to the MLE statistic scale.

For a group sequential trial, the maximum information  $I_X$  is derived in the SEQDESIGN procedure with the specified  $\alpha$ ,  $\beta$ , and  $\theta_1$ . With the maximum information

$$I_X = \frac{1}{\text{Var}(\hat{\theta})}$$

the sample size required for a specified test statistic in the trial can be evaluated or estimated from the known or estimated variance of the response variable. Note that different designs might produce different maximum information levels for the same hypothesis, and this in turn might require a different number of observations for the trial.

If each observation in the data set provides one unit of information in a hypothesis testing, such as a one-sample test for the mean, the required sample size for the sequential design can be derived from the maximum information. However, for a survival analysis, an individual in the survival time data might provide only partial information because of censoring. In this case, the required number of events can be derived from the maximum information. With addition accrual information, the sample size can also be computed.

The SEQDESIGN procedure provides sample size computation for some one-sample and two-sample tests in the SAMPLESIZE statement. It also provides sample size computation for tests of a parameter in regression models such as normal regression, logistic regression, and proportional hazards regression. In addition, the procedure can also compute the required sample size or number of events from the corresponding number in the fixed-sample design.

Table 83.11 lists the options available in the SAMPLESIZE statement.

**Table 83.11** SAMPLESIZE Statement Options

| Option                     | Description                                                    |
|----------------------------|----------------------------------------------------------------|
| <b>Fixed-Sample Models</b> |                                                                |
| INPUTNOBS                  | Specifies sample size for fixed-sample design                  |
| INPUTNEVENTS               | Specifies number of events for fixed-sample design             |
| <b>One-Sample Models</b>   |                                                                |
| ONESAMPLEMEAN              | Specifies one-sample Z test for mean                           |
| ONESAMPLEFREQ              | Specifies one-sample test for binomial proportion              |
| <b>Two-Sample Models</b>   |                                                                |
| TWOSAMPLEMEAN              | Specifies two-sample Z test for mean difference                |
| TWOSAMPLEFREQ              | Specifies two-sample test for binomial proportions             |
| TWOSAMPLESURVIVAL          | Specifies log-rank test for two survival distributions         |
| <b>Regression Models</b>   |                                                                |
| REG                        | Specifies test for a regression parameter                      |
| LOGISTIC                   | Specifies test for a logistic regression parameter             |
| PHREG                      | Specifies test for a proportional hazards regression parameter |

The MODEL=INPUTNOBS and MODEL=INPUTNEVENTS options are described next, and the remaining options are described in the next three sections.

### Input Sample Size for Fixed-Sample Design

The MODEL=INPUTNOBS option derives the sample size required for a group sequential trial from the sample size  $n_0$  for the corresponding fixed-sample design. With the N=  $n_0$  option specifying the sample size  $n_0$  for a fixed-sample design, the sample size required for a group sequential trial is then computed as

$$N_X = \frac{I_X}{I_0} n_0$$

where  $I_X$  is the maximum information for the group sequential design and  $I_0$  is the information for the corresponding fixed-sample design. The information ratio between  $I_X$  and  $I_0$  is derived in the SEQDESIGN procedure.

The SAMPLE=ONE option specifies a one-sample test, and the SAMPLE=TWO option specifies a two-sample test. For a two-sample test, the WEIGHT= option specifies the sample size allocation weights for the two groups.

### Input Number of Events for Fixed-Sample Design

The MODEL=INPUTNEVENTS option derives the number of events required for a group sequential trial from the number of events  $d_0$  for the corresponding fixed-sample design. With the D=  $d_0$  option specifying the number of events  $d_0$  for a fixed-sample survival analysis, the number of events required for a group sequential trial is then computed as

$$d_X = \frac{I_X}{I_0} d_0$$

where  $I_X$  is the maximum information for the group sequential design and  $I_0$  is the information for the corresponding fixed-sample design. The information ratio between  $I_X$  and  $I_0$  is derived in the SEQDESIGN procedure.

The SAMPLE=ONE option specifies a one-sample test, and the SAMPLE=TWO option specifies a two-sample test. For a two-sample test, the WEIGHT= option specifies the sample size allocation weights for the two groups.

The ACCRUAL= option specifies the method for individual accrual. The default ACCRUAL=UNIFORM option specifies that the individual accrual is uniform in the accrual time  $T_a$  with a constant accrual rate  $r_a$ , and the ACCRUAL=EXP(PARM= $\gamma_0$ ) option specifies that the individual accrual is truncated exponential with a scaled power parameter  $\gamma_0$ , where  $\gamma_0 \geq -10$  and  $\gamma_0 \neq 0$ . With a scaled parameter  $\gamma_0$ , the power parameter for the truncated exponential with the accrual time  $T_a$  is given by  $\gamma = \gamma_0/T_a$ .

The LOSS= option specifies the individual loss to follow up in the sample size computation. The default LOSS=NONE option specifies no loss to follow up, and the EXP(POWER= $\tau$ ) option specifies exponential loss function with a power parameter  $\tau$ .

With the computed number of events  $d_X$  for a group sequential survival design, the required total sample size and sample size at each stage can be derived from specifications of hazard rates, accrual information, and losses to follow-up information. For each study group, the hazard rate  $h$  is constant (which corresponds to an exponential survival distribution) in the sample size computation.

The next four subsections describe required sample sizes for uniform accrual (with and without losses to follow up) and for truncated exponential accrual (with and without losses to follow up).

### Uniform Accrual without Losses to Follow Up

For a study group with a constant hazard rate  $h$ , if the individual accrual is uniform in the accrual time  $T_a$  with a constant accrual rate  $r_a$ , Kim and Tsatis (1990, pp. 83–84) show that the expected number of events by time  $t$  is given by

$$D_h(t) = \begin{cases} r_a \left( t - \frac{1-e^{-ht}}{h} \right) & \text{if } t \leq T_a \\ r_a \left( T_a - \frac{e^{-ht}}{h} (e^{hT_a} - 1) \right) & \text{if } t > T_a \end{cases}$$

For a one-sample design (such as a proportional hazards regression), the expected number of events by time  $t$  is  $E(t) = D_h(t)$ , where  $h$  is the hazard rate for the group. For a two-sample design (such as a log-rank test for two survival distributions), the expected number of events by time  $t$  is

$$E(t) = \frac{R}{R+1} D_{h_a}(t) + \frac{1}{R+1} D_{h_b}(t)$$

where  $h_a$  and  $h_b$  are hazard rates in groups A and B, respectively, and  $R$  is the ratio of the sample size allocation weights  $w_a/w_b$ .



If the accrual rate  $r_a$  is specified with one of the three time parameters—the accrual time, follow-up time, and total study time—then PROC SEQDESIGN derives the other two time parameters by solving the equation for the expected number of events. Similarly, if the accrual rate  $r_a$  is not specified but two of the three time parameters are specified, then PROC SEQDESIGN derives the accrual rate.

If the accrual rate  $r_a$  is specified without the accrual time  $T_a$ , follow-up time  $T_f$ , and total study time  $T = T_a + T_f$ , the minimum and maximum accrual times can be computed from the following equation, as described in Kim and Tsiatis (1990, p. 85):

$$\frac{d_X}{r_a} \leq T_a \leq E^{-1}(d_X)$$

With the accrual rate  $r_a$  and the accrual time  $T_a$ , the total sample size is

$$N_X = r_a T_a$$

At each stage  $k$ , the number of events is given by

$$d_k = \frac{I_k}{I_X} d_X$$

The corresponding time  $T_k$  can be derived from the equation for the expected number of events,  $E(t) = d_k$ , and the resulting sample size is computed as

$$N_k = \begin{cases} r_a T_k & \text{if } T_k \leq T_a \\ r_a T_a & \text{if } T_k > T_a \end{cases}$$

### Uniform Accrual with Losses to Follow Up

With the LOSS=EXP(HAZARD= $\tau$ ) option, the individual loss to follow up has an exponential loss distribution function

$$H(t) = 1 - e^{-\tau t}$$

where  $\tau \geq 0$  is the loss hazard rate. The loss hazard rate can also be specified implicitly with the MEDTIME= $t_\tau$  suboption through the median loss time  $t_\tau$ .

For a study group with a constant hazard rate  $h$ , if the individual accrual is uniform in the accrual time  $T_a$  with a constant accrual rate  $r_a$  and the individual loss to follow up has an exponential loss distribution function  $H(t)$ , Lachin and Foulkes (1986, p. 511) derive the expected number of events by time  $t$  (where  $t > T_a$ ) as

$$D_h(t, T_a) = r_a T_a \frac{h}{h + \tau} \left( 1 - \frac{1}{(h + \tau) T_a} e^{-(h + \tau)t} (e^{(h + \tau)T_a} - 1) \right)$$

For  $t \leq T_a$ , the SEQDESIGN procedure estimates the expected number of events by time  $t$  as

$$D_h(t, T_a) = r_a t \frac{h}{h + \tau} \left( 1 - \frac{1}{(h + \tau)t} (1 - e^{-(h + \tau)t}) \right)$$

For a one-sample design (such as a proportional hazards regression), the expected number of events by time  $t$  is  $E(t, T_a) = D_h(t, T_a)$ , where  $h$  is the hazard rate for the group. For a two-sample design (such as a log-rank test for two survival distributions), the expected number of events by time  $t$  is

$$E(t, T_a) = \frac{R}{R + 1} D_{h_a}(t, T_a) + \frac{1}{R + 1} D_{h_b}(t, T_a)$$

where  $h_a$  and  $h_b$  are hazard rates in groups A and B, respectively, and  $R$  is the ratio of the sample size allocation weights  $w_a/w_b$ .

If the accrual rate  $r_a$  is specified with one of the three time parameters—the accrual time, follow-up time, and total study time—then PROC SEQDESIGN derives the other two time parameters by solving the equation for the expected number of events. Similarly, if the accrual rate  $r_a$  is not specified, but two of the three time parameters are specified, then PROC SEQDESIGN derives the accrual rate.

If the accrual rate  $r_a$  is specified without the accrual time  $T_a$ , follow-up time  $T_f$ , and total study time  $T = T_a + T_f$ , the SEQDESIGN procedure computes the minimum accrual time  $T_a$  by solving the equation

$$E(\infty, T_a) = d_X$$

A closed-form solution is then given by

$$\frac{d_X}{r_a} \left( \frac{R}{R+1} \frac{h_a}{h_a + \tau} + \frac{1}{R+1} \frac{h_b}{h_b + \tau} \right)^{-1}$$

Similarly, the SEQDESIGN procedure derives the maximum accrual time  $T_a$  by solving the equation

$$E(T_a, T_a) = d_X$$

The maximum accrual time  $T_a$  is then obtained by an iterative process.

With the accrual rate  $r_a$  and the accrual time  $T_a$ , the total sample size is

$$N_X = r_a T_a$$

At each stage  $k$ , the number of events is given by

$$d_k = \frac{I_k}{I_X} d_X$$

The corresponding time  $T_k$  can be derived from the equation for the expected number of events,  $E(t) = d_k$ , and the resulting sample size is computed as

$$N_k = \begin{cases} r_a T_k & \text{if } T_k \leq T_a \\ r_a T_a & \text{if } T_k > T_a \end{cases}$$

### Truncated Exponential Accrual without Losses to Follow Up

For a study group with a constant hazard rate  $h$ , if the individual accrual is truncated exponential with parameter  $\gamma$  over the accrual period from 0 to  $T_a$  with distribution

$$F(t) = \frac{1 - e^{-\gamma t}}{1 - e^{-\gamma T_a}} \quad \text{for } 0 \leq t \leq T_a$$

Lachin and Foulkes (1986, p. 510) derive the expected number of events by time  $t$  (where  $t > T_a$ ) as

$$D_h(t, N) = N \left( 1 + \frac{\gamma}{h - \gamma} \frac{e^{-ht} - e^{-h(t-T_a)} e^{-\gamma T_a}}{1 - e^{-\gamma T_a}} \right)$$

where  $N$  is the total sample size.

For  $t \leq T_a$ , the SEQDESIGN procedure estimates the expected number of events by time  $t$  as

$$D_h(t, N) = N F(t) \left( 1 + \frac{\gamma}{h - \gamma} \frac{e^{-ht} - e^{-\gamma t}}{1 - e^{-\gamma t}} \right)$$

For the truncated exponential accrual function with a parameter  $\gamma$  over the accrual period from 0 to  $T_a$ , you specify the scaled parameter  $\gamma_0 = \gamma T_a$  in the ACCRUAL=EXP(PARM= $\gamma_0$ ) option, where  $\gamma_0 \geq -10$  and  $\gamma_0 \neq 0$ .

For a one-sample design (such as a proportional hazards regression), the expected number of events by time  $t$  is  $E(t, N) = D_h(t, N)$ , where  $h$  is the hazard rate for the group. For a two-sample design (such as a log-rank test for two survival distributions), the expected number of events by time  $t$  is

$$E(t, N) = \frac{R}{R + 1} D_{h_a}(t, N) + \frac{1}{R + 1} D_{h_b}(t, N)$$

where  $h_a$  and  $h_b$  are hazard rates in groups A and B, respectively, and  $R$  is the ratio of the sample size allocation weights  $w_a/w_b$ .

If the total sample size  $N$  is specified, then at least one of the three time parameters—the accrual time, follow-up time, and total study time—must be specified, and then PROC SEQDESIGN derives the other two time parameters by solving the equation for the expected number of events. Similarly, if the total sample size  $N$  is not specified, then at least two of the three time parameters must be specified, and PROC SEQDESIGN derives the sample size.

If the accrual sample size  $N$  is not specified, the SEQDESIGN procedure computes the minimum accrual sample size by solving the equation

$$E(\infty, N) = d_X$$

That is,  $N = d_X$ .

Similarly, if the total sample size  $N$  is not specified but the accrual time  $T_a$  is specified, the SEQDESIGN procedure derives the maximum accrual sample size  $N$  by solving the equation

$$E(T_a, N) = d_X$$

At each stage  $k$ , the number of events is given by

$$d_k = \frac{I_k}{I_X} d_X$$

The corresponding time  $T_k$  can be derived from the equation for the expected number of events,  $E(t) = d_k$ , and the resulting sample size is computed as

$$N_k = \begin{cases} N F(T_k) & \text{if } T_k \leq T_a \\ N & \text{if } T_k > T_a \end{cases}$$

### Truncated Exponential Accrual with Losses to Follow Up

With the LOSS=EXP(HAZARD= $\tau$ ) option, the individual loss to follow up has an exponential loss distribution function

$$H(t) = 1 - e^{-\tau t}$$

where  $\tau \geq 0$  is the loss hazard rate. The loss hazard rate can also be specified implicitly with the MEDTIME= $t_\tau$  suboption through the median loss time  $t_\tau$ .

For a study group with a constant hazard rate  $h$ , if the individual accrual is truncated exponential with parameter  $\gamma$  over the accrual period from 0 to  $T_a$  with distribution

$$F(t) = \frac{1 - e^{-\gamma t}}{1 - e^{-\gamma T_a}} \quad \text{for } 0 \leq t \leq T_a$$

and the individual loss to follow up has an exponential loss distribution function  $H(t)$ , Lachin and Foulkes (1986, p. 513) derive the expected number of events by time  $t$  (where  $t > T_a$ ) as

$$D_h(t, N) = N \frac{h}{h + \tau} \left( 1 + \frac{\gamma}{h + \tau - \gamma} \frac{e^{-(h+\tau)t} - e^{-(h+\tau)(t-T_a)} e^{-\gamma T_a}}{1 - e^{-\gamma T_a}} \right)$$

For  $t \leq T_a$ , the SEQDESIGN procedure estimates the expected number of events by time  $t$  as

$$D_h(t, N) = N F(t) \frac{h}{h + \tau} \left( 1 + \frac{\gamma}{h + \tau - \gamma} \frac{e^{-(h+\tau)t} - e^{-\gamma t}}{1 - e^{-\gamma t}} \right)$$

For the truncated exponential accrual function with a parameter  $\gamma$  over the accrual period from 0 to  $T_a$ , you specify the scaled parameter  $\gamma_0 = \gamma T_a$  in the ACCRUAL=EXP(PARM= $\gamma_0$ ) option, where  $\gamma_0 \geq -10$  and  $\gamma_0 \neq 0$ .

For a one-sample design (such as a proportional hazards regression), the expected number of events by time  $t$  is  $E(t, N) = D_h(t, N)$ , where  $h$  is the hazard rate for the group. For a two-sample design (such as a log-rank test for two survival distributions), the expected number of events by time  $t$  is

$$E(t, N) = \frac{R}{R + 1} D_{h_a}(t, N) + \frac{1}{R + 1} D_{h_b}(t, N)$$

where  $h_a$  and  $h_b$  are hazard rates in groups A and B, respectively, and  $R$  is the ratio of the sample size allocation weights  $w_a/w_b$ .

If the total sample size  $N$  is specified, then at least one of the three time parameters—the accrual time, follow-up time, and total study time—must be specified, and then PROC SEQDESIGN derives the other two time parameters by solving the equation for the expected number of events. Similarly, if the total sample size  $N$  is not specified, then at least two of the three time parameters must be specified, and PROC SEQDESIGN derives the sample size.

If the accrual sample size is not specified, the SEQDESIGN procedure computes the minimum sample size  $N$  by solving the equation

$$E(\infty, N) = d_X$$

A closed-form solution is then given by

$$d_X \left( \frac{R}{R+1} \frac{h_a}{h_a + \tau} + \frac{1}{R+1} \frac{h_b}{h_b + \tau} \right)^{-1}$$

Similarly, if the accrual sample size  $N$  is not specified but the accrual time  $T_a$  is specified, the SEQDESIGN procedure derives the maximum accrual sample size  $N$  by solving the equation

$$E(T_a, N) = d_X$$

At each stage  $k$ , the number of events is given by

$$d_k = \frac{I_k}{I_X} d_X$$

The corresponding time  $T_k$  can be derived from the equation for the expected number of events,  $E(t) = d_k$ , and the resulting sample size is computed as

$$N_k = \begin{cases} N F(T_k) & \text{if } T_k \leq T_a \\ N & \text{if } T_k > T_a \end{cases}$$

The following three sections describe examples of test statistics with their resulting information levels, which can then be used to derive the required sample size. The maximum likelihood estimators are used for all tests except to compare two survival distributions with a log-rank test, where a score statistic is used.

## Applicable One-Sample Tests and Sample Size Computation

The SEQDESIGN procedure provides sample size computation for two one-sample tests: normal mean and binomial proportion. The required sample size depends on the variance of the response variable—that is, the sample proportion for a binomial proportion test.

In a typical clinical trial, a hypothesis is designed to reject, not accept, the null hypothesis to show the evidence for the alternative hypothesis. Thus, in most cases, the proportion under the alternative hypothesis is used to derive the required sample size. For a test of the binomial proportion, the REF=NULLPROP and REF=PROP options use proportions under the null and alternative hypotheses, respectively.

### Test for a Normal Mean

The MODEL=ONESAMPLEMEAN option in the SAMPLESIZE statement derives the sample size required to test a normal mean by using the sample mean statistic for the null hypothesis  $\mu = \mu_0$ . At stage  $k$ , the sample mean is computed as

$$\bar{y}_k = \frac{1}{N_k} \sum_{j=1}^{N_k} y_{kj}$$

where  $y_{kj}$  is the value of the  $j$ th observation available in the  $k$ th stage and  $N_k$  is the cumulative sample size at stage  $k$ .

An equivalent hypothesis is  $H_0 : \theta = 0$ , where  $\theta = \mu - \mu_0$ .

The MLE statistic for  $\theta$ ,

$$\hat{\theta}_k = \bar{y}_k - \mu_0 \sim N(\theta, I_k^{-1})$$

where the information

$$I_k = \frac{1}{\text{Var}(\hat{\theta})} = \frac{1}{\text{Var}(\bar{y}_k)} = \frac{N_k}{\sigma^2}$$

is the inverse of the variance.

That is, the standardized statistic

$$Z_k = \hat{\theta}_k \sqrt{I_k} = (\bar{y}_k - \mu_0) \sqrt{I_k} \sim N(\theta \sqrt{I_k}, 1)$$

Thus, to test the hypothesis  $H_0 : \theta = 0$  against a two-sided alternative  $H_1 : \theta = \theta_1$ ,  $H_0$  is rejected at stage  $k$  if the statistic  $Z_k$  is less than or equal to the lower  $\alpha$  boundary value or if  $Z_k$  is greater than or equal to the upper  $\alpha$  boundary value at stage  $k$ .

If the variance  $\sigma^2$  is unknown, the sample variance can be used if it is assumed that the sample variance is computed from a large sample such that the test statistic has an approximately normal distribution.

The maximum information is needed to derive the required sample size. If the maximum information is not specified or derived with the ALTREF= option in the procedure, the MEAN= $\theta_1$  option in the SAMPLESIZE statement is used to specify the alternative reference and thus to derive the maximum information.

In the SEQDESIGN procedure, the computed total sample size

$$N_K = \sigma^2 I_X$$

where  $I_X$  is the maximum information and  $\sigma$  is the specified standard deviation. With an available maximum information, you can specify the MODEL=ONESAMPLEMEAN( STDDEV=  $\sigma$ ) option in the SAMPLESIZE statement to compute the required total sample size and individual sample size at each stage. A procedure such as PROC MEANS can be used to derive a one-sample  $Z$  test for a normal mean.

### Test for a Binomial Proportion

The MODEL=ONESAMPLEFREQ option in the SAMPLESIZE statement derives the sample size required to test a binomial proportion by using the null hypothesis  $p = p_0$ , where  $p$  is the proportion of a binomial population. At stage  $k$ , the MLE for  $p$  is computed as

$$\hat{p}_k = \frac{1}{N_k} \sum_{j=1}^{N_k} y_{kj}$$

where  $y_{kj}$  is the value of the  $j$ th observation available in the  $k$ th stage and  $N_k$  is the cumulative sample size at stage  $k$ .

An equivalent hypothesis is  $H_0 : \theta = 0$ , where  $\theta = p - p_0$ . If  $p_0$  is not close to 0 or 1, then for a large sample,  $\hat{\theta}_k = \hat{p}_k - p_0$  has an approximately normal distribution

$$\hat{\theta}_k \sim N(\theta, I_k^{-1})$$

where the information  $I_k = (p(1-p)/N_k)^{-1}$  is the inverse of the variance  $\text{Var}(\hat{\theta})$ .

Then the standardized statistic

$$Z_k = \hat{\theta}_k \sqrt{I_k} \sim N(\theta \sqrt{I_k}, 1)$$

In practice, the estimated sample proportion  $\hat{p}$  at stage  $k$  can be used to derive the information  $I_k$  and test statistic  $Z_k$ . Thus, to test the hypothesis  $H_0$  against an upper alternative  $H_1 : \theta = \theta_1 > 0$ ,  $H_0$  is rejected at stage  $k$  if the statistic  $Z_k$  is greater than or equal to the upper  $\alpha$  boundary at stage  $k$ .

The maximum information  $I_X$  is needed to derive the required sample size. If the maximum information is not specified or derived with the ALTREF= option in the procedure, the PROP= option in the SAMPLESIZE statement is used to specify the alternative reference and to derive the maximum information for the sample size calculation.

It is assumed that the sample size is sufficiently large such that the test statistic has an approximately normal distribution. With the hypotheses  $H_0 : p = p_0$  and  $H_1 : p = p_1$ , the SEQDESIGN procedure derives the total sample size

$$N_X = p^* (1 - p^*) I_X$$

where  $p^* = p_0$  if REF=NULLPROP is specified. Otherwise,  $p^* = p_1$ .

If the PROP= option in the SAMPLESIZE statement is not specified, then the alternative reference  $\theta_1$  derived in the SEQDESIGN procedure is used to compute  $p_1 = p_0 + \theta_1$ .

The ALTREF= option in the PROC statement can be used to specify  $\theta_1$ . Otherwise, the PROP= option in the SAMPLESIZE statement must be specified.

For example, with  $H_0 : p = 0.5$ ,  $H_1 : p = 0.6$ , and REF=PROP (which is the default),

$$N_K = p^*(1 - p^*) I_X = (0.6 \times 0.4) I_X = 0.24 I_X$$

You can specify the MODEL=ONESAMPLEFREQ option in the SAMPLESIZE statement to compute the required total sample size and individual sample size at each stage. A procedure such as PROC GENMOD with the default DIST=NORMAL option in the MODEL statement can be used to derive the Z test for a binomial proportion.

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## Applicable Two-Sample Tests and Sample Size Computation

The SEQDESIGN procedure provides sample size computation for two-sample tests: the test for the difference between two normal means, tests for binomial proportions, and the log-rank test for two survival distributions. These tests for binomial proportions include the test for the difference between two binomial proportions, the log odds ratio test for binomial proportions, and the log relative risk test for binomial proportions,

For a test of difference between two sample means, the required sample size depends on the assumed sample variances. Similarly, for a test of two-sample proportions, the required sample size depends on the assumed sample proportions. For a log-rank test of two survival distributions, the required sample size depends on the assumed sample hazard rates, accrual rate, and accrual time.

If the REF=NULLPROP or REF=NULLHAZARD option is specified, the proportions or hazard rates under the null hypothesis are used to derive the required sample size or number of events. Otherwise, the REF=PROP option (which is the default in the MODEL=TWOSAMPLEFREQ option) or the REF=HAZARD option (which is the default in the MODEL=TWOSAMPLESURVIVAL option) uses proportions or hazard rates under the alternative hypothesis to derive the required sample size or number of events.

### Test for the Difference between Two Normal Means

The MODEL=TWOSAMPLEMEAN option in the SAMPLESIZE statement derives the sample size required to test the difference between the means of two normal populations  $\mu_a$  and  $\mu_b$  by using the null hypothesis  $H_0 : \theta = 0$ , where  $\theta = \mu_a - \mu_b$ .

At stage  $k$ , the MLE for  $\theta$  is computed as

$$\hat{\theta}_k = \bar{y}_{ak} - \bar{y}_{bk} = \frac{1}{N_{ak}} \sum_{j=1}^{N_{ak}} y_{akj} - \frac{1}{N_{bk}} \sum_{j=1}^{N_{bk}} y_{bjk}$$

where  $y_{akj}$  and  $y_{bjk}$  are the values of the  $j$ th observation available in the  $k$ th stage groups A and B, respectively, and  $N_{ak}$  and  $N_{bk}$  are the cumulative sample sizes at stage  $k$  for these two groups.

The statistic  $\hat{\theta}_k$  has a normal distribution

$$\hat{\theta}_k \sim N(\theta, I_k^{-1})$$

where the information  $I_k$  is the inverse of the variance  $\text{Var}(\hat{\theta}_k) = \sigma_a^2/N_{ak} + \sigma_b^2/N_{bk}$ .

Then the standardized statistic

$$Z_k = \hat{\theta}_k \sqrt{I_k} \sim N(\theta \sqrt{I_k}, 1)$$

Thus, to test the hypothesis  $H_0 : \theta = 0$  against an upper alternative  $H_1 : \theta = \theta_1, \theta_1 > 0$ ,  $H_0$  is rejected at stage  $k$  if the statistic  $Z_k \geq a_k$ , the upper  $\alpha$  boundary for the standardized  $Z$  statistic at stage  $k$ .

If the variances  $\sigma_a^2$  and  $\sigma_b^2$  are unknown, the sample variances can be used to derive the information  $I_k$  if it is assumed that each sample variance is computed from a large sample such that the test statistic has an approximately normal distribution.

The maximum information is needed to derive the required sample size. If the maximum information is not specified or derived in the procedure, the alternative reference  $\theta_1^*$  specified in the MEANDIFF option is used to derive the maximum information.

Note that in order to derive the sample sizes  $N_{ak}$  and  $N_{bk}$  uniquely from the information,  $N_{ak} = R N_{bk}$  is assumed for  $k = 1, 2, \dots, K$ , where  $R = w_a/w_b$  is the constant allocation ratio computed from the WEIGHT= $w_a w_b$  option in the SAMPLESIZE statement.



In PROC SEQDESIGN, the computed total sample sizes for the two groups are

$$N_{aK} = (\sigma_a^2 + R\sigma_b^2) I_X = R \left( \frac{\sigma_a^2}{R} + \sigma_b^2 \right) I_X$$

$$N_{bK} = \left( \frac{\sigma_a^2}{R} + \sigma_b^2 \right) I_X$$

where  $I_X$  is the maximum information derived in the SEQDESIGN procedure,  $R$  is the constant allocation ratio, and  $\sigma_a$  and  $\sigma_b$  are the specified standard deviations.

For  $R = 1$ , the two sample sizes are equal, then

$$N_{aK} = N_{bK} = \frac{N_K}{2} = (\sigma_a^2 + \sigma_b^2) I_X$$

If the variances from the two groups are equal,  $\sigma_a^2 = \sigma_b^2 = \sigma^2$ , then the total sample sizes for the two groups are

$$N_{aK} = (1 + R) \sigma^2 I_X$$

$$N_{bK} = \left( 1 + \frac{1}{R} \right) \sigma^2 I_X$$

and the total sample size is

$$N_X = N_{aK} + N_{bK} = \frac{(R + 1)^2}{R} \sigma^2 I_X$$

Furthermore, for  $R = 1$ , the two sample sizes are equal, then

$$N_{aK} = N_{bK} = \frac{N_X}{2} = 2 \sigma^2 I_X$$

With an available maximum information, you can specify the MODEL=TWOSAMPLEMEAN(WEIGHT= $R$  STDDEV= $\sigma_a$   $\sigma_b$ ) option in the SAMPLESIZE statement to compute the required total sample size and individual sample size at each stage. A procedure such as PROC GLM can be used to derive the two-sample  $Z$  test for the mean difference.

### Test for the Difference between Two Binomial Proportions

The MODEL=TWOSAMPLEFREQ(TEST=PROP) option in the SAMPLESIZE statement derives the sample size required to test the difference between two binomial populations with  $H_0 : \theta = 0$ , where  $\theta = p_a - p_b$ . At stage  $k$ , the MLE for  $\theta$  is

$$\hat{\theta}_k = \hat{p}_{ak} - \hat{p}_{bk} = \frac{1}{N_{ak}} \sum_{j=1}^{N_{ak}} y_{akj} - \frac{1}{N_{bk}} \sum_{j=1}^{N_{bk}} y_{bjk}$$

where  $y_{akj}$  and  $y_{bjk}$  are the values of the  $j$ th observation available in the  $k$ th stage for groups A and B, respectively, and  $N_{ak}$  and  $N_{bk}$  are the cumulative sample sizes at stage  $k$  for these two groups.

For sufficiently large sample sizes  $N_{ak}$  and  $N_{bk}$ , the statistic  $\hat{\theta}_k$  has an approximate normal distribution

$$\hat{\theta}_k \sim N(\theta, I_k^{-1})$$

where the information is the inverse of the variance

$$\text{Var}(\hat{\theta}_k) = \frac{p_a(1-p_a)}{N_{ak}} + \frac{p_b(1-p_b)}{N_{bk}}$$

Thus, the standardized statistic

$$Z_k = \hat{\theta}_k \sqrt{I_k} \sim N(\theta \sqrt{I_k}, 1)$$

In practice,  $p_a = \hat{p}_a$  and  $p_b = \hat{p}_b$ , the estimated sample proportions for groups A and B, respectively, at stage  $k$ , can be used to derive the information  $I_k$  and the test statistic  $Z_k$ . Thus, to test the hypothesis  $H_0$  against an upper alternative  $H_1 : \theta > 0$ ,  $H_0$  is rejected at stage  $k$  if the statistic  $Z_k \geq a_k$ , the upper  $\alpha$  boundary for the standardized  $Z$  statistic at stage  $k$ .

The maximum information  $I_X$  is needed to derive the required sample size. If the maximum information is not specified or derived with the ALTREF= option in the procedure, the PROP= option in the SAMPLESIZE statement is used to provide proportions under the alternative hypothesis for the alternative reference and then to derive the maximum information.

The proportions in the two groups are needed to derive the sample size. Also, in order to derive the sample sizes  $N_{ak}$  and  $N_{bk}$  uniquely from the information,  $N_{ak} = R N_{bk}$  is assumed for  $k = 1, 2, \dots, K$ , where  $R = w_a/w_b$  is the constant allocation ratio computed from the WEIGHT= $w_a w_b$  option in the SAMPLESIZE statement. Then

$$I_X = \left( \frac{p_a(1-p_a)}{N_{aK}} + \frac{p_b(1-p_b)}{N_{bK}} \right)^{-1} = \frac{N_{aK}}{p_a(1-p_a) + R p_b(1-p_b)}$$

In PROC SEQDESIGN, the total sample sizes in the two groups are computed as

$$N_{aK} = (p_a^*(1-p_a^*) + R p_b^*(1-p_b^*)) I_X$$

$$N_{bK} = \frac{1}{R} N_{aK}$$

where  $R = w_a/w_b$  is the constant allocation ratio, and  $p_a^*$  and  $p_b^*$  are proportions specified with the REF= option:

- REF=NULLPROP uses proportions under  $H_0$ :  $p_a^* = p_{0a}$ ,  $p_b^* = p_{0b}$
- REF=AVGNULPROP uses the average proportion under  $H_0$ :  $p_a^* = p_b^* = (R p_{0a} + p_{0b})/(R + 1)$
- REF=PROP uses proportions under  $H_1$ :  $p_a^* = p_{1a}$ ,  $p_b^* = p_{1b}$
- REF=AVGPROP uses the average proportion under  $H_1$ :  $p_a^* = p_b^* = (R p_{1a} + p_{1b})/(R + 1)$

The total sample size is given by

$$N_X = N_{aK} + N_{bK} = (R + 1) \left( \frac{1}{R} p_a^* (1 - p_a^*) + p_b^* (1 - p_b^*) \right) I_X$$

For  $R = 1$ , the two sample sizes are equal,

$$N_{aK} = N_{bK} = \frac{N_X}{2} = (p_a^* (1 - p_a^*) + p_b^* (1 - p_b^*)) I_X$$

You can specify the MODEL=TWOSAMPLEFREQ( TEST=PROP WEIGHT=R ) option in the SAMPLE-SIZE statement to compute the required total sample size and individual sample size at each stage. A procedure such as PROC GENMOD with the default DIST=NORMAL option in the MODEL statement can be used to derive the two-sample  $Z$  test for proportion difference.

### Test for Two Binomial Proportions with a Log Odds Ratio Statistic

The MODEL=TWOSAMPLEFREQ(TEST=LOGOR) option in the SAMPLESIZE statement derives the sample size required to test two binomial proportions by using a log odds ratio statistic. The odds ratio is the ratio of the odds in one group to the odds in the other group, and the log odds ratio is the logarithm of the odds ratio

$$\theta = \log \left( \frac{p_a / (1 - p_a)}{p_b / (1 - p_b)} \right) = \log \left( \frac{p_a (1 - p_b)}{p_b (1 - p_a)} \right)$$

The hypothesis of no difference between two proportions,  $p_a = p_b$ , can be tested through the null hypothesis  $H_0 : \theta = 0$ , where  $\theta$  is the log odds ratio. For example, with  $H_0 : p_a = p_b = 0.6$  and  $H_1 : p_a = 0.8, p_b = 0.6$ , it corresponds to the equivalent hypothesis  $H_0 : \theta = 0$  and  $H_1 : \theta = \log \left( \frac{0.8(1-0.6)}{0.6(1-0.8)} \right) = \log(8/3) = 0.98083$ .

The maximum likelihood estimate of  $\theta$  is given by

$$\hat{\theta} = \log \left( \frac{\hat{p}_a (1 - \hat{p}_b)}{\hat{p}_b (1 - \hat{p}_a)} \right)$$

with an asymptotic variance

$$\text{Var}(\hat{\theta}) = I^{-1} = \frac{1}{N_a p_a (1 - p_a)} + \frac{1}{N_b p_b (1 - p_b)}$$

where  $I$  is the information (Diggle et al. 2002, pp. 341–342). That is, the standardized statistic

$$Z_k = \hat{\theta}_k \sqrt{I_k} \sim N \left( \theta \sqrt{I_k}, 1 \right)$$

In practice,  $p_a = \hat{p}_a$  and  $p_b = \hat{p}_b$ , the estimated sample proportions for groups A and B, respectively, at stage  $k$ , can be used to derive the information  $I_k$  and the test statistic  $Z_k = \hat{\theta}_k \sqrt{I_k}$  if the two sample sizes  $N_a$  and  $N_b$  are sufficiently large such that the test statistic has an approximately normal distribution.

The maximum information  $I_X$  is needed to derive the required sample size. If the maximum information is not specified or derived with the ALTREF= option in the procedure, the PROP= option in the SAMPLESIZE statement is used to provide proportions under the alternative hypothesis for the alternative reference and then to derive the maximum information.

In order to derive the sample sizes  $N_{ak}$  and  $N_{bk}$  uniquely from the information,  $N_{ak} = R N_{bk}$  is assumed for  $k = 1, 2, \dots, K$ , where  $R = w_a/w_b$  is the constant allocation ratio computed from the WEIGHT= $w_a/w_b$  option in the SAMPLESIZE statement. Then with

$$I_X = N_{bK} \left( \frac{1}{R p_a(1 - p_a)} + \frac{1}{p_b(1 - p_b)} \right)^{-1}$$

the sample size can be computed.

In PROC SEQDESIGN, the total sample sizes in the two groups are computed as

$$N_{bK} = I_X \left( \frac{1}{R p_a^*(1 - p_a^*)} + \frac{1}{p_b^*(1 - p_b^*)} \right)$$

$$N_{aK} = R N_{bK}$$

where  $R = w_a/w_b$  is the constant allocation ratio, and  $p_a^*$  and  $p_b^*$  are proportions specified with the REF= option:

- REF=NULLPROP uses proportions under  $H_0$ :  $p_a^* = p_{0a}$ ,  $p_b^* = p_{0b}$
- REF=AVGNULLPROP uses the average proportion under  $H_0$ :  $p_a^* = p_b^* = (R p_{0a} + p_{0b}) / (R + 1)$
- REF=PROP uses proportions under  $H_1$ :  $p_a^* = p_{1a}$ ,  $p_b^* = p_{1b}$
- REF=AVGPROP uses the average proportion under  $H_1$ :  $p_a^* = p_b^* = (R p_{1a} + p_{1b}) / (R + 1)$

You can specify the MODEL=TWOSAMPLEFREQ( TEST=LOGOR WEIGHT= $R$ ) option in the SAMPLESIZE statement to compute the required total sample size and individual sample size at each stage. A procedure such as PROC LOGISTIC can be used to derive the log odds ratio statistic.

### Test for Two Binomial Proportions with a Log Relative Risk Statistic

The MODEL=TWOSAMPLEFREQ(TEST=LOGRR) option in the SAMPLESIZE statement derives the sample size required to test two binomial proportions by using a log relative risk statistic. The relative risk is the ratio of the proportion in one group to the proportion in the other group. The log relative risk statistic is the logarithm of the relative risk

$$\theta = \log \left( \frac{p_a}{p_b} \right)$$

The hypothesis of no difference between two proportions,  $p_a = p_b$ , can be tested through the null hypothesis  $H_0 : \theta = 0$ . For example, with  $H_0 : p_a = p_b = 0.6$  and  $H_1 : p_a = 0.8$ ,  $p_b = 0.6$ , it corresponds to the equivalent hypothesis  $H_0 : \theta = 0$  and  $H_1 : \theta = \log \left( \frac{0.8}{0.6} \right) = \log(4/3) = 0.28768$ .

The maximum likelihood estimate of  $\theta$  is given by

$$\hat{\theta} = \log\left(\frac{\hat{p}_a}{\hat{p}_b}\right)$$

with an asymptotic variance

$$I^{-1} = \frac{1 - p_a}{N_a p_a} + \frac{1 - p_b}{N_b p_b}$$

where  $I$  is the information (Chow and Liu 1998, p. 329).

In practice,  $p_a = \hat{p}_a$  and  $p_b = \hat{p}_b$ , the estimated sample proportions for groups A and B, respectively, at stage  $k$ , are used to derive the information  $I_k$  and the test statistic  $Z_k = \hat{\theta}_k \sqrt{I_k}$ .

The maximum information  $I_X$  and proportions  $p_a$  and  $p_b$  are needed to derive the required sample size. If the maximum information is not specified or derived with the ALTREF= option in the procedure, the PROP= option in the SAMPLESIZE statement is used to provide proportions under the alternative hypothesis for the alternative reference and then to derive the maximum information.

Note that in order to derive the sample sizes  $N_{ak}$  and  $N_{bk}$  uniquely from the information,  $N_{ak} = R N_{bk}$  is assumed for  $k = 1, 2, \dots, K$ , where  $R = w_a/w_b$  is the constant allocation ratio computed from the WEIGHT= $w_a w_b$  option in the SAMPLESIZE statement. Then the sample size can be computed from

$$I_X = N_{bK} \left( \frac{1 - p_a}{R p_a} + \frac{1 - p_b}{p_b} \right)^{-1}$$

In PROC SEQDESIGN, the computed sample sizes in the two groups are

$$N_{bK} = I_X \left( \frac{1 - p_a^*}{R p_a^*} + \frac{1 - p_b^*}{p_b^*} \right)$$

$$N_{aK} = R N_{bK}$$

where  $R = w_a/w_b$  is the constant allocation ratio, and  $p_a^*$  and  $p_b^*$  are proportions specified with the REF= option:

- REF=NULLPROP uses proportions under  $H_0$ :  $p_a^* = p_{0a}$ ,  $p_b^* = p_{0b}$
- REF=AVGNULPROP uses the average proportion under  $H_0$ :  $p_a^* = p_b^* = (R p_{0a} + p_{0b})/(R + 1)$
- REF=PROP uses proportions under  $H_1$ :  $p_a^* = p_{1a}$ ,  $p_b^* = p_{1b}$
- REF=AVGPROP uses the average proportion under  $H_1$ :  $p_a^* = p_b^* = (R p_{1a} + p_{1b})/(R + 1)$

You can specify the MODEL=TWOSAMPLEFREQ( TEST=LOGRR WEIGHT= $R$ ) option in the SAMPLESIZE statement to compute the required total sample size and individual sample size at each stage. A procedure such as PROC LOGISTIC can be used to derive the log relative risk statistic.

### Test for Two Survival Distributions with a Log-Rank Test

The MODEL=TWOSAMPLESURV option in the SAMPLESIZE statement derives the number of events required for a log-rank test of two survival distributions. The analysis of survival data involves the survival times for both censored and uncensored data. A noncensored survival time is the time from treatment to an event such as remission or relapse for an individual. A censored survival time is the time from treatment to the time of analysis for an individual surviving at that time, and the status is unknown beyond that time.

Let  $T$  be the random variable of the survival time. Then the survival function

$$S(t) = \Pr(T > t)$$

is the probability that an individual from the population has a survival time that exceeds  $t$ . And the hazard function is given by

$$h(t) = \frac{f(t)}{S(t)}$$

where  $f(t)$  is the density function of  $T$ .

The hazard functions can be used to test the equality of two survival distributions  $S_a(t) = S_b(t)$  with the null hypothesis  $H_0 : h_a(t) = h_b(t), t > 0$ , where  $S_a(t)$  and  $S_b(t)$  are survival functions for groups A and B, respectively, and  $h_a(t)$  and  $h_b(t)$  are the corresponding hazard functions.

If the two hazards are proportional,  $h_a(t) = \lambda h_b(t)$ , where  $\lambda$  is a constant, then an equivalent null hypothesis is

$$H_0 : \lambda = \frac{h_a(t)}{h_b(t)} = 1$$

Alternatively, another equivalent null hypothesis is given by

$$H_0 : \theta = -\log(\lambda) = 0$$

Suppose that the hazard rate  $h$  is a constant. Then with a specified median survival time  $T_m$ , the hazard rate can be derived from the equation

$$e^{-hT_m} = \frac{1}{2}$$

Denote the distinct event times at stage  $k$  as  $\tau_{kj}, j = 1, 2, \dots, t_k$ , where  $t_k$  is the total number of distinct event times. Then the score statistic is the log-rank statistic (Jennison and Turnbull 2000, pp. 259–261; Whitehead 1997, pp. 36–39)

$$S_k = \sum_{j=1}^{t_k} (d_{akj} - e_{akj})$$

where  $d_{akj}$  is the number of events from group A and  $e_{akj}$  is the number of expected events from A. The number of expected events from A is computed as

$$e_{akj} = d_{kj} \frac{r_{akj}}{r_{kj}}$$

where  $d_{kj}$  is the number of events from both groups,  $r_{akj}$  is the number of individuals from the treatment group who survived up to time  $\tau_{kj}$ , and  $r_{bkj}$  is the number of individuals from both groups who survived up to time  $\tau_{kj}$ .

If the number of events  $d_{kj}$  is small relative to  $r_{kj}$ , the number of individuals survived up to time  $\tau_{kj}$ , then with a sufficiently large sample size,  $S_k$  has an approximately normal distribution

$$S_k \sim N(\theta I_k, I_k)$$

where the variance of  $S_k$  is the estimated information

$$I_k = \sum_{j=1}^{t_k} \frac{r_{akj} r_{bkj} d_{kj}}{r_{kj}^2}$$

In order to derive the number of events from the information  $I_k$ ,  $N_{ak} = R N_{bk}$  is assumed for  $k = 1, 2, \dots, K$ , where  $R = w_a/w_b$  is the constant allocation ratio computed from the WEIGHT= $w_a w_b$  option in the SAMPLESIZE statement.

The maximum information  $I_X$  is needed to derive the required sample size. If the maximum information is specified or derived with the ALTREF= option in the procedure, the HAZARD=, MEDSURVTIME=, and HAZARDRATIO= options are not applicable. Otherwise, the HAZARD=, MEDSURVTIME=, or HAZARDRATIO= option is used to compute the alternative reference and then to derive the maximum information for the sample size calculation.

With  $N_{aK} = R N_{bK}$ , if the number of events is few relative to the number of individuals who survived, then  $r_{aKj} \approx R r_{bKj}$ , and

$$I_X \approx \sum_{j=1}^{t_K} \frac{R}{(R+1)^2} d_{Kj} = \frac{R}{(R+1)^2} D_X$$

where  $D_X$  is the total number of events.

Thus, the required total number of events

$$D_X = \frac{(R+1)^2}{R} I_X$$

For a study group, if the hazard rate is constant, corresponding to an exponential survival distribution, and the individual accrual is uniform in the accrual time  $T_a$  with a constant accrual rate  $r_a$ , then the required total sample size and sample size at each stage can be derived. See the section “[Input Number of Events for Fixed-Sample Design](#)” on page 7044 for a detailed description of the sample size computation that uses hazard rates, accrual rate, and accrual time.

You can specify the MODEL=TWOSAMPLESURVIVAL option in the SAMPLESIZE statement to compute the required total number of events and individual number of events at each stage. With the specifications of hazard rates, accrual rate, and accrual time, the required total sample size and individual sample size at each stage can also be derived. If the REF=NULLHAZARD option is specified, the hazard rates under the null hypothesis,  $h_{0a}$  and  $h_{0b}$ , are used in the sample size computation. Otherwise, the hazard rates under the alternative hypothesis,  $h_{1a}$  and  $h_{1b}$ , are used. A procedure such as PROC LIFETEST can be used to derive the log-rank statistic.

## Applicable Regression Parameter Tests and Sample Size Computation

The SEQDESIGN procedure provides sample size computation for tests of a regression parameter in three regression models: normal regression, logistic regression, and proportional hazards regression.

To test a parameter  $\beta_1$  in a regression model, the variance of the parameter estimate  $\hat{\beta}_1$  is needed for the sample size computation. In a simple regression model with one covariate X1, the variance of  $\hat{\beta}_1$  is inversely related to the variance of X1,  $\sigma_x^2$ . That is,

$$\text{Var}(\hat{\beta}_1) \propto \frac{1}{N \sigma_x^2}$$

for the normal regression and logistic regression models, where  $N$  is the sample size, and

$$\text{Var}(\hat{\beta}_1) \propto \frac{1}{D \sigma_x^2}$$

for the proportional hazards regression model, where  $D$  is the number of events.

For a regression model with more than one covariate, the variance of  $\hat{\beta}_1$  for the normal regression and logistic regression models is inversely related to the variance of X1 after adjusting for other covariates. That is,

$$\text{Var}(\hat{\beta}_1) \propto \frac{1}{N (1 - r_x^2) \sigma_x^2}$$

where  $\hat{\beta}_1$  is the estimate of the parameter  $\beta_1$  in the model and  $r_x^2$  is the R square from the regression of X1 on other covariates—that is, the proportion of the variance  $\sigma_x^2$  explained by these covariates.

Similarly, for a proportional hazards regression model,

$$\text{Var}(\hat{\beta}_1) \propto \frac{1}{D (1 - r_x^2) \sigma_x^2}$$

Thus, with the derived maximum information, the required sample size or number of events can also be computed for the testing of a parameter in a regression model with covariates.

### Test for a Parameter in the Regression Model

The MODEL=REG option in the SAMPLESIZE statement derives the sample size required for a  $Z$  test of a normal regression. For a normal linear regression model, the response variable is normally distributed with the mean equal to a linear function of the explanatory variables and the constant variance  $\sigma^2$ .

The normal linear model is

$$y \sim N(\mathbf{X}\boldsymbol{\beta}, \sigma_y^2 \mathbf{I}_{(N)})$$

where  $\mathbf{Y}_{(N \times 1)}$  is the vector of the  $N$  observed responses,  $\mathbf{X}_{(N \times p)}$  is the design matrix for these  $N$  observations,  $\boldsymbol{\beta}_{(p \times 1)}$  is the parameter vector, and  $\mathbf{I}_{(N)}$  is the  $(N \times N)$  identity matrix.

The least squares estimate is

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1} \mathbf{X}'\mathbf{Y}$$



and is normally distributed with mean  $\beta$  and variance

$$\text{Var}(\hat{\beta}) = \sigma_y^2 (\mathbf{X}'\mathbf{X})^{-1}$$

For a model with only one covariate X1,

$$\hat{\beta}_1 \sim N(\beta_1, \text{Var}(\hat{\beta}_1))$$

where the variance

$$\text{Var}(\hat{\beta}_1) = I_{\beta_1}^{-1} = \sigma_y^2 \frac{1}{N \sigma_x^2}$$

Thus, with the derived maximum information  $I_X = I_{\beta_1}$ , the required sample size is given by

$$N = I_X \frac{\sigma_y^2}{\sigma_x^2}$$

For a normal linear model with more than one covariate, the variance of a single parameter  $\beta_1$  is

$$\text{Var}(\hat{\beta}_1) = \sigma_y^2 (\mathbf{X}'\mathbf{X})_{(11)}^{-1} = \sigma_y^2 \frac{1}{N \sigma_x^2 (1 - r_x^2)}$$

where  $(\mathbf{X}'\mathbf{X})_{(11)}^{-1}$  is the diagonal element of the  $(\mathbf{X}'\mathbf{X})^{-1}$  matrix corresponding to the parameter  $\beta_1$ ,  $\sigma_x^2$  is the variance of the variable X1, and  $r_x^2$  is the proportion of variance of X1 explained by other covariates. The value  $\sigma_x^2 (1 - r_x^2)$  represents the variance of X1 after adjusting for all other covariates.

Thus, with the derived maximum information  $I_X$ , the required sample size is

$$N = I_X \frac{\sigma_y^2}{(1 - r_x^2) \sigma_x^2}$$

In the SEQDESIGN procedure, you can specify the MODEL=REG( VARIANCE= $\sigma_y^2$  XVARIANCE= $\sigma_x^2$  XRSQUARE= $r_x^2$ ) option in the SAMPLESIZE statement to compute the required total sample size and individual sample size at each stage. A SAS procedure such as PROC REG can be used to compute the parameter estimate and its standard error at each stage.

### Test for a Parameter in the Logistic Regression Model

The MODEL=LOGISTIC option in the SAMPLESIZE statement derives the sample size required for a Z test of a logistic regression parameter. The linear logistic model has the form

$$\text{logit}(p) = \log\left(\frac{p}{1-p}\right) = \mathbf{x}\beta$$

where  $p$  is the response probability to be modeled and  $\beta$  is a vector of parameters.

Following the derivation in the section “Test for a Parameter in the Regression Model” on page 7061, the required sample size for testing a parameter in  $\beta$  is given by

$$N = I_X \frac{\sigma_y^2}{(1 - r_x^2) \sigma_x^2}$$

With the variance of the logit response,  $\sigma_y^2 = 1/(p(1-p))$ ,

$$N = I_X \frac{1}{p(1-p)} \frac{1}{(1-r_x^2)\sigma_x^2}$$

where  $\sigma_x^2$  is the variance of X and  $r_x^2$  is the proportion of variance explained by other covariates.

In the SEQDESIGN procedure, you can specify the MODEL=LOGISTIC( PROP= $p$  XVARIANCE= $\sigma_x^2$  XRSQUARE= $r_x^2$ ) option in the SAMPLESIZE statement to compute the required total sample size and individual sample size at each stage.

A SAS procedure such as PROC LOGISTIC can be used to compute the parameter estimate and its standard error at each stage.

### Test for a Parameter in the Proportional Hazards Regression Model

The MODEL=PHREG option in the SAMPLESIZE statement derives the number of events required for a Z test of a proportional hazards regression parameter. For analyses of survival data, Cox's semiparametric model is often used to examine the effect of explanatory variables on hazard rates. The survival time of each observation in the population is assumed to follow its own hazard function,  $h_i(t)$ , expressed as

$$h_i(t) = h(t; \mathbf{X}_i) = h_0(t) \exp(\mathbf{X}_i' \boldsymbol{\beta})$$

where  $h_0(t)$  is an arbitrary and unspecified baseline hazard function,  $\mathbf{x}_i$  is the vector of explanatory variables for the  $i$ th individual, and  $\boldsymbol{\beta}$  is the vector of regression parameters associated with the explanatory variables.

Hsieh and Lavori (2000, p. 553) show that the required number of events for testing a parameter in  $\boldsymbol{\beta}$ ,  $\beta_1$ , associated with the variable X1 is given by

$$D_X = I_X \frac{1}{(1-r_x^2)\sigma_x^2}$$

where  $\sigma_x^2$  is the variance of X1 and  $r_x^2$  is the proportion of variance of X1 explained by other covariates.

In the SEQDESIGN procedure, you can specify the MODEL=PHREG( XVARIANCE= $\sigma_x^2$  XRSQUARE= $r_x^2$ ) option in the SAMPLESIZE statement to compute the required number of events and individual number of events at each stage.

A SAS procedure such as PROC PHREG can be used to compute the parameter estimate and its standard error at each stage.

Note that for a two-sample test, X1 is an indicator variable and is the only covariate in the model. Thus, if the two sample sizes are equal, then the variance  $\sigma_x^2 = 1/4$  and the required number of events for testing the parameter  $\beta_1$  is given by

$$D_X = I_X \frac{1}{\sigma_x^2} = 4 I_X$$

See the section "Input Number of Events for Fixed-Sample Design" on page 7044 for a detailed description of the sample size computation that uses hazard rates, accrual rate, and accrual time.

## Aspects of Group Sequential Designs

This section summarizes various aspects of group sequential designs that are encountered in applications of the SEQDESIGN procedure. Features are illustrated through two-sided designs with  $\alpha = 0.05$  and  $\beta = 0.10$ . The null hypothesis  $H_0 : \theta = 0$  and an alternative reference  $\theta_1 = \pm 0.25$  are used for the designs with early stopping only to reject the null hypothesis.

### Canonical Joint Distribution

The SEQDESIGN procedure assumes that with a total number of stages  $K$ , the sequence of the standardized test statistics  $\{Z_1, Z_2, \dots, Z_K\}$  has the canonical joint distribution with information levels  $\{I_1, I_2, \dots, I_K\}$  for the parameter  $\theta$  (Jennison and Turnbull 2000, p. 49):

- $(Z_1, Z_2, \dots, Z_K)$  is multivariate normal
- $Z_k \sim N(\theta\sqrt{I_k}, 1)$ ,  $k = 1, 2, \dots, K$
- $\text{Cov}(Z_{k_1}, Z_{k_2}) = \sqrt{(I_{k_1}/I_{k_2})}$ ,  $1 \leq k_1 \leq k_2 \leq K$

### Normality Assumption

The SEQDESIGN procedure derives the boundary values by assuming that the sequence of the standardized test statistics  $\{Z_1, Z_2, \dots, Z_K\}$  has the canonical joint distribution with information levels  $\{I_1, I_2, \dots, I_K\}$  for the parameter  $\theta$ . If the test statistic  $Z_k$  does not have a normal distribution, it is assumed that the test statistic is computed from a large sample, so that the resulting statistic has an approximately normal distribution.

### Number of Stages

For group sequential trials with fixed significance level  $\alpha$ , power  $1 - \beta$ , and alternative reference, if the number of stages is increased, the required maximum information is also increased, but the average sample number under the alternative hypothesis is likely to decrease.

For example, for two-sided designs with early stopping only to reject the null hypothesis  $H_0 : \theta = 0$ ,  $\alpha = 0.05$ , and  $\beta = 0.10$  at the alternative reference  $\theta_1 = \pm 0.25$ , the O'Brien-Fleming method increases the maximum information from 168.12 for a fixed-sample design to 169.32 for a two-stage design, 172.57 for a five-stage design, and then 174.42 for a ten-stage design. In the mean time, the average sample number (as a percentage of fixed-sample) under the alternative hypothesis decreases from 100 for a fixed-sample design to 85.11 for a two-stage design, 75.03 for a five-stage design, and then 71.80 for a ten-stage design. The reduction in average sample number decreases as the number of stages increases. Thus there seems to be little to gain from choosing a design with more than five stages (Pocock 1982, p. 155).

### Alternative Reference

The alternative reference  $\theta_1$  is the hypothetical reference under the alternative hypothesis at which the power is computed. It is a treatment value that the investigators would hope to detect with high probability (Jennison and Turnbull 2000, p. 21).

For a group sequential design with specified parameters such as  $\alpha$  and  $\beta$  errors, the drift parameter  $\theta_1\sqrt{I_X}$  is always derived in the SEQDESIGN procedure. Thus, with a smaller alternative reference  $\theta_1$ , a larger maximum information level  $I_X$  is needed. That is, in order to detect a smaller difference with the same high power, a larger sample size is required.

### Maximum Information

In a clinical trial, the amount of information about an unknown parameter available from the data can be measured by the Fisher information, the variance of the score statistic. The maximum information is the information level needed at the final stage of the group sequential trial if the trial does not stop at an interim stage. For a group sequential design, the maximum information can be derived with the specified alternative reference.

The maximum information is proportional to the sample size or number of events required for the design. Thus, it can also be used to compare different designs. Generally, a design with a larger probability to stop the trial early tends to have a larger maximum information. For example, for two-sided four-stage designs with early stopping only to reject  $H_0$ ,  $\alpha = 0.05$ , and  $\beta = 0.10$  at the alternative reference  $\theta_1 = \pm 0.25$ , the Pocock method has a maximum information of 198.91 and the O'Brien-Fleming method has a maximum information of 171.84, indicating a much larger information level required for the Pocock method.

### Drift Parameter

The drift parameter  $\theta_1\sqrt{I_X}$  is derived for each design in the SEQDESIGN procedure, where  $\theta_1$  is the alternative reference. It is proportional to the square root of maximum information required for the design and can be used to compare maximum information for different designs with the same alternative reference. For example, for two-sided four-stage designs with early stopping only to reject  $H_0$ ,  $\alpha = 0.05$ , and  $\beta = 0.10$ , the Pocock method has a drift parameter 3.526 and the O'Brien-Fleming method has a drift parameter 3.277, indicating that a larger maximum information level is required for the Pocock method than for the O'Brien-Fleming method.

### Average Sample Number

The average sample number is the expected sample size (for nonsurvival data) or expected number of events (for survival data) of the design under a specific hypothetical reference. The percent average sample numbers with respect to the corresponding fixed-sample design are displayed in the SEQDESIGN procedure.

The design that requires a larger maximum information level tends to have a smaller average sample number under the alternative hypothesis. For example, for two-sided four-stage designs with early stopping only to reject  $H_0$ ,  $\alpha = 0.05$ , and  $\beta = 0.10$  at the alternative reference  $\theta_1 = \pm 0.25$ , the Pocock design has a maximum information of 198.91 and an average sample number (in percentage of fixed-sample design) of 69.75 under the alternative hypothesis, and the O'Brien-Fleming design has a maximum information of 171.84 and an average sample number of 76.74.

### Sample Size

The maximum information for the sequential design expressed as a percentage of its corresponding fixed-sample information is derived in the SEQDESIGN procedure. The sample size or number of events needed for a group sequential trial is computed by multiplying the sample size or number of events for the corresponding fixed-sample design by the derived percentage.

If the sample size or number of events for the fixed-sample design is available, you can use the MODEL=INPUTNOBS or MODEL=INPUTNEVENTS option in the SAMPLESIZE statement to derive the sample size or number of events needed at each stage. Otherwise, with the specified or derived maximum information, you can use the MODEL= option in the SAMPLESIZE statement to specify a hypothesis test and then to derive the sample size or number of events needed at each stage. See the section “Sample Size Computation” on page 7042 for the sample size computation for commonly used tests.

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## Summary of Methods in Group Sequential Designs

There are three different types of methods available in the SEQDESIGN procedure: fixed boundary shape methods for specified boundary shape, Whitehead methods for boundaries from continuous monitoring, and error spending methods for specified error spending at each stage.

The fixed boundary shape methods include unified family methods and Haybittle-Peto methods. The unified family methods include Pocock, O’Brien-Fleming, power family, and triangular methods.

### Pocock Method

Pocock derives the constant boundary on the standardized  $Z$  scale to demonstrate the sequential design while maintaining the overall  $\alpha$  and  $\beta$  levels (Pocock 1977). The resulting boundary tends to stop the trials early with a larger  $p$ -value. This boundary is commonly called a Pocock boundary, but Pocock himself does not advocate these boundary values for stopping a trial early to reject the null hypothesis, because large  $p$ -values might not be persuasive enough (Pocock and White 1999). Also, the nominal  $p$ -value at the final stage is much smaller than the overall  $p$ -value of the design. That is, the trial might stop at the final stage with a small nominal  $p$ -value, but the test is not rejected, which might not be easy to justify.

### O’Brien-Fleming Method

O’Brien-Fleming boundary values are inversely proportional to the square root of information levels on the standardized  $Z$  scale (O’Brien and Fleming 1979). The O’Brien-Fleming boundary is conservative in the early stages and tends to stop the trials early only with a small  $p$ -value. But the nominal value at the final stage is close to the overall  $p$ -value of the design.

### Power Family Method

The power family method (Wang and Tsiatis 1987; Emerson and Fleming 1989; Pampallona and Tsiatis 1994) generalizes the Pocock and O’Brien-Fleming methods with a power parameter to allow continuous movement between the Pocock and O’Brien-Fleming methods. The power parameter is  $\rho = 0$  for the Pocock method and  $\rho = 0.5$  for the O’Brien-Fleming method.

### Triangular Method

The unified family triangular method (Kittelson and Emerson 1999) contains straight-line boundaries on the score scale. For a one-sided trial with early stopping either to reject and to accept the null hypothesis, the method produces a triangular continuation region. The boundary shape is specified with the slope parameter  $\tau$ .

## Unified Family Method

The unified family method (Kittelson and Emerson 1999) extends power family methods to incorporate the triangular method, which contains straight-line boundaries on the score scale.

## Haybittle-Peto Method

The Haybittle-Peto method (Haybittle 1971; Peto et al. 1976) uses a  $Z$  value of 3 for the critical values in interim stages and derives the critical value at the final stage. With this method, the final-stage critical value is close to the original design without interim monitoring. The SEQDESIGN procedure extends this method further to allow for different  $Z$  or nominal  $p$ -values for the boundaries.

## Whitehead Method

Whitehead methods (Whitehead and Stratton 1983; Whitehead 1997, 2001) derive the boundary values by adapting the continuous monitoring tests to the discrete monitoring of group sequential tests. With early stopping to reject or accept the null hypothesis in a one-sided test, the derived continuation region has a triangular shape on the score-scaled boundaries. Only elementary calculations are needed to derive the boundary values in Whitehead's triangular methods. The resulting Type I error probability and power are extremely close but differ slightly from the specified values due to the approximations used in deriving the tests (Jennison and Turnbull 2000, p. 106). The SEQDESIGN procedure provides the BOUNDARYKEY= option to adjust the boundary value at the final stage for the exact Type I or Type II error probability levels.

## Error Spending Method

The error spending method uses the specified  $\alpha$  and  $\beta$  errors to be used at each stage of the design to derive the boundary values.

## Error Spending Function Method

The error spending function method uses the error spending function to compute the  $\alpha$  and  $\beta$  errors to be used at each stage of the design and then to derive the boundary values for these errors. The following four error spending functions are available in the SEQDESIGN procedure:

- The Pocock-type error spending function (Lan and DeMets 1983) produces boundaries similar to those produced with Pocock's method.
- The O'Brien-Fleming-type error spending function (Lan and DeMets 1983) produces boundaries similar to those produced with the O'Brien-Fleming method.
- The gamma error spending function (Hwang, Shih, and DeCani 1990) specifies a gamma cumulative error spending function indexed by the gamma parameter  $\gamma$ . The boundaries created with  $\gamma = 1$  are similar to the boundaries from the Pocock method, and the boundaries created with  $\gamma = -4$  or  $\gamma = -5$  are similar to the boundaries from the O'Brien-Fleming method.
- The power error spending function (Jennison and Turnbull 2000, p. 148) specifies a power cumulative error spending function indexed by the power parameter  $\rho$ . The boundaries created with  $\rho = 1$  are similar to the boundaries from the Pocock method, and the boundaries created with  $\rho = 3$  are similar to the boundaries from the O'Brien-Fleming method.

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## Table Output

For each design, the SEQDESIGN procedure displays the “Design Information,” “Method Information,” and “Boundary Information” tables by default.

### Boundary Information

The “Boundary Information” table displays the following information at each stage:

- proportion of information
- actual information level, if the maximum information is either specified or derived
- alternative references with the specified statistic scale. If a  $p$ -value scale is specified, the standardized  $Z$  scale is used.
- boundary values with the specified statistic scale to reject or accept the null hypothesis

Note that implicitly, the boundary information table also contains variables for the boundary scale, stopping criterion, and type of alternative hypothesis. That is, if an ODS statement is used to save the table, the data set also contains the variables `_Scale_` for the boundary scale, `_Stop_` for the stopping criterion, and `_ALT_` for the type of alternative hypothesis.

### Design Information

The “Design Information” table displays the design specifications and derived statistics. The derived Max Information (Percent Fixed-Sample) is the maximum information for the sequential design in percentage of the corresponding fixed-sample information.

The Null Ref ASN (Percent Fixed-Sample) is the average sample number (expected sample size for nonsurvival data or expected number of events for survival data) required under the null hypothesis for the group sequential design in percentage of the corresponding fixed-sample design. Similarly, the Alt Ref ASN (Percent Fixed-Sample) is the average sample number required under the alternative reference for the group sequential design in percentage of the corresponding fixed-sample design.

If both the maximum information (MAXINFO= option) and the alternative reference  $\theta_1$  (ALTREF= option) are specified, then either the ALPHA= option is used to derive the Type II error probability  $\beta$  (BOUNDARYKEY=ALPHA) or the BETA= option is used to derive the Type I error probability  $\alpha$  (BOUNDARYKEY=BETA).

### Error Spending Information

The “Error Spending Information” table displays the following information at each stage:

- proportion of information
- actual information level, if the maximum information is either specified or derived
- cumulative error spending for each boundary

## Method Information

The “Method Information” table displays detailed method information for the design. For each boundary, it displays the following:

- the group sequential method used
- the  $\alpha$  or  $\beta$  errors
- the specified parameter  $\rho$ , if an error spending function is used
- the specified parameters  $\rho$  and  $\tau$  with the derived critical value  $C$ , if a unified family method is used
- the alternative reference  $\theta_1$ , if either the ALTREF= or the MAXINFO= option is specified
- the derived drift parameter,  $\theta_1 \sqrt{I_X}$ , where  $I_X$  is the maximum information and  $\theta_1$  is the alternative reference

Note that the alternative references are displayed with the MLE scale in the “Method Information” table. In contrast, the alternative references in the “Boundary Information” table are displayed with the specified statistic scale (if the  $p$ -value scale is not specified) or the standardized  $Z$  scale (if the  $p$ -value scale is specified).

## Powers and Expected Sample Sizes

The “Powers and Expected Sample Sizes” table displays the following information under each of the specified hypothetical references  $\theta = c_i \theta_1$ , where  $\theta_1$  is the alternative reference and  $c_i$  are values specified in the CREF= option.

- coefficient  $c_i$  for the hypothetical references. The value  $c_i = 0$  corresponds to the null hypothesis and  $c_i = 1$  corresponds to the alternative hypothesis
- power
- expected sample size, as percentage of fixed-sample size

For a one-sided design, the power and expected sample sizes under the hypothetical references  $\theta = c_i \theta_1$  are displayed.

For a two-sided symmetric design, the power and expected sample sizes under each of the hypothetical references  $\theta = c_i \theta_{1u}$  are displayed, where  $\theta_{1u}$  is the upper alternative reference.

For a two-sided asymmetric design, the power and expected sample sizes under each of the hypothetical references  $\theta = c_i \theta_{1l}$  and  $\theta = c_i \theta_{1u}$  are displayed, where  $\theta_{1l}$  and  $\theta_{1u}$  are the lower and upper alternative references, respectively.

For a two-sided design, the power is the probability of correctly rejecting the null hypothesis for the correct alternative. Thus, under the null hypothesis, the displayed power corresponds to a one-sided Type I error probability level—that is, the lower  $\alpha$  level or the upper  $\alpha$  level.



The expected sample size as a percentage of the corresponding fixed-sample design is

$$100 \times \frac{\sum_{k=1}^K p_k I_k}{I_0}$$

where  $p_k$  is the stopping probability at stage  $k$ ,  $\sum_{k=1}^K p_k I_k$  is the expected information level, and  $I_0$  is the information level for the fixed-sample design.

### Sample Size Summary

When you use the SAMPLESIZE statement with the SEQDESIGN procedure, the “Sample Size Summary” table displays parameters for the sample size computation. It also displays the expected sample sizes or numbers of events for the model under both the null and alternative hypotheses.

The expected sample size is the average sample size

$$\frac{\sum_{k=1}^K p_k I_k}{I_0} N_0$$

where  $p_k$  is the stopping probability at stage  $k$ ,  $\sum_{k=1}^K p_k I_k$  is the expected information level,  $I_0$  is the information level for the fixed-sample design, and  $N_0$  is the sample size for the fixed-sample design.

The expected number of events is the average number of events

$$\frac{\sum_{k=1}^K p_k I_k}{I_0} D_0$$

where  $D_0$  is the fixed-sample number of events for the model.

### Sample Size Information

The “Sample Sizes (N)” table displays the required sample sizes and information levels at each stage, in both fractional and integer numbers. The derived fractional sample sizes are under the heading “Fractional N.” These sample sizes are rounded up to integers under the heading “Ceiling N.” The matched integer sample sizes are also displayed for two-sample tests.

The “Required Number of Events (D)” table displays the required number of events required and information level at each stage.

The “Number of Events (D) and Sample Sizes (N)” table displays the number of events and sample size required at each stage with the study time. The derived times under the heading “Fractional Time” are not integers. These times are rounded up to integers under the heading “Ceiling Time.”

### Stopping Probabilities

The “Expected Cumulative Stopping Probabilities” table displays the following information under each of the specified hypothetical references  $\theta = c_i \theta_1$ , where  $c_i$  are values specified in the CREF= option, and  $\theta_1$  is the alternative reference:

- coefficient  $c_i$  for the hypothetical references. The value  $c_i = 0$  corresponds to the null hypothesis, and  $c_i = 1$  corresponds to the alternative hypothesis

- expected stopping stage
- source of the stopping probability: reject  $H_0$  (with STOP=REJECT or STOP=BOTH), accept  $H_0$  (with STOP=ACCEPT or STOP=BOTH), or either reject or accept  $H_0$  (with STOP=BOTH)
- expected cumulative stopping probabilities at each stage

For a one-sided design, the expected cumulative stopping probabilities under the hypothetical references  $\theta = c_i\theta_{1l}$  are displayed.

For a two-sided design, the expected cumulative stopping probabilities under each of the hypothetical references  $\theta = c_i\theta_{1l}$  and  $\theta = c_i\theta_{1u}$  are displayed, where  $\theta_{1l}$  and  $\theta_{1u}$  are the lower and upper alternative references, respectively.

Note that for a symmetric two-sided design, only the expected cumulative stopping probabilities under the hypothetical references  $\theta = c_i\theta_{1u}$  are derived.

The expected stopping stage is given by  $k_0 + d$ , where the integer  $k_0$  and the fraction  $d$  ( $0 \leq d < 1$ ) are derived from the expected information level equation

$$\sum_{k=1}^K p_k I_k = I_{k_0} + d (I_{(k_0+1)} - I_{k_0})$$

where  $p_k$  is the stopping probability at stage  $k$ .

For equally spaced information levels, the expected stopping stage is reduced to the weighted average

$$\sum_{k=1}^K p_k k$$

## ODS Table Names

PROC SEQDESIGN assigns a name to each table it creates. You must use these names to reference tables when using the Output Delivery System (ODS). These names are listed in Table 83.12. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

**Table 83.12** ODS Tables Produced by PROC SEQDESIGN

| ODS Table Name    | Description                    | Statement  | Option   |
|-------------------|--------------------------------|------------|----------|
| Boundary          | Boundary values                |            |          |
| Design            | Design information             |            |          |
| ErrSpend          | Error spending                 |            | ERRSPEND |
| Method            | Method information             |            |          |
| PowerSampleSize   | Power and expected sample size |            | PSS      |
| SampleSize        | Derived sample sizes           | SAMPLESIZE |          |
| SampleSizeSummary | Sample size summary            | SAMPLESIZE |          |
| StopProb          | Stopping probabilities         |            | STOPPROB |

## Graphics Output

This section describes the use of ODS for creating graphics with the SEQDESIGN procedure. To request these graphs, ODS Graphics must be enabled and you must specify the associated graphics options in the PROC SEQDESIGN statement. Except for the PLOTS=BOUNDARY option, where a detailed boundary plot is generated for each design separately, each option produces a plot for all designs together. For more information about ODS Graphics, see Chapter 21, “Statistical Graphics Using ODS.”

### Sequential ASN Plot

The PLOTS=ASN option displays the average sample numbers (expected sample sizes for nonsurvival data or expected numbers of events for survival data) under various hypothetical references. The average sample numbers are connected for each design, and these connected curves for all designs are displayed in the “Sequential ASN Plot” graph.

For a one-sided design, average sample numbers under the hypothetical references  $\theta = c_i\theta_1$  are displayed, where  $c_i$  are the values specified in the CREF= option and  $\theta_1$  is the alternative reference. The horizontal axis displays the  $c_i$  values of these hypothetical references.

For a two-sided design, average sample numbers under each of the hypothetical references  $\theta = c_i\theta_{1l}$  and  $\theta = c_i\theta_{1u}$  are displayed, where  $\theta_{1l}$  and  $\theta_{1u}$  are the lower and upper alternative references, respectively. The horizontal axis displays  $-c_i$  values for lower hypothetical references  $\theta = c_i\theta_{1l}$  and  $c_i$  values for upper hypothetical references  $\theta = c_i\theta_{1u}$ .

Note that for a symmetric two-sided design, only average sample numbers under the hypothetical references  $\theta = c_i\theta_{1u}$  are derived.

### Sequential Boundary Plot

The PLOTS=BOUNDARY option displays boundary values and the acceptance and rejection regions at each stage for each design separately in the “Detailed Boundary Information” graph. The BOUNDARYSCALE= option is used to specify the scale of the boundaries on the vertical axis. The keywords MLE, SCORE, STDZ, and PVALUE in the BOUNDARYSCALE= option correspond to the boundary with the MLE scale, score statistic scale, standardized normal Z scale, and  $p$ -value scale, respectively.

The stage numbers are displayed on the horizontal axis. In addition, the HSCALE= option in the PLOTS=BOUNDARY option can be used to specify the scale on the horizontal axis. The keywords INFO and SAMPLESIZE in the HSCALE= option correspond to the information levels and sample sizes, respectively.

### Combined Sequential Boundary Plot

The PLOTS=COMBINEDBOUNDARY option displays boundary values. The boundary values are connected for each boundary in each design, and these connected curves for all designs are displayed in the “Sequential Boundary Information” graph. The BOUNDARYSCALE= option is used to specify the scale of the boundaries on the vertical axis. The keywords MLE, SCORE, STDZ, and PVALUE in the BOUNDARYSCALE= option correspond to the boundary with the MLE scale, score statistic scale, standardized normal Z scale, and  $p$ -value scale, respectively.

The HSCALE= option in the PLOTS=COMBINEDBOUNDARY option can be used to specify the scale on the horizontal axis. The keywords INFO, SAMPLESIZE, and STAGE in the HSCALE= option correspond to the information levels, sample sizes, and stage numbers, respectively.

## Sequential Error Spending Plot

The PLOTS=ERRSPEND option displays the cumulative error spending at each stage on each boundary in the “Sequential Error Spending Plot” graph. A legend table uses the design labels to identify the curves for the corresponding design in the plot. Another legend table uses symbols to identify boundaries in the plot.

## Sequential Power Plot

The PLOTS=POWER option displays the powers under various hypothetical references. The powers are connected for each design, and these connected curves for all designs are displayed in the “Sequential Power Plot” graph.

For a one-sided design, powers under hypothetical references  $\theta = c_i\theta_1$  are displayed, where  $c_i$  are the values specified in the CREF= option and  $\theta_1$  is the alternative reference. The horizontal axis displays the  $c_i$  values of these hypothetical references.

For a two-sided design, powers under hypothetical references  $\theta = c_i\theta_{1l}$  and  $\theta = c_i\theta_{1u}$  are displayed, where  $\theta_{1l}$  and  $\theta_{1u}$  are the lower and upper alternative references, respectively. The horizontal axis displays  $-c_i$  values for lower hypothetical references  $\theta = c_i\theta_{1l}$  and  $c_i$  values for upper hypothetical references  $\theta = c_i\theta_{1u}$ .

Note that for a symmetric two-sided design, only powers under hypothetical references  $\theta = c_i\theta_{1u}$  are derived.

---

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “[Statistical Graphics Using ODS.](#)”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS.](#)”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “[A Primer on ODS Statistical Graphics](#)” on page 599 in Chapter 21, “[Statistical Graphics Using ODS.](#)”

PROC SEQDESIGN assigns a name to each graph it creates. You can use these names to reference the graphs when using ODS. To request these graphs, ODS Graphics must be enabled and you must specify the options indicated in [Table 83.13](#).

**Table 83.13** Graphs Produced by PROC SEQDESIGN

| ODS Graph Name       | Plot Description         | Option                 |
|----------------------|--------------------------|------------------------|
| ASNPlot              | Average sample numbers   | PLOTS=ASN              |
| BoundaryPlot         | Detailed boundary values | PLOTS=BOUNDARY         |
| CombinedBoundaryPlot | Boundary values          | PLOTS=COMBINEDBOUNDARY |
| ErrSpendPlot         | Error spending           | PLOTS=ERRSPEND         |
| PowerPlot            | Power curves             | PLOTS=POWER            |

---

## Examples: SEQDESIGN Procedure

The following examples demonstrate the usage of group sequential methods. [Example 83.1](#) uses the NSTAGES=1 option to derive boundaries of critical values for a fixed-sample design. The remaining examples use different methods to create boundaries for various group sequential designs.

---

### Example 83.1: Creating Fixed-Sample Designs

This example demonstrates a one-sided fixed-sample design and a two-sided fixed-sample design. The following statements request a fixed-sample design with an upper alternative:

```
ods graphics on;
proc seqdesign pss
 ;
 OneSidedFixedSample: design nstages=1
 alt=upper
 alpha=0.025 beta=0.10
 ;
 samplesize model=onesamplemean(mean=0.25);
run;
ods graphics off;
```

In the DESIGN statement, the label `OneSidedFixedSample` identifies the design in the output tables. The NSTAGES=1 option specifies that the design has only one stage; this corresponds to a fixed-sample design. In the SEQDESIGN procedure, the null hypothesis for the design is  $H_0 : \theta = 0$  and the ALT=UPPER option specifies an upper alternative hypothesis  $H_1 : \theta = \theta_1 > 0$ . The MEAN=0.25 option in the SAMPLESIZE statement specifies the upper alternative reference  $\theta_1 = 0.25$ .

The options ALPHA=0.025 and BETA=0.10 specify the Type I error probability level  $\alpha = 0.025$  and the Type II error probability level  $\beta = 0.10$ . That is, the design has a power  $1 - \beta = 0.90$  at  $\theta_1 = 0.25$ .

The “Design Information” table in [Output 83.1.1](#) displays design specifications and the derived statistics such as power. As expected, the derived statistics such as maximum information and average sample number (in percentage of its corresponding fixed-sample information) are 100 for the fixed-sample design (NSTAGES=1). Also, for a fixed-sample design, the STOP= and METHOD= options in the DESIGN statement are not applicable.

**Output 83.1.1** One-Sided Fixed-Sample Design Information

| The SEQDESIGN Procedure                   |                |
|-------------------------------------------|----------------|
| Design: OneSidedFixedSample               |                |
| Design Information                        |                |
| Statistic Distribution                    | Normal         |
| Boundary Scale                            | Standardized Z |
| Alternative Hypothesis                    | Upper          |
| Alternative Reference                     | 0.25           |
| Number of Stages                          | 1              |
| Alpha                                     | 0.025          |
| Beta                                      | 0.1            |
| Power                                     | 0.9            |
| Max Information (Percent of Fixed Sample) | 100            |
| Max Information                           | 168.1188       |
| Null Ref ASN (Percent of Fixed Sample)    | 100            |
| Alt Ref ASN (Percent of Fixed Sample)     | 100            |

The “Method Information” table in [Output 83.1.2](#) displays the  $\alpha$  and  $\beta$  error levels. It also displays the derived drift parameter, which is the standardized reference improvement,  $\theta_1 \sqrt{I_0}$ , where  $\theta_1$  is the alternative reference and  $I_0$  is the maximum information for the design. If either  $\theta_1$  or  $I_0$  is specified, the other statistic is derived in the SEQDESIGN procedure. For a fixed-sample design,

$$\theta_1 \sqrt{I_0} = \Phi^{-1}(1 - \alpha) + \Phi^{-1}(1 - \beta) = \Phi^{-1}(0.975) + \Phi^{-1}(0.90) = 3.2415$$

**Output 83.1.2** Method Information

| Method Information |         |         |                       |          |
|--------------------|---------|---------|-----------------------|----------|
| Boundary           | Alpha   | Beta    | Alternative Reference | Drift    |
| Upper Alpha        | 0.02500 | 0.10000 | 0.25                  | 3.241516 |

The “Boundary Information” table in [Output 83.1.3](#) displays information level, alternative reference, and boundary value at each stage. The information proportion indicates the proportion of maximum information available at the stage. With only one stage for a fixed-sample design, the proportion is 1. With the SAMPLESIZE statement, the required sample size  $N$  is also displayed under the heading “Information Level.”

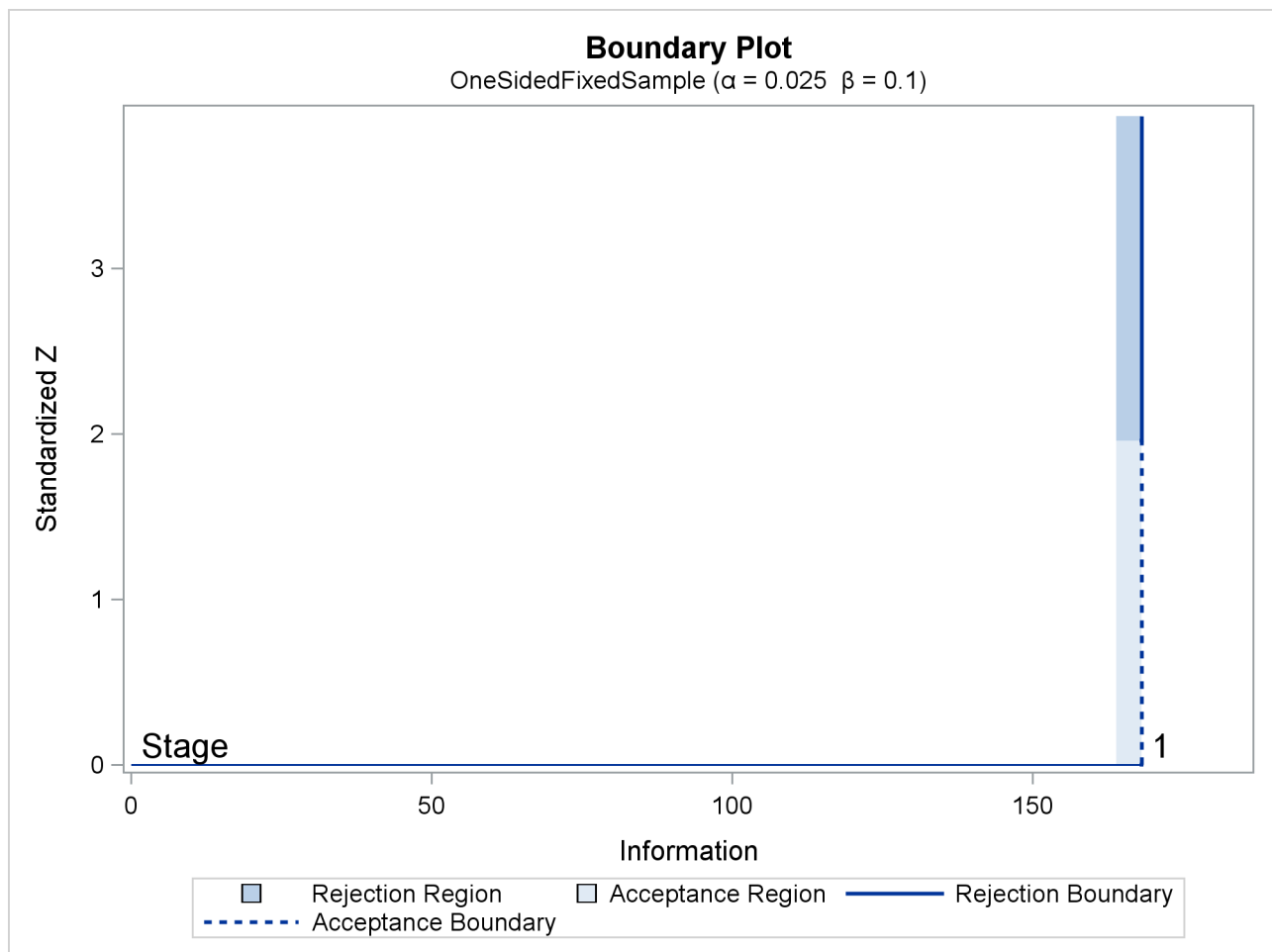
**Output 83.1.3** Boundary Information

| Boundary Information (Standardized Z Scale) |                             |          |          |                        |                          |         |
|---------------------------------------------|-----------------------------|----------|----------|------------------------|--------------------------|---------|
| Null Reference = 0                          |                             |          |          |                        |                          |         |
| _Stage_                                     | -----Information Level----- |          |          | -Alternative-          | -Boundary Values-        |         |
|                                             | Proportion                  | Actual   | N        | --Reference--<br>Upper | -----Upper-----<br>Alpha |         |
| 1                                           | 1.0000                      | 168.1188 | 168.1188 | 3.24152                |                          | 1.95996 |

By default (or equivalently if you specify BOUNDARYSCALE=STDZ), output alternative references and boundaries are displayed with the standardized normal Z scale. The alternative reference on the standardized Z scale at stage 1 is given by  $\theta_1 \sqrt{I_1}$ , where  $I_1$  is the information level at stage 1. With a boundary value 1.96, the hypothesis of  $\theta = 0$  is rejected if the standardized normal statistic  $Z \geq 1.96$ .

With ODS Graphics enabled, a detailed boundary plot with the rejection and acceptance regions is displayed, as shown in [Output 83.1.4](#). The boundary values in the “Boundary Information” table in [Figure 83.1.3](#) are displayed in the plot.

**Output 83.1.4** Boundary Plot



The “Sample Size Summary” table in [Output 83.1.5](#) displays parameters for the sample size computation of the test for a normal mean.

**Output 83.1.5** Sample Size Summary

| Sample Size Summary             |                 |
|---------------------------------|-----------------|
| Test                            | One-Sample Mean |
| Mean                            | 0.25            |
| Standard Deviation              | 1               |
| Max Sample Size                 | 168.1188        |
| Expected Sample Size (Null Ref) | 168.1188        |
| Expected Sample Size (Alt Ref)  | 168.1188        |

The “Sample Sizes (N)” table in [Output 83.1.6](#) displays the derived sample sizes, in both fractional and integer numbers. With the resulting integer sample sizes, the corresponding information level is slightly larger than the level from the design. This can increase the power slightly if the integer sample size is used in the trial.

**Output 83.1.6** Derived Sample Sizes

| Sample Sizes (N)           |                        |             |                     |             |
|----------------------------|------------------------|-------------|---------------------|-------------|
| One-Sample Z Test for Mean |                        |             |                     |             |
| _Stage_                    | -----Fractional N----- |             | -----Ceiling N----- |             |
|                            | N                      | Information | N                   | Information |
| 1                          | 168.12                 | 168.1       | 169                 | 169.0       |

The following statements request a two-sided fixed-sample design with a specified alternative reference:

```
ods graphics on;
proc seqdesign altref=1.2
 pss
 ;
 TwoSidedFixedSample: design nstages=1
 alt=twosided
 alpha=0.05 beta=0.10
 ;
 samplesize model=twosamplemean(stddev=2 weight=2);
run;
ods graphics off;
```

In the SEQDESIGN procedure, the null hypothesis for the design is  $H_0 : \theta = 0$ . The ALT=TWOSIDED option specifies a two-sided alternative hypothesis  $H_1 : \theta = \theta_1 \neq 0$ . The ALTREF=1.2 option in the PROC SEQDESIGN statement specifies the alternative reference  $\theta_1 = \pm 1.2$ .

The ALPHA=0.05 option (which is the default) specifies the two-sided Type I error probability level  $\alpha = 0.05$ . That is, the lower and upper Type I error probabilities  $\alpha_l = \alpha_u = 0.025$ . The BETA=0.10 option (which is the default) specifies the Type II error probability level  $\beta = 0.10$ , and the design has a power  $1 - \beta = 0.90$  at the alternative reference  $\theta_1 = \pm 1.2$ .



The “Design Information” table in [Output 83.1.7](#) displays design specifications and the derived power. With a specified alternative reference, the maximum information is derived.

**Output 83.1.7** Two-Sided Fixed-Sample Design Information

| The SEQDESIGN Procedure                   |                |
|-------------------------------------------|----------------|
| Design: TwoSidedFixedSample               |                |
| Design Information                        |                |
| Statistic Distribution                    | Normal         |
| Boundary Scale                            | Standardized Z |
| Alternative Hypothesis                    | Two-Sided      |
| Alternative Reference                     | 1.2            |
| Number of Stages                          | 1              |
| Alpha                                     | 0.05           |
| Beta                                      | 0.1            |
| Power                                     | 0.9            |
| Max Information (Percent of Fixed Sample) | 100            |
| Max Information                           | 7.296822       |
| Null Ref ASN (Percent of Fixed Sample)    | 100            |
| Alt Ref ASN (Percent of Fixed Sample)     | 100            |

The “Method Information” table in [Output 83.1.8](#) displays the  $\alpha$  and  $\beta$  errors, alternative references, and drift parameter. For a fixed-sample design, the derived drift parameter

$$\theta_1 \sqrt{I_0} = \Phi^{-1}\left(1 - \frac{\alpha}{2}\right) + \Phi^{-1}(1 - \beta) = \Phi^{-1}(0.975) + \Phi^{-1}(0.90) = 3.2415$$

**Output 83.1.8** Method Information

| Method Information |         |         |                       |          |
|--------------------|---------|---------|-----------------------|----------|
| Boundary           | Alpha   | Beta    | Alternative Reference | Drift    |
| Upper Alpha        | 0.02500 | 0.10000 | 1.2                   | 3.241516 |
| Lower Alpha        | 0.02500 | 0.10000 | -1.2                  | -3.24152 |

With a specified alternative reference  $\theta_1 = 1.2$ , the maximum information

$$I_0 = \left( \frac{3.2415}{1.2} \right)^2 = 7.2968$$

The default “Boundary Information” table in [Output 83.1.9](#) displays information level, alternative reference, and boundary values. By default (or equivalently if you specify BOUNDARYSCALE=STDZ), the alternative reference and boundary values are displayed with the standardized normal Z scale. Thus, the standardized alternative references  $\pm\theta_1\sqrt{I_0}$  are displayed.

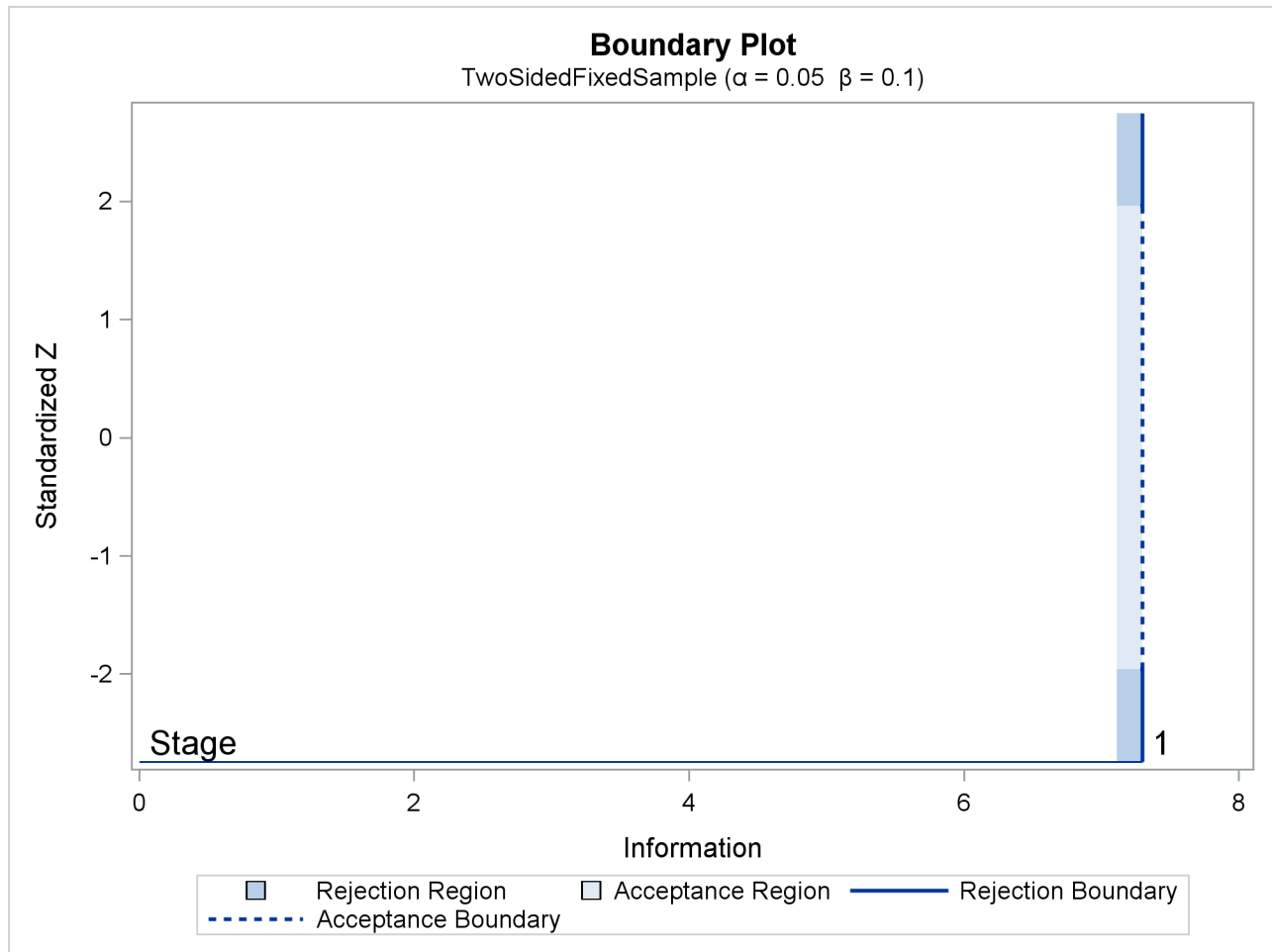
**Output 83.1.9** Boundary Information

| Boundary Information (Standardized Z Scale) |                             |          |          |                       |         |
|---------------------------------------------|-----------------------------|----------|----------|-----------------------|---------|
| Null Reference = 0                          |                             |          |          |                       |         |
| _Stage_                                     | -----Information Level----- |          |          | -----Alternative----- |         |
|                                             | Proportion                  | Actual   | N        | Lower                 | Upper   |
| 1                                           | 1.0000                      | 7.296822 | 131.3428 | -3.24152              | 3.24152 |
| Boundary Information (Standardized Z Scale) |                             |          |          |                       |         |
| Null Reference = 0                          |                             |          |          |                       |         |
| _Stage_                                     | -----Boundary Values----    |          |          |                       |         |
|                                             | Alpha                       | Alpha    |          |                       |         |
| 1                                           | -1.95996                    | 1.95996  |          |                       |         |

With boundary values of  $-1.96$  and  $1.96$ , the hypothesis of  $\theta = 0$  is rejected if the standardized normal statistic  $Z \geq 1.96$  or  $Z \leq -1.96$ .

With ODS Graphics enabled, a detailed boundary plot with the rejection and acceptance regions is displayed, as shown in [Output 83.1.10](#). The boundary values in the “Boundary Information” table in [Figure 83.1.9](#) are displayed in the plot.

**Output 83.1.10** Boundary Plot



The “Sample Size Summary” table in [Output 83.1.11](#) displays parameters for the sample size computation of the test for a normal mean.

**Output 83.1.11** Sample Size Summary

| Sample Size Summary             |                  |
|---------------------------------|------------------|
| Test                            | Two-Sample Means |
| Mean Difference                 | 1.2              |
| Standard Deviation              | 2                |
| Max Sample Size                 | 131.3428         |
| Expected Sample Size (Null Ref) | 131.3428         |
| Expected Sample Size (Alt Ref)  | 131.3428         |
| Weight (Group A)                | 2                |
| Weight (Group B)                | 1                |

The “Sample Sizes (N)” table in [Output 83.1.12](#) displays the derived sample sizes, in both fractional and integer numbers. With the WEIGHT=2 option, the allocation ratio is 2 for the first group and 1 for the second group. With the resulting integer sample sizes, the corresponding information level is slightly larger

than the level from the design. This can increase the power slightly if the integer sample size is used in the trial.

**Output 83.1.12** Derived Sample Sizes

| Sample Sizes (N)                      |        |          |          |             |
|---------------------------------------|--------|----------|----------|-------------|
| Two-Sample Z Test for Mean Difference |        |          |          |             |
| -----Fractional N-----                |        |          |          |             |
| _Stage_                               | N      | N(Grp 1) | N(Grp 2) | Information |
| 1                                     | 131.34 | 87.56    | 43.78    | 7.2968      |
| Sample Sizes (N)                      |        |          |          |             |
| Two-Sample Z Test for Mean Difference |        |          |          |             |
| -----Ceiling N-----                   |        |          |          |             |
| _Stage_                               | N      | N(Grp 1) | N(Grp 2) | Information |
| 1                                     | 132    | 88       | 44       | 7.3333      |

**Example 83.2: Creating a One-Sided O'Brien-Fleming Design**

This example demonstrates a group sequential design for a clinical study. A clinic is conducting a study on the effect of vitamin C supplements in treating flu symptoms. The study groups consist of patients in the clinic with their first sign of flu symptoms within the last 24 hours. These individuals are randomly assigned to either the control group, which receives the placebo pills, or the treatment group, which receives large doses of vitamin C supplements. At the end of a five-day period, the flu symptoms of each individual are recorded.

Suppose that from past experience, 60% of individuals experiencing flu symptoms have the symptoms disappeared within five days. The clinic wants to detect a 75% symptoms disappearance with a high probability in the trial. A test that compares the proportions directly is to specify a null hypothesis  $H_0 : \theta = p_a - p_b = 0$  with a Type I error probability level  $\alpha = 0.025$ , where  $p_a$  and  $p_b$  are the proportions of symptoms' disappearance in the treatment group and control group, respectively. A one-sided alternative  $H_1 : \theta > 0$  is also specified with a power of  $1 - \beta = 0.90$  at  $H_1 : \theta = 0.15$ .

For a one-sided fixed-sample design, the critical value for the standardized Z test statistic is given by  $C_\alpha = \Phi^{-1}(1 - \alpha) = 1.96$ . That is, at the end of study, if the test statistic  $z \geq C_\alpha$ , then the null hypothesis is rejected and the efficacy of vitamin C supplements is declared. Otherwise, the null hypothesis is not rejected and the effect of vitamin C supplements is not significant.

To achieve a  $1 - \beta = 0.90$  power at  $H_1 : \theta = 0.15$  for a fixed-sample design, the information required is given by

$$I_0 = \frac{(\Phi^{-1}(1 - \alpha) + \Phi^{-1}(1 - \beta))^2}{0.15^2} = \frac{(1.96 + 1.28155)^2}{0.0225} = 466.99$$

With an equal sample size on the treatment and control groups,  $N_a = N_b$ , the sample size required for each group under  $H_1$  is computed from the information  $I_0$ :

$$N_a = N_b = (p_{1a}(1 - p_{1a}) + p_{1b}(1 - p_{1b})) I_0$$

where  $p_{1a} = 0.75$  and  $p_{1b} = 0.60$  are proportions in the treatment and control groups under  $H_1$ . That is,

$$N_a = N_b = (0.75 \times 0.25 + 0.6 \times 0.4) \times 466.99 = 199.64$$

Thus, 200 individuals are required for each group in the fixed-sample study. See the section “[Test for the Difference between Two Binomial Proportions](#)” on page 7054 for a detailed derivation of these required sample sizes.

Instead of a fixed-sample design for the trial, a group sequential design is used to stop the trial early for ethical concerns of possible harm or an unexpected strong efficacy outcome of the new drug. It can also save time and resources in the process. The following statements invoke the SEQDESIGN procedure and request a four-stage group sequential design that uses an O’Brien-Fleming method for normally distributed statistics. The design uses a one-sided alternative hypothesis  $H_1$  with early stopping to reject or accept  $H_0$ .

```
ods graphics on;
proc seqdesign altref=0.15
 ;
 OneSidedOBrienFleming: design nstages=4
 method=obf
 alt=upper stop=both
 alpha=0.025 beta=0.10
 ;
 sample size model=twosamplefreq(nullprop=0.6 test=prop);
ods output Boundary=Bnd_Prop;
run;
ods graphics off;
```

In a sequential design, a hypothesis can be rejected, accepted, or continued to the next time point at each interim stage. The STOP=BOTH option specifies early stopping to reject or accept the null hypothesis. The “Design Information,” “Method Information,” and “Boundary Information” tables are displayed by default.

The “Design Information” table in [Output 83.2.1](#) displays design specifications and derived statistics such as power and maximum information. With a specified alternative reference, ALTREF=0.15, the maximum information  $I_X$  is derived.

**Output 83.2.1** Design Information

| The SEQDESIGN Procedure                   |                    |
|-------------------------------------------|--------------------|
| Design: OneSidedOBrienFleming             |                    |
| Design Information                        |                    |
| Statistic Distribution                    | Normal             |
| Boundary Scale                            | Standardized Z     |
| Alternative Hypothesis                    | Upper              |
| Early Stop                                | Accept/Reject Null |
| Method                                    | O'Brien-Fleming    |
| Boundary Key                              | Both               |
| Alternative Reference                     | 0.15               |
| Number of Stages                          | 4                  |
| Alpha                                     | 0.025              |
| Beta                                      | 0.1                |
| Power                                     | 0.9                |
| Max Information (Percent of Fixed Sample) | 107.6741           |
| Max Information                           | 502.8343           |
| Null Ref ASN (Percent of Fixed Sample)    | 61.12891           |
| Alt Ref ASN (Percent of Fixed Sample)     | 75.89782           |

The Max Information (Percent Fixed-Sample) is the ratio in percentage between the maximum information for the group sequential design and the information required for a corresponding fixed-sample design:

$$100 \times \frac{I_X}{I_0} = 100 \times \frac{502.83}{466.99} = 107.67$$

That is, if the group sequential trial does not stop at any interim stages, the information needed is 7.67% more than is needed for the corresponding fixed-sample design. For a two-sample test for binomial proportions, the information is proportional to the sample size. Thus, 7.67% more observations are needed for the group sequential trial.

The Null Ref ASN (Percent Fixed-Sample) is the ratio in percentage between the expected sample size required under the null hypothesis for the group sequential design and the sample size required for the corresponding fixed-sample design. With a ratio of 61.1%, the expected sample size for the group sequential trial under the null hypothesis is 61.1% of the sample size in the corresponding fixed-sample design.

Similarly, the Alt Ref ASN (Percent Fixed-Sample) is the ratio in percentage between the expected sample size required under the alternative hypothesis for the group sequential design and the sample size required for the corresponding fixed-sample design. With a ratio of 75.9%, the expected sample size for the group sequential trial under the alternative hypothesis is 75.9% of the sample size in the corresponding fixed-sample design.

For a one-sided design with an upper alternative and early stopping to reject or accept the null hypothesis, upper  $\alpha$  and  $\beta$  boundaries are created. The “Method Information” table in [Output 83.2.2](#) displays the Type I error probability  $\alpha$ , the Type II error probability  $\beta$ , and the derived drift parameter. The drift parameter is the standardized reference improvement between the alternative and null hypotheses at the final stage. It is also the standardized alternative reference at the final stage if the null reference is zero.

**Output 83.2.2** Method Information

| Method Information |                 |                       |         |                          |     |        |
|--------------------|-----------------|-----------------------|---------|--------------------------|-----|--------|
| Boundary           | Method          | Alpha                 | Beta    | -----Unified Family----- |     |        |
|                    |                 |                       |         | Rho                      | Tau | C      |
| Upper Alpha        | O'Brien-Fleming | 0.02500               | .       | 0.5                      | 0   | 1.9784 |
| Upper Beta         | O'Brien-Fleming | .                     | 0.10000 | 0.5                      | 0   | 1.3852 |
| Method Information |                 |                       |         |                          |     |        |
|                    | Boundary        | Alternative Reference |         | Drift                    |     |        |
|                    | Upper Alpha     | 0.15                  |         | 3.363595                 |     |        |
|                    | Upper Beta      | 0.15                  |         | 3.363595                 |     |        |

With the METHOD=OBF option, the O'Brien-Fleming method is used for each boundary. The O'Brien-Fleming method is one of the unified family methods, and the “Method Information” table displays the corresponding parameter  $\rho$  in the unified family method. The table also displays the critical values  $C_\alpha = 1.9784$  for the  $\alpha$  boundary and  $C_\beta = 1.3852$  for the  $\beta$  boundary. These critical values are used to create the boundary values.

The “Boundary Information” table in [Output 83.2.3](#) displays information level, alternative reference, and boundary values at each stage. By default (or equivalently if you specify BOUNDARYSCALE=STDZ), the alternative references and boundary values are displayed with the standardized Z statistic scale. The resulting standardized alternative reference at stage  $k$  is given by  $\theta_1 \sqrt{I_k}$ , where  $\theta_1$  is the alternative reference and  $I_k$  is the information level at stage  $k$ ,  $k = 1, 2, 3, 4$ .

**Output 83.2.3** Boundary Information

| Boundary Information (Standardized Z Scale) |                             |          |          |                        |                         |         |
|---------------------------------------------|-----------------------------|----------|----------|------------------------|-------------------------|---------|
| Null Reference = 0                          |                             |          |          |                        |                         |         |
| _Stage_                                     | -----Information Level----- |          |          | -Alternative-          | ----Boundary Values---- |         |
|                                             | Proportion                  | Actual   | N        | --Reference--<br>Upper | -----Upper-----<br>Beta | Alpha   |
| 1                                           | 0.2500                      | 125.7086 | 107.4808 | 1.68180                | -1.08860                | 3.95679 |
| 2                                           | 0.5000                      | 251.4171 | 214.9617 | 2.37842                | 0.41946                 | 2.79788 |
| 3                                           | 0.7500                      | 377.1257 | 322.4425 | 2.91296                | 1.31347                 | 2.28446 |
| 4                                           | 1.0000                      | 502.8343 | 429.9233 | 3.36360                | 1.97840                 | 1.97840 |

By default (or equivalently if you specify INFO=EQUAL), equally spaced information levels are used. An information proportion is the proportion of maximum information available at each stage. With the derived maximum information, the actual information level at each stage is also displayed. With the SAMPLESIZE statement, the required sample size  $N$  is also displayed under the heading “Information Level.”

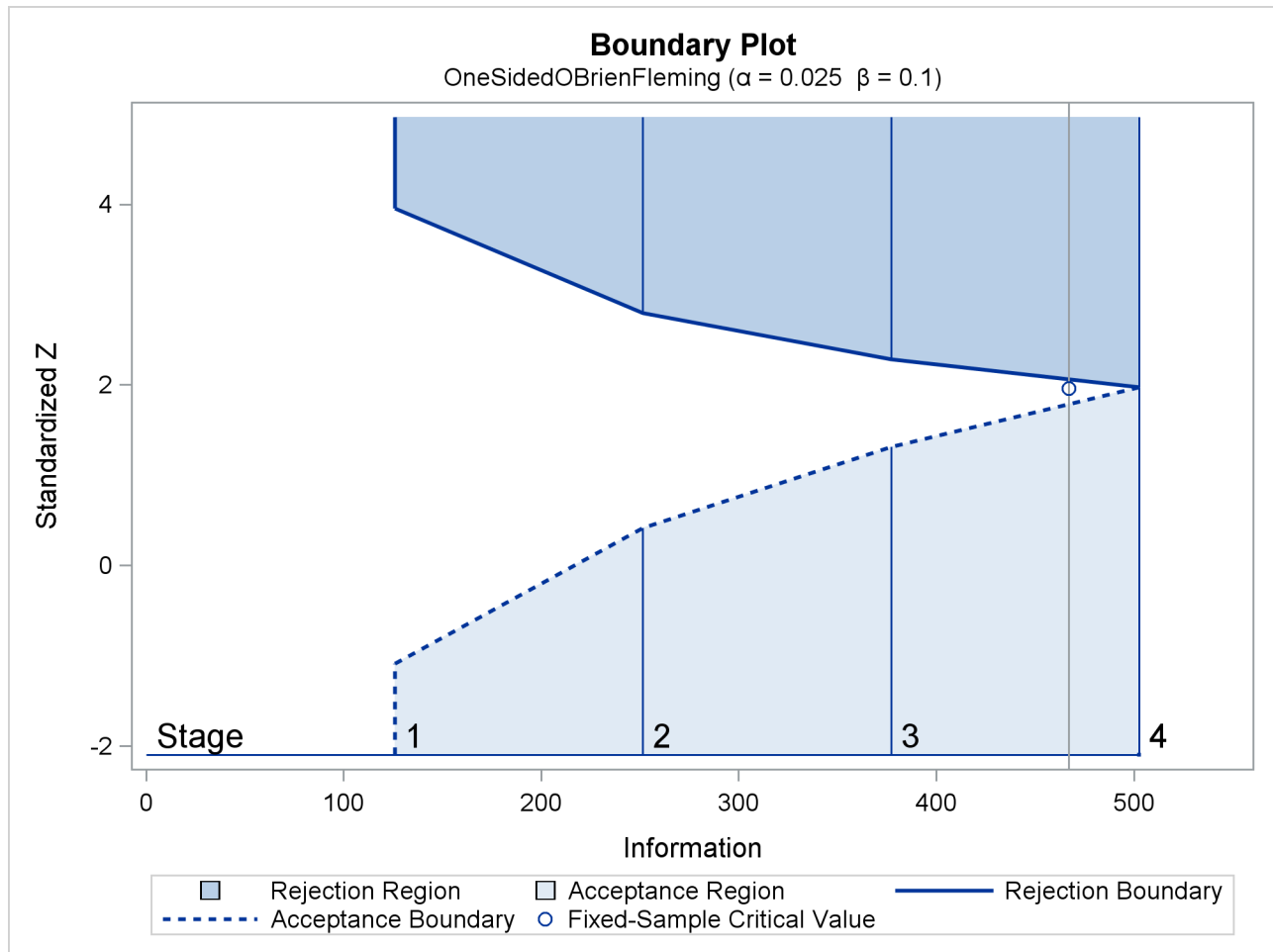
At each interim stage, if the standardized  $Z$  test statistic is larger than or equal to the corresponding upper  $\alpha$  boundary, then the hypothesis  $H_0 : \theta = 0$  is rejected. If the test statistic is less than the corresponding upper  $\beta$  boundary, then the trial is stopped and the hypothesis  $H_0$  is accepted. Otherwise, the process continues to the next stage. At the final stage, stage 4, the trial stops and the hypothesis  $H_0$  is rejected if the standardized  $Z$  statistic  $Z_4 \geq 1.9784$ . Otherwise, the trial is accepted.

The ODS OUTPUT statement with the BOUNDARY=BND\_PROP option creates an output data set that contains the resulting boundary information. After the actual data from the clinical trial are collected and analyzed at each stage with a procedure such as PROC GENMOD, the SEQTEST procedure is used to test the resulting statistics at stage 1 with the boundary information stored in the BOUND\_PROP data set.

With ODS Graphics enabled, a detailed boundary plot with the rejection and acceptance regions is displayed, as shown in [Output 83.2.4](#).



Output 83.2.4 Boundary Plot



The horizontal axis indicates the information levels for the design. The stages are indicated by vertical lines with accompanying stage numbers. If at any stage a test statistic is in a rejection region, the trial stops and the hypothesis is rejected. If a test statistic is in an acceptance region, then the trial also stops and the hypothesis is accepted. If the statistic is not in a rejection region or an acceptance region, the trial continues to the next stage. The boundary plot also displays the information level and the critical value for the corresponding fixed-sample design.

The SEQDESIGN procedure derives the drift parameter  $\theta_1 \sqrt{I_X}$ , where  $\theta_1$  is the alternative reference and  $I_X$  is the maximum information. If either  $\theta_1$  or  $I_X$  is specified, the other can be derived. With the SAMPLESIZE statement, the maximum information is used to compute the required sample size for the study.

The “Sample Size Summary” table in [Output 83.2.5](#) displays parameters for the sample size computation. With the MODEL=TWOSAMPLEFREQ( NULLPROP=0.6 TEST=PROP) option in the SAMPLESIZE statement, the total sample size in each group for testing the difference between two proportions is computed. By default (or equivalently if you specify REF=PROP in the MODEL=TWOSAMPLEFREQ option), the required sample sizes are computed under the alternative hypothesis. That is,

$$N_a = N_b = (p_{1a}(1 - p_{1a}) + p_{1b}(1 - p_{1b})) I_X$$

where  $p_{1b} = 0.60$  and  $p_{1a} = p_{1b} + \theta_1 = 0.75$  are the proportions in the control and treatment groups, respectively, under the alternative hypothesis  $H_1$ . See the section “[Test for the Difference between Two Binomial Proportions](#)” on page 7054 for a detailed description of these parameters.

**Output 83.2.5** Sample Size Summary

| Sample Size Summary             |                        |
|---------------------------------|------------------------|
| Test                            | Two-Sample Proportions |
| Null Proportion                 | 0.6                    |
| Proportion (Group A)            | 0.75                   |
| Test Statistic                  | Z for Proportion       |
| Reference Proportions           | Alt Ref                |
| Max Sample Size                 | 429.9233               |
| Expected Sample Size (Null Ref) | 244.0768               |
| Expected Sample Size (Alt Ref)  | 303.0464               |

The “Sample Sizes (N)” table in [Output 83.2.6](#) displays the required sample sizes at each stage, in both fractional and integer numbers. The derived fractional sample sizes are under the heading “Fractional N.” These sample sizes are rounded up to integers under the heading “Ceiling N.” In practice, integer sample sizes are used, and the resulting information levels increase slightly. Thus, 54, 108, 162, and 215 individuals are needed in each group for the four stages, respectively.

**Output 83.2.6** Derived Sample Sizes

| Sample Sizes (N)                            |        |          |          |             |
|---------------------------------------------|--------|----------|----------|-------------|
| Two-Sample Z Test for Proportion Difference |        |          |          |             |
| -----Fractional N-----                      |        |          |          |             |
| _Stage_                                     | N      | N(Grp 1) | N(Grp 2) | Information |
| 1                                           | 107.48 | 53.74    | 53.74    | 125.7       |
| 2                                           | 214.96 | 107.48   | 107.48   | 251.4       |
| 3                                           | 322.44 | 161.22   | 161.22   | 377.1       |
| 4                                           | 429.92 | 214.96   | 214.96   | 502.8       |

| Sample Sizes (N)                            |     |          |          |             |
|---------------------------------------------|-----|----------|----------|-------------|
| Two-Sample Z Test for Proportion Difference |     |          |          |             |
| -----Ceiling N-----                         |     |          |          |             |
| _Stage_                                     | N   | N(Grp 1) | N(Grp 2) | Information |
| 1                                           | 108 | 54       | 54       | 126.3       |
| 2                                           | 216 | 108      | 108      | 252.6       |
| 3                                           | 324 | 162      | 162      | 378.9       |
| 4                                           | 430 | 215      | 215      | 502.9       |

**Example 83.3: Creating Two-Sided Pocock and O'Brien-Fleming Designs**

This example requests two 4-stage group sequential designs for normally distributed statistics with equally spaced information levels at all stages. One design uses Pocock's method and the other uses the O'Brien-Fleming method. The following statements invoke the SEQDESIGN procedure and request these two designs:

```
proc seqdesign altref=0.4
 pss
 stopprob
 errspend
 ;
 TwoSidedPocock: design nstages=4 method=poc;
 TwoSidedOBrienFleming: design nstages=4 method=obf;
 sample size model=twosamplemean(stddev=0.8 weight=2);
run;
```

By default (or equivalently if you specify ALT=TWOSIDED and STOP=REJECT in the DESIGN statement), each design has a null hypothesis  $H_0$  with a two-sided alternative with early stopping to reject  $H_0$ .

The “Design Information” table in [Output 83.3.1](#) displays design specifications and derived statistics for the Pocock’s design. With the specified ALTREF= option, the maximum information  $I_X = 77.6984$  is also derived.

**Output 83.3.1** Pocock Design Information

| The SEQDESIGN Procedure                   |                |
|-------------------------------------------|----------------|
| Design: TwoSidedPocock                    |                |
| Design Information                        |                |
| Statistic Distribution                    | Normal         |
| Boundary Scale                            | Standardized Z |
| Alternative Hypothesis                    | Two-Sided      |
| Early Stop                                | Reject Null    |
| Method                                    | Pocock         |
| Boundary Key                              | Both           |
| Alternative Reference                     | 0.4            |
| Number of Stages                          | 4              |
| Alpha                                     | 0.05           |
| Beta                                      | 0.1            |
| Power                                     | 0.9            |
| Max Information (Percent of Fixed Sample) | 118.3143       |
| Max Information                           | 77.69844       |
| Null Ref ASN (Percent of Fixed Sample)    | 115.6074       |
| Alt Ref ASN (Percent of Fixed Sample)     | 69.74805       |

With the corresponding fixed-sample information

$$I_0 = \frac{(\Phi^{-1}(1 - \alpha/2) + \Phi^{-1}(1 - \beta))^2}{0.4^2} = \frac{(1.96 + 1.28155)^2}{0.16} = 65.6728$$

the fixed-sample information ratio is  $77.6984/65.6728 = 1.1831$ .

For a two-sided design with early stopping to reject the null hypothesis, lower and upper  $\alpha$  boundaries are created. The “Method Information” table in [Output 83.3.2](#) displays the  $\alpha$  and  $\beta$  errors, alternative references, and derived drift parameters, which are the standardized alternative references at the final stage.

**Output 83.3.2** Method Information

| Method Information |        |         |         |                          |     |         |
|--------------------|--------|---------|---------|--------------------------|-----|---------|
| Boundary           | Method | Alpha   | Beta    | -----Unified Family----- |     |         |
|                    |        |         |         | Rho                      | Tau | C       |
| Upper Alpha        | Pocock | 0.02500 | 0.10000 | 0                        | 0   | 2.36129 |
| Lower Alpha        | Pocock | 0.02500 | 0.10000 | 0                        | 0   | 2.36129 |

| Method Information |                       |          |
|--------------------|-----------------------|----------|
| Boundary           | Alternative Reference | Drift    |
| Upper Alpha        | 0.4                   | 3.525869 |
| Lower Alpha        | -0.4                  | -3.52587 |

With the METHOD=POC option, the Pocock method is used for each boundary. The Pocock method is one of the unified family methods, and the table also displays its corresponding parameters  $\rho = 0$  as a unified family method and the derived parameters  $C = 2.3613$  for the boundary values.

With the PSS option, the “Power and Expected Sample Sizes” table in [Output 83.3.3](#) displays powers and expected sample sizes under various hypothetical references  $\theta = c_i \theta_1$ , where  $\theta_1$  is the alternative reference and  $c_i$  are values specified in the CREF= option. By default,  $c_i = 0, 0.5, 1.0, 1.5$ .

**Output 83.3.3** Power and Expected Sample Size Information

| Powers and Expected Sample Sizes   |         |                                          |
|------------------------------------|---------|------------------------------------------|
| Reference = CRef * (Alt Reference) |         |                                          |
| CRef                               | Power   | -Sample Size-<br>Percent<br>Fixed-Sample |
| 0.0000                             | 0.02500 | 115.6074                                 |
| 0.5000                             | 0.34252 | 104.0615                                 |
| 1.0000                             | 0.90000 | 69.7480                                  |
| 1.5000                             | 0.99869 | 43.6600                                  |

Note that at  $c_i = 0$ , the null reference  $\theta = 0$ , and the power 0.025 corresponds to the one-sided Type I error probability 0.025. At  $c_i = 1$ ,  $\theta = \theta_1$ , the power 0.9 is the power of the design. The expected sample sizes are displayed in a percentage scale to its corresponding fixed-sample size design. With the specified SAMPLESIZE statement, the expected sample sizes for the specified model in the SAMPLESIZE statement are also displayed.

With the STOPPROB option, the “Expected Cumulative Stopping Probabilities” table in Output 83.3.4 displays the expected cumulative stopping stage and cumulative stopping probability to reject the null hypothesis  $H_0$  at each stage under various hypothetical references  $\theta = c_i \theta_1$ , where  $\theta_1$  is the alternative reference and  $c_i$  are values specified in the CREF= option. By default,  $c_i = 0, 0.5, 1.0, 1.5$ .

**Output 83.3.4** Stopping Probabilities

| Expected Cumulative Stopping Probabilities |                         |             |                                  |         |         |         |  |
|--------------------------------------------|-------------------------|-------------|----------------------------------|---------|---------|---------|--|
| Reference = CRef * (Alt Reference)         |                         |             |                                  |         |         |         |  |
| CRef                                       | Expected Stopping Stage | Source      | -----Stopping Probabilities----- |         |         |         |  |
|                                            |                         |             | Stage_1                          | Stage_2 | Stage_3 | Stage_4 |  |
| 0.0000                                     | 3.908                   | Reject Null | 0.01821                          | 0.03155 | 0.04176 | 0.05000 |  |
| 0.5000                                     | 3.518                   | Reject Null | 0.07005                          | 0.15939 | 0.25242 | 0.34327 |  |
| 1.0000                                     | 2.358                   | Reject Null | 0.27482                          | 0.58074 | 0.78638 | 0.90002 |  |
| 1.5000                                     | 1.476                   | Reject Null | 0.61145                          | 0.92348 | 0.98900 | 0.99869 |  |

Note that at  $c_i = 0$ , the cumulative stopping probability to reject  $H_0$  at the final stage is the overall Type I error probability 0.05. At  $c_i = 1$ , the alternative hypothesis  $H_1 : \theta = \theta_1$ , the cumulative stopping probability to reject  $H_0$  includes both the probability in the lower rejection region and the probability in the upper rejection region. This stopping probability to reject  $H_0$  at the final stage, 0.90002, is slightly greater than the power  $1 - \beta = 0.90$ , which corresponds to the cumulative stopping probability in the upper rejection region only. See the section “Type I and Type II Errors” on page 7022 for a detailed description of the Type II error probability  $\beta$ .

The “Boundary Information” table in Output 83.3.5 displays the information level, alternative references, and boundary values at each stage. By default (or equivalently if you specify BOUNDARYSCALE=STDZ), the standardized Z scale is used to display the alternative references and boundary values. The resulting standardized alternative reference at stage  $k$  is given by  $\theta_1 \sqrt{I_k}$ , where  $\theta_1$  is the alternative reference and  $I_k$  is the information level at stage  $k$ ,  $k = 1, 2, 3, 4$ .

**Output 83.3.5** Boundary Information

| Boundary Information (Standardized Z Scale) |                             |          |          |                       |         |
|---------------------------------------------|-----------------------------|----------|----------|-----------------------|---------|
| Null Reference = 0                          |                             |          |          |                       |         |
| _Stage_                                     | -----Information Level----- |          |          | -----Alternative----- |         |
|                                             | Proportion                  | Actual   | N        | Lower                 | Upper   |
| 1                                           | 0.2500                      | 19.42461 | 55.94288 | -1.76293              | 1.76293 |
| 2                                           | 0.5000                      | 38.84922 | 111.8858 | -2.49317              | 2.49317 |
| 3                                           | 0.7500                      | 58.27383 | 167.8286 | -3.05349              | 3.05349 |
| 4                                           | 1.0000                      | 77.69844 | 223.7715 | -3.52587              | 3.52587 |

| Boundary Information (Standardized Z Scale) |                           |         |         |
|---------------------------------------------|---------------------------|---------|---------|
| Null Reference = 0                          |                           |         |         |
| _Stage_                                     | -----Boundary Values----- |         | Alpha   |
|                                             | Lower                     | Upper   |         |
| 1                                           | -2.36129                  | 2.36129 | 2.36129 |
| 2                                           | -2.36129                  | 2.36129 | 2.36129 |
| 3                                           | -2.36129                  | 2.36129 | 2.36129 |
| 4                                           | -2.36129                  | 2.36129 | 2.36129 |

By default (or equivalently if you specify INFO=EQUAL in the DESIGN statement), equally spaced information levels are used. With the SAMPLESIZE statement, the required sample size  $N$  is also displayed under the heading “Information Level.” With the Pocock method, the standardized  $Z$  boundary values are identical at all stages for each  $\alpha$  boundary.

At each interim stage, the hypothesis of  $H_0 : \theta = 0$  is rejected if the standardized normal test statistic  $z \leq -2.36129$ , the lower  $\alpha$  boundary, or  $z \geq 2.36129$ , the upper  $\alpha$  boundary. Otherwise, the trial continues to the next stage. At the final stage, stage 4, the trial stops and the hypothesis is rejected if the test statistic  $|z_4| \geq 2.36129$ . Otherwise, the hypothesis is accepted.

The “Error Spending Information” in [Output 83.3.6](#) displays cumulative error spending at each stage for each boundary. It shows that more  $\alpha$  errors are used in early stages than in later stages.

**Output 83.3.6** Error Spending Information

| Error Spending Information |                                   |                                     |         |         |         |  |
|----------------------------|-----------------------------------|-------------------------------------|---------|---------|---------|--|
| _Stage_                    | -Information Level-<br>Proportion | -----Cumulative Error Spending----- |         |         |         |  |
|                            |                                   | Alpha                               | Beta    | Beta    | Alpha   |  |
| 1                          | 0.2500                            | 0.00911                             | 0.00002 | 0.00002 | 0.00911 |  |
| 2                          | 0.5000                            | 0.01577                             | 0.00002 | 0.00002 | 0.01577 |  |
| 3                          | 0.7500                            | 0.02088                             | 0.00002 | 0.00002 | 0.02088 |  |
| 4                          | 1.0000                            | 0.02500                             | 0.10000 | 0.10000 | 0.02500 |  |

The “Sample Size Summary” table in [Output 83.3.7](#) displays the specified parameters for the sample size computation of the two-sample test for mean difference.

**Output 83.3.7** Sample Size Summary

| Sample Size Summary             |                  |
|---------------------------------|------------------|
| Test                            | Two-Sample Means |
| Mean Difference                 | 0.4              |
| Standard Deviation              | 0.8              |
| Max Sample Size                 | 223.7715         |
| Expected Sample Size (Null Ref) | 218.652          |
| Expected Sample Size (Alt Ref)  | 131.9167         |
| Weight (Group A)                | 2                |
| Weight (Group B)                | 1                |

The “Sample Sizes (N)” table in [Output 83.3.8](#) displays the derived sample sizes at each stage, in both fractional and integer numbers. With the WEIGHT=2 option, the allocation ratio is 2 for the first group and 1 for the second group. See the section “[Test for the Difference between Two Normal Means](#)” on page 7053 for the derivation of these sample sizes. With the fixed-sample information ratio 1.1831, the derived sample sizes in fractional numbers are derived by multiplying 1.1831 by the corresponding sample sizes in the fixed-sample design.

**Output 83.3.8** Sample Sizes

| Sample Sizes (N)                      |        |          |          |             |
|---------------------------------------|--------|----------|----------|-------------|
| Two-Sample Z Test for Mean Difference |        |          |          |             |
| -----Fractional N-----                |        |          |          |             |
| _Stage_                               | N      | N(Grp 1) | N(Grp 2) | Information |
| 1                                     | 55.94  | 37.30    | 18.65    | 19.4246     |
| 2                                     | 111.89 | 74.59    | 37.30    | 38.8492     |
| 3                                     | 167.83 | 111.89   | 55.94    | 58.2738     |
| 4                                     | 223.77 | 149.18   | 74.59    | 77.6984     |

| Sample Sizes (N)                      |     |          |          |             |
|---------------------------------------|-----|----------|----------|-------------|
| Two-Sample Z Test for Mean Difference |     |          |          |             |
| -----Ceiling N-----                   |     |          |          |             |
| _Stage_                               | N   | N(Grp 1) | N(Grp 2) | Information |
| 1                                     | 57  | 38       | 19       | 19.7917     |
| 2                                     | 113 | 75       | 38       | 39.4082     |
| 3                                     | 168 | 112      | 56       | 58.3333     |
| 4                                     | 225 | 150      | 75       | 78.1250     |



These fractional sample sizes are rounded up to integers under the heading “Ceiling N.” When the resulting integer sample sizes are used, the corresponding information levels are slightly larger than the levels from the design. This can increase the power slightly if a trial uses these integer sample sizes.

Note that compared with other designs, a Pocock design can stop the trial early with a larger  $p$ -value. However, this might not be persuasive enough to make a new treatment widely accepted (Pocock and White 1999).

The “Design Information” table in [Output 83.3.9](#) displays design specifications and the derived statistics for the O’Brien-Fleming design. With the specified ALTREF= option, the maximum information  $I_X = 67.1268$  is derived.

**Output 83.3.9** O’Brien-Fleming Design Information

| The SEQDESIGN Procedure                   |                 |
|-------------------------------------------|-----------------|
| Design: TwoSidedOBrienFleming             |                 |
| Design Information                        |                 |
| Statistic Distribution                    | Normal          |
| Boundary Scale                            | Standardized Z  |
| Alternative Hypothesis                    | Two-Sided       |
| Early Stop                                | Reject Null     |
| Method                                    | O'Brien-Fleming |
| Boundary Key                              | Both            |
| Alternative Reference                     | 0.4             |
| Number of Stages                          | 4               |
| Alpha                                     | 0.05            |
| Beta                                      | 0.1             |
| Power                                     | 0.9             |
| Max Information (Percent of Fixed Sample) | 102.2163        |
| Max Information                           | 67.12682        |
| Null Ref ASN (Percent of Fixed Sample)    | 101.5728        |
| Alt Ref ASN (Percent of Fixed Sample)     | 76.7397         |

With the corresponding fixed-sample information

$$I_0 = \frac{(\Phi^{-1}(1 - \alpha/2) + \Phi^{-1}(1 - \beta))^2}{0.4^2} = \frac{(1.96 + 1.28155)^2}{0.16} = 65.6728$$

the fixed-sample information ratio is  $67.1268/65.6728 = 1.022$ . That is, the maximum information for the O’Brien-Fleming design is only 2.2% more than for the corresponding fixed-sample design.

The “Method Information” table in [Output 83.3.10](#) displays the Type I  $\alpha$  level and Type II  $\beta$  level. It also displays the derived drift parameter  $\theta_1 \sqrt{I_X}$ , which is the standardized alternative reference at the final stage.

**Output 83.3.10** Method Information

| Method Information |                 |         |         |                          |     |         |
|--------------------|-----------------|---------|---------|--------------------------|-----|---------|
| Boundary           | Method          | Alpha   | Beta    | -----Unified Family----- |     |         |
|                    |                 |         |         | Rho                      | Tau | C       |
| Upper Alpha        | O'Brien-Fleming | 0.02500 | 0.10000 | 0.5                      | 0   | 2.02429 |
| Lower Alpha        | O'Brien-Fleming | 0.02500 | 0.10000 | 0.5                      | 0   | 2.02429 |

| Method Information |                       |          |
|--------------------|-----------------------|----------|
| Boundary           | Alternative Reference | Drift    |
| Upper Alpha        | 0.4                   | 3.277238 |
| Lower Alpha        | -0.4                  | -3.27724 |

With the METHOD=OBF option, the O'Brien-Fleming method is used for each boundary. The O'Brien-Fleming method is one of the unified family methods, and the table also displays its corresponding parameters  $\rho = 0.5$  as a unified family method and the derived parameter  $C = 2.0243$  for the boundary values.

With the PSS option, the "Power and Expected Sample Sizes" table in [Output 83.3.11](#) displays powers and expected sample sizes under various hypothetical references  $\theta = c_i \theta_1$ , where  $\theta_1$  is the alternative reference and  $c_i$  are values specified in the CREF= option.

**Output 83.3.11** Power and Expected Sample Size Information

| Powers and Expected Sample Sizes   |         |                                          |
|------------------------------------|---------|------------------------------------------|
| Reference = CRef * (Alt Reference) |         |                                          |
| CRef                               | Power   | -Sample Size-<br>Percent<br>Fixed-Sample |
| 0.0000                             | 0.02500 | 101.5728                                 |
| 0.5000                             | 0.36495 | 96.3684                                  |
| 1.0000                             | 0.90000 | 76.7397                                  |
| 1.5000                             | 0.99821 | 57.2590                                  |

Compared with the corresponding Pocock design, the O'Brien-Fleming design has a smaller maximum sample size, and smaller expected sample sizes under hypothetical references  $\theta = 0$  and  $\theta = 0.5 \theta_1$ , but larger expected sample sizes under hypothetical references  $\theta = \theta_1$  and  $\theta = 1.5 \theta_1$ .

With the STOPPROB option, the "Expected Cumulative Stopping Probabilities" table in [Output 83.3.12](#) displays the expected stopping stage and cumulative stopping probability to reject the null hypothesis at each stage under various hypothetical references  $\theta = c_i \theta_1$ , where  $\theta_1$  is the alternative reference and  $c_i$  are values specified in the CREF= option.

**Output 83.3.12** Stopping Probabilities

| Expected Cumulative Stopping Probabilities |                         |             |                                  |         |         |         |  |
|--------------------------------------------|-------------------------|-------------|----------------------------------|---------|---------|---------|--|
| Reference = CRef * (Alt Reference)         |                         |             |                                  |         |         |         |  |
| CRef                                       | Expected Stopping Stage | Source      | -----Stopping Probabilities----- |         |         |         |  |
|                                            |                         |             | Stage_1                          | Stage_2 | Stage_3 | Stage_4 |  |
| 0.0000                                     | 3.975                   | Reject Null | 0.00005                          | 0.00422 | 0.02091 | 0.05000 |  |
| 0.5000                                     | 3.771                   | Reject Null | 0.00062                          | 0.04430 | 0.18392 | 0.36515 |  |
| 1.0000                                     | 3.003                   | Reject Null | 0.00798                          | 0.29296 | 0.69603 | 0.90000 |  |
| 1.5000                                     | 2.241                   | Reject Null | 0.05584                          | 0.73031 | 0.97315 | 0.99821 |  |

Compared with the corresponding Pocock design, the O'Brien-Fleming design has smaller stopping probabilities in early stages under each hypothetical reference.

The "Boundary Information" table in [Output 83.3.13](#) displays the boundary values for the design that uses the O'Brien-Fleming method. Compared with the Pocock method, the standardized statistics  $\alpha$  boundary values derived from the O'Brien-Fleming method in absolute values are larger in early stages and smaller in later stages. This makes the O'Brien-Fleming design less likely to reject the null hypothesis in early stages than the Pocock design. With the derived parameter  $C = 2.0243$  for the  $\alpha$  boundary, the  $\alpha$  boundaries at stage  $j$  are computed as  $C\sqrt{4/j}$ ,  $j = 1, \dots, 4$ .

**Output 83.3.13** Boundary Information

| Boundary Information (Standardized Z Scale) |                             |          |          |                       |         |
|---------------------------------------------|-----------------------------|----------|----------|-----------------------|---------|
| Null Reference = 0                          |                             |          |          |                       |         |
| _Stage_                                     | -----Information Level----- |          |          | -----Alternative----- |         |
|                                             | Proportion                  | Actual   | N        | Lower                 | Upper   |
| 1                                           | 0.2500                      | 16.7817  | 48.33131 | -1.63862              | 1.63862 |
| 2                                           | 0.5000                      | 33.56341 | 96.66262 | -2.31736              | 2.31736 |
| 3                                           | 0.7500                      | 50.34511 | 144.9939 | -2.83817              | 2.83817 |
| 4                                           | 1.0000                      | 67.12682 | 193.3252 | -3.27724              | 3.27724 |

| Boundary Information (Standardized Z Scale) |                           |             |  |
|---------------------------------------------|---------------------------|-------------|--|
| Null Reference = 0                          |                           |             |  |
| _Stage_                                     | -----Boundary Values----- |             |  |
|                                             | ---Lower---               | ---Upper--- |  |
|                                             | Alpha                     | Alpha       |  |
| 1                                           | -4.04859                  | 4.04859     |  |
| 2                                           | -2.86278                  | 2.86278     |  |
| 3                                           | -2.33745                  | 2.33745     |  |
| 4                                           | -2.02429                  | 2.02429     |  |

The “Error Spending Information” in [Output 83.3.14](#) displays cumulative error spending at each stage for each boundary. With smaller  $\alpha$  spending in early stages for the O'Brien-Fleming method, it also indicates that the O'Brien-Fleming design is less likely to reject the null hypothesis in early stages than the Pocock design.

**Output 83.3.14** Error Spending Information

| Error Spending Information |                                   |                                     |         |                 |         |         |
|----------------------------|-----------------------------------|-------------------------------------|---------|-----------------|---------|---------|
| _Stage_                    | -Information Level-<br>Proportion | -----Cumulative Error Spending----- |         |                 |         |         |
|                            |                                   | -----Lower-----                     |         | -----Upper----- |         |         |
|                            |                                   | Alpha                               | Beta    | Beta            | Alpha   |         |
| 1                          | 0.2500                            | 0.00003                             | 0.00000 | 0.00000         | 0.00000 | 0.00003 |
| 2                          | 0.5000                            | 0.00211                             | 0.00000 | 0.00000         | 0.00000 | 0.00211 |
| 3                          | 0.7500                            | 0.01046                             | 0.00000 | 0.00000         | 0.00000 | 0.01046 |
| 4                          | 1.0000                            | 0.02500                             | 0.10000 | 0.10000         | 0.10000 | 0.02500 |

The “Sample Size Summary” table in [Output 83.3.15](#) displays the specified parameters for the sample size computation of the two-sample test for mean difference.

**Output 83.3.15** Sample Size Summary

| Sample Size Summary             |                  |
|---------------------------------|------------------|
| Test                            | Two-Sample Means |
| Mean Difference                 | 0.4              |
| Standard Deviation              | 0.8              |
| Max Sample Size                 | 193.3252         |
| Expected Sample Size (Null Ref) | 192.1081         |
| Expected Sample Size (Alt Ref)  | 145.1404         |
| Weight (Group A)                | 2                |
| Weight (Group B)                | 1                |

The “Sample Sizes (N)” table in [Output 83.3.16](#) displays the derived sample sizes at each stage, in both fractional and integer numbers. With the fixed-sample information ratio 1.0222, the required sample sizes in fractional numbers are derived by multiplying 1.0222 by the corresponding sample sizes in the fixed-sample design.

**Output 83.3.16** Derived Sample Sizes

| Sample Sizes (N)                      |        |          |          |             |
|---------------------------------------|--------|----------|----------|-------------|
| Two-Sample Z Test for Mean Difference |        |          |          |             |
| -----Fractional N-----                |        |          |          |             |
| _Stage_                               | N      | N(Grp 1) | N(Grp 2) | Information |
| 1                                     | 48.33  | 32.22    | 16.11    | 16.7817     |
| 2                                     | 96.66  | 64.44    | 32.22    | 33.5634     |
| 3                                     | 144.99 | 96.66    | 48.33    | 50.3451     |
| 4                                     | 193.33 | 128.88   | 64.44    | 67.1268     |

| Sample Sizes (N)                      |     |          |          |             |
|---------------------------------------|-----|----------|----------|-------------|
| Two-Sample Z Test for Mean Difference |     |          |          |             |
| -----Ceiling N-----                   |     |          |          |             |
| _Stage_                               | N   | N(Grp 1) | N(Grp 2) | Information |
| 1                                     | 50  | 33       | 17       | 17.5313     |
| 2                                     | 98  | 65       | 33       | 34.1996     |
| 3                                     | 146 | 97       | 49       | 50.8669     |
| 4                                     | 194 | 129      | 65       | 67.5338     |

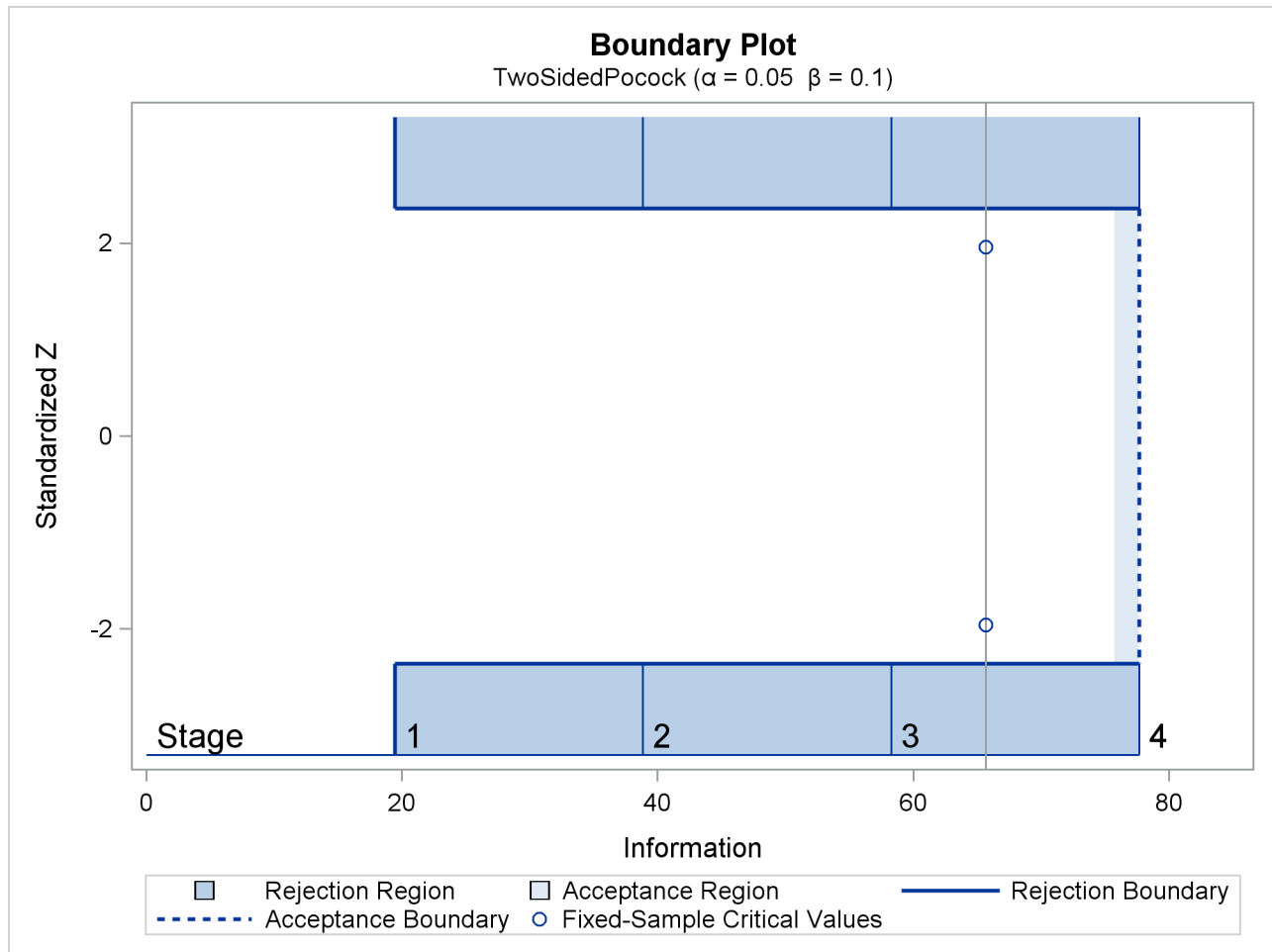
**Example 83.4: Generating Graphics Display for Sequential Designs**

This example creates the same group sequential design as in [Example 83.3](#) and creates graphics by using ODS Graphics. The following statements request all available graphs in the SEQDESIGN procedure:

```
ods graphics on;
proc seqdesign altref=0.4
 plots=all
 ;
 TwoSidedPocock: design nstages=4 method=poc;
 TwoSidedOBrienFleming: design nstages=4 method=obf;
run;
ods graphics off;
```

With the PLOTS=ALL option, a detailed boundary plot with the rejection region and acceptance region is displayed for the Pocock design, as shown in [Output 83.4.1](#). By default (or equivalently if you specify STOP=REJECT), the rejection boundaries are also generated at interim stages.

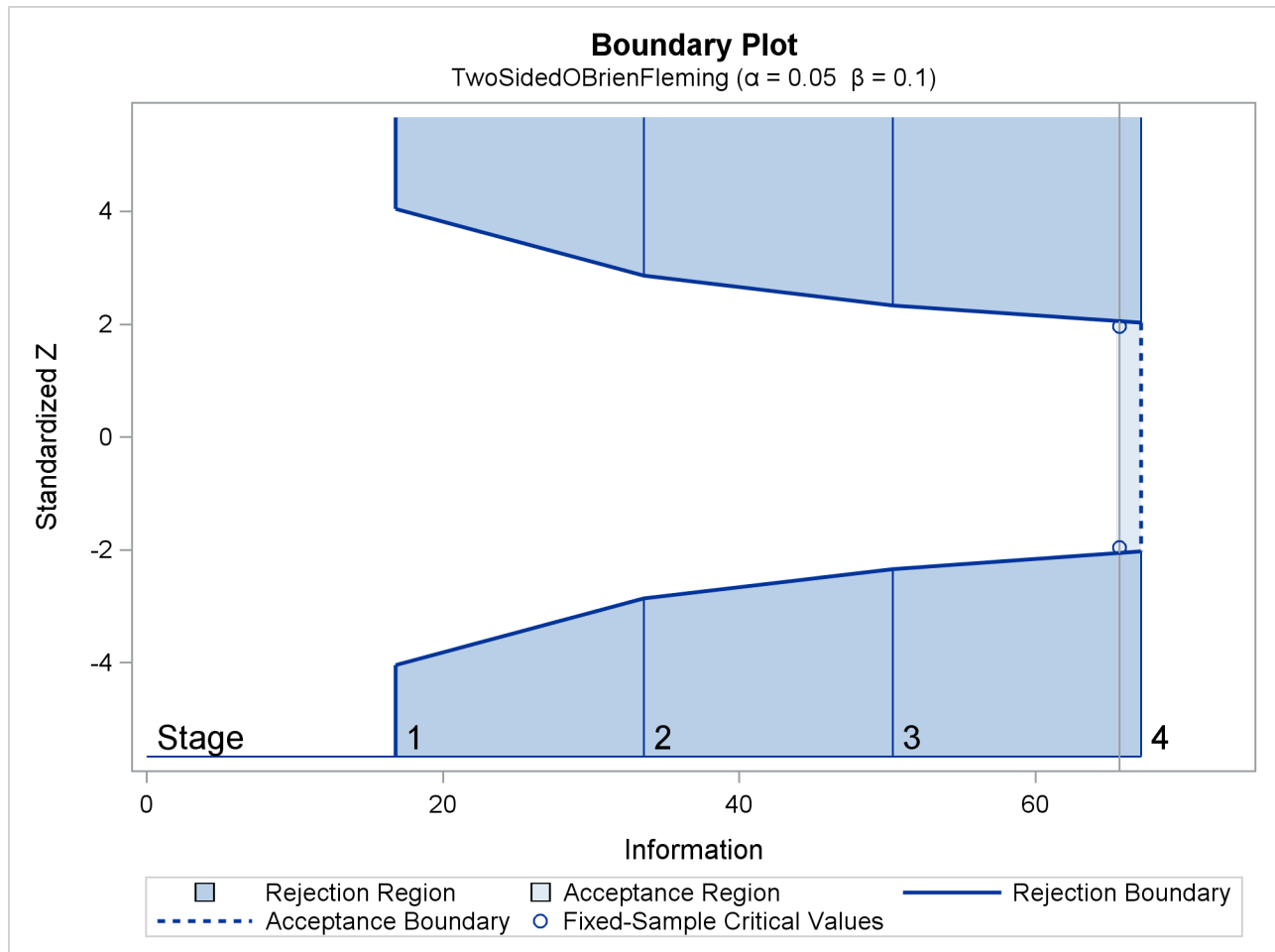
Output 83.4.1 Pocock Boundary Plot



The plot shows identical boundary values in each boundary in the standardized Z scale for the Pocock design. The information level and the critical value for the corresponding fixed-sample design are also displayed.

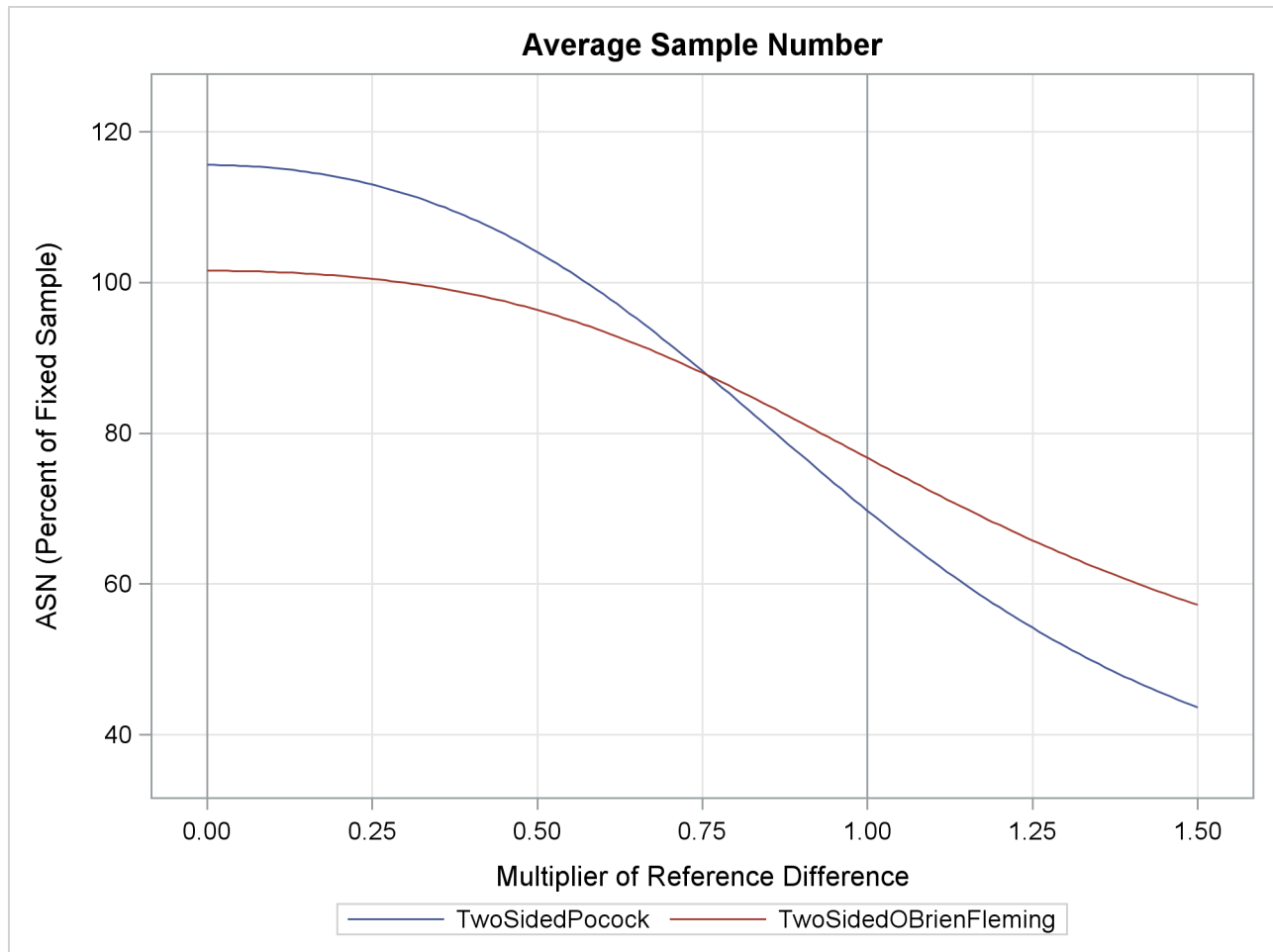
With the PLOTS=ALL option, a detailed boundary plot with the rejection region and acceptance region is also displayed for the O'Brien-Fleming design, as shown in Output 83.4.2. The plot shows that the rejection boundary values are decreasing as the trial advances in the standardized Z scale.

Output 83.4.2 O'Brien-Fleming Boundary Plot



With the PLOTS=ALL option, the procedure displays a plot of average sample numbers (expected sample sizes for nonsurvival data or expected numbers of events for survival data) under various hypothetical references for all designs simultaneously, as shown in Output 83.4.3. By default, the option CREF= 0, 0.01, 0.02, ..., 1.50 and expected sample sizes under the hypothetical references  $\theta = c_i \theta_1$  are displayed, where  $c_i$  are values specified in the CREF= option. These CREF= values are displayed on the horizontal axis.

Output 83.4.3 ASN Plot

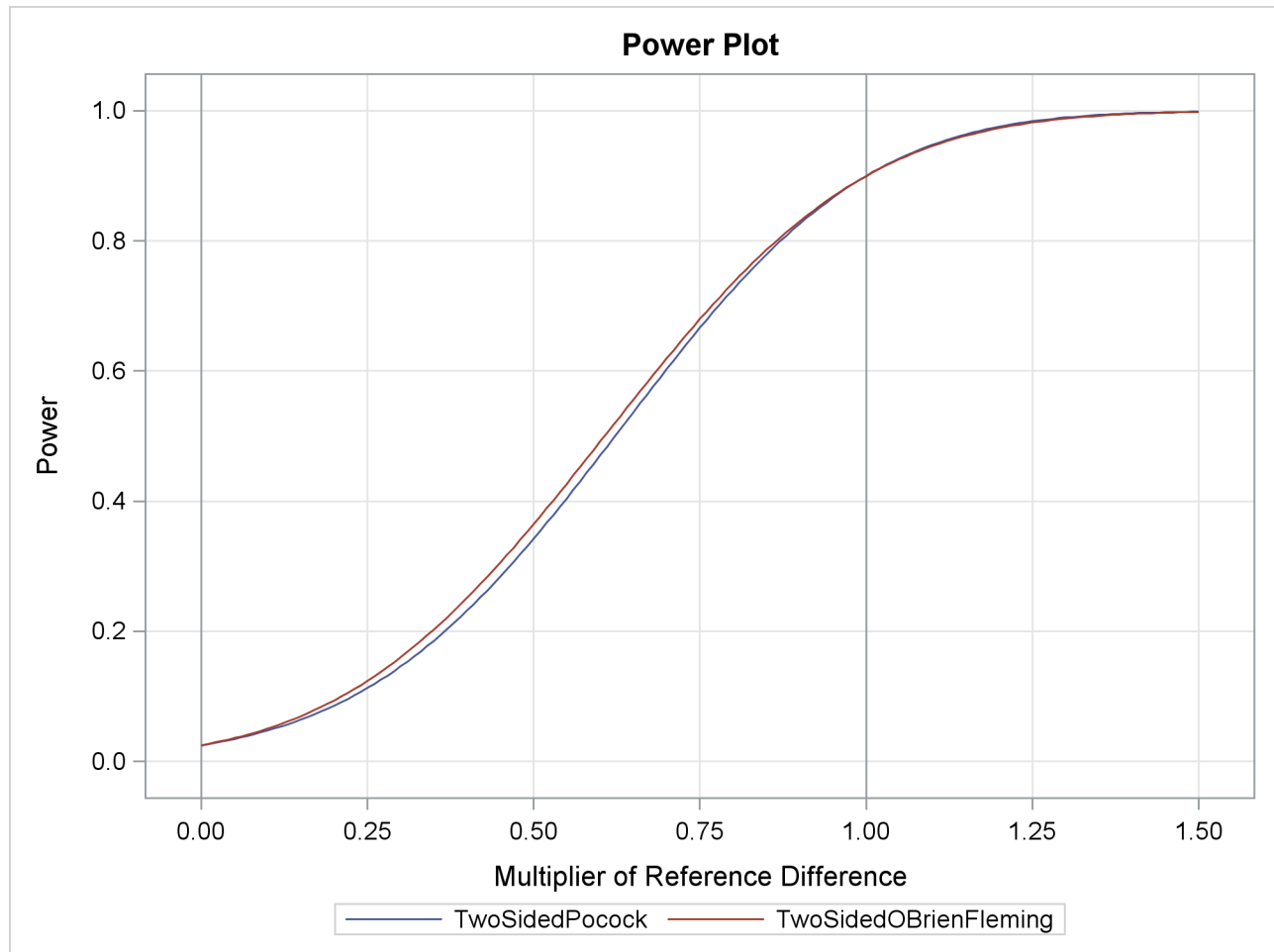


The plot shows that the Pocock design has a larger expected sample size than the O'Brien-Fleming design under the null hypothesis ( $c_i = 0$ ) and has a smaller expected sample size under the alternative hypothesis ( $c_i = 1$ ).

With the PLOTS=ALL option, the procedure displays a plot of the power curves under various hypothetical references for all designs simultaneously, as shown in Output 83.4.4. By default, the option CREF=0, 0.01, 0.02, ..., 1.50 and powers under hypothetical references  $\theta = c_i \theta_1$  are displayed, where  $c_i$  are values specified in the CREF= option. These CREF= values are displayed on the horizontal axis.



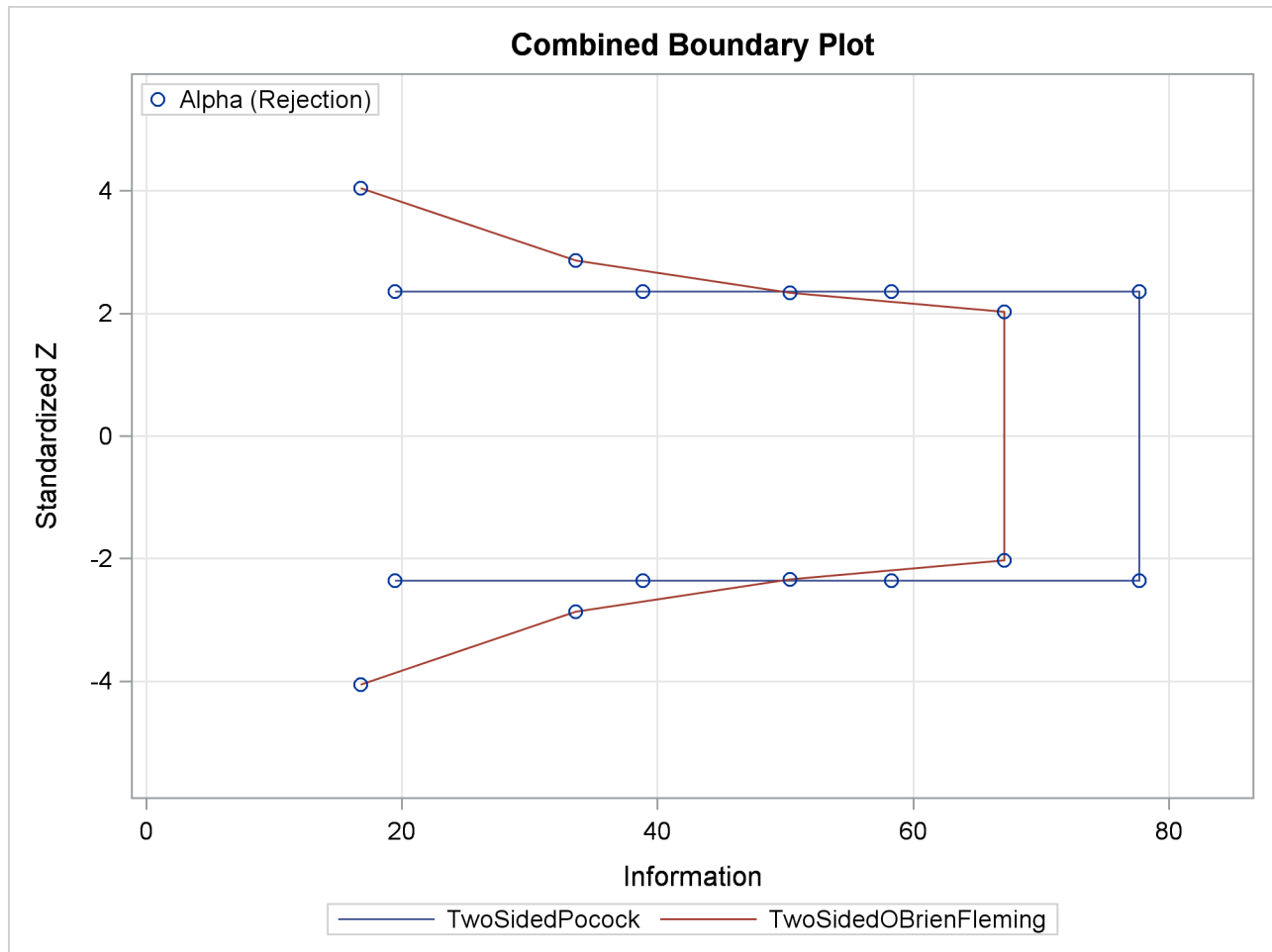
Output 83.4.4 Power Plot



Under the null hypothesis,  $c_i = 0$ , the power is 0.025, the upper Type I error probability. Under the alternative hypothesis,  $c_i = 1$ , the power is 0.9, one minus the Type II error probability. The plot shows only minor difference between the two designs.

With the PLOTS=ALL option, the procedure displays a plot of sequential boundaries for all designs simultaneously, as shown in [Output 83.4.5](#). By default (or equivalently if you specify HSCALE=INFO in the COMBINEDBOUNDARY option), the information levels are used on the horizontal axis.

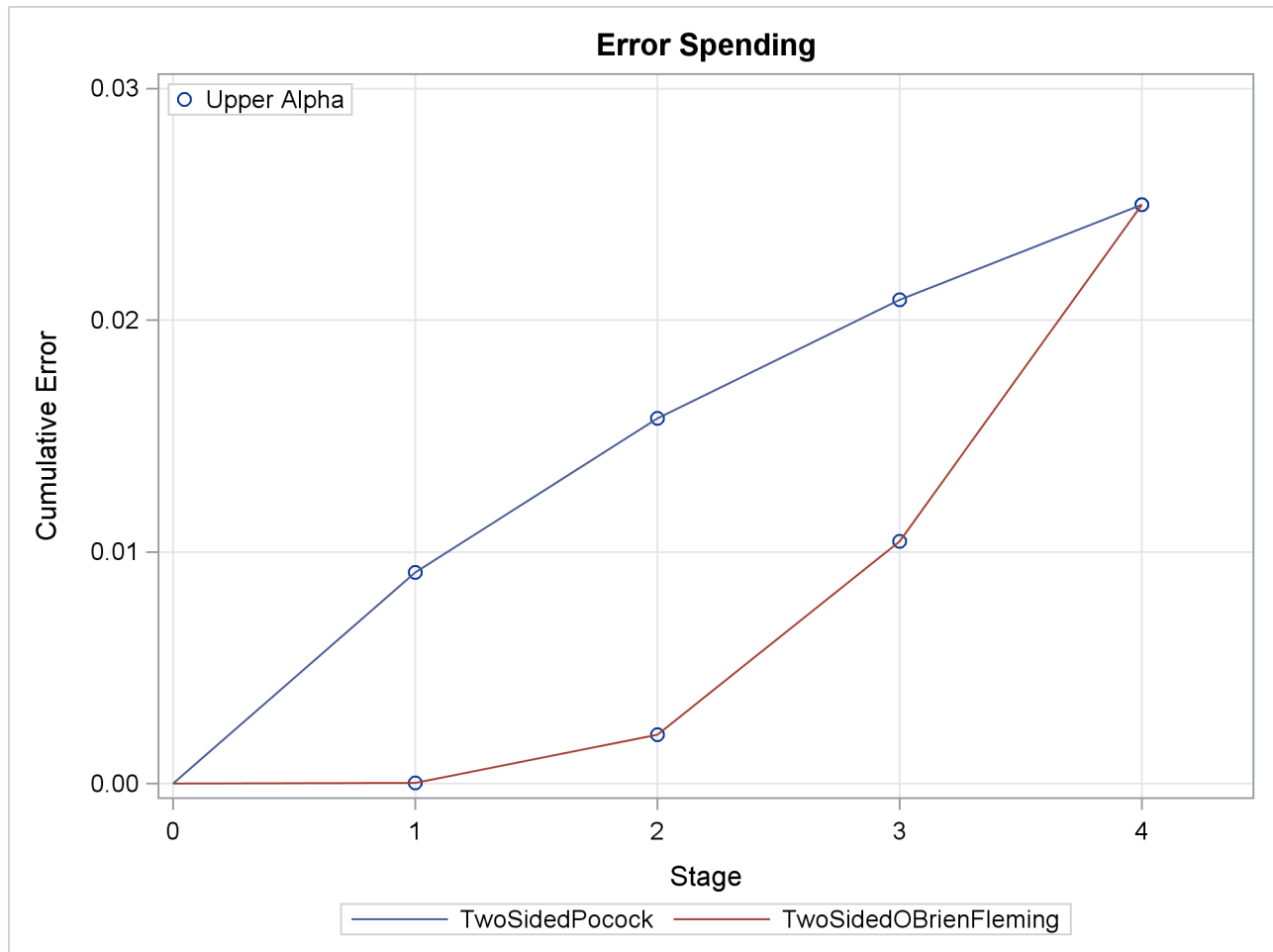
**Output 83.4.5** Combined Boundary Plot



The plot shows that the  $\alpha$  boundary values (in absolute value) created from the O'Brien-Fleming method are greater in early stages and smaller in later stages than the boundary values from the Pocock method. The plot also shows that the information level in the Pocock design is larger than the corresponding level in the O'Brien-Fleming design at each stage.

With the PLOTS=ALL option, the procedure displays a plot of cumulative error spends for all boundaries in the designs simultaneously, as shown in [Output 83.4.6](#). With a symmetric two-sided design, cumulative error spending is displayed only for the upper  $\alpha$  boundary. The plot shows that for the upper  $\alpha$  boundary, the O'Brien-Fleming method spends fewer errors in early stages and more errors in later stages than the corresponding Pocock method.

Output 83.4.6 Error Spending Plot



### Example 83.5: Creating Designs Using Haybittle-Peto Methods

This example requests two 3-stage group sequential designs for normally distributed statistics. Each design uses a Haybittle-Peto method with a two-sided alternative and early stopping to reject the hypothesis. One design uses the specified interim boundary  $Z$  values and derives the final-stage boundary value for the specified  $\alpha$  and  $\beta$  errors. The other design uses the specified boundary  $Z$  values and derives the overall  $\alpha$  and  $\beta$  errors.

The following statements specify the interim boundary  $Z$  values and derive the final-stage boundary value for the specified  $\alpha = 0.05$  and  $\beta = 0.10$ :

```
ods graphics on;
proc seqdesign altref=0.25
 errspend
 stopprob
 plots=errspend
;
```

```

OneSidedPeto: design nstages=3
 method=peto(z=3)
 alt=upper stop=reject
 alpha=0.05 beta=0.10;

run;
ods graphics off;

```

The “Design Information” table in [Output 83.5.1](#) displays design specifications and maximum information in percentage of its corresponding fixed-sample design.

**Output 83.5.1** Haybittle-Peto Design Information

| The SEQDESIGN Procedure                   |                |
|-------------------------------------------|----------------|
| Design: OneSidedPeto                      |                |
| Design Information                        |                |
| Statistic Distribution                    | Normal         |
| Boundary Scale                            | Standardized Z |
| Alternative Hypothesis                    | Upper          |
| Early Stop                                | Reject Null    |
| Method                                    | Haybittle-Peto |
| Boundary Key                              | Both           |
| Alternative Reference                     | 0.25           |
| Number of Stages                          | 3              |
| Alpha                                     | 0.05           |
| Beta                                      | 0.1            |
| Power                                     | 0.9            |
| Max Information (Percent of Fixed Sample) | 100.2466       |
| Max Information                           | 137.3592       |
| Null Ref ASN (Percent of Fixed Sample)    | 100.1192       |
| Alt Ref ASN (Percent of Fixed Sample)     | 87.35          |

The “Method Information” table in [Output 83.5.2](#) displays the  $\alpha$  and  $\beta$  errors and the derived drift parameter, which is the standardized alternative reference at the final stage.

**Output 83.5.2** Method Information

| Method Information |                |         |         |                       |          |
|--------------------|----------------|---------|---------|-----------------------|----------|
| Boundary           | Method         | Alpha   | Beta    | Alternative Reference | Drift    |
| Upper Alpha        | Haybittle-Peto | 0.05000 | 0.10000 | 0.25                  | 2.930009 |

With the STOPPROB option, the “Expected Cumulative Stopping Probabilities” table in [Output 83.5.3](#) displays the expected stopping stage and cumulative stopping probability to reject the null hypothesis at each stage under various hypothetical references  $\theta = c_i \theta_1$ , where  $\theta_1$  is the alternative reference and  $c_i = 0, 0.5, 1, 1.5$  are the default values in the CREF= option.

**Output 83.5.3** Stopping Probabilities

| Expected Cumulative Stopping Probabilities |                         |             |                                |         |         |  |
|--------------------------------------------|-------------------------|-------------|--------------------------------|---------|---------|--|
| Reference = CRef * (Alt Reference)         |                         |             |                                |         |         |  |
| CRef                                       | Expected Stopping Stage | Source      | ----Stopping Probabilities---- |         |         |  |
|                                            |                         |             | Stage_1                        | Stage_2 | Stage_3 |  |
| 0.0000                                     | 2.996                   | Reject Null | 0.00135                        | 0.00246 | 0.05000 |  |
| 0.5000                                     | 2.941                   | Reject Null | 0.01561                        | 0.04372 | 0.42762 |  |
| 1.0000                                     | 2.614                   | Reject Null | 0.09538                        | 0.29057 | 0.90000 |  |
| 1.5000                                     | 1.944                   | Reject Null | 0.32185                        | 0.73442 | 0.99698 |  |

The “Boundary Information” table in [Output 83.5.4](#) displays information level, alternative references, and boundary values. By default (or equivalently if you specify BOUNDARYSCALE=STDZ), the standardized  $Z$  scale is used to display the alternative references and boundary values. The resulting standardized alternative reference at stage  $k$  is given by  $\theta_1 \sqrt{I_k}$ , where  $\theta_1$  is the alternative reference and  $I_k$  is the information level at stage  $k$ ,  $k = 1, 2, 3$ .

**Output 83.5.4** Boundary Information

| Boundary Information (Standardized Z Scale) |                         |          |                        |                          |
|---------------------------------------------|-------------------------|----------|------------------------|--------------------------|
| Null Reference = 0                          |                         |          |                        |                          |
| _Stage_                                     | ---Information Level--- |          | -Alternative-          | -Boundary Values-        |
|                                             | Proportion              | Actual   | --Reference--<br>Upper | -----Upper-----<br>Alpha |
| 1                                           | 0.3333                  | 45.7864  | 1.69164                | 3.00000                  |
| 2                                           | 0.6667                  | 91.57281 | 2.39234                | 3.00000                  |
| 3                                           | 1.0000                  | 137.3592 | 2.93001                | 1.65042                  |

At each interim stage, if the standardized statistic  $z \geq 3$ , the trial is stopped and the null hypothesis is rejected. If the statistic  $z < 3$ , the trial continues to the next stage. At the final stage, the null hypothesis is rejected if the statistic  $z_3 > 1.65$ . Otherwise, the hypothesis is accepted. Note that the boundary values at the final stage, 1.65, are close to the critical values 1.645 in the corresponding fixed-sample design.

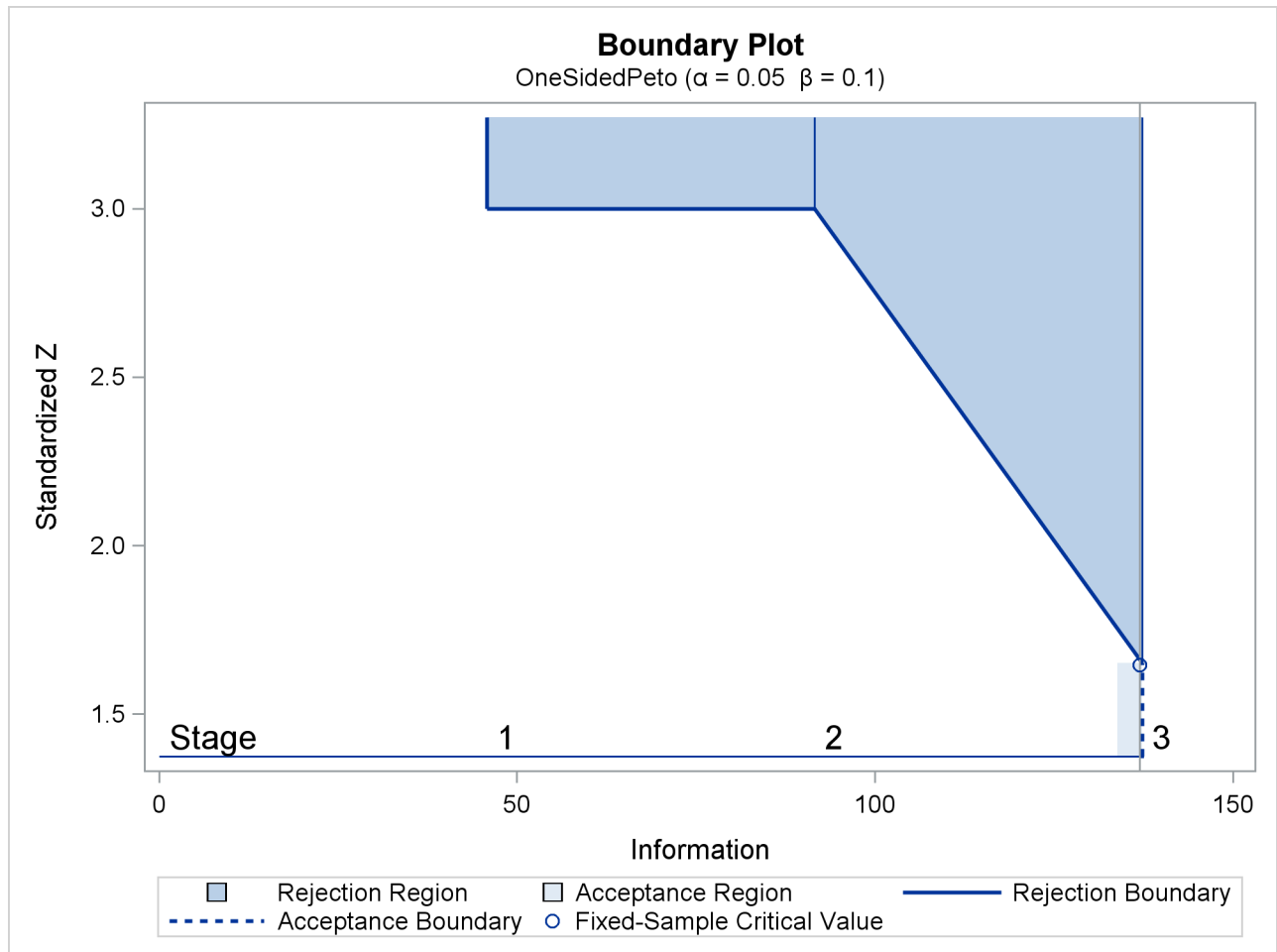
The “Error Spending Information” in [Output 83.5.5](#) displays cumulative error spending at each stage for each boundary. The stage 1  $\alpha$  spending 0.00135 corresponds to the one-sided  $p$ -value for a standardized  $Z$  statistic,  $Z > 3$ .

**Output 83.5.5** Error Spending Information

| Error Spending Information |                                   |                                                |         |  |
|----------------------------|-----------------------------------|------------------------------------------------|---------|--|
| _Stage_                    | -Information Level-<br>Proportion | -Cumulative Error Spending-<br>-----Upper----- |         |  |
|                            |                                   | Beta                                           | Alpha   |  |
| 1                          | 0.3333                            | 0.00000                                        | 0.00135 |  |
| 2                          | 0.6667                            | 0.00000                                        | 0.00246 |  |
| 3                          | 1.0000                            | 0.10000                                        | 0.05000 |  |

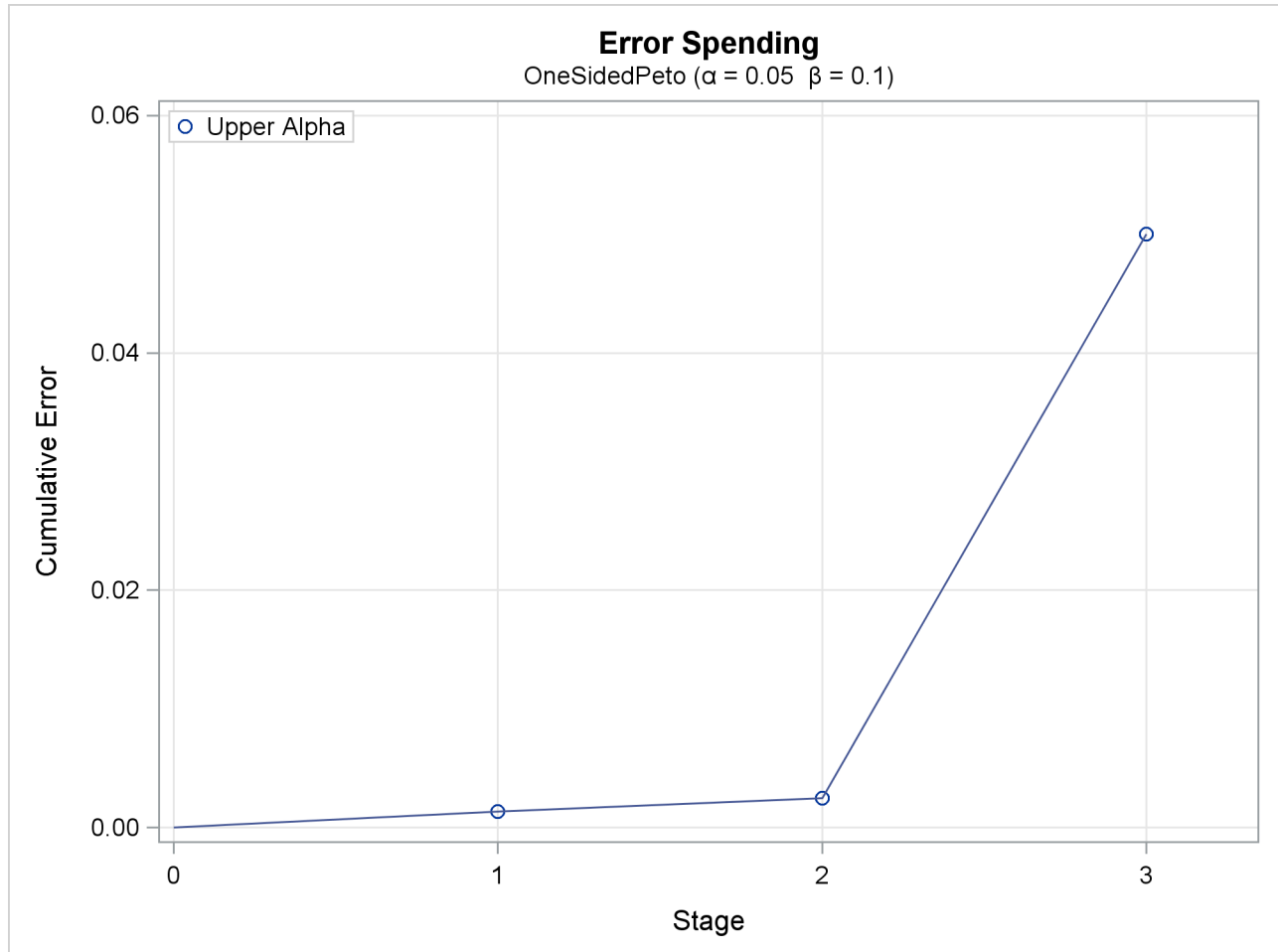
With ODS Graphics enabled, a detailed boundary plot with the rejection and acceptance regions is displayed, as shown in Output 83.5.6. With the STOP=REJECT option, the interim rejection boundaries are displayed.

**Output 83.5.6** Boundary Plot



With the PLOTS=ERRSPEND option, the procedure displays a plot of error spending for each boundary, as shown in [Output 83.5.7](#). The error spending values in the “Error Spending Information” in [Output 83.5.4](#) are displayed in the plot. As expected, the error spending at each of the first two stages is small, with the standardized  $Z$  boundary value 3.

**Output 83.5.7** Error Spending Plot



The following statements specify the boundary  $Z$  values and derive the  $\alpha$  and  $\beta$  errors from these completely specified boundary values:

```
ods graphics on;
proc seqdesign altref=0.25
 maxinfo=200
 errspend
 stopprob
 plots=errspend
 ;
 OneSidedPeto: design nstages=3
 method=peto(z=3 2.5 2)
 alt=upper stop=reject
 boundarykey=none
 ;
run;
ods graphics off;
```

The “Design Information” table in [Output 83.5.8](#) displays design specifications and derived  $\alpha$  and  $\beta$  error levels.

**Output 83.5.8** Design Information

| The SEQDESIGN Procedure                   |                |
|-------------------------------------------|----------------|
| Design: OneSidedPeto                      |                |
| Design Information                        |                |
| Statistic Distribution                    | Normal         |
| Boundary Scale                            | Standardized Z |
| Alternative Hypothesis                    | Upper          |
| Early Stop                                | Reject Null    |
| Method                                    | Haybittle-Peto |
| Boundary Key                              | None           |
| Alternative Reference                     | 0.25           |
| Number of Stages                          | 3              |
| Alpha                                     | 0.02532        |
| Beta                                      | 0.06035        |
| Power                                     | 0.93965        |
| Max Information (Percent of Fixed Sample) | 101.6769       |
| Max Information                           | 200            |
| Null Ref ASN (Percent of Fixed Sample)    | 101.3933       |
| Alt Ref ASN (Percent of Fixed Sample)     | 73.74031       |

The “Method Information” table in [Output 83.5.9](#) displays the  $\alpha$  and  $\beta$  errors and the derived drift parameter for each boundary.

**Output 83.5.9** Method Information

| Method Information |                |         |         |                       |          |
|--------------------|----------------|---------|---------|-----------------------|----------|
| Boundary           | Method         | Alpha   | Beta    | Alternative Reference | Drift    |
| Upper Alpha        | Haybittle-Peto | 0.02532 | 0.06035 | 0.25                  | 3.535534 |

With the STOPPROB option, the “Expected Cumulative Stopping Probabilities” table in [Output 83.5.10](#) displays the expected stopping stage and cumulative stopping probability to reject the null hypothesis at each stage under various hypothetical references  $\theta = c_i\theta_1$ , where  $\theta_1$  is the alternative reference and  $c_i = 0, 0.5, 1, 1.5$  are the default values in the CREF= option.



**Output 83.5.10** Stopping Probabilities

| Expected Cumulative Stopping Probabilities |                         |             |                                |         |         |  |
|--------------------------------------------|-------------------------|-------------|--------------------------------|---------|---------|--|
| Reference = CRef * (Alt Reference)         |                         |             |                                |         |         |  |
| CRef                                       | Expected Stopping Stage | Source      | ----Stopping Probabilities---- |         |         |  |
|                                            |                         |             | Stage_1                        | Stage_2 | Stage_3 |  |
| 0.0000                                     | 2.992                   | Reject Null | 0.00135                        | 0.00702 | 0.02532 |  |
| 0.5000                                     | 2.826                   | Reject Null | 0.02389                        | 0.15030 | 0.41775 |  |
| 1.0000                                     | 2.176                   | Reject Null | 0.16884                        | 0.65544 | 0.93965 |  |
| 1.5000                                     | 1.508                   | Reject Null | 0.52466                        | 0.96708 | 0.99954 |  |

The “Boundary Information” table in [Output 83.5.11](#) displays information level, alternative references, and boundary values.

**Output 83.5.11** Boundary Information

| Boundary Information (Standardized Z Scale) |                         |          |                        |                          |
|---------------------------------------------|-------------------------|----------|------------------------|--------------------------|
| Null Reference = 0                          |                         |          |                        |                          |
| _Stage_                                     | ---Information Level--- |          | -Alternative-          | -Boundary Values-        |
|                                             | Proportion              | Actual   | --Reference--<br>Upper | -----Upper-----<br>Alpha |
| 1                                           | 0.3333                  | 66.66667 | 2.04124                | 3.00000                  |
| 2                                           | 0.6667                  | 133.3333 | 2.88675                | 2.50000                  |
| 3                                           | 1.0000                  | 200      | 3.53553                | 2.00000                  |

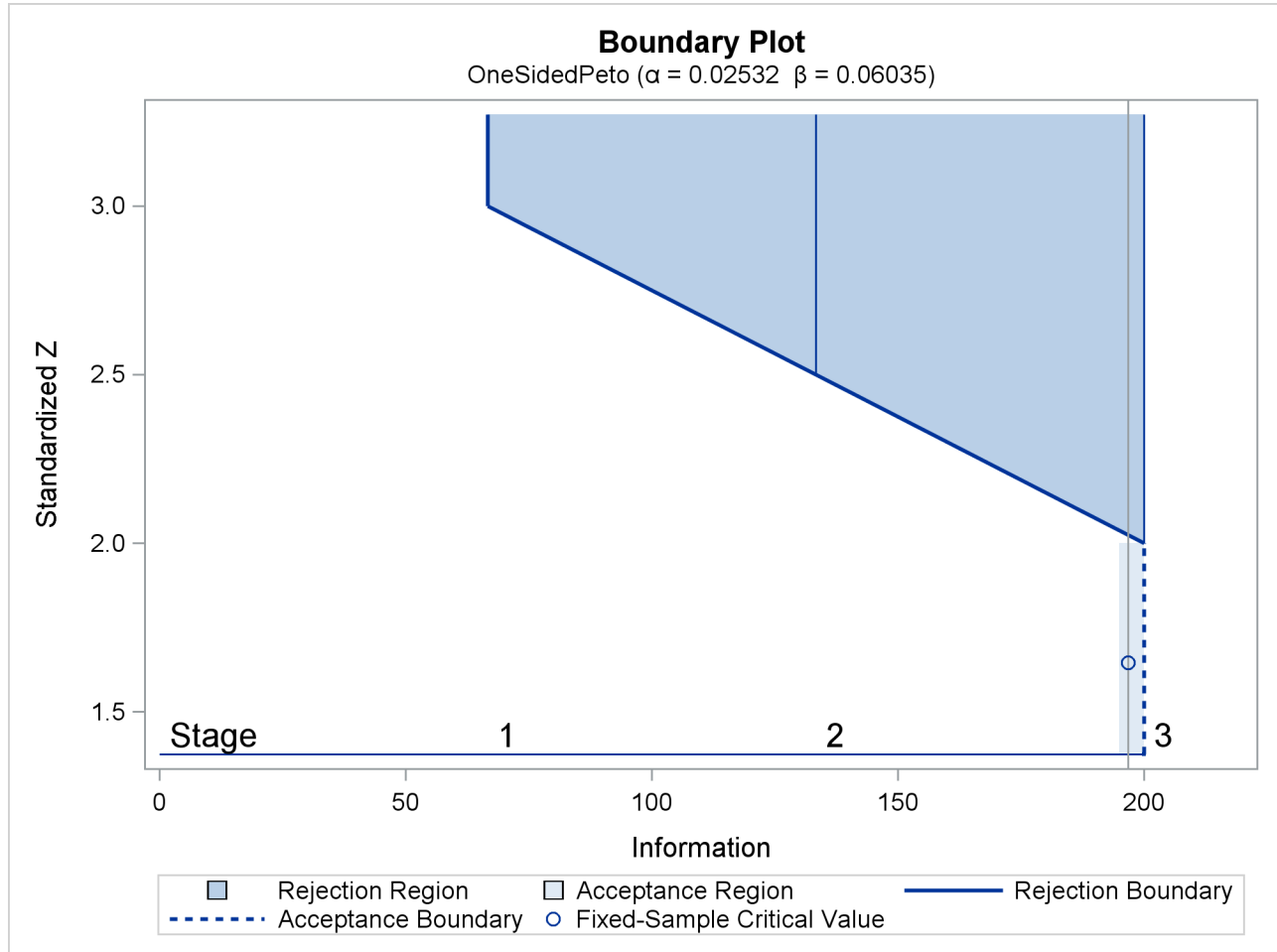
The “Error Spending Information” in [Output 83.5.12](#) displays cumulative error spending at each stage for each boundary. The first-stage  $\alpha$  spending 0.00135 corresponds to the one-sided  $p$ -value for a standardized  $Z$  statistic,  $Z > 3$ .

**Output 83.5.12** Error Spending Information

| Error Spending Information |                     |  |                             |         |
|----------------------------|---------------------|--|-----------------------------|---------|
| _Stage_                    | -Information Level- |  | -Cumulative Error Spending- |         |
|                            | Proportion          |  | -----Upper-----<br>Beta     | Alpha   |
| 1                          | 0.3333              |  | 0.00000                     | 0.00135 |
| 2                          | 0.6667              |  | 0.00000                     | 0.00702 |
| 3                          | 1.0000              |  | 0.06035                     | 0.02532 |

With ODS Graphics enabled, a detailed boundary plot with the rejection and acceptance regions is displayed, as shown in [Output 83.5.13](#). With the STOP=REJECT option, the interim rejection boundaries are displayed.

**Output 83.5.13** Boundary Plot



With the PLOTS=ERRSPEND option, the procedure displays a plot of error spending for each boundary, as shown in [Output 83.5.14](#). The error spending values in the “Error Spending Information” table in [Output 83.5.10](#) are displayed in the plot.

Output 83.5.14 Error Spending Plot



### Example 83.6: Creating Designs with Various Stopping Criteria

This example requests three 5-stage group sequential designs for normally distributed statistics. Each design uses a triangular method with the specified one-sided upper alternative reference  $\theta_1 = 0.2$ . The resulting boundary values are displayed with the score scale. Note that these unified family triangular designs are different from Whitehead's triangular designs.

The following statements request three designs with different stopping criterion:

```
ods graphics on;
proc seqdesign altref=0.2
 bscale=score
 errspend
 plots=(combinedboundary errspend(hscale=info))
 ;
 StopToRejectAccept: design nstages=5 method=tri alt=upper stop=both;
 StopToReject: design nstages=5 method=tri alt=upper stop=reject;
 StopToAccept: design nstages=5 method=tri alt=upper stop=accept;
run;
ods graphics off;
```

The first design has early stopping to reject or accept the null hypothesis  $H_0$ .

The “Design Information” table in [Output 83.6.1](#) displays design specifications and derived statistics. With the specified alternative reference, the maximum information is derived.

**Output 83.6.1** Triangular Design Information

| The SEQDESIGN Procedure                   |                    |
|-------------------------------------------|--------------------|
| Design: StopToRejectAccept                |                    |
| Design Information                        |                    |
| Statistic Distribution                    | Normal             |
| Boundary Scale                            | Score              |
| Alternative Hypothesis                    | Upper              |
| Early Stop                                | Accept/Reject Null |
| Method                                    | Triangular         |
| Boundary Key                              | Both               |
| Alternative Reference                     | 0.2                |
| Number of Stages                          | 5                  |
| Alpha                                     | 0.05               |
| Beta                                      | 0.1                |
| Power                                     | 0.9                |
| Max Information (Percent of Fixed Sample) | 140.0293           |
| Max Information                           | 299.797            |
| Null Ref ASN (Percent of Fixed Sample)    | 59.11973           |
| Alt Ref ASN (Percent of Fixed Sample)     | 66.94909           |

The “Method Information” table in [Output 83.6.2](#) displays the  $\alpha$  and  $\beta$  errors and the derived drift parameter, which is the standardized alternative reference at the final stage. The table also shows the corresponding parameters for a triangular method as a unified family method.

**Output 83.6.2** Method Information

| Method Information |             |                       |         |                          |     |         |
|--------------------|-------------|-----------------------|---------|--------------------------|-----|---------|
| Boundary           | Method      | Alpha                 | Beta    | -----Unified Family----- |     |         |
|                    |             |                       |         | Rho                      | Tau | C       |
| Upper Alpha        | Triangular  | 0.05000               | .       | 0.5                      | 1   | 0.94394 |
| Upper Beta         | Triangular  | .                     | 0.10000 | 0.5                      | 1   | 0.78753 |
| Method Information |             |                       |         |                          |     |         |
|                    | Boundary    | Alternative Reference | Drift   |                          |     |         |
|                    | Upper Alpha | 0.2                   | 3.46293 |                          |     |         |
|                    | Upper Beta  | 0.2                   | 3.46293 |                          |     |         |

The “Boundary Information” table in [Output 83.6.3](#) displays information level, alternative reference, and boundary values. With the specified BOUNDARYSCALE=SCORE option, the alternative reference and boundary values are displayed in the score statistic scale. With a score scale, the alternative reference is  $\theta_1 I_k$ , where  $\theta_1$  is the specified alternative reference and  $I_k$  is the information level at stage  $k$ ,  $k = 1, 2, \dots, 5$ .

**Output 83.6.3** Boundary Information

| Boundary Information (Score Scale) |                         |          |                        |                           |          |
|------------------------------------|-------------------------|----------|------------------------|---------------------------|----------|
| Null Reference = 0                 |                         |          |                        |                           |          |
| _Stage_                            | ---Information Level--- |          | -Alternative-          | -----Boundary Values----- |          |
|                                    | Proportion              | Actual   | --Reference--<br>Upper | -----Upper-----<br>Beta   | Alpha    |
| 1                                  | 0.2000                  | 59.9594  | 11.99188               | -4.37102                  | 19.61274 |
| 2                                  | 0.4000                  | 119.9188 | 23.98376               | 4.89371                   | 22.88154 |
| 3                                  | 0.6000                  | 179.8782 | 35.97564               | 14.15845                  | 26.15033 |
| 4                                  | 0.8000                  | 239.8376 | 47.96752               | 23.42318                  | 29.41912 |
| 5                                  | 1.0000                  | 299.797  | 59.95940               | 32.68791                  | 32.68791 |

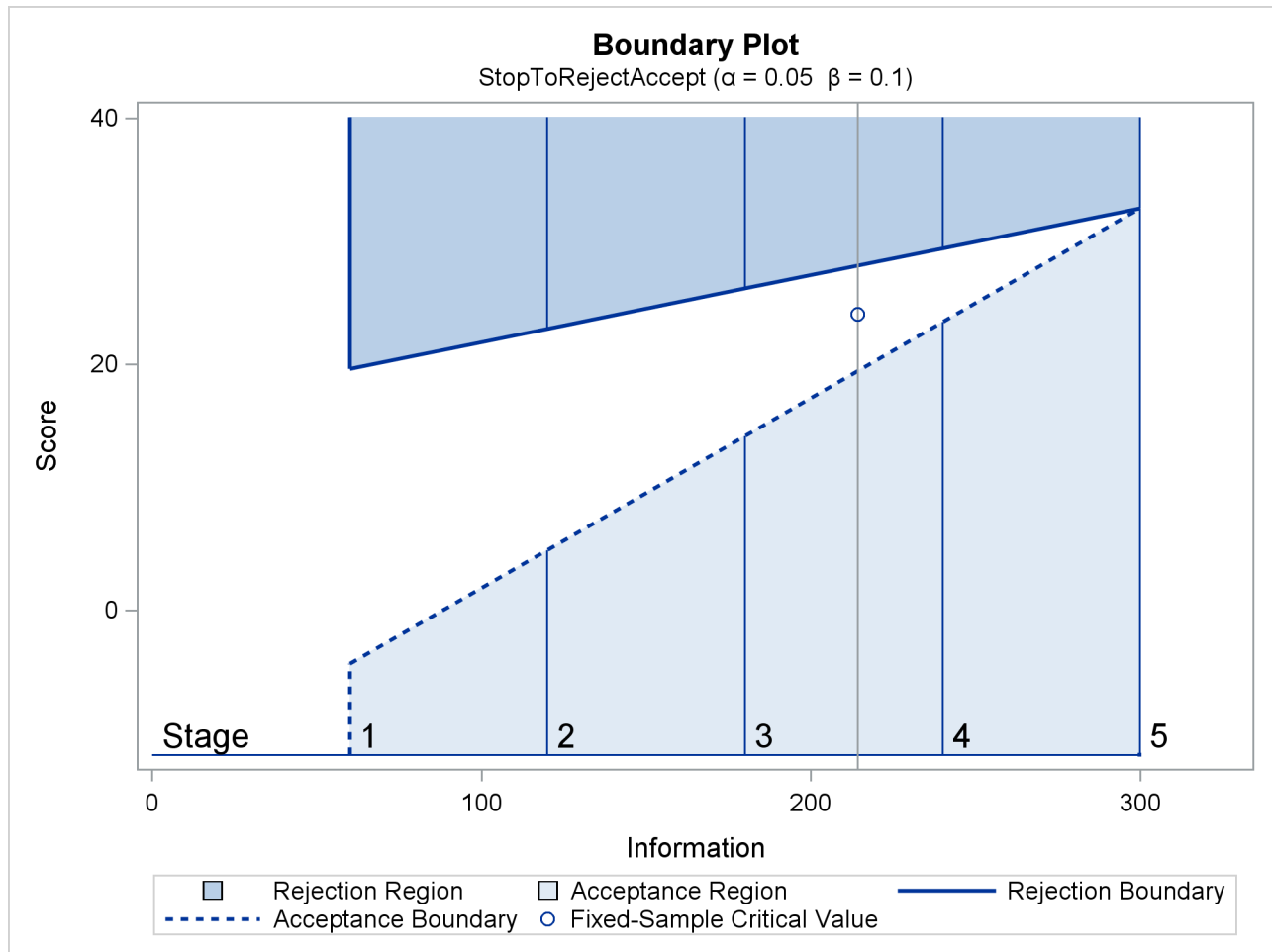
The “Error Spending Information” table in [Output 83.6.4](#) displays cumulative error spending at each stage for each boundary.

**Output 83.6.4** Error Spending Information

| Error Spending Information |                     |  |                             |         |
|----------------------------|---------------------|--|-----------------------------|---------|
| _Stage_                    | -Information Level- |  | -Cumulative Error Spending- |         |
|                            | Proportion          |  | -----Upper-----<br>Beta     | Alpha   |
| 1                          | 0.2000              |  | 0.01729                     | 0.00566 |
| 2                          | 0.4000              |  | 0.04927                     | 0.02138 |
| 3                          | 0.6000              |  | 0.07611                     | 0.03643 |
| 4                          | 0.8000              |  | 0.09357                     | 0.04641 |
| 5                          | 1.0000              |  | 0.10000                     | 0.05000 |

With ODS Graphics enabled, a detailed boundary plot with the rejection and acceptance regions is displayed, as shown in [Output 83.6.5](#). With the STOP=BOTH option, both the acceptance and rejection boundaries at interim stages are displayed. With the score scale, the acceptance and rejection boundaries are straight lines and form a triangular-shape continuation region.

**Output 83.6.5** Boundary Plot with Score Statistics



The second design has early stopping only to reject the null hypothesis  $H_0$ .

The “Design Information” table in [Output 83.6.6](#) displays design specifications and derived statistics. With the specified alternative reference, the maximum information is derived.

**Output 83.6.6** Triangular Design Information

| The SEQDESIGN Procedure                   |             |
|-------------------------------------------|-------------|
| Design: StopToReject                      |             |
| Design Information                        |             |
| Statistic Distribution                    | Normal      |
| Boundary Scale                            | Score       |
| Alternative Hypothesis                    | Upper       |
| Early Stop                                | Reject Null |
| Method                                    | Triangular  |
| Boundary Key                              | Both        |
| Alternative Reference                     | 0.2         |
| Number of Stages                          | 5           |
| Alpha                                     | 0.05        |
| Beta                                      | 0.1         |
| Power                                     | 0.9         |
| Max Information (Percent of Fixed Sample) | 113.4443    |
| Max Information                           | 242.8799    |
| Null Ref ASN (Percent of Fixed Sample)    | 111.3399    |
| Alt Ref ASN (Percent of Fixed Sample)     | 67.41968    |

The “Method Information” table in [Output 83.6.7](#) displays the  $\alpha$  and  $\beta$  errors and the derived drift parameter. The table also shows the corresponding parameters for a triangular method as a unified family method.

**Output 83.6.7** Method Information

| Method Information |             |                       |          |                          |     |        |
|--------------------|-------------|-----------------------|----------|--------------------------|-----|--------|
| Boundary           | Method      | Alpha                 | Beta     | -----Unified Family----- |     |        |
|                    |             |                       |          | Rho                      | Tau | C      |
| Upper Alpha        | Triangular  | 0.05000               | 0.10000  | 0.5                      | 1   | 0.9833 |
| Method Information |             |                       |          |                          |     |        |
|                    | Boundary    | Alternative Reference | Drift    |                          |     |        |
|                    | Upper Alpha | 0.2                   | 3.116921 |                          |     |        |

The “Boundary Information” table in [Output 83.6.8](#) displays information level, alternative reference, and boundary values. With the specified BOUNDARYSCALE=SCORE option, the alternative reference and boundary values are displayed in the score statistic scale.

**Output 83.6.8** Boundary Information

| Boundary Information (Score Scale) |                        |          |                        |                          |
|------------------------------------|------------------------|----------|------------------------|--------------------------|
| Null Reference = 0                 |                        |          |                        |                          |
| _Stage_                            | ---Information Level-- |          | -Alternative-          | -Boundary Values-        |
|                                    | Proportion             | Actual   | --Reference--<br>Upper | -----Upper-----<br>Alpha |
| 1                                  | 0.2000                 | 48.57597 | 9.71519                | 18.38919                 |
| 2                                  | 0.4000                 | 97.15194 | 19.43039               | 21.45405                 |
| 3                                  | 0.6000                 | 145.7279 | 29.14558               | 24.51891                 |
| 4                                  | 0.8000                 | 194.3039 | 38.86078               | 27.58378                 |
| 5                                  | 1.0000                 | 242.8799 | 48.57597               | 30.64864                 |

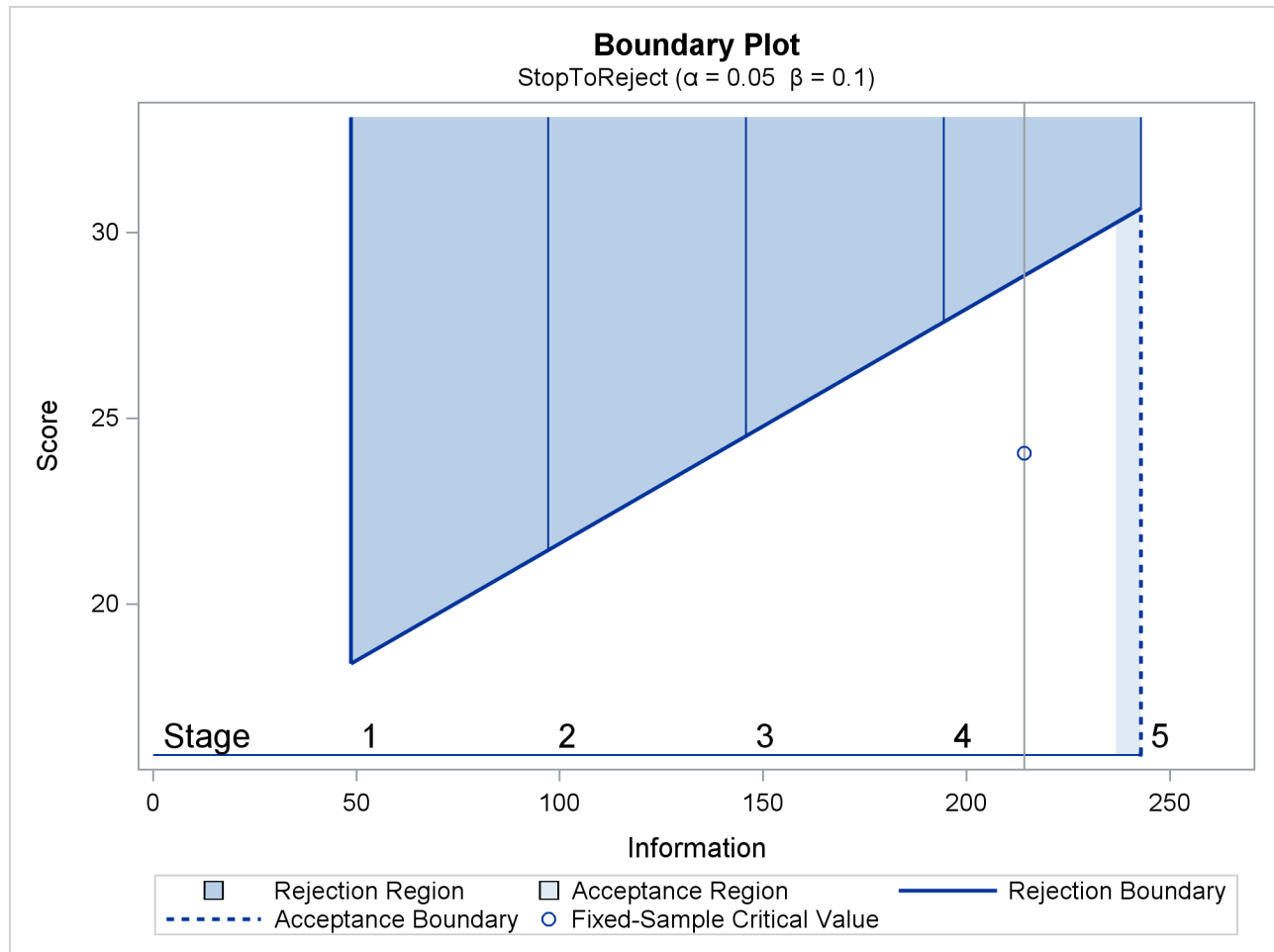
The “Error Spending Information” table in [Output 83.6.9](#) displays cumulative error spending at each stage for each boundary.

**Output 83.6.9** Error Spending Information

| Error Spending Information |                     |         |                             |         |
|----------------------------|---------------------|---------|-----------------------------|---------|
| _Stage_                    | -Information Level- |         | -Cumulative Error Spending- |         |
|                            | Proportion          |         | -----Upper-----<br>Beta     | Alpha   |
| 1                          | 0.2000              | 0.00000 | 0.00000                     | 0.00416 |
| 2                          | 0.4000              | 0.00000 | 0.00000                     | 0.01705 |
| 3                          | 0.6000              | 0.00000 | 0.00000                     | 0.03027 |
| 4                          | 0.8000              | 0.00000 | 0.00000                     | 0.04127 |
| 5                          | 1.0000              | 0.10000 | 0.10000                     | 0.05000 |

With ODS Graphics enabled, a detailed boundary plot with the rejection and acceptance regions is displayed, as shown in [Output 83.6.10](#). For a triangular design, these rejection boundaries form a straight line with the score scale.



**Output 83.6.10** Boundary Plot with Score Statistics

The third design has early stopping to accept the null hypothesis  $H_0$ .

The “Design Information” table in [Output 83.6.11](#) displays design specifications and derived statistics. With the specified alternative reference, the maximum information is derived.

**Output 83.6.11** Triangular Design Information

| The SEQDESIGN Procedure                   |             |
|-------------------------------------------|-------------|
| Design: StopToAccept                      |             |
| Design Information                        |             |
| Statistic Distribution                    | Normal      |
| Boundary Scale                            | Score       |
| Alternative Hypothesis                    | Upper       |
| Early Stop                                | Accept Null |
| Method                                    | Triangular  |
| Boundary Key                              | Both        |
| Alternative Reference                     | 0.2         |
| Number of Stages                          | 5           |
| Alpha                                     | 0.05        |
| Beta                                      | 0.1         |
| Power                                     | 0.9         |
| Max Information (Percent of Fixed Sample) | 114.9925    |
| Max Information                           | 246.1945    |
| Null Ref ASN (Percent of Fixed Sample)    | 57.83208    |
| Alt Ref ASN (Percent of Fixed Sample)     | 110.2477    |

The “Method Information” table in [Output 83.6.12](#) displays the  $\alpha$  and  $\beta$  errors and the derived drift parameter. The table also shows the corresponding parameters for a triangular method as a unified family method.

**Output 83.6.12** Method Information

| Method Information |            |                       |          |                          |     |         |
|--------------------|------------|-----------------------|----------|--------------------------|-----|---------|
| Boundary           | Method     | Alpha                 | Beta     | -----Unified Family----- |     |         |
|                    |            |                       |          | Rho                      | Tau | C       |
| Upper Beta         | Triangular | 0.05000               | 0.10000  | 0.5                      | 1   | 0.82154 |
| Method Information |            |                       |          |                          |     |         |
|                    | Boundary   | Alternative Reference | Drift    |                          |     |         |
|                    | Upper Beta | 0.2                   | 3.138117 |                          |     |         |

The “Boundary Information” table in [Output 83.6.13](#) displays information level, alternative reference, and boundary values. With the specified BOUNDARYSCALE=SCORE option, the alternative reference and boundary values are displayed in the score statistic scale.

**Output 83.6.13** Boundary Information

| Boundary Information (Score Scale) |                         |          |                        |                         |
|------------------------------------|-------------------------|----------|------------------------|-------------------------|
| Null Reference = 0                 |                         |          |                        |                         |
| _Stage_                            | ---Information Level--- |          | -Alternative-          | -Boundary Values-       |
|                                    | Proportion              | Actual   | --Reference--<br>Upper | -----Upper-----<br>Beta |
| 1                                  | 0.2000                  | 49.2389  | 9.84778                | -5.62074                |
| 2                                  | 0.4000                  | 98.4778  | 19.69556               | 1.64895                 |
| 3                                  | 0.6000                  | 147.7167 | 29.54334               | 8.91865                 |
| 4                                  | 0.8000                  | 196.9556 | 39.39112               | 16.18834                |
| 5                                  | 1.0000                  | 246.1945 | 49.23890               | 23.45803                |

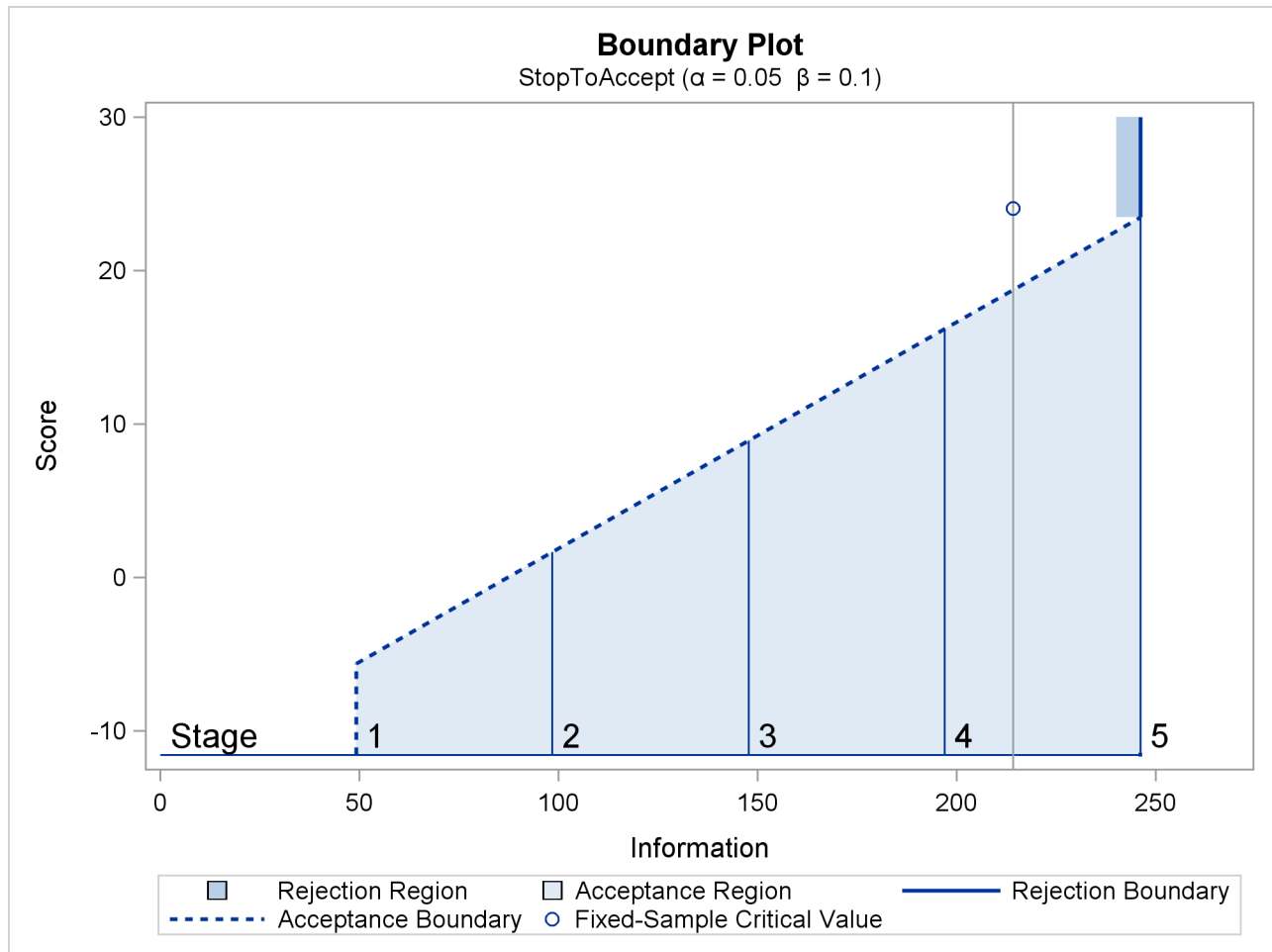
The “Error Spending Information” table in [Output 83.6.14](#) displays cumulative error spending at each stage for each boundary.

**Output 83.6.14** Error Spending Information

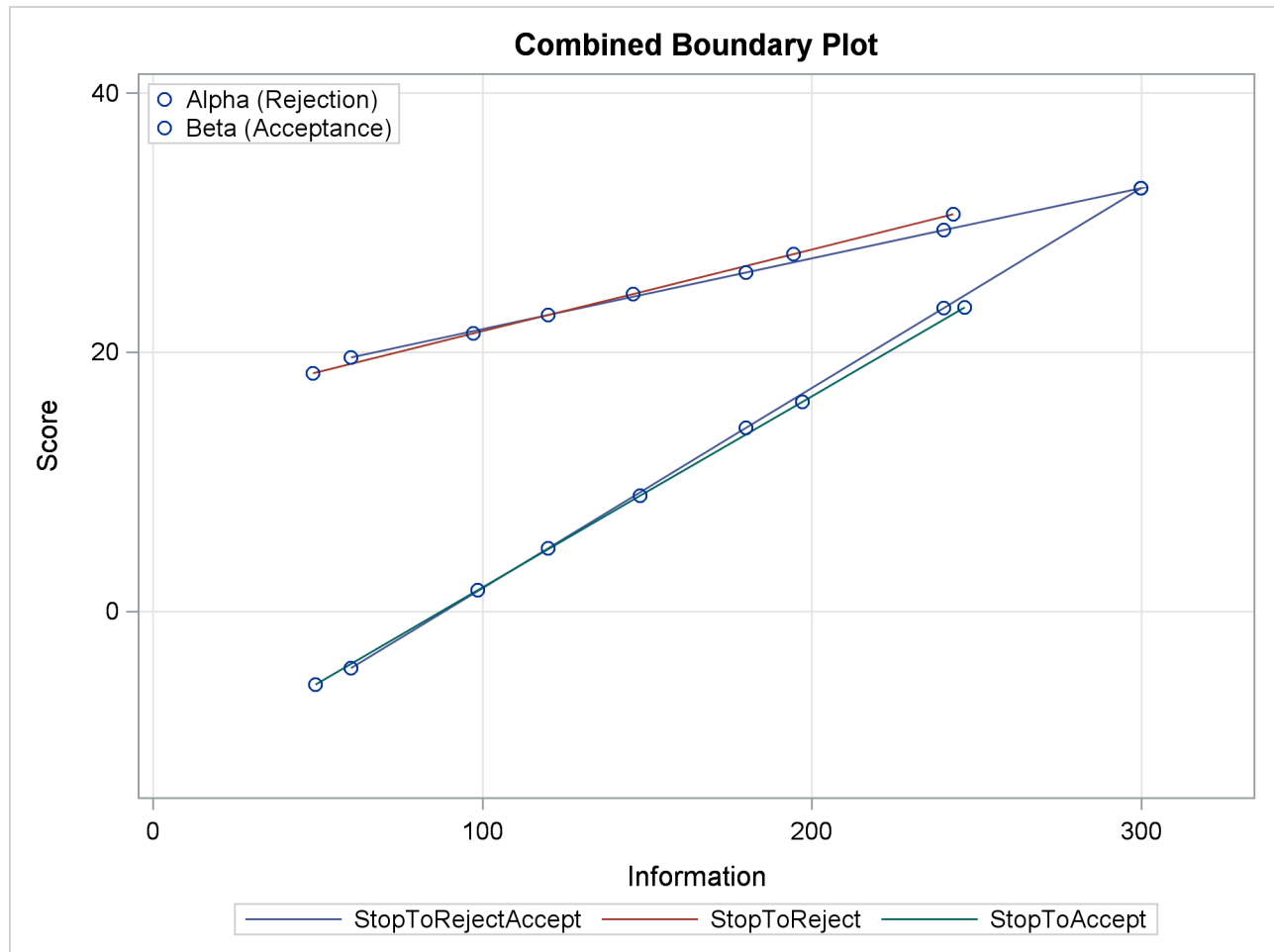
| Error Spending Information |                     |  |                             |         |
|----------------------------|---------------------|--|-----------------------------|---------|
| _Stage_                    | -Information Level- |  | -Cumulative Error Spending- |         |
|                            | Proportion          |  | -----Upper-----<br>Beta     | Alpha   |
| 1                          | 0.2000              |  | 0.01375                     | 0.00000 |
| 2                          | 0.4000              |  | 0.04149                     | 0.00000 |
| 3                          | 0.6000              |  | 0.06594                     | 0.00000 |
| 4                          | 0.8000              |  | 0.08513                     | 0.00000 |
| 5                          | 1.0000              |  | 0.10000                     | 0.05000 |

With ODS Graphics enabled, a detailed boundary plot with the rejection and acceptance regions is displayed, as shown in [Output 83.6.15](#). For a triangular design, these rejection boundaries form a straight line with the score scale.

**Output 83.6.15** Boundary Plot with Score Scale

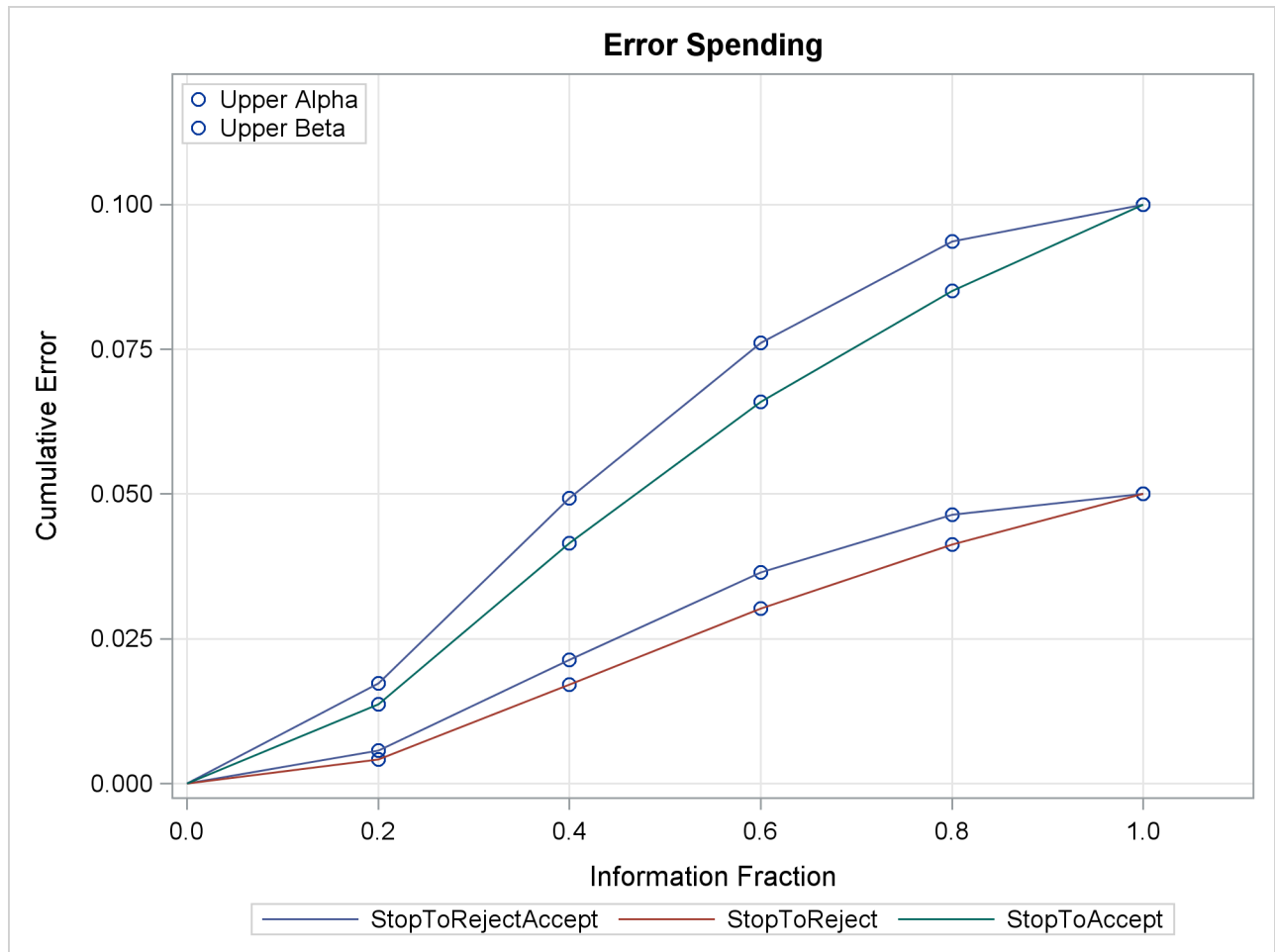


With the PLOTS=COMBINEDBOUNDARY option, a plot of the resulting sequential boundaries for all designs is displayed, as shown in [Output 83.6.16](#). The plot shows that the design with early stopping to reject and to accept  $H_0$  has larger maximum information than the other two designs.

**Output 83.6.16** Combined Boundary Plot with Score Scale

With the `PLOTS=ERRSPEND(HSCALE=INFO)` option, the error spending plot is displayed with the information level on the horizontal axis, as shown in [Output 83.6.17](#). The design with early stopping to reject or accept the null hypothesis  $H_0$  has larger  $\alpha$  spending and larger  $\beta$  spending in early stages than the other two designs.

**Output 83.6.17** Error Spending Plot



### Example 83.7: Creating Whitehead's Triangular Designs

This example requests three 4-stage Whitehead's triangular designs for normally distributed statistics. Each design has a one-sided alternative hypothesis with early stopping to reject or accept the null hypothesis  $H_0$ . Note that Whitehead's triangular designs are different from unified family triangular designs.

Suppose that a clinic is conducting a study of the effect of a new cancer treatment. The study consists of exposing mice to a carcinogen and randomly assigning them to either the control group or the treatment group. The event of interest is death from cancer induced by the carcinogen, and the response is the time from randomization to death.

Following the derivations in the section "Test for Two Survival Distributions with a Log-Rank Test" on page 7059, the hypothesis  $H_0 : \theta = -\log(\lambda) = 0$  with an alternative hypothesis  $H_1 : \theta = \theta_1 > 0$  is used, where  $\lambda$  is the hazard ratio between the treatment group and the control group.

Also suppose that from past experience, the median survival time for the control group is  $t_0 = 20$  weeks, and the study wants to detect a  $t_1 = 40$  weeks' median survival time with a 80% power in the trial. Assuming exponential survival functions for the two groups, the hazard rates can be computed from

$$S_j(t_j) = e^{-h_j t_j} = \frac{1}{2}$$

where  $j = 0, 1$ .

Thus, with  $h_0 = 0.03466$  and  $h_1 = 0.01733$ , the hazard ratio  $\lambda_1 = h_1/h_0 = 1/2$ , and the alternative reference is

$$\theta_1 = -\log(\lambda_1) = -\log\left(\frac{1}{2}\right) = 0.693147$$

The following statements invoke the SEQDESIGN procedure and specify three Whitehead's triangular designs:

```
ods graphics on;
proc seqdesign altref=0.693147
 bscale=score
 plots=combinedboundary
 ;
 BoundaryKeyNone: design nstages=4
 method=whitehead
 boundarykey=none
 alt=upper stop=both
 alpha=0.05 beta=0.20
 ;
 BoundaryKeyAlpha: design nstages=4
 method=whitehead
 boundarykey=alpha
 alt=upper stop=both
 alpha=0.05 beta=0.20
 ;
```

```

BoundaryKeyBeta: design nstages=4
 method=whitehead
 boundarykey=beta
 alt=upper stop=both
 alpha=0.05 beta=0.20
 ;

run;
ods graphics off;

```

Whitehead methods with early stopping to reject or accept the null hypothesis create boundaries that approximately satisfy the Type I and Type II error probability specification. The BOUNDARYKEY=NONE option specifies no adjustment to the boundary value at the final stage to maintain either a Type I or a Type II error probability level.

The “Design Information” table in [Output 83.7.1](#) displays design specifications and maximum information. Note that with the BOUNDARYKEY=NONE option, the derived errors  $\alpha = 0.05071$  and  $\beta = 0.19771$  are not the same as the specified errors  $\alpha = 0.05$  and  $\beta = 0.20$ .

#### Output 83.7.1 Whitehead Design Information

| The SEQDESIGN Procedure                   |                    |
|-------------------------------------------|--------------------|
| Design: BoundaryKeyNone                   |                    |
| Design Information                        |                    |
| Statistic Distribution                    | Normal             |
| Boundary Scale                            | Score              |
| Alternative Hypothesis                    | Upper              |
| Early Stop                                | Accept/Reject Null |
| Method                                    | Whitehead          |
| Boundary Key                              | None               |
| Alternative Reference                     | 0.693147           |
| Number of Stages                          | 4                  |
| Alpha                                     | 0.05071            |
| Beta                                      | 0.19771            |
| Power                                     | 0.80229            |
| Max Information (Percent of Fixed Sample) | 129.6815           |
| Max Information                           | 16.70639           |
| Null Ref ASN (Percent of Fixed Sample)    | 62.48184           |
| Alt Ref ASN (Percent of Fixed Sample)     | 73.82535           |

The “Method Information” table in [Output 83.7.2](#) displays the derived  $\alpha$  and  $\beta$  errors and the derived drift parameter. The derived errors  $\alpha = 0.05071$  and  $\beta = 0.19771$  are not exactly the same as the specified errors  $\alpha = 0.05$  and  $\beta = 0.20$  with the BOUNDARYKEY=NONE option.



**Output 83.7.2** Method Information

| Method Information |           |         |         |                            |         |
|--------------------|-----------|---------|---------|----------------------------|---------|
| Boundary           | Method    | Alpha   | Beta    | -----Whitehead-----<br>Tau | C       |
| Upper Alpha        | Whitehead | 0.05071 | .       | 0.25                       | 4.60517 |
| Upper Beta         | Whitehead | .       | 0.19771 | 0.25                       | 4.60517 |

| Method Information |                       |          |  |
|--------------------|-----------------------|----------|--|
| Boundary           | Alternative Reference | Drift    |  |
| Upper Alpha        | 0.693147              | 2.833131 |  |
| Upper Beta         | 0.693147              | 2.833131 |  |

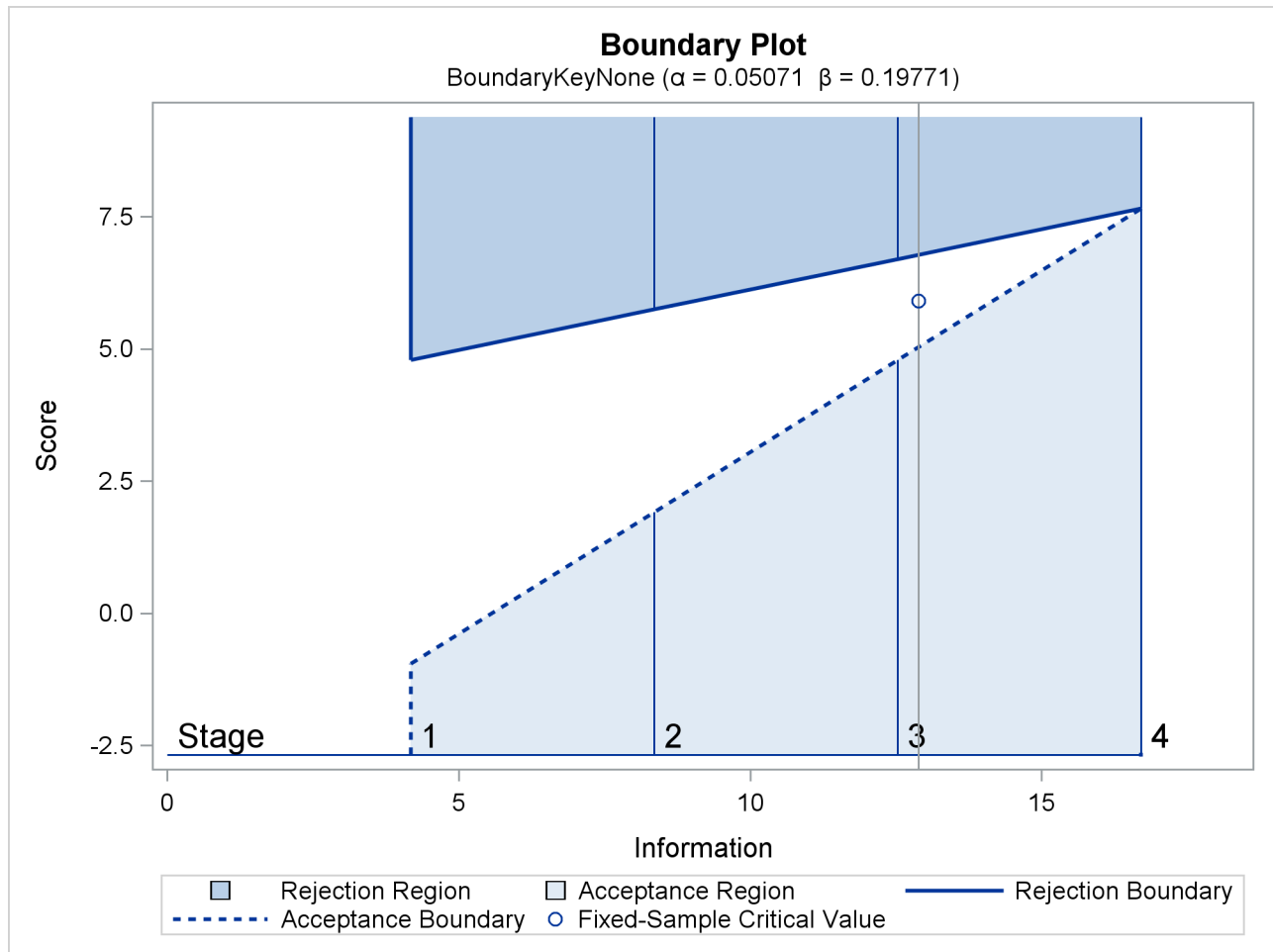
The “Boundary Information” table in [Output 83.7.3](#) displays information level, alternative reference, and boundary values. With the specified BOUNDARYSCALE=SCORE option, the alternative reference and boundary values are displayed with the score statistics scale.

**Output 83.7.3** Boundary Information

| Boundary Information (Score Scale) |                        |          |                        |                          |         |
|------------------------------------|------------------------|----------|------------------------|--------------------------|---------|
| Null Reference = 0                 |                        |          |                        |                          |         |
| _Stage_                            | ---Information Level-- |          | -Alternative-          | -----Boundary Values---- |         |
|                                    | Proportion             | Actual   | --Reference--<br>Upper | -----Upper-----<br>Beta  | Alpha   |
| 1                                  | 0.2500                 | 4.176597 | 2.89500                | -0.95755                 | 4.78775 |
| 2                                  | 0.5000                 | 8.353195 | 5.78999                | 1.91510                  | 5.74530 |
| 3                                  | 0.7500                 | 12.52979 | 8.68499                | 4.78775                  | 6.70285 |
| 4                                  | 1.0000                 | 16.70639 | 11.57998               | 7.66039                  | 7.66039 |

With ODS Graphics enabled, a detailed boundary plot with the rejection and acceptance regions is displayed, as shown in [Output 83.7.4](#).

**Output 83.7.4** Boundary Plot



The second design uses the BOUNDARYKEY=ALPHA option to adjust the boundary value at the final stage to maintain the Type I error probability level.

The “Design Information” table in [Output 83.7.5](#) displays design specifications and the derived maximum information. Note that with the BOUNDARYKEY=ALPHA option, the specified Type I error probability  $\alpha = 0.05$  is maintained.

**Output 83.7.5** Whitehead Design Information

| The SEQDESIGN Procedure                   |                    |
|-------------------------------------------|--------------------|
| Design: BoundaryKeyAlpha                  |                    |
| Design Information                        |                    |
| Statistic Distribution                    | Normal             |
| Boundary Scale                            | Score              |
| Alternative Hypothesis                    | Upper              |
| Early Stop                                | Accept/Reject Null |
| Method                                    | Whitehead          |
| Boundary Key                              | Alpha              |
| Alternative Reference                     | 0.693147           |
| Number of Stages                          | 4                  |
| Alpha                                     | 0.05               |
| Beta                                      | 0.20044            |
| Power                                     | 0.79956            |
| Max Information (Percent of Fixed Sample) | 129.9894           |
| Max Information                           | 16.70639           |
| Null Ref ASN (Percent of Fixed Sample)    | 62.6302            |
| Alt Ref ASN (Percent of Fixed Sample)     | 74.00064           |

The “Method Information” table in [Output 83.7.6](#) displays the specified and derived  $\alpha$  and  $\beta$  errors and the derived drift parameter. The derived Type I error probability is the same as the specified  $\alpha = 0.05$  and the derived Type II error probability  $\beta = 0.20044$  is not the same as the specified  $\beta = 0.20$  with the BOUNDARYKEY=ALPHA option.

**Output 83.7.6** Method Information

| Method Information |             |                          |          |                            |         |
|--------------------|-------------|--------------------------|----------|----------------------------|---------|
| Boundary           | Method      | Alpha                    | Beta     | -----Whitehead-----<br>Tau | C       |
| Upper Alpha        | Whitehead   | 0.05000                  | .        | 0.25                       | 4.60517 |
| Upper Beta         | Whitehead   | .                        | 0.20044  | 0.25                       | 4.60517 |
| Method Information |             |                          |          |                            |         |
|                    | Boundary    | Alternative<br>Reference | Drift    |                            |         |
|                    | Upper Alpha | 0.693147                 | 2.833131 |                            |         |
|                    | Upper Beta  | 0.693147                 | 2.833131 |                            |         |

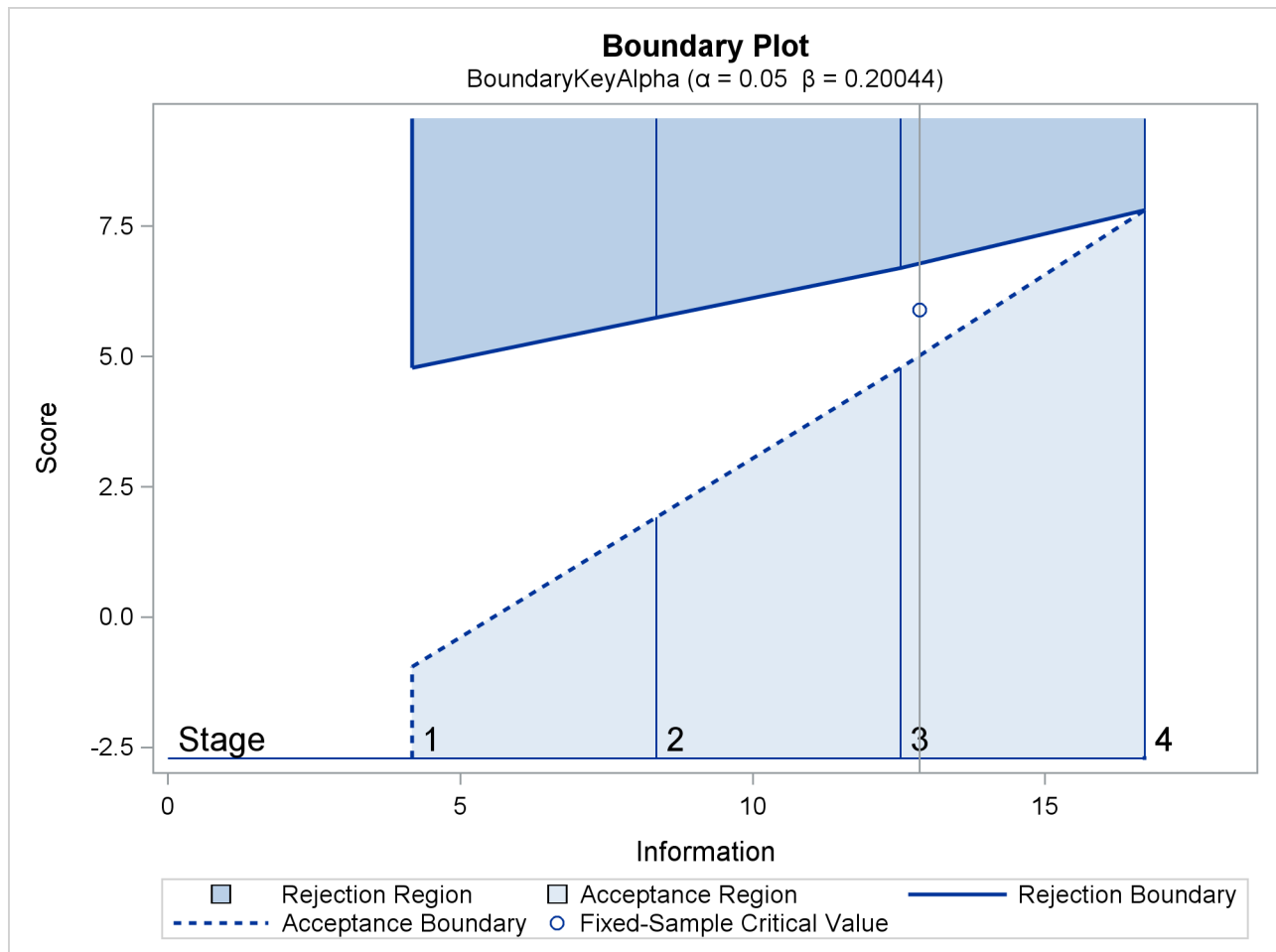
The “Boundary Information” table in [Output 83.7.7](#) displays information level, alternative reference, and boundary values.

**Output 83.7.7** Boundary Information

| Boundary Information (Score Scale) |                         |          |                        |                           |         |
|------------------------------------|-------------------------|----------|------------------------|---------------------------|---------|
| Null Reference = 0                 |                         |          |                        |                           |         |
| _Stage_                            | ---Information Level--- |          | -Alternative-          | -----Boundary Values----- |         |
|                                    | Proportion              | Actual   | --Reference--<br>Upper | -----Upper-----<br>Beta   | Alpha   |
| 1                                  | 0.2500                  | 4.176597 | 2.89500                | -0.95755                  | 4.78775 |
| 2                                  | 0.5000                  | 8.353195 | 5.78999                | 1.91510                   | 5.74530 |
| 3                                  | 0.7500                  | 12.52979 | 8.68499                | 4.78775                   | 6.70285 |
| 4                                  | 1.0000                  | 16.70639 | 11.57998               | 7.81300                   | 7.81300 |

With ODS Graphics enabled, a detailed boundary plot with the rejection and acceptance regions is displayed, as shown in [Output 83.7.8](#).

**Output 83.7.8** Boundary Plot



The third design specifies the BOUNDARYKEY=BETA option to derive the boundary values to maintain the Type II error probability level  $\beta$ .

The “Design Information” table in Output 83.7.9 displays design specifications and the derived maximum information. Note that with the BOUNDARYKEY=BETA option, the specified Type II error probability  $\beta = 0.20$  is maintained.

**Output 83.7.9** Whitehead Design Information

| The SEQDESIGN Procedure                   |                    |
|-------------------------------------------|--------------------|
| Design: BoundaryKeyBeta                   |                    |
| Design Information                        |                    |
| Statistic Distribution                    | Normal             |
| Boundary Scale                            | Score              |
| Alternative Hypothesis                    | Upper              |
| Early Stop                                | Accept/Reject Null |
| Method                                    | Whitehead          |
| Boundary Key                              | Beta               |
| Alternative Reference                     | 0.693147           |
| Number of Stages                          | 4                  |
| Alpha                                     | 0.05011            |
| Beta                                      | 0.2                |
| Power                                     | 0.8                |
| Max Information (Percent of Fixed Sample) | 129.9364           |
| Max Information                           | 16.70639           |
| Null Ref ASN (Percent of Fixed Sample)    | 62.60462           |
| Alt Ref ASN (Percent of Fixed Sample)     | 73.97042           |

The “Method Information” table in Output 83.7.10 displays the  $\alpha$  and  $\beta$  errors and the derived drift parameter. The derived Type II error probability is the same as the specified  $\beta = 0.20$  and the derived Type I error probability  $\alpha = 0.05011$  is not the same as the specified  $\alpha = 0.05$  with the BOUNDARYKEY=BETA option.

**Output 83.7.10** Method Information

| Method Information |             |                       |          |                     |         |
|--------------------|-------------|-----------------------|----------|---------------------|---------|
| Boundary           | Method      | Alpha                 | Beta     | -----Whitehead----- |         |
|                    |             |                       |          | Tau                 | C       |
| Upper Alpha        | Whitehead   | 0.05011               | .        | 0.25                | 4.60517 |
| Upper Beta         | Whitehead   | .                     | 0.20000  | 0.25                | 4.60517 |
| Method Information |             |                       |          |                     |         |
|                    | Boundary    | Alternative Reference | Drift    |                     |         |
|                    | Upper Alpha | 0.693147              | 2.833131 |                     |         |
|                    | Upper Beta  | 0.693147              | 2.833131 |                     |         |

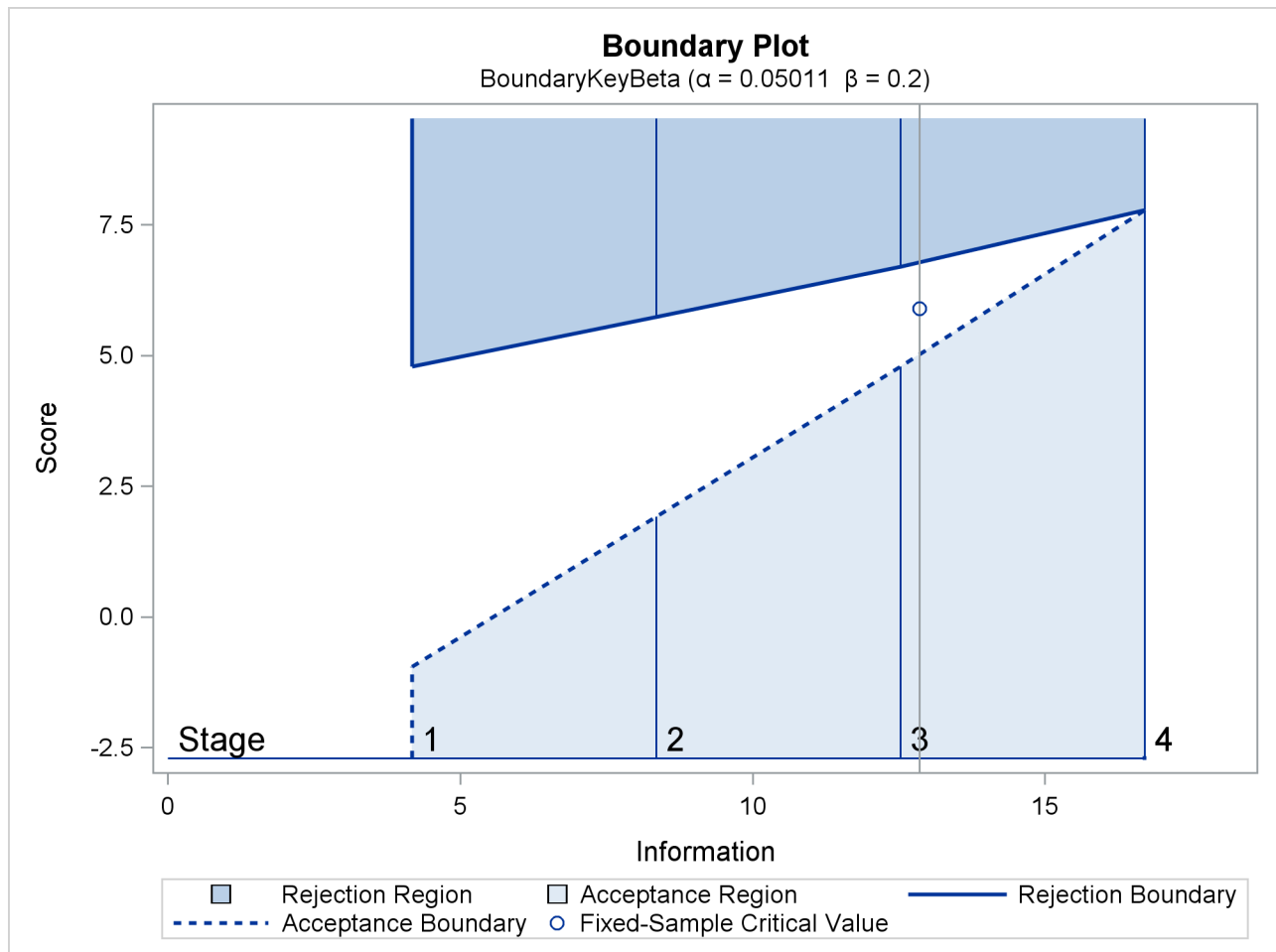
The “Boundary Information” table in [Output 83.7.11](#) displays information level, alternative reference, and boundary values.

**Output 83.7.11** Boundary Information

| Boundary Information (Score Scale) |                        |          |                        |                           |         |
|------------------------------------|------------------------|----------|------------------------|---------------------------|---------|
| Null Reference = 0                 |                        |          |                        |                           |         |
| _Stage_                            | ---Information Level-- |          | -Alternative-          | -----Boundary Values----- |         |
|                                    | Proportion             | Actual   | --Reference--<br>Upper | -----Upper-----<br>Beta   | Alpha   |
| 1                                  | 0.2500                 | 4.176597 | 2.89500                | -0.95755                  | 4.78775 |
| 2                                  | 0.5000                 | 8.353195 | 5.78999                | 1.91510                   | 5.74530 |
| 3                                  | 0.7500                 | 12.52979 | 8.68499                | 4.78775                   | 6.70285 |
| 4                                  | 1.0000                 | 16.70639 | 11.57998               | 7.78899                   | 7.78899 |

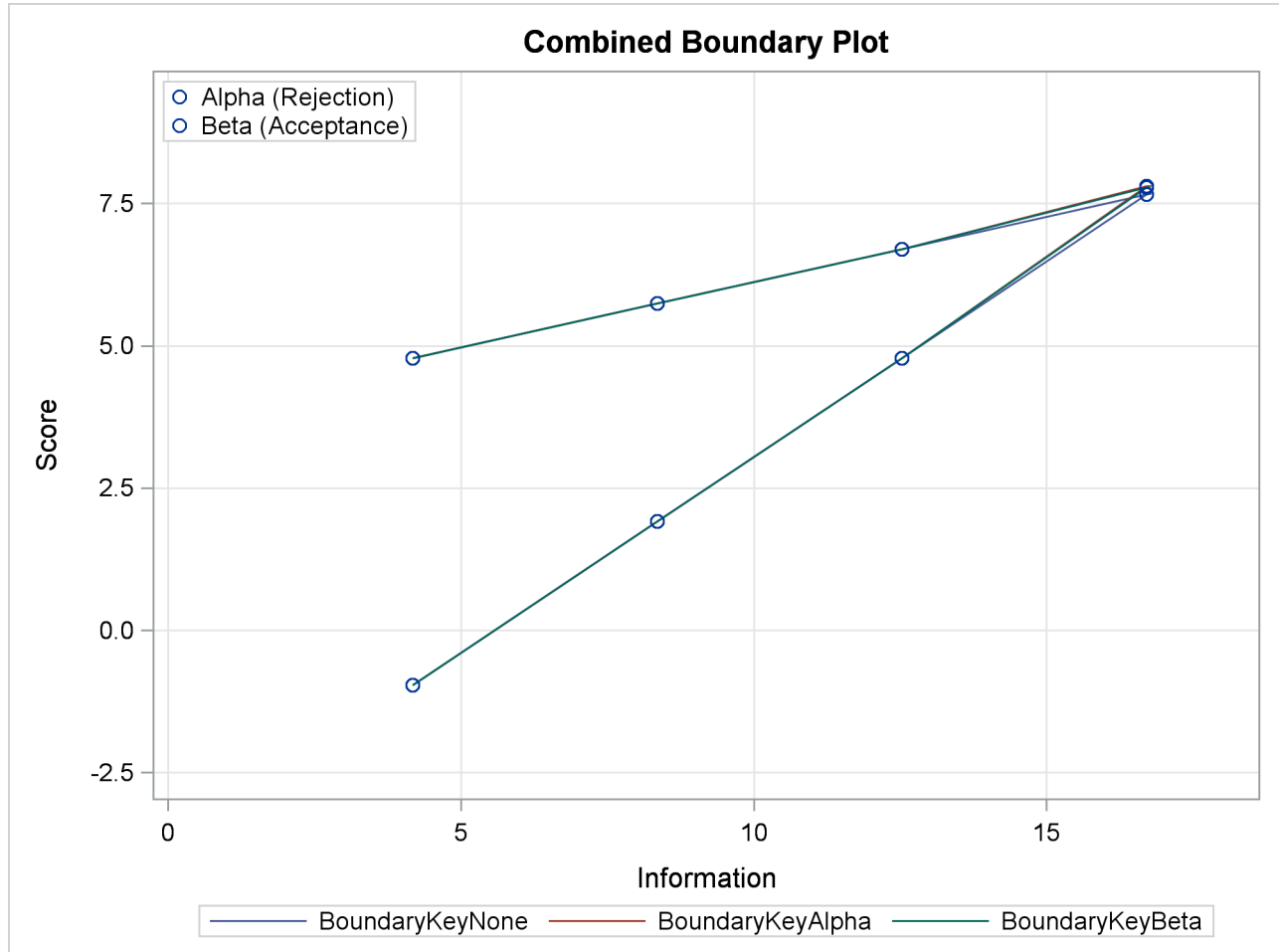
With ODS Graphics enabled, a detailed boundary plot with the rejection and acceptance regions is displayed, as shown in [Output 83.7.12](#).

**Output 83.7.12** Boundary Plot



With the PLOTS=COMBINEDBOUNDARY option, a combined plot of group sequential boundaries for all designs is displayed, as shown in [Output 83.7.13](#). It shows that three designs are similar, with a slightly smaller boundary value at the final stage for the design with the BOUNDARYKEY=NONE option.

**Output 83.7.13** Combined Boundary Plot



The following statements invoke the SEQDESIGN procedure and specify the SAMPLESIZE statement to derive required sample sizes for a log-rank test comparing two survival distributions for the treatment effect (Jennison and Turnbull 2000, pp. 77–79; Whitehead 1997, pp. 36–39):

```
proc seqdesign altref=0.693147
 bscale=score
 ;
 BoundaryKeyAlpha: design nstages=4
 method=whitehead
 boundarykey=alpha
 alt=upper stop=both
 alpha=0.05 beta=0.20
 ;
 samplesize model=twosamplesurvival
 (nullhazard=0.03466 accrate=10);
run;
```

The design is identical to the previous design with the BOUNDARYKEY=ALPHA option except with the addition of the sample size computation.

The “Sample Size Summary” table in [Output 83.7.14](#) displays parameters for the sample size computation. Since the ACCTIME= option is not specified for the accrual time, the minimum and maximum accrual times are derived for the specified accrual rate.

**Output 83.7.14** Sample Size Summary

| The SEQDESIGN Procedure  |                     |          |
|--------------------------|---------------------|----------|
| Design: BoundaryKeyAlpha |                     |          |
| Sample Size Summary      |                     |          |
| Test                     | Two-Sample Survival |          |
| Null Hazard Rate         |                     | 0.03466  |
| Hazard Rate (Group A)    |                     | 0.01733  |
| Hazard Rate (Group B)    |                     | 0.03466  |
| Hazard Ratio             |                     | 0.5      |
| log(Hazard Ratio)        |                     | -0.69315 |
| Reference Hazards        |                     | Alt Ref  |
| Accrual                  |                     | Uniform  |
| Accrual Rate             |                     | 10       |
| Min Accrual Time         |                     | 6.682556 |
| Min Sample Size          |                     | 66.82556 |
| Max Accrual Time         |                     | 25.40111 |
| Max Sample Size          |                     | 254.0111 |
| Max Number of Events     |                     | 66.82556 |

If the ACCTIME=20 option is specified in the SAMPLESIZE statement, the “Sample Size Summary” table in [Output 83.7.15](#) also displays the follow-up time and maximum sample size with the specified accrual time.

**Output 83.7.15** Sample Size Summary

| The SEQDESIGN Procedure         |                     |          |
|---------------------------------|---------------------|----------|
| Design: WhiteheadKeyAlpha       |                     |          |
| Sample Size Summary             |                     |          |
| Test                            | Two-Sample Survival |          |
| Null Hazard Rate                |                     | 0.03466  |
| Hazard Rate (Group A)           |                     | 0.01733  |
| Hazard Rate (Group B)           |                     | 0.03466  |
| Hazard Ratio                    |                     | 0.5      |
| log(Hazard Ratio)               |                     | -0.69315 |
| Reference Hazards               |                     | Alt Ref  |
| Accrual                         |                     | Uniform  |
| Accrual Rate                    |                     | 10       |
| Accrual Time                    |                     | 20       |
| Follow-up Time                  |                     | 6.474376 |
| Total Time                      |                     | 26.47438 |
| Max Number of Events            |                     | 66.82556 |
| Max Sample Size                 |                     | 200      |
| Expected Sample Size (Null Ref) |                     | 161.5941 |
| Expected Sample Size (Alt Ref)  |                     | 172.4693 |



The “Number of Events (D) and Sample Sizes (N)” table in [Output 83.7.16](#) displays the required time at each stage, in both fractional and integer numbers. The derived times under the heading “Fractional Time” are not integers. These times are rounded up to integers under the heading “Ceiling Time.” The table also displays the numbers of events and sample sizes at each stage.

**Output 83.7.16** Number of Events and Sample Sizes

| Numbers of Events (D) and Sample Sizes (N)<br>Two-Sample Log-Rank Test |       |          |          |         |        |          |          |
|------------------------------------------------------------------------|-------|----------|----------|---------|--------|----------|----------|
| -----Fractional Time-----                                              |       |          |          |         |        |          |          |
| _Stage_                                                                | D     | D(Grp 1) | D(Grp 2) | Time    | N      | N(Grp 1) | N(Grp 2) |
| 1                                                                      | 16.71 | 5.82     | 10.89    | 11.9867 | 119.87 | 59.93    | 59.93    |
| 2                                                                      | 33.41 | 11.84    | 21.57    | 17.3585 | 173.58 | 86.79    | 86.79    |
| 3                                                                      | 50.12 | 18.01    | 32.11    | 21.7480 | 200.00 | 100.00   | 100.00   |
| 4                                                                      | 66.83 | 24.46    | 42.37    | 26.4744 | 200.00 | 100.00   | 100.00   |

| Numbers of Events (D) and Sample Sizes (N)<br>Two-Sample Log-Rank Test |             |       |          |          |      |        |          |
|------------------------------------------------------------------------|-------------|-------|----------|----------|------|--------|----------|
| -Fractional<br>Time-----                                               |             |       |          |          |      |        |          |
| _Stage_                                                                | Information | D     | D(Grp 1) | D(Grp 2) | Time | N      | N(Grp 1) |
| 1                                                                      | 4.1766      | 16.74 | 5.83     | 10.91    | 12   | 120.00 | 60.00    |
| 2                                                                      | 8.3532      | 35.73 | 12.68    | 23.04    | 18   | 180.00 | 90.00    |
| 3                                                                      | 12.5298     | 51.07 | 18.37    | 32.70    | 22   | 200.00 | 100.00   |
| 4                                                                      | 16.7064     | 68.55 | 25.14    | 43.41    | 27   | 200.00 | 100.00   |

| Numbers of Events (D) and Sample Sizes (N)<br>Two-Sample Log-Rank Test |          |             |
|------------------------------------------------------------------------|----------|-------------|
| -----Ceiling Time-----                                                 |          |             |
| _Stage_                                                                | N(Grp 2) | Information |
| 1                                                                      | 60.00    | 4.1854      |
| 2                                                                      | 90.00    | 8.9322      |
| 3                                                                      | 100.00   | 12.7667     |
| 4                                                                      | 100.00   | 17.1378     |

### Example 83.8: Creating a One-Sided Error Spending Design

This example requests a five-stage, one-sided group sequential design for normally distributed statistics. The design uses an O’Brien-Fleming-type error spending function for the  $\alpha$  boundary and a Pocock-type error spending function for the  $\beta$  boundary. The following statements request a one-sided design by using different  $\alpha$  and  $\beta$  spending functions:

```
ods graphics on;
proc seqdesign altref=0.2 errspend
 pss(cref=0 0.5 1)
 stopprob(cref=0 0.5 1)
 plots=(asn power errspend)
 ;
 OneSidedErrorSpending: design nstages=5
 method(alpha)=errfuncobf
 method(beta)=errfuncpoc
 alt=upper stop=both
 alpha=0.025
 ;
run;
ods graphics off;
```

The “Design Information” table in [Output 83.8.1](#) displays design specifications and the derived statistics. With the specified alternative reference, the maximum information is derived.

**Output 83.8.1** Error Spending Method Design Information

| The SEQDESIGN Procedure                   |                    |
|-------------------------------------------|--------------------|
| Design: OneSidedErrorSpending             |                    |
| Design Information                        |                    |
| Statistic Distribution                    | Normal             |
| Boundary Scale                            | Standardized Z     |
| Alternative Hypothesis                    | Upper              |
| Early Stop                                | Accept/Reject Null |
| Method                                    | Error Spending     |
| Boundary Key                              | Both               |
| Alternative Reference                     | 0.2                |
| Number of Stages                          | 5                  |
| Alpha                                     | 0.025              |
| Beta                                      | 0.1                |
| Power                                     | 0.9                |
| Max Information (Percent of Fixed Sample) | 119.4278           |
| Max Information                           | 313.7196           |
| Null Ref ASN (Percent of Fixed Sample)    | 50.35408           |
| Alt Ref ASN (Percent of Fixed Sample)     | 78.77223           |

The “Method Information” table in [Output 83.8.2](#) displays the  $\alpha$  and  $\beta$  errors, alternative reference, and derived drift parameter, which is the standardized alternative reference at the final stage.

**Output 83.8.2** Method Information

| Method Information |                |         |         |                                    |
|--------------------|----------------|---------|---------|------------------------------------|
| Boundary           | Method         | Alpha   | Beta    | ----Error Spending----<br>Function |
| Upper Alpha        | Error Spending | 0.02500 | .       | Approx O'Brien-Fleming             |
| Upper Beta         | Error Spending | .       | 0.10000 | Approx Pocock                      |

| Method Information |                          |          |  |
|--------------------|--------------------------|----------|--|
| Boundary           | Alternative<br>Reference | Drift    |  |
| Upper Alpha        | 0.2                      | 3.542426 |  |
| Upper Beta         | 0.2                      | 3.542426 |  |

With the STOPPROB option, the “Expected Cumulative Stopping Probabilities” table in [Output 83.8.3](#) displays the expected stopping stage and cumulative stopping probability to reject the null hypothesis at each stage under various hypothetical references  $\theta = c_i\theta_1$ , where  $\theta_1$  is the alternative reference and  $c_i$  are values specified in the CREF= option.

**Output 83.8.3** Stopping Probabilities

| Expected Cumulative Stopping Probabilities |                            |             |  |
|--------------------------------------------|----------------------------|-------------|--|
| Reference = CRef * (Alt Reference)         |                            |             |  |
| CRef                                       | Expected<br>Stopping Stage | Source      |  |
| 0.0000                                     | 2.108                      | Reject Null |  |
| 0.0000                                     | 2.108                      | Accept Null |  |
| 0.0000                                     | 2.108                      | Total       |  |
| 0.5000                                     | 3.296                      | Reject Null |  |
| 0.5000                                     | 3.296                      | Accept Null |  |
| 0.5000                                     | 3.296                      | Total       |  |
| 1.0000                                     | 3.298                      | Reject Null |  |
| 1.0000                                     | 3.298                      | Accept Null |  |
| 1.0000                                     | 3.298                      | Total       |  |

| Expected Cumulative Stopping Probabilities |                                  |         |         |         |         |
|--------------------------------------------|----------------------------------|---------|---------|---------|---------|
| Reference = CRef * (Alt Reference)         |                                  |         |         |         |         |
| CRef                                       | -----Stopping Probabilities----- |         |         |         |         |
|                                            | Stage_1                          | Stage_2 | Stage_3 | Stage_4 | Stage_5 |
| 0.0000                                     | 0.00000                          | 0.00039 | 0.00381 | 0.01221 | 0.02500 |
| 0.0000                                     | 0.38080                          | 0.69133 | 0.86162 | 0.94170 | 0.97500 |
| 0.0000                                     | 0.38080                          | 0.69173 | 0.86543 | 0.95391 | 1.00000 |
| 0.5000                                     | 0.00002                          | 0.01265 | 0.09650 | 0.24465 | 0.38724 |
| 0.5000                                     | 0.13665                          | 0.28063 | 0.41080 | 0.52230 | 0.61276 |
| 0.5000                                     | 0.13667                          | 0.29328 | 0.50730 | 0.76695 | 1.00000 |
| 1.0000                                     | 0.00050                          | 0.13209 | 0.52642 | 0.80390 | 0.90000 |
| 1.0000                                     | 0.02954                          | 0.05231 | 0.07085 | 0.08648 | 0.10000 |
| 1.0000                                     | 0.03004                          | 0.18440 | 0.59728 | 0.89039 | 1.00000 |

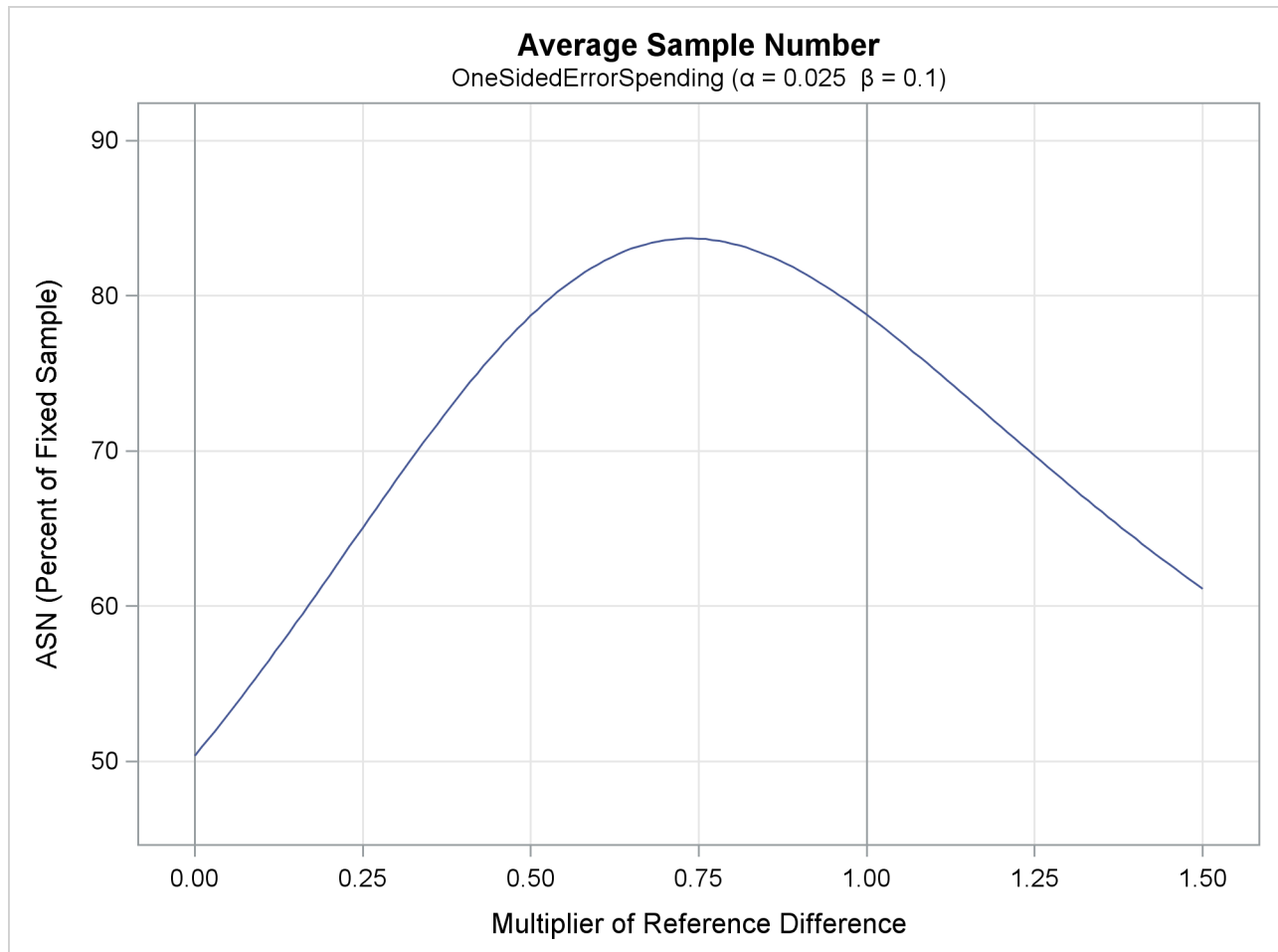
With the PSS option, the “Power and Expected Sample Sizes” table in [Output 83.8.4](#) displays powers and expected sample sizes under various hypothetical references  $\theta = c_i \theta_1$ , where  $\theta_1$  is the alternative reference and  $c_i = 0, 0.5, 1, 1.5$  are the default values in the CREF= option.

**Output 83.8.4** Power and Expected Sample Size Information

| Powers and Expected Sample Sizes<br>Reference = CRef * (Alt Reference) |         |                                          |
|------------------------------------------------------------------------|---------|------------------------------------------|
| CRef                                                                   | Power   | -Sample Size-<br>Percent<br>Fixed-Sample |
| 0.0000                                                                 | 0.02500 | 50.3541                                  |
| 0.5000                                                                 | 0.38724 | 78.7219                                  |
| 1.0000                                                                 | 0.90000 | 78.7722                                  |

With the PLOTS=ASN option, the procedure displays a plot of expected sample sizes under various hypothetical references, as shown in [Output 83.8.5](#). By default, expected sample sizes under the hypotheses  $\theta = c_i \theta_1$ ,  $c_i = 0, 0.01, 0.02, \dots, 1.50$ , are displayed, where  $\theta_1$  is the alternative reference.

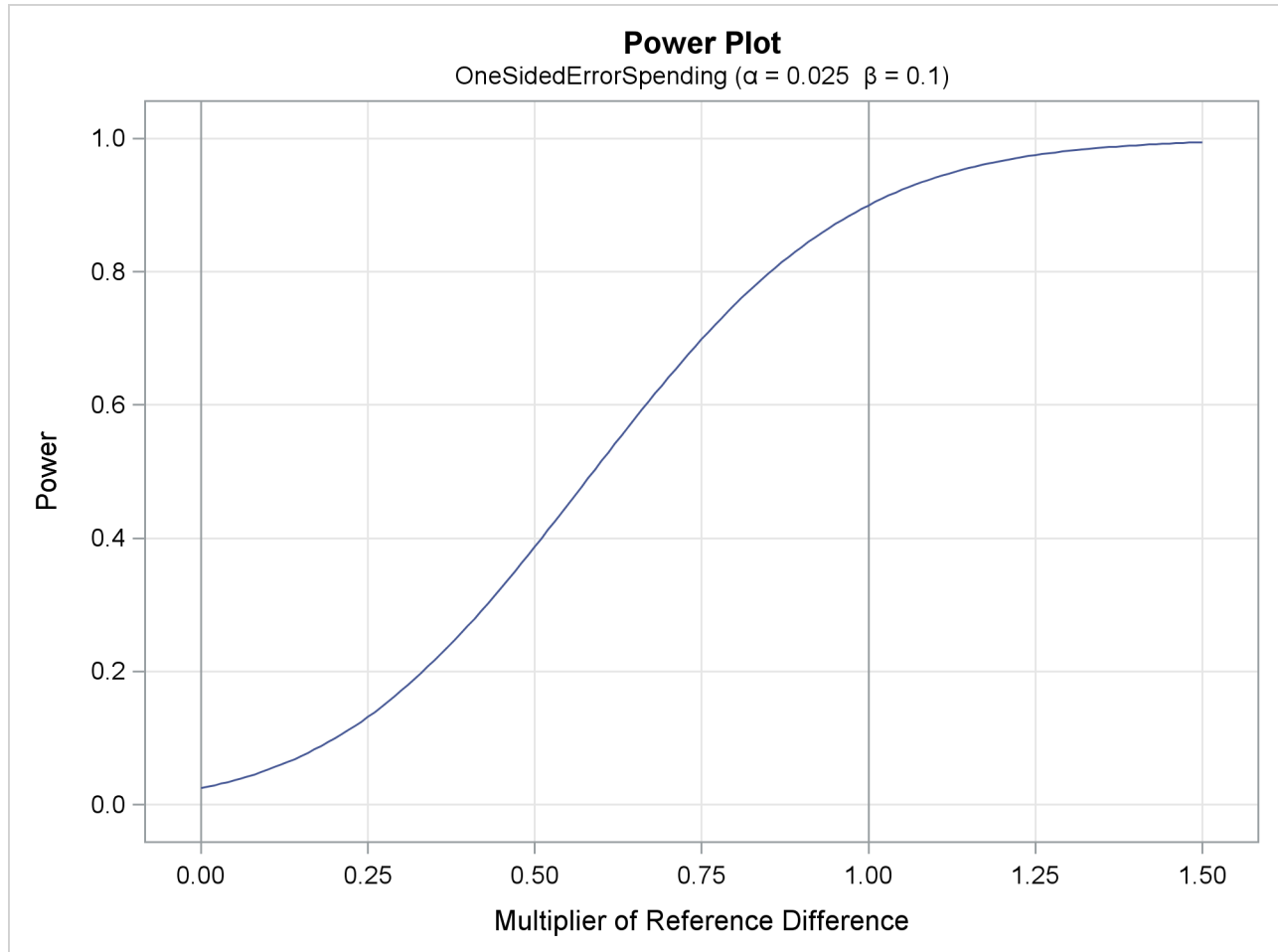
**Output 83.8.5** ASN Plot



With the PLOTS=POWER option, the procedure displays a plot of the power curves under various hypothetical references for all designs simultaneously, as shown in [Output 83.8.6](#). By default, the option CREF= 0, 0.01, 0.02, . . . , 1.50 and powers under hypothetical references  $\theta = c_i \theta_1$  are displayed, where  $c_i$  are values specified in the CREF= option. These CREF= values are displayed on the horizontal axis.

Under the null hypothesis,  $c_i = 0$ , the power is 0.025, the upper Type I error probability. Under the alternative hypothesis,  $c_i = 1$ , the power is 0.9, one minus the Type II error probability. The plot shows only minor difference between the two designs.

**Output 83.8.6** Power Plot



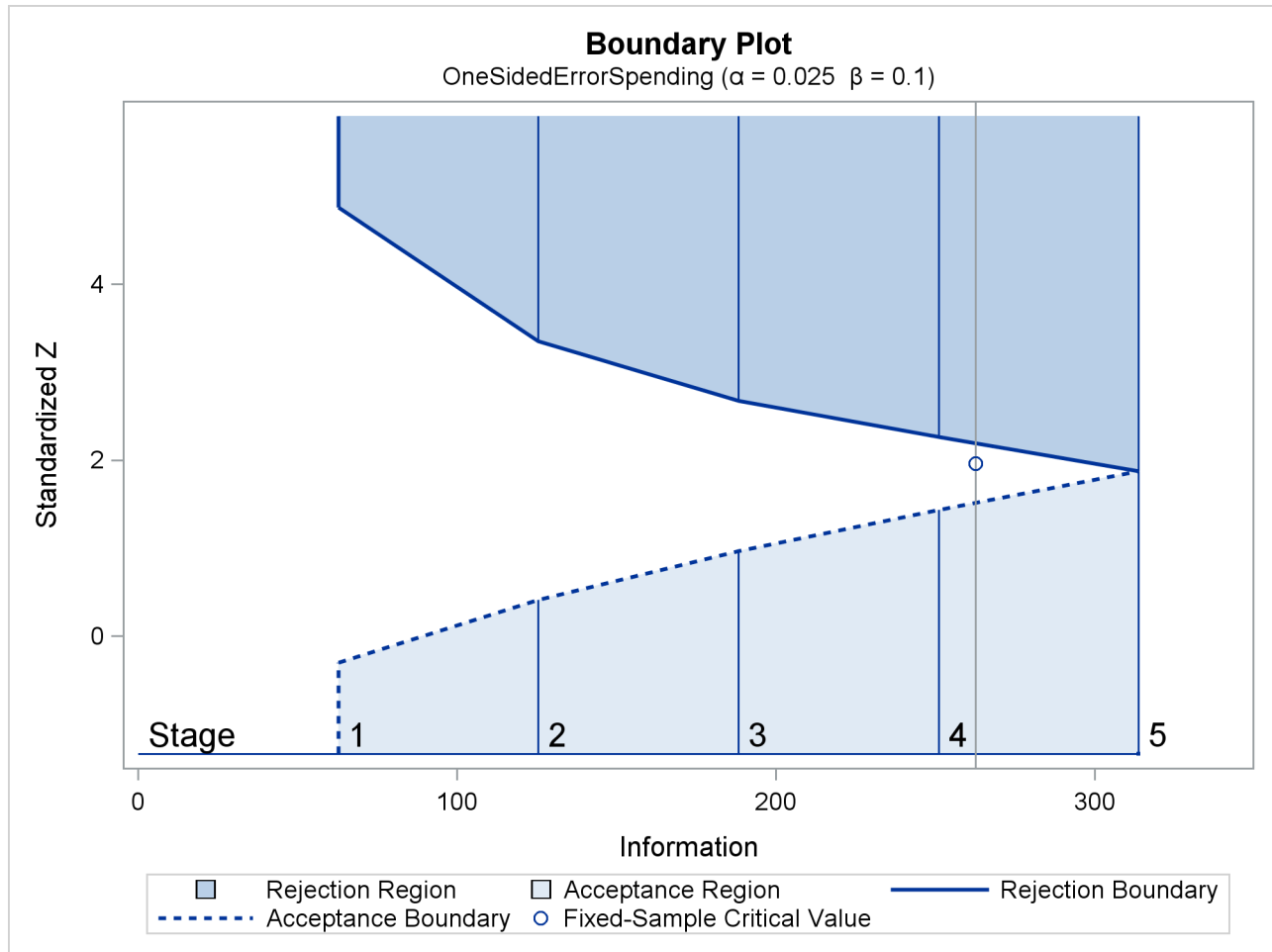
The “Boundary Information” table in [Output 83.8.7](#) displays information level, alternative reference, and boundary values. By default (or equivalently if you specify BOUNDARYSCALE=STDZ), the alternative reference and boundary values are displayed with the standardized Z scale. That is, the resulting standardized alternative reference at stage  $k$  is given by  $\theta_1 \sqrt{I_k}$ , where  $\theta_1$  is the specified alternative reference and  $I_k$  is the information level at stage  $k$ ,  $k = 1, 2, \dots, 5$ .

**Output 83.8.7** Boundary Information

| Boundary Information (Standardized Z Scale) |                         |          |                        |                           |         |
|---------------------------------------------|-------------------------|----------|------------------------|---------------------------|---------|
| Null Reference = 0                          |                         |          |                        |                           |         |
| _Stage_                                     | ---Information Level--- |          | -Alternative-          | -----Boundary Values----- |         |
|                                             | Proportion              | Actual   | --Reference--<br>Upper | -----Upper-----<br>Beta   | Alpha   |
| 1                                           | 0.2000                  | 62.74393 | 1.58422                | -0.30338                  | 4.87688 |
| 2                                           | 0.4000                  | 125.4879 | 2.24043                | 0.41667                   | 3.35706 |
| 3                                           | 0.6000                  | 188.2318 | 2.74395                | 0.97165                   | 2.67766 |
| 4                                           | 0.8000                  | 250.9757 | 3.16844                | 1.43627                   | 2.26535 |
| 5                                           | 1.0000                  | 313.7196 | 3.54243                | 1.87522                   | 1.87522 |

With ODS Graphics enabled, a detailed boundary plot with the rejection and acceptance regions is displayed, as shown in [Output 83.8.8](#). This plot displays the boundary values in the “Boundary Information” table in [Output 83.8.7](#).

**Output 83.8.8** Boundary Plot



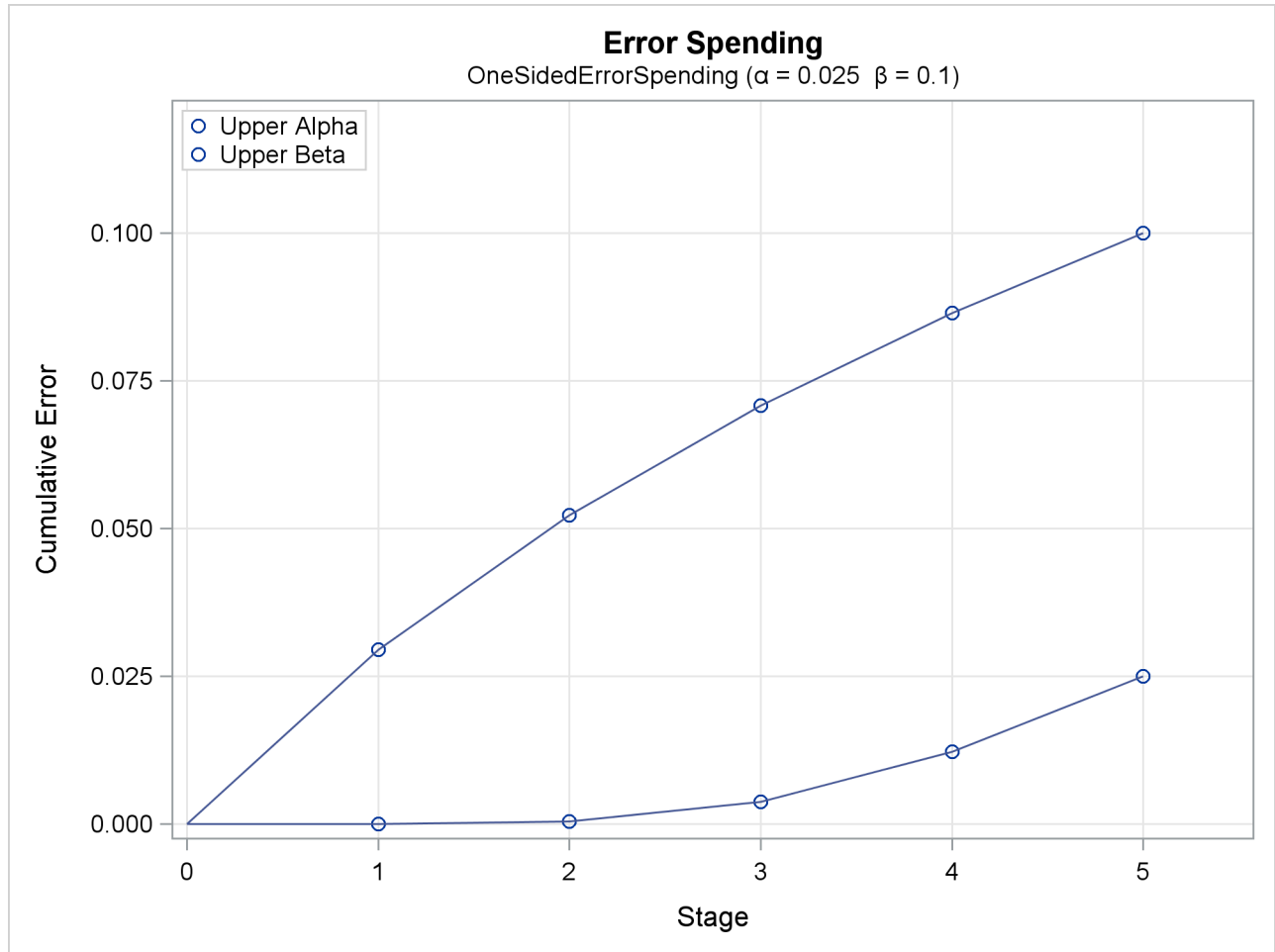
The “Error Spending Information” table in [Output 83.8.9](#) displays cumulative error spending at each stage for each boundary.

**Output 83.8.9** Error Spending Information

| Error Spending Information |                                   |                             |                          |  |
|----------------------------|-----------------------------------|-----------------------------|--------------------------|--|
| _Stage_                    | -Information Level-<br>Proportion | -Cumulative Error Spending- |                          |  |
|                            |                                   | Beta                        | -----Upper-----<br>Alpha |  |
| 1                          | 0.2000                            | 0.02954                     | 0.00000                  |  |
| 2                          | 0.4000                            | 0.05231                     | 0.00039                  |  |
| 3                          | 0.6000                            | 0.07085                     | 0.00381                  |  |
| 4                          | 0.8000                            | 0.08648                     | 0.01221                  |  |
| 5                          | 1.0000                            | 0.10000                     | 0.02500                  |  |

With the PLOTS=ERRSPEND option, the procedure displays a plot of error spending for each boundary, as shown in [Output 83.8.10](#). This plot displays the cumulative error spending at each stage in the “Error Spending Information” table in [Output 83.8.9](#). The O’Brien-Fleming-type  $\alpha$  spending function is conservative in early stages because it uses much less at early stages than in the later stages. In contrast, the Pocock-type  $\beta$  spending function uses more at early stages than in the later stages.

Output 83.8.10 Error Spending Plot





### Example 83.9: Creating Designs with Various Number of Stages

This example requests three group sequential designs for normally distributed statistics. Each design uses the power family error spending function with the default power parameter  $\rho = 2$ . The specified error spending method is between the approximated Pocock method ( $\rho = 1$ ) and the approximated O'Brien-Fleming method ( $\rho = 3$ ) (Jennison and Turnbull 2000, p. 148). The three designs are identical except for the specified number of stages. The following statements request these three group sequential designs:

```
ods graphics on;
proc seqdesign plots=(asn
 power
 combinedboundary
 errspend(hscale=info)
)
;
TwoStageDesign: design nstages=2
 method=errfuncpow
 alt=upper stop=reject
;
FiveStageDesign: design nstages=5
 method=errfuncpow
 alt=upper stop=reject
;
TenStageDesign: design nstages=10
 method=errfuncpow
 alt=upper stop=reject
;
run;
ods graphics off;
```

The “Design Information” table in [Output 83.9.1](#) displays design information for the two-stage design.

**Output 83.9.1** Design Information

| The SEQDESIGN Procedure                   |                |
|-------------------------------------------|----------------|
| Design: TwoStageDesign                    |                |
| Design Information                        |                |
| Statistic Distribution                    | Normal         |
| Boundary Scale                            | Standardized Z |
| Alternative Hypothesis                    | Upper          |
| Early Stop                                | Reject Null    |
| Method                                    | Error Spending |
| Boundary Key                              | Both           |
| Number of Stages                          | 2              |
| Alpha                                     | 0.05           |
| Beta                                      | 0.1            |
| Power                                     | 0.9            |
| Max Information (Percent of Fixed Sample) | 102.4167       |
| Null Ref ASN (Percent of Fixed Sample)    | 101.7766       |
| Alt Ref ASN (Percent of Fixed Sample)     | 79.81021       |

The “Boundary Information” table in [Output 83.9.2](#) displays the information level, alternative reference, and boundary values. By default (or equivalently if you specify BOUNDARYSCALE=STDZ), the alternative reference and boundary values are displayed with the standardized normal Z scale. The resulting standardized alternative reference at stage  $k$  is given by  $\theta_1 \sqrt{I_k}$ , where  $\theta_1$  is the alternative reference and  $I_k$  is the information level at stage  $k$ ,  $k = 1, 2$ .

**Output 83.9.2** Boundary Information in Z Scale

| Boundary Information (Standardized Z Scale) |                                           |                                                  |                                                        |
|---------------------------------------------|-------------------------------------------|--------------------------------------------------|--------------------------------------------------------|
| Null Reference = 0                          |                                           |                                                  |                                                        |
| <u>_Stage_</u>                              | <u>-Information Level-<br/>Proportion</u> | <u>-Alternative-<br/>--Reference--<br/>Upper</u> | <u>-Boundary Values-<br/>-----Upper-----<br/>Alpha</u> |
| 1                                           | 0.5000                                    | 2.09414                                          | 2.24140                                                |
| 2                                           | 1.0000                                    | 2.96156                                          | 1.69970                                                |

The “Design Information” table in [Output 83.9.3](#) displays design information for the five-stage design. Compared with the two-stage design in [Output 83.9.1](#), the maximum information increases from 102.42 to 105.62, and the average sample number under the alternative reference (Alt Ref ASN) decreases from 79.81 to 69.64.

**Output 83.9.3** Design Information

| The SEQDESIGN Procedure                   |                |
|-------------------------------------------|----------------|
| Design: FiveStageDesign                   |                |
| Design Information                        |                |
| Statistic Distribution                    | Normal         |
| Boundary Scale                            | Standardized Z |
| Alternative Hypothesis                    | Upper          |
| Early Stop                                | Reject Null    |
| Method                                    | Error Spending |
| Boundary Key                              | Both           |
| Number of Stages                          | 5              |
| Alpha                                     | 0.05           |
| Beta                                      | 0.1            |
| Power                                     | 0.9            |
| Max Information (Percent of Fixed Sample) | 105.6235       |
| Null Ref ASN (Percent of Fixed Sample)    | 104.356        |
| Alt Ref ASN (Percent of Fixed Sample)     | 69.64322       |

The “Boundary Information” table in [Output 83.9.4](#) displays the information level, alternative reference, and boundary values with the default standardized normal Z scale.

**Output 83.9.4** Boundary Information in Z Scale

| Boundary Information (Standardized Z Scale) |                                           |                                                  |                                                        |
|---------------------------------------------|-------------------------------------------|--------------------------------------------------|--------------------------------------------------------|
| Null Reference = 0                          |                                           |                                                  |                                                        |
| <u>_Stage_</u>                              | <u>-Information Level-<br/>Proportion</u> | <u>-Alternative-<br/>--Reference--<br/>Upper</u> | <u>-Boundary Values-<br/>-----Upper-----<br/>Alpha</u> |
| 1                                           | 0.2000                                    | 1.34502                                          | 2.87816                                                |
| 2                                           | 0.4000                                    | 1.90215                                          | 2.47023                                                |
| 3                                           | 0.6000                                    | 2.32965                                          | 2.20095                                                |
| 4                                           | 0.8000                                    | 2.69005                                          | 1.98182                                                |
| 5                                           | 1.0000                                    | 3.00756                                          | 1.79024                                                |

The “Design Information” table in [Output 83.9.5](#) displays design information for the ten-stage design. Compared with the five-stage design in [Output 83.9.3](#), the maximum information increases further from 105.62 to 107.26 and under the alternative reference, the average sample number decreases further from 69.64 to 66.36.

**Output 83.9.5** Design Information

| The SEQDESIGN Procedure                   |                |
|-------------------------------------------|----------------|
| Design: TenStageDesign                    |                |
| Design Information                        |                |
| Statistic Distribution                    | Normal         |
| Boundary Scale                            | Standardized Z |
| Alternative Hypothesis                    | Upper          |
| Early Stop                                | Reject Null    |
| Method                                    | Error Spending |
| Boundary Key                              | Both           |
| Number of Stages                          | 10             |
| Alpha                                     | 0.05           |
| Beta                                      | 0.1            |
| Power                                     | 0.9            |
| Max Information (Percent of Fixed Sample) | 107.256        |
| Null Ref ASN (Percent of Fixed Sample)    | 105.7276       |
| Alt Ref ASN (Percent of Fixed Sample)     | 66.35565       |

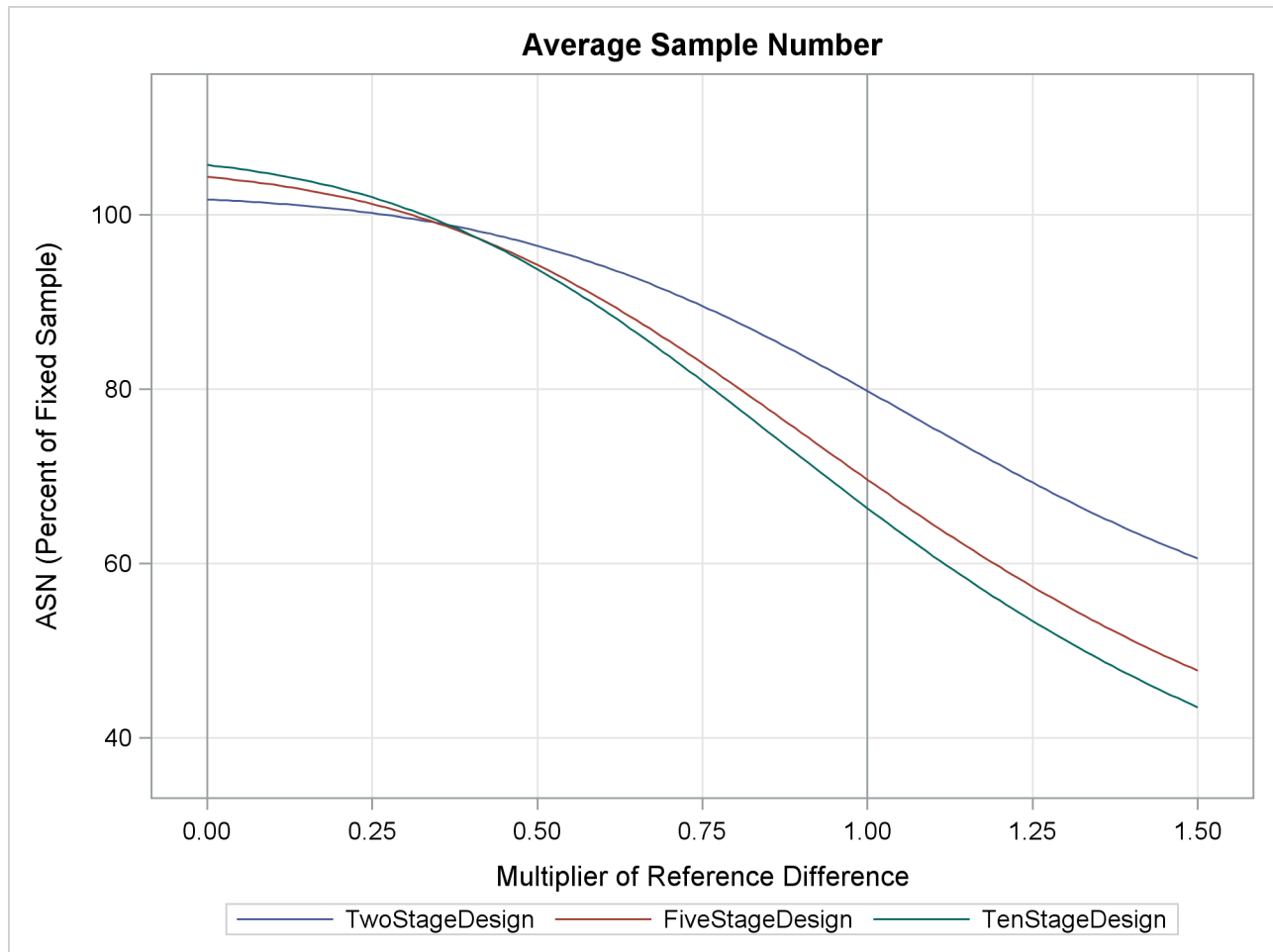
The “Boundary Information” table in [Output 83.9.6](#) displays the information level, alternative reference, and boundary values with the default standardized normal Z scale.

**Output 83.9.6** Boundary Information in Z Scale

| Boundary Information (Standardized Z Scale) |                                           |                                                  |                                                        |
|---------------------------------------------|-------------------------------------------|--------------------------------------------------|--------------------------------------------------------|
| Null Reference = 0                          |                                           |                                                  |                                                        |
| <u>_Stage_</u>                              | <u>-Information Level-<br/>Proportion</u> | <u>-Alternative-<br/>--Reference--<br/>Upper</u> | <u>-Boundary Values-<br/>-----Upper-----<br/>Alpha</u> |
| 1                                           | 0.1000                                    | 0.95840                                          | 3.29053                                                |
| 2                                           | 0.2000                                    | 1.35538                                          | 2.94037                                                |
| 3                                           | 0.3000                                    | 1.65999                                          | 2.72115                                                |
| 4                                           | 0.4000                                    | 1.91679                                          | 2.54808                                                |
| 5                                           | 0.5000                                    | 2.14304                                          | 2.40114                                                |
| 6                                           | 0.6000                                    | 2.34758                                          | 2.27127                                                |
| 7                                           | 0.7000                                    | 2.53568                                          | 2.15359                                                |
| 8                                           | 0.8000                                    | 2.71076                                          | 2.04503                                                |
| 9                                           | 0.9000                                    | 2.87519                                          | 1.94355                                                |
| 10                                          | 1.0000                                    | 3.03072                                          | 1.84765                                                |

With the PLOTS=ASN option, the procedure displays a plot of average sample numbers under various hypothetical references for all designs simultaneously, as shown in [Output 83.9.7](#). By default, the option CREF= 0, 0.01, 0.02, . . . , 1.50 and expected sample sizes under the hypothetical references  $\theta = c_i \theta_1$  are displayed, where  $c_i$  are values specified in the CREF= option. These CREF= values are displayed on the horizontal axis.

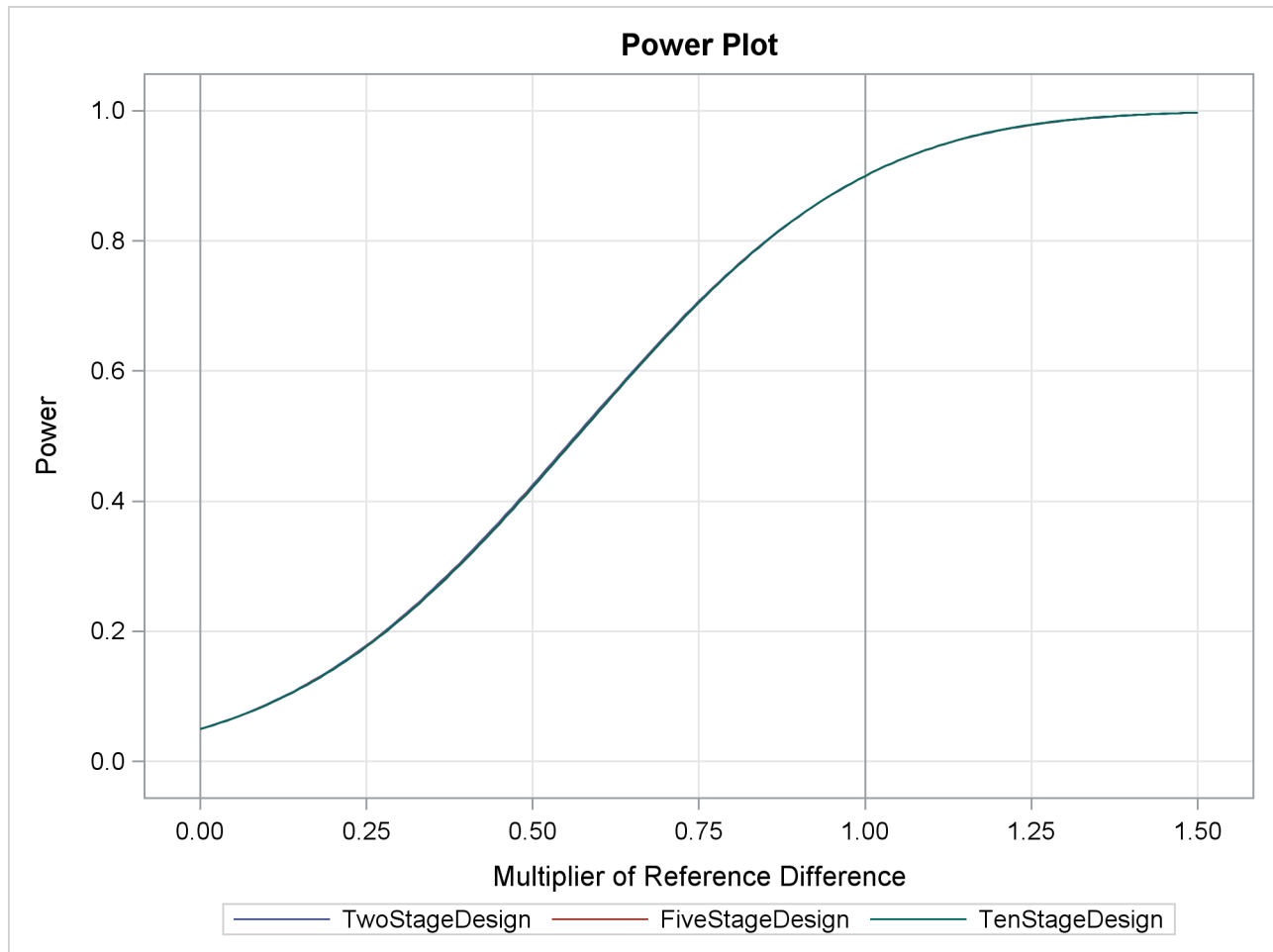
Output 83.9.7 ASN Plot



The plot shows that as the number of stages increases, the average sample number as a percentage of the fixed-sample design increases under the null hypothesis ( $c_i = 0$ ) but decreases under the alternative hypothesis ( $c_i = 1$ ).

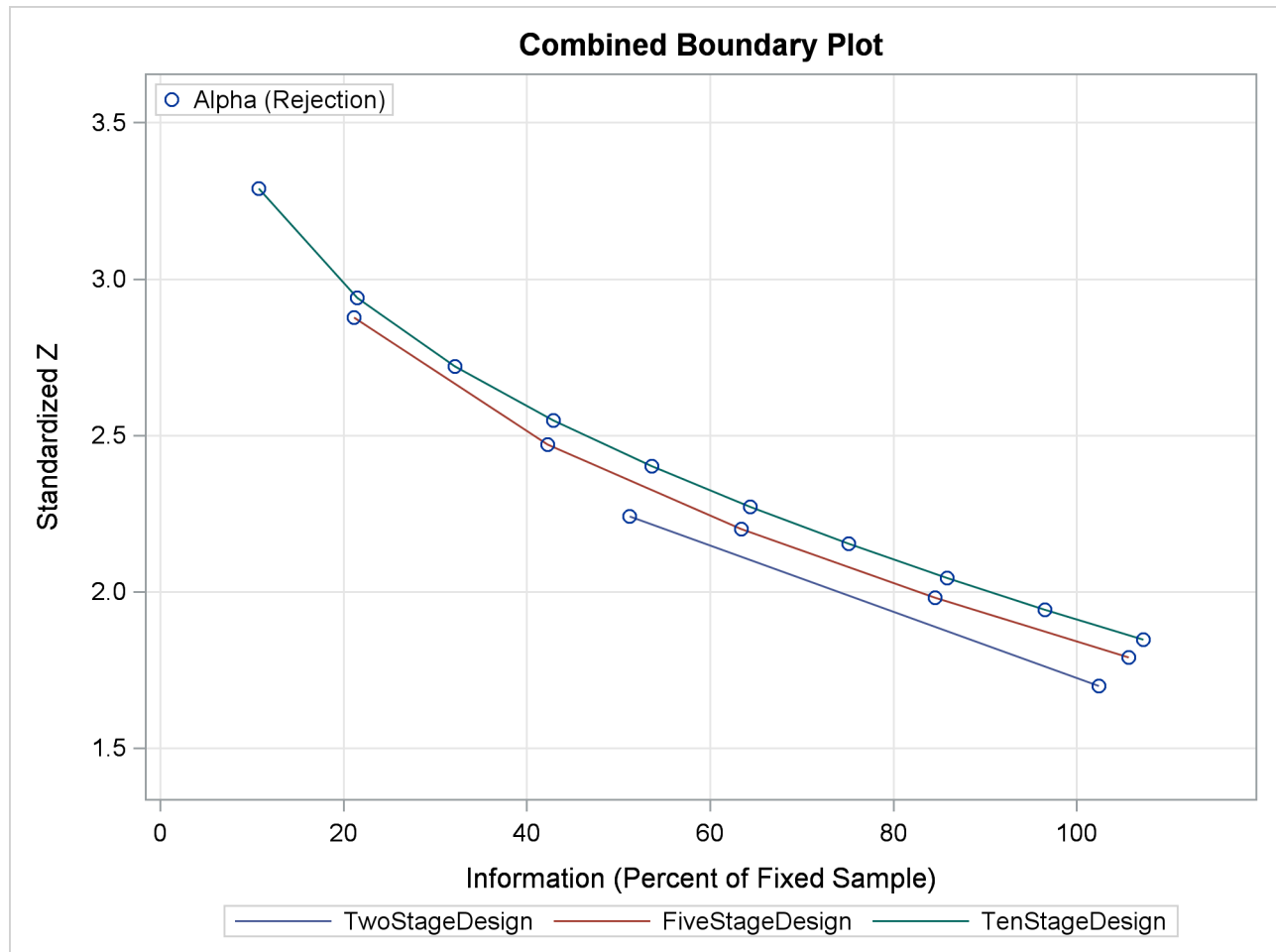
With the PLOTS=POWER option, the procedure displays a plot of the power curves under various hypothetical references for all designs simultaneously, as shown in [Output 83.9.8](#). By default, the option CREF= 0, 0.01, 0.02, ..., 1.50 and powers under hypothetical references  $\theta = c_i \theta_1$  are displayed, where  $c_i$  are values specified in the CREF= option. These CREF= values are displayed on the horizontal axis.

Output 83.9.8 Power Plot



Under the null hypothesis,  $c_i = 0$ , the power is 0.05, the upper Type I error probability. Under the alternative hypothesis,  $c_i = 1$ , the power is 0.9, one minus the Type II error probability. The plot shows only minor difference among the three designs.

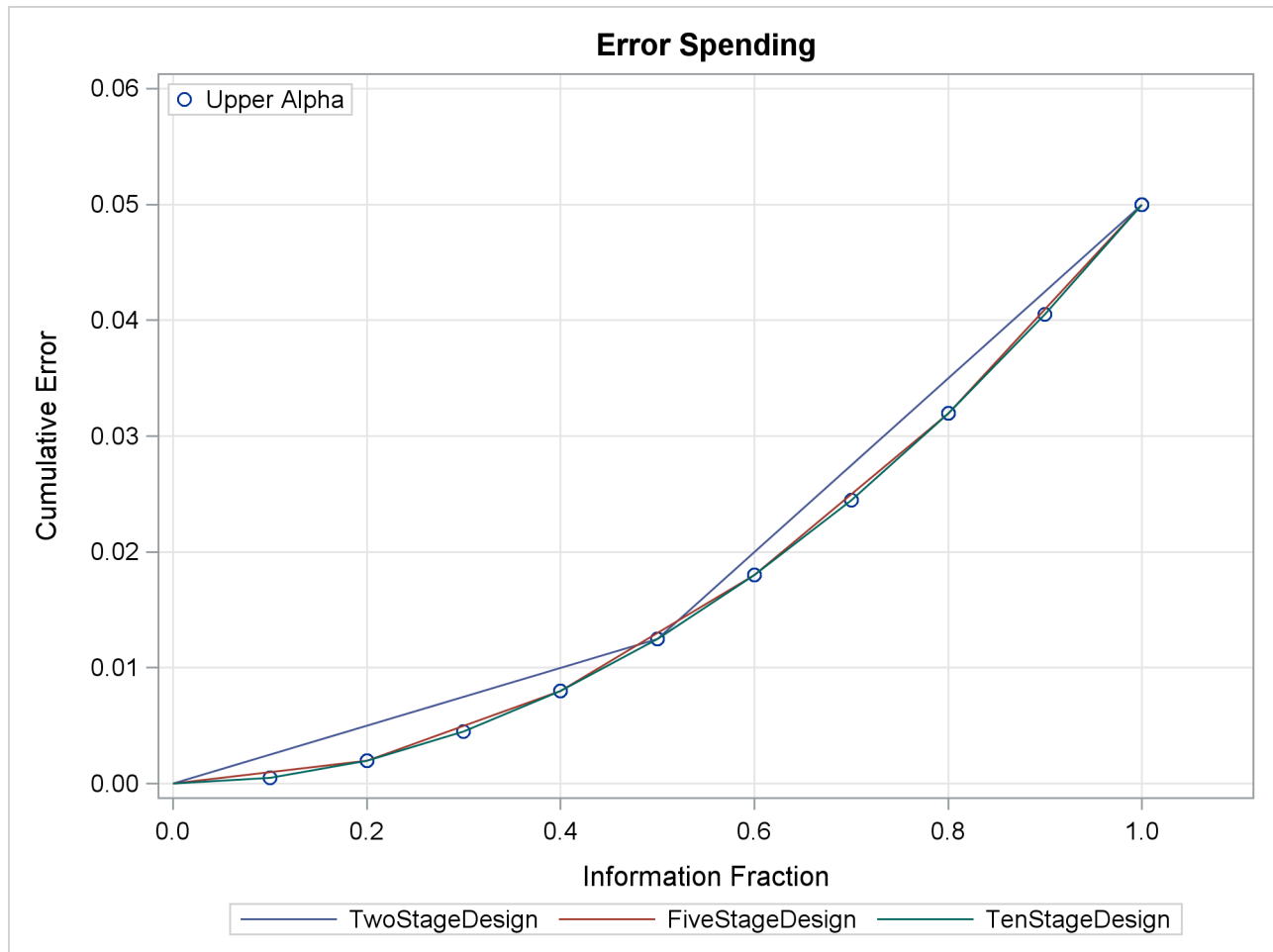
With the `PLOTS=COMBINEDBOUNDARY` option, the procedure displays a plot of sequential boundaries for all designs simultaneously, as shown in [Output 83.9.9](#). By default (or equivalently if you specify `COMBINEDBOUNDARY(HSCALE=INFO)`), the information levels are used on the horizontal axis. Since the maximum information is not available for the design, the percent information ratios with respect to the corresponding fixed-sample design are displayed in the plot.

**Output 83.9.9** Combined Boundary Plot

The plot shows that as the number of stages increases, the maximum information increases and the  $\alpha$  boundary values also increase.

With the PLOTS=ERRSPEND(HSCALE=INFO) option, the procedure displays a plot of cumulative error spends for all boundaries in the designs simultaneously, as shown in [Output 83.9.10](#).

**Output 83.9.10** Error Spending Plot



The plot shows similar error spending for these three designs since all three designs are generated from the same power family error spending function.



### Example 83.10: Creating Two-Sided Error Spending Designs with and without Overlapping Lower and Upper $\beta$ Boundaries

This example requests two three-stage group sequential designs for normally distributed statistics. Each design uses a power family error spending function with a specified two-sided alternative hypothesis  $H_1 : \theta_1 = \pm 0.2$  and early stopping only to accept the null hypothesis  $H_0$ .

The first design uses the BETAOVERLAP=NOADJUST option to derive acceptance boundary values without adjusting for the possible overlapping of the lower and upper  $\beta$  boundaries computed from the two corresponding one-sided tests. The second design uses the BETAOVERLAP=ADJUST option to test the overlapping of the  $\beta$  boundaries at each interim stage based on the two corresponding one-sided tests and then to set the  $\beta$  boundary values at the stage to missing if overlapping occurs at that stage.

The following statements request a two-sided design with the BETAOVERLAP=NOADJUST option:

```
ods graphics on;
proc seqdesign altref=0.2 errspend;
 design nstages=3
 method=errfuncpow
 alt=twosided stop=accept
 betaoverlap=noadjust
 beta=0.09
 ;
run;
ods graphics off;
```

The “Design Information” table in Output 83.10.1 displays design specifications and the derived statistics for the first design. With the specified alternative reference  $\theta_1 = 0.2$ , the maximum information is derived.

**Output 83.10.1** Design Information

| The SEQDESIGN Procedure                   |                |
|-------------------------------------------|----------------|
| Design: Design_1                          |                |
| Design Information                        |                |
| Statistic Distribution                    | Normal         |
| Boundary Scale                            | Standardized Z |
| Alternative Hypothesis                    | Two-Sided      |
| Early Stop                                | Accept Null    |
| Method                                    | Error Spending |
| Boundary Key                              | Both           |
| Alternative Reference                     | 0.2            |
| Number of Stages                          | 3              |
| Alpha                                     | 0.05           |
| Beta                                      | 0.09           |
| Power                                     | 0.91           |
| Max Information (Percent of Fixed Sample) | 103.8789       |
| Max Information                           | 282.9328       |
| Null Ref ASN (Percent of Fixed Sample)    | 79.20197       |
| Alt Ref ASN (Percent of Fixed Sample)     | 102.1476       |

The “Boundary Information” table in [Output 83.10.2](#) displays the information level, alternative reference, and boundary values. With a specified alternative reference  $\theta_1$ , the maximum information is derived from the procedure, and the actual information level at each stage is displayed in the table. By default (or equivalently if you specify `BOUNDARYSCALE=STDZ`), the alternative reference and boundary values are displayed with the standardized Z scale. The alternative reference at stage  $k$  is given by  $\theta_1\sqrt{I_k}$ , where  $\theta_1$  is the specified alternative reference and  $I_k$  is the information level at stage  $k$ ,  $k = 1, 2, 3$ .

**Output 83.10.2** Boundary Information

| Boundary Information (Standardized Z Scale) |                       |          |                       |                     |                         |             |
|---------------------------------------------|-----------------------|----------|-----------------------|---------------------|-------------------------|-------------|
| Null Reference = 0                          |                       |          |                       |                     |                         |             |
| _Stage_                                     | --Information Level-- |          | -----Alternative----- |                     | ----Boundary Values---- |             |
|                                             | Proportion            | Actual   | -----Reference-----   | -----Reference----- | ---Lower---             | ---Upper--- |
|                                             |                       |          | Lower                 | Upper               | Beta                    | Beta        |
| 1                                           | 0.3333                | 94.31094 | -1.94228              | 1.94228             | -0.08239                | 0.08239     |
| 2                                           | 0.6667                | 188.6219 | -2.74679              | 2.74679             | -0.90351                | 0.90351     |
| 3                                           | 1.0000                | 282.9328 | -3.36412              | 3.36412             | -1.92519                | 1.92519     |

The “Error Spending Information” table in [Output 83.10.3](#) displays the cumulative error spending at each stage for each boundary.

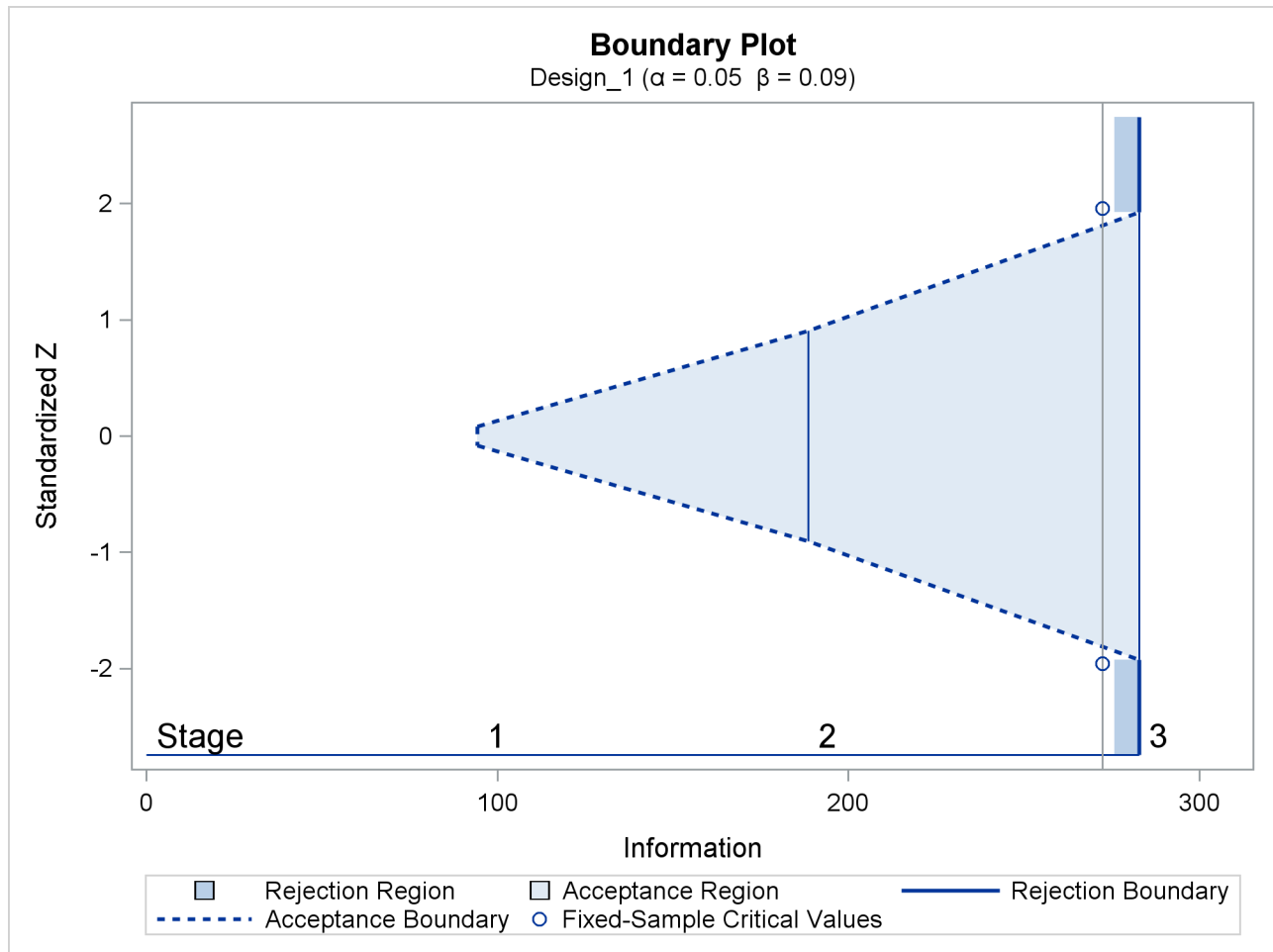
**Output 83.10.3** Error Spending Information

| Error Spending Information |                     |  |                                     |         |                 |         |
|----------------------------|---------------------|--|-------------------------------------|---------|-----------------|---------|
| _Stage_                    | -Information Level- |  | -----Cumulative Error Spending----- |         |                 |         |
|                            | Proportion          |  | -----Lower-----                     |         | -----Upper----- |         |
|                            |                     |  | Alpha                               | Beta    | Beta            | Alpha   |
| 1                          | 0.3333              |  | 0.00000                             | 0.01000 | 0.01000         | 0.00000 |
| 2                          | 0.6667              |  | 0.00000                             | 0.04000 | 0.04000         | 0.00000 |
| 3                          | 1.0000              |  | 0.02500                             | 0.09000 | 0.09000         | 0.02500 |

With the `STOP=ACCEPT` option, the design does not stop at interim stages to reject  $H_0$ , and the  $\alpha$  spending at each interim stage is zero. For the power family error spending function with the default parameter  $\rho = 2$ , the beta spending at stage 1 is  $(1/3)^\rho \beta = (1/3)^2 0.09 = 0.01$ , and the cumulative beta spending at stage 2 is  $(2/3)^\rho \beta = (2/3)^2 0.09 = 0.04$ .

With ODS Graphics enabled, a detailed boundary plot with the acceptance and rejection regions is displayed, as shown in [Output 83.10.4](#).

Output 83.10.4 Boundary Plot



The following statements request a two-sided design with the BETAOVERLAP=ADJUST option, which is the default:

```
ods graphics on;
proc seqdesign altref=0.2 errspend;
 design nstages=3
 method=errfuncpow
 alt=twosided
 stop=accept
 betaoverlap=adjust
 beta=0.09
 ;
run;
ods graphics off;
```

With the BETAOVERLAP=ADJUST option, the procedure first derives the usual  $\beta$  boundary values for the two-sided design and then checks for overlapping of the  $\beta$  boundaries for the two corresponding one-sided tests at each stage. If this type of overlapping occurs at a particular stage, the  $\beta$  boundary values for that stage are set to missing, the  $\beta$  spending values at that stage are reset to zero, and the  $\beta$  spending values at subsequent stages are adjusted proportionally.

The boundary values without adjusting for the possible overlapping of the two one-sided  $\beta$  boundaries are identical to the boundary values derived in the first design (with the BETAOVERLAP=NOADJUST option, as shown in Output 83.10.2). At stage 1, the upper  $\beta$  boundary value for the corresponding one-sided test is

$$\theta_1 \sqrt{I_1} - \Phi^{-1}(1 - \beta_1) = 0.2 \sqrt{94.31094} - \Phi^{-1}(0.99) = 1.94228 - 2.32635 = -0.38407$$

where  $\theta_1 = 0.2$  is the upper alternative reference,  $I_1 = 94.31094$  is the information level at stage 1, and  $\beta_1 = 0.01$  is the  $\beta$  spending at stage 1 (as shown in Output 83.10.3).

Similarly, the lower  $\beta$  boundary value for the corresponding one-sided test is computed as 0.38407. Since the upper  $\beta$  boundary value is less than the lower  $\beta$  boundary at stage 1, overlapping occurs, and so the  $\beta$  boundary values for the two-sided design are set to missing at stage 1.

With the  $\beta$  boundary values set to missing at stage 1 and the  $\beta$  spending  $\beta'_1 = 0$  the  $\beta$  spending values at subsequent interim stages are adjusted proportionally. In this example, the adjusted  $\beta$  spending at stage 2 is computed as

$$\beta'_2 = \beta'_1 + \frac{\beta_2 - \beta_1}{\beta_3 - \beta_1} (\beta_3 - \beta'_1) = 0 + \frac{0.04 - 0.01}{0.09 - 0.01} 0.09 = 0.03375$$

where  $\beta_k$  is the cumulative  $\beta$  spending at stage  $k$  before the adjustment,  $k = 1, 2, 3$ .

The “Design Information” table in Output 83.10.5 displays design specifications and derived statistics for the design.

**Output 83.10.5** Design Information

| The SEQDESIGN Procedure                   |                |
|-------------------------------------------|----------------|
| Design: Design_1                          |                |
| Design Information                        |                |
| Statistic Distribution                    | Normal         |
| Boundary Scale                            | Standardized Z |
| Alternative Hypothesis                    | Two-Sided      |
| Early Stop                                | Accept Null    |
| Method                                    | Error Spending |
| Boundary Key                              | Both           |
| Alternative Reference                     | 0.2            |
| Number of Stages                          | 3              |
| Alpha                                     | 0.05           |
| Beta                                      | 0.09           |
| Power                                     | 0.91           |
| Max Information (Percent of Fixed Sample) | 101.9388       |
| Max Information                           | 277.649        |
| Null Ref ASN (Percent of Fixed Sample)    | 80.56408       |
| Alt Ref ASN (Percent of Fixed Sample)     | 100.792        |

The “Boundary Information” table in [Output 83.10.6](#) displays the information levels, alternative references, and boundary values.

**Output 83.10.6** Boundary Information

| Boundary Information (Standardized Z Scale) |                       |          |                       |         |                         |             |
|---------------------------------------------|-----------------------|----------|-----------------------|---------|-------------------------|-------------|
| Null Reference = 0                          |                       |          |                       |         |                         |             |
| _Stage_                                     | --Information Level-- |          | -----Alternative----- |         | ----Boundary Values---- |             |
|                                             | Proportion            | Actual   | -----Reference-----   | Upper   | ---Lower---             | ---Upper--- |
|                                             |                       |          | Lower                 |         | Beta                    | Beta        |
| 1                                           | 0.3333                | 92.54967 | -1.92405              | 1.92405 | .                       | .           |
| 2                                           | 0.6667                | 185.0993 | -2.72102              | 2.72102 | -0.89469                | 0.89469     |
| 3                                           | 1.0000                | 277.649  | -3.33256              | 3.33256 | -1.93494                | 1.93494     |

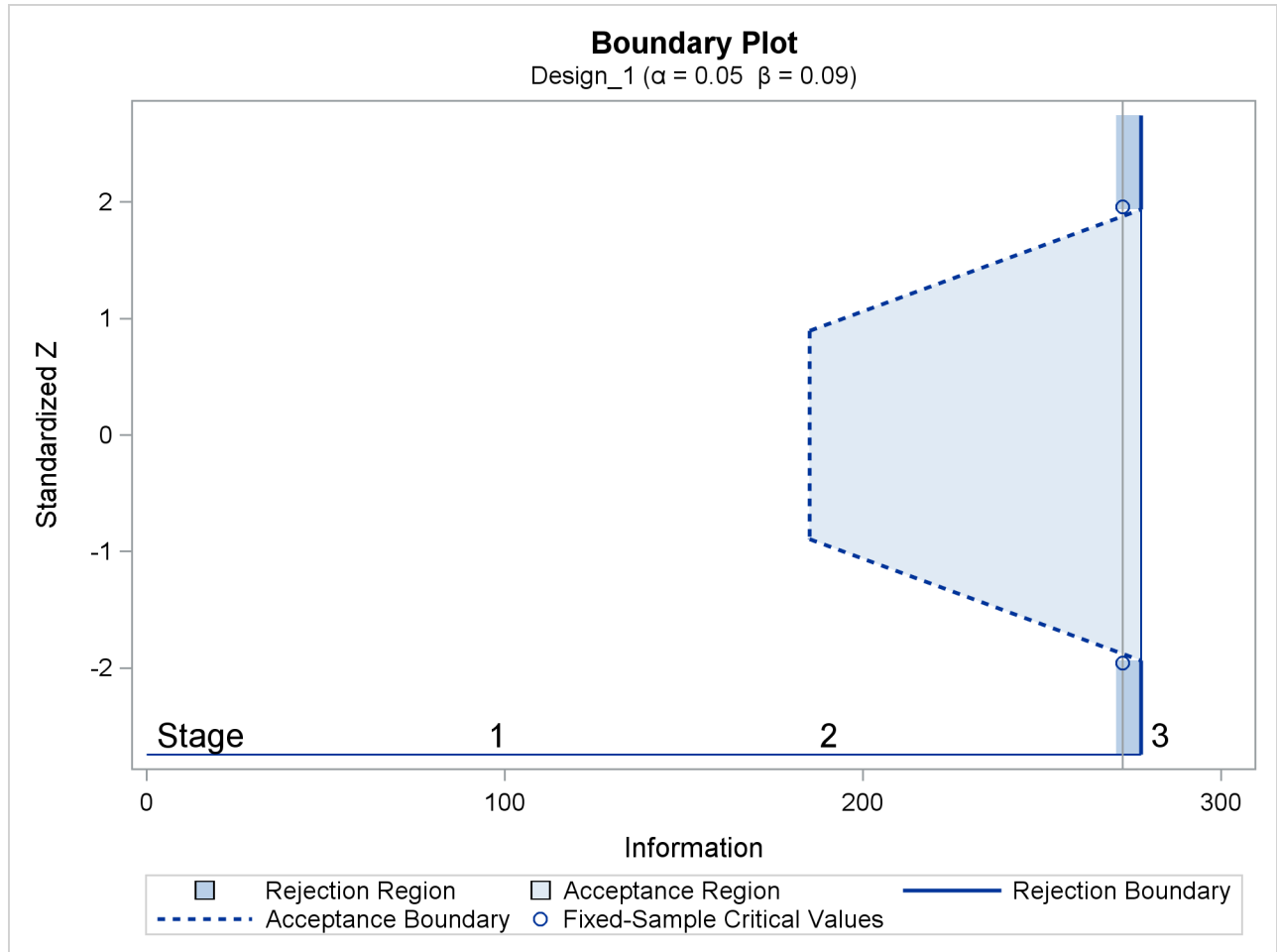
The “Error Spending Information” table in [Output 83.10.7](#) displays the cumulative error spending at each stage for each boundary.

**Output 83.10.7** Error Spending Information

| Error Spending Information |                                   |                                     |         |                 |         |  |
|----------------------------|-----------------------------------|-------------------------------------|---------|-----------------|---------|--|
| _Stage_                    | -Information Level-<br>Proportion | -----Cumulative Error Spending----- |         |                 |         |  |
|                            |                                   | -----Lower-----                     | Upper   | -----Lower----- | Upper   |  |
|                            |                                   | Alpha                               | Beta    | Beta            | Alpha   |  |
| 1                          | 0.3333                            | 0.00000                             | 0.00000 | 0.00000         | 0.00000 |  |
| 2                          | 0.6667                            | 0.00000                             | 0.03375 | 0.03375         | 0.00000 |  |
| 3                          | 1.0000                            | 0.02500                             | 0.09000 | 0.09000         | 0.02500 |  |

With ODS Graphics enabled, a detailed boundary plot with the acceptance and rejection regions is displayed, as shown in [Output 83.10.8](#).

Output 83.10.8 Boundary Plot



### Example 83.11: Creating a Two-Sided Asymmetric Error Spending Design with Early Stopping to Reject $H_0$

This example requests a three-stage two-sided asymmetric group sequential design for normally distributed statistics.

The O'Brien-Fleming boundary can be approximated using a power family error spending function with parameter  $\rho = 3$ , and the Pocock boundary can be approximated using a power family error spending function with parameter  $\rho = 1$  (Jennison and Turnbull 2000, p. 148). The following statements use the power family error spending function to create a two-sided asymmetric design with early stopping to reject the null hypothesis  $H_0$ :

```
ods graphics on;
proc seqdesign altref=1.0
 pss(cref=0 0.5 1)
 stopprob(cref=0 0.5 1)
 errspend
 plots=(asn power errspend)
;

TwoSidedErrorSpending: design nstages=3
 method(upperalpha)=errfuncpow(rho=3)
 method(loweralpha)=errfuncpow(rho=1)
 info=cum(2 3 4)
 alt=twosided
 stop=reject
 alpha=0.075(upper=0.025)
;

run;
ods graphics off;
```

The design uses power family error spending functions with  $\rho = 1$  for the lower  $\alpha$  boundary and  $\rho = 3$  for the upper  $\alpha$  boundary. Thus, the design is conservative in the early stages and tends to stop the trials early only with a small  $p$ -value for the upper  $\alpha$  boundary. The upper  $\alpha$  level 0.025 is specified explicitly, and the lower  $\alpha$  level is computed as  $0.075 - 0.025 = 0.05$ .

The “Design Information” table in [Output 83.11.1](#) displays design specifications and the derived maximum information. Note that in order to attain the same information level for the asymmetric lower and upper boundaries, the derived power at the lower alternative 0.92963 is larger than the default 0.90.

**Output 83.11.1** Design Information

| The SEQDESIGN Procedure                     |                |
|---------------------------------------------|----------------|
| Design: TwoSidedErrorSpending               |                |
| Design Information                          |                |
| Statistic Distribution                      | Normal         |
| Boundary Scale                              | Standardized Z |
| Alternative Hypothesis                      | Two-Sided      |
| Early Stop                                  | Reject Null    |
| Method                                      | Error Spending |
| Boundary Key                                | Both           |
| Alternative Reference                       | 1              |
| Number of Stages                            | 3              |
| Alpha                                       | 0.075          |
| Alpha (Lower)                               | 0.05           |
| Alpha (Upper)                               | 0.025          |
| Beta (Lower)                                | 0.07037        |
| Beta (Upper)                                | 0.1            |
| Power (Lower)                               | 0.92963        |
| Power (Upper)                               | 0.9            |
| Max Information (Percent of Fixed Sample)   | 102.4384       |
| Max Information                             | 10.76365       |
| Null Ref ASN (Percent of Fixed Sample)      | 100.4877       |
| Lower Alt Ref ASN (Percent of Fixed Sample) | 64.8288        |
| Upper Alt Ref ASN (Percent of Fixed Sample) | 75.98778       |

The “Method Information” table in [Output 83.11.2](#) displays the specified  $\alpha$  and  $\beta$  error levels and the derived drift parameter. With the same information level used for the asymmetric lower and upper boundaries, only one of the  $\beta$  levels is maintained, and the other is derived to have the level less than or equal to the default level.

**Output 83.11.2** Method Information

| Method Information |                |                          |          |                                    |
|--------------------|----------------|--------------------------|----------|------------------------------------|
| Boundary           | Method         | Alpha                    | Beta     | ----Error Spending----<br>Function |
| Upper Alpha        | Error Spending | 0.02500                  | 0.10000  | Power (Rho=3)                      |
| Lower Alpha        | Error Spending | 0.05000                  | 0.07037  | Power (Rho=1)                      |
| Method Information |                |                          |          |                                    |
|                    | Boundary       | Alternative<br>Reference | Drift    |                                    |
|                    | Upper Alpha    | 1                        | 3.280801 |                                    |
|                    | Lower Alpha    | -1                       | -3.2808  |                                    |



With the STOPPROB(CREF=0 0.5 1) option, the “Expected Cumulative Stopping Probabilities” table in **Output 83.11.3** displays the expected stopping stage and cumulative stopping probability to reject the null hypothesis  $H_0$  at each stage under hypothetical references  $\theta = 0$  (null hypothesis  $H_0$ ),  $\theta = 0.5\theta_1$ , and  $\theta = \theta_1$  (alternative hypothesis  $H_1$ ), where  $\theta_1$  is the alternative reference.

**Output 83.11.3** Stopping Probabilities

| Expected Cumulative Stopping Probabilities |           |                         |                      |
|--------------------------------------------|-----------|-------------------------|----------------------|
| Reference = CRef * (Alt Reference)         |           |                         |                      |
| CRef                                       | Ref       | Expected Stopping Stage | Source               |
| 0.0000                                     | Lower Alt | 2.924                   | Rej Null (Lower Alt) |
| 0.0000                                     | Lower Alt | 2.924                   | Rej Null (Upper Alt) |
| 0.0000                                     | Lower Alt | 2.924                   | Reject Null          |
| 0.5000                                     | Lower Alt | 2.456                   | Rej Null (Lower Alt) |
| 0.5000                                     | Lower Alt | 2.456                   | Rej Null (Upper Alt) |
| 0.5000                                     | Lower Alt | 2.456                   | Reject Null          |
| 1.0000                                     | Lower Alt | 1.531                   | Rej Null (Lower Alt) |
| 1.0000                                     | Lower Alt | 1.531                   | Rej Null (Upper Alt) |
| 1.0000                                     | Lower Alt | 1.531                   | Reject Null          |
| 0.0000                                     | Upper Alt | 2.924                   | Rej Null (Lower Alt) |
| 0.0000                                     | Upper Alt | 2.924                   | Rej Null (Upper Alt) |
| 0.0000                                     | Upper Alt | 2.924                   | Reject Null          |
| 0.5000                                     | Upper Alt | 2.758                   | Rej Null (Lower Alt) |
| 0.5000                                     | Upper Alt | 2.758                   | Rej Null (Upper Alt) |
| 0.5000                                     | Upper Alt | 2.758                   | Reject Null          |
| 1.0000                                     | Upper Alt | 1.967                   | Rej Null (Lower Alt) |
| 1.0000                                     | Upper Alt | 1.967                   | Rej Null (Upper Alt) |
| 1.0000                                     | Upper Alt | 1.967                   | Reject Null          |

| Expected Cumulative Stopping Probabilities |           |                                |         |         |
|--------------------------------------------|-----------|--------------------------------|---------|---------|
| Reference = CRef * (Alt Reference)         |           |                                |         |         |
| CRef                                       | Ref       | ----Stopping Probabilities---- |         |         |
|                                            |           | Stage_1                        | Stage_2 | Stage_3 |
| 0.0000                                     | Lower Alt | 0.02500                        | 0.03750 | 0.05000 |
| 0.0000                                     | Lower Alt | 0.00313                        | 0.01055 | 0.02500 |
| 0.0000                                     | Lower Alt | 0.02813                        | 0.04805 | 0.07500 |
| 0.5000                                     | Lower Alt | 0.21185                        | 0.33190 | 0.45370 |
| 0.5000                                     | Lower Alt | 0.00005                        | 0.00012 | 0.00021 |
| 0.5000                                     | Lower Alt | 0.21190                        | 0.33202 | 0.45391 |
| 1.0000                                     | Lower Alt | 0.64054                        | 0.82803 | 0.92963 |
| 1.0000                                     | Lower Alt | 0.00000                        | 0.00000 | 0.00000 |
| 1.0000                                     | Lower Alt | 0.64054                        | 0.82803 | 0.92963 |
| 0.0000                                     | Upper Alt | 0.02500                        | 0.03750 | 0.05000 |
| 0.0000                                     | Upper Alt | 0.00313                        | 0.01055 | 0.02500 |
| 0.0000                                     | Upper Alt | 0.02813                        | 0.04805 | 0.07500 |
| 0.5000                                     | Upper Alt | 0.00090                        | 0.00110 | 0.00120 |
| 0.5000                                     | Upper Alt | 0.05769                        | 0.18269 | 0.36458 |
| 0.5000                                     | Upper Alt | 0.05860                        | 0.18379 | 0.36578 |
| 1.0000                                     | Upper Alt | 0.00001                        | 0.00001 | 0.00001 |
| 1.0000                                     | Upper Alt | 0.33926                        | 0.69356 | 0.90000 |
| 1.0000                                     | Upper Alt | 0.33927                        | 0.69357 | 0.90001 |

“Rej Null (Lower Alt)” and “Rej Null (Upper Alt)” under the heading “Source” indicate the probabilities of rejecting the null hypothesis for the lower alternative and for the upper alternative, respectively. “Reject Null” indicates the probability of rejecting the null hypothesis for either the lower or upper alternative.

Note that with the STOP=REJECT option, the cumulative stopping probability of accepting the null hypothesis  $H_0$  at each interim stage is zero and is not displayed.

With the PSS(CREF=0.5 1.0) option, the “Power and Expected Sample Sizes” table in [Output 83.11.4](#) displays powers and expected sample sizes under hypothetical references  $\theta = 0$  (null hypothesis  $H_0$ ),  $\theta = 0.5\theta_1$ , and  $\theta = \theta_1$  (alternative hypothesis  $H_1$ ), where  $\theta_1$  is the alternative reference. The expected sample sizes are displayed in a percentage scale relative to the corresponding fixed-sample size design.

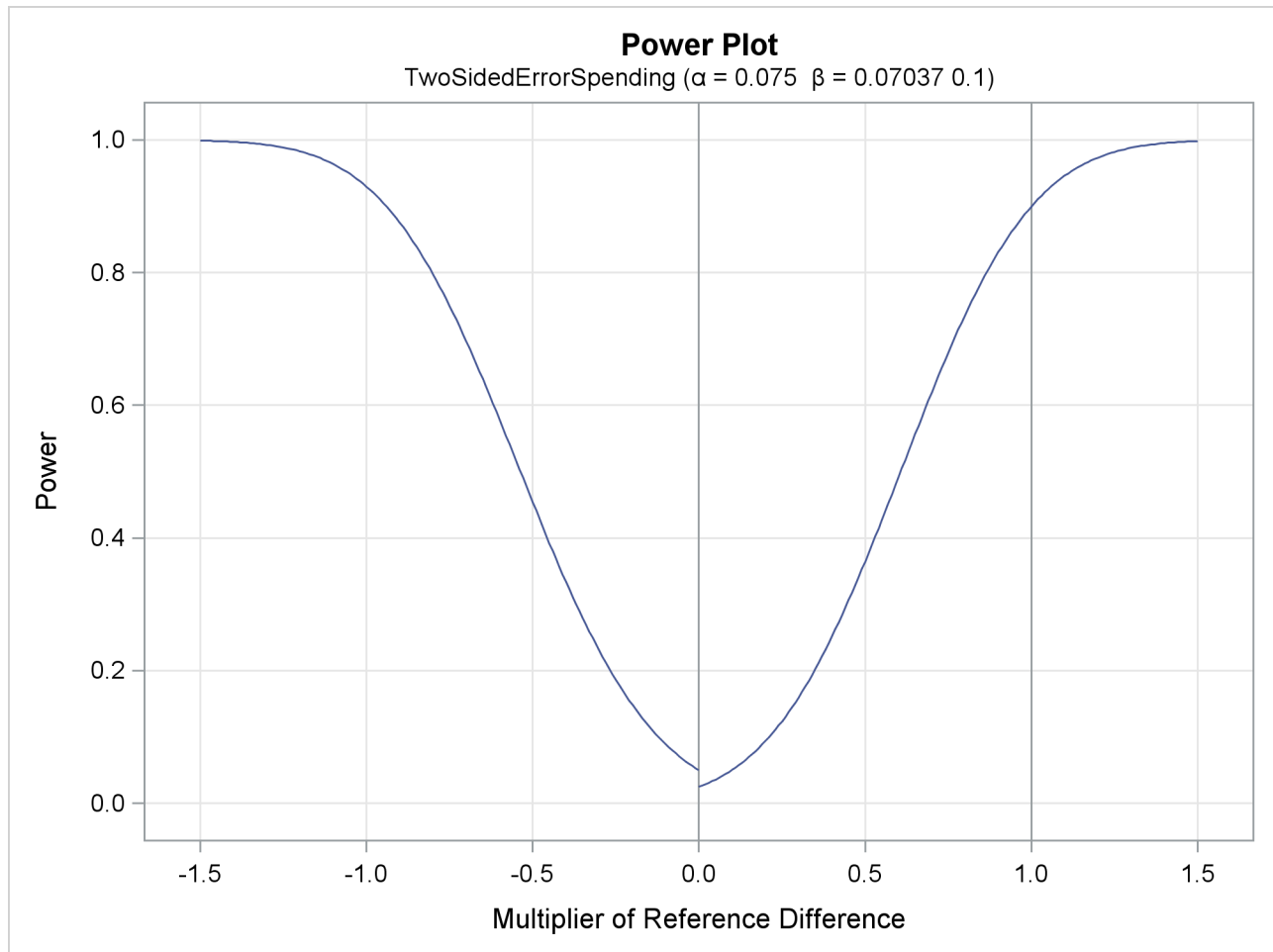
**Output 83.11.4** Power and Expected Sample Size Information

| Powers and Expected Sample Sizes   |           |         |                                          |
|------------------------------------|-----------|---------|------------------------------------------|
| Reference = CRef * (Alt Reference) |           |         |                                          |
| CRef                               | Ref       | Power   | -Sample Size-<br>Percent<br>Fixed-Sample |
| 0.0000                             | Lower Alt | 0.05000 | 100.4877                                 |
| 0.5000                             | Lower Alt | 0.45370 | 88.5090                                  |
| 1.0000                             | Lower Alt | 0.92963 | 64.8288                                  |
| 0.0000                             | Upper Alt | 0.02500 | 100.4877                                 |
| 0.5000                             | Upper Alt | 0.36458 | 96.2309                                  |
| 1.0000                             | Upper Alt | 0.90000 | 75.9878                                  |

Note that at  $c_i = 0$ , the null reference  $\theta = 0$ , the power with the lower alternative is the lower  $\alpha$  error 0.05, and the power with the upper alternative is the upper  $\alpha$  error 0.025. At  $c_i = 1$ , the alternative reference  $\theta = \theta_1$ , the power with the upper alternative is the specified power 0.90, and the power with the lower alternative 0.92963 is greater than the specified power 0.90 because the same information level is used for these two asymmetric boundaries.

With the PLOTS=POWER option, the procedure displays a plot of the power curves under various hypothetical references, as shown in [Output 83.11.5](#). By default, powers under the lower hypotheses  $\theta = c_i\theta_{1l}$  and under the upper hypotheses  $\theta = c_i\theta_{1u}$  are displayed for a two-sided asymmetric design, where  $c_i = 0, 0.01, 0.02, \dots, 1.50$  and  $\theta_{1l} = -1$  and  $\theta_{1u} = 1$  are the lower and upper alternative references, respectively.

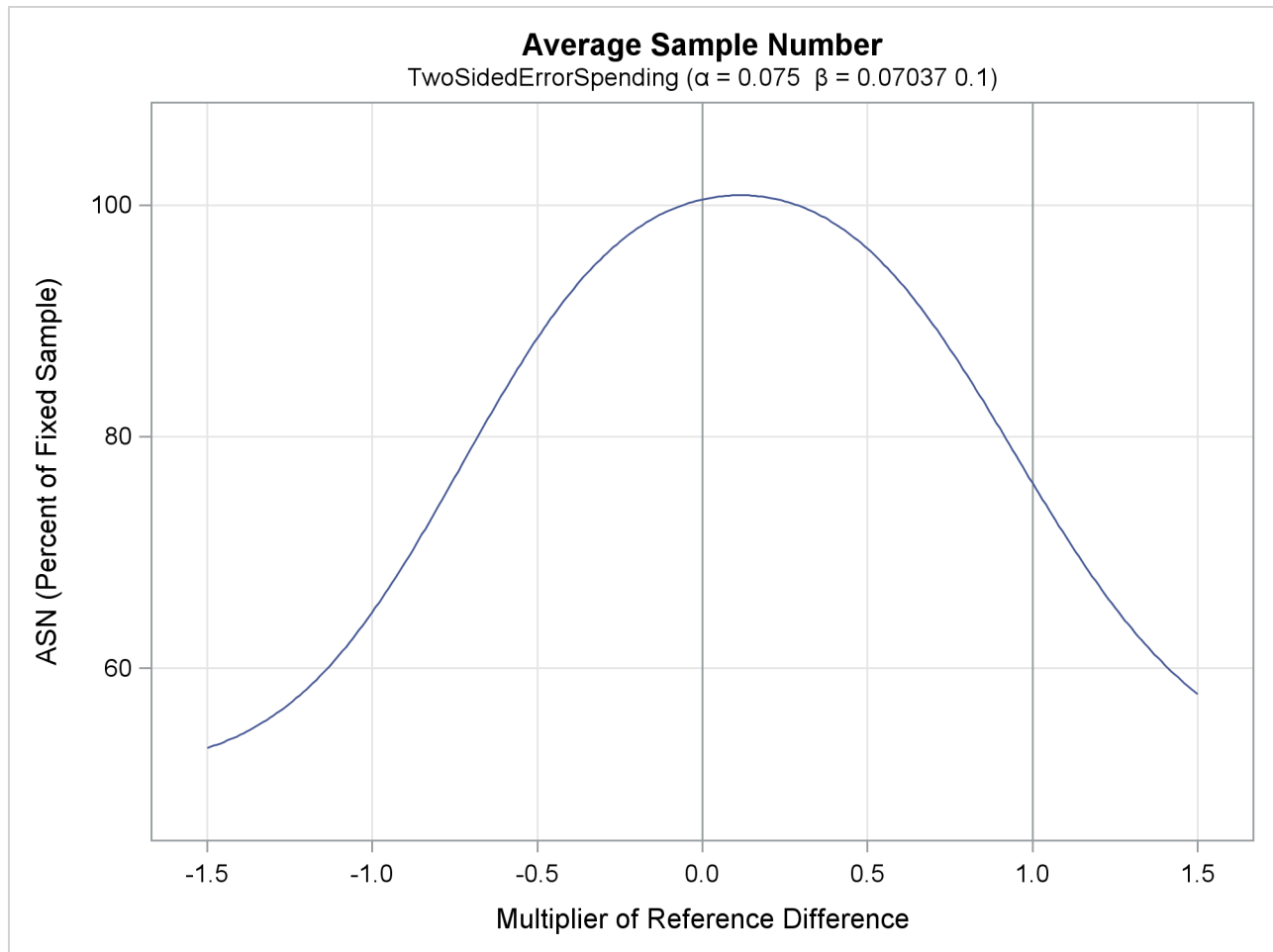
Output 83.11.5 Power Plot



The horizontal axis displays the multiplier of the reference difference. A positive multiplier corresponds to  $c_i$  for the upper alternative hypothesis, and a negative multiplier corresponds to  $-c_i$  for the lower alternative hypothesis. For lower reference hypotheses, the power is the lower  $\alpha$  error 0.05 under the null hypothesis ( $c_i = 0$ ) and is 0.92963 under the alternative hypothesis ( $c_i = 1$ ). For upper reference hypotheses, the power is the upper  $\alpha$  error 0.025 under the null hypothesis ( $c_i = 0$ ) and is 0.90 under the alternative hypothesis ( $c_i = 1$ ).

With the PLOTS=ASN option, the procedure displays a plot of expected sample sizes under various hypothetical references, as shown in [Output 83.11.6](#). By default, expected sample sizes under the lower hypotheses  $\theta = c_i \theta_{1l}$  and under the upper hypotheses  $\theta = c_i \theta_{1u}$ ,  $c_i = 0, 0.01, 0.02, \dots, 1.50$ , are displayed for a two-sided asymmetric design, where  $\theta_{1l} = -1$  and  $\theta_{1u} = 1$  are the lower and upper alternative references, respectively.

**Output 83.11.6** ASN Plot



The horizontal axis displays the multiplier of the reference difference. A positive multiplier corresponds to  $c_i$  for the upper alternative hypothesis and a negative multiplier corresponds to  $-c_i$  for the lower alternative hypothesis.

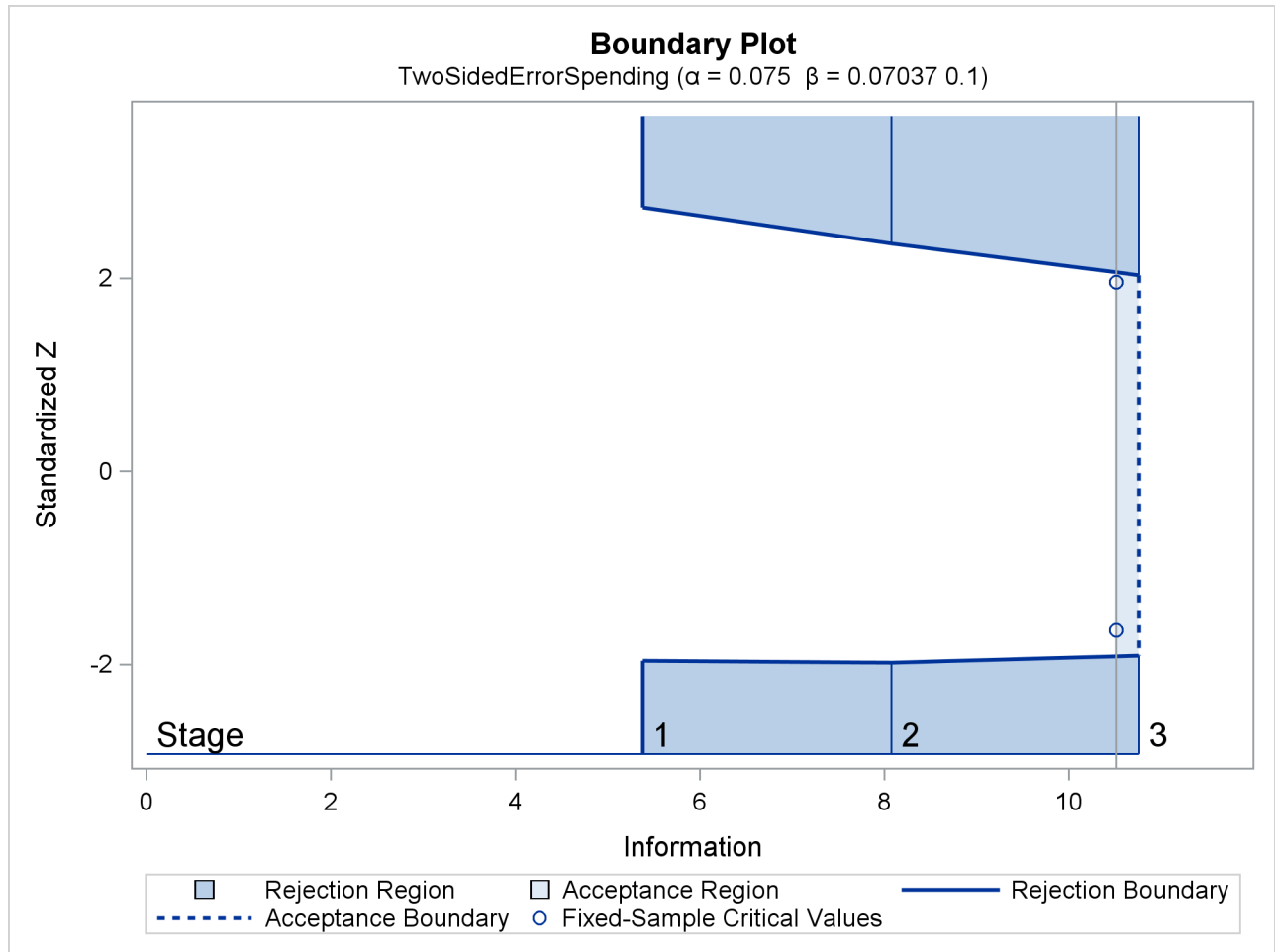
The “Boundary Information” table in [Output 83.11.7](#) displays the information levels, alternative references, and boundary values. By default (or equivalently if you specify BOUNDARYSCALE=STDZ), the standardized  $Z$  scale is used to display the alternative references and boundary values. The resulting standardized alternative references at stage  $k$  are given by  $\pm\theta_1\sqrt{I_k}$ , where  $\theta_1$  is the specified alternative reference and  $I_k$  is the information level at stage  $k$ ,  $k = 1, 2, 3$ .

**Output 83.11.7** Boundary Information

| Boundary Information (Standardized Z Scale) |                       |          |                       |                     |                         |             |
|---------------------------------------------|-----------------------|----------|-----------------------|---------------------|-------------------------|-------------|
| Null Reference = 0                          |                       |          |                       |                     |                         |             |
| _Stage_                                     | --Information Level-- |          | -----Alternative----- |                     | ----Boundary Values---- |             |
|                                             | Proportion            | Actual   | -----Reference-----   | -----Reference----- | ---Lower---             | ---Upper--- |
|                                             |                       |          | Lower                 | Upper               | Alpha                   | Alpha       |
| 1                                           | 0.5000                | 5.381827 | -2.31988              | 2.31988             | -1.95996                | 2.73437     |
| 2                                           | 0.7500                | 8.07274  | -2.84126              | 2.84126             | -1.98394                | 2.35681     |
| 3                                           | 1.0000                | 10.76365 | -3.28080              | 3.28080             | -1.90855                | 2.02853     |

With ODS Graphics enabled, a detailed boundary plot with the rejection and acceptance regions is displayed, as shown in [Output 83.11.8](#).

**Output 83.11.8** Boundary Plot



The “Error Spending Information” table in [Output 83.11.9](#) displays the cumulative error spending at each stage for each boundary.

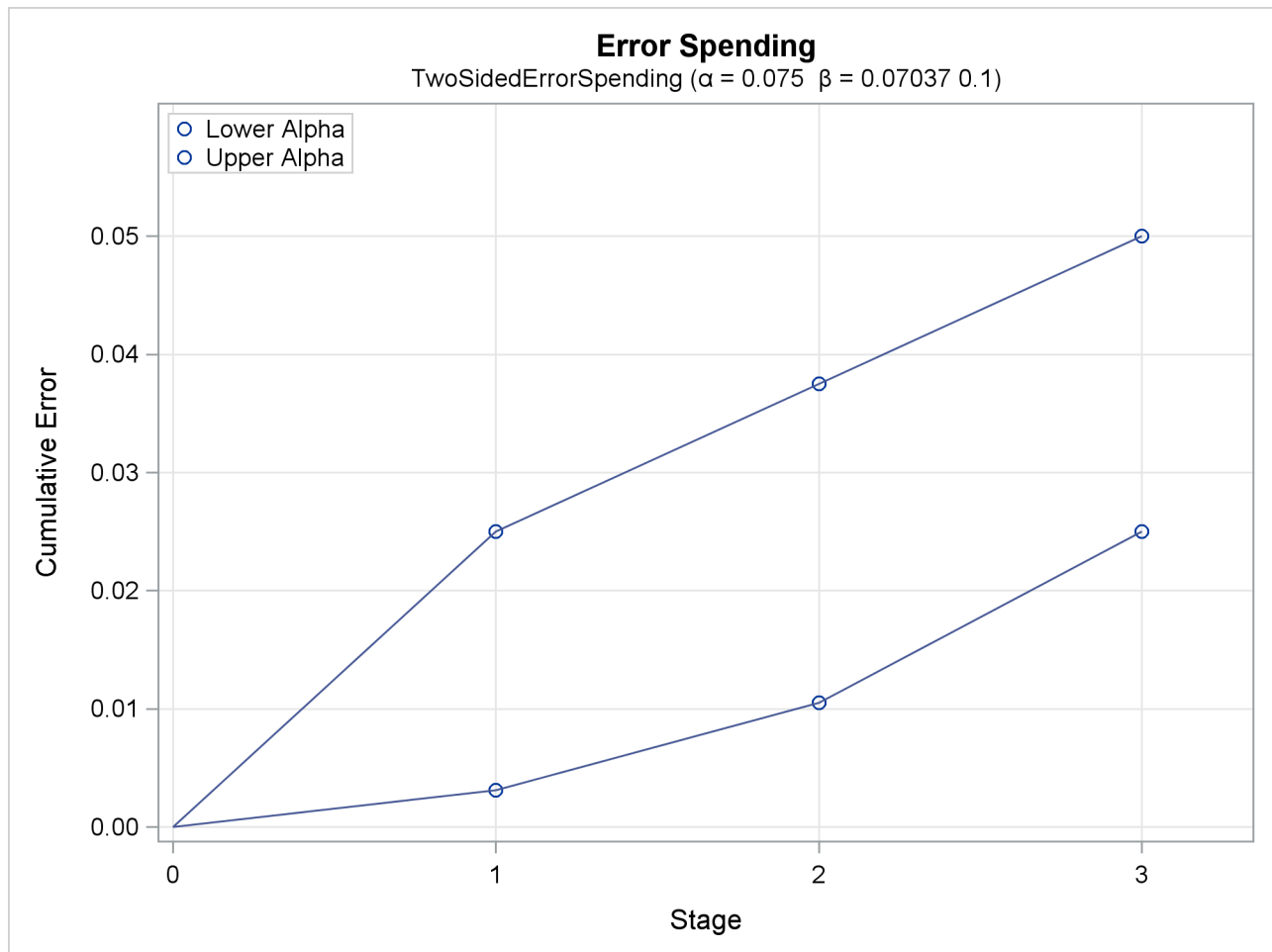
**Output 83.11.9** Error Spending Information

| _Stage_ | -Information Level-<br>Proportion | -----Cumulative Error Spending----- |         |                 |         |
|---------|-----------------------------------|-------------------------------------|---------|-----------------|---------|
|         |                                   | -----Lower-----                     |         | -----Upper----- |         |
|         |                                   | Alpha                               | Beta    | Beta            | Alpha   |
| 1       | 0.5000                            | 0.02500                             | 0.00000 | 0.00001         | 0.00313 |
| 2       | 0.7500                            | 0.03750                             | 0.00000 | 0.00001         | 0.01055 |
| 3       | 1.0000                            | 0.05000                             | 0.07037 | 0.10000         | 0.02500 |

With the STOP=REJECT option, there is no early stopping to accept  $H_0$ , and the corresponding  $\beta$  spending at an interim stage is computed from the rejection region. For example, the upper  $\beta$  spending at stage 1 (0.00001) is the probability of rejecting  $H_0$  for the lower alternative under the upper alternative reference.

With the PLOTS=ERRSPEND option, the procedure displays a plot of the cumulative error spending on each boundary at each stage, as shown in Output 83.11.10.

**Output 83.11.10** Error Spending Plot



### Example 83.12: Creating a Two-Sided Asymmetric Error Spending Design with Early Stopping to Reject or Accept $H_0$

This example requests a four-stage two-sided asymmetric group sequential design for normally distributed statistics. The O'Brien-Fleming boundary can be approximated by a gamma family error spending function with parameter  $\gamma = -4$  or  $-5$ , and the Pocock boundary can be approximated with parameter  $\gamma = 1$  (Hwang, Shih, and DeCani 1990, p. 1440). The following statements use the gamma error spending function with early stopping to reject or accept the null hypothesis  $H_0$ :

```
ods graphics on;
proc seqdesign altref=2
 pss(cref=0 0.5 1)
 stopprob(cref=0 1)
 errspend
 plots=(asn power errspend)
 ;
TwoSidedAsymmetric: design nstages=4
 method=errfuncgamma(gamma=1)
 method(beta)=errfuncgamma(gamma=-2)
 method(upperalpha)=errfuncgamma(gamma=-5)
 alt=twosided
 stop=both
 beta=0.1
 ;
run;
ods graphics off;
```

The design uses gamma family error spending functions with  $\gamma = -5$  for the upper  $\alpha$  boundary,  $\gamma = 1$  for the lower  $\alpha$  boundary, and  $\gamma = -2$  for the lower and upper  $\beta$  boundaries.

The “Design Information” table in [Output 83.12.1](#) displays design specifications and the derived maximum information. Note that in order to attain the same information level for the asymmetric lower and upper boundaries, the derived power at the upper alternative 0.93655 is larger than the specified  $1 - \beta = 0.90$ .

**Output 83.12.1** Design Information

| The SEQDESIGN Procedure                     |                    |
|---------------------------------------------|--------------------|
| Design: TwoSidedAsymmetric                  |                    |
| Design Information                          |                    |
| Statistic Distribution                      | Normal             |
| Boundary Scale                              | Standardized Z     |
| Alternative Hypothesis                      | Two-Sided          |
| Early Stop                                  | Accept/Reject Null |
| Method                                      | Error Spending     |
| Boundary Key                                | Both               |
| Alternative Reference                       | 2                  |
| Number of Stages                            | 4                  |
| Alpha                                       | 0.05               |
| Beta (Lower)                                | 0.1                |
| Beta (Upper)                                | 0.06345            |
| Power (Lower)                               | 0.9                |
| Power (Upper)                               | 0.93655            |
| Max Information (Percent of Fixed Sample)   | 104.0688           |
| Max Information                             | 3.162386           |
| Null Ref ASN (Percent of Fixed Sample)      | 74.16654           |
| Lower Alt Ref ASN (Percent of Fixed Sample) | 59.10271           |
| Upper Alt Ref ASN (Percent of Fixed Sample) | 73.78797           |

The “Method Information” table in [Output 83.11.2](#) displays the specified  $\alpha$  and  $\beta$  error levels and the derived drift parameter. With the same information level used for the asymmetric lower and upper boundaries, only one of the  $\beta$  levels is maintained and the other is derived to have the level less than or equal to the specified level.

**Output 83.12.2** Method Information

| Method Information |                |         |         |                                    |
|--------------------|----------------|---------|---------|------------------------------------|
| Boundary           | Method         | Alpha   | Beta    | ----Error Spending----<br>Function |
| Upper Alpha        | Error Spending | 0.02500 | .       | Gamma (Gamma=-5)                   |
| Upper Beta         | Error Spending | .       | 0.06345 | Gamma (Gamma=-2)                   |
| Lower Beta         | Error Spending | .       | 0.10000 | Gamma (Gamma=-2)                   |
| Lower Alpha        | Error Spending | 0.02500 | .       | Gamma (Gamma=1)                    |

| Method Information |                       |          |
|--------------------|-----------------------|----------|
| Boundary           | Alternative Reference | Drift    |
| Upper Alpha        | 2                     | 3.55662  |
| Upper Beta         | 2                     | 3.55662  |
| Lower Beta         | -2                    | -3.55662 |
| Lower Alpha        | -2                    | -3.55662 |



With the STOPPROB(CREF=0 1) option, the “Expected Cumulative Stopping Probabilities” table in Output 83.12.3 displays the expected stopping stage and cumulative stopping probabilities at each stage under the null reference  $\theta = 0$  and under the alternative reference  $\theta = \theta_1$ .

**Output 83.12.3** Stopping Probabilities

| Expected Cumulative Stopping Probabilities |           |                         |                      |  |
|--------------------------------------------|-----------|-------------------------|----------------------|--|
| Reference = CRef * (Alt Reference)         |           |                         |                      |  |
| CRef                                       | Ref       | Expected Stopping Stage | Source               |  |
| 0.0000                                     | Lower Alt | 2.851                   | Rej Null (Lower Alt) |  |
| 0.0000                                     | Lower Alt | 2.851                   | Rej Null (Upper Alt) |  |
| 0.0000                                     | Lower Alt | 2.851                   | Reject Null          |  |
| 0.0000                                     | Lower Alt | 2.851                   | Accept Null          |  |
| 0.0000                                     | Lower Alt | 2.851                   | Total                |  |
| 1.0000                                     | Lower Alt | 2.272                   | Rej Null (Lower Alt) |  |
| 1.0000                                     | Lower Alt | 2.272                   | Rej Null (Upper Alt) |  |
| 1.0000                                     | Lower Alt | 2.272                   | Reject Null          |  |
| 1.0000                                     | Lower Alt | 2.272                   | Accept Null          |  |
| 1.0000                                     | Lower Alt | 2.272                   | Total                |  |
| 0.0000                                     | Upper Alt | 2.851                   | Rej Null (Lower Alt) |  |
| 0.0000                                     | Upper Alt | 2.851                   | Rej Null (Upper Alt) |  |
| 0.0000                                     | Upper Alt | 2.851                   | Reject Null          |  |
| 0.0000                                     | Upper Alt | 2.851                   | Accept Null          |  |
| 0.0000                                     | Upper Alt | 2.851                   | Total                |  |
| 1.0000                                     | Upper Alt | 2.836                   | Rej Null (Lower Alt) |  |
| 1.0000                                     | Upper Alt | 2.836                   | Rej Null (Upper Alt) |  |
| 1.0000                                     | Upper Alt | 2.836                   | Reject Null          |  |
| 1.0000                                     | Upper Alt | 2.836                   | Accept Null          |  |
| 1.0000                                     | Upper Alt | 2.836                   | Total                |  |

| Expected Cumulative Stopping Probabilities |           |                                  |         |         |         |
|--------------------------------------------|-----------|----------------------------------|---------|---------|---------|
| Reference = CRef * (Alt Reference)         |           |                                  |         |         |         |
| CRef                                       | Ref       | -----Stopping Probabilities----- |         |         |         |
|                                            |           | Stage_1                          | Stage_2 | Stage_3 | Stage_4 |
| 0.0000                                     | Lower Alt | 0.00875                          | 0.01556 | 0.02087 | 0.02500 |
| 0.0000                                     | Lower Alt | 0.00042                          | 0.00190 | 0.00704 | 0.02500 |
| 0.0000                                     | Lower Alt | 0.00917                          | 0.01746 | 0.02791 | 0.05000 |
| 0.0000                                     | Lower Alt | 0.00000                          | 0.30125 | 0.79354 | 0.95000 |
| 0.0000                                     | Lower Alt | 0.00917                          | 0.31870 | 0.82145 | 1.00000 |
| 1.0000                                     | Lower Alt | 0.27499                          | 0.58934 | 0.79601 | 0.90000 |
| 1.0000                                     | Lower Alt | 0.00000                          | 0.00000 | 0.00000 | 0.00000 |
| 1.0000                                     | Lower Alt | 0.27499                          | 0.58934 | 0.79601 | 0.90000 |
| 1.0000                                     | Lower Alt | 0.00000                          | 0.01863 | 0.04935 | 0.10000 |
| 1.0000                                     | Lower Alt | 0.27499                          | 0.60797 | 0.84536 | 1.00000 |
| 0.0000                                     | Upper Alt | 0.00875                          | 0.01556 | 0.02087 | 0.02500 |
| 0.0000                                     | Upper Alt | 0.00042                          | 0.00190 | 0.00704 | 0.02500 |
| 0.0000                                     | Upper Alt | 0.00917                          | 0.01746 | 0.02791 | 0.05000 |
| 0.0000                                     | Upper Alt | 0.00000                          | 0.30125 | 0.79354 | 0.95000 |
| 0.0000                                     | Upper Alt | 0.00917                          | 0.31870 | 0.82145 | 1.00000 |
| 1.0000                                     | Upper Alt | 0.00002                          | 0.00002 | 0.00002 | 0.00002 |
| 1.0000                                     | Upper Alt | 0.05945                          | 0.33802 | 0.72323 | 0.93655 |
| 1.0000                                     | Upper Alt | 0.05947                          | 0.33804 | 0.72325 | 0.93657 |
| 1.0000                                     | Upper Alt | 0.00000                          | 0.01182 | 0.03131 | 0.06343 |
| 1.0000                                     | Upper Alt | 0.05947                          | 0.34986 | 0.75456 | 1.00000 |

“Rej Null (Lower Alt)” and “Rej Null (Upper Alt)” under the heading “Source” indicate the probabilities of rejecting the null hypothesis for the lower alternative and for the upper alternative, respectively. “Reject Null” indicates the probability of rejecting the null hypothesis for either the lower or upper alternative, “Accept Null” indicates the probability of accepting the null hypothesis, and “Total” indicates the total probability of stopping the trial.

With the PSS(CREF=0 0.5 1.0) option, the “Power and Expected Sample Sizes” table in [Output 83.12.4](#) displays powers and expected sample sizes under hypothetical references  $\theta = 0$  (null hypothesis  $H_0$ ),  $\theta = 0.5\theta_1$ , and  $\theta = \theta_1$  (alternative hypothesis  $H_1$ ), where  $\theta_1$  is the alternative reference. The expected sample sizes are displayed in a scale that indicates a percentage of its corresponding fixed-sample size design.

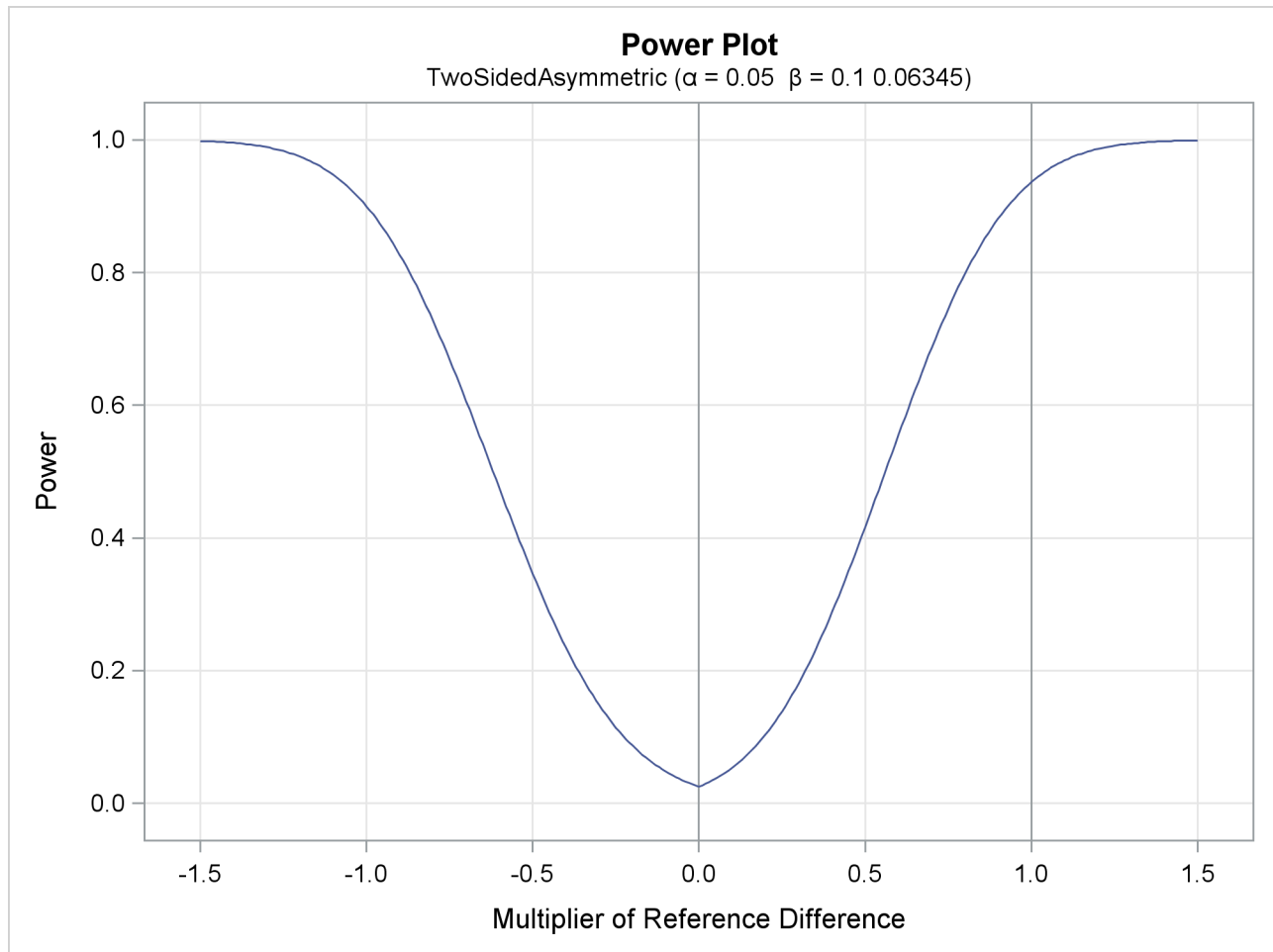
**Output 83.12.4** Power and Expected Sample Size Information

| Powers and Expected Sample Sizes   |           |         |                                          |
|------------------------------------|-----------|---------|------------------------------------------|
| Reference = CRef * (Alt Reference) |           |         |                                          |
| CRef                               | Ref       | Power   | -Sample Size-<br>Percent<br>Fixed-Sample |
| 0.0000                             | Lower Alt | 0.02500 | 74.1665                                  |
| 0.5000                             | Lower Alt | 0.34601 | 75.8425                                  |
| 1.0000                             | Lower Alt | 0.90000 | 59.1027                                  |
| 0.0000                             | Upper Alt | 0.02500 | 74.1665                                  |
| 0.5000                             | Upper Alt | 0.41647 | 85.3976                                  |
| 1.0000                             | Upper Alt | 0.93655 | 73.7880                                  |

Note that at  $c_i = 0$ , the null reference  $\theta = 0$ , the power with the lower alternative is the lower  $\alpha$  error 0.025, and the power with the upper alternative is the upper  $\alpha$  error 0.025. At  $c_i = 1$ , the alternative reference  $\theta = \theta_1$ , the power with the lower alternative is the specified power 0.90, and the power with the upper alternative 0.93655 is greater than the specified power 0.90 because the same information level is used for these two asymmetric boundaries.

With the PLOTS=POWER option, the procedure displays a plot of the power curves under various hypothetical references, as shown in [Output 83.12.5](#). By default, powers under the lower hypotheses  $\theta = c_i \theta_{1l}$  and under the upper hypotheses  $\theta = c_i \theta_{1u}$ , are displayed for a two-sided asymmetric design, where  $c_i = 0, 0.01, 0.02, \dots, 1.50$  and  $\theta_{1l} = -1$  and  $\theta_{1u} = 1$  are the lower and upper alternative references, respectively.

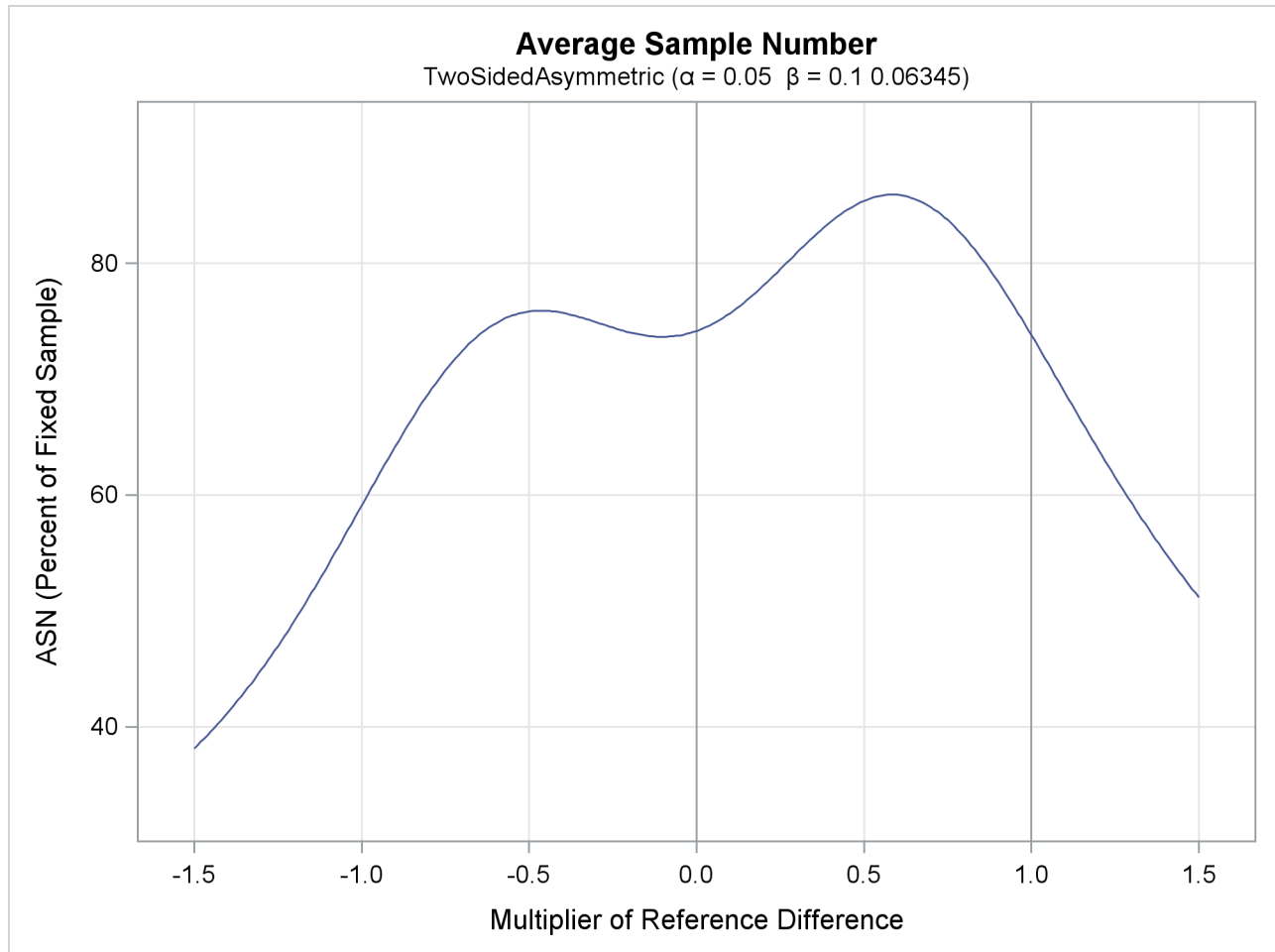
Output 83.12.5 Power Plot



The horizontal axis displays the multiplier of the reference difference. A positive multiplier corresponds to  $c_i$  for the upper alternative hypothesis, and a negative multiplier corresponds to  $-c_i$  for the lower alternative hypothesis. For lower reference hypotheses, the power is the lower  $\alpha$  error 0.025 under the null hypothesis ( $c_i = 0$ ) and is 0.90 under the alternative hypothesis ( $c_i = 1$ ). For upper reference hypotheses, the power is the upper  $\alpha$  error 0.025 under the null hypothesis ( $c_i = 0$ ) and is 0.93655 under the alternative hypothesis ( $c_i = 1$ ).

With the PLOTS=ASN option, the procedure displays a plot of expected sample sizes under various hypothetical references, as shown in Output 83.12.6. By default, expected sample sizes under the lower hypotheses  $\theta = c_i \theta_{1l}$  and under the upper hypotheses  $\theta = c_i \theta_{1u}$  are displayed for a two-sided asymmetric design, where  $c_i = 0, 0.01, 0.02, \dots, 1.50$  and  $\theta_{1l} = -1$  and  $\theta_{1u} = 1$  are the lower and upper alternative references, respectively.

**Output 83.12.6** ASN Plot



The horizontal axis displays the multiplier of the reference difference. A positive multiplier corresponds to  $c_i$  for the upper alternative hypothesis, and a negative multiplier corresponds to  $-c_i$  for the lower alternative hypothesis.

By default (or equivalently if you specify BETAOVERLAP=ADJUST), the SEQDESIGN procedure first derives boundary values without adjusting for the possible overlapping of the two one-sided  $\beta$  boundaries based on two corresponding one-sided tests. Then the procedure checks for overlapping of the  $\beta$  boundaries at the interim stages. Since the two  $\beta$  boundaries overlap at stage 1, the  $\beta$  boundary values for stage 1 are set to missing, the  $\beta$  spending values at stage 1 are set to zero, and the  $\beta$  spending values at subsequent stages are adjusted proportionally.

The “Boundary Information” table in [Output 83.12.7](#) displays the information levels, alternative references, and boundary values. By default (or equivalently if you specify BOUNDARYSCALE=STDZ), the standardized Z scale is used to display the alternative references and boundary values. The resulting standardized alternative references at stage  $k$  is given by  $\pm\theta_1\sqrt{I_k}$ , where  $\theta_1$  is the specified alternative reference and  $I_k$  is the information level at stage  $k$ ,  $k = 1, 2, 3, 4$ .

**Output 83.12.7** Boundary Information

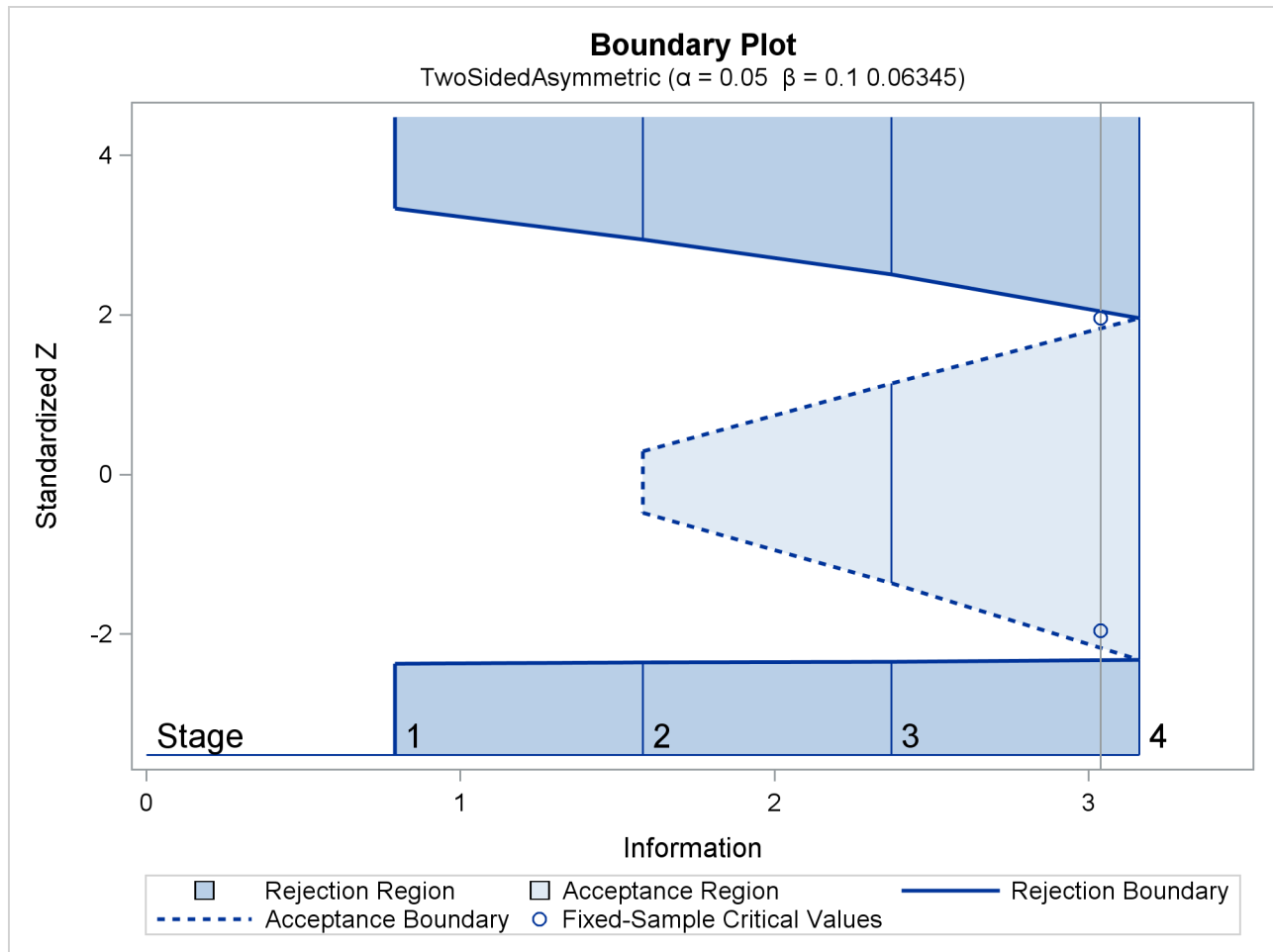
| Boundary Information (Standardized Z Scale) |                         |          |                       |         |
|---------------------------------------------|-------------------------|----------|-----------------------|---------|
| Null Reference = 0                          |                         |          |                       |         |
| _Stage_                                     | ---Information Level--- |          | -----Alternative----- |         |
|                                             | Proportion              | Actual   | Lower                 | Upper   |
| 1                                           | 0.2500                  | 0.790597 | -1.77831              | 1.77831 |
| 2                                           | 0.5000                  | 1.581193 | -2.51491              | 2.51491 |
| 3                                           | 0.7500                  | 2.37179  | -3.08012              | 3.08012 |
| 4                                           | 1.0000                  | 3.162386 | -3.55662              | 3.55662 |

| Boundary Information (Standardized Z Scale) |                           |          |         |         |
|---------------------------------------------|---------------------------|----------|---------|---------|
| Null Reference = 0                          |                           |          |         |         |
| _Stage_                                     | -----Boundary Values----- |          |         |         |
|                                             | Alpha                     | Beta     | Beta    | Alpha   |
| 1                                           | -2.37610                  | .        | .       | 3.33772 |
| 2                                           | -2.35714                  | -0.48408 | 0.29400 | 2.94871 |
| 3                                           | -2.34861                  | -1.36183 | 1.13898 | 2.50473 |
| 4                                           | -2.32105                  | -2.32105 | 1.95675 | 1.95675 |

With ODS Graphics enabled, a detailed boundary plot with the rejection and acceptance regions is displayed, as shown in [Output 83.12.8](#).

**Output 83.12.8** Boundary Plot



The “Error Spending Information” in **Output 83.12.9** displays the cumulative error spending at each stage for each boundary.

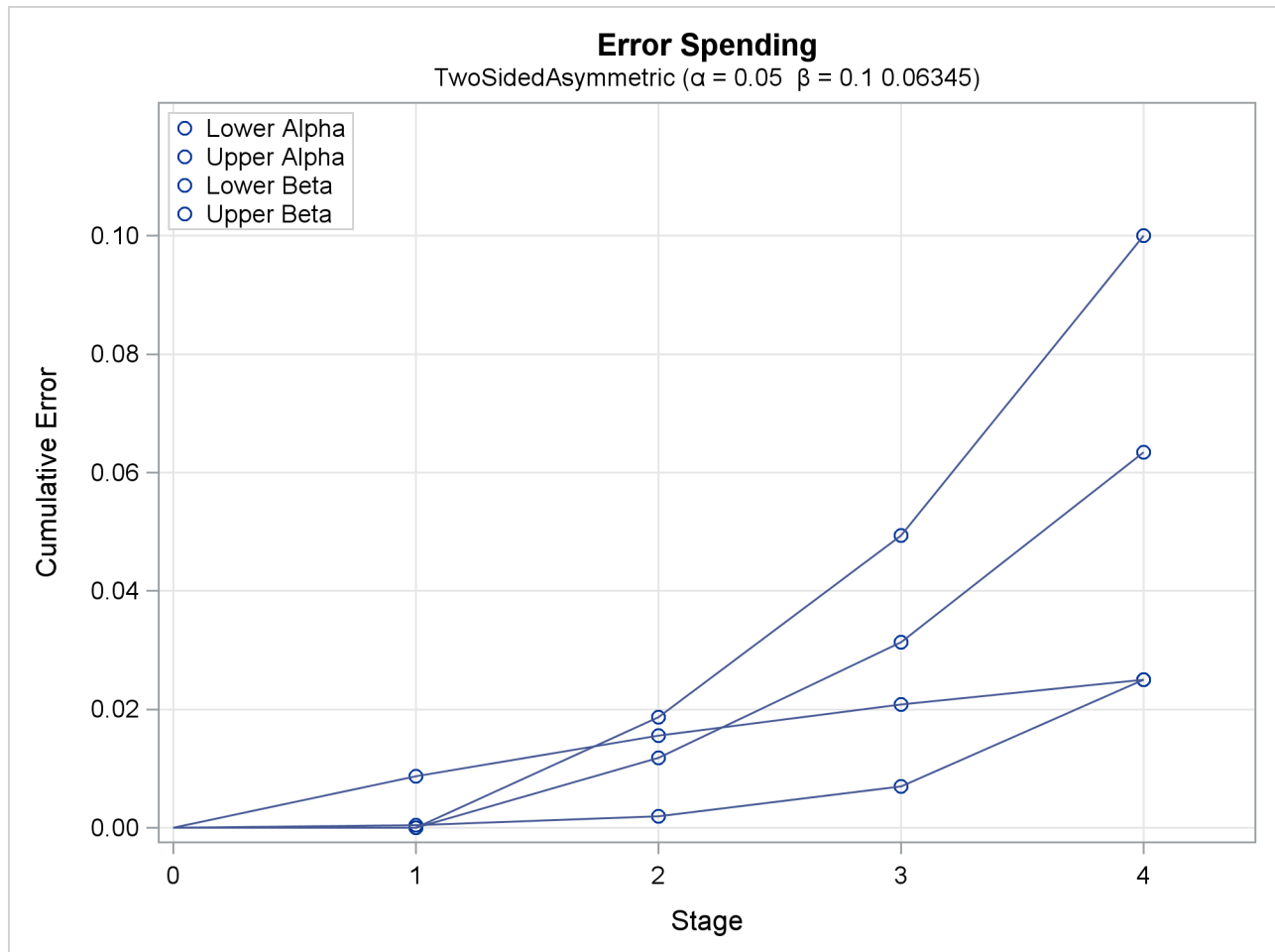
**Output 83.12.9** Error Spending Information

| _Stage_ | -Information Level-<br>Proportion | -----Cumulative Error Spending----- |         |                 |         |
|---------|-----------------------------------|-------------------------------------|---------|-----------------|---------|
|         |                                   | -----Lower-----                     |         | -----Upper----- |         |
|         |                                   | Alpha                               | Beta    | Beta            | Alpha   |
| 1       | 0.2500                            | 0.00875                             | 0.00000 | 0.00002         | 0.00042 |
| 2       | 0.5000                            | 0.01556                             | 0.01863 | 0.01184         | 0.00190 |
| 3       | 0.7500                            | 0.02087                             | 0.04935 | 0.03132         | 0.00704 |
| 4       | 1.0000                            | 0.02500                             | 0.10000 | 0.06345         | 0.02500 |

With the  $\beta$  boundary values missing at stage 1, there is no early stopping to accept  $H_0$  at stage 1, and the corresponding  $\beta$  spending at stage 1 is computed from the rejection region. For example, the upper  $\beta$  spending at stage 1 (0.00002) is the probability of rejecting  $H_0$  for the lower alternative under the upper alternative reference.

With the PLOTS=ERRSPEND option, the procedure displays a plot of the cumulative error spending on each boundary at each stage, as shown in Output 83.12.10.

**Output 83.12.10** Error Spending Plot



### Example 83.13: Creating a Design with a Nonbinding Beta Boundary

This example requests a two-sided design similar to Example 83.2, but with a nonbinding beta boundary. With a nonbinding acceptance boundary, the trial does not need to stop to accept the null hypothesis when a test statistic falls in the acceptance region at interim stages. The design maintains the specified Type I error level, but at the cost of increased sample size.

The following statements invoke the SEQDESIGN procedure and request a four-stage group sequential design with early stopping to reject or accept  $H_0$ :

```
ods graphics on;
proc seqdesign altref=0.15 errspend
 ;
 NonbindingDesign: design nstages=4
 method=obf
 alt=upper
 stop=both(betaboundary=nonbinding)
 alpha=0.025 beta=0.10
 ;
 samplesize model=twosamplefreq(nullprop=0.6 test=prop);
run;
ods graphics off;
```

The STOP=BOTH option specifies early stopping to reject or accept the null hypothesis, and the BETABOUNDARY=NONBINDING suboption requests the nonbinding beta boundary.

The “Design Information,” “Method Information,” and “Boundary Information” tables are displayed by default. The “Design Information” table in [Output 83.13.1](#) displays design specifications and derived statistics such as power and maximum information. With a specified alternative reference, ALTREF=0.15, the maximum information  $I_X$  is derived.

**Output 83.13.1** Design Information

| The SEQDESIGN Procedure                   |                                   |
|-------------------------------------------|-----------------------------------|
| Design: NonbindingDesign                  |                                   |
| Design Information                        |                                   |
| Statistic Distribution                    | Normal                            |
| Boundary Scale                            | Standardized Z                    |
| Alternative Hypothesis                    | Upper                             |
| Early Stop                                | Accept (Nonbinding) / Reject Null |
| Method                                    | O'Brien-Fleming                   |
| Boundary Key                              | Both                              |
| Alternative Reference                     | 0.15                              |
| Number of Stages                          | 4                                 |
| Alpha (Binding Beta Boundary)             | 0.02228                           |
| Alpha (Nonbinding Beta Boundary)          | 0.025                             |
| Beta                                      | 0.1                               |
| Power                                     | 0.9                               |
| Max Information (Percent of Fixed Sample) | 110.7138                          |
| Max Information                           | 517.0296                          |
| Null Ref ASN (Percent of Fixed Sample)    | 62.29796                          |
| Alt Ref ASN (Percent of Fixed Sample)     | 78.5392                           |

With the BETABOUNDARY=NONBINDING option, there are two ways to compute the Type I error level: with or without the beta boundary. Alpha (Binding Beta Boundary) displays the Type I error level with the beta boundary, and Alpha (Nonbinding Beta Boundary) displays the Type I error level without the beta boundary.

The maximum information is the information level at the final stage of the group sequential trial. The Max Information (Percent Fixed-Sample) row displays the maximum information for the sequential design



expressed as a percentage of the information for the corresponding fixed-sample design (which has a Type I error level 0.025). In [Output 83.13.1](#), Max Information (Percent Fixed-Sample) is 110.71%, which means that the information needed for the group sequential trial is 10.71% more than the information needed for the corresponding fixed-sample design if the trial does not stop at any interim stage.

Compared to the corresponding design with a binding beta boundary, which has a Max Information (Percent Fixed-Sample) of 107.67% as displayed in [Output 83.2.1](#), the nonbinding design requires a larger sample size if the trial proceeds to the final stage.

The “Method Information” table in [Output 83.13.2](#) displays the values of  $\rho = 0.5$  and  $\tau = 0$ , which are the parameters for the O’Brien-Fleming method. The table also displays the drift parameter 3.4107, which is greater than the drift parameter 3.3636 in the corresponding binding boundary design, as displayed in [Output 83.2.2](#).

**Output 83.13.2** Method Information

| Method Information |                 |         |         |                          |     |         |
|--------------------|-----------------|---------|---------|--------------------------|-----|---------|
| Boundary           | Method          | Alpha   | Beta    | -----Unified Family----- |     |         |
|                    |                 |         |         | Rho                      | Tau | C       |
| Upper Alpha        | O'Brien-Fleming | 0.02500 | .       | 0.5                      | 0   | 2.0243  |
| Upper Beta         | O'Brien-Fleming | .       | 0.10000 | 0.5                      | 0   | 1.38645 |

| Method Information |                       |             |      |
|--------------------|-----------------------|-------------|------|
| Boundary           | Alternative Reference | Drift       |      |
|                    |                       | Upper Alpha | 0.15 |
| Upper Beta         | 0.15                  | 3.410743    |      |

The “Boundary Information” table in [Output 83.13.3](#) displays information level, alternative reference, and boundary values at each stage. By default (or equivalently if you specify BOUNDARYSCALE=STDZ), the alternative reference and boundary values are displayed with the standardized Z statistic scale. The resulting standardized alternative reference at stage  $k$  is given by  $\theta_1 \sqrt{I_k}$ , where  $\theta_1$  is the alternative reference and  $I_k$  is the information level at stage  $k$ , for  $k= 1, 2, 3, 4$ .

**Output 83.13.3** Boundary Information

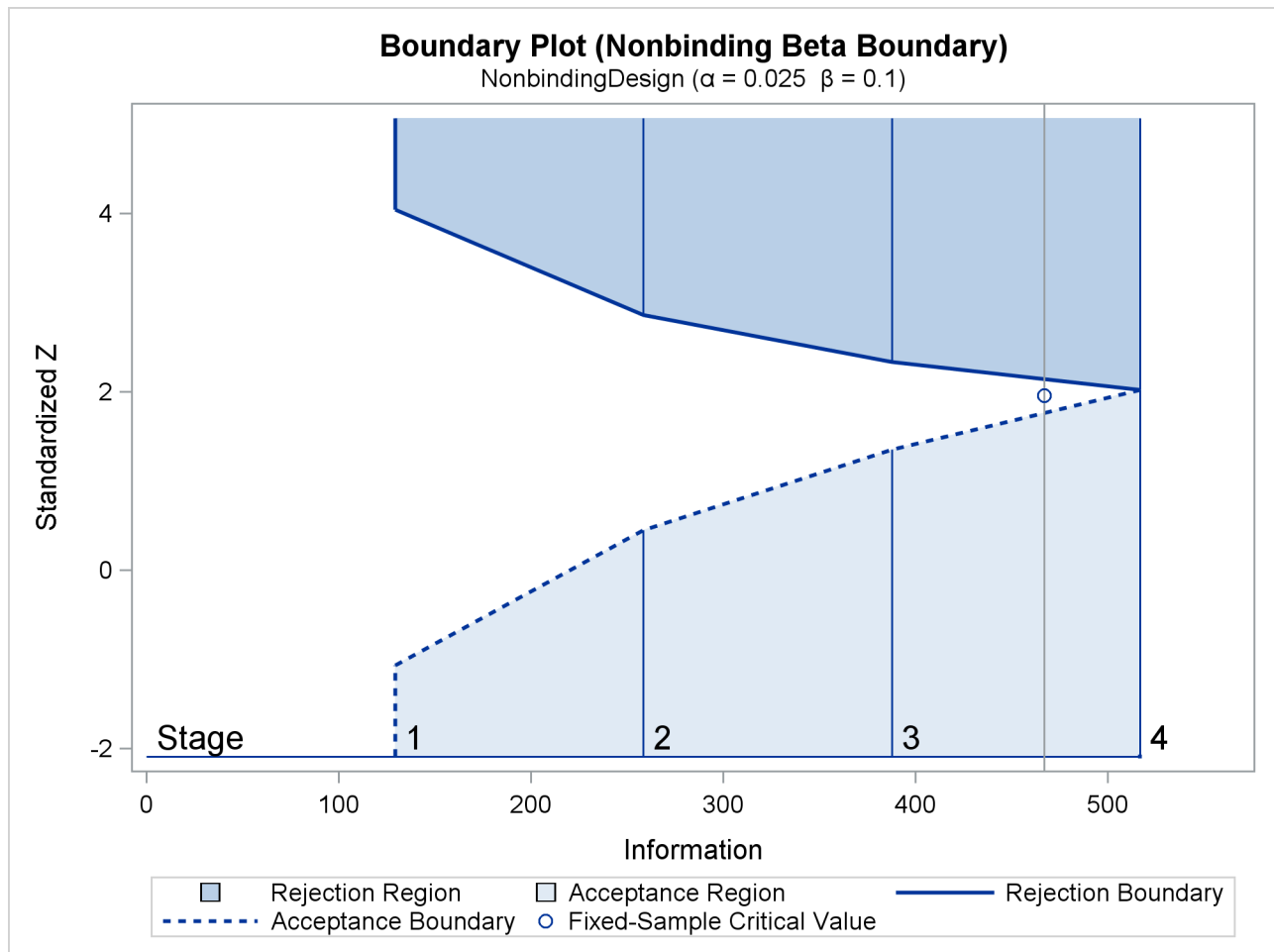
| Boundary Information (Standardized Z Scale)  |                             |          |          |                        |                         |         |
|----------------------------------------------|-----------------------------|----------|----------|------------------------|-------------------------|---------|
| Nonbinding Beta Boundary, Null Reference = 0 |                             |          |          |                        |                         |         |
| _Stage_                                      | -----Information Level----- |          |          | -Alternative-          | ----Boundary Values---- |         |
|                                              | Proportion                  | Actual   | N        | --Reference--<br>Upper | -----Upper-----<br>Beta | Alpha   |
| 1                                            | 0.2500                      | 129.2574 | 110.5151 | 1.70537                | -1.06752                | 4.04859 |
| 2                                            | 0.5000                      | 258.5148 | 221.0302 | 2.41176                | 0.45103                 | 2.86279 |
| 3                                            | 0.7500                      | 387.7722 | 331.5452 | 2.95379                | 1.35286                 | 2.33746 |
| 4                                            | 1.0000                      | 517.0296 | 442.0603 | 3.41074                | 2.02430                 | 2.02430 |

By default (or equivalently if you specify INFO=EQUAL), equally spaced information levels are used. With the derived maximum information, the actual information level at each stage is also displayed. With the SAMPLESIZE statement, the required sample size  $N$  is also displayed under the heading “Information Level.”

Note that with the standardized  $Z$  statistic scale, the rejection boundary values are identical to the boundary values that are derived in the corresponding design with early stopping to reject  $H_0$ .

With ODS Graphics enabled, a detailed boundary plot with the rejection and acceptance regions is displayed, as shown in [Output 83.13.4](#).

**Output 83.13.4** Boundary Plot



The horizontal axis indicates the information levels for the design. The stages are indicated by vertical lines with accompanying stage numbers. The boundary plot also displays the information level and the critical value for the corresponding fixed-sample design.

The “Error Spending Information (Nonbinding Beta Boundary)” table in [Output 83.13.5](#) displays cumulative error spending at each stage for each boundary. With a nonbinding beta boundary, the  $\alpha$  spending at each stage is computed by using the  $\alpha$  boundary only.

**Output 83.13.5** Error Spending Information

| Error Spending Information (Nonbinding Beta Boundary) |                                   |                             |         |  |
|-------------------------------------------------------|-----------------------------------|-----------------------------|---------|--|
| _Stage_                                               | -Information Level-<br>Proportion | -Cumulative Error Spending- |         |  |
|                                                       |                                   | -----Upper-----             |         |  |
|                                                       |                                   | Beta                        | Alpha   |  |
| 1                                                     | 0.2500                            | 0.00278                     | 0.00003 |  |
| 2                                                     | 0.5000                            | 0.02603                     | 0.00211 |  |
| 3                                                     | 0.7500                            | 0.06343                     | 0.01046 |  |
| 4                                                     | 1.0000                            | 0.10000                     | 0.02500 |  |

The SEQDESIGN procedure derives the drift parameter  $\theta_1 \sqrt{I_X}$ , where  $\theta_1$  is the alternative reference and  $I_X$  is the maximum information. With the SAMPLESIZE statement, the maximum information is used to compute the required sample size for the study.

The “Sample Size Summary” table in [Output 83.13.6](#) displays parameters for the sample size computation. With the MODEL=TWOSAMPLEFREQ(NULLPROP=0.6 TEST=PROP) option in the SAMPLESIZE statement, the total sample size and expected sample sizes under the null and alternative hypotheses for testing the difference between two proportions are displayed.

**Output 83.13.6** Sample Size Summary

| Sample Size Summary             |                        |          |
|---------------------------------|------------------------|----------|
| Test                            | Two-Sample Proportions |          |
| Null Proportion                 |                        | 0.6      |
| Proportion (Group A)            |                        | 0.75     |
| Test Statistic                  | Z for Proportion       |          |
| Reference Proportions           | Alt                    | Ref      |
| Max Sample Size                 |                        | 442.0603 |
| Expected Sample Size (Null Ref) |                        | 248.7446 |
| Expected Sample Size (Alt Ref)  |                        | 313.5929 |

The “Sample Sizes (N)” table in [Output 83.13.7](#) displays the required sample sizes at each stage, in both fractional and integer numbers. The derived fractional sample sizes are under the heading “Fractional N.” These sample sizes are rounded up to integers under the heading “Ceiling N.” As expected, the sample sizes in the table are larger than the corresponding sample sizes in the corresponding design with binding beta boundary.

**Output 83.13.7** Derived Sample Sizes

| Sample Sizes (N)                            |        |          |          |             |
|---------------------------------------------|--------|----------|----------|-------------|
| Two-Sample Z Test for Proportion Difference |        |          |          |             |
| -----Fractional N-----                      |        |          |          |             |
| _Stage_                                     | N      | N(Grp 1) | N(Grp 2) | Information |
| 1                                           | 110.52 | 55.26    | 55.26    | 129.3       |
| 2                                           | 221.03 | 110.52   | 110.52   | 258.5       |
| 3                                           | 331.55 | 165.77   | 165.77   | 387.8       |
| 4                                           | 442.06 | 221.03   | 221.03   | 517.0       |

| Sample Sizes (N)                            |     |          |          |             |
|---------------------------------------------|-----|----------|----------|-------------|
| Two-Sample Z Test for Proportion Difference |     |          |          |             |
| -----Ceiling N-----                         |     |          |          |             |
| _Stage_                                     | N   | N(Grp 1) | N(Grp 2) | Information |
| 1                                           | 112 | 56       | 56       | 131.0       |
| 2                                           | 222 | 111      | 111      | 259.6       |
| 3                                           | 332 | 166      | 166      | 388.3       |
| 4                                           | 444 | 222      | 222      | 519.3       |

**Example 83.14: Computing Sample Size for Survival Data**

This example illustrates sample size computation for survival data when the accrual is not uniform and when the data contain individual loss to follow up.

Suppose that a clinic is conducting a study of the effect of a new cancer treatment. The study consists of exposing mice to a carcinogen and randomly assigning them to either the control group or the treatment group. The event of interest is death from cancer induced by the carcinogen, and the response is the time from randomization to death.

Following the derivations in the section “Test for Two Survival Distributions with a Log-Rank Test” on page 7059, this example uses the hypothesis  $H_0 : \theta = -\log(\lambda) = 0$  with an alternative hypothesis  $H_1 : \theta = \theta_1 > 0$ , where  $\lambda$  is the hazard ratio between the treatment group and the control group.

Suppose that from past experience, the median survival time for the control group is  $t_0 = 20$  weeks, and the study wants to detect a  $t_1 = 40$  weeks’ median survival time with a 80% power in the trial. If exponential survival functions are assumed for the two groups, the hazard rates can be computed from

$$S_j(t_j) = e^{-h_j t_j} = \frac{1}{2}$$

where  $j = 0, 1$ .

Thus, with  $h_0 = 0.03466$  and  $h_1 = 0.01733$ , the hazard ratio  $\lambda_1 = h_1/h_0 = 1/2$ , and the alternative reference is

$$\theta_1 = -\log(\lambda_1) = -\log\left(\frac{1}{2}\right) = 0.693147$$

The following statements invoke the SEQDESIGN procedure:

```
proc seqdesign altref=0.693147
 ;
 OBrienFleming: design nstages=4
 method=obf
 ;
 samplesize model=twosamplesurvival
 (nullhazard=0.03466
 accrual=exp(parm=-0.1)
 loss=exp(hazard=0.05)
 acctime=20);
run;
```

The ALTREF= option specifies the alternative reference  $\theta_1 = -\log(\frac{1}{2}) = 0.693147$ . The DESIGN statement requests a group sequential design, and the METHOD=OBF option specifies the O'Brien-Fleming design. By default, the design has a two-sided alternative hypothesis in which early stopping in the interim stages occurs to reject the null hypothesis. The SAMPLESIZE statement derives required sample sizes for the test, and the MODEL=TWOSAMPLESURVIVAL option specifies a log-rank test to compare two survival distributions for the treatment effect.

The “Design Information” table in [Output 83.14.1](#) displays design specifications and four derived statistics: the actual maximum information, the maximum information, the average sample number under the null hypothesis (Null Ref ASN), and the average sample number under the alternative hypothesis (Alt Ref ASN).

**Output 83.14.1** O'Brien-Fleming Design Information

| The SEQDESIGN Procedure                   |                 |
|-------------------------------------------|-----------------|
| Design: OBrienFleming                     |                 |
| Design Information                        |                 |
| Statistic Distribution                    | Normal          |
| Boundary Scale                            | Standardized Z  |
| Alternative Hypothesis                    | Two-Sided       |
| Early Stop                                | Reject Null     |
| Method                                    | O'Brien-Fleming |
| Boundary Key                              | Both            |
| Alternative Reference                     | 0.693147        |
| Number of Stages                          | 4               |
| Alpha                                     | 0.05            |
| Beta                                      | 0.1             |
| Power                                     | 0.9             |
| Max Information (Percent of Fixed Sample) | 102.2163        |
| Max Information                           | 22.35452        |
| Null Ref ASN (Percent of Fixed Sample)    | 101.5728        |
| Alt Ref ASN (Percent of Fixed Sample)     | 76.7397         |

The “Boundary Information” table in [Output 83.14.2](#) displays the information level, including the proportion, actual level, and corresponding number of events at each stage. The table also displays the lower and upper alternative references, and the lower and upper boundary values at each stage.

**Output 83.14.2** Boundary Information

| Boundary Information (Standardized Z Scale) |                             |          |          |                       |         |
|---------------------------------------------|-----------------------------|----------|----------|-----------------------|---------|
| Null Reference = 0                          |                             |          |          |                       |         |
| _Stage_                                     | -----Information Level----- |          |          | -----Alternative----- |         |
|                                             | Proportion                  | Actual   | Events   | Lower                 | Upper   |
| 1                                           | 0.2500                      | 5.58863  | 22.35452 | -1.63862              | 1.63862 |
| 2                                           | 0.5000                      | 11.17726 | 44.70904 | -2.31736              | 2.31736 |
| 3                                           | 0.7500                      | 16.76589 | 67.06356 | -2.83817              | 2.83817 |
| 4                                           | 1.0000                      | 22.35452 | 89.41808 | -3.27724              | 3.27724 |

| Boundary Information (Standardized Z Scale) |                           |             |  |
|---------------------------------------------|---------------------------|-------------|--|
| Null Reference = 0                          |                           |             |  |
| _Stage_                                     | -----Boundary Values----- |             |  |
|                                             | ---Lower---               | ---Upper--- |  |
|                                             | Alpha                     | Alpha       |  |
| 1                                           | -4.04859                  | 4.04859     |  |
| 2                                           | -2.86278                  | 2.86278     |  |
| 3                                           | -2.33745                  | 2.33745     |  |
| 4                                           | -2.02429                  | 2.02429     |  |

In the SAMPLESIZE statement, the MODEL=TWOSAMPLESURVIVAL option specifies a log-rank test to compare two survival distributions for the treatment effect. The NULLHAZARD=0.03466 option specifies null hazard rates for the two groups under the null hypothesis. The ACCTIME= option specifies the accrual time  $T_a$ , and the ACCRUAL=EXP(POWER=-0.1) option specifies that the individual accrual is truncated exponential with a scaled power parameter  $\gamma_0 = -0.1$ . That is, the truncated exponential accrual has a power parameter  $\gamma = \gamma_0 / T_a = -0.1 / 20 = -0.005$  in the accrual time  $T_a$ . The LOSS=EXP(HAZARD=0.05) option specifies an exponential loss function with a hazard rate  $\tau = 0.05$ . Since the ACCNOBS= option is not included with the specified accrual time, the minimum and maximum sample sizes are derived from the specified accrual time. See the section “[Test for Two Survival Distributions with a Log-Rank Test](#)” on page 7059 for a detailed derivation of these required sample sizes.

The “Sample Size Summary” table in [Output 83.14.3](#) displays parameters for the sample size computation. Since the ACCNOBS= option is not included with the specified accrual time, the minimum and maximum sample sizes are derived.

**Output 83.14.3** Sample Size Summary

| Sample Size Summary          |                                   |
|------------------------------|-----------------------------------|
| Test                         | Two-Sample Survival               |
| Null Hazard Rate             | 0.03466                           |
| Hazard Rate (Group A)        | 0.01733                           |
| Hazard Rate (Group B)        | 0.03466                           |
| Hazard Ratio                 | 0.5                               |
| log(Hazard Ratio)            | -0.69315                          |
| Reference Hazards            | Alt Ref                           |
| Accrual                      | Truncated Exponential with Losses |
| Scaled Exponential Parameter | -0.1                              |
| Loss Hazard Rate             | 0.05                              |
| Accrual Time                 | 20                                |
| Min Accrual Sample Size      | 269                               |
| Max Accrual Sample Size      | 553                               |
| Max Number of Events         | 89.41808                          |

The “Numbers of Events (D)” table in [Output 83.14.4](#) displays the required number of events and corresponding information level at each stage.

**Output 83.14.4** Derived Sample Sizes

| Numbers of Events (D)<br>Two-Sample Log-Rank Test |       |             |
|---------------------------------------------------|-------|-------------|
| _Stage_                                           | D     | Information |
| 1                                                 | 22.35 | 5.5886      |
| 2                                                 | 44.71 | 11.1773     |
| 3                                                 | 67.06 | 16.7659     |
| 4                                                 | 89.42 | 22.3545     |

With the minimum and maximum sample sizes of 269 and 553, respectively, the ACCNOBS=360 option specifies an accrual sample size of 360 for the trial.

```
proc seqdesign altref=0.693147
 ;
 OBrienFleming: design nstages=4
 method=obf
 ;
 samplesize model=twosamplesurvival
 (nullhazard=0.03466
 accrual=exp(parm=-0.1)
 loss=exp(hazard=0.05)
 accnobs=360 acctime=20);
run;
```

With the specified accrual sample size and accrual time, the “Sample Size Summary” table in [Output 83.14.5](#) also displays the follow-up time and maximum sample size with the specified accrual time.

**Output 83.14.5** Sample Size Summary

| The SEQDESIGN Procedure         |                                   |
|---------------------------------|-----------------------------------|
| Design: OBrienFleming           |                                   |
| Sample Size Summary             |                                   |
| Test                            | Two-Sample Survival               |
| Null Hazard Rate                | 0.03466                           |
| Hazard Rate (Group A)           | 0.01733                           |
| Hazard Rate (Group B)           | 0.03466                           |
| Hazard Ratio                    | 0.5                               |
| log(Hazard Ratio)               | -0.69315                          |
| Reference Hazards               | Alt Ref                           |
| Accrual                         | Truncated Exponential with Losses |
| Scaled Exponential Parameter    | -0.1                              |
| Loss Hazard Rate                | 0.05                              |
| Accrual Time                    | 20                                |
| Follow-up Time                  | 9.100324                          |
| Total Time                      | 29.10032                          |
| Max Number of Events            | 89.41808                          |
| Max Sample Size                 | 360                               |
| Expected Sample Size (Null Ref) | 359.7605                          |
| Expected Sample Size (Alt Ref)  | 342.9205                          |

The “Number of Events (D) and Sample Sizes (N)” table in [Output 83.14.6](#) displays the required time at each stage, in both fractional and integer numbers. The derived times under the heading “Fractional Time” are not integers. These times are rounded up to integers under the heading “Ceiling Time.” The table also displays the numbers of events and sample sizes at each stage.



## Output 83.14.6 Number of Events and Sample Sizes

| Numbers of Events (D) and Sample Sizes (N)<br>Two-Sample Log-Rank Test |       |          |          |         |        |          |          |
|------------------------------------------------------------------------|-------|----------|----------|---------|--------|----------|----------|
| -----Fractional Time-----                                              |       |          |          |         |        |          |          |
| _Stage_                                                                | D     | D(Grp 1) | D(Grp 2) | Time    | N      | N(Grp 1) | N(Grp 2) |
| 1                                                                      | 22.35 | 7.74     | 14.62    | 11.4005 | 200.79 | 100.39   | 100.39   |
| 2                                                                      | 44.71 | 15.69    | 29.01    | 17.0454 | 304.52 | 152.26   | 152.26   |
| 3                                                                      | 67.06 | 23.81    | 43.25    | 21.9812 | 360.00 | 180.00   | 180.00   |
| 4                                                                      | 89.42 | 32.39    | 57.03    | 29.1003 | 360.00 | 180.00   | 180.00   |

| Numbers of Events (D) and Sample Sizes (N)<br>Two-Sample Log-Rank Test |             |                        |          |          |      |        |          |
|------------------------------------------------------------------------|-------------|------------------------|----------|----------|------|--------|----------|
| -Fractional<br>Time----                                                |             | -----Ceiling Time----- |          |          |      |        |          |
| _Stage_                                                                | Information | D                      | D(Grp 1) | D(Grp 2) | Time | N      | N(Grp 1) |
| 1                                                                      | 5.5886      | 24.46                  | 8.48     | 15.98    | 12   | 211.67 | 105.83   |
| 2                                                                      | 11.1773     | 48.97                  | 17.23    | 31.75    | 18   | 322.36 | 161.18   |
| 3                                                                      | 16.7659     | 67.14                  | 23.84    | 43.30    | 22   | 360.00 | 180.00   |
| 4                                                                      | 22.3545     | 91.46                  | 33.21    | 58.25    | 30   | 360.00 | 180.00   |

| Numbers of Events (D) and Sample Sizes (N)<br>Two-Sample Log-Rank Test |          |             |
|------------------------------------------------------------------------|----------|-------------|
| -----Ceiling Time-----                                                 |          |             |
| _Stage_                                                                | N(Grp 2) | Information |
| 1                                                                      | 105.83   | 6.1162      |
| 2                                                                      | 161.18   | 12.2436     |
| 3                                                                      | 180.00   | 16.7851     |
| 4                                                                      | 180.00   | 22.8649     |

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# Chapter 84

## The SEQTEST Procedure

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## Overview: SEQTEST Procedure

The purpose of the SEQTEST procedure is to perform interim analyses for clinical trials. Clinical trials are experiments on human beings to demonstrate the efficacy and safety of new drugs or treatments. A simple example is a trial to test the effectiveness of a new drug in humans by comparing the outcomes in a group of patients who receive the new drug with the outcomes in a comparable group of patients who receive a placebo.

A clinical trial is conducted according to a plan called a *protocol*. A protocol details the objectives of the trial, the data collection process, and the analyses of the data. The protocol contains information such as a null hypothesis and an alternative hypothesis, a test statistic, the probability  $\alpha$  of a Type I error (incorrectly rejecting the null hypothesis), the probability  $\beta$  of a Type II error (incorrectly accepting the null hypothesis), the sample size needed to attain a specified power (probability of correctly rejecting the null hypothesis) of  $1 - \beta$  at an alternative reference, and critical values that are associated with the test statistic for hypothesis testing.

In a fixed-sample trial, data about all individuals are first collected and then examined at the end of the study. Most major trials have data safety monitoring boards or data monitoring committees that periodically monitor safety and efficacy data during the trial and recommend that a trial be stopped for safety concerns such as an unacceptable toxicity level. In certain rare situations, the board or committee might even recommend that a trial be stopped for efficacy. In contrast to a fixed-sample trial, a group sequential trial provides for interim analyses before the formal completion of the trial while maintaining the specified overall Type I and Type II error probability levels.

A group sequential trial is most useful in situations where it is important to monitor the trial to prevent unnecessary exposure of patients to an unsafe new drug, or alternatively to a placebo treatment if the new drug shows significant improvement. If a group sequential trial stops early, then it usually requires fewer participants than a corresponding fixed-sample trial.

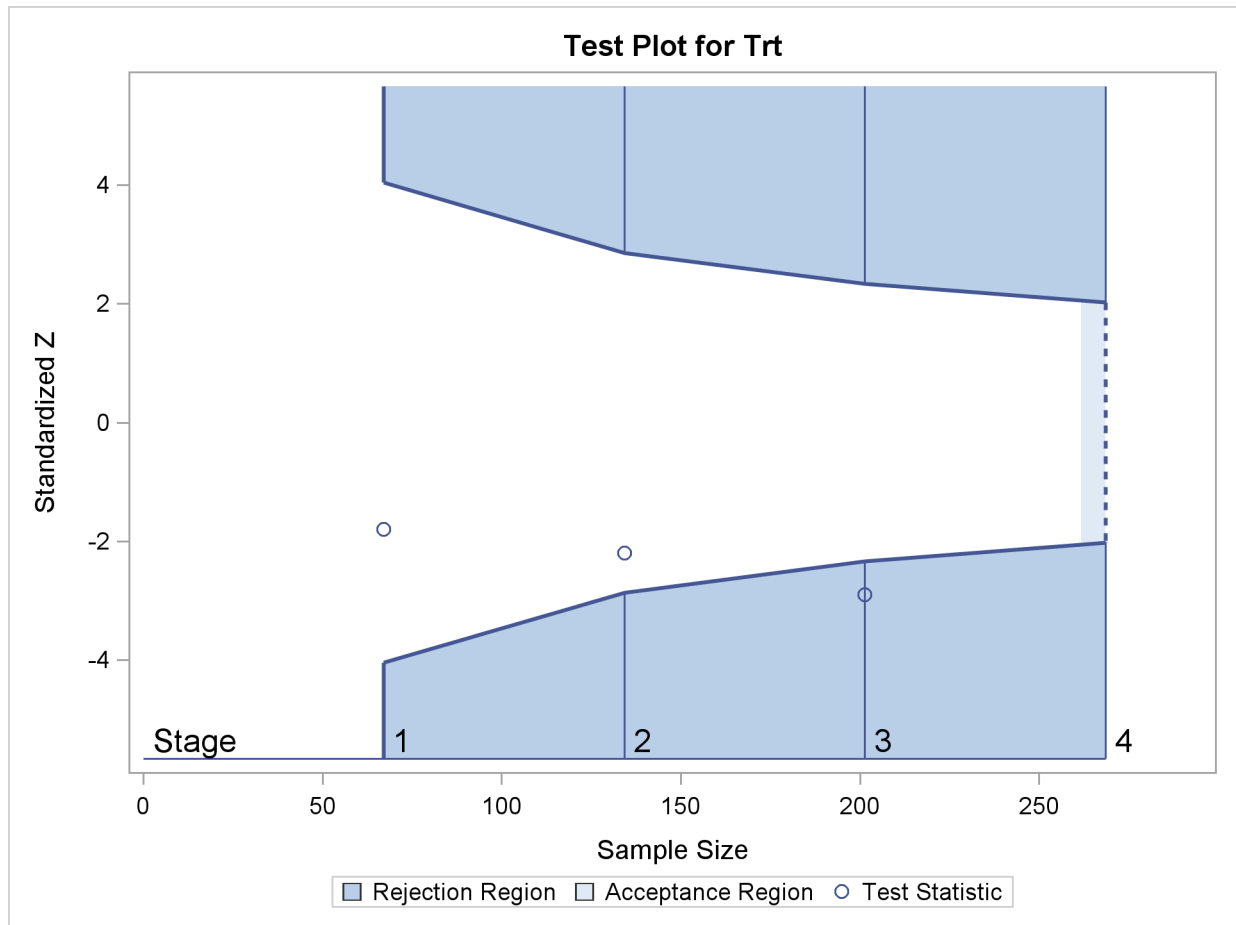
Thus, in most cases, if a group sequential trial stops early for safety of the new treatment, fewer patients will be exposed to the new treatment than in the fixed-sample trial. Also, if a trial stops early for efficacy of the new treatment, the new treatment will be available sooner than it would be in a fixed-sample trial. Furthermore, if a trial stops early, this can also save time and resources.

A group sequential design provides detailed specifications for a group sequential trial. In addition to the usual specification for a fixed-sample design, it provides the total number of stages (the number of interim stages plus a final stage) and a stopping criterion to reject, to accept, or to either reject or accept the null hypothesis at each interim stage. It also provides critical values and the sample size at each stage for the trial.

At each interim stage, the data collected at the current stage in addition to the data collected at previous stages are analyzed, and statistics such as a maximum likelihood test statistic and its associated standard error are computed. The test statistic is then compared with its corresponding critical values at the stage, and the trial is stopped or continued. If a trial continues to the final stage, the null hypothesis is either rejected or accepted. The critical values for each stage are chosen in such a way to maintain the overall  $\alpha$  level, the overall  $\beta$  level, or both the overall  $\alpha$  and  $\beta$  levels.

Figure 84.1 shows a two-sided symmetric group sequential trial that stops early to reject the null hypothesis that the parameter  $\text{Trt}$  is zero.

**Figure 84.1** Sequential Plot for Two-Sided Test



The trial has four stages, which are indicated by vertical lines with accompanying stage numbers. With early stopping to reject the null hypothesis, the lower rejection boundary is constructed by connecting the lower critical values (boundary values) for the stages. Similarly, the upper rejection boundary is constructed by connecting the upper critical values for the stages. The horizontal axis indicates the sample size for the group sequential trial, and the vertical axis indicates the boundary values and test statistics on the standardized  $Z$  scale.

At each interim stage, if the standardized  $Z$  test statistic falls into a rejection region (the darker shaded areas in Figure 84.1), the trial stops and the null hypothesis is rejected. Otherwise, the trial continues to the next stage. At the final stage (stage 4), the trial is rejected if  $Z$  falls into a rejection region. Otherwise, the trial is accepted. In Figure 84.1, the test statistic does not fall into the rejection regions for stages 1 and 2, and so the trial continues to stage 3. At stage 3, the test statistic falls into the rejection region, and the null hypothesis is rejected.



A group sequential trial usually involves six steps:

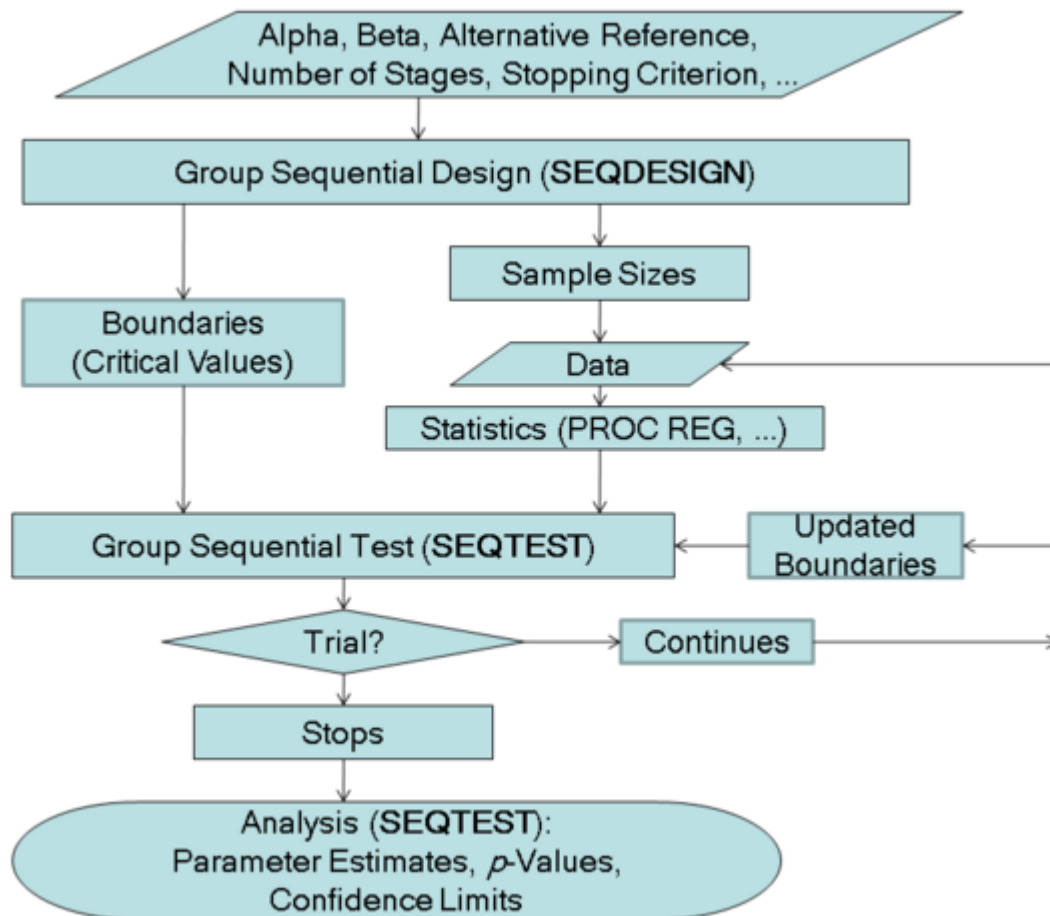
1. You specify the statistical details of the design, including the null and alternative hypotheses, a test statistic for the hypothesis test, the Type I and II error probabilities, a stopping criterion, the total number of stages, and the relative information level at each stage.
2. You compute the boundary values for the trial based on the specifications in Step 1. You also compute the sample size required at each stage for the specified hypothesis test.
3. At each stage, you collect additional data with the required sample sizes. The data available at each stage include the data collected at previous stages in addition to the data collected at the current stage.
4. At each stage, you analyze the available data with a procedure such as the REG procedure, and you compute the test statistic.
5. At each stage, you compare the test statistic with the corresponding boundary values. You stop the trial to reject or accept the hypothesis, or you continue the trial to the next stage. If you continue the trial to the final stage, you either accept or reject the hypothesis.
6. After the trial stops, you compute parameter estimates, confidence limits for the parameter, and a  $p$ -value for the hypothesis test.

You use the companion SEQDESIGN procedure at Step 2 to compute the boundary values and required sample sizes for the trial. You use the SEQTEST procedure at Step 5 to compare the test statistic with its boundary values. At stage 1, the boundary values are derived by using the boundary information tables created by the SEQDESIGN procedure. These boundary information tables are structured for input to the SEQTEST procedure. At each subsequent stage, the boundary values are derived by using the test information tables created by the SEQTEST procedure at the previous stage. These test information tables are also structured for input to the SEQTEST procedure. You also use the SEQTEST procedure at Step 6 to compute parameter estimates, confidence limits, and  $p$ -values after the trial stops.

Note that for some clinical trials, the information levels are derived from statistics based on individuals specified in the design plan and might not reach the target maximum information level. For example, if an estimate of the variance is used to compute the required sample size for a group sequential trial, the computed variance at each stage might not be the same as the estimated variance. Thus, instead of specifying the number of individuals in the protocol, the information level can be specified. You can then adjust the sample sizes with the updated variance estimates at interim stages to achieve the target maximum information level for the trial (Jennison and Turnbull 2000, p. 295).

The flowchart in [Figure 84.2](#) summarizes the steps in a typical group sequential trial and the relevant SAS procedures.

Figure 84.2 Group Sequential Trial



## Features of the SEQTEST Procedure

At each stage, the data are analyzed with a statistical procedure such as the REG procedure, and a test statistic and its associated information level are computed. The information level is the amount of information available about the unknown parameter. For a maximum likelihood statistic, the information level is the inverse of its variance.

At each stage, you use the SEQTEST procedure to compare the test statistic with its boundary values. At stage 1, the boundary values are derived by using the boundary information tables created by the SEQDESIGN procedure. At each subsequent stage, the boundary values are derived by using the test information tables created by the SEQTEST procedure at the previous stage.

If the observed information level does not match the corresponding information level in the BOUNDARY= data set, the SEQTEST procedure modifies the boundary values to adjust for new information levels at the current and subsequent stages. See the section “[Boundary Adjustments for Information Levels](#)” on page 7223 for a detailed description of these boundary adjustments.

Either you can specify the test statistic and its information level in the DATA= input data set, or you can specify the test statistic and its associated standard error in the PARMS= input data set. With the PARMS=

input data set, the information level for the test statistic is computed from its standard error. See the section “[Input Data Sets](#)” on page 7217 for a detailed description of these input data sets.

At the end of a trial, the parameter estimate is computed. The median unbiased estimate, confidence limits, and  $p$ -value depend on the specified sample space ordering. A sample space ordering specifies the ordering for test statistics that result in the stopping of a trial. That is, for all the statistics in the rejection region and in acceptance region, the SEQTEST procedure provides three different sample space orderings: the stagewise ordering uses counterclockwise ordering around the continuation region, the LR ordering uses the distance between the observed  $Z$  statistic  $z$  and its hypothetical value, and the MLE ordering uses the observed maximum likelihood estimate. See the section “[Available Sample Space Orderings in a Sequential Test](#)” on page 7230 for a detailed description of these orderings.

---

## Output from the SEQTEST Procedure

In addition to the adjusted boundary values and test results for the group sequential trial, the SEQTEST procedure also computes the following quantities:

- average sample numbers (as percentages of the corresponding fixed-sample sizes for nonsurvival data or fixed-sample numbers of events for survival data) under various hypothetical references, including the null and alternative references
- stopping probabilities at each stage under various hypothetical references to indicate how likely it is that the trial will stop at that stage
- conditional power given the most recently observed statistic under specified hypothetical references
- predictive power given the most recently observed statistic
- repeated confidence intervals for the parameter from the observed statistic at each stage
- parameter estimate,  $p$ -value for hypothesis testing, and median and confidence limits for the parameter at the conclusion of a sequential trial

---

## Getting Started: SEQTEST Procedure

The following example illustrates a clinical study that uses a two-sided O’Brien-Fleming design (O’Brien and Fleming 1979) to stop the trial early for ethical concerns about possible harm or for unexpectedly strong efficacy of the new drug.

Suppose that a pharmaceutical company is conducting a clinical trial to test the efficacy of a new cholesterol-lowering drug. The primary focus is low-density lipoprotein (LDL), the so-called bad cholesterol, which is a risk factor for coronary heart disease. LDL is measured in  $mg / dL$ , milligrams per deciliter of blood.

The trial consists of two groups of equally allocated patients with elevated LDL level: an experimental group given the new drug and a placebo control group. Suppose the changes in LDL level after the treatment for patients in the experimental and control groups are normally distributed with means  $\mu_e$  and  $\mu_c$ , respectively,

and have a common variance  $\sigma^2$ . Then the null hypothesis of no effect for the new drug is  $H_0 : \theta = \mu_e - \mu_c = 0$ . Also suppose that the alternative reference  $\theta = -10$  is the clinically meaningful difference that the trial should detect with a high probability (power), and that a good estimate of the standard deviation for the changes in LDL level is  $\hat{\sigma} = 20$ .

The following statements invoke the SEQDESIGN procedure and request a four-stage O'Brien-Fleming design for standardized normal test statistics:

```
ods graphics on;
proc seqdesign altref=-10.0;
 TwoSidedOBrienFleming: design nstages=4
 method=obf
 ;
 samplesize model=twosamplemean(stddev=20);
 ods output Boundary=Bnd_LDL;
run;
ods graphics off;
```

The ALTREF= option specifies the alternative reference, and the actual maximum information is derived in the SEQDESIGN procedure.

In the DESIGN statement, the label **TwoSidedOBrienFleming** identifies the design in the output tables. By default (or equivalently if you specify ALT=TWOSIDED and STOP=REJECT), the design has a two-sided alternative hypothesis with early stopping in the interim stages only to reject the null hypothesis. That is, at each interim stage, the trial will either be stopped to reject the null hypothesis or continue to the next stage.

The NSTAGES=4 option in the DESIGN statement specifies the total number of stages in the group sequential trial, including three interim stages and a final stage. In the SEQDESIGN procedure, the null hypothesis for the design is  $H_0 : \theta = 0$ . By default (or equivalently if you specify ALPHA=0.05 and BETA=0.10), the design has a Type I error probability  $\alpha = 0.05$ , and a Type II error probability  $\beta = 0.10$ , which corresponds to a power of  $1 - \beta = 0.90$  at the alternative reference  $H_1 : \theta = -10$ .

For a two-sided design with early stopping to reject the null hypothesis, there are two boundaries for the design: an upper  $\alpha$  (rejection) boundary that consists of upper rejection critical values and a lower  $\alpha$  boundary that consists of lower rejection critical values. Each boundary is a set of critical values, one from each stage. With the METHOD=OBF option in the DESIGN statement, the O'Brien-Fleming method is used for the two boundaries for the design; see [Figure 84.5](#).

The SAMPLESIZE statement with the MODEL=TWOSAMPLEMEAN option uses the derived maximum information to compute required sample sizes for a two-sample test for mean difference.

The ODS OUTPUT statement with the BOUNDARY=BND\_LDL option creates an output data set named BND\_LDL which contains the resulting boundary information. At each stage of the trial, data are collected and analyzed with a statistical procedure, and a test statistic and its corresponding information level are computed.

In this example, you can use the REG procedure to compute the maximum likelihood estimate  $\hat{\theta}$  for the drug effect and the corresponding standard error for  $\hat{\theta}$ . At stage 1, you can use the SEQTEST procedure to compare the test statistic with adjusted boundaries that are derived from the boundary information stored in the BOUND\_LDL data set. At each subsequent stage, you can use the SEQTEST procedure to compare the test statistic with adjusted boundaries that are derived from the boundary information stored in the test information table that was created by the SEQTEST procedure at the previous stage. The test information tables are structured for input to the SEQTEST procedure.

At each interim stage, the trial will either be stopped to reject the null hypothesis or continue to the next stage. At the final stage, the null hypothesis is either rejected or accepted.

By default (or equivalently if you specify `INFO=EQUAL`), the SEQDESIGN procedure derives boundary values with equally spaced information levels for all stages—that is, the same information increment between successive stages.

The “Design Information” table in Figure 84.3 displays design specifications and three derived statistics: the maximum information, the average sample number under the null hypothesis (Null Ref ASN), and the average sample number under the alternative hypothesis (Alt Ref ASN). Each statistic is expressed as a percentage of the identical statistic for the corresponding fixed-sample information. The average sample number is the expected sample size (for nonsurvival data) or expected number of events (for survival data). When you specify an alternative reference (in this case, `ALTREF=-10`), the actual maximum information 0.1074 is also computed. Note that for a symmetric two-sided design, the `ALTREF=-10` option implies a lower alternative reference of  $-10$  and an upper alternative reference of  $10$ .

**Figure 84.3** O'Brien-Fleming Design Information

| The SEQDESIGN Procedure                   |                 |
|-------------------------------------------|-----------------|
| Design: TwoSidedOBrienFleming             |                 |
| Design Information                        |                 |
| Statistic Distribution                    | Normal          |
| Boundary Scale                            | Standardized Z  |
| Alternative Hypothesis                    | Two-Sided       |
| Early Stop                                | Reject Null     |
| Method                                    | O'Brien-Fleming |
| Boundary Key                              | Both            |
| Alternative Reference                     | -10             |
| Number of Stages                          | 4               |
| Alpha                                     | 0.05            |
| Beta                                      | 0.1             |
| Power                                     | 0.9             |
| Max Information (Percent of Fixed Sample) | 102.2163        |
| Max Information                           | 0.107403        |
| Null Ref ASN (Percent of Fixed Sample)    | 101.5728        |
| Alt Ref ASN (Percent of Fixed Sample)     | 76.7397         |

The “Boundary Information” table in Figure 84.4 displays the information level, the lower and upper alternative references, and the lower and upper boundary values at each stage. By default (or equivalently if you specify `INFO=EQUAL`), the SEQDESIGN procedure uses equally spaced information levels for all stages.

Figure 84.4 Boundary Information

| Boundary Information (Standardized Z Scale) |                             |          |          |                       |         |
|---------------------------------------------|-----------------------------|----------|----------|-----------------------|---------|
| Null Reference = 0                          |                             |          |          |                       |         |
| _Stage_                                     | -----Information Level----- |          |          | -----Alternative----- |         |
|                                             | Proportion                  | Actual   | N        | Lower                 | Upper   |
| 1                                           | 0.2500                      | 0.026851 | 42.96116 | -1.63862              | 1.63862 |
| 2                                           | 0.5000                      | 0.053701 | 85.92233 | -2.31736              | 2.31736 |
| 3                                           | 0.7500                      | 0.080552 | 128.8835 | -2.83817              | 2.83817 |
| 4                                           | 1.0000                      | 0.107403 | 171.8447 | -3.27724              | 3.27724 |

| Boundary Information (Standardized Z Scale) |                          |            |  |
|---------------------------------------------|--------------------------|------------|--|
| Null Reference = 0                          |                          |            |  |
| _Stage_                                     | -----Boundary Values---- |            |  |
|                                             | ---Lower--               | ---Upper-- |  |
|                                             | Alpha                    | Alpha      |  |
| 1                                           | -4.04859                 | 4.04859    |  |
| 2                                           | -2.86278                 | 2.86278    |  |
| 3                                           | -2.33745                 | 2.33745    |  |
| 4                                           | -2.02429                 | 2.02429    |  |

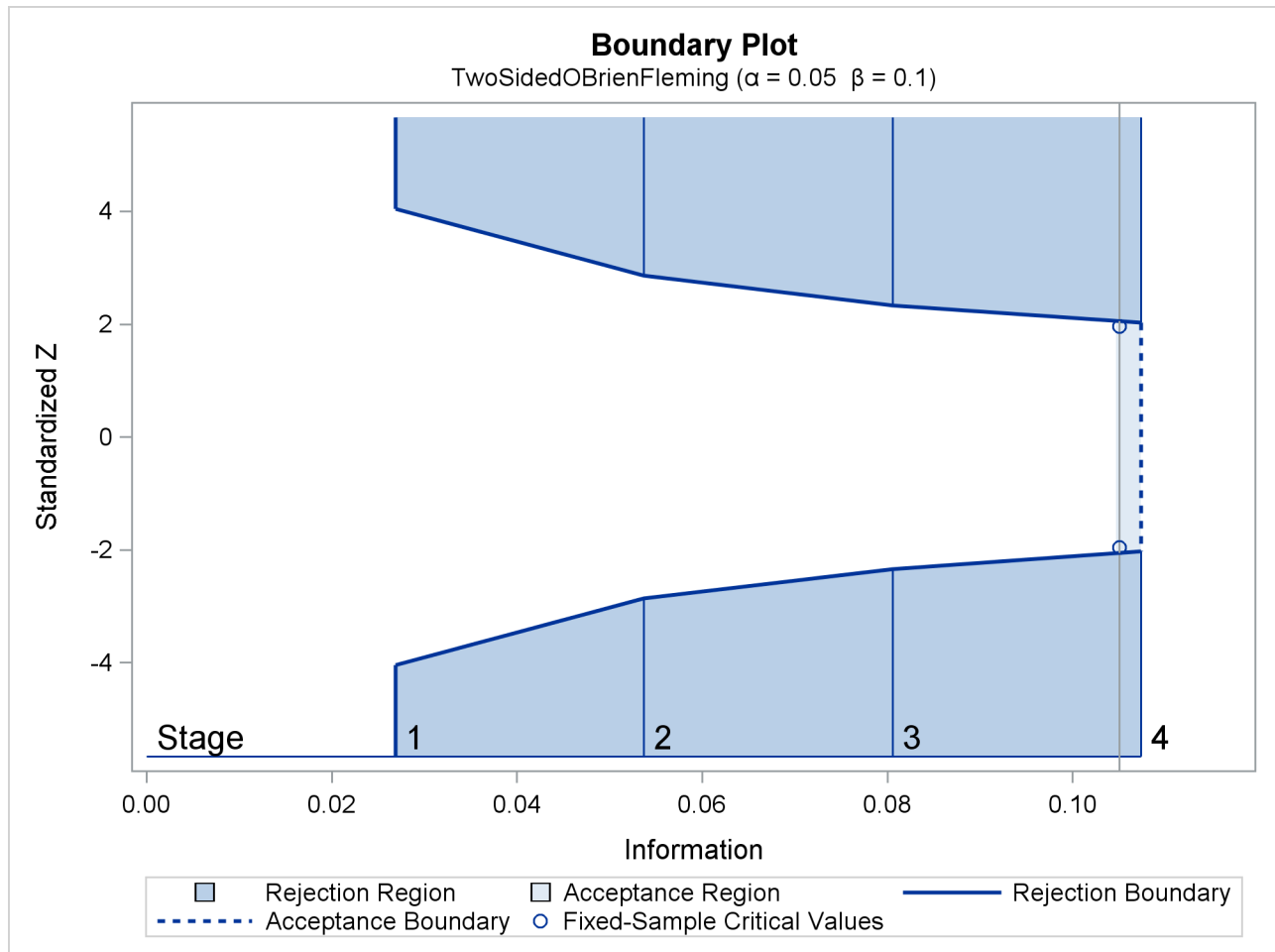
The information proportion is the proportion of maximum information available at each stage. By default (or equivalently if you specify BOUNDARYSCALE=STDZ), the alternative references and boundary values are displayed with the standardized  $Z$  statistic scale. The alternative reference in the standardized  $Z$  scale at stage  $k$  is given by  $\theta_1 \sqrt{I_k}$ , where  $\theta_1$  is the alternative reference and  $I_k$  is the information available at stage  $k$ ,  $k = 1, 2, 3, 4$ .

In this example, a standardized  $Z$  statistic is computed by standardizing the parameter estimate of the effect in LDL level. A lower  $Z$  test statistic indicates a beneficial effect. Consequently, at each interim stage, if the standardized  $Z$  test statistic is less than or equal to the corresponding lower  $\alpha$  boundary value, the hypothesis  $H_0 : \theta = 0$  is rejected for efficacy. If the test statistic is greater than or equal to the corresponding upper  $\alpha$  boundary value, the hypothesis  $H_0$  is rejected for harmful effect. Otherwise, the process continues to the next stage. At the final stage (stage 4), the hypothesis  $H_0$  is rejected for efficacy if the  $Z$  statistic is less than or equal to the corresponding lower  $\alpha$  boundary value  $-2.0243$ , and the hypothesis  $H_0$  is rejected for harmful effect if the  $Z$  statistic is greater than or equal to the corresponding upper  $\alpha$  boundary value  $2.0243$ . Otherwise, the hypothesis of no significant difference is accepted.

Note that in a typical trial, the actual information levels do not match the information levels specified in the design. Consequently, the SEQTEST procedure modifies the boundary values stored in the BND\_LDL data set to adjust for these new information levels.

If ODS Graphics is enabled, a detailed boundary plot with the rejection and acceptance regions is displayed, as shown in Figure 84.5.

**Figure 84.5** O'Brien-Fleming Boundary Plot



This boundary plot displays the boundary values in the “Boundary Information” table in Figure 84.4. The stages are indicated by vertical lines with accompanying stage numbers. The horizontal axis indicates the information levels for the stages. If a test statistic at an interim stage is in the rejection region (shaded area), the trial stops and the null hypothesis is rejected. If the statistic is not in any rejection region, the trial continues to the next stage. The plot also displays critical values for the corresponding fixed-sample design. The symbol “o” identifies the fixed-sample critical values of  $-1.96$  and  $1.96$ .

When you specify the SAMPLESIZE statement, the maximum information (either explicitly specified or derived in the SEQDESIGN procedure) is used to compute the required sample sizes for the study. The MODEL=TWOSAMPLEMEAN(STDDEV=20) option specifies the test for the difference between two normal means. See the section “Test for the Difference between Two Normal Means” in the chapter “The SEQDESIGN Procedure” for a detailed description of how these required sample sizes are calculated.

The “Sample Size Summary” table in Figure 84.6 displays the parameters for the sample size computation and the resulting maximum and expected sample sizes.

**Figure 84.6** Required Sample Size Summary

| Sample Size Summary             |                  |
|---------------------------------|------------------|
| Test                            | Two-Sample Means |
| Mean Difference                 | -10              |
| Standard Deviation              | 20               |
| Max Sample Size                 | 171.8447         |
| Expected Sample Size (Null Ref) | 170.7627         |
| Expected Sample Size (Alt Ref)  | 129.0137         |

With the derived maximum information 0.1074 and the specified MODEL=TWOSAMPLEMEAN (STDDEV=20) option in the SAMPLESIZE statement, the total sample size in each group is

$$N_a = N_b = 2\sigma^2 I_X = 2 \times 20^2 \times 0.1074 = 85.92$$

The “Sample Sizes (N)” table in Figure 84.7 displays the required sample sizes at each stage for the trial, in both fractional and integer numbers. The derived fractional sample sizes are displayed under the heading “Fractional N.” These sample sizes are rounded up to integers under the heading “Ceiling N.” By default (or equivalently if you specify WEIGHT=1 in the MODEL=TWOSAMPLEMEAN option), the sample sizes for the two groups are equal for the two-sample test.

**Figure 84.7** Required Sample Sizes

| Sample Sizes (N)                      |        |          |          |             |
|---------------------------------------|--------|----------|----------|-------------|
| Two-Sample Z Test for Mean Difference |        |          |          |             |
| -----Fractional N-----                |        |          |          |             |
| _Stage_                               | N      | N(Grp 1) | N(Grp 2) | Information |
| 1                                     | 42.96  | 21.48    | 21.48    | 0.0269      |
| 2                                     | 85.92  | 42.96    | 42.96    | 0.0537      |
| 3                                     | 128.88 | 64.44    | 64.44    | 0.0806      |
| 4                                     | 171.84 | 85.92    | 85.92    | 0.1074      |

| Sample Sizes (N)                      |     |          |          |             |
|---------------------------------------|-----|----------|----------|-------------|
| Two-Sample Z Test for Mean Difference |     |          |          |             |
| -----Ceiling N-----                   |     |          |          |             |
| _Stage_                               | N   | N(Grp 1) | N(Grp 2) | Information |
| 1                                     | 44  | 22       | 22       | 0.0275      |
| 2                                     | 86  | 43       | 43       | 0.0538      |
| 3                                     | 130 | 65       | 65       | 0.0812      |
| 4                                     | 172 | 86       | 86       | 0.1075      |

In practice, integer sample sizes are used in the trial, and the resulting information levels increase slightly. Thus, each of the two groups needs 22, 43, 65, and 86 patients for the four stages, respectively.



Suppose that 22 patients are available in each group at stage 1 and that their measurements for LDL are saved in the data set LDL\_1. Figure 84.8 lists the first 10 observations in the data set LDL\_1.

**Figure 84.8** Clinical Trial Data

| First 10 Obs in the Trial Data |     |        |
|--------------------------------|-----|--------|
| Obs                            | Trt | Ldl    |
| 1                              | 0   | 33.33  |
| 2                              | 1   | -14.89 |
| 3                              | 0   | 15.30  |
| 4                              | 1   | 4.71   |
| 5                              | 0   | 26.89  |
| 6                              | 1   | -48.74 |
| 7                              | 0   | -39.35 |
| 8                              | 1   | -8.13  |
| 9                              | 0   | -8.22  |
| 10                             | 1   | 12.35  |

The variable Trt is an indicator variable with value 1 for patients in the treatment group and value 0 for patients in the placebo control group. The variable Ldl is the LDL level of these patients.

The following statements use the REG procedure to estimate the mean treatment difference and its associated standard error at stage 1:

```
proc reg data=LDL_1;
 model Ldl=Trt;
 ods output ParameterEstimates=Parms_LDL1;
run;
```

The following statements create the data set for the mean treatment difference and its associated standard error as a PARMS= data set, which will subsequently serve as an input data set for PROC SEQTEST. Note that all of the variables are required for a PARMS= data set, as described in the section “PARMS= Data Set” on page 7219.

```
data Parms_LDL1;
 set Parms_LDL1;
 if Variable='Trt';
 Scale='MLE';
 Stage= 1;
 keep _Scale_ _Stage_ Variable Estimate StdErr;
run;

proc print data=Parms_LDL1;
 title 'Statistics Computed at Stage 1';
run;
```

Figure 84.9 displays the statistics computed at stage 1.

**Figure 84.9** Statistics Computed at Stage 1

| Statistics Computed at Stage 1 |          |          |         |         |         |
|--------------------------------|----------|----------|---------|---------|---------|
| Obs                            | Variable | Estimate | StdErr  | _Scale_ | _Stage_ |
| 1                              | Trt      | -2.52591 | 5.68572 | MLE     | 1       |

Since the sample sizes derived are based on the estimated variance at the designing phase, the information level that corresponds to the test statistic at stage 1 is estimated by

$$I_1 = \frac{1}{s_1^2} = \frac{1}{5.686^2} = 0.0309$$

where  $s_1$  is the standard error of the treatment estimate.

The following statements invoke the SEQTEST procedure to test for early stopping at stage 1:

```
ods graphics on;
proc seqtest Boundary=Bnd_LDL
 Parms(Testvar=Trt)=Parms_LDL1
 infoadj=prop
 ;
 ods output Test=Test_LDL1;
run;
ods graphics off;
```

The BOUNDARY= option specifies the input data set that provides the boundary information for the trial at stage 1, which was generated in the SEQDESIGN procedure. The PARMS=PARMS\_LDL1 option specifies the input data set PARMS\_LDL1 that contains the test statistic and its associated standard error at stage 1, and the TESTVAR=TRT option identifies the test variable TRT in the data set.

By default (or equivalently if you specify BOUNDARYKEY=ALPHA), the maximum information and the Type I error level are maintained. Furthermore, with the INFOADJ=PROP option (which is the default), the information levels at future interim stages (2 and 3) are adjusted proportionally from the levels provided in the BOUNDARY= data set.

The ODS OUTPUT statement with the TEST=TEST\_LDL1 option creates an output data set named TEST\_LDL1 which contains the updated boundary information for the test at stage 1, and the boundary information that is needed for the group sequential test at the next stage. See the section “[Boundary Adjustments for Information Levels](#)” on page 7223 for details.

The “Design Information” table in [Figure 84.10](#) displays design specifications. By default (or equivalently if you specify BOUNDARYKEY=ALPHA), the boundary values are adjusted for the updated information levels to maintain the Type I  $\alpha$  level, and the maximum information remains the same as in the BOUNDARY= data set. But the derived Type II error probability  $\beta$  and power  $1 - \beta$  are slightly different with new information levels. With the updated power  $1 - \beta$ , the corresponding fixed-sample design is also updated.

**Figure 84.10** Design Information

| The SEQTEST Procedure                     |                 |
|-------------------------------------------|-----------------|
| Design Information                        |                 |
| BOUNDARY Data Set                         | WORK.BND_LDL    |
| Data Set                                  | WORK.PARMS_LDL1 |
| Statistic Distribution                    | Normal          |
| Boundary Scale                            | Standardized Z  |
| Alternative Hypothesis                    | Two-Sided       |
| Early Stop                                | Reject Null     |
| Number of Stages                          | 4               |
| Alpha                                     | 0.05            |
| Beta                                      | 0.10074         |
| Power                                     | 0.89926         |
| Max Information (Percent of Fixed Sample) | 102.4815        |
| Max Information                           | 0.10740291      |
| Null Ref ASN (Percent of Fixed Sample)    | 101.7765        |
| Alt Ref ASN (Percent of Fixed Sample)     | 75.4928         |

The “Test Information” table in Figure 84.11 displays the boundary values for the test statistic. By default (or equivalently if you specify BOUNDARYSCALE=STDZ), these statistics are displayed with the standardized Z scale. With the INFOADJ=PROP option (which is the default), information levels at future interim stages are derived proportionally from the corresponding levels provided in the BOUNDARY= data set.

**Figure 84.11** Sequential Tests

| Test Information (Standardized Z Scale) |                       |          |                       |                 |                         |             |
|-----------------------------------------|-----------------------|----------|-----------------------|-----------------|-------------------------|-------------|
| Null Reference = 0                      |                       |          |                       |                 |                         |             |
| _Stage_                                 | --Information Level-- |          | -----Alternative----- |                 | ----Boundary Values---- |             |
|                                         | Proportion            | Actual   | -----Reference-----   | -----Upper----- | ---Lower---             | ---Upper--- |
|                                         |                       |          | Lower                 | Upper           | Alpha                   | Alpha       |
| 1                                       | 0.2880                | 0.030934 | -1.75879              | 1.75879         | -3.39532                | 3.39532     |
| 2                                       | 0.5253                | 0.056423 | -2.37536              | 2.37536         | -2.77374                | 2.77374     |
| 3                                       | 0.7627                | 0.081913 | -2.86205              | 2.86205         | -2.32412                | 2.32412     |
| 4                                       | 1.0000                | 0.107403 | -3.27724              | 3.27724         | -2.03147                | 2.03147     |

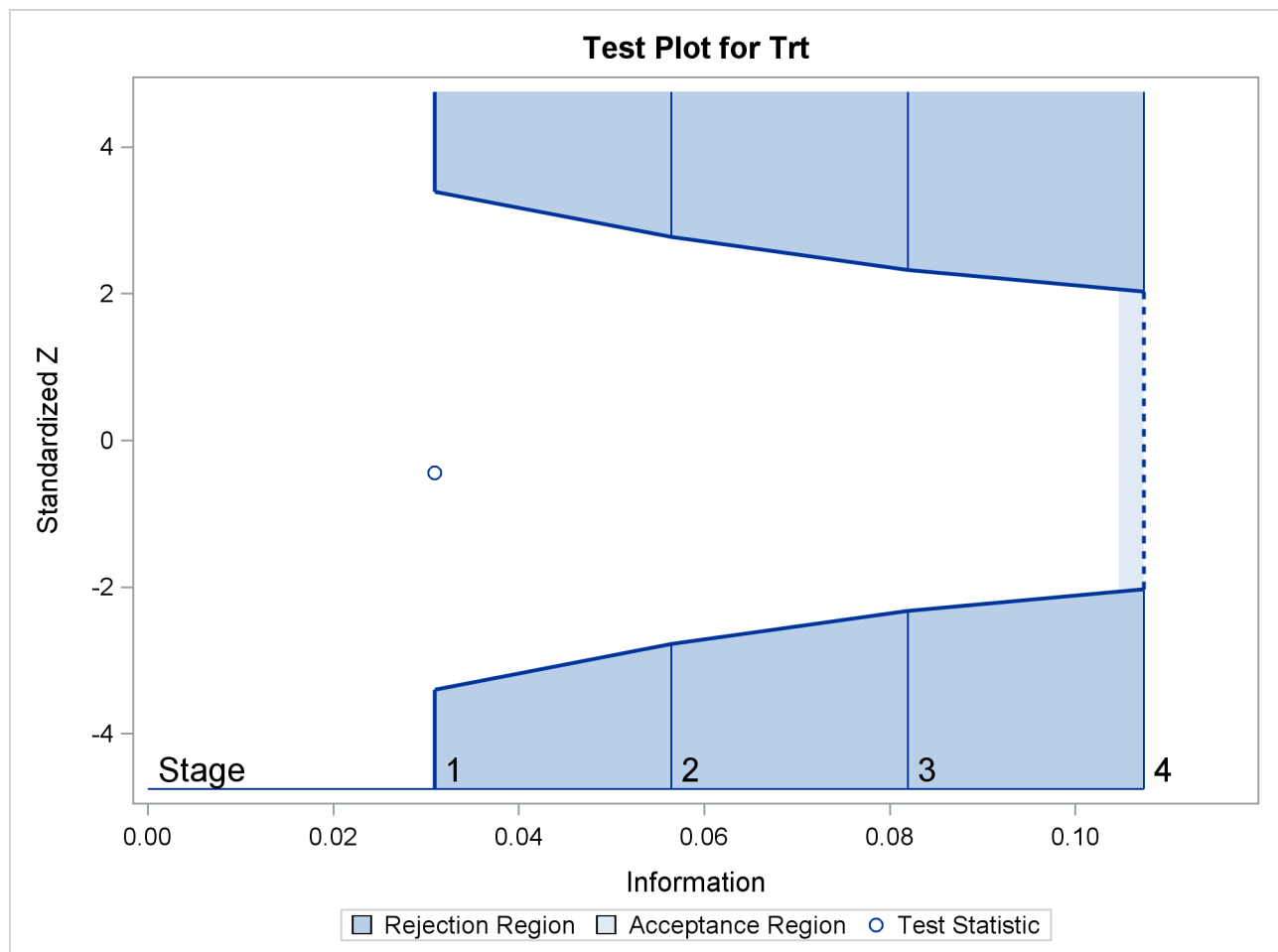
| Test Information (Standardized Z Scale) |                |               |
|-----------------------------------------|----------------|---------------|
| Null Reference = 0                      |                |               |
| _Stage_                                 | -----Test----- |               |
|                                         | Estimate       | -----Trt----- |
|                                         |                | Action        |
| 1                                       | -0.44426       | Continue      |
| 2                                       | .              |               |
| 3                                       | .              |               |
| 4                                       | .              |               |

At stage 1, the standardized  $Z$  statistic  $-0.44426$  is between the lower and upper  $\alpha$  boundary values, and so the trial continues to the next stage. With the observed information level at stage 1,  $I_1 = 0.0309$  (which is not substantially different from the target information level at stage 1), the trial continues to the next stage without adjustment of the sample size according to the study plan.

If an observed information level is different from its target level at an interim stage, the sample sizes at future stages can be adjusted to achieve the target maximum information level according to the study plan. That is, a study plan might modify the final sample size to achieve the target maximum information level if the observed information level is different from its target level by a specified amount at the interim stage. For example, if the variance estimate is used to compute the required sample size of a two-sample  $Z$  test for mean difference, the study plan might use the current variance estimate to update the required sample size for the trial (Jennison and Turnbull 2000, p. 295). See the section “Applicable Two-Sample Tests and Sample Size Computation” in “The SEQDESIGN Procedure” for a description of how to compute the sample size from the variance estimate.

If ODS Graphics is enabled, a detailed test plot with the rejection and acceptance regions is displayed, as shown in Figure 84.12. This plot displays the boundary values in the “Test Information” table in Figure 84.11. The stages are indicated by vertical lines with accompanying stage numbers. The horizontal axis indicates the information levels for the stages. As expected, the test statistic is in the continuation region between the lower and upper  $\alpha$  boundaries.

**Figure 84.12** Sequential Test Plot



The following statements use the REG procedure with the data available at the first two stages to estimate the mean treatment difference and its associated standard error at stage 2:

```
proc reg data=LDL_2;
 model Ldl=Trt;
 ods output ParameterEstimates=Parms_LDL2;
run;
```

The following statements create and display (in Figure 84.13) the data set for the mean treatment difference and its associated standard error:

```
data Parms_LDL2;
 set Parms_LDL2;
 if Variable='Trt';
 Scale='MLE';
 Stage= 2;
 keep _Scale_ _Stage_ Variable Estimate StdErr;
run;

proc print data=Parms_LDL2;
 title 'Statistics Computed at Stage 2';
run;
```

**Figure 84.13** Statistics Computed at Stage 2

| Statistics Computed at Stage 2 |          |          |         |         |         |
|--------------------------------|----------|----------|---------|---------|---------|
| Obs                            | Variable | Estimate | StdErr  | _Scale_ | _Stage_ |
| 1                              | Trt      | -8.37628 | 4.24405 | MLE     | 2       |

Using the standard error for the treatment estimate available at stage 2, the information level that corresponds to the test statistic at stage 2 is estimated by

$$I_2 = \frac{1}{s_2^2} = \frac{1}{4.244^2} = 0.0555$$

where  $s_2$  is the standard error of the treatment estimate at stage 2.

The following statements invoke the SEQTEST procedure to test for early stopping at stage 2:

```
proc seqtest Boundary=Test_LDL1
 Parms (Testvar=Trt) =Parms_LDL2
 infoadj=prop
 ;
 ods output Test=Test_LDL2;
run;
```

The BOUNDARY= option specifies the input data set that provides the boundary information for the trial at stage 2, which was generated by the SEQTEST procedure at the previous stage. The PARMS= option specifies the input data set that contains the test statistic and its associated standard error at stage 2, and the TESTVAR= option identifies the test variable in the data set.

The ODS OUTPUT statement with the TEST=TEST\_LDL2 option creates an output data set named TEST\_LDL2 which contains the updated boundary information for the test at stage 2. The data set also provides the boundary information that is needed for the group sequential test at the next stage.

The “Test Information” table in Figure 84.14 displays the boundary values for the test statistic with the default standardized Z scale

**Figure 84.14** Sequential Tests

| The SEQTEST Procedure                   |                       |          |                       |                     |                         |             |
|-----------------------------------------|-----------------------|----------|-----------------------|---------------------|-------------------------|-------------|
| Test Information (Standardized Z Scale) |                       |          |                       |                     |                         |             |
| Null Reference = 0                      |                       |          |                       |                     |                         |             |
| _Stage_                                 | --Information Level-- |          | -----Alternative----- |                     | ----Boundary Values---- |             |
|                                         | Proportion            | Actual   | -----Reference-----   | -----Reference----- | ---Lower---             | ---Upper--- |
|                                         |                       |          | Lower                 | Upper               | Alpha                   | Alpha       |
| 1                                       | 0.2880                | 0.030934 | -1.75879              | 1.75879             | -3.39532                | 3.39532     |
| 2                                       | 0.5169                | 0.055519 | -2.35624              | 2.35624             | -2.78456                | 2.78456     |
| 3                                       | 0.7585                | 0.081461 | -2.85413              | 2.85413             | -2.32908                | 2.32908     |
| 4                                       | 1.0000                | 0.107403 | -3.27724              | 3.27724             | -2.03097                | 2.03097     |

| Test Information (Standardized Z Scale) |                |               |          |
|-----------------------------------------|----------------|---------------|----------|
| Null Reference = 0                      |                |               |          |
| _Stage_                                 | -----Test----- |               | Action   |
|                                         | Estimate       | -----Trt----- |          |
| 1                                       | -0.44426       |               | Continue |
| 2                                       | -1.97365       |               | Continue |
| 3                                       | .              |               |          |
| 4                                       | .              |               |          |

At stage 2, the standardized test statistic,  $z = -8.37628/4.24405 = -1.97365$ , is between its corresponding lower and upper  $\alpha$  boundary values. Therefore, the trial continues to the next stage.

The following statements use the REG procedure with the data available at the first three stages to estimate the mean treatment difference and its associated standard error at stage 3:

```
proc reg data=LDL_3;
 model Ldl=Trt;
 ods output ParameterEstimates=Parms_LDL3;
run;
```

The following statements create and display (in Figure 84.15) the data set for the mean treatment difference and its associated standard error:

```
data Parms_LDL3;
 set Parms_LDL3;
 if Variable='Trt';
 Scale='MLE';
 Stage= 3;
 keep _Scale_ _Stage_ Variable Estimate StdErr;
run;

proc print data=Parms_LDL3;
 title 'Statistics Computed at Stage 3';
run;
```

**Figure 84.15** Statistics Computed at Stage 3

| Statistics Computed at Stage 3 |          |          |         |         |         |
|--------------------------------|----------|----------|---------|---------|---------|
| Obs                            | Variable | Estimate | StdErr  | _Scale_ | _Stage_ |
| 1                              | Trt      | -9.21369 | 3.42149 | MLE     | 3       |

The following statements invoke the SEQTEST procedure to test for early stopping at stage 3:

```
ods graphics on;
proc seqtest Boundary=Test_LDL2
 Parms(Testvar=Trt)=Parms_LDL3
 infoadj=prop
 ;
 ods output Test=Test_LDL3;
run;
ods graphics off;
```

The BOUNDARY= option specifies the input data set that provides the boundary information for the trial at stage 3, which was generated by the SEQTEST procedure at the previous stage. The PARMS= option specifies the input data set that contains the test statistic and its associated standard error at stage 3, and the TESTVAR= option identifies the test variable in the data set.

The ODS OUTPUT statement with the TEST=TEST\_LDL3 option creates an output data set named TEST\_LDL3 which contains the updated boundary information for the test at stage 3. The data set also provides the boundary information that is needed for the group sequential test at the next stage.

The “Test Information” table in Figure 84.16 displays the boundary values for the test statistic with the default standardized Z scale.

Figure 84.16 Sequential Tests

| The SEQTEST Procedure                   |                       |          |                       |                     |                         |            |
|-----------------------------------------|-----------------------|----------|-----------------------|---------------------|-------------------------|------------|
| Test Information (Standardized Z Scale) |                       |          |                       |                     |                         |            |
| Null Reference = 0                      |                       |          |                       |                     |                         |            |
| _Stage_                                 | --Information Level-- |          | -----Alternative----- |                     | ----Boundary Values---- |            |
|                                         | Proportion            | Actual   | -----Reference-----   | -----Reference----- | ---Lower--              | ---Upper-- |
|                                         |                       |          | Lower                 | Upper               | Alpha                   | Alpha      |
| 1                                       | 0.2880                | 0.030934 | -1.75879              | 1.75879             | -3.39532                | 3.39532    |
| 2                                       | 0.5169                | 0.055519 | -2.35624              | 2.35624             | -2.78456                | 2.78456    |
| 3                                       | 0.7953                | 0.085422 | -2.92271              | 2.92271             | -2.25480                | 2.25480    |
| 4                                       | 1.0000                | 0.107403 | -3.27724              | 3.27724             | -2.04573                | 2.04573    |

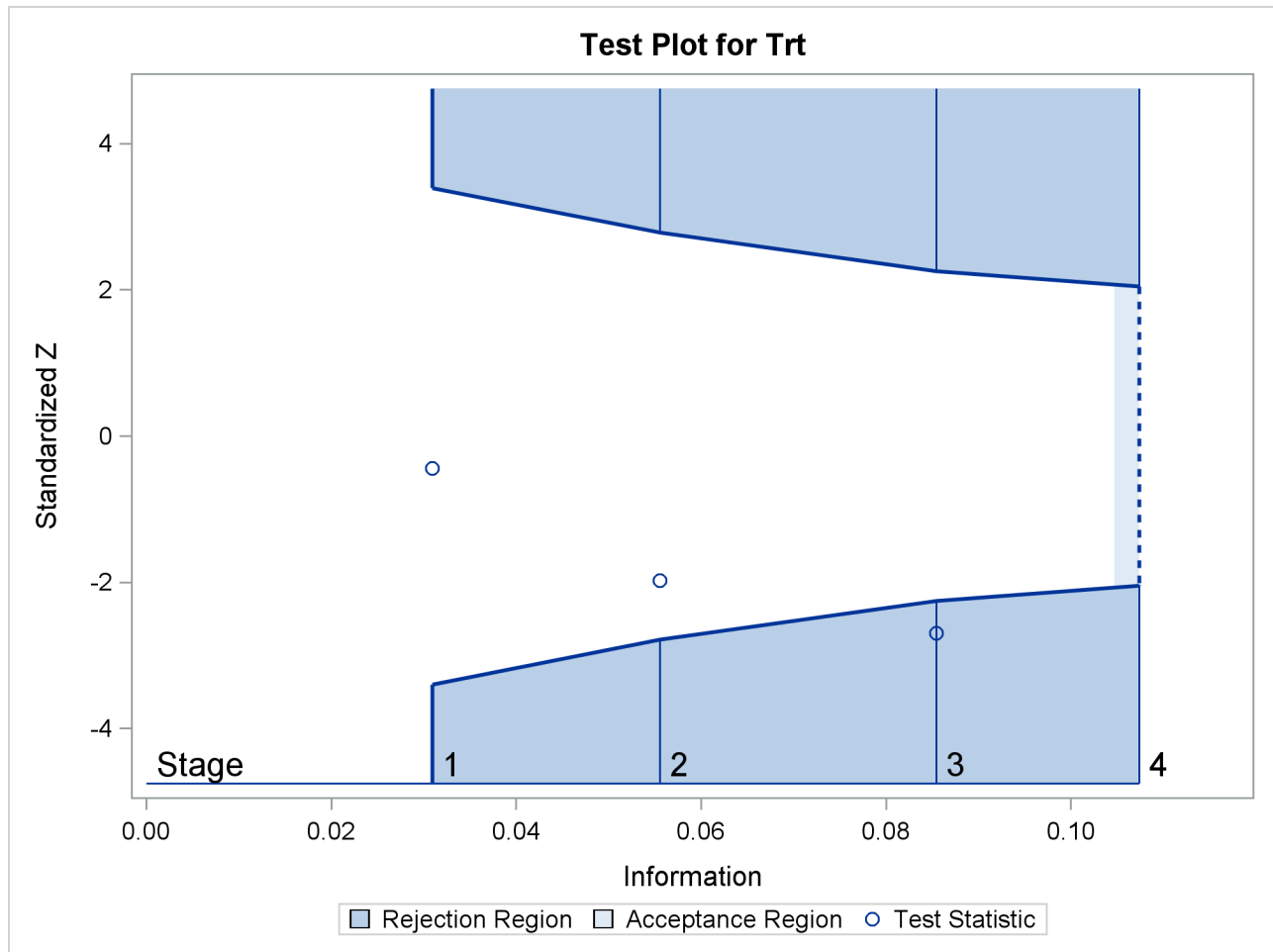
| Test Information (Standardized Z Scale) |                |             |
|-----------------------------------------|----------------|-------------|
| Null Reference = 0                      |                |             |
| _Stage_                                 | -----Test----- |             |
|                                         | Estimate       | Action      |
| 1                                       | -0.44426       | Continue    |
| 2                                       | -1.97365       | Continue    |
| 3                                       | -2.69289       | Reject Null |
| 4                                       | .              |             |

The sequential test stops at stage 3 to reject the null hypothesis for the lower alternative because the test statistic  $-2.69289$  is less than the corresponding upper  $\alpha$  boundary  $-2.25480$ . That is, the test demonstrates significant beneficial effect for the new drug.

The “Test Plot” displays boundary values for the design and the test statistic at the first three stages, as shown in Figure 84.17. It shows that the test statistic is in the “Rejection Region” below the lower  $\alpha$  boundary at stage 3.



Figure 84.17 Sequential Test Plot



When a trial stops, the “Parameter Estimates” table in Figure 84.18 displays the stopping stage, parameter estimate, unbiased median estimate, confidence limits, and  $p$ -value under the null hypothesis  $H_0 : \theta = 0$ . As expected, the  $p$ -value 0.0108 is significant at the two-sided  $\alpha$  level,  $\alpha = 0.05$ , and the confidence interval does not contain the value zero. The  $p$ -value, unbiased median estimate, and confidence limits depend on the ordering of the sample space  $(k, z)$ , where  $k$  is the stage number and  $z$  is the standardized  $Z$  statistic. See the section “Analysis after a Sequential Test” on page 7229 for a detailed description of these statistics.

Figure 84.18 Parameter Estimates

| Parameter Estimates<br>Stagewise Ordering |                       |           |                          |                 |
|-------------------------------------------|-----------------------|-----------|--------------------------|-----------------|
| Parameter                                 | Stopping Stage        | MLE       | p-Value for<br>H0:Parm=0 | Median Estimate |
| Trt                                       | 3                     | -9.213692 | 0.0108                   | -9.022891       |
| Parameter Estimates<br>Stagewise Ordering |                       |           |                          |                 |
| Parameter                                 | 95% Confidence Limits |           |                          |                 |
| Trt                                       | -15.79845    -2.13138 |           |                          |                 |

## Syntax: SEQTEST Procedure

The following statement is available in the SEQTEST procedure:

```
PROC SEQTEST < options > ;
```

## PROC SEQTEST Statement

The PROC SEQTEST statement invokes the SEQTEST procedure. Table 84.1 summarizes the options available in the PROC SEQTEST statement.

**Table 84.1** Summary of PROC SEQTEST Options

| Option                 | Description                                                                                                                         |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------|
| <b>Input Data Sets</b> |                                                                                                                                     |
| BOUNDARY=              | Specifies the data set for boundary information                                                                                     |
| DATA=                  | Specifies the data set for parameter estimates and information levels                                                               |
| PARMS=                 | Specifies the data set for parameter estimates and standard errors                                                                  |
| <b>Boundaries</b>      |                                                                                                                                     |
| BETABOUNDARY=          | Specifies whether the $\beta$ boundary is used in the computation of the Type I error level $\alpha$                                |
| BETAOVERLAP=           | Checks for overlapping of the lower and upper $\beta$ boundaries at the current and subsequent interim stages in a two-sided design |
| BOUNDARYKEY=           | Specifies the boundary key to maintain Type I and II error probability levels                                                       |
| BOUNDARYSCALE=         | Specifies the boundary scale                                                                                                        |
| ERRSPENDADJ=           | Specifies error spending methods for boundary adjustments                                                                           |
| ERRSPENDMIN=           | Specifies minimum error spending values for the boundaries                                                                          |
| INFOADJ=               | Specifies whether information levels at future interim stages should be adjusted                                                    |

Table 84.1 continued

| Option                                          | Description                                                                                          |
|-------------------------------------------------|------------------------------------------------------------------------------------------------------|
| NSTAGES=                                        | Specifies the number of stages                                                                       |
| <b>Test Statistics</b>                          |                                                                                                      |
| DATA( TESTVAR= )                                | Specifies the test variable in the DATA= data set                                                    |
| PARMS( TESTVAR= )                               | Specifies the test variable in the PARMS= data set                                                   |
| <b><i>p</i>-Values and Confidence Intervals</b> |                                                                                                      |
| CIALPHA=                                        | Specifies the significance levels for the confidence interval                                        |
| CITYPE=                                         | Specifies the types of confidence interval                                                           |
| ORDER=                                          | Specifies the ordering of the sample space used to derive the <i>p</i> -values and confidence limits |
| <b>Table Output</b>                             |                                                                                                      |
| CONDPOWER                                       | Displays conditional powers                                                                          |
| ERRSPEND                                        | Displays the cumulative error spending at each stage                                                 |
| PREDPOWER                                       | Displays the predictive powers                                                                       |
| PSS                                             | Displays the powers and expected sample sizes                                                        |
| RCI                                             | Displays the repeated confidence intervals                                                           |
| STOPPROB                                        | Displays the expected cumulative stopping probabilities                                              |
| <b>Graphics Output</b>                          |                                                                                                      |
| PLOTS=ASN                                       | Displays the expected sample numbers plot                                                            |
| PLOTS=CONDPOWER                                 | Displays the conditional powers plot                                                                 |
| PLOTS=ERRSPEND                                  | Displays the error spending plot                                                                     |
| PLOTS=POWER                                     | Displays the powers plot                                                                             |
| PLOTS=RCI                                       | Displays the repeated confidence intervals plot                                                      |
| PLOTS=TEST                                      | Displays the boundary plot with test statistics                                                      |

The BOUNDARY= option provides the information for the design and is required in the PROC SEQTEST statement. By default, the SEQTEST procedure displays tables of design information and test information. If ODS Graphics is enabled, the procedure also displays a sequential test plot.

The following options can be used in the PROC SEQTEST statement. They are listed in alphabetical order.

#### **BETABOUNDARY=BINDING | NONBINDING**

specifies whether the  $\beta$  boundary is used in the computation of the Type I error level  $\alpha$ . The BETABOUNDARY=BINDING option computes the Type I error probability with the  $\beta$  (acceptance) boundary, and the BETABOUNDARY=NONBINDING suboption computes the Type I error probability without the  $\beta$  boundary (Zhu, Ni, and Yao 2011, pp. 132–133). For a detailed description of nonbinding acceptance boundary, see the section “Acceptance ( $\beta$ ) Boundary” in Chapter 83, “The SEQDESIGN Procedure.” The default is BETABOUNDARY=BINDING.

#### **BETAOVERLAP=ADJUST | NOADJUST**

##### **OVERLAP=ADJUST | NOADJUST**

specifies whether to check for overlapping of the lower and upper  $\beta$  boundaries for the two corresponding one-sided tests at the current and subsequent interim stages. This option applies to two-sided designs with early stopping to accept  $H_0$ , or to either accept or reject  $H_0$ . This type of over-

lapping might result from a small  $\beta$  spending at an interim stage. When you specify BETAOVERLAP=ADJUST, the procedure checks for this type of overlapping at the current and subsequent interim stages. If such overlapping is found, the  $\beta$  boundaries for the two-sided design at that stage are set to missing, and the  $\beta$  spending values at subsequent stages are adjusted, as described in the section “Boundary Adjustments for Overlapping Lower and Upper  $\beta$  Boundaries” on page 7225.

You can specify BETAOVERLAP=NOADJUST to request that no adjustment be made. The default is BETAOVERLAP=ADJUST.

#### **BOUNDARY=SAS-data-set**

names the required SAS data set that contains the design boundary information. At stage 1, the data set is usually created from the “Boundary Information” table created by the SEQDESIGN procedure. At each subsequent stage, the data set is usually created from the “Test Information” table created by the SEQTEST procedure at the previous stage. The data set includes the variables `_Scale_` for the boundary scale, `_Stop_` for the stopping criterion, and `_ALT_` for the type of alternative hypothesis. It also includes `_Stage_` for the stage number, `Info_Prop` for the information proportion, and a set of the boundary variables from `Bound_LA`, `Bound_LB`, `Bound_UB`, and `Bound_UA` for boundary values at each stage.

The data set might also include `_Info_` for the actual information level, `NObs` for the number of observation, and `Events` for the number of events required at each stage.

#### **BOUNDARYKEY=ALPHA | BETA | BOTH**

specifies the boundary key to be maintained in the boundary adjustments. The BOUNDARYKEY=ALPHA option maintains the Type I  $\alpha$  level and derives the Type II error probability, and the BOUNDARYKEY=BETA option maintains the Type II  $\beta$  level and derives the Type I error probability. The BOUNDARYKEY=BOTH option maintains both  $\alpha$  and  $\beta$  levels simultaneously by deriving a new maximum information. The default is BOUNDARYKEY=ALPHA.

#### **BOUNDARYSCALE=MLE | SCORE | STDZ | PVALUE**

##### **BSCALE=MLE | SCORE | STDZ | PVALUE**

specifies the boundary scale to be displayed in the output boundary table and plot. The BOUNDARYSCALE=MLE, BOUNDARYSCALE=SCORE, BOUNDARYSCALE=STDZ, and BOUNDARYSCALE=PVALUE options correspond to the boundary with the maximum likelihood estimator scale, score statistic scale, standardized normal Z scale, and  $p$ -value scale, respectively. The default is BOUNDARYSCALE=STDZ.

With the BOUNDARYSCALE=MLE or BOUNDARYSCALE=SCORE option, either the MAXINFO= option must be specified or the `_Info_` variable must be in the BOUNDARY= data set to provide the necessary information level at each stage to derive the boundary values. Usually, these values are obtained from analysis output in SAS procedures.

Note that for a two-sided design, the  $p$ -value scale displays the one-sided fixed-sample  $p$ -value under the null hypothesis with a lower alternative hypothesis.

#### **CIALPHA= $\alpha$ (< < LOWER= $\alpha_l$ > < UPPER= $\alpha_u$ > )>**

specifies the significance levels for the confidence interval, where  $0 < \alpha < 1$ ,  $0 < \alpha_l < 0.5$ , and  $0 < \alpha_u < 0.5$ . The default is CIALPHA=0.05.

For a lower confidence interval (CITYPE=LOWER), the CIALPHA= $\alpha$  option produces a  $(1 - \alpha)$  lower confidence interval. For an upper confidence interval (CITYPE=UPPER), the CIALPHA= $\alpha$

option produces a  $(1 - \alpha)$  upper confidence interval. The LOWER= and UPPER= suboptions are applicable only for a two-sided confidence interval (CITYPE=TWOSIDED). The LOWER= suboption specifies the lower significance level  $\alpha_l$  and the upper significance level  $\alpha_u = 1 - \alpha_l$ . The UPPER= suboption specifies the upper significance level  $\alpha_u$  and the lower significance level  $\alpha_l = 1 - \alpha_u$ . If both LOWER= and UPPER= suboptions are not specified,  $\alpha_l = \alpha_u = \alpha/2$ . The significance levels  $\alpha_l$  and  $\alpha_u$  are then used for the  $(1 - \alpha_l)$  lower confidence limit and  $(1 - \alpha_u)$  upper confidence limit, respectively.

**CITYPE=LOWER | UPPER | TWOSIDED**

specifies the type of confidence interval. The CITYPE=LOWER, CITYPE=UPPER, and CITYPE=TWOSIDED options correspond to the lower confidence interval, upper confidence interval, and two-sided confidence interval, respectively. The default is CITYPE=LOWER for the design with an upper alternative, CITYPE=UPPER for the design with a lower alternative, and CITYPE=TWOSIDED for the design with a two-sided alternative.

**DATA < (TESTVAR=variable) >=SAS-data-set**

names the SAS data set that contains the test statistic and its associated information level for the stage. The data set includes the stage variable `_Stage_` and a variable to identify or derive the information level: `_Info_` for the information level, `NObs` for the number of observation, or `Events` for the number of events. If the information level that corresponds to the test statistic is not available, the information level derived in the BOUNDARY= data set is used.

If the TESTVAR= option is specified, the data set also includes the test variable specified in the TESTVAR= option and the scale variable `_Scale_` for the test statistic. Usually, these test variable values are obtained from analysis output in SAS procedures.

**ERRSPENDADJ=method**

**ERRSPENDADJ(boundary)=method**

**BOUNDARYADJ=method**

**BOUNDARYADJ(boundary)=method**

specifies methods to compute the error spending values at the current and future interim stages for the boundaries. This option is applicable only if the observed information level at the current stage does not match the value provided in the BOUNDARY= data set. These error spending values are then used to derive the updated boundary values. The default is ERRSPENDADJ=ERRLINE. Note that the information levels at future interim stages are determined by the INFOADJ= option.

The following options specify available error spending methods for boundary adjustment:

**NONE**

specifies that the cumulative error spending at each interim stage not be changed, even if the corresponding information level has been changed.

**ERRLINE**

specifies the linear interpolation method for the adjustment.

**ERRFUNCGAMMA < ( GAMMA=  $\gamma$  ) >**

specifies the gamma function method for the adjustment. The GAMMA= suboption specifies the  $\gamma$  parameter in the function, where  $\gamma \leq 3$ . The default is GAMMA=-2.

**ERRFUNCOBF**

specifies the approximate O'Brien-Fleming cumulative error spending function for the adjustment.

**ERRFUNCPOC**

specifies the approximate Pocock cumulative error spending function for the adjustment.

**ERRFUNCPOW < ( RHO=  $\rho$  ) >**

specifies the power function method for the adjustment. The RHO= suboption specifies the power parameter  $\rho$  in the function, where  $\rho \geq 0.25$ . The default is RHO=2.

See the section “[Boundary Adjustments for Information Levels](#)” on page 7223 for a detailed description of the available error spending methods for boundary adjustment in the SEQTEST procedure.

If an error spending method for boundary adjustments is used for all boundaries in a group sequential test, you can use the ERRSPENDADJ=*method* option to specify the method. Otherwise, you can use the following ERRSPENDADJ(*boundary*)=*method* options to specify different methods for the boundaries.

**ERRSPENDADJ(ALPHA)=*method***

**ERRSPENDADJ(REJECT)=*method***

**BOUNDARYADJ(ALPHA)=*method***

**BOUNDARYADJ(REJECT)=*method***

specifies the adjustment method for the  $\alpha$  (rejection) boundary of a one-sided design or the lower and upper  $\alpha$  boundaries of a two-sided design.

**ERRSPENDADJ(LOWERALPHA)=*method***

**ERRSPENDADJ(LOWERREJECT)=*method***

**BOUNDARYADJ(LOWERALPHA)=*method***

**BOUNDARYADJ(LOWERREJECT)=*method***

specifies the adjustment method for the lower  $\alpha$  boundary of a two-sided design.

**ERRSPENDADJ(UPPERALPHA)=*method***

**ERRSPENDADJ(UPPERREJECT)=*method***

**BOUNDARYADJ(UPPERALPHA)=*method***

**BOUNDARYADJ(UPPERREJECT)=*method***

specifies the adjustment method for the upper  $\alpha$  boundary of a two-sided design.

**ERRSPENDADJ(BETA)=*method***

**ERRSPENDADJ(ACCEPT)=*method***

**BOUNDARYADJ(BETA)=*method***

**BOUNDARYADJ(ACCEPT)=*method***

specifies the adjustment method for the  $\beta$  (acceptance) boundary of a one-sided design or the lower and upper  $\beta$  boundaries of a two-sided design.

**ERRSPENDADJ(LOWERBETA)=method**

**ERRSPENDADJ(LOWERACCEPT)=method**

**BOUNDARYADJ(LOWERBETA)=method**

**BOUNDARYADJ(LOWERACCEPT)=method**

specifies the adjustment method for the lower  $\beta$  boundary of a two-sided design.

**ERRSPENDADJ(UPPERBETA)=method**

**ERRSPENDADJ(UPPERACCEPT)=method**

**BOUNDARYADJ(UPPERBETA)=method**

**BOUNDARYADJ(UPPERACCEPT)=method**

specifies the adjustment method for the upper  $\beta$  boundary of a two-sided design.

**ERRSPENDMIN=numbers**

**ERRSPENDMIN(boundary)=numbers**

specifies the minimum error spending values at the current observed and future interim stages for the boundaries specified in the BOUNDARYKEY= option. The default is ERRSPENDMIN=0.

If a set of numbers is used for each boundary in the design, you can use the ERRSPENDMIN=numbers option. Otherwise, you can use the following ERRSPENDMIN(boundary)=numbers options to specify different sets of minimum error spending values for the boundaries. For a boundary, the error spending value at stage 1 is identical to its nominal  $p$ -value.

**ERRSPENDMIN(ALPHA)=numbers**

**ERRSPENDMIN(REJECT)=numbers**

specifies the minimum error spending values for the  $\alpha$  boundary of a one-sided design or the lower and upper  $\alpha$  boundaries of a two-sided design.

**ERRSPENDMIN(LOWERALPHA)=numbers**

**ERRSPENDMIN(LOWERREJECT)=numbers**

specifies the minimum error spending values for the lower  $\alpha$  boundary of a two-sided design.

**ERRSPENDMIN(UPPERALPHA)=numbers**

**ERRSPENDMIN(UPPERREJECT)=numbers**

specifies the minimum error spending values for the upper  $\alpha$  boundary of a two-sided design.

**ERRSPENDMIN(BETA)=numbers**

**ERRSPENDMIN(ACCEPT)=numbers**

specifies the minimum error spending values for the  $\beta$  boundary of a one-sided design or the lower and upper  $\beta$  boundaries of a two-sided design.

**ERRSPENDMIN(LOWERBETA)=numbers**

**ERRSPENDMIN(LOWERACCEPT)=numbers**

specifies the minimum error spending values for the lower  $\beta$  boundary of a two-sided design.

**ERRSPENDMIN(UPPERBETA)=numbers**

**ERRSPENDMIN(UPPERACCEPT)=numbers**

specifies the minimum error spending values for the upper  $\beta$  boundary of a two-sided design.

**INFOADJ=NONE | PROP**

specifies whether information levels at future interim stages are to be adjusted. If you specify INFOADJ=NONE, no adjustment is made, and the information levels are preserved at the levels provided in the BOUNDARY= data set. If you specify INFOADJ=PROP (which is the default), the information levels are adjusted proportionally from the levels provided in the BOUNDARY= data set. The section “[Information Level Adjustments at Future Stages](#)” on page 7223 describes how the adjustments are computed.

Note that if you specify BOUNDARYKEY=BOTH, the INFOADJ=NONE option is not applicable, and the INFOADJ=PROP option is used to adjust the information levels at future stages proportionally from the levels provided in the BOUNDARY= data set to maintain both  $\alpha$  and  $\beta$  levels.

**NSTAGES=*number***

specifies the number of stages for the clinical trial. The default is the number derived from the BOUNDARY= data set.

The specified NSTAGES= number might or might not be the same as the number derived in the BOUNDARY= data set. You can use the NSTAGES= option to set the next stage as the final stage to compute the conditional power, as described in the section “[Conditional Power Approach](#)” on page 7226.

**ORDER=LR | MLE | STAGEWISE**

specifies the ordering of the sample space  $(k, z)$ , where  $k$  is the stage number and  $z$  is the observed standardized  $Z$  statistic. The ordering is used to derive the  $p$ -values for the observed  $(k, z)$  statistic and to create unbiased median estimate and confidence limits from the statistic. The ORDER=LR option specifies the LR ordering that compares the distances between observed standardized  $Z$  statistics and their corresponding hypothetical values, the ORDER=MLE option specifies the MLE ordering that compares values in the MLE scale, and the ORDER=STAGEWISE specifies the stagewise ordering that uses counterclockwise ordering around the continuation region. The default is ORDER=STAGEWISE. See the section “[Available Sample Space Orderings in a Sequential Test](#)” on page 7230 for a detailed description of these sample space orderings.

**PARMS <(TESTVAR=*variable*)> =SAS-*data-set***

names the SAS data set that contains the parameter estimate and its associated standard error for the stage. The data set includes the stage variable `_Stage_`, the test statistic Estimate, the standard error of the estimate StdErr, and the test statistic scale variable `_Scale_`. The standard error is used to derive the information level. If the standard error is not available, the information level derived in the BOUNDARY= data set is used.

The data set also includes the variable Parameter, Effect, Variable, or Parm that contains the test variable specified in the TESTVAR= option. Usually, these test variable values are obtained from analysis output in SAS procedures.

**Table Output Options**

You can specify the following *options* in the PROC SEQTEST statement to display additional table output. They are listed in alphabetical order.



**CONDPOWER** < ( options ) >

displays conditional powers given the most recently observed statistic under specified hypothetical references.

You can specify the following *options*:

**CREF=**  $c_1 < c_2 \dots >$ 

specifies the hypothetical references, where  $c_i \geq 0$ . For a one-sided test, the powers are derived under the hypothetical references  $\theta = \hat{\theta}$  and  $\theta = c_i \theta_1$ , where  $\hat{\theta}$  is the observed statistic,  $\theta_1$  is the alternative reference, and  $c_i$  are the values specified in the CREF= option. For a two-sided test, the powers are derived under hypothetical references  $\theta = \hat{\theta}$ ,  $\theta = c_i \theta_{1l}$ , and  $\theta = c_i \theta_{1u}$ , where  $\theta_{1l}$  is the lower alternative reference and  $\theta_{1u}$  is the upper alternative reference. The default is CREF= 0 0.5 1.0 1.5.

**TYPE=ALLSTAGES | FINALSTAGE**

specifies the probability to be computed for the conditional power. Two types of conditional power can be computed: TYPE=ALLSTAGES computes the conditional power as the total probability of rejecting the null hypothesis at all future stages given the observed statistic, and TYPE=FINALSTAGE computes the conditional power as the probability that the test statistic at the final stage would exceed the rejection critical value given the observed statistic. The default is TYPE=ALLSTAGES.

If interim stages exist between the current stage and the final stage, the conditional power that is computed when TYPE=FINALSTAGE is not the conditional probability to reject the null hypothesis  $H_0$ . In this case, you can set the next stage as the final stage, and the resulting conditional power is the conditional probability to reject  $H_0$ .

**ERRSPEND**

displays the error spending at each stage for each sequential boundary.

**PREDPOWER**

displays predictive powers given the most recently observed statistic. The predictive power is the posterior probability that the test statistic at the final stage would exceed the rejection critical value given the observed statistic and a prior distribution of the hypothetical reference. A noninformative prior is used in the procedure.

**PSS** < ( CREF=  $c_1 < c_2 \dots >$  ) >

displays powers and expected sample sizes under various hypothetical references, where  $c_i \geq 0$ .

For a one-sided design with the null reference  $\theta_0 = 0$ , the power and expected sample sizes under hypotheses  $\theta = c_i \theta_1$  are displayed, where  $\theta_1$  is the alternative reference and  $c_i$  are the values specified in the CREF= option.

For a two-sided design, the power and expected sample sizes under hypotheses  $\theta = c_i \theta_{1l}$  and  $\theta = c_i \theta_{1u}$  are displayed, where  $\theta_{1l}$  and  $\theta_{1u}$  are the lower and upper alternative references, respectively. The default is CREF= 0 0.5 1.0 1.5.

Note that for a symmetric two-sided design, only the power and expected sample sizes under hypotheses  $\theta = c_i \theta_{1u}$  are derived.

**RCI**

displays repeated confidence intervals for the parameter from the observed statistic at each stage. Repeated confidence intervals include both rejection and acceptance confidence intervals.

With the STOP=REJECT or STOP=BOTH option, rejection confidence limits can be derived, and the null hypothesis  $H_0 : \theta = 0$  is rejected if the lower rejection confidence limit is greater than 0 or the upper rejection confidence limit is less than 0.

With the STOP=ACCEPT or STOP=BOTH option, acceptance confidence limits can be derived, and the null hypothesis is accepted with alternative hypotheses  $H_{1l} : \theta = \theta_{1l}$  and  $H_{1u} : \theta = \theta_{1u}$  if the upper acceptance confidence limit is less than  $\theta_{1u}$  and the lower acceptance confidence limit is greater than  $\theta_{1l}$ .

**STOPPROB <( CREF=  $c_1 < c_2 \dots >$  ) >**

displays expected cumulative stopping probabilities under various hypothetical references, where  $c_i \geq 0$ .

For a one-sided design, expected cumulative stopping probabilities at each stage under hypotheses  $\theta = c_i \theta_1$  are displayed, where  $\theta_1$  is the alternative reference and  $c_i$  are the values specified in the CREF= option.

For a two-sided design, expected cumulative stopping probabilities at each stage under hypotheses  $\theta = c_i \theta_{1l}$  and  $\theta = c_i \theta_{1u}$  are displayed, where  $\theta_{1l}$  and  $\theta_{1u}$  are the lower and upper alternative references, respectively. Note that for a symmetric two-sided design, only expected cumulative stopping probabilities under hypotheses  $\theta = c_i \theta_{1u}$  are derived. The default is CREF= 0 0.5 1.0 1.5.

**Graphics Output Options**

The following options can be used in the PROC SEQTEST statement to display plots with ODS Graphics. They are listed in alphabetical order.

**PLOTS <( ONLY )> <= *plot-request* >****PLOTS <( ONLY )> <= ( *plot-request* < ... *plot-request* ) >**

specifies options that control the details of the plots. The default is PLOTS=TEST. The global plot option ONLY suppresses the default plots and displays only plots specifically requested.

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;
proc seqtest Boundary=Bnd_LDL
 Parms(Testvar=Trt)=Parms_LDL1
 Plots=(test errspend);
run;
ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The plot request options include the following.

**ALL**

produces all appropriate plots.

**ASN** < ( **CREF=**  $c_1 < c_2 \dots >$  ) >

displays a plot of the average sample numbers (expected sample sizes for nonsurvival data or expected number of events for survival data) under various hypothetical references, where  $c_i \geq 0$ .

For a one-sided design, expected sample numbers under hypotheses  $\theta = c_i \theta_1$  are displayed, where  $\theta_1$  is the alternative reference and  $c_i$  are the values specified in the CREF= option.

For a two-sided design, expected sample numbers under hypotheses  $\theta = c_i \theta_{1l}$  and  $\theta = c_i \theta_{1u}$  are displayed, where  $\theta_{1l}$  and  $\theta_{1u}$  are the lower and upper alternative references, respectively. Note that for a symmetric two-sided design, only the average sample numbers under hypotheses  $\theta = c_i \theta_{1u}$  are derived. The default is CREF= 0 to 1.5 by 0.01.

**CONDPOWER** < ( *options* ) >

displays a plot of conditional powers given the most recently observed statistic under specified hypothetical references.

You can specify the following *options*:

**CREF=**  $c_1 < c_2 \dots >$

specifies the hypothetical references, where  $c_i \geq 0$ . For a one-sided test, the powers are derived under hypothetical references  $\theta = \hat{\theta}$  and  $\theta = c_i \theta_1$ , where  $\hat{\theta}$  is the observed statistic,  $\theta_1$  is the alternative reference, and  $c_i$  are the values specified in the CREF= option. For a two-sided test, the powers are derived under hypothetical references  $\theta = \hat{\theta}$ ,  $\theta = c_i \theta_{1l}$ , and  $\theta = c_i \theta_{1u}$ , where  $\theta_{1l}$  is the lower alternative reference and  $\theta_{1u}$  is the upper alternative reference. The default is CREF= 0 to 1.5 by 0.01.

**TYPE=ALLSTAGES | FINALSTAGE**

specifies the probability to be computed for the conditional power. Two types of conditional power can be computed: TYPE=ALLSTAGES computes the conditional power as the total probability of rejecting the null hypothesis at all future stages given the observed statistic, and TYPE=FINALSTAGE computes the conditional power as the probability that the test statistic at the final stage would exceed the rejection critical value given the observed statistic. The default is TYPE=ALLSTAGES.

**ERRSPEND** < ( **HSCALE=INFO | STAGE** ) >

displays a plot of the error spending for all sequential boundaries in the designs simultaneously. You can display the information level (HSCALE=INFO) or the stage number (HSCALE=STAGE) on the horizontal axis. With HSCALE=INFO, the information fractions are used in the plot. The default is HSCALE=STAGE.

**NONE**

suppresses all plots.

**POWER <( CREF=  $c_1 < c_2 \dots >$  ) >**

displays a plot of the power curves under various hypothetical references, where  $c_i \geq 0$ .

For a one-sided design, powers under hypotheses  $\theta = c_i \theta_1$  are displayed, where  $\theta_1$  is the alternative reference and  $c_i$  are the values specified in the CREF= option.

For a two-sided design, powers under hypotheses  $\theta = c_i \theta_{1l}$  and  $\theta = c_i \theta_{1u}$  are displayed, where  $\theta_{1l}$  and  $\theta_{1u}$  are the lower and upper alternative references, respectively. Note that for a symmetric two-sided design, only powers under hypotheses  $\theta = c_i \theta_{1u}$  are derived. The default is CREF= 0 to 1.5 by 0.01.

**RCI**

displays a plot of repeated confidence intervals. Repeated confidence intervals include both rejection and acceptance confidence intervals.

With the STOP=REJECT or STOP=BOTH option, rejection confidence limits can be derived and the null hypothesis  $H_0 : \theta = 0$  is rejected if the lower rejection confidence limit is greater than 0 or the upper rejection confidence limit is less than 0.

With the STOP=ACCEPT or STOP=BOTH option, acceptance confidence limits can be derived and the null hypothesis is accepted with alternative hypotheses  $H_{1l} : \theta = \theta_{1l}$  and  $H_{1u} : \theta = \theta_{1u}$  if the upper acceptance confidence limit is less than  $\theta_{1u}$  and the lower acceptance confidence limit is greater than  $\theta_{1l}$ .

**TEST <( HSCALE=INFO | SAMPLESIZE ) >**

displays a plot of the sequential boundaries and test variables. Either the information level (HSCALE=INFO) or the sample size (HSCALE=SAMPLESIZE) is displayed on the horizontal axis. The HSCALE=SAMPLESIZE option is applicable only if the sample size information is available in both the input BOUNDARY= data set and input DATA= data set. The stage number for each stage is displayed inside the plot. The default is HSCALE=INFO.

## Details: SEQTEST Procedure

### Input Data Sets

The BOUNDARY= data set option is required, and if neither the DATA= nor the PARMS= data set option is specified, the procedure derives statistics such as Type I and Type II error probabilities from the BOUNDARY= data set. The resulting boundaries are displayed with the scale specified in the BOUNDARYSCALE= option.

### BOUNDARY= Data Set

The BOUNDARY= data set provides the boundary information for the sequential test. At stage 1, the data set is usually created with an ODS OUTPUT statement from the “Boundary Information” table created by the SEQDESIGN procedure. At each subsequent stage, the data set is usually created with an ODS OUTPUT statement from the “Test Information” table that was created by the SEQTEST procedure at the

previous stage. See the section “Getting Started: SEQTEST Procedure” on page 7192 for an illustration of the BOUNDARY= data set option.

The BOUNDARY= data set contains the following variables:

- `_Scale_`, the boundary scale, with the value MLE for the maximum likelihood estimate, STDZ for the standardized Z, SCORE for the score statistic, or PVALUE for the nominal  $p$ -value. Note that for a two-sided design, the nominal  $p$ -value is the one-sided fixed-sample  $p$ -value under the null hypothesis with a lower alternative hypothesis.
- `_Stop_`, the stopping criterion, with the value REJECT for rejecting the null hypothesis  $H_0$ , ACCEPT for accepting  $H_0$ , or BOTH for both rejecting and accepting  $H_0$
- `_ALT_`, the type of alternative hypothesis, with the value UPPER for an upper alternative, LOWER for a lower alternative, or TWOSIDED for a two-sided alternative
- `_Stage_`, the stage number
- the boundary variables, a subset of Bound\_LA for lower  $\alpha$  boundary, Bound\_LB for lower  $\beta$  boundary, Bound\_UB for upper  $\beta$  boundary, and Bound\_UA for upper  $\alpha$  boundary
- AltRef\_L, the lower alternative reference, if ALT=LOWER or ALT=TWOSIDED
- AltRef\_U, the upper alternative reference, if ALT=UPPER or ALT=TWOSIDED
- `_InfoProp_`, the information proportion at each stage

Optionally, the BOUNDARY= data set also contains the following variables:

- `_Info_`, the information level at each stage
- NObs, the required number of observations for nonsurvival data at each stage
- Events, the required number of events for survival data at each stage
- Parameter, the variable specified in the DATA(TESTVAR=) or PARMS(TESTVAR=) option
- Estimate, the parameter estimate

If the BOUNDARY= data set contains the variable Parameter for the test variable that is specified in the TESTVAR= option, and the variable Estimate for the test statistics, then these test statistics are also displayed in the output test information table and output test plot.

## DATA= Data Set

The DATA= data set provides the test variable information for the current stage of the trial. Such data sets are usually created with an ODS OUTPUT statement by using a procedure such as PROC MEANS. See “Example 84.4: Testing a Binomial Proportion” on page 7284 for an illustration of the DATA= data set option.

The DATA= data set includes the following variables:

- `_Stage_`, the stage number
- `_Scale_`, the scale for the test statistic, with the value MLE for the maximum likelihood estimate, STDZ for the standardized Z, SCORE for the score statistic, or PVALUE for the nominal  $p$ -value
- `_Info_`, the information level
- NObs, the number of observations for nonsurvival data at each stage
- Events, the number of events for survival data at each stage
- test variable, specified in the TESTVAR= option, contains the test variable value in the scale specified in the `_Scale_` variable

With the specified DATA= data set, PROC SEQTEST derives boundary values from the information levels in the `_Info_` variable. If the data set does not include the `_Info_` variable, then the information levels are derived from the NObs or Events variable in the DATA= data set if that variable is also in the input BOUNDARY= data set. That is, the information level at stage  $k$  is computed as  $I_k^* = I_k \times (n_k^*/n_k)$ , where  $I_k$  and  $n_k$  are the information level and sample size, respectively, at stage  $k$  in the BOUNDARY= data set and  $n_k^*$  is the sample size at stage  $k$  in the DATA= data set. Otherwise, the information levels from the BOUNDARY= data set are used.

If the TESTVAR= option is specified, the DATA= data set must also include the test variable for the test statistic and `_Scale_` variable for the corresponding scale. Note that for a two-sided design, the nominal  $p$ -value is the one-sided fixed-sample  $p$ -value under the null hypothesis with a lower alternative hypothesis.

### PARMS= Data Set

The PARMS= data set provides a parameter estimate and associated standard error for the current stage of the trial. Such data sets are usually created with an ODS OUTPUT statement by using procedures such as the GENMOD, GLM, LOGISTIC, and REG procedures. See the section “Getting Started: SEQTEST Procedure” on page 7192 for an illustration of the PARMS= data set option.

The PARMS= data set includes the following variables:

- `_Stage_`, the stage number
- `_Scale_`, the scale for the test statistic, with the value MLE for the maximum likelihood estimate, STDZ for the standardized Z, SCORE for the score statistic, or PVALUE for the nominal  $p$ -value
- Parameter, Effect, Variable, or Parm, which contains the variable specified in the TESTVAR= option
- Estimate, the parameter estimate
- StdErr, standard error of the parameter estimate
- NObs, the number of observations for nonsurvival data at each stage
- Events, the number of events for survival data at each stage

With the specified PARMs= data set, the information level is derived from the StdErr variable. For a score statistic, the information level  $I_k$  is the variance of the statistic,  $\hat{s}_k^2$ , where  $\hat{s}_k$  is the standard error in the StdErr variable. Otherwise, the information level is the inverse of the variance of the statistic,  $\hat{s}_k^{-2}$ . If the data set does not include the StdErr variable, the information levels derived from the BOUNDARY= data set are used.

If the data set does not include the StdErr variable, then the information levels are derived from the NObs or Events variable in the PARMs= data set if that variable is also in the input BOUNDARY= data set. That is, the information level at stage  $k$  is computed as  $I_k^* = I_k \times (n_k^*/n_k)$ , where  $I_k$  and  $n_k$  are the information level and sample size, respectively, at stage  $k$  in the BOUNDARY= data set and  $n_k^*$  is the sample size at stage  $k$  in the PARMs= data set. Otherwise, the information levels from the BOUNDARY= data set are used.

If the TESTVAR= option is specified, the PARMs= data set also includes the variable Parameter, Effect, Variable, or Parm for the test variable, Estimate for the test statistic, and \_Scale\_ variable for the corresponding scale. Note that for a two-sided design, the nominal  $p$ -value is the one-sided fixed-sample  $p$ -value under the null hypothesis with a lower alternative hypothesis.

## Boundary Variables

The boundaries created in group sequential trials depend on the type of the alternative hypothesis and the early stopping criterion. Table 84.2 shows the boundaries created with various design specifications.

**Table 84.2** Boundary Variables

| Alternative Hypothesis | Specifications<br>Early Stopping | Boundary Variables |      |       |       |
|------------------------|----------------------------------|--------------------|------|-------|-------|
|                        |                                  | Lower              |      | Upper |       |
|                        |                                  | Alpha              | Beta | Beta  | Alpha |
| Lower                  | Accept $H_0$                     |                    | X    |       |       |
|                        | Reject $H_0$                     | X                  |      |       |       |
|                        | Accept/Reject $H_0$              | X                  | X    |       |       |
| Upper                  | Accept $H_0$                     |                    |      | X     |       |
|                        | Reject $H_0$                     |                    |      |       | X     |
|                        | Accept/Reject $H_0$              |                    |      | X     | X     |
| Two-sided              | Accept $H_0$                     |                    | X    | X     |       |
|                        | Reject $H_0$                     | X                  |      |       | X     |
|                        | Accept/Reject $H_0$              | X                  | X    | X     | X     |

Up to four different boundaries can be generated in a group sequential design:

- the upper  $\alpha$  boundary, used to reject the null hypothesis in favor of an upper alternative hypothesis
- the upper  $\beta$  boundary, used to accept the null hypothesis with an upper alternative hypothesis
- the lower  $\beta$  boundary, used to accept the null hypothesis with a lower alternative hypothesis

- the lower  $\alpha$  boundary, used to reject the null hypothesis in favor of a lower alternative hypothesis

For a two-sided design, the null hypothesis is accepted only if both the null hypothesis is accepted with an upper alternative hypothesis and the null hypothesis is accepted with a lower alternative hypothesis.

For a one-sided design with a lower alternative, only the lower boundaries are created. Similarly, for a one-sided design with an upper alternative, only the upper boundaries are created. For example, Figure 84.19 shows the boundary plot for a one-sided test with an upper alternative.

**Figure 84.19** Boundary Plot for One-Sided Test

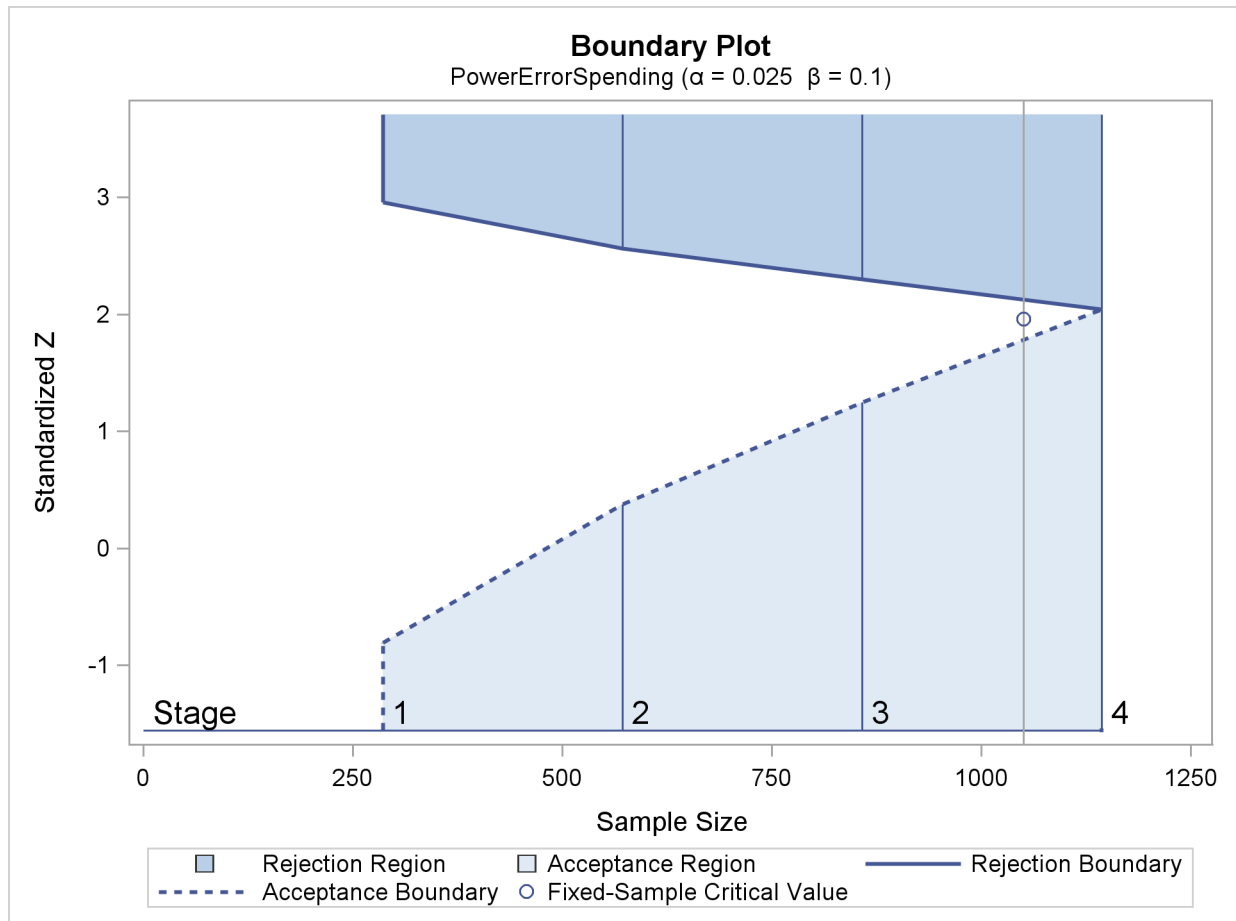


Figure 84.19 corresponds to a one-sided sequential design with early stopping to reject or accept the null hypothesis. For a sequential test with early stopping only to reject the null hypothesis, there are no acceptance boundary values at interim stages. The acceptance boundary value and its associated acceptance region are displayed only at the final stage. Similarly, for a sequential test with early stopping only to accept the null hypothesis, there are no rejection boundary values at interim stages. The rejection boundary value and its associated rejection region are displayed only at the final stage.

For a two-sided design, both the lower and upper boundaries are created. For a design with early stopping to reject the null hypothesis,  $\alpha$  boundaries are created. Similarly, for a design with early stopping to accept the null hypothesis,  $\beta$  boundaries are created. For a design with early stopping to accept or reject the null hypothesis, both the  $\alpha$  and  $\beta$  boundaries are created.



For example, Figure 84.20 shows the boundary plot for a two-sided test.

**Figure 84.20** Boundary Plot for Two-Sided Test

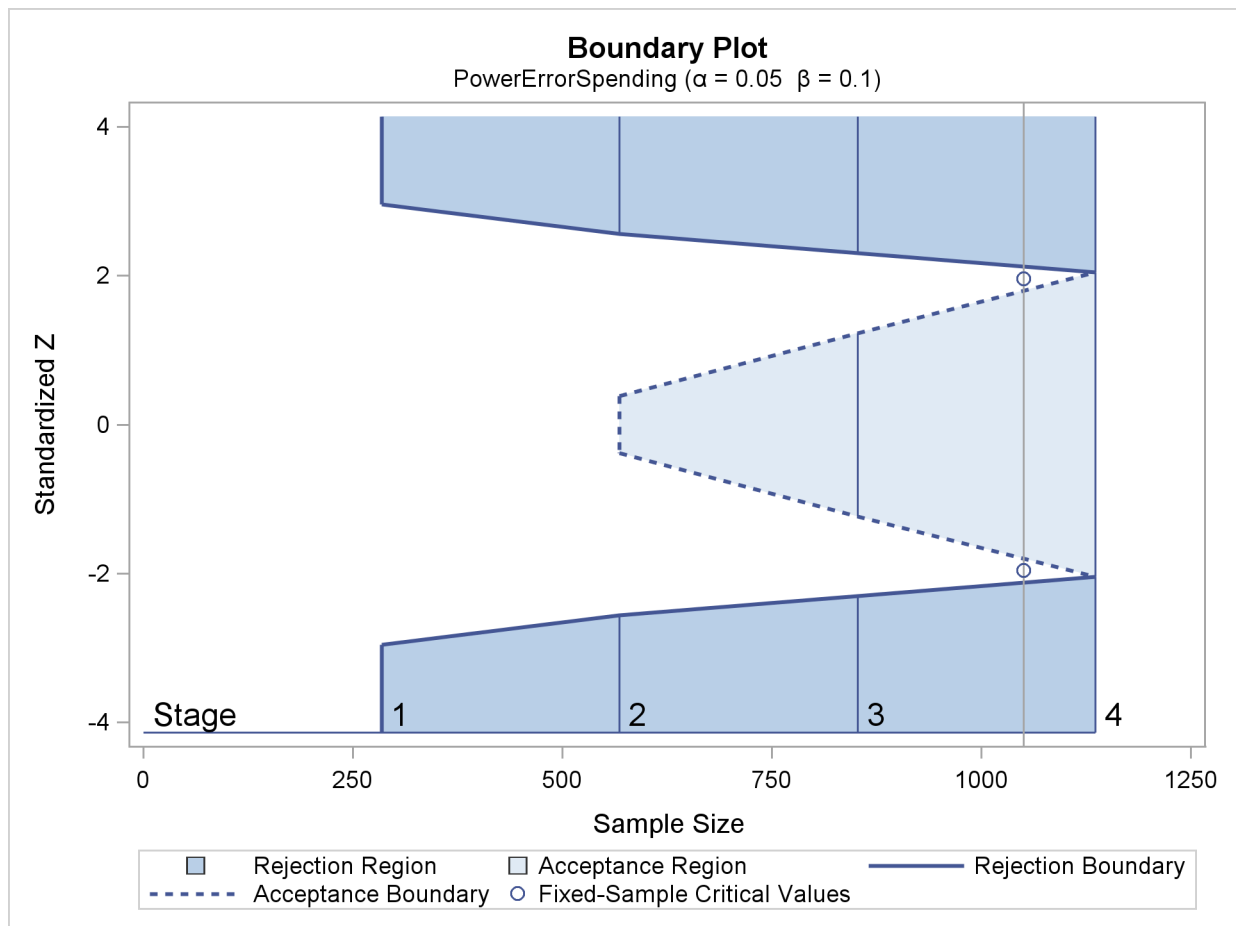


Figure 84.20 corresponds to a two-sided sequential design with early stopping to reject or accept the null hypothesis. For a sequential test with early stopping only to reject the null hypothesis, there are no acceptance boundary values at interim stages. The acceptance boundary value and its associated acceptance region are displayed only at the final stage. Similarly, for a sequential test with early stopping only to accept the null hypothesis, there are no rejection boundary values at interim stages. The rejection boundary value and its associated rejection region are displayed only at the final stage.

## Information Level Adjustments at Future Stages

In a group sequential clinical trial, the information level for the observed test statistic at the current stage generally does not match the corresponding information level in the BOUNDARY= data set. By default (or equivalently if you specify INFOADJ=PROP), the SEQTEST procedure accommodates the observed information level by adjusting the information levels at future interim stages. The adjustment of information levels depends on the boundary key to be maintained in the boundary adjustments, which in turn is determined by the BOUNDARYKEY= option.

If you specify BOUNDARYKEY=ALPHA (which is the default) or BOUNDARYKEY=BETA, the maximum information level (the information level at the final stage) provided in the BOUNDARY= data set is maintained. In this case, if an observed information level at the current stage is different from the level provided in the BOUNDARY= data set, you can use the INFOADJ= option to determine whether the information levels at subsequent interim stages are to be adjusted. Specifying INFOADJ=NONE preserves the levels provided in the BOUNDARY= data set without adjustment. Specifying INFOADJ=PROP proportionally adjusts the levels provided in the BOUNDARY= data set as follows.

Denote the information level at stage  $k$  for the  $K$ -stage design that is stored in the BOUNDARY= data set by  $I_k$ ,  $k = 1, 2, \dots, K$ . Also denote the information level that corresponds to the test statistic at an interim stage  $k_0$  by  $I'_{k_0}$ ,  $1 \leq k_0 \leq (K - 1)$ . Then for the updated design, the information level at stage  $k$ ,  $k = k_0 + 1, \dots, (K - 1)$ , is computed as

$$I'_k = I'_{k_0} + (I_K - I'_{k_0}) \frac{I_k - I_{k_0}}{I_K - I_{k_0}}$$

Note that if  $I'_{k_0} \geq I_K$ , the information level at stage  $k_0$  reaches the maximum information level in the design, the trial stops at stage  $k_0$ , and no future information levels are derived.

If you specify BOUNDARYKEY=BOTH, the maximum information level for the trial is not necessarily the same as the maximum information level saved in the BOUNDARY= data set. In this case, the INFOADJ=NONE option is not applicable, and the INFOADJ=PROP option is used to proportionally adjust the information levels at future interim stages with the updated maximum information  $I'_K$ . That is, with an updated  $I'_K$ , the information level at a future interim stage  $k$  is computed as

$$I'_k = I'_{k_0} + (I'_K - I'_{k_0}) \frac{I_k - I_{k_0}}{I'_K - I_{k_0}}$$

## Boundary Adjustments for Information Levels

In a group sequential clinical trial, if the information level for the observed test statistic does not match the corresponding information level in the BOUNDARY= data set, the INFOADJ=PROP option (which is the default) can be used to modify information levels at future stages to accommodate this observed information level. With the adjusted information levels, the ERRSPENDADJ= option provides various methods to compute error spending values at the current and future interim stages. These error spending values are then used to derive boundary values in the SEQTEST procedure. See the section “Error Spending Methods” in the chapter “The SEQDESIGN Procedure” for a detailed description of how to use these error spending values to derive boundary values.

The ERRSPENDADJ=NONE option keeps the error spending the same at each stage. The ERRSPENDADJ=ERRLINE option uses a linear interpolation on the cumulative error spending in the

design stored in the BOUNDARY= data set to derive the error spending for each unmatched information level (Kittelson and Emerson 1999, p. 882). That is, the cumulative error spending for an information level  $I$  is computed as

$$e(I) = \begin{cases} e_1 \left( \frac{I}{I_1} \right) & \text{if } I < I_1 \\ e_j + (\alpha_{j+1} - \alpha_j) \left( \frac{I - I_j}{I_{j+1} - I_j} \right) & \text{if } I_j \leq I < I_{j+1} \\ e_K & \text{if } I \geq I_K \end{cases}$$

where  $e_1, e_2, \dots, e_K$  are the cumulative errors at the  $K$  stages of the design that is stored in the BOUNDARY= data set.

The ERRSPENDADJ=ERRFUNCPOC option uses Pocock-type cumulative error spending function (Lan and DeMets 1983):

$$E(t) = \begin{cases} 1 & \text{if } t \geq 1 \\ \log(1 + (e - 1)t) & \text{if } 0 < t < 1 \\ 0 & \text{otherwise} \end{cases}$$

With an error level of  $\alpha$  or  $\beta$ , the cumulative error spending for an information level  $I$  is  $e(I) = \alpha E(I/I_K)$  or  $e(I) = \beta E(I/I_K)$ .

The ERRSPENDADJ=ERRFUNCOBF option uses O'Brien-Fleming-type cumulative error spending function (Lan and DeMets 1983):

$$E(t; a) = \begin{cases} 1 & \text{if } t \geq 1 \\ \frac{1}{a} 2 (1 - \Phi(\frac{z(1-a/2)}{\sqrt{t}})) & \text{if } 0 < t < 1 \\ 0 & \text{otherwise} \end{cases}$$

where  $a$  is either  $\alpha$  for the  $\alpha$  spending function or  $\beta$  for the  $\beta$  spending function, and  $\Phi$  is the cumulative distribution function of the standardized  $Z$  statistic. That is, with an error level of  $\alpha$  or  $\beta$ , the cumulative error spending for an information level  $I$  is  $e(I) = \alpha E(I/I_K; \alpha)$  or  $e(I) = \beta E(I/I_K; \beta)$ .

The ERRSPENDADJ=ERRFUNCGAMMA option uses gamma cumulative error spending function (Hwang, Shih, and DeCani 1990):

$$E(t; \gamma) = \begin{cases} 1 & \text{if } t \geq 1 \\ \frac{1 - e^{-\gamma t}}{1 - e^{-\gamma}} & \text{if } 0 < t < 1, \gamma \neq 0 \\ t & \text{if } 0 < t < 1, \gamma = 0 \\ 0 & \text{otherwise} \end{cases}$$

where  $\gamma$  is the parameter  $\gamma$  specified in the GAMMA= option. That is, with an error level of  $\alpha$  or  $\beta$ , the cumulative error spending for an information level  $I$  is  $e(I) = \alpha E(I/I_K; \gamma)$  or  $e(I) = \beta E(I/I_K; \gamma)$ .

The ERRSPENDADJ=ERRFUNCPOW option uses power cumulative error spending function (Jennison and Turnbull 2000, p. 148):

$$E(t; \rho) = \begin{cases} 1 & \text{if } t \geq 1 \\ t^\rho & \text{if } 0 < t < 1 \\ 0 & \text{otherwise} \end{cases}$$

where  $\rho$  is the power parameter specified in the RHO= suboption. With an error level of  $\alpha$  or  $\beta$ , the cumulative error spending for an information level  $I$  is  $e(I) = \alpha E(I/I_K; \rho)$  or  $e(I) = \beta E(I/I_K; \rho)$ .

If the BOUNDARYKEY=BOTH option is specified, the maximum information required for the trial might not be the same as the maximum information level stored in the BOUNDARY= data set. In this case, the information levels at future stages are adjusted proportionally, and the same error spending values that were computed based on the maximum information level stored in the BOUNDARY= data set are used to derive boundary values for the trial.

If an error spending function is used to create boundaries for the design in the SEQDESIGN procedure, then in order to better maintain the design features throughout the group sequential trial, the same error spending function to create boundaries for the design in the SEQDESIGN procedure should be used to modify boundaries in the SEQTEST procedure at each subsequent stage.

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## Boundary Adjustments for Minimum Error Spending

In a group sequential clinical trial, boundary values created from a design such as an O'Brien-Fleming design might be too conservative in early stages. Thus the trial is unlikely to stop in early stages. Lan and DeMets (1983, p. 662) suggest truncating boundary values to a number such as 3.5 for the trial to have a reasonable probability of stopping at early stages. Instead of truncating boundary values by a specified number, the ERRSPENDMIN= option provides individual minimum error spending at each interim stage to stop the trial early.

For a  $K$ -stage trial, denote the derived cumulative error spending at stage  $k$  after adjusting for information levels by  $e_k, k = 1, 2, \dots, K$ . Also denote the specified minimum error spending at interim stage  $k$  by  $\epsilon_k, k = 1, 2, \dots, K - 1$ . Then the cumulative error spending at stage 1 is  $e'_1 = \max(e_1, \epsilon_1)$ . If  $e_1 < e'_1$ , the error spending values at subsequent interim stages are adjusted proportionally by

$$e'_j = e'_1 + \frac{e_j - e_1}{e_K - e_1} (e_K - e'_1)$$

for  $j = 2, \dots, K - 1$ .

The process is repeated at each subsequent interim stage. That is, at stage  $k, k = 2, \dots, K - 1$ , denote the updated cumulative  $\beta$  spending at stage  $j$  by  $e_j, j = k, k + 1, \dots, K$ . Then the cumulative error spending at stage  $k$  is  $e'_k = \max(e_k, e'_{k-1} + \epsilon_k)$ . If  $e_k < e'_k$ , the error spending values at subsequent interim stages are adjusted proportionally by

$$e'_j = e'_k + \frac{e_j - e_k}{e_K - e_k} (e_K - e'_k)$$

for  $j = k + 1, \dots, K - 1$ .

Note that the ERRSPENDMIN= option is applicable only to the boundaries specified in the BOUNDARYKEY= option. That is, the ERRSPENDMIN= option is applicable to the  $\alpha$  boundaries with BOUNDARYKEY=ALPHA or BOUNDARYKEY=BOTH, and it is applicable to the  $\beta$  boundaries with BOUNDARYKEY=BETA or BOUNDARYKEY=BOTH.

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## Boundary Adjustments for Overlapping Lower and Upper $\beta$ Boundaries

In the SEQTEST procedure, the  $\alpha$  and  $\beta$  spending values at the stages are used to derive the boundary values for the trial. For a two-sided design with early stopping to accept  $H_0$ , or to either reject or accept

$H_0$ , a zero  $\beta$  spending at an interim stage sets the  $\beta$  boundary values to missing. A small  $\beta$  spending at the current or subsequent interim stage might result in overlapping of the lower and upper  $\beta$  boundaries for the two corresponding one-sided tests. Specifically, this form of overlapping occurs at an interim stage  $k$  if the upper  $\beta$  boundary value that is derived from the one-sided test for the upper alternative is less than the lower  $\beta$  boundary value that is derived from the one-sided test for the lower alternative (Kittelson and Emerson 1999, pp. 881–882; Rudser and Emerson 2007, p. 6). You can use the BETAOVERLAP= option to specify how this type of overlapping is to be handled.

If BETAOVERLAP=ADJUST (which is the default) is specified, the procedure derives the boundary values for the two-sided design and then checks for overlapping of the two one-sided  $\beta$  boundaries at the current and subsequent interim stages. If overlapping occurs at a particular stage, the  $\beta$  boundary values for the two-sided design are set to missing (so the trial does not stop to accept the null hypothesis at this stage), and the  $\beta$  spending values at subsequent stages are adjusted proportionally as follows.

If the  $\beta$  boundary values are set to missing at stage  $k$  in a  $K$ -stage trial, the adjusted  $\beta$  spending value at stage  $k$ ,  $e'_k$ , is updated for these missing  $\beta$  boundary values, and then the  $\beta$  spending values at subsequent stages are adjusted proportionally by

$$e'_j = e'_k + \frac{e_j - e_k}{e_K - e_k} (e_K - e'_k)$$

for  $j = k + 1, \dots, K$ , where  $e_j$  and  $e'_j$  are cumulative  $\beta$  spending values at stage  $j$  before and after the adjustment, respectively.

After all these adjusted  $\beta$  spending values are computed, the boundary values are then further modified for these adjusted  $\beta$  spending values.

If you specify BETAOVERLAP=NOADJUST, no adjustment is made when overlapping of one-sided  $\beta$  boundaries occurs.

## Stochastic Curtailment

Lan, Simon, and Halperin (1982) introduce stochastic curtailment to stop a trial if, given current data, it is likely to predict the outcome of the trial with high probability. That is, a trial can be stopped to reject the null hypothesis  $H_0$  if, given current data in the analyses, the conditional probability of rejecting  $H_0$  under  $H_0$  at the end of the trial is greater than  $\gamma$ , where the constant  $\gamma$  should be between 0.5 and 1 and values of 0.8 or 0.9 are recommended (Jennison and Turnbull 2000, p. 206). Similarly, a trial can be stopped to accept the null hypothesis  $H_0$  if, given current data in the analyses, the conditional probability of rejecting  $H_0$  under the alternative hypothesis  $H_1$  at the end of the trial is less than  $\gamma$ .

The following two approaches for stochastic curtailment are available in the SEQTEST procedures: conditional power approach and predictive power approach. For each approach, the derived group sequential test is used as the reference test for rejection.

## Conditional Power Approach

In the SEQTEST procedure, you can compute two types of conditional power as described in the following sections:

**TYPE=ALLSTAGES**

The default TYPE=ALLSTAGES suboption in the CONDPOWER and PLOT=CONDPOWER options computes the conditional power at an interim stage  $k$  as the total probability of rejecting the null hypothesis at all future stages given the observed statistic (Zhu, Ni, and Yao 2011, pp. 131–132).

For a one-sided test with an upper alternative, the conditional power at an interim stage  $k$  is given by

$$\begin{aligned} p_{ku}(\theta) &= P_{\theta}(z_{k+1} > a_{k+1} | z_k, \theta) \\ &+ P_{\theta}(b_{k+1} \leq z_{k+1} < a_{k+1}, z_{k+2} > a_{k+2} | z_k, \theta) \\ &+ \dots \\ &+ P_{\theta}(b_j \leq z_j < a_j, j = k + 1, \dots, K - 1, z_K > a_K | z_k, \theta) \end{aligned}$$

where  $z_k$  is the observed statistic and  $\theta$  is the hypothetical reference. The conditional power for a one-sided test with a lower alternative is similarly derived.

For a two-sided test, the conditional power for the upper alternative is given by

$$\begin{aligned} p_{ku}(\theta) &= P_{\theta}(z_{k+1} > a_{k+1} | z_k, \theta) \\ &+ P_{\theta}(\_a_{k+1} < z_{k+1} \leq \_b_{k+1} \text{ or } b_{k+1} \leq z_{k+1} < a_{k+1}, z_{k+2} > a_{k+2} | z_k, \theta) \\ &+ \dots \\ &+ \theta(\_a_j < z_j \leq \_b_j \text{ or } b_j \leq z_j < a_j, j = k + 1, \dots, K - 1, z_K > a_K | z_k, \theta) \end{aligned}$$

The conditional power for the lower alternative is similarly derived.

**TYPE=FINALSTAGE**

The TYPE=FINALSTAGE suboption in the CONDPOWER and PLOT=CONDPOWER options computes the conditional power at an interim stage  $k$  as the probability that the test statistic at the final stage (stage  $K$ ) would exceed the rejection critical value given the observed statistic (Jennison and Turnbull 2000, p. 207).

The conditional distribution of  $Z_K$  given the observed statistic  $z_k$  at the  $k$ th stage and the hypothetical reference  $\theta$  is

$$Z_K | (z_k, \theta) \sim N \left( z_k \Pi_k^{\frac{1}{2}} + \theta I_X^{\frac{1}{2}} (1 - \Pi_k), 1 - \Pi_k \right)$$

where  $\Pi_k = I_k / I_X$  is the fraction of information at the  $k$ th stage.

The power for the upper alternative,  $\text{prob}(Z_K > a_K | z_k, \theta)$ , is then given by

$$p_{ku}(\theta) = \Phi \left( (1 - \Pi_k)^{-\frac{1}{2}} (z_k \Pi_k^{\frac{1}{2}} - a_K) + \theta I_X^{\frac{1}{2}} (1 - \Pi_k)^{\frac{1}{2}} \right)$$

where  $\Phi$  is the cumulative distribution function of the standardized  $Z$  statistic and  $a_K$  is the upper critical value at the final stage.

Similarly, the power for the lower alternative,  $\text{prob}(Z_K < a_{-K} | z_k, \theta)$ , is

$$p_{kl}(\theta) = 1 - \Phi \left( (1 - \Pi_k)^{-\frac{1}{2}} (z_k \Pi_k^{\frac{1}{2}} - a_{-K}) + \theta I_X^{\frac{1}{2}} (1 - \Pi_k)^{\frac{1}{2}} \right)$$

where  $a_{-K}$  is the lower critical value at the final stage.

If  $\theta = \hat{\theta}_k = z_k I_k^{-\frac{1}{2}}$ , the maximum likelihood estimate at stage  $k$ , the powers for the upper and lower alternatives can be simplified:

$$p_{ku}(\theta) = \Phi \left( (1 - \Pi_k)^{-\frac{1}{2}} (z_k \Pi_k^{-\frac{1}{2}} - a_K) \right)$$

$$p_{kl}(\theta) = 1 - \Phi \left( (1 - \Pi_k)^{-\frac{1}{2}} (z_k \Pi_k^{-\frac{1}{2}} - a_{-K}) \right)$$

If there exist interim stages between the  $k$ th stage and the final stage,  $k < K - 1$ , the conditional power computed with TYPE=FINALSTAGE is not the conditional probability to reject the null hypothesis  $H_0$ . In this case, you can set the next stage as the final stage, and the conditional power is the conditional probability of rejecting  $H_0$ .

A special case of the conditional power is the futility index (Ware, Muller, and Braunwald 1985). It is 1 minus the conditional power under  $H_1 : \theta = \theta_1$ :

$$1 - p_{ku}(\theta_1) \text{ or } 1 - p_{kl}(\theta_1)$$

That is, it is the probability of accepting the null hypothesis under the alternative hypothesis given current data. A high futility index indicates a small probability of success (rejecting  $H_0$ ) given the current data.

### Predictive Power Approach

The conditional power depends on the specified reference  $\theta$ , which might be supported by the current data (Jennison and Turnbull 2000, p. 210). An alternative is to use the predictive power (Herson 1979), which is a weighted average of the conditional power over values of  $\theta$ . Without prior knowledge about  $\theta$ , then with  $\hat{\theta} = z_k / \sqrt{I_k}$ , the maximum likelihood estimate at stage  $k$ , the posterior distribution for  $\theta$  (Jennison and Turnbull 2000, p. 211) is

$$\theta | Z_K \sim N \left( \frac{z_k}{\sqrt{I_k}}, \frac{1}{I_k} \right)$$

Thus, the predictive power at stage  $k$  for the upper and lower alternatives can be derived as

$$p_{ku} = 1 - \Phi \left( (1 - \Pi_k)^{-\frac{1}{2}} (a_K \Pi_k^{\frac{1}{2}} - z_k) \right)$$

$$p_{kl} = \Phi \left( (1 - \Pi_k)^{-\frac{1}{2}} (a_{-K} \Pi_k^{\frac{1}{2}} - z_k) \right)$$

where  $a_K$  and  $a_{-K}$  are the upper and lower critical values at the final stage.

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### Repeated Confidence Intervals

In a group sequential test, repeated confidence intervals for a parameter  $\theta$  are defined as a sequence of intervals  $(\hat{\theta}_{kl}, \hat{\theta}_{ku})$ ,  $k = 1, 2, \dots, K$ , for which a simultaneous coverage probability is maintained (Jennison and Turnbull 2000, p. 189). That is, a  $(1 - \alpha)$  sequence of repeated confidence intervals has

$$\text{Prob}(\hat{\theta}_{kl} \leq \theta \leq \hat{\theta}_{ku}) = 1 - \alpha$$

These confidence limits  $\hat{\theta}_{kl}$  and  $\hat{\theta}_{ku}$  can be created from observed statistic and boundary values at each stage.

## Two-Sided Repeated Confidence Intervals

Two sequences of repeated confidence intervals can be derived for a two-sided test. One is a  $(1 - \alpha_l - \alpha_u)$  rejection repeated confidence intervals  $(\hat{\theta}_{kl}(\alpha), \hat{\theta}_{ku}(\alpha))$ ,  $k = 1, 2, \dots, K$ , and the other is a  $(1 - \beta_l - \beta_u)$  acceptance repeated confidence intervals  $(\hat{\theta}_{kl}(\beta), \hat{\theta}_{ku}(\beta))$ ,  $k = 1, 2, \dots, K$ , where  $\alpha_l$  and  $\alpha_u$  are the lower and upper Type I error probabilities for the test and  $\beta_l$  and  $\beta_u$  are the lower and upper Type II error probabilities for the test (Jennison and Turnbull 2000, p. 196).

The rejection lower and upper repeated confidence limits at stage  $k$  are

$$\hat{\theta}_{kl}(\alpha) = \hat{\theta}_k - \frac{a_k}{\sqrt{I_k}} \quad \hat{\theta}_{ku}(\alpha) = \hat{\theta}_k - \frac{a_k}{\sqrt{I_k}}$$

The hypothesis is rejected for upper alternative if the lower limit  $\hat{\theta}_{kl}(\alpha) > \theta_{0u}$  and is rejected for lower alternative if the upper limit  $\hat{\theta}_{ku}(\alpha) < \theta_{0l}$ . That is, the hypothesis is rejected if both  $\theta_{0l}$  and  $\theta_{0u}$  are not in a rejection repeated confidence interval  $(\hat{\theta}_{kl}(\alpha), \hat{\theta}_{ku}(\alpha))$ .

The acceptance lower and upper repeated confidence limits at stage  $k$  are

$$\hat{\theta}_{kl}(\beta) = \hat{\theta}_k + \left( \theta_{1l} - \frac{b_k}{\sqrt{I_k}} \right) \quad \hat{\theta}_{ku}(\beta) = \hat{\theta}_k + \left( \theta_{1u} - \frac{b_k}{\sqrt{I_k}} \right)$$

The hypothesis is accepted if the lower limit  $\hat{\theta}_{kl}(\beta) > \theta_{1l}$  and the upper limit  $\hat{\theta}_{ku}(\beta) < \theta_{1u}$ . That is, a repeated confidence interval is contained in the interval  $(\theta_{1l}, \theta_{1u})$ .

## One-Sided Repeated Confidence Intervals

Like the two-sided repeated confidence intervals, two sequences of repeated confidence intervals can be derived for a one-sided test. Suppose the one-sided test has an upper alternative  $\theta_{1u}$ . Then one sequence of repeated confidence intervals is a  $(1 - \alpha_u)$  rejection repeated confidence intervals  $(\hat{\theta}_{kl}(\alpha), \infty)$ ,  $k = 1, 2, \dots, K$ , and the other is a  $(1 - \beta_u)$  acceptance repeated confidence intervals  $(-\infty, \hat{\theta}_{ku}(\beta))$ ,  $k = 1, 2, \dots, K$ , where  $\alpha_u$  and  $\beta_u$  are the upper Type I and Type II error probabilities for the test. Thus, a sequence of repeated confidence intervals with confidence level greater than or equal to  $(1 - \alpha_u - \beta_u)$  is given by  $(\hat{\theta}_{kl}(\alpha), \hat{\theta}_{ku}(\beta))$ .

The rejection lower repeated confidence limit and the acceptance upper repeated confidence limit at stage  $k$  are

$$\hat{\theta}_{kl}(\alpha) = \hat{\theta}_k - \left( \frac{a_k}{\sqrt{I_k}} - \theta_{0u} \right) \quad \hat{\theta}_{ku}(\beta) = \hat{\theta}_k + \left( \theta_{1u} - \frac{b_k}{\sqrt{I_k}} \right)$$

The hypothesis is rejected if the lower limit  $\hat{\theta}_{kl}(\alpha) > \theta_{0u}$ . and it is accepted if the upper limit  $\hat{\theta}_{ku}(\beta) < \theta_{1u}$ .

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## Analysis after a Sequential Test

At the end of a trial, the hypothesis is either rejected or accepted. But the  $p$ -value, median, and confidence limits depend on the ordering the sample space  $(k, z)$ , where  $k$  is the stage number and  $z$  is the standardized  $Z$  statistic.

Following the notations used in Jennison and Turnbull (2000, pp. 179–180),  $(k', z') \succ (k, z)$  if  $(k', z')$  has a higher order or more extreme than  $(k, z)$ . Then for a given ordering, the  $p$ -value, median, and confidence limits associated with the observed statistics  $(k, z)$  can be derived.



***p*-value**

With the observed pair of statistics  $(k_0, z_0)$  when the trial is stopped, a one-sided upper *p*-value is computed as

$$\text{Prob}\{ (k, z) \succeq (k_0, z_0) \}$$

A one-sided lower *p*-value is computed as

$$\text{Prob}\{ (k, z) \preceq (k_0, z_0) \}$$

A two-sided *p*-value is twice the smaller of the lower and upper *p*-values.

**Median Unbiased Estimate**

With the observed pair  $(k_0, z_0)$ , a median unbiased estimate  $\theta_m$  is computed from

$$\text{Prob}\{ (k, z) \succeq (k_0, z_0) \mid \theta_m \} = 0.50$$

**Confidence Limits**

With the observed pair  $(k_0, z_0)$ , a lower  $(1 - \alpha_l)$  confidence limit for  $\theta$ ,  $\theta_l$ , is computed from

$$\text{Prob}\{ (k, z) \succeq (k_0, z_0) \mid \theta_l \} = \alpha_l$$

Similarly, an upper  $(1 - \alpha_u)$  confidence limit for  $\theta$ ,  $\theta_u$ , is computed from

$$\text{Prob}\{ (k, z) \preceq (k_0, z_0) \mid \theta_u \} = \alpha_u$$

**Available Sample Space Orderings in a Sequential Test**

At the end of a trial, the hypothesis is either rejected or accepted. Denote the stage number and the statistic at the end of a trial by a pair of statistics  $(k, z)$ , where  $k$  is the stage number and  $z$  is the standardized  $Z$  statistic. Then an ordering on the sample space  $(k, z)$  is needed to derive the *p*-value, median, and confidence limits associated with the observed statistics  $(k^*, z^*)$ .

The SEQTEST procedure provides the stagewise, LR, and MLE orderings. See Jennison and Turnbull (2000, pp. 179–187) for a detailed description and comparison of these orderings.

**Stagewise Ordering**

If the continuation regions of a design are intervals, the stagewise ordering (Fairbanks and Madsen 1982; Tsiatis, Rosner, and Mehta 1984; Jennison and Turnbull 2000, pp. 179–180) uses counter-clockwise ordering around the continuation region to compute the *p*-value, unbiased median estimate, and confidence limits. This ordering depends on the stopping region, stopping stage, and standardized statistic at the stopping stage. But it does not depend on information levels beyond the observed stage. For a one-sided design with an upper alternative,  $(k', z') \succ (k, z)$  if one of the following criteria holds:

- $k' = k$  and  $z' > z$
- $k' < k$  and  $z' \geq a_{k'}$ , the upper  $\alpha$  boundary at stage  $k'$
- $k' > k$  and  $z < b_k$ , the upper  $\beta$  boundary at stage  $k$

Similar criteria can be derived for a one-sided design with a lower alternative.

For a two-sided design with early stopping to reject the null hypothesis,  $(k', z') \succ (k, z)$  if one of the following criteria holds:

- $k' = k$  and  $z' > z$
- $k' < k$  and  $z' \geq a_{k'}$ , the upper  $\alpha$  boundary at stage  $k'$
- $k' > k$  and  $z \leq -a_k$ , the lower  $\alpha$  boundary at stage  $k$

Note that the stagewise ordering is not applicable for two-sided designs with early stopping to accept  $H_0$  or to either accept or reject  $H_0$ , which might have two disjoint continuous intervals at each interim stage.

For a two-sided design with early stopping either to reject or to accept the null hypothesis,  $(k', z') \succ (k, z)$  if one of the following criteria holds:

- $z' \geq a_{k'}$  and  $z < b_k$
- $z' > -b_{k'}$  and  $z \leq -a_k$

That is, each value in the continuation region is less extreme than each value in the upper rejection region and more extreme than each value in the lower rejection region. Then, combining with the ordering defined for a two-sided design with early stopping to reject the null hypothesis, the  $p$ -value, median, and confidence limits can be derived for the observed statistics in the lower or upper rejection region.

Thus, if the stagewise ordering is specified in the SEQTEST procedure for a two-sided design with early stopping to either reject or accept the null hypothesis, the stagewise ordering is used to derive these statistics only if the observed statistics is in the lower or upper rejection region. Otherwise, the LR ordering is used.

## LR Ordering

The LR ordering (Chang 1989) depends on the observed standardized  $Z$  statistic  $z$ , information levels, and a specified hypothetical reference. For the LR ordering under a given hypothesis  $H : \theta = \theta_g$ ,  $(k', z') \succ (k, z)$  if

$$(z' - \theta_g \sqrt{I_{k'}}) > (z - \theta_g \sqrt{I_k})$$

Under the null hypothesis  $H_0 : \theta = 0$ , it reduces to

$$z' > z$$

and can be used to derive statistics under  $H_0$ , such as  $p$ -values.

The LR ordering is applicable to all designs if all information levels are available. But depending on the boundary shape, some observed statistics  $(k, z)$  in the rejection region might be less extreme than the statistics in the acceptance region. That is, the  $p$ -value for observed statistics in the rejection region might be greater than the significance level.

## MLE Ordering

The MLE ordering (Emerson and Fleming 1990) depends only on the observed maximum likelihood estimate.  $(k', z') \succ (k, z)$  if

$$\frac{z'}{\sqrt{I_{k'}}} > \frac{z}{\sqrt{I_k}}$$

The MLE ordering is applicable to all designs if all information levels are available.

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## Applicable Tests and Sample Size Computation

The SEQDESIGN procedure assumes that the data are from a multivariate normal distribution and the sequence of the standardized test statistics  $\{Z_1, Z_2, \dots, Z_K\}$  have the following canonical joint distribution:

- $Z_k \sim N(\theta\sqrt{I_k}, 1)$
- $\text{Cov}(Z_{k_1}, Z_{k_2}) = \sqrt{I_{k_1}/I_{k_2}}$ ,  $1 \leq k_1 \leq k_2 \leq K$

where  $K$  is the total number of stages and  $I_k$  is the information available at stage  $k$ .

If the data are not from a normal distribution such as binomial distribution, then it is assumed that the test statistic is computed from a large sample such that the statistic has an approximately normal distribution.

In a clinical trial, the sample size required depends on the Type I error probability  $\alpha$ , reference improvement  $\theta_1$ , power  $1 - \beta$ , and variance of the response variable. Given a null hypothesis  $H_0 : \theta = 0$  with an upper alternative hypothesis  $H_1 : \theta = \theta_1$ , the information required for a fixed-sample test is given by

$$I_0 = \frac{(\Phi^{-1}(1 - \alpha) + \Phi^{-1}(1 - \beta))^2}{\theta_1^2}$$

where the parameter  $\theta$  depends on the test specified in the clinical trial. For example, if you are comparing two binomial populations  $H_0 : \theta = 0$ , then  $\theta = p_t - p_c$  is the difference between two proportions if the proportion difference statistic is used, and  $\theta = \log\left(\frac{p_t(1-p_c)}{p_c(1-p_t)}\right)$ , the log odds ratio for the two proportions if the log odds ratio statistic is used.

If the maximum likelihood estimate  $\hat{\theta}$  from the likelihood function can be derived, then the asymptotic variance for  $\hat{\theta}$  is  $\text{Var}(\hat{\theta}) = 1/I$ , where  $I$  is Fisher's information for  $\theta$ .

The resulting statistic  $\hat{\theta}$  corresponds to the MLE scale as specified in the BOUNDARYSCALE=MLE option in the PROC SEQDESIGN statement,  $\hat{\theta}\sqrt{I}$  corresponds to the standardized Z scale (BOUNDARYSCALE=STDZ), and  $\hat{\theta}I$  corresponds to the score scale (BOUNDARYSCALE=SCORE).

Alternatively, if the score statistic is derived, it can also be used as the test statistic and its asymptotic variance is given by Fisher's information.

For a group sequential trial, the maximum information  $I_X$  is derived in the SEQDESIGN procedure by using the specified  $\alpha$ ,  $\beta$ , and  $\theta_1$ . With the maximum information

$$I_X = \frac{1}{\text{Var}(\hat{\theta})}$$

the sample size required for a specified test statistic in the trial can be evaluated or estimated from the known or estimated variance of the response variable. Note that different designs might produce different maximum information levels for the same hypothesis, and this in turn might require a different number of observations for the trial.

With a specified test statistic, the required sample sizes at the stages can be computed. These tests include commonly used tests for normal means, binomial proportions, and survival distributions. See the section “Sample Size Computation” in “The SEQDESIGN Procedure” for a description of these tests.

## Table Output

The SEQTEST procedure displays the “Design Information” and “Test Information” tables by default.

### Conditional Power

The “Conditional Power Information” table displays the following information under a hypothetical reference:

- stopping stage
- MLE, observed maximum likelihood estimate
- conditional power under the hypothetical reference

For a one-sided test, the power are derived under hypothetical references  $\theta = \hat{\theta}$  and  $\theta = c_i \theta_1$ , where  $\hat{\theta}$  is the observed statistic,  $\theta_1$  is the alternative reference, and  $c_i$  are the values specified in the CREF= option. For a two-sided test, the power are derived under the hypothetical references  $\theta = \hat{\theta}$ ,  $\theta = c_i \theta_{1l}$ , and  $\theta = c_i \theta_{1u}$ , where  $\theta_{1l}$  is the lower alternative reference and  $\theta_{1u}$  is the upper alternative reference. The default is CREF= 0 0.5 1.0 1.5.

### Design Information

The “Design Information” table displays the design specifications and derived statistics. The derived Max Information (Percent Fixed-Sample) is the maximum information for the sequential design in percentage of the corresponding fixed-sample information.

The Null Ref ASN (Percent Fixed-Sample) is the average sample size required under the null hypothesis for the group sequential design in percentage of the corresponding fixed-sample design. Similarly, the Alt Ref ASN (Percent Fixed-Sample) is the average sample size required under the alternative reference for the group sequential design in percentage of the corresponding fixed-sample design.

### Error Spending Information

The “Error Spending Information” table displays the following information at each stage:

- proportion of information
- actual information level, if the maximum information is either specified or derived
- cumulative error spending for each boundary

## Parameter Estimates

The “Parameter Estimates” table displays the following information at the conclusion of a sequential trial:

- stopping stage
- parameter estimate
- median and confidence limits based on the specified ordering
- $p$ -value for the hypothesis  $H_0$  based on the specified ordering

## Powers and Expected Sample Sizes

The “Powers and Expected Sample Sizes” table displays the following information under each of the specified hypothetical references  $\theta = c_i\theta_1$ , where  $\theta_1$  is the alternative reference and  $c_i$  are values specified in the CREF= option.

- coefficient  $c_i$  for the hypothetical references. The value  $c_i = 0$  corresponds to the null hypothesis and  $c_i = 1$  corresponds to the alternative hypothesis
- power
- expected sample size, as percentage of fixed-sample size

For a one-sided design, the power and expected sample sizes under the hypothetical references  $\theta = c_i\theta_1$  are displayed.

For a two-sided symmetric design, the power and expected sample sizes under each of the hypothetical references  $\theta = c_i\theta_{1u}$  are displayed, where  $\theta_{1u}$  is the upper alternative reference.

For a two-sided asymmetric design, the power and expected sample sizes under each of the hypothetical references  $\theta = c_i\theta_{1l}$  and  $\theta = c_i\theta_{1u}$  are displayed, where  $\theta_{1l}$  and  $\theta_{1u}$  are the lower and upper alternative references, respectively.

For a two-sided design, the power is the probability of correctly rejecting the null hypothesis for the correct alternative. Thus, under the null hypothesis, the displayed power corresponds to a one-sided Type I error probability level—that is, the lower  $\alpha$  level or the upper  $\alpha$  level.

The expected sample size as a percentage of the corresponding fixed-sample design is

$$100 \times \frac{\sum_{k=1}^K p_k I_k}{I_0}$$

where  $p_k$  is the stopping probability at stage  $k$ ,  $\sum_{k=1}^K p_k I_k$  is the expected information level, and  $I_0$  is the information level for the fixed-sample design.

## Predictive Power

The “Predictive Power Information” table displays the following information:

- stopping stage
- MLE, observed maximum likelihood estimate
- predictive power

## Repeated Confidence Intervals

The “Repeated Confidence Intervals” table displays the following information for the observed statistic at each stage:

- information level
- parameter estimate
- rejection confidence limits. The null hypothesis is rejected for the upper alternative if the lower rejection confidence limit is greater than the null parameter value. Similarly, the null hypothesis is rejected for the lower alternative if the upper rejection confidence limit is less than the null parameter value.
- acceptance confidence limits. The upper alternative hypothesis is rejected if the upper acceptance confidence limit is less than the upper alternative value. Similarly, the lower alternative hypothesis is rejected if the lower acceptance confidence limit is greater than the upper alternative value. For a two-sided design, if both upper and lower alternative hypothesis are rejected, the null hypothesis is accepted.

## Stopping Probabilities

The “Expected Cumulative Stopping Probabilities” table displays the following information under each of the specified hypothetical references  $\theta = c_i \theta_1$ , where  $c_i$  are values specified in the CREF= option, and  $\theta_1$  is the alternative reference:

- coefficient  $c_i$  for the hypothetical references. The value  $c_i = 0$  corresponds to the null hypothesis, and  $c_i = 1$  corresponds to the alternative hypothesis
- expected stopping stage
- source of the stopping probability: reject  $H_0$  (with STOP=REJECT or STOP=BOTH), accept  $H_0$  (with STOP=ACCEPT or STOP=BOTH), or either reject or accept  $H_0$  (with STOP=BOTH)
- expected cumulative stopping probabilities at each stage

For a one-sided design, the expected cumulative stopping probabilities under the hypothetical references  $\theta = c_i \theta_{1l}$  are displayed.

For a two-sided design, the expected cumulative stopping probabilities under each of the hypothetical references  $\theta = c_i \theta_{1l}$  and  $\theta = c_i \theta_{1u}$  are displayed, where  $\theta_{1l}$  and  $\theta_{1u}$  are the lower and upper alternative references, respectively.

Note that for a symmetric two-sided design, only the expected cumulative stopping probabilities under the hypothetical references  $\theta = c_i \theta_{1u}$  are derived.

The expected stopping stage is given by  $k_0 + d$  and is derived from the expected information level

$$\sum_{k=1}^K p_k I_k = I_{k_0} + d (I_{(k_0+1)} - I_{k_0})$$

where  $p_k$  is the stopping probability at stage  $k$  and  $0 \leq d < 1$ .

For equally spaced information levels, the expected stopping stage is reduced to the weighted average

$$\sum_{k=1}^K p_k k$$

## Test Information

The “Test Information” table displays the following information at each stage:

- proportion of information
- actual information level, if the maximum information is available from the input BOUNDARY= data set
- alternative references with the specified statistic scale. If a  $p$ -value scale is specified, the standardized  $Z$  scale is used.
- boundary values with the specified statistic scale to reject or accept the null hypothesis

Note that implicitly, the test information table also contains variables for the boundary scale, stopping criterion, and type of alternative hypothesis. That is, if an ODS statement is used to save the table, the data set also contains the variables `_Scale_` for the boundary scale, `_Stop_` for the stopping criterion, and `_ALT_` for the type of alternative hypothesis.

If the test variable is specified, the table also displays the following:

- test statistic
- resulting action of test statistic: continue to the next stage, accept the null hypothesis  $H_0$ , or reject  $H_0$

## ODS Table Names

PROC SEQTEST assigns a name to each table it creates. You must use these names to reference tables when using the Output Delivery System (ODS). These names are listed in Table 84.3. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

**Table 84.3** ODS Tables Produced by PROC SEQTEST

| ODS Table Name     | Description                         | Option                                   |
|--------------------|-------------------------------------|------------------------------------------|
| CondPower          | Conditional power                   | CONDPOWER                                |
| Design             | Design information                  |                                          |
| ErrSpend           | Error spending                      | ERRSPEND                                 |
| ParameterEstimates | Parameter estimates                 | DATA( TESTVAR= ) or<br>PARMS( TESTVAR= ) |
| PowerSampleSize    | Power and expected sample sizes     | PSS                                      |
| PredPower          | Predictive power                    | PREDPOWER                                |
| RepeatedCI         | Repeated confidence intervals       | RCI                                      |
| StopProb           | Stopping probabilities              | STOPPROB                                 |
| Test               | Test statistics and boundary values |                                          |

## Graphics Output

This section describes the use of ODS for creating graphics with the SEQTEST procedure. To request these graphs, ODS Graphics must be enabled and you must specify the associated graphics options in the PROC SEQTEST statement. For more information about ODS Graphics, see Chapter 21, “Statistical Graphics Using ODS.”

### Sequential ASN Plot

The PLOTS=ASN option displays the average sample numbers (expected sample sizes for nonsurvival data or expected numbers of events for survival data) under various hypothetical references. The average sample numbers are connected for each design, and these connected curves for all designs are displayed in the “Sequential ASN Plot” graph.

For a one-sided design, average sample numbers under the hypothetical references  $\theta = c_i\theta_1$  are displayed, where  $c_i$  are the values specified in the CREF= option and  $\theta_1$  is the alternative reference. The horizontal axis displays the  $c_i$  values of these hypothetical references.

For a two-sided design, average sample numbers under each of the hypothetical references  $\theta = c_i\theta_{1l}$  and  $\theta = c_i\theta_{1u}$  are displayed, where  $\theta_{1l}$  and  $\theta_{1u}$  are the lower and upper alternative references, respectively. The horizontal axis displays  $-c_i$  values for lower hypothetical references  $\theta = c_i\theta_{1l}$  and  $c_i$  values for upper hypothetical references  $\theta = c_i\theta_{1u}$ . Note that for a symmetric two-sided design, only average sample numbers under the hypothetical references  $\theta = c_i\theta_{1u}$  are derived.

If the trial stops after the sequential test, the hypothetical reference corresponding to the test statistic is also indicated in the plot.



### Conditional Power Plot

The PLOTS=CONDPOWER option displays the conditional powers given the observed statistic under various hypothetical references. These powers are connected and are displayed in the “Conditional Power Plot” graph.

For a one-sided test, the power are derived under the hypothetical references  $\theta = \hat{\theta}$  and  $\theta = c_i\theta_1$ , where  $\hat{\theta}$  is the observed statistic,  $\theta_1$  is the alternative reference, and  $c_i$  are the values specified in the CREF= option. The horizontal axis displays these  $c_i$  values for hypothetical references.

For a two-sided test, the power are derived under hypothetical references  $\theta = \hat{\theta}$ ,  $\theta = c_i\theta_{1l}$ , and  $\theta = c_i\theta_{1u}$ , where  $\theta_{1l}$  is the lower alternative reference and  $\theta_{1u}$  is the upper alternative reference. The horizontal axis displays  $-c_i$  values for hypothetical references  $\theta = c_i\theta_{1l}$  and  $c_i$  values for hypothetical references  $\theta = c_i\theta_{1u}$ .

If the trial stops after the sequential test, the hypothetical reference corresponding to the test statistic is also indicated in the plot.

### Sequential Error Spending Plot

The PLOTS=ERRSPEND option displays the cumulative error spending at each stage on each boundary in the “Sequential Error Spending Plot” graph. A legend table uses the design labels to identify the curves for the corresponding design in the plot.

### Sequential Power Plot

The PLOTS=POWER option displays the powers under various hypothetical references. The powers are connected for each design, and these connected curves for all designs are displayed in the “Sequential Power Plot” graph.

For a one-sided design, powers under hypothetical references  $\theta = c_i\theta_1$  are displayed, where  $c_i$  are the values specified in the CREF= option and  $\theta_1$  is the alternative reference. The horizontal axis displays the  $c_i$  values of these hypothetical references.

For a two-sided design, powers under hypothetical references  $\theta = c_i\theta_{1l}$  and  $\theta = c_i\theta_{1u}$  are displayed, where  $\theta_{1l}$  and  $\theta_{1u}$  are the lower and upper alternative references, respectively. The horizontal axis displays  $-c_i$  values for lower hypothetical references  $\theta = c_i\theta_{1l}$  and  $c_i$  values for upper hypothetical references  $\theta = c_i\theta_{1u}$ . Note that for a symmetric two-sided design, only powers under hypothetical references  $\theta = c_i\theta_{1u}$  are derived.

If the trial stops after the sequential test, the hypothetical reference corresponding to the test statistic is also indicated in the plot.

### Repeated Confidence Intervals Plot

The PLOTS=RCI option displays repeated confidence intervals at each stage given the observed statistic at that stage. These repeated confidence intervals are displayed in the “Repeated Confidence Intervals Plot” graph.

## Sequential Test Plot

The PLOTS=TEST option displays boundary values and test statistics in the “Test Plot” graph. The boundary values are connected for each boundary, and both the stage number and the information level at each stage are displayed. The legend table identifies the acceptance and rejection regions in the plot.

---

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “Statistical Graphics Using ODS.”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “A Primer on ODS Statistical Graphics” on page 599 in Chapter 21, “Statistical Graphics Using ODS.”

PROC SEQTEST assigns a name to each graph it creates. You can use these names to reference the graphs when using ODS. To request these graphs, ODS Graphics must be enabled and you must specify the options indicated in Table 84.4.

**Table 84.4** Graphs Produced by PROC SEQTEST

| ODS Graph Name | Plot Description                    | Option          |
|----------------|-------------------------------------|-----------------|
| AsnPlot        | Average sample numbers              | PLOTS=ASN       |
| CondPowerPlot  | Conditional power curves            | PLOTS=CONDPower |
| ErrSpendPlot   | Error spending                      | PLOTS=ERRSPEND  |
| PowerPlot      | Power curves                        | PLOTS=POWER     |
| RepeatedCIPlot | Repeated confidence intervals       | PLOTS=RCI       |
| TestPlot       | Boundary values and test statistics | PLOTS=TEST      |

---

## Examples: SEQTEST Procedure

The following examples perform group sequential tests with various designs and test statistics.

Four statistic scales are available for the input boundary values, the input test statistic, and the displayed test information in the SEQTEST procedure. These are the maximum likelihood estimator scale, score statistic scale, standardized normal Z scale, and  $p$ -value scale. There is a unique one-to-one transformation between any two of the scales, and you can use different scales for the input boundary values and input test statistic. These boundary values and test statistic are displayed with the scale specified in the BOUNDARYSCALE= option in the SEQTEST procedure.

## Example 84.1: Testing the Difference between Two Proportions

This example demonstrates group sequential tests that use an O'Brien-Fleming group sequential design. A clinic is studying the effect of vitamin C supplements in treating flu symptoms. The study consists of patients in the clinic who have exhibited the first sign of flu symptoms within the last 24 hours. These patients are randomly assigned to either the control group (which receives placebo pills) or the treatment group (which receives large doses of vitamin C supplements). At the end of a five-day period, the flu symptoms of each patient are recorded.

Suppose that you know from past experience that flu symptoms disappear in five days for 60% of patients who experience flu symptoms. The clinic would like to detect a 75% symptom disappearance with a high probability. A test that compares the proportions directly specifies the null hypothesis  $H_0 : \theta = p_t - p_c = 0$  with a one-sided alternative  $H_1 : \theta > 0$  and a power of 0.90 at  $H_1 : \theta = 0.15$ , where  $p_t$  and  $p_c$  are the proportions of symptom disappearance in the treatment group and control group, respectively.

The following statements invoke the SEQDESIGN procedure and request a four-stage group sequential design by using an O'Brien-Fleming method for normally distributed data. The design uses a one-sided alternative hypothesis with early stopping either to accept or reject the null hypothesis  $H_0$ . The BOUNDARYSCALE=MLE option uses the MLE scale to display statistics in the boundary table and boundary plots.

```
ods graphics on;
proc seqdesign altref=0.15
 boundaryscale=mle
 ;
 OBrienFleming: design method=obf
 nstages=4
 alt=upper
 stop=both
 alpha=0.025
 ;
 samplesize model=twosamplefreq(nullprop=0.6 test=prop);
 ods output Boundary=Bnd_Count;
run;
ods graphics off;
```

The ODS OUTPUT statement with the BOUNDARY=BND\_COUNT option creates an output data set named BND\_COUNT which contains the resulting boundary information for the subsequent sequential tests.

The “Design Information” table in [Output 84.1.1](#) displays design specifications. With the specified alternative hypothesis  $H_1 : \theta = 0.15$ , the maximum information is derived to achieve a power of 0.90 at  $H_1$ . The derived fixed-sample information ratio 1.0767 is the maximum information needed for a group sequential design relative to its corresponding fixed-sample design.

**Output 84.1.1** O'Brien-Fleming Design Information

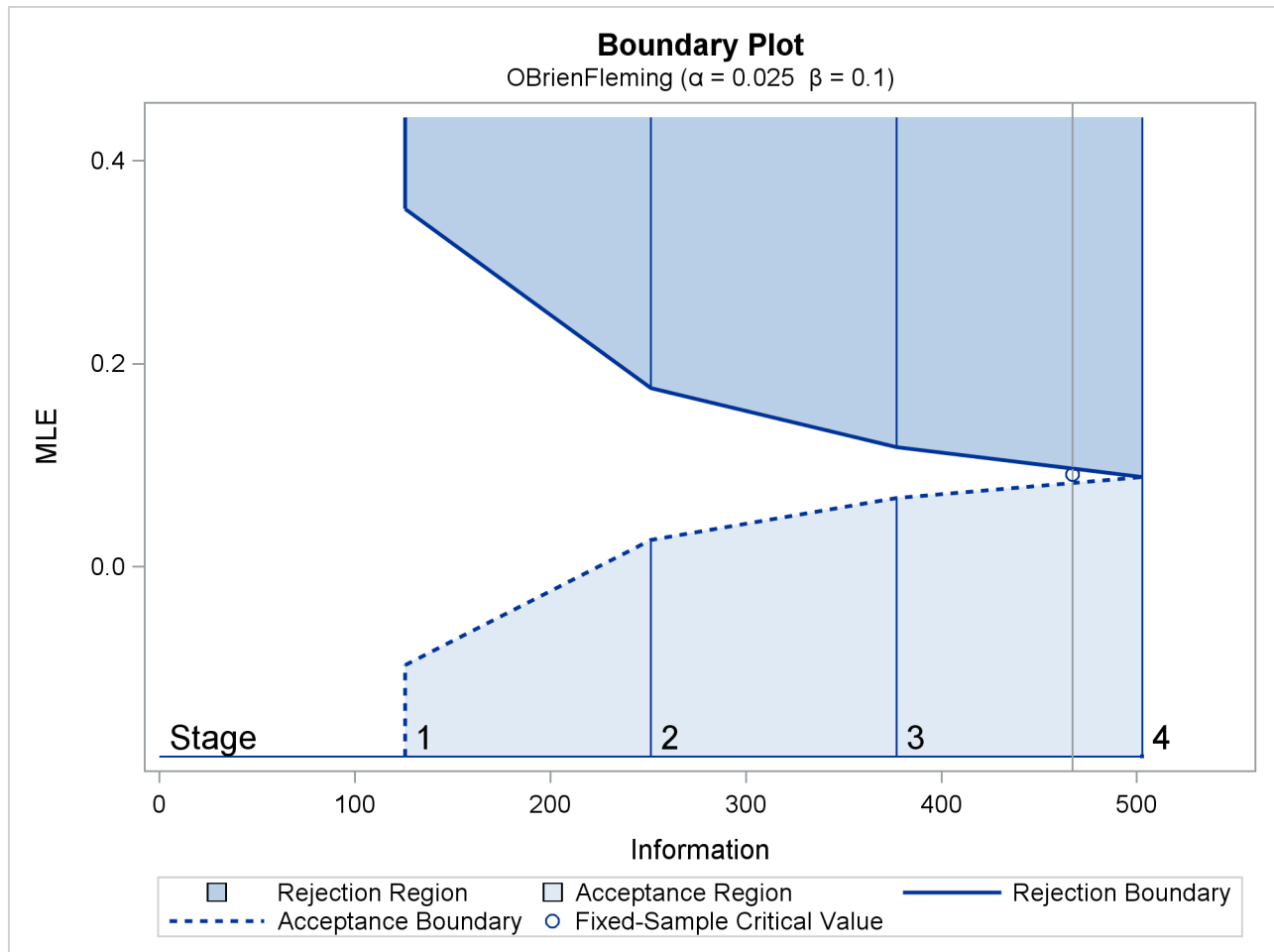
| The SEQDESIGN Procedure                   |                    |
|-------------------------------------------|--------------------|
| Design: OBrienFleming                     |                    |
| Design Information                        |                    |
| Statistic Distribution                    | Normal             |
| Boundary Scale                            | MLE                |
| Alternative Hypothesis                    | Upper              |
| Early Stop                                | Accept/Reject Null |
| Method                                    | O'Brien-Fleming    |
| Boundary Key                              | Both               |
| Alternative Reference                     | 0.15               |
| Number of Stages                          | 4                  |
| Alpha                                     | 0.025              |
| Beta                                      | 0.1                |
| Power                                     | 0.9                |
| Max Information (Percent of Fixed Sample) | 107.6741           |
| Max Information                           | 502.8343           |
| Null Ref ASN (Percent of Fixed Sample)    | 61.12891           |
| Alt Ref ASN (Percent of Fixed Sample)     | 75.89782           |

The “Boundary Information” table in [Output 84.1.2](#) displays the information level, alternative reference, and boundary values at each stage. With the BOUNDARYSCALE=MLE option, the SEQDESIGN procedure displays the output boundaries with the maximum likelihood estimator scale.

**Output 84.1.2** O'Brien-Fleming Boundary Information

| Boundary Information (MLE Scale) |                             |          |          |               |                         |         |
|----------------------------------|-----------------------------|----------|----------|---------------|-------------------------|---------|
| Null Reference = 0               |                             |          |          |               |                         |         |
| _Stage_                          | -----Information Level----- |          |          | -Alternative- | ----Boundary Values---- |         |
|                                  | Proportion                  | Actual   | N        | --Reference-- | -----Upper-----         |         |
|                                  |                             |          |          | Upper         | Beta                    | Alpha   |
| 1                                | 0.2500                      | 125.7086 | 107.4808 | 0.15000       | -0.09709                | 0.35291 |
| 2                                | 0.5000                      | 251.4171 | 214.9617 | 0.15000       | 0.02645                 | 0.17645 |
| 3                                | 0.7500                      | 377.1257 | 322.4425 | 0.15000       | 0.06764                 | 0.11764 |
| 4                                | 1.0000                      | 502.8343 | 429.9233 | 0.15000       | 0.08823                 | 0.08823 |

With ODS Graphics enabled, a detailed boundary plot with the rejection and acceptance regions is displayed, as shown in [Output 84.1.3](#). The horizontal axis indicates the information levels for the design. The stages are indicated by vertical lines with accompanying stage numbers. If the test statistic at a stage is in a rejection region, the trial stops and the hypothesis is rejected. If the test statistic is in an acceptance region, then the trial also stops and the hypothesis is accepted. If the statistic is not in a rejection or an acceptance region, the trial continues to the next stage.

**Output 84.1.3** O'Brien-Fleming Boundary Plot

The boundary plot also displays the information level and critical value for the corresponding fixed-sample design. The solid and dashed lines at the fixed-sample information level correspond to the rejection and acceptance lines, respectively.

With the SAMPLESIZE statement, the maximum information is used to derive the required sample size for the study. The “Sample Size Summary” table in [Output 84.1.4](#) displays parameters for the sample size computation.

**Output 84.1.4** Required Sample Size Summary

| Sample Size Summary             |                        |
|---------------------------------|------------------------|
| Test                            | Two-Sample Proportions |
| Null Proportion                 | 0.6                    |
| Proportion (Group A)            | 0.75                   |
| Test Statistic                  | Z for Proportion       |
| Reference Proportions           | Alt Ref                |
| Max Sample Size                 | 429.9233               |
| Expected Sample Size (Null Ref) | 244.0768               |
| Expected Sample Size (Alt Ref)  | 303.0464               |

With the derived maximum information and the specified MODEL= option in the SAMPLESIZE statement, the total sample size in each group for testing the difference between two proportions under the alternative hypothesis is

$$N_1 = N_2 = (p_{1c} (1 - p_{1c}) + p_{1t} (1 - p_{1t})) I_X$$

where  $p_{1c} = 0.6$  and  $p_{1t} = p_{1c} + \theta_1 = 0.75$ . By default (or equivalently if you specify REF=PROP in the MODEL=TWOSAMPLEFREQ option), the required sample sizes are computed under the alternative hypothesis. See the section “Test for the Difference between Two Binomial Proportions” in the chapter “The SEQDESIGN Procedure” for a description of these parameters.

The “Sample Sizes (N)” table in [Output 84.1.5](#) displays the required sample sizes at each stage, in both fractional and integer numbers. The derived sample sizes under the heading Fractional N which correspond to the design are not integers. These sample sizes are rounded up to integers under the heading Ceiling N. In practice, integer sample sizes are used, and the information levels increase slightly. Thus, 54, 108, 162, and 215 patients are needed in each group for the four stages, respectively.

**Output 84.1.5** Required Sample Sizes

| Sample Sizes (N)                            |        |          |          |             |
|---------------------------------------------|--------|----------|----------|-------------|
| Two-Sample Z Test for Proportion Difference |        |          |          |             |
| -----Fractional N-----                      |        |          |          |             |
| _Stage_                                     | N      | N(Grp 1) | N(Grp 2) | Information |
| 1                                           | 107.48 | 53.74    | 53.74    | 125.7       |
| 2                                           | 214.96 | 107.48   | 107.48   | 251.4       |
| 3                                           | 322.44 | 161.22   | 161.22   | 377.1       |
| 4                                           | 429.92 | 214.96   | 214.96   | 502.8       |

| Sample Sizes (N)                            |     |          |          |             |
|---------------------------------------------|-----|----------|----------|-------------|
| Two-Sample Z Test for Proportion Difference |     |          |          |             |
| -----Ceiling N-----                         |     |          |          |             |
| _Stage_                                     | N   | N(Grp 1) | N(Grp 2) | Information |
| 1                                           | 108 | 54       | 54       | 126.3       |
| 2                                           | 216 | 108      | 108      | 252.6       |
| 3                                           | 324 | 162      | 162      | 378.9       |
| 4                                           | 430 | 215      | 215      | 502.9       |

Suppose the trial follows the study plan, and 54 patients are available in each group at stage 1. The data set count\_1 contains these 108 patients. [Output 84.1.6](#) lists the first 10 observations of the data set.

**Output 84.1.6** Clinical Trial Data

| First 10 Obs in the Trial Data |     |      |
|--------------------------------|-----|------|
| Obs                            | Trt | Resp |
| 1                              | 0   | 0    |
| 2                              | 1   | 1    |
| 3                              | 0   | 1    |
| 4                              | 1   | 0    |
| 5                              | 0   | 0    |
| 6                              | 1   | 0    |
| 7                              | 0   | 0    |
| 8                              | 1   | 1    |
| 9                              | 0   | 1    |
| 10                             | 1   | 0    |

The Trt variable is a grouping variable with value 0 for a patient in the placebo control group and value 1 for a patient in the treatment group who is given vitamin C supplements. The Resp variable is an indicator variable with value 1 for a patient without flu symptoms after five days and value 0 for a patient with flu symptoms after five days.

The following statements use the GENMOD procedure to estimate the treatment effect at stage 1:

```
proc genmod data=count_1;
 model Resp= Trt;
 ods output ParameterEstimates=Parms_Count1;
run;
```

Output 84.1.7 displays the treatment effect at stage 1.

**Output 84.1.7** Stage 1 Treatment Difference

| The GENMOD Procedure                               |    |          |                |                            |                 |            |  |
|----------------------------------------------------|----|----------|----------------|----------------------------|-----------------|------------|--|
| Analysis Of Maximum Likelihood Parameter Estimates |    |          |                |                            |                 |            |  |
| Parameter                                          | DF | Estimate | Standard Error | Wald 95% Confidence Limits | Wald Chi-Square | Pr > ChiSq |  |
| Intercept                                          | 1  | 0.6296   | 0.0627         | 0.5066 0.7526              | 100.68          | <.0001     |  |
| Trt                                                | 1  | 0.1111   | 0.0887         | -0.0628 0.2850             | 1.57            | 0.2105     |  |
| Scale                                              | 1  | 0.4611   | 0.0314         | 0.4035 0.5269              |                 |            |  |

NOTE: The scale parameter was estimated by maximum likelihood.

The test statistic is  $\hat{\theta}_1 = \hat{p}_t - \hat{p}_c = 0.1111$ , and its associated standard error is

$$\sqrt{\text{Var}(\hat{\theta}_1)} = \sqrt{\frac{\hat{p}_c(1 - \hat{p}_c)}{54} + \frac{\hat{p}_t(1 - \hat{p}_t)}{54}} = 0.0887$$

The following statements create and display (in [Output 84.1.8](#)) the data set that contains the parameter estimate at stage 1,  $\hat{\theta}_1 = 0.1111$ , and its associated standard error  $\sqrt{\text{Var}(\hat{\theta}_1)} = 0.0887$  which are used in the SEQTEST procedure:

```
data Parms_Count1;
 set Parms_Count1;
 if Parameter='Trt';
 Scale='MLE';
 Stage= 1;
 keep _Scale_ _Stage_ Parameter Estimate StdErr;
run;

proc print data=Parms_Count1;
 title 'Statistics Computed at Stage 1';
run;
```

**Output 84.1.8** Statistics Computed at Stage 1

| Statistics Computed at Stage 1 |           |          |        |         |         |
|--------------------------------|-----------|----------|--------|---------|---------|
| Obs                            | Parameter | Estimate | StdErr | _Scale_ | _Stage_ |
| 1                              | Trt       | 0.1111   | 0.0887 | MLE     | 1       |

The initial required sample sizes are derived with the proportions  $p_c = 0.6$  and  $p_t = 0.75$ . If the observed proportions are different from these assumed values, or if the number of available patients is different from the study plan in one of the stages, then the information level that corresponds to the test statistic is estimated from

$$I_k = \frac{1}{\text{Var}(\hat{\theta}_k)}$$

The following statements invoke the SEQTEST procedure and test for early stopping at stage 1:

```
ods graphics on;
proc seqtest Boundary=Bnd_Count
 Parms (Testvar=Trt)=Parms_Count1
 infoadj=none
 errspendmin=0.001
 boundaryscale=mle
 errspend
 plots=errspend
 ;
 ods output Test=Test_Count1;
run;
ods graphics off;
```

The BOUNDARY= option specifies the input data set that provides the boundary information for the trial at stage 1, which was generated in the SEQDESIGN procedure. The PARMS=PARMS\_COUNT1 option specifies the input data set PARMS\_COUNT1 that contains the test statistic and its associated standard error at stage 1, and the TESTVAR=TRT option identifies the test variable TRT in the data set. The INFOADJ=NONE option maintains the information levels at future interim stages (2 and 3) as provided in the



BOUNDARY= data set. The BOUNDARYSCALE=MLE option displays the output boundaries in terms of the MLE scale.

The O'Brien-Fleming design is conservative in early stages and might not be desirable in a clinical trial. The ERRSPENDMIN=0.001 option specifies the minimum error spending at each stage to be 0.001, and it might increase the corresponding nominal  $p$ -value in early stages for the trial. The BOUNDARYSCALE=MLE option uses the MLE scale to display test statistics in the boundary table and boundary plots.

The ODS OUTPUT statement with the TEST=TEST\_COUNT1 option creates an output data set named TEST\_COUNT1 which contains the updated boundary information for the test at stage 1. The data set also provides the boundary information that is needed for the group sequential test at the next stage.

The “Design Information” table in [Output 84.1.9](#) displays design specifications. The derived statistics, such as the overall  $\alpha$  and  $\beta$  levels, are derived from the specified maximum information and boundary values in the BOUNDARY= data set. Note that with a minor change in the information level at stage 1, the power also changes slightly from the design provided in the BOUNDARY= data set.

**Output 84.1.9** Design Information

| The SEQTEST Procedure                     |                    |
|-------------------------------------------|--------------------|
| Design Information                        |                    |
| BOUNDARY Data Set                         | WORK.BND_COUNT     |
| Data Set                                  | WORK.PARMS_COUNT1  |
| Statistic Distribution                    | Normal             |
| Boundary Scale                            | MLE                |
| Alternative Hypothesis                    | Upper              |
| Early Stop                                | Accept/Reject Null |
| Number of Stages                          | 4                  |
| Alpha                                     | 0.025              |
| Beta                                      | 0.10147            |
| Power                                     | 0.89853            |
| Max Information (Percent of Fixed Sample) | 108.2301           |
| Max Information                           | 502.834283         |
| Null Ref ASN (Percent of Fixed Sample)    | 61.09917           |
| Alt Ref ASN (Percent of Fixed Sample)     | 73.9745            |

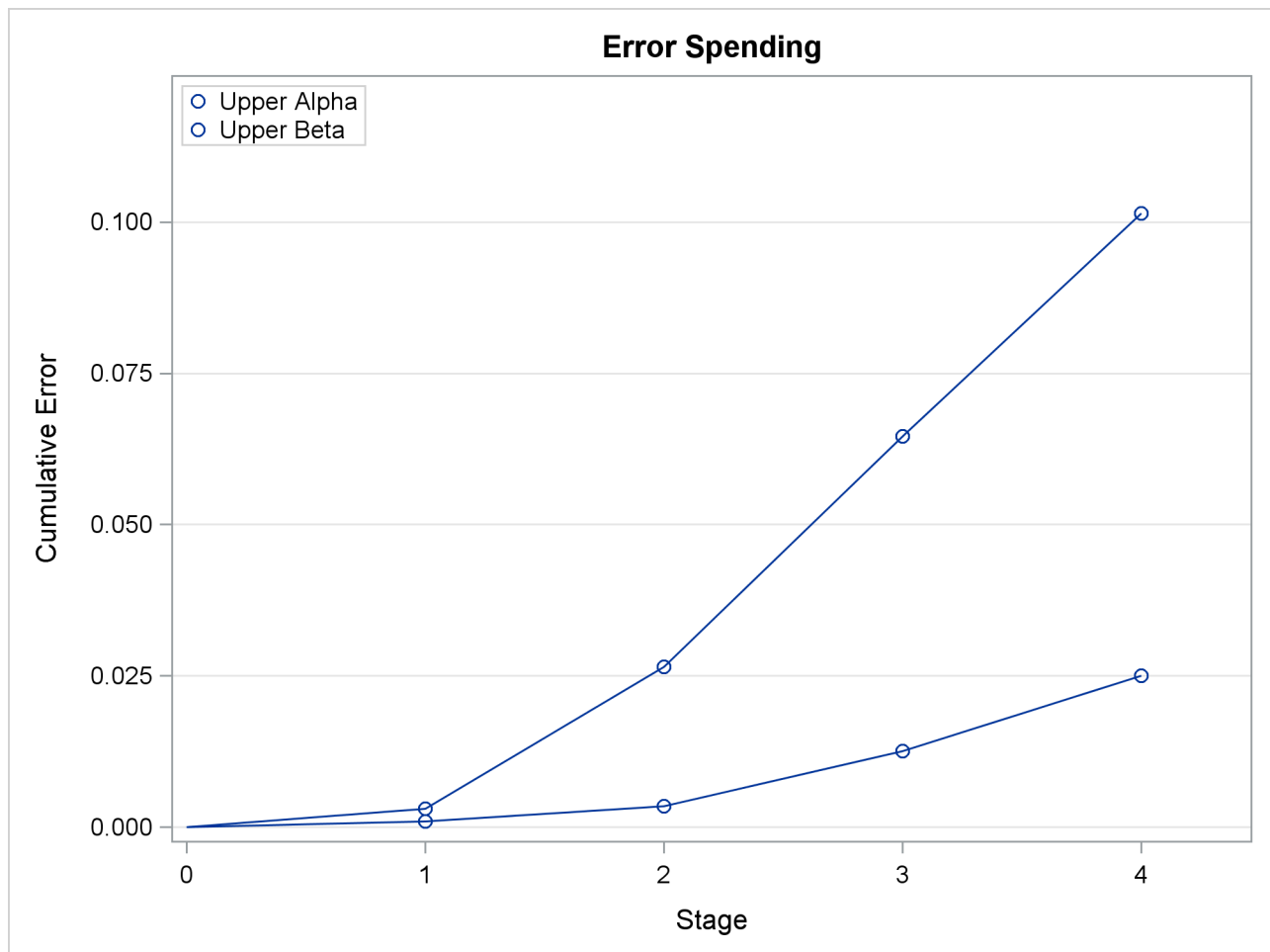
With the ERRSPEND option, the “Error Spending Information” table in [Output 84.1.10](#) displays cumulative error spending at each stage for each boundary. By default (or equivalently if you specify BOUNDARYKEY=ALPHA), the Type I error level  $\alpha = 0.025$  is maintained. Furthermore, with the ERRSPENDMIN=0.001 option, the  $\alpha$  spending at each stage is greater than or equal to 0.001.

**Output 84.1.10** Error Spending Information

| Error Spending Information |                         |          |                             |         |
|----------------------------|-------------------------|----------|-----------------------------|---------|
| _Stage_                    | ---Information Level--- |          | -Cumulative Error Spending- |         |
|                            | Proportion              | Actual   | Beta                        | Alpha   |
| 1                          | 0.2525                  | 126.9871 | 0.00308                     | 0.00100 |
| 2                          | 0.5000                  | 251.4171 | 0.02653                     | 0.00343 |
| 3                          | 0.7500                  | 377.1257 | 0.06456                     | 0.01254 |
| 4                          | 1.0000                  | 502.8343 | 0.10147                     | 0.02500 |

With the PLOTS=ERRSPEND option, the procedure displays a plot of error spending for each boundary, as shown in [Output 84.1.11](#). The error spending values in the “Error Spending Information” table in [Output 84.1.10](#) are displayed in the plot.

**Output 84.1.11** Error Spending Plot



The “Test Information” table in [Output 84.1.12](#) displays the boundary values for the design, test statistic, and resulting action at each stage. With the BOUNDARYSCALE=MLE option, the maximum likelihood

estimator scale is used for the test statistic and boundary values. The table shows that the test statistic 0.1111 is between the upper  $\alpha$  and  $\beta$  boundaries, so the trial continues to the next stage.

#### Output 84.1.12 Sequential Test

| Test Information (MLE Scale) |                        |          |                        |                          |         |
|------------------------------|------------------------|----------|------------------------|--------------------------|---------|
| Null Reference = 0           |                        |          |                        |                          |         |
| _Stage_                      | ---Information Level-- |          | -Alternative-          | -----Boundary Values---- |         |
|                              | Proportion             | Actual   | --Reference--<br>Upper | -----Upper-----<br>Beta  | Alpha   |
| 1                            | 0.2525                 | 126.9871 | 0.15000                | -0.09306                 | 0.27423 |
| 2                            | 0.5000                 | 251.4171 | 0.15000                | 0.02674                  | 0.17527 |
| 3                            | 0.7500                 | 377.1257 | 0.15000                | 0.06805                  | 0.11792 |
| 4                            | 1.0000                 | 502.8343 | 0.15000                | 0.08875                  | 0.08875 |

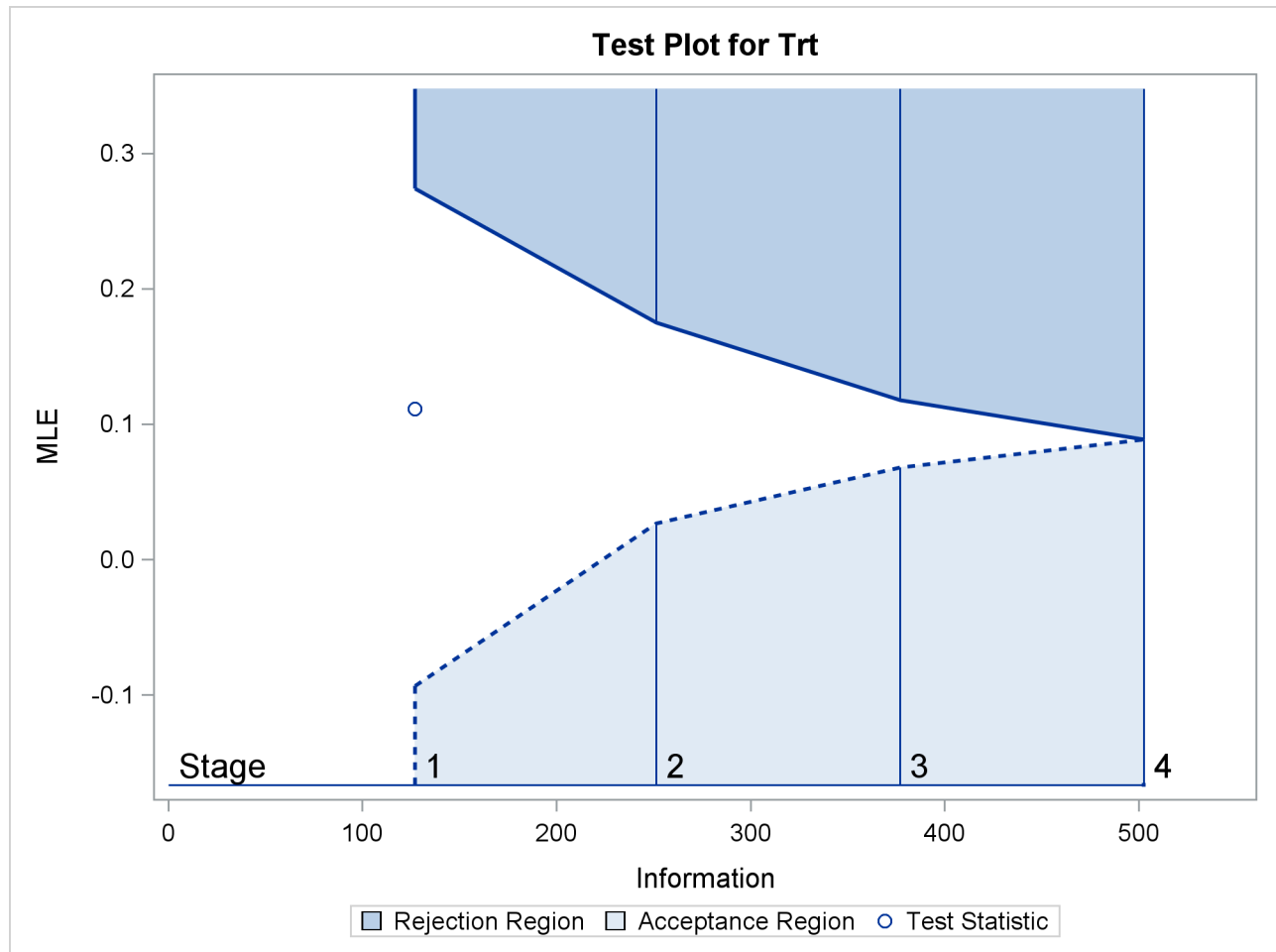
| Test Information (MLE Scale) |          |                         |
|------------------------------|----------|-------------------------|
| Null Reference = 0           |          |                         |
| _Stage_                      | Estimate | -----Test-----          |
|                              |          | -----Trt-----<br>Action |
| 1                            | 0.11111  | Continue                |
| 2                            | .        |                         |
| 3                            | .        |                         |
| 4                            | .        |                         |

The information level at stage 1 is derived from the standard error,

$$I_1 = \frac{1}{\text{Var}(\hat{\theta}_1)} = \frac{1}{(\text{s.e.}(\hat{\theta}_1))^2} = 126.987$$

By default (or equivalently if you specify PLOTS=TEST), the “Test Plot” graph displays boundary values of the design and the test statistic at stage 1, as shown in [Output 84.1.13](#). It also shows that the observed statistic is in the continuation region.

Output 84.1.13 Sequential Test Plot



The observed information level at stage 1,  $I_1 = 126.987$ , is slightly larger than the target information level at the design. If an observed information level in the study is substantially different from its target level in the design, then the sample sizes should be adjusted in the subsequent stages to achieve the target information levels.

Suppose the trial continues to the next stage, and 108 patients are available in each group at stage 2. The data set COUNT\_2 contains these 216 patients.

The following statements use the GENMOD procedure to estimate the treatment effect at stage 2:

```
proc genmod data=Count_2;
 model Resp= Trt;
 ods output ParameterEstimates=Parms_Count2;
run;
```

The following statements create the parameter estimate at stage 2,  $\hat{\theta}_2 = \hat{p}_2 - \hat{p}_1 = 0.1759$ , and its associated standard error  $\sqrt{\text{Var}(\hat{\theta}_2)} = 0.0623$  into a test data set:

```
data Parms_Count2;
 set Parms_Count2;
 if Parameter='Trt';
 Scale='MLE';
 Stage= 2;
 keep _Scale_ _Stage_ Parameter Estimate StdErr;
run;

proc print data=Parms_Count2;
 title 'Statistics Computed at Stage 2';
run;
```

Output 84.1.14 displays the test statistics at stage 2.

**Output 84.1.14** Statistics Computed at Stage 2

| Statistics Computed at Stage 2 |           |          |        |         |         |
|--------------------------------|-----------|----------|--------|---------|---------|
| Obs                            | Parameter | Estimate | StdErr | _Scale_ | _Stage_ |
| 1                              | Trt       | 0.1759   | 0.0623 | MLE     | 2       |

The following statements invoke the SEQTEST procedure and test for early stopping at stage 2:

```
ods graphics on;
proc seqtest Boundary=Test_Count1
 Parms(Testvar=Trt)=Parms_Count2
 infoadj=none
 boundaryscale=mle
 ;
 ods output Test=Test_Count2;
run;
ods graphics off;
```

The BOUNDARY= option specifies the input data set that provides the boundary information for the trial at stage 2, which was generated by the SEQTEST procedure at the previous stage. The PARMS= option specifies the input data set that contains the test statistic and its associated standard error at stage 2, and the TESTVAR= option identifies the test variable in the data set.

The ODS OUTPUT statement with the TEST=TEST\_COUNT2 option creates an output data set named TEST\_COUNT2 which contains the updated boundary information for the test at stage 2. The data set also provides the boundary information that is needed for the group sequential test at the next stage.

The “Test Information” table in [Output 84.1.15](#) displays the boundary values, test statistic, and resulting action at each stage. The table shows that the test statistic 0.17593 is larger than the corresponding upper alpha boundary value, so the trial stops to reject the hypothesis.

**Output 84.1.15** Sequential Test

```

The SEQTEST Procedure

Test Information (MLE Scale)
Null Reference = 0

---Information Level---
Stage Proportion Actual -Alternative-
 0.2525 126.9871 --Reference--
 0.5122 257.5571 --Upper
 0.7500 377.1257 Beta
 1.0000 502.8343 Alpha

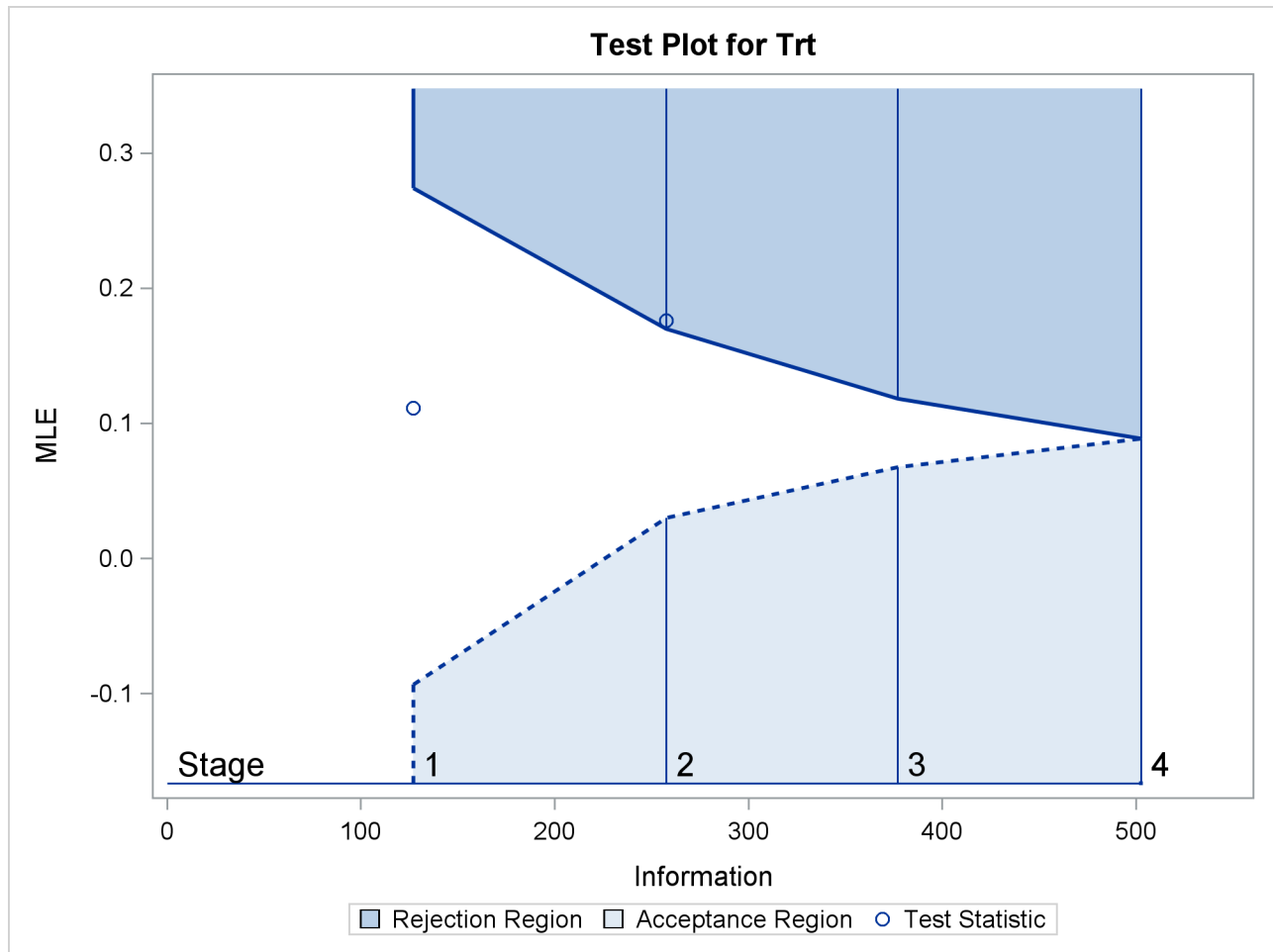
Test Information (MLE Scale)
Null Reference = 0

-----Test-----
-----Trt-----
Stage Estimate Action
 1 0.11111 Continue
 2 0.17593 Reject Null
 3 .
 4 .

```

With ODS Graphics enabled, the “Test Plot” is displayed, as shown in [Output 84.1.16](#). The plot displays boundary values of the design and the test statistics at the first two stages. As expected, the test statistic at stage 2 is in the “Upper Rejection Region” above the upper alpha boundary.

Output 84.1.16 Sequential Test Plot



After a trial is stopped, the “Parameter Estimates” table in [Output 84.1.17](#) displays the stopping stage and the maximum likelihood estimate of the parameter. It also displays the  $p$ -value, median estimate, and confidence limits for the parameter that correspond to the observed statistic by using the specified sample space ordering.

Output 84.1.17 Parameter Estimates

| Parameter Estimates<br>Stagewise Ordering |                |          |                          |                 |              |
|-------------------------------------------|----------------|----------|--------------------------|-----------------|--------------|
| Parameter                                 | Stopping Stage | MLE      | p-Value for<br>H0:Parm=0 | Median Estimate | Lower 95% CL |
| Trt                                       | 2              | 0.175926 | 0.0031                   | 0.174462        | 0.07059      |

The MLE statistic at the stopping stage is the maximum likelihood estimate of the parameter and is biased. The computation of  $p$ -value, unbiased median estimate, and confidence limits depends on the ordering of the sample space  $(k, z)$ , where  $k$  is the stage number and  $z$  is the observed standardized  $Z$  statistic. By default

(or equivalently if you specify ORDER=STAGewise), the stagewise ordering that uses counterclockwise ordering around the continuation region is used to compute the  $p$ -value, unbiased median estimate, and confidence limits. As expected, the  $p$ -value is less than 0.025, and the confidence interval does not contain the null reference zero. With the stagewise ordering, the  $p$ -value is computed as

$$P_{\theta=0}(Z_1 > a_1) + P_{\theta=0}(Z_2 > z_2 \mid b_1 < Z_1 < a_1)$$

where  $z_2$  is the observed standardized  $Z$  statistic at stage 2,  $Z_1$  is the standardized normal variate at stage 1,  $Z_2$  is the standardized normal variate at stage 2, and  $a_1$  and  $b_1$  are the stage 1 upper rejection and acceptance boundary values, respectively.

See the section “Available Sample Space Orderings in a Sequential Test” on page 7230 for a detailed description of the stagewise ordering.

## Example 84.2: Testing an Effect in a Regression Model

This example demonstrates a two-sided group sequential test that uses an error spending design with early stopping to reject the null hypothesis. A study is conducted to examine the effects of Age (years), Weight (kg), RunTime (time in minutes to run 1.5 miles), RunPulse (heart rate while running), and MaxPulse (maximum heart rate recorded while running) on Oxygen (oxygen intake rate, ml per kg body weight per minute). The primary interest is whether oxygen intake rate is associated with weight.

The hypothesis is tested using the following linear model:

$$\text{Oxygen} = \text{Age} + \text{Weight} + \text{RunTime} + \text{RunPulse} + \text{MaxPulse}$$

The null hypothesis is  $H_0 : \beta_w = 0$ , where  $\beta_w$  is the regression parameter for the variable Weight. Suppose that  $\beta_w = 0.10$  is the reference improvement that should be detected at a 0.90 level. Then the maximum information  $I_X$  can be derived in the SEQDESIGN procedure.

Following the derivations in the section “Test for a Parameter in the Regression Model” in the chapter “The SEQDESIGN Procedure,” the required sample size can be derived from

$$N = I_X \frac{\sigma_y^2}{(1 - r_x^2) \sigma_x^2}$$

where  $\sigma_y^2$  is the variance of the response variable in the regression model,  $r_x^2$  is the proportion of variance of Weight explained by other covariates, and  $\sigma_x^2$  is the variance of Weight.

Further suppose that from past experience,  $\sigma_y^2 = 5$ ,  $r_x^2 = 0.10$ , and  $\sigma_x^2 = 64$ . Then the required sample size can be derived using the SAMPLESIZE statement in the SEQDESIGN procedure.



The following statements invoke the SEQDESIGN procedure and request a three-stage group sequential design for normally distributed data to test the null hypothesis of a regression parameter  $H_0 : \beta_w = 0$  against the alternative  $H_1 : \beta_w \neq 0$ :

```
ods graphics on;
proc seqdesign altref=0.10;
 OBFErrorFunction: design method=errfuncobf
 nstages=3
 info=cum(2 3 4)
 ;
 sample size model=reg(variance=5 xvariance=64 xrsquare=0.10);
 ods output Boundary=Bnd_Fit;
run;
ods graphics off;
```

By default (or equivalently if you specify ALPHA=0.05 and BETA=0.10), the procedure uses a Type I error probability 0.05 and a Type II error probability 0.10. The ALTREF=0.10 option specifies a power of  $1 - \beta = 0.90$  at the alternative hypothesis  $H_1 : \beta_w = \pm 0.10$ . The INFO=CUM(2 3 4) option specifies that the study perform the first interim analysis with information proportion  $2/4 = 0.5$ —that is, after half of the total observations are collected.

The ODS OUTPUT statement with the BOUNDARY=BND\_FIT option creates an output data set named BND\_FIT which contains the resulting boundary information for the subsequent sequential tests.

The “Design Information” table in [Output 84.2.1](#) displays design specifications and derived statistics. Since the alternative reference is specified, the maximum information is derived.

#### Output 84.2.1 Design Information

| The SEQDESIGN Procedure                   |                |
|-------------------------------------------|----------------|
| Design: OBFErrorFunction                  |                |
| Design Information                        |                |
| Statistic Distribution                    | Normal         |
| Boundary Scale                            | Standardized Z |
| Alternative Hypothesis                    | Two-Sided      |
| Early Stop                                | Reject Null    |
| Method                                    | Error Spending |
| Boundary Key                              | Both           |
| Alternative Reference                     | 0.1            |
| Number of Stages                          | 3              |
| Alpha                                     | 0.05           |
| Beta                                      | 0.1            |
| Power                                     | 0.9            |
| Max Information (Percent of Fixed Sample) | 101.8276       |
| Max Information                           | 1069.948       |
| Null Ref ASN (Percent of Fixed Sample)    | 101.2587       |
| Alt Ref ASN (Percent of Fixed Sample)     | 77.81586       |

The “Boundary Information” table in [Output 84.2.2](#) displays information level, alternative reference, and boundary values at each stage.

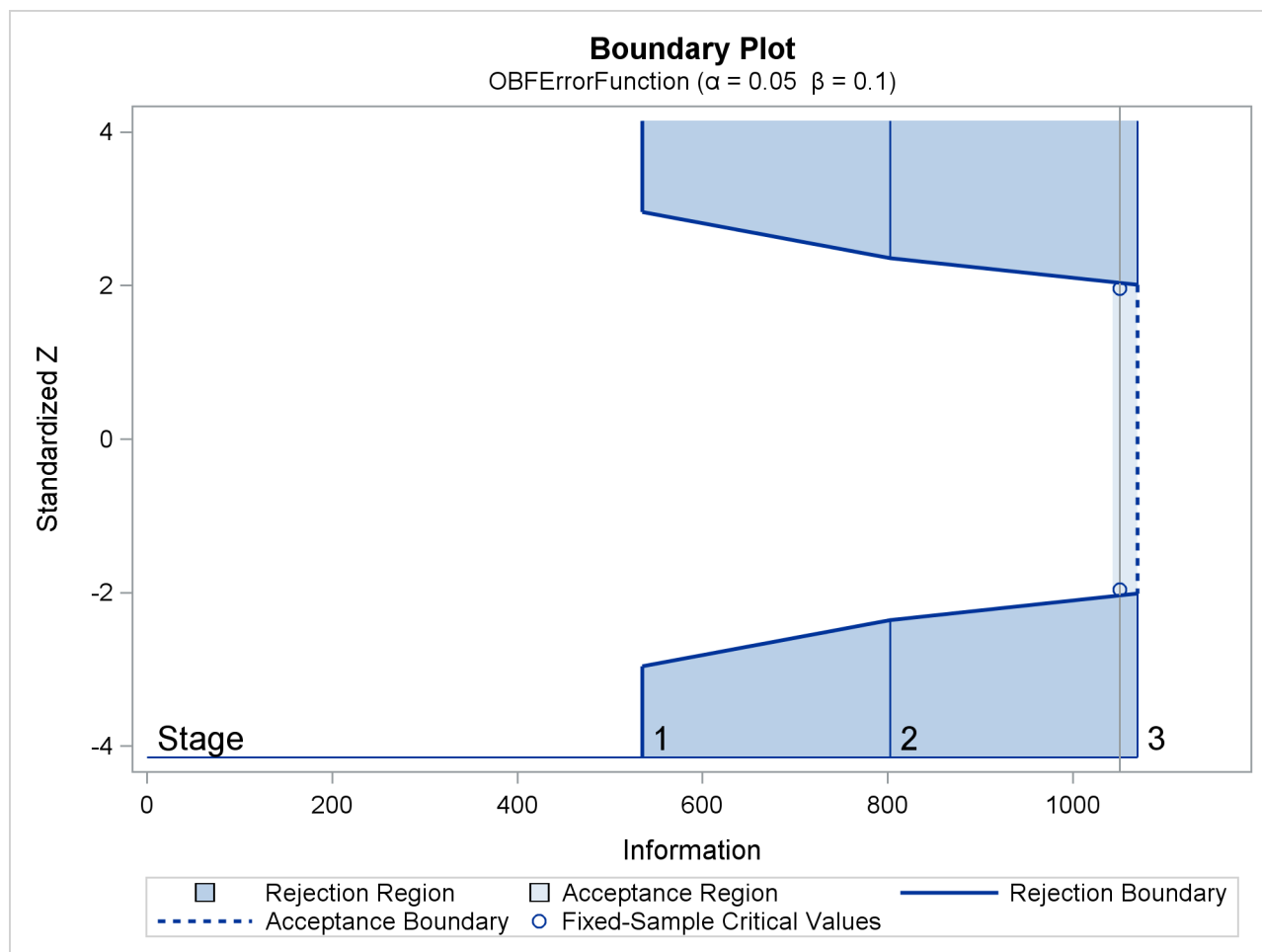
**Output 84.2.2** Boundary Information

| Boundary Information (Standardized Z Scale) |                             |          |          |                       |         |
|---------------------------------------------|-----------------------------|----------|----------|-----------------------|---------|
| Null Reference = 0                          |                             |          |          |                       |         |
| _Stage_                                     | -----Information Level----- |          |          | -----Alternative----- |         |
|                                             | Proportion                  | Actual   | N        | Lower                 | Upper   |
| 1                                           | 0.5000                      | 534.9738 | 46.43869 | -2.31295              | 2.31295 |
| 2                                           | 0.7500                      | 802.4606 | 69.65804 | -2.83277              | 2.83277 |
| 3                                           | 1.0000                      | 1069.948 | 92.87739 | -3.27101              | 3.27101 |

| Boundary Information (Standardized Z Scale) |                           |         |       |
|---------------------------------------------|---------------------------|---------|-------|
| Null Reference = 0                          |                           |         |       |
| _Stage_                                     | -----Boundary Values----- |         |       |
|                                             | Alpha                     | Alpha   | Alpha |
| 1                                           | -2.96259                  | 2.96259 |       |
| 2                                           | -2.35902                  | 2.35902 |       |
| 3                                           | -2.01409                  | 2.01409 |       |

With ODS Graphics enabled, a detailed boundary plot with the rejection and acceptance regions is displayed, as shown in [Output 84.2.3](#). The boundary plot also displays the information level and critical value for the corresponding fixed-sample design. This design has characteristics of an O’Brien-Fleming design; the probability for early stopping is low, and the maximum information and critical values at the final stage are similar to those of the corresponding fixed-sample design.

**Output 84.2.3** Boundary Plot

With the MODEL=REG option in the SAMPLESIZE statement, the “Sample Size Summary” table in [Output 84.2.4](#) displays the parameters for the sample size computation.

**Output 84.2.4** Required Sample Size Summary

| Sample Size Summary             |               |
|---------------------------------|---------------|
| Test                            | Reg Parameter |
| Parameter                       | 0.1           |
| Variance                        | 5             |
| X Variance                      | 64            |
| R Square (X)                    | 0.1           |
| Max Sample Size                 | 92.87739      |
| Expected Sample Size (Null Ref) | 92.35845      |
| Expected Sample Size (Alt Ref)  | 70.97617      |

The “Sample Sizes” table in [Output 84.2.5](#) displays the required sample sizes for the group sequential clinical trial.

**Output 84.2.5** Required Sample Sizes

| Sample Sizes (N)                |                        |             |                     |             |
|---------------------------------|------------------------|-------------|---------------------|-------------|
| Z Test for Regression Parameter |                        |             |                     |             |
| _Stage_                         | -----Fractional N----- |             | -----Ceiling N----- |             |
|                                 | N                      | Information | N                   | Information |
| 1                               | 46.44                  | 535.0       | 47                  | 541.4       |
| 2                               | 69.66                  | 802.5       | 70                  | 806.4       |
| 3                               | 92.88                  | 1069.9      | 93                  | 1071.4      |

Thus, 47, 70, and 93 individuals are needed in stages 1, 2, and 3, respectively. Since the sample sizes are derived from estimated values of  $\sigma_y^2$ ,  $r_x^2$ , and  $\sigma_x^2$ , the actual information levels might not achieve the target information levels. Thus, instead of specifying sample sizes in the protocol, you can specify the maximum information levels. Then if an actual information level is much less than the target level, you can increase the sample sizes for the remaining stages to achieve the desired information levels and power.

Suppose that 47 individuals are available at stage 1. [Output 84.2.6](#) lists the first 10 observations of the trial data.

**Output 84.2.6** Clinical Trial Data

| First 10 Obs in the Trial Data |         |     |         |         |           |           |
|--------------------------------|---------|-----|---------|---------|-----------|-----------|
| Obs                            | Oxygen  | Age | Weight  | RunTime | Run Pulse | Max Pulse |
| 1                              | 54.5521 | 44  | 87.7676 | 11.6949 | 178.435   | 181.607   |
| 2                              | 52.2821 | 40  | 75.4853 | 9.8872  | 184.433   | 183.667   |
| 3                              | 62.1871 | 44  | 89.0638 | 8.7950  | 155.540   | 167.108   |
| 4                              | 65.3269 | 42  | 67.7310 | 8.4577  | 162.926   | 173.877   |
| 5                              | 59.9809 | 37  | 93.1902 | 9.3228  | 179.033   | 180.144   |
| 6                              | 52.5588 | 47  | 75.9044 | 12.0385 | 177.753   | 175.033   |
| 7                              | 51.7838 | 40  | 73.5422 | 11.6607 | 175.838   | 178.140   |
| 8                              | 57.0024 | 43  | 81.2861 | 11.2219 | 160.963   | 171.770   |
| 9                              | 48.0775 | 44  | 85.2290 | 13.1789 | 173.722   | 176.548   |
| 10                             | 68.3357 | 38  | 80.2490 | 8.5066  | 171.824   | 184.011   |

The following statements use the REG procedure to estimate the slope  $\beta_w$  and its associated standard error at stage 1:

```
proc reg data=Fit_1;
 model Oxygen=Age Weight RunTime RunPulse MaxPulse;
 ods output ParameterEstimates=Parms_Fit1;
run;
```

The following statements create and display (in [Output 84.2.7](#)) the input data set that contains slope  $\beta_w$  and its associated standard error for the SEQTEST procedure:

```
data Parms_Fit1;
 set Parms_Fit1;
 if Variable='Weight';
 Scale='MLE';
 Stage= 1;
 keep _Scale_ _Stage_ Variable Estimate StdErr;
run;

proc print data=Parms_Fit1;
 title 'Statistics Computed at Stage 1';
run;
```

**Output 84.2.7** Statistics Computed at Stage 1

| Statistics Computed at Stage 1 |          |          |         |         |         |
|--------------------------------|----------|----------|---------|---------|---------|
| Obs                            | Variable | Estimate | StdErr  | _Scale_ | _Stage_ |
| 1                              | Weight   | 0.03772  | 0.04345 | MLE     | 1       |

The following statements invoke the SEQTEST procedure to test for early stopping at stage 1:

```
ods graphics on;
proc seqtest Boundary=Bnd_Fit
 Parms(Testvar=Weight)=Parms_Fit1
 infoadj=prop
 errspendadj=errfuncobf
 order=lr
 stopprob
 ;
 ods output Test=Test_Fit1;
run;
ods graphics off;
```

The BOUNDARY= option specifies the input data set that provides the boundary information for the trial at stage 1 (this data set was generated in the SEQDESIGN procedure). Recall that these boundary values were derived for the information levels specified with the INFO=CUM(2 3 4) option in the SEQDESIGN procedure. The PARMS=PARMS\_FIT1 option specifies the input data set PARMS\_FIT1 that contains the test statistic and its associated standard error at stage 1, and the TESTVAR=WEIGHT option identifies the test variable WEIGHT in the data set.

If the computed information level for stage 1 is not the same as the value provided in the BOUNDARY= data set, the INFOADJ=PROP option (which is the default) proportionally adjusts the information levels at future interim stages from the levels provided in the BOUNDARY= data set. The ORDER=LR option uses the LR ordering to derive the  $p$ -value, the unbiased median estimate, and the confidence limits for the regression slope estimate. The ERRSPENDADJ=ERRFUNCBOBF option adjusts the boundaries with the updated error spending values generated from an O'Brien-Fleming-type cumulative error spending function.

The ODS OUTPUT statement with the TEST=TEST\_FIT1 option creates an output data set named TEST\_FIT1 which contains the updated boundary information for the test at stage 1. The adjustment is needed because the observed information level is different from the information level in the BOUNDARY= data set. The data set TEST\_FIT1 also provides the boundary information that is needed for the group sequential test at the next stage.

The “Design Information” table in [Output 84.2.8](#) displays the design specifications. By default (or equivalently if you specify BOUNDARYKEY=ALPHA), the boundary values are modified for the new information levels to maintain the Type I  $\alpha$  level. The maximum information remains the same as in the BOUNDARY= data set, but the derived Type II error probability  $\beta$  and power  $1 - \beta$  are different because of the new information level.

**Output 84.2.8** Design Information

| The SEQTEST Procedure                     |                 |
|-------------------------------------------|-----------------|
| Design Information                        |                 |
| BOUNDARY Data Set                         | WORK.BND_FIT    |
| Data Set                                  | WORK.PARMS_FIT1 |
| Statistic Distribution                    | Normal          |
| Boundary Scale                            | Standardized Z  |
| Alternative Hypothesis                    | Two-Sided       |
| Early Stop                                | Reject Null     |
| Number of Stages                          | 3               |
| Alpha                                     | 0.05            |
| Beta                                      | 0.09994         |
| Power                                     | 0.90006         |
| Max Information (Percent of Fixed Sample) | 101.8057        |
| Max Information                           | 1069.94751      |
| Null Ref ASN (Percent of Fixed Sample)    | 101.2416        |
| Alt Ref ASN (Percent of Fixed Sample)     | 77.87607        |

With the STOPPROB option, the “Expected Cumulative Stopping Probabilities” table in [Output 84.2.9](#) displays the expected stopping stage and cumulative stopping probability to reject the null hypothesis at each stage under various hypothetical references  $\theta = c_i \theta_1$ , where  $\theta_1$  is the alternative reference and  $c_i = 0, 0.5, 1, 1.5$  by default. You can specify other values for  $c_i$  with the CREF= option.

**Output 84.2.9** Stopping Probabilities

| Expected Cumulative Stopping Probabilities |                         |             |                                |         |         |  |
|--------------------------------------------|-------------------------|-------------|--------------------------------|---------|---------|--|
| Reference = CRef * (Alt Reference)         |                         |             |                                |         |         |  |
| CRef                                       | Expected Stopping Stage | Source      | ----Stopping Probabilities---- |         |         |  |
|                                            |                         |             | Stage_1                        | Stage_2 | Stage_3 |  |
| 0.0000                                     | 2.978                   | Reject Null | 0.00289                        | 0.01906 | 0.05000 |  |
| 0.5000                                     | 2.792                   | Reject Null | 0.03373                        | 0.17443 | 0.36566 |  |
| 1.0000                                     | 2.069                   | Reject Null | 0.24884                        | 0.68206 | 0.90006 |  |
| 1.5000                                     | 1.348                   | Reject Null | 0.68172                        | 0.97032 | 0.99820 |  |

The “Test Information” table in [Output 84.2.10](#) displays the boundary values for the test statistic. By default (or equivalently if you specify BOUNDARYSCALE=STDZ), these statistics are displayed with the standardized Z scale. The information level at stage 1 is derived from the standard error  $s_1$  in the PARMS= data set,

$$I_1 = \frac{1}{s_1^2} = \frac{1}{0.043453^2} = 529.62$$

**Output 84.2.10** Sequential Tests

| Test Information (Standardized Z Scale) |                       |          |                       |         |                         |            |
|-----------------------------------------|-----------------------|----------|-----------------------|---------|-------------------------|------------|
| Null Reference = 0                      |                       |          |                       |         |                         |            |
| _Stage_                                 | --Information Level-- |          | -----Alternative----- |         | ----Boundary Values---- |            |
|                                         | Proportion            | Actual   | -----Reference-----   |         | ---Lower--              | ---Upper-- |
|                                         |                       |          | Lower                 | Upper   | Alpha                   | Alpha      |
| 1                                       | 0.4950                | 529.6232 | -2.30135              | 2.30135 | -2.97951                | 2.97951    |
| 2                                       | 0.7475                | 799.7853 | -2.82805              | 2.82805 | -2.36291                | 2.36291    |
| 3                                       | 1.0000                | 1069.948 | -3.27101              | 3.27101 | -2.01336                | 2.01336    |

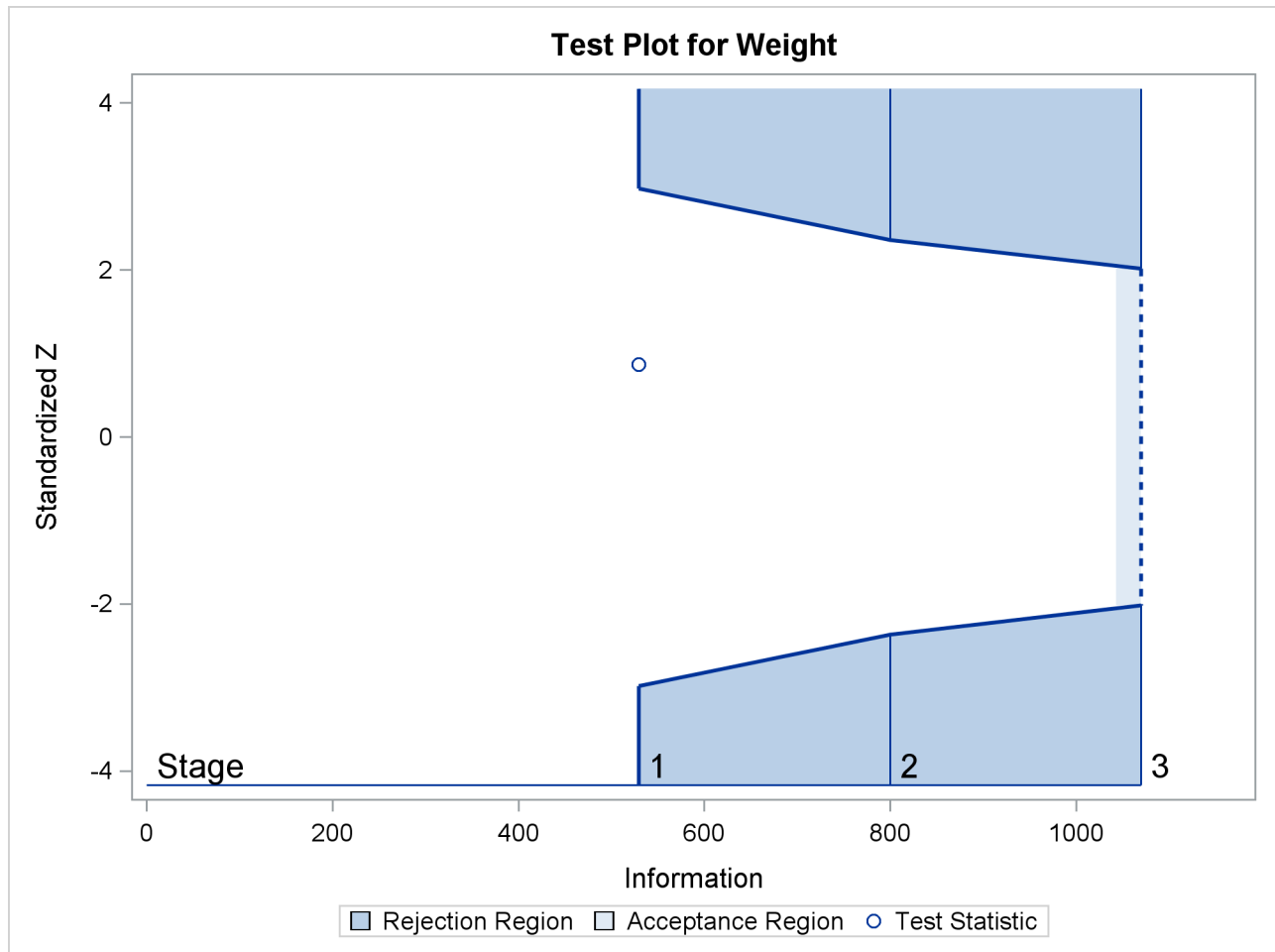
| Test Information (Standardized Z Scale) |          |                  |          |
|-----------------------------------------|----------|------------------|----------|
| Null Reference = 0                      |          |                  |          |
| _Stage_                                 | Estimate | -----Test-----   |          |
|                                         |          | -----Weight----- |          |
|                                         |          |                  | Action   |
| 1                                       | 0.86798  |                  | Continue |
| 2                                       | .        |                  |          |
| 3                                       | .        |                  |          |

With the INFOADJ=PROP option (which is the default), the information level at stage 2 is derived proportionally from the observed information at stage 1 and the information levels in the BOUNDARY= data set. See the section “[Boundary Adjustments for Information Levels](#)” on page 7223 for details about how the adjusted information levels are computed.

At stage 1, the standardized Z statistic 0.86798 is between the lower  $\alpha$  boundary  $-2.97951$  and the upper  $\alpha$  boundary  $2.97951$ , so the trial continues to the next stage.

With ODS Graphics enabled, a boundary plot with test statistics is displayed, as shown in [Output 84.2.11](#). As expected, the test statistic is in the continuation region between the lower and upper  $\alpha$  boundaries.

Output 84.2.11 Sequential Test Plot



The following statements use the REG procedure to estimate the slope  $\beta_w$  and its associated standard error at stage 2:

```
proc reg data=Fit_2;
 model Oxygen=Age Weight RunTime RunPulse MaxPulse;
 ods output ParameterEstimates=Parms_Fit2;
run;
```

Note that the data set Fit\_2 contains both the data from stage 1 and the data from stage 2.

The following statements create and display (in [Output 84.2.12](#)) the input data set that contains slope  $\beta_w$  and its associated standard error at stage 2 for the SEQTEST procedure:

```
data Parms_Fit2;
 set Parms_Fit2;
 if Variable='Weight';
 Scale='MLE';
 Stage= 2;
 keep _Scale_ _Stage_ Variable Estimate StdErr;
run;
```



```
proc print data=Parms_Fit2;
 title 'Statistics Computed at Stage 2';
run;
```

### Output 84.2.12 Statistics Computed at Stage 2

| Statistics Computed at Stage 2 |          |          |         |         |         |
|--------------------------------|----------|----------|---------|---------|---------|
| Obs                            | Variable | Estimate | StdErr  | _Scale_ | _Stage_ |
| 1                              | Weight   | 0.02932  | 0.03520 | MLE     | 2       |

The following statements invoke the SEQTEST procedure to test for early stopping at stage 2:

```
proc seqtest Boundary=Test_Fit1
 Parms(Testvar=Weight)=Parms_Fit2
 infoadj=prop
 errspendadj=errfuncobf
 order=lr
 ;
ods output Test=Test_Fit2;
run;
```

The BOUNDARY= option specifies the input data set that provides the boundary information for the trial at stage 2, which was generated by the SEQTEST procedure at the previous stage. The PARMs= option specifies the input data set that contains the test statistic and its associated standard error at stage 2, and the TESTVAR= option identifies the test variable in the data set.

The ODS OUTPUT statement with the TEST=TEST\_FIT2 option creates an output data set named TEST\_FIT2 which contains the updated boundary information for the test at stage 2. The data set also provides the boundary information that is needed for the group sequential test at the next stage.

Since the data set PARMs\_FIT2 does not contain the test information at stage 1, the information level at stage 1 in the TEST\_FIT1 data set is used to generate boundary values for the test at stage 2.

Following the process at stage 1, the slope estimate is also between its corresponding lower and upper  $\alpha$  boundary values, so the trial continues to the next stage.

The following statements use the REG procedure to estimate the slope  $\beta_w$  and its associated standard error at the final stage:

```
proc reg data=Fit_3;
 model Oxygen=Age Weight RunTime RunPulse MaxPulse;
 ods output ParameterEstimates=Parms_Fit3;
run;
```

The following statements create the input data set that contains slope  $\beta_w$  and its associated standard error at stage 3 for the SEQTEST procedure:

```
data Parms_Fit3;
 set Parms_Fit3;
 if Variable='Weight';
 Scale='MLE';
 Stage= 3;
 keep _Scale_ _Stage_ Variable Estimate StdErr;
run;
```

The following statements print (in [Output 84.2.13](#)) the test statistics at stage 3:

```
proc print data=Parms_Fit3;
 title 'Statistics Computed at Stage 3';
run;
```

**Output 84.2.13** Statistics Computed at Stage 3

| Statistics Computed at Stage 3 |          |          |         |         |         |
|--------------------------------|----------|----------|---------|---------|---------|
| Obs                            | Variable | Estimate | StdErr  | _Scale_ | _Stage_ |
| 1                              | Weight   | 0.02189  | 0.03028 | MLE     | 3       |

The following statements invoke the SEQTEST procedure to test the hypothesis:

```
ods graphics on;
proc seqtest Boundary=Test_Fit2
 Parms(testvar=Weight)=Parms_Fit3
 errspendadj=errfuncobf
 order=lr
 pss
 plots=(asn power)
 ;
 ods output Test=Test_Fit3;
run;
ods graphics off;
```

The BOUNDARY= option specifies the input data set that provides the boundary information for the trial at stage 3, which was generated by the SEQTEST procedure at the previous stage. The PARMs= option specifies the input data set that contains the test statistic and its associated standard error at stage 3, and the TESTVAR= option identifies the test variable in the data set.

The ODS OUTPUT statement with the TEST=TEST\_FIT3 option creates an output data set named TEST\_FIT3 which contains the updated boundary information for the test at stage 3.

The “Design Information” table in [Output 84.2.14](#) displays design specifications. By default (or equivalently if you specify BOUNDARYKEY=ALPHA), the boundary values are modified for the new information levels to maintain the Type I  $\alpha$  level.

**Output 84.2.14** Design Information

| The SEQTEST Procedure                     |                 |
|-------------------------------------------|-----------------|
| Design Information                        |                 |
| BOUNDARY Data Set                         | WORK.TEST_FIT2  |
| Data Set                                  | WORK.PARMS_FIT3 |
| Statistic Distribution                    | Normal          |
| Boundary Scale                            | Standardized Z  |
| Alternative Hypothesis                    | Two-Sided       |
| Early Stop                                | Reject Null     |
| Number of Stages                          | 3               |
| Alpha                                     | 0.05            |
| Beta                                      | 0.09514         |
| Power                                     | 0.90486         |
| Max Information (Percent of Fixed Sample) | 102.0102        |
| Max Information                           | 1090.63724      |
| Null Ref ASN (Percent of Fixed Sample)    | 101.4122        |
| Alt Ref ASN (Percent of Fixed Sample)     | 77.22139        |

The maximum information is derived from the standard error associated with the slope estimate at the final stage and is larger than the target level. The derived Type II error probability  $\beta$  and power  $1 - \beta$  are different because of the new information levels.

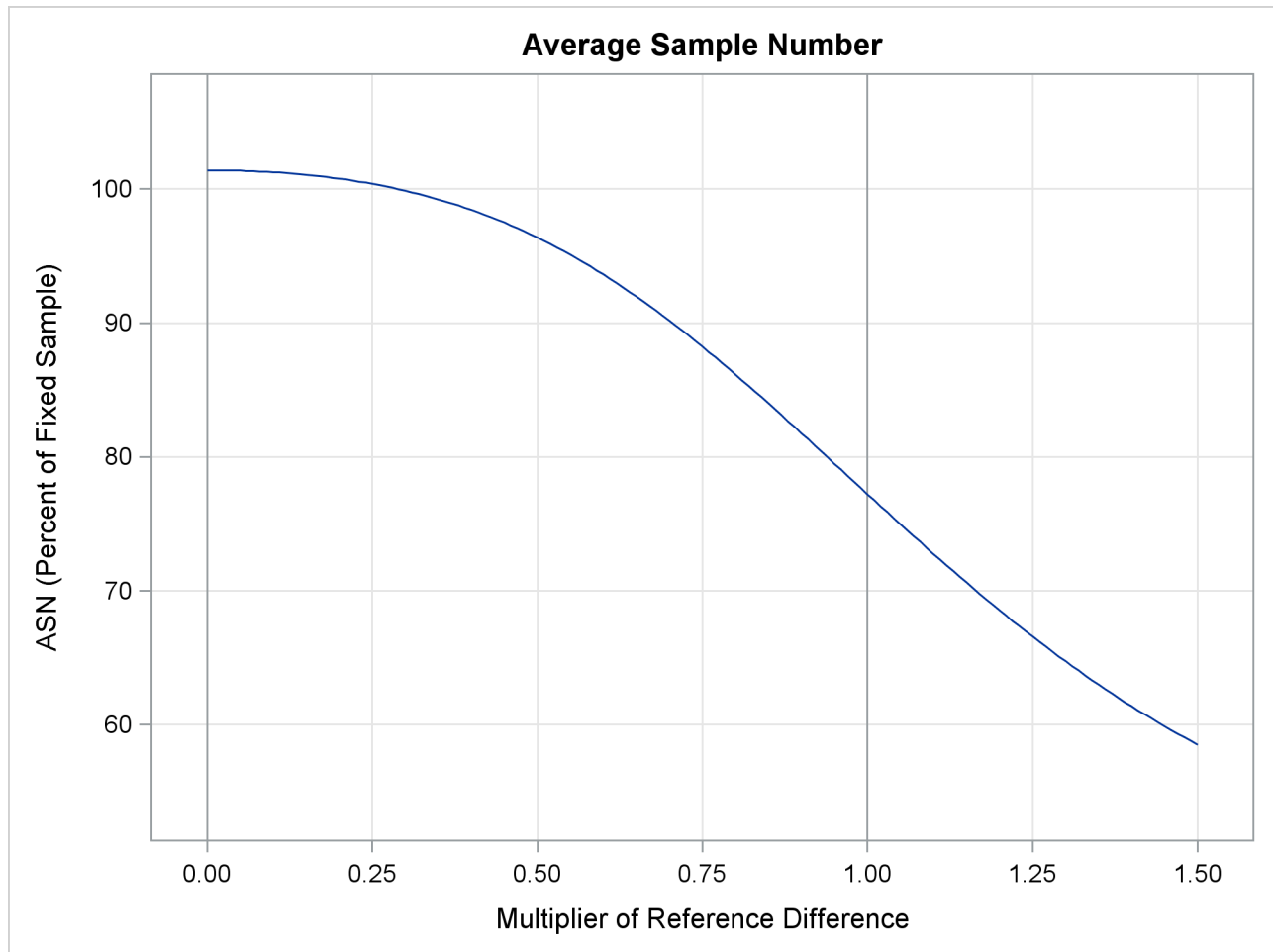
With the PSS option, the “Power and Expected Sample Sizes” table in [Output 84.2.15](#) displays powers and expected mean sample sizes under various hypothetical references  $\theta = c_i \theta_1$ , where  $\theta_1$  is the alternative reference and  $c_i = 0, 0.5, 1, 1.5$  by default. You can specify the  $c_i$  values with the CREF= option.

**Output 84.2.15** Power and Expected Sample Size Information

| Powers and Expected Sample Sizes   |         |                                          |
|------------------------------------|---------|------------------------------------------|
| Reference = CRef * (Alt Reference) |         |                                          |
| CRef                               | Power   | -Sample Size-<br>Percent<br>Fixed-Sample |
| 0.0000                             | 0.02500 | 101.4122                                 |
| 0.5000                             | 0.37046 | 96.3754                                  |
| 1.0000                             | 0.90486 | 77.2214                                  |
| 1.5000                             | 0.99844 | 58.5301                                  |

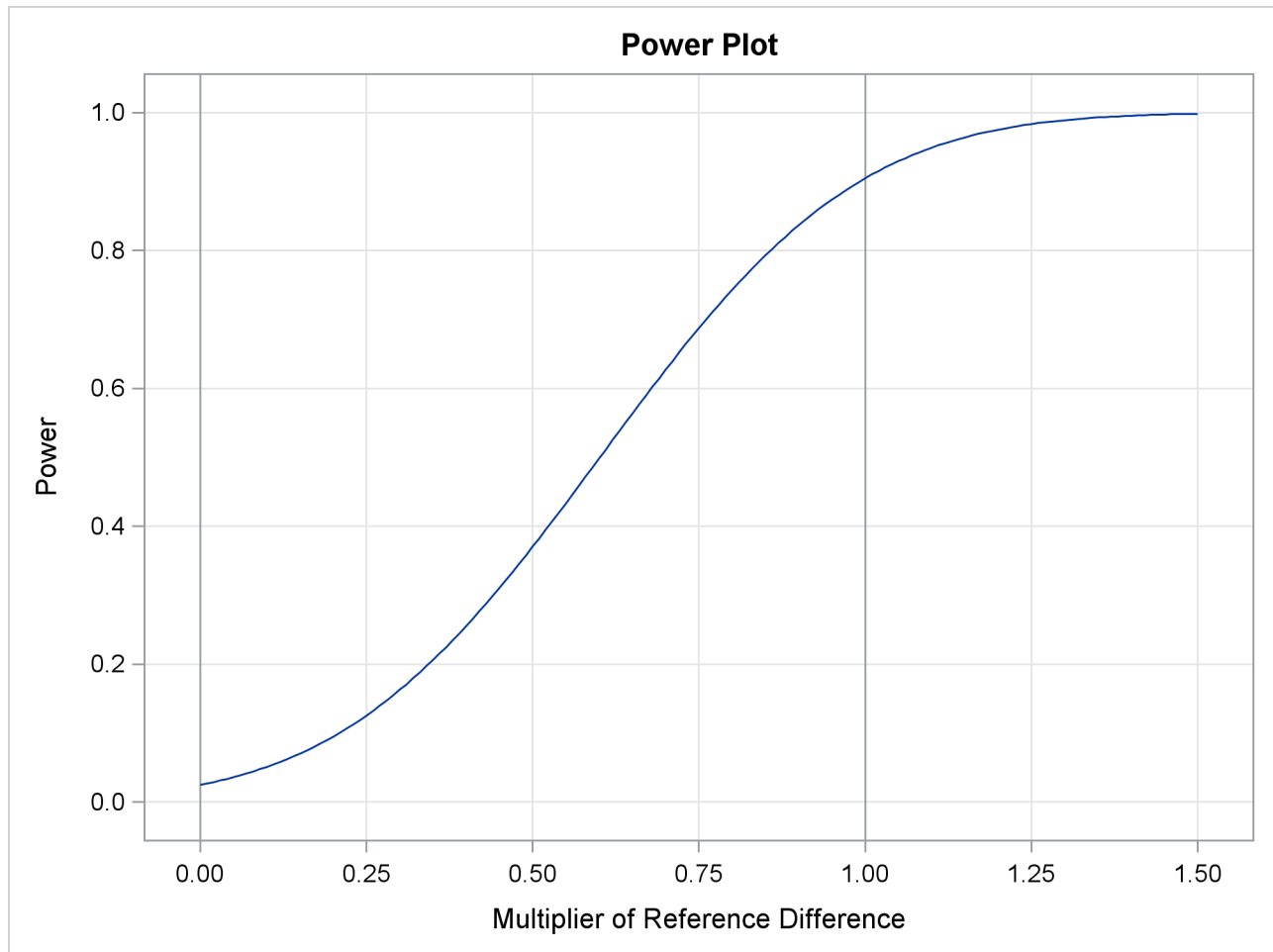
With the PLOTS=ASN option, the procedure displays a plot of expected sample sizes under various hypothetical references, as shown in [Output 84.2.16](#). By default, expected sample sizes under the hypotheses  $\theta = c_i \theta_1$ ,  $c_i = 0, 0.01, 0.02, \dots, 1.50$ , are displayed, where  $\theta_1$  is the alternative reference.

Output 84.2.16 ASN Plot



With the PLOTS=POWER option, the procedure displays a plot of powers under various hypothetical references, as shown in [Output 84.2.17](#). By default, powers under hypothetical references  $\theta = c_i \theta_1$  are displayed, where  $c_i = 0, 0.01, 0.02, \dots, 1.50$  by default. You can specify  $c_i$  values with the CREF= option. The  $c_i$  values are displayed on the horizontal axis.

Output 84.2.17 Power Plot



Under the null hypothesis,  $c_i = 0$ , the power is 0.025, which is the upper Type I error probability. Under the alternative hypothesis,  $c_i = 1$ , the power is 0.90486, which is one minus the Type II error probability.

The “Test Information” table in [Output 84.2.18](#) displays the boundary values for the test statistic with the default standardized Z scale. The information level at the current stage is derived from the standard error for the current stage in the PARMS= data set. At stage 3, the standardized slope estimate 0.72284 is still between the lower and upper  $\alpha$  boundary values. Since it is the final stage, the trial stops to accept the null hypothesis that the variable Weight has no effect on the oxygen intake rate after adjusting for other covariates.

**Output 84.2.18** Sequential Tests

| Test Information (Standardized Z Scale) |                       |          |                       |                     |                         |             |
|-----------------------------------------|-----------------------|----------|-----------------------|---------------------|-------------------------|-------------|
| Null Reference = 0                      |                       |          |                       |                     |                         |             |
| _Stage_                                 | --Information Level-- |          | -----Alternative----- |                     | ----Boundary Values---- |             |
|                                         | Proportion            | Actual   | -----Reference-----   | -----Reference----- | ---Lower---             | ---Upper--- |
|                                         |                       |          | Lower                 | Upper               | Alpha                   | Alpha       |
| 1                                       | 0.4856                | 529.6232 | -2.30135              | 2.30135             | -2.97951                | 2.97951     |
| 2                                       | 0.7401                | 807.1954 | -2.84112              | 2.84112             | -2.34945                | 2.34945     |
| 3                                       | 1.0000                | 1090.637 | -3.30248              | 3.30248             | -2.01885                | 2.01885     |

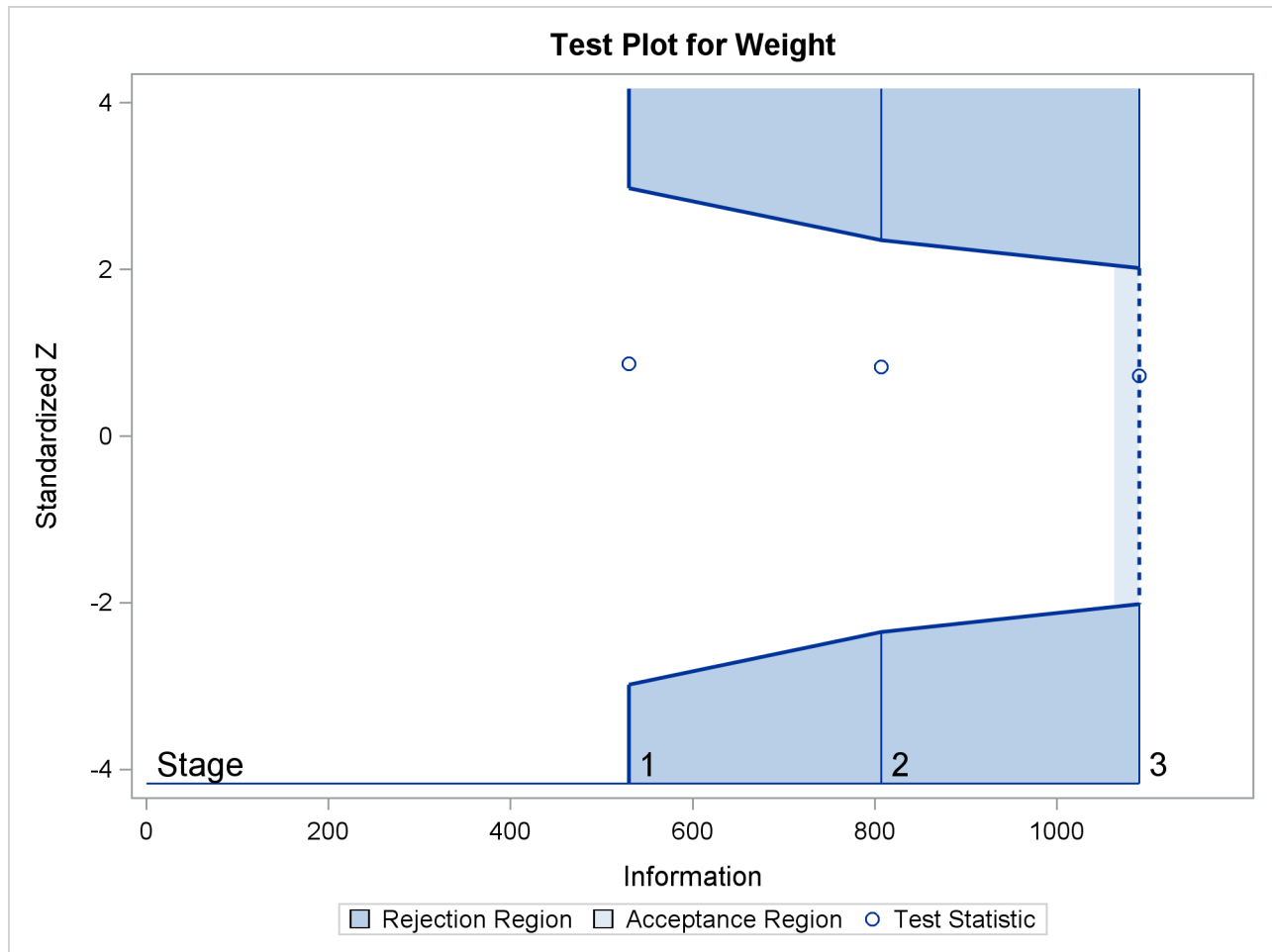
  

| Test Information (Standardized Z Scale) |                |             |
|-----------------------------------------|----------------|-------------|
| Null Reference = 0                      |                |             |
| _Stage_                                 | -----Test----- |             |
|                                         | Estimate       | Action      |
| 1                                       | 0.86798        | Continue    |
| 2                                       | 0.83305        | Continue    |
| 3                                       | 0.72284        | Accept Null |

Since the data set FIT\_3 contains the test information only at stage 3, the information levels at previous stages in the TEST\_FIT2 data set are used to generate boundary values for the test.

With ODS Graphics enabled, a boundary plot with test statistics is displayed, as shown in [Output 84.2.19](#). As expected, the test statistic is in the acceptance region between the lower and upper  $\alpha$  boundaries at the final stage.

**Output 84.2.19** Sequential Test Plot



After a trial is stopped, the “Parameter Estimates” table in [Output 84.2.20](#) displays the stopping stage, parameter estimate, unbiased median estimate, confidence limits, and the  $p$ -value under the null hypothesis  $H_0 : \beta_w = 0$ .

**Output 84.2.20** Parameter Estimates

| Parameter Estimates<br>LR Ordering |                       |          |                                  |                 |
|------------------------------------|-----------------------|----------|----------------------------------|-----------------|
| Parameter                          | Stopping Stage        | MLE      | p-Value for $H_0: \text{Parm}=0$ | Median Estimate |
| Weight                             | 3                     | 0.021888 | 0.4699                           | 0.021884        |
| Parameter Estimates<br>LR Ordering |                       |          |                                  |                 |
| Parameter                          | 95% Confidence Limits |          |                                  |                 |
| Weight                             | -0.03747              | 0.08123  |                                  |                 |

As expected, the  $p$ -value 0.4699 is not significant at the  $\alpha = 0.05$  level, and the confidence interval does contain the value zero. The  $p$ -value, unbiased median estimate, and confidence limits depend on the ordering of the sample space  $(k, z)$ , where  $k$  is the stage number and  $z$  is the standardized  $Z$  statistic. With the specified LR ordering, the  $p$ -values are computed with the ordering  $(k', z') \succ (k, z)$  if  $z' > z$ . See the section “Available Sample Space Orderings in a Sequential Test” on page 7230 for a detailed description of the LR ordering.

---

### Example 84.3: Testing an Effect with Early Stopping to Accept $H_0$

This example demonstrates a two-sided group sequential test that uses an error spending design with early stopping to accept the null hypothesis  $H_0$ . The example is similar to Example 84.2 but with early stopping to accept  $H_0$ .

A study is conducted to examine the effects of Age (years), Weight (kg), RunTime (time in minutes to run 1.5 miles), RunPulse (heart rate while running), and MaxPulse (maximum heart rate recorded while running) on Oxygen (oxygen intake rate, ml per kg body weight per minute). The primary interest is whether oxygen intake rate is associated with weight.

The hypothesis is tested using the following linear model:

$$\text{Oxygen} = \text{Age} + \text{Weight} + \text{RunTime} + \text{RunPulse} + \text{MaxPulse}$$

The null hypothesis is  $H_0 : \beta_w = 0$ , where  $\beta_w$  is the regression parameter for the variable Weight. Suppose that  $\beta_w = 0.10$  is the reference improvement that should be detected at a 0.90 level. Then the maximum information  $I_X$  can be derived in the SEQDESIGN procedure.

Following the derivations in the section “Test for a Parameter in the Regression Model” in the chapter “The SEQDESIGN Procedure,” the required sample size can be derived from

$$N = I_X \frac{\sigma_y^2}{(1 - r_x^2) \sigma_x^2}$$

where  $\sigma_y^2$  is the variance of the response variable in the regression model,  $r_x^2$  is the proportion of variance of Weight explained by other covariates, and  $\sigma_x^2$  is the variance of Weight.

Further suppose that from past experience,  $\sigma_y^2 = 5$ ,  $r_x^2 = 0.10$ , and  $\sigma_x^2 = 64$ . Then the required sample size can be derived using the SAMPLESIZE statement in the SEQDESIGN procedure.

The following statements invoke the SEQDESIGN procedure and request a three-stage group sequential design for normally distributed data to test the null hypothesis of a regression parameter  $H_0 : \beta_w = 0$  against the alternative  $H_1 : \beta_w \neq 0$ :

```
ods graphics on;
proc seqdesign altref=0.10;
 OBFErrorFunction: design method=errfuncgamma
 stop=accept
 nstages=3
 info=cum(2 3 4);

 samplesize model=reg(variance=5 xviance=64 xrsquare=0.10);
```



```
ods output Boundary=Bnd_Fit;
run;
ods graphics off;
```

By default (or equivalently if you specify ALPHA=0.05 and BETA=0.10), the procedure uses a Type I error probability 0.05 and a Type II error probability 0.10. The ALTREF=0.10 option specifies a power of  $1 - \beta = 0.90$  at the alternative hypothesis  $H_1 : \beta_w = \pm 0.10$ . The INFO=CUM(2 3 4) option specifies that the study perform the first interim analysis with information proportion  $2/4 = 0.5$ —that is, after half of the total observations are collected.

The ODS OUTPUT statement with the BOUNDARY=BND\_FIT option creates an output data set named BND\_FIT which contains the resulting boundary information for the subsequent sequential tests.

The “Design Information” table in [Output 84.3.1](#) displays design specifications and derived statistics. Since the alternative reference is specified, the maximum information is derived.

**Output 84.3.1** Error Spending Design Information

| The SEQDESIGN Procedure                   |                |
|-------------------------------------------|----------------|
| Design: OBFErrorFunction                  |                |
| Design Information                        |                |
| Statistic Distribution                    | Normal         |
| Boundary Scale                            | Standardized Z |
| Alternative Hypothesis                    | Two-Sided      |
| Early Stop                                | Accept Null    |
| Method                                    | Error Spending |
| Boundary Key                              | Both           |
| Alternative Reference                     | 0.1            |
| Number of Stages                          | 3              |
| Alpha                                     | 0.05           |
| Beta                                      | 0.1            |
| Power                                     | 0.9            |
| Max Information (Percent of Fixed Sample) | 103.9245       |
| Max Information                           | 1091.972       |
| Null Ref ASN (Percent of Fixed Sample)    | 75.00521       |
| Alt Ref ASN (Percent of Fixed Sample)     | 101.8099       |

The “Boundary Information” table in [Output 84.3.2](#) displays information level, alternative reference, and boundary values at each stage.

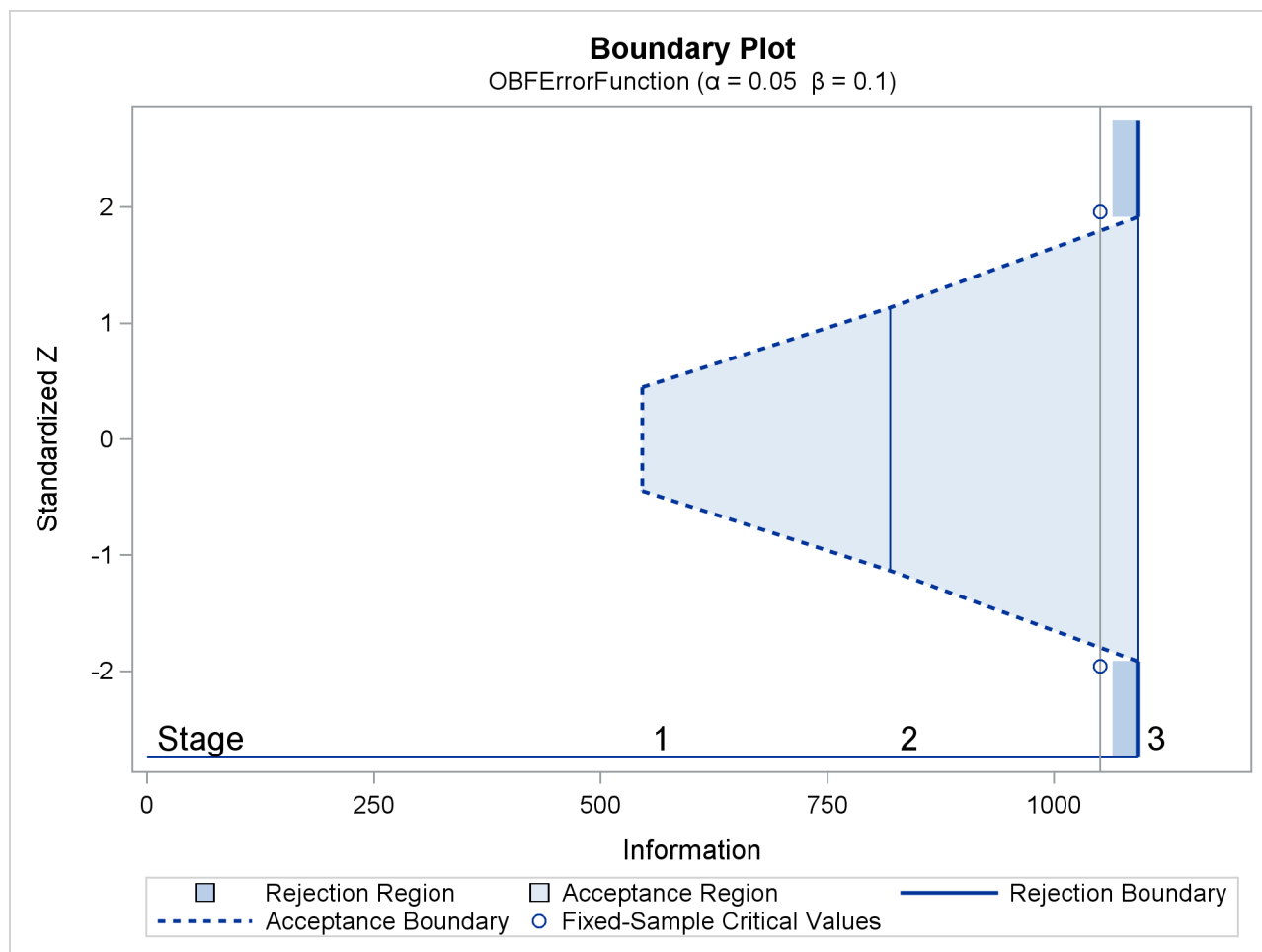
**Output 84.3.2** Boundary Information

| Boundary Information (Standardized Z Scale) |                             |          |          |                       |         |
|---------------------------------------------|-----------------------------|----------|----------|-----------------------|---------|
| Null Reference = 0                          |                             |          |          |                       |         |
| _Stage_                                     | -----Information Level----- |          |          | -----Alternative----- |         |
|                                             | Proportion                  | Actual   | N        | Lower                 | Upper   |
| 1                                           | 0.5000                      | 545.9862 | 47.39463 | -2.33663              | 2.33663 |
| 2                                           | 0.7500                      | 818.9792 | 71.09195 | -2.86178              | 2.86178 |
| 3                                           | 1.0000                      | 1091.972 | 94.78926 | -3.30450              | 3.30450 |

| Boundary Information (Standardized Z Scale) |                           |             |  |
|---------------------------------------------|---------------------------|-------------|--|
| Null Reference = 0                          |                           |             |  |
| _Stage_                                     | -----Boundary Values----- |             |  |
|                                             | ---Lower---               | ---Upper--- |  |
|                                             | Beta                      | Beta        |  |
| 1                                           | -0.44937                  | 0.44937     |  |
| 2                                           | -1.13583                  | 1.13583     |  |
| 3                                           | -1.91428                  | 1.91428     |  |

With ODS Graphics enabled, a detailed boundary plot with the rejection and acceptance regions is displayed, as shown in [Output 84.3.3](#). The boundary plot also displays the information level and critical value for the corresponding fixed-sample design.

**Output 84.3.3** Boundary Plot

With the MODEL=REG option in the SAMPLESIZE statement, the “Sample Size Summary” table in [Output 84.3.4](#) displays the parameters for the sample size computation.

**Output 84.3.4** Required Sample Size Summary

| Sample Size Summary             |               |
|---------------------------------|---------------|
| Test                            | Reg Parameter |
| Parameter                       | 0.1           |
| Variance                        | 5             |
| X Variance                      | 64            |
| R Square (X)                    | 0.1           |
| Max Sample Size                 | 94.78926      |
| Expected Sample Size (Null Ref) | 68.41207      |
| Expected Sample Size (Alt Ref)  | 92.86057      |

The “Sample Sizes” table in [Output 84.3.5](#) displays the required sample sizes for the group sequential clinical trial.

**Output 84.3.5** Required Sample Sizes

| Sample Sizes (N)                |                        |             |                     |             |
|---------------------------------|------------------------|-------------|---------------------|-------------|
| Z Test for Regression Parameter |                        |             |                     |             |
| _Stage_                         | -----Fractional N----- |             | -----Ceiling N----- |             |
|                                 | N                      | Information | N                   | Information |
| 1                               | 47.39                  | 546.0       | 48                  | 553.0       |
| 2                               | 71.09                  | 819.0       | 72                  | 829.4       |
| 3                               | 94.79                  | 1092.0      | 95                  | 1094.4      |

Thus, 48, 72, and 95 individuals are needed in stages 1, 2, and 3, respectively. Since the sample sizes are derived from estimated values of  $\sigma_y^2$ ,  $r_x^2$ , and  $\sigma_x^2$ , the actual information levels might not achieve the target information levels. Thus, instead of specifying sample sizes in the protocol, you can specify the maximum information levels. Then if an actual information level is much less than the target level, you can increase the sample sizes for the remaining stages to achieve the desired information levels and power.

Suppose that 48 individuals are available at stage 1. [Output 84.3.6](#) lists the first 10 observations of the trial data.

**Output 84.3.6** Clinical Trial Data

| First 10 Obs in the Trial Data |         |     |         |         |           |           |
|--------------------------------|---------|-----|---------|---------|-----------|-----------|
| Obs                            | Oxygen  | Age | Weight  | RunTime | Run Pulse | Max Pulse |
| 1                              | 54.5521 | 44  | 87.7676 | 11.6949 | 178.435   | 181.607   |
| 2                              | 52.2821 | 40  | 75.4853 | 9.8872  | 184.433   | 183.667   |
| 3                              | 62.1871 | 44  | 89.0638 | 8.7950  | 155.540   | 167.108   |
| 4                              | 65.3269 | 42  | 67.7310 | 8.4577  | 162.926   | 173.877   |
| 5                              | 59.9809 | 37  | 93.1902 | 9.3228  | 179.033   | 180.144   |
| 6                              | 52.5588 | 47  | 75.9044 | 12.0385 | 177.753   | 175.033   |
| 7                              | 51.7838 | 40  | 73.5422 | 11.6607 | 175.838   | 178.140   |
| 8                              | 57.0024 | 43  | 81.2861 | 11.2219 | 160.963   | 171.770   |
| 9                              | 48.0775 | 44  | 85.2290 | 13.1789 | 173.722   | 176.548   |
| 10                             | 68.3357 | 38  | 80.2490 | 8.5066  | 171.824   | 184.011   |

The following statements use the REG procedure to estimate the slope  $\beta_w$  and its associated standard error at stage 1:

```
proc reg data=Fit_1;
 model Oxygen=Age Weight RunTime RunPulse MaxPulse;
 ods output ParameterEstimates=Parms_Fit1;
run;
```

The following statements create and display (in [Output 84.3.7](#)) the input data set that contains slope  $\beta_w$  and its associated standard error for the SEQTEST procedure:

```
data Parms_Fit1;
 set Parms_Fit1;
 if Variable='Weight';
 Scale='MLE';
 Stage= 1;
 keep _Scale_ _Stage_ Variable Estimate StdErr;
run;

proc print data=Parms_Fit1;
 title 'Statistics Computed at Stage 1';
run;
```

**Output 84.3.7** Statistics Computed at Stage 1

| Statistics Computed at Stage 1 |          |          |         |         |         |
|--------------------------------|----------|----------|---------|---------|---------|
| Obs                            | Variable | Estimate | StdErr  | _Scale_ | _Stage_ |
| 1                              | Weight   | 0.04660  | 0.04308 | MLE     | 1       |

The following statements invoke the SEQTEST procedure to test for early stopping at stage 1:

```
ods graphics on;
proc seqtest Boundary=Bnd_Fit
 Parms(testvar=Weight)=Parms_Fit1
 infoadj=none
 errspendadj=errfuncgamma
 stopprob
 order=lr
 ;
 ods output Test=Test_Fit1;
run;
ods graphics off;
```

The BOUNDARY= option specifies the input data set that provides the boundary information for the trial at stage 1, which was generated in the SEQDESIGN procedure. The PARMS=PARMS\_FIT1 option specifies the input data set PARMS\_FIT1 that contains the test statistic and its associated standard error at stage 1, and the TESTVAR=WEIGHT option identifies the test variable WEIGHT in the data set. The INFOADJ=NONE option maintains the information level for stage 2 at the value provided in the BOUNDARY= data set.

The ORDER=LR option uses the LR ordering to derive the  $p$ -value, the unbiased median estimate, and the confidence limits for the regression slope estimate. The ERRSPENDADJ=ERRFUNC GAMMA option adjusts the boundaries with the updated error spending values generated from a gamma cumulative error spending function.

The ODS OUTPUT statement with the TEST=TEST\_FIT1 option creates an output data set named TEST\_FIT1 which contains the updated boundary information for the test at stage 1. The data set also provides the boundary information that is needed for the group sequential test at the next stage.

The “Design Information” table in [Output 84.3.8](#) displays the design specifications. By default (or equivalently if you specify BOUNDARYKEY=ALPHA), the boundary values are modified for the new information levels to maintain the Type I  $\alpha$  level. The maximum information remains the same as in the BOUNDARY= data set, but the derived Type II error probability  $\beta$  and power  $1 - \beta$  are different because of the new information level.

**Output 84.3.8** Design Information

| The SEQTEST Procedure                     |                 |
|-------------------------------------------|-----------------|
| Design Information                        |                 |
| BOUNDARY Data Set                         | WORK.BND_FIT    |
| Data Set                                  | WORK.PARMS_FIT1 |
| Statistic Distribution                    | Normal          |
| Boundary Scale                            | Standardized Z  |
| Alternative Hypothesis                    | Two-Sided       |
| Early Stop                                | Accept Null     |
| Number of Stages                          | 3               |
| Alpha                                     | 0.05            |
| Beta                                      | 0.10007         |
| Power                                     | 0.89993         |
| Max Information (Percent of Fixed Sample) | 103.9498        |
| Max Information                           | 1091.97232      |
| Null Ref ASN (Percent of Fixed Sample)    | 75.15846        |
| Alt Ref ASN (Percent of Fixed Sample)     | 101.8296        |

With the STOPPROB option, the “Expected Cumulative Stopping Probabilities” table in [Output 84.3.9](#) displays the expected stopping stage and the cumulative stopping probability of accepting the null hypothesis at each stage under various hypothetical references  $\theta = c_i\theta_1$ , where  $\theta_1$  is the alternative reference and  $c_i = 0, 0.5, 1, 1.5$  by default. You can specify other values for  $c_i$  with the CREF= option.

**Output 84.3.9** Stopping Probabilities

| Expected Cumulative Stopping Probabilities |                         |             |                                |         |         |  |
|--------------------------------------------|-------------------------|-------------|--------------------------------|---------|---------|--|
| Reference = CRef * (Alt Reference)         |                         |             |                                |         |         |  |
| CRef                                       | Expected Stopping Stage | Source      | ----Stopping Probabilities---- |         |         |  |
|                                            |                         |             | Stage_1                        | Stage_2 | Stage_3 |  |
| 0.0000                                     | 1.895                   | Accept Null | 0.33304                        | 0.76607 | 0.95000 |  |
| 0.5000                                     | 2.409                   | Accept Null | 0.17680                        | 0.40947 | 0.62828 |  |
| 1.0000                                     | 2.918                   | Accept Null | 0.02636                        | 0.05453 | 0.10007 |  |
| 1.5000                                     | 2.997                   | Accept Null | 0.00109                        | 0.00166 | 0.00242 |  |

The “Test Information” table in [Output 84.3.10](#) displays the boundary values for the test statistic. By default (or equivalently if you specify BOUNDARYSCALE=STDZ), these statistics are displayed with the standardized Z scale. The information level at stage 1 is derived from the standard error  $s_1$  in the PARMS= data set,

$$I_1 = \frac{1}{s_1^2} = \frac{1}{0.04308^2} = 538.8$$

**Output 84.3.10** Sequential Tests

| Test Information (Standardized Z Scale) |                         |          |                       |         |
|-----------------------------------------|-------------------------|----------|-----------------------|---------|
| Null Reference = 0                      |                         |          |                       |         |
| _Stage_                                 | ---Information Level--- |          | -----Alternative----- |         |
|                                         | Proportion              | Actual   | Lower                 | Upper   |
| 1                                       | 0.4934                  | 538.7887 | -2.32118              | 2.32118 |
| 2                                       | 0.7500                  | 818.9792 | -2.86178              | 2.86178 |
| 3                                       | 1.0000                  | 1091.972 | -3.30450              | 3.30450 |

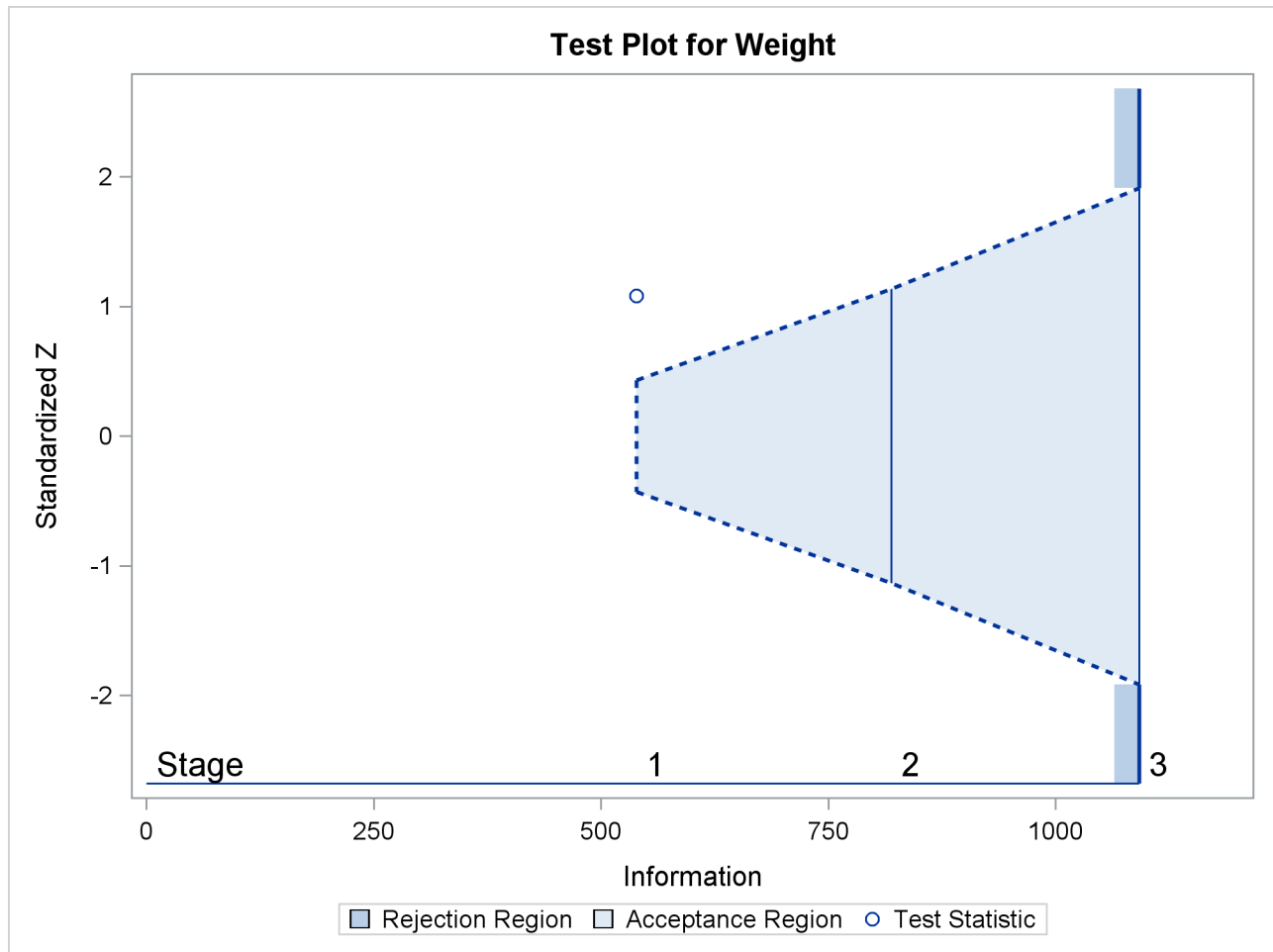
  

| Test Information (Standardized Z Scale) |                           |                     |                              |          |
|-----------------------------------------|---------------------------|---------------------|------------------------------|----------|
| Null Reference = 0                      |                           |                     |                              |          |
| _Stage_                                 | -----Boundary Values----- |                     | -----Test-----               |          |
|                                         | ---Lower---<br>Beta       | ---Upper---<br>Beta | -----Weight-----<br>Estimate | Action   |
| 1                                       | -0.43033                  | 0.43033             | 1.08174                      | Continue |
| 2                                       | -1.13623                  | 1.13623             | .                            |          |
| 3                                       | -1.91431                  | 1.91431             | .                            |          |

At stage 1, the standardized Z statistic 1.08174 is greater than the upper  $\beta$  boundary 0.43033, so the trial continues to the next stage.

With ODS Graphics enabled, a boundary plot with test statistics is displayed, as shown in [Output 84.3.11](#). As expected, the test statistic is in the continuation region.

**Output 84.3.11** Sequential Test Plot



The following statements use the REG procedure to estimate the slope  $\beta_w$  and its associated standard error at stage 2:

```
proc reg data=Fit_2;
 model Oxygen=Age Weight RunTime RunPulse MaxPulse;
 ods output ParameterEstimates=Parms_Fit2;
run;
```

Note that the data set Fit\_2 contains both the data from stage 1 and the data from stage 2,

The following statements create and display (in [Output 84.3.12](#)) the input data set that contains slope  $\beta_w$  and its associated standard error at stage 2 for the SEQTEST procedure:

```
data Parms_Fit2;
 set Parms_Fit2;
 if Variable='Weight';
 Scale='MLE';
 Stage= 2;
 keep _Scale_ _Stage_ Variable Estimate StdErr;
run;
```



```
proc print data=Parms_Fit2;
 title 'Statistics Computed at Stage 2';
run;
```

**Output 84.3.12** Statistics Computed at Stage 2

| Statistics Computed at Stage 2 |          |          |         |         |         |
|--------------------------------|----------|----------|---------|---------|---------|
| Obs                            | Variable | Estimate | StdErr  | _Scale_ | _Stage_ |
| 1                              | Weight   | 0.02925  | 0.03490 | MLE     | 2       |

The following statements invoke the SEQTEST procedure to test for early stopping at stage 2:

```
ods graphics on;
proc seqtest Boundary=Test_Fit1
 Parms(testvar=Weight)=Parms_Fit2
errspendadj=errfuncgamma
order=lr
pss
plots=(asn power)
;
ods output Test=Test_Fit2;
run;
ods graphics off;
```

The BOUNDARY= option specifies the input data set that provides the boundary information for the trial at stage 2, which was generated by the SEQTEST procedure at the previous stage. The PARMS= option specifies the input data set that contains the test statistic and its associated standard error at stage 2, and the TESTVAR= option identifies the test variable in the data set.

Since the data set PARMS\_FIT2 does not contain the test information at stage 1, the information level at stage 1 in the TEST\_FIT1 data set is used to generate boundary values for the test.

The ORDER=LR option uses the LR ordering to derive the  $p$ -value, unbiased median estimate, and confidence limits for the regression slope estimate.

The ODS OUTPUT statement with the TEST=TEST\_FIT2 option creates an output data set named TEST\_FIT2 which contains the updated boundary information for the test at stage 2. The data set also provides the boundary information that is needed for the group sequential test at the next stage.

The “Design Information” table in [Output 84.3.13](#) displays design specifications. By default (or equivalently if you specify BOUNDARYKEY=ALPHA), the boundary values are modified for the new information levels to maintain the Type I  $\alpha$  level.

**Output 84.3.13** Design Information

| The SEQTEST Procedure                     |                 |
|-------------------------------------------|-----------------|
| Design Information                        |                 |
| BOUNDARY Data Set                         | WORK.TEST_FIT1  |
| Data Set                                  | WORK.PARMS_FIT2 |
| Statistic Distribution                    | Normal          |
| Boundary Scale                            | Standardized Z  |
| Alternative Hypothesis                    | Two-Sided       |
| Early Stop                                | Accept Null     |
| Number of Stages                          | 3               |
| Alpha                                     | 0.05            |
| Beta                                      | 0.10009         |
| Power                                     | 0.89991         |
| Max Information (Percent of Fixed Sample) | 103.9566        |
| Max Information                           | 1091.97232      |
| Null Ref ASN (Percent of Fixed Sample)    | 75.18254        |
| Alt Ref ASN (Percent of Fixed Sample)     | 101.8349        |

The derived Type II error probability  $\beta$  and power  $1 - \beta$  are different because of the new information levels.

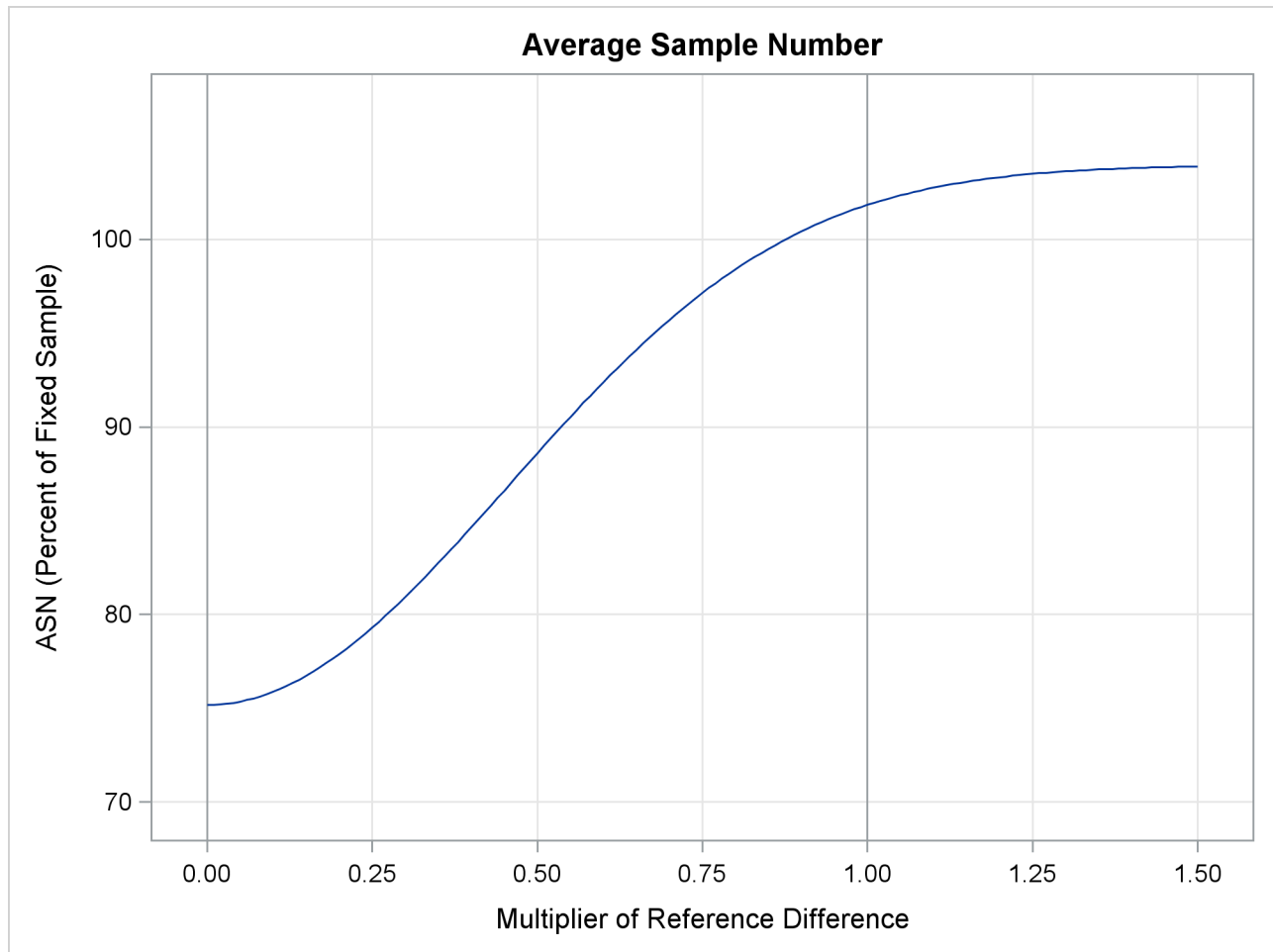
With the PSS option, the “Power and Expected Sample Sizes” table in [Output 84.3.14](#) displays powers and expected mean sample sizes under various hypothetical references  $\theta = c_i\theta_1$ , where  $\theta_1$  is the alternative reference and  $c_i = 0, 0.5, 1, 1.5$  are the default values in the CREF= option.

**Output 84.3.14** Power and Expected Sample Size Information

| Powers and Expected Sample Sizes   |         |                                          |
|------------------------------------|---------|------------------------------------------|
| Reference = CRef * (Alt Reference) |         |                                          |
| CRef                               | Power   | -Sample Size-<br>Percent<br>Fixed-Sample |
| 0.0000                             | 0.02500 | 75.1825                                  |
| 0.5000                             | 0.37154 | 88.5975                                  |
| 1.0000                             | 0.89991 | 101.8349                                 |
| 1.5000                             | 0.99758 | 103.8843                                 |

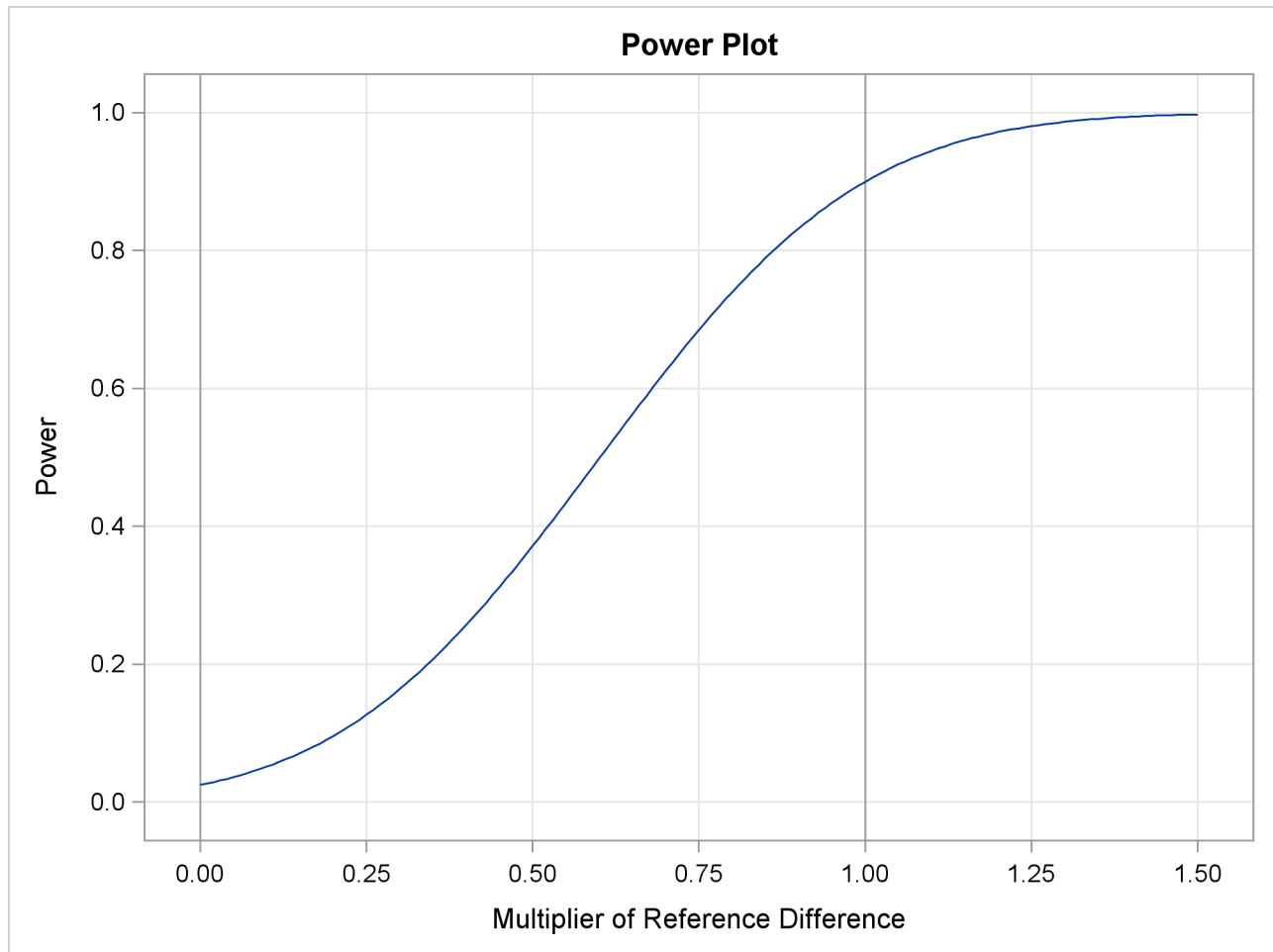
With the PLOTS=ASN option, the procedure displays a plot of expected sample sizes under various hypothetical references, as shown in [Output 84.3.15](#). By default, expected sample sizes under the hypotheses  $\theta = c_i\theta_1$ ,  $c_i = 0, 0.01, 0.02, \dots, 1.50$ , are displayed, where  $\theta_1$  is the alternative reference.

Output 84.3.15 ASN Plot



With the PLOTS=POWER option, the procedure displays a plot of the power curves under various hypothetical references for all designs simultaneously, as shown in [Output 84.3.16](#). By default, powers under hypothetical references  $\theta = c_i \theta_1$  are displayed, where  $c_i = 0, 0.01, 0.02, \dots, 1.50$  by default. You can specify  $c_i$  values with the CREF= option. The  $c_i$  values are displayed on the horizontal axis.

Output 84.3.16 Power Plot



Under the null hypothesis,  $c_i = 0$ , the power is 0.025, which is the upper Type I error probability. Under the alternative hypothesis,  $c_i = 1$ , the power is 0.89991, which is one minus the Type II error probability, as displayed in the “Design Information” table in [Output 84.3.13](#).

The “Test Information” table in [Output 84.3.17](#) displays the boundary values for the test statistic with the default standardized Z scale. At stage 2, the standardized slope estimate 0.83805 is between the lower and upper  $\beta$  boundary values. The trial stops to accept the null hypothesis that the variable Weight has no effect on the oxygen intake rate after adjusting for other covariates.

## Output 84.3.17 Sequential Tests

| Test Information (Standardized Z Scale) |                         |          |                       |         |
|-----------------------------------------|-------------------------|----------|-----------------------|---------|
| Null Reference = 0                      |                         |          |                       |         |
| _Stage_                                 | ---Information Level--- |          | -----Alternative----- |         |
|                                         | Proportion              | Actual   | Lower                 | Upper   |
| 1                                       | 0.4934                  | 538.7887 | -2.32118              | 2.32118 |
| 2                                       | 0.7517                  | 820.8509 | -2.86505              | 2.86505 |
| 3                                       | 1.0000                  | 1091.972 | -3.30450              | 3.30450 |

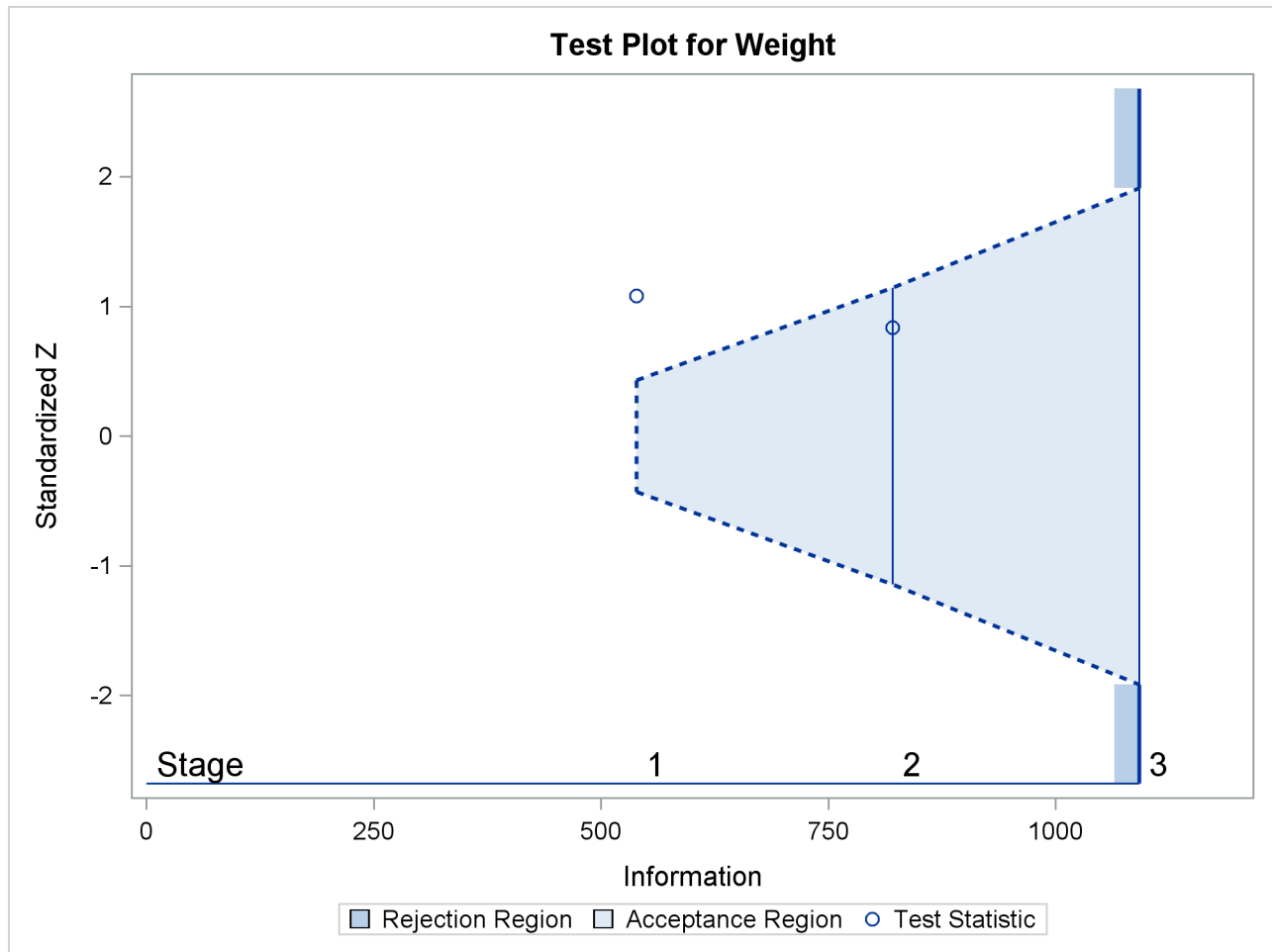
  

| Test Information (Standardized Z Scale) |                           |                     |                              |             |
|-----------------------------------------|---------------------------|---------------------|------------------------------|-------------|
| Null Reference = 0                      |                           |                     |                              |             |
| _Stage_                                 | -----Boundary Values----- |                     | -----Test-----               |             |
|                                         | ---Lower---<br>Beta       | ---Upper---<br>Beta | -----Weight-----<br>Estimate | Action      |
| 1                                       | -0.43033                  | 0.43033             | 1.08174                      | Continue    |
| 2                                       | -1.14239                  | 1.14239             | 0.83805                      | Accept Null |
| 3                                       | -1.91408                  | 1.91408             | .                            |             |

Since the data set PARMs\_FIT2 contains the test information only at stage 2, the information level at stage 1 in the TEST\_FIT1 data set is used to generate boundary values for the test.

With ODS Graphics enabled, a boundary plot with test statistics is displayed, as shown in [Output 84.3.18](#). As expected, the test statistic is in the acceptance region between the lower and upper  $\alpha$  boundaries at the final stage.

**Output 84.3.18** Sequential Test Plot



After a trial is stopped, the “Parameter Estimates” table in [Output 84.3.19](#) displays the stopping stage, parameter estimate, unbiased median estimate, confidence limits, and the  $p$ -value under the null hypothesis  $H_0 : \beta_w = 0$ . As expected, the  $p$ -value 0.3056 is not significant at the  $\alpha = 0.05$  level, and the confidence interval does contain the value zero. The  $p$ -value, unbiased median estimate, and confidence limits depend on the ordering of the sample space  $(k, z)$ , where  $k$  is the stage number and  $z$  is the standardized  $Z$  statistic. With the specified LR ordering, the  $p$ -values are computed with the ordering  $(k', z') > (k, z)$  if  $z' > z$ . See the section “[Available Sample Space Orderings in a Sequential Test](#)” on page 7230 for a detailed description of the LR ordering.

**Output 84.3.19** Parameter Estimates

| Parameter Estimates<br>LR Ordering |                       |          |                       |                 |
|------------------------------------|-----------------------|----------|-----------------------|-----------------|
| Parameter                          | Stopping Stage        | MLE      | p-Value for H0:Parm=0 | Median Estimate |
| Weight                             | 2                     | 0.029251 | 0.3056                | 0.037080        |
| Parameter Estimates<br>LR Ordering |                       |          |                       |                 |
| Parameter                          | 95% Confidence Limits |          |                       |                 |
| Weight                             | -0.03368 0.10532      |          |                       |                 |

### Example 84.4: Testing a Binomial Proportion

This example tests a binomial proportion by using a four-stage group sequential design. Suppose a supermarket is developing a new store-brand coffee. From past studies, the positive response for the current store-brand coffee from customers is around 60%. The store is interested in whether the new brand has a better positive response than the current brand.

A power family method is used for the group sequential trial with the null hypothesis  $H_0 : p = p_0 = 0.60$  and a one-sided upper alternative with a power of 0.80 at  $H_1 : p = 0.70$ . To accommodate the zero null reference that is assumed in the SEQDESIGN procedure, an equivalent hypothesis  $H_0 : \theta = 0$  with  $H_1 : \theta = 0.10$  is used, where  $\theta = p - p_0$ . The following statements request a power family method with early stopping to reject the null hypothesis:

```
ods graphics on;
proc seqdesign altref=0.10
 boundaryscale=mle
 ;
 PowerFamily: design method=pow
 nstages=4
 alt=upper
 beta=0.20
 ;
 samplesize model=onesamplefreq(nullprop=0.6);
 ods output Boundary=Bnd_Prop;
run;
ods graphics off;
```

The NULLPROP= option in the SAMPLESIZE statement specifies  $p_0 = 0.60$  for the sample size computation. The ODS OUTPUT statement with the BOUNDARY=BND\_PROP option creates an output data set named BND\_PROP which contains the resulting boundary information for the subsequent sequential tests.

With the BOUNDARYSCALE=MLE option, the procedure displays the output boundaries in terms of the maximum likelihood estimates. The “Design Information” table in [Output 84.4.1](#) displays design specifica-

tions and derived statistics. With the specified alternative reference  $\theta_1 = p_1 - p_0 = 0.7 - 0.6 = 0.1$ , the maximum information 670.38 is also derived.

**Output 84.4.1** Design Information

| The SEQDESIGN Procedure                   |              |
|-------------------------------------------|--------------|
| Design: PowerFamily                       |              |
| Design Information                        |              |
| Statistic Distribution                    | Normal       |
| Boundary Scale                            | MLE          |
| Alternative Hypothesis                    | Upper        |
| Early Stop                                | Reject Null  |
| Method                                    | Power Family |
| Boundary Key                              | Both         |
| Alternative Reference                     | 0.1          |
| Number of Stages                          | 4            |
| Alpha                                     | 0.05         |
| Beta                                      | 0.2          |
| Power                                     | 0.8          |
| Max Information (Percent of Fixed Sample) | 108.4306     |
| Max Information                           | 670.3782     |
| Null Ref ASN (Percent of Fixed Sample)    | 106.9276     |
| Alt Ref ASN (Percent of Fixed Sample)     | 78.51072     |

The “Boundary Information” table in [Output 84.4.2](#) displays the information level, alternative reference, and boundary values at each stage. With the STOP=REJECT option, only the rejection boundary values are displayed.

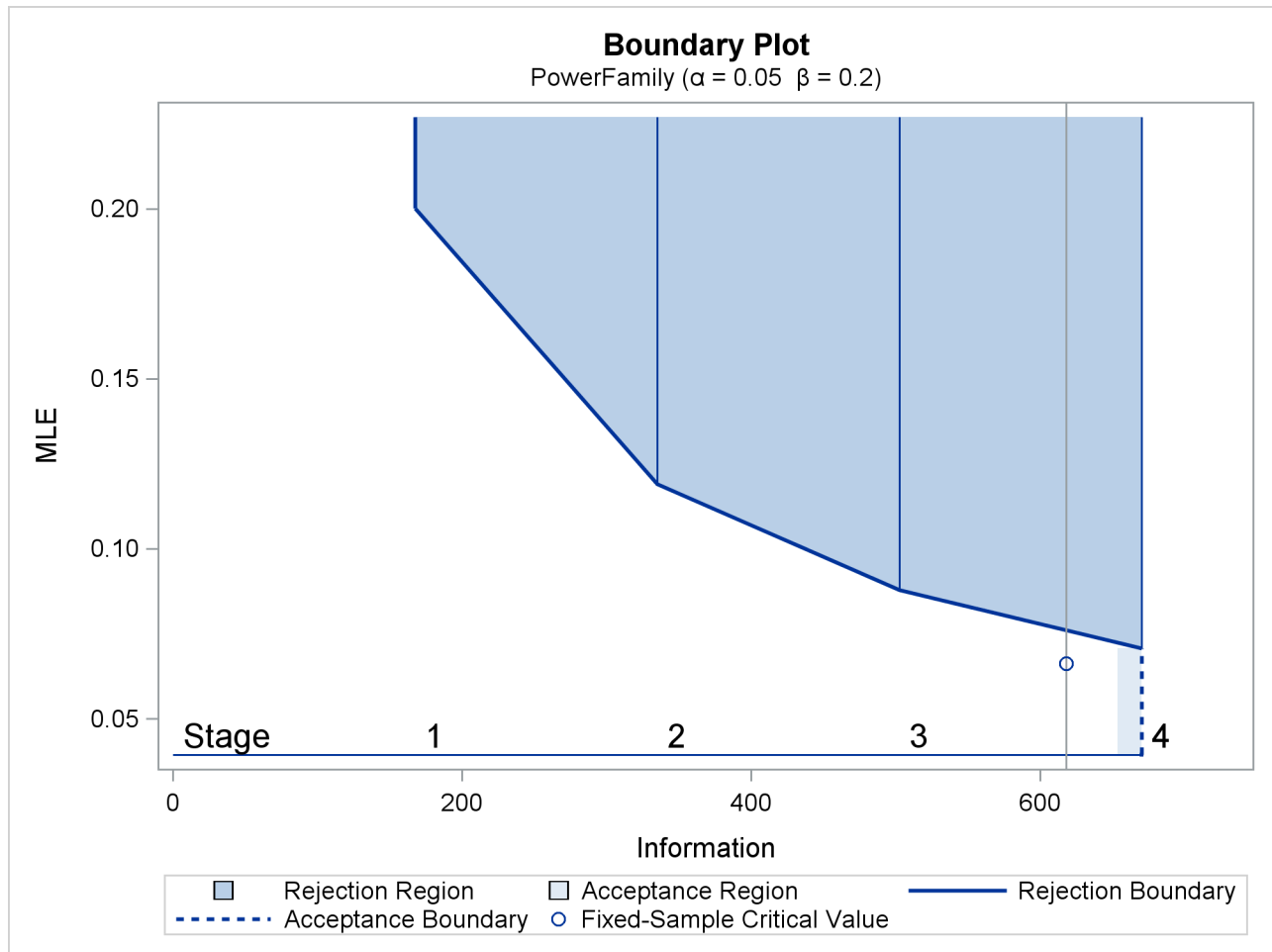
**Output 84.4.2** Boundary Information

| Boundary Information (MLE Scale) |                             |          |          |                        |                          |
|----------------------------------|-----------------------------|----------|----------|------------------------|--------------------------|
| Null Reference = 0               |                             |          |          |                        |                          |
| _Stage_                          | -----Information Level----- |          |          | -Alternative-          | -Boundary Values-        |
|                                  | Proportion                  | Actual   | N        | --Reference--<br>Upper | -----Upper-----<br>Alpha |
| 1                                | 0.2500                      | 167.5945 | 35.19485 | 0.10000                | 0.20018                  |
| 2                                | 0.5000                      | 335.1891 | 70.38971 | 0.10000                | 0.11903                  |
| 3                                | 0.7500                      | 502.7836 | 105.5846 | 0.10000                | 0.08782                  |
| 4                                | 1.0000                      | 670.3782 | 140.7794 | 0.10000                | 0.07077                  |

With ODS Graphics enabled, a detailed boundary plot with the rejection and acceptance regions is displayed, as shown in [Output 84.4.3](#).



**Output 84.4.3** Boundary Plot



With the MODEL=ONESAMPLEFREQ option in the SAMPLESIZE statement, the “Sample Size Summary” table in **Output 84.4.4** displays the parameters for the sample size computation.

**Output 84.4.4** Required Sample Size Summary

| Sample Size Summary             |                       |
|---------------------------------|-----------------------|
| Test                            | One-Sample Proportion |
| Null Proportion                 | 0.6                   |
| Proportion                      | 0.7                   |
| Test Statistic                  | Z for Proportion      |
| Reference Proportion            | Alt Ref               |
| Max Sample Size                 | 140.7794              |
| Expected Sample Size (Null Ref) | 138.828               |
| Expected Sample Size (Alt Ref)  | 101.9333              |

The “Sample Sizes” table in [Output 84.4.5](#) displays the required sample sizes for the group sequential clinical trial.

**Output 84.4.5** Required Sample Sizes

| Sample Sizes (N)                 |                        |             |                     |             |
|----------------------------------|------------------------|-------------|---------------------|-------------|
| One-Sample Z Test for Proportion |                        |             |                     |             |
| _Stage_                          | -----Fractional N----- |             | -----Ceiling N----- |             |
|                                  | N                      | Information | N                   | Information |
| 1                                | 35.19                  | 167.6       | 36                  | 171.4       |
| 2                                | 70.39                  | 335.2       | 71                  | 338.1       |
| 3                                | 105.58                 | 502.8       | 106                 | 504.8       |
| 4                                | 140.78                 | 670.4       | 141                 | 671.4       |

Thus, 36 customers are needed at stage 1, and 35 new customers are needed at each of the remaining stages. Suppose that 36 customers are available at stage 1. [Output 84.4.6](#) lists the 10 observations in the data set `count_1`.

**Output 84.4.6** Clinical Trial Data

| First 10 Obs in the Trial Data |      |  |
|--------------------------------|------|--|
| Obs                            | Resp |  |
| 1                              | 1    |  |
| 2                              | 1    |  |
| 3                              | 0    |  |
| 4                              | 0    |  |
| 5                              | 1    |  |
| 6                              | 1    |  |
| 7                              | 0    |  |
| 8                              | 1    |  |
| 9                              | 1    |  |
| 10                             | 1    |  |

The `Resp` variable is an indicator variable with a value of 1 for a customer with a positive response and a value of 0 for a customer without a positive response.

The following statements use the `MEANS` procedure to compute the mean response at stage 1:

```
proc means data=Prop_1;
 var Resp;
 ods output Summary=Data_Prop1;
run;
```

The following statements create and display (in [Output 84.4.7](#)) the data set for the centered mean positive response,  $\hat{p} - p_0$ :

```
data Data_Prop1;
 set Data_Prop1;
 Scale='MLE';
 Stage= 1;
 NObs= Resp_N;
 PDiff= Resp_Mean - 0.6;
 keep _Scale_ _Stage_ NObs PDiff;
run;
proc print data=Data_Prop1;
 title 'Statistics Computed at Stage 1';
run;
```

**Output 84.4.7** Statistics Computed at Stage 1

| Statistics Computed at Stage 1 |         |         |      |           |
|--------------------------------|---------|---------|------|-----------|
| Obs                            | _Scale_ | _Stage_ | NObs | PDiff     |
| 1                              | MLE     | 1       | 36   | -0.016667 |

The following statements invoke the SEQTEST procedure to test for early stopping at stage 1:

```
ods graphics on;
proc seqtest Boundary=Bnd_Prop
 Data(Testvar=PDiff)=Data_Prop1
 infoadj=prop
 boundarykey=both
 boundaryscale=mle
 ;
 ods output Test=Test_Prop1;
run;
ods graphics off;
```

The BOUNDARY= option specifies the input data set that provides the boundary information for the trial at stage 1, which was generated in the SEQDESIGN procedure. The DATA=DATA\_PROP1 option specifies the input data set DATA\_PROP1 that contains the test statistic and its associated sample size at stage 1, and the TESTVAR=PDIFF option identifies the test variable PDIFF in the data set.

If the computed information level for stage 1 is not the same as the value provided in the BOUNDARY= data set, the INFOADJ=PROP option (which is the default) proportionally adjusts the information levels at future interim stages from the levels provided in the BOUNDARY= data set. The BOUNDARYKEY=BOTH option maintains both the  $\alpha$  and  $\beta$  levels. The BOUNDARYSCALE=MLE option displays the output boundaries in terms of the MLE scale.

The ODS OUTPUT statement with the TEST=TEST\_PROP1 option creates an output data set named TEST\_PROP1 which contains the updated boundary information for the test at stage 1. The data set also provides the boundary information that is needed for the group sequential test at the next stage.

The “Design Information” table in [Output 84.4.8](#) displays design specifications. With the specified BOUNDARYKEY=BOTH option, the information levels and boundary values at future stages are modified to maintain both the  $\alpha$  and  $\beta$  levels.

**Output 84.4.8** Design Information

| The SEQTEST Procedure                     |                 |
|-------------------------------------------|-----------------|
| Design Information                        |                 |
| BOUNDARY Data Set                         | WORK.BND_PROP   |
| Data Set                                  | WORK.DATA_PROP1 |
| Statistic Distribution                    | Normal          |
| Boundary Scale                            | MLE             |
| Alternative Hypothesis                    | Upper           |
| Early Stop                                | Reject Null     |
| Number of Stages                          | 4               |
| Alpha                                     | 0.05            |
| Beta                                      | 0.2             |
| Power                                     | 0.8             |
| Max Information (Percent of Fixed Sample) | 108.4795        |
| Max Information                           | 670.680662      |
| Null Ref ASN (Percent of Fixed Sample)    | 106.9693        |
| Alt Ref ASN (Percent of Fixed Sample)     | 78.44835        |

The “Test Information” table in [Output 84.4.9](#) displays the boundary values for the test statistic with the specified MLE scale.

**Output 84.4.9** Sequential Tests

| Test Information (MLE Scale) |                             |          |          |                        |                          |
|------------------------------|-----------------------------|----------|----------|------------------------|--------------------------|
| Null Reference = 0           |                             |          |          |                        |                          |
| _Stage_                      | -----Information Level----- |          |          | -Alternative-          | -Boundary Values-        |
|                              | Proportion                  | Actual   | N        | --Reference--<br>Upper | -----Upper-----<br>Alpha |
| 1                            | 0.2556                      | 171.4286 | 35.98376 | 0.10000                | 0.19638                  |
| 2                            | 0.5037                      | 337.8459 | 70.91565 | 0.10000                | 0.11843                  |
| 3                            | 0.7519                      | 504.2633 | 105.8475 | 0.10000                | 0.08770                  |
| 4                            | 1.0000                      | 670.6807 | 140.7794 | 0.10000                | 0.07080                  |

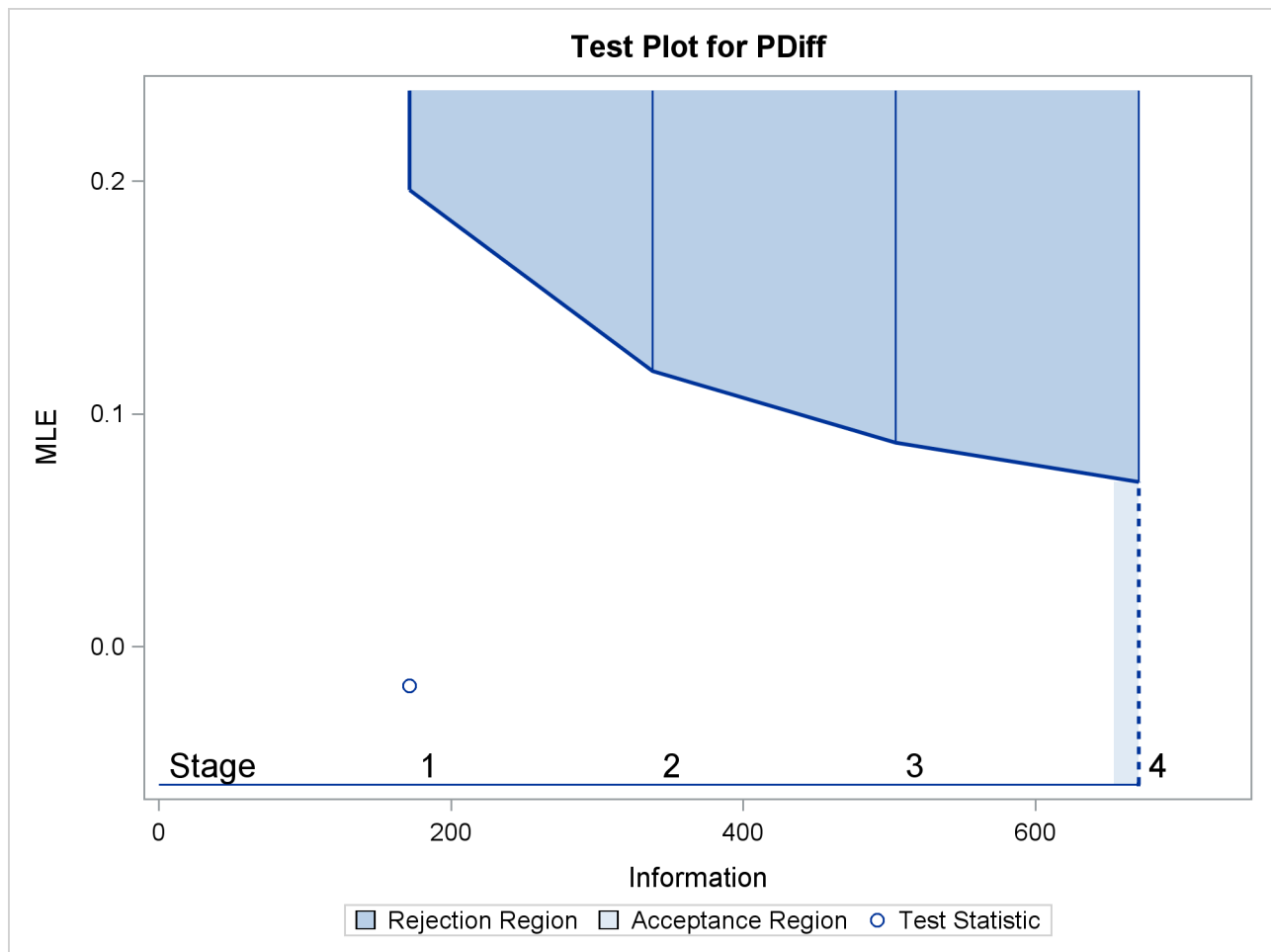
| Test Information (MLE Scale) |                |          |
|------------------------------|----------------|----------|
| Null Reference = 0           |                |          |
| _Stage_                      | -----Test----- |          |
|                              | Estimate       | PDiff    |
| 1                            | -0.01667       | Continue |
| 2                            | .              |          |
| 3                            | .              |          |
| 4                            | .              |          |

The information level at stage 1 is computed as  $I_1^* = I_1 \times (n_1^*/n_1)$ , where  $I_1$  and  $n_1$  are the information level and sample size at stage 1 in the BOUNDARY= data set, and  $n_1^* = 36$  is the available sample size at stage 1.

With the INFOADJ=PROP option (which is the default), the information levels at interim stages 2 and 3 are derived proportionally from the information levels in the BOUNDARY= data set. At stage 1, the statistic  $\hat{\theta} = \hat{p} - p_0 = 0.58333 - 0.6 = -0.01667$  is less than the upper  $\alpha$  boundary value 0.19638, so the trial continues to the next stage.

With ODS Graphics enabled, a boundary plot with the rejection and acceptance regions is displayed, as shown in [Output 84.4.10](#). As expected, the test statistic is in the continuation region.

**Output 84.4.10** Sequential Test Plot



The following statements use the MEANS procedure to compute the mean response at stage 2:

```
proc means data=Prop_2;
 var Resp;
 ods output Summary=Data_Prop2;
run;
```

The following statements create and display (in [Output 84.4.11](#)) the data set for the centered mean positive response ( $\hat{p} - p_0$ ) at stage 2:

```
data Data_Prop2;
 set Data_Prop2;
 Scale='MLE';
 Stage= 2;
 NObs= Resp_N;
 PDiff= Resp_Mean - 0.6;
 keep _Scale_ _Stage_ NObs PDiff;
run;

proc print data=Data_Prop2;
 title 'Statistics Computed at Stage 2';
run;
```

**Output 84.4.11** Statistics Computed at Stage 2

| Statistics Computed at Stage 2 |         |         |      |           |
|--------------------------------|---------|---------|------|-----------|
| Obs                            | _Scale_ | _Stage_ | NObs | PDiff     |
| 1                              | MLE     | 2       | 71   | -0.064789 |

The following statements invoke the SEQTEST procedure to test for early stopping at stage 2:

```
ods graphics on;
proc seqtest Boundary=Test_Prop1
 Data(Testvar=PDiff)=Data_Prop2
 inoadj=prop
 boundarykey=both
 boundaryscale=mle
 condpower(cref=1)
 predpower
 plots=condpower
 ;
 ods output test=Test_Prop2;
run;
ods graphics off;
```

The BOUNDARY= option specifies the input data set that provides the boundary information for the trial at stage 2, which was generated by the SEQTEST procedure at the previous stage. The DATA= option specifies the input data set that contains the test statistic and its associated sample size at stage 2, and the TESTVAR= option identifies the test variable in the data set.

The ODS OUTPUT statement with the TEST=TEST\_PROP2 option creates an output data set named TEST\_PROP2 which contains the updated boundary information for the test at stage 2. The data set also provides the boundary information that is needed for the group sequential test at the next stage.

The CONDPower(CREF=1) option requests the conditional power with the observed statistic under the alternative hypothesis, in addition to the conditional power under the hypothetical reference  $\theta = \hat{\theta}$ , the MLE estimate. The PREDPOWER option requests the noninformative predictive power with the observed statistic.

The “Test Information” table in [Output 84.4.12](#) displays the boundary values for the test statistic with the specified MLE scale. The test statistic  $\hat{\theta} = -0.06479$  is less than the corresponding upper  $\alpha$  boundary 0.11831, so the sequential test does not stop at stage 2 to reject the null hypothesis.

**Output 84.4.12** Sequential Tests

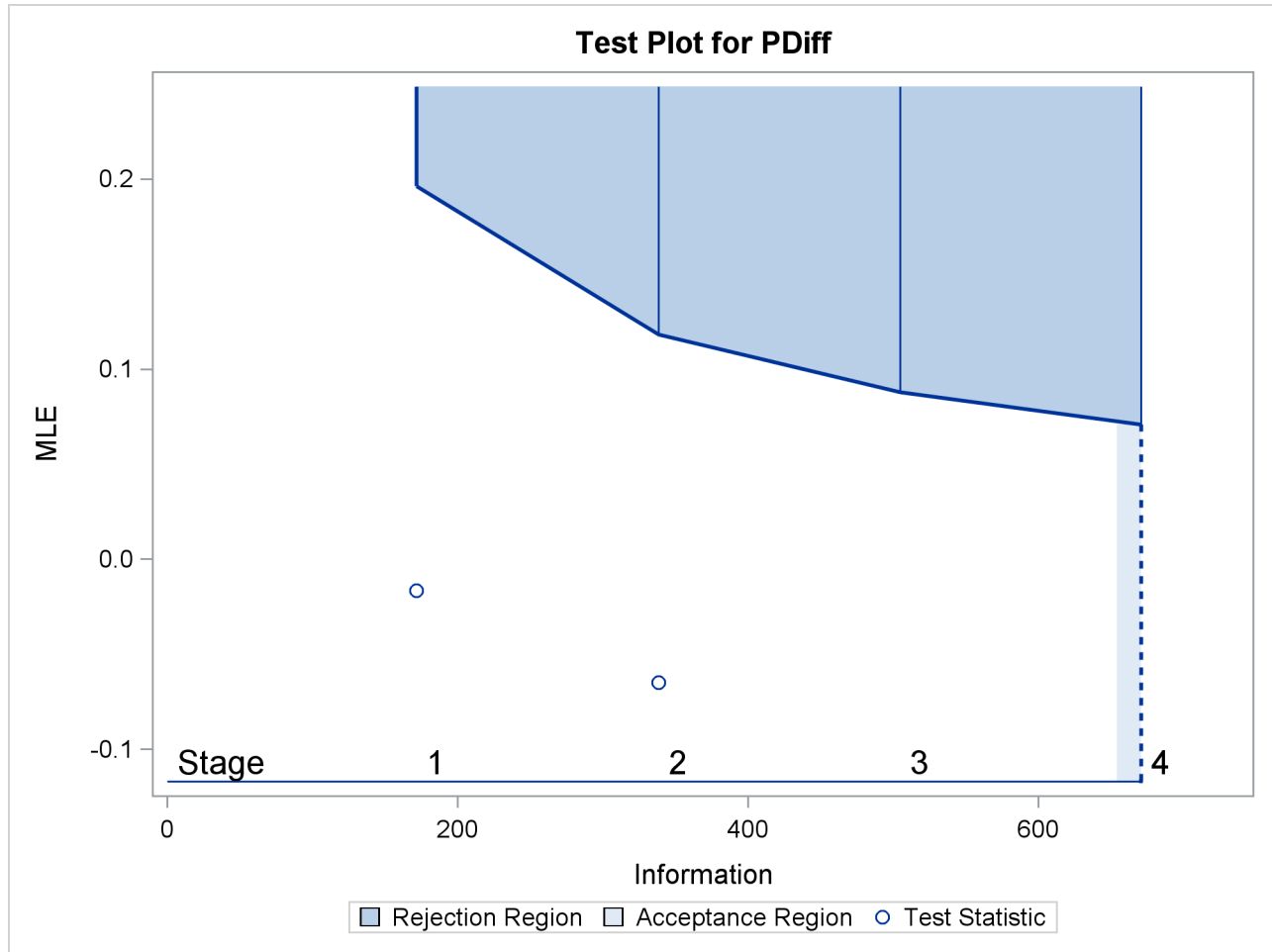
| The SEQTEST Procedure        |                             |          |          |                        |                   |         |
|------------------------------|-----------------------------|----------|----------|------------------------|-------------------|---------|
| Test Information (MLE Scale) |                             |          |          |                        |                   |         |
| Null Reference = 0           |                             |          |          |                        |                   |         |
| _Stage_                      | -----Information Level----- |          |          | -Alternative-          | -Boundary Values- |         |
|                              | Proportion                  | Actual   | N        | --Reference--<br>Upper | -----Upper-----   | Alpha   |
| 1                            | 0.2556                      | 171.4286 | 35.98223 | 0.10000                |                   | 0.19638 |
| 2                            | 0.5043                      | 338.2478 | 70.99698 | 0.10000                |                   | 0.11831 |
| 3                            | 0.7522                      | 504.4785 | 105.8882 | 0.10000                |                   | 0.08767 |
| 4                            | 1.0000                      | 670.7092 | 140.7794 | 0.10000                |                   | 0.07081 |

| Test Information (MLE Scale) |                |          |
|------------------------------|----------------|----------|
| Null Reference = 0           |                |          |
| _Stage_                      | -----Test----- |          |
|                              | Estimate       | Action   |
| 1                            | -0.01667       | Continue |
| 2                            | -0.06479       | Continue |
| 3                            | .              |          |
| 4                            | .              |          |

With ODS Graphics enabled, the “Test Plot” displays boundary values of the design and the test statistic, as shown in [Output 84.4.13](#). It also shows that the test statistic is in the “Continuation Region” below the upper  $\alpha$  boundary value at stage 2.

**Output 84.4.13** Sequential Test Plot



The “Conditional Power Information” table in [Output 84.4.14](#) displays conditional powers given the observed statistic under hypothetical references  $\theta = \hat{\theta}$ , the maximum likelihood estimate, and  $\theta = \theta_1$ . The constant  $c$  under CRef for the MLE is derived from  $\hat{\theta} = c\theta_1$ ; that is,  $c = \hat{\theta}/\theta_1 = -0.06479/0.1 = -0.6479$ .

**Output 84.4.14** Conditional Power

| Conditional Power Information      |          |                     |         |                   |
|------------------------------------|----------|---------------------|---------|-------------------|
| Reference = CRef * (Alt Reference) |          |                     |         |                   |
| Stopping Stage                     | MLE      | -----Reference----- |         | Conditional Power |
|                                    |          | Ref                 | CRef    |                   |
| 2                                  | -0.06479 | MLE                 | -0.6479 | 0.00000           |
| 2                                  | -0.06479 | Alternative         | 1.0000  | 0.02369           |

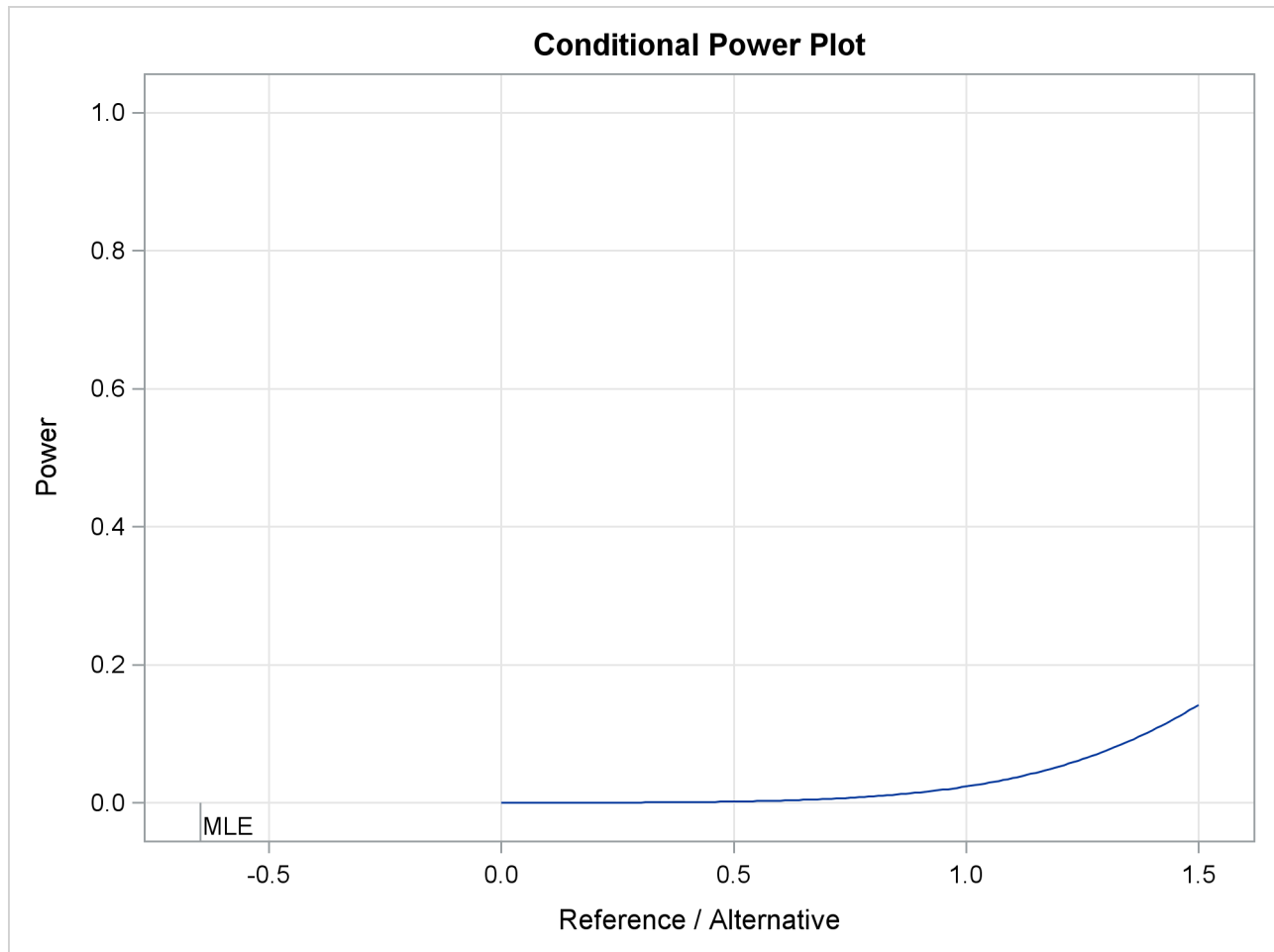
The conditional power is the probability of rejecting the null hypothesis under these hypothetical references given the observed statistic  $\hat{\theta} = -0.06479$ . The table in [Output 84.4.14](#) shows a weak conditional power of 0.02369 under the alternative hypothesis.



With the default TYPE=ALLSTAGES suboption in the CONDPOWER option, the conditional power at the interim stage 2 is the probability that the test statistic would exceed the rejection critical value at all future stages given the observed statistic  $\hat{\theta} = -0.06479$ .

The “Conditional Power Plot” displays conditional powers given the observed statistic under various hypothetical references, as shown in [Output 84.4.15](#). These references include  $\theta = \hat{\theta}$ , the maximum likelihood estimate, and  $\theta = c_i\theta_1$ , where  $\theta_1$  is the alternative reference and  $c_i = 0, 0.01, \dots, 1.50$  are constants that are specified in the CREF= option. [Output 84.4.16](#) shows that the conditional power increases as  $c_i$  increases.

**Output 84.4.15** Conditional Power Plot



The predictive power is the probability to reject the null hypothesis under the posterior distribution with a noninformative prior given the observed statistic  $\hat{\theta} = -0.06479$ . The “Predictive Power Information” table in [Output 84.4.16](#) indicates that the predictive power at  $\hat{\theta} = -0.06479$  is 0.0002.

**Output 84.4.16** Predictive Power

| Predictive Power Information |          |                  |
|------------------------------|----------|------------------|
| Stopping Stage               | MLE      | Predictive Power |
| 2                            | -0.06479 | 0.00020          |

With a predictive power 0.0002 and a conditional power of 0.02369 under  $H_1$ , the supermarket decides to stop the trial and accept the null hypothesis. That is, the positive response for the new store-brand coffee is not better than that for the current store-brand coffee.

The following statements invoke the SEQTEST procedure to test for early stopping at stage 2. The NSTAGES=3 option sets the next stage as the final stage (stage 3), and the BOUNDARYKEY=BOTH option derives the information level at stage 3 that maintain both Type I and Type II error probability levels. The CONDPOWER(CREF=1) option requests the conditional power with the observed statistic under the alternative hypothesis, in addition to the conditional power under the hypothetical reference  $\theta = \hat{\theta}$ , the MLE estimate.

```
proc seqtest Boundary=Test_Prop1
 Data (Testvar=PDiff)=Data_Prop2
 nstages=3
 boundarykey=both
 boundaryscale=mle
 condpower (cref=1)
;
run;
```

The “Test Information” table in [Output 84.4.17](#) displays the boundary values for the test statistic with the specified MLE scale, assuming that the next stage is the final stage.

**Output 84.4.17** Sequential Tests

| The SEQTEST Procedure        |                             |          |          |                        |                          |
|------------------------------|-----------------------------|----------|----------|------------------------|--------------------------|
| Test Information (MLE Scale) |                             |          |          |                        |                          |
| Null Reference = 0           |                             |          |          |                        |                          |
| _Stage_                      | -----Information Level----- |          |          | -Alternative-          | -Boundary Values-        |
|                              | Proportion                  | Actual   | N        | --Reference--<br>Upper | -----Upper-----<br>Alpha |
| 1                            | 0.2645                      | 171.4286 | 37.23405 | 0.10000                | 0.19638                  |
| 2                            | 0.5219                      | 338.2478 | 73.46696 | 0.10000                | 0.11831                  |
| 3                            | 1.0000                      | 648.1598 | 140.7794 | 0.10000                | 0.06831                  |

| Test Information (MLE Scale) |                |          |
|------------------------------|----------------|----------|
| Null Reference = 0           |                |          |
| _Stage_                      | -----Test----- |          |
|                              | Estimate       | Action   |
| 1                            | -0.01667       | Continue |
| 2                            | -0.06479       | Continue |
| 3                            | .              |          |

The “Conditional Power Information” table in [Output 84.4.18](#) displays conditional powers given the observed statistic, assuming that the next stage is the final stage.

**Output 84.4.18** Conditional Power

| Conditional Power Information      |          |                     |         |                      |
|------------------------------------|----------|---------------------|---------|----------------------|
| Reference = CRef * (Alt Reference) |          |                     |         |                      |
| Stopping<br>Stage                  | MLE      | -----Reference----- |         | Conditional<br>Power |
|                                    |          | Ref                 | CRef    |                      |
| 2                                  | -0.06479 | MLE                 | -0.6479 | 0.00000              |
| 2                                  | -0.06479 | Alternative         | 1.0000  | 0.02278              |

The conditional power is the probability of rejecting the null hypothesis under these hypothetical references given the observed statistic  $\hat{\theta} = -0.06479$ . The table in [Output 84.4.18](#) also shows a weak conditional power of 0.02278 under the alternative hypothesis.

## Example 84.5: Comparing Two Proportions with a Log Odds Ratio Test

This example compares two binomial proportions by using a log odds ratio statistic in a five-stage group sequential test. A clinic is studying the effect of vitamin C supplements in treating flu symptoms. The study consists of patients in the clinic who exhibit the first sign of flu symptoms within the last 24 hours. These patients are randomly assigned to either the control group (which receives placebo pills) or the treatment group (which receives large doses of vitamin C supplements). At the end of a five-day period, the flu symptoms of each patient are recorded.

Suppose that you know from past experience that flu symptoms disappear in five days for 60% of patients who experience flu symptoms. The clinic would like to detect a 70% symptom disappearance with a high probability. A test that compares the proportions directly specifies the null hypothesis  $H_0 : \theta = p_t - p_c = 0$  with a one-sided alternative  $H_1 : \theta > 0$  and a power of 0.90 at  $H_1 : \theta = 0.10$ , where  $p_t$  and  $p_c$  are the proportions of symptom disappearance in the treatment group and control group, respectively. An alternative trial tests an equivalent hypothesis by using the log odds ratio statistics:

$$\theta = \log \left( \frac{\left( \frac{p_t}{1-p_t} \right)}{\left( \frac{p_c}{1-p_c} \right)} \right)$$

Then the null hypothesis is  $H_0 : \theta = \theta_0 = 0$  and the alternative hypothesis is

$$H_1 : \theta = \theta_1 = \log \left( \frac{\left( \frac{0.70}{0.30} \right)}{\left( \frac{0.6}{0.4} \right)} \right) = 0.441833$$

The following statements invoke the SEQDESIGN procedure and request a five-stage group sequential design by using an error spending function method for normally distributed statistics. The design uses a two-sided alternative hypothesis with early stopping to reject the null hypothesis  $H_0$ .

```
ods graphics on;
proc seqdesign altref=0.441833
 boundaryscale=mle
 ;
 OneSidedErrorSpending: design method=errfuncpow
 nstages=5
 alt=upper
 stop=accept
 alpha=0.025;
 sample size model=twosamplefreq(nullprop=0.6 test=logor);
 ods output Boundary=Bnd_CSUP;
run;
ods graphics off;
```

The ODS OUTPUT statement with the BOUNDARY=BND\_CSUP option creates an output data set named BND\_CSUP which contains the resulting boundary information for the subsequent sequential tests.

The “Design Information” table in [Output 84.5.1](#) displays design specifications and derived statistics. With the specified alternative reference, the maximum information 56.30934 is derived.

**Output 84.5.1** Design Information

| The SEQDESIGN Procedure                   |                |
|-------------------------------------------|----------------|
| Design: OneSidedErrorSpending             |                |
| Design Information                        |                |
| Statistic Distribution                    | Normal         |
| Boundary Scale                            | MLE            |
| Alternative Hypothesis                    | Upper          |
| Early Stop                                | Accept Null    |
| Method                                    | Error Spending |
| Boundary Key                              | Both           |
| Alternative Reference                     | 0.441833       |
| Number of Stages                          | 5              |
| Alpha                                     | 0.025          |
| Beta                                      | 0.1            |
| Power                                     | 0.9            |
| Max Information (Percent of Fixed Sample) | 104.6166       |
| Max Information                           | 56.30934       |
| Null Ref ASN (Percent of Fixed Sample)    | 57.21399       |
| Alt Ref ASN (Percent of Fixed Sample)     | 102.1058       |

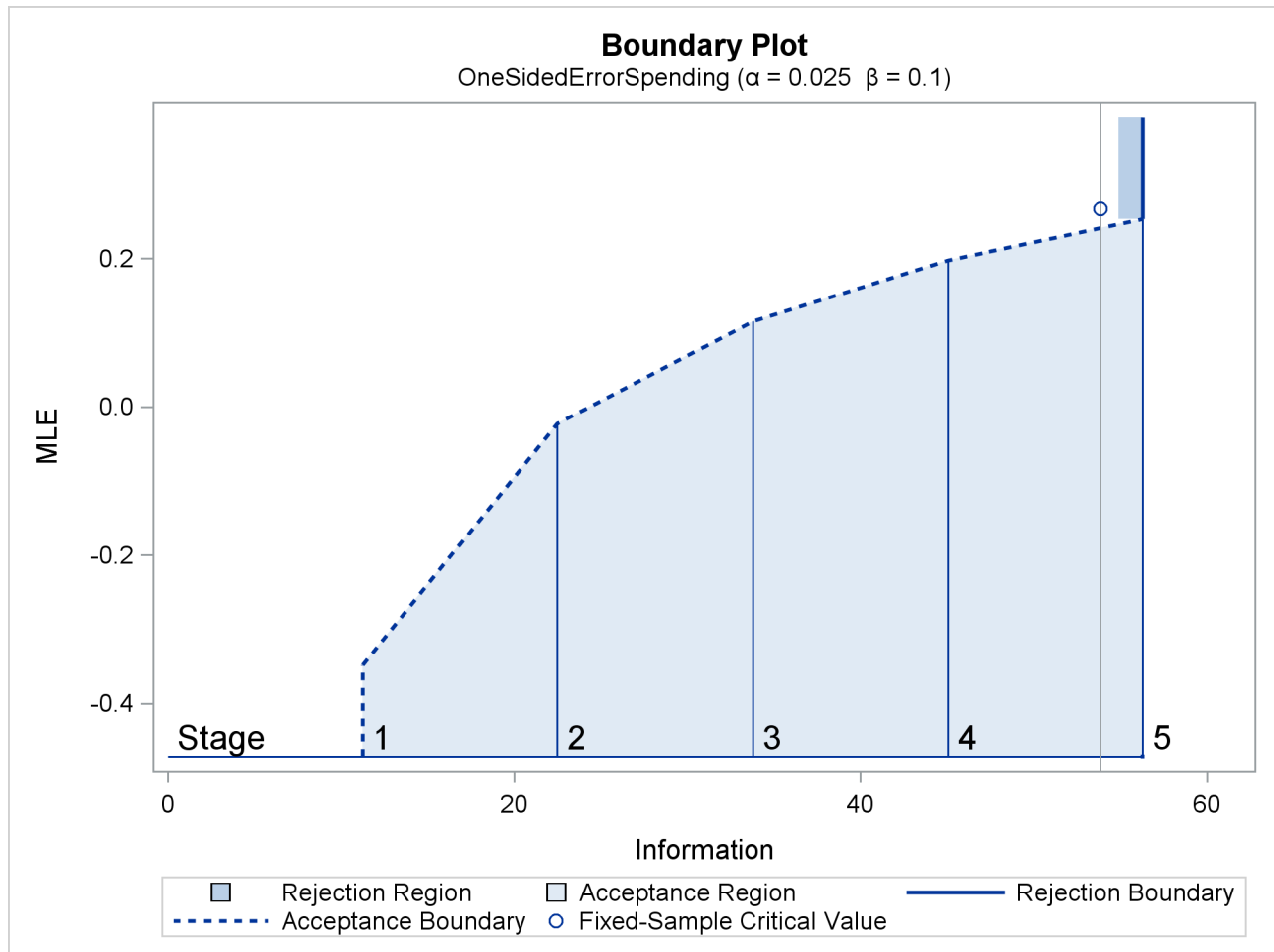
The “Boundary Information” table in [Output 84.5.2](#) displays information level, alternative reference, and boundary values at each stage. With the specified BOUNDARYSCALE=MLE option, the procedure displays the output boundaries in terms of the MLE scale.

**Output 84.5.2** Boundary Information

| Boundary Information (MLE Scale) |                             |          |          |                        |                         |
|----------------------------------|-----------------------------|----------|----------|------------------------|-------------------------|
| Null Reference = 0               |                             |          |          |                        |                         |
| _Stage_                          | -----Information Level----- |          |          | -Alternative-          | -Boundary Values-       |
|                                  | Proportion                  | Actual   | N        | --Reference--<br>Upper | -----Upper-----<br>Beta |
| 1                                | 0.2000                      | 11.26187 | 201.1048 | 0.44183                | -0.34844                |
| 2                                | 0.4000                      | 22.52374 | 402.2096 | 0.44183                | -0.02262                |
| 3                                | 0.6000                      | 33.7856  | 603.3144 | 0.44183                | 0.11527                 |
| 4                                | 0.8000                      | 45.04747 | 804.4192 | 0.44183                | 0.19708                 |
| 5                                | 1.0000                      | 56.30934 | 1005.524 | 0.44183                | 0.25345                 |

With ODS Graphics enabled, a detailed boundary plot with the rejection and acceptance regions is displayed, as shown in [Output 84.5.3](#).

**Output 84.5.3** Boundary Plot



With the SAMPLESIZE statement, the “Sample Size Summary” table in [Output 84.5.4](#) displays the parameters for the sample size computation.

**Output 84.5.4** Sample Size Summary

| Sample Size Summary             |                        |
|---------------------------------|------------------------|
| Test                            | Two-Sample Proportions |
| Null Proportion                 | 0.6                    |
| Proportion (Group A)            | 0.7                    |
| Test Statistic                  | Log Odds Ratio         |
| Reference Proportions           | Alt Ref                |
| Max Sample Size                 | 1005.524               |
| Expected Sample Size (Null Ref) | 549.9132               |
| Expected Sample Size (Alt Ref)  | 981.3914               |

The “Sample Sizes” table in [Output 84.5.5](#) displays the required sample sizes for the group sequential clinical trial.

**Output 84.5.5** Required Sample Sizes

| Sample Sizes (N)                                         |         |          |          |             |
|----------------------------------------------------------|---------|----------|----------|-------------|
| Two-Sample Log Odds Ratio Test for Proportion Difference |         |          |          |             |
| -----Fractional N-----                                   |         |          |          |             |
| _Stage_                                                  | N       | N(Grp 1) | N(Grp 2) | Information |
| 1                                                        | 201.10  | 100.55   | 100.55   | 11.2619     |
| 2                                                        | 402.21  | 201.10   | 201.10   | 22.5237     |
| 3                                                        | 603.31  | 301.66   | 301.66   | 33.7856     |
| 4                                                        | 804.42  | 402.21   | 402.21   | 45.0475     |
| 5                                                        | 1005.52 | 502.76   | 502.76   | 56.3093     |

| Sample Sizes (N)                                         |      |          |          |             |
|----------------------------------------------------------|------|----------|----------|-------------|
| Two-Sample Log Odds Ratio Test for Proportion Difference |      |          |          |             |
| -----Ceiling N-----                                      |      |          |          |             |
| _Stage_                                                  | N    | N(Grp 1) | N(Grp 2) | Information |
| 1                                                        | 202  | 101      | 101      | 11.3120     |
| 2                                                        | 404  | 202      | 202      | 22.6240     |
| 3                                                        | 604  | 302      | 302      | 33.8240     |
| 4                                                        | 806  | 403      | 403      | 45.1360     |
| 5                                                        | 1006 | 503      | 503      | 56.3360     |

Thus, 101 new patients are needed in each group at stages 1, 2, and 4, and 100 new patients are needed in each group at stages 3 and 5. Suppose that 101 patients are available in each group at stage 1. [Output 84.5.6](#) lists the 10 observations in the data set `count_1`.

**Output 84.5.6** Clinical Trial Data

| First 10 Obs in the Trial Data |         |      |
|--------------------------------|---------|------|
| Obs                            | TrtGrp  | Resp |
| 1                              | Control | 1    |
| 2                              | C_Sup   | 0    |
| 3                              | Control | 0    |
| 4                              | C_Sup   | 1    |
| 5                              | Control | 1    |
| 6                              | C_Sup   | 1    |
| 7                              | Control | 1    |
| 8                              | C_Sup   | 0    |
| 9                              | Control | 0    |
| 10                             | C_Sup   | 1    |

The `TrtGrp` variable is a grouping variable with the value `Control` for a patient in the placebo control group and the value `C_Sup` for a patient in the treatment group who receives vitamin C supplements. The `Resp` variable is an indicator variable with the value 1 for a patient without flu symptoms after five days and the value 0 for a patient with flu symptoms after five days.

The following statements use the LOGISTIC procedure to compute the log odds ratio statistic and its associated standard error at stage 1:

```
proc logistic data=CSup_1 descending;
 class TrtGrp / param=ref;
 model Resp= TrtGrp;
 ods output ParameterEstimates=Parms_CSUP1;
run;
```

The DESCENDING option is used to reverse the order for the response levels, so the LOGISTIC procedure is modeling the probability that  $\text{Resp} = 1$ .

The following statements create and display (in [Output 84.5.7](#)) the data set for the log odds ratio statistic and its associated standard error:

```
data Parms_CSUP1;
 set Parms_CSUP1;
 if Variable='TrtGrp' and ClassVal0='C_Sup';
 Scale='MLE';
 Stage= 1;
 keep _Scale_ _Stage_ Variable Estimate StdErr;
run;

proc print data=Parms_CSUP1;
 title 'Statistics Computed at Stage 1';
run;
```

**Output 84.5.7** Statistics Computed at Stage 1

| Statistics Computed at Stage 1 |          |          |        |         |         |
|--------------------------------|----------|----------|--------|---------|---------|
| Obs                            | Variable | Estimate | StdErr | _Scale_ | _Stage_ |
| 1                              | TrtGrp   | 0.3247   | 0.2856 | MLE     | 1       |

The following statements invoke the SEQTEST procedure to test for early stopping at stage 1:

```
ods graphics on;
proc seqtest Boundary=Bnd_CSUP
 Parms (Testvar=TrtGrp) =Parms_CSUP1
 infoadj=prop
 errspendadj=errfuncpow
 boundarykey=both
 boundaryscale=mle
 ;
 ods output test=Test_CSUP1;
run;
ods graphics off;
```

The BOUNDARY= option specifies the input data set that provides the boundary information for the trial at stage 1, which was generated in the SEQDESIGN procedure. The PARM=PARMS\_CSUP1 option specifies the input data set PARMS\_CSUP1 that contains the test statistic and its associated standard error at stage 1, and the TESTVAR=TRTGRP option identifies the test variable TRTGRP in the data set.



If the computed information level for stage 1 is not the same as the value provided in the BOUNDARY= data set, the INFOADJ=PROP option (which is the default) proportionally adjusts the information levels at future interim stages from the levels provided in the BOUNDARY= data set. The ERRSPENDADJ=ERRFUNCPOW option adjusts the boundaries with the updated error spending values generated from the power error spending function. The BOUNDARYKEY=BOTH option maintains both the  $\alpha$  and  $\beta$  levels. The BOUNDARYSCALE=MLE option displays the output boundaries in terms of the MLE scale.

The ODS OUTPUT statement with the TEST=TEST\_CSUP1 option creates an output data set named TEST\_CSUP1 which contains the updated boundary information for the test at stage 1. The data set also provides the boundary information that is needed for the group sequential test at the next stage.

The “Design Information” table in [Output 84.5.8](#) displays design specifications. With the specified BOUNDARYKEY=BOTH option, the information levels and boundary values at future stages are modified to maintain both the  $\alpha$  and  $\beta$  levels.

**Output 84.5.8** Design Information

| The SEQTEST Procedure                     |                  |
|-------------------------------------------|------------------|
| Design Information                        |                  |
| BOUNDARY Data Set                         | WORK.BND_CSUP    |
| Data Set                                  | WORK.PARMS_CSUP1 |
| Statistic Distribution                    | Normal           |
| Boundary Scale                            | MLE              |
| Alternative Hypothesis                    | Upper            |
| Early Stop                                | Accept Null      |
| Number of Stages                          | 5                |
| Alpha                                     | 0.025            |
| Beta                                      | 0.1              |
| Power                                     | 0.9              |
| Max Information (Percent of Fixed Sample) | 104.6673         |
| Max Information                           | 56.3361718       |
| Null Ref ASN (Percent of Fixed Sample)    | 57.02894         |
| Alt Ref ASN (Percent of Fixed Sample)     | 102.1369         |

The “Test Information” table in [Output 84.5.9](#) displays the boundary values for the test statistic with the specified MLE scale. With the INFOADJ=PROP option (which is the default), the information levels at future interim stages are derived proportionally from the observed information at stage 1 and the information levels in the BOUNDARY= data set.

Since the information level at stage 1 is derived from the PARMS= data set and other information levels are not specified, equal increments are used at remaining stages. At stage 1, the MLE statistic 0.32474 is greater than the corresponding upper  $\beta$  boundary value  $-0.29906$ , so the sequential test continues to the next stage.

**Output 84.5.9** Sequential Tests

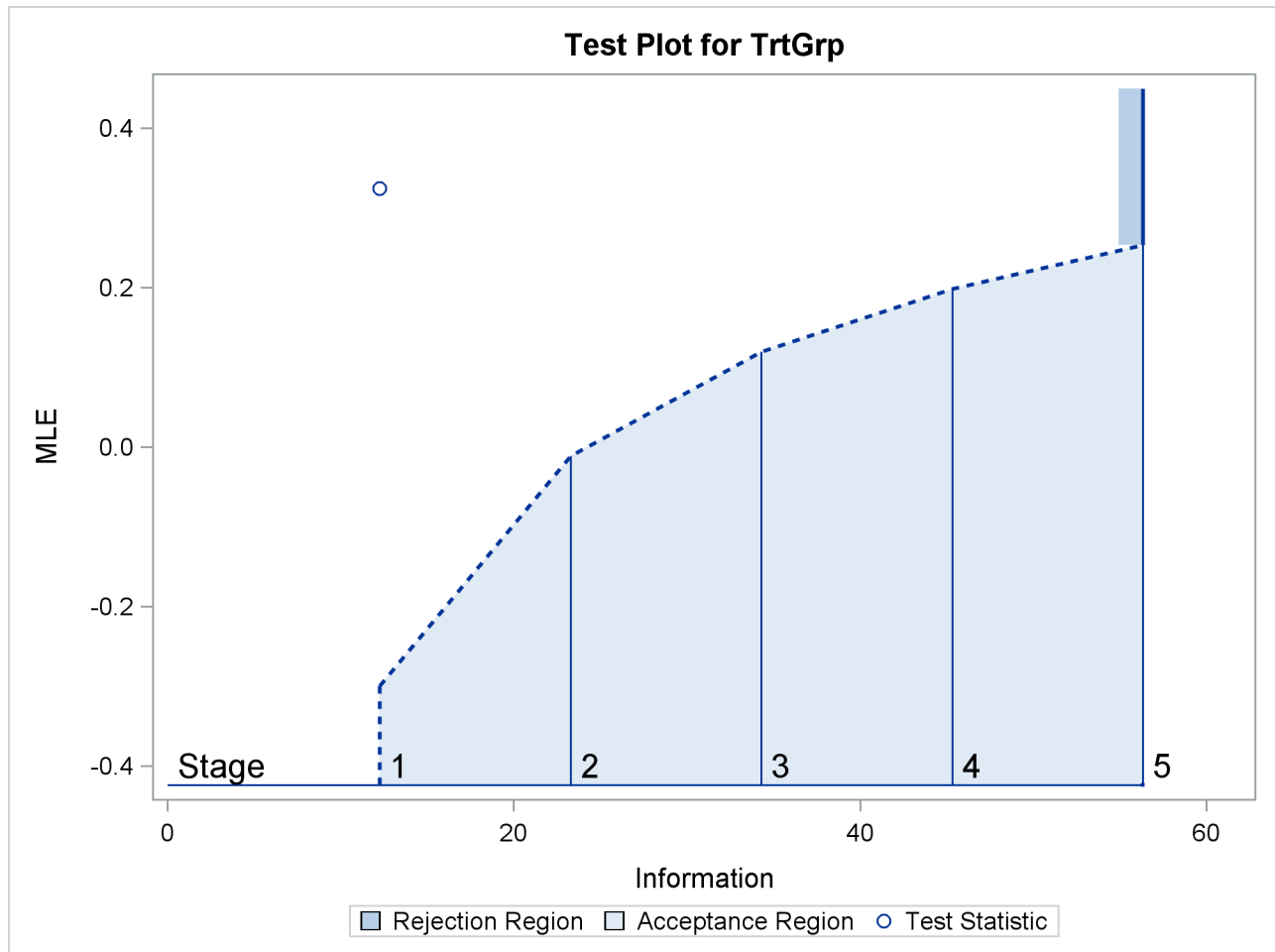
| Test Information (MLE Scale) |                         |          |                        |
|------------------------------|-------------------------|----------|------------------------|
| Null Reference = 0           |                         |          |                        |
| _Stage_                      | ---Information Level--- |          | -Alternative-          |
|                              | Proportion              | Actual   | --Reference--<br>Upper |
| 1                            | 0.2176                  | 12.26014 | 0.44183                |
| 2                            | 0.4132                  | 23.27914 | 0.44183                |
| 3                            | 0.6088                  | 34.29815 | 0.44183                |
| 4                            | 0.8044                  | 45.31716 | 0.44183                |
| 5                            | 1.0000                  | 56.33617 | 0.44183                |

| Test Information (MLE Scale) |                         |                              |          |
|------------------------------|-------------------------|------------------------------|----------|
| Null Reference = 0           |                         |                              |          |
| _Stage_                      | -Boundary Values-       | -----Test-----               |          |
|                              | -----Upper-----<br>Beta | -----TrtGrp-----<br>Estimate | Action   |
| 1                            | -0.29906                | 0.32474                      | Continue |
| 2                            | -0.01067                | .                            |          |
| 3                            | 0.11942                 | .                            |          |
| 4                            | 0.19829                 | .                            |          |
| 5                            | 0.25325                 | .                            |          |

With ODS Graphics enabled, a boundary plot with the boundary values and test statistics is displayed, as shown in [Output 84.5.10](#). As expected, the test statistic is in the continuation region.

Output 84.5.10 Sequential Test Plot



The following statements use the LOGISTIC procedure to compute the log odds ratio statistic and its associated standard error at stage 2:

```
proc logistic data=CSup_2 descending;
 class TrtGrp / param=ref;
 model Resp= TrtGrp;
 ods output ParameterEstimates=Parms_CSup2;
run;
```

The following statements create and display (in Output 84.5.11) the data set for the mean positive response and its associated standard error at stage 2:

```
data Parms_CSup2;
 set Parms_CSup2;
 if Variable='TrtGrp' and ClassVal0='C_Sup';
 Scale='MLE';
 Stage= 2;
 keep _Scale_ _Stage_ Variable Estimate StdErr;
run;
proc print data=Parms_CSup2;
 title 'Statistics Computed at Stage 2';
run;
```

**Output 84.5.11** Statistics Computed at Stage 2

| Statistics Computed at Stage 2 |          |          |        |         |         |
|--------------------------------|----------|----------|--------|---------|---------|
| Obs                            | Variable | Estimate | StdErr | _Scale_ | _Stage_ |
| 1                              | TrtGrp   | 0.2356   | 0.2073 | MLE     | 2       |

The following statements invoke the SEQTEST procedure to test for early stopping at stage 2:

```
proc seqtest Boundary=Test_CSup1
 Parms (testvar=TrtGrp)=Parms_CSup2
 infoadj=prop
 errspendadj=errfuncpow
 boundarykey=both
 boundaryscale=mle
 ;
ods output Test=Test_CSup2;
run;
```

The BOUNDARY= option specifies the input data set that provides the boundary information for the trial at stage 2, which was generated by the SEQTEST procedure at the previous stage. The PARMS= option specifies the input data set that contains the test statistic and its associated standard error at stage 2, and the TESTVAR= option identifies the test variable in the data set.

The ODS OUTPUT statement with the TEST=CSUP\_LDL2 option creates an output data set named CSUP\_LDL2 which contains the updated boundary information for the test at stage 2. The data set also provides the boundary information that is needed for the group sequential test at the next stage.

The “Test Information” table in [Output 84.5.12](#) displays the boundary values for the test statistic with the specified MLE scale. The test statistic 0.2356 is greater than the corresponding upper  $\beta$  boundary value  $-0.01068$ , so the sequential test continues to the next stage.

## Output 84.5.12 Sequential Tests

| The SEQTEST Procedure        |                         |          |                        |  |
|------------------------------|-------------------------|----------|------------------------|--|
| Test Information (MLE Scale) |                         |          |                        |  |
| Null Reference = 0           |                         |          |                        |  |
| _Stage_                      | ---Information Level--- |          | -Alternative-          |  |
|                              | Proportion              | Actual   | --Reference--<br>Upper |  |
| 1                            | 0.2176                  | 12.26014 | 0.44183                |  |
| 2                            | 0.4132                  | 23.27916 | 0.44183                |  |
| 3                            | 0.6088                  | 34.29799 | 0.44183                |  |
| 4                            | 0.8044                  | 45.31681 | 0.44183                |  |
| 5                            | 1.0000                  | 56.33563 | 0.44183                |  |

| Test Information (MLE Scale) |                   |          |                  |  |
|------------------------------|-------------------|----------|------------------|--|
| Null Reference = 0           |                   |          |                  |  |
| _Stage_                      | -Boundary Values- |          | -----Test-----   |  |
|                              | -----Upper-----   |          | -----TrtGrp----- |  |
|                              | Beta              | Estimate | Action           |  |
| 1                            | -0.29906          | 0.32474  | Continue         |  |
| 2                            | -0.01068          | 0.23560  | Continue         |  |
| 3                            | 0.11942           | .        | .                |  |
| 4                            | 0.19829           | .        | .                |  |
| 5                            | 0.25325           | .        | .                |  |

Similar results are found at stages 3 and stage 4, so the trial continues to the final stage. The following statements use the LOGISTIC procedure to compute the log odds ratio statistic and its associated standard error at stage 5:

```
proc logistic data=CSup_5 descending;
 class TrtGrp / param=ref;
 model Resp= TrtGrp;
 ods output ParameterEstimates=Parms_CSup5;
run;
```

The following statements create and display (in Output 84.5.13) the data set for the log odds ratio statistic and its associated standard error at stage 5:

```
data Parms_CSup5;
 set Parms_CSup5;
 if Variable='TrtGrp' and ClassVal0='C_Sup';
 Scale='MLE';
 Stage= 5;
 keep _Scale_ _Stage_ Variable Estimate StdErr;
run;

proc print data=Parms_CSup5;
 title 'Statistics Computed at Stage 5';
run;
```

**Output 84.5.13** Statistics Computed at Stage 5

| Statistics Computed at Stage 5 |          |          |        |         |         |
|--------------------------------|----------|----------|--------|---------|---------|
| Obs                            | Variable | Estimate | StdErr | _Scale_ | _Stage_ |
| 1                              | TrtGrp   | 0.2043   | 0.1334 | MLE     | 5       |

The following statements invoke the SEQTEST procedure to test for the hypothesis at stage 5:

```
ods graphics on;
proc seqtest Boundary=Test_CSup4
 Parms (testvar=TrtGrp)=Parms_CSup5
 errspendadj=errfuncpow
 boundaryscale=mle
 cialpha=.025
 rci
 plots=rci
 ;
run;
ods graphics off;
```

The BOUNDARY= option specifies the input data set that provides the boundary information for the trial at stage 5, which was generated by the SEQTEST procedure at the previous stage. The PARMS= option specifies the input data set that contains the test statistic and its associated standard error at stage 5, and the TESTVAR= option identifies the test variable in the data set. By default (or equivalently if you specify BOUNDARYKEY=ALPHA), the boundary value at stage 5 is derived to maintain the  $\alpha$  level.

The “Test Information” table in [Output 84.5.14](#) displays the boundary values for the test statistic with the specified MLE scale. The test statistic 0.2043 is less than the corresponding upper  $\beta$  boundary 0.25375, so the sequential test stops to accept the null hypothesis. That is, there is no reduction in duration of symptoms for the group receiving vitamin C supplements.

**Output 84.5.14** Sequential Tests

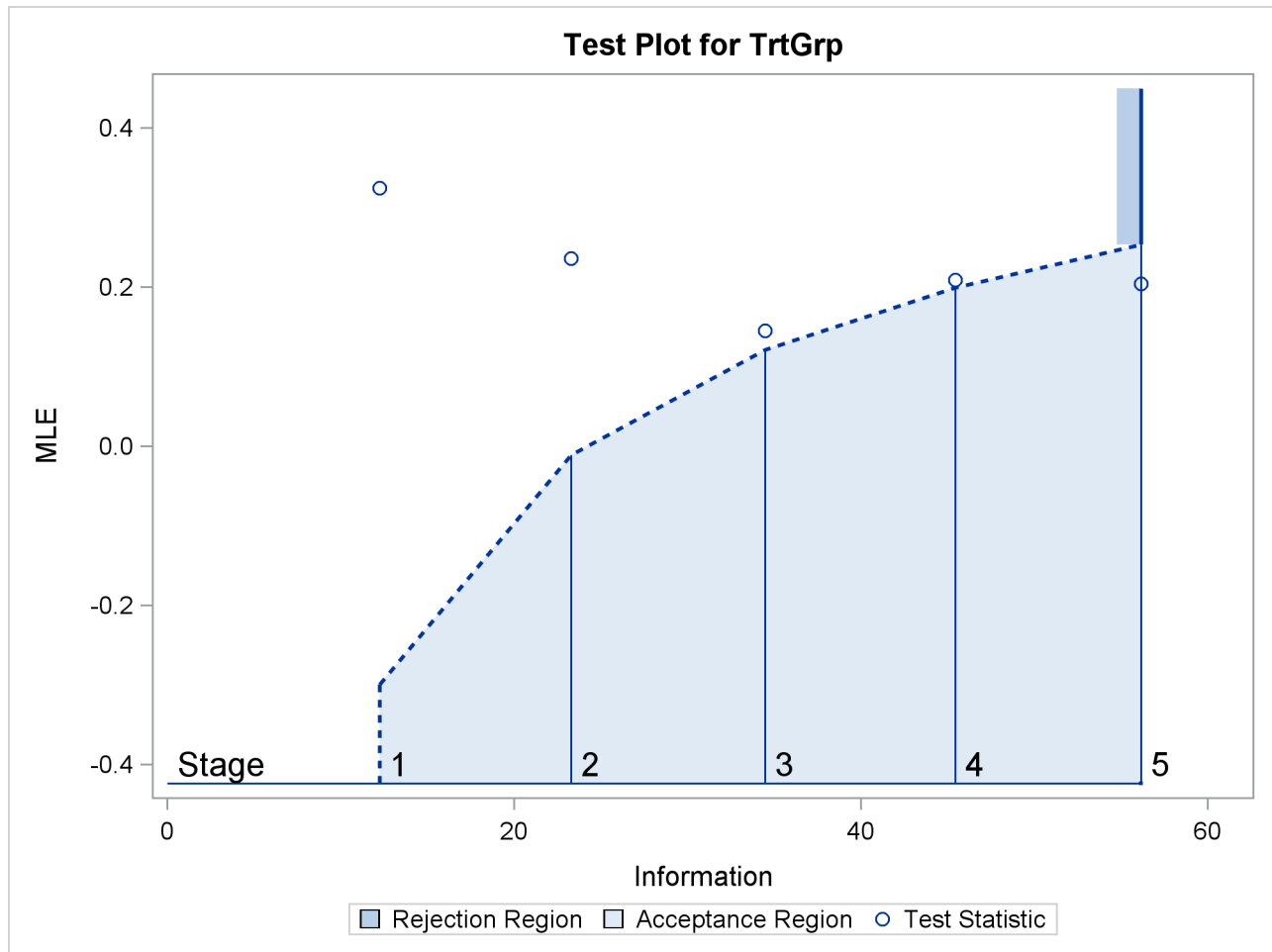
| The SEQTEST Procedure        |                        |          |                        |
|------------------------------|------------------------|----------|------------------------|
| Test Information (MLE Scale) |                        |          |                        |
| Null Reference = 0           |                        |          |                        |
| _Stage_                      | ---Information Level-- |          | -Alternative-          |
|                              | Proportion             | Actual   | --Reference--<br>Upper |
| 1                            | 0.2183                 | 12.26014 | 0.44183                |
| 2                            | 0.4145                 | 23.27916 | 0.44183                |
| 3                            | 0.6141                 | 34.48793 | 0.44183                |
| 4                            | 0.8092                 | 45.44685 | 0.44183                |
| 5                            | 1.0000                 | 56.16068 | 0.44183                |

| Test Information (MLE Scale) |                         |                |                            |
|------------------------------|-------------------------|----------------|----------------------------|
| Null Reference = 0           |                         |                |                            |
| _Stage_                      | -Boundary Values-       | -----Test----- |                            |
|                              | -----Upper-----<br>Beta | Estimate       | -----TrtGrp-----<br>Action |
| 1                            | -0.29906                | 0.32474        | Continue                   |
| 2                            | -0.01068                | 0.23560        | Continue                   |
| 3                            | 0.12134                 | 0.14482        | Continue                   |
| 4                            | 0.19899                 | 0.20855        | Continue                   |
| 5                            | 0.25375                 | 0.20430        | Accept Null                |

The “Test Plot” displays boundary values of the design and the test statistics, as shown in [Output 84.5.15](#). It also shows that the test statistic is in the “Acceptance Region” at the final stage.

**Output 84.5.15** Sequential Test Plot



After a trial is stopped, the “Parameter Estimates” table in [Output 84.5.16](#) displays the stopping stage, parameter estimate, unbiased median estimate, confidence limits, and the  $p$ -value under the null hypothesis  $H_0 : \theta = 0$ . As expected, the  $p$ -value 0.0456 is not significant at  $\alpha = 0.025$  level and the lower 97.5% confidence limit is less than the value  $\theta_0 = 0$ . The  $p$ -value, unbiased median estimate, and confidence limits depend on the ordering of the sample space  $(k, z)$ , where  $k$  is the stage number and  $z$  is the standardized  $Z$  statistic.

**Output 84.5.16** Parameter Estimates

| Parameter Estimates<br>Stagewise Ordering |                |          |                                  |                 |                |
|-------------------------------------------|----------------|----------|----------------------------------|-----------------|----------------|
| Parameter                                 | Stopping Stage | MLE      | p-Value for $H_0: \text{Parm}=0$ | Median Estimate | Lower 97.5% CL |
| TrtGrp                                    | 5              | 0.204303 | 0.0456                           | 0.234494        | -0.03712       |



Since the test is accepted at stage 5, the  $p$ -value computed by using the default stagewise ordering can be expressed as

$$\alpha_u = P_{\theta=0}(z_5 < Z_5 \mid b_k < Z_k, k < 5)$$

where  $z_5 = 1.53105$  is the test statistic at stage 5,  $Z_k$  is a standardized normal variate at stage  $k$ , and  $b_k$  is the upper  $\beta$  boundary value in the standardized  $Z$  scale at stage  $k$ ,  $k = 1, 2, \dots, 5$ .

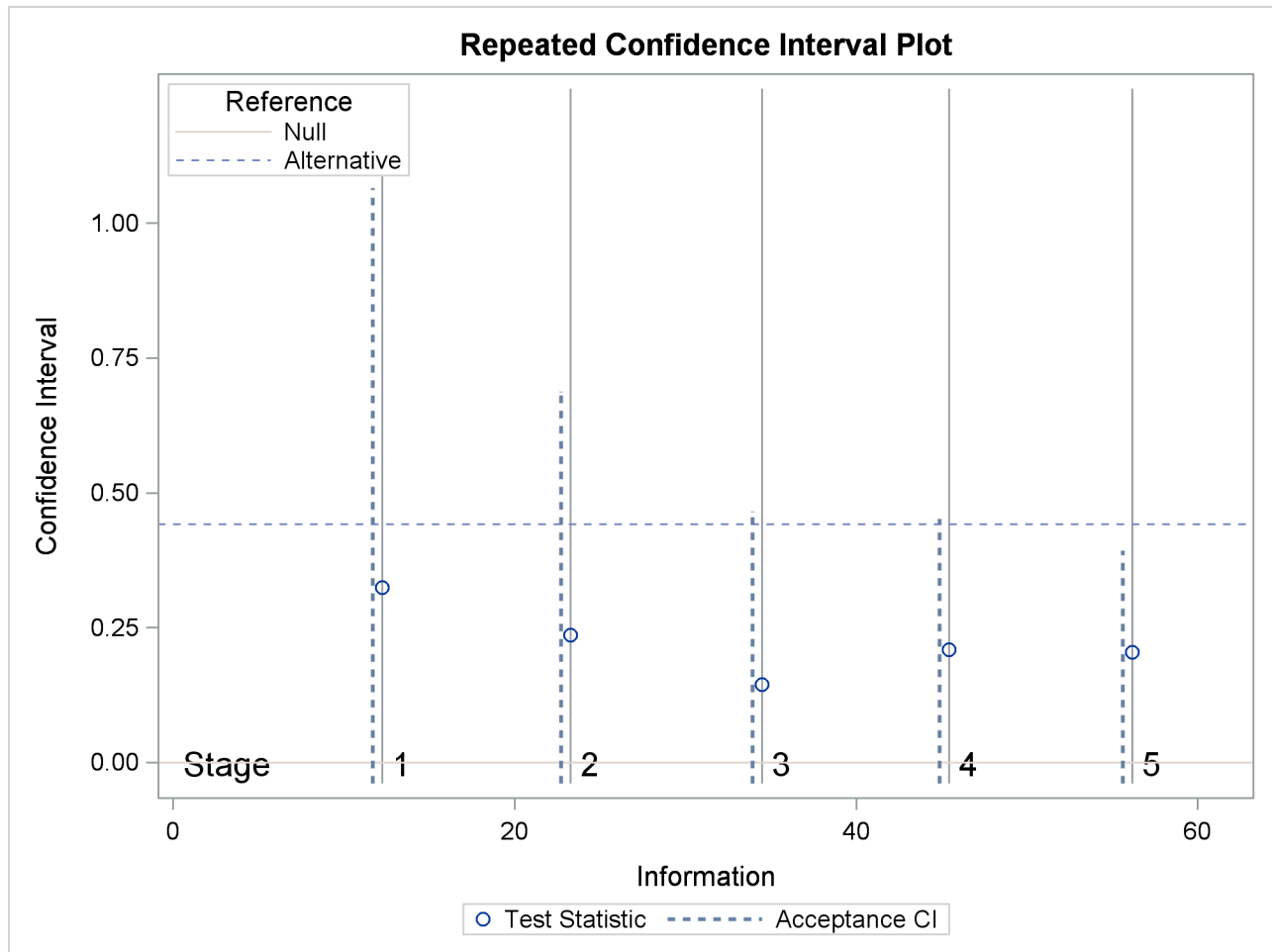
With the RCI option, the “Repeated Confidence Intervals” table in [Output 84.5.17](#) displays repeated confidence intervals for the parameter. For a one-sided test with an upper alternative hypothesis, since the upper acceptance repeated confidence limit 0.3924 at the final stage is less than the alternative reference 0.441833, the null hypothesis is accepted.

**Output 84.5.17** Repeated Confidence Intervals

| Repeated Confidence Intervals |                      |                       |                                          |
|-------------------------------|----------------------|-----------------------|------------------------------------------|
| <u>_Stage_</u>                | Information<br>Level | Parameter<br>Estimate | -Acceptance Boundary-<br>Upper 89.94% CI |
| 1                             | 12.2601              | 0.32474               | 1.0656                                   |
| 2                             | 23.2792              | 0.23560               | 0.6881                                   |
| 3                             | 34.4879              | 0.14482               | 0.4653                                   |
| 4                             | 45.4468              | 0.20855               | 0.4514                                   |
| 5                             | 56.1607              | 0.20430               | 0.3924                                   |

With the PLOTS=RCI option, the “Repeated Confidence Intervals Plot” displays repeated confidence intervals for the parameter, as shown in [Output 84.5.18](#). It shows that the upper acceptance repeated confidence limit at the final stage is less than the alternative reference 0.441833. This implies that the study accepts the null hypothesis at the final stage.

**Output 84.5.18** Repeated Confidence Intervals Plot



### Example 84.6: Comparing Two Survival Distributions with a Log-Rank Test

This example requests a log-rank test that compares two survival distributions for the treatment effect (Jenkinson and Turnbull 2000, pp. 77–79; Whitehead 1997, pp. 36–39).

A clinic is studying the effect of a new cancer treatment. The study consists of mice exposed to a carcinogen and randomized to either the control group or the treatment group. The event of interest is the death from cancer induced by the carcinogen, and the response is the time from randomization to death.

Following the derivations in the section “Test for Two Survival Distributions with a Log-Rank Test” in the chapter “The SEQDESIGN Procedure,” the hypothesis  $H_0 : \theta = -\log(\lambda) = 0$  with an alternative hypothesis  $H_1 : \theta = \theta_1 > 0$  can be used, where  $\lambda$  is the hazard ratio between the treatment group and control group.

Suppose that from past experience, the median survival time for the control group is  $t_0 = 20$  weeks, and the study would like to detect a  $t_1 = 40$  weeks median survival time with a 80% power in the trial. Assuming exponential survival functions for the two groups, the hazard rates can be computed from

$$S_j(t_j) = e^{-h_j t_j} = \frac{1}{2}$$

where  $j = 0, 1$ .

Thus, with  $h_0 = 0.03466$  and  $h_1 = 0.01733$ , the hazard ratio  $\lambda_1 = h_1/h_0 = 1/2$  and the alternative hypothesis is

$$\theta_1 = -\log(\lambda_1) = -\log\left(\frac{1}{2}\right) = 0.69315$$

The following statements invoke the SEQDESIGN procedure and request a four-stage group sequential design for normally distributed data. The design uses a one-sided alternative hypothesis with early stopping to reject and to accept the null hypothesis  $H_0$ . Whitehead's triangular method is used to derive the boundaries.

```
ods graphics on;
proc seqdesign altref=0.69315
 boundaryscale=score
 ;
 OneSidedWhitehead: design method=whitehead
 nstages=4
 boundarykey=alpha
 alt=upper stop=both
 beta=0.20;
 samplesize model=twosamplesurvival
 (nullhazard=0.03466
 accrate=10);
run;
ods graphics off;
```

A Whitehead method creates boundaries that approximately satisfy the Type I and Type II error probability level specification. The BOUNDARYKEY=ALPHA option is used to adjust the boundary value at the last stage and to meet the specified Type I probability level.

The specified ACCRATE=10 option indicates that 10 mice will be accrued each week and the resulting minimum and maximum accrual times are displayed. With the BOUNDARYSCALE=SCORE option, the procedure displays the output boundaries with the score statistics.

The “Design Information” table in [Output 84.6.1](#) displays design specifications and derived statistics.

**Output 84.6.1** Design Information

| The SEQDESIGN Procedure                   |                    |
|-------------------------------------------|--------------------|
| Design: OneSidedWhitehead                 |                    |
| Design Information                        |                    |
| Statistic Distribution                    | Normal             |
| Boundary Scale                            | Score              |
| Alternative Hypothesis                    | Upper              |
| Early Stop                                | Accept/Reject Null |
| Method                                    | Whitehead          |
| Boundary Key                              | Alpha              |
| Alternative Reference                     | 0.69315            |
| Number of Stages                          | 4                  |
| Alpha                                     | 0.05               |
| Beta                                      | 0.20044            |
| Power                                     | 0.79956            |
| Max Information (Percent of Fixed Sample) | 129.9894           |
| Max Information                           | 16.70624           |
| Null Ref ASN (Percent of Fixed Sample)    | 62.6302            |
| Alt Ref ASN (Percent of Fixed Sample)     | 74.00064           |

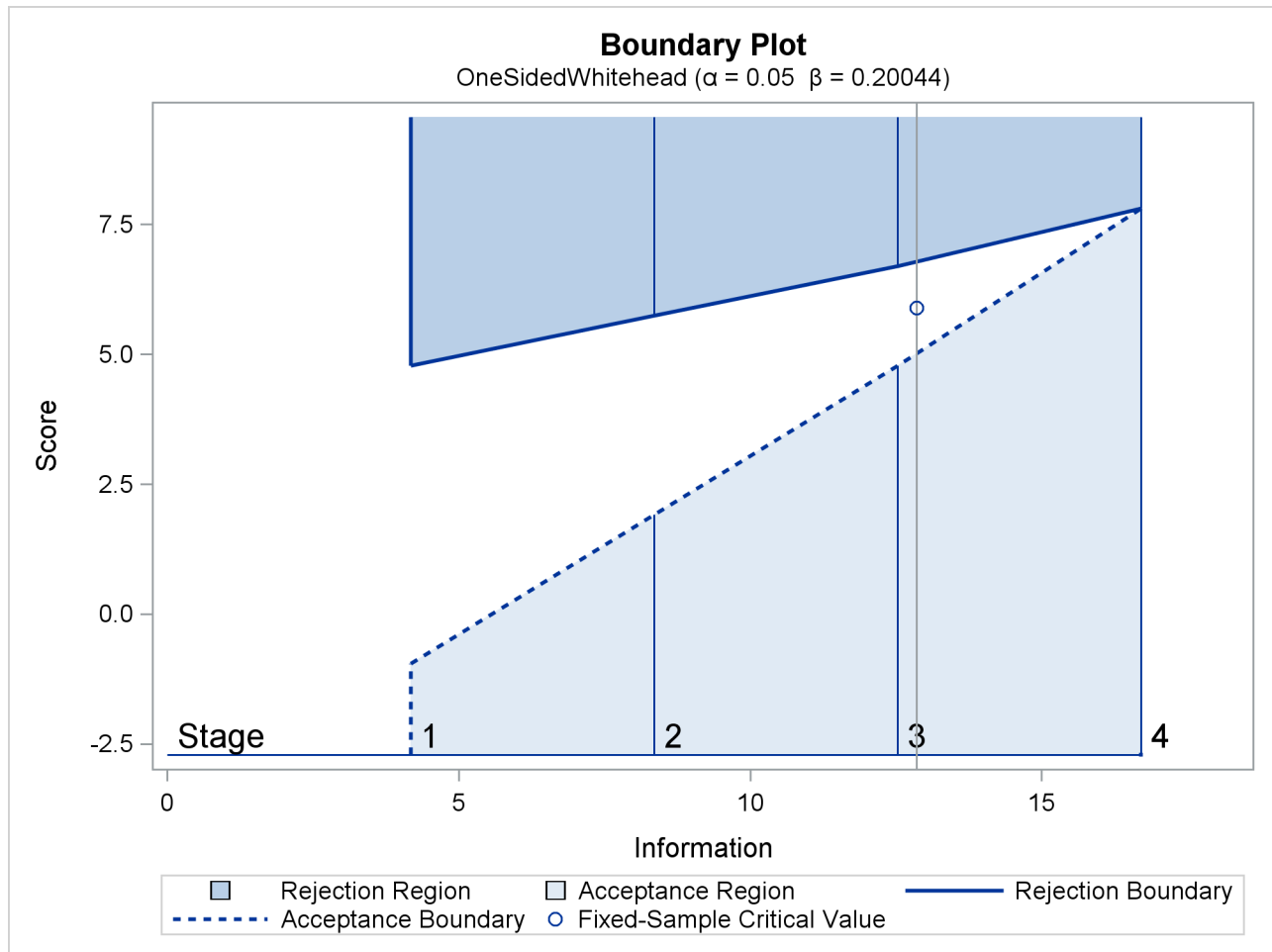
The “Boundary Information” table in [Output 84.6.2](#) displays the information level, alternative reference, and boundary values at each stage.

**Output 84.6.2** Boundary Information

| Boundary Information (Score Scale) |                             |          |          |               |                        |         |
|------------------------------------|-----------------------------|----------|----------|---------------|------------------------|---------|
| Null Reference = 0                 |                             |          |          |               |                        |         |
| _Stage_                            | -----Information Level----- |          |          | -Alternative- | ----Boundary Values--- |         |
|                                    | Proportion                  | Actual   | Events   | --Reference-- | -----Upper-----        |         |
|                                    |                             |          |          | Upper         | Beta                   | Alpha   |
| 1                                  | 0.2500                      | 4.176561 | 16.70624 | 2.89498       | -0.95755               | 4.78773 |
| 2                                  | 0.5000                      | 8.353122 | 33.41249 | 5.78997       | 1.91509                | 5.74527 |
| 3                                  | 0.7500                      | 12.52968 | 50.11873 | 8.68495       | 4.78773                | 6.70282 |
| 4                                  | 1.0000                      | 16.70624 | 66.82498 | 11.57993      | 7.81296                | 7.81296 |

With ODS Graphics enabled, a detailed boundary plot with the rejection and acceptance regions is displayed, as shown in [Output 84.6.3](#).

**Output 84.6.3** Boundary Plot



With the MODEL=TWOSAMPLESURVIVAL option in the SAMPLESIZE statement, the “Sample Size Summary” table in Output 84.6.4 displays the parameters for the sample size computation.

**Output 84.6.4** Required Sample Size Summary

| Sample Size Summary   |                     |
|-----------------------|---------------------|
| Test                  | Two-Sample Survival |
| Null Hazard Rate      | 0.03466             |
| Hazard Rate (Group A) | 0.01733             |
| Hazard Rate (Group B) | 0.03466             |
| Hazard Ratio          | 0.499999            |
| log(Hazard Ratio)     | -0.69315            |
| Reference Hazards     | Alt Ref             |
| Accrual               | Uniform             |
| Accrual Rate          | 10                  |
| Min Accrual Time      | 6.682498            |
| Min Sample Size       | 66.82498            |
| Max Accrual Time      | 25.401              |
| Max Sample Size       | 254.01              |
| Max Number of Events  | 66.82498            |

With a minimum accrual time of 6.6825 weeks and a maximum accrual time of 25.401 weeks, an accrual time of 20 weeks is used in the study.

The “Numbers of Events” table in [Output 84.6.5](#) displays the required number of events for the group sequential clinical trial.

**Output 84.6.5** Required Numbers of Events

| Numbers of Events (D)<br>Two-Sample Log-Rank Test |       |             |
|---------------------------------------------------|-------|-------------|
| _Stage_                                           | D     | Information |
| 1                                                 | 16.71 | 4.1766      |
| 2                                                 | 33.41 | 8.3531      |
| 3                                                 | 50.12 | 12.5297     |
| 4                                                 | 66.82 | 16.7062     |

The following statements invoke the SEQDESIGN procedure and provide more detailed sample size information:

```
proc seqdesign altref=0.69315
 boundaryscale=score
 ;
 OneSidedWhitehead: design method=whitehead
 nstages=4
 boundarykey=alpha
 alt=upper
 stop=both
 beta=0.20;
 samplesize model=twosamplesurvival
 (nullhazard=0.03466
 accrate=10 acctime=20);
 ods output Boundary=Bnd_Surv;
run;
```

The ODS OUTPUT statement with the BOUNDARY=BND\_SURV option creates an output data set named BND\_SURV which contains the resulting boundary information for the subsequent sequential tests.

With an accrual time of 20 weeks, the “Sample Size Summary” table in [Output 84.6.6](#) displays the follow-up time for the trial.

**Output 84.6.6** Required Sample Size Summary

| The SEQDESIGN Procedure         |                     |
|---------------------------------|---------------------|
| Design: OneSidedWhitehead       |                     |
| Sample Size Summary             |                     |
| Test                            | Two-Sample Survival |
| Null Hazard Rate                | 0.03466             |
| Hazard Rate (Group A)           | 0.01733             |
| Hazard Rate (Group B)           | 0.03466             |
| Hazard Ratio                    | 0.499999            |
| log(Hazard Ratio)               | -0.69315            |
| Reference Hazards               | Alt Ref             |
| Accrual                         | Uniform             |
| Accrual Rate                    | 10                  |
| Accrual Time                    | 20                  |
| Follow-up Time                  | 6.47422             |
| Total Time                      | 26.47422            |
| Max Number of Events            | 66.82498            |
| Max Sample Size                 | 200                 |
| Expected Sample Size (Null Ref) | 161.5937            |
| Expected Sample Size (Alt Ref)  | 172.4689            |

The “Numbers of Events and Sample Sizes” table in [Output 84.6.7](#) displays the required sample sizes for the group sequential clinical trial.

**Output 84.6.7** Numbers of Events and Sample Sizes

| Numbers of Events (D) and Sample Sizes (N)<br>Two-Sample Log-Rank Test |       |          |          |         |        |          |          |
|------------------------------------------------------------------------|-------|----------|----------|---------|--------|----------|----------|
| -----Fractional Time-----                                              |       |          |          |         |        |          |          |
| _Stage_                                                                | D     | D(Grp 1) | D(Grp 2) | Time    | N      | N(Grp 1) | N(Grp 2) |
| 1                                                                      | 16.71 | 5.82     | 10.89    | 11.9866 | 119.87 | 59.93    | 59.93    |
| 2                                                                      | 33.41 | 11.84    | 21.57    | 17.3584 | 173.58 | 86.79    | 86.79    |
| 3                                                                      | 50.12 | 18.01    | 32.11    | 21.7479 | 200.00 | 100.00   | 100.00   |
| 4                                                                      | 66.82 | 24.46    | 42.37    | 26.4742 | 200.00 | 100.00   | 100.00   |

| Numbers of Events (D) and Sample Sizes (N)<br>Two-Sample Log-Rank Test |             |                        |          |          |      |        |          |
|------------------------------------------------------------------------|-------------|------------------------|----------|----------|------|--------|----------|
| -Fractional Time----                                                   |             | -----Ceiling Time----- |          |          |      |        |          |
| _Stage_                                                                | Information | D                      | D(Grp 1) | D(Grp 2) | Time | N      | N(Grp 1) |
| 1                                                                      | 4.1766      | 16.74                  | 5.83     | 10.91    | 12   | 120.00 | 60.00    |
| 2                                                                      | 8.3531      | 35.73                  | 12.68    | 23.04    | 18   | 180.00 | 90.00    |
| 3                                                                      | 12.5297     | 51.07                  | 18.37    | 32.70    | 22   | 200.00 | 100.00   |
| 4                                                                      | 16.7062     | 68.55                  | 25.14    | 43.41    | 27   | 200.00 | 100.00   |

| Numbers of Events (D) and Sample Sizes (N)<br>Two-Sample Log-Rank Test |          |             |
|------------------------------------------------------------------------|----------|-------------|
| -----Ceiling Time-----                                                 |          |             |
| _Stage_                                                                | N(Grp 2) | Information |
| 1                                                                      | 60.00    | 4.1854      |
| 2                                                                      | 90.00    | 8.9322      |
| 3                                                                      | 100.00   | 12.7667     |
| 4                                                                      | 100.00   | 17.1377     |

Thus the study will perform three interim analyses after 12, 18, and 22 weeks and a final analysis after 27 weeks if the study does not stop at any of the interim analyses.

Note that the SEQDESIGN procedure does not compute numbers of events or sample sizes for all statistical models. If the number of events or sample size for a fixed-sample design is available, then the MODEL=INPUTNEVENTS or MODEL=INPUTNOBS option can be used to input fixed-sample information. For example, with a required fixed-sample number of events 51.4073, the following SAMPLESIZE statement can be used to produce the same sample size results:

```

samplesize model=inputnevents
 (d=51.47 sample=two
 hazard=0.03466 0.01733
 accrate=10 acctime=20);

```

Suppose that 120 mice are available after week 12 for the first interim analysis. [Output 84.6.8](#) lists the 10 observations in the data set weeks\_1.



**Output 84.6.8** Clinical Trial Data

| First 10 Obs in the Trial Data |           |       |       |
|--------------------------------|-----------|-------|-------|
| Obs                            | Trt<br>Gp | Event | Weeks |
| 1                              | 0         | 0     | 11    |
| 2                              | 1         | 0     | 11    |
| 3                              | 0         | 0     | 11    |
| 4                              | 1         | 0     | 11    |
| 5                              | 0         | 1     | 6     |
| 6                              | 1         | 0     | 11    |
| 7                              | 0         | 0     | 11    |
| 8                              | 1         | 0     | 11    |
| 9                              | 0         | 1     | 9     |
| 10                             | 1         | 0     | 11    |

The TrtGp variable is a grouping variable with the value 0 for a mouse in the placebo control group and the value 1 for a mouse in the treatment group. The Weeks variable is the survival time variable measured in weeks and the Event variable is the censoring variable with the value 0 indicating censoring. That is, the values of Weeks are considered censored if the corresponding values of Event are 0; otherwise, they are considered as event times.

The following statements use the LIFETEST procedure to estimate the log-rank statistic at stage 1:

```
proc lifetest data=Surv_1;
 time Weeks*Event(0);
 test TrtGp;
 ods output logunichisq=Parms_Surv1;
run;
```

The following statements create and display (in [Output 84.6.9](#)) the data set for the log-rank statistic and its associated standard error:

```
data Parms_Surv1;
 set Parms_Surv1(rename=(Statistic=Estimate));
 if Variable='TrtGp';
 Scale='Score';
 Stage= 1;
 keep Variable _Scale_ _Stage_ StdErr Estimate;
run;

proc print data=Parms_Surv1;
 title 'Statistics Computed at Stage 1';
run;
```

**Output 84.6.9** Statistics Computed at Stage 1

| Statistics Computed at Stage 1 |          |          |        |         |         |
|--------------------------------|----------|----------|--------|---------|---------|
| Obs                            | Variable | Estimate | StdErr | _Scale_ | _Stage_ |
| 1                              | TrtGp    | 3.2004   | 1.9979 | Score   | 1       |

The following statements invoke the SEQTEST procedure to test for early stopping at stage 1:

```
ods graphics on;
proc seqtest Boundary=Bnd_Surv
 Parms (Testvar=TrtGp)=Parms_Surv1
 infoadj=none
 boundaryscale=score
 ;
 ods output Test=Test_Surv1;
run;
ods graphics off;
```

The BOUNDARY= option specifies the input data set that provides the boundary information for the trial at stage 1, which was generated in the SEQDESIGN procedure. The PARMS=PARMS\_SURV1 option specifies the input data set PARMS\_SURV1 that contains the test statistic and its associated standard error at stage 1, and the TESTVAR=TRTGp option identifies the test variable TRTGp in the data set. The INFOADJ=NONE option maintains the information levels for future interim stages (2 and 3) at the values provided in the BOUNDARY= data set.

The ODS OUTPUT statement with the TEST=TEST\_SURV1 option creates an output data set named TEST\_SURV1 which contains the updated boundary information for the test at stage 1. The data set also provides the boundary information that is needed for the group sequential test at the next stage.

The “Design Information” table in [Output 84.6.10](#) displays design specifications. By default (or equivalently if you specify BOUNDARYKEY=ALPHA), the maximum information and the Type I error level  $\alpha$  are preserved. Since the computed information level at stage 1 is not the same as the value provided in the BOUNDARY= data set, the power has been modified.

**Output 84.6.10** Design Information

| The SEQTEST Procedure                     |                    |
|-------------------------------------------|--------------------|
| Design Information                        |                    |
| BOUNDARY Data Set                         | WORK.BND_SURV      |
| Data Set                                  | WORK.PARMS_SURV1   |
| Statistic Distribution                    | Normal             |
| Boundary Scale                            | Score              |
| Alternative Hypothesis                    | Upper              |
| Early Stop                                | Accept/Reject Null |
| Number of Stages                          | 4                  |
| Alpha                                     | 0.05               |
| Beta                                      | 0.20055            |
| Power                                     | 0.79945            |
| Max Information (Percent of Fixed Sample) | 130.0335           |
| Max Information                           | 16.7062448         |
| Null Ref ASN (Percent of Fixed Sample)    | 62.80855           |
| Alt Ref ASN (Percent of Fixed Sample)     | 74.19155           |

The “Test Information” table in [Output 84.6.11](#) displays the boundary values for the test statistic with the SCORE statistic scale. Since only the information level at stage 1 is specified in the DATA= data set, the information levels at subsequent stages are derived proportionally from the corresponding information levels provided in the BOUNDARY= data set. At stage 1, the score statistic 3.2004 is between the upper  $\beta$  boundary value  $-1.0386$  and the upper  $\alpha$  boundary value  $4.7142$ , so the trial continues to the next stage.

**Output 84.6.11** Sequential Tests

| Test Information (Score Scale) |                        |          |                        |                          |         |
|--------------------------------|------------------------|----------|------------------------|--------------------------|---------|
| Null Reference = 0             |                        |          |                        |                          |         |
| _Stage_                        | ---Information Level-- |          | -Alternative-          | -----Boundary Values---- |         |
|                                | Proportion             | Actual   | --Reference--<br>Upper | -----Upper-----<br>Beta  | Alpha   |
| 1                              | 0.2389                 | 3.991698 | 2.76685                | -1.03860                 | 4.71422 |
| 2                              | 0.5000                 | 8.353122 | 5.78997                | 1.91799                  | 5.73971 |
| 3                              | 0.7500                 | 12.52968 | 8.68495                | 4.78802                  | 6.70284 |
| 4                              | 1.0000                 | 16.70624 | 11.57993               | 7.81346                  | 7.81346 |

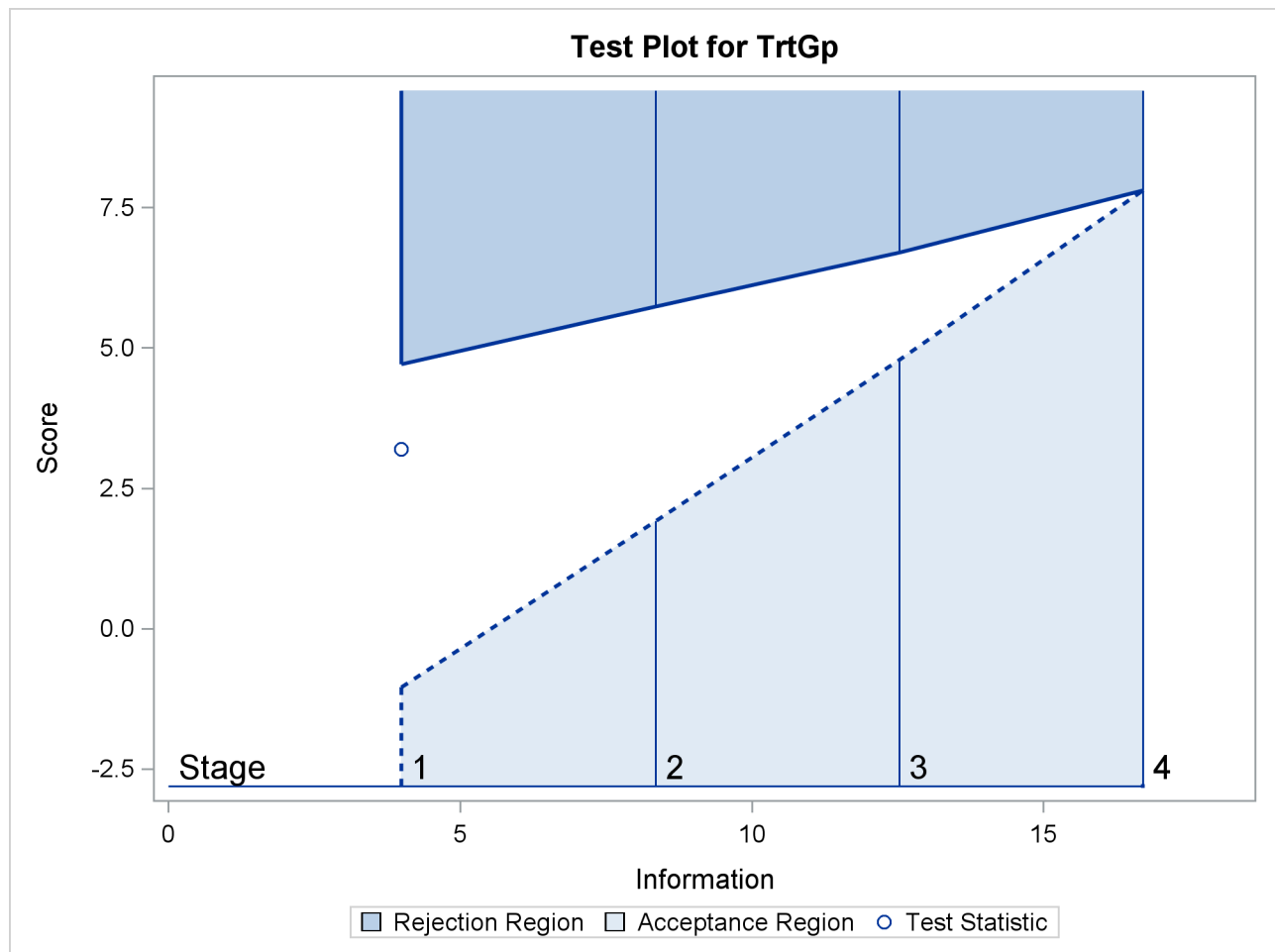
  

| Test Information (Score Scale) |          |                           |
|--------------------------------|----------|---------------------------|
| Null Reference = 0             |          |                           |
| _Stage_                        | Estimate | -----Test-----            |
|                                |          | -----TrtGp-----<br>Action |
| 1                              | 3.20040  | Continue                  |
| 2                              | .        |                           |
| 3                              | .        |                           |
| 4                              | .        |                           |

Note that the observed information level 3.9917 corresponds to a proportion of 0.2389 in information level. If the observed information level is much smaller than the target proportion of 0.25, then you need to increase the accrual rate, accrual time, or follow-up time to achieve the target maximum information level for the trial. Scharfstein and Tsiatis (1998) use the simulation and bootstrap methods to modify the trial at interim stages to achieve the target maximum information level. These modifications should be specified in the study protocol or study plan before the study starts.

With ODS Graphics enabled, a boundary plot with test statistics is displayed, as shown in [Output 84.6.12](#). As expected, the test statistic is in the continuation region between the upper  $\beta$  and  $\alpha$  boundary values.

**Output 84.6.12** Sequential Test Plot



Note that the input `DATA=` option can also be used for the test statistics. For example, the following statements create and display (in [Output 84.6.13](#)) the data set for the log-rank statistic and its associated standard error after the `LIFETEST` procedure. Since the log-rank statistic is a score statistic, the corresponding information level is the variance of the statistic.

```
proc lifetest data=Surv_1;
 time Weeks*Event(0);
 test TrtGp;
 ods output logunichisq=Parms_Surv1a;
run;
```

```

data Parms_Surv1a;
 set Parms_Surv1a(rename=(Statistic=TrtGp));
 keep _Scale_ _Stage_ _Info_ TrtGp;
 Scale='Score';
 Stage= 1;
 Info= StdErr * StdErr;
 if Variable='TrtGp';
run;

proc print data=Parms_Surv1a;
 title 'Statistics Computed at Stage 1';
run;

```

**Output 84.6.13** Statistics Computed at Stage 1

| Statistics Computed at Stage 1 |        |         |         |         |
|--------------------------------|--------|---------|---------|---------|
| Obs                            | TrtGp  | _Scale_ | _Stage_ | _Info_  |
| 1                              | 3.2004 | Score   | 1       | 3.99170 |

The following statements can be used to invoke the SEQTEST procedure to test for early stopping at stage 1:

```

ods graphics on;
proc seqtest Boundary=Bnd_Surv
 Data(Testvar=TrtGp)=Parms_Surv1a
 inoadj=none
 boundaryscale=score
 ;
 ods output Test=Test_Surv1;
run;
ods graphics off;

```

The following statements use the LIFETEST procedure to compute the log-rank statistic and its associated standard error at stage 2:

```

proc lifetest data=Surv_2;
 time Weeks*Event(0);
 test TrtGp;
 ods output logunichisq=Parms_Surv2;
run;

```

The following statements create and display (in [Output 84.6.14](#)) the data set for the log-rank statistic and its associated standard error for each of the first two stages:

```

data Parms_Surv2;
 set Parms_Surv2 (rename=(Statistic=Estimate));
 if Variable='TrtGp';
 Scale='Score';
 Stage= 2;
 keep Variable _Scale_ _Stage_ StdErr Estimate;
run;

```

```
proc print data=Parms_Surv2;
 title 'Statistics Computed at Stage 2';
run;
```

#### Output 84.6.14 Statistics Computed at Stage 2

| Statistics Computed at Stage 2 |          |          |        |         |         |
|--------------------------------|----------|----------|--------|---------|---------|
| Obs                            | Variable | Estimate | StdErr | _Scale_ | _Stage_ |
| 1                              | TrtGp    | 7.3136   | 2.9489 | Score   | 2       |

The following statements invoke the SEQTEST procedure to test for early stopping at stage 2:

```
ods graphics on;
proc seqtest Boundary=Test_Surv1
 Parms (Testvar=TrtGp) =Parms_Surv2
 infoadj=none
 boundaryscale=score
 cotype=lower
 ;
ods output Test=Test_Surv2;
run;
ods graphics off;
```

The BOUNDARY= option specifies the input data set that provides the boundary information for the trial at stage 2, which was generated by the SEQTEST procedure at the previous stage. The PARMS= option specifies the input data set that contains the test statistic and its associated standard error at stage 2, and the TESTVAR= option identifies the test variable in the data set. The INFOADJ=NONE option maintains the information level for stage 3 at the value provided in the BOUNDARY= data set.

The ODS OUTPUT statement with the TEST=TEST\_SURV2 option creates an output data set named TEST\_SURV2 which contains the updated boundary information for the test at stage 2. The data set also provides the boundary information that is needed for the group sequential test at the next stage if the trial does not stop at the current stage.

The “Test Information” table in [Output 84.6.15](#) displays the boundary values for the test statistic. The test statistic 7.31365 is larger than the corresponding upper  $\alpha$  boundary 5.79886, so the study stops and rejects the null hypothesis. That is, there is evidence of reduction in hazard rate for the new treatment.

## Output 84.6.15 Sequential Tests

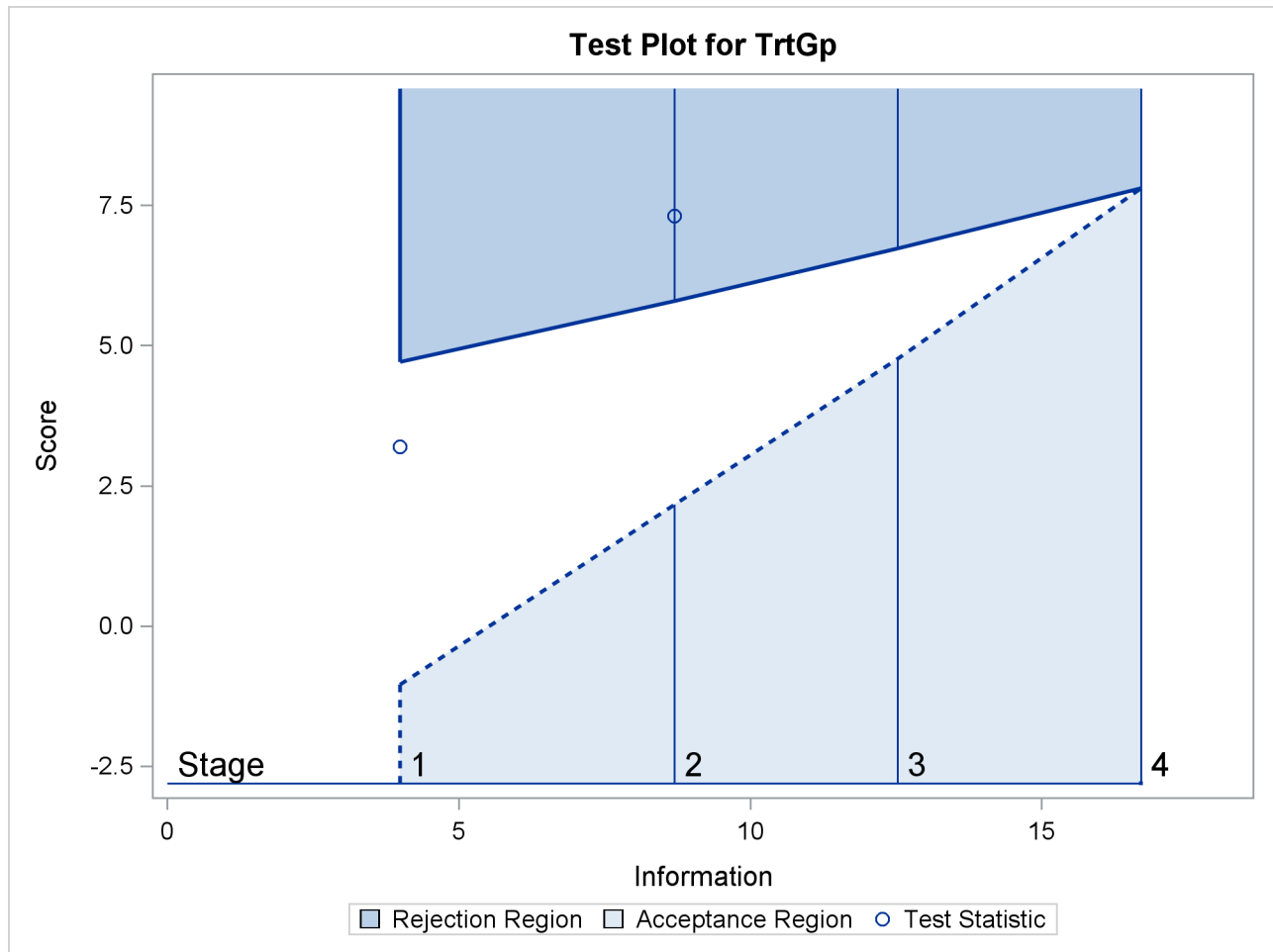
| The SEQTEST Procedure          |                        |          |                        |                          |         |
|--------------------------------|------------------------|----------|------------------------|--------------------------|---------|
| Test Information (Score Scale) |                        |          |                        |                          |         |
| Null Reference = 0             |                        |          |                        |                          |         |
| _Stage_                        | ---Information Level-- |          | -Alternative-          | -----Boundary Values---- |         |
|                                | Proportion             | Actual   | --Reference--<br>Upper | -----Upper-----<br>Beta  | Alpha   |
| 1                              | 0.2389                 | 3.991698 | 2.76685                | -1.03860                 | 4.71422 |
| 2                              | 0.5205                 | 8.696125 | 6.02772                | 2.17045                  | 5.79332 |
| 3                              | 0.7500                 | 12.52968 | 8.68495                | 4.76306                  | 6.72915 |
| 4                              | 1.0000                 | 16.70624 | 11.57993               | 7.81287                  | 7.81287 |

| Test Information (Score Scale) |                |             |
|--------------------------------|----------------|-------------|
| Null Reference = 0             |                |             |
| _Stage_                        | -----Test----- |             |
|                                | Estimate       | Action      |
| 1                              | 3.20040        | Continue    |
| 2                              | 7.31365        | Reject Null |
| 3                              | .              | .           |
| 4                              | .              | .           |

With ODS Graphics enabled, the “Test Plot” displays boundary values of the design and the test statistic at the first two stages, as shown in [Output 84.6.16](#). It also shows that the test statistic is in the “Rejection Region” above the upper  $\alpha$  boundary value at stage 2.

Output 84.6.16 Sequential Test Plot



After the stopping of a trial, the “Parameter Estimates” table in Output 84.6.17 displays the stopping stage, parameter estimate, unbiased median estimate, confidence limits, and  $p$ -value under the null hypothesis  $H_0 : \theta = 0$ .

Output 84.6.17 Parameter Estimates

| Parameter Estimates<br>Stagewise Ordering |                |          |                                  |                 |              |
|-------------------------------------------|----------------|----------|----------------------------------|-----------------|--------------|
| Parameter                                 | Stopping Stage | MLE      | p-Value for $H_0: \text{Parm}=0$ | Median Estimate | Lower 95% CL |
| TrtGp                                     | 2              | 0.841024 | 0.0139                           | 0.810329        | 0.21615      |

As expected, the  $p$ -value 0.0139 is significant at the  $\alpha = 0.05$  level and the lower 95% confidence limit is larger than  $\theta_0 = 0$ . The  $p$ -value, unbiased median estimate, and lower confidence limit depend on the ordering of the sample space  $(k, z)$ , where  $k$  is the stage number and  $z$  is the standardized  $Z$  statistic. With



the specified stagewise ordering, the  $p$ -value is  $p_1 + p_2$ , where  $p_1$  is the  $\alpha$  spending at stage 1,

$$p_1 = P_{\theta=0}(Z_1\sqrt{I_1} \geq 4.71422) = 0.00915$$

$$p_2 = P_{\theta=0}(Z_2\sqrt{I_2} \geq 7.31365 \mid -1.04069 < Z_1\sqrt{I_1} < 4.71422)$$

where  $Z_k$  is a standardized normal variate and  $I_k$  is the information level at stage  $k$  for  $k = 1, 2$ .

### Example 84.7: Testing an Effect in a Proportional Hazards Regression Model

This example compares two survival distributions for the treatment effect. The example uses a power family method to generate two-sided asymmetric boundaries and then uses a proportional hazards regression model to test the hypothesis with a covariate.

A clinic is conducting a clinical study for the effect of a new cancer treatment. The study consists of mice exposed to a carcinogen and randomized to either the control group or the treatment group. The event of interest is the death from cancer induced by the carcinogen, and the response is the time from randomization to death.

Consider the proportional hazards regression model

$$h(t; \text{TrtGp}, \text{Wgt}) = h_0(t) \exp(\beta_g \text{TrtGp} + \beta_w \text{Wgt})$$

where  $h_0(t)$  is an arbitrary and unspecified baseline hazard function,  $\text{TrtGp}$  is the grouping variable for the two groups,  $\text{Wgt}$  is the initial weight of the mice, and  $\beta_g$  and  $\beta_w$  are the regression parameters associated with the variables  $\text{TrtGp}$  and  $\text{Wgt}$ , respectively. The grouping variable has the value 0 for each mouse in the control group and the value 1 for each mouse in the treatment group.

The hypothesis  $H_0 : \beta_g = 0$  with an alternative hypothesis  $H_1 : \beta_g \neq 0$  is used for the study.

Suppose that from past experience, the median survival time for the control group is  $t_0 = 20$  weeks. The study would like to detect a  $t_1 = 40$  weeks median survival time with a 80% power in the trial. Assuming exponential survival functions for the two groups, the hazard rates can be computed from

$$S_j(t_j) = e^{-h_j t_j} = \frac{1}{2}$$

where  $j = 0, 1$ .

Thus, with the hazard rates  $h_0 = 0.03466$  and  $h_1 = 0.01733$ , the hazard ratio  $\exp(\beta_g) = h_1/h_0 = 1/2$  and the alternative hypothesis

$$\beta_{g1} = \log\left(\frac{1}{2}\right) = -0.69315$$

Following the derivations in the section “Test for a Parameter in the Proportional Hazards Regression Model” in the chapter “The SEQDESIGN Procedure,” the required number of events for testing a parameter in  $\beta$  is given by

$$D_X = I_X \frac{1}{(1 - r_x^2) \sigma_x^2}$$

where  $\sigma_x^2$  is the variance of TrtGp and  $r_x^2$  is the proportion of variance of TrtGp explained by the variable Wgt.

If the two groups have the same number of mice in the study, then the MLE of the variance is  $\hat{\sigma}_x^2 = 0.25$ . Further, if  $r_x^2 = 0.10$ , then you can specify the MODEL=PHREG( XVARIANCE=0.25 XRSQUARE=0.10) option in the SAMPLESIZE statement in the SEQDESIGN procedure to compute the required number of events and the individual number of events at each stage.

The following statements invoke the SEQDESIGN procedure and request a four-stage group sequential design for normally distributed data. The design uses a two-sided alternative hypothesis with early stopping to reject the null hypothesis  $H_0$ . A power family method is used to derive the boundaries.

```
ods graphics on;
proc seqdesign altref=0.69315;
 TwoSidedPowerFamily: design method=pow
 nstages=4
 alpha=0.075 (lower=0.025)
 beta=0.20;
 samplesize model=phreg(xvariance=0.25 xrsquare=0.10
 hazard=0.02451 accrate=10);
run;
ods graphics off;
```

The ALPHA=0.075(LOWER=0.025) option specifies a lower  $\alpha$  level 0.025 for the lower rejection boundary and an upper  $\alpha$  level  $0.05 = 0.075 - 0.025$  for the upper rejection boundary. The geometric average hazard  $\sqrt{h_0 \times h_1} = \sqrt{0.03466 \times 0.01733} = 0.02451$  is used in the HAZARD= option in the SAMPLESIZE statement to compute the required sample size. The specified ACCRATE=10 option indicates that 10 mice will be accrued each week and the resulting minimum and maximum accrual times will be displayed.

The “Design Information” table in [Output 84.7.1](#) displays the design specifications and the derived statistics.

**Output 84.7.1** Design Information

| The SEQDESIGN Procedure                   |                |
|-------------------------------------------|----------------|
| Design: TwoSidedPowerFamily               |                |
| Design Information                        |                |
| Statistic Distribution                    | Normal         |
| Boundary Scale                            | Standardized Z |
| Alternative Hypothesis                    | Two-Sided      |
| Early Stop                                | Reject Null    |
| Method                                    | Power Family   |
| Boundary Key                              | Both           |
| Alternative Reference                     | 0.69315        |
| Number of Stages                          | 4              |
| Alpha                                     | 0.075          |
| Alpha (Lower)                             | 0.025          |
| Alpha (Upper)                             | 0.05           |
| Beta (Lower)                              | 0.2            |
| Beta (Upper)                              | 0.12764        |
| Power (Lower)                             | 0.8            |
| Power (Upper)                             | 0.87236        |
| Max Information (Percent of Fixed Sample) | 106.468        |
| Max Information                           | 17.39288       |
| Null Ref ASN (Percent of Fixed Sample)    | 104.3691       |
| Lower Alt Ref ASN (Number of Events)      | 58.04014       |
| Upper Alt Ref ASN (Number of Events)      | 52.05395       |

The “Boundary Information” table in [Output 84.7.2](#) displays the information level, alternative reference, and boundary values at each stage. By default (or equivalently if you specify BOUNDARYSCALE=STDZ), the procedure displays the output boundaries with the standardized Z statistic.

**Output 84.7.2** Boundary Information

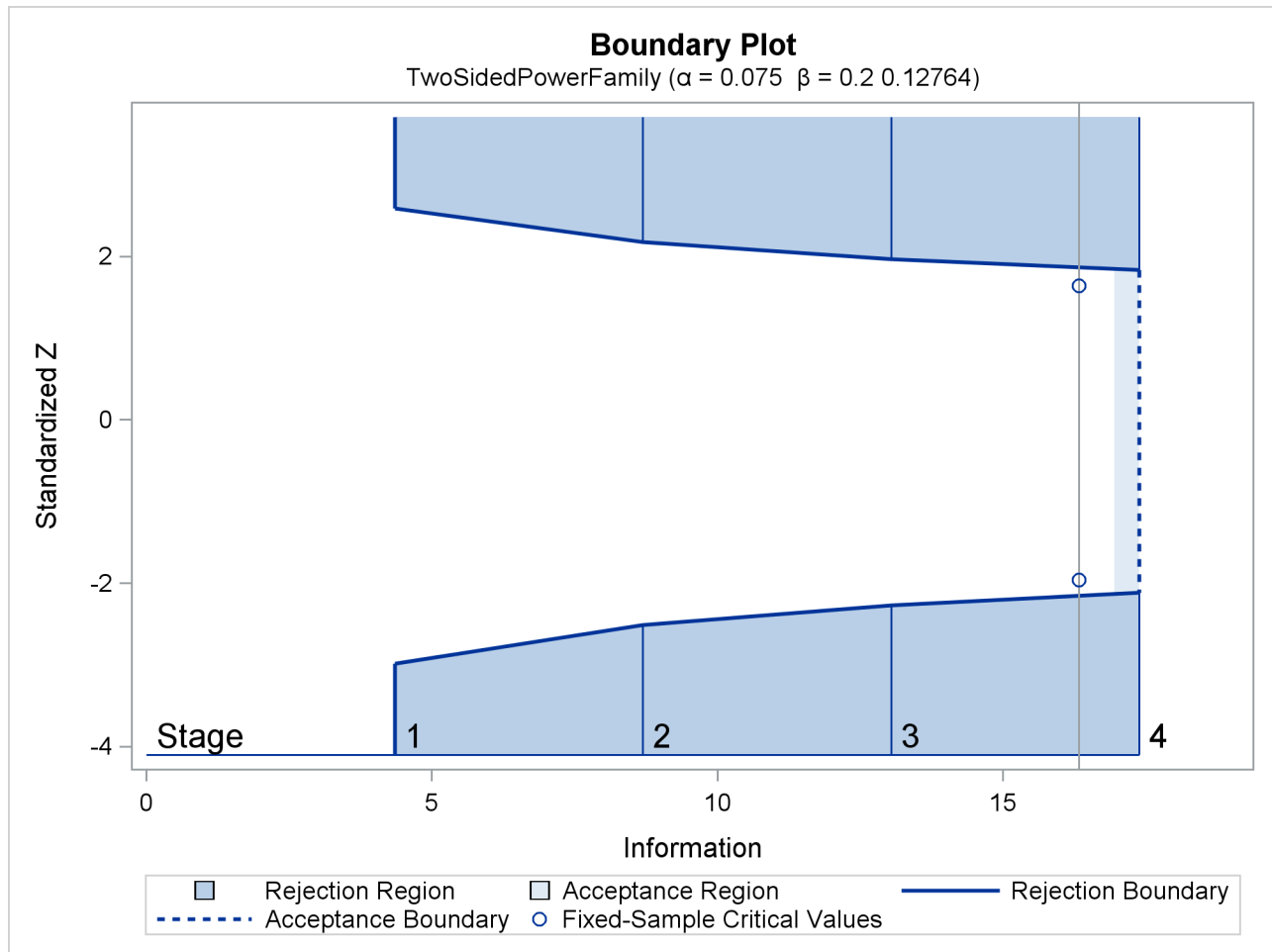
| Boundary Information (Standardized Z Scale) |                             |          |          |                       |         |
|---------------------------------------------|-----------------------------|----------|----------|-----------------------|---------|
| Null Reference = 0                          |                             |          |          |                       |         |
| _Stage_                                     | -----Information Level----- |          |          | -----Alternative----- |         |
|                                             | Proportion                  | Actual   | Events   | Lower                 | Upper   |
| 1                                           | 0.2500                      | 4.348221 | 19.32543 | -1.44538              | 1.44538 |
| 2                                           | 0.5000                      | 8.696441 | 38.65085 | -2.04408              | 2.04408 |
| 3                                           | 0.7500                      | 13.04466 | 57.97628 | -2.50348              | 2.50348 |
| 4                                           | 1.0000                      | 17.39288 | 77.3017  | -2.89077              | 2.89077 |

| Boundary Information (Standardized Z Scale) |                           |            |  |
|---------------------------------------------|---------------------------|------------|--|
| Null Reference = 0                          |                           |            |  |
| _Stage_                                     | -----Boundary Values----- |            |  |
|                                             | ---Lower--                | ---Upper-- |  |
|                                             | Alpha                     | Alpha      |  |
| 1                                           | -2.98871                  | 2.59149    |  |
| 2                                           | -2.51320                  | 2.17917    |  |
| 3                                           | -2.27093                  | 1.96910    |  |
| 4                                           | -2.11334                  | 1.83246    |  |

With ODS Graphics enabled, a detailed boundary plot with the rejection and acceptance regions is displayed, as shown in [Output 84.7.3](#).

**Output 84.7.3** Boundary Plot



With the MODEL=PHREG option in the SAMPLESIZE statement, the “Sample Size Summary” table in Output 84.7.4 displays the parameters used in the sample size computation for the proportional hazards regression model.

**Output 84.7.4** Required Sample Size Summary

| Sample Size Summary  |                  |
|----------------------|------------------|
| Test                 | PH Reg Parameter |
| Parameter            | 0.69315          |
| X Variance           | 0.25             |
| R Square (X)         | 0.1              |
| Hazard Rate          | 0.02451          |
| Accrual              | Uniform          |
| Accrual Rate         | 10               |
| Min Accrual Time     | 7.73017          |
| Min Sample Size      | 77.3017          |
| Max Accrual Time     | 27.97872         |
| Max Sample Size      | 279.7872         |
| Max Number of Events | 77.3017          |

With a minimum accrual time of 7.73 weeks and maximum accrual time of 27.98 weeks, an accrual time of 20 weeks is used in the study. The “Numbers of Events” table in [Output 84.7.5](#) displays the required numbers of events for the group sequential clinical trial.

**Output 84.7.5** Required Sample Sizes

| Numbers of Events (D)              |       |             |
|------------------------------------|-------|-------------|
| Z Test for PH Regression Parameter |       |             |
| <u>Stage</u>                       | D     | Information |
| 1                                  | 19.33 | 4.3482      |
| 2                                  | 38.65 | 8.6964      |
| 3                                  | 57.98 | 13.0447     |
| 4                                  | 77.30 | 17.3929     |

The following statements invoke the SEQDESIGN procedure and provide more detailed sample size information with a 20-week accrual time:

```
proc seqdesign altref=0.69315;
 TwoSidedPowerFamily: design method=pow
 nstages=4
 alpha=0.075 (lower=0.025)
 beta=0.20;
 samplesize model=phreg(xvariance=0.25 xrsquare=0.10
 hazard=0.02451
 accrate=10 acctime=20);
 ods output Boundary=Bnd_Time;
run;
```

The ODS OUTPUT statement with the BOUNDARY=BND\_TIME option creates an output data set named BND\_TIME which contains the resulting boundary information for the subsequent sequential tests.

With an accrual time of 20 weeks, the “Sample Size Summary” table in [Output 84.7.6](#) displays the follow-up time for the trial.

**Output 84.7.6** Sample Size Summary

| The SEQDESIGN Procedure         |                  |
|---------------------------------|------------------|
| Design: TwoSidedPowerFamily     |                  |
| Sample Size Summary             |                  |
| Test                            | PH Reg Parameter |
| Parameter                       | 0.69315          |
| X Variance                      | 0.25             |
| R Square (X)                    | 0.1              |
| Hazard Rate                     | 0.02451          |
| Accrual                         | Uniform          |
| Accrual Rate                    | 10               |
| Accrual Time                    | 20               |
| Follow-up Time                  | 10.34195         |
| Total Time                      | 30.34195         |
| Max Number of Events            | 77.3017          |
| Max Sample Size                 | 200              |
| Expected Sample Size (Null Ref) | 199.4282         |
| Expected Sample Size (Alt Ref)  | 188.6561         |

The “Numbers of Events and Sample Sizes” table in [Output 84.7.7](#) displays the required sample sizes for the group sequential clinical trial.

**Output 84.7.7** Numbers of Events and Sample Sizes

| Numbers of Events (D) and Sample Sizes (N) |       |         |        |             |
|--------------------------------------------|-------|---------|--------|-------------|
| Z Test for PH Regression Parameter         |       |         |        |             |
| -----Fractional Time-----                  |       |         |        |             |
| _Stage_                                    | D     | Time    | N      | Information |
| 1                                          | 19.33 | 13.2362 | 132.36 | 4.3482      |
| 2                                          | 38.65 | 19.1466 | 191.47 | 8.6964      |
| 3                                          | 57.98 | 24.3744 | 200.00 | 13.0447     |
| 4                                          | 77.30 | 30.3420 | 200.00 | 17.3929     |

| Numbers of Events (D) and Sample Sizes (N) |       |      |        |             |
|--------------------------------------------|-------|------|--------|-------------|
| Z Test for PH Regression Parameter         |       |      |        |             |
| -----Ceiling Time-----                     |       |      |        |             |
| _Stage_                                    | D     | Time | N      | Information |
| 1                                          | 21.49 | 14   | 140.00 | 4.8359      |
| 2                                          | 41.90 | 20   | 200.00 | 9.4281      |
| 3                                          | 60.14 | 25   | 200.00 | 13.5309     |
| 4                                          | 79.26 | 31   | 200.00 | 17.8346     |

Thus, the study will perform three interim analyses after 14, 20, and 25 weeks and a final analysis after 31 weeks if the study does not stop at any of the interim analyses.

Suppose 140 mice are available for the first interim analysis after week 14. [Output 84.7.8](#) lists the first 10 observations in the data set `weeks_1`.

**Output 84.7.8** Clinical Trial Data

| First 10 Obs in the Trial Data |           |       |         |       |  |
|--------------------------------|-----------|-------|---------|-------|--|
| Obs                            | Trt<br>Gp | Event | Wgt     | Weeks |  |
| 1                              | 0         | 0     | 22.1659 | 12    |  |
| 2                              | 1         | 0     | 28.4458 | 12    |  |
| 3                              | 0         | 0     | 26.2857 | 12    |  |
| 4                              | 1         | 0     | 25.0283 | 12    |  |
| 5                              | 0         | 0     | 21.5114 | 12    |  |
| 6                              | 1         | 0     | 23.2240 | 12    |  |
| 7                              | 0         | 1     | 22.6845 | 6     |  |
| 8                              | 1         | 0     | 27.9292 | 12    |  |
| 9                              | 0         | 0     | 22.5514 | 12    |  |
| 10                             | 1         | 1     | 27.3793 | 11    |  |

The `TrtGp` variable is a grouping variable with the value 0 for a mouse in the placebo control group and the value 1 for a mouse in the treatment group.

The `Weeks` variable is the survival time variable measured in weeks and the `Event` variable is the censoring variable with the value 0 indicating censoring. That is, the values of `Weeks` are considered censored if the corresponding values of `Event` are 0; otherwise, they are considered as event times.

The following statements use the PHREG procedure to estimate the treatment effect after adjusting for the `Wgt` variable at stage 1:

```
proc phreg data=Time_1;
 model Weeks*Event(0)= TrtGp Wgt;
 ods output parameterestimates=Parms_Time1;
run;
```

The following statements create and display (in [Output 84.7.9](#)) the data set for the treatment effect MLE statistic and its associated standard error. Note that for a MLE statistic, the inverse of the variance of the statistic is the information.

```
data Parms_Time1;
 set Parms_Time1;
 if Parameter='TrtGp';
 Scale='MLE';
 Stage= 1;
 keep _Scale_ _Stage_ Parameter Estimate StdErr;
run;

proc print data=Parms_Time1;
 title 'Statistics Computed at Stage 1';
run;
```



**Output 84.7.9** Statistics Computed at Stage 1

| Statistics Computed at Stage 1 |           |          |         |         |         |
|--------------------------------|-----------|----------|---------|---------|---------|
| Obs                            | Parameter | Estimate | StdErr  | _Scale_ | _Stage_ |
| 1                              | TrtGp     | 0.00836  | 0.46588 | MLE     | 1       |

The following statements invoke the SEQTEST procedure to test for early stopping at stage 1:

```
ods graphics on;
proc seqtest Boundary=Bnd_Time
 Parms (Testvar=TrtGp)=Parms_Time1
 infoadj=prop
 order=lr
 ;
ods output Test=Test_Time1;
run;
ods graphics off;
```

The BOUNDARY= option specifies the input data set that provides the boundary information for the trial at stage 1, which was generated in the SEQDESIGN procedure. The PARMS=PARMS\_TIME1 option specifies the input data set PARMS\_TIME1 that contains the test statistic and its associated standard error at stage 1, and the TESTVAR=TRTGP option identifies the test variable TRTGP in the data set.

If the computed information level for stage 1 is not the same as the value provided in the BOUNDARY= data set, the INFOADJ=PROP option (which is the default) proportionally adjusts the information levels at future interim stages from the levels provided in the BOUNDARY= data set. The ORDER=LR option uses the LR ordering to derive the  $p$ -value, the unbiased median estimate, and the confidence limits for the regression slope estimate.

The ODS OUTPUT statement with the TEST=TEST\_TIME1 option creates an output data set named TEST\_TIME1 which contains the updated boundary information for the test at stage 1. The data set also provides the boundary information that is needed for the group sequential test at the next stage.

The “Design Information” table in [Output 84.7.10](#) displays design specifications. By default (or equivalently if you specify BOUNDARYKEY=ALPHA), the boundary values are modified for the new information levels to maintain the Type I  $\alpha$  level. The maximum information and the power have been modified for the new information levels.

**Output 84.7.10** Design Information

```

The SEQTEST Procedure

Design Information

BOUNDARY Data Set WORK.BND_TIME
Data Set WORK.PARMS_TIME1
Statistic Distribution Normal
Boundary Scale Standardized Z
Alternative Hypothesis Two-Sided
Early Stop Reject Null
Number of Stages 4
Alpha 0.075
Alpha (Lower) 0.025
Alpha (Upper) 0.05
Beta (Lower) 0.20048
Beta (Upper) 0.12795
Power (Lower) 0.79952
Power (Upper) 0.87205
Max Information (Percent of Fixed Sample) 106.5982
Max Information 17.3928828
Null Ref ASN (Percent of Fixed Sample) 104.4715
Lower Alt Ref ASN (Percent of Fixed Sample) 79.7886
Upper Alt Ref ASN (Percent of Fixed Sample) 71.53877

```

The “Test Information” table in [Output 84.7.11](#) displays the boundary values for the test statistic with the MLE statistic scale.

**Output 84.7.11** Sequential Tests

```

Test Information (Standardized Z Scale)
Null Reference = 0

-----Alternative----- ----Boundary Values----
--Information Level- -----Reference----- ---Lower-- ---Upper--
Stage Proportion Actual Lower Upper Alpha Alpha
1 0.2649 4.607347 -1.48783 1.48783 -2.92457 2.54086
2 0.5099 8.869192 -2.06428 2.06428 -2.50505 2.17290
3 0.7550 13.13104 -2.51175 2.51175 -2.27093 1.96941
4 1.0000 17.39288 -2.89077 2.89077 -2.11635 1.83531

Test Information (Standardized Z Scale)
Null Reference = 0

-----Test-----
-----TrtGp-----
Stage Estimate Action
1 0.01795 Continue
2 .
3 .
4 .

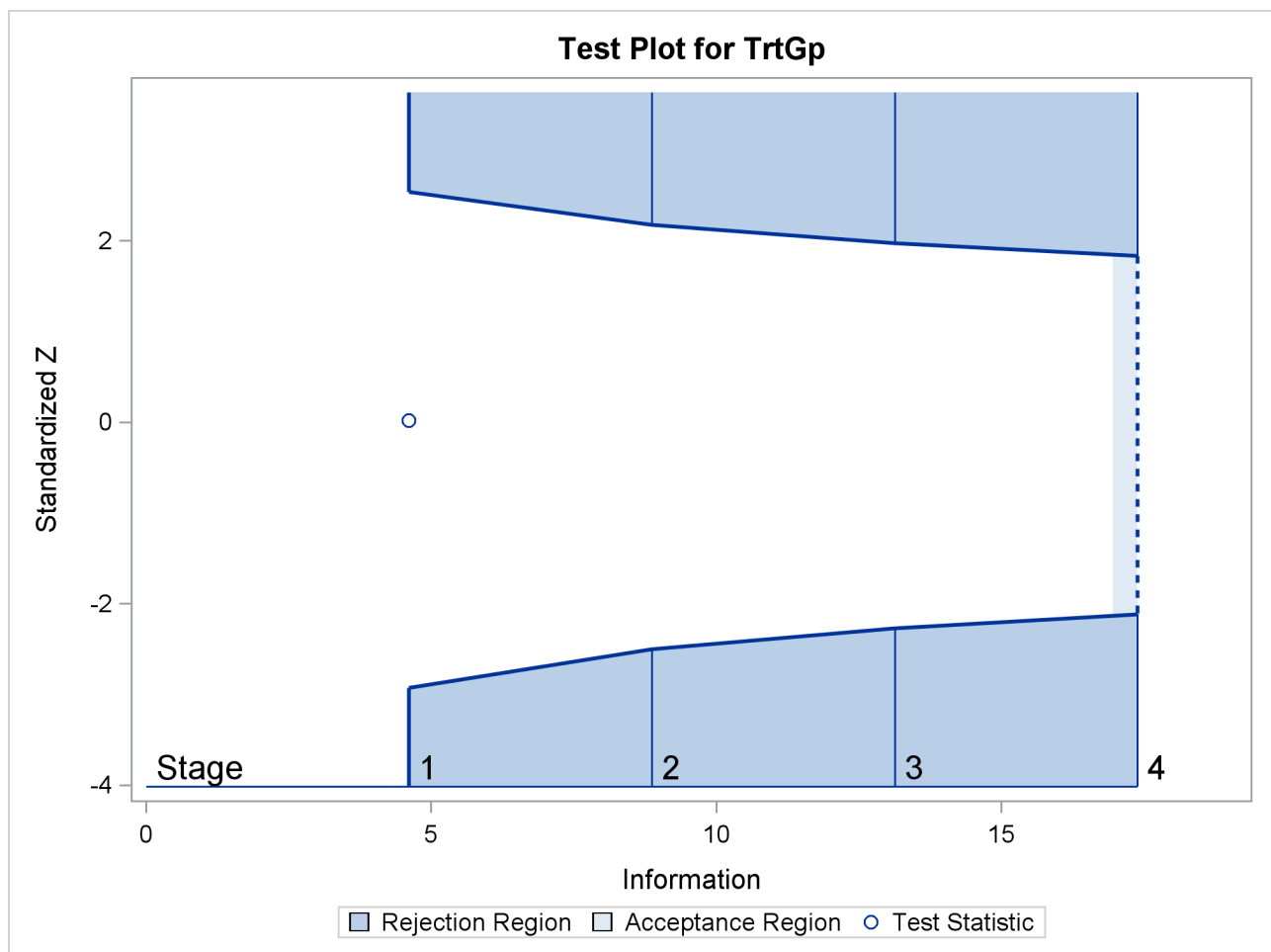
```

With the INFOADJ=PROP option (which is the default), the information levels at interim stages 2 and 3 are derived proportionally from the information levels in the BOUNDARY= data set. At stage 1, the standardized Z statistic 0.01795 is between the lower and upper  $\alpha$  boundary values of  $-2.92457$  and  $2.54086$ , so the trial continues to the next stage.

Note that the observed information level 4.6073 corresponds to a proportion of 0.2649 in the information level. If the observed information level is much larger than the target proportion of 0.25, then you can decrease the accrual rate, accrual time, or follow-up time to achieve target information levels for subsequent stages. These modifications should be specified in the study plan before the study begins.

With ODS Graphics enabled, a boundary plot with test statistics is displayed, as shown in [Output 84.7.12](#). As expected, the test statistic is in the continuation region between the lower and upper  $\alpha$  boundary values.

**Output 84.7.12** Sequential Test Plot



The following statements use the PHREG procedure to compute the MLE statistic and its associated standard error at stage 2:

```
proc phreg data=Time_2;
 model Weeks*Event(0) = TrtGp Wgt;
 ods output parameterestimates = ParmTime2;
run;
```

The following statements create the data set for the MLE statistic and its associated standard error at stage 2:

```
data Parms_Time2;
 set Parms_Time2;
 if Parameter='TrtGp';
 Scale='MLE';
 Stage= 2;
 keep _Scale_ _Stage_ Parameter Estimate StdErr;
run;
```

The following statements invoke the SEQTEST procedure to test for early stopping at stage 2:

```
proc seqtest Boundary=Test_Time1
 Parms(Testvar=TrtGp)=Parms_Time2
 infoadj=prop
 order=lr
 ;
 ods output Test=Test_Time2;
run;
```

The BOUNDARY= option specifies the input data set that provides the boundary information for the trial at stage 2, which was generated by the SEQTEST procedure at the previous stage. The PARMS= option specifies the input data set that contains the test statistic and its associated standard error at stage 2, and the TESTVAR= option identifies the test variable in the data set.

The ODS OUTPUT statement with the TEST=TEST\_TIME2 option creates an output data set named TEST\_TIME2 which contains the updated boundary information for the test at stage 2. The data set also provides the boundary information that is needed for the group sequential test at the next stage.

The “Test Information” table in [Output 84.7.13](#) displays the boundary values for the test statistic with the MLE statistic scale. At stage 2, the standardized Z statistic  $-0.43552$  is between the lower  $\alpha$  and upper boundary values,  $-2.47689$  and  $2.14819$ , respectively, so the trial continues to the next stage.

## Output 84.7.13 Sequential Tests

| The SEQTEST Procedure                   |                       |          |                       |                     |                         |             |
|-----------------------------------------|-----------------------|----------|-----------------------|---------------------|-------------------------|-------------|
| Test Information (Standardized Z Scale) |                       |          |                       |                     |                         |             |
| Null Reference = 0                      |                       |          |                       |                     |                         |             |
| _Stage_                                 | --Information Level-- |          | -----Alternative----- |                     | ----Boundary Values---- |             |
|                                         | Proportion            | Actual   | -----Reference-----   | -----Reference----- | ---Lower---             | ---Upper--- |
|                                         |                       |          | Lower                 | Upper               | Alpha                   | Alpha       |
| 1                                       | 0.2649                | 4.607347 | -1.48783              | 1.48783             | -2.92457                | 2.54086     |
| 2                                       | 0.5251                | 9.132918 | -2.09475              | 2.09475             | -2.47689                | 2.14819     |
| 3                                       | 0.7625                | 13.2629  | -2.52433              | 2.52433             | -2.26878                | 1.96770     |
| 4                                       | 1.0000                | 17.39288 | -2.89077              | 2.89077             | -2.12017                | 1.83880     |

| Test Information (Standardized Z Scale) |                |                 |          |
|-----------------------------------------|----------------|-----------------|----------|
| Null Reference = 0                      |                |                 |          |
| _Stage_                                 | -----Test----- |                 | Action   |
|                                         | Estimate       | -----TrtGp----- |          |
| 1                                       | 0.01795        |                 | Continue |
| 2                                       | -0.43552       |                 | Continue |
| 3                                       | .              |                 |          |
| 4                                       | .              |                 |          |

Since the data set PARMs\_Time2 contains the test information only at stage 2, the information level at stage 1 in the TEST\_Time1 data set is used to generate boundary values for the test.

Similarly, the test statistic at stage 3 is also between its corresponding lower and upper  $\alpha$  boundary values. The trial continues to the next stage.

The following statements use the PHREG procedure to compute the MLE statistic and its associated standard error at the final stage:

```
proc phreg data=Time_4;
 model Weeks*Event(0)= TrtGp Wgt;
 ods output parameterestimates= ParmS_Time4;
run;
```

The following statements create and display (in Output 84.7.14) the data set for the MLE statistic and its associated standard error at each stage of the study:

```
data ParmS_Time4;
 set ParmS_Time4;
 if Parameter='TrtGp';
 Scale='MLE';
 Stage= 4;
 keep _Scale_ _Stage_ Parameter Estimate StdErr;
run;

proc print data=ParmS_Time4;
 title 'Statistics Computed at Stage 4';
run;
```

**Output 84.7.14** Statistics Computed at Stage 4

| Statistics Computed at Stage 4 |           |          |         |         |         |
|--------------------------------|-----------|----------|---------|---------|---------|
| Obs                            | Parameter | Estimate | StdErr  | _Scale_ | _Stage_ |
| 1                              | TrtGp     | -0.04451 | 0.23971 | MLE     | 4       |

The following statements invoke the SEQTEST procedure to test the hypothesis at stage 4:

```
ods graphics on;
proc seqtest Boundary=Test_Time3
 Parms (Testvar=TrtGp)=Parms_Time4
 order=lr
 ;
run;
ods graphics off;
```

The BOUNDARY= option specifies the input data set that provides the boundary information for the trial at stage 4, which was generated by the SEQTEST procedure at the previous stage. The PARMS= option specifies the input data set that contains the test statistic and its associated standard error at stage 4, and the TESTVAR= option identifies the test variable in the data set.

The “Test Information” table in [Output 84.7.15](#) displays the boundary values for the test statistic. The standardized test statistic  $-0.1857$  is between the lower and upper  $\alpha$  boundary values of  $-2.10447$  and  $1.82112$ , respectively, so the study stops and accepts the null hypothesis. That is, there is no evidence of reduction in hazard rate for the new treatment.

## Output 84.7.15 Sequential Tests

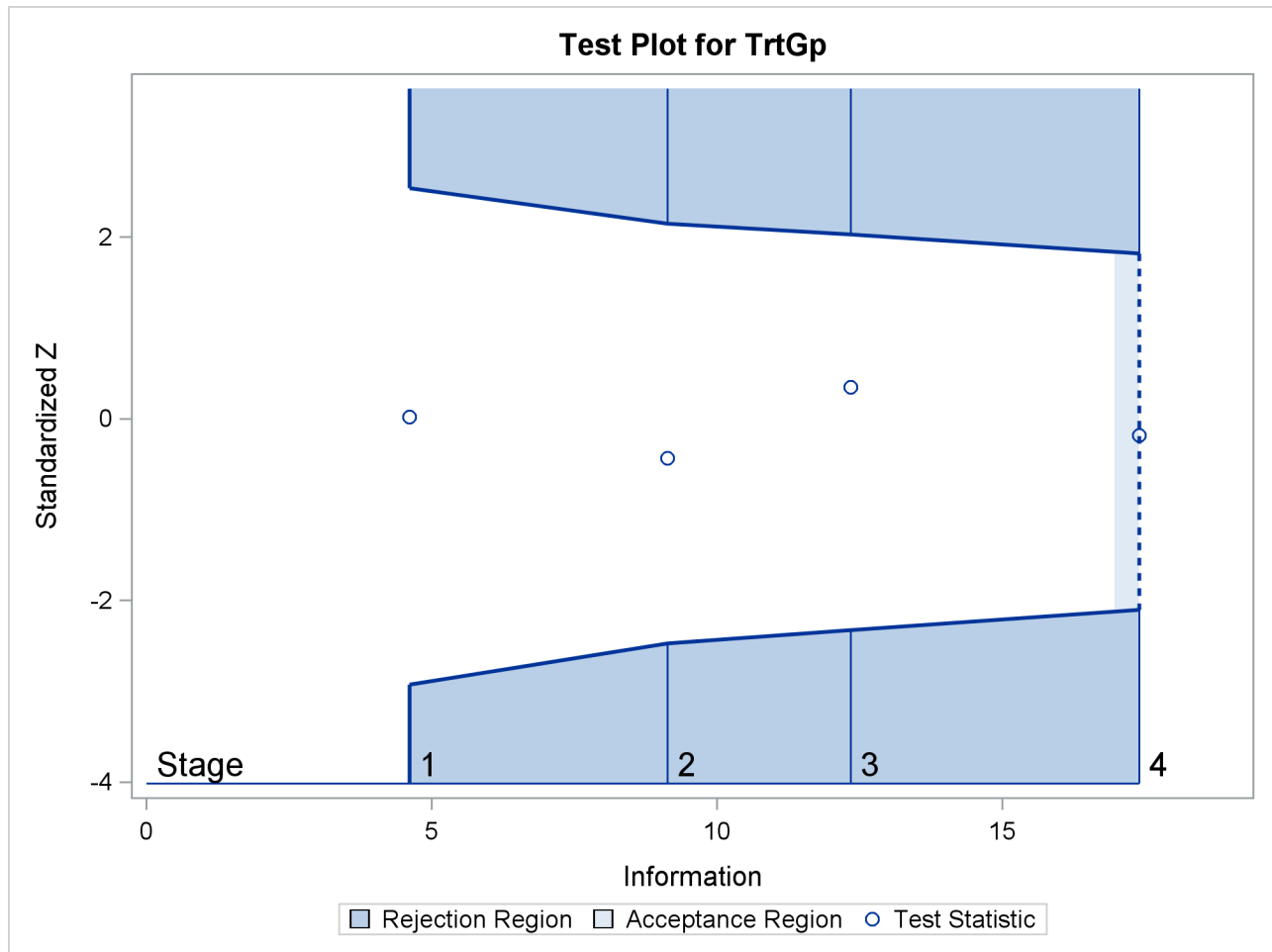
| The SEQTEST Procedure                   |                       |          |                       |                     |                         |             |
|-----------------------------------------|-----------------------|----------|-----------------------|---------------------|-------------------------|-------------|
| Test Information (Standardized Z Scale) |                       |          |                       |                     |                         |             |
| Null Reference = 0                      |                       |          |                       |                     |                         |             |
| _Stage_                                 | --Information Level-- |          | -----Alternative----- |                     | ----Boundary Values---- |             |
|                                         | Proportion            | Actual   | -----Reference-----   | -----Reference----- | ---Lower---             | ---Upper--- |
|                                         |                       |          | Lower                 | Upper               | Alpha                   | Alpha       |
| 1                                       | 0.2647                | 4.607347 | -1.48783              | 1.48783             | -2.92457                | 2.54086     |
| 2                                       | 0.5248                | 9.132918 | -2.09475              | 2.09475             | -2.47689                | 2.14819     |
| 3                                       | 0.7095                | 12.34753 | -2.43566              | 2.43566             | -2.32705                | 2.02634     |
| 4                                       | 1.0000                | 17.40274 | -2.89159              | 2.89159             | -2.10447                | 1.82112     |

| Test Information (Standardized Z Scale) |                |             |
|-----------------------------------------|----------------|-------------|
| Null Reference = 0                      |                |             |
| _Stage_                                 | -----Test----- |             |
|                                         | Estimate       | Action      |
| 1                                       | 0.01795        | Continue    |
| 2                                       | -0.43552       | Continue    |
| 3                                       | 0.34864        | Continue    |
| 4                                       | -0.18570       | Accept Null |

The “Test Plot” displays boundary values of the design and the test statistic at the first two stages, as shown in [Output 84.7.16](#). It also shows that the test statistic is in the “Acceptance Region” between the lower and upper  $\alpha$  boundary values at stage 4.

**Output 84.7.16** Sequential Test Plot



After the stopping of a trial, the “Parameter Estimates” table in **Output 84.7.17** displays the stopping stage, parameter estimate, unbiased median estimate, confidence limits, and  $p$ -value under the null hypothesis  $H_0 : \theta = 0$ .

**Output 84.7.17** Parameter Estimates

| Parameter Estimates<br>LR Ordering |                       |           |                                  |                 |
|------------------------------------|-----------------------|-----------|----------------------------------|-----------------|
| Parameter                          | Stopping Stage        | MLE       | p-Value for $H_0: \text{Parm}=0$ | Median Estimate |
| TrtGp                              | 4                     | -0.044514 | 0.8525                           | -0.044577       |
| Parameter Estimates<br>LR Ordering |                       |           |                                  |                 |
| Parameter                          | 95% Confidence Limits |           |                                  |                 |
| TrtGp                              | -0.51461      0.42538 |           |                                  |                 |



As expected, the two-sided  $p$ -value 0.8525 is not significant at the lower  $\alpha = 0.025$  level and the upper  $\alpha = 0.05$  level, and the two-sided 95% confidence interval contains the null value zero. The  $p$ -value, unbiased median estimate, and lower confidence limit depend on the ordering of the sample space  $(k, z)$ , where  $k$  is the stage number and  $z$  is the standardized  $Z$  statistic. With the specified LR ordering, the two-sided  $p$ -value is derived from the one-sided  $p$ -value

$$p_u = \sum_{k=1}^4 P_{\theta=0} (Z_k \geq z_4 \mid -a_{k'} < Z_{k'} < a_{k'}, k' < k)$$

where  $z_4 = -0.1857$  is the observed test statistic at stage 4,  $Z_k$  is a standardized normal variate at stage  $k$ , and  $-a_{k'}$  and  $a_{k'}$  are the stage  $k$  lower and upper rejection boundary values, respectively.

Thus,

$$p_u = \alpha_u + P_{\theta=0} (z_4 \leq Z_4 < a_4 \mid -a_{k'} < Z_{k'} < a_{k'}, k' < 4)$$

where  $\alpha_u = 0.05$  is the upper  $\alpha$  level and  $a_4 = 1.82112$ .

Since  $P_{\theta=0} (z_4 \leq Z_4 \leq a_4 \mid -a_{k'} < Z_{k'} < a_{k'}, k' < 4) = 0.52374$ ,  $p_u = 0.05 + 0.52374 = 0.57374$ , which is greater than 0.50. Thus, the two-sided  $p$ -value is given by  $2 \times (1.0 - p_u) = 0.8525$ .

---

### Example 84.8: Testing an Effect in a Logistic Regression Model

This example requests a two-sided test for the dose effect in a dose-response model (Whitehead 1997, pp. 262–263). Consider the logistic regression model

$$\text{logit}(p) = \log\left(\frac{p}{1-p}\right) = \beta_0 + \beta_1 \text{LDose}$$

where  $p = \text{Prob}(\text{Resp} = 1 \mid \text{LDose})$  is the response probability to be modeled for the binary response **Resp** and  $\text{LDose} = \log(\text{Dose} + 1)$  is the covariate. The dose levels are 0 for the control group, and they are 1, 3, and 6 for the three treatment groups.

Following the derivations in the section “Test for a Parameter in the Logistic Regression Model” in the chapter “The SEQDESIGN Procedure,” the required sample size can be derived from

$$N = I_X \frac{\sigma_y^2}{(1 - r_x^2) \sigma_x^2}$$

where  $\sigma_y^2$  is the variance of the response variable in the logistic regression model,  $r_x^2$  is the proportion of variance of **LDose** explained by other covariates, and  $\sigma_x^2$  is the variance of **LDose**.

Since **LDose** is the only covariate in the model,  $r_x^2 = 0$ . For a logistic model, the variance  $\sigma^2$  can be estimated by

$$\sigma_y^2 = \frac{1}{\hat{p}(1 - \hat{p})}$$

where  $\hat{p}$  is the estimated probability of the response variable **Resp**. Thus, the sample size can be computed as

$$N = I_X \frac{1}{p(1-p)} \frac{1}{\sigma_x^2}$$

The null hypothesis  $H_0 : \beta_1 = 0$  corresponds to no treatment effect. Suppose that the alternative hypothesis  $H_1 : \beta_1 = 0.5$  is the reference improvement that should be detected at a 0.90 level.

Note that  $\beta_1 = 0.5$  corresponds to an odds ratio of 2 between the treatment group with dose level 3 and the control group. The log odds ratio between the two groups is

$$\log\left(\frac{p_t(1-p_c)}{(1-p_t)p_0}\right) = \log\left(\frac{p_t}{1-p_t}\right) - \log\left(\frac{p_c}{1-p_c}\right)$$

which corresponds to

$$(\beta_0 + \beta_1 \log(3 + 1)) - (\beta_0 + \beta_1 \log(1)) = \beta_1 \log(4) = \log(2)$$

If the same number of patients are assigned in each of the four groups, then the MLE of the variance of LDose is  $\hat{\sigma}_x^2 = 0.5345$ . Further, if the response rate is 0.40, then the required sample size can be derived using the SAMPLESIZE statement in the SEQDESIGN procedure.

The following statements invoke the SEQDESIGN procedure and request a three-stage group sequential design for normally distributed data. The design has a null hypothesis of no treatment effect  $H_0 : \beta_1 = 0$  with early stopping to reject the null hypothesis with a two-sided alternative hypothesis  $H_1 : \beta_1 = \pm 0.5$ .

```
ods graphics on;
proc seqdesign altref=0.5;
 TwoSidedErrorSpending: design method=errfuncpow
 method(loweralpha)=errfuncpow(rho=1)
 method(upperalpha)=errfuncpow(rho=3)
 nstages=3
 stop=both;
 samplesize model=logistic(prop=0.4 xvariance=0.5345);
 ods output Boundary=Bnd_Dose;
run;
ods graphics off;
```

The ODS OUTPUT statement with the BOUNDARY=BND\_DOSE option creates an output data set named BND\_DOSE which contains the resulting boundary information for the subsequent sequential tests.

The “Design Information” table in [Output 84.8.1](#) displays design specifications and derived statistics. Since the alternative reference is specified, the maximum information 47.22445 is derived.

**Output 84.8.1** Error Spending Design Information

| The SEQDESIGN Procedure                   |                    |
|-------------------------------------------|--------------------|
| Design: TwoSidedErrorSpending             |                    |
| Design Information                        |                    |
| Statistic Distribution                    | Normal             |
| Boundary Scale                            | Standardized Z     |
| Alternative Hypothesis                    | Two-Sided          |
| Early Stop                                | Accept/Reject Null |
| Method                                    | Error Spending     |
| Boundary Key                              | Both               |
| Alternative Reference                     | 0.5                |
| Number of Stages                          | 3                  |
| Alpha                                     | 0.05               |
| Beta (Lower)                              | 0.1                |
| Beta (Upper)                              | 0.07871            |
| Power (Lower)                             | 0.9                |
| Power (Upper)                             | 0.92129            |
| Max Information (Percent of Fixed Sample) | 103.7223           |
| Max Information                           | 47.22445           |
| Null Ref ASN (Percent of Fixed Sample)    | 79.47628           |
| Lower Alt Ref ASN (Sample Size)           | 234.1646           |
| Upper Alt Ref ASN (Sample Size)           | 270.4058           |

The “Boundary Information” table in [Output 84.8.2](#) displays the information level, alternative reference, and boundary values at each stage. By default (or equivalently if you specify BOUNDARYSCALE=STDZ), the boundary values are displayed with the standardized Z statistic scale.

**Output 84.8.2** Boundary Information

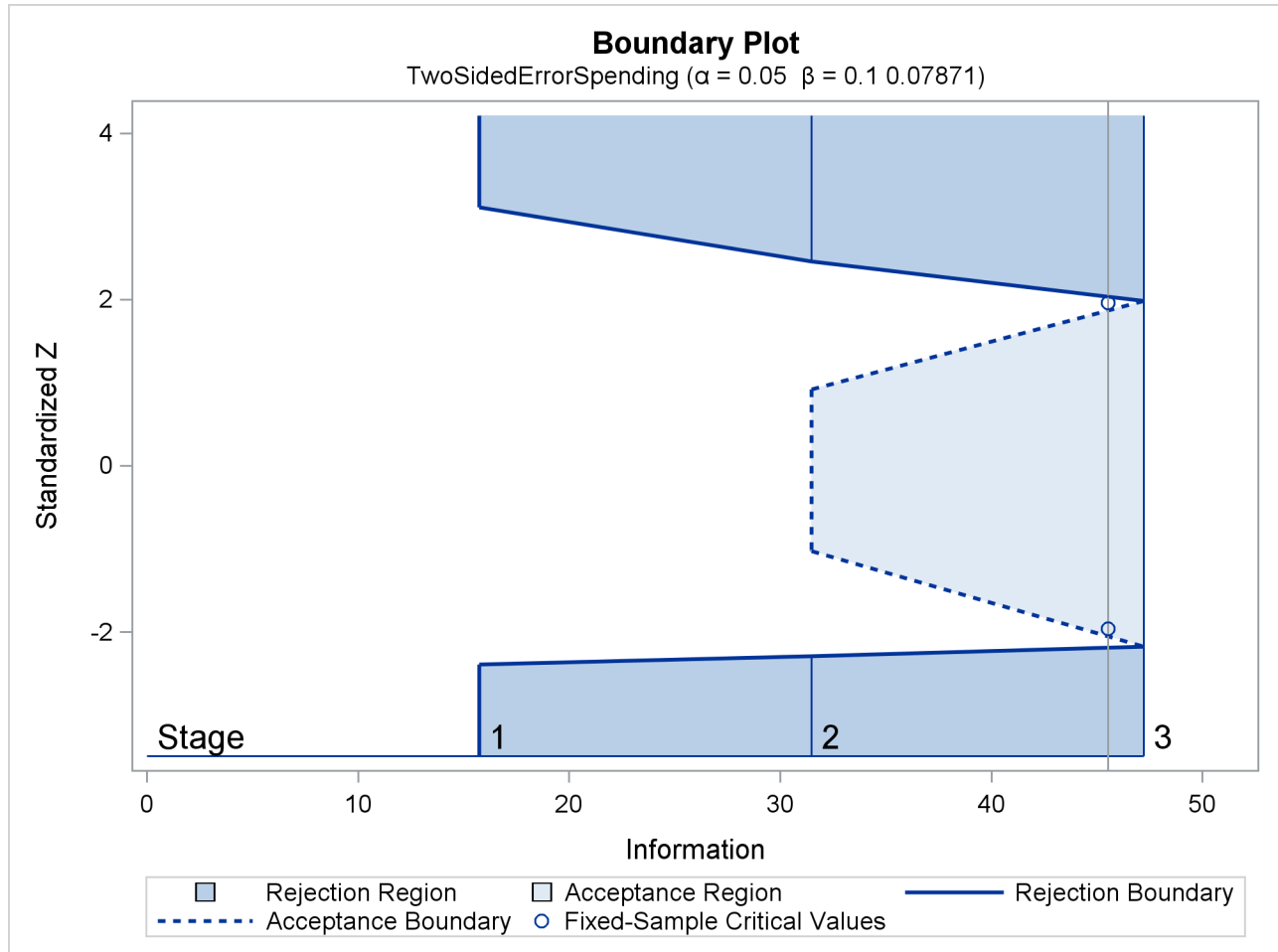
| Boundary Information (Standardized Z Scale) |                             |          |          |                       |         |
|---------------------------------------------|-----------------------------|----------|----------|-----------------------|---------|
| Null Reference = 0                          |                             |          |          |                       |         |
| _Stage_                                     | -----Information Level----- |          |          | -----Alternative----- |         |
|                                             | Proportion                  | Actual   | N        | Lower                 | Upper   |
| 1                                           | 0.3333                      | 15.74148 | 122.7119 | -1.98378              | 1.98378 |
| 2                                           | 0.6667                      | 31.48297 | 245.4238 | -2.80548              | 2.80548 |
| 3                                           | 1.0000                      | 47.22445 | 368.1357 | -3.43600              | 3.43600 |

| Boundary Information (Standardized Z Scale) |                           |          |                 |         |
|---------------------------------------------|---------------------------|----------|-----------------|---------|
| Null Reference = 0                          |                           |          |                 |         |
| _Stage_                                     | -----Boundary Values----- |          |                 |         |
|                                             | -----Lower-----           |          | -----Upper----- |         |
|                                             | Alpha                     | Beta     | Beta            | Alpha   |
| 1                                           | -2.39398                  | .        | .               | 3.11302 |
| 2                                           | -2.29380                  | -1.02812 | 0.91855         | 2.46193 |
| 3                                           | -2.17479                  | -2.17479 | 1.98311         | 1.98311 |

With ODS Graphics enabled, a detailed boundary plot with the rejection and acceptance regions is displayed, as shown in [Output 84.8.3](#).

**Output 84.8.3** Boundary Plot



With the SAMPLESIZE statement, the “Sample Size Summary” table in [Output 84.8.4](#) displays the parameters for the sample size computation.

**Output 84.8.4** Required Sample Size Summary

| Sample Size Summary             |                        |
|---------------------------------|------------------------|
| Test                            | Logistic Reg Parameter |
| Parameter                       | 0.5                    |
| Proportion                      | 0.4                    |
| X Variance                      | 0.5345                 |
| R Square (X)                    | 0                      |
| Max Sample Size                 | 368.1357               |
| Expected Sample Size (Null Ref) | 282.0807               |
| Expected Sample Size (Alt Ref)  | 270.4058               |

The “Sample Sizes” table in [Output 84.8.5](#) displays the required sample sizes for the group sequential clinical trial.

**Output 84.8.5** Required Sample Sizes

| Sample Sizes (N)                         |                        |             |                     |             |
|------------------------------------------|------------------------|-------------|---------------------|-------------|
| Z Test for Logistic Regression Parameter |                        |             |                     |             |
| _Stage_                                  | -----Fractional N----- |             | -----Ceiling N----- |             |
|                                          | N                      | Information | N                   | Information |
| 1                                        | 122.71                 | 15.7415     | 123                 | 15.7784     |
| 2                                        | 245.42                 | 31.4830     | 246                 | 31.5569     |
| 3                                        | 368.14                 | 47.2245     | 369                 | 47.3353     |

That is, 123 new patients are needed in each stage and the number is rounded up to 124 for each stage to have a multiple of four for the four dose levels in the trial. Note that since the sample sizes are derived from an estimated response probability and are rounded up, the actual information levels might not match the corresponding target information levels.

[Output 84.8.6](#) lists the first 10 observations of the trial data.

**Output 84.8.6** Clinical Trial Data

| First 10 Obs in the Trial Data |      |      |         |  |
|--------------------------------|------|------|---------|--|
| Obs                            | Resp | Dose | LDose   |  |
| 1                              | 0    | 0    | 0.00000 |  |
| 2                              | 0    | 1    | 0.69315 |  |
| 3                              | 1    | 3    | 1.38629 |  |
| 4                              | 1    | 6    | 1.94591 |  |
| 5                              | 1    | 0    | 0.00000 |  |
| 6                              | 1    | 1    | 0.69315 |  |
| 7                              | 1    | 3    | 1.38629 |  |
| 8                              | 1    | 6    | 1.94591 |  |
| 9                              | 0    | 0    | 0.00000 |  |
| 10                             | 0    | 1    | 0.69315 |  |

The following statements use the LOGISTIC procedure to estimate the slope  $\beta_1$  and its associated standard error at stage 1:

```
proc logistic data=Dose_1;
 model Resp(event='1')= LDose;
 ods output ParameterEstimates=Parms_Dose1;
run;
```

The following statements create and display (in [Output 84.8.7](#)) the input data set that contains slope  $\beta_1$  and its associated standard error for the SEQTEST procedure:

```
data Parms_Dose1;
 set Parms_Dose1;
 if Variable='LDose';
 Scale='MLE';
 Stage= 1;
 keep _Scale_ _Stage_ Variable Estimate StdErr;
run;

proc print data=Parms_Dose1;
 title 'Statistics Computed at Stage 1';
run;
```

**Output 84.8.7** Statistics Computed at Stage 1

| Statistics Computed at Stage 1 |          |          |        |         |         |
|--------------------------------|----------|----------|--------|---------|---------|
| Obs                            | Variable | Estimate | StdErr | _Scale_ | _Stage_ |
| 1                              | LDose    | 0.5741   | 0.2544 | MLE     | 1       |

The following statements invoke the SEQTEST procedure to test for early stopping at stage 1:

```
ods graphics on;
proc seqtest Boundary=Bnd_Dose
 Parms(testvar=LDose)=Parms_Dose1
 infoadj=prop
 order=mle
 boundaryscale=mle
 ;
 ods output Test=Test_Dose1;
run;
ods graphics off;
```

The BOUNDARY= option specifies the input data set that provides the boundary information for the trial at stage 1, which was generated in the SEQDESIGN procedure. The PARMS=PARMS\_DOSE1 option specifies the input data set PARMS\_DOSE1 that contains the test statistic and its associated standard error at stage 1, and the TESTVAR=LDOSE option identifies the test variable LDOSE in the data set.

If the computed information level for stage 1 is not the same as the value provided in the BOUNDARY= data set, the INFOADJ=PROP option (which is the default) proportionally adjusts the information levels at future interim stages from the levels provided in the BOUNDARY= data set. The ORDER=MLE option uses the MLE ordering to derive the  $p$ -value, the unbiased median estimate, and the confidence limits for the regression slope estimate.

The ODS OUTPUT statement with the TEST=TEST\_DOSE1 option creates an output data set named TEST\_DOSE1 which contains the updated boundary information for the test at stage 1. The data set also provides the boundary information that is needed for the group sequential test at the next stage.

The “Design Information” table in [Output 84.8.8](#) displays design specifications. By default (or equivalently if you specify BOUNDARYKEY=ALPHA), the boundary values are modified for the new information

levels to maintain the Type I  $\alpha$  level. The maximum information remains the same as the design stored in the BOUNDARY= data set, but the derived Type II error probability  $\beta$  and power  $1 - \beta$  are different because of the new information levels.

**Output 84.8.8** Design Information

| The SEQTEST Procedure                       |                    |
|---------------------------------------------|--------------------|
| Design Information                          |                    |
| BOUNDARY Data Set                           | WORK.BND_DOSE      |
| Data Set                                    | WORK.PARMS_DOSE1   |
| Statistic Distribution                      | Normal             |
| Boundary Scale                              | MLE                |
| Alternative Hypothesis                      | Two-Sided          |
| Early Stop                                  | Accept/Reject Null |
| Number of Stages                            | 3                  |
| Alpha                                       | 0.05               |
| Beta (Lower)                                | 0.09992            |
| Beta (Upper)                                | 0.07871            |
| Power (Lower)                               | 0.90008            |
| Power (Upper)                               | 0.92129            |
| Max Information (Percent of Fixed Sample)   | 103.7231           |
| Max Information                             | 47.2244524         |
| Null Ref ASN (Percent of Fixed Sample)      | 79.45049           |
| Lower Alt Ref ASN (Percent of Fixed Sample) | 66.05269           |
| Upper Alt Ref ASN (Percent of Fixed Sample) | 76.24189           |

The “Test Information” table in Output 84.8.9 displays the boundary values for the test statistic with the specified MLE scale.

**Output 84.8.9** Sequential Tests

| Test Information (MLE Scale) |                         |          |                       |         |  |  |
|------------------------------|-------------------------|----------|-----------------------|---------|--|--|
| Null Reference = 0           |                         |          |                       |         |  |  |
| _Stage_                      | ---Information Level--- |          | -----Alternative----- |         |  |  |
|                              | Proportion              | Actual   | Lower                 | Upper   |  |  |
| 1                            | 0.3272                  | 15.45062 | -0.50000              | 0.50000 |  |  |
| 2                            | 0.6636                  | 31.33753 | -0.50000              | 0.50000 |  |  |
| 3                            | 1.0000                  | 47.22445 | -0.50000              | 0.50000 |  |  |

| Test Information (MLE Scale) |                           |          |         |         |                |          |
|------------------------------|---------------------------|----------|---------|---------|----------------|----------|
| Null Reference = 0           |                           |          |         |         |                |          |
| _Stage_                      | -----Boundary Values----- |          |         |         | -----Test----- |          |
|                              | Alpha                     | Beta     | Beta    | Alpha   | Estimate       | Action   |
| 1                            | -0.61078                  | .        | .       | 0.79337 | 0.57409        | Continue |
| 2                            | -0.40974                  | -0.18169 | 0.16222 | 0.44033 | .              |          |
| 3                            | -0.31633                  | -0.31633 | 0.28860 | 0.28860 | .              |          |

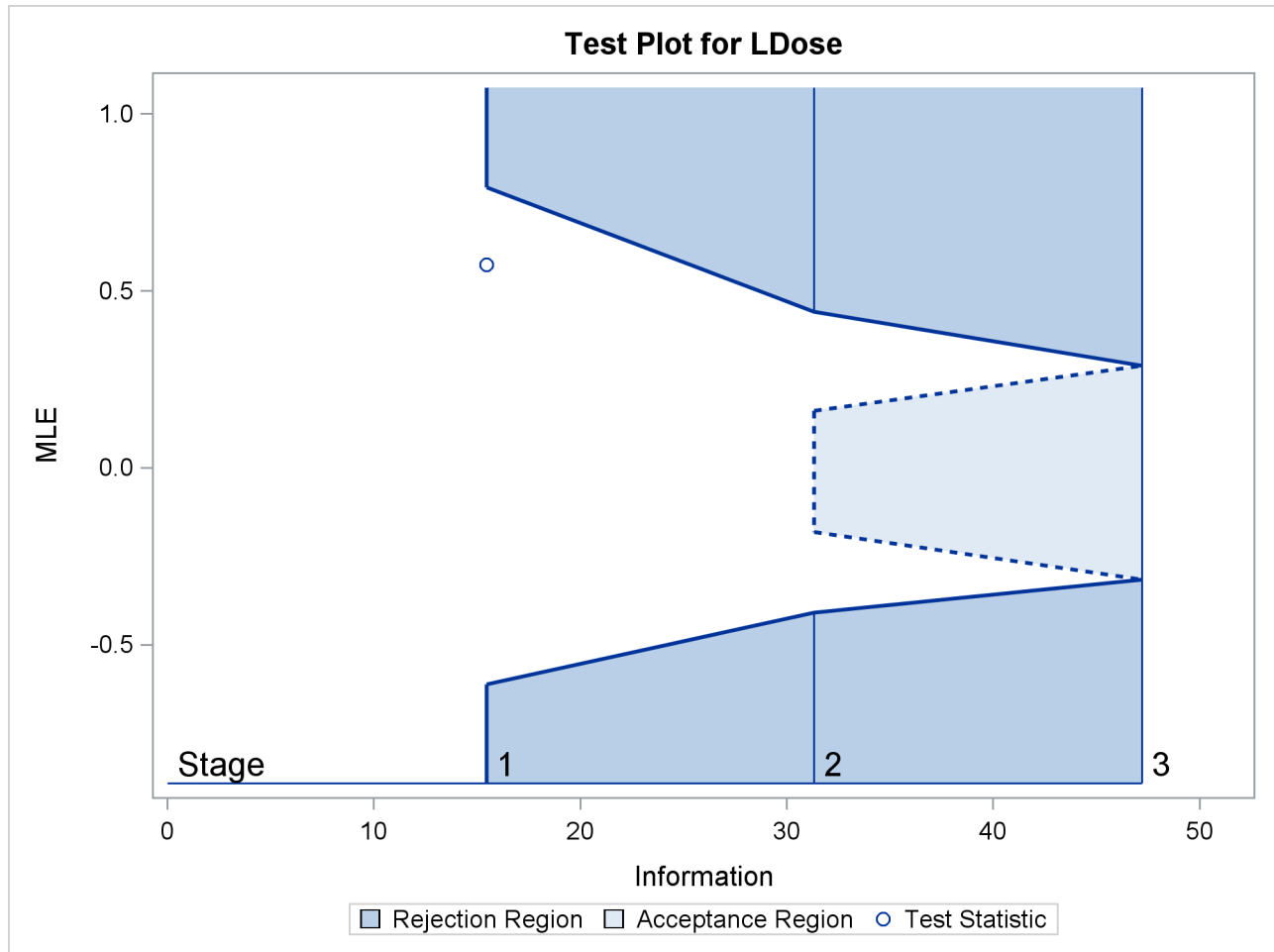
The information level at stage 1 is derived from the standard error  $s_1$  in the PARMS= data set,

$$I_1 = \frac{1}{s_1^2} = \frac{1}{0.2544^2} = 15.45$$

With the INFOADJ=PROP option (which is the default), the information level at stage 2 is derived proportionally from the observed information at stage 1 and the information levels in the BOUNDARY= data set. At stage 1, the  $\beta$  boundary values are missing and there is no early stopping to accept  $H_0$ . The MLE test statistic 0.57409 is between the lower and upper  $\alpha$  boundaries, so the trial continues to the next stage.

With ODS Graphics enabled, a boundary plot with the boundary values and test statistics is displayed, as shown in [Output 84.8.10](#). As expected, the test statistic is in the continuation region below the upper alpha boundary.

**Output 84.8.10** Sequential Test Plot





The following statements use the LOGISTIC procedure to estimate the slope  $\beta_1$  and its associated standard error at stage 2:

```
proc logistic data=dose_2;
 model Resp(event='1')=LDose;
 ods output ParameterEstimates=Parms_Dose2;
run;
```

The following statements create and display (in [Output 84.8.11](#)) the input data set that contains slope  $\beta_1$  and its associated standard error at stage 2 for the SEQTEST procedure:

```
data Parms_Dose2;
 set Parms_Dose2;
 if Variable='LDose';
 Scale='MLE';
 Stage= 2;
 keep _Scale_ _Stage_ Variable Estimate StdErr;
run;

proc print data=Parms_Dose2;
 title 'Statistics Computed at Stage 2';
run;
```

**Output 84.8.11** Statistics Computed at Stage 2

| Statistics Computed at Stage 2 |          |          |        |         |         |
|--------------------------------|----------|----------|--------|---------|---------|
| Obs                            | Variable | Estimate | StdErr | _Scale_ | _Stage_ |
| 1                              | LDose    | 0.5213   | 0.1788 | MLE     | 2       |

The following statements invoke the SEQTEST procedure to test for early stopping at stage 2:

```
ods graphics on;
proc seqtest Boundary=Test_Dose1
 Parms (Testvar=LDose) =Parms_Dose2
 infoadj=prop
 order=mle
 boundaryscale=mle
 rci
 plots=rci
 ;
 ods output Test=Test_Dose2;
run;
ods graphics off;
```

The BOUNDARY= option specifies the input data set that provides the boundary information for the trial at stage 2, which was generated by the SEQTEST procedure at the previous stage. The PARMS= option specifies the input data set that contains the test statistic and its associated standard error at stage 2, and the TESTVAR= option identifies the test variable in the data set.

The ORDER=MLE option uses the MLE ordering to derive the  $p$ -value, unbiased median estimate, and confidence limits for the regression slope estimate.

The ODS OUTPUT statement with the TEST=TEST\_DOSE2 option creates an output data set named TEST\_DOSE2 which contains the updated boundary information for the test at stage 2. The data set also provides the boundary information that is needed for the group sequential test at the next stage.

The “Design Information” table in [Output 84.8.12](#) displays design specifications. By default (or equivalently if you specify BOUNDARYKEY=ALPHA), the boundary values are modified for the new information levels to maintain the Type I  $\alpha$  level.

**Output 84.8.12** Design Information

| The SEQTEST Procedure                       |                    |
|---------------------------------------------|--------------------|
| Design Information                          |                    |
| BOUNDARY Data Set                           | WORK.TEST_DOSE1    |
| Data Set                                    | WORK.PARMS_DOSE2   |
| Statistic Distribution                      | Normal             |
| Boundary Scale                              | MLE                |
| Alternative Hypothesis                      | Two-Sided          |
| Early Stop                                  | Accept/Reject Null |
| Number of Stages                            | 3                  |
| Alpha                                       | 0.05               |
| Beta (Lower)                                | 0.0999             |
| Beta (Upper)                                | 0.07871            |
| Power (Lower)                               | 0.9001             |
| Power (Upper)                               | 0.92129            |
| Max Information (Percent of Fixed Sample)   | 103.7227           |
| Max Information                             | 47.2244524         |
| Null Ref ASN (Percent of Fixed Sample)      | 79.44086           |
| Lower Alt Ref ASN (Percent of Fixed Sample) | 66.04641           |
| Upper Alt Ref ASN (Percent of Fixed Sample) | 76.22739           |

The information is derived from the standard error associated with the slope estimate at the final stage and is larger than the target level. The derived Type II error probability  $\beta$  and power  $1 - \beta$  are different because of the new information levels.

The “Test Information” table in [Output 84.8.13](#) displays the boundary values for the test statistic with the specified MLE scale. The information levels are derived from the standard errors in the PARMS= data set. At stage 2, the slope estimate 0.52128 is larger than 0.44091, the upper  $\alpha$  boundary value, the trial stops to reject the null hypothesis of no treatment effect.

**Output 84.8.13** Sequential Tests

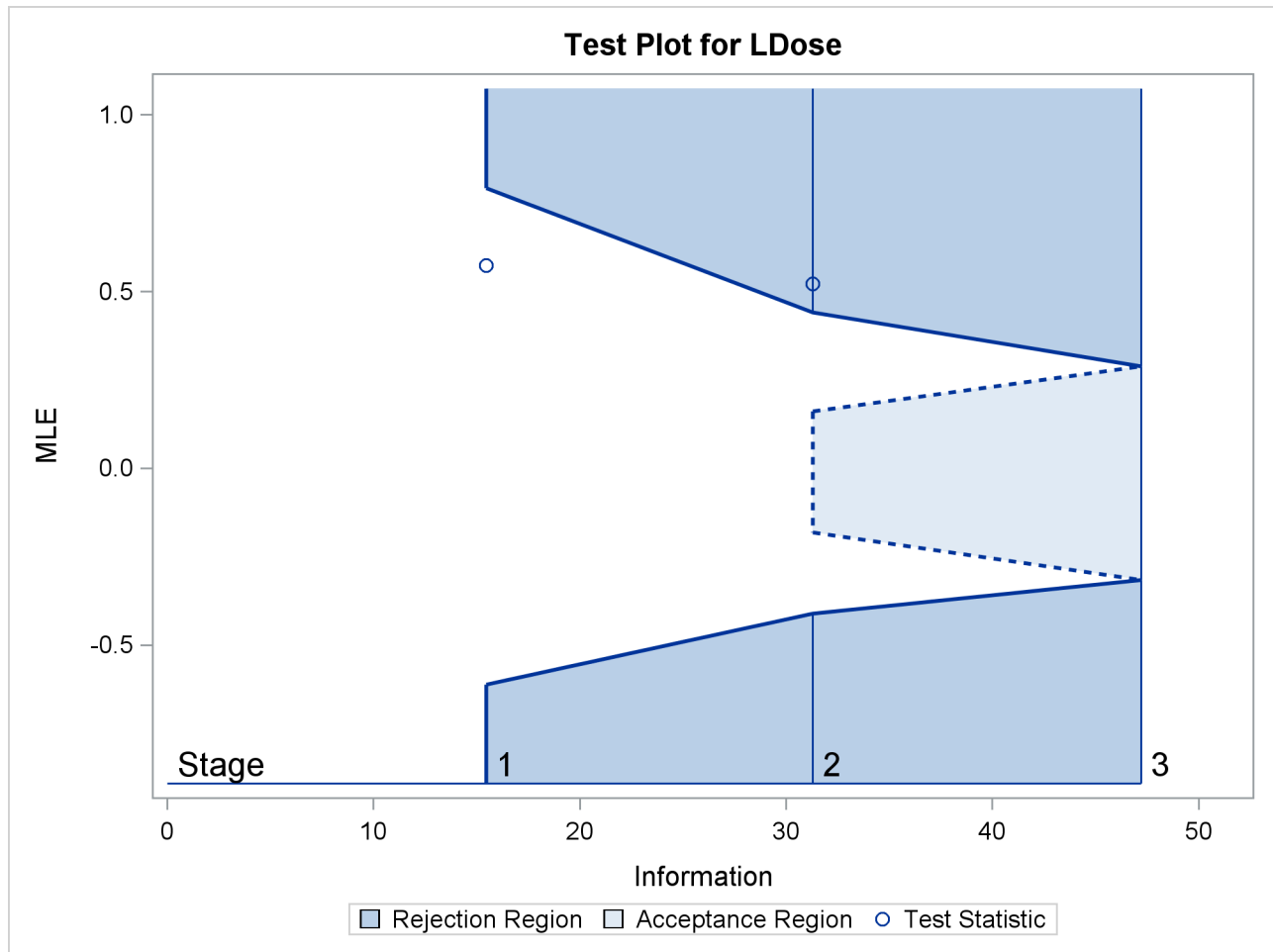
| Test Information (MLE Scale) |                         |          |                       |         |
|------------------------------|-------------------------|----------|-----------------------|---------|
| Null Reference = 0           |                         |          |                       |         |
| _Stage_                      | ---Information Level--- |          | -----Alternative----- |         |
|                              | Proportion              | Actual   | Lower                 | Upper   |
| 1                            | 0.3272                  | 15.45062 | -0.50000              | 0.50000 |
| 2                            | 0.6624                  | 31.28346 | -0.50000              | 0.50000 |
| 3                            | 1.0000                  | 47.22445 | -0.50000              | 0.50000 |

| Test Information (MLE Scale) |                           |          |                 |         |                 |             |
|------------------------------|---------------------------|----------|-----------------|---------|-----------------|-------------|
| Null Reference = 0           |                           |          |                 |         |                 |             |
| _Stage_                      | -----Boundary Values----- |          |                 |         | -----Test-----  |             |
|                              | -----Lower-----           |          | -----Upper----- |         | -----LDose----- |             |
|                              | Alpha                     | Beta     | Beta            | Alpha   | Estimate        | Action      |
| 1                            | -0.61078                  | .        | .               | 0.79337 | 0.57409         | Continue    |
| 2                            | -0.41028                  | -0.18112 | 0.16166         | 0.44091 | 0.52128         | Reject Null |
| 3                            | -0.31628                  | -0.31628 | 0.28861         | 0.28861 | .               |             |

With ODS Graphics enabled, a boundary plot with the boundary values and test statistics is displayed, as shown in [Output 84.8.14](#). As expected, the test statistic is above the upper  $\alpha$  boundary in the upper rejection region at stage 2.

Output 84.8.14 Sequential Test Plot



After a trial is stopped, the “Parameter Estimates” table in [Output 84.8.15](#) displays the stopping stage, parameter estimate, unbiased median estimate, confidence limits, and the  $p$ -value under the null hypothesis  $H_0 : \beta_1 = 0$ .

Output 84.8.15 Parameter Estimates

| Parameter Estimates<br>MLE Ordering |                       |          |                                  |                 |
|-------------------------------------|-----------------------|----------|----------------------------------|-----------------|
| Parameter                           | Stopping Stage        | MLE      | p-Value for $H_0: \text{Parm}=0$ | Median Estimate |
| LDose                               | 2                     | 0.521275 | 0.0050                           | 0.502647        |
| Parameter Estimates<br>MLE Ordering |                       |          |                                  |                 |
| Parameter                           | 95% Confidence Limits |          |                                  |                 |
| LDose                               | 0.15745               | 0.85154  |                                  |                 |

With the ORDER=MLE option, the MLE ordering is used to compute the  $p$ -value, unbiased median estimate, and confidence limits. As expected, the  $p$ -value 0.005 is significant at the  $\alpha = 0.05$  level and the confidence interval does not contain the null reference zero.

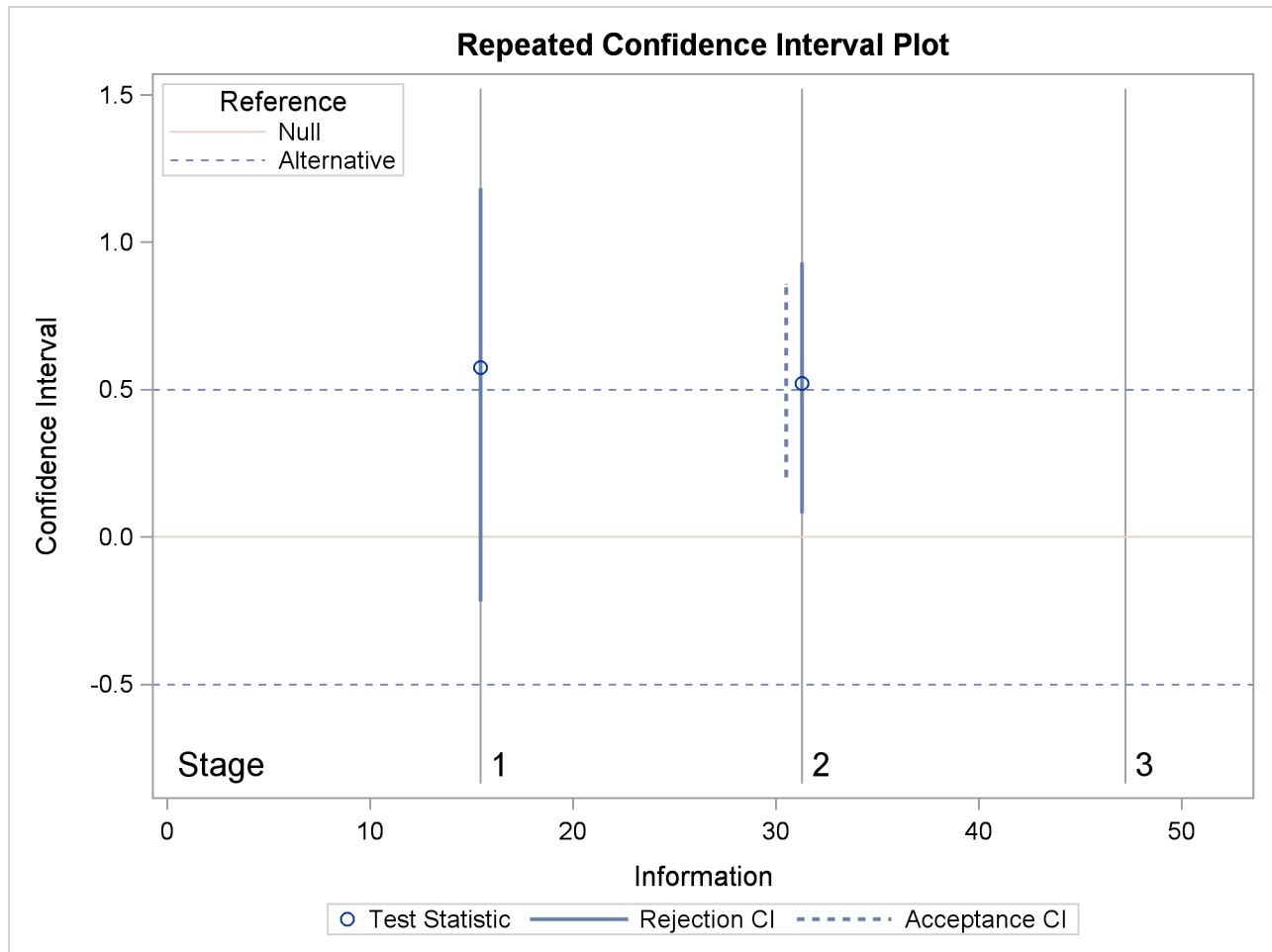
With the RCI option, the “Repeated Confidence Intervals” table in [Output 84.8.16](#) displays repeated confidence intervals for the parameter. For a two-sided test, since the rejection lower repeated confidence limit 0.0804 is greater than the null reference zero, the trial is stopped to reject the hypothesis.

**Output 84.8.16** Repeated Confidence Intervals

| Repeated Confidence Intervals |                   |                    |                         |                         |                          |                          |
|-------------------------------|-------------------|--------------------|-------------------------|-------------------------|--------------------------|--------------------------|
| _Stage_                       | Information Level | Parameter Estimate | -Rejection Boundary-    | -Rejection Boundary-    | -Acceptance Boundary-    | -Acceptance Boundary-    |
|                               |                   |                    | Lower 97.5% Repeated CL | Upper 97.5% Repeated CL | Lower 90.01% Repeated CL | Upper 92.13% Repeated CL |
| 1                             | 15.4506           | 0.57409            | -0.2193                 | 1.1849                  | .                        | .                        |
| 2                             | 31.2835           | 0.52128            | 0.0804                  | 0.9316                  | 0.2024                   | 0.8596                   |

With the PLOTS=RCI option, the “Repeated Confidence Intervals Plot” displays repeated confidence intervals for the parameter, as shown in [Output 84.8.17](#). It shows that the null reference zero is inside the rejection repeated confidence interval at stage 1 but outside the rejection repeated confidence interval at stage 2. This implies that the study stops at stage 2 to reject the hypothesis.

**Output 84.8.17** Repeated Confidence Intervals Plot



Note that the hypothesis is accepted if at any stage, the acceptance repeated confidence interval falls within the interval  $(-0.5, 0.5)$  of the alternative references.

### Example 84.9: Conducting a Trial with a Nonbinding Acceptance Boundary

This example demonstrates a trail with a nonbinding acceptance boundary. The design is similar to the design in Example 84.1, but has a nonbinding beta boundary.

A clinic is studying the effect of vitamin C supplements in treating flu symptoms. The study consists of patients in the clinic who have exhibited the first sign of flu symptoms within the last 24 hours. These patients are randomly assigned to either the control group (which receives placebo pills) or the treatment group (which receives large doses of vitamin C supplements). At the end of a five-day period, the flu symptoms of each patient are recorded.

Suppose that you know from past experience that flu symptoms disappear in five days for 60% of patients who experience flu symptoms. The clinic would like to detect a 75% symptom disappearance with a high probability. A test that compares the proportions directly specifies the null hypothesis  $H_0 : \theta = p_t - p_c = 0$

with a one-sided alternative  $H_1 : \theta > 0$  and a power of 0.90 at  $H_1 : \theta = 0.15$ , where  $p_t$  and  $p_c$  are the proportions of symptom disappearance in the treatment group and control group, respectively.

The following statements invoke the SEQDESIGN procedure and request a four-stage group sequential design by using an O'Brien-Fleming method for normally distributed data.

```
ods graphics on;
proc seqdesign altref=0.15 errspend
 ;
 NonbindingDesign: design nstages=4
 method=obf
 alt=upper
 stop=both(betaboundary=nonbinding)
 alpha=0.025
 ;
 samplesize model=twosamplefreq(nullprop=0.6 test=prop);
ods output Boundary=Bnd_Count;
run;
ods graphics off;
```

The ALT=UPPER option specifies a one-sided alternative hypothesis, and the STOP=BOTH option specifies early stopping to reject or accept the null hypothesis  $H_0$ . The BETABOUNDARY=NONBINDING suboption requests nonbinding beta boundary to have the flexibility to continue the trial when a test statistic falls in the acceptance region at interim stages (Zhu, Ni, and Yao 2011, pp. 132–133). The ODS OUTPUT statement with the BOUNDARY=BND\_COUNT option creates an output data set named BND\_COUNT which contains the resulting boundary information for the subsequent sequential tests.

The “Design Information” table in [Output 84.9.1](#) displays design specifications. With the specified alternative hypothesis  $H_1 : \theta = 0.15$ , the maximum information is derived to achieve a power of 0.90 at  $H_1$ . The derived fixed-sample information ratio 1.107 is the maximum information needed for a group sequential design relative to its corresponding fixed-sample design. Compare to the default BETABOUNDARY=BINDING option, the BETABOUNDARY=NONBINDING option requires a larger sample size for the design.

**Output 84.9.1** O'Brien-Fleming Design Information

| The SEQDESIGN Procedure                   |                                   |
|-------------------------------------------|-----------------------------------|
| Design: NonbindingDesign                  |                                   |
| Design Information                        |                                   |
| Statistic Distribution                    | Normal                            |
| Boundary Scale                            | Standardized Z                    |
| Alternative Hypothesis                    | Upper                             |
| Early Stop                                | Accept (Nonbinding) / Reject Null |
| Method                                    | O'Brien-Fleming                   |
| Boundary Key                              | Both                              |
| Alternative Reference                     | 0.15                              |
| Number of Stages                          | 4                                 |
| Alpha (Binding Beta Boundary)             | 0.02228                           |
| Alpha (Nonbinding Beta Boundary)          | 0.025                             |
| Beta                                      | 0.1                               |
| Power                                     | 0.9                               |
| Max Information (Percent of Fixed Sample) | 110.7138                          |
| Max Information                           | 517.0296                          |
| Null Ref ASN (Percent of Fixed Sample)    | 62.29796                          |
| Alt Ref ASN (Percent of Fixed Sample)     | 78.5392                           |

The “Boundary Information” table in [Output 84.9.2](#) displays the information level, alternative reference, and boundary values at each stage. With the default BOUNDARYSCALE=STDZ option, the SEQDESIGN procedure displays the output boundaries with the standardized normal Z scale.

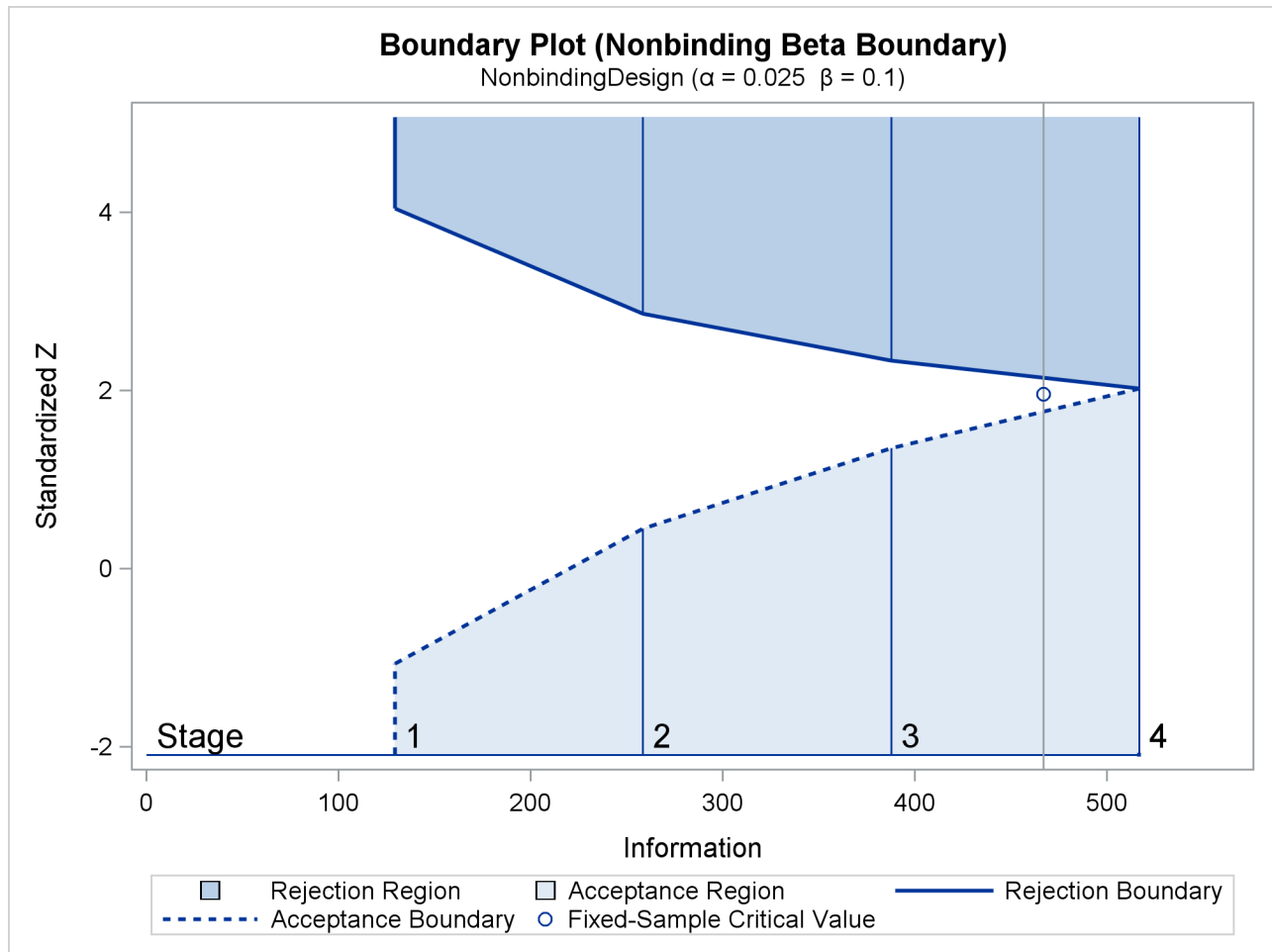
**Output 84.9.2** O'Brien-Fleming Boundary Information

| Boundary Information (Standardized Z Scale)  |                             |          |          |               |                         |         |
|----------------------------------------------|-----------------------------|----------|----------|---------------|-------------------------|---------|
| Nonbinding Beta Boundary, Null Reference = 0 |                             |          |          |               |                         |         |
| _Stage_                                      | -----Information Level----- |          |          | -Alternative- | ----Boundary Values---- |         |
|                                              | Proportion                  | Actual   | N        | --Reference-- | -----Upper-----         |         |
|                                              |                             |          |          | Upper         | Beta                    | Alpha   |
| 1                                            | 0.2500                      | 129.2574 | 110.5151 | 1.70537       | -1.06752                | 4.04859 |
| 2                                            | 0.5000                      | 258.5148 | 221.0302 | 2.41176       | 0.45103                 | 2.86279 |
| 3                                            | 0.7500                      | 387.7722 | 331.5452 | 2.95379       | 1.35286                 | 2.33746 |
| 4                                            | 1.0000                      | 517.0296 | 442.0603 | 3.41074       | 2.02430                 | 2.02430 |

With ODS Graphics enabled, a detailed boundary plot with the rejection and acceptance regions is displayed, as shown in [Output 84.1.3](#). The horizontal axis indicates the information levels for the design. The stages are indicated by vertical lines with accompanying stage numbers. If the test statistic at a stage is in a rejection region, the trial stops and the hypothesis is rejected. If the test statistic is in an acceptance region, then the trial either stops to accept the hypothesis or continues to the next stage. If the statistic is not in a rejection or an acceptance region, the trial continues to the next stage.



**Output 84.9.3** O'Brien-Fleming Boundary Plot



The boundary plot also displays the information level and critical value for the corresponding fixed-sample design. The solid and dashed lines at the fixed-sample information level correspond to the rejection and acceptance lines, respectively.

The “Error Spending Information (Nonbinding Beta Boundary)” in **Output 84.9.4** displays cumulative error spending at each stage for each boundary. With a nonbinding beta boundary, the  $\alpha$  spending at each stage is computed by using the  $\alpha$  boundary only.

**Output 84.9.4** Error Spending Information

| Error Spending Information (Nonbinding Beta Boundary) |                                   |                             |                          |  |
|-------------------------------------------------------|-----------------------------------|-----------------------------|--------------------------|--|
| _Stage_                                               | -Information Level-<br>Proportion | -Cumulative Error Spending- |                          |  |
|                                                       |                                   | Beta                        | -----Upper-----<br>Alpha |  |
| 1                                                     | 0.2500                            | 0.00278                     | 0.00003                  |  |
| 2                                                     | 0.5000                            | 0.02603                     | 0.00211                  |  |
| 3                                                     | 0.7500                            | 0.06343                     | 0.01046                  |  |
| 4                                                     | 1.0000                            | 0.10000                     | 0.02500                  |  |

With the SAMPLESIZE statement, the maximum information is used to derive the required sample size for the study. The “Sample Size Summary” table in [Output 84.9.5](#) displays parameters for the sample size computation.

**Output 84.9.5** Required Sample Size Summary

| Sample Size Summary             |                        |
|---------------------------------|------------------------|
| Test                            | Two-Sample Proportions |
| Null Proportion                 | 0.6                    |
| Proportion (Group A)            | 0.75                   |
| Test Statistic                  | Z for Proportion       |
| Reference Proportions           | Alt Ref                |
| Max Sample Size                 | 442.0603               |
| Expected Sample Size (Null Ref) | 248.7446               |
| Expected Sample Size (Alt Ref)  | 313.5929               |

With the derived maximum information and the specified MODEL= option in the SAMPLESIZE statement, the total sample size in each group for testing the difference between two proportions under the alternative hypothesis is

$$N_1 = N_2 = (p_{1c}(1 - p_{1c}) + p_{1t}(1 - p_{1t})) I_X$$

where  $p_{1c} = 0.6$  and  $p_{1t} = p_{1c} + \theta_1 = 0.75$ . By default (or equivalently if you specify REF=PROP in the MODEL=TWOSAMPLEFREQ option), the required sample sizes are computed under the alternative hypothesis. See the section “Test for the Difference between Two Binomial Proportions” in the chapter “The SEQDESIGN Procedure” for a description of these parameters.

The “Sample Sizes (N)” table in [Output 84.9.6](#) displays the required sample sizes at each stage, in both fractional and integer numbers. The derived sample sizes under the heading Fractional N which correspond to the design are not integers. These sample sizes are rounded up to integers under the heading Ceiling N. In practice, integer sample sizes are used, and the information levels increase slightly. Thus, 56, 111, 166, and 222 patients are needed in each group for the four stages, respectively.

**Output 84.9.6** Required Sample Sizes

| Sample Sizes (N)                            |        |          |          |             |
|---------------------------------------------|--------|----------|----------|-------------|
| Two-Sample Z Test for Proportion Difference |        |          |          |             |
| -----Fractional N-----                      |        |          |          |             |
| _Stage_                                     | N      | N(Grp 1) | N(Grp 2) | Information |
| 1                                           | 110.52 | 55.26    | 55.26    | 129.3       |
| 2                                           | 221.03 | 110.52   | 110.52   | 258.5       |
| 3                                           | 331.55 | 165.77   | 165.77   | 387.8       |
| 4                                           | 442.06 | 221.03   | 221.03   | 517.0       |

| Sample Sizes (N)                            |     |          |          |             |
|---------------------------------------------|-----|----------|----------|-------------|
| Two-Sample Z Test for Proportion Difference |     |          |          |             |
| -----Ceiling N-----                         |     |          |          |             |
| _Stage_                                     | N   | N(Grp 1) | N(Grp 2) | Information |
| 1                                           | 112 | 56       | 56       | 131.0       |
| 2                                           | 222 | 111      | 111      | 259.6       |
| 3                                           | 332 | 166      | 166      | 388.3       |
| 4                                           | 444 | 222      | 222      | 519.3       |

Suppose the trial follows the study plan, and 56 patients are available in each group at stage 1. The data set `count_1` contains these 108 patients. [Output 84.9.7](#) lists the first 10 observations of the data set.

**Output 84.9.7** Clinical Trial Data

| First 10 Obs in the Trial Data |     |      |  |
|--------------------------------|-----|------|--|
| Obs                            | Trt | Resp |  |
| 1                              | 0   | 0    |  |
| 2                              | 1   | 1    |  |
| 3                              | 0   | 1    |  |
| 4                              | 1   | 1    |  |
| 5                              | 0   | 1    |  |
| 6                              | 1   | 0    |  |
| 7                              | 0   | 0    |  |
| 8                              | 1   | 1    |  |
| 9                              | 0   | 1    |  |
| 10                             | 1   | 0    |  |

The `Trt` variable is a grouping variable with value 0 for a patient in the placebo control group and value 1 for a patient in the treatment group who is given vitamin C supplements. The `Resp` variable is an indicator variable with value 1 for a patient without flu symptoms after five days and value 0 for a patient with flu symptoms after five days.

The following statements use the GENMOD procedure to estimate the treatment effect at stage 1:

```
proc genmod data=count_1;
 model Resp= Trt;
 ods output ParameterEstimates=Parms_Count1;
run;
```

Output 84.9.8 displays the treatment effect at stage 1.

**Output 84.9.8** Stage 1 Treatment Difference

| The GENMOD Procedure                               |    |          |                |                            |        |                 |            |
|----------------------------------------------------|----|----------|----------------|----------------------------|--------|-----------------|------------|
| Analysis Of Maximum Likelihood Parameter Estimates |    |          |                |                            |        |                 |            |
| Parameter                                          | DF | Estimate | Standard Error | Wald 95% Confidence Limits |        | Wald Chi-Square | Pr > ChiSq |
| Intercept                                          | 1  | 0.6786   | 0.0619         | 0.5572                     | 0.7999 | 120.07          | <.0001     |
| Trt                                                | 1  | 0.0179   | 0.0876         | -0.1538                    | 0.1895 | 0.04            | 0.8384     |
| Scale                                              | 1  | 0.4634   | 0.0310         | 0.4065                     | 0.5283 |                 |            |

NOTE: The scale parameter was estimated by maximum likelihood.

The test statistic is  $\hat{\theta}_1 = \hat{p}_t - \hat{p}_c = 0.0179$ , and its associated standard error is

$$\sqrt{\text{Var}(\hat{\theta}_1)} = \sqrt{\frac{\hat{p}_c(1 - \hat{p}_c)}{56} + \frac{\hat{p}_t(1 - \hat{p}_t)}{56}} = 0.0876$$

The following statements create and display (in Output 84.9.9) the data set that contains the parameter estimate at stage 1,  $\hat{\theta}_1 = 0.0179$ , and its associated standard error  $\sqrt{\text{Var}(\hat{\theta}_1)} = 0.0876$  which are used in the SEQTEST procedure:

```
data Parms_Count1;
 set Parms_Count1;
 if Parameter='Trt';
 Scale='MLE';
 Stage= 1;
 keep _Scale_ _Stage_ Parameter Estimate StdErr;
run;

proc print data=Parms_Count1;
 title 'Statistics Computed at Stage 1';
run;
```

**Output 84.9.9** Statistics Computed at Stage 1

| Statistics Computed at Stage 1 |           |          |        |         |         |
|--------------------------------|-----------|----------|--------|---------|---------|
| Obs                            | Parameter | Estimate | StdErr | _Scale_ | _Stage_ |
| 1                              | Trt       | 0.0179   | 0.0876 | MLE     | 1       |

The initial required sample sizes are derived with the proportions  $p_c = 0.6$  and  $p_t = 0.75$ . If the observed proportions are different from these assumed values, or if the number of available patients is different from the study plan in one of the stages, then the information level that corresponds to the test statistic is estimated from

$$I_k = \frac{1}{\text{Var}(\hat{\theta}_k)}$$

The following statements invoke the SEQTEST procedure and test for early stopping at stage 1:

```
ods graphics on;
proc seqtest Boundary=Bnd_Count
 Parms (Testvar=Trt)=Parms_Count1
 betaboundary=nonbinding
 infoadj=none
 errspendmin=0.001
 errspend
 ;
ods output Test=Test_Count1;
run;
ods graphics off;
```

The BOUNDARY= option specifies the input data set that provides the boundary information for the trial at stage 1, which was generated in the SEQDESIGN procedure. The PARMS=PARMS\_COUNT1 option specifies the input data set PARMS\_COUNT1 that contains the test statistic and its associated standard error at stage 1, and the TESTVAR=TRT option identifies the test variable TRT in the data set.

The BETABOUNDARY=NONBINDING option requests nonbinding beta boundary to have the flexibility to continue the trial when the test statistic falls in the acceptance region at stage 1. The INFOADJ=NONE option maintains the information levels at future interim stages (2 and 3) as provided in the BOUNDARY= data set. The default BOUNDARYSCALE=STDZ option displays the output boundaries in terms of the standardized normal  $Z$  scale.

The O'Brien-Fleming design is conservative in early stages and might not be desirable in a clinical trial. The ERRSPENDMIN=0.001 option specifies the minimum error spending at each stage to be 0.001, and it might increase the corresponding nominal  $p$ -value in early stages for the trial. The default BOUNDARYSCALE=STDZ option uses the standardized normal  $Z$  scale to display test statistics in the boundary table and boundary plots.

The ODS OUTPUT statement with the TEST=TEST\_COUNT1 option creates an output data set named TEST\_COUNT1 which contains the updated boundary information for the test at stage 1. The data set also provides the boundary information that is needed for the group sequential test at the next stage.

The "Design Information" table in [Output 84.9.10](#) displays design specifications. The derived statistics, such as the overall  $\alpha$  and  $\beta$  levels, are derived from the specified maximum information and boundary values in the BOUNDARY= data set. Note that with a minor change in the information level at stage 1, the power also changes slightly from the design provided in the BOUNDARY= data set.

**Output 84.9.10** Design Information

| The SEQTEST Procedure                     |                                  |
|-------------------------------------------|----------------------------------|
| Design Information                        |                                  |
| BOUNDARY Data Set                         | WORK.BND_COUNT                   |
| Data Set                                  | WORK.PARMS_COUNT1                |
| Statistic Distribution                    | Normal                           |
| Boundary Scale                            | Standardized Z                   |
| Alternative Hypothesis                    | Upper                            |
| Early Stop                                | Accept (Nonbinding) /Reject Null |
| Number of Stages                          | 4                                |
| Alpha (Binding Beta Boundary)             | 0.02237                          |
| Alpha (Nonbinding Beta Boundary)          | 0.025                            |
| Beta                                      | 0.10142                          |
| Power                                     | 0.89858                          |
| Max Information (Percent of Fixed Sample) | 111.2654                         |
| Max Information                           | 517.029617                       |
| Null Ref ASN (Percent of Fixed Sample)    | 62.27694                         |
| Alt Ref ASN (Percent of Fixed Sample)     | 76.31328                         |

With the ERRSPEND option, the “Error Spending Information” table in [Output 84.9.11](#) displays cumulative error spending at each stage for each boundary. By default (or equivalently if you specify BOUNDARYKEY=ALPHA), the Type I error level with nonbinding beta boundary  $\alpha = 0.025$  is maintained. Furthermore, with the ERRSPENDMIN=0.001 option, the  $\alpha$  spending at each stage is greater than or equal to 0.001.

**Output 84.9.11** Error Spending Information

| Error Spending Information (Nonbinding Beta Boundary) |                         |          |                             |         |
|-------------------------------------------------------|-------------------------|----------|-----------------------------|---------|
| _Stage_                                               | ---Information Level--- |          | -Cumulative Error Spending- |         |
|                                                       | Proportion              | Actual   | Beta                        | Alpha   |
| 1                                                     | 0.2522                  | 130.3756 | 0.00302                     | 0.00100 |
| 2                                                     | 0.5000                  | 258.5148 | 0.02640                     | 0.00299 |
| 3                                                     | 0.7500                  | 387.7722 | 0.06433                     | 0.01101 |
| 4                                                     | 1.0000                  | 517.0296 | 0.10142                     | 0.02500 |

The “Test Information” table in [Output 84.9.12](#) displays the boundary values for the design, test statistic, and resulting action at each stage. With the default BOUNDARYSCALE=STDZ option, the standardized normal Z scale is used for the test statistic and boundary values. The table shows that the test statistic 0.2039 is between the upper  $\alpha$  and  $\beta$  boundaries, so the trial continues to the next stage.

## Output 84.9.12 Sequential Test

| Test Information (Standardized Z Scale)      |                         |          |                        |                           |         |
|----------------------------------------------|-------------------------|----------|------------------------|---------------------------|---------|
| Nonbinding Beta Boundary, Null Reference = 0 |                         |          |                        |                           |         |
| _Stage_                                      | ---Information Level--- |          | -Alternative-          | -----Boundary Values----- |         |
|                                              | Proportion              | Actual   | --Reference--<br>Upper | -----Upper-----<br>Beta   | Alpha   |
| 1                                            | 0.2522                  | 130.3756 | 1.71273                | -1.03271                  | 3.09023 |
| 2                                            | 0.5000                  | 258.5148 | 2.41176                | 0.45564                   | 2.84016 |
| 3                                            | 0.7500                  | 387.7722 | 2.95379                | 1.36069                   | 2.34211 |
| 4                                            | 1.0000                  | 517.0296 | 3.41074                | 2.03599                   | 2.03599 |

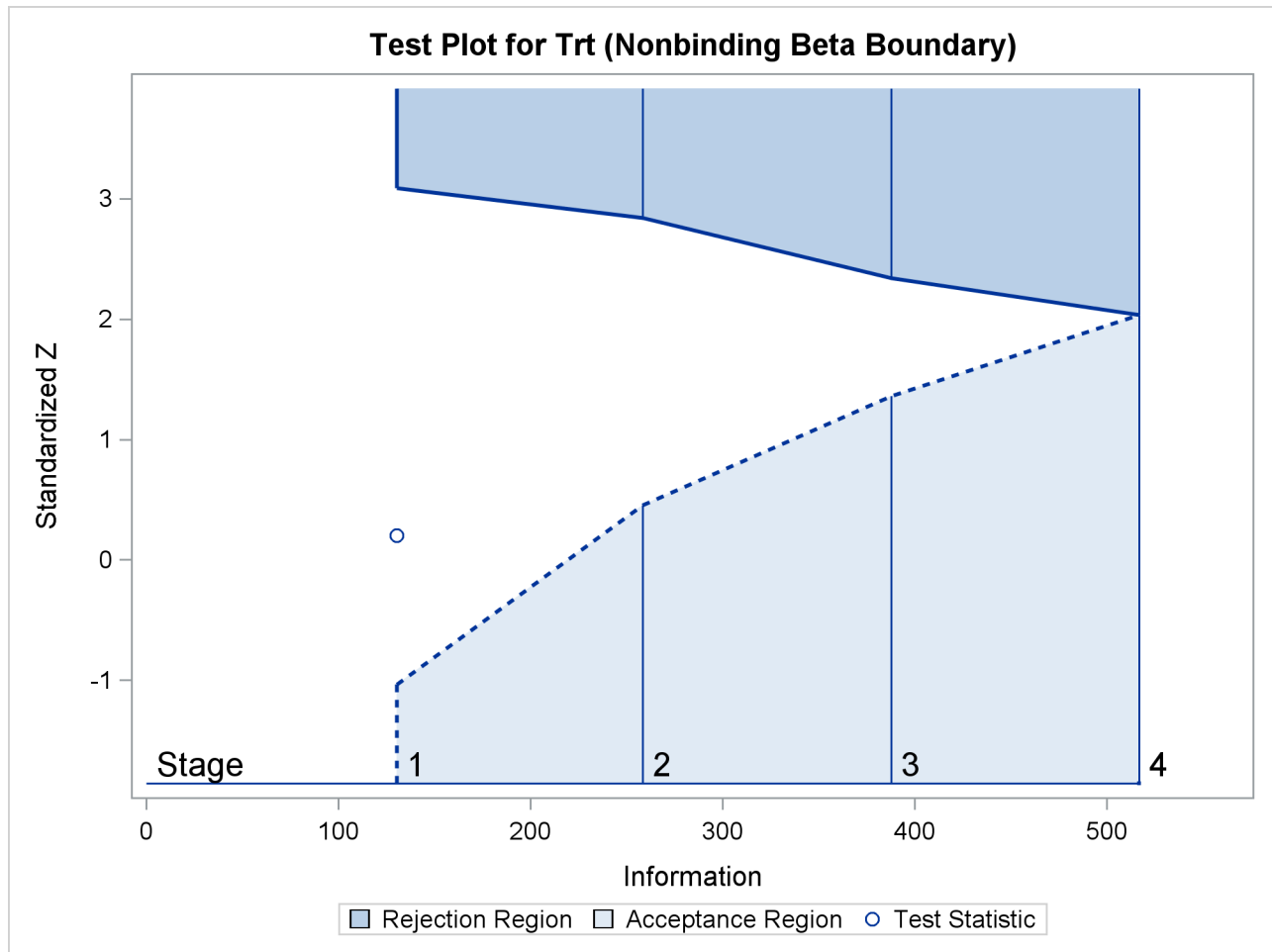
| Test Information (Standardized Z Scale)      |                |               |
|----------------------------------------------|----------------|---------------|
| Nonbinding Beta Boundary, Null Reference = 0 |                |               |
| _Stage_                                      | -----Test----- |               |
|                                              | Estimate       | Trt<br>Action |
| 1                                            | 0.20390        | Continue      |
| 2                                            | .              | .             |
| 3                                            | .              | .             |
| 4                                            | .              | .             |

The information level at stage 1 is derived from the standard error,

$$I_1 = \frac{1}{\text{Var}(\hat{\theta}_1)} = \frac{1}{(\text{s.e.}(\hat{\theta}_1))^2} = 130.376$$

By default (or equivalently if you specify PLOTS=TEST), the “Test Plot” graph displays boundary values of the design and the test statistic at stage 1, as shown in [Output 84.9.13](#). It also shows that the observed statistic is in the continuation region.

Output 84.9.13 Sequential Test Plot



The observed information level at stage 1,  $I_1 = 130.376$ , is slightly larger than the target information level at the design. If an observed information level in the study is substantially different from its target level in the design, then the sample sizes should be adjusted in the subsequent stages to achieve the target information levels.

Suppose the trial continues to the next stage, and 111 patients are available in each group at stage 2. The data set COUNT\_2 contains these 222 patients.

The following statements use the GENMOD procedure to estimate the treatment effect at stage 2:

```
proc genmod data=Count_2;
 model Resp= Trt;
 ods output ParameterEstimates=Parms_Count2;
run;
```

The following statements create the parameter estimate at stage 2,  $\hat{\theta}_2 = \hat{p}_2 - \hat{p}_1 = 0.027$ , and its associated standard error  $\sqrt{\text{Var}(\hat{\theta}_2)} = 0.0621$  into a test data set:



```

data Parms_Count2;
 set Parms_Count2;
 if Parameter='Trt';
 Scale='MLE';
 Stage= 2;
 keep _Scale_ _Stage_ Parameter Estimate StdErr;
run;

proc print data=Parms_Count2;
 title 'Statistics Computed at Stage 2';
run;

```

Output 84.9.14 displays the test statistics at stage 2.

**Output 84.9.14** Statistics Computed at Stage 2

| Statistics Computed at Stage 2 |           |          |        |         |         |
|--------------------------------|-----------|----------|--------|---------|---------|
| Obs                            | Parameter | Estimate | StdErr | _Scale_ | _Stage_ |
| 1                              | Trt       | 0.0270   | 0.0621 | MLE     | 2       |

The following statements invoke the SEQTEST procedure and test for early stopping at stage 2:

```

ods graphics on;
proc seqtest Boundary=Test_Count1
 Parms(Testvar=Trt)=Parms_Count2
 betaboundary=nonbinding
 infoadj=none
 ;
ods output Test=Test_Count2;
run;
ods graphics off;

```

The BOUNDARY= option specifies the input data set that provides the boundary information for the trial at stage 2, which was generated by the SEQTEST procedure at the previous stage. The PARMS= option specifies the input data set that contains the test statistic and its associated standard error at stage 2, and the TESTVAR= option identifies the test variable in the data set.

The ODS OUTPUT statement with the TEST=TEST\_COUNT2 option creates an output data set named TEST\_COUNT2 which contains the updated boundary information for the test at stage 2. The data set also provides the boundary information that is needed for the group sequential test at the next stage.

The “Test Information” table in [Output 84.9.15](#) displays the boundary values, test statistic, and resulting action at each stage. The table shows that the test statistic 0.43522 is less than the corresponding upper beta boundary value, so the trial can be stopped to accept the hypothesis. With the BETABOUNDARY=NONBINDING option, The clinic has the option to continue the trial while still maintaining the Type I error level.

**Output 84.9.15** Sequential Test

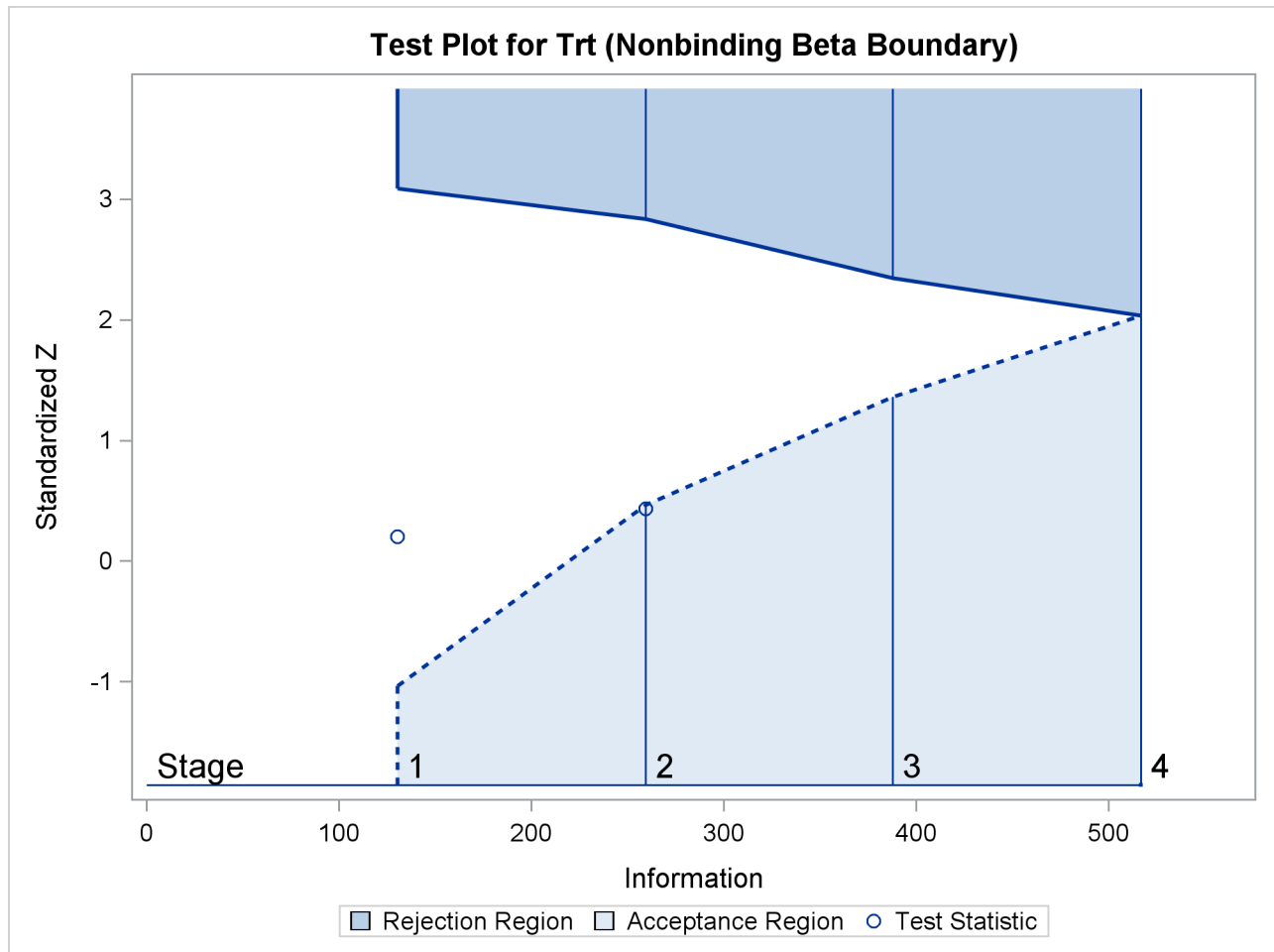
| The SEQTEST Procedure                        |                        |          |                        |                          |         |
|----------------------------------------------|------------------------|----------|------------------------|--------------------------|---------|
| Test Information (Standardized Z Scale)      |                        |          |                        |                          |         |
| Nonbinding Beta Boundary, Null Reference = 0 |                        |          |                        |                          |         |
| _Stage_                                      | ---Information Level-- |          | -Alternative-          | -----Boundary Values---- |         |
|                                              | Proportion             | Actual   | --Reference--<br>Upper | -----Upper-----<br>Beta  | Alpha   |
| 1                                            | 0.2522                 | 130.3756 | 1.71273                | -1.03271                 | 3.09023 |
| 2                                            | 0.5015                 | 259.3157 | 2.41549                | 0.46349                  | 2.83297 |
| 3                                            | 0.7500                 | 387.7722 | 2.95379                | 1.36018                  | 2.34294 |
| 4                                            | 1.0000                 | 517.0296 | 3.41074                | 2.03610                  | 2.03610 |

| Test Information (Standardized Z Scale)      |                |                          |
|----------------------------------------------|----------------|--------------------------|
| Nonbinding Beta Boundary, Null Reference = 0 |                |                          |
| _Stage_                                      | -----Test----- |                          |
|                                              | Estimate       | Action                   |
| 1                                            | 0.20390        | Continue                 |
| 2                                            | 0.43522        | Accept Null (Nonbinding) |
| 3                                            | .              |                          |
| 4                                            | .              |                          |

With ODS Graphics enabled, the “Test Plot” is displayed, as shown in [Output 84.9.16](#). The plot displays boundary values of the design and the test statistics at the first two stages. As expected, the test statistic at stage 2 is in the “Upper Acceptance Region” below the upper beta boundary.

Output 84.9.16 Sequential Test Plot



Suppose the clinic decides to continue the trial, and at the next stage, 108 patients are available in each group at stage 3. The data set COUNT\_3 contains these 332 patients.

The following statements use the GENMOD procedure to estimate the treatment effect at stage 3:

```
proc genmod data=Count_3;
 model Resp= Trt;
 ods output ParameterEstimates=Parms_Count3;
run;
```

The following statements create the parameter estimate at stage 2,  $\hat{\theta}_2 = \hat{p}_2 - \hat{p}_1 = 0.1205$ , and its associated standard error  $\sqrt{\text{Var}(\hat{\theta}_2)} = 0.0507$  into a test data set:

```
data Parms_Count3;
 set Parms_Count3;
 if Parameter='Trt';
 Scale='MLE';
 Stage= 3;
 keep _Scale_ _Stage_ Parameter Estimate StdErr;
run;
```

```
proc print data=Parms_Count3;
 title 'Statistics Computed at Stage 3';
run;
```

Output 84.9.17 displays the test statistics at stage 3.

**Output 84.9.17** Statistics Computed at Stage 3

| Statistics Computed at Stage 3 |           |          |        |         |         |
|--------------------------------|-----------|----------|--------|---------|---------|
| Obs                            | Parameter | Estimate | StdErr | _Scale_ | _Stage_ |
| 1                              | Trt       | 0.1205   | 0.0507 | MLE     | 3       |

The following statements invoke the SEQTEST procedure and test for early stopping at stage 3:

```
ods graphics on;
proc seqtest Boundary=Test_Count2
 Parms (Testvar=Trt) =Parms_Count3
 betaboundary=nonbinding
;
ods output Test=Test_Count3;
run;
ods graphics off;
```

The “Test Information” table in [Output 84.9.18](#) displays the boundary values, test statistic, and resulting action at each stage. The table shows that the test statistic 2.37437 is greater than the corresponding upper alpha boundary value, so the trial stops to reject the hypothesis.

## Output 84.9.18 Sequential Test

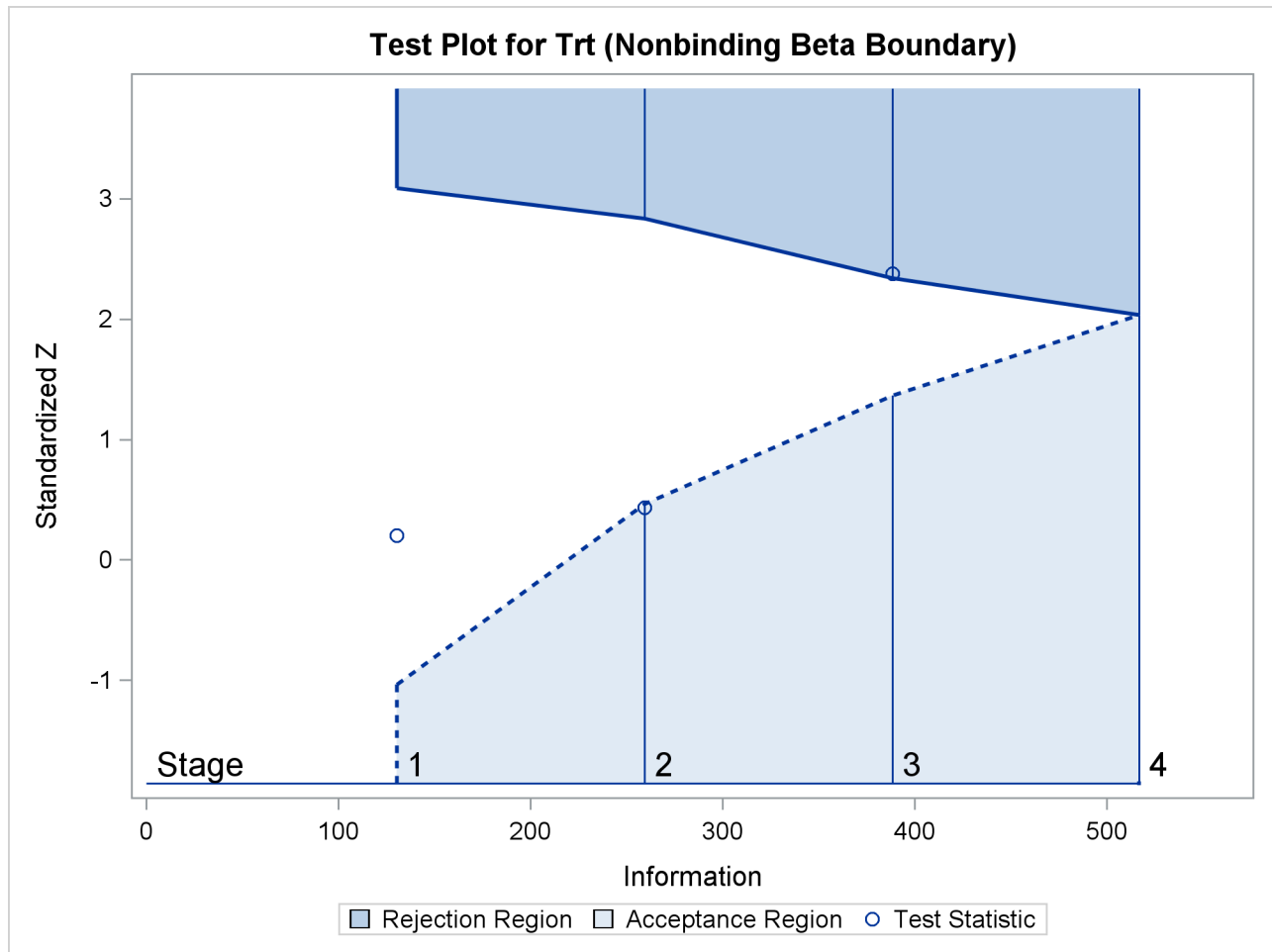
| The SEQTEST Procedure                        |                        |          |                        |                          |         |
|----------------------------------------------|------------------------|----------|------------------------|--------------------------|---------|
| Test Information (Standardized Z Scale)      |                        |          |                        |                          |         |
| Nonbinding Beta Boundary, Null Reference = 0 |                        |          |                        |                          |         |
| _Stage_                                      | ---Information Level-- |          | -Alternative-          | -----Boundary Values---- |         |
|                                              | Proportion             | Actual   | --Reference--<br>Upper | -----Upper-----<br>Beta  | Alpha   |
| 1                                            | 0.2522                 | 130.3756 | 1.71273                | -1.03271                 | 3.09023 |
| 2                                            | 0.5015                 | 259.3157 | 2.41549                | 0.46349                  | 2.83297 |
| 3                                            | 0.7512                 | 388.3763 | 2.95609                | 1.36434                  | 2.34036 |
| 4                                            | 1.0000                 | 517.0296 | 3.41074                | 2.03658                  | 2.03658 |

| Test Information (Standardized Z Scale)      |                |                          |
|----------------------------------------------|----------------|--------------------------|
| Nonbinding Beta Boundary, Null Reference = 0 |                |                          |
| _Stage_                                      | -----Test----- |                          |
|                                              | Estimate       | -----Trt-----<br>Action  |
| 1                                            | 0.20390        | Continue                 |
| 2                                            | 0.43522        | Accept Null (Nonbinding) |
| 3                                            | 2.37437        | Reject Null              |
| 4                                            | .              | .                        |

With ODS Graphics enabled, the “Test Plot” is displayed, as shown in [Output 84.9.19](#). The plot displays boundary values of the design and the test statistics at the first two stages. As expected, the test statistic at stage 3 is in the “Upper Rejection Region” above the upper alpha boundary.

**Output 84.9.19** Sequential Test Plot



After a trial is stopped, the “Parameter Estimates” table in [Output 84.9.20](#) displays the stopping stage and the maximum likelihood estimate of the parameter. It also displays the  $p$ -value, median estimate, and confidence limits for the parameter that correspond to the observed statistic by using the specified sample space ordering.

**Output 84.9.20** Parameter Estimates

| Parameter Estimates<br>Stagewise Ordering |                |          |                                  |                 |              |
|-------------------------------------------|----------------|----------|----------------------------------|-----------------|--------------|
| Parameter                                 | Stopping Stage | MLE      | p-Value for $H_0: \text{Parm}=0$ | Median Estimate | Lower 95% CL |
| Trt                                       | 3              | 0.120482 | 0.0103                           | 0.119371        | 0.03494      |

The MLE statistic at the stopping stage is the maximum likelihood estimate of the parameter and is biased. The computation of  $p$ -value, unbiased median estimate, and confidence limits depends on the ordering of the sample space  $(k, z)$ , where  $k$  is the stage number and  $z$  is the observed standardized  $Z$  statistic. By default

(or equivalently if you specify ORDER=STAGewise), the stagewise ordering that uses counterclockwise ordering around the continuation region is used to compute the  $p$ -value, unbiased median estimate, and confidence limits. As expected, the  $p$ -value is less than 0.025, and the confidence interval does not contain the null reference zero.

See the section “Available Sample Space Orderings in a Sequential Test” on page 7230 for a detailed description of the stagewise ordering.

---

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# Chapter 85

## The SIM2D Procedure

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## Overview: SIM2D Procedure

The SIM2D procedure uses an LU decomposition technique to produce a spatial simulation for a Gaussian random field with a specified mean and covariance structure in two dimensions.

The simulation can be conditional or unconditional. If it is conditional, a set of coordinates and associated field values are read from a SAS data set. The resulting simulation honors these data values.

You can specify the mean structure as a quadratic function in the coordinates. Specify the semivariance by naming the form and supplying the associated parameters, or by using the contents of an item store file that was previously created by PROC VARIOGRAM.

PROC SIM2D can handle anisotropic and nested semivariogram models. Seven covariance models are supported: Gaussian, exponential, spherical, cubic, pentaspherical, sine hole effect, and Matérn. A single nugget effect is also supported.

You can specify the locations of simulation points in a **GRID** statement, or they can be read from a SAS data set. The grid specification is most suitable for a regular grid; the data set specification can handle any irregular pattern of points.

The SIM2D procedure writes the simulated values for each grid point to an output data set. The SIM2D procedure uses ODS Graphics to create graphs as part of its output. For general information about ODS Graphics, see Chapter 21, “[Statistical Graphics Using ODS.](#)” For more information about the graphics available in PROC SIM2D, see the section “[ODS Graphics](#)” on page 7413.

---

## Introduction to Spatial Simulation

The purpose of spatial simulation is to produce a set of partial realizations of a spatial random field (SRF)  $Z(s), s \in D \subset \mathcal{R}^2$  in a way that preserves a specified mean  $\mu(s) = E[Z(s)]$  and covariance structure  $C_z(s_1 - s_2) = \text{Cov}(Z(s_1), Z(s_2))$ . The realizations are partial in the sense that they occur only at a finite set of locations  $(s_1, s_2, \dots, s_n)$ . These locations are typically on a regular grid, but they can be arbitrary locations in the plane.

PROC SIM2D produces simulations for continuous processes in two dimensions by using the lower-upper (LU) decomposition method. In these simulations the possible values of the measured quantity  $Z(s_0)$  at location  $s_0 = (x_0, y_0)$  can vary continuously over a certain range. An additional assumption, needed for computational purposes, is that the spatial random field  $Z(s)$  is Gaussian. The section “[Details: SIM2D Procedure](#)” on page 7408 provides more information about different types of spatial simulation and associated computational methods.

Spatial simulation is different from spatial prediction, where the emphasis is on predicting a point value at a given grid location. In this sense, spatial prediction is local. In contrast, spatial simulation is global; the emphasis is on the entire realization  $(Z(s_1), Z(s_2), \dots, Z(s_n))$ .

Given the correct mean  $\mu(s)$  and covariance structure  $C_z(s_1 - s_2)$ , SRF quantities that are difficult or impossible to calculate in a spatial prediction context can easily be approximated by functions of multiple simulations.

---

## Getting Started: SIM2D Procedure

Spatial simulation, just like spatial prediction, requires a model of spatial dependence, usually in terms of the covariance  $C_z(\mathbf{h})$ . For a given set of spatial data  $Z(s_i), i = 1, \dots, n$ , the covariance structure (both the form and parameter values) can be found by the VARIOGRAM procedure. This example uses the coal seam thickness data that are also used in the section “Getting Started: VARIOGRAM Procedure” on page 8561.

In this example, the data consist of coal seam thickness measurements (in feet) taken over an area of  $100 \times 100$  ( $10^6$  ft<sup>2</sup>). The coordinates are offsets from a point in the southwest corner of the measurement area, with the north and east distances in units of thousands of feet.

---

### Preliminary Spatial Data Analysis

A semivariance analysis of the coal seam thickness thick data set is performed in “Getting Started: VARIOGRAM Procedure” on page 8561 of the VARIOGRAM procedure. The analysis considers the spatial random field (SRF)  $Z(s)$  of the Thick variable to be free of surface trends. The expected value  $E[Z(s)]$  is then a constant  $\mu(s) = \mu$ , which suggests that you can work with the original thickness data rather than residuals from a trend surface fit. In fact, a reasonable approximation of the spatial process generating the coal seam data is given by

$$Z(s) = \mu + \varepsilon(s)$$

where  $\varepsilon(s)$  is a Gaussian SRF with Gaussian covariance structure

$$C_z(\mathbf{h}) = c_0 \exp\left(-\frac{h^2}{a_0^2}\right)$$

Of note, the term “Gaussian” is used in two ways in this description. For a set of locations  $s_1, s_2, \dots, s_n$ , the random vector

$$\mathbf{Z}(s) = \begin{bmatrix} Z(s_1) \\ Z(s_2) \\ \vdots \\ Z(s_n) \end{bmatrix}$$

has a multivariate Gaussian or normal distribution  $N_n(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ . The  $(i,j)$  element of  $\boldsymbol{\Sigma}$  is computed by  $C_z(s_i - s_j)$ , which happens to be a Gaussian functional form.

Any functional form for  $C_z(\mathbf{h})$  that yields a valid covariance matrix  $\Sigma$  can be used. Both the functional form of  $C_z(\mathbf{h})$  and the parameter values

$$\mu = 40.1173$$

$$c_0 = 7.4599$$

$$a_0 = 30.1111$$

are estimated by using PROC VARIOGRAM in section “[Theoretical Semivariogram Model Fitting](#)” on page 8571 in the VARIOGRAM procedure. Specifically, the expected value  $\mu$  is reported in the VARIOGRAM procedure OUTV output data set, and the parameters  $c_0$  and  $a_0$  are estimates derived from a weighted least squares fit.

The choice of a Gaussian functional form for  $C_z(\mathbf{h})$  is simply based on the data, and it is not at all crucial to the simulation. However, it *is* crucial to the simulation method used in PROC SIM2D that  $Z(s)$  be a Gaussian SRF. For details, see the section “[Computational and Theoretical Details of Spatial Simulation](#)” on page 7408.

## Investigating Variability by Simulation

The variability of  $Z(s)$ , as modeled by

$$Z(s) = \mu + \varepsilon(s)$$

with the Gaussian covariance structure  $C_z(\mathbf{h})$  found previously, is not obvious from the covariance model form and parameters. The variation around the mean of the surface is relatively small, making it difficult visually to pick up differences in surface plots of simulated realizations.

Instead, you can compute the mean for each location on a grid from a series of realizations in a simulation. Then, the standard deviation of all the simulated values at each grid location provides you with a measure of the variability of  $Z(s)$  for the given covariance structure. You can also investigate variations at selected grid points in more detail, as shown in the “[Example 85.2: Variability at Selected Locations](#)” on page 7419.

The present example shows how to use ODS Graphics with PROC SIM2D to investigate the mean and standard deviation of simulated values. You use the thick data set which is available from the SasHELP library. In the data set, the Thick variable represents simulated observations of coal seam thickness. For your goal, you produce 5,000 realizations of a simulation with PROC SIM2D, where you specify the Gaussian model with the parameters found previously. You want the simulated data to pass through the simulated values, so first you define the data with the following data step:

```

title 'Using PROC SIM2D for Spatial Simulation';

data thick;
 input East North Thick @@;
 label Thick='Coal Seam Thickness';
 datalines;
 0.7 59.6 34.1 2.1 82.7 42.2 4.7 75.1 39.5
 4.8 52.8 34.3 5.9 67.1 37.0 6.0 35.7 35.9
 6.4 33.7 36.4 7.0 46.7 34.6 8.2 40.1 35.4
 13.3 0.6 44.7 13.3 68.2 37.8 13.4 31.3 37.8
 17.8 6.9 43.9 20.1 66.3 37.7 22.7 87.6 42.8
 23.0 93.9 43.6 24.3 73.0 39.3 24.8 15.1 42.3
 24.8 26.3 39.7 26.4 58.0 36.9 26.9 65.0 37.8
 27.7 83.3 41.8 27.9 90.8 43.3 29.1 47.9 36.7
 29.5 89.4 43.0 30.1 6.1 43.6 30.8 12.1 42.8
 32.7 40.2 37.5 34.8 8.1 43.3 35.3 32.0 38.8
 37.0 70.3 39.2 38.2 77.9 40.7 38.9 23.3 40.5
 39.4 82.5 41.4 43.0 4.7 43.3 43.7 7.6 43.1
 46.4 84.1 41.5 46.7 10.6 42.6 49.9 22.1 40.7
 51.0 88.8 42.0 52.8 68.9 39.3 52.9 32.7 39.2
 55.5 92.9 42.2 56.0 1.6 42.7 60.6 75.2 40.1
 62.1 26.6 40.1 63.0 12.7 41.8 69.0 75.6 40.1
 70.5 83.7 40.9 70.9 11.0 41.7 71.5 29.5 39.8
 78.1 45.5 38.7 78.2 9.1 41.7 78.4 20.0 40.8
 80.5 55.9 38.7 81.1 51.0 38.6 83.8 7.9 41.6
 84.5 11.0 41.5 85.2 67.3 39.4 85.5 73.0 39.8
 86.7 70.4 39.6 87.2 55.7 38.8 88.1 0.0 41.6
 88.4 12.1 41.3 88.4 99.6 41.2 88.8 82.9 40.5
 88.9 6.2 41.5 90.6 7.0 41.5 90.7 49.6 38.9
 91.5 55.4 39.0 92.9 46.8 39.1 93.4 70.9 39.7
 55.8 50.5 38.1 96.2 84.3 40.3 98.2 58.2 39.5
 ;

```

Since this is a conditional simulation, you can specify the **OBSERV** option in the **PLOTS** option in PROC SIM2D to see the locations and values of the measured points in the area where you want to perform spatial simulations.

Furthermore, the **SIM** suboption in the **PLOTS** option specifies that you want to create a plot that shows the means of the simulated values across the region. The **SIM** suboption with no other arguments produces a plot that shows the contours of the simulated means in the foreground and the gradient of the simulated standard deviations in the background.

You obtain these PROC SIM2D results at the nodes of an output grid that you specify according to your application needs. In the present analysis, a convenient area that encompasses all the Thick data points is a square with a side length of 100,000 feet. You define a regular grid for your simulation in this area. Assume a distance of 2,500 feet between grid nodes in both directions for a smooth contour plot. Based on this choice, your square grid has 41 nodes on each side. This means that PROC SIM2D computes the simulated values at a total of 1,681 grid points. You use the **GRID** statement of the PROC SIM2D to specify this grid.

The **SIMULATE** statement specifies the parameters of your simulation across the output grid. In particular, the **VAR=** option specifies the conditional simulation variable. The number of realizations in the simulation is specified with the **NUMREAL=** option. The **SEED=** option specifies the seed for the simulation random number generator.

The spatial correlation model for the simulation is also specified in the **SIMULATE** statement. You specify the model type by using the **FORM=** option. The options **SCALE=** and **RANGE=** specify the covariance structure sill  $c_0$  and range  $a_0$  parameters, respectively, as discussed in the previous section.

Although it is not included in the original spatial structure, note that a minimal nugget effect is specified with the **NUGGET=** option to avoid singularity issues. Singularity can appear in the present example as a result of the combined use of the Gaussian covariance model and relatively short distances between nodes, data, or nodes and data in the simulation area.

These steps are implemented using the following **DATA** step and statements:

```
ods graphics on;

proc sim2d data=thick outsim=sim plot=(observ sim);
 coordinates xc=East yc=North;
 simulate var=Thick numreal=5000 seed=79931
 scale=7.4599 range=30.1111 nugget=1e-8 form=gauss;
 mean 40.1173;
 grid x=0 to 100 by 2.5 y=0 to 100 by 2.5;
run;
```

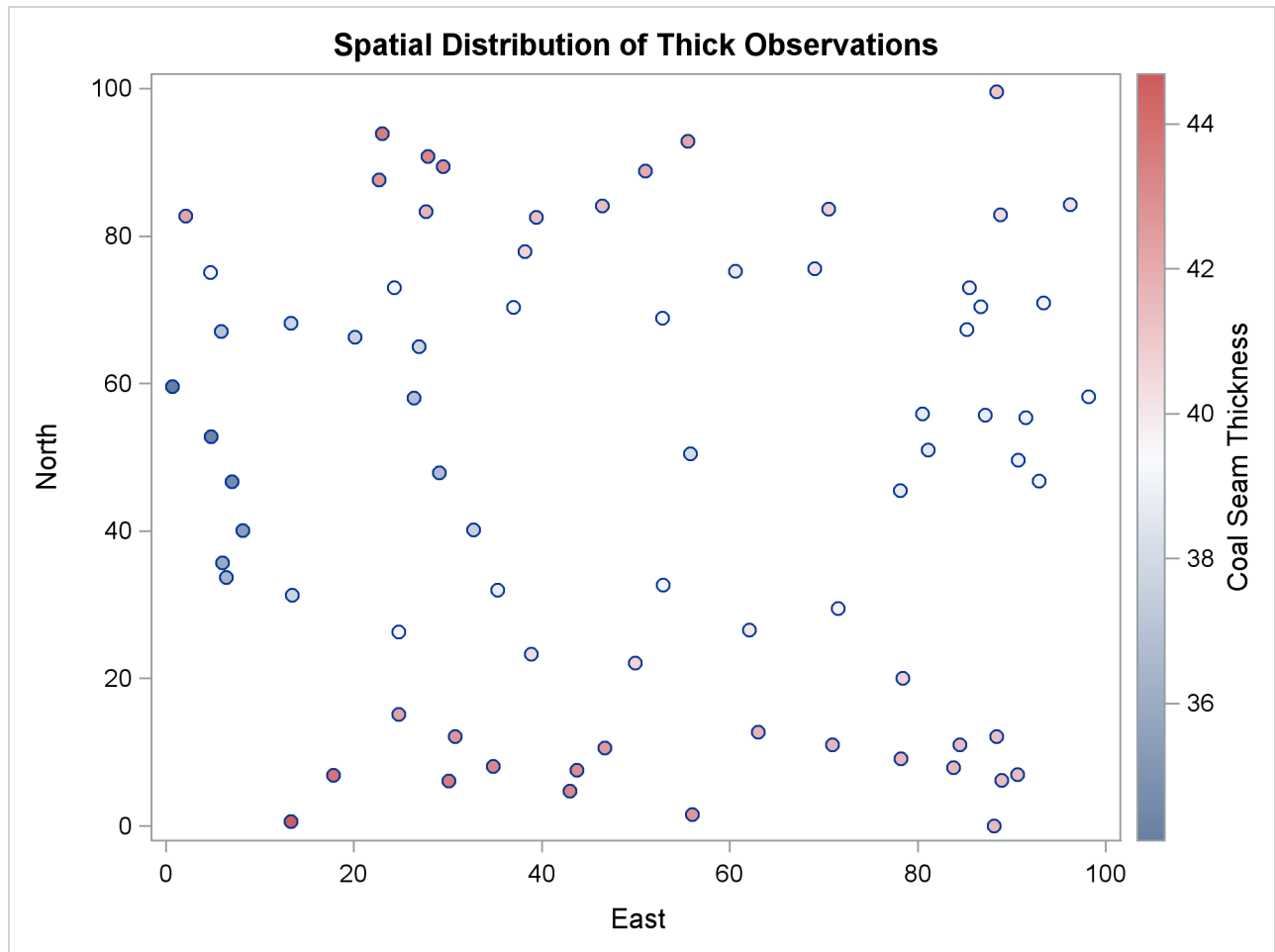
The table in [Figure 85.1](#) shows the number of observations read and used in the conditional simulation. This table can provide you with useful information in case you have missing values in the input data.

**Figure 85.1** Number of Observations for the thick Data Set

| Using PROC SIM2D for Spatial Simulation     |    |
|---------------------------------------------|----|
| The SIM2D Procedure                         |    |
| Simulation: SIM1, Dependent Variable: Thick |    |
| Number of Observations Read                 | 75 |
| Number of Observations Used                 | 75 |

The sample locations are then plotted in [Figure 85.2](#). The figure clearly shows some small-scale variation that is typical of spatial data.

**Figure 85.2** Scatter Plot of the Observations Spatial Distribution



PROC SIM2D also produces the table shown in Figure 85.3, which contains information about the type of simulation you run and the number of realizations requested.

**Figure 85.3** Simulation Analysis Information

| Simulation Information |             |
|------------------------|-------------|
| Simulation Grid Points | 1681        |
| Type                   | Conditional |
| Number of Realizations | 5000        |

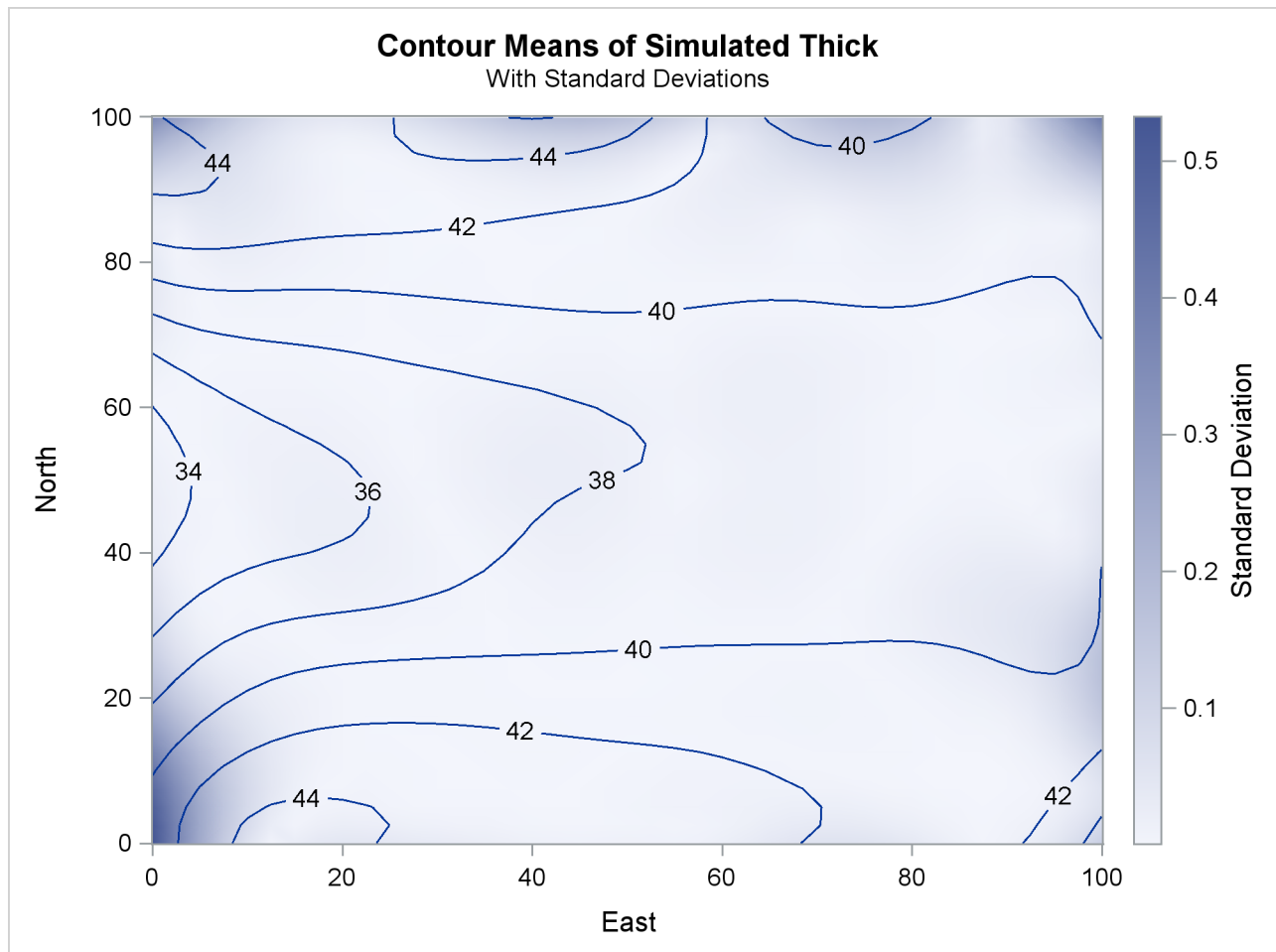
The table in Figure 85.4 displays the spatial correlation model information that is used by PROC SIM2D for the current simulation. If applicable, the table also provides the effective range. This is the distance  $r_\epsilon$  at which the covariance is 5% of its value at zero. Here you specified the Gaussian model, for which the effective range  $r_\epsilon$  is  $\sqrt{3}a_0$ .



**Figure 85.4** Simulation Covariance Model Information

| Covariance Model Information |           |
|------------------------------|-----------|
| Type                         | Gaussian  |
| Sill                         | 7.4599    |
| Range                        | 30.1111   |
| Effective Range              | 52.153955 |
| Nugget Effect                | 1E-8      |

Eventually, the SIM2D procedure produces the requested simulation plot shown in Figure 85.5. The contours of the mean of the simulated values show the average of the simulated realizations at each grid node; the average is based on the given spatial structure characteristics. In this case, these means are also conditioned by the Thick observations across the region.

**Figure 85.5** Contour Plot of Conditionally Simulated Coal Seam Thickness

Observe also the gradient that shows the standard deviation of the simulated values at each grid node. This gradient appears to be generally small throughout the region. A few exceptions are evident close to the region borders. In these areas the simulated realizations depend on a limited amount of neighboring data. The simulation at these locations relies mainly on the underlying spatial structure.

In addition to the simulation analysis, you can use the PROC SIM2D output to obtain statistical information about the simulated values at selected locations. Assume that you would like some basic statistics for the extreme southwest point at (East=0, North=0) and the point (East=75, North=75) toward the northeast corner of the region. You use the following DATA step to select the realizations for these points from the OUTSIM= output data set:

```
data selected;
 set sim(where=((gxc=0 and gyc=0) or (gxc=75 and gyc=75)));
 label gxc = "X-coord";
 label gyc = "Y-coord";
run;
```

Then, you use PROC SORT to sort the selected data set entries and PROC MEANS to produce the simulation statistics for the selected points. The following statements yield the mean, standard deviation, and maximum values of the 5,000 realizations of the Thick values at each one of the selected locations:

```
proc sort data=selected;
 by gxc gyc;
run;
proc means data=selected Mean Std Max;
 class gxc gyc;
 ways 2;
 where ((gxc = 0) & (gyc = 0)
 | ((gxc = 75) & (gyc = 75)));
 var SValue;
run;

ods graphics off;
```

The requested statistics for the grid points (East=0, North=0) and (East=75, North=75) are shown in [Figure 85.6](#).

**Figure 85.6** Simulation Statistics at Grid Points (East=0, North=0) and (East=75, North=75)

| Using PROC SIM2D for Spatial Simulation                  |         |       |            |           |            |  |
|----------------------------------------------------------|---------|-------|------------|-----------|------------|--|
| The MEANS Procedure                                      |         |       |            |           |            |  |
| Analysis Variable : SVALUE Simulated Value at Grid Point |         |       |            |           |            |  |
| X-coord                                                  | Y-coord | N Obs | Mean       | Std Dev   | Maximum    |  |
| 0                                                        | 0       | 5000  | 40.6968472 | 0.5328597 | 42.6616357 |  |
| 75                                                       | 75      | 5000  | 40.1090845 | 0.0024556 | 40.1197239 |  |

“[Example 85.2: Variability at Selected Locations](#)” on page 7419 shows you how to perform a simulation at a set of selected locations rather than on a domain-wide grid, and how to obtain more detailed statistics from the simulation.

## Syntax: SIM2D Procedure

The following statements are available in the SIM2D procedure:

```

PROC SIM2D options ;
 BY variables ;
 COORDINATES coordinate-variables ;
 GRID grid-options ;
 ID variable ;
 RESTORE store-options ;
 SIMULATE simulate-options ;
 MEAN mean-options ;

```

The **SIMULATE** and **MEAN** statements are hierarchical; you can specify any number of **SIMULATE** statements, but you must specify at least one. If you specify a **MEAN** statement, it refers to the preceding **SIMULATE** statement. If you omit the **MEAN** statement, a zero-mean model is simulated.

You must specify a single **COORDINATES** statement to identify the  $x$  and  $y$  coordinate variables in the input data set when you perform a conditional simulation. You must also specify a single **GRID** statement to specify the grid information.

Table 85.1 outlines the options available in PROC SIM2D classified by function.

**Table 85.1** Options Available in the SIM2D Procedure

| Task                                                                | Statement   | Option  |
|---------------------------------------------------------------------|-------------|---------|
| <b>Data Set Options</b>                                             |             |         |
| Specify an input data set                                           | PROC SIM2D  | DATA=   |
| Specify a grid data set                                             | GRID        | GDATA=  |
| Specify labels for individual grid points or in 1-D                 | GRID        | LABEL   |
| Specify correlation model and parameters                            | SIMULATE    | MDATA=  |
| Write simulated values                                              | PROC SIM2D  | OUTSIM= |
| Specify plot display and options                                    | PROC SIM2D  | PLOTS   |
| Specify a quadratic form data set                                   | MEAN        | QDATA=  |
| Specify plot display and options                                    | PROC SIM2D  | PLOTS   |
| <b>Declaring the Role of Variables</b>                              |             |         |
| Specify variables to define analysis subgroups                      | BY          |         |
| Specify a variable with observation labels                          | ID          |         |
| Specify the conditioning variable                                   | SIMULATE    | VAR=    |
| Specify the $x$ and $y$ coordinate variables in the DATA= data set  | COORDINATES | XC= YC= |
| Specify the $x$ and $y$ coordinate variables in the GDATA= data set | GRID        | XC= YC= |
| Specify the constant coefficient variable in the QDATA= data set    | MEAN        | CONST=  |
| Specify the linear $x$ coefficient variable in the QDATA= data set  | MEAN        | CX=     |

Table 85.1 continued

| Task                                                                   | Statement | Option                       |
|------------------------------------------------------------------------|-----------|------------------------------|
| Specify the linear $y$ coefficient variable in the QDATA= data set     | MEAN      | CY=                          |
| Specify the quadratic $x$ coefficient variable in the QDATA= data set  | MEAN      | CXX=                         |
| Specify the quadratic $y$ coefficient variable in the QDATA= data set  | MEAN      | CYY=                         |
| Specify the quadratic $xy$ coefficient variable in the QDATA= data set | MEAN      | CXY=                         |
| <b>Controlling the Simulation</b>                                      |           |                              |
| Specify the number of grid points in one-dimensional cases             | GRID      | NPTS=                        |
| Specify the number of realizations                                     | SIMULATE  | NUMREAL=                     |
| Specify the seed value for the random generator                        | SIMULATE  | SEED=                        |
| <b>Controlling the Mean Quadratic Surface</b>                          |           |                              |
| Specify the CONST term                                                 | MEAN      | CONST=                       |
| Specify the linear $x$ term                                            | MEAN      | CX=                          |
| Specify the linear $y$ term                                            | MEAN      | CY=                          |
| Specify the quadratic $x$ term                                         | MEAN      | CXX=                         |
| Specify the quadratic $y$ term                                         | MEAN      | CYY=                         |
| Specify the quadratic cross term                                       | MEAN      | CXY=                         |
| <b>Controlling the Semivariogram Model</b>                             |           |                              |
| Specify an angle for an anisotropic model                              | SIMULATE  | ANGLE=                       |
| Specify nested angles                                                  | SIMULATE  | ANGLE= $(a_1, \dots, a_k)$   |
| Specify a functional form                                              | SIMULATE  | FORM=                        |
| Specify nested functional forms                                        | SIMULATE  | FORM= $(f_1, \dots, f_k)$    |
| Specify a nugget effect                                                | SIMULATE  | NUGGET=                      |
| Specify a range parameter                                              | SIMULATE  | RANGE=                       |
| Specify nested range parameters                                        | SIMULATE  | RANGE= $(r_1, \dots, r_k)$   |
| Specify a minor-major axis ratio for an anisotropic model              | SIMULATE  | RATIO=                       |
| Specify nested minor-major axis ratios                                 | SIMULATE  | RATIO= $(ra_1, \dots, ra_k)$ |
| Specify a scale parameter                                              | SIMULATE  | SCALE=                       |
| Specify nested scale parameters                                        | SIMULATE  | SCALE= $(s_1, \dots, s_k)$   |
| Specify item store with correlation information                        | RESTORE   | IN=                          |
| Specify model and parameters from an item store                        | SIMULATE  | STORESELECT                  |

## PROC SIM2D Statement

**PROC SIM2D** *options* ;

The PROC SIM2D statement invokes the SIM2D procedure. Table 85.2 summarizes the options available in the PROC SIM2D statement.

**Table 85.2** PROC SIM2D Statement Options

| Option   | Description                                              |
|----------|----------------------------------------------------------|
| DATA=    | Specifies an input data set                              |
| IDGLOBAL | Uses ascending observation numbers across BY groups      |
| IDNUM    | Uses the observation number for the observation labels   |
| NARROW   | Restricts the variables included in the OUTSIM= data set |
| NOPRINT  | Suppresses the normal display of results                 |
| OUTSIM=  | Writes simulated values to a SAS data set                |
| PLOTS    | Specifies plot display and options                       |

You can specify the following options with the PROC SIM2D statement.

### **DATA=SAS-data-set**

specifies a SAS data set that contains the  $x$  and  $y$  coordinate variables and the VAR= variables that are used in the SIMULATE statements. This data set is required if you specify the BY statement or the COORDINATES statement or if any of the SIMULATE statements are conditional—that is, if you specify the VAR= option in any of those. Otherwise, you do not need the DATA= option, and this option is ignored if you specify it.

### **IDGLOBAL**

specifies that ascending observation numbers be used across BY groups for the observation labels in the appropriate output data sets and the OBSERVATIONS plot, instead of resetting the observation number in the beginning of each BY group. The IDGLOBAL option is ignored if no BY variables are specified. Also, if you specify the ID statement, then the IDGLOBAL option is ignored unless you also specify the IDNUM option in the PROC SIM2D statement.

### **IDNUM**

specifies that the observation number be used for the observation labels in the appropriate output data sets and the OBSERVATIONS plot. The IDNUM option takes effect when you specify the ID statement; otherwise, it is ignored.

### **NARROW**

restricts the variables included in the OUTSIM= data set. When you specify the NARROW option, only four variables are included. This option is useful when a large number of simulations are produced. Including only four variables reduces the memory required for the OUTSIM= data set. For details about the variables that are excluded with the NARROW option, see the section “Output Data Set” on page 7411.

**NOPRINT**

suppresses the normal display of results. The NOPRINT option is useful when you want only to create one or more output data sets with the procedure. **NOTE:** This option temporarily disables the Output Delivery System (ODS); see the section “[ODS Graphics](#)” on page 7413 for more information.

**OUTSIM=SAS-data-set**

specifies a SAS data set in which to store the simulation values, iteration number, simulate statement label, variable name, and grid location. For details, see the section “[Output Data Set](#)” on page 7411.

**PLOTS** <(global-plot-option)> <= plot-request <(options)>>**PLOTS** <(global-plot-option)> <= (plot-request <(options)> <... plot-request <(options)>>>

controls the plots produced through ODS Graphics. When you specify only one plot request, you can omit the parentheses around the plot request. Here are some examples:

```
plots=none
plots=observ
plots=(observ(out1) sim)
plots=(sim(fill=mean line=sd obs=grad) sim(fill=sd))
```

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;

proc sim2d data=thick outsim=sim;
 coordinates xc=East yc=North;
 simulate var=Thick numreal=5000 seed=79931
 scale=7.4599 range=30.1111 form=gauss;
 mean 40.1173;
 grid x=0 to 100 by 2.5 y=0 to 100 by 2.5;
run;

ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS](#).”

By default, no graphs are created; you must specify the PLOTS= option to make graphs.

The following *global-plot-option* is available:

**ONLY**

produces only plots that are specifically requested.

The following individual *plot-requests* and *plot options* are available:

**ALL**

produces all appropriate plots. You can specify other *options* with ALL. For example, to request all appropriate plots and an additional simulation plot, specify PLOTS=(ALL SIM).

**EQUATE**

specifies that all appropriate plots be produced in a way in which the axes coordinates have equal size units.

**NONE**

suppresses all plots.

**OBSERVATIONS** < (*observations-plot-options*) >**OBSERV** < (*observations-plot-options*) >**OBS** < (*observations-plot-options*) >

produces the observed data plot in conditional simulations. Only one observations plot is created if you specify the OBSERVATIONS option more than once within a PLOTS option.

The OBSERVATIONS option has the following suboptions:

**GRADIENT**

specifies that observations be displayed as circles colored by the observed measurement.

**LABEL** < (*label-option*) >

labels the observations. The label is the ID variable if the ID statement is specified; otherwise, it is the observation number. The *label-option* can be one of the following:

**EQ=number**

specifies that labels show for any observation whose value is equal to the specified *number*.

**MAX=number**

specifies that labels show for observations with values smaller than or equal to the specified *number*.

**MIN=number**

specifies that labels show for observations with values equal to or greater than the specified *number*.

If you specify multiple instances of the OBSERVATIONS option and you specify the LABEL suboption in any of those, then the resulting observations plot displays the observations labels. If more than one *label-option* is specified in multiple LABEL suboptions, then the prevailing *label-option* in the resulting OBSERVATIONS plot emerges by adhering to the choosing order: MIN, MAX, EQ.

**OUTLINE**

specifies that observations be displayed as circles with a border but with a completely transparent fill.

**OUTLINEGRADIENT**

is the same as OBSERVATIONS(GRADIENT) except that a border is shown around each observation.

**SHOWMISSING**

specifies that observations with missing values be displayed in addition to the observations with nonmissing values. By default, missing values locations are not shown on the

plot. If you specify multiple instances of the OBSERVATIONS option and you specify the SHOWMISSING suboption in any of those, then the resulting observations plot displays the observations with missing values.

If you omit any of the GRADIENT, OUTLINE, and OUTLINEGRADIENT suboptions, the OUTLINEGRADIENT is the default suboption. If you specify multiple instances of the OBSERVATIONS option or multiple suboptions for OBSERVATIONS, then the resulting observations plot honors the last specified GRADIENT, OUTLINE, or OUTLINEGRADIENT suboption.

### **SIMULATION** < (*sim-plot-options*) >

#### **SIM** < (*sim-plot-options*) >

specifies that simulation plots be produced. You can specify the SIM option multiple times in the same PLOTS option to request instances of plots with the following *sim-plot-options*:

#### **ALPHA=number**

specifies a parameter to obtain the confidence level for constructing confidence limits based on the simulation standard deviation. The value of *number* must be between 0 and 1, and the confidence level is  $1 - \text{number}$ . The default is ALPHA=0.05; this corresponds to the confidence level of 95%. The ALPHA= suboption is used only for simulation plots in one dimension, and it is incompatible with the FILL and LINE suboptions.

#### **CLONLY**

specifies that only the confidence limits be shown in a simulation plot without the simulation mean. This suboption can be useful for identifying confidence limits when the simulation standard deviation is small at the simulation locations. CLONLY is used only for simulation band plots of simulations on a linear grid, and it is incompatible with the FILL and LINE suboptions.

#### **CONNP**

specifies that grid points that you provide as individual simulation locations be connected with a line on the area map. This suboption is ignored when you have a single grid point, a prediction grid in two dimensions, or when you also specify the NOMAP suboption. The CONNP suboption is incompatible with the FILL and LINE suboptions.

#### **FILL=NONE | MEAN | SD**

produces a surface plot for either the values of the means or the standard deviations. FILL=SD is the default. However, if you omit the FILL suboption the behavior depends on the LINE suboption as follows: If you specify LINE=NONE or entirely omit the LINE suboption, then the FILL suboption is set to its default value. If LINE=PRED or LINE=SE, then the FILL suboption is set to the same value as the LINE suboption.

#### **LINE=NONE | MEAN | SD**

produces a contour line plot for either the values of the means or the standard deviations. LINE=MEAN is the default. However, if you omit the LINE suboption the behavior depends on the FILL suboption as follows: If you specify FILL=NONE or entirely omit the FILL suboption, then the LINE suboption is set to its default value. If FILL=PRED or FILL=SE, then the LINE suboption is set to the same value as the FILL suboption.



**NOMAP**

specifies that the simulation plot be produced without a map of the domain where you have observations. The NOMAP suboption is used in the case of simulation in one dimension or at individual points. It is ignored in the case of unconditional simulation, and it is incompatible with the FILL and LINE suboptions.

**OBS=obs-options**

produces an overlaid scatter plot of the observations in addition to the specified contour plots. The following *obs-options* are available:

**GRAD**

specifies that observations be displayed as circles colored by the observed measurement. The same color gradient displays the means surface and the observations. The conditional simulation honors the observed values, so the means surface at the observation locations has the same color as the corresponding observations.

**LINEGRAD**

is the same as OBS=GRAD except that a border is shown around each observation. This option is useful for identifying the location of observations where the standard deviations are small, because at these points the color of the observations and the color of the surface are indistinguishable.

**NONE**

specifies that no observations be displayed.

**OUTL**

specifies that observations be displayed as circles with a border but with a completely transparent fill.

OBS=NONE is the default when you have a grid in two dimensions, and OBS=LINEGRAD is the default used in the area map when you specify a conditional simulation in one dimension.

**SHOWD**

specifies that the horizontal axis in scatter plots of linear simulation grids show the distance between grid points instead of the grid points' coordinates. When the area map is displayed, the simulation locations are also connected with a line. In all other grid configurations the SHOWD suboption is ignored, and it is incompatible with the FILL and LINE suboptions.

**SHOWP**

specifies that the grid points in band plots of linear simulation grids be shown as marks on the band plot. In all other grid configurations the SHOWP suboption is ignored, and it is incompatible with the FILL and LINE suboptions.

**TYPE=BAND | BOX**

requests a particular type of plot when you have a linear grid, regardless of the default SIM plot behavior in this case. The TYPE suboption is incompatible with the FILL and LINE suboptions.

If you specify multiple instances of the ALPHA, FILL, LINE, OBS, or TYPE suboptions in the same SIM option, then the resulting simulation plot honors the last value specified for any

of the suboptions. Any combination where you specify FILL=NONE and LINE=NONE is not available. When the simulation grid is in two dimensions, only the FILL, LINE, and OBS suboptions apply. If you specify incompatible suboptions in the same SIM plot, then the plot instance is skipped.

The SIM option produces a surface or contour line plot for grids in two dimensions and a band plot or box plot for grids in one dimension or individual points. In two dimensions the plot illustrates the means and standard deviations of the simulation realizations at each grid point. By default, when you specify a linear grid with fewer than 10 points, PROC SIM2D produces a SIM box plot that depicts the simulation distribution at each point. For 10 or more points in a linear grid, the SIM plot is a band plot of the simulation means and the confidence limits at the 95% confidence level. You can override the default behavior in linear grids with the TYPE suboption. Simulation at individual locations always produces a SIM box plot.

In cases of conditional simulation in one dimension or at individual points an area map is produced that shows the observations and the grid points. Band plots of linear grids display the grid points as a line on the map. When you specify individual simulation locations, the grid points are indicated with marks on the area map. The area map appears on the side of conditional simulation band plots or box plots, unless you specify the NOMAP suboption. You can also label individual grid points or the ends of linear grid segments with the LABEL option of the GRID statement.

#### **SEMIVARIOGRAM** <(semivar-plot-option)>

##### **SEMIVAR** <(semivar-plot-option)>

specifies that the semivariogram used for the simulation be produced. You can use the following *semivar-plot-option*:

##### **MAXD=number**

specifies a positive value for the upper limit of the semivariogram horizontal axis of distance. The SEMIVARIOGRAM plot extends by default to a distance that depends on the correlation model range. You can use the MAXD= option to adjust the default maximum distance value for the plot.

The SEMIVARIOGRAM option produces a plot for each correlation model that you specify for your simulation tasks. In an anisotropic case, the plot is not produced if you assign different anisotropy angles for different model components. The only exception is when you specify zonal components at right angles with the nonzonal model components. Also, the SEMIVARIOGRAM option is ignored for models that consist of purely zonal components.

## **BY Statement**

### **BY variables ;**

You can specify a BY statement with PROC SIM2D to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the SIM2D procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

In PROC SIM2D it makes sense to use the BY statement only in conditional simulations where observations are involved. In particular, using the BY statement assumes that you have specified an input data set with the DATA= option in the PROC SIM2D statement. In PROC SIM2D if you omit the VAR= option in the SIMULATE statement, then this is a request for unconditional simulation even if you have specified the DATA= option in the PROC SIM2D statement. Therefore, it is possible to specify the BY statement and request mixed types of simulations by specifying multiple SIMULATE statements in the same PROC SIM2D step.

A special case occurs when you omit the DATA= option in the PROC SIM2D statement, your unconditional simulation correlation model input comes from an item store in the RESTORE statement, and this store has its own BY groups. The SIM2D procedure exhibits then a BY-like behavior, even though you specified no BY statement. This behavior enables you to distinguish the simulation tasks that depend on models in the different store BY groups.

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

---

## COORDINATES Statement

**COORDINATES** *coordinate-variables* ;

The two options in the COORDINATES statement give the name of the variables in the DATA= data set that contains the values of the  $x$  and  $y$  coordinates of the conditioning data. You must specify the COORDINATES statement when you specify an input data set with the DATA= option in the PROC SIM2D statement.

Only one COORDINATES statement is allowed, and it is applied to all SIMULATE statements that have the VAR= specification. In other words, it is assumed that all the VAR= variables in all SIMULATE statements have the same  $x$  and  $y$  coordinates.

You can abbreviate the COORDINATES statement as COORD.

**XCOORD**=(*variable-name*)

**XC**=(*variable-name*)

gives the name of the variable that contains the  $x$  coordinate of the data in the DATA= data set.

**YCOORD**=(*variable-name*)

**YC=(variable-name)**

gives the name of the variable that contains the y coordinate of the data locations in the **DATA=** data set.

---

## GRID Statement

**GRID** *grid-options* </ option > ;

The GRID statement specifies the grid of spatial locations at which to perform the simulations. A single GRID statement is required and is applied to all **SIMULATE** statements. Specify the grid in one of the following three ways:

- Specify the *x* and *y* coordinates explicitly for a grid in two dimensions.
- Specify the **NPTS=** option in addition to the *x* and *y* coordinates to define a grid of individual points or in one dimension.
- Specify the coordinates by using a SAS data set for a grid of individual points or in one dimension.

The GRID statement has the following *grid-options*:

**NPTS=number**

**NPTS=ALL**

controls specification of a grid in one dimension or a grid of individual simulation locations.

When you specify the **NPTS=number** option and the coordinates of two points in the **GRIDDATA=** data set or in both the **X=** and **Y=** options, you request a linear simulation grid. Its direction is across the line defined by the specified points. The grid size is equal to the *number* of points that you specify in the **NPTS=** option, where *number*  $\geq 2$ .

When you specify the **NPTS=ALL** option and the coordinates for any number of points in the **GRIDDATA=** data set or in each of the **X=** and **Y=** options, the **SIM2D** procedure performs simulation only at the specified individual locations. Use the **NPTS=ALL** option to examine a set of individual points anywhere on the **XY** plane or to specify a custom grid in one dimension.

If the number of *x* coordinates and the number of *y* coordinates in the **X=** and **Y=** options, respectively, are different, then the **NPTS=** option is ignored; in that case, a two-dimensional grid is used according to the specified **X=** and **Y=** options.

If you specify a simulation grid with any number of points other than two in the **GRIDDATA=** data set, then the option **NPTS=ALL** has the same effect as omitting the **NPTS=** option.

**X=number**

**X= $x_1, \dots, x_m$**

**X= $x_1$  to  $x_m$**

**X= $x_1$  to  $x_m$  by  $\delta x$**

specifies the *x* coordinate of the grid locations.

**Y=number**

**Y=y<sub>1</sub>, . . . , y<sub>m</sub>**

**Y=y<sub>1</sub> to y<sub>m</sub>**

**Y=y<sub>1</sub> to y<sub>m</sub> by  $\delta y$**

specifies the y coordinate of the grid locations.

Use the X= and Y= options of the GRID statement to specify a grid in one or two dimensions, or a grid of individual simulation locations.

For example, the following two GRID statements are equivalent:

```
GRID X=1, 2, 3, 4, 5 Y=0, 2, 4, 6, 8, 10;
```

```
GRID X=1 TO 5 Y=0 to 10 by 2;
```

In the following example, the first GRID statement produces a grid in two dimensions. The second statement produces simulation output only for the four individual points at the locations (1,0), (2,5), (3,7), and (4,10) on the XY plane.

```
GRID X=1 TO 4 Y=0, 5, 7, 10;
```

```
GRID X=1 TO 4 Y=0, 5, 7, 10 NPTS=ALL;
```

In the next example, the first GRID statement specifies a 2-by-2 grid in two dimensions. The second GRID statement specifies a linear grid of eight points. The grid is in the direction of the line defined by the specified points (2,8) and (3,5) on the XY plane and it extends between these two points.

```
GRID X=2, 3 Y=8, 5;
```

```
GRID x=2, 3 Y=8, 5 NPTS=8;
```

The last example shows a GRID statement that specifies a linear grid made of seven points across the Y axis. In this case, the syntax is sufficient to fully define a linear grid without the NPTS= option.

```
GRID X=5 Y=3 TO 9;
```

To specify grid locations from a SAS data set, you must provide the name of the data set and the variables that contain the values of the x and y coordinates.

**GRIDDATA=SAS-data-set**

**GDATA=SAS-data-set**

specifies a SAS data set that contains the x and y grid coordinates. Use the GRIDDATA= option of the GRID statement to specify a grid in one dimension or a grid of individual simulation locations.

**XCOORD**=(*variable-name*)

**XC**=(*variable-name*)

gives the name of the variable that contains the *x* coordinate of the grid locations in the **GRIDDATA**= data set.

**YCOORD**=(*variable-name*)

**YC**=(*variable-name*)

gives the name of the variable that contains the *y* coordinate of the grid locations in the **GRIDDATA**= data set.

You can specify the following option in the **GRID** statement after a slash (/):

**LABEL** <(suboption)> = (*character-list*)

specifies labels to tag grid points in simulation plots when you use grids in one dimension. You can specify one or more such labels as quoted strings in the *character-list*.

When the number of labels in the *character-list* exceeds the number of points in your grid, the labels in the list are used sequentially and any labels in excess are ignored. When the number of labels in the *character-list* is smaller than the number of points in your grid, the behavior is as follows:

- If an area map is included in the simulation plot, then blank labels are assigned to the remaining nonlabeled grid points on the map.
- For the simulation band and box plots, the coordinates of nonlabeled grid points are automatically assigned as their labels.

If the grid points are collinear and the horizontal axis displays distance, then two labels appear by default in the simulation plot. These are assigned to the first and the last points of the grid to help identify the ends of the linear grid segment on the plot map. This label pair is shown only when the plot includes an area map. Specifically, the two labels appear when you request simulation band plots, or simulation box plots for which you specify the **SIM(SHOWD)** suboption, if applicable. The two labels do not appear if you specify explicitly the **NOMAP** suboption in the **PLOTS=SIM** option.

The two labels have default values, unless you choose to specify your own labels with the **LABEL**= option. If you specify more than two labels in the *character-list* under these conditions, then only the first and last labels in the list are used; any additional labels in between are ignored.

The **LABEL**= option has the following *suboption*:

#### **ALL**

specifies that all individual points in the grid are assigned sequentially the labels you specify in the **LABEL(ALL)**= option when the **SIM(SHOWD)** suboption is applicable and specified in a simulation box plot. In all other cases, the **ALL** suboption is ignored.

The **ALL** suboption enables you to override the default behavior when the **SIM(SHOWD)** suboption is specified (the default behavior is to display labels only for the first and last grid points). As a result, you can use the **ALL** suboption to label grid grid points in both conditional and unconditional simulation tasks regardless of whether you specify the **NOMAP** suboption in the **PLOTS=SIM** option.

The **LABEL**= option is ignored when you produce simulation plots of grids in two dimensions.

---

## ID Statement

**ID** *variable* ;

The ID statement specifies which variable to include for identification of the observations in the labels and tool tips of the **OBSERVATIONS** plot and the tool tips of the **SIM** plot. The ID statement has an effect only when you perform conditional simulation.

In the SIM2D procedure you can specify only one ID variable in the ID statement. If no ID statement is given, then PROC SIM2D uses the observation number in the plots.

---

## RESTORE Statement

**RESTORE IN=***store-name* </ *option*> ;

The RESTORE statement specifies an item store that provides spatial correlation model input for the PROC SIM2D simulation tasks. An item store is a binary file defined by the SAS System. You cannot modify the contents of an item store. The SIM2D procedure can use only item stores created by PROC VARIOGRAM.

Item stores enable you to use saved correlation models without having to repeat specification of these models in the **SIMULATE** statement. In principle, an item store contains the chosen model from a model fitting process in PROC VARIOGRAM. If more than one model form is fitted, then all successful fits are included in the item store. In this case, you can choose any of the available models to use for simulation with the **STORESELECT(MODEL=)** option in the **SIMULATE** statement. Successfully fitted models might include questionable fits, which are so flagged when you specify the **INFO** option to display model names.

The *store-name* is a usual one- or two-level SAS name, as for SAS data sets. If you specify a one-level name, then the item store resides in the WORK library and is deleted at the end of the SAS session. Since item stores are often used for postprocessing tasks, typical usage specifies a two-level name of the form *libname.membername*.

When you specify the RESTORE statement, the default output contains some general information about the input item store. This information includes the store name, label (if assigned), the data set that was used to create the store, BY group information, the procedure that created the store, and the creation date.

You can specify the following option in the RESTORE statement after a slash (/):

**INFO** <( *info-options* )>

specifies that additional information about the input item store be printed. This information is provided in two ODS tables. One table displays the variables in the item store, in addition to the mean and standard deviation for each of them. These statistics are based on the observations that were used to produce the store results. The second table shows the model on top of the list of all fitted models for each direction angle in the item store. The INFO option has the following *info-options*:

### DETAILS

#### DET

specifies that more detailed information be displayed about the input item store. This option produces the full list of models for each direction angle in the item store, in addition to the model equivalence class. For more information about classes of equivalence, see the section

“Classes of Equivalence” on page 8634 in the VARIOGRAM procedure. The DETAILS option is ignored if the input item store contains information about a single fitted model.

### ONLY

specifies that only information about the input item store without any simulation tasks be displayed.

Each variable in an item store has a mean value that is passed to PROC SIM2D and used in simulations. If the mean in the item store is a missing value, then a zero mean is used by default. Specify the “MEAN Statement” on page 7406MEAN statement to override the mean information in the item store. For example, if you want to use only the correlation model in the item store and exclude the accompanying mean, then explicitly specify a zero mean in the “MEAN Statement” on page 7406MEAN statement.

When you specify an input item store with the RESTORE statement in PROC SIM2D, all the DATA= input data set variables must match input item store variables. If there are BY groups in the input DATA= set or in the input RESTORE variables, then PROC SIM2D handles the different cases as follows:

- If both PROC SIM2D has BY groups and the RESTORE statement has BY groups, then the analysis variables must match. This matching assumes implicitly that in each BY group of PROC SIM2D and the item store, the corresponding set of observations and correlation model comes from the same random field. This assumption is valid if you use the same data set, first in PROC VARIOGRAM to fit a model and save it in the item store, and then in PROC SIM2D to run simulations with the resulting correlation models.
- If PROC SIM2D has BY groups but the item store does not, then the item store is accepted only if the procedure and the item store analysis variables match. In this case, the same item store model choice iterates across the BY groups of the input data. You are advised to proceed with caution: each BY group in the input DATA= set corresponds to a different realization of a random field. Hence, by using the same correlation model for simulation purposes, you implicitly assume that all these different realizations are instances of the same random field.
- If PROC SIM2D has an input DATA= set and no BY groups but the item store has BY groups, then the item store is rejected
- If PROC SIM2D has no input DATA= set and the item store has BY groups, then PROC SIM2D runs unconditional simulations for the models in the store BY groups. See also the BY statement for more about the behavior in this case.

---

## SIMULATE Statement

**SIMULATE** *simulate-options* ;

The SIMULATE statement specifies details on the simulation and the covariance model used in the simulation. You can specify the following *simulate-options* with a SIMULATE statement, which can be abbreviated by SIM.

Table 85.3 summarizes the options available in the SIMULATE statement.



**Table 85.3** SIMULATE Statement Options

| Option                                | Description                                               |
|---------------------------------------|-----------------------------------------------------------|
| <b>Simulate-Options</b>               |                                                           |
| NUMREAL=                              | Specifies the number of realizations to produce           |
| VAR=                                  | Specifies the conditioning variable                       |
| <b>Covariance Model Specification</b> |                                                           |
| ANGLE=                                | Specifies the angle of the major axis                     |
| FORM=                                 | Specifies the functional form                             |
| MDATA=                                | Specifies the input data set containing parameter values  |
| NUGGET=                               | Specifies the nugget effect for the model                 |
| RANGE=                                | Specifies the range parameter                             |
| RATIO=                                | Specifies the ratio of the minor axis to the major axis   |
| SCALE=                                | Specifies the scale (or <i>sill</i> ) parameter           |
| SEED=                                 | Specifies the seed to use for the random number generator |
| SINGULAR=                             | Gives the singularity criterion                           |
| SMOOTH=                               | Specifies the smoothness parameter                        |
| STORESELECT                           | Uses information from an input item store for prediction  |

**NUMREAL=***number*

**NUMR=***number*

**NR=***number*

specifies the number of realizations to produce for the spatial process specified by the covariance model. As a result, the number of observations in the **OUTSIM=** data set contributed by a given **SIMULATE** statement is the product of the **NUMREAL=** value and the number of grid points. This can cause the **OUTSIM=** data set to become large even for moderate values of the **NUMREAL=** option.

**VAR=**(*variable-name*)

specifies the single numeric variable used as the conditioning variable in the simulation. In other words, the simulation is conditional on the values of the **VAR=** variable found in the **DATA=** data set. If you omit the **VAR=** option or if all observations of the **VAR=** variable are missing values, then the simulation is *unconditional*. Since multiple **SIMULATE** statements are allowed, you can perform both unconditional and conditional simulations with a single **PROC SIM2D** statement.

### Covariance Model Specification

You can specify a semivariogram or covariance model in three ways:

- You specify the required parameters **SCALE**, **RANGE**, **FORM**, and **SMOOTH** (if you specify the **MATERN** form), and possibly the optional parameters **NUGGET**, **ANGLE**, and **RATIO**, explicitly in the **SIMULATE** statement.
- You specify an **MDATA=** data set. This data set contains variables that correspond to the required parameters **SCALE**, **RANGE**, **FORM**, and **SMOOTH** (if you specify the **MATERN** form), and, optionally, variables for the **NUGGET**, **ANGLE**, and **RATIO** parameters.

- You can specify an input item store in the **RESTORE** statement. The item store contains one or more correlation models for one or more direction angles. You can specify these models in the **STORESELECT** option of the **SIMULATE** statement to run a simulation.

The three methods are mutually exclusive: you specify all parameters explicitly, they are all are read from the **MDATA=** data set, or you select a model and its parameters from an input item store. The following *simulate-options* are related to model specification:

**ANGLE=***angle*

**ANGLE=**(*angle1*, . . . , *anglek*)

specifies the angle of the major axis for anisotropic models, measured in degrees clockwise from the N–S axis. The default is **ANGLE=0**.

In the case of a nested semivariogram model with *k* nestings, you have the following two ways to specify the anisotropy major axis: you can specify only one *angle* which is then applied to all nested forms, or you can specify one angle for each of the *k* nestings.

**NOTE:** The syntax makes it possible to specify different angles for different forms of the nested model, but this practice is rarely used.

**FORM=***form*

**FORM=**(*form1*, . . . , *formk*)

specifies the functional form (type) of the semivariogram model. Use the syntax with the single *form* to specify a non-nested model. Use the syntax with forms *form<sub>i</sub>*, *i* = 1, . . . , *k*, to specify a nested model with *k* structures. Each of the forms can be any of the following:

**CUBIC | EXPONENTIAL | GAUSSIAN | MATERN |  
PENTASPHERICAL | SINEHOLEEFFECT | SPHERICAL**

**CUB | EXP | GAU | MAT | PEN | SHE | SPH**

specify the functional form (type).

For example, the syntax

**FORM=GAU**

specifies a model with a single Gaussian structure. Also, the syntax

**FORM= (EXP, SHE, MAT)**

specifies a nested model with an exponential, a sine hole effect, and a Matérn structure. Finally

**FORM= (EXP, EXP)**

specifies a nested model with two structures both of which are exponential.

**NOTE:** In the documentation, models are named either by using their full names or by using the first three letters of their structures. Also, the names of different structures in a nested model are separated by a hyphen (-). According to this convention, the previous examples illustrate how to specify a GAU, an EXP-SHE-MAT, and an EXP-EXP model, respectively, with the **FORM=** option.

All the supported model forms have two parameters specified by the **SCALE=** and **RANGE=** options, except for the MATERN model which has a third parameter specified by the **SMOOTH=** option. A **FORM=** value is required, unless you specify the **MDATA=** option or the **STORESELECT** option.

Computation of the MATERN covariance is numerically demanding. As a result, simulations that use Matérn covariance structures can be time-consuming.

#### **MDATA=SAS-data-set**

specifies the input data set that contains parameter values for the covariance or semivariogram model. The **MDATA=** option cannot be combined with any of the **FORM=** or **STORESELECT** options.

The **MDATA=** data set must contain variables named **SCALE**, **RANGE**, and **FORM**, and it can optionally contain variables **NUGGET**, **ANGLE**, and **RATIO**. If you specify the MATERN form, then you must also include a variable named **SMOOTH** in the **MDATA=** data set.

The **FORM** variable must be a character variable, and it can assume only the values allowed in the explicit **FORM=** syntax described previously. The **RANGE**, **SCALE** and **SMOOTH** variables must be numeric. The optional variables **ANGLE**, **RATIO**, and **NUGGET** must also be numeric if present.

The number of observations present in the **MDATA=** data set corresponds to the level of nesting of the covariance or semivariogram model. For example, to specify a non-nested model that uses a spherical covariance, an **MDATA=** data set might contain the following statements:

```
data mdl;
 input scale range form $;
 datalines;
 25 10 SPH
 ;
```

The PROC SIM2D statement to use the **MDATA=** specification is of the form shown in the following:

```
proc sim2d data=...;
 sim var=... mdata=mdl;
run;
```

This is equivalent to the following explicit specification of the covariance model parameters:

```
proc sim2d data=...;
 sim var=... scale=25 range=10 form=sph;
run;
```

The following **MDATA=** data set is an example of an anisotropic nested model:

```
data md2;
 input scale range form $ nugget angle ratio smooth;
 datalines;
 20 8 SPH 5 35 .7 .
 12 3 MAT 5 0 .8 2.8
 4 1 GAU 5 45 .5 .
 ;
```

```
proc sim2d data=...;
 sim var=.... mdata=md2;
run;
```

This is equivalent to the following explicit specification of the covariance model parameters:

```
proc sim2d data=...;
 sim var=.... scale=(20,12,4) range=(8,3,1) form=(SPH,MAT,GAU)
 angle=(35,0,45) ratio=(.7,.8,.5) nugget=5 smooth=2.8;
run;
```

This example is somewhat artificial in that it is usually hard to detect different anisotropy directions and ratios for different nestings by using an experimental semivariogram. **NOTE:** The NUGGET variable value is the same for all nestings. This is always the case; the nugget effect is a single additive term for all models. For further details, see the section “[The Nugget Effect](#)” on page 3830 in the KRIGE2D procedure.

The example also shows that if you specify a MATERN form in the nested model, then the SMOOTH variable must be specified for all nestings in the MDATA= data set. You simply specify the SMOOTH value as missing for nestings other than MATERN.

The **SIMULATE** statement can be given a label. This is useful for identification in the **OUTSIM=** data set when multiple **SIMULATE** statements are specified. For example:

```
proc sim2d data=...;
 gauss1: sim var=.... form=gau;
 mean;
 gauss2: sim var=.... form gau;
 mean;
 exp1: sim var=.... form=exp;
 mean;
 exp2: sim var=.... form=exp;
 mean;
run;
```

In the **OUTSIM=** data set, the values “GAUSS1,” “GAUSS2,” “EXP1,” and “EXP2” for the LABEL variable help to identify the realizations that correspond to the four **SIMULATE** statements. If you do not provide a label for a **SIMULATE** statement, a default label of SIM $n$  is given, where  $n$  is the number of unlabeled **SIMULATE** statements seen so far.

#### **NUGGET=***number*

specifies the nugget effect for the model. This effect is due to a discontinuity in the semivariogram as determined by plotting the sample semivariogram (see the section “[The Nugget Effect](#)” on page 3830 in the KRIGE2D procedure for details). For models without any nugget effect, the NUGGET= option is left out. The default is NUGGET=0.

#### **RANGE=***range*

#### **RANGE=**(*range1, ..., rangek*)

specifies the range parameter in the semivariogram models. In the case of a nested semivariogram model with  $k$  nestings, you must specify a range for each nesting.

The range parameter is the divisor in the exponent in all supported models. It has the units of distance or distance squared for these models, and it is related to the correlation scale for the underlying spatial process.

See the section “[Theoretical Semivariogram Models](#)” on page 3823 in the KRIGE2D procedure for details about how the RANGE= values are determined.

**RATIO=***ratio*

**RATIO=**(*ratio1*, . . . , *ratio**k*)

specifies the ratio of the length of the minor axis to the length of the major axis for anisotropic models. The value of the RATIO= option must be between 0 and 1. In the case of a nested semivariogram model with *k* nestings, you can specify a ratio for each nesting. The default is RATIO=1.

**SCALE=***scale*

**SCALE=**(*scale1*, . . . , *scale**k*)

specifies the scale (or *sill*) parameter in semivariogram models. In the case of a nested semivariogram model with *k* nestings, you must specify a scale for each nesting. The scale parameter is the multiplicative factor in all supported models; it has the same units as the variance of the VAR= variable.

See the section “[Theoretical Semivariogram Models](#)” on page 3823 in the KRIGE2D procedure for details about how the SCALE= values are determined.

**SEED=***seed-value*

specifies the seed to use for the random number generator. The SEED= option *seed-value* has to be an integer.

**SINGULAR=***number*

gives the singularity criterion for solving the set of linear equations involved in the computation of the mean and covariance of the conditional distribution associated with a given SIMULATE statement. The larger the value of the SINGULAR= option, the easier it is for the covariance matrix system to be declared singular. The default is SINGULAR=1E-8.

For more details about the use of the SINGULAR= option, see the section “[Computational and Theoretical Details of Spatial Simulation](#)” on page 7408.

**SMOOTH=***smooth*

**SMOOTH=**(*smooth1*, . . . , *smooth**m*)

specifies the smoothness parameter  $\nu > 0$  in the Matérn type of semivariance structures. The special case  $\nu = 0.5$  is equivalent to the exponential model, whereas  $\nu \rightarrow \infty$  gives the Gaussian model.

When you specify *m* different MATERN forms in the FORM= option, you must also provide *m* smoothness values in the SMOOTH option. If you must specify more than one smoothness value, the values are assigned sequentially to the MATERN nestings in the order the nestings are specified. If you specify more smoothness values than necessary, then values in excess are ignored.

**STORESELECT**(*sselect-options*)

**SSEL**(*sselect-options*)

specifies that information from an input item store be used for the prediction. You cannot combine the STORESELECT option with any of the FORM= or MDATA= options. The STORESELECT option has the following *sselect-options*:

**TYPE=***field-type*

specifies whether to perform isotropic or anisotropic simulation. You can choose the *field-type* from one of the following:

**ISO**

specifies isotropic field for the simulation.

**ANIGEO | GEO**

specifies a field with geometric anisotropy for the simulation.

**ANIZON**(*zonal-form1*, . . . , *zonal-formn*)**ZON**(*zonal-form1*, . . . , *zonal-formn*)

specifies a field with zonal anisotropy for the simulation. Each *zonal-formi*,  $i = 1, \dots, n$ , can be any of the following:

**CUB | EXP | GAU | MAT | PEN | SHE | SPH**

specify a form for the simulation.

Each *zonal-formi*,  $i = 1, \dots, n$ , is a structure in the purely zonal component of the correlation model in the direction angle of the minor anisotropy axis. For this reason, when you specify the TYPE=ANIZON suboption you must also specify the nonzonal component of the correlation model in the MODEL= suboption of the STORESELECT option. Assume the nonzonal component has  $k$  structures; these are common across all directions and each one has the same scale in all directions. In that sense, you use the TYPE=ANIZON suboption to specify only the  $n$  zonal anisotropy structures of an input store ( $k + n$ )-structure nested model in the direction angle of the minor anisotropy axis.

Given this specification,  $k + n$  must be up to the maximum number of nested model structures that is supported by the item store. See also the MODEL= suboption of the STORESELECT option.

In conclusion, you can use an input item store for prediction with zonal anisotropy if you know that every structure in the nonzonal model component has the same scale across all directions. When this condition does not apply for the item store models, specify the model parameters explicitly in the SIMULATE statement.

Computation of the MATERN covariance is numerically demanding. As a result, predictions that use Matérn covariance structures can be time-consuming.

If you omit the TYPE= option, the default behavior is TYPE=ISO when the input item store contains information for only one angle or for the omnidirectional case. If you specify an item store with information for more than one direction, then the default behavior is TYPE=ANIGEO.

When you specify TYPE=ISO to request isotropic analysis in the presence of an item store with information for multiple directions, you must specify the ANGLEID= suboption of the STORESELECT option with one argument. This argument specifies which of the direction angles information to use for the isotropic analysis.

When you indicate the presence of anisotropy with the TYPE=ANIGEO or TYPE=ANIZON suboptions of the STORESELECT option, the following conditions apply:

- You must specify the ANGLEID= suboption of the STORESELECT option to designate the major and minor anisotropy axes. See the ANGLEID= suboption of the STORESELECT option for details.

- – For TYPE=ANIGEO, ensure that you have the same scale in all anisotropy directions.
- For TYPE=ANIZON, ensure that the nonzonal component scale is the same in all anisotropy directions.

If you import a nested model, these rules also apply to each one of the nested structures.

- Model ranges in the major anisotropy axis must be longer than ranges in the minor anisotropy axis.
- Any Matérn covariance structure must maintain its smoothness parameter value in all anisotropy directions.

**ANGLEID=***angleid1*

**ANGLEID=**(*angleid1*, *angleid2*)

specifies which direction angles in the input item store be used for simulation. The angles are identified by the corresponding number in the AngleID column of the “Store Models Information” table, or by the AngleID parameter in the table title when you specify the **INFO(DETAILS)** option in the **RESTORE** statement.

If you request isotropic prediction in the **TYPE=** suboption of the **STORESELECT** option and the item store has omnidirectional contents or information about only one angle, then the **ANGLEID=** option is ignored. The simulation input comes from the omnidirectional information. In the case of a single angle, you still perform isotropic simulation and the model parameters are provided by the model in the single direction angle in the item store. However, if the item store contains information for more than one angle, then you must specify one angle ID in *angleid1*. The model information from the corresponding angle is then used in your isotropic simulation.

When you specify an anisotropic simulation in the **TYPE=** option of the **STORESELECT** option, you need to have information about two perpendicular direction angles. One of them is the major and the other is the minor anisotropy axis. You must always specify the major anisotropy axis angle ID in *angleid1* and the minor anisotropy axis angle ID in *angleid2*. This means that the range parameters of the model forms in the angle designated by the *angleid1* need to be larger than the corresponding ranges of the forms in the angle designated by the *angleid2*. Conveniently, if the item store has only two angles, then you only need to specify the ID *angleid1* of the major anisotropy axis angle. If the item store has only one angle, then you cannot perform anisotropic simulation with input from the item store.

**NOTE:** You can perform geometric anisotropic analysis even if the item store does not contain information about a direction that is perpendicular to the one specified by *angleid1*. This is possible due to the geometry of the ellipse. In particular, when you specify the major axis with *angleid1* and an angle ID for a second direction with a corresponding smaller range, then PROC SIM2D automatically computes the minor anisotropy axis range and the necessary range ratio parameter.

Anisotropic analysis is not possible when you specify instances of the same angle in the input item store. It is possible that PROC VARIOGRAM produces an item store where two or more directions can be the same if their corresponding correlation models were obtained for different angle tolerances or bandwidths in the VARIOGRAM procedure. Consequently, you cannot specify anisotropic simulation if the input store contains only two angles that are the same or if you specify *angleid1* and *angleid2* that correspond to equal angles.



**MODEL=***form*

**MODEL=**(*form1*, . . . , *formk*)

specifies the theoretical semivariogram model selection to use for the simulation. Use any combination of one, two, or three forms to describe a model in the input item store because up to three nested structures are supported. Each *form<sub>i</sub>*,  $i = 1, \dots, k$ , can be any of the following:

**CUB | EXP | GAU | MAT | PEN | SHE | SPH**

specify the selection model.

Computation of the MATERN covariance is numerically demanding. As a result, simulations that use Matérn covariance structures can be time-consuming.

All fitted models that are stored in the input item store contain information about their component parameters and also about the nugget effect if any. The SIM2D procedure retrieves this information when you make a model selection in the MODEL= option, and you do not need to individually specify a nugget effect or any other parameter of the model.

By default, the model that is ranked first among the models for a given angle in the item store is used for the simulation task. If more than one model is available in the item store, then you can specify the MODEL= option to use a different model for the simulation.

In an anisotropic simulation, the default selection is the model that is ranked first in the direction angle of the major anisotropy axis. If you specify the TYPE=ANIGEO option, then a model that consists of identical structures needs to be present in the selected minor anisotropy axis angle in the item store. If you specify the TYPE=ANIZON option, then a model with the exact same first  $k$  structures must be present in the selected minor anisotropy axis angle, and it must feature at least one more structure as a zonal component. The zonal component is specified separately in the TYPE=ANIZON suboption of the STORESELECT option. Consequently, remember that in zonal anisotropy the MODEL= suboption designates only the nonzonal component of the correlation model in the minor anisotropy axis direction. In all, if there are  $k$  common structures and  $n$  structures in the purely zonal component, then  $k + n$  must be up to the maximum number of nested model structures that is supported by the item store.

**SVAR=***store-var*

**SVAR=**(*store-varlist*)

specifies one *store-var* item store variable or a list *store-varlist* of variables that are present in the item store. This option selects one or more item store variables whose correlation models you want to use in the current simulation task.

If you are performing a conditional simulation, then PROC SIM2D searches the input item store for the variable that is specified in the VAR= option of the SIMULATE statement. Then, the procedure selects the appropriate correlation model for the task. In this case, if you specify the SVAR= option, it is ignored. However, when you request an unconditional simulation and specify input from an item store, then you must also use SVAR= to specify a source for your correlation model.

In comparison to the other two ways of specifying a correlation model in PROC SIM2D, the STORESELECT option is quite different because you can avoid explicit specification of all parameter values of a model. When you specify the STORESELECT option, then the corresponding scale, range, nugget effect, and smoothness (if appropriate) parameter values are invoked as saved attributes of the model that you select from the item store.



In the case of anisotropy, you specify the angles indirectly with the `ANGLEID=` option of the `STORESELECT` option, and the ratios are computed implicitly by using the selected model ranges. Explore how to specify valid anisotropical models imported from an input item store with the two examples that follow.

In the first example, assume the input item store `lnStoreGeo` contains exponential models in the angles  $\theta_1 = 0^\circ$ ,  $\theta_2 = 45^\circ$ , and  $\theta_3 = 90^\circ$ . You know in advance that all models have the same scale  $c_1 = c_2 = c_3$  across these directions and that the respective ranges are  $a_1 = 15$ ,  $a_2 = 20$ , and  $a_3 = 25$  in distance units. Hence, you have a case of geometric anisotropy where the major anisotropy axis is in the direction of angle  $\theta_3$  and the minor anisotropy axis is in the direction of angle  $\theta_1$ . The following statements in PROC SIM2D use the information in the item store `lnStoreGeo` to perform simulation under the assumption of geometric anisotropy:

```
proc sim2d data=...;
 restore in=lnStoreGeo;
 simulate storeselect(model=exp type=anigeo angleid=(3,1));
run;
```

For the second example, assume a case of zonal anisotropy. Consider the input item store `lnStoreZon`, which contains models in the two angles,  $\theta_1 = 30^\circ$  and  $\theta_2 = 120^\circ$ . Specifically, in  $\theta_1$  you have an exponential-spherical model: the exponential structure has scale  $c_{1E} = 3$  and range  $a_{1E} = 10$ ; the spherical structure has scale  $c_{1S} = 1$  and range  $a_{1S} = 6$ . In direction  $\theta_2$  you have an exponential model with scale  $c_{1E} = 3$  and range  $a_{1E} = 12$ . Hence, the zonal anisotropy major axis is in the direction of the lowest total variance, which is in angle  $\theta_2$ ; then, the minor axis is in the direction of angle  $\theta_1$ . The following statements in PROC SIM2D use the information in the store `lnStoreZon` to perform simulation under the assumption of zonal anisotropy:

```
proc sim2d data=...;
 restore in=lnStoreZon;
 simulate storeselect(model=exp type=anizon(sph) angleid=(2,1));
run;
```

---

## MEAN Statement

**MEAN** *spec1, ..., spec6* ;

**MEAN QDATA**=*SAS-data-set* **CONST**=*var1* **CX**=*var2* **CY**=*var3*  
**CXX**=*var4* **CYY**=*var5* **CXY**=*var6* ;

**MEAN QDATA**=*SAS-data-set* ;

A mean function  $\mu(s)$  that is a quadratic in the coordinates can be written as

$$\mu(s) = \mu(x, y) = \beta_0 + \beta_1 x + \beta_2 y + \beta_3 x^2 + \beta_4 y^2 + \beta_5 xy$$

The MEAN statement specifies the quadratic surface to use as the mean function for the simulated SRF. There are two ways to specify the MEAN statement. The MEAN statement allows the specification of the coefficients  $\beta_0, \dots, \beta_5$  either explicitly or through a QDATA= data set.

An example of an explicit specification is the following:

```
mean 1.4 + 2.5*x + 3.6*y + 0.47*x*x + 0.58*y*y + 0.69*x*y;
```

In this example, all terms have a nonzero coefficient. Any term with a zero coefficient is simply left out of the specification. For example,

```
mean 1.4;
```

is a valid quadratic form with all terms having zero coefficients except the constant term.

An equivalent way of specifying the mean function is through the QDATA= data set. For example, the MEAN statement

```
mean 1.4 + 2.5*x + 3.6*y + 0.47*x*x + 0.58*y*y + 0.69*x*y;
```

can be alternatively specified by the following DATA step and MEAN statement:

```
data q1;
 input c1 c2 c3 c4 c5 c6;
 datalines;
 1.4 2.5 3.6 0.47 0.58 0.69
 ;

proc sim2d data=...;
 simulate ...;
 mean qdata=q1 const=c1 cx=c2 cy=c3 cxx=c4 cyy=c5 cxy=c6;
run;
```

The QDATA= data set specifies the data set containing the coefficients. The parameters CONST=, CX=, CY=, CXX=, CYY=, and CYX= specify the variables in the QDATA= data set that correspond to the constant, linear x, linear y, and so on. For any coefficient not specified in this list, the QDATA= data set is checked for the presence of variables with default names of CONST, CX, CY, CXX, CYY, and CXY. If these variables are present, their values are taken as the corresponding coefficients. Hence, you can rewrite the previous example as follows:

```
data q1;
 input const cx cy cxx cyy cxy;
 datalines;
 1.4 2.5 3.6 0.47 0.58 0.69
 ;

proc sim2d data=...;
 simulate ...;
 mean qdata=q1;
run;
```

If a given coefficient does not appear in the list or in the data set with the default name, a value of zero is assumed.

If you run a simulation task with input from a [RESTORE](#) statement, then by default the simulation uses the mean of the item store variable in the simulation. You can override this default behavior if you explicitly specify the MEAN statement with a different mean function.

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## Details: SIM2D Procedure

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### Computational and Theoretical Details of Spatial Simulation

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#### Introduction

There are a number of approaches to simulating spatial random fields or, more generally, simulating sets of dependent random variables. These include sequential indicator methods, turning bands, and the Karhunen-Loeve expansion. See Christakos (1992, Chapter 8) and Deutsch and Journel (1992, Chapter V) for details.

A particularly simple method available for Gaussian spatial random fields is the LU decomposition method. This method is computationally efficient. For a given covariance matrix, the  $LU = \mathbf{LL}'$  decomposition is computed once, and the simulation proceeds by repeatedly generating a vector of independent  $N(0, 1)$  random variables and multiplying by the  $\mathbf{L}$  matrix.

One problem with this technique is memory requirements; memory is required to hold the full data and grid covariance matrix in core. While this is especially limiting in the three-dimensional case, you can use PROC SIM2D, which handles only two-dimensional data, for moderately sized simulation problems.

#### Theoretical Development

It is a simple matter to produce an  $N(0, 1)$  random number, and by stacking  $k$   $N(0, 1)$  random numbers in a column vector, you can obtain a vector with independent standard normal components  $\mathbf{W} \sim N_k(\mathbf{0}, \mathbf{I})$ . The meaning of the terms *independence* and *randomness* in the context of a deterministic algorithm required for the generation of these numbers is subtle; see Knuth (1981, Chapter 3) for details.

Rather than  $\mathbf{W} \sim N_k(\mathbf{0}, \mathbf{I})$ , what is required is the generation of a vector  $\mathbf{Z} \sim N_k(\mathbf{0}, \mathbf{C})$ —that is,

$$\mathbf{Z} = \begin{bmatrix} Z_1 \\ Z_2 \\ \vdots \\ Z_k \end{bmatrix}$$

with covariance matrix

$$\mathbf{C} = \begin{pmatrix} C_{11} & C_{12} & \cdots & C_{1k} \\ C_{21} & C_{22} & \cdots & C_{2k} \\ & \ddots & & \\ C_{k1} & C_{k2} & \cdots & C_{kk} \end{pmatrix}$$

If the covariance matrix is symmetric and positive definite, it has a Cholesky root  $\mathbf{L}$  such that  $\mathbf{C}$  can be factored as

$$\mathbf{C} = \mathbf{LL}'$$

where  $\mathbf{L}$  is lower triangular. See Ralston and Rabinowitz (1978, Chapter 9, Section 3-3) for details. This vector  $\mathbf{Z}$  can be generated by the transformation  $\mathbf{Z} = \mathbf{LW}$ . Here is where the assumption of a Gaussian SRF is crucial. When  $\mathbf{W} \sim N_k(\mathbf{0}, \mathbf{I})$ , then  $\mathbf{Z} = \mathbf{LW}$  is also Gaussian. The mean of  $\mathbf{Z}$  is

$$E(\mathbf{Z}) = \mathbf{L}(E(\mathbf{W})) = \mathbf{0}$$

and the variance is

$$\text{Var}(\mathbf{Z}) = \text{Var}(\mathbf{LW}) = E(\mathbf{LW}\mathbf{W}'\mathbf{L}') = \mathbf{L}E(\mathbf{W}\mathbf{W}')\mathbf{L}' = \mathbf{L}\mathbf{L}' = \mathbf{C}$$

Consider now an SRF  $Z(s), s \in D \subset \mathcal{R}^2$ , with spatial covariance function  $C(\mathbf{h})$ . Fix locations  $s_1, s_2, \dots, s_k$ , and let  $\mathbf{Z}$  denote the random vector

$$\mathbf{Z} = \begin{bmatrix} Z(s_1) \\ Z(s_2) \\ \vdots \\ Z(s_k) \end{bmatrix}$$

with corresponding covariance matrix

$$\mathbf{C}_Z = \begin{pmatrix} C(\mathbf{0}) & C(s_1 - s_2) & \cdots & C(s_1 - s_k) \\ C(s_2 - s_1) & C(\mathbf{0}) & \cdots & C(s_2 - s_k) \\ & & \ddots & \\ C(s_k - s_1) & C(s_k - s_2) & \cdots & C(\mathbf{0}) \end{pmatrix}$$

Since this covariance matrix is symmetric and positive definite, it has a Cholesky root, and the  $Z(s_i), i = 1, \dots, k$ , can be simulated as described previously. This is how the SIM2D procedure implements unconditional simulation in the zero-mean case. More generally,

$$Z(s) = \mu(s) + \varepsilon(s)$$

where  $\mu(s)$  is a quadratic form in the coordinates  $s = (x, y)$  and the  $\varepsilon(s)$  is an SRF that has the same covariance matrix  $\mathbf{C}_Z$  as previously. In this case, the  $\mu(s_i), i = 1, \dots, k$ , is computed once and added to the simulated vector  $\varepsilon(s_i), i = 1, \dots, k$ , for each realization.

For a conditional simulation, this distribution of

$$\mathbf{Z} = \begin{bmatrix} Z(s_1) \\ Z(s_2) \\ \vdots \\ Z(s_k) \end{bmatrix}$$

must be conditioned on the observed data. The relevant general result concerning conditional distributions of multivariate normal random variables is the following. Let  $\mathbf{X} \sim N_m(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ , where

$$\mathbf{X} = \begin{bmatrix} \mathbf{X}_1 \\ \mathbf{X}_2 \end{bmatrix}$$

$$\boldsymbol{\mu} = \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}$$

$$\boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\Sigma}_{11} & \boldsymbol{\Sigma}_{12} \\ \boldsymbol{\Sigma}_{21} & \boldsymbol{\Sigma}_{22} \end{pmatrix}$$

The subvector  $\mathbf{X}_1$  is  $k \times 1$ ,  $\mathbf{X}_2$  is  $n \times 1$ ,  $\boldsymbol{\Sigma}_{11}$  is  $k \times k$ ,  $\boldsymbol{\Sigma}_{22}$  is  $n \times n$ , and  $\boldsymbol{\Sigma}_{12} = \boldsymbol{\Sigma}'_{21}$  is  $k \times n$ , with  $k + n = m$ . The full vector  $\mathbf{X}$  is partitioned into two subvectors,  $\mathbf{X}_1$  and  $\mathbf{X}_2$ , and  $\boldsymbol{\Sigma}$  is similarly partitioned into covariances and cross covariances.

With this notation, the distribution of  $\mathbf{X}_1$  conditioned on  $\mathbf{X}_2 = \mathbf{x}_2$  is  $N_k(\tilde{\boldsymbol{\mu}}, \tilde{\boldsymbol{\Sigma}})$ , with

$$\tilde{\boldsymbol{\mu}} = \boldsymbol{\mu}_1 + \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}(\mathbf{x}_2 - \boldsymbol{\mu}_2)$$

and

$$\tilde{\boldsymbol{\Sigma}} = \boldsymbol{\Sigma}_{11} - \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}\boldsymbol{\Sigma}_{21}$$

See Searle (1971, pp. 46–47) for details. The correspondence with the conditional spatial simulation problem is as follows. Let the coordinates of the observed data points be denoted  $\tilde{s}_1, \tilde{s}_2, \dots, \tilde{s}_n$ , with values  $\tilde{z}_1, \tilde{z}_2, \dots, \tilde{z}_n$ . Let  $\tilde{\mathbf{Z}}$  denote the random vector

$$\tilde{\mathbf{Z}} = \begin{bmatrix} Z(\tilde{s}_1) \\ Z(\tilde{s}_2) \\ \vdots \\ Z(\tilde{s}_n) \end{bmatrix}$$

The random vector  $\tilde{\mathbf{Z}}$  corresponds to  $\mathbf{X}_2$ , while  $\mathbf{Z}$  corresponds to  $\mathbf{X}_1$ . Then  $(\mathbf{Z} \mid \tilde{\mathbf{Z}} = \tilde{\mathbf{z}}) \sim N_k(\tilde{\boldsymbol{\mu}}, \tilde{\mathbf{C}})$  as in the previous distribution. The matrix

$$\tilde{\mathbf{C}} = \mathbf{C}_{11} - \mathbf{C}_{12}\mathbf{C}_{22}^{-1}\mathbf{C}_{21}$$

is again positive definite, so a Cholesky factorization can be performed.

The dimension  $n$  for  $\tilde{\mathbf{Z}}$  is simply the number of nonmissing observations for the **VAR=** variable; the values  $\tilde{z}_1, \tilde{z}_2, \dots, \tilde{z}_n$  are the values of this variable. The coordinates  $\tilde{s}_1, \tilde{s}_2, \dots, \tilde{s}_n$  are also found in the **DATA=** data set, with the variables that correspond to the  $x$  and  $y$  coordinates identified in the **COORDINATES** statement. **NOTE:** All **VAR=** variables use the same set of conditioning coordinates; this fixes the matrix  $\mathbf{C}_{22}$  for all simulations.

The dimension  $k$  for  $\mathbf{Z}$  is the number of grid points specified in the **GRID** statement. Since there is a single **GRID** statement, this fixes the matrix  $\mathbf{C}_{11}$  for all simulations. Similarly,  $\mathbf{C}_{12}$  is fixed.

The Cholesky factorization  $\tilde{\mathbf{C}} = \mathbf{L}\mathbf{L}'$  is computed once, as is the mean correction

$$\tilde{\boldsymbol{\mu}} = \boldsymbol{\mu}_1 + \mathbf{C}_{12}\mathbf{C}_{22}^{-1}(\mathbf{x}_2 - \boldsymbol{\mu}_2)$$

The means  $\boldsymbol{\mu}_1$  and  $\boldsymbol{\mu}_2$  are computed using the grid coordinates  $s_1, s_2, \dots, s_k$ , the data coordinates  $\tilde{s}_1, \tilde{s}_2, \dots, \tilde{s}_n$ , and the quadratic form specification from the **MEAN** statement. The simulation is now performed exactly as in the unconditional case. A  $k \times 1$  vector of independent standard  $N(0, 1)$  random variables is generated and multiplied by  $\mathbf{L}$ , and  $\tilde{\boldsymbol{\mu}}$  is added to the transformed vector. This is repeated  $N$  times, where  $N$  is the value specified for the **NR=** option.

## Computational Details

In the computation of  $\tilde{\boldsymbol{\mu}}$  and  $\boldsymbol{\Sigma}$  described in the previous section, the inverse  $\boldsymbol{\Sigma}_{22}^{-1}$  is never actually computed; an equation of the form

$$\boldsymbol{\Sigma}_{22}\mathbf{A} = \mathbf{B}$$

is solved for  $\mathbf{A}$  by using a modified Gaussian elimination algorithm that takes advantage of the fact that  $\boldsymbol{\Sigma}_{22}$  is symmetric with constant diagonal  $C_z(0)$  that is larger than all off-diagonal elements. The **SINGULAR=** option pertains to this algorithm. The value specified for the **SINGULAR=** option is scaled by  $C_z(0)$  before comparison with the pivot element.

### Memory Usage

For conditional simulations, the largest matrix held in core memory at any one time depends on the number of grid points and data points. Using the previous notation, the data-data covariance matrix  $\mathbf{C}_{22}$  is  $n \times n$ , where  $n$  is the number of nonmissing observations for the **VAR=** variable in the **DATA=** data set. The grid-data cross covariance  $\mathbf{C}_{12}$  is  $n \times k$ , where  $k$  is the number of grid points. The grid-grid covariance  $\mathbf{C}_{11}$  is  $k \times k$ . The maximum memory required at any one time for storing these matrices is

$$\max(k(k + 1), n(n + 1) + 2(n \times k)) \times \text{sizeof}(\text{double})$$

There are additional memory requirements that add to the total memory usage, but usually these matrix calculations dominate, especially when the number of grid points is large.

---

## Output Data Set

The **SIM2D** procedure produces a single output data set: the **OUTSIM=SAS-data-set**. The **OUTSIM=** data set contains all the needed information to uniquely identify the simulated values.

The **OUTSIM=** data set contains the following variables:

- **LABEL**, which is the label for the current **SIMULATE** statement
- **VARNAME**, which is the name of the conditioning variable for the current **SIMULATE** statement
- **MODSVAR**, which is the name of the input item store variable associated with the current correlation model in an unconditional simulation

- `_ITER_`, which is the iteration number within the current `SIMULATE` statement
- `GXC`, which is the  $x$  coordinate for the current grid point
- `GYC`, which is the  $y$  coordinate for the current grid point
- `SVALUE`, which is the value of the simulated variable

If you specify the `NARROW` option in the `PROC SIM2D` statement, the `LABEL` and `VARNAME` variables are not included in the `OUTSIM=` data set. This option is useful in the case where the number of data points, grid points, and realizations are such that they generate a very large `OUTSIM=` data set. The size of the `OUTSIM=` data set is reduced when these variables are not included.

In unconditional simulation tasks where no input data set is specified, the `VARNAME` variable is excluded from the `OUTSIM=` data set. In unconditional simulation tasks where you have specified an input data set, the `VARNAME` variable is included but given a missing value. In the case of mixed conditional and unconditional simulations (that is, when multiple `SIMULATE` statements are specified, among which one or more contain a `VAR=` specification and one or more have no `VAR=` specification), the `VARNAME` variable is included but is given a missing value for those observations that correspond to an unconditional simulation.

The `MODSVAR` variable is included in the `OUTSIM=` data set only when you specify an input item store with the `RESTORE` statement, and it indicates the presence of that store. This variable helps you identify the output of different unconditional simulations when the model input comes from an item store; it is not suggesting that a simulation task is conditioned upon it.

Specifically, the `MODSVAR` variable has a missing value for conditional simulation tasks. The variable also has a missing value for unconditional simulations for which you specify a correlation model explicitly, either with the `FORM=` option or with the `MDATA=` data set in the `SIMULATE` statement. In all other cases, the `MODSVAR` variable indicates the input item store variable that is associated with the store model used for the current unconditional simulation task.

---

## Displayed Output

In addition to the output data set, the `SIM2D` procedure produces output objects as well. The `SIM2D` procedure output objects are the following:

- a default “Number of Observations” table that displays the number of observations read from the input data set and the number of observations used in the analysis.
- a map that shows the spatial distribution of the observations of the current `VAR` variable in the `SIMULATE` statement, in the case of conditional simulations. The observations are displayed by default with circled markers whose color indicates the `VAR` value at the corresponding location.
- a default table for each `SIMULATE` statement that summarizes the simulation specifications.
- a default table for each `SIMULATE` statement that shows the covariance model parameters for the corresponding simulation.
- plots of simulation outcome at each point of the specified output grid or at specified individual locations. You can produce more than one of these plots for every `SIMULATE` statement with styles that you can specify by using the available suboptions of the `PLOTS=SIM` option.

- a “Store Info” table with basic information about the input item store. This table is produced by default when you specify the **RESTORE** statement.
- a “Store Variables Information” table that describes the analysis variables of an input item store. The table is produced by default when you specify an item store with the **RESTORE** statement.
- a “Store Models Information” table with detailed information about the models and direction angles that are contained in an input item store. The table is produced by default when you specify an item store with the **RESTORE** statement.

---

## ODS Table Names

Each table created by PROC SIM2D has a name associated with it, and you must use this name to reference the table when using ODS Graphics. These names are listed in [Table 85.4](#).

**Table 85.4** ODS Tables Produced by PROC SIM2D

| ODS Table Name                 | Description                                                   | Statement | Option         |
|--------------------------------|---------------------------------------------------------------|-----------|----------------|
| <a href="#">ModelInfo</a>      | Parameters of the covariance model used in current simulation | PROC      | Default output |
| <a href="#">NObs</a>           | Number of observations read and used                          | PROC      | Default output |
| <a href="#">SimuInfo</a>       | General information about the simulation                      | PROC      | Default output |
| <a href="#">StoreInfo</a>      | Input item store identity information                         | RESTORE   | Default output |
| <a href="#">StoreModelInfo</a> | Input item store direction angles and models information      | RESTORE   | INFO           |
| <a href="#">StoreVarInfo</a>   | Input item store variables and their statistics               | RESTORE   | INFO           |

---

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “[Statistical Graphics Using ODS.](#)”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS.](#)”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “[A Primer on ODS Statistical Graphics](#)” on page 599 in Chapter 21, “[Statistical Graphics Using ODS.](#)”

For additional control of the graphics that are displayed, see the **PLOTS** option in the section “[PROC SIM2D Statement](#)” on page 7386.



## ODS Graph Names

PROC SIM2D assigns a name to each graph it creates by using ODS Graphics. You can use these names to reference the graphs when using ODS Graphics. You must also specify the PLOTS= option indicated in Table 85.5.

**Table 85.5** Graphs Produced by PROC SIM2D

| ODS Graph Name   | Plot Description                                                                                                                                                                                                                                                       | Statement | Option        |
|------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------|---------------|
| SimulationPlot   | Outlines of the observation locations, and either a contour plot of the simulated means and surface of the standard deviation in areal grids, or a band plot of the simulated means or box plot of the simulation distribution in linear grids or individual locations | PROC      | PLOTS=SIM     |
| ObservationsPlot | Scatter plot of observed data and colored markers indicating observed values                                                                                                                                                                                           | PROC      | PLOTS=OBSERV  |
| Semivariogram    | Plots of the semivariogram models used for all simulation tasks                                                                                                                                                                                                        | PROC      | PLOTS=SEMIVAR |

## Examples: SIM2D Procedure

### Example 85.1: Simulation and Economic Feasibility

You can use simulations to investigate the expected behavior of a stochastic process. Simulations with PROC SIM2D can indicate spatial characteristics in your study that might be important for decision making or general assessment. The present example and the one in section “[Example 85.3: Risk Analysis with Simulation](#)” on page 7423 are two instances of this type of analysis in different fields.

Continuing with the coal seam thickness example from the section “[Getting Started: SIM2D Procedure](#)” on page 7377, this example asks a rather complicated question of economic nature. For illustration, an (approximate) answer is provided, which requires the use of simulation.

### Simulating a Subregion for Economic Feasibility

The coal seam must be of a minimum thickness, called a *cutoff value*, for a mining operation to be profitable. Suppose that, for a subregion of the measured area, the cost of mining is higher than in the remaining areas due to the geology of the overburden. This higher cost results in a higher thickness cutoff value for the subregion. Suppose also that it is determined from a detailed cost analysis that at least 60% of the subregion must exceed a seam thickness of 39.7 feet for profitability.

How can you use the SRF model ( $\mu$  and  $C_z(s)$ ) and the measured seam thickness values  $Z(s_i), i = 1, \dots, 75$ , to determine, in some approximate way, whether at least 60% of the subregion exceeds this minimum?

Spatial prediction does not appear to be helpful in answering this question. Although it is easy to determine whether a predicted value at a location in the subregion is above the 39.7-foot cutoff value, it is not clear how to incorporate the standard error associated with the predicted value. The standard error is what characterizes the stochastic nature of the prediction (and the underlying SRF). It is clear that it must be included in any realistic approach to the problem.

A conditional simulation, on the other hand, seems to be a natural way of obtaining an approximate answer. By simulating the SRF on a sufficiently fine grid in the subregion, you can determine the proportion of grid points in which the mean value over realizations exceeds the 39.7-foot cutoff and compare it with the 60% value needed for profitability.

It is desirable in any simulation study that the quantity being estimated (in this case, the proportion that exceeds the 39.7-foot cutoff) not depend on the number of simulations performed. For example, suppose that the maximum seam thickness is simulated. It is likely that the maximum value increases as the number of simulations performed increases. Hence, a simulation is not useful for such an estimate. A simulation is useful for determining the *distribution* of the maximum, but there are general theoretical results for such distributions, making such a simulation unnecessary. See Leadbetter, Lindgren, and Rootzen (1983) for details.

In the case of simulating the proportion that exceeds the 39.7-foot cutoff, it is expected that this quantity will settle down to a fixed value as the number of realizations increases. At a fixed grid point, the quantity being compared with the cutoff value is the mean over all simulated realizations; this mean value settles down to a fixed number as the number of realizations increases. In the same manner, the proportion of the grid where the mean values exceed the cutoff also becomes constant. This can be tested using PROC SIM2D.

A crucial, nonprovable assumption in applying SRF theory to the coal seam thickness data is that the values  $Z(s_i), i = 1, \dots, 75$ , represent a *single* realization from the set of all possible realizations consistent with the SRF model ( $\mu$  and  $C_z(\mathbf{h})$ ). A conditional simulation repeatedly produces other possible simulated realizations consistent with the model and data. However, the only concern of the mining company is this single unique realization. It is not concerned about similar coal fields to be mined sometime in the future; it might never see another coal field remotely similar to this one, or it might not be in business in the future.

Hence the proportion found by generating repeated simulated realizations must somehow relate back to the unique realization that is the coal field (seam thickness). This is done by interpreting the proportion found from a simulation to the spatial mean proportion for the unique realization. The term “spatial mean” is simply an appropriate integral over the fixed (but unknown) spatial function  $z(\mathbf{s})$ . (The SRF is denoted  $Z(\mathbf{s})$ ; a particular realization, a deterministic function of the spatial coordinates, is denoted  $z(\mathbf{s})$ .)

This interpretation requires an ergodic assumption, which is also needed in the original estimation of  $C_z(\mathbf{s})$ . See Cressie (1993, pp. 53–58) for a discussion of ergodicity and Gaussian SRFs.

## Implementation Using PROC SIM2D

The subregion to be considered is the southeast corner of the field, which is a square region with a length of 40 distance units (in thousands of feet). First, you input the thickness data as the following DATA step shows:

```

title 'Simulating a Subregion for Economic Feasibility';

data thick;
 input East North Thick @@;
 label Thick='Coal Seam Thickness';

```

```

datalines;
 0.7 59.6 34.1 2.1 82.7 42.2 4.7 75.1 39.5
 4.8 52.8 34.3 5.9 67.1 37.0 6.0 35.7 35.9
 6.4 33.7 36.4 7.0 46.7 34.6 8.2 40.1 35.4
 13.3 0.6 44.7 13.3 68.2 37.8 13.4 31.3 37.8
 17.8 6.9 43.9 20.1 66.3 37.7 22.7 87.6 42.8
 23.0 93.9 43.6 24.3 73.0 39.3 24.8 15.1 42.3
 24.8 26.3 39.7 26.4 58.0 36.9 26.9 65.0 37.8
 27.7 83.3 41.8 27.9 90.8 43.3 29.1 47.9 36.7
 29.5 89.4 43.0 30.1 6.1 43.6 30.8 12.1 42.8
 32.7 40.2 37.5 34.8 8.1 43.3 35.3 32.0 38.8
 37.0 70.3 39.2 38.2 77.9 40.7 38.9 23.3 40.5
 39.4 82.5 41.4 43.0 4.7 43.3 43.7 7.6 43.1
 46.4 84.1 41.5 46.7 10.6 42.6 49.9 22.1 40.7
 51.0 88.8 42.0 52.8 68.9 39.3 52.9 32.7 39.2
 55.5 92.9 42.2 56.0 1.6 42.7 60.6 75.2 40.1
 62.1 26.6 40.1 63.0 12.7 41.8 69.0 75.6 40.1
 70.5 83.7 40.9 70.9 11.0 41.7 71.5 29.5 39.8
 78.1 45.5 38.7 78.2 9.1 41.7 78.4 20.0 40.8
 80.5 55.9 38.7 81.1 51.0 38.6 83.8 7.9 41.6
 84.5 11.0 41.5 85.2 67.3 39.4 85.5 73.0 39.8
 86.7 70.4 39.6 87.2 55.7 38.8 88.1 0.0 41.6
 88.4 12.1 41.3 88.4 99.6 41.2 88.8 82.9 40.5
 88.9 6.2 41.5 90.6 7.0 41.5 90.7 49.6 38.9
 91.5 55.4 39.0 92.9 46.8 39.1 93.4 70.9 39.7
 55.8 50.5 38.1 96.2 84.3 40.3 98.2 58.2 39.5
;

```

PROC SIM2D is run on the entire data set for conditioning, while the simulation grid covers only this subregion. It is convenient to be able to vary the seed, the grid increment, and the number of simulations performed. The following macro implements the computation of the percent area that exceeds the cutoff value by using the seed, the grid increment, and the number of simulated realizations as macro arguments.

Within the macro, the data set produced by PROC SIM2D is transposed with PROC TRANSPOSE so that each grid location is a separate variable. The MEANS procedure averages then the simulated value at each grid point over all realizations. It is this average that is compared to the cutoff value. The last DATA step does the comparison, uses an appropriate loop to determine the percent of the grid locations that exceed this cutoff value, and writes the results to the listing file in the form of a report. This sequence is implemented with the following statements:

```

/* Construct macro for conditional simulation -----*/
%let cc0=7.4599;
%let aa0=30.1111;
%let ngt=1e-8;
%let form=gauss;
%let cut=39.7;

%macro area_sim(seed=,nr=,ginc=);
 %let ngrid=%eval(40/&ginc+1);
 %let tgrid=%eval(&ngrid*&ngrid);

 proc sim2d data=thick outsim=sim1;
 coordinates xc=east yc=north;
 simulate var=thick numreal=&nr seed=&seed

```

```

 scale=&cc0 range=&aa0 nugget=&ngt form=&form;
 mean 40.1173;
 grid x=60 to 100 by &ginc
 y= 0 to 40 by &ginc;
run;

proc transpose data=sim1 out=sim2 prefix=sims;
 by _iter_;
 var svalue;
run;

proc means data=sim2 noprint n mean;
 var sims1-sims&tgrid;
 output out=msim n=numsim mean=ms1-ms&tgrid;
run;

data _null_;
 file print;
 array simss ms1-ms&tgrid;
 set msim;
 cflag=0;
 do ss=1 to &tgrid;
 tempv=simss[ss];
 if simss[ss] > &cut then do;
 cflag + 1;
 end;
 end;
 area_per=100*(cflag/&tgrid);
 put // +5 'Conditional Simulation of Coal Seam'
 ' Thickness for Subregion';
 put / +5 'Subregion is South-East Corner 40 by 40 distance units';
 put / +5 "Seed:&seed" +2 "Grid Increment:&ginc";
 put / +5 "Total Number of Grid Points:&tgrid" +2
 "Number of Simulations:&nr";
 put / +5 "Percent of Subregion Exceeding Cutoff of %left(&cut) ft.:"
 +2 area_per 5.2;
run;
%mend area_sim;

```

In the following statement, you invoke the macro three times. Each time, the macro is invoked with a different seed and combination of the grid increment and number of simulations. The macro is first invoked with a relatively coarse grid (grid increment of 10 distance units) and a small number of realizations (5). The output of this conditional simulation is shown in [Output 85.1.1](#).

```

/* Execute macro for coarse grid -----*/
%area_sim(seed=12345,nr=5,ginc=10);

```

**Output 85.1.1** Conditional Simulation of Coal Seam Thickness on a Coarse Grid

```

 Simulating a Subregion for Economic Feasibility

 Conditional Simulation of Coal Seam Thickness for Subregion

 Subregion is South-East Corner 40 by 40 distance units

 Seed:12345 Grid Increment:10

 Total Number of Grid Points:25 Number of Simulations:5

 Percent of Subregion Exceeding Cutoff of 39.7 ft.: 76.00

```

The next invocation, in the following statement, uses a finer grid and 50 realizations. The output of the second conditional simulation is shown in [Output 85.1.2](#).

```

/* Execute macro for fine grid and fewer simulations -----*/
%area_sim(seed=54321,nr=50,ginc=1);

```

**Output 85.1.2** Conditional Simulation of Coal Seam Thickness on a Fine Grid

```

 Simulating a Subregion for Economic Feasibility

 Conditional Simulation of Coal Seam Thickness for Subregion

 Subregion is South-East Corner 40 by 40 distance units

 Seed:54321 Grid Increment:1

 Total Number of Grid Points:1681 Number of Simulations:50

 Percent of Subregion Exceeding Cutoff of 39.7 ft.: 76.09

```

The final invocation, in the following statement, uses the same grid increment and 500 realizations. The output of this conditional simulation is shown in [Output 85.1.3](#).

```

/* Execute macro for fine grid and more simulations -----*/
%area_sim(seed=655311,nr=500,ginc=1);

```

**Output 85.1.3** Conditional Simulation of Coal Seam Thickness on a Fine Grid

```

Simulating a Subregion for Economic Feasibility

Conditional Simulation of Coal Seam Thickness for Subregion

Subregion is South-East Corner 40 by 40 distance units

Seed:655311 Grid Increment:1

Total Number of Grid Points:1681 Number of Simulations:500

Percent of Subregion Exceeding Cutoff of 39.7 ft.: 76.09

```

The results from the preceding simulations indicate that about 76% of the subregion exceeds the cutoff value.

**NOTE:** The number of grid points in the simulation increases with the square of the decrease in the grid increment, leading to long CPU processing times. Increasing the number of realizations results in a linear increase in processing times. Hence, using as coarse a grid as possible allows for more realizations and experimentation with different seeds.

---

## Example 85.2: Variability at Selected Locations

This example exhibits a more detailed investigation of the variation of simulated Thick variable values. You use the same thick data set from the section “Getting Started: SIM2D Procedure” on page 7377, and you are interested in the simulated values statistics at two selected grid points.

Specifically, you perform a simulation asking for 5,000 realizations (iterations) at two points of the region defined in the section “Preliminary Spatial Data Analysis” on page 7377. These are the extreme southwest point and a point toward the northeast corner of the region. Since you want to avoid performing the simulation across the whole region, you need to produce a `GDATA=` data set to specify the coordinates of the selected points. These steps are implemented using the following DATA step and statements:

```

title 'Investigation of Random Field Variability';

data thick;
 input East North Thick @@;
 label Thick='Coal Seam Thickness';
 datalines;
 0.7 59.6 34.1 2.1 82.7 42.2 4.7 75.1 39.5
 4.8 52.8 34.3 5.9 67.1 37.0 6.0 35.7 35.9
 6.4 33.7 36.4 7.0 46.7 34.6 8.2 40.1 35.4
 13.3 0.6 44.7 13.3 68.2 37.8 13.4 31.3 37.8
 17.8 6.9 43.9 20.1 66.3 37.7 22.7 87.6 42.8
 23.0 93.9 43.6 24.3 73.0 39.3 24.8 15.1 42.3
 24.8 26.3 39.7 26.4 58.0 36.9 26.9 65.0 37.8
 27.7 83.3 41.8 27.9 90.8 43.3 29.1 47.9 36.7
 29.5 89.4 43.0 30.1 6.1 43.6 30.8 12.1 42.8
 32.7 40.2 37.5 34.8 8.1 43.3 35.3 32.0 38.8
 37.0 70.3 39.2 38.2 77.9 40.7 38.9 23.3 40.5
 39.4 82.5 41.4 43.0 4.7 43.3 43.7 7.6 43.1
 46.4 84.1 41.5 46.7 10.6 42.6 49.9 22.1 40.7
 51.0 88.8 42.0 52.8 68.9 39.3 52.9 32.7 39.2
 55.5 92.9 42.2 56.0 1.6 42.7 60.6 75.2 40.1
 62.1 26.6 40.1 63.0 12.7 41.8 69.0 75.6 40.1
 70.5 83.7 40.9 70.9 11.0 41.7 71.5 29.5 39.8
 78.1 45.5 38.7 78.2 9.1 41.7 78.4 20.0 40.8
 80.5 55.9 38.7 81.1 51.0 38.6 83.8 7.9 41.6
 84.5 11.0 41.5 85.2 67.3 39.4 85.5 73.0 39.8
 86.7 70.4 39.6 87.2 55.7 38.8 88.1 0.0 41.6
 88.4 12.1 41.3 88.4 99.6 41.2 88.8 82.9 40.5
 88.9 6.2 41.5 90.6 7.0 41.5 90.7 49.6 38.9
 91.5 55.4 39.0 92.9 46.8 39.1 93.4 70.9 39.7
 55.8 50.5 38.1 96.2 84.3 40.3 98.2 58.2 39.5
 ;

data grid;
 input xc yc;
 datalines;
 0 0
 75 75
 ;

```

Then, you run PROC SIM2D with the same parameters and characteristics as those shown in the section “Preliminary Spatial Data Analysis” on page 7377. This time, however, you ask for simulated values only at the two locations you specified in the previous DATA step. The following statements execute the requested simulation:

```

proc sim2d data=thick outsim=sim1;
 coordinates xc=East yc=North;
 simulate var=Thick numreal=5000 seed=79931
 scale=7.4599 range=30.1111 form=gauss;
 mean 40.1173;
 grid gdata=grid xc=xc yc=yc;
run;

```

After the simulation is performed, summary statistics are computed for each of the specified grid points. In particular, you use PROC UNIVARIATE and a BY statement to request the quantiles and the extreme observations at these locations, as the following statements show:

```
proc sort data=sim1;
 by gxc gyc;
run;

proc univariate data=sim1;
 var svalue;
 by gxc gyc;
 ods select Quantiles ExtremeObs;
 title 'Simulation Statistics at Selected Grid Points';
run;
```

The summary statistics for the first grid point (East=0, North=0) are presented in [Output 85.2.1](#).

**Output 85.2.1** Simulation Statistics at Grid Point (East=0, North=0)

| Simulation Statistics at Selected Grid Points                                 |      |                   |          |  |
|-------------------------------------------------------------------------------|------|-------------------|----------|--|
| ----- X-coordinate of the grid point=0 Y-coordinate of the grid point=0 ----- |      |                   |          |  |
| The UNIVARIATE Procedure                                                      |      |                   |          |  |
| Variable: SVALUE (Simulated Value at Grid Point)                              |      |                   |          |  |
| Quantiles (Definition 5)                                                      |      |                   |          |  |
|                                                                               |      | Quantile          | Estimate |  |
|                                                                               |      | 100% Max          | 42.4207  |  |
|                                                                               |      | 99%               | 41.8960  |  |
|                                                                               |      | 95%               | 41.5315  |  |
|                                                                               |      | 90%               | 41.3419  |  |
|                                                                               |      | 75% Q3            | 41.0324  |  |
|                                                                               |      | 50% Median        | 40.6701  |  |
|                                                                               |      | 25% Q1            | 40.2871  |  |
|                                                                               |      | 10%               | 39.9904  |  |
|                                                                               |      | 5%                | 39.7825  |  |
|                                                                               |      | 1%                | 39.4181  |  |
|                                                                               |      | 0% Min            | 38.6864  |  |
| ----- X-coordinate of the grid point=0 Y-coordinate of the grid point=0 ----- |      |                   |          |  |
| Extreme Observations                                                          |      |                   |          |  |
| -----Lowest-----                                                              |      | -----Highest----- |          |  |
| Value                                                                         | Obs  | Value             | Obs      |  |
| 38.6864                                                                       | 2691 | 42.2952           | 1149     |  |
| 38.8611                                                                       | 1817 | 42.3114           | 3612     |  |
| 38.9013                                                                       | 3026 | 42.3305           | 3757     |  |
| 38.9467                                                                       | 2275 | 42.4177           | 135      |  |
| 38.9823                                                                       | 3100 | 42.4207           | 4536     |  |



Finally, [Output 85.2.2](#) displays the summary statistics for the second grid point (East=75, North=75).

**Output 85.2.2** Simulation Statistics at Grid Point (East=75, North=75)

```

Simulation Statistics at Selected Grid Points

----- X-coordinate of the grid point=75 Y-coordinate of the grid point=75 -----

 The UNIVARIATE Procedure
Variable: SVALUE (Simulated Value at Grid Point)

 Quantiles (Definition 5)

 Quantile Estimate

 100% Max 40.1171
 99% 40.1147
 95% 40.1131
 90% 40.1122
 75% Q3 40.1108
 50% Median 40.1092
 25% Q1 40.1075
 10% 40.1062
 5% 40.1053
 1% 40.1035
 0% Min 40.1001

----- X-coordinate of the grid point=75 Y-coordinate of the grid point=75 -----

 Extreme Observations

 -----Lowest----- -----Highest-----

 Value Obs Value Obs

 40.1001 7176 40.1167 8980
 40.1007 6262 40.1167 9272
 40.1011 7383 40.1169 5676
 40.1016 7156 40.1170 6514
 40.1017 5643 40.1171 5329

```

For each simulation location, a single realization might result in values that differ significantly from the random field mean at that location. However, the averages of progressively larger numbers of realizations tend to shorten this gap and reduce the simulation variability, as exhibited in the results for the two example locations in [Output 85.2.1](#) and [Output 85.2.2](#). At the limit of an infinite number of realizations, the simulation mean recovers the mean and covariance structure of the random field.

---

## Example 85.3: Risk Analysis with Simulation

This example is in the field of environmental risk assessment. A square region of size 500 km × 500 km has been sampled for arsenic in drinking water. The `logAsData` data set consists of 138 simulated arsenic logarithm concentration observations represented by the `logAs` variable. Section “[Example 102.1: Aspects of Semivariogram Model Fitting](#)” on page 8648 in the VARIOGRAM procedure treats these observations as actual data in order to determine the spatial continuity structure for illustration in the examples.

A preliminary analysis indicates that the population exposure to the pollutant is currently at a relatively low level, as shown in the section “[Example 49.1: Spatial Prediction of Pollutant Concentration](#)” on page 3846 in the KRIGE2D procedure. In particular, spatial prediction with kriging suggests that less than 1% of the region is affected by arsenic concentration in water that exceeds the World Health Organization (WHO) standard of 10  $\mu\text{g}/\text{lt}$ .

You want to simulate the random field of the arsenic logarithm concentration so that you can gain insight into the characteristics of this field. Your objective is to assess whether the occurrence of above-threshold arsenic concentrations is a localized phenomenon, and whether you might expect more such occurrences across the region. For the simulation you need the outcome of the spatial continuity analysis in section “[Example 102.1: Aspects of Semivariogram Model Fitting](#)” on page 8648 in the VARIOGRAM procedure. These results are the fitted semivariance models that are stored in the `SemivAsStore` item store by PROC VARIOGRAM.

Based on the discussion in the section “[Example 85.1: Simulation and Economic Feasibility](#)” on page 7414, you simulate the arsenic logarithm concentration on the premise of the ergodicity assumption. In brief, this assumption relates the mean and covariances of each individual realization to the corresponding values of the random field; see also the section “[Ergodicity](#)” on page 8615 in the VARIOGRAM procedure. In the present case you are interested in the average of a large size of realizations, rather than individual ones. A single realization could suggest possible locations where the WHO regulatory standard might be violated. The average of multiple realizations has a smoothing effect on individual excessive-concentration episodes in single realizations. The smoothing enables you to see general characteristics of the arsenic concentration field behavior on the basis of its spatial correlation description.

For illustration, assume a rectangular grid of nodes with an equal spacing of 10 km between neighboring nodes in the north and east directions. Then, simulated values are produced at a total of  $51 \times 51 = 2601$  locations.

You begin by reading the `logAsData` data set with the following DATA step:

```

title 'Risk Assessment with Simulation';

data logAsData;
 input East North logAs @@;
 label logAs='log(As) Concentration';
 datalines;
193.0 296.6 -0.68153 232.6 479.1 0.96279 268.7 312.5 -1.02908
 43.6 4.9 0.65010 152.6 54.9 1.87076 449.1 395.8 0.95932
310.9 493.6 -1.66208 287.8 164.9 -0.01779 330.0 8.0 2.06837
225.7 241.7 0.15899 452.3 83.4 -1.21217 156.5 462.5 -0.89031
 11.5 84.4 -0.24496 144.4 335.7 0.11950 149.0 431.8 -0.57251
234.3 123.2 -1.33642 37.8 197.8 -0.27624 183.1 173.9 -2.14558
149.3 426.7 -1.06506 434.4 67.5 -1.04657 439.6 237.0 -0.09074
 36.4 175.2 -1.21211 370.6 244.0 3.28091 452.0 96.5 -0.77081
247.0 86.8 0.04720 413.6 373.2 1.78235 253.5 291.7 0.56132
129.7 111.9 1.34000 352.7 42.1 0.23621 279.3 82.7 2.12350
382.6 290.7 0.86756 188.2 222.8 -1.23308 382.8 154.5 -0.94094
304.4 309.2 -1.95158 337.5 387.2 -1.31294 490.7 189.8 0.40206
159.0 100.1 -0.22272 245.5 329.2 -0.26082 372.1 379.5 -1.89078
417.8 84.1 -1.25176 173.9 407.6 -0.24240 121.5 107.7 1.54509
453.5 313.6 0.65895 143.5 346.7 -0.87196 157.4 125.5 -1.96165
371.8 353.2 -0.59464 358.9 338.2 -1.07133 8.6 437.8 1.44203
395.9 394.2 -0.24144 149.5 58.9 1.17459 453.5 420.6 -0.63951
182.3 85.0 1.00005 21.0 290.1 0.31016 11.1 352.2 -0.88418
131.2 238.4 -0.57184 104.9 6.3 1.12054 247.3 256.0 0.14019
428.4 383.7 0.92448 327.8 481.1 -2.72543 199.2 92.8 -0.05717
453.9 230.1 0.16571 205.0 250.6 0.07581 459.5 271.6 0.93700
229.5 262.8 1.83590 370.4 228.6 2.96611 330.2 281.9 1.79723
354.8 388.3 -3.18262 406.2 222.7 2.41594 254.4 393.1 2.03221
 96.7 85.2 -0.47156 407.2 256.8 0.66747 498.5 273.8 1.03041
417.2 471.4 -1.42766 368.8 424.3 -0.70506 303.0 59.1 1.43070
403.1 264.1 1.64554 21.2 360.8 0.67094 148.2 78.1 2.15323
305.5 310.7 -1.47985 228.5 180.3 -0.68386 161.1 143.3 1.07901
 70.5 155.1 0.54652 363.1 282.6 -0.43051 86.0 472.5 -1.18855
175.9 105.3 -2.08112 96.8 426.3 1.56592 475.1 453.1 -1.53776
125.7 485.4 1.40054 277.9 201.6 -0.54565 406.2 125.0 -1.38657
 60.0 275.5 -0.59966 431.3 494.6 -0.36860 399.9 399.0 -0.77265
 28.8 311.1 0.91693 166.1 348.2 -0.49056 266.6 83.5 0.67277
 54.7 356.3 0.49596 433.5 460.3 -1.61309 201.7 167.6 -1.40678
158.1 203.6 -1.32499 67.6 230.4 1.14672 81.9 250.0 0.63378
372.0 50.7 0.72445 26.4 264.6 1.00862 300.1 91.7 -0.74089
303.0 447.4 1.74589 108.4 386.2 1.12847 55.6 191.7 0.95175
 36.3 273.2 1.78880 94.5 298.3 -2.43320 366.1 187.3 -0.80526
130.7 389.2 -0.31513 37.2 324.2 0.24489 295.5 211.8 0.41899
 58.6 206.2 0.18495 346.3 142.8 -0.92038 484.2 215.9 0.08012
451.4 415.7 0.02773 58.9 86.5 0.17652 212.6 363.9 0.17215
378.7 407.6 0.51516 265.9 305.0 -0.30718 123.2 314.8 -0.90591
 26.9 471.7 1.70285 16.5 7.1 0.51736 255.1 472.6 2.02381
111.5 148.4 -0.09658 440.4 375.0 1.23285 406.4 19.5 1.01181
321.2 65.8 -0.02095 466.4 357.1 -0.49272 2.0 484.6 0.50994
200.9 205.1 0.43543 30.3 337.0 1.60882 297.0 12.7 1.79824
158.2 450.7 0.05295 122.8 105.3 1.53936 417.8 329.7 -2.08124
;

```

For this simulation you use the spatial correlation information that is saved in the SemivAsStore item store in the section “[Example 102.1: Aspects of Semivariogram Model Fitting](#)” on page 8648 in the VARIOGRAM procedure with the following statements:

```
ods graphics on;

proc variogram data=logAsData plots=none;
 store out=SemivAsStore / label='LogAs Concentration Models';
 compute lagd=5 maxlag=40;
 coord xc=East yc=North;
 model form=auto(mlist=(exp,gau,mat) nest=1 to 2);
 var logAs;
run;
```

In PROC SIM2D you specify the container item store with the **IN=** option of the **RESTORE** statement. You request correlation input from an item store by specifying the **STORESELECT** option in the **SIMULATE** statement. You request 5,000 realizations for this simulation by specifying the number in the **NUMREAL=** option of the **SIMULATE** statement.

Assume that you first want to review the saved models in the item store. Use the **INFO** option of the **RESTORE** statement to produce a table with information about the top-ranking fitted model in the item store. Use the **DET** and **ONLY** suboptions of the **INFO** option to request details about all fitted models included in the item store. The **ONLY** suboption suppresses the simulation tasks and produces only the tables about the item store. You specify the following statements:

```
proc sim2d data=logAsData outsim=Outsim plots=none;
 restore in=SemivAsStore / info(det only);
 coordinates xc=East yc=North;
 simulate var=logAs numreal=5000 storeselect seed=39841;
 grid x=0 to 500 by 10 y=0 to 500 by 10;
run;
```

PROC SIM2D produces a table with general information about the input item store identity, as shown in [Output 85.3.1](#).

### Output 85.3.1 PROC SIM2D and Input Item Store General Information

| Risk Assessment with Simulation          |                            |
|------------------------------------------|----------------------------|
| The SIM2D Procedure                      |                            |
| Correlation Model Item Store Information |                            |
| Input Item Store                         | WORK.SEMIVASSTORE          |
| Item Store Label                         | LogAs Concentration Models |
| Data Set Created From                    | WORK.LOGASDATA             |
| By-group Information                     | No By-groups Present       |
| Created By                               | PROC VARIOGRAM             |
| Date Created                             | 07JUN12:14:11:33           |

Output 85.3.2 displays the item store variables, in addition to the mean and standard deviation of their data set of origin. In this case, the logAs values come from the logAsData data set. By default, the SIM2D procedure uses the variable mean in the item store for the simulation, unless you explicitly specify the MEAN statement.

**Output 85.3.2** Variables in the Input Item Store

| Item Store Variables |          |               |
|----------------------|----------|---------------|
| Variable             | Mean     | Std Deviation |
| logAs                | 0.084309 | 1.527707      |

The models in the SemivAsStore item store that have been fitted to the arsenic logarithm logAs empirical semivariance are shown in Output 85.3.3. The default item store model selection is the model on top of the list in Output 85.3.3.

**Output 85.3.3** Angle and Models Information in the Input Item Store

| Item Store Models For logAs |                                      |
|-----------------------------|--------------------------------------|
| Class                       | Model                                |
| 1                           | Gau-Gau<br>Gau-Mat                   |
| 2                           | Exp-Gau                              |
| 3                           | Exp-Mat                              |
| 4                           | Mat                                  |
| 5                           | Gau                                  |
| 6                           | Exp<br>Exp-Exp<br>Mat-Exp<br>Gau-Exp |

You run again the SIM2D procedure without the INFO option in the RESTORE statement. This action prompts PROC SIM2D to run the simulation tasks that you specify with the SIMULATE statement. You specify the STORESELECT option in the SIMULATE statement without any suboptions, so that the simulation uses the default model selection in the SemivAsStore item store. You save the simulation output in the Outsims output data set. You also specify the SIM and the SEMIVAR suboptions in the PLOTS option of the PROC SIM2D statement to obtain output plots. You use the following statements:

```
proc sim2d data=logAsData outsims=Outsims plots=(sim semivar);
 restore in=SemivAsStore;
 coordinates xc=East yc=North;
 simulate var=logAs numreal=5000 storeselect seed=89702;
 grid x=0 to 500 by 10 y=0 to 500 by 10;
run;
```

**NOTE:** This step can take several minutes to run, and it produces a data set with over 10 million observations. When you run these statements, PROC SIM2D again produces a table about the input item store identity. This output is followed by a number of observations table and information about the simulation task, as shown in [Output 85.3.4](#).

**Output 85.3.4** Number of Observations and Simulation Information Tables

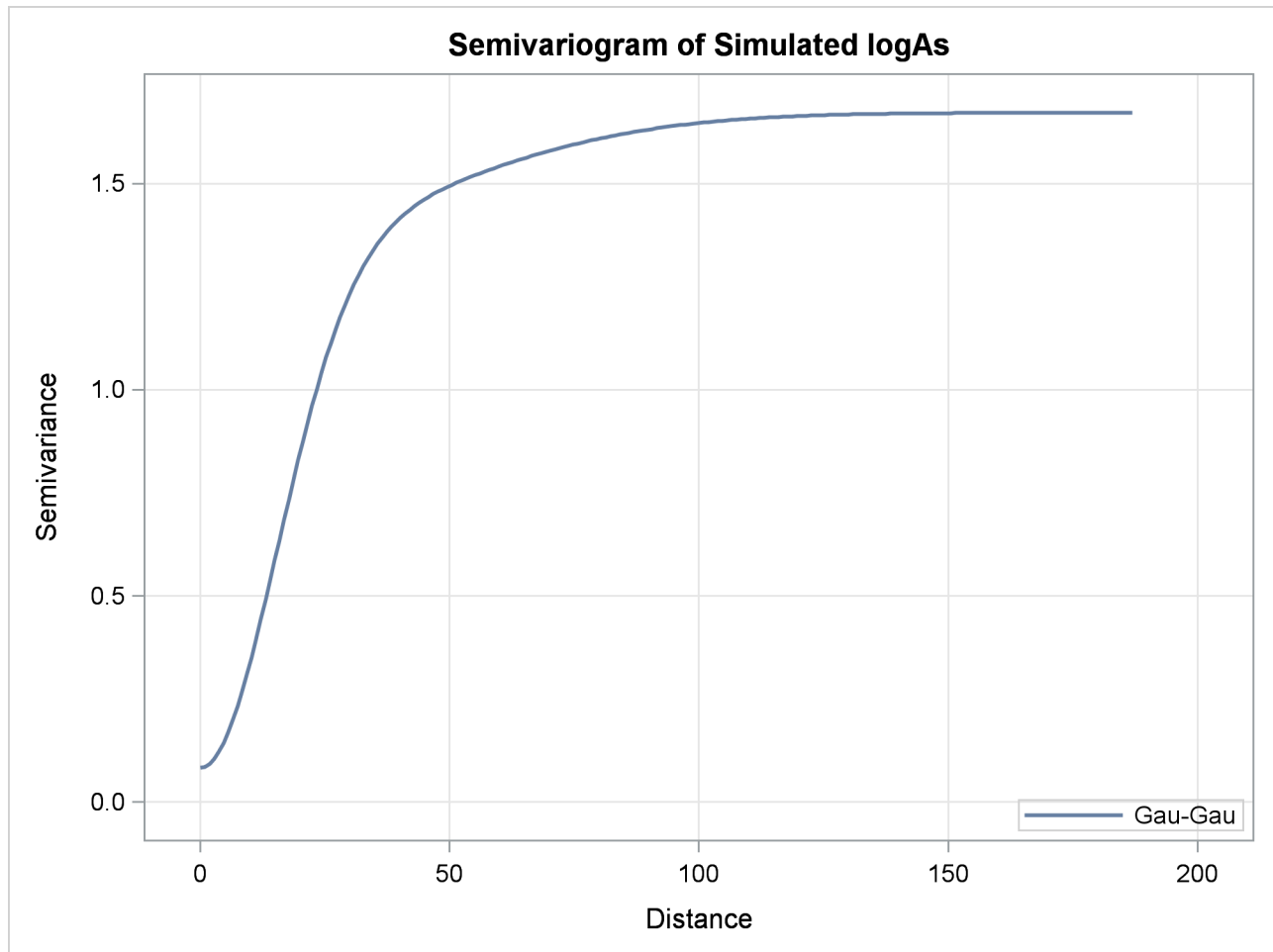
| Risk Assessment with Simulation             |             |
|---------------------------------------------|-------------|
| The SIM2D Procedure                         |             |
| Simulation: SIM1, Dependent Variable: logAs |             |
| Number of Observations Read                 | 138         |
| Number of Observations Used                 | 138         |
| Simulation Information                      |             |
| Simulation Grid Points                      | 2601        |
| Type                                        | Conditional |
| Number of Realizations                      | 5000        |

The SIM2D procedure uses the selected fitted Gaussian-Gaussian model in the SemivAsStore item store. [Output 85.3.5](#) shows the saved parameter values of the model that are used in the simulation.

**Output 85.3.5** Information about the Gaussian-Gaussian Model

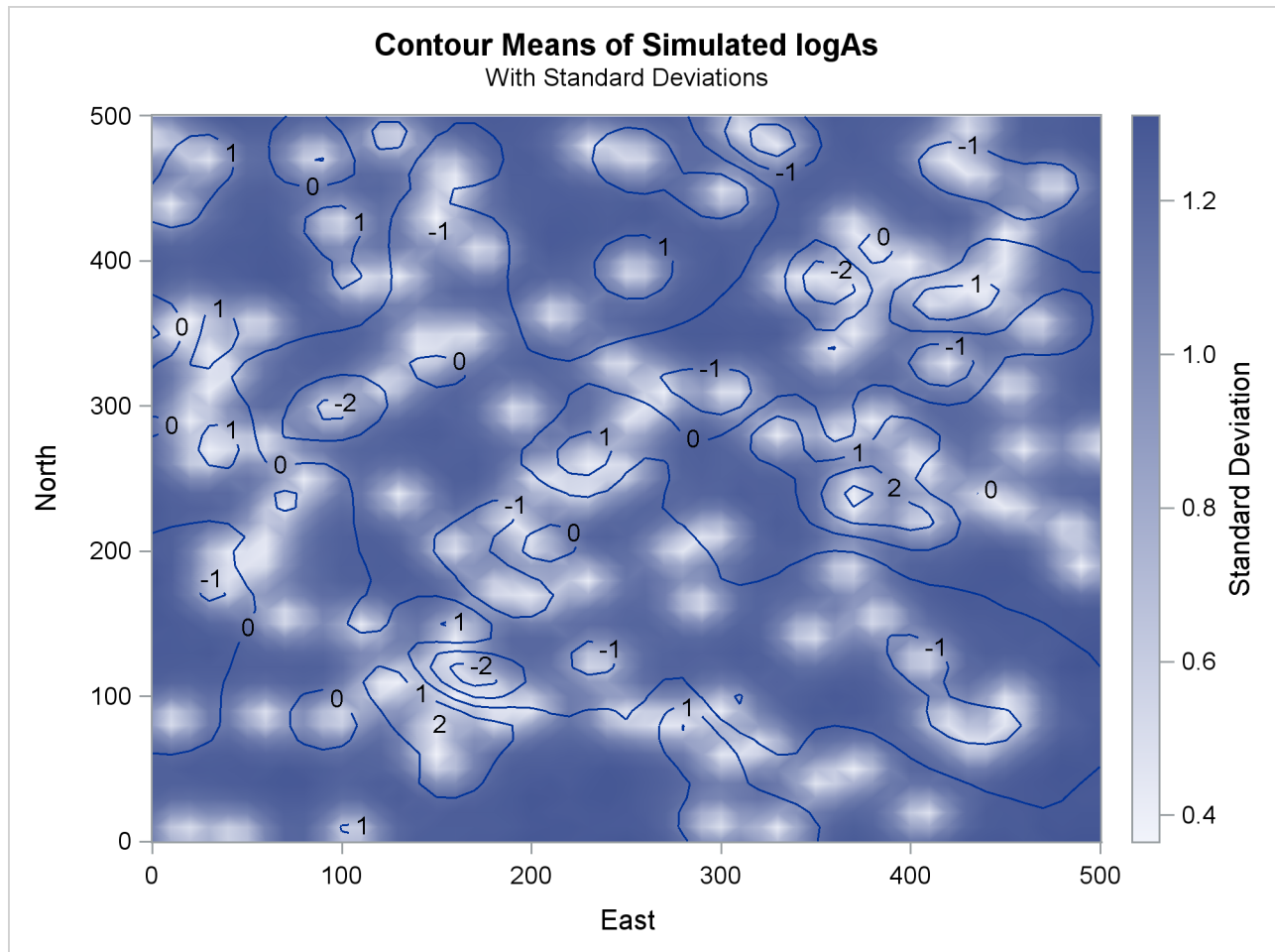
| Covariance Model Information       |           |
|------------------------------------|-----------|
| Nested Structure 1 Type            | Gaussian  |
| Nested Structure 1 Sill            | 0.3276646 |
| Nested Structure 1 Range           | 62.312728 |
| Nested Structure 1 Effective Range | 107.92881 |
| Nested Structure 2 Type            | Gaussian  |
| Nested Structure 2 Sill            | 1.261545  |
| Nested Structure 2 Range           | 21.459563 |
| Nested Structure 2 Effective Range | 37.169053 |
| Nugget Effect                      | 0.0830758 |

[Output 85.3.6](#) shows a plot of the correlation model used in the simulation. Its parameters come from the stored information in the SemivAsStore item store.

**Output 85.3.6** Gaussian-Gaussian Semivariogram Model Used in Simulation

The PLOTS=SIM option produces contours of the mean value of the 5,000 realizations for each one of the output grid locations, and a surface of the associated standard deviation. The resulting plot is shown in Output 85.3.7. The mean value contours exhibit reduced variation compared to a SIM plot of one single realization. In fact, Output 85.3.7 is very similar to the prediction plot of the same Gaussian model in the section “Example 49.1: Spatial Prediction of Pollutant Concentration” on page 3846 in the KRIGE2D procedure.

Clearly, there appears to be a small area of increased arsenic concentration values, which is located in the central-eastern part of the domain. The WHO threshold of  $10 \mu\text{g}/\text{lt}$  for the maximum allowed arsenic concentration in water translates into about 2.3 in the log scale. The indicated area is the only one within the region where the simulated means exceed the value 3. In addition, there appear to be two smaller areas of simulated means values at or above 2 in the southern part of the region.

**Output 85.3.7** Simulated Arsenic Logarithm Values with Gaussian-Gaussian Covariance

The simulation plot indicates that arsenic concentration values in excess of the WHO health standard is a rather localized phenomenon. If it were not so, then the plot would suggest that increased arsenic concentrations extend across larger areas. In turn, this means that individual realizations would tend to produce systematically higher arsenic concentrations at different neighboring locations, and their average would appear as higher logAs values in the **SIM** plot. Instead, you conclude that the Gaussian-Gaussian correlation that describes the spatial continuity for the arsenic logarithm observations leads to only localized occurrence of the WHO standard violation.

Now you want to find out whether additional localized occurrences might take place on the basis of the Gaussian-Gaussian spatial continuity behavior. The distribution of the simulation standard deviation values in **Output 85.3.7** offers important feedback about this issue. Observe the areas in the plot where the means gradient indicates increasing values. The means contours create several pools where the values increase to simulated means higher than 1.

With the clear exceptions of the isolated area in the central-eastern part of the domain and the pool in the south-west that exhibit logAs values above 2, the simulation standard deviation seems to be around 1 or less in almost all other pools with logAs values above 1. Due to those relatively low standard deviations, this visual inspection suggests that even in individual realizations you might rarely expect the arsenic logarithm to exceed the threshold value of around 2.3.



However, in the few pools of logAs values above 1, there can be patches of increased standard deviation. In these cases, you suspect that arsenic concentration could exceed occasionally the WHO regulatory standard, even if the plot of the simulated means does not explicitly portray so.

Based on these remarks, you want to quantify the percentage of the region that could be affected by excessive arsenic concentration. You begin with a DATA step that takes as input the simulation Outsim output data set. The DATA step marks the simulated arsenic logarithm means values that are in excess of the WHO concentration threshold of 10  $\mu\text{g}/\text{lt}$ , and saves the outcome into an indicator variable OverLimit. At the same time, the arsenic logarithm values are transformed back into arsenic concentration values so that they can be compared to the threshold value. The simulated means in the Outsim data set are stored in the svalue variable. You use the following statements:

```
data AsOverLimit;
 set Outsim;
 OverLimit = (exp(svalue) > 10) * 100;
run;
```

Then, you use the MEANS procedure to express the selected nodes population (where the WHO standard violation occurs) as a percentage of the entire domain area. You invoke PROC MEANS twice. The first time, you average over each realization in the PROC SIM2D output. For that purpose, you use the variable `_ITER_` in the simulation sim1 output data set as a BY variable in PROC MEANS. You save the iteration-averaged indicator values in the PctOverLimit variable. The second time, PROC MEANS averages the PctOverLimit variable to obtain the percentage you want. You also specify the P5 and P95 options in the PROC MEANS statement to request the lower and upper confidence limits, respectively, in this computation. The interval between those limits expresses the 90% interval for the true area percentage based on the stochastic simulation. You use the following statements:

```
proc means data=AsOverLimit noprint;
 by _ITER_;
 var OverLimit;
 output out=OverLimitData mean=PctOverLimit;
run;
proc means data=OverLimitData mean p5 p95;
 var PctOverLimit;
 label PctOverLimit="Percent above threshold";
run;
```

The result is shown in [Output 85.3.8](#). PROC MEANS accounts for all individual occurrences throughout the simulation where the WHO arsenic concentration threshold is exceeded. This happens at about 3.9% of the total area in 5,000 realizations. Compare this value to the less than 1% percentage in the PROC KRIGE2D prediction, as reported in the beginning of this section. On one hand, the prediction outcome tells you what goes on currently across the region within a degree of certainty given by the prediction error. On the other hand, the simulation provides you with an indicator that under the given spatial continuity estimate a relatively larger area is in potential danger of being affected by above-threshold arsenic concentration.

In fact, the 5% and 95% confidence limits in [Output 85.3.8](#) show the area percentage limits within which you can expect excessive arsenic concentration. Based on the stochastic simulation, at the 90% confidence level the arsenic concentration in drinking water is expected to violate the WHO regulatory standard in anywhere from about 2.6% to 5.4% of the study region.

**Output 85.3.8** Violation of Arsenic Concentration Threshold Using Gaussian-Gaussian Model

| Risk Assessment with Simulation                          |           |           |
|----------------------------------------------------------|-----------|-----------|
| The MEANS Procedure                                      |           |           |
| Analysis Variable : PctOverLimit Percent above threshold |           |           |
| Mean                                                     | 5th Pctl  | 95th Pctl |
| 3.9308727                                                | 2.6143791 | 5.4209919 |

You also want to compute the probability that individual areas in the region are expected to violate the WHO arsenic concentration standard. Start by identifying again the simulated arsenic logarithm means values in excess of the WHO concentration threshold of 10  $\mu\text{g}/\text{lt}$ . The following DATA step saves the outcome into the variable LocalOverLimit:

```
data LocalAsOverLimit;
 set Outsim;
 LocalOverLimit = (exp(svalue) > 10);
run;
```

Then you use the SORT procedure to sort the information based on location coordinates. This intermediate step is necessary so that you can use the MEANS procedure with the LocalAsOverLimit data set. In the following statements, PROC MEANS computes the expected violations of the WHO standard for each location in the region across all realizations of the simulation:

```
proc sort data=LocalAsOverLimit;
 by gxc gyc;
run;
proc means data=LocalAsOverLimit noprint;
 by gxc gyc;
 var LocalOverLimit;
 output out=OverLimLocI mean=ProbOverLimit;
run;
```

The output is the probability that the WHO standard is violated at each one of the simulation locations across the region. You create a plot of this probability with the help of the TEMPLATE and the SGRENDER procedures. You use the following statements:

```

proc template;
 define statgraph surfacePlot;
 dynamic _VARX _VARY _VAR _TITLE _LEGENDLABEL;
 BeginGraph;
 entrytitle _TITLE;
 layout overlay /
 xaxisopts = (offsetmax=0)
 yaxisopts = (offsetmax=0);
 contourplotparm x=_VARX y=_VARY z=_VAR /
 nhint=10 name='probplot';
 continuouslegend 'probplot' / title=_LEGENDLABEL;
 endlayout;
 EndGraph;
 end;
run;

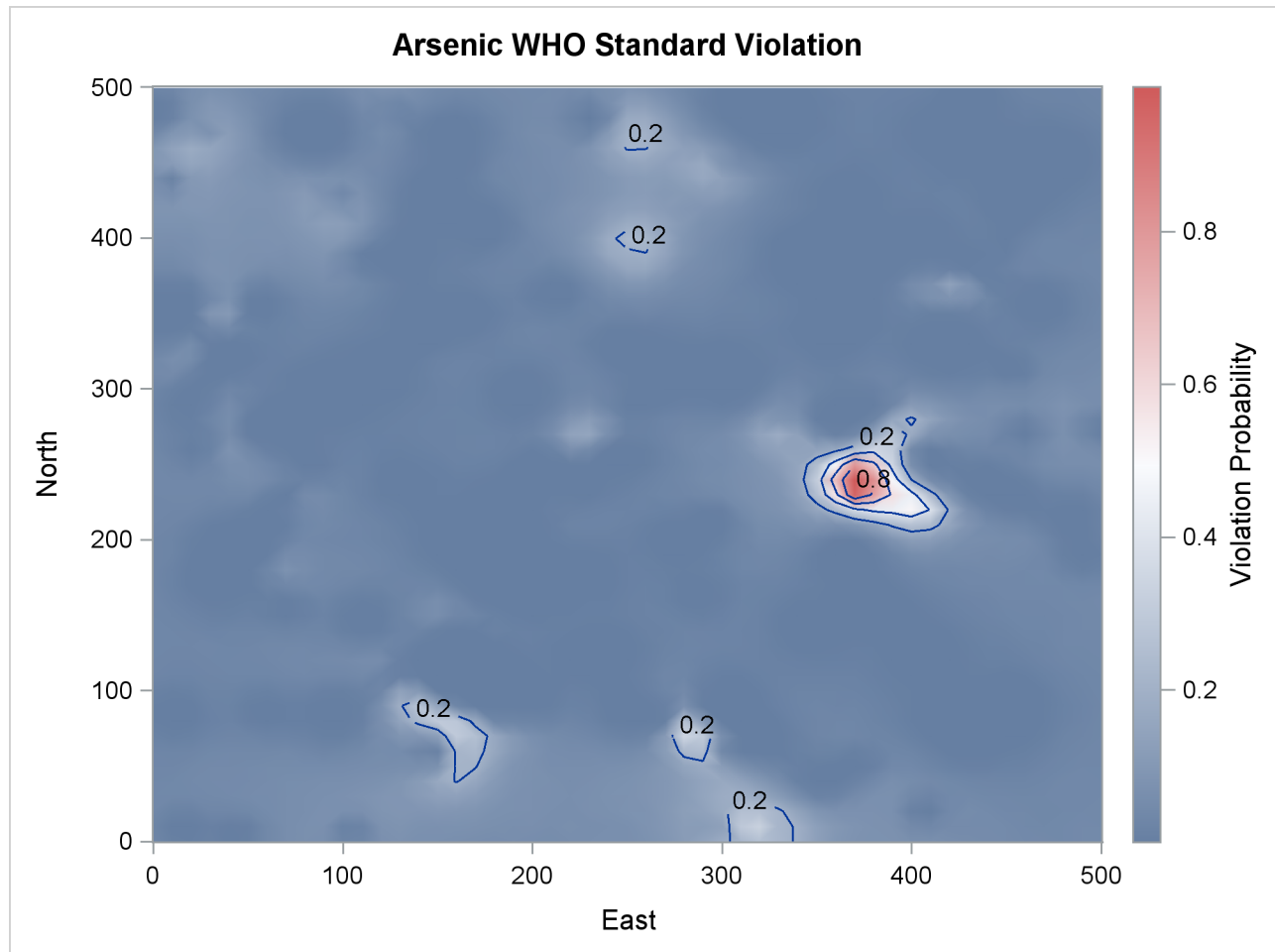
proc sgrender data=OverLimLoc1 template=surfacePlot;
 dynamic _VARX = 'gxc'
 _VARY = 'gyc'
 _VAR = 'ProbOverLimit'
 _TITLE='Arsenic WHO Standard Violation'
 _LEGENDLABEL='Violation Probability';
 label gyc='North' gxc='East';
run;

ods graphics off;

```

Output 85.3.9 shows the map of probability that the arsenic concentration WHO standard is violated in the region for the selected spatial correlation model of the pollutant. Based on the preceding analysis, the probability is very close to 1 in the area where the simulation mean values are above the standard limit. A few more areas that were indicated earlier in the analysis suggest a violation probability between 20% and 40%. The remaining areas in the region exhibit very low probability, which is notably nonzero at a few scattered locations. These findings suggest that throughout the simulation there have been realizations where the arsenic WHO standard was exceeded at locations whose simulated mean is well below that standard.

From the environmental risk assessment perspective, the preceding analysis can trigger a more detailed investigation into areas in the region where the health standard might be violated. Although the original observations in the logAsData data set indicate no existing problem in some of these areas, the present example illustrates that spatial analysis and simulation can raise flags of caution. This type of analysis can help to focus scientific, management, and policy efforts on these particular areas of the region and to monitor closely the pollutant concentration for potential health risks.

**Output 85.3.9** Map of Violation of the Arsenic WHO Standard Probability


---

## References

- Christakos, G. (1992), *Random Field Models in Earth Sciences*, New York: Academic Press.
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# Chapter 86

## The SIMNORMAL Procedure

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### Overview: SIMNORMAL Procedure

The SIMNORMAL procedure can perform conditional and unconditional simulation for a set of correlated normal or Gaussian random variables.

The means, variances, and covariances (or correlations) are read from an input TYPE=CORR or TYPE=COV data set. This data set is typically produced by the CORR procedure. Conditional simulations are performed by appending a special observation, identified by the value of 'COND' for the \_TYPE\_ variable, which contains the conditioning value.

The output data set from PROC SIMNORMAL contains simulated values for each of the analysis variables. Optionally, the output data set also contains the seed stream and the values of the conditioning variables. PROC SIMNORMAL produces no printed output.

---

### Getting Started: SIMNORMAL Procedure

The following example illustrates the use of PROC SIMNORMAL to generate variable values conditioned on a set of related or correlated variables.

Suppose you are given a sample of size 50 from ten normally distributed, correlated random variables,  $IN_{1,i}, \dots, IN_{5,i}, OUT_{1,i}, \dots, OUT_{5,i}, i = 1, \dots, 50$ . The first five variables represent input variables for a chemical manufacturing process, and the last five are output variables.

First, the data are input and the correlation structure is determined by using PROC CORR, as in the following statements. The results are shown in Figure 86.1.

```
data a ;
 input in1-in5 out1-out5 ;
 datalines ;
 9.3500 10.0964 7.3177 10.3617 10.3444 9.4612
 10.7443 9.9026 9.0144 11.7968
 7.8599 10.4560 10.0075 8.5875 10.0014 10.3869

 ... more lines ...

 8.9174 9.9623 9.5742 9.9713
run ;

proc corr data=a cov nocorr outp=outcov ;
 var in1-in5 out1-out5 ;
run ;
```

**Figure 86.1** Correlation of Chemical Process Variables

| The CORR Procedure |      |      |      |     |     |      |      |
|--------------------|------|------|------|-----|-----|------|------|
| 10 Variables:      | in1  | in2  | in3  | in4 | in5 | out1 | out2 |
|                    | out3 | out4 | out5 |     |     |      |      |

Figure 86.1 continued

| Covariance Matrix, DF = 49 |             |              |             |             |             |
|----------------------------|-------------|--------------|-------------|-------------|-------------|
|                            | in1         | in2          | in3         | in4         | in5         |
| in1                        | 1.019198331 | 0.128086799  | 0.291646382 | 0.327014916 | 0.417546732 |
| in2                        | 0.128086799 | 1.056460818  | 0.143581799 | 0.095937707 | 0.104117743 |
| in3                        | 0.291646382 | 0.143581799  | 1.384051249 | 0.058853960 | 0.326107730 |
| in4                        | 0.327014916 | 0.095937707  | 0.058853960 | 1.023128678 | 0.347916864 |
| in5                        | 0.417546732 | 0.104117743  | 0.326107730 | 0.347916864 | 1.606858140 |
| out1                       | 0.097650713 | 0.056612934  | 0.093498839 | 0.022915645 | 0.360270318 |
| out2                       | 0.206698403 | -0.121700731 | 0.078294087 | 0.125961491 | 0.297046593 |
| out3                       | 0.516271121 | 0.266581451  | 0.481576554 | 0.179627237 | 0.749212945 |
| out4                       | 0.118726106 | 0.092288067  | 0.057816322 | 0.075028230 | 0.220196337 |
| out5                       | 0.261770905 | -0.020971411 | 0.259053423 | 0.078147576 | 0.349618466 |

| Covariance Matrix, DF = 49 |              |              |             |              |              |
|----------------------------|--------------|--------------|-------------|--------------|--------------|
|                            | out1         | out2         | out3        | out4         | out5         |
| in1                        | 0.097650713  | 0.206698403  | 0.516271121 | 0.118726106  | 0.261770905  |
| in2                        | 0.056612934  | -0.121700731 | 0.266581451 | 0.092288067  | -0.020971411 |
| in3                        | 0.093498839  | 0.078294087  | 0.481576554 | 0.057816322  | 0.259053423  |
| in4                        | 0.022915645  | 0.125961491  | 0.179627237 | 0.075028230  | 0.078147576  |
| in5                        | 0.360270318  | 0.297046593  | 0.749212945 | 0.220196337  | 0.349618466  |
| out1                       | 0.807007554  | 0.217285879  | 0.064816340 | -0.053931448 | 0.037758721  |
| out2                       | 0.217285879  | 0.929455806  | 0.206825664 | 0.138551008  | 0.054039499  |
| out3                       | 0.064816340  | 0.206825664  | 1.837505268 | 0.292963975  | 0.165910481  |
| out4                       | -0.053931448 | 0.138551008  | 0.292963975 | 0.832831377  | -0.067396486 |
| out5                       | 0.037758721  | 0.054039499  | 0.165910481 | -0.067396486 | 0.697717191  |

| Simple Statistics |    |          |         |           |         |          |
|-------------------|----|----------|---------|-----------|---------|----------|
| Variable          | N  | Mean     | Std Dev | Sum       | Minimum | Maximum  |
| in1               | 50 | 10.18988 | 1.00955 | 509.49400 | 7.63500 | 12.58860 |
| in2               | 50 | 10.10673 | 1.02784 | 505.33640 | 8.12580 | 13.78310 |
| in3               | 50 | 10.14888 | 1.17646 | 507.44420 | 7.31770 | 12.40080 |
| in4               | 50 | 10.03884 | 1.01150 | 501.94200 | 7.40490 | 11.99060 |
| in5               | 50 | 10.22587 | 1.26762 | 511.29340 | 7.23350 | 12.93360 |
| out1              | 50 | 9.85347  | 0.89834 | 492.67340 | 8.01220 | 12.24660 |
| out2              | 50 | 9.96857  | 0.96408 | 498.42840 | 7.76420 | 12.09450 |
| out3              | 50 | 10.29588 | 1.35555 | 514.79410 | 7.29660 | 13.74200 |
| out4              | 50 | 10.15856 | 0.91260 | 507.92780 | 8.43090 | 12.45230 |
| out5              | 50 | 10.26023 | 0.83529 | 513.01130 | 7.86060 | 11.96000 |

After the mean and correlation structure are determined, any subset of these variables can be simulated. Suppose you are interested in a particular function of the output variables for two sets of values of the input variables for the process. In particular, you are interested in the mean and variability of the following function over 500 runs of the process conditioned on each set of input values:

$$f(out_1, \dots, out_5) = \frac{out_1 - out_3}{out_1 + out_2 + out_3 + out_4 + out_5}$$



Although the distribution of these quantities could be determined theoretically, it is simpler to perform a conditional simulation by using PROC SIMNORMAL.

To do this, you first append a `_TYPE_='COND'` observation to the covariance data set produced by PROC CORR for each group of input values:

```

data cond1 ;
 TYPE='COND' ;
 in1 = 8 ;
 in2 = 10.5 ;
 in3 = 12 ;
 in4 = 13.5 ;
 in5 = 14.4 ;
 output ;
run ;

data cond2 ;
 TYPE='COND' ;
 in1 = 15.4 ;
 in2 = 13.7 ;
 in3 = 11 ;
 in4 = 7.9 ;
 in5 = 5.5 ;
 output ;
run ;

```

Next, each of these conditioning observations is appended to a copy of the `OUTP=OUTCOV` data from the CORR procedure, as in the following statements. A new variable, `INPUT`, is added to distinguish the sets of input values. This variable is used as a `BY` variable in subsequent steps.

```

data outcov1 ;
 input=1 ;
 set outcov cond1 ;
run ;

data outcov2 ;
 input=2 ;
 set outcov cond2 ;
run ;

```

Finally, these two data sets are concatenated:

```

data outcov ;
 set outcov1 outcov2 ;
run ;
proc print data=outcov ;
 where (_type_ ne 'COV') ;
run ;

```

Figure 86.2 shows the added observations.

**Figure 86.2** OUTP= Data Set from PROC CORR with `_TYPE_=COND` Observations Appended

| Obs | input | <code>_TYPE_</code> | <code>_NAME_</code> | in1     | in2     | in3     | in4     |
|-----|-------|---------------------|---------------------|---------|---------|---------|---------|
| 11  | 1     | MEAN                |                     | 10.1899 | 10.1067 | 10.1489 | 10.0388 |
| 12  | 1     | STD                 |                     | 1.0096  | 1.0278  | 1.1765  | 1.0115  |
| 13  | 1     | N                   |                     | 50.0000 | 50.0000 | 50.0000 | 50.0000 |
| 14  | 1     | COND                |                     | 8.0000  | 10.5000 | 12.0000 | 13.5000 |
| 25  | 2     | MEAN                |                     | 10.1899 | 10.1067 | 10.1489 | 10.0388 |
| 26  | 2     | STD                 |                     | 1.0096  | 1.0278  | 1.1765  | 1.0115  |
| 27  | 2     | N                   |                     | 50.0000 | 50.0000 | 50.0000 | 50.0000 |
| 28  | 2     | COND                |                     | 15.4000 | 13.7000 | 11.0000 | 7.9000  |

| Obs | in5     | out1    | out2    | out3    | out4    | out5    |
|-----|---------|---------|---------|---------|---------|---------|
| 11  | 10.2259 | 9.8535  | 9.9686  | 10.2959 | 10.1586 | 10.2602 |
| 12  | 1.2676  | 0.8983  | 0.9641  | 1.3555  | 0.9126  | 0.8353  |
| 13  | 50.0000 | 50.0000 | 50.0000 | 50.0000 | 50.0000 | 50.0000 |
| 14  | 14.4000 | .       | .       | .       | .       | .       |
| 25  | 10.2259 | 9.8535  | 9.9686  | 10.2959 | 10.1586 | 10.2602 |
| 26  | 1.2676  | 0.8983  | 0.9641  | 1.3555  | 0.9126  | 0.8353  |
| 27  | 50.0000 | 50.0000 | 50.0000 | 50.0000 | 50.0000 | 50.0000 |
| 28  | 5.5000  | .       | .       | .       | .       | .       |

You now run PROC SIMNORMAL, specifying the input data set and the VAR and COND variables. Note that you must specify a `TYPE=COV` or `TYPE=CORR` for the input data set. PROC CORR automatically assigns a `TYPE=COV` or `TYPE=CORR` attribute for the OUTP= data set. However, since the intermediate DATA steps that appended the `_TYPE_='COND'` observations turned off this attribute, an explicit `TYPE=CORR` in the DATA= option in the PROC SIMNORMAL statement is needed.

The specification of PROC SIMNORMAL now follows from the problem description. The condition variables are IN1–IN5, the analysis variables are OUT1–OUT5, and 500 realizations are required. A seed value can be chosen arbitrarily, or the system clock can be used. Note that in the following statements, the simulation is done for each of the values of the BY variable INPUT:

```
proc simnormal data=outcov(type=cov)
 out = osim
 numreal = 500
 seed = 33179
 ;
 by input ;
 var out1-out5 ;
 cond in1-in5 ;
run;

data b;
 set osim ;
 denom = sum(of out1-out5) ;
 if abs(denom) < 1e-8 then ff = . ;
 else ff = (out1-out3)/denom ;
run ;
```

The DATA step that follows the simulation computes the function  $f(out_1, \dots, out_5)$ ; in the following statements the UNIVARIATE procedure computes the simple statistics for this function for each set of conditioning input values. This is shown in Figure 86.3, and Figure 86.4 shows the distribution of the function values for each set of input values by using the SG PANEL procedure.

```
proc univariate data=b ;
 by input ;
 var ff ;
run ;
title ;
proc sgpanel data=b ;
 panelby input ;
 REFLINE 0 / axis= x ;
 density ff ;
run ;
```

**Figure 86.3** Simple Statistics for ff for Each Set of Input Values

| ----- input=1 -----        |             |                     |            |
|----------------------------|-------------|---------------------|------------|
| The UNIVARIATE Procedure   |             |                     |            |
| Variable: ff               |             |                     |            |
| Moments                    |             |                     |            |
| N                          | 500         | Sum Weights         | 500        |
| Mean                       | -0.0134833  | Sum Observations    | -6.7416303 |
| Std Deviation              | 0.02830426  | Variance            | 0.00080113 |
| Skewness                   | 0.56773239  | Kurtosis            | 1.31522925 |
| Uncorrected SS             | 0.49066351  | Corrected SS        | 0.39976435 |
| Coeff Variation            | -209.92145  | Std Error Mean      | 0.0012658  |
| ----- input=1 -----        |             |                     |            |
| Basic Statistical Measures |             |                     |            |
| Location                   |             | Variability         |            |
| Mean                       | -0.01348    | Std Deviation       | 0.02830    |
| Median                     | -0.01565    | Variance            | 0.0008011  |
| Mode                       | .           | Range               | 0.21127    |
|                            |             | Interquartile Range | 0.03618    |
| ----- input=1 -----        |             |                     |            |
| Tests for Location: Mu0=0  |             |                     |            |
| Test                       | -Statistic- | -----p Value-----   |            |
| Student's t                | t -10.6519  | Pr >  t             | <.0001     |
| Sign                       | M -106      | Pr >=  M            | <.0001     |
| Signed Rank                | S -33682    | Pr >=  S            | <.0001     |

Figure 86.3 continued

| ----- input=1 -----      |                  |                  |                   |     |
|--------------------------|------------------|------------------|-------------------|-----|
| Quantiles (Definition 5) |                  |                  |                   |     |
|                          | Quantile         | Estimate         |                   |     |
|                          | 100% Max         | 0.11268600       |                   |     |
|                          | 99%              | 0.07245656       |                   |     |
|                          | 95%              | 0.03270269       |                   |     |
|                          | 90%              | 0.02064338       |                   |     |
|                          | 75% Q3           | 0.00370322       |                   |     |
|                          | 50% Median       | -0.01564850      |                   |     |
|                          | 25% Q1           | -0.03247389      |                   |     |
|                          | 10%              | -0.04716239      |                   |     |
|                          | 5%               | -0.05572806      |                   |     |
|                          | 1%               | -0.07201126      |                   |     |
|                          | 0% Min           | -0.09858350      |                   |     |
| ----- input=1 -----      |                  |                  |                   |     |
| Extreme Observations     |                  |                  |                   |     |
|                          | -----Lowest----- |                  | -----Highest----- |     |
|                          | Value            | Obs              | Value             | Obs |
|                          | -0.0985835       | 471              | 0.0750538         | 22  |
|                          | -0.0908179       | 472              | 0.0794747         | 245 |
|                          | -0.0802423       | 90               | 0.0840160         | 48  |
|                          | -0.0760645       | 249              | 0.1004812         | 222 |
|                          | -0.0756070       | 226              | 0.1126860         | 50  |
| ----- input=2 -----      |                  |                  |                   |     |
| The UNIVARIATE Procedure |                  |                  |                   |     |
| Variable: ff             |                  |                  |                   |     |
| Moments                  |                  |                  |                   |     |
| N                        | 500              | Sum Weights      | 500               |     |
| Mean                     | -0.0405913       | Sum Observations | -20.295631        |     |
| Std Deviation            | 0.03027008       | Variance         | 0.00091628        |     |
| Skewness                 | 0.1033062        | Kurtosis         | -0.1458848        |     |
| Uncorrected SS           | 1.28104777       | Corrected SS     | 0.4572225         |     |
| Coeff Variation          | -74.57289        | Std Error Mean   | 0.00135372        |     |

Figure 86.3 continued

```

----- input=2 -----

```

| Basic Statistical Measures |          |                     |           |
|----------------------------|----------|---------------------|-----------|
| Location                   |          | Variability         |           |
| Mean                       | -0.04059 | Std Deviation       | 0.03027   |
| Median                     | -0.04169 | Variance            | 0.0009163 |
| Mode                       | .        | Range               | 0.18332   |
|                            |          | Interquartile Range | 0.04339   |

```

----- input=2 -----

```

| Tests for Location: Mu0=0 |   |             |          |                   |
|---------------------------|---|-------------|----------|-------------------|
| Test                      |   | -Statistic- |          | -----p Value----- |
| Student's t               | t | -29.985     | Pr >  t  | <.0001            |
| Sign                      | M | -203        | Pr >=  M | <.0001            |
| Signed Rank               | S | -58745      | Pr >=  S | <.0001            |

```

----- input=2 -----

```

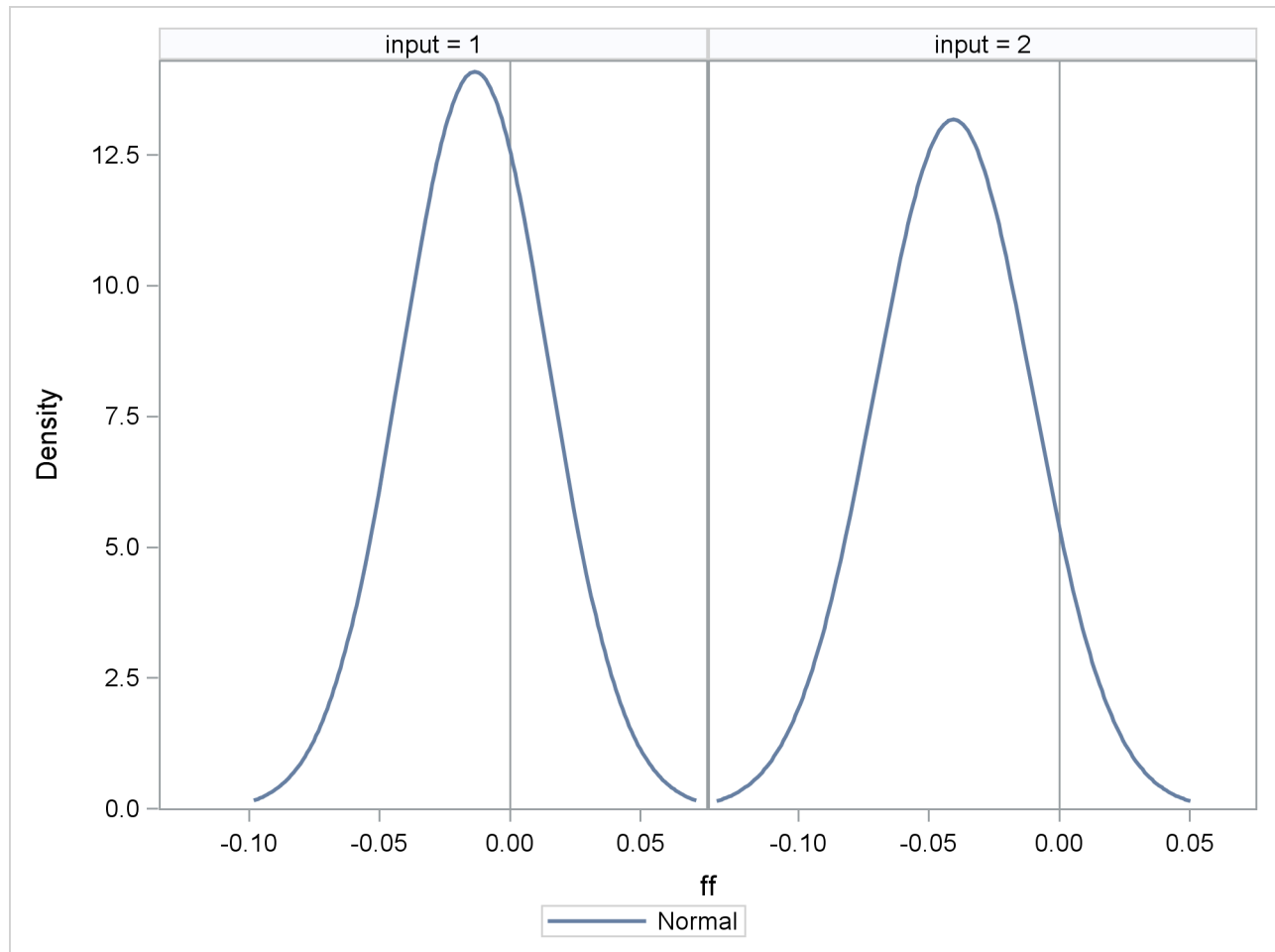
| Quantiles (Definition 5) |             |
|--------------------------|-------------|
| Quantile                 | Estimate    |
| 100% Max                 | 0.06101208  |
| 99%                      | 0.02693796  |
| 95%                      | 0.01008202  |
| 90%                      | -0.00111776 |
| 75% Q3                   | -0.01847726 |
| 50% Median               | -0.04169199 |
| 25% Q1                   | -0.06187039 |
| 10%                      | -0.07798499 |
| 5%                       | -0.08606522 |
| 1%                       | -0.11026564 |
| 0% Min                   | -0.12231183 |

```

----- input=2 -----

```

| Extreme Observations |     |                   |     |
|----------------------|-----|-------------------|-----|
| -----Lowest-----     |     | -----Highest----- |     |
| Value                | Obs | Value             | Obs |
| -0.122312            | 937 | 0.0272906         | 688 |
| -0.119884            | 980 | 0.0291769         | 652 |
| -0.113512            | 920 | 0.0388217         | 670 |
| -0.112345            | 523 | 0.0477261         | 845 |
| -0.110497            | 897 | 0.0610121         | 632 |

**Figure 86.4** Frequency Plot for ff for Each Set of Input Values


---

## Syntax: SIMNORMAL Procedure

The following statements are available in the SIMNORMAL procedure:

```

PROC SIMNORMAL DATA=SAS-data-set < options > ;
 VAR variables ;
 BY variables ;
 CONDITION variables ;

```

Both the PROC SIMNORMAL and VAR statements are required. The following statements can be used with the SIMNORMAL procedure:

---

## PROC SIMNORMAL Statement

```

PROC SIMNORMAL DATA=SAS-data-set < options > ;

```

The PROC SIMNORMAL statement invokes the SIMNORMAL procedure. Table 86.1 summarizes the options available in the PROC SIMNORMAL statement.

**Table 86.1** Summary of PROC SIMNORMAL Statement Options

| Option                                    | Description                                                                         |
|-------------------------------------------|-------------------------------------------------------------------------------------|
| <b>Specify Input and Output Data Sets</b> |                                                                                     |
| DATA=                                     | Specifies input data set (TYPE=CORR, COV, and so on)                                |
| OUT=                                      | Creates output data set that contains simulated values                              |
| <b>Seed Values</b>                        |                                                                                     |
| SEED=                                     | Specifies seed value (integer)                                                      |
| SEEDBY                                    | Requests reinitialization of seed for each BY group                                 |
| <b>Control Contents of OUT= Data Set</b>  |                                                                                     |
| OUTSEED                                   | Requests seed values written to OUT= data set                                       |
| OUTCOND                                   | Requests conditioning variable values written to OUT=data set                       |
| <b>Control Number of Simulated Values</b> |                                                                                     |
| NUMREAL=                                  | Specifies the number of realizations for each BY group written to the OUT= data set |
| <b>Singularity Criteria</b>               |                                                                                     |
| SINGULAR1=                                | Sets the singularity criterion for Cholesky decomposition                           |
| SINGULAR2=                                | Sets the singularity criterion for covariance matrix sweeping                       |

The following options can be used with the PROC SIMNORMAL statement.

**DATA=SAS-data-set**

specifies the input data set that must be a specially structured TYPE=CORR, COV, UCORR, UCOV, or SSCP SAS data set. If the DATA= option is omitted, the most recently created SAS data set is used.

**SEED=seed-value**

specifies the seed to use for the random number generator. If the SEED= value is omitted, the system clock is used. If the system clock is used, a note is written to the log; the note gives the seed value based on the system clock. In addition, the random seed stream is copied to the OUT= data set if the OUTSEED option is specified.

**SEEDBY**

specifies that the seed stream be reinitialized for each BY group. By default, a single random stream is used over all BY groups. If you specify SEEDBY, the random stream starts again at the initial seed value. This initial value is from the SEED= value that you specify. If you do not specify a SEED=value, the system clock generates this initial seed.

For example, suppose you had a TYPE=CORR data set with BY groups, and the mean, variances, and covariance or correlation values were identical for each BY group. Then if you specified SEEDBY, the simulated values in each BY group in the OUT= data set would be identical.

**OUT=SAS-data-set**

specifies a SAS data set in which to store the simulated values for the VAR variables. If you omit the OUT=option, the output data set is created and given a default name by using the DATA $n$  convention.

See the section “OUT= Output Data Set” on page 7446 for details.

**NUMREAL= $n$** 

specifies the number of realizations to generate. A value of NUMREAL=500 generates 500 observations in the OUT=dataset, or 500 observations within each BY group if a BY statement is given.

NUMREAL can be abbreviated as NUMR or NR.

**OUTSEED**

requests that the seed values be included in the OUT= data set. The variable Seed is added to the OUT= data set. The first value of Seed is the SEED= value specified in the PROC SIMNORMAL statement (or obtained from the system clock); subsequent values are produced by the random number generator.

**OUTCOND**

requests that the values of the conditioning variables be included in the OUT= data set. These values are constant for the data set or within a BY group. Note that specifying OUTCOND can greatly increase the size of the OUT= data set. This increase depends on the number of conditioning variables.

**SINGULAR1= $number$** 

specifies the first singularity criterion, which is applied to the Cholesky decomposition of the covariance matrix. The SINGULAR1= value must be in the range (0, 1). The default value is  $10^{-8}$ . SINGULAR1 can be abbreviated SING1.

**SINGULAR2= $number$** 

specifies the second singularity criterion, which is applied to the sweeping of the covariance or correlation matrix to obtain the conditional covariance. The SINGULAR2=option is applicable only when a CONDITION statement is given. The SINGULAR2= value must be in the range (0, 1). The default value is  $10^{-8}$ . SINGULAR2 can be abbreviated SING2.

## BY Statement

**BY variables ;**

A BY statement can be used with the SIMNORMAL procedure to obtain separate simulations for each covariance structure defined by the BY variables. When a BY statement appears, the procedure expects the input DATA= data set to be sorted in the order of the BY variables. If a CONDITION statement is used along with a BY statement, there must be a \_TYPE\_='COND' observation within each BY group. Note that if a BY statement is specified, the number of realizations specified by the NUMREAL= option are produced for each BY group.

## CONDITION Statement

**CONDITION | COND variables ;**



A `CONDITION` statement specifies the conditioning variables. The presence of a `CONDITION` statement requests that a conditional simulation be performed.

The lack of a `CONDITIONAL` statement simply means that an unconditional simulation for the `VAR` variables is to be performed.

If a `CONDITION` statement is given, the variables listed must be numeric variables in the `DATA=` data set. This requires a conditioning value for each of the `CONDITION` variables. This value is supplied by adding a `_TYPE_='COND'` observation for each `CONDITION` variable. Such observations are added to the `DATA=` data set by a `DATA` step.

Note that a data set created by the `CORR` procedure is automatically given the `TYPE=COV`, `UCOV`, `CORR`, or `UCORR` attribute, so you do not have to specify the `TYPE=` option in the `DATA=` option in the `PROC SIMNORMAL` statement. However, when adding the conditioning values by using a `DATA` step with a `SET` statement, you must use the `TYPE=COV`, `UCOV`, `CORR`, or `UCORR` attribute in the new data set. See the section “Getting Started: [SIMNORMAL Procedure](#)” on page 7435 for an example in which the `TYPE` is set.

## VAR Statement

**VAR** *variables* ;

Use the `VAR` statement to specify the analysis variables. Only numeric variables can be specified. If a `VAR` statement is not given, all numeric variables in the `DATA=` data set that are not in the `CONDITION` or `BY` statement are used.

## OUT= Output Data Set

The `SIMNORMAL` procedure produces a single output data set: the `OUT=SAS-data-set`.

The `OUT=` data set contains the following variables:

- all variables listed in the `VAR` statement
- all variables listed in the `BY` statement, if one is given
- `Rnum`, which is the realization number within the current `BY` group
- `Seed`, which is current seed value, if the `OUTSEED` option is specified
- all variables listed in the `CONDITION` statement, if a `CONDITION` statement is given and the `OUTCOND` option is specified

The number of observations is determined by the value of the `NUMREAL=` option. If there are no `BY` groups, the number of observations in the `OUT=` data set is equal to the value of the `NUMREAL=` option. If there are `BY` groups, there are number of observations equals the value of the `NUMREAL=` option for each `BY` group.

---

## Computational Details: SIMNORMAL Procedure

---

### Introduction

There are a number of approaches to simulating a set of dependent random variables. In the context of spatial random fields, these include sequential indicator methods, turning bands, and the Karhunen-Loeve expansion. See Christakos (1992, Chapter 8) and Deutsch and Journel (1992, Chapter 5) for details.

In addition, there is the LU decomposition method, a particularly simple and computationally efficient for normal or Gaussian variates. For a given covariance matrix, the  $\mathbf{LU} = \mathbf{LL}'$  decomposition is computed once, and the simulation proceeds by repeatedly generating a vector of independent  $N(0, 1)$  random variables and multiplying by the  $\mathbf{L}$  matrix.

One problem with this technique is that memory is required to hold the covariance matrix of all the analysis and conditioning variables in core.

---

### Unconditional Simulation

It is a simple matter to produce an  $N(0, 1)$  random number, and by stacking  $k$  such numbers in a column vector you obtain a vector with independent standard normal components  $\mathbf{W} \sim N_k(\mathbf{0}, \mathbf{I})$ . The meaning of the terms *independence* and *randomness* in the context of a deterministic algorithm required for the generation of these numbers is somewhat subtle; see Knuth (1973, Vol. 2, Chapter 3) for a discussion of these issues.

Rather than  $\mathbf{W} \sim N_k(\mathbf{0}, \mathbf{I})$ , what is required is the generation of a vector  $\mathbf{Z} \sim N_k(\mathbf{0}, \mathbf{V})$ —that is,

$$\mathbf{Z} = \begin{bmatrix} Z_1 \\ Z_2 \\ \vdots \\ Z_k \end{bmatrix}$$

with covariance matrix

$$\mathbf{V} = \begin{pmatrix} \sigma_{11} & \sigma_{12} & \cdots & \sigma_{1k} \\ \sigma_{21} & \sigma_{22} & \cdots & \sigma_{2k} \\ & \ddots & & \\ \sigma_{k1} & \sigma_{k2} & \cdots & \sigma_{kk} \end{pmatrix}$$

where

$$\sigma_{ij} = \text{Cov}(Z_i, Z_j)$$

If the covariance matrix is symmetric and positive definite, it has a Cholesky root  $\mathbf{L}$  such that  $\mathbf{V}$  can be factored as

$$\mathbf{V} = \mathbf{L}\mathbf{L}'$$

where  $\mathbf{L}$  is lower triangular. See Ralston and Rabinowitz (1978, Chapter 9, Section 3-3) for details. This vector  $\mathbf{Z}$  can be generated by the transformation  $\mathbf{Z} = \mathbf{L}\mathbf{W}$ . Note that this is where the assumption of multivariate normality is crucial. If  $\mathbf{W} \sim N_k(\mathbf{0}, \mathbf{I}_k)$ , then  $\mathbf{Z} = \mathbf{L}\mathbf{W}$  is also normal or Gaussian. The mean of  $\mathbf{Z}$  is

$$E(\mathbf{Z}) = \mathbf{L}(E(\mathbf{W})) = \mathbf{0}$$

and the variance is

$$\text{Var}(\mathbf{Z}) = \text{Var}(\mathbf{L}\mathbf{W}) = E(\mathbf{L}\mathbf{W}\mathbf{W}'\mathbf{L}') = \mathbf{L} E(\mathbf{W}\mathbf{W}') \mathbf{L}' = \mathbf{L}\mathbf{L}' = \mathbf{V}$$

Finally, let  $Y_k = Z_k + \mu_k$ ; that is, you add a mean term to each variable  $Z_k$ . The covariance structure of the  $Y_k$ 's remains the same. Unconditional simulation is done by simply repeatedly generating  $k$   $N(0, 1)$  random numbers, stacking them, and performing the transformation

$$\mathbf{W} \mapsto \mathbf{Z} = \mathbf{L}\mathbf{W} \mapsto \mathbf{Y} = \mathbf{Z} + \boldsymbol{\mu}$$

## Conditional Simulation

For a conditional simulation, this distribution of

$$\mathbf{Y} = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_k \end{bmatrix}$$

must be conditioned on the values of the CONDITION variables. The relevant general result concerning conditional distributions of multivariate normal random variables is the following. Let  $\mathbf{X} \sim N_m(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ , where

$$\mathbf{X} = \begin{bmatrix} \mathbf{X}_1 \\ \mathbf{X}_2 \end{bmatrix}$$

$$\boldsymbol{\mu} = \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}$$

$$\boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\Sigma}_{11} & \boldsymbol{\Sigma}_{12} \\ \boldsymbol{\Sigma}_{21} & \boldsymbol{\Sigma}_{22} \end{pmatrix}$$

and where  $bX_1$  is  $k \times 1$ ,  $X_2$  is  $n \times 1$ ,  $\Sigma_{11}$  is  $k \times k$ ,  $\Sigma_{22}$  is  $n \times n$ , and  $\Sigma_{12} = \Sigma'_{21}$  is  $k \times n$ , with  $k + n = m$ . The full vector  $\mathbf{X}$  has simply been partitioned into two subvectors,  $\mathbf{X}_1$  and  $\mathbf{X}_2$ , and  $\Sigma$  has been similarly partitioned into covariances and cross covariances.

With this notation, the distribution of  $\mathbf{X}_1$  conditioned on  $\mathbf{X}_2 = x_2$  is  $N_k(\tilde{\mu}, \tilde{\Sigma})$ , with

$$\tilde{\mu} = \mu_1 + \Sigma_{12}\Sigma_{22}^{-1}(x_2 - \mu_2)$$

and

$$\tilde{\Sigma} = \Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}$$

See Searle (1971, pp. 46–47) for details.

Using the SIMNORMAL procedure corresponds with the conditional simulation as follows. Let  $Y_1, \dots, Y_k$  be the VAR variables as before ( $k$  is the number of variables in the VAR list). Let the mean vector for  $\mathbf{Y}$  be denoted by  $\mu_1 = E(\mathbf{Y})$ . Let the CONDITION variables be denoted by  $C_1, \dots, C_n$  (where  $n$  is the number of variables in the COND list). Let the mean vector for  $\mathbf{C}$  be denoted by  $\mu_2 = E(\mathbf{C})$  and the conditioning values be denoted by

$$\mathbf{c} = \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{bmatrix}$$

Then stacking

$$\mathbf{X} = \begin{bmatrix} \mathbf{Y} \\ \mathbf{C} \end{bmatrix}$$

the variance of  $\mathbf{X}$  is

$$\mathbf{V} = \text{Var}(\mathbf{X}) = \Sigma = \begin{pmatrix} \mathbf{V}_{11} & \mathbf{V}_{12} \\ \mathbf{V}_{21} & \mathbf{V}_{22} \end{pmatrix}$$

where  $\mathbf{V}_{11} = \text{Var}(\mathbf{Y})$ ,  $\mathbf{V}_{12} = \text{Cov}(\mathbf{Y}, \mathbf{C})$ , and  $\mathbf{V}_{22} = \text{Var}(\mathbf{C})$ . By using the preceding general result, the relevant covariance matrix is

$$\tilde{\mathbf{V}} = \mathbf{V}_{11} - \mathbf{V}_{12}\mathbf{V}_{22}^{-1}\mathbf{V}_{21}$$

and the mean is

$$\tilde{\mu} = \mu_1 + \mathbf{V}_{12}\mathbf{V}_{22}^{-1}(\mathbf{c} - \mu_2)$$

By using  $\tilde{\mathbf{V}}$  and  $\tilde{\mu}$ , simulating  $(\mathbf{Y}|\mathbf{C} = \mathbf{c}) \sim N_k(\tilde{\mu}, \tilde{\mathbf{V}})$  now proceeds as in the unconditional case.

## References

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# Chapter 87

## The STDIZE Procedure

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### Overview: STDIZE Procedure

The STDIZE procedure standardizes one or more numeric variables in a SAS data set by subtracting a location measure and dividing by a scale measure. A variety of location and scale measures are provided, including estimates that are resistant to outliers and clustering. Some of the well-known standardization methods such as mean, median, standard deviation, range, Huber's estimate, Tukey's biweight estimate, and Andrew's wave estimate are available in the STDIZE procedure.

In addition, you can multiply each standardized value by a constant and add a constant. Thus, the final output value is

$$result = add + multiply \times \frac{original - location}{scale}$$

where

*result* = final output value  
*add* = constant to add (ADD= option)  
*multiply* = constant to multiply by (MULT= option)  
*original* = original input value  
*location* = location measure  
*scale* = scale measure

PROC STDIZE can also find quantiles in one pass of the data, a capability that is especially useful for very large data sets. With such data sets, the UNIVARIATE procedure might have high or excessive memory or time requirements.

## Getting Started: STDIZE Procedure

The following example demonstrates how you can use the STDIZE procedure to obtain location and scale measures of your data.

In the following hypothetical data set, a random sample of grade twelve students is selected from a number of coeducational schools. Each school is classified as one of two types: Urban or Rural. There are 40 observations.

The variables are id (student identification), Type (type of school attended: 'urban'=urban area and 'rural'=rural area), and total (total assessment scores in History, Geometry, and Chemistry).

The following DATA step creates the SAS data set TotalScores.

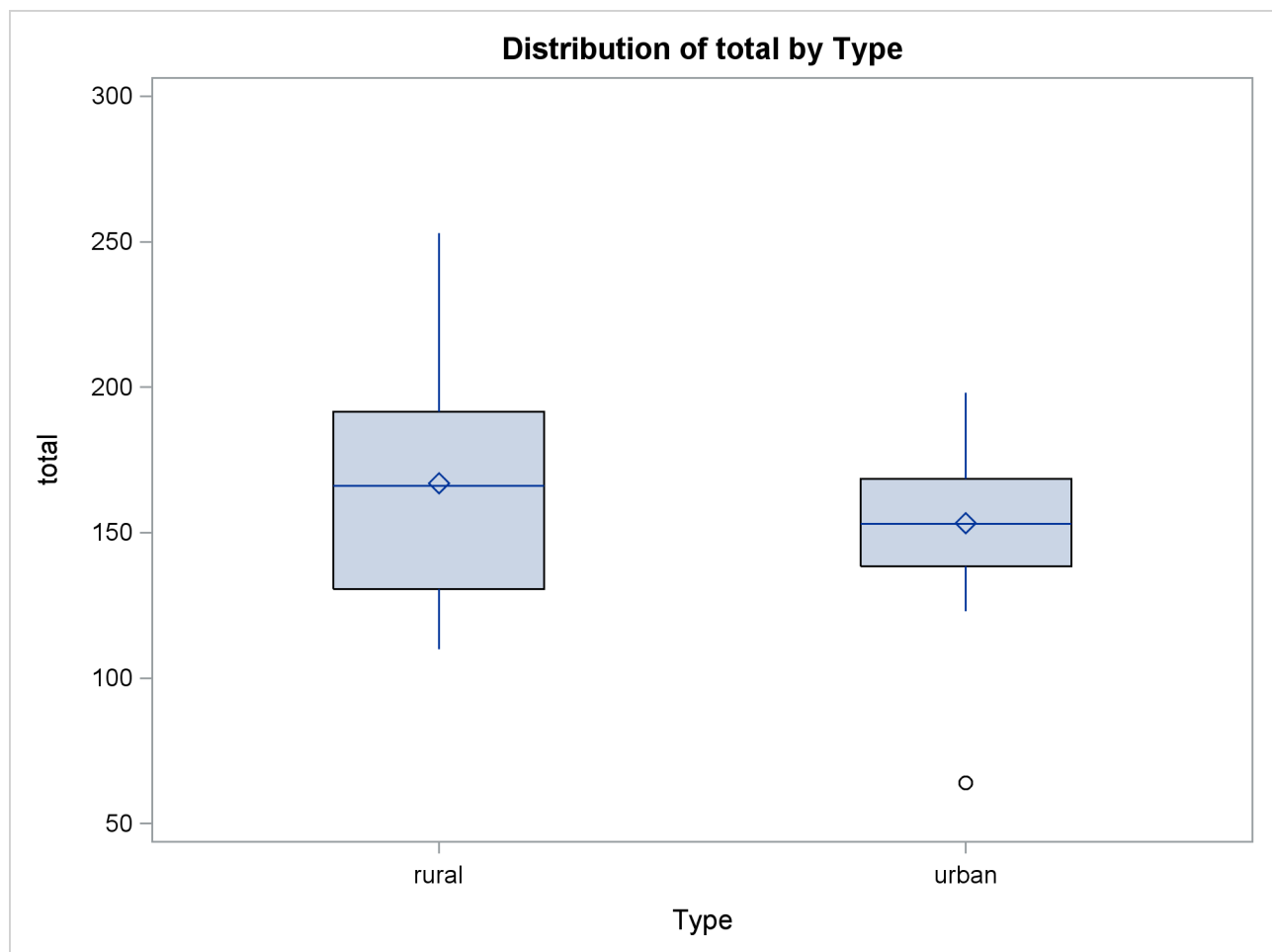
```
data TotalScores;
 title 'High School Scores Data';
 input id Type $ total @@;
 datalines;
 1 rural 135 2 rural 125 3 rural 223 4 rural 224 5 rural 133
 6 rural 253 7 rural 144 8 rural 193 9 rural 152 10 rural 178
 11 rural 120 12 rural 180 13 rural 154 14 rural 184 15 rural 187
 16 rural 111 17 rural 190 18 rural 128 19 rural 110 20 rural 217
 21 urban 192 22 urban 186 23 urban 64 24 urban 159 25 urban 133
 26 urban 163 27 urban 130 28 urban 163 29 urban 189 30 urban 144
 31 urban 154 32 urban 198 33 urban 150 34 urban 151 35 urban 152
 36 urban 151 37 urban 127 38 urban 167 39 urban 170 40 urban 123
 ;
```

Suppose you now want to standardize the total scores in different types of schools prior to any further analysis. Before standardizing the total scores, you can use the box plot from PROC BOXPLOT to summarize the total scores for both types of schools.

```
ods graphics on;
proc boxplot data=TotalScores;
 plot total*Type / boxstyle=schematic noserifs;
run;
```

The PLOT statement in the PROC BOXPLOT statement creates the schematic plots (without the serifs) when you specify `boxstyle=schematic noserifs`. Figure 87.1 displays a box plot for each type of school.

**Figure 87.1** Schematic Plots from PROC BOXPLOT





Inspection reveals that one urban score is a low outlier. Also, if you compare the lengths of two box plots, there seems to be twice as much dispersion for the rural scores as for the urban scores.

The following PROC UNIVARIATE statement reports the information about the extreme values of the Score variable for each type of school:

```
proc univariate data=TotalScores;
 var total;
 by Type;
run;
```

Figure 87.2 displays the table from PROC UNIVARIATE for the lowest and highest five total scores for urban schools. The outlier (Obs = 23), marked in Figure 87.2 by the symbol '0', has a score of 64.

**Figure 87.2** Table for Extreme Observations When Type=urban

| High School Scores Data  |     |                |     |
|--------------------------|-----|----------------|-----|
| ----- Type=urban -----   |     |                |     |
| The UNIVARIATE Procedure |     |                |     |
| Variable: total          |     |                |     |
| Extreme Observations     |     |                |     |
| ----Lowest----           |     | ----Highest--- |     |
| Value                    | Obs | Value          | Obs |
| 64                       | 23  | 170            | 39  |
| 123                      | 40  | 186            | 22  |
| 127                      | 37  | 189            | 29  |
| 130                      | 27  | 192            | 21  |
| 133                      | 25  | 198            | 32  |

The following PROC STDIZE procedure requests the METHOD=STD option for computing the location and scale measures:

```
proc stdize data=totalscores method=std pstat;
 title2 'METHOD=STD';
 var total;
 by Type;
run;
```

Figure 87.3 displays the table of location and scale measures from the PROC STDIZE statement. PROC STDIZE uses the sample mean as the location measure and the sample standard deviation as the scale measure for standardizing. The PSTAT option displays a table containing these two measures.

**Figure 87.3** Location and Scale Measures Table When METHOD=STD

| High School Scores Data<br>METHOD=STD |            |                            |    |
|---------------------------------------|------------|----------------------------|----|
| ----- Type=rural -----                |            |                            |    |
| The STDIZE Procedure                  |            |                            |    |
| Location and Scale Measures           |            |                            |    |
| Location = mean                       |            | Scale = standard deviation |    |
| Name                                  | Location   | Scale                      | N  |
| total                                 | 167.050000 | 41.956713                  | 20 |
| High School Scores Data<br>METHOD=STD |            |                            |    |
| ----- Type=urban -----                |            |                            |    |
| The STDIZE Procedure                  |            |                            |    |
| Location and Scale Measures           |            |                            |    |
| Location = mean                       |            | Scale = standard deviation |    |
| Name                                  | Location   | Scale                      | N  |
| total                                 | 153.300000 | 30.066768                  | 20 |

The ratio of the scale of rural scores to the scale of urban scores is approximately 1.4 (41.96/30.07). This ratio is smaller than the dispersion ratio observed in the previous schematic plots.

The STDIZE procedure provides several location and scale measures that are resistant to outliers. The following statements invoke three different standardization methods and display the tables for the location and scale measures:

```
proc stdize data=totalscores method=mad pstat;
 title2 'METHOD=MAD';
 var total;
 by Type;
run;
```

```
proc stdize data=totalscores method=iqr pstat;
 title2 'METHOD=IQR';
 var total;
 by Type;
run;
```

```

proc stdize data=totalscores method=abw(4) pstat;
 title2 'METHOD=ABW(4)';
 var total;
 by Type;
run;

```

Figure 87.4 displays the table of location and scale measures when the standardization method is median absolute deviation (MAD). The location measure is the median, and the scale measure is the median absolute deviation from the median. The ratio of the scale of rural scores to the scale of urban scores is approximately 2.06 (32.0/15.5) and is close to the dispersion ratio observed in the previous schematic plots.

**Figure 87.4** Location and Scale Measures Table When METHOD=MAD

| High School Scores Data<br>METHOD=MAD |            |                                    |    |
|---------------------------------------|------------|------------------------------------|----|
| ----- Type=rural -----                |            |                                    |    |
| The STDIZE Procedure                  |            |                                    |    |
| Location and Scale Measures           |            |                                    |    |
| Location = median                     |            | Scale = median abs dev from median |    |
| Name                                  | Location   | Scale                              | N  |
| total                                 | 166.000000 | 32.000000                          | 20 |
| High School Scores Data<br>METHOD=MAD |            |                                    |    |
| ----- Type=urban -----                |            |                                    |    |
| The STDIZE Procedure                  |            |                                    |    |
| Location and Scale Measures           |            |                                    |    |
| Location = median                     |            | Scale = median abs dev from median |    |
| Name                                  | Location   | Scale                              | N  |
| total                                 | 153.000000 | 15.500000                          | 20 |

Figure 87.5 displays the table of location and scale measures when the standardization method is IQR. The location measure is the median, and the scale measure is the interquartile range. The ratio of the scale of rural scores to the scale of urban scores is approximately 2.03 (61/30) and is, in fact, the dispersion ratio observed in the previous schematic plots.

**Figure 87.5** Location and Scale Measures Table When METHOD=IQR

| High School Scores Data<br>METHOD=IQR |            |                             |    |
|---------------------------------------|------------|-----------------------------|----|
| ----- Type=rural -----                |            |                             |    |
| The STDIZE Procedure                  |            |                             |    |
| Location and Scale Measures           |            |                             |    |
| Location = median                     |            | Scale = interquartile range |    |
| Name                                  | Location   | Scale                       | N  |
| total                                 | 166.000000 | 61.000000                   | 20 |
| High School Scores Data<br>METHOD=IQR |            |                             |    |
| ----- Type=urban -----                |            |                             |    |
| The STDIZE Procedure                  |            |                             |    |
| Location and Scale Measures           |            |                             |    |
| Location = median                     |            | Scale = interquartile range |    |
| Name                                  | Location   | Scale                       | N  |
| total                                 | 153.000000 | 30.000000                   | 20 |

Figure 87.6 displays the table of location and scale measures when the standardization method is ABW, for which the location measure is the biweight one-step M-estimate, and the scale measure is the biweight A-estimate. Note that the initial estimate for ABW is MAD. The following steps help to decide the value of the tuning constant:

1. For rural scores, the location estimate for MAD is 166.0, and the scale estimate for MAD is 32.0. The maximum of the rural scores is 253 (not shown), and the minimum is 110 (not shown). Thus, the tuning constant needs to be 3 so that it does not reject any observation that has a score between 110 to 253.
2. For urban scores, the location estimate for MAD is 153.0, and the scale estimate for MAD is 15.5. The maximum of the rural scores is 198, and the minimum (also an outlier) is 64. Thus, the tuning constant needs to be 4 so that it rejects the outlier (64) but includes the maximum (198) as a normal observation.
3. The maximum of the tuning constants, obtained in steps 1 and 2, is 4.

See Goodall (1983, Chapter 11) for details about the tuning constant. The ratio of the scale of rural scores to the scale of urban scores is approximately 2.06 (32.0/15.5). It is also close to the dispersion ratio observed in the previous schematic plots.

**Figure 87.6** Location and Scale Measures Table When METHOD=ABW

| High School Scores Data<br>METHOD=ABW(4) |            |                             |    |
|------------------------------------------|------------|-----------------------------|----|
| ----- Type=rural -----                   |            |                             |    |
| The STDIZE Procedure                     |            |                             |    |
| Location and Scale Measures              |            |                             |    |
| Location = biweight 1-step M-estimate    |            | Scale = biweight A-estimate |    |
| Name                                     | Location   | Scale                       | N  |
| total                                    | 162.889603 | 56.662855                   | 20 |
| High School Scores Data<br>METHOD=ABW(4) |            |                             |    |
| ----- Type=urban -----                   |            |                             |    |
| The STDIZE Procedure                     |            |                             |    |
| Location and Scale Measures              |            |                             |    |
| Location = biweight 1-step M-estimate    |            | Scale = biweight A-estimate |    |
| Name                                     | Location   | Scale                       | N  |
| total                                    | 156.014608 | 28.615980                   | 20 |

The preceding analysis shows that METHOD=MAD, METHOD=IQR, and METHOD=ABW all provide better dispersion ratios than METHOD=STD does.

You can recompute the standard deviation after deleting the outlier from the original data set for comparison. The following statements create a data set NoOutlier that excludes the outlier from the TotalScores data set and invoke PROC STDIZE with METHOD=STD.

```
data NoOutlier;
 set totalscores;
 if (total = 64) then delete;
run;

proc stdize data=NoOutlier method=std pstat;
 title2 'After Removing Outlier, METHOD=STD';
 var total;
 by Type;
run;
```

Figure 87.7 displays the location and scale measures after deleting the outlier. The lack of resistance of the standard deviation to outliers is clearly illustrated: if you delete the outlier, the sample standard deviation of urban scores changes from 30.07 to 22.09. The new ratio of the scale of rural scores to the scale of urban scores is approximately 1.90 (41.96/22.09).

**Figure 87.7** Location and Scale Measures Table When METHOD=STD without the Outlier

| High School Scores Data<br>After Removing Outlier, METHOD=STD |            |                            |    |
|---------------------------------------------------------------|------------|----------------------------|----|
| ----- Type=rural -----                                        |            |                            |    |
| The STDIZE Procedure                                          |            |                            |    |
| Location and Scale Measures                                   |            |                            |    |
| Location = mean                                               |            | Scale = standard deviation |    |
| Name                                                          | Location   | Scale                      | N  |
| total                                                         | 167.050000 | 41.956713                  | 20 |
| High School Scores Data<br>After Removing Outlier, METHOD=STD |            |                            |    |
| ----- Type=urban -----                                        |            |                            |    |
| The STDIZE Procedure                                          |            |                            |    |
| Location and Scale Measures                                   |            |                            |    |
| Location = mean                                               |            | Scale = standard deviation |    |
| Name                                                          | Location   | Scale                      | N  |
| total                                                         | 158.000000 | 22.088207                  | 19 |

---

## Syntax: STDIZE Procedure

The following statements are available in the STDIZE procedure:

```

PROC STDIZE < options > ;
 BY variables ;
 FREQ variable ;
 LOCATION variables ;
 SCALE variables ;
 VAR variables ;
 WEIGHT variable ;

```

The PROC STDIZE statement is required. The BY, LOCATION, FREQ, VAR, SCALE, and WEIGHT statements are described in alphabetical order following the PROC STDIZE statement.

## PROC STDIZE Statement

**PROC STDIZE** < options > ;

The PROC STDIZE statement invokes the STDIZE procedure. You can specify the following options in the PROC STDIZE statement. Table 87.1 summarizes the options available in the PROC STDIZE statement.

**Table 87.1** Summary of PROC STDIZE Statement Options

| Option                                 | Description                                                                                                                |
|----------------------------------------|----------------------------------------------------------------------------------------------------------------------------|
| <b>Specify standardization methods</b> |                                                                                                                            |
| METHOD=                                | Specifies the name of the standardization method                                                                           |
| INITIAL=                               | Specifies the method for computing initial estimates for the A estimates                                                   |
| <b>Unstandardize variables</b>         |                                                                                                                            |
| UNSTD                                  | Unstandardizes variables when you also specify the METHOD=IN option                                                        |
| <b>Process missing values</b>          |                                                                                                                            |
| NOMISS                                 | Omits observations with any missing values from computation                                                                |
| MISSING=                               | Specifies the method or a numeric value for replacing missing values                                                       |
| REPLACE                                | Replaces missing data with zero in the standardized data                                                                   |
| REONLY                                 | Replaces missing data with the location measure (does not standardize the data)                                            |
| <b>Specify data set details</b>        |                                                                                                                            |
| DATA=                                  | Specifies the input data set                                                                                               |
| KEEPLN                                 | Specifies that output variables inherit the length of the analysis variable                                                |
| OUT=                                   | Specifies the output data set                                                                                              |
| OPREFIX=                               | Specifies that original variables appear in the OUT= data set                                                              |
| SPREFIX=                               | Specifies a prefix for the standardized variable names                                                                     |
| OUTSTAT=                               | Specifies the output statistic data set                                                                                    |
| <b>Specify computational settings</b>  |                                                                                                                            |
| VARDEF=                                | Specifies the variances divisor                                                                                            |
| NMARKERS=                              | Specifies the number of markers when you also specify PCTLMTD=ONEPASS                                                      |
| MULT=                                  | Specifies the constant to multiply each value by after standardizing                                                       |
| ADD=                                   | Specifies the constant to add to each value after standardizing and multiplying by the value specified in the MULT= option |
| FUZZ=                                  | Specifies the relative fuzz factor for writing the output                                                                  |
| <b>Specify percentiles</b>             |                                                                                                                            |
| PCTLDEF=                               | Specifies the definition of percentiles when you also specify the PCTLMTD=ORD_STAT option                                  |

Table 87.1 continued

| Option                            | Description                                                                                                 |
|-----------------------------------|-------------------------------------------------------------------------------------------------------------|
| PCTLMTD=                          | Specifies the method used to estimate percentiles                                                           |
| PCTLPTS=                          | Writes observations containing percentiles to the data set specified in the OUTSTAT= option                 |
| <b>Normalize scale estimators</b> |                                                                                                             |
| NORM                              | Normalizes the scale estimator to be consistent for the standard deviation of a normal distribution         |
| SNORM                             | Normalizes the scale estimator to have an expectation of approximately 1 for a standard normal distribution |
| <b>Specify output</b>             |                                                                                                             |
| PSTAT                             | Displays the location and scale measures                                                                    |

These options and their abbreviations are described (in alphabetical order) in the remainder of this section.

**ADD=c**

specifies a constant, *c*, to add to each value after standardizing and multiplying by the value you specify in the MULT= option. The default value is 0.

**DATA=SAS-data-set**

specifies the input data set to be standardized. If you omit the DATA= option, the most recently created data set is used.

**FUZZ=c**

specifies the relative fuzz factor. The default value is 1E-14. For the OUT= data set, the score is computed as follows:

$$\text{if } |result| < m \times c \text{ then } result = 0$$

where *m* is the constant specified in the MULT= option, or 1 if MULT= option is not specified.

For the OUTSTAT= data set and the location and scale table, the *scale* and *location* values are computed as follows:

$$\text{if } scale < |location| \times c \text{ then } scale = 0$$

Otherwise,

$$\text{if } |location| < m \times c \text{ then } location = 0$$

**INITIAL=method**

specifies the method for computing initial estimates for the A estimates (ABW, AWAVE, and AHUBER). You cannot specify the following methods for initial estimates: INITIAL=ABW, INITIAL=AHUBER, INITIAL=AWAVE, and INITIAL=IN. The default is INITIAL=MAD.



**KEEPLN**

specifies that the standardized variables inherit the lengths of the analysis variables that PROC STDIZE uses to derive them. PROC STDIZE stores numbers in double-precision without this option.

*Caution:* The KEEPLEN option causes the standardized variables to permanently lose numeric precision by truncating or rounding the values. However, the precision of the output variables will match that of the input.

**METHOD=*name***

specifies the name of the method for computing location and scale measures. Valid values for *name* are as follows: MEAN, MEDIAN, SUM, EUCLEN, USTD, STD, RANGE, MIDRANGE, MAXABS, IQR, MAD, ABW, AHUBER, AWAVE, AGK, SPACING, L, and IN.

For details about these methods, see the descriptions in the section “[Standardization Methods](#)” on page 7468. The default is METHOD=STD.

**MISSING=*method* | *value***

specifies the method (or a numeric value) for replacing missing values. If you omit the MISSING= option, the REPLACE option replaces missing values with the location measure given by the METHOD= option. Specify the MISSING= option when you want to replace missing values with a different value. You can specify any name that is valid in the METHOD= option except the name IN. The corresponding location measure is used to replace missing values.

If a numeric value is given, the value replaces missing values after standardizing the data. However, you can specify the REONLY option with the MISSING= option to suppress standardization for cases in which you want only to replace missing values.

**MULT=*c***

specifies a constant, *c*, by which to multiply each value after standardizing. The default value is 1.

**NMARKERS=*n***

specifies the number of markers used when you specify the one-pass algorithm (PCTLMTD=ONEPASS). The value *n* must be greater than or equal to 5. The default value is 105.

**NOMISS**

omits observations with missing values for any of the analyzed variables from calculation of the location and scale measures. If you omit the NOMISS option, all nonmissing values are used.

**NORM**

normalizes the scale estimator to be consistent for the standard deviation of a normal distribution when you specify the option METHOD=AGK, METHOD=IQR, METHOD=MAD, or METHOD=SPACING.

**OPREFIX<=*o-prefix*>**

specifies that the original variables should appear in the OUT= data set. You can optionally specify an equal sign and a prefix. For example, if OPREFIX=Original, then the names of the variables are OriginalVAR1, OriginalVAR2, and so on, where VAR1 and VAR2 are the original variable names. The value of OPREFIX= must be different from the value of SPREFIX=. If you specify OPREFIX, without an equal sign and a prefix, then the default prefix is null and you must specify SPREFIX=*s-prefix*.

**OUT=SAS-data-set**

specifies the name of the SAS data set created by PROC STDIZE. By default, the output data set is a copy of the DATA= data set except that the analyzed variables have been standardized. Analyzed variables are those specified in the VAR statement or, if there is no VAR statement, all numeric variables not listed in any other statement. However, you can use the OPREFIX option to request that both the original and standardized variables be included in the output data set. You can change variable names by specifying prefixes with the OPREFIX= and SPREFIX= options. See the section “[Output Data Sets](#)” on page 7473 for more information.

If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*.

If you omit the OUT= option, PROC STDIZE creates an output data set named according to the DATA $n$  convention.

**OUTSTAT=SAS-data-set**

specifies the name of the SAS data set containing the location and scale measures and other computed statistics. See the section “[Output Data Sets](#)” on page 7473 for more information.

**PCTLDEF=percentiles**

specifies which of five definitions is used to calculate percentiles when you specify the option PCTLMTD=ORD\_STAT. By default, PCTLDEF=5. Note that the option PCTLMTD=ONEPASS implies PCTLDEF=5. See the section “[Computational Methods for the PCTLDEF= Option](#)” on page 7471 for details about percentile definition.

You cannot use PCTLDEF= when you compute weighted quantiles.

**PCTLMTD=ORD\_STAT | ONEPASS | P2**

specifies the method used to estimate percentiles. Specify the PCTLMTD=ORD\_STAT option to compute the percentiles by the order statistics method.

The PCTLMTD=ONEPASS option modifies an algorithm invented by Jain and Chlamtac (1985). See the section “[Computing Quantiles](#)” on page 7471 for more details about this algorithm.

**PCTLPTS= $n$** 

writes percentiles to the OUTSTAT= data set. Values of  $n$  can be any decimal number between 0 and 100, inclusive.

A requested percentile is identified by the \_TYPE\_ variable in the OUTSTAT= data set with a value of P $n$ . For example, suppose you specify the option PCTLPTS=10, 30. The corresponding observations in the OUTSTAT= data set that contain the 10th and the 30th percentiles would then have values \_TYPE\_=P10 and \_TYPE\_=P30, respectively.

**PSTAT**

displays the location and scale measures.

**REPLACE**

replaces missing data with the value 0 in the standardized data (this value corresponds to the location measure before standardizing). To replace missing data by other values, see the preceding description of the MISSING= option. You cannot specify both the REPLACE and REONLY options.

**REONLY**

replaces missing data only; PROC STDIZE does not standardize the data. Missing values are replaced with the location measure unless you also specify the `MISSING=value` option, in which case missing values are replaced with *value*. You cannot specify both the `REPLACE` and `REONLY` options.

**SNORM**

normalizes the scale estimator to have an expectation of approximately 1 for a standard normal distribution when you specify the `METHOD=SPACING` option.

**SPREFIX=<s-prefix>**

specifies a prefix for the standardized variables. For example, if `SPREFIX=Std`, then the names of the standardized variables are `StdVAR1`, `StdVAR2`, and so on, where `VAR1` and `VAR2` are the original variable names. The value of `SPREFIX=` must be different from the value of `OPREFIX=`. The default prefix is null. If you omit the `SPREFIX` option, the standardized variables still appear in the `OUT=` data set by default and the variable names remain the same. If you want to have the variable names changed, you need to specify a prefix with `SPREFIX=s-prefix`.

**UNSTD****UNSTDIZE**

unstandardizes variables when you specify the `METHOD=IN(ds)` option. The location and scale measures, along with constants for addition and multiplication that the unstandardization is based on, are identified by the `_TYPE_` variable in the `ds` data set.

The `ds` data set must have a `_TYPE_` variable and contain the following two observations: a `_TYPE_ = 'LOCATION'` observation and a `_TYPE_ = 'SCALE'` observation. The variable `_TYPE_` can also contain the optional observations, `'ADD'` and `'MULT'`; if these observations are not found in the `ds` data set, the constants specified in the `ADD=` and `MULT=` options (or their default values) are used for unstandardization.

See the section “`OUTSTAT= Data Set`” on page 7473 for details about the statistics that each value of `_TYPE_` represents. The formula used for unstandardization is as follows: If the final output value from the previous standardization is calculated as

$$result = add + multiply \times \frac{original - location}{scale}$$

The unstandardized variable is computed as

$$original = scale \times \frac{result - add}{multiply} + location$$

**VARDEF=DF | N | WDF | WEIGHT | WGT**

specifies the divisor to be used in the calculation of variances. By default, `VARDEF=DF`. The values and associated divisors are as follows.

| Value        | Divisor                | Formula            |
|--------------|------------------------|--------------------|
| DF           | Degrees of freedom     | $n - 1$            |
| N            | Number of observations | $n$                |
| WDF          | Sum of weights minus 1 | $(\sum_i w_i) - 1$ |
| WEIGHT   WGT | Sum of weights         | $\sum_i w_i$       |

---

## BY Statement

**BY variables ;**

You can specify a BY statement with PROC STDIZE to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the STDIZE procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

When you specify the option METHOD=IN(ds), the following rules are applied to BY-group processing:

- If the ds data set does not contain any of the BY variables, the entire DATA= data set is standardized by the location and scale measures (along with the constants for addition and multiplication) in the ds data set.
- If the ds data set contains some, but not all, of the BY variables or if some BY variables do not have the same type or length in the ds data set that they have in the DATA= data set, PROC STDIZE displays an error message and stops.
- If all of the BY variables appear in the ds data set with the same type and length as in the DATA= data set, each BY group in the DATA= data set is standardized using the location and scale measures (along with the constants for addition and multiplication) from the corresponding BY group in the ds data set. The BY groups in the ds data set must be in the same order in which they appear in the DATA= data set. All BY groups in the DATA= data set must also appear in the ds data set. If you do not specify the NOTSORTED option, some BY groups can appear in the ds data set but not in the DATA= data set; such BY groups are not used in standardizing data.

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

---

## FREQ Statement

**FREQ** *variable* ;

If one variable in the input data set represents the frequency of occurrence for other values in the observation, specify the variable name in a FREQ statement. PROC STDIZE treats the data set as if each observation appeared  $n$  times, where  $n$  is the value of the FREQ variable for the observation. Nonintegral values of the FREQ variable are truncated to the largest integer less than the FREQ value. If the FREQ variable has a value that is less than 1 or is missing, the observation is not used in the analysis.

### NOTRUNCATE

#### NOTRUNC

specifies that frequency values are not truncated to integers.

The nonintegral values of the FREQ variable can be used for the following standardization methods: AGK, ABW, AHUBER, AWAVE, EUCLLEN, IQR, L, MAD, MEAN, MEDIAN, SPACING, STD, SUM, and USTD. The nonintegral frequency values are used for the MAD, MEDIAN, or IQR method only when PCTLMTD=ORD\_STAT is specified. If PCTLMTD=ONEPASS is specified, the NOTRUNCATE option is ignored.

---

## LOCATION Statement

**LOCATION** *variables* ;

The LOCATION statement specifies a list of numeric variables that contain location measures in the input data set specified by the METHOD=IN option.

---

## SCALE Statement

**SCALE** *variables* ;

The SCALE statement specifies the list of numeric variables that contain scale measures in the input data set specified by the METHOD=IN option.

---

## VAR Statement

**VAR** *variable* ;

The VAR statement lists numeric variables to be standardized. If you omit the VAR statement, all numeric variables not listed in the BY, FREQ, and WEIGHT statements are used.

## WEIGHT Statement

**WEIGHT** *variable* ;

The WEIGHT statement specifies a numeric variable in the input data set with values that are used to weight each observation. Only one variable can be specified.

The WEIGHT variable values can be nonintegers. An observation is used in the analysis only if the value of the WEIGHT variable is greater than zero.

The WEIGHT variable applies only when you specify the following standardization methods: AGK, EUCLEN, IQR, L, MAD, MEAN, MEDIAN, STD, SUM, and USTD. Weights are used for the METHOD=MAD, MEDIAN, or IQR only when PCTLMTD=ORD\_STAT is specified; if PCTLMTD=ONEPASS is specified, the WEIGHT statement is ignored.

PROC STDIZE uses the value of the WEIGHT variable to calculate the sample mean and sample variances:

$$\bar{x}_w = \sum_i w_i x_i / \sum_i w_i \quad (\text{sample mean})$$

$$us_w^2 = \sum_i w_i x_i^2 / d \quad (\text{uncorrected sample variances})$$

$$s_w^2 = \sum_i w_i (x_i - \bar{x}_w)^2 / d \quad (\text{sample variances})$$

where  $w_i$  is the weight value of the  $i$ th observation,  $x_i$  is the value of the  $i$ th observation, and  $d$  is the divisor controlled by the VARDEF= option (see the VARDEF= option for details).

The following weighted statistics are defined accordingly:

|        |                                                                                                        |
|--------|--------------------------------------------------------------------------------------------------------|
| MEAN   | the weighted mean, $\bar{x}_w$                                                                         |
| SUM    | the weighted sum, $\sum_i w_i x_i$                                                                     |
| USTD   | the weighted uncorrected standard deviation, $\sqrt{us_w^2}$                                           |
| STD    | the weighted standard deviation, $\sqrt{s_w^2}$                                                        |
| EUCLEN | the weighted Euclidean length, computed as the square root of the weighted uncorrected sum of squares: |

$$\sqrt{\sum_i w_i x_i^2}$$

|        |                                                                                                                                                                           |
|--------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| MEDIAN | the weighted median. See the section “ <a href="#">Weighted Percentiles</a> ” on page 7472 for the formulas and descriptions.                                             |
| MAD    | the weighted median absolute deviation from the weighted median. See the section “ <a href="#">Weighted Percentiles</a> ” on page 7472 for the formulas and descriptions. |
| IQR    | the weighted median, 25th percentile, and the 75th percentile. See the section “ <a href="#">Weighted Percentiles</a> ” on page 7472 for the formulas and descriptions.   |

- AGK the AGK estimate. This estimate is documented further in the ACECLUS procedure as the METHOD=COUNT option. See the discussion of the WEIGHT statement in Chapter 23, “The ACECLUS Procedure,” for information about how the WEIGHT variable is applied to the AGK estimate.
- L the  $L_p$  estimate. This estimate is documented further in the FASTCLUS procedure as the LEAST= option. See the discussion of the WEIGHT statement in Chapter 36, “The FASTCLUS Procedure,” for information about how the WEIGHT variable is used to compute weighted cluster means. The number of clusters is always 1.

---

## Details: STDIZE Procedure

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### Standardization Methods

The following table lists standardization methods and their corresponding location and scale measures available with the METHOD= option.

**Table 87.2** Available Standardization Methods

| Method              | Location                     | Scale                                 |
|---------------------|------------------------------|---------------------------------------|
| MEAN                | Mean                         | 1                                     |
| MEDIAN              | Median                       | 1                                     |
| SUM                 | 0                            | Sum                                   |
| EUCLEN              | 0                            | Euclidean length                      |
| USTD                | 0                            | Standard deviation about origin       |
| STD                 | Mean                         | Standard deviation                    |
| RANGE               | Minimum                      | Range                                 |
| MIDRANGE            | Midrange                     | Range/2                               |
| MAXABS              | 0                            | Maximum absolute value                |
| IQR                 | Median                       | Interquartile range                   |
| MAD                 | Median                       | Median absolute deviation from median |
| ABW( <i>c</i> )     | Biweight one-step M-estimate | Biweight A-estimate                   |
| AHUBER( <i>c</i> )  | Huber one-step M-estimate    | Huber A-estimate                      |
| AWAVE( <i>c</i> )   | Wave one-step M-estimate     | Wave A-estimate                       |
| AGK( <i>p</i> )     | Mean                         | AGK estimate (ACECLUS)                |
| SPACING( <i>p</i> ) | Mid-minimum spacing          | Minimum spacing                       |
| L( <i>p</i> )       | L( <i>p</i> )                | L( <i>p</i> )                         |
| IN(ds)              | Read from data set           | Read from data set                    |

For METHOD=ABW( $c$ ), METHOD=AHUBER( $c$ ), or METHOD=AWAVE( $c$ ),  $c$  is a positive numeric tuning constant.

For METHOD=AGK( $p$ ),  $p$  is a numeric constant that gives the proportion of pairs to be included in the estimation of the within-cluster variances.

For METHOD=SPACING( $p$ ),  $p$  is a numeric constant that gives the proportion of data to be contained in the spacing.

For METHOD=L( $p$ ),  $p$  is a numeric constant greater than or equal to 1 that specifies the power to which differences are to be raised in computing an L( $p$ ) or Minkowski metric.

For METHOD=IN(ds), ds is the name of a SAS data set that meets either of the following two conditions:

- The data set contains a `_TYPE_` variable. The observation that contains the location measure corresponds to the value `_TYPE_ = 'LOCATION'`, and the observation that contains the scale measure corresponds to the value `_TYPE_ = 'SCALE'`. You can also use a data set created by the `OUTSTAT=` option from another PROC STDIZE statement as the ds data set. See the section “Output Data Sets” on page 7473 for the contents of the `OUTSTAT=` data set.
- The data set contains the location and scale variables specified by the `LOCATION` and `SCALE` statements.

PROC STDIZE reads in the location and scale variables in the ds data set by first looking for the `_TYPE_` variable in the ds data set. If it finds this variable, PROC STDIZE continues to search for all variables specified in the `VAR` statement. If it does not find the `_TYPE_` variable, PROC STDIZE searches for the location variables specified in the `LOCATION` statement and the scale variables specified in the `SCALE` statement.

The variable `_TYPE_` can also contain the optional observations, ‘ADD’ and ‘MULT’. If these observations are found in the ds data set, the values in the observation of `_TYPE_ = 'MULT'` are the multiplication constants, and the values in the observation of `_TYPE_ = 'ADD'` are the addition constants; otherwise, the constants specified in the `ADD=` and `MULT=` options (or their default values) are used.

For robust estimators, see Goodall (1983) and Iglewicz (1983). The MAD method has the highest breakdown point (50%), but it is somewhat inefficient. The ABW, AHUBER, and AWAVE methods provide a good compromise between breakdown and efficiency. The L( $p$ ) location estimates are increasingly robust as  $p$  drops from 2 (which corresponds to least squares, or mean estimation) to 1 (which corresponds to least absolute value, or median estimation). However, the L( $p$ ) scale estimates are not robust.

The SPACING method is robust to both outliers and clustering (Jannsen et al. 1995) and is, therefore, a good choice for cluster analysis or nonparametric density estimation. The mid-minimum spacing method estimates the mode for small  $p$ . The AGK method is also robust to clustering and more efficient than the SPACING method, but it is not as robust to outliers and takes longer to compute. If you expect  $g$  clusters, the argument to METHOD=SPACING or METHOD=AGK should be  $\frac{1}{g}$  or less. The AGK method is less biased than the SPACING method for small samples. As a general guide, it is reasonable to use AGK for samples of size 100 or less and SPACING for samples of size 1,000 or more, with the treatment of intermediate sample sizes depending on the available computer resources.



## Computation of the Statistics

Formulas for statistics of METHOD=MEAN, METHOD=MEDIAN, METHOD=SUM, METHOD=USTD, METHOD=STD, METHOD=RANGE, and METHOD=IQR are given in the chapter “Elementary Statistics Procedures” (*Base SAS Procedures Guide*).

Note that the computations of median and upper and lower quartiles depend on the PCTLMTD= option.

The other statistics listed in Table 87.2, except for METHOD=IN, are described as follows:

|                |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
|----------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| EUCLEN         | Euclidean length.<br>$\sqrt{\sum_{i=1}^n x_i^2}$ , where $x_i$ is the $i$ th observation and $n$ is the total number of observations in the sample.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
| L( $p$ )       | Minkowski metric. This metric is documented as the LEAST= $p$ option in the PROC FASTCLUS statement of the FASTCLUS procedure (see Chapter 36, “The FASTCLUS Procedure”).<br><br>If you specify METHOD=L( $p$ ) in the PROC STDIZE statement, your results are similar to those obtained from PROC FASTCLUS if you specify the LEAST= $p$ option with MAXCLUS=1 (and use the default values of the MAXITER= option). The difference between the two types of calculations concerns the maximum number of iterations. In PROC STDIZE, it is a criterion for convergence on all variables; in PROC FASTCLUS, it is a criterion for convergence on a single variable.<br><br>The location and scale measures for L( $p$ ) are output to the OUTSEED= data set in PROC FASTCLUS. |
| MIDRANGE       | $(\text{maximum} + \text{minimum})/2$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |
| ABW( $c$ )     | Tukey’s biweight. See Goodall (1983, pp. 376–378, p. 385) for the biweight one-step M-estimate. Also see Iglewicz (1983, pp. 416-418) for the biweight A-estimate.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
| AHUBER( $c$ )  | Hubers. See Goodall (1983, pp. 371–374) for the Huber one-step M-estimate. Also see Iglewicz (1983, pp. 416-418) for the Huber A-estimate of scale.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
| AWAVE( $c$ )   | Andrews’ wave. See Goodall (1983, p. 376) for the Wave one-step M-estimate. Also see Iglewicz (1983, pp. 416-418) for the Wave A-estimate of scale.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
| AGK( $p$ )     | The noniterative univariate form of the estimator described by Art, Gnanadesikan, and Kettenring (1982).<br><br>The AGK estimate is documented in the section on the METHOD= option in the PROC ACECLUS statement of the ACECLUS procedure (also see the section “Background” on page 814 in Chapter 23, “The ACECLUS Procedure”). Specifying METHOD=AGK( $p$ ) in the PROC STDIZE statement is the same as specifying METHOD=COUNT and P= $p$ in the PROC ACECLUS statement.                                                                                                                                                                                                                                                                                                |
| SPACING( $p$ ) | The absolute difference between two data values. The minimum spacing for a proportion $p$ is the minimum absolute difference between two data values that contain a proportion $p$ of the data between them. The mid-minimum spacing is the mean of these two data values.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |

## Computing Quantiles

PROC STDIZE offers two methods for computing quantiles: the one-pass approach and the order-statistics approach (like that used in the UNIVARIATE procedure).

The one-pass approach used in PROC STDIZE modifies the  $P^2$  algorithm for histograms proposed by Jain and Chlamtac (1985). The primary difference comes from the movement of markers. The one-pass method allows a marker to move to the right (or left) by more than one position (to the largest possible integer) as long as it does not result in two markers being in the same position. The modification is necessary in order to incorporate the `FREQ` variable.

You might obtain inaccurate results if you use the one-pass approach to estimate quantiles beyond the quartiles (that is, when you estimate quantiles  $< P25$  or quantiles  $> P75$ ). A large sample size (10,000 or more) is often required if the tail quantiles (quantiles  $\leq P10$  or quantiles  $\geq P90$ ) are requested. Note that, for variables with highly skewed or heavy-tailed distributions, tail quantile estimates might be inaccurate.

The order-statistics approach for estimating quantiles is faster than the one-pass method but requires that the entire data set be stored in memory. The accuracy in estimating the quantiles is comparable for both methods when the requested percentiles are between the lower and upper quartiles. The default is `PCTLMTD=ORD_STAT` if enough memory is available; otherwise, `PCTLMTD=ONEPASS`.

### Computational Methods for the `PCTLDEF=` Option

You can specify one of five methods for computing quantile statistics when you use the order-statistics approach (`PCTLMTD=ORD_STAT`); otherwise, the `PCTLDEF=5` method is used when you use the one-pass approach (`PCTLMTD=ONEPASS`).

**Percentile Definitions** Let  $n$  be the number of nonmissing values for a variable, and let  $x_1, x_2, \dots, x_n$  represent the ordered values of the variable. For the  $t$ th percentile, let  $p = t/100$ . In the following definitions numbered 1, 2, 3, and 5, let

$$np = j + g$$

where  $j$  is the integer part and  $g$  is the fractional part of  $np$ . For definition 4, let

$$(n + 1)p = j + g$$

Given the preceding definitions, the  $t$ th percentile,  $y$ , is defined as follows:

`PCTLDEF=1`      weighted average at  $x_{np}$

$$y = (1 - g)x_j + gx_{j+1}$$

where  $x_0$  is taken to be  $x_1$

`PCTLDEF=2`      observation numbered closest to  $np$

$$y = x_i$$

where  $i$  is the integer part of  $np + 1/2$  if  $g \neq 1/2$ . If  $g = 1/2$ , then

$y = x_j$  if  $j$  is even, or

$y = x_{j+1}$  if  $j$  is odd

|           |                                                |
|-----------|------------------------------------------------|
| PCTLDEF=3 | empirical distribution function                |
|           | $y = x_j$ if $g = 0$                           |
|           | $y = x_{j+1}$ if $g > 0$                       |
| PCTLDEF=4 | weighted average aimed at $x_{p(n+1)}$         |
|           | $y = (1 - g)x_j + gx_{j+1}$                    |
|           | where $x_{n+1}$ is taken to be $x_n$           |
| PCTLDEF=5 | empirical distribution function with averaging |
|           | $y = (x_j + x_{j+1})/2$ if $g = 0$             |
|           | $y = x_{j+1}$ if $g > 0$                       |

### Weighted Percentiles

When you specify a WEIGHT statement, or specify the NOTRUNCATE option in a FREQ statement, the percentiles are computed differently. The 100 $p$ th weighted percentile  $y$  is computed from the empirical distribution function with averaging

$$y = \begin{cases} \frac{1}{2}(x_i + x_{i+1}) & \text{if } \sum_{j=1}^i w_j = pW \\ x_{i+1} & \text{if } \sum_{j=1}^i w_j < pW < \sum_{j=1}^{i+1} w_j \end{cases}$$

where  $w_i$  is the weight associated with  $x_i$ , and where  $W = \sum_{i=1}^n w_i$  is the sum of the weights.

For PCTLMTD= ORD\_STAT, the PCTLDEF= option is not applicable when a WEIGHT statement is used, or when a NOTRUNCATE option is specified in a FREQ statement. However, in this case, if all the weights are identical, the weighted percentiles are the same as the percentiles that would be computed without a WEIGHT statement and with PCTLDEF=5.

For PCTLMTD= ONEPASS, the quantile computation currently does not use any weights.

---

### Constant Data

Constant variables are not standardized. The scale value is set to missing when the data are constant.

---

### Missing Values

Missing values can be replaced by the location measure or by any specified constant (see the REPLACE option and the MISSING= option). You can also suppress standardization if you want only to replace missing values (see the REONLY option).

If you specify the NOMISS option, PROC STDIZE omits observations with any missing values in the analyzed variables from computation of the location and scale measures.

## Output Data Sets

### OUT= Data Set

By default, the output data set is a copy of the DATA= data set except that the analyzed variables have been standardized. Analyzed variables are those specified in the VAR statement or, if there is no VAR statement, all numeric variables not listed in any other statement. However, you can use the OPREFIX option to request that both the original and standardized variables be included in the output data set. You can change variable names by specifying prefixes with the OPREFIX=*o-prefix* and SPREFIX=*s-prefix* options, but keep in mind that the two prefixes must be different. See [OPREFIX](#) and [SPREFIX](#) for more information.

### OUTSTAT= Data Set

The new data set contains the following variables:

- the BY variables, if any
- `_TYPE_`, a character variable
- the analyzed variables

Each observation in the new data set contains a type of statistic as indicated by the `_TYPE_` variable. The values of the `_TYPE_` variable are as follows:

|                |                                                                                                                                                                                                                        |
|----------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| LOCATION       | location measure of each variable                                                                                                                                                                                      |
| SCALE          | scale measure of each variable                                                                                                                                                                                         |
| ADD            | constant specified in the ADD= option. This value is the same for each variable.                                                                                                                                       |
| MULT           | constant specified in the MULT= option. This value is the same for each variable.                                                                                                                                      |
| N              | total number of nonmissing positive frequencies of each variable                                                                                                                                                       |
| NORM           | norm measure of each variable. This observation is produced only when you specify the NORM option with METHOD=AGK, METHOD=IQR, METHOD=MAD, or METHOD=SPACING or when you specify the SNORM option with METHOD=SPACING. |
| NObsRead       | number of physical records read                                                                                                                                                                                        |
| NObsUsed       | number of physical records used in the analysis                                                                                                                                                                        |
| NObsMiss       | number of physical records containing missing values                                                                                                                                                                   |
| $P_n$          | percentiles of each variable, as specified by the PCTLPTS= option. The argument $n$ is any real number such that $0 \leq n \leq 100$                                                                                   |
| SumFreqsRead   | sum of the frequency variable (or the sum of NObsUsed ones when there is no frequency variable) for all observations read                                                                                              |
| SumFreqsUsed   | sum of the frequency variable (or the sum of NObsUsed ones when there is no frequency variable) for all observations used in the analysis                                                                              |
| SumWeightsRead | sum of the weight variable (or the sum of NObsUsed ones when there is no weight variable) for all observations read                                                                                                    |

SumWeightsUsed      sum of the weight variable (or the sum of NObsUsed ones when there is no weight variable) for all observations used in the analysis

---

## Displayed Output

If you specify the PSTAT option, PROC STDIZE displays the following statistics for each variable:

- the name of the variable, Name
- the location estimate, Location
- the scale estimate, Scale
- the norm estimate, Norm (when you specify the NORM option with METHOD=AGK, METHOD=IQR, METHOD=MAD, or METHOD=SPACING or when you specify the SNORM option with METHOD=SPACING)
- sum of nonmissing positive frequencies, N
- sum of nonmissing positive weights if the WEIGHT statement is specified, Sum of Weights

---

## ODS Table Names

PROC STDIZE assigns a name to the single table it creates. You can use this name to reference the table when using the Output Delivery System (ODS) to select a table or create an output data set. This name is listed in Table 87.3. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

**Table 87.3** ODS Table Produced by PROC STDIZE

| ODS Table Name | Description                 | Statement | Option |
|----------------|-----------------------------|-----------|--------|
| Statistics     | Location and Scale Measures | PROC      | PSTAT  |

---

## Example: STDIZE Procedure

---

### Example 87.1: Standardization of Variables in Cluster Analysis

To illustrate the effect of standardization in cluster analysis, this example uses the Fish data set described in the “Getting Started” section of Chapter 36, “The FASTCLUS Procedure.” The numbers are measurements taken on 159 fish caught from the same lake (Laengelmavesi) near Tampere in Finland (Puranen 1917). The fish data set is available from the Sashelp library.

The species (bream, parkki, pike, perch, roach, smelt, and whitefish), weight, three different length measurements (measured from the nose of the fish to the beginning of its tail, the notch of its tail, and the end of its tail), height, and width of each fish are recorded.

A couple of new variables are created in the Fish data set: `Weight3` and `logLengthRatio`. The weight of a fish indicates its size—a heavier pike tends to be larger than a lighter pike. To get a one-dimensional measure of the size of a fish, take the cubic root of the weight (`Weight3`). The variables `Height`, `Width`, `Length1`, `Length2`, and `Length3` are rescaled in order to adjust for dimensionality. The `logLengthRatio` variable measures the tail length.

Because the new variables `Weight3`–`logLengthRatio` depend on the variable `Weight`, observations with missing values for `Weight` are not added to the data set. Consequently, there are 157 observations in the SAS data set `Sashelp.Fish`.

Before you perform a cluster analysis on coordinate data, it is necessary to consider scaling or transforming the variables since variables with large variances tend to have a larger effect on the resulting clusters than variables with small variances do.

This example uses three different approaches to standardize or transform the data prior to the cluster analysis. The first approach uses several standardization methods provided in the `STDIZE` procedure. However, since standardization is not always appropriate prior to the clustering (see Milligan and Cooper (1987) for a Monte Carlo study on various methods of variable standardization), the second approach performs the cluster analysis with no standardization. The third approach invokes the `ACECLUS` procedure to transform the data into a within-cluster covariance matrix.

The clustering is performed by the `FASTCLUS` procedure to find seven clusters. Note that the variables `Length2` and `Length3` are eliminated from this analysis since they both are significantly and highly correlated with the variable `Length1`. The correlation coefficients are 0.9958 and 0.9604, respectively. An output data set is created, and the `FREQ` procedure is invoked to compare the clusters with the species classification.

The DATA step is as follows:

```

title 'Fish Measurement Data';

data Fish;
 set sashelp.fish;
 if Weight <= 0 or Weight = . then delete;
 Weight3 = Weight ** (1/3);
 Height = Height / Weight3;
 Width = Width / Weight3;
 Length1 = Length1 / Weight3;
 Length2 = Length2 / Weight3;
 Length3 = Length3 / Weight3;
 LogLengthRatio = log(Length3 / Length1);
run;

```

The following macro, Std, standardizes the Fish data. The macro reads a single argument, mtd, which selects the METHOD= specification to be used in PROC STDIZE.

```

/*--- macro for standardization ---*/

%macro Std(mtd);
 title2 "Data are Standardized by PROC STDIZE with METHOD= &mtd";
 proc stdize data=fish out=sdzout method=&mtd;
 var Length1 logLengthRatio Height Width Weight3;
 run;
%mend Std;

```

The following macro, FastFreq, includes a PROC FASTCLUS statement for performing cluster analysis and a PROC FREQ statement for crosstabulating species with the cluster membership information that is derived from the previous PROC FASTCLUS statement. The macro reads a single argument, ds, which selects the input data set to be used in PROC FASTCLUS.

```

/*--- macro for clustering and crosstabulating ---*/
/*--- cluster membership with species ---*/

%macro FastFreq(ds);
 proc fastclus data=&ds out=clust maxclusters=7 maxiter=100 noprint;
 var Length1 logLengthRatio Height Width Weight3;
 run;

 proc freq data=clust;
 tables species*cluster;
 run;
%mend FastFreq;

```

The following analysis (labeled 'Approach 1') includes 18 different methods of standardization followed by clustering. Since there is a large amount of output from this approach, only results from METHOD=STD, METHOD=RANGE, METHOD=AGK(0.14), and METHOD=SPACING(0.14) are shown. The following statements produce [Output 87.1.1](#) through [Output 87.1.4](#).

```
/* Approach 1: data are standardized by PROC STDIZE */

%Std (MEAN) ;
%FastFreq (sdzout) ;

%Std (MEDIAN) ;
%FastFreq (sdzout) ;

%Std (SUM) ;
%FastFreq (sdzout) ;

%Std (EUCLLEN) ;
%FastFreq (sdzout) ;

%Std (USTD) ;
%FastFreq (sdzout) ;

%Std (STD) ;
%FastFreq (sdzout) ;

%Std (RANGE) ;
%FastFreq (sdzout) ;

%Std (MIDRANGE) ;
%FastFreq (sdzout) ;

%Std (MAXABS) ;
%FastFreq (sdzout) ;

%Std (IQR) ;
%FastFreq (sdzout) ;

%Std (MAD) ;
%FastFreq (sdzout) ;

%Std (AGK (.14)) ;
%FastFreq (sdzout) ;

%Std (SPACING (.14)) ;
%FastFreq (sdzout) ;

%Std (ABW (5)) ;
%FastFreq (sdzout) ;

%Std (AWAVE (5)) ;
%FastFreq (sdzout) ;

%Std (L (1)) ;
%FastFreq (sdzout) ;

%Std (L (1.5)) ;
%FastFreq (sdzout) ;
```



```
%Std(L(2));
%FastFreq(sdzout);
```

**Output 87.1.1** Data Are Standardized by PROC STDIZE with METHOD=STD

| Fish Measurement Data                                 |                  |       |        |       |        |        |        |        |
|-------------------------------------------------------|------------------|-------|--------|-------|--------|--------|--------|--------|
| Data are Standardized by PROC STDIZE with METHOD= STD |                  |       |        |       |        |        |        |        |
| The FREQ Procedure                                    |                  |       |        |       |        |        |        |        |
| Table of Species by CLUSTER                           |                  |       |        |       |        |        |        |        |
| Species                                               | CLUSTER(Cluster) |       |        |       |        |        |        |        |
| Frequency                                             |                  |       |        |       |        |        |        |        |
| Percent                                               |                  |       |        |       |        |        |        |        |
| Row Pct                                               |                  |       |        |       |        |        |        |        |
| Col Pct                                               | 1                | 2     | 3      | 4     | 5      | 6      | 7      | Total  |
| Bream                                                 | 0                | 0     | 0      | 0     | 0      | 34     | 0      | 34     |
|                                                       | 0.00             | 0.00  | 0.00   | 0.00  | 0.00   | 21.66  | 0.00   | 21.66  |
|                                                       | 0.00             | 0.00  | 0.00   | 0.00  | 0.00   | 100.00 | 0.00   |        |
|                                                       | 0.00             | 0.00  | 0.00   | 0.00  | 0.00   | 100.00 | 0.00   |        |
| Parkki                                                | 0                | 0     | 0      | 0     | 11     | 0      | 0      | 11     |
|                                                       | 0.00             | 0.00  | 0.00   | 0.00  | 7.01   | 0.00   | 0.00   | 7.01   |
|                                                       | 0.00             | 0.00  | 0.00   | 0.00  | 100.00 | 0.00   | 0.00   |        |
|                                                       | 0.00             | 0.00  | 0.00   | 0.00  | 100.00 | 0.00   | 0.00   |        |
| Perch                                                 | 0                | 17    | 0      | 12    | 0      | 0      | 27     | 56     |
|                                                       | 0.00             | 10.83 | 0.00   | 7.64  | 0.00   | 0.00   | 17.20  | 35.67  |
|                                                       | 0.00             | 30.36 | 0.00   | 21.43 | 0.00   | 0.00   | 48.21  |        |
|                                                       | 0.00             | 89.47 | 0.00   | 92.31 | 0.00   | 0.00   | 54.00  |        |
| Pike                                                  | 17               | 0     | 0      | 0     | 0      | 0      | 0      | 17     |
|                                                       | 10.83            | 0.00  | 0.00   | 0.00  | 0.00   | 0.00   | 0.00   | 10.83  |
|                                                       | 100.00           | 0.00  | 0.00   | 0.00  | 0.00   | 0.00   | 0.00   |        |
|                                                       | 100.00           | 0.00  | 0.00   | 0.00  | 0.00   | 0.00   | 0.00   |        |
| Roach                                                 | 0                | 0     | 0      | 0     | 0      | 0      | 19     | 19     |
|                                                       | 0.00             | 0.00  | 0.00   | 0.00  | 0.00   | 0.00   | 12.10  | 12.10  |
|                                                       | 0.00             | 0.00  | 0.00   | 0.00  | 0.00   | 0.00   | 100.00 |        |
|                                                       | 0.00             | 0.00  | 0.00   | 0.00  | 0.00   | 0.00   | 38.00  |        |
| Smelt                                                 | 0                | 0     | 13     | 0     | 0      | 0      | 1      | 14     |
|                                                       | 0.00             | 0.00  | 8.28   | 0.00  | 0.00   | 0.00   | 0.64   | 8.92   |
|                                                       | 0.00             | 0.00  | 92.86  | 0.00  | 0.00   | 0.00   | 7.14   |        |
|                                                       | 0.00             | 0.00  | 100.00 | 0.00  | 0.00   | 0.00   | 2.00   |        |
| Whitefish                                             | 0                | 2     | 0      | 1     | 0      | 0      | 3      | 6      |
|                                                       | 0.00             | 1.27  | 0.00   | 0.64  | 0.00   | 0.00   | 1.91   | 3.82   |
|                                                       | 0.00             | 33.33 | 0.00   | 16.67 | 0.00   | 0.00   | 50.00  |        |
|                                                       | 0.00             | 10.53 | 0.00   | 7.69  | 0.00   | 0.00   | 6.00   |        |
| Total                                                 | 17               | 19    | 13     | 13    | 11     | 34     | 50     | 157    |
|                                                       | 10.83            | 12.10 | 8.28   | 8.28  | 7.01   | 21.66  | 31.85  | 100.00 |

**Output 87.1.2** Data Are Standardized by PROC STDIZE with METHOD=RANGE

| Fish Measurement Data                                   |                  |        |        |        |       |        |        |        |
|---------------------------------------------------------|------------------|--------|--------|--------|-------|--------|--------|--------|
| Data are Standardized by PROC STDIZE with METHOD= RANGE |                  |        |        |        |       |        |        |        |
| The FREQ Procedure                                      |                  |        |        |        |       |        |        |        |
| Table of Species by CLUSTER                             |                  |        |        |        |       |        |        |        |
| Species                                                 | CLUSTER(Cluster) |        |        |        |       |        |        |        |
| Frequency                                               |                  |        |        |        |       |        |        |        |
| Percent                                                 |                  |        |        |        |       |        |        |        |
| Row Pct                                                 |                  |        |        |        |       |        |        |        |
| Col Pct                                                 | 1                | 2      | 3      | 4      | 5     | 6      | 7      | Total  |
| Bream                                                   | 0                | 0      | 34     | 0      | 0     | 0      | 0      | 34     |
|                                                         | 0.00             | 0.00   | 21.66  | 0.00   | 0.00  | 0.00   | 0.00   | 21.66  |
|                                                         | 0.00             | 0.00   | 100.00 | 0.00   | 0.00  | 0.00   | 0.00   |        |
|                                                         | 0.00             | 0.00   | 100.00 | 0.00   | 0.00  | 0.00   | 0.00   |        |
| Parkki                                                  | 0                | 0      | 0      | 0      | 0     | 11     | 0      | 11     |
|                                                         | 0.00             | 0.00   | 0.00   | 0.00   | 0.00  | 7.01   | 0.00   | 7.01   |
|                                                         | 0.00             | 0.00   | 0.00   | 0.00   | 0.00  | 100.00 | 0.00   |        |
|                                                         | 0.00             | 0.00   | 0.00   | 0.00   | 0.00  | 100.00 | 0.00   |        |
| Perch                                                   | 0                | 0      | 0      | 9      | 20    | 0      | 27     | 56     |
|                                                         | 0.00             | 0.00   | 0.00   | 5.73   | 12.74 | 0.00   | 17.20  | 35.67  |
|                                                         | 0.00             | 0.00   | 0.00   | 16.07  | 35.71 | 0.00   | 48.21  |        |
|                                                         | 0.00             | 0.00   | 0.00   | 29.03  | 86.96 | 0.00   | 100.00 |        |
| Pike                                                    | 17               | 0      | 0      | 0      | 0     | 0      | 0      | 17     |
|                                                         | 10.83            | 0.00   | 0.00   | 0.00   | 0.00  | 0.00   | 0.00   | 10.83  |
|                                                         | 100.00           | 0.00   | 0.00   | 0.00   | 0.00  | 0.00   | 0.00   |        |
|                                                         | 100.00           | 0.00   | 0.00   | 0.00   | 0.00  | 0.00   | 0.00   |        |
| Roach                                                   | 0                | 0      | 0      | 19     | 0     | 0      | 0      | 19     |
|                                                         | 0.00             | 0.00   | 0.00   | 12.10  | 0.00  | 0.00   | 0.00   | 12.10  |
|                                                         | 0.00             | 0.00   | 0.00   | 100.00 | 0.00  | 0.00   | 0.00   |        |
|                                                         | 0.00             | 0.00   | 0.00   | 61.29  | 0.00  | 0.00   | 0.00   |        |
| Smelt                                                   | 0                | 14     | 0      | 0      | 0     | 0      | 0      | 14     |
|                                                         | 0.00             | 8.92   | 0.00   | 0.00   | 0.00  | 0.00   | 0.00   | 8.92   |
|                                                         | 0.00             | 100.00 | 0.00   | 0.00   | 0.00  | 0.00   | 0.00   |        |
|                                                         | 0.00             | 100.00 | 0.00   | 0.00   | 0.00  | 0.00   | 0.00   |        |
| Whitefish                                               | 0                | 0      | 0      | 3      | 3     | 0      | 0      | 6      |
|                                                         | 0.00             | 0.00   | 0.00   | 1.91   | 1.91  | 0.00   | 0.00   | 3.82   |
|                                                         | 0.00             | 0.00   | 0.00   | 50.00  | 50.00 | 0.00   | 0.00   |        |
|                                                         | 0.00             | 0.00   | 0.00   | 9.68   | 13.04 | 0.00   | 0.00   |        |
| Total                                                   | 17               | 14     | 34     | 31     | 23    | 11     | 27     | 157    |
|                                                         | 10.83            | 8.92   | 21.66  | 19.75  | 14.65 | 7.01   | 17.20  | 100.00 |

## Output 87.1.3 Data Are Standardized by PROC STDIZE with METHOD=AGK(0.14)

| Fish Measurement Data                                      |                  |        |        |       |        |       |       |  |        |
|------------------------------------------------------------|------------------|--------|--------|-------|--------|-------|-------|--|--------|
| Data are Standardized by PROC STDIZE with METHOD= AGK(.14) |                  |        |        |       |        |       |       |  |        |
| The FREQ Procedure                                         |                  |        |        |       |        |       |       |  |        |
| Table of Species by CLUSTER                                |                  |        |        |       |        |       |       |  |        |
| Species                                                    | CLUSTER(Cluster) |        |        |       |        |       |       |  | Total  |
| Frequency                                                  |                  |        |        |       |        |       |       |  |        |
| Percent                                                    |                  |        |        |       |        |       |       |  |        |
| Row Pct                                                    |                  |        |        |       |        |       |       |  |        |
| Col Pct                                                    | 1                | 2      | 3      | 4     | 5      | 6     | 7     |  | Total  |
| Bream                                                      | 0                | 0      | 34     | 0     | 0      | 0     | 0     |  | 34     |
|                                                            | 0.00             | 0.00   | 21.66  | 0.00  | 0.00   | 0.00  | 0.00  |  | 21.66  |
|                                                            | 0.00             | 0.00   | 100.00 | 0.00  | 0.00   | 0.00  | 0.00  |  |        |
|                                                            | 0.00             | 0.00   | 100.00 | 0.00  | 0.00   | 0.00  | 0.00  |  |        |
| Parkki                                                     | 11               | 0      | 0      | 0     | 0      | 0     | 0     |  | 11     |
|                                                            | 7.01             | 0.00   | 0.00   | 0.00  | 0.00   | 0.00  | 0.00  |  | 7.01   |
|                                                            | 100.00           | 0.00   | 0.00   | 0.00  | 0.00   | 0.00  | 0.00  |  |        |
|                                                            | 100.00           | 0.00   | 0.00   | 0.00  | 0.00   | 0.00  | 0.00  |  |        |
| Perch                                                      | 0                | 0      | 0      | 3     | 0      | 20    | 33    |  | 56     |
|                                                            | 0.00             | 0.00   | 0.00   | 1.91  | 0.00   | 12.74 | 21.02 |  | 35.67  |
|                                                            | 0.00             | 0.00   | 0.00   | 5.36  | 0.00   | 35.71 | 58.93 |  |        |
|                                                            | 0.00             | 0.00   | 0.00   | 13.04 | 0.00   | 86.96 | 94.29 |  |        |
| Pike                                                       | 0                | 0      | 0      | 0     | 17     | 0     | 0     |  | 17     |
|                                                            | 0.00             | 0.00   | 0.00   | 0.00  | 10.83  | 0.00  | 0.00  |  | 10.83  |
|                                                            | 0.00             | 0.00   | 0.00   | 0.00  | 100.00 | 0.00  | 0.00  |  |        |
|                                                            | 0.00             | 0.00   | 0.00   | 0.00  | 100.00 | 0.00  | 0.00  |  |        |
| Roach                                                      | 0                | 0      | 0      | 17    | 0      | 0     | 2     |  | 19     |
|                                                            | 0.00             | 0.00   | 0.00   | 10.83 | 0.00   | 0.00  | 1.27  |  | 12.10  |
|                                                            | 0.00             | 0.00   | 0.00   | 89.47 | 0.00   | 0.00  | 10.53 |  |        |
|                                                            | 0.00             | 0.00   | 0.00   | 73.91 | 0.00   | 0.00  | 5.71  |  |        |
| Smelt                                                      | 0                | 14     | 0      | 0     | 0      | 0     | 0     |  | 14     |
|                                                            | 0.00             | 8.92   | 0.00   | 0.00  | 0.00   | 0.00  | 0.00  |  | 8.92   |
|                                                            | 0.00             | 100.00 | 0.00   | 0.00  | 0.00   | 0.00  | 0.00  |  |        |
|                                                            | 0.00             | 100.00 | 0.00   | 0.00  | 0.00   | 0.00  | 0.00  |  |        |
| Whitefish                                                  | 0                | 0      | 0      | 3     | 0      | 3     | 0     |  | 6      |
|                                                            | 0.00             | 0.00   | 0.00   | 1.91  | 0.00   | 1.91  | 0.00  |  | 3.82   |
|                                                            | 0.00             | 0.00   | 0.00   | 50.00 | 0.00   | 50.00 | 0.00  |  |        |
|                                                            | 0.00             | 0.00   | 0.00   | 13.04 | 0.00   | 13.04 | 0.00  |  |        |
| Total                                                      | 11               | 14     | 34     | 23    | 17     | 23    | 35    |  | 157    |
|                                                            | 7.01             | 8.92   | 21.66  | 14.65 | 10.83  | 14.65 | 22.29 |  | 100.00 |

**Output 87.1.4** Data Are Standardized by PROC STDIZE with METHOD=SPACING(0.14)

| Fish Measurement Data                                          |                  |        |        |       |        |       |        |        |
|----------------------------------------------------------------|------------------|--------|--------|-------|--------|-------|--------|--------|
| Data are Standardized by PROC STDIZE with METHOD= SPACING(.14) |                  |        |        |       |        |       |        |        |
| The FREQ Procedure                                             |                  |        |        |       |        |       |        |        |
| Table of Species by CLUSTER                                    |                  |        |        |       |        |       |        |        |
| Species                                                        | CLUSTER(Cluster) |        |        |       |        |       |        | Total  |
| Frequency                                                      |                  |        |        |       |        |       |        |        |
| Percent                                                        |                  |        |        |       |        |       |        |        |
| Row Pct                                                        |                  |        |        |       |        |       |        |        |
| Col Pct                                                        | 1                | 2      | 3      | 4     | 5      | 6     | 7      |        |
| Bream                                                          | 0                | 0      | 0      | 0     | 0      | 0     | 34     | 34     |
|                                                                | 0.00             | 0.00   | 0.00   | 0.00  | 0.00   | 0.00  | 21.66  | 21.66  |
|                                                                | 0.00             | 0.00   | 0.00   | 0.00  | 0.00   | 0.00  | 100.00 |        |
|                                                                | 0.00             | 0.00   | 0.00   | 0.00  | 0.00   | 0.00  | 100.00 |        |
| Parkki                                                         | 0                | 0      | 11     | 0     | 0      | 0     | 0      | 11     |
|                                                                | 0.00             | 0.00   | 7.01   | 0.00  | 0.00   | 0.00  | 0.00   | 7.01   |
|                                                                | 0.00             | 0.00   | 100.00 | 0.00  | 0.00   | 0.00  | 0.00   |        |
|                                                                | 0.00             | 0.00   | 100.00 | 0.00  | 0.00   | 0.00  | 0.00   |        |
| Perch                                                          | 20               | 0      | 0      | 0     | 0      | 36    | 0      | 56     |
|                                                                | 12.74            | 0.00   | 0.00   | 0.00  | 0.00   | 22.93 | 0.00   | 35.67  |
|                                                                | 35.71            | 0.00   | 0.00   | 0.00  | 0.00   | 64.29 | 0.00   |        |
|                                                                | 86.96            | 0.00   | 0.00   | 0.00  | 0.00   | 94.74 | 0.00   |        |
| Pike                                                           | 0                | 17     | 0      | 0     | 0      | 0     | 0      | 17     |
|                                                                | 0.00             | 10.83  | 0.00   | 0.00  | 0.00   | 0.00  | 0.00   | 10.83  |
|                                                                | 0.00             | 100.00 | 0.00   | 0.00  | 0.00   | 0.00  | 0.00   |        |
|                                                                | 0.00             | 100.00 | 0.00   | 0.00  | 0.00   | 0.00  | 0.00   |        |
| Roach                                                          | 0                | 0      | 0      | 17    | 0      | 2     | 0      | 19     |
|                                                                | 0.00             | 0.00   | 0.00   | 10.83 | 0.00   | 1.27  | 0.00   | 12.10  |
|                                                                | 0.00             | 0.00   | 0.00   | 89.47 | 0.00   | 10.53 | 0.00   |        |
|                                                                | 0.00             | 0.00   | 0.00   | 85.00 | 0.00   | 5.26  | 0.00   |        |
| Smelt                                                          | 0                | 0      | 0      | 0     | 14     | 0     | 0      | 14     |
|                                                                | 0.00             | 0.00   | 0.00   | 0.00  | 8.92   | 0.00  | 0.00   | 8.92   |
|                                                                | 0.00             | 0.00   | 0.00   | 0.00  | 100.00 | 0.00  | 0.00   |        |
|                                                                | 0.00             | 0.00   | 0.00   | 0.00  | 100.00 | 0.00  | 0.00   |        |
| Whitefish                                                      | 3                | 0      | 0      | 3     | 0      | 0     | 0      | 6      |
|                                                                | 1.91             | 0.00   | 0.00   | 1.91  | 0.00   | 0.00  | 0.00   | 3.82   |
|                                                                | 50.00            | 0.00   | 0.00   | 50.00 | 0.00   | 0.00  | 0.00   |        |
|                                                                | 13.04            | 0.00   | 0.00   | 15.00 | 0.00   | 0.00  | 0.00   |        |
| Total                                                          | 23               | 17     | 11     | 20    | 14     | 38    | 34     | 157    |
|                                                                | 14.65            | 10.83  | 7.01   | 12.74 | 8.92   | 24.20 | 21.66  | 100.00 |

The following analysis (labeled 'Approach 2') applies the cluster analysis directly to the original data. The following statements produce [Output 87.1.5](#).

```

/* Approach 2: data are untransformed */

title2 'Data are Untransformed';
%FastFreq(fish);

```

**Output 87.1.5** Untransformed Data

| Fish Measurement Data       |                  |       |        |        |       |        |       |        |
|-----------------------------|------------------|-------|--------|--------|-------|--------|-------|--------|
| Data are Untransformed      |                  |       |        |        |       |        |       |        |
| The FREQ Procedure          |                  |       |        |        |       |        |       |        |
| Table of Species by CLUSTER |                  |       |        |        |       |        |       |        |
| Species                     | CLUSTER(Cluster) |       |        |        |       |        |       | Total  |
| Frequency                   | 1                | 2     | 3      | 4      | 5     | 6      | 7     |        |
| Percent                     |                  |       |        |        |       |        |       |        |
| Row Pct                     |                  |       |        |        |       |        |       |        |
| Col Pct                     |                  |       |        |        |       |        |       |        |
| Bream                       | 13               | 0     | 0      | 0      | 0     | 0      | 21    | 34     |
|                             | 8.28             | 0.00  | 0.00   | 0.00   | 0.00  | 0.00   | 13.38 | 21.66  |
|                             | 38.24            | 0.00  | 0.00   | 0.00   | 0.00  | 0.00   | 61.76 |        |
|                             | 44.83            | 0.00  | 0.00   | 0.00   | 0.00  | 0.00   | 47.73 |        |
| Parkki                      | 2                | 3     | 0      | 0      | 6     | 0      | 0     | 11     |
|                             | 1.27             | 1.91  | 0.00   | 0.00   | 3.82  | 0.00   | 0.00  | 7.01   |
|                             | 18.18            | 27.27 | 0.00   | 0.00   | 54.55 | 0.00   | 0.00  |        |
|                             | 6.90             | 18.75 | 0.00   | 0.00   | 15.38 | 0.00   | 0.00  |        |
| Perch                       | 8                | 9     | 0      | 1      | 20    | 0      | 18    | 56     |
|                             | 5.10             | 5.73  | 0.00   | 0.64   | 12.74 | 0.00   | 11.46 | 35.67  |
|                             | 14.29            | 16.07 | 0.00   | 1.79   | 35.71 | 0.00   | 32.14 |        |
|                             | 27.59            | 56.25 | 0.00   | 6.67   | 51.28 | 0.00   | 40.91 |        |
| Pike                        | 0                | 0     | 10     | 0      | 1     | 4      | 2     | 17     |
|                             | 0.00             | 0.00  | 6.37   | 0.00   | 0.64  | 2.55   | 1.27  | 10.83  |
|                             | 0.00             | 0.00  | 58.82  | 0.00   | 5.88  | 23.53  | 11.76 |        |
|                             | 0.00             | 0.00  | 100.00 | 0.00   | 2.56  | 100.00 | 4.55  |        |
| Roach                       | 3                | 4     | 0      | 0      | 12    | 0      | 0     | 19     |
|                             | 1.91             | 2.55  | 0.00   | 0.00   | 7.64  | 0.00   | 0.00  | 12.10  |
|                             | 15.79            | 21.05 | 0.00   | 0.00   | 63.16 | 0.00   | 0.00  |        |
|                             | 10.34            | 25.00 | 0.00   | 0.00   | 30.77 | 0.00   | 0.00  |        |
| Smelt                       | 0                | 0     | 0      | 14     | 0     | 0      | 0     | 14     |
|                             | 0.00             | 0.00  | 0.00   | 8.92   | 0.00  | 0.00   | 0.00  | 8.92   |
|                             | 0.00             | 0.00  | 0.00   | 100.00 | 0.00  | 0.00   | 0.00  |        |
|                             | 0.00             | 0.00  | 0.00   | 93.33  | 0.00  | 0.00   | 0.00  |        |
| Whitefish                   | 3                | 0     | 0      | 0      | 0     | 0      | 3     | 6      |
|                             | 1.91             | 0.00  | 0.00   | 0.00   | 0.00  | 0.00   | 1.91  | 3.82   |
|                             | 50.00            | 0.00  | 0.00   | 0.00   | 0.00  | 0.00   | 50.00 |        |
|                             | 10.34            | 0.00  | 0.00   | 0.00   | 0.00  | 0.00   | 6.82  |        |
| Total                       | 29               | 16    | 10     | 15     | 39    | 4      | 44    | 157    |
|                             | 18.47            | 10.19 | 6.37   | 9.55   | 24.84 | 2.55   | 28.03 | 100.00 |

The following analysis (labeled 'Approach 3') transforms the original data with the ACECLUS procedure and creates a TYPE=ACE output data set that is used as an input data set for the cluster analysis. The following statements produce [Output 87.1.6](#).

```
/* Approach 3: data are transformed by PROC ACECLUS */

title2 'Data are Transformed by PROC ACECLUS';
proc aceclus data=fish out=ace p=.02 noprint;
 var Length1 logLengthRatio Height Width Weight3;
run;
%FastFreq(ace);
```

## Output 87.1.6 Data Are Transformed by PROC ACECLUS

| Fish Measurement Data                |                  |       |        |        |       |        |       |        |
|--------------------------------------|------------------|-------|--------|--------|-------|--------|-------|--------|
| Data are Transformed by PROC ACECLUS |                  |       |        |        |       |        |       |        |
| The FREQ Procedure                   |                  |       |        |        |       |        |       |        |
| Table of Species by CLUSTER          |                  |       |        |        |       |        |       |        |
| Species                              | CLUSTER(Cluster) |       |        |        |       |        |       | Total  |
| Frequency                            | 1                | 2     | 3      | 4      | 5     | 6      | 7     |        |
| Percent                              |                  |       |        |        |       |        |       |        |
| Row Pct                              |                  |       |        |        |       |        |       |        |
| Col Pct                              |                  |       |        |        |       |        |       |        |
| Bream                                | 13               | 0     | 0      | 0      | 0     | 0      | 21    | 34     |
|                                      | 8.28             | 0.00  | 0.00   | 0.00   | 0.00  | 0.00   | 13.38 | 21.66  |
|                                      | 38.24            | 0.00  | 0.00   | 0.00   | 0.00  | 0.00   | 61.76 |        |
|                                      | 44.83            | 0.00  | 0.00   | 0.00   | 0.00  | 0.00   | 47.73 |        |
| Parkki                               | 2                | 3     | 0      | 0      | 6     | 0      | 0     | 11     |
|                                      | 1.27             | 1.91  | 0.00   | 0.00   | 3.82  | 0.00   | 0.00  | 7.01   |
|                                      | 18.18            | 27.27 | 0.00   | 0.00   | 54.55 | 0.00   | 0.00  |        |
|                                      | 6.90             | 18.75 | 0.00   | 0.00   | 15.38 | 0.00   | 0.00  |        |
| Perch                                | 8                | 9     | 0      | 1      | 20    | 0      | 18    | 56     |
|                                      | 5.10             | 5.73  | 0.00   | 0.64   | 12.74 | 0.00   | 11.46 | 35.67  |
|                                      | 14.29            | 16.07 | 0.00   | 1.79   | 35.71 | 0.00   | 32.14 |        |
|                                      | 27.59            | 56.25 | 0.00   | 6.67   | 51.28 | 0.00   | 40.91 |        |
| Pike                                 | 0                | 0     | 10     | 0      | 1     | 4      | 2     | 17     |
|                                      | 0.00             | 0.00  | 6.37   | 0.00   | 0.64  | 2.55   | 1.27  | 10.83  |
|                                      | 0.00             | 0.00  | 58.82  | 0.00   | 5.88  | 23.53  | 11.76 |        |
|                                      | 0.00             | 0.00  | 100.00 | 0.00   | 2.56  | 100.00 | 4.55  |        |
| Roach                                | 3                | 4     | 0      | 0      | 12    | 0      | 0     | 19     |
|                                      | 1.91             | 2.55  | 0.00   | 0.00   | 7.64  | 0.00   | 0.00  | 12.10  |
|                                      | 15.79            | 21.05 | 0.00   | 0.00   | 63.16 | 0.00   | 0.00  |        |
|                                      | 10.34            | 25.00 | 0.00   | 0.00   | 30.77 | 0.00   | 0.00  |        |
| Smelt                                | 0                | 0     | 0      | 14     | 0     | 0      | 0     | 14     |
|                                      | 0.00             | 0.00  | 0.00   | 8.92   | 0.00  | 0.00   | 0.00  | 8.92   |
|                                      | 0.00             | 0.00  | 0.00   | 100.00 | 0.00  | 0.00   | 0.00  |        |
|                                      | 0.00             | 0.00  | 0.00   | 93.33  | 0.00  | 0.00   | 0.00  |        |
| Whitefish                            | 3                | 0     | 0      | 0      | 0     | 0      | 3     | 6      |
|                                      | 1.91             | 0.00  | 0.00   | 0.00   | 0.00  | 0.00   | 1.91  | 3.82   |
|                                      | 50.00            | 0.00  | 0.00   | 0.00   | 0.00  | 0.00   | 50.00 |        |
|                                      | 10.34            | 0.00  | 0.00   | 0.00   | 0.00  | 0.00   | 6.82  |        |
| Total                                | 29               | 16    | 10     | 15     | 39    | 4      | 44    | 157    |
|                                      | 18.47            | 10.19 | 6.37   | 9.55   | 24.84 | 2.55   | 28.03 | 100.00 |

Table 87.4 displays a table summarizing each classification results. In this table, the first column represents the standardization method, the second column represents the number of clusters that the seven species are classified into, and the third column represents the total number of observations that are misclassified.

**Table 87.4** Summary of Clustering Results

| Method of Standardization | Number of Clusters | Misclassification |
|---------------------------|--------------------|-------------------|
| MEAN                      | 5                  | 71                |
| MEDIAN                    | 5                  | 71                |
| SUM                       | 6                  | 51                |
| EUCLEN                    | 6                  | 45                |
| USTD                      | 6                  | 45                |
| STD                       | 5                  | 33                |
| RANGE                     | 7                  | 32                |
| MIDRANGE                  | 7                  | 32                |
| MAXABS                    | 7                  | 26                |
| IQR                       | 5                  | 28                |
| MAD                       | 4                  | 35                |
| ABW(5)                    | 6                  | 34                |
| AWAVE(5)                  | 6                  | 29                |
| AGK(0.14)                 | 7                  | 28                |
| SPACING(0.14)             | 7                  | 25                |
| L(1)                      | 6                  | 41                |
| L(1.5)                    | 5                  | 33                |
| L(2)                      | 5                  | 33                |
| untransformed             | 5                  | 71                |
| PROC ACECLUS              | 5                  | 71                |

Consider the results displayed in Output 87.1.1. In that analysis, the method of standardization is STD, and the number of clusters and the number of misclassifications are computed as shown in Table 87.5.

**Table 87.5** Computations of Numbers of Clusters and Misclassification When Standardization Method Is STD

| Species   | Cluster Number | Misclassification in Each Species |
|-----------|----------------|-----------------------------------|
| Bream     | 6              | 0                                 |
| Parkki    | 5              | 0                                 |
| Perch     | 7              | 29                                |
| Pike      | 1              | 0                                 |
| Roach     | 7              | 0                                 |
| Smelt     | 3              | 1                                 |
| Whitefish | 7              | 3                                 |

In Output 87.1.1, the bream species is classified as cluster 6 since all 34 bream are categorized into cluster 6 with no misclassification. A similar pattern is seen with the roach, parkki, pike, and smelt species.



For the whitefish species, two fish are categorized into cluster 2, one fish is categorized into cluster 4, and three fish are categorized into cluster 7. Because the majority of this species is categorized into cluster 7, it is recorded in Table 87.5 as being classified as cluster 7 with 3 misclassifications. A similar pattern is seen with the perch species: it is classified as cluster 7 with 29 misclassifications.

In summary, when the standardization method is STD, seven species of fish are classified into only five clusters and the total number of misclassified observations is 33.

The result of this analysis demonstrates that when variables are standardized by the STDIZE procedure with methods including RANGE, MIDRANGE, MAXABS, AGK(0.14), and SPACING(0.14), the FASTCLUS procedure produces the correct number of clusters and less misclassification than it does when other standardization methods are used. The SPACING method attains the best result, probably because the variables Length1 and Height both exhibit marked groupings (bimodality) in their distributions.

---

## References

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URL <http://www.amstat.org/publications/jse/datasets/fishcatch.txt>

# Chapter 88

## The STDRATE Procedure

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### Overview: STDRATE Procedure

Epidemiology is the study of the occurrence and distribution of health-related states or events in specified populations. Epidemiology also includes the study of the determinants that influence these states, and the application of this knowledge to control health problems (Porta 2008). It is a discipline that describes, quantifies, and postulates causal mechanisms for health phenomena in populations (Friss and Sellers 2009).

A common goal is to establish relationships between various factors (such as exposure to a specific chemical) and the event outcomes (such as incidence of disease). But the measure of an association between an exposure and an event outcome can be biased due to confounding. That is, the association of the exposure to some other variables, such as age, influences the occurrence of the event outcome. With confounding, the usual effect between an exposure and an event outcome can be biased because some of the effect might be accounted for by other variables. For example, with an event rate discrepancy among different age groups of a population, the overall crude rate might not provide a useful summary statistic to compare populations.

One strategy to control confounding is stratification. In stratification, a population is divided into several subpopulations according to specific criteria for the confounding variables, such as age and sex groups. The effect of the exposure on the event outcome is estimated within each stratum, and then these stratum-specific effect estimates are combined into an overall estimate.

Two commonly used event frequency measures are rate and risk:

- A rate is a measure of the frequency with which an event occurs in a defined population in a specified period of time. It measures the change in one quantity per unit of another quantity. For example, an event rate measures how fast the events are occurring. That is, an event rate of a population over a specified time period can be defined as the number of new events divided by population-time (Kleinbaum, Kupper, and Morgenstern 1982, p. 100) over the same time period.
- A risk is the probability that an event occurs in a specified time period. It is assumed that only one event can occur in the time period for each subject or item. The overall crude risk of a population over a specified time period is the number of new events in the time period divided by the population size at the beginning of the time period.

Standardized overall rate and risk estimates based on stratum-specific estimates can be derived with the effects of confounding variables removed. These estimates provide useful summary statistics and allow valid comparison of the populations. There are two types of standardization:

- Direct standardization computes the weighted average of stratum-specific estimates in the study population, using the weights from a standard or reference population. This standardization is applicable when the study population is large enough to provide stable stratum-specific estimates. The directly standardized estimate is the overall crude rate in the study population if it has the same strata distribution as the reference population. When standardized estimates for different populations are derived by using the same reference population, the resulting estimates can also be compared by using the estimated difference and estimated ratio statistics.
- Indirect standardization computes the weighted average of stratum-specific estimates in the reference population, using the weights from the study population. The ratio of the overall crude rate or risk in the study population and the corresponding weighted estimate in the reference population is the standardized morbidity ratio (SMR). This ratio is also the standardized mortality ratio if the event is death. SMR is used to compare rates or risks in the study and reference populations. With SMR, the indirectly standardized estimate is then computed as the product of the SMR and the overall crude estimate for the reference population. SMR and indirect standardization are applicable even when the study population is so small that the resulting stratum-specific rates are not stable.

Assuming that an effect, such as the rate difference between two populations, is homogeneous across strata, each stratum provides an estimate of the same effect. A pooled estimate of the effect can then be derived

from these stratum-specific effect estimates. One way to estimate a homogeneous effect is the Mantel-Haenszel method (Greenland and Rothman 2008, p. 271). For a homogeneous rate difference effect between two populations, the Mantel-Haenszel estimate is identical to the difference between two directly standardized rates, but with weights derived from the two populations instead of from an explicitly specified reference population. The Mantel-Haenszel method can also be applied to other homogeneous effects between populations, such as the rate ratio, risk difference, and risk ratio.

The STDRATE procedure computes directly standardized rates and risks for study populations. For two study populations with the same reference population, PROC STDRATE compares directly standardized rates or risks from these two populations. For homogeneous effects across strata, PROC STDRATE computes Mantel-Haenszel estimates. The STDRATE procedure also computes indirectly standardized rates and risks, including SMR.

The attributable fraction measures the excess event rate or risk fraction in the exposed population that can be attributed to the exposure. The rate or risk ratio statistic is required in the attributable fraction computation, and the STDRATE procedure estimates the ratio by using either SMR or the rate ratio statistic in the Mantel-Haenszel estimates.

Although the STDRATE procedure provides useful summary standardized statistics, standardization is not a substitute for individual comparisons of stratum-specific estimates. PROC STDRATE provides summary statistics, such as rate and risk estimates and their confidence limits, in each stratum. In addition, PROC STDRATE also displays these stratum-specific statistics by using ODS Graphics.

Note that the term standardization has different meanings in other statistical applications. For example, the STDIZE procedure standardizes numeric variables in a SAS data set by subtracting a location measure and dividing by a scale measure.

---

## Getting Started: STDRATE Procedure

This example illustrates indirect standardization and uses the standardized mortality ratio to compare the death rate from skin cancer between people who live in the state of Florida and people who live in the United States as a whole.

The Florida\_C43 data set contains the stratum-specific mortality information for skin cancer in year 2000 for the state of Florida (Florida Department of Health 2000, 2012). The variable Age is a grouping variable that forms the strata in the standardization, and the variables Event and PYear identify the number of events and total person-years, respectively. The COMMA11. format is specified in the DATA step to input numerical values that contain commas in PYear.

```
data Florida_C43;
 input Age $1-5 Event PYear comma11.;
 datalines;
00-04 0 953,785
05-14 0 1,997,935
15-24 4 1,885,014
25-34 14 1,957,573
35-44 43 2,356,649
45-54 72 2,088,000
55-64 70 1,548,371
65-74 126 1,447,432
```

```

75-84 136 1,087,524
85+ 73 335,944
;

```

The US\_C43 data set contains the corresponding stratum-specific mortality information for the United States in year 2000 (Miniño et al. 2002; U.S. Bureau of Census 2011). The variable `Age` is the grouping variable, and the variables `Event` and `PYear` identify the number of events and the total person-years, respectively.

```

data US_C43;
 input Age $1-5 Event comma7. PYear comma12.;
 datalines;
00-04 0 19,175,798
05-14 1 41,077,577
15-24 41 39,183,891
25-34 186 39,892,024
35-44 626 45,148,527
45-54 1,199 37,677,952
55-64 1,303 24,274,684
65-74 1,637 18,390,986
75-84 1,624 12,361,180
85+ 803 4,239,587
;

```

The following statements invoke the STD RATE procedure and request indirect standardization to compare death rates between the state of Florida and the United States:

```

ods graphics on;
proc stdrate data=Florida_C43 refdata=US_C43
 method=indirect
 stat=rate(mult=100000)
 plots=all
 ;
 population event=Event total=PYear;
 reference event=Event total=PYear;
 strata Age / stats smr;
run;
ods graphics off;

```

The `DATA=` and `REFDATA=` options name the study data set and reference data set, respectively. The `METHOD=INDIRECT` option requests indirect standardization. The `STAT=RATE` option specifies the rate as the frequency measure for standardization, and the `MULT=100000` suboption (which is the default) displays the rates per 100,000 person-years in the table output and graphics output. The `PLOTS=ALL` option requests all appropriate plots with indirect standardization.

The POPULATION statement specifies the options that are related to the study population, and the EVENT= and TOTAL= options specify variables for the number of events and person-years in the study population, respectively.

The REFERENCE statement specifies the options related to the reference population, and the EVENT= and TOTAL= options specify variables for the number of events and person-years in the reference population, respectively.

The STRATA statement lists the variable Age that forms the strata. The STATS option requests a strata information table that contains stratum-specific statistics such as rates, and the SMR option requests a table of stratum-specific SMR estimates.

The “Standardization Information” table in [Figure 88.1](#) displays the standardization information.

**Figure 88.1** Standardization Information

| The STDRATE Procedure       |                          |
|-----------------------------|--------------------------|
| Standardization Information |                          |
| Data Set                    | WORK.FLORIDA_C43         |
| Reference Data Set          | WORK.US_C43              |
| Method                      | Indirect Standardization |
| Statistic                   | Rate                     |
| Number of Strata            | 10                       |
| Rate Multiplier             | 100000                   |

The STATS option in the STRATA statement requests that the “Indirectly Standardized Strata Statistics” table in [Figure 88.2](#) display the strata information and expected number of events at each stratum. The MULT=100000 suboption in the STAT=RATE option requests that crude rates per 100,000 person-years be displayed. The Expected Events column displays the expected number of events when the stratum-specific rates in the reference data set are applied to the corresponding person-years in the study data set.

Figure 88.2 Strata Information (Indirect Standardization)

| The STD RATE Procedure                    |       |                            |                                 |            |               |                   |
|-------------------------------------------|-------|----------------------------|---------------------------------|------------|---------------|-------------------|
| Indirectly Standardized Strata Statistics |       |                            |                                 |            |               |                   |
| Rate Multiplier = 100000                  |       |                            |                                 |            |               |                   |
| Stratum<br>Index                          | Age   | -----Study Population----- |                                 |            | Crude<br>Rate | Standard<br>Error |
|                                           |       | Observed<br>Events         | ----Population-Time---<br>Value | Proportion |               |                   |
| 1                                         | 00-04 | 0                          | 953785                          | 0.0609     | 0.0000        | 0.00000           |
| 2                                         | 05-14 | 0                          | 1997935                         | 0.1276     | 0.0000        | 0.00000           |
| 3                                         | 15-24 | 4                          | 1885014                         | 0.1204     | 0.2122        | 0.10610           |
| 4                                         | 25-34 | 14                         | 1957573                         | 0.1250     | 0.7152        | 0.19114           |
| 5                                         | 35-44 | 43                         | 2356649                         | 0.1505     | 1.8246        | 0.27825           |
| 6                                         | 45-54 | 72                         | 2088000                         | 0.1333     | 3.4483        | 0.40638           |
| 7                                         | 55-64 | 70                         | 1548371                         | 0.0989     | 4.5209        | 0.54035           |
| 8                                         | 65-74 | 126                        | 1447432                         | 0.0924     | 8.7051        | 0.77551           |
| 9                                         | 75-84 | 136                        | 1087524                         | 0.0695     | 12.5055       | 1.07234           |
| 10                                        | 85+   | 73                         | 335944                          | 0.0215     | 21.7298       | 2.54328           |

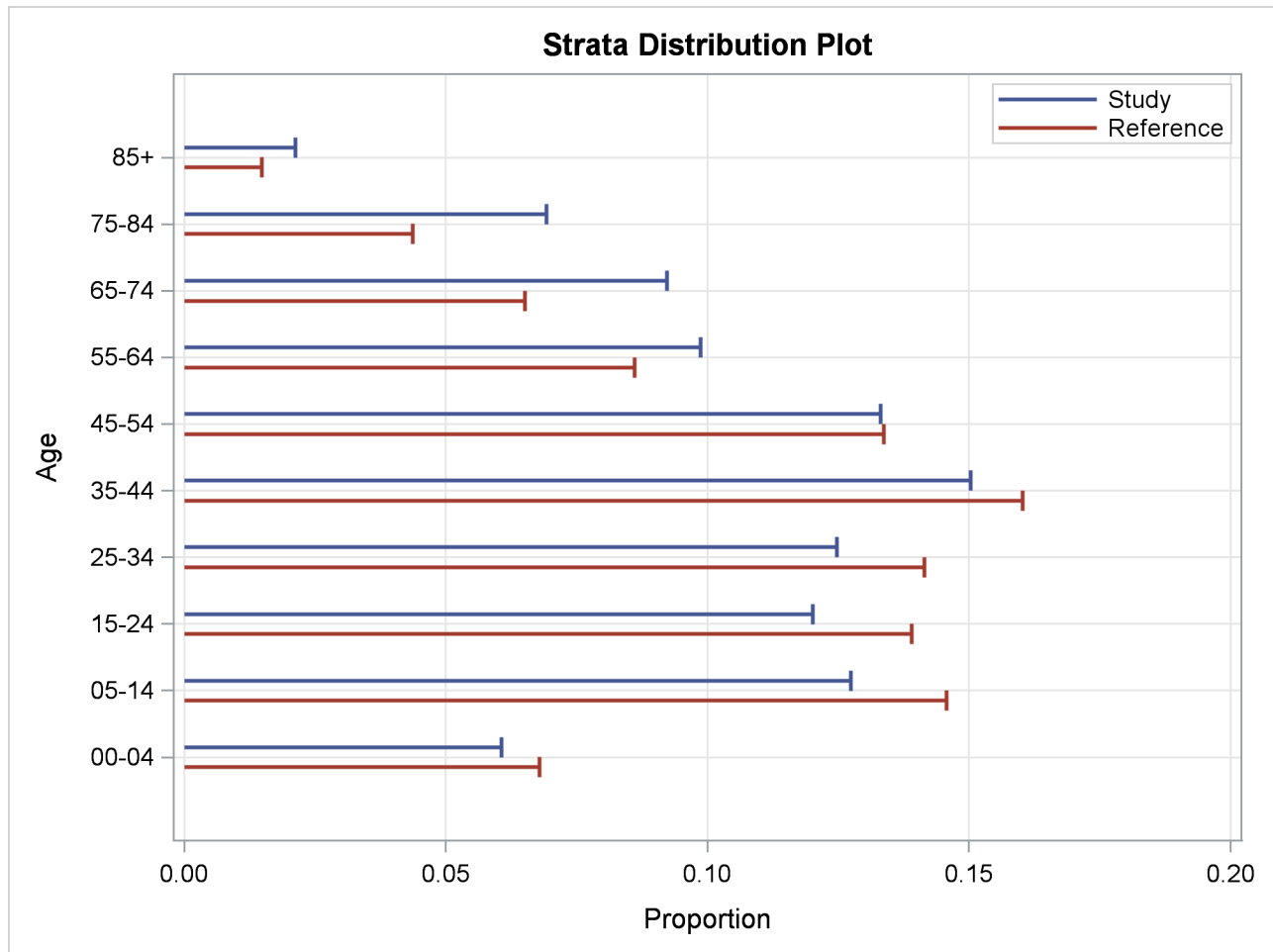
  

| Indirectly Standardized Strata Statistics |                                 |         |                                 |            |               |                    |
|-------------------------------------------|---------------------------------|---------|---------------------------------|------------|---------------|--------------------|
| Rate Multiplier = 100000                  |                                 |         |                                 |            |               |                    |
| Stratum<br>Index                          | -Study Population-              |         | -----Reference Population-----  |            | Crude<br>Rate | Expected<br>Events |
|                                           | 95% Normal<br>Confidence Limits |         | ----Population-Time---<br>Value | Proportion |               |                    |
| 1                                         | 0.0000                          | 0.0000  | 19175798                        | 0.0681     | 0.0000        | 0.000              |
| 2                                         | 0.0000                          | 0.0000  | 41077577                        | 0.1460     | 0.0024        | 0.049              |
| 3                                         | 0.0042                          | 0.4202  | 39183891                        | 0.1392     | 0.1046        | 1.972              |
| 4                                         | 0.3405                          | 1.0898  | 39892024                        | 0.1418     | 0.4663        | 9.127              |
| 5                                         | 1.2793                          | 2.3700  | 45148527                        | 0.1604     | 1.3865        | 32.676             |
| 6                                         | 2.6518                          | 4.2448  | 37677952                        | 0.1339     | 3.1822        | 66.445             |
| 7                                         | 3.4618                          | 5.5799  | 24274684                        | 0.0863     | 5.3677        | 83.112             |
| 8                                         | 7.1851                          | 10.2250 | 18390986                        | 0.0654     | 8.9011        | 128.837            |
| 9                                         | 10.4037                         | 14.6072 | 12361180                        | 0.0439     | 13.1379       | 142.878            |
| 10                                        | 16.7451                         | 26.7146 | 4239587                         | 0.0151     | 18.9405       | 63.630             |

With ODS Graphics enabled, the PLOTS=ALL option displays all appropriate plots. With indirect standardization and a rate statistic, these plots include the strata distribution plot, the strata rate plot, and the strata SMR plot. By default, strata levels are displayed on the vertical axis for these plots.

The strata distribution plot displays proportions for stratum-specific person-years in the study and reference populations, as shown in Figure 88.3.

Figure 88.3 Strata Distribution Plot

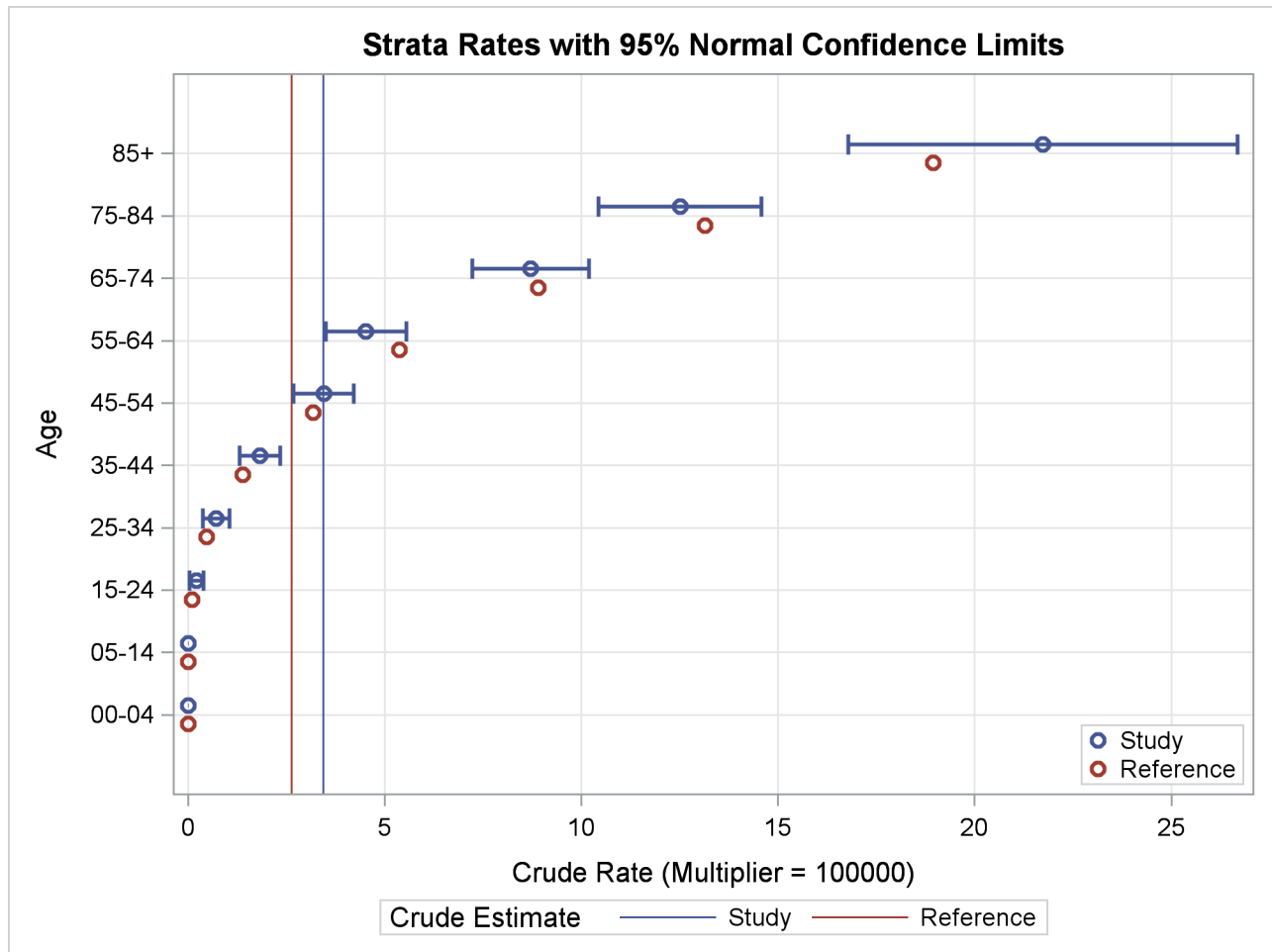


The strata distribution plot displays the proportions in the “Indirectly Standardized Strata Statistics” table in Figure 88.2. In the plot, the proportions of the study population are identified by the blue lines, and the proportions of the reference population are identified by the red lines. The plot shows that the study population has higher proportions in older age groups and lower proportions in younger age groups than the reference population.

The strata rate plot displays stratum-specific rate estimates in the study and reference populations, as shown in Figure 88.4. This plot displays the rate estimates in the “Indirectly Standardized Strata Statistics” table in Figure 88.2. In addition, the plot displays the confidence limits for the rate estimates in the study population and the overall crude rates for the two populations.



Figure 88.4 Strata Rate Plot



The SMR option in the STRATA statement requests that the “Strata SMR Estimates” table in Figure 88.5 display the strata SMR at each stratum. The MULT=100000 suboption in the STAT=RATE option requests that the reference rates per 100,000 person-years be displayed.

Figure 88.5 Strata SMR Information

| Strata SMR Estimates     |       |                          |                                |                      |                 |        |                |
|--------------------------|-------|--------------------------|--------------------------------|----------------------|-----------------|--------|----------------|
| Rate Multiplier = 100000 |       |                          |                                |                      |                 |        |                |
| Stratum Index            | Age   | ---Study Observed Events | Population-- Population-- Time | Reference Crude Rate | Expected Events | SMR    | Standard Error |
| 1                        | 00-04 | 0                        | 953785                         | 0.0000               | 0.000           | .      | .              |
| 2                        | 05-14 | 0                        | 1997935                        | 0.0024               | 0.049           | 0.0000 | .              |
| 3                        | 15-24 | 4                        | 1885014                        | 0.1046               | 1.972           | 2.0280 | 1.0140         |
| 4                        | 25-34 | 14                       | 1957573                        | 0.4663               | 9.127           | 1.5339 | 0.4099         |
| 5                        | 35-44 | 43                       | 2356649                        | 1.3865               | 32.676          | 1.3160 | 0.2007         |
| 6                        | 45-54 | 72                       | 2088000                        | 3.1822               | 66.445          | 1.0836 | 0.1277         |
| 7                        | 55-64 | 70                       | 1548371                        | 5.3677               | 83.112          | 0.8422 | 0.1007         |
| 8                        | 65-74 | 126                      | 1447432                        | 8.9011               | 128.837         | 0.9780 | 0.0871         |
| 9                        | 75-84 | 136                      | 1087524                        | 13.1379              | 142.878         | 0.9519 | 0.0816         |
| 10                       | 85+   | 73                       | 335944                         | 18.9405              | 63.630          | 1.1473 | 0.1343         |

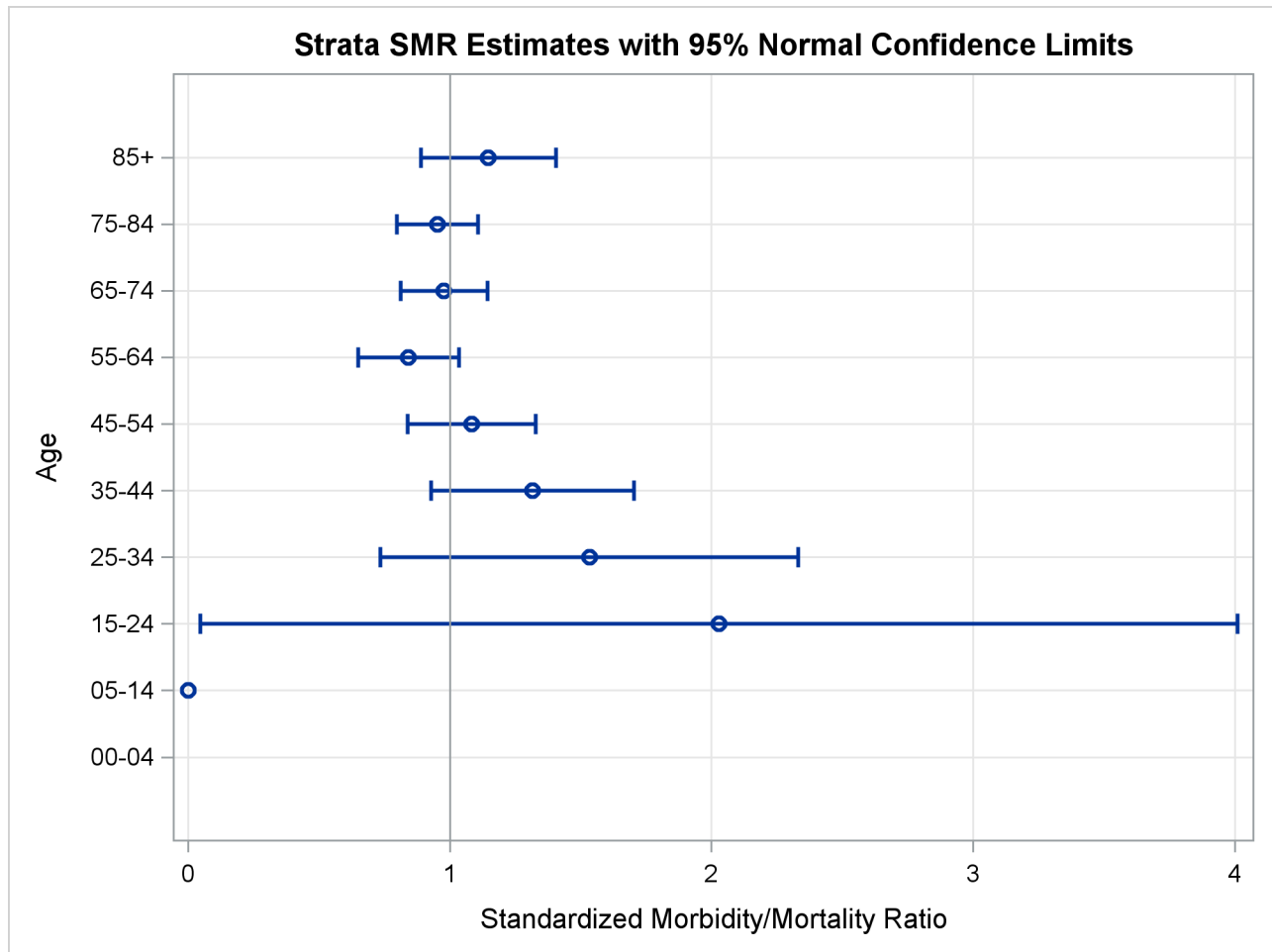
  

| Strata SMR Estimates     |                              |        |
|--------------------------|------------------------------|--------|
| Rate Multiplier = 100000 |                              |        |
| Stratum Index            | 95% Normal Confidence Limits |        |
| 1                        | .                            | .      |
| 2                        | .                            | .      |
| 3                        | 0.0406                       | 4.0154 |
| 4                        | 0.7304                       | 2.3373 |
| 5                        | 0.9226                       | 1.7093 |
| 6                        | 0.8333                       | 1.3339 |
| 7                        | 0.6449                       | 1.0395 |
| 8                        | 0.8072                       | 1.1487 |
| 9                        | 0.7919                       | 1.1118 |
| 10                       | 0.8841                       | 1.4104 |

The “Strata SMR Estimates” table shows that although SMR is less than 1 only at three age strata (55–64, 65–74, and 75–84), these three strata contain about 60% of the total events.

The strata SMR plot displays stratum-specific SMR estimates with confidence limits, as shown in Figure 88.6. The plot displays the SMR estimates in the “Strata SMR Estimates” table in Figure 88.5.

Figure 88.6 Strata SMR Plot



The METHOD=INDIRECT option requests that the “Standardized Morbidity/Mortality Ratio” table in Figure 88.7 be displayed. The table displays the SMR, its confidence limits, and the test for the null hypothesis  $H_0 : SMR = 1$ . The default ALPHA=0.05 option requests that 95% confidence limits be constructed.

Figure 88.7 Standardized Morbidity/Mortality Ratio

| Standardized Morbidity/Mortality Ratio |                 |              |                |                              |        |      |         |
|----------------------------------------|-----------------|--------------|----------------|------------------------------|--------|------|---------|
| Observed Events                        | Expected Events | Standard SMR | Standard Error | 95% Normal Confidence Limits |        | Z    | Pr >  Z |
| 538                                    | 528.726         | 1.0175       | 0.0439         | 0.9316                       | 1.1035 | 0.40 | 0.6893  |

The 95% normal confidence limits contain the null hypothesis value  $SMR = 1$ , and the hypothesis of  $SMR = 1$  is not rejected at the  $\alpha = 0.05$  level from the normal test.

The “Indirectly Standardized Rate Estimates” table in Figure 88.8 displays the indirectly standardized rate and related statistics.

**Figure 88.8** Standardized Rate Estimates (Indirect Standardization)

| Indirectly Standardized Rate Estimates |             |                   |            |          |        |  |
|----------------------------------------|-------------|-------------------|------------|----------|--------|--|
| Rate Multiplier = 100000               |             |                   |            |          |        |  |
| -----Study Population-----             |             |                   | Reference  |          |        |  |
| Observed                               | Population- | Crude             | Crude      | Expected |        |  |
| Events                                 | Time        | Rate              | Rate       | Events   | SMR    |  |
| 538                                    | 15658227    | 3.4359            | 2.6366     | 528.726  | 1.0175 |  |
| Indirectly Standardized Rate Estimates |             |                   |            |          |        |  |
| Rate Multiplier = 100000               |             |                   |            |          |        |  |
| -----Standardized Rate-----            |             |                   |            |          |        |  |
|                                        |             | Standard          | 95% Normal |          |        |  |
| Estimate                               | Error       | Confidence Limits |            |          |        |  |
| 2.6829                                 | 0.1157      | 2.4562            | 2.9096     |          |        |  |

The indirectly standardized rate estimate is the product of the SMR and the crude rate estimate for the reference population. The table shows that although the crude rate in the state of Florida (3.4359) is 30% higher than the crude rate in the U.S. (2.6366), the resulting standardized rate (2.6829) is close to the crude rate in the U.S.

---

## Syntax: STD RATE Procedure

The following statements are available in PROC STD RATE:

```

PROC STD RATE < options > ;
 BY variables ;
 POPULATION options ;
 REFERENCE options ;
 STRATA variables < / option > ;

```

The PROC STD RATE statement invokes the procedure, names the data sets, specifies the standardization method, and identifies the statistic for standardization. The BY statement requests separate analyses of groups defined by the BY variables. The required POPULATION statement specifies the rate or risk information in study populations, and the REFERENCE statement specifies the rate or risk information in the reference population. The STRATA statement lists the variables that form the strata.

The following sections describe the PROC STD RATE statement and then describe the other statements in alphabetical order.

## PROC STD RATE Statement

**PROC STD RATE** < options > ;

Table 88.1 summarizes the *options* in the PROC STD RATE statement.

**Table 88.1** Summary of PROC STD RATE Options

| Option                         | Description                                                                                               |
|--------------------------------|-----------------------------------------------------------------------------------------------------------|
| <b>Input Data Sets</b>         |                                                                                                           |
| <b>DATA=</b>                   | Names the SAS data set that contains the study populations                                                |
| <b>REFDATA=</b>                | Names the SAS data set that contains the reference population                                             |
| <b>Standardization Methods</b> |                                                                                                           |
| <b>METHOD=</b>                 | Specifies the method for standardization                                                                  |
| <b>STAT=</b>                   | Specifies the statistic for standardization                                                               |
| <b>EFFECT</b>                  | Specifies the test to compare study populations for direct standardization and Mantel-Haenszel estimation |
| <b>Displayed Output</b>        |                                                                                                           |
| <b>ALPHA=</b>                  | Specifies the significance level for confidence intervals                                                 |
| <b>CL=</b>                     | Requests the confidence limits for the standardized estimates                                             |
| <b>PLOTS</b>                   | Requests stratum-specific plots                                                                           |

You can specify the following *options* in the PROC STD RATE statement to compute standardized rates and risks in the procedure. They are listed in alphabetical order.

### **ALPHA=** $\alpha$

requests that confidence limits be constructed with confidence level  $100(1 - \alpha)\%$ , where  $0 < \alpha < 1$ . The default is ALPHA=0.05. These confidence limits include confidence limits for the stratum-specific rates or risks, standardized rate and risk, standardized morbidity/mortality ratio, and population attributable rate and risk.

### **CL=GAMMA** < (TYPE=AVERAGE | CONSERVATIVE) > | LOGNORMAL | NONE | NORMAL | POISSON

specifies the method to construct confidence limits for SMR and standardized rate and risk. You can specify the following values for this option:

#### **GAMMA**

requests confidence limits based on a gamma distribution for METHOD=DIRECT and METHOD=MH. This value applies only when STAT=RATE. You can specify the TYPE=CONSERVATIVE suboption to request conservative confidence limits that are based on a gamma distribution and were developed by Fay and Feuer (1997), or you can specify the TYPE=AVERAGE suboption to request modified confidence limits proposed by Tiwari, Clegg, and Zou (2006).

**LOGNORMAL**

requests confidence limits based on a lognormal distribution.

**NONE**

suppresses construction of confidence limits.

**NORMAL**

requests confidence limits based on a normal distribution.

**POISSON**

requests confidence limits based on a Poisson distribution. This value applies only when METHOD=INDIRECT.

The default is CL=NORMAL.

**DATA=SAS-data-set**

names the required SAS data set that contains the event information in the study populations.

**EFFECT <=DIFF | RATIO >**

displays a table of the effect estimate and associated confidence limits. This option applies only when METHOD=DIRECT with two study populations and when METHOD=MH, where two study populations are required.

EFFECT and EFFECT=RATIO display a test on the ratio effect of estimates between the study populations, and the EFFECT=DIFF option displays a test on the difference effect.

**METHOD= DIRECT | INDIRECT <(AF)> | MH <(AF)>****M= DIRECT | INDIRECT <(AF)> | MH <(AF)>**

specifies the required method for standardization. METHOD=DIRECT requests direct standardization, METHOD=INDIRECT requests indirect standardization, and METHOD=MH requests Mantel-Haenszel estimation.

The AF suboption requests the attributable fraction that measures the excess event rate or risk fraction in the exposed population that is attributable to the exposure. This suboption also requests the population attributable fraction that measures the excess event rate or risk fraction in the total population that is attributable to the exposure.

**PLOTS <( global-options )> <= plot-request >****PLOTS <( global-options )> <= ( plot-request <... plot-request > ) >**

specifies options that control the details of the plots. The default is PLOTS=RATE for STAT=RATE and PLOTS=RISK for STAT=RISK.

You can specify the following *global-options*:

**DISPLAY=INDEX | LEVEL**

specifies tick mark values for the strata axis. DISPLAY=LEVEL displays strata levels on the strata axis, and DISPLAY=INDEX displays strata indices of sequential strata identification numbers on the strata axis. The default is DISPLAY=LEVEL.

**ONLY**

suppresses the default plots and displays only plots that are specifically requested.

**STRATUM=HORIZONTAL | VERTICAL**

controls the orientation of the plots. STRATUM=VERTICAL places the strata information on the vertical axis, and STRATUM=HORIZONTAL places the strata information on the horizontal axis. The default is STRATUM=VERTICAL.

You can specify the following *plot-requests*:

**ALL**

produces all appropriate plots.

**DIST | DISTRIBUTION**

displays a plot of the proportions for stratum-specific exposed time or sample size.

**EFFECT**

displays a plot of the stratum-specific effect estimates and associated confidence limits. This option applies only when METHOD=DIRECT with two study populations and when METHOD=MH, where two study populations are required. If the EFFECT=DIFF option is specified, the stratum-specific rate or risk difference effects are displayed. Otherwise, the stratum-specific rate or risk ratio effects are displayed.

**NONE**

suppresses all plots.

**RATE**

displays a plot of the stratum-specific rates and associated confidence limits. This option applies only when STAT=RATE. If a confidence limits method is specified in the STATS(CL=) option in the STRATA statement, that method is used to compute the confidence limits. Otherwise, the normal approximation is used.

**RISK**

displays a plot of the stratum-specific risks and associated confidence limits. This option applies only when STAT=RISK. If a confidence limits method is specified in the STATS(CL=) option in the STRATA statement, that method is used to compute the confidence limits. Otherwise, the normal approximation is used.

**SMR**

displays a plot of the stratum-specific SMR estimates and associated confidence limits. This option applies only when METHOD=INDIRECT. If a method is specified in the SMR(CL=) option in the STRATA statement, that method is used to compute the confidence limits. Otherwise, the normal approximation is used.

**REFDATA=SAS-data-set**

names the required SAS data set that contains the event information in the reference population.

**STAT=RATE** < ( **MULT =c** ) >

**STAT=RISK**

specifies the statistic for standardization. **STAT=RATE** computes standardized rates, and **STAT=RISK** computes standardized risks. The default is **STAT=RATE**.

The **MULT=** suboption in the **STAT=RATE** option specifies a power of 10 constant *c*, and requests that rates per *c* population-time units be displayed in the output tables and graphics. The default is **MULT=100000**, which specifies rates per 100,000 population-time units.

## BY Statement

**BY** *variables* ;

You can specify a **BY** statement with **PROC STDRATE** to obtain separate analyses of observations in groups that are defined by the **BY** variables. When a **BY** statement appears, the procedure expects the input data set to be sorted in order of the **BY** variables. If you specify more than one **BY** statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the **SORT** procedure with a similar **BY** statement.
- Specify the **NOTSORTED** or **DESCENDING** option in the **BY** statement for the **STDRATE** procedure. The **NOTSORTED** option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the **BY** variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the **BY** variables by using the **DATASETS** procedure (in Base SAS software).

For more information about **BY**-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the **DATASETS** procedure, see the discussion in the *Base SAS Procedures Guide*.

## POPULATION Statement

**POPULATION** < *options* > ;

The required **POPULATION** statement specifies the information in the study data set. You can specify the following *options* in the **POPULATION** statement:

**EVENT=***variable*

specifies the *variable* for the number of events in the study data set.

**GROUP** < ( **ORDER=DATA** | **FORMATTED** | **INTERNAL** ) > =*variable*

specifies the *variable* whose values identify the various populations. This option is required when **METHOD=MH** and also applies when **METHOD=DIRECT** in the **PROC STDRATE** statement.



The optional ORDER= suboption specifies the order in which the values of the *variable* are to be displayed. You can specify the following values for the ORDER= suboption:

|                  |                                                                                            |
|------------------|--------------------------------------------------------------------------------------------|
| <b>DATA</b>      | sorts by the order in which the values appear in the input data set.                       |
| <b>FORMATTED</b> | sorts by their external formatted values.                                                  |
| <b>INTERNAL</b>  | sorts by the unformatted values, which yields the same order that the SORT procedure does. |

By default, ORDER=INTERNAL. For ORDER=FORMATTED and ORDER=INTERNAL, the sort order is machine-dependent.

**POPEVENT=***number*

specifies the total number of events in the study data set. This option applies only when METHOD=INDIRECT is specified in the PROC STDRATE statement and the total number of events is not available in the study data set.

**RATE < ( MULT=*c* ) > =** *variable*

specifies the *variable* for the observed rate in the study data set. This option applies only when STAT=RATE is specified in the PROC STDRATE statement. The MULT=*c* suboption specifies a power of 10 constant *c* and requests that the rates per *c* population-time units be read from the data set. The default is the value of the MULT= suboption used in the STAT=RATE option in the PROC STDRATE statement.

**RISK=***variable*

specifies the *variable* for the observed risk in the study data set. This option applies only when STAT=RISK is specified in the PROC STDRATE statement.

**TOTAL=***variable*

specifies the *variable* for either the population-time (STAT=RATE) or the number of observations (STAT=RISK) in the study data set.

---

## REFERENCE Statement

**REFERENCE** < *options* > ;

The REFERENCE statement specifies the information in the reference data set. This statement is required when METHOD=DIRECT or METHOD=INDIRECT is specified in the PROC STDRATE statement.

You can specify the following *options* in the REFERENCE statement:

**EVENT=***variable*

specifies the *variable* for the number of events in the reference data set.

**RATE < ( MULT=*c* ) > =** *variable*

specifies the *variable* for the observed rate in the reference data set. This option applies only when STAT=RATE is specified in the PROC STDRATE statement. The MULT=*c* suboption specifies a power of 10 constant *c* and requests that the rates per *c* population-time units be read from the data set. The default is the value of the MULT= suboption used in the STAT=RATE option in the PROC STDRATE statement.

**RISK=***variable*

specifies the *variable* for the observed risk in the reference data set. This option applies only when STAT=RISK is specified in the PROC STDRATE statement.

**TOTAL=***variable*

specifies the *variable* for either the population-time (STAT=RATE) or the number of observations (STAT=RISK) in the reference data set.

When METHOD=INDIRECT is specified in the PROC STDRATE statement, the overall reference population rate and risk are needed to compute indirect standardized rate and risk, respectively. If the information is not available in the reference data set, you can specify the following *options* for overall reference population rate and risk.

**REFEVENT=***number*

specifies the total *number* of events in the reference data set.

**REFRATE <( MULT=*c* )> =** *number*

specifies the crude rate in the reference data set. This option applies only when STAT=RATE is specified in the PROC STDRATE statement. The MULT=*c* suboption specifies a power of 10 constant *c*, and the *number* is the crude rate per *c* population-time units in the data set. The default is the value of the MULT= suboption in the STAT=RATE option in the PROC STDRATE statement.

**REFRISK=***number*

specifies the crude risk in the reference data set. This option applies only when STAT=RISK is specified in the PROC STDRATE statement.

**REFTOTAL=***number*

specifies either the total population-time (STAT=RATE) or the total number of observations (STAT=RISK) in the reference data set.

When STAT=RATE, the REFRATE= option specifies the crude reference rate for the indirect standardized rate. If the REFRATE= option is not specified, the REFEVENT= and REFTOTAL options can be used to compute the crude reference rate. Similarly, when STAT=RISK, the REFRISK= option specifies the crude reference risk for the indirect standardized rate. If the REFRISK= option is not specified, the REFEVENT= and REFTOTAL options can be used to compute the crude reference risk.

---

## STRATA Statement

**STRATA** *variables* </ *options*> ;

The STRATA statement names *variables* that form the strata in the standardization. The combinations of categories of STRATA variables define the strata in the population.

The STRATA variables are one or more variables in all input data sets. These variables can be either character or numeric. The formatted values of the STRATA variables determine the levels. Thus, you can use formats to group values into levels. See the FORMAT procedure in the *Base SAS Procedures Guide* and the FORMAT statement and SAS formats in *SAS Language Reference: Dictionary* for more information.

When the STRATA statement is not specified or the statement is specified without variables, all observations in a data set are treated as though they are from a single stratum.

You can specify the following *options* in the STRATA statement after a slash (/):

**EFFECT**

displays a table of the stratum-specific effect estimates and associated confidence limits. This option applies only when METHOD=DIRECT with two study populations and when METHOD=MH, where two study populations are required. If the EFFECT=DIFF option in the PROC STDRATE statement is specified, the stratum-specific rate or risk difference effects are displayed. Otherwise, the stratum-specific rate or risk ratio effects are displayed.

**MISSING**

treats missing values as a valid (nonmissing) category for all STRATA variables. When PROC STDRATE determines levels of a STRATA variable, an observation with missing values for that STRATA variable is excluded, unless the MISSING option is specified.

**ORDER=DATA | FORMATTED | INTERNAL**

specifies the order in which the values of the categorical variables are to be displayed. You can specify the following values for the ORDER= option:

|                  |                                                                                            |
|------------------|--------------------------------------------------------------------------------------------|
| <b>DATA</b>      | sorts by the order in which the values appear in the input data set.                       |
| <b>FORMATTED</b> | sorts by their external formatted values.                                                  |
| <b>INTERNAL</b>  | sorts by the unformatted values, which yields the same order that the SORT procedure does. |

By default, ORDER=INTERNAL. For ORDER=FORMATTED and ORDER=INTERNAL, the sort order is machine-dependent.

**STATS < ( CL=LOGNORMAL | NONE | NORMAL | POISSON ) >**

displays tables for stratum-specific statistics such as stratum-specific rates and risks. You can specify the following values of the CL= suboption to request confidence limits for the rate or risk estimate in each stratum:

**LOGNORMAL**

requests confidence limits based on a lognormal approximation.

**NONE**

suppresses confidence limits.

**NORMAL**

requests confidence limits based on a normal approximation and also displays the standard error for the rate estimate in each stratum.

**POISSON**

requests confidence limits based on a Poisson distribution for stratum-specific rates. This values applies only when STAT=RATE in the PROC STDRATE statement.

The default is CL=NORMAL.

**SMR < ( CL=LOGNORMAL | NONE | NORMAL | POISSON ) >**

displays tables for stratum-specific SMR estimates. This option applies only when METHOD=INDIRECT is specified in the PROC STDRATE statement. You can specify the following values of the CL= suboption to request confidence limits for the SMR estimate in each stratum:

**LOGNORMAL**

requests confidence limits based on a lognormal approximation.

**NONE**

suppresses confidence limits.

**NORMAL**

requests confidence limits based on a normal approximation and also displays the standard error for the SMR estimate in each stratum.

**POISSON**

requests confidence limits based on a Poisson distribution for stratum-specific SMR estimates. This values applies only when STAT=RATE in the PROC STDRATE statement.

The default is CL=NORMAL.

## Details: STDRATE Procedure

### Rate

A major task in epidemiology is to compare event frequencies for groups of people. Both rate and risk are commonly used to measure event frequency in the comparison. Rate is a measure of change in one quantity per unit of another quantity. An event rate measures how fast the events are occurring. In contrast, an event risk is the probability that an event occurs over a specified follow-up time period.

An event rate of a population over a specified time period can be defined as the number of new events divided by the population-time of the population over the same time period,

$$\hat{\lambda} = \frac{d}{\mathcal{T}}$$

where  $d$  is the number of events and  $\mathcal{T}$  is the population-time that is computed by adding up the time contributed by each subject in the population over the specified time period.

For a general population, the subsets (strata) might not be homogeneous enough to have a similar rate. Thus, the rate for each stratum should be computed separately to reflect this discrepancy. For a population that consists of  $K$  homogeneous strata (such as different age groups), the stratum-specific rate for the  $j$ th stratum in a population is computed as

$$\hat{\lambda}_j = \frac{d_j}{\mathcal{T}_j}$$

where  $d_j$  is the number of events and  $\mathcal{T}_j$  is the population-time for subjects in the  $j$ th stratum of the population.

Assuming the number of events in the  $j$ th stratum,  $d_j$ , has a Poisson distribution, the variance of  $\hat{\lambda}_j$  is

$$V(\hat{\lambda}_j) = V\left(\frac{d_j}{\mathcal{T}_j}\right) = \frac{1}{\mathcal{T}_j^2} V(d_j) = \frac{d_j}{\mathcal{T}_j^2} = \frac{\hat{\lambda}_j}{\mathcal{T}_j}$$

By using the method of statistical differentials (Elandt-Johnson and Johnson 1980, pp. 70–71), the variance of the logarithm of rate can be estimated by

$$V(\log(\hat{\lambda}_j)) = \frac{1}{\hat{\lambda}_j^2} V(\hat{\lambda}_j) = \frac{1}{\hat{\lambda}_j^2} \frac{\hat{\lambda}_j}{\mathcal{T}_j} = \frac{1}{\hat{\lambda}_j \mathcal{T}_j} = \frac{1}{d_j}$$

Because the rate value can be very small, especially for rare events, it is sometimes expressed in terms of the product of a multiplier and the rate itself. For example, a rate can be expressed as the number of events per 100,000 person-years.

### Normal Distribution Confidence Interval for Rate

A  $(1 - \alpha)$  confidence interval for  $\hat{\lambda}_j$  based on a normal distribution is given by

$$\left( \hat{\lambda}_j - z \sqrt{V(\hat{\lambda}_j)}, \hat{\lambda}_j + z \sqrt{V(\hat{\lambda}_j)} \right)$$

where  $z = \Phi^{-1}(1 - \alpha/2)$  is the  $(1 - \alpha/2)$  quantile of the standard normal distribution.

### Lognormal Distribution Confidence Interval for Rate

A  $(1 - \alpha)$  confidence interval for  $\log(\hat{\lambda}_j)$  based on a normal distribution is given by

$$\left( \log(\hat{\lambda}_j) - z \sqrt{V(\log(\hat{\lambda}_j))}, \log(\hat{\lambda}_j) + z \sqrt{V(\log(\hat{\lambda}_j))} \right)$$

where  $z = \Phi^{-1}(1 - \alpha/2)$  is the  $(1 - \alpha/2)$  quantile of the standard normal distribution and the variance  $V(\log(\hat{\lambda}_j)) = 1/d_j$ .

Thus, a  $(1 - \alpha)$  confidence interval for  $\hat{\lambda}_j$  based on a lognormal distribution is given by

$$\left( \hat{\lambda}_j e^{-\frac{z}{\sqrt{d_j}}}, \hat{\lambda}_j e^{\frac{z}{\sqrt{d_j}}} \right)$$

### Poisson Distribution Confidence Interval for Rate

Denote the  $(\alpha/2)$  quantile for the  $\chi^2$  distribution with  $2d_j$  degrees of freedom by

$$q_{lj} = (\chi_{2d_j}^2)^{-1}(\alpha/2)$$

Denote the  $(1 - \alpha/2)$  quantiles for the  $\chi^2$  distribution with  $2(d_j + 1)$  degrees of freedom by

$$q_{uj} = (\chi_{2(d_j+1)}^2)^{-1}(1 - \alpha/2)$$

Then a  $(1 - \alpha)$  confidence interval for  $\hat{\lambda}_j$  based on the  $\chi^2$  distribution is given by

$$\left( \frac{q_{lj}}{2\mathcal{T}_j}, \frac{q_{uj}}{2\mathcal{T}_j} \right)$$

### Confidence Interval for Rate Difference Statistic

For rate estimates from two independent samples,  $\hat{\lambda}_{1j}$  and  $\hat{\lambda}_{2j}$ , a  $(1 - \alpha)$  confidence interval for the rate difference  $\hat{\lambda}_{dj} = \hat{\lambda}_{1j} - \hat{\lambda}_{2j}$  is

$$\left( \hat{\lambda}_{dj} - z \sqrt{V(\hat{\lambda}_{dj})}, \hat{\lambda}_{dj} + z \sqrt{V(\hat{\lambda}_{dj})} \right)$$

where  $z = \Phi^{-1}(1 - \alpha/2)$  is the  $(1 - \alpha/2)$  quantile of the standard normal distribution and the variance

$$V(\hat{\lambda}_{dj}) = V(\hat{\lambda}_{1j}) + V(\hat{\lambda}_{2j})$$

### Confidence Interval for Rate Ratio Statistic

For rate estimates from two independent samples,  $\hat{\lambda}_{1j}$  and  $\hat{\lambda}_{2j}$ , a  $(1 - \alpha)$  confidence interval for the log rate ratio statistic  $\log(\hat{\lambda}_{rj}) = \log(\hat{\lambda}_{1j}/\hat{\lambda}_{2j})$  is

$$\left( \log(\hat{\lambda}_{rj}) - z \sqrt{V(\log(\hat{\lambda}_{rj}))}, \log(\hat{\lambda}_{rj}) + z \sqrt{V(\log(\hat{\lambda}_{rj}))} \right)$$

where  $z = \Phi^{-1}(1 - \alpha/2)$  is the  $(1 - \alpha/2)$  quantile of the standard normal distribution and the variance

$$V(\log(\hat{\lambda}_{rj})) = V(\log(\hat{\lambda}_{1j})) + V(\log(\hat{\lambda}_{2j}))$$

Thus, a  $(1 - \alpha)$  confidence interval for the rate ratio statistic  $\hat{\lambda}_{rj}$  is given by

$$\left( \frac{\hat{\lambda}_{1j}}{\hat{\lambda}_{2j}} e^{-z \sqrt{V(\log(\hat{\lambda}_{rj}))}}, \frac{\hat{\lambda}_{1j}}{\hat{\lambda}_{2j}} e^{z \sqrt{V(\log(\hat{\lambda}_{rj}))}} \right)$$

### Confidence Interval for Rate SMR

At stratum  $j$ , a stratum-specific standardized morbidity/mortality ratio is

$$\mathcal{R}_j = \frac{d_j}{\mathcal{E}_j}$$

where  $\mathcal{E}_j$  is the expected number of events.

With the rate

$$\hat{\lambda}_j = \frac{d_j}{\mathcal{T}_j}$$

SMR can be expressed as

$$\mathcal{R}_j = \frac{\mathcal{T}_j}{\mathcal{E}_j} \hat{\lambda}_j$$

Thus, a  $(1 - \alpha)$  confidence interval for  $\mathcal{R}_j$  is given by

$$\left( \frac{\mathcal{T}_j}{\mathcal{E}_j} \hat{\lambda}_{jl}, \frac{\mathcal{T}_j}{\mathcal{E}_j} \hat{\lambda}_{ju} \right)$$

where  $(\hat{\lambda}_{jl}, \hat{\lambda}_{ju})$  is a  $(1 - \alpha)$  confidence interval for the rate  $\hat{\lambda}_j$ .

## Risk

An event risk of a population over a specified time period can be defined as the number of new events in the follow-up time period divided by the event-free population size at the beginning of the time period,

$$\hat{\gamma} = \frac{d}{\mathcal{N}}$$

where  $\mathcal{N}$  is the population size.

For a general population, the subsets (strata) might not be homogeneous enough to have a similar risk. Thus, the risk for each stratum should be computed separately to reflect this discrepancy. For a population that consists of  $K$  homogeneous strata (such as different age groups), the stratum-specific risk for the  $j$ th stratum in a population is computed as

$$\hat{\gamma}_j = \frac{d_j}{\mathcal{N}_j}$$

where  $\mathcal{N}_j$  is the population size in the  $j$ th stratum of the population.

Assuming the number of events,  $d_j$ , has a binomial distribution, then a variance estimate of  $\hat{\gamma}_j$  is

$$V(\hat{\gamma}_j) = \frac{\hat{\gamma}_j(1 - \hat{\gamma}_j)}{\mathcal{N}_j}$$

By using the method of statistical differentials (Elandt-Johnson and Johnson 1980, pp. 70–71), the variance of the logarithm of risk can be estimated by

$$V(\log(\hat{\gamma}_j)) = \frac{1}{\hat{\gamma}_j^2} V(\hat{\gamma}_j) = \frac{1}{\hat{\gamma}_j^2} \frac{\hat{\gamma}_j(1 - \hat{\gamma}_j)}{\mathcal{N}_j} = \frac{1 - \hat{\gamma}_j}{\hat{\gamma}_j \mathcal{N}_j} = \frac{1}{d_j} - \frac{1}{\mathcal{N}_j}$$

### Normal Distribution Confidence Interval for Risk

A  $(1 - \alpha)$  confidence interval for  $\hat{\gamma}_j$  based on a normal distribution is given by

$$\left( \hat{\gamma}_j - z \sqrt{V(\hat{\gamma}_j)}, \hat{\gamma}_j + z \sqrt{V(\hat{\gamma}_j)} \right)$$

where  $z = \Phi^{-1}(1 - \alpha/2)$  is the  $(1 - \alpha/2)$  quantile of the standard normal distribution.

### Lognormal Distribution Confidence Interval for Risk

A  $(1 - \alpha)$  confidence interval for  $\log(\hat{\gamma}_j)$  based on a normal distribution is given by

$$\left( \log(\hat{\gamma}_j) - z \sqrt{V(\log(\hat{\gamma}_j))}, \log(\hat{\gamma}_j) + z \sqrt{V(\log(\hat{\gamma}_j))} \right)$$

where  $z = \Phi^{-1}(1 - \alpha/2)$  is the  $(1 - \alpha/2)$  quantile of the standard normal distribution and the variance  $V(\log(\hat{\gamma}_j)) = 1/d_j - 1/\mathcal{N}_j$ .

Thus, a  $(1 - \alpha)$  confidence interval for  $\hat{\gamma}_j$  based on a lognormal distribution is given by

$$\left( \hat{\gamma}_j e^{-z \sqrt{\frac{1}{d_j} - \frac{1}{\mathcal{N}_j}}}, \hat{\gamma}_j e^{z \sqrt{\frac{1}{d_j} - \frac{1}{\mathcal{N}_j}}} \right)$$

### Confidence Interval for Risk Difference Statistic

For rate estimates from two independent samples,  $\hat{\gamma}_{1j}$  and  $\hat{\gamma}_{2j}$ , a  $(1 - \alpha)$  confidence interval for the risk difference  $\hat{\gamma}_{dj} = \hat{\gamma}_{1j} - \hat{\gamma}_{2j}$  is

$$\left( \hat{\gamma}_{dj} - z \sqrt{V(\hat{\gamma}_{dj})}, \hat{\gamma}_{dj} + z \sqrt{V(\hat{\gamma}_{dj})} \right)$$

where  $z = \Phi^{-1}(1 - \alpha/2)$  is the  $(1 - \alpha/2)$  quantile of the standard normal distribution and the variance

$$V(\hat{\gamma}_{dj}) = V(\hat{\gamma}_{1j}) + V(\hat{\gamma}_{2j})$$

### Confidence Interval for Risk Ratio Statistic

For rate estimates from two independent samples,  $\hat{\gamma}_{1j}$  and  $\hat{\gamma}_{2j}$ , a  $(1 - \alpha)$  confidence interval for the log risk ratio statistic  $\log(\hat{\gamma}_{rj}) = \log(\hat{\gamma}_{1j}/\hat{\gamma}_{2j})$  is

$$\left( \log(\hat{\gamma}_{rj}) - z \sqrt{V(\log(\hat{\gamma}_{rj}))}, \log(\hat{\gamma}_{rj}) + z \sqrt{V(\log(\hat{\gamma}_{rj}))} \right)$$

where  $z = \Phi^{-1}(1 - \alpha/2)$  is the  $(1 - \alpha/2)$  quantile of the standard normal distribution and the variance

$$V(\log(\hat{\gamma}_{rj})) = V(\log(\hat{\gamma}_{1j})) + V(\log(\hat{\gamma}_{2j}))$$

Thus, a  $(1 - \alpha)$  confidence interval for the risk ratio statistic  $\hat{\gamma}_{rj}$  is given by

$$\left( \frac{\hat{\gamma}_{1j}}{\hat{\gamma}_{2j}} e^{-z \sqrt{V(\log(\hat{\gamma}_{rj}))}}, \frac{\hat{\gamma}_{1j}}{\hat{\gamma}_{2j}} e^{z \sqrt{V(\log(\hat{\gamma}_{rj}))}} \right)$$

### Confidence Interval for Risk SMR

At stratum  $j$ , a stratum-specific standardized morbidity/mortality ratio is

$$\mathcal{R}_j = \frac{d_j}{\mathcal{E}_j}$$

where  $\mathcal{E}_j$  is the expected number of events.

With the risk

$$\hat{\gamma}_j = \frac{d_j}{\mathcal{N}_j}$$

SMR can be expressed as

$$\mathcal{R}_j = \frac{\mathcal{N}_j}{\mathcal{E}_j} \hat{\gamma}_j$$

Thus, a  $(1 - \alpha)$  confidence interval for  $\mathcal{R}_j$  is given by

$$\left( \frac{\mathcal{N}_j}{\mathcal{E}_j} \hat{\gamma}_{jl}, \frac{\mathcal{N}_j}{\mathcal{E}_j} \hat{\gamma}_{ju} \right)$$

where  $(\hat{\gamma}_{jl}, \hat{\gamma}_{ju})$  is a  $(1 - \alpha)$  confidence interval for the risk  $\hat{\gamma}_j$ .



## Direct Standardization

Direct standardization uses the weights from a reference population to compute the standardized rate of a study group as the weighted average of stratum-specific rates in the study population. The standardized rate is computed as

$$\hat{\lambda}_{ds} = \frac{\sum_j \mathcal{T}_{rj} \hat{\lambda}_{sj}}{\mathcal{T}_r}$$

where  $\hat{\lambda}_{sj}$  is the rate in the  $j$ th stratum of the study population,  $\mathcal{T}_{rj}$  is the population-time in the  $j$ th stratum of the reference population, and  $\mathcal{T}_r = \sum_k \mathcal{T}_{rk}$  is the population-time in the reference population.

Similarly, direct standardization uses the weights from a reference population to compute the standardized risk of a study group as the weighted average of stratum-specific risks in the study population. The standardized risk is computed as

$$\hat{\gamma}_{ds} = \frac{\sum_j \mathcal{N}_{rj} \hat{\gamma}_{sj}}{\mathcal{N}_r}$$

where  $\hat{\gamma}_{sj}$  is the risk in the  $j$ th stratum of the study population,  $\mathcal{N}_{rj}$  is the number of observations in the  $j$ th stratum of the reference population, and  $\mathcal{N}_r = \sum_k \mathcal{N}_{rk}$  is the total number of observations in the reference population.

That is, the directly standardized rate and risk of a study population are weighted averages of the stratum-specific rates and risks, respectively, where the weights are the corresponding strata population sizes in the reference population. The direct standardization can be used when the study population is large enough to provide stable stratum-specific rates or risks. When the same reference population is used for multiple study populations, directly standardized rates and risks provide valid comparisons between study populations.

The variances of the directly standardized rate and risk are

$$V(\hat{\lambda}_{ds}) = V\left(\frac{\sum_j \mathcal{T}_{rj} \hat{\lambda}_{sj}}{\mathcal{T}_r}\right) = \frac{\sum_j \mathcal{T}_{rj}^2 V(\hat{\lambda}_{sj})}{\mathcal{T}_r^2}$$

$$V(\hat{\gamma}_{ds}) = V\left(\frac{\sum_j \mathcal{N}_{rj} \hat{\gamma}_{sj}}{\mathcal{N}_r}\right) = \frac{\sum_j \mathcal{N}_{rj}^2 V(\hat{\gamma}_{sj})}{\mathcal{N}_r^2}$$

By using the method of statistical differentials (Elandt-Johnson and Johnson 1980, pp. 70–71), the variance of the logarithm of directly standardized rate and risk can be estimated by

$$V(\log(\hat{\lambda}_{ds})) = \frac{1}{\hat{\lambda}_{ds}^2} V(\hat{\lambda}_{ds})$$

$$V(\log(\hat{\gamma}_{ds})) = \frac{1}{\hat{\gamma}_{ds}^2} V(\hat{\gamma}_{ds})$$

The confidence intervals for  $\hat{\lambda}_{ds}$  and  $\hat{\gamma}_{ds}$  can be constructed based on normal and lognormal distributions. A gamma distribution confidence interval can also be constructed for  $\hat{\lambda}_{ds}$ .

In the next four subsections,  $\beta = \lambda$  denotes the rate statistic and  $\beta = \gamma$  denotes the risk statistic.

### Normal Distribution Confidence Intervals for Standardized Rate and Risk

A  $(1 - \alpha)$  confidence interval for  $\hat{\beta}_{ds}$  based on a normal distribution is then given by

$$\left( \hat{\beta}_{ds} - z \sqrt{V(\hat{\beta}_{ds})}, \hat{\beta}_{ds} + z \sqrt{V(\hat{\beta}_{ds})} \right)$$

where  $z = \Phi^{-1}(1 - \alpha/2)$  is the  $(1 - \alpha/2)$  quantile of the standard normal distribution.

### Lognormal Distribution Confidence Intervals for Standardized Rate and Risk

A  $(1 - \alpha)$  confidence interval for  $\log(\hat{\beta}_{ds})$  based on a normal distribution is given by

$$\left( \log(\hat{\beta}_{ds}) - z \sqrt{V(\log(\hat{\beta}_{ds}))}, \log(\hat{\beta}_{ds}) + z \sqrt{V(\log(\hat{\beta}_{ds}))} \right)$$

where  $z = \Phi^{-1}(1 - \alpha/2)$  is the  $(1 - \alpha/2)$  quantile of the standard normal distribution.

Thus, a  $(1 - \alpha)$  confidence interval for  $\hat{\beta}_{ds}$  based on a lognormal distribution is given by

$$\left( \hat{\beta}_{ds} e^{-z \sqrt{V(\log(\hat{\beta}_{ds}))}}, \hat{\beta}_{ds} e^{z \sqrt{V(\log(\hat{\beta}_{ds}))}} \right)$$

### Gamma Distribution Confidence Interval for Standardized Rate

Fay and Feuer (1997) use the relationship between the Poisson and gamma distributions to derive approximate confidence intervals for the standardized rate  $\hat{\lambda}_{ds}$  based on the gamma distribution. As in the construction of the asymptotic normal confidence intervals, it is assumed that the number of events has a Poisson distribution, and the standardized rate is a weighted sum of independent Poisson random variables. A confidence interval for  $\hat{\lambda}_{ds}$  is then given by

$$\left( \frac{v}{2\hat{\lambda}_{ds}} (\chi^2)^{-1}_{\frac{2\hat{\lambda}_{ds}^2}{v}} \left( \frac{\alpha}{2} \right), \frac{v + w_x^2}{2(\hat{\lambda}_{ds} + w_x)} (\chi^2)^{-1}_{\frac{2(\hat{\lambda}_{ds} + w_x)^2}{v + w_x^2}} \left( 1 - \frac{\alpha}{2} \right) \right)$$

where

$$v = \sum_j w_j^2 \frac{\hat{\lambda}_{sj}}{\bar{T}_{sj}}$$

$$w_j = \frac{\bar{T}_{rj}}{\bar{T}_r} \frac{1}{\bar{T}_{sj}}$$

and  $w_x$  is the maximum  $w_j$ .

Tiwari, Clegg, and Zou (2006) propose a less conservative confidence interval for  $\hat{\lambda}_{ds}$  with a different upper confidence limit,

$$\left( \frac{v}{2\hat{\lambda}_{ds}} (\chi^2)^{-1}_{\frac{2\hat{\lambda}_{ds}^2}{v}} \left( \frac{\alpha}{2} \right), \frac{v + w_{2m}}{2(\hat{\lambda}_{ds} + w_m)} (\chi^2)^{-1}_{\frac{2(\hat{\lambda}_{ds} + w_m)^2}{v + w_{2m}}} \left( 1 - \frac{\alpha}{2} \right) \right)$$

where  $w_m$  is the average  $w_j$  and  $w_{2m}$  is the average  $w_j^2$ .

## Comparing Standardized Rates and Comparing Standardized Risks

By using the same reference population, two directly standardized rates or risks from different populations can be compared. Both the difference and ratio statistics can be used in the comparison. Assume that  $\hat{\beta}_1$  and  $\hat{\beta}_2$  are directly standardized rates or risks for two populations with variances  $V(\hat{\beta}_1)$  and  $V(\hat{\beta}_2)$ , respectively. The difference test assumes that the difference statistic

$$\hat{\beta}_1 - \hat{\beta}_2$$

has a normal distribution with mean 0 under the null hypothesis  $H_0 : \beta_1 = \beta_2$ . The variance is given by

$$V(\hat{\beta}_1 - \hat{\beta}_2) = V(\hat{\beta}_1) + V(\hat{\beta}_2)$$

The ratio test assumes that the log ratio statistic,

$$\log\left(\frac{\hat{\beta}_1}{\hat{\beta}_2}\right)$$

has a normal distribution with mean 0 under the null hypothesis  $H_0 : \beta_1 = \beta_2$ , or equivalently,  $\log(\beta_1/\beta_2) = 0$ . An estimated variance is given by

$$V\left(\log\left(\frac{\hat{\beta}_1}{\hat{\beta}_2}\right)\right) = V(\log(\hat{\beta}_1)) + V(\log(\hat{\beta}_2)) = \frac{1}{\hat{\beta}_1^2} V(\hat{\beta}_1) + \frac{1}{\hat{\beta}_2^2} V(\hat{\beta}_2)$$

## Mantel-Haenszel Effect Estimation

In direct standardization, the derived standardized rates and risks in a study population are the weighted average of the stratum-specific rates and risks in the population, respectively, where the weights are given by the population-time for standardized rate and the number of observations for standardized risk in a reference population.

Assuming that an effect, such as rate difference, rate ratio, risk difference, and risk ratio between two populations, is homogeneous across strata, the Mantel-Haenszel estimates of this effect can be constructed from directly standardized rates or risks in the two populations, where the weights are constructed from the stratum-specific population-times for rate and number of observations for risk of the two populations.

That is, for population  $k$ ,  $k=1$  and  $2$ , the standardized rate and risk are

$$\hat{\lambda}_k = \frac{\sum_j w_j \hat{\lambda}_{kj}}{\sum_j w_j} \quad \text{and} \quad \hat{\gamma}_k = \frac{\sum_j w_j \hat{\gamma}_{kj}}{\sum_j w_j}$$

where the weights are

$$w_j = \frac{\mathcal{T}_{1j} \mathcal{T}_{2j}}{\mathcal{T}_{1j} + \mathcal{T}_{2j}}$$

for standardized rate, and

$$w_j = \frac{\mathcal{N}_{1j} \mathcal{N}_{2j}}{\mathcal{N}_{1j} + \mathcal{N}_{2j}}$$

for standardized risk.

### Rate and Risk Difference Statistics

Denote  $\beta = \lambda$  for rate and  $\beta = \gamma$  for risk. The variance is

$$V(\hat{\beta}_k) = V\left(\frac{\sum_j w_j \hat{\beta}_{kj}}{\sum_j w_j}\right) = \frac{1}{(\sum_j w_j)^2} \sum_j w_j^2 V(\hat{\beta}_{kj})$$

The Mantel-Haenszel difference statistic is

$$\hat{\beta}_1 - \hat{\beta}_2$$

with variance

$$V(\hat{\beta}_1 - \hat{\beta}_2) = V(\hat{\beta}_1) + V(\hat{\beta}_2)$$

Under the null hypothesis  $H_0 : \beta_1 = \beta_2$ , the difference statistic  $\hat{\beta}_1 - \hat{\beta}_2$  has a normal distribution with mean 0.

### Rate Ratio Statistic

The Mantel-Haenszel rate ratio statistic is  $\hat{\lambda}_1/\hat{\lambda}_2$ , and the log ratio statistic is

$$\log\left(\frac{\hat{\lambda}_1}{\hat{\lambda}_2}\right)$$

Under the null hypothesis  $H_0 : \lambda_1 = \lambda_2$  (or equivalently,  $\log(\lambda_1/\lambda_2) = 0$ ), the log ratio statistic has a normal distribution with mean 0 and variance

$$V\left(\log\left(\frac{\hat{\lambda}_1}{\hat{\lambda}_2}\right)\right) = \frac{\sum_j w_j \hat{\lambda}_{pj}}{(\sum_j w_j \hat{\lambda}_{1j})(\sum_j w_j \hat{\lambda}_{2j})}$$

where

$$\hat{\lambda}_{pj} = \frac{d_{1j} + d_{2j}}{T_{1j} + T_{2j}}$$

is the combined rate estimate in stratum  $j$  under the null hypothesis of equal rates (Greenland and Robins 1985; Greenland and Rothman 2008, p. 273).

### Risk Ratio Statistic

The Mantel-Haenszel risk ratio statistic is  $\hat{\gamma}_1/\hat{\gamma}_2$ , and the log ratio statistic is

$$\log\left(\frac{\hat{\gamma}_1}{\hat{\gamma}_2}\right)$$

Under the null hypothesis  $H_0 : \gamma_1 = \gamma_2$  (or equivalently,  $\log(\gamma_1/\gamma_2) = 0$ ), the log ratio statistic has a normal distribution with mean 0 and variance

$$V\left(\log\left(\frac{\hat{\gamma}_1}{\hat{\gamma}_2}\right)\right) = \frac{\sum_j w_j (\hat{\gamma}_{pj} - \hat{\gamma}_{1j}\hat{\gamma}_{2j})}{(\sum_j w_j \hat{\gamma}_{1j})(\sum_j w_j \hat{\gamma}_{2j})}$$

where

$$\hat{\gamma}_{pj} = \frac{d_{1j} + d_{2j}}{N_{1j} + N_{2j}}$$

is the combined risk estimate in stratum  $j$  under the null hypothesis of equal risks (Greenland and Robins 1985; Greenland and Rothman 2008, p. 275).

## Indirect Standardization and Standardized Morbidity/Mortality Ratio

Indirect standardization compares the rates of the study and reference populations by applying the stratum-specific rates in the reference population to the study population, where the stratum-specific rates might not be reliable.

The expected number of events in the study population is

$$\mathcal{E} = \sum_j \mathcal{T}_{sj} \hat{\lambda}_{rj}$$

where  $\mathcal{T}_{sj}$  is the population-time in the  $j$ th stratum of the study population and  $\hat{\lambda}_{rj}$  is the rate in the  $j$ th stratum of the reference population.

With the expected number of events,  $\mathcal{E}$ , the standardized morbidity ratio or standardized mortality ratio can be expressed as

$$\mathcal{R}_{sm} = \frac{\mathcal{D}}{\mathcal{E}}$$

where  $\mathcal{D}$  is the observed number of events (Breslow and Day 1987, p. 65).

The ratio  $\mathcal{R}_{sm} > 1$  indicates that the mortality rate or risk in the study population is larger than the estimate in the reference population, and  $\mathcal{R}_{sm} < 1$  indicates that the mortality rate or risk in the study population is smaller than the estimate in the reference population.

With the ratio  $\mathcal{R}_{sm}$ , an indirectly standardized rate for the study population is computed as

$$\hat{\lambda}_{is} = \mathcal{R}_{sm} \hat{\lambda}_r$$

where  $\hat{\lambda}_r$  is the overall crude rate in the reference population.

Similarly, to compare the risks of the study and reference populations, the stratum-specific risks in the reference population are used to compute the expected number of events in the study population

$$\mathcal{E} = \sum_j N_{sj} \hat{\gamma}_{rj}$$

where  $N_{sj}$  is the number of observations in the  $j$ th stratum of the study population and  $\hat{\gamma}_{rj}$  is the risk in the  $j$ th stratum of the reference population.

Also, with the standardized morbidity ratio  $\mathcal{R}_{sm} = \mathcal{D}/\mathcal{E}$ , an indirectly standardized risk for the study population is computed as

$$\hat{\gamma}_{is} = \mathcal{R}_{sm} \hat{\gamma}_r$$

where  $\hat{\gamma}_r$  is the overall crude risk in the reference population.

The observed number of events in the study population is  $\mathcal{D} = \sum_j d_{sj}$ , where  $d_{sj}$  is the number of events in the  $j$ th stratum of the population. For the rate estimate, if  $d_{sj}$  has a Poisson distribution, then the variance of the standardized mortality ratio  $\mathcal{R}_{sm} = \mathcal{D} / \mathcal{E}$  is

$$V(\mathcal{R}_{sm}) = \frac{1}{\mathcal{E}^2} \sum_j V(d_{sj}) = \frac{1}{\mathcal{E}^2} \sum_j d_{sj} = \frac{\mathcal{D}}{\mathcal{E}^2} = \frac{\mathcal{R}_{sm}}{\mathcal{E}}$$

For the risk estimate, if  $d_{sj}$  has a binomial distribution, then the variance of  $\mathcal{R}_{sm} = \mathcal{D} / \mathcal{E}$  is

$$V(\mathcal{R}_{sm}) = V\left(\frac{1}{\mathcal{E}} \sum_j d_{sj}\right) = \frac{1}{\mathcal{E}^2} \sum_j V(d_{sj}) = \frac{1}{\mathcal{E}^2} \sum_j \mathcal{N}_{sj}^2 V(\hat{\gamma}_{sj})$$

where

$$V(\hat{\gamma}_{sj}) = \frac{\hat{\gamma}_{sj}(1 - \hat{\gamma}_{sj})}{\mathcal{N}_{sj}}$$

By using the method of statistical differentials (Elandt-Johnson and Johnson 1980, pp. 70–71), the variance of the logarithm of  $\mathcal{R}_{sm}$  can be estimated by

$$V(\log(\mathcal{R}_{sm})) = \frac{1}{\mathcal{R}_{sm}^2} V(\mathcal{R}_{sm})$$

For the rate estimate,

$$V(\log(\mathcal{R}_{sm})) = \frac{1}{\mathcal{R}_{sm}^2} V(\mathcal{R}_{sm}) = \frac{1}{\mathcal{R}_{sm}^2} \frac{\mathcal{R}_{sm}}{\mathcal{E}} = \frac{1}{\mathcal{R}_{sm}} \frac{1}{\mathcal{E}} = \frac{1}{\mathcal{D}}$$

The confidence intervals for  $\mathcal{R}_{sm}$  can be constructed based on normal, lognormal, and Poisson distributions.

### Normal Distribution Confidence Interval for SMR

A  $(1 - \alpha)$  confidence interval for  $\mathcal{R}_{sm}$  based on a normal distribution is given by

$$(\mathcal{R}_l, \mathcal{R}_u) = \left( \mathcal{R}_{sm} - z \sqrt{V(\mathcal{R}_{sm})}, \mathcal{R}_{sm} + z \sqrt{V(\mathcal{R}_{sm})} \right)$$

where  $z = \Phi^{-1}(1 - \alpha/2)$  is the  $(1 - \alpha/2)$  quantile of the standard normal distribution.

A test statistic for the null hypothesis  $H_0 : \text{SMR} = 1$  is then given by

$$\frac{\mathcal{R}_{sm} - 1}{\sqrt{V(\mathcal{R}_{sm})}}$$

The test statistic has an approximate standard normal distribution under  $H_0$ .

### Lognormal Distribution Confidence Interval for SMR

A  $(1 - \alpha)$  confidence interval for  $\log(\mathcal{R}_{sm})$  based on a normal distribution is given by

$$\left( \log(\mathcal{R}_{sm}) - z \sqrt{V(\log(\mathcal{R}_{sm}))}, \log(\mathcal{R}_{sm}) + z \sqrt{V(\log(\mathcal{R}_{sm}))} \right)$$

where  $z = \Phi^{-1}(1 - \alpha/2)$  is the  $(1 - \alpha/2)$  quantile of the standard normal distribution.

Thus, a  $(1 - \alpha)$  confidence interval for  $\mathcal{R}_{sm}$  based on a lognormal distribution is given by

$$\left( \mathcal{R}_{sm} e^{-z \sqrt{V(\log(\mathcal{R}_{sm}))}}, \mathcal{R}_{sm} e^{z \sqrt{V(\log(\mathcal{R}_{sm}))}} \right)$$

A test statistic for the null hypothesis  $H_0 : \text{SMR} = 1$  is then given by

$$\frac{\log(\mathcal{R}_{sm})}{\sqrt{V(\log(\mathcal{R}_{sm}))}}$$

The test statistic has an approximate standard normal distribution under  $H_0$ .

### Poisson Distribution Confidence Interval for Rate SMR

Denote the  $(\alpha/2)$  quantile for the  $\chi^2$  distribution with  $2\mathcal{D}$  degrees of freedom by

$$q_l = (\chi_{2\mathcal{D}}^2)^{-1}(\alpha/2)$$

Denote the  $(1 - \alpha/2)$  quantiles for the  $\chi^2$  distribution with  $2(\mathcal{D} + 1)$  degrees of freedom by

$$q_u = (\chi_{2(\mathcal{D}+1)}^2)^{-1}(1 - \alpha/2)$$

Then a  $(1 - \alpha)$  confidence interval for  $\mathcal{R}_{sm}$  based on the  $\chi^2$  distribution is given by

$$(\mathcal{R}_l, \mathcal{R}_u) = \left( \frac{q_l}{2\mathcal{E}}, \frac{q_u}{2\mathcal{E}} \right)$$

A  $p$ -value for the test of the null hypothesis  $H_0 : \text{SMR} = 1$  is given by

$$2 \min \left( \sum_{k=0}^{\mathcal{D}} \frac{e^{-\mathcal{E}} \mathcal{E}^k}{k!}, \sum_{k=\mathcal{D}}^{\infty} \frac{e^{-\mathcal{E}} \mathcal{E}^k}{k!} \right)$$

### Indirectly Standardized Rate and Its Confidence Interval

With a rate-standardized mortality ratio  $\mathcal{R}_{sm}$ , an indirectly standardized rate for the study population is computed as

$$\hat{\lambda}_{is} = \mathcal{R}_{sm} \hat{\lambda}_r$$

where  $\hat{\lambda}_r$  is the overall crude rate in the reference population.

The  $(1 - \alpha/2)$  confidence intervals for  $\hat{\lambda}_{is}$  can be constructed as

$$(\mathcal{R}_l \hat{\lambda}_r, \mathcal{R}_u \hat{\lambda}_r)$$

where  $(\mathcal{R}_l, \mathcal{R}_u)$  is the confidence interval for  $\mathcal{R}_{sm}$ .

## Indirectly Standardized Risk and Its Confidence Interval

With a risk-standardized mortality ratio  $\mathcal{R}_{sm}$ , an indirectly standardized risk for the study population is computed as

$$\hat{\gamma}_{is} = \mathcal{R}_{sm} \hat{\gamma}_r$$

where  $\hat{\gamma}_r$  is the overall crude risk in the reference population.

The  $(1 - \alpha/2)$  confidence intervals for  $\hat{\gamma}_{is}$  can be constructed as

$$(\mathcal{R}_l \hat{\gamma}_r, \mathcal{R}_u \hat{\gamma}_r)$$

where  $(\mathcal{R}_l, \mathcal{R}_u)$  is the confidence interval for  $\mathcal{R}_{sm}$ .

## Attributable Fraction and Population Attributable Fraction

The attributable fraction measures the excess event rate or risk fraction in the exposed population that is attributable to the exposure. That is, it is the proportion of event rate or risk in the exposed population that would be reduced if the exposure were not present. In contrast, the population attributable fraction measures the excess event rate or risk fraction in the total population that is attributable to the exposure.

In the STDRATE procedure, you can compute the attributable fraction by using either indirect standardization or Mantel-Haenszel estimation.

### Indirect Standardization

With indirect standardization, you specify a study population that consists of subjects who are exposed to a factor, such as smoking, and a reference population that consists of subjects who are not exposed to the factor. Denote the numbers of events in the study and reference populations by  $\mathcal{D}_s$  and  $\mathcal{D}_r$ , respectively.

For the rate estimate, denote the population-times in the study and reference populations by  $\mathcal{T}_s$  and  $\mathcal{T}_r$ , respectively. Then the event rates in the two populations can be expressed as the following equations, respectively:

$$\hat{\lambda}_s = \frac{\mathcal{D}_s}{\mathcal{T}_s} \quad \text{and} \quad \hat{\lambda}_r = \frac{\mathcal{D}_r}{\mathcal{T}_r}$$

Similarly, for the risk estimate, denote the numbers of observations in the study and reference populations by  $\mathcal{N}_s$  and  $\mathcal{N}_r$ , respectively. Then the event risks in the two populations can be expressed as the following equations, respectively:

$$\hat{\gamma}_s = \frac{\mathcal{D}_s}{\mathcal{N}_s} \quad \text{and} \quad \hat{\gamma}_r = \frac{\mathcal{D}_r}{\mathcal{N}_r}$$

In the next two subsections,  $\beta = \lambda$  denotes the rate statistic and  $\beta = \gamma$  denotes the risk statistic.



### Attributable Fraction with Indirect Standardization

The attributable fraction is the fraction of event rate or risk in the exposed population that is attributable to exposure:

$$\mathcal{R}_a = \frac{\hat{\beta}_s - \hat{\beta}_r}{\hat{\beta}_s}$$

With a standardized mortality ratio  $\mathcal{R}_{sm}$ , the attributable fraction is estimated by

$$\mathcal{R}_a = \frac{\mathcal{R}_{sm} - 1}{\mathcal{R}_{sm}}$$

The confidence intervals for the attributable fraction can be computed using the confidence intervals for  $\mathcal{R}_{sm}$ . That is, with a confidence interval  $(\mathcal{R}_l, \mathcal{R}_u)$  for  $\mathcal{R}_{sm}$ , the corresponding  $\mathcal{R}_a$  confidence interval is given by

$$\left( \frac{\mathcal{R}_l - 1}{\mathcal{R}_l}, \frac{\mathcal{R}_u - 1}{\mathcal{R}_u} \right)$$

### Population Attributable Fraction with Indirect Standardization

The population attributable fraction for a population is the fraction of event rate or risk in a given time period that is attributable to exposure. The population attributable fraction is

$$\mathcal{R}_{pa} = \frac{\hat{\beta}_0 - \hat{\beta}_r}{\hat{\beta}_0}$$

where

$$\hat{\beta}_0 = \frac{\mathcal{D}_s + \mathcal{D}_r}{\mathcal{T}_s + \mathcal{T}_r}$$

is the combined rate in the total population for the rate statistic and where

$$\hat{\beta}_0 = \frac{\mathcal{D}_s + \mathcal{D}_r}{\mathcal{N}_s + \mathcal{N}_r}$$

is the combined risk in the total population for the risk statistic.

Denote  $\rho = \mathcal{D}_s / (\mathcal{D}_s + \mathcal{D}_r)$ , the proportion of exposure among events, then  $\mathcal{R}_{pa}$  can also be expressed as

$$\mathcal{R}_{pa} = \rho \frac{\mathcal{R}_{sm} - 1}{\mathcal{R}_{sm}}$$

where  $\mathcal{R}_{sm}$  is the standardized mortality ratio.

An approximate confidence interval for the population attributable rate  $\mathcal{R}_{pa}$  can be derived by using the complementary log transformation (Greenland 2008, p. 296). That is, with

$$\mathcal{H} = \log(1 - \mathcal{R}_{pa})$$

a variance estimator for the estimated  $\mathcal{H}$  is given by

$$\text{Var}(\hat{\mathcal{H}}) = \frac{\mathcal{R}_{pa}^2}{(1 - \mathcal{R}_{pa})^2} \left( \frac{\hat{V}}{(\mathcal{R}_{sm} - 1)^2} + \frac{2}{\mathcal{D}_s (\mathcal{R}_{sm} - 1)} + \frac{\mathcal{D}_r}{\mathcal{D}_s (\mathcal{D}_s + \mathcal{D}_r)} \right)$$

where  $\hat{V}$  is a variance estimate for  $\log(\mathcal{R}_{sm})$ .

## Mantel-Haenszel Estimation

With Mantel-Haenszel estimation, you specify one study population that consists of subjects who are exposed to a factor and another study population that consists of subjects who are not exposed to the factor. Denote the numbers of events in the exposed and nonexposed study populations by  $\mathcal{D}_1$  and  $\mathcal{D}_2$ , respectively.

For the rate estimate, denote the population-times in the two populations by  $\mathcal{T}_1$  and  $\mathcal{T}_2$ , respectively. Then the event rates in the two populations can be expressed as the following equations, respectively:

$$\hat{\lambda}_1 = \frac{\mathcal{D}_1}{\mathcal{T}_1} \quad \text{and} \quad \hat{\lambda}_2 = \frac{\mathcal{D}_2}{\mathcal{T}_2}$$

Similarly, for the risk estimate, denote the numbers of observations in the two populations by  $\mathcal{N}_1$  and  $\mathcal{N}_2$ , respectively. Then the event risks in the two populations can be expressed as the following equations, respectively:

$$\hat{\gamma}_1 = \frac{\mathcal{D}_1}{\mathcal{N}_1} \quad \text{and} \quad \hat{\gamma}_2 = \frac{\mathcal{D}_2}{\mathcal{N}_2}$$

In the next two subsections,  $\beta = \lambda$  denotes the rate statistic and  $\beta = \gamma$  denotes the risk statistic.

## Attributable Fraction with Mantel-Haenszel Estimation

The attributable fraction is the fraction of event rate or risk in the exposed population that is attributable to exposure:

$$\mathcal{R}_a = \frac{\hat{\beta}_1 - \hat{\beta}_2}{\hat{\beta}_1}$$

Denote the rate or risk ratio by  $\mathcal{R} = \hat{\beta}_1/\hat{\beta}_2$ . The attributable fraction is given by

$$\mathcal{R}_a = \frac{\mathcal{R} - 1}{\mathcal{R}}$$

The confidence intervals for the attributable fraction can be computed using the confidence intervals for the rate or risk ratio  $\mathcal{R}$ . That is, with a confidence interval  $(\mathcal{R}_l, \mathcal{R}_u)$  for  $\mathcal{R}$ , the corresponding  $\mathcal{R}_a$  confidence interval is given by

$$\left( \frac{\mathcal{R}_l - 1}{\mathcal{R}_l}, \frac{\mathcal{R}_u - 1}{\mathcal{R}_u} \right)$$

For Mantel-Haenszel estimation, you can use the Mantel-Haenszel rate or risk ratio to estimate  $\mathcal{R}$ .

## Population Attributable Fraction with Mantel-Haenszel Estimation

The population attributable fraction for a population is the fraction of event rate or risk in a given time period that is attributable to exposure. The population attributable fraction is

$$\mathcal{R}_{pa} = \frac{\hat{\beta}_0 - \hat{\beta}_2}{\hat{\beta}_0}$$

where

$$\hat{\beta}_0 = \frac{\mathcal{D}_1 + \mathcal{D}_2}{\mathcal{T}_1 + \mathcal{T}_2}$$

is the combined rate in the total population for the rate statistic and where

$$\hat{\beta}_0 = \frac{\mathcal{D}_1 + \mathcal{D}_2}{\mathcal{N}_1 + \mathcal{N}_2}$$

is the combined risk in the total population for the risk statistic.

Denote the proportion of exposure among events as  $\rho = \mathcal{D}_1 / (\mathcal{D}_1 + \mathcal{D}_2)$ . Then  $\mathcal{R}_{pa}$  can also be expressed as

$$\mathcal{R}_{pa} = \rho \frac{\mathcal{R} - 1}{\mathcal{R}}$$

where  $\mathcal{R} = \hat{\beta}_1 / \hat{\beta}_2$  is the rate or risk ratio.

An approximate confidence interval for the population attributable rate  $\mathcal{R}_{pa}$  can be derived by using the complementary log transformation (Greenland 2008, p. 296). That is, with

$$\mathcal{H} = \log(1 - \mathcal{R}_{pa})$$

a variance estimator for the estimated  $\mathcal{H}$  is given by

$$\text{Var}(\hat{\mathcal{H}}) = \frac{\mathcal{R}_{pa}^2}{(1 - \mathcal{R}_{pa})^2} \left( \frac{\hat{V}}{(\mathcal{R} - 1)^2} + \frac{2}{\mathcal{D}_1 (\mathcal{R} - 1)} + \frac{\mathcal{D}_2}{\mathcal{D}_1 (\mathcal{D}_1 + \mathcal{D}_2)} \right)$$

where  $\hat{V}$  is a variance estimate for  $\log(\mathcal{R})$ .

For Mantel-Haenszel estimation, you can use the Mantel-Haenszel rate or risk ratio to estimate  $\mathcal{R}$ .

---

## Applicable Data Sets and Required Variables for Method Specifications

The METHOD= and DATA= options are required in the STDRATE procedure. The METHOD= option specifies the standardization method, and the DATA= and REFDATA= options specify the study populations and reference population, respectively. You can use the GROUP= option in the POPULATION statement to identify various study populations. Table 88.2 lists applicable data sets for each method.

**Table 88.2** Applicable Data Sets for Method Specifications

| METHOD=  | Number of Populations |                   |
|----------|-----------------------|-------------------|
|          | in DATA= Data Set     | REFDATA= Data Set |
| DIRECT   | 1                     | X                 |
|          | 2                     | X                 |
| MH       | 2                     |                   |
| INDIRECT | 1                     | X                 |

Table 88.3 lists the required variables for each method.

**Table 88.3** Required Variables for Method Specifications

| METHOD=  | STAT= | DATA= Data Set |      |       | REFDATA= Data Set |      |       |
|----------|-------|----------------|------|-------|-------------------|------|-------|
|          |       | RATE           | RISK | TOTAL | RATE              | RISK | TOTAL |
| DIRECT   | RATE  | X              |      |       |                   |      | X     |
|          | RISK  |                | X    |       |                   |      | X     |
| MH       | RATE  | X              |      | X     |                   |      |       |
|          | RISK  |                | X    | X     |                   |      |       |
| INDIRECT | RATE  |                |      | X     | X                 |      |       |
|          | RISK  |                |      | X     |                   | X    |       |

The symbol “X” indicates that the variable is either explicitly specified or implicitly available from other variables. For example, when STAT=RATE, the variable RATE is available if the corresponding variables EVENT and TOTAL are specified.

## Applicable Confidence Limits for Rate and Risk Statistics

In the STD RATE procedure, the METHOD= option specifies the standardization method, and the STAT= option specifies either either rate or risk for standardization. Table 88.4 lists applicable confidence limits for different methods with standardized rate, rate SMR, standardized risk, and risk SMR.

**Table 88.4** Applicable Confidence Limits for Standardized Rate and Risk Statistics

| Statistic | METHOD=  | Confidence Limits |           |       |         |
|-----------|----------|-------------------|-----------|-------|---------|
|           |          | Normal            | Lognormal | Gamma | Poisson |
| Rate      | DIRECT   | X                 | X         | X     |         |
|           | MH       | X                 | X         | X     |         |
|           | INDIRECT | X                 | X         |       | X       |
| Rate SMR  | INDIRECT | X                 | X         |       | X       |
| Risk      | DIRECT   | X                 | X         |       |         |
|           | MH       | X                 | X         |       |         |
|           | INDIRECT | X                 | X         |       | X       |
| Risk SMR  | INDIRECT | X                 | X         |       | X       |

Table 88.5 lists applicable confidence limits for stratum-specific rate, rate SMR, risk, and risk SMR.

**Table 88.5** Applicable Confidence Limits for Strata Rate and Risk Statistics

| Statistic | Confidence Limits |           |         |
|-----------|-------------------|-----------|---------|
|           | Normal            | Lognormal | Poisson |
| Rate      | X                 | X         | X       |
| Rate SMR  | X                 | X         | X       |
| Risk      | X                 | X         |         |
| Risk SMR  | X                 | X         |         |

## Table Output

The STD RATE procedure displays the “Standardization Information” table by default. In addition, the procedure also displays the “Standardized Rate Estimates” table (with the default STAT=RATE option in the PROC STD RATE statement) and the “Standardized Risk Estimates” table (with the STAT=RISK option) by default. The rest of this section describes the output tables in alphabetical order.

### Attributable Fraction Estimates

The “Attributable Fraction Estimates” table displays the following information:

- Parameter: attributable rate and population attributable rate for the rate statistic, and attributable risk and population attributable risk for the risk statistic
- Estimate: estimate of the parameter
- Method: method to construct confidence limits
- Lower and Upper: lower and upper confidence limits

### Effect Estimates

The “Effect Estimates” table displays the following information:

- Standardized Rate: directly standardized rates for study populations
- Standardized Risk: directly standardized risks for study populations

When EFFECT=RATIO, the table displays the following:

- Estimate: the rate or risk ratio estimate
- Log Ratio: the logarithm of rate ratio or risk ratio estimate

- Standard Error: standard error of the logarithm of the ratio estimate
- Z: the standard Z statistic
- $\text{Pr} > |Z|$ : the  $p$ -value for the test

When EFFECT=DIFF, the table displays the following:

- Estimate: the rate or risk difference estimate
- Standard Error: standard error of the difference estimate
- Z: the standard Z statistic
- $\text{Pr} > |Z|$ : the  $p$ -value for the test

### Standardization Information

The “Standardization Information” table displays the input data sets, type of statistic to be standardized, standardization method, and number of strata. The table also displays the variance divisor for the risk estimate, and the rate multiplier for the rate estimate. With a rate multiplier  $c$ , the rates per  $c$  population-time units are displayed in the output tables.

### Standardized Morbidity/Mortality Ratio

The “Standardized Morbidity/Mortality Ratio” table displays the following information:

- SMR: standardized morbidity/mortality ratio
- Standard Error: standard error for SMR
- Lower and Upper: lower and upper confidence limits for SMR
- Test Statistic:  $\text{SMR}-1$ , for the test of  $\text{SMR}=1$
- Estimate: value of test statistic
- Standard Error: standard error of the estimate
- Z: the standard Z statistic
- $\text{Pr} > |Z|$ : the  $p$ -value for the test

## Standardized Rate Estimates

The “Standardized Rate Estimates” table displays the following information:

- Population: study populations, and reference population for indirect standardization
- Number of Events: number of events in population
- Population-Time: total contributed time in population, for the rate statistic
- Crude Rate: event rate in the population
- Expected Number of Events
- SMR: standardized morbidity/mortality ratio, for indirect standardization
- Standardized Rate: for the rate statistic
- Standard Error: standard error of the standardized estimate of rate
- Confidence Limits: lower and upper confidence limits for standardized estimate

## Standardized Risk Estimates

The “Standardized Risk Estimates” table displays the following information:

- Population: study populations, and reference population for indirect standardization
- Number of Events: number of events in population
- Number of Observations: number of observations in population
- Crude Risk: event risk in the population
- Expected Number of Events
- SMR: standardized morbidity/mortality ratio, for indirect standardization
- Standardized Risk
- Standard Error: standard error of the standardized estimate of risk
- Confidence Limits: lower and upper confidence limits for standardized estimate

## Strata Effect Estimates

The “Strata Effect Estimates” table displays the following information for each stratum:

- Stratum Index: a sequential stratum identification number
- STRATA variables: the levels of STRATA variables
- Rate: rates for the study populations, for the rate statistic
- Risk: risks for the study populations, for the risk statistic

When EFFECT=DIFF, the table displays the following information for each stratum:

- Estimate: rate or risk difference estimate of the study populations
- Standard Error: the standard error of the difference estimate
- Confidence Limits: confidence limits for the difference estimate

When EFFECT=RATIO, the table displays the following information for each stratum:

- Estimate: rate or risk ratio estimate of the study populations
- Confidence Limits: confidence limits for the ratio estimate

## Strata Statistics

For each POPULATION statement, the “Strata Information” table displays the following information for each stratum:

- Stratum Index: a sequential stratum identification number
- STRATA variables: the levels of STRATA variables

If the REFERENCE statement is specified, the table displays the following information for each stratum in the reference population:

- Population-Time Value: population-time for the rate statistic for direct standardization
- Population-Time Proportion: proportion for the population-time
- Number of Observations Value: number of observations for the risk statistic for direct standardization
- Number of Observations Proportion: proportion for the number of observations
- Rate: for the rate statistic for indirect standardization
- Risk: for the risk statistic for indirect standardization



For the rate statistic, the table displays the following information for each stratum in the specified study data set:

- Number of Events
- Population-Time Value
- Population-Time Proportion
- Rate Estimate
- Standard Error: standard error for the rate estimate if the `CL=NORMAL` suboption is specified in the `STATS` option in the `STRATA` statement
- Confidence Limits: confidence limits for the risk estimate if the `CL` suboption is specified in the `STATS` option in the `STRATA` statement
- Expected Number of Events: expected number of events that use the reference population population-time for direct standardization, Mantel-Haenszel weight for Mantel-Haenszel estimation, or reference population rate for indirect standardization

For the risk statistic, the table displays the following information for each stratum in the specified study data set:

- Number of Events
- Number of Observations Value
- Number of Observations Proportion
- Risk
- Standard Error: standard error for the risk estimate, if the `CL=NORMAL` suboption is specified in the `STATS` option in the `STRATA` statement
- Confidence Limits: confidence limits for the risk estimate, if the `CL` suboption is specified in the `STATS` option in the `STRATA` statement
- Expected Number of Events: expected number of events that uses the reference population number of observations for direct standardization, Mantel-Haenszel weight for Mantel-Haenszel estimation, or reference population risk for indirect standardization

### Strata SMR Estimates

The “Strata SMR Estimates” table displays the following information for each stratum:

- Stratum Index: a sequential stratum identification number
- `STRATA` variables: the levels of `STRATA` variables
- Number of Events

- Expected Number of Observations
- SMR Estimate
- Standard Error: standard error for the SMR estimate, if the CL=NORMAL suboption is specified in the SMR option in the STRATA statement
- Confidence Limits: confidence limits for the SMR estimate, if the CL suboption is specified in the SMR option in the STRATA statement

For the rate statistic, the table also displays the following information for each stratum:

- Population-Time
- Reference Rate

For the risk statistic, the table also displays the following information for each stratum:

- Number of Observations
- Reference Risk

---

## ODS Table Names

PROC STD RATE assigns a name to each table it creates. You must use these names to refer to tables when you use the Output Delivery System (ODS). These names are listed in [Table 88.6](#). For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

**Table 88.6** ODS Tables Produced by PROC STD RATE

| ODS Table Name | Description                            | Statement     | Option              |
|----------------|----------------------------------------|---------------|---------------------|
| AttrFraction   | Attributable fraction                  | PROC STD RATE | METHOD=INDIRECT(AF) |
|                |                                        | PROC STD RATE | METHOD=MH(AF)       |
| Effect         | Effect estimates                       | PROC STD RATE | EFFECT              |
| SMR            | Standardized morbidity/mortality ratio | PROC STD RATE | METHOD=INDIRECT     |
| StdInfo        | Standardization information            | PROC STD RATE |                     |
| StdRate        | Standardized rate estimates            | PROC STD RATE | STAT=RATE           |
| StdRisk        | Standardized risk estimates            | PROC STD RATE | STAT=RISK           |
| StrataEffect   | Strata effect estimates                | STRATA        | EFFECT              |
| StrataStats    | Strata statistics                      | STRATA        | STATS               |
| StrataSMR      | Strata SMR estimates                   | STRATA        | SMR                 |

---

## Graphics Output

This section describes the use of ODS for creating graphics with the STD RATE procedure. To request these graphs, ODS Graphics must be enabled and you must specify the associated graphics options in the PROC STD RATE statement. For more information about ODS Graphics, see Chapter 21, “Statistical Graphics Using ODS.”

### Strata Distribution Plot

The PLOTS=DIST option displays the proportion of exposed time or sample size for each stratum in the populations.

### Strata Effect Plot

The PLOTS=EFFECT option displays the stratum-specific effect measure of rate difference, rate ratio, risk difference, or risk ratio. In addition, the crude effect measure and confidence limits of these stratum-specific effect estimates are also displayed.

### Strata Rate Plot

The PLOTS=RATE option displays the stratum-specific rate estimates and their confidence limits of populations. In addition, the overall crude rates of populations are also displayed.

### Strata Risk Plot

The PLOTS=RISK option displays the stratum-specific risk estimates and their confidence limits of populations. In addition, the overall crude risks of populations are also displayed.

### Strata SMR Plot

The PLOTS=SMR option displays the SMR for each stratum in the populations.

---

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “Statistical Graphics Using ODS.”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “A Primer on ODS Statistical Graphics” on page 599 in Chapter 21, “Statistical Graphics Using ODS.”

PROC STD RATE assigns a name to each graph it creates. You can use these names to refer to the graphs when you use ODS. To request the graph, ODS Graphics must be enabled and you must use the PLOTS option in the PROC STD RATE statement to specify the *plot-request* indicated in Table 88.7.

**Table 88.7** Graphs Produced by PROC STDRATE

| ODS Graph Name   | Plot Description                                                                     | <i>plot-request</i> in PLOTS Option |
|------------------|--------------------------------------------------------------------------------------|-------------------------------------|
| StrataDistPlot   | Strata proportion of exposed time or sample size                                     | DIST                                |
| StrataEffectPlot | Strata effect measure of rate difference, rate ratio, risk difference, or risk ratio | EFFECT                              |
| StrataRatePlot   | Strata rate estimates                                                                | RATE                                |
| StrataRiskPlot   | Strata risk estimates                                                                | RISK                                |
| StrataSMRPlot    | Strata SMR of rates or risks                                                         | SMR                                 |

## Examples: STDRATE Procedure

### Example 88.1: Comparing Directly Standardized Rates

This example computes directly standardized mortality rates for populations in the states of Alaska and Florida, and then compares these two standardized rates with a rate ratio statistic.

The Alaska data set contains the stratum-specific mortality information in a given period of time for the state of Alaska (Alaska Bureau of Vital Statistics 2000a, b). Variables `Sex` and `Age` are the grouping variables that form the strata in the standardization, and variables `Death` and `PYear` indicate the number of events and person-years, respectively. The `COMMA9.` format is specified in the `DATA` step to input numerical values that contain commas in `PYear`.

```

data Alaska;
 State='Alaska';
 input Sex $ Age $ Death PYear comma9.;
 datalines;
Male 00-14 37 81,205
Male 15-34 68 93,662
Male 35-54 206 108,615
Male 55-74 369 35,139
Male 75+ 556 5,491
Female 00-14 78 77,203
Female 15-34 181 85,412
Female 35-54 395 100,386
Female 55-74 555 32,118
Female 75+ 479 7,701
;

```

The Florida data set contains the corresponding stratum-specific mortality information for the state of Florida (Florida Department of Health 2000, 2012). Variables `Sex` and `Age` are the grouping variables that form the strata in the standardization, and variables `Death` and `PYear` indicate the number of events and person-years, respectively.

```

data Florida;
 State='Florida';
 input Sex $ Age $ Death comma8. PYear comma11.;
 datalines;
Male 00-14 1,189 1,505,889
Male 15-34 2,962 1,972,157
Male 35-54 10,279 2,197,912
Male 55-74 26,354 1,383,533
Male 75+ 42,443 554,632
Female 00-14 906 1,445,831
Female 15-34 1,234 1,870,430
Female 35-54 5,630 2,246,737
Female 55-74 18,309 1,612,270
Female 75+ 53,489 868,838
;

```

The TwoStates data set contains the data sets Alaska and Florida:

```

data TwoStates;
 length State $ 7.;
 set Alaska Florida;
run;

```

The US data set contains the corresponding stratum-specific person-years information for the United States (U.S. Bureau of Census 2011). Variables Sex and Age are the grouping variables that form the strata in the standardization, and the variable PYear indicates the person-years.

```

data US;
 input Sex $ Age $ PYear comma12.;
 datalines;
Male 00-14 30,854,207
Male 15-34 40,199,647
Male 35-54 40,945,028
Male 55-74 19,948,630
Male 75+ 6,106,351
Female 00-14 29,399,168
Female 15-34 38,876,268
Female 35-54 41,881,451
Female 55-74 22,717,040
Female 75+ 10,494,416
;

```

The following statements invoke the STDRATE procedure and compute the direct standardized rates for the states of Florida and Alaska by using the United States as the reference population. The DATA= option names the data set for the study populations, and the REFDATA= option names the data set for the reference population.

```

ods graphics on;
proc stdrate data=TwoStates
 refdata=US
 method=direct
 stat=rate(mult=1000)
 effect

```

```

plots(only)=(dist effect)
;
population group=State event=Death total=PYear;
reference total=PYear;
strata Sex Age / effect;
run;
ods graphics off;

```

The METHOD=DIRECT option requests direct standardization, and the STAT=RATE option specifies the rate statistic for standardization. With the EFFECT option, the procedure computes the rate effect between the study populations with the default rate ratio statistics.

The “Standardization Information” table in [Output 88.1.1](#) displays the standardization information.

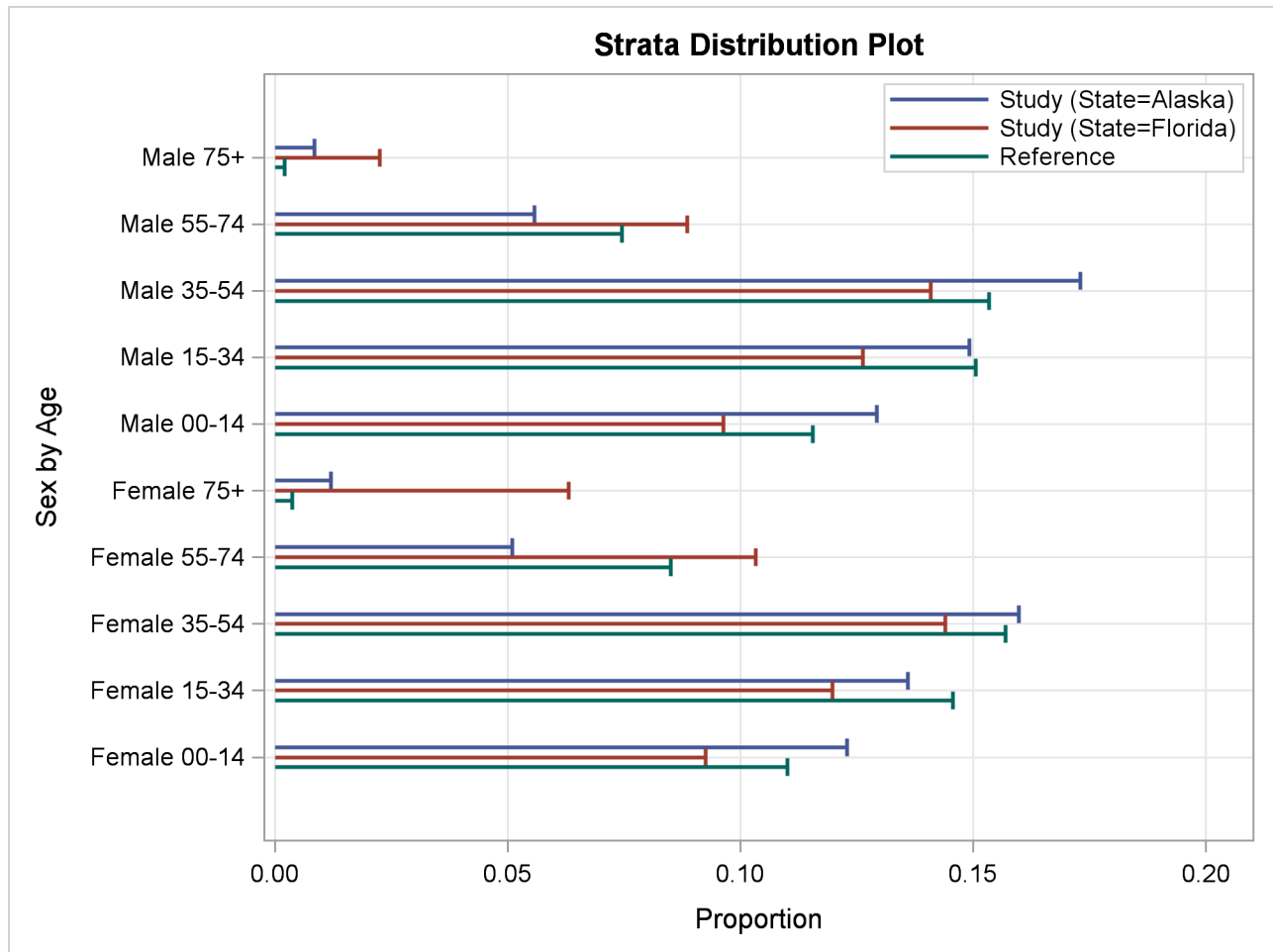
### Output 88.1.1 Standardization Information

| The STD RATE Procedure      |                        |
|-----------------------------|------------------------|
| Standardization Information |                        |
| Data Set                    | WORK.TWOSTATES         |
| Group Variable              | State                  |
| Reference Data Set          | WORK.US                |
| Method                      | Direct Standardization |
| Statistic                   | Rate                   |
| Number of Strata            | 10                     |
| Rate Multiplier             | 1000                   |

With ODS Graphics enabled, the PLOTS(ONLY)=(DIST EFFECT) option displays the strata distribution plot and the strata effect plot, but does not display the default strata rate plot.

The strata distribution plot displays proportions for stratum-specific person-years in the study populations and reference population, as shown in [Output 88.1.2](#).

Output 88.1.2 Strata Distribution Plot



The EFFECT option in the STRATA statement and the STAT=RATE option request that the “Strata Rate Effect Estimates” table in [Output 88.1.3](#) display the stratum-specific rate effect statistics between the two study populations. The default EFFECT=RATIO in the PROC STD RATE statement requests that the stratum-specific rate ratio statistics be displayed.

**Output 88.1.3** Strata Effect Estimates

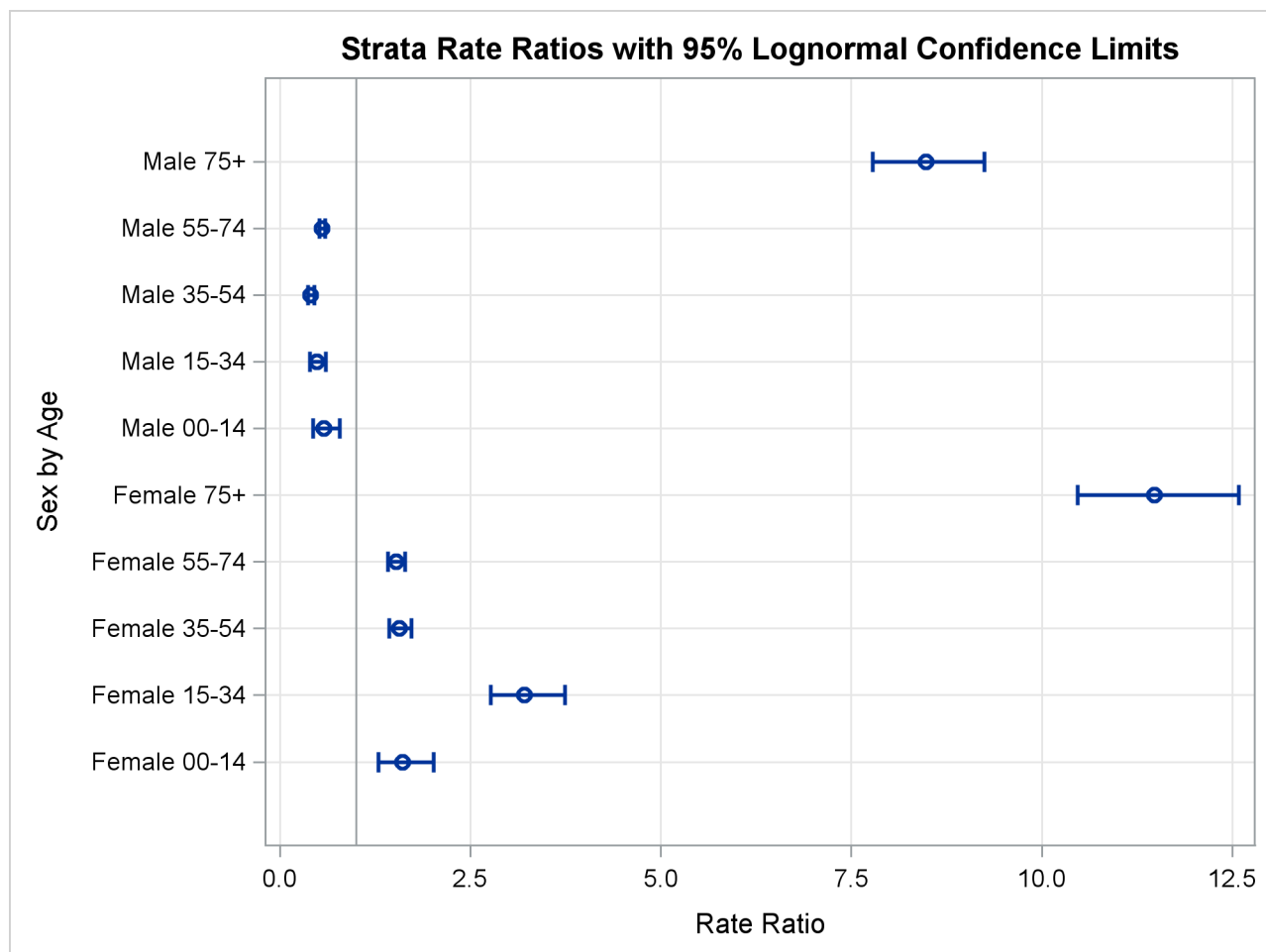
| Strata Rate Effect Estimates (Rate Multiplier = 1000) |        |       |                 |         |               |                                    |         |
|-------------------------------------------------------|--------|-------|-----------------|---------|---------------|------------------------------------|---------|
| Stratum<br>Index                                      | Sex    | Age   | -----State----- |         | Rate<br>Ratio | 95% Lognormal<br>Confidence Limits |         |
|                                                       |        |       | Alaska          | Florida |               |                                    |         |
| 1                                                     | Female | 00-14 | 1.010           | 0.6266  | 1.6123        | 1.2794                             | 2.0319  |
| 2                                                     | Female | 15-34 | 2.119           | 0.6597  | 3.2121        | 2.7481                             | 3.7544  |
| 3                                                     | Female | 35-54 | 3.935           | 2.5059  | 1.5702        | 1.4180                             | 1.7389  |
| 4                                                     | Female | 55-74 | 17.280          | 11.3560 | 1.5217        | 1.3984                             | 1.6557  |
| 5                                                     | Female | 75+   | 62.200          | 5.4191  | 11.4779       | 10.4536                            | 12.6026 |
| 6                                                     | Male   | 00-14 | 0.456           | 0.7896  | 0.5771        | 0.4160                             | 0.8004  |
| 7                                                     | Male   | 15-34 | 0.726           | 1.5019  | 0.4834        | 0.3801                             | 0.6148  |
| 8                                                     | Male   | 35-54 | 1.897           | 4.6767  | 0.4055        | 0.3533                             | 0.4655  |
| 9                                                     | Male   | 55-74 | 10.501          | 19.0483 | 0.5513        | 0.4975                             | 0.6109  |
| 10                                                    | Male   | 75+   | 101.257         | 11.9394 | 8.4809        | 7.7634                             | 9.2647  |

The “Strata Rate Effect Estimates” table shows that except for the age group 75+, Alaska has lower mortality rates for male groups and higher mortality rates for female groups than Florida. For age group 75+, Alaska has much higher mortality rates than Florida for both male and female groups.

With ODS Graphics enabled and two study populations, the PLOTS=EFFECT option displays the stratum-specific effect measures and their associated confidence limits, as shown in [Output 88.1.4](#). The STAT=RATE option and the default EFFECT=RATIO option request that the strata rate ratios be displayed. By default, confidence limits are generated with 95% confidence level. This plot displays the stratum-specific rate ratios in the “Strata Rate Effect Estimates” table in [Output 88.1.3](#).



Output 88.1.4 Strata Effect Measure Plot



The “Directly Standardized Rate Estimates” table in [Output 88.1.5](#) displays directly standardized rates and related statistics.

**Output 88.1.5** Directly Standardized Rate Estimates

| Directly Standardized Rate Estimates |                            |                 |            |                        |                 |
|--------------------------------------|----------------------------|-----------------|------------|------------------------|-----------------|
| Rate Multiplier = 1000               |                            |                 |            |                        |                 |
| State                                | -----Study Population----- |                 | Crude Rate | -Reference Population- |                 |
|                                      | Observed Events            | Population-Time |            | Expected Events        | Population-Time |
| Alaska                               | 2924                       | 626932          | 4.6640     | 1126924                | 266481515       |
| Florida                              | 76455                      | 15577105        | 4.9082     | 1076187                | 266481515       |

| Directly Standardized Rate Estimates |                             |                |            |                   |
|--------------------------------------|-----------------------------|----------------|------------|-------------------|
| Rate Multiplier = 1000               |                             |                |            |                   |
| State                                | -----Standardized Rate----- |                |            |                   |
|                                      | Estimate                    | Standard Error | 95% Normal | Confidence Limits |
| Alaska                               | 4.2289                      | 0.0901         | 4.0522     | 4.4056            |
| Florida                              | 4.0385                      | 0.0156         | 4.0079     | 4.0691            |

The MULT=1000 suboption in the STAT=RATE option requests that rates per 1,000 person-years be displayed. The table shows that although the crude rate in the Florida population (4.908) is higher than the crude rate in the Alaska population (4.664), the resulting standardized rate in the Florida population (4.0385) is lower than the crude rate in the Alaska population (4.2289).

The EFFECT option requests that the “Rate Effect Estimates” table in [Output 88.1.6](#) display the log rate ratio statistics of the two directly standardized rates by default.

**Output 88.1.6** Effect Estimates

| Rate Effect Estimates (Rate Multiplier = 1000) |         |            |                |                |      |         |
|------------------------------------------------|---------|------------|----------------|----------------|------|---------|
| -----State-----                                |         | Rate Ratio | Log Rate Ratio | Standard Error | Z    | Pr >  Z |
| Alaska                                         | Florida |            |                |                |      |         |
| 4.2289                                         | 4.0385  | 1.0471     | 0.0461         | 0.0217         | 2.13 | 0.0335  |

The table shows that with a log rate ratio statistic 1.047, the resulting *p*-value is 0.0335, which indicates that the death rate is significantly higher in Alaska than in Florida at the 5% significance level.

---

**Example 88.2: Computing Mantel-Haenszel Risk Estimation**

This example uses Mantel-Haenszel method to estimate the effect of household smoking on respiratory symptoms of school children, after adjusting for the effects of the student’s grade and household pets.

Suppose that the School data set contains the stratum-specific numbers of cases of respiratory symptoms in a given school year for a school district. Variables Pet and Grade are the grouping variables that form

the strata in the standardization, and the variable Smoking identifies students who have smokers in their households. The variables Case and Student indicate the number of cases with respiratory symptoms and the total number of students, respectively.

```
data School;
 input Smoking $ Pet $ Grade $ Case Student;
 datalines;
Yes Yes K-1 109 807
Yes Yes 2-3 106 791
Yes Yes 4-5 112 868
Yes No K-1 168 1329
Yes No 2-3 162 1337
Yes No 4-5 183 1594
No Yes K-1 284 2403
No Yes 2-3 266 2237
No Yes 4-5 273 2279
No No K-1 414 3398
No No 2-3 372 3251
No No 4-5 382 3270
;
```

The following statements invoke the STDRATE procedure and compute the Mantel-Haenszel rate difference statistic between students with household smokers and students without household smokers:

```
ods graphics on;
proc stdrate data=School
 method=mh
 stat=risk
 effect=diff
 plots=all
 ;
 population group=Smoking event=Case total=Student;
 strata Pet Grade / order=data stats(cl=none) effect;
run;
ods graphics off;
```

The ORDER=DATA option in the STRATA statement sorts the strata by the order of appearance in the input data set.

The “Standardization Information” table in [Output 88.2.1](#) displays the standardization information.

**Output 88.2.1** Standardization Information

| The STDRATE Procedure       |                 |
|-----------------------------|-----------------|
| Standardization Information |                 |
| Data Set                    | WORK.SCHOOL     |
| Group Variable              | Smoking         |
| Method                      | Mantel-Haenszel |
| Statistic                   | Risk            |
| Number of Strata            | 6               |

The `STATS` option in the `STRATA` statement requests that the `STD RATE` procedure display a “Mantel-Haenszel Standardized Strata Statistics” table for study populations, as shown in [Output 88.2.2](#). The table displays the strata information and the expected number of events in each stratum. The Expected Events column shows the expected number of events when the Mantel-Haenszel weights are applied to the corresponding stratum-specific risks in the study populations. The `CL=NONE` suboption requests that confidence limits for strata risks not be displayed.

## Output 88.2.2 Mantel-Haenszel Standardized Strata Statistics

| The STDRATE Procedure                          |               |     |       |  |
|------------------------------------------------|---------------|-----|-------|--|
| Mantel-Haenszel Standardized Strata Statistics |               |     |       |  |
| Smoking                                        | Stratum Index | Pet | Grade |  |
| No                                             | 1             | Yes | K-1   |  |
| No                                             | 2             | Yes | 2-3   |  |
| No                                             | 3             | Yes | 4-5   |  |
| No                                             | 4             | No  | K-1   |  |
| No                                             | 5             | No  | 2-3   |  |
| No                                             | 6             | No  | 4-5   |  |
| Yes                                            | 1             | Yes | K-1   |  |
| Yes                                            | 2             | Yes | 2-3   |  |
| Yes                                            | 3             | Yes | 4-5   |  |
| Yes                                            | 4             | No  | K-1   |  |
| Yes                                            | 5             | No  | 2-3   |  |
| Yes                                            | 6             | No  | 4-5   |  |

| Mantel-Haenszel Standardized Strata Statistics |               |                 |                                |            |            |
|------------------------------------------------|---------------|-----------------|--------------------------------|------------|------------|
| Smoking                                        | Stratum Index | Observed Events | -----Study Population-----     |            | Crude Risk |
|                                                |               |                 | -Number of Observations- Value | Proportion |            |
| No                                             | 1             | 284             | 2403                           | 0.1427     | 0.118186   |
| No                                             | 2             | 266             | 2237                           | 0.1329     | 0.118909   |
| No                                             | 3             | 273             | 2279                           | 0.1353     | 0.119789   |
| No                                             | 4             | 414             | 3398                           | 0.2018     | 0.121836   |
| No                                             | 5             | 372             | 3251                           | 0.1931     | 0.114426   |
| No                                             | 6             | 382             | 3270                           | 0.1942     | 0.116820   |
| Yes                                            | 1             | 109             | 807                            | 0.1200     | 0.135068   |
| Yes                                            | 2             | 106             | 791                            | 0.1176     | 0.134008   |
| Yes                                            | 3             | 112             | 868                            | 0.1291     | 0.129032   |
| Yes                                            | 4             | 168             | 1329                           | 0.1976     | 0.126411   |
| Yes                                            | 5             | 162             | 1337                           | 0.1988     | 0.121167   |
| Yes                                            | 6             | 183             | 1594                           | 0.2370     | 0.114806   |

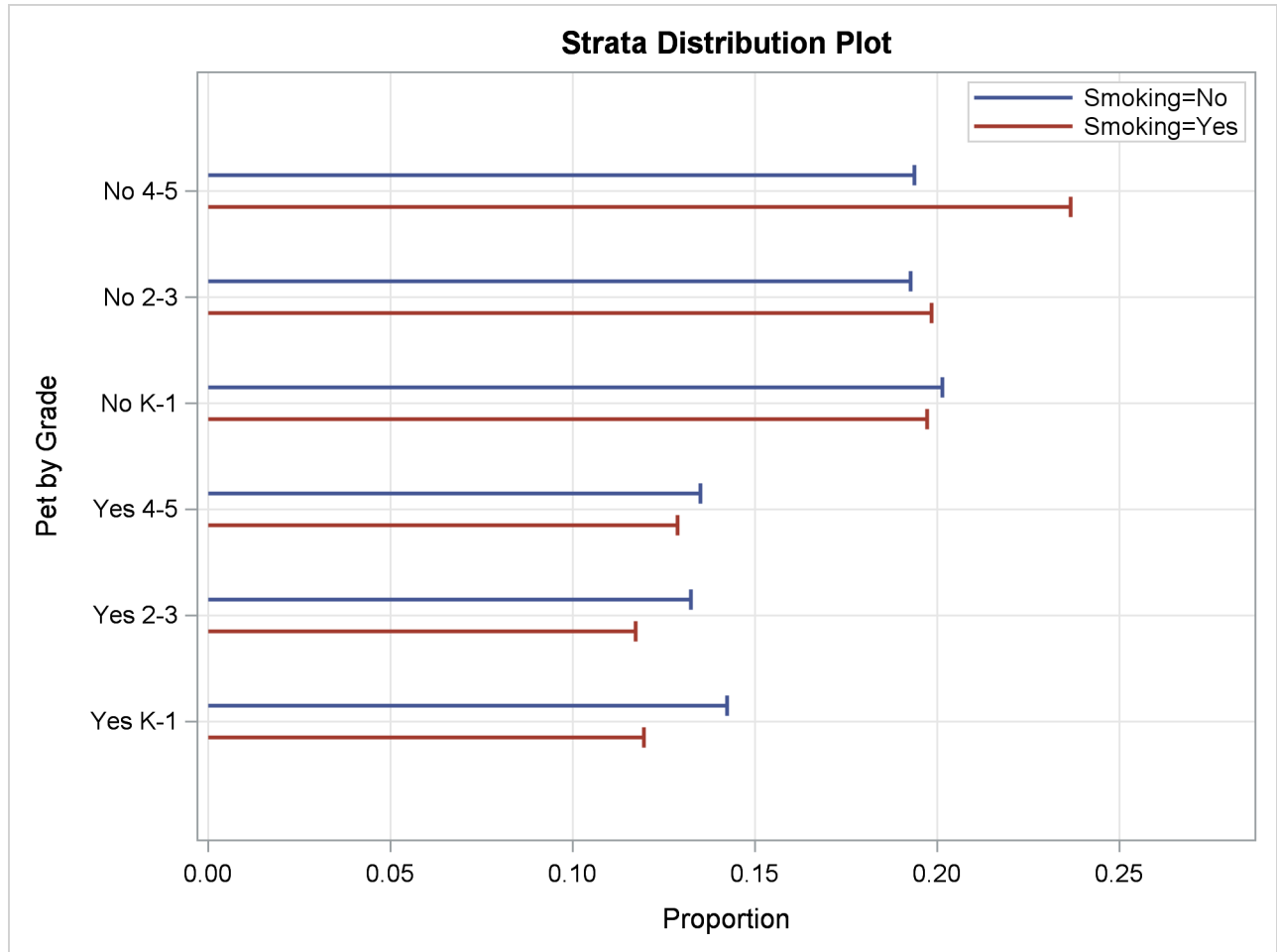
  

| Mantel-Haenszel Standardized Strata Statistics |               |                     |                 |  |
|------------------------------------------------|---------------|---------------------|-----------------|--|
| Smoking                                        | Stratum Index | --Mantel-Haenszel-- |                 |  |
|                                                |               | Weight              | Expected Events |  |
| No                                             | 1             | 604.12              | 71.398          |  |
| No                                             | 2             | 584.37              | 69.487          |  |
| No                                             | 3             | 628.59              | 75.298          |  |
| No                                             | 4             | 955.35              | 116.396         |  |
| No                                             | 5             | 947.38              | 108.405         |  |
| No                                             | 6             | 1071.62             | 125.187         |  |
| Yes                                            | 1             | 604.12              | 81.597          |  |
| Yes                                            | 2             | 584.37              | 78.310          |  |
| Yes                                            | 3             | 628.59              | 81.108          |  |
| Yes                                            | 4             | 955.35              | 120.767         |  |
| Yes                                            | 5             | 947.38              | 114.791         |  |
| Yes                                            | 6             | 1071.62             | 123.028         |  |

With ODS Graphics enabled, the PLOTS=ALL option displays all appropriate plots. With the METHOD=MH and STAT=RISK options, these plots include the strata distribution plot, strata risk plot, and strata effect plot.

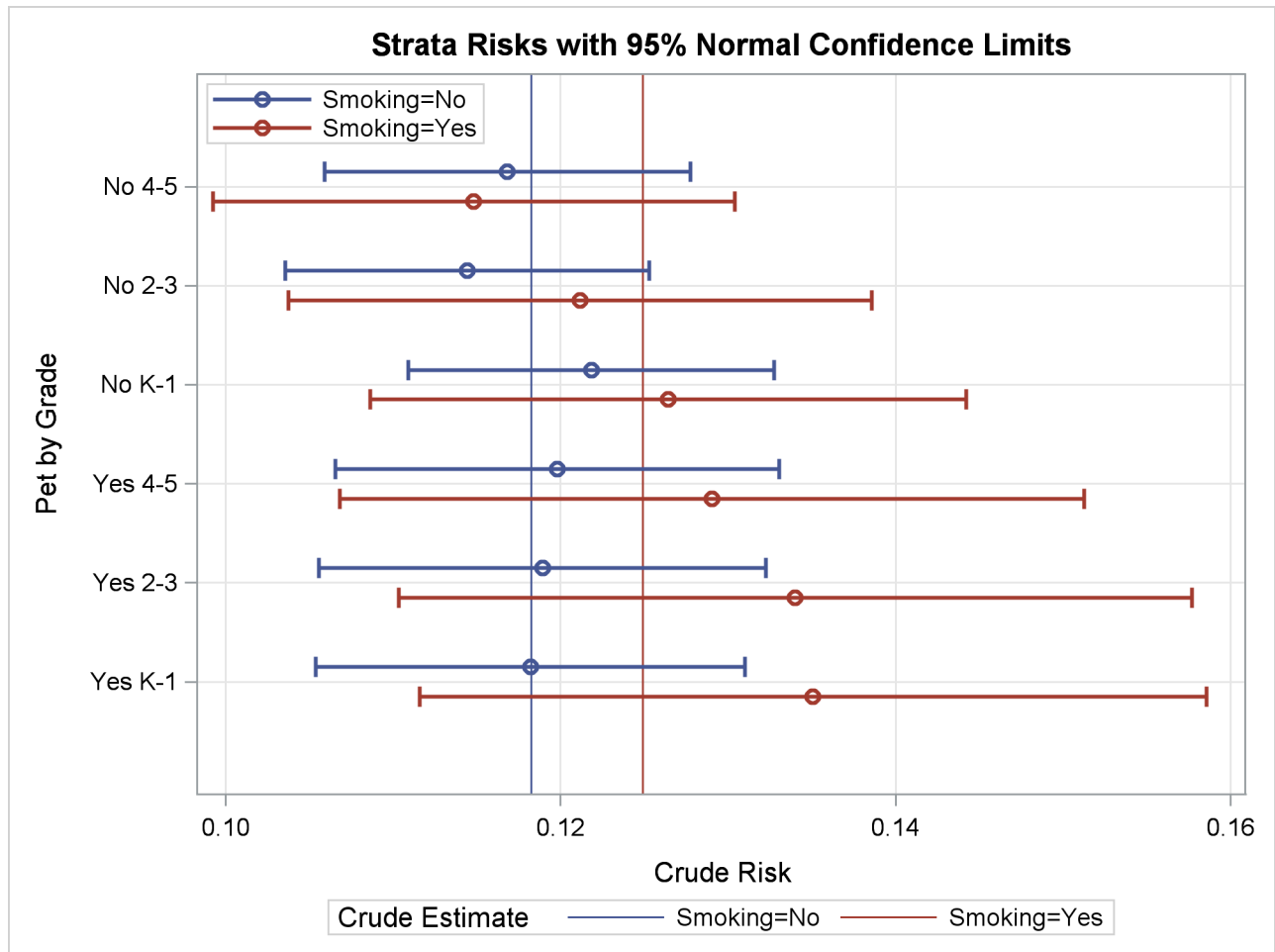
The strata distribution plot displays proportions for stratum-specific numbers of students in the study populations, as shown in Output 88.2.3.

**Output 88.2.3** Strata Distribution Plot



The strata risk plot displays stratum-specific risk estimates with confidence limits in the study populations, as shown in Output 88.2.4. This plot displays stratum-specific risk estimates in the “Mantel-Haenszel Standardized Strata Statistics” table in Output 88.2.2. In addition, the overall crude risks for the two study populations are also displayed. By default, strata levels are displayed on the vertical axis.

Output 88.2.4 Strata Risk Plot



The EFFECT option in the STRATA statement requests that the “Strata Risk Effect Estimates” table be displayed, as shown in Output 88.2.5. The EFFECT=DIFF option in the PROC STDRA TE statement requests that strata risk differences be displayed.

**Output 88.2.5** Strata Effect Estimates

| Strata Risk Effect Estimates |     |       |                   |         |                 |                |
|------------------------------|-----|-------|-------------------|---------|-----------------|----------------|
| Stratum Index                | Pet | Grade | -----Smoking----- |         | Risk Difference | Standard Error |
|                              |     |       | No                | Yes     |                 |                |
| 1                            | Yes | K-1   | 0.11819           | 0.13507 | -.016883        | 0.013716       |
| 2                            | Yes | 2-3   | 0.11891           | 0.13401 | -.015098        | 0.013912       |
| 3                            | Yes | 4-5   | 0.11979           | 0.12903 | -.009243        | 0.013257       |
| 4                            | No  | K-1   | 0.12184           | 0.12641 | -.004574        | 0.010704       |
| 5                            | No  | 2-3   | 0.11443           | 0.12117 | -.006740        | 0.010527       |
| 6                            | No  | 4-5   | 0.11682           | 0.11481 | 0.002014        | 0.009762       |

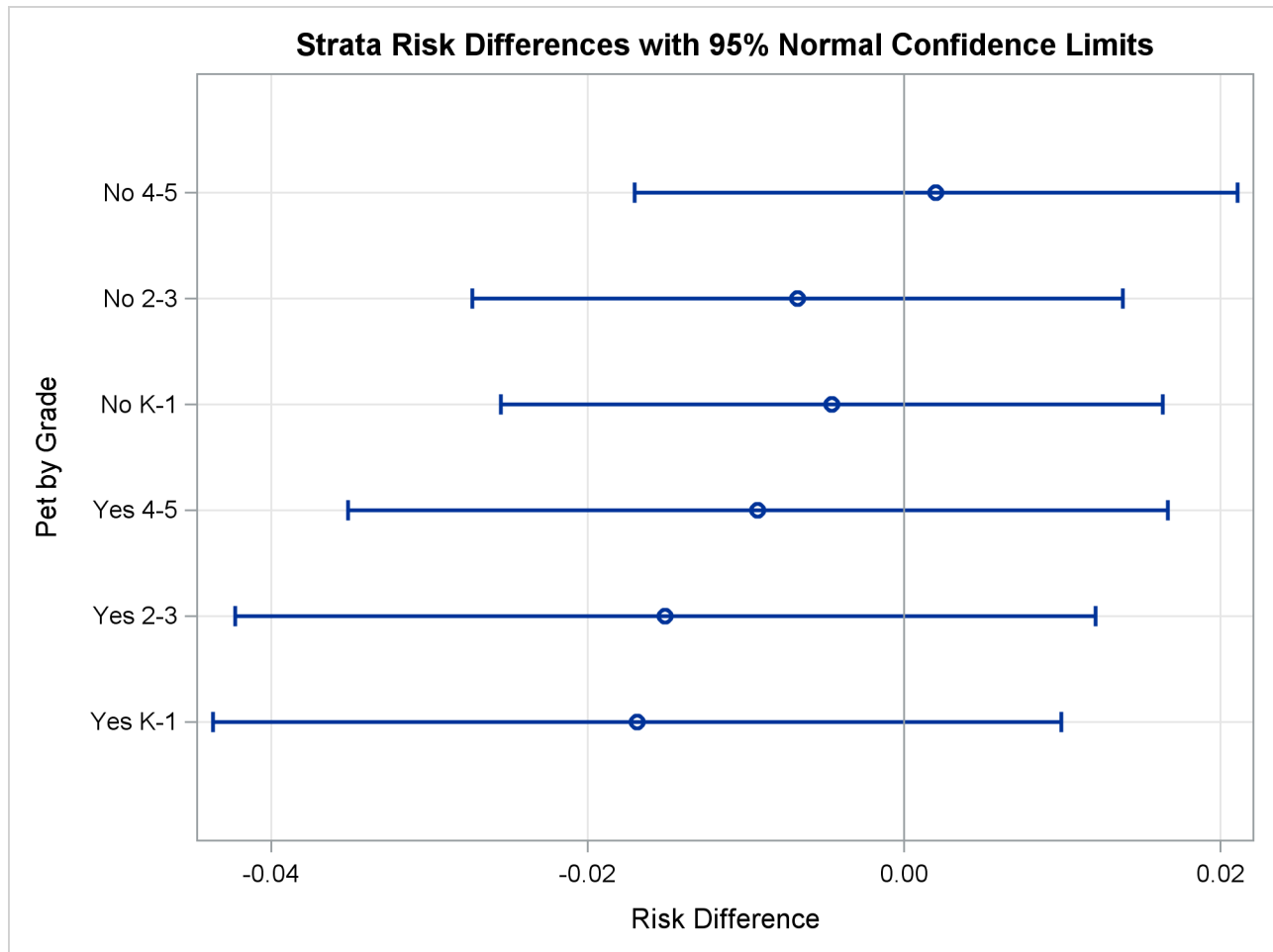
| Strata Risk Effect Estimates |                              |          |
|------------------------------|------------------------------|----------|
| Stratum Index                | 95% Normal Confidence Limits |          |
| 1                            | -.043766                     | 0.010001 |
| 2                            | -.042366                     | 0.012169 |
| 3                            | -.035225                     | 0.016740 |
| 4                            | -.025554                     | 0.016405 |
| 5                            | -.027373                     | 0.013892 |
| 6                            | -.017120                     | 0.021148 |

The “Strata Risk Effect Estimates” table shows that for the stratum of students without household pets in Grade 4–5, the risk is higher for students without household smokers than for students with household smokers. For all other strata, the risk is lower for students without household smokers than for students with household smokers. The difference is not significant in each stratum because the null value 0 is between the lower and upper confidence limits.

With ODS Graphics enabled, the PLOTS=EFFECT option displays the plot with the stratum-specific risk effect measures and their associated confidence limits, as shown in [Output 88.2.6](#). The EFFECT=DIFF option requests that the risk difference be displayed. By default, confidence limits are generated with 95% confidence level. This plot displays the stratum-specific risk differences in the “Strata Risk Effect Estimates” table in [Output 88.2.5](#).



Output 88.2.6 Strata Risk Plot



The “Mantel-Haenszel Standardized Risk Estimates” table in [Output 88.2.7](#) displays the Mantel-Haenszel standardized risks and related statistics.

**Output 88.2.7** Standardized Risk Estimates (Mantel-Haenszel Estimation)

| Mantel-Haenszel Standardized Risk Estimates |                            |                           |               |                     |         |
|---------------------------------------------|----------------------------|---------------------------|---------------|---------------------|---------|
| Smoking                                     | -----Study Population----- |                           |               | --Mantel-Haenszel-- |         |
|                                             | Observed<br>Events         | Number of<br>Observations | Crude<br>Risk | Expected<br>Events  | Weight  |
| No                                          | 1991                       | 16838                     | 0.1182        | 566.172             | 4791.43 |
| Yes                                         | 840                        | 6726                      | 0.1249        | 599.602             | 4791.43 |

| Mantel-Haenszel Standardized Risk Estimates |                             |                   |                                 |        |
|---------------------------------------------|-----------------------------|-------------------|---------------------------------|--------|
| Smoking                                     | -----Standardized Risk----- |                   |                                 |        |
|                                             | Estimate                    | Standard<br>Error | 95% Normal<br>Confidence Limits |        |
| No                                          | 0.1182                      | 0.00250           | 0.1133                          | 0.1231 |
| Yes                                         | 0.1251                      | 0.00404           | 0.1172                          | 0.1331 |

The EFFECT=DIFF option requests that the “Risk Effect Estimates” table display the risk difference statistic for the two directly standardized risks, as shown in [Output 88.2.8](#).

**Output 88.2.8** Mantel-Haenszel Effect Estimates

| Risk Effect Estimates |        |                    |                   |       |         |
|-----------------------|--------|--------------------|-------------------|-------|---------|
| -----Smoking-----     |        | Risk<br>Difference | Standard<br>Error | Z     | Pr >  Z |
| No                    | Yes    |                    |                   |       |         |
| 0.1182                | 0.1251 | -0.00698           | 0.00475           | -1.47 | 0.1418  |

The table shows that although the standardized risk for students without household smokes is lower than the standardized risk for students with household smokes, the difference (-0.00698) is not significant at the 5% significance level, (*p*-value 0.1418).

---

**Example 88.3: Computing Attributable Fraction Estimates**

This example computes the excess event risk fraction that is attributable to a specific chemical exposure for workers in a factory.

Suppose that the Factory data set contains the stratum-specific event information for exposure to a specific chemical agent. The variable Age is the grouping variable that forms the strata. The variables Event\_E and Count\_E indicate the number of events and number of workers for workers with the specific chemical exposure, respectively. The variables Event\_NE and Count\_NE indicate the number of events and number of workers for workers without the specific chemical exposure, respectively.

```

data Factory;
 input Age $ Event_E Count_E Event_NE Count_NE;
 datalines;
20-29 31 352 143 2626
30-39 57 486 392 4124
40-49 62 538 459 4662
50-59 50 455 337 3622
60-69 38 322 199 2155
70+ 9 68 35 414
;

```

The following statements invoke the STDRATE procedure and compute the attributable risk and population attributable risk for the chemical exposure:

```

ods graphics on;
proc stdrate data=Factory
 reldata=Factory
 method=indirect (af)
 stat=risk
 plots (stratum=horizontal)
;
 population event=Event_E total=Count_E;
 reference event=Event_NE total=Count_NE;
 strata Age / stats;
run;
ods graphics off;

```

The “Standardization Information” table in [Output 88.3.1](#) displays the standardization information.

### Output 88.3.1 Standardization Information

| The STDRATE Procedure       |                          |
|-----------------------------|--------------------------|
| Standardization Information |                          |
| Data Set                    | WORK.FACTORY             |
| Reference Data Set          | WORK.FACTORY             |
| Method                      | Indirect Standardization |
| Statistic                   | Risk                     |
| Number of Strata            | 6                        |

The STATS option in the STRATA statement requests that the “Indirectly Standardized Strata Statistics” table in [Output 88.3.2](#) display the strata information and the expected number of events at each stratum. The Expected Events column shows the expected numbers of events when the stratum-specific risks in the reference data set are applied to the corresponding numbers of workers in the study data set.

**Output 88.3.2** Strata Information (Indirect Standardization)

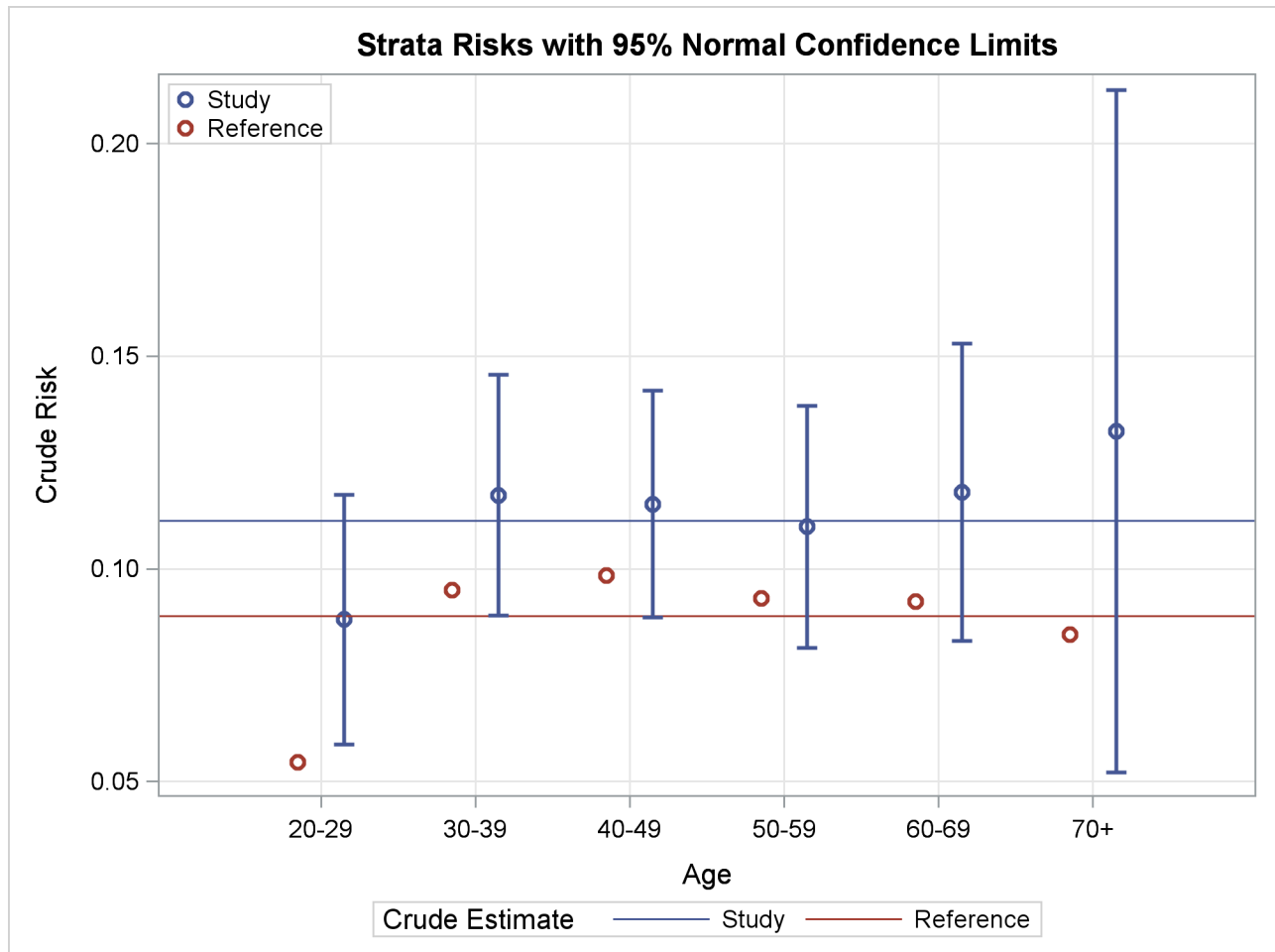
| The STDRATE Procedure                     |       |                            |                                   |            |               |                   |
|-------------------------------------------|-------|----------------------------|-----------------------------------|------------|---------------|-------------------|
| Indirectly Standardized Strata Statistics |       |                            |                                   |            |               |                   |
| Stratum<br>Index                          | Age   | -----Study Population----- |                                   |            | Crude<br>Risk | Standard<br>Error |
|                                           |       | Observed<br>Events         | -Number of Observations-<br>Value | Proportion |               |                   |
| 1                                         | 20-29 | 31                         | 352                               | 0.1585     | 0.088068      | 0.015105          |
| 2                                         | 30-39 | 57                         | 486                               | 0.2188     | 0.117284      | 0.014595          |
| 3                                         | 40-49 | 62                         | 538                               | 0.2422     | 0.115242      | 0.013767          |
| 4                                         | 50-59 | 50                         | 455                               | 0.2049     | 0.109890      | 0.014662          |
| 5                                         | 60-69 | 38                         | 322                               | 0.1450     | 0.118012      | 0.017979          |
| 6                                         | 70+   | 9                          | 68                                | 0.0306     | 0.132353      | 0.041095          |

| Indirectly Standardized Strata Statistics |                                 |          |                                   |            |               |                    |
|-------------------------------------------|---------------------------------|----------|-----------------------------------|------------|---------------|--------------------|
| Stratum<br>Index                          | -Study Population-              |          | -----Reference Population-----    |            | Crude<br>Risk | Expected<br>Events |
|                                           | 95% Normal<br>Confidence Limits |          | -Number of Observations-<br>Value | Proportion |               |                    |
| 1                                         | 0.058463                        | 0.117673 | 2626                              | 0.1492     | 0.05446       | 19.1683            |
| 2                                         | 0.088678                        | 0.145890 | 4124                              | 0.2343     | 0.09505       | 46.1959            |
| 3                                         | 0.088260                        | 0.142224 | 4662                              | 0.2648     | 0.09846       | 52.9691            |
| 4                                         | 0.081153                        | 0.138627 | 3622                              | 0.2058     | 0.09304       | 42.3343            |
| 5                                         | 0.082774                        | 0.153251 | 2155                              | 0.1224     | 0.09234       | 29.7346            |
| 6                                         | 0.051809                        | 0.212897 | 414                               | 0.0235     | 0.08454       | 5.7488             |

With ODS Graphics enabled and the specified STAT=RISK option, the default PLOTS=RISK option displays the stratum-specific risk estimates in the study and reference populations, as shown in [Output 88.3.3](#). The STRATUM=HORIZONTAL global option in the PLOTS option displays the strata information on the horizontal axis. The plot displays the stratum-specific risk estimates in the “Indirect Standardized Strata Statistics” table in [Output 88.3.2](#). In addition, confidence limits for the risk estimates in the study population and the overall crude risks for the two populations are also displayed

Output 88.3.3 Strata Risk Plot



The METHOD=INDIRECT option requests that the “Standardized Morbidity/Mortality Ratio” table in [Output 88.3.4](#) display the SMR, its 95% confidence limits, and the test for the null hypothesis  $H_0 : \text{SMR} = 1$ .

Output 88.3.4 Standardized Morbidity/Mortality Ratio

| Standardized Morbidity/Mortality Ratio |                 |        |                |                              |        |      |         |
|----------------------------------------|-----------------|--------|----------------|------------------------------|--------|------|---------|
| Observed Events                        | Expected Events | SMR    | Standard Error | 95% Normal Confidence Limits |        | Z    | Pr >  Z |
| 247                                    | 196.151         | 1.2592 | 0.0755         | 1.1113                       | 1.4072 | 3.43 | 0.0006  |

The “Standardized Morbidity/Mortality Ratio” table shows that  $\text{SMR}=1.259$ , the 95% confidence limits do not contain the null value  $\text{SMR}=1$ , and the null hypothesis of  $\text{SMR}=1$  is rejected at  $\alpha = 0.05$  level from the normal test.

The “Indirectly Standardized Risk Estimates” table in [Output 88.3.5](#) displays the standardized risks and related statistics.

**Output 88.3.5** Standardized Risks (Indirect Standardization)

| Indirectly Standardized Risk Estimates |                           |                                 |               |                    |        |  |
|----------------------------------------|---------------------------|---------------------------------|---------------|--------------------|--------|--|
| -----Study Population-----             |                           |                                 | Reference     |                    |        |  |
| Observed<br>Events                     | Number of<br>Observations | Crude<br>Risk                   | Crude<br>Risk | Expected<br>Events | SMR    |  |
| 247                                    | 2221                      | 0.1112                          | 0.0889        | 196.151            | 1.2592 |  |
| Indirectly Standardized Risk Estimates |                           |                                 |               |                    |        |  |
| -----Standardized Risk-----            |                           |                                 |               |                    |        |  |
| Estimate                               | Standard<br>Error         | 95% Normal<br>Confidence Limits |               |                    |        |  |
| 0.1120                                 | 0.00671                   | 0.0988                          | 0.1251        |                    |        |  |

The AF suboption in the METHOD=INDIRECT option requests that the “Attributable Fraction Estimates” table display the attributable risk and population attributable risk, as shown in [Output 88.3.6](#)

**Output 88.3.6** Attributable Fraction Estimates

| Attributable Fraction Estimates |          |                         |         |
|---------------------------------|----------|-------------------------|---------|
| Parameter                       | Estimate | -95% Confidence Limits- |         |
| Attributable Risk               | 0.20587  | 0.10013                 | 0.28937 |
| Population Attributable Risk    | 0.02806  | 0.01159                 | 0.04426 |

The attributable risk fraction 0.206 indicates that 20.6% of all events in the chemical exposure group are attributed to the chemical exposure, and the population attributable risk fraction 0.028 indicates that about 2.8% of all events in the total population are attributed to the chemical exposure.

The Attributable fraction can also be computed by using Mantel-Haenszel method.

Suppose that the Factory1 data set contains the stratum-specific event information for exposure to a specific chemical agent. The variable Age is the grouping variable that forms the strata, and the variable Exposure identifies workers with chemical exposure. The variables Event and Count indicate the number of events and number of workers, respectively.

```

data Factory1;
 input Exposure $ Age $ Event Count;
 datalines;
Yes 20-29 31 352
Yes 30-39 57 486
Yes 40-49 62 538
Yes 50-59 50 455
Yes 60-69 38 322
Yes 70+ 9 68
No 20-29 143 2626

```

```

No 30-39 392 4124
No 40-49 459 4662
No 50-59 337 3622
No 60-69 199 2155
No 70+ 35 414
;

```

The following statements invoke the STDRATE procedure and compute the attributable risk and population attributable risk for the chemical exposure:

```

proc stdrate data=Factory1
 method=mh (af)
 stat=risk
 effect
;
 population group(order=data)=Exposure event=Event total=Count;
 strata Age;
run;

```

The “Standardization Information” table in [Output 88.3.7](#) displays the standardization information.

#### Output 88.3.7 Standardization Information

| The STDRATE Procedure       |                 |
|-----------------------------|-----------------|
| Standardization Information |                 |
| Data Set                    | WORK.FACTORY1   |
| Group Variable              | Exposure        |
| Method                      | Mantel-Haenszel |
| Statistic                   | Risk            |
| Number of Strata            | 6               |

The “Mantel-Haenszel Standardized Risk Estimates” table in [Output 88.3.8](#) displays the Mantel-Haenszel standardized risks and related statistics.

**Output 88.3.8** Standardized Risk Estimates (Mantel-Haenszel Estimation)

| Mantel-Haenszel Standardized Risk Estimates |                            |                           |               |                     |         |
|---------------------------------------------|----------------------------|---------------------------|---------------|---------------------|---------|
| Exposure                                    | -----Study Population----- |                           |               | --Mantel-Haenszel-- |         |
|                                             | Observed<br>Events         | Number of<br>Observations | Crude<br>Risk | Expected<br>Events  | Weight  |
| Yes                                         | 247                        | 2221                      | 0.1112        | 219.122             | 1970.26 |
| No                                          | 1565                       | 17603                     | 0.0889        | 174.134             | 1970.26 |

| Mantel-Haenszel Standardized Risk Estimates |                             |                   |                                 |        |
|---------------------------------------------|-----------------------------|-------------------|---------------------------------|--------|
| Exposure                                    | -----Standardized Risk----- |                   |                                 |        |
|                                             | Estimate                    | Standard<br>Error | 95% Normal<br>Confidence Limits |        |
| Yes                                         | 0.1112                      | 0.00667           | 0.0981                          | 0.1243 |
| No                                          | 0.0884                      | 0.00214           | 0.0842                          | 0.0926 |

The EFFECT option requests that the “Risk Effect Estimates” table display the risk ratio statistic for the two directly standardized risks, as shown in [Output 88.3.9](#).

**Output 88.3.9** Mantel-Haenszel Effect Estimates

| Risk Effect Estimates |        |               |                      |                   |      |         |
|-----------------------|--------|---------------|----------------------|-------------------|------|---------|
| -----Exposure-----    |        | Risk<br>Ratio | Log<br>Risk<br>Ratio | Standard<br>Error | Z    | Pr >  Z |
| Yes                   | No     |               |                      |                   |      |         |
| 0.1112                | 0.0884 | 1.2584        | 0.2298               | 0.0647            | 3.55 | 0.0004  |

The AF suboption in the METHOD=MH option requests that the “Attributable Fraction Estimates” table display the attributable risk and population attributable risk, as shown in [Output 88.3.10](#)

**Output 88.3.10** Attributable Fraction Estimates

| Attributable Fraction Estimates |          |                         |         |
|---------------------------------|----------|-------------------------|---------|
| Parameter                       | Estimate | -95% Confidence Limits- |         |
| Attributable Risk               | 0.20531  | 0.09789                 | 0.29994 |
| Population Attributable Risk    | 0.02799  | 0.01070                 | 0.04497 |

Similar to the results of using the SMR estimates, the attributable risk fraction (0.205) indicates that 20.5% of all events in the chemical exposure group are attributed to the chemical exposure, and the population attributable risk fraction (0.028) indicates that about 2.8% of all events in the total population are attributed to the chemical exposure.



## Example 88.4: Displaying SMR Results from BY Groups

This example illustrates the use of ODS OUTPUT statement to save standardized mortality ratios for different causes and to display these statistics together in a table and in a plot.

The Florida\_Cs data set contains the stratum-specific mortality information for stomach cancer and skin cancer in year 2000 for the state of Florida (Florida Department of Health 2000, 2012). The variable Age is the grouping variable that forms the strata in the standardization. The variables Event\_C16, Event\_C43, and PYear identify the number of events for stomach cancer, the number of events for skin cancer, and the person-years, respectively. The COMMA12. format is specified in the DATA step to input numerical values that contain commas in PYear.

```
data Florida_Cs;
 input Age $1-5 Event_C16 Event_C43 PYear comma12.;
 datalines;
00-04 0 0 953,785
05-14 0 0 1,997,935
15-24 0 4 1,885,014
25-34 1 14 1,957,573
35-44 19 43 2,356,649
45-54 64 72 2,088,000
55-64 114 70 1,548,371
65-74 201 126 1,447,432
75-84 294 136 1,087,524
85+ 136 73 335,944
;
```

The following statements construct and list the mortality information by cancer cause:

```
data Florida_Cs;
 set Florida_Cs;
 Cause='Stomach'; Event=Event_C16; output;
 Cause='Skin'; Event=Event_C43; output;
 drop Event_C16 Event_C43;
run;

proc sort data=Florida_Cs;
 by Cause;
run;

proc print data=Florida_Cs;
 var Cause Age Event PYear;
run;
```

**Output 88.4.1** Florida Data

| Obs | Cause   | Age   | Event | PYear   |
|-----|---------|-------|-------|---------|
| 1   | Skin    | 00-04 | 0     | 953785  |
| 2   | Skin    | 05-14 | 0     | 1997935 |
| 3   | Skin    | 15-24 | 4     | 1885014 |
| 4   | Skin    | 25-34 | 14    | 1957573 |
| 5   | Skin    | 35-44 | 43    | 2356649 |
| 6   | Skin    | 45-54 | 72    | 2088000 |
| 7   | Skin    | 55-64 | 70    | 1548371 |
| 8   | Skin    | 65-74 | 126   | 1447432 |
| 9   | Skin    | 75-84 | 136   | 1087524 |
| 10  | Skin    | 85+   | 73    | 335944  |
| 11  | Stomach | 00-04 | 0     | 953785  |
| 12  | Stomach | 05-14 | 0     | 1997935 |
| 13  | Stomach | 15-24 | 0     | 1885014 |
| 14  | Stomach | 25-34 | 1     | 1957573 |
| 15  | Stomach | 35-44 | 19    | 2356649 |
| 16  | Stomach | 45-54 | 64    | 2088000 |
| 17  | Stomach | 55-64 | 114   | 1548371 |
| 18  | Stomach | 65-74 | 201   | 1447432 |
| 19  | Stomach | 75-84 | 294   | 1087524 |
| 20  | Stomach | 85+   | 136   | 335944  |

The US\_Cs data set contains the corresponding stratum-specific mortality information for the United States (Miniño et al. 2002; U.S. Bureau of Census 2011). The variable Age is the grouping variable that forms the strata in the standardization. The variables Event\_C16, Event\_C43, and PYear identify the number of events for stomach cancer, the number of events for skin cancer, and the person-years, respectively.

```
data US_Cs;
 input Age $1-5 Event_C16 Event_C43 PYear comma12.;
 datalines;
00-04 0 0 19,175,798
05-14 1 1 41,077,577
15-24 14 41 39,183,891
25-34 124 186 39,892,024
35-44 484 626 45,148,527
45-54 1097 1199 37,677,952
55-64 1804 1303 24,274,684
65-74 3054 1637 18,390,986
75-84 3833 1624 12,361,180
85+ 2234 803 4,239,587
;
```

The following statements construct and list the mortality information by cancer cause:

```
data US_Cs;
 set US_Cs;
 Cause='Stomach'; Event=Event_C16; output;
 Cause='Skin'; Event=Event_C43; output;
 drop Event_C16 Event_C43;
run;
```

```

proc sort data=US_Cs;
 by Cause;
run;

proc print data=US_Cs;
 var Cause Age Event PYear;
run;

```

Output 88.4.2 lists the mortality information by cancer cause.

**Output 88.4.2** Florida Data

| Obs | Cause   | Age   | Event | PYear    |
|-----|---------|-------|-------|----------|
| 1   | Skin    | 00-04 | 0     | 19175798 |
| 2   | Skin    | 05-14 | 1     | 41077577 |
| 3   | Skin    | 15-24 | 41    | 39183891 |
| 4   | Skin    | 25-34 | 186   | 39892024 |
| 5   | Skin    | 35-44 | 626   | 45148527 |
| 6   | Skin    | 45-54 | 1199  | 37677952 |
| 7   | Skin    | 55-64 | 1303  | 24274684 |
| 8   | Skin    | 65-74 | 1637  | 18390986 |
| 9   | Skin    | 75-84 | 1624  | 12361180 |
| 10  | Skin    | 85+   | 803   | 4239587  |
| 11  | Stomach | 00-04 | 0     | 19175798 |
| 12  | Stomach | 05-14 | 1     | 41077577 |
| 13  | Stomach | 15-24 | 14    | 39183891 |
| 14  | Stomach | 25-34 | 124   | 39892024 |
| 15  | Stomach | 35-44 | 484   | 45148527 |
| 16  | Stomach | 45-54 | 1097  | 37677952 |
| 17  | Stomach | 55-64 | 1804  | 24274684 |
| 18  | Stomach | 65-74 | 3054  | 18390986 |
| 19  | Stomach | 75-84 | 3833  | 12361180 |
| 20  | Stomach | 85+   | 2234  | 4239587  |

The following statements invoke the STDRATE procedure and request indirect standardization to compute the skin and stomach SMR estimates for the state of Florida. The BY statement requests separate analyses of causes that are defined by the Cause variable.

```

ods graphics on;
ods select StdInfo StrataSmrPlot Smr;
proc stdrate data=Florida_Cs refdata=US_Cs
 stat=rate
 method=indirect
 plots=smr
 ;
 population event=Event total=PYear;
 reference event=Event total=PYear;
 strata Age;
 by Cause;
ods output smr=Smr_Cs;
run;
ods graphics off;

```

Only the tables and plots that are specified in the ODS SELECT statement are displayed.

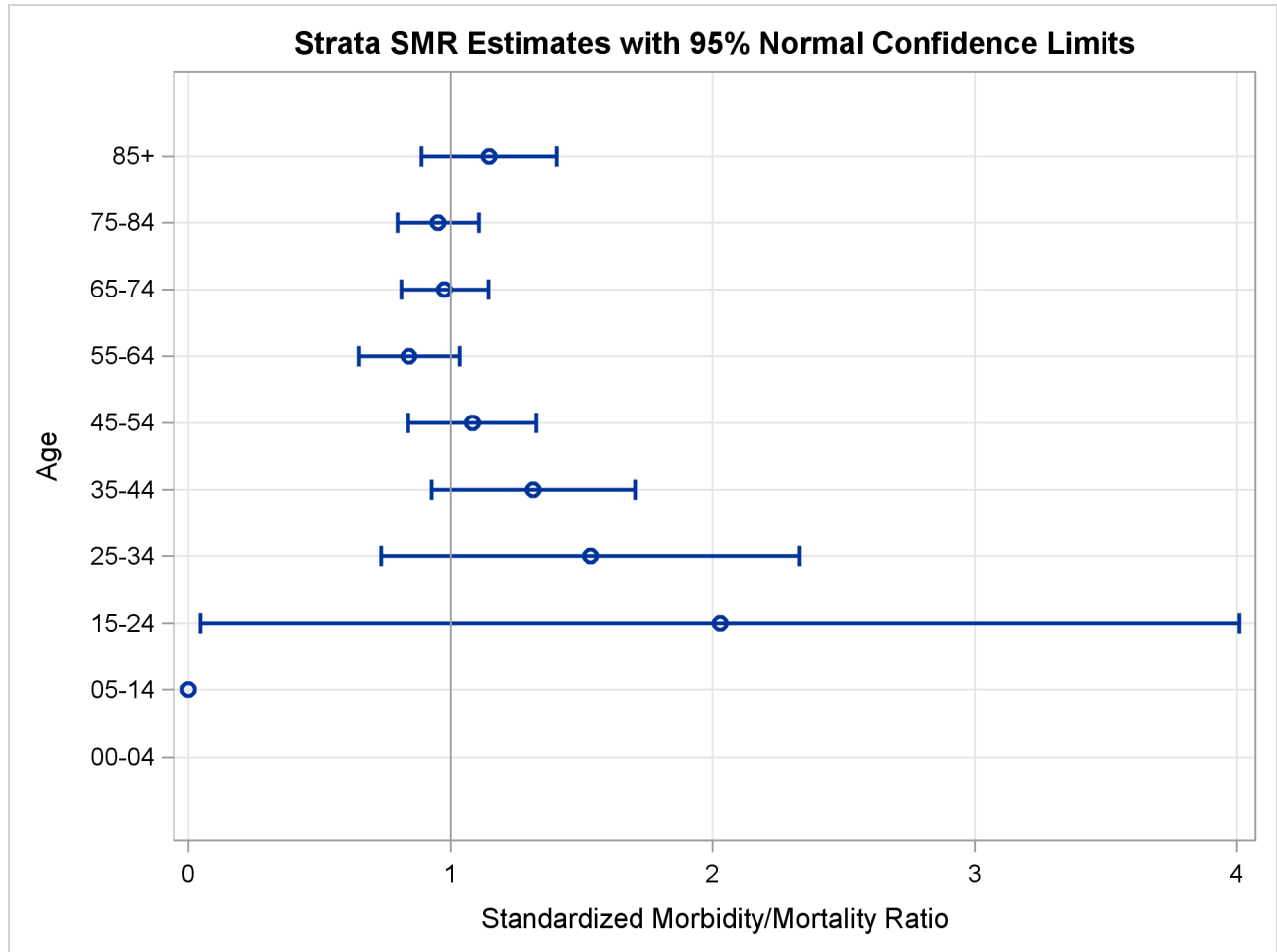
The STDINFO option in the ODS SELECT statement requests that the “Standardization Information” table display the standardization information for the first BY group, skin cancer, as shown in [Output 88.4.3](#)

### Output 88.4.3 Standardization Information

| ----- Cause=Skin -----      |                          |
|-----------------------------|--------------------------|
| The STDRATE Procedure       |                          |
| Standardization Information |                          |
| Data Set                    | WORK.FLORIDA_CS          |
| Reference Data Set          | WORK.US_CS               |
| Method                      | Indirect Standardization |
| Statistic                   | Rate                     |
| Number of Strata            | 10                       |
| Rate Multiplier             | 100000                   |

The STRATASMRPLOT option in the ODS SELECT statement requests that the strata SMR plot display stratum-specific SMR estimates for skin cancer with confidence limits, as shown in [Output 88.4.4](#).

Output 88.4.4 Strata SMR Plot



The SMR option in the ODS SELECT statement requests that the “Standardized Morbidity/Mortality Ratio” table display the SMR, its confidence limits, and the test for the null hypothesis  $H_0 : SMR = 1$  for skin cancer, as shown in Output 88.4.5. With the default ALPHA=0.05, 95% confidence limits are constructed.

Output 88.4.5 Standardized Morbidity/Mortality Ratio

| ----- Cause=Skin -----                 |                    |                 |                   |                                 |        |      |         |
|----------------------------------------|--------------------|-----------------|-------------------|---------------------------------|--------|------|---------|
| Standardized Morbidity/Mortality Ratio |                    |                 |                   |                                 |        |      |         |
| Observed<br>Events                     | Expected<br>Events | Standard<br>SMR | Standard<br>Error | 95% Normal<br>Confidence Limits |        | Z    | Pr >  Z |
| 538                                    | 528.726            | 1.0175          | 0.0439            | 0.9316                          | 1.1035 | 0.40 | 0.6893  |

Similarly, the “Standardization Information” table in Output 88.4.6 displays the standardization information for the second BY group, stomach cancer.

**Output 88.4.6** Standardization Information

```

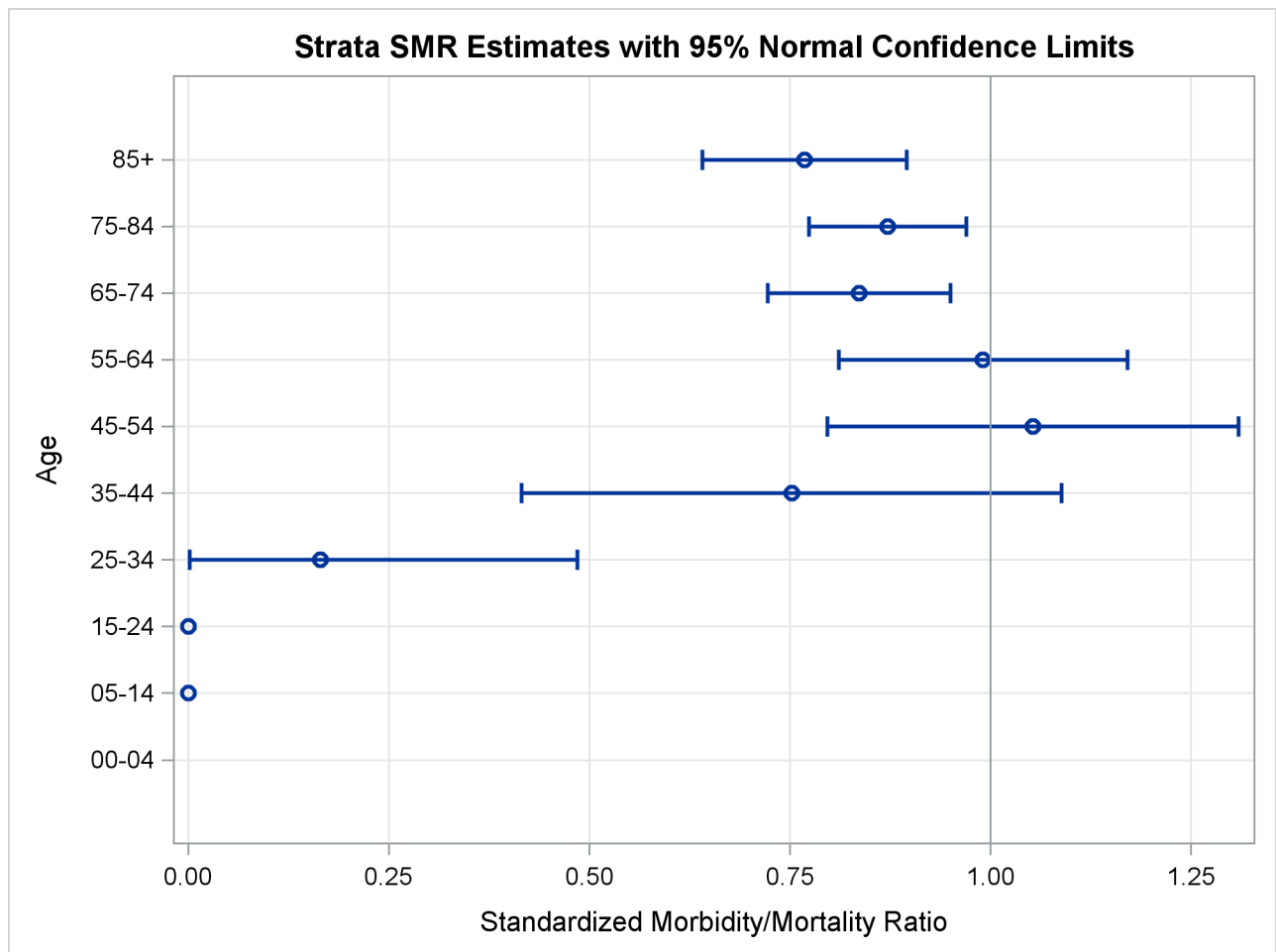
----- Cause=Stomach -----
 The STDRATE Procedure
 Standardization Information

Data Set WORK.FLORIDA_CS
Reference Data Set WORK.US_CS
Method Indirect Standardization
Statistic Rate
Number of Strata 10
Rate Multiplier 100000

```

The “Strata SMR Plot” displays stratum-specific SMR estimates with confidence limits for stomach cancer, as shown in [Output 88.4.7](#).

**Output 88.4.7** Strata SMR Plot



The “Standardized Morbidity/Mortality Ratio” table displays the SMR, its confidence limits, and the test for the null hypothesis  $H_0 : \text{SMR} = 1$  for stomach cancer, as shown in [Output 88.4.8](#).

**Output 88.4.8** Standardized Morbidity/Mortality Ratio

| ----- Cause=Stomach -----              |                    |                 |                   |                                 |        |       |         |
|----------------------------------------|--------------------|-----------------|-------------------|---------------------------------|--------|-------|---------|
| Standardized Morbidity/Mortality Ratio |                    |                 |                   |                                 |        |       |         |
| Observed<br>Events                     | Expected<br>Events | Standard<br>SMR | Standard<br>Error | 95% Normal<br>Confidence Limits |        | Z     | Pr >  Z |
| 829                                    | 962.537            | 0.8613          | 0.0299            | 0.8026                          | 0.9199 | -4.64 | <.0001  |

The ODS OUTPUT SMR=SMR\_CS statement requests that the “Standardized Morbidity/Mortality Ratio” tables for the two cancer causes be saved in the data set Smr\_Cs. The following statements display the selected output variables for the data set:

```
proc print data=Smr_Cs;
 var Cause ObservedEvents ExpectedEvents Smr SmrLcl SmrUcl;
run;
```

**Output 88.4.9** SMR Results from BY Groups

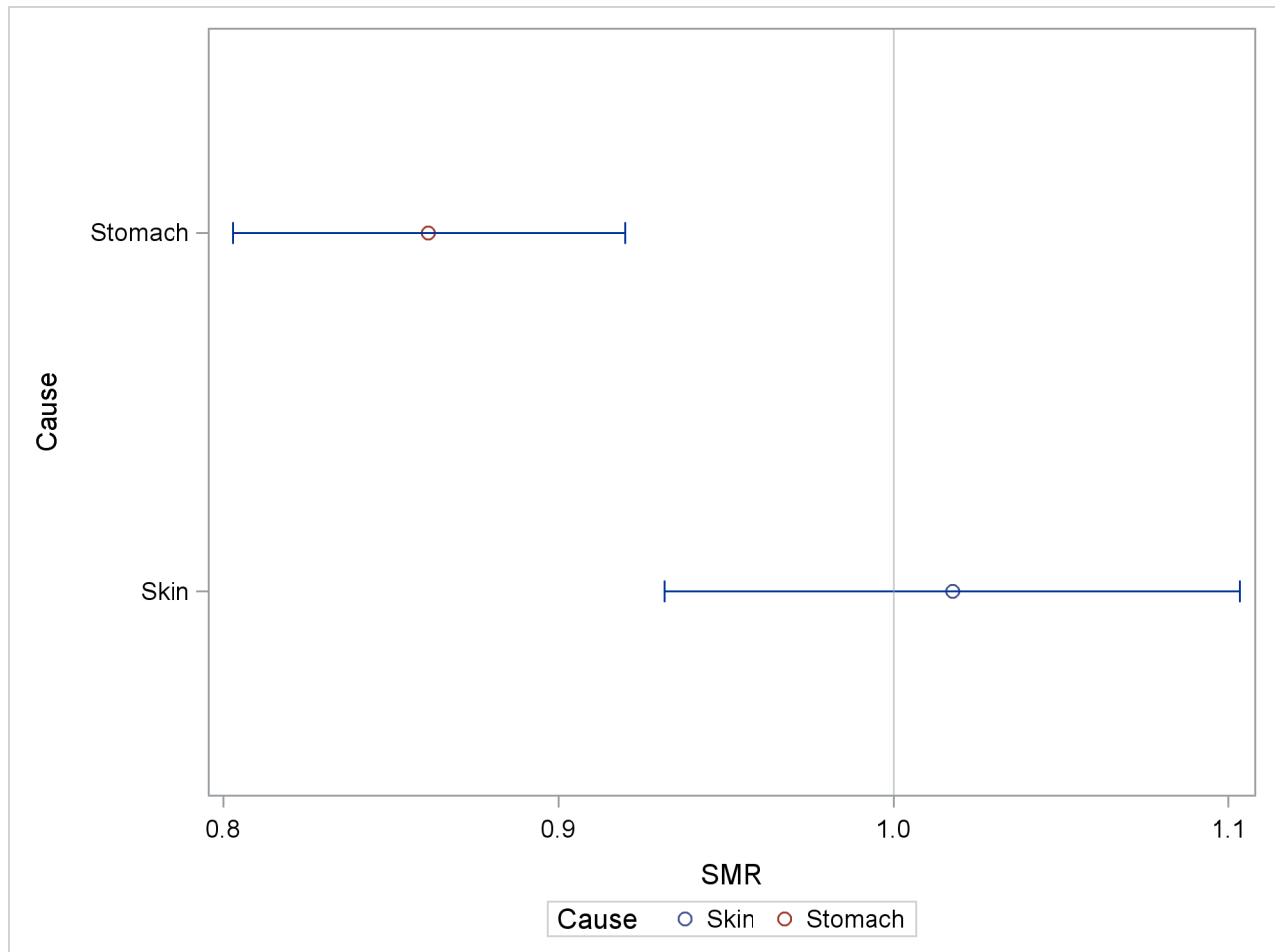
| Obs | Cause   | Observed<br>Events | Expected<br>Events | Smr    | SmrLcl | SmrUcl |
|-----|---------|--------------------|--------------------|--------|--------|--------|
| 1   | Skin    | 538                | 528.726            | 1.0175 | 0.9316 | 1.1035 |
| 2   | Stomach | 829                | 962.537            | 0.8613 | 0.8026 | 0.9199 |

The table in [Output 88.4.9](#) shows that the study population (state of Florida) has a higher skin cancer rate and a lower stomach cancer rate than the reference population (United States), but only the lower stomach cancer rate is significant because its corresponding SMR upper confidence limit (0.9199) is less than 1.

The following statements display the standardized morbidity/mortality ratios for the two causes in a plot:

```
proc sgplot data=Smr_Cs;
 scatter y=Cause x=Smr / group=Cause;
 highlow y=Cause high=SmrUcl low=SmrLcl / highcap=serif lowcap=serif;
 yaxis type=discrete;
 xaxis label="SMR";
 refline 1 / axis=x transparency=0.5;
run;
```

Output 88.4.10 SMR Results



Alternatively, you can also use the following statements to obtain separate analyses for the two cancer causes, and then to display these standardized mortality ratios together in a table and in a plot:

```

/*----- Perform Separate Analyses for Different Causes -----*/
ods graphics on;
ods select StdInfo StrataSmrPlot Smr;
proc stdrate data=Florida-Cs refdata=US-Cs
 stat=rate
 method=indirect
 plots=smr
 ;
 population event=Event_C43 total=PYear;
 reference event=Event_C43 total=PYear;
 strata Age;
ods output smr=Smr_c43;
run;

```



```

ods select StdInfo StrataSmrPlot Smr;
proc stdrate data=Florida-Cs reldata=US-Cs
 stat=rate
 method=indirect
 plots=smr
 ;
 population event=Event_C16 total=PYear;
 reference event=Event_C16 total=PYear;
 strata Age;
ods output smr=Smr_c16;
run;
ods graphics off;

/*----- Combine SMRs -----*/
data Smr_C43;
 set Smr_C43;
 length Cause $ 7.;
 Cause='Skin';
run;

data Smr_C16;
 set Smr_C16;
 length Cause $ 7.;
 Cause='Stomach';
run;

data Smr-Cs;
 set Smr_C43 Smr_C16;
run;

/*----- Display the Cause-Specific SMRs -----*/
proc print data=Smr-Cs;
 var Cause ObservedEvents ExpectedEvents Smr SmrLcl SmrUcl;
run;

proc sgplot data=Smr-Cs;
 scatter y=Cause x=Smr / group=Cause;
 highlow y=Cause high=SmrUcl low=SmrLcl / highcap=serif lowcap=serif;
 yaxis type=discrete;
 xaxis label="SMR";
 refline 1 / axis=x transparency=0.5;
run;

```

---

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# Chapter 89

## The STEPDISC Procedure

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### Overview: STEPDISC Procedure

Given a classification variable and several quantitative variables, the STEPDISC procedure performs a stepwise discriminant analysis to select a subset of the quantitative variables for use in discriminating among the classes. The set of variables that make up each class is assumed to be multivariate normal with a common covariance matrix. The STEPDISC procedure can use forward selection, backward elimination, or stepwise selection (Klecka 1980). The STEPDISC procedure is a useful prelude to further analyses with the CANDISC procedure or the DISCRIM procedure.

With PROC STEPDISC, variables are chosen to enter or leave the model according to one of two criteria:

- the significance level of an  $F$  test from an analysis of covariance, where the variables already chosen act as covariates and the variable under consideration is the dependent variable
- the squared partial correlation for predicting the variable under consideration from the CLASS variable, controlling for the effects of the variables already selected for the model

Forward selection begins with no variables in the model. At each step, PROC STEPDISC enters the variable that contributes most to the discriminatory power of the model as measured by Wilks' lambda, the likelihood ratio criterion. When none of the unselected variables meet the entry criterion, the forward selection process stops.

Backward elimination begins with all variables in the model except those that are linearly dependent on previous variables in the VAR statement. At each step, the variable that contributes least to the discriminatory power of the model as measured by Wilks' lambda is removed. When all remaining variables meet the criterion to stay in the model, the backward elimination process stops.

Stepwise selection begins, like forward selection, with no variables in the model. At each step, the model is examined. If the variable in the model that contributes least to the discriminatory power of the model as measured by Wilks' lambda fails to meet the criterion to stay, then that variable is removed. Otherwise, the variable not in the model that contributes most to the discriminatory power of the model is entered. When all variables in the model meet the criterion to stay and none of the other variables meet the criterion to enter, the stepwise selection process stops. Stepwise selection is the default method of variable selection.

It is important to realize that, in the selection of variables for entry, only one variable can be entered into the model at each step. The selection process does not take into account the relationships between variables that have not yet been selected. Thus, some important variables could be excluded in the process. Also, Wilks' lambda might not be the best measure of discriminatory power for your application. However, if you use PROC STEPDISC carefully, in combination with your knowledge of the data and careful cross validation, it can be a valuable aid in selecting variables for a discrimination model.

As with any stepwise procedure, it is important to remember that when many significance tests are performed, each at a level of, for example, 5% (0.05), the overall probability of rejecting at least one true null hypothesis is much larger than 5%. If you want to prevent including any variables that do not contribute to the discriminatory power of the model in the population, you should specify a very small significance level. In most applications, all variables considered have some discriminatory power, however small. To choose the model that provides the best discrimination by using the sample estimates, you need only to guard against estimating more parameters than can be reliably estimated with the given sample size.

Costanza and Afifi (1979) use Monte Carlo studies to compare alternative stopping rules that can be used with the forward selection method in the two-group multivariate normal classification problem. Five different numbers of variables, ranging from 10 to 30, are considered in the studies. The comparison is based on conditional and estimated unconditional probabilities of correct classification. They conclude that the use of a moderate significance level, in the range of 10 to 25 percent, often performs better than the use of a much larger or a much smaller significance level.

The significance level and the squared partial correlation criteria select variables in the same order, although they might select different numbers of variables. Increasing the sample size tends to increase the number of variables selected when you are using significance levels, but it has little effect on the number selected by using squared partial correlations.

See Chapter 10, "Introduction to Discriminant Procedures," for more information about discriminant analysis.

## Getting Started: STEPDISC Procedure

The data in this example are measurements of 159 fish caught in Finland's lake Laengelmavesi; this data set is available from the Puranen. For each of the seven species (bream, roach, whitefish, parkki, perch, pike, and smelt) the weight, length, height, and width of each fish are tallied. Three different length measurements are recorded: from the nose of the fish to the beginning of its tail, from the nose to the notch of its tail, and from the nose to the end of its tail. The height and width are recorded as percentages of the third length variable. The fish data set is available from the Sashelp library. PROC STEPDISC will select a subset of the six quantitative variables that might be useful for differentiating between the fish species. This subset is used in conjunction with PROC CANDISC and PROC DISCRIM to develop discrimination models.

The following steps use PROC STEPDISC to select a subset of potential discriminator variables. By default, PROC STEPDISC uses stepwise selection on all numeric variables that are not listed in other statements, and the significance levels for a variable to enter the subset and to stay in the subset are set to 0.15. The following statements produce [Figure 89.1](#) through [Figure 89.5](#):

```

title 'Fish Measurement Data';

proc stepdisc data=sashelp.fish;
 class Species;
run;

```

PROC STEPDISC begins by displaying summary information about the analysis (see [Figure 89.1](#)). This information includes the number of observations with nonmissing values, the number of classes in the classification variable (specified by the CLASS statement), the number of quantitative variables under consideration, the significance criteria for variables to enter and to stay in the model, and the method of variable selection being used. The frequency of each class is also displayed.

**Figure 89.1** Summary Information

|                                                       |     |                                     |      |
|-------------------------------------------------------|-----|-------------------------------------|------|
| <b>Fish Measurement Data</b>                          |     |                                     |      |
| <b>The STEPDISC Procedure</b>                         |     |                                     |      |
| <b>The Method for Selecting Variables is STEPWISE</b> |     |                                     |      |
| <b>Total Sample Size</b>                              | 158 | <b>Variable(s) in the Analysis</b>  | 6    |
| <b>Class Levels</b>                                   | 7   | <b>Variable(s) Will Be Included</b> | 0    |
|                                                       |     | <b>Significance Level to Enter</b>  | 0.15 |
|                                                       |     | <b>Significance Level to Stay</b>   | 0.15 |
| <b>Number of Observations Read</b>                    |     | 159                                 |      |
| <b>Number of Observations Used</b>                    |     | 158                                 |      |

Figure 89.1 continued

| Class Level Information |               |           |         |            |
|-------------------------|---------------|-----------|---------|------------|
| Species                 | Variable Name | Frequency | Weight  | Proportion |
| Bream                   | Bream         | 34        | 34.0000 | 0.215190   |
| Parkki                  | Parkki        | 11        | 11.0000 | 0.069620   |
| Perch                   | Perch         | 56        | 56.0000 | 0.354430   |
| Pike                    | Pike          | 17        | 17.0000 | 0.107595   |
| Roach                   | Roach         | 20        | 20.0000 | 0.126582   |
| Smelt                   | Smelt         | 14        | 14.0000 | 0.088608   |
| Whitefish               | Whitefish     | 6         | 6.0000  | 0.037975   |

For each entry step, the statistics for entry are displayed for all variables not currently selected (see Figure 89.2). The variable selected to enter at this step (if any) is displayed, as well as all the variables currently selected. Next are multivariate statistics that take into account all previously selected variables and the newly entered variable.

Figure 89.2 Step 1: Variable HEIGHT Selected for Entry

| Fish Measurement Data                 |          |         |        |           |        |
|---------------------------------------|----------|---------|--------|-----------|--------|
| The STEPDISC Procedure                |          |         |        |           |        |
| Stepwise Selection: Step 1            |          |         |        |           |        |
| Statistics for Entry, DF = 6, 151     |          |         |        |           |        |
| Variable                              | R-Square | F Value | Pr > F | Tolerance |        |
| Weight                                | 0.3750   | 15.10   | <.0001 | 1.0000    |        |
| Length1                               | 0.6017   | 38.02   | <.0001 | 1.0000    |        |
| Length2                               | 0.6098   | 39.32   | <.0001 | 1.0000    |        |
| Length3                               | 0.6280   | 42.49   | <.0001 | 1.0000    |        |
| Height                                | 0.7553   | 77.69   | <.0001 | 1.0000    |        |
| Width                                 | 0.4806   | 23.29   | <.0001 | 1.0000    |        |
| Variable Height will be entered.      |          |         |        |           |        |
| Variable(s) That Have Been Entered    |          |         |        |           |        |
| Height                                |          |         |        |           |        |
| Multivariate Statistics               |          |         |        |           |        |
| Statistic                             | Value    | F Value | Num DF | Den DF    | Pr > F |
| Wilks' Lambda                         | 0.244670 | 77.69   | 6      | 151       | <.0001 |
| Pillai's Trace                        | 0.755330 | 77.69   | 6      | 151       | <.0001 |
| Average Squared Canonical Correlation | 0.125888 |         |        |           |        |

For each removal step (Figure 89.3), the statistics for removal are displayed for all variables currently entered. The variable to be removed at this step (if any) is displayed. If no variable meets the criterion to be removed and the maximum number of steps as specified by the MAXSTEP= option has not been attained, then the procedure continues with another entry step.

**Figure 89.3** Step 2: No Variable Is Removed; Variable Length2 Added

```

Fish Measurement Data

The STEPDISC Procedure
Stepwise Selection: Step 2

Statistics for Removal, DF = 6, 151

Variable R-Square F Value Pr > F
Height 0.7553 77.69 <.0001

No variables can be removed.

Statistics for Entry, DF = 6, 150

Variable Partial
R-Square F Value Pr > F Tolerance

Weight 0.7388 70.71 <.0001 0.4690
Length1 0.9220 295.35 <.0001 0.6083
Length2 0.9229 299.31 <.0001 0.5892
Length3 0.9173 277.37 <.0001 0.5056
Width 0.8783 180.44 <.0001 0.3699

Variable Length2 will be entered.

Variable(s) That Have Been Entered

Length2 Height

Multivariate Statistics

Statistic Value F Value Num DF Den DF Pr > F
Wilks' Lambda 0.018861 157.04 12 300 <.0001
Pillai's Trace 1.554349 87.78 12 302 <.0001
Average Squared Canonical
Correlation 0.259058

```

The stepwise procedure terminates either when no variable can be removed and no variable can be entered or when the maximum number of steps as specified by the MAXSTEP= option has been attained. In this example at step 7 no variables can be either removed or entered (Figure 89.4). Steps 3 through 6 are not displayed in this document.



**Figure 89.4** Step 7: No Variables Entered or Removed

```

Fish Measurement Data

The STEPDISC Procedure
Stepwise Selection: Step 7

Statistics for Removal, DF = 6, 146

Variable Partial
 R-Square F Value Pr > F
Weight 0.4521 20.08 <.0001
Length1 0.2987 10.36 <.0001
Length2 0.5250 26.89 <.0001
Length3 0.7948 94.25 <.0001
Height 0.7257 64.37 <.0001
Width 0.5757 33.02 <.0001

No variables can be removed.

```

PROC STEPDISC ends by displaying a summary of the steps.

**Figure 89.5** Step Summary

```

No further steps are possible.

Fish Measurement Data

The STEPDISC Procedure

Stepwise Selection Summary

Number Partial Wilks' Pr < Average
Step In Entered Removed R-Square F Value Pr > F Lambda Lambda Correlation Pr >
1 1 Height 0.7553 77.69 <.0001 0.24466983 <.0001 0.12588836 <.0001
2 2 Length2 0.9229 299.31 <.0001 0.01886065 <.0001 0.25905822 <.0001
3 3 Length3 0.8826 186.77 <.0001 0.00221342 <.0001 0.38427100 <.0001
4 4 Width 0.5775 33.72 <.0001 0.00093510 <.0001 0.45200732 <.0001
5 5 Weight 0.4461 19.73 <.0001 0.00051794 <.0001 0.49488458 <.0001
6 6 Length1 0.2987 10.36 <.0001 0.00036325 <.0001 0.51744189 <.0001

```

All the variables in the data set are found to have potential discriminatory power. These variables are used to develop discrimination models in both the CANDISC and DISCRIM procedure chapters.

---

## Syntax: STEPDISC Procedure

The following statements are available in the STEPDISC procedure:

```

PROC STEPDISC < options > ;
 CLASS variable ;
 BY variables ;
 FREQ variable ;
 VAR variables ;
 WEIGHT variable ;

```

The BY, CLASS, FREQ, VAR, and WEIGHT statements are described after the PROC STEPDISC statement.

---

## PROC STEPDISC Statement

```

PROC STEPDISC < options > ;

```

The PROC STEPDISC statement invokes the STEPDISC procedure. Table 89.1 summarizes the options available in the PROC STEPDISC statement.

**Table 89.1** STEPDISC Procedure Options

| Option                            | Description                                  |
|-----------------------------------|----------------------------------------------|
| <b>Input Data Set</b>             |                                              |
| DATA=                             | Specifies input SAS data set                 |
| <b>Method Details</b>             |                                              |
| MAXMACRO=                         | Specifies maximum macro variable lists       |
| METHOD=                           | Specifies method                             |
| SINGULAR=                         | Specifies singularity                        |
| <b>Control Stepwise Selection</b> |                                              |
| SLENTY=                           | Specifies entry significance                 |
| SLSTAY=                           | Specifies staying significance               |
| PR2ENTRY=                         | Specifies entry partial R square             |
| PR2STAY=                          | Specifies staying partial R square           |
| INCLUDE=                          | Forces inclusion of variables                |
| MAXSTEP=                          | Specifies maximum number of steps            |
| START=                            | Specifies variables to begin                 |
| STOP=                             | Specifies number of variables in final model |
| <b>Control Displayed Output</b>   |                                              |
| ALL                               | Displays all                                 |
| BCORR                             | Displays between correlations                |
| BCOV                              | Displays between covariances                 |
| BSSCP                             | Displays between SSCPs                       |
| PCORR                             | Displays pooled correlations                 |
| PCOV                              | Displays pooled covariances                  |

Table 89.1 *continued*

| Option  | Description                       |
|---------|-----------------------------------|
| PSSCP   | Displays pooled SSCPs             |
| SHORT   | Suppresses output                 |
| SIMPLE  | Displays descriptive statistics   |
| STDMEAN | Displays standardized class means |
| TCORR   | Displays total correlations       |
| TCOV    | Displays total covariances        |
| TSSCP   | Displays total SSCPs              |
| WCORR   | Displays within correlations      |
| WCOV    | Displays within covariances       |
| WSSCP   | Displays within SSCPs             |

**ALL**

activates all of the display options.

**BCORR**

displays between-class correlations.

**BCOV**

displays between-class covariances. The between-class covariance matrix equals the between-class SSCP matrix divided by  $n(c - 1)/c$ , where  $n$  is the number of observations and  $c$  is the number of classes. The between-class covariances should be interpreted in comparison with the total-sample and within-class covariances, not as formal estimates of population parameters.

**BSSCP**

displays the between-class SSCP matrix.

**DATA=SAS-data-set**

specifies the data set to be analyzed. The data set can be an ordinary SAS data set or one of several specially structured data sets created by statistical procedures available with SAS/STAT software. These specially structured data sets include TYPE=CORR, COV, CSSCP, and SSCP. If the DATA= option is omitted, the procedure uses the most recently created SAS data set.

**INCLUDE=n**

includes the first  $n$  variables in the VAR statement in every model. By default, INCLUDE=0.

**MAXMACRO=n**

specifies the maximum number of macro variables with independent variable lists to create. By default, MAXMACRO=100. PROC STEPDISC saves the list of selected variables in a macro variable, &\_StdVar. Suppose your input variable list consists of x1-x10; then &\_StdVar would be set to x1 x3 x4 x10 if, for example, the first, third, fourth, and tenth variables were selected for the model. This list can be used, for example, in a subsequent procedure's VAR statement as follows:

```
var &_stdvar;
```

With BY processing, one macro variable is created for each BY group, and the macro variables are indexed by the BY-group number. The MAXMACRO= option can be used to either limit or

increase the number of these macro variables in processing data sets with many BY groups. The macro variables are created as follows:

With no BY processing, PROC STEPDISC creates the following:

|                              |                                                                   |
|------------------------------|-------------------------------------------------------------------|
| <code>_StdVar</code>         | selected variables                                                |
| <code>_StdVar1</code>        | selected variables                                                |
| <code>_StdNumBys</code>      | number of BY groups (1)                                           |
| <code>_StdNumMacroBys</code> | number of <code>_StdVari</code> macro variables actually made (1) |

With BY processing, PROC STEPDISC creates the following:

|                              |                                                                                                                                                                                                      |
|------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>_StdVar</code>         | selected variables for BY group 1                                                                                                                                                                    |
| <code>_StdVar1</code>        | selected variables for BY group 1                                                                                                                                                                    |
| <code>_StdVar2</code>        | selected variables for BY group 2                                                                                                                                                                    |
| .                            |                                                                                                                                                                                                      |
| .                            |                                                                                                                                                                                                      |
| .                            |                                                                                                                                                                                                      |
| <code>_StdVarm</code>        | selected variables for BY group $m$ , where a number is substituted for $m$                                                                                                                          |
| <code>_StdNumBys</code>      | $n$ , the number of BY groups                                                                                                                                                                        |
| <code>_StdNumMacroBys</code> | the number $m$ of <code>_StdVari</code> macro variables actually made. This value might be less than <code>_StdNumBys = n</code> , and it is less than or equal to the <code>MAXMACRO=</code> value. |

#### **MAXSTEP= $n$**

specifies the maximum number of steps. By default, `MAXSTEP=` two times the number of variables in the VAR statement.

#### **METHOD=BACKWARD | BW**

#### **METHOD=FORWARD | FW**

#### **METHOD=STEPWISE | SW**

specifies the method used to select the variables in the model. The `BACKWARD` method specifies backward elimination, `FORWARD` specifies forward selection, and `STEPWISE` specifies stepwise selection. By default, `METHOD=STEPWISE`.

#### **PCORR**

displays pooled within-class correlations (partial correlations based on the pooled within-class covariances).

#### **PCOV**

displays pooled within-class covariances.

#### **PR2ENTRY= $\rho$**

#### **PR2E= $\rho$**

specifies the partial R square for adding variables in the forward selection mode, where  $\rho \leq 1$ .

#### **PR2STAY= $\rho$**

#### **PR2S= $\rho$**

specifies the partial R square for retaining variables in the backward elimination mode, where  $\rho \leq 1$ .

**PSSCP**

displays the pooled within-class corrected SSCP matrix.

**SHORT**

suppresses the displayed output from each step.

**SIMPLE**

displays simple descriptive statistics for the total sample and within each class.

**SINGULAR= $\rho$** 

specifies the singularity criterion for entering variables, where  $0 < \rho < 1$ . PROC STEPDISC precludes the entry of a variable if the squared multiple correlation of the variable with the variables already in the model exceeds  $1 - \rho$ . With more than one variable already in the model, PROC STEPDISC also excludes a variable if it would cause any of the variables already in the model to have a squared multiple correlation (with the entering variable and the other variables in the model) exceeding  $1 - \rho$ . By default, SINGULAR= 1E-8.

**SLENTRY= $\rho$** **SLE= $\rho$** 

specifies the significance level for adding variables in the forward selection mode, where  $0 \leq \rho \leq 1$ . The default value is 0.15.

**SLSTAY= $\rho$** **SLS= $\rho$** 

specifies the significance level for retaining variables in the backward elimination mode, where  $0 \leq \rho \leq 1$ . The default value is 0.15.

**START= $n$** 

specifies that the first  $n$  variables in the VAR statement be used to begin the selection process. When you specify METHOD=FORWARD or METHOD=STEPWISE, the default value is 0; when you specify METHOD=BACKWARD, the default value is the number of variables in the VAR statement.

**STDMEAN**

displays total-sample and pooled within-class standardized class means.

**STOP= $n$** 

specifies the number of variables in the final model. The STEPDISC procedure stops the selection process when a model with  $n$  variables is found. This option applies only when you specify METHOD=FORWARD or METHOD=BACKWARD. When you specify METHOD=FORWARD, the default value is the number of variables in the VAR statement; when you specify METHOD=BACKWARD, the default value is 0.

**TCORR**

displays total-sample correlations.

**TCOV**

displays total-sample covariances.

**TSSCP**

displays the total-sample corrected SSCP matrix.

**WCORR**

displays within-class correlations for each class level.

**WCOV**

displays within-class covariances for each class level.

**WSSCP**

displays the within-class corrected SSCP matrix for each class level.

---

## BY Statement

**BY variables ;**

You can specify a BY statement with PROC STEPDISC to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the STEPDISC procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

## CLASS Statement

**CLASS** *variable* ;

The values of the CLASS variable define the groups for analysis. Class levels are determined by the formatted values of the CLASS variable. The CLASS variable can be numeric or character. A CLASS statement is required.

---

## FREQ Statement

**FREQ** *variable* ;

If a variable in the data set represents the frequency of occurrence for the other values in the observation, include the name of the variable in a FREQ statement. The procedure then treats the data set as if each observation appears  $n$  times, where  $n$  is the value of the FREQ variable for the observation. The total number of observations is considered to be equal to the sum of the FREQ variable when the procedure determines degrees of freedom for significance probabilities.

If the value of the FREQ variable is missing or is less than one, the observation is not used in the analysis. If the value is not an integer, the value is truncated to an integer.

---

## VAR Statement

**VAR** *variables* ;

The VAR statement specifies the quantitative variables eligible for selection. The default is all numeric variables not listed in other statements.

---

## WEIGHT Statement

**WEIGHT** *variable* ;

To use relative weights for each observation in the input data set, place the weights in a variable in the data set and specify the name in a WEIGHT statement. This is often done when the variance associated with each observation is different and the values of the WEIGHT variable are proportional to the reciprocals of the variances. If the value of the WEIGHT variable is missing or is less than zero, then a value of zero for the weight is assumed.

The WEIGHT and FREQ statements have a similar effect except that the WEIGHT statement does not alter the degrees of freedom.

---

## Details: STEPDISC Procedure

---

### Missing Values

Observations containing missing values are omitted from the analysis.

---

### Input Data Sets

The input data set can be an ordinary SAS data set or one of several specially structured data sets created by statistical procedures available with SAS/STAT software. For more information about these data sets, see Appendix A, “[Special SAS Data Sets](#).” The BY variable in these data sets becomes the CLASS variable in PROC STEPDISC. These specially structured data sets include the following:

- TYPE=CORR data sets created by PROC CORR by using a BY statement
- TYPE=COV data sets created by PROC PRINCOMP by using both the COV option and a BY statement
- TYPE=CSSCP data sets created by PROC CORR by using the CSSCP option and a BY statement, where the OUT= data set is assigned TYPE=CSSCP with the TYPE= data set option
- TYPE=SSCP data sets created by PROC REG by using both the OUTSSCP= option and a BY statement

When the input data set is TYPE=CORR, TYPE=COV, or TYPE=CSSCP, the STEPDISC procedure reads the number of observations for each class from the observations with `_TYPE_='N'` and the variable means in each class from the observations with `_TYPE_='MEAN'`. The procedure then reads the within-class correlations from the observations with `_TYPE_='CORR'`, the standard deviations from the observations with `_TYPE_='STD'` (data set TYPE=CORR), the within-class covariances from the observations with `_TYPE_='COV'` (data set TYPE=COV), or the within-class corrected sums of squares and crossproducts from the observations with `_TYPE_='CSSCP'` (data set TYPE=CSSCP).

When the data set does not include any observations with `_TYPE_='CORR'` (data set TYPE=CORR), `_TYPE_='COV'` (data set TYPE=COV), or `_TYPE_='CSSCP'` (data set TYPE=CSSCP) for each class, PROC STEPDISC reads the pooled within-class information from the data set. In this case, the STEPDISC procedure reads the pooled within-class correlations from the observations with `_TYPE_='PCORR'`, the pooled within-class standard deviations from the observations with `_TYPE_='PSTD'` (data set TYPE=CORR), the pooled within-class covariances from the observations with `_TYPE_='PCOV'` (data set TYPE=COV), or the pooled within-class corrected SSCP matrix from the observations with `_TYPE_='PSSCP'` (data set TYPE=CSSCP).



When the input data set is TYPE=SSCP, the STEPDISC procedure reads the number of observations for each class from the observations with `_TYPE_='N'`, the sum of weights of observations from the variable INTERCEPT in observations with `_TYPE_='SSCP'` and `_NAME_='INTERCEPT'`, the variable sums from the analysis variables in observations with `_TYPE_='SSCP'` and `_NAME_='INTERCEPT'`, and the uncorrected sums of squares and crossproducts from the analysis variables in observations with `_TYPE_='SSCP'` and `_NAME_=variable-names`.

---

## Computational Resources

In the following discussion, let

- $n$  = number of observations
- $c$  = number of class levels
- $v$  = number of variables in the VAR list
- $l$  = length of the CLASS variable
- $t$  =  $v + c - 1$

## Memory Requirements

The amount of memory in bytes for temporary storage needed to process the data is

$$c(4v^2 + 28v + 3l + 4c + 72) + 16v^2 + 92v + 4t^2 + 20t + 4l$$

Additional temporary storage of 72 bytes at each step is also required to store the results.

## Time Requirements

The following factors determine the time requirements of a stepwise discriminant analysis:

- The time needed for reading the data and computing covariance matrices is proportional to  $nv^2$ . The STEPDISC procedure must also look up each class level in the list. This is faster if the data are sorted by the CLASS variable. The time for looking up class levels is proportional to a value ranging from  $n$  to  $n \ln(c)$ .
- The time needed for stepwise discriminant analysis is proportional to the number of steps required to select the set of variables in the discrimination model. The number of steps required depends on the data set itself and the selection method and criterion used in the procedure. Each forward or backward step takes time proportional to  $(v + c)^2$ .

---

## Displayed Output

The displayed output from PROC STEPDISC includes the class level information table. For each level of the classification variable, the following information is provided: the output data set variable name, frequency sum, weight sum, and the proportion of the total sample.

The optional output from PROC STEPDISC includes the following:

The optional output includes the following:

- Within-class SSCP matrices for each group
- Pooled within-class SSCP matrix
- Between-class SSCP matrix
- Total-sample SSCP matrix
- Within-class covariance matrices for each group
- Pooled within-class covariance matrix
- Between-class covariance matrix, equal to the between-class SSCP matrix divided by  $n(c - 1)/c$ , where  $n$  is the number of observations and  $c$  is the number of classes
- Total-sample covariance matrix
- Within-class correlation coefficients and  $\text{Pr} > |r|$  to test the hypothesis that the within-class population correlation coefficients are zero
- Pooled within-class correlation coefficients and  $\text{Pr} > |r|$  to test the hypothesis that the partial population correlation coefficients are zero
- Between-class correlation coefficients and  $\text{Pr} > |r|$  to test the hypothesis that the between-class population correlation coefficients are zero
- Total-sample correlation coefficients and  $\text{Pr} > |r|$  to test the hypothesis that the total population correlation coefficients are zero
- Simple statistics, including  $N$  (the number of observations), sum, mean, variance, and standard deviation for the total sample and within each class
- Total-sample standardized class means, obtained by subtracting the grand mean from each class mean and dividing by the total-sample standard deviation
- Pooled within-class standardized class means, obtained by subtracting the grand mean from each class mean and dividing by the pooled within-class standard deviation

At each step, the following statistics are displayed:

- for each variable considered for entry or removal: partial R-square, the squared (partial) correlation, the  $F$  statistic, and  $\text{Pr} > F$ , the probability level, from a one-way analysis of covariance
- the minimum tolerance for entering each variable. A variable is entered only if its tolerance and the tolerances for all variables already in the model are greater than the value specified in the SINGULAR= option. The tolerance for the entering variable is  $1 - R^2$  from regressing the entering variable on the other variables already in the model. The tolerance for a variable already in the model is  $1 - R^2$  from regressing that variable on the entering variable and the other variables already in the model. With  $m$  variables already in the model, for each entering variable,  $m + 1$  multiple regressions are performed by using the entering variable and each of the  $m$  variables already in the model as a dependent variable. These  $m + 1$  tolerances are computed for each entering variable, and the minimum tolerance is displayed for each.

The tolerance is computed by using the total-sample correlation matrix. It is customary to compute tolerance by using the pooled within-class correlation matrix (Jennrich 1977), but it is possible for a variable with excellent discriminatory power to have a high total-sample tolerance and a low pooled within-class tolerance. For example, PROC STEPDISC enters a variable that yields perfect discrimination (that is, produces a canonical correlation of one), but a program that uses pooled within-class tolerance does not.

- the variable label, if any
- the name of the variable chosen
- the variables already selected or removed
- Wilks' lambda and the associated  $F$  approximation with degrees of freedom and  $\text{Pr} < F$ , the associated probability level after the selected variable has been entered or removed. Wilks' lambda is the likelihood ratio statistic for testing the hypothesis that the means of the classes on the selected variables are equal in the population (see the section "[Multivariate Tests](#)" on page 92 in Chapter 4, "[Introduction to Regression Procedures](#)."). Lambda is close to zero if any two groups are well separated.
- Pillai's trace and the associated  $F$  approximation with degrees of freedom and  $\text{Pr} > F$ , the associated probability level after the selected variable has been entered or removed. Pillai's trace is a multivariate statistic for testing the hypothesis that the means of the classes on the selected variables are equal in the population (see the section "[Multivariate Tests](#)" on page 92 in Chapter 4, "[Introduction to Regression Procedures](#)").
- Average squared canonical correlation (ASCC). The ASCC is Pillai's trace divided by the number of groups minus 1. The ASCC is close to 1 if all groups are well separated and if all or most directions in the discriminant space show good separation for at least two groups.
- Summary to give statistics associated with the variable chosen at each step. The summary includes the following:
  - Step number
  - Variable entered or removed

- Number in, the number of variables in the model
- Partial R-square
- the  $F$  value for entering or removing the variable
- $\text{Pr} > F$ , the probability level for the  $F$  statistic
- Wilks' lambda
- $\text{Pr} < \text{Lambda}$  based on the  $F$  approximation to Wilks' lambda
- Average squared canonical correlation
- $\text{Pr} > \text{ASCC}$  based on the  $F$  approximation to Pillai's trace
- the variable label, if any

## ODS Table Names

PROC STEPDISC assigns a name to each table it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in Table 89.2 along with the PROC STEPDISC statement options needed to produce the table. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

**Table 89.2** ODS Tables Produced by PROC STEPDISC

| ODS Table Name   | Description                                     | Option          |
|------------------|-------------------------------------------------|-----------------|
| BCorr            | Between-class correlations                      | BCORR           |
| BCov             | Between-class covariances                       | BCOV            |
| BSSCP            | Between-class SSCP matrix                       | BSSCP           |
| Counts           | Number of observations, variables, classes, df  | default         |
| CovDF            | Nonprinting table of df for covariance matrices | any *COV option |
| Levels           | Class level information                         | default         |
| Messages         | Entry/removal messages                          | default         |
| Multivariate     | Multivariate statistics                         | default         |
| NObs             | Number of observations                          | default         |
| PCorr            | Pooled within-class correlations                | PCORR           |
| PCov             | Pooled within-class covariances                 | PCOV            |
| PSSCP            | Pooled within-class SSCP matrix                 | PSSCP           |
| PStdMeans        | Pooled standardized class means                 | STDMEAN         |
| SimpleStatistics | Simple statistics                               | SIMPLE          |
| Steps            | Stepwise selection entry/removal                | default         |
| Summary          | Stepwise selection summary                      | default         |
| TCorr            | Total-sample correlations                       | TCORR           |
| TCov             | Total-sample covariances                        | TCOV            |
| TSSCP            | Total-sample SSCP matrix                        | TSSCP           |
| TStdMeans        | Total standardized class means                  | STDMEAN         |
| Variables        | Variable lists                                  | default         |
| WCorr            | Within-class correlations                       | WCORR           |
| WCov             | Within-class covariances                        | WCOV            |
| WSSCP            | Within-class SSCP matrices                      | WSSCP           |

## Example: STEPDISC Procedure

### Example 89.1: Performing a Stepwise Discriminant Analysis

The iris data published by Fisher (1936) have been widely used for examples in discriminant analysis and cluster analysis. The sepal length, sepal width, petal length, and petal width are measured in millimeters on 50 iris specimens from each of three species: *Iris setosa*, *I. versicolor*, and *I. virginica*. The iris data set is available from the Sashelp library.

A stepwise discriminant analysis is performed by using stepwise selection.

In the PROC STEPDISC statement, the BSSCP and TSSCP options display the between-class SSCP matrix and the total-sample corrected SSCP matrix. By default, the significance level of an  $F$  test from an analysis of covariance is used as the selection criterion. The variable under consideration is the dependent variable, and the variables already chosen act as covariates. The following SAS statements produce [Output 89.1.1](#) through [Output 89.1.8](#):

```

title 'Fisher (1936) Iris Data';

%let _stdvar = ;
proc stepdisc data=sashelp.iris bsscp tsscp;
 class Species;
 var SepalLength SepalWidth PetalLength PetalWidth;
run;

```

**Output 89.1.1** Iris Data: Summary Information

| Fisher (1936) Iris Data                        |               |                              |         |            |
|------------------------------------------------|---------------|------------------------------|---------|------------|
| The STEPDISC Procedure                         |               |                              |         |            |
| The Method for Selecting Variables is STEPWISE |               |                              |         |            |
| Total Sample Size                              | 150           | Variable(s) in the Analysis  | 4       |            |
| Class Levels                                   | 3             | Variable(s) Will Be Included | 0       |            |
|                                                |               | Significance Level to Enter  | 0.15    |            |
|                                                |               | Significance Level to Stay   | 0.15    |            |
| Number of Observations Read                    |               | 150                          |         |            |
| Number of Observations Used                    |               | 150                          |         |            |
| Class Level Information                        |               |                              |         |            |
| Species                                        | Variable Name | Frequency                    | Weight  | Proportion |
| Setosa                                         | Setosa        | 50                           | 50.0000 | 0.333333   |
| Versicolor                                     | Versicolor    | 50                           | 50.0000 | 0.333333   |
| Virginica                                      | Virginica     | 50                           | 50.0000 | 0.333333   |

**Output 89.1.2** Iris Data: Between-Class and Total-Sample SSCP Matrices

| Fisher (1936) Iris Data   |                   |             |             |             |             |
|---------------------------|-------------------|-------------|-------------|-------------|-------------|
| The STEPDISC Procedure    |                   |             |             |             |             |
| Between-Class SSCP Matrix |                   |             |             |             |             |
| Variable                  | Label             | SepalLength | SepalWidth  | PetalLength | PetalWidth  |
| Sepal Length              | Sepal Length (mm) | 6321.21333  | -1995.26667 | 16524.84000 | 7127.93333  |
| SepalWidth                | Sepal Width (mm)  | -1995.26667 | 1134.49333  | -5723.96000 | -2293.26667 |
| Petal Length              | Petal Length (mm) | 16524.84000 | -5723.96000 | 43710.28000 | 18677.40000 |
| PetalWidth                | Petal Width (mm)  | 7127.93333  | -2293.26667 | 18677.40000 | 8041.33333  |
| Total-Sample SSCP Matrix  |                   |             |             |             |             |
| Variable                  | Label             | SepalLength | SepalWidth  | PetalLength | PetalWidth  |
| Sepal Length              | Sepal Length (mm) | 10216.83333 | -632.26667  | 18987.30000 | 7692.43333  |
| SepalWidth                | Sepal Width (mm)  | -632.26667  | 2830.69333  | -4911.88000 | -1812.42667 |
| Petal Length              | Petal Length (mm) | 18987.30000 | -4911.88000 | 46432.54000 | 19304.58000 |
| PetalWidth                | Petal Width (mm)  | 7692.43333  | -1812.42667 | 19304.58000 | 8656.99333  |

In step 1, the tolerance is 1.0 for each variable under consideration because no variables have yet entered the model. The variable `PetalLength` is selected because its  $F$  statistic, 1180.161, is the largest among all variables.

### Output 89.1.3 Iris Data: Stepwise Selection Step 1

| Fisher (1936) Iris Data                            |                   |          |         |        |           |
|----------------------------------------------------|-------------------|----------|---------|--------|-----------|
| The STEPDISC Procedure                             |                   |          |         |        |           |
| Stepwise Selection: Step 1                         |                   |          |         |        |           |
| Statistics for Entry, DF = 2, 147                  |                   |          |         |        |           |
| Variable                                           | Label             | R-Square | F Value | Pr > F | Tolerance |
| <code>SepalLength</code>                           | Sepal Length (mm) | 0.6187   | 119.26  | <.0001 | 1.0000    |
| <code>SepalWidth</code>                            | Sepal Width (mm)  | 0.4008   | 49.16   | <.0001 | 1.0000    |
| <code>PetalLength</code>                           | Petal Length (mm) | 0.9414   | 1180.16 | <.0001 | 1.0000    |
| <code>PetalWidth</code>                            | Petal Width (mm)  | 0.9289   | 960.01  | <.0001 | 1.0000    |
| Variable <code>PetalLength</code> will be entered. |                   |          |         |        |           |
| Variable(s) That Have Been Entered                 |                   |          |         |        |           |
| <code>PetalLength</code>                           |                   |          |         |        |           |
| Multivariate Statistics                            |                   |          |         |        |           |
| Statistic                                          | Value             | F Value  | Num DF  | Den DF | Pr > F    |
| Wilks' Lambda                                      | 0.058628          | 1180.16  | 2       | 147    | <.0001    |
| Pillai's Trace                                     | 0.941372          | 1180.16  | 2       | 147    | <.0001    |
| Average Squared Canonical Correlation              | 0.470686          |          |         |        |           |

In step 2, with the variable `PetalLength` already in the model, `PetalLength` is tested for removal before a new variable is selected for entry. Since `PetalLength` meets the criterion to stay, it is used as a covariate in the analysis of covariance for variable selection. The variable `SepalWidth` is selected because its  $F$  statistic, 43.035, is the largest among all variables not in the model and because its associated tolerance, 0.8164, meets the criterion to enter. The process is repeated in steps 3 and 4. The variable `PetalWidth` is entered in step 3, and the variable `SepalLength` is entered in step 4.

**Output 89.1.4** Iris Data: Stepwise Selection Step 2

```

Fisher (1936) Iris Data

The STEPDISC Procedure
Stepwise Selection: Step 2

Statistics for Removal, DF = 2, 147

Variable Label R-Square F Value Pr > F

PetalLength Petal Length (mm) 0.9414 1180.16 <.0001

No variables can be removed.

Statistics for Entry, DF = 2, 146

Variable Label Partial
R-Square F Value Pr > F Tolerance

SepalLength Sepal Length (mm) 0.3198 34.32 <.0001 0.2400
SepalWidth Sepal Width (mm) 0.3709 43.04 <.0001 0.8164
PetalWidth Petal Width (mm) 0.2533 24.77 <.0001 0.0729

Variable SepalWidth will be entered.

Variable(s) That Have Been Entered

SepalWidth PetalLength

Multivariate Statistics

Statistic Value F Value Num DF Den DF Pr > F

Wilks' Lambda 0.036884 307.10 4 292 <.0001
Pillai's Trace 1.119908 93.53 4 294 <.0001
Average Squared Canonical
Correlation 0.559954

```



**Output 89.1.5** Iris Data: Stepwise Selection Step 3

| Fisher (1936) Iris Data                  |                   |                     |         |        |           |        |
|------------------------------------------|-------------------|---------------------|---------|--------|-----------|--------|
| The STEPDISC Procedure                   |                   |                     |         |        |           |        |
| Stepwise Selection: Step 3               |                   |                     |         |        |           |        |
| Statistics for Removal, DF = 2, 146      |                   |                     |         |        |           |        |
| Variable                                 | Label             | Partial<br>R-Square | F Value | Pr > F |           |        |
| SepalWidth                               | Sepal Width (mm)  | 0.3709              | 43.04   | <.0001 |           |        |
| PetalLength                              | Petal Length (mm) | 0.9384              | 1112.95 | <.0001 |           |        |
| No variables can be removed.             |                   |                     |         |        |           |        |
| Statistics for Entry, DF = 2, 145        |                   |                     |         |        |           |        |
| Variable                                 | Label             | Partial<br>R-Square | F Value | Pr > F | Tolerance |        |
| SepalLength                              | Sepal Length (mm) | 0.1447              | 12.27   | <.0001 | 0.1323    |        |
| PetalWidth                               | Petal Width (mm)  | 0.3229              | 34.57   | <.0001 | 0.0662    |        |
| Variable PetalWidth will be entered.     |                   |                     |         |        |           |        |
| Variable(s) That Have Been Entered       |                   |                     |         |        |           |        |
| SepalWidth PetalLength PetalWidth        |                   |                     |         |        |           |        |
| Multivariate Statistics                  |                   |                     |         |        |           |        |
| Statistic                                |                   | Value               | F Value | Num DF | Den DF    | Pr > F |
| Wilks' Lambda                            |                   | 0.024976            | 257.50  | 6      | 290       | <.0001 |
| Pillai's Trace                           |                   | 1.189914            | 71.49   | 6      | 292       | <.0001 |
| Average Squared Canonical<br>Correlation |                   | 0.594957            |         |        |           |        |

**Output 89.1.6** Iris Data: Stepwise Selection Step 4

```

Fisher (1936) Iris Data

The STEPDISC Procedure
Stepwise Selection: Step 4

Statistics for Removal, DF = 2, 145

Variable Label Partial
 Label R-Square F Value Pr > F

SepalWidth Sepal Width (mm) 0.4295 54.58 <.0001
PetalLength Petal Length (mm) 0.3482 38.72 <.0001
PetalWidth Petal Width (mm) 0.3229 34.57 <.0001

No variables can be removed.

Statistics for Entry, DF = 2, 144

Variable Label Partial
 Label R-Square F Value Pr > F Tolerance

SepalLength Sepal Length (mm) 0.0615 4.72 0.0103 0.0320

Variable SepalLength will be entered.

All variables have been entered.

Multivariate Statistics

Statistic Value F Value Num DF Den DF Pr > F

Wilks' Lambda 0.023439 199.15 8 288 <.0001
Pillai's Trace 1.191899 53.47 8 290 <.0001
Average Squared Canonical
Correlation 0.595949

```

Since no more variables can be added to or removed from the model, the procedure stops at step 5 and displays a summary of the selection process.

**Output 89.1.7** Iris Data: Stepwise Selection Step 5

| Fisher (1936) Iris Data             |                   |                     |         |        |
|-------------------------------------|-------------------|---------------------|---------|--------|
| The STEPDISC Procedure              |                   |                     |         |        |
| Stepwise Selection: Step 5          |                   |                     |         |        |
| Statistics for Removal, DF = 2, 144 |                   |                     |         |        |
| Variable                            | Label             | Partial<br>R-Square | F Value | Pr > F |
| SepalLength                         | Sepal Length (mm) | 0.0615              | 4.72    | 0.0103 |
| SepalWidth                          | Sepal Width (mm)  | 0.2335              | 21.94   | <.0001 |
| PetalLength                         | Petal Length (mm) | 0.3308              | 35.59   | <.0001 |
| PetalWidth                          | Petal Width (mm)  | 0.2570              | 24.90   | <.0001 |

No variables can be removed.

**Output 89.1.8** Iris Data: Stepwise Selection Summary

| No further steps are possible.        |                      |             |                   |                     |            |              |                  |                |  |
|---------------------------------------|----------------------|-------------|-------------------|---------------------|------------|--------------|------------------|----------------|--|
| Fisher (1936) Iris Data               |                      |             |                   |                     |            |              |                  |                |  |
| The STEPDISC Procedure                |                      |             |                   |                     |            |              |                  |                |  |
| Stepwise Selection Summary            |                      |             |                   |                     |            |              |                  |                |  |
| Step                                  | Number<br>In Entered | Removed     | Label             | Partial<br>R-Square | F Value    | Pr > F       | Wilks'<br>Lambda | Pr <<br>Lambda |  |
| 1                                     | 1                    | PetalLength | Petal Length (mm) | 0.9414              | 1180.16    | <.0001       | 0.05862828       | <.0001         |  |
| 2                                     | 2                    | SepalWidth  | Sepal Width (mm)  | 0.3709              | 43.04      | <.0001       | 0.03688411       | <.0001         |  |
| 3                                     | 3                    | PetalWidth  | Petal Width (mm)  | 0.3229              | 34.57      | <.0001       | 0.02497554       | <.0001         |  |
| 4                                     | 4                    | SepalLength | Sepal Length (mm) | 0.0615              | 4.72       | 0.0103       | 0.02343863       | <.0001         |  |
| Average Squared Canonical Correlation |                      |             |                   |                     |            |              |                  |                |  |
| Step                                  | Number<br>In Entered | Removed     |                   |                     |            | Pr ><br>ASCC |                  |                |  |
|                                       | 1                    | 1           | PetalLength       |                     | 0.47068586 | <.0001       |                  |                |  |
|                                       | 2                    | 2           | SepalWidth        |                     | 0.55995394 | <.0001       |                  |                |  |
|                                       | 3                    | 3           | PetalWidth        |                     | 0.59495691 | <.0001       |                  |                |  |
|                                       | 4                    | 4           | SepalLength       |                     | 0.59594941 | <.0001       |                  |                |  |

PROC STEPDISC automatically creates a list of the selected variables and stores it in a macro variable. You can submit the following statement to see the list of selected variables:

```
* print the macro variable list;
%put &_stdvar;
```

The macro variable `_StdVar` contains the following variable list:

```
SepalLength SepalWidth PetalLength PetalWidth
```

You could use this macro variable if you want to analyze these variables in subsequent steps as follows:

```
proc discrim data=sashelp.iris;
 class Species;
 var &_stdvar;
run;
```

The results of this step are not shown.

---

## References

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# Chapter 90

## The SURVEYFREQ Procedure

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---

## Overview: SURVEYFREQ Procedure

The SURVEYFREQ procedure produces one-way to  $n$ -way frequency and crosstabulation tables from sample survey data. These tables include estimates of population totals, population proportions, and their standard errors. Confidence limits, coefficients of variation, and design effects are also available. The procedure provides a variety of options to customize the table display.

For one-way frequency tables, PROC SURVEYFREQ provides Rao-Scott chi-square goodness-of-fit tests, which are adjusted for the sample design. You can test a null hypothesis of equal proportions for a one-way frequency table, or you can input custom null hypothesis proportions for the test. For two-way tables, PROC SURVEYFREQ provides design-adjusted tests of independence, or no association, between the row and column variables. These tests include the Rao-Scott chi-square test, the Rao-Scott likelihood ratio test, the Wald chi-square test, and the Wald log-linear chi-square test. For  $2 \times 2$  tables, PROC SURVEYFREQ computes estimates and confidence limits for risks (row proportions), the risk difference, the odds ratio, and relative risks.

PROC SURVEYFREQ computes variance estimates based on the sample design used to obtain the survey data. The design can be a complex multistage survey design with stratification, clustering, and unequal weighting. PROC SURVEYFREQ provides a choice of variance estimation methods, which include Taylor series linearization, balanced repeated replication (BRR), and the jackknife.

PROC SURVEYFREQ uses ODS Graphics to create graphs as part of its output. For general information about ODS Graphics, see Chapter 21, “[Statistical Graphics Using ODS](#).” For specific information about the statistical graphics available with the SURVEYFREQ procedure, see the `PLOTS=` option in the TABLES statement and the section “[ODS Graphics](#)” on page 7669.

## Getting Started: SURVEYFREQ Procedure

The following example shows how you can use PROC SURVEYFREQ to analyze sample survey data. The example uses data from a customer satisfaction survey for a student information system (SIS), which is a software product that provides modules for student registration, class scheduling, attendance, grade reporting, and other functions.

The software company conducted a survey of school personnel who use the SIS. A probability sample of SIS users was selected from the study population, which included SIS users at middle schools and high schools

in the three-state area of Georgia, South Carolina, and North Carolina. The sample design for this survey was a two-stage stratified design. A first-stage sample of schools was selected from the list of schools in the three-state area that use the SIS. The list of schools (the first-stage sampling frame) was stratified by state and by customer status (whether the school was a new user of the system or a renewal user). Within the first-stage strata, schools were selected with probability proportional to size and with replacement, where the size measure was school enrollment. From each sample school, five staff members were randomly selected to complete the SIS satisfaction questionnaire. These staff members included three teachers and two administrators or guidance department members.

The SAS data set `SIS_Survey` contains the survey results, as well as the sample design information needed to analyze the data. This data set includes an observation for each school staff member responding to the survey. The variable `Response` contains the staff member's response about overall satisfaction with the system.

The variable `State` contains the school's state, and the variable `NewUser` contains the school's customer status ('New Customer' or 'Renewal Customer'). These two variables determine the first-stage strata from which schools were selected. The variable `School` contains the school identification code and identifies the first-stage sampling units (clusters). The variable `SamplingWeight` contains the overall sampling weight for each respondent. Overall sampling weights were computed from the selection probabilities at each stage of sampling and were adjusted for nonresponse.

Other variables in the data set `SIS_Survey` include `SchoolType` and `Department`. The variable `SchoolType` identifies the school as a high school or a middle school. The variable `Department` identifies the staff member as a teacher, or an administrator or guidance department member.

The following PROC SURVEYFREQ statements request a one-way frequency table for the variable `Response`:

```

title 'Student Information System Survey';
proc surveyfreq data=SIS_Survey;
 tables Response;
 strata State NewUser;
 cluster School;
 weight SamplingWeight;
run;

```

The PROC SURVEYFREQ statement invokes the procedure and identifies the input data set to be analyzed. The TABLES statement requests a one-way frequency table for the variable `Response`. The table request syntax for PROC SURVEYFREQ is very similar to the table request syntax for PROC FREQ. This example shows a request for a single one-way table, but you can also request two-way tables and multiway tables. As in PROC FREQ, you can request more than one table in the same TABLES statement, and you can use multiple TABLES statements in the same invocation of the procedure.

The STRATA, CLUSTER, and WEIGHT statements provide sample design information for the procedure, so that the analysis is done according to the sample design used for the survey, and the estimates apply to the study population. The STRATA statement names the variables `State` and `NewUser`, which identify the first-stage strata. Note that the design for this example also includes stratification at the second stage of selection (by type of school personnel), but you specify only the first-stage strata for PROC SURVEYFREQ. The CLUSTER statement names the variable `School`, which identifies the clusters (primary sampling units). The WEIGHT statement names the sampling weight variable.



Figure 90.1 and Figure 90.2 display the output produced by PROC SURVEYFREQ, which includes the “Data Summary” table and the one-way table, “Table of Response.” The “Data Summary” table is produced by default unless you specify the NOSUMMARY option. This table shows there are 6 strata, 370 clusters or schools, and 1850 observations (respondents) in the SIS\_Survey data set. The sum of the sampling weights is approximately 39,000, which estimates the total number of school personnel in the study area that use the SIS.

**Figure 90.1** SIS\_Survey Data Summary

| Student Information System Survey |            |
|-----------------------------------|------------|
| The SURVEYFREQ Procedure          |            |
| Data Summary                      |            |
| Number of Strata                  | 6          |
| Number of Clusters                | 370        |
| Number of Observations            | 1850       |
| Sum of Weights                    | 38899.6482 |

Figure 90.2 displays the one-way table of Response, which provides estimates of the population total (weighted frequency) and the population percentage for each category (level) of the variable Response. The response level ‘Very Unsatisfied’ has a frequency of 304, which means that 304 sample respondents fall into this category. It is estimated that 17.17% of all school personnel in the study population fall into this category, and the standard error of this estimate is 1.29%. Note that the estimates apply to the population of all SIS users in the study area, as opposed to describing only the sample of 1850 respondents. The estimate of the total number of school personnel that are ‘Very Unsatisfied’ is 6,678, with a standard deviation of 502. The standard errors computed by PROC SURVEYFREQ are based on the multistage stratified design of the survey. This differs from some of the traditional analysis procedures, which assume the design is simple random sampling from an infinite population.

**Figure 90.2** One-Way Table of Response

| Table of Response |           |                    |                     |         |                    |
|-------------------|-----------|--------------------|---------------------|---------|--------------------|
| Response          | Frequency | Weighted Frequency | Std Dev of Wgt Freq | Percent | Std Err of Percent |
| Very Unsatisfied  | 304       | 6678               | 501.61039           | 17.1676 | 1.2872             |
| Unsatisfied       | 326       | 6907               | 495.94101           | 17.7564 | 1.2712             |
| Neutral           | 581       | 12291              | 617.20147           | 31.5965 | 1.5795             |
| Satisfied         | 455       | 9309               | 572.27868           | 23.9311 | 1.4761             |
| Very Satisfied    | 184       | 3714               | 370.66577           | 9.5483  | 0.9523             |
| Total             | 1850      | 38900              | 129.85268           | 100.000 |                    |

The following PROC SURVEYFREQ statements request confidence limits for the percentages, a chi-square goodness-of-fit test, and a weighted frequency plot for the one-way table of Response. The ODS GRAPHICS ON statement enables ODS Graphics.

```

title 'Student Information System Survey';
ods graphics on;
proc surveyfreq data=SIS_Survey nosummary;
 tables Response / clwt nopct chisq
 plots=WtFreqPlot;
 strata State NewUser;
 cluster School;
 weight SamplingWeight;
run;
ods graphics off;

```

The NOSUMMARY option in the PROC SURVEYFREQ statement suppresses the “Data Summary” table. In the TABLES statement, the CLWT option requests confidence limits for the weighted frequencies (totals). The NOPCT option suppresses display of the weighted frequencies and their standard deviations. The CHISQ option requests a Rao-Scott chi-square goodness-of-fit test, and the PLOTS= option requests a weighted frequency plot. ODS Graphics must be enabled before producing plots.

Figure 90.3 shows the one-way table of Response, which includes confidence limits for the weighted frequencies. The 95% confidence limits for the total number of users that are ‘Very Unsatisfied’ are 5692 and 7665. To change the  $\alpha$  level of the confidence limits, which equals 5% by default, you can use the ALPHA= option. Like the other estimates and standard errors produced by PROC SURVEYFREQ, these confidence limit computations take into account the complex survey design and apply to the entire study population.

**Figure 90.3** Confidence Limits for Response Totals

| Student Information System Survey |           |                       |                        |                                       |       |
|-----------------------------------|-----------|-----------------------|------------------------|---------------------------------------|-------|
| The SURVEYFREQ Procedure          |           |                       |                        |                                       |       |
| Table of Response                 |           |                       |                        |                                       |       |
| Response                          | Frequency | Weighted<br>Frequency | Std Dev of<br>Wgt Freq | 95% Confidence Limits<br>for Wgt Freq |       |
| Very Unsatisfied                  | 304       | 6678                  | 501.61039              | 5692                                  | 7665  |
| Unsatisfied                       | 326       | 6907                  | 495.94101              | 5932                                  | 7882  |
| Neutral                           | 581       | 12291                 | 617.20147              | 11077                                 | 13505 |
| Satisfied                         | 455       | 9309                  | 572.27868              | 8184                                  | 10435 |
| Very Satisfied                    | 184       | 3714                  | 370.66577              | 2985                                  | 4443  |
| Total                             | 1850      | 38900                 | 129.85268              | 38644                                 | 39155 |

Figure 90.4 displays the weighted frequency plot of Response. The plot displays weighted frequencies (totals) together with their confidence limits in the form of a vertical bar chart. You can use the PLOTS= option to request a dot plot instead of a bar chart or to plot percentages instead of weighted frequencies.

**Figure 90.4** Bar Chart of Response Totals

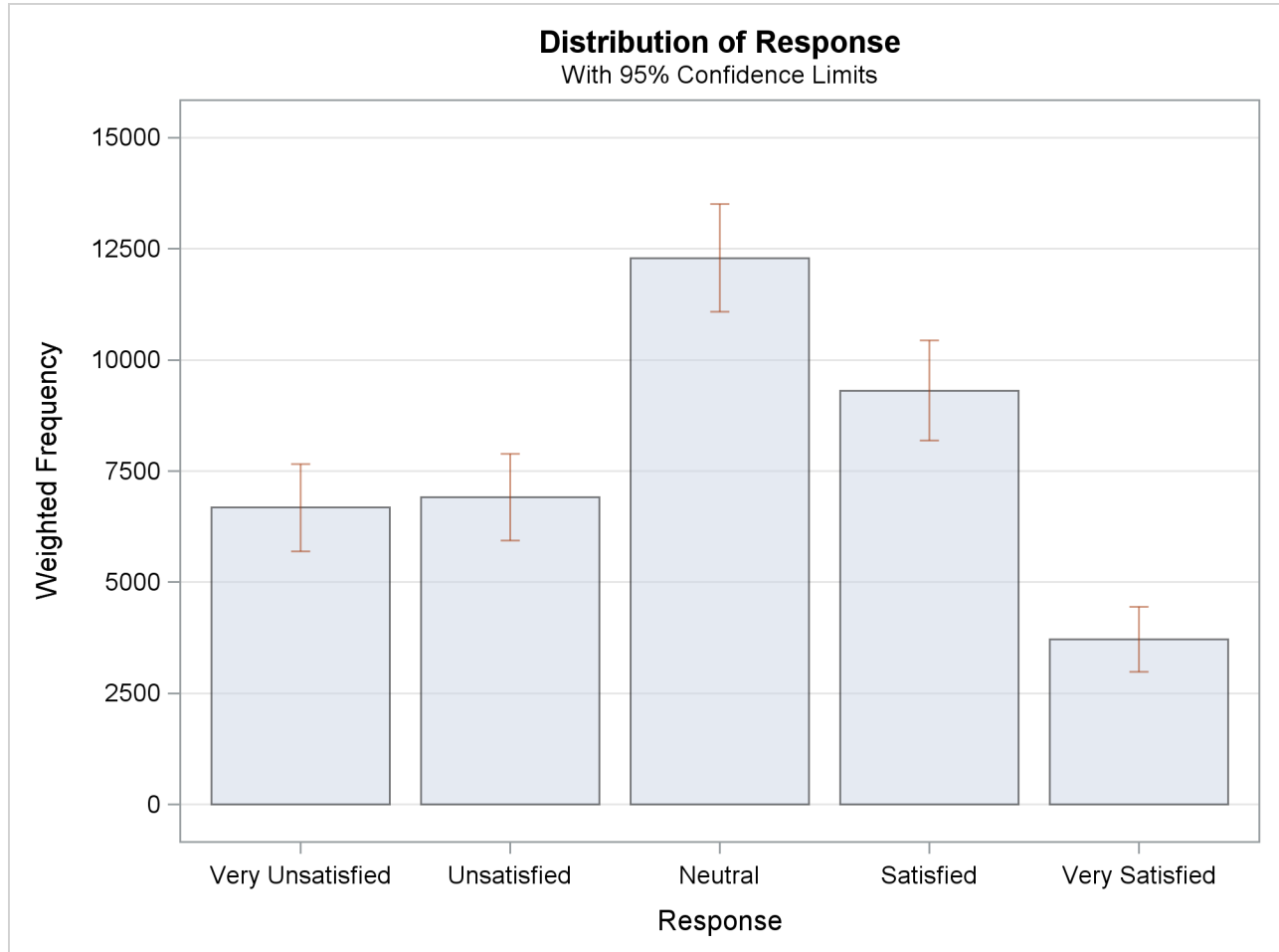


Figure 90.5 shows the chi-square goodness-of-fit results for the table of Response. The null hypothesis for this test is equal proportions for the levels of the one-way table. (To test a null hypothesis of specified proportions instead of equal proportions, you can use the TESTP= option to specify null hypothesis proportions.)

The chi-square test provided by the CHISQ option is the Rao-Scott design-adjusted chi-square test, which takes the sample design into account and provides inferences for the study population. To produce the Rao-Scott chi-square statistic, PROC SURVEYFREQ first computes the usual Pearson chi-square statistic based on the weighted frequencies, and then adjusts this value with a design correction. An  $F$  approximation is also provided. For the table of Response, the  $F$  value is 30.0972 with a  $p$ -value of  $<0.0001$ , which indicates rejection of the null hypothesis of equal proportions for all response levels.

**Figure 90.5** Chi-Square Goodness-of-Fit Test for Response

| Rao-Scott Chi-Square Test |          |
|---------------------------|----------|
| Pearson Chi-Square        | 251.8105 |
| Design Correction         | 2.0916   |
| Rao-Scott Chi-Square      | 120.3889 |
| DF                        | 4        |
| Pr > ChiSq                | <.0001   |
| F Value                   | 30.0972  |
| Num DF                    | 4        |
| Den DF                    | 1456     |
| Pr > F                    | <.0001   |
| Sample Size = 1850        |          |

Continuing to analyze the SIS\_Survey data, the following PROC SURVEYFREQ statements request a two-way table of SchoolType by Response:

```

title 'Student Information System Survey';
ods graphics on;
proc surveyfreq data=SIS_Survey nosummary;
 tables SchoolType * Response /
 plots=wtfreqplot (type=dot scale=percent groupby=row);
 strata State NewUser;
 cluster School;
 weight SamplingWeight;
run;
ods graphics off;

```

The STRATA, CLUSTER, and WEIGHT statements do not change from the one-way table analysis, because the sample design and the input data set are the same. These SURVEYFREQ statements request a different table but specify the same sample design information.

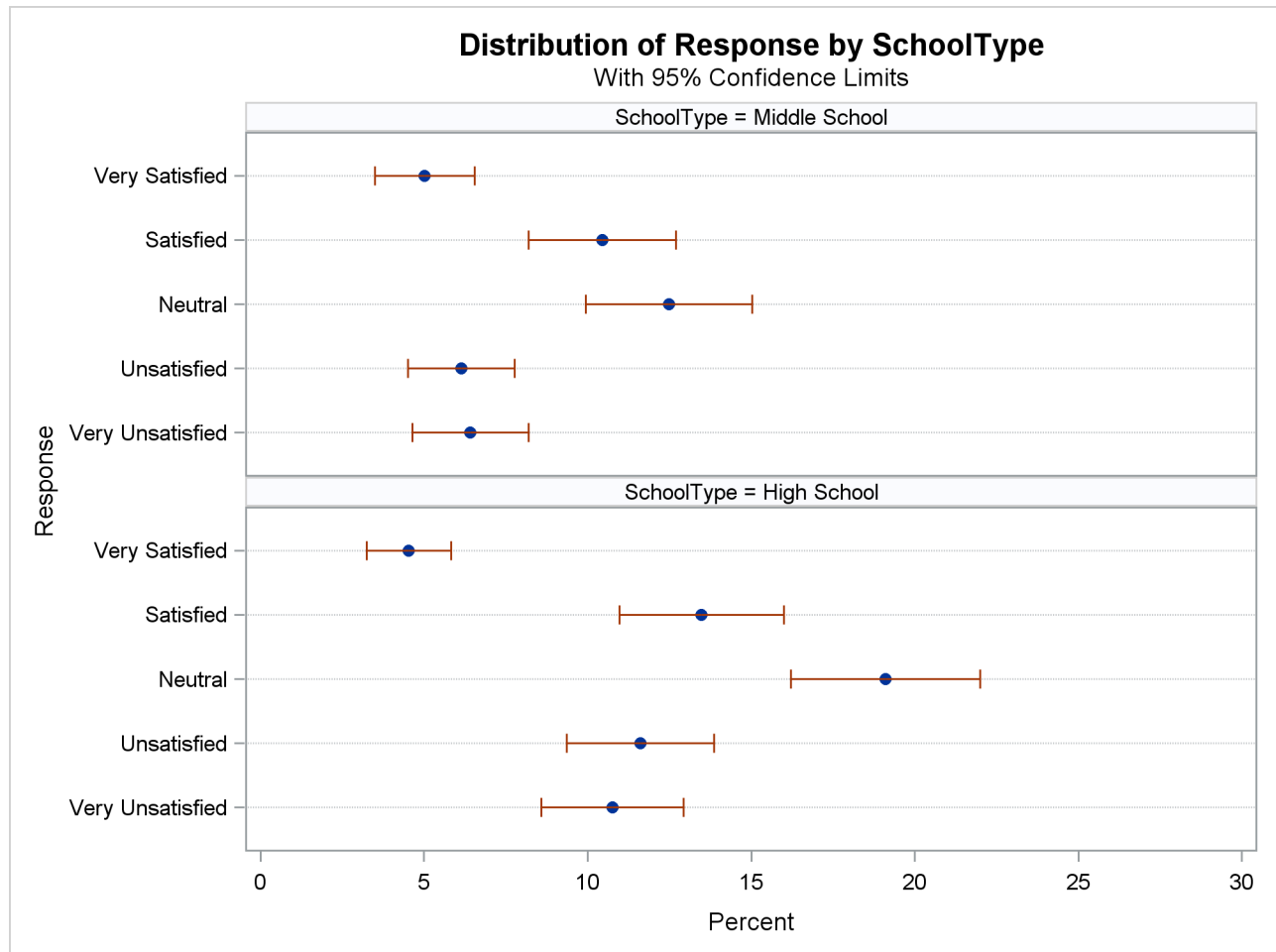
The ODS GRAPHICS ON statement enables ODS Graphics. The PLOTS= option in the TABLES statement requests a plot of SchoolType by Response, and the TYPE=DOT *plot-option* specifies a dot plot instead of the default bar chart. The SCALE=PERCENT *plot-option* requests a plot of percentages instead of totals. The GROUPBY=ROW *plot-option* groups the graph cells by the row variable (SchoolType).

Figure 90.6 shows the two-way table produced for SchoolType by Response. The first variable named in the two-way table request, SchoolType, is referred to as the *row variable*, and the second variable, Response, is referred to as the *column variable*. Two-way tables display all column variable levels for each row variable level. This two-way table lists all levels of the column variable Response for each level of the row variable SchoolType, 'Middle School' and 'High School'. Also SchoolType = 'Total' shows the distribution of Response overall for both types of schools. And Response = 'Total' provides totals over all levels of response, for each type of school and overall. To suppress these totals, you can specify the NOTOTAL option.

**Figure 90.6** Two-Way Table of SchoolType by Response

| Student Information System Survey |                  |           |                       |                        |           |                       |
|-----------------------------------|------------------|-----------|-----------------------|------------------------|-----------|-----------------------|
| The SURVEYFREQ Procedure          |                  |           |                       |                        |           |                       |
| Table of SchoolType by Response   |                  |           |                       |                        |           |                       |
| SchoolType                        | Response         | Frequency | Weighted<br>Frequency | Std Dev of<br>Wgt Freq | Percent   | Std Err of<br>Percent |
| Middle School                     | Very Unsatisfied | 116       | 2496                  | 351.43834              | 6.4155    | 0.9030                |
|                                   | Unsatisfied      | 109       | 2389                  | 321.97957              | 6.1427    | 0.8283                |
|                                   | Neutral          | 234       | 4856                  | 504.20553              | 12.4847   | 1.2953                |
|                                   | Satisfied        | 197       | 4064                  | 443.71188              | 10.4467   | 1.1417                |
|                                   | Very Satisfied   | 94        | 1952                  | 302.17144              | 5.0193    | 0.7758                |
|                                   | Total            |           | 750                   | 15758                  | 1000      | 40.5089               |
| High School                       | Very Unsatisfied | 188       | 4183                  | 431.30589              | 10.7521   | 1.1076                |
|                                   | Unsatisfied      | 217       | 4518                  | 446.31768              | 11.6137   | 1.1439                |
|                                   | Neutral          | 347       | 7434                  | 574.17175              | 19.1119   | 1.4726                |
|                                   | Satisfied        | 258       | 5245                  | 498.03221              | 13.4845   | 1.2823                |
|                                   | Very Satisfied   | 90        | 1762                  | 255.67158              | 4.5290    | 0.6579                |
|                                   | Total            |           | 1100                  | 23142                  | 1003      | 59.4911               |
| Total                             | Very Unsatisfied | 304       | 6678                  | 501.61039              | 17.1676   | 1.2872                |
|                                   | Unsatisfied      | 326       | 6907                  | 495.94101              | 17.7564   | 1.2712                |
|                                   | Neutral          | 581       | 12291                 | 617.20147              | 31.5965   | 1.5795                |
|                                   | Satisfied        | 455       | 9309                  | 572.27868              | 23.9311   | 1.4761                |
|                                   | Very Satisfied   | 184       | 3714                  | 370.66577              | 9.5483    | 0.9523                |
|                                   | Total            |           | 1850                  | 38900                  | 129.85268 | 100.000               |

Figure 90.7 displays the weighted frequency dot plot that PROC SURVEYFREQ produces for the table of SchoolType and Response. The GROUPBY=ROW *plot-option* groups the graph cells by the row variable (SchoolType). If you do not specify GROUPBY=ROW, the procedure groups the graph cells by the column variable by default. You can plot percentages instead of weighted frequencies by specifying the SCALE=PERCENT *plot-option*. You can use other *plot-options* to change the orientation of the plot or to request a different two-way layout.

**Figure 90.7** Dot Plot of Percentages for SchoolType by Response

By default, without any other TABLES statement options, a two-way table displays the frequency, the weighted frequency and its standard deviation, and the percentage and its standard error for each table cell (combination of row and column variable levels). But there are several options available to customize your table display by adding more information or by suppressing some of the default information.

The following PROC SURVEYFREQ statements request a two-way table of SchoolType by Response that displays row percentages, and also request a chi-square test of association between the two variables:

```

title 'Student Information System Survey';
proc surveyfreq data=SIS_Survey nosummary;
 tables SchoolType * Response / row nowt chisq;
 strata State NewUser;
 cluster School;
 weight SamplingWeight;
run;

```

The ROW option in the TABLES statement requests row percentages, which give the distribution of Response within each level of the row variable SchoolType. The NOWT option suppresses display of the weighted frequencies and their standard deviations. The CHISQ option requests a Rao-Scott chi-square test of association between SchoolType and Response.

Figure 90.8 displays the two-way table of SchoolType by Response. For middle schools, it is estimated that 25.79% of school personnel are satisfied with the student information system and 12.39% are very satisfied. For high schools, these estimates are 22.67% and 7.61%, respectively.

Figure 90.9 displays the chi-square test results. The Rao-Scott chi-square statistic equals 9.04, and the corresponding  $F$  value is 2.26 with a  $p$ -value of 0.0605. This indicates an association between school type (middle school or high school) and satisfaction with the student information system at the 10% significance level.

**Figure 90.8** Two-Way Table with Row Percentages

| Student Information System Survey |                  |           |         |                    |             |                        |
|-----------------------------------|------------------|-----------|---------|--------------------|-------------|------------------------|
| The SURVEYFREQ Procedure          |                  |           |         |                    |             |                        |
| Table of SchoolType by Response   |                  |           |         |                    |             |                        |
| SchoolType                        | Response         | Frequency | Percent | Std Err of Percent | Row Percent | Std Err of Row Percent |
| Middle School                     | Very Unsatisfied | 116       | 6.4155  | 0.9030             | 15.8373     | 1.9920                 |
|                                   | Unsatisfied      | 109       | 6.1427  | 0.8283             | 15.1638     | 1.8140                 |
|                                   | Neutral          | 234       | 12.4847 | 1.2953             | 30.8196     | 2.5173                 |
|                                   | Satisfied        | 197       | 10.4467 | 1.1417             | 25.7886     | 2.2947                 |
|                                   | Very Satisfied   | 94        | 5.0193  | 0.7758             | 12.3907     | 1.7449                 |
|                                   | Total            |           | 750     | 40.5089            | 2.5691      | 100.000                |
| High School                       | Very Unsatisfied | 188       | 10.7521 | 1.1076             | 18.0735     | 1.6881                 |
|                                   | Unsatisfied      | 217       | 11.6137 | 1.1439             | 19.5218     | 1.7280                 |
|                                   | Neutral          | 347       | 19.1119 | 1.4726             | 32.1255     | 2.0490                 |
|                                   | Satisfied        | 258       | 13.4845 | 1.2823             | 22.6663     | 1.9240                 |
|                                   | Very Satisfied   | 90        | 4.5290  | 0.6579             | 7.6128      | 1.0557                 |
|                                   | Total            |           | 1100    | 59.4911            | 2.5691      | 100.000                |
| Total                             | Very Unsatisfied | 304       | 17.1676 | 1.2872             |             |                        |
|                                   | Unsatisfied      | 326       | 17.7564 | 1.2712             |             |                        |
|                                   | Neutral          | 581       | 31.5965 | 1.5795             |             |                        |
|                                   | Satisfied        | 455       | 23.9311 | 1.4761             |             |                        |
|                                   | Very Satisfied   | 184       | 9.5483  | 0.9523             |             |                        |
|                                   | Total            |           | 1850    | 100.000            |             |                        |

Figure 90.9 Chi-Square Test of No Association

| Rao-Scott Chi-Square Test |         |
|---------------------------|---------|
| Pearson Chi-Square        | 18.7829 |
| Design Correction         | 2.0766  |
| Rao-Scott Chi-Square      | 9.0450  |
| DF                        | 4       |
| Pr > ChiSq                | 0.0600  |
| F Value                   | 2.2613  |
| Num DF                    | 4       |
| Den DF                    | 1456    |
| Pr > F                    | 0.0605  |
| Sample Size = 1850        |         |

## Syntax: SURVEYFREQ Procedure

The following statements are available in the SURVEYFREQ procedure:

```

PROC SURVEYFREQ < options > ;
 BY variables ;
 CLUSTER variables ;
 REPWEIGHTS variables < / options > ;
 STRATA variables < / option > ;
 TABLES requests < / options > ;
 WEIGHT variable ;

```

The PROC SURVEYFREQ statement invokes the procedure, identifies the data set to be analyzed, and specifies the variance estimation method to use. The PROC SURVEYFREQ statement is required.

The TABLES statement specifies frequency or crosstabulation tables and requests tests and statistics for those tables. The STRATA statement lists the variables that form the strata in a stratified sample design. The CLUSTER statement specifies cluster identification variables in a clustered sample design. The WEIGHT statement names the sampling weight variable. The REPWEIGHTS statement names replicate weight variables for BRR or jackknife variance estimation. The BY statement requests completely separate analyses of groups defined by the BY variables.

All statements can appear multiple times except the PROC SURVEYFREQ statement and the WEIGHT statement, which can appear only once.

The rest of this section gives detailed syntax information for the BY, CLUSTER, REPWEIGHTS, STRATA, TABLES, and WEIGHT statements in alphabetical order after the description of the PROC SURVEYFREQ statement.



## PROC SURVEYFREQ Statement

**PROC SURVEYFREQ** < options > ;

The PROC SURVEYFREQ statement invokes the SURVEYFREQ procedure. It also identifies the data set to be analyzed, specifies the variance estimation method to use, and provides sample design information. The **DATA=** option names the input data set to be analyzed. The **VARMETHOD=** option specifies the variance estimation method, which is the Taylor series method by default. For Taylor series variance estimation, you can include a finite population correction factor in the analysis by providing either the sampling rate or population total with the **RATE=** or **TOTAL=** option. If your design is stratified with different sampling rates or totals for different strata, you can input these stratum rates or totals in a SAS data set that contains the stratification variables.

Table 90.1 summarizes the options available in the PROC SURVEYFREQ statement.

**Table 90.1** PROC SURVEYFREQ Statement Options

| Option            | Description                                                      |
|-------------------|------------------------------------------------------------------|
| <b>DATA=</b>      | Names the input SAS data set                                     |
| <b>MISSING</b>    | Treats missing values as a valid level                           |
| <b>NOMCAR</b>     | Treats missing values as <i>not missing completely at random</i> |
| <b>NOSUMMARY</b>  | Suppresses the display of the “Data Summary” table               |
| <b>ORDER=</b>     | Specifies the order of variable levels                           |
| <b>PAGE</b>       | Displays only one table per page                                 |
| <b>RATE=</b>      | Specifies the first-stage sampling rate                          |
| <b>TOTAL=</b>     | Specifies the total number of primary sampling units             |
| <b>VARHEADER=</b> | Specifies the variable identification to display                 |
| <b>VARMETHOD=</b> | Specifies the variance estimation method                         |

You can specify the following *options* in the PROC SURVEYFREQ statement:

### **DATA=SAS-data-set**

names the SAS data set to be analyzed by PROC SURVEYFREQ. If you omit the **DATA=** option, the procedure uses the most recently created SAS data set.

### **MISSING**

treats missing values as a valid (nonmissing) category for all categorical variables, which include **TABLES**, **STRATA**, and **CLUSTER** variables.

By default, if you do not specify the **MISSING** option, an observation is excluded from the analysis if it has a missing value for any **STRATA** or **CLUSTER** variable. Additionally, PROC SURVEYFREQ excludes an observation from a frequency or crosstabulation table if that observation has a missing value for any of the variables in the table request, unless you specify the **MISSING** option. For more information, see the section “Missing Values” on page 7627.

### **NOMCAR**

includes observations with missing values of **TABLES** variables in the variance computation as *not missing completely at random* (NOMCAR) for Taylor series variance estimation. When you specify the **NOMCAR** option, PROC SURVEYFREQ computes variance estimates by analyzing the non-

missing values as a domain (subpopulation), where the entire population includes both nonmissing and missing domains. See the section “[Missing Values](#)” on page 7627 for details.

By default, PROC SURVEYFREQ completely excludes an observation from a frequency or crosstabulation table (and the corresponding variance computations) if that observation has a missing value for any of the variables in the table request, unless you specify the [MISSING](#) option. Note that the [NOMCAR](#) option has no effect when you specify the [MISSING](#) option, which treats missing values as a valid nonmissing level.

The [NOMCAR](#) option applies only to Taylor series variance estimation. The replication methods, which you request with the [VARMETHOD=BRR](#) and [VARMETHOD=JACKKNIFE](#) options, do not use the [NOMCAR](#) option.

### **NOSUMMARY**

suppresses the display of the “Data Summary” table, which PROC SURVEYFREQ produces by default. For details about this table, see the section “[Data Summary Table](#)” on page 7663.

### **ORDER=DATA | FORMATTED | FREQ | INTERNAL**

specifies the order of the variable levels in the frequency and crosstabulation tables, which you request in the [TABLES](#) statement. The [ORDER=](#) option also controls the order of the [STRATA](#) variable levels in the “Stratum Information” table.

The [ORDER=](#) option can take the following values:

| <b>ORDER=</b> | <b>Levels Ordered By</b>                                                                                                               |
|---------------|----------------------------------------------------------------------------------------------------------------------------------------|
| DATA          | Order of appearance in the input data set                                                                                              |
| FORMATTED     | External formatted value, except for numeric variables with no explicit format, which are sorted by their unformatted (internal) value |
| FREQ          | Descending frequency count; levels with the most observations come first in the order                                                  |
| INTERNAL      | Unformatted value                                                                                                                      |

By default, [ORDER=INTERNAL](#). The [FORMATTED](#) and [INTERNAL](#) orders are machine-dependent. Note that the frequency count used by [ORDER=FREQ](#) is the nonweighted frequency (sample size), rather than the weighted frequency.

For more information about sort order, see the chapter on the [SORT](#) procedure in the *Base SAS Procedures Guide* and the discussion of BY-group processing in *SAS Language Reference: Concepts*.

### **PAGE**

displays only one table per page. Otherwise, PROC SURVEYFREQ displays multiple tables per page as space permits.

**RATE=***value* | *SAS-data-set*

**R=***value* | *SAS-data-set*

specifies the sampling rate as a nonnegative *value*, or identifies an input data set that provides the stratum sampling rates in a variable named `_RATE_`. PROC SURVEYFREQ uses this information to compute a finite population correction for Taylor series variance estimation. The procedure does not use the [RATE=](#) option for [BRR](#) or jackknife variance estimation, which you request with the [VARMETHOD=BRR](#) or [VARMETHOD=JACKKNIFE](#) option.

If your sample design has multiple stages, you should specify the *first-stage sampling rate*, which is the ratio of the number of primary sampling units (PSUs) that are selected to the total number of PSUs in the population.

For a nonstratified sample design, or for a stratified sample design with the same sampling rate in all strata, you should specify a nonnegative *value* for the RATE= option. If your design is stratified with different sampling rates in different strata, then you should name a SAS data set that contains the stratification variables and the stratum sampling rates. See the section “Population Totals and Sampling Rates” on page 7626 for details.

The sampling rate *value* must be a nonnegative number. You can specify *value* as a number between 0 and 1. Or you can specify *value* in percentage form as a number between 1 and 100, and PROC SURVEYFREQ converts that number to a proportion. The procedure treats the value 1 as 100% instead of 1%.

If you do not specify the RATE= or TOTAL= option, then the Taylor series variance estimation does not include a finite population correction. You cannot specify both the TOTAL= option and the RATE= option in the same PROC SURVEYFREQ statement.

**TOTAL=***value* | *SAS-data-set*

**N=***value* | *SAS-data-set*

specifies the total number of primary sampling units (PSUs) in the study population as a positive *value*, or identifies an input data set that provides the stratum population totals in a variable named `_TOTAL_`. PROC SURVEYFREQ uses this information to compute a finite population correction for Taylor series variance estimation. The procedure does not use the TOTAL= option for BRR or jackknife variance estimation, which you request with the `VARMETHOD=BRR` or `VARMETHOD=JACKKNIFE` option.

For a nonstratified sample design, or for a stratified sample design with the same population total in all strata, you should specify a positive *value* for the TOTAL= option. If your sample design is stratified with different population totals in different strata, then you should name a SAS data set that contains the stratification variables and the stratum totals. See the section “Population Totals and Sampling Rates” on page 7626 for details.

If you do not specify the TOTAL= or RATE= option, then the Taylor series variance estimation does not include a finite population correction. You cannot specify both the TOTAL= option and the RATE= option in the same PROC SURVEYFREQ statement.

**VARHEADER=**LABEL | NAME | NAMELABEL

specifies the variable identification to use in the displayed output. By default VARHEADER=NAME, which displays variable names in the output. The VARHEADER= option affects the headers of the variable level columns in one-way frequency tables, crosstabulation tables, and the “Stratum Information” table. The VARHEADER= option also controls variable identification in the table headers.

The VARHEADER= option can take the following values:

| <b>VARHEADER=</b> | <b>Variable Identification Displayed</b>        |
|-------------------|-------------------------------------------------|
| LABEL             | Variable label                                  |
| NAME              | Variable name                                   |
| NAMELABEL         | Variable name and label, as <i>Name (Label)</i> |

**VARMETHOD=BRR** <(method-options)>

**VARMETHOD=JACKKNIFE** | **JK** <(method-options)>

**VARMETHOD=TAYLOR**

specifies the variance estimation method. **VARMETHOD=TAYLOR** requests the Taylor series method, which is the default if you do not specify the **VARMETHOD=** option or the **REPWEIGHTS** statement. **VARMETHOD=BRR** requests variance estimation by balanced repeated replication (BRR), and **VARMETHOD=JACKKNIFE** requests variance estimation by the delete-1 jackknife method.

For **VARMETHOD=BRR** and **VARMETHOD=JACKKNIFE**, you can specify *method-options* in parentheses after the variance method name. [Table 90.2](#) summarizes the available *method-options*.

**Table 90.2** Variance Estimation Options

| <b>VARMETHOD=</b> | <b>Variance Estimation Method</b> | <b>Method Options</b>                                                                        |
|-------------------|-----------------------------------|----------------------------------------------------------------------------------------------|
| BRR               | Balanced repeated replication     | DFADJ<br>FAY<=value><br>HADAMARD=SAS-data-set<br>OUTWEIGHTS=SAS-data-set<br>PRINTH<br>REPS=n |
| JACKKNIFE         | Jackknife                         | DFADJ<br>OUTJKCOEFS=SAS-data-set<br>OUTWEIGHTS=SAS-data-set                                  |
| TAYLOR            | Taylor series linearization       | None                                                                                         |

*Method-options* must be enclosed in parentheses after the variance method name. For example:

```
varmethod=BRR(reps=60 outweights=myReplicateWeights)
```

The following values are available for the **VARMETHOD=** option:

**BRR** < *method-options* >

requests variance estimation by balanced repeated replication (BRR). The BRR method requires a stratified sample design with two primary sampling units (PSUs) in each stratum. If you specify the **VARMETHOD=BRR** option, you must also specify a **STRATA** statement unless you provide replicate weights with a **REPWEIGHTS** statement. See the section “Balanced Repeated Replication (BRR)” on page 7637 for details.

You can specify the following *method-options* in parentheses after **VARMETHOD=BRR**:

**DFADJ**

computes the degrees of freedom as the number of nonmissing strata for the individual table request. The degrees of freedom for **VARMETHOD=BRR** equal the number of strata, which by default is based on all valid observations in the data set. But if you specify the **DFADJ** *method-option*, PROC SURVEYFREQ does not count any empty strata that occur when observations with missing values of the **TABLES** variables are removed from the analysis of that table.

See the section “Degrees of Freedom” on page 7645 for more information. See the section “Data Summary Table” on page 7663 for details about valid observations.

The DFADJ *method-option* has no effect when you specify the MISSING option, which treats missing values as a valid nonmissing level. The DFADJ *method-option* is not used when you specify the degrees of freedom in the DF= option in the TABLES statement.

The DFADJ *method-option* cannot be used when you provide replicate weights with a REPWEIGHTS statement. When you use a REPWEIGHTS statement, the degrees of freedom equal the number of REPWEIGHTS variables (or replicates), unless you specify an alternative value in the DF= option in the REPWEIGHTS or TABLES statement.

#### FAY <=value>

requests Fay’s method, which is a modification of the BRR method. See the section “Fay’s BRR Method” on page 7638 for details.

You can specify the *value* of the Fay coefficient, which is used in converting the original sampling weights to replicate weights. The Fay coefficient must be a nonnegative number less than 1. By default, the value of the Fay coefficient equals 0.5.

#### HADAMARD=SAS-data-set

##### H=SAS-data-set

names a SAS data set that contains the Hadamard matrix for BRR replicate construction. If you do not provide a Hadamard matrix with the HADAMARD= *method-option*, PROC SURVEYFREQ generates an appropriate Hadamard matrix for replicate construction. See the sections “Balanced Repeated Replication (BRR)” on page 7637 and “Hadamard Matrix” on page 7639 for details.

If a Hadamard matrix of a given dimension exists, it is not necessarily unique. Therefore, if you want to use a specific Hadamard matrix, you must provide the matrix as a SAS data set in the HADAMARD=SAS-data-set *method-option*.

In the HADAMARD= input data set, each variable corresponds to a column of the Hadamard matrix, and each observation corresponds to a row of the matrix. You can use any variable names in the HADAMARD= data set. All values in the data set must equal either 1 or –1. You must ensure that the matrix you provide is indeed a Hadamard matrix—that is,  $\mathbf{A}'\mathbf{A} = \mathbf{R}\mathbf{I}$ , where  $\mathbf{A}$  is the Hadamard matrix of dimension  $R$  and  $\mathbf{I}$  is an identity matrix. PROC SURVEYFREQ does not check the validity of the Hadamard matrix that you provide.

The HADAMARD= input data set must contain at least  $H$  variables, where  $H$  denotes the number of first-stage strata in your design. If the data set contains more than  $H$  variables, PROC SURVEYFREQ uses only the first  $H$  variables. Similarly, the HADAMARD= input data set must contain at least  $H$  observations.

If you do not specify the REPS= *method-option*, then the number of replicates is taken to be the number of observations in the HADAMARD= input data set. If you specify the number of replicates—for example, REPS=*nreps*—then the first *nreps* observations in the HADAMARD= data set are used to construct the replicates.

You can specify the PRINTH *method-option* to display the Hadamard matrix that the procedure uses to construct replicates for BRR.

**OUTWEIGHTS=SAS-data-set**

names a SAS data set to store the replicate weights that PROC SURVEYFREQ creates for BRR variance estimation. See the section “[Balanced Repeated Replication \(BRR\)](#)” on page 7637 for information about replicate weights. See the section “[Replicate Weight Output Data Set](#)” on page 7662 for details about the contents of the OUTWEIGHTS= data set.

The OUTWEIGHTS= *method-option* is not available when you provide replicate weights with a [REPWEIGHTS](#) statement.

**PRINTH**

displays the Hadamard matrix used to construct replicates for BRR. When you provide the Hadamard matrix in the [HADAMARD= method-option](#), PROC SURVEYFREQ displays only the rows and columns that are actually used to construct replicates. See the sections “[Balanced Repeated Replication \(BRR\)](#)” on page 7637 and “[Hadamard Matrix](#)” on page 7639 for more information.

The PRINTH *method-option* is not available when you provide replicate weights with a [REPWEIGHTS](#) statement because the procedure does not use a Hadamard matrix in this case.

**REPS=*n***

specifies the number of replicates for BRR variance estimation. The value of *n* must be an integer greater than 1.

If you do not provide a Hadamard matrix with the [HADAMARD= method-option](#), the number of replicates should be greater than the number of strata and should be a multiple of 4. See the section “[Balanced Repeated Replication \(BRR\)](#)” on page 7637 for more information. If a Hadamard matrix cannot be constructed for the REPS= value that you specify, the value is increased until a Hadamard matrix of that dimension can be constructed. Therefore, it is possible for the actual number of replicates used to be larger than the REPS= value that you specify.

If you provide a Hadamard matrix with the [HADAMARD= method-option](#), the value of REPS= must not be less than the number of rows in the Hadamard matrix. If you provide a Hadamard matrix and do not specify the REPS= *method-option*, the number of replicates equals the number of rows in the Hadamard matrix.

If you do not specify the REPS= or [HADAMARD= method-option](#) and do not include a [REPWEIGHTS](#) statement, the number of replicates equals the smallest multiple of 4 that is greater than the number of strata.

If you provide replicate weights with a [REPWEIGHTS](#) statement, the procedure does not use the REPS= *method-option*. With a [REPWEIGHTS](#) statement, the number of replicates equals the number of [REPWEIGHTS](#) variables.

**JACKKNIFE | JK < method-options >**

requests variance estimation by the delete-1 jackknife method. See the section “[The Jackknife Method](#)” on page 7640 for details. If you provide replicate weights with a [REPWEIGHTS](#) statement, [VARMETHOD=JACKKNIFE](#) is the default variance estimation method.

The jackknife method requires at least two primary sampling units (PSUs) in each stratum for stratified designs unless you provide replicate weights with a [REPWEIGHTS](#) statement.



You can specify the following *method-options* in parentheses after VARMETHOD=JACKKNIFE:

#### DFADJ

computes the degrees of freedom by using the number of nonmissing strata and clusters for the individual table request. The degrees of freedom for VARMETHOD=JACKKNIFE equal the number of clusters minus the number of strata, which by default is based on all valid observations in the data set. But if you specify the DFADJ *method-option*, PROC SURVEYFREQ does not count any empty strata or clusters that occur when observations with missing values of the TABLES variables are removed from the analysis of that table.

See the section “Degrees of Freedom” on page 7645 for more information. See the section “Data Summary Table” on page 7663 for details about valid observations.

The DFADJ *method-option* has no effect when you specify the MISSING option, which treats missing values as a valid nonmissing level. The DFADJ *method-option* is not used when you specify the degrees of freedom in the DF= option in the TABLES statement.

The DFADJ *method-option* cannot be used when you provide replicate weights with a REPWEIGHTS statement. When you include a REPWEIGHTS statement, the degrees of freedom equal the number of REPWEIGHTS variables (or replicates), unless you specify an alternative value in the DF= option in the REPWEIGHTS or TABLES statement.

#### OUTJKCOEFS=SAS-data-set

names a SAS data set to store the jackknife coefficients. See the section “The Jackknife Method” on page 7640 for information about jackknife coefficients. See the section “Jackknife Coefficient Output Data Set” on page 7662 for details about the contents of the OUTJKCOEFS= data set.

#### OUTWEIGHTS=SAS-data-set

names a SAS data set to store the replicate weights that PROC SURVEYFREQ creates for jackknife variance estimation. See the section “The Jackknife Method” on page 7640 for information about replicate weights. See the section “Replicate Weight Output Data Set” on page 7662 for details about the contents of the OUTWEIGHTS= data set.

The OUTWEIGHTS= *method-option* is not available when you provide replicate weights with a REPWEIGHTS statement.

#### TAYLOR

requests Taylor series variance estimation. This is the default method if you do not specify the VARMETHOD= option or a REPWEIGHTS statement. See the section “Taylor Series Variance Estimation” on page 7630 for details.

---

## BY Statement

**BY** *variables* ;

You can specify a BY statement with PROC SURVEYFREQ to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the SURVEYFREQ procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

Note that using a BY statement provides completely separate analyses of the BY groups. It does not provide a statistically valid domain (subpopulation) analysis, where the total number of units in the subpopulation is not known with certainty. You should include the domain variable(s) in your TABLES request to obtain domain analysis. See the section “[Domain Analysis](#)” on page 7626 for more details.

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

---

## CLUSTER Statement

**CLUSTER** *variables* ;

The CLUSTER statement names variables that identify the first-stage clusters in a clustered sample design. First-stage clusters are also known as primary sampling units (PSUs). The combinations of categories of CLUSTER variables define the clusters in the sample. If there is a STRATA statement, clusters are nested within strata.

If your sample design has clustering at multiple stages, you should specify only the first-stage clusters (PSUs) in the CLUSTER statement. See the section “[Specifying the Sample Design](#)” on page 7624 for more information.

If you provide replicate weights for BRR or jackknife variance estimation with the REPWEIGHTS statement, you do not need to specify a CLUSTER statement.

The CLUSTER variables are one or more variables in the DATA= input data set. These variables can be either character or numeric, but the procedure treats them as categorical variables. The formatted values of the CLUSTER variables determine the CLUSTER variable levels. Thus, you can use formats to group values into levels. See the discussion of the FORMAT procedure in the *Base SAS Procedures Guide* and the discussions of the FORMAT statement and SAS formats in *SAS Formats and Informats: Reference*.

An observation is excluded from the analysis if it has a missing value for any CLUSTER variable unless you specify the MISSING option in the PROC SURVEYFREQ statement. See the section “[Missing Values](#)” on page 7627 for more information.

You can use multiple CLUSTER statements to specify CLUSTER variables. The procedure uses variables from all CLUSTER statements to create clusters.



## REPWEIGHTS Statement

**REPWEIGHTS** *variables* </ options > ;

The REPWEIGHTS statement names variables that provide replicate weights for BRR or jackknife variance estimation, which you request with the **VARMETHOD=BRR** or **VARMETHOD=JACKKNIFE** option in the PROC SURVEYFREQ statement. If you do not provide replicate weights for these methods by using a REPWEIGHTS statement, then PROC SURVEYFREQ constructs replicate weights for the analysis. See the sections “Balanced Repeated Replication (BRR)” on page 7637 and “The Jackknife Method” on page 7640 for information about replicate weights.

Each REPWEIGHTS variable should contain the weights for a single replicate, and the number of replicates equals the number of REPWEIGHTS variables. The REPWEIGHTS variables must be numeric, and the variable values must be nonnegative numbers.

If you provide replicate weights with a REPWEIGHTS statement, you do not need to specify a **CLUSTER** or **STRATA** statement. If you use a REPWEIGHTS statement and do not specify the **VARMETHOD=** option in the PROC SURVEYFREQ statement, the procedure uses **VARMETHOD=JACKKNIFE** by default.

If you specify a REPWEIGHTS statement but do not include a **WEIGHT** statement, PROC SURVEYFREQ uses the average of each observation’s replicate weights as the observation’s weight.

You can specify the following *options* in the REPWEIGHTS statement after a slash (/):

### **DF=***df*

specifies the degrees of freedom for the analysis. The value of *df* must be a positive number. By default, the degrees of freedom equals the number of REPWEIGHTS variables. See the section “Degrees of Freedom” on page 7645 for details.

PROC SURVEYFREQ uses the DF= value in computing confidence limits for proportions, totals, and other statistics. See the section “Confidence Limits for Proportions” on page 7642 for details. PROC SURVEYFREQ also uses the DF= value in computing the denominator degrees of freedom for the *F* statistics in the Rao-Scott and Wald chi-square tests. See the sections “Rao-Scott Chi-Square Test” on page 7652, “Rao-Scott Likelihood Ratio Chi-Square Test” on page 7657, “Wald Chi-Square Test” on page 7659, and “Wald Log-Linear Chi-Square Test” on page 7660 for more information.

### **JKCOEFS=***value*

specifies the jackknife coefficient for **VARMETHOD=JACKKNIFE**. The coefficient *value* must be a nonnegative number. See the section “The Jackknife Method” on page 7640 for details about jackknife coefficients.

You can use this option to specify a single value of the jackknife coefficient, which the procedure uses for all replicates. To specify different coefficients for different replicates, use the **JKCOEFS=(values)** or **JKCOEFS=SAS-data-set** option.

### **JKCOEFS=**< (>*values*< )>

specifies jackknife coefficients for **VARMETHOD=JACKKNIFE**, where each coefficient corresponds to an individual replicate identified by a REPWEIGHTS variable. You can separate *values* with blanks or commas. The coefficient *values* must be nonnegative numbers. The number of *values* must equal the number of replicate weight variables named in the REPWEIGHTS statement. List these values in the same order in which you list the corresponding replicate weight variables in the REPWEIGHTS statement.

See the section “The Jackknife Method” on page 7640 for details about jackknife coefficients.

To specify different coefficients for different replicates, you can also use the `JKCOEFS=SAS-data-set` option. To specify a single jackknife coefficient for all replicates, use the `JKCOEFS=value` option.

#### **JKCOEFS=SAS-data-set**

names a SAS data set that contains the jackknife coefficients for `VARMETHOD=JACKKNIFE`. You provide the jackknife coefficients in the `JKCOEFS=` data set variable `JKCoefficient`. Each coefficient value must be a nonnegative number. The coefficients should correspond to the replicates that are identified by the `REPWEIGHTS` variables. Provide the coefficients as observations in the `JKCOEFS=` data set and order them to match the order in which you list the corresponding replicate weight variables in the `REPWEIGHTS` statement. The number of observations in the `JKCOEFS=` data set must not be less than the number of `REPWEIGHTS` variables.

See the section “[The Jackknife Method](#)” on page 7640 for details about jackknife coefficients.

To specify different coefficients for different replicates, you can also use the `JKCOEFS=values` option. To specify a single jackknife coefficient for all replicates, use the `JKCOEFS=value` option.

## **STRATA Statement**

**STRATA** *variables* *</ option >* ;

The `STRATA` statement names variables that identify the first-stage strata in a stratified sample design. The combinations of levels of `STRATA` variables define the strata in the sample, where strata are nonoverlapping subgroups that were sampled independently.

If your sample design has stratification at multiple stages, you should specify only the first-stage strata in the `STRATA` statement. See the section “[Specifying the Sample Design](#)” on page 7624 for more information.

If you provide replicate weights for BRR or jackknife variance estimation with a `REPWEIGHTS` statement, you do not need to specify a `STRATA` statement.

The `STRATA` variables are one or more variables in the `DATA=` input data set. These variables can be either character or numeric, but the procedure treats them as categorical variables. The formatted values of the `STRATA` variables determine the `STRATA` variable levels. Thus, you can use formats to group values into levels. See the discussion of the `FORMAT` procedure in the *Base SAS Procedures Guide* and the discussions of the `FORMAT` statement and SAS formats in *SAS Formats and Informats: Reference*.

Note that an observation is excluded from the analysis if it has a missing value for any `STRATA` variable unless you specify the `MISSING` option in the `PROC SURVEYFREQ` statement. See the section “[Missing Values](#)” on page 7627 for more information.

You can use multiple `STRATA` statements to specify `STRATA` variables. The procedure uses variables from all `STRATA` statements to define strata.

You can specify the following *option* in the `STRATA` statement after a slash (/):

#### **LIST**

displays the “Stratum Information” table, which lists all strata together with the corresponding values of the `STRATA` variables. This table provides the number of observations and the number of clusters in each stratum, as well as the sampling fraction if you specify the `RATE=` or `TOTAL=` option in the `PROC SURVEYFREQ` statement. See the section “[Stratum Information Table](#)” on page 7663 for more information.

## TABLES Statement

**TABLES** *requests* *</ options >* ;

The TABLES statement requests one-way to  $n$ -way frequency and crosstabulation tables and statistics for these tables.

If you omit the TABLES statement, PROC SURVEYFREQ generates one-way frequency tables for all **DATA=** data set variables that are not listed in the other statements.

The following argument is required in the TABLES statement:

### *requests*

specify the frequency and crosstabulation tables to produce. A *request* is composed of one variable name or several variable names separated by asterisks. To request a one-way frequency table, use a single variable. To request a two-way crosstabulation table, use an asterisk between two variables. To request a multiway table (an  $n$ -way table, where  $n > 2$ ), separate the desired variables with asterisks. The unique values of these variables form the rows, columns, and layers of the table.

For two-way tables to multiway tables, the values of the last variable form the crosstabulation table columns, while the values of the next-to-last variable form the rows. Each level (or combination of levels) of the other variables forms one layer. PROC SURVEYFREQ produces a separate crosstabulation table for each layer. For example, a specification of  $A*B*C*D$  in a TABLES statement produces  $k$  tables, where  $k$  is the number of different combinations of levels for A and B. Each table lists the levels for D (columns) within each level of C (rows).

You can use multiple TABLES statements in a single PROC SURVEYFREQ step. You can also specify any number of table requests in a single TABLES statement. To specify multiple table requests quickly, use a grouping syntax by placing parentheses around several variables and joining other variables or variable combinations. Table 90.3 shows some examples of grouping syntax.

**Table 90.3** Grouping Syntax

| TABLES Request  | Equivalent to        |
|-----------------|----------------------|
| $A*(B\ C)$      | $A*B\ A*C$           |
| $(A\ B)*(C\ D)$ | $A*C\ B*C\ A*D\ B*D$ |
| $(A\ B\ C)*D$   | $A*D\ B*D\ C*D$      |
| $A\ --\ C$      | $A\ B\ C$            |
| $(A\ --\ C)*D$  | $A*D\ B*D\ C*D$      |

The TABLES statement variables are one or more variables from the **DATA=** input data set. These variables can be either character or numeric, but the procedure treats them as categorical variables. PROC SURVEYFREQ uses the formatted values of the TABLES variable to determine the categorical variable levels. So if you assign a format to a variable with a FORMAT statement, PROC SURVEYFREQ formats the values before dividing observations into the levels of a frequency or crosstabulation table. See the discussion of the FORMAT procedure in the *Base SAS Procedures Guide* and the discussions of the FORMAT statement and SAS formats in *SAS Formats and Informats: Reference*.

By default, the frequency or crosstabulation table lists the values of both character and numeric variables in ascending order based on internal (unformatted) variable values. You can change the order of the values in the table by specifying the **ORDER=** option in the **PROC SURVEYFREQ** statement. To list the values in ascending order by formatted value, use **ORDER=FORMATTED**.

## Without Options

If you request a frequency or crosstabulation table without specifying options, **PROC SURVEYFREQ** produces the following for each table level or cell:

- frequency (sample size)
- weighted frequency, which estimates the population total
- standard deviation of the weighted frequency
- percentage, which estimates the population proportion
- standard error of the percentage

The table displays weighted frequencies if your analysis includes a **WEIGHT** statement, or if you specify the **WTFREQ** option in the **TABLES** statement. The table also displays the number of observations with missing values. See the sections “**One-Way Frequency Tables**” on page 7664 and “**Crosstabulation Tables**” on page 7665 for more information.

## Options

Table 90.4 summarizes the *options* available in the **TABLES** statement. Descriptions of the *options* follow the table in alphabetical order.

**Table 90.4** TABLES Statement Options

| Option                              | Description                                            |
|-------------------------------------|--------------------------------------------------------|
| <b>Control Statistical Analysis</b> |                                                        |
| ALPHA=                              | Sets the level for confidence limits                   |
| CHISQ                               | Requests Rao-Scott chi-square test                     |
| DF=                                 | Specifies degrees of freedom                           |
| LRCHISQ                             | Requests Rao-Scott likelihood ratio test               |
| OR                                  | Requests odds ratio and relative risks                 |
| RISK                                | Requests risks and risk difference                     |
| TESTP=                              | Specifies null proportions for one-way chi-square test |
| WCHISQ                              | Requests Wald chi-square test                          |
| WLLCHISQ                            | Requests Wald log-linear chi-square test               |

Table 90.4 continued

| Option                                      | Description                                                                                    |
|---------------------------------------------|------------------------------------------------------------------------------------------------|
| <b>Request Additional Table Information</b> |                                                                                                |
| CL                                          | Displays confidence limits for percentages and specifies confidence limit type for percentages |
| CLWT                                        | Displays confidence limits for weighted frequencies                                            |
| COLUMN                                      | Displays column percentages and standard errors                                                |
| CV                                          | Displays coefficients of variation for percentages                                             |
| CVWT                                        | Displays coefficients of variation for weighted frequencies                                    |
| DEFF                                        | Displays design effects for percentages                                                        |
| EXPECTED                                    | Displays expected weighted frequencies (two-way tables)                                        |
| ROW                                         | Displays row percentages and standard errors                                                   |
| VAR                                         | Displays variances for percentages                                                             |
| VARWT                                       | Displays variances for weighted frequencies                                                    |
| WTFREQ                                      | Displays totals and standard errors when there is no WEIGHT statement                          |
| <b>Control Displayed Output</b>             |                                                                                                |
| NOCELLPERCENT                               | Suppresses display of overall percentages                                                      |
| NOFREQ                                      | Suppresses display of frequency counts                                                         |
| NOPERCENT                                   | Suppresses display of all percentages                                                          |
| NOPRINT                                     | Suppresses display of tables but displays statistical tests                                    |
| NOSPARE                                     | Suppresses display of zero rows and columns                                                    |
| NOSTD                                       | Suppresses display of standard errors for all estimates                                        |
| NOTOTAL                                     | Suppresses display of row and column totals                                                    |
| NOWT                                        | Suppresses display of weighted frequencies                                                     |
| <b>Produce Statistical Graphics</b>         |                                                                                                |
| PLOTS=                                      | Requests plots from ODS Graphics                                                               |

You can specify the following *options* in a TABLES statement:

**ALPHA= $\alpha$** 

sets the level for confidence limits. The value of  $\alpha$  must be between 0 and 1, and the default is 0.05. A confidence level of  $\alpha$  produces  $100(1 - \alpha)\%$  confidence limits. The default of ALPHA=0.05 produces 95% confidence limits.

You request confidence limits for percentages with the CL option, and you request confidence limits for weighted frequencies with the CLWT option. See the sections “Confidence Limits for Proportions” on page 7642 and “Confidence Limits for Totals” on page 7642 for more information.

The ALPHA= option also applies to confidence limits for the risks and risk difference, which you request with the RISK option, and to confidence limits for the odds ratio and relative risks, which you request with the OR option. See the sections “Risks and Risk Difference” on page 7648 and “Odds Ratio and Relative Risks” on page 7650 for details.

**CHISQ <(options)>**

requests the Rao-Scott chi-square test. This is a design-adjusted test that is computed by applying a design correction to the weighted Pearson chi-square statistic. By default, PROC SURVEYFREQ provides a first-order Rao-Scott chi-square test. If you specify CHISQ(SECONDORDER), the pro-

cedure provides a second-order (Satterthwaite) Rao-Scott chi-square test. See the section “[Rao-Scott Chi-Square Test](#)” on page 7652 for details.

For one-way tables, the CHISQ option produces a design-based goodness-of-fit test. By default, this is a goodness-of-fit test for equal proportions. If you specify the null hypothesis proportions in the `TESTP=` option, the CHISQ option produces a chi-square goodness-of-fit test for the specified proportions.

By default for one-way tables, and for first-order tests for two-way tables, the design correction is computed from proportion estimates. If you specify `CHISQ(MODIFIED)`, the design correction is computed from null hypothesis proportions. For second-order tests for two-way tables, the design correction is always computed from null hypothesis proportions.

You can specify the following *options* in parentheses after the CHISQ option:

#### **FIRSTORDER**

requests a first-order Rao-Scott chi-square test. This is the default for the CHISQ option; if you do not specify `CHISQ(SECONDORDER)`, the procedure provides a first-order Rao-Scott test.

#### **MODIFIED**

uses the null hypothesis proportions to compute the Rao-Scott design correction. By default (if you do not specify `CHISQ(MODIFIED)`), the procedure uses proportion estimates to compute the design correction for all first-order tests and for second-order tests for one-way tables. For second-order tests for two-way tables, the procedure always uses null hypothesis proportions to compute the design correction.

#### **SECONDORDER**

requests a second-order (Satterthwaite) Rao-Scott chi-square test. See the section “[Rao-Scott Chi-Square Test](#)” on page 7652 for details.

#### **CL** <(options)>

requests confidence limits for the percentages (proportions) in the crosstabulation table. By default, PROC SURVEYFREQ computes standard Wald (“linear”) confidence limits for proportions by using the variance estimates that are based on the sample design. See the section “[Confidence Limits for Proportions](#)” on page 7642 for more information. The procedure determines the confidence coefficient from the `ALPHA=` option, which by default equals 0.05 and produces 95% confidence limits.

You can specify *options* in parentheses after the CL option to control the confidence limit computations. You can use the `TYPE=` option to request an alternative confidence limit type. In addition to Wald confidence limits, the following types of design-based confidence limits are available for proportions: modified Clopper-Pearson (exact), modified Wilson (score), and logit confidence limits.

If you specify the `PSMALL` option, PROC SURVEYFREQ uses the alternative confidence limit type for extreme (small or large) proportion estimates and uses Wald confidence limits for all other proportion estimates. If you do not specify the `PSMALL` option, PROC SURVEYFREQ computes the specified confidence limit type for all proportion values.

You can specify the following *options* in parentheses after the CL option:

#### **ADJUST=NO | YES**

controls the degrees-of-freedom adjustment to the effective sample size for the modified Clopper-Pearson and Wilson confidence limits. By default, `ADJUST=YES`. If you specify `ADJUST=NO`, the confidence limit computations do not apply the degrees-of-freedom adjustment to the effective sample size. See the section “[Modified Confidence Limits](#)” on page 7643 for details.



The ADJUST= option is available for **TYPE=CLOPPERPEARSON** and **TYPE=WILSON** confidence limits.

#### **PSMALL <=p>**

uses the alternative confidence limit type that you specify with the TYPE= option for extreme (small or large) proportion values.

The PSMALL value  $p$  defines the range of extreme proportion values, where those proportions less than or equal to  $p$  or greater than or equal to  $(1 - p)$  are considered to be extreme, and those proportions between  $p$  and  $(1 - p)$  are not extreme. If you do not specify a PSMALL value  $p$ , PROC SURVEYFREQ uses  $p = 0.25$  by default. For  $p = 0.25$ , the procedure computes Wald confidence limits for proportions between 0.25 and 0.75 and computes the alternative confidence limit type for proportions less than or equal to 0.25 or greater than or equal to 0.75.

The PSMALL value  $p$  must be a nonnegative number. You can specify  $p$  as a proportion between 0 and 0.5. Or you can specify  $p$  in percentage form as a number between 1 and 50, and PROC SURVEYFREQ converts that number to a proportion. The procedure treats the value 1 as the percentage form 1%.

The PSMALL option is available for **TYPE=CLOPPERPEARSON**, **TYPE=LOGIT**, and **TYPE=WILSON** confidence limits. See the section “Confidence Limits for Proportions” on page 7642 for details.

#### **TRUNCATE=NO | YES**

controls the truncation of the effective sample size for the modified Clopper-Pearson and Wilson confidence limits. By default, TRUNCATE=YES truncates the effective sample size if it is larger than the original sample size. If you specify TRUNCATE=NO, the effective sample size is not truncated. See the section “Modified Confidence Limits” on page 7643 for details.

The TRUNCATE= option is available for **TYPE=CLOPPERPEARSON** and **TYPE=WILSON** confidence limits.

#### **TYPE=name**

specifies the type of confidence limits to compute for proportions. If you do not specify the TYPE= option, PROC SURVEYFREQ computes Wald confidence limits (TYPE=WALD) by default.

If you specify the **CL(PSMALL)** option, the procedure uses the specified confidence limit type for extreme proportions (outside the PSMALL range) and uses Wald confidence limits for proportions that are not outside the range. If you do not specify the **CL(PSMALL)** option, the procedure uses the specified confidence limit type for all proportions.

The following *names* are available for the TYPE= option:

#### **CLOPPERPEARSON | CP**

requests modified Clopper-Pearson (exact) confidence limits for proportions. See the section “Modified Clopper-Pearson Confidence Limits” on page 7644 for details.

#### **LOGIT**

requests logit confidence limits for proportions. See the section “Logit Confidence Limits” on page 7645 for details.

**WALD**

requests standard Wald (“linear”) confidence limits for proportions. This is the default confidence limit type if you do not specify the TYPE= option. See the section “[Wald Confidence Limits](#)” on page 7643 for details.

**WILSON | SCORE**

requests modified Wilson (score) confidence limits for proportions. See the section “[Modified Wilson Confidence Limits](#)” on page 7644 for details.

**CLWT**

requests confidence limits for the weighted frequencies (totals) in the crosstabulation table. PROC SURVEYFREQ determines the confidence coefficient from the ALPHA= option, which by default equals 0.05 and produces 95% confidence limits. See the section “[Confidence Limits for Totals](#)” on page 7642 for more information.

**COLUMN <(option)>**

displays the column percentage (estimated proportion of the column total) for each cell in a two-way table. The COLUMN option also provides the standard errors of the column percentages. See the section “[Row and Column Proportions](#)” on page 7635 for more information. This option has no effect for one-way tables.

You can specify the following *option* in parentheses after the COLUMN option:

**DEFF**

displays the design effect for each column percentage in the crosstabulation table. See the section “[Design Effect](#)” on page 7646 for more information.

**CV**

displays the coefficient of variation for each percentage (proportion) estimate in the crosstabulation table. See the section “[Coefficient of Variation](#)” on page 7646 for more information.

**CVWT**

displays the coefficient of variation for each weighted frequency (estimated total), in the crosstabulation table. See the section “[Coefficient of Variation](#)” on page 7646 for more information.

**DEFF**

displays the design effect for each overall percentage (proportion) estimate in the crosstabulation table. See the section “[Design Effect](#)” on page 7646 for more information.

To request design effects for row or column percentages, specify the DEFF option in parentheses after the ROW or COLUMN option.

**DF=*df***

specifies the degrees of freedom for the analysis. The value of *df* must be a nonnegative number. By default, PROC SURVEYFREQ computes the degrees of freedom as described in the section “[Degrees of Freedom](#)” on page 7645.

PROC SURVEYFREQ uses the DF= value in computing confidence limits for proportions, totals, and other statistics. See the section “[Confidence Limits for Proportions](#)” on page 7642 for details. PROC SURVEYFREQ also uses the DF= value in computing the denominator degrees of freedom for the *F* statistics in the Rao-Scott and Wald chi-square tests. See the sections “[Rao-Scott Chi-Square Test](#)” on page 7652, “[Rao-Scott Likelihood Ratio Chi-Square Test](#)” on page 7657, “[Wald Chi-Square Test](#)” on page 7659, and “[Wald Log-Linear Chi-Square Test](#)” on page 7660 for more information.



**EXPECTED**

displays expected weighted frequencies (totals) for the table cells in a two-way table. The expected weighted frequencies are computed under the null hypothesis that the row and column variables are independent. See the section “[Expected Weighted Frequency](#)” on page 7647 for more information. This option has no effect for one-way tables.

**LRCHISQ <(options)>**

requests the Rao-Scott likelihood ratio chi-square test. This is a design-adjusted test that is computed by applying a design correction to the weighted likelihood ratio chi-square statistic. By default, PROC SURVEYFREQ provides a first-order Rao-Scott likelihood ratio test. If you specify [LRCHISQ\(SECONDORDER\)](#), the procedure provides a second-order (Satterthwaite) Rao-Scott likelihood ratio test. See the section “[Rao-Scott Likelihood Ratio Chi-Square Test](#)” on page 7657 for details.

For one-way tables, the LRCHISQ option produces a design-based likelihood ratio goodness-of-fit test. By default, the null hypothesis is equal proportions. If you specify null hypothesis proportions in the [TESTP=](#) option, the LRCHISQ option produces a design-based likelihood ratio test for the specified proportions.

By default for one-way tables, and for first-order tests for two-way tables, the design correction is computed from proportion estimates. If you specify [LRCHISQ\(MODIFIED\)](#), the design correction is computed from null hypothesis proportions. For second-order tests for two-way tables, the design correction is always computed from null hypothesis proportions.

You can specify the following *options* in parentheses after the LRCHISQ option:

**FIRSTORDER**

requests a first-order Rao-Scott likelihood ratio test. This is the default for the LRCHISQ option; if you do not specify [LRCHISQ\(SECONDORDER\)](#), the procedure provides a first-order Rao-Scott test.

**MODIFIED**

uses the null hypothesis proportions to compute the Rao-Scott design correction. By default (if you do not specify [LRCHISQ\(MODIFIED\)](#)), the procedure uses proportion estimates to compute the design correction for all first-order tests and for second-order tests for one-way tables. For second-order tests for two-way tables, the procedure always uses null hypothesis proportions to compute the design correction.

**SECONDORDER**

requests a second-order (Satterthwaite) Rao-Scott likelihood ratio test. See the section “[Rao-Scott Likelihood Ratio Chi-Square Test](#)” on page 7657 for details.

**NOCELLPERCENT**

suppresses the display of overall cell percentages in the crosstabulation table, as well as the standard errors of the percentages. The NOCELLPERCENT option does not suppress the display of row or column percentages, which you request with the [ROW](#) or [COLUMN](#) option.

**NOFREQ**

suppresses the display of cell frequencies in the crosstabulation table. The NOFREQ option also suppresses the display of row, column, and overall table frequencies.

**NOPERCENT**

suppresses the display of all percentages in the crosstabulation table. The NOPERCENT option also suppresses the display of standard errors of the percentages. Use the **NOCELLPERCENT** option to suppress display of overall cell percentages but allow display of row or column percentages.

**NOPRINT**

suppresses the display of frequency and crosstabulation tables but displays all requested statistical tests. Note that this option disables the Output Delivery System (ODS) for the suppressed tables. For more information, see Chapter 20, “Using the Output Delivery System.”

**NOSPARSE**

suppresses the display of variable levels with zero frequency in two-way tables. By default, the procedure displays all levels of the column variable within each level of the row variable, including any column variable levels with zero frequency for that row. For multiway tables, the procedure displays all levels of the row variable for each layer of the table by default, including any row variable levels with zero frequency for the layer.

**NOSTD**

suppresses the display of all standard errors in the crosstabulation table.

**NOTOTAL**

suppresses the display of row totals, column totals, and overall totals in the crosstabulation table.

**NOWT**

suppresses the display of weighted frequencies in the crosstabulation table. The NOWT option also suppresses the display of standard errors of the weighted frequencies.

**OR | RELRISK**

requests estimates of the odds ratio, the column 1 relative risk, and the column 2 relative risk for  $2 \times 2$  tables. The OR option also provides confidence limits for these statistics. See the section “Odds Ratio and Relative Risks” on page 7650 for details.

To compute confidence limits for the odds ratio and relative risks, PROC SURVEYFREQ determines the confidence coefficient from the **ALPHA=** option, which by default equals 0.05 and produces 95% confidence limits.

**PLOTS** <(global-plot-options)> <=plot-request <(plot-options)>>

**PLOTS** <(global-plot-options)>

<=(plot-request <(plot-options)> <...plot-request <(plot-options)>>>

controls the plots that are produced through ODS Graphics. *Plot-requests* identify the plots, and *plot-options* control the appearance and content of the plots. You can specify *plot-options* in parentheses after a *plot-request*. A *global-plot-option* applies to all plots for which it is available unless it is altered by a specific *plot-option*. You can specify *global-plot-options* in parentheses after the PLOTS option.

When you specify only one *plot-request*, you can omit the parentheses around the *plot-request*. For example:

```
plots=all
plots=wtfreqplot
plots=(wtfreqplot oddsratioplot)
plots(only)=(riskdiffplot relriskplot)
```

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;
proc surveyfreq;
 tables treatment*response / chisq plots=wtfreqplot;
 weight wt;
run;
ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

If ODS Graphics is enabled but you do not specify the PLOTS= option, PROC SURVEYFREQ produces all plots that are associated with the analyses that you request with the exception of weighted frequency plots and mosaic plots. To produce a weighted frequency plot or mosaic plot when ODS Graphics is enabled, you must specify the **WTFREQPLOT** or **MOSAICPLOT** *plot-request*, respectively, in the PLOTS= option, or you must specify the **PLOTS=ALL** option. PROC SURVEYFREQ produces the remaining plots (listed in Table 90.5) by default when you request the corresponding TABLES statement options. You can suppress default plots and request specific plots by using the **PLOTS(ONLY)=** option; **PLOTS(ONLY)=(*plot-requests*)** produces only the plots that are specified as *plot-requests*. You can suppress all plots by specifying the **PLOTS=NONE** option.

See Figure 90.4 and Figure 90.7 for examples of plots that PROC SURVEYFREQ produces. For general information about ODS Graphics, see Chapter 21, “Statistical Graphics Using ODS.”

### Plot Requests

Table 90.5 lists the available *plot-requests* together with their required TABLES statement options. Descriptions of the *plot-requests* follow the table in alphabetical order.

**Table 90.5** Plot Requests

| Plot Request         | Description             | Required TABLES Statement Option                                            |
|----------------------|-------------------------|-----------------------------------------------------------------------------|
| <b>ALL</b>           | All plots               | None                                                                        |
| <b>MOSAICPLOT</b>    | Mosaic plot             | Crosstabulation table request                                               |
| <b>NONE</b>          | No plots                | None                                                                        |
| <b>ODDSRATIOPLOT</b> | Odds ratio plot         | <b>OR</b> ( $h \times 2 \times 2$ table)                                    |
| <b>RELRIKSPLOT</b>   | Relative risk plot      | <b>OR</b> ( $h \times 2 \times 2$ table)                                    |
| <b>RISKDIFFPLOT</b>  | Risk difference plot    | <b>RISK</b> , <b>RISK1</b> , or <b>RISK2</b> ( $h \times 2 \times 2$ table) |
| <b>WTFREQPLOT</b>    | Weighted frequency plot | Frequency or crosstabulation table request                                  |

The following *plot-requests* are available with the PLOTS= option:

#### **ALL**

requests all plots that are associated with the specified analyses. If you specify the PLOTS=ALL option, PROC SURVEYFREQ produces the weighted frequency and mosaic plots that are associated with the tables that you request. (PROC SURVEYFREQ does not produce weighted frequency and mosaic plots by default when ODS Graphics is enabled.)

**MOSAICPLOT** <(plot-option)>

requests a mosaic plot. Mosaic plots are available for crosstabulation tables. For multiway tables, PROC SURVEYFREQ provides a mosaic plot for each two-way table layer.

To produce a mosaic plot, you must specify the MOSAICPLOT *plot-request* in the PLOTS= option, or you must specify the PLOTS=ALL option. PROC SURVEYFREQ does not produce mosaic plots by default when ODS Graphics is enabled.

Mosaic plots display tiles that correspond to the crosstabulation table cells. The areas of the tiles are proportional to the weighted frequencies of the table cells. The column variable is displayed on the X axis, and the tile widths are proportional to the relative weighted frequencies of the column variable levels. The row variable is displayed on the Y axis, and the tile heights are proportional to the relative weighted frequencies of the row levels within column levels. The colors of the tiles correspond to the row variable levels. See Friendly (2000) for more information.

You can specify the following *plot-option* in parentheses after the MOSAICPLOT *plot-request*:

**SQUARE**

produces a square mosaic plot, where the height of the Y axis equals the width of the X axis. In a square mosaic plot, the scale of the relative weighted frequencies is the same on both axes. By default, PROC SURVEYFREQ produces a rectangular mosaic plot.

**NONE**

suppresses all plots.

**ODDSRATIOPLOT** <(plot-options)>

requests a plot of odds ratios with confidence limits. Odds ratio plots are available for multiway  $2 \times 2$  tables and display the odds ratio (with confidence limits) for each  $2 \times 2$  table layer. To produce an odds ratio plot, you must also specify the OR option in the TABLES statement for a multiway  $2 \times 2$  table.

Table 90.6 lists the *plot-options* that are available for odds ratio plots. See the subsection “Plot Options for ODDSRATIOPLOT, RELRISKPLOT, and RISKDIFFPLOT” for descriptions of the *plot-options*.

**Table 90.6** Plot Options for ODDSRATIOPLOT, RELRISKPLOT, and RISKDIFFPLOT

| Plot Option | Description             | Values                  |
|-------------|-------------------------|-------------------------|
| CLDISPLAY=  | Error bar type          | SERIF*, LINE, or BAR    |
| COLUMN=**   | Risk column             | 1* or 2                 |
| LOGBASE=*** | Axis scale              | 2, E, or 10             |
| NPANELPOS=  | Statistics per graphic  | Number (All*)           |
| ORDER=      | Order of two-way levels | ASCENDING or DESCENDING |
| RANGE=      | Range to display        | Values or CLIP          |
| STATS       | Displays statistics     | None                    |

\*Default

\*\* Available for RELRISKPLOT and RISKDIFFPLOT

\*\*\* Available for ODDSRATIOPLOT and RELRISKPLOT

**RELRIKSPLOT** <(plot-options)>

requests a plot of relative risks with confidence limits. Relative risk plots are available for multiway  $2 \times 2$  tables and display the relative risk (with confidence limits) for each  $2 \times 2$  table layer. To produce a relative risk plot, you must also specify the **OR** option in the TABLES statement for a multiway  $2 \times 2$  table.

Table 90.6 lists the *plot-options* that are available for relative risk plots. See the subsection “Plot Options for ODDSRATIO PLOT, RELRIKSPLOT, and RISKDIFF PLOT” for descriptions of the *plot-options*.

**RISKDIFFPLOT** <(plot-options)>

requests a plot of risk differences with confidence limits. Risk difference plots are available for multiway  $2 \times 2$  tables and display the risk difference (with confidence limits) for each  $2 \times 2$  table layer. To produce a risk difference plot, you must also specify the **RISK**, **RISK1**, or **RISK2** option in the TABLES statement for a multiway  $2 \times 2$  table.

Table 90.6 lists the *plot-options* that are available for risk difference plots. See the subsection “Plot Options for ODDSRATIO PLOT, RELRIKSPLOT, and RISKDIFF PLOT” for descriptions of the *plot-options*.

**WTFREQPLOT** <(plot-options)>

requests a weighted frequency plot. Weighted frequency plots are available for frequency and crosstabulation tables. For multiway tables, PROC SURVEYFREQ provides a two-way weighted frequency plot for each two-way table layer.

To produce a weighted frequency plot, you must specify the WTFREQPLOT *plot-request* in the PLOTS= option, or you must specify the **PLOTS=ALL** option. PROC SURVEYFREQ does not produce weighted frequency plots by default when ODS Graphics is enabled.

By default, PROC SURVEYFREQ displays weighted frequency plots as bar charts. You can specify the **TYPE=DOTPLOT** *plot-option* to display frequency plots as dot plots. You can plot weighted percentages instead of frequencies by specifying the **SCALE=PERCENT** *plot-option*. There are four frequency plot layouts available, which you can request by specifying the **TWOWAY=** *plot-option*. See the subsection “Plot Options for WTFREQPLOT” for more information.

By default, the primary grouping of graph cells in a two-way layout is by column variable. Row variable levels are then displayed within column variable levels. You can specify the **GROUPBY=ROW** *plot-option* to group first by row variable.

Weighted frequency plots for one-way tables display confidence limits by default. For two-way tables, weighted frequency plots display confidence limits by default in the **TWOWAY=GROUPVERTICAL** and **TWOWAY=GROUPHORIZONTAL** layouts. You can suppress confidence limits by specifying the **CLBAR=NO** *plot-option*. Confidence limits are not available for two-way plots in the **TWOWAY=CLUSTER** and **TWOWAY=STACKED** layouts.

Table 90.7 lists the *plot-options* that are available for weighted frequency plots. See the subsection “Plot Options for WTFREQPLOT” for descriptions of the *plot-options*.

**Table 90.7** Plot Options for WTFREQPLOT

| Plot Option  | Description           | Values                                                |
|--------------|-----------------------|-------------------------------------------------------|
| CLBAR=       | Confidence limit bars | YES* or NO                                            |
| GROUPBY=**   | Primary group         | COLUMN* or ROW                                        |
| NPANELPOS=** | Sections per panel    | Number (4*)                                           |
| ORIENT=      | Orientation           | VERTICAL* or HORIZONTAL                               |
| SCALE=       | Scale                 | WTFREQ* or PERCENT                                    |
| TWOWAY=**    | Two-way layout        | CLUSTER, GROUPTHORIZONTAL, GROUPVERTICAL*, or STACKED |
| TYPE=        | Type                  | BARCHART* or DOTPLOT                                  |

\*Default

\*\*For two-way tables

### Global Plot Options

A *global-plot-option* applies to all plots for which the option is available unless it is altered by an individual *plot-option*. All *plot-options* that are listed in Table 90.7 and Table 90.6 are available as *global-plot-options*. The **ONLY** option is also available as a *global-plot-option*.

You can specify *global-plot-options* in parentheses after the PLOTS option. For example:

```
plots(order=ascending stats)=(riskdiffplot oddsratioplot)
plots(only)=wtfreqplot
```

In addition to the *plot-options* that are listed in Table 90.7 and Table 90.6, you can specify the following *global-plot-option* in parentheses after the PLOTS option:

#### **ONLY**

suppresses the default plots and requests only the plots that are specified as *plot-requests*.

### Plot Options for ODDSATIOPLOTT, RELRISKPLOTT, and RISKDIFFPLOTT

You can specify the following *plot-options* in parentheses after the **ODDSATIOPLOTT**, **RELRISKPLOTT**, or **RISKDIFFPLOTT** *plot-request*:

#### **CLDISPLAY=SERIF | LINE | BAR < width >**

controls the appearance of the confidence limit error bars. The default value is **CLDISPLAY=SERIF**, which displays the confidence limits as lines with serifs. **CLDISPLAY=LINE** displays the confidence limits as plain lines without serifs.

**CLDISPLAY=BAR** displays the confidence limits as bars. By default, the width of the bars equals the size of the marker for the estimate. You can control the width of the bars and the size of the marker by specifying the value of *width* as a percentage of the distance between bars,  $0 < width \leq 1$ . The bar might disappear when the value of *width* is very small.

**COLUMN=1 | 2**

specifies the  $2 \times 2$  table column to use to compute the risk (proportion). The **COLUMN=** *plot-option* is available for the relative risk plot (**RELRISKPLOT**) and the risk difference plot (**RISKDIFFPLOT**). If you specify **COLUMN=1**, the plot displays the column 1 relative risks or the column 1 risk differences. Similarly, if you specify **COLUMN=2**, the plot displays the column 2 relative risks or risk differences.

The **COLUMN=** *plot-option* does not apply to odds ratio plots. The default is **COLUMN=1** for relative risks plots.

If you request both column 1 and column 2 risk differences with the **RISK** option, **COLUMN=1** is the default for the risk difference plot. If you request computation of only column 1 (or only column 2) risk differences with the **RISK1** (or **RISK2**) option, by default the risk difference plot displays the corresponding risk differences.

**LOGBASE=2 | E | 10**

applies to the odds ratio plot (**ODDSRATIOPLOT**) and the relative risk plot (**RELRISKPLOT**). The **LOGBASE=** *plot-option* displays the odds ratio or relative risk axis on the log scale that you specify.

**NPANELPOS=*n***

divides the plot into multiple panels that display at most  $|n|$  statistics (odds ratios, relative risks, or risk differences) per panel. If  $n$  is positive, the number of statistics per panel is balanced; if  $n$  is negative, the number of statistics per panel is not balanced. For example, suppose you want to display 21 odds ratios. **NPANELPOS=20** displays two panels, the first with 11 odds ratios and the second with 10 odds ratios; **NPANELPOS=-20** displays 20 odds ratios in the first panel but only one in the second panel.

By default,  $n = 0$  and all statistics are displayed in a single panel.

**ORDER=ASCENDING | DESCENDING**

displays the statistics (odds ratios, relative risks, or risk differences) in sorted order. By default, the statistics are displayed in the order in which the two-way table layers appear in the multiway table.

**RANGE=(*< min >* *<, max >*) | CLIP**

specifies the range of values to display. If you specify **RANGE=CLIP**, the confidence limits are clipped and the display range is determined by the minimum and maximum values of the estimates. By default, the display range includes all confidence limits.

**STATS**

displays the values of the statistics and their confidence limits on the right side of the plot. If you do not specify the **STATS** option, the statistic values are not displayed.

**Plot Options for WTFREQPLOT**

You can specify the following *plot-options* in parentheses after the **WTFREQPLOT** *plot-request*:



**CLBAR=NO | YES**

controls the confidence limit error bars in the plots. CLBAR=NO suppresses confidence limit error bars. CLBAR=YES is the default for all weighted frequency plots except two-way plots that are displayed in the **TWOWAY=CLUSTER** or **TWOWAY=STACKED** layout. Confidence limit error bars are not available in the **TWOWAY=CLUSTER** and **TWOWAY=STACKED** layouts.

**GROUPBY=COLUMN | ROW**

specifies the primary grouping for two-way weighted frequency plots. The default is **GROUPBY=COLUMN**, which groups graph cells first by column variable and displays row variable levels within column variable levels. You can specify **GROUPBY=ROW** to group first by row variable. In two-way and multiway table requests, the column variable is the last variable specified and forms the columns of the crosstabulation table. The row variable is the next-to-last variable specified and forms the rows of the table.

By default for a bar chart that is displayed in the **TWOWAY=STACKED** layout, bars correspond to the column variable levels and row levels are displayed (stacked) within each column bar. By default for a bar chart that is displayed in the **TWOWAY=CLUSTER** layout, bars are first grouped by column variable levels, and row levels are displayed as adjacent bars within each column-level group. You can reverse the default row and column variable groupings by specifying **GROUPBY=ROW**.

**NPANELPOS=*n***

divides a two-way weighted frequency plot into multiple panels that display at most  $|n|$  sections per panel. Sections correspond to row or column variable levels, depending on the type of plot and the grouping.

The **NPANELPOS= *plot-option*** applies to two-way plots that are displayed in the **TWOWAY=GROUPVERTICAL** or **TWOWAY=GROUPHORIZONTAL** layout. The **NPANELPOS= *plot-option*** does not apply to the **TWOWAY=CLUSTER** and **TWOWAY=STACKED** layouts, which are always displayed in a single panel.

If  $n$  is positive, the number of sections per panel is balanced; if  $n$  is negative, the number of sections per panel is not balanced. For example, suppose your two-way table has 21 sections. **NPANELPOS=20** displays two panels, the first with 11 sections and the second with 10 sections; **NPANELPOS=-20** displays 20 sections in the first panel but only 1 section in the second panel.

By default,  $n = 4$  and each panel includes at most four sections.

**ORIENT=HORIZONTAL | VERTICAL**

controls the orientation of the weighted frequency plot. The **ORIENT=HORIZONTAL** *plot-option* places the variable levels on the Y axis and the weighted frequencies or percentages on the X axis. **ORIENT=VERTICAL** places the variable levels on the X axis. The default is **ORIENT=VERTICAL** for bar charts (**TYPE=BARCHART**) and **ORIENT=HORIZONTAL** for dot plots (**TYPE=DOTPLOT**).

**SCALE=WTFREQ | PERCENT**

specifies the scale of the frequencies to display. **SCALE=WTFREQ** displays weighted frequencies (totals), and **SCALE=PERCENT** displays percentages. The default is **SCALE=WTFREQ**.



**TWOWAY=CLUSTER | GROUPTHORIZONTAL | GROUPVERTICAL | STACKED**

specifies the layout for two-way weighted frequency plots.

All TWOWAY= layouts are available for bar charts (**TYPE=BARCHART**). All TWOWAY= layouts except TWOWAY=CLUSTER are available for dot plots (**TYPE=DOTPLOT**). Confidence limits (**CLBAR=**) can be displayed in the GROUPVERTICAL and GROUPTHORIZONTAL layouts. Confidence limits are not available in the STACKED and CLUSTER layouts. The **ORIENT=** and **GROUPBY=** *plot-options* are available for all TWOWAY= layouts.

The default two-way layout is TWOWAY=GROUPVERTICAL, which produces a grouped plot that has a vertical common baseline. By default for bar charts (**TYPE=BARCHART**, **ORIENT=VERTICAL**), the X axis displays column variable levels, and the Y axis displays weighted frequencies. The plot includes a vertical (Y-axis) block for each row variable level. The relative positions of the graph cells in this plot layout are the same as the relative positions of the table cells in the crosstabulation table. You can reverse the default row and column grouping by specifying the **GROUPBY=ROW** *plot-option*.

The TWOWAY=GROUPTHORIZONTAL layout produces a grouped plot that has a horizontal common baseline. By default (**GROUPBY=COLUMN**), the plot displays a block on the X axis for each column variable level. Within each column-level block, the plot displays row variable levels.

The TWOWAY=STACKED layout produces stacked displays of weighted frequencies. By default (**GROUPBY=COLUMN**) in a stacked bar chart, the bars correspond to column variable levels, and row levels are stacked within each column level. By default in a stacked dot plot, the dotted lines correspond to column levels, and cell weighted frequencies are plotted as data dots on the corresponding column line. The dot color identifies the row level.

The TWOWAY=CLUSTER layout, which is available only for bar charts, displays groups of adjacent bars. By default, the primary grouping is by column variable level, and row levels are displayed within each column level.

You can reverse the default row and column grouping in any layout by specifying the **GROUPBY=ROW** *plot-option*. The default is **GROUPBY=COLUMN**, which groups first by column variable.

**TYPE=BARCHART | DOTPLOT**

specifies the type of the weighted frequency plot. **TYPE=BARCHART** produces a bar chart and **TYPE=DOTPLOT** produces a dot plot. The default type is **TYPE=BARCHART**.

**RISK | RISKDIFF**

requests risk statistics for  $2 \times 2$  tables. The RISK option also provides standard errors and confidence limits for these statistics. Risk statistics include the row 1 risk (proportion), row 2 risk, overall risk, and risk difference. See the section “[Risks and Risk Difference](#)” on page 7648 for details.

The RISK option provides both column 1 and column 2 risks. To request only column 1 or column 2 risks, use the **RISK1** or **RISK2** option.

To compute confidence limits for the risks and risk difference, PROC SURVEYFREQ determines the confidence coefficient from the **ALPHA=** option, which by default equals 0.05 and produces 95% confidence limits.

**RISK1**

requests column 1 risk statistics for  $2 \times 2$  tables, together with their standard errors and confidence limits. Risk statistics include the row 1 risk (proportion), row 2 risk, overall risk, and risk difference. See the section “[Risks and Risk Difference](#)” on page 7648 for details.

To compute confidence limits for the risks and risk difference, PROC SURVEYFREQ determines the confidence coefficient from the `ALPHA=` option, which by default equals 0.05 and produces 95% confidence limits.

**RISK2**

requests column 2 risk statistics for  $2 \times 2$  tables, together with their standard errors and confidence limits. Risk statistics include the row 1 risk (proportion), row 2 risk, overall risk, and risk difference. See the section “[Risks and Risk Difference](#)” on page 7648 for details.

To compute confidence limits for the risks and risk difference, PROC SURVEYFREQ determines the confidence coefficient from the `ALPHA=` option, which by default equals 0.05 and produces 95% confidence limits.

**ROW** < option >

displays the row percentage (estimated proportion of the row total) for each cell in a two-way table. The ROW option also provides the standard errors of the row percentages. See the section “[Row and Column Proportions](#)” on page 7635 for more information. This option has no effect for one-way tables.

You can specify the following *option* in parentheses after the ROW option:

**DEFF**

displays the design effect for each row percentage in the crosstabulation table. See the section “[Design Effect](#)” on page 7646 for more information.

**TESTP=**(values)

specifies null hypothesis proportions (test percentages) for chi-square tests for one-way tables (goodness-of-fit tests). You can separate *values* with blanks or commas. Specify *values* in probability form as numbers between 0 and 1, where the proportions sum to 1. Or specify *values* in percentage form as numbers between 0 and 100, where the percentages sum to 100. PROC SURVEYFREQ treats the value 1 as the percentage form 1%. The number of TESTP= values must equal the number of variable levels in the one-way table. List these values in the same order in which the corresponding variable levels appear in the output.

When you specify the TESTP= option, PROC SURVEYFREQ displays the specified test percentages in the one-way frequency table. The TESTP= option has no effect for two-way tables.

PROC SURVEYFREQ uses the TESTP= values for the one-way Rao-Scott chi-square test (**CHISQ**) and for the one-way Rao-Scott likelihood ratio chi-square test (**LRCHISQ**). See the sections “[Rao-Scott Chi-Square Test](#)” on page 7652 and “[Rao-Scott Likelihood Ratio Chi-Square Test](#)” on page 7657 for details.

**VAR**

displays the variance estimate for each percentage in the crosstabulation table. See the section “[Proportions](#)” on page 7634 for details. By default, PROC SURVEYFREQ displays the standard errors of the percentages.

**VARWT**

displays the variance estimate for each weighted frequency, or estimated total, in the crosstabulation table. See the section “Totals” on page 7632 for details. By default, PROC SURVEYFREQ displays the standard deviations of the weighted frequencies.

**WCHISQ**

requests the Wald chi-square test for two-way tables. See the section “Wald Chi-Square Test” on page 7659 for details.

**WLLCHISQ**

requests the Wald log-linear chi-square test for two-way tables. See the section “Wald Log-Linear Chi-Square Test” on page 7660 for details.

**WTFREQ**

displays totals (weighted frequencies) and their standard errors when you do not specify a **WEIGHT** or **REPWEIGHTS** statement. PROC SURVEYFREQ displays the weighted frequencies by default when you include a **WEIGHT** or **REPWEIGHTS** statement. Without a **WEIGHT** or **REPWEIGHTS** statement, PROC SURVEYFREQ assigns all observations a weight of one.

---

## WEIGHT Statement

**WEIGHT** *variable* ;

The **WEIGHT** statement names the variable that contains the sampling weights. This variable must be numeric, and the sampling weights must be positive numbers. If an observation has a weight that is nonpositive or missing, then the procedure omits that observation from the analysis. See the section “Missing Values” on page 7627 for more information. If you specify more than one **WEIGHT** statement, the procedure uses only the first **WEIGHT** statement and ignores the rest.

If you do not specify a **WEIGHT** statement but provide replicate weights with a **REPWEIGHTS** statement, PROC SURVEYFREQ uses the average of each observation’s replicate weights as the observation’s weight.

If you do not specify a **WEIGHT** statement or a **REPWEIGHTS** statement, PROC SURVEYFREQ assigns all observations a weight of one.

---

## Details: SURVEYFREQ Procedure

### Specifying the Sample Design

PROC SURVEYFREQ produces tables and statistics that are based on the sample design used to obtain the survey data. PROC SURVEYFREQ can be used for single-stage or multistage designs, with or without stratification, and with or without unequal weighting. To analyze your survey data with PROC SURVEYFREQ, you need to provide sample design information for the procedure. This information can include design strata, clusters, and sampling weights. You can provide sample design information with the **STRATA**, **CLUSTER**, and **WEIGHT** statements, and with the **RATE=** or **TOTAL=** option in the PROC SURVEYFREQ statement.

If you provide replicate weights for BRR or jackknife variance estimation, you do not need to specify a STRATA or CLUSTER statement. Otherwise, you should specify STRATA and CLUSTER statements whenever your design includes stratification and clustering.

When there are clusters (PSUs) in the sample design, the procedure estimates variance by using the PSUs, as described in the section “[Statistical Computations](#)” on page 7630. For a multistage sample design, the variance estimation depends only on the first stage of the sample design. Therefore, the required input includes only first-stage cluster (PSU) and first-stage stratum identification. You do not need to input design information about any additional stages of sampling.

## Stratification

If your sample design is stratified at the first stage of sampling, use the [STRATA](#) statement to name the variables that form the strata. The combinations of categories of STRATA variables define the strata in the sample, where strata are nonoverlapping subgroups that were sampled independently. If your sample design has stratification at multiple stages, you should identify only the first-stage strata in the STRATA statement.

If you use a [REPWEIGHTS](#) statement to provide replicate weights for BRR or jackknife variance estimation, you do not need to specify a STRATA statement. Otherwise, you should specify a STRATA statement whenever your design includes stratification. If you do not specify a STRATA statement or a REPWEIGHTS statement, then PROC SURVEYFREQ assumes there is no stratification at the first stage.

## Clustering

If your sample design selects clusters at the first stage of sampling, use the [CLUSTER](#) statement to name the variables that identify the first-stage clusters, which are also called primary sampling units (PSUs). The combinations of categories of CLUSTER variables define the clusters in the sample. If there is a STRATA statement, clusters are nested within strata. If your sample design has clustering at multiple stages, you should specify only the first-stage clusters (PSUs) in the CLUSTER statement. PROC SURVEYFREQ assumes that each cluster that is defined by the CLUSTER statement variables represents a PSU in the sample, and that each observation belongs to one PSU.

If you use a [REPWEIGHTS](#) statement to provide replicate weights for BRR or jackknife variance estimation, you do not need to specify a CLUSTER statement. Otherwise, you should specify a CLUSTER statement whenever your design includes clustering at the first stage of sampling. If you do not specify a CLUSTER statement, then PROC SURVEYFREQ treats each observation as a PSU.

## Weighting

If your sample design includes unequal weighting, use the [WEIGHT](#) statement to name the variable that contains the sampling weights. Sampling weights must be positive numbers. If an observation has a weight that is nonpositive or missing, then the procedure omits that observation from the analysis. See the section “[Missing Values](#)” on page 7627 for more information.

If you do not specify a WEIGHT statement but include a [REPWEIGHTS](#) statement, PROC SURVEYFREQ uses the average of each observation’s replicate weights as the observation’s weight. If you do not specify a WEIGHT statement or a REPWEIGHTS statement, PROC SURVEYFREQ assigns all observations a weight of one.

## Population Totals and Sampling Rates

To include a finite population correction (*fpc*) in Taylor series variance estimation, you can input either the sampling rate or the population total by using the `RATE=` or `TOTAL=` option in the `PROC SURVEYFREQ` statement. (You cannot specify both of these options in the same `PROC SURVEYFREQ` statement.) The `RATE=` and `TOTAL=` options apply only to Taylor series variance estimation. The procedure does not use a finite population correction for BRR or jackknife variance estimation.

If you do not specify the `RATE=` or `TOTAL=` option, Taylor series variance estimation does not include a finite population correction. For fairly small sampling fractions, it is appropriate to ignore this correction. See Cochran (1977) and Kish (1965) for more information.

If your design has multiple stages of selection and you are specifying the `RATE=` option, you should input the first-stage sampling rate, which is the ratio of the number of PSUs in the sample to the total number of PSUs in the study population. If you are specifying the `TOTAL=` option for a multistage design, you should input the total number of PSUs in the study population.

For a nonstratified sample design, or for a stratified sample design with the same sampling rate or the same population total in all strata, you can use the `RATE=value` or `TOTAL=value` option. If your sample design is stratified with different sampling rates or population totals in different strata, use the `RATE=SAS-data-set` or `TOTAL=SAS-data-set` option to name a SAS data set that contains the stratum sampling rates or totals. This data set is called a *secondary data set*, as opposed to the *primary data set* that you specify with the `DATA=` option.

The secondary data set must contain all the stratification variables listed in the `STRATA` statement and all the variables in the `BY` statement. Furthermore, the `BY` groups must appear in the same order as in the primary data set. If there are formats that are associated with the `STRATA` variables and the `BY` variables, then the formats must be consistent in the primary and the secondary data sets. If you specify the `TOTAL=SAS-data-set` option, the secondary data set must have a variable named `_TOTAL_` that contains the stratum population totals. If you specify the `RATE=SAS-data-set` option, the secondary data set must have a variable named `_RATE_` that contains the stratum sampling rates. If the secondary data set contains more than one observation for any one stratum, the procedure uses the first value of `_TOTAL_` or `_RATE_` for that stratum and ignores the rest.

The *value* in the `RATE=` option or the values of `_RATE_` in the secondary data set must be nonnegative numbers. You can specify *value* as a number between 0 and 1. Or you can specify *value* in percentage form as a number between 1 and 100, and `PROC SURVEYFREQ` converts that number to a proportion. The procedure treats the value 1 as 100% instead of 1%.

If you specify the `TOTAL=value` option, *value* must not be less than the sample size. If you provide stratum population totals in a secondary data set, these values must not be less than the corresponding stratum sample sizes.

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## Domain Analysis

`PROC SURVEYFREQ` provides domain analysis through its multiway table capability. *Domain analysis* refers to the computation of statistics for domains (subpopulations), in addition to the computation of statistics for the entire study population. Formation of subpopulations can be unrelated to the sample design, and so the domain sample sizes can actually be random variables. Domain analysis takes this variability into account by using the entire sample in estimating the variance of domain estimates. Domain analysis is also

known as subgroup analysis, subpopulation analysis, and subdomain analysis. For more information about domain analysis, see Lohr (2010); Cochran (1977); Fuller et al. (1989).

To request domain analysis with PROC SURVEYFREQ, you should include the domain variable(s) in your TABLES statement request. For example, specifying DOMAIN \* A \* B in a TABLES statement produces separate two-way tables of A by B for each level of DOMAIN. If your domains are formed by more than one variable, you can specify DomainVariable\_1 \* DomainVariable\_2 \* A \* B, for example, to obtain two-way tables of A by B for each domain formed by the different combinations of levels for DomainVariable\_1 and DomainVariable\_2. See [Example 90.2](#) for an example of domain analysis.

If you specify DOMAIN \* A in a TABLES statement, the values of the variable DOMAIN form the table rows. The two-way table lists levels of the variable A within each level of the row variable DOMAIN. Specify the ROW option in the TABLES statement to obtain the row percentages and their standard errors. This provides the one-way distribution of A for each domain (level of the variable DOMAIN).

Including the domain variables in a TABLES statement request provides a different analysis from that obtained by using a BY statement, which provides completely separate analyses of the BY groups. The BY statement can also be used to analyze the data set by subgroups, but it is critical to note that this does *not* produce a valid domain analysis. The BY statement is appropriate only when the number of units in each subgroup is known with certainty. For example, the BY statement can be used to obtain stratum level estimates when you have fixed sample sizes for the strata. When the subgroup sample size is a random variable, include the domain variables in your TABLES statement request.

## Missing Values

### WEIGHT Variable

If an observation has a missing value or a nonpositive value for the WEIGHT variable, then PROC SURVEYFREQ excludes that observation from the analysis.

### REPWEIGHTS Variables

If you provide replicate weights with a REPWEIGHTS statement for BRR or jackknife variance estimation, all REPWEIGHTS variable values must be nonmissing. Similarly, if you provide jackknife coefficients with the JKCOEFS= option in the REPWEIGHTS statement, all values of the JKCoefficient variable must be nonmissing. The procedure does not perform the analysis when any replicate weight or jackknife coefficient value is missing.

### STRATA and CLUSTER Variables

An observation is excluded from the analysis if it has a missing value for any STRATA or CLUSTER variable, unless you specify the MISSING option in the PROC SURVEYFREQ statement. If you specify the MISSING option, the procedure treats missing values as a valid (nonmissing) category for all categorical variables, which include STRATA variables, CLUSTER variables, and TABLES variables.

### TABLES Variables

By default, PROC SURVEYFREQ excludes an observation from a crosstabulation table (and all associated analyses) if the observation has a missing value for any of the variables in the TABLES request, unless



you specify the **MISSING** or **NOMCAR** option in the **PROC SURVEYFREQ** statement. When the procedure excludes observations with missing values from a table, it displays the total frequency of missing observations below the table.

If you specify the **MISSING** option, the procedure treats missing values as a valid (nonmissing) level for each **TABLES** variable. These levels are displayed in the crosstabulation table and included in computations of totals, percentages, and all other table statistics.

If you specify the **NOMCAR** option in the **PROC SURVEYFREQ** statement for Taylor series variance estimation, the procedure includes observations with missing values of **TABLES** variables in the variance computations. The **NOMCAR** option does not display missing levels in the crosstabulation table or compute percentages and totals for missing levels.

### The **NOMCAR** Option

The **NOMCAR** option in the **PROC SURVEYFREQ** statement includes observations with missing values of **TABLES** variables in the variance computations as *not missing completely at random* (**NOMCAR**) for Taylor series variance estimation. By default, observations are completely excluded from the analysis if they have missing values for any of the variables in the current **TABLES** request. This default treatment is based on the assumption that the values are *missing completely at random* (**MCAR**), and assumes that the analysis results should not be substantially different between the missing and nonmissing groups. See the section “**Analysis Considerations**” on page 7629 for more information.

When you specify the **NOMCAR** option, **PROC SURVEYFREQ** computes variance estimates by analyzing the nonmissing values as a domain (subpopulation), where the entire population includes both nonmissing and missing domains.

Note that the **NOMCAR** option has no effect when you specify the **MISSING** option, which treats missing values as a valid nonmissing level. The **NOMCAR** option does not affect the inclusion of observations with missing values of the **WEIGHT**, **CLUSTER**, or **STRATA** variables. Observations with missing values of the **WEIGHT** variable are always excluded from the analysis. Observations with missing values of the **CLUSTER** or **STRATA** variables are excluded unless you specify the **MISSING** option.

The **NOMCAR** option applies only to Taylor series variance estimation **VARMETHOD=TAYLOR**. The replication methods, which you request with the **VARMETHOD=BRR** and **VARMETHOD=JACKKNIFE** options, do not use the **NOMCAR** option.

### Degrees of Freedom

**PROC SURVEYFREQ** computes degrees of freedom to obtain the *t*-percentile for confidence limits for proportions, totals, and other statistics. The procedure also uses degrees of freedom for the *F* statistics in the Rao-Scott and Wald chi-square tests. The degrees of freedom computation depends on the variance estimation method that you request. See the section “**Degrees of Freedom**” on page 7645 for details. Missing values can affect the degrees of freedom computation.

#### **Taylor Series Variance Estimation**

The degrees of freedom can depend on the number of clusters, the number of strata, and the number of observations. For Taylor series variance estimation, these numbers are based on the observations included in the analysis of the individual table. These numbers do not count observations that are excluded from the table due to missing values. If all values in a stratum are excluded from the analysis of a table as missing values, then that stratum is called an *empty stratum*. Empty strata are not counted in the total number of

strata for the table. Similarly, empty clusters and missing observations are not included in the total counts of clusters and observations that are used to compute the degrees of freedom for the analysis.

If you specify the **MISSING** option, missing values are treated as valid nonmissing levels and are included in computing degrees of freedom. If you specify the **NOMCAR** option for Taylor series variance estimation, observations with missing values of the **TABLES** variables are included in computing degrees of freedom.

### **Replicate-Based Variance Estimation**

For BRR or jackknife variance estimation, by default PROC SURVEYFREQ computes the degrees of freedom by using all valid observations in the input data set. A valid observation is an observation that has a positive value of the **WEIGHT** variable and nonmissing values of the **STRATA** and **CLUSTER** variables unless you specify the **MISSING** option. See the section “Data Summary Table” on page 7663 for details about valid observations.

If you specify the **DFADJ** *method-option* for **VARMETHOD=BRR** or **VARMETHOD=JACKKNIFE**, the procedure computes the degrees of freedom based on the nonmissing observations included in the individual table analysis. This excludes any empty strata or clusters that occur when observations with missing values of the **TABLES** variables are removed from the analysis for that table.

## **Table Summary Output Data Set**

For each table request, PROC SURVEYFREQ produces a nondisplayed ODS table, “Table Summary,” which contains the number of (nonmissing) observations, strata, and clusters that are included in the analysis of the individual table. If there are missing observations, empty strata, or empty clusters excluded from the analysis, the “Table Summary” data set also contains this information. If you request any confidence limits or chi-square tests for the table, which require degrees of freedom, the “Table Summary” data set provides the degrees of freedom.

Due to missing values, the number of observations used for an individual table analysis can differ from the number of valid observations in the input data set, which is reported in the “Data Summary” table. Similarly, a difference can also occur for the number of clusters or strata. See [Example 90.3](#) for more information about the “Table Summary” output data set.

If you specify the **NOMCAR** option for Taylor series variance estimation, the “Table Summary” data set reflects all observations used for variance estimation, which includes those observations with missing values of the **TABLES** variables.

## **Analysis Considerations**

If you have missing values in your survey data for any reason (such as nonresponse), this can compromise the quality of your survey results. An observation without missing values is called a *complete respondent*, and an observation with missing values is called an *incomplete respondent*. If the complete respondents are different from the incomplete respondents with regard to a survey effect or outcome, then survey estimates will be biased and will not accurately represent the survey population. There are a variety of techniques in sample design and survey operations that can reduce nonresponse. After data collection is complete, you can use imputation to replace missing values with acceptable values, and you can use sampling weight adjustments to compensate for nonresponse. You should complete this data preparation and adjustment before you analyze your data with PROC SURVEYFREQ. For more details, see Cochran (1977); Kalton and Kaspyzyk (1986); Brick and Kalton (1996).



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## Statistical Computations

### Variance Estimation

PROC SURVEYFREQ provides a choice of variance estimation methods for complex survey data. In addition to the Taylor series linearization method, the procedures offer two replication-based (resampling) methods—balanced repeated replication (BRR) and the delete-1 jackknife. These variance estimation methods usually give similar, satisfactory results (Lohr 2010; Särndal, Swensson, and Wretman 1992; Wolter 1985). The choice of a variance estimation method can depend on the sample design used, the sample design information available, the parameters to be estimated, and computational issues. See Lohr (2010) for more details.

#### **Taylor Series Variance Estimation**

The Taylor series linearization method can be used to estimate standard errors of proportions and other statistics for crosstabulation tables. For sample survey data, the proportion estimator is a ratio estimator formed from estimators of totals. For example, to estimate the proportion in a crosstabulation table cell, the procedure uses the ratio of the estimator of the cell total frequency to the estimator of the overall population total, where these totals are linear statistics computed from the survey data. The Taylor series expansion method obtains a first-order linear approximation for the ratio estimator and then uses the variance estimate for this approximation to estimate the variance of the estimate itself (Woodruff 1971; Fuller 1975). For more information about Taylor series variance estimation for sample survey data, see Lohr (2010); Särndal, Swensson, and Wretman (1992); Lee, Forthoffer, and Lorimor (1989); Wolter (1985).

When there are clusters (PSUs) in the sample design, the Taylor series method estimates variance from the variance among PSUs. When the design is stratified, the procedure combines stratum variance estimates to compute the overall variance estimate. For a multistage sample design, the variance estimation depends only on the first stage of the sample design. So the required input includes only first-stage cluster (PSU) and first-stage stratum identification. You do not need to input design information about any additional stages of sampling. This variance estimation method assumes that the first-stage sampling fraction is small, or the first-stage sample is drawn with replacement, as it often is in practice.

See the sections “Proportions” on page 7634, “Row and Column Proportions” on page 7635, “Risks and Risk Difference” on page 7648, and “Odds Ratio and Relative Risks” on page 7650 for details and formulas for Taylor series variance estimates.

#### **Replication-Based Variance Estimation**

Replication-based methods for variance estimation draw multiple replicates (subsamples) from the full sample by following a specific resampling scheme. Commonly used resampling schemes include *balanced repeated replication* (BRR) and the *jackknife*. PROC SURVEYFREQ estimates the parameter of interest (a proportion, total, odds ratio, or other statistic) from each replicate, and then uses the variability among replicate estimates to estimate the overall variance of the parameter estimate. See Wolter (1985) and Lohr (2010) for more information.

The BRR variance estimation method requires a stratified sample design with two PSUs in each stratum. Each replicate is obtained by deleting one PSU per stratum according to the corresponding Hadamard matrix and adjusting the original weights of the remaining PSUs. The adjusted weights are called *replicate weights*. PROC SURVEYFREQ also provides Fay’s method, which is a modification of the BRR method. See the section “Balanced Repeated Replication (BRR)” on page 7637 for details.

The jackknife method deletes one PSU at a time from the full sample to create replicates, and modifies the original weights to obtain replicate weights. The total number of replicates equals the number of PSUs. If the sample design is stratified, each stratum must contain at least two PSUs, and the jackknife is applied separately within each stratum. See the section “[The Jackknife Method](#)” on page 7640 for details.

Instead of having PROC SURVEYFREQ generate replicate weights for the analysis, you can input your own replicate weights with a [REPWEIGHTS](#) statement. This can be useful if you need to do multiple analyses with the same set of replicate weights, or if you have access to replicate weights instead of design information. See the section “[Replicate Weight Output Data Set](#)” on page 7662 for more information.

## Definitions and Notation

For a stratified clustered sample design, define the following:

|                                            |                                                                                                                                 |
|--------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------|
| $h = 1, 2, \dots, H$                       | is the stratum number,<br>with a total of $H$ strata                                                                            |
| $i = 1, 2, \dots, n_h$                     | is the cluster number within stratum $h$ ,<br>with a total of $n_h$ sample clusters in stratum $h$                              |
| $j = 1, 2, \dots, m_{hi}$                  | is the unit number within cluster $i$ of stratum $h$ ,<br>with a total of $m_{hi}$ sample units from cluster $i$ of stratum $h$ |
| $n = \sum_{h=1}^H \sum_{i=1}^{n_h} m_{hi}$ | is the total number of observations in the sample                                                                               |
| $f_h$                                      | first-stage sampling rate for stratum $h$                                                                                       |
| $W_{hij}$                                  | sampling weight of unit $j$ in cluster $i$ of stratum $h$                                                                       |

The sampling rate  $f_h$ , which is used in Taylor series variance estimation, is the fraction of first-stage units (PSUs) selected for the sample. You can specify the stratum sampling rates with the [RATE=](#) option. Or if you specify population totals with the [TOTAL=](#) option, PROC SURVEYFREQ computes  $f_h$  as the ratio of stratum sample size to the stratum total, in terms of PSUs. See the section “[Population Totals and Sampling Rates](#)” on page 7626 for details. If you do not specify the [RATE=](#) option or the [TOTAL=](#) option, then the procedure assumes that the stratum sampling rates  $f_h$  are negligible and does not use a finite population correction when computing variances.

This notation is also applicable to other sample designs. For example, for a design without stratification, you can let  $H = 1$ ; for a sample design without clustering, you can let  $m_{hi} = 1$  for every  $h$  and  $i$ , which replaces clusters with individual sampling units.

For a two-way table representing the crosstabulation of two variables, define the following, where there are  $R$  levels of the row variable and  $C$  levels of the column variable:

|                                        |                                                   |
|----------------------------------------|---------------------------------------------------|
| $r = 1, 2, \dots, R$                   | is the row number, with a total of $R$ rows       |
| $c = 1, 2, \dots, C$                   | is the column number, with a total of $C$ columns |
| $N_{rc}$                               | is the population total in row $r$ and column $c$ |
| $N_{r\cdot} = \sum_{c=1}^C N_{rc}$     | is the total in row $r$                           |
| $N_{\cdot c} = \sum_{r=1}^R N_{rc}$    | is the total in column $c$                        |
| $N = \sum_{r=1}^R \sum_{c=1}^C N_{rc}$ | is the overall total                              |

$P_{rc} = N_{rc} / N$  is the population proportion in row  $r$  and column  $c$

$P_{r.} = N_{r.} / N$  is the proportion in row  $r$

$P_{.c} = N_{.c} / N$  is the proportion in column  $c$

$P_{rc}^r = N_{rc} / N_{r.}$  is the row proportion for table cell  $(r, c)$

$P_{rc}^c = N_{rc} / N_{.c}$  is the column proportion for table cell  $(r, c)$

For a specified observation (identified by stratum, cluster, and unit number within the cluster), define the following to indicate whether or not that observation belongs to cell  $(r, c)$ , row  $r$  and column  $c$ , of the two-way table, for  $r = 1, 2, \dots, R$  and  $c = 1, 2, \dots, C$ :

$$\delta_{hij}(r, c) = \begin{cases} 1 & \text{if observation } (hij) \text{ is in cell } (r, c) \\ 0 & \text{otherwise} \end{cases}$$

Similarly, define the following functions to indicate the observation's row and column classification:

$$\delta_{hij}(r \cdot) = \begin{cases} 1 & \text{if observation } (hij) \text{ is in row } r \\ 0 & \text{otherwise} \end{cases}$$

$$\delta_{hij}(\cdot c) = \begin{cases} 1 & \text{if observation } (hij) \text{ is in column } c \\ 0 & \text{otherwise} \end{cases}$$

## Totals

PROC SURVEYFREQ estimates population frequency totals for the specified crosstabulation tables, including totals for two-way table cells, rows, columns, and overall totals. The procedure computes the estimate of the total frequency in table cell  $(r, c)$  as the weighted frequency sum,

$$\widehat{N}_{rc} = \sum_{h=1}^H \sum_{i=1}^{n_h} \sum_{j=1}^{m_{hi}} \delta_{hij}(r, c) W_{hij}$$

Similarly, PROC SURVEYFREQ computes estimates of row totals, column totals, and overall totals as

$$\widehat{N}_{r.} = \sum_{h=1}^H \sum_{i=1}^{n_h} \sum_{j=1}^{m_{hi}} \delta_{hij}(r \cdot) W_{hij}$$

$$\widehat{N}_{.c} = \sum_{h=1}^H \sum_{i=1}^{n_h} \sum_{j=1}^{m_{hi}} \delta_{hij}(\cdot c) W_{hij}$$

$$\widehat{N} = \sum_{h=1}^H \sum_{i=1}^{n_h} \sum_{j=1}^{m_{hi}} W_{hij}$$

PROC SURVEYFREQ estimates the variances of totals by using the variance estimation method that you request. If you request BRR variance estimation (by specifying the `VARMETHOD=BRR` option in the PROC SURVEYFREQ statement), the procedure estimates the variances as described in the section “Balanced

Repeated Replication (BRR)” on page 7637. If you request jackknife variance estimation (by specifying the `VARMETHOD=JACKKNIFE` option), the procedure estimates the variances as described in the section “The Jackknife Method” on page 7640.

If you do not specify the `VARMETHOD=` option or a `REPWEIGHTS` statement, the default variance estimation method is Taylor series, which you can also request with the `VARMETHOD=TAYLOR` option. Since totals are linear statistics, their variances can be estimated directly, without the approximation that is used for proportions and other nonlinear statistics. PROC SURVEYFREQ estimates the variance of the total frequency in table cell  $(r, c)$  as

$$\widehat{\text{Var}}(\widehat{N}_{rc}) = \sum_{h=1}^H \widehat{\text{Var}}_h(\widehat{N}_{rc})$$

where if  $n_h > 1$ ,

$$\begin{aligned} \widehat{\text{Var}}_h(\widehat{N}_{rc}) &= \frac{n_h(1 - f_h)}{n_h - 1} \sum_{i=1}^{n_h} (n_{rc}^{hi} - \bar{n}_{rc}^h)^2 \\ n_{rc}^{hi} &= \sum_{j=1}^{m_{hi}} \delta_{hij}(r, c) W_{hij} \\ \bar{n}_{rc}^h &= \left( \sum_{i=1}^{n_h} n_{rc}^{hi} \right) / n_h \end{aligned}$$

and if  $n_h = 1$ ,

$$\widehat{\text{Var}}_h(\widehat{N}_{rc}) = \begin{cases} \text{missing} & \text{if } n_{h'} = 1 \text{ for } h' = 1, 2, \dots, H \\ 0 & \text{if } n_{h'} > 1 \text{ for some } 1 \leq h' \leq H \end{cases}$$

The standard deviation of the total is computed as

$$\text{Std}(\widehat{N}_{rc}) = \sqrt{\widehat{\text{Var}}(\widehat{N}_{rc})}$$

The variances and standard deviations are computed in a similar manner for row totals, column totals, and overall table totals.

### Covariance of Totals

The covariance matrix of the table cell totals  $\widehat{N}_{rc}$  is an  $rc \times rc$  matrix  $\widehat{\text{V}}(\widehat{\mathbf{N}})$ , which contains the pairwise table cell covariances  $\widehat{\text{Cov}}(\widehat{N}_{rc}, \widehat{N}_{ab})$ , for  $r = 1, \dots, R; c = 1, \dots, C; a = 1, \dots, R; \text{ and } b = 1, \dots, C$ .

PROC SURVEYFREQ estimates the covariances by using the variance estimation method that you request. If you request BRR variance estimation (by specifying the `VARMETHOD=BRR` option in the PROC SURVEYFREQ statement), the procedure estimates the covariances by the method described in the section “Balanced Repeated Replication (BRR)” on page 7637. If you request jackknife variance estimation (by specifying the `VARMETHOD=JACKKNIFE` option), the procedure uses the method described in the section “The Jackknife Method” on page 7640.

Otherwise (by default, or if you request the Taylor series method), PROC SURVEYFREQ estimates the covariance between total frequency estimates for table cells  $(r, c)$  and  $(a, b)$  as

$$\widehat{\text{Cov}}(\widehat{N}_{rc}, \widehat{N}_{ab}) = \sum_{h=1}^H \left( \frac{n_h(1-f_h)}{n_h-1} \sum_{i=1}^{n_h} (n_{rc}^{hi} - \bar{n}_{rc}^h) (n_{ab}^{hi} - \bar{n}_{ab}^h) \right)$$

## Proportions

PROC SURVEYFREQ computes the estimate of the proportion in table cell  $(r, c)$  as the ratio of the estimated total for the table cell to the estimated overall total,

$$\begin{aligned} \widehat{P}_{rc} &= \widehat{N}_{rc} / \widehat{N} \\ &= \left( \sum_{h=1}^H \sum_{i=1}^{n_h} \sum_{j=1}^{m_{hi}} \delta_{hij}(r, c) W_{hij} \right) / \left( \sum_{h=1}^H \sum_{i=1}^{n_h} \sum_{j=1}^{m_{hi}} W_{hij} \right) \end{aligned}$$

If you request BRR variance estimation (by specifying the `VARMETHOD=BRR` option in the PROC SURVEYFREQ statement), the procedure estimates the variances of proportion estimates as described in the section “Balanced Repeated Replication (BRR)” on page 7637. If you request jackknife variance estimation (by specifying the `VARMETHOD=JACKKNIFE` option), the procedure estimates the variances as described in the section “The Jackknife Method” on page 7640.

If you do not specify the `VARMETHOD=` option or a `REPWEIGHTS` statement, the default variance estimation method is Taylor series, which you can also request with the `VARMETHOD=TAYLOR` option. By using Taylor series linearization, the variance of a proportion estimate can be expressed as

$$\widehat{\text{Var}}(\widehat{P}_{rc}) = \sum_{h=1}^H \widehat{\text{Var}}_h(\widehat{P}_{rc})$$

where if  $n_h > 1$ ,

$$\begin{aligned} \widehat{\text{Var}}_h(\widehat{P}_{rc}) &= \frac{n_h(1-f_h)}{n_h-1} \sum_{i=1}^{n_h} (e_{rc}^{hi} - \bar{e}_{rc}^h)^2 \\ e_{rc}^{hi} &= \left( \sum_{j=1}^{m_{hi}} (\delta_{hij}(r, c) - \widehat{P}_{rc}) W_{hij} \right) / \widehat{N} \\ \bar{e}_{rc}^h &= \left( \sum_{i=1}^{n_h} e_{rc}^{hi} \right) / n_h \end{aligned}$$

and if  $n_h = 1$ ,

$$\widehat{\text{Var}}_h(\widehat{P}_{rc}) = \begin{cases} \text{missing} & \text{if } n_{h'} = 1 \text{ for } h' = 1, 2, \dots, H \\ 0 & \text{if } n_{h'} > 1 \text{ for some } 1 \leq h' \leq H \end{cases}$$

The standard error of the proportion is computed as

$$\text{StdErr}(\widehat{P}_{rc}) = \sqrt{\widehat{\text{Var}}(\widehat{P}_{rc})}$$

Similarly, the estimate of the proportion in row  $r$  is

$$\widehat{P}_{r.} = \widehat{N}_{r.} / \widehat{N}$$

And its variance estimate is

$$\widehat{\text{Var}}(\widehat{P}_{r.}) = \sum_{h=1}^H \widehat{\text{Var}}_h(\widehat{P}_{r.})$$

where if  $n_h > 1$ ,

$$\begin{aligned} \widehat{\text{Var}}_h(\widehat{P}_{r.}) &= \frac{n_h(1-f_h)}{n_h-1} \sum_{i=1}^{n_h} (e_{r.}^{hi} - \bar{e}_{r.}^h)^2 \\ e_{r.}^{hi} &= \left( \sum_{j=1}^{m_{hi}} (\delta_{hij}(r \cdot) - \widehat{P}_{r.}) W_{hij} \right) / \widehat{N} \\ \bar{e}_{r.}^h &= \left( \sum_{i=1}^{n_h} e_{r.}^{hi} \right) / n_h \end{aligned}$$

and if  $n_h = 1$ ,

$$\widehat{\text{Var}}_h(\widehat{P}_{r.}) = \begin{cases} \text{missing} & \text{if } n_{h'} = 1 \text{ for } h' = 1, 2, \dots, H \\ 0 & \text{if } n_{h'} > 1 \text{ for some } 1 \leq h' \leq H \end{cases}$$

The standard error of the proportion in row  $r$  is computed as

$$\text{StdErr}(\widehat{P}_{r.}) = \sqrt{\widehat{\text{Var}}(\widehat{P}_{r.})}$$

Computations for the proportion in column  $c$  are done in the same way.

## Row and Column Proportions

PROC SURVEYFREQ computes the estimate of the row proportion for table cell  $(r, c)$  as the ratio of the estimated total for the table cell to the estimated total for row  $r$ ,

$$\begin{aligned} \widehat{P}_{rc}^r &= \widehat{N}_{rc} / \widehat{N}_{r.} \\ &= \left( \sum_{h=1}^H \sum_{i=1}^{n_h} \sum_{j=1}^{m_{hi}} \delta_{hij}(r, c) W_{hij} \right) / \left( \sum_{h=1}^H \sum_{i=1}^{n_h} \sum_{j=1}^{m_{hi}} \delta_{hij}(r \cdot) W_{hij} \right) \end{aligned}$$

Similarly, PROC SURVEYFREQ estimates the column proportion for table cell  $(r, c)$  as the ratio of the estimated total for the table cell to the estimated total for column  $c$ ,

$$\begin{aligned}\widehat{P}_{rc}^c &= \widehat{N}_{rc} / \widehat{N}_{\cdot c} \\ &= \left( \sum_{h=1}^H \sum_{i=1}^{n_h} \sum_{j=1}^{m_{hi}} \delta_{hij}(r, c) W_{hij} \right) / \left( \sum_{h=1}^H \sum_{i=1}^{n_h} \sum_{j=1}^{m_{hi}} \delta_{hij}(\cdot, c) W_{hij} \right)\end{aligned}$$

If you request BRR variance estimation (**VARMETHOD=BRR**), PROC SURVEYFREQ estimates the variances of the row and column proportions as described in the section “Balanced Repeated Replication (BRR)” on page 7637. If you request jackknife variance estimation (**VARMETHOD=JACKKNIFE**), the procedure estimates the variances as described in the section “The Jackknife Method” on page 7640.

If you do not specify the **VARMETHOD=** option or a **REPWEIGHTS** statement, the default variance estimation method is Taylor series (**VARMETHOD=TAYLOR**). By using Taylor series linearization, the variance of the row proportion estimate can be expressed as

$$\widehat{\text{Var}}(\widehat{P}_{rc}^r) = \sum_{h=1}^H \widehat{\text{Var}}_h(\widehat{P}_{rc}^r)$$

where if  $n_h > 1$ ,

$$\begin{aligned}\widehat{\text{Var}}_h(\widehat{P}_{rc}^r) &= \frac{n_h(1-f_h)}{n_h-1} \sum_{i=1}^{n_h} (g_{rc}^{hi} - \bar{g}_{rc}^h)^2 \\ g_{rc}^{hi} &= \left( \sum_{j=1}^{m_{hi}} (\delta_{hij}(r, c) - \widehat{P}_{rc}^r \delta_{hij}(r, \cdot)) W_{hij} \right) / \widehat{N}_{r\cdot} \\ \bar{g}_{rc}^h &= \left( \sum_{i=1}^{n_h} g_{rc}^{hi} \right) / n_h\end{aligned}$$

and if  $n_h = 1$ ,

$$\widehat{\text{Var}}_h(\widehat{P}_{rc}^r) = \begin{cases} \text{missing} & \text{if } n_{h'} = 1 \text{ for } h' = 1, 2, \dots, H \\ 0 & \text{if } n_{h'} > 1 \text{ for some } 1 \leq h' \leq H \end{cases}$$

The standard error of the row proportion is computed as

$$\text{StdErr}(\widehat{P}_{rc}^r) = \sqrt{\widehat{\text{Var}}(\widehat{P}_{rc}^r)}$$

The Taylor series variance estimate for the column proportion is computed as described previously for the row proportion, but with

$$g_{rc}^{hi} = \left( \sum_{j=1}^{m_{hi}} (\delta_{hij}(r, c) - \widehat{P}_{rc}^c \delta_{hij}(\cdot, c)) W_{hij} \right) / \widehat{N}_{\cdot c}$$

## Balanced Repeated Replication (BRR)

If you specify the `VARMETHOD=BRR` option, then PROC SURVEYFREQ uses balanced repeated replication (BRR) for variance estimation. The BRR variance estimation method requires a stratified sample design with two PSUs in each stratum. You can provide replicate weights for BRR variance estimation by using a `REPWEIGHTS` statement, or the procedure can construct replicate weights for the analysis. PROC SURVEYFREQ estimates the parameter of interest (a proportion, total, odds ratio, or other statistic) from each replicate, and then uses the variability among replicate estimates to estimate the overall variance of the parameter estimate. See Wolter (1985) and Lohr (2010) for more information about BRR variance estimation.

If you do not provide replicate weights with a `REPWEIGHTS` statement, PROC SURVEYFREQ constructs replicates based on the stratified design with two PSUs in each stratum. This section describes replicate construction by the traditional BRR method. If you specify the `FAY method-option` for `VARMETHOD=BRR`, the procedure uses Fay's modified BRR method, which is described in the section “Fay's BRR Method” on page 7638.

With the traditional BRR method, each replicate is obtained by deleting one PSU per stratum according to the corresponding Hadamard matrix of dimension  $R$ , where  $R$  is the number of replicates. The number of replicates equals the smallest multiple of 4 that is greater than the number of strata  $H$ . Alternatively, you can specify the number of replicates with the `REPS= method-option`. If a Hadamard matrix cannot be constructed for the `REPS=` value that you specify, the value is increased until a Hadamard matrix of that dimension can be constructed. Therefore, it is possible for the actual number of replicates used to be larger than the `REPS=` value that you specify.

You can provide a Hadamard matrix for BRR replicate construction by using the `HADAMARD= method-option`. Otherwise, PROC SURVEYFREQ generates an appropriate Hadamard matrix. See the section “Hadamard Matrix” on page 7639 for more information. You can display the Hadamard matrix by specifying the `PRINTH method-option`.

PROC SURVEYFREQ constructs replicates by using the first  $H$  columns of the  $R \times R$  Hadamard matrix, where  $H$  denotes the number of strata. The  $r$ th replicate ( $r = 1, 2, \dots, R$ ) is drawn from the full sample according to the  $r$ th row of the Hadamard matrix as follows:

- If element  $(r, h)$  of the Hadamard matrix equals 1, then the first PSU of stratum  $h$  is included in the  $r$ th replicate, and the second PSU of stratum  $h$  is excluded.
- If element  $(r, h)$  of the Hadamard matrix equals  $-1$ , then the second PSU of stratum  $h$  is included in the  $r$ th replicate, and the first PSU of stratum  $h$  is excluded.

For the PSUs included in replicate  $r$ , the original weights are doubled to form the replicate  $r$  weights. For the PSUs not included in replicate  $r$ , the replicate  $r$  weights equal zero. You can use the `OUTWEIGHTS=SAS-data-set method-option` to store the replicate weights in a SAS data set. See the section “Replicate Weight Output Data Set” on page 7662 for details about the contents of the `OUTWEIGHTS=` data set. You can provide these replicate weights to the procedure for subsequent analyses by using a `REPWEIGHTS` statement.

Let  $\theta$  denote the population parameter to be estimated—for example, a proportion, total, odds ratio, or other statistic. Let  $\hat{\theta}$  denote the estimate of  $\theta$  from the full sample, and let  $\hat{\theta}_r$  denote the estimate from the  $r$ th BRR



replicate, which is computed by using the replicate weights. The BRR variance estimate for  $\hat{\theta}$  is computed as

$$\widehat{V}(\hat{\theta}) = \frac{1}{R} \sum_{r=1}^R (\hat{\theta}_r - \hat{\theta})^2$$

where  $R$  is the total number of replicates.

If a parameter cannot be estimated from some replicate(s), then the variance estimate is computed by using those replicates from which the parameter can be estimated. For example, suppose the parameter is a column proportion—the proportion of column  $j$  for table cell  $(i, j)$ . If a replicate  $r$  contains no observations in column  $j$ , then the column  $j$  proportion is not estimable from replicate  $r$ . In this case, the BRR variance estimate is computed as

$$\widehat{V}(\hat{\theta}) = \frac{1}{R'} \sum_{r=1}^{R'} (\hat{\theta}_r - \hat{\theta})^2$$

where the summation is over the replicates where the parameter  $\theta$  is estimable, and  $R'$  is the number of those replicates.

#### **Fay's BRR Method**

If you specify the **FAY** *method-option* for **VARMETHOD=BRR**, then PROC SURVEYFREQ uses Fay's BRR method, which is a modification of the traditional BRR variance estimation method. As for traditional BRR, Fay's method requires a stratified sample design with two PSUs in each stratum. You can provide replicate weights by using a **REPWEIGHTS** statement, or the procedure can construct replicate weights for the analysis. PROC SURVEYFREQ estimates the parameter of interest (a proportion, total, odds ratio, or other statistic) from each replicate, and then uses the variability among replicate estimates to estimate the overall variance of the parameter estimate.

If you do not provide replicate weights with a **REPWEIGHTS** statement, PROC SURVEYFREQ constructs replicates based on the stratified design with two PSUs in each stratum. As for traditional BRR, the number of replicates  $R$  equals the smallest multiple of 4 that is greater than the number of strata  $H$ , or you can specify the number of replicates with the **REPS=** *method-option*. You can provide a Hadamard matrix for replicate construction by using the **HADAMARD=** *method-option*, or PROC SURVEYFREQ generates an appropriate Hadamard matrix.

The traditional BRR method constructs half-sample replicates by deleting one PSU per stratum according to the Hadamard matrix and doubling the original weights to form replicate weights. Fay's BRR method adjusts the original weights by a coefficient  $\epsilon$ , where  $0 \leq \epsilon < 1$ . You can specify the value of  $\epsilon$  with the **FAY=** *method-option*. If you do not specify the value of  $\epsilon$ , PROC SURVEYFREQ uses  $\epsilon = 0.5$  by default. See Judkins (1990) and Rao and Shao (1999) for information about the value of the Fay coefficient. When  $\epsilon = 0$ , Fay's method becomes the traditional BRR method. For more information, see Dipppo, Fay, and Morganstein (1984); Fay (1989); Judkins (1990).

PROC SURVEYFREQ constructs Fay BRR replicates by using the first  $H$  columns of the  $R \times R$  Hadamard matrix, where  $H$  denotes the number of strata. The  $r$ th replicate ( $r = 1, 2, \dots, R$ ) is drawn from the full sample according to the  $r$ th row of the Hadamard matrix as follows:

- If element  $(r, h)$  of the Hadamard matrix equals 1, the sampling weight of the first PSU in stratum  $h$  is multiplied by  $\epsilon$ , and the sampling weight of the second PSU is multiplied by  $(2 - \epsilon)$  to form the  $r$ th replicate weights.
- If element  $(r, h)$  of the Hadamard matrix equals  $-1$ , then the sampling weight of the second PSU in stratum  $h$  is multiplied by  $\epsilon$ , and the sampling weight of the first PSU is multiplied by  $(2 - \epsilon)$  to form the  $r$ th replicate weights.

You can use the `OUTWEIGHTS= method-option` to store the replicate weights in a SAS data set. See the section “Replicate Weight Output Data Set” on page 7662 for details about the contents of the `OUTWEIGHTS=` data set. You can provide these replicate weights to the procedure for subsequent analyses by using a `REPWEIGHTS` statement.

Let  $\theta$  denote the population parameter to be estimated—for example, a proportion, total, odds ratio, or other statistic. Let  $\hat{\theta}$  denote the estimate of  $\theta$  from the full sample, and let  $\hat{\theta}_r$  denote the estimate from the  $r$ th BRR replicate, which is computed by using the replicate weights. The Fay BRR variance estimate for  $\hat{\theta}$  is computed as

$$\widehat{V}(\hat{\theta}) = \frac{1}{R(1 - \epsilon)^2} \sum_{r=1}^R (\hat{\theta}_r - \hat{\theta})^2$$

where  $R$  is the total number of replicates and  $\epsilon$  is the Fay coefficient.

If you request Fay’s BRR method and also include a `REPWEIGHTS` statement, `PROC SURVEYFREQ` uses the replicate weights that you provide and includes the Fay coefficient  $\epsilon$  in the denominator of the variance estimate in the preceding expression.

If a parameter cannot be estimated from some replicate(s), then the variance estimate is computed by using those replicates from which the parameter can be estimated. For example, suppose the parameter is a column proportion—the proportion of column  $j$  for table cell  $(i, j)$ . If a replicate  $r$  contains no observations in column  $j$ , then the column  $j$  proportion is not estimable from replicate  $r$ . In this case, the BRR variance estimate is computed as

$$\widehat{V}(\hat{\theta}) = \frac{1}{R'(1 - \epsilon)^2} \sum_{r=1}^{R'} (\hat{\theta}_r - \hat{\theta})^2$$

where the summation is over the replicates where the parameter  $\theta$  is estimable, and  $R'$  is the number of those replicates.

### **Hadamard Matrix**

`PROC SURVEYFREQ` uses a Hadamard matrix to construct replicates for BRR variance estimation. You can provide a Hadamard matrix for replicate construction by using the `HADAMARD= method-option` for `VARMETHOD=BRR`. Otherwise, `PROC SURVEYFREQ` generates an appropriate Hadamard matrix. You can display the Hadamard matrix by specifying the `PRINTH method-option`.

A Hadamard matrix  $\mathbf{A}$  of dimension  $R$  is a square matrix that has all elements equal to 1 or  $-1$ . A Hadamard matrix must satisfy the requirement that  $\mathbf{A}'\mathbf{A} = R\mathbf{I}$ , where  $\mathbf{I}$  is an identity matrix. The dimension of a Hadamard matrix must equal 1, 2, or a multiple of 4.

For example, the following matrix is a Hadamard matrix of dimension  $k = 8$ :

```

1 1 1 1 1 1 1 1
1 -1 1 -1 1 -1 1 -1
1 1 -1 -1 1 1 -1 -1
1 -1 -1 1 1 -1 -1 1
1 1 1 1 -1 -1 -1 -1
1 -1 1 -1 -1 1 -1 1
1 1 -1 -1 -1 -1 1 1
1 -1 -1 1 -1 1 1 -1

```

For BRR replicate construction, the dimension of the Hadamard matrix must be at least  $H$ , where  $H$  denotes the number of first-stage strata in your design. If a Hadamard matrix of a given dimension exists, it is not necessarily unique. Therefore, if you want to use a specific Hadamard matrix, you must provide the matrix as a SAS data set in the `HADAMARD=SAS-data-set method-option`. You must ensure that the matrix that you provide is actually a Hadamard matrix; PROC SURVEYFREQ does not check the validity of your Hadamard matrix.

See the section “Balanced Repeated Replication (BRR)” on page 7637 and “Fay’s BRR Method” on page 7638 for details about how the Hadamard matrix is used to construct replicates for BRR variance estimation.

## The Jackknife Method

If you specify the `VARMETHOD=JACKKNIFE` option, PROC SURVEYFREQ uses the delete-1 jackknife method for variance estimation. The jackknife method can be used for stratified sample designs and for designs with no stratification. If your design is stratified, the jackknife method requires at least two PSUs in each stratum. You can provide replicate weights for jackknife variance estimation by using a `REPWEIGHTS` statement, or the procedure can construct replicate weights for the analysis. PROC SURVEYFREQ estimates the parameter of interest (a proportion, total, odds ratio, or other statistic) from each replicate, and then uses the variability among replicate estimates to estimate the overall variance of the parameter estimate. See Wolter (1985) and Lohr (2010) for more information about jackknife variance estimation.

If you do not provide replicate weights with a `REPWEIGHTS` statement, PROC SURVEYFREQ constructs the replicates. The number of replicates  $R$  equals the number of PSUs, and the procedure deletes one PSU from the full sample to form each replicate. The sampling weights are modified by the jackknife coefficient for the replicate to create the replicate weights.

If your design is not stratified (no `STRATA` statement), the jackknife coefficient has the same value for each replicate  $r$ . The jackknife coefficient equals

$$\alpha_r = (R - 1)/R \quad \text{for } r = 1, 2, \dots, R$$

where  $R$  is the total number of replicates (or total number of PSUs). For the PSUs included in a replicate, the replicate weights are computed by dividing the original sampling weights by the jackknife coefficient. For the deleted PSU, which is not included in the replicate, the replicate weights equal zero. The replicate weight for the  $j$ th member of the  $i$ th PSU can be expressed as follows when the design is not stratified:

$$W_{ij}^r = \begin{cases} W_{ij}/\alpha_r & \text{if PSU } i \text{ is included in replicate } r \\ 0 & \text{otherwise} \end{cases}$$

where  $W_{ij}$  is the original sampling weight of unit  $(ij)$ ,  $r$  is the replicate number, and  $\alpha_r$  is the jackknife coefficient.

If your design is stratified, the jackknife method requires at least two PSUs in each stratum. Let stratum  $h_r'$  be the stratum from which a PSU is deleted to form the  $r$ th replicate. Stratum  $h_r'$  is called the *donor stratum*. The jackknife coefficients are defined as

$$\alpha_r = (n_{h_r'} - 1)/n_{h_r'} \quad \text{for } r = 1, 2, \dots, R$$

where  $n_{h_r'}$  is the total number of PSUs in the donor stratum for replicate  $r$ . For all strata other than the donor stratum, the replicate  $r$  weights equal the original sampling weights. For PSUs included from the donor stratum, the replicate weights are computed by dividing the original sampling weights by the jackknife coefficient. For the deleted PSU, which is not included in the replicate, the replicate weights equal zero. The replicate weight for the  $j$ th member of the  $i$ th PSU in stratum  $h$  can be expressed as

$$W_{hij}^r = \begin{cases} W_{hij} & \text{if } h \neq h_r' \\ W_{hij}/\alpha_r & \text{if } h = h_r' \text{ and PSU } (hi) \text{ is included in replicate } r \\ 0 & \text{if } h = h_r' \text{ and PSU } (hi) \text{ is not included in replicate } r \end{cases}$$

You can use the `OUTWEIGHTS=method-option` to store the replicate weights in a SAS data set. You can also use the `OUTJKCOEFS=method-option` to store the jackknife coefficients in a SAS data set. See the sections “[Jackknife Coefficient Output Data Set](#)” on page 7662 and “[Replicate Weight Output Data Set](#)” on page 7662 for details about the contents of these output data sets. You can provide replicate weights and jackknife coefficients to the procedure for subsequent analyses by using a `REPWEIGHTS` statement. If you provide replicate weights but do not provide jackknife coefficients, PROC SURVEYFREQ uses  $\alpha_r = (R - 1)/R$  as the jackknife coefficient for all replicates.

Let  $\theta$  denote the population parameter to be estimated—for example, a proportion, total, odds ratio, or other statistic. Let  $\hat{\theta}$  denote the estimate of  $\theta$  from the full sample, and let  $\hat{\theta}_r$  be the estimate from the  $r$ th jackknife replicate, which is computed by using the replicate weights. The jackknife variance estimate for  $\hat{\theta}$  is computed as

$$\widehat{V}(\hat{\theta}) = \sum_{r=1}^R \alpha_r (\hat{\theta}_r - \hat{\theta})^2$$

where  $R$  is the total number of replicates and  $\alpha_r$  is the jackknife coefficient for replicate  $r$ .

If a parameter cannot be estimated from some replicate(s), then the variance estimate is computed by using those replicates from which the parameter can be estimated. For example, suppose the parameter is a column proportion—the proportion of column  $j$  for table cell  $(i, j)$ . If a replicate  $r$  contains no observations in column  $j$ , then the column  $j$  proportion is not estimable from replicate  $r$ . In this case, the jackknife variance estimate is computed as

$$\widehat{V}(\hat{\theta}) = \frac{R}{R'} \sum_{r=1}^{R'} \alpha_r (\hat{\theta}_r - \hat{\theta})^2$$

where the summation is over the replicates where the parameter  $\theta$  is estimable, and  $R'$  is the number of those replicates.

## Confidence Limits for Totals

If you specify the **CLWT** option in the **TABLES** statement, PROC SURVEYFREQ computes confidence limits for the weighted frequencies (totals) in the crosstabulation tables.

For the total in table cell  $(r, c)$ , the confidence limits are computed as

$$\hat{N}_{rc} \pm \left( t_{df, \alpha/2} \times \text{StdErr}(\hat{N}_{rc}) \right)$$

where  $\hat{N}_{rc}$  is the estimate of the total frequency in table cell  $(r, c)$ ,  $\text{StdErr}(\hat{N}_{rc})$  is the standard error of the estimate, and  $t_{df, \alpha/2}$  is the  $100(1-\alpha/2)$  percentile of the  $t$  distribution with  $df$  degrees of freedom calculated as described in the section “**Degrees of Freedom**” on page 7645. The confidence level  $\alpha$  is determined by the value of the **ALPHA=** option, which by default equals 0.05 and produces 95% confidence limits.

The confidence limits for row totals, column totals, and the overall total are computed similarly to the confidence limits for table cell totals.

For each table request, PROC SURVEYFREQ produces a nondisplayed ODS table, “Table Summary,” which contains the number of observations, strata, and clusters that are included in the analysis of the requested table. When you request confidence limits, the “Table Summary” data set also contains the degrees of freedom  $df$  and the value of  $t_{df, \alpha/2}$  that is used to compute the confidence limits. See [Example 90.3](#) for more information about this output data set.

## Confidence Limits for Proportions

If you specify the **CL** option in the **TABLES** statement, PROC SURVEYFREQ computes confidence limits for the proportions in the frequency and crosstabulation tables.

By default, PROC SURVEYFREQ computes Wald (“linear”) confidence limits if you do not specify an alternative confidence limit type with the **CL(TYPE=)** option. In addition to Wald confidence limits, the following types of design-based confidence limits are available for proportions: modified Clopper-Pearson (exact), modified Wilson (score), and logit confidence limits.

PROC SURVEYFREQ also provides the **CL(PSMALL)** option, which uses the alternative confidence limit type for extreme (small or large) proportions and uses the Wald confidence limits for all other proportions (not extreme). For the default **PSMALL=** value of 0.25, the procedure computes Wald confidence limits for proportions between 0.25 and 0.75 and computes the alternative confidence limit type for proportions that are outside of this range. See Curtin et al. (2006).

For details about confidence limits for proportions based on complex survey data, including comparisons of their performance, see Korn and Graubard (1999, 1998); Curtin et al. (2006); Sukasih and Jang (2005). Also, in addition to the other references cited in the following sections, for information about binomial confidence limits see Brown, Cai, and DasGupta (2001); Agresti and Coull (1998).

For each table request, PROC SURVEYFREQ produces a nondisplayed ODS table, “Table Summary,” which contains the number of observations, strata, and clusters that are included in the analysis of the requested table. When you request confidence limits, the “Table Summary” data set also contains the degrees of freedom  $df$  and the value of  $t_{df, \alpha/2}$  that is used to compute the confidence limits. See [Example 90.3](#) for more information about this output data set.

**Wald Confidence Limits**

PROC SURVEYFREQ computes standard Wald (“linear”) confidence limits for proportions by default. These confidence limits use the variance estimates that are based on the sample design. For the proportion in table cell  $(r, c)$ , the Wald confidence limits are computed as

$$\widehat{P}_{rc} \pm \left( t_{df, \alpha/2} \times \text{StdErr}(\widehat{P}_{rc}) \right)$$

where  $\widehat{P}_{rc}$  is the estimate of the proportion in table cell  $(r, c)$ ,  $\text{StdErr}(\widehat{P}_{rc})$  is the standard error of the estimate, and  $t_{df, \alpha/2}$  is the  $100(1 - \alpha/2)$  percentile of the  $t$  distribution with  $df$  degrees of freedom calculated as described in the section “[Degrees of Freedom](#)” on page 7645. The confidence level  $\alpha$  is determined by the value of the `ALPHA=` option, which by default equals 0.05 and produces 95% confidence limits.

The confidence limits for row proportions and column proportions are computed similarly to the confidence limits for table cell proportions.

**Modified Confidence Limits**

PROC SURVEYFREQ uses the modification described in Korn and Graubard (1998) to compute design-based Clopper-Pearson (exact) and Wilson (score) confidence limits. This modification substitutes the degrees-of-freedom adjusted effective sample size for the original sample size in the confidence limit computations.

The effective sample size  $n_e$  is computed as

$$n_e = n / \text{Deff}$$

where  $n$  is the original sample size (unweighted frequency) that corresponds to the total domain of the proportion estimate, and `Deff` is the design effect.

If the proportion is computed for a table cell of a two-way table, then the domain is the two-way table, and the sample size  $n$  is the frequency of the two-way table. If the proportion is a row proportion, which is based on a two-way table row, then the domain is the row, and the sample size  $n$  is the frequency of the row.

The design effect for an estimate is the ratio of the actual variance (estimated based on the sample design) to the variance of a simple random sample with the same number of observations. See the section “[Design Effect](#)” on page 7646 for details about how PROC SURVEYFREQ computes the design effect.

If you do not specify the `CL(ADJUST=NO)` option, the procedure applies a degrees-of-freedom adjustment to the effective sample size to compute the modified sample size. If you specify `CL(ADJUST=NO)`, the procedure does not apply the adjustment and uses the effective sample size  $n_e$  in the confidence limit computations.

The modified sample size  $n_e^*$  is computed by applying a degrees-of-freedom adjustment to the effective sample size  $n_e$  as

$$n_e^* = n_e \left( \frac{t_{(n-1), \alpha/2}}{t_{df, \alpha/2}} \right)^2$$

where  $df$  is the degrees of freedom and  $t_{df, \alpha/2}$  is the  $100(1 - \alpha/2)$  percentile of the  $t$  distribution with  $df$  degrees of freedom. The section “[Degrees of Freedom](#)” on page 7645 describes the computation of

the degrees of freedom  $df$ , which is based on the variance estimation method and the sample design. The confidence level  $\alpha$  is determined by the value of the `ALPHA=` option, which by default equals 0.05 and produces 95% confidence limits.

The design effect is usually greater than 1 for complex survey designs, and in that case the effective sample size is less than the actual sample size. If the adjusted effective sample size  $n_e^*$  is greater than the actual sample size  $n$ , then the procedure truncates the value of  $n_e^*$  to  $n$ , as recommended by Korn and Graubard (1998). If you specify the `CL(TRUNCATE=NO)` option, the procedure does not truncate the value of  $n_e^*$ .

**Modified Clopper-Pearson Confidence Limits** Clopper-Pearson (exact) confidence limits for the binomial proportion are constructed by inverting the equal-tailed test based on the binomial distribution. This method is attributed to Clopper and Pearson (1934). See Leemis and Trivedi (1996) for a derivation of the  $F$  distribution expression for the confidence limits.

PROC SURVEYFREQ computes modified Clopper-Pearson confidence limits according to the approach of Korn and Graubard (1998). The degrees-of-freedom adjusted effective sample size  $n_e^*$  is substituted for the sample size in the Clopper-Pearson computation, and the adjusted effective sample size times the proportion estimate  $n_e^* \hat{p}$  is substituted for the number of positive responses. (Or if you specify the `CL(ADJUST=NO)` option, the procedure uses the unadjusted effective sample size  $n_e$  instead of  $n_e^*$ .)

The modified Clopper-Pearson confidence limits for a proportion ( $P_L$  and  $P_U$ ) are computed as

$$P_L = \left( 1 + \frac{n_e^* - \hat{p}n_e^* + 1}{\hat{p}n_e^* F(\alpha/2, 2\hat{p}n_e^*, 2(n_e^* - \hat{p}n_e^* + 1))} \right)^{-1}$$

$$P_U = \left( 1 + \frac{n_e^* - \hat{p}n_e^*}{(\hat{p}n_e^* + 1) F(1 - \alpha/2, 2(\hat{p}n_e^* + 1), 2(n_e^* - \hat{p}n_e^*))} \right)^{-1}$$

where  $F(\alpha/2, b, c)$  is the  $\alpha/2$  percentile of the  $F$  distribution with  $b$  and  $c$  degrees of freedom,  $n_e^*$  is the adjusted effective sample size, and  $\hat{p}$  is the proportion estimate.

**Modified Wilson Confidence Limits** Wilson confidence limits for the binomial proportion are also known as score confidence limits and are attributed to Wilson (1927). The confidence limits are based on inverting the normal test that uses the null proportion in the variance (the score test). See Newcombe (1998) and Korn and Graubard (1999) for details.

PROC SURVEYFREQ computes modified Wilson confidence limits by substituting the degrees-of-freedom adjusted effective sample size  $n_e^*$  for the original sample size in the standard Wilson computation. (Or if you specify the `CL(ADJUST=NO)` option, the procedure substitutes the unadjusted effective sample size  $n_e$ .)

The modified Wilson confidence limits for a proportion are computed as

$$\left( \hat{p} + (\kappa)^2/2n_e^* \right) \pm \left( \kappa \sqrt{(\hat{p}(1 - \hat{p}) + (\kappa)^2)/4n_e^* / (1 + (\kappa)^2/n_e^*)} \right)$$

where  $n_e^*$  is the adjusted effective sample size and  $\hat{p}$  is the estimate of the proportion. With the degrees-of-freedom adjusted effective sample size  $n_e^*$ , the computation uses  $\kappa = z_{\alpha/2}$ . With the unadjusted effective sample size, which you request with the `ADJUST=NO` option, the computation uses  $\kappa = t_{df, \alpha/2}$ . See Curtin et al. (2006) for details.



### Logit Confidence Limits

If you specify the `CL(TYPE=LOGIT)` option, PROC SURVEYFREQ computes logit confidence limits for proportions. See Agresti (2002) and Korn and Graubard (1998) for more information.

Logit confidence limits for proportions are based on the logit transformation  $Y = \log(\hat{p}/(1 - \hat{p}))$ . The logit confidence limits  $P_L$  and  $P_U$  are computed as

$$P_L = \exp(Y_L) / (1 + \exp(Y_L))$$

$$P_U = \exp(Y_U) / (1 + \exp(Y_U))$$

where

$$(Y_L, Y_U) = \log(\hat{p}/(1 - \hat{p})) \pm (t_{df, \alpha/2} \times \text{StdErr}(\hat{p}) / (\hat{p}(1 - \hat{p})))$$

where  $\hat{p}$  is the estimate of the proportion,  $\text{StdErr}(\hat{p})$  is the standard error of the estimate, and  $t_{df, \alpha/2}$  is the  $100(1 - \alpha/2)$  percentile of the  $t$  distribution with  $df$  degrees of freedom. The degrees of freedom are calculated as described in the section “Degrees of Freedom” on page 7645. The confidence level  $\alpha$  is determined by the value of the `ALPHA=` option, which by default equals 0.05 and produces 95% confidence limits.

### Degrees of Freedom

PROC SURVEYFREQ uses the degrees of freedom of the variance estimator to obtain the  $t$ -percentile for confidence limits for proportions, totals, and other statistics. The procedure also uses the degrees of freedom in computing the  $F$  statistics for the Rao-Scott and Wald chi-square tests.

PROC SURVEYFREQ computes the degrees of freedom based on the variance estimation method and the sample design. Alternatively, you can specify the degrees of freedom in the `DF=` option in the `TABLES` statement instead of having the procedure compute it.

For Taylor series variance estimation, PROC SURVEYFREQ calculates the degrees of freedom ( $df$ ) as the number of clusters minus the number of strata. If there are no clusters, then  $df$  equals the number of observations minus the number of strata. If the design is not stratified, then  $df$  equals the number of clusters minus one. These numbers are based on the observations included in the analysis of the individual table request. These numbers do not count observations that are excluded from the table due to missing values. See the section “Missing Values” on page 7627 for details. If you specify the `MISSING` option, missing values are treated as valid nonmissing levels and are included in computing degrees of freedom. If you specify the `NOMCAR` option for Taylor series variance estimation, observations with missing values of the `TABLES` variables are included in computing degrees of freedom.

If you provide replicate weights with a `REPWEIGHTS` statement, the degrees of freedom is equal the number of replicates, which is the number of `REPWEIGHTS` variables that you provide. Alternatively, you can specify the degrees of freedom in the `DF=` option in the `REPWEIGHTS` or `TABLES` statement.

For BRR variance estimation (when you do not use a `REPWEIGHTS` statement), PROC SURVEYFREQ calculates the degrees of freedom as the number of strata. PROC SURVEYFREQ bases the number of strata on all valid observations in the data set, unless you specify the `DFADJ method-option` for `VARMETHOD=BRR`. When you specify the `DFADJ` option, the procedure computes the degrees of freedom as the number of nonmissing strata for the individual table request. This excludes any empty strata that occur when observations with missing values of the `TABLES` variables are removed from the analysis for that table.



For jackknife variance estimation (when you do not use a REPWEIGHTS statement), PROC SURVEYFREQ calculates the degrees of freedom as the number of clusters minus the number of strata. If there are no clusters, then  $df$  equals the number of observations minus the number of strata. If the design is not stratified, then  $df$  equals the number of clusters minus one. For jackknife variance estimation, PROC SURVEYFREQ bases the number of strata and clusters on all valid observations in the data set, unless you specify the DFADJ *method-option* for VARMETHOD=JACKKNIFE. When you specify the DFADJ option, the procedure computes the degrees of freedom from the number of nonmissing strata and clusters for the individual table request. This excludes any empty strata or clusters that occur when observations with missing values of the TABLES variables are removed from the analysis for that table.

For each table request, PROC SURVEYFREQ produces a nondisplayed ODS table, “Table Summary,” which contains the number of (nonmissing) observations, strata, and clusters that are included in the analysis of the table. If there are missing observations, empty strata, or empty clusters excluded from the analysis, the “Table Summary” data set also contains this information. If you request confidence limits or chi-square tests, which depend on the degrees of freedom of the variance estimator, the “Table Summary” data set provides the degrees of freedom  $df$ . See Example 90.3 for more information about this output data set.

### Coefficient of Variation

If you specify the CV option in the TABLES statement, PROC SURVEYFREQ computes the coefficients of variation for the proportion estimates in the frequency and crosstabulation tables. The coefficient of variation is the ratio of the standard error to the estimate.

For the proportion in table cell  $(r, c)$ , the coefficient of variation is computed as

$$CV(\hat{P}_{rc}) = \text{StdErr}(\hat{P}_{rc}) / \hat{P}_{rc}$$

where  $\hat{P}_{rc}$  is the estimate of the proportion in table cell  $(r, c)$ , and  $\text{StdErr}(\hat{P}_{rc})$  is the standard error of the estimate. The coefficients of variation for row proportions and column proportions are computed similarly.

If you specify the CVWT option in the TABLES statement, PROC SURVEYFREQ computes the coefficients of variation for the weighted frequencies (estimated totals) in the crosstabulation tables. For the total in table cell  $(r, c)$ , the coefficient of variation is computed as

$$CV(\hat{N}_{rc}) = \text{StdErr}(\hat{N}_{rc}) / \hat{N}_{rc}$$

where  $\hat{N}_{rc}$  is the estimate of the total in table cell  $(r, c)$ , and  $\text{StdErr}(\hat{N}_{rc})$  is the standard error of the estimate. The coefficients of variation for row totals, column totals, and the overall total are computed similarly.

### Design Effect

If you specify the DEFF option in the TABLES statement, PROC SURVEYFREQ computes design effects for the overall proportion estimates in the frequency and crosstabulation tables. If you specify the ROW(DEFF) or COLUMN(DEFF) option, the procedure provides design effects for the row or column proportion estimates, respectively. The design effect for an estimate is the ratio of the actual variance (estimated based on the sample design) to the variance of a simple random sample with the same number of observations. See Lohr (2010) and Kish (1965) for details.

For Taylor series variance estimation, PROC SURVEYFREQ computes the design effect for the proportion in table cell  $(r, c)$  as

$$\begin{aligned} \text{Deff}(\widehat{P}_{rc}) &= \widehat{\text{Var}}(\widehat{P}_{rc}) / \widehat{\text{Var}}_{\text{srs}}(\widehat{P}_{rc}) \\ &= \widehat{\text{Var}}(\widehat{P}_{rc}) / \left( (1 - f) \widehat{P}_{rc} (1 - \widehat{P}_{rc}) / (n - 1) \right) \end{aligned}$$

where  $\widehat{P}_{rc}$  is the estimate of the proportion in table cell  $(r, c)$ ,  $\widehat{\text{Var}}(\widehat{P}_{rc})$  is the variance of the estimate,  $f$  is the overall sampling fraction, and  $n$  is the sample size (unweighted frequency) for the two-way table.

For Taylor series variance estimation, PROC SURVEYFREQ determines the value of  $f$ , the overall sampling fraction, based on the **RATE=** or **TOTAL=** option. If you do not specify either of these options, PROC SURVEYFREQ assumes the value of  $f$  is negligible and does not use a finite population correction in the analysis, as described in the section “Population Totals and Sampling Rates” on page 7626. If you specify **RATE=value**, PROC SURVEYFREQ uses this value as the overall sampling fraction  $f$ . If you specify **TOTAL=value**, PROC SURVEYFREQ computes  $f$  as the ratio of the number of PSUs in the sample to the specified total.

If you specify stratum sampling rates with the **RATE=SAS-data-set** option, then PROC SURVEYFREQ computes stratum totals based on these stratum sampling rates and the number of sample PSUs in each stratum. The procedure sums the stratum totals to form the overall total, and computes  $f$  as the ratio of the number of sample PSUs to the overall total. Alternatively, if you specify stratum totals with the **TOTAL=SAS-data-set** option, then PROC SURVEYFREQ sums these totals to compute the overall total. The overall sampling fraction  $f$  is then computed as the ratio of the number of sample PSUs to the overall total.

For BRR and jackknife variance estimation, PROC SURVEYFREQ computes the design effect for the proportion in table cell  $(r, c)$  as

$$\begin{aligned} \text{Deff}(\widehat{P}_{rc}) &= \widehat{\text{Var}}(\widehat{P}_{rc}) / \widehat{\text{Var}}_{\text{srs}}(\widehat{P}_{rc}) \\ &= \widehat{\text{Var}}(\widehat{P}_{rc}) / \left( \widehat{P}_{rc} (1 - \widehat{P}_{rc}) / (n - 1) \right) \end{aligned}$$

where  $\widehat{P}_{rc}$  is the estimate of the proportion in table cell  $(r, c)$ ,  $\widehat{\text{Var}}(\widehat{P}_{rc})$  is the variance of the estimate, and  $n$  is the sample size (unweighted frequency) for the two-way table. This computation does not include the overall sampling fraction.

The procedure computes design effects similarly for proportions in one-way frequency tables, and also for row and column proportions in two-way tables. In these design effect computations, the value of  $n$  is the sample size (unweighted frequency) that corresponds to the total domain of the proportion estimate. For table cell proportions of a two-way table, the domain is the two-way table and the sample size  $n$  is the frequency of the two-way table. For row proportions, which are based on a two-way table row, the domain is the row and the sample size  $n$  is the frequency of the row.

## Expected Weighted Frequency

If you specify the **EXPECTED** option in the **TABLES** statement, PROC SURVEYFREQ computes expected weighted frequencies for the table cells in two-way tables. The expected weighted frequencies are computed

under the null hypothesis that the row and column variables are independent. The expected weighted frequency for table cell  $(r, c)$  equals

$$E_{rc} = \hat{N}_{r.} \hat{N}_{.c} / \hat{N}$$

where  $\hat{N}_{r.}$  is the estimated total for row  $r$ ,  $\hat{N}_{.c}$  is the estimated total for column  $c$ , and  $\hat{N}$  is the estimated overall total. Equivalently, the expected weighted frequency can be expressed as

$$E_{rc} = \hat{P}_{r.} \hat{P}_{.c} \hat{N}$$

These expected values are used in the design-based chi-square tests of independence, as described in the sections “Rao-Scott Chi-Square Test” on page 7652 and “Wald Chi-Square Test” on page 7659.

## Risks and Risk Difference

The **RISK** option provides estimates of risks (binomial proportions) and risk differences for  $2 \times 2$  tables, together with their standard errors and confidence limits. Risk statistics include the row 1 risk, row 2 risk, overall risk, and risk difference. If you specify the **RISK** option, PROC SURVEYFREQ provides both column 1 and column 2 risks. You can request only column 1 (or only column 2) risks by specifying the **RISK1** (or **RISK2**) option.

The column 1 risk for row 1 is the row 1 proportion for table cell (1,1). The column 1 risk estimate is computed as the ratio of the estimated total for table cell (1,1) to the estimated total for row 1,

$$\hat{P}_{11}^{(1)} = \hat{N}_{11} / \hat{N}_{1.}$$

where the total estimates are computed as described in the section “Totals” on page 7632. The column 1 risk for row 2 is the row 2 proportion for table cell (2,1), which is estimated as

$$\hat{P}_{21}^{(2)} = \hat{N}_{21} / \hat{N}_{2.}$$

The overall column 1 risk is the overall proportion in column 1, and its estimate is computed as

$$\hat{P}_{.1} = \hat{N}_{.1} / \hat{N}$$

The column 2 risk estimates are computed similarly.

The row 1 and row 2 risks are the same as the row proportions for a  $2 \times 2$  table, and their variances are computed as described in the section “Row and Column Proportions” on page 7635. The overall risk is the overall proportion in the column, and its variance computation is described in the section “Proportions” on page 7634. Confidence limits for the column 1 risk for row 1 are computed as

$$\hat{P}_{11}^{(1)} \pm \left( t_{df, \alpha/2} \times \text{StdErr}(\hat{P}_{11}^{(1)}) \right)$$

where  $\text{StdErr}(\hat{P}_{11}^{(1)})$  is the standard error of the risk estimate, and  $t_{df, \alpha/2}$  is the  $100(1 - \alpha/2)$  percentile of the  $t$  distribution with  $df$  degrees of freedom calculated as described in the section “Degrees of Freedom” on page 7645. The value of the confidence coefficient  $\alpha$  is determined by the **ALPHA=** option, which by default equals 0.05 and produces 95% confidence limits. Confidence limits for the other risks are computed similarly.

The risk difference is defined as the row 1 risk minus the row 2 risk. The estimate of the column 1 risk difference  $\widehat{RD}_1$  is computed as

$$\begin{aligned}\widehat{RD}_1 &= \widehat{P}_{11}^{(1)} - \widehat{P}_{21}^{(2)} \\ &= \left( \widehat{N}_{11} / \widehat{N}_{1\cdot} \right) - \left( \widehat{N}_{21} / \widehat{N}_{2\cdot} \right)\end{aligned}$$

The column 2 risk difference is computed similarly.

PROC SURVEYFREQ estimates the variance of the risk difference by using the variance estimation method that you request. If you request BRR variance estimation (**VARMETHOD=BRR**), the procedure estimates the variance as described in the section “Balanced Repeated Replication (BRR)” on page 7637. If you request jackknife variance estimation (**VARMETHOD=JACKKNIFE**), the procedure estimates the variance as described in the section “The Jackknife Method” on page 7640.

If you do not specify the **VARMETHOD=** option or a **REPWEIGHTS** statement, the default variance estimation method is Taylor series (**VARMETHOD=TAYLOR**). By using Taylor series linearization, the variance estimate for the column 1 risk difference  $\widehat{\text{Var}}(\widehat{RD}_1)$  can be expressed as

$$\widehat{\text{Var}}(\widehat{RD}_1) = \widehat{\mathbf{D}} \widehat{\mathbf{V}}(\widehat{\mathbf{X}}) \widehat{\mathbf{D}}'$$

where  $\widehat{\mathbf{V}}(\widehat{\mathbf{X}})$  is the covariance matrix of  $\widehat{\mathbf{X}}$ ,

$$\widehat{\mathbf{X}} = \left( \widehat{N}_{11}, \widehat{N}_{1\cdot}, \widehat{N}_{21}, \widehat{N}_{2\cdot} \right)$$

and  $\widehat{\mathbf{D}}$  is an array that contains the partial derivatives of the risk difference with respect to the elements of  $\widehat{\mathbf{X}}$ ,

$$\widehat{\mathbf{D}} = \left( 1/\widehat{N}_{1\cdot}, -\widehat{N}_{11}/\widehat{N}_{1\cdot}^2, -1/\widehat{N}_{2\cdot}, -\widehat{N}_{21}/\widehat{N}_{2\cdot}^2 \right)$$

See Wolter (1985, pp. 239–242) for details. The variance estimate for the column 2 risk difference is computed similarly.

The standard error of the column 1 risk difference is

$$\text{StdErr}(\widehat{RD}_1) = \sqrt{\widehat{\text{Var}}(\widehat{RD}_1)}$$

Confidence limits for the column 1 risk difference are computed as

$$\widehat{RD}_1 \pm \left( t_{df, \alpha/2} \times \text{StdErr}(\widehat{RD}_1) \right)$$

where  $t_{df, \alpha/2}$  is the  $100(1 - \alpha/2)$  percentile of the  $t$  distribution with  $df$  degrees of freedom calculated as described in the section “Degrees of Freedom” on page 7645. The value of the confidence coefficient  $\alpha$  is determined by the **ALPHA=** option, which by default equals 0.05 and produces 95% confidence limits. Confidence limits for the column 2 risk difference are computed in the same way.

## Odds Ratio and Relative Risks

The OR option provides estimates of the odds ratio, the column 1 relative risk, and the column 2 relative risk for  $2 \times 2$  tables, together with their confidence limits.

### Odds Ratio

For a  $2 \times 2$  table, the odds of a positive (column 1) response in row 1 is  $N_{11}/N_{12}$ . Similarly, the odds of a positive response in row 2 is  $N_{21}/N_{22}$ . The odds ratio is formed as the ratio of the row 1 odds to the row 2 odds. The estimate of the odds ratio is computed as

$$\widehat{OR} = \frac{\widehat{N}_{11} / \widehat{N}_{12}}{\widehat{N}_{21} / \widehat{N}_{22}} = \frac{\widehat{N}_{11} \widehat{N}_{22}}{\widehat{N}_{12} \widehat{N}_{21}}$$

The value of the odds ratio can be any nonnegative number. When the row and column variables are independent, the true value of the odds ratio equals 1. An odds ratio greater than 1 indicates that the odds of a positive response are higher in row 1 than in row 2. An odds ratio less than 1 indicates that the odds of positive response are higher in row 2. The strength of association increases with the deviation from 1. For details, see Stokes, Davis, and Koch (2000); Agresti (2007).

PROC SURVEYFREQ constructs confidence limits for the odds ratio by using the log transform. The  $100(1 - \alpha)\%$  confidence limits for the odds ratio are computed as

$$\left( \widehat{OR} \times \exp(-t_{df, \alpha/2} \sqrt{v}), \widehat{OR} \times \exp(t_{df, \alpha/2} \sqrt{v}) \right)$$

where

$$v = \widehat{\text{Var}}(\ln \widehat{OR}) = \widehat{\text{Var}}(\widehat{OR}) / \widehat{OR}^2$$

is the estimate of the variance of the log odds ratio, and where  $t_{df, \alpha/2}$  is the  $100(1 - \alpha/2)$  percentile of the  $t$  distribution with  $df$  degrees of freedom. The computation of  $df$  is described in the section “Degrees of Freedom” on page 7645. The value of the confidence coefficient  $\alpha$  is determined by the ALPHA= option, which by default equals 0.05 and produces 95% confidence limits.

If you request BRR variance estimation (VARMETHOD=BRR), PROC SURVEYFREQ estimates the variance of the odds ratio as described in the section “Balanced Repeated Replication (BRR)” on page 7637. If you request jackknife variance estimation (VARMETHOD=JACKKNIFE), the procedure estimates the variance as described in the section “The Jackknife Method” on page 7640.

If you do not specify the VARMETHOD= option or a REPWEIGHTS statement, the default variance estimation method is Taylor series (VARMETHOD=TAYLOR). By using Taylor series linearization, the variance estimate for the odds ratio can be expressed as

$$\widehat{\text{Var}}(\widehat{OR}) = \widehat{\mathbf{D}} \widehat{\mathbf{V}}(\widehat{\mathbf{N}}) \widehat{\mathbf{D}}'$$

where  $\widehat{\mathbf{V}}(\widehat{\mathbf{N}})$  is the covariance matrix of the estimates of the cell totals  $\widehat{\mathbf{N}}$ ,

$$\widehat{\mathbf{N}} = \begin{pmatrix} \widehat{N}_{11} & \widehat{N}_{12} & \widehat{N}_{21} & \widehat{N}_{22} \end{pmatrix}$$

and  $\widehat{\mathbf{D}}$  is an array that contains the partial derivatives of the odds ratio with respect to the elements of  $\widehat{\mathbf{N}}$ . The section “Covariance of Totals” on page 7633 describes the computation of  $\widehat{\mathbf{V}}(\widehat{\mathbf{N}})$ . The array  $\widehat{\mathbf{D}}$  is computed as

$$\widehat{\mathbf{D}} = \left( \widehat{N}_{22}/(\widehat{N}_{12}\widehat{N}_{21}), \quad -\widehat{N}_{11}\widehat{N}_{22}/(\widehat{N}_{21}\widehat{N}_{12}^2), \quad -\widehat{N}_{11}\widehat{N}_{22}/(\widehat{N}_{12}\widehat{N}_{21}^2), \quad \widehat{N}_{11}/(\widehat{N}_{12}\widehat{N}_{21}) \right)$$

See Wolter (1985, pp. 239–242) for more information.

### Relative Risks

For a  $2 \times 2$  table, the column 1 relative risk is the ratio of the column 1 risks for row 1 to row 2. As described in the section “Risks and Risk Difference” on page 7648, the column 1 risk for row 1 is the proportion of row 1 observations classified in column 1, and the column 1 risk for row 2 is the proportion of row 2 observations classified in column 1. The estimate of the column 1 relative risk is computed as

$$\widehat{RR}_1 = \frac{\widehat{N}_{11} / \widehat{N}_{1.}}{\widehat{N}_{21} / \widehat{N}_{2.}}$$

Similarly, the estimate of the column 2 relative risk is computed as

$$\widehat{RR}_2 = \frac{\widehat{N}_{12} / \widehat{N}_{1.}}{\widehat{N}_{22} / \widehat{N}_{2.}}$$

A relative risk greater than 1 indicates that the probability of positive response is greater in row 1 than in row 2. Similarly, a relative risk less than 1 indicates that the probability of positive response is less in row 1 than in row 2. The strength of association increases with the deviation from 1. For more information, see Stokes, Davis, and Koch (2000); Agresti (2007).

PROC SURVEYFREQ constructs confidence limits for the relative risk by using the log transform, which is similar to the odds ratio computations described previously. The  $100(1 - \alpha)\%$  confidence limits for the column 1 relative risk are computed as

$$\left( \widehat{RR}_1 \times \exp(-t_{df, \alpha/2} \sqrt{v}), \widehat{RR}_1 \times \exp(t_{df, \alpha/2} \sqrt{v}) \right)$$

where

$$v = \widehat{\text{Var}}(\ln \widehat{RR}_1) = \widehat{\text{Var}}(\widehat{RR}_1) / \widehat{RR}_1^2$$

is the estimate of the variance of the log column 1 relative risk, and where  $t_{df, \alpha/2}$  is the  $100(1 - \alpha/2)$  percentile of the  $t$  distribution with  $df$  degrees of freedom. The computation of  $df$  is described in the section “Degrees of Freedom” on page 7645. The value of the confidence coefficient  $\alpha$  is determined by the ALPHA= option, which by default equals 0.05 and produces 95% confidence limits.

If you request BRR variance estimation (VARMETHOD=BRR), PROC SURVEYFREQ estimates the variance of the column 1 relative risk as described in the section “Balanced Repeated Replication (BRR)” on page 7637. If you request jackknife variance estimation (VARMETHOD=JACKKNIFE), the procedure estimates the variance as described in the section “The Jackknife Method” on page 7640.

If you do not specify the VARMETHOD= option or a REPWEIGHTS statement, the default variance estimation method is Taylor series (VARMETHOD=TAYLOR). By using Taylor series linearization, the variance estimate for the column 1 relative risk can be expressed as

$$\widehat{\text{Var}}(\widehat{RR}_1) = \widehat{\mathbf{D}} \widehat{\mathbf{V}}(\widehat{\mathbf{X}}) \widehat{\mathbf{D}}'$$

where  $\widehat{\mathbf{V}}(\widehat{\mathbf{X}})$  is the covariance matrix of  $\widehat{\mathbf{X}}$ ,

$$\widehat{\mathbf{X}} = \left( \widehat{N}_{11}, \widehat{N}_{1.}, \widehat{N}_{21}, \widehat{N}_{2.} \right)$$

and  $\widehat{\mathbf{D}}$  is an array that contains the partial derivatives of the column 1 relative risk with respect to the elements of  $\widehat{\mathbf{X}}$ ,

$$\widehat{\mathbf{D}} = \left( \widehat{N}_{2.}/(\widehat{N}_{21}\widehat{N}_{1.}), -\widehat{N}_{11}\widehat{N}_{2.}/(\widehat{N}_{21}\widehat{N}_{1.}^2), -\widehat{N}_{11}\widehat{N}_{2.}/(\widehat{N}_{1.}\widehat{N}_{21}^2), \widehat{N}_{11}/(\widehat{N}_{21}\widehat{N}_{1.}) \right)$$

See Wolter (1985, pp. 239–242) for more information.

Confidence limits for the column 2 relative risk are computed similarly.

## Rao-Scott Chi-Square Test

The Rao-Scott chi-square test is a design-adjusted version of the Pearson chi-square test, which involves differences between observed and expected frequencies. For information about design-adjusted chi-square tests, see Lohr (2010, Section 10.3.2), Rao and Scott (1981, 1984, 1987); Thomas, Singh, and Roberts (1996).

PROC SURVEYFREQ provides a first-order Rao-Scott chi-square test by default. If you specify the **CHISQ(SECONDORDER)** option, PROC SURVEYFREQ provides a second-order (Satterthwaite) Rao-Scott chi-square test. The first-order design correction depends only on the design effects of the table cell proportion estimates and, for two-way tables, the design effects of the marginal proportion estimates. The second-order design correction requires computation of the full covariance matrix of the proportion estimates. The second-order test requires more computational resources than the first-order test, but it can provide some performance advantages (for Type I error and power), particularly when the design effects are variable (Thomas and Rao 1987; Rao and Thomas 1989).

### One-Way Tables

For one-way tables, the CHISQ option provides a Rao-Scott (design-based) goodness-of-fit test for one-way tables. By default, this is a test for the null hypothesis of equal proportions. If you specify null hypothesis proportions in the **TESTP=** option, the goodness-of-fit test uses the specified proportions.

**First-Order Test** The first-order Rao-Scott chi-square statistic for the goodness-of-fit test is computed as

$$Q_{RS1} = Q_P / D$$

where  $Q_P$  is the Pearson chi-square based on the estimated totals and  $D$  is the first-order design correction described in the section “[First-Order Design Correction](#)” on page 7653. See Rao and Scott (1979, 1981, 1984) for details.

For a one-way table with  $C$  levels, the Pearson chi-square is computed as

$$Q_P = (n/\hat{N}) \sum_c (\hat{N}_c - E_c)^2 / E_c$$

where  $n$  is the sample size,  $\hat{N}$  is the estimated overall total,  $\hat{N}_c$  is the estimated total for level  $c$ , and  $E_c$  is the expected total for level  $c$  under the null hypothesis. For the null hypothesis of equal proportions, the expected total for each level is

$$E_c = \hat{N} / C$$

For specified null proportions, the expected total for level  $c$  equals

$$E_c = \hat{N} \times P_c^0$$

where  $P_c^0$  is the null proportion that you specify for level  $c$ .

Under the null hypothesis, the first-order Rao-Scott chi-square  $Q_{RS1}$  approximately follows a chi-square distribution with  $(C - 1)$  degrees of freedom. A better approximation can be obtained by the  $F$  statistic,

$$F_1 = Q_{RS1} / (C - 1)$$

which has an  $F$  distribution with  $(C - 1)$  and  $\kappa(C - 1)$  degrees of freedom under the null hypothesis (Thomas and Rao 1984, 1987). The value of  $\kappa$  is the degrees of freedom for the variance estimator, which depends on the sample design and the variance estimation method. The section “[Degrees of Freedom](#)” on page 7645 describes the computation of  $\kappa$ .



**First-Order Design Correction** By default for one-way tables, the first-order design correction is computed from the proportion estimates as

$$D = \sum_c (1 - \hat{P}_c) \text{Deff}(\hat{P}_c) / (C - 1)$$

where

$$\begin{aligned} \text{Deff}(\hat{P}_c) &= \widehat{\text{Var}}(\hat{P}_c) / \text{Var}_{\text{srs}}(\hat{P}_c) \\ &= \widehat{\text{Var}}(\hat{P}_c) / \left( (1 - f) \hat{P}_c (1 - \hat{P}_c) / (n - 1) \right) \end{aligned}$$

as described in the section “**Design Effect**” on page 7646.  $\hat{P}_c$  is the proportion estimate for level  $c$ ,  $\widehat{\text{Var}}(\hat{P}_c)$  is the variance of the estimate,  $f$  is the overall sampling fraction, and  $n$  is the number of observations in the sample. The factor  $(1 - f)$  is included only for Taylor series variance estimation (**VARMETHOD=TAYLOR**) when you specify the **RATE=** or **TOTAL=** option. See the section “**Design Effect**” on page 7646 for details.

If you specify the **CHISQ(MODIFIED)** or **LRCHISQ(MODIFIED)** option, the design correction is computed by using null hypothesis proportions instead of proportion estimates. By default, null hypothesis proportions are equal proportions for all levels of the one-way table. Alternatively, you can specify null proportion values in the **TESTP=** option. The modified design correction  $D_0$  is computed from null hypothesis proportions as

$$D_0 = \sum_c (1 - P_c^0) \text{Deff}_0(\hat{P}_c) / (C - 1)$$

where

$$\begin{aligned} \text{Deff}_0(\hat{P}_c) &= \widehat{\text{Var}}(\hat{P}_c) / \text{Var}_{\text{srs}}(P_c^0) \\ &= \widehat{\text{Var}}(\hat{P}_c) / \left( (1 - f) P_c^0 (1 - P_c^0) / (n - 1) \right) \end{aligned}$$

The null hypothesis proportion  $P_c^0$  equals  $1/C$  for equal proportions (the default), or  $P_c^0$  equals the null proportion that you specify for level  $c$  if you use the **TESTP=** option.

**Second-Order Test** The second-order (Satterthwaite) Rao-Scott chi-square statistic for the goodness-of-fit test is computed as

$$Q_{RS2} = Q_{RS1} / (1 + \hat{a}^2)$$

where  $Q_{RS1}$  is the first-order Rao-Scott chi-square statistic described in the section “**First-Order Test**” on page 7652 and  $\hat{a}^2$  is the second-order design correction described in the section “**Second-Order Design Correction**” on page 7654. For details, see Rao and Scott (1979, 1981); Rao and Thomas (1989).

Under the null hypothesis, the second-order Rao-Scott chi-square  $Q_{RS2}$  approximately follows a chi-square distribution with  $(C - 1)/(1 + \hat{a}^2)$  degrees of freedom. The corresponding  $F$  statistic is

$$F_{RS2} = Q_{RS2} / (C - 1)$$

which has an  $F$  distribution with  $(C - 1)/(1 + \hat{a}^2)$  and  $\kappa(C - 1)/(1 + \hat{a}^2)$  degrees of freedom under the null hypothesis (Thomas and Rao 1984, 1987). The value of  $\kappa$  is the degrees of freedom for the variance estimator, which depends on the sample design and the variance estimation method. The section “**Degrees of Freedom**” on page 7645 describes the computation of  $\kappa$ .



**Second-Order Design Correction** The second-order (Satterthwaite) design correction for one-way tables is computed from the eigenvalues of the estimated design effects matrix  $\hat{\Delta}$ , which are known as *generalized design effects*. The design effects matrix is computed as

$$\hat{\Delta} = (n - 1)/(1 - f) \left( \text{Cov}_{\text{srs}}(\hat{\mathbf{P}})^{-1} \widehat{\text{Cov}}(\hat{\mathbf{P}}) \right)$$

where  $\text{Cov}_{\text{srs}}(\hat{\mathbf{P}})$  is the covariance under multinomial sampling (*srs* with replacement) and  $\widehat{\text{Cov}}(\hat{\mathbf{P}})$  is the covariance matrix of the first  $(C - 1)$  proportion estimates. See Rao and Scott (1979, 1981) and Rao and Thomas (1989) for details.

By default, the *srs* covariance matrix is computed from the proportion estimates as

$$\text{Cov}_{\text{srs}}(\hat{\mathbf{P}}) = \text{Diag}(\hat{\mathbf{P}}) - \hat{\mathbf{P}} \hat{\mathbf{P}}'$$

where  $\hat{\mathbf{P}}$  is an array of  $(C - 1)$  proportion estimates. If you specify the **CHISQ(MODIFIED)** or **LRCHISQ(MODIFIED)** option, the *srs* covariance matrix is computed from the null hypothesis proportions  $\mathbf{P}_0$  as

$$\text{Cov}_{\text{srs}}(\mathbf{P}_0) = \text{Diag}(\mathbf{P}_0) - \mathbf{P}_0 \mathbf{P}_0'$$

where  $\mathbf{P}_0$  is an array of  $(C - 1)$  null hypothesis proportions. The null hypothesis proportions equal  $1/C$  by default. If you use the **TESTP=** option to specify null hypothesis proportions,  $\mathbf{P}_0$  is an array of  $(C - 1)$  proportions that you specify.

The second-order design correction is computed as

$$\hat{a}^2 = \left( \sum_{c=1}^{C-1} d_c^2 / (C - 1) \bar{d}^2 \right) - 1$$

where  $d_c$  are the eigenvalues of the design effects matrix  $\hat{\Delta}$  and  $\bar{d}$  is the average of the eigenvalues.

### Two-Way Tables

For two-way tables, the **CHISQ** option provides a Rao-Scott (design-based) test of association between the row and column variables. PROC SURVEYFREQ provides a first-order Rao-Scott chi-square test by default. If you specify the **CHISQ(SECONDORDER)** option, PROC SURVEYFREQ provides a second-order (Satterthwaite) Rao-Scott chi-square test.

**First-Order Test** The first-order Rao-Scott chi-square statistic is computed as

$$Q_{RS1} = Q_P / D$$

where  $Q_P$  is the Pearson chi-square based on the estimated totals and  $D$  is the design correction described in the section “**First-Order Design Correction**” on page 7655. See Rao and Scott (1979, 1984, 1987) for details.

For a two-way tables with  $R$  rows and  $C$  columns, the Pearson chi-square is computed as

$$Q_P = (n/\hat{N}) \sum_r \sum_c (\hat{N}_{rc} - E_{rc})^2 / E_{rc}$$

where  $n$  is the sample size,  $\widehat{N}$  is the estimated overall total,  $\widehat{N}_{rc}$  is the estimated total for table cell  $(r, c)$ , and  $E_{rc}$  is the expected total for table cell  $(r, c)$  under the null hypothesis of no association,

$$E_{rc} = \widehat{N}_r \cdot \widehat{N}_{\cdot c} / \widehat{N}$$

Under the null hypothesis of no association, the first-order Rao-Scott chi-square  $Q_{RS1}$  approximately follows a chi-square distribution with  $(R - 1)(C - 1)$  degrees of freedom. A better approximation can be obtained by the  $F$  statistic,

$$F_1 = Q_{RS1} / (R - 1)(C - 1)$$

which has an  $F$  distribution with  $(R - 1)(C - 1)$  and  $\kappa(R - 1)(C - 1)$  degrees of freedom under the null hypothesis (Thomas and Rao 1984, 1987). The value of  $\kappa$  is the degrees of freedom for the variance estimator, which depends on the sample design and the variance estimation method. The section “[Degrees of Freedom](#)” on page 7645 describes the computation of  $\kappa$ .

**First-Order Design Correction** By default for a first-order test, PROC SURVEYFREQ computes the design correction from proportion estimates. If you specify the [CHISQ\(MODIFIED\)](#) or [LRCHISQ\(MODIFIED\)](#) option for a first-order test, the procedure computes the design correction from null hypothesis proportions.

Second-order tests, which you request by specifying the [CHISQ\(SECONDORDER\)](#) or [LRCHISQ\(SECONDORDER\)](#) option, are computed by applying both first-order and second-order design corrections to the weighted chi-square statistic. For second-order tests for two-way tables, PROC SURVEYFREQ always uses null hypothesis proportions to compute both the first-order and second-order design corrections.

The first-order design correction  $D$  that is based on proportion estimates is computed as

$$D = \left( \sum_r \sum_c (1 - \widehat{P}_{rc}) \text{Deff}(\widehat{P}_{rc}) - \sum_r (1 - \widehat{P}_{r\cdot}) \text{Deff}(\widehat{P}_{r\cdot}) - \sum_c (1 - \widehat{P}_{\cdot c}) \text{Deff}(\widehat{P}_{\cdot c}) \right) / (R - 1)(C - 1)$$

where

$$\begin{aligned} \text{Deff}(\widehat{P}_{rc}) &= \widehat{\text{Var}}(\widehat{P}_{rc}) / \text{Var}_{\text{srs}}(\widehat{P}_{rc}) \\ &= \text{Var}(\widehat{P}_{rc}) / \left( (1 - f) \widehat{P}_{rc} (1 - \widehat{P}_{rc}) / (n - 1) \right) \end{aligned}$$

as described in the section “[Design Effect](#)” on page 7646.  $\widehat{P}_{rc}$  is the estimate of the proportion in table cell  $(r, c)$ ,  $\widehat{\text{Var}}(\widehat{P}_{rc})$  is the variance of the estimate,  $f$  is the overall sampling fraction, and  $n$  is the number of observations in the sample. The factor  $(1 - f)$  is included only for Taylor series variance estimation ([VARMETHOD=TAYLOR](#)) when you specify the [RATE=](#) or [TOTAL=](#) option. See the section “[Design Effect](#)” on page 7646 for details.

The design effects for the estimate of the proportion in row  $r$  and the estimate of the proportion in column  $c$  ( $\text{Deff}(\widehat{P}_{r\cdot})$  and  $\text{Deff}(\widehat{P}_{\cdot c})$ , respectively) are computed in the same way.

If you specify the **CHISQ(MODIFIED)** or **LRCHISQ(MODIFIED)** option for a first-order Rao-Scott test, or if you request a second-order test for a two-way table (**CHISQ(SECONDORDER)** or **LRCHISQ(SECONDORDER)**), the procedure computes the design correction from the null hypothesis cell proportions instead of the estimated cell proportions. For two-way tables, the null hypothesis cell proportions are computed as the products of the corresponding row and column proportion estimates. The modified design correction  $D_0$  (based on null hypothesis proportions) is computed as

$$D_0 = \left( \sum_r \sum_c (1 - P_{rc}^0) \text{Deff}_0(\hat{P}_{rc}) - \sum_r (1 - \hat{P}_{r\cdot}) \text{Deff}(\hat{P}_{r\cdot}) - \sum_c (1 - \hat{P}_{\cdot c}) \text{Deff}(\hat{P}_{\cdot c}) \right) / (R - 1)(C - 1)$$

where

$$P_{rc}^0 = \hat{P}_{r\cdot} \times \hat{P}_{\cdot c}$$

and

$$\begin{aligned} \text{Deff}_0(\hat{P}_{rc}) &= \widehat{\text{Var}}(\hat{P}_{rc}) / \text{Var}_{\text{srs}}(P_{rc}^0) \\ &= \widehat{\text{Var}}(\hat{P}_{rc}) / ((1 - f) P_{rc}^0 (1 - P_{rc}^0) / (n - 1)) \end{aligned}$$

**Second-Order Test** The second-order (Satterthwaite) Rao-Scott chi-square statistic for two-way tables is computed as

$$Q_{RS2} = Q_{RS1} / (1 + \hat{a}^2)$$

where  $Q_{RS1}$  is the first-order Rao-Scott chi-square statistic described in the section “**First-Order Test**” on page 7654 and  $\hat{a}^2$  is the second-order design correction described in the section “**Second-Order Design Correction**” on page 7656. See Rao and Scott (1979, 1981) and Rao and Thomas (1989) for details.

Under the null hypothesis, the second-order Rao-Scott chi-square  $Q_{RS2}$  approximately follows a chi-square distribution with  $(R - 1)(C - 1)/(1 + \hat{a}^2)$  degrees of freedom. The corresponding  $F$  statistic is

$$F_{RS2} = Q_{RS2} (1 + \hat{a}^2) / (R - 1)(C - 1)$$

which has an  $F$  distribution with  $(R - 1)(C - 1)/(1 + \hat{a}^2)$  and  $\kappa(R - 1)(C - 1)/(1 + \hat{a}^2)$  degrees of freedom under the null hypothesis (Thomas and Rao 1984, 1987). The value of  $\kappa$  is the degrees of freedom for the variance estimator, which depends on the sample design and the variance estimation method. The section “**Degrees of Freedom**” on page 7645 describes the computation of  $\kappa$ .

**Second-Order Design Correction** The second-order (Satterthwaite) design correction for two-way tables is computed from the eigenvalues of the estimated design effects matrix  $\hat{\Delta}$ , which are known as *generalized design effects*. The design effects matrix is defined as

$$\hat{\Delta} = (n - 1)/(1 - f) \left( \text{Cov}_{\text{srs}}(\hat{\mathbf{P}})^{-1} \mathbf{H} \widehat{\text{Cov}}(\hat{\mathbf{P}}) \mathbf{H}' \right)$$

where  $\widehat{\text{Cov}}(\hat{\mathbf{P}})$  is the covariance matrix of the  $R \times C$  proportion estimates and  $\text{Cov}_{\text{srs}}(\hat{\mathbf{P}})$  is the covariance under multinomial sampling (*srs* with replacement). See Rao and Scott (1979, 1981) and Rao and Thomas (1989) for details.

The second-order design correction is computed from the design effects matrix  $\hat{\Delta}$  as

$$\hat{a}^2 = \left( \sum_{i=1}^K d_c^2 / K \bar{d}^2 \right) - 1$$

where  $K = (R - 1)(C - 1)$ ,  $d_c$  are the eigenvalues of  $\hat{\Delta}$ , and  $\bar{d}$  is the average eigenvalue.

The *srs* covariance matrix is computed as

$$\text{Cov}_{\text{srs}}(\hat{\mathbf{P}}) = \hat{\mathbf{P}}_r \otimes \hat{\mathbf{P}}_c$$

where  $\hat{\mathbf{P}}_r$  is an  $(R - 1) \times (R - 1)$  matrix that is constructed from the array of  $(R - 1)$  row proportion estimates  $\hat{\mathbf{p}}_r$  as

$$\hat{\mathbf{P}}_r = \text{Diag}(\hat{\mathbf{p}}_r) - \hat{\mathbf{p}}_r \hat{\mathbf{p}}_r'$$

Similarly,  $\hat{\mathbf{P}}_c$  is a  $(C - 1) \times (C - 1)$  matrix that is constructed from the array of  $(C - 1)$  column proportion estimates  $\hat{\mathbf{p}}_c$  as

$$\hat{\mathbf{P}}_c = \text{Diag}(\hat{\mathbf{p}}_c) - \hat{\mathbf{p}}_c \hat{\mathbf{p}}_c'$$

The  $(R - 1)(C - 1) \times (R - 1)(C - 1)$  matrix  $\mathbf{H}$  is computed as

$$\mathbf{H} = \mathbf{J}_r \otimes \mathbf{J}_c - (\hat{\mathbf{p}}_r \mathbf{l}_r') \otimes \mathbf{J}_c - \mathbf{J}_r \otimes (\hat{\mathbf{p}}_c \mathbf{l}_c')$$

where  $\mathbf{J}_r = (\mathbf{I}_{(R-1)} | \mathbf{0})$ ,  $\mathbf{J}_c = (\mathbf{I}_{(C-1)} | \mathbf{0})$ ,  $\mathbf{l}_r$  is an  $(R \times 1)$  array of ones, and  $\mathbf{l}_c$  is an  $(C \times 1)$  array of ones. See Rao and Scott (1979, p. 61) for details.

### Rao-Scott Likelihood Ratio Chi-Square Test

The Rao-Scott likelihood ratio chi-square test is a design-adjusted version of the likelihood ratio test, which involves ratios of observed and expected frequencies. For details about design-adjusted chi-square tests, see Lohr (2010, Section 10.3.2), Rao and Scott (1981, 1984, 1987); Thomas, Singh, and Roberts (1996).

PROC SURVEYFREQ provides a first-order Rao-Scott likelihood ratio test by default. If you specify the **LRCHISQ(SECONDORDER)** option, PROC SURVEYFREQ provides a second-order (Satterthwaite) likelihood ratio chi-square test.

The procedure computes the Rao-Scott likelihood ratio test by applying design adjustments to the weighted likelihood ratio statistic that is based on estimated totals. This computation is identical to the Rao-Scott chi-square test computation except that it uses the likelihood ratio statistic  $G^2$  in place of the Pearson chi-square statistic  $Q_P$ . See the section “**Rao-Scott Chi-Square Test**” on page 7652 for details.

#### One-Way Tables

For one-way tables, the LRCHISQ option provides a Rao-Scott (design-based) goodness-of-fit test for one-way tables. By default, this is a test for the null hypothesis of equal proportions. If you specify null hypothesis proportions in the **TESTP=** option, the goodness-of-fit test uses the specified proportions.

The Rao-Scott likelihood ratio test uses the likelihood ratio statistic that is based on the estimated totals,

$$G^2 = 2 (n / \hat{N}) \sum_c \hat{N}_c \ln (\hat{N}_c / E_c)$$

where  $n$  is the sample size,  $\widehat{N}$  is the estimated overall total,  $\widehat{N}_c$  is the estimated total for level  $c$ , and  $E_c$  is the expected total for level  $c$  under the null hypothesis. For the null hypothesis of equal proportions, the expected total for each level equals

$$E_c = \widehat{N} / C$$

For specified null proportions, the expected total for level  $c$  equals

$$E_c = \widehat{N} \times P_c^0$$

where  $P_c^0$  is the null proportion that you specify for level  $c$ .

The computation of the Rao-Scott likelihood ratio test for one-way tables uses  $G^2$  in place of  $Q_P$  in the Rao-Scott chi-square test computation and is otherwise identical to the chi-square test computation. See the sections “[First-Order Test](#)” on page 7652 and “[Second-Order Test](#)” on page 7653 for details.

If you specify the **LRCHISQ(MODIFIED)** option, PROC SURVEYFREQ computes the design corrections by using null hypothesis proportions instead of proportion estimates. By default, null hypothesis proportions are equal proportions for all levels of the one-way table. Alternatively, you can specify null proportion values in the **TESTP=** option.

### Two-Way Tables

For two-way tables, the **LRCHISQ** option provides a Rao-Scott (design-based) test of association between the row and column variables.

The Rao-Scott likelihood ratio test uses the likelihood ratio statistic that is based on the estimated totals,

$$G^2 = 2(n/\widehat{N}) \sum_r \sum_c \widehat{N}_{rc} \ln(\widehat{N}_{rc} / E_{rc})$$

where  $n$  is the sample size,  $\widehat{N}$  is the estimated overall total,  $\widehat{N}_{rc}$  is the estimated total for table cell  $(r, c)$ , and  $E_{rc}$  is the expected total for cell  $(r, c)$  under the null hypothesis of no association. The expected total for cell  $(r, c)$  equals

$$E_{rc} = \widehat{N}_r \cdot \widehat{N}_{\cdot c} / \widehat{N}$$

The computation of the Rao-Scott likelihood ratio test for two-way tables uses  $G^2$  in place of  $Q_P$  in the Rao-Scott chi-square test computation and is otherwise identical to the chi-square test computation. See the sections “[First-Order Test](#)” on page 7654 and “[Second-Order Test](#)” on page 7656 for details.

By default for a first-order test, PROC SURVEYFREQ computes the design correction from proportion estimates. If you specify the **LRCHISQ(MODIFIED)** option for a first-order test, the procedure computes the design correction from null hypothesis proportions.

Second-order tests, which you request by specifying the **LRCHISQ(SECONDORDER)** option, are computed by applying both first-order and second-order design corrections to the weighted likelihood ratio statistic. For second-order tests for two-way tables, PROC SURVEYFREQ always uses null hypothesis proportions to compute both the first-order and second-order design corrections.

## Wald Chi-Square Test

PROC SURVEYFREQ provides two Wald chi-square tests for independence of the row and column variables in a two-way table: a Wald chi-square test based on the difference between observed and expected weighted cell frequencies, and a Wald log-linear chi-square test based on the log odds ratios. These statistics test for independence of the row and column variables in two-way tables, taking into account the complex survey design. For information about Wald statistics and their applications to categorical data analysis, see Bedrick (1983); Koch, Freeman, and Freeman (1975); Wald (1943).

For these two tests, PROC SURVEYFREQ computes the generalized Wald chi-square statistic, the corresponding Wald  $F$  statistic, and also an adjusted Wald  $F$  statistic for tables larger than  $2 \times 2$ . Under the null hypothesis of independence, the Wald chi-square statistic approximately follows a chi-square distribution with  $(R - 1)(C - 1)$  degrees of freedom for large samples. However, it has been shown that this test can perform poorly in terms of actual significance level and power, especially for tables with a large number of cells or for samples with a relatively small number of clusters. See Thomas and Rao (1984, 1985) and Lohr (2010) for more information. See Felligi (1980) and Hidiroglou, Fuller, and Hickman (1980) for information about the adjusted Wald  $F$  statistic. Thomas and Rao (1984) found that the adjusted Wald  $F$  statistic provides a more stable test than the chi-square statistic, although its power can be low when the number of sample clusters is not large. See also Korn and Graubard (1990) and Thomas, Singh, and Roberts (1996).

If you specify the **WCHISQ** option in the TABLES statement, PROC SURVEYFREQ computes a Wald test for independence in the two-way table based on the differences between the observed (weighted) cell frequencies and the expected frequencies.

Under the null hypothesis of independence of the row and column variables, the expected cell frequencies are computed as

$$E_{rc} = \hat{N}_r \cdot \hat{N}_{\cdot c} / \hat{N}$$

where  $\hat{N}_r$  is the estimated total for row  $r$ ,  $\hat{N}_{\cdot c}$  is the estimated total for column  $c$ , and  $\hat{N}$  is the estimated overall total, as described in the section “[Expected Weighted Frequency](#)” on page 7647. The null hypothesis that the population weighted frequencies equal the expected frequencies can be expressed as

$$H_0: Y_{rc} - N_{rc} - E_{rc} = 0$$

for all  $r = 1, \dots, (R - 1)$  and  $c = 1, \dots, (C - 1)$ . This null hypothesis can be stated equivalently in terms of cell proportions, with the expected cell proportions computed as the products of the marginal row and column proportions.

The generalized Wald chi-square statistic  $Q_W$  is computed as

$$Q_W = \hat{Y}' (\mathbf{H} \hat{\mathbf{V}}(\hat{\mathbf{N}}) \mathbf{H}')^{-1} \hat{Y}$$

where  $\hat{Y}$  is an array of  $(R - 1)(C - 1)$  differences between the observed and expected weighted frequencies  $(\hat{N}_{rc} - E_{rc})$ , and  $(\mathbf{H} \hat{\mathbf{V}}(\hat{\mathbf{N}}) \mathbf{H}')$  estimates the variance of  $\hat{Y}$ .

$\hat{\mathbf{V}}(\hat{\mathbf{N}})$  is the covariance matrix of the estimates  $\hat{N}_{rc}$ , and its computation is described in the section “[Covariance of Totals](#)” on page 7633.

$\mathbf{H}$  is an  $(R - 1)(C - 1)$  by  $RC$  matrix that contains the partial derivatives of the elements of  $\hat{\mathbf{Y}}$  with respect to the elements of  $\hat{\mathbf{N}}$ . The elements of  $\mathbf{H}$  are computed as follows, where  $a$  denotes a row different from row  $r$ , and  $b$  denotes a column different from column  $c$ :

$$\partial \hat{Y}_{rc} / \partial \hat{N}_{rc} = 1 - \left( \hat{N}_{r\cdot} + \hat{N}_{\cdot c} - \hat{N}_{\cdot c} \hat{N}_{r\cdot} / \hat{N} \right) / \hat{N}$$

$$\partial \hat{Y}_{rc} / \partial \hat{N}_{ac} = - \left( \hat{N}_{r\cdot} - \hat{N}_{r\cdot} \hat{N}_{\cdot c} / \hat{N} \right) / \hat{N}$$

$$\partial \hat{Y}_{rc} / \partial \hat{N}_{rb} = - \left( \hat{N}_{\cdot c} - \hat{N}_{r\cdot} \hat{N}_{\cdot c} / \hat{N} \right) / \hat{N}$$

$$\partial \hat{Y}_{rc} / \partial \hat{Y}_{ab} = \hat{N}_{r\cdot} \hat{N}_{\cdot c} / \hat{N}^2$$

Under the null hypothesis of independence, the statistic  $Q_W$  approximately follows a chi-square distribution with  $(R - 1)(C - 1)$  degrees of freedom for large samples.

PROC SURVEYFREQ computes the Wald  $F$  statistic as

$$F_W = Q_W / (R - 1)(C - 1)$$

Under the null hypothesis of independence,  $F_W$  approximately follows an  $F$  distribution with  $(R - 1)(C - 1)$  numerator degrees of freedom. The denominator degrees of freedom are the degrees of freedom for the variance estimator and depend on the sample design and the variance estimation method. The section “Degrees of Freedom” on page 7645 describes the computation of the denominator degrees of freedom. Alternatively, you can specify the denominator degrees of freedom with the `DF=` option in the TABLES statement.

For tables larger than  $2 \times 2$ , PROC SURVEYFREQ also computes the adjusted Wald  $F$  statistic as

$$F_{Adj\_W} = Q_W (s - k + 1) / (ks)$$

where  $k = (R - 1)(C - 1)$ , and  $s$  is the degrees of freedom, which are computed as described in the section “Degrees of Freedom” on page 7645. Alternatively, you can specify the value of  $s$  with the `DF=` option in the TABLES statement. Note that for  $2 \times 2$  tables,  $k = (R - 1)(C - 1) = 1$ , and therefore the adjusted Wald  $F$  statistic equals the (unadjusted) Wald  $F$  statistic, with the same numerator and denominator degrees of freedom.

Under the null hypothesis,  $F_{Adj\_W}$  approximately follows an  $F$  distribution with  $k$  numerator degrees of freedom and  $(s - k + 1)$  denominator degrees of freedom.

### Wald Log-Linear Chi-Square Test

If you specify the `WLLCHISQ` option in the TABLES statement, PROC SURVEYFREQ computes a Wald test for independence based on the log odds ratios. See the section “Wald Chi-Square Test” on page 7659 for more information about Wald tests.

For a two-way table of  $R$  rows and  $C$  columns, the Wald log-linear test is based on the  $(R - 1)(C - 1)$ -dimensional array of elements  $\hat{Y}_{rc}$ ,

$$\hat{Y}_{rc} = \log \hat{N}_{rc} - \log \hat{N}_{rC} - \log \hat{N}_{RC} + \log \hat{N}_{RC}$$

where  $\hat{N}_{rc}$  is the estimated total for table cell  $(r, c)$ . The null hypothesis of independence between the row and column variables can be expressed as  $H_0: Y_{rc} = 0$  for all  $r = 1, \dots, (R - 1)$  and  $c = 1, \dots, (C - 1)$ . This null hypothesis can be stated equivalently in terms of cell proportions.

The generalized Wald log-linear chi-square statistic is computed as

$$Q_L = \hat{\mathbf{Y}}' \hat{\mathbf{V}}(\hat{\mathbf{Y}})^{-1} \hat{\mathbf{Y}}$$

where  $\hat{\mathbf{Y}}$  is the  $(R - 1)(C - 1)$ -dimensional array of the  $\hat{Y}_{rc}$ , and  $\hat{\mathbf{V}}(\hat{\mathbf{Y}})$  estimates the variance of  $\hat{\mathbf{Y}}$ ,

$$\hat{\mathbf{V}}(\hat{\mathbf{Y}}) = \mathbf{A} \mathbf{D}^{-1} \hat{\mathbf{V}}(\hat{\mathbf{N}}) \mathbf{D}^{-1} \mathbf{A}'$$

where  $\hat{\mathbf{V}}(\hat{\mathbf{N}})$  is the covariance matrix of the estimates  $\hat{N}_{rc}$ , which is computed as described in the section “Covariance of Totals” on page 7633.  $\mathbf{D}$  is a diagonal matrix with the estimated totals  $\hat{N}_{rc}$  on the diagonal, and  $\mathbf{A}$  is the  $(R - 1)(C - 1)$  by  $RC \times RC$  linear contrast matrix.

Under the null hypothesis of independence, the statistic  $Q_L$  approximately follows a chi-square distribution with  $(R - 1)(C - 1)$  degrees of freedom for large samples.

PROC SURVEYFREQ computes the Wald log-linear  $F$  statistic as

$$F_L = Q_L / (R - 1)(C - 1)$$

Under the null hypothesis of independence,  $F_L$  approximately follows an  $F$  distribution with  $(R - 1)(C - 1)$  numerator degrees of freedom. PROC SURVEYFREQ computes the denominator degrees of freedom as described in the section “Degrees of Freedom” on page 7645. Alternatively, you can specify the denominator degrees of freedom with the **DF=** option in the TABLES statement.

For tables larger than  $2 \times 2$ , PROC SURVEYFREQ also computes the adjusted Wald log-linear  $F$  statistic as

$$F_{Adj\_L} = Q_L (s - k + 1) / (ks)$$

where  $k = (R - 1)(C - 1)$ , and  $s$  is the denominator degrees of freedom, which is computed as described in the section “Degrees of Freedom” on page 7645. Alternatively, you can specify the value of  $s$  with the **DF=** option in the TABLES statement. Note that for  $2 \times 2$  tables,  $k = (R - 1)(C - 1) = 1$ , and therefore the adjusted Wald  $F$  statistic equals the (unadjusted) Wald  $F$  statistic, with the same numerator and denominator degrees of freedom.

Under the null hypothesis,  $F_{Adj\_L}$  approximately follows an  $F$  distribution with  $k$  numerator degrees of freedom and  $(s - k + 1)$  denominator degrees of freedom.

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## Output Data Sets

You can use the Output Delivery System to create a SAS data set from any piece of PROC SURVEYFREQ output. See the section “ODS Table Names” on page 7668 and [Example 90.3](#) for more information.

PROC SURVEYFREQ also provides an output data set that stores the replicate weights for BRR or jackknife variance estimation and an output data set that stores the jackknife coefficients for jackknife variance estimation.



## Replicate Weight Output Data Set

If you specify the `OUTWEIGHTS= method-option` for `VARMETHOD=BRR` or `VARMETHOD=JACKKNIFE`, PROC SURVEYFREQ stores the replicate weights in an output data set. The `OUTWEIGHTS=` output data set contains all observations from the `DATA=` input data set that are valid (used in the analysis). A valid observation must have a positive value of the `WEIGHT` variable. A valid observations must also have nonmissing values of the `STRATA` and `CLUSTER` variables unless you specify the `MISSING` option in the PROC SURVEYFREQ statement. See the section “Data Summary Table” on page 7663 for details about valid observations.

The `OUTWEIGHTS=` data set contains the following variables:

- all variables in the `DATA=` input data set
- `RepWt_1`, `RepWt_2`, . . . , `RepWt_n`, which are the replicate weight variables, where `n` is the total number of replicates in the analysis

Each replicate weight variable contains the replicate weights for the corresponding replicate. Replicate weights equal zero for those observations not included in the replicate.

After the procedure creates and stores replicate weights for a particular input data set and survey design, you can use them again in subsequent analyses, either in PROC SURVEYFREQ or in another survey procedure. You use a `REPWEIGHTS` statement to provide replicate weights to the procedure.

## Jackknife Coefficient Output Data Set

If you specify the `OUTJKCOEFS= method-option` for `VARMETHOD=JACKKNIFE`, PROC SURVEYFREQ stores the jackknife coefficients in an output data set. The `OUTJKCOEFS=` output data set contains one observation for each replicate. The `OUTJKCOEFS=` data set contains the following variables:

- `Replicate`, which is the replicate number for the jackknife coefficient
- `JKCoefficient`, which is the jackknife coefficient
- `DonorStratum`, which is the stratum of the PSU that was deleted to construct the replicate, if you specify a `STRATA` statement

After the procedure creates jackknife coefficients for a particular input data set and survey design, you can use the `OUTJKCOEFS= method-option` to store these coefficients and then use them again in subsequent analyses, either in PROC SURVEYFREQ or in another survey procedure. You use the `JKCOEFS=` option in the `REPWEIGHTS` statement to provide jackknife coefficients for the procedure.

---

## Displayed Output

### Data Summary Table

The “Data Summary” table provides information about the input data set and the sample design. PROC SURVEYFREQ displays this table unless you specify the **NOSUMMARY** option in the PROC SURVEYFREQ statement.

The “Data Summary” table displays the total number of valid observations. To be considered *valid*, an observation must have a nonmissing, positive sampling weight value if you specify a **WEIGHT** statement. If you do not specify the **MISSING** option, a valid observation must also have nonmissing values for all **STRATA** and **CLUSTER** variables. The number of valid observations can differ from the number of nonmissing observations for an individual table request, which the procedure displays in the frequency or crosstabulation tables. See the section “Missing Values” on page 7627 for more information.

PROC SURVEYFREQ displays the following information in the “Data Summary” table:

- Number of Strata, if you specify a **STRATA** statement
- Number of Clusters, if you specify a **CLUSTER** statement
- Number of Observations, which is the total number of valid observations
- Sum of Weights, which is the sum over all valid observations, if you specify a **WEIGHT** or **REPWEIGHTS** statement

### Stratum Information Table

If you specify the **LIST** option in the **STRATA** statement, PROC SURVEYFREQ displays a “Stratum Information” table. This table provides the following information for each stratum:

- Stratum Index, which is a sequential stratum identification number
- **STRATA** variables, which list the levels of **STRATA** variables for the stratum
- Number of Observations, which is the number of valid observations in the stratum
- Population Total for the stratum, if you specify the **TOTAL=** option
- Sampling Rate for the stratum, if you specify the **TOTAL=** or **RATE=** option. If you specify the **TOTAL=** option, the sampling rate is based on the number of valid observations in the stratum.
- Number of Clusters, which is the number of clusters in the stratum, if you specify a **CLUSTER** statement

## Variance Estimation Table

If you specify the `VARMETHOD=BRR`, `VARMETHOD=JACKKNIFE`, or `NOMCAR` option in the PROC SURVEYFREQ statement, the procedure displays a “Variance Estimation” table. If you do not specify any of these options, the procedure creates a “Variance Estimation” table but does not display it. You can store this nondisplayed table in an output data set by using the Output Delivery System (ODS). See the section “ODS Table Names” on page 7668 for more information.

The “Variance Estimation” table provides the following information:

- Method, which is the variance estimation method—Taylor Series, Balanced Repeated Replication, or Jackknife
- Replicate Weights input data set name, if you provide replicate weights with a `REPWEIGHTS` statement
- Number of Replicates, for `VARMETHOD=BRR` or `VARMETHOD=JACKKNIFE`
- Hadamard Data Set name, if you specify the `HADAMARD= method-option` for `VARMETHOD=BRR`
- Fay Coefficient, if you specify the `FAY method-option` for `VARMETHOD=BRR`
- Missing Levels Included (MISSING), if you specify the `MISSING` option
- Missing Levels Included (NOMCAR), if you specify the `NOMCAR` option

## Hadamard Matrix

If you specify the `PRINTH method-option` for `VARMETHOD=BRR`, PROC SURVEYFREQ displays the Hadamard matrix used to construct replicates for BRR variance estimation. If you provide a Hadamard matrix with the `HADAMARD= method-option` for `VARMETHOD=BRR` but the procedure does not use the entire matrix, the procedure displays only the rows and columns that are actually used to construct replicates.

## One-Way Frequency Tables

PROC SURVEYFREQ displays one-way frequency tables for all one-way table requests in the `TABLES` statements, unless you specify the `NOPRINT` option in the `TABLES` statement. A one-way table shows the sample frequency distribution of a single variable, and provides estimates for its population distribution in terms of totals and proportions.

If you request a one-way table without specifying options, PROC SURVEYFREQ displays the following information for each level of the variable:

- Frequency count, which is the number of sample observations in the level
- Weighted Frequency, which estimates the population total for the level
- Standard Deviation of Weighted Frequency
- Percent, which estimates the population proportion for the level
- Standard Error of Percent

The one-way table displays weighted frequencies if your analysis includes a **WEIGHT** or **REPWEIGHTS** statement, or if you specify the **WTFREQ** option in the **TABLES** statement.

The one-way table also displays the Frequency Missing, which is the number of observations with missing values.

You can suppress the frequency counts by specifying the **NOFREQ** option in the **TABLES** statement. Also, the **NOWT** option suppresses the weighted frequencies and their standard deviations. The **NOPERCENT** option suppresses the percentages and their standard errors. The **NOSTD** option suppresses the standard errors of the percentages and the standard deviations of the weighted frequencies. The **NOTOTAL** option suppresses the total row of the one-way table.

**PROC SURVEYFREQ** optionally displays the following information in a one-way table:

- Variance of Weighted Frequency, if you specify the **VARWT** option
- Confidence Limits for Weighted Frequency, if you specify the **CLWT** option
- Coefficient of Variation for Weighted Frequency, if you specify the **CVWT** option
- Test Percent, if you specify the **TESTP=** option
- Variance of Percent, if you specify the **VAR** option
- Confidence Limits for Percent, if you specify the **CL** option
- Coefficient of Variation for Percent, if you specify the **CV** option
- Design Effect for Percent, if you specify the **DEFF** option

## Crosstabulation Tables

**PROC SURVEYFREQ** displays all table requests in the **TABLES** statements, unless you specify the **NOPRINT** option in the **TABLES** statement. For two-way to multiway crosstabulation tables, the values of the last variable in the table request form the table columns. The values of the next-to-last variable form the rows. Each level (or combination of levels) of the other variables forms one layer. **PROC SURVEYFREQ** produces a separate two-way crosstabulation table for each layer of a multiway table.

For each layer, the crosstabulation table displays the row and column variable names and values (levels). Each two-way table lists levels of the column variable within each level of the row variable.

By default, the procedure displays all levels of the column variable within each level of the row variables, including any column variable levels with zero frequency for that row. For multiway tables, the procedure displays all levels of the row variable for each layer of the table by default, including any row levels with zero frequency for that layer. You can suppress the display of zero frequency levels by specifying the **NOSPARE** option.

If you request a crosstabulation table without specifying options, the table displays the following information for each combination of variable levels (table cell):

- Frequency, which is the number of sample observations in the table cell
- Weighted Frequency, which estimates the population total for the table cell

- Standard Deviation of Weighted Frequency
- Percent, which estimates the population proportion for the table cell
- Standard Error of Percent

The two-way table displays weighted frequencies if your analysis includes a **WEIGHT** or **REPWEIGHTS** statement, or if you specify the **WTFREQ** option in the **TABLES** statement.

The two-way table also displays the Frequency Missing, which is the number of observations with missing values.

You can suppress the frequency counts by specifying the **NOFREQ** option in the **TABLES** statement. Also, the **NOWT** option suppresses the weighted frequencies and their standard deviations. The **NOPERCENT** option suppresses all percentages and their standard errors. The **NOCELLPERCENT** option suppresses overall cell percentages and their standard errors, but displays any other percentages (and standard errors) that you request, such as row or column percentages. The **NOSTD** option suppresses the standard errors of the percentages and the standard deviations of the weighted frequencies. The **NOTOTAL** option suppresses the row totals and column totals, as well as the overall total.

PROC SURVEYFREQ optionally displays the following information in a two-way table:

- Expected Weighted Frequency, if you specify the **EXPECTED** option
- Variance of Weighted Frequency, if you specify the **VARWT** option
- Confidence Limits for Weighted Frequency, if you specify the **CLWT** option
- Coefficient of Variation for Weighted Frequency, if you specify the **CVWT** option
- Variance of Percent, if you specify the **VAR** option
- Confidence Limits for Percent, if you specify the **CL** option
- Coefficient of Variation for Percent, if you specify the **CV** option
- Design Effect for Percent, if you specify the **DEFF** option
- Row Percent, which estimates the population proportion of the row total, if you specify the **ROW** option
- Standard Error of Row Percent, if you specify the **ROW** option
- Variance of Row Percent, if you specify the **VAR** option and the **ROW** option
- Confidence Limits for Row Percent, if you specify the **CL** option and the **ROW** option
- Coefficient of Variation for Row Percent, if you specify the **CV** option and the **ROW** option
- Design Effect for Row Percent, if you specify the **ROW(DEFF)** option
- Column Percent, which estimates the population proportion of the column total, if you specify the **COLUMN** option
- Standard Error of Column Percent, if you specify the **COLUMN** option

- Variance of Column Percent, if you specify the **VAR** option and the **COLUMN** option
- Confidence Limits for Column Percent, if you specify the **CL** option and the **COLUMN** option
- Coefficient of Variation for Column Percent, if you specify the **CV** option and the **COLUMN** option
- Design Effects for Column Percent, if you specify the **COLUMN(DEFF)** option

## Statistical Tests

If you specify the **CHISQ** option for the Rao-Scott chi-square test or the **LRCHISQ** option for the Rao-Scott likelihood ratio chi-square test, PROC SURVEYFREQ displays the following information:

- Pearson Chi-Square, if you specify the **CHISQ** option
- Likelihood Ratio Chi-Square, if you specify the **LRCHISQ** option
- Design Correction
- Rao-Scott Chi-Square, by default or if you specify the **FIRSTORDER** option
- First-Order Chi-Square, if you specify the **SECONDORDER** option
- Second-Order Chi-Square, if you specify the **SECONDORDER** option
- DF, which is the degrees of freedom for the chi-square test
- Pr > ChiSq, which is the  $p$ -value for the chi-square test
- F Value
- Num DF, which is the numerator degrees of freedom for F
- Den DF, which is the denominator degrees of freedom for F
- Pr > F, which is the  $p$ -value for the  $F$  test

If you specify the **WCHISQ** option for the Wald chi-square test or the **WLLCHISQ** option for the Wald log-linear chi-square test, PROC SURVEYFREQ displays the following information:

- Wald Chi-Square, if you specify the **WCHISQ** option
- Wald Log-Linear Chi-Square, if you specify the **WLLCHISQ** option
- F Value
- Num DF, which is the numerator degrees of freedom for F
- Den DF, which is the denominator degrees of freedom for F
- Pr > F, which is the  $p$ -value for the  $F$  test
- Adjusted F Value, for tables larger than  $2 \times 2$

- Num DF, which is the numerator degrees of freedom for Adjusted F
- Den DF, which is the denominator degrees of freedom for Adjusted F
- Pr > Adj F, which is the  $p$ -value for the Adjusted  $F$  test

## Risks and Risk Difference

If you specify the **RISK** option in the TABLES statement for a  $2 \times 2$  table, PROC SURVEYFREQ displays “Column 1 Risk Estimates” and “Column 2 Risk Estimates” tables. You can display only column 1 or column 2 risks by specifying the **RISK1** or **RISK2** option, respectively.

The “Risk Estimates” table displays the following information for Row 1, Row 2, Total, and Difference:

- Row, which identifies the risk as Row 1, Row 2, Total, or Difference
- Risk estimate
- Standard Error
- Confidence Limits

In the “Column 1 Risk Estimates” table, the row 1 risk is the column 1 percentage of row 1. The row 2 risk is the column 1 percentage of row 2, and the total risk is the column 1 percentage of the entire table. The risk difference is the row 1 risk minus the row 2 risk. In the “Column 2 Risk Estimates” table, these computations are based on column 2.

## Odds Ratio and Relative Risks

If you specify the **OR** option in the TABLES statement for a  $2 \times 2$  table, PROC SURVEYFREQ displays the “Odds Ratio” table. This table includes the following information:

- Statistic, which identifies the statistic as the Odds Ratio, the Column 1 Relative Risk, or the Column 2 Relative Risk
- Estimate
- Confidence Limits

---

## ODS Table Names

PROC SURVEYFREQ assigns a name to each table that it creates. You can use these names to refer to tables when you use the Output Delivery System (ODS) to select tables and create output data sets. For more information about ODS, see Chapter 20, “Using the Output Delivery System.” See Example 90.3 for examples of storing PROC SURVEYFREQ tables as output data sets.

Table 90.8 lists the ODS table names together with their descriptions and the options required to produce the tables.

**Table 90.8** ODS Tables Produced by PROC SURVEYFREQ

| ODS Table Name     | Description                     | Statement         | Option                                              |
|--------------------|---------------------------------|-------------------|-----------------------------------------------------|
| ChiSq              | Chi-square test                 | TABLES            | CHISQ                                               |
| ChiSq1             | Modified chi-square test        | TABLES            | CHISQ(MODIFIED)                                     |
| CrossTabs          | Crosstabulation table           | TABLES            | <i>n</i> -way table request, <i>n</i> > 1           |
| HadamardMatrix     | Hadamard matrix                 | PROC              | VARMETHOD=BRR(PRINTH)                               |
| LRChiSq            | Likelihood ratio test           | TABLES            | LRCHISQ                                             |
| LRChiSq1           | Modified likelihood ratio test  | TABLES            | LRCHISQ(MODIFIED)                                   |
| OddsRatio          | Odds ratio and relative risks   | TABLES            | OR (2 × 2 table)                                    |
| OneWay             | One-way frequency table         | PROC<br>or TABLES | No TABLES statement<br>One-way table request        |
| Risk1              | Column 1 risk estimates         | TABLES            | RISK or RISK1 (2 × 2 table)                         |
| Risk2              | Column 2 risk estimates         | TABLES            | RISK or RISK2 (2 × 2 table)                         |
| StrataInfo         | Stratum information             | STRATA            | LIST                                                |
| Summary            | Data summary                    | PROC              | Default                                             |
| TableSummary       | Table summary (not displayed)   | TABLES            | Default                                             |
| VarianceEstimation | Variance estimation             | PROC              | VARMETHOD=BRR,<br>VARMETHOD=JACKKNIFE,<br>or NOMCAR |
| WChiSq             | Wald chi-square test            | TABLES            | WCHISQ (two-way table)                              |
| WLLChiSq           | Wald log-linear chi-square test | TABLES            | WLLCHISQ (two-way table)                            |

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “Statistical Graphics Using ODS.”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “A Primer on ODS Statistical Graphics” on page 599 in Chapter 21, “Statistical Graphics Using ODS.”

When ODS Graphics is enabled, you can request specific plots with the PLOTS= option in the TABLES statement. To produce a weighted frequency plot, you must specify the WTFREQPLOT *plot-request* in the PLOTS= option. By default, PROC SURVEYFREQ produces all other plots that are associated with the analyses that you request in the TABLES statement. You can suppress default plots and request specific plots by using the PLOTS(ONLY)= option. See the description of the PLOTS= option for more information.

PROC SURVEYFREQ assigns a name to each graph that it creates with ODS Graphics. You can use these names to refer to the graphs. Table 90.9 lists the names of the graphs that PROC SURVEYFREQ generates together with their descriptions, their PLOTS= options (*plot-requests*), and the TABLES statement options that are required to produce the graphs.



**Table 90.9** ODS Graphs Produced by PROC SURVEYFREQ

| ODS Graph Name | Description             | PLOTS= Option | TABLES Statement Option             |
|----------------|-------------------------|---------------|-------------------------------------|
| WtFreqPlot     | Weighted frequency plot | WTFREQPLOT    | Any table request                   |
| ORPlot         | Odds ratio plot         | ODDSRATIOPLOT | OR ( $h \times 2 \times 2$ table)   |
| RelRiskPlot    | Relative risk plot      | RELRIKSPLOT   | OR ( $h \times 2 \times 2$ table)   |
| RiskDiffPlot   | Risk difference plot    | RISKDIFFPLOT  | RISK ( $h \times 2 \times 2$ table) |

## Examples: SURVEYFREQ Procedure

### Example 90.1: Two-Way Tables

This example uses the SIS\_Survey data set from the section “Getting Started: SURVEYFREQ Procedure” on page 7588. The data set contains results from a customer satisfaction survey for a student information system (SIS).

The following PROC SURVEYFREQ statements request a two-way table for Department by Response and customize the crosstabulation table display:

```

title 'Student Information System Survey';
proc surveyfreq data=SIS_Survey;
 tables Department * Response / cv deff nowt nostd nototal;
 strata State NewUser / list;
 cluster School;
 weight SamplingWeight;
run;

```

The TABLES statement requests a two-way table of Department by Response. The CV option requests coefficients of variation for the percentage estimates. The DEFF option requests design effects for the percentage estimates. The NOWT option suppresses display of the weighted frequencies, and the NOSTD option suppresses display of standard errors for the estimates. The NOTOTAL option suppresses the row totals, column totals, and overall totals.

The STRATA, CLUSTER, and WEIGHT statements provide sample design information for the procedure, so that the analysis is done according to the sample design used for the survey. The STRATA statement names the variables State and NewUser, which identify the first-stage strata. The LIST option in the STRATA statement requests a “Stratum Information” table. The CLUSTER statement names the variable School, which identifies the clusters (primary sampling units). The WEIGHT statement names the sampling weight variable.

Output 90.1.1 displays the “Data Summary” and “Stratum Information” tables produced by PROC SURVEYFREQ. The “Stratum Information” table lists the six strata in the survey and shows the number of observations and the number of clusters (schools) in each stratum.

**Output 90.1.1** Data Summary and Stratum Information

```

Student Information System Survey

The SURVEYFREQ Procedure

Data Summary

Number of Strata 6
Number of Clusters 370
Number of Observations 1850
Sum of Weights 38899.6482

Stratum Information

Stratum Index State NewUser Number of Number of
 State NewUser Obs Clusters

1 GA Renewal Customer 315 63
2 GA New Customer 355 71
3 NC Renewal Customer 280 56
4 NC New Customer 420 84
5 SC Renewal Customer 210 42
6 SC New Customer 270 54

```

Output 90.1.2 displays the two-way table of Department by Response. According to the TABLES statement options that are specified, this two-way table includes coefficients of variation and design effects for the percentage estimates, and it does not show the weighted frequencies or the standard errors of the estimates. It also does not show the row, column, and overall totals.

**Output 90.1.2** Two-Way Table of Department by Response

```

Table of Department by Response

Department Response Frequency Percent CV for Design
 State Frequency Percent Percent Effect

Faculty Very Unsatisfied 209 13.4987 0.0865 2.1586
Faculty Unsatisfied 203 13.0710 0.0868 2.0962
Faculty Neutral 346 22.4127 0.0629 2.1157
Faculty Satisfied 254 16.2006 0.0806 2.3232
Faculty Very Satisfied 98 6.2467 0.1362 2.2842

Admin/Guidance Very Unsatisfied 95 3.6690 0.1277 1.1477
Admin/Guidance Unsatisfied 123 4.6854 0.1060 1.0211
Admin/Guidance Neutral 235 9.1838 0.0700 0.9166
Admin/Guidance Satisfied 201 7.7305 0.0756 0.8848
Admin/Guidance Very Satisfied 86 3.3016 0.1252 0.9892

```

The following PROC SURVEYFREQ statements request a two-way table of Department by Response that includes row percentages, and also a Wald chi-square test of association between the two table variables:

```

title 'Student Information System Survey';
proc surveyfreq data=SIS_Survey nosummary;
 tables Department * Response / row nowt wchisq;
 strata State NewUser;
 cluster School;
 weight SamplingWeight;
run;

```

Output 90.1.3 displays the two-way table. The row percentages show the distribution of Response for Department = 'Faculty' and for Department = 'Admin/Guidance'. This is equivalent to a domain (subpopulation) analysis of Response, where the domains are Department = 'Faculty' and Department = 'Admin/Guidance'.

Output 90.1.4 displays the Wald chi-square test of association between Department and Response. The Wald chi-square is 11.44, and the corresponding adjusted  $F$  value is 2.84 with a  $p$ -value of 0.0243. This indicates a significant association between department (faculty or admin/guidance) and satisfaction with the student information system.

**Output 90.1.3** Table of Department by Response with Row Percentages

| Student Information System Survey |                  |           |         |                       |                |                           |
|-----------------------------------|------------------|-----------|---------|-----------------------|----------------|---------------------------|
| The SURVEYFREQ Procedure          |                  |           |         |                       |                |                           |
| Table of Department by Response   |                  |           |         |                       |                |                           |
| Department                        | Response         | Frequency | Percent | Std Err of<br>Percent | Row<br>Percent | Std Err of<br>Row Percent |
| Faculty                           | Very Unsatisfied | 209       | 13.4987 | 1.1675                | 18.8979        | 1.6326                    |
|                                   | Unsatisfied      | 203       | 13.0710 | 1.1350                | 18.2992        | 1.5897                    |
|                                   | Neutral          | 346       | 22.4127 | 1.4106                | 31.3773        | 1.9705                    |
|                                   | Satisfied        | 254       | 16.2006 | 1.3061                | 22.6805        | 1.8287                    |
|                                   | Very Satisfied   | 98        | 6.2467  | 0.8506                | 8.7452         | 1.1918                    |
|                                   | Total            |           | 1110    | 71.4297               | 0.1468         | 100.000                   |
| Admin/Guidance                    | Very Unsatisfied | 95        | 3.6690  | 0.4684                | 12.8419        | 1.6374                    |
|                                   | Unsatisfied      | 123       | 4.6854  | 0.4966                | 16.3995        | 1.7446                    |
|                                   | Neutral          | 235       | 9.1838  | 0.6430                | 32.1447        | 2.2300                    |
|                                   | Satisfied        | 201       | 7.7305  | 0.5842                | 27.0579        | 2.0406                    |
|                                   | Very Satisfied   | 86        | 3.3016  | 0.4133                | 11.5560        | 1.4466                    |
|                                   | Total            |           | 740     | 28.5703               | 0.1468         | 100.000                   |
| Total                             | Very Unsatisfied | 304       | 17.1676 | 1.2872                |                |                           |
|                                   | Unsatisfied      | 326       | 17.7564 | 1.2712                |                |                           |
|                                   | Neutral          | 581       | 31.5965 | 1.5795                |                |                           |
|                                   | Satisfied        | 455       | 23.9311 | 1.4761                |                |                           |
|                                   | Very Satisfied   | 184       | 9.5483  | 0.9523                |                |                           |
|                                   | Total            |           | 1850    | 100.000               |                |                           |

**Output 90.1.4** Wald Chi-Square Test

| Wald Chi-Square Test |         |
|----------------------|---------|
| Chi-Square           | 11.4454 |
| F Value              | 2.8613  |
| Num DF               | 4       |
| Den DF               | 364     |
| Pr > F               | 0.0234  |
| Adj F Value          | 2.8378  |
| Num DF               | 4       |
| Den DF               | 361     |
| Pr > Adj F           | 0.0243  |
| Sample Size = 1850   |         |

**Example 90.2: Multiway Tables (Domain Analysis)**

Continuing to use the SIS\_Survey data set from the section “Getting Started: SURVEYFREQ Procedure” on page 7588, this example shows how to produce multiway tables. The following PROC SURVEYFREQ statements request a table of Department by SchoolType by Response for the student information system survey:

```

title 'Student Information System Survey';
proc surveyfreq data=SIS_Survey;
 tables Department * SchoolType * Response
 SchoolType * Response;
 strata State NewUser;
 cluster School;
 weight SamplingWeight;
run;

```

The TABLES statement requests a multiway table with SchoolType as the row variable, Response as the column variable, and Department as the layer variable. This request produces a separate two-way table of SchoolType by Response for each level of the variable Department. The TABLES statement also requests a two-way table of SchoolType by Response, which totals the multiway table over both levels of Department. As in the previous examples, the STRATA, CLUSTER, and WEIGHT statements provide sample design information, so that the analysis will be done according to the design used for this survey.

Output 90.2.1 displays the multiway table produced by PROC SURVEYFREQ, which includes a table of SchoolType by Response for Department = ‘Faculty’ and for Department = ‘Admin/Guidance’. This is equivalent to a domain (subpopulation) analysis of SchoolType by Response, where the domains are Department = ‘Faculty’ and Department = ‘Admin/Guidance’.

## Output 90.2.1 Multiway Table of Department by SchoolType by Response

## Student Information System Survey

## The SURVEYFREQ Procedure

Table of SchoolType by Response  
Controlling for Department=Faculty

| SchoolType    | Response         | Frequency | Weighted<br>Frequency | Std Dev of<br>Wgt Freq | Percent   | Std Err of<br>Percent |
|---------------|------------------|-----------|-----------------------|------------------------|-----------|-----------------------|
| Middle School | Very Unsatisfied | 74        | 1846                  | 301.22637              | 6.6443    | 1.0838                |
|               | Unsatisfied      | 78        | 1929                  | 283.11476              | 6.9428    | 1.0201                |
|               | Neutral          | 130       | 3289                  | 407.80855              | 11.8369   | 1.4652                |
|               | Satisfied        | 113       | 2795                  | 368.85087              | 10.0597   | 1.3288                |
|               | Very Satisfied   | 55        | 1378                  | 261.63311              | 4.9578    | 0.9411                |
|               | Total            |           | 450                   | 11237                  | 714.97120 | 40.4415               |
| High School   | Very Unsatisfied | 135       | 3405                  | 389.42313              | 12.2536   | 1.3987                |
|               | Unsatisfied      | 125       | 3155                  | 384.56734              | 11.3563   | 1.3809                |
|               | Neutral          | 216       | 5429                  | 489.37826              | 19.5404   | 1.7564                |
|               | Satisfied        | 141       | 3507                  | 417.54773              | 12.6208   | 1.5040                |
|               | Very Satisfied   | 43        | 1052                  | 221.59367              | 3.7874    | 0.7984                |
|               | Total            |           | 660                   | 16549                  | 719.61536 | 59.5585               |
| Total         | Very Unsatisfied | 209       | 5251                  | 454.82598              | 18.8979   | 1.6326                |
|               | Unsatisfied      | 203       | 5085                  | 442.39032              | 18.2992   | 1.5897                |
|               | Neutral          | 346       | 8718                  | 550.81735              | 31.3773   | 1.9705                |
|               | Satisfied        | 254       | 6302                  | 507.01711              | 22.6805   | 1.8287                |
|               | Very Satisfied   | 98        | 2430                  | 330.97602              | 8.7452    | 1.1918                |
|               | Total            |           | 1110                  | 27786                  | 119.25529 | 100.000               |

Table of SchoolType by Response  
Controlling for Department=Admin/Guidance

| SchoolType    | Response         | Frequency | Weighted<br>Frequency | Std Dev of<br>Wgt Freq | Percent   | Std Err of<br>Percent |
|---------------|------------------|-----------|-----------------------|------------------------|-----------|-----------------------|
| Middle School | Very Unsatisfied | 42        | 649.43427             | 133.06194              | 5.8435    | 1.1947                |
|               | Unsatisfied      | 31        | 460.35557             | 100.80158              | 4.1422    | 0.9076                |
|               | Neutral          | 104       | 1568                  | 186.99946              | 14.1042   | 1.6804                |
|               | Satisfied        | 84        | 1269                  | 165.71127              | 11.4142   | 1.4896                |
|               | Very Satisfied   | 39        | 574.93878             | 110.37243              | 5.1732    | 0.9942                |
|               | Total            |           | 300                   | 4521                   | 287.86832 | 40.6774               |
| High School   | Very Unsatisfied | 53        | 777.77725             | 136.41869              | 6.9983    | 1.2285                |
|               | Unsatisfied      | 92        | 1362                  | 175.40862              | 12.2573   | 1.5806                |
|               | Neutral          | 131       | 2005                  | 212.34804              | 18.0404   | 1.8990                |
|               | Satisfied        | 117       | 1739                  | 190.07798              | 15.6437   | 1.7118                |
|               | Very Satisfied   | 47        | 709.37033             | 126.54394              | 6.3828    | 1.1371                |
|               | Total            |           | 440                   | 6593                   | 288.92483 | 59.3226               |
| Total         | Very Unsatisfied | 95        | 1427                  | 182.28132              | 12.8419   | 1.6374                |
|               | Unsatisfied      | 123       | 1823                  | 193.43045              | 16.3995   | 1.7446                |
|               | Neutral          | 235       | 3572                  | 250.22739              | 32.1447   | 2.2300                |
|               | Satisfied        | 201       | 3007                  | 226.82311              | 27.0579   | 2.0406                |
|               | Very Satisfied   | 86        | 1284                  | 160.83434              | 11.5560   | 1.4466                |
|               | Total            |           | 740                   | 11114                  | 60.78850  | 100.000               |

## Example 90.3: Output Data Sets

PROC SURVEYFREQ uses the Output Delivery System (ODS) to create output data sets. This is a departure from older SAS procedures that provide OUTPUT statements for similar functionality. By using ODS, you can create a SAS data set from any piece of PROC SURVEYFREQ output. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

When selecting tables for ODS output data sets, you refer to tables by their ODS table names. Each table created by PROC SURVEYFREQ is assigned a name. See the section “ODS Table Names” on page 7668 for a list of the table names provided by PROC SURVEYFREQ.

To save the one-way table of Response from Figure 90.3 in an output data set, use an ODS OUTPUT statement as follows:

```
proc surveyfreq data=SIS_Survey;
 tables Response / cl nowt;
 ods output OneWay=ResponseTable;
 strata State NewUser;
 cluster School;
 weight SamplingWeight;
run;
```

Output 90.3.1 displays the output data set ResponseTable, which contains the one-way table of Response. This data set has six observations, and each of these observations corresponds to a row of the one-way table. The first five observations correspond to the five levels of Response, as they are ordered in the one-way table display, and the last observation corresponds to the overall total, which is the last row of the one-way table. The data set ResponseTable includes a variable corresponding to each column of the one-way table. For example, the variable Percent contains the percentage estimates, and the variables LowerCL and UpperCL contain the lower and upper confidence limits for the percentage estimates.

**Output 90.3.1** ResponseTable Output Data Set

| Obs | Table          | Response         | Frequency | Percent | StdErr | LowerCL | UpperCL |
|-----|----------------|------------------|-----------|---------|--------|---------|---------|
| 1   | Table Response | Very Unsatisfied | 304       | 17.1676 | 1.2872 | 14.6364 | 19.6989 |
| 2   | Table Response | Unsatisfied      | 326       | 17.7564 | 1.2712 | 15.2566 | 20.2562 |
| 3   | Table Response | Neutral          | 581       | 31.5965 | 1.5795 | 28.4904 | 34.7026 |
| 4   | Table Response | Satisfied        | 455       | 23.9311 | 1.4761 | 21.0285 | 26.8338 |
| 5   | Table Response | Very Satisfied   | 184       | 9.5483  | 0.9523 | 7.6756  | 11.4210 |
| 6   | Table Response | .                | 1850      | 100.000 | —      | —       | —       |

PROC SURVEYFREQ also creates a table summary that is not displayed. Some of the information in this table is similar to that contained in the “Data Summary” table, but the table summary describes the data that are used to analyze the specified table, while the data summary describes the entire input data set. Due to missing values, for example, the number of observations (or strata or clusters) used to analyze a particular table can differ from the number of observations (or strata or clusters) reported for the input data set in the “Data Summary” table. See the section “Missing Values” on page 7627 for more details. If you request confidence limits, the “Table Summary” table also contains the degrees of freedom and the *t*-value used to compute the confidence limits.

The following statements store the nondisplayed “Table Summary” table in the output data set ResponseSummary:

```
proc surveyfreq data=SIS_Survey;
 tables Response / cl nowt;
 ods output TableSummary=ResponseSummary;
 strata State NewUser;
 cluster School;
 weight SamplingWeight;
run;
```

Output 90.3.2 displays the output data set ResponseSummary.

**Output 90.3.2** ResponseSummary Output Data Set

| Obs | Table          | Number of Observations | Number of Strata | Number of Clusters | Degrees of Freedom | t Percentile |
|-----|----------------|------------------------|------------------|--------------------|--------------------|--------------|
| 1   | Table Response | 1850                   | 6                | 370                | 364                | 1.966503     |

---

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# Chapter 91

## The SURVEYLOGISTIC Procedure

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## Overview: SURVEYLOGISTIC Procedure

Categorical responses arise extensively in sample survey. Common examples of responses include the following:

- binary: for example, attended graduate school or not
- ordinal: for example, mild, moderate, and severe pain
- nominal: for example, ABC, NBC, CBS, FOX TV network viewed at a certain hour

Logistic regression analysis is often used to investigate the relationship between such discrete responses and a set of explanatory variables. For a description of logistic regression for sample survey data, see Binder (1981, 1983); Roberts, Rao, and Kumar (1987); Skinner, Holt, and Smith (1989); Morel (1989); Lehtonen and Pahkinen (1995).

For binary response models, the response of a sampling unit can take a specified value or not (for example, attended graduate school or not). Suppose  $\mathbf{x}$  is a row vector of explanatory variables and  $\pi$  is the response probability to be modeled. The linear logistic model has the form

$$\text{logit}(\pi) \equiv \log\left(\frac{\pi}{1-\pi}\right) = \alpha + \mathbf{x}\boldsymbol{\beta}$$

where  $\alpha$  is the intercept parameter and  $\boldsymbol{\beta}$  is the vector of slope parameters.

The logistic model shares a common feature with the more general class of generalized linear models—namely, that a function  $g = g(\mu)$  of the expected value,  $\mu$ , of the response variable is assumed to be linearly related to the explanatory variables. Since  $\mu$  implicitly depends on the stochastic behavior of the response, and since the explanatory variables are assumed to be fixed, the function  $g$  provides the link between the random (stochastic) component and the systematic (deterministic) component of the response variable. For this reason, Nelder and Wedderburn (1972) refer to  $g(\cdot)$  as a link function. One advantage of the logit function over other link functions is that differences on the logistic scale are interpretable regardless

of whether the data are sampled prospectively or retrospectively (McCullagh and Nelder 1989, Chapter 4). Other link functions that are widely used in practice are the probit function and the complementary log-log function. The SURVEYLOGISTIC procedure enables you to choose one of these link functions, resulting in fitting a broad class of binary response models of the form

$$g(\pi) = \alpha + \mathbf{x}\boldsymbol{\beta}$$

For ordinal response models, the response  $Y$  of an individual or an experimental unit might be restricted to one of a usually small number of ordinal values, denoted for convenience by  $1, \dots, D, D + 1$  ( $D \geq 1$ ). For example, pain severity can be classified into three response categories as 1=mild, 2=moderate, and 3=severe. The SURVEYLOGISTIC procedure fits a common slopes cumulative model, which is a parallel lines regression model based on the cumulative probabilities of the response categories rather than on their individual probabilities. The cumulative model has the form

$$g(\Pr(Y \leq d | \mathbf{x})) = \alpha_d + \mathbf{x}\boldsymbol{\beta}, \quad 1 \leq d \leq D$$

where  $\alpha_1, \dots, \alpha_k$  are  $k$  intercept parameters and  $\boldsymbol{\beta}$  is the vector of slope parameters. This model has been considered by many researchers. Aitchison and Silvey (1957) and Ashford (1959) employ a probit scale and provide a maximum likelihood analysis; Walker and Duncan (1967) and Cox and Snell (1989) discuss the use of the log-odds scale. For the log-odds scale, the cumulative logit model is often referred to as the *proportional odds* model.

For nominal response logistic models, where the  $D + 1$  possible responses have no natural ordering, the logit model can also be extended to a *generalized logit* model, which has the form

$$\log \left( \frac{\Pr(Y = i | \mathbf{x})}{\Pr(Y = D + 1 | \mathbf{x})} \right) = \alpha_i + \mathbf{x}\boldsymbol{\beta}_i, \quad i = 1, \dots, D$$

where the  $\alpha_1, \dots, \alpha_D$  are  $D$  intercept parameters and the  $\boldsymbol{\beta}_1, \dots, \boldsymbol{\beta}_D$  are  $D$  vectors of parameters. These models were introduced by McFadden (1974) as the *discrete choice* model, and they are also known as *multinomial* models.

The SURVEYLOGISTIC procedure fits linear logistic regression models for discrete response survey data by the method of maximum likelihood. For statistical inferences, PROC SURVEYLOGISTIC incorporates complex survey sample designs, including designs with stratification, clustering, and unequal weighting.

The maximum likelihood estimation is carried out with either the Fisher scoring algorithm or the Newton-Raphson algorithm. You can specify starting values for the parameter estimates. The logit link function in the ordinal logistic regression models can be replaced by the probit function or the complementary log-log function.

Odds ratio estimates are displayed along with parameter estimates. You can also specify the change in the explanatory variables for which odds ratio estimates are desired.

Variances of the regression parameters and odds ratios are computed by using either the Taylor series (linearization) method or replication (resampling) methods to estimate sampling errors of estimators based on complex sample designs (Binder 1983; Särndal, Swensson, and Wretman 1992; Wolter 2007; Rao, Wu, and Yue 1992).

The SURVEYLOGISTIC procedure enables you to specify categorical variables (also known as CLASS variables) as explanatory variables. It also enables you to specify interaction terms in the same way as in the LOGISTIC procedure.

Like many procedures in SAS/STAT software that allow the specification of CLASS variables, the SURVEYLOGISTIC procedure provides a CONTRAST statement for specifying customized hypothesis tests concerning the model parameters. The CONTRAST statement also provides estimation of individual rows of contrasts, which is particularly useful for obtaining odds ratio estimates for various levels of the CLASS variables.

## Getting Started: SURVEYLOGISTIC Procedure

The SURVEYLOGISTIC procedure is similar to the LOGISTIC procedure and other regression procedures in the SAS System. See Chapter 54, “The LOGISTIC Procedure,” for general information about how to perform logistic regression by using SAS. PROC SURVEYLOGISTIC is designed to handle sample survey data, and thus it incorporates the sample design information into the analysis.

The following example illustrates how to use PROC SURVEYLOGISTIC to perform logistic regression for sample survey data.

In the customer satisfaction survey example in the section “Getting Started: SURVEYSELECT Procedure” on page 8021 of Chapter 95, “The SURVEYSELECT Procedure,” an Internet service provider conducts a customer satisfaction survey. The survey population consists of the company’s current subscribers from four states: Alabama (AL), Florida (FL), Georgia (GA), and South Carolina (SC). The company plans to select a sample of customers from this population, interview the selected customers and ask their opinions on customer service, and then make inferences about the entire population of subscribers from the sample data. A stratified sample is selected by using the probability proportional to size (PPS) method. The sample design divides the customers into strata depending on their types (‘Old’ or ‘New’) and their states (AL, FL, GA, SC). There are eight strata in all. Within each stratum, customers are selected and interviewed by using the PPS with replacement method, where the size variable is Usage. The stratified PPS sample contains 192 customers. The data are stored in the SAS data set SampleStrata. Figure 91.1 displays the first 10 observations of this data set.

**Figure 91.1** Stratified PPS Sample (First 10 Observations)

| Customer Satisfaction Survey<br>Stratified PPS Sampling<br>(First 10 Observations) |       |      |             |                       |       |                 |
|------------------------------------------------------------------------------------|-------|------|-------------|-----------------------|-------|-----------------|
| Obs                                                                                | State | Type | Customer ID | Rating                | Usage | Sampling Weight |
| 1                                                                                  | AL    | New  | 24394278    | Neutral               | 13.17 | 26.358          |
| 2                                                                                  | AL    | New  | 64798692    | Extremely Unsatisfied | 15.53 | 22.352          |
| 3                                                                                  | AL    | New  | 75375074    | Unsatisfied           | 99.11 | 3.501           |
| 4                                                                                  | AL    | New  | 262831809   | Neutral               | 5.40  | 64.228          |
| 5                                                                                  | AL    | New  | 294428658   | Extremely Satisfied   | 1.17  | 297.488         |
| 6                                                                                  | AL    | New  | 336222949   | Unsatisfied           | 38.69 | 8.970           |
| 7                                                                                  | AL    | New  | 351929023   | Extremely Satisfied   | 2.72  | 127.475         |
| 8                                                                                  | AL    | New  | 366142640   | Satisfied             | 2.61  | 132.958         |
| 9                                                                                  | AL    | New  | 371478614   | Neutral               | 14.36 | 24.173          |
| 10                                                                                 | AL    | New  | 477172230   | Neutral               | 4.06  | 85.489          |



In the SAS data set `SampleStrata`, the variable `CustomerID` uniquely identifies each customer. The variable `State` contains the state of the customer's address. The variable `Type` equals 'Old' if the customer has subscribed to the service for more than one year; otherwise, the variable `Type` equals 'New'. The variable `Usage` contains the customer's average monthly service usage, in hours. The variable `Rating` contains the customer's responses to the survey. The sample design uses an unequal probability sampling method, with the sampling weights stored in the variable `SamplingWeight`.

The following SAS statements fit a cumulative logistic model between the satisfaction levels and the Internet usage by using the stratified PPS sample:

```

title 'Customer Satisfaction Survey';
proc surveylogistic data=SampleStrata;
 strata state type/list;
 model Rating (order=internal) = Usage;
 weight SamplingWeight;
run;

```

The PROC SURVEYLOGISTIC statement invokes the SURVEYLOGISTIC procedure. The STRATA statement specifies the stratification variables `State` and `Type` that are used in the sample design. The LIST option requests a summary of the stratification. In the MODEL statement, `Rating` is the response variable and `Usage` is the explanatory variable. The ORDER=internal is used for the response variable `Rating` to ask the procedure to order the response levels by using the internal numerical value (1–5) instead of the formatted character value. The WEIGHT statement specifies the variable `SamplingWeight` that contains the sampling weights.

The results of this analysis are shown in the following figures.

**Figure 91.2** Stratified PPS Sample, Model Information

| Customer Satisfaction Survey |                         |                 |
|------------------------------|-------------------------|-----------------|
| The SURVEYLOGISTIC Procedure |                         |                 |
| Model Information            |                         |                 |
| Data Set                     | WORK.SAMPLESTRATA       |                 |
| Response Variable            | Rating                  |                 |
| Number of Response Levels    | 5                       |                 |
| Stratum Variables            | State                   |                 |
|                              | Type                    |                 |
| Number of Strata             | 8                       |                 |
| Weight Variable              | SamplingWeight          | Sampling Weight |
| Model                        | Cumulative Logit        |                 |
| Optimization Technique       | Fisher's Scoring        |                 |
| Variance Adjustment          | Degrees of Freedom (DF) |                 |

PROC SURVEYLOGISTIC first lists the following model fitting information and sample design information in Figure 91.2:

- The link function is the logit of the cumulative of the lower response categories.
- The Fisher scoring optimization technique is used to obtain the maximum likelihood estimates for the regression coefficients.
- The response variable is Rating, which has five response levels.
- The stratification variables are State and Type.
- There are eight strata in the sample.
- The weight variable is SamplingWeight.
- The **variance adjustment method** used for the regression coefficients is the default degrees of freedom adjustment.

Figure 91.3 lists the number of observations in the data set and the number of observations used in the analysis. Since there is no missing value in this example, observations in the entire data set are used in the analysis. The sums of weights are also reported in this table.

**Figure 91.3** Stratified PPS Sample, Number of Observations

|                             |          |
|-----------------------------|----------|
| Number of Observations Read | 192      |
| Number of Observations Used | 192      |
| Sum of Weights Read         | 11326.25 |
| Sum of Weights Used         | 11326.25 |

The “Response Profile” table in Figure 91.4 lists the five response levels, their ordered values, and their total frequencies and total weights for each category. Due to the ORDER=INTERNAL option for the response variable Rating, the category “Extremely Unsatisfied” has the Ordered Value 1, the category “Unsatisfied” has the Ordered Value 2, and so on.

**Figure 91.4** Stratified PPS Sample, Response Profile

| Response Profile |                       |                 |              |
|------------------|-----------------------|-----------------|--------------|
| Ordered Value    | Rating                | Total Frequency | Total Weight |
| 1                | Extremely Unsatisfied | 58              | 2368.8598    |
| 2                | Unsatisfied           | 47              | 1606.9657    |
| 3                | Neutral               | 44              | 2594.3564    |
| 4                | Satisfied             | 35              | 1898.5839    |
| 5                | Extremely Satisfied   | 8               | 2857.4848    |

Probabilities modeled are cumulated over the lower Ordered Values.

Figure 91.5 displays the output of the stratification summary. There are a total of eight strata, and each stratum is defined by the customer types within each state. The table also shows the number of customers within each stratum.

**Figure 91.5** Stratified PPS Sample, Stratification Summary

| Stratum Information |       |      |       |
|---------------------|-------|------|-------|
| Stratum Index       | State | Type | N Obs |
| 1                   | AL    | New  | 24    |
| 2                   |       | Old  | 23    |
| 3                   | FL    | New  | 25    |
| 4                   |       | Old  | 22    |
| 5                   | GA    | New  | 25    |
| 6                   |       | Old  | 24    |
| 7                   | SC    | New  | 24    |
| 8                   |       | Old  | 25    |

Figure 91.6 shows the chi-square test for testing the proportional odds assumption. The test is highly significant, which indicates that the cumulative logit model might not adequately fit the data.

**Figure 91.6** Stratified PPS Sample, Testing the Proportional Odds Assumption

| Score Test for the Proportional Odds Assumption |    |            |
|-------------------------------------------------|----|------------|
| Chi-Square                                      | DF | Pr > ChiSq |
| 617.8597                                        | 3  | <.0001     |

Figure 91.7 shows the iteration algorithm converged to obtain the MLE for this example. The “Model Fit Statistics” table contains the Akaike information criterion (AIC), the Schwarz criterion (SC), and the negative of twice the log likelihood ( $-2 \log L$ ) for the intercept-only model and the fitted model. AIC and SC can be used to compare different models, and the ones with smaller values are preferred.

**Figure 91.7** Stratified PPS Sample, Model Fitting Information

| Model Convergence Status                      |                |                          |
|-----------------------------------------------|----------------|--------------------------|
| Convergence criterion (GCONV=1E-8) satisfied. |                |                          |
| Model Fit Statistics                          |                |                          |
| Criterion                                     | Intercept Only | Intercept and Covariates |
| AIC                                           | 35996.656      | 35312.584                |
| SC                                            | 36009.686      | 35328.872                |
| -2 Log L                                      | 35988.656      | 35302.584                |

The table “Testing Global Null Hypothesis: BETA=0” in Figure 91.8 shows the likelihood ratio test, the efficient score test, and the Wald test for testing the significance of the explanatory variable (Usage). All tests are significant.

**Figure 91.8** Stratified PPS Sample

| Testing Global Null Hypothesis: BETA=0 |            |    |            |
|----------------------------------------|------------|----|------------|
| Test                                   | Chi-Square | DF | Pr > ChiSq |
| Likelihood Ratio                       | 686.0718   | 1  | <.0001     |
| Score                                  | 420.7314   | 1  | <.0001     |
| Wald                                   | 3.9793     | 1  | 0.0461     |

Figure 91.9 shows the parameter estimates of the logistic regression and their standard errors.

**Figure 91.9** Stratified PPS Sample, Parameter Estimates

| Analysis of Maximum Likelihood Estimates |    |          |                |                 |            |  |
|------------------------------------------|----|----------|----------------|-----------------|------------|--|
| Parameter                                | DF | Estimate | Standard Error | Wald Chi-Square | Pr > ChiSq |  |
| Intercept Extremely Unsatisfied          | 1  | -1.6784  | 0.3874         | 18.7741         | <.0001     |  |
| Intercept Unsatisfied                    | 1  | -0.9356  | 0.3645         | 6.5900          | 0.0103     |  |
| Intercept Neutral                        | 1  | 0.0438   | 0.4177         | 0.0110          | 0.9165     |  |
| Intercept Satisfied                      | 1  | 0.8440   | 0.5699         | 2.1930          | 0.1386     |  |
| Usage                                    | 1  | 0.0350   | 0.0175         | 3.9793          | 0.0461     |  |

Figure 91.10 displays the odds ratio estimate and its confidence limits.

**Figure 91.10** Stratified PPS Sample, Odds Ratios

| Odds Ratio Estimates |                |                            |       |
|----------------------|----------------|----------------------------|-------|
| Effect               | Point Estimate | 95% Wald Confidence Limits |       |
| Usage                | 1.036          | 1.001                      | 1.072 |

## Syntax: SURVEYLOGISTIC Procedure

The following statements are available in the SURVEYLOGISTIC procedure:

```

PROC SURVEYLOGISTIC < options > ;
 BY variables ;
 CLASS variable < (v-options) > < variable < (v-options) > ... > < / v-options > ;
 CLUSTER variables ;
 CONTRAST 'label' effect values < , ... effect values > < / options > ;
 DOMAIN variables < variable*variable variable*variable*variable ... > ;
 EFFECT name = effect-type (variables < / options >) ;
 ESTIMATE < 'label' > estimate-specification < / options > ;
 FREQ variable ;
 LSMEANS < model-effects > < / options > ;
 LSMESTIMATE model-effect lsmestimate-specification < / options > ;
 MODEL events/trials = < effects < / options > > ;
 MODEL variable < (v-options) > = < effects > < / options > ;
 OUTPUT < OUT=SAS-data-set > < options > < / option > ;
 REPWEIGHTS variables < / options > ;
 SLICE model-effect < / options > ;
 STORE < OUT= > item-store-name < / LABEL='label' > ;
 STRATA variables < / option > ;
 < label: > TEST equation1 < , ... , equationk > < / options > ;
 UNITS independent1 = list1 < ... independentk = listk > < / option > ;
 WEIGHT variable ;

```

The PROC SURVEYLOGISTIC and MODEL statements are required.

The CLASS, CLUSTER, CONTRAST, EFFECT, ESTIMATE, LSMEANS, LSMESTIMATE, REPWEIGHTS, SLICE, STRATA, TEST statements can appear multiple times. You should use only one of each following statements: MODEL, WEIGHT, STORE, OUTPUT, and UNITS.

The CLASS statement (if used) must precede the MODEL statement, and the CONTRAST statement (if used) must follow the MODEL statement.

The rest of this section provides detailed syntax information for each of the preceding statements, except the EFFECT, ESTIMATE, LSMEANS, LSMESTIMATE, SLICE, STORE statements. These statements are also available in many other procedures. Summary descriptions of functionality and syntax for these statements are shown in this chapter, and full documentation about them is available in Chapter 19, “Shared Concepts and Topics.”

The syntax descriptions begin with the PROC SURVEYLOGISTIC statement; the remaining statements are covered in alphabetical order.

## PROC SURVEYLOGISTIC Statement

**PROC SURVEYLOGISTIC** < options > ;

The PROC SURVEYLOGISTIC statement invokes the SURVEYLOGISTIC procedure. Optionally, it identifies input data sets, controls the ordering of the response levels, and specifies the variance estimation method. The PROC SURVEYLOGISTIC statement is required.

Table 91.1 summarizes the options available in the PROC SURVEYLOGISTIC statement.

**Table 91.1** PROC SURVEYLOGISTIC Statement Options

| Option     | Description                                                      |
|------------|------------------------------------------------------------------|
| ALPHA=     | Sets the confidence level for confidence limits                  |
| DATA=      | Names the SAS data set containing the data to be analyze         |
| INEST=     | Names the SAS data set that contains initial estimates           |
| MISSING    | Treats missing values as a nonmissing category                   |
| NAMELEN=   | Specifies the length of effect names                             |
| NOMCAR     | Treats missing values as <i>not missing completely at random</i> |
| NOSORT     | Suppresses the internal sorting process                          |
| ORDER=     | Specifies the sort order                                         |
| RATE=      | Specifies the sampling rate                                      |
| TOTAL=     | Specifies the total number of primary sampling units             |
| VARMETHOD= | Specifies the variance estimation method                         |

### ALPHA=*value*

sets the confidence level for confidence limits. The value of the ALPHA= option must be between 0 and 1, and the default value is 0.05. A confidence level of  $\alpha$  produces  $100(1 - \alpha)\%$  confidence limits. The default of ALPHA=0.05 produces 95% confidence limits.

### DATA=*SAS-data-set*

names the SAS data set containing the data to be analyzed. If you omit the DATA= option, the procedure uses the most recently created SAS data set.

### INEST=*SAS-data-set*

names the SAS data set that contains initial estimates for all the parameters in the model. BY-group processing is allowed in setting up the INEST= data set. See the section “[INEST= Data Set](#)” on page 7733 for more information.

### MISSING

treats missing values as a valid (nonmissing) category for all categorical variables, which include [CLASS](#), [STRATA](#), [CLUSTER](#), and [DOMAIN](#) variables.

By default, if you do not specify the MISSING option, an observation is excluded from the analysis if it has a missing value. For more information, see the section “[Missing Values](#)” on page 7723.

**NAMELEN=*n***

specifies the length of effect names in tables and output data sets to be *n* characters, where *n* is a value between 20 and 200. The default length is 20 characters.

**NOMCAR**

requests that the procedure treat missing values in the variance computation as *not missing completely at random* (NOMCAR) for Taylor series variance estimation. When you specify the NOMCAR option, PROC SURVEYLOGISTIC computes variance estimates by analyzing the nonmissing values as a domain or subpopulation, where the entire population includes both nonmissing and missing domains. See the section “Missing Values” on page 7723 for more details.

By default, PROC SURVEYLOGISTIC completely excludes an observation from analysis if that observation has a missing value, unless you specify the MISSING option. Note that the NOMCAR option has no effect on a classification variable when you specify the MISSING option, which treats missing values as a valid nonmissing level.

The NOMCAR option applies only to Taylor series variance estimation. The replication methods, which you request with the VARMETHOD=BRR and VARMETHOD=JACKKNIFE options, do not use the NOMCAR option.

**NOSORT**

suppresses the internal sorting process to shorten the computation time if the data set is presorted by the STRATA and CLUSTER variables. By default, the procedure sorts the data by the STRATA variables if you use the STRATA statement; then the procedure sorts the data by the CLUSTER variables within strata. If your data are already stored by the order of STRATA and CLUSTER variables, then you can specify this option to omit this sorting process to reduce the usage of computing resources, especially when your data set is very large. However, if you specify this NOSORT option while your data are not presorted by STRATA and CLUSTER variables, then any changes in these variables creates a new stratum or cluster.

**ORDER=DATA | FORMATTED | FREQ | INTERNAL**

specifies the sort order for the levels of the response variable. This option, except for ORDER=FREQ, also determines the sort order for the levels of CIUSTER and DOMAIN variables and controls STRATA variable levels in the “Stratum Information” table. By default, ORDER=INTERNAL. However, if an ORDER= option is specified after the response variable, in the MODEL statement, it overrides this option for the response variable. This option does not affect the ordering of the CLASS variable levels; see the ORDER= option in the CLASS statement for more information.

**RATE=*value* | SAS-data-set****R=*value* | SAS-data-set**

specifies the sampling rate as a nonnegative *value*, or specifies an input data set that contains the stratum sampling rates. The procedure uses this information to compute a finite population correction for Taylor series variance estimation. The procedure does not use the RATE= option for BRR or jackknife variance estimation, which you request with the VARMETHOD=BRR or VARMETHOD=JACKKNIFE option.

If your sample design has multiple stages, you should specify the *first-stage sampling rate*, which is the ratio of the number of PSUs selected to the total number of PSUs in the population.

For a nonstratified sample design, or for a stratified sample design with the same sampling rate in all strata, you should specify a nonnegative *value* for the RATE= option. If your design is stratified with different sampling rates in the strata, then you should name a SAS data set that contains the stratification variables and the sampling rates. See the section “[Specification of Population Totals and Sampling Rates](#)” on page 7734 for more details.

The *value* in the RATE= option or the values of `_RATE_` in the secondary data set must be nonnegative numbers. You can specify *value* as a number between 0 and 1. Or you can specify *value* in percentage form as a number between 1 and 100, and PROC SURVEYLOGISTIC converts that number to a proportion. The procedure treats the value 1 as 100% instead of 1%.

If you do not specify the TOTAL= or RATE= option, then the Taylor series variance estimation does not include a finite population correction. You cannot specify both the TOTAL= and RATE= options.

**TOTAL=***value* | *SAS-data-set*

**N=***value* | *SAS-data-set*

specifies the total number of primary sampling units in the study population as a positive *value*, or specifies an input data set that contains the stratum population totals. The procedure uses this information to compute a finite population correction for Taylor series variance estimation. The procedure does not use the TOTAL= option for BRR or jackknife variance estimation, which you request with the `VARMETHOD=BRR` or `VARMETHOD=JACKKNIFE` option.

For a nonstratified sample design, or for a stratified sample design with the same population total in all strata, you should specify a positive *value* for the TOTAL= option. If your sample design is stratified with different population totals in the strata, then you should name a SAS data set that contains the stratification variables and the population totals. See the section “[Specification of Population Totals and Sampling Rates](#)” on page 7734 for more details.

If you do not specify the TOTAL= or RATE= option, then the Taylor series variance estimation does not include a finite population correction. You cannot specify both the TOTAL= and RATE= options.

**VARMETHOD=BRR** <(method-options)>

**VARMETHOD=JACKKNIFE** | **JK** <(method-options)>

**VARMETHOD=TAYLOR**

specifies the variance estimation method. `VARMETHOD=TAYLOR` requests the Taylor series method, which is the default if you do not specify the `VARMETHOD=` option or the `REPWEIGHTS` statement. `VARMETHOD=BRR` requests variance estimation by balanced repeated replication (BRR), and `VARMETHOD=JACKKNIFE` requests variance estimation by the delete-1 jackknife method.

For `VARMETHOD=BRR` and `VARMETHOD=JACKKNIFE` you can specify *method-options* in parentheses. [Table 91.2](#) summarizes the available *method-options*.



**Table 91.2** Variance Estimation Options

| <b>VARMETHOD=</b> | <b>Variance Estimation Method</b> | <i>Method-Options</i>                                                                                                          |
|-------------------|-----------------------------------|--------------------------------------------------------------------------------------------------------------------------------|
| BRR               | Balanced repeated replication     | FAY <i>&lt;=value&gt;</i><br>HADAMARD= <i>SAS-data-set</i><br>OUTWEIGHTS= <i>SAS-data-set</i><br>PRINTH<br>REPS= <i>number</i> |
| JACKKNIFE         | Jackknife                         | OUTJKCOEFS= <i>SAS-data-set</i><br>OUTWEIGHTS= <i>SAS-data-set</i>                                                             |
| TAYLOR            | Taylor series linearization       | None                                                                                                                           |

*Method-options* must be enclosed in parentheses following the method keyword. For example:

```
varmethod=BRR (reps=60 outweights=myReplicateWeights)
```

The following values are available for the VARMETHOD= option:

**BRR** *<(method-options)>*

requests **balanced repeated replication** (BRR) variance estimation. The BRR method requires a stratified sample design with two primary sampling units (PSUs) per stratum. See the section “**Balanced Repeated Replication (BRR) Method**” on page 7740 for more information.

You can specify the following *method-options* in parentheses following VARMETHOD=BRR:

**FAY** *<=value>*

requests **Fay’s method**, a modification of the BRR method, for variance estimation. See the section “**Fay’s BRR Method**” on page 7741 for more information.

You can specify the *value* of the Fay coefficient, which is used in converting the original sampling weights to replicate weights. The Fay coefficient must be a nonnegative number less than 1. By default, the value of the Fay coefficient equals 0.5.

**HADAMARD**=*SAS-data-set*

**H**=*SAS-data-set*

names a SAS data set that contains the **Hadamard matrix** for BRR replicate construction. If you do not provide a Hadamard matrix with the HADAMARD= *method-option*, PROC SURVEYLOGISTIC generates an appropriate Hadamard matrix for replicate construction. See the sections “**Balanced Repeated Replication (BRR) Method**” on page 7740 and “**Hadamard Matrix**” on page 7743 for details.

If a Hadamard matrix of a given dimension exists, it is not necessarily unique. Therefore, if you want to use a specific Hadamard matrix, you must provide the matrix as a SAS data set in the HADAMARD= *method-option*.

In the HADAMARD= input data set, each variable corresponds to a column of the Hadamard matrix, and each observation corresponds to a row of the matrix. You can use any variable names in the HADAMARD= data set. All values in the data set must equal either 1 or -1. You must ensure that the matrix you provide is indeed a Hadamard matrix—that is,  $\mathbf{A}'\mathbf{A} = R\mathbf{I}$ , where  $\mathbf{A}$  is the Hadamard matrix of dimension  $R$  and  $\mathbf{I}$  is an identity matrix. PROC SURVEYLOGISTIC does not check the validity of the Hadamard matrix that you provide.

The HADAMARD= input data set must contain at least  $H$  variables, where  $H$  denotes the number of first-stage strata in your design. If the data set contains more than  $H$  variables, the procedure uses only the first  $H$  variables. Similarly, the HADAMARD= input data set must contain at least  $H$  observations.

If you do not specify the REPS= *method-option*, then the number of replicates is taken to be the number of observations in the HADAMARD= input data set. If you specify the number of replicates—for example, REPS=*nreps*—then the first *nreps* observations in the HADAMARD= data set are used to construct the replicates.

You can specify the PRINTH option to display the Hadamard matrix that the procedure uses to construct replicates for BRR.

#### **OUTWEIGHTS=SAS-data-set**

names a SAS data set that contains replicate weights. See the section “Balanced Repeated Replication (BRR) Method” on page 7740 for information about replicate weights. See the section “Replicate Weights Output Data Set” on page 7751 for more details about the contents of the OUTWEIGHTS= data set.

The OUTWEIGHTS= *method-option* is not available when you provide replicate weights with the REPWEIGHTS statement.

#### **PRINTH**

displays the Hadamard matrix.

When you provide your own Hadamard matrix with the HADAMARD= *method-option*, only the rows and columns of the Hadamard matrix that are used by the procedure are displayed. See the sections “Balanced Repeated Replication (BRR) Method” on page 7740 and “Hadamard Matrix” on page 7743 for details.

The PRINTH *method-option* is not available when you provide replicate weights with the REPWEIGHTS statement because the procedure does not use a Hadamard matrix in this case.

#### **REPS=number**

specifies the number of replicates for BRR variance estimation. The value of *number* must be an integer greater than 1.

If you do not provide a Hadamard matrix with the HADAMARD= *method-option*, the number of replicates should be greater than the number of strata

and should be a multiple of 4. See the section “Balanced Repeated Replication (BRR) Method” on page 7740 for more information. If a Hadamard matrix cannot be constructed for the REPS= value that you specify, the value is increased until a Hadamard matrix of that dimension can be constructed. Therefore, it is possible for the actual number of replicates used to be larger than the REPS= value that you specify.

If you provide a Hadamard matrix with the HADAMARD= *method-option*, the value of REPS= must not be less than the number of rows in the Hadamard matrix. If you provide a Hadamard matrix and do not specify the REPS= *method-option*, the number of replicates equals the number of rows in the Hadamard matrix.

If you do not specify the REPS= or HADAMARD= *method-option* and do not include a REPWEIGHTS statement, the number of replicates equals the smallest multiple of 4 that is greater than the number of strata.

If you provide replicate weights with the REPWEIGHTS statement, the procedure does not use the REPS= *method-option*. With a REPWEIGHTS statement, the number of replicates equals the number of REPWEIGHTS variables.

#### JACKKNIFE | JK <(method-options)>

requests variance estimation by the delete-1 jackknife method. See the section “Jackknife Method” on page 7742 for details. If you provide replicate weights with a REPWEIGHTS statement, VARMETHOD=JACKKNIFE is the default variance estimation method.

You can specify the following *method-options* in parentheses following VARMETHOD=JACKKNIFE:

##### **OUTJKCOEFS=SAS-data-set**

names a SAS data set that contains jackknife coefficients. See the section “Jackknife Method” on page 7742 for information about jackknife coefficients. See the section “Jackknife Coefficients Output Data Set” on page 7751 for more details about the contents of the OUTJKCOEFS= data set.

##### **OUTWEIGHTS=SAS-data-set**

names a SAS data set that contains replicate weights. See the section “Jackknife Method” on page 7742 for information about replicate weights. See the section “Replicate Weights Output Data Set” on page 7751 for more details about the contents of the OUTWEIGHTS= data set.

The OUTWEIGHTS= *method-option* is not available when you provide replicate weights with the REPWEIGHTS statement.

#### TAYLOR

requests Taylor series variance estimation. This is the default method if you do not specify the VARMETHOD= option or a REPWEIGHTS statement. See the section “Taylor Series (Linearization)” on page 7739 for more information.

---

## BY Statement

**BY** *variables* ;

You can specify a BY statement with PROC SURVEYLOGISTIC to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the SURVEYLOGISTIC procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

Note that using a BY statement provides completely separate analyses of the BY groups. It does not provide a statistically valid domain (subpopulation) analysis, where the total number of units in the subpopulation is not known with certainty. You should use the DOMAIN statement to obtain domain analysis. For more information about subpopulation analysis for sample survey data, see Cochran (1977).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

---

## CLASS Statement

**CLASS** *variable* <(v-options)> <*variable* <(v-options)> ... > </v-options> ;

The CLASS statement names the classification variables to be used in the analysis. The CLASS statement must precede the MODEL statement. You can specify various *v-options* for each variable by enclosing them in parentheses after the variable name. You can also specify global *v-options* for the CLASS statement by placing them after a slash (/). Global *v-options* are applied to all the variables specified in the CLASS statement. However, individual CLASS variable *v-options* override the global *v-options*.

**CPREFIX=** *n*

specifies that, at most, the first *n* characters of a CLASS variable name be used in creating names for the corresponding dummy variables. The default is  $32 - \min(32, \max(2, f))$ , where *f* is the formatted length of the CLASS variable.

**DESCENDING**

**DESC**

reverses the sort order of the classification variable.

**LPREFIX= *n***

specifies that, at most, the first *n* characters of a CLASS variable label be used in creating labels for the corresponding dummy variables.

**ORDER=DATA | FORMATTED | FREQ | INTERNAL**

specifies the order in which to sort the levels of the classification variables.

This option applies to the levels for all classification variables, except when you use the (default) ORDER=FORMATTED option with numeric classification variables that have no explicit format. With this option, the levels of such variables are ordered by their internal value.

The ORDER= option can take the following values:

| Value of ORDER=  | Levels Sorted By                                                                                                                       |
|------------------|----------------------------------------------------------------------------------------------------------------------------------------|
| <b>DATA</b>      | Order of appearance in the input data set                                                                                              |
| <b>FORMATTED</b> | External formatted value, except for numeric variables with no explicit format, which are sorted by their unformatted (internal) value |
| <b>FREQ</b>      | Descending frequency count; levels with the most observations come first in the order                                                  |
| <b>INTERNAL</b>  | Unformatted value                                                                                                                      |

By default, ORDER=FORMATTED. For ORDER=FORMATTED and ORDER=INTERNAL, the sort order is machine-dependent. For more information about sort order, see the chapter on the SORT procedure in the *Base SAS Procedures Guide* and the discussion of BY-group processing in *SAS Language Reference: Concepts*.

**PARAM=keyword**

specifies the parameterization method for the classification variable or variables. Design matrix columns are created from CLASS variables according to the following coding schemes; the default is PARAM=EFFECT.

|                          |                                                                                                       |
|--------------------------|-------------------------------------------------------------------------------------------------------|
| EFFECT                   | specifies effect coding                                                                               |
| GLM                      | specifies less-than-full-rank, reference cell coding; this option can be used only as a global option |
| ORDINAL                  | specifies the cumulative parameterization for an ordinal CLASS variable                               |
| POLYNOMIAL   POLY        | specifies polynomial coding                                                                           |
| REFERENCE   REF          | specifies reference cell coding                                                                       |
| ORTHEFFECT               | orthogonalizes PARAM=EFFECT                                                                           |
| ORTHORDINAL   ORTHOTHERM | orthogonalizes PARAM=ORDINAL                                                                          |
| ORTHPOLY                 | orthogonalizes PARAM=POLYNOMIAL                                                                       |
| ORTHREF                  | orthogonalizes PARAM=REFERENCE                                                                        |

If PARAM=ORTHPOLY or PARAM=POLY, and the CLASS levels are numeric, then the ORDER= option in the CLASS statement is ignored, and the internal, unformatted values are used.

EFFECT, POLYNOMIAL, REFERENCE, ORDINAL, and their orthogonal parameterizations are full rank. The REF= option in the CLASS statement determines the reference level for EFFECT, REFERENCE, and their orthogonal parameterizations.

Parameter names for a CLASS predictor variable are constructed by concatenating the CLASS variable name with the CLASS levels. However, for the POLYNOMIAL and orthogonal parameterizations, parameter names are formed by concatenating the CLASS variable name and keywords that reflect the parameterization.

**REFERENCE=** 'level' | keyword

**REF=** 'level' | keyword

specifies the reference level for PARAM=EFFECT or PARAM=REFERENCE. For an individual (but not a global) variable REF= *option*, you can specify the *level* of the variable to use as the reference level. For a global or individual variable REF= *option*, you can use one of the following *keywords*. The default is REF=LAST.

|       |                                                 |
|-------|-------------------------------------------------|
| FIRST | designates the first ordered level as reference |
| LAST  | designates the last ordered level as reference  |

---

## CLUSTER Statement

**CLUSTER** *variables* ;

The CLUSTER statement names variables that identify the clusters in a clustered sample design. The combinations of categories of CLUSTER variables define the clusters in the sample. If there is a STRATA statement, clusters are nested within strata.

If you provide replicate weights for BRR or jackknife variance estimation with the REPWEIGHTS statement, you do not need to specify a CLUSTER statement.

If your sample design has clustering at multiple stages, you should identify only the first-stage clusters (primary sampling units (PSUs)), in the CLUSTER statement. See the section “Primary Sampling Units (PSUs)” on page 7734 for more information.

The CLUSTER *variables* are one or more variables in the DATA= input data set. These variables can be either character or numeric. The formatted values of the CLUSTER variables determine the CLUSTER variable levels. Thus, you can use formats to group values into levels. See the FORMAT procedure in the *Base SAS Procedures Guide* and the FORMAT statement and SAS formats in *SAS Formats and Informats: Reference* for more information.

When determining levels of a CLUSTER variable, an observation with missing values for this CLUSTER variable is excluded, unless you specify the MISSING option. For more information, see the section “Missing Values” on page 7723.

You can use multiple CLUSTER statements to specify cluster variables. The procedure uses variables from all CLUSTER statements to create clusters.

## CONTRAST Statement

**CONTRAST** *'label'* *row-description* <, ..., *row-description* </ options>> ;

where a *row-description* is defined as follows:

*effect values* <, ..., *effect values*>

The CONTRAST statement provides a mechanism for obtaining customized hypothesis tests. It is similar to the CONTRAST statement in PROC LOGISTIC and PROC GLM, depending on the coding schemes used with any classification variables involved.

The CONTRAST statement enables you to specify a matrix,  $\mathbf{L}$ , for testing the hypothesis  $\mathbf{L}\boldsymbol{\theta} = 0$ , where  $\boldsymbol{\theta}$  is the parameter vector. You must be familiar with the details of the model parameterization that PROC SURVEYLOGISTIC uses (for more information, see the [PARAM=](#) option in the section “[CLASS Statement](#)” on page 7697). Optionally, the CONTRAST statement enables you to estimate each row,  $\mathbf{l}_i\boldsymbol{\theta}$ , of  $\mathbf{L}\boldsymbol{\theta}$  and test the hypothesis  $\mathbf{l}_i\boldsymbol{\theta} = 0$ . Computed statistics are based on the asymptotic chi-square distribution of the Wald statistic.

There is no limit to the number of CONTRAST statements that you can specify, but they must appear after the [MODEL](#) statement.

The following parameters can be specified in the CONTRAST statement:

- label* identifies the contrast on the output. A label is required for every contrast specified, and it must be enclosed in quotes.
- effect* identifies an effect that appears in the MODEL statement. The name INTERCEPT can be used as an effect when one or more intercepts are included in the model. You do not need to include all effects that are included in the MODEL statement.
- values* are constants that are elements of the  $\mathbf{L}$  matrix associated with the effect. To correctly specify your contrast, it is crucial to know the ordering of parameters within each effect and the variable levels associated with any parameter. The “Class Level Information” table shows the ordering of levels within variables. The E option, described later in this section, enables you to verify the proper correspondence of *values* to parameters.

The rows of  $\mathbf{L}$  are specified in order and are separated by commas. Multiple degree-of-freedom hypotheses can be tested by specifying multiple *row-descriptions*. For any of the full-rank parameterizations, if an effect is not specified in the CONTRAST statement, all of its coefficients in the  $\mathbf{L}$  matrix are set to 0. If too many values are specified for an effect, the extra ones are ignored. If too few values are specified, the remaining ones are set to 0.

When you use effect coding (by default or by specifying [PARAM=EFFECT](#) in the CLASS statement), all parameters are directly estimable (involve no other parameters).

For example, suppose an effect that is coded CLASS variable A has four levels. Then there are three parameters ( $\alpha_1, \alpha_2, \alpha_3$ ) that represent the first three levels, and the fourth parameter is represented by

$$-\alpha_1 - \alpha_2 - \alpha_3$$

To test the first versus the fourth level of A, you would test

$$\alpha_1 = -\alpha_1 - \alpha_2 - \alpha_3$$

or, equivalently,

$$2\alpha_1 + \alpha_2 + \alpha_3 = 0$$

which, in the form  $\mathbf{L}\boldsymbol{\theta} = 0$ , is

$$\begin{bmatrix} 2 & 1 & 1 \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{bmatrix} = 0$$

Therefore, you would use the following CONTRAST statement:

```
contrast '1 vs. 4' A 2 1 1;
```

To contrast the third level with the average of the first two levels, you would test

$$\frac{\alpha_1 + \alpha_2}{2} = \alpha_3$$

or, equivalently,

$$\alpha_1 + \alpha_2 - 2\alpha_3 = 0$$

Therefore, you would use the following CONTRAST statement:

```
contrast '1&2 vs. 3' A 1 1 -2;
```

Other CONTRAST statements are constructed similarly. For example:

```
contrast '1 vs. 2' A 1 -1 0;
contrast '1&2 vs. 4' A 3 3 2;
contrast '1&2 vs. 3&4' A 2 2 0;
contrast 'Main Effect' A 1 0 0,
 A 0 1 0,
 A 0 0 1;
```

When you use the less-than-full-rank parameterization (by specifying `PARAM=GLM` in the `CLASS` statement), each row is checked for estimability. If `PROC SURVEYLOGISTIC` finds a contrast to be nonestimable, it displays missing values in corresponding rows in the results. `PROC SURVEYLOGISTIC` handles missing level combinations of classification variables in the same manner as `PROC LOGISTIC`. Parameters corresponding to missing level combinations are not included in the model. This convention can affect the way in which you specify the `L` matrix in your `CONTRAST` statement. If the elements of `L` are not specified for an effect that contains a specified effect, then the elements of the specified effect are distributed over the levels of the higher-order effect just as the `LOGISTIC` procedure does for its `CONTRAST` and `ESTIMATE` statements. For example, suppose that the model contains effects `A` and `B` and their interaction `A*B`. If you specify a `CONTRAST` statement involving `A` alone, the `L` matrix contains nonzero terms for both `A` and `A*B`, since `A*B` contains `A`.

The degrees of freedom is the number of linearly independent constraints implied by the `CONTRAST` statement—that is, the rank of `L`.



You can specify the following options after a slash (/):

**ALPHA=***value*

sets the confidence level for confidence limits. The value of the ALPHA= option must be between 0 and 1, and the default value is 0.05. A confidence level of  $\alpha$  produces  $100(1 - \alpha)\%$  confidence limits. The default of ALPHA=0.05 produces 95% confidence limits.

**E**

requests that the **L** matrix be displayed.

**ESTIMATE=***keyword*

requests that each individual contrast (that is, each row,  $\mathbf{l}_i\boldsymbol{\beta}$ , of  $\mathbf{L}\boldsymbol{\beta}$ ) or exponentiated contrast ( $e^{\mathbf{l}_i\boldsymbol{\beta}}$ ) be estimated and tested. PROC SURVEYLOGISTIC displays the point estimate, its standard error, a Wald confidence interval, and a Wald chi-square test for each contrast. The significance level of the confidence interval is controlled by the ALPHA= option. You can estimate the contrast or the exponentiated contrast ( $e^{\mathbf{l}_i\boldsymbol{\beta}}$ ), or both, by specifying one of the following *keywords*:

|      |                                                                              |
|------|------------------------------------------------------------------------------|
| PARM | specifies that the contrast itself be estimated                              |
| EXP  | specifies that the exponentiated contrast be estimated                       |
| BOTH | specifies that both the contrast and the exponentiated contrast be estimated |

**SINGULAR=***value*

tunes the estimability checking. If  $\mathbf{v}$  is a vector, define  $\text{ABS}(\mathbf{v})$  to be the largest absolute value of the elements of  $\mathbf{v}$ . For a row vector  $\mathbf{l}$  of the matrix **L**, define

$$c = \begin{cases} \text{ABS}(\mathbf{l}) & \text{if } \text{ABS}(\mathbf{l}) > 0 \\ 1 & \text{otherwise} \end{cases}$$

If  $\text{ABS}(\mathbf{l} - \mathbf{I}\mathbf{H})$  is greater than  $c*\textit{value}$ , then  $\mathbf{l}\boldsymbol{\beta}$  is declared nonestimable. The **H** matrix is the Hermite form matrix  $\mathbf{I}_0^{-1}\mathbf{I}_0$ , where  $\mathbf{I}_0^{-1}$  represents a generalized inverse of the information matrix  $\mathbf{I}_0$  of the null model. The *value* must be between 0 and 1; the default is  $10^{-4}$ .

## DOMAIN Statement

**DOMAIN** *variables* < *variable\*variable variable\*variable\*variable ...* > ;

The DOMAIN statement requests analysis for domains (subpopulations) in addition to analysis for the entire study population. The DOMAIN statement names the variables that identify domains, which are called domain variables.

It is common practice to compute statistics for domains. The formation of these domains might be unrelated to the sample design. Therefore, the sample sizes for the domains are random variables. Use a DOMAIN statement to incorporate this variability into the variance estimation.

Note that a DOMAIN statement is different from a BY statement. In a BY statement, you treat the sample sizes as fixed in each subpopulation, and you perform analysis within each BY group independently. See the section “[Domain Analysis](#)” on page 7744 for more details.

Use the DOMAIN statement on the entire data set to perform a domain analysis. Creating a new data set from a single domain and analyzing that with PROC SURVEYLOGISTIC yields inappropriate estimates of variance.

A domain variable can be either character or numeric. The procedure treats domain variables as categorical variables. If a variable appears by itself in a DOMAIN statement, each level of this variable determines a domain in the study population. If two or more variables are joined by asterisks (\*), then every possible combination of levels of these variables determines a domain. The procedure performs a descriptive analysis within each domain that is defined by the domain variables.

When determining levels of a DOMAIN variable, an observation with missing values for this DOMAIN variable is excluded, unless you specify the **MISSING** option. For more information, see the section “Missing Values” on page 7723.

The formatted values of the domain variables determine the categorical variable levels. Thus, you can use formats to group values into levels. See the **FORMAT** procedure in the *Base SAS Procedures Guide* and the **FORMAT** statement and SAS formats in *SAS Formats and Informats: Reference* for more information.

---

## EFFECT Statement

**EFFECT** *name=effect-type (variables < / options >)* ;

The **EFFECT** statement enables you to construct special collections of columns for design matrices. These collections are referred to as *constructed effects* to distinguish them from the usual model effects that are formed from continuous or classification variables, as discussed in the section “GLM Parameterization of Classification Variables and Effects” on page 383 in Chapter 19, “Shared Concepts and Topics.”

You can specify the following *effect-types*:

|                          |                                                                                                                                                                                                           |
|--------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>COLLECTION</b>        | is a collection effect that defines one or more variables as a single effect with multiple degrees of freedom. The variables in a collection are considered as a unit for estimation and inference.       |
| <b>LAG</b>               | is a classification effect in which the level that is used for a given period corresponds to the level in the preceding period.                                                                           |
| <b>MULTIMEMBER   MM</b>  | is a multimember classification effect whose levels are determined by one or more variables that appear in a <b>CLASS</b> statement.                                                                      |
| <b>POLYNOMIAL   POLY</b> | is a multivariate polynomial effect in the specified numeric variables.                                                                                                                                   |
| <b>SPLINE</b>            | is a regression spline effect whose columns are univariate spline expansions of one or more variables. A spline expansion replaces the original variable with an expanded or larger set of new variables. |

Table 91.3 summarizes the *options* available in the **EFFECT** statement.

**Table 91.3** EFFECT Statement Options

| Option                            | Description                                                                   |
|-----------------------------------|-------------------------------------------------------------------------------|
| <b>Collection Effects Options</b> |                                                                               |
| <b>DETAILS</b>                    | Displays the constituents of the collection effect                            |
| <b>Lag Effects Options</b>        |                                                                               |
| <b>DESIGNROLE=</b>                | Names a variable that controls to which lag design an observation is assigned |

Table 91.3 continued

| Option                             | Description                                                                                                                                          |
|------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------|
| DETAILS                            | Displays the lag design of the lag effect                                                                                                            |
| NLAG=                              | Specifies the number of periods in the lag                                                                                                           |
| PERIOD=                            | Names the variable that defines the period                                                                                                           |
| WITHIN=                            | Names the variable or variables that define the group within which each period is defined                                                            |
| <b>Multimember Effects Options</b> |                                                                                                                                                      |
| NOEFFECT                           | Specifies that observations with all missing levels for the multimember variables should have zero values in the corresponding design matrix columns |
| WEIGHT=                            | Specifies the weight variable for the contributions of each of the classification effects                                                            |
| <b>Polynomial Effects Options</b>  |                                                                                                                                                      |
| DEGREE=                            | Specifies the degree of the polynomial                                                                                                               |
| MDEGREE=                           | Specifies the maximum degree of any variable in a term of the polynomial                                                                             |
| STANDARDIZE=                       | Specifies centering and scaling suboptions for the variables that define the polynomial                                                              |
| <b>Spline Effects Options</b>      |                                                                                                                                                      |
| BASIS=                             | Specifies the type of basis (B-spline basis or truncated power function basis) for the spline expansion                                              |
| DEGREE=                            | Specifies the degree of the spline transformation                                                                                                    |
| KNOTMETHOD=                        | Specifies how to construct the knots for spline effects                                                                                              |

For more information about the syntax of these *effect-types* and how columns of constructed effects are computed, see the section “EFFECT Statement” on page 393 in Chapter 19, “Shared Concepts and Topics.”

## ESTIMATE Statement

```
ESTIMATE <'label'> estimate-specification <(divisor=n)>
 < , ... <'label'> estimate-specification <(divisor=n)> >
 </options> ;
```

The ESTIMATE statement provides a mechanism for obtaining custom hypothesis tests. Estimates are formed as linear estimable functions of the form  $L\beta$ . You can perform hypothesis tests for the estimable functions, construct confidence limits, and obtain specific nonlinear transformations.

Table 91.4 summarizes the options available in the ESTIMATE statement.

**Table 91.4** ESTIMATE Statement Options

| Option                                                     | Description                                                                     |
|------------------------------------------------------------|---------------------------------------------------------------------------------|
| <b>Construction and Computation of Estimable Functions</b> |                                                                                 |
| DIVISOR=                                                   | Specifies a list of values to divide the coefficients                           |
| NOFILL                                                     | Suppresses the automatic fill-in of coefficients for higher-order effects       |
| SINGULAR=                                                  | Tunes the estimability checking difference                                      |
| <b>Degrees of Freedom and <math>p</math>-values</b>        |                                                                                 |
| ADJUST=                                                    | Determines the method for multiple comparison adjustment of estimates           |
| ALPHA= $\alpha$                                            | Determines the confidence level ( $1 - \alpha$ )                                |
| LOWER                                                      | Performs one-sided, lower-tailed inference                                      |
| STEPDOWN                                                   | Adjusts multiplicity-corrected $p$ -values further in a step-down fashion       |
| TESTVALUE=                                                 | Specifies values under the null hypothesis for tests                            |
| UPPER                                                      | Performs one-sided, upper-tailed inference                                      |
| <b>Statistical Output</b>                                  |                                                                                 |
| CL                                                         | Constructs confidence limits                                                    |
| CORR                                                       | Displays the correlation matrix of estimates                                    |
| COV                                                        | Displays the covariance matrix of estimates                                     |
| E                                                          | Prints the <b>L</b> matrix                                                      |
| JOINT                                                      | Produces a joint $F$ or chi-square test for the estimable functions             |
| SEED=                                                      | Specifies the seed for computations that depend on random numbers               |
| <b>Generalized Linear Modeling</b>                         |                                                                                 |
| CATEGORY=                                                  | Specifies how to construct estimable functions with multinomial data            |
| EXP                                                        | Exponentiates and displays estimates                                            |
| ILINK                                                      | Computes and displays estimates and standard errors on the inverse linked scale |

For details about the syntax of the ESTIMATE statement, see the section “ESTIMATE Statement” on page 437 in Chapter 19, “Shared Concepts and Topics.”

## FREQ Statement

**FREQ** *variable* ;

The *variable* in the FREQ statement identifies a variable that contains the frequency of occurrence of each observation. PROC SURVEYLOGISTIC treats each observation as if it appears  $n$  times, where  $n$  is the value of the FREQ variable for the observation. If it is not an integer, the frequency value is truncated to

an integer. If the frequency value is less than 1 or missing, the observation is not used in the model fitting. When the FREQ statement is not specified, each observation is assigned a frequency of 1.

If you use the `events/trials` syntax in the MODEL statement, the FREQ statement is not allowed because the event and trial variables represent the frequencies in the data set.

If you use the FREQ statement and specify the `VARMETHOD=BRR` or `VARMETHOD=JACKKNIFE` option to estimate the variance, then you must identify the primary sampling units with a CLUSTER statement unless you also provide replicate weights with a REPWEIGHTS statement.

---

## LSMEANS Statement

**LSMEANS** < *model-effects* > < / *options* > ;

The LSMEANS statement computes and compares least squares means (LS-means) of fixed effects. LS-means are *predicted margins*—that is, they estimate the marginal means over a hypothetical balanced population.

Table 91.5 summarizes available options in the LSMEANS statement.

**Table 91.5** LSMEANS Statement Options

| Option                                          | Description                                                                                 |
|-------------------------------------------------|---------------------------------------------------------------------------------------------|
| <b>Construction and Computation of LS-Means</b> |                                                                                             |
| AT                                              | Modifies the covariate value in computing LS-means                                          |
| BYLEVEL                                         | Computes separate margins                                                                   |
| DIFF                                            | Requests differences of LS-means                                                            |
| OM=                                             | Specifies the weighting scheme for LS-means computation as determined by the input data set |
| SINGULAR=                                       | Tunes estimability checking                                                                 |
| <b>Degrees of Freedom and <i>p</i>-values</b>   |                                                                                             |
| ADJUST=                                         | Determines the method for multiple-comparison adjustment of LS-means differences            |
| ALPHA= $\alpha$                                 | Determines the confidence level $(1 - \alpha)$                                              |
| STEPDOWN                                        | Adjusts multiple-comparison <i>p</i> -values further in a step-down fashion                 |
| <b>Statistical Output</b>                       |                                                                                             |
| CL                                              | Constructs confidence limits for means and mean differences                                 |
| CORR                                            | Displays the correlation matrix of LS-means                                                 |
| COV                                             | Displays the covariance matrix of LS-means                                                  |
| E                                               | Prints the <b>L</b> matrix                                                                  |
| LINES                                           | Produces a “Lines” display for pairwise LS-means differences                                |
| MEANS                                           | Prints the LS-means                                                                         |
| PLOTS=                                          | Requests graphs of means and mean comparisons                                               |
| SEED=                                           | Specifies the seed for computations that depend on random numbers                           |

---

Table 91.5 *continued*

| Option                             | Description                                                                                                       |
|------------------------------------|-------------------------------------------------------------------------------------------------------------------|
| <b>Generalized Linear Modeling</b> |                                                                                                                   |
| EXP                                | Exponentiates and displays estimates of LS-means or LS-means differences                                          |
| ILINK                              | Computes and displays estimates and standard errors of LS-means (but not differences) on the inverse linked scale |
| ODDSRATIO                          | Reports (simple) differences of least squares means in terms of odds ratios if permitted by the link function     |

For details about the syntax of the LSMEANS statement, see the section “LSMEANS Statement” on page 453 of Chapter 19, “Shared Concepts and Topics.”

## LSMESTIMATE Statement

```
LSMESTIMATE model-effect <'label'> values <divisor=n>
 < , ... <'label'> values <divisor=n> >
 </options> ;
```

The LSMESTIMATE statement provides a mechanism for obtaining custom hypothesis tests among least squares means.

Table 91.6 summarizes the options available in the LSMESTIMATE statement.

Table 91.6 LSMESTIMATE Statement Options

| Option                                              | Description                                                                         |
|-----------------------------------------------------|-------------------------------------------------------------------------------------|
| <b>Construction and Computation of LS-Means</b>     |                                                                                     |
| AT                                                  | Modifies covariate values in computing LS-means                                     |
| BYLEVEL                                             | Computes separate margins                                                           |
| DIVISOR=                                            | Specifies a list of values to divide the coefficients                               |
| OM=                                                 | Specifies the weighting scheme for LS-means computation as determined by a data set |
| SINGULAR=                                           | Tunes estimability checking                                                         |
| <b>Degrees of Freedom and <math>p</math>-values</b> |                                                                                     |
| ADJUST=                                             | Determines the method for multiple-comparison adjustment of LS-means differences    |
| ALPHA= $\alpha$                                     | Determines the confidence level ( $1 - \alpha$ )                                    |
| LOWER                                               | Performs one-sided, lower-tailed inference                                          |
| STEPDOWN                                            | Adjusts multiple-comparison $p$ -values further in a step-down fashion              |
| TESTVALUE=                                          | Specifies values under the null hypothesis for tests                                |
| UPPER                                               | Performs one-sided, upper-tailed inference                                          |

Table 91.6 *continued*

| Option                             | Description                                                                                                       |
|------------------------------------|-------------------------------------------------------------------------------------------------------------------|
| <b>Statistical Output</b>          |                                                                                                                   |
| CL                                 | Constructs confidence limits for means and mean differences                                                       |
| CORR                               | Displays the correlation matrix of LS-means                                                                       |
| COV                                | Displays the covariance matrix of LS-means                                                                        |
| E                                  | Prints the <b>L</b> matrix                                                                                        |
| ELSM                               | Prints the <b>K</b> matrix                                                                                        |
| JOINT                              | Produces a joint <i>F</i> or chi-square test for the LS-means and LS-means differences                            |
| SEED=                              | Specifies the seed for computations that depend on random numbers                                                 |
| <b>Generalized Linear Modeling</b> |                                                                                                                   |
| CATEGORY=                          | Specifies how to construct estimable functions with multinomial data                                              |
| EXP                                | Exponentiates and displays LS-means estimates                                                                     |
| ILINK                              | Computes and displays estimates and standard errors of LS-means (but not differences) on the inverse linked scale |

For details about the syntax of the LSMESTIMATE statement, see the section “[LSMESTIMATE Statement](#)” on page 470 in Chapter 19, “[Shared Concepts and Topics](#).”

## MODEL Statement

**MODEL** *events/trials* = < *effects* </ *options* >> ;

**MODEL** *variable* <( *v-options*) > = < *effects* > </ *options* > ;

The MODEL statement names the response variable and the explanatory effects, including covariates, main effects, interactions, and nested effects; see the section “[Specification of Effects](#)” on page 3324 of Chapter 42, “[The GLM Procedure](#),” for more information. If you omit the explanatory variables, the procedure fits an intercept-only model. [Model options](#) can be specified after a slash (/).

Two forms of the MODEL statement can be specified. The first form, referred to as *single-trial* syntax, is applicable to binary, ordinal, and nominal response data. The second form, referred to as *events/trials* syntax, is restricted to the case of binary response data. The single-trial syntax is used when each observation in the DATA= data set contains information about only a single trial, such as a single subject in an experiment. When each observation contains information about multiple binary-response trials, such as the counts of the number of subjects observed and the number responding, then events/trials syntax can be used.

In the events/trials syntax, you specify two variables that contain count data for a binomial experiment. These two variables are separated by a slash. The value of the first variable, *events*, is the number of positive responses (or events), and it must be nonnegative. The value of the second variable, *trials*, is the number of trials, and it must not be less than the value of *events*.

In the single-trial syntax, you specify one variable (on the left side of the equal sign) as the response variable. This variable can be character or numeric. [Options](#) specific to the response variable can be specified immediately after the response variable with parentheses around them.

For both forms of the MODEL statement, explanatory *effects* follow the equal sign. Variables can be either continuous or classification variables. Classification variables can be character or numeric, and they must be declared in the CLASS statement. When an effect is a classification variable, the procedure enters a set of coded columns into the design matrix instead of directly entering a single column containing the values of the variable.

## Response Variable Options

You specify the following options by enclosing them in parentheses after the response variable:

### DESCENDING

#### DESC

reverses the order of response categories. If both the DESCENDING and the [ORDER=](#) options are specified, PROC SURVEYLOGISTIC orders the response categories according to the ORDER= option and then reverses that order. See the section “[Response Level Ordering](#)” on page 7724 for more detail.

#### EVENT=*'category'* | *keyword*

specifies the event category for the binary response model. PROC SURVEYLOGISTIC models the probability of the event category. The EVENT= option has no effect when there are more than two response categories. You can specify the value (formatted if a format is applied) of the event category in quotes or you can specify one of the following keywords. The default is EVENT=FIRST.

FIRST                    designates the first ordered category as the event

LAST                     designates the last ordered category as the event

One of the most common sets of response levels is  $\{0,1\}$ , with 1 representing the event for which the probability is to be modeled. Consider the example where Y takes the values 1 and 0 for event and nonevent, respectively, and Exposure is the explanatory variable. To specify the value 1 as the event category, use the following MODEL statement:

```
model Y(event='1') = Exposure;
```

### ORDER=DATA | FORMATTED | FREQ | INTERNAL

specifies the sort order for the levels of the response variable. By default, ORDER=INTERNAL. For ORDER=FORMATTED and ORDER=INTERNAL, the sort order is machine-dependent.

When the default ORDER=FORMATTED is in effect for numeric variables for which you have supplied no explicit format,



| Value of ORDER= | Levels Sorted By                                                                                                                       |
|-----------------|----------------------------------------------------------------------------------------------------------------------------------------|
| DATA            | Order of appearance in the input data set                                                                                              |
| FORMATTED       | External formatted value, except for numeric variables with no explicit format, which are sorted by their unformatted (internal) value |
| FREQ            | Descending frequency count; levels with the most observations come first in the order                                                  |
| INTERNAL        | Unformatted value                                                                                                                      |

For more information about sort order, see the chapter on the SORT procedure in the *Base SAS Procedures Guide* and the discussion of BY-group processing in *SAS Language Reference: Concepts*.

**REFERENCE=**'category' | keyword

**REF=**'category' | keyword

specifies the reference category for the generalized logit model and the binary response model. For the generalized logit model, each nonreference category is contrasted with the reference category. For the binary response model, specifying one response category as the reference is the same as specifying the other response category as the event category. You can specify the value (formatted if a format is applied) of the reference category in quotes or you can specify one of the following keywords. The default is REF=LAST.

FIRST            designates the first ordered category as the reference

LAST             designates the last ordered category as the reference

## Model Options

Model options can be specified after a slash (/). [Table 91.7](#) summarizes the options available in the MODEL statement.

**Table 91.7** MODEL Statement Options

| Option                               | Description                                                                                                            |
|--------------------------------------|------------------------------------------------------------------------------------------------------------------------|
| <b>Model Specification Options</b>   |                                                                                                                        |
| LINK=                                | Specifies link function                                                                                                |
| NOINT                                | Suppresses intercept(s)                                                                                                |
| OFFSET=                              | Specifies offset variable                                                                                              |
| <b>Convergence Criterion Options</b> |                                                                                                                        |
| ABSFCNV=                             | Specifies absolute function convergence criterion                                                                      |
| FCNV=                                | Specifies relative function convergence criterion                                                                      |
| GCONV=                               | Specifies relative gradient convergence criterion                                                                      |
| XCONV=                               | Specifies relative parameter convergence criterion                                                                     |
| MAXITER=                             | Specifies maximum number of iterations                                                                                 |
| NOCHECK                              | Suppresses checking for infinite parameters                                                                            |
| RIDGING=                             | Specifies technique used to improve the log-likelihood function when its value is worse than that of the previous step |
| SINGULAR=                            | Specifies tolerance for testing singularity                                                                            |

Table 91.7 (continued)

| Option                                               | Description                                                         |
|------------------------------------------------------|---------------------------------------------------------------------|
| TECHNIQUE=                                           | Specifies iterative algorithm for maximization                      |
| <b>Options for Adjustment to Variance Estimation</b> |                                                                     |
| VADJUST=                                             | Chooses variance estimation adjustment method                       |
| <b>Options for Confidence Intervals</b>              |                                                                     |
| ALPHA=                                               | Specifies $\alpha$ for the $100(1 - \alpha)\%$ confidence intervals |
| CLPARM                                               | Computes confidence intervals for parameters                        |
| CLODDS                                               | Computes confidence intervals for odds ratios                       |
| <b>Options for Display of Details</b>                |                                                                     |
| CORRB                                                | Displays correlation matrix                                         |
| COVB                                                 | Displays covariance matrix                                          |
| EXPB                                                 | Displays exponentiated values of estimates                          |
| ITPRINT                                              | Displays iteration history                                          |
| NODUMMYPRINT                                         | Suppresses “Class Level Information” table                          |
| PARMLABEL                                            | Displays parameter labels                                           |
| RSQUARE                                              | Displays generalized $R^2$                                          |
| STB                                                  | Displays standardized estimates                                     |

The following list describes these options:

**ABSFCNV=value**

specifies the absolute function convergence criterion. Convergence requires a small change in the log-likelihood function in subsequent iterations:

$$|l^{(i)} - l^{(i-1)}| < value$$

where  $l^{(i)}$  is the value of the log-likelihood function at iteration  $i$ . See the section “Convergence Criteria” on page 7731.

**ALPHA=value**

sets the level of significance  $\alpha$  for  $100(1 - \alpha)\%$  confidence intervals for regression parameters or odds ratios. The value  $\alpha$  must be between 0 and 1. By default,  $\alpha$  is equal to the value of the ALPHA= option in the PROC SURVEYLOGISTIC statement, or  $\alpha = 0.05$  if the ALPHA= option is not specified. This option has no effect unless confidence limits for the parameters or odds ratios are requested.

**CLODDS**

requests confidence intervals for the odds ratios. Computation of these confidence intervals is based on individual Wald tests. The confidence coefficient can be specified with the ALPHA= option.

See the section “Wald Confidence Intervals for Parameters” on page 7745 for more information.

**CLPARM**

requests confidence intervals for the parameters. Computation of these confidence intervals is based on the individual Wald tests. The confidence coefficient can be specified with the ALPHA= option.

See the section “Wald Confidence Intervals for Parameters” on page 7745 for more information.

**CORRB**

displays the correlation matrix of the parameter estimates.

**COVB**

displays the covariance matrix of the parameter estimates.

**EXPB****EXPEST**

displays the exponentiated values ( $e^{\hat{\theta}_i}$ ) of the parameter estimates  $\hat{\theta}_i$  in the “Analysis of Maximum Likelihood Estimates” table for the logit model. These exponentiated values are the estimated odds ratios for the parameters corresponding to the continuous explanatory variables.

**FCONV=value**

specifies the relative function convergence criterion. Convergence requires a small relative change in the log-likelihood function in subsequent iterations:

$$\frac{|l^{(i)} - l^{(i-1)}|}{|l^{(i-1)}| + 1\text{E-}6} < \text{value}$$

where  $l^{(i)}$  is the value of the log likelihood at iteration  $i$ . See the section “Convergence Criteria” on page 7731 for details.

**GCONV=value**

specifies the relative gradient convergence criterion. Convergence requires that the normalized prediction function reduction is small:

$$\frac{\mathbf{g}^{(i)'} \mathbf{I}^{(i)} \mathbf{g}^{(i)}}{|l^{(i)}| + 1\text{E-}6} < \text{value}$$

where  $l^{(i)}$  is the value of the log-likelihood function,  $\mathbf{g}^{(i)}$  is the gradient vector, and  $\mathbf{I}^{(i)}$  the (expected) information matrix. All of these functions are evaluated at iteration  $i$ . This is the default convergence criterion, and the default value is 1E–8. See the section “Convergence Criteria” on page 7731 for details.

**ITPRINT**

displays the iteration history of the maximum-likelihood model fitting. The ITPRINT option also displays the last evaluation of the gradient vector and the final change in the  $-2 \log L$ .

**LINK=keyword****L=keyword**

specifies the link function that links the response probabilities to the linear predictors. You can specify one of the following keywords. The default is LINK=LOGIT.

**CLOGLOG** specifies the complementary log-log function. PROC SURVEYLOGISTIC fits the binary complementary log-log model for binary response and fits the cumulative complementary log-log model when there are more than two response categories. Aliases: CCLOGLOG, CCLL, CUMCLOGLOG.

**GLOGIT** specifies the generalized logit function. PROC SURVEYLOGISTIC fits the generalized logit model where each nonreference category is contrasted with the reference category. You can use the response variable option REF= to specify the reference category.

|        |                                                                                                                                                                                                                                                                                  |
|--------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| LOGIT  | specifies the cumulative logit function. PROC SURVEYLOGISTIC fits the binary logit model when there are two response categories and fits the cumulative logit model when there are more than two response categories. Aliases: CLOGIT, CUMLOGIT.                                 |
| PROBIT | specifies the inverse standard normal distribution function. PROC SURVEYLOGISTIC fits the binary probit model when there are two response categories and fits the cumulative probit model when there are more than two response categories. Aliases: NORMIT, CPROBIT, CUMPROBIT. |

See the section “[Link Functions and the Corresponding Distributions](#)” on page 7727 for details.

**MAXITER=*n***

specifies the maximum number of iterations to perform. By default, MAXITER=25. If convergence is not attained in *n* iterations, the displayed output created by the procedure contains results that are based on the last maximum likelihood iteration.

**NOCHECK**

disables the checking process to determine whether maximum likelihood estimates of the regression parameters exist. If you are sure that the estimates are finite, this option can reduce the execution time when the estimation takes more than eight iterations. For more information, see the section “[Existence of Maximum Likelihood Estimates](#)” on page 7731.

**NODUMMYPRINT**

suppresses the “Class Level Information” table, which shows how the design matrix columns for the CLASS variables are coded.

**NOINT**

suppresses the intercept for the binary response model or the first intercept for the ordinal response model.

**OFFSET=*name***

names the offset variable. The regression coefficient for this variable is fixed at 1.

**PARMLABEL**

displays the labels of the parameters in the “Analysis of Maximum Likelihood Estimates” table.

**RIDGING=ABSOLUTE | RELATIVE | NONE**

specifies the technique used to improve the log-likelihood function when its value in the current iteration is less than that in the previous iteration. If you specify the RIDGING=ABSOLUTE option, the diagonal elements of the negative (expected) Hessian are inflated by adding the ridge value. If you specify the RIDGING=RELATIVE option, the diagonal elements are inflated by a factor of 1 plus the ridge value. If you specify the RIDGING=NONE option, the crude line search method of taking half a step is used instead of ridging. By default, RIDGING=RELATIVE.

**RSQUARE**

requests a generalized  $R^2$  measure for the fitted model.

For more information, see the section “[Generalized Coefficient of Determination](#)” on page 7733.

**SINGULAR=***value*

specifies the tolerance for testing the singularity of the Hessian matrix (Newton-Raphson algorithm) or the expected value of the Hessian matrix (Fisher scoring algorithm). The Hessian matrix is the matrix of second partial derivatives of the log likelihood. The test requires that a pivot for sweeping this matrix be at least this *value* times a norm of the matrix. Values of the SINGULAR= option must be numeric. By default, SINGULAR= $10^{-12}$ .

**STB**

displays the standardized estimates for the parameters for the continuous explanatory variables in the “Analysis of Maximum Likelihood Estimates” table. The standardized estimate of  $\theta_i$  is given by  $\hat{\theta}_i/(s/s_i)$ , where  $s_i$  is the total sample standard deviation for the  $i$ th explanatory variable and

$$s = \begin{cases} \pi/\sqrt{3} & \text{Logistic} \\ 1 & \text{Normal} \\ \pi/\sqrt{6} & \text{Extreme-value} \end{cases}$$

For the intercept parameters and parameters associated with a CLASS variable, the standardized estimates are set to missing.

**TECHNIQUE=FISHER | NEWTON****TECH=FISHER | NEWTON**

specifies the optimization technique for estimating the regression parameters. NEWTON (or NR) is the Newton-Raphson algorithm and FISHER (or FS) is the Fisher scoring algorithm. Both techniques yield the same estimates, but the estimated covariance matrices are slightly different except for the case where the LOGIT link is specified for binary response data. The default is TECHNIQUE=FISHER. If the LINK=GLOGIT option is specified, then Newton-Raphson is the default and only available method. See the section “[Iterative Algorithms for Model Fitting](#)” on page 7729 for details.

**VADJUST=DF****VADJUST=MOREL** < (*Morel-options*) >**VADJUST=NONE**

specifies an [adjustment to the variance estimation](#) for the regression coefficients.

By default, PROC SURVEYLOGISTIC uses the degrees of freedom adjustment VADJUST=DF.

If you do not want to use any variance adjustment, you can specify the VADJUST=NONE option. You can specify the VADJUST=MOREL option for the variance adjustment proposed by Morel (1989).

You can specify the following *Morel-options* within parentheses after the VADJUST=MOREL option:

**ADJBOUND=** $\phi$ 

sets the upper bound coefficient  $\phi$  in the variance adjustment. This upper bound must be positive. By default, the procedure uses  $\phi = 0.5$ . See the section “[Adjustments to the Variance Estimation](#)” on page 7740 for more details on how this upper bound is used in the variance estimation.

**DEFFBOUND=** $\delta$ 

sets the lower bound of the estimated design effect in the variance adjustment. This lower bound must be positive. By default, the procedure uses  $\delta = 1$ . See the section “[Adjustments to the Variance Estimation](#)” on page 7740 for more details about how this lower bound is used in the variance estimation.

**XCONV=value**

specifies the relative parameter convergence criterion. Convergence requires a small relative parameter change in subsequent iterations:

$$\max_j |\delta_j^{(i)}| < value$$

where

$$\delta_j^{(i)} = \begin{cases} \theta_j^{(i)} - \theta_j^{(i-1)} & |\theta_j^{(i-1)}| < 0.01 \\ \frac{\theta_j^{(i)} - \theta_j^{(i-1)}}{\theta_j^{(i-1)}} & \text{otherwise} \end{cases}$$

and  $\theta_j^{(i)}$  is the estimate of the  $j$ th parameter at iteration  $i$ . See the section “Convergence Criteria” on page 7731 for details.

## OUTPUT Statement

**OUTPUT** < **OUT=SAS-data-set** > < options > < / option > ;

The OUTPUT statement creates a new SAS data set that contains all the variables in the input data set and, optionally, the estimated linear predictors and their standard error estimates, the estimates of the cumulative or individual response probabilities, and the confidence limits for the cumulative probabilities. Formulas for the statistics are given in the section “Linear Predictor, Predicted Probability, and Confidence Limits” on page 7749.

If you use the single-trial syntax, the data set also contains a variable named `_LEVEL_`, which indicates the level of the response that the given row of output is referring to. For example, the value of the cumulative probability variable is the probability that the response variable is as large as the corresponding value of `_LEVEL_`. For details, see the section “OUT= Data Set in the OUTPUT Statement” on page 7750.

The estimated linear predictor, its standard error estimate, all predicted probabilities, and the confidence limits for the cumulative probabilities are computed for all observations in which the explanatory variables have no missing values, even if the response is missing. By adding observations with missing response values to the input data set, you can compute these statistics for new observations, or for settings of the explanatory variables not present in the data, without affecting the model fit.

Table 91.8 summarizes the options available in the OUTPUT statement.

**Table 91.8** OUTPUT Statement Options

| Option     | Description                                                            |
|------------|------------------------------------------------------------------------|
| ALPHA=     | Sets the level of significance                                         |
| LOWER      | Names the variable that contains the lower confidence limits           |
| OUT=       | Names the output data set                                              |
| PREDICTED  | Names the variable that contains the predicted probabilities           |
| PREDPROBS= | Requests predicted probabilities                                       |
| STDXBETA=  | Names the variable that contains the standard error estimates          |
| UPPER      | Names the variable that contains the upper confidence limits           |
| XBETA=     | Names the variable that contains the estimates of the linear predictor |

You can specify the following options in the OUTPUT statement:

**LOWER | L=name**

names the variable that contains the lower confidence limits for  $\pi$ , where  $\pi$  is the probability of the event response if events/trials syntax or the single-trial syntax with binary response is specified;  $\pi$  is cumulative probability (that is, the probability that the response is less than or equal to the value of `_LEVEL_`) for a cumulative model; and  $\pi$  is the individual probability (that is, the probability that the response category is represented by the value of `_LEVEL_`) for the generalized logit model. See the [ALPHA=](#) option for information about setting the confidence level.

**OUT=SAS-data-set**

names the output data set. If you omit the OUT= option, the output data set is created and given a default name by using the `DATAn` convention.

The statistic options in the OUTPUT statement specify the statistics to be included in the output data set and name the new variables that contain the statistics.

**PREDICTED | P=name**

names the variable that contains the predicted probabilities. For the events/trials syntax or the single-trial syntax with binary response, it is the predicted event probability. For a cumulative model, it is the predicted cumulative probability (that is, the probability that the response variable is less than or equal to the value of `_LEVEL_`); and for the generalized logit model, it is the predicted individual probability (that is, the probability of the response category represented by the value of `_LEVEL_`).

**PREDPROBS=(keywords)**

requests individual, cumulative, or cross validated predicted probabilities. Descriptions of the *keywords* are as follows.

**INDIVIDUAL | I** requests the predicted probability of each response level. For a response variable *Y* with three levels, 1, 2, and 3, the individual probabilities are  $\Pr(Y=1)$ ,  $\Pr(Y=2)$ , and  $\Pr(Y=3)$ .

**CUMULATIVE | C** requests the cumulative predicted probability of each response level. For a response variable *Y* with three levels, 1, 2, and 3, the cumulative probabilities are  $\Pr(Y \leq 1)$ ,  $\Pr(Y \leq 2)$ , and  $\Pr(Y \leq 3)$ . The cumulative probability for the last response level always has the constant value of 1. For generalized logit models, the cumulative predicted probabilities are not computed and are set to missing.

**CROSSVALIDATE | XVALIDATE | X** requests the cross validated individual predicted probability of each response level. These probabilities are derived from the leave-one-out principle; that is, dropping the data of one subject and reestimating the parameter estimates. PROC SURVEYLOGISTIC uses a less expensive one-step approximation to compute the parameter estimates. This option is valid only for binary response models; for nominal and ordinal models, the cross validated probabilities are not computed and are set to missing.

See the section “[Details of the PREDPROBS= Option](#)” on page 7717 at the end of this section for further details.



**STDXBETA=***name*

names the variable that contains the standard error estimates of **XBETA** (the definition of which follows).

**UPPER | U=***name*

names the variable that contains the upper confidence limits for  $\pi$ , where  $\pi$  is the probability of the event response if events/trials syntax or single-trial syntax with binary response is specified;  $\pi$  is cumulative probability (that is, the probability that the response is less than or equal to the value of `_LEVEL_`) for a cumulative model; and  $\pi$  is the individual probability (that is, the probability that the response category is represented by the value of `_LEVEL_`) for the generalized logit model. See the **ALPHA=** option for information about setting the confidence level.

**XBETA=***name*

names the variable that contains the estimates of the linear predictor  $\alpha_i + \mathbf{x}\boldsymbol{\beta}$ , where  $i$  is the corresponding ordered value of `_LEVEL_`.

You can specify the following option in the OUTPUT statement after a slash (/):

**ALPHA=***value*

sets the level of significance  $\alpha$  for  $100(1 - \alpha)\%$  confidence limits for the appropriate response probabilities. The value  $\alpha$  must be between 0 and 1. By default,  $\alpha$  is equal to the value of the **ALPHA=** option in the PROC SURVEYLOGISTIC statement, or 0.05 if the ALPHA= option is not specified.

### Details of the PREDPROBS= Option

You can request any of the three given types of predicted probabilities. For example, you can request both the individual predicted probabilities and the cross validated probabilities by specifying **PREDPROBS=(I X)**.

When you specify the **PREDPROBS=** option, two automatic variables `_FROM_` and `_INTO_` are included for the single-trial syntax and only one variable, `_INTO_`, is included for the events/trials syntax. The `_FROM_` variable contains the formatted value of the observed response. The variable `_INTO_` contains the formatted value of the response level with the largest individual predicted probability.

If you specify **PREDPROBS=INDIVIDUAL**, the OUTPUT data set contains  $k$  additional variables representing the individual probabilities, one for each response level, where  $k$  is the maximum number of response levels across all BY groups. The names of these variables have the form `IP_`*xxx*, where *xxx* represents the particular level. The representation depends on the following situations:

- If you specify the events/trials syntax, *xxx* is either Event or Nonevent. Thus, the variable that contains the event probabilities is named `IP_Event` and the variable containing the nonevent probabilities is named `IP_Nonevent`.
- If you specify the single-trial syntax with more than one BY group, *xxx* is 1 for the first ordered level of the response, 2 for the second ordered level of the response, and so forth, as given in the “Response Profile” table. The variable that contains the predicted probabilities  $\Pr(Y=1)$  is named `IP_1`, where  $Y$  is the response variable. Similarly, `IP_2` is the name of the variable containing the predicted probabilities  $\Pr(Y=2)$ , and so on.
- If you specify the single-trial syntax with no BY-group processing, *xxx* is the left-justified formatted value of the response level (the value can be truncated so that `IP_`*xxx* does not exceed 32 characters).



For example, if  $Y$  is the response variable with response levels ‘None,’ ‘Mild,’ and ‘Severe,’ the variables representing individual probabilities  $\Pr(Y=\text{‘None’})$ ,  $\Pr(Y=\text{‘Mild’})$ , and  $\Pr(Y=\text{‘Severe’})$  are named `IP_None`, `IP_Mild`, and `IP_Severe`, respectively.

If you specify `PREDPROBS=CUMULATIVE`, the OUTPUT data set contains  $k$  additional variables that represent the cumulative probabilities, one for each response level, where  $k$  is the maximum number of response levels across all BY groups. The names of these variables have the form `CP_xxx`, where `xxx` represents the particular response level. The naming convention is similar to that given by `PREDPROBS=INDIVIDUAL`. The `PREDPROBS=CUMULATIVE` values are the same as those output by the `PREDICT=keyword`, but they are arranged in variables in each output observation rather than in multiple output observations.

If you specify `PREDPROBS=CROSSVALIDATE`, the OUTPUT data set contains  $k$  additional variables representing the cross validated predicted probabilities of the  $k$  response levels, where  $k$  is the maximum number of response levels across all BY groups. The names of these variables have the form `XP_xxx`, where `xxx` represents the particular level. The representation is the same as that given by `PREDPROBS=INDIVIDUAL`, except that for the events/trials syntax there are four variables for the cross validated predicted probabilities instead of two:

`XP_EVENT_R1E` is the cross validated predicted probability of an event when a current event trial is removed.

`XP_NONEVENT_R1E` is the cross validated predicted probability of a nonevent when a current event trial is removed.

`XP_EVENT_R1N` is the cross validated predicted probability of an event when a current nonevent trial is removed.

`XP_NONEVENT_R1N` is the cross validated predicted probability of a nonevent when a current nonevent trial is removed.

---

## REPWEIGHTS Statement

**REPWEIGHTS** *variables* </ options > ;

The `REPWEIGHTS` statement names variables that provide replicate weights for BRR or jackknife variance estimation, which you request with the `VARMETHOD=BRR` or `VARMETHOD=JACKKNIFE` option in the `PROC SURVEYLOGISTIC` statement. If you do not provide replicate weights for these methods by using a `REPWEIGHTS` statement, then the procedure constructs replicate weights for the analysis. See the sections “Balanced Repeated Replication (BRR) Method” on page 7740 and “Jackknife Method” on page 7742 for information about replicate weights.

Each `REPWEIGHTS` variable should contain the weights for a single replicate, and the number of replicates equals the number of `REPWEIGHTS` variables. The `REPWEIGHTS` variables must be numeric, and the variable values must be nonnegative numbers.

If you provide replicate weights with a `REPWEIGHTS` statement, you do not need to specify a `CLUSTER` or `STRATA` statement. If you use a `REPWEIGHTS` statement and do not specify the `VARMETHOD=` option in the `PROC SURVEYLOGISTIC` statement, the procedure uses `VARMETHOD=JACKKNIFE` by default.

If you specify a **REPWEIGHTS** statement but do not include a **WEIGHT** statement, the procedure uses the average of replicate weights of each observation as the observation's weight.

You can specify the following options in the **REPWEIGHTS** statement after a slash (/):

**DF=***df*

specifies the degrees of freedom for the analysis. The value of *df* must be a positive number. By default, the degrees of freedom equals the number of **REPWEIGHTS** variables.

**JKCOEFS=***value*

specifies a **jackknife coefficient** for **VARMETHOD=JACKKNIFE**. The coefficient *value* must be a nonnegative number. See the section “**Jackknife Method**” on page 7742 for details about jackknife coefficients.

You can use this option to specify a single value of the jackknife coefficient, which the procedure uses for all replicates. To specify different coefficients for different replicates, use the **JKCOEFS=values** or **JKCOEFS=SAS-data-set** option.

**JKCOEFS=***values*

specifies jackknife coefficients for **VARMETHOD=JACKKNIFE**, where each coefficient corresponds to an individual replicate that is identified by a **REPWEIGHTS** variable. You can separate *values* with blanks or commas. The coefficient *values* must be nonnegative numbers. The number of *values* must equal the number of replicate weight variables named in the **REPWEIGHTS** statement. List these values in the same order in which you list the corresponding replicate weight variables in the **REPWEIGHTS** statement.

See the section “**Jackknife Method**” on page 7742 for details about jackknife coefficients.

To specify different coefficients for different replicates, you can also use the **JKCOEFS=SAS-data-set** option. To specify a single jackknife coefficient for all replicates, use the **JKCOEFS=value** option.

**JKCOEFS=SAS-data-set**

names a SAS data set that contains the jackknife coefficients for **VARMETHOD=JACKKNIFE**. You provide the jackknife coefficients in the **JKCOEFS=** data set variable **JKCoefficient**. Each coefficient value must be a nonnegative number. The observations in the **JKCOEFS=** data set should correspond to the replicates that are identified by the **REPWEIGHTS** variables. Arrange the coefficients or observations in the **JKCOEFS=** data set in the same order in which you list the corresponding replicate weight variables in the **REPWEIGHTS** statement. The number of observations in the **JKCOEFS=** data set must not be less than the number of **REPWEIGHTS** variables.

See the section “**Jackknife Method**” on page 7742 for details about jackknife coefficients.

To specify different coefficients for different replicates, you can also use the **JKCOEFS=values** option. To specify a single jackknife coefficient for all replicates, use the **JKCOEFS=value** option.

---

## SLICE Statement

**SLICE** *model-effect* </ options > ;

The **SLICE** statement provides a general mechanism for performing a partitioned analysis of the LS-means for an interaction. This analysis is also known as an analysis of simple effects.

The SLICE statement uses the same options as the LSMEANS statement, which are summarized in Table 19.21. For details about the syntax of the SLICE statement, see the section “SLICE Statement” on page 498 in Chapter 19, “Shared Concepts and Topics.”

## STORE Statement

```
STORE <OUT=>item-store-name </ LABEL='label'> ;
```

The STORE statement requests that the procedure save the context and results of the statistical analysis. The resulting item store has a binary file format that cannot be modified. The contents of the item store can be processed with the PLM procedure.

For details about the syntax of the STORE statement, see the section “STORE Statement” on page 501 in Chapter 19, “Shared Concepts and Topics.”

## STRATA Statement

```
STRATA variables </ option> ;
```

The STRATA statement specifies variables that form the strata in a stratified sample design. The combinations of categories of STRATA variables define the strata in the sample.

If your sample design has stratification at multiple stages, you should identify only the first-stage strata in the STRATA statement. See the section “Specification of Population Totals and Sampling Rates” on page 7734 for more information.

If you provide replicate weights for BRR or jackknife variance estimation with the REPWEIGHTS statement, you do not need to specify a STRATA statement.

The STRATA variables are one or more variables in the DATA= input data set. These variables can be either character or numeric. The formatted values of the STRATA variables determine the levels. Thus, you can use formats to group values into levels. See the FORMAT procedure in the *Base SAS Procedures Guide* and the FORMAT statement and SAS formats in *SAS Formats and Informats: Reference* for more information.

When determining levels of a STRATA variable, an observation with missing values for this STRATA variable is excluded, unless you specify the MISSING option. For more information, see the section “Missing Values” on page 7723.

You can use multiple STRATA statements to specify stratum variables.

You can specify the following option in the STRATA statement after a slash (/):

### LIST

displays a “Stratum Information” table, which includes values of the STRATA variables and the number of observations, number of clusters, population total, and sampling rate for each stratum. See the section “Stratum Information” on page 7754 for more details.

---

## TEST Statement

`< label: > TEST equation1 <, equation2, ... > </ option > ;`

The TEST statement tests linear hypotheses about the regression coefficients. The Wald test is used to jointly test the null hypotheses ( $H_0: \mathbf{L}\boldsymbol{\theta} = \mathbf{c}$ ) specified in a single TEST statement. When  $\mathbf{c} = \mathbf{0}$  you should specify a CONTRAST statement instead.

Each *equation* specifies a linear hypothesis (a row of the  $\mathbf{L}$  matrix and the corresponding element of the  $\mathbf{c}$  vector); multiple *equations* are separated by commas. The label, which must be a valid SAS name, is used to identify the resulting output and should always be included. You can submit multiple TEST statements.

The form of an *equation* is as follows:

`term < ± term ... > < = ± term < ± term ... >>`

where *term* is a parameter of the model, or a constant, or a constant times a parameter. For a binary response model, the intercept parameter is named INTERCEPT; for an ordinal response model, the intercept parameters are named INTERCEPT, INTERCEPT2, INTERCEPT3, and so on. When no equal sign appears, the expression is set to 0. The following illustrates possible uses of the TEST statement:

```
proc surveylogistic;
 model y= a1 a2 a3 a4;
 test1: test intercept + .5 * a2 = 0;
 test2: test intercept + .5 * a2;
 test3: test a1=a2=a3;
 test4: test a1=a2, a2=a3;
run;
```

Note that the first and second TEST statements are equivalent, as are the third and fourth TEST statements.

You can specify the following option in the TEST statement after a slash (/):

### PRINT

displays intermediate calculations in the testing of the null hypothesis  $H_0: \mathbf{L}\boldsymbol{\theta} = \mathbf{c}$ . This includes  $\mathbf{L}\widehat{\mathbf{V}}(\hat{\boldsymbol{\theta}})\mathbf{L}'$  bordered by  $(\mathbf{L}\hat{\boldsymbol{\theta}} - \mathbf{c})$  and  $[\mathbf{L}\widehat{\mathbf{V}}(\hat{\boldsymbol{\theta}})\mathbf{L}']^{-1}$  bordered by  $[\mathbf{L}\widehat{\mathbf{V}}(\hat{\boldsymbol{\theta}})\mathbf{L}']^{-1}(\mathbf{L}\hat{\boldsymbol{\theta}} - \mathbf{c})$ , where  $\hat{\boldsymbol{\theta}}$  is the pseudo-estimator of  $\boldsymbol{\theta}$  and  $\widehat{\mathbf{V}}(\hat{\boldsymbol{\theta}})$  is the estimated covariance matrix of  $\hat{\boldsymbol{\theta}}$ .

For more information, see the section “Testing Linear Hypotheses about the Regression Coefficients” on page 7745.

---

## UNITS Statement

`UNITS independent1 = list1 <... independentk = listk > </ option > ;`

The UNITS statement enables you to specify units of change for the continuous explanatory variables so that customized odds ratios can be estimated. An estimate of the corresponding odds ratio is produced for each unit of change specified for an explanatory variable. The UNITS statement is ignored for CLASS variables. If the CLODDS option is specified in the MODEL statement, the corresponding confidence limits for the odds ratios are also displayed.

The term *independent* is the name of an explanatory variable, and *list* represents a list of units of change, separated by spaces, that are of interest for that variable. Each unit of change in a list has one of the following forms:

- *number*
- SD or -SD
- *number* \* SD

where *number* is any nonzero number and SD is the sample standard deviation of the corresponding independent variable. For example,  $X = -2$  requests an odds ratio that represents the change in the odds when the variable  $X$  is decreased by two units.  $X = 2*SD$  requests an estimate of the change in the odds when  $X$  is increased by two sample standard deviations.

You can specify the following option in the UNITS statement after a slash (/):

**DEFAULT=*list***

gives a list of units of change for all explanatory variables that are not specified in the UNITS statement. Each unit of change can be in any of the forms described previously. If the DEFAULT= option is not specified, PROC SURVEYLOGISTIC does not produce customized odds ratio estimates for any explanatory variable that is not listed in the UNITS statement.

For more information, see the section “Odds Ratio Estimation” on page 7745.

## WEIGHT Statement

**WEIGHT** *variable* ;

The WEIGHT statement names the variable that contains the sampling weights. This variable must be numeric, and the sampling weights must be positive numbers. If an observation has a weight that is nonpositive or missing, then the procedure omits that observation from the analysis. See the section “Missing Values” on page 7723 for more information. If you specify more than one WEIGHT statement, the procedure uses only the first WEIGHT statement and ignores the rest.

If you do not specify a WEIGHT statement but provide replicate weights with a REPWEIGHTS statement, PROC SURVEYLOGISTIC uses the average of replicate weights of each observation as the observation’s weight.

If you do not specify a WEIGHT statement or a REPWEIGHTS statement, PROC SURVEYLOGISTIC assigns all observations a weight of one.

---

## Details: SURVEYLOGISTIC Procedure

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### Missing Values

If you have missing values in your survey data for any reason, such as nonresponse, this can compromise the quality of your survey results. If the respondents are different from the nonrespondents with regard to a survey effect or outcome, then survey estimates might be biased and cannot accurately represent the survey population. There are a variety of techniques in sample design and survey operations that can reduce nonresponse. After data collection is complete, you can use imputation to replace missing values with acceptable values, and/or you can use sampling weight adjustments to compensate for nonresponse. You should complete this data preparation and adjustment before you analyze your data with PROC SURVEYLOGISTIC. For more information, see Cochran (1977); Kalton and Kaspyzyk (1986); Brick and Kalton (1996).

If an observation has a missing value or a nonpositive value for the **WEIGHT** or **FREQ** variable, then that observation is excluded from the analysis.

An observation is also excluded if it has a missing value for any design (**STRATA**, **CLUSTER**, or **DOMAIN**) variable, unless you specify the **MISSING** option in the PROC SURVEYLOGISTIC statement. If you specify the **MISSING** option, the procedure treats missing values as a valid (nonmissing) category for all categorical variables.

By default, if an observation contains missing values for the response, offset, or any explanatory variables used in the independent effects, the observation is excluded from the analysis. This treatment is based on the assumption that the missing values are missing completely at random (MCAR). However, this assumption is not true sometimes. For example, evidence from other surveys might suggest that observations with missing values are systematically different from observations without missing values. If you believe that missing values are not missing completely at random, then you can specify the **NOMCAR** option to include these observations with missing values in the dependent variable and the independent variables in the variance estimation.

Whether or not the **NOMCAR** option is used, observations with missing or invalid values for **WEIGHT**, **FREQ**, **STRATA**, **CLUSTER**, or **DOMAIN** variables are always excluded, unless the **MISSING** option is also specified.

When you specify the **NOMCAR** option, the procedure treats observations with and without missing values for variables in the regression model as two different domains, and it performs a domain analysis in the domain of nonmissing observations.

If you use a **REPWEIGHTS** statement, all **REPWEIGHTS** variables must contain nonmissing values.

## Model Specification

### Response Level Ordering

Response level ordering is important because, by default, PROC SURVEYLOGISTIC models the probabilities of response levels with lower *Ordered Values*. Ordered Values, displayed in the “Response Profile” table, are assigned to response levels in ascending sorted order. That is, the lowest response level is assigned Ordered Value 1, the next lowest is assigned Ordered Value 2, and so on. For example, if your response variable  $Y$  takes values in  $\{1, \dots, D + 1\}$ , then the functions of the response probabilities modeled with the cumulative model are

$$\text{logit}(\Pr(Y \leq i|\mathbf{x})), i = 1, \dots, D$$

and for the generalized logit model they are

$$\log \left( \frac{\Pr(Y = i|\mathbf{x})}{\Pr(Y = D + 1|\mathbf{x})} \right), i = 1, \dots, D$$

where the highest Ordered Value  $Y = D + 1$  is the reference level. You can change these default functions by specifying the **EVENT=**, **REF=**, **DESCENDING**, or **ORDER=** response variable options in the MODEL statement.

For binary response data with event and nonevent categories, the procedure models the function

$$\text{logit}(p) = \log \left( \frac{p}{1 - p} \right)$$

where  $p$  is the probability of the response level assigned to Ordered Value 1 in the “Response Profiles” table. Since

$$\text{logit}(p) = -\text{logit}(1 - p)$$

the effect of reversing the order of the two response levels is to change the signs of  $\alpha$  and  $\beta$  in the model  $\text{logit}(p) = \alpha + \mathbf{x}\beta$ .

If your event category has a higher Ordered Value than the nonevent category, the procedure models the nonevent probability. You can use response variable options to model the event probability. For example, suppose the binary response variable  $Y$  takes the values 1 and 0 for event and nonevent, respectively, and **Exposure** is the explanatory variable. By default, the procedure assigns Ordered Value 1 to response level  $Y=0$ , and Ordered Value 2 to response level  $Y=1$ . Therefore, the procedure models the probability of the nonevent (Ordered Value=1) category. To model the event probability, you can do the following:

- Explicitly state which response level is to be modeled by using the response variable option **EVENT=** in the MODEL statement:

```
model Y(event='1') = Exposure;
```

- Specify the response variable option **DESCENDING** in the MODEL statement:

```
model Y(descending)=Exposure;
```

- Specify the response variable option **REF=** in the MODEL statement as the nonevent category for the response variable. This option is most useful when you are fitting a generalized logit model.

```
model Y(ref='0') = Exposure;
```

- Assign a format to Y such that the first formatted value (when the formatted values are put in sorted order) corresponds to the event. For this example, Y=1 is assigned formatted value 'event' and Y=0 is assigned formatted value 'nonevent.' Since **ORDER= FORMATTED** by default, Ordered Value 1 is assigned to response level Y=1 so the procedure models the event.

```
proc format;
 value Disease 1='event' 0='nonevent';
run;

proc surveylogistic;
 format Y Disease.;
 model Y=Exposure;
run;
```

## CLASS Variable Parameterization

Consider a model with one **CLASS** variable A with four levels: 1, 2, 5, and 7. Details of the possible choices for the **PARAM=** option follow.

**EFFECT** Three columns are created to indicate group membership of the nonreference levels. For the reference level, all three dummy variables have a value of  $-1$ . For instance, if the reference level is 7 (**REF=7**), the design matrix columns for A are as follows.

| Design Matrix |    |    |    |
|---------------|----|----|----|
| A             | A1 | A2 | A5 |
| 1             | 1  | 0  | 0  |
| 2             | 0  | 1  | 0  |
| 5             | 0  | 0  | 1  |
| 7             | -1 | -1 | -1 |

For **CLASS** main effects that use the **EFFECT** coding scheme, individual parameters correspond to the difference between the effect of each nonreference level and the average over all four levels.

**GLM** As in **PROC GLM**, four columns are created to indicate group membership. The design matrix columns for A are as follows.



| Design Matrix |    |    |    |    |
|---------------|----|----|----|----|
| A             | A1 | A2 | A5 | A7 |
| 1             | 1  | 0  | 0  | 0  |
| 2             | 0  | 1  | 0  | 0  |
| 5             | 0  | 0  | 1  | 0  |
| 7             | 0  | 0  | 0  | 1  |

For CLASS main effects that use the GLM coding scheme, individual parameters correspond to the difference between the effect of each level and the last level.

**ORDINAL**

Three columns are created to indicate group membership of the higher levels of the effect. For the first level of the effect (which for A is 1), all three dummy variables have a value of 0. The design matrix columns for A are as follows.

| Design Matrix |    |    |    |
|---------------|----|----|----|
| A             | A2 | A5 | A7 |
| 1             | 0  | 0  | 0  |
| 2             | 1  | 0  | 0  |
| 5             | 1  | 1  | 0  |
| 7             | 1  | 1  | 1  |

The first level of the effect is a control or baseline level.

For CLASS main effects that use the ORDINAL coding scheme, the first level of the effect is a control or baseline level; individual parameters correspond to the difference between effects of the current level and the preceding level. When the parameters for an ordinal main effect have the same sign, the response effect is monotonic across the levels.

**POLYNOMIAL | POLY** Three columns are created. The first represents the linear term ( $x$ ), the second represents the quadratic term ( $x^2$ ), and the third represents the cubic term ( $x^3$ ), where  $x$  is the level value. If the CLASS levels are not numeric, they are translated into 1, 2, 3, ... according to their sort order. The design matrix columns for A are as follows.

| Design Matrix |        |        |        |
|---------------|--------|--------|--------|
| A             | APOLY1 | APOLY2 | APOLY3 |
| 1             | 1      | 1      | 1      |
| 2             | 2      | 4      | 8      |
| 5             | 5      | 25     | 125    |
| 7             | 7      | 49     | 343    |

**REFERENCE | REF** Three columns are created to indicate group membership of the nonreference levels. For the reference level, all three dummy variables have a value of 0. For instance, if the reference level is 7 (REF=7), the design matrix columns for A are as follows.

| Design Matrix |    |    |    |
|---------------|----|----|----|
| A             | A1 | A2 | A5 |
| 1             | 1  | 0  | 0  |
| 2             | 0  | 1  | 0  |
| 5             | 0  | 0  | 1  |
| 7             | 0  | 0  | 0  |

For CLASS main effects that use the REFERENCE coding scheme, individual parameters correspond to the difference between the effect of each nonreference level and the reference level.

**ORTHEFFECT** The columns are obtained by applying the Gram-Schmidt orthogonalization to the columns for PARAM=EFFECT. The design matrix columns for A are as follows.

| Design Matrix |          |          |          |
|---------------|----------|----------|----------|
| A             | AOEFF1   | AOEFF2   | AOEFF3   |
| 1             | 1.41421  | -0.81650 | -0.57735 |
| 2             | 0.00000  | 1.63299  | -0.57735 |
| 5             | 0.00000  | 0.00000  | 1.73205  |
| 7             | -1.41421 | -0.81649 | -0.57735 |

**ORTHORDINAL** | **ORTHOTHERM** The columns are obtained by applying the Gram-Schmidt orthogonalization to the columns for PARAM=ORDINAL. The design matrix columns for A are as follows.

| Design Matrix |          |          |          |
|---------------|----------|----------|----------|
| A             | AOORD1   | AOORD2   | AOORD3   |
| 1             | -1.73205 | 0.00000  | 0.00000  |
| 2             | 0.57735  | -1.63299 | 0.00000  |
| 5             | 0.57735  | 0.81650  | -1.41421 |
| 7             | 0.57735  | 0.81650  | 1.41421  |

**ORTHPOLY** The columns are obtained by applying the Gram-Schmidt orthogonalization to the columns for PARAM=POLY. The design matrix columns for A are as follows.

| Design Matrix |         |         |         |
|---------------|---------|---------|---------|
| A             | AOPOLY1 | AOPOLY2 | AOPOLY5 |
| 1             | -1.153  | 0.907   | -0.921  |
| 2             | -0.734  | -0.540  | 1.473   |
| 5             | 0.524   | -1.370  | -0.921  |
| 7             | 1.363   | 1.004   | 0.368   |

**ORTHREF** The columns are obtained by applying the Gram-Schmidt orthogonalization to the columns for PARAM=REFERENCE. The design matrix columns for A are as follows.

| Design Matrix |          |          |          |
|---------------|----------|----------|----------|
| A             | AOREF1   | AOREF2   | AOREF3   |
| 1             | 1.73205  | 0.00000  | 0.00000  |
| 2             | -0.57735 | 1.63299  | 0.00000  |
| 5             | -0.57735 | -0.81650 | 1.41421  |
| 7             | -0.57735 | -0.81650 | -1.41421 |

## Link Functions and the Corresponding Distributions

Four link functions are available in the SURVEYLOGISTIC procedure. The logit function is the default. To specify a different link function, use the **LINK=** option in the MODEL statement. The link functions and the corresponding distributions are as follows:

- The **logit** function

$$g(p) = \log\left(\frac{p}{1-p}\right)$$

is the inverse of the cumulative logistic distribution function, which is

$$F(x) = \frac{1}{1 + e^{-x}}$$

- The **probit** (or normit) function

$$g(p) = \Phi^{-1}(p)$$

is the inverse of the cumulative standard normal distribution function, which is

$$F(x) = \Phi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^x e^{-\frac{1}{2}z^2} dz$$

Traditionally, the probit function includes an additive constant 5, but throughout PROC SURVEYLOGISTIC, the terms probit and normit are used interchangeably, previously defined as  $g(p)$ .

- The **complementary log-log** function

$$g(p) = \log(-\log(1-p))$$

is the inverse of the cumulative extreme-value function (also called the Gompertz distribution), which is

$$F(x) = 1 - e^{-e^x}$$

- The **generalized logit** function extends the binary logit link to a vector of levels  $(\pi_1, \dots, \pi_{k+1})$  by contrasting each level with a fixed level

$$g(\pi_i) = \log\left(\frac{\pi_i}{\pi_{k+1}}\right) \quad i = 1, \dots, k$$

The variances of the normal, logistic, and extreme-value distributions are not the same. Their respective means and variances are

| Distribution  | Mean      | Variance  |
|---------------|-----------|-----------|
| Normal        | 0         | 1         |
| Logistic      | 0         | $\pi^2/3$ |
| Extreme-value | $-\gamma$ | $\pi^2/6$ |

where  $\gamma$  is the Euler constant. In comparing parameter estimates that use different link functions, you need to take into account the different scalings of the corresponding distributions and, for the complementary log-log function, a possible shift in location. For example, if the fitted probabilities are in the neighborhood of 0.1 to 0.9, then the parameter estimates from using the logit link function should be about  $\pi/\sqrt{3} \approx 1.8$  larger than the estimates from the probit link function.

## Model Fitting

### Determining Observations for Likelihood Contributions

If you use the events/trials syntax, each observation is split into two observations. One has the response value 1 with a frequency equal to the value of the *events* variable. The other observation has the response value 2 and a frequency equal to the value of (*trials* – *events*). These two observations have the same explanatory variable values and the same WEIGHT values as the original observation.

For either the single-trial or the events/trials syntax, let  $j$  index all observations. In other words, for the single-trial syntax,  $j$  indexes the actual observations. And, for the events/trials syntax,  $j$  indexes the observations after splitting (as described previously). If your data set has 30 observations and you use the single-trial syntax,  $j$  has values from 1 to 30; if you use the events/trials syntax,  $j$  has values from 1 to 60.

Suppose the response variable in a cumulative response model can take on the ordered values  $1, \dots, k, k + 1$ , where  $k$  is an integer  $\geq 1$ . The likelihood for the  $j$ th observation with ordered response value  $y_j$  and explanatory variables vector (row vectors)  $\mathbf{x}_j$  is given by

$$L_j = \begin{cases} F(\alpha_1 + \mathbf{x}_j \boldsymbol{\beta}) & y_j = 1 \\ F(\alpha_i + \mathbf{x}_j \boldsymbol{\beta}) - F(\alpha_{i-1} + \mathbf{x}_j \boldsymbol{\beta}) & 1 < y_j = i \leq k \\ 1 - F(\alpha_k + \mathbf{x}_j \boldsymbol{\beta}) & y_j = k + 1 \end{cases}$$

where  $F(\cdot)$  is the logistic, normal, or extreme-value distribution function;  $\alpha_1, \dots, \alpha_k$  are ordered intercept parameters; and  $\boldsymbol{\beta}$  is the slope parameter vector.

For the generalized logit model, letting the  $k + 1$ st level be the reference level, the intercepts  $\alpha_1, \dots, \alpha_k$  are unordered and the slope vector  $\boldsymbol{\beta}_i$  varies with each logit. The likelihood for the  $j$ th observation with ordered response value  $y_j$  and explanatory variables vector  $\mathbf{x}_j$  (row vectors) is given by

$$L_j = \Pr(Y = y_j | \mathbf{x}_j) = \begin{cases} \frac{e^{\alpha_i + \mathbf{x}_j \boldsymbol{\beta}_i}}{1 + \sum_{i=1}^k e^{\alpha_i + \mathbf{x}_j \boldsymbol{\beta}_i}} & 1 \leq y_j = i \leq k \\ \frac{1}{1 + \sum_{i=1}^k e^{\alpha_i + \mathbf{x}_j \boldsymbol{\beta}_i}} & y_j = k + 1 \end{cases}$$

### Iterative Algorithms for Model Fitting

Two iterative maximum likelihood algorithms are available in PROC SURVEYLOGISTIC to obtain the pseudo-estimate  $\hat{\boldsymbol{\theta}}$  of the model parameter  $\boldsymbol{\theta}$ . The default is the Fisher scoring method, which is equivalent to fitting by iteratively reweighted least squares. The alternative algorithm is the Newton-Raphson method. Both algorithms give the same parameter estimates; the covariance matrix of  $\hat{\boldsymbol{\theta}}$  is estimated in the section “Variance Estimation” on page 7738. For a generalized logit model, only the Newton-Raphson technique is available. You can use the `TECHNIQUE=` option in the MODEL statement to select a fitting algorithm.

**Iteratively Reweighted Least Squares Algorithm (Fisher Scoring)**

Let  $Y$  be the response variable that takes values  $1, \dots, k, k+1$  ( $k \geq 1$ ). Let  $j$  index all observations and  $Y_j$  be the value of response for the  $j$ th observation. Consider the multinomial variable  $\mathbf{Z}_j = (Z_{1j}, \dots, Z_{kj})'$  such that

$$Z_{ij} = \begin{cases} 1 & \text{if } Y_j = i \\ 0 & \text{otherwise} \end{cases}$$

and  $Z_{(k+1)j} = 1 - \sum_{i=1}^k Z_{ij}$ . With  $\pi_{ij}$  denoting the probability that the  $j$ th observation has response value  $i$ , the expected value of  $\mathbf{Z}_j$  is  $\boldsymbol{\pi}_j = (\pi_{1j}, \dots, \pi_{kj})'$ , and  $\pi_{(k+1)j} = 1 - \sum_{i=1}^k \pi_{ij}$ . The covariance matrix of  $\mathbf{Z}_j$  is  $\mathbf{V}_j$ , which is the covariance matrix of a multinomial random variable for one trial with parameter vector  $\boldsymbol{\pi}_j$ . Let  $\boldsymbol{\theta}$  be the vector of regression parameters—for example,  $\boldsymbol{\theta} = (\alpha_1, \dots, \alpha_k, \boldsymbol{\beta})'$  for cumulative logit model. Let  $\mathbf{D}_j$  be the matrix of partial derivatives of  $\boldsymbol{\pi}_j$  with respect to  $\boldsymbol{\theta}$ . The estimating equation for the regression parameters is

$$\sum_j \mathbf{D}'_j \mathbf{W}_j (\mathbf{Z}_j - \boldsymbol{\pi}_j) = \mathbf{0}$$

where  $\mathbf{W}_j = w_j f_j \mathbf{V}_j^{-1}$ , and  $w_j$  and  $f_j$  are the WEIGHT and FREQ values of the  $j$ th observation.

With a starting value of  $\boldsymbol{\theta}^{(0)}$ , the pseudo-estimate of  $\boldsymbol{\theta}$  is obtained iteratively as

$$\boldsymbol{\theta}^{(i+1)} = \boldsymbol{\theta}^{(i)} + \left( \sum_j \mathbf{D}'_j \mathbf{W}_j \mathbf{D}_j \right)^{-1} \sum_j \mathbf{D}'_j \mathbf{W}_j (\mathbf{Z}_j - \boldsymbol{\pi}_j)$$

where  $\mathbf{D}_j$ ,  $\mathbf{W}_j$ , and  $\boldsymbol{\pi}_j$  are evaluated at the  $i$ th iteration  $\boldsymbol{\theta}^{(i)}$ . The expression after the plus sign is the step size. If the log likelihood evaluated at  $\boldsymbol{\theta}^{(i+1)}$  is less than that evaluated at  $\boldsymbol{\theta}^{(i)}$ , then  $\boldsymbol{\theta}^{(i+1)}$  is recomputed by step-halving or ridging. The iterative scheme continues until convergence is obtained—that is, until  $\boldsymbol{\theta}^{(i+1)}$  is sufficiently close to  $\boldsymbol{\theta}^{(i)}$ . Then the maximum likelihood estimate of  $\boldsymbol{\theta}$  is  $\hat{\boldsymbol{\theta}} = \boldsymbol{\theta}^{(i+1)}$ .

By default, starting values are zero for the slope parameters, and starting values are the observed cumulative logits (that is, logits of the observed cumulative proportions of response) for the intercept parameters. Alternatively, the starting values can be specified with the **INEST=** option in the PROC SURVEYLOGISTIC statement.

**Newton-Raphson Algorithm**

Let

$$\mathbf{g} = \sum_j w_j f_j \frac{\partial l_j}{\partial \boldsymbol{\theta}}$$

$$\mathbf{H} = \sum_j -w_j f_j \frac{\partial^2 l_j}{\partial \boldsymbol{\theta}^2}$$

be the gradient vector and the Hessian matrix, where  $l_j = \log L_j$  is the log likelihood for the  $j$ th observation. With a starting value of  $\boldsymbol{\theta}^{(0)}$ , the pseudo-estimate  $\hat{\boldsymbol{\theta}}$  of  $\boldsymbol{\theta}$  is obtained iteratively until convergence is obtained:

$$\boldsymbol{\theta}^{(i+1)} = \boldsymbol{\theta}^{(i)} + \mathbf{H}^{-1} \mathbf{g}$$

where  $\mathbf{H}$  and  $\mathbf{g}$  are evaluated at the  $i$ th iteration  $\boldsymbol{\theta}^{(i)}$ . If the log likelihood evaluated at  $\boldsymbol{\theta}^{(i+1)}$  is less than that evaluated at  $\boldsymbol{\theta}^{(i)}$ , then  $\boldsymbol{\theta}^{(i+1)}$  is recomputed by step-halving or ridging. The iterative scheme continues until convergence is obtained—that is, until  $\boldsymbol{\theta}^{(i+1)}$  is sufficiently close to  $\boldsymbol{\theta}^{(i)}$ . Then the maximum likelihood estimate of  $\boldsymbol{\theta}$  is  $\hat{\boldsymbol{\theta}} = \boldsymbol{\theta}^{(i+1)}$ .

## Convergence Criteria

Four convergence criteria are allowed: `ABSFCONV=`, `FCONV=`, `GCONV=`, and `XCONV=`. If you specify more than one convergence criterion, the optimization is terminated as soon as one of the criteria is satisfied. If none of the criteria is specified, the default is `GCONV=1E-8`.

## Existence of Maximum Likelihood Estimates

The likelihood equation for a logistic regression model does not always have a finite solution. Sometimes there is a nonunique maximum on the boundary of the parameter space, at infinity. The existence, finiteness, and uniqueness of pseudo-estimates for the logistic regression model depend on the patterns of data points in the observation space (Albert and Anderson 1984; Santner and Duffy 1986).

Consider a binary response model. Let  $Y_j$  be the response of the  $i$ th subject, and let  $\mathbf{x}_j$  be the row vector of explanatory variables (including the constant 1 associated with the intercept). There are three mutually exclusive and exhaustive types of data configurations: complete separation, quasi-complete separation, and overlap.

**Complete separation**                      There is a complete separation of data points if there exists a vector  $\mathbf{b}$  that correctly allocates all observations to their response groups; that is,

$$\begin{cases} \mathbf{x}_j \mathbf{b} > 0 & Y_j = 1 \\ \mathbf{x}_j \mathbf{b} < 0 & Y_j = 2 \end{cases}$$

This configuration gives nonunique infinite estimates. If the iterative process of maximizing the likelihood function is allowed to continue, the log likelihood diminishes to zero, and the dispersion matrix becomes unbounded.

**Quasi-complete separation**            The data are not completely separable, but there is a vector  $\mathbf{b}$  such that

$$\begin{cases} \mathbf{x}_j \mathbf{b} \geq 0 & Y_j = 1 \\ \mathbf{x}_j \mathbf{b} \leq 0 & Y_j = 2 \end{cases}$$

and equality holds for at least one subject in each response group. This configuration also yields nonunique infinite estimates. If the iterative process of maximizing the likelihood function is allowed to continue, the dispersion matrix becomes unbounded and the log likelihood diminishes to a nonzero constant.

**Overlap**                                      If neither complete nor quasi-complete separation exists in the sample points, there is an overlap of sample points. In this configuration, the pseudo-estimates exist and are unique.

Complete separation and quasi-complete separation are problems typically encountered with small data sets. Although complete separation can occur with any type of data, quasi-complete separation is not likely with truly continuous explanatory variables.

The SURVEYLOGISTIC procedure uses a simple empirical approach to recognize the data configurations that lead to infinite parameter estimates. The basis of this approach is that any convergence method of maximizing the log likelihood must yield a solution that gives complete separation, if such a solution exists. In maximizing the log likelihood, there is no checking for complete or quasi-complete separation if convergence is attained in eight or fewer iterations. Subsequent to the eighth iteration, the probability of the observed response is computed for each observation. If the probability of the observed response is one for all observations, there is a complete separation of data points and the iteration process is stopped. If the complete separation of data has not been determined and an observation is identified to have an extremely large probability ( $\geq 0.95$ ) of the observed response, there are two possible situations. First, there is overlap in the data set, and the observation is an atypical observation of its own group. The iterative process, if allowed to continue, stops when a maximum is reached. Second, there is quasi-complete separation in the data set, and the asymptotic dispersion matrix is unbounded. If any of the diagonal elements of the dispersion matrix for the standardized observations vectors (all explanatory variables standardized to zero mean and unit variance) exceeds 5,000, quasi-complete separation is declared and the iterative process is stopped. If either complete separation or quasi-complete separation is detected, a warning message is displayed in the procedure output.

Checking for quasi-complete separation is less foolproof than checking for complete separation. The **NOCHECK** option in the MODEL statement turns off the process of checking for infinite parameter estimates. In cases of complete or quasi-complete separation, turning off the checking process typically results in the procedure failing to converge.

## Model Fitting Statistics

Suppose the model contains  $s$  explanatory effects. For the  $j$ th observation, let  $\hat{\pi}_j$  be the estimated probability of the observed response. The three criteria displayed by the SURVEYLOGISTIC procedure are calculated as follows:

- $-2 \log$  likelihood:

$$-2 \text{ Log L} = -2 \sum_j w_j f_j \log(\hat{\pi}_j)$$

where  $w_j$  and  $f_j$  are the weight and frequency values, respectively, of the  $j$ th observation. For binary response models that use the events/trials syntax, this is equivalent to

$$-2 \text{ Log L} = -2 \sum_j w_j f_j \{r_j \log(\hat{\pi}_j) + (n_j - r_j) \log(1 - \hat{\pi}_j)\}$$

where  $r_j$  is the number of events,  $n_j$  is the number of trials, and  $\hat{\pi}_j$  is the estimated event probability.

- Akaike information criterion:

$$\text{AIC} = -2 \text{ Log L} + 2p$$

where  $p$  is the number of parameters in the model. For cumulative response models,  $p = k + s$ , where  $k$  is the total number of response levels minus one, and  $s$  is the number of explanatory effects. For the generalized logit model,  $p = k(s + 1)$ .

- Schwarz criterion:

$$SC = -2 \text{Log } L + p \log\left(\sum_j f_j\right)$$

where  $p$  is the number of parameters in the model. For cumulative response models,  $p = k + s$ , where  $k$  is the total number of response levels minus one, and  $s$  is the number of explanatory effects. For the generalized logit model,  $p = k(s + 1)$ .

The  $-2 \log$  likelihood statistic has a chi-square distribution under the null hypothesis (that all the explanatory effects in the model are zero), and the procedure produces a  $p$ -value for this statistic. The AIC and SC statistics give two different ways of adjusting the  $-2 \log$  likelihood statistic for the number of terms in the model and the number of observations used.

### Generalized Coefficient of Determination

Cox and Snell (1989, pp. 208–209) propose the following generalization of the coefficient of determination to a more general linear model:

$$R^2 = 1 - \left\{ \frac{L(\mathbf{0})}{L(\hat{\boldsymbol{\theta}})} \right\}^{\frac{2}{n}}$$

where  $L(\mathbf{0})$  is the likelihood of the intercept-only model,  $L(\hat{\boldsymbol{\theta}})$  is the likelihood of the specified model, and  $n$  is the sample size. The quantity  $R^2$  achieves a maximum of less than 1 for discrete models, where the maximum is given by

$$R_{\max}^2 = 1 - \{L(\mathbf{0})\}^{\frac{2}{n}}$$

Nagelkerke (1991) proposes the following adjusted coefficient, which can achieve a maximum value of 1:

$$\tilde{R}^2 = \frac{R^2}{R_{\max}^2}$$

Properties and interpretation of  $R^2$  and  $\tilde{R}^2$  are provided in Nagelkerke (1991). In the “Testing Global Null Hypothesis: BETA=0” table,  $R^2$  is labeled as “RSquare” and  $\tilde{R}^2$  is labeled as “Max-rescaled RSquare.” Use the **RSQUARE** option to request  $R^2$  and  $\tilde{R}^2$ .

### INEST= Data Set

You can specify starting values for the iterative algorithm in the **INEST=** data set.

The **INEST=** data set contains one observation for each **BY** group. The **INEST=** data set must contain the intercept variables (named **Intercept** for binary response models and **Intercept**, **Intercept2**, **Intercept3**, and so forth, for ordinal response models) and all explanatory variables in the **MODEL** statement. If **BY** processing is used, the **INEST=** data set should also include the **BY** variables, and there must be one observation for each **BY** group. If the **INEST=** data set also contains the **\_TYPE\_** variable, only observations with **\_TYPE\_** value ‘**PARMS**’ are used as starting values.



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## Survey Design Information

### Specification of Population Totals and Sampling Rates

To include a finite population correction (*fpc*) in Taylor series variance estimation, you can input either the sampling rate or the population total by using the `RATE=` or `TOTAL=` option in the PROC SURVEYLOGISTIC statement. (You cannot specify both of these options in the same PROC SURVEYLOGISTIC statement.) The `RATE=` and `TOTAL=` options apply only to Taylor series variance estimation. The procedure does not use a finite population correction for BRR or jackknife variance estimation.

If you do not specify the `RATE=` or `TOTAL=` option, the Taylor series variance estimation does not include a finite population correction. For fairly small sampling fractions, it is appropriate to ignore this correction. See Cochran (1977) and Kish (1965) for more information.

If your design has multiple stages of selection and you are specifying the `RATE=` option, you should input the first-stage sampling rate, which is the ratio of the number of PSUs in the sample to the total number of PSUs in the study population. If you are specifying the `TOTAL=` option for a multistage design, you should input the total number of PSUs in the study population. See the section “Primary Sampling Units (PSUs)” on page 7734 for more details.

For a nonstratified sample design, or for a stratified sample design with the same sampling rate or the same population total in all strata, you can use the `RATE=value` or `TOTAL=value` option. If your sample design is stratified with different sampling rates or population totals in different strata, use the `RATE=SAS-data-set` or `TOTAL=SAS-data-set` option to name a SAS data set that contains the stratum sampling rates or totals. This data set is called a *secondary data set*, as opposed to the *primary data set* that you specify with the `DATA=` option.

The secondary data set must contain all the stratification variables listed in the STRATA statement and all the variables in the BY statement. If there are formats associated with the STRATA variables and the BY variables, then the formats must be consistent in the primary and the secondary data sets. If you specify the `TOTAL=SAS-data-set` option, the secondary data set must have a variable named `_TOTAL_` that contains the stratum population totals. Or if you specify the `RATE=SAS-data-set` option, the secondary data set must have a variable named `_RATE_` that contains the stratum sampling rates. If the secondary data set contains more than one observation for any one stratum, then the procedure uses the first value of `_TOTAL_` or `_RATE_` for that stratum and ignores the rest.

The *value* in the `RATE=` option or the values of `_RATE_` in the secondary data set must be nonnegative numbers. You can specify *value* as a number between 0 and 1. Or you can specify *value* in percentage form as a number between 1 and 100, and PROC SURVEYLOGISTIC converts that number to a proportion. The procedure treats the value 1 as 100% instead of 1%.

If you specify the `TOTAL=value` option, *value* must not be less than the sample size. If you provide stratum population totals in a secondary data set, these values must not be less than the corresponding stratum sample sizes.

### Primary Sampling Units (PSUs)

When you have clusters, or primary sampling units (PSUs), in your sample design, the procedure estimates variance from the variation among PSUs when the Taylor series variance method is used. See the section “Taylor Series (Linearization)” on page 7739 for more information.

BRR or jackknife variance estimation methods draw multiple replicates (or subsamples) from the full sample by following a specific resampling scheme. These subsamples are constructed by deleting PSUs from the full sample.

If you use a **REPWEIGHTS** statement to provide replicate weights for BRR or jackknife variance estimation, you do not need to specify a **CLUSTER** statement. Otherwise, you should specify a **CLUSTER** statement whenever your design includes clustering at the first stage of sampling. If you do not specify a **CLUSTER** statement, then PROC SURVEYLOGISTIC treats each observation as a PSU.

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## Logistic Regression Models and Parameters

The SURVEYLOGISTIC procedure fits a logistic regression model and estimates the corresponding regression parameters. Each model uses the link function you specified in the **LINK=** option in the MODEL statement. There are four types of model you can use with the procedure: cumulative logit model, complementary log-log model, probit model, and generalized logit model.

### Notation

Let  $Y$  be the response variable with categories  $1, 2, \dots, D, D + 1$ . The  $p$  covariates are denoted by a  $p$ -dimension row vector  $\mathbf{x}$ .

For a stratified clustered sample design, each observation is represented by a row vector,  $(w_{hij}, \mathbf{y}'_{hij}, y_{hij(D+1)}, \mathbf{x}_{hij})$ , where

- $h = 1, 2, \dots, H$  is the stratum index
- $i = 1, 2, \dots, n_h$  is the cluster index within stratum  $h$
- $j = 1, 2, \dots, m_{hi}$  is the unit index within cluster  $i$  of stratum  $h$
- $w_{hij}$  denotes the sampling weight
- $\mathbf{y}_{hij}$  is a  $D$ -dimensional column vector whose elements are indicator variables for the first  $D$  categories for variable  $Y$ . If the response of the  $j$ th unit of the  $i$ th cluster in stratum  $h$  falls in category  $d$ , the  $d$ th element of the vector is one, and the remaining elements of the vector are zero, where  $d = 1, 2, \dots, D$ .
- $y_{hij(D+1)}$  is the indicator variable for the  $(D + 1)$  category of variable  $Y$
- $\mathbf{x}_{hij}$  denotes the  $k$ -dimensional row vector of explanatory variables for the  $j$ th unit of the  $i$ th cluster in stratum  $h$ . If there is an intercept, then  $x_{hij1} \equiv 1$ .
- $\tilde{n} = \sum_{h=1}^H n_h$  is the total number of clusters in the sample
- $n = \sum_{h=1}^H \sum_{i=1}^{n_h} m_{hi}$  is the total sample size

The following notations are also used:

- $f_h$  denotes the sampling rate for stratum  $h$
- $\boldsymbol{\pi}_{hij}$  is the expected vector of the response variable:

$$\begin{aligned}\boldsymbol{\pi}_{hij} &= E(\mathbf{y}_{hij}|\mathbf{x}_{hij}) \\ &= (\pi_{hij1}, \pi_{hij2}, \dots, \pi_{hijD})' \\ \pi_{hij(D+1)} &= E(y_{hij(D+1)}|\mathbf{x}_{hij})\end{aligned}$$

Note that  $\pi_{hij(D+1)} = 1 - \mathbf{1}'\boldsymbol{\pi}_{hij}$ , where  $\mathbf{1}$  is a  $D$ -dimensional column vector whose elements are 1.

## Logistic Regression Models

If the response categories of the response variable  $Y$  can be restricted to a number of ordinal values, you can fit cumulative probabilities of the response categories with a cumulative logit model, a complementary log-log model, or a probit model. Details of cumulative logit models (or proportional odds models) can be found in McCullagh and Nelder (1989). If the response categories of  $Y$  are nominal responses without natural ordering, you can fit the response probabilities with a generalized logit model. Formulation of the generalized logit models for nominal response variables can be found in Agresti (2002). For each model, the procedure estimates the model parameter  $\boldsymbol{\theta}$  by using a pseudo-log-likelihood function. The procedure obtains the pseudo-maximum likelihood estimator  $\hat{\boldsymbol{\theta}}$  by using iterations described in the section “[Iterative Algorithms for Model Fitting](#)” on page 7729 and estimates its variance described in the section “[Variance Estimation](#)” on page 7738.

### Cumulative Logit Model

A cumulative logit model uses the **logit** function

$$g(t) = \log\left(\frac{t}{1-t}\right)$$

as the link function.

Denote the cumulative sum of the expected proportions for the first  $d$  categories of variable  $Y$  by

$$F_{hijd} = \sum_{r=1}^d \pi_{hijr}$$

for  $d = 1, 2, \dots, D$ . Then the cumulative logit model can be written as

$$\log\left(\frac{F_{hijd}}{1-F_{hijd}}\right) = \alpha_d + \mathbf{x}_{hij}\boldsymbol{\beta}$$

with the model parameters

$$\begin{aligned}\boldsymbol{\beta} &= (\beta_1, \beta_2, \dots, \beta_k)' \\ \boldsymbol{\alpha} &= (\alpha_1, \alpha_2, \dots, \alpha_D)', \quad \alpha_1 < \alpha_2 < \dots < \alpha_D \\ \boldsymbol{\theta} &= (\boldsymbol{\alpha}', \boldsymbol{\beta}')'\end{aligned}$$

**Complementary Log-Log Model**

A complementary log-log model uses the **complementary log-log** function

$$g(t) = \log(-\log(1 - t))$$

as the link function. Denote the cumulative sum of the expected proportions for the first  $d$  categories of variable  $Y$  by

$$F_{hijd} = \sum_{r=1}^d \pi_{hijr}$$

for  $d = 1, 2, \dots, D$ . Then the complementary log-log model can be written as

$$\log(-\log(1 - F_{hijd})) = \alpha_d + \mathbf{x}_{hij} \boldsymbol{\beta}$$

with the model parameters

$$\begin{aligned} \boldsymbol{\beta} &= (\beta_1, \beta_2, \dots, \beta_k)' \\ \boldsymbol{\alpha} &= (\alpha_1, \alpha_2, \dots, \alpha_D)', \quad \alpha_1 < \alpha_2 < \dots < \alpha_D \\ \boldsymbol{\theta} &= (\boldsymbol{\alpha}', \boldsymbol{\beta}')' \end{aligned}$$

**Probit Model**

A probit model uses the **probit** (or normit) function, which is the inverse of the cumulative standard normal distribution function,

$$g(t) = \Phi^{-1}(t)$$

as the link function, where

$$\Phi(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^t e^{-\frac{1}{2}z^2} dz$$

Denote the cumulative sum of the expected proportions for the first  $d$  categories of variable  $Y$  by

$$F_{hijd} = \sum_{r=1}^d \pi_{hijr}$$

for  $d = 1, 2, \dots, D$ . Then the probit model can be written as

$$F_{hijd} = \Phi(\alpha_d + \mathbf{x}_{hij} \boldsymbol{\beta})$$

with the model parameters

$$\begin{aligned} \boldsymbol{\beta} &= (\beta_1, \beta_2, \dots, \beta_k)' \\ \boldsymbol{\alpha} &= (\alpha_1, \alpha_2, \dots, \alpha_D)', \quad \alpha_1 < \alpha_2 < \dots < \alpha_D \\ \boldsymbol{\theta} &= (\boldsymbol{\alpha}', \boldsymbol{\beta}')' \end{aligned}$$

### Generalized Logit Model

For nominal response, a generalized logit model is to fit the ratio of the expected proportion for each response category over the expected proportion of a reference category with a logit link function.

Without loss of generality, let category  $D + 1$  be the reference category for the response variable  $Y$ . Denote the expected proportion for the  $d$ th category by  $\pi_{hij d}$  as in the section “Notation” on page 7735. Then the generalized logit model can be written as

$$\log \left( \frac{\pi_{hij d}}{\pi_{hij(D+1)}} \right) = \mathbf{x}_{hij} \boldsymbol{\beta}_d$$

for  $d = 1, 2, \dots, D$ , with the model parameters

$$\begin{aligned} \boldsymbol{\beta}_d &= (\beta_{d1}, \beta_{d2}, \dots, \beta_{dk})' \\ \boldsymbol{\theta} &= (\boldsymbol{\beta}'_1, \boldsymbol{\beta}'_2, \dots, \boldsymbol{\beta}'_D)' \end{aligned}$$

### Likelihood Function

Let  $g(\cdot)$  be a link function such that

$$\boldsymbol{\pi} = \mathbf{g}(\mathbf{x}, \boldsymbol{\theta})$$

where  $\boldsymbol{\theta}$  is a column vector for regression coefficients. The pseudo-log likelihood is

$$l(\boldsymbol{\theta}) = \sum_{h=1}^H \sum_{i=1}^{n_h} \sum_{j=1}^{m_{hi}} w_{hij} \left( (\log(\boldsymbol{\pi}_{hij}))' \mathbf{y}_{hij} + \log(\pi_{hij(D+1)}) y_{hij(D+1)} \right)$$

Denote the pseudo-estimator as  $\hat{\boldsymbol{\theta}}$ , which is a solution to the estimating equations:

$$\sum_{h=1}^H \sum_{i=1}^{n_h} \sum_{j=1}^{m_{hi}} w_{hij} \mathbf{D}_{hij} \left( \text{diag}(\boldsymbol{\pi}_{hij}) - \boldsymbol{\pi}_{hij} \boldsymbol{\pi}'_{hij} \right)^{-1} (\mathbf{y}_{hij} - \boldsymbol{\pi}_{hij}) = \mathbf{0}$$

where  $\mathbf{D}_{hij}$  is the matrix of partial derivatives of the link function  $\mathbf{g}$  with respect to  $\boldsymbol{\theta}$ .

To obtain the pseudo-estimator  $\hat{\boldsymbol{\theta}}$ , the procedure uses iterations with a starting value  $\boldsymbol{\theta}^{(0)}$  for  $\boldsymbol{\theta}$ . See the section “Iterative Algorithms for Model Fitting” on page 7729 for more details.

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### Variance Estimation

Due to the variability of characteristics among items in the population, researchers apply scientific sample designs in the sample selection process to reduce the risk of a distorted view of the population, and they make inferences about the population based on the information from the sample survey data. In order to make statistically valid inferences for the population, they must incorporate the sample design in the data analysis.

The SURVEYLOGISTIC procedure fits linear logistic regression models for discrete response survey data by using the maximum likelihood method. In the variance estimation, the procedure uses the Taylor series

(linearization) method or replication (resampling) methods to estimate sampling errors of estimators based on complex sample designs, including designs with stratification, clustering, and unequal weighting (Binder 1981, 1983; Roberts, Rao, and Kumar 1987; Skinner, Holt, and Smith 1989; Binder and Roberts 2003; Morel 1989; Lehtonen and Pahkinen 1995; Woodruff 1971; Fuller 1975; Särndal, Swensson, and Wretman 1992; Fuller 2009; Wolter 2007; Rust 1985; Dippo, Fay, and Morganstein 1984; Rao and Shao 1999; Rao, Wu, and Yue 1992; Rao and Shao 1996).

You can use the `VARMETHOD=` option to specify a variance estimation method to use. By default, the Taylor series method is used. However, replication methods have recently gained popularity for estimating variances in complex survey data analysis. One reason for this popularity is the relative simplicity of replication-based estimates, especially for nonlinear estimators; another is that modern computational capacity has made replication methods feasible for practical survey analysis.

Replication methods draw multiple replicates (also called subsamples) from a full sample according to a specific resampling scheme. The most commonly used resampling schemes are the *balanced repeated replication* (BRR) method and the *jackknife* method. For each replicate, the original weights are modified for the PSUs in the replicates to create replicate weights. The parameters of interest are estimated by using the replicate weights for each replicate. Then the variances of parameters of interest are estimated by the variability among the estimates derived from these replicates. You can use the `REPWEIGHTS` statement to provide your own replicate weights for variance estimation.

The following sections provide details about how the variance-covariance matrix of the estimated regression coefficients is estimated for each variance estimation method.

### Taylor Series (Linearization)

The Taylor series (linearization) method is the most commonly used method to estimate the covariance matrix of the regression coefficients for complex survey data. It is the default variance estimation method used by PROC SURVEYLOGISTIC.

Using the notation described in the section “Notation” on page 7735, the estimated covariance matrix of model parameters  $\hat{\theta}$  by the Taylor series method is

$$\widehat{V}(\hat{\theta}) = \widehat{Q}^{-1} \widehat{G} \widehat{Q}^{-1}$$

where

$$\begin{aligned} \widehat{Q} &= \sum_{h=1}^H \sum_{i=1}^{n_h} \sum_{j=1}^{m_{hi}} w_{hij} \widehat{D}_{hij} \left( \text{diag}(\hat{\boldsymbol{\pi}}_{hij}) - \hat{\boldsymbol{\pi}}_{hij} \hat{\boldsymbol{\pi}}'_{hij} \right)^{-1} \widehat{D}'_{hij} \\ \widehat{G} &= \frac{n-1}{n-p} \sum_{h=1}^H \frac{n_h(1-f_h)}{n_h-1} \sum_{i=1}^{n_h} (\mathbf{e}_{hi\cdot} - \bar{\mathbf{e}}_{h\cdot\cdot}) (\mathbf{e}_{hi\cdot} - \bar{\mathbf{e}}_{h\cdot\cdot})' \\ \mathbf{e}_{hi\cdot} &= \sum_{j=1}^{m_{hi}} w_{hij} \widehat{D}_{hij} \left( \text{diag}(\hat{\boldsymbol{\pi}}_{hij}) - \hat{\boldsymbol{\pi}}_{hij} \hat{\boldsymbol{\pi}}'_{hij} \right)^{-1} (\mathbf{y}_{hij} - \hat{\boldsymbol{\pi}}_{hij}) \\ \bar{\mathbf{e}}_{h\cdot\cdot} &= \frac{1}{n_h} \sum_{i=1}^{n_h} \mathbf{e}_{hi\cdot} \end{aligned}$$

and  $\mathbf{D}_{hij}$  is the matrix of partial derivatives of the link function  $g$  with respect to  $\boldsymbol{\theta}$  and  $\widehat{D}_{hij}$  and the response probabilities  $\hat{\boldsymbol{\pi}}_{hij}$  are evaluated at  $\hat{\boldsymbol{\theta}}$ .

If you specify the `TECHNIQUE=NEWTON` option in the `MODEL` statement to request the **Newton-Raphson algorithm**, the matrix  $\widehat{\mathbf{Q}}$  is replaced by the negative (expected) Hessian matrix when the estimated covariance matrix  $\widehat{\mathbf{V}}(\widehat{\boldsymbol{\theta}})$  is computed.

### Adjustments to the Variance Estimation

The factor  $(n - 1)/(n - p)$  in the computation of the matrix  $\widehat{\mathbf{G}}$  reduces the small sample bias associated with using the estimated function to calculate deviations (Morel 1989; Hidioglou, Fuller, and Hickman 1980). For simple random sampling, this factor contributes to the degrees-of-freedom correction applied to the residual mean square for ordinary least squares in which  $p$  parameters are estimated. By default, the procedure uses this adjustment in Taylor series variance estimation. It is equivalent to specifying the `VADJUST=DF` option in the `MODEL` statement. If you do not want to use this multiplier in the variance estimation, you can specify the `VADJUST=NONE` option in the `MODEL` statement to suppress this factor.

In addition, you can specify the `VADJUST=MOREL` option to request an adjustment to the variance estimator for the model parameters  $\widehat{\boldsymbol{\theta}}$ , introduced by Morel (1989):

$$\widehat{\mathbf{V}}(\widehat{\boldsymbol{\theta}}) = \widehat{\mathbf{Q}}^{-1}\widehat{\mathbf{G}}\widehat{\mathbf{Q}}^{-1} + \kappa\lambda\widehat{\mathbf{Q}}^{-1}$$

where for given nonnegative constants  $\delta$  and  $\phi$ ,

$$\begin{aligned}\kappa &= \max\left(\delta, p^{-1}\text{tr}\left(\widehat{\mathbf{Q}}^{-1}\widehat{\mathbf{G}}\right)\right) \\ \lambda &= \min\left(\phi, \frac{p}{\bar{n} - p}\right)\end{aligned}$$

The adjustment  $\kappa\lambda\widehat{\mathbf{Q}}^{-1}$  does the following:

- reduces the small sample bias reflected in inflated Type I error rates
- guarantees a positive-definite estimated covariance matrix provided that  $\widehat{\mathbf{Q}}^{-1}$  exists
- is close to zero when the sample size becomes large

In this adjustment,  $\kappa$  is an estimate of the design effect, which has been bounded below by the positive constant  $\delta$ . You can use `DEFFBOUND= $\delta$`  in the `VADJUST=MOREL` option in the `MODEL` statement to specify this lower bound; by default, the procedure uses  $\delta = 1$ . The factor  $\lambda$  converges to zero when the sample size becomes large, and  $\lambda$  has an upper bound  $\phi$ . You can use `ADJBOUND= $\phi$`  in the `VADJUST=MOREL` option in the `MODEL` statement to specify this upper bound; by default, the procedure uses  $\phi = 0.5$ .

### Balanced Repeated Replication (BRR) Method

The balanced repeated replication (BRR) method requires that the full sample be drawn by using a stratified sample design with two primary sampling units (PSUs) per stratum. Let  $H$  be the total number of strata. The total number of replicates  $R$  is the smallest multiple of 4 that is greater than  $H$ . However, if you prefer a larger number of replicates, you can specify the `REPS=number` option. If a *number*  $\times$  *number* Hadamard matrix cannot be constructed, the number of replicates is increased until a Hadamard matrix becomes available.

Each replicate is obtained by deleting one PSU per stratum according to the corresponding **Hadamard matrix** and adjusting the original weights for the remaining PSUs. The new weights are called replicate weights.

Replicates are constructed by using the first  $H$  columns of the  $R \times R$  **Hadamard matrix**. The  $r$ th ( $r = 1, 2, \dots, R$ ) replicate is drawn from the full sample according to the  $r$ th row of the Hadamard matrix as follows:

- If the  $(r, h)$  element of the Hadamard matrix is 1, then the first PSU of stratum  $h$  is included in the  $r$ th replicate and the second PSU of stratum  $h$  is excluded.
- If the  $(r, h)$  element of the Hadamard matrix is  $-1$ , then the second PSU of stratum  $h$  is included in the  $r$ th replicate and the first PSU of stratum  $h$  is excluded.

Note that the “first” and “second” PSUs are determined by data order in the input data set. Thus, if you reorder the data set and perform the same analysis by using BRR method, you might get slightly different results, because the contents in each replicate sample might change.

The replicate weights of the remaining PSUs in each half-sample are then doubled to their original weights. For more details about the BRR method, see Wolter (2007) and Lohr (2010).

By default, an appropriate Hadamard matrix is generated automatically to create the replicates. You can request that the Hadamard matrix be displayed by specifying the **VARMETHOD=BRR(PRINTH)** *method-option*. If you provide a Hadamard matrix by specifying the **VARMETHOD=BRR(HADAMARD=)** *method-option*, then the replicates are generated according to the provided Hadamard matrix.

You can use the **VARMETHOD=BRR(OUTWEIGHTS=)** *method-option* to save the replicate weights into a SAS data set.

Let  $\hat{\theta}$  be the estimated regression coefficients from the full sample for  $\theta$ , and let  $\hat{\theta}_r$  be the estimated regression coefficient from the  $r$ th replicate by using replicate weights. PROC SURVEYLOGISTIC estimates the covariance matrix of  $\hat{\theta}$  by

$$\widehat{V}(\hat{\theta}) = \frac{1}{R} \sum_{r=1}^R (\hat{\theta}_r - \hat{\theta}) (\hat{\theta}_r - \hat{\theta})'$$

with  $H$  degrees of freedom, where  $H$  is the number of strata.

## Fay's BRR Method

Fay's method is a modification of the **BRR** method, and it requires a stratified sample design with two primary sampling units (PSUs) per stratum. The total number of replicates  $R$  is the smallest multiple of 4 that is greater than the total number of strata  $H$ . However, if you prefer a larger number of replicates, you can specify the **REPS=** *method-option*.

For each replicate, Fay's method uses a Fay coefficient  $0 \leq \epsilon < 1$  to impose a perturbation of the original weights in the full sample that is gentler than using only half-samples, as in the traditional BRR method. The Fay coefficient  $0 \leq \epsilon < 1$  can be set by specifying the **FAY =  $\epsilon$**  *method-option*. By default,  $\epsilon = 0.5$  if the **FAY** *method-option* is specified without providing a value for  $\epsilon$  (Judkins 1990; Rao and Shao 1999). When  $\epsilon = 0$ , Fay's method becomes the traditional **BRR** method. For more details, see Dippo, Fay, and Morganstein (1984); Fay (1984, 1989); Judkins (1990).



Let  $H$  be the number of strata. Replicates are constructed by using the first  $H$  columns of the  $R \times R$  Hadamard matrix, where  $R$  is the number of replicates,  $R > H$ . The  $r$ th ( $r = 1, 2, \dots, R$ ) replicate is created from the full sample according to the  $r$ th row of the Hadamard matrix as follows:

- If the  $(r, h)$  element of the Hadamard matrix is 1, then the full sample weight of the first PSU in stratum  $h$  is multiplied by  $\epsilon$  and the full sample weight of the second PSU is multiplied by  $2 - \epsilon$  to obtain the  $r$ th replicate weights.
- If the  $(r, h)$  element of the Hadamard matrix is  $-1$ , then the full sample weight of the first PSU in stratum  $h$  is multiplied by  $2 - \epsilon$  and the full sample weight of the second PSU is multiplied by  $\epsilon$  to obtain the  $r$ th replicate weights.

You can use the `VARMETHOD=BRR(OUTWEIGHTS=)` *method-option* to save the replicate weights into a SAS data set.

By default, an appropriate Hadamard matrix is generated automatically to create the replicates. You can request that the Hadamard matrix be displayed by specifying the `VARMETHOD=BRR(PRINTH)` *method-option*. If you provide a Hadamard matrix by specifying the `VARMETHOD=BRR(HADAMARD=)` *method-option*, then the replicates are generated according to the provided Hadamard matrix.

Let  $\hat{\theta}$  be the estimated regression coefficients from the full sample for  $\theta$ . Let  $\hat{\theta}_r$  be the estimated regression coefficient obtained from the  $r$ th replicate by using replicate weights. PROC SURVEYLOGISTIC estimates the covariance matrix of  $\hat{\theta}$  by

$$\widehat{V}(\hat{\theta}) = \frac{1}{R(1 - \epsilon)^2} \sum_{r=1}^R (\hat{\theta}_r - \hat{\theta}) (\hat{\theta}_r - \hat{\theta})'$$

with  $H$  degrees of freedom, where  $H$  is the number of strata.

## Jackknife Method

The jackknife method of variance estimation deletes one PSU at a time from the full sample to create replicates. The total number of replicates  $R$  is the same as the total number of PSUs. In each replicate, the sample weights of the remaining PSUs are modified by the jackknife coefficient  $\alpha_r$ . The modified weights are called replicate weights.

The jackknife coefficient and replicate weights are described as follows.

**Without Stratification** If there is no stratification in the sample design (no `STRATA` statement), the jackknife coefficients  $\alpha_r$  are the same for all replicates:

$$\alpha_r = \frac{R - 1}{R} \quad \text{where } r = 1, 2, \dots, R$$

Denote the original weight in the full sample for the  $j$ th member of the  $i$ th PSU as  $w_{ij}$ . If the  $i$ th PSU is included in the  $r$ th replicate ( $r = 1, 2, \dots, R$ ), then the corresponding replicate weight for the  $j$ th member of the  $i$ th PSU is defined as

$$w_{ij}^{(r)} = w_{ij} / \alpha_r$$

**With Stratification** If the sample design involves stratification, each stratum must have at least two PSUs to use the jackknife method.

Let stratum  $\tilde{h}_r$  be the stratum from which a PSU is deleted for the  $r$ th replicate. Stratum  $\tilde{h}_r$  is called the *donor stratum*. Let  $n_{\tilde{h}_r}$  be the total number of PSUs in the donor stratum  $\tilde{h}_r$ . The jackknife coefficients are defined as

$$\alpha_r = \frac{n_{\tilde{h}_r} - 1}{n_{\tilde{h}_r}} \quad \text{where } r = 1, 2, \dots, R$$

Denote the original weight in the full sample for the  $j$ th member of the  $i$ th PSU as  $w_{ij}$ . If the  $i$ th PSU is included in the  $r$ th replicate ( $r = 1, 2, \dots, R$ ), then the corresponding replicate weight for the  $j$ th member of the  $i$ th PSU is defined as

$$w_{ij}^{(r)} = \begin{cases} w_{ij} & \text{if } i\text{th PSU is not in the donor stratum } \tilde{h}_r \\ w_{ij}/\alpha_r & \text{if } i\text{th PSU is in the donor stratum } \tilde{h}_r \end{cases}$$

You can use the `VARMETHOD=JACKKNIFE(OUTJKCOEFS=)` *method-option* to save the jackknife coefficients into a SAS data set and use the `VARMETHOD=JACKKNIFE(OUTWEIGHTS=)` *method-option* to save the replicate weights into a SAS data set.

If you provide your own replicate weights with a `REPWEIGHTS` statement, then you can also provide corresponding jackknife coefficients with the `JKCOEFS=` option.

Let  $\hat{\theta}$  be the estimated regression coefficients from the full sample for  $\theta$ . Let  $\hat{\theta}_r$  be the estimated regression coefficient obtained from the  $r$ th replicate by using replicate weights. PROC SURVEYLOGISTIC estimates the covariance matrix of  $\hat{\theta}$  by

$$\widehat{V}(\hat{\theta}) = \sum_{r=1}^R \alpha_r (\hat{\theta}_r - \hat{\theta}) (\hat{\theta}_r - \hat{\theta})'$$

with  $R - H$  degrees of freedom, where  $R$  is the number of replicates and  $H$  is the number of strata, or  $R - 1$  when there is no stratification.

### Hadamard Matrix

A Hadamard matrix  $\mathbf{H}$  is a square matrix whose elements are either 1 or -1 such that

$$\mathbf{H}\mathbf{H}' = k\mathbf{I}$$

where  $k$  is the dimension of  $\mathbf{H}$  and  $\mathbf{I}$  is the identity matrix of order  $k$ . The order  $k$  is necessarily 1, 2, or a positive integer that is a multiple of 4.

For example, the following matrix is a Hadamard matrix of dimension  $k = 8$ :

$$\begin{matrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 \end{matrix}$$

## Domain Analysis

A **DOMAIN** statement requests that the procedure perform logistic regression analysis for each domain.

For a domain  $\Omega$ , let  $I_\Omega$  be the corresponding indicator variable:

$$I_\Omega(h, i, j) = \begin{cases} 1 & \text{if observation } (h, i, j) \text{ belongs to } \Omega \\ 0 & \text{otherwise} \end{cases}$$

Let

$$v_{hij} = w_{hij} I_\Omega(h, i, j) = \begin{cases} w_{hij} & \text{if observation } (h, i, j) \text{ belongs to } \Omega \\ 0 & \text{otherwise} \end{cases}$$

The regression in domain  $\Omega$  uses  $v$  as the weight variable.

## Hypothesis Testing and Estimation

### Score Statistics and Tests

To understand the general form of the score statistics, let  $\mathbf{g}(\boldsymbol{\theta})$  be the vector of first partial derivatives of the log likelihood with respect to the parameter vector  $\boldsymbol{\theta}$ , and let  $\mathbf{H}(\boldsymbol{\theta})$  be the matrix of second partial derivatives of the log likelihood with respect to  $\boldsymbol{\theta}$ . That is,  $\mathbf{g}(\boldsymbol{\theta})$  is the gradient vector, and  $\mathbf{H}(\boldsymbol{\theta})$  is the Hessian matrix. Let  $\mathbf{I}(\boldsymbol{\theta})$  be either  $-\mathbf{H}(\boldsymbol{\theta})$  or the expected value of  $-\mathbf{H}(\boldsymbol{\theta})$ . Consider a null hypothesis  $H_0$ . Let  $\hat{\boldsymbol{\theta}}$  be the MLE of  $\boldsymbol{\theta}$  under  $H_0$ . The chi-square score statistic for testing  $H_0$  is defined by

$$\mathbf{g}'(\hat{\boldsymbol{\theta}})\mathbf{I}^{-1}(\hat{\boldsymbol{\theta}})\mathbf{g}(\hat{\boldsymbol{\theta}})$$

It has an asymptotic  $\chi^2$  distribution with  $r$  degrees of freedom under  $H_0$ , where  $r$  is the number of restrictions imposed on  $\boldsymbol{\theta}$  by  $H_0$ .

### Testing the Parallel Lines Assumption

For an ordinal response, PROC SURVEYLOGISTIC performs a test of the parallel lines assumption. In the displayed output, this test is labeled “Score Test for the Equal Slopes Assumption” when the **LINK=** option is **NORMIT** or **CLOGLOG**. When **LINK=LOGIT**, the test is labeled as “Score Test for the Proportional Odds Assumption” in the output. This section describes the methods used to calculate the test.

For this test, the number of response levels,  $D + 1$ , is assumed to be strictly greater than 2. Let  $Y$  be the response variable taking values  $1, \dots, D, D + 1$ . Suppose there are  $k$  explanatory variables. Consider the general cumulative model without making the parallel lines assumption:

$$g(\Pr(Y \leq d \mid \mathbf{x})) = (\mathbf{1}, \mathbf{x})\boldsymbol{\theta}_d, \quad 1 \leq d \leq D$$

where  $g(\cdot)$  is the link function, and  $\boldsymbol{\theta}_d = (\alpha_d, \beta_{d1}, \dots, \beta_{dk})'$  is a vector of unknown parameters consisting of an intercept  $\alpha_d$  and  $k$  slope parameters  $\beta_{k1}, \dots, \beta_{kd}$ . The parameter vector for this general cumulative model is

$$\boldsymbol{\theta} = (\boldsymbol{\theta}'_1, \dots, \boldsymbol{\theta}'_D)'$$

Under the null hypothesis of parallelism  $H_0: \beta_{1i} = \beta_{2i} = \dots = \beta_{Di}, 1 \leq i \leq k$ , there is a single common slope parameter for each of the  $s$  explanatory variables. Let  $\beta_1, \dots, \beta_k$  be the common slope parameters. Let  $\hat{\alpha}_1, \dots, \hat{\alpha}_D$  and  $\hat{\beta}_1, \dots, \hat{\beta}_k$  be the MLEs of the intercept parameters and the common slope parameters. Then, under  $H_0$ , the MLE of  $\theta$  is

$$\hat{\theta} = (\hat{\theta}'_1, \dots, \hat{\theta}'_D)' \quad \text{with} \quad \hat{\theta}_d = (\hat{\alpha}_d, \hat{\beta}_1, \dots, \hat{\beta}_k)', \quad 1 \leq d \leq D$$

and the chi-square score statistic  $\mathbf{g}'(\hat{\theta})\mathbf{I}^{-1}(\hat{\theta})\mathbf{g}(\hat{\theta})$  has an asymptotic chi-square distribution with  $k(D - 1)$  degrees of freedom. This tests the parallel lines assumption by testing the equality of separate slope parameters simultaneously for all explanatory variables.

### Wald Confidence Intervals for Parameters

Wald confidence intervals are sometimes called normal confidence intervals. They are based on the asymptotic normality of the parameter estimators. The  $100(1 - \alpha)\%$  Wald confidence interval for  $\theta_j$  is given by

$$\hat{\theta}_j \pm z_{1-\alpha/2} \hat{\sigma}_j$$

where  $z_{1-\alpha/2}$  is the  $100(1 - \alpha/2)$  percentile of the standard normal distribution,  $\hat{\theta}_j$  is the pseudo-estimate of  $\theta_j$ , and  $\hat{\sigma}_j$  is the standard error estimate of  $\hat{\theta}_j$  in the section “Variance Estimation” on page 7738.

### Testing Linear Hypotheses about the Regression Coefficients

Linear hypotheses for  $\theta$  are expressed in matrix form as

$$H_0: \mathbf{L}\theta = \mathbf{c}$$

where  $\mathbf{L}$  is a matrix of coefficients for the linear hypotheses and  $\mathbf{c}$  is a vector of constants. The vector of regression coefficients  $\theta$  includes slope parameters as well as intercept parameters. The Wald chi-square statistic for testing  $H_0$  is computed as

$$\chi^2_W = (\mathbf{L}\hat{\theta} - \mathbf{c})'[\mathbf{L}\hat{\mathbf{V}}(\hat{\theta})\mathbf{L}']^{-1}(\mathbf{L}\hat{\theta} - \mathbf{c})$$

where  $\hat{\mathbf{V}}(\hat{\theta})$  is the estimated covariance matrix in the section “Variance Estimation” on page 7738. Under  $H_0$ ,  $\chi^2_W$  has an asymptotic chi-square distribution with  $r$  degrees of freedom, where  $r$  is the rank of  $\mathbf{L}$ .

### Odds Ratio Estimation

Consider a dichotomous response variable with outcomes *event* and *nonevent*. Let a dichotomous risk factor variable  $X$  take the value 1 if the risk factor is present and 0 if the risk factor is absent. According to the logistic model, the log odds function,  $g(X)$ , is given by

$$g(X) \equiv \log\left(\frac{\Pr(\text{event} | X)}{\Pr(\text{nonevent} | X)}\right) = \beta_0 + \beta_1 X$$

The odds ratio  $\psi$  is defined as the ratio of the odds for those with the risk factor ( $X = 1$ ) to the odds for those without the risk factor ( $X = 0$ ). The log of the odds ratio is given by

$$\log(\psi) \equiv \log(\psi(X = 1, X = 0)) = g(X = 1) - g(X = 0) = \beta_1$$

The parameter,  $\beta_1$ , associated with  $X$  represents the change in the log odds from  $X = 0$  to  $X = 1$ . So the odds ratio is obtained by simply exponentiating the value of the parameter associated with the risk factor. The odds ratio indicates how the odds of *event* change as you change  $X$  from 0 to 1. For instance,  $\psi = 2$  means that the odds of an event when  $X = 1$  are twice the odds of an event when  $X = 0$ .

Suppose the values of the dichotomous risk factor are coded as constants  $a$  and  $b$  instead of 0 and 1. The odds when  $X = a$  become  $\exp(\beta_0 + a\beta_1)$ , and the odds when  $X = b$  become  $\exp(\beta_0 + b\beta_1)$ . The odds ratio corresponding to an increase in  $X$  from  $a$  to  $b$  is

$$\psi = \exp[(b - a)\beta_1] = [\exp(\beta_1)]^{b-a} \equiv [\exp(\beta_1)]^c$$

Note that for any  $a$  and  $b$  such that  $c = b - a = 1$ ,  $\psi = \exp(\beta_1)$ . So the odds ratio can be interpreted as the change in the odds for any increase of one unit in the corresponding risk factor. However, the change in odds for some amount other than one unit is often of greater interest. For example, a change of one pound in body weight might be too small to be considered important, while a change of 10 pounds might be more meaningful. The odds ratio for a change in  $X$  from  $a$  to  $b$  is estimated by raising the odds ratio estimate for a unit change in  $X$  to the power of  $c = b - a$ , as shown previously.

For a polytomous risk factor, the computation of odds ratios depends on how the risk factor is parameterized. For illustration, suppose that **Race** is a risk factor with four categories: White, Black, Hispanic, and Other.

For the effect parameterization scheme (PARAM=EFFECT) with White as the reference group, the design variables for **Race** are as follows.

| Race     | Design Variables |       |       |
|----------|------------------|-------|-------|
|          | $X_1$            | $X_2$ | $X_3$ |
| Black    | 1                | 0     | 0     |
| Hispanic | 0                | 1     | 0     |
| Other    | 0                | 0     | 1     |
| White    | -1               | -1    | -1    |

The log odds for Black is

$$\begin{aligned} g(\text{Black}) &= \beta_0 + \beta_1(X_1 = 1) + \beta_2(X_2 = 0) + \beta_3(X_3 = 0) \\ &= \beta_0 + \beta_1 \end{aligned}$$

The log odds for White is

$$\begin{aligned} g(\text{White}) &= \beta_0 + \beta_1(X_1 = -1) + \beta_2(X_2 = -1) + \beta_3(X_3 = -1) \\ &= \beta_0 - \beta_1 - \beta_2 - \beta_3 \end{aligned}$$

Therefore, the log odds ratio of Black versus White becomes

$$\begin{aligned} \log(\psi(\text{Black, White})) &= g(\text{Black}) - g(\text{White}) \\ &= 2\beta_1 + \beta_2 + \beta_3 \end{aligned}$$

For the reference cell parameterization scheme (PARAM=REF) with White as the reference cell, the design variables for race are as follows.

| Race     | Design Variables |       |       |
|----------|------------------|-------|-------|
|          | $X_1$            | $X_2$ | $X_3$ |
| Black    | 1                | 0     | 0     |
| Hispanic | 0                | 1     | 0     |
| Other    | 0                | 0     | 1     |
| White    | 0                | 0     | 0     |

The log odds ratio of Black versus White is given by

$$\begin{aligned}
 \log(\psi(\text{Black}, \text{White})) &= g(\text{Black}) - g(\text{White}) \\
 &= (\beta_0 + \beta_1(X_1 = 1) + \beta_2(X_2 = 0) + \beta_3(X_3 = 0)) - \\
 &\quad (\beta_0 + \beta_1(X_1 = 0) + \beta_2(X_2 = 0) + \beta_3(X_3 = 0)) \\
 &= \beta_1
 \end{aligned}$$

For the GLM parameterization scheme (PARAM=GLM), the design variables are as follows.

| Race     | Design Variables |       |       |       |
|----------|------------------|-------|-------|-------|
|          | $X_1$            | $X_2$ | $X_3$ | $X_4$ |
| Black    | 1                | 0     | 0     | 0     |
| Hispanic | 0                | 1     | 0     | 0     |
| Other    | 0                | 0     | 1     | 0     |
| White    | 0                | 0     | 0     | 1     |

The log odds ratio of Black versus White is

$$\begin{aligned}
 \log(\psi(\text{Black}, \text{White})) &= g(\text{Black}) - g(\text{White}) \\
 &= (\beta_0 + \beta_1(X_1 = 1) + \beta_2(X_2 = 0) + \beta_3(X_3 = 0) + \beta_4(X_4 = 0)) - \\
 &\quad (\beta_0 + \beta_1(X_1 = 0) + \beta_2(X_2 = 0) + \beta_3(X_3 = 0) + \beta_4(X_4 = 1)) \\
 &= \beta_1 - \beta_4
 \end{aligned}$$

Consider the hypothetical example of heart disease among race in Hosmer and Lemeshow (2000, p. 51). The entries in the following contingency table represent counts.

| Disease Status | Race  |       |          |       |
|----------------|-------|-------|----------|-------|
|                | White | Black | Hispanic | Other |
| Present        | 5     | 20    | 15       | 10    |
| Absent         | 20    | 10    | 10       | 10    |

The computation of odds ratio of Black versus White for various parameterization schemes is shown in Table 91.9.

**Table 91.9** Odds Ratio of Heart Disease Comparing Black to White

| PARAM= | Parameter Estimates |                 |                 |                 | Odds Ratio Estimates                          |
|--------|---------------------|-----------------|-----------------|-----------------|-----------------------------------------------|
|        | $\hat{\beta}_1$     | $\hat{\beta}_2$ | $\hat{\beta}_3$ | $\hat{\beta}_4$ |                                               |
| EFFECT | 0.7651              | 0.4774          | 0.0719          |                 | $\exp(2 \times 0.7651 + 0.4774 + 0.0719) = 8$ |
| REF    | 2.0794              | 1.7917          | 1.3863          |                 | $\exp(2.0794) = 8$                            |
| GLM    | 2.0794              | 1.7917          | 1.3863          | 0.0000          | $\exp(2.0794) = 8$                            |

Since the log odds ratio ( $\log(\psi)$ ) is a linear function of the parameters, the Wald confidence interval for  $\log(\psi)$  can be derived from the parameter estimates and the estimated covariance matrix. Confidence intervals for the odds ratios are obtained by exponentiating the corresponding confidence intervals for the log odds ratios. In the displayed output of PROC SURVEYLOGISTIC, the “Odds Ratio Estimates” table contains the odds ratio estimates and the corresponding 95% Wald confidence intervals computed by using the covariance matrix in the section “Variance Estimation” on page 7738. For continuous explanatory variables, these odds ratios correspond to a unit increase in the risk factors.

To customize odds ratios for specific units of change for a continuous risk factor, you can use the UNITS statement to specify a list of relevant units for each explanatory variable in the model. Estimates of these customized odds ratios are given in a separate table. Let  $(L_j, U_j)$  be a confidence interval for  $\log(\psi)$ . The corresponding lower and upper confidence limits for the customized odds ratio  $\exp(c\beta_j)$  are  $\exp(cL_j)$  and  $\exp(cU_j)$ , respectively, (for  $c > 0$ ); or  $\exp(cU_j)$  and  $\exp(cL_j)$ , respectively, (for  $c < 0$ ). You use the CLODDS option in the MODEL statement to request confidence intervals for the odds ratios.

For a generalized logit model, odds ratios are computed similarly, except  $D$  odds ratios are computed for each effect, corresponding to the  $D$  logits in the model.

### Rank Correlation of Observed Responses and Predicted Probabilities

The predicted mean score of an observation is the sum of the Ordered Values (shown in the “Response Profile” table) minus one, weighted by the corresponding predicted probabilities for that observation; that is, the predicted mean score is  $\sum_{d=1}^{D+1} (d-1)\hat{\pi}_d$ , where  $D+1$  is the number of response levels and  $\hat{\pi}_d$  is the predicted probability of the  $d$ th (ordered) response.

A pair of observations with different observed responses is said to be *concordant* if the observation with the lower ordered response value has a lower predicted mean score than the observation with the higher ordered response value. If the observation with the lower ordered response value has a higher predicted mean score than the observation with the higher ordered response value, then the pair is *discordant*. If the pair is neither concordant nor discordant, it is a *tie*. Enumeration of the total numbers of concordant and discordant pairs is carried out by categorizing the predicted mean score into intervals of length  $D/500$  and accumulating the corresponding frequencies of observations.

Let  $N$  be the sum of observation frequencies in the data. Suppose there are a total of  $t$  pairs with different responses,  $n_c$  of them are concordant,  $n_d$  of them are discordant, and  $t - n_c - n_d$  of them are tied. PROC SURVEYLOGISTIC computes the following four indices of rank correlation for assessing the predictive ability of a model:

$$c = (n_c + 0.5(t - n_c - n_d))/t$$

$$\text{Somers' } D = (n_c - n_d)/t$$

$$\text{Goodman-Kruskal Gamma} = (n_c - n_d)/(n_c + n_d)$$

$$\text{Kendall's Tau-}a = (n_c - n_d)/(0.5N(N - 1))$$

Note that  $c$  also gives an estimate of the area under the receiver operating characteristic (ROC) curve when the response is binary (Hanley and McNeil 1982).

For binary responses, the predicted mean score is equal to the predicted probability for Ordered Value 2. As such, the preceding definition of concordance is consistent with the definition used in previous releases for the binary response model.

## Linear Predictor, Predicted Probability, and Confidence Limits

This section describes how predicted probabilities and confidence limits are calculated by using the pseudo-estimates (MLEs) obtained from PROC SURVEYLOGISTIC. For a specific example, see the section “Getting Started: SURVEYLOGISTIC Procedure” on page 7685. Predicted probabilities and confidence limits can be output to a data set with the OUTPUT statement.

### Cumulative Response Models

For a row vector of explanatory variables  $\mathbf{x}$ , the linear predictor

$$\eta_i = g(\text{Pr}(Y \leq i | \mathbf{x})) = \alpha_i + \mathbf{x}\boldsymbol{\beta}, \quad 1 \leq i \leq k$$

is estimated by

$$\hat{\eta}_i = \hat{\alpha}_i + \mathbf{x}\hat{\boldsymbol{\beta}}$$

where  $\hat{\alpha}_i$  and  $\hat{\boldsymbol{\beta}}$  are the MLEs of  $\alpha_i$  and  $\boldsymbol{\beta}$ . The estimated standard error of  $\eta_i$  is  $\hat{\sigma}(\hat{\eta}_i)$ , which can be computed as the square root of the quadratic form  $(1, \mathbf{x}')\hat{\mathbf{V}}_b(1, \mathbf{x}')$ , where  $\hat{\mathbf{V}}_b$  is the estimated covariance matrix of the parameter estimates. The asymptotic  $100(1 - \alpha)\%$  confidence interval for  $\eta_i$  is given by

$$\hat{\eta}_i \pm z_{\alpha/2}\hat{\sigma}(\hat{\eta}_i)$$

where  $z_{\alpha/2}$  is the  $100(1 - \alpha/2)$  percentile point of a standard normal distribution.

The predicted value and the  $100(1 - \alpha)\%$  confidence limits for  $\text{Pr}(Y \leq i | \mathbf{x})$  are obtained by back-transforming the corresponding measures for the linear predictor.

| Link    | Predicted Probability       | $100(1 - \alpha)$ Confidence Limits                                    |
|---------|-----------------------------|------------------------------------------------------------------------|
| LOGIT   | $1/(1 + e^{-\hat{\eta}_i})$ | $1/(1 + e^{-\hat{\eta}_i \pm z_{\alpha/2}\hat{\sigma}(\hat{\eta}_i)})$ |
| PROBIT  | $\Phi(\hat{\eta}_i)$        | $\Phi(\hat{\eta}_i \pm z_{\alpha/2}\hat{\sigma}(\hat{\eta}_i))$        |
| CLOGLOG | $1 - e^{-e^{\hat{\eta}_i}}$ | $1 - e^{-e^{\hat{\eta}_i \pm z_{\alpha/2}\hat{\sigma}(\hat{\eta}_i)}}$ |



## Generalized Logit Model

For a vector of explanatory variables  $\mathbf{x}$ , let  $\pi_i$  denote the probability of obtaining the response value  $i$ :

$$\pi_i = \begin{cases} \frac{\pi_{k+1} e^{\alpha_i + \mathbf{x}\boldsymbol{\beta}_i}}{1 + \sum_{j=1}^k e^{\alpha_j + \mathbf{x}\boldsymbol{\beta}_j}} & 1 \leq i \leq k \\ 1 & i = k + 1 \end{cases}$$

By the *delta method*,

$$\sigma^2(\pi_i) = \left( \frac{\partial \pi_i}{\partial \boldsymbol{\theta}} \right)' \mathbf{V}(\boldsymbol{\theta}) \frac{\partial \pi_i}{\partial \boldsymbol{\theta}}$$

A 100(1- $\alpha$ )% confidence level for  $\pi_i$  is given by

$$\hat{\pi}_i \pm z_{\alpha/2} \hat{\sigma}(\hat{\pi}_i)$$

where  $\hat{\pi}_i$  is the estimated expected probability of response  $i$  and  $\hat{\sigma}(\hat{\pi}_i)$  is obtained by evaluating  $\sigma(\pi_i)$  at  $\boldsymbol{\theta} = \hat{\boldsymbol{\theta}}$ .

## Output Data Sets

You can use the Output Delivery System (ODS) to create a SAS data set from any piece of PROC SURVEYLOGISTIC output. See the section “ODS Table Names” on page 7757 for more information. For a more detailed description of using ODS, see Chapter 20, “Using the Output Delivery System.”

PROC SURVEYLOGISTIC also provides an **OUTPUT** statement to create a data set that contains estimated linear predictors, the estimates of the cumulative or individual response probabilities, and their confidence limits.

If you use BRR or jackknife variance estimation, PROC SURVEYLOGISTIC provides an output data set that stores the replicate weights and an output data set that stores the jackknife coefficients for jackknife variance estimation.

### OUT= Data Set in the OUTPUT Statement

The OUT= data set in the **OUTPUT** statement contains all the variables in the input data set along with statistics you request by using *keyword=name* options or the PREDPROBS= option in the OUTPUT statement. In addition, if you use the single-trial syntax and you request any of the XBETA=, STDXBETA=, PREDICTED=, LCL=, and UCL= options, the OUT= data set contains the automatic variable `_LEVEL_`. The value of `_LEVEL_` identifies the response category upon which the computed values of XBETA=, STDXBETA=, PREDICTED=, LCL=, and UCL= are based.

When there are more than two response levels, only variables named by the XBETA=, STDXBETA=, PREDICTED=, LOWER=, and UPPER= options and the variables given by PREDPROBS=(INDIVIDUAL CUMULATIVE) have their values computed; the other variables have missing values. If you fit a generalized logit model, the cumulative predicted probabilities are not computed.

When there are only two response categories, each input observation produces one observation in the OUT= data set.

If there are more than two response categories and you specify only the PREDPROBS= option, then each input observation produces one observation in the OUT= data set. However, if you fit an ordinal (cumulative) model and specify options other than the PREDPROBS= options, each input observation generates as many output observations as one fewer than the number of response levels, and the predicted probabilities and their confidence limits correspond to the cumulative predicted probabilities. If you fit a generalized logit model and specify options other than the PREDPROBS= options, each input observation generates as many output observations as the number of response categories; the predicted probabilities and their confidence limits correspond to the probabilities of individual response categories.

For observations in which only the response variable is missing, values of the XBETA=, STDXBETA=, PREDICTED=, UPPER=, LOWER=, and PREDPROBS= options are computed even though these observations do not affect the model fit. This enables, for instance, predicted probabilities to be computed for new observations.

### Replicate Weights Output Data Set

If you specify the OUTWEIGHTS= *method-option* for VARMETHOD=BRR or VARMETHOD=JACKKNIFE, PROC SURVEYLOGISTIC stores the replicate weights in an output data set. The OUTWEIGHTS= output data set contains all observations from the DATA= input data set that are valid (used in the analysis). (A valid observation is an observation that has a positive value of the WEIGHT variable. Valid observations must also have nonmissing values of the STRATA and CLUSTER variables, unless you specify the MISSING option.)

The OUTWEIGHTS= data set contains the following variables:

- all variables in the DATA= input data set
- RepWt\_1, RepWt\_2, . . . , RepWt\_n, which are the replicate weight variables

where  $n$  is the total number of replicates in the analysis. Each replicate weight variable contains the replicate weights for the corresponding replicate. Replicate weights equal zero for those observations not included in the replicate.

After the procedure creates replicate weights for a particular input data set and survey design, you can use the OUTWEIGHTS= *method-option* to store these replicate weights and then use them again in subsequent analyses, either in PROC SURVEYLOGISTIC or in the other survey procedures. You can use the REPWEIGHTS statement to provide replicate weights for the procedure.

### Jackknife Coefficients Output Data Set

If you specify the OUTJKCOEFS= *method-option* for VARMETHOD=JACKKNIFE, PROC SURVEYLOGISTIC stores the jackknife coefficients in an output data set. The OUTJKCOEFS= output data set contains one observation for each replicate. The OUTJKCOEFS= data set contains the following variables:

- Replicate, which is the replicate number for the jackknife coefficient
- JKCoefficient, which is the jackknife coefficient
- DonorStratum, which is the stratum of the PSU that was deleted to construct the replicate, if you specify a STRATA statement

After the procedure creates jackknife coefficients for a particular input data set and survey design, you can use the `OUTJKCOEFS=` *method-option* to store these coefficients and then use them again in subsequent analyses, either in PROC SURVEYLOGISTIC or in the other survey procedures. You can use the `JKCOEFS=` option in the `REPWEIGHTS` statement to provide jackknife coefficients for the procedure.

---

## Displayed Output

The SURVEYLOGISTIC procedure produces output that is described in the following sections.

Output that is generated by the `EFFECT`, `ESTIMATE`, `LSMEANS`, `LSMESTIMATE`, and `SLICE` statements are not listed below. For information about the output that is generated by these statements, see the corresponding sections of Chapter 19, “[Shared Concepts and Topics](#).”

## Model Information

By default, PROC SURVEYLOGISTIC displays the following information in the “Model Information” table:

- name of the input Data Set
- name and label of the Response Variable if the single-trial syntax is used
- number of Response Levels
- name of the Events Variable if the events/trials syntax is used
- name of the Trials Variable if the events/trials syntax is used
- name of the Offset Variable if the `OFFSET=` option is specified
- name of the Frequency Variable if the `FREQ` statement is specified
- name(s) of the Stratum Variable(s) if the `STRATA` statement is specified
- total Number of Strata if the `STRATA` statement is specified
- name(s) of the Cluster Variable(s) if the `CLUSTER` statement is specified
- total Number of Clusters if the `CLUSTER` statement is specified
- name of the Weight Variable if the `WEIGHT` statement is specified
- Variance Adjustment method
- Upper Bound `ADJBOUND` parameter used in the `VADJUST=MOREL(ADJBOUND= )` option
- Lower Bound `DEFFBOUND` parameter used in the `VADJUST=MOREL(DEFFBOUND= )` option
- whether FPC (finite population correction) is used

## Variance Estimation

By default, PROC SURVEYLOGISTIC displays the following variance estimation information in the “Variance Estimation” table:

- Method, which is the variance estimation method
- Variance Adjustment method
- Upper Bound ADJBOUND parameter specified in the `VADJUST=MOREL(ADJBOUND= )` option
- Lower Bound DEFFBOUND parameter specified in the `VADJUST=MOREL(DEFFBOUND= )` option
- whether FPC (finite population correction) is used
- Number of Replicates, if you specify the `VARMETHOD=BRR` or `VARMETHOD=JACKKNIFE` option
- Number of Replicates Used, if you specify the `VARMETHOD=BRR` or `VARMETHOD=JACKKNIFE` option and some of the replicates are excluded due to unattained convergence
- Hadamard Data Set name, if you specify the `VARMETHOD=BRR(HADAMARD=) method-option`
- Fay Coefficient, if you specify the `VARMETHOD=BRR(FAY) method-option`
- Replicate Weights input data set name, if you use a `REPWEIGHTS` statement
- whether Missing Levels are created for categorical variables by the `MISSING` option
- whether observations with Missing Values are included in the analysis by the `NOMCAR` option

## Data Summary

By default, PROC SURVEYLOGISTIC displays the following information for the entire data set:

- Number of Observations read from the input data set
- Number of Observations used in the analysis

If there is a `DOMAIN` statement, PROC SURVEYLOGISTIC also displays the following:

- Number of Observations in the current domain
- Number of Observations not in the current domain

If there is a `FREQ` statement, PROC SURVEYLOGISTIC also displays the following:

- Sum of Frequencies of all the observations read from the input data set
- Sum of Frequencies of all the observations used in the analysis

If there is a WEIGHT statement, PROC SURVEYLOGISTIC also displays the following:

- Sum of Weights of all the observations read from the input data set
- Sum of Weights of all the observations used in the analysis
- Sum of Weights of all the observations in the current domain, if DOMAIN statement is also specified.

## Response Profile

By default, PROC SURVEYLOGISTIC displays a “Response Profile” table, which gives, for each response level, the ordered value (an integer between one and the number of response levels, inclusive); the value of the response variable if the single-trial syntax is used or the values “EVENT” and “NO EVENT” if the events/trials syntax is used; the count or frequency; and the sum of weights if the WEIGHT statement is specified.

## Class Level Information

If you use a CLASS statement to name classification variables, PROC SURVEYLOGISTIC displays a "Class Level Information" table. This table contains the following information for each classification variable:

- Class, which lists each CLASS variable name
- Value, which lists the values of the classification variable. The values are separated by a white space character; therefore, to avoid confusion, you should not include a white space character within a classification variable value.
- Design Variables, which lists the parameterization used for the classification variables

## Stratum Information

When you specify the LIST option in the STRATA statement, PROC SURVEYLOGISTIC displays a "Stratum Information" table, which provides the following information for each stratum:

- Stratum Index, which is a sequential stratum identification number
- STRATA variable(s), which lists the levels of STRATA variables for the stratum
- Population Total, if you specify the TOTAL= option
- Sampling Rate, if you specify the TOTAL= or RATE= option. If you specify the TOTAL= option, the sampling rate is based on the number of nonmissing observations in the stratum.
- N Obs, which is the number of observations
- number of Clusters, if you specify a CLUSTER statement

## Maximum Likelihood Iteration History

The “Maximum Likelihood Iterative Phase” table gives the iteration number, the step size (in the scale of 1.0, 0.5, 0.25, and so on) or the ridge value,  $-2 \log$  likelihood, and parameter estimates for each iteration. Also displayed are the last evaluation of the gradient vector and the last change in the  $-2 \log$  likelihood. You need to use the ITPRINT option in the MODEL statement to obtain this table.

## Score Test

The “Score Test” table displays the score test result for testing the parallel lines assumption, if an ordinal response model is fitted. If LINK=CLOGLOG or LINK=PROBIT, this test is labeled “Score Test for the Parallel Slopes Assumption.” The proportion odds assumption is a special case of the parallel lines assumption when LINK=LOGIT. In this case, the test is labeled “Score Test for the Proportional Odds Assumption.”

## Model Fit Statistics

By default, PROC SURVEYLOGISTIC displays the following information in the “Model Fit Statistics” table:

- “Model Fit Statistics” and “Testing Global Null Hypothesis: BETA=0” tables, which give the various criteria ( $-2 \log L$ , AIC, SC) based on the likelihood for fitting a model with intercepts only and for fitting a model with intercepts and explanatory variables. If you specify the NOINT option, these statistics are calculated without considering the intercept parameters. The third column of the table gives the chi-square statistics and  $p$ -values for the  $-2 \log L$  statistic and for the Score statistic. These test the joint effect of the explanatory variables included in the model. The Score criterion is always missing for the models identified by the first two columns of the table. Note also that the first two rows of the Chi-Square column are always missing, since tests cannot be performed for AIC and SC.
- generalized  $R^2$  measures for the fitted model if you specify the RSQUARE option in the MODEL statement

## Type III Analysis of Effects

PROC SURVEYLOGISTIC displays the “Type III Analysis of Effects” table if the model contains an effect involving a CLASS variable. This table gives the degrees of freedom, the Wald Chi-square statistic, and the  $p$ -value for each effect in the model.

## Analysis of Maximum Likelihood Estimates

By default, PROC SURVEYLOGISTIC displays the following information in the “Analysis of Maximum Likelihood Estimates” table:

- the degrees of freedom for Wald chi-square test
- maximum likelihood estimate of the parameter
- estimated standard error of the parameter estimate, computed as the square root of the corresponding diagonal element of the estimated covariance matrix

- Wald chi-square statistic, computed by squaring the ratio of the parameter estimate divided by its standard error estimate
- $p$ -value of the Wald chi-square statistic with respect to a chi-square distribution with one degree of freedom
- standardized estimate for the slope parameter, given by  $\hat{\beta}_i / (s/s_i)$ , where  $s_i$  is the total sample standard deviation for the  $i$ th explanatory variable and

$$s = \begin{cases} \pi/\sqrt{3} & \text{logistic} \\ 1 & \text{normal} \\ \pi/\sqrt{6} & \text{extreme-value} \end{cases}$$

You need to specify the STB option in the MODEL statement to obtain these estimates. Standardized estimates of the intercept parameters are set to missing.

- value of  $(e^{\hat{\beta}_i})$  for each slope parameter  $\beta_i$  if you specify the EXPB option in the MODEL statement. For continuous variables, this is equivalent to the estimated odds ratio for a one-unit change.
- label of the variable (if space permits) if you specify the PARMLABEL option in the MODEL statement. Due to constraints on the line size, the variable label might be suppressed in order to display the table in one panel. Use the SAS system option LINESIZE= to specify a larger line size to accommodate variable labels. A shorter line size can break the table into two panels, allowing labels to be displayed.

### Odds Ratio Estimates

The “Odds Ratio Estimates” table displays the odds ratio estimates and the corresponding 95% Wald confidence intervals. For continuous explanatory variables, these odds ratios correspond to a unit increase in the risk factors.

### Association of Predicted Probabilities and Observed Responses

The “Association of Predicted Probabilities and Observed Responses” table displays measures of association between predicted probabilities and observed responses, which include a breakdown of the number of pairs with different responses, and four rank correlation indexes: Somers’  $D$ , Goodman-Kruskal Gamma, and Kendall’s Tau- $a$ , and  $c$ .

### Wald Confidence Interval for Parameters

The “Wald Confidence Interval for Parameters” table displays confidence intervals for all the parameters if you use the CLPARM option in the MODEL statement.

### Wald Confidence Interval for Odds Ratios

The “Wald Confidence Interval for Odds Ratios” table displays confidence intervals for all the odds ratios if you use the CLODDS option in the MODEL statement.

## Estimated Covariance Matrix

PROC SURVEYLOGISTIC displays the following information in the “Estimated Covariance Matrix” table:

- estimated covariance matrix of the parameter estimates if you use the COVB option in the MODEL statement
- estimated correlation matrix of the parameter estimates if you use the CORRB option in the MODEL statement

## Linear Hypotheses Testing Results

The “Linear Hypothesis Testing” table gives the result of the Wald test for each TEST statement (if specified).

## Hadamard Matrix

If you specify the `VARMETHOD=BRR(PRINTH)` *method-option* in the PROC SURVEYLOGISTIC statement, the procedure displays the Hadamard matrix.

When you provide a Hadamard matrix with the `VARMETHOD=BRR(HADAMARD=)` *method-option*, the procedure displays only used rows and columns of the Hadamard matrix.

---

## ODS Table Names

PROC SURVEYLOGISTIC assigns a name to each table it creates; these names are listed in Table 91.10. You can use these names to refer the table when using the Output Delivery System (ODS) to select tables and create output data sets. The EFFECT, ESTIMATE, LSMEANS, LSMESTIMATE, and SLICE statements also create tables, which are not listed in Table 91.10. For information about these tables, see the corresponding sections of Chapter 19, “Shared Concepts and Topics.”

For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

**Table 91.10** ODS Tables Produced by PROC SURVEYLOGISTIC

| ODS Table Name    | Description                                                   | Statement | Option                            |
|-------------------|---------------------------------------------------------------|-----------|-----------------------------------|
| Association       | Association of predicted probabilities and observed responses | MODEL     | Default                           |
| ClassLevelInfo    | Class variable levels and design variables                    | MODEL     | Default<br>(with CLASS variables) |
| CLOddsWald        | Wald’s confidence limits for odds ratios                      | MODEL     | CLODDS                            |
| CLparmWald        | Wald’s confidence limits for parameters                       | MODEL     | CLPARAM                           |
| ContrastCoeff     | L matrix from CONTRAST                                        | CONTRAST  | E                                 |
| ContrastEstimate  | Estimates from CONTRAST                                       | CONTRAST  | ESTIMATE=                         |
| ContrastTest      | Wald test for CONTRAST                                        | CONTRAST  | Default                           |
| ConvergenceStatus | Convergence status                                            | MODEL     | Default                           |



Table 91.10 continued

| ODS Table Name      | Description                                                                                                         | Statement | Option                            |
|---------------------|---------------------------------------------------------------------------------------------------------------------|-----------|-----------------------------------|
| CorrB               | Estimated correlation matrix of parameter estimators                                                                | MODEL     | CORRB                             |
| CovB                | Estimated covariance matrix of parameter estimators                                                                 | MODEL     | COVB                              |
| CumulativeModelTest | Test of the cumulative model assumption                                                                             | MODEL     | (Ordinal response)                |
| DomainSummary       | Domain summary                                                                                                      | DOMAIN    | Default                           |
| FitStatistics       | Model fit statistics                                                                                                | MODEL     | Default                           |
| GlobalTests         | Test for global null hypothesis                                                                                     | MODEL     | Default                           |
| HadamardMatrix      | Hadamard matrix                                                                                                     | PROC      | PRINTH                            |
| IterHistory         | Iteration history                                                                                                   | MODEL     | ITPRINT                           |
| LastGradient        | Last evaluation of gradient                                                                                         | MODEL     | ITPRINT                           |
| Linear              | Linear combination                                                                                                  | PROC      | Default                           |
| LogLikeChange       | Final change in the log likelihood                                                                                  | MODEL     | ITPRINT                           |
| ModelInfo           | Model information                                                                                                   | PROC      | Default                           |
| NObs                | Number of observations                                                                                              | PROC      | Default                           |
| OddsEst             | Adjusted odds ratios                                                                                                | UNITS     | Default                           |
| OddsRatios          | Odds ratios                                                                                                         | MODEL     | Default                           |
| ParameterEstimates  | Maximum likelihood estimates of model parameters                                                                    | MODEL     | Default                           |
| RSquare             | R-square                                                                                                            | MODEL     | RSQUARE                           |
| ResponseProfile     | Response profile                                                                                                    | PROC      | Default                           |
| StrataInfo          | Stratum information                                                                                                 | STRATA    | LIST                              |
| TestPrint1          | $L[\text{cov}(\mathbf{b})]L'$ and $L\mathbf{b} - \mathbf{c}$                                                        | TEST      | PRINT                             |
| TestPrint2          | $G\text{inv}(L[\text{cov}(\mathbf{b})]L')$ and $G\text{inv}(L[\text{cov}(\mathbf{b})]L')(L\mathbf{b} - \mathbf{c})$ | TEST      | PRINT                             |
| TestStmts           | Linear hypotheses testing results                                                                                   | TEST      | Default                           |
| Type3               | Type III tests of effects                                                                                           | MODEL     | Default<br>(with CLASS variables) |
| VarianceEstimation  | Variance estimation                                                                                                 | PROC      | Default                           |

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “Statistical Graphics Using ODS.”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “A Primer on ODS Statistical Graphics” on page 599 in Chapter 21, “Statistical Graphics Using ODS.”

When ODS Graphics is enabled, then the ESTIMATE, LSMEANS, LSMESTIMATE, and SLICE statements can produce plots that are associated with their analyses. For information about these plots, see the corresponding sections of Chapter 19, “Shared Concepts and Topics.”

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## Examples: SURVEYLOGISTIC Procedure

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### Example 91.1: Stratified Cluster Sampling

A market research firm conducts a survey among undergraduate students at a certain university to evaluate three new Web designs for a commercial Web site targeting undergraduate students at the university.

The sample design is a stratified sample where the strata are students' classes. Within each class, 300 students are randomly selected by using simple random sampling without replacement. The total number of students in each class in the fall semester of 2001 is shown in the following table:

| Class         | Enrollment |
|---------------|------------|
| 1 - Freshman  | 3,734      |
| 2 - Sophomore | 3,565      |
| 3 - Junior    | 3,903      |
| 4 - Senior    | 4,196      |

This total enrollment information is saved in the SAS data set Enrollment by using the following SAS statements:

```
proc format;
 value Class
 1='Freshman' 2='Sophomore'
 3='Junior' 4='Senior';
run;

data Enrollment;
 format Class Class.;
 input Class _TOTAL_;
 datalines;
1 3734
2 3565
3 3903
4 4196
;
```

In the data set Enrollment, the variable `_TOTAL_` contains the enrollment figures for all classes. They are also the population size for each stratum in this example.

Each student selected in the sample evaluates one randomly selected Web design by using the following scale:

|   |                   |
|---|-------------------|
| 1 | Dislike very much |
| 2 | Dislike           |
| 3 | Neutral           |
| 4 | Like              |
| 5 | Like very much    |

The survey results are collected and shown in the following table, with the three different Web designs coded as A, B, and C.

| Evaluation of New Web Designs |        |               |    |    |    |    |
|-------------------------------|--------|---------------|----|----|----|----|
| Strata                        | Design | Rating Counts |    |    |    |    |
|                               |        | 1             | 2  | 3  | 4  | 5  |
| Freshman                      | A      | 10            | 34 | 35 | 16 | 15 |
|                               | B      | 5             | 6  | 24 | 30 | 25 |
|                               | C      | 11            | 14 | 20 | 34 | 21 |
| Sophomore                     | A      | 19            | 12 | 26 | 18 | 25 |
|                               | B      | 10            | 18 | 32 | 23 | 26 |
|                               | C      | 15            | 22 | 34 | 9  | 20 |
| Junior                        | A      | 8             | 21 | 23 | 26 | 22 |
|                               | B      | 1             | 4  | 15 | 33 | 47 |
|                               | C      | 16            | 19 | 30 | 23 | 12 |
| Senior                        | A      | 11            | 14 | 24 | 33 | 18 |
|                               | B      | 8             | 15 | 25 | 30 | 22 |
|                               | C      | 2             | 34 | 30 | 18 | 16 |

The survey results are stored in a SAS data set WebSurvey by using the following SAS statements:

```
proc format;
 value Design 1='A' 2='B' 3='C';
 value Rating
 1='dislike very much'
 2='dislike'
 3='neutral'
 4='like'
 5='like very much';
run;

data WebSurvey;
 format Class Class. Design Design. Rating Rating.;
 do Class=1 to 4;
 do Design=1 to 3;
 do Rating=1 to 5;
 input Count @@;
 output;
 end;
 end;
 end;
end;
```

```

datalines;
10 34 35 16 15 8 21 23 26 22 5 10 24 30 21
 1 14 25 23 37 11 14 20 34 21 16 19 30 23 12
19 12 26 18 25 11 14 24 33 18 10 18 32 23 17
 8 15 35 30 12 15 22 34 9 20 2 34 30 18 16
;

data WebSurvey;
 set WebSurvey;
 if Class=1 then Weight=3734/300;
 if Class=2 then Weight=3565/300;
 if Class=3 then Weight=3903/300;
 if Class=4 then Weight=4196/300;
run;

```

The data set WebSurvey contains the variables Class, Design, Rating, Count, and Weight. The variable class is the stratum variable, with four strata: freshman, sophomore, junior, and senior. The variable Design specifies the three new Web designs: A, B, and C. The variable Rating contains students' evaluations of the new Web designs. The variable counts gives the frequency with which each Web design received each rating within each stratum. The variable weight contains the sampling weights, which are the reciprocals of selection probabilities in this example.

Output 91.1.1 shows the first 20 observations of the data set.

**Output 91.1.1** Web Design Survey Sample (First 20 Observations)

| Obs | Class     | Design | Rating            | Count | Weight  |
|-----|-----------|--------|-------------------|-------|---------|
| 1   | Freshman  | A      | dislike very much | 10    | 12.4467 |
| 2   | Freshman  | A      | dislike           | 34    | 12.4467 |
| 3   | Freshman  | A      | neutral           | 35    | 12.4467 |
| 4   | Freshman  | A      | like              | 16    | 12.4467 |
| 5   | Freshman  | A      | like very much    | 15    | 12.4467 |
| 6   | Freshman  | B      | dislike very much | 8     | 12.4467 |
| 7   | Freshman  | B      | dislike           | 21    | 12.4467 |
| 8   | Freshman  | B      | neutral           | 23    | 12.4467 |
| 9   | Freshman  | B      | like              | 26    | 12.4467 |
| 10  | Freshman  | B      | like very much    | 22    | 12.4467 |
| 11  | Freshman  | C      | dislike very much | 5     | 12.4467 |
| 12  | Freshman  | C      | dislike           | 10    | 12.4467 |
| 13  | Freshman  | C      | neutral           | 24    | 12.4467 |
| 14  | Freshman  | C      | like              | 30    | 12.4467 |
| 15  | Freshman  | C      | like very much    | 21    | 12.4467 |
| 16  | Sophomore | A      | dislike very much | 1     | 11.8833 |
| 17  | Sophomore | A      | dislike           | 14    | 11.8833 |
| 18  | Sophomore | A      | neutral           | 25    | 11.8833 |
| 19  | Sophomore | A      | like              | 23    | 11.8833 |
| 20  | Sophomore | A      | like very much    | 37    | 11.8833 |

The following SAS statements perform the logistic regression:

```
proc surveylogistic data=WebSurvey total=Enrollment;
 stratum Class;
 freq Count;
 class Design;
 model Rating (order=internal) = design;
 weight Weight;
run;
```

The PROC SURVEYLOGISTIC statement invokes the procedure. The TOTAL= option specifies the data set Enrollment, which contains the population totals in the strata. The population totals are used to calculate the finite population correction factor in the variance estimates. The response variable Rating is in the ordinal scale. A cumulative logit model is used to investigate the responses to the Web designs. In the MODEL statement, rating is the response variable, and Design is the effect in the regression model. The ORDER=INTERNAL option is used for the response variable Rating to sort the ordinal response levels of Rating by its internal (numerical) values rather than by the formatted values (for example, 'like very much'). Because the sample design involves stratified simple random sampling, the STRATA statement is used to specify the stratification variable Class. The WEIGHT statement specifies the variable Weight for sampling weights.

The sample and analysis summary is shown in [Output 91.1.2](#). There are five response levels for the Rating, with 'dislike very much' as the lowest ordered value. The regression model is modeling lower cumulative probabilities by using logit as the link function. Because the TOTAL= option is used, the finite population correction is included in the variance estimation. The sampling weight is also used in the analysis.

#### Output 91.1.2 Web Design Survey, Model Information

| The SURVEYLOGISTIC Procedure |                         |
|------------------------------|-------------------------|
| Model Information            |                         |
| Data Set                     | WORK.WEBSURVEY          |
| Response Variable            | Rating                  |
| Number of Response Levels    | 5                       |
| Frequency Variable           | Count                   |
| Stratum Variable             | Class                   |
| Number of Strata             | 4                       |
| Weight Variable              | Weight                  |
| Model                        | Cumulative Logit        |
| Optimization Technique       | Fisher's Scoring        |
| Variance Adjustment          | Degrees of Freedom (DF) |
| Finite Population Correction | Used                    |

**Output 91.1.2** *continued*

| Response Profile |                   |                 |              |
|------------------|-------------------|-----------------|--------------|
| Ordered Value    | Rating            | Total Frequency | Total Weight |
| 1                | dislike very much | 116             | 1489.0733    |
| 2                | dislike           | 227             | 2933.0433    |
| 3                | neutral           | 338             | 4363.3767    |
| 4                | like              | 283             | 3606.8067    |
| 5                | like very much    | 236             | 3005.7000    |

Probabilities modeled are cumulated over the lower Ordered Values.

In [Output 91.1.3](#), the score chi-square for testing the proportional odds assumption is 98.1957, which is highly significant. This indicates that the cumulative logit model might not adequately fit the data.

**Output 91.1.3** Web Design Survey, Testing the Proportional Odds Assumption

| Score Test for the Proportional Odds Assumption |    |            |
|-------------------------------------------------|----|------------|
| Chi-Square                                      | DF | Pr > ChiSq |
| 98.1957                                         | 6  | <.0001     |

An alternative model is to use the generalized logit model with the LINK=GLOGIT option, as shown in the following SAS statements:

```
proc surveylogistic data=WebSurvey total=Enrollment;
 stratum Class;
 freq Count;
 class Design;
 model Rating (ref='neutral') = Design /link=glogit;
 weight Weight;
run;
```

The REF='neutral' option is used for the response variable Rating to indicate that all other response levels are referenced to the level 'neutral.' The option LINK=GLOGIT option requests that the procedure fit a generalized logit model.

The summary of the analysis is shown in [Output 91.1.4](#), which indicates that the generalized logit model is used in the analysis.

**Output 91.1.4** Web Design Survey, Model Information

| The SURVEYLOGISTIC Procedure                                   |                         |                 |              |
|----------------------------------------------------------------|-------------------------|-----------------|--------------|
| Model Information                                              |                         |                 |              |
| Data Set                                                       | WORK.WEBSURVEY          |                 |              |
| Response Variable                                              | Rating                  |                 |              |
| Number of Response Levels                                      | 5                       |                 |              |
| Frequency Variable                                             | Count                   |                 |              |
| Stratum Variable                                               | Class                   |                 |              |
| Number of Strata                                               | 4                       |                 |              |
| Weight Variable                                                | Weight                  |                 |              |
| Model                                                          | Generalized Logit       |                 |              |
| Optimization Technique                                         | Newton-Raphson          |                 |              |
| Variance Adjustment                                            | Degrees of Freedom (DF) |                 |              |
| Finite Population Correction                                   | Used                    |                 |              |
| Response Profile                                               |                         |                 |              |
| Ordered Value                                                  | Rating                  | Total Frequency | Total Weight |
| 1                                                              | dislike                 | 227             | 2933.0433    |
| 2                                                              | dislike very much       | 116             | 1489.0733    |
| 3                                                              | like                    | 283             | 3606.8067    |
| 4                                                              | like very much          | 236             | 3005.7000    |
| 5                                                              | neutral                 | 338             | 4363.3767    |
| Logits modeled use Rating='neutral' as the reference category. |                         |                 |              |

Output 91.1.5 shows the parameterization for the main effect Design.

**Output 91.1.5** Web Design Survey, Class Level Information

| Class Level Information |       |                  |    |
|-------------------------|-------|------------------|----|
| Class                   | Value | Design Variables |    |
| Design                  | A     | 1                | 0  |
|                         | B     | 0                | 1  |
|                         | C     | -1               | -1 |

The parameter and odds ratio estimates are shown in [Output 91.1.6](#). For each odds ratio estimate, the 95% confidence limits shown in the table contain the value 1.0. Therefore, no conclusion about which Web design is preferred can be made based on this survey.

**Output 91.1.6** Web Design Survey, Parameter and Odds Ratio Estimates

| Analysis of Maximum Likelihood Estimates |                     |    |          |                |                 |            |
|------------------------------------------|---------------------|----|----------|----------------|-----------------|------------|
| Parameter                                | Rating              | DF | Estimate | Standard Error | Wald Chi-Square | Pr > ChiSq |
| Intercept                                | dislike             | 1  | -0.3964  | 0.0832         | 22.7100         | <.0001     |
| Intercept                                | dislike very much   | 1  | -1.0826  | 0.1045         | 107.3889        | <.0001     |
| Intercept                                | like                | 1  | -0.1892  | 0.0780         | 5.8888          | 0.0152     |
| Intercept                                | like very much      | 1  | -0.3767  | 0.0824         | 20.9223         | <.0001     |
| Design                                   | A dislike           | 1  | -0.0942  | 0.1166         | 0.6518          | 0.4195     |
| Design                                   | A dislike very much | 1  | -0.0647  | 0.1469         | 0.1940          | 0.6596     |
| Design                                   | A like              | 1  | -0.1370  | 0.1104         | 1.5400          | 0.2146     |
| Design                                   | A like very much    | 1  | 0.0446   | 0.1130         | 0.1555          | 0.6933     |
| Design                                   | B dislike           | 1  | 0.0391   | 0.1201         | 0.1057          | 0.7451     |
| Design                                   | B dislike very much | 1  | 0.2721   | 0.1448         | 3.5294          | 0.0603     |
| Design                                   | B like              | 1  | 0.1669   | 0.1102         | 2.2954          | 0.1298     |
| Design                                   | B like very much    | 1  | 0.1420   | 0.1174         | 1.4641          | 0.2263     |

| Odds Ratio Estimates |                   |                |                            |       |
|----------------------|-------------------|----------------|----------------------------|-------|
| Effect               | Rating            | Point Estimate | 95% Wald Confidence Limits |       |
| Design A vs C        | dislike           | 0.861          | 0.583                      | 1.272 |
| Design A vs C        | dislike very much | 1.153          | 0.692                      | 1.923 |
| Design A vs C        | like              | 0.899          | 0.618                      | 1.306 |
| Design A vs C        | like very much    | 1.260          | 0.851                      | 1.865 |
| Design B vs C        | dislike           | 0.984          | 0.659                      | 1.471 |
| Design B vs C        | dislike very much | 1.615          | 0.975                      | 2.675 |
| Design B vs C        | like              | 1.218          | 0.838                      | 1.768 |
| Design B vs C        | like very much    | 1.389          | 0.925                      | 2.086 |

**Example 91.2: The Medical Expenditure Panel Survey (MEPS)**

The U.S. Department of Health and Human Services conducts the Medical Expenditure Panel Survey (MEPS) to produce national and regional estimates of various aspects of health care. The MEPS has a complex sample design that includes both stratification and clustering. The sampling weights are adjusted for nonresponse and raked with respect to population control totals from the Current Population Survey. See the MEPS Survey Background (2006) and Machlin, Yu, and Zodet (2005) for details.

In this example, the 1999 full-year consolidated data file HC-038 (MEPS HC-038, 2002) from the MEPS is used to investigate the relationship between medical insurance coverage and the demographic variables. The data can be downloaded directly from the Agency for Healthcare Research and Quality (AHRQ) Web site at [http://www.meps.ahrq.gov/mepsweb/data\\_stats/download\\_data\\_files\\_detail.jsp?cboPufNumber=HC-038](http://www.meps.ahrq.gov/mepsweb/data_stats/download_data_files_detail.jsp?cboPufNumber=HC-038) in either ASCII format or SAS transport format. The Web site includes a detailed description of the data as well as the SAS program used to access and format it.

For this example, the SAS transport format data file for HC-038 is downloaded to 'C:H38.ssp' on a Windows-based PC. The instructions on the Web site lead to the following SAS statements for creating



a SAS data set MEPS, which contains only the sample design variables and other variables necessary for this analysis.

```

proc format;
 value racex
 -9 = 'NOT ASCERTAINED'
 -8 = 'DK'
 -7 = 'REFUSED'
 -1 = 'INAPPLICABLE'
 1 = 'AMERICAN INDIAN'
 2 = 'ALEUT, ESKIMO'
 3 = 'ASIAN OR PACIFIC ISLANDER'
 4 = 'BLACK'
 5 = 'WHITE'
 91 = 'OTHER'
 ;
 value sex
 -9 = 'NOT ASCERTAINED'
 -8 = 'DK'
 -7 = 'REFUSED'
 -1 = 'INAPPLICABLE'
 1 = 'MALE'
 2 = 'FEMALE'
 ;
 value povcat9h
 1 = 'NEGATIVE OR POOR'
 2 = 'NEAR POOR'
 3 = 'LOW INCOME'
 4 = 'MIDDLE INCOME'
 5 = 'HIGH INCOME'
 ;
 value inscov9f
 1 = 'ANY PRIVATE'
 2 = 'PUBLIC ONLY'
 3 = 'UNINSURED'
 ;
run;

libname mylib '';
filename in1 'H38.SSP';
proc xcopy in=in1 out=mylib import;
run;

data meps;
 set mylib.H38;
 label racex= sex= inscov99= povcat99=
 varstr99= varpsu99= perwt99f= totexp99=;
 format racex racex. sex sex.
 povcat99 povcat9h. inscov99 inscov9f.;
 keep inscov99 sex racex povcat99 varstr99
 varpsu99 perwt99f totexp99;
run;

```

There are a total of 24,618 observations in this SAS data set. Each observation corresponds to a person in the survey. The stratification variable is VARSTR99, which identifies the 143 strata in the sample. The variable VARPSU99 identifies the 460 PSUs in the sample. The sampling weights are stored in the variable PERWT99F. The response variable is the health insurance coverage indicator variable, INSCOV99, which has three values:

- 
- 1 The person had any private insurance coverage any time during 1999
  - 2 The person had only public insurance coverage during 1999
  - 3 The person was uninsured during all of 1999
- 

The demographic variables include gender (SEX), race (RACEX), and family income level as a percent of the poverty line (POVCAT99). The variable RACEX has five categories:

- 
- 1 American Indian
  - 2 Aleut, Eskimo
  - 3 Asian or Pacific Islander
  - 4 Black
  - 5 White
- 

The variable POVCAT99 is constructed by dividing family income by the applicable poverty line (based on family size and composition), with the resulting percentages grouped into five categories:

- 
- 1 Negative or poor (less than 100%)
  - 2 Near poor (100% to less than 125%)
  - 3 Low income (125% to less than 200%)
  - 4 Middle income (200% to less than 400%)
  - 5 High income (greater than or equal to 400%)
- 

The data set also contains the total health care expenditure in 1999, TOTEXP99, which is used as a covariate in the analysis.

Output 91.2.1 displays the first 30 observations of this data set.

**Output 91.2.1** 1999 Full-Year MEPS (First 30 Observations)

| O  | S      | R     | P                | I           | T           | P    | V        | V   |    |
|----|--------|-------|------------------|-------------|-------------|------|----------|-----|----|
| b  | E      | A     | O                | N           | O           | E    | A        | A   |    |
| s  | X      | C     | V                | S           | T           | R    | R        | R   |    |
|    |        | X     | C                | C           | E           | W    | S        | P   |    |
|    |        |       | A                | O           | X           | T    | T        | S   |    |
|    |        |       | T                | V           | P           | 9    | R        | U   |    |
|    |        |       | 9                | 9           | 9           | 9    | 9        | 9   |    |
|    |        |       | 9                | 9           | 9           | F    | 9        | 9   |    |
| 1  | MALE   | WHITE | MIDDLE           | INCOME      | PUBLIC ONLY | 2735 | 14137.86 | 131 | 2  |
| 2  | FEMALE | WHITE | MIDDLE           | INCOME      | ANY PRIVATE | 6687 | 17050.99 | 131 | 2  |
| 3  | MALE   | WHITE | MIDDLE           | INCOME      | ANY PRIVATE | 60   | 35737.55 | 131 | 2  |
| 4  | MALE   | WHITE | MIDDLE           | INCOME      | ANY PRIVATE | 60   | 35862.67 | 131 | 2  |
| 5  | FEMALE | WHITE | MIDDLE           | INCOME      | ANY PRIVATE | 786  | 19407.11 | 131 | 2  |
| 6  | MALE   | WHITE | MIDDLE           | INCOME      | ANY PRIVATE | 345  | 18499.83 | 131 | 2  |
| 7  | MALE   | WHITE | MIDDLE           | INCOME      | ANY PRIVATE | 680  | 18499.83 | 131 | 2  |
| 8  | MALE   | WHITE | MIDDLE           | INCOME      | ANY PRIVATE | 3226 | 22394.53 | 136 | 1  |
| 9  | FEMALE | WHITE | MIDDLE           | INCOME      | ANY PRIVATE | 2852 | 27008.96 | 136 | 1  |
| 10 | MALE   | WHITE | MIDDLE           | INCOME      | ANY PRIVATE | 112  | 25108.71 | 136 | 1  |
| 11 | MALE   | WHITE | MIDDLE           | INCOME      | ANY PRIVATE | 3179 | 17569.81 | 136 | 1  |
| 12 | MALE   | WHITE | MIDDLE           | INCOME      | ANY PRIVATE | 168  | 21478.06 | 136 | 1  |
| 13 | FEMALE | WHITE | MIDDLE           | INCOME      | ANY PRIVATE | 1066 | 21415.68 | 136 | 1  |
| 14 | MALE   | WHITE | NEGATIVE OR POOR | PUBLIC ONLY |             | 0    | 12254.66 | 125 | 1  |
| 15 | MALE   | WHITE | NEGATIVE OR POOR | ANY PRIVATE |             | 0    | 17699.75 | 125 | 1  |
| 16 | FEMALE | WHITE | NEGATIVE OR POOR | UNINSURED   |             | 0    | 18083.15 | 125 | 1  |
| 17 | MALE   | BLACK | NEGATIVE OR POOR | PUBLIC ONLY |             | 230  | 6537.97  | 78  | 10 |
| 18 | MALE   | WHITE | LOW INCOME       | UNINSURED   |             | 408  | 8951.36  | 95  | 2  |
| 19 | FEMALE | WHITE | LOW INCOME       | UNINSURED   |             | 0    | 11833.00 | 95  | 2  |
| 20 | MALE   | WHITE | LOW INCOME       | UNINSURED   |             | 40   | 12754.07 | 95  | 2  |
| 21 | FEMALE | WHITE | LOW INCOME       | UNINSURED   |             | 51   | 14698.57 | 95  | 2  |
| 22 | MALE   | WHITE | LOW INCOME       | UNINSURED   |             | 0    | 3890.20  | 92  | 19 |
| 23 | FEMALE | WHITE | LOW INCOME       | UNINSURED   |             | 610  | 5882.29  | 92  | 19 |
| 24 | MALE   | WHITE | LOW INCOME       | PUBLIC ONLY |             | 24   | 8610.47  | 92  | 19 |
| 25 | FEMALE | BLACK | MIDDLE INCOME    | UNINSURED   |             | 1758 | 0.00     | 64  | 1  |
| 26 | MALE   | BLACK | MIDDLE INCOME    | PUBLIC ONLY |             | 551  | 7049.70  | 64  | 1  |
| 27 | MALE   | BLACK | MIDDLE INCOME    | ANY PRIVATE |             | 65   | 34067.03 | 64  | 1  |
| 28 | FEMALE | BLACK | NEGATIVE OR POOR | PUBLIC ONLY |             | 0    | 9313.84  | 73  | 12 |
| 29 | FEMALE | BLACK | NEGATIVE OR POOR | PUBLIC ONLY |             | 10   | 14697.03 | 73  | 12 |
| 30 | MALE   | BLACK | NEGATIVE OR POOR | PUBLIC ONLY |             | 0    | 4574.73  | 73  | 12 |

The following SAS statements fit a generalized logit model for the 1999 full-year consolidated MEPS data:

```
proc surveylogistic data=meps;
 stratum VARSTR99;
 cluster VARPSU99;
 weight PERWT99F;
 class SEX RACEX POVCAT99;
 model INSCOV99 = TOTEXP99 SEX RACEX POVCAT99 / link=glogit;
run;
```

The STRATUM statement specifies the stratification variable VARSTR99. The CLUSTER statement specifies the PSU variable VARPSU99. The WEIGHT statement specifies the sample weight variable PERWT99F. The demographic variables SEX, RACEX, and POV99 are listed in the CLASS statement to indicate that they are categorical independent variables in the MODEL statement. In the MODEL statement, the response variable is INSCOV99, and the independent variables are TOTEXP99 along with the selected demographic variables. The LINK= option requests that the procedure fit the generalized logit model because the response variable INSCOV99 has nominal responses.

The results of this analysis are shown in the following outputs.

PROC SURVEYLOGISTIC lists the model fitting information and sample design information in [Output 91.2.2](#).

**Output 91.2.2** MEPS, Model Information

| The SURVEYLOGISTIC Procedure |                         |
|------------------------------|-------------------------|
| Model Information            |                         |
| Data Set                     | WORK.MEPS               |
| Response Variable            | INSCOV99                |
| Number of Response Levels    | 3                       |
| Stratum Variable             | VARSTR99                |
| Number of Strata             | 143                     |
| Cluster Variable             | VARPSU99                |
| Number of Clusters           | 460                     |
| Weight Variable              | PERWT99F                |
| Model                        | Generalized Logit       |
| Optimization Technique       | Newton-Raphson          |
| Variance Adjustment          | Degrees of Freedom (DF) |

[Output 91.2.3](#) displays the number of observations and the total of sampling weights both in the data set and used in the analysis. Only the observations with positive person-level weight are used in the analysis. Therefore, 1,053 observations with zero person-level weights were deleted.

**Output 91.2.3** MEPS, Number of Observations

|                             |          |
|-----------------------------|----------|
| Number of Observations Read | 24618    |
| Number of Observations Used | 23565    |
| Sum of Weights Read         | 2.7641E8 |
| Sum of Weights Used         | 2.7641E8 |

[Output 91.2.4](#) lists the three insurance coverage levels for the response variable INSCOV99. The “UNINSURED” category is used as the reference category in the model.

**Output 91.2.4** MEPS, Response Profile

| Response Profile |             |                 |              |
|------------------|-------------|-----------------|--------------|
| Ordered Value    | INSCOV99    | Total Frequency | Total Weight |
| 1                | ANY PRIVATE | 16130           | 204403997    |
| 2                | PUBLIC ONLY | 4241            | 41809572     |
| 3                | UNINSURED   | 3194            | 30197198     |

Logits modeled use INSCOV99='UNINSURED' as the reference category.

Output 91.2.5 shows the parameterization in the regression model for each categorical independent variable.

**Output 91.2.5** MEPS, Classification Levels

| Class Level Information |                           |    |                  |    |    |  |
|-------------------------|---------------------------|----|------------------|----|----|--|
| Class                   | Value                     |    | Design Variables |    |    |  |
| SEX                     | FEMALE                    | 1  |                  |    |    |  |
|                         | MALE                      | -1 |                  |    |    |  |
| RACEX                   | ALEUT, ESKIMO             | 1  | 0                | 0  | 0  |  |
|                         | AMERICAN INDIAN           | 0  | 1                | 0  | 0  |  |
|                         | ASIAN OR PACIFIC ISLANDER | 0  | 0                | 1  | 0  |  |
|                         | BLACK                     | 0  | 0                | 0  | 1  |  |
|                         | WHITE                     | -1 | -1               | -1 | -1 |  |
| POVCAT99                | HIGH INCOME               | 1  | 0                | 0  | 0  |  |
|                         | LOW INCOME                | 0  | 1                | 0  | 0  |  |
|                         | MIDDLE INCOME             | 0  | 0                | 1  | 0  |  |
|                         | NEAR POOR                 | 0  | 0                | 0  | 1  |  |
|                         | NEGATIVE OR POOR          | -1 | -1               | -1 | -1 |  |

Output 91.2.6 displays the parameter estimates and their standard errors.

Output 91.2.7 displays the odds ratio estimates and their standard errors.

For example, after adjusting for the effects of sex, race, and total health care expenditures, a person with high income is estimated to be 11.595 times more likely than a poor person to choose private health care insurance over no insurance, but only 0.274 times as likely to choose public health insurance over no insurance.

Output 91.2.6 MEPS, Parameter Estimates

| Analysis of Maximum Likelihood Estimates |                           |             |    |          |                |                 |
|------------------------------------------|---------------------------|-------------|----|----------|----------------|-----------------|
| Parameter                                |                           | INSCOV99    | DF | Estimate | Standard Error | Wald Chi-Square |
| Intercept                                |                           | ANY PRIVATE | 1  | 2.7703   | 0.1906         | 211.3648        |
| Intercept                                |                           | PUBLIC ONLY | 1  | 1.9216   | 0.1561         | 151.4590        |
| TOTEXP99                                 |                           | ANY PRIVATE | 1  | 0.000215 | 0.000071       | 9.1895          |
| TOTEXP99                                 |                           | PUBLIC ONLY | 1  | 0.000241 | 0.000072       | 11.1509         |
| SEX                                      | FEMALE                    | ANY PRIVATE | 1  | 0.1208   | 0.0248         | 23.7173         |
| SEX                                      | FEMALE                    | PUBLIC ONLY | 1  | 0.1741   | 0.0308         | 31.9571         |
| RACEX                                    | ALEUT, ESKIMO             | ANY PRIVATE | 1  | 7.1457   | 0.6976         | 104.9258        |
| RACEX                                    | ALEUT, ESKIMO             | PUBLIC ONLY | 1  | 7.6303   | 0.5022         | 230.8760        |
| RACEX                                    | AMERICAN INDIAN           | ANY PRIVATE | 1  | -2.0904  | 0.2615         | 63.8878         |
| RACEX                                    | AMERICAN INDIAN           | PUBLIC ONLY | 1  | -1.8992  | 0.2909         | 42.6095         |
| RACEX                                    | ASIAN OR PACIFIC ISLANDER | ANY PRIVATE | 1  | -1.8055  | 0.2299         | 61.6848         |
| RACEX                                    | ASIAN OR PACIFIC ISLANDER | PUBLIC ONLY | 1  | -1.9914  | 0.2285         | 75.9479         |
| RACEX                                    | BLACK                     | ANY PRIVATE | 1  | -1.7517  | 0.1983         | 78.0146         |
| RACEX                                    | BLACK                     | PUBLIC ONLY | 1  | -1.7038  | 0.1691         | 101.4970        |
| POVCAT99                                 | HIGH INCOME               | ANY PRIVATE | 1  | 1.4560   | 0.0685         | 452.1829        |
| POVCAT99                                 | HIGH INCOME               | PUBLIC ONLY | 1  | -0.6092  | 0.0903         | 45.5392         |
| POVCAT99                                 | LOW INCOME                | ANY PRIVATE | 1  | -0.3066  | 0.0666         | 21.1762         |
| POVCAT99                                 | LOW INCOME                | PUBLIC ONLY | 1  | -0.0239  | 0.0754         | 0.1007          |
| POVCAT99                                 | MIDDLE INCOME             | ANY PRIVATE | 1  | 0.6467   | 0.0587         | 121.1736        |
| POVCAT99                                 | MIDDLE INCOME             | PUBLIC ONLY | 1  | -0.3496  | 0.0807         | 18.7732         |
| POVCAT99                                 | NEAR POOR                 | ANY PRIVATE | 1  | -0.8015  | 0.1076         | 55.4443         |
| POVCAT99                                 | NEAR POOR                 | PUBLIC ONLY | 1  | 0.2985   | 0.0952         | 9.8308          |

| Analysis of Maximum Likelihood Estimates |                           |             |            |
|------------------------------------------|---------------------------|-------------|------------|
| Parameter                                |                           | INSCOV99    | Pr > ChiSq |
| Intercept                                |                           | ANY PRIVATE | <.0001     |
| Intercept                                |                           | PUBLIC ONLY | <.0001     |
| TOTEXP99                                 |                           | ANY PRIVATE | 0.0024     |
| TOTEXP99                                 |                           | PUBLIC ONLY | 0.0008     |
| SEX                                      | FEMALE                    | ANY PRIVATE | <.0001     |
| SEX                                      | FEMALE                    | PUBLIC ONLY | <.0001     |
| RACEX                                    | ALEUT, ESKIMO             | ANY PRIVATE | <.0001     |
| RACEX                                    | ALEUT, ESKIMO             | PUBLIC ONLY | <.0001     |
| RACEX                                    | AMERICAN INDIAN           | ANY PRIVATE | <.0001     |
| RACEX                                    | AMERICAN INDIAN           | PUBLIC ONLY | <.0001     |
| RACEX                                    | ASIAN OR PACIFIC ISLANDER | ANY PRIVATE | <.0001     |
| RACEX                                    | ASIAN OR PACIFIC ISLANDER | PUBLIC ONLY | <.0001     |
| RACEX                                    | BLACK                     | ANY PRIVATE | <.0001     |
| RACEX                                    | BLACK                     | PUBLIC ONLY | <.0001     |
| POVCAT99                                 | HIGH INCOME               | ANY PRIVATE | <.0001     |
| POVCAT99                                 | HIGH INCOME               | PUBLIC ONLY | <.0001     |
| POVCAT99                                 | LOW INCOME                | ANY PRIVATE | <.0001     |
| POVCAT99                                 | LOW INCOME                | PUBLIC ONLY | 0.7510     |
| POVCAT99                                 | MIDDLE INCOME             | ANY PRIVATE | <.0001     |
| POVCAT99                                 | MIDDLE INCOME             | PUBLIC ONLY | <.0001     |
| POVCAT99                                 | NEAR POOR                 | ANY PRIVATE | <.0001     |
| POVCAT99                                 | NEAR POOR                 | PUBLIC ONLY | 0.0017     |

## Output 91.2.7 MEPS, Odds Ratios

| Odds Ratio Estimates |                                    |             |                |
|----------------------|------------------------------------|-------------|----------------|
| Effect               |                                    | INSCOV99    | Point Estimate |
| TOTEXP99             |                                    | ANY PRIVATE | 1.000          |
| TOTEXP99             |                                    | PUBLIC ONLY | 1.000          |
| SEX                  | FEMALE vs MALE                     | ANY PRIVATE | 1.273          |
| SEX                  | FEMALE vs MALE                     | PUBLIC ONLY | 1.417          |
| RACEX                | ALEUT, ESKIMO vs WHITE             | ANY PRIVATE | >999.999       |
| RACEX                | ALEUT, ESKIMO vs WHITE             | PUBLIC ONLY | >999.999       |
| RACEX                | AMERICAN INDIAN vs WHITE           | ANY PRIVATE | 0.553          |
| RACEX                | AMERICAN INDIAN vs WHITE           | PUBLIC ONLY | 1.146          |
| RACEX                | ASIAN OR PACIFIC ISLANDER vs WHITE | ANY PRIVATE | 0.735          |
| RACEX                | ASIAN OR PACIFIC ISLANDER vs WHITE | PUBLIC ONLY | 1.045          |
| RACEX                | BLACK vs WHITE                     | ANY PRIVATE | 0.776          |
| RACEX                | BLACK vs WHITE                     | PUBLIC ONLY | 1.394          |
| POV99                | HIGH INCOME vs NEGATIVE OR POOR    | ANY PRIVATE | 11.595         |
| POV99                | HIGH INCOME vs NEGATIVE OR POOR    | PUBLIC ONLY | 0.274          |
| POV99                | LOW INCOME vs NEGATIVE OR POOR     | ANY PRIVATE | 1.990          |
| POV99                | LOW INCOME vs NEGATIVE OR POOR     | PUBLIC ONLY | 0.492          |
| POV99                | MIDDLE INCOME vs NEGATIVE OR POOR  | ANY PRIVATE | 5.162          |
| POV99                | MIDDLE INCOME vs NEGATIVE OR POOR  | PUBLIC ONLY | 0.356          |
| POV99                | NEAR POOR vs NEGATIVE OR POOR      | ANY PRIVATE | 1.213          |
| POV99                | NEAR POOR vs NEGATIVE OR POOR      | PUBLIC ONLY | 0.680          |

| Odds Ratio Estimates |                            |          |
|----------------------|----------------------------|----------|
|                      | 95% Wald Confidence Limits |          |
|                      | 1.000                      | 1.000    |
|                      | 1.000                      | 1.000    |
|                      | 1.155                      | 1.403    |
|                      | 1.255                      | 1.598    |
|                      | >999.999                   | >999.999 |
|                      | >999.999                   | >999.999 |
|                      | 0.339                      | 0.901    |
|                      | 0.603                      | 2.178    |
|                      | 0.499                      | 1.083    |
|                      | 0.656                      | 1.665    |
|                      | 0.638                      | 0.944    |
|                      | 1.132                      | 1.717    |
|                      | 9.301                      | 14.455   |
|                      | 0.213                      | 0.353    |
|                      | 1.607                      | 2.464    |
|                      | 0.395                      | 0.614    |
|                      | 4.200                      | 6.343    |
|                      | 0.280                      | 0.451    |
|                      | 0.903                      | 1.630    |
|                      | 0.527                      | 0.877    |

---

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## Chapter 92

# The SURVEYMEANS Procedure

### Contents

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## Overview: SURVEYMEANS Procedure

The SURVEYMEANS procedure estimates characteristics of a survey population by using statistics computed from a survey sample. It enables you to estimate statistics such as means, totals, proportions, quantiles, geometric means, and ratios. PROC SURVEYMEANS also provides domain analysis, which computes estimates for subpopulations or domains. The procedure also estimates variances and confidence limits and performs  $t$  tests for these statistics. PROC SURVEYMEANS uses either the Taylor series (linearization) method or replication (subsampling) methods to estimate sampling errors of estimators based on complex sample designs. The sample design can be a complex survey sample design with stratification, clustering, and unequal weighting. For more information, see Fuller (2009); Lohr (2010); Särndal, Swensson, and Wretman (1992); Wolter (2007).

---

## Getting Started: SURVEYMEANS Procedure

This section demonstrates how you can use the SURVEYMEANS procedure to produce descriptive statistics from sample survey data. For a complete description of PROC SURVEYMEANS, see the section “Syntax: SURVEYMEANS Procedure” on page 7785. The section “Examples: SURVEYMEANS Procedure” on page 7839 provides more complicated examples to illustrate the applications of PROC SURVEYMEANS.

---

## Simple Random Sampling

This example illustrates how you can use PROC SURVEYMEANS to estimate population means and proportions from sample survey data. The study population is a junior high school with a total of 4,000 students in grades 7, 8, and 9. Researchers want to know how much these students spend weekly for ice cream, on average, and what percentage of students spend at least \$10 weekly for ice cream.

To answer these questions, 40 students were selected from the entire student population by using simple random sampling (SRS). Selection by simple random sampling means that all students have an equal chance of being selected and no student can be selected more than once. Each student selected for the sample was asked how much he or she spends for ice cream per week, on average. The SAS data set IceCream saves the responses of the 40 students:

```
data IceCream;
 input Grade Spending @@;
 if (Spending < 10) then Group='less';
 else Group='more';
 datalines;
7 7 7 7 8 12 9 10 7 1 7 10 7 3 8 20 8 19 7 2
7 2 9 15 8 16 7 6 7 6 7 6 9 15 8 17 8 14 9 8
9 8 9 7 7 3 7 12 7 4 9 14 8 18 9 9 7 2 7 1
7 4 7 11 9 8 8 10 8 13 7 2 9 6 9 11 7 2 7 9
;
```

The variable Grade contains a student's grade. The variable Spending contains a student's response regarding how much he spends per week for ice cream, in dollars. The variable Group is created to indicate

whether a student spends at least \$10 weekly for ice cream: Group='more' if a student spends at least \$10, or Group='less' if a student spends less than \$10.

You can use PROC SURVEYMEANS to produce estimates for the entire student population, based on this random sample of 40 students:

```

title1 'Analysis of Ice Cream Spending';
title2 'Simple Random Sample Design';
proc surveymeans data=IceCream total=4000;
 var Spending Group;
run;

```

The PROC SURVEYMEANS statement invokes the procedure. The TOTAL=4000 option specifies the total number of students in the study population, or school. The procedure uses this total to adjust variance estimates for the effects of sampling from a finite population. The VAR statement names the variables to analyze, Spending and Group.

Figure 92.1 displays the results from this analysis. There are a total of 40 observations used in the analysis. The “Class Level Information” table lists the two levels of the variable Group. This variable is a character variable, and so PROC SURVEYMEANS provides a categorical analysis for it, estimating the relative frequency or proportion for each level. If you want a categorical analysis for a numeric variable, you can name that variable in the CLASS statement.

**Figure 92.1** Analysis of Ice Cream Spending

| Analysis of Ice Cream Spending |        |           |          |                      |                 |            |
|--------------------------------|--------|-----------|----------|----------------------|-----------------|------------|
| Simple Random Sample Design    |        |           |          |                      |                 |            |
| The SURVEYMEANS Procedure      |        |           |          |                      |                 |            |
| Data Summary                   |        |           |          |                      |                 |            |
| Number of Observations         |        |           |          |                      |                 | 40         |
| Class Level Information        |        |           |          |                      |                 |            |
| Class                          |        |           |          |                      |                 |            |
| Variable                       | Levels | Values    |          |                      |                 |            |
| Group                          | 2      | less more |          |                      |                 |            |
| Statistics                     |        |           |          |                      |                 |            |
| Variable                       | Level  | N         | Mean     | Std Error<br>of Mean | 95% CL for Mean |            |
| Spending                       |        | 40        | 8.750000 | 0.845139             | 7.04054539      | 10.4594546 |
| Group                          | less   | 23        | 0.575000 | 0.078761             | 0.41568994      | 0.7343101  |
|                                | more   | 17        | 0.425000 | 0.078761             | 0.26568994      | 0.5843101  |

The “Statistics” table displays the estimates for each analysis variable. By default, PROC SURVEYMEANS displays the number of observations, the estimate of the mean, its standard error, and the 95% confidence limits for the mean. You can obtain other statistics by specifying the corresponding *statistic-keywords* in the PROC SURVEYMEANS statement.

The estimate of the average weekly ice cream expense is \$8.75 for students at this school. The standard error of this estimate is \$0.85, and the 95% confidence interval for weekly ice cream expense is from \$7.04 to \$10.46. The analysis variable Group is a character variable, and so PROC SURVEYMEANS analyzes it as categorical, estimating the relative frequency or proportion for each level or category. These estimates are displayed in the Mean column of the “Statistics” table. It is estimated that 57.5% of all students spend less than \$10 weekly on ice cream, while 42.5% of the students spend at least \$10 weekly. The standard error of each estimate is 7.9%.

---

## Stratified Sampling

Suppose that the sample of students described in the previous section was actually selected by using stratified random sampling. In stratified sampling, the study population is divided into nonoverlapping strata, and samples are selected from each stratum independently.

The list of students in this junior high school was stratified by grade, yielding three strata: grades 7, 8, and 9. A simple random sample of students was selected from each grade. Table 92.1 shows the total number of students in each grade.

**Table 92.1** Number of Students by Grade

| Grade | Number of Students |
|-------|--------------------|
| 7     | 1,824              |
| 8     | 1,025              |
| 9     | 1,151              |
| Total | 4,000              |

To analyze this stratified sample, you need to provide the population totals for each stratum to PROC SURVEYMEANS. The SAS data set StudentTotals contains the information from Table 92.1:

```
data StudentTotals;
 input Grade _total_;
 datalines;
7 1824
8 1025
9 1151
;
```

The variable Grade is the stratum identification variable, and the variable \_TOTAL\_ contains the total number of students for each stratum. PROC SURVEYMEANS requires you to use the variable name \_TOTAL\_ for the stratum population totals.

The procedure uses the stratum population totals to adjust variance estimates for the effects of sampling from a finite population. If you do not provide population totals or sampling rates, then the procedure assumes



that the proportion of the population in the sample is very small, and the computation does not involve a finite population correction.

In a stratified sample design, when the sampling rates in the strata are unequal, you need to use sampling weights to reflect this information in order to produce an unbiased mean estimator. In this example, the appropriate sampling weights are reciprocals of the probabilities of selection. You can use the following DATA step to create the sampling weights:

```
data IceCream;
 set IceCream;
 if Grade=7 then Prob=20/1824;
 if Grade=8 then Prob=9/1025;
 if Grade=9 then Prob=11/1151;
 Weight=1/Prob;
run;
```

When you use PROC SURVEYSELECT to select your sample, the procedure creates these sampling weights for you.

The following SAS statements perform the stratified analysis of the survey data:

```
title1 'Analysis of Ice Cream Spending';
title2 'Stratified Sample Design';
proc surveymeans data=IceCream total=StudentTotals;
 stratum Grade / list;
 var Spending Group;
 weight Weight;
run;
```

The PROC SURVEYMEANS statement invokes the procedure. The DATA= option names the SAS data set IceCream as the input data set to be analyzed. The TOTAL= option names the data set StudentTotals as the input data set that contains the stratum population totals. Comparing this to the analysis in the section “[Simple Random Sampling](#)” on page 7779, notice that the TOTAL=StudentTotals option is used here instead of the TOTAL=4000 option. In this stratified sample design, the population totals are different for different strata, and so you need to provide them to PROC SURVEYMEANS in a SAS data set.

The STRATA statement identifies the stratification variable Grade. The LIST option in the STRATA statement requests that the procedure display stratum information. The WEIGHT statement tells the procedure that the variable Weight contains the sampling weights.

[Figure 92.2](#) displays information about the input data set. There are three strata in the design and 40 observations in the sample. The categorical variable Group has two levels, ‘less’ and ‘more.’

[Figure 92.3](#) displays information for each stratum. The table displays a stratum index and the values of the STRATA variable. The stratum index identifies each stratum by a sequentially assigned number. For each stratum, the table gives the population total (total number of students), the sampling rate, and the sample size. The stratum sampling rate is the ratio of the number of students in the sample to the number of students in the population for that stratum. The table also lists each analysis variable and the number of stratum observations for that variable. For categorical variables, the table lists each level and the number of sample observations in that level.

**Figure 92.2** Data Summary

```

Analysis of Ice Cream Spending
Stratified Sample Design

The SURVEYMEANS Procedure

Data Summary

Number of Strata 3
Number of Observations 40
Sum of Weights 4000

Class Level Information

Class
Variable Levels Values

Group 2 less more

```

**Figure 92.3** Stratum Information

```

Stratum Information

Stratum Index Grade Population Total Sampling Rate N Obs Variable Level

1 7 1824 1.10% 20 Spending Group less more
2 8 1025 0.88% 9 Spending Group less more
3 9 1151 0.96% 11 Spending Group less more

Stratum Information

Stratum Index Grade Population Total Sampling Rate N Obs Variable N

1 7 1824 1.10% 20 Spending Group 20
1 7 1824 1.10% 17 Spending Group 17
1 7 1824 1.10% 3 Spending Group 3
2 8 1025 0.88% 9 Spending Group 9
2 8 1025 0.88% 0 Spending Group 0
2 8 1025 0.88% 9 Spending Group 9
3 9 1151 0.96% 11 Spending Group 11
3 9 1151 0.96% 6 Spending Group 6
3 9 1151 0.96% 5 Spending Group 5

```

Figure 92.4 shows the following:

- The estimate of average weekly ice cream expense is \$9.14 for students in this school, with a standard error of \$0.53, and a 95% confidence interval from \$8.06 to \$10.22.
- An estimate of 54.5% of all students spend less than \$10 weekly on ice cream, and 45.5% spend more, with a standard error of 5.8%.

**Figure 92.4** Analysis of Ice Cream Spending

|          |       | Statistics |          |                      |                 |            |
|----------|-------|------------|----------|----------------------|-----------------|------------|
| Variable | Level | N          | Mean     | Std Error<br>of Mean | 95% CL for Mean |            |
| Spending |       | 40         | 9.141298 | 0.531799             | 8.06377052      | 10.2188254 |
| Group    | less  | 23         | 0.544555 | 0.058424             | 0.42617678      | 0.6629323  |
|          | more  | 17         | 0.455445 | 0.058424             | 0.33706769      | 0.5738232  |

## Output Data Sets

PROC SURVEYMEANS uses the Output Delivery System (ODS) to create output data sets. This is a departure from older SAS procedures that provide OUTPUT statements for similar functionality. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

For example, to save the “Statistics” table shown in Figure 92.4 in the previous section in an output data set, you use the ODS OUTPUT statement as follows:

```
title1 'Analysis of Ice Cream Spending';
title2 'Stratified Sample Design';
proc surveymeans data=IceCream total=StudentTotals;
 stratum Grade / list;
 var Spending Group;
 weight Weight;
 ods output Statistics=MyStat;
run;
```

The statement

```
ods output Statistics=MyStat;
```

requests that the “Statistics” table that appears in Figure 92.4 be placed in a SAS data set MyStat.

The PRINT procedure displays observations of the data set MyStat:

```
proc print data=MyStat;
run;
```

Figure 92.5 displays the data set MyStat. The section “ODS Table Names” on page 7838 gives the complete list of tables produced by PROC SURVEYMEANS.

**Figure 92.5** Output Data Set MyStat

| Analysis of Ice Cream Spending<br>Stratified Sample Design |          |              |    |          |          |                 |                 |
|------------------------------------------------------------|----------|--------------|----|----------|----------|-----------------|-----------------|
| Obs                                                        | VarName  | Var<br>Level | N  | Mean     | StdErr   | Lower<br>CLMean | Upper<br>CLMean |
| 1                                                          | Spending |              | 40 | 9.141298 | 0.531799 | 8.06377052      | 10.2188254      |
| 2                                                          | Group    | less         | 23 | 0.544555 | 0.058424 | 0.42617678      | 0.6629323       |
| 3                                                          | Group    | more         | 17 | 0.455445 | 0.058424 | 0.33706769      | 0.5738232       |

## Syntax: SURVEYMEANS Procedure

The following statements are available in the SURVEYMEANS procedure:

```

PROC SURVEYMEANS < options > < statistic-keywords > ;
 BY variables ;
 CLASS variables ;
 CLUSTER variables ;
 DOMAIN variables < variable*variable variable*variable*variable ... > < / option > ;
 POSTSTRATA variables / PSTOTAL= < option > ;
 POSTSTRATA variables / PSPCT= < option > ;
 RATIO < 'label' > variables / variables ;
 REPWEIGHTS variables < / options > ;
 STRATA variables < / option > ;
 VAR variables ;
 WEIGHT variable ;

```

The PROC SURVEYMEANS statement invokes the procedure. It optionally names the input data sets, specifies statistics for the procedure to compute, and specifies the variance estimation method. The PROC SURVEYMEANS statement is required.

The VAR statement identifies the variables to be analyzed. The CLASS statement identifies numeric variables that are to be analyzed as categorical variables. The STRATA statement lists the variables that form the strata in a stratified sample design. The CLUSTER statement specifies cluster identification variables in a clustered sample design. The DOMAIN statement lists the variables that define domains for subpopulation analysis. The RATIO statement requests ratio analysis for means or proportions of analysis variables. The WEIGHT statement names the sampling weight variable. The POSTSTRATA statement lists the variables that are used to form poststrata for poststratification. The REPWEIGHTS statement names replicate weight variables for BRR or jackknife variance estimation. You can use a BY statement with PROC SURVEYMEANS to obtain separate analyses for groups defined by the BY variables.

All statements can appear multiple times except the PROC SURVEYMEANS statement, POSTSTRATA statement, and WEIGHT statement, which can appear only once.

The rest of this section gives detailed syntax information for the BY, CLASS, CLUSTER, DOMAIN, POSTSTRATA, RATIO, REPWEIGHTS, STRATA, VAR, and WEIGHT statements in alphabetical order after the description of the PROC SURVEYMEANS statement.

## PROC SURVEYMEANS Statement

**PROC SURVEYMEANS** < options > *statistic-keywords* ;

The PROC SURVEYMEANS statement invokes the SURVEYMEANS procedure. In this statement, you identify the data set to be analyzed, specify the variance estimation method, and provide sample design information. The DATA= option names the input data set to be analyzed. The VARMETHOD= option specifies the variance estimation method, which is the Taylor series method by default. For Taylor series variance estimation, you can include a finite population correction factor in the analysis by providing either the sampling rate or population total with the RATE= or TOTAL= option. If your design is stratified, with different sampling rates or totals for different strata, then you can input these stratum rates or totals in a SAS data set that contains the stratification variables.

In the PROC SURVEYMEANS statement, you also can use *statistic-keywords* to specify statistics, such as population mean and population total, for the procedure to compute. You can also request data set summary information and sample design information.

Table 92.2 summarizes the options available in the PROC SURVEYMEANS statement.

**Table 92.2** PROC SURVEYMEANS Statement Options

| Option      | Description                                                                    |
|-------------|--------------------------------------------------------------------------------|
| ALPHA=      | Sets the confidence level for confidence limits                                |
| DATA=       | Specifies the SAS data set to be analyzed                                      |
| MISSING     | Treats missing values as a valid                                               |
| NOMCAR      | Computes variance estimates by analyzing the nonmissing values as a domain     |
| NONSYMCL    | Requests nonsymmetric confidence limits for quantiles                          |
| NOPARSE     | Suppresses the display of analysis variables with zero frequency               |
| ORDER=      | Specifies the order in which to report the values of the categorical variables |
| PERCENTILE= | Specifies percentiles that you want the procedure to compute                   |
| QUANTILE=   | Specifies quantiles that you want the procedure to compute                     |
| RATE=       | Specifies the sampling rate                                                    |
| STACKING    | Produces the output data sets by using a stacking table structure              |
| TOTAL=      | Specifies the total number of primary sampling units                           |
| VARMETHOD=  | Specifies the variance estimation method                                       |

You can specify the following options in the PROC SURVEYMEANS statement:

### ALPHA= $\alpha$

sets the confidence level for confidence limits. The value of the ALPHA= option must be between 0 and 1, and the default value is 0.05. A confidence level of  $\alpha$  produces  $100(1 - \alpha)\%$  confidence limits. The default of ALPHA=0.05 produces 95% confidence limits.

**DATA=SAS-data-set**

specifies the SAS data set to be analyzed by PROC SURVEYMEANS. If you omit the DATA= option, the procedure uses the most recently created SAS data set.

**MISSING**

treats missing values as a valid (nonmissing) category for all categorical variables, which include CLASS, STRATA, CLUSTER, DOMAIN, and POSTSTRATA variables.

By default, if you do not specify the MISSING option, an observation is excluded from the analysis if it has a missing value. For more information, see the section “Missing Values” on page 7804.

**NOMCAR**

requests that the procedure treat missing values in the variance computation as *not missing completely at random* (NOMCAR) for Taylor series variance estimation. When you specify the NOMCAR option, PROC SURVEYMEANS computes variance estimates by analyzing the nonmissing values as a domain (subpopulation), where the entire population includes both nonmissing and missing domains. See the section “Missing Values” on page 7804 for more details.

By default, PROC SURVEYMEANS completely excludes an observation from analysis if that observation has a missing value, unless you specify the MISSING option for categorical variables. Note that the NOMCAR option has no effect on a categorical variable when you specify the MISSING option, which treats missing values as a valid nonmissing level.

The NOMCAR option applies only to Taylor series variance estimation. The replication methods, which you request with the VARMETHOD=BRR and VARMETHOD=JACKKNIFE options, do not use the NOMCAR option.

The NOMCAR option is not available for geometric means or poststratification.

**NONSYMCL**

requests nonsymmetric confidence limits for quantiles when you request quantiles with PERCENTILE= or QUANTILE= option. See the section “Confidence Limits” on page 7818 for more details. This option applies only to the default VARMETHOD=TAYLOR option.

**NOSPARE**

suppresses the display of analysis variables with zero frequency. By default, the procedure displays all continuous variables and all levels of categorical variables.

**ORDER=DATA | FORMATTED | INTERNAL**

specifies the order in which the values of the categorical variables are to be reported.

This option also determines the sort order for the levels of CIUSTER and DOMAIN variables and controls STRATA variable levels in the “Stratum Information” table.

The following shows how PROC SURVEYMEANS interprets values of the ORDER= option:

|           |                                                                                                                                                     |
|-----------|-----------------------------------------------------------------------------------------------------------------------------------------------------|
| DATA      | orders values according to their order in the input data set.                                                                                       |
| FORMATTED | orders values by their formatted values. This order is operating environment dependent. By default, the order is ascending.                         |
| INTERNAL  | orders values by their unformatted values, which yields the same order that the SORT procedure does. This order is operating environment dependent. |

By default, ORDER=INTERNAL. For ORDER=FORMATTED and ORDER=INTERNAL, the sort order is machine-dependent.

For more information about sort order, see the chapter on the SORT procedure in the *Base SAS Procedures Guide* and the discussion of BY-group processing in *SAS Language Reference: Concepts*.

#### PERCENTILE=(*values*)

specifies percentiles you want the procedure to compute. You can separate values with blanks or commas. Each value must be between 0 and 100. You can also use the *statistic-keywords* DECILES, MEDIAN, Q1, Q3, and QUARTILES to request common percentiles.

PROC SURVEYMEANS uses Woodruff's method (Dorfman and Valliant 1993; Särndal, Swensson, and Wretman 1992; Francisco and Fuller 1991) to estimate the variances of quantiles. See the section "Quantiles" on page 7817 for more details.

#### QUANTILE=(*values*)

specifies quantiles you want the procedure to compute. You can separate values with blanks or commas. Each value must be between 0 and 1. You can also use the *statistic-keywords* DECILES, MEDIAN, Q1, Q3, and QUARTILES to request common quantiles.

PROC SURVEYMEANS uses Woodruff's method (Dorfman and Valliant 1993; Särndal, Swensson, and Wretman 1992; Francisco and Fuller 1991) to estimate the variances of quantiles. See the section "Quantiles" on page 7817 for more details.

#### RATE=*value* | SAS-data-set

#### R=*value* | SAS-data-set

specifies the sampling rate as a nonnegative *value*, or specifies an input data set that contains the stratum sampling rates. The procedure uses this information to compute a finite population correction for Taylor series variance estimation. The procedure does not use the RATE= option for BRR or jackknife variance estimation, which you request with the VARMETHOD=BRR or VARMETHOD=JACKKNIFE option.

If your sample design has multiple stages, you should specify the *first-stage sampling rate*, which is the ratio of the number of PSUs selected to the total number of PSUs in the population.

For a nonstratified sample design, or for a stratified sample design with the same sampling rate in all strata, you should specify a nonnegative *value* for the RATE= option. If your design is stratified with different sampling rates in the strata, then you should name a SAS data set that contains the stratification variables and the sampling rates. See the section "Specification of Population Totals and Sampling Rates" on page 7805 for more details.

The *value* in the RATE= option or the values of \_RATE\_ in the secondary data set must be nonnegative numbers. You can specify *value* as a number between 0 and 1. Or you can specify *value* in percentage form as a number between 1 and 100, and PROC SURVEYMEANS converts that number to a proportion. The procedure treats the value 1 as 100% instead of 1%.

If you do not specify the TOTAL= or RATE= option, then the Taylor series variance estimation does not include a finite population correction. You cannot specify both the TOTAL= and RATE= options.

#### STACKING

requests that the procedure produce the output data sets by using a stacking table structure, which was the default before SAS 9. The new default is to produce a rectangular table structure in the output data sets.



A rectangular structure creates one observation for each analysis variable in the data set. A stacking structure creates only one observation in the output data set for all analysis variables.

The STACKING option affects the following tables:

- Domain
- Ratio
- Statistics
- StrataInfo

See the section “[Rectangular and Stacking Structures in an Output Data Set](#)” on page 7831 for more details.

**TOTAL=***value* | *SAS-data-set*

**N=***value* | *SAS-data-set*

specifies the total number of primary sampling units in the study population as a positive *value*, or specifies an input data set that contains the stratum population totals. The procedure uses this information to compute a finite population correction for Taylor series variance estimation. The procedure does not use the TOTAL= option for BRR or jackknife variance estimation, which you request with the [VARMETHOD=BRR](#) or [VARMETHOD=JACKKNIFE](#) option.

For a nonstratified sample design, or for a stratified sample design with the same population total in all strata, you should specify a positive *value* for the TOTAL= option. If your sample design is stratified with different population totals in the strata, then you should name a SAS data set that contains the stratification variables and the population totals. See the section “[Specification of Population Totals and Sampling Rates](#)” on page 7805 for more details.

If you do not specify the TOTAL= or [RATE=](#) option, then the Taylor series variance estimation does not include a finite population correction. You cannot specify both the TOTAL= and RATE= options.

*statistic-keywords*

specifies the statistics for the procedure to compute. If you do not specify any *statistic-keywords*, PROC SURVEYMEANS computes the NOBS, MEAN, STDERR, and CLM statistics by default.

The statistics produced depend on the type of the analysis variable. If you name a numeric variable in the CLASS statement, then the procedure analyzes that variable as a categorical variable. The procedure always analyzes character variables as categorical. See the section “[CLASS Statement](#)” on page 7796 for more information.

PROC SURVEYMEANS computes MIN, MAX, and RANGE for numeric variables but not for categorical variables. For numeric variables, the keyword MEAN produces the mean, but for categorical variables it produces the proportion in each category or level. Also, for categorical variables, the keyword NOBS produces the number of observations for each variable level, and the keyword NMISS produces the number of missing observations for each level. If you request the keyword NCLUSTER for a categorical variable, PROC SURVEYMEANS displays for each level the number of clusters with observations in that level. PROC SURVEYMEANS computes SUMWGT in the same way for both categorical and numeric variables, as the sum of the weights over all nonmissing observations.

PROC SURVEYMEANS performs univariate analysis, analyzing each variable separately. Thus the number of nonmissing and missing observations might not be the same for all analysis variables. See the section “[Missing Values](#)” on page 7804 for more information.



The following statistics are available for ratios (which you request with a **RATIO** statement): N, NCLU, SUMWGT, RATIO, STDERR, DF, T, PROBT, and CLM, as shown in the following list. If no statistics are requested, the procedure computes the ratio and its standard error by default.

The valid *statistic-keywords* are as follows:

|           |                                                                                                                                                                |
|-----------|----------------------------------------------------------------------------------------------------------------------------------------------------------------|
| ALL       | all available statistics except those associated with geometric means                                                                                          |
| ALLGEO    | all available statistics associated with geometric means                                                                                                       |
| CLM       | 100(1 - $\alpha$ )% two-sided confidence limits for the MEAN, where $\alpha$ is determined by the <b>ALPHA=</b> option; the default is $\alpha = 0.05$         |
| CLSUM     | 100(1 - $\alpha$ )% two-sided confidence limits for the SUM, where $\alpha$ is determined by the <b>ALPHA=</b> option; the default is $\alpha = 0.05$          |
| CV        | coefficient of variation for MEAN                                                                                                                              |
| CVSUM     | coefficient of variation for SUM                                                                                                                               |
| DECILES   | the 10th, the 20th, . . . , and the 90th percentiles including their standard errors and confidence limits                                                     |
| DF        | degrees of freedom for the <i>t</i> test                                                                                                                       |
| GEOMEAN   | geometric mean of a numeric variable that contains positive values                                                                                             |
| GMCLM     | 100(1 - $\alpha$ )% two-sided confidence limits for the GEOMEAN, where $\alpha$ is determined by the <b>ALPHA=</b> option; the default is $\alpha = 0.05$      |
| GMSTDERR  | standard error of the GEOMEAN. When you request GEOMEAN, the procedure computes GMSTDERR by default.                                                           |
| LCLM      | 100(1 - $\alpha$ )% one-sided lower confidence limit for the MEAN, where $\alpha$ is determined by the <b>ALPHA=</b> option; the default is $\alpha = 0.05$    |
| LCLSUM    | 100(1 - $\alpha$ )% one-sided lower confidence limit for the SUM, where $\alpha$ is determined by the <b>ALPHA=</b> option; the default is $\alpha = 0.05$     |
| LGMCLM    | 100(1 - $\alpha$ )% one-sided lower confidence limit for the GEOMEAN, where $\alpha$ is determined by the <b>ALPHA=</b> option; the default is $\alpha = 0.05$ |
| MAX       | maximum value                                                                                                                                                  |
| MEAN      | mean for a numeric variable, or the proportion in each category for a categorical variable                                                                     |
| MEDIAN    | median for a numeric variable                                                                                                                                  |
| MIN       | minimum value                                                                                                                                                  |
| NCLUSTER  | number of clusters                                                                                                                                             |
| NMISS     | number of missing observations                                                                                                                                 |
| NOBS      | number of nonmissing observations                                                                                                                              |
| Q1        | lower quartile                                                                                                                                                 |
| Q3        | upper quartile                                                                                                                                                 |
| QUARTILES | lower quartile (25%th percentile), median (50%th percentile), and upper quartile (75%th percentile), including their standard errors and confidence limits     |

|        |                                                                                                                                                         |
|--------|---------------------------------------------------------------------------------------------------------------------------------------------------------|
| RANGE  | range, MAX–MIN                                                                                                                                          |
| STD    | standard deviation of the SUM. When you request SUM, the procedure computes STD by default.                                                             |
| STDERR | standard error of the MEAN or RATIO. When you request MEAN or RATIO, the procedure computes STDERR by default.                                          |
| SUM    | weighted sum, $\sum w_i y_i$ , or estimated population total when the appropriate sampling weights are used                                             |
| SUMWGT | sum of the weights, $\sum w_i$                                                                                                                          |
| T      | $t$ -value and its corresponding $p$ -value with DF degrees of freedom for $H_0 : \theta = 0$ , where $\theta$ is a requested statistic                 |
| UCLM   | 100(1 – $\alpha$ )% one-sided upper confidence limit for the MEAN, where $\alpha$ is determined by the ALPHA= option; the default is $\alpha = 0.05$    |
| UCLSUM | 100(1 – $\alpha$ )% one-sided upper confidence limit for the SUM, where $\alpha$ is determined by the ALPHA= option; the default is $\alpha = 0.05$     |
| UGMCLM | 100(1 – $\alpha$ )% one-sided upper confidence limit for the GEOMEAN, where $\alpha$ is determined by the ALPHA= option; the default is $\alpha = 0.05$ |
| VAR    | variance of the MEAN or RATIO                                                                                                                           |
| VARSUM | variance of the SUM                                                                                                                                     |

See the section “Statistical Computations” on page 7807 for details about how PROC SURVEYMEANS computes these statistics.

**VARMETHOD=BRR** <(method-options)>

**VARMETHOD=JACKKNIFE** | **JK** <(method-options)>

**VARMETHOD=TAYLOR**

specifies the variance estimation method. VARMETHOD=TAYLOR requests the Taylor series method, which is the default if you do not specify the VARMETHOD= option or the REPWEIGHTS statement. VARMETHOD=BRR requests variance estimation by balanced repeated replication (BRR), and VARMETHOD=JACKKNIFE requests variance estimation by the delete-1 jackknife method.

For VARMETHOD=BRR and VARMETHOD=JACKKNIFE you can specify *method-options* in parentheses. Table 92.3 summarizes the available *method-options*.

**Table 92.3** Variance Estimation Options

| <b>VARMETHOD=</b> | <b>Variance Estimation Method</b> | <i>Method-Options</i>                                                                              |
|-------------------|-----------------------------------|----------------------------------------------------------------------------------------------------|
| BRR               | Balanced repeated replication     | DFADJ<br>FAY <=value><br>HADAMARD=SAS-data-set<br>OUTWEIGHTS=SAS-data-set<br>PRINTH<br>REPS=number |
| JACKKNIFE         | Jackknife                         | DFADJ<br>OUTJKCOEFS=SAS-data-set<br>OUTWEIGHTS=SAS-data-set                                        |
| TAYLOR            | Taylor series linearization       | None                                                                                               |

*Method-options* must be enclosed in parentheses following the method keyword. For example:

```
varmethod=BRR (reps=60 outweights=myReplicateWeights)
```

The following values are available for the VARMETHOD= option:

#### **BRR** <(method-options)>

requests **balanced repeated replication** (BRR) variance estimation. The BRR method requires a stratified sample design with two primary sampling units (PSUs) per stratum. See the section “**Balanced Repeated Replication (BRR) Method**” on page 7824 for more information.

You can specify the following *method-options* in parentheses following VARMETHOD=BRR:

#### **DFADJ**

computes the degrees of freedom as the number of nonmissing strata for an analysis variable. The degrees of freedom for VARMETHOD=BRR equal the number of strata, which by default is based on all valid observations in the data set. But if you specify the *DFADJ method-option*, PROC SURVEYMEANS does not count any empty strata that are due to all observations containing missing values for an analysis variable.

See the section “**Degrees of Freedom**” on page 7810 for more information. See the section “**Data and Sample Design Summary**” on page 7832 for details about valid observations.

The *DFADJ method-option* has no effect on categorical variables when you specify the **MISSING** option, which treats missing values as a valid nonmissing level.

The *DFADJ method-option* cannot be used when you provide replicate weights with a **REPWEIGHTS** statement. When you use a **REPWEIGHTS** statement, the degrees of freedom equal the number of **REPWEIGHTS** variables (or replicates), unless you specify an alternative value in the **DF=** option in the **REPWEIGHTS** statement.

#### **FAY** <=value>

requests **Fay’s method**, a modification of the **BRR** method, for variance estimation. See the section “**Fay’s BRR Method**” on page 7825 for more information.

You can specify the *value* of the Fay coefficient, which is used in converting the original sampling weights to replicate weights. The Fay coefficient must be a nonnegative number less than 1. By default, the value of the Fay coefficient equals 0.5.

#### **HADAMARD**=SAS-data-set

#### **H**=SAS-data-set

names a SAS data set that contains the **Hadamard matrix** for BRR replicate construction. If you do not provide a Hadamard matrix with the

HADAMARD= *method-option*, PROC SURVEYMEANS generates an appropriate Hadamard matrix for replicate construction. See the sections “Balanced Repeated Replication (BRR) Method” on page 7824 and “Hadamard Matrix” on page 7827 for details.

If a Hadamard matrix of a given dimension exists, it is not necessarily unique. Therefore, if you want to use a specific Hadamard matrix, you must provide the matrix as a SAS data set in the HADAMARD= *method-option*.

In the HADAMARD= input data set, each variable corresponds to a column of the Hadamard matrix, and each observation corresponds to a row of the matrix. You can use any variable names in the HADAMARD= data set. All values in the data set must equal either 1 or -1. You must ensure that the matrix you provide is indeed a Hadamard matrix—that is,  $\mathbf{A}'\mathbf{A} = R\mathbf{I}$ , where  $\mathbf{A}$  is the Hadamard matrix of dimension  $R$  and  $\mathbf{I}$  is an identity matrix. PROC SURVEYMEANS does not check the validity of the Hadamard matrix that you provide.

The HADAMARD= input data set must contain at least  $H$  variables, where  $H$  denotes the number of first-stage strata in your design. If the data set contains more than  $H$  variables, the procedure uses only the first  $H$  variables. Similarly, the HADAMARD= input data set must contain at least  $H$  observations.

If you do not specify the REPS= *method-option*, then the number of replicates is taken to be the number of observations in the HADAMARD= input data set. If you specify the number of replicates—for example, REPS= $nreps$ —then the first  $nreps$  observations in the HADAMARD= data set are used to construct the replicates.

You can specify the PRINTH option to display the Hadamard matrix that the procedure uses to construct replicates for BRR.

#### **OUTWEIGHTS=SAS-data-set**

names a SAS data set that contains replicate weights. See the section “Balanced Repeated Replication (BRR) Method” on page 7824 for information about replicate weights. See the section “Replicate Weights Output Data Set” on page 7829 for more details about the contents of the OUTWEIGHTS= data set.

The OUTWEIGHTS= *method-option* is not available when you provide replicate weights with the REPWEIGHTS statement.

#### **PRINTH**

displays the Hadamard matrix.

When you provide your own Hadamard matrix with the HADAMARD= *method-option*, only the rows and columns of the Hadamard matrix that are used by the procedure are displayed. See the sections “Balanced Repeated Replication (BRR) Method” on page 7824 and “Hadamard Matrix” on page 7827 for details.

The PRINTH *method-option* is not available when you provide replicate weights with the REPWEIGHTS statement because the procedure does not use a Hadamard matrix in this case.

**REPS=*number***

specifies the number of replicates for BRR variance estimation. The value of *number* must be an integer greater than 1.

If you do not provide a Hadamard matrix with the HADAMARD= *method-option*, the number of replicates should be greater than the number of strata and should be a multiple of 4. See the section “Balanced Repeated Replication (BRR) Method” on page 7824 for more information. If a Hadamard matrix cannot be constructed for the REPS= value that you specify, the value is increased until a Hadamard matrix of that dimension can be constructed. Therefore, it is possible for the actual number of replicates used to be larger than the REPS= value that you specify.

If you provide a Hadamard matrix with the HADAMARD= *method-option*, the value of REPS= must not be less than the number of rows in the Hadamard matrix. If you provide a Hadamard matrix and do not specify the REPS= *method-option*, the number of replicates equals the number of rows in the Hadamard matrix.

If you do not specify the REPS= or HADAMARD= *method-option* and do not include a REPWEIGHTS statement, the number of replicates equals the smallest multiple of 4 that is greater than the number of strata.

If you provide replicate weights with the REPWEIGHTS statement, the procedure does not use the REPS= *method-option*. With a REPWEIGHTS statement, the number of replicates equals the number of REPWEIGHTS variables.

**JACKKNIFE | JK <(method-options)>**

requests variance estimation by the delete-1 jackknife method. See the section “Jackknife Method” on page 7826 for details. If you provide replicate weights with a REPWEIGHTS statement, VARMETHOD=JACKKNIFE is the default variance estimation method.

You can specify the following *method-options* in parentheses following VARMETHOD=JACKKNIFE:

**DFADJ**

computes the degrees of freedom as the number of nonmissing strata for an analysis variable. The degrees of freedom for VARMETHOD=JACKKNIFE equal the number of clusters (or number of observations if there is no clusters) minus the number of strata (or one if there is no strata). By default, the number of strata is based on all valid observations in the data set. But if you specify the DFADJ *method-option*, PROC SURVEYMEANS does not count any empty strata that are due to all observations containing missing values for an analysis variable.

See the section “Degrees of Freedom” on page 7810 for more information. See the section “Data and Sample Design Summary” on page 7832 for details about valid observations.

The DFADJ *method-option* has no effect on categorical variables when you specify the MISSING option, which treats missing values as a valid nonmissing level.

The DFADJ *method-option* cannot be used when you provide replicate weights with a REPWEIGHTS statement. When you use a REPWEIGHTS statement, the degrees of freedom equal the number of REPWEIGHTS variables (or replicates), unless you specify an alternative value in the DF= option in the REPWEIGHTS statement.

**OUTJKCOEFS=SAS-data-set**

names a SAS data set that contains jackknife coefficients. See the section “Jackknife Method” on page 7826 for information about jackknife coefficients. See the section “Jackknife Coefficients Output Data Set” on page 7830 for more details about the contents of the OUTJKCOEFS= data set.

**OUTWEIGHTS=SAS-data-set**

names a SAS data set that contains replicate weights. See the section “Jackknife Method” on page 7826 for information about replicate weights. See the section “Replicate Weights Output Data Set” on page 7829 for more details about the contents of the OUTWEIGHTS= data set.

The OUTWEIGHTS= *method-option* is not available when you provide replicate weights with the REPWEIGHTS statement.

**TAYLOR**

requests Taylor series variance estimation. This is the default method if you do not specify the VARMETHOD= option or a REPWEIGHTS statement. See the section “Taylor Series Method” on page 7809 for more information.

---

## BY Statement

**BY variables ;**

You can specify a BY statement with PROC SURVEYMEANS to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the SURVEYMEANS procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.

- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

Note that using a BY statement provides completely separate analyses of the BY groups. It does not provide a statistically valid domain (subpopulation) analysis, where the total number of units in the subpopulation is not known with certainty. You should use the DOMAIN statement to obtain domain analysis. For more information about subpopulation analysis for sample survey data, see Cochran (1977).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

## CLASS Statement

**CLASS** *variables* ;

The CLASS statement names variables to be analyzed as categorical variables. For categorical variables, PROC SURVEYMEANS estimates the proportion in each category or level, instead of the overall mean. PROC SURVEYMEANS always analyzes character variables as categorical. If you want categorical analysis for a numeric variable, you must include that variable in the CLASS statement.

The CLASS *variables* are one or more variables in the DATA= input data set. These variables can be either character or numeric. The formatted values of the CLASS variables determine the categorical variable levels. Thus, you can use formats to group values into levels. See the FORMAT procedure in the *Base SAS Procedures Guide* and the FORMAT statement and SAS formats in *SAS Formats and Informats: Reference* for more information.

When determining levels of a CLASS variable, an observation with missing values for this CLASS variable is excluded, unless you specify the MISSING option. For more information, see the section “Missing Values” on page 7804.

You can use multiple CLASS statements to specify categorical variables.

When you specify classification variables, you can use the SAS system option SUMSIZE= to limit (or to specify) the amount of memory that is available for data analysis. See the chapter on SAS system options in *SAS System Options: Reference* for a description of the SUMSIZE= option.

## CLUSTER Statement

**CLUSTER** *variables* ;

The CLUSTER statement names variables that identify the clusters in a clustered sample design. The combinations of categories of CLUSTER variables define the clusters in the sample. If there is a STRATA statement, clusters are nested within strata.

If you provide replicate weights for BRR or jackknife variance estimation with the REPWEIGHTS statement, you do not need to specify a CLUSTER statement.

If your sample design has clustering at multiple stages, you should identify only the first-stage clusters (primary sampling units (PSUs)), in the CLUSTER statement. See the section “Primary Sampling Units (PSUs)” on page 7806 for more information.



The CLUSTER *variables* are one or more variables in the DATA= input data set. These variables can be either character or numeric. The formatted values of the CLUSTER variables determine the CLUSTER variable levels. Thus, you can use formats to group values into levels. See the FORMAT procedure in the *Base SAS Procedures Guide* and the FORMAT statement and SAS formats in *SAS Formats and Informats: Reference* for more information.

When determining levels of a CLUSTER variable, an observation with missing values for this CLUSTER variable is excluded, unless you specify the MISSING option. For more information, see the section “Missing Values” on page 7804.

You can use multiple CLUSTER statements to specify cluster variables. The procedure uses variables from all CLUSTER statements to create clusters.

---

## DOMAIN Statement

**DOMAIN** *variables* < *variable\*variable variable\*variable\*variable . . .* > < / *option* > ;

The DOMAIN statement requests analysis for domains (subpopulations) in addition to analysis for the entire study population. The DOMAIN statement names the variables that identify domains, which are called domain variables.

It is common practice to compute statistics for domains. The formation of these domains might be unrelated to the sample design. Therefore, the sample sizes for the domains are random variables. Use a DOMAIN statement to incorporate this variability into the variance estimation.

Note that a DOMAIN statement is different from a BY statement. In a BY statement, you treat the sample sizes as fixed in each subpopulation, and you perform analysis within each BY group independently. See the section “Domain Analysis” on page 7806 for more details.

Use the DOMAIN statement on the entire data set to perform a domain analysis. Creating a new data set from a single domain and analyzing that with PROC SURVEYMEANS yields inappropriate estimates of variance.

A domain variable can be either character or numeric. The procedure treats domain variables as categorical variables. If a variable appears by itself in a DOMAIN statement, each level of this variable determines a domain in the study population. If two or more variables are joined by asterisks (\*), then every possible combination of levels of these variables determines a domain. The procedure performs a descriptive analysis within each domain that is defined by the domain variables.

When determining levels of a DOMAIN variable, an observation with missing values for this DOMAIN variable is excluded, unless you specify the MISSING option. For more information, see the section “Missing Values” on page 7804.

The formatted values of the domain variables determine the categorical variable levels. Thus, you can use formats to group values into levels. See the FORMAT procedure in the *Base SAS Procedures Guide* and the FORMAT statement and SAS formats in *SAS Formats and Informats: Reference* for more information.



You can specify the following option in the DOMAIN statement after a slash (/):

### DFADJ

computes the degrees of freedom by using the number of non-empty strata for an analysis variable in a domain.

In a domain analysis, it is possible that some strata contain no sampling units for a specific domain. Or some strata in the domain might be empty due to missing values. By default, the procedure counts these empty strata when computing the degrees of freedom.

However, if you specify the DFADJ option, the procedure excludes any empty strata when computing the degrees of freedom. Prior to SAS 9.2, the procedure excluded empty strata by default.

See the section “Degrees of Freedom” on page 7810 for more information. See the section “Data and Sample Design Summary” on page 7832 for details about valid observations.

The DFADJ option has no effect on categorical variables when you specify the MISSING option, which treats missing values as a valid nonmissing level.

## POSTSTRATA Statement

**POSTSTRATA** *variables* / **PSTOTAL=** *< option >* ;

**POSTSTRATA** *variables* / **PSPCT=** *< option >* ;

The POSTSTRATA statement names variables that form the poststrata to adjust the sampling weight for analyzing the survey. The combinations of categories of POSTSTRATA variables define the poststrata in the sample.

The POSTSTRATA *variables* are one or more variables in the DATA= input data set. These variables can be either character or numeric. The formatted values of the POSTSTRATA *variables* determine the categorical levels. Thus, you can use formats to group values into levels. See the FORMAT procedure in the *Base SAS Procedures Guide* and the FORMAT statement and SAS formats in *SAS Formats and Informats: Reference* for more information.

You must specify either poststratification totals or poststratification proportions, but not both, in the POSTSTRATA statement after a slash (/).

**PSTOTAL=***SAS-data-set* | *values*

**POSTTOTAL=***SAS-data-set* | *values*

**PSCONTROL=***SAS-data-set* | *values*

specifies an input data set that contains the poststratum totals or specifies the population poststratum totals as positive *values*. The SURVEYMEANS procedure uses this information to compute weight adjustment for poststratification.

You can provide poststratification totals by specifying **PSTOTAL=***SAS-data-set*, which names a SAS data set that contains the poststratification variables and the poststratum totals. This data set is called the *poststratum total data set*.

A poststratum total data set must contain all the poststratification variables that are listed in the POSTSTRATA statement and all the variables listed in the BY statement. If there are formats associated with the POSTSTRATA variables and the BY variables, then the formats in the poststratum

total data set for these variables must be consistent with those in the **DATA=** data set in the PROC SURVEYMEANS statement.

A poststratum total data set must have a variable named **\_PSTOTAL\_** that contains the poststratum totals. The value of **\_PSTOTAL\_** must be positive.

When poststratum levels are easy to identify, their corresponding poststratum totals can be specified as a list of positive numbers.

**ORDER=FORMATTED** is used to order the levels of poststratum levels.

You can separate *values* in the **PSTOTAL=** option with blanks or commas. The number of *values* must equal the number of poststrata in the data. List the *values* in the order of the corresponding poststratum level. The sum of the *values* should equal the total sampling weights.

**PSPCT=SAS-data-set | values**

**POSTPCT=SAS-data-set | values**

specifies an input data set that contains the population poststratum proportions or specifies the population poststratum proportions as positive *values*. The SURVEYMEANS procedure uses this information to compute weight adjustment for poststratification.

You can provide poststratification proportions by specifying **POSTPCT=SAS-data-set**, which names a SAS data set that contains the poststratification variables and the poststratum poststratification. This data set is called the *poststratum proportion data set*.

A poststratum proportion data set must contain all the poststratification variables that are listed in the POSTSTRATA statement and all the variables listed in the BY statement. If there are formats associated with the POSTSTRATA variables and the BY variables, then the formats in the poststratum proportion data set for these variables must be consistent with those in the **DATA=** data set in the PROC SURVEYMEANS statement.

A poststratum proportion data set must have a variable named **\_PSPCT\_** that contains the poststratum proportions. The value of **\_PSPCT\_** must be positive.

You can provide poststratum proportions either as positive decimal numbers between 0 and 1 for all poststrata or as positive percentages that must be less than 100 for all poststrata. If any value of the proportions is greater than 1, the procedure treats all proportions as percentages instead of decimal numbers.

When poststratum levels are easy to identify, their corresponding poststratum proportions can be specified as a list of positive numbers.

**ORDER=FORMATTED** is used to order the levels of poststratum levels.

You can separate *values* in the **POSTPCT=** option with blanks or commas. The number of *values* must equal the number of poststrata in the data. List the *values* in the order of the corresponding poststratum level.

If you provide the proportions as decimal numbers, then the sum of these values over all poststrata must be 1.

If you provide the proportions as percentages, then the sum of these percentages over all poststrata must be 100.

You can also optionally specify the following option to create an output data set to store the poststratification weights.

**OUTPSWGT=SAS-data-set**

**OUT=SAS-data-set**

names a SAS data set to contain poststratification weights. See the section “Poststratification” on page 7820 for information about poststratification weights.

If you also specify an **OUTWEIGHTS=** *method-option* for **VARMETHOD=BRR** or **VARMETHOD=JACKKNIFE** in the **PROC SURVEYMEANS** statement, the **OUTPSWGT=** option is ignored. The poststratification weights for the full sample and the replication weights adjusted for poststratification are stored in the **OUTWEIGHTS=** data set.

See the section “Poststratification Weights Output Data Set” on page 7830 for more information about the contents of the **OUTPSWGT=** data set and the section “Replicate Weights Output Data Set” on page 7829 for more information about the contents of the **OUTWEIGHTS=** data set.

## RATIO Statement

**RATIO** < 'label' > *variables / variables* ;

The **RATIO** statement requests ratio analysis for means or proportions of analysis variables. A ratio statement names the variables whose means are used as numerators or denominators in a ratio. Variables that appear before the slash (/) are called *numerator variables* and are used as numerators. Variables that appear after the slash (/) are called *denominator variables* and are used as denominators. These *variables* can be any number of analysis variables, either continuous or categorical, except those named in the **BY**, **CLUSTER**, **STRATA**, **DOMAIN**, **POSTSTRATA**, **REPWEIGHTS**, and **WEIGHT** statements.

You can optionally specify a label for each **RATIO** statement to identify the ratios in the output. Labels must be enclosed in single quotes.

The computation of ratios depends on whether the numerator and denominator variables are continuous or categorical.

For continuous variables, ratios are calculated from the variable means. For example, for continuous variables X, Y, Z, and T, the following **RATIO** statement requests that the procedure analyze the ratios  $\bar{x}/\bar{z}$ ,  $\bar{x}/\bar{t}$ ,  $\bar{y}/\bar{z}$ , and  $\bar{y}/\bar{t}$ :

```
ratio x y / z t;
```

If a continuous variable appears as both a numerator and a denominator variable, the ratio of this variable to itself is ignored.

For categorical variables, ratios are calculated with the proportions for the categories. For example, if the categorical variable Gender has the values ‘Male’ and ‘Female,’ with the proportions  $p_m = \text{Pr}(\text{Gender}=\text{‘Male’})$  and  $p_f = \text{Pr}(\text{Gender}=\text{‘Female’})$ , and Y is a continuous variable, then the following **RATIO** statement requests that the procedure analyze the ratios  $p_m/p_f$ ,  $p_f/p_m$ ,  $\bar{y}/p_m$ , and  $\bar{y}/p_f$ :

```
ratio Gender y / Gender;
```

If a categorical variable appears as both a numerator and denominator variable, then the ratios of the proportions for all categories are computed, except the ratio of each category to itself.

You can have more than one RATIO statement. Each RATIO statement produces ratios independently by using its own numerator and denominator variables. Each RATIO statement also produces its own ratio analysis table.

Available statistics for a ratio are as follows:

- N, number of observations used to compute the ratio
- NCLU, number of clusters
- SUMWGT, sum of weights
- RATIO, ratio
- STDERR, standard error of ratio
- VAR, variance of ratio
- T, *t*-value of ratio
- PROBT, *p*-value of *t*
- DF, degrees of freedom of *t*
- CLM, two-sided confidence limits for ratio
- UCLM, one-sided upper confidence limit for ratio
- LCLM, one-sided lower confidence limit for ratio

The procedure calculates these statistics based on the *statistic-keywords* that you specify in the PROC SURVEYMEANS statement. If a *statistic-keyword* is not appropriate for a RATIO statement, that *statistic-keyword* is ignored for the ratios. If no valid statistics are requested for a RATIO statement, the procedure computes the ratio and its standard error by default.

When the means or proportions for the numerator and denominator variables in a ratio are calculated, an observation is excluded if it has a missing value for a continuous numerator or denominator variable. The procedure also excludes an observation with a missing value for a categorical numerator or denominator variable unless you specify the **MISSING** option.

When the denominator for a ratio is zero, then the value of the ratio is displayed as ‘-Infy’, ‘Infy’, or a missing value, depending on whether the numerator is negative, positive, or zero, respectively, and the corresponding internal value is the special missing value ‘.M’, the special missing value ‘.I’, or the usual missing value, respectively.

---

## REPWEIGHTS Statement

**REPWEIGHTS** *variables* </ options > ;

The REPWEIGHTS statement names variables that provide replicate weights for BRR or jackknife variance estimation, which you request with the **VARMETHOD=BRR** or **VARMETHOD=JACKKNIFE** option in the PROC SURVEYMEANS statement. If you do not provide replicate weights for these methods by using a

REPWEIGHTS statement, then the procedure constructs replicate weights for the analysis. See the sections “Balanced Repeated Replication (BRR) Method” on page 7824 and “Jackknife Method” on page 7826 for information about replicate weights.

Each REPWEIGHTS variable should contain the weights for a single replicate, and the number of replicates equals the number of REPWEIGHTS variables. The REPWEIGHTS variables must be numeric, and the variable values must be nonnegative numbers.

If you provide replicate weights with a REPWEIGHTS statement, you do not need to specify a CLUSTER or STRATA statement. If you use a REPWEIGHTS statement and do not specify the VARMETHOD= option in the PROC SURVEYMEANS statement, the procedure uses VARMETHOD=JACKKNIFE by default.

If you specify a REPWEIGHTS statement but do not include a WEIGHT statement, the procedure uses the average of replicate weights of each observation as the observation’s weight.

You can specify the following options in the REPWEIGHTS statement after a slash (/):

**DF=*df***

specifies the degrees of freedom for the analysis. The value of *df* must be a positive number. By default, the degrees of freedom equals the number of REPWEIGHTS variables.

**JKCOEFS=*value***

specifies a jackknife coefficient for VARMETHOD=JACKKNIFE. The coefficient *value* must be a nonnegative number. See the section “Jackknife Method” on page 7826 for details about jackknife coefficients.

You can use this option to specify a single value of the jackknife coefficient, which the procedure uses for all replicates. To specify different coefficients for different replicates, use the JKCOEFS=*values* or JKCOEFS=*SAS-data-set* option.

**JKCOEFS=*values***

specifies jackknife coefficients for VARMETHOD=JACKKNIFE, where each coefficient corresponds to an individual replicate that is identified by a REPWEIGHTS variable. You can separate *values* with blanks or commas. The coefficient *values* must be nonnegative numbers. The number of *values* must equal the number of replicate weight variables named in the REPWEIGHTS statement. List these values in the same order in which you list the corresponding replicate weight variables in the REPWEIGHTS statement.

See the section “Jackknife Method” on page 7826 for details about jackknife coefficients.

To specify different coefficients for different replicates, you can also use the JKCOEFS=*SAS-data-set* option. To specify a single jackknife coefficient for all replicates, use the JKCOEFS=*value* option.

**JKCOEFS=*SAS-data-set***

names a SAS data set that contains the jackknife coefficients for VARMETHOD=JACKKNIFE. You provide the jackknife coefficients in the JKCOEFS= data set variable JKCoefficient. Each coefficient value must be a nonnegative number. The observations in the JKCOEFS= data set should correspond to the replicates that are identified by the REPWEIGHTS variables. Arrange the coefficients or observations in the JKCOEFS= data set in the same order in which you list the corresponding replicate weight variables in the REPWEIGHTS statement. The number of observations in the JKCOEFS= data set must not be less than the number of REPWEIGHTS variables.

See the section “Jackknife Method” on page 7826 for details about jackknife coefficients.

To specify different coefficients for different replicates, you can also use the `JKCOEFS=values` option. To specify a single jackknife coefficient for all replicates, use the `JKCOEFS=value` option.

---

## STRATA Statement

**STRATA** *variables* </ option > ;

The STRATA statement specifies variables that form the strata in a stratified sample design. The combinations of categories of STRATA variables define the strata in the sample.

If your sample design has stratification at multiple stages, you should identify only the first-stage strata in the STRATA statement. See the section “Specification of Population Totals and Sampling Rates” on page 7805 for more information.

If you provide replicate weights for BRR or jackknife variance estimation with the `REPWEIGHTS` statement, you do not need to specify a STRATA statement.

The STRATA *variables* are one or more variables in the DATA= input data set. These variables can be either character or numeric. The formatted values of the STRATA variables determine the levels. Thus, you can use formats to group values into levels. See the `FORMAT` procedure in the *Base SAS Procedures Guide* and the `FORMAT` statement and SAS formats in *SAS Formats and Informats: Reference* for more information.

When determining levels of a STRATA variable, an observation with missing values for this STRATA variable is excluded, unless you specify the `MISSING` option. For more information, see the section “Missing Values” on page 7804.

You can use multiple STRATA statements to specify stratum variables.

You can specify the following option in the STRATA statement after a slash (/):

### LIST

displays a “Stratum Information” table, which includes values of the STRATA variables and the number of observations, number of clusters, population total, and sampling rate for each stratum. See the section “Stratum Information” on page 7833 for more details.

---

## VAR Statement

**VAR** *variables* ;

The VAR statement names the variables to be analyzed.

A *variable* in the VAR statement should not appear in any of the `BY`, `CLUSTER`, `DOMAIN`, `POSTSTRATA`, `REPWEIGHTS`, `STRATA`, and `WEIGHT` statements.

If you want a categorical analysis for a numeric variable, you must also name that variable in the `CLASS` statement. For categorical variables, PROC SURVEYMEANS estimates the proportion in each category or level, instead of the overall mean. Character variables are always analyzed as categorical variables. See the section “CLASS Statement” on page 7796 for more information.

When you specify a variable in a `RATIO` statement but not in a VAR statement, PROC SURVEYMEANS includes this variable as an analysis variable.

If you do not specify a VAR statement, then PROC SURVEYMEANS analyzes all variables in the DATA= input data set, except those named in the BY, CLUSTER, DOMAIN, POSTSTRATA, REPWEIGHTS, STRATA, and WEIGHT statements.

---

## WEIGHT Statement

**WEIGHT** *variable* ;

The WEIGHT statement names the variable that contains the sampling weights. This variable must be numeric, and the sampling weights must be positive numbers. If an observation has a weight that is nonpositive or missing, then the procedure omits that observation from the analysis. See the section “Missing Values” on page 7804 for more information. If you specify more than one WEIGHT statement, the procedure uses only the first WEIGHT statement and ignores the rest.

If you do not specify a WEIGHT statement but provide replicate weights with a REPWEIGHTS statement, PROC SURVEYMEANS uses the average of replicate weights of each observation as the observation’s weight.

If you do not specify a WEIGHT statement or a REPWEIGHTS statement, PROC SURVEYMEANS assigns all observations a weight of one.

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## Details: SURVEYMEANS Procedure

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### Missing Values

If you have missing values in your survey data for any reason, such as nonresponse, this can compromise the quality of your survey results. If the respondents are different from the nonrespondents with regard to a survey effect or outcome, then survey estimates might be biased and cannot accurately represent the survey population. There are a variety of techniques in sample design and survey operations that can reduce nonresponse. After data collection is complete, you can use imputation to replace missing values with acceptable values, and/or you can use sampling weight adjustments to compensate for nonresponse. You should complete this data preparation and adjustment before you analyze your data with PROC SURVEYMEANS. For more information, see Cochran (1977); Kalton and Kaspyzyk (1986); Brick and Kalton (1996).

If an observation has a missing value or a nonpositive value for the WEIGHT variable, then that observation is excluded from the analysis.

An observation is also excluded from the analysis if it has a missing value for any design (STRATA, CLUSTER, DOMAIN, or POSTSTRATA) variable, unless you specify the MISSING option in the PROC SURVEYMEANS statement. If you specify the MISSING option, the procedure treats missing values as a valid (nonmissing) category for all categorical variables.

By default, when computing statistics for an analysis variable, PROC SURVEYMEANS omits observations with missing values for that analysis variable. The procedure computes statistics for each variable based only on observations that have nonmissing values for that variable. This treatment is based on the assumption that the missing values are missing completely at random (MCAR). However, this assumption is sometimes



not true. For example, evidence from other surveys might suggest that observations with missing values are systematically different from observations without missing values. If you believe that missing values are not missing completely at random, then you can specify the **NOMCAR** option to let variance estimation include these observations with missing values in the analysis variables.

Whether or not you specify the **NOMCAR** option, the procedure always excludes observations with missing or invalid values for the **WEIGHT**, **STRATA**, **CLUSTER**, and **DOMAIN** variables, unless you specify the **MISSING** option.

When you specify the **NOMCAR** option, the procedure treats observations with and without missing values for analysis variables as two different domains, and it performs a domain analysis in the domain of nonmissing observations.

The procedure performs univariate analysis and analyzes each **VAR** variable separately. Thus, the number of missing observations might be different for different variables. You can specify the keyword **NMISS** in the **PROC SURVEYMEANS** statement to display the number of missing values for each analysis variable in the “Statistics” table.

When you specify a **RATIO** statement, the procedure excludes any observation that has a missing value for a continuous numerator or denominator variable. The procedure also excludes an observation with a missing value for a categorical numerator or denominator variable unless you specify the **MISSING** option.

If you use a **REPWEIGHTS** statement, all **REPWEIGHTS** variables must contain nonmissing values.

## Survey Data Analysis

### Specification of Population Totals and Sampling Rates

To include a finite population correction (*fpc*) in Taylor series variance estimation, you can input either the sampling rate or the population total by using the **RATE=** or **TOTAL=** option in the **PROC SURVEYMEANS** statement. (You cannot specify both of these options in the same **PROC SURVEYMEANS** statement.) The **RATE=** and **TOTAL=** options apply only to Taylor series variance estimation. The procedure does not use a finite population correction for **BRR** or jackknife variance estimation.

If you do not specify the **RATE=** or **TOTAL=** option, the Taylor series variance estimation does not include a finite population correction. For fairly small sampling fractions, it is appropriate to ignore this correction. For more information, see Cochran (1977); Kish (1965).

If your design has multiple stages of selection and you are specifying the **RATE=** option, you should input the first-stage sampling rate, which is the ratio of the number of PSUs in the sample to the total number of PSUs in the study population. If you are specifying the **TOTAL=** option for a multistage design, you should input the total number of PSUs in the study population. See the section “**Primary Sampling Units (PSUs)**” on page 7806 for more details.

For a nonstratified sample design, or for a stratified sample design with the same sampling rate or the same population total in all strata, you can use the **RATE=value** or **TOTAL=value** option. If your sample design is stratified with different sampling rates or population totals in different strata, use the **RATE=SAS-data-set** or **TOTAL=SAS-data-set** option to name a SAS data set that contains the stratum sampling rates or totals. This data set is called a *secondary data set*, as opposed to the *primary data set* that you specify with the **DATA=** option.



The secondary data set must contain all the stratification variables listed in the STRATA statement and all the variables in the BY statement. If there are formats associated with the STRATA variables and the BY variables, then the formats must be consistent in the primary and the secondary data sets. If you specify the TOTAL=*SAS-data-set* option, the secondary data set must have a variable named `_TOTAL_` that contains the stratum population totals. Or if you specify the RATE=*SAS-data-set* option, the secondary data set must have a variable named `_RATE_` that contains the stratum sampling rates. If the secondary data set contains more than one observation for any one stratum, then the procedure uses the first value of `_TOTAL_` or `_RATE_` for that stratum and ignores the rest.

The *value* in the RATE= option or the values of `_RATE_` in the secondary data set must be nonnegative numbers. You can specify *value* as a number between 0 and 1. Or you can specify *value* in percentage form as a number between 1 and 100, and PROC SURVEYMEANS converts that number to a proportion. The procedure treats the value 1 as 100% instead of 1%.

If you specify the TOTAL=*value* option, *value* must not be less than the sample size. If you provide stratum population totals in a secondary data set, these values must not be less than the corresponding stratum sample sizes.

### Primary Sampling Units (PSUs)

When you have clusters, or primary sampling units (PSUs), in your sample design, the procedure estimates variance from the variation among PSUs when the Taylor series variance method is used. See the section “Variance and Standard Error of the Mean” on page 7809 and the section “Variance and Standard Deviation of the Total” on page 7812 for more information.

BRR or jackknife variance estimation methods draw multiple replicates (or subsamples) from the full sample by following a specific resampling scheme. These subsamples are constructed by deleting PSUs from the full sample.

If you use a `REPWEIGHTS` statement to provide replicate weights for BRR or jackknife variance estimation, you do not need to specify a `CLUSTER` statement. Otherwise, you should specify a `CLUSTER` statement whenever your design includes clustering at the first stage of sampling. If you do not specify a `CLUSTER` statement, then PROC SURVEYMEANS treats each observation as a PSU.

### Domain Analysis

It is common practice to compute statistics for domains (subpopulations), in addition to computing statistics for the entire study population. Analysis for domains that uses the entire sample is called *domain analysis* (also called subgroup analysis, subpopulation analysis, or subdomain analysis). The formation of these subpopulations of interest might be unrelated to the sample design. Therefore, the sample sizes for the subpopulations might actually be random variables.

Use a `DOMAIN` statement to incorporate this variability into the variance estimation. Note that using a `BY` statement provides completely separate analyses of the BY groups. It does not provide a statistically valid subpopulation or domain analysis, where the total number of units in the subpopulation is not known with certainty.

For more detailed information about domain analysis, see Kish (1965).

## Statistical Computations

The SURVEYMEANS procedure uses the Taylor series (linearization) method or replication (resampling) methods to estimate sampling errors of estimators based on complex sample designs. For more information, see Fuller (2009); Wolter (2007); Lohr (2010); Kalton (1983); Hidiroglou, Fuller, and Hickman (1980); Fuller et al. (1989); Lee, Forthoffer, and Lorimor (1989); Cochran (1977); Kish (1965); Hansen, Hurwitz, and Madow (1953); Rust (1985); Dippo, Fay, and Morganstein (1984); Rao and Shao (1999); Rao, Wu, and Yue (1992); Rao and Shao (1996). You can use the `VARMETHOD=` option to specify a variance estimation method to use. By default, the Taylor series method is used.

The Taylor series method obtains a linear approximation for the estimator and then uses the variance estimate for this approximation to estimate the variance of the estimate itself (Woodruff 1971; Fuller 1975). When there are clusters, or PSUs, in the sample design, the procedure estimates variance from the variation among PSUs. When the design is stratified, the procedure pools stratum variance estimates to compute the overall variance estimate. For  $t$  tests of the estimates, the degrees of freedom equal the number of clusters minus the number of strata in the sample design.

For a multistage sample design, the Taylor series estimation depends only on the first stage of the sample design. Therefore, the required input includes only first-stage cluster (PSU) and first-stage stratum identification. You do not need to input design information about any additional stages of sampling. This variance estimation method assumes that the first-stage sampling fraction is small, or that the first-stage sample is drawn with replacement, as it often is in practice.

Quite often in complex surveys, respondents have unequal weights, which reflect unequal selection probabilities and adjustments for nonresponse. In such surveys, the appropriate sampling weights must be used to obtain valid estimates for the study population.

However, replication methods have recently gained popularity for estimating variances in complex survey data analysis. One reason for this popularity is the relative simplicity of replication-based estimates, especially for nonlinear estimators; another is that modern computational capacity has made replication methods feasible for practical survey analysis.

Replication methods draw multiple replicates (also called subsamples) from a full sample according to a specific resampling scheme. The most commonly used resampling schemes are the *balanced repeated replication* (BRR) method and the *jackknife* method. For each replicate, the original weights are modified for the PSUs in the replicates to create replicate weights. The population parameters of interest are estimated by using the replicate weights for each replicate. Then the variances of parameters of interest are estimated by the variability among the estimates derived from these replicates. You can use a `REPWEIGHTS` statement to provide your own replicate weights for variance estimation. For more information about using replication methods to analyze sample survey data, see the section “Replication Methods for Variance Estimation” on page 7824.

## Definitions and Notation

For a stratified clustered sample design, together with the sampling weights, the sample can be represented by an  $n \times (P + 1)$  matrix

$$\begin{aligned} (\mathbf{w}, \mathbf{Y}) &= (w_{hij}, \mathbf{y}_{hij}) \\ &= (w_{hij}, y_{hij}^{(1)}, y_{hij}^{(2)}, \dots, y_{hij}^{(P)}) \end{aligned}$$

where

- $h = 1, 2, \dots, H$  is the stratum index
- $i = 1, 2, \dots, n_h$  is the cluster index within stratum  $h$
- $j = 1, 2, \dots, m_{hi}$  is the unit index within cluster  $i$  of stratum  $h$
- $p = 1, 2, \dots, P$  is the analysis variable number, with a total of  $P$  variables
- $n = \sum_{h=1}^H \sum_{i=1}^{n_h} m_{hi}$  is the total number of observations in the sample
- $w_{hij}$  denotes the sampling weight for unit  $j$  in cluster  $i$  of stratum  $h$
- $y_{hij} = (y_{hij}^{(1)}, y_{hij}^{(2)}, \dots, y_{hij}^{(P)})$  are the observed values of the analysis variables for unit  $j$  in cluster  $i$  of stratum  $h$ , including both the values of numerical variables and the values of indicator variables for levels of categorical variables.

For a categorical variable  $C$ , let  $l$  denote the number of levels of  $C$ , and denote the level values as  $c_1, c_2, \dots, c_l$ . Let  $y^{(q)}$  ( $q \in \{1, 2, \dots, P\}$ ) be an indicator variable for the category  $C = c_k$  ( $k = 1, 2, \dots, l$ ) with the observed value in unit  $j$  in cluster  $i$  of stratum  $h$ :

$$y_{hij}^{(q)} = I_{\{C=c_k\}}(h, i, j) = \begin{cases} 1 & \text{if } C_{hij} = c_k \\ 0 & \text{otherwise} \end{cases}$$

Note that the indicator variable  $y_{hij}^{(q)}$  is set to missing when  $C_{hij}$  is missing. Therefore, the total number of analysis variables,  $P$ , is the total number of numerical variables plus the total number of levels of all categorical variables.

The sampling rate  $f_h$  for stratum  $h$ , which is used in Taylor series variance estimation, is the fraction of first-stage units (PSUs) selected for the sample. You can use the TOTAL= or RATE= option to input population totals or sampling rates. See the section “[Specification of Population Totals and Sampling Rates](#)” on page 7805 for details. If you input stratum totals, PROC SURVEYMEANS computes  $f_h$  as the ratio of the stratum sample size to the stratum total. If you input stratum sampling rates, PROC SURVEYMEANS uses these values directly for  $f_h$ . If you do not specify the TOTAL= or RATE= option, then the procedure assumes that the stratum sampling rates  $f_h$  are negligible, and a finite population correction is not used when computing variances. Replication methods specified by the [VARMETHOD=BRR](#) or the [VARMETHOD=JACKKNIFE](#) option do not use this finite population correction  $f_h$ .

## Mean

When you specify the keyword MEAN, the procedure computes the estimate of the mean (mean per element) from the survey data. Also, the procedure computes the mean by default if you do not specify any *statistic-keywords* in the PROC SURVEYMEANS statement.

PROC SURVEYMEANS computes the estimate of the mean as

$$\hat{Y} = \left( \sum_{h=1}^H \sum_{i=1}^{n_h} \sum_{j=1}^{m_{hi}} w_{hij} y_{hij} \right) / w_{..}$$

where

$$w_{\dots} = \sum_{h=1}^H \sum_{i=1}^{n_h} \sum_{j=1}^{m_{hi}} w_{hij}$$

is the sum of the weights over all observations in the sample.

## Variance and Standard Error of the Mean

When you specify the keyword `STDERR`, the procedure computes the standard error of the mean. Also, the procedure computes the standard error by default if you specify the keyword `MEAN`, or if you do not specify any *statistic-keywords* in the `PROC SURVEYMEANS` statement. The keyword `VAR` requests the variance of the mean.

### Taylor Series Method

When you use `VARMETHOD=TAYLOR`, or by default if you do not specify the `VARMETHOD=` option, `PROC SURVEYMEANS` uses the Taylor series method to estimate the variance of the mean  $\widehat{Y}$ . The procedure computes the estimated variance as

$$\widehat{V}(\widehat{Y}) = \sum_{h=1}^H \widehat{V}_h(\widehat{Y})$$

where, if  $n_h > 1$ , then

$$\begin{aligned} \widehat{V}_h(\widehat{Y}) &= \frac{n_h(1-f_h)}{n_h-1} \sum_{i=1}^{n_h} (e_{hi\cdot} - \bar{e}_{h\cdot\cdot})^2 \\ e_{hi\cdot} &= \left( \sum_{j=1}^{m_{hi}} w_{hij} (y_{hij} - \widehat{Y}) \right) / w_{\dots} \\ \bar{e}_{h\cdot\cdot} &= \left( \sum_{i=1}^{n_h} e_{hi\cdot} \right) / n_h \end{aligned}$$

and if  $n_h = 1$ , then

$$\widehat{V}_h(\widehat{Y}) = \begin{cases} \text{missing} & \text{if } n_{h'} = 1 \text{ for } h' = 1, 2, \dots, H \\ 0 & \text{if } n_{h'} > 1 \text{ for some } 1 \leq h' \leq H \end{cases}$$

### Replication Methods

When you specify `VARMETHOD=BRR` or `VARMETHOD=JACKKNIFE`, the procedure computes the variance  $\widehat{V}(\widehat{Y})$  with replication methods by using the variability among replicate estimates to estimate the overall variance. See the section “Replication Methods for Variance Estimation” on page 7824 for more details.

**Standard Error**

The standard error of the mean is the square root of the estimated variance.

$$\text{StdErr}(\hat{Y}) = \sqrt{\hat{V}(\hat{Y})}$$

**t Test for the Mean**

If you specify the keyword T, PROC SURVEYMEANS computes the  $t$ -value for testing that the population mean equals zero,  $H_0 : \bar{Y} = 0$ . The test statistic equals

$$t(\hat{Y}) = \hat{Y} / \text{StdErr}(\hat{Y})$$

The two-sided  $p$ -value for this test is

$$\text{Prob}(|T| > |t(\hat{Y})|)$$

where  $T$  is a random variable with the  $t$  distribution with  $df$  degrees of freedom.

**Degrees of Freedom**

PROC SURVEYMEANS computes degrees of freedom  $df$  to obtain the  $100(1 - \alpha)\%$  confidence limits for means, proportions, totals, ratios, and other statistics. The degrees of freedom computation depends on the variance estimation method that you request. Missing values can affect the degrees of freedom computation. See the section “Missing Values” on page 7804 for details.

**Taylor Series Variance Estimation**

For the Taylor series method, PROC SURVEYMEANS calculates the degrees of freedom for the  $t$  test as the number of clusters minus the number of strata. If there are no clusters, then the degrees of freedom equal the number of observations minus the number of strata. If the design is not stratified, then the degrees of freedom equal the number of PSUs minus one.

If all observations in a stratum are excluded from the analysis due to missing values, then that stratum is called an *empty stratum*. Empty strata are not counted in the total number of strata for the table. Similarly, empty clusters and missing observations are not included in the total counts of cluster and observations that are used to compute the degrees of freedom for the analysis.

If you specify the MISSING option, missing values are treated as valid nonmissing levels for a categorical variable and are included in computing degrees of freedom. If you specify the NOMCAR option for Taylor series variance estimation, observations with missing values for an analysis variable are included in computing degrees of freedom.

**Replicate-Based Variance Estimation**

When there is a REPWEIGHTS statement, the degrees of freedom equal the number of REPWEIGHTS variables, unless you specify an alternative in the DF= option in a REPWEIGHTS statement.

For BRR or jackknife variance estimation without a REPWEIGHT statement, by default PROC SURVEYMEANS computes the degrees of freedom by using all valid observations in the input data set. A valid observation is an observation that has a positive value of the WEIGHT variable and nonmissing values of the STRATA and CLUSTER variables unless you specify the MISSING option. See the section “Data and Sample Design Summary” on page 7832 for details about valid observations.

For BRR variance estimation (including [Fay's method](#)) without a REPWEIGHTS statement, PROC SURVEYMEANS calculates the degrees of freedom as the number of strata. PROC SURVEYMEANS bases the number of strata on all valid observations in the data set, unless you specify the *DFADJ method-option* for `VARMETHOD=BRR`. When you specify the DFADJ option, the procedure computes the degrees of freedom as the number of nonmissing strata for an analysis variable. This excludes any empty strata that occur when observations with missing values of that analysis variable are removed.

For jackknife variance estimation without a REPWEIGHTS statement, PROC SURVEYMEANS calculates the degrees of freedom as the number of clusters (or number of observations if there are no clusters) minus the number of strata (or one if there are no strata). For jackknife variance estimation, PROC SURVEYMEANS bases the number of strata and clusters on all valid observations in the data set, unless you specify the *DFADJ method-option* for `VARMETHOD=JACKKNIFE`. When you specify the DFADJ option, the procedure computes the degrees of freedom from the number of nonmissing strata and clusters for an analysis variable. This excludes any empty strata or clusters that occur when observations with missing values of an analysis variable are removed.

The procedure displays the degrees of freedom for the  $t$  test if you specify the keyword DF in the PROC SURVEYMEANS statement.

## Confidence Limits for the Mean

If you specify the keyword CLM, the procedure computes two-sided confidence limits for the mean. Also, the procedure includes the confidence limits by default if you do not specify any *statistic-keywords* in the PROC SURVEYMEANS statement.

The confidence coefficient is determined by the value of the ALPHA= option, which by default equals 0.05 and produces 95% confidence limits. The confidence limits are computed as

$$\hat{Y} \pm \text{StdErr}(\hat{Y}) \cdot t_{df, \alpha/2}$$

where  $\hat{Y}$  is the estimate of the mean,  $\text{StdErr}(\hat{Y})$  is the standard error of the mean, and  $t_{df, \alpha/2}$  is the  $100(1 - \alpha/2)$  percentile of the  $t$  distribution with  $df$  calculated as in the section "[t Test for the Mean](#)" on page 7810.

If you specify the keyword UCLM, the procedure computes the one-sided upper  $100(1 - \alpha)\%$  confidence limit for the mean:

$$\hat{Y} + \text{StdErr}(\hat{Y}) \cdot t_{df, \alpha}$$

If you specify the keyword LCLM, the procedure computes the one-sided lower  $100(1 - \alpha)\%$  confidence limit for the mean:

$$\hat{Y} - \text{StdErr}(\hat{Y}) \cdot t_{df, \alpha}$$

## Coefficient of Variation

If you specify the keyword CV, PROC SURVEYMEANS computes the coefficient of variation, which is the ratio of the standard error of the mean to the estimated mean:

$$cv(\bar{Y}) = \text{StdErr}(\bar{Y}) / \bar{Y}$$

If you specify the keyword CVSUM, PROC SURVEYMEANS computes the coefficient of variation for the estimated total, which is the ratio of the standard deviation of the sum to the estimated total:

$$cv(Y) = \text{Std}(\hat{Y}) / \hat{Y}$$

## Proportions

If you specify the keyword MEAN for a categorical variable, PROC SURVEYMEANS estimates the proportion, or relative frequency, for each level of the categorical variable. If you do not specify any *statistic-keywords* in the PROC SURVEYMEANS statement, the procedure estimates the proportions for levels of the categorical variables, together with their standard errors and confidence limits.

The procedure estimates the proportion in level  $c_k$  for variable  $C$  as

$$\hat{p} = \frac{\sum_{h=1}^H \sum_{i=1}^{n_h} \sum_{j=1}^{m_{hi}} w_{hij} y_{hij}^{(q)}}{\sum_{h=1}^H \sum_{i=1}^{n_h} \sum_{j=1}^{m_{hi}} w_{hij}}$$

where  $y_{hij}^{(q)}$  is the value of the indicator function for level  $C = c_k$ , defined in the section “Definitions and Notation” on page 7807, and  $y_{hij}^{(q)}$  equals 1 if the observed value of variable  $C$  equals  $c_k$ , and  $y_{hij}^{(q)}$  equals 0 otherwise. Since the proportion estimator is actually an estimator of the mean for an indicator variable, the procedure computes its variance and standard error according to the method outlined in the section “Variance and Standard Error of the Mean” on page 7809. Similarly, the procedure computes confidence limits for proportions as in the section “Confidence Limits for the Mean” on page 7811.

## Total

If you specify the keyword SUM, the procedure computes the estimate of the population total from the survey data. The estimate of the total is the weighted sum over the sample:

$$\hat{Y} = \sum_{h=1}^H \sum_{i=1}^{n_h} \sum_{j=1}^{m_{hi}} w_{hij} y_{hij}$$

For a categorical variable level,  $\hat{Y}$  estimates its total frequency in the population.

## Variance and Standard Deviation of the Total

When you specify the keyword STD or the keyword SUM, the procedure estimates the standard deviation of the total. The keyword VARSUM requests the variance of the total.

### Taylor Series Method

When you use `VARMETHOD=TAYLOR`, or by default, PROC SURVEYMEANS uses the Taylor series method to estimate the variance of the total as

$$\hat{V}(\hat{Y}) = \sum_{h=1}^H \hat{V}_h(\hat{Y})$$

where, if  $n_h > 1$ , then

$$\widehat{V}_h(\widehat{Y}) = \frac{n_h(1 - f_h)}{n_h - 1} \sum_{i=1}^{n_h} (y_{hi\cdot} - \bar{y}_{h\cdot\cdot})^2$$

$$y_{hi\cdot} = \sum_{j=1}^{m_{hi}} w_{hij} y_{hij}$$

$$\bar{y}_{h\cdot\cdot} = \left( \sum_{i=1}^{n_h} y_{hi\cdot} \right) / n_h$$

and if  $n_h = 1$ , then

$$\widehat{V}_h(\widehat{Y}) = \begin{cases} \text{missing} & \text{if } n_{h'} = 1 \text{ for } h' = 1, 2, \dots, H \\ 0 & \text{if } n_{h'} > 1 \text{ for some } 1 \leq h' \leq H \end{cases}$$

### Replication Methods

When you specify `VARMETHOD=BRR` or `VARMETHOD=JACKKNIFE` option, the procedure computes the variance  $\widehat{V}(\widehat{Y})$  with replication methods by measuring the variability among the estimates derived from these replicates. See the section “Replication Methods for Variance Estimation” on page 7824 for more details.

### Standard Deviation

The standard deviation of the total equals

$$\text{Std}(\widehat{Y}) = \sqrt{\widehat{V}(\widehat{Y})}$$

### Confidence Limits for the Total

If you specify the keyword `CLSUM`, the procedure computes confidence limits for the total. The confidence coefficient is determined by the value of the `ALPHA=` option, which by default equals 0.05 and produces 95% confidence limits. The confidence limits are computed as

$$\widehat{Y} \pm \text{Std}(\widehat{Y}) \cdot t_{df, \alpha/2}$$

where  $\widehat{Y}$  is the estimate of the total,  $\text{Std}(\widehat{Y})$  is the estimated standard deviation, and  $t_{df, \alpha/2}$  is the  $100(1 - \alpha/2)$  percentile of the  $t$  distribution with  $df$  calculated as described in the section “*t* Test for the Mean” on page 7810.

If you specify the keyword `UCLSUM`, the procedure computes the one-sided upper  $100(1 - \alpha)\%$  confidence limit for the sum:

$$\widehat{Y} + \text{Std}(\widehat{Y}) \cdot t_{df, \alpha}$$

If you specify the keyword `LCLSUM`, the procedure computes the one-sided lower  $100(1 - \alpha)\%$  confidence limit for the sum:

$$\widehat{Y} - \text{Std}(\widehat{Y}) \cdot t_{df, \alpha}$$



## Ratio

When you use a **RATIO** statement, the procedure produces statistics requested by the *statistic-keywords* in the PROC SURVEYMEANS statement.

Suppose that you want to calculate the ratio of variable  $Y$  to variable  $X$ . Let  $x_{hij}$  be the value of variable  $X$  for the  $j$ th member in cluster  $i$  in the  $h$ th stratum.

The ratio of  $Y$  to  $X$  is

$$\widehat{R} = \frac{\sum_{h=1}^H \sum_{i=1}^{n_h} \sum_{j=1}^{m_{hi}} w_{hij} y_{hij}}{\sum_{h=1}^H \sum_{i=1}^{n_h} \sum_{j=1}^{m_{hi}} w_{hij} x_{hij}}$$

PROC SURVEYMEANS uses the Taylor series method to estimate the variance of the ratio  $\widehat{R}$  as

$$\widehat{V}(\widehat{R}) = \sum_{h=1}^H \widehat{V}_h(\widehat{R})$$

where, if  $n_h > 1$ , then

$$\begin{aligned} \widehat{V}_h(\widehat{R}) &= \frac{n_h(1-f_h)}{n_h-1} \sum_{i=1}^{n_h} (g_{hi\cdot} - \bar{g}_{h\cdot\cdot})^2 \\ g_{hi\cdot} &= \frac{\sum_{j=1}^{m_{hi}} w_{hij} (y_{hij} - x_{hij} \widehat{R})}{\sum_{h=1}^H \sum_{i=1}^{n_h} \sum_{j=1}^{m_{hi}} w_{hij} x_{hij}} \\ \bar{g}_{h\cdot\cdot} &= \left( \sum_{i=1}^{n_h} g_{hi\cdot} \right) / n_h \end{aligned}$$

and if  $n_h = 1$ , then

$$\widehat{V}_h(\widehat{R}) = \begin{cases} \text{missing} & \text{if } n_{h'} = 1 \text{ for } h' = 1, 2, \dots, H \\ 0 & \text{if } n_{h'} > 1 \text{ for some } 1 \leq h' \leq H \end{cases}$$

The standard error of the ratio is the square root of the estimated variance:

$$\text{StdErr}(\widehat{R}) = \sqrt{\widehat{V}(\widehat{R})}$$

When the denominator for a ratio is zero, then the value of the ratio is displayed as ‘-Infy’, ‘Infy’, or a missing value, depending on whether the numerator is negative, positive, or zero, respectively; and the corresponding internal value is the special missing value ‘.M’, the special missing value ‘.I’, or the usual missing value, respectively.

## Domain Statistics

When you use a **DOMAIN** statement to request a domain analysis, the procedure computes the requested statistics for each domain.

For a domain  $D$ , let  $I_D$  be the corresponding indicator variable:

$$I_D(h, i, j) = \begin{cases} 1 & \text{if observation } (h, i, j) \text{ belongs to } D \\ 0 & \text{otherwise} \end{cases}$$

Let

$$v_{hij} = w_{hij} I_D(h, i, j) = \begin{cases} w_{hij} & \text{if observation } (h, i, j) \text{ belongs to } D \\ 0 & \text{otherwise} \end{cases}$$

The requested statistics for variable  $y$  in domain  $D$  are computed by using the new weights  $v$ .

**Domain Mean**

The estimated mean of  $y$  in the domain  $D$  is

$$\widehat{Y}_D = \left( \sum_{h=1}^H \sum_{i=1}^{n_h} \sum_{j=1}^{m_{hi}} v_{hij} y_{hij} \right) / v_{\dots}$$

where

$$v_{\dots} = \sum_{h=1}^H \sum_{i=1}^{n_h} \sum_{j=1}^{m_{hi}} v_{hij}$$

The variance of  $\widehat{Y}_D$  is estimated by

$$\widehat{V}(\widehat{Y}_D) = \sum_{h=1}^H \widehat{V}_h(\widehat{Y}_D)$$

where, if  $n_h > 1$ , then

$$\begin{aligned} \widehat{V}_h(\widehat{Y}_D) &= \frac{n_h(1 - f_h)}{n_h - 1} \sum_{i=1}^{n_h} (r_{hi\cdot} - \bar{r}_{h\cdot\cdot})^2 \\ r_{hi\cdot} &= \left( \sum_{j=1}^{m_{hi}} v_{hij} (y_{hij} - \widehat{Y}_D) \right) / v_{\dots} \\ \bar{r}_{h\cdot\cdot} &= \left( \sum_{i=1}^{n_h} r_{hi\cdot} \right) / n_h \end{aligned}$$

and if  $n_h = 1$ , then

$$\widehat{V}_h(\widehat{Y}_D) = \begin{cases} \text{missing} & \text{if } n_{h'} = 1 \text{ for } h' = 1, 2, \dots, H \\ 0 & \text{if } n_{h'} > 1 \text{ for some } 1 \leq h' \leq H \end{cases}$$

**Domain Total**

The estimated total in domain  $D$  is

$$\widehat{Y}_D = \sum_{h=1}^H \sum_{i=1}^{n_h} \sum_{j=1}^{m_{hi}} v_{hij} y_{hij}$$

and its estimated variance is

$$\widehat{V}(\widehat{Y}_D) = \sum_{h=1}^H \widehat{V}_h(\widehat{Y}_D)$$

where, if  $n_h > 1$ , then

$$\begin{aligned} \widehat{V}_h(\widehat{Y}_D) &= \frac{n_h(1-f_h)}{n_h-1} \sum_{i=1}^{n_h} (z_{hi\cdot} - \bar{z}_{h\cdot\cdot})^2 \\ z_{hi\cdot} &= \sum_{j=1}^{m_{hi}} v_{hij} z_{hij} \\ \bar{z}_{h\cdot\cdot} &= \left( \sum_{i=1}^{n_h} z_{hi\cdot} \right) / n_h \end{aligned}$$

and if  $n_h = 1$ , then

$$\widehat{V}_h(\widehat{Y}_D) = \begin{cases} \text{missing} & \text{if } n_{h'} = 1 \text{ for } h' = 1, 2, \dots, H \\ 0 & \text{if } n_{h'} > 1 \text{ for some } 1 \leq h' \leq H \end{cases}$$

**Domain Ratio**

The estimated ratio of  $Y$  to  $X$  in domain  $D$  is

$$\widehat{R}_D = \frac{\sum_{h=1}^H \sum_{i=1}^{n_h} \sum_{j=1}^{m_{hi}} v_{hij} y_{hij}}{\sum_{h=1}^H \sum_{i=1}^{n_h} \sum_{j=1}^{m_{hi}} v_{hij} x_{hij}}$$

and its estimated variance is

$$\widehat{V}(\widehat{R}_D) = \sum_{h=1}^H \widehat{V}_h(\widehat{R}_D)$$

where, if  $n_h > 1$ , then

$$\begin{aligned} \widehat{V}_h(\widehat{R}_D) &= \frac{n_h(1-f_h)}{n_h-1} \sum_{i=1}^{n_h} (g_{hi\cdot} - \bar{g}_{h\cdot\cdot})^2 \\ g_{hi\cdot} &= \frac{\sum_{j=1}^{m_{hi}} v_{hij} (y_{hij} - x_{hij} \widehat{R}_D)}{\sum_{h=1}^H \sum_{i=1}^{n_h} \sum_{j=1}^{m_{hi}} v_{hij} x_{hij}} \\ \bar{g}_{h\cdot\cdot} &= \left( \sum_{i=1}^{n_h} g_{hi\cdot} \right) / n_h \end{aligned}$$

and if  $n_h = 1$ , then

$$\widehat{V}_h(\widehat{R}_D) = \begin{cases} \text{missing} & \text{if } n_{h'} = 1 \text{ for } h' = 1, 2, \dots, H \\ 0 & \text{if } n_{h'} > 1 \text{ for some } 1 \leq h' \leq H \end{cases}$$

### Quantiles

Let  $Y$  be the variable of interest in a complex survey. Denote  $F(t) = \Pr(Y \leq t)$  as the cumulative distribution for  $Y$ . For  $0 < p < 1$ , the  $p$ th quantile of the population cumulative distribution function is

$$Y_p = \inf\{y : F(y) \geq p\}$$

#### Estimate of Quantile

Let  $\{y_{hij}, w_{hij}\}$  be the observed values for variable  $Y$  associated with sampling weights, where  $(h, i, j)$  are the stratum index, cluster index, and member index, respectively, as shown in the section “Definitions and Notation” on page 7807. Let  $y_{(1)} < y_{(2)} < \dots < y_{(d)}$  denote the sample order statistics for variable  $Y$ .

An estimate of quantile  $Y_p$  is

$$\hat{Y}_p = \begin{cases} y_{(1)} & \text{if } p < \hat{F}(y_{(1)}) \\ y_{(k)} + \frac{p - \hat{F}(y_{(k)})}{\hat{F}(y_{(k+1)}) - \hat{F}(y_{(k)})} (y_{(k+1)} - y_{(k)}) & \text{if } \hat{F}(y_{(k)}) \leq p < \hat{F}(y_{(k+1)}) \\ y_{(d)} & \text{if } p = 1 \end{cases}$$

where  $\hat{F}(t)$  is the estimated cumulative distribution for  $Y$ :

$$\hat{F}(t) = \frac{\sum_{h=1}^H \sum_{i=1}^{n_h} \sum_{j=1}^{m_{hi}} w_{hij} I(y_{hij} \leq t)}{\sum_{h=1}^H \sum_{i=1}^{n_h} \sum_{j=1}^{m_{hi}} w_{hij}}$$

and  $I(\cdot)$  is the indicator function.

#### Standard Error

When you use `VARMETHOD=TAYLOR`, or by default if you do not specify the `VARMETHOD=` option, PROC SURVEYMEANS uses Woodruff’s method (Dorfman and Valliant 1993; Särndal, Swensson, and Wretman 1992; Francisco and Fuller 1991) to estimate the variances of quantiles. This method first constructs a confidence interval on a quantile. Then it uses the width of the confidence interval to estimate the standard error of a quantile.

In order to estimate the variance for  $\hat{Y}_p$ , first the procedure estimates the variance of the estimated distribution function  $\hat{F}(\hat{Y}_p)$  by

$$\hat{V}(\hat{F}(\hat{Y}_p)) = \sum_{h=1}^H \frac{n_h(1 - f_h)}{n_h - 1} \sum_{i=1}^{n_h} (d_{hi\cdot} - \bar{d}_{h\cdot})^2$$

where

$$d_{hi\cdot} = \left( \sum_{j=1}^{m_{hi}} w_{hij} (I(y_{hij} \leq \hat{Y}_p) - \hat{F}(\hat{Y}_p)) \right) / w_{\dots}$$

$$\bar{d}_{h\cdot} = \left( \sum_{i=1}^{n_h} d_{hi\cdot} \right) / n_h$$

Then  $100(1 - \alpha)\%$  confidence limits for  $\hat{F}(\hat{Y}_p)$  can be constructed by

$$(\hat{p}_L, \hat{p}_U) = \left( \hat{F}(\hat{Y}_p) - t_{df, \alpha/2} \sqrt{\hat{V}(\hat{F}(\hat{Y}_p))}, \quad \hat{F}(\hat{Y}_p) + t_{df, \alpha/2} \sqrt{\hat{V}(\hat{F}(\hat{Y}_p))} \right)$$

where  $t_{df, \alpha/2}$  is the  $100(1 - \alpha/2)$  percentile of the  $t$  distribution with  $df$  degrees of freedom, described in the section “[Degrees of Freedom](#)” on page 7810.

When  $(\hat{p}_L, \hat{p}_U)$  is out of the range of  $[0, 1]$ , the procedure does not compute the standard error.

The  $\hat{p}_L$ th quantile is defined as

$$\hat{Y}_{\hat{p}_L} = \begin{cases} y_{(1)} & \text{if } \hat{p}_L < \hat{F}(y_{(1)}) \\ y_{(k_L)} + \frac{\hat{p}_L - \hat{F}(y_{(k_L)})}{\hat{F}(y_{(k_L+1)}) - \hat{F}(y_{(k_L)})} (y_{(k_L+1)} - y_{(k_L)}) & \text{if } \hat{F}(y_{(k_L)}) \leq \hat{p}_L < \hat{F}(y_{(k_L+1)}) \\ y_{(d)} & \text{if } \hat{p}_L = 1 \end{cases}$$

and the  $\hat{p}_U$ th quantile is defined as

$$\hat{Y}_{\hat{p}_U} = \begin{cases} y_{(1)} & \text{if } \hat{p}_U < \hat{F}(y_{(1)}) \\ y_{(k_U)} + \frac{\hat{p}_U - \hat{F}(y_{(k_U)})}{\hat{F}(y_{(k_U+1)}) - \hat{F}(y_{(k_U)})} (y_{(k_U+1)} - y_{(k_U)}) & \text{if } \hat{F}(y_{(k_U)}) \leq \hat{p}_U < \hat{F}(y_{(k_U+1)}) \\ y_{(d)} & \text{if } \hat{p}_U = 1 \end{cases}$$

The standard error of  $\hat{Y}_p$  then is estimated by

$$\text{sd}(\hat{Y}_p) = \frac{\hat{Y}_{\hat{p}_U} - \hat{Y}_{\hat{p}_L}}{2t_{df, \alpha/2}}$$

where  $t_{df, \alpha/2}$  is the  $100(1 - \alpha/2)$  percentile of the  $t$  distribution with  $df$  degrees of freedom.

When you use the replication method, PROC SURVEYMEANS uses the usual variance estimates for a quantile as described in the section “[Replication Methods for Variance Estimation](#)” on page 7824. However, you should proceed cautiously because this variance estimator can have poor properties (Dorfman and Valliant 1993).

### Confidence Limits

Symmetric  $100(1 - \alpha)\%$  confidence limits are computed as

$$\left( \hat{Y}_p - \text{sd}(\hat{Y}_p) \cdot t_{df, \alpha/2}, \quad \hat{Y}_p + \text{sd}(\hat{Y}_p) \cdot t_{df, \alpha/2} \right)$$

If you specify the `NONSYMCL` option in the SURVEYMEANS statement when you use `VARMETHOD=TAYLOR` option, the procedure computes  $100(1 - \alpha)\%$  nonsymmetric confidence limits:

$$\left( \hat{Y}_{\hat{p}_L}, \quad \hat{Y}_{\hat{p}_U} \right)$$

### Geometric Mean

For a continuous variable  $Y$  that has positive values, the SURVEYMEANS procedure can compute its geometric mean and associated standard error and confidence limits. To request these statistics, you can specify *statistic-keywords* such as GEOMEAN, GEOSTDERR, and GEOMLCLM.

The geometric mean of  $Y$  from a sample is computed as

$$\begin{aligned} \widehat{Y}_G &= \left( \prod_{h=1}^H \prod_{i=1}^{n_h} \prod_{j=1}^{m_{hi}} y_{hij}^{w_{hij}} \right)^{\frac{1}{w_{\dots}}} \\ &= \exp \left( \frac{1}{w_{\dots}} \sum_{h=1}^H \sum_{i=1}^{n_h} \sum_{j=1}^{m_{hi}} w_{hij} \ln(y_{hij}) \right) \end{aligned}$$

where

$$w_{\dots} = \sum_{h=1}^H \sum_{i=1}^{n_h} \sum_{j=1}^{m_{hi}} w_{hij}$$

is the sum of the weights over all observations in the data set.

When you use the Taylor series method, the variance estimation for the geometric mean is computed as

$$\widehat{V}(\widehat{Y}_G) = \left(\widehat{Y}_G\right)^2 \sum_{h=1}^H \frac{n_h(1-f_h)}{n_h-1} \sum_{i=1}^{n_h} (r_{hi\cdot} - \bar{r}_{h\cdot})^2$$

where

$$\begin{aligned} r_{hi\cdot} &= \left( \sum_{j=1}^{m_{hi}} w_{hij} (\ln(y_{hij}) - \ln(\widehat{Y}_G)) \right) / w_{\dots} \\ \bar{r}_{h\cdot} &= \left( \sum_{i=1}^{n_h} r_{hi\cdot} \right) / n_h \end{aligned}$$

The standard error of the geometric mean is the square root of the estimated variance:

$$\text{StdErr}(\widehat{Y}_G) = \sqrt{\widehat{V}(\widehat{Y}_G)}$$

The confidence limits for the geometric means are computed based on the confidence limits for the log transformation of the  $Y$  variable as

$$\left( \exp(\ln(\widehat{Y}_G) - \gamma), \quad \exp(\ln(\widehat{Y}_G) + \gamma) \right)$$

where

$$\gamma = t_{df, \alpha/2} * \text{StdErr}(\widehat{Y}_G) / \widehat{Y}_G$$

and  $t_{df, \alpha/2}$  is the  $100(1 - \alpha/2)$  percentile of the  $t$  distribution, with  $df$  calculated as in the section “*t* Test for the Mean” on page 7810.

If you use replication methods to estimate the variance by specifying `VARMETHOD=BRR` or `VARMETHOD=JACKKNIFE`, the procedure computes the variance of a geometric means  $\widehat{V}_R(\widehat{Y}_G)$  by using the variability among replicate estimates to estimate the overall variance. See the section “*Replication Methods for Variance Estimation*” on page 7824 for more information.

Then the standard error is the square root of the estimated variance:

$$\text{StdErr}_R(\widehat{Y}_G) = \sqrt{\widehat{V}_R(\widehat{Y}_G)}$$

The confidence limits for the geometric means are computed based on the confidence limits for the log transformation of the variable  $Y$  as

$$\left( \exp(\ln(\widehat{Y}_G) - \lambda), \quad \exp(\ln(\widehat{Y}_G) + \lambda) \right)$$

where

$$\lambda = t_{df, \alpha/2} * \text{StdErr}_R(\widehat{Y}_G) / \widehat{Y}_G$$

and  $t_{df, \alpha/2}$  is the  $100(1 - \alpha/2)$  percentile of the  $t$  distribution, with  $df$  calculated as in the section “*t* Test for the Mean” on page 7810.

## Poststratification

After a probability sample is drawn and survey data are collected, researchers sometimes want to stratify the sample according to auxiliary information about the sampled population. This process is often called *poststratification*.

When poststratification is done properly, it can improve efficiency. It can also be used to adjust the sampling weights such that the marginal distribution of the sampling weights is in agreement with known auxiliary information from other resources, such as the census. The adjusted weight is often called the *poststratification weight*. It is quite common for researchers to use poststratification techniques in survey data analysis.

Poststratification is also used by epidemiologists, who frequently analyze health survey data. They often compute statistics based on a process called *direct standardization*, a form of poststratification. For example, certain diseases, such as cancer, are more common among older populations. Therefore, to compare the prevalence rates among geographic regions that are populated with different age groups, it is necessary to make adjustments according to such demographic categories and to compute relative prevalence rates of the diseases.

For more information about poststratification, see Fuller (2009); Lohr (2010); Wolter (2007); Rao, Yung, and Hidiroglou (2002).

After you provide the population controls for each poststratum that is defined by the poststratification variables, the SURVEYMEANS procedure creates the poststratification weights accordingly. Then the procedure computes statistics that you request by using poststratification weights.

You can save the poststratification weights in an `OUTPSWGT=` data to be used in subsequent analyses.

For a select sample, let  $p = 1, 2, \dots, P$  be the poststratum index; let  $Z_1, Z_2, \dots, Z_P$  be the population totals for each corresponding poststratum; and let  $I_p$  be a corresponding indicator variable for the poststratum  $p$  defined by

$$I_p(h, i, j) = \begin{cases} 1 & \text{if observation } (h, i, j) \text{ belongs to } p\text{th poststratum} \\ 0 & \text{otherwise} \end{cases}$$

Denote the total sum of original weights in the sample for each poststratum as

$$\psi_p = \sum_{h=1}^H \sum_{i=1}^{n_h} \sum_{j=1}^{m_{hi}} w_{hij} I_p(h, i, j)$$

Then the poststratification weight for the observation  $(h, i, j)$  is

$$\tilde{w}_{hij} = w_{hij} \frac{Z_p}{\psi_p}$$

The SURVEYMEANS procedure computes statistics by using the poststratification weights  $\tilde{w}_{hij}$  instead of the original weights  $w_{hij}$ .

The standard error and confidence intervals of computed statistics are based on the estimated variance, using either a replication method or the Taylor series method.

### **Replication Methods**

When you specify `VARMETHOD=BRR` or `VARMETHOD=JACKKNIFE`, PROC SURVEYMEANS computes the variance of a statistic by using replication methods, as described in the section “[Replication Methods for Variance Estimation](#)” on page 7824. However, with poststratification, an extra step is needed to adjust the weights.

First, PROC SURVEYMEANS constructs a replicate and computes appropriate replicate weights for the replicate. Then, by using the poststratification control totals, the procedure adjusts these replicate weights in the same way as described previously for constructing the poststratification weights for the full sample. Finally, PROC SURVEYMEANS computes the estimate for a desired statistics by using the poststratification weights that are adjusted from the replicate weights in the current replicate. Then the final variance is estimated by the variability among replicate estimates, as described in the section “[Replication Methods for Variance Estimation](#)” on page 7824.



**Taylor Series Method**

When you specify `VARMETHOD=TAYLOR`, or by default when you do not specify the `VARMETHOD=` option, PROC SURVEYMEANS uses the Taylor series method to estimate the variances of requested statistics.

**Variance of the Mean** The mean of variable  $Y$  under poststratification is

$$\hat{Y}_{PS} = \left( \sum_{h=1}^H \sum_{i=1}^{n_h} \sum_{j=1}^{m_{hi}} \tilde{w}_{hij} y_{hij} \right) / \tilde{w}_{\dots}$$

where

$$\tilde{w}_{\dots} = \sum_{h=1}^H \sum_{i=1}^{n_h} \sum_{j=1}^{m_{hi}} \tilde{w}_{hij}$$

is the sum of the poststratification weights over all observations in the sample.

For each poststratum  $p = 1, 2, \dots, P$ , let the mean of variable  $Y$  in each poststratum be

$$\hat{Y}^{(p)} = \left( \sum_{h=1}^H \sum_{i=1}^{n_h} \sum_{j=1}^{m_{hi}} I_p(h, i, j) \tilde{w}_{hij} y_{hij} \right) / \tilde{w}_{\dots}^{(p)}$$

where

$$\tilde{w}_{\dots}^{(p)} = \sum_{h=1}^H \sum_{i=1}^{n_h} \sum_{j=1}^{m_{hi}} I_p(h, i, j) \tilde{w}_{hij}$$

is the total of the poststratification weights in poststratum  $p$ .

For observation  $(h, i, j)$ , let  $p$  be the poststratum to which it belongs. Let

$$\tilde{y}_{hij} = y_{hij} - \hat{Y}^{(p)}$$

PROC SURVEYMEANS estimates the variance of  $\hat{Y}_{PS}$  as

$$\hat{V}(\hat{Y}_{PS}) = \sum_{h=1}^H \hat{V}_h$$

where, if  $n_h > 1$ , then

$$\hat{V}_h = \frac{n_h(1-f_h)}{n_h-1} \sum_{i=1}^{n_h} (e_{hi\cdot} - \bar{e}_{h\cdot\cdot})^2$$

$$e_{hi\cdot} = \left( \sum_{j=1}^{m_{hi}} \tilde{w}_{hij} \tilde{y}_{hij} \right) / \tilde{w}_{h\cdot\cdot}$$

$$\bar{e}_{h\cdot\cdot} = \left( \sum_{i=1}^{n_h} e_{hi\cdot} \right) / n_h$$

and if  $n_h = 1$ , then

$$\hat{V}_h = \begin{cases} \text{missing} & \text{if } n_{h'} = 1 \text{ for } h' = 1, 2, \dots, H \\ 0 & \text{if } n_{h'} > 1 \text{ for some } 1 \leq h' \leq H \end{cases}$$

**Variance of the Ratio** Suppose you want to calculate the ratio of variable Y to variable X. Let  $x_{hij}$  and  $y_{hij}$  be the values of variable X and variable Y, respectively, for observation  $(h, i, j)$ .

The ratio of Y to X after poststratification is

$$\hat{R}_{PS} = \frac{\sum_{h=1}^H \sum_{i=1}^{n_h} \sum_{j=1}^{m_{hi}} \tilde{w}_{hij} y_{hij}}{\sum_{h=1}^H \sum_{i=1}^{n_h} \sum_{j=1}^{m_{hi}} \tilde{w}_{hij} x_{hij}}$$

where  $\tilde{w}_{hij}$  is the poststratification weight for observation  $(h, i, j)$ .

Let

$$\tilde{y}_{hij} = y_{hij} - \hat{Y}^{(p)}$$

$$\tilde{x}_{hij} = x_{hij} - \hat{X}^{(p)}$$

where  $\hat{Y}^{(p)}$  and  $\hat{X}^{(p)}$  are the means of variable Y and variable X, respectively, in poststratum  $p$ .

The variance of  $\hat{R}_{PS}$  is estimated by

$$\hat{V}(\hat{R}_{PS}) = \sum_{h=1}^H \hat{V}_h(\hat{R}_{PS})$$

where, if  $n_h > 1$ , then

$$\hat{V}_h(\hat{R}_{PS}) = \frac{n_h(1-f_h)}{n_h-1} \sum_{i=1}^{n_h} (g_{hi\cdot} - \bar{g}_{h\cdot\cdot})^2$$

$$g_{hi\cdot} = \frac{\sum_{j=1}^{m_{hi}} \tilde{w}_{hij} (\tilde{y}_{hij} - \tilde{x}_{hij} \hat{R}_{PS})}{\sum_{h=1}^H \sum_{i=1}^{n_h} \sum_{j=1}^{m_{hi}} \tilde{w}_{hij} x_{hij}}$$

$$\bar{g}_{h\cdot\cdot} = \left( \sum_{i=1}^{n_h} g_{hi\cdot} \right) / n_h$$

and if  $n_h = 1$ , then

$$\hat{V}_h(\hat{R}_{PS}) = \begin{cases} \text{missing} & \text{if } n_{h'} = 1 \text{ for } h' = 1, 2, \dots, H \\ 0 & \text{if } n_{h'} > 1 \text{ for some } 1 \leq h' \leq H \end{cases}$$

## Replication Methods for Variance Estimation

Recently replication methods have gained popularity for estimating variances in complex survey data analysis. One reason for this popularity is the relative simplicity of replication-based estimates, especially for nonlinear estimators; another is that modern computational capacity has made replication methods feasible for practical survey analysis. For more information, see Lohr (2010); Wolter (2007); Rust (1985); Dippo, Fay, and Morganstein (1984); Rao and Shao (1999); Rao, Wu, and Yue (1992); Rao and Shao (1996).

Replication methods draw multiple replicates (also called subsamples) from a full sample according to a specific resampling scheme. The most commonly used resampling schemes are the *balanced repeated replication* (BRR) method and the *jackknife* method. For each replicate, the original weights are modified for the PSUs in the replicates to create replicate weights. The statistics of interest are estimated by using the replicate weights for each replicate. Then the variances of parameters of interest are estimated by the variability among the estimates derived from these replicates. You can use the `REPWEIGHTS` statement to provide your own replicate weights for variance estimation.

### Balanced Repeated Replication (BRR) Method

The balanced repeated replication (BRR) method requires that the full sample be drawn by using a stratified sample design with two primary sampling units (PSUs) per stratum. Let  $H$  be the total number of strata. The total number of replicates  $R$  is the smallest multiple of 4 that is greater than  $H$ . However, if you prefer a larger number of replicates, you can specify the `REPS=number` option. If a  $number \times number$  Hadamard matrix cannot be constructed, the number of replicates is increased until a Hadamard matrix becomes available.

Each replicate is obtained by deleting one PSU per stratum according to the corresponding Hadamard matrix and adjusting the original weights for the remaining PSUs. The new weights are called replicate weights.

Replicates are constructed by using the first  $H$  columns of the  $R \times R$  Hadamard matrix. The  $r$ th ( $r = 1, 2, \dots, R$ ) replicate is drawn from the full sample according to the  $r$ th row of the Hadamard matrix as follows:

- If the  $(r, h)$  element of the Hadamard matrix is 1, then the first PSU of stratum  $h$  is included in the  $r$ th replicate and the second PSU of stratum  $h$  is excluded.
- If the  $(r, h)$  element of the Hadamard matrix is  $-1$ , then the second PSU of stratum  $h$  is included in the  $r$ th replicate and the first PSU of stratum  $h$  is excluded.

Note that the “first” and “second” PSUs are determined by data order in the input data set. Thus, if you reorder the data set and perform the same analysis by using BRR method, you might get slightly different results, because the contents in each replicate sample might change.

The replicate weights of the remaining PSUs in each half-sample are then doubled to their original weights. For more details about the BRR method, see Wolter (2007) and Lohr (2010).

By default, an appropriate Hadamard matrix is generated automatically to create the replicates. You can request that the Hadamard matrix be displayed by specifying the `VARMETHOD=BRR(PRINTH)` *method-option*. If you provide a Hadamard matrix by specifying the `VARMETHOD=BRR(HADAMARD=)` *method-option*, then the replicates are generated according to the provided Hadamard matrix.

You can use the `VARMETHOD=BRR(OUTWEIGHTS=)` *method-option* to save the replicate weights into a SAS data set.

Suppose that  $\theta$  is a population parameter of interest. Let  $\hat{\theta}$  be the estimate from the full sample for  $\theta$ . Let  $\hat{\theta}_r$  be the estimate from the  $r$ th replicate subsample by using replicate weights. PROC SURVEYMEANS estimates the variance of  $\hat{\theta}$  by

$$\widehat{V}(\hat{\theta}) = \frac{1}{R} \sum_{r=1}^R (\hat{\theta}_r - \hat{\theta})^2$$

with  $H$  degrees of freedom, where  $H$  is the number of strata.

If a parameter cannot be computed from one or more replicates, then the variance estimate is computed by using those replicates from which the parameter can be estimated. For example, suppose the parameter is a ratio. If a replicate  $r$  contains observations such that the denominator of the ratio is zero, then the ratio cannot be computed from replicate  $r$ . In this case, the BRR variance estimate is computed as

$$\widehat{V}(\hat{\theta}) = \frac{1}{R'} \sum_{r=1}^{R'} (\hat{\theta}_r - \hat{\theta})^2$$

where the summation is over the replicates where the parameter  $\theta$  can be computed, and  $R'$  is the number of those replicates.

## Fay's BRR Method

Fay's method is a modification of the BRR method, and it requires a stratified sample design with two primary sampling units (PSUs) per stratum. The total number of replicates  $R$  is the smallest multiple of 4 that is greater than the total number of strata  $H$ . However, if you prefer a larger number of replicates, you can specify the `REPS=` *method-option*.

For each replicate, Fay's method uses a Fay coefficient  $0 \leq \epsilon < 1$  to impose a perturbation of the original weights in the full sample that is gentler than using only half-samples, as in the traditional BRR method. The Fay coefficient  $0 \leq \epsilon < 1$  can be set by specifying the `FAY =  $\epsilon$`  *method-option*. By default,  $\epsilon = 0.5$  if the `FAY` *method-option* is specified without providing a value for  $\epsilon$  (Judkins 1990; Rao and Shao 1999). When  $\epsilon = 0$ , Fay's method becomes the traditional BRR method. For more details, see Dippo, Fay, and Morganstein (1984); Fay (1984, 1989); Judkins (1990).

Let  $H$  be the number of strata. Replicates are constructed by using the first  $H$  columns of the  $R \times R$  Hadamard matrix, where  $R$  is the number of replicates,  $R > H$ . The  $r$ th ( $r = 1, 2, \dots, R$ ) replicate is created from the full sample according to the  $r$ th row of the Hadamard matrix as follows:

- If the  $(r, h)$  element of the Hadamard matrix is 1, then the full sample weight of the first PSU in stratum  $h$  is multiplied by  $\epsilon$  and the full sample weight of the second PSU is multiplied by  $2 - \epsilon$  to obtain the  $r$ th replicate weights.

- If the  $(r, h)$  element of the Hadamard matrix is  $-1$ , then the full sample weight of the first PSU in stratum  $h$  is multiplied by  $2 - \epsilon$  and the full sample weight of the second PSU is multiplied by  $\epsilon$  to obtain the  $r$ th replicate weights.

You can use the `VARMETHOD=BRR(OUTWEIGHTS=)` *method-option* to save the replicate weights into a SAS data set.

By default, an appropriate Hadamard matrix is generated automatically to create the replicates. You can request that the Hadamard matrix be displayed by specifying the `VARMETHOD=BRR(PRINTH)` *method-option*. If you provide a Hadamard matrix by specifying the `VARMETHOD=BRR(HADAMARD=)` *method-option*, then the replicates are generated according to the provided Hadamard matrix.

Suppose that  $\theta$  is a population parameter of interest. Let  $\hat{\theta}$  be the estimate from the full sample for  $\theta$ . Let  $\hat{\theta}_r$  be the estimate from the  $r$ th replicate subsample by using replicate weights. PROC SURVEYMEANS estimates the variance of  $\hat{\theta}$  by

$$\widehat{V}(\hat{\theta}) = \frac{1}{R(1 - \epsilon)^2} \sum_{r=1}^R (\hat{\theta}_r - \hat{\theta})^2$$

with  $H$  degrees of freedom, where  $H$  is the number of strata.

## Jackknife Method

The jackknife method of variance estimation deletes one PSU at a time from the full sample to create replicates. The total number of replicates  $R$  is the same as the total number of PSUs. In each replicate, the sample weights of the remaining PSUs are modified by the jackknife coefficient  $\alpha_r$ . The modified weights are called replicate weights.

The jackknife coefficient and replicate weights are described as follows.

**Without Stratification** If there is no stratification in the sample design (no `STRATA` statement), the jackknife coefficients  $\alpha_r$  are the same for all replicates:

$$\alpha_r = \frac{R - 1}{R} \quad \text{where } r = 1, 2, \dots, R$$

Denote the original weight in the full sample for the  $j$ th member of the  $i$ th PSU as  $w_{ij}$ . If the  $i$ th PSU is included in the  $r$ th replicate ( $r = 1, 2, \dots, R$ ), then the corresponding replicate weight for the  $j$ th member of the  $i$ th PSU is defined as

$$w_{ij}^{(r)} = w_{ij} / \alpha_r$$

**With Stratification** If the sample design involves stratification, each stratum must have at least two PSUs to use the jackknife method.

Let stratum  $\tilde{h}_r$  be the stratum from which a PSU is deleted for the  $r$ th replicate. Stratum  $\tilde{h}_r$  is called the *donor stratum*. Let  $n_{\tilde{h}_r}$  be the total number of PSUs in the donor stratum  $\tilde{h}_r$ . The jackknife coefficients are defined as

$$\alpha_r = \frac{n_{\tilde{h}_r} - 1}{n_{\tilde{h}_r}} \quad \text{where } r = 1, 2, \dots, R$$

Denote the original weight in the full sample for the  $j$ th member of the  $i$ th PSU as  $w_{ij}$ . If the  $i$ th PSU is included in the  $r$ th replicate ( $r = 1, 2, \dots, R$ ), then the corresponding replicate weight for the  $j$ th member of the  $i$ th PSU is defined as

$$w_{ij}^{(r)} = \begin{cases} w_{ij} & \text{if } i\text{th PSU is not in the donor stratum } \tilde{h}_r \\ w_{ij}/\alpha_r & \text{if } i\text{th PSU is in the donor stratum } \tilde{h}_r \end{cases}$$

You can use the `VARMETHOD=JACKKNIFE(OUTJKCOEFS=)` *method-option* to save the jackknife coefficients into a SAS data set and use the `VARMETHOD=JACKKNIFE(OUTWEIGHTS=)` *method-option* to save the replicate weights into a SAS data set.

If you provide your own replicate weights with a `REPWEIGHTS` statement, then you can also provide corresponding jackknife coefficients with the `JKCOEFS=` option.

Suppose that  $\theta$  is a population parameter of interest. Let  $\hat{\theta}$  be the estimate from the full sample for  $\theta$ . Let  $\hat{\theta}_r$  be the estimate from the  $r$ th replicate subsample by using replicate weights. PROC SURVEYMEANS estimates the variance of  $\hat{\theta}$  by

$$\widehat{V}(\hat{\theta}) = \sum_{r=1}^R \alpha_r (\hat{\theta}_r - \hat{\theta})^2$$

with  $R - H$  degrees of freedom, where  $R$  is the number of replicates and  $H$  is the number of strata, or  $R - 1$  when there is no stratification.

## Hadamard Matrix

A Hadamard matrix  $\mathbf{H}$  is a square matrix whose elements are either 1 or  $-1$  such that

$$\mathbf{H}\mathbf{H}' = k\mathbf{I}$$

where  $k$  is the dimension of  $\mathbf{H}$  and  $\mathbf{I}$  is the identity matrix of order  $k$ . The order  $k$  is necessarily 1, 2, or a positive integer that is a multiple of 4.

For example, the following matrix is a Hadamard matrix of dimension  $k = 8$ :

$$\begin{matrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 \end{matrix}$$

---

## Computational Resources

Due to the complex nature of survey data analysis, the SURVEYMEANS procedure usually requires more memory than an analysis by the MEANS procedure for the same analysis variables. PROC SURVEYMEANS requires memory resources to keep a copy of each unique value of the STRATUM, CLUSTER, and DOMAIN variables in addition to the memory needed for the categorical analysis variables and other computations.

The estimated memory needed by the SURVEYMEANS procedure is described as follows.

Let:

- $T_{\text{str}}$  be the total number of STRATUM variables
- $L_{\text{str}}(t)$  be the number of unique values for the  $t$ th STRATUM variable, where  $t = 1, 2, \dots, T_{\text{str}}$
- $H$  be the total number of strata
- $T_{\text{clu}}$  be the total number of CLUSTER variables
- $L_{\text{clu}}(t)$  be the number of unique values for the  $t$ th CLUSTER variable, where  $t = 1, 2, \dots, T_{\text{clu}}$
- $T_{\text{dom}}$  be the total number of DOMAIN variables in a domain (you might have multiple domains defined in a DOMAIN statement)
- $L_{\text{dom}}(t)$  be the number of unique values for the  $t$ th DOMAIN variable, where  $t = 1, 2, \dots, T_{\text{dom}}$
- $D$  be the total number of domains
- $T_{\text{cont}}$  be the total number of continuous analysis variables
- $T_{\text{clas}}$  be the total number of categorical analysis variables (CLASS variable)
- $L_{\text{clas}}(t)$  be the number of unique values for the  $t$ th CLASS variable, where  $t = 1, 2, \dots, T_{\text{clas}}$
- $T_{\text{ratio}}$  be the total number of ratios
- $T_{\text{pctl}}$  be the total number of percentiles
- $c$  be a constant on the order of 32 bytes (64 for 64-bit architectures) plus the maximum combined unformatted and formatted length among all the STRATUM, CLUSTER, DOMAIN, and CLASS variables

If all combinations of levels of categorical variables exist, the maximum potential memory (in bytes) requirements for the analysis is estimated by

$$c * P * Q + 2000 * (H + 1) * (D + 1) * Q$$

where

$$P = \prod_{t=1}^{T_{\text{str}}} L_{\text{str}}(t) \prod_{t=1}^{T_{\text{clu}}} L_{\text{clu}}(t) \prod_{t=1}^{T_{\text{dom}}} L_{\text{dom}}(t)$$

$$Q = T_{\text{cont}} + \sum_{t=1}^{T_{\text{clas}}} L_{\text{clas}}(t) + T_{\text{ratio}} + T_{\text{pctl}}$$

A relatively small amount of memory, compared to the memory usage described in the preceding calculation, is also needed for the analysis.

When the data-dependent memory usage overwhelms what is available in the computer system, the procedure might open one or more utility files to complete the analysis. This process can be controlled by the SAS system option `SUMSIZE=`, which sets the memory threshold where utility file operations begin. For best results, set `SUMSIZE=` to be less than the amount of real memory that is likely to be available for the task. See the chapter on SAS system options in *SAS System Options: Reference* for a description of the `SUMSIZE=` option.

If PROC SURVEYMEANS reports that there is insufficient memory, increase `SUMSIZE=`. A `SUMSIZE=` value greater than `MEMSIZE=` has no effect. Therefore, you might also need to increase `MEMSIZE=`.

The `MEMSIZE` option can be specified at system invocation, on the SAS command line, or in a configuration file. However, the `MEMSIZE` system option is not available in some operating environments. See the *SAS Companion* for your operating environment for more information and for the syntax specification.

To report a procedure's memory consumption, you can use the `FULLSTIMER` option. The syntax is described in the *SAS Companion* for your operating environment.

Also see the *SAS System Options: Reference* for more information about how to adjust your computation resource parameters for your operating environment.

For additional information about the memory usage for categorical variables, see the section “Computational Resources” in the chapter “The MEANS Procedure” in the *Base SAS Procedures Guide: Statistical Procedures*.

## Output Data Sets

You can use the Output Delivery System to create a SAS data set from any piece of PROC SURVEYMEANS output. See the section “ODS Table Names” on page 7838 for more information.

PROC SURVEYMEANS also provides an output data set that stores the replicate weights for BRR or jackknife variance estimation and an output data set that stores the jackknife coefficients for jackknife variance estimation.

### Replicate Weights Output Data Set

If you specify the `OUTWEIGHTS= method-option` for `VARMETHOD=BRR` or `VARMETHOD=JACKKNIFE`, PROC SURVEYMEANS stores the replicate weights in an output data set. The `OUTWEIGHTS=` output data set contains all observations from the `DATA=` input data set that are valid (used in the analysis). (A valid observation is an observation that has a positive value of the `WEIGHT` variable. Valid observations must also have nonmissing values of the `STRATA` and `CLUSTER` variables, unless you specify the `MISSING` option. See the section “Data and Sample Design Summary” on page 7832 for details about valid observations.)

The `OUTWEIGHTS=` data set contains the following variables:

- all variables in the `DATA=` input data set
- `RepWt_1`, `RepWt_2`, . . . , `RepWt_n`, which are the replicate weight variables

where  $n$  is the total number of replicates in the analysis. Each replicate weight variable contains the replicate weights for the corresponding replicate. Replicate weights equal zero for those observations not included in the replicate.



After the procedure creates replicate weights for a particular input data set and survey design, you can use the `OUTWEIGHTS= method-option` to store these replicate weights and then use them again in subsequent analyses, either in PROC SURVEYMEANS or in the other survey procedures. You can use the `REPWEIGHTS` statement to provide replicate weights for the procedure.

### Jackknife Coefficients Output Data Set

If you specify the `OUTJKCOEFS= method-option` for `VARMETHOD=JACKKNIFE`, PROC SURVEYMEANS stores the jackknife coefficients in an output data set. The `OUTJKCOEFS=` output data set contains one observation for each replicate. The `OUTJKCOEFS=` data set contains the following variables:

- Replicate, which is the replicate number for the jackknife coefficient
- JKCoefficient, which is the jackknife coefficient
- DonorStratum, which is the stratum of the PSU that was deleted to construct the replicate, if you specify a `STRATA` statement

After the procedure creates jackknife coefficients for a particular input data set and survey design, you can use the `OUTJKCOEFS= method-option` to store these coefficients and then use them again in subsequent analyses, either in PROC SURVEYMEANS or in the other survey procedures. You can use the `JKCOEFS=` option in the `REPWEIGHTS` statement to provide jackknife coefficients for the procedure.

### Poststratification Weights Output Data Set

If you specify the `OUTPSWGT=` option in the `POSTSTRATA` statement, PROC SURVEYMEANS stores the poststratification weights in an output data set. The `OUTPSWGT=` output data set contains all observations from the `DATA=` input data set that are valid (used in the analysis). (A valid observation is an observation that has a positive value of the `WEIGHT` variable. Valid observations must also have non-missing values of the `STRATA` and `CLUSTER` variables, unless you specify the `MISSING` option. See the section “Data and Sample Design Summary” on page 7832 for more information about valid observations.)

For `VARMETHOD=TAYLOR`, the `OUTPSWGT=` data set contains the following variables:

- all variables in the `DATA=` input data set
- `_PSWt_`, which contains poststratification weights

For `VARMETHOD=BRR` and `VARMETHOD=JACKKNIFE`, the `OUTPSWGT=` option is the same `OUTWEIGHTS= method-option` that you specify in the PROC SURVEYMEANS statement, except that it also contains the variable `_PSWt_`, which contains poststratification weights for the full sample. The replication weights, adjusted for poststratification, are stored in the `OUTWEIGHTS=` data set. See the section “Replicate Weights Output Data Set” on page 7829 for the contents of the `OUTWEIGHTS=` data set.

However, if you also specify an `OUTWEIGHTS= method-option` in the PROC SURVEYMEANS statement and use a different data set name, the data set in `OUTPSWGT=` option is ignored.

If you provide your own replicate weights by using a `REPWEIGHTS` statement for `VARMETHOD=BRR` or `VARMETHOD=JACKKNIFE`, the poststratification replicate weights replace the original replicate weights in the `OUTPSWGT=` data set.

## Rectangular and Stacking Structures in an Output Data Set

When you use an ODS output statement to create SAS data sets for certain tables in PROC SURVEYMEANS, there are two possible types of table structure for the output data sets: *rectangular* and *stacking*. A rectangular structure creates one observation for each analysis variable in the data set. A stacking structure creates only one observation in the output data set for all analysis variables.

Before SAS 9, the stacking table structure, similar to the table structure in PROC MEANS, was the default in PROC SURVEYMEANS. Since SAS 9, the new default is to produce a rectangular table in the output data sets. You can use the **STACKING** option to request that the procedure produce the output data sets by using a stacking table structure.

The STACKING option affects the following tables:

- Domain
- Ratio
- Statistics
- StrataInfo

Figure 92.6 and Figure 92.7 shows these two structures for analyzing the following data set:

```
data new;
 input sex$ x;
 datalines;
M 12
F 5
M 13
F 23
F 11
;
```

The following statements request the default rectangular structure of the output data set for the statistics table:

```
proc surveymeans data=new mean;
 ods output statistics=rectangle;
run;

proc print data=rectangle;
run;
```

Figure 92.6 shows the rectangular structure.

**Figure 92.6** Rectangular Structure in the Output Data Set

| Rectangular Structure in the Output Data Set |             |              |           |          |
|----------------------------------------------|-------------|--------------|-----------|----------|
| Obs                                          | Var<br>Name | Var<br>Level | Mean      | StdErr   |
| 1                                            | x           |              | 12.800000 | 2.905168 |
| 2                                            | sex         | F            | 0.600000  | 0.244949 |
| 3                                            | sex         | M            | 0.400000  | 0.244949 |

The following statements specify the **STACKING** option to request that the output data set have a stacking structure:

```
proc surveymeans data=new mean stacking;
 ods output statistics=stacking;
run;

proc print data=stacking;
run;
```

Figure 92.7 shows the stacking structure of the output data set for the statistics table requested by the **STACKING** option.

**Figure 92.7** Stacking Structure in the Output Data Set Requested by the **STACKING** option

| Stacking Structure in the Output Data Set |              |           |            |              |            |
|-------------------------------------------|--------------|-----------|------------|--------------|------------|
| Obs                                       | x            | x_Mean    | x_StdErr   | sex_F        | sex_F_Mean |
| 1                                         | x            | 12.800000 | 2.905168   | sex=F        | 0.600000   |
| Obs                                       | sex_F_StdErr | sex_M     | sex_M_Mean | sex_M_StdErr |            |
| 1                                         | 0.244949     | sex=M     | 0.400000   | 0.244949     |            |

---

## Displayed Output

The SURVEYMEANS procedure produces output that is described in the following sections.

### Data and Sample Design Summary

The “Data Summary” table provides information about the input data set and the sample design. This table displays the total number of valid observations, where an observation is considered *valid* if it has nonmissing values for all procedure variables other than the analysis variables—that is, for all specified

**STRATA**, **CLUSTER**, **DOMAIN**, **POSTSTRATA**, and **WEIGHT** variables. This number might differ from the number of nonmissing observations for an individual analysis variable, which the procedure displays in the “Statistics” table. See the section “Missing Values” on page 7804 for more information.

PROC SURVEYMEANS displays the following information in the “Data Summary” table:

- Number of Strata, if you specify a STRATA statement
- Number of Poststrata, if you specify a POSTSTRATA statement
- Number of Clusters, if you specify a CLUSTER statement
- Number of Observations, which is the total number of valid observations
- Sum of Weights, which is the sum over all valid observations, if you specify a WEIGHT statement

### Class Level Information

If you use a **CLASS** statement to name classification variables for categorical analysis, or if you list any character variables in the VAR statement, then PROC SURVEYMEANS displays a “Class Level Information” table. This table contains the following information for each classification variable:

- Class Variable, which lists each CLASS variable name
- Levels, which is the number of values or levels of the classification variable
- Values, which lists the values of the classification variable. The values are separated by a white space character; therefore, to avoid confusion, you should not include a white space character within a classification variable value.

### Stratum Information

If you specify the **LIST** option in the STRATA statement, PROC SURVEYMEANS displays a “Stratum Information” table. This table displays the number of valid observations in each stratum, as well as the number of nonmissing stratum observations for each analysis variable. The “Stratum Information” table provides the following for each stratum:

- Stratum Index, which is a sequential stratum identification number
- STRATA variable(s), which lists the levels of STRATA variables for the stratum
- Population Total, if you specify the **TOTAL=** option
- Sampling Rate, if you specify the **TOTAL=** or **RATE=** option. If you specify the **TOTAL=** option, the sampling rate is based on the number of valid observations in the stratum.
- N Obs, which is the number of valid observations
- Variable, which lists each analysis variable name
- Levels, which identifies each level for categorical variables

- N, which is the number of nonmissing observations for the analysis variable
- Clusters, which is the number of clusters, if you specify a **CLUSTER** statement

## Variance Estimation

If the variance method is not Taylor series or if the **NOMCAR** option is used, by default, PROC SURVEYMEANS displays the following variance estimation specifications in the “Variance Estimation” table:

- Method, which is the variance estimation method
- Replicate Weights Data Set, which is the name of the SAS data set that contains the replicate weights
- Number of Replicates, which is the number of replicates if you specify the **VARMETHOD=BRR** or **VARMETHOD=JACKKNIFE** option
- Hadamard Data Set, which is the name of the SAS data set for the HADAMARD matrix if you specify the **VARMETHOD=BRR(HADAMARD=)** *method-option*
- Fay Coefficient, which is the value of the FAY coefficient if you specify the **VARMETHOD=BRR(FAY)** *method-option*
- Missing Levels Included (MISSING), if you specify the **MISSING** option
- Missing Levels Included (NOMCAR), if you specify the **NOMCAR** option

## Statistics

The “Statistics” table displays all of the statistics that you request with *statistic-keywords* in the PROC SURVEYMEANS statement, except DECILES, MEDIAN, Q1, Q3, and QUARTILES, which are displayed in the “Quantiles” table. If you do not specify any *statistic-keywords*, then by default this table displays the following information for each analysis variable: the sample size, the mean, the standard error of the mean, and the confidence limits for the mean. The “Statistics” table can contain the following information for each analysis variable, depending on which *statistic-keywords* you request:

- Variable name
- Variable Label
- Level, which identifies each level for categorical variables
- N, which is the number of nonmissing observations
- N Miss, which is the number of missing observations
- Minimum
- Maximum
- Range

- Number of Clusters
- Sum of Weights
- DF, which is the degrees of freedom for the  $t$  test
- Mean
- Std Error of Mean, which is the standard error of the mean
- Var of Mean, which is the variance of the mean
- $t$  Value, for testing  $H_0$  : population MEAN = 0
- $\text{Pr} > |t|$ , which is the two-sided  $p$ -value for the  $t$  test
- $100(1 - \alpha)\%$  CL for Mean, which are two-sided confidence limits for the mean
- $100(1 - \alpha)\%$  Upper CL for Mean, which is a one-sided upper confidence limit for the mean
- $100(1 - \alpha)\%$  Lower CL for Mean, which is a one-sided lower confidence limit for the mean
- Coeff of Variation, which is the coefficient of variation for the mean
- Sum
- Std Dev, which is the standard deviation of the sum
- Var of Sum, which is the variance of the sum
- $100(1 - \alpha)\%$  CL for Sum, which are two-sided confidence limits for the sum
- $100(1 - \alpha)\%$  Upper CL for Sum, which is a one-sided upper confidence limit for the sum
- $100(1 - \alpha)\%$  Lower CL for Sum, which is a one-sided lower confidence limit for the Sum
- Coeff of Variation for sum, which is the coefficient of variation for the sum

## Quantiles

The “Quantiles” table displays all the quantiles that you request with either *statistic-keywords* such as DECILES, MEDIAN, Q1, Q3, and QUARTILES, or the `PERCENTILE=` option, or the `QUANTILE=` option in the PROC SURVEYMEANS statement.

The “Quantiles” table contains the following information for each quantile:

- Variable name
- Variable Label
- Percentile, which is the requested quantile in the format of %
- Percentile Label, which is the corresponding common name for a percentile if it exists—for example, *Median* for 50th percentile

- Estimate, which is the estimate for a requested quantile with respect to the population distribution
- Std Error, which is the standard error of the quantile
- $100(1 - \alpha)\%$  Confidence Limits, which are two-sided confidence limits for the quantile

## Domain Analysis

If you specify a **DOMAIN** statement, the procedure displays domain statistics in a “Domain Analysis” table. A “Domain Analysis” table displays all the requested statistics for each level of the domain request. The procedure produces a separate “Domain Analysis” for each separate domain request. For example, the **DOMAIN** statement

```
domain A B*C*D A*C C;
```

specifies four domain requests:

- A: all the levels of A
- C: all the levels of C
- A\*C: all the interactive levels of A and C
- B\*C\*D: all the interactive levels of B, C, and D

The procedure displays four “Domain Analysis” tables, one for each domain definition. If you use an **ODS OUTPUT** statement to create an output data set for domain analysis, the output data set contains a variable **Domain** whose values are these domain definitions. It contains all the columns in the “Statistics” table plus columns of domain variable values.

## Ratio Analysis

The “Ratio Analysis” table displays statistics for all the ratios that you request in the **RATIO** statement. If you do not specify any *statistic-keywords* in the **PROC SURVEYMEANS** statement, then by default this table displays the ratios and standard errors. The “Ratio Analysis” table can contain the following information for each ratio, depending on which *statistic-keywords* you request:

- Numerator, which identifies the numerator variable of the ratio
- Denominator, which identifies the denominator variable of the ratio
- N, which is the number of observations used in the ratio analysis
- number of Clusters
- Sum of Weights
- DF, which is the degrees of freedom for the *t* test
- Ratio
- Std Err of Ratio, which is the standard error of the ratio

- Var, which is the variance of the ratio
- $t$  Value, for testing  $H_0$  : population RATIO = 0
- $\Pr > |t|$ , which is the two-sided  $p$ -value for the  $t$  test
- $100(1 - \alpha)\%$  CL for Ratio, which are two-sided confidence limits for the Ratio
- Upper  $100(1 - \alpha)\%$  CL for Ratio, which are one-sided upper confidence limits for the Ratio
- Lower  $100(1 - \alpha)\%$  CL for Ratio, which are one-sided lower confidence limits for the Ratio

When you use the ODS OUTPUT statement to create an output data set, if you use labels for your RATIO statement, these labels are saved in the variable Ratio Statement in the output data set.

### Domain Ratio Analysis

If you specify a DOMAIN statement with a RATIO statement, the procedure displays domain ratios in a “Domain Ratio Analysis” table. A “Domain Ratio Analysis” table displays all the ratio statistics for each level of the domain request. It contains all the columns in the “Ratio Analysis” table plus columns of domain variable values.

### Hadamard Matrix

If you specify the `VARMETHOD=BRR(PRINTH)` *method-option* in the PROC SURVEYMEANS statement, PROC SURVEYMEANS displays the Hadamard matrix that is used to construct replicates for BRR variance estimation.

If you provide a Hadamard matrix with the `VARMETHOD=BRR(HADAMARD=)` *method-option* but the procedure does not use the entire matrix, the procedure displays only the rows and columns that are actually used to construct replicates.

### Geometric Means

The “Geometric Means” table displays all the statistics related to geometric mean that you request with *statistic-keywords* in the PROC SURVEYMEANS statement. The “Geometric Means” table can contain the following information for each analysis variable, depending on which *statistic-keywords* you request:

- Variable Name
- Variable Label
- Geometric Mean
- Std Error of Geometric Mean
- $100(1 - \alpha)\%$  CL for Geometric Mean, which are two-sided confidence limits for the geometric mean
- $100(1 - \alpha)\%$  Lower CL for Geometric Mean, which is a one-sided lower confidence limit for the geometric mean
- $100(1 - \alpha)\%$  Upper CL for Geometric Mean, which is a one-sided upper confidence limit for the geometric mean



## Domain Geometric Means

If you specify a **DOMAIN** statement and request any statistics related to geometric mean with *statistic-keywords* in the PROC SURVEYMEANS statement, the procedure displays these statistics for each domain level in a “Domain Geometric Means” table. It contains all the columns in the “Geometric Means” table plus columns of domain variable values.

## ODS Table Names

PROC SURVEYMEANS assigns a name to each table it creates; these names are listed in Table 92.4. You can use these names to refer to tables when you use the Output Delivery System (ODS) to select tables and create output data sets. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

**Table 92.4** ODS Tables Produced by PROC SURVEYMEANS

| ODS Table Name     | Description                                      | Statement                      | Option                                        |
|--------------------|--------------------------------------------------|--------------------------------|-----------------------------------------------|
| ClassVarInfo       | Class level information                          | <b>CLASS</b>                   | Default                                       |
| Domain             | Statistics in domains                            | <b>DOMAIN</b>                  | Default                                       |
| DomainRatio        | Statistics for ratios in domains                 | <b>DOMAIN</b> and <b>RATIO</b> | Default                                       |
| DomainGeoMeans     | Statistics related to geometric means in domains | <b>PROC</b> and <b>DOMAIN</b>  | <b>Keywords</b>                               |
| GeoMeans           | Statistics related to geometric means            | <b>PROC</b>                    | <b>Keywords</b>                               |
| HadamardMatrix     | Hadamard matrix                                  | <b>PROC</b>                    | <b>PRINTH</b>                                 |
| Ratio              | Statistics for ratios                            | <b>RATIO</b>                   | Default                                       |
| Quantiles          | Quantiles                                        | <b>PROC</b>                    | Default                                       |
| Statistics         | Statistics                                       | <b>PROC</b>                    | Default                                       |
| StrataInfo         | Stratum information                              | <b>STRATA</b>                  | <b>LIST</b>                                   |
| Summary            | Data summary                                     | <b>PROC</b>                    | Default                                       |
| VarianceEstimation | Variance estimation                              | <b>PROC</b>                    | <b>VARMETHOD=JK   BRR</b><br>or <b>NOMCAR</b> |

For example, the following statements create an output data set MyStrata, which contains the “StrataInfo” table, and an output data set MyStat, which contains the “Statistics” table for the ice cream study discussed in the section “Stratified Sampling” on page 7781:

```

title1 'Analysis of Ice Cream Spending';
proc surveymeans data=IceCream total=StudentTotals;
 strata Grade / list;
 var Spending Group;
 weight Weight;
 ods output
 StrataInfo = MyStrata
 Statistics = MyStat;
run;

```

## Examples: SURVEYMEANS Procedure

The section “Getting Started: SURVEYMEANS Procedure” on page 7779 contains examples of analyzing data from simple random sampling and stratified simple random sample designs. This section provides more examples that illustrate how to use PROC SURVEYMEANS.

### Example 92.1: Stratified Cluster Sample Design

Consider the example in the section “Stratified Sampling” on page 7781. The study population is a junior high school with a total of 4,000 students in grades 7, 8, and 9. Researchers want to know how much these students spend weekly for ice cream, on the average, and what percentage of students spend at least \$10 weekly for ice cream.

The example in the section “Stratified Sampling” on page 7781 assumes that the sample of students was selected using a stratified simple random sample design. This example shows analysis based on a more complex sample design.

Suppose that every student belongs to a study group and that study groups are formed within each grade level. Each study group contains between two and four students. Table 92.5 shows the total number of study groups for each grade.

**Table 92.5** Study Groups and Students by Grade

| Grade | Number of Study Groups | Number of Students |
|-------|------------------------|--------------------|
| 7     | 608                    | 1,824              |
| 8     | 252                    | 1,025              |
| 9     | 403                    | 1,151              |
| Total | 1263                   | 4,000              |

It is quicker and more convenient to collect data from students in the same study group than to collect data from students individually. Therefore, this study uses a stratified clustered sample design. The primary sampling units, or clusters, are study groups. The list of all study groups in the school is stratified by grade level. From each grade level, a sample of study groups is randomly selected, and all students in each selected study group are interviewed. The sample consists of eight study groups from the 7th grade, three groups from the 8th grade, and five groups from the 9th grade.

The SAS data set IceCreamStudy saves the responses of the selected students:

```
data IceCreamStudy;
 input Grade StudyGroup Spending @@;
 if (Spending < 10) then Group='less';
 else Group='more';
 datalines;
7 34 7 7 34 7 7 412 4 9 27 14
7 34 2 9 230 15 9 27 15 7 501 2
9 230 8 9 230 7 7 501 3 8 59 20
7 403 4 7 403 11 8 59 13 8 59 17
```

```

8 143 12 8 143 16 8 59 18 9 235 9
8 143 10 9 312 8 9 235 6 9 235 11
9 312 10 7 321 6 8 156 19 8 156 14
7 321 3 7 321 12 7 489 2 7 489 9
7 78 1 7 78 10 7 489 2 7 156 1
7 78 6 7 412 6 7 156 2 9 301 8
;

```

In the data set `IceCreamStudy`, the variable `Grade` contains a student's grade. The variable `StudyGroup` identifies a student's study group. It is possible for students from different grades to have the same study group number because study groups are sequentially numbered within each grade. The variable `Spending` contains a student's response regarding how much he spends per week for ice cream, in dollars. The variable `GROUP` indicates whether a student spends at least \$10 weekly for ice cream. It is not necessary to store the data in order of grade and study group.

The SAS data set `StudyGroup` is created to provide PROC SURVEYMEANS with the sample design information shown in [Table 92.5](#):

```

data StudyGroups;
 input Grade _total_;
 datalines;
7 608
8 252
9 403
;

```

The variable `Grade` identifies the strata, and the variable `_TOTAL_` contains the total number of study groups in each stratum. As discussed in the section “[Specification of Population Totals and Sampling Rates](#)” on page 7805, the population totals stored in the variable `_TOTAL_` should be expressed in terms of the primary sampling units (PSUs), which are study groups in this example. Therefore, the variable `_TOTAL_` contains the total number of study groups for each grade, rather than the total number of students.

In order to obtain unbiased estimates, you create sampling weights by using the following SAS statements:

```

data IceCreamStudy;
 set IceCreamStudy;
 if Grade=7 then Prob=8/608;
 if Grade=8 then Prob=3/252;
 if Grade=9 then Prob=5/403;
 Weight=1/Prob;
run;

```

The sampling weights are the reciprocals of the probabilities of selections. The variable `Weight` contains the sampling weights. Because the sampling design is clustered and all students from each selected cluster are interviewed, the sampling weights equal the inverse of the cluster (or study group) selection probabilities.

The following SAS statements perform the analysis for this sample design:

```

title1 'Analysis of Ice Cream Spending';
proc surveymeans data=IceCreamStudy total=StudyGroups;
 strata Grade / list;
 cluster StudyGroup;
 var Spending Group;
 weight Weight;
run;

```

[Output 92.1.1](#) provides information about the sample design and the input data set. There are three strata in the sample design, and the sample contains 16 clusters and 40 observations. The variable `Group` has two levels, 'less' and 'more.'

**Output 92.1.1** Data Summary and Class Information

| Analysis of Ice Cream Spending |        |           |
|--------------------------------|--------|-----------|
| The SURVEYMEANS Procedure      |        |           |
| Data Summary                   |        |           |
| Number of Strata               |        | 3         |
| Number of Clusters             |        | 16        |
| Number of Observations         |        | 40        |
| Sum of Weights                 |        | 3162.6    |
| Class Level Information        |        |           |
| Class                          |        |           |
| Variable                       | Levels | Values    |
| Group                          | 2      | less more |

[Output 92.1.2](#) displays information for each stratum. Since the primary sampling units in this design are study groups, the population totals shown in [Output 92.1.2](#) are the total numbers of study groups for each stratum or grade. This differs from [Output 92.3](#), which provides the population totals in terms of students since students were the primary sampling units for that design. [Output 92.1.2](#) also displays the number of clusters for each stratum and analysis variable.

## Output 92.1.2 Stratum Information

| Stratum Information |       |                  |               |       |                |           |
|---------------------|-------|------------------|---------------|-------|----------------|-----------|
| Stratum Index       | Grade | Population Total | Sampling Rate | N Obs | Variable       | Level     |
| 1                   | 7     | 608              | 1.32%         | 20    | Spending Group | less more |
| 2                   | 8     | 252              | 1.19%         | 9     | Spending Group | less more |
| 3                   | 9     | 403              | 1.24%         | 11    | Spending Group | less more |

| Stratum Information |       |                  |               |       |                |               |
|---------------------|-------|------------------|---------------|-------|----------------|---------------|
| Stratum Index       | Grade | Population Total | Sampling Rate | N Obs | Variable       | N             |
| 1                   | 7     | 608              | 1.32%         | 20    | Spending Group | 20<br>17<br>3 |
| 2                   | 8     | 252              | 1.19%         | 9     | Spending Group | 9<br>0<br>9   |
| 3                   | 9     | 403              | 1.24%         | 11    | Spending Group | 11<br>6<br>5  |

| Stratum Information |       |                  |               |       |                |             |
|---------------------|-------|------------------|---------------|-------|----------------|-------------|
| Stratum Index       | Grade | Population Total | Sampling Rate | N Obs | Variable       | Clusters    |
| 1                   | 7     | 608              | 1.32%         | 20    | Spending Group | 8<br>8<br>3 |
| 2                   | 8     | 252              | 1.19%         | 9     | Spending Group | 3<br>0<br>3 |
| 3                   | 9     | 403              | 1.24%         | 11    | Spending Group | 5<br>4<br>4 |

Output 92.1.3 displays the estimates of the average weekly ice cream expenditure and the percentage of students spending at least \$10 weekly for ice cream.

**Output 92.1.3** Statistics

| Statistics |       |    |          |                      |                 |            |
|------------|-------|----|----------|----------------------|-----------------|------------|
| Variable   | Level | N  | Mean     | Std Error<br>of Mean | 95% CL for Mean |            |
| Spending   |       | 40 | 8.923860 | 0.650859             | 7.51776370      | 10.3299565 |
| Group      | less  | 23 | 0.561437 | 0.056368             | 0.43966057      | 0.6832130  |
|            | more  | 17 | 0.438563 | 0.056368             | 0.31678698      | 0.5603394  |

**Example 92.2: Domain Analysis**

Suppose that you are studying profiles of 800 top-performing companies to provide information about their impact on the economy. You are also interested in the company profiles within each market type. A sample of 66 companies is selected with unequal probability across market types. However, market type is not included in the sample design. Thus, the number of companies within each market type is a random variable in your sample. To obtain statistics within each market type, you should use domain analysis. The data of the 66 companies are saved in the following data set:

```

data Company;
 length Type $14;
 input Type$ Asset Sale Value Profit Employee Weight;
 datalines;
Other 2764.0 1828.0 1850.3 144.0 18.7 9.6
Energy 13246.2 4633.5 4387.7 462.9 24.3 42.6
Finance 3597.7 377.8 93.0 14.0 1.1 12.2
Transportation 6646.1 6414.2 2377.5 348.2 47.1 21.8
HiTech 1068.4 1689.8 1430.2 72.9 4.6 4.3
Manufacturing 1125.0 1719.4 1057.5 98.1 20.4 4.5
Other 1459.0 1241.4 452.7 24.5 20.1 5.5
Finance 2672.3 262.5 296.2 23.1 2.2 9.3
Finance 311.0 566.2 932.0 52.8 2.7 1.9
Energy 1148.6 1014.6 485.1 60.6 4.0 4.5
Finance 5327.0 572.4 372.9 25.2 4.2 17.7
Energy 1602.7 678.4 653.0 75.6 2.8 6.0
Energy 5808.8 1288.4 2007.0 318.8 5.9 19.2
Medical 268.8 204.4 820.9 45.6 3.7 1.8
Transportation 5222.6 2627.8 1910.0 245.6 22.8 17.4
Other 872.7 1419.4 939.3 69.7 12.2 3.7
Retail 4461.7 8946.8 4662.7 289.0 132.1 15.0
HiTech 6719.2 6942.0 8240.2 381.3 85.8 22.1
Retail 833.4 1538.8 1090.3 64.9 15.4 3.5
Finance 415.9 167.3 1126.8 56.8 0.7 2.2
HiTech 442.4 1139.9 1039.9 57.6 22.7 2.3
Other 801.5 1157.0 664.2 56.9 15.5 3.4
Finance 4954.8 468.8 366.4 41.7 3.0 16.5
Finance 2661.9 257.9 181.1 21.2 2.1 9.3
Finance 5345.8 530.1 337.4 36.4 4.3 17.8

```

|                |         |         |        |       |       |      |
|----------------|---------|---------|--------|-------|-------|------|
| Energy         | 3334.3  | 1644.7  | 1407.8 | 157.6 | 6.4   | 11.4 |
| Manufacturing  | 1826.6  | 2671.7  | 483.2  | 71.3  | 25.3  | 6.7  |
| Retail         | 618.8   | 2354.7  | 767.7  | 58.6  | 19.0  | 2.9  |
| Retail         | 1529.1  | 6534.0  | 826.3  | 58.3  | 65.8  | 5.7  |
| Manufacturing  | 4458.4  | 4824.5  | 3132.1 | 28.9  | 67.0  | 15.0 |
| HiTech         | 5831.7  | 6611.1  | 9464.7 | 459.6 | 86.7  | 19.3 |
| Medical        | 6468.3  | 4199.2  | 3170.4 | 270.1 | 59.5  | 21.3 |
| Energy         | 1720.7  | 473.1   | 811.1  | 86.6  | 1.6   | 6.3  |
| Energy         | 1679.7  | 1379.9  | 721.1  | 91.8  | 4.5   | 6.2  |
| Retail         | 4018.2  | 16823.4 | 2038.3 | 178.1 | 162.0 | 13.6 |
| Other          | 227.1   | 575.8   | 1083.8 | 62.6  | 1.9   | 1.6  |
| Finance        | 3872.8  | 362.0   | 209.3  | 27.6  | 2.4   | 13.1 |
| Retail         | 3359.3  | 4844.7  | 2651.4 | 224.1 | 75.6  | 11.5 |
| Energy         | 1295.6  | 356.9   | 180.8  | 162.3 | 0.6   | 5.0  |
| Energy         | 1658.0  | 626.6   | 688.0  | 126.0 | 3.5   | 6.1  |
| Finance        | 12156.7 | 1345.5  | 680.7  | 106.6 | 9.4   | 39.2 |
| HiTech         | 3982.6  | 4196.0  | 3946.8 | 313.9 | 64.3  | 13.5 |
| Finance        | 8760.7  | 886.4   | 1006.9 | 90.0  | 7.5   | 28.5 |
| Manufacturing  | 2362.2  | 3153.3  | 1080.0 | 137.0 | 25.2  | 8.4  |
| Transportation | 2499.9  | 3419.0  | 992.6  | 47.2  | 25.3  | 8.8  |
| Energy         | 1430.4  | 1610.0  | 664.3  | 77.7  | 3.5   | 5.4  |
| Energy         | 13666.5 | 15465.4 | 2736.7 | 411.4 | 26.6  | 43.9 |
| Manufacturing  | 4069.3  | 4174.7  | 2907.6 | 289.2 | 38.2  | 13.7 |
| Energy         | 2924.7  | 711.9   | 1067.8 | 146.7 | 3.4   | 10.1 |
| Transportation | 1262.1  | 1716.0  | 364.3  | 71.2  | 14.5  | 4.9  |
| Medical        | 684.4   | 672.9   | 287.4  | 61.8  | 6.0   | 3.1  |
| Energy         | 3069.3  | 1719.0  | 1439.0 | 196.4 | 4.9   | 10.6 |
| Medical        | 246.5   | 318.8   | 924.1  | 43.8  | 3.1   | 1.7  |
| Finance        | 11562.2 | 1128.5  | 580.4  | 64.2  | 6.7   | 37.3 |
| Finance        | 9316.0  | 1059.4  | 816.5  | 95.9  | 8.0   | 30.2 |
| Retail         | 1094.3  | 3848.0  | 563.3  | 29.4  | 44.7  | 4.4  |
| Retail         | 1102.1  | 4878.3  | 932.4  | 65.2  | 47.3  | 4.4  |
| HiTech         | 466.4   | 675.8   | 845.7  | 64.5  | 5.2   | 2.4  |
| Manufacturing  | 10839.4 | 5468.7  | 1895.4 | 232.8 | 47.8  | 35.0 |
| Manufacturing  | 733.5   | 2135.3  | 96.6   | 10.9  | 2.7   | 3.2  |
| Manufacturing  | 10354.2 | 14477.4 | 5607.2 | 321.9 | 188.5 | 33.5 |
| Energy         | 1902.1  | 2697.9  | 329.3  | 34.2  | 2.2   | 6.9  |
| Other          | 2245.2  | 2132.2  | 2230.4 | 198.9 | 8.0   | 8.0  |
| Transportation | 949.4   | 1248.3  | 298.9  | 35.4  | 10.4  | 3.9  |
| Retail         | 2834.4  | 2884.6  | 458.2  | 41.2  | 49.8  | 9.8  |
| Retail         | 2621.1  | 6173.8  | 1992.7 | 183.7 | 115.1 | 9.2  |

;

For each company in your sample, the variables are defined as follows:

- Type identifies the type of market for the company.
- Asset contains the company's assets, in millions of dollars.
- Sale contains sales, in millions of dollars.
- Value contains the market value of the company, in millions of dollars.
- Profit contains the profit, in millions of dollars.

- Employee contains the number of employees, in thousands.
- Weight contains the sampling weight.

The following SAS statements use PROC SURVEYMEANS to perform the domain analysis, estimating means, and other statistics for the overall population and also for the subpopulations (or domain) defined by market type. The DOMAIN statement specifies Type as the domain variable:

```

title 'Top Companies Profile Study';
proc surveymeans data=Company total=800 mean sum;
 var Asset Sale Value Profit Employee;
 weight Weight;
 domain Type;
run;

```

Output 92.2.1 shows that there are 66 observations in the sample. The sum of the sampling weights equals 799.8, which is close to the total number of companies in the study population.

**Output 92.2.1** Company Profile Study

| Top Companies Profile Study |             |                      |         |             |
|-----------------------------|-------------|----------------------|---------|-------------|
| The SURVEYMEANS Procedure   |             |                      |         |             |
| Data Summary                |             |                      |         |             |
| Number of Observations      |             | 66                   |         |             |
| Sum of Weights              |             | 799.8                |         |             |
| Statistics                  |             |                      |         |             |
| Variable                    | Mean        | Std Error<br>of Mean | Sum     | Std Dev     |
| Asset                       | 6523.488510 | 720.557075           | 5217486 | 1073829     |
| Sale                        | 4215.995799 | 839.132506           | 3371953 | 847885      |
| Value                       | 2145.935121 | 342.531720           | 1716319 | 359609      |
| Profit                      | 188.788210  | 25.057876            | 150993  | 30144       |
| Employee                    | 36.874869   | 7.787857             | 29493   | 7148.003298 |

The “Statistics” table in Output 92.2.1 displays the estimates of the mean and total for all analysis variables for the entire set of 800 companies, while Output 92.2.2 shows the mean and total estimates for each company type.



## Output 92.2.2 Domain Analysis for Company Profile Study

| Domain Analysis: Type |          |             |                      |             |             |
|-----------------------|----------|-------------|----------------------|-------------|-------------|
| Type                  | Variable | Mean        | Std Error<br>of Mean | Sum         | Std Dev     |
| Energy                | Asset    | 7868.302932 | 1941.699163          | 1449341     | 785962      |
|                       | Sale     | 5419.679099 | 2416.214417          | 998305      | 673373      |
|                       | Value    | 2249.297177 | 520.295162           | 414321      | 213580      |
|                       | Profit   | 289.564658  | 52.512141            | 53338       | 25927       |
|                       | Employee | 14.151194   | 3.974697             | 2606.650000 | 1481.777769 |
| Finance               | Asset    | 7890.190264 | 1057.185336          | 1855773     | 704506      |
|                       | Sale     | 829.210502  | 115.762531           | 195030      | 74436       |
|                       | Value    | 565.068197  | 76.964547            | 132904      | 48156       |
|                       | Profit   | 63.716837   | 10.099341            | 14986       | 5801.108513 |
|                       | Employee | 5.806293    | 0.811555             | 1365.640000 | 519.658410  |
| HiTech                | Asset    | 5031.959781 | 732.436967           | 321542      | 183302      |
|                       | Sale     | 5464.292019 | 731.296997           | 349168      | 196013      |
|                       | Value    | 6707.828482 | 1194.160584          | 428630      | 249154      |
|                       | Profit   | 346.407042  | 42.299004            | 22135       | 12223       |
|                       | Employee | 70.766980   | 8.683595             | 4522.010000 | 2524.778281 |
| Manufacturing         | Asset    | 7403.004250 | 1454.921083          | 888361      | 492577      |
|                       | Sale     | 7207.638833 | 2112.444703          | 864917      | 501679      |
|                       | Value    | 2986.442750 | 799.121544           | 358373      | 196979      |
|                       | Profit   | 211.933583  | 39.993255            | 25432       | 13322       |
|                       | Employee | 83.314333   | 31.089019            | 9997.720000 | 6294.309490 |
| Medical               | Asset    | 5046.570609 | 1218.444638          | 140799      | 131942      |
|                       | Sale     | 3313.219713 | 758.216303           | 92439       | 85655       |
|                       | Value    | 2561.614695 | 530.802245           | 71469       | 64663       |
|                       | Profit   | 218.682796  | 44.051447            | 6101.250000 | 5509.560969 |
|                       | Employee | 46.518996   | 11.135955            | 1297.880000 | 1213.651734 |
| Other                 | Asset    | 1850.250000 | 338.128984           | 58838       | 31375       |
|                       | Sale     | 1620.784906 | 168.686773           | 51541       | 24593       |
|                       | Value    | 1432.820755 | 297.869828           | 45564       | 24204       |
|                       | Profit   | 115.089937  | 27.970560            | 3659.860000 | 2018.201371 |
|                       | Employee | 14.306604   | 2.313733             | 454.950000  | 216.327710  |
| Retail                | Asset    | 2939.845750 | 393.692369           | 235188      | 94605       |
|                       | Sale     | 7395.453500 | 1746.187580          | 591636      | 263263      |
|                       | Value    | 2103.863125 | 529.756409           | 168309      | 78304       |
|                       | Profit   | 157.171875  | 31.734253            | 12574       | 5478.281027 |
|                       | Employee | 93.624000   | 15.726743            | 7489.920000 | 3093.832061 |
| Transportation        | Asset    | 4712.047359 | 888.954411           | 267644      | 163516      |
|                       | Sale     | 4030.233275 | 1015.555708          | 228917      | 142669      |
|                       | Value    | 1703.330282 | 313.841326           | 96749       | 58947       |
|                       | Profit   | 224.762324  | 56.168925            | 12767       | 8287.585418 |
|                       | Employee | 30.946303   | 6.786270             | 1757.750000 | 1066.586615 |

### Example 92.3: Ratio Analysis

Suppose you are interested in the profit per employee and the sale per employee among the 800 top-performing companies in the data in the previous example. The following SAS statements illustrate how you can use PROC SURVEYMEANS to estimate these ratios:

```

title 'Ratio Analysis in Top Companies Profile Study';
proc surveymeans data=Company total=800 ratio;
 var Profit Sale Employee;
 weight Weight;
 ratio Profit Sale / Employee;
run;

```

The RATIO statement requests the ratio of the profit and the sales to the number of employees.

Output 92.3.1 shows the estimated ratios and their standard errors. Because the profit and the sales figures are in millions of dollars, and the employee numbers are in thousands, the profit per employee is estimated as \$5,120 with a standard error of \$1,059, and the sales per employee are \$114,332 with a standard error of \$20,503.

**Output 92.3.1** Estimate Ratios

| Ratio Analysis in Top Companies Profile Study |             |            |           |
|-----------------------------------------------|-------------|------------|-----------|
| The SURVEYMEANS Procedure                     |             |            |           |
| Ratio Analysis                                |             |            |           |
| Numerator                                     | Denominator | Ratio      | Std Err   |
| Sale                                          | Employee    | 114.332497 | 20.502742 |
| Profit                                        | Employee    | 5.119698   | 1.058939  |

### Example 92.4: Analyzing Survey Data with Missing Values

As described in the section “Missing Values” on page 7804, the SURVEYMEANS procedure excludes an observation from the analysis if it has a missing value for the analysis variable or a nonpositive value for the WEIGHT variable.

However, if there is evidence indicating that the nonrespondents are different from the respondents for your study, you can use the NOMCAR option to compute descriptive statistics among respondents while still counting the number of nonrespondents.

We use the ice cream example in the section “Stratified Sampling” on page 7781 to illustrate how to perform similar analysis when there are missing values.

Suppose that some of the students failed to provide the amounts spent on ice cream, as shown in the following data set, IceCream:

```

data IceCream;
 input Grade Spending @@;
 if Grade=7 then Prob=20/1824;
 if Grade=8 then Prob=9/1025;
 if Grade=9 then Prob=11/1151;
 Weight=1/Prob;
 datalines;
7 7 7 7 8 . 9 10 7 . 7 10 7 3 8 20 8 19 7 2
7 . 9 15 8 16 7 6 7 6 7 6 9 15 8 17 8 14 9 .
9 8 9 7 7 3 7 12 7 4 9 14 8 18 9 9 7 2 7 1
7 4 7 11 9 8 8 . 8 13 7 . 9 . 9 11 7 2 7 9
;

data StudentTotals;
 input Grade _total_;
 datalines;
7 1824
8 1025
9 1151
;

```

Considering the possibility that those students who did not respond spend differently than those students who did respond, you can use the NOMCAR option to request the analysis to treat the respondents as a domain rather than exclude the nonrespondents.

The following SAS statements produce the desired analysis:

```

title 'Analysis of Ice Cream Spending';
proc surveymeans data=IceCream total=StudentTotals nomcar mean sum;
 strata Grade;
 var Spending;
 weight Weight;
run;

```

Output 92.4.1 summarizes the analysis including the variance estimation method.

#### Output 92.4.1 Analysis of Incomplete Ice Cream Data Excluding Observations with Missing Values

| Analysis of Ice Cream Spending |               |
|--------------------------------|---------------|
| The SURVEYMEANS Procedure      |               |
| Data Summary                   |               |
| Number of Strata               | 3             |
| Number of Observations         | 40            |
| Sum of Weights                 | 4000          |
| Variance Estimation            |               |
| Method                         | Taylor Series |
| Missing Values                 | NOMCAR        |

Output 92.4.2 shows the mean and total estimates when treating respondents as a domain in the student population. Although the point estimates are the same as the analysis without the NOMCAR option, for this particular example, the variance estimations are slightly higher when you assume that the missingness is not completely at random.

**Output 92.4.2** Analysis of Incomplete Ice Cream Data Excluding Observations with Missing Values

| Variable | Statistics |                      |       |             |
|----------|------------|----------------------|-------|-------------|
|          | Mean       | Std Error<br>of Mean | Sum   | Std Dev     |
| Spending | 9.770542   | 0.652347             | 32139 | 3515.126876 |

### Example 92.5: Variance Estimation Using Replication Methods

In order to improve service, the San Francisco Municipal Railway (MUNI) conducts a survey to estimate passenger’s average waiting time for MUNI’s subway system.

The study uses a stratified cluster sample design. Each MUNI subway line is a stratum. The subway lines included in the study are ‘J-Church,’ ‘K-Ingleside,’ ‘L-Taraval,’ ‘M-Ocean View,’ ‘N-Judah,’ and the street car ‘F-Market & Wharves.’ The MUNI vehicles in service for these lines during a day are primary sampling units. Within each stratum, two vehicles (PSUs) are randomly selected. Then the waiting times of passengers for a selected MUNI vehicle are collected.

Table 92.6 shows the number of passengers that are interviewed in each of the selected MUNI vehicles.

**Table 92.6** The Sample of the MUNI Waiting Time Study

| MUNI Line          | Vehicle | Number of Passengers |
|--------------------|---------|----------------------|
| F-Market & Wharves | 1       | 65                   |
|                    | 2       | 102                  |
| J-Church           | 1       | 101                  |
|                    | 2       | 142                  |
| K-Ingleside        | 1       | 145                  |
|                    | 2       | 180                  |
| L-Taraval          | 1       | 135                  |
|                    | 2       | 185                  |
| M-Ocean View       | 1       | 139                  |
|                    | 2       | 203                  |
| N-Judah            | 1       | 306                  |
|                    | 2       | 234                  |

The collected data are saved in the SAS data set MUNISURVEY. The variable Line indicates which MUNI line a passenger is riding. The variable vehicle identifies the vehicle that a passenger is boarding. The variable

Waittime is the time (in minutes) that a passenger waited. The variable weight contains the sampling weights, which are determined by selection probabilities within each stratum.

Output 92.5.1 displays the first 10 observations of the data set MUNIsurvey.

**Output 92.5.1** First 10 Observations in the Data Set from the MUNI Subway Survey

| MUNI Subway Passenger Waiting Time Survey Data |                    |         |           |          |        |
|------------------------------------------------|--------------------|---------|-----------|----------|--------|
| Obs                                            | line               | vehicle | passenger | waittime | weight |
| 1                                              | F-Market & Wharves | 1       | 1         | 18       | 59     |
| 2                                              | F-Market & Wharves | 1       | 2         | 0        | 59     |
| 3                                              | F-Market & Wharves | 1       | 3         | 16       | 59     |
| 4                                              | F-Market & Wharves | 1       | 4         | 13       | 59     |
| 5                                              | F-Market & Wharves | 1       | 5         | 5        | 59     |
| 6                                              | F-Market & Wharves | 1       | 6         | 13       | 59     |
| 7                                              | F-Market & Wharves | 1       | 7         | 7        | 59     |
| 8                                              | F-Market & Wharves | 1       | 8         | 5        | 59     |
| 9                                              | F-Market & Wharves | 1       | 9         | 16       | 59     |
| 10                                             | F-Market & Wharves | 1       | 10        | 5        | 59     |

Using the VARMETHOD=BRR option, the following SAS statements analyze the MUNI subway survey by using the BRR method to estimate the variance:

```

title 'MUNI Passenger Waiting Time Analysis Using BRR';
proc surveymeans data=MUNIsurvey mean varmethod=brr mean clm;
 strata line;
 cluster vehicle;
 var waittime;
 weight weight;
run;

```

The STRATUM variable is line, which corresponds to MUNI lines. The two clusters within each stratum are identified by the variable vehicle. The sampling weights are stored in the variable weight. The mean and confident limits for passenger waiting time (in minutes) are requested statistics.

Output 92.5.2 summarizes the data and indicates that the variance estimation method is BRR with 8 replicates.

**Output 92.5.2** MUNI Passenger Waiting Time Analysis Using the BRR Method

| MUNI Passenger Waiting Time Analysis Using BRR |        |
|------------------------------------------------|--------|
| The SURVEYMEANS Procedure                      |        |
| Data Summary                                   |        |
| Number of Strata                               | 6      |
| Number of Clusters                             | 12     |
| Number of Observations                         | 1937   |
| Sum of Weights                                 | 143040 |
| Variance Estimation                            |        |
| Method                                         | BRR    |
| Number of Replicates                           | 8      |

Output 92.5.3 reports that the average passenger waiting time for a MUNI vehicle is 7.33 minutes, with an estimated standard of 0.24 minutes, using the BRR method. The 95% confident limits for the mean are estimated as 6.75 to 7.91 minutes.

**Output 92.5.3** MUNI Passenger Waiting Time Analysis Using the BRR Method

| Statistics |          |                      |                       |
|------------|----------|----------------------|-----------------------|
| Variable   | Mean     | Std Error<br>of Mean | 95% CL for Mean       |
| waittime   | 7.333012 | 0.237557             | 6.75172983 7.91429366 |

Alternatively, the variance can be estimated using the jackknife method if the VARMETHOD=JACKKNIFE option is used. The following SAS statements analyze the MUNI subway survey by using the jackknife method to estimate the variance:

```

title 'MUNI Passenger Waiting Time Analysis Using Jackknife';
proc surveymeans data=MUNISURVEY mean varmethod=jackknife mean clm;
 strata line;
 cluster vehicle;
 var waittime;
 weight weight;
run;

```

Output 92.5.4 summarizes the data and indicates that the variance estimation method is jackknife with 12 replicates.

**Output 92.5.4** MUNI Passenger Waiting Time Analysis Using the Jackknife Method

| MUNI Passenger Waiting Time Analysis Using Jackknife |           |
|------------------------------------------------------|-----------|
| The SURVEYMEANS Procedure                            |           |
| Data Summary                                         |           |
| Number of Strata                                     | 6         |
| Number of Clusters                                   | 12        |
| Number of Observations                               | 1937      |
| Sum of Weights                                       | 143040    |
| Variance Estimation                                  |           |
| Method                                               | Jackknife |
| Number of Replicates                                 | 12        |

Output 92.5.5 reports the statistics computed using the jackknife method. Although the average passenger waiting time remains the same (7.33 minutes), the standard error is slightly smaller 0.23 minutes when the jackknife method is used, as opposed to 0.24 minutes when the BRR method is used. The 95% confidence limits are between 6.76 and 7.90 minutes when the jackknife method is used.

**Output 92.5.5** MUNI Passenger Waiting Time Analysis Using the Jackknife Method

| Statistics |          |                      |                       |
|------------|----------|----------------------|-----------------------|
| Variable   | Mean     | Std Error<br>of Mean | 95% CL for Mean       |
| waittime   | 7.333012 | 0.232211             | 6.76481105 7.90121244 |

---

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# Chapter 93

## The SURVEYPHREG Procedure

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## Overview: SURVEYPHREG Procedure

The SURVEYPHREG procedure performs regression analysis based on the Cox proportional hazards model for sample survey data. Cox’s semiparametric model is widely used in the analysis of survival data to estimate hazard rates when adequate explanatory variables are available. The procedure provides design-based variance estimates, confidence intervals, and hypothesis tests concerning the parameters and model effects. See Chapter 3, “Introduction to Statistical Modeling with SAS/STAT Software,” and Chapter 14, “Introduction to Survey Procedures,” for an introduction to the basic concepts of survey data analysis; see Chapter 13, “Introduction to Survival Analysis Procedures,” for an introduction to the basic concepts of survival analysis.

The survival time of each member of a finite population is assumed to follow its own hazard function,  $\lambda_i(t)$ , expressed as

$$\lambda_i(t) = \lambda(t; \mathbf{Z}_i(t)) = \lambda_0(t) \exp(\mathbf{Z}_i'(t)\boldsymbol{\beta})$$

where  $\lambda_0(t)$  is an arbitrary and unspecified baseline hazard function,  $\mathbf{Z}_i(t)$  is the vector of explanatory variables for the  $i$ th population unit at time  $t$ , and  $\boldsymbol{\beta}$  is the vector of unknown regression parameters.

The finite population regression parameter  $\boldsymbol{\beta}_N$  is defined as the maximizer of the partial log likelihood when the entire finite population is observed. The SURVEYPHREG procedure produces a sample-based estimate  $\hat{\boldsymbol{\beta}}$  of the proportional hazards regression parameters  $\boldsymbol{\beta}_N$  for the finite population by maximizing the partial pseudo-log-likelihood  $l_\pi(\boldsymbol{\beta}; \mathbf{Z}_i(t), t_i)$  based on observed covariates  $\mathbf{Z}_i(t)$  and observed survival time  $t_i$ . The procedure also produces an estimate of the sampling variance  $V(\hat{\boldsymbol{\beta}}|\mathcal{F}_N)$ , which assumes that the values of

the finite population  $\mathcal{F}_N$  are fixed. For statistical inference, PROC SURVEYPHREG incorporates complex survey sample designs, including designs with stratification, clustering, and unequal weighting.

The procedure also allows time-dependent explanatory variables. An explanatory variable is time-dependent if its value for any given individual can change over time. Time-dependent variables have many useful applications in survival analysis. You can include time-dependent variables such as blood pressure or blood chemistry measures that vary with time during the course of a study. You can also use time-dependent variables to test the validity of the proportional hazards model.

Several optimization techniques are available in SURVEYPHREG to maximize the log likelihood. Hazard ratio estimates can also be obtained along with parameter estimates. Sampling errors of the regression parameters and hazard ratios are computed by using either the Taylor series (linearization) method or one of the replication (resampling) methods that are based on complex sample designs (Binder 1983; Wolter 2007; Särndal, Swensson, and Wretman 1992; Binder 1992; Lohr 2010; Fuller 2009). These variance estimators essentially assume the finite population as fixed and estimate the variability due to the random sample selection mechanism.

The remaining sections of this chapter contain information about how to use PROC SURVEYPHREG, information about the underlying statistical methodology, and some applications of the procedure. The section “[Getting Started: SURVEYPHREG Procedure](#)” on page 7857 introduces PROC SURVEYPHREG with an example. The section “[Syntax: SURVEYPHREG Procedure](#)” on page 7861 describes the syntax of the procedure. The section “[Details: SURVEYPHREG Procedure](#)” on page 7884 summarizes the statistical techniques employed in PROC SURVEYPHREG. The section “[Examples: SURVEYPHREG Procedure](#)” on page 7913 includes some additional examples of useful applications. Experienced SAS/STAT software users might decide to proceed to the “Syntax” section, while other users might choose to read both the “Getting Started” and “Examples” sections before proceeding to “Syntax” and “Details.”

---

## Getting Started: SURVEYPHREG Procedure

This section uses a data set that is obtained by stratified random sampling from a simulated finite population to illustrate some of the basic features of PROC SURVEYPHREG.

Suppose the library system for a small county wants to study the length of time that books are borrowed over a specified study period, adjusting for the age of the borrower and accounting for the fact that some books are never returned. Suppose there are 10 branch libraries in the county. Assume that a list of 11,617 (simulated) transactions is available for the study period October 1, 2008, to December 31, 2008, and assume that this list can be used as the sampling frame. A stratified random sample with replacement is used to select 100 transactions, where branch libraries are the strata. The total number of transactions within branches range from 510 to 2,011 for the study period. The total sample size of 100 transactions is allocated proportionally across branches based on the number of transactions. For each selected transaction, telephone interviews were conducted to find out additional characteristics of the borrower. The data set LibrarySurvey contains the following variables for all units (transactions) in the sample:

- Branch, the library branch from which the book was borrowed
- SampleWeight, the survey sampling weight for the transaction
- CheckOut, the date the book was borrowed

- CheckIn, the date the book was returned, with a missing value if the book was not returned by December 31, 2008
- Age, the age of the borrower

```

data LibrarySurvey;
 input Branch 2.
 SamplingWeight 7.2
 CheckOut date10.
 CheckIn date10.
 Age;
 datalines;
1 103.60 08NOV2008 13NOV2008 18
1 103.60 01OCT2008 07OCT2008 30
1 103.60 05NOV2008 06NOV2008 73
1 103.60 25OCT2008 26OCT2008 53
1 103.60 09NOV2008 10NOV2008 55
2 127.50 10DEC2008 15DEC2008 39
2 127.50 19DEC2008 . 33
2 127.50 26NOV2008 27NOV2008 41
2 127.50 03NOV2008 07NOV2008 33

... more lines ...

10 118.35 14NOV2008 17NOV2008 29
10 118.35 11DEC2008 13DEC2008 35
10 118.35 21NOV2008 23NOV2008 46
;

data LibrarySurvey;
 set LibrarySurvey;
 Returned = (CheckIn ^= .);
 if (Returned) then
 lenBorrow = CheckIn - CheckOut;
 else
 lenBorrow = input('31Dec2008',date9.) - CheckOut;
run;

```

PROC SURVEYPHREG can be used to estimate the regression parameters of a proportional hazards model and the design-based variance of the estimated coefficients. The design-based variance is useful when the finite population is considered fixed, as in this example. See Lohr (2010) and Särndal, Swensson, and Wretman (1992) for details.

The following statements request a proportional hazards regression of lenBorrow on Age with Returned as the censor indicator. A transaction is considered to be censored if its check-in date is missing. The WEIGHT statement specifies the sampling weight variable (SamplingWeight), and the STRATA statement specifies the stratification variable (Branch).

```

proc surveypHreg data = LibrarySurvey;
 weight SamplingWeight;
 strata Branch;
 model lenBorrow*Returned(0) = Age;
run;

```

Summary information about the model, number of observations, survey design, censored values, and variance estimation method are shown in [Output 93.1](#). The “Model Information” table summarizes the model you fit. The “Number of Observations” table displays the number of observations read and used by the procedure. This table also displays the sum of weights read and used. The sum of weights read (11,616.79) can be used as an estimator of the population size, and the sum of weights used can be used as an estimator of the respondent size in the population. The “Design Summary” table displays survey design information such as stratification and clustering. This example implements a stratified design with 10 strata. The “Censored Summary” and “Weighted Censored Summary” tables display the (weighted) number of censored and event units. Weighted counts can be used as estimators of the corresponding finite population quantities. For example, [Output 93.1](#) shows that 10% of the sampled units are censored and an estimated 10.05% of the population units are censored.

**Figure 93.1** Summary Statistics

| The SURVEYPHREG Procedure                          |                    |       |                  |
|----------------------------------------------------|--------------------|-------|------------------|
| Model Information                                  |                    |       |                  |
| Data Set                                           | WORK.LIBRARYSURVEY |       |                  |
| Dependent Variable                                 | lenBorrow          |       |                  |
| Censoring Variable                                 | Returned           |       |                  |
| Censoring Value(s)                                 | 0                  |       |                  |
| Weight Variable                                    | SamplingWeight     |       |                  |
| Stratum Variable                                   | Branch             |       |                  |
| Ties Handling                                      | BRESLOW            |       |                  |
|                                                    |                    |       |                  |
| Number of Observations Read                        |                    |       | 100              |
| Number of Observations Used                        |                    |       | 100              |
| Sum of Weights Read                                |                    |       | 11616.79         |
| Sum of Weights Used                                |                    |       | 11616.79         |
|                                                    |                    |       |                  |
| Design Summary                                     |                    |       |                  |
| Number of Strata                                   |                    | 10    |                  |
|                                                    |                    |       |                  |
| Summary of the Number of Event and Censored Values |                    |       |                  |
|                                                    | Total              | Event | Censored         |
|                                                    |                    |       | Percent Censored |
|                                                    | 100                | 90    | 10               |
|                                                    |                    |       | 10.00            |

Figure 93.1 continued

| Summary of the Weighted Number of Event and Censored Values |               |          |                  |
|-------------------------------------------------------------|---------------|----------|------------------|
| Total                                                       | Event         | Censored | Percent Censored |
| 11616.79                                                    | 10449.22      | 1167.57  | 10.05            |
| Variance Estimation                                         |               |          |                  |
| Method                                                      | Taylor Series |          |                  |

Parameter estimates and their standard errors are shown in [Output 93.2](#). The estimated regression coefficient is highly significant with a value of 0.062, indicating a positive association between age and the length of time books are borrowed (recall that these are simulated data). In this example, the procedure uses the STRATA and WEIGHT statements to incorporate stratification and unequal weighting, respectively, into variance estimation. The degrees of freedom are calculated as the number of sampling units (100) minus the number of strata (10). Note that the estimated variance reported in [Output 93.2](#) ignores the finite population correction (*fpc*). You can use the TOTAL= or RATE= option in the PROC statement to include an *fpc* in your variance estimator.

Figure 93.2 Weighted Estimates and Their Standard Errors

| Analysis of Maximum Likelihood Estimates |    |          |                |         |         |              |
|------------------------------------------|----|----------|----------------|---------|---------|--------------|
| Parameter                                | DF | Estimate | Standard Error | t Value | Pr >  t | Hazard Ratio |
| Age                                      | 90 | 0.061593 | 0.008366       | 7.36    | <.0001  | 1.064        |

## Syntax: SURVEYPHREG Procedure

The following statements are available in the SURVEYPHREG procedure. Items within < > are optional.

```

PROC SURVEYPHREG < options > ;
 BY variables ;
 CLASS variable < (options) > < ... variable < (options) > > < / options > ;
 CLUSTER variables ;
 DOMAIN variables < variable* variable variable* variable* variable ... > ;
 ESTIMATE < 'label' > estimate-specification < / options > ;
 FREQ variable ;
 LSMEANS < model-effects > < / options > ;
 LSMESTIMATE model-effect lsmestimate-specification < / options > ;
 MODEL response < * censor(list) > = effects < / options > ;
 NLOPTIONS < options > ;
 OUTPUT < OUT=SAS-data-set > < keyword=name ... keyword=name > < / options > ;
 Programming statements ;
 REPWEIGHTS variables < / options > ;
 SLICE model-effect < / options > ;
 STRATA variables < / option > ;
 STORE < OUT= > item-store-name < / LABEL='label' > ;
 TEST < model-effects > < / options > ;
 WEIGHT variable ;

```

The PROC SURVEYPHREG and MODEL statements are required. The CLASS statement, if present, must precede the MODEL statement.

The MODEL statement specifies the analysis model. The CLASS statement specifies the categorical variables. The STRATA statement lists the variables that form the strata in a stratified sample design. The CLUSTER statement specifies cluster identification variables in a clustered sample design. The WEIGHT statement names the sampling weight variable. The NLOPTIONS statement specifies the optimization techniques. The REPWEIGHTS statement names replicate weight variables for BRR or jackknife variance estimation. The DOMAIN statement lists the variables that define domains for subpopulation analysis. The BY statement requests completely separate analyses of groups defined by the BY variables.

The rest of this section provides detailed syntax information for each statement, beginning with the PROC SURVEYPHREG statement. The remaining statements are covered in alphabetical order.

The ESTIMATE, LSMEANS, LSMESTIMATE, SLICE, STORE, and TEST statements are also available in other procedures. Summary descriptions of functionality and syntax for these statements are provided in this chapter, and you can find full documentation about them in Chapter 19, “[Shared Concepts and Topics](#).”



## PROC SURVEYPHREG Statement

**PROC SURVEYPHREG** <options> ;

The PROC SURVEYPHREG statement invokes the SURVEYPHREG procedure. It also identifies the data set to be analyzed. Table 93.1 summarizes the options available in the PROC SURVEYPHREG statement.

**Table 93.1** PROC SURVEYPHREG Statement Options

| Option     | Description                                                                    |
|------------|--------------------------------------------------------------------------------|
| DATA=      | Names the input SAS data set                                                   |
| MISSING    | Treats missing values as a valid category                                      |
| NOPRINT    | Suppresses all displayed output                                                |
| NOMCAR     | Uses missing observations specified as <i>not missing completely at random</i> |
| ORDER=     | Specifies the sort order of CLASS variables                                    |
| RATE=      | Specifies the sampling rate                                                    |
| TOTAL=     | Specifies the total number of primary sampling units                           |
| VARMETHOD= | Specifies the variance estimation method                                       |

You can specify the following options in the PROC SURVEYPHREG statement:

### DATA=SAS-data-set

names the SAS data set that contains the data to be analyzed. If you omit the DATA= option, the procedure uses the most recently created SAS data set.

### MISSING

treats missing values as a valid (nonmissing) category for all categorical variables, which include CLASS, STRATA, CLUSTER, and DOMAIN variables. By default, if you do not specify the MISSING option, an observation is excluded from the analysis if it has a missing value for any of these categorical variables. For more information, see the section “Missing Values” on page 7893.

### NOPRINT

suppresses all displayed output. Note that this option temporarily disables the Output Delivery System (ODS); see Chapter 20, “Using the Output Delivery System,” for more information.

### NOMCAR

includes observations with missing values of the analysis variables that are specified in the MODEL statement as *not missing completely at random* (NOMCAR) for Taylor series variance estimation. When you specify the NOMCAR option, PROC SURVEYPHREG computes variance estimates by analyzing the nonmissing values as a domain (subpopulation), where the entire population includes both nonmissing and missing domains. See the section “Missing Values” on page 7893 for details.

By default, PROC SURVEYPHREG excludes an observation from analyses (and the corresponding variance computations) if that observation has a missing value for any of the variables in the MODEL statement. Note that if you specify the MISSING option for classification variables, then the procedure treats the missing values as a valid nonmissing level.

The NOMCAR option applies only to Taylor series variance estimation. The replication methods, which you request with the VARMETHOD=BRR and VARMETHOD=JACKKNIFE options, do not use the NOMCAR option.

**ORDER=DATA | FORMATTED | FREQ | INTERNAL**

specifies the sort order for the levels of the classification variables (which are specified in the **CLASS** statement). This option applies to the levels for all classification variables, except when you use the (default) **ORDER=FORMATTED** option with numeric classification variables that have no explicit format. With this option, the levels of such variables are ordered by their internal value.

The **ORDER=** option can take the following values:

| Value of <b>ORDER=</b> | Levels Sorted By                                                                                                                       |
|------------------------|----------------------------------------------------------------------------------------------------------------------------------------|
| <b>DATA</b>            | Order of appearance in the input data set                                                                                              |
| <b>FORMATTED</b>       | External formatted value, except for numeric variables with no explicit format, which are sorted by their unformatted (internal) value |
| <b>FREQ</b>            | Descending frequency count; levels with the most observations come first in the order                                                  |
| <b>INTERNAL</b>        | Unformatted value                                                                                                                      |

By default, **ORDER=FORMATTED**. For **ORDER=FORMATTED** and **ORDER=INTERNAL**, the sort order is machine-dependent. For more information about sort order, see the chapter on the **SORT** procedure in the *Base SAS Procedures Guide* and the discussion of BY-group processing in *SAS Language Reference: Concepts*.

**RATE=***value* | *SAS-data-set*

**R=***value* | *SAS-data-set*

specifies the sampling rate as a nonnegative *value*, or identifies an input data set that gives the stratum sampling rates in a variable named `_RATE_`. PROC SURVEYPHREG uses this information to compute a finite population correction for Taylor series variance estimation. The procedure does not use the **RATE=** option for BRR or jackknife variance estimation, which you request with the **VARMETHOD=BRR** or **VARMETHOD=JACKKNIFE** option.

If your sample design has multiple stages, you should specify the *first-stage sampling rate*, which is the ratio of the number of primary sampling units (PSUs) that are selected to the total number of PSUs in the population.

For a nonstratified sample design, or for a stratified sample design with the same sampling rate in all strata, you should specify a nonnegative *value* for the **RATE=** option. If your design is stratified with different sampling rates in different strata, then you should name a SAS data set that contains the stratification variables and the stratum sampling rates. See the section “[Population Totals and Sampling Rates](#)” on page 7892 for details.

The sampling rate *value* must be a nonnegative number. You can specify *value* as a number between 0 and 1. Or you can specify *value* in percentage form as a number between 1 and 100, and PROC SURVEYPHREG converts that number to a proportion. The procedure treats the value 1 as 100% instead of 1%.

If you do not specify the **RATE=** or **TOTAL=** option, then the Taylor series variance estimation does not include a finite population correction. You cannot specify both the **TOTAL=** option and the **RATE=** option in the same PROC SURVEYPHREG statement.

**TOTAL=***value* | *SAS-data-set*

**N=***value* | *SAS-data-set*

specifies the total number of primary sampling units (PSUs) in the study population as a positive *value*, or identifies an input data set that gives the stratum population totals in a variable named `_TOTAL_`. PROC SURVEYPHREG uses this information to compute a finite population correction for Taylor series variance estimation. The procedure does not use the TOTAL= option for BRR or jackknife variance estimation, which you request with the **VARMETHOD=BRR** or **VARMETHOD=JACKKNIFE** option.

For a nonstratified sample design, or for a stratified sample design with the same population total in all strata, you should specify a positive *value* for the TOTAL= option, which refers to the total number of PSUs in each stratum. If your sample design is stratified with different population totals in different strata, then you should name a SAS data set that contains the stratification variables and the stratum totals. See the section “Population Totals and Sampling Rates” on page 7892 for details.

If you do not specify the TOTAL= or RATE= option, then the Taylor series variance estimation does not include a finite population correction. You cannot specify both the TOTAL= option and the RATE= option in the same PROC SURVEYPHREG statement.

**VARMETHOD=BRR** < (*method-options*) > | **JACKKNIFE** < (*method-options*) > | **TAYLOR**

specifies the variance estimation method. **VARMETHOD=TAYLOR** requests the Taylor series method, which is the default if you do not specify the VARMETHOD= option or a **REPWEIGHTS** statement. **VARMETHOD=BRR** requests variance estimation by balanced repeated replication (BRR), and **VARMETHOD=JACKKNIFE** requests variance estimation by the delete-1 jackknife method.

For **VARMETHOD=BRR** and **VARMETHOD=JACKKNIFE**, you can specify *method-options* in parentheses following the variance method name. Table 93.2 summarizes the available *method-options*.

**Table 93.2** Variance Estimation Options

| <b>VARMETHOD=</b> | <b>Variance Estimation Method</b> | <i>Method-Options</i>                                                                                                                                                                 |
|-------------------|-----------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| BRR               | Balanced repeated replication     | <b>CENTER=FULLSAMPLE</b>   <b>REPLICATES</b><br><b>FAY</b> <= <i>value</i> ><br><b>HADAMARD=SAS-data-set</b><br><b>OUTWEIGHTS=SAS-data-set</b><br><b>PRINTH</b><br><b>REPS=number</b> |
| JACKKNIFE         | Jackknife                         | <b>CENTER=FULLSAMPLE</b>   <b>REPLICATES</b><br><b>OUTJKCOEFS=SAS-data-set</b><br><b>OUTWEIGHTS=SAS-data-set</b>                                                                      |
| TAYLOR            | Taylor series linearization       | None                                                                                                                                                                                  |

The following values are available for the VARMETHOD= option:

**BRR** < (*method-options*) >

requests variance estimation by balanced repeated replication (BRR). The BRR method requires a stratified sample design with two primary sampling units (PSUs) in each stratum. If you specify the VARMETHOD=BRR option, you must also specify a STRATA statement unless you provide replicate weights with a REPWEIGHTS statement. See the section “Balanced Repeated Replication (BRR) Method” on page 7896 for details.

You can specify the following *method-options* in parentheses after the VARMETHOD=BRR option:

**CENTER=FULLSAMPLE | REPLICATES**

defines how to compute the deviations for the BRR method. CENTER=FULLSAMPLE is the default, which computes the deviations of the replicate estimates from the full sample estimate. Alternatively, you can specify CENTER=REPLICATES to compute the deviations of the replicate estimates from the average of the replicate estimates. See the section “Balanced Repeated Replication (BRR) Method” on page 7896 for details.

**FAY** < =*value* >

requests Fay’s method, which is a modification of the BRR method. See the section “Fay’s BRR Method” on page 7898 for details.

You can specify the *value* of the Fay coefficient, which is used in converting the original sampling weights to replicate weights. The Fay coefficient must be a nonnegative number less than 1. By default, the value of the Fay coefficient equals 0.5.

**HADAMARD=***SAS-data-set*

**H=***SAS-data-set*

names a SAS data set that contains the Hadamard matrix for BRR replicate construction. If you do not provide a Hadamard matrix with the HADAMARD= *method-option*, PROC SURVEYPHREG generates an appropriate Hadamard matrix for replicate construction. See the sections “Balanced Repeated Replication (BRR) Method” on page 7896 and “Hadamard Matrix” on page 7898 for details.

If a Hadamard matrix of a given dimension exists, it is not necessarily unique. Therefore, if you want to use a specific Hadamard matrix, you must provide the matrix as a SAS data set in the HADAMARD= *method-option*.

In the HADAMARD= input data set, each variable corresponds to a column of the Hadamard matrix, and each observation corresponds to a row of the matrix. You can use any variable names in the HADAMARD= data set. All values in the data set must equal either 1 or –1. You must ensure that the matrix you provide is indeed a Hadamard matrix—that is,  $\mathbf{A}'\mathbf{A} = \mathbf{R}\mathbf{I}$ , where  $\mathbf{A}$  is the Hadamard matrix of dimension  $R$  and  $\mathbf{I}$  is an identity matrix. PROC SURVEYPHREG does not check the validity of the Hadamard matrix that you provide.

The HADAMARD= input data set must contain at least  $H$  variables, where  $H$  denotes the number of first-stage strata in your design. If the data set contains more than  $H$  variables, PROC SURVEYPHREG uses only the first  $H$  variables. Similarly, the HADAMARD= input data set must contain at least  $H$  observations.

If you do not specify the REPS= *method-option*, then the number of replicates is taken to be the number of observations in the HADAMARD= input data set. If you specify the number of replicates—for example, REPS=*nreps*—then the first *nreps* observations in the HADAMARD= data set are used to construct the replicates.

You can specify the PRINTH *method-option* to display the Hadamard matrix that the procedure uses to construct replicates for BRR.

#### **OUTWEIGHTS=SAS-data-set**

names an output SAS data set to store the replicate weights that PROC SURVEYPHREG creates for BRR variance estimation. See the section “Balanced Repeated Replication (BRR) Method” on page 7896 for information about replicate weights. See the section “Replicate Weights Output Data Set” on page 7908 for details about the contents of the OUTWEIGHTS= data set.

The OUTWEIGHTS= *method-option* is not available when you provide replicate weights with a REPWEIGHTS statement.

#### **PRINTH**

displays the Hadamard matrix used to construct replicates for BRR. When you provide the Hadamard matrix in the HADAMARD= *method-option*, PROC SURVEYPHREG displays only the rows and columns that are actually used to construct replicates. See the sections “Balanced Repeated Replication (BRR) Method” on page 7896 and “Hadamard Matrix” on page 7898 for more information.

The PRINTH *method-option* is not available when you provide replicate weights with a REPWEIGHTS statement because the procedure does not use a Hadamard matrix in this case.

#### **REPS=number**

specifies the number of replicates for BRR variance estimation. The value of *number* must be an integer greater than 1.

If you do not provide a Hadamard matrix with the HADAMARD= *method-option*, the number of replicates should be greater than the number of strata and should be a multiple of 4. See the section “Balanced Repeated Replication (BRR) Method” on page 7896 for more information. If a Hadamard matrix cannot be constructed for the REPS= value that you specify, the value is increased until a Hadamard matrix of that dimension can be constructed. Therefore, it is possible for the actual number of replicates used to be larger than the REPS= value that you specify.

If you provide a Hadamard matrix with the HADAMARD= *method-option*, the value of REPS= must not be less than the number of rows in the Hadamard matrix. If you provide a Hadamard matrix and do not specify the REPS= *method-option*, the number of replicates equals the number of rows in the Hadamard matrix.

If you do not specify the REPS= or HADAMARD= *method-option* and do not include a **REPWEIGHTS** statement, the number of replicates equals the smallest multiple of 4 that is greater than the number of strata.

If you provide replicate weights with a **REPWEIGHTS** statement, the procedure does not use the REPS= *method-option*. With a **REPWEIGHTS** statement, the number of replicates equals the number of **REPWEIGHTS** variables.

### **JACKKNIFE | JK** <(method-options)>

requests variance estimation by the delete-1 jackknife method. See the section “[Jackknife Method](#)” on page 7899 for details. If you provide replicate weights with a **REPWEIGHTS** statement, **VARMETHOD=JACKKNIFE** is the default variance estimation method. The **JACKKNIFE** method requires at least two primary sampling units (PSUs) in each stratum for stratified designs unless you provide replicate weights with a **REPWEIGHTS** statement.

You can specify the following *method-options* in parentheses following **VARMETHOD=JACKKNIFE**:

#### **CENTER=FULLSAMPLE | REPLICATES**

defines how to compute the deviations for the jackknife method. **CENTER=FULLSAMPLE** is the default, which computes the deviations of the replicate estimates from the full sample estimate. Alternatively, you can specify **CENTER=REPLICATES** to compute the deviations of the replicate estimates from the average of the replicate estimates. See the section “[Jackknife Method](#)” on page 7899 for details.

#### **OUTWEIGHTS=SAS-data-set**

names an output SAS data set that contains replicate weights. See the section “[Jackknife Method](#)” on page 7899 for information about replicate weights. See the section “[Replicate Weights Output Data Set](#)” on page 7908 for more details about the contents of the **OUTWEIGHTS=** data set.

The **OUTWEIGHTS=** *method-option* is not available when you provide replicate weights with the **REPWEIGHTS** statement.

#### **OUTJKCOEFS=SAS-data-set**

names an output SAS data set that contains [jackknife coefficients](#). See the section “[Jackknife Coefficients Output Data Set](#)” on page 7909 for more details about the contents of the **OUTJKCOEFS=** data set.

### **TAYLOR**

requests [Taylor series](#) variance estimation. This is the default method if you do not specify the **VARMETHOD=** option or a **REPWEIGHTS** statement. See the section “[Taylor Series Linearization](#)” on page 7895 for more information.

---

## **BY Statement**

**BY variables ;**

You can specify a **BY** statement with **PROC SURVEYPHREG** to obtain separate analyses of observations in groups that are defined by the **BY** variables. When a **BY** statement appears, the procedure expects the input data set to be sorted in order of the **BY** variables. If you specify more than one **BY** statement, only the last one specified is used.



If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the SURVEYPHREG procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

Note that using a BY statement provides completely separate analyses of the BY groups. It does not provide a domain (subpopulation) analysis, where the total number of units in the subpopulation is not known at the time the survey is designed. For such an analysis use the DOMAIN statement.

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

---

## CLASS Statement

```
CLASS variable <(options)> ... <variable <(options)>> </options> ;
```

The CLASS statement names the classification variables to be used as explanatory variables in the analysis. The CLASS statement must precede the MODEL statement. Most *options* can be specified either as individual variable *options* or as global *options*. You can specify *options* for each variable by enclosing the options in parentheses after the variable name. You can also specify global *options* for the CLASS statement by placing the *options* after a slash (/). Global *options* are applied to all the variables specified in the CLASS statement. If you specify more than one CLASS statement, the global *options* specified in any one CLASS statement apply to all CLASS statements. However, individual CLASS variable *options* override the global *options*. The following *options* are available:

### DESCENDING

#### DESC

reverses the sort order of the classification variable. If both the DESCENDING and ORDER= options are specified, PROC SURVEYPHREG orders the categories according to the ORDER= option and then reverses that order.

### MISSING

treats missing values (“.”, “.A”, ..., “.Z” for numeric variables and blanks for character variables) as valid values for the CLASS variable.

### ORDER=DATA | FORMATTED | FREQ | INTERNAL

specifies the sort order for the levels of classification variables. This ordering determines which parameters in the model correspond to each level in the data, so the ORDER= option can be useful when you use the CONTRAST statement. By default, ORDER=FORMATTED. For ORDER=FORMATTED and ORDER=INTERNAL, the sort order is machine-dependent. When ORDER=FORMATTED is in effect for numeric variables for which you have supplied no explicit format, the levels are ordered by their internal values.

The following table shows how PROC SURVEYPHREG interprets values of the ORDER= option.

| Value of ORDER= | Levels Sorted By                                                                                                                         |
|-----------------|------------------------------------------------------------------------------------------------------------------------------------------|
| DATA            | Order of appearance in the input data set                                                                                                |
| FORMATTED       | External formatted values, except for numeric variables with no explicit format, which are sorted by their unformatted (internal) values |
| FREQ            | Descending frequency count; levels with more observations come earlier in the order                                                      |
| INTERNAL        | Unformatted value                                                                                                                        |

For more information about sort order, see the chapter on the SORT procedure in the *Base SAS Procedures Guide* and the discussion of BY-group processing in *SAS Language Reference: Concepts*.

**PARAM=keyword**

specifies the parameterization method for the classification variable or variables. You can specify any of the *keywords* shown in the following table;

Design matrix columns are created from CLASS variables according to the corresponding coding schemes:

| Value of PARAM=           | Coding                                                                                              |
|---------------------------|-----------------------------------------------------------------------------------------------------|
| EFFECT                    | Effect coding                                                                                       |
| GLM                       | Less-than-full-rank reference cell coding (this <i>keyword</i> can be used only in a global option) |
| ORDINAL<br>THERMOMETER    | Cumulative parameterization for an ordinal CLASS variable                                           |
| POLYNOMIAL<br>POLY        | Polynomial coding                                                                                   |
| REFERENCE<br>REF          | Reference cell coding                                                                               |
| ORTHEFFECT                | Orthogonalizes PARAM=EFFECT coding                                                                  |
| ORTHORDINAL<br>ORTHOTHERM | Orthogonalizes PARAM=ORDINAL coding                                                                 |
| ORTHPOLY                  | Orthogonalizes PARAM=POLYNOMIAL coding                                                              |
| ORTHREF                   | Orthogonalizes PARAM=REFERENCE coding                                                               |

All parameterizations are full rank, except for the GLM parameterization. The REF= option in the CLASS statement determines the reference level for EFFECT and REFERENCE coding and for their orthogonal parameterizations. It also indirectly determines the reference level for a singular GLM parameterization through the order of levels.

If PARAM=ORTHPOLY or PARAM=POLY and the classification variable is numeric, then the ORDER= option in the CLASS statement is ignored, and the internal unformatted values are used. See



the section “Other Parameterizations” on page 387 of Chapter 19, “Shared Concepts and Topics,” for further details.

**REF=** *'level' | keyword*

specifies the reference level for **PARAM=EFFECT**, **PARAM=REFERENCE**, and their orthogonalizations. For **PARAM=GLM**, the **REF=** option specifies a level of the classification variable to be put at the end of the list of levels. This level thus corresponds to the reference level in the usual interpretation of the linear estimates with a singular parameterization.

For an individual variable **REF=** option (but not for a global **REF=** option), you can specify the *level* of the variable to use as the reference level. Specify the formatted value of the variable if a format is assigned. For a global or individual variable **REF=** option, you can use one of the following *keywords*. The default is **REF=LAST**.

**FIRST**     designates the first ordered level as reference.

**LAST**      designates the last ordered level as reference.

**TRUNCATE**< *=n* >

specifies the length *n* of **CLASS** variable values to use in determining **CLASS** variable levels. The default is to use the full formatted length of the **CLASS** variable. If you specify **TRUNCATE** without the length *n*, the first 16 characters of the formatted values are used. When formatted values are longer than 16 characters, you can use this option to revert to the levels as determined in releases before SAS 9. The **TRUNCATE** option is available only as a global option.

## CLUSTER Statement

**CLUSTER** *variables* ;

The **CLUSTER** statement names variables that identify the first-stage clusters in a clustered sample design. First-stage clusters are also known as primary sampling units (PSUs). The combinations of categories of **CLUSTER** variables define the clusters in the sample. If there is a **STRATA** statement, clusters are nested within strata.

If your sample design has clustering at multiple stages, you should specify only the first-stage clusters (PSUs) in the **CLUSTER** statement. See the section “Specifying the Sample Design” on page 7891 for more information.

If you provide replicate weights for BRR or jackknife variance estimation with a **REPWEIGHTS** statement, you do not need to specify a **CLUSTER** statement.

The **CLUSTER variables** are one or more variables in the **DATA=** input data set. These variables can be either character or numeric, but the procedure treats them as categorical variables. The formatted values of the **CLUSTER** variables determine the **CLUSTER** variable levels. Thus, you can use formats to group values into levels. See the discussion of the **FORMAT** procedure in the *Base SAS Procedures Guide* and the discussions of the **FORMAT** statement and SAS formats in *SAS Formats and Informats: Reference*.

You can use multiple **CLUSTER** statements to specify **CLUSTER** variables. The procedure uses variables from all **CLUSTER** statements to create clusters. Cluster variables must not occur in the **CLASS** statement.

---

## DOMAIN Statement

**DOMAIN** *variables* < *variable\** *variable* *variable\** *variable\** *variable* ... > ;

The DOMAIN statement requests analysis for domains (subpopulations), in addition to analysis for the entire study population. The DOMAIN statement names the variables that identify domains, which are called domain variables.

It is common practice to compute statistics for domains. The formation of these domains might not be known at the design stage. Therefore, the sample sizes for the domains are often random. Use a DOMAIN statement to incorporate this variability into the variance estimation.

Note that a DOMAIN statement is different from a BY statement. In a BY statement, you treat the sample sizes as fixed in each subpopulation, and you perform analysis within each BY group independently.

Use the DOMAIN statement on the entire data set to perform a domain analysis. Creating a new data set from a single domain and analyzing that with PROC SURVEYPHREG yields inappropriate estimates of variance.

A domain variable can be either character or numeric. The procedure treats domain variables as categorical variables. If a variable appears by itself in a DOMAIN statement, each level of this variable determines a domain in the study population. If two or more variables are joined by asterisks (\*), then every possible combination of levels of these variables determines a domain. The procedure performs a descriptive analysis within each domain that is defined by the domain variables. Domain variables must not occur in the CLASS statement.

The formatted values of the domain variables determine the categorical variable levels. Thus, you can use formats to group values into levels. For more information, see the FORMAT procedure in the *Base SAS Procedures Guide* and the FORMAT statement and SAS formats in the *SAS Formats and Informats: Reference*.

---

## ESTIMATE Statement

**ESTIMATE** < '*label*' > *estimate-specification* < (*divisor*=*n*) >  
 < , ... < '*label*' > *estimate-specification* < (*divisor*=*n*) > >  
 < / *options* > ;

The ESTIMATE statement provides a mechanism for obtaining custom hypothesis tests. Estimates are formed as linear estimable functions of the form  $\mathbf{L}\boldsymbol{\beta}$ . You can perform hypothesis tests for the estimable functions, construct confidence limits, and obtain specific nonlinear transformations.

Table 93.3 summarizes the options available in the ESTIMATE statement.

**Table 93.3** ESTIMATE Statement Options

| Option                                                     | Description                                                               |
|------------------------------------------------------------|---------------------------------------------------------------------------|
| <b>Construction and Computation of Estimable Functions</b> |                                                                           |
| DIVISOR=                                                   | Specifies a list of values to divide the coefficients                     |
| NOFILL                                                     | Suppresses the automatic fill-in of coefficients for higher-order effects |
| SINGULAR=                                                  | Tunes the estimability checking difference                                |
| <b>Degrees of Freedom and <math>p</math>-values</b>        |                                                                           |
| ADJUST=                                                    | Determines the method for multiple comparison adjustment of estimates     |
| ALPHA= $\alpha$                                            | Determines the confidence level ( $1 - \alpha$ )                          |
| LOWER                                                      | Performs one-sided, lower-tailed inference                                |
| STEPDOWN                                                   | Adjusts multiplicity-corrected $p$ -values further in a step-down fashion |
| TESTVALUE=                                                 | Specifies values under the null hypothesis for tests                      |
| UPPER                                                      | Performs one-sided, upper-tailed inference                                |
| <b>Statistical Output</b>                                  |                                                                           |
| CL                                                         | Constructs confidence limits                                              |
| CORR                                                       | Displays the correlation matrix of estimates                              |
| COV                                                        | Displays the covariance matrix of estimates                               |
| E                                                          | Prints the $L$ matrix                                                     |
| JOINT                                                      | Produces a joint $F$ or chi-square test for the estimable functions       |
| SEED=                                                      | Specifies the seed for computations that depend on random numbers         |

For details about the syntax of the ESTIMATE statement, see the section “ESTIMATE Statement” on page 437 in Chapter 19, “Shared Concepts and Topics.”

## FREQ Statement

**FREQ** *variable* ;

The FREQ statement names a numeric *variable* that provides a frequency for each observation in the input data set. PROC SURVEYPHREG treats each observation as if it appears  $n$  times, where  $n$  is the value of the FREQ variable for the observation. If not an integer, the frequency value is truncated to an integer. If the frequency value is missing, the observation is not used in the analysis. The FREQ statement allows one frequency variable.

If you use the FREQ statement and request the jackknife or BRR variance estimator by specifying the VARMETHOD=JACKKNIFE or VARMETHOD=BRR option in the PROC SURVEYPHREG statement, then you must identify the primary sampling units with a CLUSTER statement unless you also provide replicate weights with a REPWEIGHTS statement.

## LSMEANS Statement

**LSMEANS** < model-effects > < / options > ;

The LSMEANS statement computes and compares least squares means (LS-means) of fixed effects. LS-means are *predicted population margins*—that is, they estimate the marginal means over a balanced population. In a sense, LS-means are to unbalanced designs as class and subclass arithmetic means are to balanced designs.

Table 93.4 summarizes the options available in the LSMEANS statement.

**Table 93.4** LSMEANS Statement Options

| Option                                          | Description                                                                                 |
|-------------------------------------------------|---------------------------------------------------------------------------------------------|
| <b>Construction and Computation of LS-Means</b> |                                                                                             |
| AT                                              | Modifies the covariate value in computing LS-means                                          |
| BYLEVEL                                         | Computes separate margins                                                                   |
| DIFF                                            | Requests differences of LS-means                                                            |
| OM=                                             | Specifies the weighting scheme for LS-means computation as determined by the input data set |
| SINGULAR=                                       | Tunes estimability checking                                                                 |
| <b>Degrees of Freedom and <i>p</i>-values</b>   |                                                                                             |
| ADJUST=                                         | Determines the method for multiple-comparison adjustment of LS-means differences            |
| ALPHA= $\alpha$                                 | Determines the confidence level ( $1 - \alpha$ )                                            |
| STEPDOWN                                        | Adjusts multiple-comparison <i>p</i> -values further in a step-down fashion                 |
| <b>Statistical Output</b>                       |                                                                                             |
| CL                                              | Constructs confidence limits for means and mean differences                                 |
| CORR                                            | Displays the correlation matrix of LS-means                                                 |
| COV                                             | Displays the covariance matrix of LS-means                                                  |
| E                                               | Prints the <b>L</b> matrix                                                                  |
| LINES                                           | Produces a “Lines” display for pairwise LS-means differences                                |
| MEANS                                           | Prints the LS-means                                                                         |
| PLOTS=                                          | Requests graphs of means and mean comparisons                                               |
| SEED=                                           | Specifies the seed for computations that depend on random numbers                           |

For details about the syntax of the LSMEANS statement, see the section “LSMEANS Statement” on page 453 in Chapter 19, “Shared Concepts and Topics.”

## LSMESTIMATE Statement

```
LSMESTIMATE model-effect <'label'> values <divisor=n>
 <,...<'label'> values <divisor=n>>
 </options>;
```

The LSMESTIMATE statement provides a mechanism for obtaining custom hypothesis tests among least squares means.

Table 93.5 summarizes the options available in the LSMESTIMATE statement.

**Table 93.5** LSMESTIMATE Statement Options

| Option                                          | Description                                                                            |
|-------------------------------------------------|----------------------------------------------------------------------------------------|
| <b>Construction and Computation of LS-Means</b> |                                                                                        |
| AT                                              | Modifies covariate values in computing LS-means                                        |
| BYLEVEL                                         | Computes separate margins                                                              |
| DIVISOR=                                        | Specifies a list of values to divide the coefficients                                  |
| OM=                                             | Specifies the weighting scheme for LS-means computation as determined by a data set    |
| SINGULAR=                                       | Tunes estimability checking                                                            |
| <b>Degrees of Freedom and <i>p</i>-values</b>   |                                                                                        |
| ADJUST=                                         | Determines the method for multiple-comparison adjustment of LS-means differences       |
| ALPHA= $\alpha$                                 | Determines the confidence level ( $1 - \alpha$ )                                       |
| LOWER                                           | Performs one-sided, lower-tailed inference                                             |
| STEPDOWN                                        | Adjusts multiple-comparison <i>p</i> -values further in a step-down fashion            |
| TESTVALUE=                                      | Specifies values under the null hypothesis for tests                                   |
| UPPER                                           | Performs one-sided, upper-tailed inference                                             |
| <b>Statistical Output</b>                       |                                                                                        |
| CL                                              | Constructs confidence limits for means and mean differences                            |
| CORR                                            | Displays the correlation matrix of LS-means                                            |
| COV                                             | Displays the covariance matrix of LS-means                                             |
| E                                               | Prints the <b>L</b> matrix                                                             |
| ELSM                                            | Prints the <b>K</b> matrix                                                             |
| JOINT                                           | Produces a joint <i>F</i> or chi-square test for the LS-means and LS-means differences |
| SEED=                                           | Specifies the seed for computations that depend on random numbers                      |

For details about the syntax of the LSMESTIMATE statement, see the section “LSMESTIMATE Statement” on page 470 in Chapter 19, “Shared Concepts and Topics.”

## MODEL Statement

**MODEL** *response* < \* *censor (list)* > = *effects* < / *options* > ;

The MODEL statement identifies the variable to be used as the failure time variable, the optional censoring variable, and the explanatory effects, including covariates, main effects, and interactions; see the section “Specification of Effects” on page 3324 of Chapter 42, “The GLM Procedure,” for more information. A note of caution: specifying the effect T\*A in the MODEL statement, where T is the time variable and A is a CLASS variable, does not make the effect time-dependent. You must specify exactly one MODEL statement.

The MODEL statement allows one response variable. In the MODEL statement, the failure time variable precedes the equal sign. This can optionally be followed by an asterisk, the name of the censoring variable, and a list of censoring values (separated by blanks or commas if there is more than one) enclosed in parentheses. If the censoring variable takes on one of these values, the corresponding failure time is considered to be censored. The variables following the equal sign are the explanatory variables (sometimes called independent variables or covariates) for the model.

The censoring variable must be numeric. The failure time variable must contain nonnegative values. Any observation with a negative failure time is excluded from the analysis, as is any observation with a missing value for any of the variables listed in the MODEL statement. See “Missing Values” on page 7893 for details.

Table 93.6 summarizes the options available in the MODEL statement, which can be specified after a slash (/).

**Table 93.6** MODEL Statement Options

| Option     | Description                                                                  |
|------------|------------------------------------------------------------------------------|
| ALPHA=     | Specifies $\alpha$ for the 100(1 - $\alpha$ )% confidence limits             |
| CLPARM     | Computes confidence limits for regression parameters                         |
| COVB       | Displays covariance matrix                                                   |
| DF=        | Specifies the denominator degrees of freedom                                 |
| HESS       | Displays the Hessian matrix                                                  |
| INVHESS    | Displays the inverse of the Hessian matrix                                   |
| RISKLIMITS | Computes confidence limits for the exponentials of the regression parameters |
| SERATIO=   | Computes the ratio of two standard errors for the regression coefficients    |
| SINGULAR=  | Specifies tolerance for testing singularity                                  |
| TIES=      | Specifies the method of handling ties in failure times                       |
| VADJUST=   | Specifies a variance adjustment factor                                       |
| VARRATIO=  | Computes the ratio of two variances for the regression coefficients          |

**ALPHA= $\alpha$** 

sets the level of the confidence limits for the estimated regression parameters and the hazard ratios. The value of *alpha* must be between 0 and 1, and the default is 0.05. A confidence level of  $\alpha$  produces  $100(1 - \alpha)\%$  confidence limits. The default of ALPHA=0.05 produces 95% confidence limits.

The ALPHA= option has no effect unless the CLPARM or RISKLIMITS option is also specified.

**CLPARM**

produces confidence limits for regression parameters of Cox proportional hazards models. The confidence coefficient can be specified with the ALPHA= option. Classification main effects that use parameterizations other than REF, EFFECT, or GLM are ignored. See “Confidence Intervals” on page 7905 for details.

**COVB**

displays the estimated covariance matrix of the parameter estimates.

**DF=value | keyword**

specifies the denominator degrees of freedom for hypothesis tests and the degrees of freedom to use for confidence limits. If a *value* is specified, it must be a nonnegative number. By default, PROC SURVEYPHREG computes the degrees of freedom as described in the section “Degrees of Freedom” on page 7901. Instead of a *value*, you can specify one of the following key words:

**NONE**

specifies the denominator degrees of freedom to be infinite. Use this option if you want to compute chi-square tests and normal confidence intervals. This option is applicable to both the Taylor series linearization and the replication methods.

**PARMADJ**

computes the denominator degrees of freedom as the number of clusters (or observations if no CLUSTER statement is specified) minus the number of strata (or one if no STRATA statement is specified) minus the number of nonsingular parameters plus one in the model. This option can be useful if you are fitting a model with many parameters relative to the number of clusters minus the number of strata. See Korn and Graubard (1999, section 5.2) for further details. This option is applicable only for the Taylor series linearization method.

**ALLREPS**

computes the denominator degrees of freedom for replication methods by using the total number of replicate samples. By default, PROC SURVEYPHREG computes the denominator degrees of freedom based on the number of replicate samples used. See “Degrees of Freedom” on page 7901 for details.

**HESS**

displays the last evaluation of the Hessian matrix.

**INVHESS**

displays the inverse of the Hessian matrix that is evaluated at the estimated regression parameters.

**RISKLIMITS****RL**

produces confidence limits for hazard ratios and related quantities. See the section “[Hazard Ratios](#)” on page 7905 for details. The confidence coefficient can be specified with the **ALPHA=** option. Great care needs to be taken with any interpretation of the estimates and their confidence limits if interaction effects are involved in the model or if parameterizations other than REF, EFFECT, or GLM are used.

**SERATIO=ALL | MODEL | IND**

computes the ratio of two standard errors for the regression parameters. The standard error in the numerator uses the complete design information that you specify. You can specify the following options to compute different standard errors for the denominator:

**ALL**

requests both MODEL and IND standard error ratios.

**MODEL**

computes the standard errors in the denominator as the square root of the diagonals of the inverse Hessian matrix evaluated at the estimated regression parameters. See the section “[Variance Ratios and Standard Error Ratios](#)” on page 7902 for more information.

**IND**

computes the standard errors in the denominator by ignoring stratification and clustering. See the section “[Variance Ratios and Standard Error Ratios](#)” on page 7902 for more information.

**SINGULAR=value**

specifies the singularity criterion for determining linear dependencies in the set of explanatory variables. The default value is  $10^{-12}$ .

**TIES=method**

specifies how to handle ties in the failure time. The available *methods* are as follows:

**BRESLOW**

uses the approximate partial likelihood of Breslow (1974). This is the default value.

**EFRON**

uses the approximate partial likelihood of Efron (1977).

If there are no ties, both methods result in the same likelihood and yield identical estimates. The default, TIES=BRESLOW, is the most efficient method when there are no ties.

**VADJUST=DF | PARMADJ | NONE | AVGREPSS**

specifies variance adjustment factors. You can use the following key words:

**DF****PARMADJ**

requests degrees of freedom adjustment  $(n - 1)/(n - p)$  in the computation of the matrix **G** for the Taylor series linearization [variance estimation](#). By default, VADJUST=DF.



**NONE**

excludes the degrees of freedom adjustment  $(n - 1)/(n - p)$  from the computation of the matrix **G** for the Taylor series linearization [variance estimation](#).

**AVGREPSS**

use the average sum of squares from all the usable replicate samples for the unusable replicates. This option is applicable only for the jackknife replication method. AVGREPSS multiplies the default jackknife variance estimator by the factor  $R/R_a$ , where  $R_a$  is the number of usable replicates and  $R$  is the total number of replicates. See the section “[Variance Adjustment Factors](#)” on page 7902 for details.

**VARRATIO=ALL | MODEL | IND**

computes the ratio of two variances for the regression parameters. The variance in the numerator uses the complete design information. You can specify the following options to compute different variances for the denominator:

**ALL**

requests both MODEL and IND variance ratios.

**MODEL**

computes the variances in the denominator as the diagonals of the inverse Hessian matrix evaluated at the estimated regression parameters. See the section “[Variance Ratios and Standard Error Ratios](#)” on page 7902 for more information.

**IND**

computes the variances in the denominator by ignoring stratification and clustering. See the section “[Variance Ratios and Standard Error Ratios](#)” on page 7902 for more information.

**NLOPTIONS Statement**

**NLOPTIONS** < options > ;

The NLOPTIONS statement specifies details of the nonlinear optimization used by PROC SURVEYPHREG to maximize the log likelihood function. By default, the procedure uses the Newton-Raphson optimization technique. For more information about the NLOPTIONS statement, see the section “[NLOPTIONS Statement](#)” on page 482 in Chapter 19, “[Shared Concepts and Topics](#).”

**OUTPUT Statement**

**OUTPUT** < OUT=SAS-data-set > < keyword=name . . . keyword=name > < / options > ;

The OUTPUT statement creates a new SAS data set that contains statistics that are calculated for each observation unit. These statistics can include the estimated linear predictor ( $\mathbf{z}'_j \hat{\boldsymbol{\beta}}$ ) and its standard error, residuals, and influence statistics. In addition, this data set includes all the variables from the DATA= input data set.

Only score residuals are available in the OUTPUT data set if the model contains a time-dependent variable that is defined by means of programming statements.

The following list explains specifications in the OUTPUT statement:

**OUT=SAS-data-set**

names the output data set. If you omit the OUT= option, the OUTPUT data set is named by using the DATA*n* convention. See the section “[OUT= Data Set for the OUTPUT statement](#)” on page 7908 for more information.

*keyword=name*

specifies the statistics to include in the OUTPUT data set and names the new variables that contain the statistics. Specify a keyword for each desired statistic (see the following list of keywords), and optionally an equal sign with either a variable or a list of variables in parentheses to contain the statistics. If you specify a keyword without a variable name, then the procedure uses default names. The keywords that accept a list of variables are RESSCH, RESSCO, and WTRESSCH. For these keywords, you can specify as many names in *name* as the number of explanatory variables in the MODEL statement. If you specify *k* names and *k* is less than the total number of explanatory variables, only the first *k* names are taken from the list; the procedure assigns default names for the rest of the statistics. The keywords and the corresponding statistics are as follows:

**ATRISK**

specifies the number of subjects at risk at the observation time  $\tau_j$ .

**RESDEV**

specifies the deviance residual  $\hat{D}_j$ . This is a transform of the martingale residual to achieve a more symmetric distribution.

**RESMART**

specifies the martingale residual  $\hat{M}_j$ . The residual at the observation time  $\tau_j$  can be interpreted as the difference over  $[0, \tau_j]$  in the observed number of events minus the expected number of events given by the model.

**RESSCH**

specifies the Schoenfeld residuals. These residuals are useful in assessing the proportional hazards assumption.

**RESSCO**

specifies the score residuals. These residuals are a decomposition of the first partial derivative of the log likelihood. They can be used to assess the leverage that is exerted by each subject in the parameter estimation. They are also useful in constructing design-based variance estimators.

**STDXBETA**

specifies the standard error of the estimated linear predictor,  $\sqrt{\mathbf{z}'_j \hat{\mathbf{V}}(\hat{\boldsymbol{\beta}}|F) \mathbf{z}_j}$ .

**WTATRISK**

specifies the weighted number of subjects at risk at the observation time  $\tau_j$ .

**XBETA**

specifies the estimate of the linear predictor,  $\mathbf{z}'_j \hat{\boldsymbol{\beta}}$ .

## Programming Statements

Programming statements are used to create or modify the values of the explanatory variables in the MODEL statement. They are especially useful in fitting models with time-dependent explanatory variables. Programming statements can also be used to create explanatory variables that are not time-dependent. PROC SURVEYPHREG programming statements cannot be used to create or modify the values of the response variable, the censoring variable, the frequency variable, the weight variable, the class variables, the strata variables, the cluster variables, or the domain variables.

The following DATA step statements are available in PROC SURVEYPHREG:

```

ABORT;
ARRAY arrayname < [dimensions] > < $ > < variables-and-constants >;
CALL name < (expression < , expression ... >) >;
DELETE;
DO < variable = expression < TO expression > < BY expression > >
 < , expression < TO expression > < BY expression > > ...
 < WHILE expression > < UNTIL expression >;
END;
GOTO statement-label;
IF expression;
IF expression THEN program-statement;
 ELSE program-statement;
variable = expression;
variable + expression;
LINK statement-label;
PUT < variable > < = > ...;
RETURN;
SELECT < (expression) >;
STOP;
SUBSTR(variable, index, length)= expression;
WHEN (expression)program-statement;
 OTHERWISE program-statement;

```

By default, the PUT statement in PROC SURVEYPHREG writes results to the Output window instead of the Log window. If you want the results of the PUT statements to go to the Log window, add the following statement before the PUT statement:

```
FILE LOG;
```

DATA step functions are also available. Use these programming statements the same way you use them in the DATA step. For detailed information, see the *SAS Functions and CALL Routines: Reference*.

Consider the following example of using programming statements in PROC SURVEYPHREG. Suppose blood pressure is measured at multiple times during the course of a study that investigates the effect of blood pressure on some survival time. By treating the blood pressure as a time-dependent explanatory variable, you can use the value of the most recent blood pressure at each specific point of time in the modeling process rather than using the initial blood pressure or the final blood pressure. The values of the following variables are recorded for each patient, if they are available. Otherwise, the variables contain missing values.

|        |                                                     |
|--------|-----------------------------------------------------|
| Time   | survival time                                       |
| Censor | censoring indicator (with 0 as the censoring value) |
| BP0    | blood pressure on entry to the study                |
| T1     | time 1                                              |
| BP1    | blood pressure at T1                                |
| T2     | time 2                                              |
| BP2    | blood pressure at T2                                |
| WT     | design weight                                       |
| PSU    | identification of primary sampling units            |

The following programming statements create a variable BP. At each time T, the value of BP is the blood pressure reading for that time, if available. Otherwise, it is the last blood pressure reading.

```
proc surveyphreg;
 weight WT;
 model Time*Censor(0)=BP;
 cluster PSU;
 BP = BP0;
 if Time>=T1 and T1^=. then BP=BP1;
 if Time>=T2 and T2^=. then BP=BP2;
run;
```

---

## REPWEIGHTS Statement

**REPWEIGHTS** *variables* *</ options >* ;

The REPWEIGHTS statement names variables that provide replicate weights for BRR or jackknife variance estimation, which you request with the **VARMETHOD=BRR** or **VARMETHOD=JACKKNIFE** option in the PROC SURVEYPHREG statement. If you do not provide replicate weights for these methods by using a REPWEIGHTS statement, then PROC SURVEYPHREG constructs replicate weights for the analysis. See the sections “Balanced Repeated Replication (BRR) Method” on page 7896 and “Jackknife Method” on page 7899 for more information.

Each REPWEIGHTS variable should contain the weights for a single replicate, and the number of replicates equals the number of REPWEIGHTS variables. The REPWEIGHTS variables must be numeric, and the variable values must be nonnegative numbers.

If you provide replicate weights with a REPWEIGHTS statement, you do not need to specify a **CLUSTER** or **STRATA** statement. If you use a REPWEIGHTS statement and do not specify the **VARMETHOD=** option in the PROC SURVEYPHREG statement, the procedure uses **VARMETHOD=JACKKNIFE** by default.

If you specify a REPWEIGHTS statement but do not include a **WEIGHT** statement, PROC SURVEYPHREG uses the average of each observation’s replicate weights as the observation’s weight.

You can specify the following options in the REPWEIGHTS statement after a slash (/):

**DF=***df*

specifies the degrees of freedom for the analysis. The value of *df* must be a positive number. See the section “Degrees of Freedom” on page 7901 for details.

PROC SURVEYPHREG also use the DF= value in computing the denominator degrees of freedom for the *F* statistics in Wald type tests and confidence intervals.

**JKCOEFS=***jackknife-coefficient-specification*

specifies jackknife coefficients for **VARMETHOD=JACKKNIFE**. The default value for the jackknife coefficient is  $(R - 1)/R$ , where *R* is the total number of replicates. You can specify an alternative value with one of the following three forms:

**JKCOEFS=***value*

specifies a single jackknife coefficient for all replicates. The coefficient *value* must be a non-negative number.

**JKCOEFS=**(*values*)

specifies jackknife coefficients for **VARMETHOD=JACKKNIFE**, where each coefficient corresponds to an individual replicate identified by a REPWEIGHTS variable. You can separate *values* with blanks or commas. The coefficient *values* must be nonnegative numbers. The number of *values* must equal the number of replicate weight variables named in the REPWEIGHTS statement. List these values in the same order in which you list the corresponding replicate weight variables in the REPWEIGHTS statement.

**JKCOEFS=***SAS-data-set*

names a SAS data set that contains the jackknife coefficients for **VARMETHOD=JACKKNIFE**. You provide the jackknife coefficients in the JKCOEFS= data set variable JKCoefficient. Each coefficient value must be a nonnegative number. The observations in the JKCOEFS= data set should correspond to the replicates that are identified by the REPWEIGHTS variables. Arrange the coefficients or observations in the JKCOEFS= data set in the same order in which you list the corresponding replicate weight variables in the REPWEIGHTS statement. The number of observations in the JKCOEFS= data set must not be less than the number of REPWEIGHTS variables.

See the section “Jackknife Method” on page 7899 for details about jackknife coefficients.

---

## SLICE Statement

**SLICE** *model-effect* < / *options* > ;

The SLICE statement provides a general mechanism for performing a partitioned analysis of the LS-means for an interaction. This analysis is also known as an analysis of simple effects.

The SLICE statement uses the same options as the LSMEANS statement, which are summarized in Table 19.21. For details about the syntax of the SLICE statement, see the section “SLICE Statement” on page 498 in Chapter 19, “Shared Concepts and Topics.”

---

## STORE Statement

**STORE** < **OUT=** > *item-store-name* < / **LABEL=** 'label' > ;

The STORE statement requests that the procedure save the context and results of the statistical analysis. The resulting item store has a binary file format that cannot be modified. The contents of the item store can be processed with the PLM procedure.

For details about the syntax of the STORE statement, see the section “STORE Statement” on page 501 in Chapter 19, “Shared Concepts and Topics.”

---

## STRATA Statement

**STRATA** *variables* < / *option* > ;

The STRATA statement names variables that form the strata in a stratified sample design. The combinations of levels of STRATA variables define the strata in the sample, where strata are nonoverlapping subgroups that were sampled independently.

If your sample design has stratification at multiple stages, you should identify only the first-stage strata in the STRATA statement. See the section “Specifying the Sample Design” on page 7891 for more information.

If you provide replicate weights for BRR or jackknife variance estimation with a REPWEIGHTS statement, you do not need to specify a STRATA statement.

The STRATA *variables* are one or more variables in the DATA= input data set. These variables can be either character or numeric, but the procedure treats them as categorical variables. The formatted values of the STRATA variables determine the STRATA variable levels. Thus, you can use formats to group values into levels. See the discussion of the FORMAT procedure in the *Base SAS Procedures Guide* and the discussions of the FORMAT statement and SAS formats in the *SAS Formats and Informats: Reference*. Strata variables must not occur in the CLASS statement.

The STRATA statement in PROC SURVEYPHREG is different from the STRATA statement in PROC PHREG (Chapter 67, “The PHREG Procedure”). PROC PHREG fits different baseline hazard functions in different strata, which is useful if the proportional hazards assumption is not satisfied.

You can specify the following option in the STRATA statement after a slash (/):

### LIST

displays a “Stratum Information” table, which lists all strata together with the corresponding values of the STRATA variables. This table provides the number of observations and the number of clusters in each stratum, as well as the sampling fraction if you specify the RATE= or TOTAL= option.

---

## TEST Statement

**TEST** < *model-effects* > < / *options* > ;

The TEST statement enables you to perform  $F$  tests for model effects that test Type I, Type II, or Type III hypotheses. See Chapter 15, “The Four Types of Estimable Functions,” for details about the construction of Type I, II, and III estimable functions.

Table 93.7 summarizes the options available in the TEST statement.

**Table 93.7** TEST Statement Options

| Option    | Description                                                |
|-----------|------------------------------------------------------------|
| CHISQ     | Requests chi-square tests                                  |
| DDF=      | Specifies denominator degrees of freedom for fixed effects |
| E         | Requests Type I, Type II, and Type III coefficients        |
| E1        | Requests Type I coefficients                               |
| E2        | Requests Type II coefficients                              |
| E3        | Requests Type III coefficients                             |
| HTYPE=    | Indicates the type of hypothesis test to perform           |
| INTERCEPT | Adds a row that corresponds to the overall intercept       |

For details about the syntax of the TEST statement, see the section “TEST Statement” on page 502 in Chapter 19, “Shared Concepts and Topics.”

## WEIGHT Statement

**WEIGHT** *variable* ;

The WEIGHT statement names the variable that contains the sampling weights. This variable must be numeric, and the sampling weights must be positive numbers. If an observation has a weight that is nonpositive or missing, then the procedure omits that observation from the analysis. See the section “Missing Values” on page 7893 for more information. The WEIGHT statement allows one weight variable.

If you do not specify a WEIGHT statement but provide replicate weights with a REPWEIGHTS statement, PROC SURVEYPHREG uses the average of each observation’s replicate weights as the observation’s weight.

If you specify neither a WEIGHT statement nor a REPWEIGHTS statement, PROC SURVEYPHREG assigns all observations a weight of one.

## Details: SURVEYPHREG Procedure

### Notation and Estimation

Let  $U = \{1, 2, \dots, N\}$  be the set of indices and let  $\mathcal{F}_N$  be the set of values for a finite population of size  $N$ . The survival time of each member of the finite population is assumed to follow its own hazard function,  $\lambda_i(t)$ , expressed as

$$\lambda_i(t) = \lambda(t; \mathbf{Z}_i(t)) = \lambda_0(t) \exp(\mathbf{Z}_i'(t)\boldsymbol{\beta})$$

where  $\lambda_0(t)$  is an arbitrary and unspecified baseline hazard function,  $\mathbf{Z}_i(t)$  is the vector of explanatory variables for the  $i$ th unit at time  $t$ , and  $\boldsymbol{\beta}$  is the vector of unknown regression parameters that are associated with the explanatory variables. The vector  $\boldsymbol{\beta}$  is assumed to be the same for all individuals.

The partial likelihood function introduced by Cox (1972, 1975) eliminates the unknown baseline hazard  $\lambda_0(t)$  and accounts for censored survival times. If the entire population is observed, then this partial likelihood can be used to estimate  $\boldsymbol{\beta}$ . Let  $\boldsymbol{\beta}_N$  be the desired estimator. Assuming a working model with uncorrelated responses,  $\boldsymbol{\beta}_N$  is obtained by maximizing the partial log likelihood,

$$l(\boldsymbol{\beta}) = \sum_{i \in U} \log \left\{ L(\boldsymbol{\beta}; \mathbf{Z}_i(t), t_i) \right\}$$

with respect to  $\boldsymbol{\beta}$ , where  $L(\boldsymbol{\beta}; \mathbf{Z}_i(t), t_i)$  is Cox's partial likelihood function.

Assume that probability sample  $A$  is selected from the finite population  $U$  and  $\pi_i$  is the selection probability for unit  $i$ . Further assume that covariates  $\mathbf{Z}_i(t)$  and survival time  $t_i$  are available for every unit in the sample  $A$ . An estimator of the finite population log likelihood is

$$l_\pi(\boldsymbol{\beta}) = \sum_{i \in A} \pi_i^{-1} \log \left\{ L(\boldsymbol{\beta}; \mathbf{Z}_i(t), t_i) \right\}$$

See “Partial Likelihood Function for the Cox Model” on page 7890 for more details.

A sample-based estimator  $\hat{\boldsymbol{\beta}}$  for the finite population quantity  $\boldsymbol{\beta}_N$  can be obtained by maximizing the partial pseudo-log-likelihood  $l_\pi(\boldsymbol{\beta}; \mathbf{Z}_i(t), t_i)$  with respect to  $\boldsymbol{\beta}$ . The design-based variance for  $\hat{\boldsymbol{\beta}}$  is obtained by assuming the set of finite population values  $\mathcal{F}_N$  as fixed. For more information about maximum pseudo-likelihood estimators and other inferential approaches for survey data, see Kish and Frankel (1974); Godambe and Thompson (1986); Pfeiffermann (1993), Korn and Graubard (1999, chapter 3), Chambers and Skinner (2003, chapter 2), and Fuller (2009, section 6.5). Maximum pseudo-likelihood estimators and their properties for Cox's proportional hazards model for survey data are discussed in Binder (1990, 1992); Lin and Wei (1989); Lin (2000); Boudreau and Lawless (2006).

Without loss of generality, the rest of this section uses indices for stratified clustered designs. For a stratified clustered sample design, observations are represented by a matrix

$$(\mathbf{w}, \mathbf{t}, \mathbf{\Delta}, \mathbf{Z}) = (w_{hij}, t_{hij}, \Delta_{hij}, \mathbf{z}_{hij})$$

where

- $\mathbf{w}$  denotes the vector of sampling weights
- $\mathbf{t}$  denotes the event time variable
- $\mathbf{\Delta}$  denotes the event indicator
- $\mathbf{Z}$  denotes the  $n \times p$  matrix of auxiliary information
- $h = 1, 2, \dots, H$  is the stratum index
- $i = 1, 2, \dots, n_h$  is the cluster index within stratum  $h$
- $j = 1, 2, \dots, m_{hi}$  is the unit index within cluster  $i$  of stratum  $h$
- $p$  is the total number of parameters
- $n = \sum_{h=1}^H \sum_{i=1}^{n_h} m_{hi}$  is the total number of observations in the sample
- $y_{hij}(t) = I(t_{hij} \geq t)$ , where  $I(\cdot)$  is an indicator function
- $n_{hij}(t) = I(t_{hij} \leq t)$ , where  $I(\cdot)$  is an indicator function



Let  $\sum_B = \sum_{(h,i,j) \in B}$  denote the summation over the set of indices such that the observation unit  $j$  in PSU  $i$  and stratum  $h$  belongs to the index set  $B$ . Typically,  $B$  is the set of all population indices that are in the sample, the risk set, or the set of all units with a failure.

The first-stage sampling rate (fraction of PSUs selected for the sample) is denoted by  $f_h$ . The first-stage sampling rate is used in Taylor series variance estimation. You can specify the stratum sampling rates with the `RATE=` option. Or if you specify population totals with the `TOTAL=` option, PROC SURVEYFREQ computes  $f_h$  as the ratio of stratum sample size to the stratum total, in terms of PSUs. See the section “Population Totals and Sampling Rates” on page 7892 for details. If you do not specify the `RATE=` option or the `TOTAL=` option, then the procedure assumes that the stratum sampling rates  $f_h$  are negligible and does not use a finite population correction when computing variances.

## Failure Time Distribution

Let  $T$  be a nonnegative random variable that represents the failure time of an individual from a homogeneous superpopulation. The survival distribution function (also known as the survivor function) of  $T$  is written as

$$S(t) = \Pr(T \geq t)$$

A mathematically equivalent way of specifying the distribution of  $T$  is through its hazard function. The hazard function  $\lambda(t)$  specifies the instantaneous failure rate at  $t$ . If  $T$  is a continuous random variable,  $\lambda(t)$  is expressed as

$$\lambda(t) = \lim_{\Delta t \rightarrow 0^+} \frac{\Pr(t \leq T < t + \Delta t \mid T \geq t)}{\Delta t} = \frac{f(t)}{S(t)}$$

where  $f(t)$  is the probability density function of  $T$ .

## Time and CLASS Variables Usage

The following DATA step creates an artificial data set, `Test`, to be used in this section. There are six variables in `Test`: the variable `T` contains the failure times; the variable `Status` is the censoring indicator variable with the value 1 for an uncensored failure time and the value 0 for a censored time; the variable `A` is a categorical variable with values 1, 2, and 3 representing three different categories; the variable `MirrorT` is an exact copy of `T`; the variable `W` is the observation weight; and the variable `S` is the strata indicator.

```
data Test;
 input T Status A W S @@;
 MirrorT = T;
 datalines;
23 1 1 10 1 7 0 1 20 2
23 1 1 10 1 10 1 1 20 2
20 0 1 10 1 13 0 1 20 2
24 1 1 10 1 10 1 1 20 2
18 1 2 10 1 6 1 2 20 2
18 0 2 10 1 6 1 2 20 2
13 0 2 10 1 13 1 2 20 2
 9 0 2 10 1 15 1 2 20 2
 8 1 3 10 1 6 1 3 20 2
```

```

12 0 3 10 1 4 1 3 20 2
11 1 3 10 1 8 1 1 20 2
 6 1 3 10 1 7 1 3 20 2
 7 1 3 10 1 12 1 3 20 2
 9 1 2 10 1 15 1 2 20 2
 3 1 2 10 1 14 0 3 20 2
 6 1 1 10 1 13 1 2 20 2
;

```

### Time Variable on the Right Side of the MODEL Statement

The time variable cannot be used explicitly as an explanatory effect in the MODEL statement. The following statements produce an error message:

```

proc surveypreg data=Test;
 weight W;
 strata S;
 class A;
 model T*Status(0)=T*A;
run;

```

To use the time variable as an explanatory effect, replace T by MirrorT as an effect, which is an exact copy of T, as in the following statements:

```

proc surveypreg data=Test;
 weight W;
 strata S;
 class A;
 model T*Status(0)=A*MirrorT;
run;

```

Note that neither T\*A nor MirrorT\*A in the MODEL statement is time-dependent. The results of fitting this model are shown in Figure 93.3.

**Figure 93.3** T\*A Effect

| The SURVEYPHREG Procedure                |    |            |                   |         |         |                 |
|------------------------------------------|----|------------|-------------------|---------|---------|-----------------|
| Analysis of Maximum Likelihood Estimates |    |            |                   |         |         |                 |
| Parameter                                | DF | Estimate   | Standard<br>Error | t Value | Pr >  t | Hazard<br>Ratio |
| MirrorT*A 1                              | 30 | -17.560699 | 0.337239          | -52.07  | <.0001  | 0.000           |
| MirrorT*A 2                              | 30 | -17.424235 | 0.331186          | -52.61  | <.0001  | 0.000           |
| MirrorT*A 3                              | 30 | -17.448672 | 0.290159          | -60.13  | <.0001  | 0.000           |

### CLASS Variables and Programming Statements

In PROC SURVEYPHREG, the levels of CLASS variables are determined by the CLASS statement and the input data and are not affected by user-supplied programming statements. Consider the following state-

ments, which produce the results in Figure 93.4. Variable A is declared as a CLASS variable in the CLASS statement.

```
proc surveypHreg data=Test;
 weight W;
 strata S;
 class A;
 model T*Status(0)=A;
run;
```

Figure 93.4 shows the parameters that correspond to A and their respective regression coefficients estimates.

**Figure 93.4** Design Variable and Regression Coefficient Estimates

| The SURVEYPHREG Procedure                |        |           |                |         |         |              |
|------------------------------------------|--------|-----------|----------------|---------|---------|--------------|
| Class Level Information                  |        |           |                |         |         |              |
| Class                                    | Levels | Values    |                |         |         |              |
| A                                        | 3      | 1         | 2              | 3       |         |              |
| Analysis of Maximum Likelihood Estimates |        |           |                |         |         |              |
| Parameter                                | DF     | Estimate  | Standard Error | t Value | Pr >  t | Hazard Ratio |
| A 1                                      | 30     | -1.162184 | 0.655136       | -1.77   | 0.0862  | 0.313        |
| A 2                                      | 30     | -0.616962 | 0.521841       | -1.18   | 0.2464  | 0.540        |
| A 3                                      | 30     | 0         | .              | .       | .       | 1.000        |

Now consider the programming statement that attempts to change the value of the CLASS variable A as in the following specification:

```
proc surveypHreg data=Test;
 weight W;
 strata S;
 class A;
 model T*Status(0)=A;
 if A=3 then A=2;
run;
```

Results of this analysis are shown in Figure 93.5 and are identical to those in Figure 93.4. The `if A=3 then A=2` programming statement has no effect on the explanatory variable for A, which have already been determined.

**Figure 93.5** Design Variable and Regression Coefficient Estimates

| The SURVEYPHREG Procedure                |        |           |                |         |         |              |
|------------------------------------------|--------|-----------|----------------|---------|---------|--------------|
| Class Level Information                  |        |           |                |         |         |              |
| Class                                    | Levels | Values    |                |         |         |              |
| A                                        | 3      | 1         | 2              | 3       |         |              |
| Analysis of Maximum Likelihood Estimates |        |           |                |         |         |              |
| Parameter                                | DF     | Estimate  | Standard Error | t Value | Pr >  t | Hazard Ratio |
| A 1                                      | 30     | -1.162184 | 0.655136       | -1.77   | 0.0862  | 0.313        |
| A 2                                      | 30     | -0.616962 | 0.521841       | -1.18   | 0.2464  | 0.540        |
| A 3                                      | 30     | 0         | .              | .       | .       | 1.000        |

Additionally any variable used in a programming statement that has already been declared in the CLASS statement is *not* treated as a collection of the corresponding design variables. Consider the following statements:

```
proc surveypreg data=Test;
 class A;
 model T*Status(0)=A X;
 X=T*A;
run;
```

The CLASS variable A generates two design variables as explanatory variables. The variable X created by the `X=T*A` programming statement is a single time-dependent covariate whose values are evaluated using the exact values of A given in the data, not the dummy coded values that represent A. In the data set Test, A has the values of 1, 2, and 3, and these values are multiplied by the values of T to produce X. If A were a character variable with values 'Bird', 'Cat', and 'Dog', the programming statement `X=T*A` would have produced an error in the attempt to multiply a number with a character value.

**Figure 93.6** Single Time-Dependent Variable X\*A

| The SURVEYPHREG Procedure                |    |          |                |         |         |              |
|------------------------------------------|----|----------|----------------|---------|---------|--------------|
| Analysis of Maximum Likelihood Estimates |    |          |                |         |         |              |
| Parameter                                | DF | Estimate | Standard Error | t Value | Pr >  t | Hazard Ratio |
| A 1                                      | 31 | 0.158010 | 1.222654       | 0.13    | 0.8980  | 1.171        |
| A 2                                      | 31 | 0.008993 | 0.674629       | 0.01    | 0.9894  | 1.009        |
| A 3                                      | 31 | 0        | .              | .       | .       | 1.000        |
| X                                        | 31 | 0.092679 | 0.073746       | 1.26    | 0.2182  | 1.097        |

The following statements are not the same as in the preceding program. If you want to create time-dependent covariates from the values of a CLASS variable, you could use syntax like the following:

```
proc surveypHreg data=Test;
 class A;
 model T*Status(0)=A X1 X2;
 X1= T*(A=1);
 X2= T*(A=2);
run;
```

The Boolean parenthetical expressions (A=1) and (A=2) resolve to a value of 1 or 0, depending on whether the expression is true or false, respectively.

Results of this test are shown in Figure 93.7.

**Figure 93.7** Simple Test of Proportional Hazards Assumption

| The SURVEYPHREG Procedure                |    |           |                |         |         |              |
|------------------------------------------|----|-----------|----------------|---------|---------|--------------|
| Analysis of Maximum Likelihood Estimates |    |           |                |         |         |              |
| Parameter                                | DF | Estimate  | Standard Error | t Value | Pr >  t | Hazard Ratio |
| A 1                                      | 31 | -0.007655 | 1.284875       | -0.01   | 0.9953  | 0.992        |
| A 2                                      | 31 | -0.881383 | 1.834533       | -0.48   | 0.6343  | 0.414        |
| A 3                                      | 31 | 0         | .              | .       | .       | 1.000        |
| X1                                       | 31 | -0.155220 | 0.172914       | -0.90   | 0.3763  | 0.856        |
| X2                                       | 31 | 0.011554  | 0.198796       | 0.06    | 0.9540  | 1.012        |

In general, when your model contains a categorical explanatory variable that is time-dependent, it might be necessary to use hardcoded dummy variables to represent the categories of the categorical variable.

## Partial Likelihood Function for the Cox Model

Let  $t_{(1)} < t_{(2)} < \dots < t_{(K)}$  denote the  $K$  distinct, ordered event times. Let  $d_k$  denote the multiplicity of failures at  $t_{(k)}$ ; that is,  $d_k$  is the size of the set  $\mathcal{D}_k$  of individuals that fail at  $t_{(k)}$ . Let  $w_{hij}$  be the weight associated with the  $j$ th observation unit in the  $i$ th cluster in stratum  $h$ . Using this notation, the pseudo-likelihood functions used in PROC SURVEYPHREG to estimate  $\beta_N$  are described in the following sections.

### Continuous Time Scale

Let  $\mathcal{R}_k$  denote the risk set just before the  $k$ th ordered event time  $t_{(k)}$ .

The Breslow likelihood is expressed as

$$L_{\text{Breslow}}(\beta) = \prod_{k=1}^K \frac{\exp(\beta' \sum_{\mathcal{D}_k} w_{hij} \mathbf{Z}_{hij}(t))}{\left\{ \sum_{\mathcal{R}_k} w_{hij} \exp(\beta' \mathbf{Z}_{hij}(t)) \right\}^{\sum_{\mathcal{D}_k} w_{hij}}}$$

The Efron likelihood is expressed as

$$L_{\text{Efron}}(\boldsymbol{\beta}) = \prod_{k=1}^K \frac{\exp(\boldsymbol{\beta}' \sum_{\mathcal{D}_k} w_{hij} \mathbf{Z}_{hij}(t))}{\{\phi(\boldsymbol{\beta}, \mathbf{Z}, \mathbf{w}, k)\}^{\frac{1}{d_k}} \sum_{\mathcal{D}_k} w_{hij}}$$

where  $\phi(\boldsymbol{\beta}, \mathbf{Z}, \mathbf{w}, k)$  is

$$\phi(\boldsymbol{\beta}, \mathbf{Z}, \mathbf{w}, k) = \prod_{l=1}^{d_k} \left\{ \sum_{\mathcal{R}_k} w_{hij} \exp(\boldsymbol{\beta}' \mathbf{Z}_{hij}(t)) - \frac{l-1}{d_k} \sum_{\mathcal{D}_k} w_{hij} \exp(\boldsymbol{\beta}' \mathbf{Z}_{hij}(t)) \right\}$$

## Specifying the Sample Design

PROC SURVEYPHREG produces statistics that are based on the sample design used to obtain the survey data. PROC SURVEYPHREG can be used for single-stage or multistage designs, with or without stratification, and with or without unequal weighting. To analyze your survey data with PROC SURVEYPHREG, you need to provide sample design information for the procedure. This information can include design (or variance) strata, clusters, and sampling weights. You provide sample design information with the **STRATA**, **CLUSTER**, and **WEIGHT** statements, and with the **RATE=** or **TOTAL=** option in the PROC SURVEYPHREG statement.

If you provide replicate weights for BRR or jackknife variance estimation, you do not need to specify a **STRATA** or **CLUSTER** statement. Otherwise, you should specify **STRATA** and **CLUSTER** statements whenever your design includes stratification and clustering.

When there are clusters (PSUs) in the sample design, the procedure estimates variance by using the PSUs, as described in the section “[Variance Estimation](#)” on page 7895. For a multistage sample design, PROC SURVEYPHREG uses only the first stage of the sample design for variance estimation. So, the required input includes only first-stage cluster (PSU) and first-stage stratum identification. You do not need to input design information about any additional stages of sampling.

### Stratification

If your sample design is stratified at the first stage of sampling, use the **STRATA** statement to name the variables that form the strata. The combinations of categories of **STRATA** variables define the strata in the sample, where strata are nonoverlapping subgroups that were sampled independently. If your sample design has stratification at multiple stages, you should identify only the first-stage strata in the **STRATA** statement.

If you use a **REPWEIGHTS** statement to provide replicate weights for BRR or jackknife variance estimation, you do not need to specify a **STRATA** statement. Otherwise, you should specify a **STRATA** statement whenever your design includes stratification. If you do not specify a **STRATA** statement or a **REPWEIGHTS** statement, then PROC SURVEYPHREG assumes there is no stratification at the first stage. In other words, in this case, the procedure assumes that all observation units are in the same stratum.

### Clustering

If your sample design selects clusters at the first stage of sampling, use the **CLUSTER** statement to name the variables that identify the first-stage clusters, which are also called primary sampling units (PSUs). The combinations of categories of **CLUSTER** variables define the clusters in the sample. If there is a **STRATA**

statement, clusters are nested within strata. If your sample design has clustering at multiple stages, you should specify only the first-stage clusters (PSUs) in the CLUSTER statement. PROC SURVEYPHREG assumes that each cluster that is defined by the CLUSTER statement variables represents a PSU in the sample.

If you use a REPWEIGHTS statement to provide replicate weights for BRR or jackknife variance estimation, you do not need to specify a CLUSTER statement. Otherwise, you should specify a CLUSTER statement whenever your design includes clustering at the first stage of sampling. If you do not specify a CLUSTER statement, then PROC SURVEYPHREG treats each observation as a PSU.

## Weighting

If your sample design includes unequal weighting, use the WEIGHT statement to name the variable that contains the sampling weights. Sampling weights must be positive numbers. If an observation has a weight that is nonpositive or missing, then the procedure omits that observation from the analysis. See the section “Missing Values” on page 7893 for more information.

If you do not specify a WEIGHT statement but include a REPWEIGHTS statement, PROC SURVEYPHREG uses the average of each observation’s replicate weights as the observation’s weight. If you specify neither a WEIGHT statement nor a REPWEIGHTS statement, PROC SURVEYPHREG assumes all observations have a weight of one.

## Population Totals and Sampling Rates

To include a finite population correction (*fpc*) in Taylor series variance estimation, you can input either the sampling rate or the population total by using the RATE= or TOTAL= option in the PROC SURVEYPHREG statement. You cannot specify both of these options in the same PROC SURVEYPHREG statement. The RATE= and TOTAL= options apply only to Taylor series variance estimation. The procedure does not use a finite population correction for BRR or jackknife variance estimation.

If you do not specify the RATE= or TOTAL= option, the Taylor series variance estimation does not include a finite population correction. For fairly small sampling fractions, this correction is often ignored. See Cochran (1977) and Kish (1965) for more information.

If your design has multiple stages of selection and you are specifying the RATE= option, you should input the first-stage sampling rate, which is the ratio of the number of PSUs in the sample to the total number of PSUs in the study population. If you are specifying the TOTAL= option for a multistage design, you should input the total number of PSUs in the study population.

For a nonstratified sample design, or for a stratified sample design with the same sampling rate or the same population total in all strata, you can use the RATE=*value* or TOTAL=*value* option. If your sample design is stratified with different sampling rates or population totals in different strata, use the RATE=*SAS-data-set* or TOTAL=*SAS-data-set* option to name a SAS data set that contains the stratum sampling rates or totals. This data set is called a *secondary data set*, as opposed to the *primary data set* that you specify with the DATA= option.

The secondary data set must contain all the stratification variables listed in the STRATA statement and all the variables in the BY statement. Furthermore, the BY groups must appear in the same order as in the primary data set. If there are formats associated with the STRATA variables and the BY variables, then the formats must be consistent in the primary and the secondary data sets. If you specify the TOTAL=*SAS-data-set* option, the secondary data set must have a variable named `_TOTAL_` that contains the stratum population

totals. If you specify the `RATE=SAS-data-set` option, the secondary data set must have a variable named `_RATE_` that contains the stratum sampling rates. If the secondary data set contains more than one observation for any one stratum, the procedure uses the first value of `_TOTAL_` or `_RATE_` for that stratum and ignores the rest.

The *value* in the `RATE=` option or the values of `_RATE_` in the secondary data set must be nonnegative numbers. You can specify *value* as a number between 0 and 1. Or you can specify *value* in percentage form as a number between 1 and 100, and PROC SURVEYPHREG converts that number to a proportion. The procedure treats the value 1 as 100% instead of 1%.

If you specify the `TOTAL=value` option, *value* must not be less than the sample size. If you provide stratum population totals in a secondary data set, these values must not be less than the corresponding stratum sample sizes.

---

## Missing Values

Missing values in your survey data can compromise the quality of your survey results. Some missing values for survey data are because of nonresponses. An observation whose response to every survey item is available is called a *complete respondent*, and an observation whose response to one or more survey items are missing is called an *incomplete respondent*. If the complete respondents are different from the incomplete respondents with regard to a survey effect or outcome, then survey estimates will be biased and will not accurately represent the survey population. There are a variety of techniques in sample design and survey operations that can reduce nonresponse. After data collection is complete, you can use imputation to replace missing values with acceptable values, and you can use sampling weight adjustments to compensate for nonresponse. You should complete this data preparation and adjustment before you analyze your data with PROC SURVEYPHREG. For more details, see Cochran (1977); Kalton and Kaspyzyk (1986); Brick and Kalton (1996).

### WEIGHT Variable

If an observation has a missing value or a nonpositive value for the `WEIGHT` variable, then PROC SURVEYPHREG excludes that observation from the analysis.

### REPWEIGHTS Variables

If you provide replicate weights with a `REPWEIGHTS` statement for BRR or jackknife variance estimation, all `REPWEIGHTS` variable values must be nonmissing. Similarly, if you provide jackknife coefficients with the `JKCOEFS=` option in the `REPWEIGHTS` statement, all values of the `JKCoefficient` variable must be nonmissing. The procedure does not perform the analysis when any replicate weight or jackknife coefficient value is missing.

### CLASS, STRATA, CLUSTER, and DOMAIN Variables

An observation is excluded from the analysis if it has a missing value for any `CLASS`, `STRATA`, `CLUSTER`, or `DOMAIN` variable, unless you specify the `MISSING` option in the PROC SURVEYPHREG statement. If you specify the `MISSING` option, the procedure treats missing values as a valid (nonmissing) category for all categorical variables, which include `STRATA` variables, `CLUSTER` variables, `CLASS` variables, and `DOMAIN` variables.



## Analysis Variables

By default, PROC SURVEYPHREG excludes an observation from the likelihood estimation and all associated analyses if the observation has a missing value for any of the variables in the **MODEL** statement, unless you specify the **MISSING** or **NOMCAR** option in the PROC SURVEYPHREG statement. When the procedure excludes observations with missing values from analyses, it displays the total frequency of observations used in the “NObs” table.

If you specify time-dependent covariates by using **programming statements**, the procedure computes the values of the covariates for all observations in the risk set at every event time. If an observation contains missing values for any of the time-dependent covariates at a given event time, then the observation is not used at that event time. However, that same observation can be used at some other event times where it contains no missing values. Therefore, an observation with missing time-dependent covariates can be used at some event times but ignored at other event times, depending on whether any of the corresponding time-dependent covariates are missing.

If you specify the **MISSING** option, the procedure treats missing levels as a valid (nonmissing) level for each categorical analysis variable.

If you specify the **NOMCAR** option for Taylor series variance estimation, the procedure includes observations with missing values of analysis variables in the variance computations.

## The NOMCAR Option

When you specify the **NOMCAR** option, PROC SURVEYPHREG computes variance estimates by analyzing the nonmissing values for variables in the regression model as a domain or subpopulation, where the entire population includes both nonmissing and missing domains. By default, if an observation contains missing values for the dependent variable or for any variable used in the independent effects, the observation is excluded from the analysis. See the section “**Missing Values**” on page 7893 for more information.

Note that the **NOMCAR** option has no effect on categorical predictors when you specify the **MISSING** option, which treats missing values as a valid nonmissing level. The **NOMCAR** option does not affect the inclusion of observations with missing values of the **WEIGHT**, **FREQ**, **CLUSTER**, **STRATA**, or **DOMAIN** variables. Observations with missing values of the **WEIGHT** and **FREQ** variables are always excluded from the analysis. Observations with missing values of the **CLUSTER**, **DOMAIN**, or **STRATA** variables are excluded unless you specify the **MISSING** option.

The **NOMCAR** option applies only to Taylor series variance estimation. The replication methods, which you request with the **VARMETHOD=BRR** and **VARMETHOD=JACKKNIFE** options, do not use the **NOMCAR** option.

## Degrees of Freedom

PROC SURVEYPHREG computes degrees of freedom to compute confidence limits and  $F$  statistics. The degrees of freedom computation depends on the variance estimation method that you request. See the section “**Degrees of Freedom**” on page 7901 for details. Missing values can affect the degrees of freedom computation.

### **Taylor Series Variance Estimation**

The degrees of freedom can depend on the number of clusters, the number of strata, and the number of observations. For Taylor series variance estimation, these numbers are based on the observations included

in the analysis. These numbers do not count observations that are excluded from the analysis due to missing values. If all values in a stratum are excluded from the analysis as missing values, then that stratum is called an *empty stratum*. Empty strata are not counted in the total number of strata for the analysis. Similarly, empty clusters and missing observations are not included in the totals counts of clusters and observations that are used to compute the degrees of freedom for the analysis.

If you specify the **MISSING** option, missing values are treated as valid nonmissing levels and are included in computing degrees of freedom. If you specify the **NOMCAR** option for Taylor series variance estimation, observations with missing values for variables in the regression model are included in computing degrees of freedom.

### Replicate-Based Variance Estimation

For BRR or jackknife variance estimation, by default PROC SURVEYPHREG computes the degrees of freedom by using all valid observations in the input data set. A valid observation is an observation that has a positive value of the **WEIGHT** variable and nonmissing values of the **STRATA** and **CLUSTER** variables unless you specify the **MISSING** option.

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## Variance Estimation

PROC SURVEYPHREG uses the Taylor series method or replication (resampling) methods to estimate sampling errors of estimators that are based on complex sample designs (Fuller 1975; Särndal, Swensson, and Wretman 1992; Wolter 2007; Rust 1985; Dippo, Fay, and Morganstein 1984; Rao and Shao 1999, 1996; and Binder 1992). You can use the **VARMETHOD=** option in the PROC statement to specify the variance estimation method. By default, PROC SURVEYPHREG uses the Taylor series method.

However, replication methods have recently gained popularity for estimating variances in complex survey data analysis. One reason for this popularity is the relative simplicity of replication-based estimates, especially for nonlinear estimators; another is that modern computational capacity has made replication methods feasible for practical survey analysis.

Replication methods draw multiple replicates (also called subsamples) from a full sample according to a specific resampling scheme. The most commonly used resampling schemes are the *balanced repeated replication* (BRR) method and the *jackknife* method. For each replicate, the original weights are modified for the PSUs in the replicates to create replicate weights. The parameters of interest are estimated by using the replicate weights for each replicate. Then the variances of parameters of interest are estimated by the variability among the estimates derived from these replicates. The procedure automatically creates replicate weights based on the replication method you specify; alternatively you can use the **REPWEIGHTS** statement to provide your own replicate weights for variance estimation.

The following sections provide details about how the variance-covariance matrix of the estimated regression coefficients is estimated for each variance estimation method.

### Taylor Series Linearization

The Taylor series linearization method is the default variance estimation method used by PROC SURVEYPHREG. See the section “**Notation and Estimation**” on page 7884 for definitions of the notation used in this section. Let

$$S^{(r)}(\boldsymbol{\beta}, t) = \sum_A w_{hij} y_{hij}(t) \exp(\boldsymbol{\beta}' \mathbf{Z}_{hij}(t)) \mathbf{Z}_{hij}^{\otimes r}(t)$$

where  $r = 0, 1$ . Let  $A$  be the set of indices in the selected sample. Let

$$\mathbf{a}^{\otimes r} = \begin{cases} \mathbf{a}\mathbf{a}' & , r = 1 \\ I_{\dim(\mathbf{a})} & , r = 0 \end{cases}$$

and let  $I_{\dim(\mathbf{a})}$  be the identity matrix of appropriate dimension.

Let  $\bar{\mathbf{Z}}(\boldsymbol{\beta}, t) = \frac{S^{(1)}(\boldsymbol{\beta}, t)}{S^{(0)}(\boldsymbol{\beta}, t)}$ . The score residual for the  $(h, i, j)$  subject is

$$\begin{aligned} \mathbf{L}_{hij}(\boldsymbol{\beta}) &= \Delta_{hij} \left\{ \mathbf{Z}_{hij}(t_{hij}) - \bar{\mathbf{Z}}(\boldsymbol{\beta}, t_{hij}) \right\} \\ &\quad - \sum_{(h', i', j') \in A} \Delta_{h'i'j'} \frac{w_{h'i'j'} Y_{hij}(t_{h'i'j'}) \exp(\boldsymbol{\beta}' \mathbf{Z}_{hij}(t_{h'i'j'}))}{S^{(0)}(\boldsymbol{\beta}, t_{h'i'j'})} \left\{ \mathbf{Z}_{hij}(t_{h'i'j'}) - \bar{\mathbf{Z}}(\boldsymbol{\beta}, t_{h'i'j'}) \right\} \end{aligned}$$

For TIES=EFRON, the computation of the score residuals is modified to comply with the Efron partial likelihood. See the section “Residuals” on page 7906 for more information.

The Taylor series estimate of the covariance matrix of  $\hat{\boldsymbol{\beta}}$  is

$$\hat{\mathbf{V}}(\hat{\boldsymbol{\beta}}) = \mathcal{I}^{-1}(\hat{\boldsymbol{\beta}}) \mathbf{G} \mathcal{I}^{-1}(\hat{\boldsymbol{\beta}})$$

where  $\mathcal{I}(\hat{\boldsymbol{\beta}})$  is the observed information matrix and the  $p \times p$  matrix  $\mathbf{G}$  is defined as

$$\mathbf{G} = \frac{n-1}{n-p} \sum_{h=1}^H \frac{n_h(1-f_h)}{n_h-1} \sum_{i=1}^{n_h} (\mathbf{e}_{hi+} - \bar{\mathbf{e}}_{h..})' (\mathbf{e}_{hi+} - \bar{\mathbf{e}}_{h..})$$

The observed residuals, their sums and means are defined as follows:

$$\begin{aligned} \mathbf{e}_{hij} &= w_{hij} \mathbf{L}_{hij}(\hat{\boldsymbol{\beta}}) \\ \mathbf{e}_{hi+} &= \sum_{j=1}^{m_{hi}} \mathbf{e}_{hij} \\ \bar{\mathbf{e}}_{h..} &= \frac{1}{n_h} \sum_{i=1}^{n_h} \mathbf{e}_{hi+} \end{aligned}$$

The factor  $(n-1)/(n-p)$  in the computation of the matrix  $\mathbf{G}$  reduces the small sample bias that is associated with using the estimated function to calculate deviations (Fuller et al. (1989), pp. 77–81). For simple random sampling, this factor contributes to the degrees of freedom correction applied to the residual mean square for ordinary least squares in which  $p$  parameters are estimated. By default, the procedure uses this adjustment in the variance estimation. If you do not want to use this multiplier in the variance estimator, then specify the VADJUST=NONE option in the MODEL statement.

### Balanced Repeated Replication (BRR) Method

The balanced repeated replication (BRR) method requires that the full sample be drawn by using a stratified sample design with two primary sampling units (PSUs) per stratum. The BRR method constructs half-sample replicates by deleting one PSU per stratum according to a Hadamard matrix and doubling the original

weight of the other PSU in that stratum. Let  $H$  be the total number of strata. The total number of replicates  $R$  is the smallest multiple of 4 that is greater than  $H$ . However, if you prefer a larger number of replicates, you can specify the `REPS= $n$  method-option`. If a  $n \times n$  Hadamard matrix cannot be constructed, the number of replicates is increased until a Hadamard matrix becomes available.

Each replicate is obtained by deleting one PSU per stratum according to a corresponding Hadamard matrix and adjusting the original weights for the remaining PSUs. The new weights are called replicate weights.

Replicates are constructed by using the first  $H$  columns of the  $R \times R$  Hadamard matrix. The  $r$ th ( $r = 1, 2, \dots, R$ ) replicate is drawn from the full sample according to the  $r$ th row of the Hadamard matrix as follows:

- If the  $(r, h)$  element of the Hadamard matrix is 1, then the first PSU of stratum  $h$  is included in the  $r$ th replicate and the second PSU of stratum  $h$  is excluded.
- If the  $(r, h)$  element of the Hadamard matrix is  $-1$ , then the second PSU of stratum  $h$  is included in the  $r$ th replicate and the first PSU of stratum  $h$  is excluded.

The replicate weights of the remaining PSUs in each half sample are then doubled to their original weights. For more detail about the BRR method, see Wolter (2007) and Lohr (2010).

By default, an appropriate Hadamard matrix is generated automatically to create the replicates. You can display the Hadamard matrix by specifying the `VARMETHOD=BRR(PRINTH) method-option`. If you provide a Hadamard matrix by specifying the `VARMETHOD=BRR(HADAMARD=) method-option`, then the replicates are generated according to the provided Hadamard matrix. You can use the `VARMETHOD=BRR(OUTWEIGHTS=) method-option` to store the replicate weights in a SAS data set.

Let  $\hat{\beta}$  be the estimated proportional hazards regression coefficients from the full sample, and let  $\hat{\beta}_r$  be the estimated proportional hazards regression coefficients from the  $r$ th replicate by using replicate weights. PROC SURVEYPHREG estimates the covariance matrix of  $\hat{\beta}$  by

$$\widehat{V}(\hat{\beta}) = \frac{1}{R} \sum_{r=1}^R (\hat{\beta}_r - \hat{\beta}) (\hat{\beta}_r - \hat{\beta})'$$

with  $H$  degrees of freedom, where  $H$  is the number of strata.

If you specify the `CENTER=REPLICATES method-option`, then PROC SURVEYPHREG computes the covariance matrix of  $\hat{\beta}$  by

$$\widehat{V}(\hat{\beta}) = \frac{1}{R} \sum_{r=1}^R (\hat{\beta}_r - \overline{\hat{\beta}}_r) (\hat{\beta}_r - \overline{\hat{\beta}}_r)'$$

where  $\overline{\hat{\beta}}_r$  is the average of the replicate estimates as follows:

$$\overline{\hat{\beta}}_r = \frac{1}{R} \sum_{r=1}^R \hat{\beta}_r$$

If one or more components of  $\hat{\beta}_r$  cannot be calculated for some replicates, then the variance estimate is computed by using only the replicates for which the proportional hazards regression coefficients can

be estimated. Estimability and nonconvergence are the two most common reasons why  $\hat{\beta}_r$  might not be available for a replicate sample even if  $\hat{\beta}$  is defined for the full sample. Let  $R_a$  be the number of replicates where  $\hat{\beta}_r$  is available, and let  $R - R_a$  be the number of replicates where  $\hat{\beta}_r$  is not available. Without loss of generality, assume that  $\hat{\beta}_r$  is available only for the first  $R_a$  replicates; then the BRR variance estimator is

$$\widehat{V}(\hat{\beta}) = \frac{1}{R_a} \sum_{r=1}^{R_a} (\hat{\beta}_r - \hat{\beta})(\hat{\beta}_r - \hat{\beta})'$$

with degrees of freedom equal to the minimum of  $H$  and  $R_a$ , where  $H$  is the number of strata. Alternatively, you can use the `FAY=method-option` to request Fay's BRR method, as discussed in the following section.

### Fay's BRR Method

The traditional BRR method constructs half-sample replicates by deleting one PSU per stratum according to a Hadamard matrix and doubling the original weight of the other PSU. Fay's BRR method uses the Fay coefficient,  $\epsilon$  ( $0 \leq \epsilon < 1$ ), and instead of deleting one PSU per stratum, it multiplies the original weight by the coefficient  $\epsilon$ . The original weight of the remaining PSU in that stratum is multiplied by  $2 - \epsilon$ . PROC SURVEYPHREG uses  $\epsilon = 0.5$  as the default value; alternatively, you can specify a value for  $\epsilon$  with the `FAY=method-option`. When  $\epsilon = 0$ , Fay's method becomes the traditional BRR method. For more details, see Dipppo, Fay, and Morganstein (1984); Fay (1984, 1989); Judkins (1990). Because the traditional BRR method uses only half of the total sample in every replicate, several replicate estimators ( $\hat{\beta}_r$ ) might be undefined even when the full sample estimator ( $\hat{\beta}$ ) is defined. Fay's BRR method is especially useful for this situation because it uses all the sampled units in every replicate.

Let  $\hat{\beta}$  be the estimated proportional hazards regression coefficients from the full sample, and let  $\hat{\beta}_r$  be the estimated regression coefficients that are obtained from the  $r$ th replicate by using replicate weights. PROC SURVEYPHREG estimates the covariance matrix of  $\hat{\beta}$  by

$$\widehat{V}(\hat{\beta}) = \frac{1}{R(1-\epsilon)^2} \sum_{r=1}^R (\hat{\beta}_r - \hat{\beta})(\hat{\beta}_r - \hat{\beta})'$$

with  $H$  degrees of freedom, where  $H$  is the number of strata.

### Hadamard Matrix

PROC SURVEYPHREG uses a Hadamard matrix to construct replicates for BRR variance estimation. You can provide a Hadamard matrix for replicate construction by using the `HADAMARD=method-option` for `VARMETHOD=BRR`. Otherwise, PROC SURVEYPHREG generates an appropriate Hadamard matrix. You can display the Hadamard matrix by specifying the `PRINTH method-option`.

A Hadamard matrix  $\mathbf{A}$  of dimension  $R$  is a square matrix that has all elements equal to 1 or  $-1$  such that  $\mathbf{A}'\mathbf{A} = R\mathbf{I}$ , where  $\mathbf{I}$  is an identity matrix of appropriate order. The dimension of a Hadamard matrix must equal 1, 2, or a multiple of 4.

For example, the following matrix is a Hadamard matrix of dimension  $k = 8$ :

$$\begin{matrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 \end{matrix}$$

For BRR replicate construction, the dimension of the Hadamard matrix must be at least  $H$ , where  $H$  denotes the number of first-stage strata in your design. If a Hadamard matrix of a given dimension exists, it is not necessarily unique. Therefore, if you want to use a specific Hadamard matrix, you must provide the matrix as a SAS data set in the `HADAMARD=method-option`. You must ensure that the matrix that you provide is actually a Hadamard matrix; PROC SURVEYPHREG does not check the validity of your Hadamard matrix.

See the section “Balanced Repeated Replication (BRR) Method” on page 7896 for details about how the Hadamard matrix is used to construct replicates for BRR variance estimation.

## Jackknife Method

The jackknife method of variance estimation deletes one PSU at a time from the full sample to create replicates. This method is also known as the delete-1 jackknife method because it deletes exactly one PSU in every replicate. The total number of replicates  $R$  is the same as the total number of PSUs. In each replicate, the sampling weights of the remaining PSUs are modified by the *jackknife coefficient*  $\alpha_r$ . The modified weights are called replicate weights.

Let PSU  $i$  in stratum  $h_r$  be omitted for the  $r$ th replicate; then the jackknife coefficient and replicate weights are computed as

$$\alpha_r = \begin{cases} \frac{n_{hr}-1}{n_{hr}} & \text{for a stratified design} \\ \frac{R-1}{R} & \text{for designs without stratification} \end{cases}$$

and

$$w_{hij}^{(r)} = \begin{cases} w_{hij} & \text{if observation unit } j \text{ is not in donor stratum } h_r \\ 0 & \text{if observation unit } j \text{ is in PSU } i \text{ of donor stratum } h_r \\ w_{hij}/\alpha_r & \text{if observation unit } j \text{ is not in PSU } i \text{ but in donor stratum } h_r \end{cases}$$

You can use the `VARMETHOD=JACKKNIFE(OUTJKCOEFS=)` *method-option* to store the jackknife coefficients in a SAS data set and use the `VARMETHOD=JACKKNIFE(OUTWEIGHTS=)` *method-option* to store the replicate weights in a SAS data set.

If you provide your own replicate weights with a `REPWEIGHTS` statement, then you can also provide corresponding jackknife coefficients with the `JKCOEFS=` option. If you provide replicate weights with a `REPWEIGHTS` statement but do not provide jackknife coefficients, then the procedure uses  $(R - 1)/R$  as the default jackknife coefficient for every replicate, where  $R$  is the total number of replicates.

Let  $\hat{\beta}$  be the estimated proportional hazards regression coefficients from the full sample, and let  $\hat{\beta}_r$  be the estimated regression coefficients for the  $r$ th replicate. PROC SURVEYPHREG estimates the covariance matrix of  $\hat{\beta}$  by

$$\widehat{V}(\hat{\beta}) = \sum_{r=1}^R \alpha_r (\hat{\beta}_r - \hat{\beta}) (\hat{\beta}_r - \hat{\beta})'$$

with  $R - H$  degrees of freedom, where  $R$  is the number of replicates and  $H$  is the number of strata, or  $R - 1$  when there is no stratification.

If you specify the `CENTER=REPLICATES` *method-option*, then PROC SURVEYPHREG computes the covariance matrix of  $\hat{\beta}$  by

$$\widehat{V}(\hat{\beta}) = \sum_{r=1}^R \alpha_r (\hat{\beta}_r - \overline{\hat{\beta}_r}) (\hat{\beta}_r - \overline{\hat{\beta}_r})'$$

where  $\overline{\hat{\beta}_r}$  is the average of the replicate estimates as follows:

$$\overline{\hat{\beta}_r} = \frac{1}{R} \sum_{r=1}^R \hat{\beta}_r$$

If one or more components of  $\hat{\beta}_r$  cannot be calculated for some replicates, then the variance estimator uses only the replicates for which the proportional hazards regression coefficients can be estimated. Estimability and nonconvergence are two common reasons why  $\hat{\beta}_r$  might not be available for a replicate sample even if  $\hat{\beta}$  is defined for the full sample. Let  $R_a$  be the number of replicates where  $\hat{\beta}_r$  are available, and let  $R - R_a$  be the number of replicates where  $\hat{\beta}_r$  are not available. Without loss of generality, assume that  $\hat{\beta}_r$  is available only for the first  $R_a$  replicates; then the jackknife variance estimator is

$$\widehat{V}(\hat{\beta}) = \sum_{r=1}^{R_a} \alpha_r (\hat{\beta}_r - \hat{\beta}) (\hat{\beta}_r - \hat{\beta})'$$

with  $R_a - H$  degrees of freedom, where  $H$  is the number of strata. Alternatively, you can use the `VADJUST=AVGREPSS` option in the MODEL statement to use the average sum of squares for the invalid replicate samples. See “[Variance Adjustment Factors](#)” on page 7902 for details.



## Degrees of Freedom

PROC SURVEYPHREG uses the degrees of freedom of the variance estimator to obtain  $t$  confidence limits and Wald type  $F$  tests. PROC SURVEYPHREG computes the degrees of freedom based on the variance estimation method and the sample design. Alternatively, you can specify the degrees of freedom in the **DF=** option in the **MODEL** statement.

For Taylor series variance estimation, PROC SURVEYPHREG calculates the degrees of freedom ( $df$ ) as the number of clusters minus the number of strata. If the **CLUSTER** statement is not specified, then the procedure treats each observation as a cluster. If the **STRATA** statement is not specified, then the procedure assumes that all observations are in the same stratum. These numbers are based on the observations included in the analysis. These numbers do not count observations that are excluded from the analysis due to missing values. See the section “Missing Values” on page 7893 for details. If you specify the **MISSING** option in the **CLASS** statement, missing values are treated as valid nonmissing levels and are included in computing degrees of freedom. If you specify the **NOMCAR** option for Taylor series variance estimation, observations with missing values of the analysis variables are included in computing the degrees of freedom.

If you provide replicate weights with a **REPWEIGHTS** statement, the degrees of freedom is equal the number of replicates used, which is the number of **REPWEIGHTS** variables that provide replicate estimates. Alternatively, you can specify the degrees of freedom in the **DF=** option in the **REPWEIGHTS** or **MODEL** statement.

For BRR variance estimation (when you do not use a **REPWEIGHTS** statement), PROC SURVEYPHREG calculates the degrees of freedom as the number of strata. PROC SURVEYPHREG bases the number of strata on all valid observations in the data set. If some replicate samples are not usable in the sense that these replicate samples cannot be used for parameter estimation (say, for nonconvergence or inestimability), then  $df$  equals the minimum of the number of strata and the number of replicates used. Alternatively, you can use the **DF=ALLREPS** option in the **MODEL** statement to specify that  $df$  equals the number of strata.

For jackknife variance estimation (when you do not use a **REPWEIGHTS** statement), PROC SURVEYPHREG calculates the degrees of freedom as the number of clusters minus the number of strata. If the **CLUSTER** statement is not specified, then the procedure treats each observation as a cluster. If the **STRATA** statement is not specified, then the procedure assumes that all observations are in the same stratum. For jackknife variance estimation, PROC SURVEYPHREG bases the number of strata and clusters on all valid observations in the data set. If some replicate samples are not usable in the sense that these replicate samples cannot be used for parameter estimation (say, for nonconvergence or inestimability), then  $df$  equals the number of clusters (or observations if no **CLUSTER** statement is specified) minus the number of strata (or one in if no **STRATA** statement is specified) minus the number of replicate samples that are not used. Alternatively, you can use the **DF=ALLREPS** option in the **MODEL** statement to specify that  $df$  equals the number of clusters minus the number of strata.



## Variance Adjustment Factors

PROC SURVEYPHREG provides options for adjustment of the default variance estimators. VADJUST=NONE and VADJUST=DF are available for the Taylor series linearization variance estimator. VADJUST=AVGREPSS is available for the jackknife replication variance estimators.

For models with large number of parameters, it is reasonable to adjust the Taylor series linearized variance estimator by the number of estimable parameters in the analysis model. Fuller et al. (1989, pp. 77–81) use an adjustment factor  $(n - 1)/(n - p)$  to estimate the linearized variance for regression coefficients, where  $n$  is the total number of observation units and  $p$  is the number of estimable parameters in the analysis model. By default, PROC SURVEYPHREG uses this adjustment in the computation of the matrix  $\mathbf{G}$  for the Taylor series linearization **variance estimation**. If you do not want to use this adjustment, then specify VADJUST=NONE.

Variance adjustment factors can be useful for replication variance estimations, especially if some replicate samples are not usable. A replicate sample might not provide useful parameter estimates (replicate estimates) for reasons such as nonconvergence of the optimization or inestimability of some parameters in that subsample. For example, consider the **jackknife variance estimator** with  $R$  replicates. Suppose that only  $R_a (< R)$  replicates are used to obtain replicate estimates and  $R - R_a$  replicates cannot be used due to, say, nonconvergence of the optimization. Without loss of generality, assume that the first  $R_a$  replicates are used. By default SURVEYPHREG uses

$$\widehat{\mathbf{V}}(\hat{\boldsymbol{\beta}}) = \sum_{r=1}^{R_a} \alpha_r (\hat{\boldsymbol{\beta}}_r - \hat{\boldsymbol{\beta}}) (\hat{\boldsymbol{\beta}}_r - \hat{\boldsymbol{\beta}})'$$

as the jackknife variance estimator. An alternative estimator is

$$\begin{aligned} \widehat{\mathbf{V}}(\hat{\boldsymbol{\beta}}) &= \sum_{r=1}^{R_a} \alpha_r (\hat{\boldsymbol{\beta}}_r - \hat{\boldsymbol{\beta}}) (\hat{\boldsymbol{\beta}}_r - \hat{\boldsymbol{\beta}})' + (R - R_a) \left\{ \frac{1}{R_a} \sum_{r=1}^{R_a} \alpha_r (\hat{\boldsymbol{\beta}}_r - \hat{\boldsymbol{\beta}}) (\hat{\boldsymbol{\beta}}_r - \hat{\boldsymbol{\beta}})' \right\} \\ &= \frac{R}{R_a} \sum_{r=1}^{R_a} \alpha_r (\hat{\boldsymbol{\beta}}_r - \hat{\boldsymbol{\beta}}) (\hat{\boldsymbol{\beta}}_r - \hat{\boldsymbol{\beta}})' \end{aligned}$$

which uses the average replicate sum of squares for the  $R - R_a$  unusable replicate samples. If you specify the VADJUST=AVGREPSS option, PROC SURVEYPHREG uses the second variance estimator for the jackknife replication method. Note that you can specify the **FAY method-option** for the BRR method to avoid nonconvergence of the optimization or inestimability of some parameters in subsamples.

## Variance Ratios and Standard Error Ratios

PROC SURVEYPHREG provides options to compute different variance ratios and standard error ratios.

If you specify the VARRATIO=MODEL option, then the procedure computes the variance ratio of the estimated regression parameter  $\hat{\beta}_j$  as  $\frac{\widehat{V}(\hat{\beta}_j)}{\widehat{V}_M(\hat{\beta}_j)}$ , where  $\widehat{V}(\hat{\beta}_j)$ , the estimated variance of  $\hat{\beta}_j$ , uses the complete design information and  $\widehat{V}_M(\hat{\beta}_j)$  is the  $j$ th diagonal element of the observed information matrix  $\mathcal{I}^{-1}(\hat{\boldsymbol{\beta}})$ .

If you specify the VARRATIO=IND option, then the procedure computes the variance ratio of the estimated regression parameter  $\hat{\beta}_j$  as  $\frac{\widehat{V}(\hat{\beta}_j)}{\widehat{V}_{\text{IND}}(\hat{\beta}_j)}$ , where  $\widehat{V}(\hat{\beta}_j)$ , the estimated variance of  $\hat{\beta}_j$ , uses the complete design information and  $\widehat{V}_{\text{IND}}(\hat{\beta}_j)$  is the  $j$ th diagonal element of  $\widehat{V}_{\text{IND}}(\hat{\boldsymbol{\beta}})$ .  $\widehat{V}_{\text{IND}}(\hat{\boldsymbol{\beta}})$  is the sandwich variance

estimator, which ignores the strata and the clusters and is computed as

$$\hat{V}_{\text{IND}}(\hat{\beta}) = \mathcal{I}^{-1}(\hat{\beta}) \left\{ \frac{n}{n-1} (1-f) \sum_h \sum_i \sum_j (e_{hij} - \bar{e}_{\dots})' (e_{hij} - \bar{e}_{\dots}) \right\} \mathcal{I}^{-1}(\hat{\beta})$$

where  $e_{hij}$  are the weighted score residuals,  $f$  is the overall sampling fraction, and  $n$  is the number of observation units. The three sums are over the observation units ( $j$ ) across the PSUs ( $i$ ) and the strata ( $h$ ).

For Taylor series variance estimation, PROC SURVEYPHREG determines the value of  $f$ , the overall sampling fraction, based on the **RATE=** or **TOTAL=** option. If you do not specify either of these options, PROC SURVEYPHREG assumes that the value of  $f$  is negligible and does not use a finite population correction in the analysis. If you specify **RATE=value**, PROC SURVEYPHREG uses *value* as the overall sampling fraction  $f$ . If you specify **TOTAL=value**, PROC SURVEYPHREG computes  $f$  as the ratio of the number of PSUs in the sample to the specified total.

If you specify stratum sampling rates by using the **RATE=SAS-data-set** option, then PROC SURVEYPHREG computes stratum totals based on these stratum sampling rates and the number of sample PSUs in each stratum. The procedure sums the stratum totals to form the overall total and then computes  $f$  as the ratio of the number of sample PSUs to the overall total. Alternatively, if you specify stratum totals with the **TOTAL=SAS-data-set** option, then PROC SURVEYPHREG sums these totals to compute the overall total. The overall sampling fraction  $f$  is then computed as the ratio of the number of sample PSUs to the overall total.

The replication methods do not use the finite population correction factor  $(1 - f)$  in the denominator.

Standard error ratios are computed as the square root of the variance ratios.

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## Domain Analysis

*Domain analysis* refers to the computation of statistics for domains (subpopulations). Formation of subpopulations can be unrelated to the sample design, and so the domain sample sizes can actually be random variables. Domain analysis takes this variability into account to compute variance estimates for estimated model parameters. Domain analysis is also known as subgroup analysis, subpopulation analysis, and subdomain analysis. For more information about domain analysis, see Lohr (2010); Särndal, Swensson, and Wretman (1992); Cochran (1977).

To request domain analysis with PROC SURVEYPHREG, use the **DOMAIN** statement. If your domains are formed by more than one variable, you can specify **DomainVariable\_1 \* DomainVariable\_2** in the **DOMAIN** statement. If you use the **DOMAIN** statement, the procedure performs separate analyses for all domains, in addition to the overall analysis.

Including the domain variables in a **DOMAIN** statement request provides a different analysis from that obtained by using a **BY** statement, which provides completely separate analyses of the **BY** groups. The **BY** statement can also be used to analyze the data set by subgroups, but it is critical to note that this does *not* account for random sample sizes that often occur for domain analyses. The **BY** statement is appropriate only when the number of units in each subgroup is known with certainty. For example, the **BY** statement can be used to obtain stratum level estimates when you have fixed sample sizes for the strata. When the subgroup sample size is random, include the domain variables in **DOMAIN** statement.

## Hypothesis Tests, Confidence Intervals, and Residuals

### Testing the Global Null Hypothesis

The following statistics can be used to test the global null hypothesis  $H_0: \boldsymbol{\beta} = \mathbf{0}$ . Let  $d$  be the number of clusters (or observations) minus the number of strata (or one) and  $p$  be the number of estimable parameters in the analysis model.

The likelihood ratio test is expressed as

$$\chi_{LR}^2 = 2 \left[ \log \{L(\hat{\boldsymbol{\beta}})\} - \log \{L(\mathbf{0})\} \right]$$

where  $L(\cdot)$  denotes the partial pseudo-likelihood described in “[Partial Likelihood Function for the Cox Model](#)” on page 7890. The  $p$ -value is computed by using a chi-square distribution with  $p$  degrees of freedom. The usual assumptions required for a likelihood ratio test do not hold for the pseudo-likelihood that is used by PROC SURVEYPHREG, leading to other methods for testing the global null hypothesis, such as the Wald test discussed below.

Wald’s test is expressed as

$$W_F = \left( \frac{d - p + 1}{dp} \right) \hat{\boldsymbol{\beta}}' \left[ \widehat{\mathbf{V}}(\hat{\boldsymbol{\beta}}) \right]^{-1} \hat{\boldsymbol{\beta}}$$

The  $p$ -value is computed by using an  $F$  distribution with  $(p, d)$  degrees of freedom. For the Taylor series linearization method, the `DF=PARMADJ` option in the MODEL statement computes the  $p$ -value by using an  $F$  distribution with  $(p, d - p + 1)$  degrees of freedom.

If you specify the `DF=NONE` option in the MODEL statement, then the procedure computes

$$W_{\chi^2} = \hat{\boldsymbol{\beta}}' \left[ \widehat{\mathbf{V}}(\hat{\boldsymbol{\beta}}) \right]^{-1} \hat{\boldsymbol{\beta}}$$

and the  $p$ -value is computed by using a chi-square distribution with  $p$  degrees of freedom.

### Model Fit Statistics

Suppose the model contains  $p$  estimable parameters. Then the following two criteria are displayed for model fit statistics:

- $-2 \log$  likelihood:

$$-2 \text{ Log L} = -2 \log(L(\hat{\boldsymbol{\beta}}))$$

where  $L(\cdot)$  is a partial pseudo-likelihood function for the corresponding `TIES=` option as described in the section “[Partial Likelihood Function for the Cox Model](#)” on page 7890, and  $\hat{\boldsymbol{\beta}}$  is the maximum pseudo-log-likelihood estimate of the proportional hazards regression coefficients.

- Akaike’s information criterion (AIC):

$$\text{AIC} = -2 \text{ Log L} + 2p$$

The AIC statistics gives a different way of adjusting the  $-2 \log$  likelihood statistic for the number of estimable parameters in the model.

## Contrasts

For a testable hypothesis  $H_0: \mathbf{L}\boldsymbol{\beta} = 0$ , the Wald  $F$  statistic is computed as

$$F_{\text{Wald}} = \frac{(\mathbf{L}^* \hat{\boldsymbol{\beta}})' (\mathbf{L}^* \hat{\mathbf{V}} \mathbf{L}^*)^{-1} (\mathbf{L}^* \hat{\boldsymbol{\beta}})}{\text{rank}(\mathbf{L})}$$

where  $\mathbf{L}$  is a contrast vector or matrix that you specify,  $\boldsymbol{\beta}$  is the vector of regression parameters,  $\hat{\boldsymbol{\beta}}$  is the estimated regression coefficients,  $\hat{\mathbf{V}}$  is the estimated covariance matrix of  $\hat{\boldsymbol{\beta}}$ ,  $\text{rank}(\mathbf{L})$  is the rank of  $\mathbf{L}$ , and  $\mathbf{L}^*$  is a matrix such that

- $\mathbf{L}^*$  has the same number of columns as  $\mathbf{L}$
- $\mathbf{L}^*$  has full row rank
- the rank of  $\mathbf{L}^*$  equals the rank of the  $\mathbf{L}$  matrix
- all rows of  $\mathbf{L}^*$  are estimable functions
- the Wald  $F$  statistic computed by using the  $\mathbf{L}^*$  matrix is equivalent to the Wald  $F$  statistic computed by using the  $\mathbf{L}$  matrix with any row deleted that is a linear combination of previous rows

If  $\mathbf{L}$  is a full-rank matrix and all rows of  $\mathbf{L}$  are estimable functions, then  $\mathbf{L}^*$  is the same as  $\mathbf{L}$ . It is possible that  $\mathbf{L}$  matrix cannot be constructed for a given set of linear contrasts, in which case the contrasts are not testable.

If the **DF=NONE** option in the MODEL statement is specified, then the procedure performs a chi-square significance test.

## Confidence Intervals

By default, the SURVEYPHREG procedure computes  $t$  confidence limits for the estimated regression coefficients. Alternatively, you can specify the **DF=NONE** option in the MODEL statement to request standard normal confidence intervals. The  $t$  confidence interval for a linear combination  $\mathbf{L}'\boldsymbol{\beta}$  of the regression coefficients is computed as

$$\left( \mathbf{L}'\hat{\boldsymbol{\beta}} \pm t_{df, \alpha/2} \sqrt{\mathbf{L}'\hat{\mathbf{V}}(\hat{\boldsymbol{\beta}})\mathbf{L}} \right)$$

where  $t_{df, \alpha/2}$  is the  $100(1 - \alpha/2)$  percentile point of the  $t$  distribution with  $df$  degrees of freedom. See the section “**Degrees of Freedom**” on page 7901 for more information about  $df$ . If you use the **DF=NONE** option in the MODEL statement, then the procedure uses the  $100(1 - \alpha/2)$  percentile point of the standard normal distribution.

## Hazard Ratios

The hazard ratio for a quantitative effect with regression coefficient  $\beta_j = \mathbf{e}'_j \boldsymbol{\beta}$  is defined as  $\exp(\beta_j)$ , where  $\mathbf{e}_j$  denotes the  $j$ th unit vector. In general, a log-hazard ratio can be written as  $\mathbf{L}'\boldsymbol{\beta}$ , a linear combination of the regression coefficients, and the hazard ratio  $\exp(\mathbf{L}'\boldsymbol{\beta})$  is obtained by replacing  $\mathbf{e}_j$  with  $\mathbf{l}$ .

The confidence intervals for hazard ratios are obtained by exponentiating the confidence limits of the corresponding linear combination. Thus, the  $100(1 - \alpha)$  confidence limits are

$$\exp\left(\mathbf{e}'_j \hat{\boldsymbol{\beta}} \pm t_{df, \alpha/2} \sqrt{\mathbf{e}'_j \hat{\mathbf{V}}(\hat{\boldsymbol{\beta}}) \mathbf{e}_j}\right)$$

where  $t_{df, \alpha/2}$  is the  $100(1 - \alpha/2)$  percentile point of the  $t$  distribution with  $df$  degrees of freedom. See the section “[Degrees of Freedom](#)” on page 7901 for more information about  $df$ . If you use the `DF=NONE` option in the MODEL statement, then the procedure uses the  $100(1 - \alpha/2)$  percentile point of the standard normal distribution.

## Residuals

This section describes the computation of residuals (RESMART, RESDEV, RESSCH, and RESSCO in the OUTPUT statement). See the section “[Notation and Estimation](#)” on page 7884 for definition of notation that is used in this section. The residuals are calculated based on the `TIES=` option in the MODEL statement.

### **TIES=BRESLOW**

This is the default option. Let

$$S^{(r)}(\boldsymbol{\beta}, t) = \sum_A w_{hij} y_{hij}(t) \exp(\boldsymbol{\beta}' \mathbf{Z}_{hij}(t)) \mathbf{Z}_{hij}^{\otimes r}(t)$$

$$\bar{\mathbf{Z}}(\boldsymbol{\beta}, t) = \frac{S^{(1)}(\boldsymbol{\beta}, t)}{S^{(0)}(\boldsymbol{\beta}, t)}$$

where  $r = 0, 1$ ; and  $A$  be the set of indices in the selected sample.

Further let

$$\begin{aligned} d\Lambda_0(\boldsymbol{\beta}, t) &= \sum_A \frac{w_{hij} dn_{hij}(t)}{S^{(0)}(\boldsymbol{\beta}, t)} \\ dM_{hij}(\boldsymbol{\beta}, t) &= dn_{hij}(t) - y_{hij}(t) \exp(\boldsymbol{\beta}' \mathbf{Z}_{hij}(t)) d\Lambda_0(\boldsymbol{\beta}, t) \end{aligned}$$

The martingale residual at  $t$  is defined as

$$\begin{aligned} \hat{M}_{hij}(t) &= \int_0^t dM_{hij}(\hat{\boldsymbol{\beta}}, \tau) \\ &= n_{hij}(t) - \int_0^t y_{hij}(\tau) \exp(\hat{\boldsymbol{\beta}}' \mathbf{Z}_{hij}(\tau)) d\Lambda_0(\hat{\boldsymbol{\beta}}, \tau) \end{aligned}$$

Here  $\hat{M}_{hij}(t)$  estimates the difference over  $(0, t]$  between the observed number of events for the  $(h, i, j)$  observation unit and a conditional expected number of events. The quantity  $\hat{M}_{hij} \equiv \hat{M}_{hij}(\infty)$  is referred to as the martingale residual for the  $(h, i, j)$  observation unit. For the Cox model with no time-dependent explanatory variables, the martingale residual for the  $(h, i, j)$  unit with observation time  $t_{(h,i,j)}$  and event status  $\Delta_{(h,i,j)}$  is

$$\hat{M}_{(h,i,j)} = \Delta_{(h,i,j)} - e^{\hat{\boldsymbol{\beta}}' \mathbf{Z}_{(h,i,j)}} \int_0^{t_{(h,i,j)}} d\Lambda_0(\hat{\boldsymbol{\beta}}, s)$$

The deviance residual  $D_{hij}$  for the  $(h, i, j)$  observation unit is a transformation of the corresponding martingale residuals,

$$D_{hij} = \text{sign}(\hat{M}_{hij}) \sqrt{2 \left[ -\hat{M}_{hij} - n_{hij}(\infty) \log \left( \frac{n_{hij}(\infty) - \hat{M}_{hij}}{n_{hij}(\infty)} \right) \right]}$$

The square root shrinks large negative martingale residuals, while the logarithmic transformation expands martingale residuals that are close to unity. As such, the deviance residuals are more symmetrically distributed around zero than the martingale residuals. For the Cox model, the deviance residual reduces to the form

$$D_{hij} = \text{sign}(\hat{M}_{hij}) \sqrt{2[-\hat{M}_{hij} - \Delta_{hij} \log(\Delta_{hij} - \hat{M}_{hij})]}$$

The Schoenfeld (1982) residual vector is calculated on a per-event-time basis. At the  $k$ th event time  $t_{hij,k}$  of the  $(h, i, j)$  observation unit, the Schoenfeld residual

$$\hat{U}_{hij}(t_{hij,k}) = \mathbf{Z}_{hij}(t_{hij,k}) - \bar{\mathbf{Z}}(\hat{\boldsymbol{\beta}}, t_{hij,k})$$

is the difference between the observed covariate vector for the  $(h, i, j)$  observation unit and the average of the covariate vectors over the risk set at  $t_{hij,k}$ . Under the proportional hazards assumption, the Schoenfeld residuals have the sample path of a random walk; therefore, they are useful in assessing time trend or lack of proportionality.

The score process for the  $(h, i, j)$  subject at time  $t$  is

$$\mathbf{L}_{hij}(\boldsymbol{\beta}, t) = \int_0^t [\mathbf{Z}_{hij}(\tau) - \bar{\mathbf{Z}}(\boldsymbol{\beta}, \tau)] dM_{hij}(\boldsymbol{\beta}, \tau)$$

The vector  $\hat{\mathbf{L}}_{hij} \equiv \mathbf{L}_{hij}(\hat{\boldsymbol{\beta}}, \infty)$  is the score residual for the  $(h, i, j)$  observation unit.

The score residuals are a decomposition of the first partial derivative of the log likelihood. They are useful in assessing the influence of each subject on individual parameter estimates. They also play an important role in the computation of the variance estimators.

### TIES=EFRON

For TIES=EFRON, the preceding computation is modified to comply with the Efron partial likelihood. For a given uncensored time  $t$ , let  $\delta_{hij}(t) = 1$  if  $t$  is an event time for the  $(h, i, j)$  observation, and 0 otherwise. Let  $d(t) = \sum_{hij \in A} \delta_{hij}(t)$ , which is the number of observation units that have an event at  $t$ . For  $1 \leq l \leq d(t)$ , let

$$\begin{aligned} S^{(r)}(\boldsymbol{\beta}, l, t) &= \sum_A w_{hij} y_{hij}(t) \left\{ 1 - \frac{l-1}{d(t)} \delta_{hij}(t) \right\} \exp(\boldsymbol{\beta}' \mathbf{Z}_{hij}(t)) \mathbf{Z}_{hij}^{\otimes r}(t) \\ \bar{\mathbf{Z}}(\boldsymbol{\beta}, l, t) &= \frac{S^{(1)}(\boldsymbol{\beta}, l, t)}{S^{(0)}(\boldsymbol{\beta}, l, t)} \\ d\Lambda_0(\boldsymbol{\beta}, l, t) &= \sum_A \frac{w_{hij} d n_{hij}(t)}{S^{(0)}(\boldsymbol{\beta}, l, t)} \\ dM_{hij}(\boldsymbol{\beta}, l, t) &= d n_{hij}(t) - y_{hij}(t) \left( 1 - \delta_{hij}(t) \frac{l-1}{d(t)} \right) \exp(\boldsymbol{\beta}' \mathbf{Z}_{hij}(t)) d\Lambda_0(\boldsymbol{\beta}, l, t) \end{aligned}$$

where  $r = 0, 1$ , and  $A$  are the set of indices in the selected sample.

The martingale residual at  $t$  for the  $(h, i, j)$  observation unit is defined as

$$\begin{aligned}\hat{M}_{hij}(t) &= \int_0^t \frac{1}{d(\tau)} \sum_{l=1}^{d(\tau)} dM_{hij}(\hat{\beta}, l, \tau) \\ &= n_{hij}(t) - \int_0^t \frac{1}{d(\tau)} \sum_{l=1}^{d(\tau)} y_{hij}(\tau) \left(1 - \delta_{hij}(\tau) \frac{l-1}{d(\tau)}\right) \exp\left(\hat{\beta}' \mathbf{Z}_{hij}(\tau)\right) d\Lambda_0(\hat{\beta}, l, \tau)\end{aligned}$$

Deviance residuals are computed by using the same transform on the corresponding martingale residuals as in TIES=BRESLOW.

The Schoenfeld residual vector for the  $(h, i, j)$  observation unit at event time  $t_{hij,k}$  is

$$\hat{\mathbf{U}}_{hij}(t_{hij,k}) = \mathbf{Z}_{hij}(t_{hij,k}) - \frac{1}{d(t_{hij,k})} \sum_{l=1}^{d(t_{hij,k})} \bar{\mathbf{Z}}(\hat{\beta}, l, t_{hij,k})$$

The score process for the  $(h, i, j)$  observation unit at time  $t$  is

$$\mathbf{L}_{hij}(\beta, t) = \int_0^t \frac{1}{d(\tau)} \sum_{l=1}^{d(\tau)} \left(\mathbf{Z}_{hij}(\tau) - \bar{\mathbf{Z}}(\beta, l, \tau)\right) dM_{hij}(\beta, l, \tau)$$

## Output Data Sets

You can use the Output Delivery System to create a SAS data set from any piece of PROC SURVEYPHREG output. See the section “ODS Table Names” on page 7912 for more information. PROC SURVEYPHREG also provides an output data set to store observation-level statistics, an output data set to store the replicate weights for BRR or jackknife variance estimation, and an output data set to store the jackknife coefficients for jackknife variance estimation.

### OUT= Data Set for the OUTPUT statement

The **OUTPUT** statement can be used to store observation-level statistics, such as the predicted values and their standard errors, the (weighted) number of observation units at risk, martingale residuals, Schoenfeld residuals, score residuals, and deviance residuals. See the section “Residuals” on page 7906 for details about how these statistics are calculated.

### Replicate Weights Output Data Set

If you specify the **OUTWEIGHTS=** *method-option* for **VARMETHOD=BRR** or **JACKKNIFE**, PROC SURVEYPHREG stores the replicate weights in an output data set. The **OUTWEIGHTS=** output data set contains all observations that are used in the analysis or all valid observations in the **DATA=** input data set. See the section “Missing Values” on page 7893 for details about valid observations.

The OUTWEIGHTS= data set contains the following variables:

- all variables in the DATA= input data set
- RepWt\_1, RepWt\_2, . . . , RepWt\_R, which are the replicate weight variables, where R is the total number of replicates in the analysis

Each replicate weight variable contains the replicate weights for the corresponding replicate. Replicate weights equal zero for those observations not included in the replicate.

After the procedure creates replicate weights for a particular input data set and survey design, you can use the OUTWEIGHTS= *method-option* to store these replicate weights and then use them again in subsequent analyses, either in PROC SURVEYPHREG or in the other survey procedures. You can use a REPWEIGHTS statement to provide replicate weights for the procedure.

### Jackknife Coefficients Output Data Set

If you specify the OUTJKCOEFS= *method-option* for VARMETHOD=JACKKNIFE, PROC SURVEYPHREG stores the jackknife coefficients in an output data set. The OUTJKCOEFS= output data set contains one observation for each replicate. The OUTJKCOEFS= data set contains the following variables:

- Replicate, which is the replicate number for the jackknife coefficient
- JKCoefficient, which is the jackknife coefficient for the replicate
- DonorStratum, which is the stratum of the PSU that was deleted to construct the replicate, if you specify a STRATA statement

After the procedure creates jackknife coefficients for a particular input data set and survey design, you can use the OUTJKCOEFS= *method-option* to store these coefficients and then use them again in subsequent analyses, either in PROC SURVEYPHREG or in the other survey procedures. You can use the JKCOEFS= option in the REPWEIGHTS statement to provide jackknife coefficients for the procedure.

---

## Displayed Output

If you use the NOPRINT option in the PROC SURVEYPHREG statement, the procedure does not display any output. Otherwise, PROC SURVEYPHREG displays results of the analysis in a collection of tables.

### Model Information

The “Model Information” table displays the two-level name of the input data set, the name and label of the failure time variable, the name and label of the censoring variable and the values that indicate censored times, the model, the name and label of the FREQ variable, the name and label of the WEIGHT variable, the name and label of the STRATA variables, the name and label of the CLUSTER variables, and the method of handling ties in the failure time for the Cox model. The ODS name of the “Model Information” table is “ModelInfo.”



## Number of Observations

The “Number of Observations” table displays the number of observations that are read and used, the sum of frequencies read and used, the sum of weights read and used, and the weighted sum of frequencies that are read and used in the analysis. The ODS name of the “Number of Observations” table is “NObs.”

## Summary of the Number of Event and Censored Values

The “Summary of the Number of Event and Censored Values” table displays the number of events and censored values. The ODS name of the “Summary of the Number of Event and Censored Values” table is “CensoredSummary.”

## Summary of the Weighted Number of Event and Censored Values

The “Summary of the Weighted Number of Event and Censored Values” table displays the weighted number of events and censored values. The ODS name of the “Summary of the Weighted Number of Event and Censored Values” table is “WeightedCensoredSummary.”

## Class Level Information

The “Class Level Information” table is displayed when there are CLASS variables in the model. The table lists the categories of every CLASS variable that is used in the model and the corresponding design variable values. The ODS name of the “Class Level Information” table is “ClassLevelInfo.”

## Design Summary Table

The “Design Summary” table provides information about the sample design. The table displays the total number of strata that are read and used, and the total number of clusters read and used. The table is displayed only if you specify a STRATA or CLUSTER statement. The ODS name of the “Design Summary” table is “DesignSummary.”

## Stratum Information Table

If you specify the LIST option in the STRATA statement, PROC SURVEYPHREG displays a “Stratum Information” table. The ODS name of the “Stratum Information Table” is “StrataInfo.” This table provides the following information for each stratum:

- Stratum Index, which is a sequential stratum identification number
- STRATA variables, which list the levels of STRATA variables for the stratum
- Number of Observations, which is the number of observations used in the stratum
- Population Total for the stratum, if you specify the TOTAL= option
- Sampling Rate for the stratum, if you specify the TOTAL= or RATE= option. If you specify the TOTAL= option, the sampling rate is based on the number of valid observations in the stratum.
- Number of Clusters, which is the number of clusters in the stratum, if you specify a CLUSTER statement

## Convergence Status

The “Convergence Status” table displays the convergence status of the optimization routine. The procedure displays this table only when you specify the NLOPTIONS statement. The ODS name of the “Convergence Status” table is “ConvergenceStatus.”

## Model Fit Statistics

The “Model Fit Statistics” table displays the values of  $-2 \log$  likelihood and the AIC for the null model and the fitted model. The ODS name of the “Model Fit Statistics” table is “FitStatistics.”

## Testing Global Null Hypothesis: BETA=0

The “Testing Global Null Hypothesis: BETA=0” table displays results of the likelihood ratio test and the Wald test for testing the hypothesis that all parameters are zero. The ODS name of the “Testing Global Null Hypothesis: BETA=0” table is “GlobalTests.”

## Analysis of Maximum Likelihood Estimates

The “Analysis of Maximum Likelihood Estimates” table displays the denominator degrees of freedom, which is computed as described in the section “Degrees of Freedom” on page 7901; the maximum likelihood estimate of the parameter; the estimated standard error, computed as the square root of the corresponding diagonal element of the estimated covariance matrix; the  $t$  statistic, computed as the parameter estimate divided by the standard error; the  $p$ -value of the  $t$  statistic with respect to a  $t$  distribution with denominator degrees of freedom; and the hazard ratio estimate. The  $t$  confidence limits for the parameter estimates and estimated hazard ratios are displayed if you specify the CLPARM or RISKLIMITS option in the MODEL statement. You can specify the DF=NONE option in the MODEL statement to request  $p$ -values and confidence intervals from a standard normal distribution. If you specify the VARRATIO=ALL | MODEL | IND option in the MODEL statement, then the variance ratios for model or independence (or both) are displayed. If you specify the SERATIO=ALL | MODEL | IND option in the MODEL statement, then the standard error ratios for model or independence (or both) are displayed.

The ODS name of the “Analysis of Maximum Likelihood Estimates” table is “ParameterEstimates.”

## Covariance Matrix

The “Covariance Matrix” table is displayed if you specify the COVB option in the MODEL statement. The table contains the estimated covariance matrix for the parameter estimates. The ODS name of the “Covariance Matrix” table is “CovB.”

## Hessian Matrix

The “Hessian Matrix” table is displayed if you specify the HESS option in the MODEL statement. The table contains the Hessian matrix that is evaluated at the estimated regression parameters. The ODS name of the “Hessian Matrix” table is “Hessian.”

## Inverse Hessian Matrix

The “Inverse Hessian Matrix” table is displayed if you specify the INVHESS option in the MODEL statement. The table contains the inverse of the Hessian matrix evaluated at the estimated regression parameters. The ODS name of the “Inverse Hessian Matrix” table is “InvHessian.”

## Variance Estimation Table

The “Variance Estimation” table provides the following information:

- Method, which is the variance estimation method—Taylor Series, Balanced Repeated Replication, or Jackknife
- Replicate Weights input data set name, if you provide replicate weights with a `REPWEIGHTS` statement
- Number of Replicates, for `VARMETHOD=BRR` or `VARMETHOD=JACKKNIFE`
- Hadamard Data Set name, if you specify the `HADAMARD= method-option` for `VARMETHOD=BRR`
- Fay Coefficient, if you specify the `FAY method-option` for `VARMETHOD=BRR`
- Missing Values Included (MISSING), if you specify the `MISSING` option
- Missing Values Included (NOMCAR), if you specify the `NOMCAR` option
- Missing Values Excluded, if you have missing values and you do not specify the `NOMCAR` option

## Hadamard Matrix

If you specify the `PRINTH method-option` for `VARMETHOD=BRR`, PROC SURVEYPHREG displays the Hadamard matrix that is used to construct replicates for BRR variance estimation. If you provide a Hadamard matrix with the `HADAMARD= method-option` for `VARMETHOD=BRR` but the procedure does not use the entire matrix, the procedure displays only the rows and columns that are actually used to construct replicates. The ODS name of the “Hadamard Matrix” table is “HadamardMatrix.”

---

## ODS Table Names

PROC SURVEYPHREG assigns a name to each table it creates. You can use this name to refer to the table when using the Output Delivery System (ODS) to select tables and create output data sets. For more information about ODS, see Chapter 20, “Using the Output Delivery System.” Table 93.8 lists the table names, along with the corresponding analysis options.

**Table 93.8** ODS Tables Produced by PROC SURVEYPHREG

| ODS Table Name    | Description                                | Statement / Option |
|-------------------|--------------------------------------------|--------------------|
| CensoredSummary   | Summary of event and censored observations | Default            |
| ClassLevelInfo    | CLASS variable levels                      | CLASS              |
| ConvergenceStatus | Convergence status                         | NLOPTIONS / PALL   |
| CovB              | Covariance of parameter estimates          | MODEL / COVB       |
| DesignSummary     | Design summary                             | STRATA or CLUSTER  |
| FitStatistics     | Model fit statistics                       | Default            |
| GlobalTests       | Tests of the global null hypothesis        | Default            |

Table 93.8 *continued*

| ODS Table Name          | Description                                                   | Statement / Option    |
|-------------------------|---------------------------------------------------------------|-----------------------|
| Hadamard                | Hadamard matrix                                               | VARMETHOD=BRR(PRINTH) |
| Hessian                 | Observed Hessian matrix                                       | MODEL / HESSIAN       |
| InvHessian              | Inverse of the observed Hessian matrix                        | MODEL / INVHESS       |
| IterHist                | Iteration history                                             | NLOPTIONS / PHISTORY  |
| ModelInfo               | Model information                                             | Default               |
| NObs                    | Number of observations                                        | Default               |
| ParameterEstimates      | Maximum likelihood Estimates of model parameters              | Default               |
| ParameterEstimatesStart | Initial parameter values for optimization                     | NLOPTIONS / PALL      |
| StrataInfo              | Stratum information                                           | STRATA / LIST         |
| VarianceEstimation      | Variance estimation                                           | Default               |
| WeightedCensoredSummary | Summary of weighted number of event and censored observations | WEIGHT                |

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “Statistical Graphics Using ODS.”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “A Primer on ODS Statistical Graphics” on page 599 in Chapter 21, “Statistical Graphics Using ODS.”

When ODS Graphics is enabled, the ESTIMATE, LSMEANS, LSMESTIMATE, and SLICE statements can produce plots that are associated with their analyses. For information about these plots, see the corresponding sections of Chapter 19, “Shared Concepts and Topics.”

## Examples: SURVEYPHREG Procedure

### Example 93.1: Analysis of Clustered Data

When experimental units are naturally or artificially clustered, failure times of experimental units within a cluster are correlated. Lee, Wei, and Amato (1992) estimate the regression parameters in the Cox model by maximizing a partial likelihood function under an independent working correlation assumption and estimate

the variance of the estimated regression coefficients by using a robust sandwich variance estimator that accounts for the intracluster dependence.

The Diabetic Retinopathy Study (DRS) is a randomized, controlled clinical trial of more than 1,700 patients across 15 medical centers. One objective of this study was to determine if photocoagulation treatment delays the occurrence of blindness. One eye of each patient was randomly assigned to treatment and the other eye to control. See [Example 67.11](#) in Chapter 67, “The PHREG Procedure,” for more information about the data set and a similar analysis; see <http://www.nei.nih.gov/neitrials/static/study62.asp> for more information about the DRS.

Each patient is a cluster that contributes two observations to the input data set, one for each eye. The following variables are available:

- ID, patient’s identification
- Time, failure time
- Status, event indicator (0=censored, and 1=uncensored)
- Treatment, treatment received (1=laser photocoagulation, and 0=otherwise)
- DiabeticType, type of diabetes (0=juvenile onset with age of onset at 20 or under, and 1= adult onset with age of onset over 20)

The following DATA step creates the data set Blind, which represents 197 diabetic patients from the DRS:

```
data Blind;
 input ID Time Status DiabeticType Treatment @@;
 datalines;
 5 46.23 0 1 1 5 46.23 0 1 0 14 42.50 0 0 1 14 31.30 1 0 0
 16 42.27 0 0 1 16 42.27 0 0 0 25 20.60 0 0 1 25 20.60 0 0 0
 29 38.77 0 0 1 29 0.30 1 0 0 46 65.23 0 0 1 46 54.27 1 0 0
 49 63.50 0 0 1 49 10.80 1 0 0 56 23.17 0 0 1 56 23.17 0 0 0
 61 1.47 0 0 1 61 1.47 0 0 0 71 58.07 0 1 1 71 13.83 1 1 0
100 46.43 1 1 1 100 48.53 0 1 0 112 44.40 0 1 1 112 7.90 1 1 0
120 39.57 0 1 1 120 39.57 0 1 0 127 30.83 1 1 1 127 38.57 1 1 0
133 66.27 0 1 1 133 14.10 1 1 0 150 20.17 1 0 1 150 6.90 1 0 0
167 58.43 0 1 1 167 41.40 1 1 0 176 58.20 0 0 1 176 58.20 0 0 0
185 57.43 0 1 1 185 57.43 0 1 0 190 56.03 0 0 1 190 56.03 0 0 0

 ... more lines ...

1705 8.00 0 0 1 1705 8.00 0 0 0 1717 51.60 0 1 1 1717 42.33 1 1 0
1727 49.97 0 1 1 1727 2.90 1 1 0 1746 45.90 0 0 1 1746 1.43 1 0 0
1749 41.93 0 1 1 1749 41.93 0 1 0

;
```

The following SAS statements request a proportional hazards regression of Time on Treatment, DiabeticType, and the Treatment × DiabeticType interaction, with Status as the censoring indicator. The CLUSTER statement indicates the observations that came from the same patient.

```
proc surveypreg data=Blind;
 model Time*Status(0) = Treatment DiabeticType Treatment*DiabeticType;
 cluster id;
run;
```

Output 93.1.1 displays some summary information. There are 394 observations and 197 patients (clusters). Almost 61% of the observations are censored. The  $p$ -values for the null model are less than 0.0001 for both the likelihood ratio test and the Wald test (Output 93.1.2), which indicates that the survival time is highly dependent on Treatment and DiabeticType. In this example, the likelihood ratio statistic has a chi-square distribution with 3 degrees of freedom and the Wald statistics has the  $F$  distribution with the numerator degrees of freedom 3 and the denominator degrees of freedom 196. The denominator degrees of freedom are calculated as the number of clusters (197) minus one.

**Output 93.1.1** Summary Information

| The SURVEYPHREG Procedure                          |               |          |                  |
|----------------------------------------------------|---------------|----------|------------------|
| Number of Observations Read                        | 394           |          |                  |
| Number of Observations Used                        | 394           |          |                  |
| Design Summary                                     |               |          |                  |
| Number of Clusters                                 | 197           |          |                  |
| Summary of the Number of Event and Censored Values |               |          |                  |
| Total                                              | Event         | Censored | Percent Censored |
| 394                                                | 155           | 239      | 60.66            |
| Variance Estimation                                |               |          |                  |
| Method                                             | Taylor Series |          |                  |

**Output 93.1.2** Global Test Results

| Testing Global Null Hypothesis: BETA=0 |                |        |        |         |
|----------------------------------------|----------------|--------|--------|---------|
| Test                                   | Test Statistic | Num DF | Den DF | p-Value |
| Likelihood Ratio                       | 28.4556        | 3      | Infty  | <.0001  |
| Wald                                   | 11.3872        | 3      | 196    | <.0001  |

Output 93.1.3 displays parameter estimates, standard errors,  $t$  statistics, denominator degrees of freedom,  $p$ -values, and hazard ratios. In this example data set, Treatment and Treatment  $\times$  DiabeticType interaction

are significant with  $p$ -values 0.023 and 0.006, respectively. Since the model contains Treatment  $\times$  DiabeticType interaction, the exponential of the estimated regression coefficient is not the hazard ratio. Use the ESTIMATE statement to calculate the hazard ratios.

### Output 93.1.3 Parameter Estimates

| Analysis of Maximum Likelihood Estimates |     |           |                |         |         |
|------------------------------------------|-----|-----------|----------------|---------|---------|
| Parameter                                | DF  | Estimate  | Standard Error | t Value | Pr >  t |
| Treatment                                | 196 | -0.424672 | 0.185912       | -2.28   | 0.0234  |
| DiabeticType                             | 196 | 0.340841  | 0.196577       | 1.73    | 0.0845  |
| Treatment*DiabeticTy                     | 196 | -0.845665 | 0.305081       | -2.77   | 0.0061  |

| Analysis of Maximum Likelihood Estimates |              |
|------------------------------------------|--------------|
| Parameter                                | Hazard Ratio |
| Treatment                                | 0.654        |
| DiabeticType                             | 1.406        |
| Treatment*DiabeticTy                     | 0.429        |

### Example 93.2: Stratification, Clustering, and Unequal Weights

This example uses a data set from the National Health and Nutrition Examination Survey I (NHANES I) Epidemiologic Followup Study (NHEFS). The NHEFS is a national longitudinal survey that is conducted by the National Center for Health Statistics, the National Institute on Aging, and some other agencies of the Public Health Service in the United States. Some important objectives of this survey are to determine the relationships between clinical, nutritional, and behavioral factors; to determine mortality and hospital utilizations; and to monitor changes in risk factors for the initial cohort that represents the NHANES I population. A cohort of size 14,407, which includes all persons 25 to 74 years old who completed a medical examination at NHANES I in 1971–1975, was selected for the NHEFS. Personal interviews were conducted for every selected unit during the first wave of data collection from the year 1982 to 1984. Follow-up studies were conducted in 1986, 1987, and 1992. In the year 1986, only nondeceased persons 55 to 74 years old (as reported in the base year survey) were interviewed. The 1987 and 1992 NHEFS contain the entire nondeceased NHEFS cohort. Vital and tracing status data, interview data, health care facility stay data, and mortality data for all four waves are available for public use. See <http://www.cdc.gov/nchs/nhanes/nhefs/nhefs.htm> for more information about the survey and the data sets.

For illustration purposes, 1,018 observations from the 1987 NHEFS public use interview data are used to create the data set cancer. The observations are obtained from 10 strata that contain 596 PSUs. The sum of observation weights for these selected units is over 19 million. Observation weights range from 359 to 129,359 with a mean of 18,747.69 and a median of 11,414. Several observation weights have large values; therefore it is reasonable to rescale the observation weights to facilitate the optimization routine. Different scaling techniques are proposed in the literature. For example, Binder (1992) uses scaled weights such that the sum of weights over the sampled units is one. Without loss of generality, the analysis weights in this example are obtained by dividing each observation weight by a large number (130,000). Because of this rescaling, you must be careful interpreting some results from PROC SURVEYPHREG.

The following variables are used in this example:

- ObsNo, unit identification
- Strata, stratum identification
- PSU, identification for primary sampling units
- ObservationWt, sampling weight associated with each unit
- AnalysisWt, obtained from the sampling weights by dividing each ObservationWt by 130,000
- Smoke, smoking status (–1 = not applicable, 1 = never smoked, 2 = current or former smoker in 1982–1984 follow-up, and 3 = current or former smoker in 1987 follow-up)
- Age, the event-time variable, defined as follows:
  - age of the subject when the first cancer was reported for subjects with reported cancer
  - age of the subject at death for deceased subjects without reported cancer
  - age of the subject as reported in 1987 follow-up (this value is used for nondeceased subjects who never reported cancer)
  - age of the subject for the entry year 1971–1975 survey if the subject has cancer (or is deceased) but the date of incident is not reported
- Cancer, cancer indicator (1 = cancer reported, 0 = cancer not reported)
- BodyWeight, body weight of the subject as reported in the 1987 follow-up, or an imputed body weight based on the subject’s age in the entry year 1971–1975 survey

The following SAS statements create the data set cancer. Note that BodyWeight for a few observations (8%) is imputed based on Age by using a deterministic regression imputation model (Särndal and Lundström (2005, chapter 12)). The imputed values are treated as observed values in this example. In other words, this example treats the data set Cancer as the observed data set.

```

data cancer;
 input ObsNo Strata PSU AnalysisWt ObservationWt Smoke
 Age Cancer BodyWeight;
 datalines;
 1 3 002 0.02927 3805 2 53 1 175
 2 3 002 0.04698 6107 2 77 0 175
 3 3 039 0.02283 2968 2 50 0 160
 4 3 084 0.23414 30438 2 52 0 145
 5 3 007 0.03908 5081 1 80 0 127
 6 3 009 0.02993 3891 1 62 0 180
 7 3 009 0.02754 3580 2 50 0 157
 8 3 022 0.02283 2968 2 56 0 142
 9 3 050 0.18268 23748 2 60 0 140

 ... more lines ...

1016 4 002 0.02068 2689 2 40 0 120
1017 4 092 0.35298 45888 2 52 0 166
1018 4 035 0.03344 4347 -1 58 0 156
;

```



Suppose you want to study the occurrence of cancer for the base year survey population and its relation to smoking status and body weight. The following statements request a proportional hazards regression of Age on BodyWeight and Smoke with Cancer as the censor indicator. The STRATA, CLUSTER, and WEIGHT statements identify the variance strata, PSUs, and analysis weights respectively. The CLASS statement specifies that Smoke is a categorical variable, and the MODEL statement provides information about the analysis model. The TIES= option in the MODEL statement requests the Efron likelihood to handle tied events. If you do not specify the TIES= option in the MODEL statement, then the procedure uses the Breslow likelihood. The PHISTORY option in the NLOPTIONS statement is used to display the iteration history table. The ESTIMATE statement computes a contrast between subjects who are reported as current (or former) smokers and the others. The EXP option in the ESTIMATE statement requests that the linear contrast be estimated in the exponential scale, which is the hazard ratio. The TEST statement requests the Type 3 test for each effect that is specified in the MODEL statement.

```
proc surveypHreg data = cancer;
 strata strata;
 cluster psu;
 weight analysiswt;
 class smoke;
 model age*cancer(0) = bodyweight smoke / ties = efron;
 nloptions phistory;
 estimate smoke 0.5 0.5 -0.5 -0.5 / exp;
 test ;
run;
```

Some summary statistics are shown in [Output 93.2.1](#). The “Model Information” table contains information about the model such as the names for the dependent and censoring variables, and the likelihood. The “Number of Observations” table displays the number of observations and the sum of weights. A total of 1,018 observations are read from the Cancer data set, but one observation is not used in the analysis because it has a zero sampling weight. The sum of weights is 146.81, which gives an estimated population size of 19,085,105 ( $= 146.8085 \times 130,000$ ). Note that the estimated population size would be 19,085,151 if you use the sampling weights (ObservationWt) instead of the analysis weights (AnalysisWt). The difference is due to the rounding errors in AnalysisWt. For simplicity, analysis weights are rounded at the fifth decimal place. The “Design Summary” table shows that there are 596 PSUs and 10 strata. From the censored summary tables, 11.7% subjects in the sample have reported cancer and an estimated 11.6% subjects in the study population have cancer. The “Variance Estimation” table shows that the Taylor series linearization variance estimation method is used and the observation units with missing values are excluded from the analysis. Note that the only missing unit in this data set has a zero sampling weight and hence it is not included in the analysis.

**Output 93.2.1** Model Information, Data Summary, Design Summary, and Information about Variance Estimation

```

The SURVEYPHREG Procedure

Model Information

Data Set WORK.CANCER
Dependent Variable Age
Censoring Variable Cancer
Censoring Value(s) 0
Weight Variable AnalysisWt
Stratum Variable Strata
Cluster Variable PSU
Ties Handling EFRON

Number of Observations Read 1018
Number of Observations Used 1017
Sum of Weights Read 146.8085
Sum of Weights Used 146.8085

Design Summary

Number of Strata 10
Number of Clusters 596

Summary of the Number of Event and Censored Values

Total Event Censored Percent
 Censored

1017 119 898 88.30

Summary of the Weighted Number of Event and Censored Values

Total Event Censored Percent
 Censored

146.8085 17.01185 129.7966 88.41

Variance Estimation

Method Taylor Series
Missing Values Excluded

```

The “Iteration History” table in [Output 93.2.2](#) shows that the procedure converged after four iterations. The “Objective Function” column contains the value of the likelihood after every iteration. The “Objective Function Change” column measures the change in the objective function between iterations; however, this is not the monitored convergence criterion. The SURVEYPHREG procedure monitors several features simultaneously to determine whether to stop an optimization.

**Output 93.2.2** Iteration History

| Maximum Likelihood Iteration History |              |               |            |                       |                   |                                |       |                                  |
|--------------------------------------|--------------|---------------|------------|-----------------------|-------------------|--------------------------------|-------|----------------------------------|
| Iter                                 | Rest<br>arts | Func<br>Calls | Act<br>Con | Objective<br>Function | Obj Fun<br>Change | Max Abs<br>Gradient<br>Element | Ridge | Actual<br>Over<br>Pred<br>Change |
| 1                                    | 0            | 4             | 0          | -63.34004             | 1.6501            | 21.9620                        | 0     | 0.916                            |
| 2                                    | 0            | 6             | 0          | -63.29819             | 0.0418            | 0.2005                         | 0     | 1.052                            |
| 3                                    | 0            | 8             | 0          | -63.29776             | 0.000430          | 0.00293                        | 0     | 1.012                            |
| 4                                    | 0            | 10            | 0          | -63.29776             | 1.528E-7          | 1.102E-6                       | 0     | 1.000                            |

Estimates for proportional hazards regression coefficients and their standard errors are shown in [Output 93.2.3](#). The categorical variable Smoke has four levels, and GLM parameterization is used by PROC SURVEYPHREG. You can use the PARAM= option in the CLASS statement to specify other types of parameterizations. The estimated regression coefficient for BodyWeight is 0.012 with a standard error of 0.003. The degrees of freedom for the *t* test are equal to the number of PSUs (596) minus the number of strata (10). The “Estimates” table displays the estimated contrast and the corresponding hypothesis test. The estimated value for the contrast is -0.75. The estimated hazard for the nonsmokers is 0.47 times the estimated hazard for the current or former smokers. In this example data set, the contrast of interest is not significant at 0.05 levels. The “Type III Tests of Model Effects” table displays the Type 3 analysis. The effect variable Smoke has four levels. The F Value for Smoke is 1.49 with three numerator degrees of freedom and 586 denominator degrees of freedom.

**Output 93.2.3** Parameter Estimates

| Analysis of Maximum Likelihood Estimates |     |           |                   |         |         |                 |
|------------------------------------------|-----|-----------|-------------------|---------|---------|-----------------|
| Parameter                                | DF  | Estimate  | Standard<br>Error | t Value | Pr >  t | Hazard<br>Ratio |
| BodyWeight                               | 586 | 0.011920  | 0.003155          | 3.78    | 0.0002  | 1.012           |
| Smoke -1                                 | 586 | -1.174048 | 0.739450          | -1.59   | 0.1129  | 0.309           |
| Smoke 1                                  | 586 | -1.006515 | 0.578810          | -1.74   | 0.0826  | 0.365           |
| Smoke 2                                  | 586 | -0.674183 | 0.558412          | -1.21   | 0.2278  | 0.510           |
| Smoke 3                                  | 586 | 0         | .                 | .       | .       | 1.000           |

| Type III Tests of Model Effects |           |           |         |        |
|---------------------------------|-----------|-----------|---------|--------|
| Effect                          | Num<br>DF | Den<br>DF | F Value | Pr > F |
| BodyWeight                      | 1         | 586       | 14.27   | 0.0002 |
| Smoke                           | 3         | 586       | 1.49    | 0.2160 |

**Output 93.2.3** *continued*

| Label | Estimate |                |     |         |         | Exponentiated |
|-------|----------|----------------|-----|---------|---------|---------------|
|       | Estimate | Standard Error | DF  | t Value | Pr >  t |               |
| Row 1 | -0.7532  | 0.3870         | 586 | -1.95   | 0.0521  | 0.4709        |

**Example 93.3: Domain Analysis**

This example uses a data set from the NHANES I Epidemiologic Followup Study (NHEFS); see [Example 93.2](#) for more information about the NHEFS.

For illustration purposes, 1,891 observations from the 1992 NHEFS vital and tracing status data set are used to estimate the regression coefficients of a proportional hazards model. The observations are obtained from 22 strata; each stratum contains either two or three primary sampling units. The sum of observation weights for these selected units is almost 103 million. Observation weights range from 1,498 to 470,154 with a mean of 54,457.11 and a median of 45,246. The following variables are used in this example. Although this example uses the observation weights directly, Binder (1992) suggests that a scaled version of the observation weights would be useful to improve the performance of the optimization routine.

The following variables are created in the data set mortality:

- ID, unit identification
- VARSTRATA, stratum identification
- VARPSU, identification for primary sampling units
- SWEIGHT, sampling weight associated with each unit
- AGE, the subject's reported age at the 1992 interview if the subject was alive at that time; otherwise, the subject's age at death
- VITALSTATUS, vital status of subject in 1992 (1 = alive, 3 = dead, 4 = unknown, 5 = traced alive with direct subject contact, 6 = traced alive without direct subject contact)
- POVARIND, indicator for poverty area where subject's household was located at NHANES I (1971–1975) exam, (1 = poverty area, 2 = non-poverty area)
- GENDER, (1 = male, 2 = female)

**data mortality;**

```
input ID VARSTRATA VARPSU SWEIGHT AGE VITALSTATUS POVARIND GENDER;
datalines;
```

```
1 03 1 13312 66 1 1 1
2 03 1 7941 71 3 1 2
3 03 1 16048 . 4 1 1
4 03 3 9298 58 3 1 1
5 03 2 15336 56 3 1 2
6 03 1 14744 63 1 1 1
```

```

 7 03 2 83729 70 1 2 2
 8 03 3 106492 57 1 2 1
 9 03 3 78083 81 3 2 2
 10 03 3 55957 79 3 2 1

... more lines ...

 1890 13 1 88939 59 1 2 1
 1891 13 1 59218 75 1 2 2
;

```

Suppose you want to estimate the hazard function for mortality time after adjusting for the poverty area indicator in the base year survey population. The following SAS statements request a proportional hazards regression of age (AGE) on poverty indicator (POVARIND):

```

proc surveypHreg data = mortality nomcar;
 class povarind;
 strata varstrata;
 cluster varpsu;
 weight sweight;
 model age*vitalstatus(1 4 5 6) = povarind;
 domain gender;
run;

```

Subjects with VITALSTATUS 1, 4, 5, or 6 are considered alive. The CLASS statement specifies that POVARIND is a categorical variable, the WEIGHT statement identifies the sampling weights, the STRATA statement identifies variance strata, and the CLUSTER statement identifies variance PSUs. The DOMAIN statement requests three separate analyses: for the overall data set, the male subpopulation, and the female subpopulation respectively. There are 223 observation units with missing values on age. All the units with missing age have vital status 1, 4, 5, or 6. Therefore, these subjects are considered to be alive in the current survey year 1992. Age for every observation unit in the base year survey was known from 1971–1975 NHANES I. One reasonable approach is to determine the age of these 223 units based on their age from the NHANES I data set. However, for illustration purposes, this example does not include the observation units with missing age when estimating the regression coefficients. Instead, an analysis of just the set of respondents is requested by specifying the NOMCAR option in the PROC SURVEYPHREG statement. This option uses a variance estimator that accounts for the random size of the set of respondents.

Output 93.3.1 shows summary statistics for the overall analysis. A total of 1,891 observations are read from the input DATA= data set, but only 1,668 observations are used in the analysis. The remaining 223 observations have missing values in the variable age. The respondent data set represents almost 89.5 million units in the population. There are 22 strata and 55 clusters. Although only 57% observation units in the sample are alive, an estimated 69% observation units in the population are alive. This difference is reasonable because selection probabilities for observation units are not the same. If you do not use the sampling weights, then your sample-based estimators might be biased for the corresponding finite population quantities. The “Variance Estimation” table indicates that the NOMCAR option is used for variance estimation.

**Output 93.3.1** Summary Statistics for the Entire Population

| The SURVEYPHREG Procedure                                   |          |               |          |                  |
|-------------------------------------------------------------|----------|---------------|----------|------------------|
| Number of Observations Read                                 |          |               | 1891     |                  |
| Number of Observations Used                                 |          |               | 1668     |                  |
| Sum of Weights Read                                         |          |               | 1.0298E8 |                  |
| Sum of Weights Used                                         |          |               | 89439590 |                  |
| Design Summary                                              |          |               |          |                  |
| Number of Strata                                            |          |               | 22       |                  |
| Number of Clusters                                          |          |               | 55       |                  |
| Summary of the Number of Event and Censored Values          |          |               |          |                  |
|                                                             | Total    | Event         | Censored | Percent Censored |
|                                                             | 1668     | 717           | 951      | 57.01            |
| Summary of the Weighted Number of Event and Censored Values |          |               |          |                  |
|                                                             | Total    | Event         | Censored | Percent Censored |
|                                                             | 89439590 | 27650348      | 61789242 | 69.08            |
| Variance Estimation                                         |          |               |          |                  |
| Method                                                      |          | Taylor Series |          |                  |
| Missing Values                                              |          | NOMCAR        |          |                  |

Output 93.3.2 displays the estimated regression coefficients and their standard errors. Poverty index has two levels, and only one level is estimable. By default, PROC SURVEYPHREG estimates the first level (POVARIND 1) and assigns a zero value for the second level. The estimated regression coefficient is 0.385 with a standard error of 0.078. The estimated hazard for the poverty areas is 1.47 times higher than the estimated hazard for the non-poverty areas. The degrees of freedom are equal to the number of PSUs (55) minus the number of strata (22).

**Output 93.3.2** Inference for the Entire Population

| Analysis of Maximum Likelihood Estimates |    |          |                |         |         |              |
|------------------------------------------|----|----------|----------------|---------|---------|--------------|
| Parameter                                | DF | Estimate | Standard Error | t Value | Pr >  t | Hazard Ratio |
| POVARIND 1                               | 33 | 0.384961 | 0.077586       | 4.96    | <.0001  | 1.470        |
| POVARIND 2                               | 33 | 0        | .              | .       | .       | 1.000        |

Output 93.3.3 shows that 813 observation units in the sample are male, and they account for over 42.6 million males in the base year survey population. Approximately half of these observation units in the sample are censored, and an estimated 64.5% observation units are censored for the male subpopulation.

### Output 93.3.3 Summary Statistics for the Male Subpopulation

| The SURVEYPHREG Procedure                                   |          |          |                  |
|-------------------------------------------------------------|----------|----------|------------------|
| Domain Analysis for domain GENDER=1                         |          |          |                  |
| Number of Observations Read                                 |          |          | 1891             |
| Number of Observations Used                                 |          |          | 813              |
| Sum of Weights Read                                         |          |          | 48887067         |
| Sum of Weights Used                                         |          |          | 42629905         |
| Summary of the Number of Event and Censored Values          |          |          |                  |
| Total                                                       | Event    | Censored | Percent Censored |
| 813                                                         | 404      | 409      | 50.31            |
| Summary of the Weighted Number of Event and Censored Values |          |          |                  |
| Total                                                       | Event    | Censored | Percent Censored |
| 42629905                                                    | 15126321 | 27503584 | 64.52            |

Output 93.3.4 shows that the estimated regression coefficient for POVARIND 1 is 0.425 with a standard error of 0.157. The estimated hazard for the males in the poverty areas is 1.53 times higher than the estimated hazard for the males in the non-poverty areas. The degrees of freedom for the  $t$  significant test for the male subpopulation are equal to the total number of PSUs (55) minus the total number of strata (22).

### Output 93.3.4 Inference for the Male Subpopulation

| Analysis of Maximum Likelihood Estimates |    |          |                |         |         |              |
|------------------------------------------|----|----------|----------------|---------|---------|--------------|
| Parameter                                | DF | Estimate | Standard Error | t Value | Pr >  t | Hazard Ratio |
| POVARIND 1                               | 33 | 0.424922 | 0.156583       | 2.71    | 0.0105  | 1.529        |
| POVARIND 2                               | 33 | 0        | .              | .       | .       | 1.000        |

Output 93.3.5 displays some summary statistics for the female subpopulation. There are 855 observation units for females in the sample, and they represent over 46.8 million females in the base year survey population. Although 63.4% females in the sample are alive, an estimated 73.2% females in the subpopulation are alive.

**Output 93.3.5** Summary Statistics for the Female Subpopulation

| The SURVEYPHREG Procedure                                   |          |          |                  |
|-------------------------------------------------------------|----------|----------|------------------|
| Domain Analysis for domain GENDER=2                         |          |          |                  |
| Number of Observations Read                                 |          |          | 1891             |
| Number of Observations Used                                 |          |          | 855              |
| Sum of Weights Read                                         |          |          | 54091604         |
| Sum of Weights Used                                         |          |          | 46809685         |
| Summary of the Number of Event and Censored Values          |          |          |                  |
| Total                                                       | Event    | Censored | Percent Censored |
| 855                                                         | 313      | 542      | 63.39            |
| Summary of the Weighted Number of Event and Censored Values |          |          |                  |
| Total                                                       | Event    | Censored | Percent Censored |
| 46809685                                                    | 12524027 | 34285658 | 73.24            |

Output 93.3.6 shows that the estimated proportional hazards regression coefficients for POVARIND for the females subpopulation (0.435) is higher than the estimated proportional hazards regression coefficients for POVARIND for the males subpopulation. The estimated hazard for the females in the poverty areas is 1.54 times higher than the estimated hazard for the females in the non-poverty areas. The degrees of freedom for the *t* significant test for the female subpopulation are equal to the total number of PSUs (55) minus the total number of strata (22).

**Output 93.3.6** Inference for the Female Subpopulation

| Analysis of Maximum Likelihood Estimates |    |          |                |         |         |              |
|------------------------------------------|----|----------|----------------|---------|---------|--------------|
| Parameter                                | DF | Estimate | Standard Error | t Value | Pr >  t | Hazard Ratio |
| POVARIND 1                               | 33 | 0.434579 | 0.115766       | 3.75    | 0.0007  | 1.544        |
| POVARIND 2                               | 33 | 0        | .              | .       | .       | 1.000        |

**Example 93.4: Variance Estimation by Using Replicate Weights**

Consider the data set LibrarySurvey from “Getting Started: SURVEYPHREG Procedure” on page 7857. The selected sample contains 100 transactions from ten branch libraries. A set of replicate weights and jackknife coefficients are created by randomly assigning observation units in disjoint groups of nearly equal size within each stratum. A total of 46 different groups are created. The data set LibraryRepWeights is



similar to the data set LibrarySurvey except that it also contains replicate weights repwt\_1 to repwt\_46. Each column of replicate weights is obtained by deleting one group of observations and adjusting the sampling weights for the other groups in that stratum (Rust 1985).

The data set LibraryJKCOEF contains the jackknife coefficient for every replicate sample. The variable replicate denotes the replicate number, donorstratum denotes the stratum identification for that replicate, and jkcoefficient denotes the jackknife coefficient for that replicate sample.

```

data LibrarySurvey;
 set LibrarySurvey;
 randomorder = ranuni(12345);
run;
proc sort data = LibrarySurvey out = LibrarySurvey;
 by Branch randomorder;
run;
data LibrarySurvey;
 set LibrarySurvey;
 array nGroup{10} (2 2 2 4 4 4 4 8 8 8);
 GroupPSU = mod(_N_, nGroup{Branch});
 drop randomorder nGroup1 nGroup2 nGroup3 nGroup4
 nGroup5 nGroup6 nGroup7 nGroup8 nGroup9 nGroup10;
run;

proc surveymeans data = LibrarySurvey varmethod = jk
 (outweights = LibraryRepWeights outjkcoefs = LibraryJKCOEF);
 weight SamplingWeight;
 strata Branch;
 cluster GroupPSU;
 var Age;
run;

```

It is not necessary to provide replicate weights to compute jackknife variance estimates using the SURVEYPHREG procedure. If you do not specify the replicate weights, then the procedure creates replicate weights for you. For this illustration, assume that LibraryRepWeights and LibraryJKCOEF are the only two data sets available for analysis.

The following SAS statements request a proportional hazards regression of lenBorrow on Age. The variable Returned is the censor indicator, and the value 0 indicates a censored observation. The WEIGHT statement specifies the sampling weight variable, and the REPWEIGHTS statement specifies replicate weight variables RepWt\_1 to RepWt\_46. The JKCOEFS= option in the REPWEIGHTS statement specifies the jackknife coefficient for each replicate sample. The VARMETHOD= option in the MODEL statement requests the jackknife variance estimation method. A STRATA statement is not required when the REPWEIGHTS statement is specified.

```

proc surveypHreg data = LibraryRepWeights varmethod = jk;
 weight SamplingWeight;
 repweights RepWt_: / jkcoefs = LibraryJKCOEF;
 model lenBorrow*Returned(0) = Age;
run;

```

Output 93.4.1 displays some summary information. The “Number of Observations,” “Censored Summary,” and “Weighted Censored Summary” tables are exactly the same as in the example discussed in “Getting Started: SURVEYPHREG Procedure” on page 7857. The “Variance Estimation” table displays information about the variance estimation, such as the name of the variance estimation method and the number of replicate samples.

**Output 93.4.1** Summary Statistics for Overall Analysis

| The SURVEYPHREG Procedure                                   |          |                        |           |                  |
|-------------------------------------------------------------|----------|------------------------|-----------|------------------|
| Number of Observations Read                                 |          |                        | 100       |                  |
| Number of Observations Used                                 |          |                        | 100       |                  |
| Sum of Weights Read                                         |          |                        | 11616.79  |                  |
| Sum of Weights Used                                         |          |                        | 11616.79  |                  |
| Summary of the Number of Event and Censored Values          |          |                        |           |                  |
|                                                             | Total    | Event                  | Censored  | Percent Censored |
|                                                             | 100      | 90                     | 10        | 10.00            |
| Summary of the Weighted Number of Event and Censored Values |          |                        |           |                  |
|                                                             | Total    | Event                  | Censored  | Percent Censored |
|                                                             | 11616.79 | 10449.22               | 1167.57   | 10.05            |
| Variance Estimation                                         |          |                        |           |                  |
| Method                                                      |          |                        | Jackknife |                  |
| Replicate Weights                                           |          | WORK.LIBRARYREPWEIGHTS |           |                  |
| Number of Replicates                                        |          |                        | 46        |                  |

Output 93.4.2 shows that the estimated regression coefficient is 0.0616 with a standard error of 0.009. The denominator degrees of freedom (46) for the *t* test is equal to the number of replicates used. Note that the estimated proportional hazards regression coefficient is the same as the estimated proportional hazards regression coefficient in the example in “Getting Started: SURVEYPHREG Procedure” on page 7857, but the standard error and the denominator degrees of freedom are different. This is not surprising because these two examples use the same estimator to estimate the regression coefficients but different estimators to estimate the variance.

**Output 93.4.2** Inferences Based on Survey Design for Overall Analysis

| Analysis of Maximum Likelihood Estimates |    |          |                |         |         |              |
|------------------------------------------|----|----------|----------------|---------|---------|--------------|
| Parameter                                | DF | Estimate | Standard Error | t Value | Pr >  t | Hazard Ratio |
| Age                                      | 46 | 0.061593 | 0.009159       | 6.73    | <.0001  | 1.064        |

## Example 93.5: A Test of the Proportional Hazards Assumption by Using the Programming Statements

You can use programming statements in PROC SURVEYPHREG to create time-dependent covariates to test the proportional hazards assumption for complex survey data. Consider the data set mortality from Example 93.3. The data set contains 1,891 observations from the 1992 NHANES I Epidemiologic Followup study (NHEFS) vital and tracing status.

Suppose you want to fit a proportional hazards model to this data and construct a test for the proportional hazards assumption on gender. The following statements request a proportional hazards regression of age on gender and x, where the time-dependent covariate x is created using the programming statements. The explanatory variable x assumes the value of the time variable age for the male subgroup. The variable vitalstatus is the censor indicator, and a value of 1, 4, 5, or 6 indicates a censored observation. The WEIGHT statement specifies the sampling weight, and the CLASS statement specifies that gender is a classification variable.

```
proc surveypHreg data = mortality nomcar;
 class gender;
 strata varstrata;
 cluster varpsu;
 weight sweight;
 model age*vitalstatus(1 4 5 6) = gender x;
 x = age*(gender=1);
run;
```

Output 93.5.1 displays some summary information. The “Number of Observations,” “Censored Summary,” and “Weighted Censored Summary” tables are exactly the same as in the example discussed in “Example 93.3: Domain Analysis” on page 7921.

### Output 93.5.1 Data Summary, Censored Summary, and Information about Variance Estimation

| The SURVEYPHREG Procedure                                   |          |          |                  |  |
|-------------------------------------------------------------|----------|----------|------------------|--|
| Number of Observations Read                                 |          | 1891     |                  |  |
| Number of Observations Used                                 |          | 1891     |                  |  |
| Sum of Weights Read                                         |          | 1.0298E8 |                  |  |
| Sum of Weights Used                                         |          | 1.0298E8 |                  |  |
| Summary of the Number of Event and Censored Values          |          |          |                  |  |
| Total                                                       | Event    | Censored | Percent Censored |  |
| 1891                                                        | 717      | 1174     | 62.08            |  |
| Summary of the Weighted Number of Event and Censored Values |          |          |                  |  |
| Total                                                       | Event    | Censored | Percent Censored |  |
| 1.0298E8                                                    | 27650348 | 75328323 | 73.15            |  |

**Output 93.5.1** *continued*

| Variance Estimation |               |
|---------------------|---------------|
| Method              | Taylor Series |
| Missing Values      | NOMCAR        |

**Output 93.5.2** displays the estimated regression coefficients and their standard errors. The variable gender has two levels, and only one level is estimable. By default, PROC SURVEYPHREG estimates the first level (GENDER 1) and assigns a zero value for the second level. The estimated regression coefficient is 1.61 with a standard error of 0.71. The estimated regression coefficient for  $x$  is  $-0.02$  with a standard error of 0.01. The  $t$  statistic for  $x$  is  $-1.55$  with a  $p$ -value of 0.13 on 33 degrees of freedom. This test suggests that an interaction between the time variable age and gender is not significant. Therefore, there is little evidence of an exponential trend over time in the hazard ratio for gender.

**Output 93.5.2** Parameter Estimates

| Analysis of Maximum Likelihood Estimates |    |             |                |         |         |              |
|------------------------------------------|----|-------------|----------------|---------|---------|--------------|
| Parameter                                | DF | Estimate    | Standard Error | t Value | Pr >  t | Hazard Ratio |
| GENDER 1                                 | 33 | 1.605505    | 0.709269       | 2.26    | 0.0303  | 4.980        |
| GENDER 2                                 | 33 | 0           | .              | .       | .       | 1.000        |
| $x$                                      | 33 | $-0.015648$ | 0.010082       | $-1.55$ | 0.1302  | 0.984        |

---

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# Chapter 94

## The SURVEYREG Procedure

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## Overview: SURVEYREG Procedure

The SURVEYREG procedure performs regression analysis for sample survey data. This procedure can handle complex survey sample designs, including designs with stratification, clustering, and unequal weighting. The procedure fits linear models for survey data and computes regression coefficients and their variance-covariance matrix. The procedure also provides significance tests for the model effects and for any specified estimable linear functions of the model parameters. Using the regression model, the procedure can compute predicted values for the sample survey data.

PROC SURVEYREG uses elementwise regression to compute the regression coefficient estimators by generalized least squares estimation. The procedure assumes that the regression coefficients are the same across strata and primary sampling units (PSUs). To estimate the variance-covariance matrix for the regression coefficients, PROC SURVEYREG uses either the Taylor series (linearization) method or replication (resampling) methods to estimate sampling errors of estimators, based on complex sample designs. For details see Woodruff (1971); Fuller (1975); Särndal, Swensson, and Wretman (1992); Wolter (2007); Rust (1985); Dippo, Fay, and Morganstein (1984); Rao and Shao (1999); Rao, Wu, and Yue (1992); and Rao and Shao (1996).

---

## Getting Started: SURVEYREG Procedure

This section demonstrates how you can use PROC SURVEYREG to perform a regression analysis for sample survey data. For a complete description of the usage of PROC SURVEYREG, see the section “[Syntax: SURVEYREG Procedure](#)” on page 7942. The section “[Examples: SURVEYREG Procedure](#)” on page 7985 provides more detailed examples that illustrate the applications of PROC SURVEYREG.

---

## Simple Random Sampling

Suppose that, in a junior high school, there are a total of 4,000 students in grades 7, 8, and 9. You want to know how household income and the number of children in a household affect students’ average weekly spending for ice cream.

In order to answer this question, you draw a sample by using simple random sampling from the student population in the junior high school. You randomly select 40 students and ask them their average weekly expenditure for ice cream, their household income, and the number of children in their household. The answers from the 40 students are saved as the following SAS data set `IceCream`:

```
data IceCream;
 input Grade Spending Income Kids @@;
 datalines;
7 7 39 2 7 7 38 1 8 12 47 1
9 10 47 4 7 1 34 4 7 10 43 2
7 3 44 4 8 20 60 3 8 19 57 4
7 2 35 2 7 2 36 1 9 15 51 1
8 16 53 1 7 6 37 4 7 6 41 2
7 6 39 2 9 15 50 4 8 17 57 3
```

```

8 14 46 2 9 8 41 2 9 8 41 1
9 7 47 3 7 3 39 3 7 12 50 2
7 4 43 4 9 14 46 3 8 18 58 4
9 9 44 3 7 2 37 1 7 1 37 2
7 4 44 2 7 11 42 2 9 8 41 2
8 10 42 2 8 13 46 1 7 2 40 3
9 6 45 1 9 11 45 4 7 2 36 1
7 9 46 1
;

```

In the data set `IceCream`, the variable `Grade` indicates a student's grade. The variable `Spending` contains the dollar amount of each student's average weekly spending for ice cream. The variable `Income` specifies the household income, in thousands of dollars. The variable `Kids` indicates how many children are in a student's family.

The following PROC SURVEYREG statements request a regression analysis:

```

title1 'Ice Cream Spending Analysis';
title2 'Simple Random Sample Design';
proc surveyreg data=IceCream total=4000;
 class Kids;
 model Spending = Income Kids / solution;
run;

```

The PROC SURVEYREG statement invokes the procedure. The `TOTAL=4000` option specifies the total in the population from which the sample is drawn. The `CLASS` statement requests that the procedure use the variable `Kids` as a classification variable in the analysis. The `MODEL` statement describes the linear model that you want to fit, with `Spending` as the dependent variable and `Income` and `Kids` as the independent variables. The `SOLUTION` option in the `MODEL` statement requests that the procedure output the regression coefficient estimates.

Figure 94.1 displays the summary of the data, the summary of the fit, and the levels of the classification variable `Kids`. The "Fit Statistics" table displays the denominator degrees of freedom, which are used in  $F$  tests and  $t$  tests in the regression analysis.

**Figure 94.1** Summary of Data

|                                                     |           |
|-----------------------------------------------------|-----------|
| Ice Cream Spending Analysis                         |           |
| Simple Random Sample Design                         |           |
| The SURVEYREG Procedure                             |           |
| Regression Analysis for Dependent Variable Spending |           |
| Data Summary                                        |           |
| Number of Observations                              | 40        |
| Mean of Spending                                    | 8.75000   |
| Sum of Spending                                     | 350.00000 |

Figure 94.1 *continued*

| Fit Statistics          |        |         |
|-------------------------|--------|---------|
| R-square                |        | 0.8132  |
| Root MSE                |        | 2.4506  |
| Denominator DF          |        | 39      |
| Class Level Information |        |         |
| Class Variable          | Levels | Values  |
| Kids                    | 4      | 1 2 3 4 |

Figure 94.2 displays the tests for model effects. The effect Income is significant in the linear regression model, while the effect Kids is not significant at the 5% level.

Figure 94.2 Testing Effects in the Regression

| Tests of Model Effects |        |         |        |
|------------------------|--------|---------|--------|
| Effect                 | Num DF | F Value | Pr > F |
| Model                  | 4      | 119.15  | <.0001 |
| Intercept              | 1      | 153.32  | <.0001 |
| Income                 | 1      | 324.45  | <.0001 |
| Kids                   | 3      | 0.92    | 0.4385 |

NOTE: The denominator degrees of freedom for the F tests is 39.

The regression coefficient estimates and their standard errors and associated  $t$  tests are displayed in Figure 94.3.

Figure 94.3 Regression Coefficients

| Estimated Regression Coefficients |            |                |         |         |
|-----------------------------------|------------|----------------|---------|---------|
| Parameter                         | Estimate   | Standard Error | t Value | Pr >  t |
| Intercept                         | -26.084677 | 2.46720403     | -10.57  | <.0001  |
| Income                            | 0.775330   | 0.04304415     | 18.01   | <.0001  |
| Kids 1                            | 0.897655   | 1.12352876     | 0.80    | 0.4292  |
| Kids 2                            | 1.494032   | 1.24705263     | 1.20    | 0.2381  |
| Kids 3                            | -0.513181  | 1.33454891     | -0.38   | 0.7027  |
| Kids 4                            | 0.000000   | 0.00000000     | .       | .       |

NOTE: The denominator degrees of freedom for the  $t$  tests is 39.  
Matrix X'X is singular and a generalized inverse was used to solve the normal equations. Estimates are not unique.

## Stratified Sampling

Suppose that the previous student sample is actually drawn using a stratified sample design. The strata are grades in the junior high school: 7, 8, and 9. Within strata, simple random samples are selected. Table 94.1 provides the number of students in each grade.

**Table 94.1** Students in Grades

| Grade        | Number of Students |
|--------------|--------------------|
| 7            | 1,824              |
| 8            | 1,025              |
| 9            | 1,151              |
| <b>Total</b> | <b>4,000</b>       |

In order to analyze this sample by using PROC SURVEYREG, you need to input the stratification information by creating a SAS data set with the information in Table 94.1. The following SAS statements create such a data set called StudentTotals:

```
data StudentTotals;
 input Grade _TOTAL_;
 datalines;
7 1824
8 1025
9 1151
;
```

The variable Grade is the stratification variable, and the variable \_TOTAL\_ contains the total numbers of students in each stratum in the survey population. PROC SURVEYREG requires you to use the keyword \_TOTAL\_ as the name of the variable that contains the population total information.

In a stratified sample design, when the sampling rates in the strata are unequal, you need to use sampling weights to reflect this information. For this example, the appropriate sampling weights are the reciprocals of the probabilities of selection. You can use the following DATA step to create the sampling weights:

```
data IceCream;
 set IceCream;
 if Grade=7 then Prob=20/1824;
 if Grade=8 then Prob=9/1025;
 if Grade=9 then Prob=11/1151;
 Weight=1/Prob;
run;
```

If you use PROC SURVEYSELECT to select your sample, PROC SURVEYSELECT creates these sampling weights for you.

The following statements demonstrate how you can fit a linear model while incorporating the sample design information (stratification):

```

title1 'Ice Cream Spending Analysis';
title2 'Stratified Sample Design';
proc surveyreg data=IceCream total=StudentTotals;
 strata Grade /list;
 class Kids;
 model Spending = Income Kids / solution;
 weight Weight;
run;

```

Comparing these statements to those in the section “[Simple Random Sampling](#)” on page 7935, you can see how the TOTAL=StudentTotals option replaces the previous TOTAL=4000 option.

The STRATA statement specifies the stratification variable Grade. The LIST option in the STRATA statement requests that the stratification information be included in the output. The WEIGHT statement specifies the weight variable.

[Figure 94.4](#) summarizes the data information, the sample design information, and the fit information. Note that, due to the stratification, the denominator degrees of freedom for  $F$  tests and  $t$  tests are 37, which is different from the analysis in [Figure 94.1](#).

**Figure 94.4** Summary of the Regression

|                                                     |         |
|-----------------------------------------------------|---------|
| Ice Cream Spending Analysis                         |         |
| Stratified Sample Design                            |         |
| The SURVEYREG Procedure                             |         |
| Regression Analysis for Dependent Variable Spending |         |
| Data Summary                                        |         |
| Number of Observations                              | 40      |
| Sum of Weights                                      | 4000.0  |
| Weighted Mean of Spending                           | 9.14130 |
| Weighted Sum of Spending                            | 36565.2 |
| Design Summary                                      |         |
| Number of Strata                                    | 3       |
| Fit Statistics                                      |         |
| R-square                                            | 0.8219  |
| Root MSE                                            | 2.4185  |
| Denominator DF                                      | 37      |

For each stratum, [Figure 94.5](#) displays the value of identifying variables, the number of observations (sample size), the total population size, and the calculated sampling rate or fraction.

**Figure 94.5** Stratification and Classification Information

| Stratum Information |       |       |                  |               |
|---------------------|-------|-------|------------------|---------------|
| Stratum Index       | Grade | N Obs | Population Total | Sampling Rate |
| 1                   | 7     | 20    | 1824             | 1.10%         |
| 2                   | 8     | 9     | 1025             | 0.88%         |
| 3                   | 9     | 11    | 1151             | 0.96%         |

| Class Level Information |        |        |       |
|-------------------------|--------|--------|-------|
| Class Variable          | Levels | Values |       |
| Kids                    | 4      | 1      | 2 3 4 |

Figure 94.6 displays the tests for the significance of model effects under the stratified sample design. The Income effect is strongly significant, while the Kids effect is not significant at the 5% level.

**Figure 94.6** Testing Effects

| Tests of Model Effects |        |         |        |
|------------------------|--------|---------|--------|
| Effect                 | Num DF | F Value | Pr > F |
| Model                  | 4      | 124.85  | <.0001 |
| Intercept              | 1      | 150.95  | <.0001 |
| Income                 | 1      | 326.89  | <.0001 |
| Kids                   | 3      | 0.99    | 0.4081 |

NOTE: The denominator degrees of freedom for the F tests is 37.

The regression coefficient estimates for the stratified sample, along with their standard errors and associated  $t$  tests, are displayed in Figure 94.7.

**Figure 94.7** Regression Coefficients

| Estimated Regression Coefficients |            |                |         |         |
|-----------------------------------|------------|----------------|---------|---------|
| Parameter                         | Estimate   | Standard Error | t Value | Pr >  t |
| Intercept                         | -26.086882 | 2.44108058     | -10.69  | <.0001  |
| Income                            | 0.776699   | 0.04295904     | 18.08   | <.0001  |
| Kids 1                            | 0.888631   | 1.07000634     | 0.83    | 0.4116  |
| Kids 2                            | 1.545726   | 1.20815863     | 1.28    | 0.2087  |
| Kids 3                            | -0.526817  | 1.32748011     | -0.40   | 0.6938  |
| Kids 4                            | 0.000000   | 0.00000000     | .       | .       |

NOTE: The denominator degrees of freedom for the t tests is 37.  
Matrix X'WX is singular and a generalized inverse was used to solve the normal equations. Estimates are not unique.

You can request other statistics and tests by using PROC SURVEYREG. You can also analyze data from a more complex sample design. The remainder of this chapter provides more detailed information.

---

## Output Data Sets

You can use the OUTPUT statement to create a new SAS data set that contains the estimated linear predictors and their standard error estimates, the residuals from the linear regression, and the confidence limits for the predictors. See the section “[OUTPUT Statement](#)” on page 7960 for more details.

You can use the Output Delivery System (ODS) to create SAS data sets that capture the outputs from PROC SURVEYREG. For more information about ODS, see Chapter 20, “[Using the Output Delivery System.](#)”

For example, to save the “ParameterEstimates” table ([Figure 94.7](#)) in the previous section in an output data set, you use the ODS OUTPUT statement as follows:

```

title1 'Ice Cream Spending Analysis';
title2 'Stratified Sample Design';
proc surveyreg data=IceCream total=StudentTotals;
 strata Grade /list;
 class Kids;
 model Spending = Income Kids / solution;
 weight Weight;
 ods output ParameterEstimates = MyParmEst;
run;

```

The statement

```
ods output ParameterEstimates = MyParmEst;
```

requests that the “ParameterEstimates” table that appears in [Figure 94.7](#) be placed into a SAS data set MyParmEst.



The PRINT procedure displays observations of the data set MyParmEst:

```
proc print data=MyParmEst;
run;
```

Figure 94.8 displays the observations in the data set MyParmEst. The section “ODS Table Names” on page 7983 gives the complete list of the tables produced by PROC SURVEYREG.

**Figure 94.8** The Data Set MyParmEst

| Ice Cream Spending Analysis<br>Stratified Sample Design |           |            |            |       |        |        |
|---------------------------------------------------------|-----------|------------|------------|-------|--------|--------|
| Obs                                                     | Parameter | Estimate   | StdErr     | DenDF | tValue | Probt  |
| 1                                                       | Intercept | -26.086882 | 2.44108058 | 37    | -10.69 | <.0001 |
| 2                                                       | Income    | 0.776699   | 0.04295904 | 37    | 18.08  | <.0001 |
| 3                                                       | Kids 1    | 0.888631   | 1.07000634 | 37    | 0.83   | 0.4116 |
| 4                                                       | Kids 2    | 1.545726   | 1.20815863 | 37    | 1.28   | 0.2087 |
| 5                                                       | Kids 3    | -0.526817  | 1.32748011 | 37    | -0.40  | 0.6938 |
| 6                                                       | Kids 4    | 0.000000   | 0.00000000 | 37    | .      | .      |

## Syntax: SURVEYREG Procedure

The following statements are available in the SURVEYREG procedure:

```
PROC SURVEYREG < options > ;
 BY variables ;
 CLASS variables ;
 CLUSTER variables ;
 CONTRAST 'label' effect values < ... effect values > < / options > ;
 DOMAIN variables < variable*variable variable*variable*variable ... > ;
 EFFECT name = effect-type (variables < / options >) ;
 ESTIMATE < 'label' > estimate-specification < / options > ;
 LSMEANS < model-effects > < / options > ;
 LSMESTIMATE model-effect lsmestimate-specification < / options > ;
 MODEL dependent = < effects > < / options > ;
 OUTPUT < keyword < =variable-name > ... keyword < =variable-name > > < / option > ;
 REPWEIGHTS variables < / options > ;
 SLICE model-effect < / options > ;
 STORE < OUT= > item-store-name < / LABEL='label' > ;
 STRATA variables < / options > ;
 TEST < model-effects > < / options > ;
 WEIGHT variable ;
```

The PROC SURVEYREG and MODEL statements are required. If your model contains classification effects, you must list the classification variables in a CLASS statement, and the CLASS statement must pre-

cede the MODEL statement. If you use a CONTRAST statement or an ESTIMATE statement, the MODEL statement must precede the CONTRAST or ESTIMATE statement.

The rest of this section provides detailed syntax information for each of the preceding statements, except the EFFECT, ESTIMATE, LSMEANS, LSMESTIMATE, SLICE, STORE, and TEST statements. These statements are also available in many other procedures. Summary descriptions of functionality and syntax for these statements are shown in this chapter, and full documentation about them is available in Chapter 19, “Shared Concepts and Topics.”

The CLASS, CLUSTER, CONTRAST, EFFECT, ESTIMATE, LSMEANS, LSMESTIMATE, REPWEIGHTS, SLICE, STRATA, TEST statements can appear multiple times. You should use only one of each of the following statements: MODEL, WEIGHT, STORE, and OUTPUT.

The syntax descriptions begin with the PROC SURVEYREG statement; the remaining statements are covered in alphabetical order.

---

## PROC SURVEYREG Statement

**PROC SURVEYREG** < options > ;

The PROC SURVEYREG statement invokes the SURVEYREG procedure. It optionally names the input data sets and specifies the variance estimation method.

Table 94.2 summarizes the options available in the PROC SURVEYREG statement.

**Table 94.2** PROC SURVEYREG Statement Options

| Option     | Description                                                                               |
|------------|-------------------------------------------------------------------------------------------|
| ALPHA=     | Sets the confidence level                                                                 |
| DATA=      | Specifies the SAS data set to be analyzed                                                 |
| MISSING    | Treats missing values as a nonmissing                                                     |
| NOMCAR     | Treats missing values as <i>not missing completely at random</i>                          |
| ORDER=     | Specifies the sort order                                                                  |
| RATE=      | Specifies the sampling rate                                                               |
| TOTAL=     | Specifies the total number of primary sampling units                                      |
| TRUNCATE   | Specifies class levels using no more than the first 16 characters of the formatted values |
| VARMETHOD= | Specifies the variance estimation method                                                  |

You can specify the following options in the PROC SURVEYREG statement:

### **ALPHA=** $\alpha$

sets the confidence level for confidence limits. The value of the ALPHA= option must be between 0 and 1, and the default value is 0.05. A confidence level of  $\alpha$  produces  $100(1 - \alpha)\%$  confidence limits. The default of ALPHA=0.05 produces 95% confidence limits.

**DATA=SAS-data-set**

specifies the SAS data set to be analyzed by PROC SURVEYREG. If you omit the DATA= option, the procedure uses the most recently created SAS data set.

**MISSING**

treats missing values as a valid (nonmissing) category for all categorical variables, which include **CLASS**, **STRATA**, **CLUSTER**, and **DOMAIN** variables.

By default, if you do not specify the MISSING option, an observation is excluded from the analysis if it has a missing value. For more information, see the section “Missing Values” on page 7964.

**NOMCAR**

requests that the procedure treat missing values in the variance computation as *not missing completely at random* (NOMCAR) for Taylor series variance estimation. When you specify the NOMCAR option, PROC SURVEYREG computes variance estimates by analyzing the nonmissing values as a domain or subpopulation, where the entire population includes both nonmissing and missing domains. See the section “Missing Values” on page 7964 for more details.

By default, PROC SURVEYREG completely excludes an observation from analysis if that observation has a missing value, unless you specify the MISSING option. Note that the NOMCAR option has no effect on a classification variable when you specify the MISSING option, which treats missing values as a valid nonmissing level.

The NOMCAR option applies only to Taylor series variance estimation. The replication methods, which you request with the **VARMETHOD=BRR** and **VARMETHOD=JACKKNIFE** options, do not use the NOMCAR option.

**ORDER=DATA | FORMATTED | FREQ | INTERNAL**

specifies the sort order for the levels of the classification variables (which are specified in the **CLASS** statement).

This option also determines the sort order for the levels of **DOMAIN** variables.

This option applies to the levels for all classification variables, except when you use the (default) **ORDER=FORMATTED** option with numeric classification variables that have no explicit format. With this option, the levels of such variables are ordered by their internal value.

The ORDER= option can take the following values:

| Value of ORDER=  | Levels Sorted By                                                                                                                       |
|------------------|----------------------------------------------------------------------------------------------------------------------------------------|
| <b>DATA</b>      | Order of appearance in the input data set                                                                                              |
| <b>FORMATTED</b> | External formatted value, except for numeric variables with no explicit format, which are sorted by their unformatted (internal) value |
| <b>FREQ</b>      | Descending frequency count; levels with the most observations come first in the order                                                  |
| <b>INTERNAL</b>  | Unformatted value                                                                                                                      |

By default, ORDER=FORMATTED. For ORDER=FORMATTED and ORDER=INTERNAL, the

sort order is machine-dependent. For more information about sort order, see the chapter on the SORT procedure in the *Base SAS Procedures Guide* and the discussion of BY-group processing in *SAS Language Reference: Concepts*.

**RATE=***value* | *SAS-data-set*

**R=***value* | *SAS-data-set*

specifies the sampling rate as a nonnegative *value*, or specifies an input data set that contains the stratum sampling rates. The procedure uses this information to compute a finite population correction for Taylor series variance estimation. The procedure does not use the RATE= option for BRR or jackknife variance estimation, which you request with the **VARMETHOD=BRR** or **VARMETHOD=JACKKNIFE** option.

If your sample design has multiple stages, you should specify the *first-stage sampling rate*, which is the ratio of the number of PSUs selected to the total number of PSUs in the population.

For a nonstratified sample design, or for a stratified sample design with the same sampling rate in all strata, you should specify a nonnegative *value* for the RATE= option. If your design is stratified with different sampling rates in the strata, then you should name a SAS data set that contains the stratification variables and the sampling rates. See the section “[Specification of Population Totals and Sampling Rates](#)” on page 7965 for more details.

The *value* in the RATE= option or the values of `_RATE_` in the secondary data set must be nonnegative numbers. You can specify *value* as a number between 0 and 1. Or you can specify *value* in percentage form as a number between 1 and 100, and PROC SURVEYREG converts that number to a proportion. The procedure treats the value 1 as 100%, and not the percentage form 1%.

If you do not specify the **TOTAL=** or RATE= option, then the Taylor series variance estimation does not include a finite population correction. You cannot specify both the **TOTAL=** and RATE= options.

**TOTAL=***value* | *SAS-data-set*

**N=***value* | *SAS-data-set*

specifies the total number of primary sampling units in the study population as a positive *value*, or specifies an input data set that contains the stratum population totals. The procedure uses this information to compute a finite population correction for Taylor series variance estimation. The procedure does not use the TOTAL= option for BRR or jackknife variance estimation, which you request with the **VARMETHOD=BRR** or **VARMETHOD=JACKKNIFE** option.

For a nonstratified sample design, or for a stratified sample design with the same population total in all strata, you should specify a positive *value* for the TOTAL= option. If your sample design is stratified with different population totals in the strata, then you should name a SAS data set that contains the stratification variables and the population totals. See the section “[Specification of Population Totals and Sampling Rates](#)” on page 7965 for more details.

If you do not specify the **TOTAL=** or **RATE=** option, then the Taylor series variance estimation does not include a finite population correction. You cannot specify both the **TOTAL=** and **RATE=** options.

**TRUNCATE**

specifies that class levels should be determined using no more than the first 16 characters of the formatted values of the CLASS, STRATA, and CLUSTER variables. When formatted values are longer than 16 characters, you can use this option in order to revert to the levels as determined in releases before SAS 9.

**VARMETHOD=BRR** <(method-options)>

**VARMETHOD=JACKKNIFE** | **JK** <(method-options)>

**VARMETHOD=TAYLOR**

specifies the variance estimation method. **VARMETHOD=TAYLOR** requests the Taylor series method, which is the default if you do not specify the **VARMETHOD=** option or the **REPWEIGHTS** statement. **VARMETHOD=BRR** requests variance estimation by balanced repeated replication (BRR), and **VARMETHOD=JACKKNIFE** requests variance estimation by the delete-1 jackknife method.

For **VARMETHOD=BRR** and **VARMETHOD=JACKKNIFE** you can specify *method-options* in parentheses. Table 94.3 summarizes the available *method-options*.

**Table 94.3** Variance Estimation Options

| <b>VARMETHOD=</b> | <b>Variance Estimation Method</b> | <i>Method-Options</i>                                                                     |
|-------------------|-----------------------------------|-------------------------------------------------------------------------------------------|
| BRR               | Balanced repeated replication     | FAY <=value><br>HADAMARD=SAS-data-set<br>OUTWEIGHTS=SAS-data-set<br>PRINTH<br>REPS=number |
| JACKKNIFE         | Jackknife                         | OUTJKCOEFS=SAS-data-set<br>OUTWEIGHTS=SAS-data-set                                        |
| TAYLOR            | Taylor series linearization       | None                                                                                      |

*Method-options* must be enclosed in parentheses following the method keyword. For example:

```
varmethod=BRR(reps=60 outweights=myReplicateWeights)
```

The following values are available for the **VARMETHOD=** option:

**BRR** <(method-options)>

requests **balanced repeated replication** (BRR) variance estimation. The BRR method requires a stratified sample design with two primary sampling units (PSUs) per stratum. See the section “**Balanced Repeated Replication (BRR) Method**” on page 7971 for more information.

You can specify the following *method-options* in parentheses following **VARMETHOD=BRR**:

**FAY** <=value>

requests **Fay’s method**, a modification of the BRR method, for variance estimation. See the section “**Fay’s BRR Method**” on page 7972 for more information.

You can specify the *value* of the Fay coefficient, which is used in converting the original sampling weights to replicate weights. The Fay coefficient must be a nonnegative number less than 1. By default, the value of the Fay coefficient equals 0.5.

**HADAMARD=SAS-data-set****H=SAS-data-set**

names a SAS data set that contains the [Hadamard matrix](#) for BRR replicate construction. If you do not provide a Hadamard matrix with the `HADAMARD= method-option`, PROC SURVEYREG generates an appropriate Hadamard matrix for replicate construction. See the sections “[Balanced Repeated Replication \(BRR\) Method](#)” on page 7971 and “[Hadamard Matrix](#)” on page 7973 for details.

If a Hadamard matrix of a given dimension exists, it is not necessarily unique. Therefore, if you want to use a specific Hadamard matrix, you must provide the matrix as a SAS data set in the `HADAMARD= method-option`.

In the `HADAMARD=` input data set, each variable corresponds to a column of the Hadamard matrix, and each observation corresponds to a row of the matrix. You can use any variable names in the `HADAMARD=` data set. All values in the data set must equal either 1 or -1. You must ensure that the matrix you provide is indeed a Hadamard matrix—that is,  $\mathbf{A}'\mathbf{A} = R\mathbf{I}$ , where  $\mathbf{A}$  is the Hadamard matrix of dimension  $R$  and  $\mathbf{I}$  is an identity matrix. PROC SURVEYREG does not check the validity of the Hadamard matrix that you provide.

The `HADAMARD=` input data set must contain at least  $H$  variables, where  $H$  denotes the number of first-stage strata in your design. If the data set contains more than  $H$  variables, the procedure uses only the first  $H$  variables. Similarly, the `HADAMARD=` input data set must contain at least  $H$  observations.

If you do not specify the `REPS= method-option`, then the number of replicates is taken to be the number of observations in the `HADAMARD=` input data set. If you specify the number of replicates—for example, `REPS=nreps`—then the first  $nreps$  observations in the `HADAMARD=` data set are used to construct the replicates.

You can specify the `PRINTH` option to display the Hadamard matrix that the procedure uses to construct replicates for BRR.

**OUTWEIGHTS=SAS-data-set**

names a SAS data set that contains replicate weights. See the section “[Balanced Repeated Replication \(BRR\) Method](#)” on page 7971 for information about replicate weights. See the section “[Replicate Weights Output Data Set](#)” on page 7978 for more details about the contents of the `OUTWEIGHTS=` data set.

The `OUTWEIGHTS= method-option` is not available when you provide replicate weights with the `REPWEIGHTS` statement.

**PRINTH**

displays the Hadamard matrix.

When you provide your own Hadamard matrix with the `HADAMARD= method-option`, only the rows and columns of the Hadamard matrix that

are used by the procedure are displayed. See the sections “Balanced Repeated Replication (BRR) Method” on page 7971 and “Hadamard Matrix” on page 7973 for details.

The PRINTH *method-option* is not available when you provide replicate weights with the REPWEIGHTS statement because the procedure does not use a Hadamard matrix in this case.

**REPS=*number***

specifies the number of replicates for BRR variance estimation. The value of *number* must be an integer greater than 1.

If you do not provide a Hadamard matrix with the HADAMARD= *method-option*, the number of replicates should be greater than the number of strata and should be a multiple of 4. See the section “Balanced Repeated Replication (BRR) Method” on page 7971 for more information. If a Hadamard matrix cannot be constructed for the REPS= value that you specify, the value is increased until a Hadamard matrix of that dimension can be constructed. Therefore, it is possible for the actual number of replicates used to be larger than the REPS= value that you specify.

If you provide a Hadamard matrix with the HADAMARD= *method-option*, the value of REPS= must not be less than the number of rows in the Hadamard matrix. If you provide a Hadamard matrix and do not specify the REPS= *method-option*, the number of replicates equals the number of rows in the Hadamard matrix.

If you do not specify the REPS= or HADAMARD= *method-option* and do not include a REPWEIGHTS statement, the number of replicates equals the smallest multiple of 4 that is greater than the number of strata.

If you provide replicate weights with the REPWEIGHTS statement, the procedure does not use the REPS= *method-option*. With a REPWEIGHTS statement, the number of replicates equals the number of REPWEIGHTS variables.

**JACKKNIFE | JK <(method-options)>**

requests variance estimation by the delete-1 jackknife method. See the section “Jackknife Method” on page 7972 for details. If you provide replicate weights with a REPWEIGHTS statement, VARMETHOD=JACKKNIFE is the default variance estimation method.

You can specify the following *method-options* in parentheses following VARMETHOD=JACKKNIFE:

**OUTJKCOEFS=*SAS-data-set***

names a SAS data set that contains jackknife coefficients. See the section “Jackknife Method” on page 7972 for information about jackknife coefficients. See the section “Jackknife Coefficients Output Data Set” on page 7978 for more details about the contents of the OUTJKCOEFS= data set.



**OUTWEIGHTS=SAS-data-set**

names a SAS data set that contains replicate weights. See the section “[Jackknife Method](#)” on page 7972 for information about replicate weights. See the section “[Replicate Weights Output Data Set](#)” on page 7978 for more details about the contents of the OUTWEIGHTS= data set.

The OUTWEIGHTS= *method-option* is not available when you provide replicate weights with the [REPWEIGHTS](#) statement.

**TAYLOR**

requests Taylor series variance estimation. This is the default method if you do not specify the [VARMETHOD=](#) option or a [REPWEIGHTS](#) statement. See the section “[Taylor Series \(Linearization\)](#)” on page 7970 for more information.

---

## BY Statement

**BY variables ;**

You can specify a BY statement with PROC SURVEYREG to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the SURVEYREG procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

Note that using a BY statement provides completely separate analyses of the BY groups. It does not provide a statistically valid domain (subpopulation) analysis, where the total number of units in the subpopulation is not known with certainty. You should use the DOMAIN statement to obtain domain analysis. For more information about subpopulation analysis for sample survey data, see Cochran (1977).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.



---

## CLASS Statement

**CLASS** *variables* ;

The CLASS statement names the classification variables to be used in the model. Typical classification variables are Treatment, Sex, Race, Group, and Replication. If you use the CLASS statement, it must appear before the MODEL statement.

Classification variables can be either character or numeric. By default, class levels are determined from the entire set of formatted values of the CLASS variables.

**NOTE:** Prior to SAS 9, class levels were determined by using no more than the first 16 characters of the formatted values. To revert to this previous behavior, you can use the TRUNCATE option in the PROC SURVEYREG statement.

In any case, you can use formats to group values into levels. See the discussion of the FORMAT procedure in the *Base SAS Procedures Guide* and the discussions of the FORMAT statement and SAS formats in *SAS Formats and Informats: Reference*. You can adjust the order of CLASS variable levels with the ORDER= option in the PROC SURVEYREG statement.

You can use multiple CLASS statements to specify classification variables.

---

## CLUSTER Statement

**CLUSTER** *variables* ;

The CLUSTER statement names variables that identify the clusters in a clustered sample design. The combinations of categories of CLUSTER variables define the clusters in the sample. If there is a STRATA statement, clusters are nested within strata.

If you provide replicate weights for BRR or jackknife variance estimation with the REPWEIGHTS statement, you do not need to specify a CLUSTER statement.

If your sample design has clustering at multiple stages, you should identify only the first-stage clusters (primary sampling units (PSUs)), in the CLUSTER statement. See the section “Primary Sampling Units (PSUs)” on page 7966 for more information.

The CLUSTER *variables* are one or more variables in the DATA= input data set. These variables can be either character or numeric. The formatted values of the CLUSTER variables determine the CLUSTER variable levels. Thus, you can use formats to group values into levels. See the FORMAT procedure in the *Base SAS Procedures Guide* and the FORMAT statement and SAS formats in *SAS Formats and Informats: Reference* for more information.

When determining levels of a CLUSTER variable, an observation with missing values for this CLUSTER variable is excluded, unless you specify the MISSING option. For more information, see the section “Missing Values” on page 7964.

You can use multiple CLUSTER statements to specify cluster variables. The procedure uses variables from all CLUSTER statements to create clusters.

Prior to SAS 9, clusters were determined by using no more than the first 16 characters of the formatted values. If you want to revert to this previous behavior, you can use the TRUNCATE option in the PROC SURVEYREG statement.

## CONTRAST Statement

**CONTRAST** *'label'* effect values *</ options >* ;

**CONTRAST** *'label'* effect values *< . . . effect values >* *</ options >* ;

The CONTRAST statement provides custom hypothesis tests for linear combinations of the regression parameters  $H_0: \mathbf{L}\boldsymbol{\beta} = \mathbf{0}$ , where  $\mathbf{L}$  is the vector or matrix you specify and  $\boldsymbol{\beta}$  is the vector of regression parameters. Thus, to use this feature, you must be familiar with the details of the model parameterization used by PROC SURVEYREG. For information about the parameterization, see the section “GLM Parameterization of Classification Variables and Effects” on page 383 in Chapter 19, “Shared Concepts and Topics.”

Each term in the MODEL statement, called an *effect*, is a variable or a combination of variables. You can specify an effect with a variable name or a special notation by using variable names and operators. For more details about how to specify an effect, see the section “Specification of Effects” on page 3324 in Chapter 42, “The GLM Procedure.”

For each CONTRAST statement, PROC SURVEYREG computes Wald’s  $F$  test. The procedure displays this value with the degrees of freedom, and identifies it with the contrast label. The numerator degrees of freedom for Wald’s  $F$  test equal  $\text{rank}(\mathbf{L})$ . The denominator degrees of freedom equal the number of clusters (or the number of observations if there is no CLUSTER statement) minus the number of strata. Alternatively, you can use the **DF=** option in the MODEL statement to specify the denominator degrees of freedom.

You can specify any number of CONTRAST statements, but they must appear after the MODEL statement.

In the CONTRAST statement,

|               |                                                                                                                                                                                                                            |
|---------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <i>label</i>  | identifies the contrast in the output. A label is required for every contrast specified. Labels must be enclosed in single quotes.                                                                                         |
| <i>effect</i> | identifies an effect that appears in the MODEL statement. You can use the INTERCEPT keyword as an effect when an intercept is fitted in the model. You do not need to include all effects that are in the MODEL statement. |
| <i>values</i> | are constants that are elements of $\mathbf{L}$ associated with the effect.                                                                                                                                                |

You can specify the following options in the CONTRAST statement after a slash (/):

### **E**

displays the entire coefficient  $\mathbf{L}$  vector or matrix.

### **NOFILL**

requests no filling in higher-order effects. When you specify only certain portions of  $\mathbf{L}$ , by default PROC SURVEYREG constructs the remaining elements from the context. (For more information, see the section “Specification of ESTIMATE Expressions” on page 3345 in Chapter 42, “The GLM Procedure.”)

When you specify the NOFILL option, PROC SURVEYREG does not construct the remaining portions and treats the vector or matrix  $\mathbf{L}$  as it is defined in the CONTRAST statement.

**SINGULAR=value**

tunes the estimability checking. If  $\mathbf{v}$  is a vector, define  $\text{ABS}(\mathbf{v})$  to be the largest absolute value of the elements of  $\mathbf{v}$ . For a row vector  $\mathbf{l}$  of the matrix  $\mathbf{L}$ , define

$$c = \begin{cases} \text{ABS}(\mathbf{l}) & \text{if } \text{ABS}(\mathbf{l}) > 0 \\ 1 & \text{otherwise} \end{cases}$$

If  $\text{ABS}(\mathbf{l} - \mathbf{lH})$  is greater than  $c \cdot \text{value}$ , then  $\mathbf{l}\boldsymbol{\beta}$  is declared nonestimable. Here,  $\mathbf{H}$  is the matrix  $(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{X}$ . The *value* must be between 0 and 1; the default is  $10^{-7}$ .

As stated previously, the CONTRAST statement enables you to perform hypothesis tests  $H_0: \mathbf{L}\boldsymbol{\beta} = 0$ .

If the  $\mathbf{L}$  matrix contains more than one contrast, then you can separate the rows of the  $\mathbf{L}$  matrix with commas.

For example, for the model

```
proc surveyreg;
 class A B;
 model Y=A B;
run;
```

with A at 5 levels and B at 2 levels, the parameter vector is

$$(\mu \ \alpha_1 \ \alpha_2 \ \alpha_3 \ \alpha_4 \ \alpha_5 \ \beta_1 \ \beta_2)$$

To test the hypothesis that the pooled A linear and A quadratic effect is zero, you can use the following  $\mathbf{L}$  matrix:

$$\mathbf{L} = \begin{bmatrix} 0 & -2 & -1 & 0 & 1 & 2 & 0 & 0 \\ 0 & 2 & -1 & -2 & -1 & 2 & 0 & 0 \end{bmatrix}$$

The corresponding CONTRAST statement is

```
contrast 'A Linear & Quadratic'
 a -2 -1 0 1 2,
 a 2 -1 -2 -1 2;
```

## DOMAIN Statement

**DOMAIN** *variables* < *variable\*variable variable\*variable\*variable ...* > ;

The DOMAIN statement requests analysis for domains (subpopulations) in addition to analysis for the entire study population. The DOMAIN statement names the variables that identify domains, which are called domain variables.

It is common practice to compute statistics for domains. The formation of these domains might be unrelated to the sample design. Therefore, the sample sizes for the domains are random variables. Use a DOMAIN statement to incorporate this variability into the variance estimation.

Note that a DOMAIN statement is different from a BY statement. In a BY statement, you treat the sample sizes as fixed in each subpopulation, and you perform analysis within each BY group independently. See the section “[Domain Analysis](#)” on page 7976 for more details.

Use the DOMAIN statement on the entire data set to perform a domain analysis. Creating a new data set from a single domain and analyzing that with PROC SURVEYREG yields inappropriate estimates of variance.

A domain variable can be either character or numeric. The procedure treats domain variables as categorical variables. If a variable appears by itself in a DOMAIN statement, each level of this variable determines a domain in the study population. If two or more variables are joined by asterisks (\*), then every possible combination of levels of these variables determines a domain. The procedure performs a descriptive analysis within each domain that is defined by the domain variables.

When determining levels of a DOMAIN variable, an observation with missing values for this DOMAIN variable is excluded, unless you specify the MISSING option. For more information, see the section “Missing Values” on page 7964.

The formatted values of the domain variables determine the categorical variable levels. Thus, you can use formats to group values into levels. See the FORMAT procedure in the *Base SAS Procedures Guide* and the FORMAT statement and SAS formats in *SAS Formats and Informats: Reference* for more information.

---

## EFFECT Statement

**EFFECT** *name=effect-type (variables < / options>);*

The EFFECT statement enables you to construct special collections of columns for design matrices. These collections are referred to as *constructed effects* to distinguish them from the usual model effects that are formed from continuous or classification variables, as discussed in the section “GLM Parameterization of Classification Variables and Effects” on page 383 in Chapter 19, “Shared Concepts and Topics.”

You can specify the following *effect-types*:

|                          |                                                                                                                                                                                                           |
|--------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>COLLECTION</b>        | is a collection effect that defines one or more variables as a single effect with multiple degrees of freedom. The variables in a collection are considered as a unit for estimation and inference.       |
| <b>LAG</b>               | is a classification effect in which the level that is used for a given period corresponds to the level in the preceding period.                                                                           |
| <b>MULTIMEMBER   MM</b>  | is a multimember classification effect whose levels are determined by one or more variables that appear in a CLASS statement.                                                                             |
| <b>POLYNOMIAL   POLY</b> | is a multivariate polynomial effect in the specified numeric variables.                                                                                                                                   |
| <b>SPLINE</b>            | is a regression spline effect whose columns are univariate spline expansions of one or more variables. A spline expansion replaces the original variable with an expanded or larger set of new variables. |

Table 94.4 summarizes the *options* available in the EFFECT statement.

**Table 94.4** EFFECT Statement Options

| Option                            | Description                                        |
|-----------------------------------|----------------------------------------------------|
| <b>Collection Effects Options</b> |                                                    |
| DETAILS                           | Displays the constituents of the collection effect |

Table 94.4 continued

| Option                             | Description                                                                                                                                          |
|------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Lag Effects Options</b>         |                                                                                                                                                      |
| DESIGNROLE=                        | Names a variable that controls to which lag design an observation is assigned                                                                        |
| DETAILS                            | Displays the lag design of the lag effect                                                                                                            |
| NLAG=                              | Specifies the number of periods in the lag                                                                                                           |
| PERIOD=                            | Names the variable that defines the period                                                                                                           |
| WITHIN=                            | Names the variable or variables that define the group within which each period is defined                                                            |
| <b>Multimember Effects Options</b> |                                                                                                                                                      |
| NOEFFECT                           | Specifies that observations with all missing levels for the multimember variables should have zero values in the corresponding design matrix columns |
| WEIGHT=                            | Specifies the weight variable for the contributions of each of the classification effects                                                            |
| <b>Polynomial Effects Options</b>  |                                                                                                                                                      |
| DEGREE=                            | Specifies the degree of the polynomial                                                                                                               |
| MDEGREE=                           | Specifies the maximum degree of any variable in a term of the polynomial                                                                             |
| STANDARDIZE=                       | Specifies centering and scaling suboptions for the variables that define the polynomial                                                              |
| <b>Spline Effects Options</b>      |                                                                                                                                                      |
| BASIS=                             | Specifies the type of basis (B-spline basis or truncated power function basis) for the spline expansion                                              |
| DEGREE=                            | Specifies the degree of the spline transformation                                                                                                    |
| KNOTMETHOD=                        | Specifies how to construct the knots for spline effects                                                                                              |

For more information about the syntax of these *effect-types* and how columns of constructed effects are computed, see the section “EFFECT Statement” on page 393 in Chapter 19, “Shared Concepts and Topics.”

## ESTIMATE Statement

```
ESTIMATE <'label'> estimate-specification <(divisor=n)>
 < , ... <'label'> estimate-specification <(divisor=n)> >
 </ options > ;
```

The ESTIMATE statement provides a mechanism for obtaining custom hypothesis tests. Estimates are formed as linear estimable functions of the form  $\mathbf{L}\boldsymbol{\beta}$ . You can perform hypothesis tests for the estimable functions, construct confidence limits, and obtain specific nonlinear transformations.

Table 94.5 summarizes the options available in the ESTIMATE statement.

**Table 94.5** ESTIMATE Statement Options

| Option                                                     | Description                                                               |
|------------------------------------------------------------|---------------------------------------------------------------------------|
| <b>Construction and Computation of Estimable Functions</b> |                                                                           |
| DIVISOR=                                                   | Specifies a list of values to divide the coefficients                     |
| NOFILL                                                     | Suppresses the automatic fill-in of coefficients for higher-order effects |
| SINGULAR=                                                  | Tunes the estimability checking difference                                |
| <b>Degrees of Freedom and <math>p</math>-values</b>        |                                                                           |
| ADJUST=                                                    | Determines the method for multiple comparison adjustment of estimates     |
| ALPHA= $\alpha$                                            | Determines the confidence level ( $1 - \alpha$ )                          |
| LOWER                                                      | Performs one-sided, lower-tailed inference                                |
| STEPDOWN                                                   | Adjusts multiplicity-corrected $p$ -values further in a step-down fashion |
| TESTVALUE=                                                 | Specifies values under the null hypothesis for tests                      |
| UPPER                                                      | Performs one-sided, upper-tailed inference                                |
| <b>Statistical Output</b>                                  |                                                                           |
| CL                                                         | Constructs confidence limits                                              |
| CORR                                                       | Displays the correlation matrix of estimates                              |
| COV                                                        | Displays the covariance matrix of estimates                               |
| E                                                          | Prints the <b>L</b> matrix                                                |
| JOINT                                                      | Produces a joint $F$ or chi-square test for the estimable functions       |
| SEED=                                                      | Specifies the seed for computations that depend on random numbers         |

For details about the syntax of the ESTIMATE statement, see the section “ESTIMATE Statement” on page 437 in Chapter 19, “Shared Concepts and Topics.”

## LSMEANS Statement

```
LSMEANS < model-effects > < / options > ;
```

The LSMEANS statement computes and compares least squares means (LS-means) of fixed effects. LS-means are *predicted margins*—that is, they estimate the marginal means over a hypothetical balanced population.

Table 94.6 summarizes available options in the LSMEANS statement.

**Table 94.6** LSMEANS Statement Options

| Option                                              | Description                                                                                 |
|-----------------------------------------------------|---------------------------------------------------------------------------------------------|
| <b>Construction and Computation of LS-Means</b>     |                                                                                             |
| AT                                                  | Modifies the covariate value in computing LS-means                                          |
| BYLEVEL                                             | Computes separate margins                                                                   |
| DIFF                                                | Requests differences of LS-means                                                            |
| OM=                                                 | Specifies the weighting scheme for LS-means computation as determined by the input data set |
| SINGULAR=                                           | Tunes estimability checking                                                                 |
| <b>Degrees of Freedom and <math>p</math>-values</b> |                                                                                             |
| ADJUST=                                             | Determines the method for multiple-comparison adjustment of LS-means differences            |
| ALPHA= $\alpha$                                     | Determines the confidence level $(1 - \alpha)$                                              |
| STEPDOWN                                            | Adjusts multiple-comparison $p$ -values further in a step-down fashion                      |
| <b>Statistical Output</b>                           |                                                                                             |
| CL                                                  | Constructs confidence limits for means and mean differences                                 |
| CORR                                                | Displays the correlation matrix of LS-means                                                 |
| COV                                                 | Displays the covariance matrix of LS-means                                                  |
| E                                                   | Prints the L matrix                                                                         |
| LINES                                               | Produces a “Lines” display for pairwise LS-means differences                                |
| MEANS                                               | Prints the LS-means                                                                         |
| PLOTS=                                              | Requests graphs of means and mean comparisons                                               |
| SEED=                                               | Specifies the seed for computations that depend on random numbers                           |

For details about the syntax of the LSMEANS statement, see the section “LSMEANS Statement” on page 453 of Chapter 19, “Shared Concepts and Topics.”

## LSMESTIMATE Statement

```
LSMESTIMATE model-effect <'label'> values <divisor=n>
 < , ... <'label'> values <divisor=n> >
 </options> ;
```

The LSMESTIMATE statement provides a mechanism for obtaining custom hypothesis tests among least squares means.

Table 94.7 summarizes the options available in the LSMESTIMATE statement.

**Table 94.7** LSMESTIMATE Statement Options

| Option                                          | Description                                                                            |
|-------------------------------------------------|----------------------------------------------------------------------------------------|
| <b>Construction and Computation of LS-Means</b> |                                                                                        |
| AT                                              | Modifies covariate values in computing LS-means                                        |
| BYLEVEL                                         | Computes separate margins                                                              |
| DIVISOR=                                        | Specifies a list of values to divide the coefficients                                  |
| OM=                                             | Specifies the weighting scheme for LS-means computation as determined by a data set    |
| SINGULAR=                                       | Tunes estimability checking                                                            |
| <b>Degrees of Freedom and <i>p</i>-values</b>   |                                                                                        |
| ADJUST=                                         | Determines the method for multiple-comparison adjustment of LS-means differences       |
| ALPHA= $\alpha$                                 | Determines the confidence level ( $1 - \alpha$ )                                       |
| LOWER                                           | Performs one-sided, lower-tailed inference                                             |
| STEPDOWN                                        | Adjusts multiple-comparison <i>p</i> -values further in a step-down fashion            |
| TESTVALUE=                                      | Specifies values under the null hypothesis for tests                                   |
| UPPER                                           | Performs one-sided, upper-tailed inference                                             |
| <b>Statistical Output</b>                       |                                                                                        |
| CL                                              | Constructs confidence limits for means and mean differences                            |
| CORR                                            | Displays the correlation matrix of LS-means                                            |
| COV                                             | Displays the covariance matrix of LS-means                                             |
| E                                               | Prints the <b>L</b> matrix                                                             |
| ELSM                                            | Prints the <b>K</b> matrix                                                             |
| JOINT                                           | Produces a joint <i>F</i> or chi-square test for the LS-means and LS-means differences |
| SEED=                                           | Specifies the seed for computations that depend on random numbers                      |

For details about the syntax of the LSMESTIMATE statement, see the section “LSMESTIMATE Statement” on page 470 in Chapter 19, “Shared Concepts and Topics.”

## MODEL Statement

**MODEL** *dependent* = < effects > < / options > ;

The MODEL statement specifies the dependent (response) variable and the independent (regressor) variables or effects. The dependent variable must be numeric. Each term in a MODEL statement, called an *effect*, is a variable or a combination of variables. You can specify an effect with a variable name or with special notation by using variable names and operators. For more information about how to specify an effect, see the section “Specification of Effects” on page 3324 in Chapter 42, “The GLM Procedure.”



Only one MODEL statement is allowed for each PROC SURVEYREG statement. If you specify more than one MODEL statement, the procedure uses the first model and ignores the rest.

Table 94.8 summarizes the options available in the MODEL statement.

**Table 94.8** MODEL Statement Options

| Option    | Description                                                         |
|-----------|---------------------------------------------------------------------|
| ADJRSQ    | Compute the adjusted multiple R-square                              |
| ANOVA     | Produces the ANOVA table                                            |
| CLPARM    | Requests confidence limits                                          |
| COVB      | Displays the estimated covariance matrix                            |
| DEFF      | Displays design effects                                             |
| DF=       | Specifies the denominator degrees of freedom                        |
| I         | Displays the inverse or the generalized inverse of the $X'X$ matrix |
| NOINT     | Omits the intercept                                                 |
| PARMLABEL | Displays the labels of the parameters                               |
| SINGULAR= | Tunes the estimability checking                                     |
| SOLUTION  | Displays parameter estimates                                        |
| STB       | Displays standardized parameter estimates                           |
| VADJUST=  | Specifies whether to use degrees of freedom adjustment              |
| X         | Displays the $X'X$ matrix, or the $X'WX$ matrix                     |

You can specify the following options in the MODEL statement after a slash (/):

#### **ADJRSQ**

requests the procedure compute the adjusted multiple R-square.

#### **ANOVA**

requests the ANOVA table be produced in the output. By default, the ANOVA table is not printed in the output.

#### **CLPARM**

requests confidence limits for the parameter estimates. The SURVEYREG procedure determines the confidence coefficient by using the **ALPHA=** option, which by default equals 0.05 and produces 95% confidence bounds. The CLPARM option also requests confidence limits for all the estimable linear functions of regression parameters in the **ESTIMATE** statements.

Note that when there is a **CLASS** statement, you need to use the **SOLUTION** option with the CLPARM option to obtain the parameter estimates and their confidence limits.

#### **COVB**

displays the estimated covariance matrix of the estimated regression estimates.

#### **DEFF**

displays design effects for the regression coefficient estimates.

**DF=value**

specifies the denominator degrees of freedom for the  $F$  tests and the degrees of freedom for the  $t$  tests. For details about the default denominator degrees of freedom, see the section “Denominator Degrees of Freedom” on page 7974 for details.

**I | INVERSE**

displays the inverse or the generalized inverse of the  $X'X$  matrix. When there is a WEIGHT variable, the procedure displays the inverse or the generalized inverse of the  $X'WX$  matrix, where  $W$  is the diagonal matrix constructed from WEIGHT variable values.

**NOINT**

omits the intercept from the model.

**PARMLABEL**

displays the labels of the parameters in the “Estimated Regression Coefficients” table, if the effect contains a single continuous variable that has a label.

**SINGULAR=value**

tunes the estimability checking. If  $\mathbf{v}$  is a vector, define  $ABS(\mathbf{v})$  to be the largest absolute value of the elements of  $\mathbf{v}$ . For a row vector  $\mathbf{l}$  of the matrix  $L$ , define

$$c = \begin{cases} ABS(\mathbf{l}) & \text{if } ABS(\mathbf{l}) > 0 \\ 1 & \text{otherwise} \end{cases}$$

If  $ABS(\mathbf{l} - \mathbf{IH})$  is greater than  $c*value$ , then  $\mathbf{l}\beta$  is declared nonestimable. Here,  $\mathbf{H}$  is the matrix  $(X'X)^{-1}X'X$ . The *value* must be between 0 and 1; the default is  $10^{-4}$ .

**SOLUTION**

displays a solution to the normal equations, which are the parameter estimates. The SOLUTION option is useful only when you use a CLASS statement. If you do not specify a CLASS statement, PROC SURVEYREG displays parameter estimates by default. But if you specify a CLASS statement, PROC SURVEYREG does not display parameter estimates unless you also specify the SOLUTION option.

**STB**

produces standardized regression coefficients. A standardized regression coefficient is computed by dividing a parameter estimate by the ratio of the sample standard deviation of the dependent variable to the sample standard deviation of the regressor.

**VADJUST=DF | NONE**

specifies whether to use degrees of freedom adjustment  $(n - 1)/(n - p)$  in the computation of the matrix  $G$  for the variance estimation. If you do not specify the VADJUST= option, by default, PROC SURVEYREG uses the degrees-of-freedom adjustment that is equivalent to the VARADJ=DF option. If you do not want to use this variance adjustment, you can specify the VADJUST=NONE option.

**X | XPX**

displays the  $X'X$  matrix, or the  $X'WX$  matrix when there is a WEIGHT variable, where  $W$  is the diagonal matrix constructed from WEIGHT variable values. The X option also displays the crossproducts vector  $X'y$  or  $X'Wy$ .

## OUTPUT Statement

```
OUTPUT < OUT=SAS-data-set > < keyword < =variable-name > . . . keyword < =variable-name > >
< / option > ;
```

The OUTPUT statement creates a new SAS data set that contains all the variables in the input data set and, optionally, the estimated linear predictors and their standard error estimates, the residuals from the linear regression, and the confidence limits for the predictors.

You can specify the following options in the OUTPUT statement:

### **OUT=SAS-data-set**

gives the name of the new output data set. By default, the procedure uses the DATA*n* convention to name the new data set.

### *keyword* < =*variable-name* >

specifies the statistics to include in the output data set and names the new variables that contain the statistics. You can specify a keyword for each desired statistic (see the following list of keywords). Optionally, you can name a statistic by providing a variable name followed an equal sign to contain the statistic. For example,

```
output out=myOutDataSet p=myPredictor;
```

creates a SAS data set myOutDataSet that contains the predicted values in the variable myPredictor.

The keywords allowed and the statistics they represent are as follows:

|                      |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |
|----------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| LCLM   L             | lower bound of a $100(1 - \alpha)\%$ confidence interval for the expected value (mean) of the predicted value. The $\alpha$ level is equal to the value of the ALPHA= option in the OUTPUT statement or, if this option is not specified, to the ALPHA= option in the PROC SURVEYREG statement. If neither of these options is set, then $\alpha = 0.05$ by default, resulting in the lower bound for a 95% confidence interval. If no variable name is given for this keyword, the default variable name is _LCLM_. |
| PREDICTED   PRED   P | predicted values. If no variable name is given for this keyword, the default variable name is _PREDICTED_.                                                                                                                                                                                                                                                                                                                                                                                                           |
| RESIDUAL   R         | residuals, calculated as ACTUAL – PREDICTED. If no variable name is given for this keyword, the default variable name is _RESIDUAL_.                                                                                                                                                                                                                                                                                                                                                                                 |
| STDP   STD           | standard error of the mean predicted value. If no variable name is given for this keyword, the default variable name is _STD_.                                                                                                                                                                                                                                                                                                                                                                                       |
| UCLM   U             | upper bound of a $100(1 - \alpha)\%$ confidence interval for the expected value (mean) of the predicted value. The $\alpha$ level is equal to the value of the ALPHA= option in the OUTPUT statement or, if this option is not specified, to the ALPHA= option in the PROC SURVEYREG statement. If neither of these options is set, then $\alpha = 0.05$ by default, resulting in the upper bound for a 95% confidence interval. If no variable name is given for this keyword, the default variable name is _UCLM_. |

The following option is available in the OUTPUT statement and is specified after a slash (/):

**ALPHA= $\alpha$** 

specifies the level of significance  $\alpha$  for  $100(1 - \alpha)\%$  confidence intervals. By default,  $\alpha$  is equal to the value of the **ALPHA=** option in the PROC SURVEYREG statement or 0.05 if that option is not specified. You can use values between 0 and 1.

---

## REPWEIGHTS Statement

**REPWEIGHTS** *variables* *</ options >* ;

The REPWEIGHTS statement names variables that provide replicate weights for BRR or jackknife variance estimation, which you request with the **VARMETHOD=BRR** or **VARMETHOD=JACKKNIFE** option in the PROC SURVEYREG statement. If you do not provide replicate weights for these methods by using a REPWEIGHTS statement, then the procedure constructs replicate weights for the analysis. See the sections “Balanced Repeated Replication (BRR) Method” on page 7971 and “Jackknife Method” on page 7972 for information about replicate weights.

Each REPWEIGHTS variable should contain the weights for a single replicate, and the number of replicates equals the number of REPWEIGHTS variables. The REPWEIGHTS variables must be numeric, and the variable values must be nonnegative numbers.

If you provide replicate weights with a REPWEIGHTS statement, you do not need to specify a **CLUSTER** or **STRATA** statement. If you use a REPWEIGHTS statement and do not specify the **VARMETHOD=** option in the PROC SURVEYREG statement, the procedure uses **VARMETHOD=JACKKNIFE** by default.

If you specify a REPWEIGHTS statement but do not include a **WEIGHT** statement, the procedure uses the average of replicate weights of each observation as the observation’s weight.

You can specify the following options in the REPWEIGHTS statement after a slash (/):

**DF=*df***

specifies the degrees of freedom for the analysis. The value of *df* must be a positive number. By default, the degrees of freedom equals the number of REPWEIGHTS variables.

**JKCOEFS=*value***

specifies a jackknife coefficient for **VARMETHOD=JACKKNIFE**. The coefficient *value* must be a nonnegative number. See the section “Jackknife Method” on page 7972 for details about jackknife coefficients.

You can use this option to specify a single value of the jackknife coefficient, which the procedure uses for all replicates. To specify different coefficients for different replicates, use the **JKCOEFS=values** or **JKCOEFS=SAS-data-set** option.

**JKCOEFS=*values***

specifies jackknife coefficients for **VARMETHOD=JACKKNIFE**, where each coefficient corresponds to an individual replicate that is identified by a REPWEIGHTS variable. You can separate *values* with blanks or commas. The coefficient *values* must be nonnegative numbers. The number of *values* must equal the number of replicate weight variables named in the REPWEIGHTS statement. List these values in the same order in which you list the corresponding replicate weight variables in the REPWEIGHTS statement.

See the section “Jackknife Method” on page 7972 for details about jackknife coefficients.

To specify different coefficients for different replicates, you can also use the `JKCOEFS=SAS-data-set` option. To specify a single jackknife coefficient for all replicates, use the `JKCOEFS=value` option.

#### **JKCOEFS=SAS-data-set**

names a SAS data set that contains the jackknife coefficients for `VARMETHOD=JACKKNIFE`. You provide the jackknife coefficients in the `JKCOEFS=` data set variable `JKCoefficient`. Each coefficient value must be a nonnegative number. The observations in the `JKCOEFS=` data set should correspond to the replicates that are identified by the `REPWEIGHTS` variables. Arrange the coefficients or observations in the `JKCOEFS=` data set in the same order in which you list the corresponding replicate weight variables in the `REPWEIGHTS` statement. The number of observations in the `JKCOEFS=` data set must not be less than the number of `REPWEIGHTS` variables.

See the section “[Jackknife Method](#)” on page 7972 for details about jackknife coefficients.

To specify different coefficients for different replicates, you can also use the `JKCOEFS=values` option. To specify a single jackknife coefficient for all replicates, use the `JKCOEFS=value` option.

## **SLICE Statement**

**SLICE** *model-effect* < / options > ;

The SLICE statement provides a general mechanism for performing a partitioned analysis of the LS-means for an interaction. This analysis is also known as an analysis of simple effects.

The SLICE statement uses the same options as the `LSMEANS` statement, which are summarized in [Table 19.21](#). For details about the syntax of the SLICE statement, see the section “[SLICE Statement](#)” on page 498 in Chapter 19, “[Shared Concepts and Topics](#).”

## **STORE Statement**

**STORE** < **OUT=** > *item-store-name* < / **LABEL=** 'label' > ;

The STORE statement requests that the procedure save the context and results of the statistical analysis. The resulting item store has a binary file format that cannot be modified. The contents of the item store can be processed with the PLM procedure.

For details about the syntax of the STORE statement, see the section “[STORE Statement](#)” on page 501 in Chapter 19, “[Shared Concepts and Topics](#).”

## **STRATA Statement**

**STRATA** *variables* < / options > ;

The STRATA statement specifies variables that form the strata in a stratified sample design. The combinations of categories of STRATA variables define the strata in the sample.

If your sample design has stratification at multiple stages, you should identify only the first-stage strata in the STRATA statement. See the section “[Specification of Population Totals and Sampling Rates](#)” on page 7965 for more information.

If you provide replicate weights for BRR or jackknife variance estimation with the **REPWEIGHTS** statement, you do not need to specify a STRATA statement.

The STRATA *variables* are one or more variables in the DATA= input data set. These variables can be either character or numeric. The formatted values of the STRATA variables determine the levels. Thus, you can use formats to group values into levels. See the **FORMAT** procedure in the *Base SAS Procedures Guide* and the **FORMAT** statement and SAS formats in *SAS Formats and Informats: Reference* for more information.

When determining levels of a STRATA variable, an observation with missing values for this STRATA variable is excluded, unless you specify the **MISSING** option. For more information, see the section “**Missing Values**” on page 7964.

You can use multiple STRATA statements to specify stratum variables.

You can specify the following options in the STRATA statement after a slash (/):

#### **LIST**

displays a “Stratum Information” table, which includes values of the STRATA variables and the number of observations, number of clusters, population total, and sampling rate for each stratum. See the section “**Stratum Information**” on page 7980 for more details.

#### **NOCOLLAPSE**

prevents the procedure from collapsing (combining) strata that have only one sampling unit for the Taylor series variance estimation. By default, the procedure **collapses** strata that contain only one sampling unit for the Taylor series method. See the section “**Stratum Collapse**” on page 7968 for details.

---

## **TEST Statement**

**TEST** < *model-effects* > < / *options* > ;

The TEST statement enables you to perform *F* tests for model effects that test Type I, Type II, or Type III hypotheses. See Chapter 15, “**The Four Types of Estimable Functions**,” for details about the construction of Type I, II, and III estimable functions.

Table 94.9 summarizes the options available in the TEST statement.

**Table 94.9** TEST Statement Options

| <b>Option</b>    | <b>Description</b>                                         |
|------------------|------------------------------------------------------------|
| <b>CHISQ</b>     | Requests chi-square tests                                  |
| <b>DDF=</b>      | Specifies denominator degrees of freedom for fixed effects |
| <b>E</b>         | Requests Type I, Type II, and Type III coefficients        |
| <b>E1</b>        | Requests Type I coefficients                               |
| <b>E2</b>        | Requests Type II coefficients                              |
| <b>E3</b>        | Requests Type III coefficients                             |
| <b>HTYPE=</b>    | Indicates the type of hypothesis test to perform           |
| <b>INTERCEPT</b> | Adds a row that corresponds to the overall intercept       |

For details about the syntax of the TEST statement, see the section “TEST Statement” on page 502 in Chapter 19, “Shared Concepts and Topics.”

---

## WEIGHT Statement

**WEIGHT** *variable* ;

The WEIGHT statement names the variable that contains the sampling weights. This variable must be numeric, and the sampling weights must be positive numbers. If an observation has a weight that is nonpositive or missing, then the procedure omits that observation from the analysis. See the section “Missing Values” on page 7964 for more information. If you specify more than one WEIGHT statement, the procedure uses only the first WEIGHT statement and ignores the rest.

If you do not specify a WEIGHT statement but provide replicate weights with a REPWEIGHTS statement, PROC SURVEYREG uses the average of replicate weights of each observation as the observation’s weight.

If you do not specify a WEIGHT statement or a REPWEIGHTS statement, PROC SURVEYREG assigns all observations a weight of one.

---

## Details: SURVEYREG Procedure

---

### Missing Values

If you have missing values in your survey data for any reason, such as nonresponse, this can compromise the quality of your survey results. If the respondents are different from the nonrespondents with regard to a survey effect or outcome, then survey estimates might be biased and cannot accurately represent the survey population. There are a variety of techniques in sample design and survey operations that can reduce nonresponse. After data collection is complete, you can use imputation to replace missing values with acceptable values, and/or you can use sampling weight adjustments to compensate for nonresponse. You should complete this data preparation and adjustment before you analyze your data with PROC SURVEYREG. For more information, see Cochran (1977); Kalton and Kaspyzyk (1986); Brick and Kalton (1996).

If an observation has a missing value or a nonpositive value for the WEIGHT variable, then that observation is excluded from the analysis.

An observation is also excluded from the analysis if it has a missing value for any design (STRATA, CLUSTER, or DOMAIN) variable, unless you specify the MISSING option in the PROC SURVEYREG statement. If you specify the MISSING option, the procedure treats missing values as a valid (nonmissing) category for all categorical variables.

By default, if an observation contains missing values for the dependent variable or for any variable used in the independent effects, the observation is excluded from the analysis. This treatment is based on the assumption that the missing values are missing completely at random (MCAR). However, this assumption sometimes is not true. For example, evidence from other surveys might suggest that observations with missing values are systematically different from observations without missing values. If you believe that missing values are not missing completely at random, then you can specify the NOMCAR option to include these



observations with missing values in the dependent variable and the independent variables in the variance estimation.

Whether or not you specify the **NOMCAR** option, the procedure always excludes observations with missing or invalid values for the **WEIGHT**, **STRATA**, **CLUSTER**, and **DOMAIN** variables, unless you specify the **MISSING** option.

When you specify the **NOMCAR** option, the procedure treats observations with and without missing values for variables in the regression model as two different domains, and it performs a domain analysis in the domain of nonmissing observations.

If you use a **REPWEIGHTS** statement, all **REPWEIGHTS** variables must contain nonmissing values.

## Survey Design Information

### Specification of Population Totals and Sampling Rates

To include a finite population correction (*fpc*) in Taylor series variance estimation, you can input either the sampling rate or the population total by using the **RATE=** or **TOTAL=** option in the **PROC SURVEYREG** statement. (You cannot specify both of these options in the same **PROC SURVEYREG** statement.) The **RATE=** and **TOTAL=** options apply only to Taylor series variance estimation. The procedure does not use a finite population correction for **BRR** or jackknife variance estimation.

If you do not specify the **RATE=** or **TOTAL=** option, the Taylor series variance estimation does not include a finite population correction. For fairly small sampling fractions, it is appropriate to ignore this correction. See Cochran (1977) and Kish (1965) for more information.

If your design has multiple stages of selection and you are specifying the **RATE=** option, you should input the first-stage sampling rate, which is the ratio of the number of PSUs in the sample to the total number of PSUs in the study population. If you are specifying the **TOTAL=** option for a multistage design, you should input the total number of PSUs in the study population. See the section “**Primary Sampling Units (PSUs)**” on page 7966 for more details.

For a nonstratified sample design, or for a stratified sample design with the same sampling rate or the same population total in all strata, you can use the **RATE=value** or **TOTAL=value** option. If your sample design is stratified with different sampling rates or population totals in different strata, use the **RATE=SAS-data-set** or **TOTAL=SAS-data-set** option to name a SAS data set that contains the stratum sampling rates or totals. This data set is called a *secondary data set*, as opposed to the *primary data set* that you specify with the **DATA=** option.

The secondary data set must contain all the stratification variables listed in the **STRATA** statement and all the variables in the **BY** statement. If there are formats associated with the **STRATA** variables and the **BY** variables, then the formats must be consistent in the primary and the secondary data sets. If you specify the **TOTAL=SAS-data-set** option, the secondary data set must have a variable named **\_TOTAL\_** that contains the stratum population totals. Or if you specify the **RATE=SAS-data-set** option, the secondary data set must have a variable named **\_RATE\_** that contains the stratum sampling rates. If the secondary data set contains more than one observation for any one stratum, then the procedure uses the first value of **\_TOTAL\_** or **\_RATE\_** for that stratum and ignores the rest.

The *value* in the **RATE=** option or the values of **\_RATE\_** in the secondary data set must be nonnegative numbers. You can specify *value* as a number between 0 and 1. Or you can specify *value* in percentage



form as a number between 1 and 100, and PROC SURVEYREG converts that number to a proportion. The procedure treats the value 1 as 100%, and not the percentage form 1%.

If you specify the `TOTAL=value` option, *value* must not be less than the sample size. If you provide stratum population totals in a secondary data set, these values must not be less than the corresponding stratum sample sizes.

### Primary Sampling Units (PSUs)

When you have clusters, or primary sampling units (PSUs), in your sample design, the procedure estimates variance from the variation among PSUs when the Taylor series variance method is used. See the section “Variance Estimation” on page 7969 for more information.

BRR or jackknife variance estimation methods draw multiple replicates (or subsamples) from the full sample by following a specific resampling scheme. These subsamples are constructed by deleting PSUs from the full sample.

If you use a `REPWEIGHTS` statement to provide replicate weights for BRR or jackknife variance estimation, you do not need to specify a `CLUSTER` statement. Otherwise, you should specify a `CLUSTER` statement whenever your design includes clustering at the first stage of sampling. If you do not specify a `CLUSTER` statement, then PROC SURVEYREG treats each observation as a PSU.

## Computational Details

### Notation

For a stratified clustered sample design, observations are represented by an  $n \times (p + 2)$  matrix

$$(\mathbf{w}, \mathbf{y}, \mathbf{X}) = (w_{hij}, y_{hij}, \mathbf{x}_{hij})$$

where

- $\mathbf{w}$  denotes the sampling weight vector
- $\mathbf{y}$  denotes the dependent variable
- $\mathbf{X}$  denotes the  $n \times p$  design matrix. (When an effect contains only classification variables, the columns of  $\mathbf{X}$  that correspond this effect contain only 0s and 1s; no reparameterization is made.)
- $h = 1, 2, \dots, H$  is the stratum index
- $i = 1, 2, \dots, n_h$  is the cluster index within stratum  $h$
- $j = 1, 2, \dots, m_{hi}$  is the unit index within cluster  $i$  of stratum  $h$
- $p$  is the total number of parameters (including an intercept if the `INTERCEPT` effect is included in the `MODEL` statement)
- $n = \sum_{h=1}^H \sum_{i=1}^{n_h} m_{hi}$  is the total number of observations in the sample

Also,  $f_h$  denotes the sampling rate for stratum  $h$ . You can use the `TOTAL=` or `RATE=` option to input population totals or sampling rates. See the section “[Specification of Population Totals and Sampling Rates](#)” on page 7965 for details. If you input stratum totals, PROC SURVEYREG computes  $f_h$  as the ratio of the stratum sample size to the stratum total. If you input stratum sampling rates, PROC SURVEYREG uses these values directly for  $f_h$ . If you do not specify the `TOTAL=` or `RATE=` option, then the procedure assumes that the stratum sampling rates  $f_h$  are negligible, and a finite population correction is not used when computing variances.

## Regression Coefficients

PROC SURVEYREG solves the normal equations  $\mathbf{X}'\mathbf{W}\mathbf{X}\boldsymbol{\beta} = \mathbf{X}'\mathbf{W}\mathbf{y}$  by using a modified sweep routine that produces a generalized (g2) inverse  $(\mathbf{X}'\mathbf{W}\mathbf{X})^-$  and a solution (Pringle and Rayner 1971)

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{W}\mathbf{X})^- \mathbf{X}'\mathbf{W}\mathbf{y}$$

where  $\mathbf{W}$  is the diagonal matrix constructed from `WEIGHT` variable values.

For models with class variables, there are more design matrix columns than there are degrees of freedom ( $df$ ) for the effect. Thus, there are linear dependencies among the columns. In this case, the parameters are not estimable; there is an infinite number of least squares solutions. PROC SURVEYREG uses a generalized (g2) inverse to obtain values for the estimates. The solution values are not displayed unless you specify the `SOLUTION` option in the `MODEL` statement. The solution has the characteristic that estimates are zero whenever the design column for that parameter is a linear combination of previous columns. (In strict terms, the solution values should not be called estimates.) With this full parameterization, hypothesis tests are constructed to test linear functions of the parameters that are estimable.

## Design Effect

If you specify the `DEFF` option in the `MODEL` statement, PROC SURVEYREG calculates the design effects for the regression coefficients. The design effect of an estimate is the ratio of the actual variance to the variance computed under the assumption of simple random sampling:

$$\text{DEFF} = \frac{\text{variance under the sample design}}{\text{variance under simple random sampling}}$$

See Kish (1965, p. 258) for more details. PROC SURVEYREG computes the numerator as described in the section “[Variance Estimation](#)” on page 7969. And the denominator is computed under the assumption that the sample design is simple random sampling, with no stratification and no clustering.

To compute the variance under the assumption of simple random sampling, PROC SURVEYREG calculates the sampling rate as follows. If you specify both sampling weights and sampling rates (or population totals) for the analysis, then the sampling rate under simple random sampling is calculated as

$$f_{\text{SRS}} = n / w_{..}$$

where  $n$  is the sample size and  $w_{..}$  (the sum of the weights over all observations) estimates the population size. If the sum of the weights is less than the sample size,  $f_{\text{SRS}}$  is set to zero. If you specify sampling rates for the analysis but not sampling weights, then PROC SURVEYREG computes the sampling rate under simple random sampling as the average of the stratum sampling rates:

$$f_{\text{SRS}} = \frac{1}{H} \sum_{h=1}^H f_h$$

If you do not specify sampling rates (or population totals) for the analysis, then the sampling rate under simple random sampling is assumed to be zero:

$$f_{\text{SRS}} = 0$$

## Stratum Collapse

If there is only one sampling unit in a stratum, then PROC SURVEYREG cannot estimate the variance for this stratum for the Taylor series method. To estimate stratum variances, by default the procedure collapses, or combines, those strata that contain only one sampling unit. If you specify the **NOCOLLAPSE** option in the STRATA statement, PROC SURVEYREG does not collapse strata and uses a variance estimate of zero for any stratum that contains only one sampling unit.

Note that stratum collapse only applies to Taylor series variance estimation (the default method, also specified by **VARMETHOD=TAYLOR**). The procedure does not collapse strata for BRR or jackknife variance estimation, which you request with the **VARMETHOD=BRR** or **VARMETHOD=JACKKNIFE** option.

If you do not specify the **NOCOLLAPSE** option for the Taylor series method, PROC SURVEYREG collapses strata according to the following rules. If there are multiple strata that contain only one sampling unit each, then the procedure collapses, or combines, all these strata into a new pooled stratum. If there is only one stratum with a single sampling unit, then PROC SURVEYREG collapses that stratum with the preceding stratum, where strata are ordered by the **STRATA** variable values. If the stratum with one sampling unit is the first stratum, then the procedure combines it with the following stratum.

If you specify stratum sampling rates by using the **RATE=SAS-data-set** option, PROC SURVEYREG computes the sampling rate for the new pooled stratum as the weighted average of the sampling rates for the collapsed strata. See the section “Computational Details” on page 7966 for details. If the specified sampling rate equals 0 for any of the collapsed strata, then the pooled stratum is assigned a sampling rate of 0. If you specify stratum totals by using the **TOTAL=SAS-data-set** option, PROC SURVEYREG combines the totals for the collapsed strata to compute the sampling rate for the new pooled stratum.

## Sampling Rate of the Pooled Stratum from Collapse

Assuming that PROC SURVEYREG collapses single-unit strata  $h_1, h_2, \dots, h_c$  into the pooled stratum, the procedure calculates the sampling rate for the pooled stratum as

$$f_{\text{Pooled Stratum}} = \begin{cases} 0 & \text{if any of } f_{h_l} = 0 \text{ where } l = 1, 2, \dots, c \\ \left( \sum_{l=1}^c n_{h_l} f_{h_l}^{-1} \right)^{-1} \sum_{l=1}^c n_{h_l} & \text{otherwise} \end{cases}$$

## Analysis of Variance (ANOVA)

PROC SURVEYREG produces an analysis of variance table for the model specified in the **MODEL** statement. This table is identical to the one produced by the GLM procedure for the model. PROC SURVEYREG computes ANOVA table entries by using the sampling weights, but not the sample design information about stratification and clustering.

The degrees of freedom (*df*) displayed in the ANOVA table are the same as those in the ANOVA table produced by PROC GLM. The Total DF is the total degrees of freedom used to obtain the regression coefficient

estimates. The Total DF equals the total number of observations minus 1 if the model includes an intercept. If the model does not include an intercept, the Total DF equals the total number of observations. The Model DF equals the degrees of freedom for the effects in the MODEL statement, not including the intercept. The Error DF equals the Total DF minus the Model DF.

### Multiple R-Square

PROC SURVEYREG computes a multiple R-square for the weighted regression as

$$R^2 = 1 - \frac{SS_{error}}{SS_{total}}$$

where  $SS_{error}$  is the error sum of squares in the ANOVA table

$$SS_{error} = \mathbf{r}'\mathbf{W}\mathbf{r}$$

and  $SS_{total}$  is the total sum of squares

$$SS_{total} = \begin{cases} \mathbf{y}'\mathbf{W}\mathbf{y} & \text{if no intercept} \\ \mathbf{y}'\mathbf{W}\mathbf{y} - \left( \sum_{h=1}^H \sum_{i=1}^{n_h} \sum_{j=1}^{m_{hi}} w_{hij} y_{hij} \right)^2 / w_{\dots} & \text{otherwise} \end{cases}$$

where  $w_{\dots}$  is the sum of the sampling weights over all observations.

### Adjusted R-Square

If you specify the **ADJRSQ** option in the MODEL statement, PROC SURVEYREG computes an multiple R-square adjusted as the weighted regression as

$$ADJRSQ = \begin{cases} 1 - \frac{n(1 - R^2)}{n - p} & \text{if no intercept} \\ 1 - \frac{(n - 1)(1 - R^2)}{n - p} & \text{otherwise} \end{cases}$$

where  $R^2$  is the multiple R-square.

### Root Mean Square Errors

PROC SURVEYREG computes the square root of mean square errors as

$$\sqrt{MSE} = \sqrt{n SS_{error} / (n - p) w_{\dots}}$$

where  $w_{\dots}$  is the sum of the sampling weights over all observations.

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## Variance Estimation

PROC SURVEYREG uses the Taylor series method or replication (resampling) methods to estimate sampling errors of estimators based on complex sample designs (Fuller 2009; Woodruff 1971; Fuller 1975;

Fuller et al. 1989; Särndal, Swensson, and Wretman 1992; Wolter 2007; Rust 1985; Dippo, Fay, and Morganstein 1984; Rao and Shao 1999; Rao, Wu, and Yue 1992; Rao and Shao 1996). You can use the **VARMETHOD=** option to specify a variance estimation method to use. By default, the Taylor series method is used. However, replication methods have recently gained popularity for estimating variances in complex survey data analysis. One reason for this popularity is the relative simplicity of replication-based estimates, especially for nonlinear estimators; another is that modern computational capacity has made replication methods feasible for practical survey analysis.

Replication methods draw multiple replicates (also called subsamples) from a full sample according to a specific resampling scheme. The most commonly used resampling schemes are the *balanced repeated replication* (BRR) method and the *jackknife* method. For each replicate, the original weights are modified for the PSUs in the replicates to create replicate weights. The parameters of interest are estimated by using the replicate weights for each replicate. Then the variances of parameters of interest are estimated by the variability among the estimates derived from these replicates. You can use the **REPWEIGHTS** statement to provide your own replicate weights for variance estimation.

The following sections provide details about how the variance-covariance matrix of the estimated regression coefficients is estimated for each variance estimation method.

### Taylor Series (Linearization)

The Taylor series (linearization) method is the most commonly used method to estimate the covariance matrix of the regression coefficients for complex survey data. It is the default variance estimation method used by PROC SURVEYREG.

Use the notation described in the section “**Notation**” on page 7966 to denote the residuals from the linear regression as

$$\mathbf{r} = \mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}}$$

with  $r_{hij}$  as its elements. Let the  $p \times p$  matrix  $\mathbf{G}$  be defined as

$$\mathbf{G} = \frac{n-1}{n-p} \sum_{h=1}^H \frac{n_h(1-f_h)}{n_h-1} \sum_{i=1}^{n_h} (\mathbf{e}_{hi\cdot} - \bar{\mathbf{e}}_{h\cdot\cdot})' (\mathbf{e}_{hi\cdot} - \bar{\mathbf{e}}_{h\cdot\cdot})$$

where

$$\mathbf{e}_{hij} = w_{hij} r_{hij} \mathbf{x}_{hij}$$

$$\mathbf{e}_{hi\cdot} = \sum_{j=1}^{m_{hi}} \mathbf{e}_{hij}$$

$$\bar{\mathbf{e}}_{h\cdot\cdot} = \frac{1}{n_h} \sum_{i=1}^{n_h} \mathbf{e}_{hi\cdot}$$

The Taylor series estimate of the covariance matrix of  $\hat{\boldsymbol{\beta}}$  is

$$\widehat{\mathbf{V}}(\hat{\boldsymbol{\beta}}) = (\mathbf{X}'\mathbf{W}\mathbf{X})^{-1} \mathbf{G} (\mathbf{X}'\mathbf{W}\mathbf{X})^{-1}$$

The factor  $(n - 1)/(n - p)$  in the computation of the matrix  $\mathbf{G}$  reduces the small sample bias associated with using the estimated function to calculate deviations (Hidiroglou, Fuller, and Hickman 1980). For simple random sampling, this factor contributes to the degrees of freedom correction applied to the residual mean square for ordinary least squares in which  $p$  parameters are estimated. By default, the procedure use this adjustment in the variance estimation. If you do not want to use this multiplier in variance estimation, you can specify the `VADJUST=NONE` option in the `MODEL` statement to suppress this factor.

### Balanced Repeated Replication (BRR) Method

The balanced repeated replication (BRR) method requires that the full sample be drawn by using a stratified sample design with two primary sampling units (PSUs) per stratum. Let  $H$  be the total number of strata. The total number of replicates  $R$  is the smallest multiple of 4 that is greater than  $H$ . However, if you prefer a larger number of replicates, you can specify the `REPS=number` option. If a  $number \times number$  Hadamard matrix cannot be constructed, the number of replicates is increased until a Hadamard matrix becomes available.

Each replicate is obtained by deleting one PSU per stratum according to the corresponding Hadamard matrix and adjusting the original weights for the remaining PSUs. The new weights are called replicate weights.

Replicates are constructed by using the first  $H$  columns of the  $R \times R$  Hadamard matrix. The  $r$ th ( $r = 1, 2, \dots, R$ ) replicate is drawn from the full sample according to the  $r$ th row of the Hadamard matrix as follows:

- If the  $(r, h)$  element of the Hadamard matrix is 1, then the first PSU of stratum  $h$  is included in the  $r$ th replicate and the second PSU of stratum  $h$  is excluded.
- If the  $(r, h)$  element of the Hadamard matrix is  $-1$ , then the second PSU of stratum  $h$  is included in the  $r$ th replicate and the first PSU of stratum  $h$  is excluded.

Note that the “first” and “second” PSUs are determined by data order in the input data set. Thus, if you reorder the data set and perform the same analysis by using BRR method, you might get slightly different results, because the contents in each replicate sample might change.

The replicate weights of the remaining PSUs in each half-sample are then doubled to their original weights. For more details about the BRR method, see Wolter (2007) and Lohr (2010).

By default, an appropriate Hadamard matrix is generated automatically to create the replicates. You can request that the Hadamard matrix be displayed by specifying the `VARMETHOD=BRR(PRINTH)` *method-option*. If you provide a Hadamard matrix by specifying the `VARMETHOD=BRR(HADAMARD=)` *method-option*, then the replicates are generated according to the provided Hadamard matrix.

You can use the `VARMETHOD=BRR(OUTWEIGHTS=)` *method-option* to save the replicate weights into a SAS data set.

Let  $\hat{\boldsymbol{\beta}}$  be the estimated regression coefficients from the full sample for  $\boldsymbol{\beta}$ , and let  $\hat{\boldsymbol{\beta}}_r$  be the estimated regression coefficient from the  $r$ th replicate by using replicate weights. PROC SURVEYREG estimates the covariance matrix of  $\hat{\boldsymbol{\beta}}$  by

$$\widehat{\mathbf{V}}(\hat{\boldsymbol{\beta}}) = \frac{1}{R} \sum_{r=1}^R (\hat{\boldsymbol{\beta}}_r - \hat{\boldsymbol{\beta}}) (\hat{\boldsymbol{\beta}}_r - \hat{\boldsymbol{\beta}})'$$

with  $H$  degrees of freedom, where  $H$  is the number of strata.

## Fay's BRR Method

Fay's method is a modification of the BRR method, and it requires a stratified sample design with two primary sampling units (PSUs) per stratum. The total number of replicates  $R$  is the smallest multiple of 4 that is greater than the total number of strata  $H$ . However, if you prefer a larger number of replicates, you can specify the `REPS=method-option`.

For each replicate, Fay's method uses a Fay coefficient  $0 \leq \epsilon < 1$  to impose a perturbation of the original weights in the full sample that is gentler than using only half-samples, as in the traditional BRR method. The Fay coefficient  $0 \leq \epsilon < 1$  can be set by specifying the `FAY =  $\epsilon$  method-option`. By default,  $\epsilon = 0.5$  if the `FAY method-option` is specified without providing a value for  $\epsilon$  (Judkins 1990; Rao and Shao 1999). When  $\epsilon = 0$ , Fay's method becomes the traditional BRR method. For more details, see Dipbo, Fay, and Morganstein (1984); Fay (1984, 1989); Judkins (1990).

Let  $H$  be the number of strata. Replicates are constructed by using the first  $H$  columns of the  $R \times R$  Hadamard matrix, where  $R$  is the number of replicates,  $R > H$ . The  $r$ th ( $r = 1, 2, \dots, R$ ) replicate is created from the full sample according to the  $r$ th row of the Hadamard matrix as follows:

- If the  $(r, h)$  element of the Hadamard matrix is 1, then the full sample weight of the first PSU in stratum  $h$  is multiplied by  $\epsilon$  and the full sample weight of the second PSU is multiplied by  $2 - \epsilon$  to obtain the  $r$ th replicate weights.
- If the  $(r, h)$  element of the Hadamard matrix is  $-1$ , then the full sample weight of the first PSU in stratum  $h$  is multiplied by  $2 - \epsilon$  and the full sample weight of the second PSU is multiplied by  $\epsilon$  to obtain the  $r$ th replicate weights.

You can use the `VARMETHOD=BRR(OUTWEIGHTS=) method-option` to save the replicate weights into a SAS data set.

By default, an appropriate Hadamard matrix is generated automatically to create the replicates. You can request that the Hadamard matrix be displayed by specifying the `VARMETHOD=BRR(PRINTH) method-option`. If you provide a Hadamard matrix by specifying the `VARMETHOD=BRR(HADAMARD=) method-option`, then the replicates are generated according to the provided Hadamard matrix.

Let  $\hat{\beta}$  be the estimated regression coefficients from the full sample for  $\beta$ . Let  $\hat{\beta}_r$  be the estimated regression coefficient obtained from the  $r$ th replicate by using replicate weights. PROC SURVEYREG estimates the covariance matrix of  $\hat{\beta}$  by

$$\widehat{V}(\hat{\beta}) = \frac{1}{R(1 - \epsilon)^2} \sum_{r=1}^R (\hat{\beta}_r - \hat{\beta}) (\hat{\beta}_r - \hat{\beta})'$$

with  $H$  degrees of freedom, where  $H$  is the number of strata.

## Jackknife Method

The jackknife method of variance estimation deletes one PSU at a time from the full sample to create replicates. The total number of replicates  $R$  is the same as the total number of PSUs. In each replicate, the sample weights of the remaining PSUs are modified by the jackknife coefficient  $\alpha_r$ . The modified weights are called replicate weights.

The jackknife coefficient and replicate weights are described as follows.



**Without Stratification** If there is no stratification in the sample design (no **STRATA** statement), the jackknife coefficients  $\alpha_r$  are the same for all replicates:

$$\alpha_r = \frac{R-1}{R} \quad \text{where } r = 1, 2, \dots, R$$

Denote the original weight in the full sample for the  $j$ th member of the  $i$ th PSU as  $w_{ij}$ . If the  $i$ th PSU is included in the  $r$ th replicate ( $r = 1, 2, \dots, R$ ), then the corresponding replicate weight for the  $j$ th member of the  $i$ th PSU is defined as

$$w_{ij}^{(r)} = w_{ij}/\alpha_r$$

**With Stratification** If the sample design involves stratification, each stratum must have at least two PSUs to use the jackknife method.

Let stratum  $\tilde{h}_r$  be the stratum from which a PSU is deleted for the  $r$ th replicate. Stratum  $\tilde{h}_r$  is called the *donor stratum*. Let  $n_{\tilde{h}_r}$  be the total number of PSUs in the donor stratum  $\tilde{h}_r$ . The jackknife coefficients are defined as

$$\alpha_r = \frac{n_{\tilde{h}_r} - 1}{n_{\tilde{h}_r}} \quad \text{where } r = 1, 2, \dots, R$$

Denote the original weight in the full sample for the  $j$ th member of the  $i$ th PSU as  $w_{ij}$ . If the  $i$ th PSU is included in the  $r$ th replicate ( $r = 1, 2, \dots, R$ ), then the corresponding replicate weight for the  $j$ th member of the  $i$ th PSU is defined as

$$w_{ij}^{(r)} = \begin{cases} w_{ij} & \text{if } i\text{th PSU is not in the donor stratum } \tilde{h}_r \\ w_{ij}/\alpha_r & \text{if } i\text{th PSU is in the donor stratum } \tilde{h}_r \end{cases}$$

You can use the **VARMETHOD=JACKKNIFE(OUTJKCOEFS=)** *method-option* to save the jackknife coefficients into a SAS data set and use the **VARMETHOD=JACKKNIFE(OUTWEIGHTS=)** *method-option* to save the replicate weights into a SAS data set.

If you provide your own replicate weights with a **REPWEIGHTS** statement, then you can also provide corresponding jackknife coefficients with the **JKCOEFS=** option.

Let  $\hat{\beta}$  be the estimated regression coefficients from the full sample for  $\beta$ . Let  $\hat{\beta}_r$  be the estimated regression coefficient obtained from the  $r$ th replicate by using replicate weights. PROC SURVEYREG estimates the covariance matrix of  $\hat{\beta}$  by

$$\widehat{V}(\hat{\beta}) = \sum_{r=1}^R \alpha_r (\hat{\beta}_r - \hat{\beta}) (\hat{\beta}_r - \hat{\beta})'$$

with  $R-H$  degrees of freedom, where  $R$  is the number of replicates and  $H$  is the number of strata, or  $R-1$  when there is no stratification.

## Hadamard Matrix

A Hadamard matrix **H** is a square matrix whose elements are either 1 or  $-1$  such that

$$\mathbf{H}\mathbf{H}' = k\mathbf{I}$$



where  $k$  is the dimension of  $\mathbf{H}$  and  $\mathbf{I}$  is the identity matrix of order  $k$ . The order  $k$  is necessarily 1, 2, or a positive integer that is a multiple of 4.

For example, the following matrix is a Hadamard matrix of dimension  $k = 8$ :

```

1 1 1 1 1 1 1 1
1 -1 1 -1 1 -1 1 -1
1 1 -1 -1 1 1 -1 -1
1 -1 -1 1 1 -1 -1 1
1 1 1 1 -1 -1 -1 -1
1 -1 1 -1 -1 1 -1 1
1 1 -1 -1 -1 -1 1 1
1 -1 -1 1 -1 1 1 -1

```

## Degrees of Freedom

PROC SURVEYREG produces tests for the significance of model effects, regression parameters, estimable functions specified in the **ESTIMATE** statement, and contrasts specified in the **CONTRAST** statement. It computes all these tests taking into account the sample design. The degrees of freedom for these tests differ from the degrees of freedom for the ANOVA table, which does not consider the sample design.

### Denominator Degrees of Freedom

The denominator  $df$  refers to the denominator degrees of freedom for  $F$  tests and to the degrees of freedom for  $t$  tests in the analysis.

For the **Taylor series** method, the denominator  $df$  equals the number of clusters minus the actual number of strata. If there are no clusters, the denominator  $df$  equals the number of observations minus the actual number of strata. The *actual number of strata* equals the following:

- one, if there is no **STRATA** statement
- the number of strata in the sample, if there is a **STRATA** statement but the procedure does not collapse any strata
- the number of strata in the sample after collapsing, if there is a **STRATA** statement and the procedure collapses strata that have only one sampling unit

Alternatively, you can specify your own denominator  $df$  by using the **DF=** option in the **MODEL** statement.

For the **BRR** method (including **Fay's method**) without a **REPWEIGHTS** statement, the denominator  $df$  equals the number of strata.

For the **jackknife** method without a **REPWEIGHTS** statement, the denominator  $df$  is equal to the number of replicates minus the *actual number of strata*.

When there is a **REPWEIGHTS** statement, the denominator  $df$  equals the number of **REPWEIGHTS** variables, unless you specify an alternative in the **DF=** option in a **REPWEIGHTS** statement.

### Numerator Degrees of Freedom

The numerator *df* refers to the numerator degrees of freedom for the Wald *F* statistic associated with an effect or with a contrast. The procedure computes the Wald *F* statistic for an effect as a Type III test; that is, the test has the following properties:

- The hypothesis for an effect does not involve parameters of other effects except for containing effects (which it must involve to be estimable).
- The hypotheses to be tested are invariant to the ordering of effects in the model.

See the section “Testing Effects” on page 7975 for more information. The numerator *df* for the Wald *F* statistic for a contrast is the rank of the **L** matrix that defines the contrast.

## Testing

### Testing Effects

For each effect in the model, PROC SURVEYREG computes an **L** matrix such that every element of **Lβ** is estimable; the **L** matrix has the maximum possible rank that is associated with the effect. To test the effect, the procedure uses the Wald *F* statistic for the hypothesis  $H_0: \mathbf{L}\boldsymbol{\beta} = 0$ . The Wald *F* statistic equals

$$F_{\text{Wald}} = \frac{(\mathbf{L}\hat{\boldsymbol{\beta}})'(\mathbf{L}'\hat{\mathbf{V}}\mathbf{L})^{-1}(\mathbf{L}\hat{\boldsymbol{\beta}})}{\text{rank}(\mathbf{L}'\hat{\mathbf{V}}\mathbf{L})}$$

with numerator degrees of freedom equal to  $\text{rank}(\mathbf{L}'\hat{\mathbf{V}}\mathbf{L})$ .

In the Taylor series method, the denominator degrees of freedom is equal to the number of clusters minus the number of strata (unless you specify the denominator degrees of freedom with the **DF=** option in the MODEL statement). For details about denominator degrees of freedom in replication methods, see the section “Denominator Degrees of Freedom” on page 7974. It is possible that the **L** matrix cannot be constructed for an effect, in which case that effect is not testable. For more information about how the matrix **L** is constructed, see the discussion in Chapter 15, “The Four Types of Estimable Functions.”

You can use the TEST statement to perform *F* tests that test Type I, Type II, or Type III hypotheses. For details about the syntax of the TEST statement, see the section “TEST Statement” on page 502 of Chapter 19, “Shared Concepts and Topics.”

### Contrasts

You can use the CONTRAST statement to perform custom hypothesis tests. If the hypothesis is testable in the univariate case, the Wald *F* statistic for  $H_0: \mathbf{L}\boldsymbol{\beta} = 0$  is computed as

$$F_{\text{Wald}} = \frac{(\mathbf{L}_{\text{Full}}\hat{\boldsymbol{\beta}})'(\mathbf{L}'_{\text{Full}}\hat{\mathbf{V}}\mathbf{L}_{\text{Full}})^{-1}(\mathbf{L}_{\text{Full}}\hat{\boldsymbol{\beta}})}{\text{rank}(\mathbf{L})}$$

where  $\mathbf{L}$  is the contrast vector or matrix you specify,  $\boldsymbol{\beta}$  is the vector of regression parameters,  $\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{W}\mathbf{X})^{-1}\mathbf{X}'\mathbf{W}\mathbf{Y}$ ,  $\widehat{\mathbf{V}}$  is the estimated covariance matrix of  $\hat{\boldsymbol{\beta}}$ ,  $\text{rank}(\mathbf{L})$  is the rank of  $\mathbf{L}$ , and  $\mathbf{L}_{\text{Full}}$  is a matrix such that

- $\mathbf{L}_{\text{Full}}$  has the same number of columns as  $\mathbf{L}$
- $\mathbf{L}_{\text{Full}}$  has full row rank
- the rank of  $\mathbf{L}_{\text{Full}}$  equals the rank of the  $\mathbf{L}$  matrix
- all rows of  $\mathbf{L}_{\text{Full}}$  are estimable functions
- the Wald  $F$  statistic computed using the  $\mathbf{L}_{\text{Full}}$  matrix is equivalent to the Wald  $F$  statistic computed by using the  $\mathbf{L}$  matrix with any row deleted that is a linear combination of previous rows

If  $\mathbf{L}$  is a full-rank matrix and all rows of  $\mathbf{L}$  are estimable functions, then  $\mathbf{L}_{\text{Full}}$  is the same as  $\mathbf{L}$ . It is possible that  $\mathbf{L}_{\text{Full}}$  matrix cannot be constructed for contrasts in a CONTRAST statement, in which case the contrasts are not testable.

---

## Domain Analysis

A **DOMAIN** statement requests that the procedure perform regression analysis for each domain.

For a domain  $D$ , let  $I_D$  be the corresponding indicator variable:

$$I_D(h, i, j) = \begin{cases} 1 & \text{if observation } (h, i, j) \text{ belongs to domain } D \\ 0 & \text{otherwise} \end{cases}$$

Let

$$v_{hij} = w_{hij} I_D(h, i, j) = \begin{cases} w_{hij} & \text{if observation } (h, i, j) \text{ belongs to domain } D \\ 0 & \text{otherwise} \end{cases}$$

The regression in domain  $D$  uses  $v$  as the weight variable.

---

## Computational Resources

Due to the complex nature of survey data analysis, the SURVEYREG procedure requires more memory than an analysis of the same regression model by the GLM procedure. For details about the amount of memory related to the modeling, see the section “[Computational Resources](#)” on page 3379 in Chapter 42, “[The GLM Procedure](#).”

The memory needed by the SURVEYREG procedure to handle the survey design is described as follows.

Let

- $H$  be the total number of strata
- $n_c$  be the total number of clusters in your sample across all  $H$  strata, if you specify a **CLUSTER** statement
- $p$  be the total number of parameters in the model

The memory needed (in bytes) is

$$48H + 8pH + 4p(p + 1)H$$

For a cluster sample, the additional memory needed (in bytes) is

$$48H + 8pH + 4p(p + 1)H + 4p(p + 1)n_c + 16n_c$$

The SURVEYREG procedure also uses other small amounts of additional memory. However, when you have a large number of clusters or strata, or a large number of parameters in your model, the memory described previously dominates the total memory required by the procedure.

## Output Data Sets

You can use the Output Delivery System (ODS) to create a SAS data set from any piece of PROC SURVEYREG output. See the section “[ODS Table Names](#)” on page 7983 for more information. For a more detailed description of using ODS, see Chapter 20, “[Using the Output Delivery System](#).”

PROC SURVEYREG also provides an **OUTPUT** statement to create a data set that contains estimated linear predictors and their standard error estimates, the residuals from the linear regression, and the confidence limits for the predictors.

If you use BRR or jackknife variance estimation, PROC SURVEYREG provides an output data set that stores the replicate weights and an output data set that stores the jackknife coefficients for jackknife variance estimation.

### OUT= Data Set Created by the OUTPUT Statement

The **OUTPUT** statement produces an output data set that contains the following:

- all original data from the SAS data set input to PROC SURVEYREG
- the new variables corresponding to the diagnostic measures specified with statistics keywords in the **OUTPUT** statement (**PREDICTED=**, **RESIDUAL=**, and so on)

When any independent variable in the analysis (including all classification variables) is missing for an observation, then all new variables that correspond to diagnostic measures are missing for the observation in the output data set.

When a dependent variable in the analysis is missing for an observation, then the residual variable that corresponds to **R** is also missing in the output data set. However, the variables corresponding to **LCLM**, **P**, **STDP**, and **UCLM** are not missing.

## Replicate Weights Output Data Set

If you specify the `OUTWEIGHTS= method-option` for `VARMETHOD=BRR` or `VARMETHOD=JACKKNIFE`, PROC SURVEYREG stores the replicate weights in an output data set. The `OUTWEIGHTS=` output data set contains all observations from the `DATA=` input data set that are valid (used in the analysis). (A valid observation is an observation that has a positive value of the `WEIGHT` variable. Valid observations must also have nonmissing values of the `STRATA` and `CLUSTER` variables, unless you specify the `MISSING` option.)

The `OUTWEIGHTS=` data set contains the following variables:

- all variables in the `DATA=` input data set
- `RepWt_1`, `RepWt_2`, . . . , `RepWt_n`, which are the replicate weight variables

where  $n$  is the total number of replicates in the analysis. Each replicate weight variable contains the replicate weights for the corresponding replicate. Replicate weights equal zero for those observations not included in the replicate.

After the procedure creates replicate weights for a particular input data set and survey design, you can use the `OUTWEIGHTS= method-option` to store these replicate weights and then use them again in subsequent analyses, either in PROC SURVEYREG or in the other survey procedures. You can use the `REPWEIGHTS` statement to provide replicate weights for the procedure.

## Jackknife Coefficients Output Data Set

If you specify the `OUTJKCOEFS= method-option` for `VARMETHOD=JACKKNIFE`, PROC SURVEYREG stores the jackknife coefficients in an output data set. The `OUTJKCOEFS=` output data set contains one observation for each replicate. The `OUTJKCOEFS=` data set contains the following variables:

- `Replicate`, which is the replicate number for the jackknife coefficient
- `JKCoefficient`, which is the jackknife coefficient
- `DonorStratum`, which is the stratum of the PSU that was deleted to construct the replicate, if you specify a `STRATA` statement

After the procedure creates jackknife coefficients for a particular input data set and survey design, you can use the `OUTJKCOEFS= method-option` to store these coefficients and then use them again in subsequent analyses, either in PROC SURVEYREG or in the other survey procedures. You can use the `JKCOEFS=` option in the `REPWEIGHTS` statement to provide jackknife coefficients for the procedure.

---

## Displayed Output

The SURVEYREG procedure produces output that is described in the following sections.

Output that is generated by the `EFFECT`, `ESTIMATE`, `LSMEANS`, `LSMESTIMATE`, and `SLICE` statements is not listed below. For information about the output that is generated by these statements, see the corresponding sections of Chapter 19, “[Shared Concepts and Topics](#).”

## Data Summary

By default, PROC SURVEYREG displays the following information in the “Data Summary” table:

- Number of Observations, which is the total number of observations used in the analysis, excluding observations with missing values
- Sum of Weights, if you specify a WEIGHT statement
- Mean of the dependent variable in the MODEL statement, or Weighted Mean if you specify a WEIGHT statement
- Sum of the dependent variable in the MODEL statement, or Weighted Sum if you specify a WEIGHT statement

## Design Summary

When you specify a CLUSTER statement or a STRATA statement, the procedure displays a “Design Summary” table, which provides the following sample design information:

- Number of Strata, if you specify a STRATA statement
- Number of Strata Collapsed, if the procedure collapses strata
- Number of Clusters, if you specify a CLUSTER statement
- Overall Sampling Rate used to calculate the design effect, if you specify the DEFF option in the MODEL statement

## Domain Summary

By default, PROC SURVEYREG displays the following information in the “Domain Summary” table:

- Number of Observations, which is the total number of observations used in the analysis
- total number of observations in the current domain
- total number of observations not in the current domain
- Sum of Weights for the observations in the current domain, if you specify a WEIGHT statement

## Fit Statistics

By default, PROC SURVEYREG displays the following regression statistics in the “Fit Statistics” table:

- R-square for the regression
- Root MSE, which is the square root of the mean square error
- Denominator DF, which is the denominator degrees of freedom for the  $F$  tests and also the degrees of freedom for the  $t$  tests produced by the procedure

## Variance Estimation

If the variance method is not Taylor series (see the section “Variance Estimation” on page 7969) or if the `NOMCAR` option is used, by default, PROC SURVEYREG displays the following variance estimation information in the “Variance Estimation” table:

- Method, which is the variance estimation method
- Number of Replicates, if you specify the `VARMETHOD=BRR` or `VARMETHOD=JACKKNIFE` option
- Hadamard Data Set name, if you specify the `VARMETHOD=BRR(HADAMARD=)` *method-option*
- Fay Coefficient, if you specify the `VARMETHOD=BRR(FAY)` *method-option*
- Replicate Weights input data set name, if you provide replicate weights with a `REPWEIGHTS` statement
- Missing Levels, which indicates whether missing levels of categorical variables are included by the `MISSING` option
- Missing Values, which indicates whether observations with missing values are included in the analysis by the `NOMCAR` option

## Stratum Information

When you specify the `LIST` option in the `STRATA` statement, PROC SURVEYREG displays a “Stratum Information” table, which provides the following information for each stratum:

- Stratum Index, which is a sequential stratum identification number
- `STRATA` variable(s), which lists the levels of `STRATA` variables for the stratum
- Population Total, if you specify the `TOTAL=` option
- Sampling Rate, if you specify the `TOTAL=` option or the `RATE=` option. If you specify the `TOTAL=` option, the sampling rate is based on the number of nonmissing observations in the stratum.
- N Obs, which is the number of observations
- number of Clusters, if you specify a `CLUSTER` statement
- Collapsed, which has the value ‘Yes’ if the stratum is collapsed with another stratum before analysis

If PROC SURVEYREG collapses strata, the “Stratum Information” table also displays stratum information for the new, collapsed stratum. The new stratum has a Stratum Index of 0 and is labeled ‘Pooled.’

## Class Level Information

If you use a CLASS statement to name classification variables, PROC SURVEYREG displays a “Class Level Information” table. This table contains the following information for each classification variable:

- Class Variable, which lists each CLASS variable name
- Levels, which is the number of values or levels of the classification variable
- Values, which lists the values of the classification variable. The values are separated by a white space character; therefore, to avoid confusion, you should not include a white space character within a classification variable value.

## X'X Matrix

If you specify the XPX option in the MODEL statement, PROC SURVEYREG displays the  $X'X$  matrix. When there is a WEIGHT variable, the procedure displays the  $X'WX$  matrix. This option also displays the crossproducts vector  $X'y$  or  $X'Wy$ , where  $y$  is the response vector (dependent variable).

## Inverse Matrix of X'X

If you specify the INVERSE option in the MODEL statement, PROC SURVEYREG displays the inverse or the generalized inverse of the  $X'X$  matrix. When there is a WEIGHT variable, the procedure displays the inverse or the generalized inverse of the  $X'WX$  matrix.

## ANOVA for Dependent Variable

If you specify the ANOVA option in the model statement, PROC SURVEYREG displays an analysis of variance table for the dependent variable. This table is identical to the ANOVA table displayed by the GLM procedure.

## Tests of Model Effects

By default, PROC SURVEYREG displays a “Tests of Model Effects” table, which provides Wald’s  $F$  test for each effect in the model. The table contains the following information for each effect:

- Effect, which is the effect name
- Num DF, which is the numerator degrees of freedom for Wald’s  $F$  test
- F Value, which is Wald’s  $F$  statistic
- Pr > F, which is the significance probability corresponding to the F Value

A footnote displays the denominator degrees of freedom, which is the same for all effects.



## Estimated Regression Coefficients

PROC SURVEYREG displays the “Estimated Regression Coefficients” table by default when there is no CLASS statement. Also, the procedure displays this table when you specify a CLASS statement and also specify the SOLUTION option in the MODEL statement. This table contains the following information for each regression parameter:

- Parameter, which identifies the effect or regressor variable
- Estimate, which is the estimate of the regression coefficient
- Standardized Estimate, which is the standardized regression coefficient
- Standard Error, which is the standard error of the estimate
- t Value, which is the  $t$  statistic for testing  $H_0: \text{Parameter} = 0$
- Pr > |t|, which is the two-sided significance probability corresponding to the t Value
- Pr > |t|, which is the two-sided significance probability corresponding to the t Value

## Covariance of Estimated Regression Coefficients

When you specify the COVB option in the MODEL statement, PROC SURVEYREG displays the “Covariance of Estimated Regression Coefficients” matrix.

## Coefficients of Contrast

When you specify the E option in a CONTRAST statement, PROC SURVEYREG displays a “Coefficients of Contrast” table for the contrast. You can use this table to check the coefficients you specified in the CONTRAST statement. Also, this table gives a note for a nonestimable contrast.

## Analysis of Contrasts

If you specify a CONTRAST statement, PROC SURVEYREG produces an “Analysis of Contrasts” table, which displays Wald’s  $F$  test for the contrast. If you use more than one CONTRAST statement, the procedure displays all results in the same table. The “Analysis of Contrasts” table contains the following information for each contrast:

- Contrast, which is the label of the contrast
- Num DF, which is the numerator degrees of freedom for Wald’s  $F$  test
- F Value, which is Wald’s  $F$  statistic for testing  $H_0: \text{Contrast} = 0$
- Pr > F, which is the significance probability corresponding to the F Value

## Hadamard Matrix

If you specify the `VARMETHOD=BRR(PRINTH)` *method-option* in the PROC SURVEYREG statement, the procedure displays the Hadamard matrix.

When you provide a Hadamard matrix with the `VARMETHOD=BRR(HADAMARD=)` *method-option* but the procedure does not use the entire matrix, the procedure displays only the rows and columns that are actually used to construct replicates.

---

## ODS Table Names

PROC SURVEYREG assigns a name to each table it creates; these names are listed in Table 94.10. You can use these names to refer to tables when you use the Output Delivery System (ODS) to select tables and create output data sets. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

To improve the consistency among procedures, tables that are generated by the ESTIMATE statements are changed slightly in appearance and formatting compared to releases prior to SAS/STAT 9.22. However, the statistics in the “Estimates” table remain unchanged. The “Coef” table replaces the previous “EstimateCoef” table that displays the L matrix coefficients of an estimable function of the parameters.

The EFFECT, ESTIMATE, LSMEANS, LSMESTIMATE, and SLICE statements also create tables, which are not listed in Table 94.10. For information about these tables, see the corresponding sections of Chapter 19, “Shared Concepts and Topics.”

**Table 94.10** ODS Tables Produced by PROC SURVEYREG

| ODS Table Name     | Description                                     | Statement        | Option   |
|--------------------|-------------------------------------------------|------------------|----------|
| ANOVA              | ANOVA for dependent variable                    | MODEL            | ANOVA    |
| ClassVarInfo       | Class level information                         | CLASS            | Default  |
| ContrastCoef       | Coefficients of contrast                        | CONTRAST         | E        |
| Contrasts          | Analysis of contrasts                           | CONTRAST         | Default  |
| CovB               | Covariance of estimated regression coefficients | MODEL            | COVB     |
| DataSummary        | Data summary                                    | PROC             | Default  |
| DesignSummary      | Design summary                                  | STRATA   CLUSTER | Default  |
| DomainSummary      | Domain summary                                  | DOMAIN           | Default  |
| Effects            | Tests of model effects                          | MODEL            | Defect   |
| FitStatistics      | Fit statistics                                  | MODEL            | Default  |
| HadamardMatrix     | Hadamard matrix                                 | PROC             | PRINTH   |
| InvXPX             | Inverse matrix of $X'X$                         | MODEL            | I        |
| ParameterEstimates | Estimated regression coefficients               | MODEL            | SOLUTION |
| StrataInfo         | Stratum information                             | STRATA           | LIST     |
| VarianceEstimation | Variance estimation                             | PROC             | Default  |
| XPX                | $X'X$ matrix                                    | MODEL            | XPX      |

By referring to the names of such tables, you can use the ODS OUTPUT statement to place one or more of these tables in output data sets.

For example, the following statements create an output data set MyStrata, which contains the “StrataInfo” table, an output data set MyParmEst, which contains the “ParameterEstimates” table, and an output data set Cov, which contains the “CovB” table for the ice cream study discussed in the section “Stratified Sampling” on page 7938:

```

title1 'Ice Cream Spending Analysis';
title2 'Stratified Sample Design';
proc surveyreg data=IceCream total=StudentTotals;
 strata Grade /list;
 class Kids;
 model Spending = Income Kids / solution covb;
 weight Weight;
 ods output StrataInfo = MyStrata
 ParameterEstimates = MyParmEst
 CovB = Cov;
run;

```

Note that the option CovB is specified in the MODEL statement in order to produce the covariance matrix table.

---

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “Statistical Graphics Using ODS.”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “A Primer on ODS Statistical Graphics” on page 599 in Chapter 21, “Statistical Graphics Using ODS.”

When ODS Graphics is enabled, the ESTIMATE, LSMEANS, LSMESTIMATE, and SLICE statements can produce plots that are associated with their analyses. For information about these plots, see the corresponding sections of Chapter 19, “Shared Concepts and Topics.”

---

## Examples: SURVEYREG Procedure

---

### Example 94.1: Simple Random Sampling

This example investigates the relationship between the labor force participation rate (LFPR) of women in 1968 and 1972 in large cities in the United States. A simple random sample of 19 cities is drawn from a total of 200 cities. For each selected city, the LFPRs are recorded and saved in a SAS data set Labor. In the following DATA step, LFPR in 1972 is contained in the variable LFPR1972, and the LFPR in 1968 is identified by the variable LFPR1968:

```
data Labor;
 input City $ 1-16 LFPR1972 LFPR1968;
 datalines;
New York .45 .42
Los Angeles .50 .50
Chicago .52 .52
Philadelphia .45 .45
Detroit .46 .43
San Francisco .55 .55
Boston .60 .45
Pittsburgh .49 .34
St. Louis .35 .45
Connecticut .55 .54
Washington D.C. .52 .42
Cincinnati .53 .51
Baltimore .57 .49
Newark .53 .54
Minn/St. Paul .59 .50
Buffalo .64 .58
Houston .50 .49
Patterson .57 .56
Dallas .64 .63
;
```

Assume that the LFPRs in 1968 and 1972 have a linear relationship, as shown in the following model:

$$\text{LFPR1972} = \beta_0 + \beta_1 * \text{LFPR1968} + \text{error}$$

You can use PROC SURVEYREG to obtain the estimated regression coefficients and estimated standard errors of the regression coefficients. The following statements perform the regression analysis:

```
title 'Study of Labor Force Participation Rates of Women';
proc surveyreg data=Labor total=200;
 model LFPR1972 = LFPR1968;
run;
```

Here, the TOTAL=200 option specifies the finite population total from which the simple random sample of 19 cities is drawn. You can specify the same information by using the sampling rate option RATE=0.095 (19/200=.095).

Output 94.1.1 summarizes the data information and the fit information.

**Output 94.1.1** Summary of Regression Using Simple Random Sampling

| Study of Labor Force Participation Rates of Women   |          |
|-----------------------------------------------------|----------|
| The SURVEYREG Procedure                             |          |
| Regression Analysis for Dependent Variable LFPR1972 |          |
| Data Summary                                        |          |
| Number of Observations                              | 19       |
| Mean of LFPR1972                                    | 0.52684  |
| Sum of LFPR1972                                     | 10.01000 |
| Fit Statistics                                      |          |
| R-square                                            | 0.3970   |
| Root MSE                                            | 0.05657  |
| Denominator DF                                      | 18       |

Output 94.1.2 presents the significance tests for the model effects and estimated regression coefficients. The  $F$  tests and  $t$  tests for the effects in the model are also presented in these tables.

**Output 94.1.2** Regression Coefficient Estimates

| Tests of Model Effects                                          |            |                |         |         |
|-----------------------------------------------------------------|------------|----------------|---------|---------|
| Effect                                                          | Num DF     | F Value        | Pr > F  |         |
| Model                                                           | 1          | 13.84          | 0.0016  |         |
| Intercept                                                       | 1          | 4.63           | 0.0452  |         |
| LFPR1968                                                        | 1          | 13.84          | 0.0016  |         |
| NOTE: The denominator degrees of freedom for the F tests is 18. |            |                |         |         |
| Estimated Regression Coefficients                               |            |                |         |         |
| Parameter                                                       | Estimate   | Standard Error | t Value | Pr >  t |
| Intercept                                                       | 0.20331056 | 0.09444296     | 2.15    | 0.0452  |
| LFPR1968                                                        | 0.65604048 | 0.17635810     | 3.72    | 0.0016  |
| NOTE: The denominator degrees of freedom for the t tests is 18. |            |                |         |         |

From the regression performed by PROC SURVEYREG, you obtain a positive estimated slope for the linear relationship between the LFPR in 1968 and the LFPR in 1972. The regression coefficients are all significant at the 5% level. The effects Intercept and LFPR1968 are significant in the model at the 5% level. In this example, the  $F$  test for the overall model without intercept is the same as the effect LFPR1968.

## Example 94.2: Cluster Sampling

This example illustrates the use of regression analysis in a simple random cluster sample design. The data are from Särndal, Swensson, and Wretman (1992, p. 652). A total of 284 Swedish municipalities are grouped into 50 clusters of neighboring municipalities. Five clusters with a total of 32 municipalities are randomly selected. The results from the regression analysis in which clusters are used in the sample design are compared to the results of a regression analysis that ignores the clusters. The linear relationship between the population in 1975 and in 1985 is investigated.

The 32 selected municipalities in the sample are saved in the data set `Municipalities`:

```
data Municipalities;
 input Municipality Cluster Population85 Population75;
 datalines;
205 37 5 5
206 37 11 11
207 37 13 13
208 37 8 8
209 37 17 19
6 2 16 15
7 2 70 62
8 2 66 54
9 2 12 12
10 2 60 50
94 17 7 7
95 17 16 16
96 17 13 11
97 17 12 11
98 17 70 67
99 17 20 20
100 17 31 28
101 17 49 48
276 50 6 7
277 50 9 10
278 50 24 26
279 50 10 9
280 50 67 64
281 50 39 35
282 50 29 27
283 50 10 9
284 50 27 31
52 10 7 6
53 10 9 8
54 10 28 27
55 10 12 11
56 10 107 108
;
```

The variable `Municipality` identifies the municipalities in the sample; the variable `Cluster` indicates the cluster to which a municipality belongs; and the variables `Population85` and `Population75` contain the municipality populations in 1985 and in 1975 (in thousands), respectively. A regression analysis is performed by PROC SURVEYREG with a `CLUSTER` statement:

```

title1 'Regression Analysis for Swedish Municipalities';
title2 'Cluster Sampling';
proc surveyreg data=Municipalities total=50;
 cluster Cluster;
 model Population85=Population75;
run;

```

The TOTAL=50 option specifies the total number of clusters in the sampling frame.

Output 94.2.1 displays the data and design summary. Since the sample design includes clusters, the procedure displays the total number of clusters in the sample in the “Design Summary” table.

**Output 94.2.1** Regression Analysis for Cluster Sampling

|                                                         |           |
|---------------------------------------------------------|-----------|
| Regression Analysis for Swedish Municipalities          |           |
| Cluster Sampling                                        |           |
| The SURVEYREG Procedure                                 |           |
| Regression Analysis for Dependent Variable Population85 |           |
| Data Summary                                            |           |
| Number of Observations                                  | 32        |
| Mean of Population85                                    | 27.50000  |
| Sum of Population85                                     | 880.00000 |
| Design Summary                                          |           |
| Number of Clusters                                      | 5         |

Output 94.2.2 displays the fit statistics and regression coefficient estimates. In the “Estimated Regression Coefficients” table, the estimated slope for the linear relationship is 1.05, which is significant at the 5% level; but the intercept is not significant. This suggests that a regression line crossing the original can be established between populations in 1975 and in 1985.

**Output 94.2.2** Regression Analysis for Cluster Sampling

|                |        |
|----------------|--------|
| Fit Statistics |        |
| R-square       | 0.9860 |
| Root MSE       | 3.0488 |
| Denominator DF | 4      |

**Output 94.2.2** *continued*

| Estimated Regression Coefficients |            |                |         |         |
|-----------------------------------|------------|----------------|---------|---------|
| Parameter                         | Estimate   | Standard Error | t Value | Pr >  t |
| Intercept                         | -0.0191292 | 0.89204053     | -0.02   | 0.9839  |
| Population75                      | 1.0546253  | 0.05167565     | 20.41   | <.0001  |

NOTE: The denominator degrees of freedom for the t tests is 4.

The CLUSTER statement is necessary in PROC SURVEYREG in order to incorporate the sample design. If you do not specify a CLUSTER statement in the regression analysis, as in the following statements, the standard deviation of the regression coefficients are incorrectly estimated.

```

title1 'Regression Analysis for Swedish Municipalities';
title2 'Simple Random Sampling';
proc surveyreg data=Municipalities total=284;
 model Population85=Population75;
run;

```

The analysis ignores the clusters in the sample, assuming that the sample design is a simple random sampling. Therefore, the TOTAL= option specifies the total number of municipalities, which is 284.

Output 94.2.3 displays the regression results ignoring the clusters. Compared to the results in Output 94.2.2, the regression coefficient estimates are the same. However, without using clusters, the regression coefficients have a smaller variance estimate, as in Output 94.2.3. By using clusters in the analysis, the estimated regression coefficient for effect Population75 is 1.05, with the estimated standard error 0.05, as displayed in Output 94.2.2; without using the clusters, the estimate is 1.05, but with the estimated standard error 0.04, as displayed in Output 94.2.3. To estimate the variance of the regression coefficients correctly, you should include the clustering information in the regression analysis.

**Output 94.2.3** Regression Analysis for Simple Random Sampling

| Regression Analysis for Swedish Municipalities<br>Simple Random Sampling |           |
|--------------------------------------------------------------------------|-----------|
| The SURVEYREG Procedure                                                  |           |
| Regression Analysis for Dependent Variable Population85                  |           |
| Data Summary                                                             |           |
| Number of Observations                                                   | 32        |
| Mean of Population85                                                     | 27.50000  |
| Sum of Population85                                                      | 880.00000 |



**Output 94.2.3** *continued*

| Fit Statistics                                                  |            |                |         |         |
|-----------------------------------------------------------------|------------|----------------|---------|---------|
| R-square                                                        |            |                | 0.9860  |         |
| Root MSE                                                        |            |                | 3.0488  |         |
| Denominator DF                                                  |            |                | 31      |         |
| Estimated Regression Coefficients                               |            |                |         |         |
| Parameter                                                       | Estimate   | Standard Error | t Value | Pr >  t |
| Intercept                                                       | -0.0191292 | 0.67417606     | -0.03   | 0.9775  |
| Population75                                                    | 1.0546253  | 0.03668414     | 28.75   | <.0001  |
| NOTE: The denominator degrees of freedom for the t tests is 31. |            |                |         |         |

**Example 94.3: Regression Estimator for Simple Random Sample**

By using auxiliary information, you can construct regression estimators to provide more accurate estimates of population characteristics. With ESTIMATE statements in PROC SURVEYREG, you can specify a regression estimator as a linear function of the regression parameters to estimate the population total. This example illustrates this application by using the data set Municipalities from [Example 94.2](#).

In this sample, a linear model between the Swedish populations in 1975 and in 1985 is established:

$$\text{Population85} = \alpha + \beta * \text{Population75} + \text{error}$$

Assuming that the total population in 1975 is known to be 8200 (in thousands), you can use the ESTIMATE statement to predict the 1985 total population by using the following statements:

```

title1 'Regression Analysis for Swedish Municipalities';
title2 'Estimate Total Population';
proc surveyreg data=Municipalities total=50;
 cluster Cluster;
 model Population85=Population75;
 estimate '1985 population' Intercept 284 Population75 8200;
run;

```

Since each observation in the sample is a municipality and there is a total of 284 municipalities in Sweden, the coefficient for Intercept ( $\alpha$ ) in the ESTIMATE statement is 284 and the coefficient for Population75 ( $\beta$ ) is the total population in 1975 (8.2 million).

[Output 94.3.1](#) displays the regression results and the estimation of the total population. By using the linear model, you can predict the total population in 1985 to be 8.64 million, with a standard error of 0.26 million.

**Output 94.3.1** Use the Regression Estimator to Estimate the Population Total

| Regression Analysis for Swedish Municipalities<br>Estimate Total Population |          |                |    |         |         |
|-----------------------------------------------------------------------------|----------|----------------|----|---------|---------|
| The SURVEYREG Procedure                                                     |          |                |    |         |         |
| Regression Analysis for Dependent Variable Population85                     |          |                |    |         |         |
|                                                                             | Estimate |                |    |         |         |
| Label                                                                       | Estimate | Standard Error | DF | t Value | Pr >  t |
| 1985 population                                                             | 8642.49  | 258.56         | 4  | 33.43   | <.0001  |

**Example 94.4: Stratified Sampling**

This example illustrates the use of the SURVEYREG procedure to perform a regression in a stratified sample design. Consider a population of 235 farms producing corn in Nebraska and Iowa. You are interested in the relationship between corn yield (CornYield) and total farm size (FarmArea).

Each state is divided into several regions, and each region is used as a stratum. Within each stratum, a simple random sample with replacement is drawn. A total of 19 farms is selected by using a stratified simple random sample. The sample size and population size within each stratum are displayed in Table 94.11.

**Table 94.11** Number of Farms in Each Stratum

| Stratum      | State    | Region | Number of Farms |           |
|--------------|----------|--------|-----------------|-----------|
|              |          |        | Population      | Sample    |
| 1            | Iowa     | 1      | 100             | 3         |
| 2            |          | 2      | 50              | 5         |
| 3            |          | 3      | 15              | 3         |
| 4            | Nebraska | 1      | 30              | 6         |
| 5            |          | 2      | 40              | 2         |
| <b>Total</b> |          |        | <b>235</b>      | <b>19</b> |

Three models for the data are considered:

- Model I — Common intercept and slope:

$$\text{Corn Yield} = \alpha + \beta * \text{Farm Area}$$

- Model II — Common intercept, different slope:

$$\text{Corn Yield} = \begin{cases} \alpha + \beta_{\text{Iowa}} * \text{Farm Area} & \text{if the farm is in Iowa} \\ \alpha + \beta_{\text{Nebraska}} * \text{Farm Area} & \text{if the farm is in Nebraska} \end{cases}$$

- Model III — Different intercept and different slope:

$$\text{Corn Yield} = \begin{cases} \alpha_{\text{Iowa}} + \beta_{\text{Iowa}} * \text{Farm Area} & \text{if the farm is in Iowa} \\ \alpha_{\text{Nebraska}} + \beta_{\text{Nebraska}} * \text{Farm Area} & \text{if the farm is in Nebraska} \end{cases}$$

Data from the stratified sample are saved in the SAS data set Farms. In the data set Farms, the variable Weight represents the sampling weight. In the following DATA step, the sampling weights are the reciprocals of selection probabilities:

```
data Farms;
 input State $ Region FarmArea CornYield Weight;
 datalines;
Iowa 1 100 54 33.333
Iowa 1 83 25 33.333
Iowa 1 25 10 33.333
Iowa 2 120 83 10.000
Iowa 2 50 35 10.000
Iowa 2 110 65 10.000
Iowa 2 60 35 10.000
Iowa 2 45 20 10.000
Iowa 3 23 5 5.000
Iowa 3 10 8 5.000
Iowa 3 350 125 5.000
Nebraska 1 130 20 5.000
Nebraska 1 245 25 5.000
Nebraska 1 150 33 5.000
Nebraska 1 263 50 5.000
Nebraska 1 320 47 5.000
Nebraska 1 204 25 5.000
Nebraska 2 80 11 20.000
Nebraska 2 48 8 20.000
;
```

The information about population size in each stratum is saved in the SAS data set StratumTotals:

```
data StratumTotals;
 input State $ Region _TOTAL_;
 datalines;
Iowa 1 100
Iowa 2 50
Iowa 3 15
Nebraska 1 30
Nebraska 2 40
;
```

Using the sample data from the data set Farms and the control information data from the data set StratumTotals, you can fit Model I by using PROC SURVEYREG with the following statements:

```

title1 'Analysis of Farm Area and Corn Yield';
title2 'Model I: Same Intercept and Slope';
proc surveyreg data=Farms total=StratumTotals;
 strata State Region / list;
 model CornYield = FarmArea / covB;
 weight Weight;
run;

```

Output 94.4.1 displays the data summary and stratification information fitting Model I. The sampling rates are automatically computed by the procedure based on the sample sizes and the population totals in strata.

**Output 94.4.1** Data Summary and Stratum Information Fitting Model I

| Analysis of Farm Area and Corn Yield                 |          |           |       |                  |               |  |
|------------------------------------------------------|----------|-----------|-------|------------------|---------------|--|
| Model I: Same Intercept and Slope                    |          |           |       |                  |               |  |
| The SURVEYREG Procedure                              |          |           |       |                  |               |  |
| Regression Analysis for Dependent Variable CornYield |          |           |       |                  |               |  |
| Data Summary                                         |          |           |       |                  |               |  |
| Number of Observations                               |          | 19        |       |                  |               |  |
| Sum of Weights                                       |          | 234.99900 |       |                  |               |  |
| Weighted Mean of CornYield                           |          | 31.56029  |       |                  |               |  |
| Weighted Sum of CornYield                            |          | 7416.6    |       |                  |               |  |
| Design Summary                                       |          |           |       |                  |               |  |
| Number of Strata                                     |          | 5         |       |                  |               |  |
| Fit Statistics                                       |          |           |       |                  |               |  |
| R-square                                             |          | 0.3882    |       |                  |               |  |
| Root MSE                                             |          | 20.6422   |       |                  |               |  |
| Denominator DF                                       |          | 14        |       |                  |               |  |
| Stratum Information                                  |          |           |       |                  |               |  |
| Stratum Index                                        | State    | Region    | N Obs | Population Total | Sampling Rate |  |
| 1                                                    | Iowa     | 1         | 3     | 100              | 3.00%         |  |
| 2                                                    |          | 2         | 5     | 50               | 10.0%         |  |
| 3                                                    |          | 3         | 3     | 15               | 20.0%         |  |
| 4                                                    | Nebraska | 1         | 6     | 30               | 20.0%         |  |
| 5                                                    |          | 2         | 2     | 40               | 5.00%         |  |

Output 94.4.2 displays tests of model effects and the estimated regression coefficients.

**Output 94.4.2** Estimated Regression Coefficients and the Estimated Covariance Matrix

| Tests of Model Effects |        |         |        |
|------------------------|--------|---------|--------|
| Effect                 | Num DF | F Value | Pr > F |
| Model                  | 1      | 21.74   | 0.0004 |
| Intercept              | 1      | 4.93    | 0.0433 |
| FarmArea               | 1      | 21.74   | 0.0004 |

NOTE: The denominator degrees of freedom for the F tests is 14.

| Estimated Regression Coefficients |            |                |         |         |
|-----------------------------------|------------|----------------|---------|---------|
| Parameter                         | Estimate   | Standard Error | t Value | Pr >  t |
| Intercept                         | 11.8162978 | 5.31981027     | 2.22    | 0.0433  |
| FarmArea                          | 0.2126576  | 0.04560949     | 4.66    | 0.0004  |

NOTE: The denominator degrees of freedom for the t tests is 14.

| Covariance of Estimated Regression Coefficients |              |              |
|-------------------------------------------------|--------------|--------------|
|                                                 | Intercept    | FarmArea     |
| Intercept                                       | 28.300381277 | -0.146471538 |
| FarmArea                                        | -0.146471538 | 0.0020802259 |

Alternatively, you can assume that the linear relationship between corn yield (CornYield) and farm area (FarmArea) is different among the states (Model II). In order to analyze the data by using this model, you create auxiliary variables FarmAreaNE and FarmAreaIA to represent farm area in different states:

$$\text{FarmAreaNE} = \begin{cases} 0 & \text{if the farm is in Iowa} \\ \text{FarmArea} & \text{if the farm is in Nebraska} \end{cases}$$

$$\text{FarmAreaIA} = \begin{cases} \text{FarmArea} & \text{if the farm is in Iowa} \\ 0 & \text{if the farm is in Nebraska} \end{cases}$$

The following statements create these variables in a new data set called FarmsByState and use PROC SURVEYREG to fit Model II:

```
data FarmsByState;
 set Farms;
 if State='Iowa' then do;
 FarmAreaIA=FarmArea;
 FarmAreaNE=0;
 end;
```

```

else do;
 FarmAreaIA=0;
 FarmAreaNE=FarmArea;
end;
run;

```

The following statements perform the regression by using the new data set FarmsByState. The analysis uses the auxiliary variables FarmAreaIA and FarmAreaNE as the regressors:

```

title1 'Analysis of Farm Area and Corn Yield';
title2 'Model II: Same Intercept, Different Slopes';
proc surveyreg data=FarmsByState total=StratumTotals;
 strata State Region;
 model CornYield = FarmAreaIA FarmAreaNE / covB;
 weight Weight;
run;

```

Output 94.4.3 displays the fit statistics and parameter estimates. The estimated slope parameters for each state are quite different from the estimated slope in Model I. The results from the regression show that Model II fits these data better than Model I.

**Output 94.4.3** Regression Results from Fitting Model II

| Analysis of Farm Area and Corn Yield                            |              |                |              |         |
|-----------------------------------------------------------------|--------------|----------------|--------------|---------|
| Model II: Same Intercept, Different Slopes                      |              |                |              |         |
| The SURVEYREG Procedure                                         |              |                |              |         |
| Regression Analysis for Dependent Variable CornYield            |              |                |              |         |
| Fit Statistics                                                  |              |                |              |         |
| R-square                                                        |              |                | 0.8158       |         |
| Root MSE                                                        |              |                | 11.6759      |         |
| Denominator DF                                                  |              |                | 14           |         |
| Estimated Regression Coefficients                               |              |                |              |         |
| Parameter                                                       | Estimate     | Standard Error | t Value      | Pr >  t |
| Intercept                                                       | 4.04234816   | 3.80934848     | 1.06         | 0.3066  |
| FarmAreaIA                                                      | 0.41696069   | 0.05971129     | 6.98         | <.0001  |
| FarmAreaNE                                                      | 0.12851012   | 0.02495495     | 5.15         | 0.0001  |
| NOTE: The denominator degrees of freedom for the t tests is 14. |              |                |              |         |
| Covariance of Estimated Regression Coefficients                 |              |                |              |         |
|                                                                 | Intercept    | FarmAreaIA     | FarmAreaNE   |         |
| Intercept                                                       | 14.511135861 | -0.118001232   | -0.079908772 |         |
| FarmAreaIA                                                      | -0.118001232 | 0.0035654381   | 0.0006501109 |         |
| FarmAreaNE                                                      | -0.079908772 | 0.0006501109   | 0.0006227496 |         |

For Model III, different intercepts are used for the linear relationship in two states. The following statements illustrate the use of the NOINT option in the MODEL statement associated with the CLASS statement to fit Model III:

```

title1 'Analysis of Farm Area and Corn Yield';
title2 'Model III: Different Intercepts and Slopes';
proc surveyreg data=FarmsByState total=StratumTotals;
 strata State Region;
 class State;
 model CornYield = State FarmAreaIA FarmAreaNE / noint covB solution;
 weight Weight;
run;

```

The model statement includes the classification effect State as a regressor. Therefore, the parameter estimates for effect State present the intercepts in two states.

Output 94.4.4 displays the regression results for fitting Model III, including parameter estimates, and covariance matrix of the regression coefficients. The estimated covariance matrix shows a lack of correlation between the regression coefficients from different states. This suggests that Model III might be the best choice for building a model for farm area and corn yield in these two states.

However, some statistics remain the same under different regression models—for example, Weighted Mean of CornYield. These estimators do not rely on the particular model you use.

#### Output 94.4.4 Regression Results for Fitting Model III

| Analysis of Farm Area and Corn Yield                            |            |                |         |         |
|-----------------------------------------------------------------|------------|----------------|---------|---------|
| Model III: Different Intercepts and Slopes                      |            |                |         |         |
| The SURVEYREG Procedure                                         |            |                |         |         |
| Regression Analysis for Dependent Variable CornYield            |            |                |         |         |
| Fit Statistics                                                  |            |                |         |         |
| R-square                                                        |            | 0.9300         |         |         |
| Root MSE                                                        |            | 11.9810        |         |         |
| Denominator DF                                                  |            | 14             |         |         |
| Estimated Regression Coefficients                               |            |                |         |         |
| Parameter                                                       | Estimate   | Standard Error | t Value | Pr >  t |
| State Iowa                                                      | 5.27797099 | 5.27170400     | 1.00    | 0.3337  |
| State Nebraska                                                  | 0.65275201 | 1.70031616     | 0.38    | 0.7068  |
| FarmAreaIA                                                      | 0.40680971 | 0.06458426     | 6.30    | <.0001  |
| FarmAreaNE                                                      | 0.14630563 | 0.01997085     | 7.33    | <.0001  |
| NOTE: The denominator degrees of freedom for the t tests is 14. |            |                |         |         |

**Output 94.4.4** *continued*

| Covariance of Estimated Regression Coefficients |              |                |              |              |
|-------------------------------------------------|--------------|----------------|--------------|--------------|
|                                                 | State Iowa   | State Nebraska | FarmAreaIA   | FarmAreaNE   |
| State Iowa                                      | 27.790863033 | 0              | -0.205517205 | 0            |
| State Nebraska                                  | 0            | 2.8910750385   | 0            | -0.027354011 |
| FarmAreaIA                                      | -0.205517205 | 0              | 0.0041711265 | 0            |
| FarmAreaNE                                      | 0            | -0.027354011   | 0            | 0.0003988349 |

**Example 94.5: Regression Estimator for Stratified Sample**

This example uses the corn yield data set FARMS from Example 94.4 to illustrate how to construct a regression estimator for a stratified sample design.

As in Example 94.3, by incorporating auxiliary information into a regression estimator, the procedure can produce more accurate estimates of the population characteristics that are of interest. In this example, the sample design is a stratified sample design. The auxiliary information is the total farm areas in regions of each state, as displayed in Table 94.12. You want to estimate the total corn yield by using this information under the three linear models given in Example 94.4.

**Table 94.12** Information for Each Stratum

| Stratum      | State    | Number of Farms |            | Sample    | Total Farm Area |
|--------------|----------|-----------------|------------|-----------|-----------------|
|              |          | Region          | Population |           |                 |
| 1            | Iowa     | 1               | 100        | 3         | 13,200          |
| 2            |          | 2               | 50         | 5         |                 |
| 3            |          | 3               | 15         | 3         |                 |
| 4            | Nebraska | 1               | 30         | 6         | 8,750           |
| 5            |          | 2               | 40         | 2         |                 |
| <b>Total</b> |          |                 | <b>235</b> | <b>19</b> | <b>21,950</b>   |

The regression estimator to estimate the total corn yield under Model I can be obtained by using PROC SURVEYREG with an ESTIMATE statement:

```

title1 'Estimate Corn Yield from Farm Size';
title2 'Model I: Same Intercept and Slope';
proc surveyreg data=Farms total=StratumTotals;
 strata State Region / list;
 class State Region;
 model CornYield = FarmArea State*Region /solution;
 weight Weight;
 estimate 'Estimate of CornYield under Model I'
 INTERCEPT 235 FarmArea 21950
 State*Region 100 50 15 30 40 /e;
run;

```



To apply the constraint in each stratum that the weighted total number of farms equals to the total number of farms in the stratum, you can include the strata as an effect in the MODEL statement, effect State\*Region. Thus, the CLASS statement must list the STRATA variables, State and Region, as classification variables. The following ESTIMATE statement specifies the regression estimator, which is a linear function of the regression parameters:

```
estimate 'Estimate of CornYield under Model I'
 INTERCEPT 235 FarmArea 21950
 State*Region 100 50 15 30 40 /e;
```

This linear function contains the total for each explanatory variable in the model. Because the sampling units are farms in this example, the coefficient for Intercept in the ESTIMATE statement is the total number of farms (235); the coefficient for FarmArea is the total farm area listed in Table 94.12 (21950); and the coefficients for effect State\*Region are the total number of farms in each strata (as displayed in Table 94.12).

Output 94.5.1 displays the results of the ESTIMATE statement. The regression estimator for the total of CornYield in Iowa and Nebraska is 7464 under Model I, with a standard error of 927.

**Output 94.5.1** Regression Estimator for the Total of CornYield under Model I

| Estimate Corn Yield from Farm Size<br>Model I: Same Intercept and Slope |          |                |    |         |
|-------------------------------------------------------------------------|----------|----------------|----|---------|
| The SURVEYREG Procedure                                                 |          |                |    |         |
| Regression Analysis for Dependent Variable CornYield                    |          |                |    |         |
| Estimate                                                                |          |                |    |         |
| Label                                                                   | Estimate | Standard Error | DF | t Value |
| Estimate of CornYield under Model I                                     | 7463.52  | 926.84         | 14 | 8.05    |
| Estimate                                                                |          |                |    |         |
| Label                                                                   | Pr >  t  |                |    |         |
| Estimate of CornYield under Model I                                     | <.0001   |                |    |         |

Under Model II, a regression estimator for totals can be obtained by using the following statements:

```
title1 'Estimate Corn Yield from Farm Size';
title2 'Model II: Same Intercept, Different Slopes';
proc surveyreg data=FarmsByState total=StratumTotals;
 strata State Region;
 class State Region;
 model CornYield = FarmAreaIA FarmAreaNE
 state*region /solution;
 weight Weight;
 estimate 'Total of CornYield under Model II'
 INTERCEPT 235 FarmAreaIA 13200 FarmAreaNE 8750
 State*Region 100 50 15 30 40 /e;
run;
```

In this model, you also need to include strata as a fixed effect in the MODEL statement. Other regressors are the auxiliary variables FarmAreaIA and FarmAreaNE (defined in Example 94.4). In the following ESTIMATE statement, the coefficient for Intercept is still the total number of farms; and the coefficients for FarmAreaIA and FarmAreaNE are the total farm area in Iowa and Nebraska, respectively, as displayed in Table 94.12. The total number of farms in each strata are the coefficients for the strata effect:

```
estimate 'Total of CornYield under Model II'
 INTERCEPT 235 FarmAreaIA 13200 FarmAreaNE 8750
 State*Region 100 50 15 30 40 /e;
```

Output 94.5.2 displays that the results of the regression estimator for the total of corn yield in two states under Model II is 7580 with a standard error of 859. The regression estimator under Model II has a slightly smaller standard error than under Model I.

**Output 94.5.2** Regression Estimator for the Total of CornYield under Model II

| Estimate Corn Yield from Farm Size                   |          |                |    |         |         |
|------------------------------------------------------|----------|----------------|----|---------|---------|
| Model II: Same Intercept, Different Slopes           |          |                |    |         |         |
| The SURVEYREG Procedure                              |          |                |    |         |         |
| Regression Analysis for Dependent Variable CornYield |          |                |    |         |         |
|                                                      | Estimate |                |    |         |         |
| Label                                                | Estimate | Standard Error | DF | t Value | Pr >  t |
| Total of CornYield under Model II                    | 7580.49  | 859.18         | 14 | 8.82    | <.0001  |

Finally, you can apply Model III to the data and estimate the total corn yield. Under Model III, you can also obtain the regression estimators for the total corn yield for each state. Three ESTIMATE statements are used in the following statements to create the three regression estimators:

```
title1 'Estimate Corn Yield from Farm Size';
title2 'Model III: Different Intercepts and Slopes';
proc surveyreg data=FarmsByState total=StratumTotals;
 strata State Region;
 class State Region;
 model CornYield = state FarmAreaIA FarmAreaNE
 State*Region /noint solution;
 weight Weight;
 estimate 'Total CornYield in Iowa under Model III'
 State 165 0 FarmAreaIA 13200 FarmAreaNE 0
 State*region 100 50 15 0 0 /e;
 estimate 'Total CornYield in Nebraska under Model III'
 State 0 70 FarmAreaIA 0 FarmAreaNE 8750
 State*Region 0 0 0 30 40 /e;
 estimate 'Total CornYield in both states under Model III'
 State 165 70 FarmAreaIA 13200 FarmAreaNE 8750
 State*Region 100 50 15 30 40 /e;
run;
```

The fixed effect State is added to the MODEL statement to obtain different intercepts in different states, by using the NOINT option. Among the ESTIMATE statements, the coefficients for explanatory variables are different depending on which regression estimator is estimated. For example, in the ESTIMATE statement

```
estimate 'Total CornYield in Iowa under Model III'
 State 165 0 FarmAreaIA 13200 FarmAreaNE 0
 State*region 100 50 15 0 0 /e;
```

the coefficients for the effect State are 165 and 0, respectively. This indicates that the total number of farms in Iowa is 165 and the total number of farms in Nebraska is 0, because the estimation is the total corn yield in Iowa only. Similarly, the total numbers of farms in three regions in Iowa are used for the coefficients of the strata effect State\*Region, as displayed in Table 94.12. Output 94.5.3 displays the results from the three regression estimators by using Model III. Since the estimations are independent in each state, the total corn yield from both states is equal to the sum of the estimated total of corn yield in Iowa and Nebraska,  $6246 + 1334 = 7580$ . This regression estimator is the same as the one under Model II. The variance of regression estimator of the total corn yield in both states is the sum of variances of regression estimators for total corn yield in each state. Therefore, it is not necessary to use Model III to obtain the regression estimator for the total corn yield unless you need to estimate the total corn yield for each individual state.

**Output 94.5.3** Regression Estimator for the Total of CornYield under Model III

| Estimate Corn Yield from Farm Size                   |          |                |    |         |
|------------------------------------------------------|----------|----------------|----|---------|
| Model III: Different Intercepts and Slopes           |          |                |    |         |
| The SURVEYREG Procedure                              |          |                |    |         |
| Regression Analysis for Dependent Variable CornYield |          |                |    |         |
| Estimate                                             |          |                |    |         |
| Label                                                | Estimate | Standard Error | DF | t Value |
| Total CornYield in Iowa under Model III              | 6246.11  | 851.27         | 14 | 7.34    |
| Estimate                                             |          |                |    |         |
| Label                                                | Pr >  t  |                |    |         |
| Total CornYield in Iowa under Model III              | <.0001   |                |    |         |

## Example 94.6: Stratum Collapse

In a stratified sample, it is possible that some strata might have only one sampling unit. When this happens, PROC SURVEYREG collapses the strata that contain a single sampling unit into a pooled stratum. For more detailed information about stratum collapse, see the section “Stratum Collapse” on page 7968.

Suppose that you have the following data:

```

data Sample;
 input Stratum X Y W;
 datalines;
10 0 0 5
10 1 1 5
11 1 1 10
11 1 2 10
12 3 3 16
33 4 4 45
14 6 7 50
12 3 4 16
;

```

The variable `Stratum` is again the stratification variable, the variable `X` is the independent variable, and the variable `Y` is the dependent variable. You want to regress `Y` on `X`. In the data set `Sample`, both `Stratum=33` and `Stratum=14` contain one observation. By default, PROC SURVEYREG collapses these strata into one pooled stratum in the regression analysis.

To input the finite population correction information, you create the SAS data set `StratumTotals`:

```

data StratumTotals;
 input Stratum _TOTAL_;
 datalines;
10 10
11 20
12 32
33 40
33 45
14 50
15 .
66 70
;

```

The variable `Stratum` is the stratification variable, and the variable `_TOTAL_` contains the stratum totals. The data set `StratumTotals` contains more strata than the data set `Sample`. Also in the data set `StratumTotals`, more than one observation contains the stratum totals for `Stratum=33`:

```

33 40
33 45

```

PROC SURVEYREG allows this type of input. The procedure simply ignores strata that are not present in the data set `Sample`; for the multiple entries of a stratum, the procedure uses the first observation. In this example, `Stratum=33` has the stratum total `_TOTAL_=40`.

The following SAS statements perform the regression analysis:

```

title1 'Stratified Sample with Single Sampling Unit in Strata';
title2 'With Stratum Collapse';
proc surveyreg data=Sample total=StratumTotals;
 strata Stratum/list;
 model Y=X;
 weight W;
run;

```

Output 94.6.1 shows that there are a total of five strata in the input data set and two strata are collapsed into a pooled stratum. The denominator degrees of freedom is 4, due to the collapse (see the section “Denominator Degrees of Freedom” on page 7974).

**Output 94.6.1** Summary of Data and Regression

| Stratified Sample with Single Sampling Unit in Strata<br>With Stratum Collapse |           |
|--------------------------------------------------------------------------------|-----------|
| The SURVEYREG Procedure                                                        |           |
| Regression Analysis for Dependent Variable Y                                   |           |
| Data Summary                                                                   |           |
| Number of Observations                                                         | 8         |
| Sum of Weights                                                                 | 157.00000 |
| Weighted Mean of Y                                                             | 4.31210   |
| Weighted Sum of Y                                                              | 677.00000 |
| Design Summary                                                                 |           |
| Number of Strata                                                               | 5         |
| Number of Strata Collapsed                                                     | 2         |
| Fit Statistics                                                                 |           |
| R-square                                                                       | 0.9564    |
| Root MSE                                                                       | 0.5111    |
| Denominator DF                                                                 | 4         |

Output 94.6.2 displays the stratification information, including stratum collapse. Under the column Collapsed, the fourth stratum (Stratum=14) and the fifth (Stratum=33) are marked as ‘Yes,’ which indicates that these two strata are collapsed into the pooled stratum (Stratum Index=0). The sampling rate for the pooled stratum is 2% (see the section “Sampling Rate of the Pooled Stratum from Collapse” on page 7968).

Output 94.6.3 displays the parameter estimates and the tests of the significance of the model effects.

**Output 94.6.2** Stratification Information

| Stratum Information |           |         |       |                  |               |
|---------------------|-----------|---------|-------|------------------|---------------|
| Stratum Index       | Collapsed | Stratum | N Obs | Population Total | Sampling Rate |
| 1                   |           | 10      | 2     | 10               | 20.0%         |
| 2                   |           | 11      | 2     | 20               | 10.0%         |
| 3                   |           | 12      | 2     | 32               | 6.25%         |
| 4                   | Yes       | 14      | 1     | 50               | 2.00%         |
| 5                   | Yes       | 33      | 1     | 40               | 2.50%         |
| 0                   | Pooled    |         | 2     | 90               | 2.22%         |

NOTE: Strata with only one observation are collapsed into the stratum with Stratum Index "0".

**Output 94.6.3** Parameter Estimates and Effect Tests

| Tests of Model Effects |        |         |        |
|------------------------|--------|---------|--------|
| Effect                 | Num DF | F Value | Pr > F |
| Model                  | 1      | 173.01  | 0.0002 |
| Intercept              | 1      | 0.00    | 0.9961 |
| X                      | 1      | 173.01  | 0.0002 |

NOTE: The denominator degrees of freedom for the F tests is 4.

| Estimated Regression Coefficients |            |                |         |         |
|-----------------------------------|------------|----------------|---------|---------|
| Parameter                         | Estimate   | Standard Error | t Value | Pr >  t |
| Intercept                         | 0.00179469 | 0.34306373     | 0.01    | 0.9961  |
| X                                 | 1.12598708 | 0.08560466     | 13.15   | 0.0002  |

NOTE: The denominator degrees of freedom for the t tests is 4.

Alternatively, if you prefer not to collapse strata with a single sampling unit, you can specify the NOCOLLAPSE option in the STRATA statement:

```

title1 'Stratified Sample with Single Sampling Unit in Strata';
title2 'Without Stratum Collapse';
proc surveyreg data=Sample total=StratumTotals;
 strata Stratum/list nocollapse;
 model Y = X;
 weight W;
run;

```

Output 94.6.4 does not contain the stratum collapse information displayed in Output 94.6.1, and the denominator degrees of freedom are 3 instead of 4.

#### Output 94.6.4 Summary of Data and Regression

| Stratified Sample with Single Sampling Unit in Strata<br>Without Stratum Collapse |           |
|-----------------------------------------------------------------------------------|-----------|
| The SURVEYREG Procedure                                                           |           |
| Regression Analysis for Dependent Variable Y                                      |           |
| Data Summary                                                                      |           |
| Number of Observations                                                            | 8         |
| Sum of Weights                                                                    | 157.00000 |
| Weighted Mean of Y                                                                | 4.31210   |
| Weighted Sum of Y                                                                 | 677.00000 |
| Design Summary                                                                    |           |
| Number of Strata                                                                  | 5         |
| Fit Statistics                                                                    |           |
| R-square                                                                          | 0.9564    |
| Root MSE                                                                          | 0.5111    |
| Denominator DF                                                                    | 3         |

In Output 94.6.5, although the fourth stratum and the fifth stratum contain only one observation, no stratum collapse occurs.

#### Output 94.6.5 Stratification Information

| Stratum Information |         |       |                  |               |  |
|---------------------|---------|-------|------------------|---------------|--|
| Stratum Index       | Stratum | N Obs | Population Total | Sampling Rate |  |
| 1                   | 10      | 2     | 10               | 20.0%         |  |
| 2                   | 11      | 2     | 20               | 10.0%         |  |
| 3                   | 12      | 2     | 32               | 6.25%         |  |
| 4                   | 14      | 1     | 50               | 2.00%         |  |
| 5                   | 33      | 1     | 40               | 2.50%         |  |

As a result of not collapsing strata, the standard error estimates of the parameters, shown in Output 94.6.6, are different from those in Output 94.6.3, as are the tests of the significance of model effects.

**Output 94.6.6** Parameter Estimates and Effect Tests

| Tests of Model Effects |        |         |        |
|------------------------|--------|---------|--------|
| Effect                 | Num DF | F Value | Pr > F |
| Model                  | 1      | 347.27  | 0.0003 |
| Intercept              | 1      | 0.00    | 0.9962 |
| X                      | 1      | 347.27  | 0.0003 |

NOTE: The denominator degrees of freedom for the F tests is 3.

| Estimated Regression Coefficients |            |                |         |         |
|-----------------------------------|------------|----------------|---------|---------|
| Parameter                         | Estimate   | Standard Error | t Value | Pr >  t |
| Intercept                         | 0.00179469 | 0.34302581     | 0.01    | 0.9962  |
| X                                 | 1.12598708 | 0.06042241     | 18.64   | 0.0003  |

NOTE: The denominator degrees of freedom for the t tests is 3.

**Example 94.7: Domain Analysis**

Recall the example in the section “Getting Started: SURVEYREG Procedure” on page 7935, which analyzed a stratified simple random sample from a junior high school to examine how household income and the number of children in a household affect students’ average weekly spending for ice cream. You can use the same sample to analyze the average weekly spending among male and female students. Because student gender is unrelated to the design of the sample, this kind of analysis is called domain analysis (subgroup analysis).

This example shows how you can use PROC SURVEYREG to perform domain analysis. The data set follows:

```
data IceCreamDataDomain;
 input Grade Spending Income Gender$ @@;
 datalines;
7 7 39 M 7 7 38 F 8 12 47 F
9 10 47 M 7 1 34 M 7 10 43 M
7 3 44 M 8 20 60 F 8 19 57 M
7 2 35 M 7 2 36 F 9 15 51 F
8 16 53 F 7 6 37 F 7 6 41 M
7 6 39 M 9 15 50 M 8 17 57 F
8 14 46 M 9 8 41 M 9 8 41 F
9 7 47 F 7 3 39 F 7 12 50 M
7 4 43 M 9 14 46 F 8 18 58 M
9 9 44 F 7 2 37 F 7 1 37 M
7 4 44 M 7 11 42 M 9 8 41 M
8 10 42 M 8 13 46 F 7 2 40 F
9 6 45 F 9 11 45 M 7 2 36 F
7 9 46 F
;
```



```

data IceCreamDataDomain;
 set IceCreamDataDomain;
 if Grade=7 then Prob=20/1824;
 if Grade=8 then Prob=9/1025;
 if Grade=9 then Prob=11/1151;
 Weight=1/Prob;
run;

```

In the data set `IceCreamDataDomain`, the variable `Grade` indicates a student's grade, which is the stratification variable. The variable `Spending` contains the dollar amount of each student's average weekly spending for ice cream. The variable `Income` specifies the household income, in thousands of dollars. The variable `Gender` indicates a student's gender. The sampling weights are created by using the reciprocals of the probabilities of selection, as follows:

```

data StudentTotals;
 input Grade _TOTAL_;
 datalines;
7 1824
8 1025
9 1151
;

```

In the data set `StudentTotals`, the variable `Grade` is the stratification variable, and the variable `_TOTAL_` contains the total numbers of students in the strata in the survey population.

The following statements demonstrate how you can analyze the relationship between spending and income among male and female students:

```

title1 'Ice Cream Spending Analysis';
title2 'Domain Analysis by Gender';
proc surveyreg data=IceCreamDataDomain total=StudentTotals;
 strata Grade;
 model Spending = Income;
 domain Gender;
 weight Weight;
run;

```

Output 94.7.1 gives a summary of the domains.

### Output 94.7.1 Domain Analysis Summary

|                                                  |         |
|--------------------------------------------------|---------|
| Ice Cream Spending Analysis                      |         |
| Domain Analysis by Gender                        |         |
| The SURVEYREG Procedure                          |         |
| Gender=F                                         |         |
| Domain Regression Analysis for Variable Spending |         |
| Domain Summary                                   |         |
| Number of Observations                           | 40      |
| Number of Observations in Domain                 | 19      |
| Number of Observations Not in Domain             | 21      |
| Sum of Weights in Domain                         | 1926.9  |
| Weighted Mean of Spending                        | 9.37611 |
| Weighted Sum of Spending                         | 18066.5 |
| Ice Cream Spending Analysis                      |         |
| Domain Analysis by Gender                        |         |
| The SURVEYREG Procedure                          |         |
| Gender=M                                         |         |
| Domain Regression Analysis for Variable Spending |         |
| Domain Summary                                   |         |
| Number of Observations                           | 40      |
| Number of Observations in Domain                 | 21      |
| Number of Observations Not in Domain             | 19      |
| Sum of Weights in Domain                         | 2073.1  |
| Weighted Mean of Spending                        | 8.92305 |
| Weighted Sum of Spending                         | 18498.7 |

Output 94.7.2 shows the parameter estimates for the model within each domain.

**Output 94.7.2** Parameter Estimates within Domain

|                                                                 |            |                   |         |         |
|-----------------------------------------------------------------|------------|-------------------|---------|---------|
| Ice Cream Spending Analysis<br>Domain Analysis by Gender        |            |                   |         |         |
| The SURVEYREG Procedure                                         |            |                   |         |         |
| Gender=F                                                        |            |                   |         |         |
| Domain Regression Analysis for Variable Spending                |            |                   |         |         |
| Estimated Regression Coefficients                               |            |                   |         |         |
| Parameter                                                       | Estimate   | Standard<br>Error | t Value | Pr >  t |
| Intercept                                                       | -23.751681 | 2.30795437        | -10.29  | <.0001  |
| Income                                                          | 0.735366   | 0.04757001        | 15.46   | <.0001  |
| NOTE: The denominator degrees of freedom for the t tests is 37. |            |                   |         |         |
| Ice Cream Spending Analysis<br>Domain Analysis by Gender        |            |                   |         |         |
| The SURVEYREG Procedure                                         |            |                   |         |         |
| Gender=M                                                        |            |                   |         |         |
| Domain Regression Analysis for Variable Spending                |            |                   |         |         |
| Estimated Regression Coefficients                               |            |                   |         |         |
| Parameter                                                       | Estimate   | Standard<br>Error | t Value | Pr >  t |
| Intercept                                                       | -23.213291 | 2.13361241        | -10.88  | <.0001  |
| Income                                                          | 0.729419   | 0.04589801        | 15.89   | <.0001  |
| NOTE: The denominator degrees of freedom for the t tests is 37. |            |                   |         |         |

For this particular example, the effect Income is significant for both models built within subgroups of male and female students, and the models are quite similar. In many other cases, regression models vary from subgroup to subgroup.

## Example 94.8: Compare Domain Statistics

This example is a continuation of [Example 94.7](#) in which domain analyses for male and female students were performed. Suppose that you are now interested in estimating the gender domain means of weekly ice cream spending (that is, the average spending for males and females, respectively). You can use the SURVEYMEANS procedure to produce these domain statistics by using the following statements:

```
proc surveymeans data=IceCreamDataDomain total=StudentTotals;
 strata Grade;
 var spending;
 domain Gender;
 weight Weight;
run;
```

Output 94.8.1 shows the estimated spending among male and female students.

**Output 94.8.1** Estimated Domain Means

| The SURVEYMEANS Procedure |          |    |          |                      |
|---------------------------|----------|----|----------|----------------------|
| Domain Analysis: Gender   |          |    |          |                      |
| Gender                    | Variable | N  | Mean     | Std Error<br>of Mean |
| F                         | Spending | 19 | 9.376111 | 1.077927             |
| M                         | Spending | 21 | 8.923052 | 1.003423             |

| Domain Analysis: Gender |          |                 |            |  |
|-------------------------|----------|-----------------|------------|--|
| Gender                  | Variable | 95% CL for Mean |            |  |
| F                       | Spending | 7.19202418      | 11.5601988 |  |
| M                       | Spending | 6.88992385      | 10.9561807 |  |

You can also use PROC SURVEYREG to estimate these domain means. The benefit of this alternative approach is that PROC SURVEYREG provides more tools for additional analysis, such as domain means comparisons in a LSMEANS statement.

Suppose that you want to test whether there is a significant difference for the ice cream spending between male and female students. You can use the following statements to perform the test:

```

title1 'Ice Cream Spending Analysis';
title2 'Compare Domain Statistics';
proc surveyreg data=IceCreamDataDomain total=StudentTotals;
 strata Grade;
 class Gender;
 model Spending = Gender / vadjust=none;
 lsmeans Gender / diff;
 weight Weight;
run;

```

The variable Gender is used as a model effect. The `VADJUST=NONE` option is used to produce variance estimates for domain means that are identical to those produced by PROC SURVEYMEANS. The `LSMEANS` statement requests that PROC SURVEYREG estimate the average spending in each gender group. The `DIFF` option requests that the procedure compute the difference among domain means.

Output 94.8.2 displays the estimated weekly spending on ice cream among male and female students, respectively, and their standard errors. Female students spend \$9.38 per week on average, and male students spend \$8.92 per week on average. These domain means, including their standard errors, are identical to those in Output 94.8.1 which are produced by PROC SURVEYMEANS.

**Output 94.8.2** Domain Means between Gender

| Ice Cream Spending Analysis                         |          |                |    |         |         |
|-----------------------------------------------------|----------|----------------|----|---------|---------|
| Compare Domain Statistics                           |          |                |    |         |         |
| The SURVEYREG Procedure                             |          |                |    |         |         |
| Regression Analysis for Dependent Variable Spending |          |                |    |         |         |
| Gender Least Squares Means                          |          |                |    |         |         |
| Gender                                              | Estimate | Standard Error | DF | t Value | Pr >  t |
| F                                                   | 9.3761   | 1.0779         | 37 | 8.70    | <.0001  |
| M                                                   | 8.9231   | 1.0034         | 37 | 8.89    | <.0001  |

Output 94.8.3 shows the estimated difference for weekly ice cream spending between the two gender groups. The female students spend \$0.45 more than male students on average, and the difference is not statistically significant based on the  $t$  test.

**Output 94.8.3** Domain Means Comparison

| Differences of Gender Least Squares Means |         |          |                |    |         |         |
|-------------------------------------------|---------|----------|----------------|----|---------|---------|
| Gender                                    | _Gender | Estimate | Standard Error | DF | t Value | Pr >  t |
| F                                         | M       | 0.4531   | 1.7828         | 37 | 0.25    | 0.8008  |

If you want to investigate whether there is any significant difference in ice cream spending among grades, you can use the following similar statements to compare:

```

title1 'Ice Cream Spending Analysis';
title2 'Compare Domain Statistics';
ods graphics on;
proc surveyreg data=IceCreamDataDomain total=StudentTotals;
 strata Grade;
 class Grade;
 model Spending = Grade / vadjust=none;
 lsmeans Grade / diff plots=(diff meanplot(cl));
 weight Weight;
run;
ods graphics off;

```

The Grade is specified in the CLASS statement to be used as an effect in the MODEL statement. The DIFF option in the LSMEANS statement requests that the procedure compute the difference among the domain means for the effect Grade. The ODS GRAPHICS statement enables ODS to create graphics. The PLOTS=(DIFF MEANPLOT(CL)) option requests two graphics: the domain means plot “MeanPlot” and their pairwise difference plot “DiffPlot”. The CL suboption requests the “MeanPlot” to display confidence. For information about ODS Graphics, see Chapter 21, “Statistical Graphics Using ODS.”

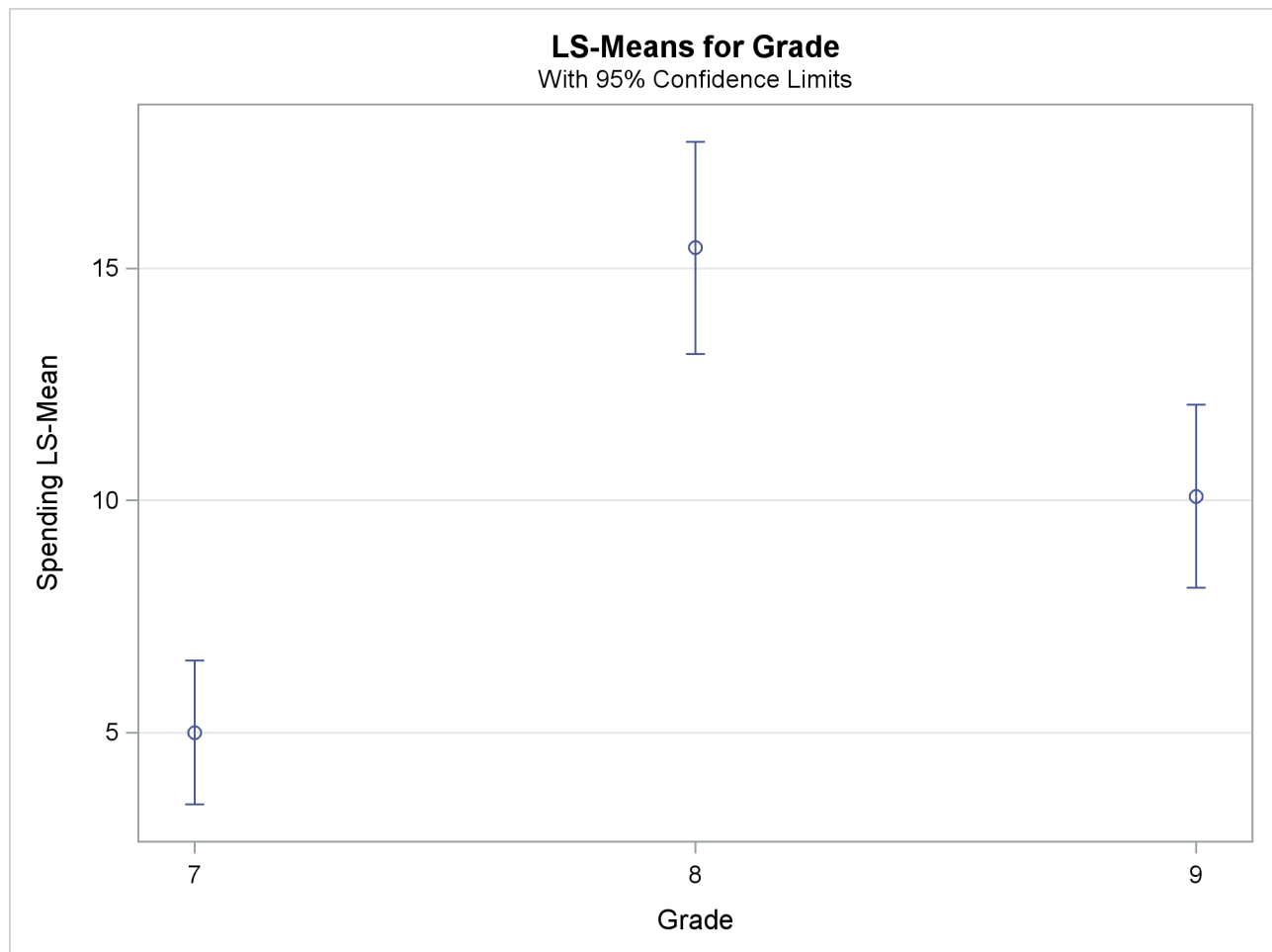
Output 94.8.4 shows the estimated weekly spending on ice cream for students within each grade. Students in Grade 7 spend the least, only \$5.00 per week. Students in Grade 8 spend the most, \$15.44 per week. Students in Grade 9 spend a little less at \$10.09 per week.

**Output 94.8.4** Domain Means among Grades

| Ice Cream Spending Analysis<br>Compare Domain Statistics |          |                |    |         |         |
|----------------------------------------------------------|----------|----------------|----|---------|---------|
| The SURVEYREG Procedure                                  |          |                |    |         |         |
| Regression Analysis for Dependent Variable Spending      |          |                |    |         |         |
| Grade Least Squares Means                                |          |                |    |         |         |
| Grade                                                    | Estimate | Standard Error | DF | t Value | Pr >  t |
| 7                                                        | 5.0000   | 0.7636         | 37 | 6.55    | <.0001  |
| 8                                                        | 15.4444  | 1.1268         | 37 | 13.71   | <.0001  |
| 9                                                        | 10.0909  | 0.9719         | 37 | 10.38   | <.0001  |

Output 94.8.5 plots the weekly spending results that are shown in Output 94.8.4.

**Output 94.8.5** Plot of Means of Ice Cream Spending within Grades



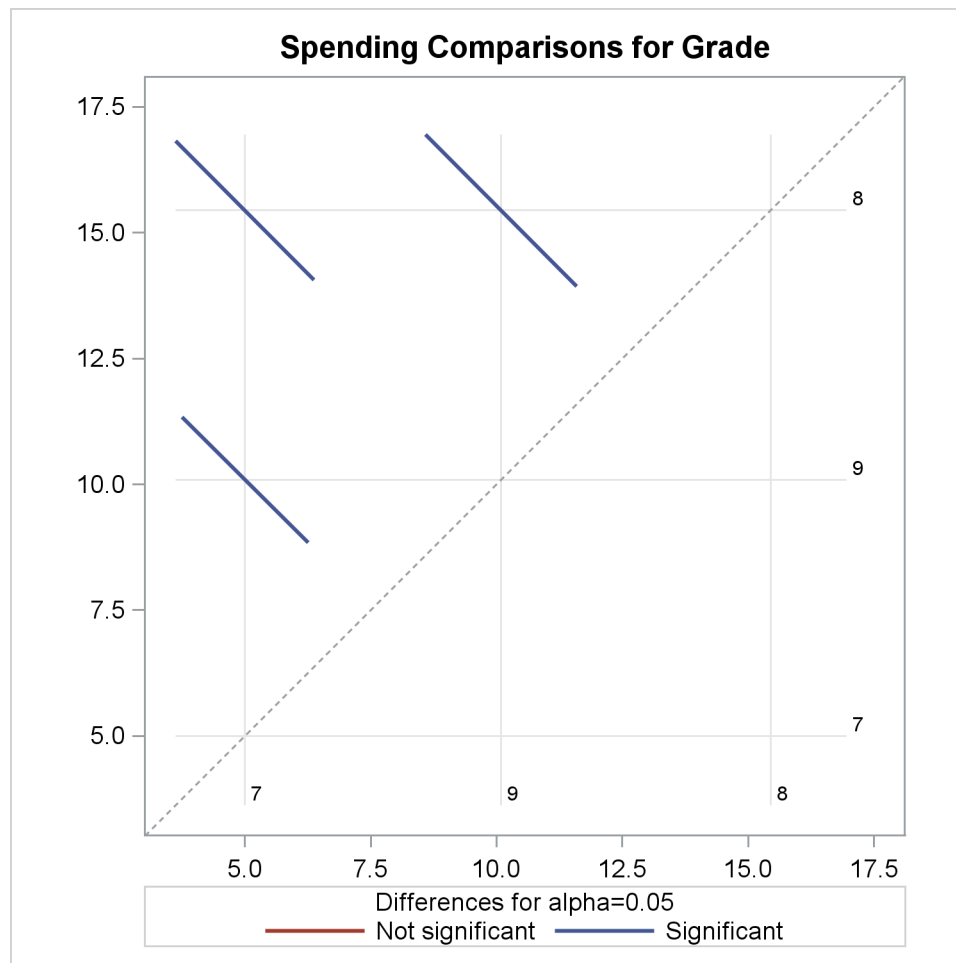
Output 94.8.6 displays pairwise comparisons for weekly ice cream spending among grades. All the differences are significant based on  $t$  tests.

**Output 94.8.6** Domain Means Comparison

| Differences of Grade Least Squares Means |        |          |                |    |         |         |
|------------------------------------------|--------|----------|----------------|----|---------|---------|
| Grade                                    | _Grade | Estimate | Standard Error | DF | t Value | Pr >  t |
| 7                                        | 8      | -10.4444 | 1.3611         | 37 | -7.67   | <.0001  |
| 7                                        | 9      | -5.0909  | 1.2360         | 37 | -4.12   | 0.0002  |
| 8                                        | 9      | 5.3535   | 1.4880         | 37 | 3.60    | 0.0009  |

Output 94.8.7 plots the comparisons that are shown in Output 94.8.6.

**Output 94.8.7** Plot of Pairwise Comparisons of Spending among Grades



In Output 94.8.7, the spending for each grade is shown in the background grid on both axes. Comparisons for each pair of domain means are shown by colored bars at intersections of these grids. The length of each bar represents the width of the confidence intervals for the corresponding difference between domain means. The significance of these pairwise comparisons are indicated in the plot by whether these bars cross the 45-degree background dash-line across the plot. Since none of the three bars cross the dash-line, all pairwise comparisons are significant, as shown in Output 94.8.6.

## Example 94.9: Variance Estimate Using the Jackknife Method

This example uses the stratified sample from the section “Getting Started: SURVEYREG Procedure” on page 7935 to illustrate how to estimate the variances with replication methods.

As shown in the section “Stratified Sampling” on page 7938, the sample is saved in the SAS data set IceCream. The variable Grade that indicates a student’s grade is the stratification variable. The variable Spending contains the dollar amount of each student’s average weekly spending for ice cream. The variable



Income specifies the household income, in thousands of dollars. The variable Kids indicates how many children are in a student's family. The variable Weight contains sampling weights.

In this example, we use the jackknife method to estimate the variance, saving the replicate weights generated by the procedure into a SAS data set:

```

title1 'Ice Cream Spending Analysis';
title2 'Use the Jackknife Method to Estimate the Variance';
proc surveyreg data=IceCream
 varmethod=JACKKNIFE(outweights=JKWeights);
 strata Grade;
 class Kids;
 model Spending = Income Kids / solution;
 weight Weight;
run;

```

The `VARMETHOD=JACKKNIFE` option requests the procedure to estimate the variance by using the jackknife method. The `OUTWEIGHTS=JKWeights` option provides a SAS data set named JKWeights that contains the replicate weights used in the computation.

Output 94.9.1 shows the summary of the data and the variance estimation method. There are a total of 40 replicates generated by the procedure.

#### Output 94.9.1 Variance Estimation Using the Jackknife Method

|                                                     |           |
|-----------------------------------------------------|-----------|
| Ice Cream Spending Analysis                         |           |
| Use the Jackknife Method to Estimate the Variance   |           |
| The SURVEYREG Procedure                             |           |
| Regression Analysis for Dependent Variable Spending |           |
| Data Summary                                        |           |
| Number of Observations                              | 40        |
| Sum of Weights                                      | 4000.0    |
| Weighted Mean of Spending                           | 9.14130   |
| Weighted Sum of Spending                            | 36565.2   |
| Design Summary                                      |           |
| Number of Strata                                    | 3         |
| Variance Estimation                                 |           |
| Method                                              | Jackknife |
| Number of Replicates                                | 40        |

Output 94.9.2 displays the parameter estimates and their standard errors, as well as the tests of model effects that use the jackknife method.

**Output 94.9.2** Variance Estimation Using the Jackknife Method

| Tests of Model Effects |        |         |        |  |
|------------------------|--------|---------|--------|--|
| Effect                 | Num DF | F Value | Pr > F |  |
| Model                  | 4      | 110.48  | <.0001 |  |
| Intercept              | 1      | 133.30  | <.0001 |  |
| Income                 | 1      | 289.16  | <.0001 |  |
| Kids                   | 3      | 0.90    | 0.4525 |  |

NOTE: The denominator degrees of freedom for the F tests is 37.

| Estimated Regression Coefficients |            |                |         |         |
|-----------------------------------|------------|----------------|---------|---------|
| Parameter                         | Estimate   | Standard Error | t Value | Pr >  t |
| Intercept                         | -26.086882 | 2.58771182     | -10.08  | <.0001  |
| Income                            | 0.776699   | 0.04567521     | 17.00   | <.0001  |
| Kids 1                            | 0.888631   | 1.12799263     | 0.79    | 0.4358  |
| Kids 2                            | 1.545726   | 1.25598146     | 1.23    | 0.2262  |
| Kids 3                            | -0.526817  | 1.42555453     | -0.37   | 0.7138  |
| Kids 4                            | 0.000000   | 0.00000000     | .       | .       |

NOTE: The denominator degrees of freedom for the t tests is 37.  
 Matrix X'WX is singular and a generalized inverse was used to solve the normal equations. Estimates are not unique.

Output 94.9.3 prints the first 6 observation in the output data set JKWeights, which contains the replicate weights.

The data set JKWeights contains all the variable in the data set IceCream, in addition to the replicate weights variables named RepWt\_1, RepWt\_2, ..., RepWt\_40.

For example, the first observation (student) from stratum Grade=7 is deleted to create the first replicate. Therefore, stratum Grade=7 is the donor stratum for the first replicate, and the corresponding replicate weights are saved in the variable RepWt\_1.

Because the first observation is deleted in the first replicate, RepWt\_1=0 for the first observation. For observations from strata other than the donor stratum Grade=7, their replicate weights remain the same as in the variable Weight, while the rest of the observations in stratum Grade=7 are multiplied by the reciprocal of the corresponding jackknife coefficient, 0.95 for the first replicate.

**Output 94.9.3** The Jackknife Replicate Weights for the First 6 Observations

| The Jackknife Weights for the First 6 Obs |          |          |          |          |          |          |          |          |          |         |
|-------------------------------------------|----------|----------|----------|----------|----------|----------|----------|----------|----------|---------|
| Obs                                       | Grade    | Spending | Income   | Kids     | Prob     | Weight   | RepWt_1  | RepWt_2  | RepWt_3  | RepWt_4 |
| 1                                         | 7        | 7        | 39       | 2        | 0.010965 | 91.200   | 0.000    | 96.000   | 91.200   | 91.200  |
| 2                                         | 7        | 7        | 38       | 1        | 0.010965 | 91.200   | 96.000   | 0.000    | 91.200   | 91.200  |
| 3                                         | 8        | 12       | 47       | 1        | 0.008780 | 113.889  | 113.889  | 113.889  | 0.000    | 113.889 |
| 4                                         | 9        | 10       | 47       | 4        | 0.009557 | 104.636  | 104.636  | 104.636  | 104.636  | 0.000   |
| 5                                         | 7        | 1        | 34       | 4        | 0.010965 | 91.200   | 96.000   | 96.000   | 91.200   | 91.200  |
| 6                                         | 7        | 10       | 43       | 2        | 0.010965 | 91.200   | 96.000   | 96.000   | 91.200   | 91.200  |
| Obs                                       | RepWt_5  | RepWt_6  | RepWt_7  | RepWt_8  | RepWt_9  | RepWt_10 | RepWt_11 | RepWt_12 | RepWt_13 |         |
| 1                                         | 96.000   | 96.000   | 96.000   | 91.200   | 91.200   | 96.000   | 96.000   | 91.200   | 91.200   |         |
| 2                                         | 96.000   | 96.000   | 96.000   | 91.200   | 91.200   | 96.000   | 96.000   | 91.200   | 91.200   |         |
| 3                                         | 113.889  | 113.889  | 113.889  | 128.125  | 128.125  | 113.889  | 113.889  | 113.889  | 128.125  |         |
| 4                                         | 104.636  | 104.636  | 104.636  | 104.636  | 104.636  | 104.636  | 104.636  | 115.100  | 104.636  |         |
| 5                                         | 0.000    | 96.000   | 96.000   | 91.200   | 91.200   | 96.000   | 96.000   | 91.200   | 91.200   |         |
| 6                                         | 96.000   | 0.000    | 96.000   | 91.200   | 91.200   | 96.000   | 96.000   | 91.200   | 91.200   |         |
| Obs                                       | RepWt_14 | RepWt_15 | RepWt_16 | RepWt_17 | RepWt_18 | RepWt_19 | RepWt_20 | RepWt_21 | RepWt_22 |         |
| 1                                         | 96.000   | 96.000   | 96.000   | 91.200   | 91.200   | 91.200   | 91.200   | 91.200   | 91.200   |         |
| 2                                         | 96.000   | 96.000   | 96.000   | 91.200   | 91.200   | 91.200   | 91.200   | 91.200   | 91.200   |         |
| 3                                         | 113.889  | 113.889  | 113.889  | 113.889  | 128.125  | 128.125  | 113.889  | 113.889  | 113.889  |         |
| 4                                         | 104.636  | 104.636  | 104.636  | 115.100  | 104.636  | 104.636  | 115.100  | 115.100  | 115.100  |         |
| 5                                         | 96.000   | 96.000   | 96.000   | 91.200   | 91.200   | 91.200   | 91.200   | 91.200   | 91.200   |         |
| 6                                         | 96.000   | 96.000   | 96.000   | 91.200   | 91.200   | 91.200   | 91.200   | 91.200   | 91.200   |         |
| Obs                                       | RepWt_23 | RepWt_24 | RepWt_25 | RepWt_26 | RepWt_27 | RepWt_28 | RepWt_29 | RepWt_30 | RepWt_31 |         |
| 1                                         | 96.000   | 96.000   | 96.000   | 91.200   | 91.200   | 91.200   | 96.000   | 96.000   | 96.000   |         |
| 2                                         | 96.000   | 96.000   | 96.000   | 91.200   | 91.200   | 91.200   | 96.000   | 96.000   | 96.000   |         |
| 3                                         | 113.889  | 113.889  | 113.889  | 113.889  | 128.125  | 113.889  | 113.889  | 113.889  | 113.889  |         |
| 4                                         | 104.636  | 104.636  | 104.636  | 115.100  | 104.636  | 115.100  | 104.636  | 104.636  | 104.636  |         |
| 5                                         | 96.000   | 96.000   | 96.000   | 91.200   | 91.200   | 91.200   | 96.000   | 96.000   | 96.000   |         |
| 6                                         | 96.000   | 96.000   | 96.000   | 91.200   | 91.200   | 91.200   | 96.000   | 96.000   | 96.000   |         |
| Obs                                       | RepWt_32 | RepWt_33 | RepWt_34 | RepWt_35 | RepWt_36 | RepWt_37 | RepWt_38 | RepWt_39 | RepWt_40 |         |
| 1                                         | 96.000   | 91.200   | 91.200   | 91.200   | 96.000   | 91.200   | 91.200   | 96.000   | 96.000   |         |
| 2                                         | 96.000   | 91.200   | 91.200   | 91.200   | 96.000   | 91.200   | 91.200   | 96.000   | 96.000   |         |
| 3                                         | 113.889  | 113.889  | 128.125  | 128.125  | 113.889  | 113.889  | 113.889  | 113.889  | 113.889  |         |
| 4                                         | 104.636  | 115.100  | 104.636  | 104.636  | 104.636  | 115.100  | 115.100  | 104.636  | 104.636  |         |
| 5                                         | 96.000   | 91.200   | 91.200   | 91.200   | 96.000   | 91.200   | 91.200   | 96.000   | 96.000   |         |
| 6                                         | 96.000   | 91.200   | 91.200   | 91.200   | 96.000   | 91.200   | 91.200   | 96.000   | 96.000   |         |

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# Chapter 95

## The SURVEYSELECT Procedure

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## Overview: SURVEYSELECT Procedure

The SURVEYSELECT procedure provides a variety of methods for selecting probability-based random samples. The procedure can select a simple random sample or can sample according to a complex multistage sample design that includes stratification, clustering, and unequal probabilities of selection. With probability sampling, each unit in the survey population has a known, positive probability of selection. This property of probability sampling avoids selection bias and enables you to use statistical theory to make valid inferences from the sample to the survey population.

To select a sample with PROC SURVEYSELECT, you input a SAS data set that contains the sampling frame, which is the list of units from which the sample is to be selected. The sampling units can be individual observations or groups of observations (clusters). You also specify the selection method, the desired sample size or sampling rate, and other selection parameters. PROC SURVEYSELECT selects the sample and produces an output data set that contains the selected units, their selection probabilities, and their sampling weights. When you select a sample in multiple stages, you invoke the procedure separately for each stage of selection, inputting the frame and selection parameters for each current stage.

PROC SURVEYSELECT provides methods for both equal probability sampling and probability proportional to size (PPS) sampling. In equal probability sampling, each unit in the sampling frame, or in a stratum, has the same probability of being selected for the sample. In PPS sampling, a unit's selection probability is proportional to its size measure. For details about probability sampling methods, see Lohr (2010); Kish (1965, 1987); Kalton (1983); Cochran (1977).

PROC SURVEYSELECT provides the following equal probability sampling methods:

- simple random sampling (without replacement)
- unrestricted random sampling (with replacement)
- systematic random sampling
- sequential random sampling
- Bernoulli sampling

This procedure also provides Poisson sampling and the following probability proportional to size (PPS) sampling methods:

- PPS sampling without replacement
- PPS sampling with replacement
- PPS systematic sampling
- PPS algorithms for selecting two units per stratum
- sequential PPS sampling with minimum replacement

The procedure uses fast, efficient algorithms for these sample selection methods. Thus, it performs well even for large input data sets or sampling frames.

PROC SURVEYSELECT can perform stratified sampling by selecting samples independently within strata, which are nonoverlapping subgroups of the survey population. Stratification controls the distribution of the sample size in the strata. It is widely used in practice toward meeting a variety of survey objectives. For example, with stratification you can ensure adequate sample sizes for subgroups of interest, including small subgroups, or you can use stratification toward improving the precision of the overall estimates. When you use a systematic or sequential selection method, PROC SURVEYSELECT can also sort by control variables within strata for the additional control of implicit stratification.

For stratified sampling, PROC SURVEYSELECT provides survey design methods to allocate the total sample size among the strata. Available allocation methods include proportional, Neyman, and optimal allocation. Optimal allocation maximizes the estimation precision within the available resources, taking into account stratum sizes, costs, and variances.

PROC SURVEYSELECT provides replicated sampling, where the total sample is composed of a set of replicates, and each replicate is selected in the same way. You can use replicated sampling to study variable nonsampling errors, such as variability in the results obtained by different interviewers. You can also use replication to estimate standard errors for combined sample estimates and to perform a variety of other resampling and simulation tasks.

---

## Getting Started: SURVEYSELECT Procedure

In this example, an Internet service provider conducts a customer satisfaction survey. The survey population consists of the company's current subscribers. The company plans to select a sample of customers from this population, interview the selected customers, and then make inferences about the entire survey population from the sample data.

The SAS data set `Customers` contains the sampling frame, which is the list of units in the survey population. The sample of customers will be selected from this sampling frame. The data set `Customers` is constructed from the company's customer database. It contains one observation for each customer, with a total of 13,471 observations.



The following PROC PRINT statements display the first 10 observations of the data set Customers and produce Figure 95.1:

```
title1 'Customer Satisfaction Survey';
title2 'First 10 Observations';
proc print data=Customers(obs=10);
run;
```

**Figure 95.1** Customers Data Set (First 10 Observations)

| Customer Satisfaction Survey |             |       |      |       |  |
|------------------------------|-------------|-------|------|-------|--|
| First 10 Observations        |             |       |      |       |  |
| Obs                          | CustomerID  | State | Type | Usage |  |
| 1                            | 416-87-4322 | AL    | New  | 839   |  |
| 2                            | 288-13-9763 | GA    | Old  | 224   |  |
| 3                            | 339-00-8654 | GA    | Old  | 2451  |  |
| 4                            | 118-98-0542 | GA    | New  | 349   |  |
| 5                            | 421-67-0342 | FL    | New  | 562   |  |
| 6                            | 623-18-9201 | SC    | New  | 68    |  |
| 7                            | 324-55-0324 | FL    | Old  | 137   |  |
| 8                            | 832-90-2397 | AL    | Old  | 1563  |  |
| 9                            | 586-45-0178 | GA    | New  | 615   |  |
| 10                           | 801-24-5317 | SC    | New  | 728   |  |

In the SAS data set Customers, the variable CustomerID uniquely identifies each customer. The variable State contains the state of the customer's address. The company has customers in four states: Georgia (GA), Alabama (AL), Florida (FL), and South Carolina (SC). The variable Type equals 'Old' if the customer has subscribed to the service for more than one year; otherwise, the variable Type equals 'New'. The variable Usage contains the customer's average monthly service usage, in minutes.

The following sections illustrate the use of PROC SURVEYSELECT for probability sampling with three different designs for the customer satisfaction survey. All three designs are one-stage, with customers as the sampling units. The first design is simple random sampling without stratification. In the second design, customers are stratified by state and type, and the sample is selected by simple random sampling within strata. In the third design, customers are sorted within strata by usage, and the sample is selected by systematic random sampling within strata.

---

## Simple Random Sampling

The following PROC SURVEYSELECT statements select a probability sample of customers from the Customers data set by using simple random sampling:

```
title1 'Customer Satisfaction Survey';
title2 'Simple Random Sampling';
proc surveyselect data=Customers method=srs n=100
 out=SampleSRS;
run;
```

The PROC SURVEYSELECT statement invokes the procedure. The DATA= option names the SAS data set Customers as the input data set from which to select the sample. The METHOD=SRS option specifies simple random sampling as the sample selection method. In simple random sampling, each unit has an equal probability of selection, and sampling is without replacement. Without-replacement sampling means that a unit cannot be selected more than once. The N= option specifies a sample size of 100 customers. The OUT= option stores the sample in the SAS data set named SampleSRS.

Figure 95.2 displays the output from PROC SURVEYSELECT, which summarizes the sample selection. A sample of 100 customers is selected from the data set Customers by simple random sampling. With simple random sampling and no stratification in the sample design, the selection probability is the same for all units in the sample. In this sample, the selection probability for each customer equals 0.007423, which is the sample size (100) divided by the population size (13,471). The sampling weight equals 134.71 for each customer in the sample, where the weight is the inverse of the selection probability. If you specify the STATS option, PROC SURVEYSELECT includes the selection probabilities and sampling weights in the output data set. (This information is always included in the output data set for more complex designs.)

The random number seed is 39647. PROC SURVEYSELECT uses this number as the initial seed for random number generation. Because the SEED= option is not specified in the PROC SURVEYSELECT statement, the seed value is obtained by using the time of day from the computer's clock. You can specify SEED=39647 to reproduce this sample.

**Figure 95.2** Sample Selection Summary

| Customer Satisfaction Survey<br>Simple Random Sampling |                        |
|--------------------------------------------------------|------------------------|
| The SURVEYSELECT Procedure                             |                        |
| Selection Method                                       | Simple Random Sampling |
| Input Data Set                                         | CUSTOMERS              |
| Random Number Seed                                     | 39647                  |
| Sample Size                                            | 100                    |
| Selection Probability                                  | 0.007423               |
| Sampling Weight                                        | 134.71                 |
| Output Data Set                                        | SAMPLESRS              |

The sample of 100 customers is stored in the SAS data set SampleSRS. PROC SURVEYSELECT does not display this output data set. The following PROC PRINT statements display the first 20 observations of SampleSRS:

```

title1 'Customer Satisfaction Survey';
title2 'Sample of 100 Customers, Selected by SRS';
title3 '(First 20 Observations)';
proc print data=SampleSRS(obs=20);
run;

```

Figure 95.3 displays the first 20 observations of the output data set SampleSRS, which contains the sample of customers. This data set includes all the variables from the DATA= input data set Customers. If you do not want to include all variables, you can use the ID statement to specify which variables to copy from the input data set to the output (sample) data set.

**Figure 95.3** Customer Sample (First 20 Observations)

| Customer Satisfaction Survey<br>Sample of 100 Customers, Selected by SRS<br>(First 20 Observations) |             |       |      |       |
|-----------------------------------------------------------------------------------------------------|-------------|-------|------|-------|
| Obs                                                                                                 | CustomerID  | State | Type | Usage |
| 1                                                                                                   | 017-27-4096 | GA    | New  | 168   |
| 2                                                                                                   | 026-37-3895 | AL    | New  | 59    |
| 3                                                                                                   | 038-54-9276 | GA    | New  | 785   |
| 4                                                                                                   | 046-40-3131 | FL    | New  | 60    |
| 5                                                                                                   | 070-37-6924 | GA    | New  | 524   |
| 6                                                                                                   | 100-58-3342 | FL    | New  | 302   |
| 7                                                                                                   | 107-61-9029 | AL    | New  | 235   |
| 8                                                                                                   | 110-95-0432 | FL    | New  | 12    |
| 9                                                                                                   | 112-81-9251 | SC    | New  | 347   |
| 10                                                                                                  | 137-33-0478 | GA    | New  | 551   |
| 11                                                                                                  | 143-83-4677 | AL    | New  | 203   |
| 12                                                                                                  | 147-19-9164 | GA    | New  | 172   |
| 13                                                                                                  | 159-51-0606 | FL    | New  | 102   |
| 14                                                                                                  | 164-14-7799 | GA    | Old  | 388   |
| 15                                                                                                  | 165-05-7323 | SC    | New  | 606   |
| 16                                                                                                  | 174-69-3566 | AL    | Old  | 111   |
| 17                                                                                                  | 177-69-6934 | FL    | New  | 202   |
| 18                                                                                                  | 181-58-3508 | AL    | Old  | 261   |
| 19                                                                                                  | 207-41-8446 | AL    | Old  | 183   |
| 20                                                                                                  | 207-64-7308 | GA    | New  | 193   |

---

## Stratified Sampling

In this section, stratification is added to the sample design for the customer satisfaction survey. The sampling frame, which is the list of all customers, is stratified by State and Type. This divides the sampling frame into nonoverlapping subgroups formed from the values of the State and Type variables. Samples are then selected independently within the strata.

PROC SURVEYSELECT requires that the input data set be sorted by the STRATA variables. The following PROC SORT statements sort the Customers data set by the stratification variables State and Type:

```
proc sort data=Customers;
 by State Type;
run;
```

The following PROC FREQ statements display the crosstabulation of the Customers data set by State and Type:

```
title1 'Customer Satisfaction Survey';
title2 'Strata of Customers';
proc freq data=Customers;
 tables State*Type;
run;
```

Figure 95.4 presents the table of State by Type for the 13,471 customers. There are four states and two levels of Type, forming a total of eight strata.

**Figure 95.4** Stratification of Customers by State and Type

| Customer Satisfaction Survey   |       |       |        |
|--------------------------------|-------|-------|--------|
| Strata of Customers            |       |       |        |
| The FREQ Procedure             |       |       |        |
| Table of State by Type         |       |       |        |
| State                          | Type  |       |        |
| Frequency                      |       |       |        |
| Percent                        |       |       |        |
| Row Pct                        |       |       |        |
| Col Pct                        | New   | Old   | Total  |
| -----+-----+-----+-----+-----+ |       |       |        |
| AL                             | 1238  | 706   | 1944   |
|                                | 9.19  | 5.24  | 14.43  |
|                                | 63.68 | 36.32 |        |
|                                | 14.43 | 14.43 |        |
| -----+-----+-----+-----+-----+ |       |       |        |
| FL                             | 2170  | 1370  | 3540   |
|                                | 16.11 | 10.17 | 26.28  |
|                                | 61.30 | 38.70 |        |
|                                | 25.29 | 28.01 |        |
| -----+-----+-----+-----+-----+ |       |       |        |
| GA                             | 3488  | 1940  | 5428   |
|                                | 25.89 | 14.40 | 40.29  |
|                                | 64.26 | 35.74 |        |
|                                | 40.65 | 39.66 |        |
| -----+-----+-----+-----+-----+ |       |       |        |
| SC                             | 1684  | 875   | 2559   |
|                                | 12.50 | 6.50  | 19.00  |
|                                | 65.81 | 34.19 |        |
|                                | 19.63 | 17.89 |        |
| -----+-----+-----+-----+-----+ |       |       |        |
| Total                          | 8580  | 4891  | 13471  |
|                                | 63.69 | 36.31 | 100.00 |

The following PROC SURVEYSELECT statements select a probability sample of customers from the Customers data set according to the stratified sample design:

```

title1 'Customer Satisfaction Survey';
title2 'Stratified Sampling';
proc surveyselect data=Customers method=srs n=15
 seed=1953 out=SampleStrata;
 strata State Type;
run;

```

The STRATA statement names the stratification variables State and Type. In the PROC SURVEYSELECT statement, the METHOD=SRS option specifies simple random sampling. The N= option specifies a sample size of 15 customers for each stratum. If you want to specify different sample sizes for different strata, you can use the N=SAS-*data-set* option to name a secondary data set that contains the stratum sample sizes. The SEED= option specifies 1953 as the initial seed for random number generation.

Figure 95.5 displays the output from PROC SURVEYSELECT, which summarizes the sample selection. A total of 120 customers are selected.

**Figure 95.5** Sample Selection Summary

| Customer Satisfaction Survey<br>Stratified Sampling |                        |
|-----------------------------------------------------|------------------------|
| The SURVEYSELECT Procedure                          |                        |
| Selection Method                                    | Simple Random Sampling |
| Strata Variables                                    | State<br>Type          |
| Input Data Set                                      | CUSTOMERS              |
| Random Number Seed                                  | 1953                   |
| Stratum Sample Size                                 | 15                     |
| Number of Strata                                    | 8                      |
| Total Sample Size                                   | 120                    |
| Output Data Set                                     | SAMPLESTRATA           |

The following PROC PRINT statements display the first 30 observations of the output data set SampleStrata:

```

title1 'Customer Satisfaction Survey';
title2 'Sample Selected by Stratified Design';
title3 '(First 30 Observations)';
proc print data=SampleStrata(obs=30);
run;

```

Figure 95.6 displays the first 30 observations of the output data set SampleStrata, which contains the sample of 120 customers, 15 customers from each of the eight strata. The variable SelectionProb contains the selection probability for each customer in the sample. Because customers are selected with equal probability within strata in this design, the selection probability equals the stratum sample size (15) divided by the stratum population size. The selection probabilities differ from stratum to stratum because the stratum population sizes differ. The selection probability for each customer in the first stratum (State='AL' and Type='New') is 0.012116, and the selection probability for customers in the second stratum is 0.021246. The variable SamplingWeight contains the sampling weights, which are computed as inverse selection probabilities.

**Figure 95.6** Customer Sample (First 30 Observations)

| Customer Satisfaction Survey<br>Sample Selected by Stratified Design<br>(First 30 Observations) |       |      |             |       |                |                 |
|-------------------------------------------------------------------------------------------------|-------|------|-------------|-------|----------------|-----------------|
| Obs                                                                                             | State | Type | CustomerID  | Usage | Selection Prob | Sampling Weight |
| 1                                                                                               | AL    | New  | 015-57-9903 | 26    | 0.012116       | 82.5333         |
| 2                                                                                               | AL    | New  | 052-18-5029 | 576   | 0.012116       | 82.5333         |
| 3                                                                                               | AL    | New  | 064-72-0145 | 88    | 0.012116       | 82.5333         |
| 4                                                                                               | AL    | New  | 291-22-2497 | 1221  | 0.012116       | 82.5333         |
| 5                                                                                               | AL    | New  | 305-62-6833 | 187   | 0.012116       | 82.5333         |
| 6                                                                                               | AL    | New  | 309-63-9722 | 534   | 0.012116       | 82.5333         |
| 7                                                                                               | AL    | New  | 413-76-0209 | 435   | 0.012116       | 82.5333         |
| 8                                                                                               | AL    | New  | 492-18-7867 | 70    | 0.012116       | 82.5333         |
| 9                                                                                               | AL    | New  | 508-16-8324 | 189   | 0.012116       | 82.5333         |
| 10                                                                                              | AL    | New  | 561-82-0366 | 392   | 0.012116       | 82.5333         |
| 11                                                                                              | AL    | New  | 685-24-1718 | 74    | 0.012116       | 82.5333         |
| 12                                                                                              | AL    | New  | 800-20-2155 | 21    | 0.012116       | 82.5333         |
| 13                                                                                              | AL    | New  | 857-94-2672 | 77    | 0.012116       | 82.5333         |
| 14                                                                                              | AL    | New  | 918-29-9618 | 540   | 0.012116       | 82.5333         |
| 15                                                                                              | AL    | New  | 963-93-4916 | 33    | 0.012116       | 82.5333         |
| 16                                                                                              | AL    | Old  | 000-88-0484 | 401   | 0.021246       | 47.0667         |
| 17                                                                                              | AL    | Old  | 005-80-0241 | 114   | 0.021246       | 47.0667         |
| 18                                                                                              | AL    | Old  | 171-99-9085 | 210   | 0.021246       | 47.0667         |
| 19                                                                                              | AL    | Old  | 182-45-1938 | 160   | 0.021246       | 47.0667         |
| 20                                                                                              | AL    | Old  | 208-99-1105 | 60    | 0.021246       | 47.0667         |
| 21                                                                                              | AL    | Old  | 229-48-6213 | 1169  | 0.021246       | 47.0667         |
| 22                                                                                              | AL    | Old  | 265-55-4763 | 1370  | 0.021246       | 47.0667         |
| 23                                                                                              | AL    | Old  | 467-73-7465 | 14    | 0.021246       | 47.0667         |
| 24                                                                                              | AL    | Old  | 509-38-7128 | 173   | 0.021246       | 47.0667         |
| 25                                                                                              | AL    | Old  | 601-71-3629 | 142   | 0.021246       | 47.0667         |
| 26                                                                                              | AL    | Old  | 603-40-7787 | 302   | 0.021246       | 47.0667         |
| 27                                                                                              | AL    | Old  | 702-39-0977 | 270   | 0.021246       | 47.0667         |
| 28                                                                                              | AL    | Old  | 861-79-5340 | 101   | 0.021246       | 47.0667         |
| 29                                                                                              | AL    | Old  | 908-20-0603 | 340   | 0.021246       | 47.0667         |
| 30                                                                                              | AL    | Old  | 937-69-9106 | 182   | 0.021246       | 47.0667         |

## Stratified Sampling with Control Sorting

The next sample design for the customer satisfaction survey uses stratification by State and also control sorting by Type and Usage within State. After stratification and control sorting, customers are selected by systematic random sampling within strata. Selection by systematic sampling, together with control sorting before selection, spreads the sample uniformly over the range of type and usage values within each stratum (state). The following PROC SURVEYSELECT statements select a probability sample of customers from the Customers data set according to this design:

```

title1 'Customer Satisfaction Survey';
title2 'Stratified Sampling with Control Sorting';
proc surveyselect data=Customers method=sys rate=.02
 seed=1234 out=SampleControl;
 strata State;
 control Type Usage;
run;

```

The STRATA statement names the stratification variable State. The CONTROL statement names the control variables Type and Usage. In the PROC SURVEYSELECT statement, the METHOD=SYS option requests systematic random sampling. The RATE= option specifies a sampling rate of 2% for each stratum. The SEED= option specifies the initial seed for random number generation.

Figure 95.7 displays the output from PROC SURVEYSELECT, which summarizes the sample selection. A sample of 271 customers is selected by using systematic random sampling within strata determined by State. The sampling frame Customers is sorted by control variables Type and Usage within strata. The type of sorting is serpentine, which is the default when SORT=NEST is not specified. See the section “Sorting by CONTROL Variables” on page 8057 for a description of serpentine sorting. The sorted data set replaces the input data set. (To leave the input data set unsorted and store the sorted input data in another data set, use the OUTSORT= option.) The output data set SampleControl contains the sample of customers.

**Figure 95.7** Sample Selection Summary

|                                          |                            |
|------------------------------------------|----------------------------|
| Customer Satisfaction Survey             |                            |
| Stratified Sampling with Control Sorting |                            |
| The SURVEYSELECT Procedure               |                            |
| Selection Method                         | Systematic Random Sampling |
| Strata Variable                          | State                      |
| Control Variables                        | Type<br>Usage              |
| Control Sorting                          | Serpentine                 |
| Input Data Set                           | CUSTOMERS                  |
| Random Number Seed                       | 1234                       |
| Stratum Sampling Rate                    | 0.02                       |
| Number of Strata                         | 4                          |
| Total Sample Size                        | 270                        |
| Output Data Set                          | SAMPLECONTROL              |

---

## Syntax: SURVEYSELECT Procedure

The following statements are available in the SURVEYSELECT procedure:

```
PROC SURVEYSELECT options ;
 CONTROL variables ;
 FREQ variable ;
 ID variables ;
 SAMPLINGUNIT | CLUSTER variables </ options > ;
 SIZE variable ;
 STRATA variables </ options > ;
```

The **PROC SURVEYSELECT** statement invokes the SURVEYSELECT procedure. Optionally, it identifies input and output data sets. It also specifies the selection method, the sample size, and other sample design parameters. The **PROC SURVEYSELECT** statement is required.

The **SIZE** statement identifies the variable that contains the size measures of the sampling units. This statement is required for any probability proportional to size (PPS) selection method unless you specify the **PPS** option in the **SAMPLINGUNIT** statement.

The remaining statements are optional. The **STRATA** statement identifies a variable or set of variables that stratify the input data set. When you specify a **STRATA** statement, **PROC SURVEYSELECT** selects samples independently from the strata that are formed by the **STRATA** variables. The **STRATA** statement also provides options to allocate the total sample size among the strata.

The **SAMPLINGUNIT** statement identifies a variable or set of variables that group the input data set observations into sampling units (clusters). Sampling units are nested within strata. When you specify a **SAMPLINGUNIT** statement, **PROC SURVEYSELECT** selects clusters instead of individual observations.

The **CONTROL** statement identifies variables for ordering units within strata. It can be used for systematic and sequential sampling methods. The **ID** statement identifies variables to copy from the input data set to the output data set of selected units.

The **FREQ** statement identifies a variable that contains the frequency of occurrence for each observation. The **FREQ** statement is available only for sample allocation when no sample is selected, which you can request by specifying the **ALLOC=** and **NOSAMPLE** options in the **STRATA** statement.

The rest of this section gives detailed syntax information for the **CONTROL**, **FREQ**, **ID**, **SAMPLINGUNIT**, **SIZE**, and **STRATA** statements in alphabetical order after the description of the **PROC SURVEYSELECT** statement.

---

## PROC SURVEYSELECT Statement

```
PROC SURVEYSELECT options ;
```

The **PROC SURVEYSELECT** statement invokes the SURVEYSELECT procedure. Optionally, it identifies input and output data sets. If you do not name a **DATA=** input data set, the procedure selects the sample from the most recently created SAS data set. If you do not name an **OUT=** output data set to contain the sample of selected units, the procedure still creates an output data set and names it according to the **DATA<sub>n</sub>** convention.



The PROC SURVEYSELECT statement also specifies the sample selection method, the sample size, and other sample design parameters.

If you do not specify a selection method, PROC SURVEYSELECT uses simple random sampling (**METHOD=SRS**) by default unless you specify a **SIZE** statement or the **PPS** option in the **SAMPLINGUNIT** statement. If you do specify a **SIZE** statement (or the **PPS** option), PROC SURVEYSELECT uses probability proportional to size selection without replacement (**METHOD=PPS**) by default. See the description of the **METHOD=** option for more information.

You must specify the sample size or sampling rate except when you request Poisson sampling (**METHOD=POISSON**), request a method that selects two units from each stratum (**METHOD=PPS\_BREWER** or **METHOD=PPS\_MURTHY**), or specify the **MARGIN=** option in the **STRATA** statement for sample allocation. You can use the **SAMPSIZE=*n*** option to specify the sample size, or you can use the **SAMPSIZE=SAS-data-set** option to name a secondary input data set that contains stratum sample sizes.

You can also provide stratum sampling rates, minimum size measures, maximum size measures, and certainty size measures in the secondary input data set. See the descriptions of the **SAMPSIZE=**, **SAMPRATE=**, **MINSIZE=**, **MAXSIZE=**, **CERTSIZE=**, and **CERTSIZE=P=** options for more information. You can name only one secondary input data set in each invocation of the procedure. See the section “Secondary Input Data Set” on page 8071 for details.

Table 95.1 summarizes the *options* available in the PROC SURVEYSELECT statement. Descriptions of the *options* follow in alphabetical order.

**Table 95.1** PROC SURVEYSELECT Statement Options

| Option                            | Description                                                        |
|-----------------------------------|--------------------------------------------------------------------|
| <b>Input and Output Data Sets</b> |                                                                    |
| <b>DATA=</b>                      | Names the input SAS data set                                       |
| <b>OUT=</b>                       | Names the output SAS data set that contains the sample             |
| <b>OUTSORT=</b>                   | Names an output SAS data set that stores the sorted input data set |
| <b>Selection Method</b>           |                                                                    |
| <b>METHOD=</b>                    | Specifies the sample selection method                              |
| <b>Sample Size</b>                |                                                                    |
| <b>SAMPSIZE=</b>                  | Specifies the sample size                                          |
| <b>SELECTALL</b>                  | Selects all stratum units when the sample size exceeds the total   |
| <b>Sampling Rate</b>              |                                                                    |
| <b>SAMPRATE=</b>                  | Specifies the sampling rate                                        |
| <b>NMIN=</b>                      | Specifies the minimum stratum sample size                          |
| <b>NMAX=</b>                      | Specifies the maximum stratum sample size                          |
| <b>Replicated Sampling</b>        |                                                                    |
| <b>REPS=</b>                      | Specifies the number of sample replicates                          |
| <b>Size Measures</b>              |                                                                    |
| <b>MINSIZE=</b>                   | Specifies the minimum size measure                                 |
| <b>MAXSIZE=</b>                   | Specifies the maximum size measure                                 |
| <b>CERTSIZE=</b>                  | Specifies the certainty size measure                               |
| <b>CERTSIZE=P=</b>                | Specifies the certainty proportion                                 |

Table 95.1 *continued*

| Option                          | Description                                               |
|---------------------------------|-----------------------------------------------------------|
| <b>Control Sorting</b>          |                                                           |
| <b>SORT=</b>                    | Specifies the type of sorting                             |
| <b>Random Number Generation</b> |                                                           |
| <b>SEED=</b>                    | Specifies the initial seed                                |
| <b>RANUNI</b>                   | Requests the RANUNI random number generator               |
| <b>Displayed Output</b>         |                                                           |
| <b>NOPRINT</b>                  | Suppresses the display of all output                      |
| <b>OUT= Data Set Contents</b>   |                                                           |
| <b>JTPROBS</b>                  | Includes joint probabilities of selection                 |
| <b>OUTALL</b>                   | Includes all observations from the DATA= input data set   |
| <b>OUTHITS</b>                  | Includes a distinct copy of each selected unit            |
| <b>OUTSEED</b>                  | Includes the initial seed for each stratum                |
| <b>OUTSIZE</b>                  | Includes additional design and sampling frame information |
| <b>STATS</b>                    | Includes selection probabilities and sampling weights     |

You can specify the following *options* in the PROC SURVEYSELECT statement:

### **CERTSIZE**

requests certainty selection, where the certainty size values are provided in the secondary input data set. Use the CERTSIZE option when you have already named the secondary data set in another option, such as the **SAMPSIZE=SAS-data-set** option. See the section “Secondary Input Data Set” on page 8071 for details.

The CERTSIZE option is available for **METHOD=PPS** and **METHOD=PPS\_SAMPFORD**. The CERTSIZE option is not available with the **SAMPLINGUNIT** statement.

In certainty selection, PROC SURVEYSELECT automatically selects all sampling units that have size measures greater than or equal to the stratum certainty size values. After identifying the certainty units, PROC SURVEYSELECT selects the remainder of the sample according to the method that is specified in the **METHOD=** option.

You provide the stratum certainty size values in the secondary input data set variable **\_CERTSIZE\_**. Each certainty size value must be a positive number. The variable **Certain** in the **OUT=** data set identifies the certainty selections, which have selection probabilities equal to 1.

If you want to specify a single certainty size value for all strata, you can use the **CERTSIZE=certain** option.

### **CERTSIZE=certain**

specifies the certainty size value, which must be a positive number. PROC SURVEYSELECT automatically selects all sampling units that have size measures greater than or equal to the value *certain*. After identifying the certainty units, PROC SURVEYSELECT selects the remainder of the sample according to the method that is specified in the **METHOD=** option.

The **CERTSIZE=** option is available for **METHOD=PPS** and **METHOD=PPS\_SAMPFORD**. The **CERTSIZE=** option is not available with the **SAMPLINGUNIT** statement.

The variable **Certain** in the **OUT=** data set identifies the certainty selections, which have selection probabilities equal to 1.

If you request a stratified sample design with the **STRATA** statement and specify the **CERTSIZE=certain** option, PROC SURVEYSELECT uses the value *certain* for all strata. If you do not want to use the same certainty size for all strata, use the **CERTSIZE=SAS-data-set** option to specify a certainty size value for each stratum.

#### **CERTSIZE=SAS-data-set**

names a SAS data set that contains certainty size values for the strata. PROC SURVEYSELECT automatically selects all sampling units that have size measures greater than or equal to the stratum certainty size values. After identifying the certainty units, PROC SURVEYSELECT selects the remainder of the sample according to the method that is specified in the **METHOD=** option.

The **CERTSIZE=** option is available for **METHOD=PPS** and **METHOD=PPS\_SAMPFORD**. The **CERTSIZE=** option is not available with the **SAMPLINGUNIT** statement.

You provide the stratum certainty size values in the **CERTSIZE=** data set variable **\_CERTSIZE\_**. Each certainty size value must be a positive number. The variable **Certain** in the **OUT=** data set identifies the certainty selections, which have selection probabilities equal to 1.

The **CERTSIZE=** input data set should contain all the **STRATA** variables, with the same type and length as in the **DATA=** data set. The **STRATA** groups should appear in the same order in the **CERTSIZE=** data set as in the **DATA=** data set. The **CERTSIZE=** data set must include a variable named **\_CERTSIZE\_** that contains the certainty size value for each stratum. The **CERTSIZE=** data set is a secondary input data set. See the section “**Secondary Input Data Set**” on page 8071 for details. You can name only one secondary input data set in each invocation of the procedure.

If you want to specify a single certainty size value for all strata, you can use the **CERTSIZE=certain** option.

#### **CERTSIZE=P**

requests certainty proportion selection, where the stratum certainty proportions are provided in the secondary input data set. Use the **CERTSIZE=P** option when you have already named the secondary data set in another option, such as the **SAMPSIZE=SAS-data-set** option. See the section “**Secondary Input Data Set**” on page 8071 for details.

The **CERTSIZE=P** option is available for **METHOD=PPS** and **METHOD=PPS\_SAMPFORD**. The **CERTSIZE=P** option is not available with the **SAMPLINGUNIT** statement.

In certainty proportion selection, PROC SURVEYSELECT automatically selects all sampling units that have size measures greater than or equal to the stratum certainty proportion of the total stratum size. The procedure repeats this process with the remaining units until no more certainty units are selected. After identifying the certainty units, PROC SURVEYSELECT selects the remainder of the sample according to the method that is specified in the **METHOD=** option.

You provide the stratum certainty proportions in the secondary input data set variable **\_CERTP\_**. Each certainty proportion must be a positive number. You can specify a proportion value as a number between 0 and 1. Or you can specify a proportion value in percentage form as a number between 1 and 100, and PROC SURVEYSELECT converts that number to a proportion. The procedure treats the value 1 as 100% instead of 1%.

The variable **Certain** in the **OUT=** data set identifies the certainty selections, which have selection probabilities equal to 1.

If you want to specify a single certainty proportion for all strata, you can use the **CERTSIZE=P=p** option.

**CERTSIZE=P= $\rho$** 

specifies the certainty proportion. PROC SURVEYSELECT automatically selects all sampling units that have size measures greater than or equal to the proportion  $\rho$  of the total stratum size. The procedure repeats this process with the remaining units until no more certainty units are selected. After identifying the certainty units, PROC SURVEYSELECT selects the remainder of the sample according to the method that is specified in the **METHOD=** option.

The CERTSIZE=P= option is available for **METHOD=PPS** and **METHOD=PPS\_SAMPFORD**. The CERTSIZE=P= option is not available with the **SAMPLINGUNIT** statement.

The value of the certainty proportion  $\rho$  must be a positive number. You can specify  $\rho$  as a number between 0 and 1. Or you can specify  $\rho$  in percentage form as a number between 1 and 100, and PROC SURVEYSELECT converts that number to a proportion. The procedure treats the value 1 as 100% instead of 1%.

The variable **Certain** in the **OUT=** data set identifies the certainty selections, which have selection probabilities equal to 1.

If you request a stratified sample design with the **STRATA** statement and specify the CERTSIZE=P= $\rho$  option, PROC SURVEYSELECT uses the certainty proportion  $\rho$  for all strata. If you do not want to use the same certainty proportion for all strata, use the **CERTSIZE=P=SAS-data-set** option to specify a certainty proportion for each stratum.

**CERTSIZE=P=SAS-data-set**

names a SAS data set that contains certainty proportions for the strata. PROC SURVEYSELECT automatically selects all sampling units with size measures greater than or equal to the certainty proportion of the total stratum size. The procedure repeats this process with the remaining units until no more certainty units are selected. After identifying the certainty units, PROC SURVEYSELECT selects the remainder of the sample according to the method that is specified in the **METHOD=** option.

The CERTSIZE=P= option is available for **METHOD=PPS** and **METHOD=PPS\_SAMPFORD**. The CERTSIZE=P= option is not available with the **SAMPLINGUNIT** statement.

You provide the stratum certainty proportions in the CERTSIZE=P= data set variable **\_CERTP\_**. Each certainty proportion must be a positive number. You can specify a proportion value as a number between 0 and 1. Or you can specify a proportion value in percentage form as a number between 1 and 100, and PROC SURVEYSELECT converts that number to a proportion. The procedure treats the value 1 as 100% instead of 1%.

The variable **Certain** in the **OUT=** data set identifies the certainty selections, which have selection probabilities equal to 1.

The CERTSIZE=P= input data set should contain all the **STRATA** variables, with the same type and length as in the **DATA=** data set. The **STRATA** groups should appear in the same order in the CERTSIZE=P= data set as in the **DATA=** data set. The CERTSIZE=P= data set must include a variable named **\_CERTP\_** that contains the certainty proportion for each stratum. The CERTSIZE=P= data set is a secondary input data set. See the section “**Secondary Input Data Set**” on page 8071 for details. You can name only one secondary input data set in each invocation of the procedure.

If you want to specify a single certainty proportion for all strata, you can use the **CERTSIZE=P= $\rho$**  option.

**DATA=SAS-data-set**

names the SAS data set from which PROC SURVEYSELECT selects the sample. If you omit the DATA= option, the procedure uses the most recently created SAS data set. In sampling terminology, the input data set is the *sampling frame* (the list of units from which the sample is selected).

By default, the procedure uses input data set observations as sampling units and selects a sample of these units. Alternatively, you can use the **SAMPLINGUNIT** statement to define sampling units as groups of observations (clusters).

**JTPROBS**

includes joint probabilities of selection in the OUT= output data set. This option is available for the following probability proportional to size selection methods: **METHOD=PPS**, **METHOD=PPS\_SAMPFORD**, and **METHOD=PPS\_WR**. By default, PROC SURVEYSELECT outputs joint selection probabilities for **METHOD=PPS\_BREWER** and **METHOD=PPS\_MURTHY**, which select two units per stratum.

For details about computation of joint selection probabilities for a particular sampling method, see the method description in the section “[Sample Selection Methods](#)” on page 8058. For more information about the contents of the output data set, see the section “[Sample Output Data Set](#)” on page 8072.

**MAXSIZE**

requests adjustment of size measures according to the stratum maximum size values provided in the secondary input data set. Use the MAXSIZE option when you have already named the secondary input data set in another option, such as the **SAMPSIZE=SAS-data-set** option. See the section “[Secondary Input Data Set](#)” on page 8071 for details.

The MAXSIZE option is available when you use size measures for any PPS selection method and also include a **STRATA** statement. You provide size measures by specifying the **SIZE** statement or the **PPS** option in the **SAMPLINGUNIT** statement.

You provide the stratum maximum size values in the secondary input data set variable **\_MAXSIZE\_**. Each maximum size value must be a positive number.

When a size measure exceeds the specified maximum value for its stratum, PROC SURVEYSELECT adjusts the size measure downward to equal the maximum size value. If your sampling units are individual observations, the variable **AdjustedSize** in the OUT= data set contains the adjusted size measures.

If you use a **SAMPLINGUNIT** statement to define sampling units (clusters), then the procedure applies the MAXSIZE adjustment to the sampling unit size. The sampling unit size equals the number of observations in the sampling unit if you specify the **PPS** option, or the sum of the observation size measures if you specify a **SIZE** statement. The output data set variable **UnitSize** contains the adjusted sampling unit size measures.

If you want to specify a single maximum size value for all strata, you can use the **MAXSIZE=max** option.

**MAXSIZE=max**

specifies the maximum size value. The value of *max* must be a positive number.

When a size measure exceeds the value *max*, PROC SURVEYSELECT adjusts the size measure downward to equal *max*. If your sampling units are individual observations, the variable **AdjustedSize** in the OUT= data set contains the adjusted size measures.

If you use a **SAMPLINGUNIT** statement to define sampling units (clusters), then the procedure applies the **MAXSIZE** adjustment to the sampling unit size. The sampling unit size equals the number of observations in the sampling unit if you specify the **PPS** option, or the sum of the observation size measures if you specify a **SIZE** statement. The output data set variable **UnitSize** contains the adjusted sampling unit size measures.

The **MAXSIZE=***max* option is available when you use size measures for any PPS selection method. You provide size measures by specifying the **SIZE** statement or the **PPS** option in the **SAMPLINGUNIT** statement.

If you request a stratified sample design with the **STRATA** statement and specify the **MAXSIZE=***max* option, PROC SURVEYSELECT uses the maximum size *max* for all strata. If you do not want to use the same maximum size for all strata, use the **MAXSIZE=***SAS-data-set* option to specify a maximum size value for each stratum.

#### **MAXSIZE=***SAS-data-set*

names a SAS data set that contains maximum size values for the strata. You provide the stratum maximum size values in the **MAXSIZE=** data set variable **\_MAXSIZE\_**. Each maximum size value must be a positive number.

The **MAXSIZE=***SAS-data-set* option is available when you use size measures for any PPS selection method and also include a **STRATA** statement. You provide size measures by specifying the **SIZE** statement or the **PPS** option in the **SAMPLINGUNIT** statement.

When a size measure exceeds the maximum size value for its stratum, PROC SURVEYSELECT adjusts the size measure downward to equal the maximum size value. If your sampling units are individual observations, the variable **AdjustedSize** in the **OUT=** data set contains the adjusted size measures.

If you use a **SAMPLINGUNIT** statement to define sampling units (clusters), then the procedure applies the **MAXSIZE** adjustment to the sampling unit size. The sampling unit size equals the number of observations in the sampling unit if you specify the **PPS** option, or the sum of the observation size measures if you specify a **SIZE** statement. The output data set variable **UnitSize** contains the adjusted sampling unit size measures.

The **MAXSIZE=** input data set should contain all the **STRATA** variables, with the same type and length as in the **DATA=** data set. The **STRATA** groups should appear in the same order in the **MAXSIZE=** data set as in the **DATA=** data set. The **MAXSIZE=** data set must include a variable named **\_MAXSIZE\_** that contains the maximum size value for each stratum. The **MAXSIZE=** data set is a secondary input data set. See the section “**Secondary Input Data Set**” on page 8071 for details. You can name only one secondary input data set in each invocation of the procedure.

If you want to specify a single maximum size value for all strata, you can use the **MAXSIZE=***max* option.

#### **METHOD=***name*

##### **M=***name*

specifies the method for sample selection.

If you do not specify the **METHOD=** option, PROC SURVEYSELECT uses simple random sampling (**METHOD=****SRS**) by default unless you specify a **SIZE** statement or the **PPS** option in the **SAMPLINGUNIT** statement. If you do specify a **SIZE** statement (or the **PPS** option), PROC SURVEYSELECT uses probability proportional to size selection without replacement (**METHOD=****PPS**) by default.



The following values are available for the METHOD= option:

### **BERNOULLI**

requests Bernoulli sampling, which consists of  $N$  independent selection trials, each with constant inclusion probability  $\pi$ , where  $N$  is the total number of sampling units in the stratum or data set. The sample size is not fixed but is a random variable. See the section “[Bernoulli Sampling](#)” on page 8061 for details.

When you specify METHOD=BERNOULLI, you must provide the sampling rate (inclusion probability  $\pi$ ) by using the SAMPRATE= option. For stratified sampling (which you request with the STRATA statement), you can specify the same sampling rate for each stratum with the SAMPRATE= $r$  option. Or you can specify different sampling rates for different strata by using the SAMPRATE=(*values*) or SAMPRATE=SAS-data-set option.

Because Bernoulli sampling is based on a specified inclusion probability instead of a fixed sample size, METHOD=BERNOULLI does not use the SAMPSIZE= option. Also, the ALLOC= option in the STRATA statement (which allocates the total sample size among strata) is not available with METHOD=BERNOULLI.

### **POISSON**

requests Poisson sampling. A generalization of Bernoulli sampling, Poisson sampling consists of  $N$  independent selection trials with a separate inclusion probability specified for each unit, where  $N$  is the total number of sampling units in the stratum or data set. The sample size is not fixed but is a random variable. See the section “[Poisson Sampling](#)” on page 8062 for details.

You must provide inclusion probabilities for Poisson sampling in the SIZE variable. The probability values should be between 0 and 1. If a value of the SIZE variable is missing, nonpositive, or greater than 1, PROC SURVEYSELECT omits the observation from sample selection.

Because Poisson sampling is based on specified inclusion probabilities instead of a fixed sample size, METHOD=POISSON does not use the SAMPSIZE= option. Also, the ALLOC= option in the STRATA statement (which allocates the total sample size among strata) is not available with METHOD=POISSON.

The SAMPLINGUNIT statement is not available with METHOD=POISSON.

When METHOD=POISSON is specified with the SAMPRATE= option and without a SIZE statement, PROC SURVEYSELECT uses METHOD=BERNOULLI.

### **PPS**

requests selection with probability proportional to size and without replacement. See the section “[PPS Sampling without Replacement](#)” on page 8062 for details. If you specify METHOD=PPS, you must name a size measure variable in the SIZE statement or specify the PPS option in the SAMPLINGUNIT statement.

### **PPS\_BREWER | BREWER**

requests selection according to Brewer’s method. Brewer’s method selects two units from each stratum with probability proportional to size and without replacement. See the section “[Brewer’s PPS Method](#)” on page 8066 for details. If you specify METHOD=PPS\_BREWER, you must name a size measure variable in the SIZE statement or specify the PPS option in the SAMPLINGUNIT statement. You do not need to specify the sample size with the SAMPSIZE= option because Brewer’s method selects two units from each stratum.

**PPS\_MURTHY | MURTHY**

requests selection according to Murthy's method. Murthy's method selects two units from each stratum with probability proportional to size and without replacement. See the section “[Murthy's PPS Method](#)” on page 8066 for details. If you specify `METHOD=PPS_MURTHY`, you must name a size measure variable in the `SIZE` statement or specify the `PPS` option in the `SAMPLINGUNIT` statement. You do not need to specify the sample size with the `SAMPsize=` option because Murthy's method selects two units from each stratum.

**PPS\_SAMPFORD | SAMPFORD**

requests selection according to Sampford's method. Sampford's method selects units with probability proportional to size and without replacement. See the section “[Sampford's PPS Method](#)” on page 8067 for details. If you specify `METHOD=PPS_SAMPFORD`, you must name a size measure variable in the `SIZE` statement or specify the `PPS` option in the `SAMPLINGUNIT` statement.

**PPS\_SEQ | CHROMY**

requests sequential selection with probability proportional to size and with minimum replacement. This method is also known as Chromy's method. See the section “[PPS Sequential Sampling](#)” on page 8064 for details. If you specify `METHOD=PPS_SEQ`, you must name a size measure variable in the `SIZE` statement or specify the `PPS` option in the `SAMPLINGUNIT` statement.

**PPS\_SYS**

requests systematic selection with probability proportional to size. See the section “[PPS Systematic Sampling](#)” on page 8064 for details. If you specify `METHOD=PPS_SYS`, you must name a size measure variable in the `SIZE` statement or specify the `PPS` option in the `SAMPLINGUNIT` statement.

**PPS\_WR**

requests selection with probability proportional to size and with replacement. See the section “[PPS Sampling with Replacement](#)” on page 8064 for details. If you specify `METHOD=PPS_WR`, you must name a size measure variable in the `SIZE` statement or specify the `PPS` option in the `SAMPLINGUNIT` statement.

**SEQ**

requests sequential selection according to Chromy's method. If you specify `METHOD=SEQ` and do not specify a `SIZE` statement (or the `PPS` option in the `SAMPLINGUNIT` statement), PROC SURVEYSELECT uses sequential zoned selection with equal probability and without replacement. See the section “[Sequential Random Sampling](#)” on page 8060 for details.

If you specify `METHOD=SEQ` and also specify a `SIZE` statement (or the `PPS` option in the `SAMPLINGUNIT` statement), PROC SURVEYSELECT uses `METHOD=PPS_SEQ`, which is sequential selection with probability proportional to size and with minimum replacement. See the section “[PPS Sequential Sampling](#)” on page 8064 for more information.

**SRS**

requests simple random sampling, which is selection with equal probability and without replacement. See the section “[Simple Random Sampling](#)” on page 8059 for details. `METHOD=SRS` is the default if you do not specify the `METHOD=` option and also do not specify a `SIZE` statement (or the `PPS` option in the `SAMPLINGUNIT` statement).



**SYS**

requests systematic random sampling. If you specify `METHOD=SYS` and do not specify a `SIZE` statement (or the `PPS` option in the `SAMPLINGUNIT` statement), PROC SURVEYSELECT uses systematic selection with equal probability. See the section “Systematic Random Sampling” on page 8060 for more information.

If you specify `METHOD=SYS` and also specify a `SIZE` statement (or the `PPS` option in the `SAMPLINGUNIT` statement), PROC SURVEYSELECT uses `METHOD=PPS_SYS`, which is systematic selection with probability proportional to size. See the section “PPS Systematic Sampling” on page 8064 for details.

**URS**

requests unrestricted random sampling, which is selection with equal probability and with replacement. See the section “Unrestricted Random Sampling” on page 8059 for details.

**MINSIZE**

requests adjustment of size measures according to the stratum minimum size values provided in the secondary input data set. Use the `MINSIZE` option when you have already named the secondary input data set in another option, such as the `SAMPsize=SAS-data-set` option. See the section “Secondary Input Data Set” on page 8071 for details.

The `MINSIZE` option is available when you use size measures for any PPS selection method and also include a `STRATA` statement. You provide size measures by specifying the `SIZE` statement or the `PPS` option in the `SAMPLINGUNIT` statement.

You provide the stratum minimum size values in the secondary input data set variable `_MINSIZE_`. Each minimum size value must be a positive number.

When a size measure is less than the specified minimum value for its stratum, PROC SURVEYSELECT adjusts the size measure upward to equal the minimum size value. If your sampling units are individual observations, the variable `AdjustedSize` in the `OUT=` data set contains the adjusted size measures.

If you use a `SAMPLINGUNIT` statement to define sampling units (clusters), then the procedure applies the `MINSIZE` adjustment to the sampling unit size. The sampling unit size equals the number of observations in the sampling unit if you specify the `PPS` option, or the sum of the observation size measures if you specify a `SIZE` statement. The output data set variable `UnitSize` contains the adjusted sampling unit size measures.

If you want to specify a single minimum size value for all strata, you can use the `MINSIZE=min` option.

**MINSIZE=min**

specifies the minimum size value. The value of *min* must be a positive number.

When a size measure is less than the value *min*, PROC SURVEYSELECT adjusts the size measure upward to equal *min*. If your sampling units are individual observations, the variable `AdjustedSize` in the `OUT=` data set contains the adjusted size measures.

If you use a `SAMPLINGUNIT` statement to define sampling units (clusters), then the procedure applies the `MINSIZE` adjustment to the sampling unit size. The sampling unit size equals the number of observations in the sampling unit if you specify the `PPS` option, or the sum of the observation size

measures if you specify a [SIZE](#) statement. The output data set variable `UnitSize` contains the adjusted sampling unit size measures.

The `MINSIZE=min` option is available when you use size measures for any PPS selection method. You provide size measures by specifying the [SIZE](#) statement or the [PPS](#) option in the [SAMPLINGUNIT](#) statement.

If you request a stratified sample design with the [STRATA](#) statement and specify the `MINSIZE=min` option, PROC SURVEYSELECT uses the minimum size *min* for all strata. If you do not want to use the same minimum size for all strata, use the `MINSIZE=SAS-data-set` option to specify a minimum size value for each stratum.

#### **MINSIZE=*SAS-data-set***

names a SAS data set that contains minimum size values for the strata. You provide the stratum minimum size values in the `MINSIZE=` data set variable `_MINSIZE_`. Each minimum size value must be a positive number.

The `MINSIZE=SAS-data-set` option is available when you use size measures for any PPS selection method and also include a [STRATA](#) statement. You provide size measures by specifying the [SIZE](#) statement or the [PPS](#) option in the [SAMPLINGUNIT](#) statement.

When a size measure is less than the minimum size value for its stratum, PROC SURVEYSELECT adjusts the size measure upward to equal the minimum size measure. If your sampling units are individual observations, the variable `AdjustedSize` in the `OUT=` data set contains the adjusted size measures.

If you use a [SAMPLINGUNIT](#) statement to define sampling units (clusters), then the procedure applies the `MINSIZE` adjustment to the sampling unit size. The sampling unit size equals the number of observations in the sampling unit if you specify the [PPS](#) option, or the sum of the observation size measures if you specify a [SIZE](#) statement. The output data set variable `UnitSize` contains the adjusted sampling unit size measures.

The `MINSIZE=` input data set should contain all the [STRATA](#) variables, with the same type and length as in the `DATA=` data set. The [STRATA](#) groups should appear in the same order in the `MINSIZE=` data set as in the `DATA=` data set. The `MINSIZE=` data set must include a variable named `_MINSIZE_` that contains the minimum size measure for each stratum. The `MINSIZE=` data set is a secondary input data set. See the section “[Secondary Input Data Set](#)” on page 8071 for details. You can name only one secondary input data set in each invocation of the procedure.

If you want to specify a single minimum size value for all strata, you can use the `MINSIZE=min` option.

#### **NMAX=*n***

specifies the maximum stratum sample size *n* for the [SAMPRATE=](#) option. When you specify the [SAMPRATE=](#) option, PROC SURVEYSELECT calculates the stratum sample size by multiplying the total number of units in the stratum by the specified sampling rate. If this sample size is greater than the value `NMAX=n`, then PROC SURVEYSELECT selects only *n* units.

The maximum sample size *n* must be a positive integer. The `NMAX=` option is available only with the [SAMPRATE=](#) option, which can be used with equal probability selection methods ([METHOD=SRS](#), [METHOD=URS](#), [METHOD=SYS](#), and [METHOD=SEQ](#)). The `NMAX=` option is not available with [METHOD=BERNOULLI](#), where the [SAMPRATE=](#) option specifies the constant inclusion probability.

**NMIN=*n***

specifies the minimum stratum sample size  $n$  for the **SAMPRATE=** option. When you specify the **SAMPRATE=** option, PROC SURVEYSELECT calculates the stratum sample size by multiplying the total number of units in the stratum by the specified sampling rate. If this sample size is less than the value **NMIN= $n$** , then PROC SURVEYSELECT selects  $n$  units.

The minimum sample size  $n$  must be a positive integer. The **NMIN=** option is available only with the **SAMPRATE=** option, which can be used with equal probability selection methods (**METHOD=SRS**, **METHOD=URS**, **METHOD=SYS**, and **METHOD=SEQ**). The **NMIN=** option is not available with **METHOD=BERNOULLI**, where the **SAMPRATE=** option specifies the constant inclusion probability.

**NOPRINT**

suppresses the display of all output. You can use the **NOPRINT** option when you want only to create an output data set. Note that this option temporarily disables the Output Delivery System (ODS). For more information, see Chapter 20, “Using the Output Delivery System.”

**OUT=*SAS-data-set***

names the output data set that contains the sample. If you omit the **OUT=** option, the data set is named **DATA $n$** , where  $n$  is the smallest integer that makes the name unique.

The output data set contains the units that are selected for the sample, in addition to design information and selection statistics, depending on the selection method and output options that you request. See descriptions of the options **JTPROBS**, **OUTALL**, **OUTHITS**, **OUTSEED**, **OUTSIZE**, and **STATS**, which specify information to include in the output data set. See the section “Sample Output Data Set” on page 8072 for details about the contents of the output data set.

By default, the output data set contains only those units that are selected for the sample. To include all observations from the input data set in the output data set, use the **OUTALL** option.

By default, the output data set includes one copy of each selected unit, even when a unit is selected more than once, which can occur when you use with-replacement or with-minimum-replacement selection methods. For with-replacement or with-minimum-replacement selection methods, the output data set includes a variable **NumberHits** that records the number of hits (selections) for each unit. To include a distinct copy of each selection in the output data set when the same unit is selected more than once, use the **OUTHITS** option.

If you specify the **NOSAMPLE** option in the **STRATA** statement, PROC SURVEYFREQ allocates the total sample size among the strata but does not select the sample. In this case, the **OUT=** data set contains the allocated sample sizes. See the section “Allocation Output Data Set” on page 8075 for details.

**OUTALL**

includes all observations from the **DATA=** input data set in the **OUT=** output data set. By default, the output data set includes only those units selected for the sample. When you specify the **OUTALL** option, the output data set includes all observations from the input data set and also contains a variable that indicates each observation’s selection status. The variable **Selected** equals 1 for an observation that is selected for the sample, and equals 0 for an observation that is not selected. For information about the contents of the output data set, see the section “Sample Output Data Set” on page 8072.

The **OUTALL** option is available for equal probability selection methods (**METHOD=SRS**, **METHOD=URS**, **METHOD=SYS**, **METHOD=SEQ**, and **METHOD=BERNOULLI**). The **OUTALL** option is also available for **METHOD=POISSON**.

**OUTHITS**

includes a distinct copy of each selected unit in the **OUT=** output data set when the same sampling unit is selected more than once. By default, the output data set contains a single copy of each unit selected, even when a unit is selected more than once, and the variable `NumberHits` records the number of hits (selections) for each unit. If you specify the **OUTHITS** option, the output data set contains  $m$  copies of a sampling unit for which `NumberHits` equals  $m$ . For example, with the **OUTHITS** option a unit that is selected three times is represented by three copies in the output data set.

A sampling unit can be selected more than once by with-replacement and with-minimum-replacement selection methods, which include **METHOD=URS**, **METHOD=PPS\_WR**, **METHOD=PPS\_SYS**, and **METHOD=PPS\_SEQ**. The **OUTHITS** option is available for these selection methods.

See the section “[Sample Output Data Set](#)” on page 8072 for details about the contents of the output data set.

**OUTSEED**

includes the initial seed for each stratum in the **OUT=** output data set. The variable `InitialSeed` contains the stratum initial seeds. See the section “[Sample Output Data Set](#)” on page 8072 for details about the contents of the output data set.

To reproduce the same sample for any stratum in a subsequent execution of PROC SURVEYSELECT, you can specify the same stratum initial seed with the **SEED=SAS-data-set** option, along with the same sample selection parameters. See the section “[Random Number Generation](#)” on page 8058 for more information.

The “[Sample Selection Summary](#)” table displays the initial random number seed for the entire sample selection, which is the same as the initial seed for the first stratum when the design is stratified. To reproduce the entire sample, you can specify this same seed value in the **SEED=** option, along with the same sample selection parameters.

Beginning in SAS/STAT 12.1, PROC SURVEYSELECT uses the Mersenne-Twister random number generator by default. In previous releases, PROC SURVEYSELECT used the RANUNI random number generator, which you can now request by specifying the **RANUNI** option. To reproduce samples that PROC SURVEYSELECT selected in releases prior to SAS/STAT 12.1, specify the **RANUNI** option with the **SEED=** option (for the same input data set and sample selection parameters).

**OUTSIZE**

includes additional design and sampling frame information in the **OUT=** output data set.

If you use a **STRATA** statement, the **OUTSIZE** option provides stratum-level values in the output data set. Otherwise, the **OUTSIZE** option provides overall values.

The **OUTSIZE** option includes the sample size or sampling rate in the output data set, depending on whether you specify the **SAMPSIZE=** option or the **SAMPRATE=** option, respectively. For PPS selection methods, the **OUTSIZE** option includes the total size measure in the output data set. If you do not provide size measures, or if you specify a **SAMPLINGUNIT** statement, the **OUTSIZE** option includes the total number of sampling units.

If you request size measure adjustment or certainty selection, the **OUTSIZE** option includes the following information in the output data set: the minimum size measure if you specify the **MINSIZE=** option, the maximum size measure if you specify the **MAXSIZE=** option, the certainty size measure if you specify the **CERTSIZE=** option, and the certainty proportion if you specify the **CERTSIZE=P=** option.

For **METHOD=BERNOULLI**, the **OUTSIZE** option includes the following information in the output data set: total number of sampling units, selection probability (sampling rate), expected sample size, and actual sample size. See the section “[Bernoulli Sampling](#)” on page 8061 for descriptions of these statistics.

For more information about the contents of the output data set, see the section “[Sample Output Data Set](#)” on page 8072.

#### **OUTSORT=SAS-data-set**

names an output data set to store the sorted input data set. This option is available when you specify a **CONTROL** statement to sort the **DATA=** input data set for systematic or sequential selection methods (**METHOD=SYS**, **METHOD=PPS\_SYS**, **METHOD=SEQ**, and **METHOD=PPS\_SEQ**).

If you specify **CONTROL** variables but do not name an output data set with the **OUTSORT=** option, then the sorted data set replaces the input data set.

#### **RANUNI**

requests uniform random number generation by the method of Fishman and Moore (1982), which PROC SURVEYSELECT used in releases prior to SAS/STAT 12.1. This is the same random number generator that the RANUNI function provides.

Beginning in SAS/STAT 12.1, PROC SURVEYSELECT uses the Mersenne-Twister random number generator by default. Developed by Matsumoto and Nishimura (1998), the Mersenne-Twister random number generator has a very long period and good statistical properties. This is the random number generator that the RAND function provides for the uniform distribution.

See the section “[Random Number Generation](#)” on page 8058 for details, and see *SAS Functions and CALL Routines: Reference* for information about the RANUNI and RAND functions.

You can specify the RANUNI option with the **SEED=** option to reproduce samples that PROC SURVEYSELECT selected in releases prior to SAS/STAT 12.1. To reproduce a sample by using the RANUNI and **SEED=** options, you must also specify the same input data set and sample selection parameters.

#### **REPS=nreps**

specifies the number of sample replicates. The value of *nreps* must be a positive integer.

When you specify the **REPS=** option, PROC SURVEYSELECT selects *nreps* independent samples, each with the same sample size or sampling rate and the same sample design that you request. The variable Replicate in the **OUT=** data set contains the sample replicate number.

You can use replicated sampling to provide a simple method of variance estimation for any form of statistic, and also to evaluate variable nonsampling errors such as interviewer differences. For information about replicated sampling, see Lohr (2010); Wolter (2007); Kish (1965, 1987); Kalton (1983). You can also use the **REPS=** option to perform a variety of other resampling and simulation tasks. See Cassell (2007) for more information.

#### **SAMPRATE=r**

#### **RATE=r**

specifies the sampling rate, which is the proportion of units to select for the sample. The sampling rate *r* must be a positive number. You can specify *r* as a number between 0 and 1. Or you can specify

$r$  in percentage form as a number between 1 and 100, and PROC SURVEYSELECT converts that number to a proportion. The procedure treats the value 1 as 100% instead of 1%.

The SAMPRATE= option is available only for equal probability selection methods (METHOD=SRS, METHOD=URS, METHOD=SYS, METHOD=SEQ, and METHOD=BERNOULLI). For systematic random sampling (METHOD=SYS), PROC SURVEYSELECT uses the inverse of the sampling rate  $r$  as the selection interval. See the section “Systematic Random Sampling” on page 8060 for details. For Bernoulli sampling (METHOD=BERNOULLI), PROC SURVEYSELECT uses the sampling rate  $r$  as the inclusion probability. See the section “Bernoulli Sampling” on page 8061 for details. For the other equal probability selection methods, PROC SURVEYSELECT converts the sampling rate  $r$  to the sample size before selection by multiplying the total number of units in the stratum or frame by the sampling rate and rounding up to the nearest integer.

If you request a stratified sample design with the STRATA statement and specify the SAMPRATE= $r$  option, PROC SURVEYSELECT uses the sampling rate  $r$  for each stratum. If you do not want to use the same sampling rate for each stratum, use the SAMPRATE=(values) option or the SAMPRATE=SAS-data-set option to specify a sampling rate for each stratum.

#### **SAMPRATE=(values)**

#### **RATE=(values)**

specifies stratum sampling rates, where the stratum sampling rate is the proportion of units to select from the stratum. You can separate values with blanks or commas. The number of SAMPRATE= values must equal the number of strata in the input data set.

List the stratum sampling rate values in the order in which the strata appear in the input data set. When you use the SAMPRATE=(values) option, the input data set must be sorted by the STRATA variables in ascending order. You cannot use the DESCENDING or NOTSORTED option in the STRATA statement.

Each stratum sampling rate value must be a nonnegative. You can specify a rate value as a number between 0 and 1. Or you can specify a rate value in percentage form as a number between 1 and 100, and PROC SURVEYSELECT converts that number to a proportion. The procedure treats the value 1 as 100% instead of 1%.

To select a sample from a stratum, the value of the stratum sampling rate must be positive. If you specify a stratum sampling rate of 0, then PROC SURVEYSELECT does not select a sample from the stratum. This has the effect of subsetting the input data set before sample selection; the stratum that you omit is not included in the sampling frame or represented in the sample.

The SAMPRATE= option is available only for equal probability selection methods (METHOD=SRS, METHOD=URS, METHOD=SYS, METHOD=SEQ, and METHOD=BERNOULLI). For systematic random sampling (METHOD=SYS), PROC SURVEYSELECT uses the inverse of the stratum sampling rate as the stratum selection interval. See the section “Systematic Random Sampling” on page 8060 for details. For Bernoulli sampling (METHOD=BERNOULLI), PROC SURVEYSELECT uses the stratum sampling rate as the inclusion probability for the stratum. See the section “Bernoulli Sampling” on page 8061 for details. For the other equal probability selection methods, PROC SURVEYSELECT converts the stratum sampling rate to the stratum sample size before selection by multiplying the total number of units in the stratum by the sampling rate and rounding up to the nearest integer.



**SAMPRATE=SAS-data-set**

**RATE=SAS-data-set**

names a SAS data set that contains stratum sampling rates, where the stratum sampling rate is the proportion of units to select from the stratum. The SAMPRATE= data set should include a variable `_RATE_` that contains the stratum sampling rates.

Each sampling rate value must be a nonnegative number. You can specify a rate value as a number between 0 and 1. Or you can specify a rate value in percentage form as a number between 1 and 100, and PROC SURVEYSELECT converts that number to a proportion. The procedure treats the value 1 as 100% instead of 1%.

To select a sample from a stratum, the value of the stratum sampling rate must be positive. If you specify a stratum sampling rate of 0, then PROC SURVEYSELECT does not select a sample from the stratum. This has the effect of subsetting the input data set before sample selection; the stratum that you omit is not included in the sampling frame or represented in the sample.

The SAMPRATE= input data set should contain all the STRATA variables, with the same type and length as in the DATA= data set. The STRATA groups should appear in the same order in the SAMPRATE= data set as in the DATA= data set.

The SAMPRATE= option is available only for equal probability selection methods ([METHOD=SRS](#), [METHOD=URS](#), [METHOD=SYS](#), [METHOD=SEQ](#), and [METHOD=BERNOULLI](#)). For systematic random sampling ([METHOD=SYS](#)), PROC SURVEYSELECT uses the inverse of the stratum sampling rate as the stratum selection interval. See the section “[Systematic Random Sampling](#)” on page 8060 for details. For Bernoulli sampling ([METHOD=BERNOULLI](#)), PROC SURVEYSELECT uses the stratum sampling rate as the inclusion probability for the stratum. See the section “[Bernoulli Sampling](#)” on page 8061 for details. For the other equal probability selection methods, PROC SURVEYSELECT converts the stratum sampling rate to the stratum sample size before selection by multiplying the total number of units in the stratum by the sampling rate and rounding up to the nearest integer.

**SAMPsize=*n***

**N=*n***

specifies the sample size, which is the number of units to select for the sample. The sample size *n* must be a positive integer. For selection methods that select without replacement, the sample size *n* must not exceed the number of units in the input data set.

If you do not specify a [SAMPLINGUNIT](#) statement, then your sampling units are observations, and PROC SURVEYSELECT selects *n* observations. If you use a [SAMPLINGUNIT](#) statement to define sampling units as groups of observations (clusters), then the procedure selects *n* clusters.

If you specify the SAMPsize=*n* option and request stratified selection with the [STRATA](#) statement, PROC SURVEYSELECT selects *n* units from each stratum unless you also specify the [ALLOC=](#) option in the [STRATA](#) statement to allocate the total sample size among the strata.

If you specify the [ALLOC=](#) option in the [STRATA](#) statement and the SAMPsize=*n* option, PROC SURVEYSELECT allocates the total sample size *n* among the strata according to the allocation method that you request. See the section “[Sample Size Allocation](#)” on page 8067 for details. If you specify the [MARGIN=](#) option with the [ALLOC=](#) option in the [STRATA](#) statement, PROC SURVEYSELECT determines the stratum sample sizes that provide the requested margin of error for the allocation. Therefore, you cannot use the SAMPsize= option with the [MARGIN=](#) option.

For methods that select without replacement, the sample size  $n$  must not exceed the number of units in any stratum. If you do not want to select the same number of units from each stratum, use the **SAMPSIZE=(values)** option or the **SAMPSIZE=SAS-data-set** option to specify a sample size for each stratum.

For without-replacement selection methods, by default, PROC SURVEYSELECT does not allow you to specify a stratum sample size that is greater than the total number of units available in the stratum. If you specify the **SELECTALL** option, PROC SURVEYSELECT selects all stratum units when the stratum sample size exceeds the number of units in the stratum.

### **SAMPSIZE=(values)**

#### **N=(values)**

specifies stratum sample sizes, where the stratum sample size is the number of units to select from the stratum. You can separate *values* with blanks or commas. The number of SAMPSIZE= values must equal the number of strata in the input data set.

List the stratum sample size values in the order in which the strata appear in the input data set. When you use the SAMPSIZE=(values) option, the input data set must be sorted by the STRATA variables in ascending order. You cannot use the DESCENDING or NOTSORTED option in the STRATA statement.

Each stratum sample size value must be a nonnegative integer. To select a sample from a stratum, the value of the stratum sample size must be positive. If you specify a stratum sample size of 0, then PROC SURVEYSELECT does not select a sample from the stratum. This has the effect of subsetting the input data set before sample selection; the stratum that you omit is not included in the sampling frame or represented in the sample.

For without-replacement selection methods, by default, PROC SURVEYSELECT does not allow you to specify a stratum sample size that is greater than the total number of units available in the stratum. If you specify the **SELECTALL** option, PROC SURVEYSELECT selects all stratum units when the stratum sample size exceeds the number of units in the stratum.

### **SAMPSIZE=SAS-data-set**

#### **N=SAS-data-set**

names a SAS data set that contains stratum sample sizes, where the stratum sample size is the number of units to select from the stratum. The SAMPSIZE= input data set should include a variable named `_NSIZE_` or `SampleSize` that contains the stratum sample sizes.

Each stratum sample size value must be a nonnegative integer. To select a sample from a stratum, the value of the stratum sample size must be positive. If you specify a stratum sample size of 0, then PROC SURVEYSELECT does not select a sample from the stratum. This has the effect of subsetting the input data set before sample selection; the stratum that you omit is not included in the sampling frame or represented in the sample.

The SAMPSIZE= input data set should contain all the STRATA variables, with the same type and length as in the DATA= data set. The STRATA groups should appear in the same order in the SAMPSIZE= data set as in the DATA= data set. The SAMPSIZE= data set is a secondary input data set. See the section “[Secondary Input Data Set](#)” on page 8071 for details. You can name only one secondary input data set in each invocation of the procedure.

For without-replacement selection methods, by default, PROC SURVEYSELECT does not allow you to specify a stratum sample size that is greater than the total number of units available in the stratum. If you specify the **SELECTALL** option, PROC SURVEYSELECT selects all stratum units when the stratum sample size exceeds the number of units in the stratum.



**SEED**

indicates that stratum-level initial seeds are included in the secondary input data set. Use the SEED option when you have already named the secondary input data set in another option, such as the `SAMPsize=SAS-data-set` option. See the section “[Secondary Input Data Set](#)” on page 8071 for details. You can name only one secondary input data set in each invocation of the procedure.

You provide the stratum initial seeds in the secondary input data set variable named `_SEED_` or `InitialSeed`. The initial seeds must be positive integers.

See the description of the `SEED=SAS-data-set` option for more information about initial seeds for random number generation.

**SEED=number**

specifies the initial seed for random number generation. The SEED= value must be a positive integer. If you do not specify the SEED= option, or if the SEED= value is negative or 0, PROC SURVEYSELECT uses the time of day from the computer’s clock to obtain the initial seed. See the section “[Random Number Generation](#)” on page 8058 for more information.

If you request a stratified sample design with the STRATA statement, you can use the `SEED=SAS-data-set` option to specify an initial seed for each stratum. Otherwise, PROC SURVEYSELECT generates random numbers continuously across strata from the random number stream initialized by the SEED= value.

You can use the `OUTSEED` option to include the stratum initial seeds in the output data set.

Whether or not you specify the SEED= option, PROC SURVEYSELECT displays the value of the initial seed in the “Sample Selection Summary” table. If you need to reproduce the same sample in a subsequent execution of PROC SURVEYSELECT, you can specify this same seed value in the SEED= option, along with the same sample selection parameters, and PROC SURVEYSELECT will reproduce the sample.

Beginning in SAS/STAT 12.1, PROC SURVEYSELECT uses the Mersenne-Twister random number generator by default. In previous releases, PROC SURVEYSELECT used the RANUNI random number generator, which you can now request by specifying the `RANUNI` option. To reproduce samples that PROC SURVEYSELECT selected in releases prior to SAS/STAT 12.1, use the `RANUNI` option with the SEED= option (for the same input data set and sample selection parameters).

**SEED=SAS-data-set**

names a SAS data set that contains initial seeds for the strata. You provide the stratum seeds in the SEED= input data set variable `_SEED_` or `InitialSeed`.

The initial seed values must be positive integers. If the initial seed value for the first stratum is not a positive integer, PROC SURVEYSELECT uses the time of day from the computer’s clock to obtain the initial seed. If the initial seed value for a subsequent stratum is not a positive integer, PROC SURVEYSELECT continues to use the random number stream already initialized by the seed for the previous stratum. See the section “[Sample Selection Methods](#)” on page 8058 for more information.

The SEED= input data set should contain all the STRATA variables, with the same type and length as in the DATA= data set. The STRATA groups should appear in the same order in the SEED= data set as in the DATA= data set. The SEED= data set is a secondary input data set. See the section “[Secondary Input Data Set](#)” on page 8071 for details. You can name only one secondary input data set in each invocation of the procedure.

You can use the `OUTSEED` option to include the stratum initial seeds in the output data set.

Whether or not you specify the SEED= option, PROC SURVEYSELECT displays the value of the initial seed in the “Sample Selection Summary” table. If you need to reproduce the same sample in a subsequent execution of PROC SURVEYSELECT, you can specify this same seed value in the SEED= option, along with the same sample selection parameters, and PROC SURVEYSELECT will reproduce the sample.

If you specify initial seeds by strata with the SEED=*SAS-data-set* option, you can reproduce the same sample in a subsequent execution of PROC SURVEYSELECT by specifying these same stratum initial seeds, along with the same sample selection parameters. If you need to reproduce the same sample for only a subset of the strata, you can use the same initial seeds for those strata in the subset.

Beginning in SAS/STAT 12.1, PROC SURVEYSELECT uses the Mersenne-Twister random number generator by default. In previous releases, PROC SURVEYSELECT used the RANUNI random number generator, which you can now request by specifying the RANUNI option. To reproduce samples that PROC SURVEYSELECT selected in releases prior to SAS/STAT 12.1, use the RANUNI option with the SEED= option (for the same input data set and sample selection parameters).

### SELECTALL

requests that PROC SURVEYSELECT select all stratum units when the stratum sample size exceeds the total number of units in the stratum. By default, PROC SURVEYSELECT does not allow you to specify a stratum sample size that is greater than the total number of units in the stratum, unless you are using a with-replacement selection method.

The SELECTALL option is available for the following without-replacement selection methods: METHOD=SRS, METHOD=SYS, METHOD=SEQ, METHOD=PPS, and METHOD=PPS\_SAMPFORD.

The SELECTALL option is not available for with-replacement selection methods, with-minimum-replacement methods, or those PPS methods that select two units per stratum.

### SORT=NEST | SERP

specifies the type of sorting by CONTROL variables. The option SORT=NEST requests nested sorting, and SORT=SERP requests hierarchic serpentine sorting. The default is SORT=SERP. See the section “[Sorting by CONTROL Variables](#)” on page 8057 for descriptions of serpentine and nested sorting. Where there is only one CONTROL variable, the two types of sorting are equivalent.

The SORT= option is available when you specify a CONTROL statement for systematic or sequential selection methods (METHOD=SYS, METHOD=PPS\_SYS, METHOD=SEQ, and METHOD=PPS\_SEQ). When you specify a CONTROL statement, PROC SURVEYSELECT sorts the input data set by the CONTROL variables within strata before selecting the sample.

The SORT= option and the CONTROL statement are not available with a SAMPLINGUNIT statement. See the descriptions of the CONTROL and SAMPLINGUNIT statements for more information.

When you specify a CONTROL statement, you can also use the OUTSORT= option to name an output data set that contains the sorted input data set. Otherwise, if you do not specify the OUTSORT= option, the sorted data set replaces the input data set.

### STATS

includes the selection probability and sampling weight in the OUT= output data set for equal probability selection methods when you do not specify a STRATA statement. By default, the output data set does not include these values for equal probability selection methods unless you specify a STRATA statement. The STATS option applies to the following selection methods: METHOD=SRS, METHOD=URS, METHOD=SYS, METHOD=SEQ, and METHOD=BERNOULLI.

In addition to the selection probability and sampling weight, the **STATS** option includes the following statistics in the output data set for **METHOD=BERNOULLI**: total number of sampling units, expected sample size, actual sample size, and adjusted sampling weight. See the section “[Bernoulli Sampling](#)” on page 8061 for more information.

For PPS selection methods, the output data set contains selection probabilities and sampling weights by default. The **STATS** option has no effect for PPS methods.

For more information about the contents of the output data set, see the section “[Sample Output Data Set](#)” on page 8072.

## CONTROL Statement

**CONTROL** *variables* ;

The **CONTROL** statement names variables for sorting the input data set before sample selection. The **CONTROL** variables can be character or numeric. If you also specify a **STRATA** statement, **PROC SURVEYSELECT** sorts by **CONTROL** variables within strata.

Control sorting is available for systematic and sequential selection methods (**METHOD=SYS**, **METHOD=PPS\_SYS**, **METHOD=SEQ**, and **METHOD=PPS\_SEQ**). Ordering the sampling units before systematic or sequential selection can provide additional control over the distribution of the sample.

Control sorting is not available when you use a **SAMPLINGUNIT** statement, which defines groups of observations as units (clusters) for sample selection. See the description of the **SAMPLINGUNIT** statement for information about ordering clusters before systematic or sequential selection.

By default (or if you specify the **SORT=SERP** option in the **PROC SURVEYSELECT** statement), **PROC SURVEYSELECT** uses hierarchic serpentine sorting by the **CONTROL** variables. If you specify the **SORT=NEST** option, the procedure uses nested sorting. For more information about serpentine and nested sorting, see the section “[Sorting by CONTROL Variables](#)” on page 8057.

You can use the **OUTSORT=** option in the **PROC SURVEYSELECT** statement to name an output data set that contains the sorted input data set. If you do not specify the **OUTSORT=** option when you use the **CONTROL** statement, then the sorted data set replaces the input data set.

## FREQ Statement

**FREQ** *variable* ;

The **FREQ** statement names a numeric variable that contains the frequency of occurrence of each observation. If you use a **FREQ** statement, **PROC SURVEYSELECT** assumes that an observation represents  $n$  observations, where  $n$  is the value of the **FREQ** variable for the observation. The **FREQ** statement is not available when you specify a **SAMPLINGUNIT** statement.

The **FREQ** statement is available only for sample allocation when no sample is selected, which you can request by specifying the **ALLOC=** and **NOSAMPLE** options in the **STRATA** statement. The **ALLOC=** option requests allocation of the total sample size among the strata, and the **NOSAMPLE** option requests that no sample be selected after allocation. When you specify the **NOSAMPLE** option, the procedure computes stratum sample sizes according to the allocation method that you request, but does not select the

sample. See the sections “Allocation Options” on page 8052 and “Sample Size Allocation” on page 8067 for details.

The sum of the FREQ variable values (frequencies) represents the total number of sampling units. The sum of the frequencies in a stratum represents the total number of sampling units in the stratum. When you use a FREQ statement, the sample size allocation is based on the expanded total and stratum frequencies.

Values of the FREQ variable must be nonmissing and nonnegative. If a value of the FREQ variable is 0, PROC SURVEYSELECT ignores the observation. If a value of the FREQ variable is not an integer, PROC SURVEYSELECT uses only the integer portion as the frequency of the observation.

## ID Statement

**ID** *variables* ;

The ID statement names one or more variables from the **DATA=** input data set to include in the **OUT=** output data set of selected units. If there is no ID statement, PROC SURVEYSELECT includes all variables from the input data set in the output data set. The ID variables can be either character or numeric.

## SAMPLINGUNIT | CLUSTER Statement

**SAMPLINGUNIT | CLUSTER** *variables* < / options > ;

The SAMPLINGUNIT statement names variables that identify the sampling units as groups of observations (clusters). The combinations of categories of SAMPLINGUNIT variables define the sampling units. If there is a STRATA statement, sampling units are nested within strata.

When you use a SAMPLINGUNIT statement to define units (clusters), PROC SURVEYSELECT selects a sample of these units by using the selection method and design parameters that you specify in the PROC SURVEYSELECT statement. If you do not use a SAMPLINGUNIT statement, then PROC SURVEYSELECT uses the input data set observations as sampling units by default.

The SAMPLINGUNIT variables are one or more variables in the **DATA=** input data set. These variables can be either character or numeric. The formatted values of the SAMPLINGUNIT variables determine the SAMPLINGUNIT variable levels. Thus, you can use formats to group values into levels. See the FORMAT procedure in the *Base SAS Procedures Guide* and the FORMAT statement and SAS formats in *SAS Formats and Informats: Reference* for more information.

You can use a SAMPLINGUNIT statement with any equal probability selection method or PPS selection method. The SAMPLINGUNIT statement is not available for Poisson sampling (**METHOD=POISSON**).

If you specify the **PPS** option in the SAMPLINGUNIT statement and do not specify a **SIZE** statement, then the procedure computes sampling unit size as the number of observations in the sampling unit. If you specify a **SIZE** statement with a SAMPLINGUNIT statement, then the procedure computes sampling unit size by summing the size measures of all observations in the sampling unit.

By default, PROC SURVEYSELECT sorts the input data set by the SAMPLINGUNIT variables within strata before sample selection. This groups the observations into sampling units and orders the sampling units by the SAMPLINGUNIT variables. If you do not want the procedure to sort the input data set by the SAMPLINGUNIT variables, then specify the **PRESORTED** option in the SAMPLINGUNIT statement. By

using the **PRESORTED** option, you can provide the order of the sampling units for systematic and sequential selection methods. The **CONTROL** statement is not available with the **SAMPLINGUNIT** statement.

Note that the **SAMPLINGUNIT** statement defines groups of observations (clusters) to use as sampling units, and **PROC SURVEYSELECT** selects a sample of these units. When you use a **SAMPLINGUNIT** statement, **PROC SURVEYSELECT** does not select samples of observations from within the sampling units (clusters). To select independent samples within groups, use the **STRATA** statement.

You can specify the following *options* in the **SAMPLINGUNIT** statement after a slash (/):

### **PPS**

computes a sampling unit's size measure as the number of observations in the sampling unit. The procedure then uses these size measures to select a sample according to the PPS selection method that you specify with the **METHOD=** option in the **PROC SURVEYSELECT** statement.

This option has no effect when you specify a **SIZE** statement. When you specify a **SIZE** statement, the procedure computes sampling unit size by summing the size measures of all observations that belong to the sampling unit.

### **PRESORTED**

requests that **PROC SURVEYSELECT** not sort the input data set by the **SAMPLINGUNIT** variables within strata. By default, the procedure sorts the input data set by the **SAMPLINGUNIT** variables, which groups the observations into sampling units and orders the units by the **SAMPLINGUNIT** variables.

The **PRESORTED** option enables you to provide the order of the sampling units. For systematic and sequential selection methods, ordering provides additional control over the distribution of the sample and gives some benefits of proportionate stratification. Systematic and sequential methods include **METHOD=SYS**, **METHOD=PPS\_SYS**, **METHOD=SEQ**, and **METHOD=PPS\_SEQ**. See the descriptions of these methods in the section “Sample Selection Methods” on page 8058 for more information.

When you specify the **PRESORTED** option, the procedure treats the sampling unit groups as **NOTSORTED**. Like the **BY** statement option **NOTSORTED**, this does not mean that the data are unsorted by the **SAMPLINGUNIT** variables, but rather that the data are arranged in groups (according to values of the **SAMPLINGUNIT** variables) and that these groups are not necessarily in alphabetical or increasing numeric order. For more information about the **BY** statement **NOTSORTED** option, see *SAS Language Reference: Concepts*.

## **SIZE Statement**

**SIZE** *variable* ;

The **SIZE** statement names one and only one variable that contains size measures that are used for PPS selection. The **SIZE** variable must be numeric.

If you specify a **SAMPLINGUNIT** statement with a **SIZE** statement, the procedure computes a sampling unit's size by summing the size measures of all observations that belong to the sampling unit. Alternatively, if you specify the **PPS** option in the **SAMPLINGUNIT** statement and do not use a **SIZE** statement, the procedure computes sampling unit size as the number of observations in the sampling unit.

When the value of a sampling unit's size measure is missing or nonpositive, that sampling unit is excluded from the sample selection. See the section “[Missing Values](#)” on page 8056 for more information.

You can adjust the size measure values by using the `MAXSIZE=` option, the `MINSIZE=` option, or both of these options in the `PROC SURVEYSELECT` statement.

All PPS selection methods require size measures, which you can provide by specifying a `SIZE` statement (or by specifying the `PPS` option in the `SAMPLINGUNIT` statement). PPS selection methods include the following: `METHOD=PPS`, `METHOD=PPS_BREWER`, `METHOD=PPS_MURTHY`, `METHOD=PPS_SAMPFORD`, `METHOD=PPS_SEQ`, `METHOD=PPS_SYS`, and `METHOD=PPS_WR`. For details about how size measures are used in sample selection, see the descriptions of PPS selection methods in the section “[Sample Selection Methods](#)” on page 8058.

Note that a sampling unit's size measure, which you provide for PPS selection by specifying a `SIZE` statement, is not the same as the *sample size*. The sample size is the number of units to select for the sample; you specify the sample size with the `SAMPSIZE=` option in the `PROC SURVEYSELECT` statement.

For `METHOD=POISSON`, the variable that is specified in the `SIZE` statement provides inclusion probabilities for Poisson sampling. See the section “[Poisson Sampling](#)” on page 8062 for details. When the value of the `SIZE` variable is missing, nonpositive, or greater than 1, the sampling unit is not included in the sample selection.

## STRATA Statement

**STRATA** *variables* </ *options* > ;

The `STRATA` statement names variables that partition the input data set into nonoverlapping subgroups (strata). The combinations of levels of `STRATA` variables define the strata. `PROC SURVEYSELECT` then selects independent samples from these strata, according to the selection method and design parameters that you specify in the `PROC SURVEYSELECT` statement. For information about the use of stratification in sample design, see Lohr (2010); Kalton (1983); Kish (1965, 1987); Cochran (1977).

The `STRATA` variables are one or more variables in the `DATA=` input data set. These variables can be either character or numeric, but the procedure treats them as categorical variables. The formatted values of the `STRATA` variables determine the `STRATA` variable levels. Thus, you can use formats to group values into levels. See the `FORMAT` procedure in the *Base SAS Procedures Guide* and the `FORMAT` statement and SAS formats in *SAS Formats and Informats: Reference*.

The `STRATA` variables function much like `BY` variables, and `PROC SURVEYSELECT` expects the input data set to be sorted in order of the `STRATA` variables.

If you specify a `CONTROL` statement, or if you specify `METHOD=PPS`, the input data set must be sorted in ascending order by the `STRATA` variables. This means you cannot use the `STRATA` option `NOTSORTED` or `DESCENDING` when you specify a `CONTROL` statement or `METHOD=PPS`.

If your input data set is not sorted by the `STRATA` variables in ascending order, use one of the following alternatives:

- Sort the data by using the `SORT` procedure with the `STRATA` variables in a `BY` statement.
- Specify the `NOTSORTED` or `DESCENDING` option in the `STRATA` statement (when you do not specify a `CONTROL` statement or `METHOD=PPS`). The `NOTSORTED` option does not mean that the



data are unsorted but rather that the data are arranged in groups (according to values of the STRATA variables) and that these groups are not necessarily in alphabetical or increasing numeric order.

- Create an index on the STRATA variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

## Allocation Options

The STRATA options request allocation of the total sample size among the strata. You can use the ALLOC= option to specify the allocation method. Available allocation methods include proportional allocation (ALLOC=PROP), optimal allocation (ALLOC=OPTIMAL), and Neyman allocation (ALLOC=NEYMAN). See the section “Sample Size Allocation” on page 8067 for details about these methods.

Instead of requesting that PROC SURVEYSELECT compute the sample allocation, you can provide the allocation proportions by using the ALLOC=(values) option or the ALLOC=SAS-data-set option. Then PROC SURVEYSELECT allocates the total sample size among the strata according to the proportions that you provide. Allocation proportions are relative stratum sample sizes,  $n_h/n$ , where  $n_h$  is the stratum  $h$  sample size and  $n$  is the total sample size.

You can use the SAMPSIZE= option in the PROC SURVEYSELECT statement to specify the total sample size to be allocated among the strata. Alternatively, you can specify the desired margin of error in the MARGIN= option, and the procedure determines the stratum sample sizes that are required to achieve that margin. See the section “Specifying the Margin of Error” on page 8069 for details.

When you request sample allocation, by default PROC SURVEYSELECT computes the allocation of the total sample size among the strata and then selects the sample. If you specify the NOSAMPLE option, the procedure computes the allocation but does not select the sample. In this case the OUT= output data set contains the stratum sample sizes that are computed according to the specified allocation method. See the section “Allocation Output Data Set” on page 8075 for details.

You can use the ALLOC= option with any selection method except METHOD=PPS\_BREWER and METHOD=PPS\_MURTHY, which select two units from each stratum.

Table 95.2 summarizes the options available in the STRATA statement. Descriptions of the options follow in alphabetical order.

**Table 95.2** STRATA Statement Options for Sample Allocation

| Option         | Description                                   |
|----------------|-----------------------------------------------|
| ALLOC=name     | Specifies the allocation method               |
| ALLOC=(values) | Provides allocation proportions               |
| ALLOCMIN=      | Specifies the minimum sample size per stratum |
| ALPHA=         | Specifies the confidence level                |
| COST=          | Provides stratum costs                        |
| MARGIN=        | Specifies the margin of error                 |
| NOSAMPLE       | Allocates but does not select the sample      |
| STATS          | Displays additional allocation statistics     |
| VAR=           | Provides stratum variances                    |

You can specify the following *options* in the STRATA statement after a slash (/):

**ALLOC=*name***

specifies the method for allocating the total sample size among the strata. The following values for *name* are available:

**PROPORTIONAL | PROP**

requests proportional allocation, which allocates the total sample size in proportion to the stratum sizes, where the stratum size is the number of sampling units in the stratum. See the section “[Proportional Allocation](#)” on page 8068 for details.

**OPTIMAL | OPT**

requests optimal allocation, which allocates the total sample size among the strata in proportion to stratum sizes, stratum variances, and stratum costs. See the section “[Optimal Allocation](#)” on page 8068 for more information. If you specify ALLOC=OPTIMAL, you must provide the stratum variances with the [VAR=\(values\)](#), [VAR=SAS-data-set](#), or [VAR](#) option. You must provide the stratum costs with the [COST=\(values\)](#), [COST=SAS-data-set](#), or [COST](#) option.

**NEYMAN**

requests Neyman allocation, which allocates the total sample size among the strata in proportion to the stratum sizes and variances. See the section “[Neyman Allocation](#)” on page 8069 for more information. If you specify ALLOC=NEYMAN, you must provide the stratum variances with the [VAR=\(values\)](#), [VAR=SAS-data-set](#), or [VAR](#) option.

**ALLOC=(*values*)**

lists stratum allocation proportions. You can separate *values* with blanks or commas.

Each allocation proportion specifies the percent of the total sample size to allocate to the corresponding stratum. The number of ALLOC= values must equal the number of strata in the input data set. The sum of the allocation proportions must equal 1.

Each allocation proportion must be a positive number. You can specify each value as a number between 0 and 1. Or you can specify a value in percentage form as a number between 1 and 100, and PROC SURVEYSELECT converts that number to a proportion. The procedure treats the value 1 as 100% instead of 1%.

List the allocation proportions in the order in which the strata appear in the input data set. If you use the ALLOC=(*values*) option, the input data set must be sorted by the STRATA variables in ascending order. You cannot use the DESCENDING or NOTSORTED option in the STRATA statement.

**ALLOC=*SAS-data-set***

names a SAS data set that contains stratum allocation proportions. You provide the stratum allocation proportions in the ALLOC= data set variable `_ALLOC_`.

Each allocation proportion specifies the percent of the total sample size to allocate to the corresponding stratum. The sum of the allocation proportions must equal 1.

Each allocation proportion must be a positive number. You can specify the value as a number between 0 and 1. Or you can specify the value in percentage form as a number between 1 and 100, and PROC SURVEYSELECT converts that number to a proportion. The procedure treats the value 1 as 100% instead of 1%.



The ALLOC= data set should contain all the STRATA variables, with the same type and length as in the DATA= input data set. The STRATA groups should appear in the same order in the ALLOC= data set as in the DATA= data set. The ALLOC= data set is a secondary input data set. See the section “[Secondary Input Data Set](#)” on page 8071 for details. You can name only one secondary data set in each invocation of the procedure.

**ALLOCMIN=*n***

specifies the minimum sample size to allocate to a stratum. When you specify ALLOCMIN=*n*, PROC SURVEYSELECT allocates at least *n* sampling units to each stratum. If you do not specify the ALLOCMIN= option, PROC SURVEYSELECT allocates at least one sampling unit to each stratum by default.

The minimum stratum sample size *n* must be a positive integer. The ALLOCMIN value *n* times the number of strata should not exceed the total sample size to be allocated. For without-replacement selection methods, the ALLOCMIN value should not exceed the number of sampling units in any stratum.

**ALPHA= $\alpha$** 

specifies the level of the confidence interval for the [MARGIN=](#) determination of stratum sample sizes. See the section “[Specifying the Margin of Error](#)” on page 8069 for details.

The value of  $\alpha$  must be between 0 and 1; the default is 0.05. A confidence level of  $\alpha$  produces a  $100(1 - \alpha)\%$  confidence interval. The default of ALPHA=0.05 produces a 95% confidence interval.

**COST**

indicates that stratum costs are included in the secondary input data set. Use the COST option when you have already named the secondary input data set in another option, such as the [VAR=SAS-data-set](#) option. You provide the stratum costs in the secondary input data set variable `_COST_`.

A stratum cost represents the per-unit cost (the survey cost of a single unit in the stratum). Each stratum cost must be a positive number. Cost values are required if you specify the [ALLOC=OPTIMAL](#) option.

**COST=(*values*)**

specifies stratum costs, which are required if you specify the [ALLOC=OPTIMAL](#) option. You can separate *values* with blanks or commas.

A stratum cost represents the per-unit cost (the survey cost of a single unit in the stratum). Each stratum cost must be a positive number.

The number of COST= values must equal the number of strata in the input data set. List the stratum costs in the order in which the strata appear in the input data set. If you use the COST=*values* option, the input data set must be sorted by the STRATA variables in ascending order. You cannot use the DESCENDING or NOTSORTED option in the STRATA statement.

**COST=SAS-data-set**

names a SAS data set that contains the stratum costs. You provide the stratum costs in the COST= data set variable `_COST_`.

A stratum cost represents the per-unit cost (the survey cost of a single unit in the stratum). Each stratum cost must be a positive number. Stratum costs are required if you specify the [ALLOC=OPTIMAL](#) option.

The COST= data set should contain all the STRATA variables, with the same type and length as in the DATA= input data set. The STRATA groups should appear in the same order in the COST= data set as in the DATA= data set. The COST= data set is a secondary input data set. See the section “[Secondary Input Data Set](#)” on page 8071 for details. You can name only one secondary input data set in each invocation of the procedure.

### **MARGIN=***value*

specifies the desired margin of error for estimating the overall mean from the stratified sample. When you specify the MARGIN= option, PROC SURVEYSELECT determines the stratum sample sizes required to achieve this margin for the allocation method or proportions that you specify in the ALLOC= option. See the section “[Specifying the Margin of Error](#)” on page 8069 for details.

The MARGIN= *value* must be a positive number. When you specify the MARGIN= option, you must also provide the stratum variances in the VAR=(*values*), VAR=*SAS-data-set*, or VAR option.

You can use the ALPHA= option to set the level of the confidence interval that the MARGIN= computation uses. The default of ALPHA=0.05 specifies a 95% confidence interval.

You can request the MARGIN= option for any allocation method (proportional, optimal, or Neyman) or for allocation proportions that you provide (ALLOC=(*values*) or ALLOC=*SAS-data-set*). When you use the MARGIN= option, you cannot specify a total sample size in the SAMPSIZE= option in the PROC SURVEYSELECT statement.

### **NOSAMPLE**

requests that PROC SURVEYSELECT allocate the total sample size among the strata but not select the sample. When you specify the NOSAMPLE option, the OUT= output data set contains the stratum sample sizes that PROC SURVEYSELECT computes. See the section “[Allocation Output Data Set](#)” on page 8075 for details.

### **STATS**

displays statistics for the sample allocation. If you specify the MARGIN= option, the STATS option displays the expected margin of error for the allocation. See the section “[Specifying the Margin of Error](#)” on page 8069 for details. If you request ALLOC=OPTIMAL or ALLOC=NEYMAN without the MARGIN= option, the STATS option displays the expected variance, which is computed from the stratum variances that you provide and the allocated stratum sample sizes. If you request ALLOC=OPTIMAL, the STATS option also displays the total stratum cost, which is computed from the stratum costs that you provide and the allocated stratum sample sizes.

### **VAR**

indicates that stratum variances are included in the secondary input data set. Use the VAR option when you have already named the secondary input data set in another option, such as the COST=*SAS-data-set* option. You provide the stratum variances in the secondary input data set variable `_VAR_`.

Each stratum variance must be a positive number. Stratum variances are required if you specify the ALLOC=OPTIMAL, ALLOC=NEYMAN, or MARGIN= option.

### **VAR=(*values*)**

lists stratum variances, which are required if you specify the ALLOC=OPTIMAL, ALLOC=NEYMAN, or MARGIN= option. You can separate *values* with blanks or commas.

Each stratum variance must be a positive number. The number of VAR= values must equal the number of strata in the input data set. List the stratum variances in the order in which the strata appear in the

input data set. If you use the `VAR=(values)` option, the input data set must be sorted by the STRATA variables in ascending order. You cannot use the `DESCENDING` or `NOTSORTED` option in the STRATA statement.

**VAR=SAS-data-set**

names a SAS data set that contains the stratum variances. You provide the stratum variances in the `VAR=` data set variable `_VAR_`.

Each stratum variance must be a positive number. Stratum variances are required if you specify the `ALLOC=OPTIMAL`, `ALLOC=NEYMAN`, or `MARGIN=` option.

The `VAR=` data set should contain all the STRATA variables, with the same type and length as in the `DATA=` input data set. The STRATA groups should appear in the same order in the `VAR=` data set as in the `DATA=` data set. The `VAR=` data set is a secondary input data set. See the section “[Secondary Input Data Set](#)” on page 8071 for details. You can name only one secondary input data set in each invocation of the procedure.

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## Details: SURVEYSELECT Procedure

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### Missing Values

PROC SURVEYSELECT treats missing values of `STRATA` and `SAMPLINGUNIT` variables like any other STRATA or SAMPLINGUNIT variable value. The missing values form a separate, valid variable level.

When you use a `FREQ` statement for sample size allocation, all values of the frequency variable must be nonmissing. If there is a missing or nonpositive frequency, PROC SURVEYSELECT does not perform the allocation.

When you specify a `SIZE` variable, any sampling units that have missing or nonpositive size measures are excluded from the sample selection. The procedure provides a log note that reports the number of observations omitted due to missing or nonpositive size measures.

If you do not use a `SAMPLINGUNIT` statement with the `SIZE` statement, your sampling units are input data set observations, and observations that have missing or nonpositive size measures are excluded from the sample selection. If you do use a `SAMPLINGUNIT` statement with the `SIZE` statement, the procedure computes sampling unit size by summing the size measures of all observations in the unit. When summing the observation size measures, the procedure omits any observations that have missing or nonpositive size measures. If the size of an entire sampling unit is missing or nonpositive, the procedure excludes that unit from the sample selection. When a sampling unit is selected, the output data set includes all observations that belong to the selected unit, regardless of whether an observation’s size measure is missing.

If you provide stratum-level design or allocation information in a secondary input data set, the variable values should be nonmissing. For example, if a stratum value of `_NSIZE_` (or `SampleSize`) in the `SAMPSIZE=` secondary input data set is missing or negative, PROC SURVEYSELECT cannot select a sample from the stratum. The procedure gives an error message and skips the stratum. Similarly, if other secondary data

set variables have missing values for a stratum, a sample cannot be selected from the stratum. These variables include `_NRATE_`, `_MINSIZE_`, `_MAXSIZE_`, `_CERTSIZE_`, and `_CERTP_`. Additionally, if any of the sample allocation variables in the secondary input data set have missing or nonpositive values, PROC SURVEYSELECT cannot compute the sample allocation. Variables that provide information for allocation include `_ALLOC_`, `_VAR_`, and `_COST_`. See the section “Secondary Input Data Set” on page 8071 for details.

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## Sorting by CONTROL Variables

If you specify a `CONTROL` statement, PROC SURVEYSELECT sorts the input data set by the CONTROL variables before selecting the sample. If you also specify a `STRATA` statement, the procedure sorts by CONTROL variables within strata. Sorting by CONTROL variables is available for systematic and sequential selection methods, which include `METHOD=SYS`, `METHOD=PPS_SYS`, `METHOD=SEQ`, and `METHOD=PPS_SEQ`. Sorting provides additional control over the distribution of the sample and gives some benefits of proportionate stratification.

Control sorting is not available when you use a `SAMPLINGUNIT` statement, which defines groups of observations as units (clusters) for sample selection. See the description of the `SAMPLINGUNIT` statement for information about ordering clusters before systematic or sequential selection.

When you specify a `CONTROL` statement, the sorted data set replaces the input data set by default. Alternatively, you can use the `OUTSORT=` option to name an output data set that contains the sorted input data set.

PROC SURVEYSELECT provides two types of sorting: hierarchic serpentine sorting and nested sorting. By default (or if you specify the `SORT=SERP` option), the procedure uses serpentine sorting. If you specify the `SORT=NEST` option, then the procedure sorts by the CONTROL variables according to nested sorting. These two types of sorting are equivalent when there is only one CONTROL variable.

If you request nested sorting, PROC SURVEYSELECT sorts observations in the same order as PROC SORT does for an ascending sort by the CONTROL variables. See the chapter “The SORT Procedure” in the *Base SAS Procedures Guide* for more information. PROC SURVEYSELECT sorts within strata if you also specify a `STRATA` statement. The procedure first arranges the input observations in ascending order of the first CONTROL variable. Then within each level of the first control variable, the procedure arranges the observations in ascending order of the second CONTROL variable. This continues for all CONTROL variables that are specified.

In hierarchic serpentine sorting, PROC SURVEYSELECT sorts by the first CONTROL variable in ascending order. Then within the first level of the first CONTROL variable, the procedure sorts by the second CONTROL variable in ascending order. Within the second level of the first CONTROL variable, the procedure sorts by the second CONTROL variable in descending order. Sorting by the second CONTROL variable continues to alternate between ascending and descending sorting throughout all levels of the first CONTROL variable. If there is a third CONTROL variable, the procedure sorts by that variable within levels formed from the first two CONTROL variables, again alternating between ascending and descending sorting. This continues for all CONTROL variables that are specified. This sorting algorithm minimizes the change from one observation to the next with respect to the CONTROL variable values, thus making nearby observations more similar. For more information about serpentine sorting, see Chromy (1979) and Williams and Chromy (1980).

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## Random Number Generation

The probability sampling methods provided by PROC SURVEYSELECT use random numbers in their selection algorithms, as described in the following sections and in the references cited. PROC SURVEYSELECT uses a uniform random number function to generate streams of pseudo-random numbers from an initial starting point, or *seed*. You can use the **SEED=** option to specify the initial seed. If you do not specify the **SEED=** option, PROC SURVEYSELECT uses the time of day from the computer's clock to obtain the initial seed. See the description of the **SEED=** option for details about specifying initial seeds for strata, storing stratum seeds in the output data set, and reproducing samples.

Beginning in SAS/STAT 12.1, PROC SURVEYSELECT uses the Mersenne-Twister random number generator by default. The Mersenne-Twister generator (Matsumoto and Nishimura 1998) has a very long period ( $2^{19937} - 1$ ) and very good statistical properties. The algorithm is a twisted generalized feedback shift register. This is the same random number generator that the RAND function provides for the uniform distribution. See *SAS Functions and CALL Routines: Reference* for more information.

In previous releases, PROC SURVEYSELECT used the RANUNI random number generator, which you can now request by specifying the **RANUNI** option. This uniform random number generator is based on the method of Fishman and Moore (1982), which uses a prime modulus multiplicative generator with modulus  $2^{31}$  and multiplier 397,204,094. This is the same uniform random number generator that the RANUNI function provides. For more information about the RANUNI function, see *SAS Functions and CALL Routines: Reference*.

To reproduce samples that PROC SURVEYSELECT selected in releases prior to SAS/STAT 12.1, you can use the **RANUNI** option with the **SEED=** option (for the same input data set and selection parameters).

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## Sample Selection Methods

PROC SURVEYSELECT provides a variety of methods for selecting probability-based random samples. With probability sampling, each unit in the survey population has a known, positive probability of selection. This property of probability sampling avoids selection bias and enables you to use statistical theory to make valid inferences from the sample to the survey population. For more information about probability sampling, see Lohr (2010); Kish (1965, 1987); Kalton (1983); Cochran (1977).

In equal probability sampling, each unit in the sampling frame, or in a stratum, has the same probability of being selected for the sample. PROC SURVEYSELECT provides the following methods that select units with equal probability: simple random sampling, unrestricted random sampling, systematic random sampling, sequential random sampling, and Bernoulli sampling. In simple random sampling, units are selected *without replacement*, which means that a unit cannot be selected more than once. Both systematic and sequential equal probability sampling are also without replacement. In unrestricted random sampling, units are selected *with replacement*, which means that a unit can be selected more than once. In with-replacement sampling, the *number of hits* refers to the number of times a unit is selected.

In probability proportional to size (PPS) sampling, a unit's selection probability is proportional to its size measure. PROC SURVEYSELECT provides the following methods that select units with probability proportional to size (PPS): PPS sampling without replacement, PPS sampling with replacement, PPS systematic sampling, PPS sequential sampling, Brewer's method, Murthy's method, and Sampford's method. PPS sampling is often used in cluster sampling, where you select clusters (or groups of sampling units) of varying

size in the first stage of selection. For example, clusters might be schools, hospitals, or geographical areas, and the final sampling units might be students, patients, or citizens. Cluster sampling can provide efficiencies in frame construction and other survey operations. For more information, see Lohr (2010); Kalton (1983); Kish (1965), in addition to the other references cited in the following sections.

The following sections give detailed descriptions of the sample selection methods available in PROC SURVEYSELECT. In these sections,  $n_h$  denotes the sample size (the number of units in the sample) for stratum  $h$ , and  $N_h$  denotes the population size (number of units in the population) for stratum  $h$ , for  $h = 1, 2, \dots, H$ . When the sample design is not stratified,  $n$  denotes the sample size, and  $N$  denotes the population size. For PPS sampling,  $M_{hi}$  represents the size measure for unit  $i$  in stratum  $h$ ,  $M_h$  is the total of all size measures for the population of stratum  $h$ , and  $Z_{hi} = M_{hi}/M_h$  is the relative size of unit  $i$  in stratum  $h$ .

### Simple Random Sampling

The method of simple random sampling (**METHOD=SRS**) selects units with equal probability and without replacement. Each possible sample of  $n$  different units out of  $N$  has the same probability of being selected. The selection probability for each individual unit equals  $n/N$ . When you request stratified sampling with a **STRATA** statement, PROC SURVEYSELECT selects samples independently within strata. The selection probability for a unit in stratum  $h$  equals  $n_h/N_h$  for stratified simple random sampling.

By default, PROC SURVEYSELECT uses Floyd's ordered hash table algorithm for simple random sampling. This algorithm is fast, efficient, and appropriate for large data sets. See Bentley and Floyd (1987) and Bentley and Knuth (1986) for details.

If there is not enough memory available for Floyd's algorithm, PROC SURVEYSELECT switches to the sequential algorithm of Fan, Muller, and Rezucha (1962), which requires less memory but might require more time to select the sample. When PROC SURVEYSELECT uses the alternative sequential algorithm, it writes a note to the log. To request the sequential algorithm, even if enough memory is available for Floyd's algorithm, you can specify **METHOD=SRS2** in the PROC SURVEYSELECT statement.

### Unrestricted Random Sampling

The method of unrestricted random sampling (**METHOD=URS**) selects units with equal probability and with replacement. Because units are selected with replacement, a unit can be selected for the sample more than once. The expected number of hits (selections) for each unit equals  $n/N$  when sampling without stratification. For stratified sampling, the expected number of hits for a unit in stratum  $h$  equals  $n_h/N_h$ . Note that the expected number of hits exceeds 1 when the sample size  $n$  is greater than the population size  $N$ .

For unrestricted random sampling, by default, the output data set contains a single copy of each unit selected, even when a unit is selected more than once, and the variable **NumberHits** records the number of hits (selections) for each unit. If you specify the **OUTHITS** option, the output data set contains  $m$  copies of a sampling unit for which **NumberHits** equals  $m$ . For example, with the **OUTHITS** option a unit that is selected three times is represented by three copies in the output data set. For information about the contents of the output data set, see the section “**Sample Output Data Set**” on page 8072.



## Systematic Random Sampling

The method of systematic random sampling (**METHOD=SYS**) selects units at a fixed interval throughout the sampling frame or stratum after a random start. If you specify the sample size (or the stratum sample sizes) with the **SAMPSIZE=** option, PROC SURVEYSELECT uses a fractional interval to provide exactly the specified sample size. The interval equals  $N/n$ , or  $N_h/n_h$  for stratified sampling. The selection probability for each unit equals  $n/N$ , or  $n_h/N_h$  for stratified sampling. If you specify the sampling rate (or the stratum sampling rates) with the **SAMPRATE=** option, PROC SURVEYSELECT uses the inverse of the rate as the interval for systematic selection. The selection probability for each unit equals the specified rate.

Systematic random sampling controls the distribution of the sample by spreading it throughout the sampling frame or stratum at equal intervals, thus providing implicit stratification. You can use the **CONTROL** statement to order the input data set by the CONTROL variables before sample selection. If you also use a **STRATA** statement, PROC SURVEYSELECT sorts by the CONTROL variables within strata. If you do not specify a CONTROL statement, PROC SURVEYSELECT applies systematic selection to the observations in the order in which they appear in the input data set.

## Sequential Random Sampling

If you specify the **METHOD=SEQ** option and do not include a **SIZE** statement, PROC SURVEYSELECT uses the equal probability version of Chromy's method for sequential random sampling. This method selects units sequentially with equal probability and without replacement. See Chromy (1979) and Williams and Chromy (1980) for details. See the section "PPS Sequential Sampling" on page 8064 for a description of Chromy's PPS selection method.

Sequential random sampling controls the distribution of the sample by spreading it throughout the sampling frame or stratum, thus providing implicit stratification according to the order of units in the frame or stratum. You can use the **CONTROL** statement to sort the input data set by the CONTROL variables before sample selection. If you also use a **STRATA** statement, PROC SURVEYSELECT sorts by the CONTROL variables within strata. By default (or if you specify the **SORT=SERP** option), the procedure uses hierarchic serpentine ordering for sorting. If you specify the **SORT=NEST** option, the procedure uses nested sorting. See the section "Sorting by CONTROL Variables" on page 8057 for descriptions of serpentine and nested sorting. If you do not specify a CONTROL statement, PROC SURVEYSELECT applies sequential selection to the observations in the order in which they appear in the input data set.

Following Chromy's method of sequential selection, PROC SURVEYSELECT randomly chooses a starting unit from the entire stratum (or frame, if the design is not stratified). With this unit as the first one, the procedure treats the stratum units as a closed loop. This is done so that all pairwise (joint) selection probabilities are positive and an unbiased variance estimator can be obtained. The procedure numbers units sequentially from the random start to the end of the stratum and then continues from the beginning of the stratum until all units are numbered.

Beginning with the randomly chosen starting unit, PROC SURVEYSELECT accumulates the expected number of selections (hits), where the expected number of selections  $E(S_{hi})$  equals  $n_h/N_h$  for all units  $i$  in stratum  $h$ . The procedure computes

$$I_{hi} = \text{Int}\left(\sum_{j=1}^i E(S_{hj})\right) = \text{Int}(in_h/N_h)$$

$$F_{hi} = \text{Frac}\left(\sum_{j=1}^i E(S_{hj})\right) = \text{Frac}(in_h/N_h)$$

where  $\text{Int}(\cdot)$  denotes the integer part of the number, and  $\text{Frac}(\cdot)$  denotes the fractional part.

Considering each unit sequentially, Chromy's method determines whether unit  $i$  is selected by comparing the total number of selections for the first  $(i - 1)$  units,

$$T_{h(i-1)} = \sum_{j=1}^{i-1} S_{hj}$$

with the value of  $I_{h(i-1)}$ .

If  $T_{h(i-1)} = I_{h(i-1)}$ , Chromy's method determines whether or not unit  $i$  is selected as follows. If  $F_{hi} = 0$  or  $F_{h(i-1)} > F_{hi}$ , then unit  $i$  is selected with certainty. Otherwise, unit  $i$  is selected with probability

$$(F_{hi} - F_{h(i-1)}) / (1 - F_{h(i-1)})$$

If  $T_{h(i-1)} = (I_{h(i-1)} + 1)$ , Chromy's method determines whether or not unit  $i$  is selected as follows. If  $F_{hi} = 0$  or  $F_{hi} > F_{h(i-1)}$ , then the unit is not selected. Otherwise, unit  $i$  is selected with probability

$$F_{hi} / F_{h(i-1)}$$

## Bernoulli Sampling

Bernoulli sampling, which you request by specifying the `METHOD=BERNOULLI` option, is an equal probability selection method for which the total sample size is not fixed. PROC SURVEYSELECT performs an independent random selection trial for each of the  $N$  sampling units in the input data set by using the constant inclusion probability (sampling rate) that you specify. You can specify a single value of the inclusion probability  $\pi$  to use for all  $N$  sampling units, or you can specify separate stratum-level values of  $\pi_h$  to use for the  $N_h$  units in each stratum.

You provide the inclusion probability (or probabilities) by specifying the `SAMPRATE=` option. For stratified sampling (which you request with the `STRATA` statement), you can specify the same sampling rate for each stratum by using the `SAMPRATE=r` option. Or you can specify different sampling rates for different strata by using the `SAMPRATE=(values)` or `SAMPRATE=SAS-data-set` option.

In Bernoulli sampling, the sample size  $n$  (number of units selected) is not fixed; it is a random variable that has a binomial distribution with parameters  $N$  and  $\pi$ . The possible values of  $n$  range from 0 to  $N$ . The expected value of the sample size is  $\pi N$  (or  $\pi_h N_h$  for stratified sampling), and the variance of the sample size is  $\pi(1 - \pi)N$ .

For Bernoulli sampling, the selection probability is the inclusion probability that you specify by using the `SAMPRATE=` option. PROC SURVEYSELECT computes the sampling weight as the inverse of the selection probability, which is  $1/\pi$ . For Bernoulli sampling, the procedure also computes an adjusted sampling weight as the ratio of the total number of sampling units to the actual sample size,  $N/n$  (or  $N_h/n_h$  for stratified sampling). The joint selection probability for any two distinct units is  $\pi^2$ . See Särndal, Swensson, and Wretman (1992) for more information.

You can specify the `STATS` option to include the following information in the `OUT=` output data set for `METHOD=BERNOULLI`: total number of sampling units, selection probability, expected sample size, actual sample size, sampling weight, and adjusted sampling weight.



## Poisson Sampling

Poisson sampling, which you request by specifying the `METHOD=POISSON` option, is an unequal probability sampling method for which the total sample size is not fixed. A generalization of Bernoulli sampling, Poisson sampling also consists of independent random selection trials for the  $N$  sampling units in the input data set, but the sampling units can have different inclusion probabilities. You provide inclusion probabilities for Poisson sampling in the variable that you specify in the `SIZE` statement.

The expected value of the sample size for Poisson sampling is  $\sum_i \pi_i$ , where  $\pi_i$  is the inclusion probability for sampling unit  $i$ . The variance of the sample size is  $\sum_i \pi_i(1 - \pi_i)$ .

For Poisson sampling, the selection probability for unit  $i$  is the inclusion probability  $\pi_i$  that you specify by using the `SIZE` statement. PROC SURVEYSELECT computes the sampling weight for unit  $i$  as the inverse of the selection probability, which is  $1/\pi_i$ . The joint selection probability for any two distinct units  $i$  and  $j$  is  $\pi_i \pi_j$  for Poisson sampling. See Särndal, Swensson, and Wretman (1992) for more information.

## PPS Sampling without Replacement

If you specify the `METHOD=PPS` option, PROC SURVEYSELECT selects units with probability proportional to size and without replacement. The selection probability for unit  $i$  in stratum  $h$  equals  $n_h Z_{hi}$ , where  $n_h$  is the sample size for stratum  $h$ , and  $Z_{hi}$  is the relative size of unit  $i$  in stratum  $h$ . The relative size equals  $M_{hi}/M_{h\cdot}$ , which is the ratio of the size measure for unit  $i$  in stratum  $h$  ( $M_{hi}$ ) to the total of all size measures for stratum  $h$  ( $M_{h\cdot}$ ).

Because selection probabilities cannot exceed 1, the relative size for each unit must not exceed  $1/n_h$  for `METHOD=PPS`. This requirement can be expressed as  $Z_{hi} \leq 1/n_h$ , or equivalently,  $M_{hi} \leq M_{h\cdot}/n_h$ . If your size measures do not meet this requirement, you can adjust the size measures by using the `MAXSIZE=` or `MINSIZE=` option. Or you can request certainty selection for the larger units by using the `CERTSIZE=` or `CERTSIZE=P=` option. Alternatively, you can use a selection method that does not have this relative size restriction, such as PPS with minimum replacement (`METHOD=PPS_SEQ`).

PROC SURVEYSELECT uses the Hanurav-Vijayan algorithm for PPS selection without replacement. Hanurav (1967) introduced this algorithm for the selection of two units per stratum, and Vijayan (1968) generalized it for the selection of more than two units. The algorithm enables computation of joint selection probabilities and provides joint selection probability values that usually ensure nonnegativity and stability of the Sen-Yates-Grundy variance estimator. For details, see Fox (1989); Golmant (1990); Watts (1991).

Notation in the remainder of this section drops the stratum subscript  $h$  for simplicity, but selection is still done independently within strata if you specify a stratified design. For a stratified design,  $n$  now denotes the sample size for the current stratum,  $N$  denotes the stratum population size, and  $M_i$  denotes the size measure for unit  $i$  in the stratum. If the design is not stratified, this notation applies to the entire sampling frame.

According to the Hanurav-Vijayan algorithm, PROC SURVEYSELECT first orders units within the stratum in ascending order by size measure, so that  $M_1 \leq M_2 \leq \dots \leq M_N$ . Then the procedure selects the PPS sample of  $n$  observations as follows:

1. The procedure randomly chooses one of the integers  $1, 2, \dots, n$  with probability  $\theta_1, \theta_2, \dots, \theta_n$ , where

$$\theta_i = n(Z_{N-n+i+1} - Z_{N-n+i})(T + iZ_{N-n+1})/T$$

where  $Z_j = M_j/M$  and

$$T = \sum_{j=1}^{N-n} Z_j$$

By definition,  $Z_{N+1} = 1/n$  to ensure that  $\sum_{i=1}^n \theta_i = 1$ .

2. If  $i$  is the integer selected in step 1, the procedure includes the last  $(n - i)$  units of the stratum in the sample, where the units are ordered by size measure as described previously. The procedure then selects the remaining  $i$  units according to steps 3 through 6.
3. The procedure defines new normed size measures for the remaining  $(N - n + i)$  stratum units that were not selected in steps 1 and 2:

$$Z_j^* = \begin{cases} Z_j/(T + iZ_{N-n+1}) & \text{for } j = 1, \dots, N - n + 1 \\ Z_{N-n+1}/(T + iZ_{N-n+1}) & \text{for } j = N - n + 2, \dots, N - n + i \end{cases}$$

4. The procedure selects the next unit from the first  $(N - n + 1)$  stratum units with probability proportional to  $a_j(1)$ , where

$$\begin{aligned} a_1(1) &= iZ_1^* \\ a_j(1) &= iZ_j^* \prod_{k=1}^{j-1} (1 - (i - 1) P_k) \quad \text{for } j = 2, \dots, N - n + 1 \end{aligned}$$

and

$$P_k = M_k/(M_{k+1} + M_{k+2} + \dots + M_{N-n+i})$$

5. If stratum unit  $j_1$  is the unit selected in step 4, then the procedure selects the next unit from units  $(j_1 + 1)$  through  $(N - n + 2)$  with probability proportional to  $a_j(2, j_1)$ , where

$$\begin{aligned} a_{j_1+1}(2, j_1) &= (i - 1)Z_{j_1+1}^* \\ a_j(2, j_1) &= (i - 1)Z_j^* \prod_{k=j_1+1}^{j-1} (1 - (i - 2)P_k) \quad \text{for } j = j_1 + 2, \dots, N - n + 2 \end{aligned}$$

6. The procedure repeats step 5 until all  $n$  sample units are selected.

If you specify the **JTPROBS** option, PROC SURVEYSELECT computes the joint selection probabilities for all pairs of selected units in each stratum. The joint selection probability for units  $i$  and  $j$  in the stratum equals

$$P_{(ij)} = \sum_{r=1}^n \theta_r K_{ij}^{(r)}$$

where

$$K_{ij} = \begin{cases} 1 & N - n + r < i \leq N - 1 \\ rZ_{N-n+1}/(T + rZ_{N-n+1}) & N - n < i \leq N - n + r, \quad j > N - n + r \\ rZ_i/(T + rZ_{N-n+1}) & 1 \leq i \leq N - n, \quad j > N - n + r \\ \pi_{ij}^{(r)} & j \leq N - n + r \end{cases}$$

$$\pi_{ij}^{(r)} = \frac{r(r - 1)}{2} P_i Z_j \prod_{k=1}^{i-1} (1 - P_k)$$

$$P_k = M_k/(M_{k+1} + M_{k+2} + \dots + M_{N-n+r})$$

## PPS Sampling with Replacement

If you specify the `METHOD=PPS_WR` option, PROC SURVEYSELECT selects units with probability proportional to size and with replacement. The procedure makes  $n_h$  independent random selections from the stratum of  $N_h$  units, selecting with probability  $Z_{hi} = M_{hi}/M_h$ . Because units are selected with replacement, a unit can be selected for the sample more than once. The expected number of hits (selections) for unit  $i$  in stratum  $h$  equals  $n_h Z_{hi}$ . If you specify the `JTPROBS` option, PROC SURVEYSELECT computes the joint expected number of hits for all pairs of selected units in each stratum. The joint expected number of hits for units  $i$  and  $j$  in stratum  $h$  equals

$$P_{h(ij)} = \begin{cases} n_h(n_h - 1)Z_{hi}Z_{hj} & \text{for } j \neq i \\ n_h(n_h - 1)Z_{hi}Z_{hi}/2 & \text{for } j = i \end{cases}$$

## PPS Systematic Sampling

If you specify the `METHOD=PPS_SYS` option, PROC SURVEYSELECT selects units by systematic random sampling with probability proportional to size. Systematic sampling selects units at a fixed interval throughout the stratum or sampling frame after a random start. PROC SURVEYSELECT uses a fractional interval to provide exactly the specified sample size. The interval equals  $M_h/n_h$  for stratified sampling and  $M/n$  for sampling without stratification. Depending on the sample size and the values of the size measures, it might be possible for a unit to be selected more than once. The expected number of hits (selections) for unit  $i$  in stratum  $h$  equals  $n_h M_{hi}/M_h = n_h Z_{hi}$ . See Cochran (1977, pp. 265–266) and Madow (1949) for details.

Systematic random sampling controls the distribution of the sample by spreading it throughout the sampling frame or stratum at equal intervals, thus providing implicit stratification. You can use the `CONTROL` statement to order the input data set by the `CONTROL` variables before sample selection. If you also use a `STRATA` statement, PROC SURVEYSELECT sorts by the `CONTROL` variables within strata. If you do not specify a `CONTROL` statement, PROC SURVEYSELECT applies systematic selection to the observations in the order in which they appear in the input data set.

## PPS Sequential Sampling

If you specify the `METHOD=PPS_SEQ` option, PROC SURVEYSELECT uses Chromy's method of sequential random sampling. See Chromy (1979) and Williams and Chromy (1980) for details. Chromy's method selects units sequentially with probability proportional to size and with minimum replacement. Selection *with minimum replacement* means that the actual number of hits for a unit can equal the integer part of the expected number of hits for that unit, or the next largest integer. This can be compared to selection *without replacement*, where each unit can be selected only once, so the number of hits can equal 0 or 1. The other alternative is selection *with replacement*, where there is no restriction on the number of hits for each unit, so the number of hits can equal  $0, 1, \dots, n_h$ , where  $n_h$  is the stratum sample size.

Sequential random sampling controls the distribution of the sample by spreading it throughout the sampling frame or stratum, thus providing implicit stratification according to the order of units in the frame or stratum. You can use the `CONTROL` statement to sort the input data set by the `CONTROL` variables before sample selection. If you also use a `STRATA` statement, PROC SURVEYSELECT sorts by the `CONTROL` variables within strata. By default (or if you specify the `SORT=SERP` option), the procedure uses hierarchic

serpentine ordering to sort the sampling frame by the CONTROL variables within strata. If you specify the **`SORT=NEST`** option, the procedure uses nested sorting. See the section “**Sorting by CONTROL Variables**” on page 8057 for descriptions of serpentine and nested sorting. If you do not specify a CONTROL statement, PROC SURVEYSELECT applies sequential selection to the observations in the order in which they appear in the input data set.

According to Chromy’s method of sequential selection, PROC SURVEYSELECT first chooses a starting unit randomly from the entire stratum, with probability proportional to size. The procedure uses this unit as the first one and treats the stratum observations as a closed loop. This is done so that all pairwise (joint) expected number of hits are positive and an unbiased variance estimator can be obtained. The procedure numbers observations sequentially from the random start to the end of the stratum and then continues from the beginning of the stratum until all units are numbered.

Beginning with the randomly chosen starting unit, Chromy’s method partitions the ordered stratum sampling frame into  $n_h$  zones of equal size. There is one selection from each zone and a total of  $n_h$  hits (selections), although fewer than  $n_h$  distinct units might be selected. Beginning with the random start, the procedure accumulates the expected number of hits and computes

$$E(S_{hi}) = n_h Z_{hi}$$

$$I_{hi} = \text{Int}\left(\sum_{j=1}^i E(S_{hj})\right)$$

$$F_{hi} = \text{Frac}\left(\sum_{j=1}^i E(S_{hj})\right)$$

where  $E(S_{hi})$  represents the expected number of hits for unit  $i$  in stratum  $h$ ,  $\text{Int}(\cdot)$  denotes the integer part of the number, and  $\text{Frac}(\cdot)$  denotes the fractional part.

Considering each unit sequentially, Chromy’s method determines the actual number of hits for unit  $i$  by comparing the total number of hits for the first  $(i - 1)$  units,

$$T_{h(i-1)} = \sum_{j=1}^{i-1} S_{hj}$$

with the value of  $I_{h(i-1)}$ .

If  $T_{h(i-1)} = I_{h(i-1)}$ , Chromy’s method determines the total number of hits for the first  $i$  units as follows. If  $F_{hi} = 0$  or  $F_{h(i-1)} > F_{hi}$ , then  $T_{hi} = I_{hi}$ . Otherwise,  $T_{hi} = I_{hi} + 1$  with probability

$$(F_{hi} - F_{h(i-1)}) / (1 - F_{h(i-1)})$$

And the number of hits for unit  $i$  equals  $T_{hi} - T_{h(i-1)}$ .

If  $T_{h(i-1)} = (I_{h(i-1)} + 1)$ , Chromy’s method determines the total number of hits for the first  $i$  units as follows. If  $F_{hi} = 0$ , then  $T_{hi} = I_{hi}$ . If  $F_{hi} > F_{h(i-1)}$ , then  $T_{hi} = I_{hi} + 1$ . Otherwise,  $T_{hi} = I_{hi} + 1$  with probability

$$F_{hi} / F_{h(i-1)}$$

### Brewer's PPS Method

Brewer's method (`METHOD=PPS_BREWER`) selects two units from each stratum, with probability proportional to size and without replacement. The selection probability for unit  $i$  in stratum  $h$  equals  $2M_{hi}/M_h = 2Z_{hi}$ . (Because selection probabilities cannot exceed 1, the relative size for each unit,  $Z_{hi}$ , must not exceed  $1/2$ .)

Brewer's algorithm first selects a unit with probability

$$\frac{Z_{hi}(1 - Z_{hi})}{D_h(1 - 2Z_{hi})}$$

where

$$D_h = \sum_{i=1}^{N_h} \frac{Z_{hi}(1 - Z_{hi})}{1 - 2Z_{hi}}$$

Then a second unit is selected from the remaining units with probability

$$\frac{Z_{hj}}{1 - Z_{hi}}$$

where unit  $i$  is the first unit selected. The joint selection probability for units  $i$  and  $j$  in stratum  $h$  equals

$$P_{h(ij)} = \frac{2Z_{hi}Z_{hj}}{D_h} \left( \frac{1 - Z_{hi} - Z_{hj}}{(1 - 2Z_{hi})(1 - 2Z_{hj})} \right)$$

See Cochran (1977, pp. 261–263) and Brewer (1963) for details. Brewer's method yields the same selection probabilities and joint selection probabilities as Durbin's method. See Cochran (1977) and Durbin (1967) for details.

### Murthy's PPS Method

Murthy's method (`METHOD=PPS_MURTHY`) selects two units from each stratum, with probability proportional to size and without replacement. The selection probability for unit  $i$  in stratum  $h$  equals

$$P_{hi} = Z_{hi}(1 + K_h - (Z_{hi}/(1 - Z_{hi})))$$

where  $Z_{hi} = M_{hi}/M_h$  and

$$K_h = \sum_{j=1}^{N_h} (Z_{hj}/(1 - Z_{hj}))$$

Murthy's algorithm first selects a unit with probability  $Z_{hi}$ . Then a second unit is selected from the remaining units with probability  $Z_{hj}/(1 - Z_{hi})$ , where unit  $i$  is the first unit selected. The joint selection probability for units  $i$  and  $j$  in stratum  $h$  equals

$$P_{h(ij)} = Z_{hi}Z_{hj} \left( \frac{2 - Z_{hi} - Z_{hj}}{(1 - Z_{hi})(1 - Z_{hj})} \right)$$

See Cochran (1977, pp. 263–265) and Murthy (1957) for details.

## Sampford's PPS Method

Sampford's method (METHOD=PPS\_SAMPFORD) is an extension of Brewer's method that selects more than two units from each stratum, with probability proportional to size and without replacement. The selection probability for unit  $i$  in stratum  $h$  equals  $n_h M_{hi} / M_h = n_h Z_{hi}$ . (Because selection probabilities cannot exceed 1, the relative size for each unit,  $Z_{hi}$ , must not exceed  $1/n_h$ .)

Sampford's method first selects a unit from stratum  $h$  with probability  $Z_{hi}$ . Then subsequent units are selected with probability proportional to

$$\lambda_{hi} = Z_{hi} / (1 - n_h Z_{hi})$$

and with replacement. If the same unit appears more than once in the sample of size  $n_h$ , then Sampford's algorithm rejects that sample and selects a new sample. The sample is accepted if it contains  $n_h$  distinct units.

If you specify the JTPROBS option, PROC SURVEYSELECT computes the joint selection probabilities for all pairs of selected units in each stratum. The joint selection probability for units  $i$  and  $j$  in stratum  $h$  equals

$$P_{h(ij)} = K_h \lambda_{hi} \lambda_{hj} \sum_{t=2}^{n_h} \left( [t - n_h (Z_{hi} + Z_{hj})] L_{h,(n_h-t)}(\bar{ij}) \right) / n_h^{t-2}$$

where

$$K_h = 1 / \sum_{t=1}^{n_h} (t L_{h,(n_h-t)} / n_h^t)$$

$$L_{h,m} = \sum_{S_h(m)} \lambda_{hi_1} \lambda_{hi_2} \cdots \lambda_{hi_m}$$

and  $S_h(m)$  denotes all possible samples of size  $m$ , for  $m = 1, 2, \dots, N_h$ . The sum  $L_{h,m}(\bar{ij})$  is defined similarly to  $L_{h,m}$  but sums over all possible samples of size  $m$  that do not include units  $i$  and  $j$ . See Cochran (1977, pp. 262–263) and Sampford (1967) for details.

## Sample Size Allocation

If you specify the ALLOC= option in the STRATA statement, PROC SURVEYSELECT allocates the total sample size among the strata according to the method that you request. PROC SURVEYSELECT provides proportional allocation (ALLOC=PROP), optimal allocation (ALLOC=OPTIMAL), and Neyman allocation (ALLOC=NEYMAN). For more information about these allocation methods, see Lohr (2010); Kish (1965); Cochran (1977). You can also directly provide the allocation proportions by using the ALLOC=(values) option or the ALLOC=SAS-data-set option. Then PROC SURVEYSELECT allocates the sample size among the strata according to the proportions that you provide. Allocation proportions are the relative stratum sample sizes,  $n_h/n$ , where  $n_h$  is the sample size for stratum  $h$  and  $n$  is the total sample size.

You can use the SAMPSIZE= $n$  option in the PROC SURVEYSELECT statement to specify the total sample size to allocate among the strata. Or you can specify the desired margin of error in the MARGIN= option in the STRATA statement, and PROC SURVEYSELECT computes the stratum sample sizes necessary to achieve that margin of error for the allocation method that you request. See the section “Specifying the Margin of Error” on page 8069 for details.

## Proportional Allocation

When you specify the `ALLOC=PROP` option in the `STRATA` statement, PROC SURVEYSELECT allocates the total sample size among the strata in proportion to the stratum sizes, where the stratum size is the number of sampling units in the stratum. The allocation proportion of the total sample size for stratum  $h$  equals

$$f_h^* = N_h/N$$

where  $N_h$  is the number of sampling units in stratum  $h$  and  $N$  is the total number of sampling units for all strata. If you specify the total sample size  $n$  in the `SAMPsize=` option in the `PROC SURVEYSELECT` statement, the procedure computes the target sample size for stratum  $h$  as

$$n_h^* = f_h^* \times n$$

The target sample size values,  $n_h^*$ , might not be integers, but the stratum sample sizes are required to be integers. PROC SURVEYSELECT uses a rounding algorithm to convert the  $n_h^*$  to integer values  $n_h$  and maintain the requested total sample size  $n$ . The rounding algorithm includes the restriction that all values of  $n_h$  must be at least 1, so that at least one unit is selected from each stratum. If you specify a minimum stratum sample size  $n_{min}$  in the `ALLOCmin=` option in the `STRATA` statement, then all values of  $n_h$  are required to be at least  $n_{min}$ . For without-replacement selection methods, PROC SURVEYSELECT also requires that each stratum sample size must not exceed the total number of sampling units in the stratum,  $n_h \leq N_h$ . If a target stratum sample size exceeds the number of units in the stratum, PROC SURVEYSELECT allocates the maximum number of units,  $N_h$ , to the stratum, and then allocates the remaining total sample size proportionally among the remaining strata.

PROC SURVEYSELECT provides the target allocation proportions  $f_h^*$  in the output data set variable `AllocProportion`. The variable `ActualProportion` contains the actual proportions for the allocated sample sizes  $n_h$ . For stratum  $h$ , the actual proportion is computed as

$$f_h = n_h/n$$

where  $n_h$  is the allocated sample size for stratum  $h$  and  $n$  is the total sample size. The actual proportions  $f_h$  can differ from the target allocation proportions  $f_h^*$  due to rounding, the requirement that  $n_h \geq 1$  (or  $n_h \geq n_{min}$ ), and the requirement that  $n_h \leq N_h$  for without-replacement selection methods.

## Optimal Allocation

When you specify the `ALLOC=OPTIMAL` option in the `STRATA` statement, PROC SURVEYSELECT allocates the total sample size among the strata in proportion to stratum sizes, stratum costs, and stratum variances. You provide the stratum costs and variances by using the `COST=` and `VAR=` options, respectively.

Optimal allocation minimizes the overall variance for a specified cost, or equivalently minimizes the overall cost for a specified variance. For details, see Lohr (2010); Cochran (1977); Kish (1965). For optimal allocation, PROC SURVEYSELECT computes the proportion of the total sample size for stratum  $h$  as

$$f_h^* = \frac{N_h S_h}{\sqrt{C_h}} / \sum_{i=1}^H \frac{N_i S_i}{\sqrt{C_i}}$$

where  $N_h$  is the number of sampling units in stratum  $h$ ,  $S_h$  is the standard deviation within stratum  $h$ ,  $C_h$  is the unit cost within stratum  $h$ , and  $H$  is the total number of strata.



If you specify the total sample size  $n$  in the `SAMPsize=` option in the `PROC SURVEYSELECT` statement, the procedure computes the target sample size for stratum  $h$  as

$$n_h^* = f_h^* \times n$$

As described in the section “Proportional Allocation” on page 8068, the values of  $n_h^*$  are converted to integer sample sizes  $n_h$  by using a rounding algorithm that requires the sum of the stratum sample sizes to equal  $n$ . The final stratum sample sizes  $n_h$  are also required to be at least 1, or at least  $n_{min}$  if you specify a minimum stratum sample size in the `ALLOCmin=` option in the `STRATA` statement. For without-replacement selection methods, the final sample sizes cannot exceed the stratum sizes.

## Neyman Allocation

When you specify the `ALLOC=NEYMAN` option in the `STRATA` statement, `PROC SURVEYSELECT` allocates the total sample size among the strata in proportion to stratum sizes and stratum variances. Neyman allocation is a special case of optimal allocation (described in the section “Optimal Allocation” on page 8068), where the costs per unit are the same for all strata. For Neyman allocation, the proportion of the total sample size for stratum  $h$  is computed as

$$f_h^* = N_h S_h / \sum_{i=1}^H N_i S_i$$

If you specify the total sample size  $n$  in the `SAMPsize=` option in the `PROC SURVEYSELECT` statement, the procedure computes the target sample size for stratum  $h$  as  $n_h^* = f_h^* \times n$ . The  $n_h^*$  are converted to integer sample sizes  $n_h$  by using a rounding algorithm that requires the sum of the stratum sizes to equal  $n$ . The final sample sizes  $n_h$  are required to be at least 1, or at least  $n_{min}$  if you specify a minimum sample size in the `ALLOCmin=` option in the `STRATA` statement. For without-replacement selection methods, the final sample sizes must not exceed the stratum sizes.

## Specifying the Margin of Error

Instead of specifying the total sample size to allocate among the strata, you can specify the desired margin of error for estimating the overall mean from the stratified sample. Based on the requested allocation method and the stratum variances that you provide, `PROC SURVEYSELECT` computes the stratum sample sizes that are required to achieve this margin of error. You specify the margin of error in the `MARGIN=` option in the `STRATA` statement, and you provide stratum variances in the `VAR=` option. You can use the `MARGIN=` option with any allocation method (proportional, optimal, or Neyman) or with allocation proportions that you provide (`ALLOC=(values)` or `ALLOC=SAS-data-set`).

The margin of error  $e$  is the half-width of the  $100(1 - \alpha)\%$  confidence interval for the overall mean based on the stratified sample,

$$e = z_{\alpha/2} \times \sqrt{\text{Var}(\bar{y}_{str})}$$

where  $\text{Var}(\bar{y}_{str})$  is the variance of the estimate of the mean from the stratified sample and  $z_{\alpha/2}$  is the  $100(1 - \alpha/2)$  percentile of the standard normal distribution. You can specify the value of  $\alpha$  in the `ALPHA=` option in the `STRATA` statement. By default, `PROC SURVEYSELECT` uses a 95% confidence interval (`ALPHA=0.05`).



For the specified margin of error  $e$ , PROC SURVEYSELECT computes the target stratum sample sizes  $n_h^*$  for without-replacement selection methods as

$$n_h^* = f_h^* \left( \sum_{i=1}^H N_i^2 S_i^2 / f_i^* \right) / \left( (eN/z_{\alpha/2})^2 + \sum_{i=1}^H N_i S_i^2 \right)$$

where  $N_i$  is the number of sampling units in stratum  $i$ ,  $S_i^2$  is the variance within stratum  $i$ ,  $N$  is the total number of sampling units for all strata, and  $H$  is the total number of strata.

The values of  $f_h^*$  are the stratum allocation proportions, which PROC SURVEYSELECT computes according to the allocation method that you request. See the sections “[Proportional Allocation](#)” on page 8068, “[Optimal Allocation](#)” on page 8068, and “[Neyman Allocation](#)” on page 8069 for details.

For with-replacement selection methods, PROC SURVEYSELECT computes the target stratum sample sizes as

$$n_h^* = f_h^* \left( \sum_{i=1}^H N_i^2 S_i^2 / f_i^* \right) / (eN/z_{\alpha/2})^2$$

See Lohr (2010, p. 91), Cochran (1977, Chapter 5), and Arkin (1984, Chapter 10) for more information.

The target sample size values  $n_h^*$  might not be integers, but the stratum sample sizes are required to be integers. PROC SURVEYSELECT rounds all fractional target sample sizes up to integer sample sizes. If you specify a minimum stratum sample size  $n_{min}$  in the `ALLOCMIN=` option in the `STRATA` statement, then all stratum sample sizes  $n_h$  are required to be at least  $n_{min}$ .

For without-replacement selection methods, a stratum sample size cannot exceed the number of units in the stratum. If a target stratum sample size does exceed the number of units in the stratum, the procedure sets  $n_h = N_h$  for that stratum, removes the stratum from the variance computation (because it contributes nothing to the sampling error), revises the allocation proportions  $f_h^*$  for the remaining strata, and computes the stratum sample sizes again. If a stratum sample size equals the number of units in its stratum, the procedure also removes that stratum from the variance computation and revises the sample sizes for the remaining strata. See Cochran (1977, p. 104) and Arkin (1984, p. 176) for details.

When you specify the `STATS` option with the `MARGIN=` option in the `STRATA` statement, PROC SURVEYSELECT displays the expected margin of error for the sample allocation. The expected margin of error (for the overall mean based on the stratified sample) is computed from the stratum sizes ( $N_i$ ), the stratum variances that you provide ( $S_i^2$ ), and the allocated stratum sample sizes that the procedure computes ( $n_i$ ). For without-replacement selection methods, the expected margin of error is

$$e = z_{\alpha/2} \times \frac{1}{N} \sqrt{\sum_{i=1}^H \frac{N_i^2 S_i^2}{n_i} \left(1 - \frac{n_i}{N}\right)}$$

For with-replacement selection methods, the expected margin of error is

$$e = z_{\alpha/2} \times \frac{1}{N} \sqrt{\sum_{i=1}^H \frac{N_i^2 S_i^2}{n_i}}$$

The expected margin of error should be less than or equal to the value specified in the `MARGIN=` option. Any difference between the expected margin and the specified value is due to rounding the target stratum sample sizes up to integer values and increasing stratum sample sizes to equal the required minimum value (`ALLOCMIN=`).

## Secondary Input Data Set

The primary input data set for PROC SURVEYSELECT is the `DATA=` data set, which contains the list of units from which the sample is selected. You can use a secondary input data set to provide stratum-level design and selection information, such as sample sizes or rates, certainty size values, or stratum costs. This secondary input data set is sometimes called the `SAMPSIZE=` input data set. You can provide stratum sample sizes in the `_NSIZE_` (or `SampleSize`) variable in the `SAMPSIZE=` data set.

The secondary input data set must contain all the `STRATA` variables, with the same type and length as in the `DATA=` data set. The `STRATA` groups should appear in the same order in the secondary data set as in the `DATA=` data set. You can name only one secondary data set in each invocation of the procedure.

You must name the secondary input data set in the appropriate `PROC SURVEYSELECT` or `STRATA` option, and use the designated variable name to provide the stratum-level values. For example, if you want to provide stratum-level costs for sample allocation, you name the secondary data set in the `COST=SAS-data-set` option in the `STRATA` statement. The data set must include the stratum costs in a variable named `_COST_`. You can use the secondary input data set for more than one option if it is appropriate for your design. For example, the secondary data set can include both stratum costs and stratum variances, which are required for optimal allocation (`ALLOC=OPTIMAL`).

Instead of using a separate secondary input data set, you can include secondary information in the `DATA=` data set along with the sampling frame. When you include secondary information in the `DATA=` data set, name the `DATA=` data set in the appropriate options, and include the required variables in the `DATA=` data set.

Table 95.3 lists the available secondary data set variables, together with their descriptions and the corresponding options.

**Table 95.3** PROC SURVEYSELECT Secondary Data Set Variables

| Variable                | Description           | Statement           | Option                   |
|-------------------------|-----------------------|---------------------|--------------------------|
| <code>_ALLOC_</code>    | Allocation proportion | <code>STRATA</code> | <code>ALLOC=</code>      |
| <code>_CERTP_</code>    | Certainty proportion  | <code>PROC</code>   | <code>CERTSIZE=P=</code> |
| <code>_CERTSIZE_</code> | Certainty size        | <code>PROC</code>   | <code>CERTSIZE=</code>   |
| <code>_COST_</code>     | Cost                  | <code>STRATA</code> | <code>COST=</code>       |
| <code>_MAXSIZE_</code>  | Maximum size          | <code>PROC</code>   | <code>MAXSIZE=</code>    |
| <code>_MINSIZE_</code>  | Minimum size          | <code>PROC</code>   | <code>MINSIZE=</code>    |
| <code>_NSIZE_</code>    | Sample size           | <code>PROC</code>   | <code>SAMPSIZE=</code>   |
| <code>_RATE_</code>     | Sampling rate         | <code>PROC</code>   | <code>SAMPRATE=</code>   |
| <code>_SEED_</code>     | Random number seed    | <code>PROC</code>   | <code>SEED=</code>       |
| <code>_VAR_</code>      | Variance              | <code>STRATA</code> | <code>VAR=</code>        |

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## Sample Output Data Set

PROC SURVEYSELECT selects a sample and creates a SAS data set that contains the sample of selected units, unless you specify the **NOSAMPLE** option in the **STRATA** statement. If you specify the **NOSAMPLE** option, PROC SURVEYSELECT allocates the total sample size among the strata but does not select the sample. When you specify the **NOSAMPLE** option, the output data set contains the allocated sample sizes. See the section “Allocation Output Data Set” on page 8075 for details.

You can specify the name of the sample output data set in the **OUT=** option in the PROC SURVEYSELECT statement. If you omit the **OUT=** option, the data set is named **DATA $n$** , where  $n$  is the smallest integer that makes the name unique.

The output data set contains the units that are selected for the sample. These units are either observations or groups of observations (clusters) that you define by specifying the **SAMPLINGUNIT** statement. If you do not specify the **SAMPLINGUNIT** statement to define units (clusters), then PROC SURVEYSELECT uses observations as sampling units by default.

By default, the output data set contains only those units that are selected for the sample. But if you specify the **OUTALL** option, the output data set includes all observations from the input data set and also contains a variable that indicates each observation’s selection status. The variable **Selected** equals 1 for an observation selected for the sample, and equals 0 for an observation not selected. The **OUTALL** option is available for equal probability selection methods.

By default, the output data set contains a single copy of each selected unit, even if the unit is selected more than once, and the variable **NumberHits** records the number of hits (selections) for each unit. A unit can be selected more than once if you use a with-replacement or with-minimum-replacement selection method (**METHOD=URS**, **METHOD=PPS\_WR**, **METHOD=PPS\_SYS**, or **METHOD=PPS\_SEQ**). If you specify the **OUTHITS** option, the output data set includes a distinct copy of each selected unit in the output data set. For example, with the **OUTHITS** option a unit that is selected three times is represented by three copies in the output data set.

The output data set also contains design information and selection statistics, depending on the selection method and output options you specify. The output data set can include the following variables:

- **Selected**, which indicates whether or not the observation is selected for the sample. This variable is included if you specify the **OUTALL** option. **Selected** equals 1 for an observation that is selected for the sample, or 0 for an observation that is not selected.
- **STRATA** variables, which you specify in the **STRATA** statement.
- **Replicate**, which is the sample replicate number. This variable is included when you request replicated sampling with the **REPS=** option.
- **SAMPLINGUNIT (CLUSTER)** variables, which you specify in the **SAMPLINGUNIT** statement.
- **ID** variables, which you name in the **ID** statement.
- **CONTROL** variables, which you specify in the **CONTROL** statement.

- Zone, which is the selection zone. This variable is included for `METHOD=PPS_SEQ`.
- SIZE variable, which you specify in the `SIZE` statement.
- AdjustedSize, which is the adjusted size measure. This variable is included if you request adjusted sizes with the `MINSIZE=` or `MAXSIZE=` option when your sampling units are observations.
- UnitSize, which is the sampling unit (or cluster) size measure. This variable is included if you specify the `SAMPLINGUNIT` statement.
- Certain, which indicates certainty selection. This variable is included if you specify the `CERTSIZE=` or `CERTSIZE=P=` option. Certain equals 1 for units that are included with certainty because their size measures exceed the certainty size value or the certainty proportion; otherwise, Certain equals 0.
- NumberHits, which is the number of hits (selections). This variable is included for selection methods that are with replacement or with minimum replacement (`METHOD=URS`, `METHOD=PPS_WR`, `METHOD=PPS_SYS`, and `METHOD=PPS_SEQ`).

The output data set includes the following variables if you request a PPS selection method or if you specify the `STATS` option in the PROC SURVEYSELECT statement for other methods:

- ExpectedHits, which is the expected number of hits (selections). This variable is included for selection methods that are with replacement or with minimum replacement, where the same unit can be selected more than once (`METHOD=URS`, `METHOD=PPS_WR`, `METHOD=PPS_SYS`, and `METHOD=PPS_SEQ`).
- SelectionProb, which is the probability of selection. This variable is included for selection methods that are without replacement.
- SamplingWeight, which is the sampling weight. This variable equals the inverse of ExpectedHits or SelectionProb.

If you specify the `STATS` or `OUTSIZE` option for `METHOD=BERNOULLI`, the output data set contains the following variables. If you specify a `STRATA` statement, the output data set includes stratum-level values of these variables; otherwise, the output data set includes overall values.

- Total, which is the total number of sampling units
- SelectionProb, which is the selection probability that you specify by using the `SAMPRATE=` option
- ExpectedN, which is the expected value of the sample size
- SampleSize, which is the actual sample size

If you specify the `STATS` option for `METHOD=BERNOULLI`, the output data set also contains the following variable:

- AdjSamplingWeight, which is the adjusted sampling weight

For `METHOD=PPS_BREWER` and `METHOD=PPS_MURTHY`, which select two units from each stratum with probability proportional to size, the output data set contains the following variable:

- `JtSelectionProb`, which is the joint probability of selection for the two units selected from the stratum.

If you specify the `JTPROBS` option to compute joint probabilities of selection for `METHOD=PPS` or `METHOD=PPS_SAMPFORD`, then the output data set contains the following variables:

- `Unit`, which is an identification variable that numbers the selected units sequentially within each stratum.
- `JtProb_1`, `JtProb_2`, `JtProb_3`, ..., where the variable `JtProb_1` contains the joint probability of selection for the current unit and unit 1. Similarly, `JtProb_2` contains the joint probability of selection for the current unit and unit 2, and so on.

If you specify the `JTPROBS` option for `METHOD=PPS_WR`, then the output data set contains the following variables:

- `Unit`, which is an identification variable that numbers the selected units sequentially within each stratum.
- `JtHits_1`, `JtHits_2`, `JtHits_3`, ..., where the variable `JtHits_1` contains the joint expected number of hits for the current unit and unit 1. Similarly, `JtHits_2` contains the joint expected number of hits for the current unit and unit 2, and so on.

If you specify the `OUTSIZE` option, the output data set contains the following variables. If you specify a `STRATA` statement, the output data set includes stratum-level values of these variables; otherwise, the output data set includes overall values.

- `MinimumSize`, which is the minimum size measure specified with the `MINSIZE=` option. This variable is included if you specify the `MINSIZE=` option.
- `MaximumSize`, which is the maximum size measure specified with the `MAXSIZE=` option. This variable is included if you specify the `MAXSIZE=` option.
- `CertaintySize`, which is the certainty size measure specified with the `CERTSIZE=` option. This variable is included if you specify the `CERTSIZE=` option.
- `CertaintyProp`, which is the certainty proportion specified with the `CERTSIZE=P=` option. This variable is included if you specify the `CERTSIZE=P=` option.
- `Total`, which is the total number of sampling units in the stratum. This variable is included if there is no `SIZE` statement, or if you specify a `SAMPLINGUNIT` statement.
- `TotalSize`, which is the total of size measures in the stratum. This variable is included if there is a `SIZE` statement, or if you specify the `PPS` option in the `SAMPLINGUNIT` statement.

- TotalAdjSize, which is the total of adjusted size measures in the stratum. This variable is included if you request adjusted sizes with the `MAXSIZE=` or `MINSIZE=` option.
- SamplingRate, which is the sampling rate. This variable is included if you specify the `SAMPRATE=` option.
- SampleSize, which is the sample size. This variable is included if you specify the `SAMPSIZE=` option, or if you specify `METHOD=PPS_BREWER` or `METHOD=PPS_MURTHY`, which selects two units from each stratum.

If you specify the `OUTSEED` option, the output data set contains the following variable:

- InitialSeed, which is the initial seed for the stratum.

If you specify the `ALLOC=` option in the `STRATA` statement, the output data set contains the following variables:

- Total, which is the total number of sampling units in the stratum.
- Variance, which is the stratum variance. This variable is included if you specify the `VAR`, `VAR=(values)`, or `VAR=SAS-data-set` option for the `ALLOC=OPTIMAL`, `ALLOC=NEYMAN`, or `MARGIN=` allocation option.
- Cost, which is the stratum cost. This variable is included if you specify the `COST`, `COST=(values)`, or `COST=SAS-data-set` option for `ALLOC=OPTIMAL`.
- AllocProportion, which is the target allocation proportion (the proportion of the total sample size to allocate to the stratum). PROC SURVEYSELECT computes this proportion by using the specified allocation method.
- SampleSize, which is the sample size allocated to the stratum.
- ActualProportion, which is the actual proportion allocated to the stratum. The value of ActualProportion equals the allocated stratum sample size divided by the total sample size. This value can differ from the target AllocProportion due to rounding and other restrictions. See the section “Sample Size Allocation” on page 8067 for details.

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## Allocation Output Data Set

When you specify the `NOSAMPLE` option in the `STRATA` statement, PROC SURVEYSELECT allocates the total sample size among the strata but does not select the sample. In this case, the `OUT=` data set contains the allocated sample sizes.

You can specify the name of the allocation output data set with the `OUT=` option in the PROC SURVEYSELECT statement. If you omit the `OUT=` option, the data set is named `DATAn`, where `n` is the smallest integer that makes the name unique.

The allocation output data set contains one observation for each stratum. The data set can include the following variables:

- STRATA variables, which you specify in the **STRATA** statement.
- Total, which is the total number of sampling units in the stratum.
- Variance, which is the stratum variance. This variable is included if you specify the **VAR**, **VAR=(values)**, or **VAR=SAS-data-set** option for the **ALLOC=OPTIMAL**, **ALLOC=NEYMAN**, or **MARGIN=** allocation option.
- Cost, which is the stratum cost. This variable is included if you specify the **COST**, **COST=(values)**, or **COST=SAS-data-set** option for **ALLOC=OPTIMAL**.
- AllocProportion, which is the target allocation proportion (the proportion of the total sample size to allocate to the stratum). PROC SURVEYSELECT computes this proportion by using the specified allocation method.
- SampleSize, which is the sample size allocated to the stratum.
- ActualProportion, which is the actual proportion allocated to the stratum. The value of ActualProportion equals the allocated stratum sample size divided by the total sample size. This value can differ from the target AllocProportion due to rounding and other restrictions. See the section “Sample Size Allocation” on page 8067 for details.

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## Displayed Output

By default, PROC SURVEYSELECT displays two tables that summarize the sample selection: the “Sample Selection Method” table and the “Sample Selection Summary” table.

If you request sample allocation but no sample selection, PROC SURVEYSELECT displays two tables that summarize the allocation: the “Sample Allocation Method” table and the “Sample Allocation Summary” table.

You can suppress display of these tables by specifying the **NOPRINT** option.

PROC SURVEYSELECT creates an output data set that contains the units that are selected for the sample. Or if you request sample allocation but no sample selection, PROC SURVEYSELECT creates an output data set that contains the sample size allocation results. (See the sections “Sample Output Data Set” on page 8072 and “Allocation Output Data Set” on page 8075 for information about these output data sets.) The procedure does not display the output data set that it creates. Use PROC PRINT, PROC REPORT, or any other SAS reporting tool to display the output data set.

PROC SURVEYSELECT displays the following information in the “Sample Selection Method” table:

- Selection Method
- Sampling Unit Variables, if you specify a **SAMPLINGUNIT** statement
- Size Measure variable, if you specify a **SIZE** statement



- Size Measure: Number of Observations, if you specify the `PPS` option in the `SAMPLINGUNIT` statement and do not specify a `SIZE` statement
- Minimum Size Measure, if you specify the `MINSIZE=` option
- Maximum Size Measure, if you specify the `MAXSIZE=` option
- Certainty Size Measure, if you specify the `CERTSIZE=` option
- Certainty Proportion, if you specify the `CERTSIZE=P=` option
- Strata Variables, if you specify a `STRATA` statement
- Control Variables, if you specify a `CONTROL` statement
- Control Sorting (Serpentine or Nested), if you specify a `CONTROL` statement
- Allocation (Proportional, Neyman, Optimal, or Input), if you specify the `ALLOC=` option in the `STRATA` statement
- Margin of Error, if you specify the `MARGIN=` option in the `STRATA` statement
- Confidence Level, if you specify the `ALPHA=` option in the `STRATA` statement

PROC SURVEYSELECT displays the following information in the “Sample Selection Summary” table:

- Input Data Set name
- Sorted Data Set name, if you specify the `OUTSORT=` option
- Random Number Seed
- Sample Size or Stratum Sample Size, if you specify the `SAMPSIZE=n` option
- Sample Size Data Set, if you specify the `SAMPSIZE=SAS-data-set` option
- Sampling Rate or Stratum Sampling Rate, if you specify the `SAMPRATE=r` option for `METHOD=SRS`, `METHOD=URS`, `METHOD=SYS`, or `METHOD=SEQ`.
- Selection Probability or Stratum Selection Probability, if you specify the `SAMPRATE=r` option for `METHOD=BERNOULLI`
- Sampling Rate Data Set, if you specify the `SAMPRATE=SAS-data-set` option
- Minimum Sample Size or Stratum Minimum Sample Size, if you specify the `NMIN=` option with the `SAMPRATE=` option
- Maximum Sample Size or Stratum Maximum Sample Size, if you specify the `NMAX=` option with the `SAMPRATE=` option
- Allocation Input Data Set name, if you specify the `ALLOC=SAS-data-set` option in the `STRATA` statement
- Variance Input Data Set name, if you specify the `VAR=SAS-data-set` option in the `STRATA` statement



- Cost Input Data Set name, if you specify the `COST=SAS-data-set` option in the `STRATA` statement
- Selection Probability, if you specify `METHOD=SRS`, `METHOD=SYS`, or `METHOD=SEQ` and do not specify a `SIZE` statement or a `STRATA` statement
- Expected Number of Hits, if you specify `METHOD=URS` and do not specify a `STRATA` statement
- Total Number of Units, if you specify `METHOD=BERNOULLI` or `METHOD=POISSON` and do not specify a `STRATA` statement
- Expected Sample Size, if you specify `METHOD=BERNOULLI` or `METHOD=POISSON` and do not specify a `STRATA` statement
- Sample Size, if you specify `METHOD=BERNOULLI` or `METHOD=POISSON` and do not specify a `STRATA` statement
- Sampling Weight, if you specify an equal probability selection method (`METHOD=SRS`, `METHOD=URS`, `METHOD=SYS`, `METHOD=SEQ`, or `METHOD=BERNOULLI`) and do not specify a `STRATA` statement
- Adjusted Sampling Weight, if you specify `METHOD=BERNOULLI` and do not specify a `STRATA` statement
- Number of Strata, if you specify a `STRATA` statement
- Stratum Minimum Sample Size, if you specify the `ALLOCMIN=` option in the `STRATA` statement
- Number of Replicates, if you specify the `REPS=` option
- Total Sample Size, if you specify a `STRATA` statement or the `REPS=` option
- Expected Margin of Error, if you specify the `STATS` option with the `MARGIN=` option in the `STRATA` statement
- Expected Variance, if you specify the `STATS` option without the `MARGIN=` option in the `STRATA` statement for `ALLOC=OPTIMAL` or `ALLOC=NEYMAN`
- Total Stratum Costs, if you specify the `STATS` option with `ALLOC=OPTIMAL` in the `STRATA` statement
- Output Data Set name

If you specify the `NOSAMPLE` option in the `STRATA` statement, PROC SURVEYSELECT allocates the total sample among the strata but does not select the sample. When you specify the `NOSAMPLE` option, PROC SURVEYSELECT displays the “Sample Allocation Method” table and the “Sample Allocation Summary” table. The “Sample Allocation Method” table includes the following information:

- Allocation (Proportional, Neyman, Optimal, or Input)
- Margin of Error, if you specify the `MARGIN=` option in the `STRATA` statement
- Confidence Level, if you specify the `ALPHA=` option in the `STRATA` statement
- Sampling Unit Variables, if you specify a `SAMPLINGUNIT` statement

- Strata Variables
- Frequency Variable
- Selection Method, if you specify the `METHOD=` option

PROC SURVEYSELECT displays the following information in the “Sample Allocation Summary” table.

- Input Data Set name
- Allocation Input Data Set name, if you specify the `ALLOC=SAS-data-set` option in the `STRATA` statement
- Variance Input Data Set name, if you specify the `VAR=SAS-data-set` option in the `STRATA` statement
- Cost Input Data Set name, if you specify the `COST=SAS-data-set` option in the `STRATA` statement
- Number of Strata
- Stratum Minimum Sample Size, if you specify the `ALLOCMIN=` option in the `STRATA` statement
- Total Sample Size
- Expected Margin of Error, if you specify the `STATS` option with the `MARGIN=` option in the `STRATA` statement
- Expected Variance, if you specify the `STATS` option without the `MARGIN=` option in the `STRATA` statement for `ALLOC=OPTIMAL` or `ALLOC=NEYMAN`
- Total Stratum Costs, if you specify the `STATS` option with `ALLOC=OPTIMAL` in the `STRATA` statement
- Allocation Output Data Set name

---

## ODS Table Names

PROC SURVEYSELECT assigns a name to each table that it creates. You can use these names to refer to tables when you use the Output Delivery System (ODS) to select tables and create output data sets. For more information about ODS, see Chapter 20, “Using the Output Delivery System.” Table 95.4 lists the table names.

**Table 95.4** ODS Tables Produced by PROC SURVEYSELECT

| ODS Table Name | Description               | Statement | Option   |
|----------------|---------------------------|-----------|----------|
| Method         | Sample selection method   | PROC      | Default  |
| Method         | Sample allocation method  | STRATA    | NOSAMPLE |
| Summary        | Sample selection summary  | PROC      | Default  |
| Summary        | Sample allocation summary | STRATA    | NOSAMPLE |

---

## Examples: SURVEYSELECT Procedure

---

### Example 95.1: Replicated Sampling

This example uses the Customers data set from the section “Getting Started: SURVEYSELECT Procedure” on page 8021. The data set Customers contains an Internet service provider’s current subscribers, and the service provider wants to select a sample from this population for a customer satisfaction survey.

This example illustrates replicated sampling, which selects multiple samples from the survey population according to the same design. You can use replicated sampling to provide a simple method of variance estimation, or to evaluate variable nonsampling errors such as interviewer differences. For information about replicated sampling, see Lohr (2010); Wolter (2007); Kish (1965, 1987); Kalton (1983).

This design includes four replicates, each with a sample size of 50 customers. The sampling frame is stratified by State and sorted by Type and Usage within strata. Customers are selected by sequential random sampling with equal probability within strata. The following PROC SURVEYSELECT statements select a probability sample of customers from the Customers data set by using this design:

```
title1 'Customer Satisfaction Survey';
title2 'Replicated Sampling';
proc surveyselect data=Customers method=seq n=(8 12 20 10)
 reps=4 seed=40070 ranuni out=SampleRep;
 strata State;
 control Type Usage;
run;
```

The STRATA statement names the stratification variable State. The CONTROL statement names the control variables Type and Usage.

In the PROC SURVEYSELECT statement, the METHOD=SEQ option requests sequential random sampling. The REPS= option specifies four replicates of this sample. The N=(8 12 20 10) option lists the stratum sample sizes for each replicate. The N= option lists the stratum sample sizes in the same order as the strata appear in the Customers data set, which has been sorted by State. The sample size of eight customers corresponds to the first stratum, State = ‘AL’. The sample size 12 corresponds to the next stratum, State = ‘FL’, and so on.

The SEED= option specifies 40070 as the initial seed for random number generation. The RANUNI option requests random number generation by the RANUNI generator, which PROC SURVEYSELECT used in releases prior to SAS/STAT 12.1. (Beginning in SAS/STAT 12.1, PROC SURVEYSELECT uses the Mersenne-Twister random number generator by default.) You can specify the RANUNI option with the SEED= option to reproduce samples that PROC SURVEYSELECT selected in releases prior to SAS/STAT 12.1. To reproduce a sample by using the RANUNI and SEED= options, you must also specify the same input data set and sample selection parameters.

**Output 95.1.1** displays the output from PROC SURVEYSELECT, which summarizes the sample selection. A total of 200 customers is selected in four replicates. PROC SURVEYSELECT selects each replicate by using sequential random sampling within strata determined by State. The sampling frame Customers is sorted by the control variables Type and Usage within strata, according to hierarchic serpentine sorting. The output data set SampleRep contains the sample.

### Output 95.1.1 Sample Selection Summary

| Customer Satisfaction Survey |                                                      |
|------------------------------|------------------------------------------------------|
| Replicated Sampling          |                                                      |
| The SURVEYSELECT Procedure   |                                                      |
| Selection Method             | Sequential Random Sampling<br>With Equal Probability |
| Strata Variable              | State                                                |
| Control Variables            | Type<br>Usage                                        |
| Control Sorting              | Serpentine                                           |
| Input Data Set               | CUSTOMERS                                            |
| Random Number Seed           | 40070                                                |
| Number of Strata             | 4                                                    |
| Number of Replicates         | 4                                                    |
| Total Sample Size            | 200                                                  |
| Output Data Set              | SAMPLEREP                                            |

The following PROC PRINT statements display the selected customers for the first stratum, State = 'AL', from the output data set SampleRep:

```

title1 'Customer Satisfaction Survey';
title2 'Sample Selected by Replicated Design';
title3 '(First Stratum)';
proc print data=SampleRep;
 where State = 'AL';
run;

```

**Output 95.1.2** displays the 32 sample customers of the first stratum (State = 'AL') from the output data set SampleRep, which includes the entire sample of 200 customers. The variable SelectionProb contains the selection probability, and SamplingWeight contains the sampling weight. Because customers are selected with equal probability within strata in this design, all customers in the same stratum have the same selection probability. These selection probabilities and sampling weights apply to a single replicate, and the variable Replicate contains the sample replicate number.

## Output 95.1.2 Customer Sample (First Stratum)

| Customer Satisfaction Survey<br>Sample Selected by Replicated Design<br>(First Stratum) |       |           |             |      |       |                |                 |
|-----------------------------------------------------------------------------------------|-------|-----------|-------------|------|-------|----------------|-----------------|
| Obs                                                                                     | State | Replicate | CustomerID  | Type | Usage | Selection Prob | Sampling Weight |
| 1                                                                                       | AL    | 1         | 882-37-7496 | New  | 572   | .004115226     | 243             |
| 2                                                                                       | AL    | 1         | 581-32-5534 | New  | 863   | .004115226     | 243             |
| 3                                                                                       | AL    | 1         | 980-29-2898 | Old  | 571   | .004115226     | 243             |
| 4                                                                                       | AL    | 1         | 172-56-4743 | Old  | 128   | .004115226     | 243             |
| 5                                                                                       | AL    | 1         | 998-55-5227 | Old  | 35    | .004115226     | 243             |
| 6                                                                                       | AL    | 1         | 625-44-3396 | New  | 60    | .004115226     | 243             |
| 7                                                                                       | AL    | 1         | 627-48-2509 | New  | 114   | .004115226     | 243             |
| 8                                                                                       | AL    | 1         | 257-66-6558 | New  | 172   | .004115226     | 243             |
| 9                                                                                       | AL    | 2         | 622-83-1680 | New  | 22    | .004115226     | 243             |
| 10                                                                                      | AL    | 2         | 343-57-1186 | New  | 53    | .004115226     | 243             |
| 11                                                                                      | AL    | 2         | 976-05-3796 | New  | 110   | .004115226     | 243             |
| 12                                                                                      | AL    | 2         | 859-74-0652 | New  | 303   | .004115226     | 243             |
| 13                                                                                      | AL    | 2         | 476-48-1066 | New  | 839   | .004115226     | 243             |
| 14                                                                                      | AL    | 2         | 109-27-8914 | Old  | 2102  | .004115226     | 243             |
| 15                                                                                      | AL    | 2         | 743-25-0298 | Old  | 376   | .004115226     | 243             |
| 16                                                                                      | AL    | 2         | 722-08-2215 | Old  | 105   | .004115226     | 243             |
| 17                                                                                      | AL    | 3         | 668-57-7696 | New  | 200   | .004115226     | 243             |
| 18                                                                                      | AL    | 3         | 300-72-0129 | New  | 471   | .004115226     | 243             |
| 19                                                                                      | AL    | 3         | 073-60-0765 | New  | 656   | .004115226     | 243             |
| 20                                                                                      | AL    | 3         | 526-87-0258 | Old  | 672   | .004115226     | 243             |
| 21                                                                                      | AL    | 3         | 726-61-0387 | Old  | 150   | .004115226     | 243             |
| 22                                                                                      | AL    | 3         | 632-29-9020 | Old  | 51    | .004115226     | 243             |
| 23                                                                                      | AL    | 3         | 417-17-8378 | New  | 56    | .004115226     | 243             |
| 24                                                                                      | AL    | 3         | 091-26-2366 | New  | 93    | .004115226     | 243             |
| 25                                                                                      | AL    | 4         | 336-04-1288 | New  | 419   | .004115226     | 243             |
| 26                                                                                      | AL    | 4         | 827-04-7407 | New  | 650   | .004115226     | 243             |
| 27                                                                                      | AL    | 4         | 317-70-6496 | Old  | 452   | .004115226     | 243             |
| 28                                                                                      | AL    | 4         | 002-38-4582 | Old  | 206   | .004115226     | 243             |
| 29                                                                                      | AL    | 4         | 181-83-3990 | Old  | 33    | .004115226     | 243             |
| 30                                                                                      | AL    | 4         | 675-34-7393 | New  | 47    | .004115226     | 243             |
| 31                                                                                      | AL    | 4         | 228-07-6671 | New  | 65    | .004115226     | 243             |
| 32                                                                                      | AL    | 4         | 298-46-2434 | New  | 161   | .004115226     | 243             |

## Example 95.2: PPS Selection of Two Units per Stratum

This example describes hospital selection for a survey by using PROC SURVEYSELECT. A state health agency plans to conduct a statewide survey of a variety of different hospital services. The agency plans to select a probability sample of individual discharge records within hospitals by using a two-stage sample design. First-stage units are hospitals, and second-stage units are patient discharges during the study period. Hospitals are stratified first according to geographic region and then by rural/urban type and size of hospital. Two hospitals are selected from each stratum with probability proportional to size.

The data set HospitalFrame contains all hospitals in the first geographical region of the state:

```
data HospitalFrame;
 input Hospital$ Type$ SizeMeasure @@;
 if (SizeMeasure < 20) then Size='Small ';
 else if (SizeMeasure < 50) then Size='Medium';
 else Size='Large ';
 datalines;
034 Rural 0.870 107 Rural 1.316
079 Rural 2.127 223 Rural 3.960
236 Rural 5.279 165 Rural 5.893
086 Rural 0.501 141 Rural 11.528
042 Urban 3.104 124 Urban 4.033
006 Urban 4.249 261 Urban 4.376
195 Urban 5.024 190 Urban 10.373
038 Urban 17.125 083 Urban 40.382
259 Urban 44.942 129 Urban 46.702
133 Urban 46.992 218 Urban 48.231
026 Urban 61.460 058 Urban 65.931
119 Urban 66.352
;
```

In the SAS data set HospitalFrame, the variable Hospital identifies the hospital. The variable Type equals 'Urban' if the hospital is located in an urban area, and 'Rural' otherwise. The variable SizeMeasure contains the hospital's size measure, which is constructed from past data on service utilization for the hospital together with the desired sampling rates for each service. This size measure reflects the amount of relevant survey information expected from the hospital. See Drummond et al. (1982) for details about this type of size measure. The variable Size equals 'Small', 'Medium', or 'Large', depending on the value of the hospital's size measure.

The following PROC PRINT statements display the data set Hospital Frame and produce [Output 95.2.1](#):

```
title1 'Hospital Utilization Survey';
title2 'Sampling Frame, Region 1';
proc print data=HospitalFrame;
run;
```

## Output 95.2.1 Sampling Frame

| Hospital Utilization Survey<br>Sampling Frame, Region 1 |          |       |              |        |
|---------------------------------------------------------|----------|-------|--------------|--------|
| Obs                                                     | Hospital | Type  | Size Measure | Size   |
| 1                                                       | 034      | Rural | 0.870        | Small  |
| 2                                                       | 107      | Rural | 1.316        | Small  |
| 3                                                       | 079      | Rural | 2.127        | Small  |
| 4                                                       | 223      | Rural | 3.960        | Small  |
| 5                                                       | 236      | Rural | 5.279        | Small  |
| 6                                                       | 165      | Rural | 5.893        | Small  |
| 7                                                       | 086      | Rural | 0.501        | Small  |
| 8                                                       | 141      | Rural | 11.528       | Small  |
| 9                                                       | 042      | Urban | 3.104        | Small  |
| 10                                                      | 124      | Urban | 4.033        | Small  |
| 11                                                      | 006      | Urban | 4.249        | Small  |
| 12                                                      | 261      | Urban | 4.376        | Small  |
| 13                                                      | 195      | Urban | 5.024        | Small  |
| 14                                                      | 190      | Urban | 10.373       | Small  |
| 15                                                      | 038      | Urban | 17.125       | Small  |
| 16                                                      | 083      | Urban | 40.382       | Medium |
| 17                                                      | 259      | Urban | 44.942       | Medium |
| 18                                                      | 129      | Urban | 46.702       | Medium |
| 19                                                      | 133      | Urban | 46.992       | Medium |
| 20                                                      | 218      | Urban | 48.231       | Medium |
| 21                                                      | 026      | Urban | 61.460       | Large  |
| 22                                                      | 058      | Urban | 65.931       | Large  |
| 23                                                      | 119      | Urban | 66.352       | Large  |

The following PROC SURVEYSELECT statements select a probability sample of hospitals from the HospitalFrame data set by using a stratified design with PPS selection of two units from each stratum:

```

title1 'Hospital Utilization Survey';
title2 'Stratified PPS Sampling';
proc surveyselect data=HospitalFrame method=pps_brewer
 seed=48702 out=SampleHospitals;
 size SizeMeasure;
 strata Type Size notsorted;
run;

```

The STRATA statement names the stratification variables Type and Size. The NOTSORTED option specifies that observations with the same STRATA variable values are grouped together but are not necessarily sorted in alphabetical or increasing numerical order. In the HospitalFrame data set, Size = 'Small' precedes Size = 'Medium'.

In the PROC SURVEYSELECT statement, the METHOD=PPS\_BREWER option requests sample selection by Brewer's method, which selects two units per stratum with probability proportional to size. The SEED= option specifies 48702 as the initial seed for random number generation. The SIZE statement names SizeMeasure as the size measure variable. It is not necessary to specify the sample size with the N= option, because Brewer's method always selects two units from each stratum.

Output 95.2.2 displays the output from PROC SURVEYSELECT. A total of eight hospitals were selected from the four strata. The data set SampleHospitals contains the selected hospitals.

**Output 95.2.2** Sample Selection Summary

| Hospital Utilization Survey<br>Stratified PPS Sampling |                     |
|--------------------------------------------------------|---------------------|
| The SURVEYSELECT Procedure                             |                     |
| Selection Method                                       | Brewer's PPS Method |
| Size Measure                                           | SizeMeasure         |
| Strata Variables                                       | Type<br>Size        |
| Input Data Set                                         | HOSPITALFRAME       |
| Random Number Seed                                     | 48702               |
| Stratum Sample Size                                    | 2                   |
| Number of Strata                                       | 4                   |
| Total Sample Size                                      | 8                   |
| Output Data Set                                        | SAMPLEHOSPITALS     |

The following PROC PRINT statements display the sample hospitals and produce Output 95.2.3:

```

title1 'Hospital Utilization Survey';
title2 'Sample Selected by Stratified PPS Design';
proc print data=SampleHospitals;
run;

```

**Output 95.2.3** Sample Hospitals

| Hospital Utilization Survey<br>Sample Selected by Stratified PPS Design |       |        |          |              |                |                 |                   |
|-------------------------------------------------------------------------|-------|--------|----------|--------------|----------------|-----------------|-------------------|
| Obs                                                                     | Type  | Size   | Hospital | Size Measure | Selection Prob | Sampling Weight | Jt Selection Prob |
| 1                                                                       | Rural | Small  | 165      | 5.893        | 0.37447        | 2.67046         | 0.22465           |
| 2                                                                       | Rural | Small  | 141      | 11.528       | 0.73254        | 1.36511         | 0.22465           |
| 3                                                                       | Urban | Small  | 006      | 4.249        | 0.17600        | 5.68181         | 0.01454           |
| 4                                                                       | Urban | Small  | 195      | 5.024        | 0.20810        | 4.80533         | 0.01454           |
| 5                                                                       | Urban | Medium | 129      | 46.702       | 0.41102        | 2.43297         | 0.11211           |
| 6                                                                       | Urban | Medium | 218      | 48.231       | 0.42448        | 2.35584         | 0.11211           |
| 7                                                                       | Urban | Large  | 058      | 65.931       | 0.68060        | 1.46929         | 0.36555           |
| 8                                                                       | Urban | Large  | 119      | 66.352       | 0.68495        | 1.45996         | 0.36555           |

The variable SelectionProb contains the selection probability for each hospital in the sample. The variable JtSelectionProb contains the joint probability of selection for the two sample hospitals in the same stratum. The variable SamplingWeight contains the sampling weight component for this first stage of the design. The final-stage weight components, which correspond to patient record selection within hospitals, can be multiplied by the hospital weight components to obtain the overall sampling weights.



### Example 95.3: PPS (Dollar-Unit) Sampling

A small company wants to audit employee travel expenses in an effort to improve the expense reporting procedure and possibly reduce expenses. The company does not have resources to examine all expense reports and wants to use statistical sampling to objectively select expense reports for audit.

The data set `TravelExpense` contains the dollar amount of all employee travel expense transactions during the past month:

```
data TravelExpense;
 input ID$ Amount @@;
 if (Amount < 500) then Level='1_Low ';
 else if (Amount > 1500) then Level='3_High';
 else Level='2_Avg ';
 datalines;
110 237.18 002 567.89 234 118.50
743 74.38 411 1287.23 782 258.10
216 325.36 174 218.38 568 1670.80
302 134.71 285 2020.70 314 47.80
139 1183.45 775 330.54 425 780.10
506 895.80 239 620.10 011 420.18
672 979.66 142 810.25 738 670.85
192 314.58 243 87.50 263 1893.40
496 753.30 332 540.65 486 2580.35
614 230.56 654 185.60 308 688.43
784 505.14 017 205.48 162 650.42
289 1348.34 691 30.50 545 2214.80
517 940.35 382 217.85 024 142.90
478 806.90 107 560.72
;
```

In the SAS data set `TravelExpense`, the variable `ID` identifies the travel expense report. The variable `Amount` contains the dollar amount of the reported expense. The variable `Level` equals '1\_Low', '2\_Avg', or '3\_High', depending on the value of `Amount`.

In the sample design for this audit, expense reports are stratified by `Level`. This ensures that each of these expense levels is included in the sample and also permits a disproportionate allocation of the sample, selecting proportionately more of the expense reports from the higher levels. Within strata, the sample of expense reports is selected with probability proportional to the amount of the expense, thus giving a greater chance of selection to larger expenses. In auditing terms, this is known as monetary-unit sampling. See Wilburn (1984) for details.

`PROC SURVEYSELECT` requires that the input data set be sorted by the `STRATA` variables. The following `PROC SORT` statements sort the `TravelExpense` data set by the stratification variable `Level`.

```
proc sort data=TravelExpense;
 by Level;
run;
```

Output 95.3.1 displays the sampling frame data set `TravelExpense`, which contains 41 observations.

**Output 95.3.1** Sampling Frame

| Travel Expense Audit |     |         |        |
|----------------------|-----|---------|--------|
| Obs                  | ID  | Amount  | Level  |
| 1                    | 110 | 237.18  | 1_Low  |
| 2                    | 234 | 118.50  | 1_Low  |
| 3                    | 743 | 74.38   | 1_Low  |
| 4                    | 782 | 258.10  | 1_Low  |
| 5                    | 216 | 325.36  | 1_Low  |
| 6                    | 174 | 218.38  | 1_Low  |
| 7                    | 302 | 134.71  | 1_Low  |
| 8                    | 314 | 47.80   | 1_Low  |
| 9                    | 775 | 330.54  | 1_Low  |
| 10                   | 011 | 420.18  | 1_Low  |
| 11                   | 192 | 314.58  | 1_Low  |
| 12                   | 243 | 87.50   | 1_Low  |
| 13                   | 614 | 230.56  | 1_Low  |
| 14                   | 654 | 185.60  | 1_Low  |
| 15                   | 017 | 205.48  | 1_Low  |
| 16                   | 691 | 30.50   | 1_Low  |
| 17                   | 382 | 217.85  | 1_Low  |
| 18                   | 024 | 142.90  | 1_Low  |
| 19                   | 002 | 567.89  | 2_Avg  |
| 20                   | 411 | 1287.23 | 2_Avg  |
| 21                   | 139 | 1183.45 | 2_Avg  |
| 22                   | 425 | 780.10  | 2_Avg  |
| 23                   | 506 | 895.80  | 2_Avg  |
| 24                   | 239 | 620.10  | 2_Avg  |
| 25                   | 672 | 979.66  | 2_Avg  |
| 26                   | 142 | 810.25  | 2_Avg  |
| 27                   | 738 | 670.85  | 2_Avg  |
| 28                   | 496 | 753.30  | 2_Avg  |
| 29                   | 332 | 540.65  | 2_Avg  |
| 30                   | 308 | 688.43  | 2_Avg  |
| 31                   | 784 | 505.14  | 2_Avg  |
| 32                   | 162 | 650.42  | 2_Avg  |
| 33                   | 289 | 1348.34 | 2_Avg  |
| 34                   | 517 | 940.35  | 2_Avg  |
| 35                   | 478 | 806.90  | 2_Avg  |
| 36                   | 107 | 560.72  | 2_Avg  |
| 37                   | 568 | 1670.80 | 3_High |
| 38                   | 285 | 2020.70 | 3_High |
| 39                   | 263 | 1893.40 | 3_High |
| 40                   | 486 | 2580.35 | 3_High |
| 41                   | 545 | 2214.80 | 3_High |

The following PROC SURVEYSELECT statements select a probability sample of expense reports from the TravelExpense data set by using the stratified design with PPS selection within strata:

```

title1 'Travel Expense Audit';
title2 'Stratified PPS (Dollar-Unit) Sampling';
proc surveyselect data=TravelExpense method=pps n=(6 10 4)
 seed=47279 out=AuditSample;
 size Amount;
 strata Level;
run;

```

The STRATA statement names the stratification variable Level. The SIZE statement specifies the size measure variable Amount. In the PROC SURVEYSELECT statement, the METHOD=PPS option requests sample selection with probability proportional to size and without replacement. The N=(6 10 4) option specifies the stratum sample sizes, listing the sample sizes in the same order as the strata appear in the TravelExpense data set. The sample size of 6 corresponds to the first stratum, Level = '1\_Low'; the sample size of 10 corresponds to the second stratum, Level = '2\_Avg'; and 4 corresponds to the last stratum, Level = '3\_High'. The SEED= option specifies 47279 as the initial seed for random number generation.

Output 95.3.2 displays the output from PROC SURVEYSELECT. A total of 20 expense reports are selected for audit. The data set AuditSample contains the sample of travel expense reports.

#### Output 95.3.2 Sample Selection Summary

| Travel Expense Audit                  |                          |
|---------------------------------------|--------------------------|
| Stratified PPS (Dollar-Unit) Sampling |                          |
| The SURVEYSELECT Procedure            |                          |
| Selection Method                      | PPS, Without Replacement |
| Size Measure                          | Amount                   |
| Strata Variable                       | Level                    |
| Input Data Set                        | TRAVELEXPENSE            |
| Random Number Seed                    | 47279                    |
| Number of Strata                      | 3                        |
| Total Sample Size                     | 20                       |
| Output Data Set                       | AUDITSAMPLE              |

The following PROC PRINT statements display the audit sample, which is shown in Output 95.3.3:

```

title1 'Travel Expense Audit';
title2 'Sample Selected by Stratified PPS Design';
proc print data=AuditSample;
run;

```

**Output 95.3.3** Audit Sample

| Travel Expense Audit<br>Sample Selected by Stratified PPS Design |        |     |         |                |                 |
|------------------------------------------------------------------|--------|-----|---------|----------------|-----------------|
| Obs                                                              | Level  | ID  | Amount  | Selection Prob | Sampling Weight |
| 1                                                                | 1_Low  | 024 | 142.90  | 0.23949        | 4.17553         |
| 2                                                                | 1_Low  | 614 | 230.56  | 0.38640        | 2.58797         |
| 3                                                                | 1_Low  | 110 | 237.18  | 0.39750        | 2.51574         |
| 4                                                                | 1_Low  | 782 | 258.10  | 0.43256        | 2.31183         |
| 5                                                                | 1_Low  | 192 | 314.58  | 0.52721        | 1.89676         |
| 6                                                                | 1_Low  | 216 | 325.36  | 0.54528        | 1.83392         |
| 7                                                                | 2_Avg  | 332 | 540.65  | 0.37057        | 2.69853         |
| 8                                                                | 2_Avg  | 239 | 620.10  | 0.42503        | 2.35278         |
| 9                                                                | 2_Avg  | 162 | 650.42  | 0.44581        | 2.24310         |
| 10                                                               | 2_Avg  | 738 | 670.85  | 0.45981        | 2.17479         |
| 11                                                               | 2_Avg  | 506 | 895.80  | 0.61400        | 1.62866         |
| 12                                                               | 2_Avg  | 517 | 940.35  | 0.64454        | 1.55151         |
| 13                                                               | 2_Avg  | 672 | 979.66  | 0.67148        | 1.48925         |
| 14                                                               | 2_Avg  | 139 | 1183.45 | 0.81116        | 1.23280         |
| 15                                                               | 2_Avg  | 411 | 1287.23 | 0.88229        | 1.13341         |
| 16                                                               | 2_Avg  | 289 | 1348.34 | 0.92418        | 1.08204         |
| 17                                                               | 3_High | 568 | 1670.80 | 0.64385        | 1.55316         |
| 18                                                               | 3_High | 263 | 1893.40 | 0.72963        | 1.37056         |
| 19                                                               | 3_High | 285 | 2020.70 | 0.77869        | 1.28421         |
| 20                                                               | 3_High | 545 | 2214.80 | 0.85348        | 1.17167         |

**Example 95.4: Proportional Allocation**

This example uses the Customers data set from the section “Getting Started: SURVEYSELECT Procedure” on page 8021. The data set Customers contains an Internet service provider’s current subscribers, and the service provider wants to select a sample from this population for a customer satisfaction survey. This example illustrates proportional allocation, which allocates the total sample size among the strata in proportion to the strata sizes.

The section “Getting Started: SURVEYSELECT Procedure” on page 8021 gives an example of stratified sampling, where the list of customers is stratified by State and Type. Figure 95.4 displays the strata in a table of State by Type for the 13,471 customers. There are four states and two levels of Type, forming a total of eight strata. A sample of 15 customers was selected from each stratum by using the following PROC SURVEYSELECT statements:

```

title1 'Customer Satisfaction Survey';
title2 'Stratified Sampling';
proc surveyselect data=Customers method=srs n=15
 seed=1953 out=SampleStrata;
 strata State Type;
run;

```

The STRATA statement names the stratification variables State and Type. In the PROC SURVEYSELECT statement, the N= option specifies a sample size of 15 customers for each stratum.

Instead of specifying the number of customers to select from each stratum, you can specify the total sample size and request allocation of the total sample size among the strata. The following PROC SURVEYSELECT statements request proportional allocation, which allocates the total sample size in proportion to the stratum sizes:

```

title1 'Customer Satisfaction Survey';
title2 'Proportional Allocation';
proc surveyselect data=Customers n=1000
 out=SampleSizes;
 strata State Type / alloc=prop nosample;
run;

```

The STRATA statement names the stratification variables State and Type. In the STRATA statement, the ALLOC=PROP option requests proportional allocation. The NOSAMPLE option requests that no sample be selected after the procedure computes the sample size allocation. In the PROC SURVEYSELECT statement, the N= option specifies a total sample size of 1000 customers to be allocated among the strata.

Output 95.4.1 displays the output from PROC SURVEYSELECT, which summarizes the sample allocation. The total sample size of 1000 is allocated among the eight strata by using proportional allocation. The allocated sample sizes are stored in the SAS data set SampleSizes.

**Output 95.4.1** Proportional Allocation Summary

| Customer Satisfaction Survey<br>Proportional Allocation |                               |
|---------------------------------------------------------|-------------------------------|
| The SURVEYSELECT Procedure                              |                               |
| Allocation<br>Strata Variables                          | Proportional<br>State<br>Type |
| Input Data Set                                          | CUSTOMERS                     |
| Number of Strata                                        | 8                             |
| Total Sample Size                                       | 1000                          |
| Allocation Output Data Set                              | SAMPLESIZES                   |

The following PROC PRINT statements display the allocation output data set SampleSizes, which is shown in Output 95.4.2:

```

title1 'Customer Satisfaction Survey';
title2 'Proportional Allocation';
proc print data=SampleSizes;
run;

```

**Output 95.4.2** Stratum Sample Sizes

| Customer Satisfaction Survey<br>Proportional Allocation |       |      |       |                     |                |                      |
|---------------------------------------------------------|-------|------|-------|---------------------|----------------|----------------------|
| Obs                                                     | State | Type | Total | Alloc<br>Proportion | Sample<br>Size | Actual<br>Proportion |
| 1                                                       | AL    | New  | 1238  | 0.09190             | 92             | 0.092                |
| 2                                                       | AL    | Old  | 706   | 0.05241             | 52             | 0.052                |
| 3                                                       | FL    | New  | 2170  | 0.16109             | 161            | 0.161                |
| 4                                                       | FL    | Old  | 1370  | 0.10170             | 102            | 0.102                |
| 5                                                       | GA    | New  | 3488  | 0.25893             | 259            | 0.259                |
| 6                                                       | GA    | Old  | 1940  | 0.14401             | 144            | 0.144                |
| 7                                                       | SC    | New  | 1684  | 0.12501             | 125            | 0.125                |
| 8                                                       | SC    | Old  | 875   | 0.06495             | 65             | 0.065                |

The output data set `SampleSizes` includes one observation for each of the eight strata, which are identified by the stratification variables `State` and `Type`. The variable `Total` contains the number of sampling units in the stratum, and the variable `AllocProportion` contains the proportion of the total sample size to allocate to the stratum. The variable `SampleSize` contains the allocated stratum sample size. For the first stratum (`State='AL'` and `Type='New'`), the total number of sampling units is 1238 customers, the allocation proportion is 0.09190, and the allocated sample size is 92 customers. The sum of the allocated sample sizes equals the requested total sample size of 1000 customers.

The output data set also includes the variable `ActualProportion`, which contains actual stratum proportions of the total sample size. The actual proportion for a stratum equals the stratum sample size divided by the total sample size. For the first stratum (`State='AL'` and `Type='New'`), the actual proportion is 0.092, while the allocation proportion is 0.09190. The target sample sizes computed from the allocation proportions are often not integers, and PROC SURVEYSELECT uses a rounding algorithm to obtain integer sample sizes and maintain the requested total sample size. Due to rounding and other restrictions, the actual proportions can differ from the target allocation proportions. See the section “[Sample Size Allocation](#)” on page 8067 for details.

If you want to use the allocated sample sizes in a later invocation of PROC SURVEYSELECT, you can name the allocation data set in the `N=SAS-data-set` option, as shown in the following PROC SURVEYSELECT statements:

```

title1 'Customer Satisfaction Survey';
title2 'Stratified Sampling';
proc surveyselect data=Customers method=srs n=SampleSizes
 seed=1953 out=SampleStrata;
 strata State Type;
run;

```

---

## References

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# Chapter 96

## The TPSPLINE Procedure

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### Overview: TPSPLINE Procedure

The TPSPLINE procedure uses the penalized least squares method to fit a nonparametric regression model. It computes thin-plate smoothing splines to approximate smooth multivariate functions observed with noise. The TPSPLINE procedure allows great flexibility in the possible form of the regression surface. In particular, PROC TPSPLINE makes no assumptions of a parametric form for the model. The generalized cross validation (GCV) function can be used to select the amount of smoothing.

The TPSPLINE procedure complements the methods provided by the standard SAS regression procedures such as the GLM, REG, and NLIN procedures. These procedures can handle most situations in which you

specify the regression model and the model is known up to a fixed number of parameters. However, when you have no prior knowledge about the model, or when you know that the data cannot be represented by a model with a fixed number of parameters, you can use the TPSPLINE procedure to model the data.

The TPSPLINE procedure uses the penalized least squares method to fit the data with a flexible model in which the number of effective parameters can be as large as the number of unique design points. Hence, as the sample size increases, the model space also increases, enabling the thin-plate smoothing spline to fit more complicated situations.

The main features of the TPSPLINE procedure are as follows:

- provides penalized least squares estimates
- supports the use of multidimensional data
- supports multiple SCORE statements
- fits both semiparametric models and nonparametric models
- provides options for handling large data sets
- supports multiple dependent variables
- enables you to choose a particular model by specifying the model degrees of freedom or smoothing parameter
- produces graphs with ODS Graphics

---

## Penalized Least Squares Estimation

Penalized least squares estimation provides a way to balance fitting the data closely and avoiding excessive roughness or rapid variation. A penalized least squares estimate is a surface that minimizes the penalized squared error over the class of all surfaces that satisfy sufficient regularity conditions.

Define  $\mathbf{x}_i$  as a  $d$ -dimensional covariate vector from an  $n \times d$  matrix  $\mathbf{X}$ ,  $\mathbf{z}_i$  as a  $p$ -dimensional covariate vector, and  $y_i$  as the observation associated with  $(\mathbf{x}_i, \mathbf{z}_i)$ . Assuming that the relation between  $\mathbf{z}_i$  and  $y_i$  is linear but the relation between  $\mathbf{x}_i$  and  $y_i$  is unknown, you can fit the data by using a semiparametric model as follows:

$$y_i = f(\mathbf{x}_i) + \mathbf{z}_i \boldsymbol{\beta} + \epsilon_i$$

where  $f$  is an unknown function that is assumed to be reasonably smooth,  $\epsilon_i, i = 1, \dots, n$ , are independent, zero-mean random errors, and  $\boldsymbol{\beta}$  is a  $p$ -dimensional unknown parameter vector.

This model consists of two parts. The  $\mathbf{z}_i \boldsymbol{\beta}$  is the parametric part of the model, and the  $\mathbf{z}_i$  are the regression variables. The  $f(\mathbf{x}_i)$  is the nonparametric part of the model, and the  $\mathbf{x}_i$  are the smoothing variables. The ordinary least squares method estimates  $f(\mathbf{x}_i)$  and  $\boldsymbol{\beta}$  by minimizing the quantity:

$$\frac{1}{n} \sum_{i=1}^n (y_i - f(\mathbf{x}_i) - \mathbf{z}_i \boldsymbol{\beta})^2$$

However, the functional space of  $f(\mathbf{x})$  is so large that you can always find a function  $f$  that interpolates the data points. In order to obtain an estimate that fits the data well and has some degree of smoothness, you can use the penalized least squares method.

The penalized least squares function is defined as

$$S_\lambda(f) = \frac{1}{n} \sum_{i=1}^n (y_i - f(\mathbf{x}_i) - \mathbf{z}_i \boldsymbol{\beta})^2 + \lambda J_2(f)$$

where  $J_2(f)$  is the penalty on the roughness of  $f$  and is defined, in most cases, as the integral of the square of the second derivative of  $f$ .

The first term measures the goodness of fit and the second term measures the smoothness associated with  $f$ . The  $\lambda$  term is the smoothing parameter, which governs the tradeoff between smoothness and goodness of fit. When  $\lambda$  is large, it more heavily penalizes rougher fits. Conversely, a small value of  $\lambda$  puts more emphasis on the goodness of fit.

The estimate  $f_\lambda$  is selected from a reproducing kernel Hilbert space, and it can be represented as a linear combination of a sequence of basis functions. Hence, the final estimates of  $f$  can be written as

$$\hat{f}_\lambda(\mathbf{x}_i) = \theta_0 + \sum_{j=1}^d \theta_j \mathbf{x}_{i,j} + \sum_{j=1}^p \delta_j B_j(\mathbf{x}_j)$$

where  $B_j$  is the basis function, which depends on where the data  $\mathbf{x}_i$  are located, and  $\boldsymbol{\theta} = \{\theta_0, \dots, \theta_d\}$  and  $\boldsymbol{\delta} = \{\delta_1, \dots, \delta_p\}$  are the coefficients that need to be estimated.

For a fixed  $\lambda$ , the coefficients  $(\boldsymbol{\theta}, \boldsymbol{\delta}, \boldsymbol{\beta})$  can be estimated by solving an  $n \times n$  system.

The smoothing parameter can be chosen by minimizing the generalized cross validation (GCV) function.

If you write

$$\hat{\mathbf{y}} = \mathbf{A}(\lambda)\mathbf{y}$$

then  $\mathbf{A}(\lambda)$  is referred to as the *hat* or *smoothing* matrix, and the GCV function  $\text{GCV}(\lambda)$  is defined as

$$\text{GCV}(\lambda) = \frac{(1/n)\|(\mathbf{I} - \mathbf{A}(\lambda))\mathbf{y}\|^2}{[(1/n)\text{tr}(\mathbf{I} - \mathbf{A}(\lambda))]^2}$$

---

## PROC TPSPLINE with Large Data Sets

The calculation of the penalized least squares estimate is computationally intensive. The amount of memory and CPU time needed for the analysis depends on the number of unique design points, which corresponds to the number of unknown parameters to be estimated.

You can specify the `D=` option in the `MODEL` statement to reduce the number of unknown parameters. The option groups design points by the specified range (see the `D=` option on page 8114).

`PROC TPSPLINE` selects one design point from the group and treats all observations in the group as replicates of that design point. Calculation of the thin-plate smoothing spline estimates is based on the reprocessed data. The way to choose the design point from a group depends on the order of the data. Hence, different orders of input data might result in different estimates.

By combining several design points into one, this option reduces the number of unique design points, thereby approximating the original data. The value you specify for the `D=` option determines the width of the range used to group the data.

---

## Getting Started: TPSPLINE Procedure

The following example demonstrates how you can use the `TPSPLINE` procedure to fit a semiparametric model.

Suppose that  $y$  is a continuous variable and  $x_1$  and  $x_2$  are two explanatory variables of interest. To fit a bivariate thin-plate spline model, you can use a `MODEL` statement similar to that used in many regression procedures in the SAS System:

```
proc tpspline;
 model y = (x1 x2);
run;
```

The `TPSPLINE` procedure can fit semiparametric models; the parentheses in the preceding `MODEL` statement separate the smoothing variables from the regression variables. The following statements illustrate this syntax:

```
proc tpspline;
 model y = z1 (x1 x2);
run;
```

This model assumes a linear relation with  $z_1$  and an unknown functional relation with  $x_1$  and  $x_2$ .

If you want to fit several responses by using the same explanatory variables, you can save computation time by using the multiple responses feature in the `MODEL` statement. For example, if  $y_1$  and  $y_2$  are two response variables, the following `MODEL` statement can be used to fit two models. Separate analyses are then performed for each response variable.

```
proc tpspline;
 model y1 y2 = (x1 x2);
run;
```

The following example illustrates the use of PROC TPSPLINE. The data are from Bates et al. (1987).

```
data Measure;
 input x1 x2 y @@;
 datalines;
-1.0 -1.0 15.54483570 -1.0 -1.0 15.76312613
-.5 -1.0 18.67397826 -.5 -1.0 18.49722167
.0 -1.0 19.66086310 .0 -1.0 19.80231311
.5 -1.0 18.59838649 .5 -1.0 18.51904737
1.0 -1.0 15.86842815 1.0 -1.0 16.03913832
-1.0 -.5 10.92383867 -1.0 -.5 11.14066546
-.5 -.5 14.81392847 -.5 -.5 14.82830425
.0 -.5 16.56449698 .0 -.5 16.44307297
.5 -.5 14.90792284 .5 -.5 15.05653924
1.0 -.5 10.91956264 1.0 -.5 10.94227538
-1.0 .0 9.61492010 -1.0 .0 9.64648093
-.5 .0 14.03133439 -.5 .0 14.03122345
.0 .0 15.77400253 .0 .0 16.00412514
.5 .0 13.99627680 .5 .0 14.02826553
1.0 .0 9.55700164 1.0 .0 9.58467047
-1.0 .5 11.20625177 -1.0 .5 11.08651907
-.5 .5 14.83723493 -.5 .5 14.99369172
.0 .5 16.55494349 .0 .5 16.51294369
.5 .5 14.98448603 .5 .5 14.71816070
1.0 .5 11.14575565 1.0 .5 11.17168689
-1.0 1.0 15.82595514 -1.0 1.0 15.96022497
-.5 1.0 18.64014953 -.5 1.0 18.56095997
.0 1.0 19.54375504 .0 1.0 19.80902641
.5 1.0 18.56884576 .5 1.0 18.61010439
1.0 1.0 15.86586951 1.0 1.0 15.90136745
;
```

The data set Measure contains three variables x1, x2, and y. Suppose that you want to fit a surface by using the variables x1 and x2 to model the response y. The variables x1 and x2 are spaced evenly on a  $[-1 \times 1] \times [-1 \times 1]$  square, and the response y is generated by adding a random error to a function  $f(x_1, x_2)$ . The raw data are plotted in three-dimensional scatter plot by using the G3D procedure. In order to visualize those replicates, half of the data are shifted a little bit by adding a small value (0.001) to x1 values, as in the following statements:

```
data Measure1;
 set Measure;
run;

proc sort data=Measure1;
 by x2 x1;
run;
```

```

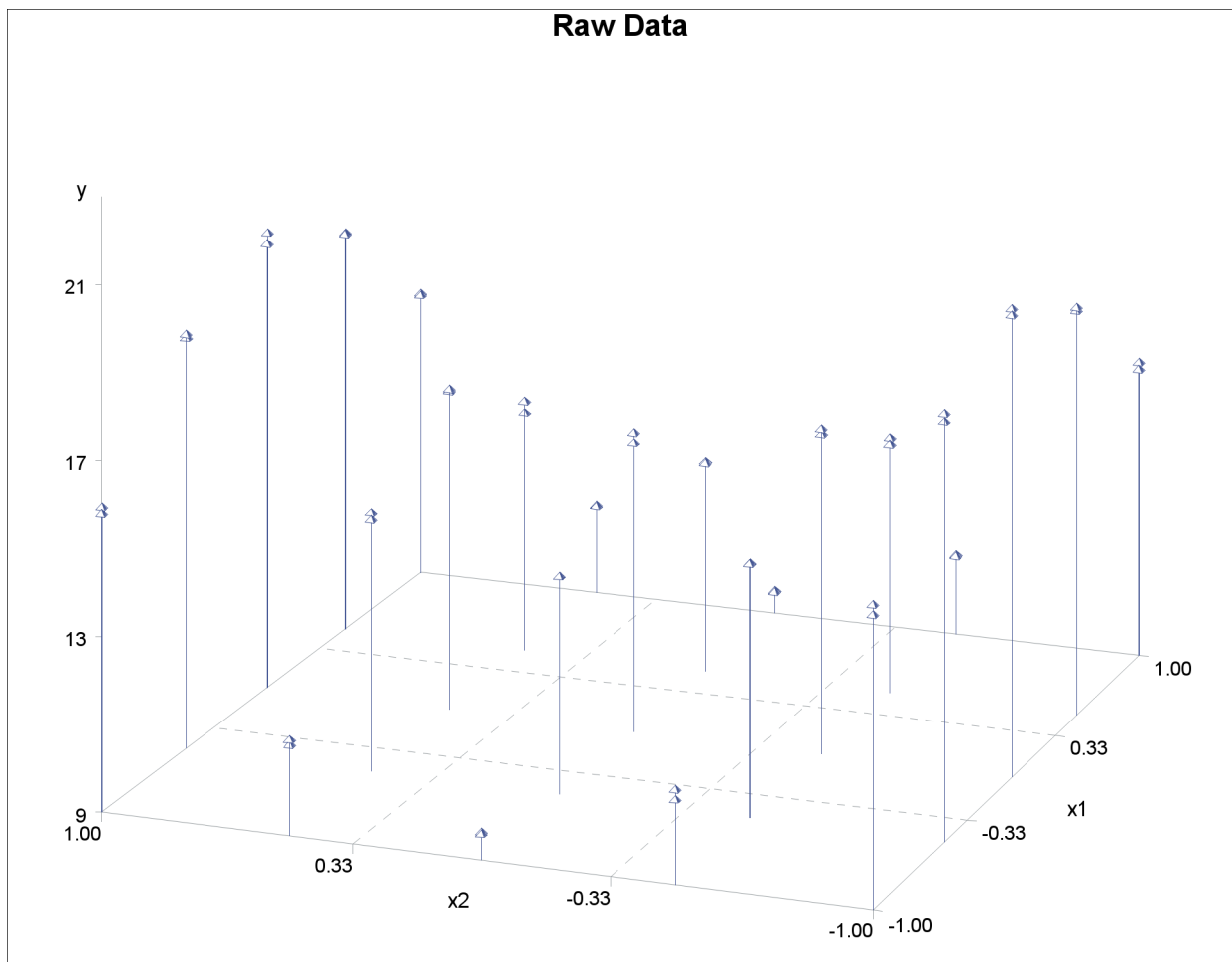
data Measure1;
 set Measure1;
 if mod(_N_, 2) = 0 then x1=x1+0.001;
run;

proc g3d data=Measure1;
 scatter x2*x1=y /size=.5
 zmin=9 zmax=21
 zticknum=4;
 title "Raw Data";
run;

```

Figure 96.1 displays the raw data.

**Figure 96.1** Plot of Data Set MEASURE



The following statements invoke the TPSPLINE procedure, to analyze the Measure data set as input. In the MODEL statement, the x1 and x2 variables are listed as smoothing variables. The LOGNLAMBDA= option specifies that PROC TPSPLINE examine a list of models with  $\log_{10}(n\lambda)$  ranging from -4 to -2.5. The OUTPUT statement creates the data set estimate to contain the predicted values and the 95% upper and lower confidence limits from the best model selected by the GCV criterion.

```
ods graphics on;
proc tpspline data=Measure;
 model y=(x1 x2) /lognlambda=(-4 to -2.5 by 0.1);
 output out=estimate pred uclm lclm;
run;

proc print data=estimate;
run;
```

When ODS Graphics is enabled, PROC TPSPLINE produces several default plots. One of the default plots is the contour plot of the fitted surface, shown in Figure 96.2. The surface exhibits nonlinear patterns along the directions of both predictors.

**Figure 96.2** Fitted Surface from PROC TPSPLINE

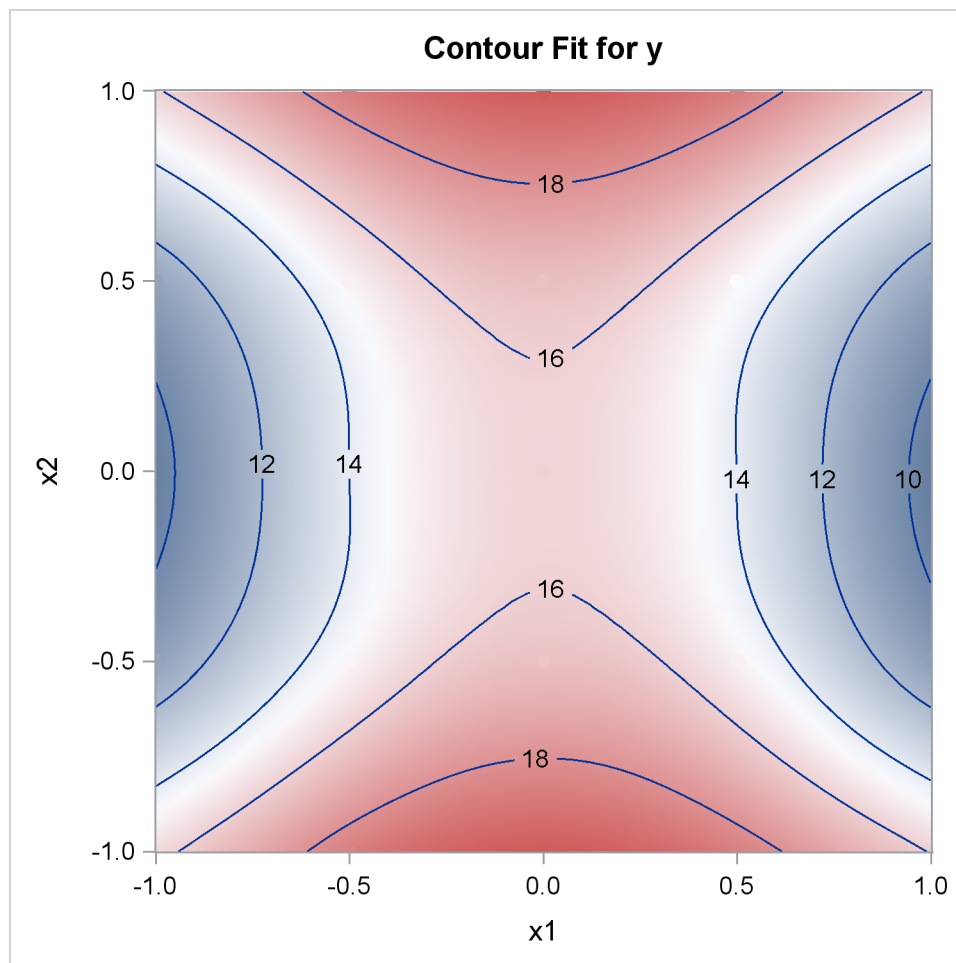




Figure 96.3 shows the “Criterion Plot” that provides a graphical display of the GCV selection process. Three sets of values are shown in the plot: the specified smoothing values and their GCV values, the examined smoothing values and their GCV values during the optimization process, and the best smoothing parameter and its GCV value. The final thin-plate smoothing spline estimate is based on  $\log_{10}(n\lambda) = -3.4762$ , which minimizes the GCV.

**Figure 96.3** The GCV Criterion by  $\log_{10}(n\lambda)$

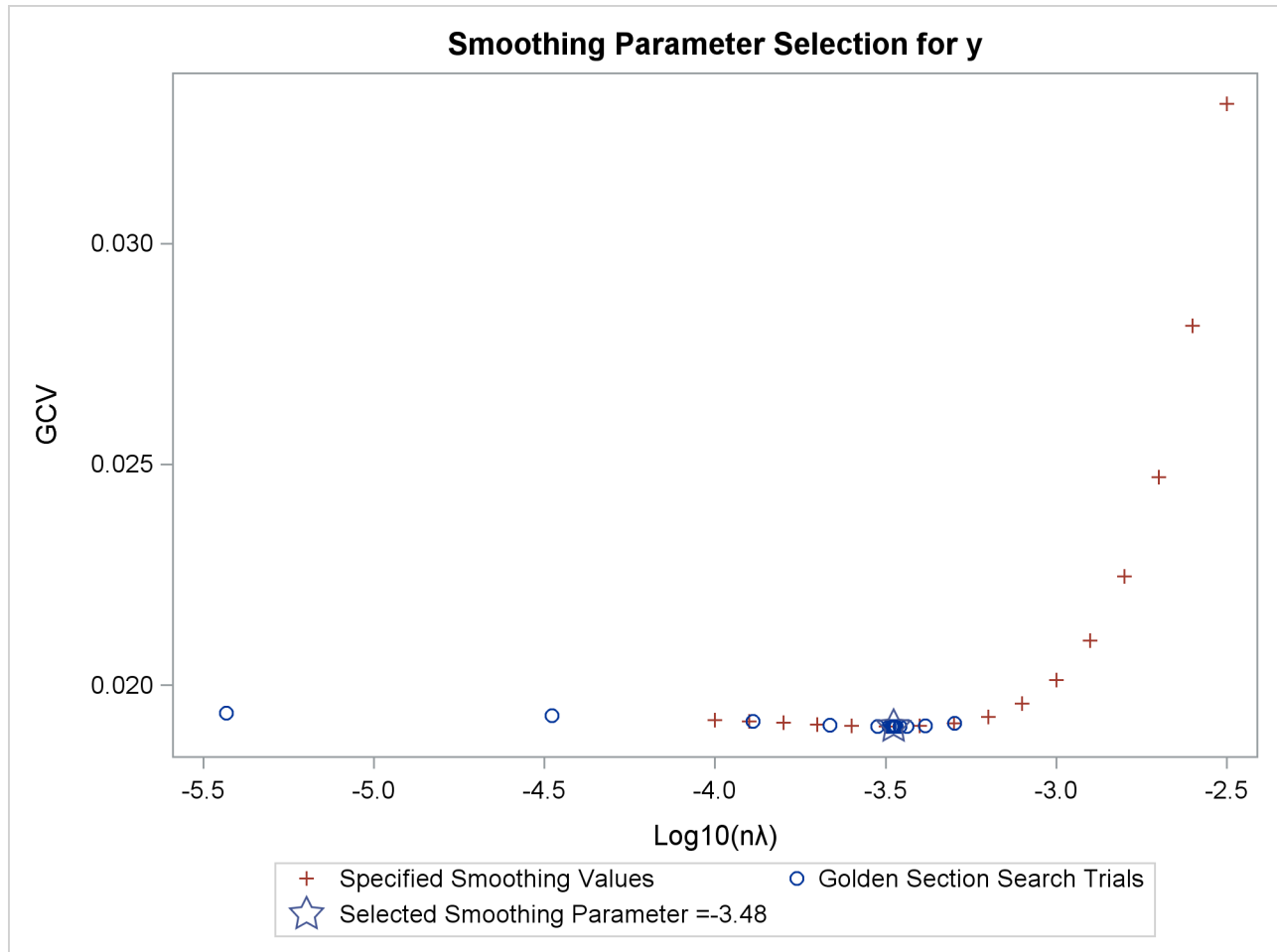


Figure 96.4 shows that the data set Measure contains 50 observations with 25 unique design points. The final model contains no parametric regression terms and two smoothing variables. The order of the derivative in the penalty is 2 by default, and the dimension of polynomial space is 3. See the section “Computational Formulas” on page 8117 for definitions.

Figure 96.4 also lists the GCV values along with the supplied values of  $\log_{10}(n\lambda)$ . The value that minimizes the GCV function is  $-3.5$  among the given list of  $\log_{10}(n\lambda)$ .

The residual sum of squares from the fitted model is 0.246110, and the model degrees of freedom are 24.593203. The standard deviation, defined as  $\text{RSS}/(\text{tr}(\mathbf{I} - \mathbf{A}))$ , is 0.098421. The predictions and 95% confidence limits are displayed in Figure 96.5.

Figure 96.4 Fitted Model Summaries from PROC TPSPLINE

| Raw Data                                  |           |
|-------------------------------------------|-----------|
| The TPSPLINE Procedure                    |           |
| Dependent Variable: y                     |           |
| Summary of Input Data Set                 |           |
| Number of Non-Missing Observations        | 50        |
| Number of Missing Observations            | 0         |
| Unique Smoothing Design Points            | 25        |
| Summary of Final Model                    |           |
| Number of Regression Variables            | 0         |
| Number of Smoothing Variables             | 2         |
| Order of Derivative in the Penalty        | 2         |
| Dimension of Polynomial Space             | 3         |
| GCV Function                              |           |
| log10(n*Lambda)                           | GCV       |
| -4.000000                                 | 0.019215  |
| -3.900000                                 | 0.019183  |
| -3.800000                                 | 0.019148  |
| -3.700000                                 | 0.019113  |
| -3.600000                                 | 0.019082  |
| -3.500000                                 | 0.019064* |
| -3.400000                                 | 0.019074  |
| -3.300000                                 | 0.019135  |
| -3.200000                                 | 0.019286  |
| -3.100000                                 | 0.019584  |
| -3.000000                                 | 0.020117  |
| -2.900000                                 | 0.021015  |
| -2.800000                                 | 0.022462  |
| -2.700000                                 | 0.024718  |
| -2.600000                                 | 0.028132  |
| -2.500000                                 | 0.033165  |
| Note: * indicates minimum GCV value.      |           |
| Summary Statistics<br>of Final Estimation |           |
| log10(n*Lambda)                           | -3.4762   |
| Smoothing Penalty                         | 2558.1432 |
| Residual SS                               | 0.2461    |
| Tr(I-A)                                   | 25.4068   |
| Model DF                                  | 24.5932   |
| Standard Deviation                        | 0.0984    |
| GCV                                       | 0.0191    |

Figure 96.5 Data Set ESTIMATE

| Raw Data |      |      |         |         |         |         |
|----------|------|------|---------|---------|---------|---------|
| Obs      | x1   | x2   | y       | P_y     | LCLM_y  | UCLM_y  |
| 1        | -1.0 | -1.0 | 15.5448 | 15.6474 | 15.5115 | 15.7832 |
| 2        | -1.0 | -1.0 | 15.7631 | 15.6474 | 15.5115 | 15.7832 |
| 3        | -0.5 | -1.0 | 18.6740 | 18.5783 | 18.4430 | 18.7136 |
| 4        | -0.5 | -1.0 | 18.4972 | 18.5783 | 18.4430 | 18.7136 |
| 5        | 0.0  | -1.0 | 19.6609 | 19.7270 | 19.5917 | 19.8622 |
| 6        | 0.0  | -1.0 | 19.8023 | 19.7270 | 19.5917 | 19.8622 |
| 7        | 0.5  | -1.0 | 18.5984 | 18.5552 | 18.4199 | 18.6905 |
| 8        | 0.5  | -1.0 | 18.5190 | 18.5552 | 18.4199 | 18.6905 |
| 9        | 1.0  | -1.0 | 15.8684 | 15.9436 | 15.8077 | 16.0794 |
| 10       | 1.0  | -1.0 | 16.0391 | 15.9436 | 15.8077 | 16.0794 |
| 11       | -1.0 | -0.5 | 10.9238 | 11.0467 | 10.9114 | 11.1820 |
| 12       | -1.0 | -0.5 | 11.1407 | 11.0467 | 10.9114 | 11.1820 |
| 13       | -0.5 | -0.5 | 14.8139 | 14.8246 | 14.6896 | 14.9597 |
| 14       | -0.5 | -0.5 | 14.8283 | 14.8246 | 14.6896 | 14.9597 |
| 15       | 0.0  | -0.5 | 16.5645 | 16.5102 | 16.3752 | 16.6452 |
| 16       | 0.0  | -0.5 | 16.4431 | 16.5102 | 16.3752 | 16.6452 |
| 17       | 0.5  | -0.5 | 14.9079 | 14.9812 | 14.8461 | 15.1162 |
| 18       | 0.5  | -0.5 | 15.0565 | 14.9812 | 14.8461 | 15.1162 |
| 19       | 1.0  | -0.5 | 10.9196 | 10.9497 | 10.8144 | 11.0850 |
| 20       | 1.0  | -0.5 | 10.9423 | 10.9497 | 10.8144 | 11.0850 |
| 21       | -1.0 | 0.0  | 9.6149  | 9.6372  | 9.5019  | 9.7724  |
| 22       | -1.0 | 0.0  | 9.6465  | 9.6372  | 9.5019  | 9.7724  |
| 23       | -0.5 | 0.0  | 14.0313 | 14.0188 | 13.8838 | 14.1538 |
| 24       | -0.5 | 0.0  | 14.0312 | 14.0188 | 13.8838 | 14.1538 |
| 25       | 0.0  | 0.0  | 15.7740 | 15.8822 | 15.7472 | 16.0171 |
| 26       | 0.0  | 0.0  | 16.0041 | 15.8822 | 15.7472 | 16.0171 |
| 27       | 0.5  | 0.0  | 13.9963 | 14.0006 | 13.8656 | 14.1356 |
| 28       | 0.5  | 0.0  | 14.0283 | 14.0006 | 13.8656 | 14.1356 |
| 29       | 1.0  | 0.0  | 9.5570  | 9.5769  | 9.4417  | 9.7122  |
| 30       | 1.0  | 0.0  | 9.5847  | 9.5769  | 9.4417  | 9.7122  |
| 31       | -1.0 | 0.5  | 11.2063 | 11.1614 | 11.0261 | 11.2967 |
| 32       | -1.0 | 0.5  | 11.0865 | 11.1614 | 11.0261 | 11.2967 |
| 33       | -0.5 | 0.5  | 14.8372 | 14.9182 | 14.7831 | 15.0532 |
| 34       | -0.5 | 0.5  | 14.9937 | 14.9182 | 14.7831 | 15.0532 |
| 35       | 0.0  | 0.5  | 16.5549 | 16.5386 | 16.4036 | 16.6736 |
| 36       | 0.0  | 0.5  | 16.5129 | 16.5386 | 16.4036 | 16.6736 |
| 37       | 0.5  | 0.5  | 14.9845 | 14.8549 | 14.7199 | 14.9900 |
| 38       | 0.5  | 0.5  | 14.7182 | 14.8549 | 14.7199 | 14.9900 |
| 39       | 1.0  | 0.5  | 11.1458 | 11.1727 | 11.0374 | 11.3080 |
| 40       | 1.0  | 0.5  | 11.1717 | 11.1727 | 11.0374 | 11.3080 |
| 41       | -1.0 | 1.0  | 15.8260 | 15.8851 | 15.7493 | 16.0210 |
| 42       | -1.0 | 1.0  | 15.9602 | 15.8851 | 15.7493 | 16.0210 |
| 43       | -0.5 | 1.0  | 18.6401 | 18.5946 | 18.4593 | 18.7299 |
| 44       | -0.5 | 1.0  | 18.5610 | 18.5946 | 18.4593 | 18.7299 |
| 45       | 0.0  | 1.0  | 19.5438 | 19.6729 | 19.5376 | 19.8081 |
| 46       | 0.0  | 1.0  | 19.8090 | 19.6729 | 19.5376 | 19.8081 |
| 47       | 0.5  | 1.0  | 18.5688 | 18.5832 | 18.4478 | 18.7185 |
| 48       | 0.5  | 1.0  | 18.6101 | 18.5832 | 18.4478 | 18.7185 |
| 49       | 1.0  | 1.0  | 15.8659 | 15.8761 | 15.7402 | 16.0120 |
| 50       | 1.0  | 1.0  | 15.9014 | 15.8761 | 15.7402 | 16.0120 |

You can also use the `TEMPLATE` and `SGRENDER` procedures to create a perspective plot for visualizing the fitted surface. Because the data in the data set `Measure` are very sparse, the fitted surface is not smooth. To produce a smoother surface, the following statements generate the data set `pred` in order to obtain a finer grid. The `LOGNLAMBDA0=` option requests that `PROC TPSPLINE` fit a model with a fixed  $\log_{10}(n\lambda)$  value of  $-3.4762$ . The `SCORE` statement evaluates the fitted surface at those new design points.

```

data pred;
 do x1=-1 to 1 by 0.1;
 do x2=-1 to 1 by 0.1;
 output;
 end;
 end;
run;

proc tpspline data=measure;
 model y=(x1 x2)/lognlambda0=-3.4762;
 score data=pred out=predy;
run;

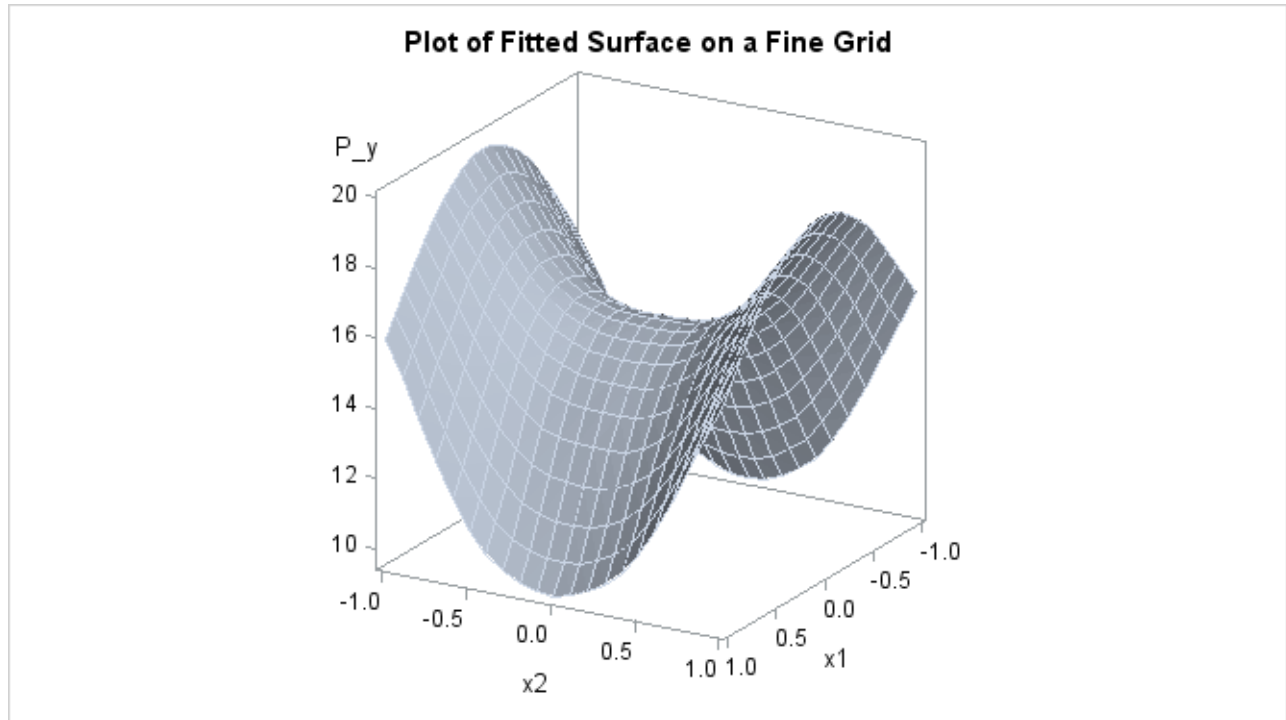
proc template;
 define statgraph surface;
 dynamic _X _Y _Z _T;
 begingraph /designheight=360;
 entrytitle _T;
 layout overlay3d/rotate=120 cube=false xaxisopts=(label="x1")
 yaxisopts=(label="x2") zaxisopts=(label="P_y");
 surfaceplotparm x=_X y=_Y z=_Z;
 endlayout;
 endgraph;
end;
run;

proc sgrender data=predy template=surface;
 dynamic _X='x1' _Y='x2' _Z='P_y'
 _T='Plot of Fitted Surface on a Fine Grid';
run;

```

The surface plot based on the finer grid is displayed in [Figure 96.6](#). The plot indicates that a parametric model with quadratic terms of  $x_1$  and  $x_2$  provides a reasonable fit to the data.

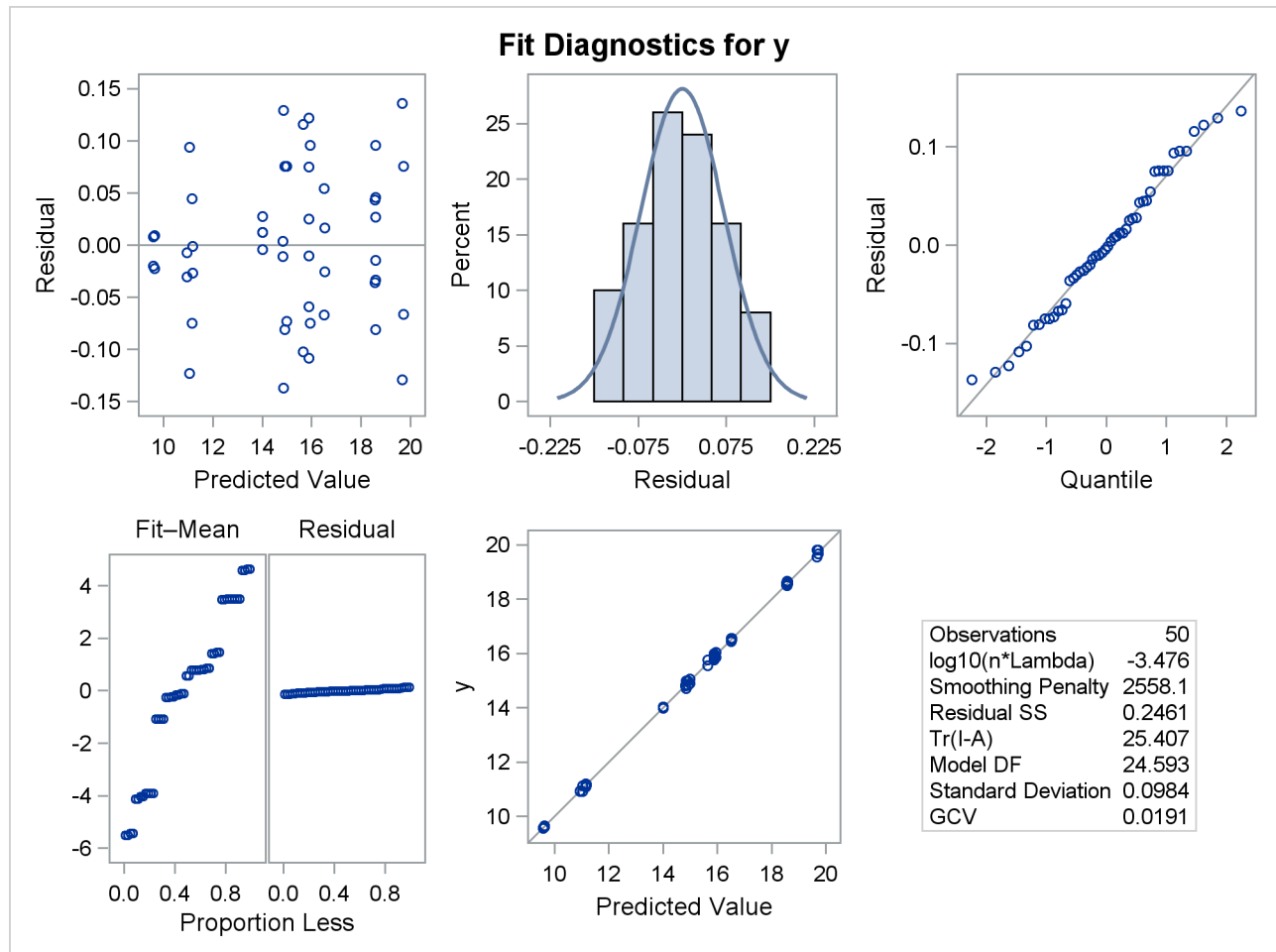
**Figure 96.6** Plot of TPSPLINE Fit



[Figure 96.7](#) shows a panel of fit diagnostics for the selected model that indicate a reasonable fit:

- The predicted values closely approximate the observed values.
- The residuals are approximately normally distributed and do not show obvious systematic patterns.
- The [RFPLOT](#) shows that much variation in the response variable is addressed by the fit and only a little remains in the residuals.

Figure 96.7 Fit Diagnostics



## Syntax: TPSPLINE Procedure

The following statements are available in the TPSPLINE procedure:

```

PROC TPSPLINE < options > ;
 MODEL dependents = < variables > (variables) < / options > ;
 SCORE DATA=SAS-data-set OUT=SAS-data-set < keyword ... keyword > ;
 OUTPUT < OUT=SAS-data-set > keyword ... keyword ;
 BY variables ;
 FREQ variable ;
 ID variables ;

```

The syntax in PROC TPSPLINE is similar to that of other regression procedures in the SAS System. The PROC TPSPLINE and MODEL statements are required. The SCORE statement can appear multiple times; all other statements appear no more than once.

The statements available for PROC TPSPLINE are described in alphabetical order after the description of the PROC TPSPLINE statement.

## PROC TPSPLINE Statement

**PROC TPSPLINE** < options > ;

The PROC TPSPLINE statement invokes the TPSPLINE procedure. Table 96.1 summarizes the options available in the TPSPLINE statement.

**Table 96.1** PROC TPSPLINE Statement Options

| Option       | Description                                               |
|--------------|-----------------------------------------------------------|
| <b>DATA=</b> | Specifies the SAS data set to be read                     |
| <b>PLOTS</b> | Controls the plots that are produced through ODS Graphics |

You can specify the following options:

**DATA=SAS-data-set**

specifies the SAS data set to be read by PROC TPSPLINE. The default value is the most recently created data set.

**PLOTS** < (global-plot-options) > <= plot-request < (options) > >

**PLOTS** < (global-plot-options) > <= (plot-request < (options) > <...plot-request < (options) > > >

controls the plots that are produced through ODS Graphics. When you specify only one plot request, you can omit the parentheses around the plot request. Here are some examples:

```
plots=none
plots=residuals(smooth)
plots(unpack)=diagnostics
plots(only)=(fit residualHistogram)
```

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;

proc tpspline;
 model y = (x);
run;

ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

If ODS Graphics is enabled but you do not specify the PLOTS= option, then PROC TPSPLINE produces a default set of plots. The following table lists the plots that are produced.

**Table 96.2** Graphs Produced

| Plot            | Conditional on:                                                |
|-----------------|----------------------------------------------------------------|
| ContourFitPanel | LAMBDA= or LOGNLAMBDA= option specified in the MODEL statement |
| ContourFit      | Model with two predictors                                      |

Table 96.2 continued

| Plot             | Conditional On                                                 |
|------------------|----------------------------------------------------------------|
| CriterionPlot    | Multiple values for the smoothing parameter                    |
| DiagnosticsPanel | Unconditional                                                  |
| ResidualBySmooth | LAMBDA= or LOGNLAMBDA= option specified in the MODEL statement |
| ResidualPanel    | Unconditional                                                  |
| FitPanel         | LAMBDA= or LOGNLAMBDA= option specified in the MODEL statement |
| FitPlot          | Model with one predictor                                       |
| ScorePlot        | One or more SCORE statements and a model with one predictor    |

For models with multiple dependent variables, separate plots are produced for each dependent variable. For models in which multiple smoothing parameters are specified with the LAMBDA= or LOGNLAMBDA= option in the MODEL statement, the plots are produced for the selected model only.

## Global Plot Options

The *global-plot-options* apply to all relevant plots generated by the TPSPLINE procedure, unless they are overridden by a *specific-plot-option*. The following *global-plot-options* are supported by the TPSPLINE procedure:

### ONLY

suppresses the default plots. Only the plots specifically requested are produced.

### UNPACK

suppresses paneling. By default, multiple plots can appear in some output panels. Specify UNPACK to get each plot individually. You can specify PLOTS(UNPACK) to unpack the default plots. You can also specify UNPACK as a suboption with the CONTOURFITPANEL, DIAGNOSTICS, FITPANEL, RESIDUALS and RESIDUALSBYSMOOTH options.

## Plot Requests

You can specify the following specific *plot-requests* and controls for them:

### ALL

produces all plots appropriate for the particular analysis. You can specify other options with ALL; for example, to request that all plots be produced and that only the residual plots be unpacked, specify PLOTS=(ALL RESIDUALS(UNPACK)).

### CONTOURFIT <(OBS=*contour-options*)>

produces a contour plot of the fitted surface overlaid with a scatter plot of the data for models with two predictors. You can use the following *contour-options* to control how the observations are displayed:

### GRADIENT

displays observations as circles colored by the observed response. The same color gradient is used to display the fitted surface and the observations. Observations where the predicted response is close to the observed response have similar colors—the greater the contrast between the color of an observation and the surface, the larger the residual is at that point. OBS=GRADIENT is the default if you do not specify any *contour-options*.



**NONE**

suppresses the observations.

**OUTLINE**

displays observations as circles with a border but with a completely transparent fill.

**OUTLINEGRADIENT**

is the same as `OBS=GRADIENT` except that a border is shown around each observation. This option is useful for identifying the location of observations where the residuals are small, because at these points the color of the observations and the color of the surface are indistinguishable.

**CONTOURFITPANEL <(options)>**

produces panels of contour plots overlaid with a scatter plot of the data for each smoothing parameter specified in the `LAMBDA=` or `LOGNLAMBDA=` option in the `MODEL` statement, for models with two predictors. If you do not specify the `LAMBDA=` or `LOGNLAMBDA=` option or if the model does not have two predictors, then this plot is not produced. Each panel contains at most six plots, and multiple panels are used when there are more than six smoothing parameters in the `LAMBDA=` or `LOGNLAMBDA=` option. The following *options* are available:

**OBS=contour-options**

specifies how the observations are displayed. See *contour-options* for the `CONTOURFIT` option for details.

**UNPACK**

suppresses paneling.

**CRITERIONPLOT | CRITERION <(NOPATH)>**

displays a scatter plot of the value of the GCV criterion versus the smoothing parameter value for all smoothing parameter values examined in the selection process. This plot is not produced when you specify one smoothing parameter with either the `LAMBDA0=` or `LOGNLAMBDA0=` option in the `MODEL` statement. When you supply a list of values for the smoothing parameter with the `LAMBDA=` or `LOGNLAMBDA=` option and PROC TPSPLINE obtains the optimal smoothing parameter by minimizing the GCV criterion, then the plot contains the supplied list of smoothing values and the optimal smoothing parameter in addition to the values examined during the optimization process. You can use the `NOPATH` suboption to disable the display of the optimization path in the plot in this case.

**DIAGNOSTICSPANEL | DIAGNOSTICS <(UNPACK)>**

produces a summary panel of fit diagnostics that consists of the following:

- residuals versus the predicted values
- a histogram of the residuals
- a normal quantile plot of the residuals
- a “Residual-Fit” (RF) plot that consists of side-by-side quantile plots of the centered fit and the residuals
- response values versus the predicted values

You can request the five plots in this panel as individual plots by specifying the `UNPACK` option. You can also request individual plots in the panel by name without having to unpack the panel. The fit diagnostics panel is produced by default whenever ODS Graphics is enabled.

**FITPANEL** < (*options*) >

produces panels of plots that show the fitted TPSPLINE curve overlaid on a scatter plot of the input data for each smoothing parameter specified in the **LAMBDA=** or **LOGNLAMBDA=** option in the MODEL statement. If you do not specify the **LAMBDA=** or **LOGNLAMBDA=** option or the model has more than one predictor, then this plot is not produced. Each panel contains at most six plots, and multiple panels are used when there are more than six smoothing parameters in the **LAMBDA=** or **LOGNLAMBDA=** option. The following *options* are available:

**CLM**

includes a confidence band at the significance level specified in the **ALPHA=** option in the MODEL statement in each plot in the panels.

**UNPACK**

suppresses paneling.

**FITPLOT | FIT** < (**CLM**) >

produces a scatter plot of the input data with the fitted TPSPLINE curve overlaid for models with a single predictor. If the **CLM** option is specified, then a confidence band at the significance level specified in the **ALPHA=** option in the MODEL statement is included in the plot.

**NONE**

suppresses all plots.

**OBSERVEDBYPREDICTED**

produces a scatter plot of the dependent variable values by the predicted values.

**QQPLOT | QQ**

produces a normal quantile plot of the residuals.

**RESIDUALBYSMOOTH** < (**SMOOTH**) >

produces, for each predictor, panels of plots that show the residuals of the TPSPLINE fit versus the predictor for each smoothing parameter specified in the **LAMBDA=** or **LOGNLAMBDA=** option in the MODEL statement. If you do not specify the **LAMBDA=** or **LOGNLAMBDA=** option, then this plot is not produced. Each panel contains at most six plots, and multiple panels are used when there are more than six smoothing parameters in the **LAMBDA=** or **LOGNLAMBDA=** option in the MODEL statement. The **SMOOTH** option displays a nonparametric fit line in each plot in the panel. The type of nonparametric fit and the options used are controlled by the underlying template for this plot. In the standard template that is provided, the nonparametric smooth is specified to be a loess fit that corresponds to the default options of PROC LOESS, except that the **PRESEARCH** suboption in the **SELECT** statement is always used. It is important to note that the loess fit that is shown in each of the residual plots is computed independently of the smoothing spline fit that is used to obtain the residuals.

**RESIDUALBYPREDICTED**

produces a scatter plot of the residuals by the predicted values.

**RESIDUALHISTOGRAM**

produces a histogram of the residuals.

**RESIDUALPANEL | RESIDUALS** <(options)>

produces panels of the residuals versus the predictors in the model. Each panel contains at most six plots, and multiple panels are used when there are more than six predictors in the model.

The following *options* are available:

**SMOOTH**

displays a nonparametric fit line in each plot in the panel. The type of nonparametric fit and the options used are controlled by the underlying template for this plot. In the standard template that is provided, the nonparametric smooth is specified to be a loess fit that corresponds to the default options of PROC LOESS, except that the PRESEARCH suboption in the SELECT statement is always used. It is important to note that the loess fit that is shown in each of the residual plots is computed independently of the smoothing spline fit that is used to obtain the residuals.

**UNPACK**

suppresses paneling.

**RFPLOT | RF**

produces a “Residual-Fit” (RF) plot that consists of side-by-side quantile plots of the centered fit and the residuals. This plot “shows how much variation in the data is explained by the fit and how much remains in the residuals” (Cleveland 1993).

**SCOREPLOT | SCORE**

produces a scatter plot of the scored values at the score points for each SCORE statement. SCORE plots are not produced for models with more than one predictor.

**BY Statement**

**BY** *variables* ;

You can specify a BY statement with PROC TPSPLINE to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the TPSPLINE procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

---

## FREQ Statement

**FREQ** *variable* ;

If one variable in your input data set represents the frequency of occurrence for other values in the observation, specify the variable's name in a FREQ statement. PROC TPSPLINE treats the data as if each observation appears  $n$  times, where  $n$  is the value of the FREQ variable for the observation. If the value of the FREQ variable is less than one, the observation is not used in the analysis. Only the integer portion of the value is used.

---

## ID Statement

**ID** *variables* ;

The ID statement is optional, and more than one ID statement can be used. If variables are specified in the ID statement, their values are displayed in tooltips to identify observations in the plots produced by PROC TPSPLINE.

---

## MODEL Statement

**MODEL** *dependent-variables* = < *regression-variables* > (*smoothing-variables*)< / *options* > ;

The MODEL statement specifies the dependent variables, the independent regression variables, which are listed with no parentheses, and the independent smoothing variables, which are listed inside parentheses.

The regression variables are optional. At least one smoothing variable is required, and it must be listed after the regression variables. No variables can be listed in both the regression variable list and the smoothing variable list.

If you specify more than one dependent variable, PROC TPSPLINE calculates a thin-plate smoothing spline estimate for each dependent variable by using the regression variables and smoothing variables specified on the right side.

If you specify regression variables, PROC TPSPLINE fits a semiparametric model by using the regression variables as the linear part of the model.

Table 96.3 summarizes the options available in the MODEL statement.

**Table 96.3** MODEL Statement Options

| Option       | Description                                                                              |
|--------------|------------------------------------------------------------------------------------------|
| ALPHA=       | Specifies the significance level                                                         |
| DF=          | Specifies the degrees of freedom                                                         |
| DISTANCE=    | Defines a range in which points are treated as replicates                                |
| LAMBDA0=     | Specifies the smoothing parameter                                                        |
| LAMBDA=      | Specifies a set of values for the $\lambda$ parameter                                    |
| LOGNLAMBDA0= | Specifies the smoothing parameter on the $\log_{10}(n\lambda)$ scale                     |
| LOGNLAMBDA=  | Specifies a set of values for the $\lambda$ parameter on the $\log_{10}(n\lambda)$ scale |
| M=           | Specifies the order of the derivative                                                    |
| RANGE=       | Specifies the range for smoothing values to be evaluated                                 |

You can specify the following options in the MODEL statement:

**ALPHA=number**

specifies the significance level  $\alpha$  of the confidence limits on the final thin-plate smoothing spline estimate when you request confidence limits to be included in the output data set. Specify *number* as a value between 0 and 1. The default value is 0.05. See the section “OUTPUT Statement” on page 8116 for more information about the OUTPUT statement.

**DF=df**

specifies the degrees of freedom of the thin-plate smoothing spline estimate, defined as

$$df = \text{tr}(\mathbf{A}(\lambda))$$

where  $\mathbf{A}(\lambda)$  is the *hat* matrix. Specify *df* as a value between zero and the number of unique design points  $n_q$ . Smaller *df* values cause more penalty on the roughness and thus smoother fits.

**DISTANCE=number**

**D=number**

defines a range such that if the  $L_\infty$  distance between two data points  $(\mathbf{x}_i, \mathbf{z}_i)$  and  $(\mathbf{x}_j, \mathbf{z}_j)$  satisfies

$$\|\mathbf{x}_i - \mathbf{x}_j\|_\infty \leq D/2$$

then these data points are treated as replicates, where  $\mathbf{x}_i$  are the smoothing variables and  $\mathbf{z}_i$  are the regression variables.

You can use the DISTANCE= option to reduce the number of unique design points by treating nearby data as replicates. This can be useful when you have a large data set. Larger DISTANCE= option values cause fewer  $n_q$  points. The default value is 0.

PROC TPSPLINE uses the DISTANCE= value to group points as follows: The data are first sorted by the smoothing variables in the order in which they appear in the MODEL statement. The first point in the sorted data becomes the first unique point. Subsequent points have their values set equal to that point until the first point where the maximum distance in one dimension is larger than  $D/2$ . This point becomes the next unique point, and so on. Because of this sequential processing, the set of unique points differs depending on the order of the smoothing variables in the MODEL statement.

For example, with a model that has two smoothing variables ( $x_1$ ,  $x_2$ ), the data are first sorted by  $x_1$  and  $x_2$  (in that order), and then uniqueness is assessed sequentially. The first point in the sorted data  $x_1 = (x_{1_1}, x_{2_1})$  becomes the first unique point,  $u_1 = (u_{1_1}, u_{2_1})$ . Subsequent points  $x_i = (x_{1_i}, x_{2_i})$  are set equal to  $u_1$  until the algorithm comes to a point with  $\max(|x_{1_i} - u_{1_1}|, |x_{2_i} - u_{2_1}|) > D/2$ . This point becomes the second unique point  $u_2$ , and data sorting proceeds from there.

**LAMBDA0=number**

specifies the smoothing parameter,  $\lambda_0$ , to be used in the thin-plate smoothing spline estimate. By default, PROC TPSPLINE uses the  $\lambda$  parameter that minimizes the GCV function for the final fit. The LAMBDA0= value must be positive. Larger  $\lambda_0$  values cause smoother fits.

**LAMBDA=list-of-values**

specifies a set of values for the  $\lambda$  parameter. PROC TPSPLINE returns a GCV value for each  $\lambda$  point that you specify. You can use the LAMBDA= option to study the GCV function curve for a set of values for  $\lambda$ . All values listed in the LAMBDA= option must be positive.

**LOGNLAMBDA0=number**

**LOGNL0=number**

specifies the smoothing parameter  $\lambda_0$  on the  $\log_{10}(n\lambda)$  scale. If you specify both the LOGNL0= and LAMBDA0= options, only the value provided by the LOGNL0= option is used. Larger  $\log_{10}(n\lambda_0)$  values cause smoother fits. By default, PROC TPSPLINE uses the  $\lambda$  parameter that minimizes the GCV function for the estimate.

**LOGNLAMBDA=list-of-values**

**LOGNL=list-of-values**

specifies a set of values for the  $\lambda$  parameter on the  $\log_{10}(n\lambda)$  scale. PROC TPSPLINE returns a GCV value for each  $\lambda$  point that you specify. You can use the LOGNLAMBDA= option to study the GCV function curve for a set of  $\lambda$  values. If you specify both the LOGNL= and LAMBDA= options, only the list of values provided by the LOGNL= option is used.

In some cases, the LOGNL= option might be preferred over the LAMBDA= option. Because the LAMBDA= value must be positive, a small change in that value can result in a major change in the GCV value. If you instead specify  $\lambda$  on the  $\log_{10}(n\lambda)$  scale, the allowable range is enlarged to include negative values. Thus, the GCV function is less sensitive to changes in LOGNLAMBDA.

The DF= option, LAMBDA0= option, and LOGNLAMBDA0= option all specify exact smoothness of a nonparametric fit. If you want to fit a model with specified smoothness, the DF= option is preferable to the other two options because  $(0, n_q)$ , the range of  $df$ , is much smaller in length than  $(0, \infty)$  of  $\lambda$  and  $(-\infty, \infty)$  of  $\log_{10}(n\lambda)$ .

**M=number**

specifies the order of the derivative in the penalty term. The *number* must be a positive integer. The default value is  $\max(2, \text{int}(d/2) + 1)$ , where  $d$  is the number of smoothing variables.

**RANGE=(lower, upper)**

specifies that on the  $\log_{10}(n\lambda)$  scale only smoothing values greater than or equal to *lower* and less than or equal to *upper* be evaluated to minimize the GCV function.

## OUTPUT Statement

**OUTPUT** **OUT**=SAS-data-set < keyword ... keyword > ;

The OUTPUT statement creates a new SAS data set that contains diagnostic measures calculated after fitting the model.

All the variables in the original data set are included in the new data set, along with variables created by specifying *keywords* in the OUTPUT statement. These new variables contain the values of a variety of statistics and diagnostic measures that are calculated for each observation in the data set. If no *keyword* is present, the data set contains only the original data set and predicted values.

Details about the specifications in the OUTPUT statement are as follows.

### **OUT**=SAS-data-set

specifies the name of the new data set to contain the diagnostic measures. This specification is required.

### *keyword*

specifies the statistics to include in the output data set. The names of the new variables that contain the statistics are formed by using a prefix of one or more characters to identify the statistic, followed by an underscore (\_), followed by the dependent variable name.

For example, suppose that you have two dependent variables—say, *y1* and *y2*—and you specify the keywords PRED, ADIAG, and UCLM. The output SAS data set will contain the following variables:

- P\_y1 and P\_y2
- ADIAG\_y1 and ADIAG\_y2
- UCLM\_y1 and UCLM\_y2

The keywords and the statistics they represent are as follows:

|           |                                                                                                                                                                                                                                                                                   |
|-----------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| RESID   R | residual values, calculated as fitted values subtracted from the observed response values: $y - \hat{y}$ . The default prefix is R_.                                                                                                                                              |
| PRED      | predicted values. The default prefix is P_.                                                                                                                                                                                                                                       |
| STD       | standard error of the mean predicted value. The default prefix is STD_.                                                                                                                                                                                                           |
| UCLM      | upper limit of the Bayesian confidence interval for the expected value of the dependent variables. By default, PROC TPSPLINE computes 95% confidence limits. The default prefix is UCLM_.                                                                                         |
| LCLM      | lower limit of the Bayesian confidence interval for the expected value of the dependent variables. By default, PROC TPSPLINE computes 95% confidence limits. The default prefix is LCLM_.                                                                                         |
| ADIAG     | diagonal element of the hat matrix associated with the observation. The default prefix is ADIAG_.                                                                                                                                                                                 |
| COEF      | coefficients arranged in the order of $(\theta_0, \theta_1, \dots, \theta_d, \delta_1, \dots, \delta_{n_q})$ , where $n_q$ is the number of unique data points. This option can be used only when there is only one dependent variable in the model. The default prefix is COEF_. |

---

## SCORE Statement

**SCORE DATA=SAS-data-set OUT=SAS-data-set < keyword . . . keyword > ;**

The SCORE statement calculates predicted statistics for a new data set. If you have multiple data sets to predict, you can specify multiple SCORE statements. You must use a SCORE statement for each data set.

You can request diagnostic measures that are calculated for each observation in the SCORE data set. The new data set contains all the variables in the SCORE data set in addition to the requested variables. If no *keyword* is present, the data set contains only the predicted values.

The following keywords must be specified in the SCORE statement:

**DATA=SAS-data-set**

specifies the input SAS data set that contains the smoothing variables  $\mathbf{x}$  and regression variables  $\mathbf{z}$ . The predicted response ( $\hat{y}$ ) value is computed for each  $(\mathbf{x}, \mathbf{z})$  pair. The data set must include all independent variables specified in the MODEL statement.

**OUT=SAS-data-set**

specifies the name of the SAS data set to contain the predictions.

*keyword*

specifies the statistics to include in the output data set for the current SCORE statement. The names of the new variables that contain the statistics are formed by using a prefix of one or more characters to identify the statistic, followed by an underscore ( $\_$ ), followed by the dependent variable name. The keywords and the statistics they represent are as follows:

|      |                                                                                                                                                              |
|------|--------------------------------------------------------------------------------------------------------------------------------------------------------------|
| PRED | predicted values                                                                                                                                             |
| STD  | standard error of the mean predicted value                                                                                                                   |
| UCLM | upper limit of the Bayesian confidence interval for the expected value of the dependent variables. By default, PROC TPSPLINE computes 95% confidence limits. |
| LCLM | lower limit of the Bayesian confidence interval for the expected value of the dependent variables. By default, PROC TPSPLINE computes 95% confidence limits. |

---

## Details: TPSPLINE Procedure

---

### Computational Formulas

The theoretical foundations for the thin-plate smoothing spline are described in Duchon (1976, 1977) and Meinguet (1979). Further results and applications are given in: Wahba and Wendelberger (1980); Hutchinson and Bischof (1983); Seaman and Hutchinson (1985).

Suppose that  $\mathcal{H}_m$  is a space of functions whose partial derivatives of total order  $m$  are in  $L_2(E^d)$ , where  $E^d$  is the domain of  $\mathbf{x}$ .



Now, consider the data model

$$y_i = f(\mathbf{x}_i) + \epsilon_i, i = 1, \dots, n$$

where  $f \in \mathcal{H}_m$ .

Using the notation from the section “[Penalized Least Squares Estimation](#)” on page 8096, for a fixed  $\lambda$ , estimate  $f$  by minimizing the penalized least squares function

$$\frac{1}{n} \sum_{i=1}^n (y_i - f(\mathbf{x}_i) - \mathbf{z}_i \boldsymbol{\beta})^2 + \lambda J_m(f)$$

$\lambda J_m(f)$  is the penalty term to enforce smoothness on  $f$ . There are several ways to define  $J_m(f)$ . For the thin-plate smoothing spline, with  $\mathbf{x} = (x_1, \dots, x_d)$  of dimension  $d$ , define  $J_m(f)$  as

$$J_m(f) = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \sum \frac{m!}{\alpha_1! \cdots \alpha_d!} \left( \frac{\partial^m f}{\partial x_1^{\alpha_1} \cdots \partial x_d^{\alpha_d}} \right)^2 dx_1 \cdots dx_d$$

where  $\sum_i \alpha_i = m$ . Under this definition,  $J_m(f)$  gives zero penalty to some functions. The space that is spanned by the set of polynomials that contribute zero penalty is called the polynomial space. The dimension of the polynomial space  $M$  is a function of dimension  $d$  and order  $m$  of the smoothing penalty,  $M = \binom{m+d-1}{d}$ .

Given the condition that  $2m > d$ , the function that minimizes the penalized least squares criterion has the form

$$\hat{f}(\mathbf{x}) = \sum_{j=1}^M \theta_j \phi_j(\mathbf{x}) + \sum_{i=1}^n \delta_i \eta_{md}(\|\mathbf{x} - \mathbf{x}_i\|)$$

where  $\boldsymbol{\theta}$  and  $\boldsymbol{\delta}$  are vectors of coefficients to be estimated. The  $M$  functions  $\phi_j$  are linearly independent polynomials that span the space of functions for which  $J_m(f)$  is zero. The basis functions  $\eta_{md}$  are defined as

$$\eta_{md}(r) = \begin{cases} \frac{(-1)^{m+1+d/2}}{2^{2m-1} \pi^{d/2} (m-1)! (m-d/2)!} r^{2m-d} \log(r) & \text{if } d \text{ is even} \\ \frac{\Gamma(d/2-m)}{2^{2m} \pi^{d/2} (m-1)!} r^{2m-d} & \text{if } d \text{ is odd} \end{cases}$$

When  $d = 2$  and  $m = 2$ , then  $M = \binom{3}{2} = 3$ ,  $\phi_1(\mathbf{x}) = 1$ ,  $\phi_2(\mathbf{x}) = x_1$ , and  $\phi_3(\mathbf{x}) = x_2$ .  $J_m(f)$  is as follows:

$$J_2(f) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left( \left( \frac{\partial^2 f}{\partial x_1^2} \right)^2 + 2 \left( \frac{\partial^2 f}{\partial x_1 \partial x_2} \right)^2 + \left( \frac{\partial^2 f}{\partial x_2^2} \right)^2 \right) dx_1 dx_2$$

For the sake of simplicity, the formulas and equations that follow assume  $m = 2$ . See Wahba (1990) and Bates et al. (1987) for more details.

Duchon (1976) showed that  $f_\lambda$  can be represented as

$$f_\lambda(\mathbf{x}_i) = \theta_0 + \sum_{j=1}^d \theta_j \mathbf{x}_{i j} + \sum_{j=1}^n \delta_j E_2(\mathbf{x}_i - \mathbf{x}_j)$$

where  $E_2(\mathbf{s}) = \frac{1}{2^{3\pi}} \|\mathbf{s}\|^2 \log(\|\mathbf{s}\|)$  for  $d = 2$ . For derivations of  $E_2(\mathbf{s})$  for other values of  $d$ , see Villalobos and Wahba (1987).

If you define  $\mathbf{K}$  with elements  $\mathbf{K}_{ij} = E_2(\mathbf{x}_i - \mathbf{x}_j)$  and  $\mathbf{T}$  with elements  $\mathbf{T}_{ij} = (\mathbf{X}_{ij})$ , the goal is to find vectors of coefficients  $\boldsymbol{\beta}$ ,  $\boldsymbol{\theta}$ , and  $\boldsymbol{\delta}$  that minimize

$$S_\lambda(\boldsymbol{\beta}, \boldsymbol{\theta}, \boldsymbol{\delta}) = \frac{1}{n} \|\mathbf{y} - \mathbf{T}\boldsymbol{\theta} - \mathbf{K}\boldsymbol{\delta} - \mathbf{Z}\boldsymbol{\beta}\|^2 + \lambda \boldsymbol{\delta}'\mathbf{K}\boldsymbol{\delta}$$

A unique solution is guaranteed if the matrix  $\mathbf{T}$  is of full rank and  $\boldsymbol{\delta}'\mathbf{K}\boldsymbol{\delta} \geq 0$ .

If  $\boldsymbol{\alpha} = \begin{pmatrix} \boldsymbol{\theta} \\ \boldsymbol{\beta} \end{pmatrix}$  and  $\mathbf{X} = (\mathbf{T} \ \mathbf{Z})$ , the expression for  $S_\lambda$  becomes

$$\frac{1}{n} \|\mathbf{y} - \mathbf{X}\boldsymbol{\alpha} - \mathbf{K}\boldsymbol{\delta}\|^2 + \lambda \boldsymbol{\delta}'\mathbf{K}\boldsymbol{\delta}$$

The coefficients  $\boldsymbol{\alpha}$  and  $\boldsymbol{\delta}$  can be obtained by solving

$$\begin{aligned} (\mathbf{K} + n\lambda\mathbf{I}_n)\boldsymbol{\delta} + \mathbf{X}\boldsymbol{\alpha} &= \mathbf{y} \\ \mathbf{X}'\boldsymbol{\delta} &= \mathbf{0} \end{aligned}$$

To compute  $\boldsymbol{\alpha}$  and  $\boldsymbol{\delta}$ , let the QR decomposition of  $\mathbf{X}$  be

$$\mathbf{X} = (\mathbf{Q}_1 \ \mathbf{Q}_2) \begin{pmatrix} \mathbf{R} \\ \mathbf{0} \end{pmatrix}$$

where  $(\mathbf{Q}_1 \ \mathbf{Q}_2)$  is an orthogonal matrix and  $\mathbf{R}$  is an upper triangular, with  $\mathbf{X}'\mathbf{Q}_2 = \mathbf{0}$  (Dongarra et al. 1979).

Since  $\mathbf{X}'\boldsymbol{\delta} = \mathbf{0}$ ,  $\boldsymbol{\delta}$  must be in the column space of  $\mathbf{Q}_2$ . Therefore,  $\boldsymbol{\delta}$  can be expressed as  $\boldsymbol{\delta} = \mathbf{Q}_2\boldsymbol{\gamma}$  for a vector  $\boldsymbol{\gamma}$ . Substituting  $\boldsymbol{\delta} = \mathbf{Q}_2\boldsymbol{\gamma}$  into the preceding equation and multiplying through by  $\mathbf{Q}_2'$  gives

$$\mathbf{Q}_2'(\mathbf{K} + n\lambda\mathbf{I})\mathbf{Q}_2\boldsymbol{\gamma} = \mathbf{Q}_2'\mathbf{y}$$

or

$$\boldsymbol{\delta} = \mathbf{Q}_2\boldsymbol{\gamma} = \mathbf{Q}_2[\mathbf{Q}_2'(\mathbf{K} + n\lambda\mathbf{I})\mathbf{Q}_2]^{-1}\mathbf{Q}_2'\mathbf{y}$$

The coefficient  $\boldsymbol{\alpha}$  can be obtained by solving

$$\mathbf{R}\boldsymbol{\alpha} = \mathbf{Q}_1'[\mathbf{y} - (\mathbf{K} + n\lambda\mathbf{I})\boldsymbol{\delta}]$$

The influence matrix  $\mathbf{A}(\lambda)$  is defined as

$$\hat{\mathbf{y}} = \mathbf{A}(\lambda)\mathbf{y}$$

and has the form

$$\mathbf{A}(\lambda) = \mathbf{I} - n\lambda\mathbf{Q}_2[\mathbf{Q}_2'(\mathbf{K} + n\lambda\mathbf{I})\mathbf{Q}_2]^{-1}\mathbf{Q}_2'$$

Similar to the regression case, if you consider the trace of  $\mathbf{A}(\lambda)$  as the degrees of freedom for the model and the trace of  $(\mathbf{I} - \mathbf{A}(\lambda))$  as the degrees of freedom for the error, the estimate  $\sigma^2$  can be represented as

$$\hat{\sigma}^2 = \frac{\text{RSS}(\lambda)}{\text{tr}(\mathbf{I} - \mathbf{A}(\lambda))}$$

where  $\text{RSS}(\lambda)$  is the residual sum of squares. Theoretical properties of these estimates have not yet been published. However, good numerical results in simulation studies have been described by several authors. For more information, see O'Sullivan and Wong (1987); Nychka (1986a, b, 1988); Hall and Titterton (1987).

## Confidence Intervals

Viewing the spline model as a Bayesian model, Wahba (1983) proposed Bayesian confidence intervals for smoothing spline estimates as

$$\hat{f}_\lambda(\mathbf{x}_i) \pm z_{\alpha/2} \sqrt{\hat{\sigma}^2 a_{ii}(\lambda)}$$

where  $a_{ii}(\lambda)$  is the  $i$ th diagonal element of the  $\mathbf{A}(\lambda)$  matrix and  $z_{\alpha/2}$  is the  $1 - \alpha/2$  quantile of the standard normal distribution. The confidence intervals are interpreted as intervals “across the function” as opposed to pointwise intervals.

For SCORE data sets, the hat matrix  $\mathbf{A}(\lambda)$  is not available. To compute the Bayesian confidence interval for a new point  $\mathbf{x}_{\text{new}}$ , let

$$\mathbf{S} = \mathbf{X}, \quad \mathbf{M} = \mathbf{K} + n\lambda\mathbf{I}$$

and let  $\boldsymbol{\xi}$  be an  $n \times 1$  vector with  $i$ th entry

$$\eta_{md}(\|\mathbf{x}_{\text{new}} - \mathbf{x}_i\|)$$

When  $d = 2$  and  $m = 2$ ,  $\xi_i$  is computed with

$$E_2(\mathbf{x}_i - \mathbf{x}_{\text{new}}) = \frac{1}{2^3 \pi} \|\mathbf{x}_i - \mathbf{x}_{\text{new}}\|^2 \log(\|\mathbf{x}_i - \mathbf{x}_{\text{new}}\|)$$

$\boldsymbol{\phi}$  is a vector of evaluations of  $\mathbf{x}_{\text{new}}$  by the polynomials that span the functional space where  $J_m(f)$  is zero. The details for  $\mathbf{X}$ ,  $\mathbf{K}$ , and  $E_2$  are discussed in the previous section. Wahba (1983) showed that the Bayesian posterior variance of  $\mathbf{x}_{\text{new}}$  satisfies

$$n\lambda \text{Var}(\mathbf{x}_{\text{new}}) = \boldsymbol{\phi}'(\mathbf{S}'\mathbf{M}^{-1}\mathbf{S})^{-1}\boldsymbol{\phi} - 2\boldsymbol{\phi}'\mathbf{d}_\xi - \boldsymbol{\xi}'\mathbf{c}_\xi$$

where

$$\begin{aligned} \mathbf{c}_\xi &= (\mathbf{M}^{-1} - \mathbf{M}^{-1}\mathbf{S}(\mathbf{S}'\mathbf{M}^{-1}\mathbf{S})^{-1}\mathbf{S}'\mathbf{M}^{-1})\boldsymbol{\xi} \\ \mathbf{d}_\xi &= (\mathbf{S}'\mathbf{M}^{-1}\mathbf{S})^{-1}\mathbf{S}'\mathbf{M}^{-1}\boldsymbol{\xi} \end{aligned}$$

Suppose that you fit a spline estimate that consists of a true function  $f$  and a random error term  $\epsilon_i$  to experimental data. In repeated experiments, it is likely that about  $100(1 - \alpha)\%$  of the confidence intervals cover the corresponding true values, although some values are covered every time and other values are not covered by the confidence intervals most of the time. This effect is more pronounced when the true surface or surface has small regions of particularly rapid change.

## Smoothing Parameter

The quantity  $\lambda$  is called the smoothing parameter, which controls the balance between the goodness of fit and the smoothness of the final estimate.

A large  $\lambda$  heavily penalizes the  $m$ th derivative of the function, thus forcing  $f^{(m)}$  close to 0. A small  $\lambda$  places less of a penalty on rapid change in  $f^{(m)}(\mathbf{x})$ , resulting in an estimate that tends to interpolate the data points.

The smoothing parameter greatly affects the analysis, and it should be selected with care. One method is to perform several analyses with different values for  $\lambda$  and compare the resulting final estimates.

A more objective way to select the smoothing parameter  $\lambda$  is to use the “leave-out-one” cross validation function, which is an approximation of the predicted mean squares error. A generalized version of the leave-out-one cross validation function is proposed by Wahba (1990) and is easy to calculate. This generalized cross validation (GCV) function is defined as

$$\text{GCV}(\lambda) = \frac{(1/n)\|(\mathbf{I} - \mathbf{A}(\lambda))\mathbf{y}\|^2}{[(1/n)\text{tr}(\mathbf{I} - \mathbf{A}(\lambda))]^2}$$

The justification for using the GCV function to select  $\lambda$  relies on asymptotic theory. Thus, you cannot expect good results for very small sample sizes or when there is not enough information in the data to separate the model from the error component. Simulation studies suggest that for independent and identically distributed Gaussian noise, you can obtain reliable estimates of  $\lambda$  for  $n$  greater than 25 or 30. Note that, even for large values of  $n$  (say,  $n \geq 50$ ), in extreme Monte Carlo simulations there might be a small percentage of unwarranted extreme estimates in which  $\hat{\lambda} = 0$  or  $\hat{\lambda} = \infty$  (Wahba 1983). Generally, if  $\sigma^2$  is known to within an order of magnitude, the occasional extreme case can be readily identified. As  $n$  gets larger, the effect becomes weaker.

The GCV function is fairly robust against nonhomogeneity of variances and non-Gaussian errors (Villalobos and Wahba 1987). Andrews (1988) has provided favorable theoretical results when variances are unequal. However, this selection method is likely to give unsatisfactory results when the errors are highly correlated.

The GCV value might be suspect when  $\lambda$  is extremely small because computed values might become indistinguishable from zero. In practice, calculations with  $\lambda = 0$  or  $\lambda$  near 0 can cause numerical instabilities that result in an unsatisfactory solution. Simulation studies have shown that a  $\lambda$  with  $\log_{10}(n\lambda) > -8$  is small enough that the final estimate based on this  $\lambda$  almost interpolates the data points. A GCV value based on a  $\lambda \leq 10^{-8}$  might not be accurate.

---

## ODS Table Names

PROC TPSPLINE assigns a name to each table it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. [Table 96.4](#) lists these names. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

**Table 96.4** ODS Tables Produced by PROC TPSPLINE

| ODS Table Name | Description                    | Statement | Option             |
|----------------|--------------------------------|-----------|--------------------|
| DataSummary    | Data summary                   | PROC      | Default            |
| FitSummary     | Fit parameters and fit summary | PROC      | Default            |
| FitStatistics  | Model fit statistics           | PROC      | Default            |
| GCVFunction    | GCV table                      | MODEL     | LOGNLAMBDA, LAMBDA |

By referring to the names of such tables, you can use the ODS OUTPUT statement to place one or more of these tables in output data sets.

For example, the following statements create an output data set named `FitStats` which contains the `FitStatistics` table, an output data set named `DataInfo` which contains the `DataSummary` table, an output data set named `ModelInfo` which contains the `FitSummary` table, and an output data set named `GCVFunc` which contains the `GCVFunction` table.

```
proc tpspline data=Melanoma;
 model Incidences=Year /LOGNLAMBDA=(-4 to 0 by 0.2);
 ods output FitStatistics = FitStats
 DataSummary = DataInfo
 FitSummary = ModelInfo
 GCVFunction = GCVFunc;
run;
```

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “[Statistical Graphics Using ODS.](#)”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the `ODS GRAPHICS ON` statement). For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS.](#)”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “[A Primer on ODS Statistical Graphics](#)” on page 599 in Chapter 21, “[Statistical Graphics Using ODS.](#)”

You can reference every graph produced through ODS Graphics with a name. [Table 96.5](#) lists the names of the graphs, along with the relevant `PLOTS=` options.

**Table 96.5** Graphs Produced by PROC TPSPLINE

| ODS Graph Name      | Plot Description                                                              | PLOTS Option        |
|---------------------|-------------------------------------------------------------------------------|---------------------|
| ContourFitPanel     | Panel of thin-plate spline contour surfaces overlaid on scatter plots of data | CONTOURFITPANEL     |
| ContourFit          | Thin-plate spline contour surface overlaid on scatter plot of data            | CONTOURFITPANEL     |
| DiagnosticsPanel    | Panel of fit diagnostics                                                      | DIAGNOSTICS         |
| FitPanel            | Panel of thin-plate spline curves overlaid on scatter plots of data           | FITPANEL            |
| FitPlot             | Thin-plate spline curve overlaid on scatter plot of data                      | FIT                 |
| ObservedByPredicted | Dependent variable versus thin-plate spline fit                               | OBSERVEDBYPREDICTED |
| QQPlot              | Normal quantile plot of residuals                                             | QQPLOT              |
| ResidualBySmooth    | Panel of residuals versus predictor by smoothing parameter values             | RESIDUALBYSMOOTH    |
| ResidualByPredicted | Residuals versus thin-plate spline fit                                        | RESIDUALBYPREDICTED |
| ResidualHistogram   | Histogram of fit residuals                                                    | RESIDUALHISTOGRAM   |

Table 96.5 *continued*

| ODS Graph Name | Plot Description                                                         | PLOTS Option |
|----------------|--------------------------------------------------------------------------|--------------|
| ResidualPanel  | Panel of residuals versus predictors for fixed smoothing parameter value | RESIDUALS    |
| ResidualPlot   | Plot of residuals versus predictor                                       | RESIDUALS    |
| RFPlot         | Side-by-side plots of quantiles of centered fit and residuals            | RFPLOT       |
| ScorePlot      | Thin-plate spline fit evaluated at scoring points                        | SCOREPLOT    |
| CriterionPlot  | GCV criterion versus smoothing parameter                                 | CRITERION    |

## Examples: TPSPLINE Procedure

### Example 96.1: Partial Spline Model Fit

This example analyzes the data set `Measure` that was introduced in the section “Getting Started: TPSPLINE Procedure” on page 8098. That analysis determined that the final estimated surface can be represented by a quadratic function for one or both of the independent variables. This example illustrates how you can use PROC TPSPLINE to fit a partial spline model. The data set `Measure` is fit by using the following model:

$$y = \beta_0 + \beta_1 x_1 + \beta x_1^2 + f(x_2)$$

The model has a parametric component (associated with the  $x_1$  variable) and a nonparametric component (associated with the  $x_2$  variable). The following statements fit a partial spline model:

```
data Measure;
 set Measure;
 x1sq = x1*x1;
run;

data pred;
 do x1=-1 to 1 by 0.1;
 do x2=-1 to 1 by 0.1;
 x1sq = x1*x1;
 output;
 end;
 end;
run;

proc tpspline data= measure;
 model y = x1 x1sq (x2);
 score data = pred out = predy;
run;
```

Output 96.1.1 displays the results from these statements.

**Output 96.1.1** Output from PROC TPSPLINE

| Raw Data                                  |          |
|-------------------------------------------|----------|
| The TPSPLINE Procedure                    |          |
| Dependent Variable: y                     |          |
| Summary of Input Data Set                 |          |
| Number of Non-Missing Observations        | 50       |
| Number of Missing Observations            | 0        |
| Unique Smoothing Design Points            | 5        |
| Summary of Final Model                    |          |
| Number of Regression Variables            | 2        |
| Number of Smoothing Variables             | 1        |
| Order of Derivative in the Penalty        | 2        |
| Dimension of Polynomial Space             | 4        |
| Summary Statistics<br>of Final Estimation |          |
| log10(n*Lambda)                           | -2.2374  |
| Smoothing Penalty                         | 205.3461 |
| Residual SS                               | 8.5821   |
| Tr(I-A)                                   | 43.1534  |
| Model DF                                  | 6.8466   |
| Standard Deviation                        | 0.4460   |
| GCV                                       | 0.2304   |

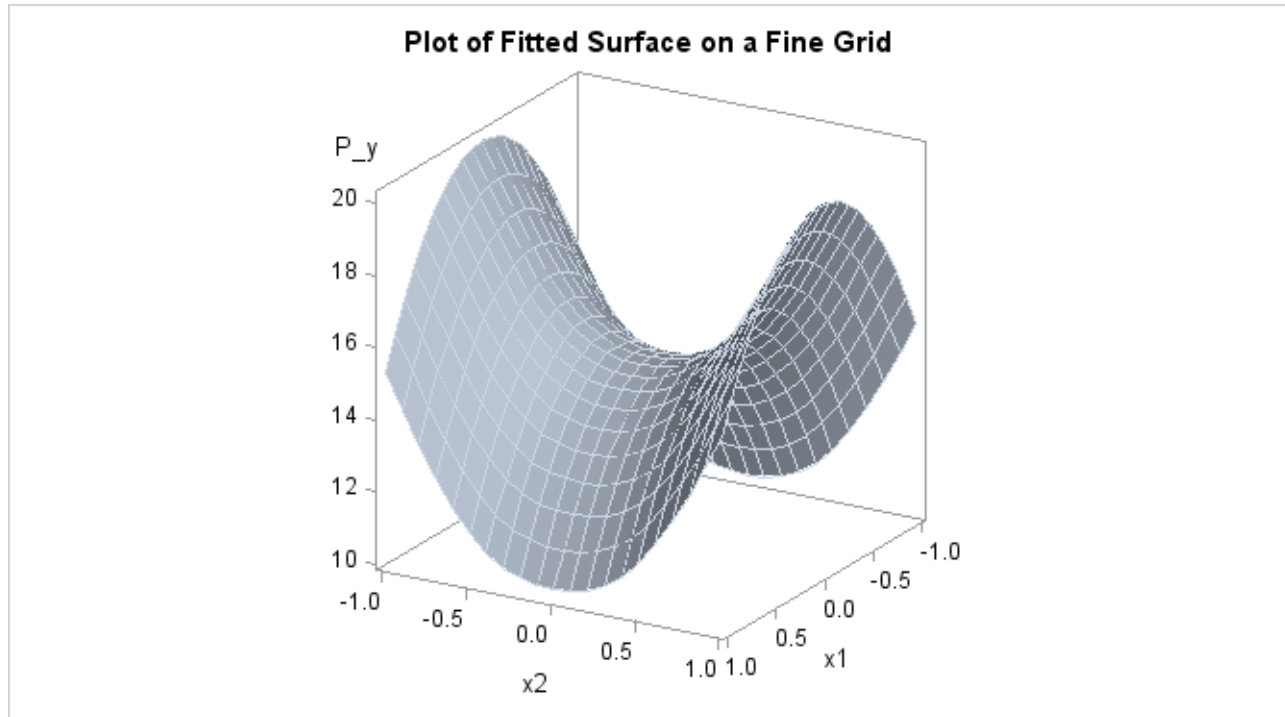
As displayed in [Output 96.1.1](#), there are five unique design points for the smoothing variable  $x_2$  and two regression variables in the model  $(x_1, x_1^2)$ . The dimension of the polynomial space is the number of columns in  $(\{1, x_1, x_1^2, x_2\}) = 4$ . The standard deviation of the estimate is much larger than the one based on the model with both  $x_1$  and  $x_2$  as smoothing variables (0.445954 compared to 0.098421). One of the many possible explanations might be that the number of unique design points of the smoothing variable is too small to warrant an accurate estimate for  $f(x_2)$ .

The following statements produce a surface plot for the partial spline model by using the surface template that is defined in the section “Getting Started: TPSPLINE Procedure” on page 8098.

```
proc sgrender data=predy template=surface;
 dynamic _X='x1' _Y='x2' _Z='P_y' _T='Plot of Fitted Surface on a Fine Grid';
run;
```

The surface displayed in [Output 96.1.2](#) is similar to the one estimated by using the full nonparametric model (displayed in [Output 96.2](#) and [Output 96.6](#)).

**Output 96.1.2** Plot of PROC TPSPLINE Fit from the Partial Spline Model





---

## Example 96.2: Spline Model with Higher-Order Penalty

This example continues the analysis of the data set `Measure` to illustrate how you can use PROC TPSPLINE to fit a spline model with a higher-order penalty term. Spline models with high-order penalty terms move low-order polynomial terms into the polynomial space. Hence, there is no penalty for these terms, and they can vary without constraint.

As shown in the previous analyses, the final model for the data set `Measure` must include quadratic terms for both  $x_1$  and  $x_2$ . This example fits the following model:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_1^2 + \beta_3 x_2 + \beta_4 x_2^2 + \beta_5 x_1 x_2 + f(x_1, x_2)$$

The model includes quadratic terms for both variables, although it differs from the usual linear model. The nonparametric term  $f(x_1, x_2)$  explains the variation of the data that is unaccounted for by a simple quadratic surface.

To modify the order of the derivative in the penalty term, specify the `M=` option. The following statements specify the option `M=3` in order to include the quadratic terms in the polynomial space:

```
data Measure;
 set Measure;
 x1sq = x1*x1;
 x2sq = x2*x2;
 x1x2 = x1*x2;
run;

proc tpspline data= Measure;
 model y = (x1 x2) / m=3;
 score data = pred out = predy;
run;
```

Output 96.2.1 displays the results from these statements.

**Output 96.2.1** Output from PROC TPSPLINE with M=3

| Raw Data                                  |           |
|-------------------------------------------|-----------|
| The TPSPLINE Procedure                    |           |
| Dependent Variable: y                     |           |
| Summary of Input Data Set                 |           |
| Number of Non-Missing Observations        | 50        |
| Number of Missing Observations            | 0         |
| Unique Smoothing Design Points            | 25        |
| Summary of Final Model                    |           |
| Number of Regression Variables            | 0         |
| Number of Smoothing Variables             | 2         |
| Order of Derivative in the Penalty        | 3         |
| Dimension of Polynomial Space             | 6         |
| Summary Statistics<br>of Final Estimation |           |
| log10(n*Lambda)                           | -3.7831   |
| Smoothing Penalty                         | 2092.4495 |
| Residual SS                               | 0.2731    |
| Tr(I-A)                                   | 29.1716   |
| Model DF                                  | 20.8284   |
| Standard Deviation                        | 0.0968    |
| GCV                                       | 0.0160    |

The model contains six terms in the polynomial space is the number of columns in  $(\{1, x_1, x_1^2, x_1x_2, x_2, x_2^2\}) = 6$ . Compare Output 96.2.1 with Output 96.1.1: the  $\log_{10}(n\lambda)$  value and the smoothing penalty differ significantly. In general, these terms are not directly comparable for different models. The final estimate based on this model is close to the estimate based on the model by using the default, M=2.

In the following statements, the REG procedure fits a quadratic surface model to the data set Measure:

```
proc reg data= Measure;
 model y = x1 x1sq x2 x2sq x1x2;
run;
```

The results are displayed in [Output 96.2.2](#).

**Output 96.2.2** Quadratic Surface Model: The REG Procedure

| Raw Data              |                |                    |                |         |         |
|-----------------------|----------------|--------------------|----------------|---------|---------|
| The REG Procedure     |                |                    |                |         |         |
| Model: MODEL1         |                |                    |                |         |         |
| Dependent Variable: y |                |                    |                |         |         |
| Analysis of Variance  |                |                    |                |         |         |
| Source                | DF             | Sum of Squares     | Mean Square    | F Value | Pr > F  |
| Model                 | 5              | 443.20502          | 88.64100       | 436.33  | <.0001  |
| Error                 | 44             | 8.93874            | 0.20315        |         |         |
| Corrected Total       | 49             | 452.14376          |                |         |         |
|                       | Root MSE       | 0.45073            | R-Square       | 0.9802  |         |
|                       | Dependent Mean | 15.08548           | Adj R-Sq       | 0.9780  |         |
|                       | Coeff Var      | 2.98781            |                |         |         |
| Parameter Estimates   |                |                    |                |         |         |
| Variable              | DF             | Parameter Estimate | Standard Error | t Value | Pr >  t |
| Intercept             | 1              | 14.90834           | 0.12519        | 119.09  | <.0001  |
| x1                    | 1              | 0.01292            | 0.09015        | 0.14    | 0.8867  |
| x1sq                  | 1              | -4.85194           | 0.15237        | -31.84  | <.0001  |
| x2                    | 1              | 0.02618            | 0.09015        | 0.29    | 0.7729  |
| x2sq                  | 1              | 5.20624            | 0.15237        | 34.17   | <.0001  |
| x1x2                  | 1              | -0.04814           | 0.12748        | -0.38   | 0.7076  |

The REG procedure produces slightly different results. To fit a similar model with PROC TPSPLINE, you can use a MODEL statement that specifies the degrees of freedom with the DF= option. You can also use a large value for the LOGNLAMBDA0= option to force a parametric model fit.

Because there is one degree of freedom for each of the terms intercept, x1, x2, x1sq, x2sq, and x1x2, the DF=6 option is used as follows:

```
proc tpspline data=measure;
 model y=(x1 x2) /m=3 df=6 lognlambda=(-4 to 1 by 0.5);
 score data = pred
 out = predy;
run;
```

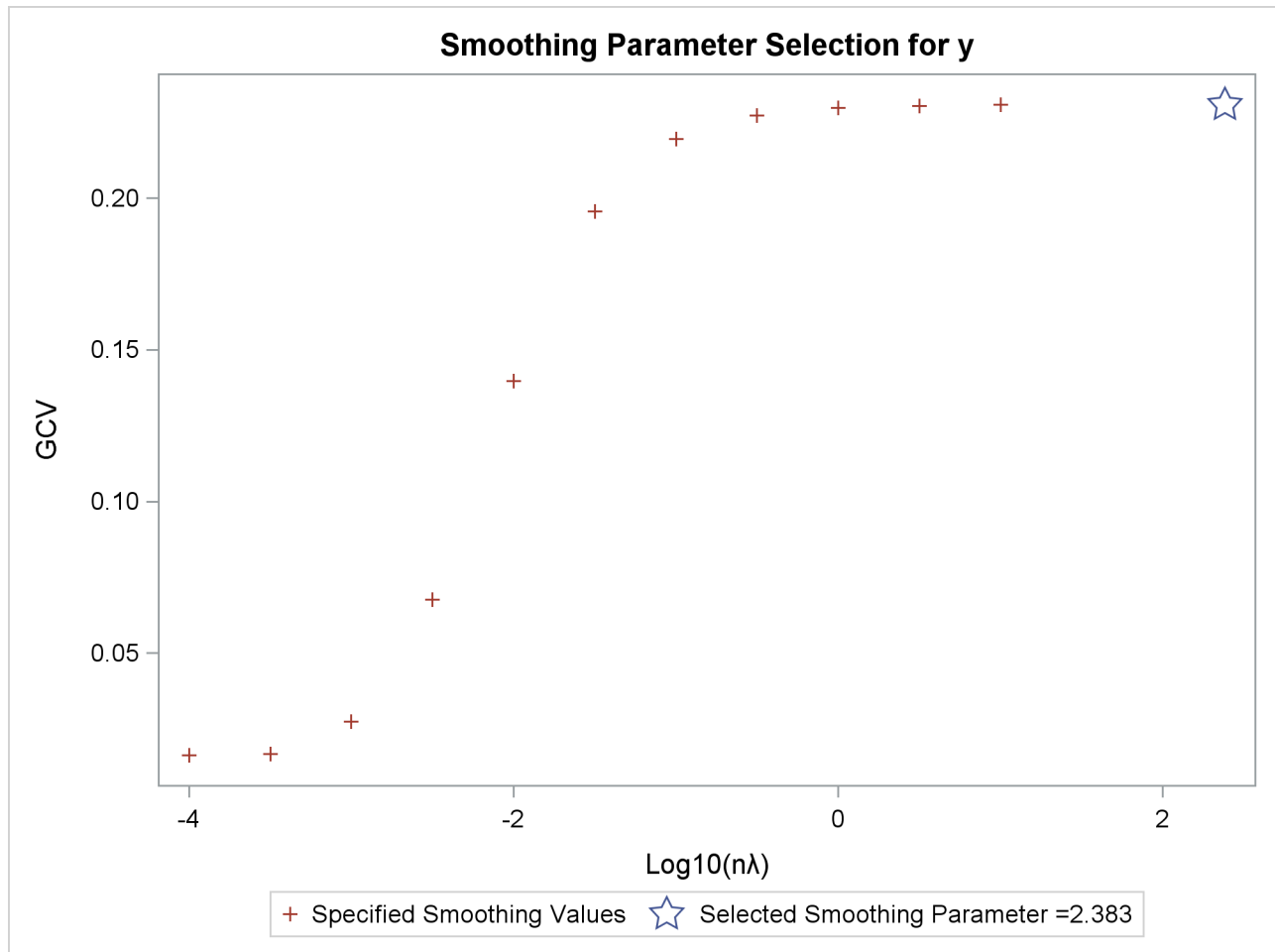
The fit statistics are displayed in [Output 96.2.3](#).

**Output 96.2.3** Output from PROC TPSPLINE Using M=3 and DF=6

| Raw Data                                  |           |
|-------------------------------------------|-----------|
| The TPSPLINE Procedure                    |           |
| Dependent Variable: y                     |           |
| Summary of Final Model                    |           |
| Number of Regression Variables            | 0         |
| Number of Smoothing Variables             | 2         |
| Order of Derivative in the Penalty        | 3         |
| Dimension of Polynomial Space             | 6         |
| GCV Function                              |           |
| log10 (n*Lambda)                          | GCV       |
| -4.00000                                  | 0.016330* |
| -3.50000                                  | 0.016889  |
| -3.00000                                  | 0.027496  |
| -2.50000                                  | 0.067672  |
| -2.00000                                  | 0.139642  |
| -1.50000                                  | 0.195727  |
| -1.00000                                  | 0.219512  |
| -0.50000                                  | 0.227306  |
| 0                                         | 0.229740  |
| 0.50000                                   | 0.230504  |
| 1.00000                                   | 0.230745  |
| Note: * indicates minimum GCV value.      |           |
| Summary Statistics<br>of Final Estimation |           |
| log10 (n*Lambda)                          | 2.3830    |
| Smoothing Penalty                         | 0.0000    |
| Residual SS                               | 8.9384    |
| Tr (I-A)                                  | 43.9997   |
| Model DF                                  | 6.0003    |
| Standard Deviation                        | 0.4507    |
| GCV                                       | 0.2309    |

Output 96.2.4 shows the GCV values for the list of supplied  $\log_{10}(n\lambda)$  values in addition to the fitted model with fixed degrees of freedom 6. The fitted model has a larger GCV value than all other examined models.

**Output 96.2.4** Criterion Plot



The final estimate is based on 6.000330 degrees of freedom because there are already 6 degrees of freedom in the polynomial space and the search range for  $\lambda$  is not large enough (in this case, setting DF=6 is equivalent to setting  $\lambda = \infty$ ).

The standard deviation and RSS (Output 96.2.3) are close to the sum of squares for the error term and the root MSE from the linear regression model (Output 96.2.2), respectively.

For this model, the optimal  $\log_{10}(n\lambda)$  is around  $-3.8$ , which produces a standard deviation estimate of 0.096765 (see Output 96.2.1) and a GCV value of 0.016051, while the model that specifies DF=6 results in a  $\log_{10}(n\lambda)$  larger than 1 and a GCV value larger than 0.23074. The nonparametric model, based on the GCV, should provide better prediction, but the linear regression model can be more easily interpreted.

## Example 96.3: Multiple Minima of the GCV Function

The data in this example represent the deposition of sulfate (SO<sub>4</sub>) at 179 sites in the 48 contiguous states of the United States in 1990. Each observation records the latitude and longitude of the site in addition to the SO<sub>4</sub> deposition at the site measured in grams per square meter ( $g/m^2$ ).

You can use PROC TPSPLINE to fit a surface that reflects the general trend and that reveals underlying features of the data, which are shown in the following DATA step:

```
data so4;
 input latitude longitude so4 @@;
 datalines;
32.45833 87.24222 1.403 34.28778 85.96889 2.103
33.07139 109.86472 0.299 36.07167 112.15500 0.304
31.95056 112.80000 0.263 33.60500 92.09722 1.950
34.17944 93.09861 2.168 36.08389 92.58694 1.578

... more lines ...

43.87333 104.19222 0.306 44.91722 110.42028 0.210
45.07611 72.67556 2.646
;

data pred;
 do latitude = 25 to 47 by 1;
 do longitude = 68 to 124 by 1;
 output;
 end;
 end;
run;
```

The preceding statements create the SAS data set so4 and the data set pred in order to make predictions on a regular grid. The following statements fit a surface for SO<sub>4</sub> deposition:

```
ods graphics on;
proc tpspline data=so4 plots(only)=criterion;
 model so4 = (latitude longitude) /lognlambda=(-6 to 1 by 0.1);
 score data=pred out=prediction1;
run;
```

Partial output from these statements is displayed in [Output 96.3.1](#) and [Output 96.3.2](#).

**Output 96.3.1** Partial Output from PROC TPSPLINE for Data Set SO<sub>4</sub>

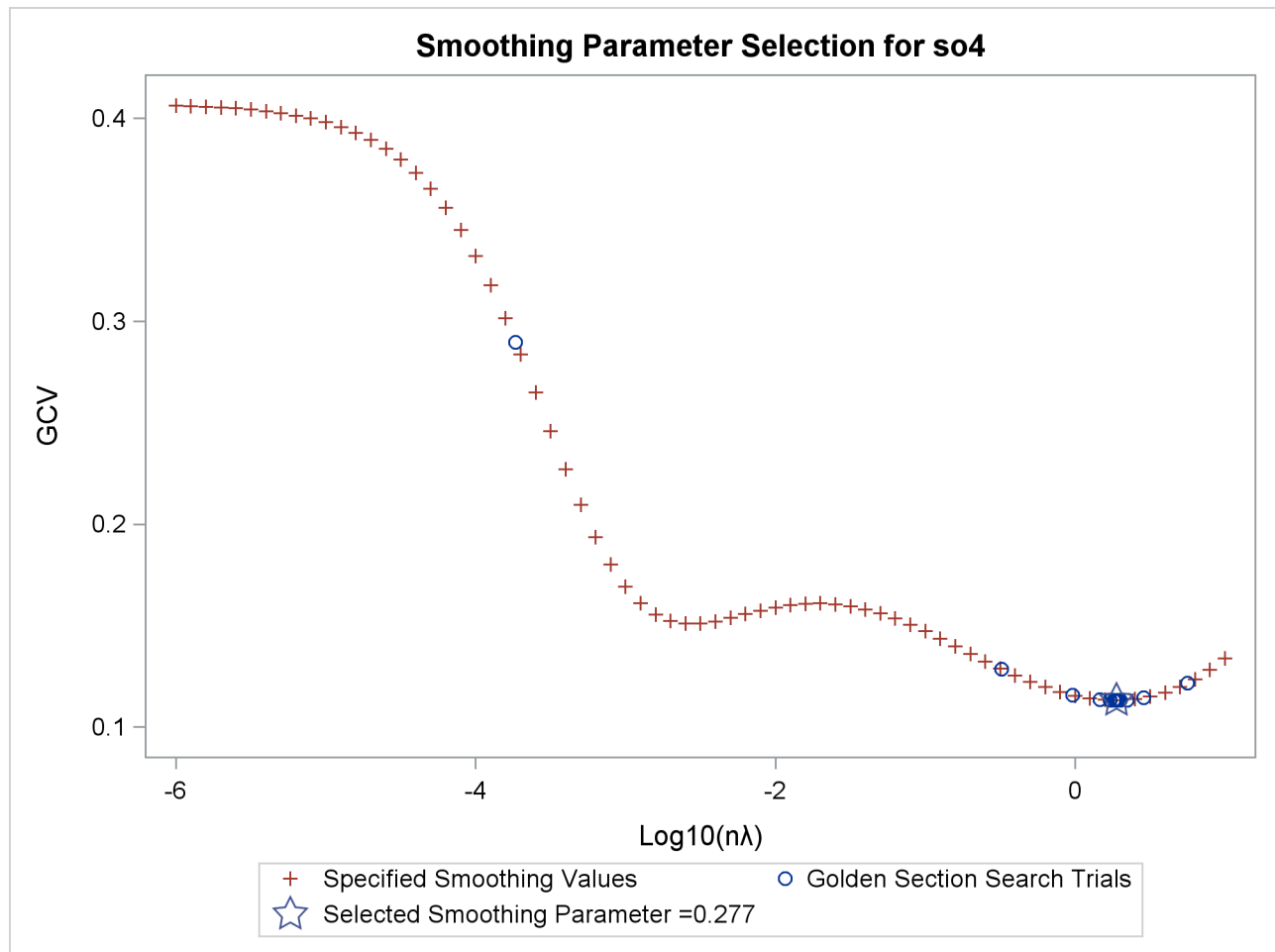
| Raw Data                           |     |
|------------------------------------|-----|
| The TPSPLINE Procedure             |     |
| Dependent Variable: so4            |     |
| Summary of Input Data Set          |     |
| Number of Non-Missing Observations | 179 |
| Number of Missing Observations     | 0   |
| Unique Smoothing Design Points     | 179 |
| Summary of Final Model             |     |
| Number of Regression Variables     | 0   |
| Number of Smoothing Variables      | 2   |
| Order of Derivative in the Penalty | 2   |
| Dimension of Polynomial Space      | 3   |

**Output 96.3.2** Partial Output from PROC TPSPLINE for Data Set SO<sub>4</sub>

| Summary Statistics<br>of Final Estimation |          |
|-------------------------------------------|----------|
| log10(n*Lambda)                           | 0.2770   |
| Smoothing Penalty                         | 2.4588   |
| Residual SS                               | 12.4450  |
| Tr(I-A)                                   | 140.2750 |
| Model DF                                  | 38.7250  |
| Standard Deviation                        | 0.2979   |
| GCV                                       | 0.1132   |

Output 96.3.3 displays the CriterionPlot of the GCV function versus  $\log_{10}(n\lambda)$ .

**Output 96.3.3** GCV Function of SO<sub>4</sub> Data Set



The GCV function has two minima. PROC TPSPLINE locates the global minimum at 0.277005. The plot also displays a local minimum located around  $-2.56$ . The TPSPLINE procedure might not always find the global minimum, although it did in this case. If there is a predetermined search range based on prior knowledge, you can use the **RANGE=** option to narrow the search range in order to find a desired smoothing value. For example, if you believe a better smoothing parameter should be within the  $(-4, -2)$  range, you can obtain the model with  $\log_{10}(n\lambda) = -2.56$  with the following statements.

```
proc tpspline data=so4;
 model so4 = (latitude longitude) / range=(-4,-2);
 score data=pred out=prediction2;
run;
```



Output 96.3.4 displays the output from PROC TPSPLINE with a specified search range from the smoothing parameter.

**Output 96.3.4** Output from PROC TPSPLINE for Data Set SO<sub>4</sub> with  $\log_{10}(n\lambda) = -2.56$

|                                           |          |
|-------------------------------------------|----------|
| Raw Data                                  |          |
| The TPSPLINE Procedure                    |          |
| Dependent Variable: so4                   |          |
| Summary of Input Data Set                 |          |
| Number of Non-Missing Observations        | 179      |
| Number of Missing Observations            | 0        |
| Unique Smoothing Design Points            | 179      |
| Summary of Final Model                    |          |
| Number of Regression Variables            | 0        |
| Number of Smoothing Variables             | 2        |
| Order of Derivative in the Penalty        | 2        |
| Dimension of Polynomial Space             | 3        |
| Summary Statistics<br>of Final Estimation |          |
| log10(n*Lambda)                           | -2.5600  |
| Smoothing Penalty                         | 177.2160 |
| Residual SS                               | 0.0438   |
| Tr(I-A)                                   | 7.2083   |
| Model DF                                  | 171.7917 |
| Standard Deviation                        | 0.0779   |
| GCV                                       | 0.1508   |

The smoothing penalty in Output 96.3.4 is much larger than that displayed in Output 96.3.2. The estimate in Output 96.3.2 uses a large  $\lambda$  value; therefore, the surface is smoother than the estimate by using  $\log_{10}(n\lambda) = -2.56$  (Output 96.3.4).

The estimate based on  $\log_{10}(n\lambda) = -2.56$  has a larger value of degrees of freedom, and it has a much smaller standard deviation.

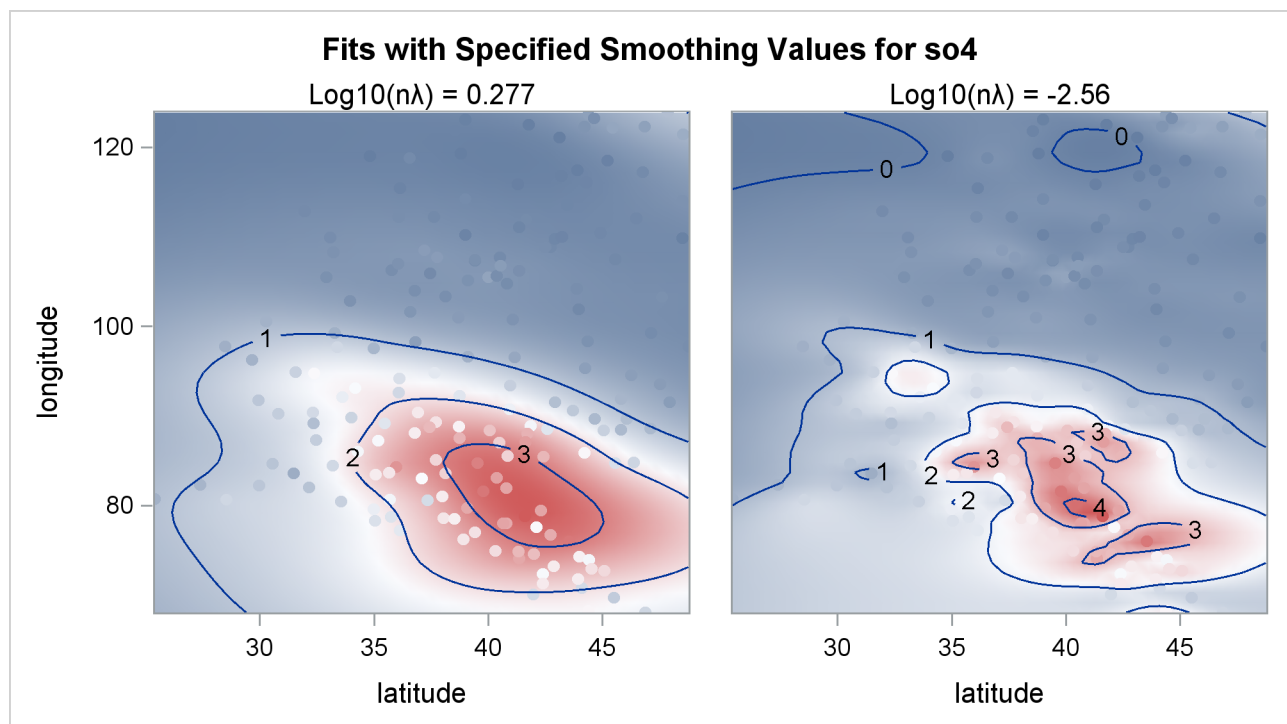
However, a smaller standard deviation in nonparametric regression does not necessarily mean that the estimate is good: a small  $\lambda$  value always produces an estimate closer to the data and, therefore, a smaller standard deviation.

When ODS Graphics is enabled, you can compare the two fits by supplying 0.277 and  $-2.56$  to the `LOGN-LAMBDA=` option:

```
proc tpspline data=so4;
 model so4 = (latitude longitude) / lognlambda=(0.277 -2.56);
run;
```

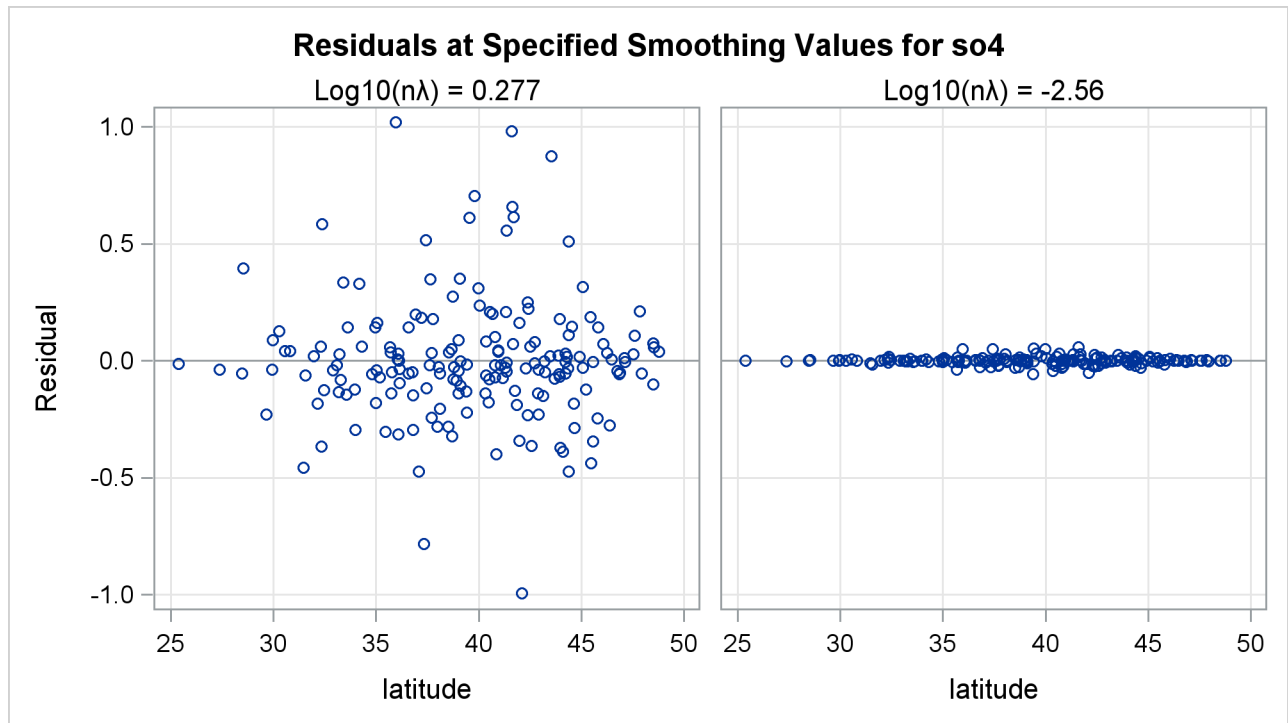
**Output 96.3.5** shows the contour surfaces of two models with the two minima. The fit that corresponds to the global minimum 0.277 shows a smoother fit that captures the general structure in the data set. The fit at the local minimum  $-2.56$  is a rougher fit that captures local details. The response values are also displayed as circles with the same color gradient by the default `GRADIENT contour-option`. The contrast between the predicted and observed  $\text{SO}_4$  deposition is greater for the smoother fit than for the other one, which means the smoother fit has larger absolute residual values.

**Output 96.3.5** Panel of Contour Fit Plots by 0.277 and  $-2.56$

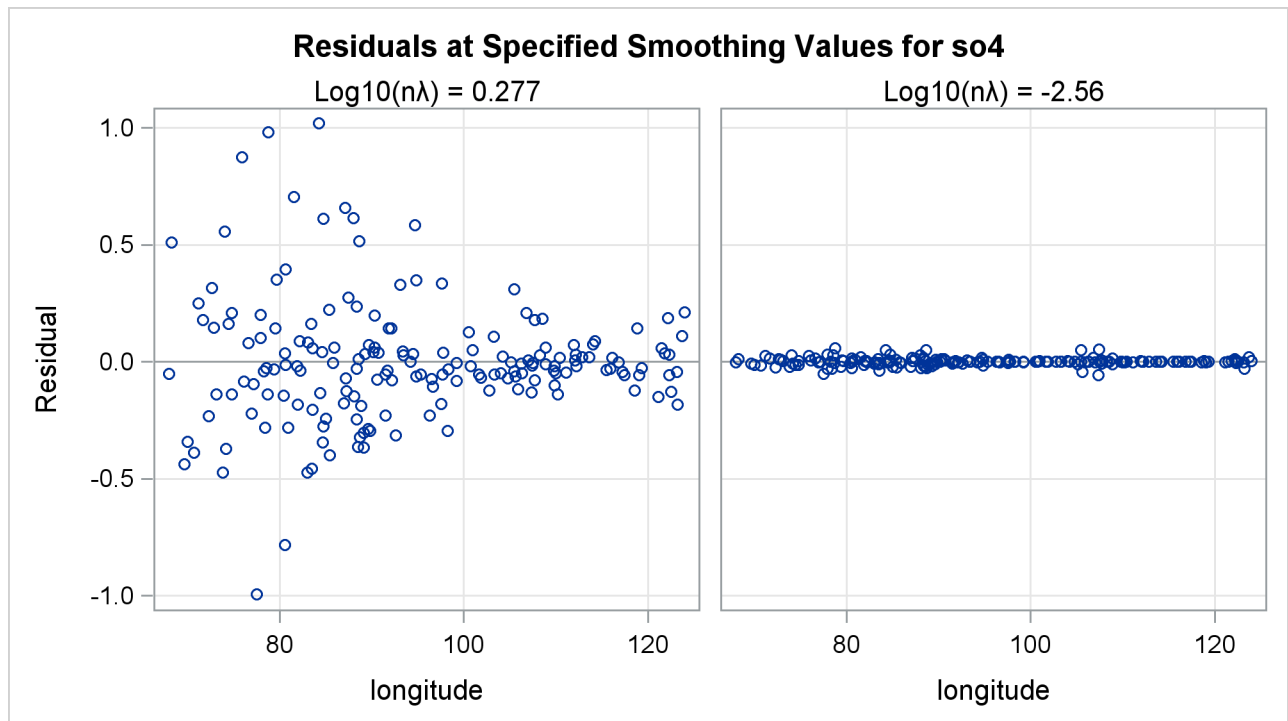


The residuals for the two fits can be visualized in `RESIDUALBYSMOOTH` panels. **Output 96.3.6** is a panel of plots of residuals against smoothing variable Latitude. **Output 96.3.7** is a panel of plots of residuals against smoothing variable Longitude. Both panels show that the residuals from the model with the global minimum are larger in absolute values than the ones from the local minimum. This is expected, since the optimal model achieves the smallest GCV value by significantly increasing the smoothness of fit and sacrificing a little in the goodness of fit.

**Output 96.3.6** Panel of Residuals by Latitude Plots



**Output 96.3.7** Panel of Residuals by Longitude Plots



In summary, the fit with  $\log_{10}(n\lambda) = 0.277$  represents the underlying surface, while the fit with the  $\log_{10}(n\lambda) = -2.56$  overfits the data and captures the additional noise component.

## Example 96.4: Large Data Set Application

This example illustrates how you can use the `D=` option to decrease the computation time needed by the TPSPLINE procedure. Although the `D=` option can be helpful in decreasing computation time for large data sets, it might produce unexpected results when used with small data sets.

The following statements generate the data set large:

```
data large;
 do x=-5 to 5 by 0.02;
 y=5*sin(3*x)+1*rannor(57391);
 output;
 end;
run;
```

The data set large contains 501 observations with one independent variable `x` and one dependent variable `y`. The following statements invoke PROC TPSPLINE to produce a thin-plate smoothing spline estimate and the associated 99% confidence interval. The output statistics are saved in the data set fit1.

```
proc tpspline data=large;
 model y =(x) /lognlambda=(-5 to -1 by 0.2) alpha=0.01;
 output out=fit1 pred lclm uclm;
run;
```

The results from this MODEL statement are displayed in [Output 96.4.1](#).

**Output 96.4.1** Output from PROC TPSPLINE without the `D=` Option

|                                    |     |
|------------------------------------|-----|
| Raw Data                           |     |
| The TPSPLINE Procedure             |     |
| Dependent Variable: y              |     |
| Summary of Input Data Set          |     |
| Number of Non-Missing Observations | 501 |
| Number of Missing Observations     | 0   |
| Unique Smoothing Design Points     | 501 |
| Summary of Final Model             |     |
| Number of Regression Variables     | 0   |
| Number of Smoothing Variables      | 1   |
| Order of Derivative in the Penalty | 2   |
| Dimension of Polynomial Space      | 2   |

## Output 96.4.1 continued

| GCV Function     |           |
|------------------|-----------|
| log10 (n*Lambda) | GCV       |
| -5.000000        | 1.258653  |
| -4.800000        | 1.228743  |
| -4.600000        | 1.205835  |
| -4.400000        | 1.188371  |
| -4.200000        | 1.174644  |
| -4.000000        | 1.163102  |
| -3.800000        | 1.152627  |
| -3.600000        | 1.142590  |
| -3.400000        | 1.132700  |
| -3.200000        | 1.122789  |
| -3.000000        | 1.112755  |
| -2.800000        | 1.102642  |
| -2.600000        | 1.092769  |
| -2.400000        | 1.083779  |
| -2.200000        | 1.076636  |
| -2.000000        | 1.072763* |
| -1.800000        | 1.074636  |
| -1.600000        | 1.087152  |
| -1.400000        | 1.120339  |
| -1.200000        | 1.194023  |
| -1.000000        | 1.344213  |

Note: \* indicates minimum GCV value.

| Summary Statistics<br>of Final Estimation |           |
|-------------------------------------------|-----------|
| log10 (n*Lambda)                          | -1.9483   |
| Smoothing Penalty                         | 9953.7066 |
| Residual SS                               | 475.0984  |
| Tr (I-A)                                  | 471.0861  |
| Model DF                                  | 29.9139   |
| Standard Deviation                        | 1.0042    |
| GCV                                       | 1.0726    |

The following statements specify an identical model, but with the additional specification of the `D=` option. The estimates are obtained by treating nearby points as replicates.

```
proc tpspline data=large;
 model y =(x) /lognlambda=(-5 to -1 by 0.2) d=0.05 alpha=0.01;
 output out=fit2 pred lclm uclm;
run;
```

The output is displayed in Output 96.4.2.

**Output 96.4.2** Output from PROC TPSPLINE with the D= Option

| Raw Data                             |           |
|--------------------------------------|-----------|
| The TPSPLINE Procedure               |           |
| Dependent Variable: y                |           |
| Summary of Input Data Set            |           |
| Number of Non-Missing Observations   | 501       |
| Number of Missing Observations       | 0         |
| Unique Smoothing Design Points       | 251       |
| Summary of Final Model               |           |
| Number of Regression Variables       | 0         |
| Number of Smoothing Variables        | 1         |
| Order of Derivative in the Penalty   | 2         |
| Dimension of Polynomial Space        | 2         |
| GCV Function                         |           |
| log10 (n*Lambda)                     | GCV       |
| -5.00000                             | 1.306536  |
| -4.80000                             | 1.261692  |
| -4.60000                             | 1.226881  |
| -4.40000                             | 1.200060  |
| -4.20000                             | 1.179284  |
| -4.00000                             | 1.162776  |
| -3.80000                             | 1.149072  |
| -3.60000                             | 1.137120  |
| -3.40000                             | 1.126220  |
| -3.20000                             | 1.115884  |
| -3.00000                             | 1.105766  |
| -2.80000                             | 1.095730  |
| -2.60000                             | 1.085972  |
| -2.40000                             | 1.077066  |
| -2.20000                             | 1.069954  |
| -2.00000                             | 1.066076* |
| -1.80000                             | 1.067929  |
| -1.60000                             | 1.080419  |
| -1.40000                             | 1.113564  |
| -1.20000                             | 1.187172  |
| -1.00000                             | 1.337252  |
| Note: * indicates minimum GCV value. |           |

Output 96.4.2 *continued*

| Summary Statistics<br>of Final Estimation |           |
|-------------------------------------------|-----------|
| log10(n*Lambda)                           | -1.9477   |
| Smoothing Penalty                         | 9943.5618 |
| Residual SS                               | 472.1424  |
| Tr(I-A)                                   | 471.0901  |
| Model DF                                  | 29.9099   |
| Standard Deviation                        | 1.0011    |
| GCV                                       | 1.0659    |

The difference between the two estimates is minimal. However, the CPU time for the second MODEL statement is only about 1/7 of the CPU time used in the first model fit.

The following statements produce a plot for comparison of the two estimates:

```

data fit2;
 set fit2;
 P1_y = P_y;
 LCLM1_y = LCLM_y;
 UCLM1_y = UCLM_y;
 drop P_y LCLM_y UCLM_y;
run;

proc sort data=fit1;
 by x y;
run;

proc sort data=fit2;
 by x y;
run;

data comp;
 merge fit1 fit2;
 by x y;
 label p1_y ="Yhat1" p_y="Yhat0"
 lclm_y ="Lower CL"
 uclm_y ="Upper CL";
run;

proc sgplot data=comp;
 title "Comparison of Two Estimates";
 title2 "with and without the D= Option";

 yaxis label="Predicted y Values";
 xaxis label="x";

 band x=x lower=lclm_y upper=uclm_y /name="range"
 legendlabel="99% CI of Predicted y without D=";
 series x=x y=P_y/ name="P_y" legendlabel="Predicted y without D="
 lineattrs=graphfit(thickness=1px pattern=shortdash);
 series x=x y=P1_y/ name="P1_y" legendlabel="Predicted y with D="

```

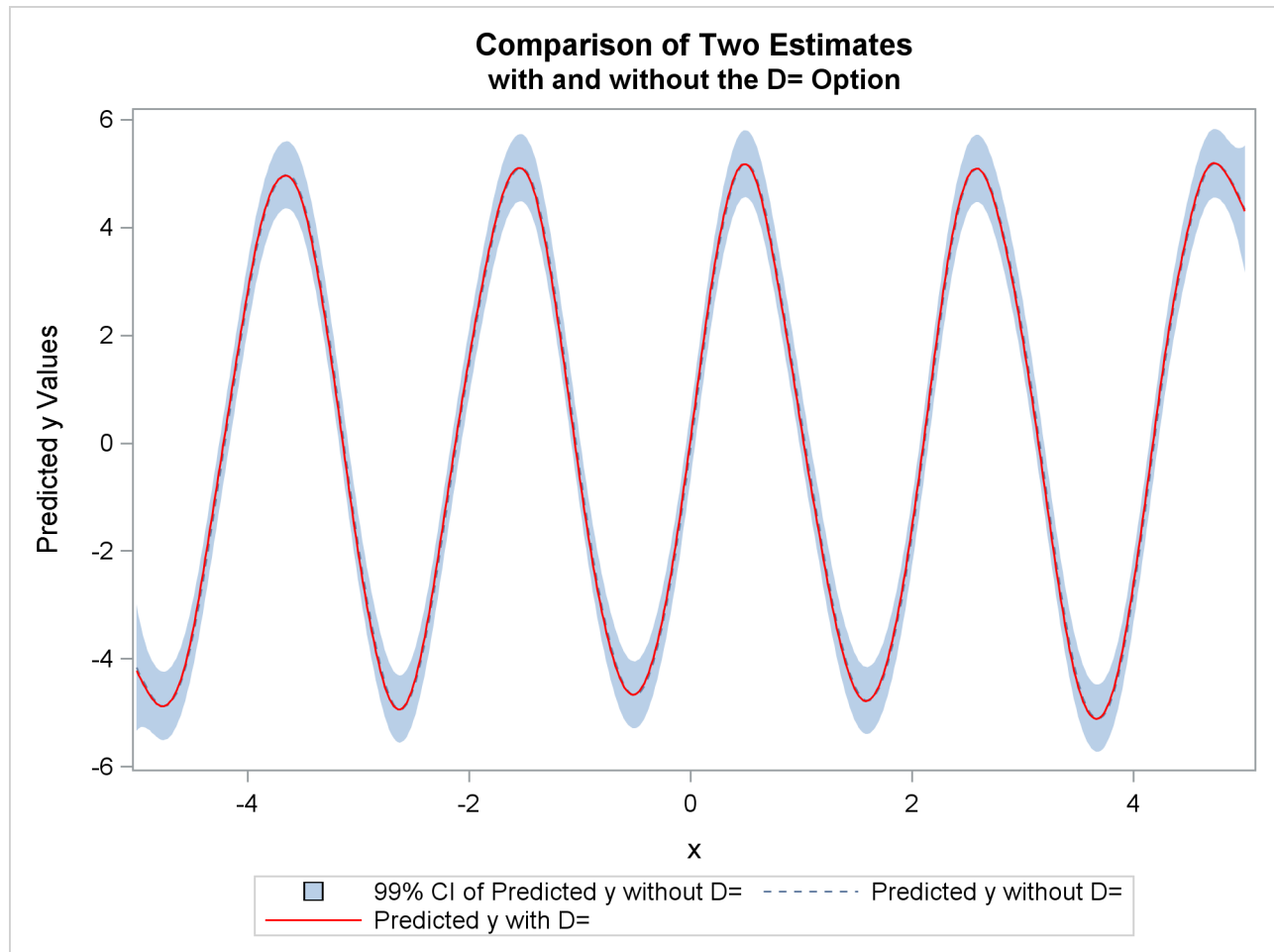
```

lineattrs=graphfit(thickness=1px color=red);
discretelegend "range" "P_y" "Pl_y";
run;

```

The estimates from fit1 and fit2 are displayed in [Output 96.4.3](#) with the 99% confidence interval from the fit1 output data set.

**Output 96.4.3** Comparison of Two PROC TPSPLINE Fits with and without the D= Option



## Example 96.5: Computing a Bootstrap Confidence Interval

This example illustrates how you can construct a bootstrap confidence interval by using the multiple responses feature in PROC TPSPLINE.

Numerous epidemiological observations have indicated that exposure to solar radiation is an important factor in the etiology of melanoma. The following data present age-adjusted melanoma incidences for 37 years from the Connecticut Tumor Registry (Houghton, Flannery, and Viola 1980). The data are analyzed by Ramsay and Silverman (1997).



```

data melanoma;
 input year incidences @@;
 datalines;
1936 0.9 1937 0.8 1938 0.8 1939 1.3
1940 1.4 1941 1.2 1942 1.7 1943 1.8
1944 1.6 1945 1.5 1946 1.5 1947 2.0
1948 2.5 1949 2.7 1950 2.9 1951 2.5
1952 3.1 1953 2.4 1954 2.2 1955 2.9
1956 2.5 1957 2.6 1958 3.2 1959 3.8
1960 4.2 1961 3.9 1962 3.7 1963 3.3
1964 3.7 1965 3.9 1966 4.1 1967 3.8
1968 4.7 1969 4.4 1970 4.8 1971 4.8
1972 4.8
;

```

The variable incidences records the number of melanoma cases per 100,000 people for the years 1936 to 1972. The following model fits the data and requests a 90% Bayesian confidence interval along with the estimate:

```

ods graphics on;
proc tpspline data=melanoma plots(only)=(criterionplot fitplot(clm));
 model incidences = (year) /alpha = 0.1;
 output out = result pred uclm lclm;
run;

```

The output is displayed in [Output 96.5.1](#)

**Output 96.5.1** Output from PROC TPSPLINE for the MELANOMA Data

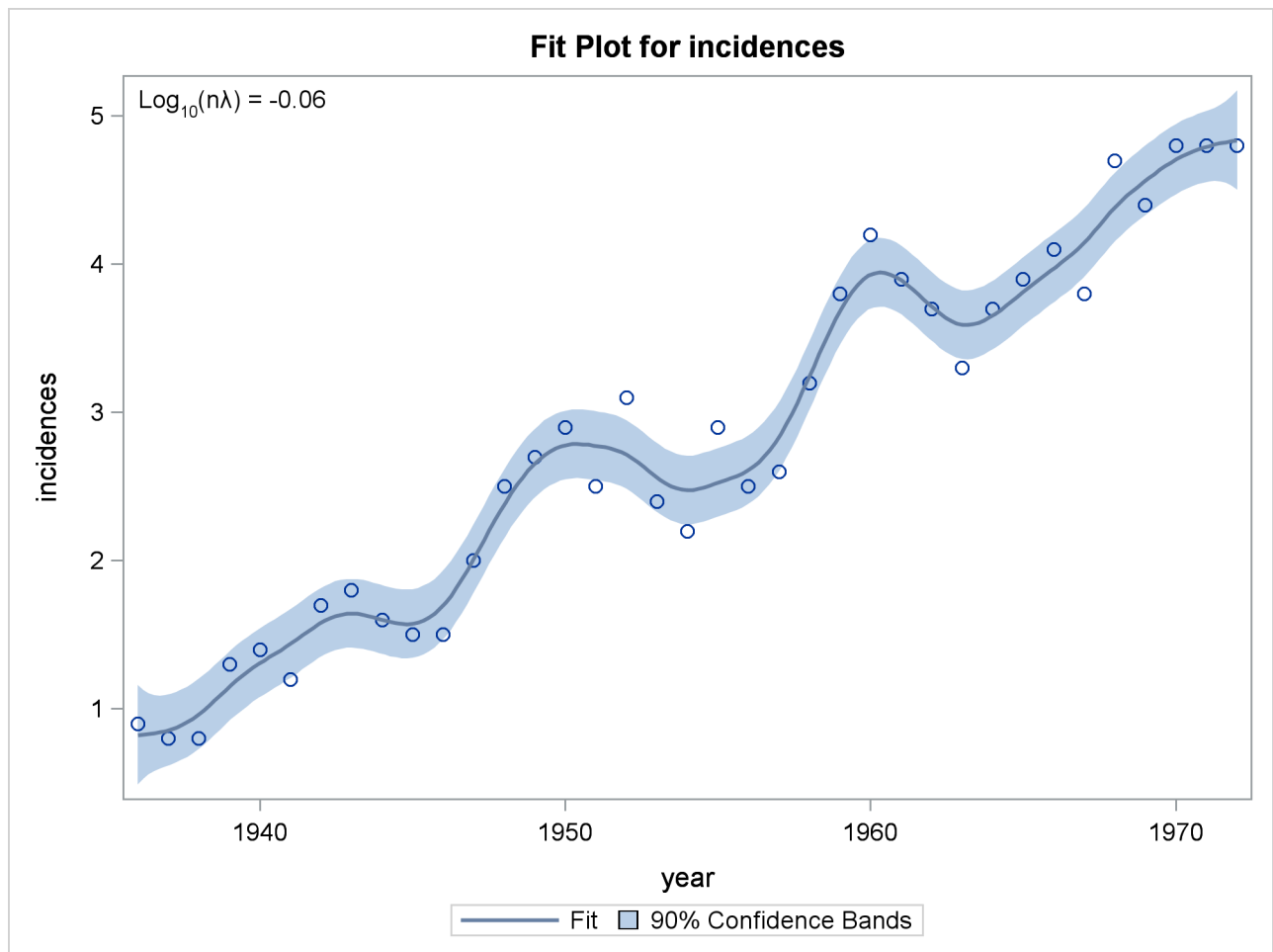
|                                                               |    |
|---------------------------------------------------------------|----|
| Comparison of Two Estimates<br>with and without the D= Option |    |
| The TPSPLINE Procedure<br>Dependent Variable: incidences      |    |
| Summary of Input Data Set                                     |    |
| Number of Non-Missing Observations                            | 37 |
| Number of Missing Observations                                | 0  |
| Unique Smoothing Design Points                                | 37 |
| Summary of Final Model                                        |    |
| Number of Regression Variables                                | 0  |
| Number of Smoothing Variables                                 | 1  |
| Order of Derivative in the Penalty                            | 2  |
| Dimension of Polynomial Space                                 | 2  |

**Output 96.5.1** *continued*

| Summary Statistics<br>of Final Estimation |         |
|-------------------------------------------|---------|
| log10(n*Lambda)                           | -0.0607 |
| Smoothing Penalty                         | 0.5171  |
| Residual SS                               | 1.2243  |
| Tr(I-A)                                   | 22.5852 |
| Model DF                                  | 14.4148 |
| Standard Deviation                        | 0.2328  |
| GCV                                       | 0.0888  |

The estimated curve is displayed with 90% confidence interval bands in [Output 96.5.2](#). The number of melanoma incidences exhibits a periodic pattern and increases over the years. The periodic pattern is related to sunspot activity and the accompanying fluctuations in solar radiation.

**Output 96.5.2** PROC TPSPLINE Estimate and 90% Confidence Interval of Data Set MELANOMA



Wang and Wahba (1995) compare several bootstrap confidence intervals to Bayesian confidence intervals for smoothing splines. Both bootstrap and Bayesian confidence intervals are across-the-curve intervals, not pointwise intervals. They concluded that bootstrap confidence intervals work as well as Bayesian intervals concerning average coverage probability. Additionally, bootstrap confidence intervals appear to be better for small sample sizes. Based on their simulation, the “percentile- $t$  interval” bootstrap interval performs better than the other types of bootstrap intervals.

Suppose that  $\hat{f}_\lambda$  and  $\hat{\sigma}$  are the estimates of  $f$  and  $\sigma$  from the data. Assume that  $f_\lambda$  is the “true”  $f$ , and generate the bootstrap sample as

$$y_i^* = \hat{f}_\lambda(\mathbf{x}_i) + \epsilon_i^*, \quad i = 1, \dots, n$$

where  $\epsilon^* = (\epsilon_1^*, \dots, \epsilon_n^*)' \sim N(0, \hat{\sigma}\mathbf{I})$ . Denote  $f_\lambda^*(\mathbf{x}_i)$  as the random variable of the bootstrap estimate at  $\mathbf{x}_i$ . Repeat this process  $K$  times, so that at each point  $\mathbf{x}_i$ , you have  $K$  bootstrap estimates  $\hat{f}_\lambda^*(\mathbf{x}_i)$  or  $K$  realizations of  $f_\lambda^*(\mathbf{x}_i)$ . For each fixed  $\mathbf{x}_i$ , consider the statistic  $D_i^*$ , which is similar to the Student’s  $t$  statistic,

$$D_i^* = \left( f_\lambda^*(\mathbf{x}_i) - \hat{f}_\lambda(\mathbf{x}_i) \right) / \hat{\sigma}_i^*$$

where  $\hat{\sigma}_i^*$  is the estimate of  $\hat{\sigma}$  based on the  $i$ th bootstrap sample.

Suppose  $\chi_{\alpha/2}$  and  $\chi_{1-\alpha/2}$  are the lower and upper  $\alpha/2$  points, respectively, of the empirical distribution of  $D_i^*$ . The  $(1 - \alpha)100\%$  bootstrap confidence interval is defined as

$$\left( \hat{f}_\lambda(\mathbf{x}_i) - \chi_{1-\alpha/2}\hat{\sigma}, \hat{f}_\lambda(\mathbf{x}_i) - \chi_{\alpha/2}\hat{\sigma} \right)$$

Bootstrap confidence intervals are easy to interpret and can be used with any distribution. However, because they require  $K$  model fits, their construction is computationally intensive.

The feature of multiple dependent variables in PROC TPSPLINE enables you to fit multiple models with the same independent variables. The procedure calculates the matrix decomposition part of the calculations only once, regardless of the number of dependent variables in the model. These calculations are responsible for most of the computing time used by the TPSPLINE procedure. This feature is particularly useful when you need to generate a bootstrap confidence interval.

To construct a bootstrap confidence interval, perform the following tasks:

- Fit the data by using PROC TPSPLINE and obtain estimates  $\hat{f}_\lambda(\mathbf{x}_i)$  and  $\hat{\sigma}$ .
- Generate  $K$  bootstrap samples based on  $\hat{f}_\lambda(\mathbf{x}_i)$  and  $\hat{\sigma}$ .
- Fit the  $K$  bootstrap samples with the TPSPLINE procedure to obtain estimates of  $\hat{f}_\lambda^*(\mathbf{x}_i)$  and  $\hat{\sigma}_i^*$ .
- Compute  $D_i^*$  and the values  $\chi_{\alpha/2}$  and  $\chi_{1-\alpha/2}$ .

The following statements illustrate this process:

```
proc tpspline data=melanoma plots(only)=fitplot(clm);
 model incidences = (year) /alpha = 0.1;
 output out=result pred uclm lclm;
run;
```

The output from the initial PROC TPSPLINE analysis is displayed in [Output 96.5.3](#). The data set result contains the predicted values and confidence limits from the analysis.

**Output 96.5.3** Output from PROC TPSPLINE for the MELANOMA Data

|                                                               |         |
|---------------------------------------------------------------|---------|
| Comparison of Two Estimates<br>with and without the D= Option |         |
| The TPSPLINE Procedure<br>Dependent Variable: incidences      |         |
| Summary of Input Data Set                                     |         |
| Number of Non-Missing Observations                            | 37      |
| Number of Missing Observations                                | 0       |
| Unique Smoothing Design Points                                | 37      |
| Summary of Final Model                                        |         |
| Number of Regression Variables                                | 0       |
| Number of Smoothing Variables                                 | 1       |
| Order of Derivative in the Penalty                            | 2       |
| Dimension of Polynomial Space                                 | 2       |
| Summary Statistics<br>of Final Estimation                     |         |
| log10(n*Lambda)                                               | -0.0607 |
| Smoothing Penalty                                             | 0.5171  |
| Residual SS                                                   | 1.2243  |
| Tr(I-A)                                                       | 22.5852 |
| Model DF                                                      | 14.4148 |
| Standard Deviation                                            | 0.2328  |
| GCV                                                           | 0.0888  |

The following statements illustrate how you can obtain a bootstrap confidence interval for the Melanoma data set. The following statements create the data set bootstrap. The observations are created with information from the preceding PROC TPSPLINE execution; as displayed in [Output 96.5.3](#),  $\hat{\sigma} = 0.232823$ . The values of  $\hat{f}_{\hat{\lambda}}(x_i)$  are stored in the data set result in the variable P\_incidence.

```

data bootstrap;
 set result;
 array y{1070} y1-y1070;
 do i=1 to 1070;
 y{i} = p_incidences + 0.232823*rannor(123456789);
 end;
 keep y1-y1070 p_incidences year;
run;

ods listing close;
proc tpspline data=bootstrap plots=none;
 ods output FitStatistics=FitResult;
 id p_incidences;
 model y1-y1070 = (year);
 output out=result2;
run;
ods listing;

```

The DATA step generates 1,070 bootstrap samples based on the previous estimate from PROC TPSPLINE. For this data set, some of the bootstrap samples result in  $\lambda$ s (selected by the GCV function) that cause problematic behavior. Thus, an additional 70 bootstrap samples are generated.

The ODS listing destination is closed before PROC TPSPLINE is invoked. The PLOTS=NONE option suppresses all graphical output. The model fits all the  $y_1 \dots y_{1070}$  variables as dependent variables, and the models are fit for all bootstrap samples simultaneously. The output data set result2 contains the variables year,  $y_1 \dots y_{1070}$ ,  $p_{y_1} \dots p_{y_{1070}}$ , and p\_incidences.

The ODS OUTPUT statement writes the FitStatistics table to the data set FitResult. The data set FitResult contains the two variables Parameter and Value. The FitResult data set is used in subsequent calculations for  $D_i^*$ .

In the data set FitResult, there are 63 estimates with a standard deviation of zero, suggesting that the estimates provide perfect fits of the data and are caused by  $\hat{\lambda}$ s that are approximately equal to zero. For small sample sizes, there is a positive probability that the  $\lambda$  chosen by the GCV function will be zero (Wang and Wahba 1995).

In the following steps, these cases are removed from the bootstrap samples as “bad” samples: they represent failure of the GCV function.

The following SAS statements manipulate the data set FitResult, retaining the standard deviations for all bootstrap samples and merging FitResult with the data set result2, which contains the estimates for bootstrap samples. In the final data set boot, the  $D_i^*$  statistics are calculated.

```

data FitResult;
 set FitResult;
 if Parameter="Standard Deviation";
 keep Value;
run;

proc transpose data=FitResult out=sd prefix=sd;

data result2;
 if _N_ = 1 then set sd;
 set result2;
run;

```

```

data boot;
 set result2;
 array y{1070} p_y1-p_y1070;
 array sd{1070} sd1-sd1070;
 do i=1 to 1070;
 if sd{i} > 0 then do;
 d = (y{i} - P_incidences)/sd{i};
 obs = _N_;
 output;
 end;
 end;
 keep d obs P_incidences year;
run;

```

The following SAS statements retain the first 1,000 bootstrap samples and calculate the values  $\chi_{\alpha/2}$  and  $\chi_{1-\alpha/2}$  with  $\alpha = 0.1$ .

```

proc sort data=boot;
 by obs;
run;

data boot;
 set boot;
 by obs;
 retain n;

 if first.obs then n=1;
 else n=n+1;
 if n > 1000 then delete;
run;

proc sort data=boot;
 by obs d;
run;

data chi1 chi2 ;
 set boot;
 if (_N_ = (obs-1)*1000+50) then output chi1;
 if (_N_ = (obs-1)*1000+950) then output chi2;
run;

proc sort data=result;
 by year;
run;

proc sort data=chi1;
 by year;
run;

proc sort data=chi2;
 by year;
run;

```

```

data result;
 merge result
 chi1(rename=(d=chi05))
 chi2(rename=(d=chi95));
 keep year incidences P_incidences lower upper
 LCLM_incidences UCLM_incidences;

 lower = -chi95*0.232823 + P_incidences;
 upper = -chi05*0.232823 + P_incidences;

 label lower="Lower 90% CL (Bootstrap)"
 upper="Upper 90% CL (Bootstrap)"
 lclm_incidences="Lower 90% CL (Bayesian)"
 uclm_incidences="Upper 90% CL (Bayesian)";
run;

```

The data set result contains the variables year and incidences, the PROC TPSPLINE estimate P\_incidences, and the 90% Bayesian and 90% bootstrap confidence intervals.

The following statements produce [Output 96.5.4](#):

```

proc sgplot data=result;
 title "Age-adjusted Melanoma Incidence for 37 Years";

 xaxis label="year";
 yaxis label="Incidences";

 band x=year lower=lclm_incidences upper=uclm_incidences/name="bayesian"
 legendlabel="90% Bayesian CI of Predicted incidences"
 fillattrs=(color=red);
 band x=year lower=lower upper=upper/name="bootstrap"
 legendlabel="90% Bootstrap CI of Predicted incidences"
 transparency=0.05;
 scatter x=year y=incidences/name="obs" legendlabel="incidences";
 series x=year y=p_incidences/name="pred"
 legendlabel="predicted values of incidences"
 lineattrs=graphfit(thickness=1px);

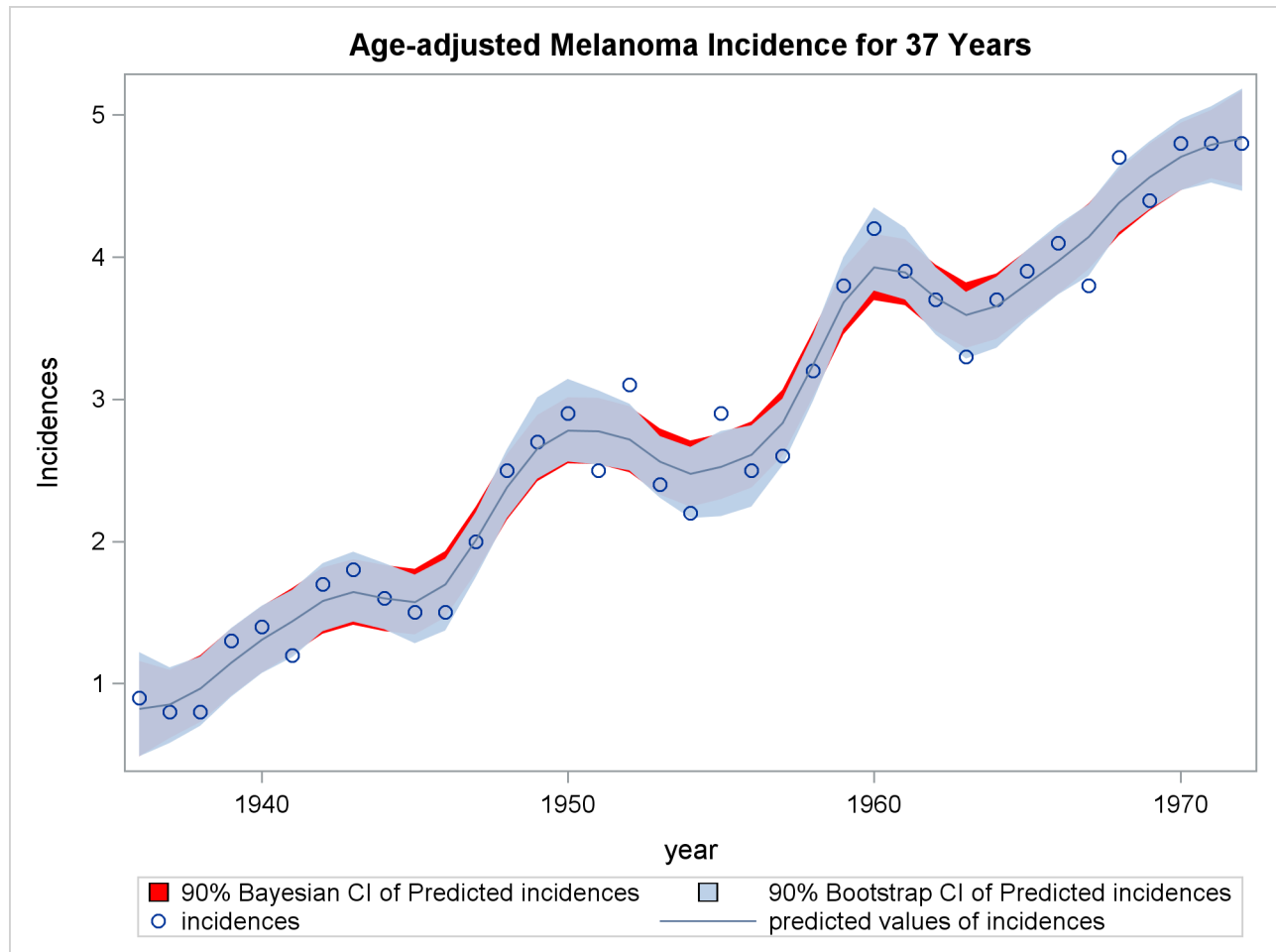
 discretelegend "bayesian" "bootstrap" "obs" "pred";
run;

ods graphics off;

```

[Output 96.5.4](#) displays the plot of the variable incidences, the predicted values, and the Bayesian and bootstrap confidence intervals.

The plot shows that the bootstrap confidence interval is similar to the Bayesian confidence interval. However, the Bayesian confidence interval is symmetric around the estimates, while the bootstrap confidence interval is not.

**Output 96.5.4** Comparison of Bayesian and Bootstrap Confidence Interval for Data Set MELANOMA

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# Chapter 97

## The TRANSREG Procedure

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## Overview: TRANSREG Procedure

The TRANSREG (transformation regression) procedure fits linear models, optionally with smooth, spline, Box-Cox, and other nonlinear transformations of the variables. You can use PROC TRANSREG to fit a curve through a scatter plot or fit multiple curves, one for each level of a classification variable. You can also constrain the functions to be parallel or monotone or have the same intercept. PROC TRANSREG can be used to code experimental designs and classification variables prior to their use in other analyses.

The TRANSREG procedure fits many types of linear models, including the following:

- ordinary regression and ANOVA
- metric and nonmetric conjoint analysis (Green and Wind 1975; de Leeuw, Young, and Takane 1976)
- linear models with Box-Cox (1964) transformations of the dependent variables
- regression with a smooth (Reinsch 1967), spline (de Boor 1978; van Rijckevorsel 1982), monotone spline (Winsberg and Ramsay 1980), or penalized B-spline (Eilers and Marx 1996) fit function
- metric and nonmetric vector and ideal point preference mapping (Carroll 1972)
- simple, multiple, and multivariate regression with variable transformations (Young, de Leeuw, and Takane 1976; Winsberg and Ramsay 1980; Breiman and Friedman 1985)
- redundancy analysis (Stewart and Love 1968) with variable transformations (Israels 1984)
- canonical correlation analysis with variable transformations (van der Burg and de Leeuw 1983)
- response surface regression (Meyers 1976; Khuri and Cornell 1987) with variable transformations

The data set can contain variables measured on nominal, ordinal, interval, and ratio scales (Siegel 1956). You can specify any mix of these variable types for the dependent and independent variables. PROC TRANSREG can do the following:

- transform nominal variables by scoring the categories to minimize squared error (Fisher 1938), or treat nominal variables as classification variables
- transform ordinal variables by monotonically scoring the ordered categories so that order is weakly preserved (adjacent categories can be merged) and squared error is minimized. Ties can be optimally untied or left tied (Kruskal 1964). Ordinal variables can also be transformed to ranks.
- transform interval and ratio scale of measurement variables linearly or nonlinearly with spline (de Boor 1978; van Rijckevorsel 1982), monotone spline (Winsberg and Ramsay 1980), penalized B-spline (Eilers and Marx 1996), smooth (Reinsch 1967), or Box-Cox (Box and Cox 1964) transformations. In addition, logarithmic, exponential, power, logit, and inverse trigonometric sine transformations are available.

Transformations produced by the PROC TRANSREG multiple regression algorithm, requesting spline transformations, are often similar to transformations produced by the ACE smooth regression method of Breiman and Friedman (1985). However, ACE does not explicitly optimize a loss function (de Leeuw 1986), while PROC TRANSREG explicitly minimizes a squared-error criterion.

PROC TRANSREG extends the ordinary general linear model by providing optimal variable transformations that are iteratively derived. PROC TRANSREG iterates until convergence, alternating two major steps: finding least squares estimates of the model parameters given the current scoring of the data, and finding least squares estimates of the scoring parameters given the current set of model parameters. This is called the method of alternating least squares (Young 1981).

For more background on alternating least squares optimal scaling methods and transformation regression methods, see Young, de Leeuw, and Takane (1976); Winsberg and Ramsay (1980); Young (1981); Gifi (1990); Schiffman, Reynolds, and Young (1981); van der Burg and de Leeuw (1983); Israels (1984); Breiman and Friedman (1985); Hastie and Tibshirani (1986). (These are just a few of the many relevant sources.)

---

## Getting Started: TRANSREG Procedure

This section provides several examples that illustrate a few of the more basic features of PROC TRANSREG.

---

### Fitting a Curve through a Scatter Plot

PROC TRANSREG can fit curves through data and detect nonlinear relationships among variables. This example uses a subset of the data from an experiment in which nitrogen oxide emissions from a single cylinder engine are measured for various combinations of fuel and equivalence ratio (Brinkman 1981). This gas data set is available from the Sashelp library. The following step creates a subset of the data for analysis:

```
title 'Gasoline and Emissions Data';

data gas;
 set sashelp.gas;
 if fuel in ('Ethanol', '82rongas', 'Gasohol');
run;
```

The next step fits a spline or curve through the data and displays the regression results. For information about splines and knots, see the sections “Smoothing Splines” on page 8263, “Linear and Nonlinear Regression Functions” on page 8250, “Simultaneously Fitting Two Regression Functions” on page 8254, and “Using Splines and Knots” on page 8233, as well as [Example 97.1](#). The following statements produce [Figure 97.1](#):

```
ods graphics on;

* Request a Spline Transformation of Equivalence Ratio;
proc transreg data=Gas solve ss2 plots=(transformation obp residuals);
 model identity(nox) = spline(EqRatio / nknots=4);
 where fuel in ('Ethanol', '82rongas', 'Gasohol');
run;
```

The **SOLVE** algorithm option, or *a-option*, requests a direct solution for both the transformation and the parameter estimates. For many models, PROC TRANSREG with the SOLVE *a-option* can produce exact results without iteration. The **SS2** (Type II sums of squares) *a-option* requests regression and ANOVA results. The **PLOTS=** option requests plots of the variable transformations, a plot of the observed values by the predicted values, and a plot of the residuals. The dependent variable NOx was specified with an **IDENTITY** transformation, which means that it will not be transformed, just as in ordinary regression. The independent variable EqRatio, in contrast, is transformed by using a cubic spline with four knots. The **NKNOTS=** option is known as a transformation option, or *t-option*. Graphical results are enabled when ODS Graphics is enabled. The results are shown in Figure 97.1 through Figure 97.5.

**Figure 97.1** Iteration, ANOVA, and Regression Results

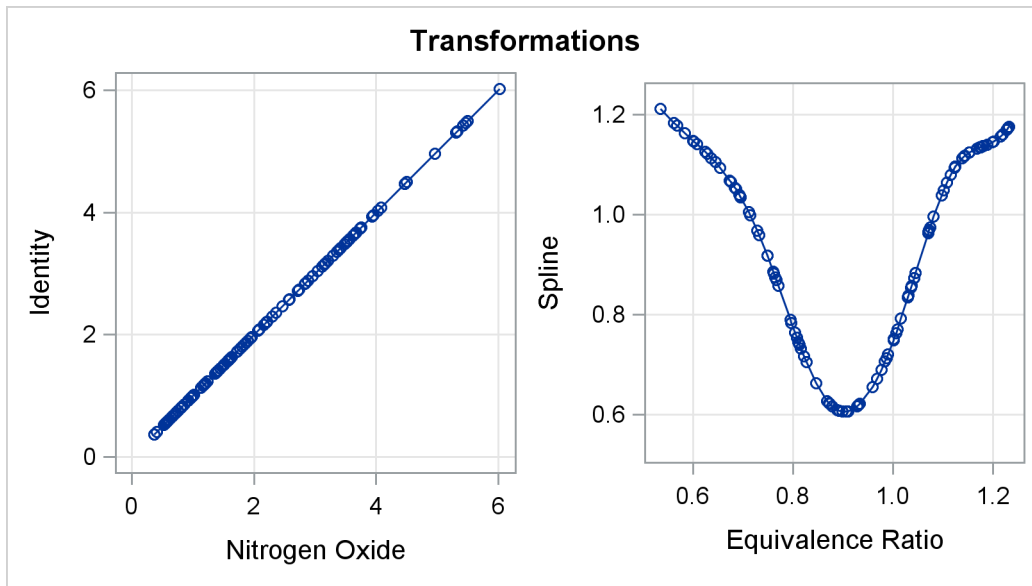
| Gasoline and Emissions Data                                   |                   |                   |          |                     |           |
|---------------------------------------------------------------|-------------------|-------------------|----------|---------------------|-----------|
| The TRANSREG Procedure                                        |                   |                   |          |                     |           |
| Dependent Variable Identity(NOx)                              |                   |                   |          |                     |           |
| Nitrogen Oxide                                                |                   |                   |          |                     |           |
| Number of Observations Read                                   |                   |                   |          |                     | 112       |
| Number of Observations Used                                   |                   |                   |          |                     | 110       |
| TRANSREG MORALS Algorithm Iteration History for Identity(NOx) |                   |                   |          |                     |           |
| Iteration<br>Number                                           | Average<br>Change | Maximum<br>Change | R-Square | Criterion<br>Change | Note      |
| 0                                                             | 1.04965           | 3.46121           | 0.00917  |                     |           |
| 1                                                             | 0.00000           | 0.00000           | 0.82429  | 0.81512             | Converged |
| Algorithm converged.                                          |                   |                   |          |                     |           |

Figure 97.1 continued

| The TRANSREG Procedure Hypothesis Tests for Identity (NOx)<br>Nitrogen Oxide |     |                |                |             |         |        |                   |
|------------------------------------------------------------------------------|-----|----------------|----------------|-------------|---------|--------|-------------------|
| Univariate ANOVA Table Based on the Usual Degrees of Freedom                 |     |                |                |             |         |        |                   |
| Source                                                                       | DF  | Sum of Squares | Mean Square    | F Value     | Pr > F  |        |                   |
| Model                                                                        | 7   | 180.0951       | 25.72788       | 68.36       | <.0001  |        |                   |
| Error                                                                        | 102 | 38.3891        | 0.37636        |             |         |        |                   |
| Corrected Total                                                              | 109 | 218.4842       |                |             |         |        |                   |
| Root MSE                                                                     |     | 0.61348        | R-Square       | 0.8243      |         |        |                   |
| Dependent Mean                                                               |     | 2.25022        | Adj R-Sq       | 0.8122      |         |        |                   |
| Coeff Var                                                                    |     | 27.26334       |                |             |         |        |                   |
| Univariate Regression Table Based on the Usual Degrees of Freedom            |     |                |                |             |         |        |                   |
| Variable                                                                     | DF  | Coefficient    | Type II        |             | F Value | Pr > F | Label             |
|                                                                              |     |                | Sum of Squares | Mean Square |         |        |                   |
| Intercept                                                                    | 1   | 8.3165407      | 324.065        | 324.065     | 861.04  | <.0001 | Intercept         |
| Spline(EqRatio)                                                              | 7   | -6.5740158     | 180.095        | 25.728      | 68.36   | <.0001 | Equivalence Ratio |

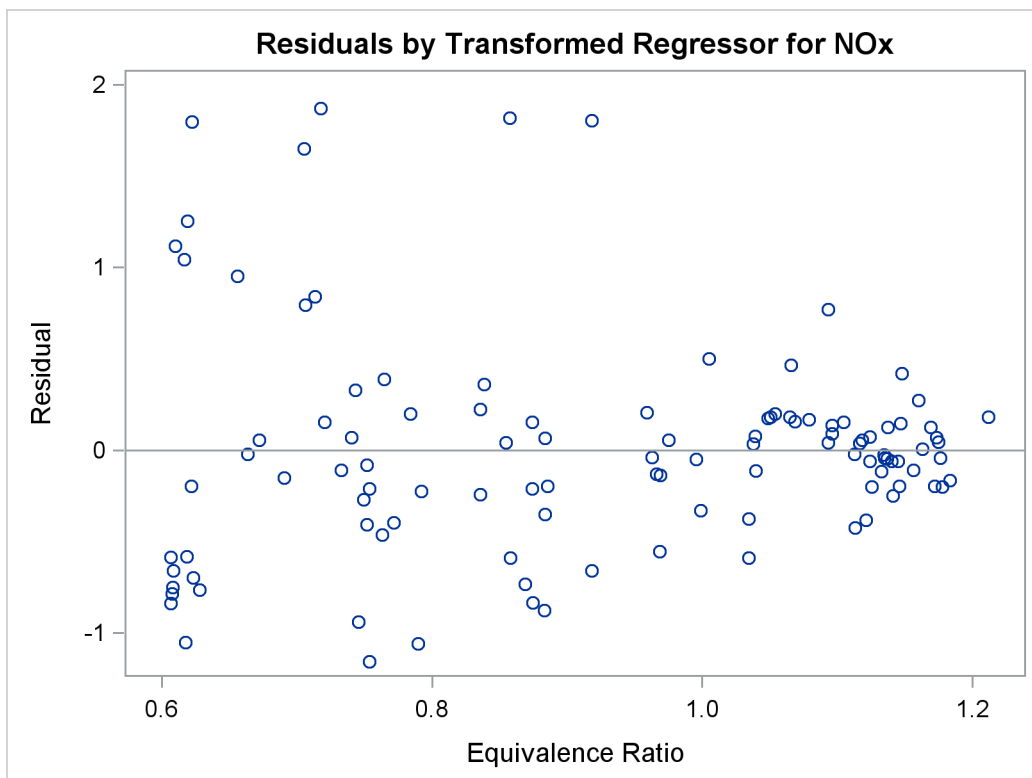
PROC TRANSREG increases the squared multiple correlation from the original value of 0.00917 to 0.82429. Iteration 0 shows the fit before the data are transformed, and iteration 1 shows the fit after the transformation, which was directly solved for in the initial iteration. The change values for iteration 0 show the change from the original EqRatio variable to the transformed EqRatio variable. For this model, no improvement on the initial solution is possible, so in iteration 1, all change values are zero. The ANOVA and regression results show that you are fitting a model with 7 model parameters, 4 knots plus a degree 3 or cubic spline. The overall model fit is identical to the test for the spline transformation, since there is only one term in the model besides the intercept, and the results are significant at the 0.0001 level. The transformations are shown next in Figure 97.2.

Figure 97.2 Transformations



The transformation plots show the identity transformation of NO<sub>x</sub> and the nonlinear spline transformation of EqRatio. These plots are requested with the `PLOTS=TRANSFORMATION` option. The plot on the left shows that NO<sub>x</sub> is unchanged, which is always the case with the `IDENTITY` transformation. In contrast, the spline transformation of EqRatio is nonlinear. It is this nonlinear transformation of EqRatio that accounts for the increase in fit that is shown in the iteration history table.

Figure 97.3 Residuals

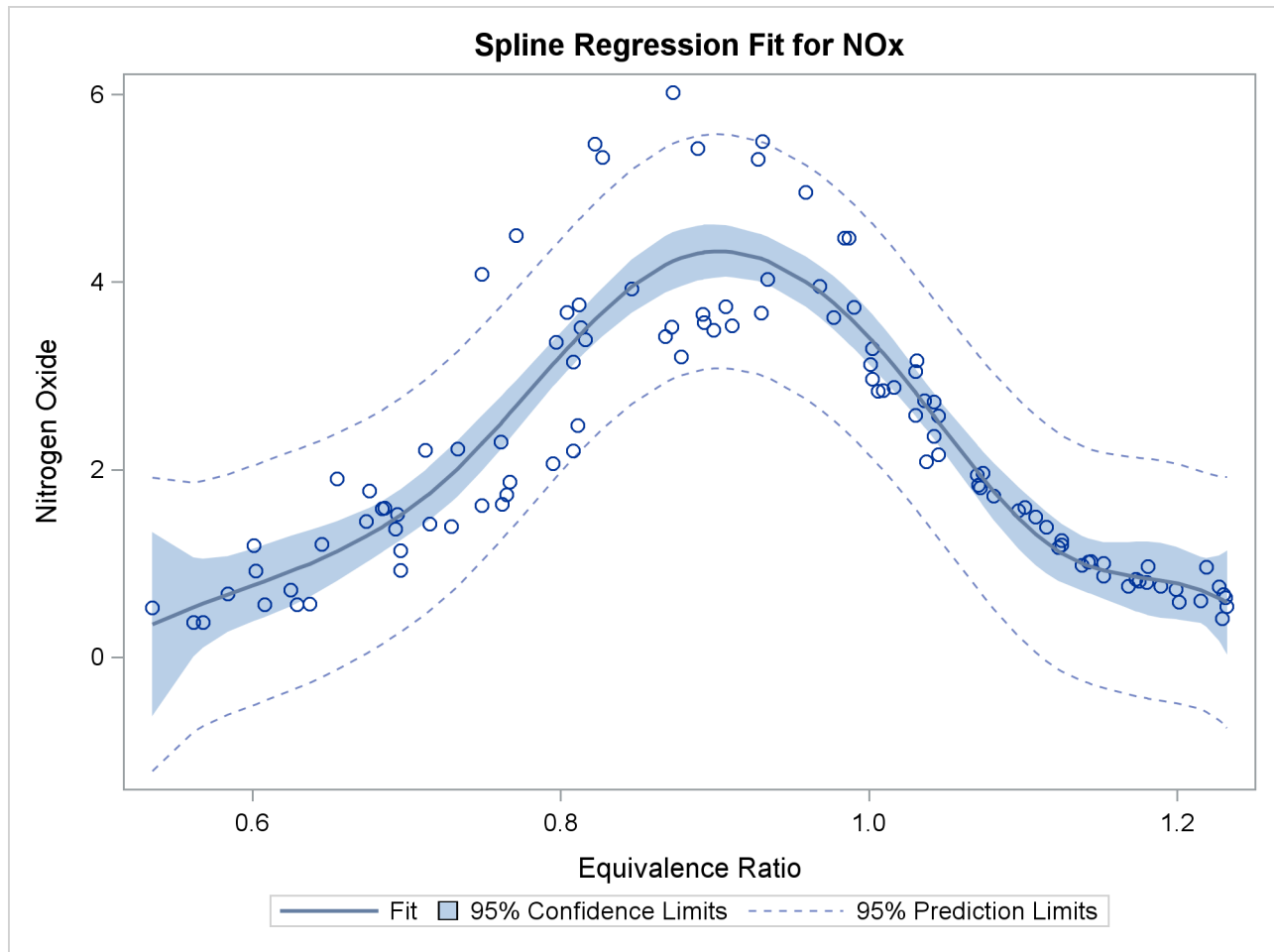




The residuals plot in Figure 97.3 shows the residuals as a function of the transformed independent variable.

The “Spline Regression Fit” plot in Figure 97.4 displays the nonlinear regression function plotted through the original data, along with 95% confidence and prediction limits. This plot clearly shows that nitrous oxide emissions are largest in the middle range of equivalence ratio, 0.08 to 1.0, and are much lower for the extreme values of equivalence ratio, such as around 0.6 and 1.2.

**Figure 97.4** Fitting a Curve through a Scatter Plot

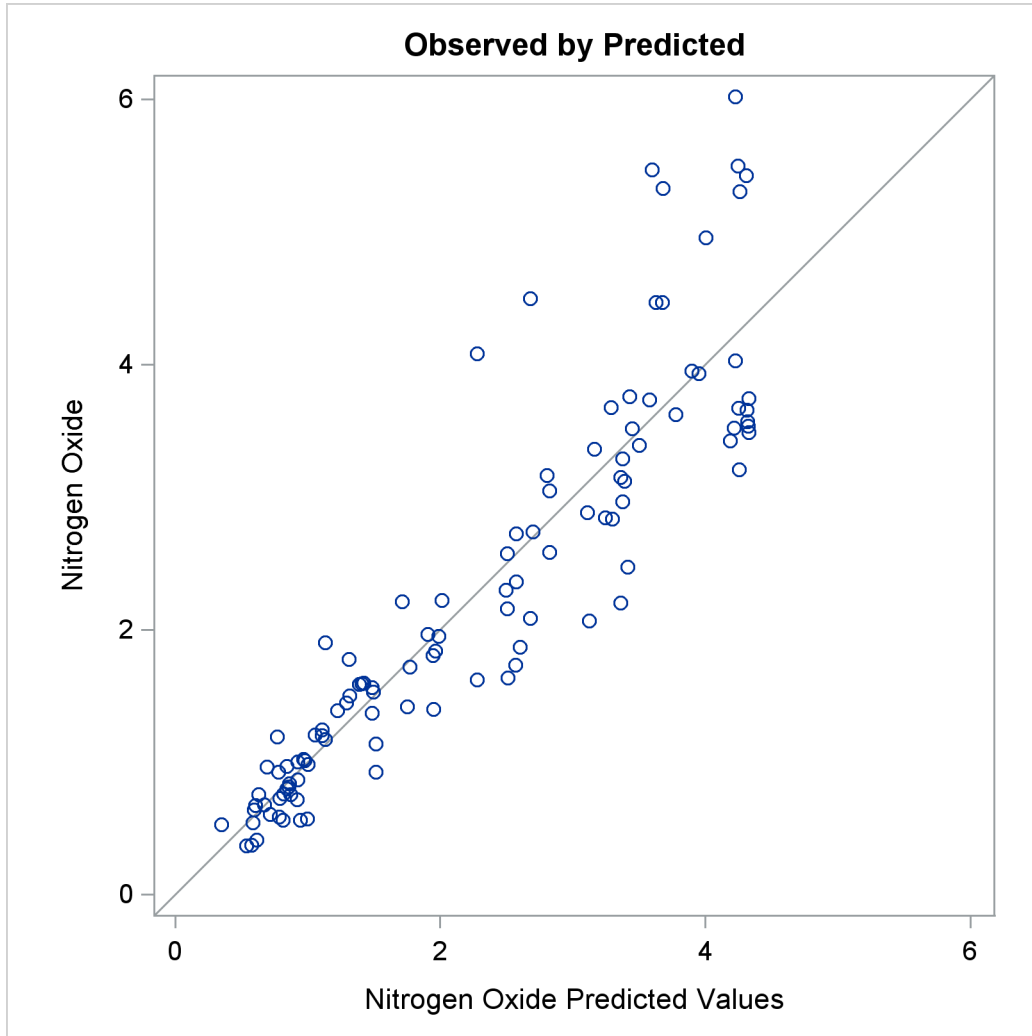


This plot is produced by default when ODS Graphics is enabled and when there is an IDENTITY dependent variable and one non-CLASS independent variable. The plot consists of an ordinary scatter plot of NOx plotted as a function of EqRatio. It also contains the predicted values of NOx, which are a function of the spline transformation of EqRatio (or TEqRatio shown previously), and are plotted as a function of EqRatio. Similarly, it contains confidence limits based on NOx and TEqRatio.

The “Observed by Predicted” values plot in Figure 97.5 displays the dependent variable plotted as a function of the regression predicted values along with a linear regression line, which for this plot always has a slope of 1. This plot was requested with the OBP or OBSERVEDBYPREDICTED suboption in the PLOTS= option. The residual differences between the transformed data and the regression line show how well the nonlinearly transformed data fit a linear-regression model. The residuals look mostly random; however, they are larger for larger values of NOx, suggesting that maybe this is not the optimal model. You can also see this by examining the fit of the function through the original scatter plot in Figure 97.4. Near the

middle of the function, the residuals are much larger. You can refit the model, this time requesting separate functions for each type of fuel. You can request the original scatter plot, without any regression information and before the variables are transformed, by specifying the SCATTER suboption in the PLOTS= option.

**Figure 97.5** Observed by Predicted



These next statements fit an additive model with separate functions for each of the different fuels. The statements produce [Figure 97.6](#) through [Figure 97.9](#).

```
* Separate Curves and Intercepts;
proc transreg data=Gas solve ss2 additive plots=(transformation obp);
 model identity(nox) = class(Fuel / zero=none) |
 spline(EqRatio / nknots=4 after);
run;
```

The **ADDITIVE** *a-option* requests an additive model, where the regression coefficients are absorbed into the transformations, and so the final regression coefficients are all one. The specification **CLASS(Fuel / ZERO=NONE)** recodes fuel into a set of three binary variables, one for each of the three fuels in this data set. The vertical bar between the **CLASS** and **SPLINE** specifications request both main effects and interactions. For this model, it requests both a separate intercept and a separate spline function for each fuel. The original

two variables, Fuel and EqRatio, are replaced by six variables—three binary intercept terms and three spline variables. The three spline variables are zero when their corresponding intercept binary variable is zero, and nonzero otherwise. The nonzero parts are optimally transformed by the analysis. The *AFTER t-option* specified with the SPLINE transformation specifies that the four knots should be selected independently for each of the three spline transformations, *after* EqRatio is crossed with the CLASS variable. Alternatively, and by default, the knots are chosen by examining EqRatio before it is crossed with the CLASS variable, and the same knots are used for all three transformations. The results are shown in Figure 97.6.

**Figure 97.6** Iteration, ANOVA, and Regression Results

```

Gasoline and Emissions Data

The TRANSREG Procedure

Dependent Variable Identity(NOx)
Nitrogen Oxide

Class Level Information

Class Levels Values
Fuel 3 82rongas Ethanol Gasohol

Number of Observations Read 112
Number of Observations Used 110
Implicit Intercept Model

TRANSREG MORALS Algorithm Iteration History for Identity(NOx)

Iteration Average Maximum
Number Change Change R-Square Criterion
 Change Change R-Square Change Note

0 0.12476 1.13866 0.18543
1 0.00000 0.00000 0.95870 0.77327 Converged

Algorithm converged.

Hypothesis Test Iterations Excluding Spline(Fuel82rongasEqRatio)
TRANSREG MORALS Algorithm Iteration History for Identity(NOx)

Iteration Average Maximum
Number Change Change R-Square Criterion
 Change Change R-Square Change Note

0 0.00000 0.00000 0.80234
1 0.00000 0.00000 0.80234 -.00000 Converged

Algorithm converged.

```

Figure 97.6 continued

| Hypothesis Test Iterations Excluding Spline(FuelEthanolEqRatio) |                |                |             |                  |           |
|-----------------------------------------------------------------|----------------|----------------|-------------|------------------|-----------|
| TRANSREG MORALS Algorithm Iteration History for Identity(NOx)   |                |                |             |                  |           |
| Iteration Number                                                | Average Change | Maximum Change | R-Square    | Criterion Change | Note      |
| 0                                                               | 0.00000        | 0.00000        | 0.48801     |                  |           |
| 1                                                               | 0.00000        | 0.00000        | 0.48801     | -.00000          | Converged |
| Algorithm converged.                                            |                |                |             |                  |           |
| Hypothesis Test Iterations Excluding Spline(FuelGasoholEqRatio) |                |                |             |                  |           |
| TRANSREG MORALS Algorithm Iteration History for Identity(NOx)   |                |                |             |                  |           |
| Iteration Number                                                | Average Change | Maximum Change | R-Square    | Criterion Change | Note      |
| 0                                                               | 0.00000        | 0.00000        | 0.80052     |                  |           |
| 1                                                               | 0.00000        | 0.00000        | 0.80052     | -.00000          | Converged |
| Algorithm converged.                                            |                |                |             |                  |           |
| The TRANSREG Procedure Hypothesis Tests for Identity(NOx)       |                |                |             |                  |           |
| Nitrogen Oxide                                                  |                |                |             |                  |           |
| Univariate ANOVA Table Based on the Usual Degrees of Freedom    |                |                |             |                  |           |
| Source                                                          | DF             | Sum of Squares | Mean Square | F Value          | Pr > F    |
| Model                                                           | 23             | 209.4613       | 9.107012    | 86.80            | <.0001    |
| Error                                                           | 86             | 9.0229         | 0.104918    |                  |           |
| Corrected Total                                                 | 109            | 218.4842       |             |                  |           |
| Root MSE                                                        |                | 0.32391        | R-Square    | 0.9587           |           |
| Dependent Mean                                                  |                | 2.25022        | Adj R-Sq    | 0.9477           |           |
| Coeff Var                                                       |                | 14.39461       |             |                  |           |

Figure 97.6 continued

| Univariate Regression Table Based on the Usual Degrees of Freedom |    |             |                              |                |         |        |
|-------------------------------------------------------------------|----|-------------|------------------------------|----------------|---------|--------|
| Variable                                                          | DF | Coefficient | Type II<br>Sum of<br>Squares | Mean<br>Square | F Value | Pr > F |
| Class.Fuel82rongas                                                | 1  | 1.00000000  | 32.634                       | 32.6338        | 311.04  | <.0001 |
| Class.FuelEthanol                                                 | 1  | 1.00000000  | 97.406                       | 97.4058        | 928.40  | <.0001 |
| Class.FuelGasohol                                                 | 1  | 1.00000000  | 34.672                       | 34.6720        | 330.47  | <.0001 |
| Spline(Fuel82rongasEq<br>Ratio)                                   | 7  | 1.00000000  | 34.162                       | 4.8803         | 46.52   | <.0001 |
| Spline(FuelEthanolEq<br>Ratio)                                    | 7  | 1.00000000  | 102.840                      | 14.6914        | 140.03  | <.0001 |
| Spline(FuelGasoholEq<br>Ratio)                                    | 7  | 1.00000000  | 34.561                       | 4.9372         | 47.06   | <.0001 |

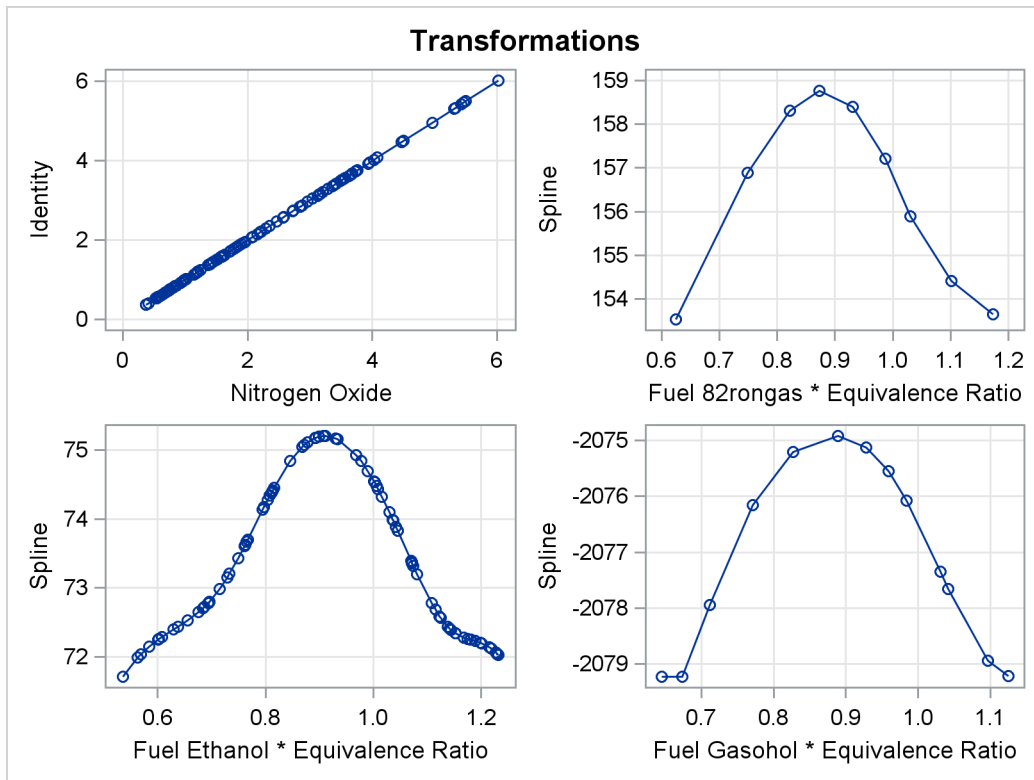
  

| Variable                        | DF | Label                             |
|---------------------------------|----|-----------------------------------|
| Class.Fuel82rongas              | 1  | Fuel 82rongas                     |
| Class.FuelEthanol               | 1  | Fuel Ethanol                      |
| Class.FuelGasohol               | 1  | Fuel Gasohol                      |
| Spline(Fuel82rongasEq<br>Ratio) | 7  | Fuel 82rongas * Equivalence Ratio |
| Spline(FuelEthanolEq<br>Ratio)  | 7  | Fuel Ethanol * Equivalence Ratio  |
| Spline(FuelGasoholEq<br>Ratio)  | 7  | Fuel Gasohol * Equivalence Ratio  |

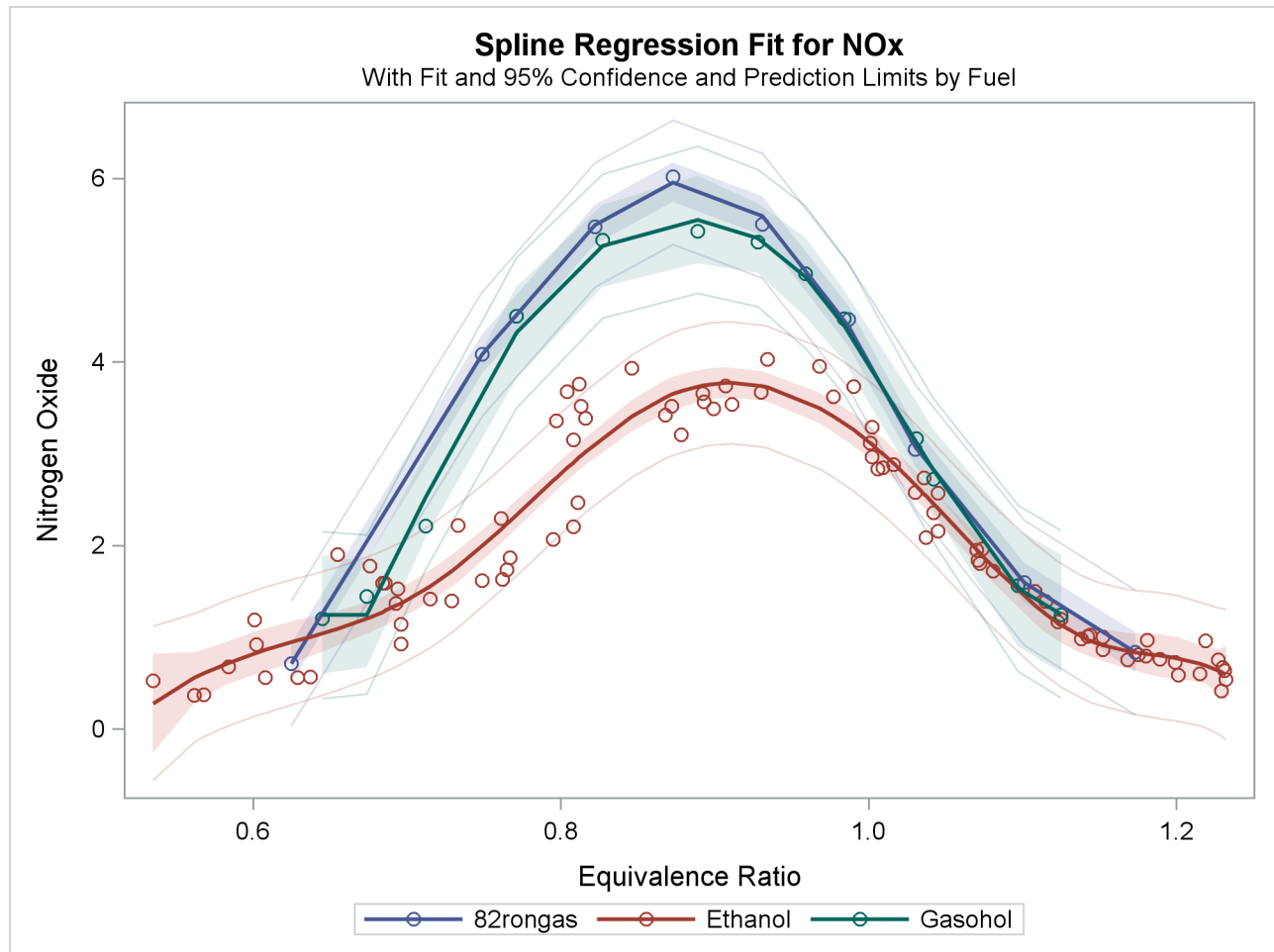
ZERO=SUM and ZERO=NONE coefficient tests are not exact when there are iterative transformations. Those tests are performed holding all transformations fixed, and so are generally liberal.

The first iteration history table in Figure 97.6 shows that PROC TRANSREG increases the squared multiple correlation from the original value of 0.18543 to 0.95870. The remaining iteration histories pertain to PROC TRANSREG's process of comparing models to test hypotheses. The important thing to look for is convergence in all of the tables.

Figure 97.7 Transformations

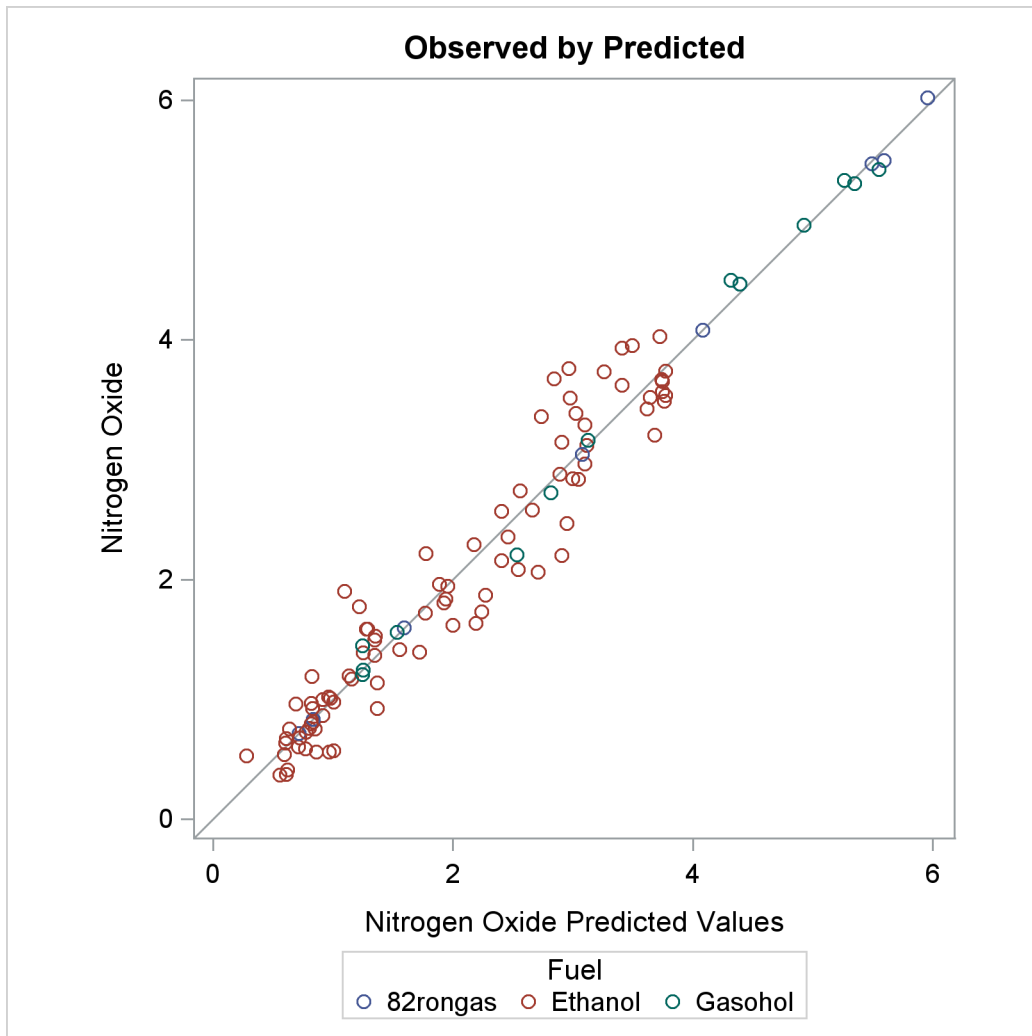


The transformations, shown in Figure 97.7, show that for all three groups, the transformation of EqRatio is approximately quadratic.

**Figure 97.8** Fitting Curves through a Scatter Plot

The fit plot, shown in [Figure 97.8](#), shows that there are in fact three distinct functions in the data. The increase in fit over the previous model comes from individually fitting each group instead of providing an aggregate fit.

Figure 97.9 Observed by Predicted



The residuals in the observed by predicted plot displayed in [Figure 97.9](#) are much better for this analysis.

You could fit a model that is “in between” the two models shown previously. This next model provides for separate intercepts for each group, but calls for a common function. There are still three functions, one per group, but their shapes are the same, and they are equidistant or parallel. This model is requested by omitting the vertical bar so that separate intercepts are requested, but not separate curves within each group. The following statements fit the separate intercepts model and create [Figure 97.10](#):

```
* Separate Intercepts;
proc transreg data=Gas solve ss2 additive;
 model identity(nox) = class(Fuel / zero=none)
 spline(EqRatio / nknots=4);
run;
```

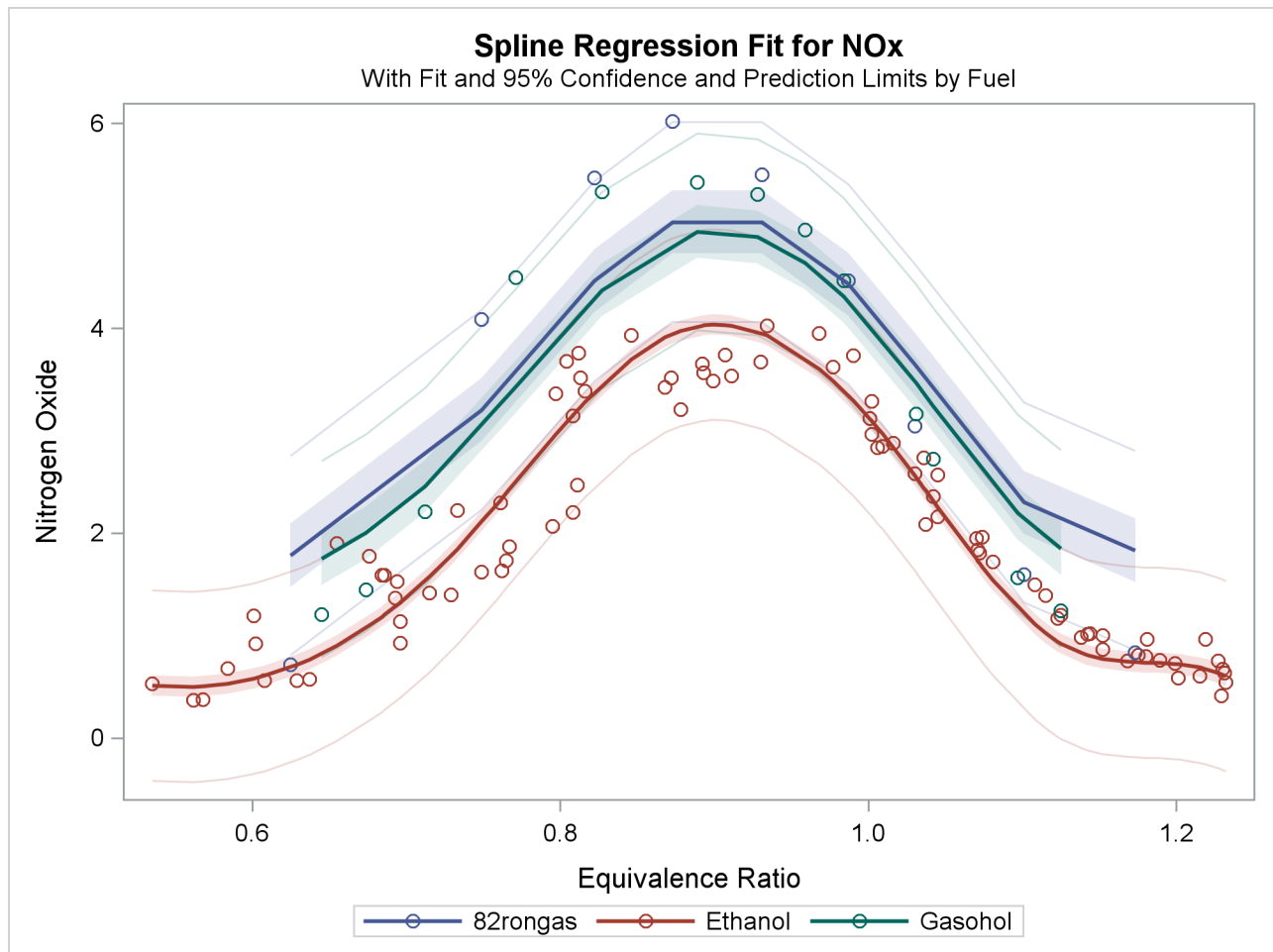
The ANOVA table and fit plot are shown in [Figure 97.10](#).



**Figure 97.10** Separate Intercepts Only

| Gasoline and Emissions Data                                  |     |                |             |         |        |
|--------------------------------------------------------------|-----|----------------|-------------|---------|--------|
| The TRANSREG Procedure                                       |     |                |             |         |        |
| Univariate ANOVA Table Based on the Usual Degrees of Freedom |     |                |             |         |        |
| Source                                                       | DF  | Sum of Squares | Mean Square | F Value | Pr > F |
| Model                                                        | 9   | 196.7548       | 21.86165    | 100.61  | <.0001 |
| Error                                                        | 100 | 21.7294        | 0.21729     |         |        |
| Corrected Total                                              | 109 | 218.4842       |             |         |        |

**Figure 97.10** continued



Now, squared multiple correlation is 0.9005, which is smaller than the model with the unconstrained separate curves, but larger than the model with only one curve. Because of the restrictions on the shapes, these curves do not track the data as well as the previous model. However, this model is more parsimonious with many fewer parameters.

There are other ways to fit curves through scatter plots in PROC TRANSREG. For example, you could use smoothing splines or penalized B-splines, as is illustrated next. The following statements fit separate curves through each group by using penalized B-splines and produce Figure 97.11:

```
* Separate Curves and Intercepts with Penalized B-Splines;
proc transreg data=Gas ss2 plots=transformation lprefix=0;
 model identity(nox) = class(Fuel / zero=none) * pbspline(EqRatio);
run;
```

This example asks for a separate penalized B-spline transformation, **PBSPLINE**, of equivalence ratio for each type of fuel. The **LPREFIX=0** *a-option* is specified in the PROC statement so that zero characters of the **CLASS** variable name (Fuel) are used in constructing the labels for the coded variables. The result is label components like “Ethanol” instead of the more redundant “Fuel Ethanol”. The results of this analysis are shown in Figure 97.11.

**Figure 97.11** Penalized B-Splines

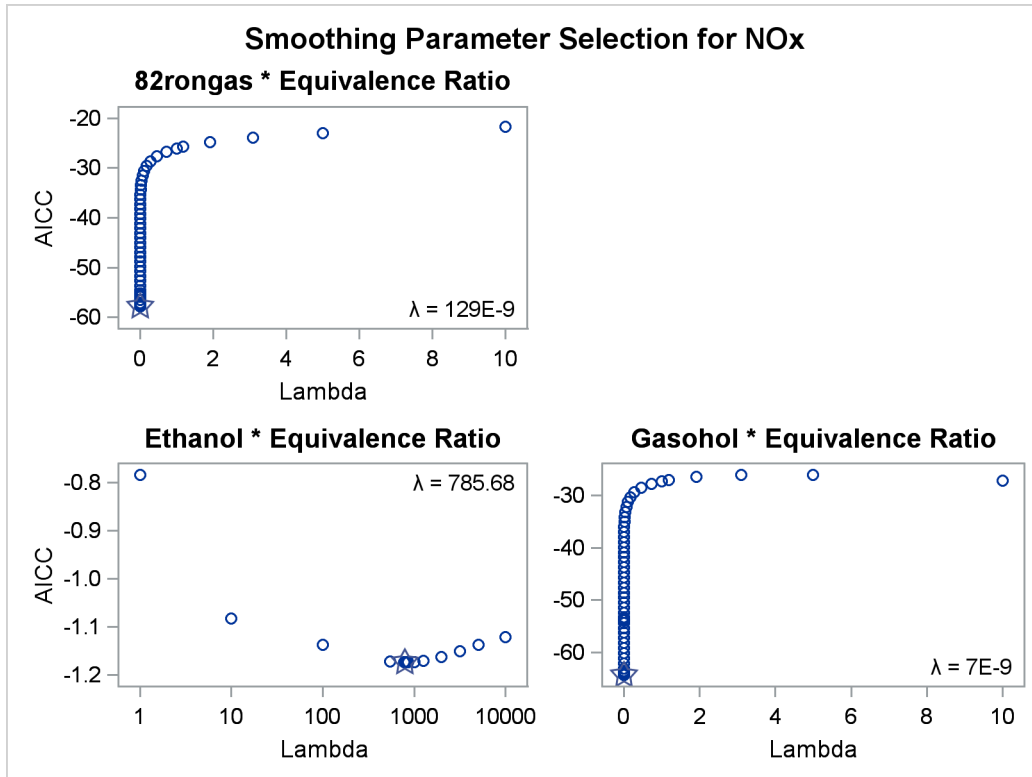


Figure 97.11 continued

| Dependent Variable Identity (NOx)<br>Nitrogen Oxide                          |                |                          |             |         |        |
|------------------------------------------------------------------------------|----------------|--------------------------|-------------|---------|--------|
| Class Level Information                                                      |                |                          |             |         |        |
| Class                                                                        | Levels         | Values                   |             |         |        |
| Fuel                                                                         | 3              | 82rongas Ethanol Gasohol |             |         |        |
| Number of Observations Read                                                  |                |                          |             |         | 112    |
| Number of Observations Used                                                  |                |                          |             |         | 110    |
| Implicit Intercept Model                                                     |                |                          |             |         |        |
| TRANSREG Univariate Algorithm Iteration History for Identity (NOx)           |                |                          |             |         |        |
| Iteration Number                                                             | Average Change | Maximum Change           | Note        |         |        |
| 1                                                                            | 0.00000        | 0.00000                  | Converged   |         |        |
| Algorithm converged.                                                         |                |                          |             |         |        |
| The TRANSREG Procedure Hypothesis Tests for Identity (NOx)<br>Nitrogen Oxide |                |                          |             |         |        |
| Univariate ANOVA Table, Penalized B-Spline Transformation                    |                |                          |             |         |        |
| Source                                                                       | DF             | Sum of Squares           | Mean Square | F Value | Pr > F |
| Model                                                                        | 33.194         | 211.4818                 | 6.371106    | 68.97   | <.0001 |
| Error                                                                        | 75.806         | 7.0024                   | 0.092373    |         |        |
| Corrected Total                                                              | 109            | 218.4842                 |             |         |        |
| Root MSE                                                                     |                | 0.30393                  | R-Square    | 0.9680  |        |
| Dependent Mean                                                               |                | 2.25022                  | Adj R-Sq    | 0.9539  |        |
| Coeff Var                                                                    |                | 13.50663                 |             |         |        |

Figure 97.11 continued

| Penalized B-Spline Transformation |       |             |          |          |                              |
|-----------------------------------|-------|-------------|----------|----------|------------------------------|
| Variable                          | DF    | Coefficient | Lambda   | AICC     | Label                        |
| Pbspline (Fuel82rongasEq Ratio)   | 9.000 | 1.000       | 1.287E-7 | -57.7841 | 82rongas * Equivalence Ratio |
| Pbspline (FuelEthanolEq Ratio)    | 12.19 | 1.000       | 785.7    | -1.1736  | Ethanol * Equivalence Ratio  |
| Pbspline (FuelGasoholEq Ratio)    | 13.00 | 1.000       | 7.019E-9 | -64.2961 | Gasohol * Equivalence Ratio  |

Figure 97.11 continued

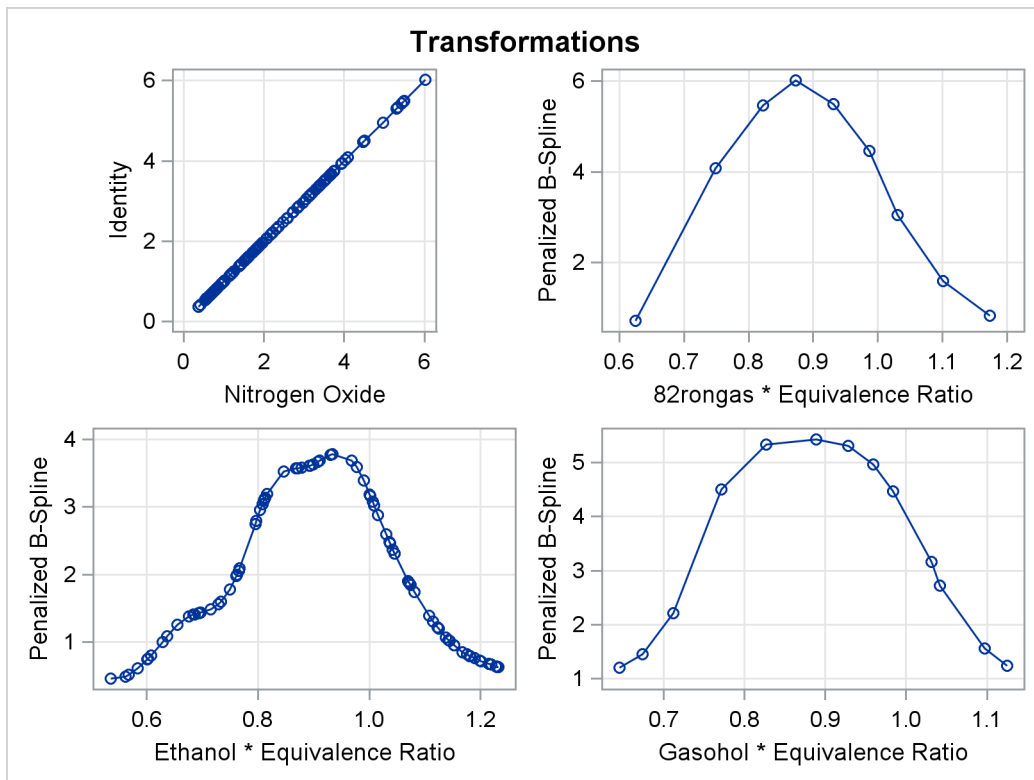
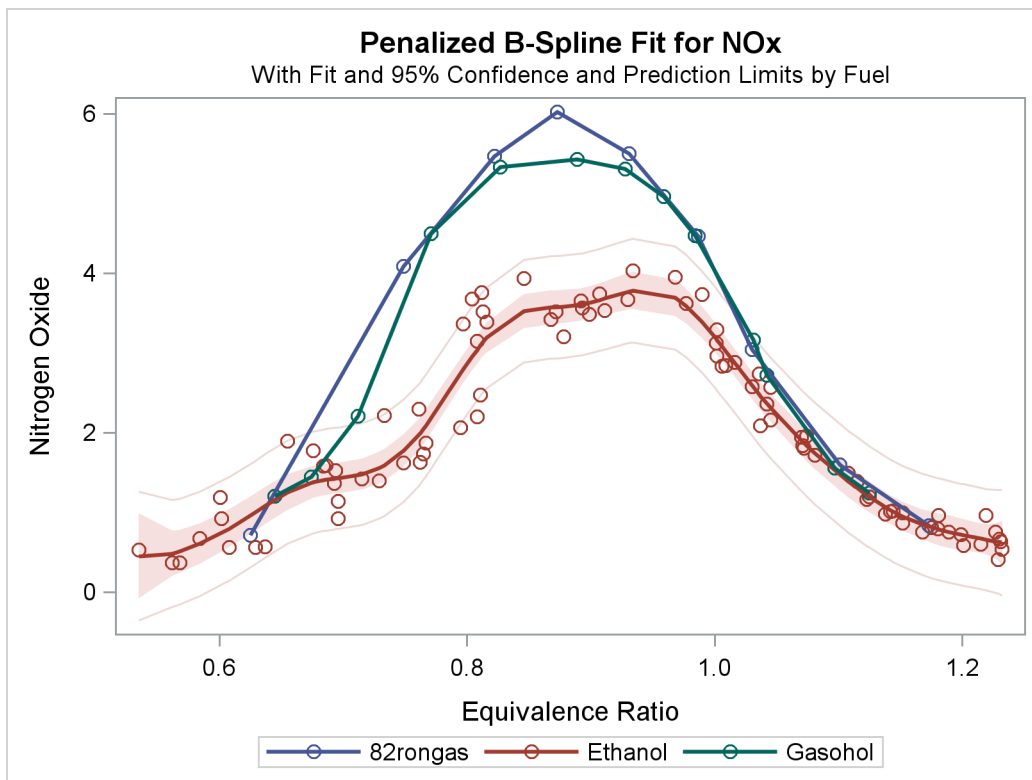


Figure 97.11 continued



With penalized B-splines, the degrees of freedom are based on the trace of the transformation hat matrix and are typically not integers. The first panel of plots shows AICC as a function of lambda, the smoothing parameter. The smoothing parameter is automatically chosen, and since the smoothing parameters range from essentially 0 to almost 800, it is clear that some functions are smoother than others. The plots of the criterion (AICC in this example) as a function of lambda use a linear scale for the horizontal axis when the range of lambdas is small, as in the first and third plot, and a log scale when the range is large, as in the second plot. The transformation for equivalence ratio for Ethanol required more smoothing than for the other two fuels. All three have an overall quadratic shape, but for Ethanol, the function more closely follows the smaller variations in the data. You could get similar results with `SPLINE` by using more knots.

For other examples of curve fitting by using PROC TRANSREG, see the sections “Smoothing Splines” on page 8263, “Linear and Nonlinear Regression Functions” on page 8250, “Simultaneously Fitting Two Regression Functions” on page 8254, and “Using Splines and Knots” on page 8233, as well as Example 97.3. These examples include cases where multiple curves are fit through scatter plots with multiple groups. Special cases include linear models with separate slopes and separate intercepts. Many constraints on the slopes, curves, and intercepts are possible.

## Main-Effects ANOVA

This example shows how to use PROC TRANSREG to code and fit a main-effects ANOVA model. PROC TRANSREG has very extensive and versatile options for coding or creating so-called dummy variables. PROC TRANSREG is commonly used to code classification variables before they are used for analysis

in other procedures. See the sections “Using the DESIGN Output Option” on page 8331 and “Discrete Choice Experiments: DESIGN, NORESTORE, NOZERO” on page 8335. In this example, the input data set contains the dependent variables *y*, factors *x1* and *x2*, and 12 observations. PROC TRANSREG can be useful for coding even before running procedures with a CLASS statement because of its detailed options that enable you to control how the coded variable names and labels are constructed. The following statements perform a main-effects ANOVA and display the results in Figure 97.12 and Figure 97.13:

```

title 'Introductory Main-Effects ANOVA Example';

data a;
 input y x1 $ x2 $;
 datalines;
8 a a
7 a a
4 a b
3 a b
5 b a
4 b a
2 b b
1 b b
8 c a
7 c a
5 c b
2 c b
;

* Fit a main-effects ANOVA model with 1, 0, -1 coding;
proc transreg ss2;
 model identity(y) = class(x1 x2 / effects);
 output coefficients replace;
run;

* Display TRANSREG output data set;
proc print label;
 format intercept -- x2a 5.2;
run;

```

The *SS2 a-option* requests results based on Type II sums of squares. The simple ANOVA model is fit by designating *y* as an **IDENTITY** variable, which specifies no transformation. The independent variables are specified with a **CLASS** expansion, which replaces them with coded variables. There are  $(3-1)+(2-1) = 3$  coded variables created by the CLASS specification, since the two CLASS variables have 3 and 2 different values or levels. In this case, the **EFFECTS t-option** is specified. This option requests an *effects coding* (displayed in Figure 97.13), which is also called a deviations from means or 0, 1, -1 coding. The **OUTPUT** statement requests an output data set with the data and coded variables. The **COEFFICIENTS** output option, or *o-option*, adds the parameter estimates and marginal means to the data set. The **REPLACE o-option** specifies that the transformed variables should replace the original variables in the output data set. The output data set variable names are the same as the original variable name. In an example like this, there are no nonlinear transformations; the transformed variables are the same as the original variables. The **REPLACE o-option** is used to eliminate unnecessary and redundant transformed variables from the output data set. The results of the PROC TRANSREG step are shown in Figure 97.12.

Figure 97.12 ANOVA Example Output from PROC TRANSREG

```

Introductory Main-Effects ANOVA Example

The TRANSREG Procedure

Dependent Variable Identity(y)

Class Level Information

Class Levels Values

x1 3 a b c
x2 2 a b

Number of Observations Read 12
Number of Observations Used 12

The TRANSREG Procedure Hypothesis Tests for Identity(y)

Univariate ANOVA Table Based on the Usual Degrees of Freedom

Source DF Sum of Mean
 DF Squares Square F Value Pr > F

Model 3 57.00000 19.00000 19.83 0.0005
Error 8 7.66667 0.95833
Corrected Total 11 64.66667

Root MSE 0.97895 R-Square 0.8814
Dependent Mean 4.66667 Adj R-Sq 0.8370
Coeff Var 20.97739

Univariate Regression Table Based on the Usual Degrees of Freedom

Variable DF Coefficient Type II
 DF Coefficient Sum of
 DF Coefficient Squares Mean
 DF Coefficient Squares Square F Value Pr > F Label

Intercept 1 4.6666667 261.333 261.333 272.70 <.0001 Intercept
Class.x1a 1 0.8333333 4.167 4.167 4.35 0.0705 x1 a
Class.x1b 1 -1.6666667 16.667 16.667 17.39 0.0031 x1 b
Class.x2a 1 1.8333333 40.333 40.333 42.09 0.0002 x2 a

```

Figure 97.12 shows the ANOVA results, fit statistics, and regression tables. The output data set, with the coded design, parameter estimates and means, is shown in Figure 97.13. For more information about PROC TRANSREG for ANOVA and other codings, see the section “ANOVA Codings” on page 8270.

Figure 97.13 Output Data Set from PROC TRANSREG

| Introductory Main-Effects ANOVA Example |          |        |   |           |       |       |       |    |    |
|-----------------------------------------|----------|--------|---|-----------|-------|-------|-------|----|----|
| Obs                                     | _TYPE_   | _NAME_ | y | Intercept | x1 a  | x1 b  | x2 a  | x1 | x2 |
| 1                                       | SCORE    | ROW1   | 8 | 1.00      | 1.00  | 0.00  | 1.00  | a  | a  |
| 2                                       | SCORE    | ROW2   | 7 | 1.00      | 1.00  | 0.00  | 1.00  | a  | a  |
| 3                                       | SCORE    | ROW3   | 4 | 1.00      | 1.00  | 0.00  | -1.00 | a  | b  |
| 4                                       | SCORE    | ROW4   | 3 | 1.00      | 1.00  | 0.00  | -1.00 | a  | b  |
| 5                                       | SCORE    | ROW5   | 5 | 1.00      | 0.00  | 1.00  | 1.00  | b  | a  |
| 6                                       | SCORE    | ROW6   | 4 | 1.00      | 0.00  | 1.00  | 1.00  | b  | a  |
| 7                                       | SCORE    | ROW7   | 2 | 1.00      | 0.00  | 1.00  | -1.00 | b  | b  |
| 8                                       | SCORE    | ROW8   | 1 | 1.00      | 0.00  | 1.00  | -1.00 | b  | b  |
| 9                                       | SCORE    | ROW9   | 8 | 1.00      | -1.00 | -1.00 | 1.00  | c  | a  |
| 10                                      | SCORE    | ROW10  | 7 | 1.00      | -1.00 | -1.00 | 1.00  | c  | a  |
| 11                                      | SCORE    | ROW11  | 5 | 1.00      | -1.00 | -1.00 | -1.00 | c  | b  |
| 12                                      | SCORE    | ROW12  | 2 | 1.00      | -1.00 | -1.00 | -1.00 | c  | b  |
| 13                                      | M COEFFI | y      | . | 4.67      | 0.83  | -1.67 | 1.83  |    |    |
| 14                                      | MEAN     | y      | . | .         | 5.50  | 3.00  | 6.50  |    |    |

The output data set has three kinds of observations, identified by values of `_TYPE_` as follows:

- When `_TYPE_='SCORE'`, the observation contains the following information about the dependent and independent variables:
  - `y` is the original dependent variable.
  - `x1` and `x2` are the independent classification variables, and the `Intercept` through `x2 a` columns contain the main-effects design matrix that PROC TRANSREG creates. The variable names are `Intercept`, `x1a`, `x1b`, and `x2a`. Their labels are shown in the listing.
- When `_TYPE_='M COEFFI'`, the observation contains coefficients of the final linear model (parameter estimates).
- When `_TYPE_='MEAN'`, the observation contains the marginal means.

The observations with `_TYPE_='SCORE'` form the score or data partition of the output data set, and the observations with `_TYPE_='M COEFFI'` and `_TYPE_='MEAN'` form the output statistics partition of the output data set.



---

## Syntax: TRANSREG Procedure

The following statements are available in the TRANSREG procedure:

```

PROC TRANSREG < DATA=SAS-data-set>
 < PLOTS=(plot-requests)>
 < OUTTEST=SAS-data-set> < a-options> < o-options> ;
MODEL < transform(dependents </ t-options>)>
 < transform(dependents </ t-options>)...=>
 transform(independents </ t-options>)
 < transform(independents </ t-options>)... > </ a-options> ;
OUTPUT < OUT=SAS-data-set> < o-options> ;
ID variables ;
FREQ variable ;
WEIGHT variable ;
BY variables ;

```

To use PROC TRANSREG, you need both the PROC TRANSREG and MODEL statements. To produce an OUT= output data set, the OUTPUT statement is required. PROC TRANSREG enables you to specify the same options in more than one statement. All of the MODEL statement *a-options* (algorithm options) and all of the OUTPUT statement *o-options* (output options) can also be specified in the PROC TRANSREG statement. You can abbreviate all *a-options*, *o-options*, and *t-options* (transformation options) to their first three letters. This is a special feature of PROC TRANSREG and is not generally true of other SAS/STAT procedures. See [Table 97.1](#) for a list of options available in the PROC TRANSREG statement.

The PROC TRANSREG statement starts the TRANSREG procedure. Optionally, this statement identifies an input and an OUTTEST= data set, specifies the algorithm and other computational details, requests displayed output, and controls the contents of the OUT= data set (which is created with the OUTPUT statement). The DATA= and OUTTEST= options can appear only in the PROC TRANSREG statement. All *a-options* and *o-options* are described in the sections on either the MODEL or OUTPUT statement, in which these options can also be specified.

The rest of this section provides detailed syntax information for each of the preceding statements, beginning with the PROC TRANSREG statement. The remaining statements are described in alphabetical order.

---

### PROC TRANSREG Statement

```

PROC TRANSREG < DATA=SAS-data-set>
 < PLOTS=(plot-requests)>
 < OUTTEST=SAS-data-set> < a-options> < o-options> ;

```

The PROC TRANSREG statement invokes the TRANSREG procedure. Optionally, this statement identifies an input and an OUTTEST= data set, specifies the algorithm and other computational details, requests displayed output, and controls the contents of the OUT= data set (which is created with the OUTPUT statement). The DATA=, OUTTEST=, and PLOTS= options can appear only in the PROC TRANSREG statement. [Table 97.1](#) summarizes the options available in the PROC TRANSREG statement. The *a-options* are also available in the MODEL statement, and the *o-options* are also available in the OUTPUT statement.

**Table 97.1** Options Available in the PROC TRANSREG Statement

| Option                                               | Description                                    |
|------------------------------------------------------|------------------------------------------------|
| <b>Data Set Options (PROC Statement)</b>             |                                                |
| DATA=                                                | Specifies input SAS data set                   |
| OUTTEST=                                             | Specifies output test statistics data set      |
| <b>ODS Graphics (PROC Statement)</b>                 |                                                |
| PLOTS=                                               | Specifies ODS Graphics selection               |
| <b>Input Control (PROC or MODEL)</b>                 |                                                |
| REITERATE                                            | Restarts the iterations                        |
| TYPE=                                                | Specifies input observation type               |
| <b>Method and Iterations (PROC or MODEL)</b>         |                                                |
| CCONVERGE=                                           | Specifies minimum criterion change             |
| CONVERGE=                                            | Specifies minimum data change                  |
| MAXITER=                                             | Specifies maximum number of iterations         |
| METHOD=                                              | Specifies iterative algorithm                  |
| NCAN=                                                | Specifies number of canonical variables        |
| NSR                                                  | Specifies no restrictions on smoothing models  |
| SINGULAR=                                            | Specifies singularity criterion                |
| SOLVE                                                | Attempts direct solution instead of iteration  |
| <b>Missing Data Handling (PROC or MODEL)</b>         |                                                |
| INDIVIDUAL                                           | Fits each model individually (METHOD=MORALS)   |
| MONOTONE=                                            | Includes monotone special missing values       |
| NOMISS                                               | Excludes observations with missing values      |
| UNTIE=                                               | Unties special missing values                  |
| <b>Intercept and CLASS Variables (PROC or MODEL)</b> |                                                |
| CPREFIX=                                             | Specifies CLASS coded variable name prefix     |
| LPREFIX=                                             | Specifies CLASS coded variable label prefix    |
| NOINT                                                | Specifies no intercept or centering            |
| ORDER=                                               | Specifies order of CLASS variable levels       |
| REFERENCE=                                           | Controls output of reference levels            |
| SEPARATORS=                                          | Controls CLASS coded variable label separators |
| <b>Control Displayed Output (PROC or MODEL)</b>      |                                                |
| ALPHA=                                               | Specifies confidence limits alpha              |
| CL                                                   | Displays parameter estimate confidence limits  |
| DETAIL                                               | Displays model specification details           |
| HISTORY                                              | Displays iteration histories                   |
| NOPRINT                                              | Suppresses displayed output                    |
| PBOXCOXTABLE                                         | Prints the Box-Cox log likelihood table        |
| RSQUARE                                              | Displays the R square                          |
| SHORT                                                | Suppresses the iteration histories             |
| SS2                                                  | Displays regression results                    |
| TEST                                                 | Displays ANOVA table                           |
| TSUFFIX=                                             | Shortens transformed variable labels           |

Table 97.1 *continued*

| Option                                                         | Description                                     |
|----------------------------------------------------------------|-------------------------------------------------|
| UTILITIES                                                      | Displays conjoint part-worth utilities          |
| <b>Standardization (PROC or MODEL)</b>                         |                                                 |
| ADDITIVE                                                       | Fits additive model                             |
| NOZEROCONSTANT                                                 | Does not zero constant variables                |
| TSTANDARD=                                                     | Specifies transformation standardization        |
| <b>Predicted Values, Residuals, Scores (PROC or OUTPUT)</b>    |                                                 |
| CANONICAL                                                      | Outputs canonical scores                        |
| CLI                                                            | Outputs individual confidence limits            |
| CLM                                                            | Outputs mean confidence limits                  |
| DESIGN=                                                        | Specifies design matrix coding                  |
| DREPLACE                                                       | Replaces dependent variables                    |
| IREPLACE                                                       | Replaces independent variables                  |
| LEVERAGE                                                       | Outputs leverage                                |
| NORESTOREMISSING                                               | Does not restore missing values                 |
| NOSCORES                                                       | Suppresses output of scores                     |
| PREDICTED                                                      | Outputs predicted values                        |
| REDUNDANCY=                                                    | Outputs redundancy variables                    |
| REPLACE                                                        | Replaces all variables                          |
| RESIDUALS                                                      | Outputs residuals                               |
| <b>Output Data Set Coefficients (PROC or OUTPUT)</b>           |                                                 |
| COEFFICIENTS                                                   | Outputs coefficients                            |
| COORDINATES=                                                   | Outputs ideal point coordinates                 |
| MEANS                                                          | Outputs marginal means                          |
| MREDUNDANCY                                                    | Outputs redundancy analysis coefficients        |
| <b>Output Data Set Variable Name Prefixes (PROC or OUTPUT)</b> |                                                 |
| ADPREFIX=                                                      | Specifies dependent variable approximations     |
| AIPREFIX=                                                      | Specifies independent variable approximations   |
| CDPREFIX=                                                      | Specifies canonical dependent variables         |
| CILPREFIX=                                                     | Specifies conservative individual lower CL      |
| CIPREFIX=                                                      | Specifies canonical independent variables       |
| CIUPREFIX=                                                     | Specifies conservative-individual-upper CL      |
| CMLPREFIX=                                                     | Specifies conservative-mean-lower CL            |
| CMUPREFIX=                                                     | Specifies conservative-mean-upper CL            |
| DEPENDENT=                                                     | Specifies METHOD=MORALS untransformed dependent |
| LILPREFIX=                                                     | Specifies liberal-individual-lower CL           |
| LIUPREFIX=                                                     | Specifies liberal-individual-upper CL           |
| LMLPREFIX=                                                     | Specifies liberal-mean-lower CL                 |
| LMUPREFIX=                                                     | Specifies liberal-mean-upper CL                 |
| PPREFIX=                                                       | Specifies predicted values                      |
| RDPREFIX=                                                      | Specifies residuals                             |
| RPREFIX=                                                       | Specifies redundancy variables                  |
| TDPREFIX=                                                      | Specifies transformed dependents                |

Table 97.1 *continued*

| Option                                   | Description                                        |
|------------------------------------------|----------------------------------------------------|
| TIPREFIX=                                | Specifies transformed independents                 |
| <b>Macros Variables (PROC or OUTPUT)</b> |                                                    |
| MACRO                                    | Creates macro variables                            |
| <b>Other Options (PROC or OUTPUT)</b>    |                                                    |
| APPROXIMATIONS                           | Outputs dependent and independent approximations   |
| CCC                                      | Outputs canonical correlation coefficients         |
| CEC                                      | Outputs canonical elliptical point coordinates     |
| CPC                                      | Outputs canonical point coordinates                |
| CQC                                      | Outputs canonical quadratic point coordinates      |
| DAPPROXIMATIONS                          | Outputs approximations to transformed dependents   |
| IAPPROXIMATIONS                          | Outputs approximations to transformed independents |
| MEC                                      | Outputs elliptical point coordinates               |
| MPC                                      | Outputs point coordinates                          |
| MQC                                      | Outputs quadratic point coordinates                |
| MRC                                      | Outputs multiple regression coefficients           |

**DATA=SAS-data-set**

specifies the SAS data set to be analyzed. If you do not specify the DATA= option, PROC TRANSREG uses the most recently created SAS data set. The data set must be an ordinary SAS data set; it cannot be a special TYPE= data set.

**OUTTEST=SAS-data-set**

specifies an output data set to contain hypothesis tests results. When you specify the OUTTEST= option, the data set contains ANOVA results. When you specify the SS2 *a-option*, regression tables are also output. When you specify the UTILITIES *o-option*, conjoint analysis part-worth utilities are also output. For more information about the OUTTEST= data set, see the section “OUTTEST= Output Data Set” on page 8313.

**PLOTS <(global-plot-options)> <= plot-request <(options)>>****PLOTS <(global-plot-options)> <= (plot-request <(options)> <... plot-request <(options)>>>**

controls the plots produced through ODS Graphics. When you specify only one plot request, you can omit the parentheses around the plot request. Here are some examples:

```
plots=none
plots=(residuals transformation)
plots(unpack)=boxcox
plots(unpack)=(transformation boxcox(p=0))
plots=(residuals(unpack) transformation(dep unpk) boxcox(t rmse))
```

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;

proc transreg plots=all;
 model identity(y) = pbspline(x);
run;

ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS](#).”

If ODS Graphics is enabled, but you do not specify the PLOTS= option, then PROC TRANSREG produces a default set of plots. The fit, scatter, residual, and observed-by-predicted plots are available with [METHOD=MORALS](#) and also with [METHOD=UNIVARIATE](#) when there is only one dependent variable. When no method is specified and there is more than one dependent variable, and when regression plots are requested, the default method is set to [METHOD=MORALS](#). When there is more than one dependent variable, when [METHOD=](#) is not specified, or when [METHOD=MORALS](#) is specified and [PLOTS=ALL](#) is specified, the plots that are produced might be different from those you would see with [METHOD=UNIVARIATE](#) and [PLOTS=ALL](#). Certain plots appear by default when ODS Graphics is enabled and certain combinations of options are specified. The Box-Cox  $F = t^2$  and log-likelihood plots appear when a [BOXCOX](#) dependent variable transformation is specified. The regression fit plot appears for models with a single dependent variable that is not transformed (for example, [IDENTITY\(y\)](#)), a single quantitative independent variable that might or might not be transformed, and at most one [CLASS](#) independent variable. Preference mapping plots appear when the [COORDINATES o-option](#) is used.

The global plot options include the following:

## **INTERPOLATE**

### **INT**

uses observations that are excluded from the analysis for interpolation in the fit and transformation plots. By default, observations with zero weight are excluded from all plots. These include observations with a zero, negative, or missing weight or frequency and observations excluded due to missing and invalid values. You can specify [PLOTS\(INTERPOLATE\)=\(plot-requests\)](#) to include some of these observations in the plots. You might want to use this option, for example, with sparse data sets to show smoother functions over the range of the data (see the section “[The PLOTS\(INTERPOLATE\) Option](#)” on page 8340). Observations with missing values in [CLASS](#) variables are excluded from the plots even when [PLOTS\(INTERPOLATE\)](#) is specified.

### **ONLY**

### **ONL**

suppresses the default plots. Only plots specifically requested are displayed.

## **UNPACKPANEL**

### **UNPACK**

### **UNP**

suppresses paneling. By default, multiple plots can appear in some output panels. Specify [UNPACKPANEL](#) to get each plot in a separate panel. You can specify [PLOTS\(UNPACKPANEL\)](#) to unpack the default plots. You can also specify [UNPACKPANEL](#) as a suboption with [TRANSFORMATION](#), [RESIDUALS](#), [PBSPLINE](#), and [BOXCOX](#).

The plot requests include the following:

**ALL**

produces all appropriate plots. You can specify other options with ALL; for example, to request all plots and unpack only the residuals, specify PLOTS=(ALL RES(UNP)).

**BOXCOX** <(options)>

**BOX** <(options)>

requests a display of the results of the Box-Cox transformation. These results are displayed by default when there is a Box-Cox transformation. The BOXCOX plot request has the following options:

**P=*n***

adds  $t$  or  $F = t^2$  curves to the legend for the functions where  $p(t) < n$ , where  $t$  is the  $t$  statistic corresponding to the optimal lambda. You can specify P=0 to suppress the legend and P=1 to see all curves in the legend. The default value comes from the BOXCOX(variable / ALPHA=p) specification, which by default is 0.05.

**RMSE**

**RMS**

plots the root mean square error as a function of lambda.

**T**

plots  $t$  statistics rather than  $F = t^2$  statistics.

**UNPACKPANEL**

**UNPACK**

**UNP**

plots the  $t$  or  $F = t^2$  and log-likelihood plots in separate panels.

**FIT** <(options)>

requests a regression fit plot. This plot is produced by default whenever it is appropriate. It is produced when the dependent variable is specified with the IDENTITY *transform*, and when there is one quantitative independent variable (for example, IDENTITY for linear fit, SPLINE or one of the other transformations for a nonlinear fit, or PSPLINE) and at most one CLASS variable. When there is a CLASS variable, separate fits are produced within levels based on your model. You would specify the FIT plot request only to specify a FIT option or with the ONLY global plot option. The FIT plot request has the following options:

**FORMULA**

**FOR**

displays the fit function as an equation in regression fit plots. This option is valid when a fit plot is produced and either an IDENTITY *transform* or a PSPLINE *expansion* with degree less than ten and no knots is specified for a single independent variable. When this option is specified, you can output the formula to a data set by using the ods output **formula**=SAS-data-set statement. This is the formula, complete with Unicode specifications for polynomials, that is used in the fit plot template to make the formula.

**NOCLM**

suppresses the confidence limits in regression fit plots.

**NOCLI**

suppresses the individual prediction limits in regression fit plots.

**NOOBS**

suppresses the observations showing only the fit function and optionally the confidence and prediction limits.

**NONE**

suppresses all plots.

**OBSERVEDBYPREDICTED****OBP****OBS**

plots the transformed dependent variable as a function of the regression predicted values.

**PBSPLINE <(UNPACKPANEL)>****PBS <(UNPACK)>**

requests the penalized B-spline criterion plots. You would specify the PBSPLINE plot request only to specify a PBSPLINE option or with the ONLY global plot option. The PBSPLINE plot request has the following option:

**UNPACKPANEL****UNPACK****UNP**

plots each criterion plot in a separate panel.

**PREFMAP****PRE**

plots ideal point or vector preference mapping results when either two **IDENTITY** or two **POINT** independent variables are specified along with the **COORDINATES** option.

**RESIDUALS <(options)>****RES <(options)>**

plots the residuals as a function of each of the transformed independent variables, except coded **CLASS** variables. The RESIDUALS plot request has the following options:

**CLASS****CLA**

plots the residuals as a function of each of the transformed independent variables, including coded **CLASS** variables. Note that the **ALL** plot request, which you use to request all plots, specifies the RESIDUALS plot request without the **CLASS** option.

**UNPACKPANEL****UNPACK****UNP**

plots the residuals in separate plots, not several per panel.

**SMOOTH****SMO**

adds a LOESS smooth function to the residuals plots.

**SCATTER****SCA**

plots the scatter plot of observed data, before the transformations, for models with a single quantitative dependent variable, a single quantitative independent variable, and at most one CLASS independent variable.

**TRANSFORMATION** <(options)>**TRA** <(options)>

plots the variable transformations. The TRANSFORMATION plot request has the following options:

**DEPENDENTS****DEP**

plots only the dependent variable transformations.

**INDEPENDENTS****IND**

plots only the independent variable transformations.

**UNPACKPANEL****UNPACK****UNP**

plots the transformations in separate plots, not several per panel.

**BY Statement**

**BY** *variables* ;

You can specify a BY statement with PROC TRANSREG to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.



- Specify the NOTSORTED or DESCENDING option in the BY statement for the TRANSREG procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

---

## FREQ Statement

**FREQ** *variable* ;

If one variable in the input data set represents the frequency of occurrence for other values in the observation, specify the variable's name in a FREQ statement. PROC TRANSREG then treats the data set as if each observation appeared  $n$  times, where  $n$  is the value of the FREQ variable for the observation. Noninteger values of the FREQ variable are truncated to the largest integer less than the FREQ value. The observation is used in the analysis only if the value of the FREQ statement variable is greater than or equal to 1.

---

## ID Statement

**ID** *variables* ;

The ID statement includes additional character or numeric variables in the **OUT=** data set. The variables must be contained in the input data set. The first variable is used to label points in PREFMAP plots. These variables are also used in some plots as tip variables.

---

## MODEL Statement

```
MODEL < transform(dependents </ t-options>)>
 < transform(dependents </ t-options>)...=>
 transform(independents </ t-options>)
 < transform(independents </ t-options>)... > </ a-options> ;
```

The MODEL statement specifies the dependent and independent variables (*dependents* and *independents*, respectively) and specifies the transformation (*transform*) to apply to each variable. Only one MODEL statement can appear in PROC TRANSREG. The *t-options* are transformation options, and the *a-options* are algorithm options. The *t-options* provide details for the transformation; these depend on the *transform* chosen. The *t-options* are listed after a slash in the parentheses that enclose the variable list (either *dependents* or *independents*). The *a-options* control the algorithm used, details of iteration, details of how the intercept and coded variables are generated, and displayed output details. The *a-options* are listed after the entire model specification (the *dependents*, *independents*, transformations, and *t-options*) and after a slash. You can also specify the algorithm options in the PROC TRANSREG statement. When you specify the

**DESIGN** *o-option*, *dependents* and an equal sign are not required. The operators \*, |, and @ from the GLM procedure are available for interactions with the **CLASS** expansion and the **IDENTITY** transformation. They are used as follows:

```

Class(a * b ...
 c | d ...
 e | f ... @ n)
Identity(a * b ...
 c | d ...
 e | f ... @ n)

```

In addition, transformations and spline expansions can be crossed with classification variables as follows:

```

transform(var) * class(group)
transform(var) | class(group)

```

See the section “Types of Effects” on page 3325 in Chapter 42, “The GLM Procedure,” for a description of the @, \*, and | operators and see the section “Model Statement Usage” on page 8220 for information about how to use these operators in PROC TRANSREG. Note that nesting is not implemented in PROC TRANSREG.

The next three sections discuss the transformations available (*transforms*) (see the section “Families of Transformations” on page 8183), the transformation options (*t-options*) (see the section “Transformation Options (t-options)” on page 8190), and the algorithm options (*a-options*) (see the section “Algorithm Options (a-options)” on page 8200).

## Families of Transformations

In the MODEL statement, *transform* specifies a transformation in one of the following five families:

|                               |                                                                                                                                                                                                                                                                              |
|-------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Variable expansions           | preprocess the specified variables, replacing them with more variables.                                                                                                                                                                                                      |
| Nonoptimal transformations    | preprocess the specified variables, replacing each one with a single new nonoptimal, nonlinear transformation.                                                                                                                                                               |
| Nonlinear fit transformations | preprocess the specified variable, replacing it with a smooth transformation, fitting one or more nonlinear functions through a scatter plot.                                                                                                                                |
| Optimal transformations       | replace the specified variables with new, iteratively derived optimal transformation variables that fit the specified model better than the original variable (except for contrived cases where the transformation fits the model exactly as well as the original variable). |
| Other transformations         | are the <b>IDENTITY</b> and <b>SSPLINE</b> transformations. These do not fit into the preceding categories.                                                                                                                                                                  |

The transformations and expansions listed in [Table 97.2](#) are available in the MODEL statement.

**Table 97.2** Transformation Families

| Transformation                       | Description                         |
|--------------------------------------|-------------------------------------|
| <b>Variable Expansions</b>           |                                     |
| BSPLINE                              | B-spline basis                      |
| CLASS                                | set of coded variables              |
| EPOINT                               | elliptical response surface         |
| POINT                                | circular response surface & PREFMAP |
| PSPLINE                              | piecewise polynomial basis          |
| QPOINT                               | quadratic response surface          |
| <b>Nonoptimal Transformations</b>    |                                     |
| ARSIN                                | inverse trigonometric sine          |
| EXP                                  | exponential                         |
| LOG                                  | logarithm                           |
| LOGIT                                | logit                               |
| POWER                                | raises variables to specified power |
| RANK                                 | transforms to ranks                 |
| <b>Nonlinear Fit Transformations</b> |                                     |
| BOXCOX                               | Box-Cox                             |
| PBSPLINE                             | penalized B-splines                 |
| SMOOTH                               | noniterative smoothing spline       |
| <b>Optimal Transformations</b>       |                                     |
| LINEAR                               | linear                              |
| MONOTONE                             | monotonic, ties preserved           |
| MSPLINE                              | monotonic B-spline                  |
| OPSCORE                              | optimal scoring                     |
| SPLINE                               | B-spline                            |
| UNTIE                                | monotonic, ties not preserved       |
| <b>Other Transformations</b>         |                                     |
| IDENTITY                             | identity, no transformation         |
| SSPLINE                              | iterative smoothing spline          |

You can use any transformation with either dependent or independent variables (except the **SMOOTH** and **PBSPLINE** transformations, which can be used only with independent variables, and **BOXCOX**, which can be used only with dependent variables). However, the variable expansions are usually more appropriate for independent variables.

The *transform* is followed by a variable (or list of variables) enclosed in parentheses. Here is an example:

```
model log(y) = class(x);
```

This example finds a **LOG** transformation of *y* and performs a **CLASS** expansion of *x*. Optionally, depending on the *transform*, the parentheses can also contain *t-options*, which follow the variables and a slash. Here is an example:

```
model identity(y) = spline(x1 x2 / nknots=3);
```

The preceding statement finds **SPLINE** transformations of *x1* and *x2*. The **NKNOTS=** *t-option* used with the **SPLINE** transformation specifies three knots. The **identity(y)** transformation specifies that *y* is not to be transformed.

The rest of this section provides syntax details for members of the five families of transformations listed at the beginning of this section. The *t-options* are discussed in the section “Transformation Options (t-options)” on page 8190.

## Variable Expansions

PROC TRANSREG performs variable expansions before iteration begins. Variable expansions expand the original variables into a typically larger set of new variables. The original variables are those that are listed in parentheses after *transform*, and they are sometimes referred to by the name of the *transform*. For example, in `CLASS(x1 x2)`, `x1` and `x2` are sometimes referred to as CLASS expansion variables or simply CLASS variables, and the expanded variables are referred to as coded or sometimes “dummy” variables. Similarly, in `POINT(Dim1 Dim2)`, `Dim1` and `Dim2` are sometimes referred to as POINT variables.

The resulting variables are not transformed by the iterative algorithms after the initial preprocessing. Observations with missing values for these types of variables are excluded from the analysis.

The `POINT`, `EPOINT`, and `QPOINT` variable expansions are used in preference mapping analyses (also called PREFMAP, external unfolding, ideal point regression) (Carroll 1972) and for response surface regressions. These three expansions create circular, elliptical, and quadratic response or preference surfaces (see the section “Point Models” on page 8294 and Example 97.6). The `CLASS` variable expansion is used for main-effects ANOVA.

The following list provides syntax and details for the variable expansion *transforms*.

### BSPLINE

#### BSP

expands each variable to a B-spline basis. You can specify the `DEGREE=`, `KNOTS=`, `NKNOTS=`, and `EVENLY=` *t-options* with the BSPLINE expansion. When `DEGREE=n` (3 by default) with *k* knots (0 by default),  $n + k + 1$  variables are created. In addition, the original variable appears in the `OUT=` data set before the `ID` variables. For example, `bspline(x)` expands `x` into `x_0 x_1 x_2 x_3` and outputs `x` as well. The `x_:` variables contain the B-spline basis vectors (which are the same basis vectors that the `SPLINE` and `MSPLINE` transformations use internally). The columns of the BSPLINE expansion sum to a column of ones, so an implicit intercept model is fit when the BSPLINE expansion is specified. If you specify the BSPLINE expansion for more than one variable, the model is less than full rank. Variables specified in a BSPLINE expansion must be numeric, and they are typically continuous. See the sections “SPLINE and MSPLINE Transformations” on page 8300 and “SPLINE, BSPLINE, and PSPLINE Comparisons” on page 8302 for more information about B-splines.

### CLASS

#### CLA

expands the variables to a set of coded or “dummy” variables. PROC TRANSREG uses the values of the formatted variables to determine class membership. The specification `class(x1 x2)` fits a simple main-effects model, `class(x1 | x2)` fits a main-effects and interactions model, and `class(x1|x2|x3|x4@2 x1*x2*x3)` fits a model with all main effects, all two-way interactions, and one three-way interaction. Variables specified with the CLASS expansion can be either character or numeric; numeric variables should be discrete. See the section “ANOVA Codings” on page 8270 for more information about CLASS variables. See the section “Model Statement Usage” on page 8220 for information about how to use the operators @, \*, and | in PROC TRANSREG.

**EPOINT****EPO**

expands the variables for an elliptical response surface regression or for an elliptical ideal point regression. Specify the **COORDINATES** *o-option* to output PREFMAP ideal elliptical point model coordinates to the **OUT=** data set. Each axis of the ellipse (or ellipsoid) is oriented in the same direction as one of the variables. The EPOINT expansion creates a new variable for each original variable. The value of each new variable is the square of each observed value for the corresponding original variable. The regression analysis then uses both sets of variables (original and squared). Variables specified with the EPOINT expansion must be numeric, and they are typically continuous. See the section “**Point Models**” on page 8294 and **Example 97.6** for more information about point models.

**POINT****POI**

expands the variables for a circular response surface regression or for a circular ideal point regression. Specify the **COORDINATES** *o-option* to output PREFMAP ideal point model coordinates to the **OUT=** data set. The POINT expansion creates a new variable having a value for each observation that is the sum of squares of all the POINT variables. This new variable is added to the set of variables and is used in the regression analysis. For more information about ideal point regression, see Carroll (1972). Variables specified with the POINT expansion must be numeric, and they are typically continuous. See the section “**Point Models**” on page 8294 and **Example 97.6** for more information about point models.

**PSPLINE****PSP**

expands each variable to a piecewise polynomial basis. You can specify the **DEGREE=**, **KNOTS=**, **NKNOTS=**, and **EVENLY** *t-options* with PSPLINE. When **DEGREE=n** (3 by default) with *k* knots (0 by default),  $n + k$  variables are created. In addition, the original variable appears in the **OUT=** data set before the **ID** variables. For example, **pspline(x / nknots=1)** expands *x* into  $x_1$   $x_2$   $x_3$   $x_4$  and outputs *x* as well. Unlike BSPLINE, an intercept is not implicit in the columns of PSPLINE. Variables specified with the PSPLINE expansion must be numeric, and they are typically continuous. See the sections “**SPLINE, BSPLINE, and PSPLINE Comparisons**” on page 8302 and “**Using Splines and Knots**” on page 8233 for more information about splines. Also see Smith (1979) for a good introduction to piecewise polynomial splines.

**QPOINT****QPO**

expands the variables for a quadratic response surface regression or for a quadratic ideal point regression. Specify the **COORDINATES** *o-option* to output PREFMAP quadratic ideal point model coordinates to the **OUT=** data set. For *m* QPOINT variables,  $m(m + 1)/2$  new variables are created containing the squares and crossproducts of the original variables. The regression analysis uses both sets (original and crossed). Variables specified with the QPOINT expansion must be numeric, and they are typically continuous. See the section “**Point Models**” on page 8294 and **Example 97.6** for more information about point models.

## Nonoptimal Transformations

The nonoptimal transformations, like the variable expansions, are computed before the iterative algorithm begins. Nonoptimal transformations create a single new transformed variable that replaces the original variable. The new variable is not transformed by the subsequent iterative algorithms (except for a possible linear transformation with missing value estimation). The following list provides syntax and details for nonoptimal variable transformations.

### ARSIN

#### ARS

finds an inverse trigonometric sine transformation. Variables specified in the ARSIN *transform* must be numeric and in the interval  $(-1.0 \leq x \leq 1.0)$ , and they are typically continuous.

### EXP

exponentiates variables ( $x$  is transformed to  $a^x$ ). To specify the value of  $a$ , use the **PARAMETER=** *t-option*. By default,  $a$  is the mathematical constant  $e = 2.718\dots$ . Variables specified with the EXP *transform* must be numeric, and they are typically continuous.

### LOG

transforms variables to logarithms ( $x$  is transformed to  $\log_a(x)$ ). To specify the base of the logarithm, use the **PARAMETER=** *t-option*. The default is a natural logarithm with base  $e = 2.718\dots$ . Variables specified with the LOG *transform* must be numeric and positive, and they are typically continuous.

### LOGIT

finds a logit transformation on the variables. The logit of  $x$  is  $\log(x/(1-x))$ . Unlike other transformations, LOGIT does not have a three-letter abbreviation. Variables specified with the LOGIT *transform* must be numeric and in the interval  $(0.0 < x < 1.0)$ , and they are typically continuous.

### POWER

#### POW

raises variables to a specified power ( $x$  is transformed to  $x^a$ ). You must specify the power parameter  $a$  by specifying the **PARAMETER=** *t-option* following the variables. Here is an example:

```
power(variable / parameter=number)
```

You can use POWER for squaring variables (PARAMETER=2), reciprocal transformations (PARAMETER=-1), square roots (PARAMETER=0.5), and so on. Variables specified with the POWER *transform* must be numeric, and they are typically continuous.

### RANK

#### RAN

transforms variables to ranks. Ranks are averaged within ties. The smallest input value is assigned the smallest rank. Variables specified in the RANK *transform* must be numeric.

## Nonlinear Fit Transformations

Nonlinear fit transformations, like nonoptimal transformations, are computed before the iterative algorithm begins. Nonlinear fit transformations create a single new transformed variable that replaces the original variable and provides one or more smooth functions through a scatter plot. The new variable is not transformed by the subsequent iterative algorithms. The nonlinear fit transformations, unlike the nonoptimal

transformations, use information in the other variables in the model to find the transformations. The nonlinear fit transformations, unlike the optimal transformations, do not minimize a squared-error criterion. The following list provides syntax and details for nonoptimal variable transformations.

## BOXCOX

### BOX

finds a Box-Cox (1964) transformation of the specified variables. The BOXCOX transformation can be used only with dependent variables. The `ALPHA=`, `CLL=`, `CONVENIENT`, `GEOMETRICMEAN`, `LAMBDA=`, and `PARAMETER=` *t-options* can be used with the BOXCOX transformation. Variables specified in the BOXCOX *transform* must be numeric, and they are typically continuous. See the section “[Box-Cox Transformations](#)” on page 8222 and [Example 97.2](#) for more information about Box-Cox transformations.

## PBSPLINE

### PBS

is a noniterative penalized B-spline transformation (Eilers and Marx 1996). The PBSPLINE transformation can be used only with independent variables. By default with PBSPLINE, a cubic spline is fit with 100 evenly spaced knots, three evenly spaced exterior knots, and a difference matrix of order three (`DEGREE=3` `NKNOTS=100` `EVENLY=3` `PARAMETER=3`). Variables specified in the PBSPLINE *transform* must be numeric, and they are typically continuous. See the section “[Penalized B-Splines](#)” on page 8260 and [Example 97.3](#) for more information about penalized B-splines.

## SMOOTH

### SMO

is a noniterative smoothing spline transformation (Reinsch 1967). You can specify the smoothing parameter with either the `SM=` or the `PARAMETER=` *t-option*. The default smoothing parameter is `SM=0`. The SMOOTH transformation can be used only with independent variables. Variables specified with the SMOOTH *transform* must be numeric, and they are typically continuous. See the sections “[Smoothing Splines](#)” on page 8263 and “[Smoothing Splines Changes and Enhancements](#)” on page 8267 for more information about smoothing splines.

## Optimal Transformations

Optimal transformations are iteratively derived. Missing values for these types of variables can be optimally estimated (see the section “[Missing Values](#)” on page 8289). The following list provides syntax and details for optimal transformations.

## LINEAR

### LIN

finds an optimal linear transformation of each variable. For variables with no missing values, the transformed variable is the same as the original variable. For variables with missing values, the transformed nonmissing values have a different scale and origin than the original values. Variables specified in the LINEAR *transform* must be numeric. See the section “[OPSCORE, MONOTONE, UNTIE, and LINEAR Transformations](#)” on page 8298 for more information about optimal scaling.



**MONOTONE****MON**

finds a monotonic transformation of each variable, with the restriction that ties are preserved. The Kruskal (1964) secondary least squares monotonic transformation is used. This transformation weakly preserves order and category membership (ties). Variables specified with the **MONOTONE** *transform* must be numeric, and they are typically discrete. See the section “**OPSCORE, MONOTONE, UNTIE, and LINEAR Transformations**” on page 8298 for more information about optimal scaling.

**MSPLINE****MSP**

finds a monotonically increasing B-spline transformation with monotonic coefficients (de Boor 1978; de Leeuw 1986) of each variable. You can specify the **DEGREE=**, **KNOTS=**, **NKNOTS=**, and **EVENLY=** *t-options* with **MSPLINE**. By default, PROC TRANSREG fits a quadratic spline with no knots. Variables specified with the **MSPLINE** *transform* must be numeric, and they are typically continuous. See the section “**SPLINE and MSPLINE Transformations**” on page 8300 for more information about monotone splines.

**OPSCORE****OPS**

finds an optimal scoring of each variable. The **OPSCORE** transformation assigns scores to each class (level) of the variable. The Fisher (1938) optimal scoring method is used. Variables specified with the **OPSCORE** *transform* can be either character or numeric; numeric variables should be discrete. See the sections “**Character OPSCORE Variables**” on page 8293 and “**OPSCORE, MONOTONE, UNTIE, and LINEAR Transformations**” on page 8298 for more information about optimal scaling.

**SPLINE****SPL**

finds a B-spline transformation (de Boor 1978) of each variable. By default, PROC TRANSREG fits a cubic spline with no knots. You can specify the **DEGREE=**, **KNOTS=**, **NKNOTS=**, and **EVENLY=** *t-options* with **SPLINE**. Variables specified with the **SPLINE** *transform* must be numeric, and they are typically continuous. See the sections “**SPLINE and MSPLINE Transformations**” on page 8300, “**Specifying the Number of Knots**” on page 8301, and “**SPLINE, BSPLINE, and PSPLINE Comparisons**” on page 8302, and “**Using Splines and Knots**” on page 8233 for more information about splines.

**UNTIE****UNT**

finds a monotonic transformation of each variable without the restriction that ties are preserved. PROC TRANSREG uses the Kruskal (1964) primary least squares monotonic transformation method. This transformation weakly preserves order but not category membership (it might untie some previously tied values). Variables specified with the **UNTIE** *transform* must be numeric, and they are typically discrete. See the section “**OPSCORE, MONOTONE, UNTIE, and LINEAR Transformations**” on page 8298 for more information about optimal scaling.



## Other Transformations

### IDENTITY

#### IDE

specifies variables that are not changed by the iterations. Typically, the IDENTITY transformation is used with a simple variable list, such as `identity(x1-x5)`. However, you can also specify interaction terms. For example, `identity(x1 | x2)` creates  $x_1$ ,  $x_2$ , and the product  $x_1*x_2$ ; and `identity(x1 | x2 | x3)` creates  $x_1$ ,  $x_2$ ,  $x_1*x_2$ ,  $x_3$ ,  $x_1*x_3$ ,  $x_2*x_3$ , and  $x_1*x_2*x_3$ . See the section “Model Statement Usage” on page 8220 for information about how to use the operators @, \*, and | in PROC TRANSREG. Variables specified in the IDENTITY *transform* must be numeric.

The IDENTITY transformation is used for variables when no transformation and no missing data estimation are desired. However, the REFLECT *t-option*, the ADDITIVE *a-option*, and the TSTANDARD=Z, and TSTANDARD=CENTER options can linearly transform all variables, including IDENTITY variables, after the iterations. Observations with missing values in IDENTITY variables are excluded from the analysis, and no optimal scores are computed for missing values in IDENTITY variables.

### SSPLINE

#### SSP

finds an iterative smoothing spline transformation of each variable. The SSPLINE transformation does not generally minimize squared error. You can specify the smoothing parameter with either the SM= *t-option* or the PARAMETER= *t-option*. The default smoothing parameter is SM=0. Variables specified with the SSPLINE *transform* must be numeric, and they are typically continuous.

## Transformation Options (t-options)

If you use a nonoptimal, nonlinear fit, optimal, or other transformation, you can use *t-options*, which specify additional details of the transformation. The *t-options* are specified within the parentheses that enclose variables and are listed after a slash. You can use *t-options* with both the dependent and the independent variables. Here is an example of using just one *t-option*:

```
proc transreg;
 model identity(y)=spline(x / nknots=3);
 output;
run;
```

The preceding statements find an optimal variable transformation (SPLINE) of the independent variable, and they use a *t-option* to specify the number of knots (NKNOTS=). The following is a more complex example:

```
proc transreg;
 model mspline(y / nknots=3)=class(x1 x2 / effects);
 output;
run;
```

These statements find a monotone spline transformation (MSPLINE with three knots) of the dependent variable and perform a CLASS expansion with effects coding of the independents.

Table 97.3 summarizes the *t-options* available in the MODEL statement.

**Table 97.3** Transformation Options

| Option                           | Description                                     |
|----------------------------------|-------------------------------------------------|
| <b>Nonoptimal Transformation</b> |                                                 |
| ORIGINAL                         | Uses original mean and variance                 |
| <b>Parameter Specification</b>   |                                                 |
| PARAMETER=                       | Specifies miscellaneous parameters              |
| SM=                              | Specifies smoothing parameter                   |
| <b>Penalized B-Spline</b>        |                                                 |
| AIC                              | Uses Akaike's information criterion             |
| AICC                             | Uses corrected AIC                              |
| CV                               | Uses cross validation criterion                 |
| GCV                              | Uses generalized cross validation criterion     |
| LAMBDA=                          | Specifies smoothing parameter list or range     |
| RANGE                            | Specifies a LAMBDA= range, not a list           |
| SBC                              | Uses Schwarz's Bayesian criterion               |
| <b>Spline</b>                    |                                                 |
| DEGREE=                          | Specifies the degree of the spline              |
| EVENLY=                          | Spaces the knots evenly                         |
| EXKNOTS=                         | Specifies exterior knots                        |
| KNOTS=                           | Specifies the interior knots or break points    |
| NKNOTS=                          | Creates <i>n</i> knots                          |
| <b>CLASS Variable</b>            |                                                 |
| CPREFIX=                         | Specifies CLASS coded variable name prefix      |
| DEVIATIONS                       | Specifies a deviations-from-means coding        |
| EFFECTS                          | Specifies a deviations-from-means coding        |
| LPREFIX=                         | Specifies CLASS coded variable label prefix     |
| ORDER=                           | Specifies order of CLASS variable levels        |
| ORTHOGONAL                       | Specifies an orthogonal-contrast coding         |
| SEPARATORS=                      | Specifies CLASS coded variable label separators |
| STANDORTH                        | Specifies a standardized-orthogonal coding      |
| ZERO=                            | Controls reference levels                       |
| <b>Box-Cox</b>                   |                                                 |
| ALPHA=                           | Specifies confidence interval alpha             |
| CLL=                             | Specifies convenient lambda list                |
| CONVENIENT                       | Uses a convenient lambda                        |
| GEOMETRICMEAN                    | Scales transformation using geometric mean      |
| LAMBDA=                          | Specifies power parameter list                  |

Table 97.3 continued

| Option                 | Description                                    |
|------------------------|------------------------------------------------|
| <b>Other t-options</b> |                                                |
| AFTER                  | Specifies operations occur after the expansion |
| CENTER                 | Specifies center before the analysis begins    |
| NAME=                  | Renames variables                              |
| REFLECT                | Reflects the variable around the mean          |
| TSTANDARD=             | Specifies transformation standardization       |
| Z                      | Standardizes before the analysis begins        |

The following sections discuss the *t-options* available for nonoptimal, nonlinear fit, optimal, and other transformations.

### Nonoptimal Transformation t-options

#### ORIGINAL

#### ORI

matches the variable's final mean and variance to the mean and variance of the original variable. By default, the mean and variance are based on the transformed values. The ORIGINAL *t-option* is available for all of the nonoptimal transformations.

### Parameter t-options

#### PARAMETER=*number*

#### PAR=*number*

specifies the transformation parameter. The PARAMETER= *t-option* is available for the BOXCOX, EXP, LOG, POWER, SMOOTH, SSPLINE, and PBSPLINE transformations. For BOXCOX, the parameter is the value to add to each value of the variable before a Box-Cox transformation. For EXP, the parameter is the value to be exponentiated; for LOG, the parameter is the base value; and for POWER, the parameter is the power. For SMOOTH and SSPLINE, the parameter is the raw smoothing parameter. (See the SM= option for an alternative way to specify the smoothing parameter.) The default for the PARAMETER= *t-option* for the BOXCOX transformation is 0 and for the LOG and EXP transformations is  $e = 2.718\dots$ . The default parameter for SMOOTH and SSPLINE is computed from SM=0. For the POWER transformation, you must specify the PARAMETER= *t-option*; there is no default. For PBSPLINE, the parameter is the order of the difference matrix, which provides some control over the smoothness of the transformation. The default order parameter with PBSPLINE is the maximum of the DEGREE= *t-option*, and 1. With PBSPLINE, the default is DEGREE=3 and PARAMETER=3, which works well for most problems.

#### SM=*n*

specifies a smoothing parameter in the range 0 to 100, just like PROC GLOT uses. For example, SM=50 in PROC TRANSREG is equivalent to I=SM50 in the SYMBOL statement with PROC GLOT. You can specify the SM= *t-option* only with the SMOOTH and SSPLINE transformations. The smoothness of the function increases as the value of the smoothing parameter increases. By default, SM=0.

## Spline t-options

The following *t-options* are available with the **SPLINE**, **MSPLINE** and **PBSPLINE** transformations and with the **PSPLINE** and **BSPLINE** expansions.

### **DEGREE=*n***

#### **DEG=*n***

specifies the degree of the spline transformation. The degree must be a nonnegative integer. The defaults are **DEGREE=3** for **SPLINE**, **PSPLINE**, and **BSPLINE** variables and **DEGREE=2** for **MSPLINE** variables.

The polynomial degree should be a small integer, usually 0, 1, 2, or 3. Larger values are rarely useful. If you have any doubt as to what degree to specify, use the default.

### **EVENLY<=*n*>**

#### **EVE<=*n*>**

is used with the **NKNOTS=** *t-option* to space the knots evenly. The differences between adjacent knots are constant.

If you specify **NKNOTS=*k*** and **EVENLY**, *k* knots are created at

$$\text{minimum} + i((\text{maximum} - \text{minimum}) / (k + 1))$$

for  $i = 1, \dots, k$ . Here is an example:

```
spline(x / nknots=2 evenly)
```

When the variable *x* has a minimum of 4 and a maximum of 10, then the two interior knots are 6 and 8. Without the **EVENLY** *t-option*, the **NKNOTS=** *t-option* places knots at percentiles, so the knots are not evenly spaced. By default for the **BSPLINE** expansion and the **SPLINE** and **MSPLINE** transformations, the smaller exterior knots are all the same and all just a little smaller than the minimum. Similarly, by default, the larger exterior knots are all the same and all just a little larger than the maximum. However, if you specify **EVENLY=*n***, then the *n* exterior knots are evenly spaced as well. The number of exterior knots must be greater than or equal to the degree. You can specify values larger than the degree when you want to interpolate slightly beyond the range or your data. The exterior knots must be less than the minimum or greater than the maximum; hence the knots across all sets are not precisely equally spaced. For example, with data ranging from 0 to 10, and with **EVENLY=3** and **NKNOTS=4**, the first exterior knots are  $-4.000000000001$ ,  $-2.000000000001$ , and  $-0.000000000001$ , the interior knots are 2, 4, 6, and 8, and the second exterior knots are  $10.000000000001$ ,  $12.000000000001$ , and  $14.000000000001$ .

With the **BSPLINE** and **PSPLINE** expansions and the **SPLINE** and **MSPLINE** transformations, evenly spaced knots are not the default. With the **PBSPLINE** transformation, evenly spaced interior and exterior knots are the default. If you want unevenly spaced knots with **PBSPLINE**, you must use the **KNOTS=** *t-option*.

### **EXKNOTS=number-list**

#### **EXK=number-list**

specifies exterior knots for **SPLINE** and **MSPLINE** transformations and **BSPLINE** expansions. Usually, this *t-option* is not needed; PROC TRANSREG automatically picks suitable exterior knots. The only time you need to use this option is when you want to ensure that the exact same basis is used for

different splines, such as when you apply coefficients from one spline transformation to a variable in a different data set (see the section “[Scoring Spline Variables](#)” on page 8245).

Specify one or two values. If the minimum EXKNOTS= value is less than the minimum data value, it is used as the exterior knot. If the maximum EXKNOTS= value is greater than the maximum data value, it is used as the exterior knot. Otherwise these values are ignored. When EXKNOTS= is specified with the [CENTER](#) or [Z](#) *t-options*, the knots apply to the original variable, not to the centered or standardized variable.

The B-spline transformations and expansions use a knot list consisting of exterior knots (values just smaller than the minimum), the specified (interior) knots, and exterior knots (values just larger than the minimum). You can use the [DETAIL](#) *a-option* to see all of these knots. If you use different exterior knots, you get different but equivalent B-spline bases. You can specify exterior knots in either the [KNOTS=](#) or [EXKNOTS=](#) *t-options*; however, for the [BSPLINE](#) expansion, the [KNOTS=](#) *t-option* creates extra all-zero basis columns, whereas the [EXKNOTS=](#) *t-option* gives you the correct basis. See the [EVENLY=](#) *t-option* for an alternative way to specify exterior knots.

**KNOTS=***number-list* | *n* TO *m* BY *p*

**KNO=***number-list* | *n* TO *m* BY *p*

specifies the interior knots or break points. By default, there are no knots. The first time you specify a value in the knot list, it indicates a discontinuity in the *n*th (from [DEGREE=\*n\*](#)) derivative of the transformation function at the value of the knot. The second mention of a value indicates a discontinuity in the (*n* – 1) derivative of the transformation function at the value of the knot. Knots can be repeated any number of times for decreasing smoothness at the break points, but the values in the knot list can never decrease.

You cannot use the [KNOTS=](#) *t-option* with the [NKNOTS=](#) *t-option*. You should keep the number of knots small (see the section “[Specifying the Number of Knots](#)” on page 8301).

**NKNOTS=***n*

**NKN=***n*

creates *n* knots, the first at the 100/(*n* + 1) percentile, the second at the 200/(*n* + 1) percentile, and so on. Knots are always placed at data values; there is no interpolation. For example, if [NKNOTS=3](#), knots are placed at the 25th percentile, the median, and the 75th percentile. You can use the [EVENLY=](#) *t-option* along with [NKNOTS=](#) to get evenly spaced knots. By default, with the [BSPLINE](#) and [PSPLINE](#) expansions and the [SPLINE](#) and [MSPLINE](#) transformations, [NKNOTS=0](#). By default, with the [PBSPLINE](#) transformation, [NKNOTS=100](#).

The value specified for the [NKNOTS=](#) *t-option* must be  $\geq 0$ .

You cannot use the [NKNOTS=](#) *t-option* with the [KNOTS=](#) *t-option*.

You should keep the number of knots small (see the section “[Specifying the Number of Knots](#)” on page 8301).

## Penalized B-Spline *t-options*

The following *t-options* are available with the [PBSPLINE](#) transformation.

**AIC**

specifies that the procedure should select the smoothing parameter,  $\lambda$ , that minimizes the (Akaike 1973) information criterion (AIC). By default, the (AICC) criterion is minimized.

**AICC**

specifies that the procedure should select the smoothing parameter,  $\lambda$ , that minimizes the corrected Akaike information criterion (Hurvich, Simonoff, and Tsai 1998). This is the default criterion unless the **AIC**, **CV**, **GCV**, or **SBC** *t-option* is specified.

**CV**

specifies that the procedure should select the smoothing parameter,  $\lambda$ , that minimizes the cross validation criterion (CV). By default, the (AICC) criterion is minimized.

**GCV**

specifies that the procedure should select the smoothing parameter,  $\lambda$ , that minimizes the generalized cross validation criterion (Craven and Wahba 1979). By default, the (AICC) criterion is minimized.

**LAMBDA=***number-list*

**LAM=***number-list*

specifies a list of penalized B-spline smoothing parameters. By default, PROC TRANSREG considers lambdas in the range 0 to 1E6. Alternatively, you can specify the **RANGE** *t-option* with **LAMBDA=**, such as **LAMBDA=1E3 1E5 RANGE**, to only consider lambdas in a narrower range. Note that the algorithm might not actually evaluate the criterion at the minimum and maximum if it does not have to. In particular, it avoids evaluating the criterion at **LAMBDA=0** (no smoothing) unless it is the only **LAMBDA=** value specified. You can also specify a list of lambdas, such as **LAMBDA=1 TO 10**, and the procedure selects the best lambda from the list. In all cases, the lambda that minimizes the specified criterion (or **AICC** by default) is chosen.

**RANGE****RAN**

specifies that the **LAMBDA=** *t-option* specifies two lambdas that define a range of values, from which an optimal lambda is selected. By default, PROC TRANSREG considers lambdas in the range 0 to 1E6.

**SBC**

specifies that the procedure should select the smoothing parameter,  $\lambda$ , that minimizes Schwarz's Bayesian criterion (Schwarz 1978; Judge et al. 1980). By default, the (AICC) criterion is minimized.

**Class Variable t-options**

**CPREFIX=***n* | *number-list*

**CPR=***n* | *number-list*

specifies the number of first characters of a **CLASS** expansion variable's name to use in constructing names for coded variables. When you specify **CPREFIX=** as an *a-option* or an *o-option*, it specifies the default for all **CLASS** variables. When you specify **CPREFIX=** as a *t-option*, it overrides the default only for selected variables. A different **CPREFIX=** value can be specified for each **CLASS** variable by specifying the **CPREFIX=number-list** *t-option*, like the **ZERO=formatted-value** *t-option*.

**DEVIATIONS****DEV**

requests a deviations-from-means coding of **CLASS** variables. The coded design matrix has values of 0, 1, and -1 for reference levels. This coding is referred to as “deviations-from-means,” “effects,” “center-point,” or “full-rank” coding. For example, here is the coding for two-, three-, four-, and five-level factors:

|   | Number of Levels |       |    |      |    |    |      |    |    |
|---|------------------|-------|----|------|----|----|------|----|----|
|   | Two              | Three |    | Four |    |    | Five |    |    |
| a | 1                | 1     | 0  | 1    | 0  | 0  | 1    | 0  | 0  |
| b | -1               | 0     | 1  | 0    | 1  | 0  | 0    | 1  | 0  |
| c |                  | -1    | -1 | 0    | 0  | 1  | 0    | 0  | 1  |
| d |                  |       |    | -1   | -1 | -1 | 0    | 0  | 0  |
| e |                  |       |    |      |    |    | -1   | -1 | -1 |

**EFFECTS****EFF**

See the **DEVIATIONS** *t-option*.

**LPREFIX=*n*** | *number-list*

**LPR=*n*** | *number-list*

specifies the number of first characters of a **CLASS** expansion variable’s label (or name if no label is specified) to use in constructing labels for the coded variables. When you specify **LPREFIX=** as an *a-option* or an *o-option*, it specifies the default for all **CLASS** variables. When you specify **LPREFIX=** as a *t-option*, it overrides the default only for selected variables. A different **LPREFIX=** value can be specified for each **CLASS** variable by specifying the **LPREFIX=number-list** *t-option*, like the **ZERO=formatted-value** *t-option*.

**ORDER=DATA** | **FREQ** | **FORMATTED** | **INTERNAL**

**ORD=DAT** | **FRE** | **FOR** | **INT**

specifies the order in which the **CLASS** variable levels are to be reported. The default is **ORDER=INTERNAL**. For **ORDER=FORMATTED** and **ORDER=INTERNAL**, the sort order is machine dependent. When you specify **ORDER=** as an *a-option* or an *o-option*, it specifies the default ordering for all **CLASS** variables. When you specify **ORDER=** as a *t-option*, it overrides the default ordering only for selected variables. You can specify a different **ORDER=** value for each **CLASS** specification.

**ORTHOGONAL****ORT**

requests an orthogonal-contrast coding of **CLASS** variables. For example, here is the orthogonal-contrast coding for two-, three-, four-, and five-level factors:

|   | Number of Levels |       |    |      |    |    |      |    |    |
|---|------------------|-------|----|------|----|----|------|----|----|
|   | Two              | Three |    | Four |    |    | Five |    |    |
| a | 1                | 1     | -1 | 1    | -1 | -1 | 1    | -1 | -1 |
| b | -1               | 0     | 2  | 0    | 2  | -1 | 0    | 2  | -1 |
| c |                  | -1    | -1 | 0    | 0  | 3  | 0    | 0  | 3  |
| d |                  |       |    | -1   | -1 | -1 | 0    | 0  | 0  |
| e |                  |       |    |      |    |    | -1   | -1 | -1 |

The sum of the coded values within each column is zero, all columns within a factor are orthogonal, and the *i*th column represents a contrast between the *i*th level and the combination of all preceding



levels and the last level. The  $X$  matrix is orthogonal and  $X'X$  is diagonal with this coding only if the experimental design is orthogonal.

**SEPARATORS=**'string-1' < 'string-2' >

**SEP=**'string-1' < 'string-2' >

specifies separators for creating **CLASS** expansion variable labels. By default, SEPARATORS=' ' \* ' ("blank" and "blank asterisk blank"). When you specify SEPARATORS= as an *a-option* or an *o-option*, it specifies the default separators for all **CLASS** variables. When you specify SEPARATORS= as a *t-option*, it overrides the default only for selected variables. You can specify a different SEPARATORS= value for each **CLASS** specification.

## STANDORTH

### STA

### ORTHEFFECT

requests a standardized-orthogonal coding of **CLASS** variables. For example, here is the standardized-orthogonal coding for two-, three-, four-, and five-level factors:

|   | Number of Levels |       |       |       |       |       |       |       |       |       |
|---|------------------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
|   | Two              | Three |       | Four  |       |       | Five  |       |       |       |
| a | 1                | 1.22  | -0.71 | 1.41  | -0.82 | -0.58 | 1.58  | -0.91 | -0.65 | -0.50 |
| b | -1               | 0.00  | 1.41  | 0.00  | 1.63  | -0.58 | 0.00  | 1.83  | -0.65 | -0.50 |
| c |                  | -1.22 | -0.71 | 0.00  | 0.00  | 1.73  | 0.00  | 0.00  | 1.94  | -0.50 |
| d |                  |       |       | -1.41 | -0.82 | -0.58 | 0.00  | 0.00  | 0.00  | 2.00  |
| e |                  |       |       |       |       |       | -1.58 | -0.91 | -0.65 | -0.50 |

The sum of the coded values within each column is zero, the sum of squares of the coded values within each column is equal to the number of levels, all columns within a factor are orthogonal, and the *i*th column represents a contrast between the *i*th level and the combination of all preceding levels and the last level. The  $X$  matrix is orthogonal and  $X'X$  is diagonal ( $X'X = nI$ , the number of observations times an identity matrix) with this coding only if the experimental design is orthogonal.

**ZERO=FIRST | LAST | NONE | SUM**

**ZER=FIR | LAS | NON | SUM**

**ZERO=**'formatted-value' < 'formatted-value' ... >

is used with **CLASS** variables. The default is ZERO=LAST.

The specification CLASS(variable / ZERO=FIRST) sets to missing the coded variable for the first of the sorted categories, implying a zero coefficient for that category.

The specification CLASS(variable / ZERO=LAST) sets to missing the coded variable for the last of the sorted categories, implying a zero coefficient for that category.

The specification CLASS(variable / ZERO='formatted-value') sets to missing the coded variable for the category with a formatted value that matches 'formatted-value', implying a zero coefficient for that category. With ZERO=formatted-value, the first formatted value applies to the first variable in the specification, the second formatted value applies to the next variable that was not previously mentioned, and so on. For example, `class(a a*b b b*c c / zero='x' 'y' 'z')` specifies that the reference level for a is 'x', for b is 'y', and for c is 'z'. With ZERO='formatted-value', the procedure first looks for exact matches between the formatted values and the specified value. If none are found, leading blanks are stripped from both and the values are compared again. If zero or two or more matches are found, warnings are issued.



The specifications ZERO=FIRST, ZERO=LAST, and ZERO='formatted-value' are used for reference cell models. The Intercept parameter estimate is the marginal mean for the reference cell, and the other marginal means are obtained by adding the intercept to the coded variable coefficients.

The specification CLASS(variable / ZERO=NONE) sets to missing none of the coded variables. The columns of the expansion sum to a column of ones, so an implicit intercept model is fit. If you specify ZERO=NONE for more than one variable, the model is less than full rank. In the model `model identity(y) = class(x / zero=none)`, the coefficients are cell means.

The specification CLASS(variable / ZERO=SUM) sets to missing none of the coded variables, and the coefficients for the coded variables created from the variable sum to 0. This creates a less-than-full-rank model, but the coefficients are uniquely determined due to the sum-to-zero constraint.

In the presence of iterative transformations, hypothesis tests for ZERO=NONE and ZERO=SUM levels are not exact; they are liberal because a model with an explicit intercept is fit inside the iterations. There is no provision for adjusting the transformations while setting to 0 a parameter that is redundant given the explicit intercept and the other parameters.

## Box-Cox t-options

The following *t-options* are available only with the BOXCOX transformation of the dependent variable (see the section “Box-Cox Transformations” on page 8222 and Example 97.2).

### ALPHA= $\rho$

#### ALP= $\rho$

specifies the Box-Cox alpha for the confidence interval for the power parameter. By default, ALPHA=0.05.

### CLL=*number-list*

specifies the Box-Cox convenient lambda list. When the confidence interval for the power parameter includes one of the values in this list, PROC TRANSREG reports it and can optionally use the convenient power parameter instead of the more optimal power parameter. The default is CLL=1.0 0.0 0.5 -1.0 -0.5 2.0 -2.0 3.0 -3.0. By default, a linear transformation is preferred over log, square root, inverse, inverse square root, quadratic, inverse quadratic, cubic, and inverse cubic. If you specify the CONVENIENT *t-option*, then PROC TRANSREG uses the first convenient power parameter in the list that is in the confidence interval. For example, if the optimal power parameter is 0.25 and 0.0 is in the confidence interval but not 1.0, then the convenient power parameter is 0.0.

### CONVENIENT

#### CON

specifies that a power parameter from the CLL= *t-option* list is to be used for the final transformation instead of the LAMBDA= *t-option* value if a CLL= value is in the confidence interval. See the CLL= *t-option* for more information about its usage.

### GEOMETRICMEAN

#### GEO

divides the Box-Cox transformation by  $\bar{y}^{\lambda-1}$ , where  $\bar{y}$  is the geometric mean of the variable to be transformed. This form of the Box-Cox transformation essentially converts the transformation back to original units, and hence it permits direct comparison of the residual sums of squares for models with different power parameters.

**LAMBDA=***number-list*

**LAM=***number-list*

specifies a list of Box-Cox power parameters. The default is LAMBDA=−3 TO 3 BY 0.25. PROC TRANSREG tries each power parameter in the list and picks the best one. However, when the **CONVENIENT** *t-option* is specified, PROC TRANSREG chooses a convenient value from the confidence interval instead of the optimal value. For example, if the optimal power parameter is 0.25 and 0.0 is in the confidence interval but not 1.0, then the convenient power parameter 0.0 (log transformation) is chosen instead of the more optimal parameter 0.25. See the **CLL=** *t-option* for more information about its usage.

## Other t-options

**AFTER**

**AFT**

requests that certain operations occur after the expansion. This *t-option* affects the **NKNOTS=** *t-option* when the **SPLINE** or **MSPLINE** transformation is crossed with a **CLASS** specification. For example, if the original spline variable (1 2 3 4 5 6 7 8 9) is expanded into the three variables (1 2 3 0 0 0 0 0 0), (0 0 0 4 5 6 0 0 0), and (0 0 0 0 0 0 7 8 9), then, by default, **NKNOTS=1** would use the overall median of 5 as the knot for all three variables. When you specify the **AFTER** *t-option*, the knots for the three variables are 2, 5, and 8. Note that the structural zeros are ignored when the internal knot list is created, but they are not ignored for the exterior knots.

You can also specify the **AFTER** *t-option* with the **RANK**, **SMOOTH**, and **PBSPLINE** transformations. The following specifications compute ranks and smooth transformations within groups, after crossing, ignoring the structural zeros:

```
class(x / zero=none) | rank(z / after)
class(x / zero=none) | smooth(z / after)
```

**CENTER**

**CEN**

centers the variables before the analysis begins (in contrast to the **TSTANDARD=CENTER** option, which centers after the analysis ends). The **CENTER** *t-option* can be used instead of running PROC STANDARD before PROC TRANSREG (see the section “Centering” on page 8336). When the **KNOTS=** *t-option* is specified with **CENTER**, the knots apply to the original variable, not to the centered variable. PROC TRANSREG centers the knots.

**NAME=***(variable-list)*

**NAM=***(variable-list)*

renames variables as they are used in the MODEL statement. This *t-option* lets you use a variable more than once.

For example, if x is a character variable, then the following step stores both the original character variable x and a numeric variable xc that contains category numbers in the **OUT=** data set:

```
proc transreg data=a;
 model identity(y) = opscore(x / name=(xc));
 output;
 id x;
run;
```

With the **CLASS** and **IDENTITY** transformations, which can contain interaction effects, the first name applies to the first variable in the specification, the second name applies to the next variable that was not previously mentioned, and so on. For example, `identity(a a * b b b * c c / name=(g h i))` specifies that the new name for **a** is **g**, for **b** is **h**, and for **c** is **i**. The same assignment is used for the (not useful) specification `identity(a a b b c c / name=(g h i))`. For all *transforms* other than **CLASS** and **IDENTITY** (all those in which interactions are not supported), repeated variables are not handled specially. For example, `spline(a a b b c c / name=(a g b h c i))` creates six variables: a copy of **a** named **a**, another copy of **a** named **g**, a copy of **b** named **b**, another copy of **b** named **h**, a copy of **c** named **c**, and another copy of **c** named **i**.

**REFLECT****REF**

reflects the transformation

$$y = -(y - \bar{y}) + \bar{y}$$

after the iterations are completed and before the final standardization and results calculations. This *t-option* is particularly useful with the dependent variable in a conjoint analysis. When the dependent variable consists of ranks with the most preferred combination assigned 1.0, the **REFLECT** *t-option* reflects the transformation so that positive utilities mean high preference. (See [Example 97.4](#).)

**TSTANDARD=CENTER | NOMISS | ORIGINAL | Z****TST=CEN | NOM | ORI | Z**

specifies the standardization of the transformed variables for the hypothesis tests and in the **OUT=** data set (see the section “[Centering](#)” on page 8336). By default, **TSTANDARD=ORIGINAL**. When you specify **TSTANDARD=** as an *a-option* or an *o-option*, it determines the default standardization for all variables. When you specify **TSTANDARD=** as a *t-option*, it overrides the default standardization only for selected variables. You can specify a different **TSTANDARD=** value for each transformation. For example, to perform a redundancy analysis with standardized dependent variables, specify the following:

```
model identity(y1-y4 / tstandard=z) = identity(x1-x10);
```

**Z**

centers and standardizes the variables to variance one before the analysis begins (in contrast to the **TSTANDARD=Z** option, which standardizes after the analysis ends). The **Z** *t-option* can be used instead of running **PROC STANDARD** before **PROC TRANSREG** (see the section “[Centering](#)” on page 8336). When the **KNOTS=** *t-option* is specified with **Z**, the knots apply to the original variable, not to the standardized variable. **PROC TRANSREG** standardizes the knots.

**Algorithm Options (a-options)**

This section discusses the options that can appear in the **PROC TRANSREG** or **MODEL** statement as *a-options*. They are listed after the entire model specification and after a slash. Here is an example:

```

proc transreg;
 model spline(y / nknots=3)=log(x1 x2 / parameter=2)
 / nomiss maxiter=50;
 output;
run;

```

In the preceding statements, **NOMISS** and **MAXITER=** are *a-options*. (**SPLINE** and **LOG** are *transforms*, and **NKNOTS=** and **PARAMETER=** are *t-options*.) The statements find a spline transformation with 3 knots on *y* and a base 2 logarithmic transformation on *x1* and *x2*. The **NOMISS** *a-option* excludes all observations with missing values, and the **MAXITER=** *a-option* specifies the maximum number of iterations.

Table 97.4 summarizes the *a-options* available in the PROC TRANSREG or MODEL statement.

**Table 97.4** Options Available in the PROC TRANSREG or MODEL Statement

| Option                               | Description                                     |
|--------------------------------------|-------------------------------------------------|
| <b>Input Control</b>                 |                                                 |
| REITERATE                            | Restarts iterations                             |
| TYPE=                                | Specifies input observation type                |
| <b>Method and Iterations</b>         |                                                 |
| CCONVERGE=                           | Specifies minimum criterion change              |
| CONVERGE=                            | Specifies minimum data change                   |
| MAXITER=                             | Specifies maximum number of iterations          |
| METHOD=                              | Specifies iterative algorithm                   |
| NCAN=                                | Specifies number of canonical variables         |
| NSR                                  | Specifies no restrictions on smoothing models   |
| SINGULAR=                            | Specifies singularity criterion                 |
| SOLVE                                | Attempts direct solution instead of iteration   |
| <b>Missing Data Handling</b>         |                                                 |
| INDIVIDUAL                           | Fits each model individually (METHOD=MORALS)    |
| MONOTONE=                            | Includes monotone special missing values        |
| NOMISS                               | Excludes observations with missing values       |
| UNTIE=                               | Unties special missing values                   |
| <b>Intercept and CLASS Variables</b> |                                                 |
| CPREFIX=                             | Specifies CLASS coded variable name prefix      |
| LPREFIX=                             | Specifies CLASS coded variable label prefix     |
| NOINT                                | Specifies no intercept or centering             |
| ORDER=                               | Specifies order of CLASS variable levels        |
| REFERENCE=                           | Controls output of reference levels             |
| SEPARATORS=                          | Specifies CLASS coded variable label separators |
| <b>Control Displayed Output</b>      |                                                 |
| ALPHA=                               | Specifies confidence limits alpha               |
| CL                                   | Displays parameter estimate confidence limits   |
| DETAIL                               | Displays model specification details            |
| HISTORY                              | Displays iteration histories                    |
| NOPRINT                              | Suppresses displayed output                     |
| PBOXCOXTABLE                         | Prints the Box-Cox log likelihood table         |

Table 97.4 continued

| Option                 | Description                              |
|------------------------|------------------------------------------|
| RSQUARE                | Displays the R square                    |
| SHORT                  | Suppresses the iteration histories       |
| SS2                    | Displays regression results              |
| TEST                   | Displays ANOVA table                     |
| TSUFFIX=               | Shortens transformed variable labels     |
| UTILITIES              | Displays conjoint part-worth utilities   |
| <b>Standardization</b> |                                          |
| ADDITIVE               | Fits additive model                      |
| NOZEROCONSTANT         | Does not zero constant variables         |
| TSTANDARD=             | Specifies transformation standardization |

The following list provides details about these *a-options*. The *a-options* are available in the PROC TRANSREG or MODEL statement.

**ADDITIVE****ADD**

creates an additive model by multiplying the values of each independent variable (after the **TSTANDARD=** standardization) by that variable's corresponding multiple regression coefficient. This process scales the independent variables so that the predicted-values variable for the final dependent variable is simply the sum of the final independent variables. An additive model is a univariate multiple regression model. As a result, the **ADDITIVE a-option** is not valid if **METHOD=CANALS**, or if **METHOD=REDUNDANCY** or **METHOD=UNIVARIATE** with more than one dependent variable.

**ALPHA=number****ALP=number**

specifies the level of significance for all of the confidence limits. By default, ALPHA=0.05.

**CCONVERGE=n****CCO=n**

specifies the minimum change in the criterion being optimized (squared multiple correlation for **METHOD=MORALS** and **METHOD=UNIVARIATE**, average squared multiple correlation for **METHOD=REDUNDANCY**, average squared canonical correlation for **METHOD=CANALS**) that is required to continue iterating. By default, CCONVERGE=0.0.

**CL**

requests confidence limits on the parameter estimates in the displayed output.

**CONVERGE=n****CON=n**

specifies the minimum average absolute change in standardized variable scores that is required to continue iterating. By default, CONVERGE=0.00001. Average change is computed over only those variables that can be transformed by the iterations; that is, all **LINEAR**, **OPSCORE**, **MONOTONE**, **UNTIE**, **SPLINE**, **MSPLINE**, and **SSPLINE** variables and nonoptimal transformation variables with missing values.

**CPREFIX=*n*****CPR=*n***

specifies the number of first characters of a **CLASS** expansion variable's name to use in constructing names for coded variables. Coded variable names are constructed from the first *n* characters of the **CLASS** expansion variable's name and the first  $32 - n$  characters of the formatted **CLASS** expansion variable's value. For example, if the variable **ClassVariable** has values 1, 2, and 3, then, by default, the coded variables are named **ClassVariable1**, **ClassVariable2**, and **ClassVariable3**. However, with **CPREFIX=5**, the coded variables are named **Class1**, **Class2**, and **Class3**. When **CPREFIX=0**, coded variable names are created entirely from the **CLASS** expansion variable's formatted values. Valid values range from  $-1$  to  $31$ , where  $-1$  indicates the default calculation and  $0$  to  $31$  are the number of prefix characters to use. The default,  $-1$ , sets *n* to  $32 - \min(32, \max(2, fl))$ , where *fl* is the format length. When you specify **CPREFIX=** as an *a-option* or an *o-option*, it specifies the default for all **CLASS** variables. When you specify **CPREFIX=** as a *t-option*, it overrides the default only for selected variables.

**DETAIL****DET**

reports on details of the model specification. For example, it reports the knots and coefficients for splines, reference levels for **CLASS** variables, Box-Cox results, the smoothing parameter, and so on. The **DETAIL** option can take two optional suboptions, **NOCOEFFICIENTS** and **NOKNOTS** (or **NOC** and **NOK**). To suppress knots from the details listing, specify **DETAIL(NOKNOTS)**. To suppress coefficients from the details listing, specify **DETAIL(NOCOEFFICIENTS)**. To suppress both knots and coefficients from the details listing, specify **DETAIL(NOKNOTS NOCOEFFICIENTS)**.

**SOLVE****SOL****DUMMY****DUM**

provides a canonical initialization. When there are no monotonicity constraints, when there is at most one canonical variable in each set, and when there is enough available memory, **PROC TRANSREG** (with the **SOLVE a-option**) can usually directly solve for the optimal solution in only one iteration. The initialization iteration is number 0, which is slower and uses more memory than other iterations. However, for some models, specifying the **SOLVE a-option** can greatly decrease the amount of time required to find the optimal transformations. During iteration 0, each variable is replaced by an expanded variable and the model is fit to the larger, expanded set of variables. For example, an **OPSCORE** variable is expanded into coded (or "dummy") variables, as if **CLASS** were specified, and a **SPLINE** variable is expanded into a B-spline basis, as if **BSPLINE** were specified. Then for each expanded variable, the results of iteration zero are constructed by multiplying the expanded basis times the  $\beta$  subvector to get the optimal transformation. This *a-option* can be useful even in models where a direct solution is not possible, because it provides good initial transformations of all the variables.

**HISTORY****HIS**

displays the iteration histories even when the **NOPRINT a-option** is specified.

**INDIVIDUAL****IND**

fits each model for each dependent variable individually. This means, for example, that when INDIVIDUAL is specified, missing values in one dependent variable will not cause that observation to be deleted for the other models with the other dependent variables. In contrast, by default, missing values in any variable in any model can cause the observation to be deleted for all models. The INDIVIDUAL *a-option* can be specified only with **METHOD=MORALS**.

This *a-option* also affects the order of the output. By default, the number of observations table is printed once at the beginning of the output. With INDIVIDUAL, a number of observations table appears for each model.

**LPREFIX=*n*****LPR=*n***

specifies the number of first characters of a **CLASS** expansion variable's label (or name if no label is specified) to use in constructing labels for coded variables. Coded variable labels are constructed from the first *n* characters of the CLASS expansion variable's name and the first 127 – Argument*n* characters of the formatted CLASS expansion variable's value. Valid values range from –1 to 127. Values of 0 to 127 specify the number of name or label characters to use. The default is –1, which specifies that PROC TRANSREG should pick a value depending on the length of the prefix and the formatted class value. When you specify LPREFIX= as an *a-option* or an *o-option*, it determines the default for all CLASS variables. When you specify LPREFIX= as a *t-option*, it overrides the default only for selected variables.

**MAXITER=*n*****MAX=*n***

specifies the maximum number of iterations (see the section “Controlling the Number of Iterations” on page 8290). By default, MAXITER=30. You can specify MAXITER=0 to save time when no transformations are requested.

**METHOD=CANALS | MORALS | REDUNDANCY | UNIVARIATE****MET=CAN | MOR | RED | UNI**

specifies the iterative algorithm. By default, METHOD=UNIVARIATE, unless you specify options that cannot be handled by the UNIVARIATE algorithm. Specifically, the default is METHOD=MORALS for the following situations:

- if you specify **LINEAR**, **OPSCORE**, **MONOTONE**, **UNTIE**, **SPLINE**, **MSPLINE**, or **SSPLINE** transformations for the independent variables
- if you specify the **ADDITIVE** *a-option* with more than one dependent variable
- if you specify the **IAPPROXIMATIONS** *o-option*
- if you specify the **INDIVIDUAL** *a-option*
- if ODS Graphics is enabled, regression plots are produced, and there is more than one dependent variable

**CANALS**

specifies canonical correlation with alternating least squares. This jointly transforms all dependent and independent variables to maximize the average of the first *n* squared canonical correlations, where *n* is the value of the **NCAN=** *a-option*.



- MORALS** specifies multiple optimal regression with alternating least squares. This transforms each dependent variable, along with the set of independent variables, to maximize the squared multiple correlation.
- REDUNDANCY** jointly transforms all dependent and independent variables to maximize the average of the squared multiple correlations (see the section “[Redundancy Analysis](#)” on page 8295).
- UNIVARIATE** transforms each dependent variable to maximize the squared multiple correlation, while the independent variables are not transformed.

**MONOTONE=***two-letters*

**MON=***two-letters*

specifies the first and last special missing value in the list of those special missing values to be estimated with within-variable order and category constraints. By default, there are no order constraints on missing value estimates. The *two-letters* value must consist of two letters in alphabetical order. For example, MONOTONE=DF means that the estimate of .D must be less than or equal to the estimate of .E, which must be less than or equal to the estimate of .F; no order constraints are placed on estimates of .\_, .A through .C, and .G through .Z. For details, see the section “[Missing Values](#)” on page 8289.

**NCAN=***n*

**NCA=***n*

specifies the number of canonical variables to use in the METHOD=CANALS algorithm. By default, NCAN=1. The value of the NCAN= *a-option* must be  $\geq 1$ .

When canonical coefficients and coordinates are included in the OUT= data set, the NCAN= *a-option* also controls the number of rows of the canonical coefficient matrices in the data set. If you specify an NCAN= value larger than the minimum of the number of dependent variables and the number of independent variables, PROC TRANSREG displays a warning and sets the NCAN= *a-option* to the maximum value.

**NOINT**

**NOI**

omits the intercept from the OUT= data set and suppresses centering of data. You cannot specify the NOINT *a-option* with iterative transformations since there is no provision for optimal scaling without an intercept. The NOINT *a-option* can be specified only when there is no implicit intercept and when all of the data in a BY group absolutely will not change during the iterations.

**NOMISS**

**NOM**

excludes all observations with missing values from the analysis, but does not exclude them from the OUT= data set. If you omit the NOMISS *a-option*, PROC TRANSREG simultaneously computes the optimal transformations of the nonmissing values and estimates the missing values that minimize squared error. For details, see the section “[Missing Values](#)” on page 8289.

Casewise deletion of observations with missing values occurs when the NOMISS *a-option* is specified, when there are missing values in expansions, when there are missing values in METHOD=UNIVARIATE independent variables, when there are weights less than or equal to 0, or when there are frequencies less than 1. Excluded observations are output with a blank value for the \_TYPE\_ variable, and they have a weight of 0. They do not contribute to the analysis but are scored and transformed as *supplementary* or *passive* observations.



See the section “[Passive Observations](#)” on page 8294 for more information about excluded observations.

## **NOPRINT**

### **NOP**

suppresses the display of all output unless you specify the [HISTORY](#) *a-option*. The **NOPRINT** *a-option* without the [HISTORY](#) *a-option* disables the Output Delivery System (ODS), including ODS Graphics, for the duration of the procedure run. The **NOPRINT** *a-option* with the [HISTORY](#) *a-option* disables all output except the iteration history, again including ODS Graphics, for the duration of the procedure run. For more information, see Chapter 20, “[Using the Output Delivery System](#).”

## **NOZEROCONSTANT**

### **NOZERO**

### **NOZ**

specifies that constant variables are expected and should not be zeroed. By default, constant variables are zeroed. This option is useful when PROC TRANSREG is used to code experimental designs for discrete choice models (see the section “[Discrete Choice Experiments: DESIGN, NORESTORE, NOZERO](#)” on page 8335). When these designs are very large, it might be more efficient to use the [DESIGN=\*n\*](#) *a-option*. It might be that attributes are constant within a block of *n* observations, so you need to specify the **NOZEROCONSTANT** *a-option* to get the correct results. You can specify this option in the PROC TRANSREG, MODEL, and OUTPUT statements.

## **NSR**

specifies that no restrictions are placed on the use of [SMOOTH](#) and [SSPLINE](#) and the ordinary least squares is used to find the coefficients and predicted values. By default, only certain types of models can be specified with [SMOOTH](#) and ordinary least squares is not used to find the coefficients and predicted values. See the section “[Smoothing Splines Changes and Enhancements](#)” on page 8267 for more information about the **NSR** option and smooth transformations.

## **ORDER=DATA | FREQ | FORMATTED | INTERNAL**

### **ORD=DAT | FRE | FOR | INT**

specifies the order in which the [CLASS](#) variable levels are to be reported. The default is **ORDER=INTERNAL**. For **ORDER=FORMATTED** and **ORDER=INTERNAL**, the sort order is machine dependent. When you specify **ORDER=** as an *a-option* or an *o-option*, it determines the default ordering for all [CLASS](#) variables. When you specify **ORDER=** as a *t-option*, it overrides the default ordering only for selected variables.

|                  |                                                                                      |
|------------------|--------------------------------------------------------------------------------------|
| <b>DATA</b>      | sorts by order of appearance in the input data set.                                  |
| <b>FORMATTED</b> | sorts by formatted value.                                                            |
| <b>FREQ</b>      | sorts by descending frequency count; levels with the most observations appear first. |
| <b>INTERNAL</b>  | sorts by unformatted value.                                                          |

## **PBOXCOXTABLE**

**PBO**

prints the Box-Cox table with the log likelihood displayed as a function of lambda. The important information in this table is displayed in the Box-Cox plot, so when ODS Graphics is enabled and the plot is produced, the table is not produced by default. When ODS Graphics is not enabled or when the plot is not produced, the table is produced by default. Specify the PBOXCOXTABLE option if you want to see the table in addition to the plot.

**REFERENCE=NONE | MISSING | ZERO****REF=NON | MIS | ZER**

specifies how reference levels of **CLASS** variables are to be treated. The options are REFERENCE=NONE, the default, in which reference levels are suppressed; REFERENCE=MISSING, in which reference levels are displayed and output with missing values; and REFERENCE=ZERO, in which reference levels are displayed and output with zeros. You can specify the REFERENCE= option in the PROC TRANSREG, MODEL, or OUTPUT statement, and you can specify it independently for the **OUT=** data set and the displayed output. When you specify it in only one statement, it sets the option for both the displayed output and the **OUT=** data set.

**REITERATE****REI**

enables PROC TRANSREG to use previous transformations as starting points. The REITERATE *a-option* affects only variables that are iteratively transformed (specified as **LINEAR**, **OPSCORE**, **MONOTONE**, **UNTIE**, **SPLINE**, **MSPLINE**, and **SSPLINE**). For iterative transformations, the REITERATE *a-option* requests a search in the input data set for a variable that consists of the value of the **TDPREFIX=** or **TIPREFIX=** *o-option* followed by the original variable name. If such a variable is found, it is used to provide the initial values for the first iteration. The final transformation is a member of the transformation family defined by the original variable, not the transformation family defined by the initialization variable. See the section “Using the REITERATE Algorithm Option” on page 8291 for more information about the REITERATE option.

**RSQUARE****RSQ**

prints a table with only the model R square.

**SEPARATORS='string-1' <'string-2'>****SEP='string-1' <'string-2'>**

specifies separators for creating **CLASS** expansion variable labels. By default, SEPARATORS=' ' \* ' (“blank” and “blank asterisk blank”). The first value is used to separate variable names and values in interactions. The second value is used to separate interaction components. For example, the label for the coded variable for the A=1 and B=2 cell is, by default, 'A 1 \* B 2'. If SEPARATORS='=' 'x' is specified, then the label is 'A=1xB=2'. When you specify SEPARATORS= as an *a-option* or an *o-option*, it determines the default separators for all **CLASS** variables. When you specify SEPARATORS= as a *t-option*, it overrides the default only for selected variables.

**SHORT****SHO**

suppresses the iteration histories.

**SINGULAR=*n*****SIN=*n***

specifies the largest value within rounding error of zero. By default, SINGULAR=1E-12. PROC TRANSREG uses the value of the SINGULAR= *a-option* for checking  $1 - R^2$  when constructing full-rank matrices of predictor variables, checking denominators before dividing, and so on. PROC TRANSREG computes the regression coefficients by sweeping with rational pivoting.

**SS2**

produces a regression table based on Type II sums of squares. Tests of the contribution of each transformation to the overall model are displayed and output to the OUTTEST= data set when you specify the OUTTEST= option. When you specify the SS2 *a-option*, the TEST *a-option* is automatically specified for you. See the section “Hypothesis Tests” on page 8303 for more information about the TEST and SS2 options. You can suppress the variable labels in the regression tables by specifying the NOLABEL option in the OPTIONS statement.

**TEST****TES**

generates an ANOVA table. PROC TRANSREG tests the null hypothesis that the vector of scoring coefficients for all of the transformations is zero. See the section “Hypothesis Tests” on page 8303 for more information about the TEST option.

**TSUFFIX=*n*****TSU=*n***

specifies the number of characters in “Transformation” to append to variable labels for transformed variables. By default, all characters are used.

**TSTANDARD=CENTER | NOMISS | ORIGINAL | Z****TST=CEN | NOM | ORI | Z**

specifies the standardization of the transformed variables for the hypothesis tests and in the OUT= data set. By default, TSTANDARD=ORIGINAL. When you specify TSTANDARD= as an *a-option* or an *o-option*, it determines the default standardization for all variables. When you specify TSTANDARD= as a *t-option*, it overrides the default standardization only for selected variables.

**CENTER** centers the output variables to mean zero, but the variances are the same as the variances of the input variables.

**NOMISS** sets the means and variances of the transformed variables in the OUT= data set, computed over all output values that correspond to nonmissing values in the input data set, to the means and variances computed from the nonmissing observations of the original variables. The TSTANDARD=NOMISS specification is useful with missing data. When a variable is linearly transformed, the final variable contains the original nonmissing values and the missing value estimates. In other words, the nonmissing values are unchanged. If your data have no missing values, TSTANDARD=NOMISS and TSTANDARD=ORIGINAL produce the same results.

**ORIGINAL** sets the means and variances of the transformed variables to the means and variances of the original variables. This is the default.

**Z** standardizes the variables to mean zero, variance one.

The final standardization is affected by other options. If you also specify the **ADDITIVE** *a-option*, the **TSTANDARD=** option specifies an intermediate step in computing the final means and variances. The final independent variables, along with their means and standard deviations, are scaled by the regression coefficients, creating an additive model with all coefficients equal to one.

For nonoptimal variable transformations, the means and variances of the original variables are actually the means and variances of the nonlinearly transformed variables, unless you specify the **ORIGINAL** nonoptimal *t-option* in the MODEL statement. For example, if a variable *x* with no missing values is specified as **LOG**, then, by default, the final transformation of *x* is simply the log of *x*, not the log of *x* standardized to the mean of *x* and variance of *x*.

**TYPE=**'text'|name

**TYP=**'text'|name

specifies the valid value for the `_TYPE_` variable in the input data set. If PROC TRANSREG finds an input `_TYPE_` variable, it uses only observations with a `_TYPE_` value that matches the **TYPE=** value. This enables a PROC TRANSREG **OUT=** data set containing coefficients to be used as input to PROC TRANSREG without requiring a WHERE statement to exclude the coefficients. If a `_TYPE_` variable is not in the data set, all observations are used. The default is **TYPE='SCORE'**, so if you do not specify the **TYPE=** *a-option*, only observations with `_TYPE_='SCORE'` are used. Do not confuse this *a-option* with the data set **TYPE=** option. The **DATA=** data set must be an ordinary SAS data set.

PROC TRANSREG displays a note when it reads observations with blank values of `_TYPE_`, but it does not automatically exclude those observations. Data sets created by the TRANSREG and PRINQUAL procedures have blank `_TYPE_` values for those observations that were excluded from the analysis due to nonpositive weights, nonpositive frequencies, or missing data. When these observations are read again, they are excluded for the same reason that they were excluded from their original analysis, not because their `_TYPE_` value is blank.

**UNTIE=**two-letters

**UNT=**two-letters

specifies the first and last special missing values in the list of those special missing values that are to be estimated with within-variable order constraints but no category constraints. The *two-letters* value must consist of two letters in alphabetical order. By default, there are category constraints but no order constraints on special missing value estimates. For details, see the sections “[Missing Values](#)” on page 8289 and “[Optimal Scaling](#)” on page 8298.

## UTILITIES

### UTI

produces a table of the part-worth utilities from a conjoint analysis. Utilities, their standard errors, and the relative importance of each factor are displayed and output to the **OUTTEST=** data set when you specify the **OUTTEST=** option. When you specify the UTILITIES *a-option*, the **TEST** *a-option* is automatically specified for you. See [Example 97.4](#) and [Example 97.5](#) for more information about conjoint analysis.

## OUTPUT Statement

**OUTPUT** **OUT**=SAS-data-set < o-options > ;

The OUTPUT statement creates a new SAS data set that contains coefficients, marginal means, and information about the original and transformed variables. The information about original and transformed variables composes the score partition of the data set; observations have `_TYPE_='SCORE'`. The coefficients and marginal means compose the coefficient partition of the data set; observations have `_TYPE_='M COEFFI'` or `_TYPE_='MEAN'`. Other values of `_TYPE_` are possible; for details, see “`_TYPE_` and `_NAME_` Variables” later in this chapter. For details about data set structure, see the section “Output Data Set” on page 8305. To specify the name of the output data set, use the **OUT=** option.

### **OUT**=SAS-data-set

specifies the output data set for the data, transformed data, predicted values, residuals, scores, coefficients, and so on. When you use an OUTPUT statement but do not use the **OUT=** specification, PROC TRANSREG creates a data set and uses the `DATAn` convention. If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*.

To control the contents of the data set and variable names, use one or more of the *o-options*. You can also specify these options in the PROC TRANSREG statement.

## Output Options (o-options)

Table 97.5 summarizes the options available in the OUTPUT statement. These options include the **OUT=** option and all of the *o-options*. Many of the statistics created in the OUTPUT statement are exactly the same as statistics created by PROC REG. More details are given in the sections “Predicted and Residual Values” on page 6708, “Model Fit and Diagnostic Statistics” on page 6715 in Chapter 79, “The REG Procedure,” and Chapter 4, “Introduction to Regression Procedures.”

**Table 97.5** Options Available in the OUTPUT Statement

| Option                                     | Description                          |
|--------------------------------------------|--------------------------------------|
| <b>Identify output data set</b>            |                                      |
| <b>OUT=</b>                                | Outputs data set                     |
| <b>Predicted Values, Residuals, Scores</b> |                                      |
| <b>CANONICAL</b>                           | Outputs canonical scores             |
| <b>CLI</b>                                 | Outputs individual confidence limits |
| <b>CLM</b>                                 | Outputs mean confidence limits       |
| <b>DESIGN=</b>                             | Specifies design matrix coding       |
| <b>DREPLACE</b>                            | Replaces dependent variables         |
| <b>IREPLACE</b>                            | Replaces independent variables       |
| <b>LEVERAGE</b>                            | Outputs leverage                     |
| <b>NORESTOREMISSING</b>                    | Does not restore missing values      |
| <b>NOSCORES</b>                            | Suppresses output of scores          |
| <b>PREDICTED</b>                           | Outputs predicted values             |
| <b>REDUNDANCY=</b>                         | Outputs redundancy variables         |
| <b>REPLACE</b>                             | Replaces all variables               |
| <b>RESIDUALS</b>                           | Outputs residuals                    |

Table 97.5 *continued*

| Option                                        | Description                                        |
|-----------------------------------------------|----------------------------------------------------|
| <b>Output Data Set Coefficients</b>           |                                                    |
| COEFFICIENTS                                  | Outputs coefficients                               |
| COORDINATES=                                  | Outputs ideal point coordinates                    |
| MEANS                                         | Outputs marginal means                             |
| MREDUNDANCY                                   | Outputs redundancy analysis coefficients           |
| <b>Output Data Set Variable Name Prefixes</b> |                                                    |
| ADPREFIX=                                     | Specifies dependent variable approximations        |
| AIPREFIX=                                     | Specifies independent variable approximations      |
| CDPREFIX=                                     | Specifies canonical dependent variables            |
| CILPREFIX=                                    | Specifies conservative individual lower CL         |
| CIPREFIX=                                     | Specifies canonical independent variables          |
| CIUPREFIX=                                    | Specifies conservative-individual-upper CL         |
| CMLPREFIX=                                    | Specifies conservative-mean-lower CL               |
| CMUPREFIX=                                    | Specifies conservative-mean-upper CL               |
| DEPENDENT=                                    | Specifies METHOD=MORALS untransformed dependent    |
| LILPREFIX=                                    | Specifies liberal-individual-lower CL              |
| LIUPREFIX=                                    | Specifies liberal-individual-upper CL              |
| LMLPREFIX=                                    | Specifies liberal-mean-lower CL                    |
| LMUPREFIX=                                    | Specifies liberal-mean-upper CL                    |
| RDPREFIX=                                     | Specifies residuals                                |
| PPREFIX=                                      | Specifies predicted values                         |
| RPREFIX=                                      | Specifies redundancy variables                     |
| TDPREFIX=                                     | Specifies transformed dependents                   |
| TIPREFIX=                                     | Specifies transformed independents                 |
| <b>Macros Variables</b>                       |                                                    |
| MACRO                                         | Creates macro variables                            |
| <b>Other Options</b>                          |                                                    |
| APPROXIMATIONS                                | Outputs dependent and independent approximations   |
| CCC                                           | Outputs canonical correlation coefficients         |
| CEC                                           | Outputs canonical elliptical point coordinates     |
| CPC                                           | Outputs canonical point coordinates                |
| CQC                                           | Outputs canonical quadratic point coordinates      |
| DAPPROXIMATIONS                               | Outputs approximations to transformed dependents   |
| IAPPROXIMATIONS                               | Outputs approximations to transformed independents |
| MEC                                           | Outputs elliptical point coordinates               |
| MPC                                           | Outputs point coordinates                          |
| MQC                                           | Outputs quadratic point coordinates                |
| MRC                                           | Outputs multiple regression coefficients           |

For the coefficients partition, the **COEFFICIENTS**, **COORDINATES**, and **MEANS** *o-options* provide the coefficients that are appropriate for your model. For more explicit control of the coefficient partition, use the options that control details and prefixes. The following list provides details about these options.

**ADPREFIX=***name***ADP=***name*

specifies a prefix for naming the dependent variable predicted values. The default is ADPREFIX=P when you specify the **PREDICTED** *o-option*; otherwise, it is ADPREFIX=A. When you specify the ADPREFIX= *o-option*, the **PREDICTED** *o-option* is automatically specified for you. The ADPREFIX= *o-option* is the same as the **PPREFIX=** *o-option*.

**AIPREFIX=***name***AIP=***name*

specifies a prefix for naming the independent variable approximations. The default is AIPREFIX=A. When you specify the AIPREFIX= *o-option*, the **IAPPROXIMATIONS** *o-option* is automatically specified for you.

**APPROXIMATIONS****APPROX****APP**

is equivalent to specifying both the **DAPPROXIMATIONS** and the **IAPPROXIMATIONS** *o-options*. If you specify **METHOD=UNIVARIATE**, then the **APPROXIMATIONS** *o-option* specifies only the **DAPPROXIMATIONS** *o-option*.

**CANONICAL****CAN**

outputs canonical variables to the **OUT=** data set. When you specify **METHOD=CANALS**, the **CANONICAL** *o-option* is automatically specified for you. The **CDPREFIX=** *o-option* specifies a prefix for naming the dependent canonical variables (default Cand), and the **CIPREFIX=** *o-option* specifies a prefix for naming the independent canonical variables (default Cani).

**CCC**

outputs canonical correlation coefficients to the **OUT=** data set.

**CDPREFIX=***name***CDP=***name*

provides a prefix for naming the canonical dependent variables. The default is CDPREFIX=Cand. When you specify the CDPREFIX= *o-option*, the **CANONICAL** *o-option* is automatically specified for you.

**CEC**

outputs canonical elliptical point model coordinates to the **OUT=** data set.

**CILPREFIX=***name***CIL=***name*

specifies a prefix for naming the conservative-individual-lower confidence limits. The default prefix is CIL. When you specify the CILPREFIX= *o-option*, the **CLI** *o-option* is automatically specified for you.



**CIPREFIX=***name***CIP=***name*

provides a prefix for naming the canonical independent variables. The default is CIPREFIX=Cani. When you specify the CIPREFIX= *o-option*, the **CANONICAL** *o-option* is automatically specified for you.

**CIUPREFIX=***name***CIU=***name*

specifies a prefix for naming the conservative-individual-upper confidence limits. The default prefix is CIU. When you specify the CIUPREFIX= *o-option*, the **CLI** *o-option* is automatically specified for you.

**CLI**

outputs individual confidence limits to the **OUT=** data set. The names of the confidence limits variables are constructed from the original dependent variable names and the prefixes specified in the following *o-options*: **LILPREFIX=** (default LIL for liberal individual lower), **CILPREFIX=** (default CIL for conservative individual lower), **LIUPREFIX=** (default LIU for liberal individual upper), and **CIUPREFIX=** (default CIU for conservative individual upper). When there are no monotonicity constraints, the liberal and conservative limits are the same.

**CLM**

outputs mean confidence limits to the **OUT=** data set. The names of the confidence limits variables are constructed from the original dependent variable names and the prefixes specified in the following *o-options*: **LMLPREFIX=** (default LML for liberal mean lower), **CMLPREFIX=** (default CML for conservative mean lower), **LMUPREFIX=** (default LMU for liberal mean upper), and **CMUPREFIX=** (default CMU for conservative mean upper). When there are no monotonicity constraints, the liberal and conservative limits are the same.

**CMLPREFIX=***name***CML=***name*

specifies a prefix for naming the conservative-mean-lower confidence limits. The default prefix is CML. When you specify the CMLPREFIX= *o-option*, the **CLM** *o-option* is automatically specified for you.

**CMUPREFIX=***name***CMU=***name*

specifies a prefix for naming the conservative-mean-upper confidence limits. The default prefix is CMU. When you specify the CMUPREFIX= *o-option*, the **CLM** *o-option* is automatically specified for you.

**COEFFICIENTS****COE**

outputs either multiple regression coefficients or raw canonical coefficients to the **OUT=** data set. If you specify **METHOD=CANALS** (in the MODEL or PROC TRANSREG statement), then the **COEFFICIENTS** *o-option* outputs the first *n* canonical variables, where *n* is the value of the **NCAN=** *a-option* (specified in the MODEL or PROC TRANSREG statement). Otherwise, the **COEFFICIENTS** *o-option* includes multiple regression coefficients in the **OUT=** data set. In addition, when you specify the **CLASS** expansion for any independent variable, the **COEFFICIENTS** *o-option* also outputs marginal means.



**COORDINATES**<=*n*>**COO**<=*n*>

outputs either ideal point or vector model coordinates for preference mapping to the **OUT=** data set. When **METHOD=CANALS**, these coordinates are computed from canonical coefficients; otherwise, the coordinates are computed from multiple regression coefficients. For details, see the section “[Point Models](#)” on page 8294.

When ODS Graphics is enabled and vector model coordinates are requested, a plot is produced with points for each row and vectors for each column. If the vectors are plotted based on the actual computed coordinates, then often the vectors are short. A better graphical display is produced when the vectors are stretched. The absolute lengths of each vector can optionally be changed by specifying **COORDINATES=*n***. Then the vector coordinates are all multiplied by *n*. Usually, *n* is a value such as 2, 2.5, or 3. The default is 2.5. Specify **COORDINATES=1** if you want to see the vectors without any stretching. The relative lengths of the different vectors are important and interpretable, and these are preserved by the stretching.

**CPC**

outputs canonical point model coordinates to the **OUT=** data set.

**CQC**

outputs canonical quadratic point model coordinates to the **OUT=** data set.

**DAPPROXIMATIONS****DAP**

outputs the approximations of the transformed dependent variables to the **OUT=** data set. These are the target values for the optimal transformations. With **METHOD=UNIVARIATE** and **METHOD=MORALS**, the dependent variable approximations are the ordinary predicted values from the linear model. The names of the approximation variables are constructed from the **ADPREFIX= *o-option*** (default A) and the original dependent variable names. For ordinary predicted values, use the **PREDICTED *o-option*** instead of the **DAPPROXIMATIONS *o-option***, since the **PREDICTED *o-option*** uses a more relevant prefix (“P” instead of “A”) and a more relevant variable label suffix (“Predicted Values” instead of “Approximations”).

**DESIGN**<=*n*>**DES**<=*n*>

specifies that your primary goal is design matrix coding, not analysis. Specifying the **DESIGN *o-option*** makes the procedure run faster. The **DESIGN *o-option*** sets the default method to **UNIVARIATE** and the default **MAXITER=** value to zero. It suppresses computing the regression coefficients, unless they are needed for some other option. Furthermore, when the **DESIGN *o-option*** is specified, the **MODEL** statement is not required to have an equal sign. When no **MODEL** statement equal sign is specified, all variables are considered independent variables, all options that require dependent variables are ignored, and the **IREPLACE *o-option*** is automatically specified for you.

You can use **DESIGN=*n*** for coding very large data sets, where *n* is the number of observations to code at one time. For example, to code a data set with a large number of observations, you can specify **DESIGN=100** or **DESIGN=1000** to process the data set in blocks of 100 or 1000 observations. If you specify the **DESIGN *o-option*** rather than **DESIGN=*n***, PROC TRANSREG tries to process all observations at once, which might not work with very large data sets. Specify the **NOZEROCONSTANT *a-option*** with **DESIGN=*n*** to ensure that constant variables within blocks are not zeroed. See the sections “[Using the DESIGN Output Option](#)” on page 8331 and “[Discrete Choice Experiments: DESIGN, NORESTORE, NOZERO](#)” on page 8335 for more information about the **DESIGN** option.

**DEPENDENT=***name*

**DEP=***name*

specifies the untransformed dependent variable for **OUT=** data sets with **METHOD=MORALS** when there is more than one dependent variable. The default is **DEPENDENT=\_DEPEND\_**.

**DREPLACE**

**DRE**

replaces the original dependent variables with the transformed dependent variables in the **OUT=** data set. The names of the transformed variables in the **OUT=** data set correspond to the names of the original dependent variables in the input data set. By default, both the original dependent variables and the transformed dependent variables (with names constructed from the **TDPREFIX=** (default T) *o-option* and the original dependent variable names) are included in the **OUT=** data set.

**IAPPROXIMATIONS**

**IAP**

outputs the approximations of the transformed independent variables to the **OUT=** data set. These are the target values for the optimal transformations. The names of the approximation variables are constructed from the **AIPREFIX=** *o-option* (default A) and the original independent variable names. When you specify the **AIPREFIX=** *o-option*, the **IAPPROXIMATIONS** *o-option* is automatically specified for you. The **IAPPROXIMATIONS** *o-option* is not valid when **METHOD=UNIVARIATE**.

**IREPLACE**

**IRE**

replaces the original independent variables with the transformed independent variables in the **OUT=** data set. The names of the transformed variables in the **OUT=** data set correspond to the names of the original independent variables in the input data set. By default, both the original independent variables and the transformed independent variables (with names constructed from the **TIPREFIX=** *o-option* (default T) and the original independent variable names) are included in the **OUT=** data set.

**LEVERAGE<=***name***>**

**LEV<=***name***>**

creates a variable with the specified name in the **OUT=** data set that contains leverages. Specifying the **LEVERAGE** *o-option* is equivalent to specifying **LEVERAGE=Leverage**.

**LILPREFIX=***name*

**LIL=***name*

specifies a prefix for naming the liberal-individual-lower confidence limits. The default prefix is LIL. When you specify the **LILPREFIX=** *o-option*, the **CLI** *o-option* is automatically specified for you.

**LIUPREFIX=***name*

**LIU=***name*

specifies a prefix for naming the liberal-individual-upper confidence limits. The default prefix is LIU. When you specify the **LIUPREFIX=** *o-option*, the **CLI** *o-option* is automatically specified for you.

**LMLPREFIX=***name***LML=***name*

specifies a prefix for naming the liberal-mean-lower confidence limits. The default prefix is LML. When you specify the LMLPREFIX= *o-option*, the **CLM** *o-option* is automatically specified for you.

**LMUPREFIX=***name***LMU=***name*

specifies a prefix for naming the liberal-mean-upper confidence limits. The default prefix is LMU. When you specify the LMUPREFIX= *o-option*, the **CLM** *o-option* is automatically specified for you.

**MACRO**(*keyword=name. . .*)**MAC**(*keyword=name. . .*)

creates macro variables. Most of the options available within the MACRO *o-option* are rarely needed. By default, PROC TRANSREG creates a macro variable named `_TrgInd` with a complete list of independent variables created by the procedure. When PROC TRANSREG is being used for design matrix creation prior to running a procedure without a CLASS statement, this macro provides a convenient way to use the results from PROC TRANSREG. For example, a PROC LOGISTIC step that uses a design matrix coded by PROC TRANSREG can use the following MODEL statement:

```
model y=&_trgind;
```

PROC TRANSREG, also by default, creates a macro variable named `_TrgIndN`, which contains the number of variables in the `_TrgInd` list. These macro variables can be used in an ARRAY statement as follows:

```
array indvars[&_trgindn] &_trgind;
```

See the sections “Using the DESIGN Output Option” on page 8331 and “Discrete Choice Experiments: DESIGN, NORESTORE, NOZERO” on page 8335 for examples of using the default macro variables.

The available *keywords* are as follows.

**DN=***name* specifies the name of a macro variable that contains the number of dependent variables. By default, a macro variable named `_TrgDepN` is created. This is the number of variables in the DL= list and the number of macro variables created by the DV= and DE= specifications.

**IN=***name* specifies the name of a macro variable that contains the number of independent variables. By default, a macro variable named `_TrgIndN` is created. This is the number of variables in the IL= list and the number of macro variables created by the IV= and IE= specifications.

**DL=***name* specifies the name of a macro variable that contains the list of the dependent variables. By default, a macro variable named `_TrgDep` is created. These are the variable names of the final transformed variables in the OUT= data set. For example, if there are three dependent variables, `y1–y3`, then `_TrgDep` contains, by default, `Ty1 Ty2 Ty3` (or `y1 y2 y3` if you specify the REPLACE *o-option*).

**IL=name** specifies the name of a macro variable that contains the list of the independent variables. By default, a macro variable named `_TrgInd` is created. These are the variable names of the final transformed variables in the `OUT=` data set. For example, if there are three independent variables, `x1–x3`, then `_TrgInd` contains, by default, `Tx1 Tx2 Tx3` (or `x1 x2 x3` if you specify the `REPLACE o-option`).

**DV=prefix** specifies a prefix for creating a list of macro variables, each of which contains one dependent variable name. For example, if there are three dependent variables, `y1–y3`, and you specify `macro (dv=Dep)`, then three macro variables, `Dep1`, `Dep2`, and `Dep3`, are created, containing `Ty1`, `Ty2`, and `Ty3`, respectively (or `y1`, `y2`, and `y3` if you specify the `REPLACE o-option`). By default, no list is created.

**IV=prefix** specifies a prefix for creating a list of macro variables, each of which contains one independent variable name. For example, if there are three independent variables, `x1–x3`, and you specify `macro (iv=Ind)`, then three macro variables, `Ind1`, `Ind2`, and `Ind3`, are created, containing `Tx1`, `Tx2`, and `TX3`, respectively (or `x1`, `x2`, and `x3` if you specify the `REPLACE o-option`). By default, no list is created.

**DE=prefix** specifies a prefix for creating a list of macro variables, each of which contains one dependent variable effect. This list shows the origin of each model term. Each effect consists of two or more parts, and each part consists of a value in 32 columns followed by a blank. For example, if you specify `macro (de=d)`, then a macro variable `d1` is created for `identity(y)`. The `d1` macro variable is shown next, wrapped onto two lines:

```

4 TY
IDENTITY Y

```

The first part is the number of parts (4), the second part is the transformed variable name, the third part is the transformation, and the last part is the input variable name. By default, no list is created.

**IE=prefix** specifies a prefix for creating a list of macro variables, each of which contains one independent variable effect. This list shows the origin of each model term. Each effect consists of two or more parts, and each part consists of a value in 32 columns followed by a blank. For example, if you specify `macro (ie=I)`, then three macro variables, `I1`, `I2`, and `I3`, are created for `class(x1 | x2)` when both `x1` and `x2` have values of 1 and 2. These macro variables are shown next, with extra white space removed:

```

5 Tx11 CLASS x1 1
5 Tx21 CLASS x2 1
8 Tx11x21 CLASS x1 1 CLASS x2 1

```

For `CLASS` variables, the formatted level appears after the variable name. The first two effects are the main effects, and the last is the interaction term. By default, no list is created.

**MEANS****MEA**

outputs marginal means for **CLASS** variable expansions to the **OUT=** data set.

**MEC**

outputs multiple regression elliptical point model coordinates to the **OUT=** data set.

**MPC**

outputs multiple regression point model coordinates to the **OUT=** data set.

**MQC**

outputs multiple regression quadratic point model coordinates to the **OUT=** data set.

**MRC**

outputs multiple regression coefficients to the **OUT=** data set.

**MREDUNDANCY****MRE**

outputs multiple redundancy analysis coefficients to the **OUT=** data set.

**NORESTOREMISSING****NORESTORE****NOR**

specifies that missing values should not be restored when the **OUT=** data set is created. By default, the coded **CLASS** variable contains a row of missing values for observations in which the **CLASS** variable is missing. When you specify the **NORESTOREMISSING** *o-option*, these observations contain a row of zeros instead. This is useful when PROC TRANSREG is used to code experimental designs for discrete choice models and there is a constant alternative indicated by a missing value.

**NOSCORES****NOS**

excludes original variables, transformed variables, predicted values, residuals, and scores from the **OUT=** data set. You can use the **NOSCORES** *o-option* with various other options to create an **OUT=** data set that contains only a coefficient partition (for example, a data set consisting entirely of coefficients and coordinates).

**PREDICTED****PRE****P**

outputs predicted values, which for **METHOD=UNIVARIATE** and **METHOD=MORALS** are the ordinary predicted values from the linear model, to the **OUT=** data set. The names of the predicted values' variables are constructed from the **PPREFIX=** *o-option* (default **P**) and the original dependent variable names. When you specify the **PPREFIX=** *o-option*, the **PREDICTED** *o-option* is automatically specified for you.

**PPREFIX=name**

**PDPREFIX=name**

**PDP=name**

specifies a prefix for naming the dependent variable predicted values. The default is **PPREFIX=P** when you specify the **PREDICTED** *o-option*; otherwise, it is **PPREFIX=A**. When you specify the **PPREFIX=** *o-option*, the **PREDICTED** *o-option* is automatically specified for you. The **PPREFIX=** *o-option* is the same as the **ADPREFIX=** *o-option*.

**RDPREFIX=***name*

**RDP=***name*

specifies a prefix for naming the residual (dependent) variables to the **OUT=** data set. The default is **RDPREFIX=R**. When you specify the **RDPREFIX=** *o-option*, the **RESIDUALS** *o-option* is automatically specified for you.

**REDUNDANCY**< **=STANDARDIZE** | **UNSTANDARDIZE** >

**RED**< **=STA** | **UNS** >

outputs redundancy variables to the **OUT=** data set, either standardized or unstandardized. Specifying the **REDUNDANCY** *o-option* is the same as specifying **REDUNDANCY=STANDARDIZE**. The results of the **REDUNDANCY** *o-option* depends on the **TSTANDARD=** option. You must specify **TSTANDARD=Z** to get results based on standardized data. The **TSTANDARD=** option controls how the data that go into the redundancy analysis are scaled, and **REDUNDANCY=STANDARDIZE|UNSTANDARDIZE** controls how the redundancy variables are scaled. The **REDUNDANCY** *o-option* is automatically specified for you when you specify the **METHOD=REDUNDANCY** *a-option*. The **RPREFIX=** *o-option* specifies a prefix (default Red) for naming the redundancy variables.

**REFERENCE=NONE** | **MISSING** | **ZERO**

**REF=NON** | **MIS** | **ZER**

specifies how reference levels of **CLASS** variables are to be treated. The options are **REFERENCE=NONE**, the default, in which reference levels are suppressed; **REFERENCE=MISSING**, in which reference levels are displayed and output with missing values; and **REFERENCE=ZERO**, in which reference levels are displayed and output with zeros. You can specify the **REFERENCE=** option in the **PROC TRANSREG**, **MODEL**, or **OUTPUT** statement, and you can specify it independently for the **OUT=** data set and the displayed output. When you specify it in only one statement, it sets the option for both the displayed output and the **OUT=** data set.

**REPLACE**

**REP**

is equivalent to specifying both the **DREPLACE** and the **IREPLACE** *o-options*.

**RESIDUALS**

**RES**

**R**

outputs the differences between the transformed dependent variables and their predicted values. The names of the residual variables are constructed from the **RDPREFIX=** *o-option* (default R) and the original dependent variable names.

**RPREFIX=***name*

**RPR=***name*

provides a prefix for naming the redundancy variables. The default is **RPREFIX=Red**. When you specify the **RPREFIX=** *o-option*, the **REDUNDANCY** *o-option* is automatically specified for you.

**TDPREFIX=***name*

**TDP=***name*

specifies a prefix for naming the transformed dependent variables. By default, **TDPREFIX=T**. The **TDPREFIX=** *o-option* is ignored when you specify the **DREPLACE** *o-option*.

**TIPREFIX**=*name*

**TIP**=*name*

specifies a prefix for naming the transformed independent variables. By default, TIPREFIX=T. The TIPREFIX= *o-option* is ignored when you specify the IREPLACE *o-option*.

## WEIGHT Statement

**WEIGHT** *variable* ;

When you use a WEIGHT statement, a weighted residual sum of squares is minimized. The WEIGHT statement has no effect on degrees of freedom or number of observations, but the weights affect most other calculations. The observation is used in the analysis only if the value of the WEIGHT statement variable is greater than 0.

## Details: TRANSREG Procedure

### Model Statement Usage

```
MODEL < transform(dependents </ t-options>)>
 < transform(dependents </ t-options>)...=>
 transform(independents </ t-options>)
 < transform(independents </ t-options>)... > </ a-options> ;
```

Here are some examples of model statements:

- linear regression

```
model identity(y) = identity(x);
```

- a linear model with a nonlinear regression function

```
model identity(y) = spline(x / nknots=5);
```

- multiple regression

```
model identity(y) = identity(x1-x5);
```

- multiple regression with nonlinear transformations

```
model spline(y / nknots=3) = spline(x1-x5 / nknots=3);
```

- multiple regression with nonlinear but monotone transformations

```
model mspline(y / nknots=3) = mspline(x1-x5 / nknots=3);
```

- multivariate multiple regression

```
model identity(y1-y4) = identity(x1-x5);
```

- canonical correlation

```
model identity(y1-y4) = identity(x1-x5) / method=canals;
```

- redundancy analysis

```
model identity(y1-y4) = identity(x1-x5) / method=redundancy;
```

- preference mapping, vector model (Carroll 1972)

```
model identity(Attrib1-Attrib3) = identity(Dim1-Dim2);
```

- preference mapping, ideal point model (Carroll 1972)

```
model identity(Attrib1-Attrib3) = point(Dim1-Dim2);
```

- preference mapping, ideal point model, elliptical (Carroll 1972)

```
model identity(Attrib1-Attrib3) = epoint(Dim1-Dim2);
```

- preference mapping, ideal point model, quadratic (Carroll 1972)

```
model identity(Attrib1-Attrib3) = qpoint(Dim1-Dim2);
```

- metric conjoint analysis

```
model identity(Subj1-Subj50) = class(a b c d e f / zero=sum);
```

- nonmetric conjoint analysis

```
model monotone(Subj1-Subj50) = class(a b c d e f / zero=sum);
```

- main effects, two-way interaction

```
model identity(y) = class(a|b);
```

- less-than-full-rank model—main effects and two-way interaction are constrained to sum to zero

```
model identity(y) = class(a|b / zero=sum);
```

- main effects and all two-way interactions

```
model identity(y) = class(a|b|c@2);
```

- main effects and all two- and three-way interactions

```
model identity(y) = class(a|b|c);
```

- main effects and only the b\*c two-way interaction



```
model identity(y) = class(a b c b*c);
```

- seven main effects, three two-way interactions

```
model identity(y) = class(a b c d e f g a*b a*c a*d);
```

- deviations-from-means (effects or (1, 0, -1)) coding, with an a reference level of '1' and a b reference level of '2'

```
model identity(y) = class(a|b / deviations zero='1' '2');
```

- cell-means coding (implicit intercept)

```
model identity(y) = class(a*b / zero=none);
```

- reference cell model

```
model identity(y) = class(a|b / zero='1' '1');
```

- reference line with change in line parameters

```
model identity(y) = class(a) | identity(x);
```

- reference curve with change in curve parameters

```
model identity(y) = class(a) | spline(x);
```

- separate curves and intercepts

```
model identity(y) = class(a / zero=none) | spline(x);
```

- quantitative effects with interaction

```
model identity(y) = identity(x1 | x2);
```

- separate quantitative effects with interaction within each cell

```
model identity(y) = class(a * b / zero=none) | identity(x1 | x2);
```

---

## Box-Cox Transformations

Box-Cox (1964) transformations are used to find potentially nonlinear transformations of a dependent variable. The Box-Cox transformation has the form

$$\begin{array}{ll} (y^\lambda - 1)/\lambda & \lambda \neq 0 \\ \log(y) & \lambda = 0 \end{array}$$

This family of transformations of the positive dependent variable  $y$  is controlled by the parameter  $\lambda$ . Transformations linearly related to square root, inverse, quadratic, cubic, and so on are all special cases. The limit

as  $\lambda$  approaches 0 is the log transformation. More generally, Box-Cox transformations of the following form can be fit:

$$\begin{aligned} ((y + c)^\lambda - 1)/(\lambda g) & \quad \lambda \neq 0 \\ \log(y + c)/g & \quad \lambda = 0 \end{aligned}$$

By default,  $c = 0$ . The parameter  $c$  can be used to rescale  $y$  so that it is strictly positive. By default,  $g = 1$ . Alternatively,  $g$  can be  $\bar{y}^{\lambda-1}$ , where  $\bar{y}$  is the geometric mean of  $y$ .

The **BOXCOX** transformation in PROC TRANSREG can be used to perform a Box-Cox transformation of the dependent variable. You can specify a list of power parameters by using the **LAMBDA=** *t-option*. By default, **LAMBDA=** -3 TO 3 BY 0.25. The procedure chooses the optimal power parameter by using a maximum likelihood criterion (Draper and Smith 1981, pp. 225–226). You can specify the **PARAMETER=**  $c$  transformation option when you want to shift the values of  $y$ , usually to avoid negatives. To divide by  $\bar{y}^{\lambda-1}$ , specify the **GEOMETRICMEAN** *t-option*.

Here are three examples of using the **LAMBDA=** *t-option*:

```
model BoxCox(y / lambda=0) = identity(x1-x5);
model BoxCox(y / lambda=-2 to 2 by 0.1) = identity(x1-x5);
model BoxCox(y) = identity(x1-x5);
```

Here is the first example:

```
model BoxCox(y / lambda=0) = identity(x1-x5);
```

**LAMBDA=0** specifies a Box-Cox transformation with a power parameter of 0. Since a single value of 0 was specified for **LAMBDA=**, there is no difference between the following models:

```
model BoxCox(y / lambda=0) = identity(x1-x5);
model log(y) = identity(x1-x5);
```

Here is the second example:

```
model BoxCox(y / lambda=-2 to 2 by 0.1) = identity(x1-x5);
```

**LAMBDA=** specifies a list of power parameters. PROC TRANSREG tries each power parameter in the list and picks the best transformation. A maximum likelihood approach (Draper and Smith 1981, pp. 225–226) is used. With Box-Cox transformations, PROC TRANSREG finds the transformation before the usual iterations begin. Note that this is quite different from PROC TRANSREG's usual approach of iteratively finding optimal transformations with ordinary and alternating least squares. It is analogous to **SMOOTH** and **PBSPLINE**, which also find transformations before the iterations begin based on a criterion other than least squares.

Here is the third example:

```
model BoxCox(y) = identity(x1-x5);
```

The default **LAMBDA=** list of -3 TO 3 BY 0.25 is used.

The procedure prints the optimal power parameter, a confidence interval on the power parameter (based on the **ALPHA=** *t-option*), a “convenient” power parameter (selected from the **CLL=** *t-option* list), and the log likelihood for each power parameter tried (see [Example 97.2](#)).

To illustrate how Box-Cox transformations work, data were generated from the model

$$y = e^{x+\epsilon}$$

where  $\epsilon \sim N(0, 1)$ . The transformed data can be fit with a linear model

$$\log(y) = x + \epsilon$$

The following statements produce [Figure 97.14](#) through [Figure 97.15](#):

```
title 'Basic Box-Cox Example';

data x;
 do x = 1 to 8 by 0.025;
 y = exp(x + normal(7));
 output;
 end;
run;

ods graphics on;

title2 'Default Options';

proc transreg data=x test;
 model BoxCox(y) = identity(x);
run;
```

Figure 97.14 Basic Box-Cox Example, Default Output

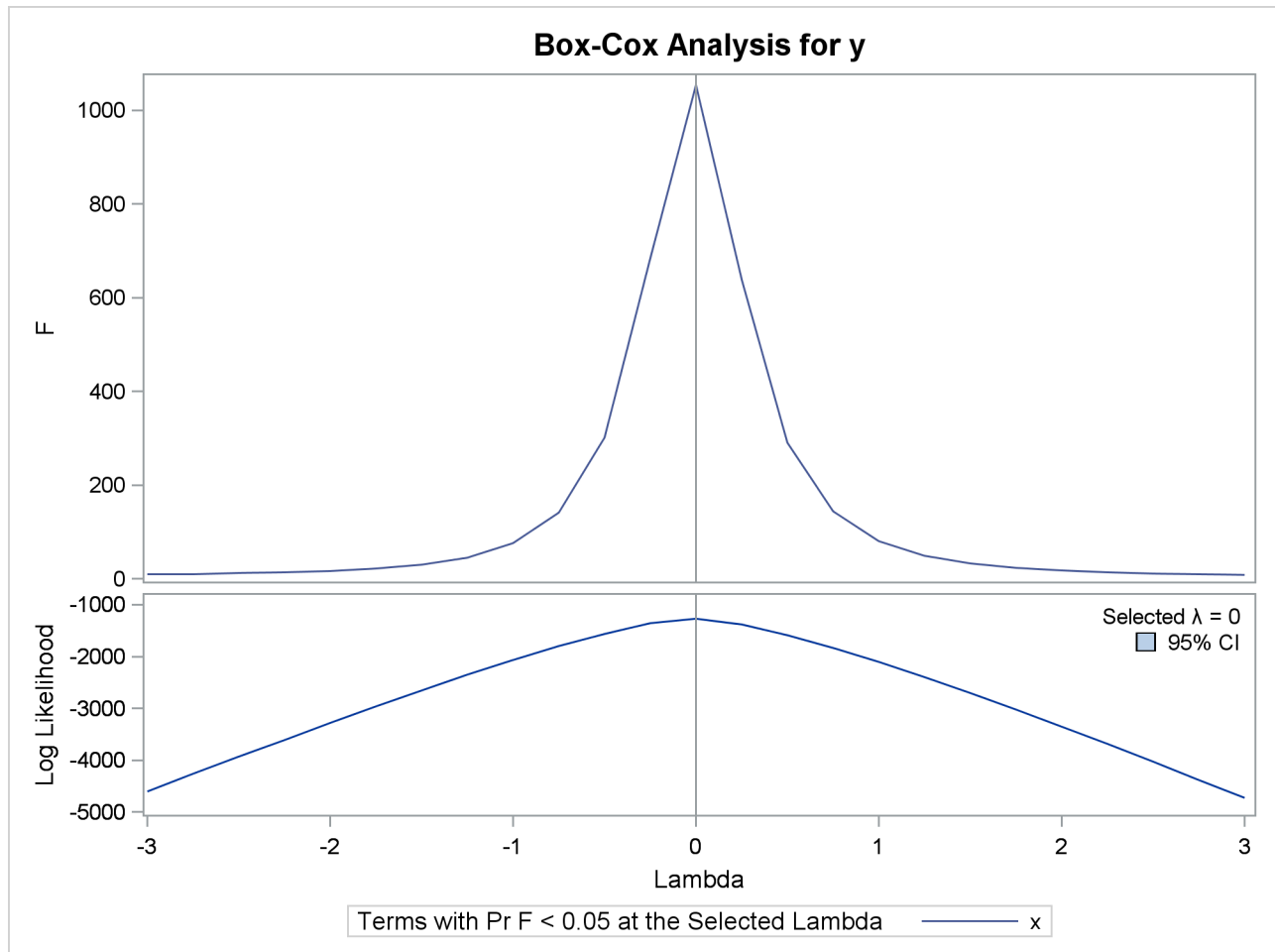


Figure 97.14 shows that PROC TRANSREG correctly selects the log transformation  $\lambda = 0$ , with a narrow confidence interval. The  $F = t^2$  plot shows that  $F$  is at its largest in the vicinity of the optimal Box-Cox transformation.

The rest of the output, which contains the ANOVA results, is shown in Figure 97.15.

Figure 97.15 Basic Box-Cox Example, Default Output

| Dependent Variable BoxCox(y) |     |
|------------------------------|-----|
| Number of Observations Read  | 281 |
| Number of Observations Used  | 281 |

Figure 97.15 continued

| The TRANSREG Procedure Hypothesis Tests for BoxCox(y)                                                                        |                |                |             |         |           |
|------------------------------------------------------------------------------------------------------------------------------|----------------|----------------|-------------|---------|-----------|
| Univariate ANOVA Table Based on the Usual Degrees of Freedom                                                                 |                |                |             |         |           |
| Source                                                                                                                       | DF             | Sum of Squares | Mean Square | F Value | Liberal p |
| Model                                                                                                                        | 1              | 1145.884       | 1145.884    | 1053.66 | >= <.0001 |
| Error                                                                                                                        | 279            | 303.421        | 1.088       |         |           |
| Corrected Total                                                                                                              | 280            | 1449.305       |             |         |           |
| The above statistics are not adjusted for the fact that the dependent variable was transformed and so are generally liberal. |                |                |             |         |           |
|                                                                                                                              | Root MSE       | 1.04285        | R-Square    | 0.7906  |           |
|                                                                                                                              | Dependent Mean | 4.49653        | Adj R-Sq    | 0.7899  |           |
|                                                                                                                              | Coeff Var      | 23.19225       | Lambda      | 0.0000  |           |

This next example uses several options. The `LAMBDA=` *t-option* specifies power parameters sparsely from  $-2$  to  $-0.5$  and  $0.5$  to  $2$  just to get the general shape of the log-likelihood function in that region. Between  $-0.5$  and  $0.5$ , more power parameters are tried. The `CONVENIENT` *t-option* is specified so that if a power parameter like  $\lambda = 1$  or  $\lambda = 0$  is found in the confidence interval, it is used instead of the optimal power parameter. `PARAMETER=2` is specified to add 2 to each  $y$  before performing the transformations. `ALPHA=0.00001` specifies a wide confidence interval.

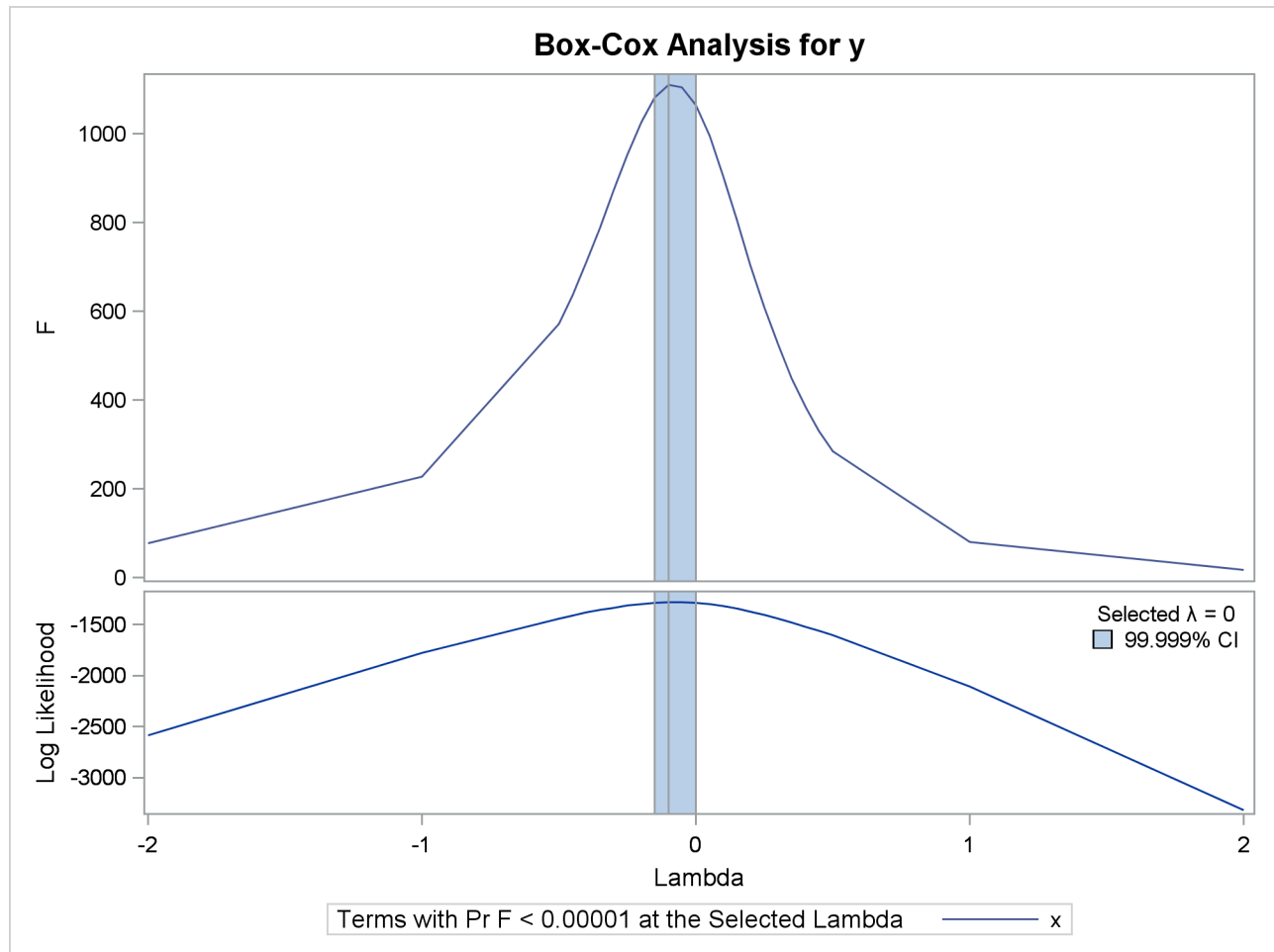
These next statements perform the Box-Cox analysis and produce Figure 97.16 and Figure 97.17:

```

title2 'Several Options Demonstrated';

proc transreg data=x ss2 details
 plots=(transformation(dependent) scatter
 observedbypredicted);
 model BoxCox(y / lambda=-2 -1 -0.5 to 0.5 by 0.05 1 2
 convenient parameter=2 alpha=0.00001) =
 identity(x);
run;

```

**Figure 97.16** Basic Box-Cox Example, Several Options Demonstrated

The results in [Figure 97.16](#) and [Figure 97.17](#) show that the optimal power parameter is  $-0.1$ , but  $0$  is in the confidence interval, and hence a log transformation is chosen. The actual Box-Cox transformation, the original scatter plot, and observed by predicted values plot are shown in [Figure 97.17](#).

**Figure 97.17** Basic Box-Cox Example, Several Options Demonstrated

| Dependent Variable BoxCox(y) |     |
|------------------------------|-----|
| Number of Observations Read  | 281 |
| Number of Observations Used  | 281 |

Figure 97.17 continued

| Model Statement Specification Details |    |             |                                |
|---------------------------------------|----|-------------|--------------------------------|
| Type                                  | DF | Variable    | Description Value              |
| Dep                                   | 1  | BoxCox(y)   | Lambda Used 0                  |
|                                       |    |             | Lambda -0.1                    |
|                                       |    |             | Log Likelihood -1280.1         |
|                                       |    |             | Conv. Lambda 0                 |
|                                       |    |             | Conv. Lambda LL -1287.7        |
|                                       |    |             | CI Limit -1289.9               |
|                                       |    |             | Alpha 0.00001                  |
|                                       |    |             | Parameter 2                    |
|                                       |    |             | Options Convenient Lambda Used |
| Ind                                   | 1  | Identity(x) | DF 1                           |

The TRANSREG Procedure Hypothesis Tests for BoxCox(y)

Univariate ANOVA Table Based on the Usual Degrees of Freedom

| Source          | DF  | Sum of Squares | Mean Square | F Value | Liberal p |
|-----------------|-----|----------------|-------------|---------|-----------|
| Model           | 1   | 999.438        | 999.4381    | 1064.82 | >= <.0001 |
| Error           | 279 | 261.868        | 0.9386      |         |           |
| Corrected Total | 280 | 1261.306       |             |         |           |

The above statistics are not adjusted for the fact that the dependent variable was transformed and so are generally liberal.

|                |          |          |        |
|----------------|----------|----------|--------|
| Root MSE       | 0.96881  | R-Square | 0.7924 |
| Dependent Mean | 4.61429  | Adj R-Sq | 0.7916 |
| Coeff Var      | 20.99591 | Lambda   | 0.0000 |

Univariate Regression Table Based on the Usual Degrees of Freedom

| Variable    | DF | Coefficient | Type II Sum of Squares | Mean Square | F Value | Liberal p |
|-------------|----|-------------|------------------------|-------------|---------|-----------|
| Intercept   | 1  | 0.42939328  | 8.746                  | 8.746       | 9.32    | >= 0.0025 |
| Identity(x) | 1  | 0.92997620  | 999.438                | 999.438     | 1064.82 | >= <.0001 |

The above statistics are not adjusted for the fact that the dependent variable was transformed and so are generally liberal.

Figure 97.17 continued

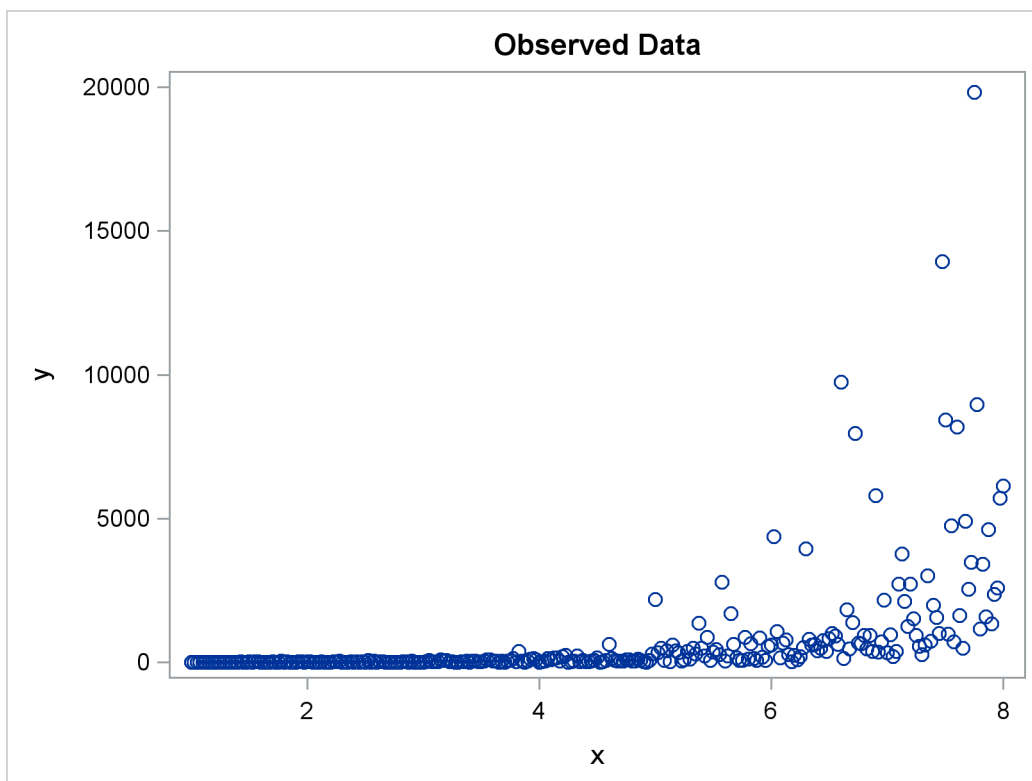
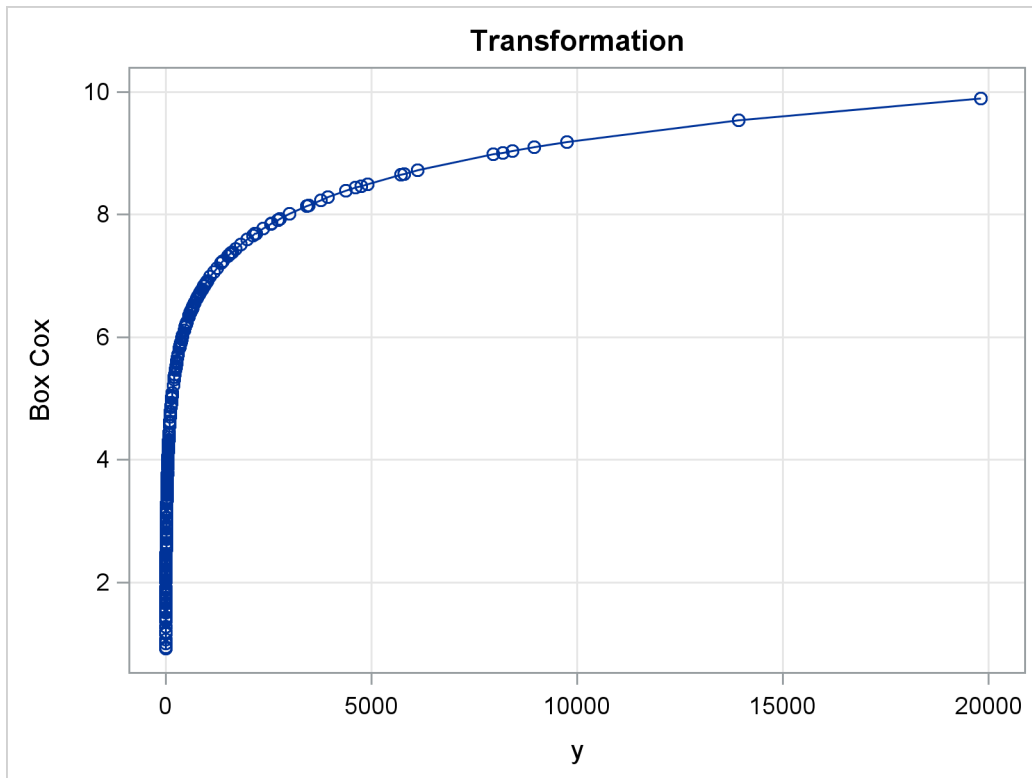
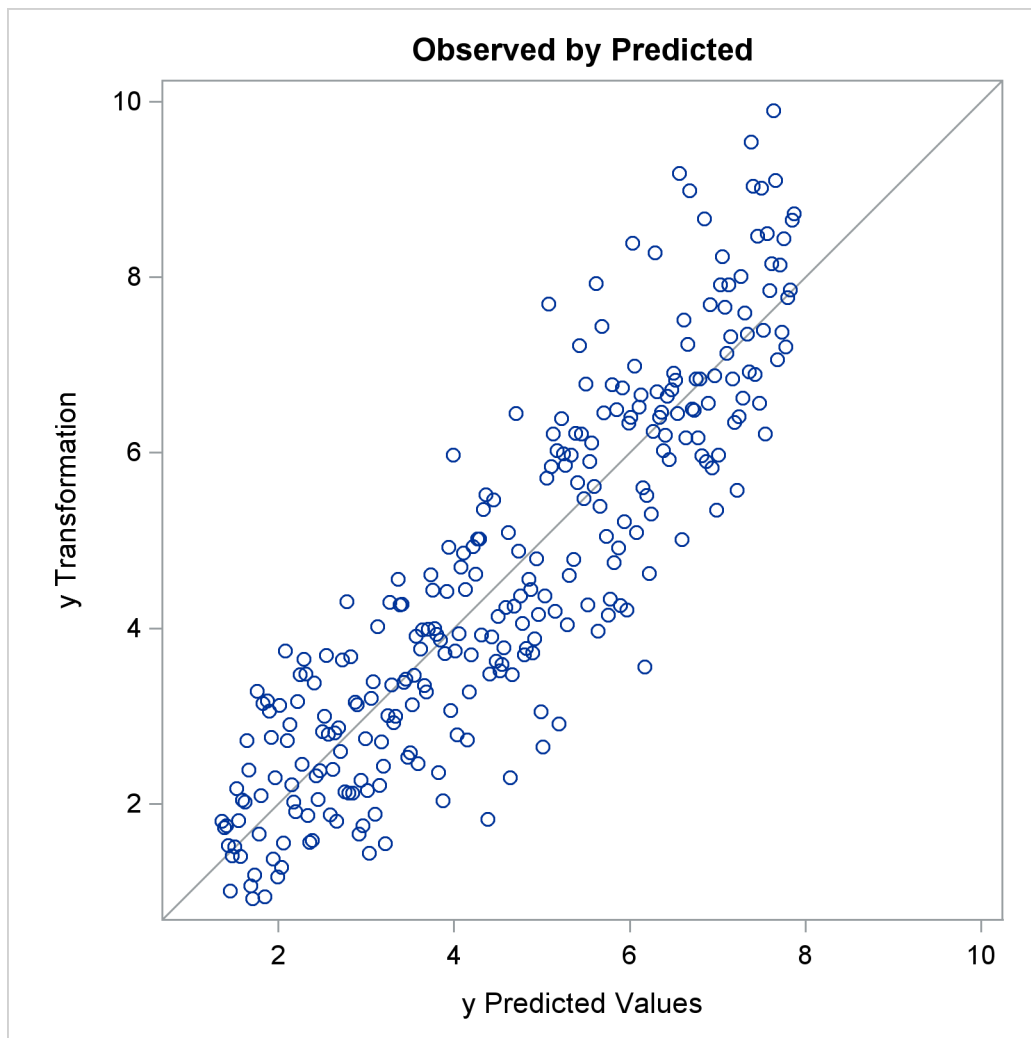




Figure 97.17 continued



The next example shows how to find a Box-Cox transformation without an independent variable. This seeks to normalize the univariate histogram. This example generates 500 random observations from a lognormal distribution. In addition, a constant variable  $z$  is created that is all zero. This is because PROC TRANSREG requires some independent variable to be specified, even if it is constant. Two options are specified in the PROC TRANSREG statement. `MAXITER=0` is specified because the Box-Cox transformation is performed before any iterations are begun. No iterations are needed since no other work is required. The `NOZERO-CONSTANT` *a-option* (which can be abbreviated `NOZ`) is specified so that PROC TRANSREG does not print any warnings when it encounters the constant independent variable. The MODEL statement asks for a Box-Cox transformation of  $y$  and an IDENTITY transformation (which does nothing) of the constant variable  $z$ . Finally, PROC UNIVARIATE is run to show a histogram of the original variable  $y$ , and the Box-Cox transformation,  $T_y$ . The following statements fit the univariate Box-Cox model and produce Figure 97.18:

```

title 'Univariate Box-Cox';

data x;
 call streaminit(17);
 z = 0;
 do i = 1 to 500;
 y = rand('lognormal');
 output;
 end;
run;

proc transreg maxiter=0 nozeroconstant;
 model BoxCox(y) = identity(z);
 output;
run;

proc univariate noprint;
 histogram y ty;
run;

```

The PROC TRANSREG results in Figure 97.18 show that zero is chosen for lambda, so a log transformation is chosen. The first histogram shows that the original data are skewed, but a log transformation makes the data appear much more nearly normal.

**Figure 97.18** Box-Cox with No Independent Variable

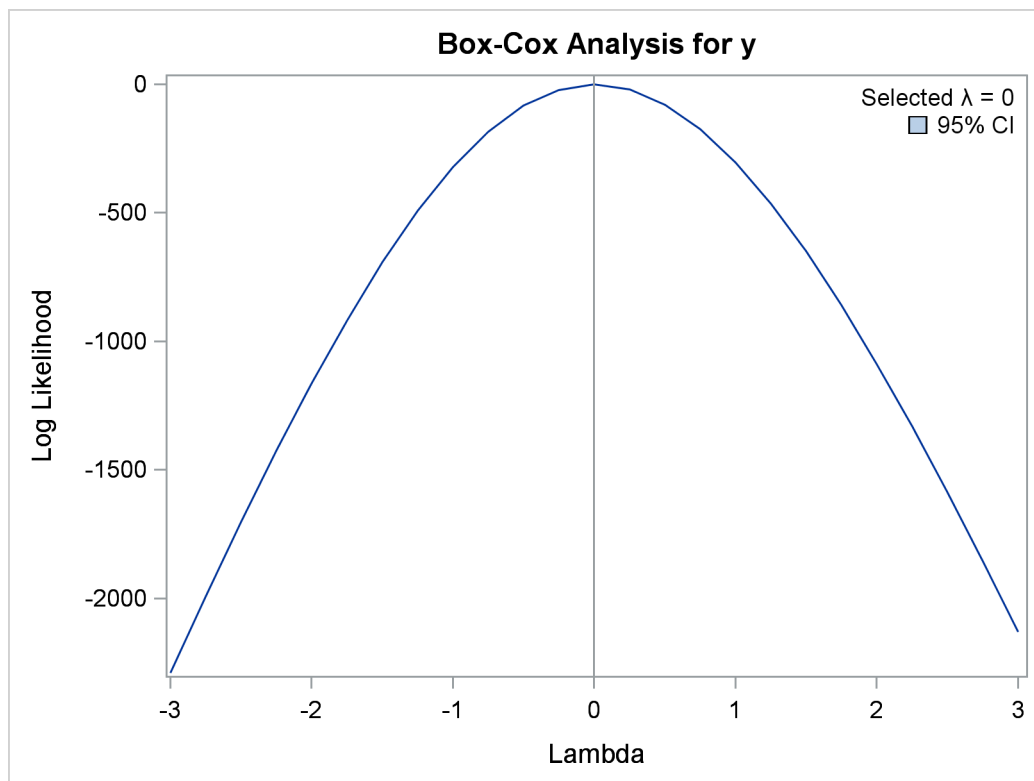
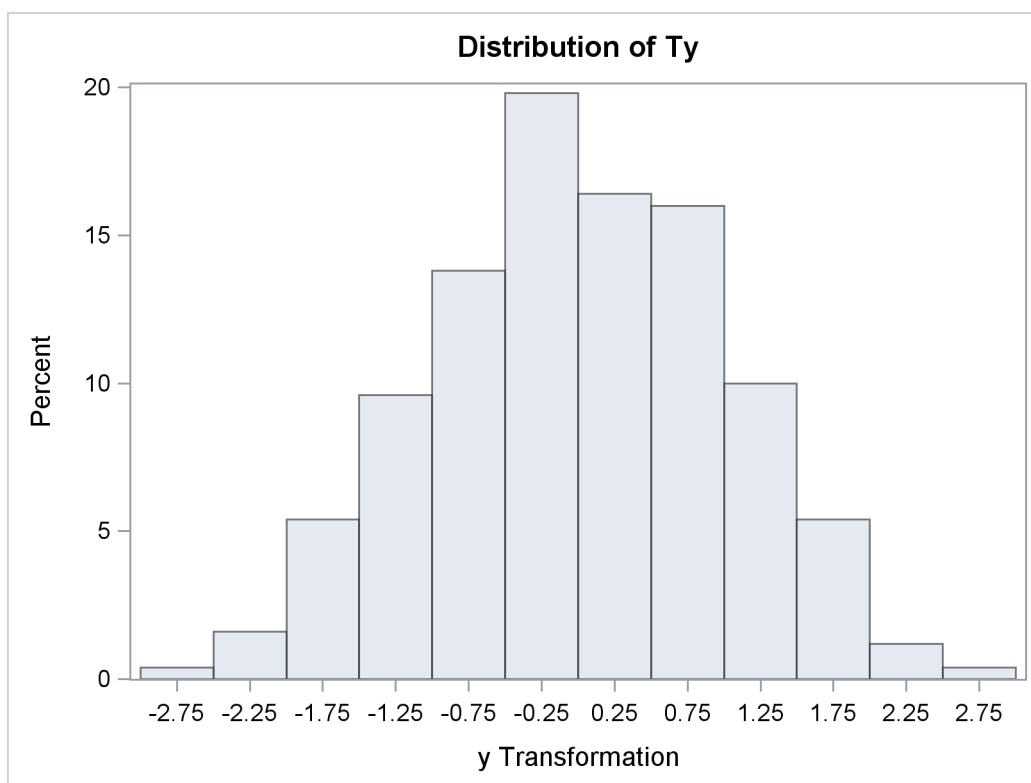
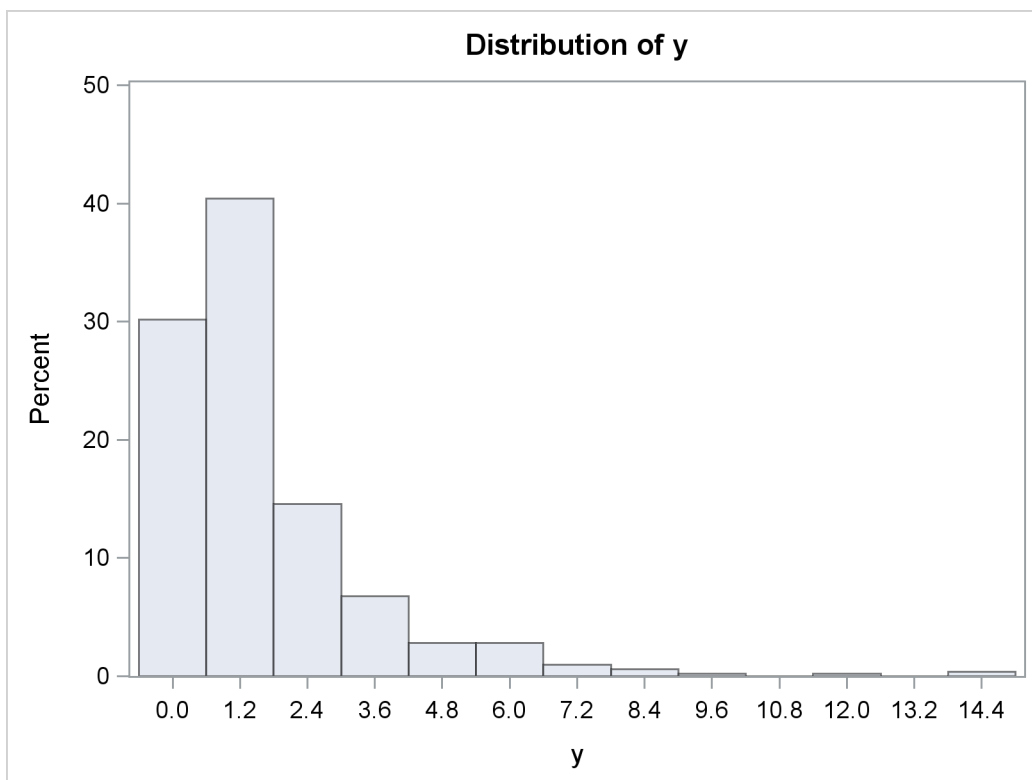


Figure 97.18 continued



## Using Splines and Knots

This section illustrates some properties of splines. *Splines* are curves, and they are usually required to be continuous and smooth. Splines are usually defined as piecewise polynomials of degree  $n$  with function values and first  $n - 1$  derivatives that agree at the points where they join. The abscissa or X-axis values of the join points are called *knots*. The term “spline” is also used for polynomials (splines with no knots) and piecewise polynomials with more than one discontinuous derivative. Splines with no knots are generally smoother than splines with knots, which are generally smoother than splines with multiple discontinuous derivatives. Splines with few knots are generally smoother than splines with many knots; however, increasing the number of knots usually increases the fit of the spline function to the data. Knots give the curve freedom to bend to more closely follow the data. See Smith (1979) for an excellent introduction to splines.

In this section, an artificial data set is created with a variable  $y$  that is a discontinuous function of  $x$ . (See Figure 97.20.) Notice that the function has four unconnected parts, each of which is a curve. Notice too that there is an overall quadratic trend—that is, ignoring the shapes of the individual curves, at first the  $y$  values tend to decrease as  $x$  increases, then  $y$  values tend to increase. While these artificial data are clearly not realistic, their distinct pattern helps illustrate how splines work. The following statements create the data set, fit a simple linear regression model, and produce Figure 97.19 through Figure 97.20:

```

title 'An Illustration of Splines and Knots';

* Create in y a discontinuous function of x.;

data a;
 x = -0.000001;
 do i = 0 to 199;
 if mod(i, 50) = 0 then do;
 c = ((x / 2) - 5)**2;
 if i = 150 then c = c + 5;
 y = c;
 end;
 x = x + 0.1;
 y = y - sin(x - c);
 output;
 end;
run;

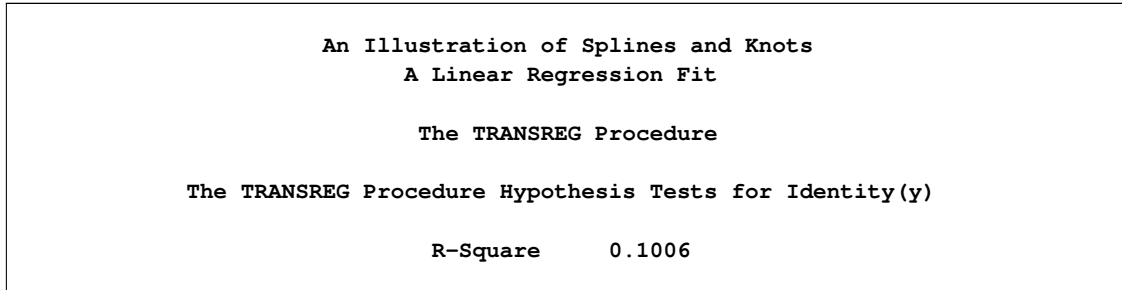
ods graphics on;

title2 'A Linear Regression Fit';
proc transreg data=a plots=scatter rsquare;
 model identity(y) = identity(x);
run;

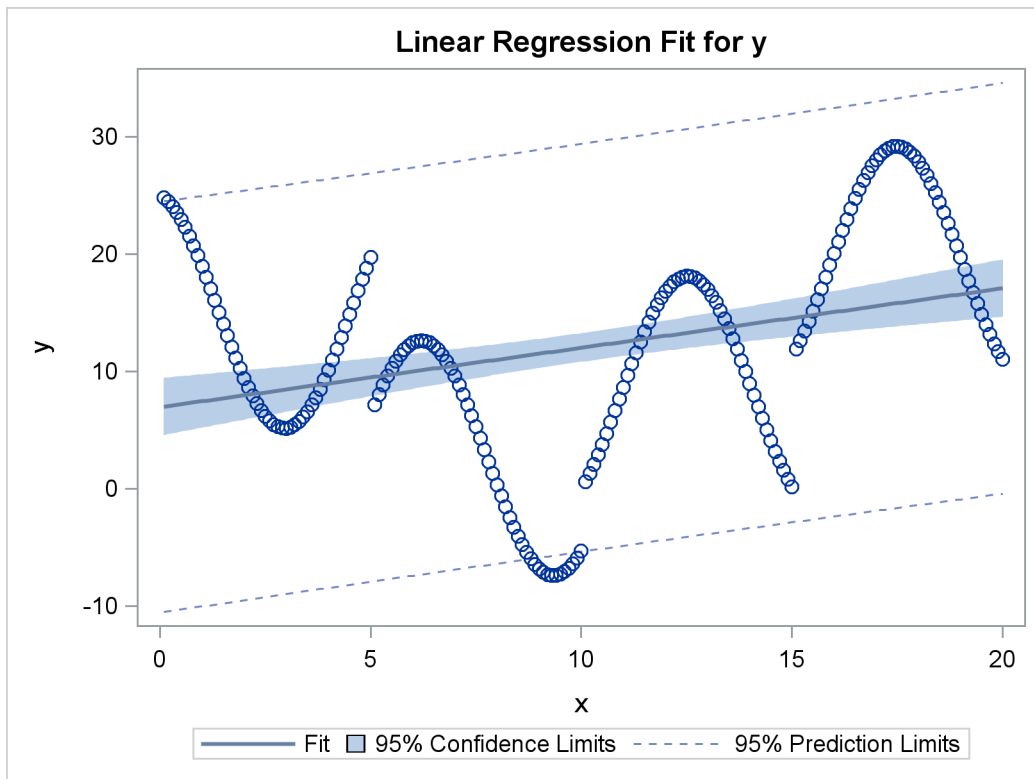
```

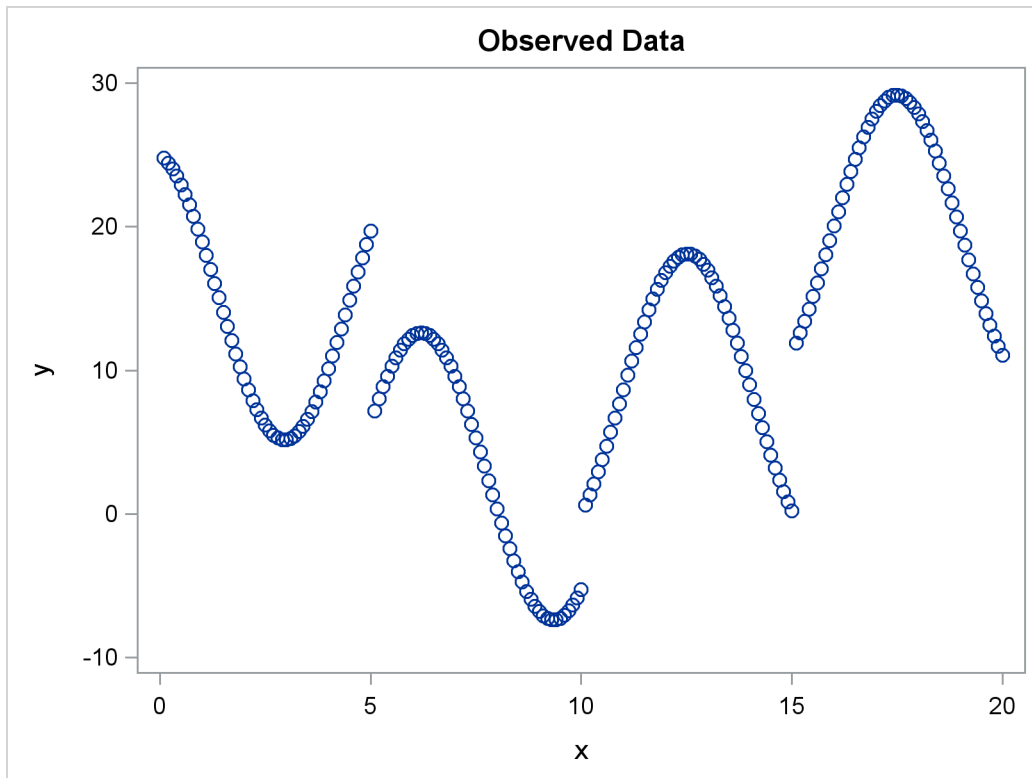
The R square for the linear regression is 0.1006. The linear fit results in Figure 97.19 show the predicted values of y given x. It can clearly be seen in Figure 97.19 that the linear regression model is not appropriate for these data.

**Figure 97.19** A Linear Regression Fit



**Figure 97.19** continued



**Figure 97.20** The Original Scatter Plot

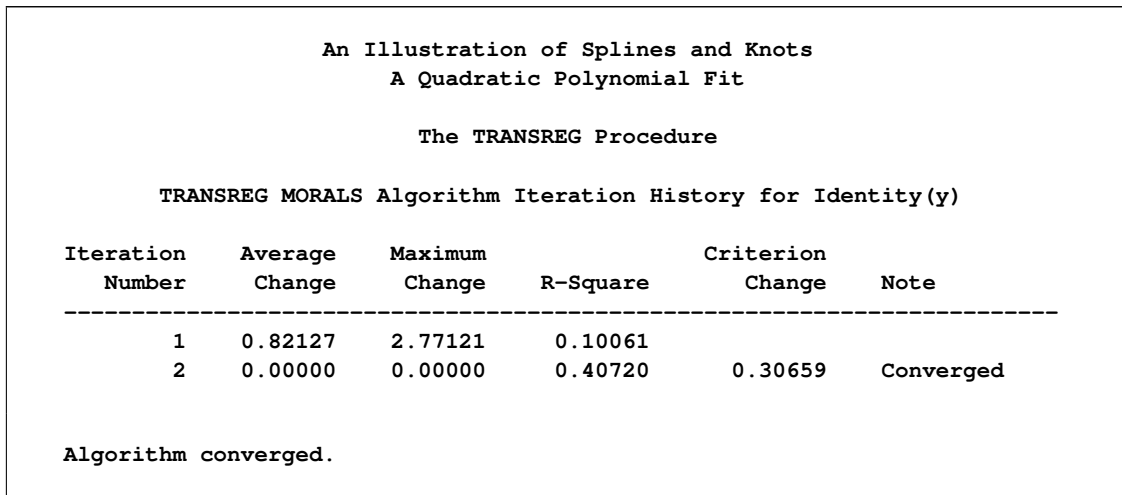
The next PROC TRANSREG step finds a degree-two spline transformation with no knots, which is a quadratic polynomial. The spline is a weighted sum of a single constant, a single straight line, and a single quadratic curve. The following statements perform the quadratic analysis and produce Figure 97.21:

```
title2 'A Quadratic Polynomial Fit';

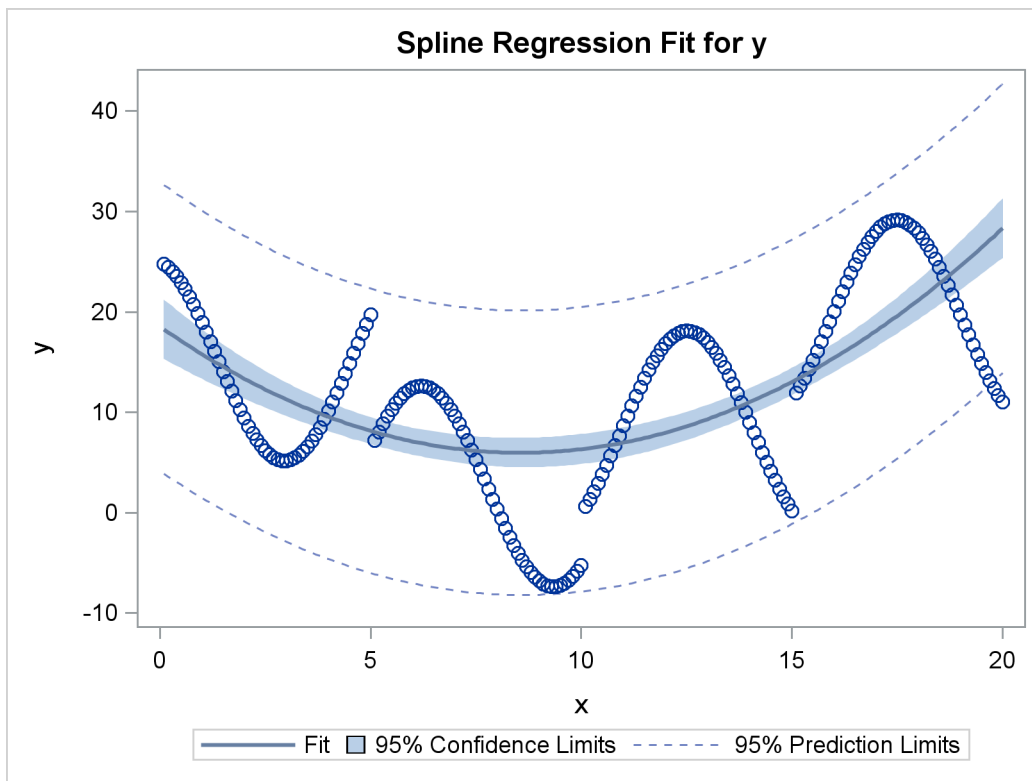
proc transreg data=A;
 model identity(y)=spline(x / degree=2);
run;
```

The R square in Figure 97.21 increases from 0.10061, which is the linear fit value from before, to 0.40720. The plot shows that the quadratic regression function does not fit any of the individual curves well, but it does follow the overall trend in the data. Since the overall trend is quadratic, if you were to fit a degree-three spline with no knots (not shown) would increase R square by only a small amount.

**Figure 97.21** A Quadratic Polynomial Fit



**Figure 97.21** continued



The next step uses the default degree of three, for a piecewise cubic polynomial, and requests knots at the known break points,  $x=5$ , 10, and 15. This requests a spline that is continuous, has continuous first and second derivatives, and has a third derivative that is discontinuous at 5, 10, and 15. The spline is a weighted sum of a single constant, a single straight line, a single quadratic curve, a cubic curve for the portion of  $x$  less than 5, a different cubic curve for the portion of  $x$  between 5 and 10, a different cubic curve for the portion of  $x$  between 10 and 15, and another cubic curve for the portion of  $x$  greater than 15. The following statements fit the spline model and produce [Figure 97.22](#):

```
title2 'A Cubic Spline Fit with Knots at X=5, 10, 15';

proc transreg data=a;
 model identity(y) = spline(x / knots=5 10 15);
run;
```

The new R square in [Figure 97.22](#) is 0.61730. The plot shows that the spline is less smooth than the quadratic polynomial and follows the data more closely than the quadratic polynomial.

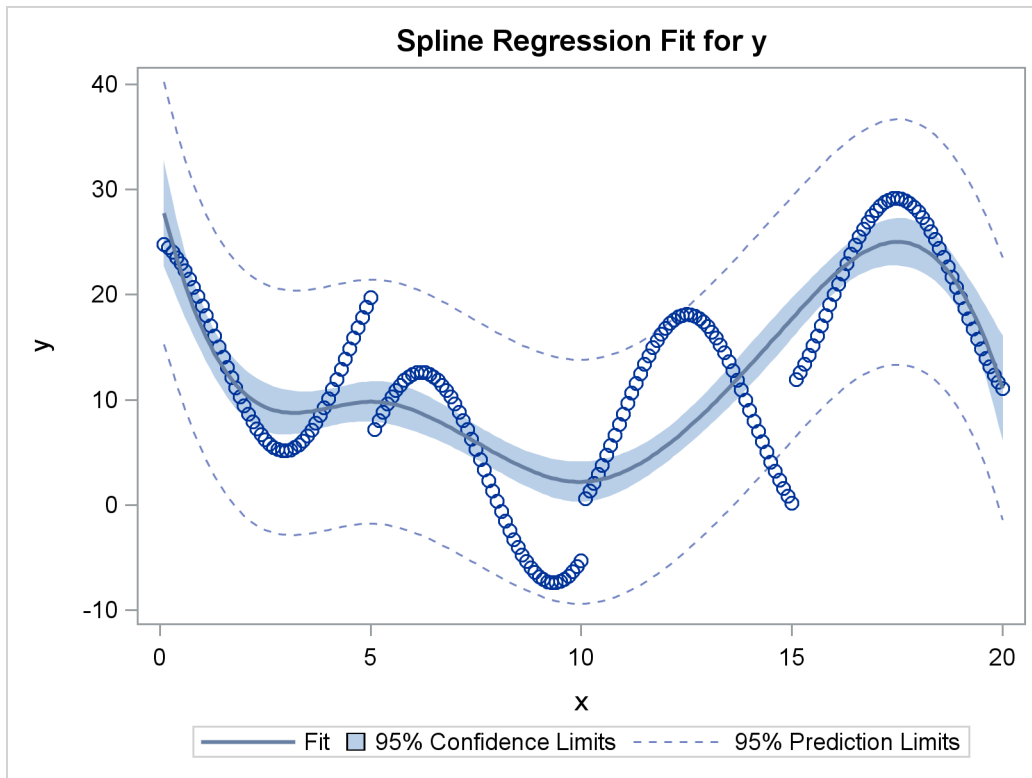
**Figure 97.22** A Cubic Spline Fit

| An Illustration of Splines and Knots                        |                   |                   |          |                     |           |
|-------------------------------------------------------------|-------------------|-------------------|----------|---------------------|-----------|
| A Cubic Spline Fit with Knots at X=5, 10, 15                |                   |                   |          |                     |           |
| The TRANSREG Procedure                                      |                   |                   |          |                     |           |
| TRANSREG MORALS Algorithm Iteration History for Identity(y) |                   |                   |          |                     |           |
| Iteration<br>Number                                         | Average<br>Change | Maximum<br>Change | R-Square | Criterion<br>Change | Note      |
| 1                                                           | 0.85367           | 3.88449           | 0.10061  |                     |           |
| 2                                                           | 0.00000           | 0.00000           | 0.61730  | 0.51670             | Converged |

Algorithm converged.



Figure 97.22 continued



The same model could be fit with a DATA step and PROC REG, as follows:

```

data b; /* A is the data set used by transreg */
 set a(keep=x y);
 x1=x; /* x */
 x2=x**2; /* x squared */
 x3=x**3; /* x cubed */
 x4=(x> 5)*((x-5)**3); /* change in x**3 after 5 */
 x5=(x>10)*((x-10)**3); /* change in x**3 after 10 */
 x6=(x>15)*((x-15)**3); /* change in x**3 after 15 */
run;

proc reg;
 model y=x1-x6;
run; quit;

```

The output from these previous statements is not displayed. The assignment statements and comments show how you can construct terms that can be used to fit the same model.

In the next step, each knot is repeated three times, so the first, second, and third derivatives are discontinuous at  $x=5$ , 10, and 15, but the spline is continuous at the knots. The spline is a weighted sum of the following:

- a single constant
- a line for the portion of  $x$  less than 5
- a quadratic curve for the portion of  $x$  less than 5
- a cubic curve for the portion of  $x$  less than 5
- a different line for the portion of  $x$  between 5 and 10
- a different quadratic curve for the portion of  $x$  between 5 and 10
- a different cubic curve for the portion of  $x$  between 5 and 10
- a different line for the portion of  $x$  between 10 and 15
- a different quadratic curve for the portion of  $x$  between 10 and 15
- a different cubic curve for the portion of  $x$  between 10 and 15
- another line for the portion of  $x$  greater than 15
- another quadratic curve for the portion of  $x$  greater than 15
- another cubic curve for the portion of  $x$  greater than 15

The spline is continuous since there is not a separate constant or separate intercept in the formula for the spline for each knot. The following statements perform this analysis and produce [Figure 97.23](#):

```
title3 'First - Third Derivatives Discontinuous at X=5, 10, 15';

proc transreg data=a;
 model identity(y) = spline(x / knots=5 5 5 10 10 10 15 15 15);
run;
```

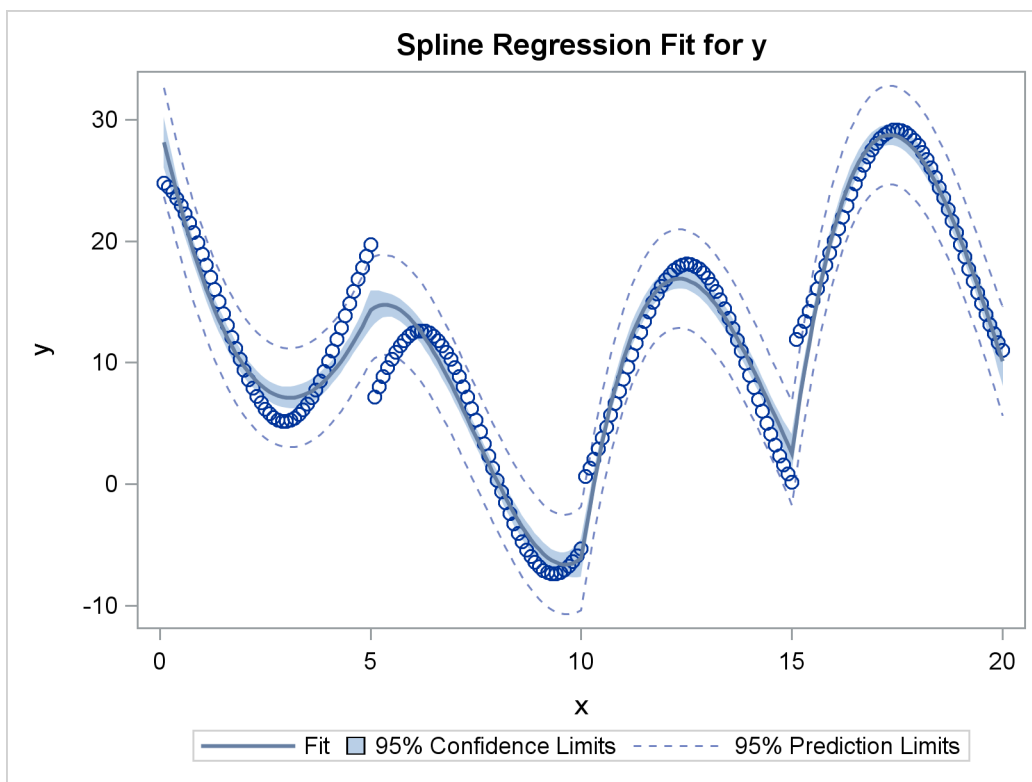
Now the R square in [Figure 97.23](#) is 0.95542, and the spline closely follows the data, except at the knots.

**Figure 97.23** Spline with Discontinuous Derivatives

| An Illustration of Splines and Knots                        |                   |                   |          |                     |           |
|-------------------------------------------------------------|-------------------|-------------------|----------|---------------------|-----------|
| A Cubic Spline Fit with Knots at X=5, 10, 15                |                   |                   |          |                     |           |
| First - Third Derivatives Discontinuous at X=5, 10, 15      |                   |                   |          |                     |           |
| The TRANSREG Procedure                                      |                   |                   |          |                     |           |
| TRANSREG MORALS Algorithm Iteration History for Identity(y) |                   |                   |          |                     |           |
| Iteration<br>Number                                         | Average<br>Change | Maximum<br>Change | R-Square | Criterion<br>Change | Note      |
| 1                                                           | 0.92492           | 3.50038           | 0.10061  |                     |           |
| 2                                                           | 0.00000           | 0.00000           | 0.95542  | 0.85481             | Converged |

Algorithm converged.

Figure 97.23 continued



The same model could be fit with a DATA step and PROC REG, as follows:

```

data b;
 set a(keep=x y);
 x1=x; /* x */
 x2=x**2; /* x squared */
 x3=x**3; /* x cubed */
 x4=(x>5) * (x-5); /* change in x after 5 */
 x5=(x>10) * (x-10); /* change in x after 10 */
 x6=(x>15) * (x-15); /* change in x after 15 */
 x7=(x>5) * ((x-5)**2); /* change in x**2 after 5 */
 x8=(x>10) * ((x-10)**2); /* change in x**2 after 10 */
 x9=(x>15) * ((x-15)**2); /* change in x**2 after 15 */
 x10=(x>5) * ((x-5)**3); /* change in x**3 after 5 */
 x11=(x>10) * ((x-10)**3); /* change in x**3 after 10 */
 x12=(x>15) * ((x-15)**3); /* change in x**3 after 15 */
run;

proc reg;
 model y=x1-x12;
run; quit;

```

The output from these previous statements is not displayed. The assignment statements and comments show how you can construct terms that can be used to fit the same model.

Each knot is repeated four times in the next step. Now the spline function is discontinuous at the knots, and it can follow the data more closely. The following statements perform this analysis and produce [Figure 97.24](#):

```

title3 'Discontinuous Function and Derivatives';

proc transreg data=a;
 model identity(y) = spline(x / knots=5 5 5 5 10 10 10 10
 15 15 15 15);
run;

```

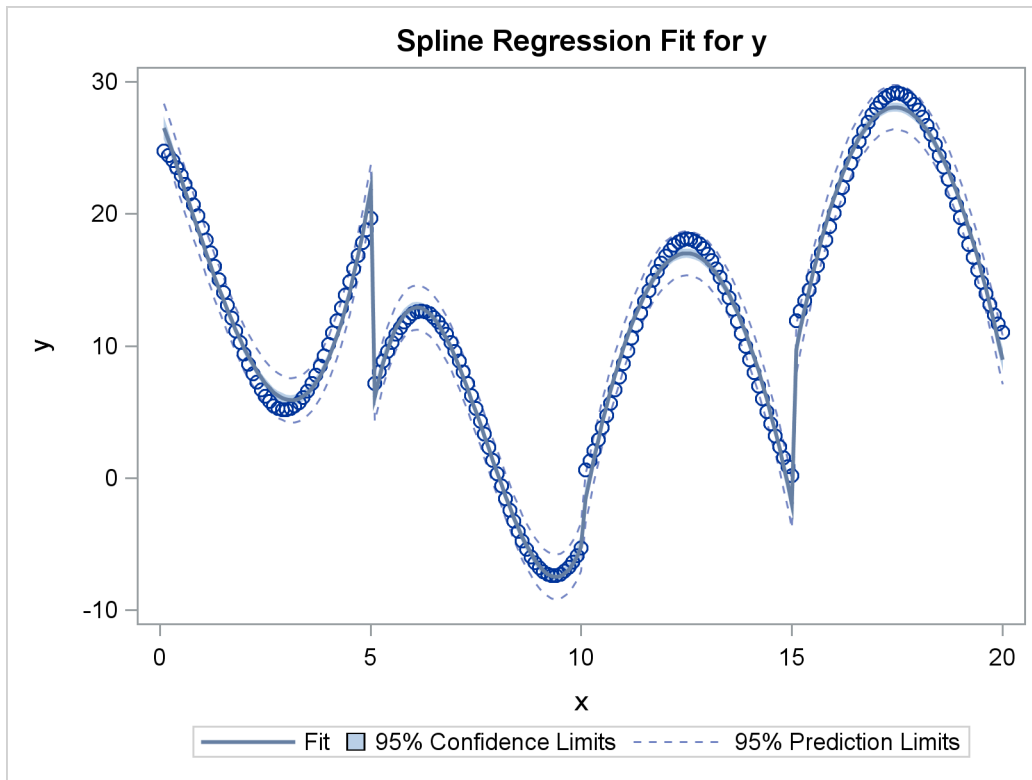
Now the R square in [Figure 97.24](#) is 0.99254. In this step, each separate curve is approximated by a cubic polynomial (with no knots within the separate polynomials). (Note, however, that the separate functions are connected in the plot, because PROC TRANSREG cannot currently produce separate functions for a model like this. Usually, you would use a CLASS variable to get separate functions.)

**Figure 97.24** Discontinuous Spline Fit

| An Illustration of Splines and Knots<br>A Cubic Spline Fit with Knots at X=5, 10, 15<br>Discontinuous Function and Derivatives |                   |                   |          |                     |           |
|--------------------------------------------------------------------------------------------------------------------------------|-------------------|-------------------|----------|---------------------|-----------|
| The TRANSREG Procedure                                                                                                         |                   |                   |          |                     |           |
| TRANSREG MORALS Algorithm Iteration History for Identity(y)                                                                    |                   |                   |          |                     |           |
| Iteration<br>Number                                                                                                            | Average<br>Change | Maximum<br>Change | R-Square | Criterion<br>Change | Note      |
| 1                                                                                                                              | 0.90271           | 3.29184           | 0.10061  |                     |           |
| 2                                                                                                                              | 0.00000           | 0.00000           | 0.99254  | 0.89193             | Converged |

Algorithm converged.

Figure 97.24 continued



To solve this problem with a DATA step and PROC REG, you would need to create all of the variables in the preceding DATA step (the B data set for the piecewise polynomial with discontinuous third derivatives), plus the following three variables:

```
x13=(x > 5); /* intercept change after 5 */
x14=(x > 10); /* intercept change after 10 */
x15=(x > 15); /* intercept change after 15 */
```

The next two examples use the `NKNOTS=` *t-option* to specify the number of knots but not their location. `NKNOTS=4` places knots at the quintiles, whereas `NKNOTS=9` places knots at the deciles. The spline and its first two derivatives are continuous. The following statements produce [Figure 97.25](#) and [Figure 97.26](#):

```
title3 'Four Knots';

proc transreg data=a;
 model identity(y) = spline(x / nknots=4);
run;

title3 'Nine Knots';

proc transreg data=a;
 model identity(y) = spline(x / nknots=9);
run;
```

The R-square values displayed in [Figure 97.25](#) and [Figure 97.26](#) are 0.74450 and 0.95256, respectively. Even though the knots are not optimally placed, the spline can closely follow the data with `NKNOTS=9`.

**Figure 97.25** Spline Fit with Knots at the Quintiles

| An Illustration of Splines and Knots                        |                   |                   |          |                     |           |
|-------------------------------------------------------------|-------------------|-------------------|----------|---------------------|-----------|
| A Cubic Spline Fit with Knots at X=5, 10, 15                |                   |                   |          |                     |           |
| Four Knots                                                  |                   |                   |          |                     |           |
| The TRANSREG Procedure                                      |                   |                   |          |                     |           |
| TRANSREG MORALS Algorithm Iteration History for Identity(y) |                   |                   |          |                     |           |
| Iteration<br>Number                                         | Average<br>Change | Maximum<br>Change | R-Square | Criterion<br>Change | Note      |
| 1                                                           | 0.90305           | 4.46027           | 0.10061  |                     |           |
| 2                                                           | 0.00000           | 0.00000           | 0.74450  | 0.64389             | Converged |

Algorithm converged.

Figure 97.25 continued

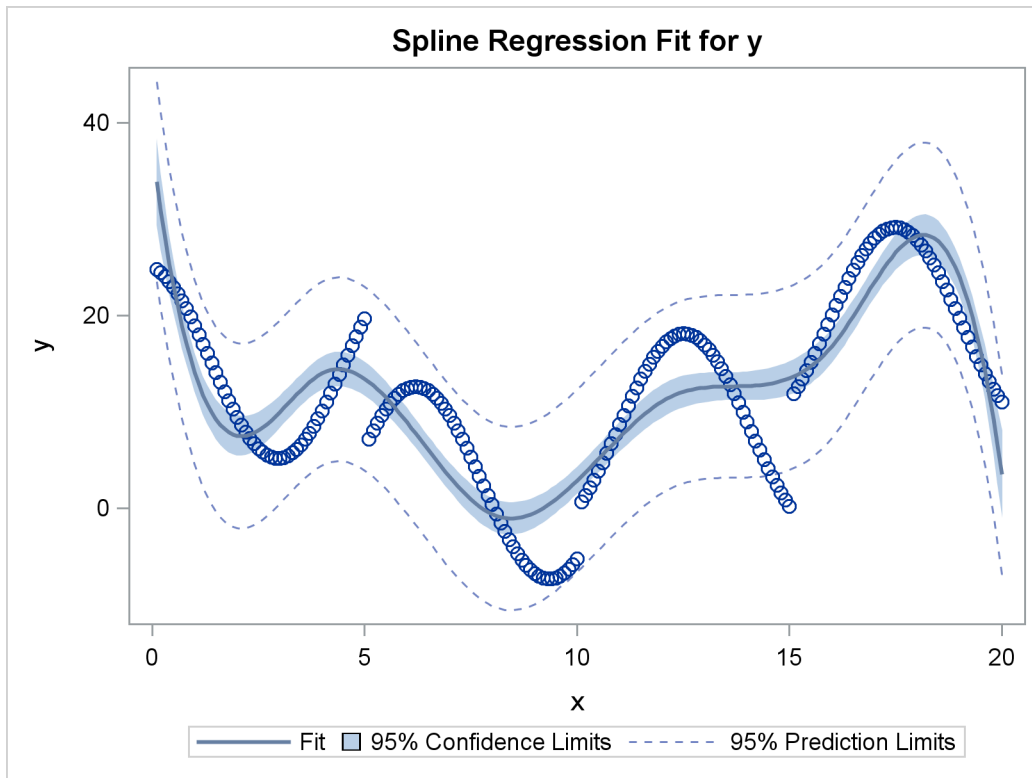


Figure 97.26 Spline Fit with Knots at the Deciles

An Illustration of Splines and Knots  
A Cubic Spline Fit with Knots at X=5, 10, 15  
Nine Knots

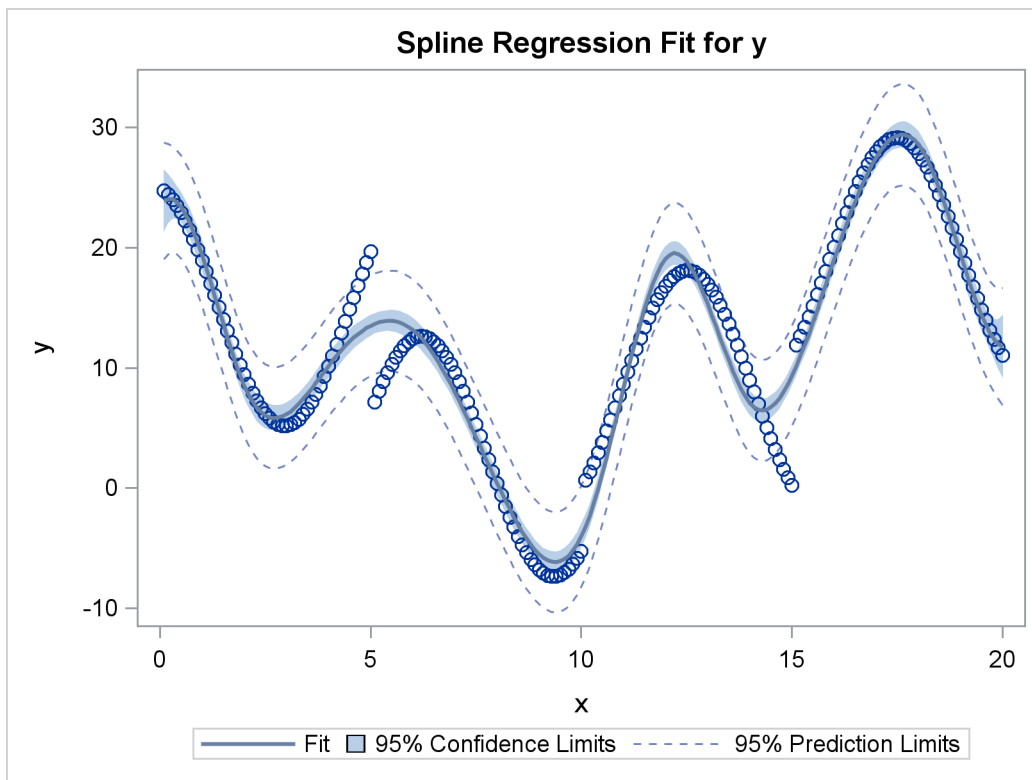
The TRANSREG Procedure

TRANSREG MORALS Algorithm Iteration History for Identity(y)

| Iteration Number | Average Change | Maximum Change | R-Square | Criterion Change | Note      |
|------------------|----------------|----------------|----------|------------------|-----------|
| 1                | 0.94832        | 3.03488        | 0.10061  |                  |           |
| 2                | 0.00000        | 0.00000        | 0.95256  | 0.85196          | Converged |

Algorithm converged.

Figure 97.26 continued



## Scoring Spline Variables

This section shows you how to find spline transformations of variables in one data set and apply the same transformations to variables in another data set. This is illustrated with artificial data. In these data sets, the variable  $y$  is approximately a linear function of nonlinear transformations of the variables  $x$ ,  $w$ , and  $z$ . The model is fit using data set  $X$ , and those results are used to score data set  $Z$ . The following statements create the two data sets:

```

title 'An Illustration of Splines and Knots';
title2 'Scoring Spline Variables';

data x;
 do i = 1 to 5000;
 w = normal(7);
 x = normal(7);
 z = normal(7);
 y = w * w + log(5 + x) + sin(z) + normal(7);
 output;
 end;
run;

```



```

data z;
 do i = 1 to 5000;
 w = normal(1);
 x = normal(1);
 z = normal(1);
 y = w * w + log(5 + x) + sin(z) + normal(1);
 output;
 end;
run;

```

First, you run PROC TRANSREG to fit the transformation regression model asking for spline transformations of the three independent variables. You must use the `EXKNOTS= t-option`, because you need to use the same knots, both interior and exterior, with both data sets. By default, the exterior knots will be different if the minima and maxima are different in the two data sets, so you get the wrong results if you do not specify the `EXKNOTS= t-option` with values less than the minima and greater than the maxima of the six `x`, `y`, and `w` variables. If the ranges in all three pairs were different, you would need separate spline transformation for each variable with different knot and exterior knot specifications. The following statements fit the spline model:

```

proc transreg data=x solve details ss2;
 ods output splinecoef=c;
 model identity(y) = spline(w x z / knots=-1.5 to 1.5 by 0.5
 exknots=-5 5);
 output out=d;
run;

```

The results of this step are not displayed. The nonprinting “SplineCoef” table is output to a SAS data set. This data set contains the coefficients that were used to get the spline transformations and can be used to transform variables in other data sets. These coefficients are also in the details table. However, in the “SplineCoef” table, they are in a form directly suitable for use with PROC SCORE.

The next step reads the second input data set, `Z`, and generates an output data set with the B-spline basis for each of the variables:

```

proc transreg data=z design;
 model bspl(w x z / knots=-1.5 to 1.5 by 0.5 exknots=-5 5);
 output out=b;
run;

```

Note that the same interior and exterior knots are used in both of the previous steps. The next three steps score the B-spline bases created in the previous step by using the coefficients generated in the first PROC TRANSREG step. PROC SCORE is run once for each `SPLINE` variable in the statements that follow:

```

proc score data=b score=c out=o1(rename=(spline=bw w=nw));
 var w;;
run;

proc score data=b score=c out=o2(rename=(spline=bx x=nx));
 var x;;
run;

proc score data=b score=c out=o3(rename=(spline=bz z=nz));
 var z;;
run;

```

The following steps merge the three transformations with the original data and plot the results:

```

data all;
 merge d(keep=w x z tw tx tz) o1(keep=nw bw)
 o2(keep=nx bx) o3(keep=nz bz);
run;

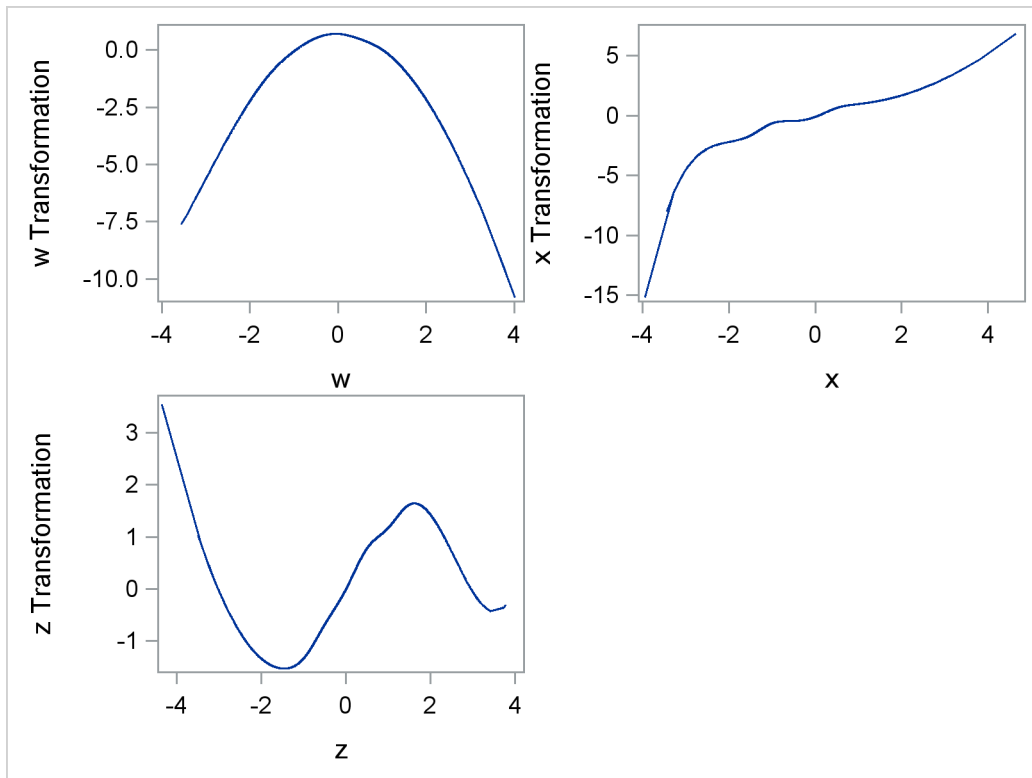
proc template;
 define statgraph twobytwo;
 begingraph;
 layout lattice / rows=2 columns=2;
 layout overlay;
 seriesplot y=tw x=w / connectorder=xaxis;
 seriesplot y=bw x=nw / connectorder=xaxis;
 endlayout;
 layout overlay;
 seriesplot y=tx x=x / connectorder=xaxis;
 seriesplot y=bx x=nx / connectorder=xaxis;
 endlayout;
 layout overlay;
 seriesplot y=tz x=z / connectorder=xaxis;
 seriesplot y=bz x=nz / connectorder=xaxis;
 endlayout;
 endlayout;
 endgraph;
 end;
run;

proc sgrender data=all template=twobytwo;
run;

```

The plots in [Figure 97.27](#) show that the two transformations for each variable, original and scored, are the same function. The two functions in each plot are on top of each other and are indistinguishable. Furthermore, PROC TRANSREG found the functional forms that were used to generate the data: quadratic for w, log for x, and sine for z.

Figure 97.27 Scoring Spline Variables Example



The next statements show how to run PROC TRANSREG, output the interior and exterior knots to an output data set with ODS, extract the knots, and use them in a DATA step to re-create the B-spline basis that PROC TRANSREG makes. In practice, you would never need to use a DATA step to make the B-spline basis since PROC TRANSREG does it automatically. The following statements show how you could do it yourself:

```
data x;
 input x @@;
 datalines;
1 2 3 4 5 6 7 8 9 10
;

ods output details=d;
proc transreg details design;
 model bspline(x / nkn=3);
 output out=y;
run;
```

```

%let k = 0;
data d;
 set d;
 length d $ 20;
 retain d ' ';
 if description ne ' ' then d = description;
 if d = 'Degree' then call symput('d', compress(formattedvalue));
 if d = 'Number of Knots'
 then call symput('k', compress(formattedvalue));
 if index(d, 'Knots') and not index(d, 'Number');
 keep d numericvalue;
run;

%let nkn = %eval(&d * 2 + &k); /* total number of knots */
%let nb = %eval(&d + 1 + &k); /* number of cols in basis */

proc transpose data=d out=k(drop=_name_) prefix=Knot;
run;

proc print; format k: 20.16;
run;

data b(keep=x:);
 if _n_ = 1 then set k; /* read knots from transreg */
 array k[&nkn] knot1-knot&nkn; /* knots */
 array b[&nb] x_0 - x_%eval(&nb - 1); /* basis */
 array w[%eval(2 * &d)]; /* work */
 set x;
 do i = 1 to &nb; b[i] = 0; end;

 * find the index of first knot greater than current data value;
 do ki = 1 to &nkn while(k[ki] le x); end;
 kki = ki - &d - 1;

 * make the basis;
 b[1 + kki] = 1;
 do j = 1 to &d;
 w[&d + j] = k[ki + j - 1] - x;
 w[j] = x - k[ki - j];
 s = 0;
 do i = 1 to j;
 t = w[&d + i] + w[j + 1 - i];
 if t ne 0.0 then t = b[i + kki] / t;
 b[i + kki] = s + w[&d + i] * t;
 s = w[j + 1 - i] * t;
 end;
 b[j + 1 + kki] = s;
 end;
run;

proc compare data=y(keep=x:) compare=b
 criterion=1e-12 note nosummary;
 title3 "should be no differences";
run;

```

The output from these steps is not shown. There are several things to note about the DATA step. It produces the same basis as PROC TRANSREG only because it uses exactly the same interior and exterior knots. The exterior knots (0.999999999999 and 10.000000000001) are just slightly smaller than 1 (the minimum in  $x$ ) and just slightly greater than 10 (the maximum in  $x$ ). Both exterior knots appear in the list three times, because a cubic (degree 3) polynomial was requested. The complete knot list is: 0.999999999999 0.999999999999 0.999999999999 3 6 8 10.000000000001 10.000000000001 10.000000000001. The exterior knots do not have any particular interpretation, but they are needed by the algorithm to construct the proper basis. The construction method computes differences between each value and the nearby knots. The algorithm that makes the B-spline basis is not very obvious, particularly compared to the polynomial spline basis. However, the B-spline basis is much better behaved numerically than a polynomial-spline basis, so that is why it is used.

---

## Linear and Nonlinear Regression Functions

This section shows how to use PROC TRANSREG in simple regression (one dependent variable and one independent variable) to find the optimal regression line, a nonlinear but monotone regression function, and a nonlinear and nonmonotone regression function. To find a linear regression function, specify the **IDENTITY** transformation of the independent variable. For a monotone curve, specify the **MSPLINE** transformation of the independent variable. To relax the monotonicity constraint, specify the **SPLINE** transformation. You can get more flexibility in spline functions by specifying knots. The more knots you specify, the more freedom the function has to follow minor variations in the data. This example uses artificial data. While these artificial data are clearly not realistic, their distinct pattern helps illustrate how splines work. The following statements generate the data and produce [Figure 97.28](#) through [Figure 97.31](#):

```

title 'Linear and Nonlinear Regression Functions';

* Generate an Artificial Nonlinear Scatter Plot;
data a;
 do i = 1 to 500;
 x = i / 2.5;
 y = -((x/50)-1.5)**2 + sin(x/8) + sqrt(x)/5 + 2*log(x) + cos(x);
 x = x / 21;
 if y > 2 then output;
 end;
run;

ods graphics on;
ods select fitplot(persist);

title2 'Linear Regression';

proc transreg data=a;
 model identity(y)=identity(x);
run;

title2 'A Monotone Regression Function';

```

```

proc transreg data=a;
 model identity(y)=mspline(x / nknots=9);
run;

title2 'A Nonlinear Regression Function';

proc transreg data=a;
 model identity(y)=spline(x / nknots=9);
run;

title2 'A Nonlinear Regression Function, 100 Knots';

proc transreg data=a;
 model identity(y)=spline(x / nknots=100);
run;

ods select all;

```

Figure 97.28 Linear Regression

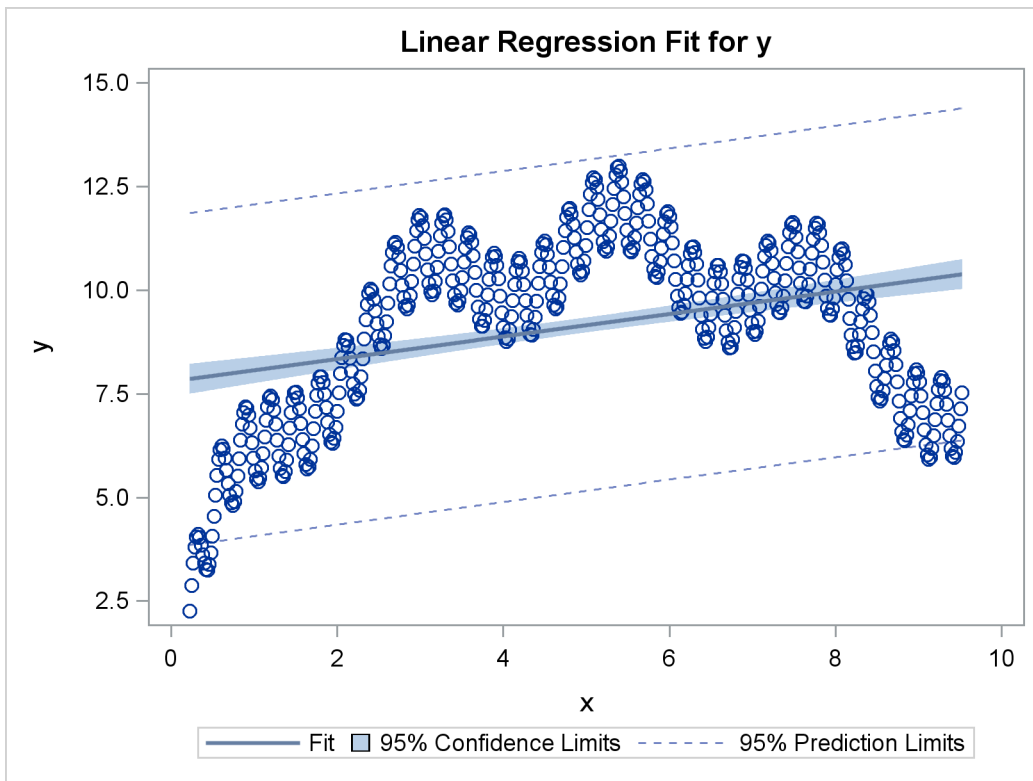


Figure 97.29 A Monotone Regression Function

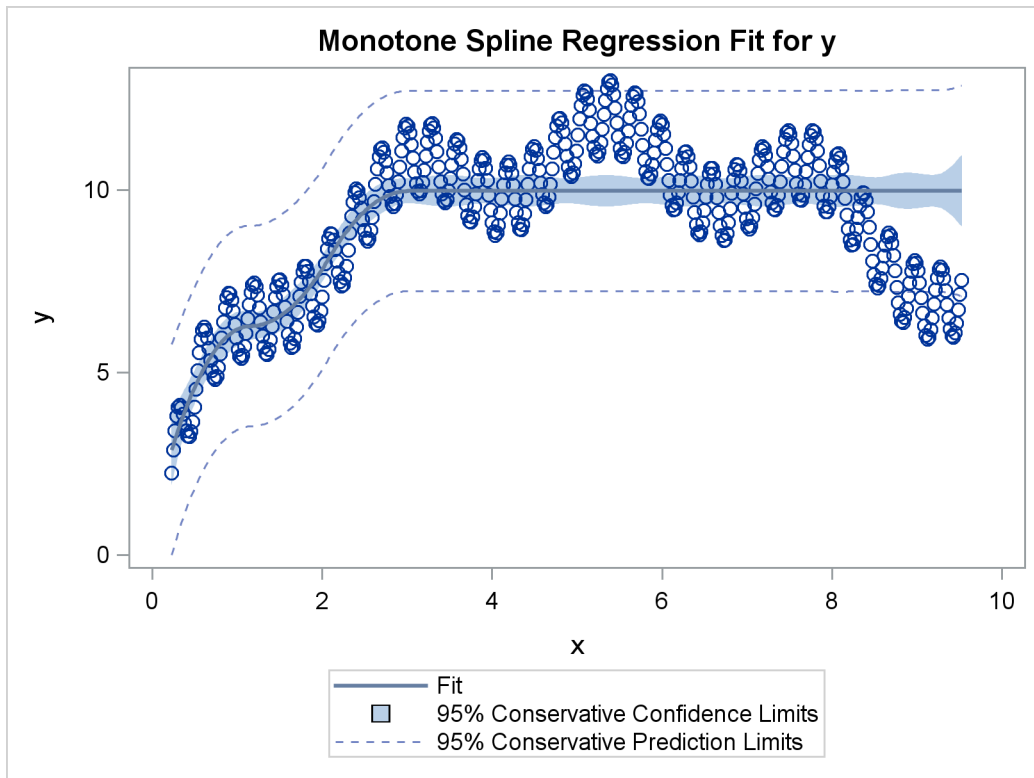
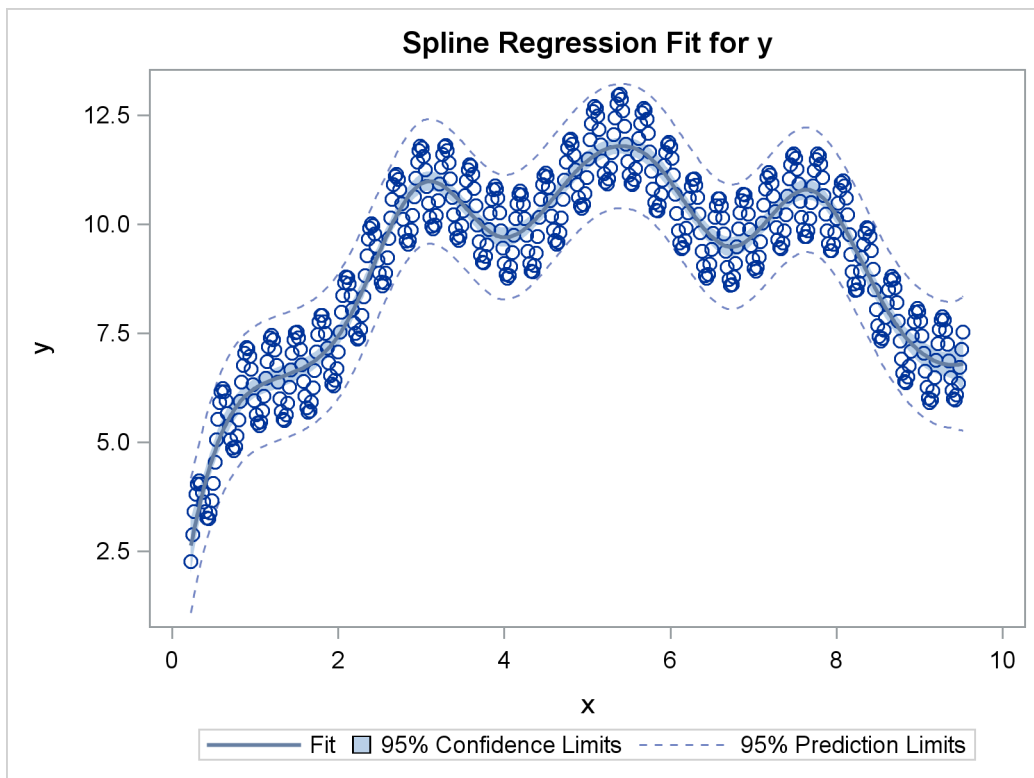
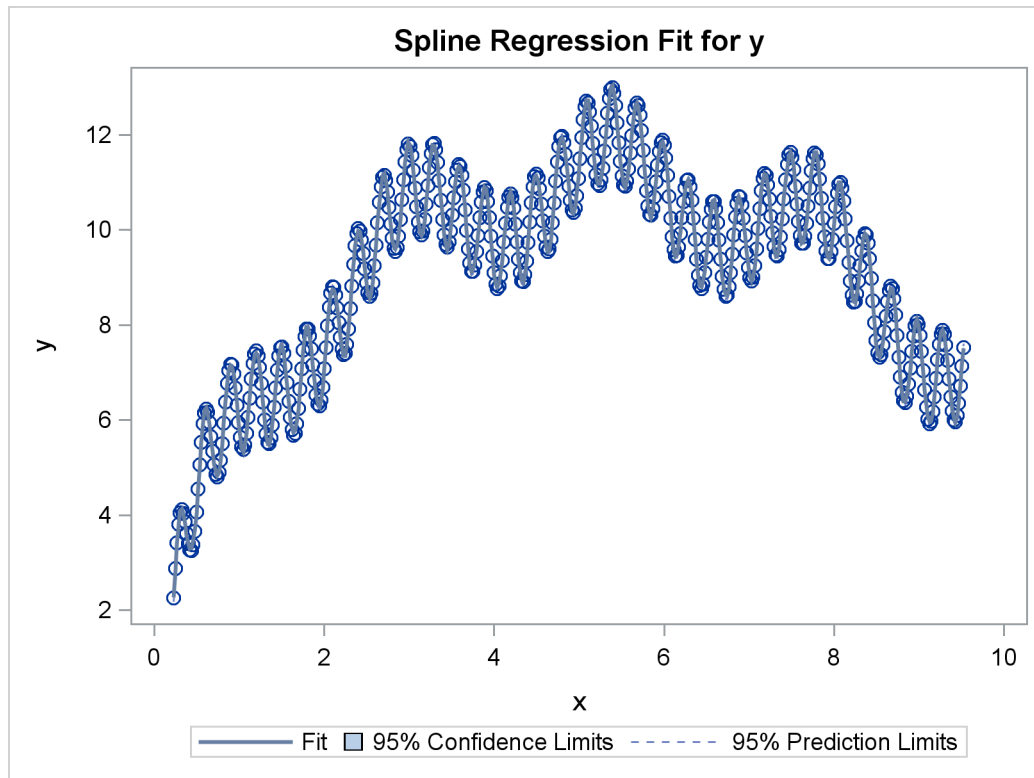


Figure 97.30 A Nonlinear Regression Function



**Figure 97.31** A Less-Smooth Nonlinear Regression Function

The squared correlation is only 0.15 for the linear regression in Figure 97.28. Clearly, a simple linear regression model is not appropriate for these data. By relaxing the constraints placed on the regression line, the proportion of variance accounted for increases from 0.15 (linear) to 0.61 (monotone in Figure 97.29) to 0.90 (nonlinear but smooth in Figure 97.30) to almost 1.0 with 100 knots (nonlinear and not very smooth in Figure 97.28). Relaxing the linearity constraint permits the regression function to bend and more closely follow the right portion of the scatter plot. Relaxing the monotonicity constraint permits the regression function to follow the periodic portion of the left side of the plot more closely. The nonlinear **MSPLINE** transformation is a quadratic spline with knots at the deciles. The first nonlinear nonmonotonic **SPLINE** transformation is a cubic spline with knots at the deciles.

Different knots and different degrees would produce slightly different results. The two nonlinear regression functions could be closely approximated by simpler piecewise linear regression functions. The monotone function could be approximated by a two-piece line with a single knot at the elbow. The first nonmonotone function could be approximated by a six-piece function with knots at the five elbows.

With this type of problem (one dependent variable with no missing values that is not transformed and one independent variable that is nonlinearly transformed), PROC TRANSREG always iterates exactly twice (although only one iteration is necessary). The first iteration reports the R square for the linear regression line and finds the optimal transformation of  $x$ . Since the data change in the first iteration, a second iteration is performed, which reports the R square for the final nonlinear regression function, and zero data change. The predicted values, which are a linear function of the optimal transformation of  $x$ , contain the  $Y$  coordinates for the nonlinear regression function. The variance of the predicted values divided by the variance of  $y$  is the R square for the fit of the nonlinear regression function. When  $x$  is monotonically transformed, the transformation of  $x$  is always monotonically increasing, but the predicted values increase if the correlation is positive and decrease for negative correlations.



## Simultaneously Fitting Two Regression Functions

One application of ordinary multiple regression is fitting two or more regression lines through a single scatter plot. With PROC TRANSREG, this application can easily be generalized to fit separate or parallel curves. To illustrate, consider a data set with two groups and a group membership variable *g* that has the value 1 for one group and 2 for the other group. The data set also has a continuous independent variable *x* and a continuous dependent variable *y*. When *g* is crossed with *x*, the variables *g1x* and *g2x* both have a large partition of zeros. For this reason, the `KNOTS= t-option` is specified instead of the `NKNOTS= t-option`. (The latter would put a number of knots in the partition of zeros.) The following example generates an artificial data set with two curves. While these artificial data are clearly not realistic, their distinct pattern helps illustrate how fitting simultaneous regression functions works. The following statements generate data and show how PROC TRANSREG fits lines, curves, and monotone curves through a scatter plot:

```

title 'Separate Curves, Separate Intercepts';

data a;
 do x = -2 to 3 by 0.025;
 g = 1;
 y = 8*(x*x + 2*cos(x*6)) + 15*normal(7654321);
 output;
 g = 2;
 y = 4*(-x*x + 4*sin(x*4)) - 40 + 15*normal(7654321);
 output;
 end;
run;

ods graphics on;
ods select fitplot(persist);

title 'Parallel Lines, Separate Intercepts';

proc transreg data=a solve;
 model identity(y)=class(g) identity(x);
run;

title 'Parallel Monotone Curves, Separate Intercepts';

proc transreg data=a;
 model identity(y)=class(g) mspline(x / knots=-1.5 to 2.5 by 0.5);
run;

title 'Parallel Curves, Separate Intercepts';

proc transreg data=a solve;
 model identity(y)=class(g) spline(x / knots=-1.5 to 2.5 by 0.5);
run;

title 'Separate Slopes, Same Intercept';

```

```

proc transreg data=a;
 model identity(y)=class(g / zero=none) * identity(x);
run;

title 'Separate Monotone Curves, Same Intercept';

proc transreg data=a;
 model identity(y) = class(g / zero=none) *
 mspline(x / knots=-1.5 to 2.5 by 0.5);
run;

title 'Separate Curves, Same Intercept';

proc transreg data=a solve;
 model identity(y) = class(g / zero=none) *
 spline(x / knots=-1.5 to 2.5 by 0.5);
run;

title 'Separate Slopes, Separate Intercepts';

proc transreg data=a;
 model identity(y) = class(g / zero=none) | identity(x);
run;

title 'Separate Monotone Curves, Separate Intercepts';

proc transreg data=a;
 model identity(y) = class(g / zero=none) |
 mspline(x / knots=-1.5 to 2.5 by 0.5);
run;

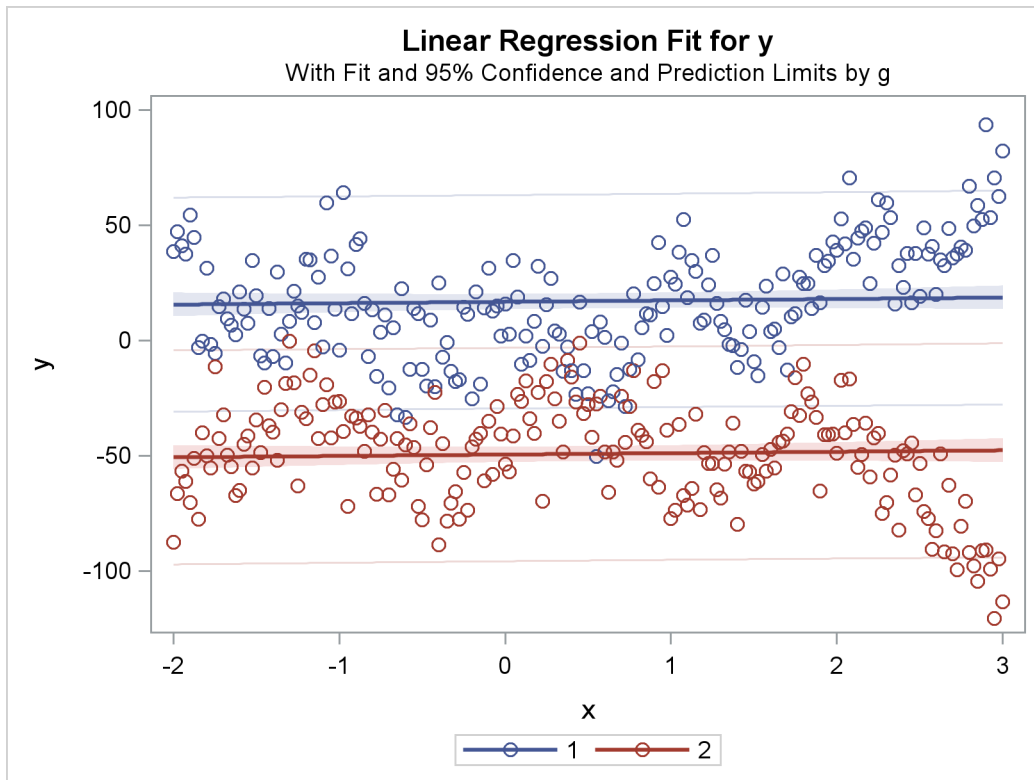
title 'Separate Curves, Separate Intercepts';

proc transreg data=a solve;
 model identity(y) = class(g / zero=none) |
 spline(x / knots=-1.5 to 2.5 by 0.5);
run;
ods select all;

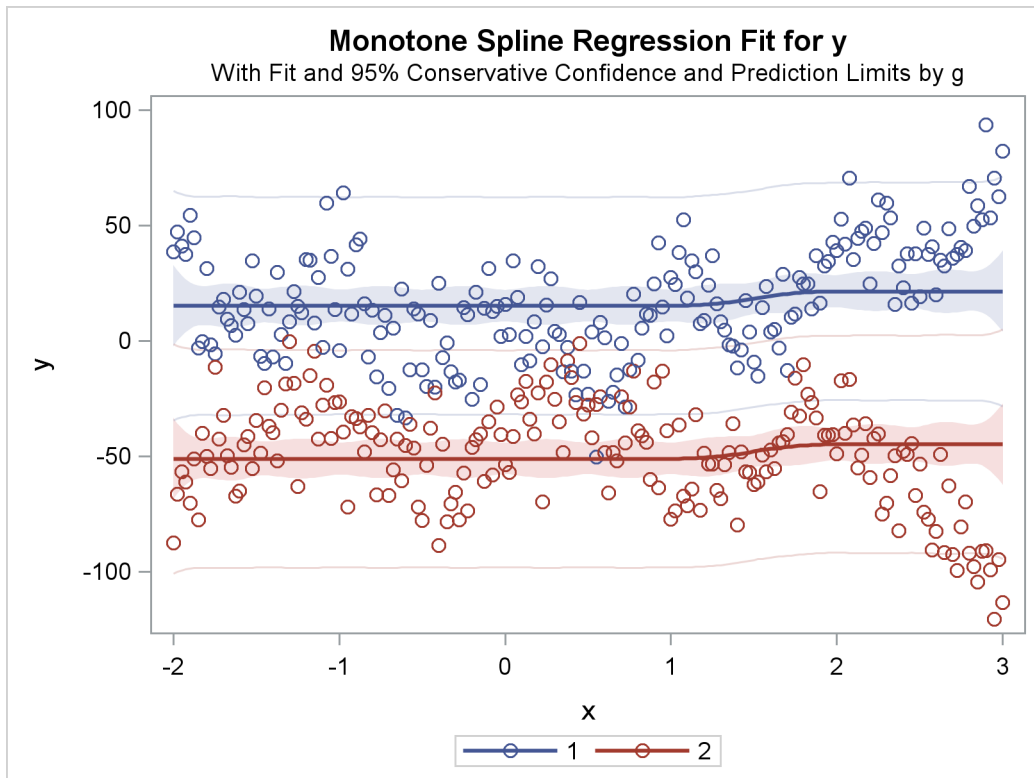
```

The previous statements produce [Figure 97.32](#) through [Figure 97.40](#). Only the fit plots are generated and displayed.

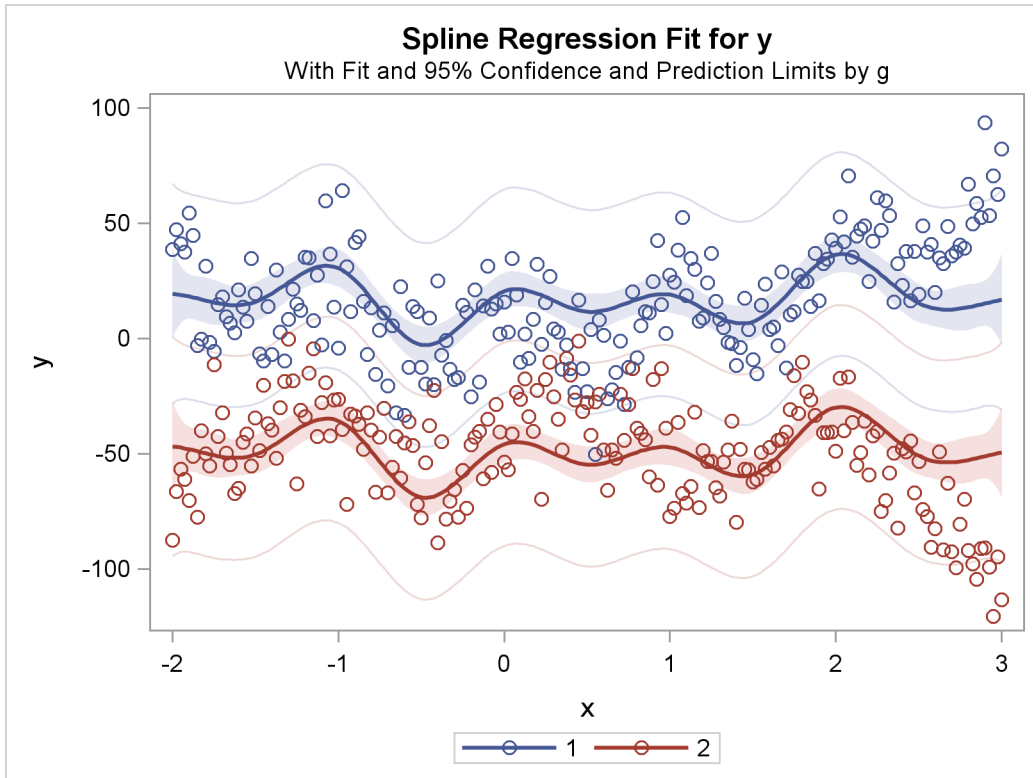
**Figure 97.32** Parallel Lines, Separate Intercepts



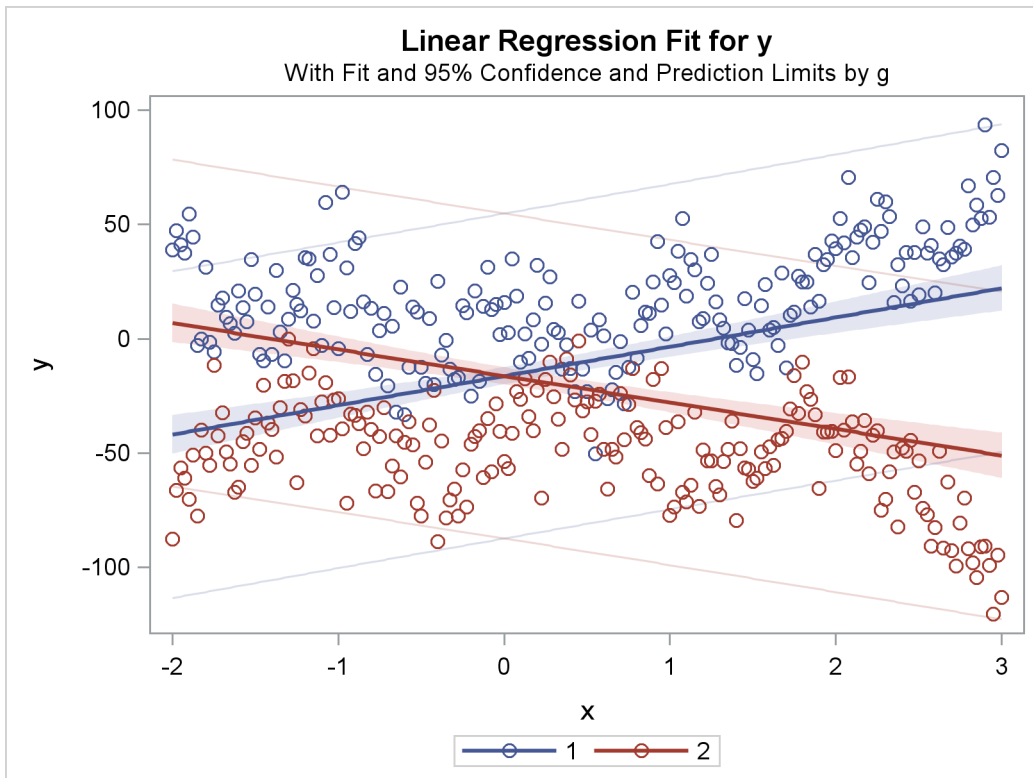
**Figure 97.33** Parallel Monotone Curves, Separate Intercepts



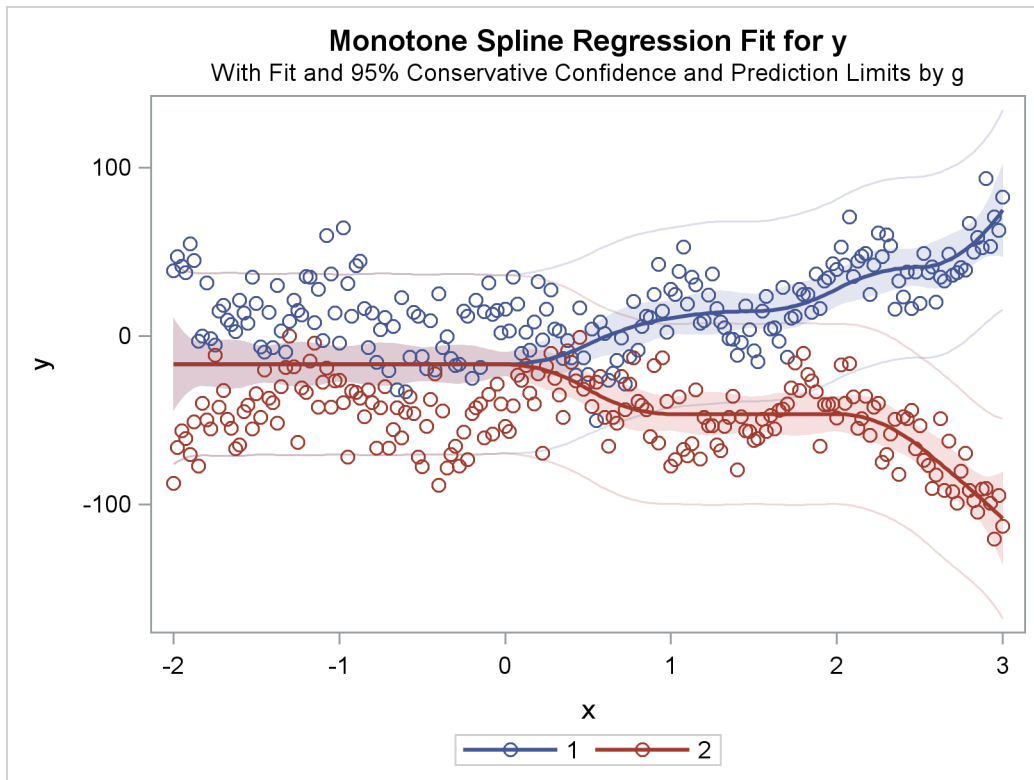
**Figure 97.34** Parallel Curves, Separate Intercepts



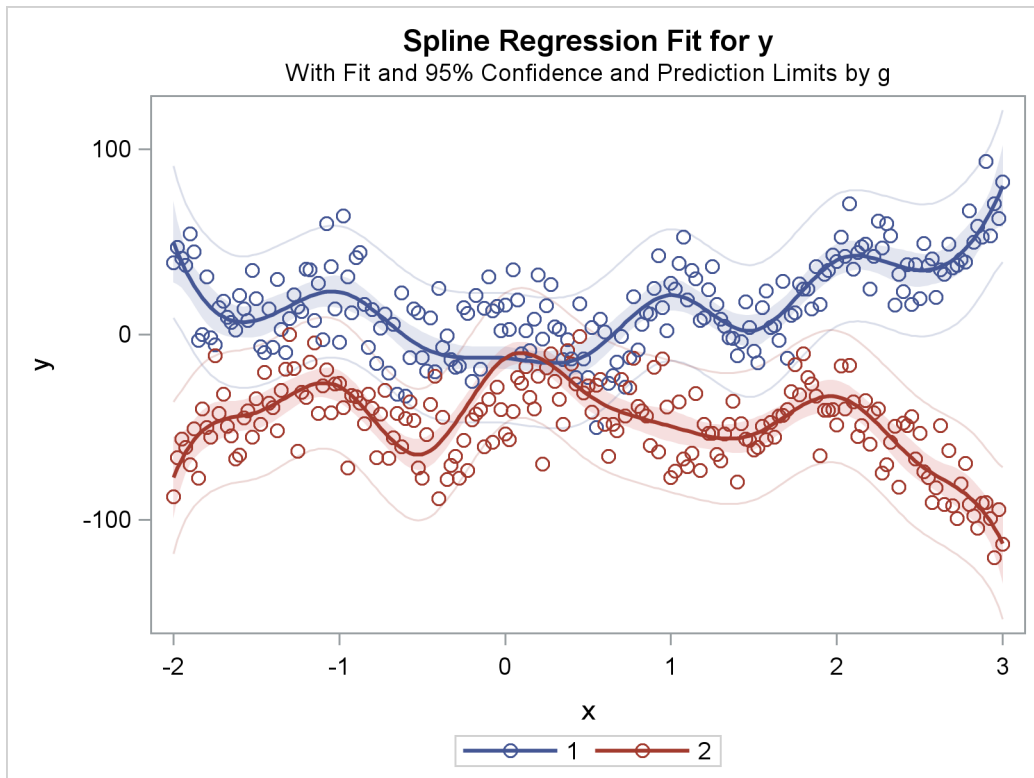
**Figure 97.35** Separate Slopes, Same Intercept



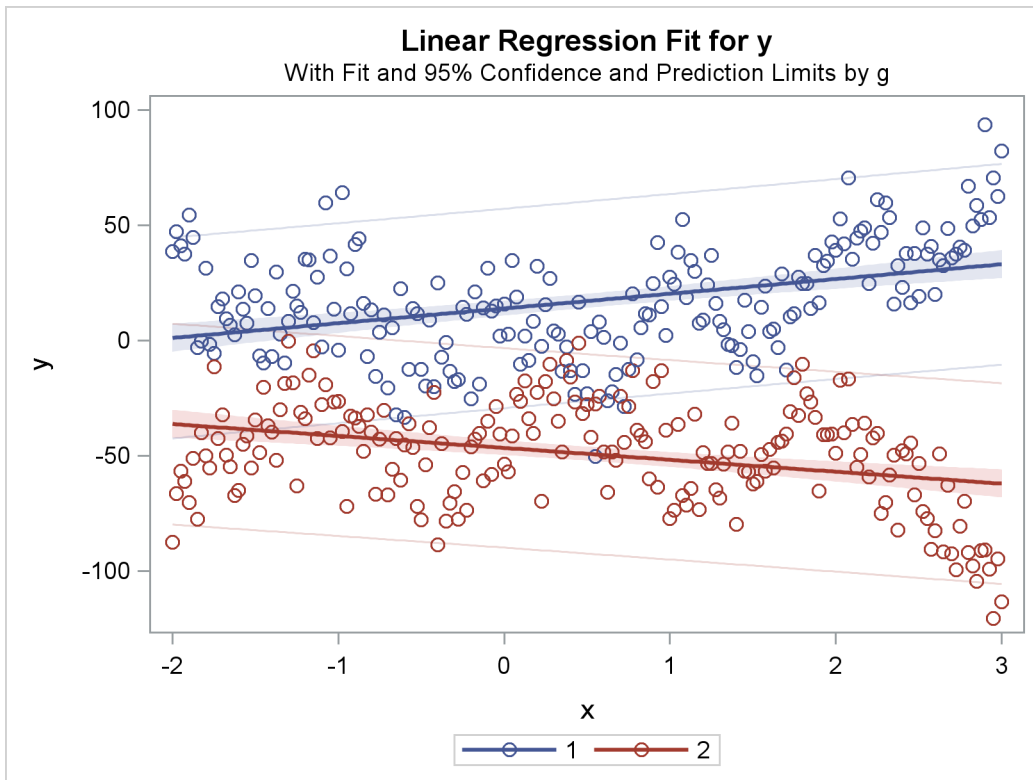
**Figure 97.36** Separate Monotone Curves, Same Intercept



**Figure 97.37** Separate Curves, Same Intercept



**Figure 97.38** Separate Slopes, Separate Intercepts



**Figure 97.39** Separate Monotone Curves, Separate Intercepts

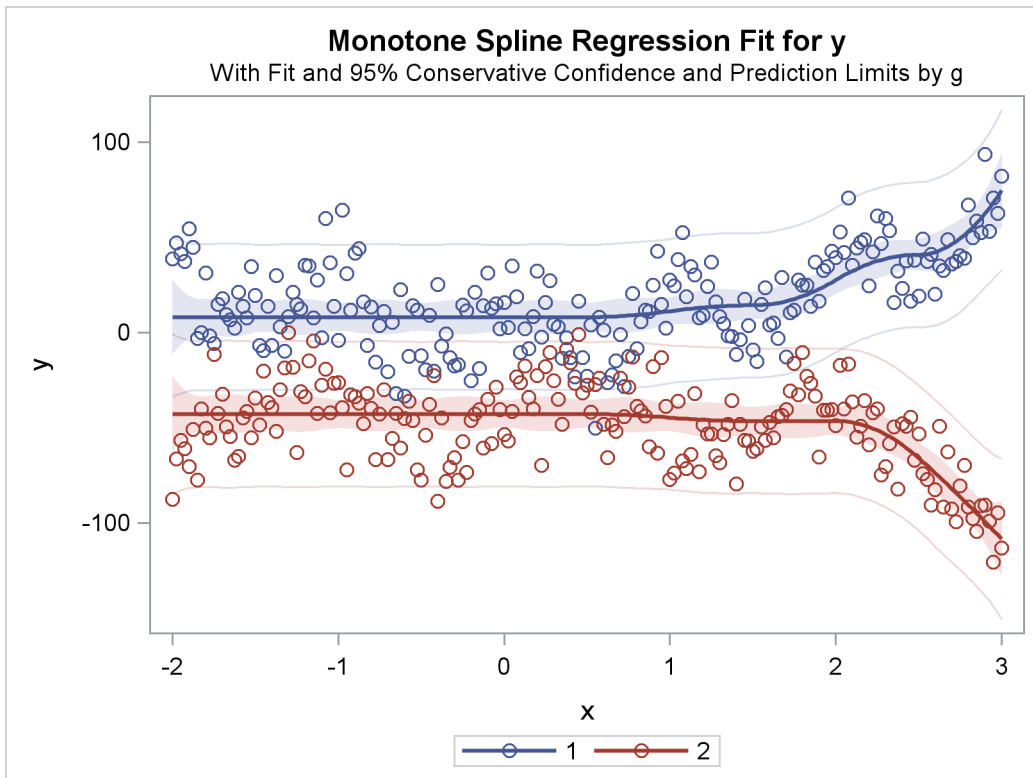
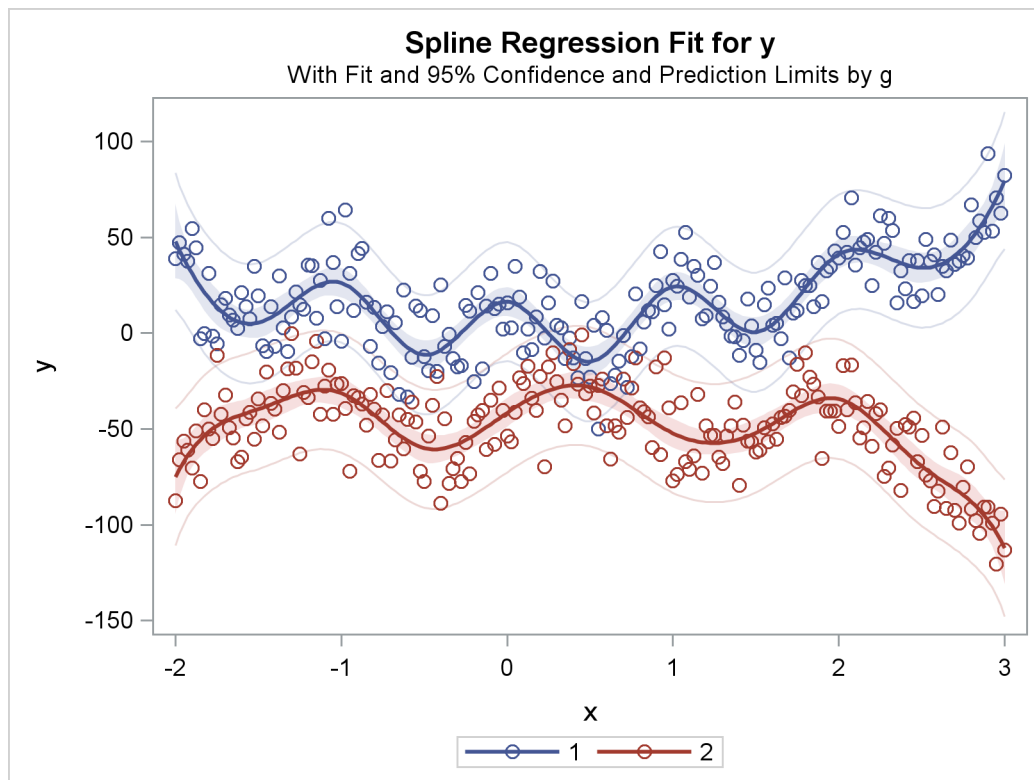


Figure 97.40 Separate Curves, Separate Intercepts



## Penalized B-Splines

You can use penalized B-splines (Eilers and Marx 1996) to fit a smooth curve through a scatter plot with an automatic selection of the smoothing parameter. See [Example 97.3](#) for an example. With penalized B-splines, you can find a transformation that minimizes any of the following criteria: **CV**, **GCV**, **AIC**, **AICC**, or **SBC**. These criteria are all functions of  $\lambda$ . For many problems, all of these criteria produce nearly identical results. However, for some problems, the choice of criterion can have a large effect. When the default results are not satisfactory, try the other criteria. Information criteria such as AIC and AICC are defined in different ways in the statistical literature, and these differences can be seen in different SAS procedures. Typically, the definitions differ only by a positive (additive or multiplicative) constant, so they are equivalent, and each of the definitions of the same criterion produces the same selection of  $\lambda$ . The definitions that PROC TRANSREG uses match the definitions that PROC REG uses. The penalized B-spline matrices, statistics, and criteria are defined as follows:

|                                                                                                           |                                                 |
|-----------------------------------------------------------------------------------------------------------|-------------------------------------------------|
| $n$                                                                                                       | number of observations                          |
| $y$                                                                                                       | dependent variable                              |
| $\mathbf{W}$                                                                                              | diagonal matrix of observation weights          |
| $w_i$                                                                                                     | weight for the $i$ th observation               |
| $\mathbf{B}$                                                                                              | B-spline basis for the independent variable     |
| $\lambda$                                                                                                 | nonnegative smoothing parameter                 |
| $\mathbf{D}$                                                                                              | difference matrix, penalizes lack of smoothness |
| $\mathbf{H} = \mathbf{B}(\mathbf{B}'\mathbf{W}\mathbf{B} + \lambda\mathbf{D}'\mathbf{D})^{-1}\mathbf{B}'$ | hat matrix                                      |

|                                                                        |                                                   |
|------------------------------------------------------------------------|---------------------------------------------------|
| $h_{ii}$                                                               | $i$ th diagonal element of $\mathbf{H}$           |
| $\hat{\mathbf{y}} = \mathbf{H}\mathbf{y}$                              | penalized B-spline transformation of $\mathbf{y}$ |
| $\text{SSE} = \sum_{i=1}^n w_i (y_i - \hat{y}_i)^2$                    | error sum of squares                              |
| $t = \sum_{i=1}^n w_i h_{ii}$                                          | weighted trace of $\mathbf{H}$                    |
| $\sum_{i=1}^n w_i \left( \frac{y_i - \hat{y}_i}{1 - h_{ii}} \right)^2$ | CV - cross validation criterion                   |
| $\sum_{i=1}^n w_i \left( \frac{y_i - \hat{y}_i}{n - t} \right)^2$      | GCV - generalized cross validation criterion      |
| $n \log(\text{SSE}/n) + 2t$                                            | AIC - Akaike's information criterion              |
| $1 + \log(\text{SSE}/n) + \frac{2(t + 1)}{n - t - 2}$                  | AICC - corrected AIC (default)                    |
| $n \log(\text{SSE}/n) + t \log(n)$                                     | SBC - Schwarz's Bayesian criterion                |

For more information about constructing the B-spline basis, see “[SPLINE and MSPLINE Transformations](#)” on page 8300 and the section “[Using Splines and Knots](#)” on page 8233. The nonzero elements of  $\mathbf{D}$ , order 1 are (1 -1), order 2 are (1 -2 1), order 3 (the default) are (1 -3 3 -1), order 4 are (1 -4 6 -4 1), and so on. The nonzero elements for each order are made from the nonzero elements from the preceding order by subtraction:  $\mathbf{d}'_{i+1} = (\mathbf{d}'_i \ 0) - (0 \ \mathbf{d}'_i)$ . Within an order, the first nonzero element of row  $i$  is in column  $i$ —that is, each row of  $\mathbf{D}$  is made from the preceding row by shifting the nonzero elements to the right one position. For example, with  $k = 4$  knots, order  $o = 3$ , and degree  $d = 3$ ,  $\mathbf{D}$  is the  $((d + 1 + k - o) \times (d + 1 + k))$  matrix:

$$\begin{bmatrix} 1 & -3 & 3 & -1 & 0 & 0 & 0 & 0 \\ 0 & 1 & -3 & 3 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & -3 & 3 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 & -3 & 3 & -1 & 0 \\ 0 & 0 & 0 & 0 & 1 & -3 & 3 & -1 \end{bmatrix} \text{ where } \begin{array}{c} 1 \quad -1 \quad 0 \\ - \quad 0 \quad 1 \quad -1 \\ \hline 1 \quad -2 \quad 1 \quad 0 \\ - \quad 0 \quad 1 \quad -2 \quad 1 \\ \hline 1 \quad -3 \quad 3 \quad -1 \end{array}$$

The weighted trace of the hat matrix,  $t = \sum_{i=1}^n w_i h_{ii}$ , provides an estimate of the number of parameters needed to find the transformation and is used in  $df$  calculations. Note, however, that in some cases, particularly with error-free or nearly error-free data, this value can be *much* larger than you might expect. You might be able to directly create a function by using [SPLINE](#) or [BSPLINE](#) with many fewer parameters that fits essentially just as well as the penalized B-spline function.

By default with [PBSPLINE](#), a cubic spline is fit with 100 evenly spaced knots, three evenly spaced exterior knots, and a difference matrix of order three. Options are specified as follows: [PBSPLINE\(x / DEGREE=3 NKNOTS=100 EVENLY=3 PARAMETER=3\)](#). By default, PROC TRANSREG searches for an optimal



lambda in the range 0 to 1E6 by using parabolic interpolation and Brent's (Brent 1973; Press et al. 1989) method. Alternatively, you can specify a lambda range or a list of lambdas by using the **LAMBDA=** option. Be aware, however, **LAMBDA=0** and values near zero might cause numerical problems including floating point errors. Also be aware that larger lambdas might cause numerical problems—for example, the error sum of squares for the model,  $\Sigma(y - \hat{y})^2$ , might be greater than the total sum of squares,  $\Sigma(y - \bar{y})^2$ —implying that the model with the transformation fits less well than simply predicting by using the mean. When this happens, you will see this message: ERROR: Degenerate transformation with PBSPLINE.

You can fit a single curve through a scatter plot ( $y \times x$ ) as follows:

```
model identity(y) = pbspline(x);
```

Alternatively, you can fit multiple curves through a scatter plot, one for each level of Group, as follows:

```
model identity(y) = class(group / zero=none) * pbspline(x);
```

There are several options for how the smoothing parameter,  $\lambda$ , is chosen. Usually, you do not specify the smoothing parameter,  $\lambda$ , and you let PROC TRANSREG choose  $\lambda$  for you by minimizing one of the information or cross validation criteria. By default, PROC TRANSREG first considers ranges defined by  $\lambda = 0$  and  $\lambda = 1, 10, 100, 1000, 10,000, 100,000, 1,000,000$ . If it finds a range that includes the minimum, it stops and does not consider larger  $\lambda$  values. Then it performs further searches in that range. For example, if the initial evaluations at  $\lambda = 1$  and  $\lambda = 10$  show that there is at least a local minimum in the range 0 to 10, then larger values are not considered. Note that the zero smoothing case,  $\lambda = 0$ , provides a boundary on the range even though the criterion is not evaluated at  $\lambda = 0$ . The criterion is not evaluated at  $\lambda = 0$  unless **LAMBDA=0** is the only value specified. Also note that the default approach is not the same as specifying the options **LAMBDA=0 1E6 RANGE**. When a range of values is specified, along with the **RANGE t-option**, PROC TRANSREG does not try to find smaller ranges based on powers of 10.

PROC TRANSREG avoids evaluating the criterion for **LAMBDA=** values at or near zero unless you force it to consider them. This is because zero smoothing is rarely interesting and the results are numerically unstable. Values of  $\lambda$  at or near zero often result in predicted values that are far outside the range of the data, particularly with interpolation and  $x$  values that do not appear in the data set. Also, zero smoothing is prone to numerical problems including floating point errors. This is particularly true when there is a small number of observations, a large number of knots, a high degree, or a perfect or near perfect fit. If you force PROC TRANSREG to evaluate the criterion at or near  $\lambda = 0$ , you can easily get bad results.

Note that when some observations appear more than once, such as when you have the kind of data where you can use a **FREQ** statement, then you should consider directly specifying lambda based on a preliminary analysis, ignoring the frequencies. Alternatively, specify a range of  $\lambda$  values, such as **LAMBDA=0.1 1E6 RANGE**, that steers  $\lambda$  away from values near zero. With the default lambda list, a cross validation criterion does not perform well in choosing a smoothing parameter with replicated data. Leaving one observation out of the computations changes the frequency for that observation from one positive integer to the next smaller positive integer, so in some sense, the point corresponding to that observation is never really left out of any computations. The resulting fit will be undersmoothed unless you specify a larger  $\lambda$ .

---

## Smoothing Splines

You can use PROC TRANSREG to plot and output to a SAS data set the same smoothing spline function that the GPLOT procedure creates. You request a smoothing spline transformation by specifying **SMOOTH** in the MODEL statement. The smoothing parameter can be specified with either the **SM=** or the **PARAMETER=** *o-option*. The results are saved in the independent variable transformation (for example, Tx, when the independent variable is x) and the predicted values variable (for example, Py, when the dependent variable is y).

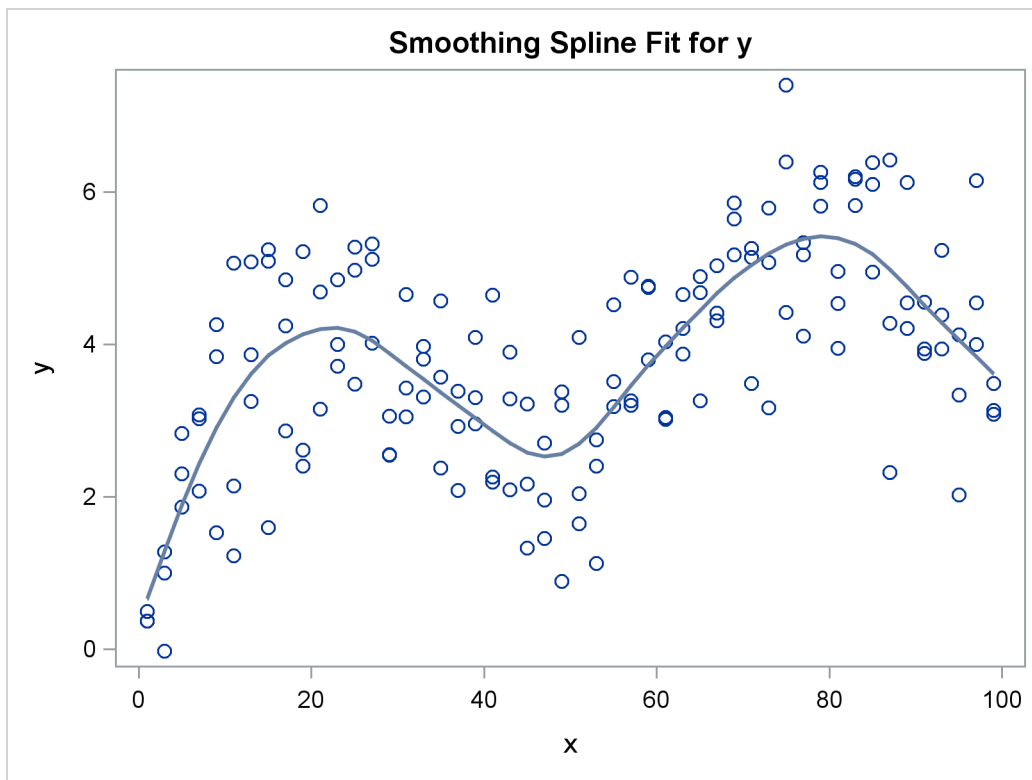
You can display the smoothing spline by using PROC TRANSREG and ODS Graphics (as shown in Figure 97.41). The following statements produce Figure 97.41:

```
title h=1.5 'Smoothing Splines';

ods graphics on;

data x;
 do x = 1 to 100 by 2;
 do rep = 1 to 3;
 y = log(x) + sin(x / 10) + normal(7);
 output;
 end;
 end;
run;

proc transreg;
 model identity(y) = smooth(x / sm=50);
 output p;
run;
```

**Figure 97.41** Smoothing Spline Displayed with ODS Graphics

You can also use PROC GPLOT to verify that the two procedures produce the same results. The PROC GPLOT plot request `y * x = 1` displays the data as stars. The specification `y * x = 2` with `I=SM50` requests the smooth curve through the scatter plot. It is overlaid with `Py * x = 3`, which displays with large dots the smooth function created by PROC TRANSREG. The results of the following step are not displayed:

```
proc gplot;
 axis1 minor=none label=(angle=90 rotate=0);
 axis2 minor=none;
 symbol1 color=blue v=circle i=none; /* data */
 symbol2 color=blue v=none i=sm50; /* gplot's smooth */
 symbol3 color=red v=dot i=none; /* transreg's smooth */
 plot y*x=1 y*x=2 py*x=3 / overlay haxis=axis2 vaxis=axis1 frame;
run; quit;
```

You can plot multiple nonlinear functions, one for each of several groups as defined by the levels of a **CLASS** variable. When you cross a **SMOOTH** variable with a **CLASS** variable, specify `ZERO=NONE` with the **CLASS** expansion. The following statements create artificial data and produce Figure 97.42:

```
title2 'Two Groups';

data x;
 do x = 1 to 100;
 Group = 1;
 do rep = 1 to 3;
 y = log(x) + sin(x / 10) + normal(7);
 end;
 end;
```

```

 output;
 end;
 group = 2;
 do rep = 1 to 3;
 y = -log(x) + cos(x / 10) + normal(7);
 output;
 end;
end;
run;

proc transreg ss2 data=x;
 model identity(y) = class(group / zero=none) *
 smooth(x / sm=50);

 output p;
run;

```

The ANOVA table in Figure 97.42 shows the overall model fit. The degrees of freedom are based on the trace of the transformation hat matrix, and are typically not integers. The “Smooth Transformation” table reports the degrees of freedom for each term, which includes an intercept for each group; the regression coefficients, which are always 1 with smoothing splines; the 0 to 100 smoothing parameter (like the one PROC GPLOT uses); the actual computed smoothing parameter; and the name and label for each term.

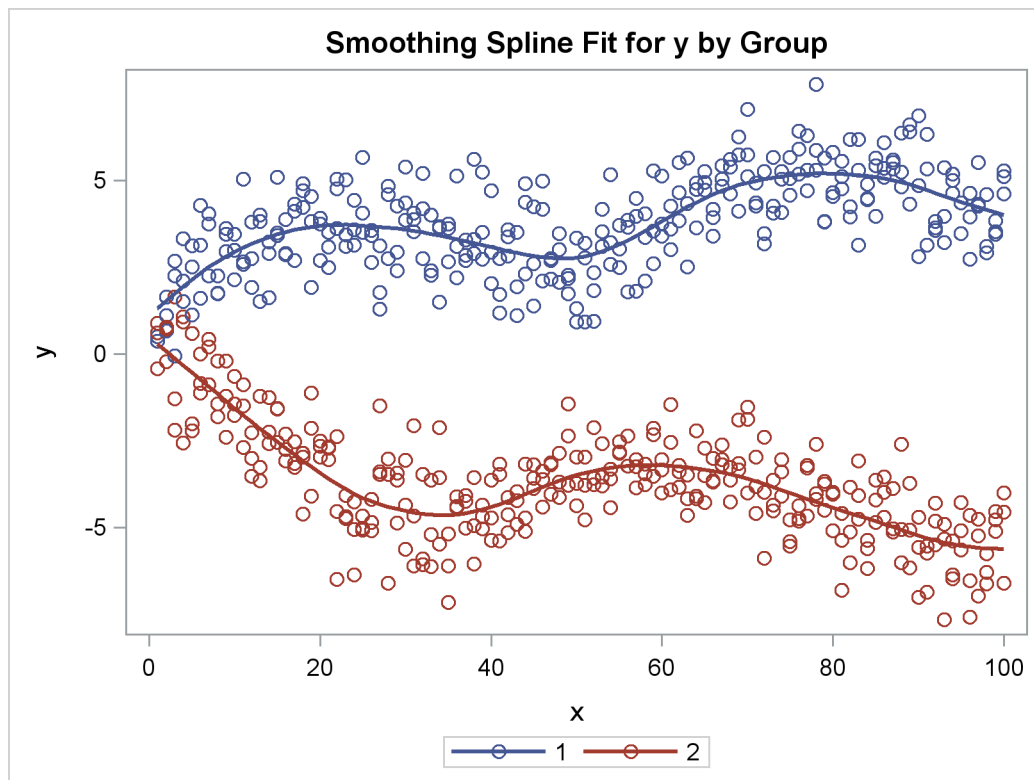
**Figure 97.42** Smoothing Spline Example 2

| Smoothing Splines                                       |        |                |             |         |        |
|---------------------------------------------------------|--------|----------------|-------------|---------|--------|
| Two Groups                                              |        |                |             |         |        |
| The TRANSREG Procedure                                  |        |                |             |         |        |
| Dependent Variable Identity(y)                          |        |                |             |         |        |
| Class Level Information                                 |        |                |             |         |        |
| Class                                                   | Levels | Values         |             |         |        |
| Group                                                   | 2      | 1              | 2           |         |        |
| Number of Observations Read                             |        | 600            |             |         |        |
| Number of Observations Used                             |        | 600            |             |         |        |
| Implicit Intercept Model                                |        |                |             |         |        |
| The TRANSREG Procedure Hypothesis Tests for Identity(y) |        |                |             |         |        |
| Univariate ANOVA Table, Smooth Transformation           |        |                |             |         |        |
| Source                                                  | DF     | Sum of Squares | Mean Square | F Value | Pr > F |
| Model                                                   | 16.794 | 9195.493       | 547.5365    | 562.03  | <.0001 |
| Error                                                   | 582.21 | 567.195        | 0.9742      |         |        |
| Corrected Total                                         | 599    | 9762.688       |             |         |        |

Figure 97.42 continued

|                       |            |             |        |           |             |
|-----------------------|------------|-------------|--------|-----------|-------------|
| Root MSE              | 0.98702    | R-Square    | 0.9419 |           |             |
| Dependent Mean        | 0.03651    | Adj R-Sq    | 0.9402 |           |             |
| Coeff Var             | 2703.13908 |             |        |           |             |
| Smooth Transformation |            |             |        |           |             |
| Variable              | DF         | Coefficient | SM     | Parameter | Label       |
| Smooth(Group1x)       | 8.8971     | 1.000       | 50     | 2405.265  | Group 1 * x |
| Smooth(Group2x)       | 8.8971     | 1.000       | 50     | 2405.265  | Group 2 * x |

Figure 97.42 continued



The **SMOOTH** transformation is valid only with independent variables. Typically, it is used only, as in the two preceding examples, in models with a single dependent variable, a single independent variable, and optionally, a single classification variable that is crossed with the independent variable. The various standardization options such as **TSTANDARD=**, **CENTER**, **Z**, and **REFLECT** are by default not permitted when the **SMOOTH** transformation is part of the model.

The **SMOOTH** transformation can also be used in other ways, but only when you specify the **NSR** *a-option*. (See the section “[Smoothing Splines Changes and Enhancements](#)” on page 8267.) When you specify the **NSR** *a-option*, and there are multiple independent variables designated as **SMOOTH**, **PROC TRANSREG**

tries to smooth the  $i$ th independent variable by using the  $i$ th dependent variable as a target. When there are more independent variables than dependent variables, the last dependent variable is reused as often as is necessary. For example, consider the following statements:

```
proc transreg nsr;
 model identity(y1-y3) = smooth(x1-x5);
run;
```

Smoothing is based on the pairs  $(y_1, x_1)$ ,  $(y_2, x_2)$ ,  $(y_3, x_3)$ ,  $(y_3, x_4)$ , and  $(y_3, x_5)$ .

The SMOOTH transformation is a noniterative transformation. The smoothing of each variable occurs before the iterations begin. In contrast, SSPLINE provides an iterative smoothing spline transformation. It does not generally minimize squared error; hence, divergence is possible with SSPLINE.

## Smoothing Splines Changes and Enhancements

How the results of the transformation are processed in PROC TRANSREG has changed with SAS 9.2. In particular, some aspects of the syntax along the coefficients and predicted values have changed. The new behavior was required to make the smoothing splines work properly with ODS Graphics and to make SMOOTH work consistently with the new PBSPLINE (penalized B-spline; see the section “Penalized B-Splines” on page 8260) capabilities. However, you can use the new NSR *a-option*, if you want the old functionality. Here are two typical uses of the SMOOTH transformation:

```
proc transreg;
 model identity(y) = smooth(x / sm=50);
 output p;
run;

proc transreg;
 model identity(y) = class(group / zero=none) * smooth(x / sm=50);
 output p;
run;
```

For the first model, the variable  $x$  is smoothly transformed by using a smoothing parameter of  $SM=50$ , and the results are stored in the transformed variable  $Tx$ . The second model has two groups of observations corresponding to  $group=1$  and  $Group=2$ . Separate curves are fit through each group. The results for the first group are stored in the transformed variable  $TGroup1x$ , and the results for the second group are stored in the transformed variable  $TGroup2x$ . The predicted values are stored in  $Py$ . In the first case,  $Py = Tx$ , and in the second case,  $Py = TGroup1x + TGroup2x$ . These represent the two standard usages of the SMOOTH transformation, and you can use ODS Graphics to display fit plots with a single or multiple smooth functions. For the first model, which is the most typical usage, the syntax has not changed, nor has the transformed variable. For the second model, the syntax has slightly changed, but the transformed variables have not. The details of the syntax changes are discussed later in this section. The primary change involves what happens after the SMOOTH transformation is found. Now, by default, ordinary least squares (OLS) is no longer used to find the coefficients when there are smooth transformations, and in the iteration history table the OLS R square is no longer produced.

Here is some background for the change. The first three of the four models shown next have much in common:

```

model identity(y) = smooth(x / sm=50);
model identity(y) = rank(x);
model identity(y) = log(x);
model identity(y) = spline(x);

```

Before SAS 9.2, the **SMOOTH**, **RANK**, and **LOG** transformations all requested that PROC TRANSREG preprocess the data, nonlinearly transforming  $x$  before using OLS to fit a model to the preprocessed results. All of these first three transformations of  $x$  are nonoptimal in the sense that none of them is based in any way on the OLS regression model that follows the preprocessing of the data. In contrast, the fourth model requests a spline transformation. In this model, both the nonlinear transformation and the final regression model seek to minimize the same OLS criterion. Some PROC TRANSREG transformations, such as **SPLINE**, **MSPLINE**, **OPSCORE**, **MONOTONE**, and so on, seek to minimize squared error, whereas others, such as **SMOOTH**, **LOG**, **EXP**, and **RANK**, do not. For the latter, the data are simply preprocessed before analysis. There is a philosophical difference, however, between **SMOOTH** and the nonoptimal transformations. The **SMOOTH** and **PBSPLINE** transformations use the dependent variable and a model (but not OLS) to compute the transformation, whereas **LOG**, **EXP**, **RANK**, and the other nonoptimal transformations do not. A log transformation, for example, would be the same, regardless of context, whereas the **SMOOTH** and **PBSPLINE** transformations depend on the model.

The principal change to **SMOOTH** in PROC TRANSREG with SAS 9.2 involves making PROC TRANSREG aware of the underlying smoothing spline model. This makes **SMOOTH** and **PBSPLINE** perform similarly, and less like **LOG**, **EXP**, **RANK**, and the other nonoptimal transformations. Previously, if you specified **SMOOTH** and then examined the regression coefficients, you would probably get an intercept very close to but not exactly 0, and the remaining coefficients would be very close to but not exactly 1. This is because PROC TRANSREG was using OLS to find the coefficients. This has changed. Now, PROC TRANSREG recognizes that the **SMOOTH** transformation has an implicit intercept (see the section “**Implicit and Explicit Intercepts**” on page 8294); hence there is no separate intercept. Furthermore, now the other parameters are exactly 1, which are the correct parameters for the non-OLS smoothing spline model. Hence, the predicted values are now the sum of the transformed variables. When there is no **CLASS** variable, the predicted values exactly match the transformed variable. The **SMOOTH** transformation is no longer a form of preprocessing; it now changes the nature of the model from OLS to a true smoothing-spline model. If you still want the old behavior, preprocessing and then OLS, you can get the old default functionality by specifying the **NSR a-option**.

The new, default functionality assumes that you either want to fit a smooth function through the data or fit separate functions, one for each level of a **CLASS** variable. It also recognizes the smoothing-spline model as a model with an implicit intercept. For these reasons, the syntax for models with a **CLASS** variable has slightly changed, as is shown next:

```

proc transreg nsr; /* old */
 model identity(y) = class(group / zero=none) |
 smooth(x / after sm=50);

 output p;
run;

proc transreg; /* new */
 model identity(y) = class(group / zero=none) *
 smooth(x / sm=50);

 output p;
run;

```

Previously, the **AFTER** *t-option* was required when you wanted to fit separate and independent functions within each group. This *t-option* specifies that PROC TRANSREG should find the smoothing spline transformations *after* it crosses the independent variable with the CLASS variable. Previously, by default, PROC TRANSREG found an overall smooth transformation and then crossed it with the CLASS variable, which is probably not what you want. You can still specify the **AFTER** *t-option*, but now it is assumed with CLASS \* SMOOTH. If you specify **AFTER** without the **NSR** *a-option*, PROC TRANSREG suppresses the note that **AFTER** is assumed. It does not affect the model. If you do not want **AFTER** to be in effect by default, you must specify the **NSR** *a-option*. Also previously, you typically needed to specify the vertical bar instead of the asterisk to cross the CLASS and SMOOTH variables. The difference is that the bar adds both crossed variables and separate group intercepts to the model, whereas the asterisk adds only the crossed variables to the model. Since the SMOOTH transformation is now recognized as providing an implicit intercept, you should use the asterisk and not the vertical bar.

The default behavior of the SMOOTH transformation needed to change for several reasons. SMOOTH was originally provided as nothing more than a way to get PROC GPLOT's smoothing splines into an output data set in the transformed variables. However, with new enhancements to PROC TRANSREG such as ODS Graphics and PBSPLINE, the old method for SMOOTH did not fit well. The old method produced predicted values that were not the correct values to plot in order to show the smoothing spline fit. Now, with this change, ODS Graphics can always plot the predicted values. PBSPLINE and SMOOTH are similar in spirit, and for both, OLS results are not truly appropriate. Before SAS 9.2, PROC TRANSREG fit linear models, linear models with nonlinearly preprocessed variables, and linear models with optimal nonlinear transformations that minimized squared error. Now it also has the ability to fit non-OLS models for scatter plot smoothing.

One aspect of the SMOOTH transformation has unconditionally changed with SAS 9.2. Previously, PROC TRANSREG did not evaluate the effective degrees of freedom by examining the trace of the transformation hat matrix. It simply used the number of categories in the *df* calculations, which for continuous variables is the number of observations. This made it impossible to get a sensible ANOVA test for the overall fit. With SAS 9.2, the degrees of freedom are always based on the trace. This *df* change also affects the **SSPLINE** transformation, which finds a smooth transformation by using the same algorithm as SMOOTH. The difference is that the SMOOTH transformation occurs once, as an analysis preprocessing step, whereas **SSPLINE** transformations occur iteratively and in the body of the alternating least squares algorithm.



---

## Iteration History Changes and Enhancements

With SAS 9.2, PROC TRANSREG no longer always prints an iteration history table by default, and in some cases, the table it prints is not the same as it was previously. This change is due to the increasing use of PROC TRANSREG with transformations that are not based on alternating least squares. Here is some background for the change. PROC TRANSREG's processing can be divided into three steps. In the first step, the data are read and certain transformations, such as **SMOOTH**, **PBSPLINE**, **BOXCOX**, **RANK**, **LOG** and the other nonoptimal transformations, are performed. These transformations are not based on OLS. In the second step, the alternating least squares iterations are performed according to **METHOD=UNIVARIATE**, **MORALS**, **REDUNDANCY**, or **CANALS**. It is in the second step that the alternating least squares transformations (**SPLINE**, **MSPLINE**, **MONOTONE**, **OPSCORE**, **LINEAR**, and **UNTIE**) are iteratively found. In the third step, the results are displayed. In some cases, the results are appropriately based on using the method of OLS applied to the optimally transformed variables. In other cases, such as with smoothing splines and penalized B-splines, OLS-based results are not appropriate. Furthermore, for many of these types of models, nothing changes in the iterations, so the computations needed to realize that nothing changes are not needed, nor is the iteration history table.

With SAS 9.2, the iteration history is not printed for models where it is known that nothing will change in the iterations. Suppose the **NOMISS** option is specified or there are no missing data. If **METHOD=UNIVARIATE**, if there are no iterative transformations (**SPLINE**, **MSPLINE**, **MONOTONE**, **OPSCORE**, **LINEAR**, and **UNTIE**), and if the **MAXITER=** option is not specified, then by default, an iteration history table is not produced. If you want to see an iteration history, there are many things you can do, such as specifying **MAXITER=**, changing the method to **MORALS**, or changing **IDENTITY** to **LINEAR**.

With models with smoothing splines or penalized B-splines, the iteration history will not contain an R square. This is because the iterations are based on the method of alternating least squares, but the smoothing splines and penalized B-splines are not based on a least squares model. Hence, an ordinary R square in the iterations, based on a computed intercept, which is typically not exactly zero, and a computed slope, which is typically not exactly one, will not be exactly the same as the correct R square, which is based on an intercept and slope of zero and one. The final reported results include the correct R square in the fit statistics table after the ANOVA table. If you want to see only the correct R square from the results, without the iteration history, you can specify the new **RSQUARE** option.

---

## ANOVA Codings

This section illustrates several different codings of classification variables and hence several different ways of fitting two-way ANOVA models to some data. Each example fits an ANOVA model, displays the ANOVA table and parameter estimates, and displays the coded design matrix. Note throughout that the ANOVA tables and R squares are identical for all of the models, showing that the codings are equivalent. For each model, the parameter estimates are stated as a function of the cell means. The formulas are appropriate for a design such as this one, which is balanced and orthogonal (every level and every pair of levels occurs equally often). They will not work with unequal frequencies. Since this data set has  $3 \times 2 = 6$  cells, the full-rank codings all have six parameters. The following statements create the input data set, and display it in Figure 97.43:

```

title 'Two-Way ANOVA Models';

data x;
 input a b @@;
 do i = 1 to 2; input y @@; output; end;
 drop i;
 datalines;
1 1 16 14 1 2 15 13
2 1 1 9 2 2 12 20
3 1 14 8 3 2 18 20
;

proc print label;
run;

```

**Figure 97.43** Input Data Set

| Two-Way ANOVA Models |   |   |    |    |
|----------------------|---|---|----|----|
| Obs                  | a | b | y  |    |
| 1                    | 1 | 1 | 16 | 14 |
| 2                    | 1 | 1 | 15 | 13 |
| 3                    | 1 | 2 | 12 | 20 |
| 4                    | 1 | 2 | 18 | 20 |
| 5                    | 2 | 1 | 1  | 9  |
| 6                    | 2 | 1 | 14 | 8  |
| 7                    | 2 | 2 | 12 | 20 |
| 8                    | 2 | 2 | 18 | 20 |
| 9                    | 3 | 1 | 14 | 8  |
| 10                   | 3 | 1 | 18 | 20 |
| 11                   | 3 | 2 | 18 | 20 |
| 12                   | 3 | 2 | 18 | 20 |

The following statements fit a cell-means model and produce [Figure 97.44](#) and [Figure 97.45](#):

```

proc transreg data=x ss2 short;
 title2 'Cell-Means Model';
 model identity(y) = class(a * b / zero=none);
 output replace;
run;

proc print label;
run;

```

Figure 97.44 Cell-Means Model

```

Two-Way ANOVA Models
Cell-Means Model

The TRANSREG Procedure

Dependent Variable Identity(y)

Class Level Information

Class Levels Values
a 3 1 2 3
b 2 1 2

Number of Observations Read 12
Number of Observations Used 12
Implicit Intercept Model

The TRANSREG Procedure Hypothesis Tests for Identity(y)

Univariate ANOVA Table Based on the Usual Degrees of Freedom

Source DF Sum of Mean
 DF Squares Square F Value Pr > F

Model 5 234.6667 46.93333 3.20 0.0946
Error 6 88.0000 14.66667
Corrected Total 11 322.6667

Root MSE 3.82971 R-Square 0.7273
Dependent Mean 13.33333 Adj R-Sq 0.5000
Coeff Var 28.72281

Univariate Regression Table Based on the Usual Degrees of Freedom

Type II
Sum of Mean
Variable DF Coefficient Squares Square F Value Pr > F Label

Class.a1b1 1 15.0000000 450.000 450.000 30.68 0.0015 a 1 * b 1
Class.a1b2 1 14.0000000 392.000 392.000 26.73 0.0021 a 1 * b 2
Class.a2b1 1 5.0000000 50.000 50.000 3.41 0.1144 a 2 * b 1
Class.a2b2 1 16.0000000 512.000 512.000 34.91 0.0010 a 2 * b 2
Class.a3b1 1 11.0000000 242.000 242.000 16.50 0.0066 a 3 * b 1
Class.a3b2 1 19.0000000 722.000 722.000 49.23 0.0004 a 3 * b 2

```

The parameter estimates are

$$\hat{\mu}_{11} = \bar{y}_{11} = 15$$

$$\hat{\mu}_{12} = \bar{y}_{12} = 14$$

$$\hat{\mu}_{21} = \bar{y}_{21} = 5$$

$$\hat{\mu}_{22} = \bar{y}_{22} = 16$$

$$\hat{\mu}_{31} = \bar{y}_{31} = 11$$

$$\hat{\mu}_{32} = \bar{y}_{32} = 19$$

**Figure 97.45** Cell-Means Model, Design Matrix

| Two-Way ANOVA Models |        |        |    |           |       |       |       |       |       |       |     |
|----------------------|--------|--------|----|-----------|-------|-------|-------|-------|-------|-------|-----|
| Cell-Means Model     |        |        |    |           |       |       |       |       |       |       |     |
| Obs                  | _TYPE_ | _NAME_ | y  | Intercept | a 1 * | a 1 * | a 2 * | a 2 * | a 3 * | a 3 * | a b |
|                      |        |        |    |           | b 1   | b 2   | b 1   | b 2   | b 1   | b 2   |     |
| 1                    | SCORE  | ROW1   | 16 | .         | 1     | 0     | 0     | 0     | 0     | 0     | 1 1 |
| 2                    | SCORE  | ROW2   | 14 | .         | 1     | 0     | 0     | 0     | 0     | 0     | 1 1 |
| 3                    | SCORE  | ROW3   | 15 | .         | 0     | 1     | 0     | 0     | 0     | 0     | 1 2 |
| 4                    | SCORE  | ROW4   | 13 | .         | 0     | 1     | 0     | 0     | 0     | 0     | 1 2 |
| 5                    | SCORE  | ROW5   | 1  | .         | 0     | 0     | 1     | 0     | 0     | 0     | 2 1 |
| 6                    | SCORE  | ROW6   | 9  | .         | 0     | 0     | 1     | 0     | 0     | 0     | 2 1 |
| 7                    | SCORE  | ROW7   | 12 | .         | 0     | 0     | 0     | 1     | 0     | 0     | 2 2 |
| 8                    | SCORE  | ROW8   | 20 | .         | 0     | 0     | 0     | 1     | 0     | 0     | 2 2 |
| 9                    | SCORE  | ROW9   | 14 | .         | 0     | 0     | 0     | 0     | 1     | 0     | 3 1 |
| 10                   | SCORE  | ROW10  | 8  | .         | 0     | 0     | 0     | 0     | 1     | 0     | 3 1 |
| 11                   | SCORE  | ROW11  | 18 | .         | 0     | 0     | 0     | 0     | 0     | 1     | 3 2 |
| 12                   | SCORE  | ROW12  | 20 | .         | 0     | 0     | 0     | 0     | 0     | 1     | 3 2 |

The next model is a reference cell model, and the default reference cell is the last cell, which in this case is the (3,2) cell. The following statements fit a reference cell model and produce [Figure 97.46](#) and [Figure 97.47](#):

```
proc transreg data=x ss2 short;
 title2 'Reference Cell Model, (3,2) Reference Cell';
 model identity(y) = class(a | b);
 output replace;
run;

proc print label;
run;
```

Figure 97.46 Reference Cell Model, (3,2) Reference Cell

```

Two-Way ANOVA Models
Reference Cell Model, (3,2) Reference Cell

The TRANSREG Procedure

Dependent Variable Identity(y)

Class Level Information

Class Levels Values
a 3 1 2 3
b 2 1 2

Number of Observations Read 12
Number of Observations Used 12

The TRANSREG Procedure Hypothesis Tests for Identity(y)

Univariate ANOVA Table Based on the Usual Degrees of Freedom

Source DF Sum of Mean
 DF Squares Square F Value Pr > F

Model 5 234.6667 46.93333 3.20 0.0946
Error 6 88.0000 14.66667
Corrected Total 11 322.6667

Root MSE 3.82971 R-Square 0.7273
Dependent Mean 13.33333 Adj R-Sq 0.5000
Coeff Var 28.72281

Univariate Regression Table Based on the Usual Degrees of Freedom

Type II
Sum of Mean
Variable DF Coefficient Squares Square F Value Pr > F Label

Intercept 1 19.0000000 722.000 722.000 49.23 0.0004 Intercept
Class.a1 1 -5.0000000 25.000 25.000 1.70 0.2395 a 1
Class.a2 1 -3.0000000 9.000 9.000 0.61 0.4632 a 2
Class.b1 1 -8.0000000 64.000 64.000 4.36 0.0817 b 1
Class.a1b1 1 9.0000000 40.500 40.500 2.76 0.1476 a 1 * b 1
Class.a2b1 1 -3.0000000 4.500 4.500 0.31 0.5997 a 2 * b 1

```

The parameter estimates are

$$\begin{aligned}\hat{\mu}_{32} &= \bar{y}_{32} = 19 \\ \hat{\alpha}_1 &= \bar{y}_{12} - \bar{y}_{32} = 14 - 19 = -5 \\ \hat{\alpha}_2 &= \bar{y}_{22} - \bar{y}_{32} = 16 - 19 = -3 \\ \hat{\beta}_1 &= \bar{y}_{31} - \bar{y}_{32} = 11 - 19 = -8 \\ \hat{\gamma}_{11} &= \bar{y}_{11} - (\hat{\mu}_{32} + \hat{\alpha}_1 + \hat{\beta}_1) = 15 - (19 + -5 + -8) = 9 \\ \hat{\gamma}_{21} &= \bar{y}_{21} - (\hat{\mu}_{32} + \hat{\alpha}_2 + \hat{\beta}_1) = 5 - (19 + -3 + -8) = -3\end{aligned}$$

**Figure 97.47** Reference Cell Model, (3,2) Reference Cell, Design Matrix

| Two-Way ANOVA Models                       |        |        |    |           |     |     |     |       |       |   |   |
|--------------------------------------------|--------|--------|----|-----------|-----|-----|-----|-------|-------|---|---|
| Reference Cell Model, (3,2) Reference Cell |        |        |    |           |     |     |     |       |       |   |   |
| Obs                                        | _TYPE_ | _NAME_ | y  | Intercept | a 1 | a 2 | b 1 | a 1 * | a 2 * | a | b |
| 1                                          | SCORE  | ROW1   | 16 | 1         | 1   | 0   | 1   | 1     | 0     | 1 | 1 |
| 2                                          | SCORE  | ROW2   | 14 | 1         | 1   | 0   | 1   | 1     | 0     | 1 | 1 |
| 3                                          | SCORE  | ROW3   | 15 | 1         | 1   | 0   | 0   | 0     | 0     | 1 | 2 |
| 4                                          | SCORE  | ROW4   | 13 | 1         | 1   | 0   | 0   | 0     | 0     | 1 | 2 |
| 5                                          | SCORE  | ROW5   | 1  | 1         | 0   | 1   | 1   | 0     | 1     | 2 | 1 |
| 6                                          | SCORE  | ROW6   | 9  | 1         | 0   | 1   | 1   | 0     | 1     | 2 | 1 |
| 7                                          | SCORE  | ROW7   | 12 | 1         | 0   | 1   | 0   | 0     | 0     | 2 | 2 |
| 8                                          | SCORE  | ROW8   | 20 | 1         | 0   | 1   | 0   | 0     | 0     | 2 | 2 |
| 9                                          | SCORE  | ROW9   | 14 | 1         | 0   | 0   | 1   | 0     | 0     | 3 | 1 |
| 10                                         | SCORE  | ROW10  | 8  | 1         | 0   | 0   | 1   | 0     | 0     | 3 | 1 |
| 11                                         | SCORE  | ROW11  | 18 | 1         | 0   | 0   | 0   | 0     | 0     | 3 | 2 |
| 12                                         | SCORE  | ROW12  | 20 | 1         | 0   | 0   | 0   | 0     | 0     | 3 | 2 |

The next model is a deviations-from-means model. This coding is also called effects coding. The default reference cell is the last cell (3,2). The following statements produce [Figure 97.48](#) and [Figure 97.49](#):

```
proc transreg data=x ss2 short;
 title2 'Deviations from Means, (3,2) Reference Cell';
 model identity(y) = class(a | b / deviations);
 output replace;
run;

proc print label;
run;
```

**Figure 97.48** Deviations-from-Means Model, (3,2) Reference Cell

| Two-Way ANOVA Models                                              |        |                |                |             |         |        |           |
|-------------------------------------------------------------------|--------|----------------|----------------|-------------|---------|--------|-----------|
| Deviations from Means, (3,2) Reference Cell                       |        |                |                |             |         |        |           |
| The TRANSREG Procedure                                            |        |                |                |             |         |        |           |
| Dependent Variable Identity(y)                                    |        |                |                |             |         |        |           |
| Class Level Information                                           |        |                |                |             |         |        |           |
| Class                                                             | Levels | Values         |                |             |         |        |           |
| a                                                                 | 3      | 1 2 3          |                |             |         |        |           |
| b                                                                 | 2      | 1 2            |                |             |         |        |           |
| Number of Observations Read                                       |        |                |                |             |         | 12     |           |
| Number of Observations Used                                       |        |                |                |             |         | 12     |           |
| The TRANSREG Procedure Hypothesis Tests for Identity(y)           |        |                |                |             |         |        |           |
| Univariate ANOVA Table Based on the Usual Degrees of Freedom      |        |                |                |             |         |        |           |
| Source                                                            | DF     | Sum of Squares | Mean Square    | F Value     | Pr > F  |        |           |
| Model                                                             | 5      | 234.6667       | 46.93333       | 3.20        | 0.0946  |        |           |
| Error                                                             | 6      | 88.0000        | 14.66667       |             |         |        |           |
| Corrected Total                                                   | 11     | 322.6667       |                |             |         |        |           |
| Root MSE                                                          |        | 3.82971        | R-Square       | 0.7273      |         |        |           |
| Dependent Mean                                                    |        | 13.33333       | Adj R-Sq       | 0.5000      |         |        |           |
| Coeff Var                                                         |        | 28.72281       |                |             |         |        |           |
| Univariate Regression Table Based on the Usual Degrees of Freedom |        |                |                |             |         |        |           |
| Variable                                                          | DF     | Coefficient    | Type II        |             | F Value | Pr > F | Label     |
|                                                                   |        |                | Sum of Squares | Mean Square |         |        |           |
| Intercept                                                         | 1      | 13.3333333     | 2133.33        | 2133.33     | 145.45  | <.0001 | Intercept |
| Class.a1                                                          | 1      | 1.1666667      | 8.17           | 8.17        | 0.56    | 0.4837 | a 1       |
| Class.a2                                                          | 1      | -2.8333333     | 48.17          | 48.17       | 3.28    | 0.1199 | a 2       |
| Class.b1                                                          | 1      | -3.0000000     | 108.00         | 108.00      | 7.36    | 0.0349 | b 1       |
| Class.a1b1                                                        | 1      | 3.5000000      | 73.50          | 73.50       | 5.01    | 0.0665 | a 1 * b 1 |
| Class.a2b1                                                        | 1      | -2.5000000     | 37.50          | 37.50       | 2.56    | 0.1609 | a 2 * b 1 |

The parameter estimates are

$$\begin{aligned}\hat{\mu} &= \bar{y} = 13.3333 \\ \hat{\alpha}_1 &= (\bar{y}_{11} + \bar{y}_{12})/2 - \bar{y} = (15 + 14)/2 - 13.3333 = 1.1667 \\ \hat{\alpha}_2 &= (\bar{y}_{21} + \bar{y}_{22})/2 - \bar{y} = (5 + 16)/2 - 13.3333 = -2.8333 \\ \hat{\beta}_1 &= (\bar{y}_{11} + \bar{y}_{21} + \bar{y}_{31})/3 - \bar{y} = (15 + 5 + 11)/3 - 13.3333 = -3 \\ \hat{\gamma}_{11} &= \bar{y}_{11} - (\bar{y} + \hat{\alpha}_1 + \hat{\beta}_1) = 15 - (13.3333 + 1.1667 + -3) = 3.5 \\ \hat{\gamma}_{21} &= \bar{y}_{21} - (\bar{y} + \hat{\alpha}_2 + \hat{\beta}_1) = 5 - (13.3333 + -2.8333 + -3) = -2.5\end{aligned}$$

**Figure 97.49** Deviations-from-Means Model, (3,2) Reference Cell, Design Matrix

| Two-Way ANOVA Models<br>Deviations from Means, (3,2) Reference Cell |       |       |    |           |     |     |     |       |       |   |   |
|---------------------------------------------------------------------|-------|-------|----|-----------|-----|-----|-----|-------|-------|---|---|
| Obs                                                                 | TYPE  | NAME  | y  | Intercept | a 1 | a 2 | b 1 | a 1 * | a 2 * | a | b |
| 1                                                                   | SCORE | ROW1  | 16 | 1         | 1   | 0   | 1   | 1     | 0     | 1 | 1 |
| 2                                                                   | SCORE | ROW2  | 14 | 1         | 1   | 0   | 1   | 1     | 0     | 1 | 1 |
| 3                                                                   | SCORE | ROW3  | 15 | 1         | 1   | 0   | -1  | -1    | 0     | 1 | 2 |
| 4                                                                   | SCORE | ROW4  | 13 | 1         | 1   | 0   | -1  | -1    | 0     | 1 | 2 |
| 5                                                                   | SCORE | ROW5  | 1  | 1         | 0   | 1   | 1   | 0     | 1     | 2 | 1 |
| 6                                                                   | SCORE | ROW6  | 9  | 1         | 0   | 1   | 1   | 0     | 1     | 2 | 1 |
| 7                                                                   | SCORE | ROW7  | 12 | 1         | 0   | 1   | -1  | 0     | -1    | 2 | 2 |
| 8                                                                   | SCORE | ROW8  | 20 | 1         | 0   | 1   | -1  | 0     | -1    | 2 | 2 |
| 9                                                                   | SCORE | ROW9  | 14 | 1         | -1  | -1  | 1   | -1    | -1    | 3 | 1 |
| 10                                                                  | SCORE | ROW10 | 8  | 1         | -1  | -1  | 1   | -1    | -1    | 3 | 1 |
| 11                                                                  | SCORE | ROW11 | 18 | 1         | -1  | -1  | -1  | 1     | 1     | 3 | 2 |
| 12                                                                  | SCORE | ROW12 | 20 | 1         | -1  | -1  | -1  | 1     | 1     | 3 | 2 |

The next model is a less-than-full-rank model. The parameter estimates are constrained to sum to zero within each effect. The following statements produce [Figure 97.50](#) and [Figure 97.51](#):

```
proc transreg data=x ss2 short;
 title2 'Less-Than-Full-Rank Model';
 model identity(y) = class(a | b / zero=sum);
 output replace;
run;

proc print label;
run;
```



Figure 97.50 Less-Than-Full-Rank Model

```

Two-Way ANOVA Models
Less-Than-Full-Rank Model

The TRANSREG Procedure

Dependent Variable Identity(y)

Class Level Information

Class Levels Values
a 3 1 2 3
b 2 1 2

Number of Observations Read 12
Number of Observations Used 12

The TRANSREG Procedure Hypothesis Tests for Identity(y)

Univariate ANOVA Table Based on the Usual Degrees of Freedom

Source DF Sum of Mean
 DF Squares Square F Value Pr > F
Model 5 234.6667 46.93333 3.20 0.0946
Error 6 88.0000 14.66667
Corrected Total 11 322.6667

Root MSE 3.82971 R-Square 0.7273
Dependent Mean 13.33333 Adj R-Sq 0.5000
Coeff Var 28.72281

```

Figure 97.50 continued

| Univariate Regression Table Based on the Usual Degrees of Freedom |    |             |                              |                |         |        |           |
|-------------------------------------------------------------------|----|-------------|------------------------------|----------------|---------|--------|-----------|
| Variable                                                          | DF | Coefficient | Type II<br>Sum of<br>Squares | Mean<br>Square | F Value | Pr > F | Label     |
| Intercept                                                         | 1  | 13.3333333  | 2133.33                      | 2133.33        | 145.45  | <.0001 | Intercept |
| Class.a1                                                          | 1  | 1.1666667   | 8.17                         | 8.17           | 0.56    | 0.4837 | a 1       |
| Class.a2                                                          | 1  | -2.8333333  | 48.17                        | 48.17          | 3.28    | 0.1199 | a 2       |
| Class.a3                                                          | 1  | 1.6666667   | 16.67                        | 16.67          | 1.14    | 0.3274 | a 3       |
| Class.b1                                                          | 1  | -3.0000000  | 108.00                       | 108.00         | 7.36    | 0.0349 | b 1       |
| Class.b2                                                          | 1  | 3.0000000   | 108.00                       | 108.00         | 7.36    | 0.0349 | b 2       |
| Class.a1b1                                                        | 1  | 3.5000000   | 73.50                        | 73.50          | 5.01    | 0.0665 | a 1 * b 1 |
| Class.a1b2                                                        | 1  | -3.5000000  | 73.50                        | 73.50          | 5.01    | 0.0665 | a 1 * b 2 |
| Class.a2b1                                                        | 1  | -2.5000000  | 37.50                        | 37.50          | 2.56    | 0.1609 | a 2 * b 1 |
| Class.a2b2                                                        | 1  | 2.5000000   | 37.50                        | 37.50          | 2.56    | 0.1609 | a 2 * b 2 |
| Class.a3b1                                                        | 1  | -1.0000000  | 6.00                         | 6.00           | 0.41    | 0.5461 | a 3 * b 1 |
| Class.a3b2                                                        | 1  | 1.0000000   | 6.00                         | 6.00           | 0.41    | 0.5461 | a 3 * b 2 |

The sum of the regression table DF's, minus one for the intercept, will be greater than the model df when there are ZERO=SUM constraints.

The parameter estimates are

$$\begin{aligned}
\hat{\mu} &= \bar{y} = 13.3333 \\
\hat{\alpha}_1 &= (\bar{y}_{11} + \bar{y}_{12})/2 - \bar{y} = (15 + 14)/2 - 13.3333 = 1.1667 \\
\hat{\alpha}_2 &= (\bar{y}_{21} + \bar{y}_{22})/2 - \bar{y} = (5 + 16)/2 - 13.3333 = -2.8333 \\
\hat{\alpha}_3 &= (\bar{y}_{31} + \bar{y}_{32})/2 - \bar{y} = (11 + 19)/2 - 13.3333 = 1.6667 \\
\hat{\beta}_1 &= (\bar{y}_{11} + \bar{y}_{21} + \bar{y}_{31})/3 - \bar{y} = (15 + 5 + 11)/3 - 13.3333 = -3 \\
\hat{\beta}_2 &= (\bar{y}_{12} + \bar{y}_{22} + \bar{y}_{32})/3 - \bar{y} = (14 + 16 + 19)/3 - 13.3333 = 3 \\
\hat{\gamma}_{11} &= \bar{y}_{11} - (\bar{y} + \hat{\alpha}_1 + \hat{\beta}_1) = 15 - (13.3333 + 1.1667 + -3) = 3.5 \\
\hat{\gamma}_{12} &= \bar{y}_{12} - (\bar{y} + \hat{\alpha}_1 + \hat{\beta}_2) = 14 - (13.3333 + 1.1667 + 3) = -3.5 \\
\hat{\gamma}_{21} &= \bar{y}_{21} - (\bar{y} + \hat{\alpha}_2 + \hat{\beta}_1) = 5 - (13.3333 + -2.8333 + -3) = -2.5 \\
\hat{\gamma}_{22} &= \bar{y}_{22} - (\bar{y} + \hat{\alpha}_2 + \hat{\beta}_2) = 16 - (13.3333 + -2.8333 + 3) = 2.5 \\
\hat{\gamma}_{31} &= \bar{y}_{31} - (\bar{y} + \hat{\alpha}_3 + \hat{\beta}_1) = 11 - (13.3333 + 1.6667 + -3) = -1 \\
\hat{\gamma}_{32} &= \bar{y}_{32} - (\bar{y} + \hat{\alpha}_3 + \hat{\beta}_2) = 19 - (13.3333 + 1.6667 + 3) = 1
\end{aligned}$$

The constraints are

$$\alpha_1 + \alpha_2 + \alpha_3 \equiv \beta_1 + \beta_2 \equiv 0$$

$$\gamma_{11} + \gamma_{12} \equiv \gamma_{21} + \gamma_{22} \equiv \gamma_{31} + \gamma_{32} \equiv \gamma_{11} + \gamma_{21} + \gamma_{31} \equiv \gamma_{12} + \gamma_{22} + \gamma_{32} \equiv 0$$

Only four of the five interaction constraints are needed. The fifth constraint is implied by the other four. (Given a  $2 \times 3$  table with four marginal sum-to-zero constraints, you can freely fill in only two cells. The values in the other four cells are determined from the first two cells and the constraints.) A full-rank model has six estimable parameters. This less-than-full-rank model has one parameter for the intercept, two for

the first main effect (plus one more as determined by the first constraint), one for the second main effect (plus one more as determined by the second constraint), and two for the interactions (plus four more as determined by the next four constraints). Six of the twelve parameters are determined given the other six and the constraints. Notice that  $\hat{\mu}$ ,  $\hat{\alpha}_1$ ,  $\hat{\alpha}_2$ ,  $\hat{\beta}_1$ ,  $\hat{\gamma}_{11}$ , and  $\hat{\gamma}_{21}$  match the corresponding estimates from the effects coding.

**Figure 97.51** Less-Than-Full-Rank Model, Design Matrix

| Two-Way ANOVA Models<br>Less-Than-Full-Rank Model |        |              |              |              |              |              |              |     |   |
|---------------------------------------------------|--------|--------------|--------------|--------------|--------------|--------------|--------------|-----|---|
| Obs                                               | _TYPE_ | _NAME_       | y            | Intercept    | a 1          | a 2          | a 3          | b 1 |   |
| 1                                                 | SCORE  | ROW1         | 16           | 1            | 1            | 0            | 0            | 1   |   |
| 2                                                 | SCORE  | ROW2         | 14           | 1            | 1            | 0            | 0            | 1   |   |
| 3                                                 | SCORE  | ROW3         | 15           | 1            | 1            | 0            | 0            | 0   |   |
| 4                                                 | SCORE  | ROW4         | 13           | 1            | 1            | 0            | 0            | 0   |   |
| 5                                                 | SCORE  | ROW5         | 1            | 1            | 0            | 1            | 0            | 1   |   |
| 6                                                 | SCORE  | ROW6         | 9            | 1            | 0            | 1            | 0            | 1   |   |
| 7                                                 | SCORE  | ROW7         | 12           | 1            | 0            | 1            | 0            | 0   |   |
| 8                                                 | SCORE  | ROW8         | 20           | 1            | 0            | 1            | 0            | 0   |   |
| 9                                                 | SCORE  | ROW9         | 14           | 1            | 0            | 0            | 1            | 1   |   |
| 10                                                | SCORE  | ROW10        | 8            | 1            | 0            | 0            | 1            | 1   |   |
| 11                                                | SCORE  | ROW11        | 18           | 1            | 0            | 0            | 1            | 0   |   |
| 12                                                | SCORE  | ROW12        | 20           | 1            | 0            | 0            | 1            | 0   |   |
| Obs                                               | b 2    | a 1 *<br>b 1 | a 1 *<br>b 2 | a 2 *<br>b 1 | a 2 *<br>b 2 | a 3 *<br>b 1 | a 3 *<br>b 2 | a   | b |
| 1                                                 | 0      | 1            | 0            | 0            | 0            | 0            | 0            | 1   | 1 |
| 2                                                 | 0      | 1            | 0            | 0            | 0            | 0            | 0            | 1   | 1 |
| 3                                                 | 1      | 0            | 1            | 0            | 0            | 0            | 0            | 1   | 2 |
| 4                                                 | 1      | 0            | 1            | 0            | 0            | 0            | 0            | 1   | 2 |
| 5                                                 | 0      | 0            | 0            | 1            | 0            | 0            | 0            | 2   | 1 |
| 6                                                 | 0      | 0            | 0            | 1            | 0            | 0            | 0            | 2   | 1 |
| 7                                                 | 1      | 0            | 0            | 0            | 1            | 0            | 0            | 2   | 2 |
| 8                                                 | 1      | 0            | 0            | 0            | 1            | 0            | 0            | 2   | 2 |
| 9                                                 | 0      | 0            | 0            | 0            | 0            | 1            | 0            | 3   | 1 |
| 10                                                | 0      | 0            | 0            | 0            | 0            | 1            | 0            | 3   | 1 |
| 11                                                | 1      | 0            | 0            | 0            | 0            | 0            | 1            | 3   | 2 |
| 12                                                | 1      | 0            | 0            | 0            | 0            | 0            | 1            | 3   | 2 |

The next model is a reference cell model, but this time the reference cell is the first cell (1,1). The following statements produce [Figure 97.52](#) and [Figure 97.53](#):

```
proc transreg data=x ss2 short;
 title2 'Reference Cell Model, (1,1) Reference Cell';
 model identity(y) = class(a | b / zero=first);
 output replace;
run;

proc print label;
run;
```

**Figure 97.52** Reference Cell Model, (1,1) Reference Cell

| Two-Way ANOVA Models                                              |        |                |                        |             |         |        |           |
|-------------------------------------------------------------------|--------|----------------|------------------------|-------------|---------|--------|-----------|
| Reference Cell Model, (1,1) Reference Cell                        |        |                |                        |             |         |        |           |
| The TRANSREG Procedure                                            |        |                |                        |             |         |        |           |
| Dependent Variable Identity(y)                                    |        |                |                        |             |         |        |           |
| Class Level Information                                           |        |                |                        |             |         |        |           |
| Class                                                             | Levels | Values         |                        |             |         |        |           |
| a                                                                 | 3      | 1 2 3          |                        |             |         |        |           |
| b                                                                 | 2      | 1 2            |                        |             |         |        |           |
| Number of Observations Read                                       |        |                |                        |             |         |        | 12        |
| Number of Observations Used                                       |        |                |                        |             |         |        | 12        |
| The TRANSREG Procedure Hypothesis Tests for Identity(y)           |        |                |                        |             |         |        |           |
| Univariate ANOVA Table Based on the Usual Degrees of Freedom      |        |                |                        |             |         |        |           |
| Source                                                            | DF     | Sum of Squares | Mean Square            | F Value     | Pr > F  |        |           |
| Model                                                             | 5      | 234.6667       | 46.93333               | 3.20        | 0.0946  |        |           |
| Error                                                             | 6      | 88.0000        | 14.66667               |             |         |        |           |
| Corrected Total                                                   | 11     | 322.6667       |                        |             |         |        |           |
| Root MSE                                                          |        | 3.82971        | R-Square               | 0.7273      |         |        |           |
| Dependent Mean                                                    |        | 13.33333       | Adj R-Sq               | 0.5000      |         |        |           |
| Coeff Var                                                         |        | 28.72281       |                        |             |         |        |           |
| Univariate Regression Table Based on the Usual Degrees of Freedom |        |                |                        |             |         |        |           |
| Variable                                                          | DF     | Coefficient    | Type II Sum of Squares | Mean Square | F Value | Pr > F | Label     |
| Intercept                                                         | 1      | 15.000000      | 450.000                | 450.000     | 30.68   | 0.0015 | Intercept |
| Class.a2                                                          | 1      | -10.000000     | 100.000                | 100.000     | 6.82    | 0.0401 | a 2       |
| Class.a3                                                          | 1      | -4.000000      | 16.000                 | 16.000      | 1.09    | 0.3365 | a 3       |
| Class.b2                                                          | 1      | -1.000000      | 1.000                  | 1.000       | 0.07    | 0.8027 | b 2       |
| Class.a2b2                                                        | 1      | 12.000000      | 72.000                 | 72.000      | 4.91    | 0.0686 | a 2 * b 2 |
| Class.a3b2                                                        | 1      | 9.000000       | 40.500                 | 40.500      | 2.76    | 0.1476 | a 3 * b 2 |

The parameter estimates are

$$\begin{aligned}\hat{\mu}_{11} &= \bar{y}_{11} = 15 \\ \hat{\alpha}_2 &= \bar{y}_{21} - \bar{y}_{11} = 5 - 15 = -10 \\ \hat{\alpha}_3 &= \bar{y}_{31} - \bar{y}_{11} = 11 - 15 = -4 \\ \hat{\beta}_2 &= \bar{y}_{12} - \bar{y}_{11} = 14 - 15 = -1 \\ \hat{\gamma}_{22} &= \bar{y}_{22} - (\hat{\mu}_{11} + \hat{\alpha}_2 + \hat{\beta}_2) = 16 - (15 + -10 + -1) = 12 \\ \hat{\gamma}_{32} &= \bar{y}_{32} - (\hat{\mu}_{11} + \hat{\alpha}_3 + \hat{\beta}_2) = 19 - (15 + -4 + -1) = 9\end{aligned}$$

**Figure 97.53** Reference Cell Model, (1,1) Reference Cell, Design Matrix

| Two-Way ANOVA Models                       |        |        |    |           |     |     |     |       |       |     |     |
|--------------------------------------------|--------|--------|----|-----------|-----|-----|-----|-------|-------|-----|-----|
| Reference Cell Model, (1,1) Reference Cell |        |        |    |           |     |     |     |       |       |     |     |
| Obs                                        | _TYPE_ | _NAME_ | y  | Intercept | a 2 | a 3 | b 2 | a 2 * | a 3 * | b 2 | b 2 |
| 1                                          | SCORE  | ROW1   | 16 | 1         | 0   | 0   | 0   | 0     | 0     | 1   | 1   |
| 2                                          | SCORE  | ROW2   | 14 | 1         | 0   | 0   | 0   | 0     | 0     | 1   | 1   |
| 3                                          | SCORE  | ROW3   | 15 | 1         | 0   | 0   | 1   | 0     | 0     | 1   | 2   |
| 4                                          | SCORE  | ROW4   | 13 | 1         | 0   | 0   | 1   | 0     | 0     | 1   | 2   |
| 5                                          | SCORE  | ROW5   | 1  | 1         | 1   | 0   | 0   | 0     | 0     | 2   | 1   |
| 6                                          | SCORE  | ROW6   | 9  | 1         | 1   | 0   | 0   | 0     | 0     | 2   | 1   |
| 7                                          | SCORE  | ROW7   | 12 | 1         | 1   | 0   | 1   | 1     | 0     | 2   | 2   |
| 8                                          | SCORE  | ROW8   | 20 | 1         | 1   | 0   | 1   | 1     | 0     | 2   | 2   |
| 9                                          | SCORE  | ROW9   | 14 | 1         | 0   | 1   | 0   | 0     | 0     | 3   | 1   |
| 10                                         | SCORE  | ROW10  | 8  | 1         | 0   | 1   | 0   | 0     | 0     | 3   | 1   |
| 11                                         | SCORE  | ROW11  | 18 | 1         | 0   | 1   | 1   | 0     | 1     | 3   | 2   |
| 12                                         | SCORE  | ROW12  | 20 | 1         | 0   | 1   | 1   | 0     | 1     | 3   | 2   |

The next model is a deviations-from-means model, but this time the reference cell is the first cell (1,1). This coding is also called effects coding. The following statements produce [Figure 97.54](#) and [Figure 97.55](#):

```
proc transreg data=x ss2 short;
 title2 'Deviations from Means, (1,1) Reference Cell';
 model identity(y) = class(a | b / deviations zero=first);
 output replace;
run;

proc print label;
run;
```

**Figure 97.54** Deviations-from-Means Model, (1,1) Reference Cell

```

Two-Way ANOVA Models
Deviations from Means, (1,1) Reference Cell

The TRANSREG Procedure

Dependent Variable Identity(y)

Class Level Information

Class Levels Values
a 3 1 2 3
b 2 1 2

Number of Observations Read 12
Number of Observations Used 12

The TRANSREG Procedure Hypothesis Tests for Identity(y)

Univariate ANOVA Table Based on the Usual Degrees of Freedom

Source DF Sum of Mean
 DF Squares Square F Value Pr > F

Model 5 234.6667 46.93333 3.20 0.0946
Error 6 88.0000 14.66667
Corrected Total 11 322.6667

Root MSE 3.82971 R-Square 0.7273
Dependent Mean 13.33333 Adj R-Sq 0.5000
Coeff Var 28.72281

Univariate Regression Table Based on the Usual Degrees of Freedom

Type II
Sum of Mean
Variable DF Coefficient Squares Square F Value Pr > F Label

Intercept 1 13.3333333 2133.33 2133.33 145.45 <.0001 Intercept
Class.a2 1 -2.8333333 48.17 48.17 3.28 0.1199 a 2
Class.a3 1 1.6666667 16.67 16.67 1.14 0.3274 a 3
Class.b2 1 3.0000000 108.00 108.00 7.36 0.0349 b 2
Class.a2b2 1 2.5000000 37.50 37.50 2.56 0.1609 a 2 * b 2
Class.a3b2 1 1.0000000 6.00 6.00 0.41 0.5461 a 3 * b 2

```

The parameter estimates are

$$\begin{aligned}\hat{\mu} &= \bar{y} = 13.3333 \\ \hat{\alpha}_2 &= (\bar{y}_{21} + \bar{y}_{22})/2 - \bar{y} = (5 + 16)/2 - 13.3333 = -2.8333 \\ \hat{\alpha}_3 &= (\bar{y}_{31} + \bar{y}_{32})/2 - \bar{y} = (11 + 19)/2 - 13.3333 = 1.6667 \\ \hat{\beta}_2 &= (\bar{y}_{12} + \bar{y}_{22} + \bar{y}_{32})/3 - \bar{y} = (14 + 16 + 19)/3 - 13.3333 = 3 \\ \hat{\gamma}_{22} &= \bar{y}_{22} - (\bar{y} + \hat{\alpha}_2 + \hat{\beta}_2) = 16 - (13.3333 + -2.8333 + 3) = 2.5 \\ \hat{\gamma}_{32} &= \bar{y}_{32} - (\bar{y} + \hat{\alpha}_3 + \hat{\beta}_2) = 19 - (13.3333 + 1.6667 + 3) = 1\end{aligned}$$

Notice that all of the parameter estimates match the corresponding estimates from the less-than-full-rank coding.

**Figure 97.55** Deviations-from-Means Model, (1,1) Reference Cell, Design Matrix

| Two-Way ANOVA Models                        |        |        |    |           |     |     |     |       |       |     |   |
|---------------------------------------------|--------|--------|----|-----------|-----|-----|-----|-------|-------|-----|---|
| Deviations from Means, (1,1) Reference Cell |        |        |    |           |     |     |     |       |       |     |   |
| Obs                                         | _TYPE_ | _NAME_ | y  | Intercept | a 2 | a 3 | b 2 | a 2 * | a 3 * | b 2 | b |
| 1                                           | SCORE  | ROW1   | 16 | 1         | -1  | -1  | -1  | 1     | 1     | 1   | 1 |
| 2                                           | SCORE  | ROW2   | 14 | 1         | -1  | -1  | -1  | 1     | 1     | 1   | 1 |
| 3                                           | SCORE  | ROW3   | 15 | 1         | -1  | -1  | 1   | -1    | -1    | 1   | 2 |
| 4                                           | SCORE  | ROW4   | 13 | 1         | -1  | -1  | 1   | -1    | -1    | 1   | 2 |
| 5                                           | SCORE  | ROW5   | 1  | 1         | 1   | 0   | -1  | -1    | 0     | 2   | 1 |
| 6                                           | SCORE  | ROW6   | 9  | 1         | 1   | 0   | -1  | -1    | 0     | 2   | 1 |
| 7                                           | SCORE  | ROW7   | 12 | 1         | 1   | 0   | 1   | 1     | 0     | 2   | 2 |
| 8                                           | SCORE  | ROW8   | 20 | 1         | 1   | 0   | 1   | 1     | 0     | 2   | 2 |
| 9                                           | SCORE  | ROW9   | 14 | 1         | 0   | 1   | -1  | 0     | -1    | 3   | 1 |
| 10                                          | SCORE  | ROW10  | 8  | 1         | 0   | 1   | -1  | 0     | -1    | 3   | 1 |
| 11                                          | SCORE  | ROW11  | 18 | 1         | 0   | 1   | 1   | 0     | 1     | 3   | 2 |
| 12                                          | SCORE  | ROW12  | 20 | 1         | 0   | 1   | 1   | 0     | 1     | 3   | 2 |

The following statements fit a model with an orthogonal-contrast coding and produce [Figure 97.56](#) and [Figure 97.57](#):

```
proc transreg data=x ss2 short;
 title2 'Orthogonal Contrast Coding';
 model identity(y) = class(a | b / orthogonal);
 output replace;
run;

proc print label;
run;
```

Figure 97.56 Orthogonal-Contrast Coding

```

Two-Way ANOVA Models
Orthogonal Contrast Coding

The TRANSREG Procedure

Dependent Variable Identity(y)

Class Level Information

Class Levels Values
a 3 1 2 3
b 2 1 2

Number of Observations Read 12
Number of Observations Used 12

The TRANSREG Procedure Hypothesis Tests for Identity(y)

Univariate ANOVA Table Based on the Usual Degrees of Freedom

Source DF Sum of Mean
 DF Squares Square F Value Pr > F
Model 5 234.6667 46.93333 3.20 0.0946
Error 6 88.0000 14.66667
Corrected Total 11 322.6667

Root MSE 3.82971 R-Square 0.7273
Dependent Mean 13.33333 Adj R-Sq 0.5000
Coeff Var 28.72281

Univariate Regression Table Based on the Usual Degrees of Freedom

Type II
Sum of Mean
Variable DF Coefficient Squares Square F Value Pr > F Label
Intercept 1 13.3333333 2133.33 2133.33 145.45 <.0001 Intercept
Class.a1 1 -0.2500000 0.50 0.50 0.03 0.8596 a 1
Class.a2 1 -1.4166667 48.17 48.17 3.28 0.1199 a 2
Class.b1 1 -3.0000000 108.00 108.00 7.36 0.0349 b 1
Class.a1b1 1 2.2500000 40.50 40.50 2.76 0.1476 a 1 * b 1
Class.a2b1 1 -1.2500000 37.50 37.50 2.56 0.1609 a 2 * b 1

```



The parameter estimates are

$$\begin{aligned}\hat{\mu} &= \bar{y} = 13.3333 \\ \hat{\alpha}_1 &= ((\bar{y}_{11} + \bar{y}_{12}) - (\bar{y}_{31} + \bar{y}_{32}))/4 = ((15 + 14) - (11 + 19))/4 = -0.25 \\ \hat{\alpha}_2 &= ((\bar{y}_{21} + \bar{y}_{22}) - (\bar{y}_{11} + \bar{y}_{12} + \bar{y}_{31} + \bar{y}_{32}))/2)/6 \\ &= ((5 + 16) - (15 + 14 + 11 + 19)/2)/6 = -1.417 \\ \hat{\beta}_1 &= ((\bar{y}_{11} + \bar{y}_{21} + \bar{y}_{31}) - (\bar{y}_{12} + \bar{y}_{22} + \bar{y}_{32}))/6 \\ &= ((15 + 5 + 11) - (14 + 16 + 19))/6 = -3 \\ \hat{\gamma}_{11} &= (\bar{y}_{11} - \bar{y}_{12} - \bar{y}_{31} + \bar{y}_{32})/4 = (15 - 14 - 11 + 19)/4 = 2.25 \\ \hat{\gamma}_{21} &= ((-\bar{y}_{11} + \bar{y}_{12} - \bar{y}_{31} + \bar{y}_{32})/2 + (\bar{y}_{21} - \bar{y}_{22}))/6 \\ &= ((-15 + 14 - 11 + 19)/2 + (5 - 16))/6 = -1.25\end{aligned}$$

**Figure 97.57** Orthogonal-Contrast Coding, Design Matrix

| Two-Way ANOVA Models<br>Orthogonal Contrast Coding |        |        |    |           |     |     |     |       |       |     |   |
|----------------------------------------------------|--------|--------|----|-----------|-----|-----|-----|-------|-------|-----|---|
| Obs                                                | _TYPE_ | _NAME_ | y  | Intercept | a 1 | a 2 | b 1 | a 1 * | a 2 * | b 1 | b |
| 1                                                  | SCORE  | ROW1   | 16 | 1         | 1   | -1  | 1   | 1     | -1    | 1   | 1 |
| 2                                                  | SCORE  | ROW2   | 14 | 1         | 1   | -1  | 1   | 1     | -1    | 1   | 1 |
| 3                                                  | SCORE  | ROW3   | 15 | 1         | 1   | -1  | -1  | -1    | 1     | 1   | 2 |
| 4                                                  | SCORE  | ROW4   | 13 | 1         | 1   | -1  | -1  | -1    | 1     | 1   | 2 |
| 5                                                  | SCORE  | ROW5   | 1  | 1         | 0   | 2   | 1   | 0     | 2     | 2   | 1 |
| 6                                                  | SCORE  | ROW6   | 9  | 1         | 0   | 2   | 1   | 0     | 2     | 2   | 1 |
| 7                                                  | SCORE  | ROW7   | 12 | 1         | 0   | 2   | -1  | 0     | -2    | 2   | 2 |
| 8                                                  | SCORE  | ROW8   | 20 | 1         | 0   | 2   | -1  | 0     | -2    | 2   | 2 |
| 9                                                  | SCORE  | ROW9   | 14 | 1         | -1  | -1  | 1   | -1    | -1    | 3   | 1 |
| 10                                                 | SCORE  | ROW10  | 8  | 1         | -1  | -1  | 1   | -1    | -1    | 3   | 1 |
| 11                                                 | SCORE  | ROW11  | 18 | 1         | -1  | -1  | -1  | 1     | 1     | 3   | 2 |
| 12                                                 | SCORE  | ROW12  | 20 | 1         | -1  | -1  | -1  | 1     | 1     | 3   | 2 |

The following statements fit a model with a standardized-orthogonal coding and produce [Figure 97.58](#) and [Figure 97.59](#):

```
proc transreg data=x ss2 short;
 title2 'Standardized-Orthogonal Coding';
 model identity(y) = class(a | b / standorth);
 output replace;
run;

proc print label;
run;
```

Figure 97.58 Standardized-Orthogonal Coding

```

Two-Way ANOVA Models
Standardized-Orthogonal Coding

The TRANSREG Procedure

Dependent Variable Identity(y)

Class Level Information

Class Levels Values
a 3 1 2 3
b 2 1 2

Number of Observations Read 12
Number of Observations Used 12

The TRANSREG Procedure Hypothesis Tests for Identity(y)

Univariate ANOVA Table Based on the Usual Degrees of Freedom

Source DF Sum of Mean
 DF Squares Square F Value Pr > F
Model 5 234.6667 46.93333 3.20 0.0946
Error 6 88.0000 14.66667
Corrected Total 11 322.6667

Root MSE 3.82971 R-Square 0.7273
Dependent Mean 13.33333 Adj R-Sq 0.5000
Coeff Var 28.72281

Univariate Regression Table Based on the Usual Degrees of Freedom

Type II
Sum of Mean
Variable DF Coefficient Squares Square F Value Pr > F Label
Intercept 1 13.3333333 2133.33 2133.33 145.45 <.0001 Intercept
Class.a1 1 -0.2041241 0.50 0.50 0.03 0.8596 a 1
Class.a2 1 -2.0034692 48.17 48.17 3.28 0.1199 a 2
Class.b1 1 -3.0000000 108.00 108.00 7.36 0.0349 b 1
Class.a1b1 1 1.8371173 40.50 40.50 2.76 0.1476 a 1 * b 1
Class.a2b1 1 -1.7677670 37.50 37.50 2.56 0.1609 a 2 * b 1

```

The parameter estimates are

$$\begin{aligned}\hat{\mu} &= \bar{y} = 13.3333 \\ \hat{\alpha}_1 &= (((\bar{y}_{11} + \bar{y}_{12}) - (\bar{y}_{31} + \bar{y}_{32}))/4) \times \sqrt{2/3} \\ &= (((15 + 14) - (11 + 19))/4) \times \sqrt{2/3} = -0.2041 \\ \hat{\alpha}_2 &= (((\bar{y}_{21} + \bar{y}_{22}) - (\bar{y}_{11} + \bar{y}_{12} + \bar{y}_{31} + \bar{y}_{32})/2)/6) \times \sqrt{6/3} \\ &= (((5 + 16) - (15 + 14 + 11 + 19)/2)/6) \times \sqrt{6/3} = -2.0035 \\ \hat{\beta}_1 &= (((\bar{y}_{11} + \bar{y}_{21} + \bar{y}_{31}) - (\bar{y}_{12} + \bar{y}_{22} + \bar{y}_{32}))/6) \times \sqrt{2/2} \\ &= (((15 + 5 + 11) - (14 + 16 + 19))/6) \times \sqrt{2/2} = -3 \\ \hat{\gamma}_{11} &= ((\bar{y}_{11} - \bar{y}_{12} - \bar{y}_{31} + \bar{y}_{32})/4) \times \sqrt{2/3} \times \sqrt{2/2} \\ &= ((15 - 14 - 11 + 19)/4) \times \sqrt{2/3} \times \sqrt{2/2} = 1.8371 \\ \hat{\gamma}_{21} &= (((-\bar{y}_{11} + \bar{y}_{12} - \bar{y}_{31} + \bar{y}_{32})/2 + (\bar{y}_{21} - \bar{y}_{22}))/6) \times \sqrt{6/3} \times \sqrt{2/2} \\ &= (((-15 + 14 - 11 + 19)/2 + (5 - 16))/6) \times \sqrt{6/3} \times \sqrt{2/2} = -1.7678\end{aligned}$$

The numerators in the square roots are sums of squares of the coded values for the unstandardized-orthogonal codings, and the denominators are the numbers of levels. These terms convert the estimates from the orthogonal contrast coding to the standardized-orthogonal coding. The term  $\sqrt{2/2}$ , which is 1 and could be dropped, is included in the preceding formulas to show the general pattern. Notice the regression tables for the orthogonal-contrast coding and the standardized-orthogonal coding. Some of the coefficients are different, but the rest of the table is the same since the coded variables for the two models differ only by a constant.

**Figure 97.59** Standardized-Orthogonal Coding, Design Matrix

| Two-Way ANOVA Models<br>Standardized-Orthogonal Coding |        |        |    |           |          |          |     |          |          |     |
|--------------------------------------------------------|--------|--------|----|-----------|----------|----------|-----|----------|----------|-----|
| Obs                                                    | _TYPE_ | _NAME_ | y  | Intercept | a 1      | a 2      | b 1 | a 1 *    | a 2 *    | a b |
|                                                        |        |        |    |           |          |          |     | b 1      | b 1      |     |
| 1                                                      | SCORE  | ROW1   | 16 | 1         | 1.22474  | -0.70711 | 1   | 1.22474  | -0.70711 | 1 1 |
| 2                                                      | SCORE  | ROW2   | 14 | 1         | 1.22474  | -0.70711 | 1   | 1.22474  | -0.70711 | 1 1 |
| 3                                                      | SCORE  | ROW3   | 15 | 1         | 1.22474  | -0.70711 | -1  | -1.22474 | 0.70711  | 1 2 |
| 4                                                      | SCORE  | ROW4   | 13 | 1         | 1.22474  | -0.70711 | -1  | -1.22474 | 0.70711  | 1 2 |
| 5                                                      | SCORE  | ROW5   | 1  | 1         | 0.00000  | 1.41421  | 1   | 0.00000  | 1.41421  | 2 1 |
| 6                                                      | SCORE  | ROW6   | 9  | 1         | 0.00000  | 1.41421  | 1   | 0.00000  | 1.41421  | 2 1 |
| 7                                                      | SCORE  | ROW7   | 12 | 1         | 0.00000  | 1.41421  | -1  | 0.00000  | -1.41421 | 2 2 |
| 8                                                      | SCORE  | ROW8   | 20 | 1         | 0.00000  | 1.41421  | -1  | 0.00000  | -1.41421 | 2 2 |
| 9                                                      | SCORE  | ROW9   | 14 | 1         | -1.22474 | -0.70711 | 1   | -1.22474 | -0.70711 | 3 1 |
| 10                                                     | SCORE  | ROW10  | 8  | 1         | -1.22474 | -0.70711 | 1   | -1.22474 | -0.70711 | 3 1 |
| 11                                                     | SCORE  | ROW11  | 18 | 1         | -1.22474 | -0.70711 | -1  | 1.22474  | 0.70711  | 3 2 |
| 12                                                     | SCORE  | ROW12  | 20 | 1         | -1.22474 | -0.70711 | -1  | 1.22474  | 0.70711  | 3 2 |

---

## Missing Values

PROC TRANSREG can estimate missing values, with or without category or monotonicity constraints, so that the regression model fit is optimized. Several approaches to missing data handling are provided. All observations with missing values in **IDENTITY**, **CLASS**, **POINT**, **EPOINT**, **QPOINT**, **SMOOTH**, **PBSPLINE**, **PSPLINE**, and **BSPLINE** variables are excluded from the analysis. When **METHOD=UNIVARIATE** (specified in the PROC TRANSREG or MODEL statement), observations with missing values in any of the independent variables are excluded from the analysis. When you specify the **NOMISS** *a-option*, observations with missing values in the other analysis variables are excluded. Otherwise, missing data are estimated, and the variable means are the initial estimates.

You can specify the **LINEAR**, **OPSCORE**, **MONOTONE**, **UNTIE**, **SPLINE**, **MSPLINE**, **SSPLINE**, **LOG**, **LOGIT**, **POWER**, **ARSIN**, **BOXCOX**, **RANK**, and **EXP** transformations in any combination with nonmissing values, ordinary missing values, and special missing values, as long as the nonmissing values in each variable have positive variance. No category or order restrictions are placed on the estimates of ordinary missing values. You can force missing value estimates within a variable to be identical by using special missing values (see “DATA Step Processing” in *SAS Language Reference: Concepts*). You can specify up to 27 categories of missing values, in which within-category estimates must be the same, by coding the missing values with **.\_** and **.A** through **.Z**.

You can also specify an ordering of some missing value estimates. You can use the **MONOTONE=** *a-option* in the PROC TRANSREG or MODEL statement to indicate a range of special missing values (a subset of the list from **.A** to **.Z**) with estimates that must be weakly ordered within each variable in which they appear. For example, if **MONOTONE=AI**, the nine classes, **.A**, **.B**, . . . , **.I**, are monotonically scored and optimally scaled just as **MONOTONE** transformation values are scored. In this case, category but not order restrictions are placed on the missing values **.\_** and **.J** through **.Z**. You can also use the **UNTIE=** *a-option* (in the PROC TRANSREG or MODEL statement) to indicate a range of special missing values with estimates that must be weakly ordered within each variable in which they appear but can be untied.

The missing value estimation facilities enable you to have partitioned or mixed-type variables. For example, a variable can be considered part nominal and part ordinal. Nominal classes of otherwise ordinal variables are coded with special missing values. This feature can be useful with survey research. The class “unfamiliar with the product” in the variable “Rate your preference for ‘Brand X’ on a 1 to 9 scale, or if you are unfamiliar with the product, check ‘unfamiliar with the product’” is an example. You can code “unfamiliar with the product” as a special missing value, such as **.A**. The 1s to 9s can be monotonically transformed, while no monotonic restrictions are placed on the quantification of the “unfamiliar with the product” class.

A variable specified for a **LINEAR** transformation, with special missing values and ordered categorical missing values, can be part interval, part ordinal, and part nominal. A variable specified for a **MONOTONE** transformation can have two independent ordinal parts. A variable specified for an **UNTIE** transformation can have an ordered categorical part and an ordered part without category restrictions. Many other mixes are possible.

---

## Missing Values, UNTIE, and Hypothesis Tests

PROC TRANSREG can estimate missing data and monotonically transform variables while untying tied values. Estimates of ordinary missing values (**.**) are all permitted to be different. Analyses with **UNTIE** transformations, the **UNTIE=** *a-option*, and ordinary missing data estimation are all prone to degeneracy

problems. Consider the following example. A perfect fit is found by collapsing all observations except the one with two missing values into a single value in  $y$  and  $x_1$ . The following statements produce Figure 97.60:

```

title 'Missing Data';

data x;
 input y x1 x2 @@;
 datalines;
1 3 7 8 3 9 1 8 6 . . 9 3 3 9
8 5 1 6 7 3 2 7 2 1 8 2 . 9 1
;

proc transreg solve;
 model linear(y) = linear(x1 x2);
 output;
run;

proc print;
run;

```

Figure 97.60 Missing Values Example

| Missing Data |        |        |   |         |           |    |    |            |         |     |
|--------------|--------|--------|---|---------|-----------|----|----|------------|---------|-----|
| Obs          | _TYPE_ | _NAME_ | y | Ty      | Intercept | x1 | x2 | TIntercept | Tx1     | Tx2 |
| 1            | SCORE  | ROW1   | 1 | 2.7680  | 1         | 3  | 7  | 1          | 5.1233  | 7   |
| 2            | SCORE  | ROW2   | 8 | 2.7680  | 1         | 3  | 9  | 1          | 5.1233  | 9   |
| 3            | SCORE  | ROW3   | 1 | 2.7680  | 1         | 8  | 6  | 1          | 5.1233  | 6   |
| 4            | SCORE  | ROW4   | . | 12.5878 | 1         | .  | 9  | 1          | 12.7791 | 9   |
| 5            | SCORE  | ROW5   | 3 | 2.7680  | 1         | 3  | 9  | 1          | 5.1233  | 9   |
| 6            | SCORE  | ROW6   | 8 | 2.7680  | 1         | 5  | 1  | 1          | 5.1233  | 1   |
| 7            | SCORE  | ROW7   | 6 | 2.7680  | 1         | 7  | 3  | 1          | 5.1233  | 3   |
| 8            | SCORE  | ROW8   | 2 | 2.7680  | 1         | 7  | 2  | 1          | 5.1233  | 2   |
| 9            | SCORE  | ROW9   | 1 | 2.7680  | 1         | 8  | 2  | 1          | 5.1233  | 2   |
| 10           | SCORE  | ROW10  | . | 2.7680  | 1         | 9  | 1  | 1          | 5.1233  | 1   |

Generally, the use of ordinary missing data estimation, the UNTIE transformation, and the UNTIE= *a-option* should be avoided, particularly with hypothesis tests. With these options, parameters are estimated based on only a single observation, and they can exert tremendous influence over the results. Each of these parameters has one model degree of freedom associated with it, so small or zero error degrees of freedom can also be a problem.

## Controlling the Number of Iterations

Several *a-options* in the PROC TRANSREG or MODEL statement control the number of iterations performed. Iteration terminates when any one of the following conditions is satisfied:

- The number of iterations equals the value of the `MAXITER=` *a-option*.

- The average absolute change in variable scores from one iteration to the next is less than the value of the `CONVERGE= a-option`.
- The criterion change is less than the value of the `CCONVERGE= a-option`.

You can specify negative values for either convergence *a-option* if you want to define convergence only in terms of the other option. The criterion change can become negative when the data have converged, so it is numerically impossible, within machine precision, to increase the criterion. Usually, a negative criterion change is the result of very small amounts of rounding error, since the algorithms are (usually) convergent. However, there are cases where a negative criterion change is a sign of divergence, which is not necessarily an error. When you specify an `SSPLINE` transformation or the `REITERATE` or `SOLVE a-option`, divergence is perfectly normal.

When there are no monotonicity constraints and there is only one canonical variable in each set, PROC TRANSREG (with the `SOLVE a-option`) can usually find the optimal solution in only one iteration. (There are no monotonicity constraints when none of the following is specified: `MONOTONE`, `MSPLINE`, or `UNTIE` transformation or the `UNTIE=` or `MONOTONE= a-option`. There is only one canonical variable in each set when `METHOD=MORALS` or `METHOD=UNIVARIATE`, or when `METHOD=REDUNDANCY` with only one dependent variable, or when `METHOD=CANALS` and `NCAN=1`.)

The initialization iteration is number 0. When there are no monotonicity constraints and there is only one canonical variable in each set, the next iteration shows no change, and iteration stops. At least two iterations (0 and 1) are performed with the `SOLVE a-option` even if nothing changes in iteration 0. The `MONOTONE`, `MSPLINE`, and `UNTIE` variables are not transformed by the canonical initialization. Note that divergence with the `SOLVE a-option`, particularly in the second iteration, is not an error. The initialization iteration is slower and uses more memory than other iterations. However, for many models, specifying the `SOLVE a-option` can greatly decrease the amount of time required to find the optimal transformations.

You can increase the number of iterations to ensure convergence by increasing the value of the `MAXITER= a-option` and decreasing the value of the `CONVERGE= a-option`. Since the average absolute change in standardized variable scores seldom decreases below  $1E-11$ , you should not specify a value for the `CONVERGE= a-option` less than  $1E-8$  or  $1E-10$ . Most of the data changes occur during the first few iterations, but the data can still change after 50 or even 100 iterations. You can try different combinations of values for the `CONVERGE=` and `MAXITER= a-options` to ensure convergence without extreme overiteration. If the data do not converge with the default specifications, try `CONVERGE=1E-8` and `MAXITER=50`, or `CONVERGE=1E-10` and `MAXITER=200`. Note that you can specify the `REITERATE a-option` to start iterating where the previous analysis stopped.

---

## Using the REITERATE Algorithm Option

You can use the `REITERATE a-option` to perform additional iterations when PROC TRANSREG stops before the data have adequately converged. For example, suppose that you execute the following step:

```
proc transreg data=a;
 model mspline(y) = mspline(x1-x5);
 output out=b coefficients;
run;
```

If the transformations do not converge in the default 30 iterations, you can perform more iterations without repeating the first 30 iterations, as follows:

```
proc transreg data=b reiterate;
 model mspline(y) = mspline(x1-x5);
 output out=b coefficients;
run;
```

Note that a WHERE statement is not necessary to exclude the coefficient observations. They are automatically excluded because their `_TYPE_` value is not SCORE.

You can also use the REITERATE *a-option* to specify starting values other than the original values for the transformations. Providing alternate starting points might help avoid local optima. Here are two examples:

```
proc transreg data=a;
 model rank(y) = rank(x1-x5);
 output out=b;
run;

proc transreg data=b reiterate;
 /* Use ranks as the starting point. */
 model mspline(y) = mspline(x1-x5);
 output out=c coefficients;
run;

data b;
 set a;
 array tx[6] ty tx1-tx5;
 do j = 1 to 6;
 tx[j] = normal(7);
 end;
run;

proc transreg data=b reiterate;
 /* Use a random starting point. */
 model mspline(y) = mspline(x1-x5);
 output out=c coefficients;
run;
```

Note that divergence with the REITERATE *a-option*, particularly in the second iteration, is not an error since the initial transformation is not required to be a valid member of the transformation family. When you specify the REITERATE *a-option*, the iteration does not terminate when the criterion change is negative during the first 10 iterations.

---

## Avoiding Constant Transformations

There are times when the optimal scaling produces a constant transformed variable. This can happen with the MONOTONE, UNTIE, and MSPLINE transformations when the target is negatively correlated with the original input variable. It can happen with all transformations when the target is uncorrelated with the original input variable. When this happens, the procedure modifies the target to avoid a constant transformation. This strategy avoids certain nonoptimal solutions.

If the transformation is monotonic and a constant transformed variable results, the procedure multiplies the target by  $-1$  and tries the optimal scaling again. If the transformation is not monotonic or if the multiplication by  $-1$  did not help, the procedure tries using a random target. If the transformation is still constant, the

previous nonconstant transformation is retained. When a constant transformation is avoided by any strategy, this message is displayed: “A constant transformation was avoided for *name*.”

With extreme collinearity, small amounts of rounding error might interact with the instability of the coefficients to produce target vectors that are not positively correlated with the original scaling. If a regression coefficient for a variable is zero, the formula for the target for that variable contains a zero divide. In a multiple regression model, after many iterations, one independent variable can be scaled the same way as the current scaling of the dependent variable, so the other independent variables have coefficients of zero. When the constant transformation warning appears, you should interpret your results with extreme caution, and recheck your model.

---

## Constant Variables

Constant and almost constant variables are zeroed and ignored. When constant variables are expected and should not be zeroed, specify the `NOZEROCONSTANT` *a-option*.

---

## Character OPSCORE Variables

Character `OPSCORE` variables are replaced by a numeric variable containing category numbers before the iterations, and the character values are discarded. Only the first eight characters are considered in determining category membership. If you want the original character variable in the output data set, give it a different name in the `OPSCORE` specification (`OPSCORE(x / name=(x2))`) and name the original variable in the `ID` statement (`ID x;`).

---

## Convergence and Degeneracies

When you specify the `SSPLINE` transformation, divergence is normal. The rest of this section assumes that you did not specify `SSPLINE`. For all the methods available in `PROC TRANSREG`, the algorithms are convergent, in terms of both the criterion being optimized and the parameters being estimated. The value of the criterion being maximized (squared multiple correlation, average squared multiple correlation, or average squared canonical correlation) can, theoretically, never decrease from one iteration to the next. The values of the parameters being solved for (the scores and weights of the transformed variables) become stable after sufficient iteration.

In practice, the criterion being maximized can decrease with overiteration. When the statistic has very nearly reached its maximum, further iterations might report a decrease in the criterion in the last few decimal places. This is a normal result of very small amounts of rounding error. By default, iteration terminates when this occurs because, by default, `CCONVERGE=0.0`. Specifying `CCONVERGE=-1`, an impossible change, turns off this check for convergence.

Even though the algorithms are convergent, they might not converge to a global optimum. Also, under extreme circumstances, the solution might degenerate. Because two points always form a straight line, the algorithms sometimes try to reach this degenerate optimum. This sometimes occurs when one observation is an ordinal outlier (when one observation has the extreme rank on all variables). The algorithm can reach an optimal solution that ties all other categories producing two points. Similar results can occur when there



are many missing values. More generally, whenever there are very few constraints on the scoring of one or more points, degeneracies can be a problem. In a well-behaved analysis, the maximum data change, average data change, and criterion change all decrease at a rapid rate with each iteration. When the rate of change increases for several iterations, the solution might be degenerating.

---

## Implicit and Explicit Intercepts

Depending on several options, the model intercept is nonzero, zero, or implicit, or there is no intercept. Ordinarily, the model contains an explicit nonzero intercept, and the Intercept variable in the `OUT=` data set contains ones. When `TSTANDARD=CENTER` or `TSTANDARD=Z` is specified, the model contains an explicit, zero intercept and the Intercept variable contains zeros. When `METHOD=CANALS`, the model is fit with centered variables and the Intercept variable is set to missing.

If you specify `CLASS` with `ZERO=NONE` or `BSPLINE` for one or more independent variables, and `TSTANDARD=NOMISS` or `TSTANDARD=ORIGINAL` (the default), an implicit intercept model is fit. The intercept is implicit in a set of the independent variables since there exists a set of independent variables the sum of which is a column of ones. All statistics are mean corrected. The implicit intercept is not an option; it is implied by the model. Specifying `SMOOTH` or `PBSPLINE` also implies an implicit intercept model.

With `METHOD=CANALS`, the Intercept variable contains the *canonical intercept* for canonical coefficients observations:  $\hat{\beta}_0 = \bar{y}'\hat{\alpha} - \bar{x}'\hat{\beta}$  where  $\mathbf{Y}\hat{\alpha} \approx \mathbf{X}\hat{\beta}$ .

---

## Passive Observations

Observations can be excluded from the analysis for several reasons; these include zero weight; zero frequency; missing values in variables designated `IDENTITY`, `CLASS`, `POINT`, `EPOINT`, `QPOINT`, `SMOOTH`, `PBSPLINE`, `PSPLINE`, or `BSPLINE`; and missing values with the `NOMISS a-option` specified. These observations are passive in that they do not contribute to determining transformations, R square, sums of squares, degrees of freedom, and so on. However, some information can be computed for them. For example, if no independent variable values are missing, predicted values and redundancy variable values can both be computed. Residuals can be computed for observations with a nonmissing dependent and nonmissing predicted value. Canonical variables for dependent variables can be computed when no dependent variables are missing; canonical variables for independent variables can be computed when no independent variables are missing, and so on. Passive observations in the `OUT=` data set have a blank value for `_TYPE_`.

---

## Point Models

The expanded set of independent variables generated from the `POINT`, `EPOINT`, and `QPOINT` expansions can be used to perform ideal point regressions (Carroll 1972) and compute ideal point coordinates for plotting in a biplot (Gabriel 1981). The three types of ideal point coordinates can all be described as transformed coefficients. Assume that  $m$  independent variables are specified in one of the three point expansions. Let  $\mathbf{b}'$  be a  $1 \times m$  row vector of coefficients for these variables and one of the dependent variables. Let  $\mathbf{R}$  be a matrix created from the coefficients of the extra variables. When coordinates are requested with the `MPC`, `MEC`, or `MQC o-option`,  $\mathbf{b}'$  and  $\mathbf{R}$  are created from multiple regression coefficients. When coordinates are requested with the `CPC`, `CEC`, or `CQC o-option`,  $\mathbf{b}'$  and  $\mathbf{R}$  are created from canonical coefficients.

If you specify the **POINT** expansion in the **MODEL** statement, **R** is an  $m \times m$  identity matrix times the coefficient for the sums of squares (**\_ISSQ\_**) variable. If you specify the **EPOINT** expansion, **R** is an  $m \times m$  diagonal matrix of coefficients from the squared variables. If you specify the **QPOINT** expansion, **R** is an  $m \times m$  symmetric matrix of coefficients from the squared variables on the diagonal and crossproduct variables off the diagonal. The **MPC**, **MEC**, **MQC**, **CPC**, **CEC**, and **CQC** ideal point coordinates are defined as  $-0.5\mathbf{b}'\mathbf{R}^{-1}$ . When **R** is singular, the ideal point coordinates are infinitely far away and are set to missing, so you should try a simpler version of the model. The version that is simpler than the **POINT** model is the vector model, where no extra variables are created. In the vector model, designate all independent variables as **IDENTITY**. Then draw vectors from the origin to the **COEFFICIENTS** points.

Typically, when you request ideal point coordinates, the **MODEL** statement should consist of a single transformation for the dependent variables (usually **IDENTITY**, **MONOTONE**, or **MSPLINE**) and a single expansion for the independent variables (one of **POINT**, **EPOINT**, or **QPOINT**).

---

## Redundancy Analysis

Redundancy analysis (Stewart and Love 1968) is a principal component analysis of multivariate regression predicted values. These first steps show the redundancy analysis results produced by **PROC TRANSREG**. The specification **TSTANDARD=Z** sets all variables to mean zero and variance one. **METHOD=REDUNDANCY** specifies redundancy analysis and outputs the redundancy variables to the **OUT=** data set. The **MREDUNDANCY** *o-option* outputs two sets of redundancy analysis coefficients to the **OUT=** data set.

The following statements produce [Figure 97.61](#):

```

title 'Redundancy Analysis';

data x;
 input y1-y3 x1-x4;
 datalines;
6 8 8 15 18 26 27
1 12 16 18 9 20 8
5 6 15 20 17 29 31
6 9 15 14 10 16 22
7 5 12 14 6 13 9
3 6 7 2 14 26 22
3 5 9 13 18 10 22
6 3 11 3 15 22 29
6 3 7 10 20 21 27
7 5 9 8 10 12 18
;

proc transreg data=x tstandard=z method=redundancy;
 model identity(y1-y3) = identity(x1-x4);
 output out=red mredundancy replace;
run;

proc print data=red(drop=Intercept);
 format _numeric_ 4.1;
run;

```

Figure 97.61 Redundancy Analysis Example

| Redundancy Analysis |          |        |      |      |      |      |      |      |      |      |      |      |
|---------------------|----------|--------|------|------|------|------|------|------|------|------|------|------|
| Obs                 | _TYPE_   | _NAME_ | y1   | y2   | y3   | x1   | x2   | x3   | x4   | Red1 | Red2 | Red3 |
| 1                   | SCORE    | ROW1   | 0.5  | 0.6  | -0.8 | 0.6  | 0.9  | 1.0  | 0.7  | 0.2  | -0.5 | -0.9 |
| 2                   | SCORE    | ROW2   | -2.0 | 2.1  | 1.5  | 1.1  | -1.0 | 0.1  | -1.7 | 1.6  | -1.5 | 0.4  |
| 3                   | SCORE    | ROW3   | 0.0  | -0.1 | 1.2  | 1.4  | 0.7  | 1.5  | 1.2  | 1.0  | 0.8  | -1.3 |
| 4                   | SCORE    | ROW4   | 0.5  | 1.0  | 1.2  | 0.4  | -0.8 | -0.5 | 0.1  | 0.5  | 1.7  | 0.1  |
| 5                   | SCORE    | ROW5   | 1.0  | -0.4 | 0.3  | 0.4  | -1.6 | -1.0 | -1.6 | 1.0  | 0.1  | 0.9  |
| 6                   | SCORE    | ROW6   | -1.0 | -0.1 | -1.1 | -1.6 | 0.1  | 1.0  | 0.1  | -0.8 | -0.9 | 1.4  |
| 7                   | SCORE    | ROW7   | -1.0 | -0.4 | -0.6 | 0.2  | 0.9  | -1.5 | 0.1  | -1.0 | -0.4 | -1.3 |
| 8                   | SCORE    | ROW8   | 0.5  | -1.2 | 0.0  | -1.5 | 0.3  | 0.4  | 1.0  | -1.2 | 0.8  | 0.7  |
| 9                   | SCORE    | ROW9   | 0.5  | -1.2 | -1.1 | -0.3 | 1.3  | 0.2  | 0.7  | -1.0 | -0.9 | -0.8 |
| 10                  | SCORE    | ROW10  | 1.0  | -0.4 | -0.6 | -0.6 | -0.8 | -1.1 | -0.4 | -0.4 | 0.8  | 0.7  |
| 11                  | M REDUND | Red1   | .    | .    | .    | 0.7  | -0.6 | 0.4  | -0.1 | .    | .    | .    |
| 12                  | M REDUND | Red2   | .    | .    | .    | 0.3  | -1.5 | -0.6 | 1.9  | .    | .    | .    |
| 13                  | M REDUND | Red3   | .    | .    | .    | -0.7 | -0.7 | 0.3  | -0.3 | .    | .    | .    |
| 14                  | R REDUND | x1     | .    | .    | .    | .    | .    | .    | .    | 0.8  | -0.0 | -0.6 |
| 15                  | R REDUND | x2     | .    | .    | .    | .    | .    | .    | .    | -0.6 | -0.2 | -0.7 |
| 16                  | R REDUND | x3     | .    | .    | .    | .    | .    | .    | .    | 0.1  | -0.2 | -0.1 |
| 17                  | R REDUND | x4     | .    | .    | .    | .    | .    | .    | .    | -0.5 | 0.3  | -0.5 |

The `_TYPE_='SCORE'` observations of the Red1–Red3 variables contain the redundancy variables. The nonmissing “M REDUND” values are coefficients for predicting the redundancy variables from the independent variables. The nonmissing “R REDUND” values are coefficients for predicting the independent variables from the redundancy variables.

The next steps show how to generate the same results manually. The data set is standardized, predicted values are computed, and principal components of the predicted values are computed. The following statements produce the redundancy variables, shown in Figure 97.62:

```
proc standard data=x out=std m=0 s=1;
 title2 'Manually Generate Redundancy Variables';
run;

proc reg noprint data=std;
 model y1-y3 = x1-x4;
 output out=p p=ay1-ay3;
run; quit;

proc princomp data=p cov noprint std out=p;
 var ay1-ay3;
run;

proc print data=p(keep=Prin:);
 format _numeric_ 4.1;
run;
```

**Figure 97.62** Redundancy Analysis Example

| Redundancy Analysis                    |       |       |       |  |
|----------------------------------------|-------|-------|-------|--|
| Manually Generate Redundancy Variables |       |       |       |  |
| Obs                                    | Prin1 | Prin2 | Prin3 |  |
| 1                                      | 0.2   | -0.5  | -0.9  |  |
| 2                                      | 1.6   | -1.5  | 0.4   |  |
| 3                                      | 1.0   | 0.8   | -1.3  |  |
| 4                                      | 0.5   | 1.7   | 0.1   |  |
| 5                                      | 1.0   | 0.1   | 0.9   |  |
| 6                                      | -0.8  | -0.9  | 1.4   |  |
| 7                                      | -1.0  | -0.4  | -1.3  |  |
| 8                                      | -1.2  | 0.8   | 0.7   |  |
| 9                                      | -1.0  | -0.9  | -0.8  |  |
| 10                                     | -0.4  | 0.8   | 0.7   |  |

The following statements produce the coefficients for predicting the redundancy variables from the independent variables, shown in [Figure 97.63](#):

```
proc reg data=p outest=redcoef noprint;
 title2 'Manually Create Redundancy Coefficients';
 model Prin1-Prin3 = x1-x4;
run; quit;

proc print data=redcoef(keep=x1-x4);
 format _numeric_ 4.1;
run;
```

**Figure 97.63** Redundancy Analysis Example

| Redundancy Analysis                     |      |      |      |      |
|-----------------------------------------|------|------|------|------|
| Manually Create Redundancy Coefficients |      |      |      |      |
| Obs                                     | x1   | x2   | x3   | x4   |
| 1                                       | 0.7  | -0.6 | 0.4  | -0.1 |
| 2                                       | 0.3  | -1.5 | -0.6 | 1.9  |
| 3                                       | -0.7 | -0.7 | 0.3  | -0.3 |

The following statements produce the coefficients for predicting the independent variables from the redundancy variables, shown in [Figure 97.64](#):

```
proc reg data=p outest=redcoef2 noprint;
 title2 'Manually Create Other Coefficients';
 model x1-x4 = prin1-prin3;
run; quit;

proc print data=redcoef2(keep=Prin1-Prin3);
 format _numeric_ 4.1;
run;
```

Figure 97.64 Redundancy Analysis Example

| Redundancy Analysis                |       |       |       |
|------------------------------------|-------|-------|-------|
| Manually Create Other Coefficients |       |       |       |
| Obs                                | Prin1 | Prin2 | Prin3 |
| 1                                  | 0.8   | -0.0  | -0.6  |
| 2                                  | -0.6  | -0.2  | -0.7  |
| 3                                  | 0.1   | -0.2  | -0.1  |
| 4                                  | -0.5  | 0.3   | -0.5  |

## Optimal Scaling

An alternating least squares optimal scaling algorithm can be divided into two major stages. The first major stage estimates the parameters of the linear model. These parameters are used to create the predicted values or target for each variable that can be transformed. Each target minimizes squared error (as explained in the discussion of the algorithms in *SAS Technical Report R-108*). The definition of the target depends on many factors, such as whether a variable is independent or dependent, which algorithm is used (for example, regression, redundancy, CANALS, or principal components), and so on. The definition of the target is independent of the transformation family you specify for the variable. However, the target values for a variable typically do not fit the prescribed transformation family for the variable. They might not have the right category structure; they might not have the right order; they might not be a linear combination of the columns of a B-spline basis; and so on.

The second major stage is optimal scaling. Optimal scaling can be defined as a possibly constrained, least squares regression problem. When you specify an optimal transformation, or when missing data are estimated for any variable, the full representation of the variable is not simply a vector; it is a matrix with more than one column. The optimal scaling phase finds the vector that is a linear combination of the columns of this matrix that is closest to the target (in terms of minimum squared error), among those that do not violate any of the constraints imposed by the transformation family. Optimal scaling methods are independent of the data analysis method that generated the target. In all cases, optimal scaling can be accomplished by creating a design matrix based on the original scaling of the variable and the transformation family specified for that variable. The optimally scaled variable is a linear combination of the columns of the design matrix. The coefficients of the linear combination are found by using (possibly constrained) least squares. Many optimal scaling problems are solved without actually constructing design and projection matrices. The next two sections describe the algorithms used by PROC TRANSREG for optimal scaling. The first section discusses optimal scaling for **OPSCORE**, **MONOTONE**, **UNTIE**, and **LINEAR** transformations, including how missing values are handled. The second section addresses **SPLINE** and **MSPLINE** transformations.

## OPSCORE, MONOTONE, UNTIE, and LINEAR Transformations

Two vectors of information are needed to produce the optimally scaled variable: the initial variable scaling vector  $x$  and the target vector  $y$ . For convenience, both vectors are first sorted on the values of the initial scaling vector. If you request an **UNTIE** transformation, the target vector is sorted within ties in the initial

scaling vector. The normal SAS collating sequence for missing and nonmissing values is used. Sorting simply permits the constraints to be specified in terms of relationships among adjoining coefficients. The sorting process partitions  $x$  and  $y$  into missing and nonmissing parts  $(x'_m x'_n)'$ , and  $(y'_m y'_n)'$ .

Next, PROC TRANSREG determines category membership. Every ordinary missing value (.) forms a separate category. (Three ordinary missing values form three categories.) Every special missing value within the range specified in the UNTIE= *a-option* forms a separate category. (If UNTIE= BC and there are three .B and two .C missing values, five categories are formed from them.) For all other special missing values, a separate category is formed for each different value. (If there are four .A missing values, one category is formed from them.)

Each distinct nonmissing value forms a separate category for OPSCORE and MONOTONE transformations (1 1 1 2 2 3 form three categories). Each nonmissing value forms a separate category for all other transformations (1 1 1 2 2 3 form six categories). When category membership is determined, category means are computed. Here is an example:

```

x: (. . .A .A .B 1 1 1 2 2 3 3 3 4)'
y: (5 6 2 4 2 1 2 3 4 6 4 5 6 7)'

OPSCORE and
MONOTONE means: (5 6 3 2 2 5 5 7)'
other means: (5 6 3 2 1 2 3 4 6 4 5 6 7)'

```

The category means are the coefficients of a category indicator design matrix. The category means are the Fisher (1938) optimal scores. For MONOTONE and UNTIE transformations, order constraints are imposed on the category means for the nonmissing partition by merging categories that are out of order. The algorithm checks upward until an order violation is found, and then averages downward until the order violation is averaged away. (The average of  $\bar{x}_1$  computed from  $n_1$  observations and  $\bar{x}_2$  computed from  $n_2$  observations is  $(n_1\bar{x}_1 + n_2\bar{x}_2)/(n_1 + n_2)$ .) The MONOTONE algorithm (Kruskal 1964, secondary approach to ties) for this example with means for the nonmissing values  $(2\ 5\ 5\ 7)'$  would do the following checks:  $2 < 5$ : OK,  $5 = 5$ : OK,  $5 < 7$ : OK. The means are in the proper order, so no work is needed.

The UNTIE transformation (Kruskal 1964, primary approach to ties) uses the same algorithm on the means of the nonmissing values  $(1\ 2\ 3\ 4\ 6\ 4\ 5\ 6\ 7)'$  but with different results for this example:  $1 < 2$ : OK,  $2 < 3$ : OK,  $3 < 4$ : OK,  $4 < 6$ : OK,  $6 > 4$ : average 6 and 4 and replace 6 and 4 by the average. The new means of the nonmissing values are  $(1\ 2\ 3\ 4\ 5\ 5\ 6\ 7)'$ . The check resumes:  $4 < 5$ : OK,  $5 = 5$ : OK,  $5 = 5$ : OK,  $5 < 6$ : OK,  $6 < 7$ : OK. If some of the special missing values are ordered, the upward-checking, downward-averaging algorithm is applied to them also, independently of the other missing and nonmissing partitions. When the means conform to any required category or order constraints, an optimally scaled vector is produced from the means. The following example results from a MONOTONE transformation:

```

x: (. . .A .A .B 1 1 1 2 2 3 3 3 4)'
y: (5 6 2 4 2 1 2 3 4 6 4 5 6 7)'
result: (5 6 3 3 2 2 2 2 5 5 5 5 5 7)'

```

The upward-checking, downward-averaging algorithm is equivalent to creating a category indicator design matrix, solving for least squares coefficients with order constraints, and then computing the linear combination of design matrix columns.

For the optimal transformation LINEAR and for nonoptimal transformations, missing values are handled as just described. The nonmissing target values are regressed onto the matrix defined by the nonmissing initial

scaling values and an intercept. In this example, the target vector  $y_n = (1\ 2\ 3\ 4\ 6\ 4\ 5\ 6\ 7)'$  is regressed onto the design matrix

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 2 & 2 & 3 & 3 & 3 & 4 \end{bmatrix}'$$

Although only a linear transformation is performed, the effect of a linear regression optimal scaling is not eliminated by the later standardization step (unless the variable has no missing values). In the presence of missing values, the linear regression is necessary to minimize squared error.

## SPLINE and MSPLINE Transformations

The missing portions of variables subjected to **SPLINE** or **MSPLINE** transformations are handled the same way as for **OPSCORE**, **MONOTONE**, **UNTIE**, and **LINEAR** transformations (see the previous section). The nonmissing partition is handled by first creating a B-spline basis of the specified degree with the specified knots for the nonmissing partition of the initial scaling vector and then regressing the target onto the basis. The optimally scaled vector is a linear combination of the B-spline basis vectors. Ordinary least squares regression coefficients are used. An algorithm for generating the B-spline basis is given in de Boor (1978, pp. 134–135). B-splines are both a computationally accurate and efficient way of constructing a basis for piecewise polynomials; however, they are not the most natural method of describing splines.

Consider an initial scaling vector  $x = (1\ 2\ 3\ 4\ 5\ 6\ 7\ 8\ 9)'$  and a degree-three spline with interior knots at 3.5 and 6.5. The B-spline basis for the transformation is the left matrix, and the natural piecewise polynomial spline basis is the right matrix.

| B-Spline Basis                                                                                                                                                                                                                                                                                                                                                                                                | Piecewise Polynomial Splines                                                                                                                                                                                                                                                                                              |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| $\begin{bmatrix} 1.000 & 0.000 & 0.000 & 0.000 & 0 & 0 \\ 0.216 & 0.608 & 0.167 & 0.009 & 0 & 0 \\ 0.008 & 0.458 & 0.461 & 0.073 & 0 & 0 \\ 0 & 0.172 & 0.585 & 0.241 & 0.001 & 0 \\ 0 & 0.037 & 0.463 & 0.463 & 0.037 & 0 \\ 0 & 0.001 & 0.241 & 0.585 & 0.172 & 0 \\ 0 & 0 & 0.073 & 0.461 & 0.458 & 0.008 \\ 0 & 0 & 0.009 & 0.167 & 0.608 & 0.216 \\ 0 & 0 & 0.000 & 0.000 & 0.000 & 1.000 \end{bmatrix}$ | $\begin{bmatrix} 1 & 1 & 1 & 1 & 0 & 0 \\ 1 & 2 & 4 & 8 & 0 & 0 \\ 1 & 3 & 9 & 27 & 0 & 0 \\ 1 & 4 & 16 & 64 & 0.125 & 0 \\ 1 & 5 & 25 & 125 & 3.375 & 0 \\ 1 & 6 & 36 & 216 & 15.625 & 0 \\ 1 & 7 & 49 & 343 & 42.875 & 0.125 \\ 1 & 8 & 64 & 512 & 91.125 & 3.375 \\ 1 & 9 & 81 & 729 & 166.375 & 15.625 \end{bmatrix}$ |

The two matrices span the same column space. The natural basis has an intercept, a linear term, a quadratic term, a cubic term, and two more terms since there are two interior knots. These terms are generated (for knot  $k$  and  $x$  element  $x$ ) by the formula  $(x - k)^3 \times I_{(x > k)}$ . The indicator variable  $I_{(x > k)}$  evaluates to 1.0 if  $x$  is greater than  $k$  and to 0.0 otherwise. If knot  $k$  had been repeated, there would be a  $(x - k)^2 \times I_{(x > k)}$  term also. Notice that the fifth column makes no contribution to the curve before 3.5, makes zero contribution at 3.5 (the transformation is continuous), and makes an increasing contribution beyond 3.5. The same pattern of results holds for the last term with knot 6.5. The coefficient of the fifth column represents the change in the cubic portion of the curve after 3.5. The coefficient of the sixth column represents the change in the cubic portion of the curve after 6.5.



The numbers in the B-spline basis do not have a simple interpretation like the numbers in the natural piecewise polynomial basis. The B-spline basis has a diagonally banded structure. The band shifts one column to the right after every knot. The number of entries in each row that can potentially be nonzero is one greater than the degree. The elements within a row always sum to one. The B-spline basis is accurate because of the smallness of the numbers and the lack of extreme collinearity inherent in the natural polynomials. B-splines are efficient because PROC TRANSREG can take advantage of the sparseness of the B-spline basis when it accumulates crossproducts. The number of required multiplications and additions to accumulate the crossproduct matrix does not increase with the number of knots but does increase with the degree of the spline, so it is much more computationally efficient to increase the number of knots than to increase the degree of the polynomial.

MSPLINE transformations are handled like SPLINE transformations except that constraints are placed on the coefficients to ensure monotonicity. When the coefficients of the B-spline basis are monotonically increasing, the transformation is monotonically increasing. When the polynomial degree is two or less, monotone coefficient splines, integrated splines (Winsberg and Ramsay 1980), and the general class of all monotone splines are equivalent.

---

## Specifying the Number of Knots

Keep the number of knots small (usually less than 10, although you can specify more). A degree-three spline with nine knots, one at each decile, can closely follow a large variety of curves. Each spline transformation of degree  $p$  with  $q$  knots fits a model with  $p + q$  parameters. The total number of parameters should be much less than the number of observations. Usually in regression analyses, it is recommended that there be at least five or ten observations for each parameter in order to get stable results. For example, when spline transformations of degree three with nine knots are requested for six variables, the number of observations in the data set should be at least 5 or 10 times 72 (since  $6 \times (3 + 9)$  is the total number of parameters). The overall model can also have a parameter for the intercept and one or more parameters for each nonspline variable in the model.

Increasing the number of knots gives the spline more freedom to bend and follow the data. Increasing the degree also gives the spline more freedom, but to a lesser extent. Specifying a large number of knots is much better than increasing the degree beyond three.

When you specify `NKNOTS= $q$`  for a variable with  $n$  observations, then each of the  $q + 1$  segments of the spline contains  $n/(q + 1)$  observations on the average. When you specify `KNOTS=number-list`, make sure that there is a reasonable number of observations in each interval.

The following statements find a cubic polynomial transformation of  $x$  and no transformation of  $y$ :

```
proc transreg;
 model identity(y)=spline(x);
 output;
run;
```

The following statements find a cubic-spline transformation for  $x$  that consists of the weighted sum of a single constant, a single straight line, a quadratic curve for the portion of the variable less than 3.0, a different quadratic curve for the portion greater than 3.0 (since the 3.0 knot is repeated), and a different cubic curve for each of the intervals: (minimum to 1.5), (1.5 to 2.4), (2.4 to 3.0), (3.0 to 4.0), and (4.0 to maximum):



```
proc transreg;
 model identity(y)=spline(x / knots=1.5 2.4 3.0 3.0 4.0);
 output;
run;
```

The transformation is continuous everywhere, its first derivative is continuous everywhere, its second derivative is continuous everywhere except at 3.0, and its third derivative is continuous everywhere except at 1.5, 2.4, 3.0, and 4.0.

The following statements find a quadratic spline transformation that consists of a polynomial  $x_t = b_0 + b_1x + b_2x^2$  for the range ( $x < 3.0$ ) and a completely different polynomial  $x_t = b_3 + b_4x + b_5x^2$  for the range ( $x > 3.0$ ):

```
proc transreg;
 model identity(y)=spline(x / knots=3 3 3 degree=2);
 output;
run;
```

The two curves are not required to be continuous at 3.0.

The following statements categorize  $y$  into 10 intervals and find a step-function transformation:

```
proc transreg;
 model identity(y)=spline(x / degree=0 nknots=9);
 output;
run;
```

One aspect of this transformation family is unlike all other optimal transformation families. The initial scaling of the data does not fit the restrictions imposed by the transformation family. This is because the initial variable can be continuous, but a discrete step-function transformation is sought. Zero-degree spline variables are categorized before the first iteration.

The following statements find a continuous, piecewise linear transformation of  $x$ :

```
proc transreg;
 model identity(y)=spline(x / degree=1 nknots=8);
 output;
run;
```

---

## SPLINE, BSPLINE, and PSPLINE Comparisons

**SPLINE** is a transformation. It takes a variable as input and produces a transformed variable as output. Internally, with **SPLINE**, a B-spline basis is used to find the transformation, which is a linear combination of the columns of the B-spline basis. However, with **SPLINE**, the basis is not made available in any output.

**BSPLINE** is an expansion. It takes a variable as input and produces more than one variable as output. The output variables are the same B-spline basis that is used internally by **SPLINE**.

**PSPLINE** is an expansion. It takes a variable as input and produces more than one variable as output. The difference between **PSPLINE** and **BSPLINE** is that **PSPLINE** produces a piecewise polynomial, whereas **BSPLINE** produces a B-spline. A matrix consisting of a piecewise polynomial basis and an intercept spans the same space as the B-spline matrix, but the basis vectors are quite different. The numbers in the piecewise

polynomials can get quite large; the numbers in the B-spline basis range between 0 and 1. There are many more zeros in the B-spline basis.

Interchanging SPLINE, BSPLINE, and PSPLINE should have no effect on the fit of the overall model except for the fact that PSPLINE is much more prone to numerical problems. Similarly, interchanging a CLASS expansion and an OPSCORE transformation should have no effect on the fit of the overall model.

---

## Hypothesis Tests

PROC TRANSREG has a set of options for testing hypotheses in models with a single dependent variable. The **TEST** *a-option* produces an ANOVA table. It tests the null hypothesis that the vector of coefficients for all of the transformations is zero. The **SS2** *a-option* produces a regression table with Type II tests of the contribution of each transformation to the overall model. In some cases, exact tests are provided; in other cases, the tests are approximate, liberal, or conservative.

There are two reasons why it is typically not appropriate to test hypotheses by using the output from PROC TRANSREG as input to other procedures such as the REG procedure. First, PROC REG has no way of determining how many degrees of freedom were used for each transformation. Second, the Type II sums of squares for the tests of the individual regression coefficients are not correct for the transformation regression model because PROC REG, as it evaluates the effect of each variable, cannot change the transformations of the other variables. PROC TRANSREG uses the correct degrees of freedom and sums of squares.

In an ordinary univariate linear model, there is one parameter for each independent variable, including the intercept. In the transformation regression model, many of the “variables” are used internally in the bases for the transformations. Each basis column has one parameter or *scoring* coefficient, and each linearly independent column has one model degree of freedom associated with it. Coefficients applied to transformed variables, *model coefficients*, do not enter into the degrees-of-freedom calculations. They are byproducts of the standardizations and can be absorbed into the transformations by specifying the **ADDITIVE** *a-option*. The word *parameter* is reserved for model and scoring coefficients that have a degree of freedom associated with them.

For expansions, there is one model parameter for each variable created by the expansion (except for all missing **CLASS** columns and expansions that have an implicit intercept). Each **IDENTITY** variable has one model parameter. If there are  $m$  **POINT** variables, they expand to  $m + 1$  variables and hence have  $m + 1$  model parameters. For  $m$  **EPOINT** variables, there are  $2m$  model parameters. For  $m$  **QPOINT** variables, there are  $m(m + 3)/2$  model parameters. If a variable with  $m$  categories is designated **CLASS**, there are  $m - 1$  parameters. For **BSPLINE** and **PSPLINE** variables of **DEGREE**= $n$  with **NKNOTS**= $k$ , there are  $n + k$  parameters. Note that one of the  $n + k + 1$  **BSPLINE** columns and one of the  $m$  **CLASS**(variable / **ZERO**=**NONE**) columns are not counted due to the implicit intercept.

There are scoring parameters for missing values in nonexcluded observations. Each ordinary missing value (.) has one scoring parameter. Each different special missing value (.\_ and .A through .Z) within each variable has one scoring parameter. Missing values specified in the **UNTIE**= and **MONOTONE**= options follow the rules for **UNTIE** and **MONOTONE** transformations, which are described later in this chapter.

For all nonoptimal transformations (**LOG**, **LOGIT**, **ARSIN**, **POWER**, **EXP**, **RANK**, **BOXCOX**), there is one parameter per variable in addition to any missing value scoring parameters.

For **SPLINE**, **OPSCORE**, and **LINEAR** transformations, the number of scoring parameters is the number of basis columns that are used internally to find the transformations minus 1 for the intercept. The number of

scoring parameters for SPLINE variables is the same as the number of model parameters for BSPLINE and PSPLINE variables. If DEGREE= $n$  and NKNOTS= $k$ , there are  $n + k$  scoring parameters. The number of scoring parameters for OPSCORE, SMOOTH, and SSPLINE variables is the same as the number of model parameters for CLASS variables. If there are  $m$  categories, there are  $m - 1$  scoring parameters. There is one parameter for each LINEAR variable. For SPLINE, OPSCORE, LINEAR, MONOTONE, UNTIE, and MSPLINE transformations, missing value scoring parameters are computed as described previously with the nonoptimal transformations.

The number of scoring parameters for MONOTONE, UNTIE, and MSPLINE transformations is less precise than for SPLINE, OPSCORE, and LINEAR transformations. One way of handling a MONOTONE transformation is to treat it as if it were the same as an OPSCORE transformation. If there are  $m$  categories, there are  $m - 1$  potential scoring parameters. However, there are typically fewer than  $m - 1$  unique parameter estimates, since some of those  $m - 1$  scoring parameter estimates might be tied during the optimal scaling to impose the order constraints. Imposing ties on the scoring parameter estimates is equivalent to fitting a model with fewer parameters. So there are two available scoring parameter counts:  $m - 1$  and a smaller number that is determined during the analysis. Using  $m - 1$  as the model degrees of freedom for MONOTONE variables (treating OPSCORE and MONOTONE transformations the same way) is *conservative*, since the MONOTONE scoring parameter estimates are more restricted than the OPSCORE scoring parameter estimates. Using the smaller count (the number of scoring parameter estimates that are different, minus 1 for the intercept) in the model degrees of freedom is *liberal*, since the data and the model together are being used to determine the number of parameters. PROC TRANSREG reports tests that use both liberal and conservative degrees of freedom to provide lower and upper bounds on the “true”  $p$ -values.

For the UNTIE transformation, the conservative scoring parameter count is the number of distinct observations, whereas the liberal scoring parameter count is the number of scoring parameter estimates that are different, minus 1 for the intercept. Hence, when you specify UNTIE, conservative tests have zero error degrees of freedom unless there are replicated observations.

For MSPLINE variables of DEGREE= $n$  and NKNOTS= $k$ , the conservative scoring parameter count is  $n + k$ , whereas the liberal parameter count is the number of scoring parameter estimates that are different, minus 1 for the intercept. A liberal degrees of freedom of 1 does not necessarily imply a linear transformation. It implies only that  $n$  plus  $k$  minus the number of ties imposed equals 1. An example of a one-degree-of-freedom nonlinear transformation is a two-piece linear transformation in which the slope of one piece is 0.

The number of scoring parameters is determined during each iteration. After the last iteration, enough information is available for the TEST *a-option* to produce an ANOVA table that reports the overall fit of the model. If you specify the SS2 *a-option*, further iterations are necessary to test the contribution of each transformation to the overall model.

The liberal tests do not compensate for overparameterization. For example, requesting a spline transformation with  $k$  knots when a linear transformation will suffice results in “liberal” tests that are actually conservative because too many degrees of freedom are being used for the transformations. To avoid this problem, use as few knots as possible.

In ordinary multiple regression, an  $F$  test of the null hypothesis that the coefficient for variable  $x_j$  is zero can be constructed by comparing two linear models. One model is the full model with all parameters, and the other is a reduced model that has all parameters except the parameter for variable  $x_j$ . The difference between the model sum of squares for the full model and the model sum of squares for the reduced model is the Type II sum of squares for the test of the null hypothesis that the coefficient for variable  $x_j$  is 0. The numerator of the  $F$  test has one degree of freedom. The mean square error for the full model is the denominator of the

$F$  test of variable  $x_j$ . Note that the estimates of the coefficients for the two models are not usually the same. When variable  $x_j$  is removed, the coefficients for the other variables change to compensate for the removal of  $x_j$ . In a transformation regression model, the transformations of the other variables must be permitted to change and the numerator degrees of freedom are not always ones. It is not correct to simply let the model coefficients for the transformed variables change and apply the new model coefficients to the old transformations computed with the old scoring parameter estimates. In a transformation regression model, further iteration is needed to test each transformation, because all the scoring parameter estimates for other variables must be permitted to change to test the effect of variable  $x_j$ . This can be quite time-consuming for a large model if the *SOLVE a-option* cannot be used to solve directly for the transformations.

---

## Output Data Set

The OUT= output data set can contain a great deal of information; however, in most cases, the output data set contains a small portion of the entire range of available information.

### Output Data Set Examples

This section provides three brief examples, illustrating some typical OUT= output data sets. See the section “Output Data Set Contents” on page 8310 for a complete list of the contents of the OUT= data set.

The first example shows the output data set from a two-way ANOVA model. The following statements produce Figure 97.65:

```

title 'ANOVA Output Data Set Example';

data ReferenceCell;
 input y x1 $ x2 $;
 datalines;
11 a a
12 a a
10 a a
 4 a b
 5 a b
 3 a b
 5 b a
 6 b a
 4 b a
 2 b b
 3 b b
 1 b b
;

* Fit Reference Cell Two-Way ANOVA Model;
proc transreg data=ReferenceCell;
 model identity(y) = class(x1 | x2);
 output coefficients replace predicted residuals;
run;

* Print the Results;
proc print;
run;

```

```
proc contents position;
 ods select position;
run;
```

Figure 97.65 ANOVA Example Output Data Set Contents

| ANOVA Output Data Set Example |          |        |    |    |    |           |     |     |        |    |    |
|-------------------------------|----------|--------|----|----|----|-----------|-----|-----|--------|----|----|
| Obs                           | _TYPE_   | _NAME_ | y  | Py | Ry | Intercept | x1a | x2a | x1ax2a | x1 | x2 |
| 1                             | SCORE    | ROW1   | 11 | 11 | 0  | 1         | 1.0 | 1   | 1      | a  | a  |
| 2                             | SCORE    | ROW2   | 12 | 11 | 1  | 1         | 1.0 | 1   | 1      | a  | a  |
| 3                             | SCORE    | ROW3   | 10 | 11 | -1 | 1         | 1.0 | 1   | 1      | a  | a  |
| 4                             | SCORE    | ROW4   | 4  | 4  | 0  | 1         | 1.0 | 0   | 0      | a  | b  |
| 5                             | SCORE    | ROW5   | 5  | 4  | 1  | 1         | 1.0 | 0   | 0      | a  | b  |
| 6                             | SCORE    | ROW6   | 3  | 4  | -1 | 1         | 1.0 | 0   | 0      | a  | b  |
| 7                             | SCORE    | ROW7   | 5  | 5  | 0  | 1         | 0.0 | 1   | 0      | b  | a  |
| 8                             | SCORE    | ROW8   | 6  | 5  | 1  | 1         | 0.0 | 1   | 0      | b  | a  |
| 9                             | SCORE    | ROW9   | 4  | 5  | -1 | 1         | 0.0 | 1   | 0      | b  | a  |
| 10                            | SCORE    | ROW10  | 2  | 2  | 0  | 1         | 0.0 | 0   | 0      | b  | b  |
| 11                            | SCORE    | ROW11  | 3  | 2  | 1  | 1         | 0.0 | 0   | 0      | b  | b  |
| 12                            | SCORE    | ROW12  | 1  | 2  | -1 | 1         | 0.0 | 0   | 0      | b  | b  |
| 13                            | M COEFFI | y      | .  | .  | .  | 2         | 2.0 | 3   | 4      |    |    |
| 14                            | MEAN     | y      | .  | .  | .  | .         | 7.5 | 8   | 11     |    |    |

| ANOVA Output Data Set Example |           |      |     |                    |  |
|-------------------------------|-----------|------|-----|--------------------|--|
| The CONTENTS Procedure        |           |      |     |                    |  |
| Variables in Creation Order   |           |      |     |                    |  |
| #                             | Variable  | Type | Len | Label              |  |
| 1                             | _TYPE_    | Char | 8   |                    |  |
| 2                             | _NAME_    | Char | 32  |                    |  |
| 3                             | y         | Num  | 8   |                    |  |
| 4                             | Py        | Num  | 8   | y Predicted Values |  |
| 5                             | Ry        | Num  | 8   | y Residuals        |  |
| 6                             | Intercept | Num  | 8   | Intercept          |  |
| 7                             | x1a       | Num  | 8   | x1 a               |  |
| 8                             | x2a       | Num  | 8   | x2 a               |  |
| 9                             | x1ax2a    | Num  | 8   | x1 a * x2 a        |  |
| 10                            | x1        | Char | 32  |                    |  |
| 11                            | x2        | Char | 32  |                    |  |

The `_TYPE_` variable indicates observation type: score, multiple regression coefficient (parameter estimates), and marginal means. The `_NAME_` variable contains the default observation labels, “ROW1”, “ROW2”, and so on, and contains the dependent variable name (y) for the remaining observations. If you specify an `ID` statement, `_NAME_` contains the values of the first ID variable for score observations. The y variable is the dependent variable, Py contains the predicted values, Ry contains the residuals, and the variables Intercept through x1ax2a contain the design matrix. The x1 and x2 variables are the original CLASS variables.

The next example shows the contents of the output data set from fitting a curve through a scatter plot. The following statements produce [Figure 97.66](#):

```

title 'Output Data Set for Curve Fitting Example';

data a;
 do x = 1 to 100;
 y = log(x) + sin(x / 10) + normal(7);
 output;
 end;
run;

proc transreg;
 model identity(y) = spline(x / nknots=9);
 output predicted out=b;
run;

proc contents position;
 ods select position;
run;

```

**Figure 97.66** Predicted Values Example Output Data Set Contents

| Output Data Set for Curve Fitting Example |               |      |     |                          |
|-------------------------------------------|---------------|------|-----|--------------------------|
| The CONTENTS Procedure                    |               |      |     |                          |
| Variables in Creation Order               |               |      |     |                          |
| #                                         | Variable      | Type | Len | Label                    |
| 1                                         | <u>_TYPE_</u> | Char | 8   |                          |
| 2                                         | <u>_NAME_</u> | Char | 32  |                          |
| 3                                         | y             | Num  | 8   |                          |
| 4                                         | Ty            | Num  | 8   | y Transformation         |
| 5                                         | Py            | Num  | 8   | y Predicted Values       |
| 6                                         | Intercept     | Num  | 8   | Intercept                |
| 7                                         | x             | Num  | 8   |                          |
| 8                                         | TIntercept    | Num  | 8   | Intercept Transformation |
| 9                                         | Tx            | Num  | 8   | x Transformation         |

The `OUT=` data set contains `_TYPE_` and `_NAME_` variables. Since no coefficients or coordinates are requested, all observations are `_TYPE_='SCORE'`. The `y` variable is the original dependent variable, `Ty` is the transformed dependent variable, `Py` contains the predicted values, `x` is the original independent variable, and `Tx` is the transformed independent variable. The data set also contains an `Intercept` and transformed intercept `TIntercept` variable. (In this case, the transformed intercept is the same as the intercept. However, if you specify the `TSTANDARD=` and `ADDITIVE` options, these are not always the same.)

The following example shows the results from specifying `METHOD=MORALS` when there is more than one dependent variable:

```
title 'METHOD=MORALS Output Data Set Example';

data x;
 input y1 y2 x1 $ x2 $;
 datalines;
11 1 a a
10 4 b a
 5 2 a b
 5 9 b b
 4 3 c c
 3 6 b a
 1 8 a b
;

* Fit Reference Cell Two-Way ANOVA Model;
proc transreg data=x noprint solve;
 model spline(y1 y2) = opscore(x1 x2 / name=(n1 n2));
 output coefficients predicted residuals;
 id x1 x2;
run;

* Print the Results;
proc print;
run;

proc contents position;
 ods select position;
run;
```

These statements produce [Figure 97.67](#).

Figure 97.67 METHOD=MORALS Rolled Output Data Set

| METHOD=MORALS Output Data Set Example |            |          |      |            |          |          |          |    |
|---------------------------------------|------------|----------|------|------------|----------|----------|----------|----|
| Obs                                   | DEPVAR     | TYPE     | NAME | DEPEND     | T_DEPEND | P_DEPEND | R_DEPEND |    |
| 1                                     | Spline(y1) | SCORE    | a    | 11         | 13.1600  | 11.1554  | 2.00464  |    |
| 2                                     | Spline(y1) | SCORE    | b    | 10         | 6.1931   | 6.8835   | -0.69041 |    |
| 3                                     | Spline(y1) | SCORE    | a    | 5          | 2.4467   | 4.7140   | -2.26724 |    |
| 4                                     | Spline(y1) | SCORE    | b    | 5          | 2.4467   | 0.4421   | 2.00464  |    |
| 5                                     | Spline(y1) | SCORE    | c    | 4          | 4.2076   | 4.2076   | 0.00000  |    |
| 6                                     | Spline(y1) | SCORE    | b    | 3          | 5.5693   | 6.8835   | -1.31422 |    |
| 7                                     | Spline(y1) | SCORE    | a    | 1          | 4.9766   | 4.7140   | 0.26261  |    |
| 8                                     | Spline(y1) | M COEFFI | y1   | .          | .        | .        | .        |    |
| 9                                     | Spline(y2) | SCORE    | a    | 1          | -0.5303  | -0.5199  | -0.01043 |    |
| 10                                    | Spline(y2) | SCORE    | b    | 4          | 5.5487   | 4.5689   | 0.97988  |    |
| 11                                    | Spline(y2) | SCORE    | a    | 2          | 3.8940   | 4.5575   | -0.66347 |    |
| 12                                    | Spline(y2) | SCORE    | b    | 9          | 9.6358   | 9.6462   | -0.01043 |    |
| 13                                    | Spline(y2) | SCORE    | c    | 3          | 5.6210   | 5.6210   | 0.00000  |    |
| 14                                    | Spline(y2) | SCORE    | b    | 6          | 3.5994   | 4.5689   | -0.96945 |    |
| 15                                    | Spline(y2) | SCORE    | a    | 8          | 5.2314   | 4.5575   | 0.67390  |    |
| 16                                    | Spline(y2) | M COEFFI | y2   | .          | .        | .        | .        |    |
| Obs                                   | Intercept  | n1       | n2   | TIntercept | Tn1      | Tn2      | x1       | x2 |
| 1                                     | 1          | 0        | 0    | 1.0000     | 0.06711  | -0.09384 | a        | a  |
| 2                                     | 1          | 1        | 0    | 1.0000     | 1.51978  | -0.09384 | b        | a  |
| 3                                     | 1          | 0        | 1    | 1.0000     | 0.06711  | 1.32038  | a        | b  |
| 4                                     | 1          | 1        | 1    | 1.0000     | 1.51978  | 1.32038  | b        | b  |
| 5                                     | 1          | 2        | 2    | 1.0000     | 0.23932  | 1.32038  | c        | c  |
| 6                                     | 1          | 1        | 0    | 1.0000     | 1.51978  | -0.09384 | b        | a  |
| 7                                     | 1          | 0        | 1    | 1.0000     | 0.06711  | 1.32038  | a        | b  |
| 8                                     | .          | .        | .    | 10.9253    | -2.94071 | -4.55475 | y1       | y1 |
| 9                                     | 1          | 0        | 0    | 1.0000     | 0.03739  | -0.09384 | a        | a  |
| 10                                    | 1          | 1        | 0    | 1.0000     | 1.51395  | -0.09384 | b        | a  |
| 11                                    | 1          | 0        | 1    | 1.0000     | 0.03739  | 1.32038  | a        | b  |
| 12                                    | 1          | 1        | 1    | 1.0000     | 1.51395  | 1.32038  | b        | b  |
| 13                                    | 1          | 2        | 2    | 1.0000     | 0.34598  | 1.32038  | c        | c  |
| 14                                    | 1          | 1        | 0    | 1.0000     | 1.51395  | -0.09384 | b        | a  |
| 15                                    | 1          | 0        | 1    | 1.0000     | 0.03739  | 1.32038  | a        | b  |
| 16                                    | .          | .        | .    | -0.3119    | 3.44636  | 3.59024  | y2       | y2 |



Figure 97.67 continued

| METHOD=MORALS Output Data Set Example |            |      |     |                                          |
|---------------------------------------|------------|------|-----|------------------------------------------|
| The CONTENTS Procedure                |            |      |     |                                          |
| Variables in Creation Order           |            |      |     |                                          |
| #                                     | Variable   | Type | Len | Label                                    |
| 1                                     | _DEPVAR_   | Char | 42  | Dependent Variable Transformation (Name) |
| 2                                     | _TYPE_     | Char | 8   |                                          |
| 3                                     | _NAME_     | Char | 32  |                                          |
| 4                                     | _DEPEND_   | Num  | 8   | Dependent Variable                       |
| 5                                     | T_DEPEND_  | Num  | 8   | Dependent Variable Transformation        |
| 6                                     | P_DEPEND_  | Num  | 8   | Dependent Variable Predicted Values      |
| 7                                     | R_DEPEND_  | Num  | 8   | Dependent Variable Residuals             |
| 8                                     | Intercept  | Num  | 8   | Intercept                                |
| 9                                     | n1         | Num  | 8   |                                          |
| 10                                    | n2         | Num  | 8   |                                          |
| 11                                    | TIntercept | Num  | 8   | Intercept Transformation                 |
| 12                                    | Tn1        | Num  | 8   | n1 Transformation                        |
| 13                                    | Tn2        | Num  | 8   | n2 Transformation                        |
| 14                                    | x1         | Char | 32  |                                          |
| 15                                    | x2         | Char | 32  |                                          |

If you specify **METHOD=MORALS** with multiple dependent variables, PROC TRANSREG performs separate univariate analyses and stacks the results in the **OUT=** data set. For this example, the results of the first analysis are in the partition designated by **\_DEPVAR\_='Spline(y1)'** and the results of the second analysis are in the partition designated by **\_DEPVAR\_='Spline(y2)'**, which are the transformation and dependent variable names. Each partition has **\_TYPE\_='SCORE'** observations for the variables and a **\_TYPE\_='M COEFFI'** observation for the coefficients. In this example, an **ID** variable is specified, so the **\_NAME\_** variable contains the formatted values of the first **ID** variable. Since both dependent variables have to go into the same column, the dependent variable is given a new name, **\_DEPEND\_**. The dependent variable transformation is named **T\_DEPEND\_**, the predicted values variable is named **P\_DEPEND\_**, and the residuals variable is named **R\_DEPEND\_**.

The independent variables are character **OPSCORE** variables. By default, PROC TRANSREG replaces character **OPSCORE** variables with category numbers and discards the original character variables. To avoid this, the input variables are renamed from **x1** and **x2** to **n1** and **n2** and the original **x1** and **x2** are added to the data set as **ID** variables. The **n1** and **n2** variables contain the initial values for the **OPSCORE** transformations, and the **Tn1** and **Tn2** variables contain optimal scores. The data set also contains an **Intercept** and transformed intercept **TIntercept** variable. The regression coefficients are in the transformation columns, which also contain the variables to which they apply.

## Output Data Set Contents

Table 97.7 summarizes the various matrices that can result from PROC TRANSREG processing and that appear in the **OUT=** data set. The exact contents of an **OUT=** data set depends on many options.

**Table 97.7** PROC TRANSREG OUT= Data Set Contents

| <b>_TYPE_</b> | <b>Contents</b>                        | <b>Options, Default Prefix</b>       |
|---------------|----------------------------------------|--------------------------------------|
| SCORE         | dependent variables                    | DREPLACE not specified               |
| SCORE         | independent variables                  | IREPLACE not specified               |
| SCORE         | transformed dependent variables        | default, TDPREFIX=T                  |
| SCORE         | transformed independent variables      | default, TIPREFIX=T                  |
| SCORE         | predicted values                       | PREDICTED, PPREFIX=P                 |
| SCORE         | residuals                              | RESIDUALS, RDPREFIX=R                |
| SCORE         | leverage                               | LEVERAGE, LEVERAGE=Leverage          |
| SCORE         | lower individual confidence limits     | CLI, LILPREFIX=LIL,<br>CILPREFIX=CIL |
| SCORE         | upper individual confidence limits     | CLI, LIUPREFIX=LIU,<br>CIUPREFIX=CIU |
| SCORE         | lower mean confidence limits           | CLM, LMLPREFIX=LML,<br>CMLPREFIX=CML |
| SCORE         | upper mean confidence limits           | CLM, LMUPREFIX=LMU,<br>CMUPREFIX=CMU |
| SCORE         | dependent canonical variables          | CANONICAL, CDPREFIX=Cand             |
| SCORE         | independent canonical variables        | CANONICAL, CIPREFIX=Cani             |
| SCORE         | redundancy variables                   | REDUNDANCY, RPREFIX=Red              |
| SCORE         | ID, CLASS, BSPLINE variables           | ID, CLASS, BSPLINE,                  |
| SCORE         | independent variables approximations   | IAPPROXIMATIONS, AIPREFIX=A          |
| M COEFFI      | multiple regression coefficients       | COEFFICIENTS, MRC                    |
| C COEFFI      | canonical coefficients                 | COEFFICIENTS, CCC                    |
| MEAN          | marginal means                         | COEFFICIENTS, MEANS                  |
| M REDUND      | multiple redundancy coefficients       | MREDUNDANCY                          |
| R REDUND      | multiple redundancy coefficients       | MREDUNDANCY                          |
| M POINT       | point coordinates                      | COORDINATES or MPC, POINT            |
| M EPOINT      | elliptical point coordinates           | COORDINATES or MEC, EPOINT           |
| M QPOINT      | quadratic point coordinates            | COORDINATES or MQC, QPOINT           |
| C POINT       | canonical point coordinates            | COORDINATES or CPC, POINT            |
| C EPOINT      | canonical elliptical point coordinates | COORDINATES or CEC, EPOINT           |
| C QPOINT      | canonical quadratic point coordinates  | COORDINATES or CQC, QPOINT           |

The independent and dependent variables are created from the original input data. Several potential differences exist between these variables and the actual input data. An intercept variable can be added, new variables can be added for POINT, EPOINT, QPOINT, CLASS, IDENTITY, PSPLINE, and BSPLINE variables, and category numbers are substituted for character OPSCORE variables. These matrices are not always what is input to the first iteration. After the expanded data set is stored for inclusion in the output data set, several things happen to the data before they are input to the first iteration: column means are substituted for missing values; zero-degree SPLINE and MSPLINE variables are transformed so that the iterative algorithms get step-function data as input, which conform to the zero-degree transformation family restrictions; and the nonoptimal transformations are performed.

**Details for the UNIVARIATE Method**

When you specify `METHOD=UNIVARIATE` (in the `MODEL` or `PROC TRANSREG` statement), `PROC TRANSREG` can perform several analyses, one for each dependent variable. While each dependent variable can be transformed, their independent variables are not transformed. The `OUT=` data set optionally contains all of the `_TYPE_='SCORE'` observations, optionally followed by coefficients or coordinates.

**Details for the MORALS Method**

When you specify `METHOD=MORALS` (in the `MODEL` or `PROC TRANSREG` statement), successive analyses are performed, one for each dependent variable. Each analysis transforms one dependent variable and the entire set of the independent variables. All information for the first dependent variable (scores then, optionally, coefficients) appears first. Then all information for the second dependent variable (scores then, optionally, coefficients) appears next. This arrangement is repeated for all dependent variables.

**Details for the CANALS and REDUNDANCY Methods**

For `METHOD=CANALS` and `METHOD=REDUNDANCY` (specified in either the `MODEL` or `PROC TRANSREG` statement), one analysis is performed that simultaneously transforms all dependent and independent variables. The `OUT=` data set optionally contains all of the `_TYPE_='SCORE'` observations, optionally followed by coefficients or coordinates.

**Variable Names**

As shown in the preceding examples, some variables in the output data set directly correspond to input variables, and some are created. All original optimal and nonoptimal transformation variable names are unchanged.

The names of the `POINT`, `QPOINT`, and `EPOINT` expansion variables are also left unchanged, but new variables are created. When independent `POINT` variables are present, the sum-of-squares variable `_ISSQ_` is added to the output data set. For each `EPOINT` and `QPOINT` variable, a new squared variable is created by appending “\_2”. For example, `Dim1` and `Dim2` are expanded into `Dim1`, `Dim2`, `Dim1_2`, and `Dim2_2`. In addition, for each pair of `QPOINT` variables, a new crossproduct variable is created by combining the two names—for example, `Dim1Dim2`.

The names of the `CLASS` variables are constructed from original variable names and levels. Lengths are controlled by the `CPREFIX= a-option`. For example, when `x1` and `x2` both have values of 'a' and 'b', `CLASS(x1 | x2 / ZERO=NONE)` creates `x1` main-effect variable names `x1a` `x1b`, `x2` main-effect variable names `x2a` `x2b`, and interaction variable names `x1ax2a` `x1ax2b` `x1bx2a` `x1bx2b`.

`PROC TRANSREG` then uses these variable names when creating the transformed, predicted, and residual variable names by affixing the relevant prefix and dropping extra characters if necessary.

**METHOD=MORALS Variable Names**

When you specify `METHOD=MORALS` and only one dependent variable is present, the output data set is structured exactly as if `METHOD=REDUNDANCY` (see the section “[Details for the CANALS and REDUNDANCY Methods](#)” on page 8312). When more than one dependent variable is present, the dependent variables are output in the variable `_DEPEND_`, transformed dependent variables are output in the variable `T_DEPEND_`, predicted values are output in the variable `P_DEPEND_`, and residuals are output in the variable `R_DEPEND_`. You can partition the data set into `BY` groups, one per dependent variable, by referring to the character variable `_DEPVAR_`, which contains the original dependent variable names and transformations.

**Duplicate Variable Names**

When the same name is generated from multiple variables in the **OUT=** data set, new names are created by appending '2', '3', or '4', and so on, until a unique name is created. For 32-character names, the last character is replaced with a numeric suffix until a unique name is created. For example, if there are two output variables that otherwise would be named *x*, then *x* and *x2* are created instead. If there are two output variables that otherwise would be named *ThisIsAThirtyTwoCharacterVarName*, then *ThisIsAThirtyTwoCharacterVarName* and *ThisIsAThirtyTwoCharacterVarNam2* are created instead.

**OUTTEST= Output Data Set**

The **OUTTEST=** data set contains hypothesis test results. The **OUTTEST=** data set always contains ANOVA results. When you specify the **SS2** *a-option*, regression tables are also output. When you specify the **UTILITIES** *a-option*, conjoint analysis part-worth utilities are also output. The **OUTTEST=** data set has the following variables:

|                    |                                                                                                                                                                                                                                                                                                                                                                                                     |
|--------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>_DEPVAR_</b>    | is a 42-character variable that contains the dependent variable transformation and name.                                                                                                                                                                                                                                                                                                            |
| <b>_TYPE_</b>      | is an 8-character variable that contains the table type. The first character is “U” for univariate or “M” for multivariate. The second character is blank. The third character is “A” for ANOVA, “2” for Type II sum of squares, or “U” for <b>UTILITIES</b> . The fourth character is blank. The fifth character is “L” for liberal tests, “C” for conservative tests, or “U” for the usual tests. |
| <b>Title</b>       | is an 80-character variable that contains the table title.                                                                                                                                                                                                                                                                                                                                          |
| <b>Variable</b>    | is a 42-character variable that contains the independent variable transformations and names for regression tables and blanks for ANOVA tables.                                                                                                                                                                                                                                                      |
| <b>Coefficient</b> | contains the multiple regression coefficients for regression tables and underscore special missing values for ANOVA tables.                                                                                                                                                                                                                                                                         |
| <b>Statistic</b>   | is a 24-character variable that contains the names for statistics in other variables, such as <b>Value</b> .                                                                                                                                                                                                                                                                                        |
| <b>Value</b>       | contains multivariate test statistics and all other information that does not fit in one of the other columns including R square, dependent mean, adjusted R square, and coefficient of variation. Whenever <b>Value</b> is not an underscore special missing value, the <b>Statistic</b> variable describes the contents of the <b>Value</b> variable.                                             |
| <b>NumDF</b>       | contains numerator degrees of freedom for <i>F</i> tests.                                                                                                                                                                                                                                                                                                                                           |
| <b>DenDF</b>       | contains denominator degrees of freedom for <i>F</i> tests.                                                                                                                                                                                                                                                                                                                                         |
| <b>SSq</b>         | contains sums of squares.                                                                                                                                                                                                                                                                                                                                                                           |
| <b>MeanSquare</b>  | contains mean squares.                                                                                                                                                                                                                                                                                                                                                                              |
| <b>F</b>           | contains <i>F</i> statistics.                                                                                                                                                                                                                                                                                                                                                                       |
| <b>NumericP</b>    | contains the <i>p</i> -value for the <i>F</i> statistic, stored in a numeric variable.                                                                                                                                                                                                                                                                                                              |
| <b>P</b>           | is a 9-character variable that contains the formatted <i>p</i> -value for the <i>F</i> statistic, including the appropriate ~, <=, >=, or blank symbols.                                                                                                                                                                                                                                            |
| <b>LowerLimit</b>  | contains lower confidence limits on the parameter estimates.                                                                                                                                                                                                                                                                                                                                        |

|            |                                                                                                                                                   |
|------------|---------------------------------------------------------------------------------------------------------------------------------------------------|
| UpperLimit | contains upper confidence limits on the parameter estimates.                                                                                      |
| StdError   | contains standard errors. For <b>SS2</b> and <b>UTILITIES</b> tables, standard errors are output for each coefficient with one degree of freedom. |
| Importance | contains the relative importance of each factor for <b>UTILITIES</b> tables.                                                                      |
| Label      | is a 256-character variable that contains variable labels.                                                                                        |

There are several possible tables in the **OUTTEST=** data set corresponding to combinations of univariate and multivariate tests; ANOVA and regression results; and liberal, conservative, and the usual tests. Each table is composed of only a subset of the variables. Numeric variables contain underscore special missing values when they are not a column in a table. Ordinary missing values (.) appear in variables that are part of a table when a nonmissing value cannot be produced. For example, the *F* is missing for a test with zero degrees of freedom.

---

## Computational Resources

This section provides information about the computational resources required to use PROC TRANSREG.

Let

- $n$  = number of observations
- $q$  = number of expanded independent variables
- $r$  = number of expanded dependent variables
- $k$  = maximum spline degree
- $p$  = maximum number of knots

More than  $56(q + r)$  plus the maximum of the data matrix size, the optimal scaling work space, and the covariance matrix size bytes of array space are required. The data matrix size is  $8n(q + r)$  bytes. The optimal scaling work space requires less than  $8(6n + (p + k + 2)(p + k + 11))$  bytes. The covariance matrix size is  $4(q + r)(q + r + 1)$  bytes.

PROC TRANSREG tries to store the original and transformed data in memory. If there is not enough memory, a utility data set is used, potentially resulting in a large increase in execution time. The amount of memory for the preceding data formulas is an underestimate of the amount of memory needed to handle most problems. These formulas give the absolute minimum amount of memory required. If a utility data set is used, and if memory can be used with perfect efficiency, then roughly the amount of memory stated previously is needed. In reality, most problems require at least two or three times the minimum.

PROC TRANSREG sorts the data once. The sort time is roughly proportional to  $(q + r)n^{3/2}$ .

One regression analysis per iteration is required to compute model parameters (or two canonical correlation analyses per iteration for **METHOD=CANALS**). The time required to accumulate the crossproducts matrix is roughly proportional to  $n(q + r)^2$ . The time required to compute the regression coefficients is roughly proportional to  $q^3$ .

Each optimal scaling is a multiple regression problem, although some transformations are handled with faster special-case algorithms. The number of regressors for the optimal scaling problems depends on the

original values of the variable and the type of transformation. For each monotone spline transformation, an unknown number of multiple regressions is required to find a set of coefficients that satisfies the constraints. The B-spline basis is generated twice for each `SPLINE` and `MSPLINE` transformation for each iteration. The time required to generate the B-spline basis is roughly proportional to  $nk^2$ .

---

## Unbalanced ANOVA without CLASS Variables

This section illustrates that an analysis of variance model can be formulated as a simple regression model with optimal scoring. The purpose of the example is to explain one aspect of how PROC TRANSREG works, not to propose an alternative way of performing an analysis of variance.

Finding the overall fit of a large, unbalanced analysis of variance model can be handled as an optimal scoring problem without creating large, sparse design matrices. For example, consider an unbalanced full main-effects and interactions ANOVA model with six factors. Assume that a SAS data set is created with factor-level indicator variables `c1` through `c6` and dependent variable `y`. If each factor level consists of nonblank single characters, you can create a cell indicator in a DATA step with the statement as follows:

```
x=compress(c1||c2||c3||c4||c5||c6);
```

The following statements optimally score `x` (by using the `OPSCORE` transformation) and do not transform `y`:

```
proc transreg;
 model identity(y)=opscore(x);
 output;
run;
```

The final R square reported is the R square for the full analysis of variance model. This R square is the same R square that would be reported by both of the following PROC GLM steps:

```
proc glm;
 class x;
 model y=x;
run;

proc glm;
 class c1-c6;
 model y=c1|c2|c3|c4|c5|c6;
run;
```

PROC TRANSREG optimally scores the classes of `x`, within the space of a single variable with values linearly related to the cell means, so the full ANOVA problem is reduced to a simple regression problem with an optimal independent variable. PROC TRANSREG requires only one iteration to find the optimal scoring of `x` but, by default, performs a second iteration, which reports no data changes.

## Hypothesis Tests for Simple Univariate Models

If the dependent variable has one parameter (`IDENTITY`, `LINEAR` with no missing values, and so on) and if there are no monotonicity constraints, PROC TRANSREG fits univariate models, which can also be fit with a DATA step and PROC REG. This is illustrated with the following artificial data set:

```
data htex;
 do i = 0.5 to 10 by 0.5;
 x1 = log(i);
 x2 = sqrt(i) + sin(i);
 x3 = 0.05 * i * i + cos(i);
 y = x1 - x2 + x3 + 3 * normal(7);
 x1 = x1 + normal(7);
 x2 = x2 + normal(7);
 x3 = x3 + normal(7);
 output;
 end;
run;
```

Both PROC TRANSREG and PROC REG are run to fit the same polynomial regression model as follows:

```
proc transreg data=htex ss2 short;
 title 'Fit a Polynomial Regression Model with PROC TRANSREG';
 model identity(y) = spline(x1);
run;

data htex2;
 set htex;
 x1_1 = x1;
 x1_2 = x1 * x1;
 x1_3 = x1 * x1 * x1;
run;

proc reg;
 title 'Fit a Polynomial Regression Model with PROC REG';
 model y = x1_1 - x1_3;
run; quit;
```

The ANOVA and regression tables from PROC TRANSREG are displayed in [Figure 97.68](#). The ANOVA and regression tables from PROC REG are displayed in [Figure 97.69](#). The `SHORT` *a-option* is specified with PROC TRANSREG to suppress the iteration history.

Figure 97.68 ANOVA and Regression Output from PROC TRANSREG

```

Fit a Polynomial Regression Model with PROC TRANSREG

The TRANSREG Procedure

Dependent Variable Identity(y)

Number of Observations Read 20
Number of Observations Used 20

Identity(y)
Algorithm converged.

The TRANSREG Procedure Hypothesis Tests for Identity(y)

Univariate ANOVA Table Based on the Usual Degrees of Freedom

Source DF Sum of Mean
 DF Squares Square F Value Pr > F
Model 3 5.8365 1.94550 0.14 0.9329
Error 16 218.3073 13.64421
Corrected Total 19 224.1438

Root MSE 3.69381 R-Square 0.0260
Dependent Mean 0.85490 Adj R-Sq -0.1566
Coeff Var 432.07258

Univariate Regression Table Based on the Usual Degrees of Freedom

Variable DF Coefficient Type II
 DF Coefficient Sum of
 DF Coefficient Squares Mean
 DF Coefficient Squares Square F Value Pr > F
Intercept 1 1.4612767 18.8971 18.8971 1.38 0.2565
Spline(x1) 3 -0.3924013 5.8365 1.9455 0.14 0.9329

```

Figure 97.69 ANOVA and Regression Output from PROC REG

```

Fit a Polynomial Regression Model with PROC REG

The REG Procedure
Model: MODEL1
Dependent Variable: y

Number of Observations Read 20
Number of Observations Used 20

```



Figure 97.69 continued

| Analysis of Variance |    |                    |                |         |         |
|----------------------|----|--------------------|----------------|---------|---------|
| Source               | DF | Sum of Squares     | Mean Square    | F Value | Pr > F  |
| Model                | 3  | 5.83651            | 1.94550        | 0.14    | 0.9329  |
| Error                | 16 | 218.30729          | 13.64421       |         |         |
| Corrected Total      | 19 | 224.14380          |                |         |         |
| Root MSE             |    | 3.69381            | R-Square       | 0.0260  |         |
| Dependent Mean       |    | 0.85490            | Adj R-Sq       | -0.1566 |         |
| Coeff Var            |    | 432.07258          |                |         |         |
| Parameter Estimates  |    |                    |                |         |         |
| Variable             | DF | Parameter Estimate | Standard Error | t Value | Pr >  t |
| Intercept            | 1  | 1.22083            | 1.47163        | 0.83    | 0.4190  |
| x1_1                 | 1  | 0.79743            | 1.75129        | 0.46    | 0.6550  |
| x1_2                 | 1  | -0.49381           | 1.50449        | -0.33   | 0.7470  |
| x1_3                 | 1  | 0.04422            | 0.32956        | 0.13    | 0.8949  |

The PROC TRANSREG regression table differs in several important ways from the parameter estimate table produced by PROC REG. The REG procedure displays standard errors and  $t$  statistics. PROC TRANSREG displays Type II sums of squares, mean squares, and  $F$  statistics. The difference is because the numerator degrees of freedom are not always 1, so  $t$  tests are not uniformly appropriate. When the degrees of freedom for variable  $x_j$  is 1, the following relationships hold between the standard errors ( $s_{\beta_j}$ ) and the Type II sums of squares ( $SS_j$ ):

$$s_{\beta_j} = (\hat{\beta}_j^2 / F_j)^{1/2}$$

and

$$SS_j = \hat{\beta}_j^2 \times \text{MSE} / s_{\beta_j}^2$$

PROC TRANSREG does not provide tests of the individual terms that go into the transformation. (However, it could if **BSPLINE** or **PSPLINE** had been specified instead of **SPLINE**.) The test of **spline(x1)** is the same as the test of the overall model. The intercepts are different due to the different numbers of variables and their standardizations.

In the next example, both  $x_1$  and  $x_2$  are transformed in the first PROC TRANSREG step, and PROC TRANSREG is used instead of a DATA step to create the polynomials for PROC REG. Both PROC TRANSREG and PROC REG fit the same polynomial regression model. The following statements run PROC TRANSREG and PROC REG and produce Figure 97.70 and Figure 97.71:

```

title 'Two-Variable Polynomial Regression';

proc transreg data=htex ss2 solve;
 model identity(y) = spline(x1 x2);
run;

proc transreg noprint data=htex maxiter=0;
 /* Use PROC TRANSREG to prepare input to PROC REG */
 model identity(y) = pspline(x1 x2);
 output out=htex2;
run;

proc reg data=htex2;
 model y = x1_1-x1_3 x2_1-x2_3;
 test x1_1, x1_2, x1_3;
 test x2_1, x2_2, x2_3;
run; quit;

```

**Figure 97.70** Two-Variable Polynomial Regression Output from PROC TRANSREG

| Two-Variable Polynomial Regression                          |                |                |          |                  |           |
|-------------------------------------------------------------|----------------|----------------|----------|------------------|-----------|
| The TRANSREG Procedure                                      |                |                |          |                  |           |
| Dependent Variable Identity(y)                              |                |                |          |                  |           |
| Number of Observations Read                                 |                |                |          | 20               |           |
| Number of Observations Used                                 |                |                |          | 20               |           |
| TRANSREG MORALS Algorithm Iteration History for Identity(y) |                |                |          |                  |           |
| Iteration Number                                            | Average Change | Maximum Change | R-Square | Criterion Change | Note      |
| 0                                                           | 0.69502        | 4.73421        | 0.08252  |                  |           |
| 1                                                           | 0.00000        | 0.00000        | 0.17287  | 0.09035          | Converged |
| Algorithm converged.                                        |                |                |          |                  |           |
| Hypothesis Test Iterations Excluding Spline(x1)             |                |                |          |                  |           |
| TRANSREG MORALS Algorithm Iteration History for Identity(y) |                |                |          |                  |           |
| Iteration Number                                            | Average Change | Maximum Change | R-Square | Criterion Change | Note      |
| 0                                                           | 0.03575        | 0.32390        | 0.15097  |                  |           |
| 1                                                           | 0.00000        | 0.00000        | 0.15249  | 0.00152          | Converged |
| Algorithm converged.                                        |                |                |          |                  |           |

Figure 97.70 continued

| Hypothesis Test Iterations Excluding Spline(x2)             |                |                |          |                  |           |
|-------------------------------------------------------------|----------------|----------------|----------|------------------|-----------|
| TRANSREG MORALS Algorithm Iteration History for Identity(y) |                |                |          |                  |           |
| Iteration Number                                            | Average Change | Maximum Change | R-Square | Criterion Change | Note      |
| 0                                                           | 0.45381        | 1.43736        | 0.00717  |                  |           |
| 1                                                           | 0.00000        | 0.00000        | 0.02604  | 0.01886          | Converged |

Algorithm converged.

The TRANSREG Procedure Hypothesis Tests for Identity(y)

Univariate ANOVA Table Based on the Usual Degrees of Freedom

| Source          | DF | Sum of Squares | Mean Square | F Value | Pr > F |
|-----------------|----|----------------|-------------|---------|--------|
| Model           | 6  | 38.7478        | 6.45796     | 0.45    | 0.8306 |
| Error           | 13 | 185.3960       | 14.26123    |         |        |
| Corrected Total | 19 | 224.1438       |             |         |        |

|                |           |          |         |
|----------------|-----------|----------|---------|
| Root MSE       | 3.77640   | R-Square | 0.1729  |
| Dependent Mean | 0.85490   | Adj R-Sq | -0.2089 |
| Coeff Var      | 441.73431 |          |         |

Univariate Regression Table Based on the Usual Degrees of Freedom

| Variable   | DF | Coefficient | Type II Sum of Squares | Mean Square | F Value | Pr > F |
|------------|----|-------------|------------------------|-------------|---------|--------|
| Intercept  | 1  | 3.5437125   | 35.2282                | 35.2282     | 2.47    | 0.1400 |
| Spline(x1) | 3  | 0.3644562   | 4.5682                 | 1.5227      | 0.11    | 0.9546 |
| Spline(x2) | 3  | -1.3551738  | 32.9112                | 10.9704     | 0.77    | 0.5315 |

There are three iteration histories: one for the overall model and two for the two independent variables. The first PROC TRANSREG iteration history shows the R square of 0.17287 for the fit of the overall model. The second is for the following model:

```
model identity(y) = spline(x2);
```

This model excludes `spline(x1)`. The third iteration history is for the following model:

```
model identity(y) = spline(x1);
```

This model excludes `spline(x2)`. The difference between the first and second R square times the total sum of squares is the model sum of squares for `spline(x1)`:

$$(0.17287 - 0.15249) \times 224.143800 = 4.568165$$

The difference between the first and third R square times the total sum of squares is the model sum of squares for `spline(x2)`:

$$(0.17287 - 0.02604) \times 224.143800 = 32.911247$$

Figure 97.71 displays the PROC REG results. The TEST statement in PROC REG tests the null hypothesis that the vector of parameters for `x1_1 x1_2 x1_3` is zero. This is the same test as the `spline(x1)` test used by PROC TRANSREG. Similarly, the PROC REG test that the vector of parameters for `x2_1 x2_2 x2_3` is zero is the same as the PROC TRANSREG `SPLINE(x2)` test. So for models with no monotonicity constraints and no dependent variable transformations, PROC TRANSREG provides little more than a different packaging of standard least squares methodology.

**Figure 97.71** Two-Variable Polynomial Regression Output from PROC REG

| Two-Variable Polynomial Regression |           |                |                    |                |         |         |
|------------------------------------|-----------|----------------|--------------------|----------------|---------|---------|
| The REG Procedure                  |           |                |                    |                |         |         |
| Model: MODEL1                      |           |                |                    |                |         |         |
| Dependent Variable: y              |           |                |                    |                |         |         |
| Number of Observations Read        |           |                |                    |                |         | 20      |
| Number of Observations Used        |           |                |                    |                |         | 20      |
| Analysis of Variance               |           |                |                    |                |         |         |
| Source                             | DF        | Sum of Squares | Mean Square        | F Value        | Pr > F  |         |
| Model                              | 6         | 38.74775       | 6.45796            | 0.45           | 0.8306  |         |
| Error                              | 13        | 185.39605      | 14.26123           |                |         |         |
| Corrected Total                    | 19        | 224.14380      |                    |                |         |         |
| Root MSE                           |           | 3.77640        | R-Square           | 0.1729         |         |         |
| Dependent Mean                     |           | 0.85490        | Adj R-Sq           | -0.2089        |         |         |
| Coeff Var                          |           | 441.73431      |                    |                |         |         |
| Parameter Estimates                |           |                |                    |                |         |         |
| Variable                           | Label     | DF             | Parameter Estimate | Standard Error | t Value | Pr >  t |
| Intercept                          | Intercept | 1              | 10.77824           | 7.55244        | 1.43    | 0.1771  |
| x1_1                               | x1 1      | 1              | 0.40112            | 1.81024        | 0.22    | 0.8281  |
| x1_2                               | x1 2      | 1              | 0.25652            | 1.66023        | 0.15    | 0.8796  |
| x1_3                               | x1 3      | 1              | -0.11639           | 0.36775        | -0.32   | 0.7567  |
| x2_1                               | x2 1      | 1              | -14.07054          | 12.50521       | -1.13   | 0.2809  |
| x2_2                               | x2 2      | 1              | 5.95610            | 5.97952        | 1.00    | 0.3374  |
| x2_3                               | x2 3      | 1              | -0.80608           | 0.87291        | -0.92   | 0.3726  |

Figure 97.71 continued

| Two-Variable Polynomial Regression      |    |             |         |        |
|-----------------------------------------|----|-------------|---------|--------|
| The REG Procedure                       |    |             |         |        |
| Model: MODEL1                           |    |             |         |        |
| Test 1 Results for Dependent Variable y |    |             |         |        |
| Source                                  | DF | Mean Square | F Value | Pr > F |
| Numerator                               | 3  | 1.52272     | 0.11    | 0.9546 |
| Denominator                             | 13 | 14.26123    |         |        |

| Two-Variable Polynomial Regression      |    |             |         |        |
|-----------------------------------------|----|-------------|---------|--------|
| The REG Procedure                       |    |             |         |        |
| Model: MODEL1                           |    |             |         |        |
| Test 2 Results for Dependent Variable y |    |             |         |        |
| Source                                  | DF | Mean Square | F Value | Pr > F |
| Numerator                               | 3  | 10.97042    | 0.77    | 0.5315 |
| Denominator                             | 13 | 14.26123    |         |        |

## Hypothesis Tests with Monotonicity Constraints

Now consider a model with monotonicity constraints. This model has no counterpart in PROC REG. The following statements fit a monotone-spline model and produce Figure 97.72:

```

title 'Monotone Splines';

proc transreg data=htex ss2 short;
 model identity(y) = mspline(x1-x3 / nknots=3);
run;

```

The *SHORT a-option* is specified to suppress the iteration histories. Two ANOVA tables are displayed—one by using liberal degrees of freedom and one by using conservative degrees of freedom. All sums of squares and the R squares are the same for both tables. What differs are the degrees of freedom and statistics that use degrees of freedom. The liberal test has 8 model degrees of freedom and 11 error degrees of freedom, whereas the conservative test has 15 model degrees of freedom and only 4 error degrees of freedom. The “true” *p*-value is between 0.8462 and 0.9997, so clearly you would fail to reject the null hypothesis. Unfortunately, results are not always this clear. (See Figure 97.72.)

Figure 97.72 Monotone Spline Transformations

| Monotone Splines                                                |    |                |             |         |                |
|-----------------------------------------------------------------|----|----------------|-------------|---------|----------------|
| The TRANSREG Procedure                                          |    |                |             |         |                |
| Dependent Variable Identity(y)                                  |    |                |             |         |                |
| Number of Observations Read                                     |    |                |             | 20      |                |
| Number of Observations Used                                     |    |                |             | 20      |                |
| Identity(y)                                                     |    |                |             |         |                |
| Algorithm converged.                                            |    |                |             |         |                |
| The TRANSREG Procedure Hypothesis Tests for Identity(y)         |    |                |             |         |                |
| Univariate ANOVA Table Based on Liberal Degrees of Freedom      |    |                |             |         |                |
| Source                                                          | DF | Sum of Squares | Mean Square | F Value | Liberal p      |
| Model                                                           | 8  | 58.0534        | 7.25667     | 0.48    | >= 0.8462      |
| Error                                                           | 11 | 166.0904       | 15.09913    |         |                |
| Corrected Total                                                 | 19 | 224.1438       |             |         |                |
| Root MSE                                                        |    | 3.88576        | R-Square    | 0.2590  |                |
| Dependent Mean                                                  |    | 0.85490        | Adj R-Sq    | -0.2799 |                |
| Coeff Var                                                       |    | 454.52581      |             |         |                |
| Univariate ANOVA Table Based on Conservative Degrees of Freedom |    |                |             |         |                |
| Source                                                          | DF | Sum of Squares | Mean Square | F Value | Conservative p |
| Model                                                           | 15 | 58.0534        | 3.87022     | 0.09    | <= 0.9997      |
| Error                                                           | 4  | 166.0904       | 41.52261    |         |                |
| Corrected Total                                                 | 19 | 224.1438       |             |         |                |
| Root MSE                                                        |    | 6.44380        | R-Square    | 0.2590  |                |
| Dependent Mean                                                  |    | 0.85490        | Adj R-Sq    | -2.5197 |                |
| Coeff Var                                                       |    | 753.74578      |             |         |                |

Figure 97.72 continued

| Univariate Regression Table Based on Liberal Degrees of Freedom |    |             |                              |                |         |           |
|-----------------------------------------------------------------|----|-------------|------------------------------|----------------|---------|-----------|
| Variable                                                        | DF | Coefficient | Type II<br>Sum of<br>Squares | Mean<br>Square | F Value | Liberal p |
| Intercept                                                       | 1  | 4.8687676   | 54.7372                      | 54.7372        | 3.63    | >= 0.0834 |
| Mspline (x1)                                                    | 2  | -0.6886834  | 12.1943                      | 6.0972         | 0.40    | >= 0.6773 |
| Mspline (x2)                                                    | 3  | -1.8237319  | 46.3155                      | 15.4385        | 1.02    | >= 0.4199 |
| Mspline (x3)                                                    | 3  | 0.8646155   | 24.6840                      | 8.2280         | 0.54    | >= 0.6616 |

| Univariate Regression Table Based on Conservative Degrees of Freedom |    |             |                              |                |         |                   |
|----------------------------------------------------------------------|----|-------------|------------------------------|----------------|---------|-------------------|
| Variable                                                             | DF | Coefficient | Type II<br>Sum of<br>Squares | Mean<br>Square | F Value | Conservative<br>p |
| Intercept                                                            | 1  | 4.8687676   | 54.7372                      | 54.7372        | 1.32    | <= 0.3149         |
| Mspline (x1)                                                         | 5  | -0.6886834  | 12.1943                      | 2.4389         | 0.06    | <= 0.9959         |
| Mspline (x2)                                                         | 5  | -1.8237319  | 46.3155                      | 9.2631         | 0.22    | <= 0.9344         |
| Mspline (x3)                                                         | 5  | 0.8646155   | 24.6840                      | 4.9368         | 0.12    | <= 0.9809         |

## Hypothesis Tests with Dependent Variable Transformations

PROC TRANSREG can also provide approximate tests of hypotheses when the dependent variable is transformed, but the output is more complicated. When a dependent variable has more than one degree of freedom, the problem becomes multivariate. Hypothesis tests are performed in the context of a multivariate linear model with the number of dependent variables equal to the number of scoring parameters for the dependent variable transformation. The transformation regression model with a dependent variable transformation differs from the usual multivariate linear model in two important ways. First, the usual assumption of multivariate normality is always violated. This fact is simply ignored. This is one reason why all hypothesis tests in the presence of a dependent variable transformation should be considered approximate at best. Multivariate normality is assumed even though it is known that the assumption is violated.

The second difference concerns the usual multivariate test statistics: Pillai's trace, Wilks' lambda, Hotelling-Lawley trace, and Roy's greatest root. The first three statistics are defined in terms of all the squared canonical correlations. Here, there is only one linear combination (the transformation), and hence only one squared canonical correlation of interest, which is equal to the R square. It might seem that Roy's greatest root, which uses only the largest squared canonical correlation, is the only statistic of interest. Unfortunately, Roy's greatest root is very liberal and provides only a lower bound on the  $p$ -value. Approximate upper bounds are provided by adjusting the other three statistics for the one linear combination case. Wilks' lambda, Pillai's trace, and Hotelling-Lawley trace are a conservative adjustment of the usual statistics.

These statistics are normally defined in terms of the squared canonical correlations, which are the eigenvalues of the matrix  $\mathbf{H}(\mathbf{H} + \mathbf{E})^{-1}$ , where  $\mathbf{H}$  is the hypothesis sum-of-squares matrix and  $\mathbf{E}$  is the error sum-of-squares matrix. Here the R square is used for the first eigenvalue, and all other eigenvalues are set to 0 since only one linear combination is used. Degrees of freedom are computed assuming that all linear

combinations contribute to the lambda and trace statistics, so the  $F$  tests for those statistics are conservative. The  $p$ -values for the liberal and conservative statistics provide approximate lower and upper bounds on  $p$ . In practice, the adjusted Pillai's trace is very conservative—perhaps too conservative to be useful. Wilks' lambda is less conservative, and the Hotelling-Lawley trace seems to be the least conservative. The conservative statistics and the liberal Roy's greatest root provide a bound on the true  $p$ -value. Unfortunately, they sometimes report a bound of 0.0001 and 1.0000.

The following example has a dependent variable transformation and produces [Figure 97.73](#):

```
title 'Transform Dependent and Independent Variables';

proc transreg data=htex ss2 solve short;
 model spline(y) = spline(x1-x3);
run;
```

The univariate results match Roy's greatest root results. Clearly, the proper action is to fail to reject the null hypothesis. However, as stated previously, results are not always this clear.

**Figure 97.73** Transform Dependent and Independent Variables

| Transform Dependent and Independent Variables                                                                                |    |                |             |         |           |
|------------------------------------------------------------------------------------------------------------------------------|----|----------------|-------------|---------|-----------|
| The TRANSREG Procedure                                                                                                       |    |                |             |         |           |
| Dependent Variable Spline(y)                                                                                                 |    |                |             |         |           |
| Number of Observations Read                                                                                                  |    | 20             |             |         |           |
| Number of Observations Used                                                                                                  |    | 20             |             |         |           |
| Spline(y)                                                                                                                    |    |                |             |         |           |
| Algorithm converged.                                                                                                         |    |                |             |         |           |
| The TRANSREG Procedure Hypothesis Tests for Spline(y)                                                                        |    |                |             |         |           |
| Univariate ANOVA Table Based on the Usual Degrees of Freedom                                                                 |    |                |             |         |           |
| Source                                                                                                                       | DF | Sum of Squares | Mean Square | F Value | Liberal p |
| Model                                                                                                                        | 9  | 110.8822       | 12.32025    | 1.09    | >= 0.4452 |
| Error                                                                                                                        | 10 | 113.2616       | 11.32616    |         |           |
| Corrected Total                                                                                                              | 19 | 224.1438       |             |         |           |
| The above statistics are not adjusted for the fact that the dependent variable was transformed and so are generally liberal. |    |                |             |         |           |
| Root MSE                                                                                                                     |    | 3.36544        | R-Square    | 0.4947  |           |
| Dependent Mean                                                                                                               |    | 0.85490        | Adj R-Sq    | 0.0399  |           |
| Coeff Var                                                                                                                    |    | 393.66234      |             |         |           |



Figure 97.73 continued

| Adjusted Multivariate ANOVA Table Based on the Usual Degrees of Freedom |          |         |        |        |           |
|-------------------------------------------------------------------------|----------|---------|--------|--------|-----------|
| Dependent Variable Scoring Parameters=3 S=3 M=2.5 N=3                   |          |         |        |        |           |
| Statistic                                                               | Value    | F Value | Num DF | Den DF | p         |
| Wilks' Lambda                                                           | 0.505308 | 0.23    | 27     | 24.006 | <= 0.9998 |
| Pillai's Trace                                                          | 0.494692 | 0.22    | 27     | 30     | <= 0.9999 |
| Hotelling-Lawley Trace                                                  | 0.978992 | 0.26    | 27     | 11.589 | <= 0.9980 |
| Roy's Greatest Root                                                     | 0.978992 | 1.09    | 9      | 10     | >= 0.4452 |

The Wilks' Lambda, Pillai's Trace, and Hotelling-Lawley Trace statistics are a conservative adjustment of the normal statistics. Roy's Greatest Root is liberal. These statistics are normally defined in terms of the squared canonical correlations which are the eigenvalues of the matrix  $H \cdot \text{inv}(H+E)$ . Here the R-Square is used for the first eigenvalue and all other eigenvalues are set to zero since only one linear combination is used. Degrees of freedom are computed assuming all linear combinations contribute to the Lambda and Trace statistics, so the F tests for those statistics are conservative. The p values for the liberal and conservative statistics provide approximate lower and upper bounds on p. A liberal test statistic with conservative degrees of freedom and a conservative test statistic with liberal degrees of freedom yield at best an approximate p value, which is indicated by a "~" before the p value.

| Univariate Regression Table Based on the Usual Degrees of Freedom |    |             |                              |                |         |           |
|-------------------------------------------------------------------|----|-------------|------------------------------|----------------|---------|-----------|
| Variable                                                          | DF | Coefficient | Type II<br>Sum of<br>Squares | Mean<br>Square | F Value | Liberal p |
| Intercept                                                         | 1  | 6.9089087   | 117.452                      | 117.452        | 10.37   | >= 0.0092 |
| Spline(x1)                                                        | 3  | -1.0832321  | 32.493                       | 10.831         | 0.96    | >= 0.4504 |
| Spline(x2)                                                        | 3  | -2.1539191  | 45.251                       | 15.084         | 1.33    | >= 0.3184 |
| Spline(x3)                                                        | 3  | 0.4779207   | 10.139                       | 3.380          | 0.30    | >= 0.8259 |

The above statistics are not adjusted for the fact that the dependent variable was transformed and so are generally liberal.

Figure 97.73 continued

| Adjusted Multivariate Regression Table Based on the Usual Degrees of Freedom |             |                        |          |         |        |        |           |  |
|------------------------------------------------------------------------------|-------------|------------------------|----------|---------|--------|--------|-----------|--|
| Variable                                                                     | Coefficient | Statistic              | Value    | F Value | Num DF | Den DF | p         |  |
| Intercept                                                                    | 6.9089087   | Wilks' Lambda          | 0.49092  | 2.77    | 3      | 8      | 0.1112    |  |
|                                                                              |             | Pillai's Trace         | 0.50908  | 2.77    | 3      | 8      | 0.1112    |  |
|                                                                              |             | Hotelling-Lawley Trace | 1.036993 | 2.77    | 3      | 8      | 0.1112    |  |
|                                                                              |             | Roy's Greatest Root    | 1.036993 | 2.77    | 3      | 8      | 0.1112    |  |
|                                                                              |             |                        |          |         |        |        |           |  |
| Spline(x1)                                                                   | -1.0832321  | Wilks' Lambda          | 0.777072 | 0.24    | 9      | 19.621 | <= 0.9840 |  |
|                                                                              |             | Pillai's Trace         | 0.222928 | 0.27    | 9      | 30     | <= 0.9787 |  |
|                                                                              |             | Hotelling-Lawley Trace | 0.286883 | 0.24    | 9      | 9.8113 | <= 0.9784 |  |
|                                                                              |             | Roy's Greatest Root    | 0.286883 | 0.96    | 3      | 10     | >= 0.4504 |  |
|                                                                              |             |                        |          |         |        |        |           |  |
| Spline(x2)                                                                   | -2.1539191  | Wilks' Lambda          | 0.714529 | 0.32    | 9      | 19.621 | <= 0.9572 |  |
|                                                                              |             | Pillai's Trace         | 0.285471 | 0.35    | 9      | 30     | <= 0.9494 |  |
|                                                                              |             | Hotelling-Lawley Trace | 0.399524 | 0.33    | 9      | 9.8113 | <= 0.9424 |  |
|                                                                              |             | Roy's Greatest Root    | 0.399524 | 1.33    | 3      | 10     | >= 0.3184 |  |
|                                                                              |             |                        |          |         |        |        |           |  |
| Spline(x3)                                                                   | 0.4779207   | Wilks' Lambda          | 0.917838 | 0.08    | 9      | 19.621 | <= 0.9998 |  |
|                                                                              |             | Pillai's Trace         | 0.082162 | 0.09    | 9      | 30     | <= 0.9996 |  |
|                                                                              |             | Hotelling-Lawley Trace | 0.089517 | 0.07    | 9      | 9.8113 | <= 0.9997 |  |
|                                                                              |             | Roy's Greatest Root    | 0.089517 | 0.30    | 3      | 10     | >= 0.8259 |  |
|                                                                              |             |                        |          |         |        |        |           |  |

These statistics are adjusted in the same way as the multivariate statistics above.

## Hypothesis Tests with One-Way ANOVA

One-way ANOVA models are fit with either an explicit or implicit intercept. In implicit intercept models, the ANOVA table of PROC TRANSREG is the correct table for a model with an intercept, and the regression table is the correct table for a model that does not have a separate explicit intercept. The PROC TRANSREG implicit intercept ANOVA table matches the PROC REG table when the NOINT *a-option* is not specified, and the PROC TRANSREG implicit intercept regression table matches the PROC REG table when the NOINT *a-option* is specified. The following statements illustrate this relationship and produce Figure 97.74:

```

data oneway;
 input y x $;
 datalines;
0 a
1 a
2 a
7 b
8 b
9 b
3 c
4 c
5 c
;

title 'Implicit Intercept Model';

proc transreg ss2 data=oneway short;
 model identity(y) = class(x / zero=none);
 output out=oneway2;
run;

proc reg data=oneway2;
 model y = xa xb xc; /* Implicit Intercept ANOVA */
 model y = xa xb xc / noint; /* Implicit Intercept Regression */
run; quit;

```

Figure 97.74 Implicit Intercept Model

```

Implicit Intercept Model

The TRANSREG Procedure

Dependent Variable Identity(y)

Class Level Information

Class Levels Values
x 3 a b c

Number of Observations Read 9
Number of Observations Used 9
Implicit Intercept Model

```

Figure 97.74 continued

| The TRANSREG Procedure Hypothesis Tests for Identity(y)           |                             |                |                        |             |         |        |       |
|-------------------------------------------------------------------|-----------------------------|----------------|------------------------|-------------|---------|--------|-------|
| Univariate ANOVA Table Based on the Usual Degrees of Freedom      |                             |                |                        |             |         |        |       |
| Source                                                            | DF                          | Sum of Squares | Mean Square            | F Value     | Pr > F  |        |       |
| Model                                                             | 2                           | 74.00000       | 37.00000               | 37.00       | 0.0004  |        |       |
| Error                                                             | 6                           | 6.00000        | 1.00000                |             |         |        |       |
| Corrected Total                                                   | 8                           | 80.00000       |                        |             |         |        |       |
|                                                                   | Root MSE                    | 1.00000        | R-Square               | 0.9250      |         |        |       |
|                                                                   | Dependent Mean              | 4.33333        | Adj R-Sq               | 0.9000      |         |        |       |
|                                                                   | Coeff Var                   | 23.07692       |                        |             |         |        |       |
| Univariate Regression Table Based on the Usual Degrees of Freedom |                             |                |                        |             |         |        |       |
| Variable                                                          | DF                          | Coefficient    | Type II Sum of Squares | Mean Square | F Value | Pr > F | Label |
| Class.xa                                                          | 1                           | 1.00000000     | 3.000                  | 3.000       | 3.00    | 0.1340 | x a   |
| Class.xb                                                          | 1                           | 8.00000000     | 192.000                | 192.000     | 192.00  | <.0001 | x b   |
| Class.xc                                                          | 1                           | 4.00000000     | 48.000                 | 48.000      | 48.00   | 0.0004 | x c   |
| Implicit Intercept Model                                          |                             |                |                        |             |         |        |       |
| The REG Procedure                                                 |                             |                |                        |             |         |        |       |
| Model: MODEL1                                                     |                             |                |                        |             |         |        |       |
| Dependent Variable: y                                             |                             |                |                        |             |         |        |       |
|                                                                   | Number of Observations Read |                |                        |             | 9       |        |       |
|                                                                   | Number of Observations Used |                |                        |             | 9       |        |       |
| Analysis of Variance                                              |                             |                |                        |             |         |        |       |
| Source                                                            | DF                          | Sum of Squares | Mean Square            | F Value     | Pr > F  |        |       |
| Model                                                             | 2                           | 74.00000       | 37.00000               | 37.00       | 0.0004  |        |       |
| Error                                                             | 6                           | 6.00000        | 1.00000                |             |         |        |       |
| Corrected Total                                                   | 8                           | 80.00000       |                        |             |         |        |       |
|                                                                   | Root MSE                    | 1.00000        | R-Square               | 0.9250      |         |        |       |
|                                                                   | Dependent Mean              | 4.33333        | Adj R-Sq               | 0.9000      |         |        |       |
|                                                                   | Coeff Var                   | 23.07692       |                        |             |         |        |       |

Figure 97.74 continued

NOTE: Model is not full rank. Least-squares solutions for the parameters are not unique. Some statistics will be misleading. A reported DF of 0 or B means that the estimate is biased.

NOTE: The following parameters have been set to 0, since the variables are a linear combination of other variables as shown.

$$xc = \text{Intercept} - xa - xb$$

Parameter Estimates

| Variable  | Label     | DF | Parameter Estimate | Standard Error | t Value | Pr >  t |
|-----------|-----------|----|--------------------|----------------|---------|---------|
| Intercept | Intercept | B  | 4.00000            | 0.57735        | 6.93    | 0.0004  |
| xa        | x a       | B  | -3.00000           | 0.81650        | -3.67   | 0.0104  |
| xb        | x b       | B  | 4.00000            | 0.81650        | 4.90    | 0.0027  |
| xc        | x c       | 0  | 0                  | .              | .       | .       |

Implicit Intercept Model

The REG Procedure  
Model: MODEL2  
Dependent Variable: y

|                             |   |
|-----------------------------|---|
| Number of Observations Read | 9 |
| Number of Observations Used | 9 |

NOTE: No intercept in model. R-Square is redefined.

Analysis of Variance

| Source            | DF | Sum of Squares | Mean Square | F Value | Pr > F |
|-------------------|----|----------------|-------------|---------|--------|
| Model             | 3  | 243.00000      | 81.00000    | 81.00   | <.0001 |
| Error             | 6  | 6.00000        | 1.00000     |         |        |
| Uncorrected Total | 9  | 249.00000      |             |         |        |

|                |          |          |        |
|----------------|----------|----------|--------|
| Root MSE       | 1.00000  | R-Square | 0.9759 |
| Dependent Mean | 4.33333  | Adj R-Sq | 0.9639 |
| Coeff Var      | 23.07692 |          |        |

Parameter Estimates

| Variable | Label | DF | Parameter Estimate | Standard Error | t Value | Pr >  t |
|----------|-------|----|--------------------|----------------|---------|---------|
| xa       | x a   | 1  | 1.00000            | 0.57735        | 1.73    | 0.1340  |
| xb       | x b   | 1  | 8.00000            | 0.57735        | 13.86   | <.0001  |
| xc       | x c   | 1  | 4.00000            | 0.57735        | 6.93    | 0.0004  |

## Using the DESIGN Output Option

This example uses PROC TRANSREG and the DESIGN *o-option* to prepare an input data set with classification variables for the LOGISTIC procedure. The DESIGN *o-option* specifies that the goal is design matrix creation, not analysis. When you specify DESIGN, dependent variables are not required. The DEVIATIONS (or EFFECTS) *t-option* requests a deviations-from-means (1, 0, -1) coding of the classification variables, which is the same coding the CATMOD procedure uses. PROC TRANSREG automatically creates a macro variable `&_TrgInd` that contains the list of independent variables created. This macro is used in the PROC LOGISTIC MODEL statement. (See Figure 97.75.) For comparison, the same analysis is also performed with PROC CATMOD. The following statements create Figure 97.75:

```

title 'Using PROC TRANSREG to Create a Design Matrix';

data a;
 do y = 1, 2;
 do a = 1 to 4;
 do b = 1 to 3;
 w = ceil(uniform(1) * 10 + 10);
 output;
 end;
 end;
 end;
run;

proc transreg data=a design;
 model class(a b / deviations);
 id y w;
 output out=coded;
run;

proc print;
 title2 'PROC TRANSREG Output Data Set';
run;

title2 'PROC LOGISTIC with Classification Variables';

proc logistic;
 freq w;
 model y = &_trgind;
run;

title2 'PROC CATMOD Should Produce the Same Results';

proc catmod data=a;
 model y = a b;
 weight w;
run;

```

Figure 97.75 The PROC TRANSREG Design Matrix

```

Using PROC TRANSREG to Create a Design Matrix
PROC LOGISTIC with Classification Variables

The LOGISTIC Procedure

Model Information

Data Set WORK.CODED
Response Variable y
Number of Response Levels 2
Frequency Variable w
Model binary logit
Optimization Technique Fisher's scoring

Number of Observations Read 24
Number of Observations Used 24
Sum of Frequencies Read 375
Sum of Frequencies Used 375

Response Profile

Ordered Value y Total Frequency
1 1 188
2 2 187

Probability modeled is y=1.

Model Convergence Status

Convergence criterion (GCONV=1E-8) satisfied.

Model Fit Statistics

Criterion Intercept Only Intercept and Covariates
AIC 521.858 524.378
SC 525.785 547.939
-2 Log L 519.858 512.378

Testing Global Null Hypothesis: BETA=0

Test Chi-Square DF Pr > ChiSq
Likelihood Ratio 7.4799 5 0.1873
Score 7.4312 5 0.1905
Wald 7.3356 5 0.1969

```

Figure 97.75 continued

| Analysis of Maximum Likelihood Estimates |    |          |                |                 |            |
|------------------------------------------|----|----------|----------------|-----------------|------------|
| Parameter                                | DF | Estimate | Standard Error | Wald Chi-Square | Pr > ChiSq |
| Intercept                                | 1  | -0.00040 | 0.1044         | 0.0000          | 0.9969     |
| a1                                       | 1  | -0.0802  | 0.1791         | 0.2007          | 0.6542     |
| a2                                       | 1  | 0.2001   | 0.1800         | 1.2363          | 0.2662     |
| a3                                       | 1  | -0.1350  | 0.1819         | 0.5514          | 0.4578     |
| b1                                       | 1  | -0.2392  | 0.1500         | 2.5436          | 0.1107     |
| b2                                       | 1  | 0.3433   | 0.1474         | 5.4223          | 0.0199     |

| Odds Ratio Estimates |                |                            |       |
|----------------------|----------------|----------------------------|-------|
| Effect               | Point Estimate | 95% Wald Confidence Limits |       |
| a1                   | 0.923          | 0.650                      | 1.311 |
| a2                   | 1.222          | 0.858                      | 1.738 |
| a3                   | 0.874          | 0.612                      | 1.248 |
| b1                   | 0.787          | 0.587                      | 1.056 |
| b2                   | 1.410          | 1.056                      | 1.882 |

| Association of Predicted Probabilities and Observed Responses |       |           |       |  |
|---------------------------------------------------------------|-------|-----------|-------|--|
| Percent Concordant                                            | 54.0  | Somers' D | 0.163 |  |
| Percent Discordant                                            | 37.8  | Gamma     | 0.177 |  |
| Percent Tied                                                  | 8.2   | Tau-a     | 0.082 |  |
| Pairs                                                         | 35156 | c         | 0.581 |  |

Using PROC TRANSREG to Create a Design Matrix  
PROC CATMOD Should Produce the Same Results

The CATMOD Procedure

| Data Summary      |   |                 |     |
|-------------------|---|-----------------|-----|
| Response          | y | Response Levels | 2   |
| Weight Variable   | w | Populations     | 12  |
| Data Set          | A | Total Frequency | 375 |
| Frequency Missing | 0 | Observations    | 24  |



Figure 97.75 continued

| Population Profiles |   |   |             |
|---------------------|---|---|-------------|
| Sample              | a | b | Sample Size |
| 1                   | 1 | 1 | 31          |
| 2                   | 1 | 2 | 31          |
| 3                   | 1 | 3 | 34          |
| 4                   | 2 | 1 | 26          |
| 5                   | 2 | 2 | 33          |
| 6                   | 2 | 3 | 37          |
| 7                   | 3 | 1 | 36          |
| 8                   | 3 | 2 | 29          |
| 9                   | 3 | 3 | 28          |
| 10                  | 4 | 1 | 26          |
| 11                  | 4 | 2 | 35          |
| 12                  | 4 | 3 | 29          |

| Response Profiles |   |
|-------------------|---|
| Response          | y |
| 1                 | 1 |
| 2                 | 2 |

Maximum Likelihood Analysis

Maximum likelihood computations converged.

Maximum Likelihood Analysis of Variance

| Source           | DF | Chi-Square | Pr > ChiSq |
|------------------|----|------------|------------|
| Intercept        | 1  | 0.00       | 0.9969     |
| a                | 3  | 1.50       | 0.6823     |
| b                | 2  | 5.64       | 0.0597     |
| Likelihood Ratio | 6  | 2.81       | 0.8329     |

Analysis of Maximum Likelihood Estimates

| Parameter | Estimate | Standard Error | Chi-Square | Pr > ChiSq |
|-----------|----------|----------------|------------|------------|
| Intercept | -0.00040 | 0.1044         | 0.00       | 0.9969     |
| a         |          |                |            |            |
| 1         | -0.0802  | 0.1791         | 0.20       | 0.6542     |
| 2         | 0.2001   | 0.1800         | 1.24       | 0.2662     |
| 3         | -0.1350  | 0.1819         | 0.55       | 0.4578     |
| b         |          |                |            |            |
| 1         | -0.2392  | 0.1500         | 2.54       | 0.1107     |
| 2         | 0.3434   | 0.1474         | 5.42       | 0.0199     |

## Discrete Choice Experiments: DESIGN, NORESTORE, NOZERO

A discrete choice experiment is constructed consisting of four product brands, each available at three different prices, \$1.49, \$1.99, \$2.49. In addition, each choice set contains a constant “other” alternative available at \$1.49. In the fifth choice set, price is constant. PROC TRANSREG is used to code the design, and the PHREG procedure fits the multinomial logit choice model (not shown). See [http://support.sas.com/resources/papers/tnote/tnote\\_marketresearch.html](http://support.sas.com/resources/papers/tnote/tnote_marketresearch.html) (Kuhfeld 2005) for more information about discrete choice modeling and the multinomial logit model; look for the latest “Discrete Choice” report. The following statements produce Figure 97.76:

```

title 'Choice Model Coding';

data design;
 array p[4];
 input p1-p4 @@;
 set = _n_;
 do brand = 1 to 4;
 price = p[brand];
 output;
 end;
 brand = .; price = 1.49; output; /* constant alternative */
 keep set brand price;
 datalines;
1.49 1.99 1.49 1.99 1.99 1.99 2.49 1.49 1.99 1.49 1.99 1.49
1.99 1.49 2.49 1.99 1.49 1.49 1.49 1.49 2.49 1.49 1.99 2.49
1.49 1.49 2.49 2.49 2.49 2.49 1.49 1.49 1.49 2.49 2.49 1.99
2.49 2.49 2.49 1.49 1.99 2.49 1.49 2.49 2.49 1.99 2.49 2.49
2.49 1.49 1.49 1.99 1.49 1.99 1.99 1.49 2.49 1.99 1.99 1.99
1.99 1.99 1.49 2.49 1.99 2.49 1.99 1.99 1.49 2.49 1.99 2.49
;

proc transreg data=design design norestoremissing nozeroconstant;
 model class(brand / zero=none) identity(price);
 output out=coded;
 by set;
run;

proc print data=coded(firstobs=21 obs=25);
 var set brand &_trgind;
run;

```

In the interest of space, only the fifth choice set is displayed in Figure 97.76.

Figure 97.76 The Fifth Choice Set

| Choice Model Coding |     |       |        |        |        |        |       |
|---------------------|-----|-------|--------|--------|--------|--------|-------|
| Obs                 | set | brand | brand1 | brand2 | brand3 | brand4 | price |
| 21                  | 5   | 1     | 1      | 0      | 0      | 0      | 1.49  |
| 22                  | 5   | 2     | 0      | 1      | 0      | 0      | 1.49  |
| 23                  | 5   | 3     | 0      | 0      | 1      | 0      | 1.49  |
| 24                  | 5   | 4     | 0      | 0      | 0      | 1      | 1.49  |
| 25                  | 5   | .     | 0      | 0      | 0      | 0      | 1.49  |

For the constant alternative (Brand = .), the brand coding is a row of zeros due to the **NORESTOREMISSING** *o-option*, and Price is a constant \$1.49 (instead of 0) due to the **NOZEROCONSTANT**.

The data set was coded by choice set (BY set;). This is a small problem. With very large problems, it might be necessary to restrict the number of observations that are coded at one time so that the procedure uses less time and memory. Coding by choice set is one option. When coding is performed after the data are merged in, coding by subject and choice set combinations is another option. Alternatively, you can specify **DESIGN=n**, where *n* is the number of observations to code at one time. For example, you can specify **DESIGN=100** or **DESIGN=1000** to process the data set in blocks of 100 or 1000 observations. Specify the **NOZEROCONSTANT** *a-option* to ensure that constant variables within blocks are not zeroed. When you specify **DESIGN=n**, or perform coding after the data are merged in, specify the dependent variable and any other variables needed for analysis as **ID** variables.

---

## Centering

You can use transformation options to center and standardize the variables in several ways. For example, the following **MODEL** statement creates three independent variables,  $x$ ,  $x^2$ , and  $x^3$ :

```
model identity(y) = pspline(x);
```

The variables are not centered.

When the **CENTER** *t-option* is specified, as in the following statement, the independent variable is centered before squaring and cubing:

```
model identity(y) = pspline(x / center);
```

The three independent variables are  $x - \bar{x}$ ,  $(x - \bar{x})^2$ , and  $(x - \bar{x})^3$ .

Since operations such as squaring occur after the centering, the resulting variables are not always centered. The **CENTER** *t-option* is particularly useful with polynomials since centering before squaring and cubing can help reduce collinearity and numerical problems. For example, if one of your variables is year, with values all greater than 1900, squaring and cubing without centering first will create variables that are all essentially perfectly correlated.

When the `TSTANDARD=CENTER` *t-option* is specified, as in the following model, the three independent variables are squared and cubed and then centered:

```
model identity(y) = pspline(x / tstandard=center);
```

The three independent variables are  $x - \bar{x}$ ,  $x^2 - \overline{x^2}$ , and  $x^3 - \overline{x^3}$ .

You can specify both the `CENTER` and `TSTANDARD=CENTER` *t-options* to center the variables, then square and cube them, and then center the results, as in the following statement:

```
model identity(y) = pspline(x / center tstandard=center);
```

The three independent variables are  $x - \bar{x}$ ,  $(x - \bar{x})^2 - \overline{(x - \bar{x})^2}$ , and  $(x - \bar{x})^3 - \overline{(x - \bar{x})^3}$ .

## Displayed Output

The display options control the amount of displayed output. The displayed output can contain the following:

- an iteration history and convergence status table (by default when there are iterations)
- an ANOVA table when the `TEST`, `SS2`, or `UTILITIES` *a-option* is specified
- a regression table when the `SS2` *a-option* is specified
- conjoint analysis part-worth utilities when the `UTILITIES` *a-option* is specified
- model details when the `DETAIL` *a-option* is specified
- a multivariate ANOVA table when the dependent variable is transformed and the `TEST` or `SS2` *a-option* is specified
- a multivariate regression table when the dependent variable is transformed and it is specified
- liberal and conservative ANOVA, multivariate ANOVA, regression, and multivariate regression tables when there is a `MONOTONE`, `UNTIE`, or `MSPLINE` transformation and the `TEST` or `SS2` *a-option* is specified

## ODS Table Names

PROC TRANSREG assigns a name to each table it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in Table 97.8. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

**Table 97.8** ODS Tables Produced by PROC TRANSREG

| ODS Table Name | Description                    | Statement & Option                        |
|----------------|--------------------------------|-------------------------------------------|
| ANOVA          | ANOVA                          | MODEL/PROC, <code>TEST/SS2</code>         |
| BoxCox         | Box-Cox transformation results | MODEL, <code>BOXCOX</code>                |
| CANALS         | CANALS iteration history       | MODEL/PROC,<br><code>METHOD=CANALS</code> |
| ClassLevels    | ANOVA                          | MODEL/PROC, <code>TEST/SS2</code>         |

Table 97.8 continued

| ODS Table Name       | Description                                  | Statement & Option                      |
|----------------------|----------------------------------------------|-----------------------------------------|
| Coef                 | Regression results                           | MODEL/PROC, <b>SS2</b>                  |
| ConservANOVA         | ANOVA, *1                                    | MODEL/PROC, <b>TEST/SS2</b>             |
| ConservCoef          | Regression results, *1                       | MODEL/PROC, <b>SS2</b>                  |
| ConservFitStatistics | Fit statistics, *1                           | MODEL/PROC, <b>TEST/SS2</b>             |
| ConservMVANOVA       | Multivariate ANOVA, *1, *2                   | MODEL/PROC, <b>TEST/SS2</b>             |
| ConservMVCoef        | Multivariate regression results, *1, *2      | MODEL/PROC, <b>SS2</b>                  |
| ConservUtilities     | Conjoint analysis utilities, *1              | MODEL/PROC, <b>UTILITIES</b>            |
| ConvergenceStatus    | Convergence status                           | default                                 |
| Details              | Model Details                                | MODEL/PROC, <b>DETAIL</b>               |
| Equation             | Linear dependency equation                   | less-than-full-rank model               |
| FitStatistics        | Fit statistics like R square                 | MODEL/PROC, <b>TEST/SS2</b>             |
| Footnotes            | Iteration history footnotes                  | default                                 |
| Formula              | Fit plot formula (nonprinting)               | PROC,<br><b>PLOTS=FIT(FORMULA)</b>      |
| LiberalANOVA         | ANOVA, *1                                    | MODEL/PROC, <b>TEST/SS2</b>             |
| LiberalCoef          | Regression results, *1                       | MODEL/PROC, <b>SS2</b>                  |
| LiberalFitStatistics | Fit statistics, *1                           | MODEL/PROC, <b>TEST/SS2</b>             |
| LiberalMVANOVA       | Multivariate ANOVA, *1, *2                   | MODEL/PROC, <b>TEST/SS2</b>             |
| LiberalMVCoef        | Multivariate regression results, *1, *2      | MODEL/PROC, <b>SS2</b>                  |
| LiberalUtilities     | Conjoint analysis utilities, *1              | MODEL/PROC, <b>UTILITIES</b>            |
| MORALS               | MORALS iteration history                     | MODEL/PROC,<br><b>METHOD=MORALS</b>     |
| MVANOVA              | Multivariate ANOVA, *2                       | MODEL/PROC, <b>TEST/SS2</b>             |
| MVCoef               | Multivariate regression results, *2          | MODEL/PROC, <b>SS2</b>                  |
| NObs                 | ANOVA                                        | MODEL/PROC, <b>TEST/SS2</b>             |
| PBSplineCriteria     | Penalized B-spline criteria (nonprinting)    | MODEL, <b>PBSPLINE</b>                  |
| RSquare              | R square                                     | MODEL/PROC, <b>RSQUARE</b>              |
| Redundancy           | Redundancy iteration history                 | MODEL/PROC,<br><b>METHOD=REDUNDANCY</b> |
| SplineCoef           | Spline coefficients (nonprinting)            | MODEL, <b>SPLINE/MSPLINE</b>            |
| TestIterations       | Hypothesis test iterations iteration history | MODEL/PROC, <b>SS2</b>                  |
| Univariate           | Univariate iteration history                 | MODEL/PROC,<br><b>METHOD=UNIVARIATE</b> |
| Utilities            | Conjoint analysis utilities                  | MODEL/PROC, <b>UTILITIES</b>            |

\*1. Liberal and conservative test tables are produced when a **MONOTONE**, **UNTIE**, or **MSPLINE** transformation is requested.

\*2. Multivariate tables are produced when the dependent variable is iteratively transformed.

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “Statistical Graphics Using ODS.”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “A Primer on ODS Statistical Graphics” on page 599 in Chapter 21, “Statistical Graphics Using ODS.”

Some graphs are produced by default; other graphs are produced by using statements and options. You can reference every graph produced through ODS Graphics with a name. The names of the graphs that PROC TRANSREG generates are listed in Table 97.9, along with the required statements and options.

**Table 97.9** Graphs Produced by PROC TRANSREG

| ODS Graph Name      | Plot Description                                 | Statement & Option                                                                                                      |
|---------------------|--------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------|
| BoxCoxFPlot         | Box-Cox $F = t^2$                                | MODEL & PROC, <b>BOXCOX</b> transform & PLOTS(UNPACK)                                                                   |
| BoxCoxLogLikePlot   | Box-Cox Log Likelihood                           | MODEL & PROC, <b>BOXCOX</b> transform & PLOTS(UNPACK)                                                                   |
| BoxCoxPlot          | Box-Cox $t$ or $F = t^2$ & Log Likelihood        | MODEL, <b>BOXCOX</b> transform                                                                                          |
| BoxCoxtPlot         | Box-Cox $t$                                      | MODEL & PROC, <b>BOXCOX</b> transform & PLOTS(UNPACK)=BOXCOX(T)                                                         |
| FitPlot             | Simple Regression and Separate Group Regressions | MODEL, a dependent variable that is not transformed, one non-CLASS independent variable, and at most one CLASS variable |
| ObservedByPredicted | Dependent Variable by Predicted Values           | MODEL, <b>PLOTS=OBSERVEDBYPREDICTED</b>                                                                                 |
| PBSplineCritPlot    | Penalized B-Spline Criterion Plot                | MODEL, <b>PBSPLINE</b> transform                                                                                        |
| PrefMapVecPlot      | Preference Mapping Vector Plot                   | MODEL & PROC, <b>IDENTITY</b> transform & <b>COORDINATES</b>                                                            |
| PrefMapIdealPlot    | Preference Mapping Ideal Point Plot              | MODEL & PROC, <b>POINT</b> expansion & <b>COORDINATES</b>                                                               |
| ResidualPlot        | Residuals                                        | PROC, <b>PLOTS=RESIDUALS</b>                                                                                            |
| RMSEPlot            | Box-Cox Root Mean Square Error                   | MODEL & PROC, <b>BOXCOX</b> transform & <b>PLOTS=BOXCOX(RMSE)</b>                                                       |
| ScatterPlot         | Scatter Plot of Observed Data                    | MODEL, one non-CLASS independent variable, and at most one CLASS variable, <b>PLOTS=SCATTER</b>                         |
| TransformationPlot  | Variable Transformations                         | PROC, <b>PLOTS=TRANSFORMATION</b>                                                                                       |

## The PLOTS(INTERPOLATE) Option

This section illustrates one use of the PLOTS(INTERPOLATE) option for use with ODS Graphics. The data set has two groups of observations,  $c = 1$  and  $c = 2$ . Each group is sparse, having only five observations, so the plots of the transformations and fit functions are not smooth. A second DATA step adds additional observations to the data set, over the range of  $x$ , with  $y$  missing. These observations do not contribute to the analysis, but they are used in computations of transformed and predicted values. The resulting plots are much smoother in the latter case than in the former. The other results of the analysis are the same. The following statements produce [Figure 97.77](#) and [Figure 97.78](#):

```

title 'Smoother Interpolation with PLOTS(INTERPOLATE)';

data a;
 input c y x;
 output;
 datalines;
1 1 1
1 2 2
1 4 3
1 6 4
1 7 5
2 3 1
2 4 2
2 5 3
2 4 4
2 5 5
;

ods graphics on;

proc transreg data=a plots=(tran fit) ss2;
 model ide(y) = pbs(x) * class(c / zero=none);
run;

data b;
 set a end=eof;
 output;
 if eof then do;
 y = .;
 do x = 1 to 5 by 0.05;
 c = 1; output;
 c = 2; output;
 end;
 end;
run;

proc transreg data=b plots(interpolate)=(tran fit) ss2;
 model ide(y) = pbs(x) * class(c / zero=none);
run;

```

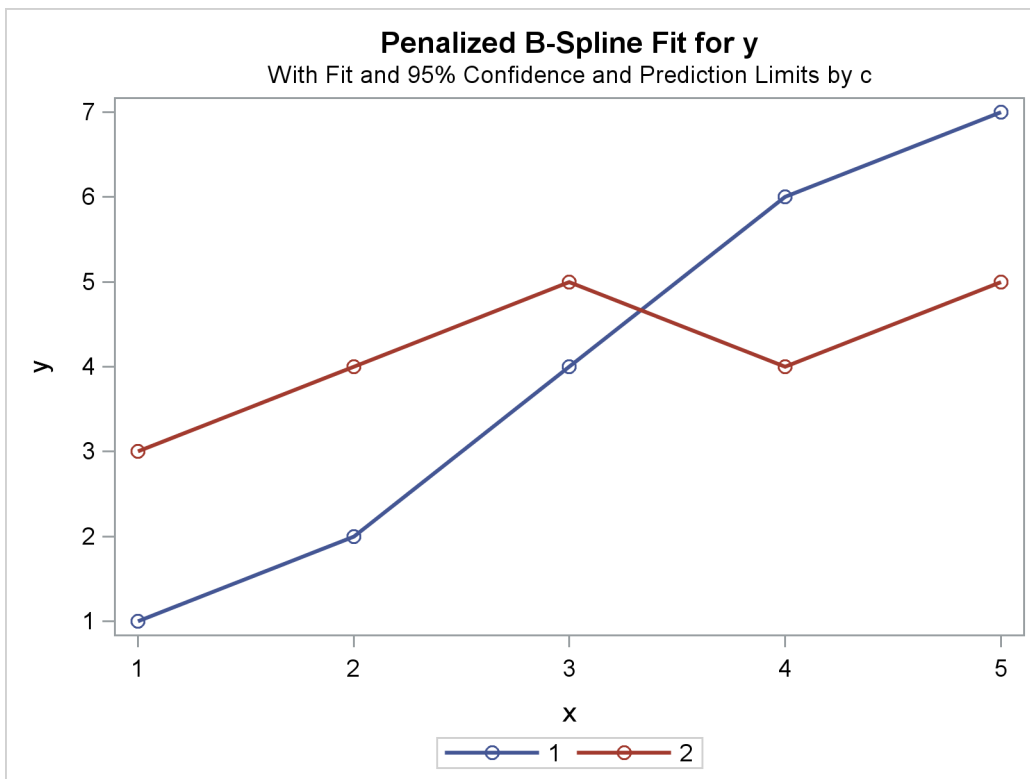
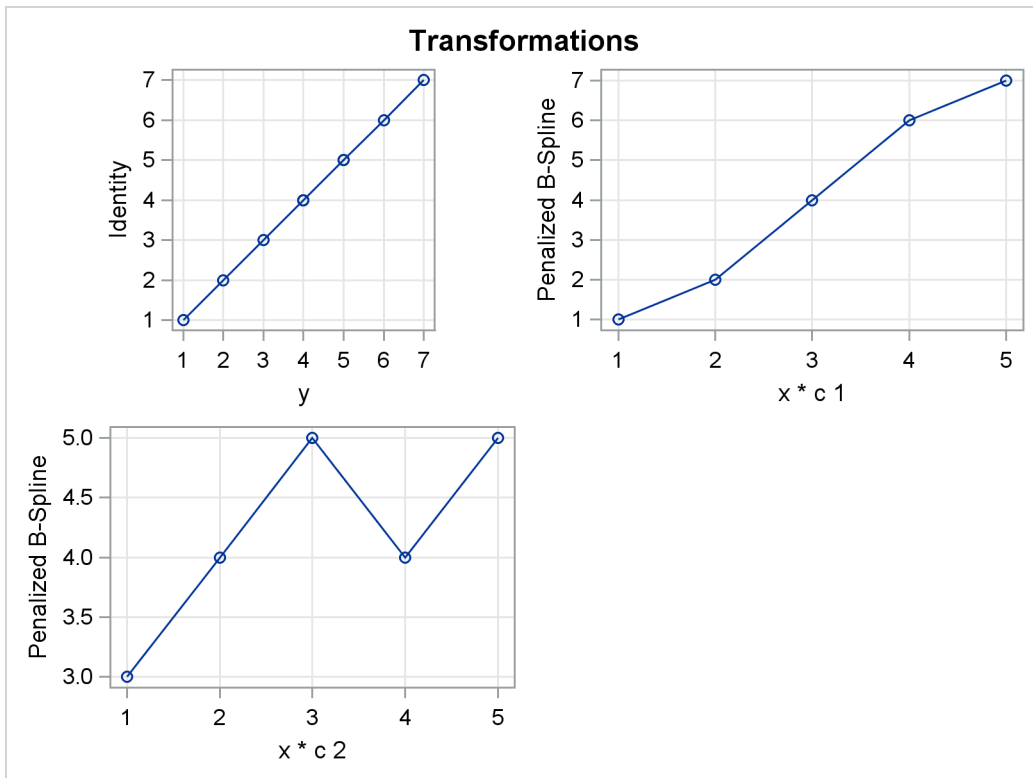
The results with no interpolation are shown in Figure 97.77. The transformation and fit functions are not at all smooth. The results with interpolation are shown in Figure 97.78. The transformation and fit functions are smooth in Figure 97.78, because there are intermediate points to plot.

**Figure 97.77** No Interpolation

| Smoother Interpolation with PLOTS (INTERPOLATE)           |        |                |             |          |         |
|-----------------------------------------------------------|--------|----------------|-------------|----------|---------|
| The TRANSREG Procedure                                    |        |                |             |          |         |
| Univariate ANOVA Table, Penalized B-Spline Transformation |        |                |             |          |         |
| Source                                                    | DF     | Sum of Squares | Mean Square | F Value  | Pr > F  |
| Model                                                     | 9      | 28.90000       | 3.211111    | Infty    | <.0001  |
| Error                                                     | 12E-10 | 0.00000        | 0.000000    |          |         |
| Corrected Total                                           | 9      | 28.90000       |             |          |         |
| Root MSE                                                  |        | 0              | R-Square    | 1.0000   |         |
| Dependent Mean                                            |        | 4.10000        | Adj R-Sq    | 1.0000   |         |
| Coeff Var                                                 |        | 0              |             |          |         |
| Penalized B-Spline Transformation                         |        |                |             |          |         |
| Variable                                                  | DF     | Coefficient    | Lambda      | AICC     | Label   |
| Pbspline(xc1)                                             | 5.0000 | 1.000          | 2.642E-7    | -66.4281 | x * c 1 |
| Pbspline(xc2)                                             | 5.0000 | 1.000          | 2.516E-7    | -60.6430 | x * c 2 |



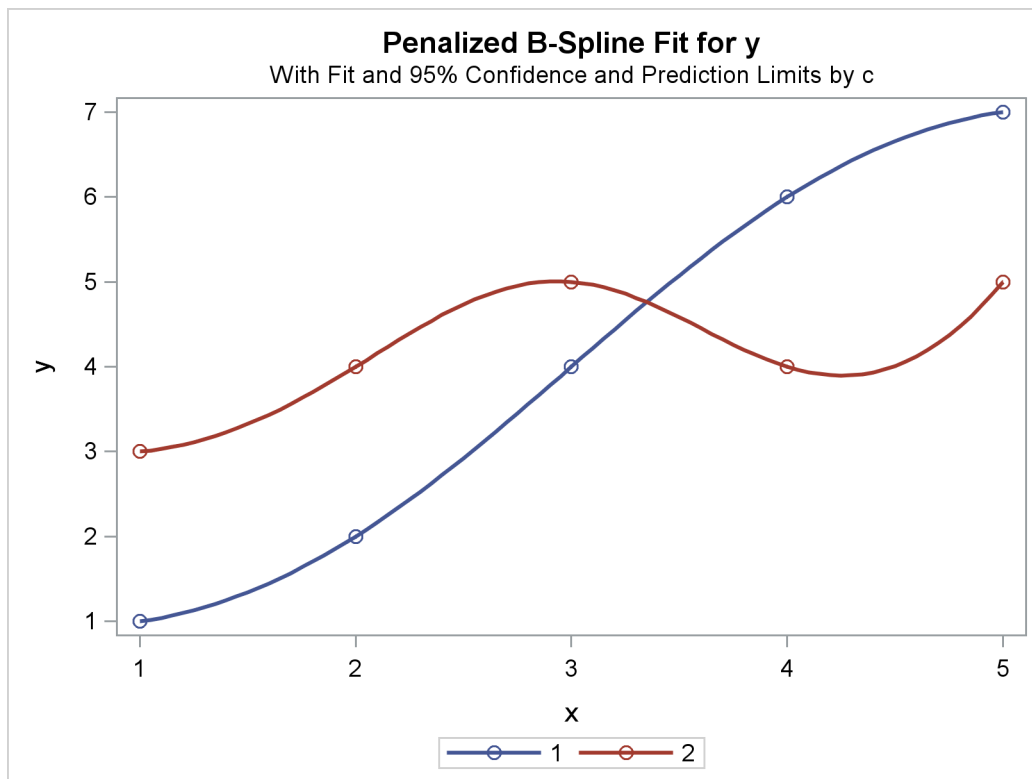
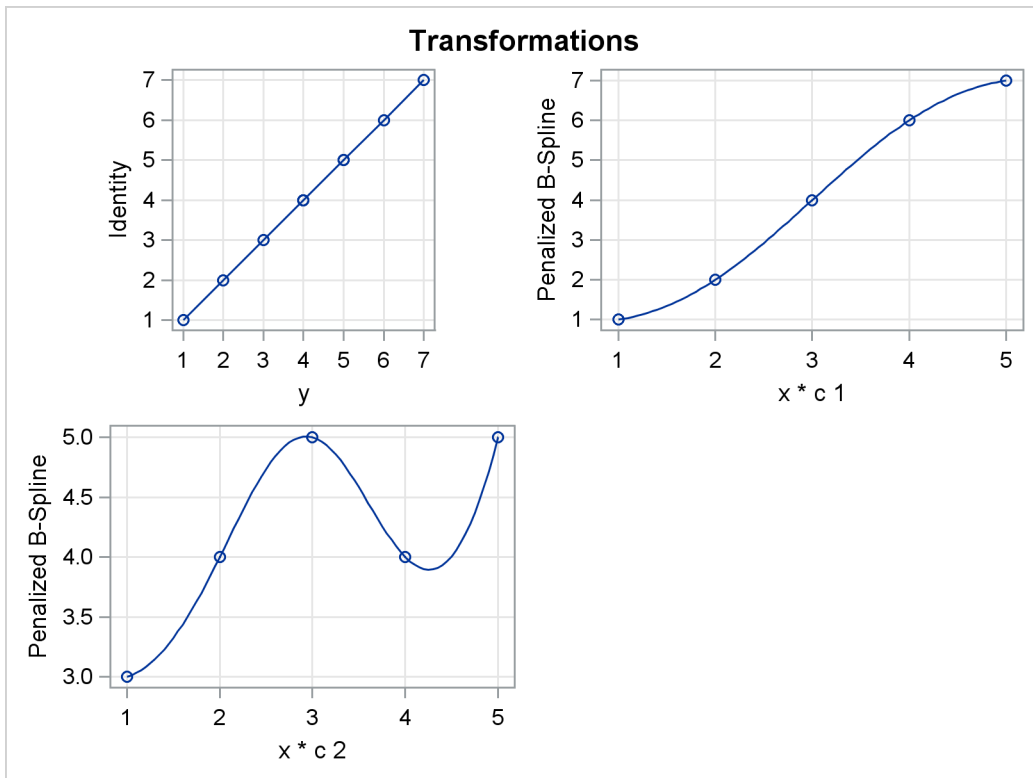
Figure 97.77 continued



**Figure 97.78** Interpolation with PLOTS(INTERPOLATE)

| Smoother Interpolation with PLOTS(INTERPOLATE)            |        |                |             |          |         |
|-----------------------------------------------------------|--------|----------------|-------------|----------|---------|
| The TRANSREG Procedure                                    |        |                |             |          |         |
| Univariate ANOVA Table, Penalized B-Spline Transformation |        |                |             |          |         |
| Source                                                    | DF     | Sum of Squares | Mean Square | F Value  | Pr > F  |
| Model                                                     | 9      | 28.90000       | 3.211111    | Infty    | <.0001  |
| Error                                                     | 12E-10 | 0.00000        | 0.000000    |          |         |
| Corrected Total                                           | 9      | 28.90000       |             |          |         |
| Root MSE                                                  |        | 0              | R-Square    | 1.0000   |         |
| Dependent Mean                                            |        | 4.10000        | Adj R-Sq    | 1.0000   |         |
| Coeff Var                                                 |        | 0              |             |          |         |
| Penalized B-Spline Transformation                         |        |                |             |          |         |
| Variable                                                  | DF     | Coefficient    | Lambda      | AICC     | Label   |
| Pbspline(xc1)                                             | 5.0000 | 1.000          | 2.642E-7    | -66.4281 | x * c 1 |
| Pbspline(xc2)                                             | 5.0000 | 1.000          | 2.516E-7    | -60.6430 | x * c 2 |

Figure 97.78 continued



## Examples: TRANSREG Procedure

### Example 97.1: Transformation Regression of Exhaust Emissions Data

In this example, the data are from an experiment in which nitrogen oxide emissions from a single cylinder engine are measured for various combinations of fuel, compression ratio, and equivalence ratio. The data are provided by Brinkman (1981). This gas data set is available from the Sashelp library.

The equivalence ratio and nitrogen oxide variables are continuous and numeric, so spline transformations of these variables are requested. The spline transformation of the dependent variable is restricted to be monotonic. Each spline is degree three with nine knots (one at each decile) in order to give PROC TRANSREG a great deal of freedom in finding transformations. The compression ratio variable has only five discrete values, so an optimal scoring is requested with monotonicity constraints. The character variable Fuel is nominal, so it is optimally scored without any monotonicity constraints. Observations with missing values are excluded with the *NOMISS a-option*.

```
ods graphics on;

title 'Gasoline Example';
title2 'Iteratively Estimate NOx, CpRatio, EqRatio, and Fuel';

* Fit the Nonparametric Model;
proc transreg data=sashelp.Gas solve test nomiss plots=all;
 ods exclude where=(_path_ ? 'MV');
 model mspline(NOx / nknots=9) = spline(EqRatio / nknots=9)
 monotone(CpRatio) opscore(Fuel);
run;
```

#### Output 97.1.1 Transformation Regression Example: The Nonparametric Model

|                                                      |     |
|------------------------------------------------------|-----|
| Gasoline Example                                     |     |
| Iteratively Estimate NOx, CpRatio, EqRatio, and Fuel |     |
| The TRANSREG Procedure                               |     |
| Dependent Variable Mspline(NOx)                      |     |
| Nitrogen Oxide                                       |     |
| Number of Observations Read                          | 171 |
| Number of Observations Used                          | 169 |

## Output 97.1.1 continued

| TRANSREG MORALS Algorithm Iteration History for Mspline(NOx) |                |                |          |                  |               |
|--------------------------------------------------------------|----------------|----------------|----------|------------------|---------------|
| Iteration Number                                             | Average Change | Maximum Change | R-Square | Criterion Change | Note          |
| 0                                                            | 0.41900        | 3.80550        | 0.05241  |                  |               |
| 1                                                            | 0.11984        | 0.83327        | 0.91028  | 0.85787          |               |
| 2                                                            | 0.03727        | 0.17688        | 0.93981  | 0.02953          |               |
| 3                                                            | 0.02795        | 0.10880        | 0.94969  | 0.00987          |               |
| 4                                                            | 0.02088        | 0.07279        | 0.95382  | 0.00413          |               |
| 5                                                            | 0.01530        | 0.05031        | 0.95582  | 0.00201          |               |
| 6                                                            | 0.01130        | 0.03922        | 0.95688  | 0.00106          |               |
| 7                                                            | 0.00852        | 0.03197        | 0.95748  | 0.00060          |               |
| 8                                                            | 0.00657        | 0.02531        | 0.95783  | 0.00035          |               |
| 9                                                            | 0.00510        | 0.01975        | 0.95805  | 0.00022          |               |
| 10                                                           | 0.00398        | 0.01534        | 0.95818  | 0.00013          |               |
| 11                                                           | 0.00314        | 0.01200        | 0.95827  | 0.00009          |               |
| 12                                                           | 0.00250        | 0.00953        | 0.95832  | 0.00005          |               |
| 13                                                           | 0.00199        | 0.00752        | 0.95836  | 0.00003          |               |
| 14                                                           | 0.00159        | 0.00594        | 0.95838  | 0.00002          |               |
| 15                                                           | 0.00127        | 0.00470        | 0.95839  | 0.00001          |               |
| 16                                                           | 0.00102        | 0.00373        | 0.95840  | 0.00001          |               |
| 17                                                           | 0.00081        | 0.00297        | 0.95841  | 0.00001          |               |
| 18                                                           | 0.00065        | 0.00237        | 0.95841  | 0.00000          |               |
| 19                                                           | 0.00052        | 0.00189        | 0.95841  | 0.00000          |               |
| 20                                                           | 0.00042        | 0.00151        | 0.95842  | 0.00000          |               |
| 21                                                           | 0.00033        | 0.00120        | 0.95842  | 0.00000          |               |
| 22                                                           | 0.00027        | 0.00096        | 0.95842  | 0.00000          |               |
| 23                                                           | 0.00021        | 0.00077        | 0.95842  | 0.00000          |               |
| 24                                                           | 0.00017        | 0.00061        | 0.95842  | 0.00000          |               |
| 25                                                           | 0.00014        | 0.00049        | 0.95842  | 0.00000          |               |
| 26                                                           | 0.00011        | 0.00039        | 0.95842  | 0.00000          |               |
| 27                                                           | 0.00009        | 0.00031        | 0.95842  | 0.00000          |               |
| 28                                                           | 0.00007        | 0.00025        | 0.95842  | 0.00000          |               |
| 29                                                           | 0.00006        | 0.00020        | 0.95842  | 0.00000          |               |
| 30                                                           | 0.00005        | 0.00016        | 0.95842  | 0.00000          | Not Converged |

WARNING: Failed to converge, however criterion change is less than 0.0001.

The TRANSREG Procedure Hypothesis Tests for Mspline(NOx)  
Nitrogen Oxide

Univariate ANOVA Table Based on the Usual Degrees of Freedom

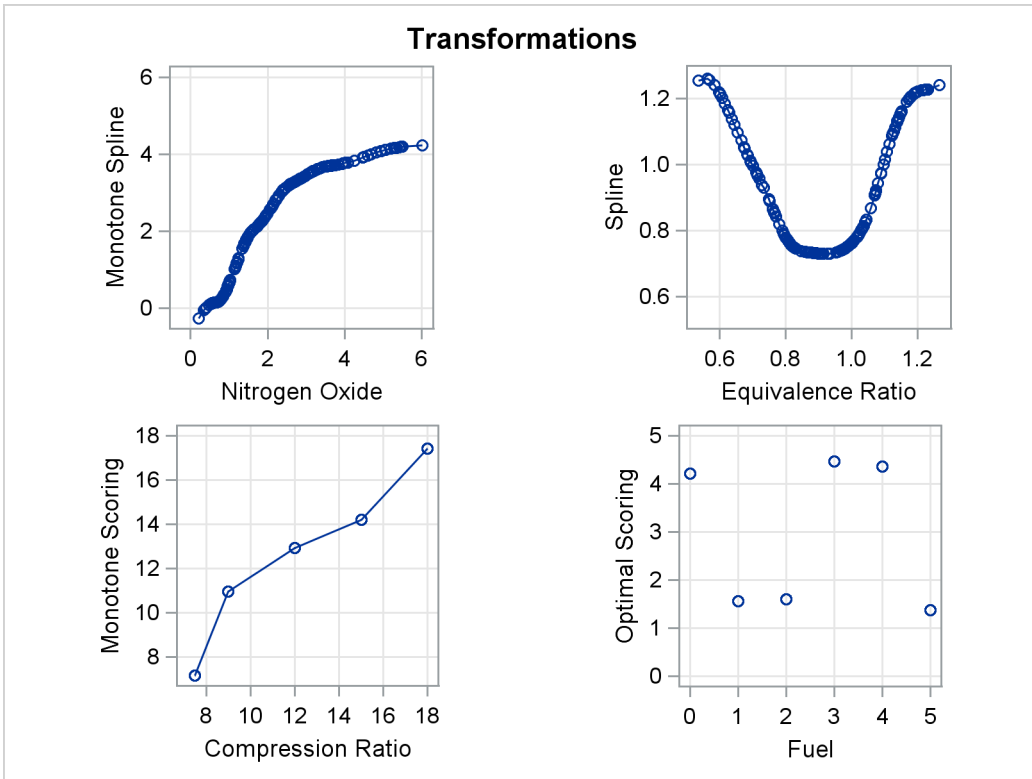
| Source          | DF  | Sum of Squares | Mean Square | F Value | Liberal p |
|-----------------|-----|----------------|-------------|---------|-----------|
| Model           | 21  | 326.0176       | 15.52465    | 161.35  | >= <.0001 |
| Error           | 147 | 14.1443        | 0.09622     |         |           |
| Corrected Total | 168 | 340.1619       |             |         |           |

The above statistics are not adjusted for the fact that the dependent variable was transformed and so are generally liberal.

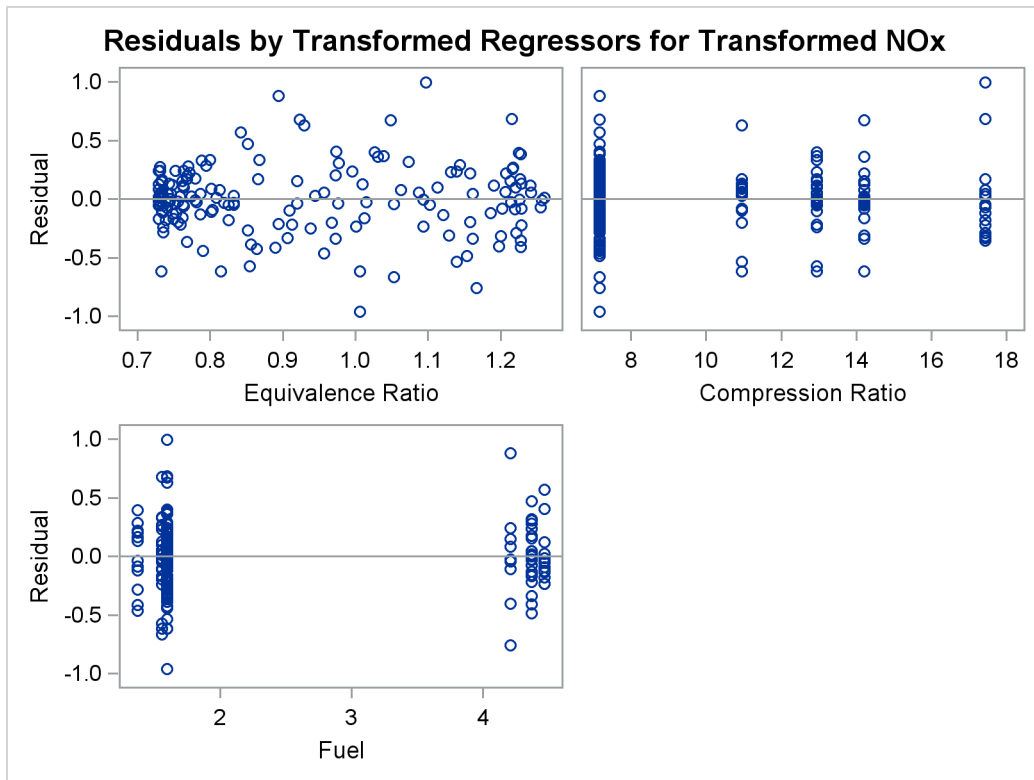
**Output 97.1.1** continued

|                |          |          |        |
|----------------|----------|----------|--------|
| Root MSE       | 0.31019  | R-Square | 0.9584 |
| Dependent Mean | 2.34593  | Adj R-Sq | 0.9525 |
| Coeff Var      | 13.22262 |          |        |

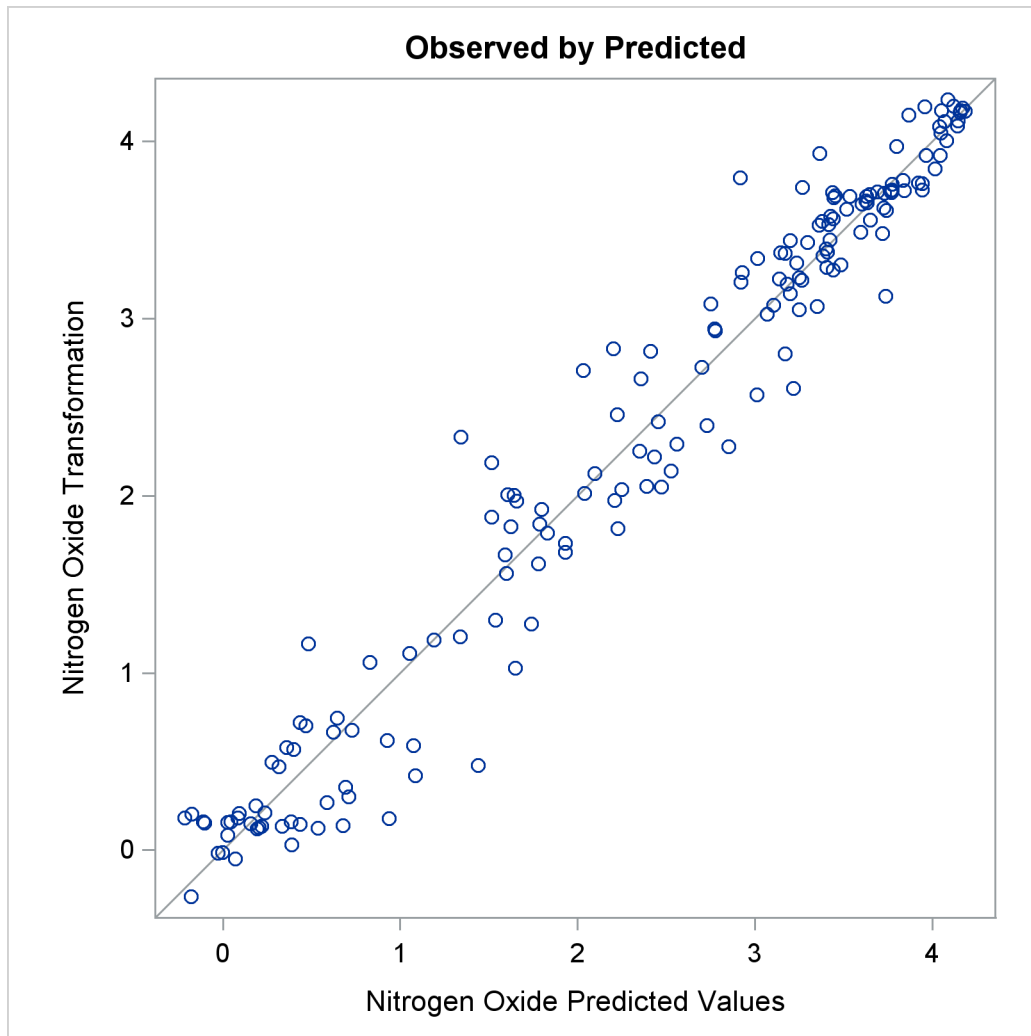
**Output 97.1.1** continued



Output 97.1.1 continued



## Output 97.1.1 continued



The squared multiple correlation for the initial model is approximately 0.05. PROC TRANSREG increases the R square to over 0.95 by transforming the variables. The transformation plots show how each variable is transformed. The transformation of compression ratio (TCpRatio) is nearly linear. The transformation of equivalence ratio (TEqRatio) is nearly parabolic. It can be seen from this plot that the optimal transformation of equivalence ratio is nearly uncorrelated with the original scoring. This suggests that the large increase in R square is due to this transformation. The transformation of nitrogen oxide (TNOx) is similar to a log transformation. The final plot shows the transformed dependent variable plotted as a function of the predicted values. This plot is reasonably linear, showing that the nonlinearities in the data are being accounted for fairly well by the TRANSREG model.

These results suggest the parametric model



$$\log(\text{NOx}) = b_0 + b_1 \times \text{EqRatio} + b_2 \times \text{EqRatio}^2 + b_3 \times \text{CpRatio} \\ + \sum_j b_j \text{class}_j(\text{Fuel}) + \text{error}$$

You can perform this analysis with PROC TRANSREG. The following statements produce [Output 97.1.2](#):

```

title2 'Now fit log(NOx) = b0 + b1*EqRatio + b2*EqRatio**2 +';
title3 'b3*CpRatio + Sum b(j)*Fuel(j) + Error';

*-Fit the Parametric Model Suggested by the Nonparametric Analysis-;
proc transreg data=sashelp.Gas solve ss2 short nomiss plots=all;
 model log(NOx) = pspline(EqRatio / deg=2) identity(CpRatio)
 opscore(Fuel);
run;

```

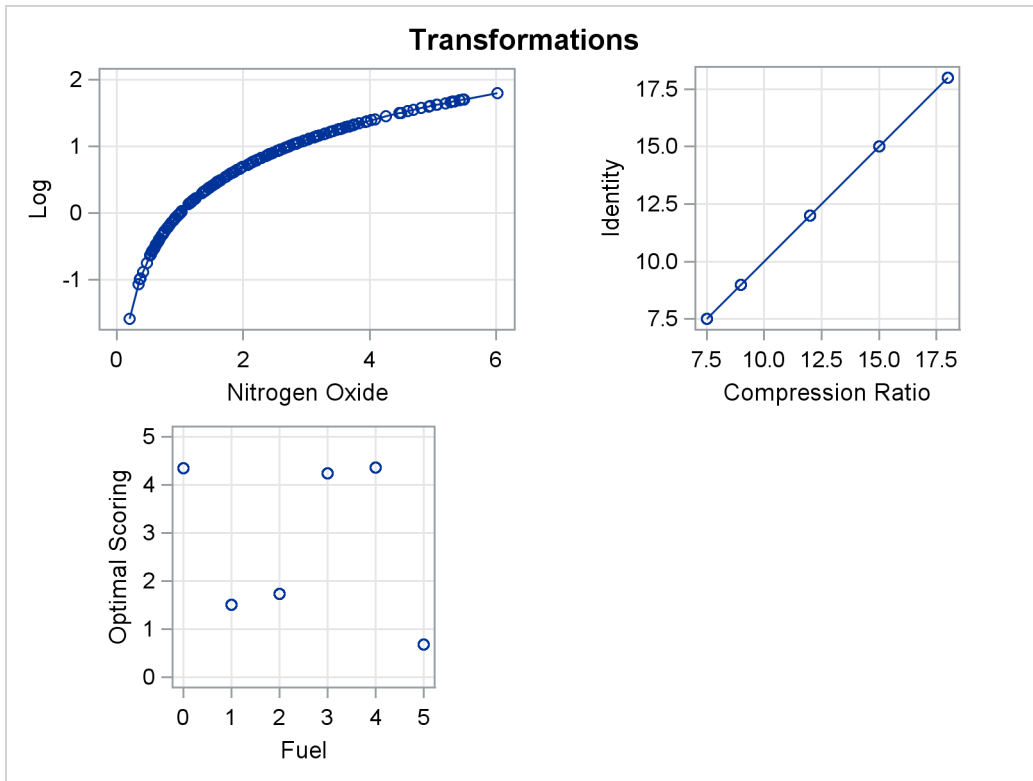
**Output 97.1.2** Transformation Regression Example: The Parametric Model

|                                                              |     |                |             |         |        |
|--------------------------------------------------------------|-----|----------------|-------------|---------|--------|
| Gasoline Example                                             |     |                |             |         |        |
| Now fit log(NOx) = b0 + b1*EqRatio + b2*EqRatio**2 +         |     |                |             |         |        |
| b3*CpRatio + Sum b(j)*Fuel(j) + Error                        |     |                |             |         |        |
| The TRANSREG Procedure                                       |     |                |             |         |        |
| Dependent Variable Log(NOx)                                  |     |                |             |         |        |
| Nitrogen Oxide                                               |     |                |             |         |        |
|                                                              |     |                |             |         |        |
| Number of Observations Read                                  |     |                |             |         |        |
| 171                                                          |     |                |             |         |        |
| Number of Observations Used                                  |     |                |             |         |        |
| 169                                                          |     |                |             |         |        |
|                                                              |     |                |             |         |        |
| Log(NOx)                                                     |     |                |             |         |        |
| Algorithm converged.                                         |     |                |             |         |        |
|                                                              |     |                |             |         |        |
| The TRANSREG Procedure Hypothesis Tests for Log(NOx)         |     |                |             |         |        |
| Nitrogen Oxide                                               |     |                |             |         |        |
|                                                              |     |                |             |         |        |
| Univariate ANOVA Table Based on the Usual Degrees of Freedom |     |                |             |         |        |
| Source                                                       | DF  | Sum of Squares | Mean Square | F Value | Pr > F |
| Model                                                        | 8   | 79.33838       | 9.917298    | 213.09  | <.0001 |
| Error                                                        | 160 | 7.44659        | 0.046541    |         |        |
| Corrected Total                                              | 168 | 86.78498       |             |         |        |
|                                                              |     |                |             |         |        |
| Root MSE                                                     |     | 0.21573        | R-Square    | 0.9142  |        |
| Dependent Mean                                               |     | 0.63130        | Adj R-Sq    | 0.9099  |        |
| Coeff Var                                                    |     | 34.17294       |             |         |        |

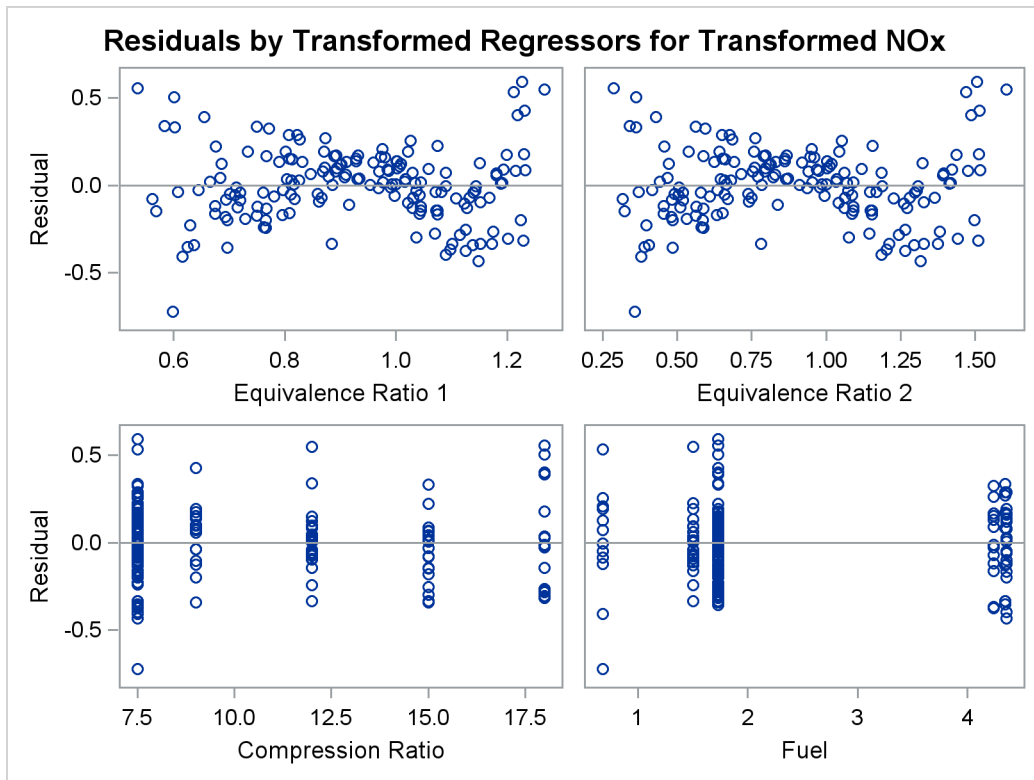
Output 97.1.2 continued

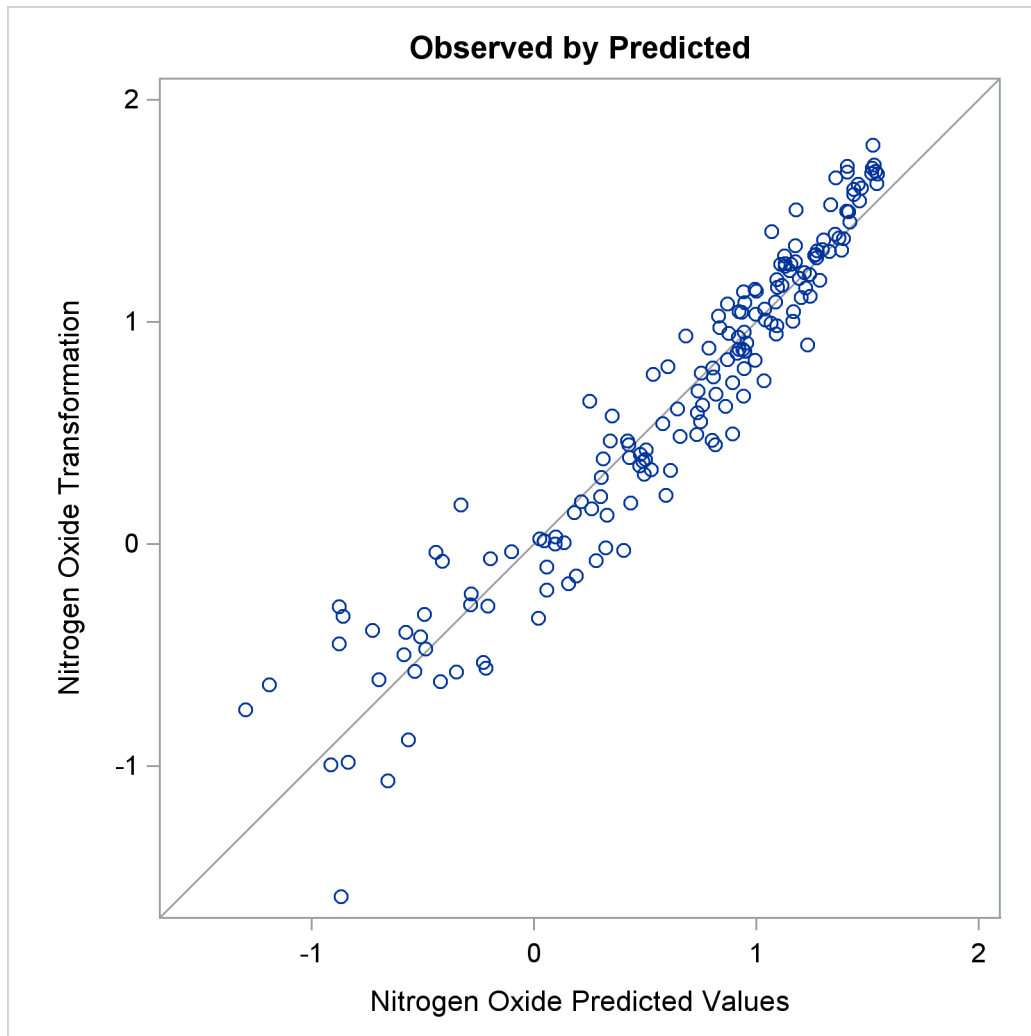
| Univariate Regression Table Based on the Usual Degrees of Freedom |    |             |                |             |         |        |                     |
|-------------------------------------------------------------------|----|-------------|----------------|-------------|---------|--------|---------------------|
| Variable                                                          | DF | Coefficient | Type II        |             | F Value | Pr > F | Label               |
|                                                                   |    |             | Sum of Squares | Mean Square |         |        |                     |
| Intercept                                                         | 1  | -15.274649  | 57.1338        | 57.1338     | 1227.60 | <.0001 | Intercept           |
| Pspline.EqRatio_1                                                 | 1  | 35.102914   | 62.7478        | 62.7478     | 1348.22 | <.0001 | Equivalence Ratio 1 |
| Pspline.EqRatio_2                                                 | 1  | -19.386468  | 64.6430        | 64.6430     | 1388.94 | <.0001 | Equivalence Ratio 2 |
| Identity(CpRatio)                                                 | 1  | 0.032058    | 1.4445         | 1.4445      | 31.04   | <.0001 | Compression Ratio   |
| Opscore(Fuel)                                                     | 5  | 0.158388    | 5.5619         | 1.1124      | 23.90   | <.0001 | Fuel                |

Output 97.1.2 continued



Output 97.1.2 continued



Output 97.1.2 *continued*

The **LOG** transformation computes the natural log. The **PSPLINE** expansion expands EqRatio into a linear term, EqRatio, and a squared term, EqRatio<sup>2</sup>. An identity transformation of CpRatio and an optimal scoring of Fuel is requested. These should provide a good parametric operationalization of the optimal transformations. The final model has an R square of 0.91 (smaller than before since the model has fewer parameters, but still quite good).

---

## Example 97.2: Box-Cox Transformations

This example shows Box-Cox transformations with a yarn failure data set. For more information about Box-Cox transformations, including using a Box-Cox transformation in a model with no independent variable, to normalize the distribution of the data, see the section “Box-Cox Transformations” on page 8222. In this example, a simple 3<sup>3</sup> design was used to study the effects of different factors on the failure of a yarn manufacturing process. The design factors are as follows:

- the length of test specimens of yarn, with levels of 250, 300, and 350 mm
- the amplitude of the loading cycle, with levels of 8, 9, and 10 mmd
- the load with levels of 40, 45, and 50 grams

The measured response was time (in cycles) until failure. However, you could just as well have measured the inverse of time until failure (in other words, the failure rate). Hence, the correct metric with which to analyze the response is not apparent. You can use PROC TRANSREG to find an optimum power transformation for the analysis. The following statements create the input SAS data set:

```

title 'Yarn Strength';

proc format;
 value a -1 = 8 0 = 9 1 = 10;
 value l -1 = 250 0 = 300 1 = 350;
 value o -1 = 40 0 = 45 1 = 50;
run;

data yarn;
 input Fail Amplitude Length Load @@;
 format amplitude a. length l. load o.;
 label fail = 'Time in Cycles until Failure';
 datalines;
674 -1 -1 -1 370 -1 -1 0 292 -1 -1 1 338 0 -1 -1
266 0 -1 0 210 0 -1 1 170 1 -1 -1 118 1 -1 0
 90 1 -1 1 1414 -1 0 -1 1198 -1 0 0 634 -1 0 1
1022 0 0 -1 620 0 0 0 438 0 0 1 442 1 0 -1
332 1 0 0 220 1 0 1 3636 -1 1 -1 3184 -1 1 0
2000 -1 1 1 1568 0 1 -1 1070 0 1 0 566 0 1 1
1140 1 1 -1 884 1 1 0 360 1 1 1
;

```

PROC TRANSREG is run to find the Box-Cox transformation. The lambda list is  $-2$  TO  $2$  BY  $0.05$ , which produces 81 lambdas, and a convenient lambda is requested. This many power parameters makes a nice graphical display with plenty of detail around the confidence interval. In the interest of space, only part of this table is displayed. The independent variables are designated with the QPOINT expansion. QPOINT, for quadratic point model, gets its name from PROC TRANSREG's ideal point modeling capabilities, which process variables for a response surface analysis. What QPOINT does is create a set of independent variables consisting of the following: the  $m$  original variables (Length Amplitude Load), the  $m$  original variables squared (Length\_2 Amplitude\_2 Load\_2), and the  $m \times (m - 1)/2 = 3$  pairs of products between the  $m$  variables (LengthAmplitude LengthLoad AmplitudeLoad). The following statements produce Output 97.2.1:

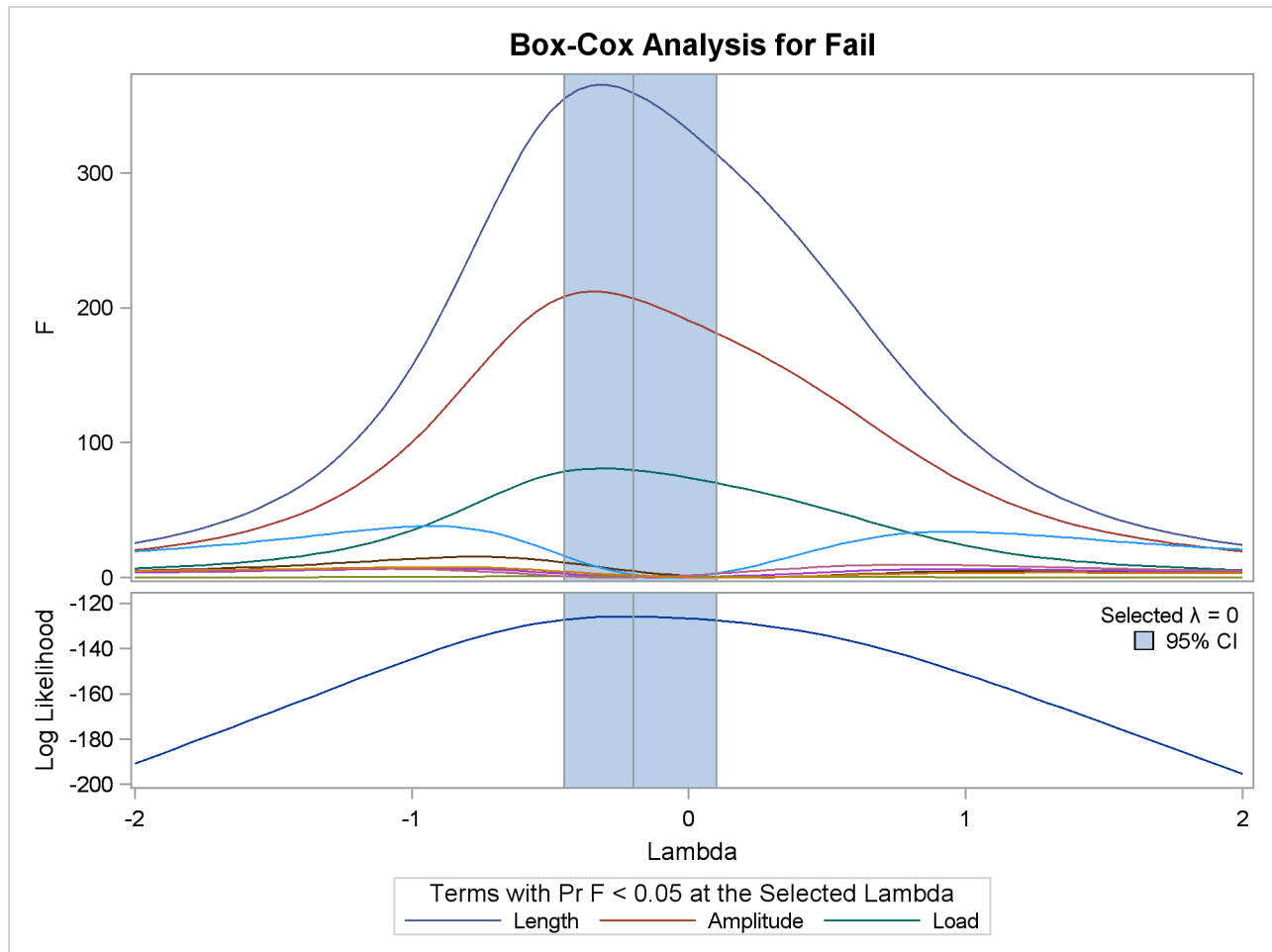
```

ods graphics on;

proc transreg details data=yarn ss2
 plots=(transformation(dependent) obp);
 model BoxCox(fail / convenient lambda=-2 to 2 by 0.05) =
 qpoint(length amplitude load);
run;

```

Output 97.2.1 Box-Cox Yarn Data



Output 97.2.1 continued

```

Dependent Variable BoxCox(Fail)
Time in Cycles until Failure

Number of Observations Read 27
Number of Observations Used 27

```

## Output 97.2.1 continued

| Model Statement Specification Details                                                                                               |    |                        |                 |                              |           |
|-------------------------------------------------------------------------------------------------------------------------------------|----|------------------------|-----------------|------------------------------|-----------|
| Type                                                                                                                                | DF | Variable               | Description     | Value                        |           |
| Dep                                                                                                                                 | 1  | BoxCox(Fail)           | Lambda Used     | 0                            |           |
|                                                                                                                                     |    |                        | Lambda          | -0.2                         |           |
|                                                                                                                                     |    |                        | Log Likelihood  | -125.9                       |           |
|                                                                                                                                     |    |                        | Conv. Lambda    | 0                            |           |
|                                                                                                                                     |    |                        | Conv. Lambda LL | -126.7                       |           |
|                                                                                                                                     |    |                        | CI Limit        | -127.8                       |           |
|                                                                                                                                     |    |                        | Alpha           | 0.05                         |           |
|                                                                                                                                     |    |                        | Options         | Convenient Lambda Used       |           |
|                                                                                                                                     |    |                        | Label           | Time in Cycles until Failure |           |
| Ind                                                                                                                                 | 1  | Qpoint.Length          | DF              | 1                            |           |
| Ind                                                                                                                                 | 1  | Qpoint.Amplitude       | DF              | 1                            |           |
| Ind                                                                                                                                 | 1  | Qpoint.Load            | DF              | 1                            |           |
| Ind                                                                                                                                 | 1  | Qpoint.Length_2        | DF              | 1                            |           |
| Ind                                                                                                                                 | 1  | Qpoint.Amplitude_2     | DF              | 1                            |           |
| Ind                                                                                                                                 | 1  | Qpoint.Load_2          | DF              | 1                            |           |
| Ind                                                                                                                                 | 1  | Qpoint.LengthAmplitude | DF              | 1                            |           |
| Ind                                                                                                                                 | 1  | Qpoint.LengthLoad      | DF              | 1                            |           |
| Ind                                                                                                                                 | 1  | Qpoint.AmplitudeLoad   | DF              | 1                            |           |
| <p>The TRANSREG Procedure Hypothesis Tests for BoxCox(Fail)<br/>Time in Cycles until Failure</p>                                    |    |                        |                 |                              |           |
| <p>Univariate ANOVA Table Based on the Usual Degrees of Freedom</p>                                                                 |    |                        |                 |                              |           |
| Source                                                                                                                              | DF | Sum of Squares         | Mean Square     | F Value                      | Liberal p |
| Model                                                                                                                               | 9  | 22.56498               | 2.507220        | 66.73                        | >= <.0001 |
| Error                                                                                                                               | 17 | 0.63871                | 0.037571        |                              |           |
| Corrected Total                                                                                                                     | 26 | 23.20369               |                 |                              |           |
| <p>The above statistics are not adjusted for the fact that the dependent variable was transformed and so are generally liberal.</p> |    |                        |                 |                              |           |
| Root MSE                                                                                                                            |    | 0.19383                | R-Square        | 0.9725                       |           |
| Dependent Mean                                                                                                                      |    | 6.33466                | Adj R-Sq        | 0.9579                       |           |
| Coeff Var                                                                                                                           |    | 3.05987                | Lambda          | 0.0000                       |           |

Output 97.2.1 continued

Univariate Regression Table Based on the Usual Degrees of Freedom

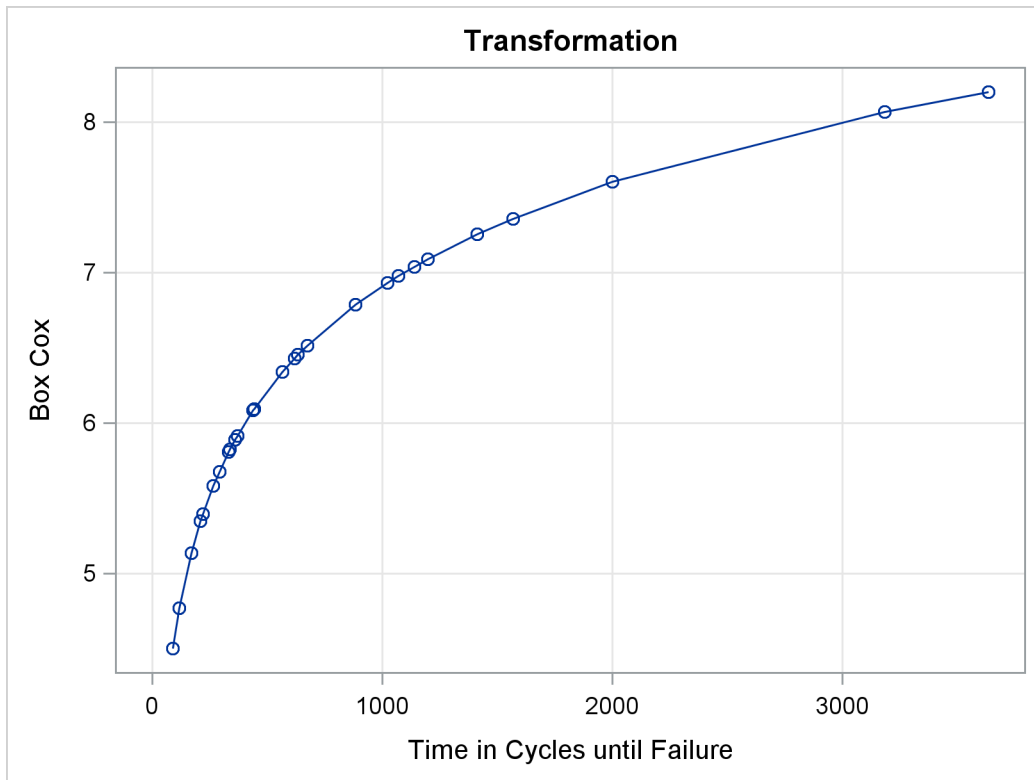
| Variable               | DF | Coefficient | Type II<br>Sum of<br>Squares | Mean<br>Square | F Value | Liberal p |
|------------------------|----|-------------|------------------------------|----------------|---------|-----------|
| Intercept              | 1  | 6.4206207   | 159.008                      | 159.008        | 4232.19 | >= <.0001 |
| Qpoint.Length          | 1  | 0.8323842   | 12.472                       | 12.472         | 331.94  | >= <.0001 |
| Qpoint.Amplitude       | 1  | -0.6309916  | 7.167                        | 7.167          | 190.75  | >= <.0001 |
| Qpoint.Load            | 1  | -0.3924940  | 2.773                        | 2.773          | 73.80   | >= <.0001 |
| Qpoint.Length_2        | 1  | -0.0856974  | 0.044                        | 0.044          | 1.17    | >= 0.2939 |
| Qpoint.Amplitude_2     | 1  | 0.0242183   | 0.004                        | 0.004          | 0.09    | >= 0.7633 |
| Qpoint.Load_2          | 1  | -0.0674555  | 0.027                        | 0.027          | 0.73    | >= 0.4058 |
| Qpoint.LengthAmplitude | 1  | -0.0382414  | 0.018                        | 0.018          | 0.47    | >= 0.5035 |
| Qpoint.LengthLoad      | 1  | -0.0684146  | 0.056                        | 0.056          | 1.49    | >= 0.2381 |
| Qpoint.AmplitudeLoad   | 1  | -0.0208340  | 0.005                        | 0.005          | 0.14    | >= 0.7142 |

| Variable               | DF | Label           |
|------------------------|----|-----------------|
| Intercept              | 1  | Intercept       |
| Qpoint.Length          | 1  | Length          |
| Qpoint.Amplitude       | 1  | Amplitude       |
| Qpoint.Load            | 1  | Load            |
| Qpoint.Length_2        | 1  | Length_2        |
| Qpoint.Amplitude_2     | 1  | Amplitude_2     |
| Qpoint.Load_2          | 1  | Load_2          |
| Qpoint.LengthAmplitude | 1  | LengthAmplitude |
| Qpoint.LengthLoad      | 1  | LengthLoad      |
| Qpoint.AmplitudeLoad   | 1  | AmplitudeLoad   |

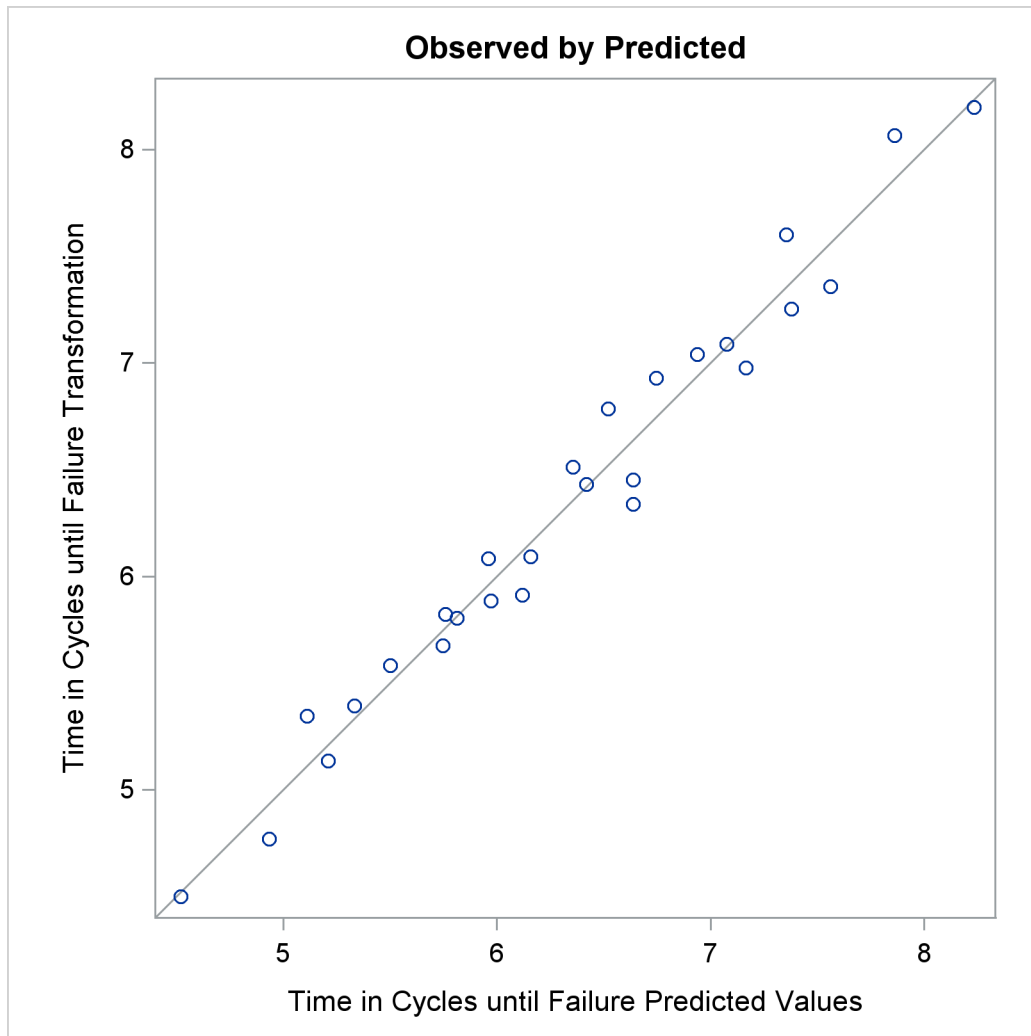
The above statistics are not adjusted for the fact that the dependent variable was transformed and so are generally liberal.



Output 97.2.1 continued



## Output 97.2.1 continued



The optimal power parameter is  $-0.20$ , but since  $0.0$  is in the confidence interval, and since the **CONVE-NIENT** *t-option* was specified, the procedure chooses a log transformation. The  $F = t^2$  plot shows in the vicinity of the optimal Box-Cox transformation, the parameters for the three original variables (Length Amplitude Load), particularly Length, are significant and the others become essentially zero.

### Example 97.3: Penalized B-Spline

The ENSO data set contains measurements of monthly averaged atmospheric pressure differences between Easter Island and Darwin, Australia, for a period of 168 months (National Institute of Standards and Technology 1998). The ENSO data set is available from the Sashelp library.

You can fit a curve through these data by using a penalized B-spline (Eilers and Marx 1996) function and the following statements:

```

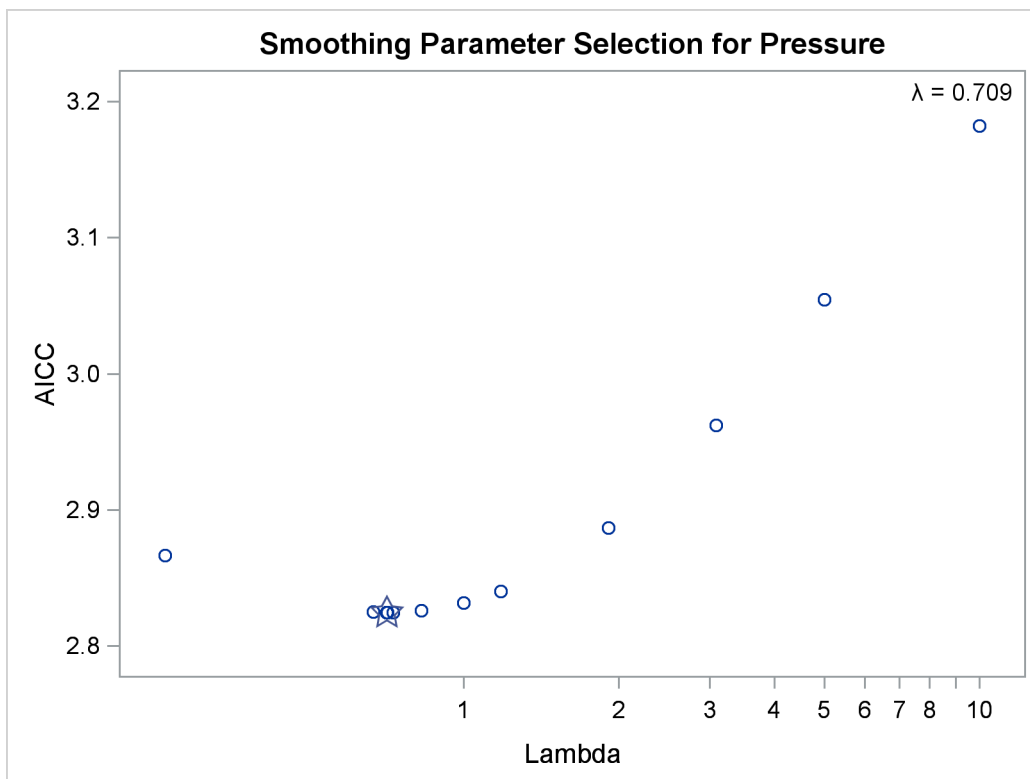
title 'Atmospheric Pressure Changes Between'
 'Easter Island & Darwin, Australia';
ods graphics on;

proc transreg data=sashelp.enso;
 model identity(pressure) = pbspline(year);
run;

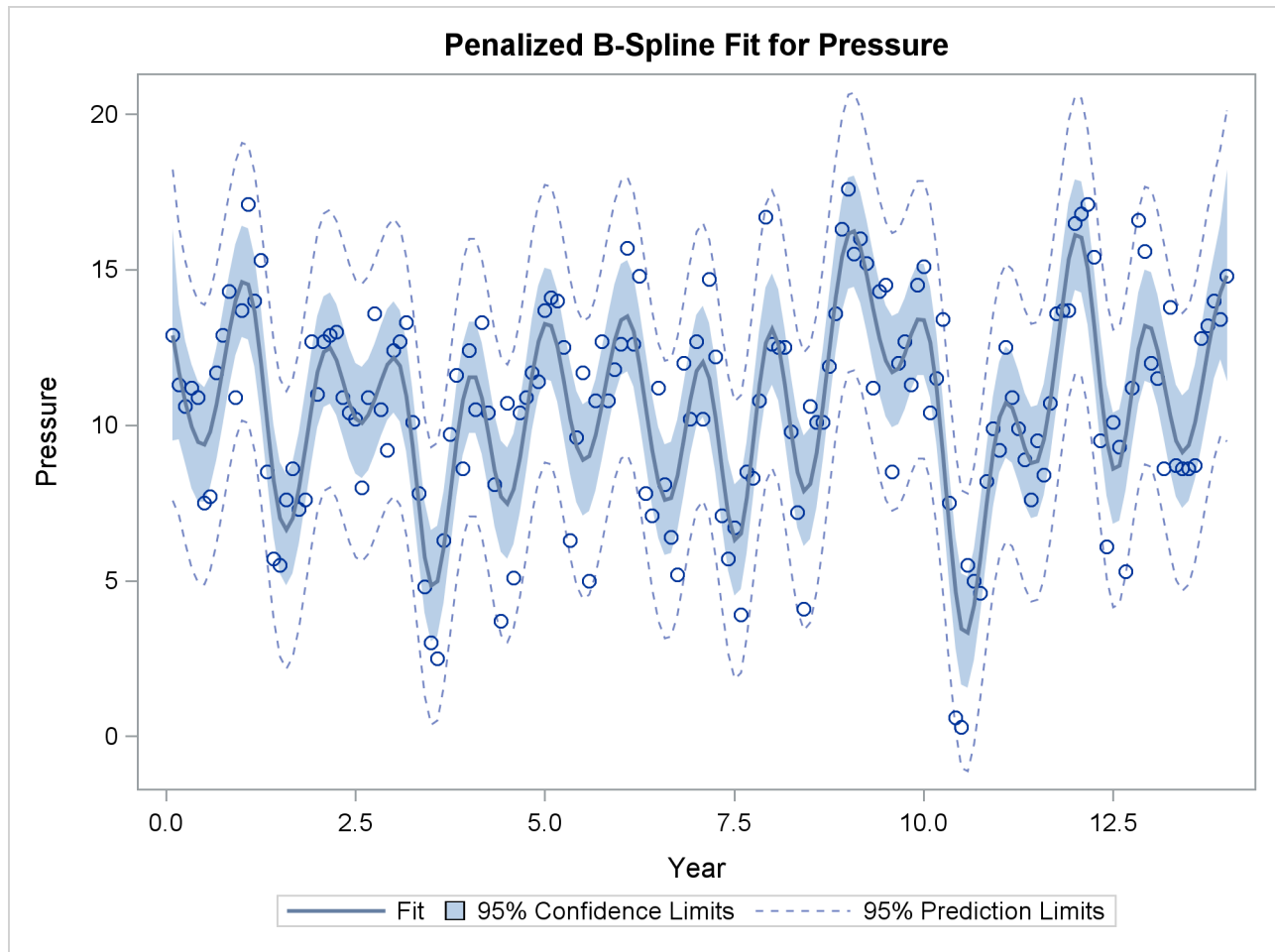
```

The dependent variable Pressure is specified along with an **IDENTITY** transformation, so Pressure is analyzed as is, with no transformations. The independent variable Year is specified with a **PBSPLINE** transformation, so a penalized B-spline model is fit. By default, a **DEGREE=3** B-spline basis is used along with 100 evenly spaced knots and three evenly spaced exterior knots on each side of the data. The penalized spline function is typically much smoother than you would get by using a **SPLINE** transformation or a **BSPLINE** expansion since changes in the coefficients of the basis are penalized to make a smoother fit. The output is shown next in [Output 97.3.1](#).

**Output 97.3.1** Change in Atmospheric Pressure, AICC



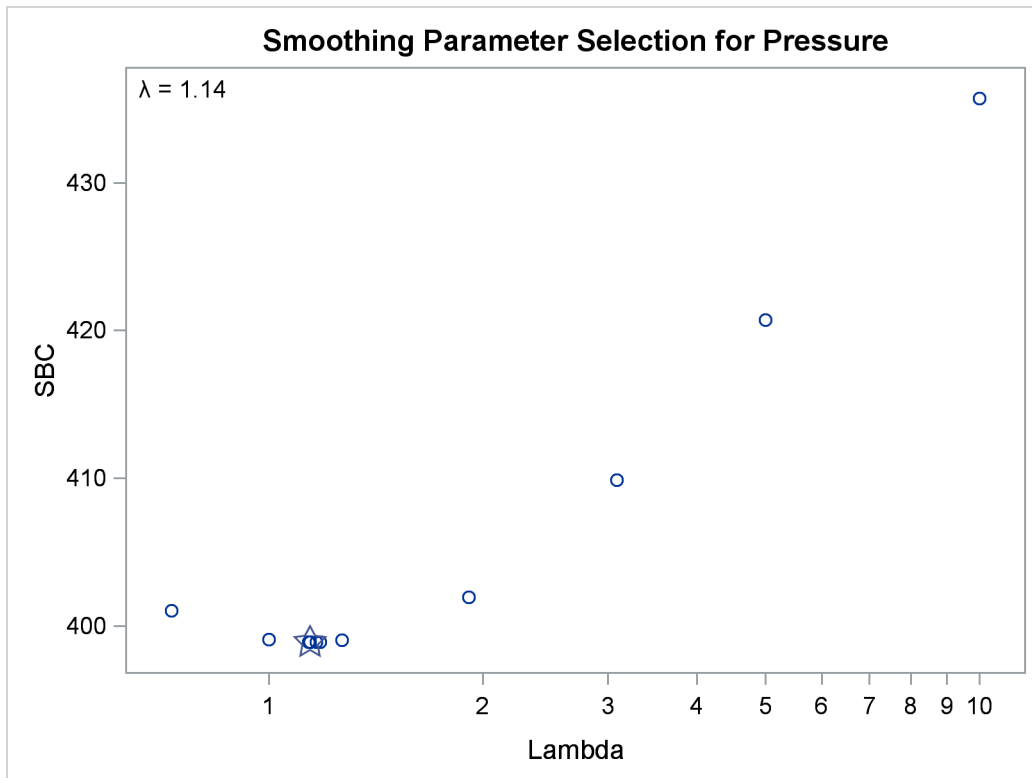
Output 97.3.1 continued



The results show a yearly cycle of pressure change. The procedure chose a smoothing parameter of  $\lambda = 0.709$ . With data such as these, with many peaks and valleys, it might be useful to perform another analysis, this time asking for a smoother plot. The Schwarz Bayesian criterion (SBC) is sometimes a better choice than the default criterion when you want a smoother plot. The following PROC TRANSREG step requests a penalized B-spline analysis minimizing the SBC criterion:

```
proc transreg data=sashelp.enso;
 model identity(pressure) = pbspline(year / sbc);
run;
```

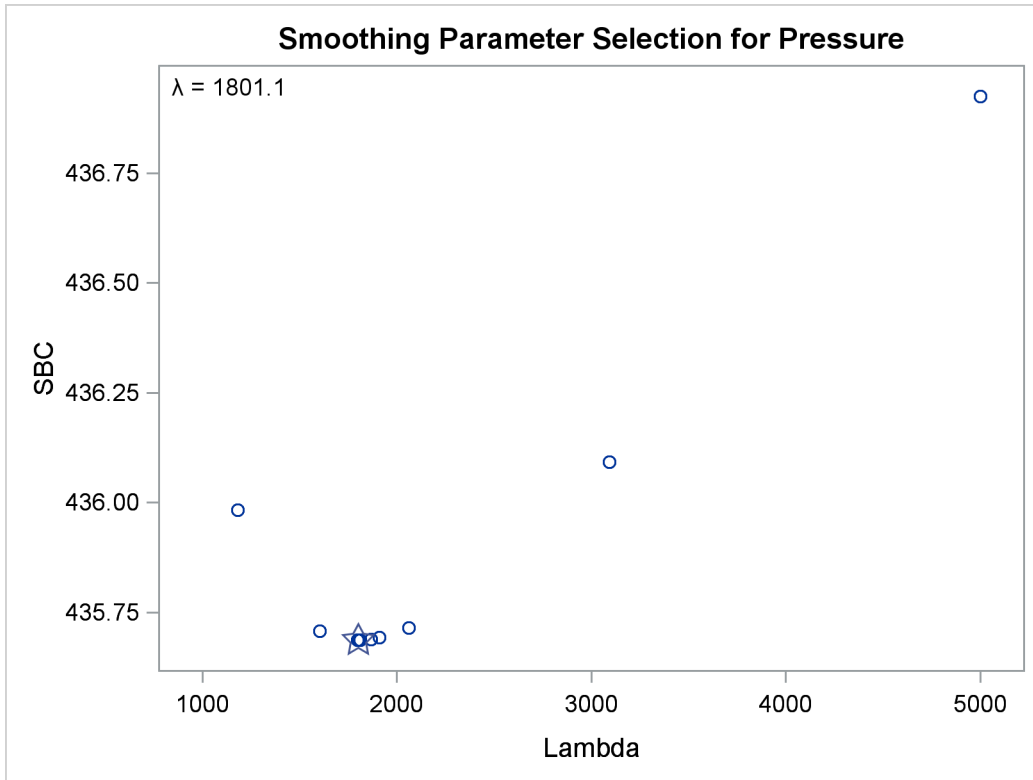
The plot of SBC as a function of  $\lambda$  is shown in [Output 97.3.2](#).

**Output 97.3.2** Change in Atmospheric Pressure, SBC

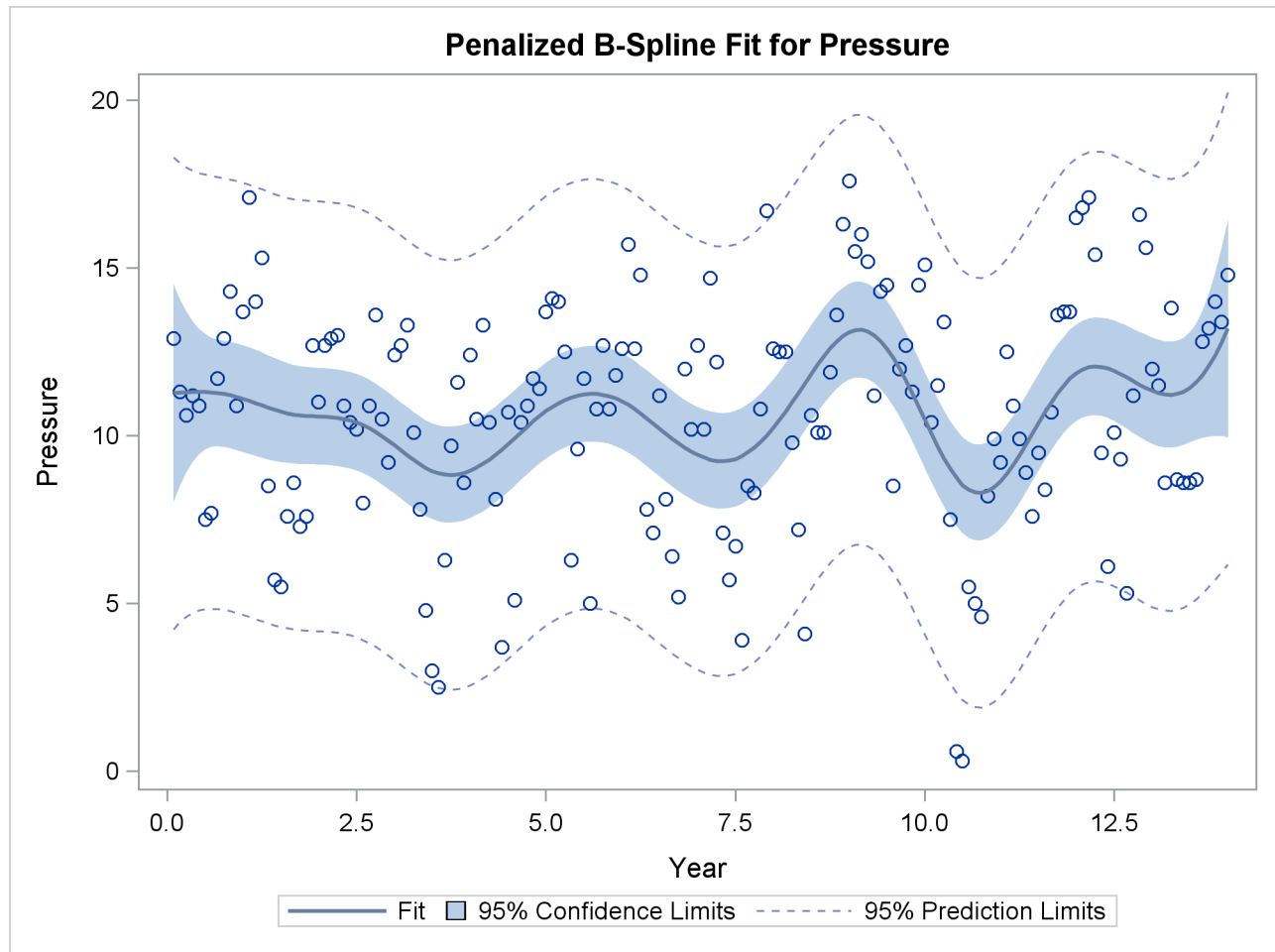
The fit plot (not shown) is essentially the same as the one shown in [Output 97.3.1](#) due to the similar choice of smoothing parameters:  $\lambda = 0.709$  versus  $\lambda = 1.14$ . You can analyze these data again, this time forcing PROC TRANSREG to consider only larger smoothing parameters. The specification `LAMBDA=2 10000 RANGE` eliminates from consideration the two lambdas that you previously saw and considers only  $2 \leq \lambda \leq 10,000$ . The following statements produce [Output 97.3.3](#):

```
proc transreg data=sashelp.enso;
 model identity(pressure) = pbspline(year / sbc lambda=2 10000 range);
run;
```

**Output 97.3.3** Change in Atmospheric Pressure, SBC, Lambda > 1



Output 97.3.3 continued

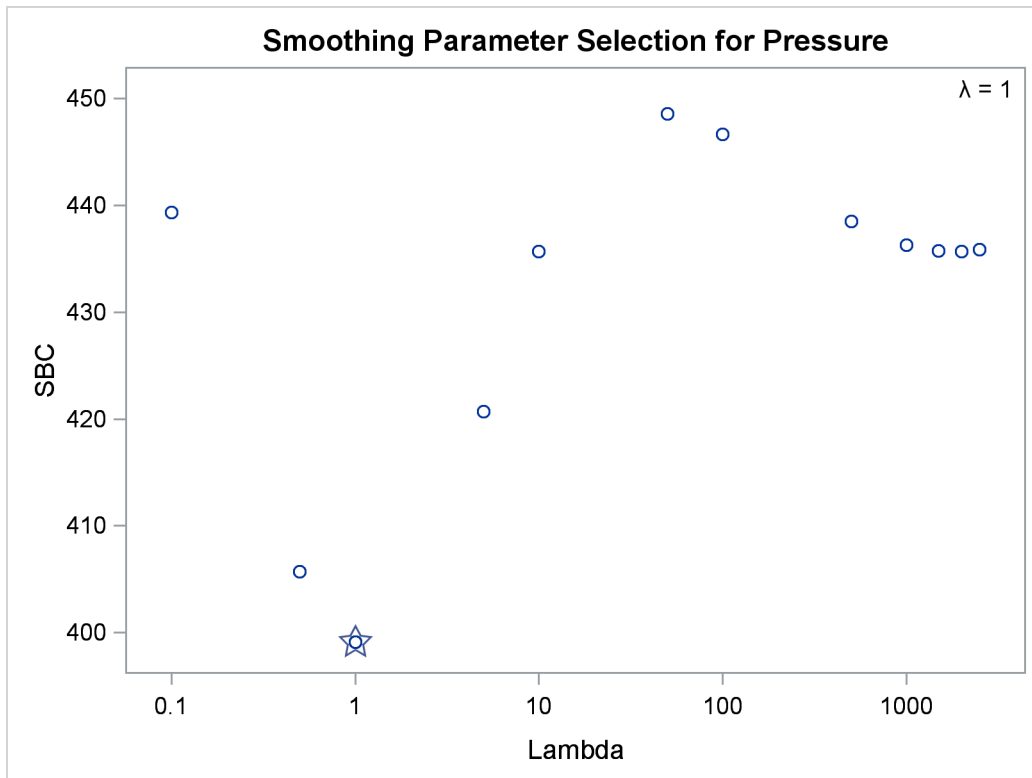


The results clearly show that there is a local minimum in the  $SBC(\lambda)$  function at  $\lambda = 1801.1$ . Using this lambda results in a much smoother regression function with a longer cycle than you saw previously. This second cycle can be identified as the periodic warming of the Pacific Ocean known as “El Niño.” The  $SBC(\lambda)$  function has at least two minima since there are at least two trends in the data. In the first analysis, PROC TRANSREG found what is probably the globally optimal solution, and in the second set of analyses, with a little nudging away from the global optimum, it found a very interesting locally optimal solution.

You can specify a list of lambdas to see SBC as a function of lambda over the range that includes both minima as follows:

```
proc transreg data=sashelp.enso;
 model identity(pressure) = pbspline(year / sbc lambda=.1 .5 1 5
 10 50 100 500 to 2500 by 500);
run;
```

The plot of SBC as a function of  $\lambda$  is shown in Output 97.3.4.

**Output 97.3.4** Change in Atmospheric Pressure, SBC, Over the Range of Both Minima

### Example 97.4: Nonmetric Conjoint Analysis of Tire Data

This example uses PROC TRANSREG to perform a nonmetric conjoint analysis of tire preference data. Conjoint analysis decomposes rank-ordered evaluation judgments of products or services into components based on qualitative product attributes. For each level of each attribute of interest, a numerical “part-worth utility” value is computed. The sum of the part-worth utilities for each product is an estimate of the utility for that product. The goal is to compute part-worth utilities such that the product utilities are as similar as possible to the original rank ordering. (This example is a greatly simplified introductory example.)

The stimuli for the experiment are 18 hypothetical tires. The stimuli represent different brands (Goodstone, Pirogi, Machismo),<sup>1</sup> prices (\$69.99, \$74.99, \$79.99), expected tread life (50,000, 60,000, 70,000 miles), and road hazard insurance plans (Yes, No). There are  $3 \times 3 \times 3 \times 2 = 54$  possible combinations. From these, 18 combinations are selected that form an efficient experimental design for a main-effects model. The combinations are then ranked from 1 (most preferred) to 18 (least preferred). In this simple example, there is one set of rankings. A real conjoint study would have many more.

First, the FORMAT procedure is used to specify the meanings of the factor levels, which are entered as numbers in the DATA step along with the ranks. PROC TRANSREG is used to perform the conjoint analysis. A maximum of 50 iterations is requested. The specification `monotone(Rank / reflect)` in the MODEL statement requests that the dependent variable Rank should be monotonically transformed and reflected so that positive utilities mean high preference. The variables Brand, Price, Life, and Hazard are

<sup>1</sup>In real conjoint experiments, real brand names would be used.



designated as **CLASS** variables, and the part-worth utilities are constrained by **ZERO=SUM** to sum to zero within each factor. The **UTILITIES** *a-option* displays the conjoint analysis results.

The importance column of the utilities table shows that price is the most important attribute in determining preference (57%), followed by expected tread life (18%), brand (15%), and road hazard insurance (10%). Looking at the utilities table for the maximum part-worth utility within each attribute, you see from the results that the most preferred combination is Pirogi brand tires, at \$69.99, with a 70,000-mile expected tread life and road hazard insurance. This product is not actually in the data set. The sum of the part-worth utilities for this combination is as follows:

$$20.64 = 9.50 + 1.90 + 5.87 + 2.41 + 0.96$$

The following statements produce [Output 97.4.1](#).

```

title 'Nonmetric Conjoint Analysis of Ranks';

proc format;
 value BrandF
 1 = 'Goodstone'
 2 = 'Pirogi '
 3 = 'Machismo ';
 value PriceF
 1 = '$69.99'
 2 = '$74.99'
 3 = '$79.99';
 value LifeF
 1 = '50,000'
 2 = '60,000'
 3 = '70,000';
 value HazardF
 1 = 'Yes'
 2 = 'No ';
run;

```

```

data Tires;
 input Brand Price Life Hazard Rank;
 format Brand BrandF9. Price PriceF9. Life LifeF6. Hazard HazardF3.;
 datalines;
1 1 2 1 3
1 1 3 2 2
1 2 1 2 14
1 2 2 2 10
1 3 1 1 17
1 3 3 1 12
2 1 1 2 7
2 1 3 2 1
2 2 1 1 8
2 2 3 1 5
2 3 2 1 13
2 3 2 2 16
3 1 1 1 6
3 1 2 1 4
3 2 2 2 15
3 2 3 1 9
3 3 1 2 18
3 3 3 2 11
;

proc transreg maxiter=50 utilities short;
 ods select TestsNote ConvergenceStatus FitStatistics Utilities;
 model monotone(Rank / reflect) =
 class(Brand Price Life Hazard / zero=sum);
 output ireplace predicted;
run;

proc print label;
 var Rank TRank PRank Brand Price Life Hazard;
 label PRank = 'Predicted Ranks';
run;

```

### Output 97.4.1 Simple Conjoint Analysis

| Nonmetric Conjoint Analysis of Ranks                       |         |          |        |
|------------------------------------------------------------|---------|----------|--------|
| The TRANSREG Procedure                                     |         |          |        |
| Monotone(Rank)                                             |         |          |        |
| Algorithm converged.                                       |         |          |        |
| The TRANSREG Procedure Hypothesis Tests for Monotone(Rank) |         |          |        |
| Root MSE                                                   | 0.49759 | R-Square | 0.9949 |
| Dependent Mean                                             | 9.50000 | Adj R-Sq | 0.9913 |
| Coeff Var                                                  | 5.23783 |          |        |

## Output 97.4.1 continued

| Utilities Table Based on the Usual Degrees of Freedom |         |                |                              |                      |
|-------------------------------------------------------|---------|----------------|------------------------------|----------------------|
| Label                                                 | Utility | Standard Error | Importance (% Utility Range) | Variable             |
| Intercept                                             | 9.5000  | 0.11728        |                              | Intercept            |
| Brand Goodstone                                       | -1.1718 | 0.16586        | 15.463                       | Class.BrandGoodstone |
| Brand Pirogi                                          | 1.8980  | 0.16586        |                              | Class.BrandPirogi    |
| Brand Machismo                                        | -0.7262 | 0.16586        |                              | Class.BrandMachismo  |
| Price \$69.99                                         | 5.8732  | 0.16586        | 56.517                       | Class.Price_69_99    |
| Price \$74.99                                         | -0.5261 | 0.16586        |                              | Class.Price_74_99    |
| Price \$79.99                                         | -5.3471 | 0.16586        |                              | Class.Price_79_99    |
| Life 50,000                                           | -1.2350 | 0.16586        | 18.361                       | Class.Life50_000     |
| Life 60,000                                           | -1.1751 | 0.16586        |                              | Class.Life60_000     |
| Life 70,000                                           | 2.4101  | 0.16586        |                              | Class.Life70_000     |
| Hazard Yes                                            | 0.9588  | 0.11728        | 9.659                        | Class.HazardYes      |
| Hazard No                                             | -0.9588 | 0.11728        |                              | Class.HazardNo       |

The standard errors are not adjusted for the fact that the dependent variable was transformed and so are generally liberal (too small).

## Output 97.4.1 continued

| Nonmetric Conjoint Analysis of Ranks |      |                     |                 |           |         |        |        |
|--------------------------------------|------|---------------------|-----------------|-----------|---------|--------|--------|
| Obs                                  | Rank | Rank Transformation | Predicted Ranks | Brand     | Price   | Life   | Hazard |
| 1                                    | 3    | 14.4462             | 13.9851         | Goodstone | \$69.99 | 60,000 | Yes    |
| 2                                    | 2    | 15.6844             | 15.6527         | Goodstone | \$69.99 | 70,000 | No     |
| 3                                    | 14   | 5.7229              | 5.6083          | Goodstone | \$74.99 | 50,000 | No     |
| 4                                    | 10   | 5.7229              | 5.6682          | Goodstone | \$74.99 | 60,000 | No     |
| 5                                    | 17   | 2.6699              | 2.7049          | Goodstone | \$79.99 | 50,000 | Yes    |
| 6                                    | 12   | 5.7229              | 6.3500          | Goodstone | \$79.99 | 70,000 | Yes    |
| 7                                    | 7    | 14.4462             | 15.0774         | Pirogi    | \$69.99 | 50,000 | No     |
| 8                                    | 1    | 18.7699             | 18.7225         | Pirogi    | \$69.99 | 70,000 | No     |
| 9                                    | 8    | 11.1143             | 10.5957         | Pirogi    | \$74.99 | 50,000 | Yes    |
| 10                                   | 5    | 14.4462             | 14.2408         | Pirogi    | \$74.99 | 70,000 | Yes    |
| 11                                   | 13   | 5.7229              | 5.8346          | Pirogi    | \$79.99 | 60,000 | Yes    |
| 12                                   | 16   | 3.8884              | 3.9170          | Pirogi    | \$79.99 | 60,000 | No     |
| 13                                   | 6    | 14.4462             | 14.3708         | Machismo  | \$69.99 | 50,000 | Yes    |
| 14                                   | 4    | 14.4462             | 14.4307         | Machismo  | \$69.99 | 60,000 | Yes    |
| 15                                   | 15   | 5.7229              | 6.1139          | Machismo  | \$74.99 | 60,000 | No     |
| 16                                   | 9    | 11.1143             | 11.6166         | Machismo  | \$74.99 | 70,000 | Yes    |
| 17                                   | 18   | 1.1905              | 1.2330          | Machismo  | \$79.99 | 50,000 | No     |
| 18                                   | 11   | 5.7229              | 4.8780          | Machismo  | \$79.99 | 70,000 | No     |

## Example 97.5: Metric Conjoint Analysis of Tire Data

This example, which is more detailed than the previous one, uses PROC TRANSREG to perform a metric conjoint analysis of tire preference data. Conjoint analysis can be used to decompose preference ratings of products or services into components based on qualitative product attributes. For each level of each attribute of interest, a numerical “part-worth utility” value is computed. The sum of the part-worth utilities for each product is an estimate of the utility for that product. The goal is to compute part-worth utilities such that the product utilities are as similar as possible to the original ratings. Metric conjoint analysis, as shown in this example, fits an ordinary linear model directly to data assumed to be measured on an interval scale. Nonmetric conjoint analysis, as shown in [Example 97.4](#), finds an optimal monotonic transformation of original data before fitting an ordinary linear model to the transformed data.

This example has three parts. In the first part, an experimental design is created. In the second part, a DATA step creates descriptions of the stimuli for the experiment. The third part of the example performs the conjoint analyses.

The stimuli for the experiment are 18 hypothetical tires. The stimuli represent different brands (Goodstone, Pirogi, Machismo),<sup>2</sup> prices (\$69.99, \$74.99, \$79.99), expected tread life (50,000, 60,000, 70,000 miles), and road hazard insurance plans (Yes, No).

For a conjoint study such as this, you need to create an experimental design with 3 three-level factors, 1 two-level factor, and 18 combinations or *runs*. The easiest way to get this design is with the %MktEx autocall macro. The %MktEx macro requires you to specify the number of levels of each of the four factors, followed by N=18, the number of runs. Specifying a random number seed, while not strictly necessary, helps ensure that the design is reproducible. The %MktLab macro assigns the actual factor names instead of the default names x1, x2, and so on, and it assigns formats to the factor levels. The %MktEval macro helps you evaluate the design. It shows how correlated or independent the factors are, how often each factor level appears in the design, how often each pair occurs for every factor pair, and how often each product profile or run occurs in the design. See [http://support.sas.com/resources/papers/tnote/tnote\\_marketresearch.html](http://support.sas.com/resources/papers/tnote/tnote_marketresearch.html) (Kuhfeld 2005) for more information about experimental design and conjoint analysis; look for the latest “Conjoint Analysis” report. The following statements create, evaluate, and display the design:

```

title 'Tire Study, Experimental Design';

proc format;
 value BrandF
 1 = 'Goodstone'
 2 = 'Pirogi '
 3 = 'Machismo ';
 value PriceF
 1 = '$69.99'
 2 = '$74.99'
 3 = '$79.99';
 value LifeF
 1 = '50,000'
 2 = '60,000'
 3 = '70,000';
 value HazardF

```

<sup>2</sup>In real conjoint experiments, real brand names would be used.

```

1 = 'Yes'
2 = 'No ';

run;

%mktext(3 3 3 2, n=18, seed=448)

%mktlab(vars=Brand Price Life Hazard, out=sasuser.TireDesign,
statements=format Brand BrandF9. Price PriceF9.
Life LifeF6. Hazard HazardF3.)

%mkteval;

proc print data=sasuser.TireDesign;
run;

```

The %MktEx macro (Kuhfeld 2005) output displayed in [Output 97.5.1](#) shows you that the design is 100% efficient, which means it is orthogonal and balanced. The %MktEval macro output displayed in [Output 97.5.2](#) shows you that all of the factors are uncorrelated or orthogonal, the design is balanced (each level occurs once), and every pair of factor levels occurs equally often (again showing that the design is orthogonal). The *n*-way frequencies show that each product profile occurs once (there are no duplicates). The design is shown in [Output 97.5.3](#). The design is automatically randomized (the profiles were sorted into a random order and the original levels are randomly reassigned). Orthogonality, balance, randomization, and other design concepts are discussed in detail in Kuhfeld (2005), in the “Experimental Design, Efficiency, Coding, and Choice Designs” report.

**Output 97.5.1** Tire Study, Design Efficiency

| Tire Study, Experimental Design |          |                         |                      |       |
|---------------------------------|----------|-------------------------|----------------------|-------|
| Algorithm Search History        |          |                         |                      |       |
| Tire Study, Experimental Design |          |                         |                      |       |
| Design                          | Row, Col | Current<br>D-Efficiency | Best<br>D-Efficiency | Notes |
| 1                               | Start    | 100.0000                | 100.0000             | Tab   |
| 1                               | End      | 100.0000                |                      |       |
| Tire Study, Experimental Design |          |                         |                      |       |
| The OPTEX Procedure             |          |                         |                      |       |
| Class Level Information         |          |                         |                      |       |
| Class                           | Levels   | Values                  |                      |       |
| x1                              | 3        | 1                       | 2                    | 3     |
| x2                              | 3        | 1                       | 2                    | 3     |
| x3                              | 3        | 1                       | 2                    | 3     |
| x4                              | 2        | 1                       | 2                    |       |

**Output 97.5.1** *continued*

| Tire Study, Experimental Design |              |              |              |                                            |
|---------------------------------|--------------|--------------|--------------|--------------------------------------------|
| Design<br>Number                | D-Efficiency | A-Efficiency | G-Efficiency | Average<br>Prediction<br>Standard<br>Error |
| 1                               | 100.0000     | 100.0000     | 100.0000     | 0.6667                                     |

**Output 97.5.2** Tire Study, Design Evaluation

| Tire Study, Experimental Design                       |       |       |      |        |
|-------------------------------------------------------|-------|-------|------|--------|
| Canonical Correlations Between the Factors            |       |       |      |        |
| There are 0 Canonical Correlations Greater Than 0.316 |       |       |      |        |
|                                                       | Brand | Price | Life | Hazard |
| Brand                                                 | 1     | 0     | 0    | 0      |
| Price                                                 | 0     | 1     | 0    | 0      |
| Life                                                  | 0     | 0     | 1    | 0      |
| Hazard                                                | 0     | 0     | 0    | 1      |

| Tire Study, Experimental Design                       |   |   |   |   |
|-------------------------------------------------------|---|---|---|---|
| Summary of Frequencies                                |   |   |   |   |
| There are 0 Canonical Correlations Greater Than 0.316 |   |   |   |   |
| Frequencies                                           |   |   |   |   |
| Brand                                                 | 6 | 6 | 6 |   |
| Price                                                 | 6 | 6 | 6 |   |
| Life                                                  | 6 | 6 | 6 |   |
| Hazard                                                | 9 | 9 |   |   |
| Brand Price                                           | 2 | 2 | 2 | 2 |
| Brand Life                                            | 2 | 2 | 2 | 2 |
| Brand Hazard                                          | 3 | 3 | 3 | 3 |
| Price Life                                            | 2 | 2 | 2 | 2 |
| Price Hazard                                          | 3 | 3 | 3 | 3 |
| Life Hazard                                           | 3 | 3 | 3 | 3 |
| N-Way                                                 | 1 | 1 | 1 | 1 |

**Output 97.5.3** Tire Study, Design

| Tire Study, Experimental Design |           |         |        |        |
|---------------------------------|-----------|---------|--------|--------|
| Obs                             | Brand     | Price   | Life   | Hazard |
| 1                               | Pirogi    | \$79.99 | 50,000 | No     |
| 2                               | Machismo  | \$79.99 | 60,000 | No     |
| 3                               | Machismo  | \$74.99 | 70,000 | Yes    |
| 4                               | Machismo  | \$74.99 | 50,000 | No     |
| 5                               | Goodstone | \$74.99 | 60,000 | Yes    |
| 6                               | Pirogi    | \$69.99 | 60,000 | Yes    |
| 7                               | Goodstone | \$69.99 | 50,000 | Yes    |
| 8                               | Machismo  | \$69.99 | 50,000 | Yes    |
| 9                               | Pirogi    | \$74.99 | 60,000 | Yes    |
| 10                              | Pirogi    | \$74.99 | 50,000 | No     |
| 11                              | Goodstone | \$79.99 | 60,000 | No     |
| 12                              | Goodstone | \$69.99 | 70,000 | No     |
| 13                              | Pirogi    | \$79.99 | 70,000 | Yes    |
| 14                              | Goodstone | \$74.99 | 70,000 | No     |
| 15                              | Machismo  | \$69.99 | 60,000 | No     |
| 16                              | Machismo  | \$79.99 | 70,000 | Yes    |
| 17                              | Pirogi    | \$69.99 | 70,000 | No     |
| 18                              | Goodstone | \$79.99 | 50,000 | Yes    |

The %MktEx macro requires SAS/STAT, SAS/QC, and SAS/IML software. Alternatively, you can make a design for this experiment using the %MktDes macro, which requires only SAS/STAT and SAS/QC software. The %MktDes macro contains a small subset of the functionality of the %MktEx macro. It can be used as follows:

```
%mktdes(factors=Brand=3 Price=3 Life=3 Hazard=2, n=18)
```

The results of this step are not shown or used.

Next, the questionnaires are printed and given to the subjects, who are asked to rate the tires.

The following statements produce [Output 97.5.4](#):

```

data _null_;
 title;
 set sasuser.TireDesign;
 file print;
 if mod(_n_,4) eq 1 then do;
 put _page_;
 put +55 'Subject _____';
 end;
 length hazardstring $ 7.;
 if put(hazard, hazardf3.) = 'Yes'
 then hazardstring = 'with';
 else hazardstring = 'without';

 s = 3 + (_n_ >= 10);
 put // _n_ +(-1) ') For your next tire purchase, '
 'how likely are you to buy this product?'
 // +s Brand 'brand tires at ' Price +(-1) ', '
 / +s 'with a ' Life 'tread life guarantee, '
 / +s 'and ' hazardstring 'road hazard insurance.'
 // +s 'Definitely Would Definitely Would'
 / +s 'Not Purchase Purchase'
 // +s '1 2 3 4 5 6 7 8 9 ';
run;

```

This output in [Output 97.5.4](#) is abbreviated in the interest of conserving space; the statements actually produce stimuli for all combinations.



**Output 97.5.4** Conjoint Analysis, Stimuli Descriptions

|                                                                                                               |   |   |   |   |                              |   |   |   |  |
|---------------------------------------------------------------------------------------------------------------|---|---|---|---|------------------------------|---|---|---|--|
| Subject _____                                                                                                 |   |   |   |   |                              |   |   |   |  |
| 1) For your next tire purchase, how likely are you to buy this product?                                       |   |   |   |   |                              |   |   |   |  |
| Pirogi brand tires at \$79.99,<br>with a 50,000 tread life guarantee,<br>and without road hazard insurance.   |   |   |   |   |                              |   |   |   |  |
| Definitely Would<br>Not Purchase                                                                              |   |   |   |   | Definitely Would<br>Purchase |   |   |   |  |
| 1                                                                                                             | 2 | 3 | 4 | 5 | 6                            | 7 | 8 | 9 |  |
| 2) For your next tire purchase, how likely are you to buy this product?                                       |   |   |   |   |                              |   |   |   |  |
| Machismo brand tires at \$79.99,<br>with a 60,000 tread life guarantee,<br>and without road hazard insurance. |   |   |   |   |                              |   |   |   |  |
| Definitely Would<br>Not Purchase                                                                              |   |   |   |   | Definitely Would<br>Purchase |   |   |   |  |
| 1                                                                                                             | 2 | 3 | 4 | 5 | 6                            | 7 | 8 | 9 |  |
| 3) For your next tire purchase, how likely are you to buy this product?                                       |   |   |   |   |                              |   |   |   |  |
| Machismo brand tires at \$74.99,<br>with a 70,000 tread life guarantee,<br>and with road hazard insurance.    |   |   |   |   |                              |   |   |   |  |
| Definitely Would<br>Not Purchase                                                                              |   |   |   |   | Definitely Would<br>Purchase |   |   |   |  |
| 1                                                                                                             | 2 | 3 | 4 | 5 | 6                            | 7 | 8 | 9 |  |
| 4) For your next tire purchase, how likely are you to buy this product?                                       |   |   |   |   |                              |   |   |   |  |
| Machismo brand tires at \$74.99,<br>with a 50,000 tread life guarantee,<br>and without road hazard insurance. |   |   |   |   |                              |   |   |   |  |
| Definitely Would<br>Not Purchase                                                                              |   |   |   |   | Definitely Would<br>Purchase |   |   |   |  |
| 1                                                                                                             | 2 | 3 | 4 | 5 | 6                            | 7 | 8 | 9 |  |

The third part of the example performs the conjoint analyses. The DATA step reads the data. Only the ratings are entered, one row per subject. Real conjoint studies have many more subjects than five. The TRANSPOSE procedure transposes this (5 × 18) data set into an (18 × 5) data set that can be merged with the factor level data set sasuser.TireDesign. The next DATA step does the merge. The PRINT procedure displays the input data set.

PROC TRANSREG fits the five individual conjoint models, one for each subject. The UTILITIES *a-option* displays the conjoint analysis results. The SHORT *a-option* suppresses the iteration histories, OUTTEST=UTILS creates an output data set with all of the conjoint results, and the SEPARATORS= option requests that the labels constructed for each category contain two blanks between the variable name and the level value. The ODS SELECT statement is used to limit the displayed output. The MODEL statement specifies IDENTITY for the ratings, which specifies a metric conjoint analysis—the ratings are not transformed. The variables Brand, Price, Life, and Hazard are designated as CLASS variables, and the part-worth utilities are constrained to sum to zero within each factor.

The following statements produce [Output 97.5.5](#):

```

title 'Tire Study, Data Entry, Preprocessing';

data Results;
 input (c1-c18) (1.);
 datalines;
233279766526376493
124467885349168274
262189456534275794
184396375364187754
133379775526267493
;

* Create an Object by Subject Data Matrix;
proc transpose data=Results out=Results(drop=_name_) prefix=Subj;
run;

* Merge the Factor Levels with the Data Matrix;
data Both;
 merge sasuser.TireDesign Results;
run;

proc print;
 title2 'Data Set for Conjoint Analysis';
run;

title 'Tire Study, Individual Conjoint Analyses';

* Fit Each Subject Individually;
proc transreg data=Both utilities short outtest=utils separators=' ';
 ods select TestsNote FitStatistics Utilities;
 model identity(Subj1-Subj5) =
 class(Brand Price Life Hazard / zero=sum);
run;

```

The output contains two tables per subject, one with overall fit statistics and one with the conjoint analysis results.

### Output 97.5.5 Conjoint Analysis

| Tire Study, Data Entry, Preprocessing<br>Data Set for Conjoint Analysis |           |         |        |        |       |       |       |       |       |
|-------------------------------------------------------------------------|-----------|---------|--------|--------|-------|-------|-------|-------|-------|
| Obs                                                                     | Brand     | Price   | Life   | Hazard | Subj1 | Subj2 | Subj3 | Subj4 | Subj5 |
| 1                                                                       | Pirogi    | \$79.99 | 50,000 | No     | 2     | 1     | 2     | 1     | 1     |
| 2                                                                       | Machismo  | \$79.99 | 60,000 | No     | 3     | 2     | 6     | 8     | 3     |
| 3                                                                       | Machismo  | \$74.99 | 70,000 | Yes    | 3     | 4     | 2     | 4     | 3     |
| 4                                                                       | Machismo  | \$74.99 | 50,000 | No     | 2     | 4     | 1     | 3     | 3     |
| 5                                                                       | Goodstone | \$74.99 | 60,000 | Yes    | 7     | 6     | 8     | 9     | 7     |
| 6                                                                       | Pirogi    | \$69.99 | 60,000 | Yes    | 9     | 7     | 9     | 6     | 9     |
| 7                                                                       | Goodstone | \$69.99 | 50,000 | Yes    | 7     | 8     | 4     | 3     | 7     |
| 8                                                                       | Machismo  | \$69.99 | 50,000 | Yes    | 6     | 8     | 5     | 7     | 7     |
| 9                                                                       | Pirogi    | \$74.99 | 60,000 | Yes    | 6     | 5     | 6     | 5     | 5     |
| 10                                                                      | Pirogi    | \$74.99 | 50,000 | No     | 5     | 3     | 5     | 3     | 5     |
| 11                                                                      | Goodstone | \$79.99 | 60,000 | No     | 2     | 4     | 3     | 6     | 2     |
| 12                                                                      | Goodstone | \$69.99 | 70,000 | No     | 6     | 9     | 4     | 4     | 6     |
| 13                                                                      | Pirogi    | \$79.99 | 70,000 | Yes    | 3     | 1     | 2     | 1     | 2     |
| 14                                                                      | Goodstone | \$74.99 | 70,000 | No     | 7     | 6     | 7     | 8     | 6     |
| 15                                                                      | Machismo  | \$69.99 | 60,000 | No     | 6     | 8     | 5     | 7     | 7     |
| 16                                                                      | Machismo  | \$79.99 | 70,000 | Yes    | 4     | 2     | 7     | 7     | 4     |
| 17                                                                      | Pirogi    | \$69.99 | 70,000 | No     | 9     | 7     | 9     | 5     | 9     |
| 18                                                                      | Goodstone | \$79.99 | 50,000 | Yes    | 3     | 4     | 4     | 4     | 3     |

### Output 97.5.5 continued

| Tire Study, Individual Conjoint Analyses                    |          |          |        |
|-------------------------------------------------------------|----------|----------|--------|
| The TRANSREG Procedure                                      |          |          |        |
| The TRANSREG Procedure Hypothesis Tests for Identity(Subj1) |          |          |        |
| Root MSE                                                    | 1.34164  | R-Square | 0.8043 |
| Dependent Mean                                              | 5.00000  | Adj R-Sq | 0.6674 |
| Coeff Var                                                   | 26.83282 |          |        |

**Output 97.5.5** *continued*

| Utilities Table Based on the Usual Degrees of Freedom |         |                |                              |                      |
|-------------------------------------------------------|---------|----------------|------------------------------|----------------------|
| Label                                                 | Utility | Standard Error | Importance (% Utility Range) | Variable             |
| Intercept                                             | 5.0000  | 0.31623        |                              | Intercept            |
| Brand Goodstone                                       | 0.3333  | 0.44721        | 20.833                       | Class.BrandGoodstone |
| Brand Pirogi                                          | 0.6667  | 0.44721        |                              | Class.BrandPirogi    |
| Brand Machismo                                        | -1.0000 | 0.44721        |                              | Class.BrandMachismo  |
| Price \$69.99                                         | 2.1667  | 0.44721        | 54.167                       | Class.Price_69_99    |
| Price \$74.99                                         | 0.0000  | 0.44721        |                              | Class.Price_74_99    |
| Price \$79.99                                         | -2.1667 | 0.44721        |                              | Class.Price_79_99    |
| Life 50,000                                           | -0.8333 | 0.44721        | 16.667                       | Class.Life50_000     |
| Life 60,000                                           | 0.5000  | 0.44721        |                              | Class.Life60_000     |
| Life 70,000                                           | 0.3333  | 0.44721        |                              | Class.Life70_000     |
| Hazard Yes                                            | 0.3333  | 0.31623        | 8.333                        | Class.HazardYes      |
| Hazard No                                             | -0.3333 | 0.31623        |                              | Class.HazardNo       |

Tire Study, Individual Conjoint Analyses

The TRANSREG Procedure

The TRANSREG Procedure Hypothesis Tests for Identity(Subj2)

|                |          |          |        |
|----------------|----------|----------|--------|
| Root MSE       | 0.56765  | R-Square | 0.9710 |
| Dependent Mean | 4.94444  | Adj R-Sq | 0.9506 |
| Coeff Var      | 11.48049 |          |        |

Output 97.5.5 *continued*

| Utilities Table Based on the Usual Degrees of Freedom |         |                |                              |                      |
|-------------------------------------------------------|---------|----------------|------------------------------|----------------------|
| Label                                                 | Utility | Standard Error | Importance (% Utility Range) | Variable             |
| Intercept                                             | 4.9444  | 0.13380        |                              | Intercept            |
| Brand Goodstone                                       | 1.2222  | 0.18922        | 25.658                       | Class.BrandGoodstone |
| Brand Pirogi                                          | -0.9444 | 0.18922        |                              | Class.BrandPirogi    |
| Brand Machismo                                        | -0.2778 | 0.18922        |                              | Class.BrandMachismo  |
| Price \$69.99                                         | 2.8889  | 0.18922        | 65.132                       | Class.Price_69_99    |
| Price \$74.99                                         | -0.2778 | 0.18922        |                              | Class.Price_74_99    |
| Price \$79.99                                         | -2.6111 | 0.18922        |                              | Class.Price_79_99    |
| Life 50,000                                           | -0.2778 | 0.18922        | 7.895                        | Class.Life50_000     |
| Life 60,000                                           | 0.3889  | 0.18922        |                              | Class.Life60_000     |
| Life 70,000                                           | -0.1111 | 0.18922        |                              | Class.Life70_000     |
| Hazard Yes                                            | 0.0556  | 0.13380        | 1.316                        | Class.HazardYes      |
| Hazard No                                             | -0.0556 | 0.13380        |                              | Class.HazardNo       |

Tire Study, Individual Conjoint Analyses

The TRANSREG Procedure

The TRANSREG Procedure Hypothesis Tests for Identity(Subj3)

|                |          |          |         |
|----------------|----------|----------|---------|
| Root MSE       | 2.48104  | R-Square | 0.3902  |
| Dependent Mean | 4.94444  | Adj R-Sq | -0.0367 |
| Coeff Var      | 50.17832 |          |         |

**Output 97.5.5** *continued*

| Utilities Table Based on the Usual Degrees of Freedom |         |                |                              |                      |
|-------------------------------------------------------|---------|----------------|------------------------------|----------------------|
| Label                                                 | Utility | Standard Error | Importance (% Utility Range) | Variable             |
| Intercept                                             | 4.9444  | 0.58479        |                              | Intercept            |
| Brand Goodstone                                       | 0.0556  | 0.82701        | 18.261                       | Class.BrandGoodstone |
| Brand Pirogi                                          | 0.5556  | 0.82701        |                              | Class.BrandPirogi    |
| Brand Machismo                                        | -0.6111 | 0.82701        |                              | Class.BrandMachismo  |
| Price \$69.99                                         | 1.0556  | 0.82701        | 31.304                       | Class.Price_69_99    |
| Price \$74.99                                         | -0.1111 | 0.82701        |                              | Class.Price_74_99    |
| Price \$79.99                                         | -0.9444 | 0.82701        |                              | Class.Price_79_99    |
| Life 50,000                                           | -1.4444 | 0.82701        | 41.739                       | Class.Life50_000     |
| Life 60,000                                           | 1.2222  | 0.82701        |                              | Class.Life60_000     |
| Life 70,000                                           | 0.2222  | 0.82701        |                              | Class.Life70_000     |
| Hazard Yes                                            | 0.2778  | 0.58479        | 8.696                        | Class.HazardYes      |
| Hazard No                                             | -0.2778 | 0.58479        |                              | Class.HazardNo       |

Tire Study, Individual Conjoint Analyses

The TRANSREG Procedure

The TRANSREG Procedure Hypothesis Tests for Identity(Subj4)

|                |          |          |        |
|----------------|----------|----------|--------|
| Root MSE       | 1.90321  | R-Square | 0.6185 |
| Dependent Mean | 5.05556  | Adj R-Sq | 0.3514 |
| Coeff Var      | 37.64598 |          |        |

## Output 97.5.5 continued

| Utilities Table Based on the Usual Degrees of Freedom |         |                |                              |                      |
|-------------------------------------------------------|---------|----------------|------------------------------|----------------------|
| Label                                                 | Utility | Standard Error | Importance (% Utility Range) | Variable             |
| Intercept                                             | 5.0556  | 0.44859        |                              | Intercept            |
| Brand Goodstone                                       | 0.6111  | 0.63440        | 36.885                       | Class.BrandGoodstone |
| Brand Pirogi                                          | -1.5556 | 0.63440        |                              | Class.BrandPirogi    |
| Brand Machismo                                        | 0.9444  | 0.63440        |                              | Class.BrandMachismo  |
| Price \$69.99                                         | 0.2778  | 0.63440        | 12.295                       | Class.Price_69_99    |
| Price \$74.99                                         | 0.2778  | 0.63440        |                              | Class.Price_74_99    |
| Price \$79.99                                         | -0.5556 | 0.63440        |                              | Class.Price_79_99    |
| Life 50,000                                           | -1.5556 | 0.63440        | 49.180                       | Class.Life50_000     |
| Life 60,000                                           | 1.7778  | 0.63440        |                              | Class.Life60_000     |
| Life 70,000                                           | -0.2222 | 0.63440        |                              | Class.Life70_000     |
| Hazard Yes                                            | 0.0556  | 0.44859        | 1.639                        | Class.HazardYes      |
| Hazard No                                             | -0.0556 | 0.44859        |                              | Class.HazardNo       |

Tire Study, Individual Conjoint Analyses

The TRANSREG Procedure

The TRANSREG Procedure Hypothesis Tests for Identity(Subj5)

|                |          |          |        |
|----------------|----------|----------|--------|
| Root MSE       | 1.36219  | R-Square | 0.8162 |
| Dependent Mean | 4.94444  | Adj R-Sq | 0.6875 |
| Coeff Var      | 27.54987 |          |        |

Output 97.5.5 *continued*

| Utilities Table Based on the Usual Degrees of Freedom |         |                |                              |                      |
|-------------------------------------------------------|---------|----------------|------------------------------|----------------------|
| Label                                                 | Utility | Standard Error | Importance (% Utility Range) | Variable             |
| Intercept                                             | 4.9444  | 0.32107        |                              | Intercept            |
| Brand Goodstone                                       | 0.2222  | 0.45406        | 9.023                        | Class.BrandGoodstone |
| Brand Pirogi                                          | 0.2222  | 0.45406        |                              | Class.BrandPirogi    |
| Brand Machismo                                        | -0.4444 | 0.45406        |                              | Class.BrandMachismo  |
| Price \$69.99                                         | 2.5556  | 0.45406        | 67.669                       | Class.Price_69_99    |
| Price \$74.99                                         | -0.1111 | 0.45406        |                              | Class.Price_74_99    |
| Price \$79.99                                         | -2.4444 | 0.45406        |                              | Class.Price_79_99    |
| Life 50,000                                           | -0.6111 | 0.45406        | 15.789                       | Class.Life50_000     |
| Life 60,000                                           | 0.5556  | 0.45406        |                              | Class.Life60_000     |
| Life 70,000                                           | 0.0556  | 0.45406        |                              | Class.Life70_000     |
| Hazard Yes                                            | 0.2778  | 0.32107        | 7.519                        | Class.HazardYes      |
| Hazard No                                             | -0.2778 | 0.32107        |                              | Class.HazardNo       |

The next steps summarize the results. Three tables are displayed, showing the following: all of the importance values, the average importance, and the part-worth utilities. The first DATA step selects the importance information from the UTILS data set. The final assignment statement stores just the variable name from the label, relying on the fact that the separator is two blanks. PROC TRANSPOSE creates the data set of importances, one row per subject, and PROC PRINT displays the results. The MEANS procedure displays the average importance of each attribute across the subjects. The next DATA step selects the part-worth utilities information from the UTILS data set. PROC TRANSPOSE creates the data set of utilities, one row per subject, and PROC PRINT displays the results. The following statements produce [Output 97.5.6](#):

```

title 'Tire Study Results';

* Gather the Importance Values;
data Importance;
 set utils(keep=_depvar_ Importance Label);
 if n(Importance);
 label = substr(label, 1, index(label, ' '));
run;

proc transpose out=Importance2(drop=_:);
 by _depvar_;
 id Label;
run;

proc print;
 title2 'Importance Values';
run;

proc means;

```



```

 title2 'Average Importance';
run;

* Gather the Part-Worth Utilities;
data Utilities;
 set utils(keep=_depvar_ Coefficient Label);
 if n(Coefficient);
run;

proc transpose out=Utilities2(drop=_:);
 by _depvar_;
 id Label;
 idlabel Label;
run;

proc print label;
 title2 'Utilities';
run;

```

**Output 97.5.6** Summary of Conjoint Analysis Results

| Tire Study Results<br>Importance Values |         |         |         |         |  |
|-----------------------------------------|---------|---------|---------|---------|--|
| Obs                                     | Brand   | Price   | Life    | Hazard  |  |
| 1                                       | 20.8333 | 54.1667 | 16.6667 | 8.33333 |  |
| 2                                       | 25.6579 | 65.1316 | 7.8947  | 1.31579 |  |
| 3                                       | 18.2609 | 31.3043 | 41.7391 | 8.69565 |  |
| 4                                       | 36.8852 | 12.2951 | 49.1803 | 1.63934 |  |
| 5                                       | 9.0226  | 67.6692 | 15.7895 | 7.51880 |  |

**Output 97.5.6** *continued*

| Tire Study Results<br>Average Importance |   |            |            |            |            |
|------------------------------------------|---|------------|------------|------------|------------|
| The MEANS Procedure                      |   |            |            |            |            |
| Variable                                 | N | Mean       | Std Dev    | Minimum    | Maximum    |
| Brand                                    | 5 | 22.1319800 | 10.2301014 | 9.0225564  | 36.8852459 |
| Price                                    | 5 | 46.1133697 | 23.7391251 | 12.2950820 | 67.6691729 |
| Life                                     | 5 | 26.2540671 | 18.0547195 | 7.8947368  | 49.1803279 |
| Hazard                                   | 5 | 5.5005832  | 3.6989117  | 1.3157895  | 8.6956522  |

**Output 97.5.6** *continued*

| Tire Study Results |           |                    |                 |                   |                  |                  |
|--------------------|-----------|--------------------|-----------------|-------------------|------------------|------------------|
| Utilities          |           |                    |                 |                   |                  |                  |
| Obs                | Intercept | Brand<br>Goodstone | Brand<br>Pirogi | Brand<br>Machismo | Price<br>\$69.99 | Price<br>\$74.99 |
| 1                  | 5.00000   | 0.33333            | 0.66667         | -1.00000          | 2.16667          | 0.00000          |
| 2                  | 4.94444   | 1.22222            | -0.94444        | -0.27778          | 2.88889          | -0.27778         |
| 3                  | 4.94444   | 0.05556            | 0.55556         | -0.61111          | 1.05556          | -0.11111         |
| 4                  | 5.05556   | 0.61111            | -1.55556        | 0.94444           | 0.27778          | 0.27778          |
| 5                  | 4.94444   | 0.22222            | 0.22222         | -0.44444          | 2.55556          | -0.11111         |

| Obs | Price<br>\$79.99 | Life<br>50,000 | Life<br>60,000 | Life<br>70,000 | Hazard<br>Yes | Hazard<br>No |
|-----|------------------|----------------|----------------|----------------|---------------|--------------|
| 1   | -2.16667         | -0.83333       | 0.50000        | 0.33333        | 0.33333       | -0.33333     |
| 2   | -2.61111         | -0.27778       | 0.38889        | -0.11111       | 0.05556       | -0.05556     |
| 3   | -0.94444         | -1.44444       | 1.22222        | 0.22222        | 0.27778       | -0.27778     |
| 4   | -0.55556         | -1.55556       | 1.77778        | -0.22222       | 0.05556       | -0.05556     |
| 5   | -2.44444         | -0.61111       | 0.55556        | 0.05556        | 0.27778       | -0.27778     |

Based on the importance values, price is the most important attribute for some of the respondents, but expected tread life is most important for others. On the average, price is most important, followed by expected tread life and brand. Road hazard insurance is less important. Each of the brands is preferred by some of the respondents. All respondents preferred a lower price over a higher price, a longer tread life, and road hazard insurance.

---

### Example 97.6: Preference Mapping of Automobile Data

This example uses PROC TRANSREG to perform a preference mapping (PREFMAP) analysis (Carroll 1972) of automobile preference data after a PROC PRINQUAL principal component analysis. The PREFMAP analysis is a response surface regression that locates ideal points for each dependent variable in a space defined by the independent variables.

The data are ratings obtained from 25 judges of their preference for each of 17 automobiles. The ratings were made on a scale of zero (very weak preference) to nine (very strong preference). These judgments were made in 1980 about that year's products. There are two character variables that indicate the manufacturer and model of the automobile. The data set also contains three ratings: miles per gallon (MPG), projected reliability (Reliability), and quality of the ride (Ride). These ratings are on a scale of one (bad) to five (good). PROC PRINQUAL creates an `OUT=` data set containing standardized principal component scores (Prin1 and Prin2), along with the `ID` variables Model, MPG, Reliability, and Ride.

While this data set contains all of the information needed for the subsequent preference mapping, you can make slightly more informative plots by adding new variable labels to the principal component score variables. The default labels are 'Component 1', 'Component 2', and so on. These are by necessity rather generic since they are created before any data are read, and they must be appropriate across BY groups when a BY variable is specified. In contrast, the MDPREF plot in PROC PRINQUAL has axis labels of the form 'Component 1 (43.54%)' and 'Component 2 (23.4%)' that show the proportion of variance accounted for

by each component. You can create an output data set from the MDPREF plot by using the ODS OUTPUT statement and then use only the label information from it to reset the labels in the output data set from PROC PRINQUAL. In the DATA PLOT step, the SET statement for the MD data set is specified before the SET statement for the PRESULTS data set. The `if 0` ensures that no data are actually read from it, but nevertheless the properties of the Prin1 and Prin2 variables including the variable labels are set based on the properties of those variables in the MD data set.

The first PROC TRANSREG step fits univariate regression models for MPG and Reliability. All variables are designated **IDENTITY**. A vector drawn in the plot of Prin1 and Prin2 from the origin to the point defined by an attribute's regression coefficients approximately shows how the autos differ on that attribute. See Carroll (1972) for more information. The Prin1 and Prin2 columns of the TResult1 **OUT=** data set contain the automobile coordinates (`_Type_='SCORE'` observations) and endpoints of the MPG and Reliability vectors (`_Type_='M COEFFI'` observations).

The second PROC TRANSREG step fits a univariate regression model with Ride designated **IDENTITY**, and Prin1 and Prin2 designated **POINT**. The **POINT** expansion creates an additional independent variable `_ISSQ_`, which contains the sum of Prin1 squared and Prin2 squared. The **OUT=** data set TResult2 contains no `_Type_='SCORE'` observations, only ideal point (`_Type_='M POINT'`) coordinates for Ride. The coordinates of both the vectors and the ideal points are output by specifying **COORDINATES** in the OUTPUT statement in PROC TRANSREG.

A vector model is used for MPG and Reliability because perfectly efficient and reliable automobiles do not exist in the data set. The ideal points for MPG and Reliability are far removed from the plot of the automobiles. It is more likely that an ideal point for quality of the ride is in the plot, so an ideal point model is used for the ride variable. See Carroll (1972) and Schiffman, Reynolds, and Young (1981) for discussions of the vector model and point models (including the **EPOINT** and **QPOINT** versions of the point model that are not used in this example). For the vector model, the default coordinates stretch factor of 2.5 was used. This extends the vectors by a factor of 2.5 from their standard lengths, making a better graphical display. Sometimes the default vectors are short and near the origin, and they look better when they are extended.

The following statements produce [Output 97.6.1](#) through [Output 97.6.5](#):

```

title 'Preference Ratings for Automobiles Manufactured in 1980';

options validvarname=any;

data CarPreferences;
 input Make $ 1-10 Model $ 12-22 @25 ('1'n-'25'n') (1.)
 MPG Reliability Ride;
 datalines;
Cadillac Eldorado 8007990491240508971093809 3 2 4
Chevrolet Chevette 0051200423451043003515698 5 3 2
Chevrolet Citation 4053305814161643544747795 4 1 5
Chevrolet Malibu 6027400723121345545668658 3 3 4
Ford Fairmont 2024006715021443530648655 3 3 4
Ford Mustang 5007197705021101850657555 3 2 2
Ford Pinto 0021000303030201500514078 4 1 1
Honda Accord 5956897609699952998975078 5 5 3
Honda Civic 4836709507488852567765075 5 5 3
Lincoln Continental 7008990592230409962091909 2 4 5
Plymouth Gran Fury 7006000434101107333458708 2 1 5
Plymouth Horizon 3005005635461302444675655 4 3 3

```

```

Plymouth Volare 4005003614021602754476555 2 1 3
Pontiac Firebird 0107895613201206958265907 1 1 5
Volkswagen Dasher 4858696508877795377895000 5 3 4
Volkswagen Rabbit 4858509709695795487885000 5 4 3
Volvo DL 9989998909999987989919000 4 5 5
;

ods graphics on;

* Compute Coordinates for a 2-Dimensional Scatter Plot of Automobiles;
proc prinqual data=CarPreferences out=PResults(drop='1'n-'25'n)
 n=2 replace standard scores mdpref=2;
 id Model MPG Reliability Ride;
 transform identity('1'n-'25'n);
 title2 'Multidimensional Preference (MDPREF) Analysis';
 ods output mdprefplot=md;
run;

options validvarname=v7;

title2 'Preference Mapping (PREFMAP) Analysis';

* Add the Labels from the Plot to the Results Data Set;
data plot;
 if 0 then set md(keep=prin:);
 set presults;
run;

* Compute Endpoints for MPG and Reliability Vectors;
proc transreg data=plot rsquare;
 Model identity(MPG Reliability)=identity(Prin1 Prin2);
 output tstandard=center coordinates replace out=TResult1;
 id Model;
run;

* Compute Ride Ideal Point Coordinates;
proc transreg data=plot rsquare;
 Model identity(Ride)=point(Prin1 Prin2);
 output tstandard=center coordinates replace noscores out=TResult2;
 id Model;
run;

proc print;
run;

```

**Output 97.6.1** Preference Ratings Example Output

Preference Ratings for Automobiles Manufactured in 1980  
Multidimensional Preference (MDPREF) Analysis

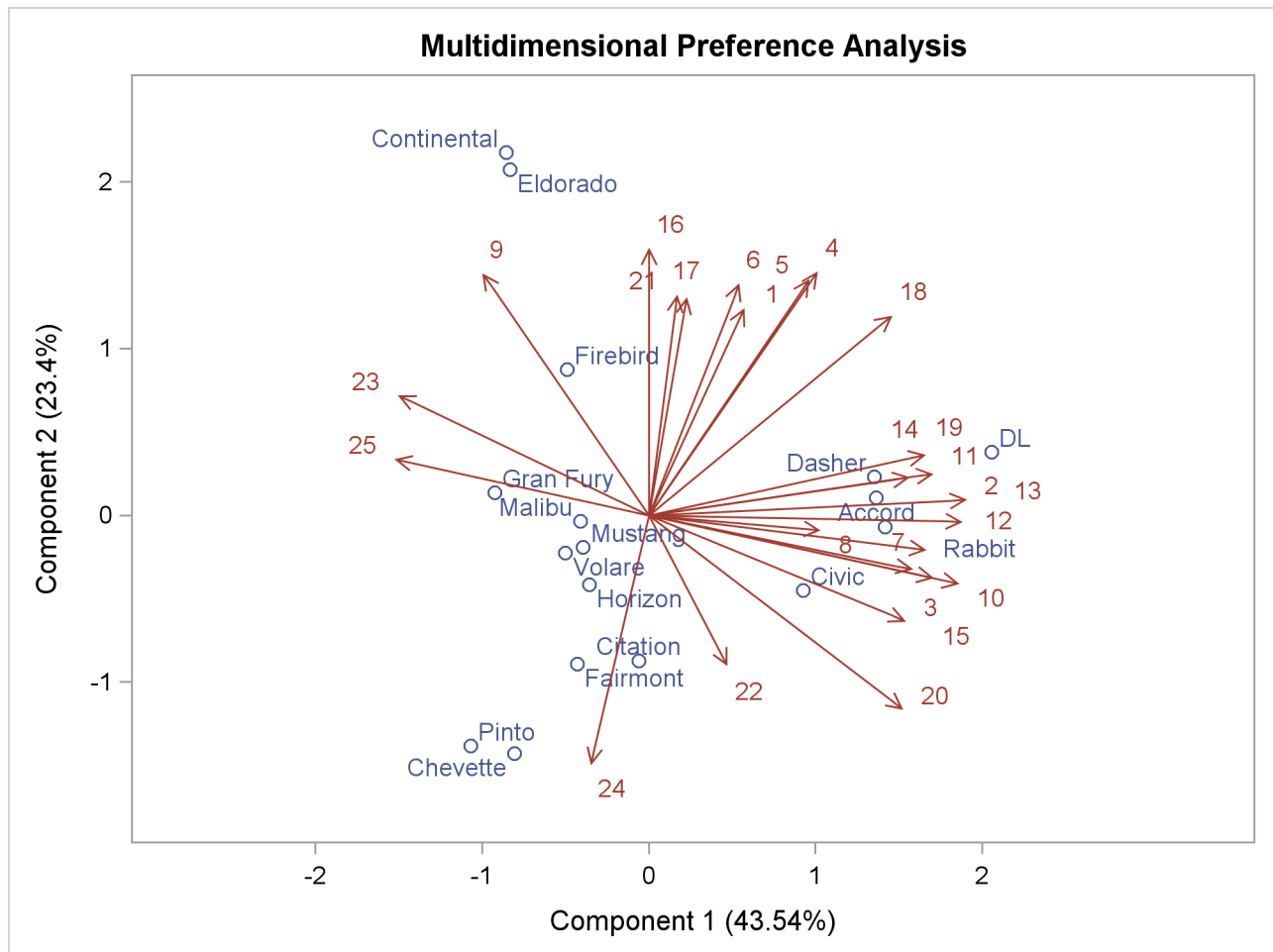
The PRINQUAL Procedure

PRINQUAL MTV Algorithm Iteration History

| Iteration Number | Average Change | Maximum Change | Proportion of Variance | Criterion Change | Note      |
|------------------|----------------|----------------|------------------------|------------------|-----------|
| 1                | 0.00000        | 0.00000        | 0.66946                |                  | Converged |

Algorithm converged.

**Output 97.6.2** MDPREF Plot



Output 97.6.3 shows that an unreliable-to-reliable direction extends from the left and slightly below the origin to the right and slightly above the origin. The Japanese and European automobiles are rated, on the

average, as more reliable. A low MPG to good MPG direction extends from the top left of the plot to the bottom right. The smaller automobiles, on the average, get better gas mileage.

**Output 97.6.3** Preference Mapping Vector Plot

```

Preference Ratings for Automobiles Manufactured in 1980
Preference Mapping (PREFMAP) Analysis

The TRANSREG Procedure

The TRANSREG Procedure Hypothesis Tests for Identity (MPG)

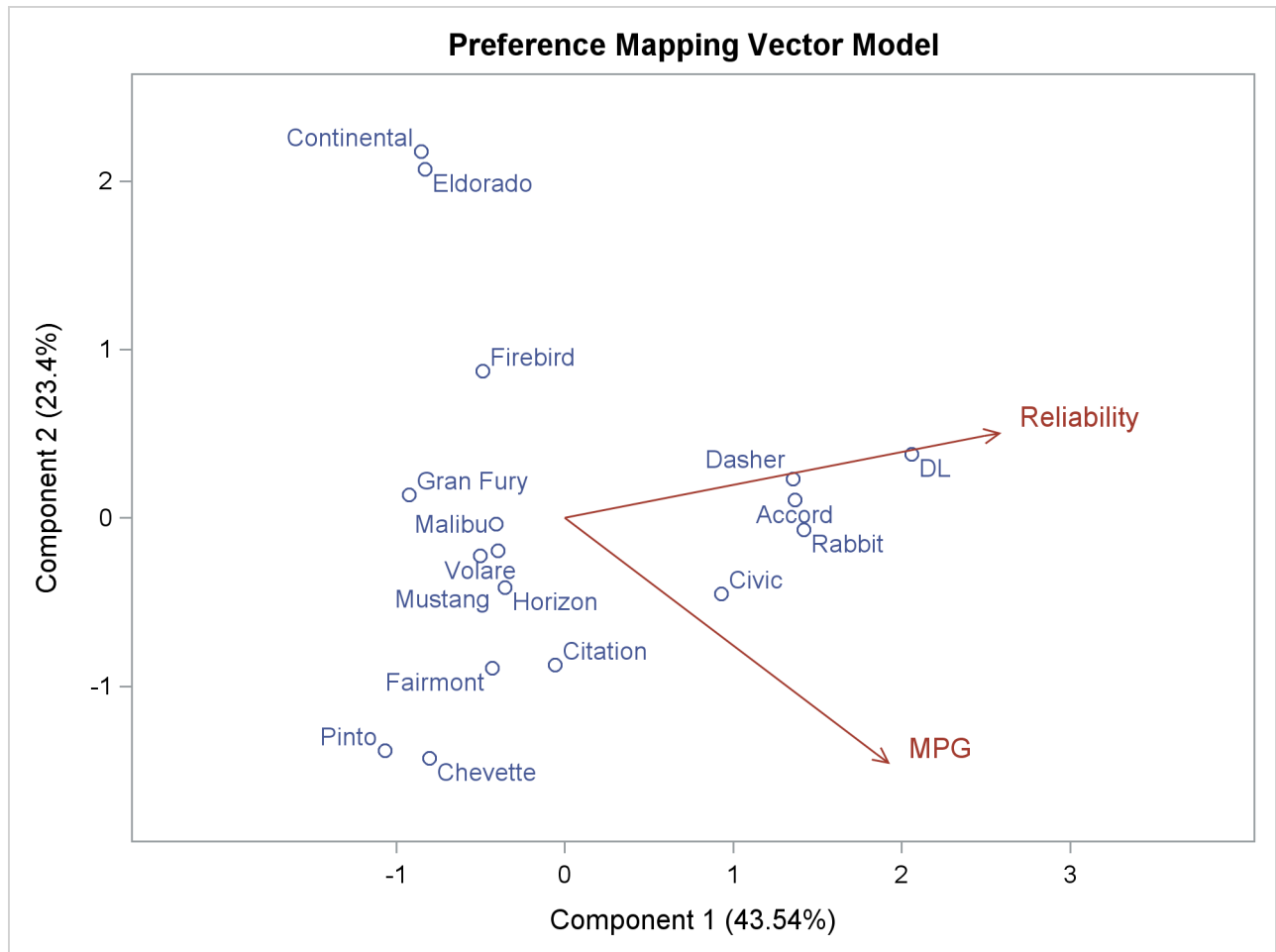
R-Square 0.5720

The TRANSREG Procedure Hypothesis Tests for Identity (Reliability)

R-Square 0.5086

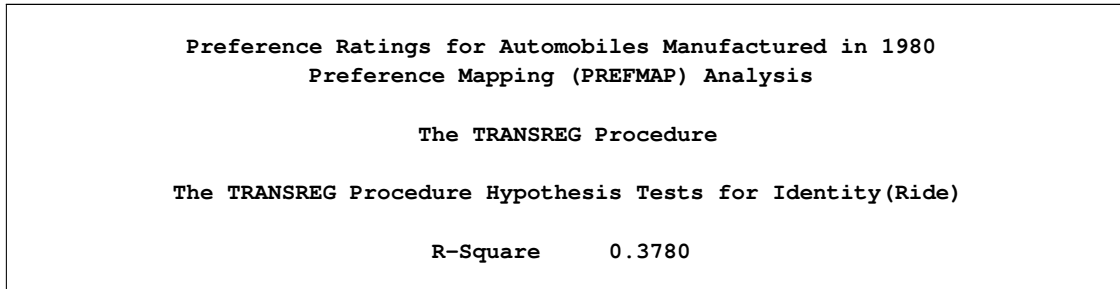
```

**Output 97.6.3** continued

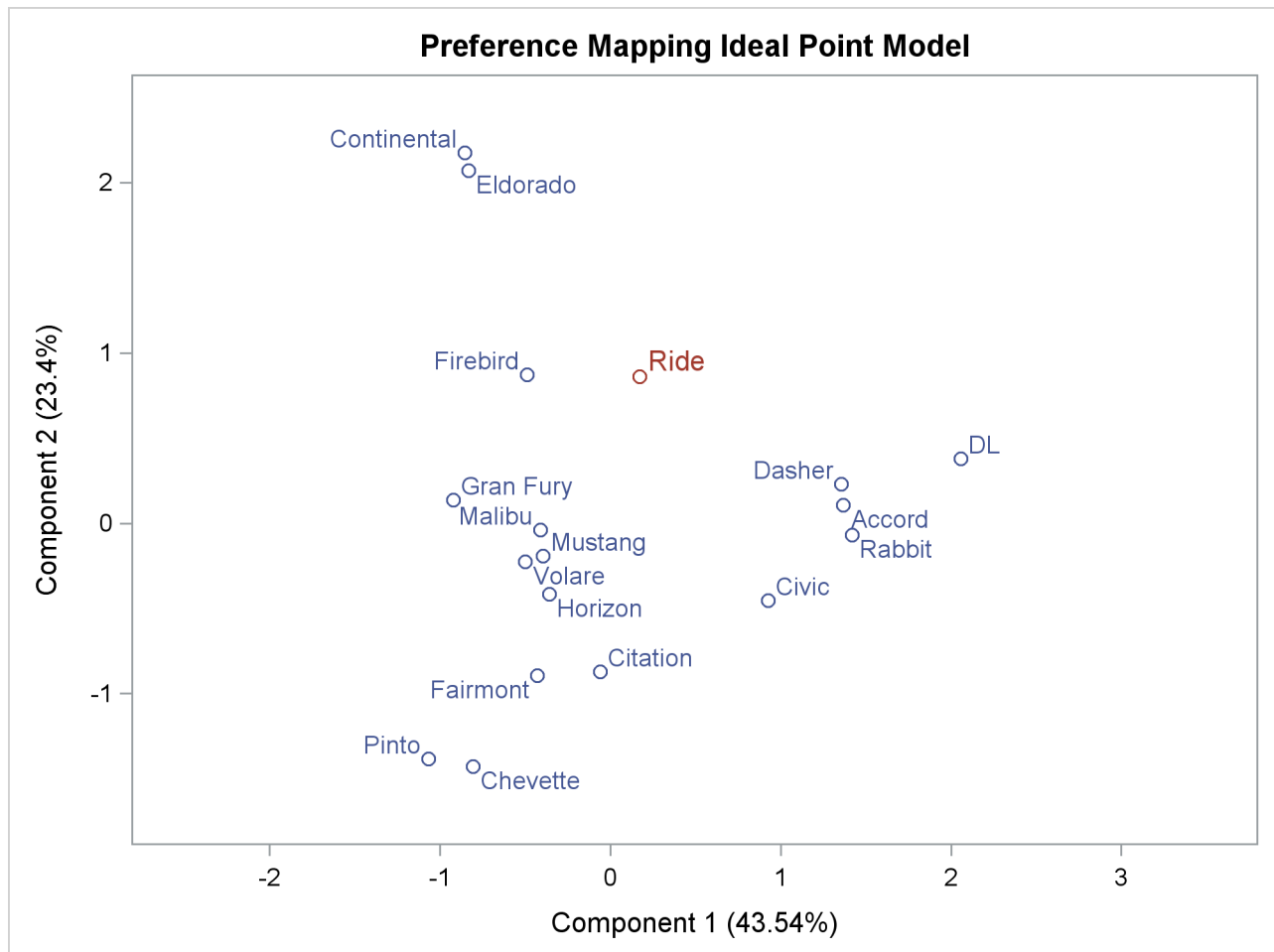


The ideal point for Ride in [Output 97.6.4](#) is in the top, just right of the center of the plot. Automobiles near the Ride ideal point tend to have a better ride than automobiles far away. It can be seen from the R squares that none of these ratings perfectly fits the model, so all of the interpretations are approximate.

**Output 97.6.4** Preference Mapping Ideal Point Plot



**Output 97.6.4** continued



The Ride point is a “negative-negative” ideal point. The point models assume that small ratings mean the object (automobile) is similar to the rating name and large ratings imply dissimilarity to the rating name. Because the opposite scoring is used, the interpretation of the Ride point must be reversed to a negative

ideal point (bad ride). However, the coefficient for the `_ISSQ_` variable in [Output 97.6.5](#) is negative, so the interpretation is reversed again, back to the original interpretation.

### Output 97.6.5 Preference Mapping Ideal Point Coefficients

| Preference Ratings for Automobiles Manufactured in 1980 |         |        |      |           |         |         |          |       |
|---------------------------------------------------------|---------|--------|------|-----------|---------|---------|----------|-------|
| Preference Mapping (PREFMAP) Analysis                   |         |        |      |           |         |         |          |       |
| Obs                                                     | _TYPE_  | _NAME_ | Ride | Intercept | Prin1   | Prin2   | _ISSQ_   | Model |
| 1                                                       | M POINT | Ride   | .    | .         | 0.49461 | 2.46539 | -0.17448 | Ride  |

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# Chapter 98

## The TREE Procedure

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## Overview: TREE Procedure

The TREE procedure reads a data set created by the CLUSTER or VARCLUS procedure and produces a tree diagram (also known as a *dendrogram* or *phenogram*), which displays the results of a hierarchical clustering analysis as a tree structure. The TREE procedure uses the data set to produce a diagram of the tree structure in the style of Johnson (1967), with the root at the top. Alternatively, the diagram can be oriented horizontally, with the root at the left. Any numeric variable in the output data set can be used to specify the heights of the clusters. PROC TREE can also create an output data set that contains a variable to indicate the disjoint clusters at a specified level in the tree.

Tree diagrams are discussed in the context of cluster analysis by Duran and Odell (1974); Hartigan (1975); Everitt (1980). Knuth (1973) provides a general treatment of tree diagrams in computer programming.

The literature on tree diagrams contains a mixture of botanical and genealogical terminology. The objects that are clustered are *leaves*. The cluster that contains all objects is the *root*. A cluster that contains at least two objects but not all of them is a *branch*. The general term for leaves, branches, and roots is *node*. If a cluster A is the union of clusters B and C, then A is the *parent* of B and C, and B and C are *children* of A. A leaf is thus a node with no children, and a root is a node with no parent. If every cluster has at most two children, the tree diagram is a *binary tree*. The CLUSTER procedure always produces binary trees. The VARCLUS procedure can produce tree diagrams with clusters that have many children.

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## Getting Started: TREE Procedure

The TREE procedure creates tree diagrams from a SAS data set that contains the tree structure. You can create this type of data set with the CLUSTER or VARCLUS procedure. See Chapter 31, “The CLUSTER Procedure,” and Chapter 100, “The VARCLUS Procedure,” for more information.

In the following example, the VARCLUS procedure is used to divide a set of variables into hierarchical clusters and to create the SAS data set that contains the tree structure. The TREE procedure then generates the tree diagrams.

The following data, from Hand et al. (1994), represent the amount of protein consumed from nine food groups for each of 25 European countries. The nine food groups are red meat (RedMeat), white meat (WhiteMeat), eggs (Eggs), milk (Milk), fish (Fish), cereal (Cereal), starch (Starch), nuts (Nuts), and fruits and vegetables (FruVeg).

The following SAS statements create the data set Protein:

```

data Protein;
 input Country $15. RedMeat WhiteMeat Eggs Milk
 Fish Cereal Starch Nuts FruVeg;
 datalines;
Albania 10.1 1.4 0.5 8.9 0.2 42.3 0.6 5.5 1.7
Austria 8.9 14.0 4.3 19.9 2.1 28.0 3.6 1.3 4.3
Belgium 13.5 9.3 4.1 17.5 4.5 26.6 5.7 2.1 4.0
Bulgaria 7.8 6.0 1.6 8.3 1.2 56.7 1.1 3.7 4.2
Czechoslovakia 9.7 11.4 2.8 12.5 2.0 34.3 5.0 1.1 4.0
Denmark 10.6 10.8 3.7 25.0 9.9 21.9 4.8 0.7 2.4
E Germany 8.4 11.6 3.7 11.1 5.4 24.6 6.5 0.8 3.6
Finland 9.5 4.9 2.7 33.7 5.8 26.3 5.1 1.0 1.4
France 18.0 9.9 3.3 19.5 5.7 28.1 4.8 2.4 6.5
Greece 10.2 3.0 2.8 17.6 5.9 41.7 2.2 7.8 6.5
Hungary 5.3 12.4 2.9 9.7 0.3 40.1 4.0 5.4 4.2
Ireland 13.9 10.0 4.7 25.8 2.2 24.0 6.2 1.6 2.9
Italy 9.0 5.1 2.9 13.7 3.4 36.8 2.1 4.3 6.7
Netherlands 9.5 13.6 3.6 23.4 2.5 22.4 4.2 1.8 3.7
Norway 9.4 4.7 2.7 23.3 9.7 23.0 4.6 1.6 2.7
Poland 6.9 10.2 2.7 19.3 3.0 36.1 5.9 2.0 6.6
Portugal 6.2 3.7 1.1 4.9 14.2 27.0 5.9 4.7 7.9
Romania 6.2 6.3 1.5 11.1 1.0 49.6 3.1 5.3 2.8
Spain 7.1 3.4 3.1 8.6 7.0 29.2 5.7 5.9 7.2
Sweden 9.9 7.8 3.5 4.7 7.5 19.5 3.7 1.4 2.0
Switzerland 13.1 10.1 3.1 23.8 2.3 25.6 2.8 2.4 4.9
UK 17.4 5.7 4.7 20.6 4.3 24.3 4.7 3.4 3.3
USSR 9.3 4.6 2.1 16.6 3.0 43.6 6.4 3.4 2.9
W Germany 11.4 12.5 4.1 18.8 3.4 18.6 5.2 1.5 3.8
Yugoslavia 4.4 5.0 1.2 9.5 0.6 55.9 3.0 5.7 3.2
;

```

The data set Protein contains the character variable Country and the nine numeric variables that represent the food groups. The \$15. in the INPUT statement specifies that the variable Country is a character variable with a length of 15.

The following statements cluster the variables in the data set Protein:

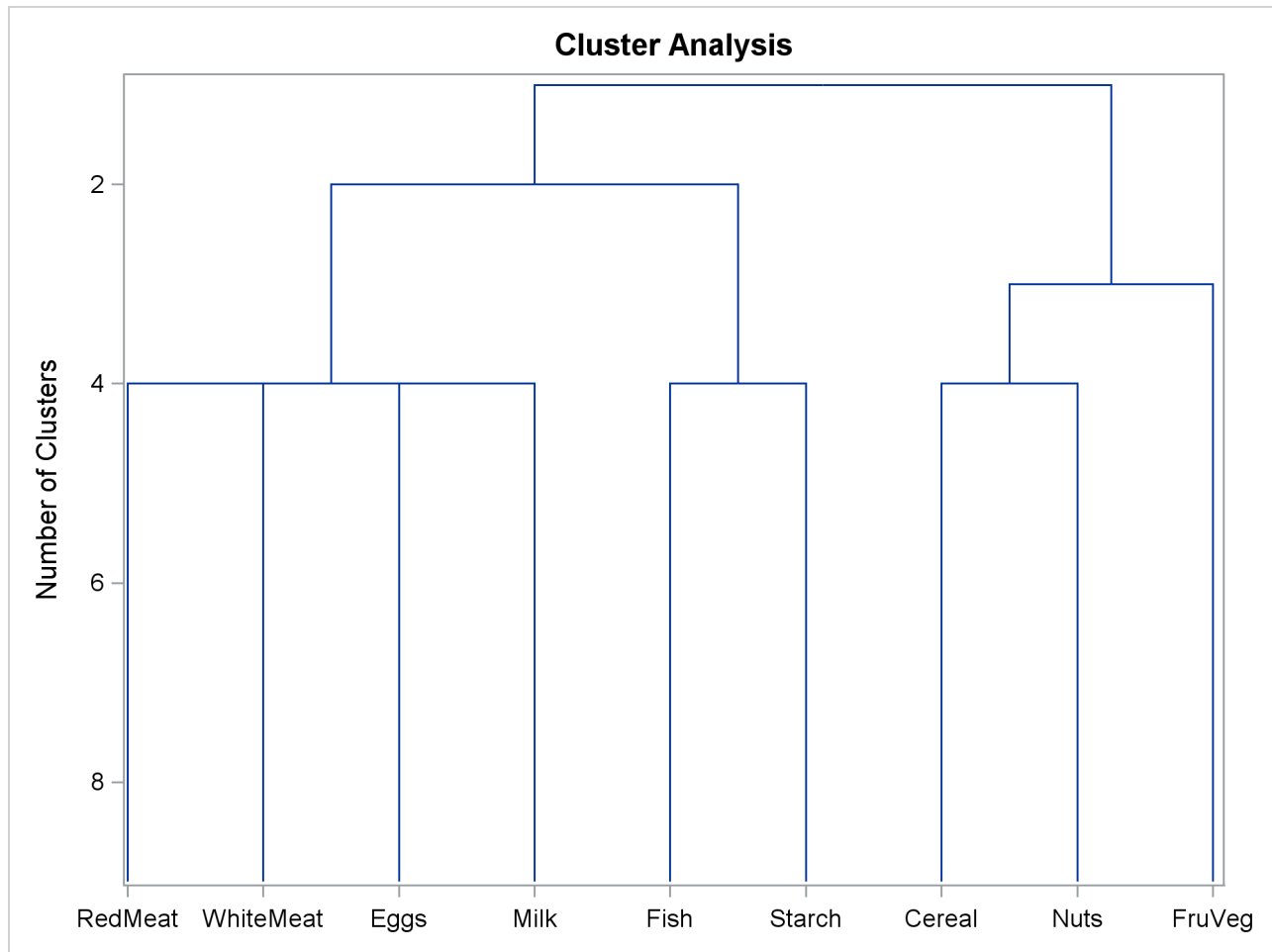
```

ods graphics on;

proc varclus data=Protein outtree=Tree centroid maxclusters=4
 plots=dendrogram(vertical height=ncl);
 var RedMeat--FruVeg;
run;

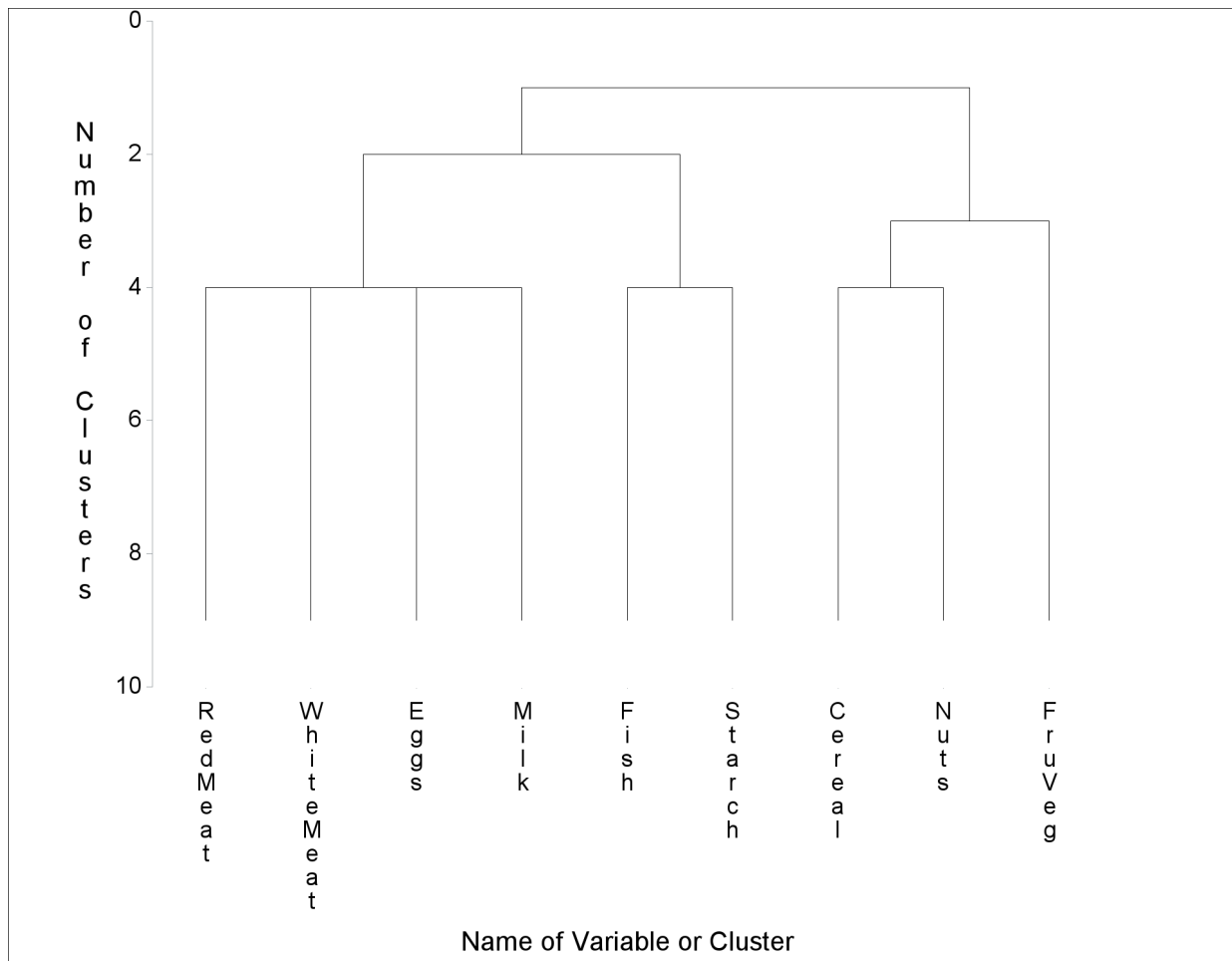
```

The OUTTREE= option creates an output data set named Tree to contain the tree structure. The CENTROID option specifies the centroid clustering method, and the MAXCLUSTERS= option specifies that the largest number of clusters desired is four. The VAR statement specifies that all numeric variables (RedMeat—FruVeg) are used by the procedure. Since ODS Graphics is enabled, PROC VARCLUS creates a dendrogram, which is displayed in [Figure 98.1](#). The option `plots=dendrogram(vertical height=ncl)` specifies a vertical dendrogram with the number of clusters on the vertical axis. The default is a horizontal dendrogram with, for this cluster analysis, the proportion of variance explained on the horizontal axis.

**Figure 98.1** Dendrogram from PROC VARCLUS and ODS Graphics

The output data set `Tree`, created by the `OUTTREE=` option in the previous statements, contains the following variables:

|                         |                                                                                               |
|-------------------------|-----------------------------------------------------------------------------------------------|
| <code>_NAME_</code>     | the name of the cluster                                                                       |
| <code>_PARENT_</code>   | the parent of the cluster                                                                     |
| <code>_NCL_</code>      | the number of clusters                                                                        |
| <code>_VAREXP_</code>   | the amount of variance explained by the cluster                                               |
| <code>_PROPOR_</code>   | the proportion of variance explained by the clusters at the current level of the tree diagram |
| <code>_MINPRO_</code>   | the minimum proportion of variance explained by a cluster                                     |
| <code>_MAXEIGEN_</code> | the maximum second eigenvalue of a cluster                                                    |

**Figure 98.2** Graphical Tree Diagram from PROC TREE

The following statements use PROC TREE to produce tree diagrams of the clusters created by PROC VARCLUS:

```
proc tree data=tree;
run;
```

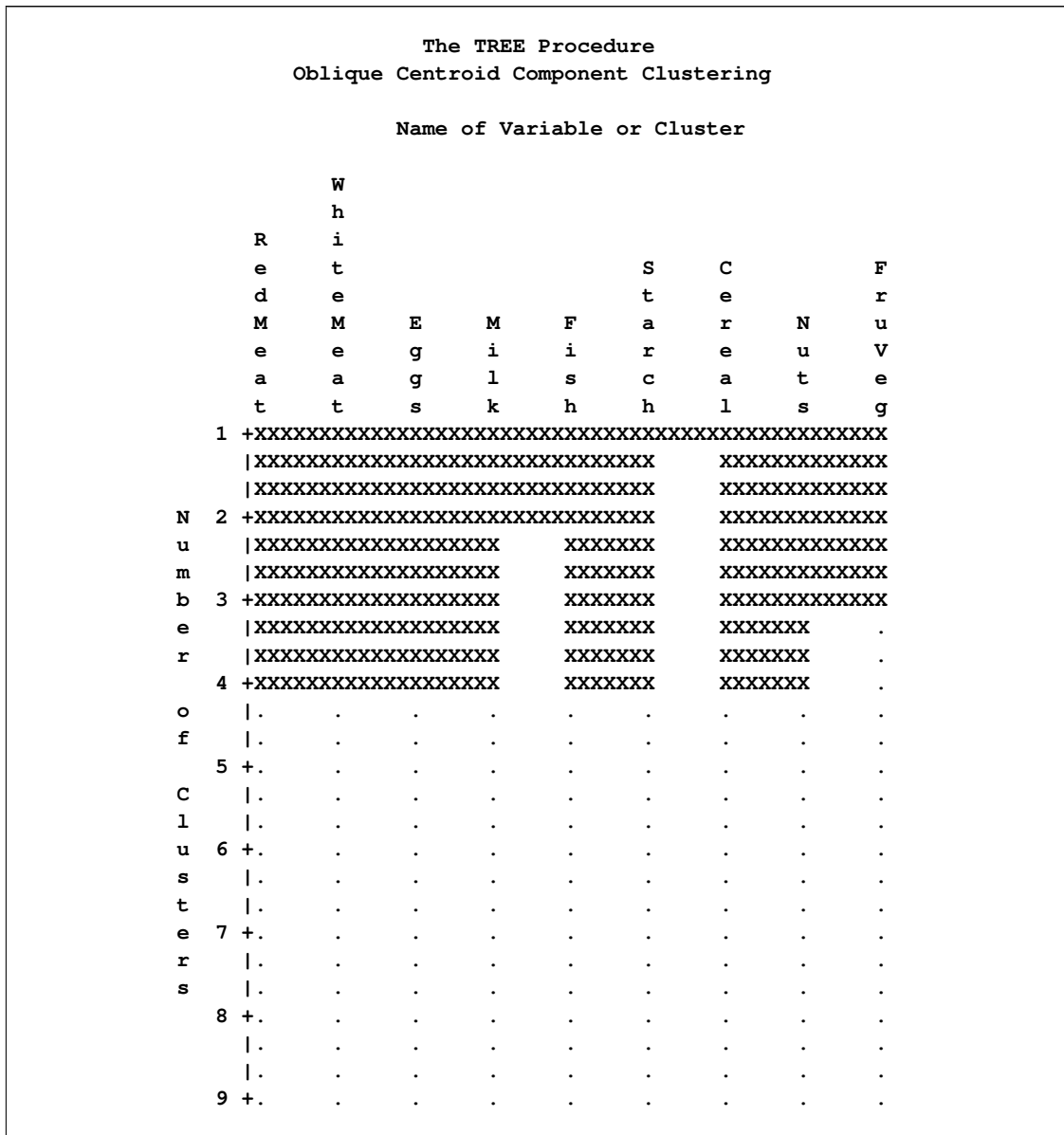
```
proc tree data=tree lineprinter;
run;
```

PROC TREE is invoked twice. In the first invocation, the tree diagram is presented using the default graphical output. In the second invocation, the LINEPRINTER option specifies line printer output.

Figure 98.2 displays the default graphical representation of the tree diagram. Figure 98.3 displays the same information as Figure 98.2 by using line printer output.



**Figure 98.3** Line Printer Representation of the Tree Diagram



In each diagram the name of the cluster is displayed on the horizontal axis and the number of clusters is displayed on the vertical (height) axis.

As you look up from the bottom of either diagram, clusters are progressively joined until a single, all-encompassing cluster is formed at the top (or root) of the tree. Clusters exist at each level of the diagram. For example, at the level where the diagram indicates three clusters, the clusters are as follows:

- Cluster 1: RedMeat WhiteMeat Eggs Milk
- Cluster 2: Fish Starch
- Cluster 3: Cereal Nuts FruVeg

As you proceed up the diagram one level, the number of clusters is two:

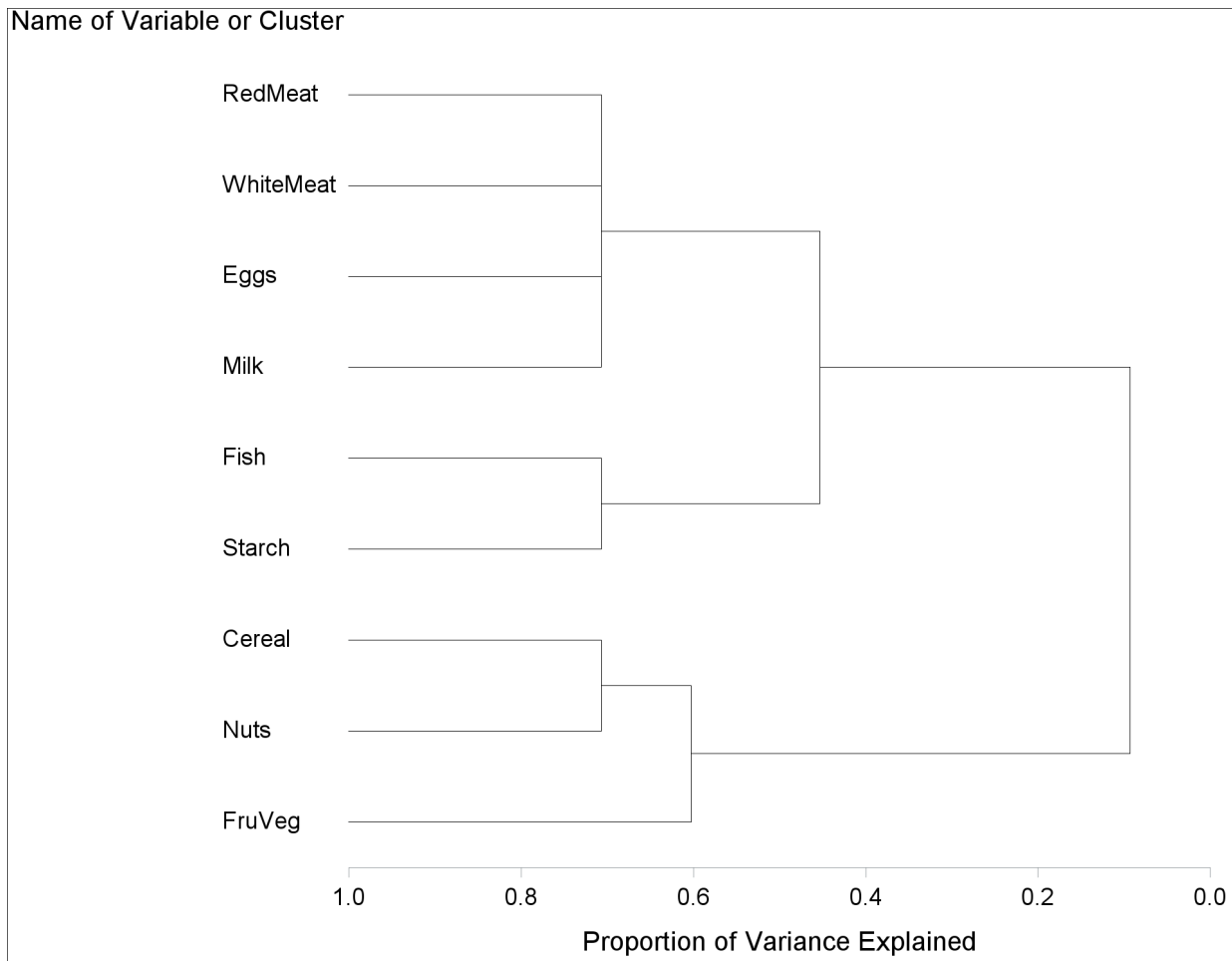
- Cluster 1: RedMeat WhiteMeat Eggs Milk Fish Starch
- Cluster 2: Cereal Nuts FruVeg

The following statements illustrate how you can specify the numeric variable that defines the height of each node (cluster) in the tree:

```
axis1 order=(0 to 1 by 0.2);
proc tree data=Tree horizontal haxis=axis1;
 height _PROPOR_;
run;
```

The ORDER= option in the AXIS1 statement (see *SAS/GRAPH: Reference*) specifies the data values in the order in which they are to appear on the axis. The HORIZONTAL option in the PROC TREE statement orients the tree diagram horizontally. The HAXIS= option specifies that the AXIS1 statement be used to customize the appearance of the horizontal axis. The HEIGHT statement specifies the variable \_PROPOR\_ (the proportion of variance explained) as the height variable.

The resulting tree diagram is shown in [Figure 98.4](#).

**Figure 98.4** Horizontal Tree Diagram with `_PROPOR_` as the HEIGHT Variable

As you look from left to right in the diagram, objects and clusters are progressively joined until a single, all-encompassing cluster is formed at the right (or root) of the tree.

Clusters exist at each level of the diagram, represented by horizontal line segments. Each vertical line segment represents a point where leaves and branches are connected into progressively larger clusters.

For example, three clusters are formed at the leftmost point along the axis where three horizontal line segments exist. At that point, where a vertical line segment connects the Cereal-Nuts and FruVeg clusters, the proportion of variance explained is about 0.6 (`_PROPOR_ = 0.6`). At the next clustering level the variables Fish and Starch are clustered with variables RedMeat through Milk, resulting in a total of two clusters. The proportion of variance explained is about 0.45 at that point.

---

## Syntax: TREE Procedure

The following statements are available in the TREE procedure:

```

PROC TREE < options > ;
 NAME variables ;
 HEIGHT variable ;
 PARENT variables ;
 BY variables ;
 COPY variables ;
 FREQ variable ;
 ID variable ;

```

If the input data set has been created by CLUSTER or VARCLUS, the only statement required is the PROC TREE statement. The BY, COPY, FREQ, HEIGHT, ID, NAME, and PARENT statements are described after the PROC TREE statement.

---

## PROC TREE Statement

```

PROC TREE < options > ;

```

The PROC TREE statement invokes the TREE procedure.

Table 98.1 summarizes the options available in the PROC TREE statement.

**Table 98.1** PROC TREE Statement Options

| Option                  | Description                                                   |
|-------------------------|---------------------------------------------------------------|
| <b>Data Sets</b>        |                                                               |
| DATA=                   | specifies input data set                                      |
| DOCK=                   | specifies that small clusters not be counted in OUT= data set |
| LEVEL=                  | defines disjoint cluster in OUT= data set                     |
| NCLUSTERS=              | specifies number of clusters in OUT= data set                 |
| OUT=                    | specifies output data set                                     |
| ROOT=                   | displays root of a subtree                                    |
| <b>Cluster Heights</b>  |                                                               |
| HEIGHT=                 | specifies variable for the height axis                        |
| DISSIMILAR              | specifies that height values indicate dissimilarity           |
| SIMILAR                 | specifies that height values indicate similarity              |
| <b>Horizontal Trees</b> |                                                               |
| HORIZONTAL              | specifies that height axis be horizontal                      |
| <b>Sort Order</b>       |                                                               |
| DESCENDING              | reverses sort order                                           |
| SORT                    | sorts children by HEIGHT variable                             |
| <b>Displayed Output</b> |                                                               |
| INC=                    | specifies increment between tick values                       |

Table 98.1 *continued*

| Option                       | Description                                                |
|------------------------------|------------------------------------------------------------|
| LINEPRINTER                  | displays tree by using line printer graphics               |
| LIST                         | displays all nodes in tree                                 |
| MAXHEIGHT=                   | specifies maximum value on axis                            |
| MINHEIGHT=                   | specifies minimum value on axis                            |
| NOPRINT                      | suppresses display of tree                                 |
| NTICK=                       | specifies number of tick intervals                         |
| <b>Graphics</b>              |                                                            |
| CFRAME=                      | specifies color of the frame                               |
| DESCRIPTION=                 | specifies catalog description                              |
| GOUT=                        | specifies catalog name                                     |
| HAXIS=                       | customizes horizontal axis                                 |
| HORDISPLAY=                  | displays horizontal tree with leaves on right              |
| HPAGES=                      | specifies number of pages to expand tree horizontally      |
| LINES=                       | specifies line color and thickness, dots at nodes          |
| NAME=                        | specifies name of graph in catalog                         |
| VAXIS=                       | customizes vertical axis                                   |
| VPAGES=                      | specifies number of pages to expand tree vertically        |
| <b>Line Printer Graphics</b> |                                                            |
| PAGES=                       | specifies number of pages                                  |
| POS=                         | specifies number of column positions                       |
| SPACES=                      | specifies number of spaces between objects                 |
| TICKPOS=                     | specifies number of column positions between ticks         |
| FILLCHAR=                    | specifies fill character between unjoined leaves           |
| JOINCHAR=                    | specifies character displayed between joined leaves        |
| LEAFCHAR=                    | specifies character representing clusters with no children |
| TREECHAR=                    | specifies character representing clusters with children    |

**CFRAME=***color*

specifies a color for the frame, which is the rectangle bounded by the axes.

**DATA=***SAS-data-set*

specifies the input data set that defines the tree. If you omit the DATA= option, the most recently created SAS data set is used.

**DESCENDING****DES**

reverses the sort order for the SORT option.

**DESCRIPTION=***entry-description*

specifies a description for the graph in the GOUT= catalog. The default is “Proc Tree Graph Output.”

**DISSIMILAR****DIS**

specifies that the values of the HEIGHT variable are dissimilarities; that is, a large height value means that the clusters are very dissimilar or far apart.

If neither the SIMILAR nor the DISSIMILAR option is specified, PROC TREE attempts to infer from the data whether the height values are similarities or dissimilarities. If PROC TREE cannot tell this from the data, it issues an error message and does not display a tree diagram.

**DOCK=*n***

causes observations in the OUT= data set that have a frequency of *n* or less to be given missing values for the output variables CLUSTER and CLUSNAME. If the NCLUSTERS= option is also specified, DOCK= also prevents clusters with a frequency of *n* or less from being counted toward the number of clusters requested by the NCLUSTERS= option. By default, DOCK=0.

**FILLCHAR='c'****FC='c'**

specifies the character displayed between leaves that are not joined into a cluster. The character should be enclosed in single quotes. The default is a blank. The LINEPRINTER option must also be specified.

**GOUT=< libref.>member-name**

specifies the catalog in which the generated graph is stored. The default is Work.Gseg.

**HAXIS=AXIS*n***

specifies that the AXIS*n* statement be used to customize the appearance of the horizontal axis.

**HEIGHT=*name*****H=*name***

specifies certain conventional variables to be used for the height axis of the tree diagram. For many situations, the only option you need is the HEIGHT= option. Valid values for *name* and their meanings are as follows:

|            |                                                                                                                                        |
|------------|----------------------------------------------------------------------------------------------------------------------------------------|
| HEIGHT   H | specifies the <code>_HEIGHT_</code> variable.                                                                                          |
| LENGTH   L | defines the height of each node as its path length from the root. This can also be interpreted as the number of ancestors of the node. |
| MODE   M   | specifies the <code>_MODE_</code> variable.                                                                                            |
| NCL   N    | specifies the <code>_NCL_</code> (number of clusters) variable.                                                                        |
| RSQ   R    | specifies the <code>_RSQ_</code> variable.                                                                                             |

See also the section “[HEIGHT Statement](#)” on page 8408. The HEIGHT statement can specify any variable in the input data set to be used for the height axis. In rare cases, you might need to specify either the DISSIMILAR option or the SIMILAR option.

**HORDISPLAY=RIGHT**

specifies that the graph be oriented horizontally with the leaf nodes on the right side, when the HORIZONTAL option is also specified. By default, the leaf nodes are on the left side.

**HORIZONTAL****HOR**

displays the tree diagram with the height axis oriented horizontally. The leaf nodes are on the side specified in the HORDISPLAY= option. If you do not specify the HORIZONTAL option, the height axis is vertical, with the root at the top. When the tree takes up more than one page, horizontal orientation can make the tree diagram considerably easier to read.

**HPAGES=*n1***

specifies that the original graph be enlarged to cover *n1* pages. If you also specify the VPAGES=*n2* option, the original graph is enlarged to cover  $n1 \times n2$  graphs. For example, if HPAGES=2 and VPAGES=3, then the original graph is generated, followed by  $2 \times 3 = 6$  more graphs. In these six graphs, the original is enlarged by a factor of 2 in the horizontal direction and by a factor of 3 in the vertical direction. The graphs are generated in left-to-right and top-to-bottom order.

**INC=*n***

specifies the increment between tick values on the height axis. If the HEIGHT variable is \_NCL\_, the default is usually 1, although a different value can be specified for consistency with other options. For any other HEIGHT variable, the default is some power of 10 times 1, 2, 2.5, or 5.

**JOINCHAR='c'****JC='c'**

specifies the character displayed between leaves that are joined into a cluster. The character should be enclosed in single quotes. The default is 'X'. The LINEPRINTER option must also be specified.

**LEAFCHAR='c'****LC='c'**

specifies the character used to represent clusters that have no children. The character should be enclosed in single quotes. The default is a period. The LINEPRINTER option must also be specified.

**LEVEL=*n***

specifies the level of the tree that defines disjoint clusters for the OUT= data set. The LEVEL= option also causes only clusters between the root and a height of *n* to be displayed. The clusters in the output data set are those that exist at a height of *n* on the tree diagram. For example, if the HEIGHT variable is \_NCL\_ (number of clusters) and LEVEL=5 is specified, then the OUT= data set contains five disjoint clusters. If the HEIGHT variable is \_RSQ\_ (R square) and LEVEL=0.9 is specified, then the OUT= data set contains the smallest number of clusters that yields an R square of at least 0.9.

**LINEPRINTER**

specifies that the tree diagram be displayed using line printer graphics.

**LINES=( < COLOR=*color* > < WIDTH=*n* > < DOTS > )**

specifies the color and the thickness of the lines of the tree, and whether a dot is drawn at each leaf node. If the frame and the lines are specified to be the same color, PROC TREE selects a different color for the lines.

**LIST**

lists all the nodes in the tree, displaying the height, parent, and children of each node.

**MAXHEIGHT=*n*****MAXH=*n***

specifies the maximum value displayed on the height axis.

**MINHEIGHT=*n*****MINH=*n***

specifies the minimum value displayed on the height axis.

**NAME=*name***

specifies the entry name for the generated graph in the GOUT= catalog. Each time another graph is generated with the same name, the name is modified by appending a number to make it unique.

**NCLUSTERS=*n*****NCL=*n*****N=*n***

specifies the number of clusters desired in the OUT= data set. The number of clusters obtained might not equal the number specified if (1) there are fewer than *n* leaves in the tree, (2) there are more than *n* unconnected trees in the data set, (3) a multiway tree does not contain a level with the specified number of clusters, or (4) the DOCK= option eliminates too many clusters.

The NCLUSTERS= option uses the `_NCL_` variable to determine the order in which the clusters are formed. If there is no `_NCL_` variable, the height variable (as determined by the HEIGHT statement or HEIGHT= option) is used instead.

**NTICK=*n***

specifies the number of tick intervals on the height axis. The default depends on the values of other options.

**NOPRINT**

suppresses the display of the tree. Specify the NOPRINT option if you want only to create an OUT= data set.

**OUT=*SAS-data-set***

creates an output data set that contains one observation for each object in the tree or subtree being processed and variables called CLUSTER and CLUSNAME that show cluster membership at any specified level in the tree. If you specify the OUT= option, you must also specify either the NCLUSTERS= or LEVEL= option in order to define the output partition level. If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*.

**PAGES=*n***

specifies the number of pages over which the tree diagram (from root to leaves) is to extend. The default is 1. The LINEPRINTER option must also be specified.

**POS=*n***

specifies the number of column positions on the height axis. The default depends on the value of the PAGES= option, the orientation of the tree diagram, and the values specified by the PAGESIZE= and LINESIZE= options. The LINEPRINTER option must also be specified.



**ROOT='name'**

specifies the value of the NAME statement variable for the root of a subtree to be displayed if you do not want to display the entire tree. If you also specify the OUT= option, the output data set contains only objects that belong to the subtree specified by the ROOT= option.

**SIMILAR****SIM**

specifies that the values of the HEIGHT variable represent similarities; that is, a large height value means that the clusters are very similar or close together.

If neither the SIMILAR nor the DISSIMILAR option is specified, PROC TREE attempts to infer from the data whether the height values are similarities or dissimilarities. If PROC TREE cannot tell this from the data, it issues an error message and does not display a tree diagram.

**SORT**

sorts the children of each node by the HEIGHT variable, in the order of cluster formation. See the DESCENDING option for details.

**SPACES=s****S=s**

specifies the number of spaces between objects in the output. The default depends on the number of objects, the orientation of the tree diagram, and the values specified by the PAGESIZE= and LINE-SIZE= options. The LINEPRINTER option must also be specified.

**TICKPOS=n**

specifies the number of column positions per tick interval on the height axis. The default value is usually between 5 and 10, although a different value can be specified for consistency with other options.

**TREECHAR='c'****TC='c'**

specifies the character used to represent clusters with children. The character should be enclosed in single quotes. The default is 'X'. The LINEPRINTER option must also be specified.

**VAXIS=AXISn**

specifies that the AXISn statement be used to customize the appearance of the vertical axis.

**VPAGES=n2**

specifies that the original graph be enlarged to cover  $n2$  pages. If you also specify the HPAGES= $n1$  option, the original graph is enlarged to cover  $n1 \times n2$  pages. For example, if HPAGES=2 and VPAGES=3, then the original graph is generated, followed by  $2 \times 3 = 6$  more graphs. In these six graphs, the original is enlarged by a factor of 2 in the horizontal direction and by a factor of 3 in the vertical direction. The graphs are generated in left-to-right and top-to-bottom order.

---

## BY Statement

**BY variables ;**

You can specify a BY statement with PROC TREE to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the TREE procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

---

## COPY Statement

**COPY variables ;**

The COPY statement specifies one or more character or numeric variables to be copied to the OUT= data set.

---

## FREQ Statement

**FREQ variable ;**

The FREQ statement specifies one numeric variable that tells how many clustering observations belong to the cluster. If the FREQ statement is omitted, PROC TREE uses the variable `_FREQ_` to specify the number of observations per cluster. If neither the FREQ statement nor the `_FREQ_` variable is present, each leaf is assumed to represent one clustering observation, and the frequency for each internal node is found by summing the frequencies of its children.

---

## HEIGHT Statement

**HEIGHT** *variable* ;

The HEIGHT statement specifies the name of a numeric variable to define the height of each node (cluster) in the tree. The height variable can also be specified by the HEIGHT= option in the PROC TREE statement. If both the HEIGHT statement and the HEIGHT= option are omitted, PROC TREE uses the variable `_HEIGHT_`. If the data set does not contain `_HEIGHT_`, PROC TREE uses the variable `_NCL_`. If `_NCL_` is not present either, the height of each node is defined to be its path length from the root.

---

## ID Statement

**ID** *variable* ;

The ID variable is used to identify the objects (leaves) in the tree on the output. The ID variable can be a character or numeric variable of any length. If the ID statement is omitted, the variable in the NAME statement is used instead. If both the ID and NAME statements are omitted, PROC TREE uses the variable `_NAME_`. If the `_NAME_` variable is not found in the data set, PROC TREE issues an error message and stops. The ID variable is copied to the OUT= data set.

---

## NAME Statement

**NAME** *variable* ;

The NAME statement specifies a character or numeric variable that identifies the node represented by each observation. The NAME statement variable and the PARENT statement variable jointly define the tree structure. If the NAME statement is omitted, PROC TREE uses the variable `_NAME_`. If the `_NAME_` variable is not found in the data set, PROC TREE issues an error message and stops.

---

## PARENT Statement

**PARENT** *variable* ;

The PARENT statement specifies a character or numeric variable that identifies the node in the tree that is the parent of each observation. The PARENT statement variable must have the same formatted length as the NAME statement variable. If the PARENT statement is omitted, PROC TREE uses the variable `_PARENT_`. If the `_PARENT_` variable is not found in the data set, PROC TREE issues an error message and stops.

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## Details: TREE Procedure

---

### Missing Values

An observation with a missing value for the NAME statement variable is omitted from processing. If the PARENT statement variable has a missing value but the NAME statement variable is present, the observation is treated as the root of a tree. A data set can contain several roots and, hence, several trees.

Missing values of the HEIGHT variable are set to upper or lower bounds determined from the nonmissing values under the assumption that the heights are monotonic with respect to the tree structure.

Missing values of the FREQ variable are inferred from nonmissing values where possible; otherwise, they are treated as zero.

---

### Output Data Set

The OUT= data set contains one observation for each leaf in the tree or subtree being processed. The variables are as follows:

- the BY variables, if any
- the ID variable, or the NAME statement variable if the ID statement is not used
- the COPY variables
- a numeric variable CLUSTER that takes values from 1 to  $c$ , where  $c$  is the number of disjoint clusters. The cluster to which the first observation belongs is given the number 1, the cluster to which the next observation belongs that does not belong to cluster 1 is given the number 2, and so on.
- a character variable CLUSNAME that gives the value of the NAME statement variable of the cluster to which the observation belongs

The CLUSTER and CLUSNAME variables are missing if the corresponding leaf has a nonpositive frequency.

---

### Displayed Output

The displayed output from the TREE procedure includes the following:

- the names of the objects in the tree
- the height axis
- the tree diagram.

The leaves of the tree diagram are displayed at the bottom of the graph. Horizontal lines connect the leaves into branches, while the topmost horizontal line indicates the root.

If the `LINEPRINTER` option is specified, the root (the cluster that contains all the objects) is indicated by a solid line of the character specified by the `TREECHAR=` option (the default character is 'X'). At each level of the tree, clusters are shown by unbroken lines of the `TREECHAR=` symbol with the `FILLCHAR=` symbol (the default is a blank) separating the clusters. The `LEAFCHAR=` symbol (the default character is a period) represents single-member clusters.

By default, the tree diagram is oriented with the height axis vertical and the object names at the top of the diagram. If the `HORIZONTAL` option is specified, then the height axis is horizontal and the object names are on the left.

---

## ODS Table Names

`PROC TREE` assigns a name to each table it creates. You can use table names to refer to tables when using the Output Delivery System (ODS) to select tables and create output data sets. The name of `PROC TREE`'s only table is listed in Table 98.2. For more information about ODS, see Chapter 20, "Using the Output Delivery System."

**Table 98.2** ODS Tables Produced by `PROC TREE`

| ODS Table Name | Description                      | Statement | Option |
|----------------|----------------------------------|-----------|--------|
| TreeListing    | Listing of all nodes in the tree | PROC      | LIST   |

---

## Examples: TREE Procedure

---

### Example 98.1: Mammals' Teeth

The following statements produce a data set that contains the numbers of different kinds of teeth for a variety of mammals:

```
data teeth;
 title 'Mammals' Teeth';
 input mammal & $16. v1-v8 @@;
 label v1='Right Top Incisors'
 v2='Right Bottom Incisors'
 v3='Right Top Canines'
 v4='Right Bottom Canines'
 v5='Right Top Premolars'
 v6='Right Bottom Premolars'
 v7='Right Top Molars'
 v8='Right Bottom Molars';
 datalines;
Brown Bat 2 3 1 1 3 3 3 3 Mole 3 2 1 0 3 3 3 3
Silver Hair Bat 2 3 1 1 2 3 3 3 Pigmy Bat 2 3 1 1 2 2 3 3
House Bat 2 3 1 1 1 2 3 3 Red Bat 1 3 1 1 2 2 3 3
Pika 2 1 0 0 2 2 3 3 Rabbit 2 1 0 0 3 2 3 3
Beaver 1 1 0 0 2 1 3 3 Groundhog 1 1 0 0 2 1 3 3
Gray Squirrel 1 1 0 0 1 1 3 3 House Mouse 1 1 0 0 0 0 3 3
Porcupine 1 1 0 0 1 1 3 3 Wolf 3 3 1 1 4 4 2 3
Bear 3 3 1 1 4 4 2 3 Raccoon 3 3 1 1 4 4 3 2
Marten 3 3 1 1 4 4 1 2 Weasel 3 3 1 1 3 3 1 2
Wolverine 3 3 1 1 4 4 1 2 Badger 3 3 1 1 3 3 1 2
River Otter 3 3 1 1 4 3 1 2 Sea Otter 3 2 1 1 3 3 1 2
Jaguar 3 3 1 1 3 2 1 1 Cougar 3 3 1 1 3 2 1 1
Fur Seal 3 2 1 1 4 4 1 1 Sea Lion 3 2 1 1 4 4 1 1
Grey Seal 3 2 1 1 3 3 2 2 Elephant Seal 2 1 1 1 4 4 1 1
Reindeer 0 4 1 0 3 3 3 3 Elk 0 4 1 0 3 3 3 3
Deer 0 4 0 0 3 3 3 3 Moose 0 4 0 0 3 3 3 3
;

```

The following statements use the CLUSTER procedure to cluster the mammals by average linkage and use ODS Graphics and the TREE procedure to produce a horizontal tree diagram that uses the average-linkage distance as its height axis:

```
ods graphics on;

proc cluster method=average std pseudo noeigen outtree=tree;
 id mammal;
 var v1-v8;
run;

proc tree horizontal;
run;

```

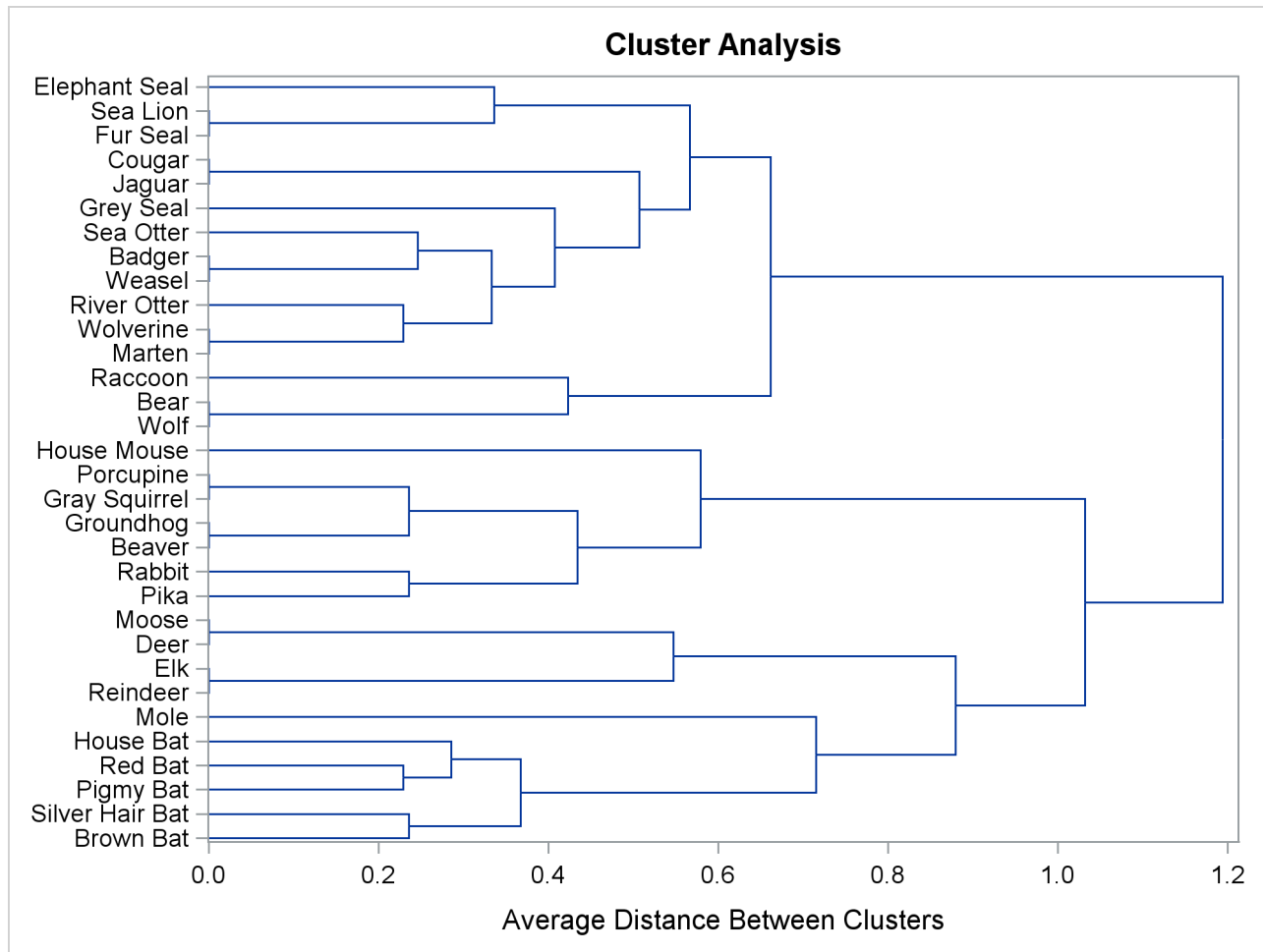
Output 98.1.1 displays the information about how the clusters are joined. For example, the cluster history shows that the mammals ‘Wolf’ and ‘Bear’ form cluster 29, which is merged with ‘Raccoon’ to form cluster 11.

### Output 98.1.1 Output from PROC CLUSTER

| Mammals' Teeth                                           |                           |      |      |      |                           |
|----------------------------------------------------------|---------------------------|------|------|------|---------------------------|
| The CLUSTER Procedure                                    |                           |      |      |      |                           |
| Average Linkage Cluster Analysis                         |                           |      |      |      |                           |
| The data have been standardized to mean 0 and variance 1 |                           |      |      |      |                           |
| Root-Mean-Square Total-Sample Standard Deviation         |                           |      |      |      | 1                         |
| Root-Mean-Square Distance Between Observations           |                           |      |      |      | 4                         |
| Cluster History                                          |                           |      |      |      |                           |
| NCL                                                      | -----Clusters Joined----- | Freq | Ps F | PsT2 | Norm T<br>RMS i<br>Dist e |
| 31                                                       | Beaver Groundhog          | 2    | .    | .    | 0 T                       |
| 30                                                       | Gray Squirrel Porcupine   | 2    | .    | .    | 0 T                       |
| 29                                                       | Wolf Bear                 | 2    | .    | .    | 0 T                       |
| 28                                                       | Marten Wolverine          | 2    | .    | .    | 0 T                       |
| 27                                                       | Weasel Badger             | 2    | .    | .    | 0 T                       |
| 26                                                       | Jaguar Cougar             | 2    | .    | .    | 0 T                       |
| 25                                                       | Fur Seal Sea Lion         | 2    | .    | .    | 0 T                       |
| 24                                                       | Reindeer Elk              | 2    | .    | .    | 0 T                       |
| 23                                                       | Deer Moose                | 2    | .    | .    | 0                         |
| 22                                                       | Pigmy Bat Red Bat         | 2    | 281  | .    | 0.2289                    |
| 21                                                       | CL28 River Otter          | 3    | 139  | .    | 0.2292                    |
| 20                                                       | CL31 CL30                 | 4    | 83.2 | .    | 0.2357 T                  |
| 19                                                       | Brown Bat Silver Hair Bat | 2    | 76.7 | .    | 0.2357 T                  |
| 18                                                       | Pika Rabbit               | 2    | 73.2 | .    | 0.2357                    |
| 17                                                       | CL27 Sea Otter            | 3    | 67.4 | .    | 0.2462                    |
| 16                                                       | CL22 House Bat            | 3    | 62.9 | 1.7  | 0.2859                    |
| 15                                                       | CL21 CL17                 | 6    | 47.4 | 6.8  | 0.3328                    |
| 14                                                       | CL25 Elephant Seal        | 3    | 45.0 | .    | 0.3362                    |
| 13                                                       | CL19 CL16                 | 5    | 40.8 | 3.5  | 0.3672                    |
| 12                                                       | CL15 Grey Seal            | 7    | 38.9 | 2.8  | 0.4078                    |
| 11                                                       | CL29 Raccoon              | 3    | 38.0 | .    | 0.423                     |
| 10                                                       | CL18 CL20                 | 6    | 34.5 | 10.3 | 0.4339                    |
| 9                                                        | CL12 CL26                 | 9    | 30.0 | 7.3  | 0.5071                    |
| 8                                                        | CL24 CL23                 | 4    | 28.7 | .    | 0.5473                    |
| 7                                                        | CL9 CL14                  | 12   | 25.7 | 7.0  | 0.5668                    |
| 6                                                        | CL10 House Mouse          | 7    | 28.3 | 4.1  | 0.5792                    |
| 5                                                        | CL11 CL7                  | 15   | 26.8 | 6.9  | 0.6621                    |
| 4                                                        | CL13 Mole                 | 6    | 31.9 | 7.2  | 0.7156                    |
| 3                                                        | CL4 CL8                   | 10   | 31.0 | 12.7 | 0.8799                    |
| 2                                                        | CL3 CL6                   | 17   | 27.8 | 16.1 | 1.0316                    |
| 1                                                        | CL2 CL5                   | 32   | .    | 27.8 | 1.1938                    |

Output 98.1.2 shows the tree diagram produced by PROC CLUSTER.

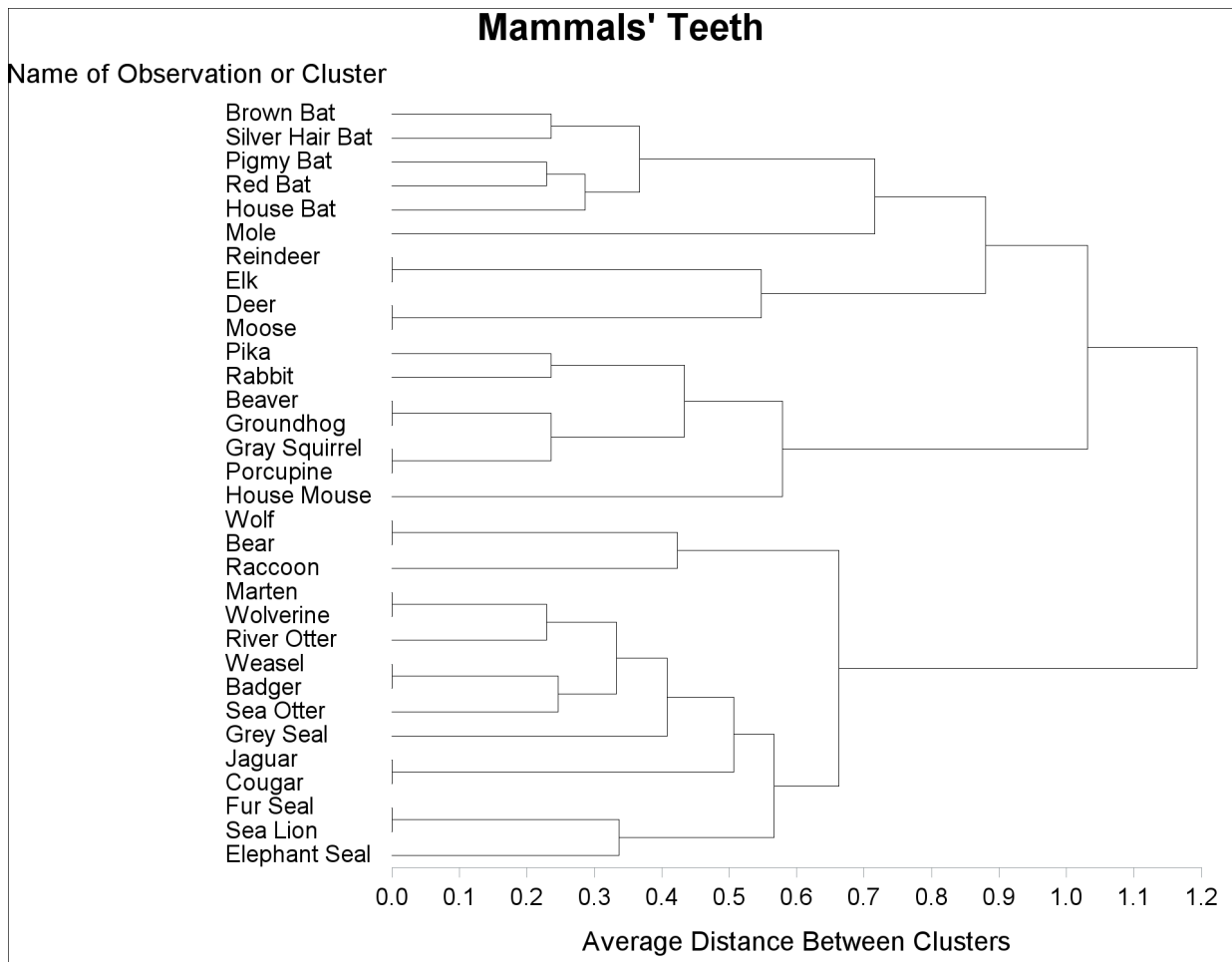
**Output 98.1.2** Dendrogram from PROC CLUSTER





Output 98.1.3 shows the corresponding tree diagram produced by PROC TREE.

**Output 98.1.3** Tree Diagram of Mammal Teeth Clusters



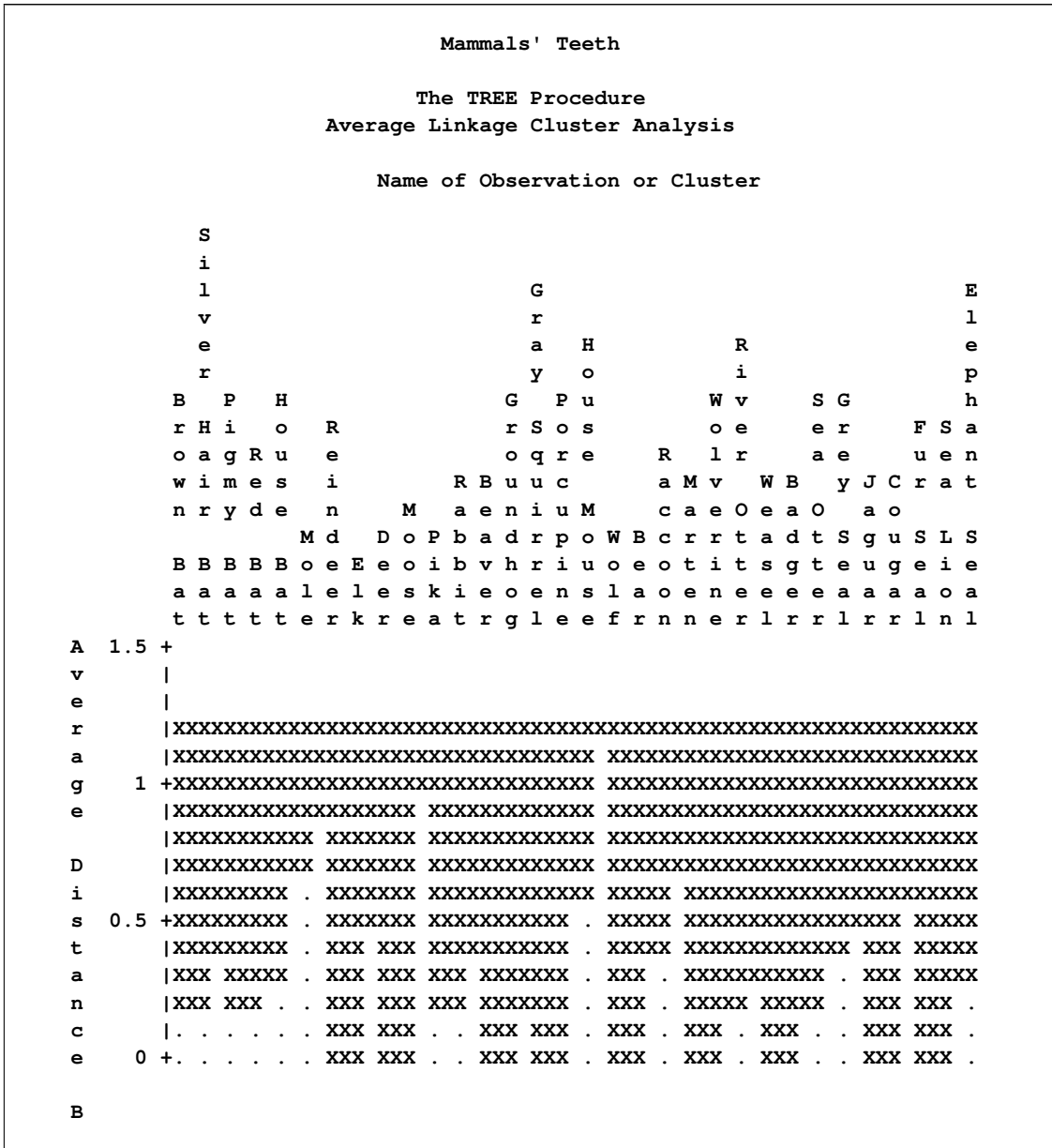
As you view the diagram in [Output 98.1.3](#) from left to right, objects and clusters are progressively joined until a single, all-encompassing cluster is formed at the right (or root) of the tree. Clusters exist at each level of the diagram, and every vertical line connects leaves and branches into progressively larger clusters. For example, the five bats form a cluster at the 0.6 level, while the next cluster consists only of the mole. The mammals ‘Reindeer’, ‘Elk’, ‘Deer’, and ‘Moose’ form the next cluster at the 0.6 level, the mammals ‘Pika’ through ‘House Mouse’ are in the fourth cluster, the mammals ‘Wolf’, ‘Bear’, and ‘Raccoon’ form the fifth cluster, and the last cluster contains the mammals ‘Marten’ through ‘Elephant Seal’.

The following statements create the same tree with line printer graphics in a vertical orientation:

```
proc tree lineprinter;
run;
```

The tree is displayed in [Output 98.1.4](#).

**Output 98.1.4** PROC TREE with the LINEPRINTER Option



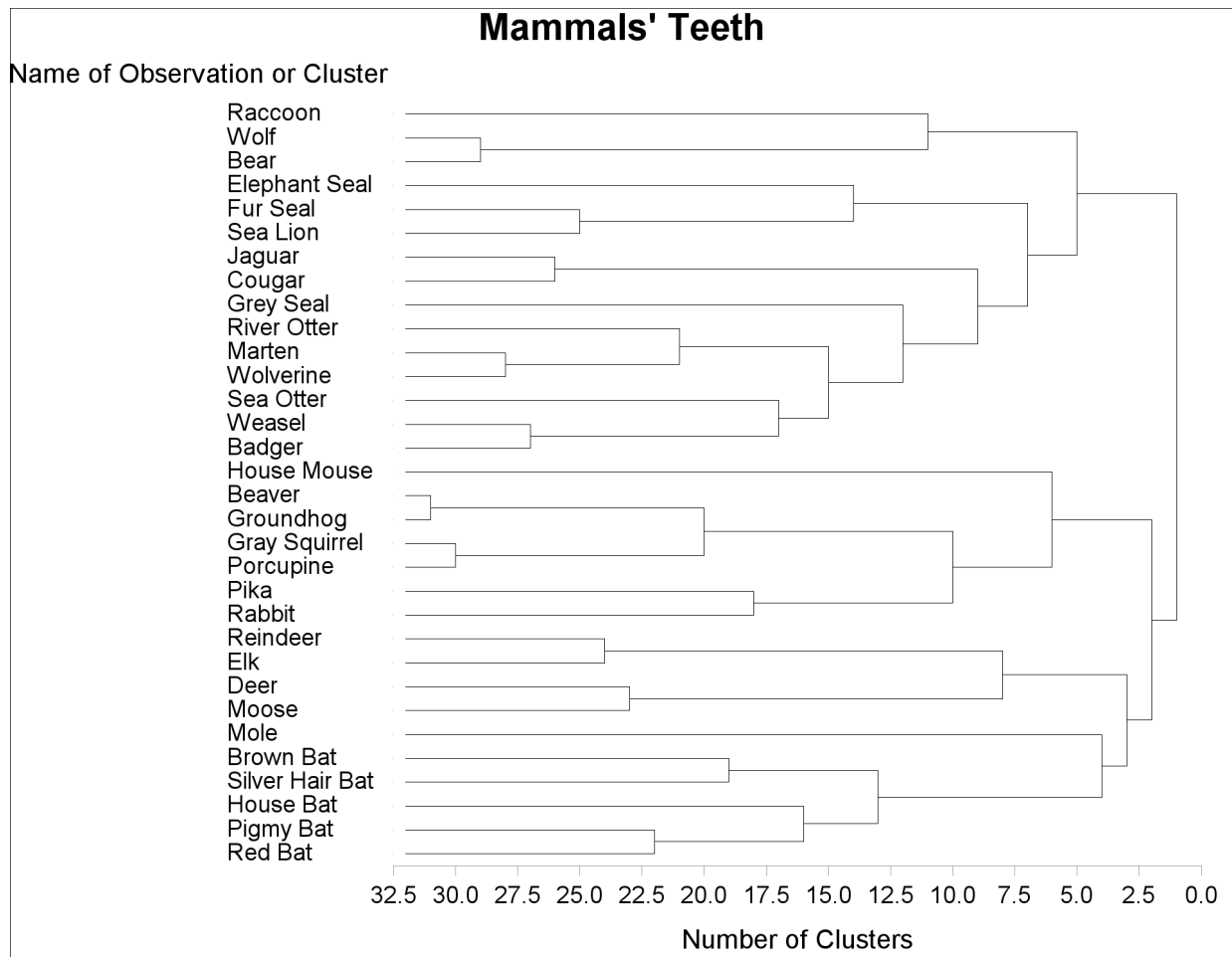
As you look up from the bottom of the diagram, objects and clusters are progressively joined until a single, all-encompassing cluster is formed at the top (or root) of the root. Clusters exist at each level of the diagram. For example, the unbroken line of Xs at the leftmost side of the 0.6 level indicates that the five bats have formed a cluster. The next cluster is represented by a period because it contains only one mammal, 'Mole'. The mammals 'Reindeer', 'Elk', 'Deer', and 'Moose' form the next cluster, indicated by Xs again. The mammals 'Pika' through 'House Mouse' are in the fourth cluster. The mammals 'Wolf', 'Bear', and 'Raccoon' form the fifth cluster, while the last cluster contains the mammals 'Marten' through 'Elephant Seal'.

The next statements sort the clusters at each branch in order of formation and use the number of clusters as the height axis:

```
proc tree sort height=n horizontal;
run;
```

The resulting tree is displayed in [Output 98.1.5](#).

**Output 98.1.5** PROC TREE with SORT and HEIGHT= Options



Because the CLUSTER procedure always produces binary trees, the number of internal (root and branch) nodes in the tree is one less than the number of leaves. Therefore 31 clusters are formed from the 32 mammals in the input data set. These are represented by the 31 vertical line segments in the tree diagram, each at a different value along the horizontal axis.

As you examine the tree from left to right, the first vertical line segment is where 'Beaver' and 'Groundhog' are clustered and the number of clusters is 31. The next cluster is formed from 'Gray Squirrel' and 'Porcupine'. The third contains 'Wolf' and 'Bear'. Note how the tree graphically displays the clustering order information that was presented in tabular form by the CLUSTER procedure in [Output 98.1.1](#).

The same clusters as in [Output 98.1.3](#) and [Output 98.1.4](#) can be seen at the six-cluster level of the tree diagram in [Output 98.1.5](#), although the SORT and HEIGHT= options make them appear in a different order.

The following statements create these six clusters and save the result in the output data set part:

```
proc tree noprint out=part nclusters=6;
 id mammal;
 copy v1-v8;
run;

proc sort;
 by cluster;
run;
```

PROC TREE with the NOPRINT option displays no output but creates an output data set that indicates the cluster to which each observation belongs at the six-cluster level in the tree. The following statements print the data set part, with the results shown in [Output 98.1.6](#):

```
proc print label uniform;
 id mammal;
 var v1-v8;
 format v1-v8 1.;
 by cluster;
run;
```

**Output 98.1.6** PROC TREE OUT= Data Set

| Mammals' Teeth        |                          |                              |                         |                            |
|-----------------------|--------------------------|------------------------------|-------------------------|----------------------------|
| ----- CLUSTER=1 ----- |                          |                              |                         |                            |
| mammal                | Right<br>Top<br>Incisors | Right<br>Bottom<br>Incisors  | Right<br>Top<br>Canines | Right<br>Bottom<br>Canines |
| Beaver                | 1                        | 1                            | 0                       | 0                          |
| Groundhog             | 1                        | 1                            | 0                       | 0                          |
| Gray Squirrel         | 1                        | 1                            | 0                       | 0                          |
| Porcupine             | 1                        | 1                            | 0                       | 0                          |
| Pika                  | 2                        | 1                            | 0                       | 0                          |
| Rabbit                | 2                        | 1                            | 0                       | 0                          |
| House Mouse           | 1                        | 1                            | 0                       | 0                          |
| mammal                | Right Top<br>Premolars   | Right<br>Bottom<br>Premolars | Right<br>Top<br>Molars  | Right<br>Bottom<br>Molars  |
| Beaver                | 2                        | 1                            | 3                       | 3                          |
| Groundhog             | 2                        | 1                            | 3                       | 3                          |
| Gray Squirrel         | 1                        | 1                            | 3                       | 3                          |
| Porcupine             | 1                        | 1                            | 3                       | 3                          |
| Pika                  | 2                        | 2                            | 3                       | 3                          |
| Rabbit                | 3                        | 2                            | 3                       | 3                          |
| House Mouse           | 0                        | 0                            | 3                       | 3                          |

Output 98.1.6 *continued*

| Mammals' Teeth        |                          |                              |                         |                            |
|-----------------------|--------------------------|------------------------------|-------------------------|----------------------------|
| ----- CLUSTER=2 ----- |                          |                              |                         |                            |
| mammal                | Right<br>Top<br>Incisors | Right<br>Bottom<br>Incisors  | Right<br>Top<br>Canines | Right<br>Bottom<br>Canines |
| Wolf                  | 3                        | 3                            | 1                       | 1                          |
| Bear                  | 3                        | 3                            | 1                       | 1                          |
| Raccoon               | 3                        | 3                            | 1                       | 1                          |
| mammal                | Right Top<br>Premolars   | Right<br>Bottom<br>Premolars | Right<br>Top<br>Molars  | Right<br>Bottom<br>Molars  |
| Wolf                  | 4                        | 4                            | 2                       | 3                          |
| Bear                  | 4                        | 4                            | 2                       | 3                          |
| Raccoon               | 4                        | 4                            | 3                       | 2                          |
| ----- CLUSTER=3 ----- |                          |                              |                         |                            |
| mammal                | Right<br>Top<br>Incisors | Right<br>Bottom<br>Incisors  | Right<br>Top<br>Canines | Right<br>Bottom<br>Canines |
| Marten                | 3                        | 3                            | 1                       | 1                          |
| Wolverine             | 3                        | 3                            | 1                       | 1                          |
| Weasel                | 3                        | 3                            | 1                       | 1                          |
| mammal                | Right Top<br>Premolars   | Right<br>Bottom<br>Premolars | Right<br>Top<br>Molars  | Right<br>Bottom<br>Molars  |
| Marten                | 4                        | 4                            | 1                       | 2                          |
| Wolverine             | 4                        | 4                            | 1                       | 2                          |
| Weasel                | 3                        | 3                            | 1                       | 2                          |

Output 98.1.6 *continued*

| Mammals' Teeth        |                          |                              |                         |                            |
|-----------------------|--------------------------|------------------------------|-------------------------|----------------------------|
| ----- CLUSTER=3 ----- |                          |                              |                         |                            |
| (continued)           |                          |                              |                         |                            |
| mammal                | Right<br>Top<br>Incisors | Right<br>Bottom<br>Incisors  | Right<br>Top<br>Canines | Right<br>Bottom<br>Canines |
| Badger                | 3                        | 3                            | 1                       | 1                          |
| Jaguar                | 3                        | 3                            | 1                       | 1                          |
| Cougar                | 3                        | 3                            | 1                       | 1                          |
| Fur Seal              | 3                        | 2                            | 1                       | 1                          |
| Sea Lion              | 3                        | 2                            | 1                       | 1                          |
| River Otter           | 3                        | 3                            | 1                       | 1                          |
| Sea Otter             | 3                        | 2                            | 1                       | 1                          |
| Elephant Seal         | 2                        | 1                            | 1                       | 1                          |
| Grey Seal             | 3                        | 2                            | 1                       | 1                          |
| mammal                | Right Top<br>Premolars   | Right<br>Bottom<br>Premolars | Right<br>Top<br>Molars  | Right<br>Bottom<br>Molars  |
| Badger                | 3                        | 3                            | 1                       | 2                          |
| Jaguar                | 3                        | 2                            | 1                       | 1                          |
| Cougar                | 3                        | 2                            | 1                       | 1                          |
| Fur Seal              | 4                        | 4                            | 1                       | 1                          |
| Sea Lion              | 4                        | 4                            | 1                       | 1                          |
| River Otter           | 4                        | 3                            | 1                       | 2                          |
| Sea Otter             | 3                        | 3                            | 1                       | 2                          |
| Elephant Seal         | 4                        | 4                            | 1                       | 1                          |
| Grey Seal             | 3                        | 3                            | 2                       | 2                          |

Output 98.1.6 *continued*

| Mammals' Teeth        |                          |                              |                         |                            |
|-----------------------|--------------------------|------------------------------|-------------------------|----------------------------|
| ----- CLUSTER=4 ----- |                          |                              |                         |                            |
| mammal                | Right<br>Top<br>Incisors | Right<br>Bottom<br>Incisors  | Right<br>Top<br>Canines | Right<br>Bottom<br>Canines |
| Reindeer              | 0                        | 4                            | 1                       | 0                          |
| Elk                   | 0                        | 4                            | 1                       | 0                          |
| Deer                  | 0                        | 4                            | 0                       | 0                          |
| Moose                 | 0                        | 4                            | 0                       | 0                          |
| mammal                | Right Top<br>Premolars   | Right<br>Bottom<br>Premolars | Right<br>Top<br>Molars  | Right<br>Bottom<br>Molars  |
| Reindeer              | 3                        | 3                            | 3                       | 3                          |
| Elk                   | 3                        | 3                            | 3                       | 3                          |
| Deer                  | 3                        | 3                            | 3                       | 3                          |
| Moose                 | 3                        | 3                            | 3                       | 3                          |
| ----- CLUSTER=5 ----- |                          |                              |                         |                            |
| mammal                | Right<br>Top<br>Incisors | Right<br>Bottom<br>Incisors  | Right<br>Top<br>Canines | Right<br>Bottom<br>Canines |
| Pigmy Bat             | 2                        | 3                            | 1                       | 1                          |
| Red Bat               | 1                        | 3                            | 1                       | 1                          |
| mammal                | Right Top<br>Premolars   | Right<br>Bottom<br>Premolars | Right<br>Top<br>Molars  | Right<br>Bottom<br>Molars  |
| Pigmy Bat             | 2                        | 2                            | 3                       | 3                          |
| Red Bat               | 2                        | 2                            | 3                       | 3                          |

**Output 98.1.6** *continued*

| Mammals' Teeth        |                          |                              |                         |                            |
|-----------------------|--------------------------|------------------------------|-------------------------|----------------------------|
| ----- CLUSTER=5 ----- |                          |                              |                         |                            |
| (continued)           |                          |                              |                         |                            |
| mammal                | Right<br>Top<br>Incisors | Right<br>Bottom<br>Incisors  | Right<br>Top<br>Canines | Right<br>Bottom<br>Canines |
| Brown Bat             | 2                        | 3                            | 1                       | 1                          |
| Silver Hair Bat       | 2                        | 3                            | 1                       | 1                          |
| House Bat             | 2                        | 3                            | 1                       | 1                          |
| mammal                | Right Top<br>Premolars   | Right<br>Bottom<br>Premolars | Right<br>Top<br>Molars  | Right<br>Bottom<br>Molars  |
| Brown Bat             | 3                        | 3                            | 3                       | 3                          |
| Silver Hair Bat       | 2                        | 3                            | 3                       | 3                          |
| House Bat             | 1                        | 2                            | 3                       | 3                          |
| ----- CLUSTER=6 ----- |                          |                              |                         |                            |
| mammal                | Right<br>Top<br>Incisors | Right<br>Bottom<br>Incisors  | Right<br>Top<br>Canines | Right<br>Bottom<br>Canines |
| Mole                  | 3                        | 2                            | 1                       | 0                          |
| mammal                | Right Top<br>Premolars   | Right<br>Bottom<br>Premolars | Right<br>Top<br>Molars  | Right<br>Bottom<br>Molars  |
| Mole                  | 3                        | 3                            | 3                       | 3                          |



---

## Example 98.2: Iris Data

Fisher (1936)'s iris data give sepal and petal dimensions for three different species of iris. The data, which are available in the Sashelp library, are clustered by *k*th-nearest-neighbor density linkage by using the CLUSTER procedure with *K*=8. Observations are identified by species ('Setosa', 'Versicolor', or 'Virginica') in the tree diagram, which is oriented with the height axis horizontal.

The following statements produce the results shown in [Output 98.2.1](#) and [Output 98.2.2](#):

```
title 'Fisher (1936) Iris Data';
ods graphics on;

proc cluster data=sashelp.iris method=twostage print=10
 outtree=tree k=8 noeigen;
 var SepalLength SepalWidth PetalLength PetalWidth;
 copy Species;
run;

proc tree data=tree horizontal lineprinter pages=1 maxh=10;
 id species;
run;
```

The PAGES=1 option specifies that the tree diagram extend over one page from tree to root. Since the HORIZONTAL option is also specified, the horizontal extent of the diagram is one page. The number of vertical pages required for the diagram is dictated by the number of leaves in the tree.

The MAXH=10 limits the values displayed on the height axis to a maximum of 10. This prunes the tree diagram so that only the portion from the leaves to level 10 is displayed. You can see this pruning effect in [Output 98.2.2](#).

**Output 98.2.1** Clustering of Fisher's Iris Data

| Fisher (1936) Iris Data                          |                              |       |      |                                 |                                    |          |     |
|--------------------------------------------------|------------------------------|-------|------|---------------------------------|------------------------------------|----------|-----|
| The CLUSTER Procedure                            |                              |       |      |                                 |                                    |          |     |
| Two-Stage Density Linkage Clustering             |                              |       |      |                                 |                                    |          |     |
| K = 8                                            |                              |       |      |                                 |                                    |          |     |
| Root-Mean-Square Total-Sample Standard Deviation |                              |       |      |                                 |                                    | 10.69224 |     |
| Cluster History                                  |                              |       |      |                                 |                                    |          |     |
| Number<br>of<br>Clusters                         | -----Clusters<br>Joined----- |       | Freq | Normalized<br>Fusion<br>Density | Maximum Density<br>in Each Cluster |          |     |
|                                                  |                              |       |      |                                 | Lesser                             | Greater  | Tie |
| 10                                               | CL11                         | OB79  | 48   | 0.2879                          | 0.1479                             | 8.3678   |     |
| 9                                                | CL13                         | OB112 | 46   | 0.2802                          | 0.2005                             | 3.5156   |     |
| 8                                                | CL10                         | OB113 | 49   | 0.2699                          | 0.1372                             | 8.3678   |     |
| 7                                                | CL8                          | OB91  | 50   | 0.2586                          | 0.1372                             | 8.3678   |     |
| 6                                                | CL9                          | OB120 | 47   | 0.1412                          | 0.0832                             | 3.5156   |     |
| 5                                                | CL6                          | OB118 | 48   | 0.107                           | 0.0605                             | 3.5156   |     |
| 4                                                | CL5                          | OB110 | 49   | 0.0969                          | 0.0541                             | 3.5156   |     |
| 3                                                | CL4                          | OB135 | 50   | 0.0715                          | 0.0370                             | 3.5156   |     |
| 2                                                | CL7                          | CL3   | 100  | 2.6277                          | 3.5156                             | 8.3678   |     |

3 modal clusters have been formed.











Output 98.2.2 *continued*

```

 XXXXXX
Virginica XXXXXX.....
 XXXXXX
Virginica XXXXXX.....
 XXXXXX
Virginica XXXXXX.....
 XXXX
Virginica XXXX.....
 XXXX
Virginica XXXX.....
 XXX
Virginica XXX.....
 XX
Virginica XX.....
 X
Virginica X.....

```

---

## References

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- Everitt, B. S. (1980), *Cluster Analysis*, Second Edition, London: Heineman Educational Books.
- Fisher, R. A. (1936), "The Use of Multiple Measurements in Taxonomic Problems," *Annals of Eugenics*, 7, 179–188.
- Hand, D. J., Daly, F., Lunn, A. D., McConway, K. J., and Ostrowski, E. (1994), *A Handbook of Small Data Sets*, London: Chapman & Hall.
- Hartigan, J. A. (1975), *Clustering Algorithms*, New York: John Wiley & Sons.
- Johnson, S. C. (1967), "Hierarchical Clustering Schemes," *Psychometrika*, 32, 241–254.
- Knuth, D. E. (1973), *The Art of Computer Programming, Volume 1, Fundamental Algorithms*, Reading, MA: Addison-Wesley.





# Chapter 99

## The TTEST Procedure

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---

## Overview: TTEST Procedure

The TTEST procedure performs  $t$  tests and computes confidence limits for one sample, paired observations, two independent samples, and the AB/BA crossover design. Two-sided, TOST (two one-sided test) equivalence, and upper and lower one-sided hypotheses are supported for means, mean differences, and mean ratios for either normal or lognormal data.

Table 99.1 summarizes the designs, analysis criteria, hypotheses, and distributional assumptions supported in the TTEST procedure, along with the syntax used to specify them.

**Table 99.1** Features Supported in the TTEST Procedure

| Feature                   | Syntax                                |
|---------------------------|---------------------------------------|
| <b>Design</b>             |                                       |
| One-sample                | VAR statement                         |
| Paired                    | PAIRED statement                      |
| Two-independent-sample    | CLASS statement, VAR statement        |
| AB/BA crossover           | VAR / CROSSOVER=                      |
| <b>Analysis Criterion</b> |                                       |
| Mean difference           | PROC TTEST TEST=DIFF                  |
| Mean ratio                | PROC TTEST TEST=RATIO                 |
| <b>Hypothesis</b>         |                                       |
| Two-sided                 | PROC TTEST SIDES=2                    |
| Equivalence               | PROC TTEST TOST ( < lower , > upper ) |
| Lower one-sided           | PROC TTEST SIDES=L                    |
| Upper one-sided           | PROC TTEST SIDES=U                    |
| <b>Distribution</b>       |                                       |
| Normal                    | PROC TTEST DIST=NORMAL                |
| Lognormal                 | PROC TTEST DIST=LOGNORMAL             |

FREQ and WEIGHT statements are available. Data can be input in the form of observations or, in certain cases, summary statistics. Output includes summary statistics; confidence limits for means, standard deviations, and coefficients of variation; hypothesis tests; and a variety of graphical displays, including histograms, densities, box plots, confidence intervals, Q-Q plots, profiles, and agreement plots.

PROC TTEST uses ODS Graphics to create graphs as part of its output. For general information about ODS Graphics, see Chapter 21, “Statistical Graphics Using ODS.” For specific information about the statistical graphics available with the TTEST procedure, see the PLOTS option in the PROC TTEST statement and the section “ODS Graphics” on page 8465.

## Getting Started: TTEST Procedure

### One-Sample $t$ Test

A one-sample  $t$  test can be used to compare a sample mean to a given value. This example, taken from Huntsberger and Billingsley (1989, p. 290), tests whether the mean length of a certain type of court case is more than 80 days by using 20 randomly chosen cases. The data are read by the following DATA step:

```
data time;
 input time @@;
 datalines;
 43 90 84 87 116 95 86 99 93 92
 121 71 66 98 79 102 60 112 105 98
 ;
```

The only variable in the data set, time, is assumed to be normally distributed. The trailing at signs (@@) indicate that there is more than one observation on a line. The following statements invoke PROC TTEST for a one-sample  $t$  test:

```
ods graphics on;

proc ttest h0=80 plots(showh0) sides=u alpha=0.1;
 var time;
run;

ods graphics off;
```

The VAR statement indicates that the time variable is being studied, while the H0= option specifies that the mean of the time variable should be compared to the null value 80 rather than the default of 0. The PLOTS(SHOWH0) option requests that this null value be displayed on all relevant graphs. The SIDES=U option reflects the focus of the research question, namely whether the mean court case length is *greater than* 80 days, rather than *different than* 80 days (in which case you would use the default SIDES=2 option). The ALPHA=0.1 option requests 90% confidence intervals rather than the default 95% confidence intervals. The output is displayed in Figure 99.1.

**Figure 99.1** One-Sample  $t$  Test Results

| The TTEST Procedure |             |         |                |         |         |
|---------------------|-------------|---------|----------------|---------|---------|
| Variable: time      |             |         |                |         |         |
| N                   | Mean        | Std Dev | Std Err        | Minimum | Maximum |
| 20                  | 89.8500     | 19.1456 | 4.2811         | 43.0000 | 121.0   |
| Mean                | 90% CL Mean | Std Dev | 90% CL Std Dev |         |         |
| 89.8500             | 84.1659     | Infty   | 19.1456        | 15.2002 | 26.2374 |

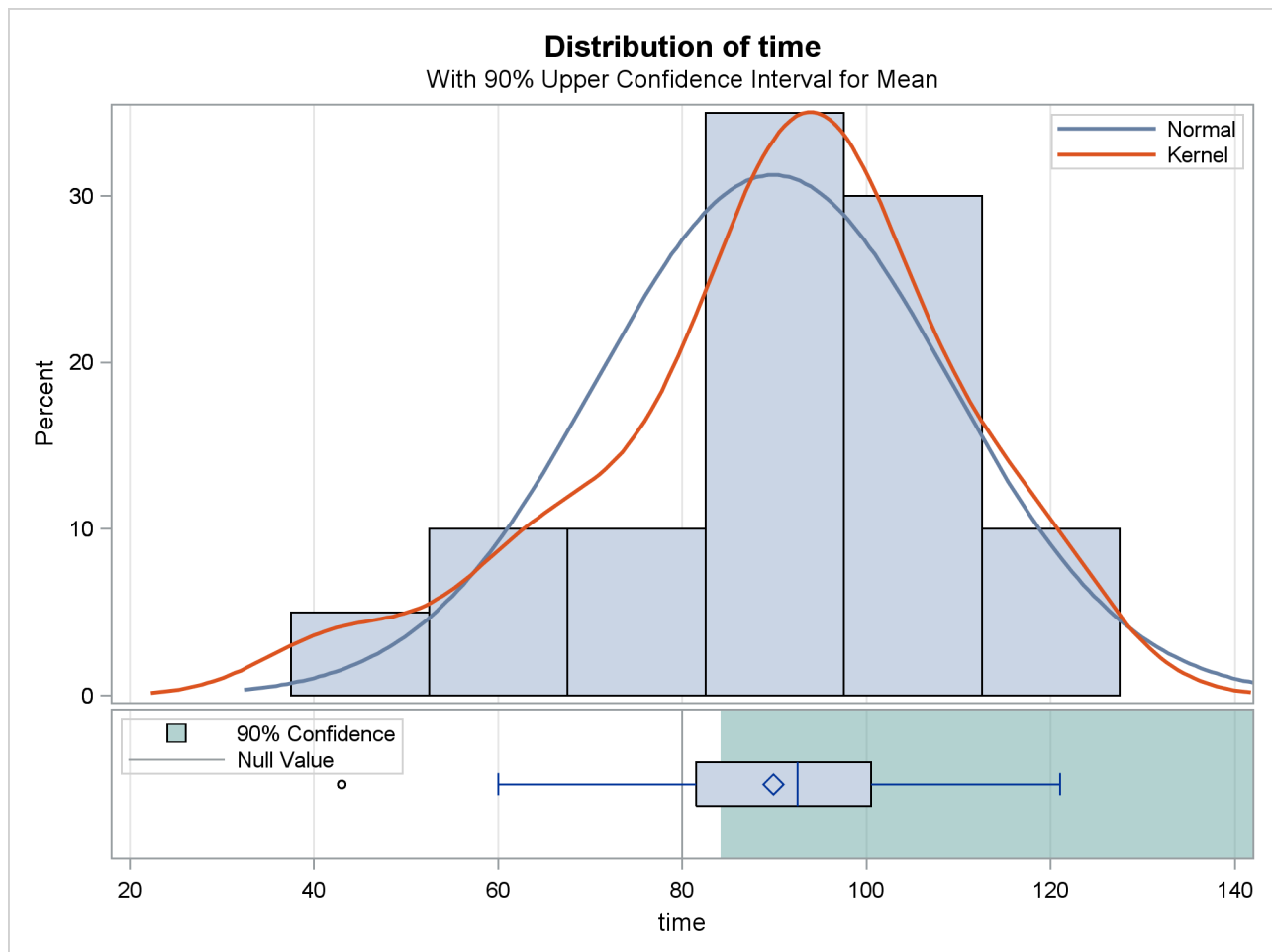
Figure 99.1 continued

| DF | t Value | Pr > t |
|----|---------|--------|
| 19 | 2.30    | 0.0164 |

Summary statistics appear at the top of the output. The sample size (N), mean, standard deviation, and standard error are displayed with the minimum and maximum values of the time variable. The 90% confidence limits for the mean and standard deviation are shown next. Due to the `SIDES=U` option, the interval for the mean is an upper one-sided interval with a finite lower bound (84.1659 days). The limits for the standard deviation are the equal-tailed variety, per the default `CI=EQUAL` option in the `PROC TTEST` statement. At the bottom of the output are the degrees of freedom, *t* statistic value, and *p*-value for the *t* test. At the 10%  $\alpha$  level, this test indicates that the mean length of the court cases is significantly greater than from 80 days ( $t = 2.30, p = 0.0164$ ).

The summary panel in Figure 99.2 shows a histogram with overlaid normal and kernel densities, a box plot, the 90% confidence interval for the mean, and the null value of 80 days.

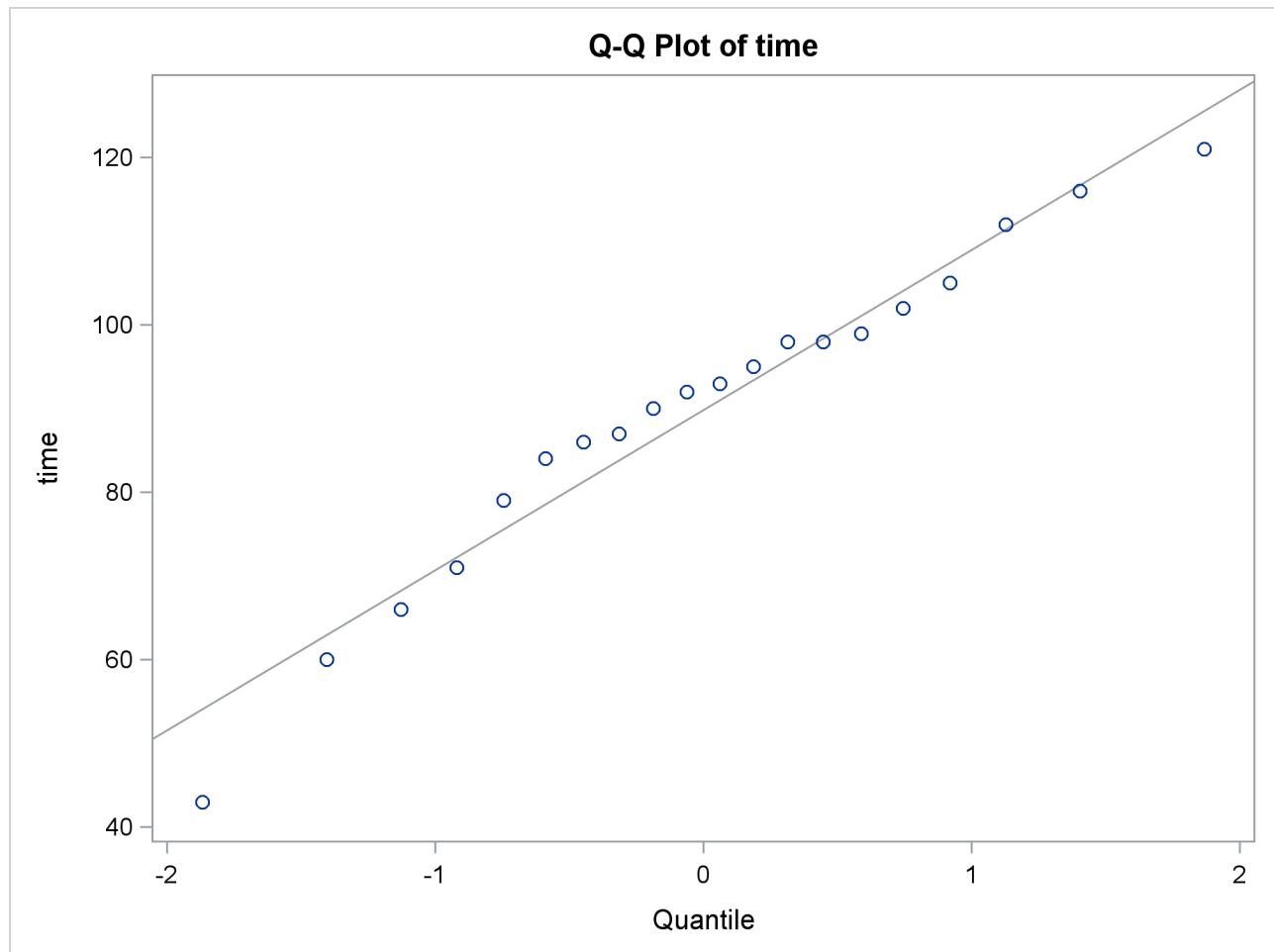
Figure 99.2 Summary Panel



The confidence interval excludes the null value, consistent with the rejection of the null hypothesis at  $\alpha = 0.1$ .

The Q-Q plot in Figure 99.3 assesses the normality assumption.

**Figure 99.3** Q-Q Plot



The curvilinear shape of the Q-Q plot suggests a possible slight deviation from normality. You could use the UNIVARIATE procedure with the NORMAL option to numerically check the normality assumptions.

## Comparing Group Means

If you want to compare values obtained from two different groups, and if the groups are independent of each other and the data are normally or lognormally distributed in each group, then a group  $t$  test can be used. Examples of such group comparisons include the following:

- test scores for two third-grade classes, where one of the classes receives tutoring
- fuel efficiency readings of two automobile nameplates, where each nameplate uses the same fuel

- sunburn scores for two sunblock lotions, each applied to a different group of people
- political attitude scores of males and females

In the following example, the golf scores for males and females in a physical education class are compared. The sample sizes from each population are equal, but this is not required for further analysis. The scores are thought to be approximately normally distributed within gender. The data are read by the following statements:

```
data scores;
 input Gender $ Score @@;
 datalines;
f 75 f 76 f 80 f 77 f 80 f 77 f 73
m 82 m 80 m 85 m 85 m 78 m 87 m 82
;
```

The dollar sign (\$) following Gender in the INPUT statement indicates that Gender is a character variable. The trailing @ signs (@@) enable the procedure to read more than one observation per line.

You can use a group *t* test to determine whether the mean golf score for the men in the class differs significantly from the mean score for the women. If you also suspect that the distributions of the golf scores of males and females have unequal variances, then you might want to specify the **COCHRAN** option in order to use the Cochran approximation (in addition to the Satterthwaite approximation, which is included by default). The following statements invoke PROC TTEST for the case of unequal variances, along with both types of confidence limits for the pooled standard deviation.

```
ods graphics on;

proc ttest cochran ci=equal umpu;
 class Gender;
 var Score;
run;

ods graphics off;
```

The **CLASS** statement contains the variable that distinguishes the groups being compared, and the **VAR** statement specifies the response variable to be used in calculations. The **COCHRAN** option produces *p*-values for the unequal variance situation by using the Cochran and Cox (1950) approximation. Equal-tailed and uniformly most powerful unbiased (UMPU) confidence intervals for  $\sigma$  are requested by the **CI=** option. Output from these statements is displayed in Figure 99.4 through Figure 99.7.

**Figure 99.4** Simple Statistics

| The TTEST Procedure |   |         |         |         |         |         |
|---------------------|---|---------|---------|---------|---------|---------|
| Variable: Score     |   |         |         |         |         |         |
| Gender              | N | Mean    | Std Dev | Std Err | Minimum | Maximum |
| f                   | 7 | 76.8571 | 2.5448  | 0.9619  | 73.0000 | 80.0000 |
| m                   | 7 | 82.7143 | 3.1472  | 1.1895  | 78.0000 | 87.0000 |
| Diff (1-2)          |   | -5.8571 | 2.8619  | 1.5298  |         |         |

Simple statistics for the two populations being compared, as well as for the difference of the means between the populations, are displayed in Figure 99.4. The Gender column indicates the population corresponding to the statistics in that row. The sample size (N), mean, standard deviation, standard error, and minimum and maximum values are displayed.

Confidence limits for means and standard deviations are shown in Figure 99.5.

**Figure 99.5** Simple Statistics

| Gender     | Method        | Mean    | 95% CL Mean |         | Std Dev |
|------------|---------------|---------|-------------|---------|---------|
| f          |               | 76.8571 | 74.5036     | 79.2107 | 2.5448  |
| m          |               | 82.7143 | 79.8036     | 85.6249 | 3.1472  |
| Diff (1-2) | Pooled        | -5.8571 | -9.1902     | -2.5241 | 2.8619  |
| Diff (1-2) | Satterthwaite | -5.8571 | -9.2064     | -2.5078 |         |

| Gender     | Method        | 95% CL | Std Dev | 95% UMPU CL<br>Std Dev |        |
|------------|---------------|--------|---------|------------------------|--------|
| f          |               | 1.6399 | 5.6039  | 1.5634                 | 5.2219 |
| m          |               | 2.0280 | 6.9303  | 1.9335                 | 6.4579 |
| Diff (1-2) | Pooled        | 2.0522 | 4.7242  | 2.0019                 | 4.5727 |
| Diff (1-2) | Satterthwaite |        |         |                        |        |

For the mean differences, both pooled (assuming equal variances for males and females) and Satterthwaite (assuming unequal variances) 95% intervals are shown. The confidence limits for the standard deviations are of the equal-tailed variety.

The test statistics, associated degrees of freedom, and  $p$ -values are displayed in Figure 99.6.

**Figure 99.6**  $t$  Tests

| Method        | Variances | DF     | t Value | Pr >  t |
|---------------|-----------|--------|---------|---------|
| Pooled        | Equal     | 12     | -3.83   | 0.0024  |
| Satterthwaite | Unequal   | 11.496 | -3.83   | 0.0026  |
| Cochran       | Unequal   | 6      | -3.83   | 0.0087  |

The Method column denotes which  $t$  test is being used for that row, and the Variances column indicates what assumption about variances is being made. The pooled test assumes that the two populations have equal variances and uses degrees of freedom  $n_1 + n_2 - 2$ , where  $n_1$  and  $n_2$  are the sample sizes for the two populations. The remaining two tests do not assume that the populations have equal variances. The Satterthwaite test uses the Satterthwaite approximation for degrees of freedom, while the Cochran test uses the Cochran and Cox approximation for the  $p$ -value. All three tests result in highly significant  $p$ -values, supporting the conclusion of a significant difference between males' and females' golf scores.

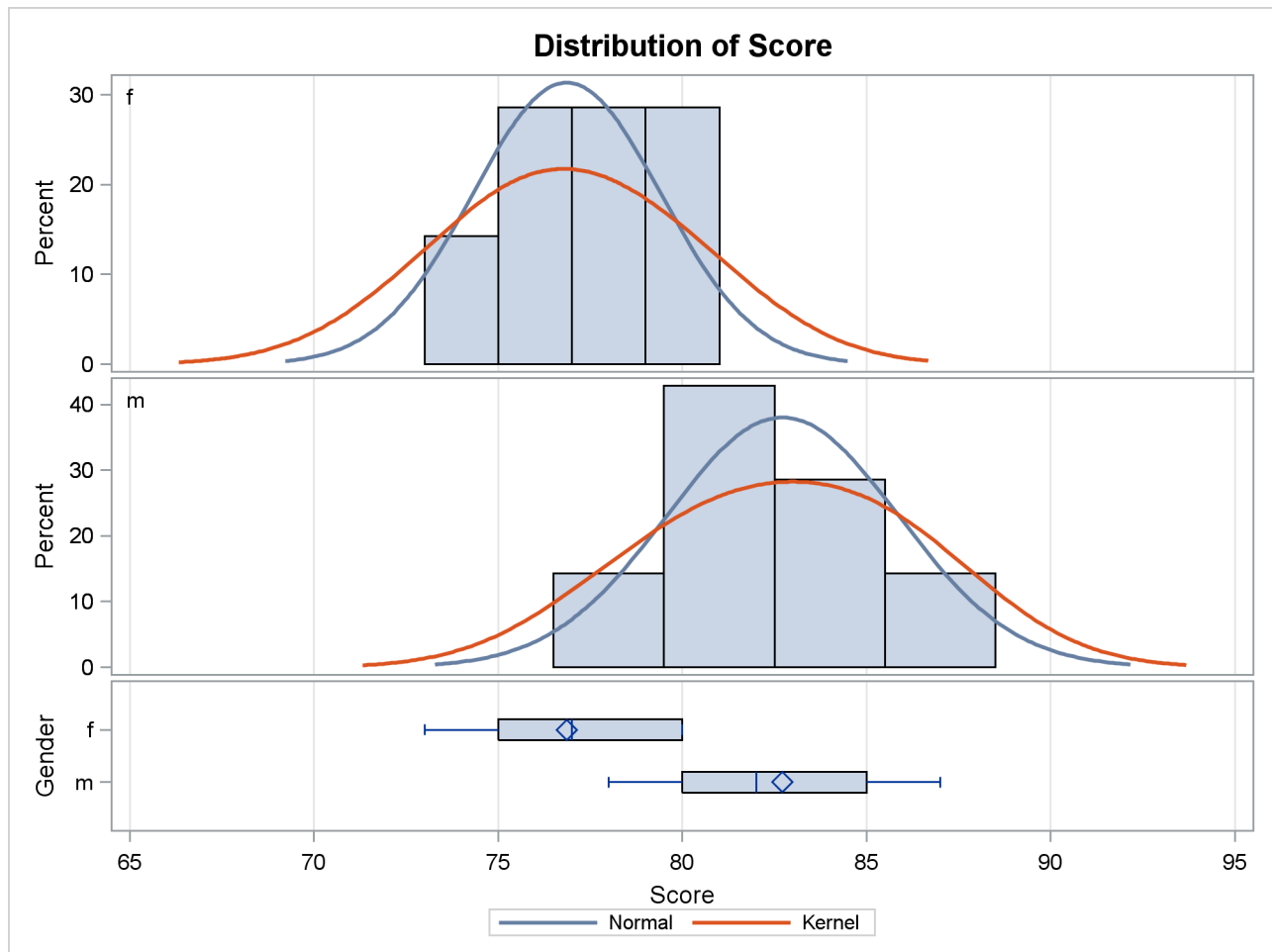
The "Equality of Variances" test in Figure 99.7 reveals insufficient evidence of unequal variances (the Folded F statistic  $F' = 1.53$ , with  $p = 0.6189$ ).



**Figure 99.7** Tests of Equality of Variances

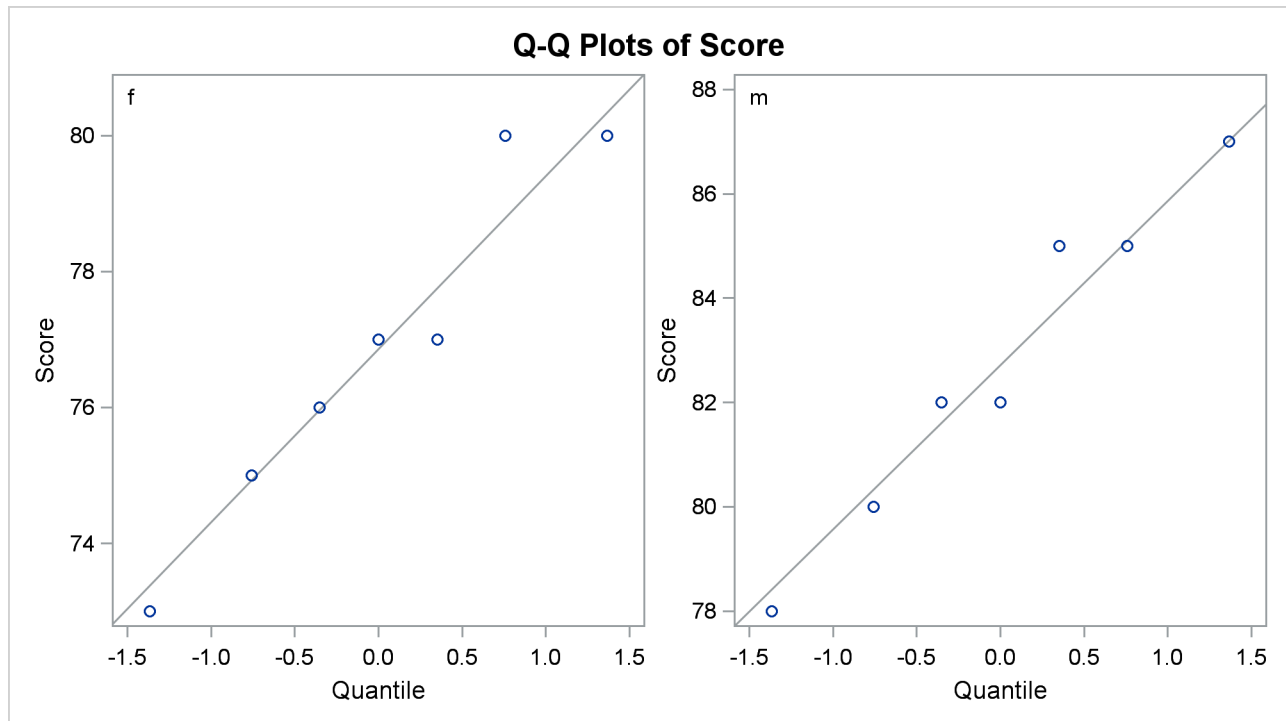
| Equality of Variances |        |        |         |        |
|-----------------------|--------|--------|---------|--------|
| Method                | Num DF | Den DF | F Value | Pr > F |
| Folded F              | 6      | 6      | 1.53    | 0.6189 |

The summary panel in [Figure 99.8](#) shows comparative histograms, normal and kernel densities, and box plots, comparing the distribution of golf scores between genders.

**Figure 99.8** Summary Panel

The Q-Q plots in [Output 99.9](#) assess the normality assumption for each gender.

Figure 99.9 Q-Q Plot



The plots for both males and females show no obvious deviations from normality. You can check the assumption of normality more rigorously by using PROC UNIVARIATE with the NORMAL option; if the assumption of normality is not reasonable, you should analyze the data with the nonparametric Wilcoxon rank sum test by using PROC NPAR1WAY.

---

## Syntax: TTEST Procedure

The following statements are available in the TTEST procedure:

```

PROC TTEST < options > ;
 CLASS variable ;
 PAIRED variables ;
 BY variables ;
 VAR variables < / options > ;
 FREQ variable ;
 WEIGHT variable ;

```

No statement can be used more than once. There is no restriction on the order of the statements after the PROC TTEST statement.

## PROC TTEST Statement

**PROC TTEST** < options > ;

The **PROC TTEST** statement invokes the TTEST procedure. Table 99.2 summarizes the options available in the **PROC TTEST** statement. The options are then described fully in alphabetical order.

**Table 99.2** PROC TTEST Statement Options

| Option                  | Description                                                                             |
|-------------------------|-----------------------------------------------------------------------------------------|
| <b>Basic Options</b>    |                                                                                         |
| <b>DATA=</b>            | Specifies input data set                                                                |
| <b>ORDER=</b>           | Determines sort order of <b>CLASS</b> variable or <b>CROSSOVER=</b> treatment variables |
| <b>Analysis Options</b> |                                                                                         |
| <b>ALPHA=</b>           | Specifies 1 – confidence level                                                          |
| <b>DIST=</b>            | Specifies distributional assumption (normal or lognormal)                               |
| <b>H0=</b>              | Specifies null value                                                                    |
| <b>SIDES=</b>           | Specifies number of sides and direction                                                 |
| <b>TEST=</b>            | Specifies test criterion (difference or ratio)                                          |
| <b>TOST</b>             | Requests equivalence test and specifies bounds                                          |
| <b>Displayed Output</b> |                                                                                         |
| <b>CI=</b>              | Requests confidence interval for standard deviation or CV                               |
| <b>COCHRAN</b>          | Requests Cochran <i>t</i> test                                                          |
| <b>PLOTS</b>            | Produces ODS statistical graphics                                                       |
| <b>Output Ordering</b>  |                                                                                         |
| <b>BYVAR</b>            | Groups results by <b>PAIRED</b> or <b>VAR</b> variables                                 |
| <b>NOBYVAR</b>          | Groups results by tables                                                                |

The following options can appear in the **PROC TTEST** statement.

### **ALPHA=***p*

specifies that confidence intervals (except test-based mean confidence intervals when the **TOST** option is used) are to be  $100(1 - p)\%$  confidence intervals, where  $0 < p < 1$ . When the **TOST** option is used, the test-based mean confidence intervals are  $100(1 - 2p)\%$  confidence intervals. By default, **PROC TTEST** uses **ALPHA=0.05**. If *p* is 0 or less, or 1 or more, an error message is printed.

### **BYVAR**

groups the results by the **PAIRED** or **VAR** variables. The **BYVAR** option is enabled by default. Note that this represents a change from previous releases for how the results are grouped with respect to variables and tables. Prior to SAS 9.2, multiple variables were included in each table, similar to the new **NOBYVAR** option.

**CI=EQUAL | UMPU | NONE****CL=EQUAL | UMPU | NONE**

specifies whether a confidence interval is displayed for  $\sigma$  and, if so, what kind. The **CI=EQUAL** option specifies an equal-tailed confidence interval, and it is the default. The **CI=UMPU** option specifies an interval based on the uniformly most powerful unbiased test of  $H_0: \sigma = \sigma_0$ . The **CI=NONE** option requests that no confidence interval be displayed for  $\sigma$ . The values **EQUAL** and **UMPU** together request that both types of confidence intervals be displayed. If the value **NONE** is specified with one or both of the values **EQUAL** and **UMPU**, **NONE** takes precedence. For more information, see the section “[Two-Independent-Sample Design](#)” on page 8455.

**COCHRAN**

requests the Cochran and Cox (1950) approximation of the probability level for the unequal variances situation. For more information, see the section “[Two-Independent-Sample Design](#)” on page 8455.

**DATA=SAS-data-set**

names the SAS data set for the procedure to use. By default, PROC TTEST uses the most recently created SAS data set. The input data set can contain summary statistics of the observations instead of the observations themselves. The number, mean, and standard deviation of the observations are required for each **BY** group (one sample and paired differences) or for each class within each **BY** group (two samples). For more information about the **DATA=** option, see the section “[Input Data Set of Statistics](#)” on page 8449.

**DIST=LOGNORMAL | NORMAL**

specifies the underlying distribution assumed for the data. The default is **NORMAL**, unless **TEST=RATIO** is specified, in which case the default is **LOGNORMAL**.

**H0=m**

requests tests against a null value of  $m$ , unless the **TOST** option is used, in which case  $m$  is merely used to derive the lower and upper equivalence bounds. For the crossover design, the value  $m$  applies for both treatment and period tests. By default, PROC TTEST uses **H0=0** when **TEST=DIFF** (or **DIST=NORMAL** for a one-sample design) and **H0=1** when **TEST=RATIO** (or **DIST=LOGNORMAL** for a one-sample design).

**NOBYVAR**

includes all **PAIRED** or **VAR** variables together in each output table. If the **NOBYVAR** option is not specified, then the **BYVAR** option is enabled, grouping the results by the **PAIRED** and **VAR** variables.

**ORDER=DATA | FORMATTED | FREQ | INTERNAL | MIXED**

specifies the order in which to sort the levels of the classification variables (which are specified in the **CLASS** statement) and treatment variables (which are specified in the **CROSSOVER=** option in the **VAR** statement). The default is **ORDER=MIXED**, which corresponds to the ordering in releases previous to SAS 9.2.

This option applies to the levels for all classification or treatment variables, except when you use the **ORDER=FORMATTED** option with numeric classification or treatment variables that have no explicit format. With this option, the levels of such variables are ordered by their internal value.

The ORDER= option can take the following values:

| Value of ORDER= | Levels Sorted By                                                                                                                                        |
|-----------------|---------------------------------------------------------------------------------------------------------------------------------------------------------|
| DATA            | Order of appearance in the input data set.                                                                                                              |
| FORMATTED       | External formatted value, except for numeric variables with no explicit format, which are sorted by their unformatted (internal) value.                 |
| FREQ            | Descending frequency count; levels with the most observations come first in the order. In the event of a tie, ORDER=MIXED is used.                      |
| INTERNAL        | Unformatted value.                                                                                                                                      |
| MIXED           | Same as ORDER=FORMATTED if the unformatted variable is character-valued; same as ORDER=INTERNAL otherwise (the unformatted variable is numeric-valued). |

For FORMATTED and INTERNAL, the sort order is machine-dependent.

For more information about sort order, see the chapter on the SORT procedure in the *Base SAS Procedures Guide* and the discussion of BY-group processing in *SAS Language Reference: Concepts*.

**PLOTS** <(global-plot-options)> <= plot-request <(options)>>

**PLOTS** <(global-plot-options)> <= (plot-request <(options)> <... plot-request <(options)>>>

controls the plots produced through ODS Graphics. When you specify only one plot request, you can omit the parentheses around the plot request. Here are some examples:

```
plots=none
plots=(histogram boxplot interval qq profiles agreement)
plots(unpack)=summary
plots(showh0)=interval(type=pergroup)
plots=(summary(unpack) interval(type=period))
```

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;

proc ttest plots=all;
 var oxygen;
run;

ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

If ODS Graphics is enabled but you do not specify the PLOTS option, then PROC TTEST produces a default set of plots. (NOTE: The graphical results are unavailable if your input data set contains summary statistics rather than observation values.)

For a one-sample design, the default plots are the following:

- summary plot (histogram with overlaid normal and kernel densities, box plot, and confidence interval band)
- Q-Q plot

For a two-independent-sample design, the default plots are the following:

- summary plot (comparative histograms with overlaid densities and box plots)
- Q-Q plot

For a paired design, the default plots are the following:

- summary plot (histogram, densities, box plot, and confidence interval) of the difference or ratio
- Q-Q plot of the difference or ratio
- profiles plot
- agreement plot

For a crossover design, the default plots are the following:

- comparative histograms with overlaid densities by treatment and period
- comparative box plots by treatment and period
- Q-Q plots by treatment and period
- profiles over treatment plot
- agreement of treatments plot

For more detailed descriptions of plots, see the section “[Interpreting Graphs](#)” on page 8466.

The global plot options include the following:

**ONLY**

suppresses the default plots. Only plots specifically requested are displayed.

**SHOWH0**

**SHOWNULL**

shows the null value (as specified by the `H0=` option in the `PROC TTEST` statement) in all relevant plots. For one-sample and paired designs, the null value can appear in `SUMMARY`, `BOX`, and `INTERVAL`. For two-independent-sample and crossover designs, the null value can appear only in `INTERVAL`.

**UNPACKPANEL**

**UNPACK**

suppresses paneling. By default, multiple plots can appear in some output panels. Specify `UNPACKPANEL` to get each plot in a separate panel. You can specify `PLOTS(UNPACKPANEL)` to unpack the default plots. You can also specify `UNPACK` as a suboption with `SUMMARY`.

The plot requests include the following:

### **ALL**

produces all appropriate plots. You can specify other options with **ALL**; for example, to request all plots and specify that intervals should be for the period difference in a crossover design, specify **PLOTS=(ALL INTERVAL(TYPE=PERIOD))**.

### **AGREEMENT**

#### **AGREEMENTPLOT**

requests an agreement plot. This plot is produced by default for paired and crossover designs, the only designs for which the **AGREEMENT** option is valid.

For paired designs, the second response in each pair is plotted against the first response. See the section “[Agreement Plots for Paired Designs](#)” on page 8466 for further details.

For crossover designs, the **AGREEMENT** plot request has the following options:

#### **TYPE=PERIOD**

plots the response in the second period against the response in the first period. See the section “[Period Agreement Plots for Crossover Designs](#)” on page 8466 for further details.

#### **TYPE=TREATMENT**

plots the response associated with the second treatment against the response associated with the first treatment. This is the default **TYPE=** option for crossover designs. See the section “[Treatment Agreement Plots for Crossover Designs](#)” on page 8467 for further details.

### **BOX**

#### **BOXPLOT**

requests a box plot or comparative box plots. This plot is produced by default for crossover designs. For other designs, a box plot appears as part of the **SUMMARY** plot by default.

For one-sample and paired designs, a confidence interval for the mean is shown as a band in the background, along with the equivalence bounds if the **TOST** option is used in the **PROC TTEST** statement.

For a two-independent-sample design, comparative box plots (one for each class) are shown. For a crossover design, comparative box plots for all four combinations of the two treatments and two periods are shown.

See the section “[Box Plots](#)” on page 8467 for further details.

### **HISTOGRAM**

#### **HIST**

#### **HISTDENS**

requests a histogram or comparative histograms with overlaid normal and kernel densities. This plot is produced by default for crossover designs. For other designs, it appears as part of the **SUMMARY** plot by default.

For one-sample and paired designs, the histogram and densities are based on the test criterion (which is the mean difference or ratio for a paired design). For a two-independent-sample design, comparative histograms (one for each class) are shown. For a crossover design, histograms for all four combinations of the two treatments and two periods are shown.

See the section “[Histograms](#)” on page 8467 for further details.

**INTERVAL****INTERVALPLOT**

requests plots of confidence interval for means.

For a two-independent-sample design, the **INTERVAL** plot request has the following options:

**TYPE=PERGROUP**

shows two separate two-sided confidence intervals, one for each class. This option cannot be used along with the **SHOWHO** global plot option.

**TYPE=TEST**

shows pooled and Satterthwaite confidence intervals. This is the default **TYPE=** option for two-independent-sample designs.

For a crossover design, The **INTERVAL** plot request has the following options:

**TYPE=PERGROUP**

shows four separate two-sided intervals, one for each treatment-by-period combination. This option cannot be used along with the **SHOWHO** global plot option.

**TYPE=PERIOD**

shows pooled and Satterthwaite confidence intervals for the period difference or ratio. This option is invalid if the **IGNOREPERIOD** option is used in the **VAR** statement.

**TYPE=TREATMENT**

shows pooled and Satterthwaite confidence intervals for the treatment difference or ratio. This is the default **TYPE=** option for crossover designs.

See the section “[Confidence Intervals](#)” on page 8467 for further details.

**NONE**

suppresses all plots.

**PROFILES****PROFILESPLOT**

requests a profiles plot. This plot is produced by default for paired and crossover designs, the only designs for which the **PROFILES** option is valid.

For paired designs, a line is drawn for each observation from left to right connecting the first response to the second response. See the section “[Profiles for Paired Designs](#)” on page 8468 for further details.

For crossover designs, the **PROFILES** plot request has the following options:

**TYPE=PERIOD**

shows response profiles over period, connecting the first period on the left to the second period on the right for each subject. See the section “[Profiles over Period for Crossover Designs](#)” on page 8468 for further details.

**TYPE=TREATMENT**

shows response profiles over treatment values, connecting the first treatment on the left to the second treatment on the right for each observation. This is the default **TYPE=** option for crossover designs. See the section “[Profiles over Treatment for Crossover Designs](#)” on page 8468 for further details.



**QQ****QQPLOT**

requests a normal quantile-quantile (Q-Q) plot. This plot is produced by default for all designs.

For two-sample designs, separate plots are shown for each class in a single panel. For crossover design, separate plots are shown for each treatment-by-period combination in a single panel.

See the section “Q-Q Plots” on page 8468 for further details.

**SUMMARY****SUMMARYPLOT**

requests **HISTOGRAM** and **BOX** plots together in a single panel, sharing common X axes. This plot is produced by default for one-sample, paired, and two-independent-sample designs, the only designs for which the **SUMMARY** option is valid. See the documentation for the **BOX** and **HISTOGRAM** plot requests for details. The **SUMMARY** plot request has the following option:

**UNPACK**

plots histograms with overlaid densities in one panel and box plots (along with confidence interval bands, if one-sample or paired design) in another. Note that specifying **PLOTS(ONLY)=SUMMARY(UNPACK)** is exactly the same as specifying **PLOTS(ONLY)=(BOX HISTOGRAM)**.

**SIDES=2 | L | U****SIDED=2 | L | U****SIDE=2 | L | U**

specifies the number of sides (or tails) and direction of the statistical tests and test-based confidence intervals. The values are interpreted as follows:

- SIDES=2** (the default) specifies two-sided tests and confidence intervals for means.
- SIDES=L** specifies lower one-sided tests, in which the alternative hypothesis indicates a mean less than the null value, and lower one-sided confidence intervals between minus infinity and the upper confidence limit.
- SIDES=U** specifies upper one-sided tests, in which the alternative hypothesis indicates a mean greater than the null value, and upper one-sided confidence intervals between the lower confidence limit and infinity.

**TEST=DIFF | RATIO**

specifies the test criterion. Use **TEST=DIFF** to test the difference of means and **TEST=RATIO** to test the ratio of means. The default is **DIFF**, unless **DIST=LOGNORMAL** is specified, in which case the default is **RATIO**. This option is ignored for one-sample designs.

**TOST ( < lower , > upper )**

requests Schuirmann’s TOST equivalence test. The *upper* equivalence bound must be specified. If **TEST=DIFF**, then the default value for the *lower* equivalence bound is  $2m - upper$ , where  $m$  is the value of the **H0=** option. If **TEST=RATIO**, then the default value for *lower* is  $m / upper$ .

---

## BY Statement

**BY** *variables* ;

You can specify a BY statement with PROC TTEST to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the TTEST procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

---

## CLASS Statement

**CLASS** *variable* ;

A CLASS statement giving the name of the classification (or grouping) variable must accompany the PROC TTEST statement in the two-independent-sample case. It should be omitted for the one-sample, paired, and AB/BA crossover designs. If it is used without the VAR statement, all numeric variables in the input data set (except those that appear in the CLASS, BY, FREQ, or WEIGHT statement) are included in the analysis.

The classification variable must have two, and only two, levels. PROC TTEST divides the observations into the two groups for the *t* test by using the levels of this variable. You can use either a numeric or a character variable in the CLASS statement.

Class levels are determined from the formatted values of the CLASS variable. Thus, you can use formats to define group levels. See the discussions of the FORMAT procedure, the FORMAT statement, formats, and informats in *SAS Formats and Informats: Reference*.

---

## FREQ Statement

**FREQ** *variable* ;

The *variable* in the FREQ statement identifies a variable that contains the frequency of occurrence of each observation. PROC TTEST treats each observation as if it appears *n* times, where *n* is the value of the FREQ

variable for the observation. If the value is not an integer, only the integer portion is used. If the frequency value is less than 1 or is missing, the observation is not used in the analysis. When the **FREQ** statement is not specified, each observation is assigned a frequency of 1. The **FREQ** statement cannot be used if the **DATA=** data set contains statistics instead of the original observations.

---

## PAIRED Statement

**PAIRED** *pair-lists* ;

The *pair-lists* in the **PAIRED** statement identifies the variables to be compared in paired comparisons. You can use one or more *pair-lists*. Variables or lists of variables are separated by an asterisk (\*) or a colon (:). The asterisk requests comparisons between each variable on the left with each variable on the right. The colon requests comparisons between the first variable on the left and the first on the right, the second on the left and the second on the right, and so forth. The number of variables on the left must equal the number on the right when the colon is used. The differences are calculated by taking the variable on the left minus the variable on the right for both the asterisk and colon. A pair formed by a variable with itself is ignored. Use the **PAIRED** statement only for paired comparisons. The **CLASS** and **VAR** statements cannot be used with the **PAIRED** statement.

Examples of the use of the asterisk and the colon are shown in Table 99.3.

**Table 99.3** PAIRED Statement in the TTEST Procedure

| These PAIRED statements...        | yield these comparisons        |
|-----------------------------------|--------------------------------|
| <b>PAIRED</b> A*B;                | A-B                            |
| <b>PAIRED</b> A*B C*D;            | A-B and C-D                    |
| <b>PAIRED</b> (A B) * (C D) ;     | A-C, A-D, B-C, and B-D         |
| <b>PAIRED</b> (A B) * (C B) ;     | A-C, A-B, and B-C              |
| <b>PAIRED</b> (A1-A2) * (B1-B2) ; | A1-B1, A1-B2, A2-B1, and A2-B2 |
| <b>PAIRED</b> (A1-A2) : (B1-B2) ; | A1-B1 and A2-B2                |

---

## VAR Statement

**VAR** *variables* </ options > ;

The **VAR** statement names the variables to be used in the analyses. One-sample comparisons are conducted when the **VAR** statement is used without the **CROSSOVER=** option or **CLASS** statement. Two-independent-sample comparisons are conducted when the **VAR** statement is used with a **CLASS** statement.

An AB/BA crossover analysis is conducted when the **CROSSOVER=** option is used in the **VAR** statement. In this case, you must specify an even number of variables. Each set of two variables represents the responses in the first and second periods of the AB/BA crossover design. For example, if you use the **CROSSOVER=** option and specify **VAR x1 x2 x3 x4**, then you will get two analyses. One analysis will have x1 as the period 1 response and x2 as the period 2 response. The other analysis will have x3 as the period 1 response and x4 as the period 2 response.

The **VAR** statement cannot be used with the **PAIRED** statement. If the **VAR** statement is omitted, all numeric variables in the input data set (except a numeric variable appearing in the **BY**, **CLASS**, **FREQ**, or **WEIGHT** statement) are included in the analysis.

You can specify the following options after a slash (/):

**CROSSOVER=** ( *variable1 variable2* )

specifies the variables representing the treatment applied in each of the two periods in an AB/BA crossover design. The treatment variables must have two, and only two, levels. For any given observation, the levels for the two variables must be different, due to the restrictions of the AB/BA crossover design. You can use either numeric or character variables.

Treatment levels are determined from the formatted values of the variables. Thus, you can use formats to define the treatment levels. See the discussions of the **FORMAT** procedure, the **FORMAT** statement, **formats**, and **informats** in *SAS Formats and Informats: Reference*.

**IGNOREPERIOD**

indicates that the period effect shall be ignored—that is, assumed to be equal to 0 (if **TEST=DIFF**) or 1 (if **TEST=RATIO**). This assumption increases the degrees of freedom for the test of the treatment difference by one and is usually more powerful, but it risks incorrect results if there is actually a period effect.

## WEIGHT Statement

**WEIGHT** *variable* ;

The **WEIGHT** statement weights each observation in the input data set by the value of the **WEIGHT** variable. The values of the **WEIGHT** variable can be nonintegral, and they are not truncated. Observations with negative, zero, or missing values for the **WEIGHT** variable are not used in the analyses. Each observation is assigned a weight of 1 when the **WEIGHT** statement is not used. The **WEIGHT** statement cannot be used with an input data set of summary statistics.

## Details: TTEST Procedure

### Input Data Set of Statistics

PROC TTEST accepts data containing either observation values or summary statistics. Observation values are supported for all analyses, whereas summary statistics are supported only for a subset of analyses. If the analysis involves the paired design, the AB/BA crossover design, or the lognormal distributional assumption (**DIST=LOGNORMAL**), then observation values must be used. The graphical results are unavailable if your input data set contains summary statistics rather than raw observed values.

PROC TTEST assumes that the **DATA=** data set contains statistics if it contains a character variable with name **\_TYPE\_** or **\_STAT\_**. The TTEST procedure expects this character variable to contain the names of statistics. If both **\_TYPE\_** and **\_STAT\_** variables exist and are of type character, PROC TTEST expects **\_TYPE\_** to contain the names of statistics including 'N', 'MEAN', and 'STD' for each **BY** group (or for

each class within each **BY** group for two-sample *t* tests). If no ‘N’, ‘MEAN’, or ‘STD’ statistics exist, an error message is printed.

**FREQ**, **WEIGHT**, and **PAIRED** statements cannot be used with input data sets of statistics. **BY**, **CLASS**, and **VAR** statements are the same regardless of data set type. For paired comparisons, see the **\_DIF\_** values for the **\_TYPE\_=T** observations in output produced by the **OUTSTATS=** option in the **PROC COMPARE** statement (see the *Base SAS Procedures Guide*).

## Missing Values

An observation is omitted from the calculations if it has a missing value for either the **CLASS** variable, a **CROSSOVER=** variable, a **PAIRED** variable, the variable to be tested (in a one-sample or two-independent-sample design), or either of the two response variables (in a crossover design). If more than one variable or pair of variables is listed in the **VAR** statement, a missing value in one variable or pair does not eliminate the observation from the analysis of other nonmissing variables or variable pairs.

## Computational Methods

This section describes the computational formulas for the estimates, confidence limits, and tests for each analysis in the TTEST procedure. The first subsection defines some common notation. The second subsection discusses the distinction between arithmetic and geometric means. The third subsection explains the concept of the coefficient of variation. The following four subsections address the four supported designs (one-sample, paired, two-independent-sample, and AB/BA crossover). The content in each of those subsections is divided into separate discussions according to different values of the **DIST=** and **TEST=** options in the **PROC TTEST** statement. The last subsection describes TOST equivalence analyses.

## Common Notation

Table 99.4 displays notation for some of the commonly used symbols.

**Table 99.4** Common Notation

| Symbol          | Description                                                                                                                                    |
|-----------------|------------------------------------------------------------------------------------------------------------------------------------------------|
| $\mu$           | Population value of (arithmetic) mean                                                                                                          |
| $\mu_0$         | Null value of test (value of <b>H0=</b> option in <b>PROC TTEST</b> statement)                                                                 |
| $\sigma^2$      | Population variance                                                                                                                            |
| $\sigma$        | Population value of standard deviation                                                                                                         |
| $\gamma$        | Population value of geometric mean                                                                                                             |
| CV              | Population value of coefficient of variation (ratio of population standard deviation and population arithmetic mean)                           |
| $\alpha$        | Value of <b>ALPHA=</b> option in <b>PROC TTEST</b> statement                                                                                   |
| $t_{p,v}$       | <i>p</i> th percentile of <i>t</i> distribution with <i>v</i> degrees of freedom ( <i>df</i> )                                                 |
| $F_{p,v_1,v_2}$ | <i>p</i> th percentile of <i>F</i> distribution with <i>v</i> <sub>1</sub> numerator <i>df</i> and <i>v</i> <sub>2</sub> denominator <i>df</i> |
| $\chi^2_{p,v}$  | <i>p</i> th percentile of chi-square distribution with <i>v</i> <i>df</i>                                                                      |

## Arithmetic and Geometric Means

The *arithmetic mean* (more commonly called simply the *mean*) of the distribution of a random variable  $X$  is its expected value,  $E(X)$ . The arithmetic mean is the natural parameter of interest for a normal distribution because the distribution of the difference of normal random variables has a known normal distribution, and the arithmetic mean of a normal difference is equal to the difference of the individual arithmetic means. (No such convenient property holds for geometric means with normal data, with either differences or ratios.)

The usual estimate of an arithmetic mean is the sum of the values divided by the number of values:

$$\text{arithmetic mean} = \frac{1}{n} \sum_{i=1}^n y_i$$

The *geometric mean* of the distribution of a random variable  $X$  is  $\exp(E(\log(X)))$ , the exponentiation of the mean of the natural logarithm. The geometric mean is the natural parameter of interest for a lognormal distribution because the distribution of a ratio of lognormal random variables has a known lognormal distribution, and the geometric mean of a lognormal ratio is equal to the ratio of the individual geometric means. (No such convenient property holds for arithmetic means with lognormal data, with either differences or ratios.)

The usual estimate of a geometric mean is the product of the values raised to the power  $1/n$ , where  $n$  is the number of values:

$$\text{geometric mean} = \left( \prod_{i=1}^n y_i \right)^{\frac{1}{n}}$$

## Coefficient of Variation

The *coefficient of variation* (abbreviated “CV”) of the distribution of a random variable  $X$  is the ratio of the standard deviation to the (arithmetic) mean, or  $\sqrt{\text{Var}(X)}/E(X)$ . Conceptually, it is a measure of the variability of  $X$  expressed in units corresponding to the mean of  $X$ .

For lognormal data, the CV is the natural measure of variability (rather than the standard deviation) because the CV is invariant to multiplication of a lognormal variable by a constant. For a two-independent-sample design, the assumption of equal CVs on a lognormal scale is analogous to the assumption of equal variances on the normal scale. When the CVs of two independent samples of lognormal data are assumed equal, the pooled estimate of variability is used.

## One-Sample Design

Define the following notation:

$n^*$  = number of observations in data set

$y_i$  = value of  $i$ th observation,  $i \in \{1, \dots, n^*\}$

$f_i$  = frequency of  $i$ th observation,  $i \in \{1, \dots, n^*\}$

$w_i$  = weight of  $i$ th observation,  $i \in \{1, \dots, n^*\}$

$$n = \text{sample size} = \sum_i^{n^*} f_i$$

**Normal Data (DIST=NORMAL)**

The mean estimate  $\bar{y}$ , standard deviation estimate  $s$ , and standard error SE are computed as follows:

$$\bar{y} = \frac{\sum_i^{n^*} f_i w_i y_i}{\sum_i^{n^*} f_i w_i}$$

$$s = \left( \frac{\sum_i^{n^*} f_i w_i (y_i - \bar{y})^2}{n - 1} \right)^{\frac{1}{2}}$$

$$SE = \frac{s}{\sum_i^{n^*} f_i w_i}$$

The  $100(1 - \alpha)\%$  confidence interval for the mean  $\mu$  is

$$\left( \bar{y} - t_{1-\frac{\alpha}{2}, n-1} SE, \bar{y} + t_{1-\frac{\alpha}{2}, n-1} SE \right), \text{ SIDES}=2$$

$$\left( -\infty, \bar{y} + t_{1-\alpha, n-1} SE \right), \text{ SIDES}=L$$

$$\left( \bar{y} - t_{1-\alpha, n-1} SE, \infty \right), \text{ SIDES}=U$$

The  $t$  value for the test is computed as

$$t = \frac{\bar{y} - \mu_0}{SE}$$

The  $p$ -value of the test is computed as

$$p\text{-value} = \begin{cases} P(t^2 > F_{1-\alpha, 1, n-1}) & , \text{ 2-sided} \\ P(t < t_{\alpha, n-1}) & , \text{ lower 1-sided} \\ P(t > t_{1-\alpha, n-1}) & , \text{ upper 1-sided} \end{cases}$$

The equal-tailed confidence interval for the standard deviation (CI=EQUAL) is based on the acceptance region of the test of  $H_0: \sigma = \sigma_0$  that places an equal amount of area ( $\frac{\alpha}{2}$ ) in each tail of the chi-square distribution:

$$\left\{ \chi_{\frac{\alpha}{2}, n-1}^2 \leq \frac{(n-1)s^2}{\sigma_0^2} \leq \chi_{\frac{1-\alpha}{2}, n-1}^2 \right\}$$

The acceptance region can be algebraically manipulated to give the following  $100(1 - \alpha)\%$  confidence interval for  $\sigma^2$ :

$$\left( \frac{(n-1)s^2}{\chi_{1-\frac{\alpha}{2}, n-1}^2}, \frac{(n-1)s^2}{\chi_{\frac{\alpha}{2}, n-1}^2} \right)$$

Taking the square root of each side yields the  $100(1 - \alpha)\%$  CI=EQUAL confidence interval for  $\sigma$ :

$$\left( \left( \frac{(n-1)s^2}{\chi_{1-\frac{\alpha}{2}, n-1}^2} \right)^{\frac{1}{2}}, \left( \frac{(n-1)s^2}{\chi_{\frac{\alpha}{2}, n-1}^2} \right)^{\frac{1}{2}} \right)$$

The other confidence interval for the standard deviation (CI=UMPU) is derived from the uniformly most powerful unbiased test of  $H_0: \sigma = \sigma_0$  (Lehmann 1986). This test has acceptance region

$$\left\{ c_1 \leq \frac{(n-1)s^2}{\sigma_0^2} \leq c_2 \right\}$$

where the critical values  $c_1$  and  $c_2$  satisfy

$$\int_{c_1}^{c_2} f_{n-1}(y)dy = 1 - \alpha$$

and

$$\int_{c_1}^{c_2} y f_{n-1}(y)dy = (n-1)(1 - \alpha)$$

where  $f_\nu(y)$  is the PDF of the chi-square distribution with  $\nu$  degrees of freedom. This acceptance region can be algebraically manipulated to arrive at

$$P \left\{ \frac{(n-1)s^2}{c_2} \leq \sigma^2 \leq \frac{(n-1)s^2}{c_1} \right\} = 1 - \alpha$$

where  $c_1$  and  $c_2$  solve the preceding two integrals. To find the area in each tail of the chi-square distribution to which these two critical values correspond, solve  $c_1 = \chi_{1-\alpha_2, n-1}^2$  and  $c_2 = \chi_{\alpha_1, n-1}^2$  for  $\alpha_1$  and  $\alpha_2$ ; the resulting  $\alpha_1$  and  $\alpha_2$  sum to  $\alpha$ . Hence, a  $100(1 - \alpha)\%$  confidence interval for  $\sigma^2$  is given by

$$\left( \frac{(n-1)s^2}{\chi_{1-\alpha_2, n-1}^2}, \frac{(n-1)s^2}{\chi_{\alpha_1, n-1}^2} \right)$$

Taking the square root of each side yields the  $100(1 - \alpha)\%$  CI=UMPU confidence interval for  $\sigma$ :

$$\left( \left( \frac{(n-1)s^2}{\chi_{1-\alpha_2, n-1}^2} \right)^{\frac{1}{2}}, \left( \frac{(n-1)s^2}{\chi_{\alpha_1, n-1}^2} \right)^{\frac{1}{2}} \right)$$

### **Lognormal Data (DIST=LOGNORMAL)**

The DIST=LOGNORMAL analysis is handled by log-transforming the data and null value, performing a DIST=NORMAL analysis, and then transforming the results back to the original scale. This simple technique is based on the properties of the lognormal distribution as discussed in Johnson, Kotz, and Balakrishnan (1994, Chapter 14).

Taking the natural logarithms of the observation values and the null value, define

$$z_i = \log(y_i), \quad i \in \{1, \dots, n^*\}$$

$$\gamma_0 = \log(\mu_0)$$

First a DIST=NORMAL analysis is performed on  $z_i$  in place of  $y_i$ . The geometric mean estimate  $\hat{\gamma}$  and CV estimate  $\widehat{CV}$  of the original lognormal data are computed as follows:

$$\hat{\gamma} = \exp(\bar{y})$$

$$\widehat{CV} = (\exp(s^2) - 1)^{\frac{1}{2}}$$

The  $t$  value and  $p$ -value remain the same. The confidence limits for the geometric mean and CV on the original lognormal scale are computed from the confidence limits for the arithmetic mean and standard deviation in the DIST=NORMAL analysis on the log-transformed data, in the same way that  $\hat{\gamma}$  is derived from  $\bar{y}$  and  $\widehat{CV}$  is derived from  $s$ .



## Paired Design

Define the following notation:

$n^*$  = number of observations in data set

$y_{1i}$  = value of  $i$ th observation for first PAIRED variable,  $i \in \{1, \dots, n^*\}$

$y_{2i}$  = value of  $i$ th observation for second PAIRED variable,  $i \in \{1, \dots, n^*\}$

$f_i$  = frequency of  $i$ th observation,  $i \in \{1, \dots, n^*\}$

$w_i$  = weight of  $i$ th observation,  $i \in \{1, \dots, n^*\}$

$$n = \text{sample size} = \sum_i^{n^*} f_i$$

### Normal Difference (DIST=NORMAL TEST=DIFF)

The analysis is the same as the analysis for the one-sample design in the section “Normal Data (DIST=NORMAL)” on page 8452 based on the differences

$$d_i = y_{1i} - y_{2i} \quad , \quad i \in \{1, \dots, n^*\}$$

### Lognormal Ratio (DIST=LOGNORMAL TEST=RATIO)

The analysis is the same as the analysis for the one-sample design in the section “Lognormal Data (DIST=LOGNORMAL)” on page 8453 based on the ratios

$$r_i = y_{1i}/y_{2i} \quad , \quad i \in \{1, \dots, n^*\}$$

### Normal Ratio (DIST=NORMAL TEST=RATIO)

The hypothesis  $H_0: \mu_1/\mu_2 = \mu_0$ , where  $\mu_1$  and  $\mu_2$  are the means of the first and second PAIRED variables, respectively, can be rewritten as  $H_0: \mu_1 - \mu_0\mu_2 = 0$ . The  $t$  value and  $p$ -value are computed in the same way as in the one-sample design in the section “Normal Data (DIST=NORMAL)” on page 8452 based on the transformed values

$$z_i = y_{1i} - \mu_0 y_{2i} \quad , \quad i \in \{1, \dots, n^*\}$$

Estimates and confidence limits are not computed for this situation.

## Two-Independent-Sample Design

Define the following notation:

$$\begin{aligned}
 n_1^* &= \text{number of observations at first class level} \\
 n_2^* &= \text{number of observations at second class level} \\
 y_{1i} &= \text{value of } i\text{th observation at first class level, } i \in \{1, \dots, n_1^*\} \\
 y_{2i} &= \text{value of } i\text{th observation at second class level, } i \in \{1, \dots, n_2^*\} \\
 f_{1i} &= \text{frequency of } i\text{th observation at first class level, } i \in \{1, \dots, n_1^*\} \\
 f_{2i} &= \text{frequency of } i\text{th observation at second class level, } i \in \{1, \dots, n_2^*\} \\
 w_{1i} &= \text{weight of } i\text{th observation at first class level, } i \in \{1, \dots, n_1^*\} \\
 w_{2i} &= \text{weight of } i\text{th observation at second class level, } i \in \{1, \dots, n_2^*\} \\
 n_1 &= \text{sample size for first class level} = \sum_i^{n_1^*} f_{1i} \\
 n_2 &= \text{sample size for second class level} = \sum_i^{n_2^*} f_{2i}
 \end{aligned}$$

### Normal Difference (DIST=NORMAL TEST=DIFF)

Observations at the first class level are assumed to be distributed as  $N(\mu_1, \sigma_1^2)$ , and observations at the second class level are assumed to be distributed as  $N(\mu_2, \sigma_2^2)$ , where  $\mu_1, \mu_2, \sigma_1$ , and  $\sigma_2$  are unknown.

The within-class-level mean estimates ( $\bar{y}_1$  and  $\bar{y}_2$ ), standard deviation estimates ( $s_1$  and  $s_2$ ), standard errors ( $SE_1$  and  $SE_2$ ), and confidence limits for means and standard deviations are computed in the same way as for the one-sample design in the section “Normal Data (DIST=NORMAL)” on page 8452.

The mean difference  $\mu_1 - \mu_2 = \mu_d$  is estimated by

$$\bar{y}_d = \bar{y}_1 - \bar{y}_2$$

Under the assumption of equal variances ( $\sigma_1^2 = \sigma_2^2$ ), the pooled estimate of the common standard deviation is

$$s_p = \left( \frac{(n_1 - 1)s_1^2 + (n_2 - 1)s_2^2}{n_1 + n_2 - 2} \right)^{\frac{1}{2}}$$

The pooled standard error (the estimated standard deviation of  $\bar{y}_d$  assuming equal variances) is

$$SE_p = s_p \left( \frac{1}{\sum_{i=1}^{n_1^*} f_{1i} w_{1i}} + \frac{1}{\sum_{i=1}^{n_2^*} f_{2i} w_{2i}} \right)^{\frac{1}{2}}$$

The pooled  $100(1 - \alpha)\%$  confidence interval for the mean difference  $\mu_d$  is

$$\begin{aligned}
 &(\bar{y}_d - t_{1-\frac{\alpha}{2}, n_1+n_2-2} SE_p, \bar{y}_d + t_{1-\frac{\alpha}{2}, n_1+n_2-2} SE_p), \text{ SIDES=2} \\
 &(-\infty, \bar{y}_d + t_{1-\alpha, n_1+n_2-2} SE_p), \text{ SIDES=L} \\
 &(\bar{y}_d - t_{1-\alpha, n_1+n_2-2} SE_p, \infty), \text{ SIDES=U}
 \end{aligned}$$

The  $t$  value for the pooled test is computed as

$$t_p = \frac{\bar{y}_d - \mu_0}{SE_p}$$

The  $p$ -value of the test is computed as

$$p\text{-value} = \begin{cases} P(t_p^2 > F_{1-\alpha, 1, n_1+n_2-2}) & , \quad 2\text{-sided} \\ P(t_p < t_{\alpha, n_1+n_2-2}) & , \quad \text{lower 1-sided} \\ P(t_p > t_{1-\alpha, n_1+n_2-2}) & , \quad \text{upper 1-sided} \end{cases}$$

Under the assumption of unequal variances (the Behrens-Fisher problem), the unpooled standard error is computed as

$$SE_u = \left( \frac{s_1^2}{\sum_{i=1}^{n_1^*} f_{1i} w_{1i}} + \frac{s_2^2}{\sum_{i=1}^{n_2^*} f_{2i} w_{2i}} \right)^{\frac{1}{2}}$$

Satterthwaite's (1946) approximation for the degrees of freedom, extended to accommodate weights, is computed as

$$df_u = \frac{SE_u^4}{\frac{s_1^4}{(n_1-1)\left(\sum_{i=1}^{n_1^*} f_{1i} w_{1i}\right)^2} + \frac{s_2^4}{(n_2-1)\left(\sum_{i=1}^{n_2^*} f_{2i} w_{2i}\right)^2}}$$

The unpooled Satterthwaite  $100(1 - \alpha)\%$  confidence interval for the mean difference  $\mu_d$  is

$$\begin{aligned} & \left( \bar{y}_d - t_{1-\frac{\alpha}{2}, df_u} SE_u, \bar{y}_d + t_{1-\frac{\alpha}{2}, df_u} SE_u \right), \quad \text{SIDES=2} \\ & \left( -\infty, \bar{y}_d + t_{1-\alpha, df_u} SE_u \right), \quad \text{SIDES=L} \\ & \left( \bar{y}_d - t_{1-\alpha, df_u} SE_u, \infty \right), \quad \text{SIDES=U} \end{aligned}$$

The  $t$  value for the unpooled Satterthwaite test is computed as

$$t_u = \frac{\bar{y}_d - \mu_0}{SE_u}$$

The  $p$ -value of the unpooled Satterthwaite test is computed as

$$p\text{-value} = \begin{cases} P(t_u^2 > F_{1-\alpha, 1, df_u}) & , \quad 2\text{-sided} \\ P(t_u < t_{\alpha, df_u}) & , \quad \text{lower 1-sided} \\ P(t_u > t_{1-\alpha, df_u}) & , \quad \text{upper 1-sided} \end{cases}$$

When the **COCHRAN** option is specified in the **PROC TTEST** statement, the Cochran and Cox (1950) approximation of the  $p$ -value of the  $t_u$  statistic is the value of  $p$  such that

$$t_u = \frac{\left( \frac{s_1^2}{\sum_{i=1}^{n_1^*} f_{1i} w_{1i}} \right) t_1 + \left( \frac{s_2^2}{\sum_{i=1}^{n_2^*} f_{2i} w_{2i}} \right) t_2}{\left( \frac{s_1^2}{\sum_{i=1}^{n_1^*} f_{1i} w_{1i}} \right) + \left( \frac{s_2^2}{\sum_{i=1}^{n_2^*} f_{2i} w_{2i}} \right)}$$

where  $t_1$  and  $t_2$  are the critical values of the  $t$  distribution corresponding to a significance level of  $p$  and sample sizes of  $n_1$  and  $n_2$ , respectively. The number of degrees of freedom is undefined when  $n_1 \neq n_2$ . In general, the Cochran and Cox test tends to be conservative (Lee and Gurland 1975).

The  $100(1 - \alpha)\%$  **CI=EQUAL** and **CI=UMPU** confidence intervals for the common population standard deviation  $\sigma$  assuming equal variances are computed as discussed in the section “**Normal Data (DIST=NORMAL)**” on page 8452 for the one-sample design, except replacing  $s^2$  by  $s_p^2$  and  $(n - 1)$  by  $(n_1 + n_2 - 1)$ .

The folded form of the  $F$  statistic,  $F'$ , tests the hypothesis that the variances are equal (Steel and Torrie 1980), where

$$F' = \frac{\max(s_1^2, s_2^2)}{\min(s_1^2, s_2^2)}$$

A test of  $F'$  is a two-tailed  $F$  test because you do not specify which variance you expect to be larger. The  $p$ -value gives the probability of a greater  $F$  value under the null hypothesis that  $\sigma_1^2 = \sigma_2^2$ . Note that this test is not very robust to violations of the assumption that the data are normally distributed, and thus it is not recommended without confidence in the normality assumption.

#### **Lognormal Ratio (DIST=LOGNORMAL TEST=RATIO)**

The **DIST=LOGNORMAL** analysis is handled by log-transforming the data and null value, performing a **DIST=NORMAL** analysis, and then transforming the results back to the original scale. See the section “**Normal Data (DIST=NORMAL)**” on page 8452 for the one-sample design for details on how the **DIST=NORMAL** computations for means and standard deviations are transformed into the **DIST=LOGNORMAL** results for geometric means and CVs. As mentioned in the section “**Coefficient of Variation**” on page 8451, the assumption of equal CVs on the lognormal scale is analogous to the assumption of equal variances on the normal scale.

#### **Normal Ratio (DIST=NORMAL TEST=RATIO)**

The distributional assumptions, equality of variances test, and within-class-level mean estimates ( $\bar{y}_1$  and  $\bar{y}_2$ ), standard deviation estimates ( $s_1$  and  $s_2$ ), standard errors ( $SE_1$  and  $SE_2$ ), and confidence limits for means and standard deviations are the same as in the section “**Normal Difference (DIST=NORMAL TEST=DIFF)**” on page 8455 for the two-independent-sample design.

The mean ratio  $\mu_1/\mu_2 = \mu_r$  is estimated by

$$\hat{\mu}_r = \bar{y}_1/\bar{y}_2$$

No estimates or confidence intervals for the ratio of standard deviations are computed.

Under the assumption of equal variances ( $\sigma_1^2 = \sigma_2^2$ ), the pooled confidence interval for the mean ratio is the Fieller (1954) confidence interval, extended to accommodate weights. Let

$$a_p = \frac{s_p^2 t_{1-\frac{\alpha}{2}, n_1+n_2-2}^2}{\sum_{i=1}^{n_2^*} f_{2i} w_{2i}} - \bar{y}_2^2$$

$$b_p = \bar{y}_1 \bar{y}_2$$

$$c_p = \frac{s_p^2 t_{1-\frac{\alpha}{2}, n_1+n_2-2}^2}{\sum_{i=1}^{n_1^*} f_{1i} w_{1i}} - \bar{y}_1^2$$

where  $s_p$  is the pooled standard deviation defined in the section “Normal Difference (DIST=NORMAL TEST=DIFF)” on page 8455 for the two-independent-sample design. If  $a_p \geq 0$  (which occurs when  $\bar{y}_2$  is too close to zero), then the pooled two-sided  $100(1 - \alpha)\%$  Fieller confidence interval for  $\mu_r$  does not exist. If  $a < 0$ , then the interval is

$$\left( -\frac{b_p}{a_p} + \frac{(b_p^2 - a_p c_p)^{\frac{1}{2}}}{a_p}, -\frac{b_p}{a_p} - \frac{(b_p^2 - a_p c_p)^{\frac{1}{2}}}{a_p} \right)$$

For the one-sided intervals, let

$$a_p^* = \frac{s_p^2 t_{1-\alpha, n_1+n_2-2}^2}{\sum_{i=1}^{n_2^*} f_{2i} w_{2i}} - \bar{y}_2^2$$

$$c_p^* = \frac{s_p^2 t_{1-\alpha, n_1+n_2-2}^2}{\sum_{i=1}^{n_1^*} f_{1i} w_{1i}} - \bar{y}_1^2$$

which differ from  $a_p$  and  $c_p$  only in the use of  $\alpha$  in place of  $\alpha/2$ . If  $a_p^* \geq 0$ , then the pooled one-sided  $100(1 - \alpha)\%$  Fieller confidence intervals for  $\mu_r$  do not exist. If  $a_p^* < 0$ , then the intervals are

$$\left( -\infty, -\frac{b_p}{a_p^*} - \frac{(b_p^2 - a_p^* c_p^*)^{\frac{1}{2}}}{a_p^*} \right), \text{ SIDES=L}$$

$$\left( -\frac{b_p}{a_p^*} + \frac{(b_p^2 - a_p^* c_p^*)^{\frac{1}{2}}}{a_p^*}, \infty \right), \text{ SIDES=U}$$

The pooled  $t$  test assuming equal variances is the Sasabuchi (1988a, b) test. The hypothesis  $H_0: \mu_r = \mu_0$  is rewritten as  $H_0: \mu_1 - \mu_0 \mu_2 = 0$ , and the pooled  $t$  test in the section “Normal Difference (DIST=NORMAL TEST=DIFF)” on page 8455 for the two-independent-sample design is conducted on the original  $y_{1i}$  values ( $i \in \{1, \dots, n_1^*\}$ ) and transformed values of  $y_{2i}$

$$y_{2i}^* = \mu_0 y_{2i}, \quad i \in \{1, \dots, n_2^*\}$$

with a null difference of 0. The  $t$  value for the Sasabuchi pooled test is computed as

$$t_p = \frac{\bar{y}_1 - \mu_0 \bar{y}_2}{s_p \left( \frac{1}{\sum_{i=1}^{n_1^*} f_{1i} w_{1i}} + \frac{\mu_0^2}{\sum_{i=1}^{n_2^*} f_{2i} w_{2i}} \right)^{\frac{1}{2}}}$$

The  $p$ -value of the test is computed as

$$p\text{-value} = \begin{cases} P(t_p^2 > F_{1-\alpha, 1, n_1+n_2-2}) & , \text{ 2-sided} \\ P(t_p < t_{\alpha, n_1+n_2-2}) & , \text{ lower 1-sided} \\ P(t_p > t_{1-\alpha, n_1+n_2-2}) & , \text{ upper 1-sided} \end{cases}$$

Under the assumption of unequal variances, the unpooled Satterthwaite-based confidence interval for the mean ratio  $\mu_r$  is computed according to the method in Dilba, Schaarschmidt, and Hothorn (2006), extended

to accommodate weights. The degrees of freedom are computed as

$$df_u = \frac{\left( \frac{s_1^2}{\sum_{i=1}^{n_1^*} f_{1i} w_{1i}} + \frac{\hat{\mu}_r^2 s_2^2}{\sum_{i=1}^{n_2^*} f_{2i} w_{2i}} \right)^2}{\frac{s_1^4}{(n_1-1) \left( \sum_{i=1}^{n_1^*} f_{1i} w_{1i} \right)^2} + \frac{\hat{\mu}_r^4 s_2^4}{(n_2-1) \left( \sum_{i=1}^{n_2^*} f_{2i} w_{2i} \right)^2}}$$

Note that the estimate  $\hat{\mu}_r = \bar{y}_1 / \bar{y}_2$  is used in  $df_u$ . Let

$$\begin{aligned} a_u &= \frac{s_2^2 t_{1-\frac{\alpha}{2}, df_u}^2}{\sum_{i=1}^{n_2^*} f_{2i} w_{2i}} - \bar{y}_2^2 \\ b_u &= \bar{y}_1 \bar{y}_2 \\ c_u &= \frac{s_1^2 t_{1-\frac{\alpha}{2}, df_u}^2}{\sum_{i=1}^{n_1^*} f_{1i} w_{1i}} - \bar{y}_1^2 \end{aligned}$$

where  $s_1$  and  $s_2$  are the within-class-level standard deviations defined in the section “**Normal Difference (DIST=NORMAL TEST=DIFF)**” on page 8455 for the two-independent-sample design. If  $a_u \geq 0$  (which occurs when  $\bar{y}_2$  is too close to zero), then the unpooled Satterthwaite-based two-sided  $100(1 - \alpha)\%$  confidence interval for  $\mu_r$  does not exist. If  $a_u < 0$ , then the interval is

$$\left( -\frac{b_u}{a_u} + \frac{(b_u^2 - a_u c_u)^{\frac{1}{2}}}{a_u}, -\frac{b_u}{a_u} - \frac{(b_u^2 - a_u c_u)^{\frac{1}{2}}}{a_u} \right)$$

The  $t$  test assuming unequal variances is the test derived in Tamhane and Logan (2004). The hypothesis  $H_0: \mu_r = \mu_0$  is rewritten as  $H_0: \mu_1 - \mu_0 \mu_2 = 0$ , and the Satterthwaite  $t$  test in the section “**Normal Difference (DIST=NORMAL TEST=DIFF)**” on page 8455 for the two-independent-sample design is conducted on the original  $y_{1i}$  values ( $i \in \{1, \dots, n_1^*\}$ ) and transformed values of  $y_{2i}$

$$y_{2i}^* = \mu_0 y_{2i}, \quad i \in \{1, \dots, n_2^*\}$$

with a null difference of 0. The degrees of freedom used in the unpooled  $t$  test differs from the  $df_u$  used in the unpooled confidence interval. The mean ratio  $\mu_0$  under the null hypothesis is used in place of the estimate  $\hat{\mu}_r$ :

$$df_u^* = \frac{\left( \frac{s_1^2}{\sum_{i=1}^{n_1^*} f_{1i} w_{1i}} + \frac{\mu_0^2 s_2^2}{\sum_{i=1}^{n_2^*} f_{2i} w_{2i}} \right)^2}{\frac{s_1^4}{(n_1-1) \left( \sum_{i=1}^{n_1^*} f_{1i} w_{1i} \right)^2} + \frac{\mu_0^4 s_2^4}{(n_2-1) \left( \sum_{i=1}^{n_2^*} f_{2i} w_{2i} \right)^2}}$$

The  $t$  value for the Satterthwaite-based unpooled test is computed as

$$t_u = \frac{\bar{y}_1 - \mu_0 \bar{y}_2}{\left( \frac{s_1^2}{\sum_{i=1}^{n_1^*} f_{1i} w_{1i}} + \frac{\mu_0^2 s_2^2}{\sum_{i=1}^{n_2^*} f_{2i} w_{2i}} \right)^{\frac{1}{2}}}$$

The  $p$ -value of the test is computed as

$$p\text{-value} = \begin{cases} P\left(t_u^2 > F_{1-\alpha, 1, df_u^*}\right) & , \text{ 2-sided} \\ P\left(t_u < t_{\alpha, df_u^*}\right) & , \text{ lower 1-sided} \\ P\left(t_u > t_{1-\alpha, df_u^*}\right) & , \text{ upper 1-sided} \end{cases}$$

## AB/BA Crossover Design

Let “A” and “B” denote the two treatment values. Define the following notation:

$n_1^*$  = number of observations with treatment sequence AB

$n_2^*$  = number of observations with treatment sequence BA

$y_{11i}$  = response value of  $i$ th observation in sequence AB during period 1,  $i \in \{1, \dots, n_1^*\}$

$y_{12i}$  = response value of  $i$ th observation in sequence AB during period 2,  $i \in \{1, \dots, n_1^*\}$

$y_{21i}$  = response value of  $i$ th observation in sequence BA during period 1,  $i \in \{1, \dots, n_2^*\}$

$y_{22i}$  = response value of  $i$ th observation in sequence BA during period 2,  $i \in \{1, \dots, n_2^*\}$

So  $\{y_{11i}, \dots, y_{11n_1^*}\}$  and  $\{y_{22i}, \dots, y_{22n_2^*}\}$  are all observed at treatment level A, and  $\{y_{12i}, \dots, y_{12n_1^*}\}$  and  $\{y_{21i}, \dots, y_{21n_1^*}\}$  are all observed at treatment level B.

Define the *period difference* for an observation as the difference between period 1 and period 2 response values:

$$pd_{kji} = y_{k1i} - y_{k2i}$$

for  $k \in \{1, 2\}$  and  $i \in \{1, \dots, n_k^*\}$ . Similarly, the *period ratio* is the ratio between period 1 and period 2 response values:

$$pr_{kji} = y_{k1i} / y_{k2i}$$

The *crossover difference* for an observation is the difference between treatment A and treatment B response values:

$$cd_{kji} = \begin{cases} y_{k1i} - y_{k2i} & , \quad k = 1 \\ y_{k2i} - y_{k1i} & , \quad k = 2 \end{cases}$$

Similarly, the *crossover ratio* is the ratio between treatment A and treatment B response values:

$$cr_{kji} = \begin{cases} y_{k1i} / y_{k2i} & , \quad k = 1 \\ y_{k2i} / y_{k1i} & , \quad k = 2 \end{cases}$$

In the absence of the **IGNOREPERIOD** option in the **PROC TTEST** statement, the data are split into two groups according to treatment sequence and analyzed as a two-independent-sample design. If **DIST=NORMAL**, then the analysis of the treatment effect is based on the half period differences  $\{pd_{kji}/2\}$ , and the analysis for the period effect is based on the half crossover differences  $\{cd_{kji}/2\}$ . The computations for the normal difference analysis are the same as in the section “**Normal Difference (DIST=NORMAL TEST=DIFF)**” on page 8455 for the two-independent-sample design. The normal ratio analysis without the **IGNOREPERIOD** option is not supported for the AB/BA crossover design. If **DIST=LOGNORMAL**, then

the analysis of the treatment effect is based on the square root of the period ratios  $\{\sqrt{Pr_{kji}}\}$ , and the analysis for the period effect is based on the square root of the crossover ratios  $\{\sqrt{Cr_{kji}}\}$ . The computations are the same as in the section “Lognormal Ratio (DIST=LOGNORMAL TEST=RATIO)” on page 8457 for the two-independent-sample design.

If the **IGNOREPERIOD** option is specified, then the treatment effect is analyzed as a paired analysis on the (treatment A, treatment B) response value pairs, regardless of treatment sequence. So the set of pairs is taken to be the concatenation of  $\{(y_{111}, y_{121}), \dots, (y_{11n_1^*}, y_{12n_1^*})\}$  and  $\{(y_{221}, y_{211}), \dots, (y_{22n_2^*}, y_{21n_2^*})\}$ . The computations are the same as in the section “Paired Design” on page 8454.

See Senn (2002, Chapter 3) for a more detailed discussion of the AB/BA crossover design.

## TOST Equivalence Test

The hypotheses for an equivalence test are

$$H_0: \mu < \theta_L \quad \text{or} \quad \mu > \theta_U$$

$$H_1: \theta_L \leq \mu \leq \theta_U$$

where  $\theta_L$  and  $\theta_U$  are the lower and upper bounds specified in the **TOST** option in the **PROC TTEST** statement, and  $\mu$  is the analysis criterion (mean, mean ratio, or mean difference, depending on the analysis). Following the two one-sided tests (TOST) procedure of Schuirmann (1987), the equivalence test is conducted by performing two separate tests:

$$H_{a0}: \mu < \theta_L$$

$$H_{a1}: \mu \geq \theta_L$$

and

$$H_{b0}: \mu > \theta_U$$

$$H_{b1}: \mu \leq \theta_U$$

The overall  $p$ -value is the larger of the two  $p$ -values of those tests.

Rejection of  $H_0$  in favor of  $H_1$  at significance level  $\alpha$  occurs if and only if the  $100(1 - 2\alpha)\%$  confidence interval for  $\mu$  is contained completely within  $(\theta_L, \theta_U)$ . So, the  $100(1 - 2\alpha)\%$  confidence interval for  $\mu$  is displayed in addition to the usual  $100(1 - \alpha)\%$  interval.

For further discussion of equivalence testing for the designs supported in the **TTEST** procedure, see Phillips (1990); Diletti, Hauschke, and Steijns (1991); Hauschke et al. (1999).

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## Displayed Output

For an AB/BA crossover design, the “CrossoverVarInfo” table shows the variables specified for the response and treatment values in each period of the design.

The summary statistics in the “Statistics” table and confidence limits in the “ConfLimits” table are displayed for certain variables and/or transformations or subgroups of the variables in the analysis, depending on the design. For a one-sample design, summary statistics are displayed for all variables in the analysis. For a paired design, statistics are displayed for the difference if you specify the **TEST=DIFF** option in the **PROC**



TTEST statement, or for the ratio if you specify TEST=RATIO. For a two-independent-sample design, the statistics for each of the two groups and for the difference (if TEST=DIFF) or ratio (if TEST=RATIO) are displayed. For an AB/BA crossover design, statistics are displayed for each of the four cells in the design (all four combinations of the two periods and two treatments). If the IGNOREPERIOD option is absent, then if TEST=DIFF is specified, statistics are displayed for the treatment difference within each sequence and overall, and also for the period difference. If TEST=RATIO, statistics are displayed for the treatment ratio within each sequence and overall, and also for the period ratio. If the IGNOREPERIOD option is specified in the VAR statement, then statistics are displayed for the overall treatment difference if TEST=DIFF or for the overall treatment ratio if TEST=RATIO.

The “Statistics” table displays the following summary statistics:

- the name of the variable(s), displayed if the NOBYVAR option is used in the PROC TTEST statement
- the name of the classification variable (if two-independent-sample design) or treatment and period (if AB/BA crossover design)
- N, the number of nonmissing values
- the (arithmetic) Mean, displayed if the DIST=NORMAL option is specified in the PROC TTEST statement
- the Geometric Mean, displayed if the DIST=LOGNORMAL option is specified in the PROC TTEST statement
- Std Dev, the standard deviation, displayed if the DIST=NORMAL option is specified in the PROC TTEST statement
- the Coefficient of Variation, displayed if the DIST=LOGNORMAL option is specified in the PROC TTEST statement
- Std Err, the standard error of the mean, displayed if the DIST=NORMAL option is specified in the PROC TTEST statement
- the Minimum value
- the Maximum value

The “ConfLimits” table displays the following:

- the name of the variable(s), displayed if the NOBYVAR option is used in the PROC TTEST statement
- the name of the classification variable (if two-independent-sample design) or treatment and period (if AB/BA crossover design)
- the (arithmetic) Mean, displayed if the DIST=NORMAL option is specified in the PROC TTEST statement
- the Geometric Mean, displayed if the DIST=LOGNORMAL option is specified in the PROC TTEST statement

- $100(1 - \alpha)\%$  CL Mean, the lower and upper confidence limits for the mean. Separate pooled and Satterthwaite confidence limits are shown for the difference or ratio transformations in two-independent-sample designs and AB/BA crossover designs without the `IGNOREPERIOD` option.
- Std Dev, the standard deviation, displayed if the `DIST=NORMAL` option is specified in the `PROC TTEST` statement
- the Coefficient of Variation, displayed if the `DIST=LOGNORMAL` option is specified in the `PROC TTEST` statement
- $100(1 - \alpha)\%$  CL Std Dev, the equal-tailed confidence limits for the standard deviation, displayed if the `DIST=NORMAL` and `CI=EQUAL` options are specified in the `PROC TTEST` statement
- $100(1 - \alpha)\%$  UMPU CL Std Dev, the UMPU confidence limits for the standard deviation, displayed if the `DIST=NORMAL` and `CI=UMPU` options are specified in the `PROC TTEST` statement
- $100(1 - \alpha)\%$  CL CV, the equal-tailed confidence limits for the coefficient of variation, displayed if the `DIST=LOGNORMAL` and `CI=EQUAL` options are specified in the `PROC TTEST` statement
- $100(1 - \alpha)\%$  UMPU CL CV, the UMPU confidence limits for the coefficient of variation, displayed if the `DIST=LOGNORMAL` and `CI=UMPU` options are specified in the `PROC TTEST` statement

The confidence limits in the “EquivLimits” table and test results in the “TTests” and “EquivTests” tables are displayed only for the test criteria—that is, the variables or transformations being tested. For a one-sample design, results are displayed for all variables in the analysis. For a paired design, results are displayed for the difference if you specify the `TEST=DIFF` option in the `PROC TTEST` statement, or for the ratio if you specify `TEST=RATIO`. For a two-independent-sample design, the results for the difference (if `TEST=DIFF`) or ratio (if `TEST=RATIO`) are displayed. For an AB/BA crossover design, results are displayed for the treatment difference (if `TEST=DIFF`) or ratio (if `TEST=RATIO`). If the `IGNOREPERIOD` option is absent, then results are also displayed for the period difference (if `TEST=DIFF`) or ratio (if `TEST=RATIO`).

The “EquivLimits” table, produced only if the `TOST` option is specified in the `PROC TTEST` statement, displays the following:

- the name of the variable(s), displayed if the `NOBYVAR` option is used in the `PROC TTEST` statement
- the (arithmetic) Mean, displayed if the `DIST=NORMAL` option is specified in the `PROC TTEST` statement
- the Geometric Mean, displayed if the `DIST=LOGNORMAL` option is specified in the `PROC TTEST` statement
- Lower Bound, the lower equivalence bound for the mean specified in the `TOST` option in the `PROC TTEST` statement
- $100(1 - 2\alpha)\%$  CL Mean, the lower and upper confidence limits for the mean relevant to the equivalence test. Separate pooled and Satterthwaite confidence limits are shown for two-independent-sample designs and AB/BA crossover designs without the `IGNOREPERIOD` option.
- Upper Bound, the upper equivalence bound for the mean specified in the `TOST` option in the `PROC TTEST` statement

- Assessment, the result of the equivalence test at the significance level specified by the ALPHA= option in the PROC TTEST statement, either “Equivalent” or “Not equivalent”

The “TTests” table is produced only if the TOST option is *not* specified in the PROC TTEST statement. Separate results for pooled and Satterthwaite tests (and also the Cochran and Cox test, if the COCHRAN option is specified in the PROC TTEST statement) are displayed for two-independent-sample designs and AB/BA crossover designs without the IGNOREPERIOD option. The table includes the following results:

- the name of the variable(s), displayed if the NOBYVAR option is used in the PROC TTEST statement
- t Value, the  $t$  statistic for comparing the mean to the null value as specified by the H0= option in the PROC TTEST statement
- DF, the degrees of freedom
- the  $p$ -value, the probability of obtaining a  $t$  statistic at least as extreme as the observed  $t$  value under the null hypothesis

The “EquivTests” table is produced only if the TOST option is specified in the PROC TTEST statement. Separate results for pooled and Satterthwaite tests are displayed for two-independent-sample designs and AB/BA crossover designs without the IGNOREPERIOD option. Each test consists of two separate one-sided tests. The overall  $p$ -value is the larger  $p$ -value from these two tests. The table includes the following results:

- the name of the variable(s), displayed if the NOBYVAR option is used in the PROC TTEST statement
- Null, the lower equivalence bound for the Upper test or the upper equivalence bound for the Lower test, as specified by the TOST option in the PROC TTEST statement
- t Value, the  $t$  statistic for comparing the mean to the Null value
- DF, the degrees of freedom
- the  $p$ -value, the probability of obtaining a  $t$  statistic at least as extreme as the observed  $t$  value under the null hypothesis

The “Equality” table gives the results of the test of equality of variances. It is displayed for two-independent-sample designs and AB/BA crossover designs without the IGNOREPERIOD option. The table includes the following results:

- the name of the variable(s), displayed if the NOBYVAR option is used in the PROC TTEST statement
- Num DF and Den DF, the numerator and denominator degrees of freedom
- F Value, the  $F'$  (folded) statistic
- Pr > F, the probability of a greater  $F'$  value. This is the two-tailed  $p$ -value.

## ODS Table Names

PROC TTEST assigns a name to each table it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in Table 99.5. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

**Table 99.5** ODS Tables Produced by PROC TTEST

| ODS Table Name | Description                                                                                            | Syntax                                                    |
|----------------|--------------------------------------------------------------------------------------------------------|-----------------------------------------------------------|
| ConfLimits     | 100(1 – $\alpha$ )% confidence limits for means, standard deviations, and/or coefficients of variation | By default                                                |
| Equality       | Tests for equality of variance                                                                         | CLASS statement or<br>VAR / CROSSEVER=<br>PROC TTEST TOST |
| EquivLimits    | 100(1 – 2 $\alpha$ )% confidence limits for means                                                      | PROC TTEST TOST                                           |
| EquivTests     | Equivalence <i>t</i> tests                                                                             | PROC TTEST TOST                                           |
| Statistics     | Univariate summary statistics                                                                          | By default                                                |
| TTests         | <i>t</i> tests                                                                                         | By default                                                |

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “Statistical Graphics Using ODS.”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “A Primer on ODS Statistical Graphics” on page 599 in Chapter 21, “Statistical Graphics Using ODS.”

## ODS Graph Names

You can reference every graph produced through ODS Graphics with a name. The names of the graphs that PROC TTEST generates are listed in Table 99.6, along with the required statements and options.

**Table 99.6** Graphs Produced by PROC TTEST

| ODS Graph Name        | Plot Description                                                                               | Option                                           |
|-----------------------|------------------------------------------------------------------------------------------------|--------------------------------------------------|
| AgreementOfPeriods    | Plot of period 2 against period 1 response values for an AB/BA crossover design                | VAR / CROSSEVER=<br>PLOTS=AGREEMENT(TYPE=PERIOD) |
| AgreementOfTreatments | Plot of second treatment against first treatment response values for an AB/BA crossover design | VAR / CROSSEVER=<br>PLOTS=AGREEMENT              |

Table 99.6 continued

| ODS Graph Name  | Plot Description                                                                                                                                                                 | Option                                          |
|-----------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------|
| AgreementPlot   | Plot of second response against first response for a paired design                                                                                                               | PAIRED statement<br>PLOTS=AGREEMENT             |
| BoxPlot         | Box plots, also with confidence band for one-sample or paired design                                                                                                             | PLOTS=BOX<br>PLOTS=SUMMARY(UNPACK)              |
| Histogram       | Histograms with overlaid kernel densities, and also normal densities if <code>DIST=NORMAL</code>                                                                                 | PLOTS=HISTOGRAM<br>PLOTS=SUMMARY(UNPACK)        |
| Interval        | Confidence intervals for means                                                                                                                                                   | PLOTS=INTERVAL                                  |
| ProfilesOverPrd | Plot of response profiles over periods 1 and 2 for an AB/BA crossover design                                                                                                     | VAR / CROSSOVER=<br>PLOTS=PROFILES(TYPE=PERIOD) |
| ProfilesOverTrt | Plot of response profiles over first and second treatments for an AB/BA crossover design                                                                                         | VAR / CROSSOVER=<br>PLOTS=PROFILES              |
| ProfilesPlot    | Plot of response profiles over first and second response values for a paired design                                                                                              | PAIRED statement<br>PLOTS=PROFILES              |
| QQPlot          | Normal quantile-quantile plots                                                                                                                                                   | PLOTS=QQ                                        |
| SummaryPanel    | Histograms with overlaid kernel densities (and also normal densities if <code>DIST=NORMAL</code> ) and box plots (and also with confidence band for one-sample or paired design) | PLOTS=SUMMARY                                   |

## Interpreting Graphs

### Agreement Plots for Paired Designs

For paired designs, the second response of each pair is plotted against the first response, with the mean shown as a large bold symbol. If the `WEIGHT` statement is used, then the mean is the weighted mean. A diagonal line with slope=0 and y-intercept=1 is overlaid. The location of the points with respect to the diagonal line reveals the strength and direction of the difference or ratio. The tighter the clustering along the same direction as the line, the stronger the positive correlation of the two measurements for each subject. Clustering along a direction perpendicular to the line indicates negative correlation.

### Period Agreement Plots for Crossover Designs

The response in the second period is plotted against the response in the first period, with plot symbols distinguishing the two treatment sequences and the two sequence means shown larger in bold. If the `WEIGHT`

statement is used, then the means are weighted means. A diagonal line with slope=0 and y-intercept=1 is overlaid.

In the absence of a strong period effect, the points from each sequence will appear as mirror images about the diagonal line, farther apart with stronger treatment effects. Deviations from symmetry about the diagonal line indicate a period effect. The spread of points within each treatment sequence is an indicator of between-subject variability. The tighter the clustering along the same direction as the line (within each treatment sequence), the stronger the positive correlation of the two measurements for each subject. Clustering along a direction perpendicular to the line indicates negative correlation.

The period agreement plot is usually less informative than the treatment agreement plot. The exception is when the period effect is stronger than the treatment effect.

### **Treatment Agreement Plots for Crossover Designs**

The response associated with the second treatment is plotted against the response associated with the first treatment, with plot symbols distinguishing the two treatment sequences and the two sequence means shown larger in bold. If the **WEIGHT** statement is used, then the means are weighted means. A diagonal line with slope=0 and y-intercept=1 is overlaid.

The location of the points with respect to the diagonal line reveals the strength and direction of the treatment effect. Substantial location differences between the two sequences indicates a strong period effect. The spread of points within each treatment sequence is an indicator of between-subject variability. The tighter the clustering along the same direction as the line (within each treatment sequence), the stronger the positive correlation of the two measurements for each subject. Clustering along a direction perpendicular to the line indicates negative correlation.

### **Box Plots**

The box is drawn from the 25th percentile (lower quartile) to the 75th percentile (upper quartile). The vertical line inside the box shows the location of the median. If **DIST=NORMAL**, then a diamond symbol shows the location of the mean. The whiskers extend to the minimum and maximum observations, and circles beyond the whiskers identify outliers.

For one-sample and paired designs, a confidence interval for the mean is shown as a band in the background. If the analysis is an equivalence analysis (with the **TOST** option in the **PROC TTEST** statement), then the interval is a  $100(1 - 2\alpha)\%$  confidence interval shown along with the equivalence bounds. The inclusion of this interval completely within the bounds is indicative of a significant  $p$ -value. If the analysis is not an equivalence analysis, then the confidence level is  $100(1 - \alpha)\%$ . If the **SHOWHO** global plot option is used, then the null value for the test is shown. If the **WEIGHT** statement is used, then weights are incorporated in the confidence intervals.

### **Histograms**

The **WEIGHT** statement is ignored in the computation of the normal and kernel densities.

### **Confidence Intervals**

If the analysis is an equivalence analysis (with the **TOST** option in the **PROC TTEST** statement), then unless the **TYPE=PERGROUP** option is used, the interval is a  $100(1 - 2\alpha)\%$  mean confidence interval shown along with the equivalence bounds. The inclusion of this interval completely within the bounds is indicative of a significant  $p$ -value.

If the analysis is not an equivalence analysis, or if the `TYPE=PERGROUP` option is used, then the confidence level is  $100(1 - \alpha)\%$ . If the `SHOWHO` global plot option is used, then the null value for the test is shown.

If the `SIDES=L` or `SIDES=U` option is used in the `PROC TTEST` statement, then the unbounded side of the one-sided interval is represented with an arrowhead. Note that the actual location of the arrowhead is irrelevant.

If the `WEIGHT` statement is used, then weights are incorporated in the confidence intervals.

### **Profiles for Paired Designs**

For paired designs, a line is drawn for each observation from left to right connecting the first response to the second response. The mean first response and mean second response are connected with a bold line. If the `WEIGHT` statement is used, then the means are weighted means. The more extreme the slope, the stronger the effect. A wide spread of profiles indicates high between-subject variability. Consistent positive slopes indicate strong positive correlation. Widely varying slopes indicate lack of correlation, while consistent negative slopes indicate strong negative correlation.

### **Profiles over Period for Crossover Designs**

For each observation, the response for the first period is connected to the response for second period, regardless of the treatment applied in each period. The means for each treatment sequence are shown in bold. If the `WEIGHT` statement is used, then the means are weighted means.

In the absence of a strong period effect, the profiles for each sequence will appear as mirror images about an imaginary horizontal line in the center. Deviations from symmetry about this imaginary horizontal line indicate a period effect. A wide spread of profiles within sequence indicates high between-subject variability.

The `TYPE=PERIOD` plot is usually less informative than the `TYPE=TREATMENT` plot. The exception is when the period effect is stronger than the treatment effect.

### **Profiles over Treatment for Crossover Designs**

For each observation, the response for the first treatment is connected to the response for the second treatment, regardless of the periods in which they occur. The means for each treatment sequence are shown in bold. If the `WEIGHT` statement is used, then the means are weighted means.

In general, the more extreme the slope, the stronger the treatment effect. Slope differences between the two treatment sequences measure the period effect. A wide spread of profiles within sequence indicates high between-subject variability.

### **Q-Q Plots**

Q-Q plots are useful for diagnosing violations of the normality and homoscedasticity assumptions. If the data in a Q-Q plot come from a normal distribution, the points will cluster tightly around the reference line. You can use the `UNIVARIATE` procedure with the `NORMAL` option to numerically check the normality assumption.



---

## Examples: TTEST Procedure

---

### Example 99.1: Using Summary Statistics to Compare Group Means

This example, taken from Huntsberger and Billingsley (1989), compares two grazing methods using 32 steers. Half of the steers are allowed to graze continuously while the other half are subjected to controlled grazing time. The researchers want to know if these two grazing methods affect weight gain differently. The data are read by the following DATA step:

```
data graze;
 length GrazeType $ 10;
 input GrazeType $ WtGain @@;
 datalines;
controlled 45 controlled 62
controlled 96 controlled 128
controlled 120 controlled 99
controlled 28 controlled 50
controlled 109 controlled 115
controlled 39 controlled 96
controlled 87 controlled 100
controlled 76 controlled 80
continuous 94 continuous 12
continuous 26 continuous 89
continuous 88 continuous 96
continuous 85 continuous 130
continuous 75 continuous 54
continuous 112 continuous 69
continuous 104 continuous 95
continuous 53 continuous 21
;
```

The variable `GrazeType` denotes the grazing method: “controlled” is controlled grazing and “continuous” is continuous grazing. The dollar sign (\$) following `GrazeType` makes it a character variable, and the trailing at signs (@@) tell the procedure that there is more than one observation per line.

If you have summary data—that is, just means and standard deviations, as computed by PROC MEANS—then you can still use PROC TTEST to perform a simple *t* test analysis. This example demonstrates this mode of input for PROC TTEST. Note, however, that graphics are unavailable when summary statistics are used as input.

The MEANS procedure is invoked to create a data set of summary statistics with the following statements:

```
proc sort;
 by GrazeType;
run;

proc means data=graze noprint;
 var WtGain;
 by GrazeType;
 output out=newgraze;
run;
```



The NOPRINT option eliminates all printed output from the MEANS procedure. The VAR statement tells PROC MEANS to compute summary statistics for the WtGain variable, and the BY statement requests a separate set of summary statistics for each level of GrazeType. The OUTPUT OUT= statement tells PROC MEANS to put the summary statistics into a data set called newgraze so that it can be used in subsequent procedures. This new data set is displayed in Output 99.1.1 by using PROC PRINT as follows:

```
proc print data=newgraze;
run;
```

The \_STAT\_ variable contains the names of the statistics, and the GrazeType variable indicates which group the statistic is from.

**Output 99.1.1** Output Data Set of Summary Statistics

| Obs | GrazeType  | _TYPE_ | _FREQ_ | _STAT_ | WtGain  |
|-----|------------|--------|--------|--------|---------|
| 1   | continuous | 0      | 16     | N      | 16.000  |
| 2   | continuous | 0      | 16     | MIN    | 12.000  |
| 3   | continuous | 0      | 16     | MAX    | 130.000 |
| 4   | continuous | 0      | 16     | MEAN   | 75.188  |
| 5   | continuous | 0      | 16     | STD    | 33.812  |
| 6   | controlled | 0      | 16     | N      | 16.000  |
| 7   | controlled | 0      | 16     | MIN    | 28.000  |
| 8   | controlled | 0      | 16     | MAX    | 128.000 |
| 9   | controlled | 0      | 16     | MEAN   | 83.125  |
| 10  | controlled | 0      | 16     | STD    | 30.535  |

The following statements invoke PROC TTEST with the newgraze data set, as denoted by the DATA= option:

```
proc ttest data=newgraze;
 class GrazeType;
 var WtGain;
run;
```

The CLASS statement contains the variable that distinguishes between the groups being compared, in this case GrazeType. The summary statistics and confidence intervals are displayed first, as shown in Output 99.1.2.

**Output 99.1.2** Summary Statistics and Confidence Limits

| The TTEST Procedure |    |         |         |         |         |         |
|---------------------|----|---------|---------|---------|---------|---------|
| Variable: WtGain    |    |         |         |         |         |         |
| GrazeType           | N  | Mean    | Std Dev | Std Err | Minimum | Maximum |
| continuous          | 16 | 75.1875 | 33.8117 | 8.4529  | 12.0000 | 130.0   |
| controlled          | 16 | 83.1250 | 30.5350 | 7.6337  | 28.0000 | 128.0   |
| Diff (1-2)          |    | -7.9375 | 32.2150 | 11.3897 |         |         |

**Output 99.1.2** *continued*

| GrazeType  | Method        | Mean    | 95% CL Mean |         | Std Dev |
|------------|---------------|---------|-------------|---------|---------|
| continuous |               | 75.1875 | 57.1705     | 93.2045 | 33.8117 |
| controlled |               | 83.1250 | 66.8541     | 99.3959 | 30.5350 |
| Diff (1-2) | Pooled        | -7.9375 | -31.1984    | 15.3234 | 32.2150 |
| Diff (1-2) | Satterthwaite | -7.9375 | -31.2085    | 15.3335 |         |

| GrazeType  | Method        | 95% CL  | Std Dev |
|------------|---------------|---------|---------|
| continuous |               | 24.9768 | 52.3300 |
| controlled |               | 22.5563 | 47.2587 |
| Diff (1-2) | Pooled        | 25.7434 | 43.0609 |
| Diff (1-2) | Satterthwaite |         |         |

In **Output 99.1.2**, The GrazeType column specifies the group for which the statistics are computed. For each class, the sample size, mean, standard deviation and standard error, and maximum and minimum values are displayed. The confidence bounds for the mean are also displayed; however, since summary statistics are used as input, the confidence bounds for the standard deviation of the groups are not calculated.

**Output 99.1.3** shows the results of tests for equal group means and equal variances.

**Output 99.1.3** *t* Tests

| Method        | Variances | DF     | t Value | Pr >  t |
|---------------|-----------|--------|---------|---------|
| Pooled        | Equal     | 30     | -0.70   | 0.4912  |
| Satterthwaite | Unequal   | 29.694 | -0.70   | 0.4913  |

| Equality of Variances |        |        |         |        |
|-----------------------|--------|--------|---------|--------|
| Method                | Num DF | Den DF | F Value | Pr > F |
| Folded F              | 15     | 15     | 1.23    | 0.6981 |

A group test statistic for the equality of means is reported for both equal and unequal variances. Both tests indicate a lack of evidence for a significant difference between grazing methods ( $t = -0.70$  and  $p = 0.4912$  for the pooled test,  $t = -0.70$  and  $p = 0.4913$  for the Satterthwaite test). The equality of variances test does not indicate a significant difference in the two variances ( $F' = 1.23$ ,  $p = 0.6981$ ). Note that this test assumes that the observations in both data sets are normally distributed; this assumption can be checked in PROC UNIVARIATE by using the NORMAL option with the raw data.

Although the ability to use summary statistics as input is useful if you lack access to the original data, some of the output that would otherwise be produced in an analysis on the original data is unavailable. There are also limitations on the designs and distributional assumptions that can be used with summary statistics as input. For more information, see the section “Input Data Set of Statistics” on page 8449.

## Example 99.2: One-Sample Comparison with the FREQ Statement

This example examines children's reading skills. The data consist of Degree of Reading Power (DRP) test scores from 44 third-grade children and are taken from Moore (1995, p. 337). Their scores are given in the following DATA step:

```
data read;
 input score count @@;
 datalines;
40 2 47 2 52 2 26 1 19 2
25 2 35 4 39 1 26 1 48 1
14 2 22 1 42 1 34 2 33 2
18 1 15 1 29 1 41 2 44 1
51 1 43 1 27 2 46 2 28 1
49 1 31 1 28 1 54 1 45 1
;
```

The following statements invoke the TTEST procedure to test if the mean test score is equal to 30.

```
ods graphics on;

proc ttest data=read h0=30;
 var score;
 freq count;
run;

ods graphics off;
```

The count variable contains the frequency of occurrence of each test score; this is specified in the FREQ statement. The output, shown in [Output 99.2.1](#), contains the results.

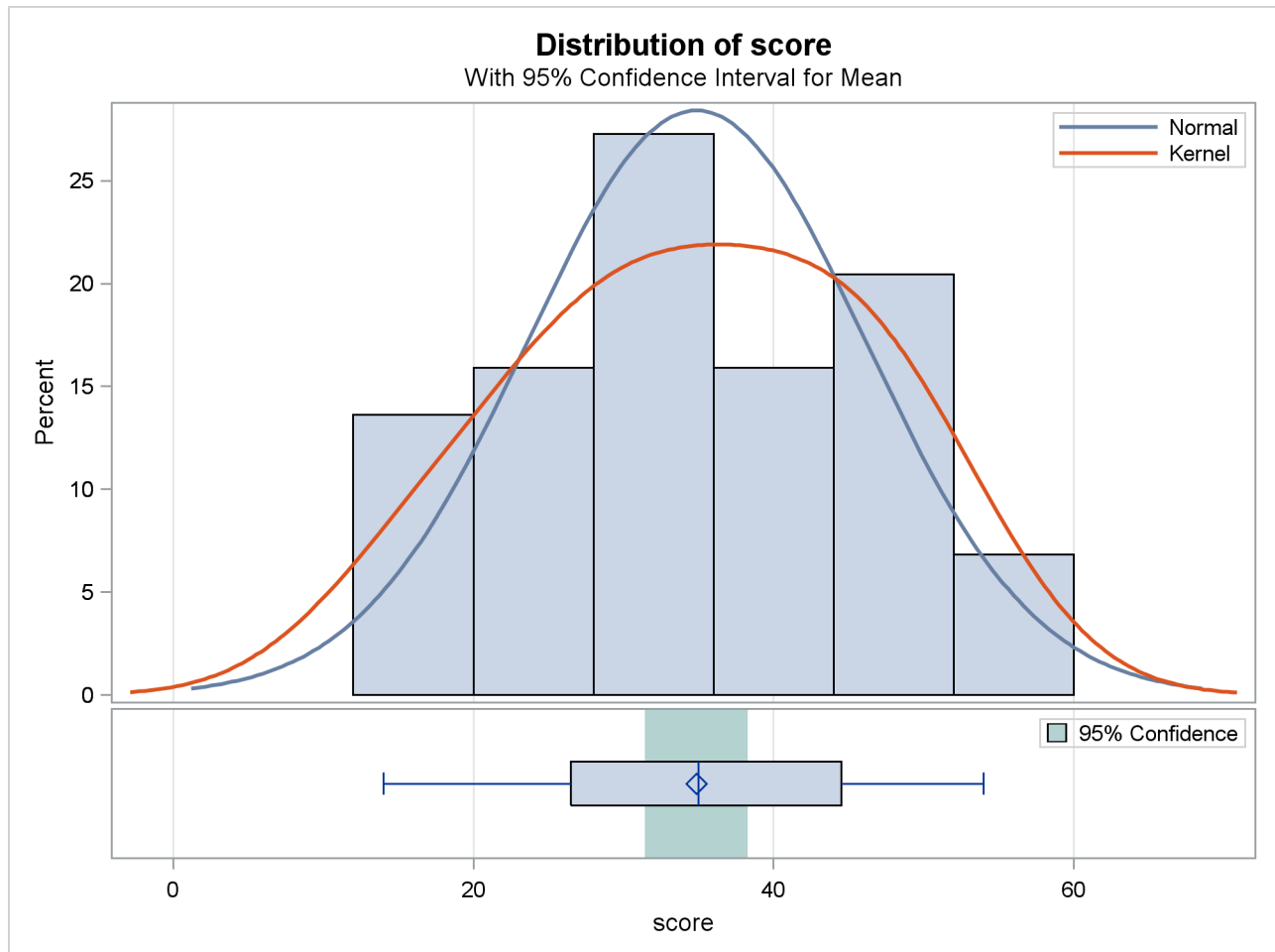
**Output 99.2.1** TTEST Results

| The TTEST Procedure |                 |         |                |         |         |
|---------------------|-----------------|---------|----------------|---------|---------|
| Variable: score     |                 |         |                |         |         |
| N                   | Mean            | Std Dev | Std Err        | Minimum | Maximum |
| 44                  | 34.8636         | 11.2303 | 1.6930         | 14.0000 | 54.0000 |
| Mean                | 95% CL Mean     | Std Dev | 95% CL Std Dev |         |         |
| 34.8636             | 31.4493 38.2780 | 11.2303 | 9.2788 14.2291 |         |         |
| DF                  | t Value         | Pr >  t |                |         |         |
| 43                  | 2.87            | 0.0063  |                |         |         |

The SAS log states that 30 observations and two variables have been read. However, the sample size given in the TTEST output is N=44. This is due to specifying the count variable in the **FREQ** statement. The test is significant ( $t = 2.87$ ,  $p = 0.0063$ ) at the 5% level, so you can conclude that the mean test score is different from 30.

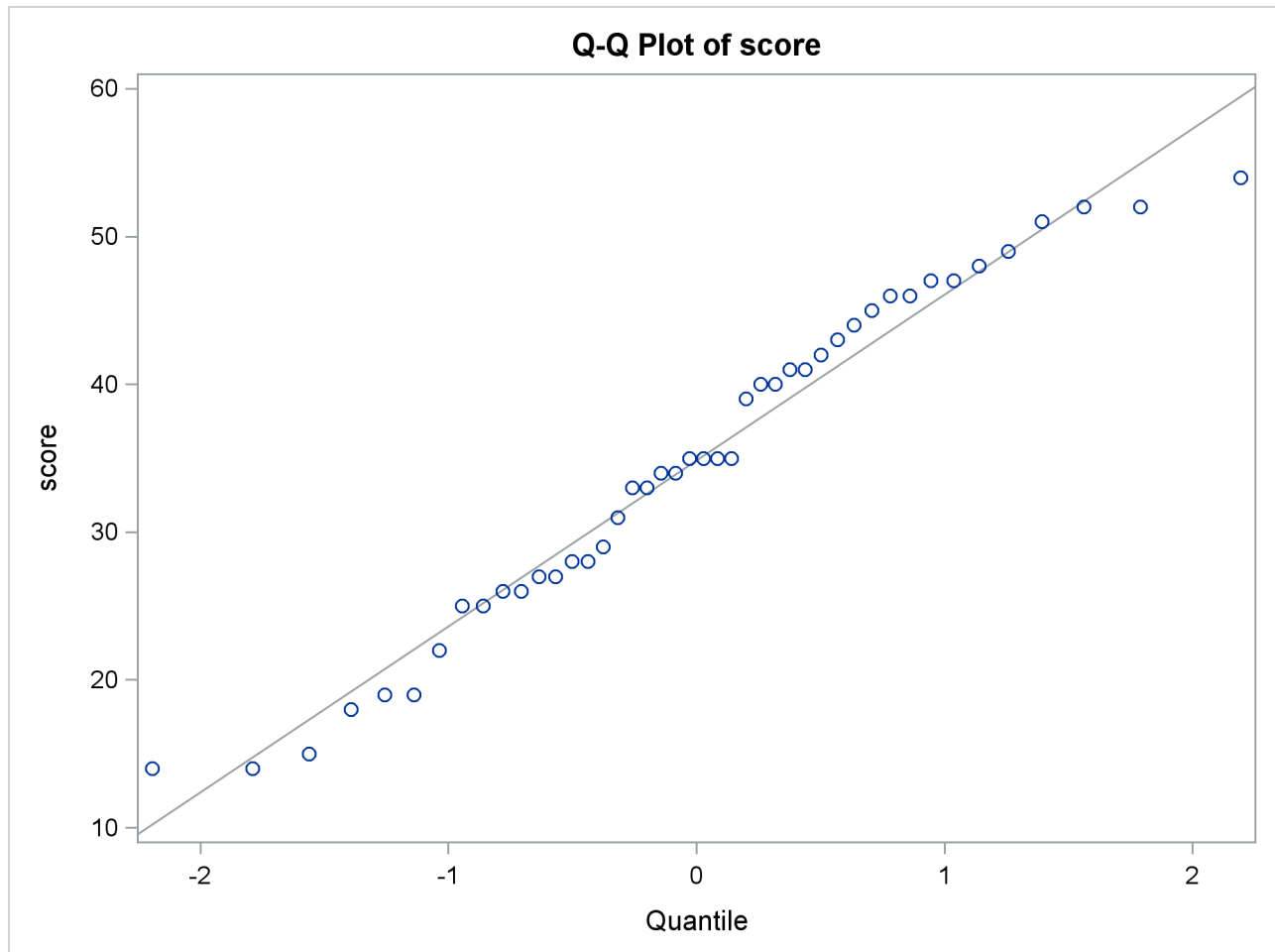
The summary panel in **Output 99.2.2** shows a histogram with overlaid normal and kernel densities, a box plot, and the 95% confidence interval for the mean.

**Output 99.2.2** Summary Panel



The Q-Q plot in **Output 99.2.3** assesses the normality assumption.

Output 99.2.3 Q-Q Plot



The tight clustering of the points around the diagonal line is consistent with the normality assumption. You could use the UNIVARIATE procedure with the NORMAL option to numerically check the normality assumption.

### Example 99.3: Paired Comparisons

When it is not feasible to assume that two groups of data are independent, and a natural pairing of the data exists, it is advantageous to use an analysis that takes the correlation into account. Using this correlation results in higher power to detect existing differences between the means. The differences between paired observations are assumed to be normally distributed. Some examples of this natural pairing are as follows:

- pre- and post-test scores for a student receiving tutoring
- fuel efficiency readings of two fuel types observed on the same automobile
- sunburn scores for two sunblock lotions, one applied to the individual's right arm, one to the left arm
- political attitude scores of husbands and wives

In this example, taken from the *SUGI Supplemental Library User's Guide, Version 5 Edition*, a stimulus is being examined to determine its effect on systolic blood pressure. Twelve men participate in the study. Each man's systolic blood pressure is measured both before and after the stimulus is applied. The following statements input the data:

```
data pressure;
 input SBPbefore SBPafter @@;
 datalines;
120 128 124 131 130 131 118 127
140 132 128 125 140 141 135 137
126 118 130 132 126 129 127 135
;
```

The variables SBPbefore and SBPafter denote the systolic blood pressure before and after the stimulus, respectively.

The statements to perform the test follow:

```
ods graphics on;

proc ttest;
 paired SBPbefore*SBPafter;
run;

ods graphics off;
```

The **PAIRED** statement is used to test whether the mean change in systolic blood pressure is significantly different from zero. The tabular output is displayed in [Output 99.3.1](#).

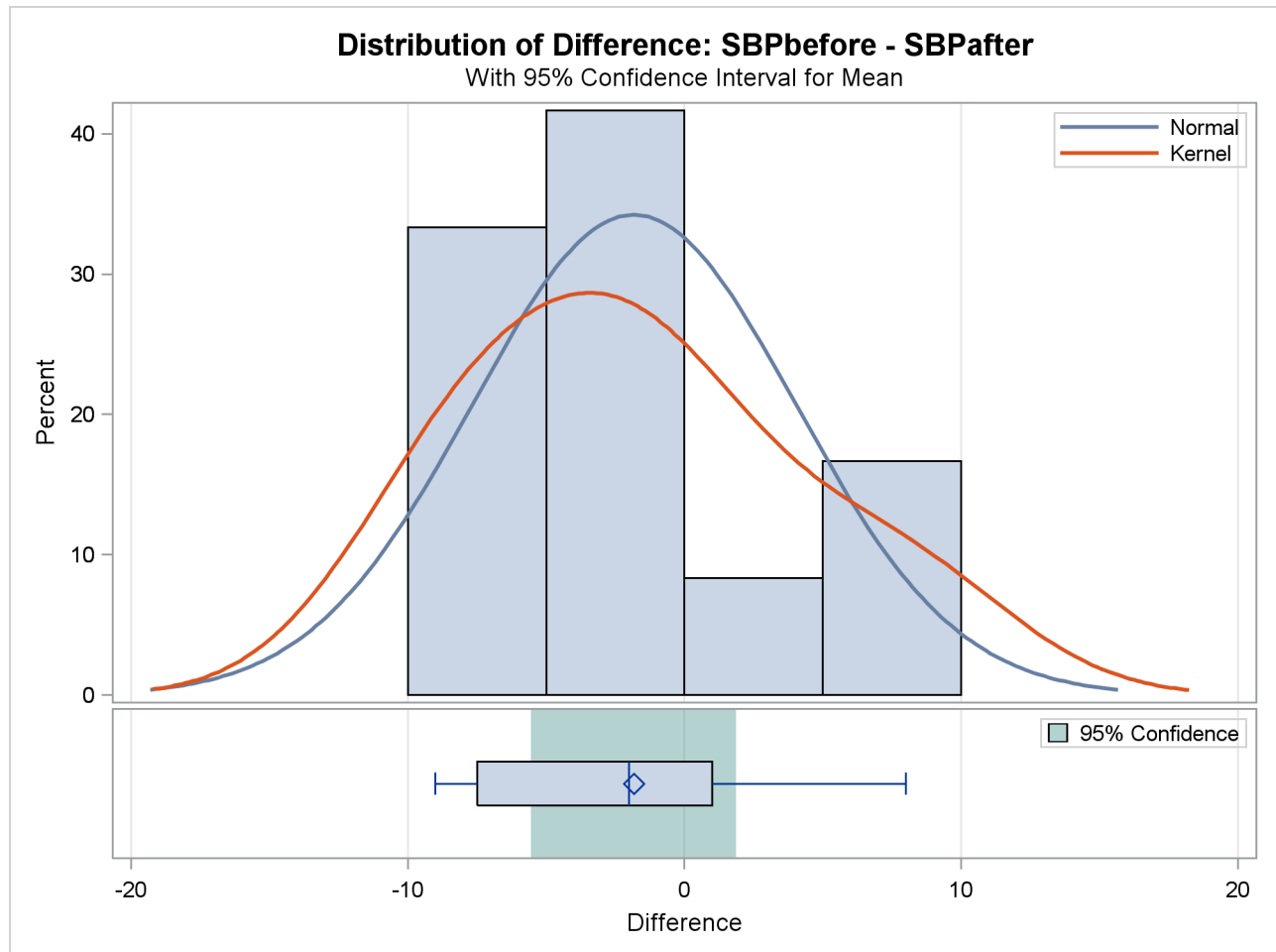
**Output 99.3.1** TTEST Results

| The TTEST Procedure              |             |         |         |         |         |
|----------------------------------|-------------|---------|---------|---------|---------|
| Difference: SBPbefore - SBPafter |             |         |         |         |         |
| N                                | Mean        | Std Dev | Std Err | Minimum | Maximum |
| 12                               | -1.8333     | 5.8284  | 1.6825  | -9.0000 | 8.0000  |
| Mean                             | 95% CL Mean | Std Dev | 95% CL  | Std Dev |         |
| -1.8333                          | -5.5365     | 1.8698  | 4.1288  | 9.8958  |         |
| DF                               | t Value     | Pr >  t |         |         |         |
| 11                               | -1.09       | 0.2992  |         |         |         |

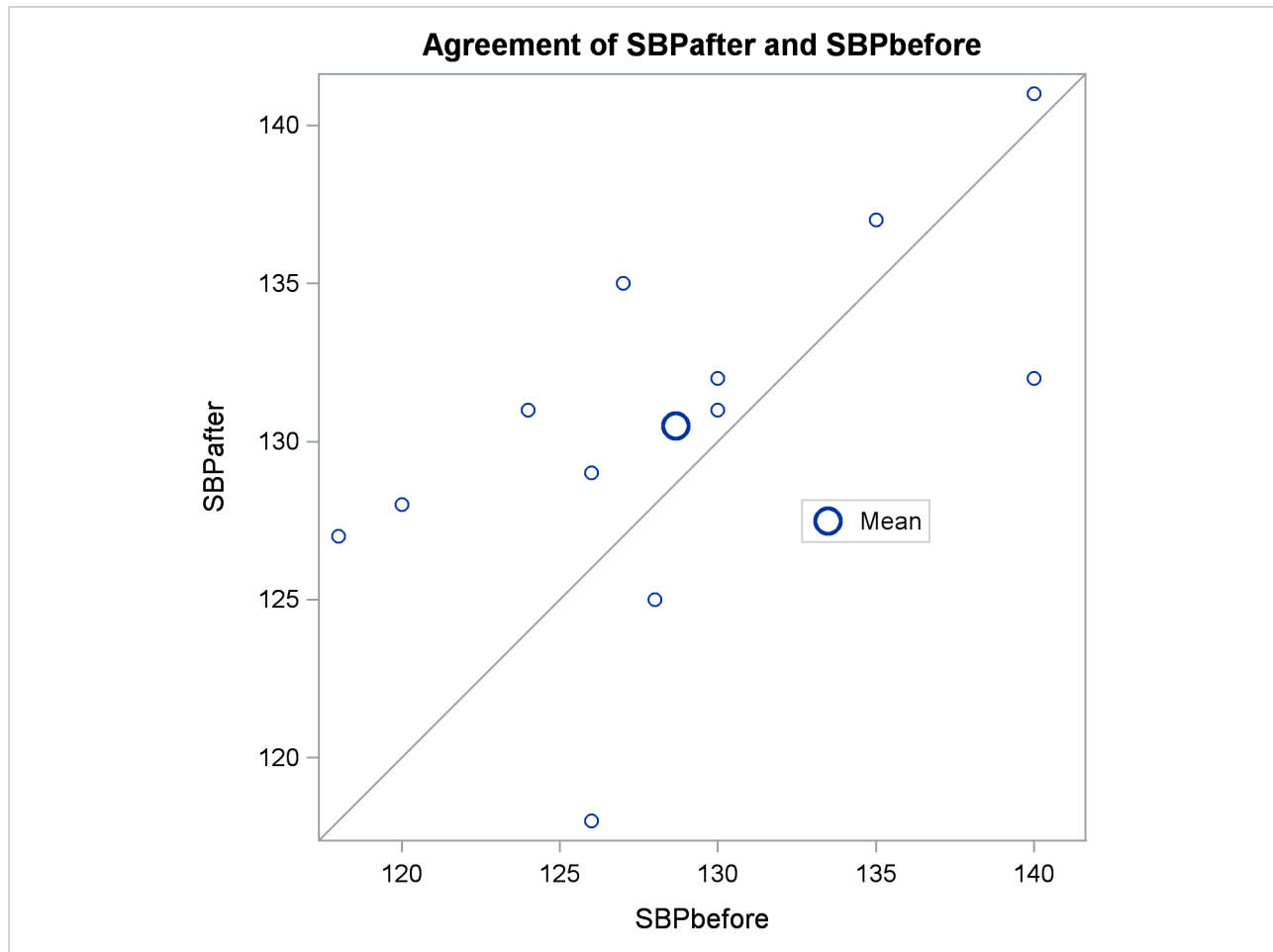
The variables SBPbefore and SBPafter are the paired variables with a sample size of 12. The summary statistics of the difference are displayed (mean, standard deviation, and standard error) along with their confidence limits. The minimum and maximum differences are also displayed. The *t* test is not significant ( $t = -1.09$ ,  $p = 0.2992$ ), indicating that the stimuli did not significantly affect systolic blood pressure.

The summary panel in [Output 99.3.2](#) shows a histogram, normal and kernel densities, box plot, and  $100(1 - \alpha)\% = 95\%$  confidence interval of the SBPbefore – SBPafter difference.

**Output 99.3.2** Summary Panel



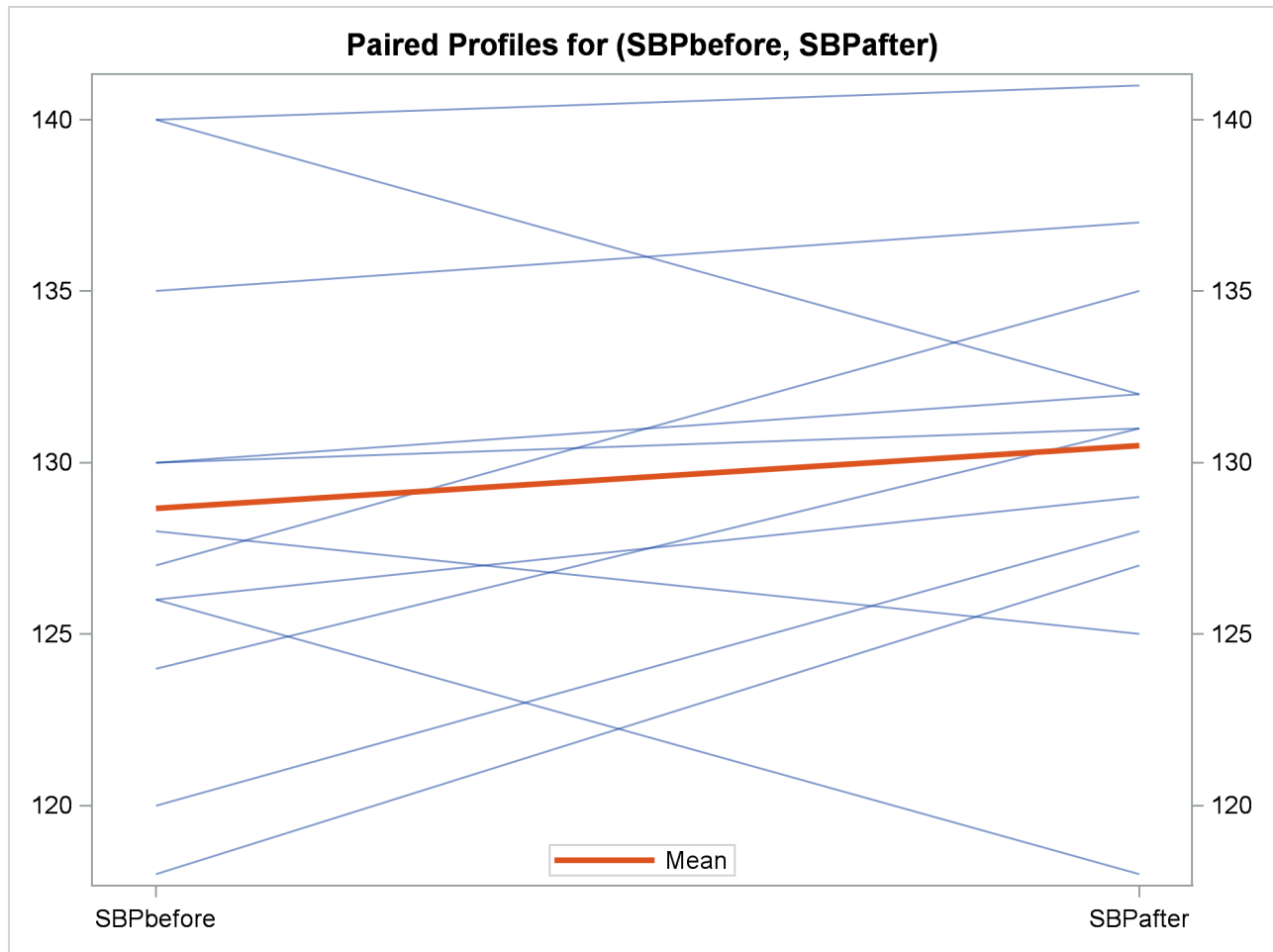
The agreement plot in [Output 99.3.3](#) reveals that only three men have higher blood pressure before the stimulus than after.

**Output 99.3.3** Agreement of Treatments

But the differences for these men are relatively large, keeping the mean difference only slightly negative.

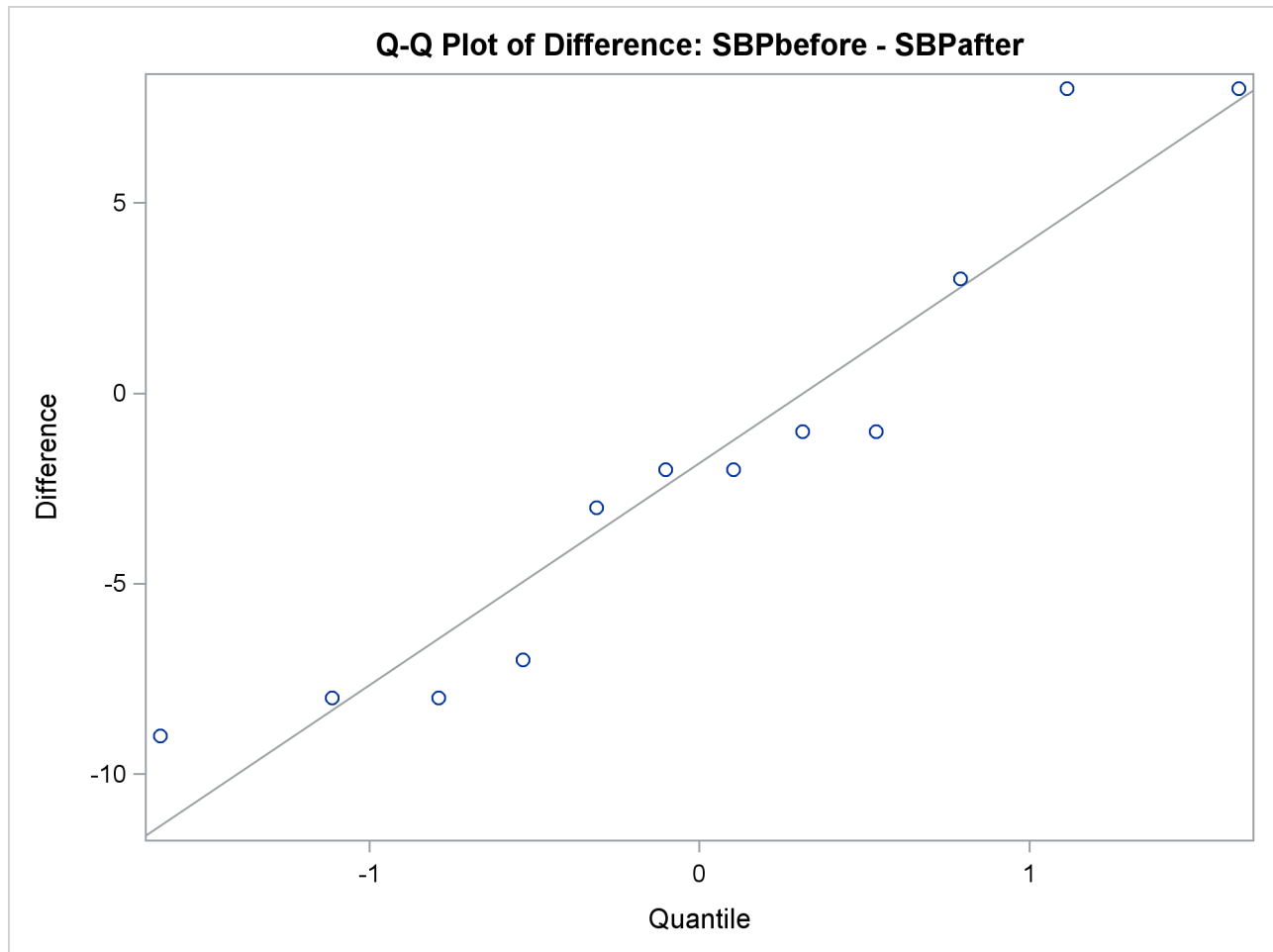
The profiles plot in [Output 99.3.4](#) is a different view of the same information contained in [Output 99.3.3](#), plotting the blood pressure from before to after the stimulus.



**Output 99.3.4** Profiles over Treatments

The Q-Q plot in [Output 99.3.5](#) assesses the normality assumption.

Output 99.3.5 Q-Q Plot



The Q-Q plot shows no obvious deviations from normality. You can check the assumption of normality more rigorously by using PROC UNIVARIATE with the NORMAL option.

---

### Example 99.4: AB/BA Crossover Design

Senn (2002, Chapter 3) discusses a study comparing the effectiveness of two bronchodilators, formoterol (“for”) and salbutamol (“sal”), in the treatment of childhood asthma. A total of 13 children are recruited for an AB/BA crossover design. A random sample of 7 of the children are assigned to the treatment sequence for/sal, receiving a dose of formoterol upon an initial visit (“period 1”) and then a dose of salbutamol upon a later visit (“period 2”). The other 6 children are assigned to the sequence sal/for, receiving the treatments in the reverse order but otherwise in a similar manner. Periods 1 and 2 are sufficiently spaced so that no carryover effects are suspected. After a child inhales a dose of a bronchodilator, peak expiratory flow (PEF) is measured. Higher PEF indicates greater effectiveness. The data are assumed to be approximately normally distributed.

The data set is generated with the following statements:

```
data asthma;
 input Drug1 $ Drug2 $ PEF1 PEF2 @@;
 datalines;
for sal 310 270 for sal 310 260 for sal 370 300
for sal 410 390 for sal 250 210 for sal 380 350
for sal 330 365
sal for 370 385 sal for 310 400 sal for 380 410
sal for 290 320 sal for 260 340 sal for 90 220
;
```

You can display the data by using the following statements, which produce [Output 99.4.1](#):

```
proc print data=asthma;
run;
```

**Output 99.4.1** Asthma Study Data

| Obs | Drug1 | Drug2 | PEF1 | PEF2 |
|-----|-------|-------|------|------|
| 1   | for   | sal   | 310  | 270  |
| 2   | for   | sal   | 310  | 260  |
| 3   | for   | sal   | 370  | 300  |
| 4   | for   | sal   | 410  | 390  |
| 5   | for   | sal   | 250  | 210  |
| 6   | for   | sal   | 380  | 350  |
| 7   | for   | sal   | 330  | 365  |
| 8   | sal   | for   | 370  | 385  |
| 9   | sal   | for   | 310  | 400  |
| 10  | sal   | for   | 380  | 410  |
| 11  | sal   | for   | 290  | 320  |
| 12  | sal   | for   | 260  | 340  |
| 13  | sal   | for   | 90   | 220  |

The variables PEF1 and PEF2 represent the responses for the first and second periods, respectively. The variables Drug1 and Drug2 represent the treatment in each period.

You can analyze this crossover design by using the `CROSSOVER=` option after a slash (/) in the `VAR` statement:

```
ods graphics on;

proc ttest data=asthma plots=interval;
 var PEF1 PEF2 / crossover= (Drug1 Drug2);
run;

ods graphics off;
```

With the default `PROC TTEST` options `TEST=DIFF` and `DIST=NORMAL` and the lack of the `IGNOREPERIOD` option in the `VAR` statement, both the treatment difference and the period difference are assessed. The `PROC TTEST` default options `H0=0`, `SIDES=2`, and `ALPHA=0.05` specify a two-sided analysis with 95% confidence limits comparing treatment and period differences to a default difference of zero. The default `CI=EQUAL` option in the `PROC TTEST` statement requests equal-tailed confidence intervals for

standard deviations. The `PLOTS=INTERVAL` option produces `TYPE=TREATMENT` confidence intervals, in addition to the default plots `AGREEMENT(TYPE=TREATMENT)`, `BOX`, `HISTOGRAM`, `PROFILES(TYPE=TREATMENT)`, and `QQ`.

Output 99.4.2 summarizes the response and treatment variables for each period.

**Output 99.4.2** Crossover Variable Information

| The TTEST Procedure            |          |           |
|--------------------------------|----------|-----------|
| Response Variables: PEF1, PEF2 |          |           |
| Crossover Variable Information |          |           |
| Period                         | Response | Treatment |
| 1                              | PEF1     | Drug1     |
| 2                              | PEF2     | Drug2     |

Output 99.4.3 displays basic summary statistics (sample size, mean, standard deviation, standard error, minimum, and maximum) for each of the four cells in the design, the treatment difference within each treatment sequence, the overall treatment difference, and the overall period difference.

**Output 99.4.3** Statistics

| Sequence | Treatment  | Period     | N | Mean     | Std Dev | Std Err |
|----------|------------|------------|---|----------|---------|---------|
| 1        | for        | 1          | 7 | 337.1    | 53.7631 | 20.3206 |
| 2        | for        | 2          | 6 | 345.8    | 70.8814 | 28.9372 |
| 2        | sal        | 1          | 6 | 283.3    | 105.4   | 43.0245 |
| 1        | sal        | 2          | 7 | 306.4    | 64.7247 | 24.4636 |
| 1        | Diff (1-2) |            | 7 | 30.7143  | 32.9682 | 12.4608 |
| 2        | Diff (1-2) |            | 6 | 62.5000  | 44.6934 | 18.2460 |
| Both     | Diff (1-2) |            |   | 46.6071  | 19.3702 | 10.7766 |
| Both     |            | Diff (1-2) |   | -15.8929 | 19.3702 | 10.7766 |
| Sequence | Treatment  | Period     |   | Minimum  | Maximum |         |
| 1        | for        | 1          |   | 250.0    | 410.0   |         |
| 2        | for        | 2          |   | 220.0    | 410.0   |         |
| 2        | sal        | 1          |   | 90.0000  | 380.0   |         |
| 1        | sal        | 2          |   | 210.0    | 390.0   |         |
| 1        | Diff (1-2) |            |   | -35.0000 | 70.0000 |         |
| 2        | Diff (1-2) |            |   | 15.0000  | 130.0   |         |
| Both     | Diff (1-2) |            |   |          |         |         |
| Both     |            | Diff (1-2) |   |          |         |         |

The treatment difference “Diff (1-2)” corresponds to the “for” treatment minus the “sal” treatment, because “for” appears before “sal” in the output, according to the `ORDER=MIXED` default `PROC TTEST` option. Its mean estimate is 46.6071, favoring formoterol over salbutamol.

The standard deviation (Std Dev) reported for a “difference” is actually the pooled standard deviation across

both treatment sequence (for/sal and sal/for), assuming equal variances. The standard error (Std Err) is the standard deviation of the mean estimate.

The top half of the table in [Output 99.4.4](#) shows 95% two-sided confidence limits for the means for the same criteria addressed in the table in [Output 99.4.3](#).

**Output 99.4.4** Confidence Limits

| Sequence | Treatment  | Period     | Method        | Mean     | 95% CL   | Mean    |
|----------|------------|------------|---------------|----------|----------|---------|
| 1        | for        | 1          |               | 337.1    | 287.4    | 386.9   |
| 2        | for        | 2          |               | 345.8    | 271.4    | 420.2   |
| 2        | sal        | 1          |               | 283.3    | 172.7    | 393.9   |
| 1        | sal        | 2          |               | 306.4    | 246.6    | 366.3   |
| 1        | Diff (1-2) |            |               | 30.7143  | 0.2238   | 61.2048 |
| 2        | Diff (1-2) |            |               | 62.5000  | 15.5972  | 109.4   |
| Both     | Diff (1-2) |            | Pooled        | 46.6071  | 22.8881  | 70.3262 |
| Both     | Diff (1-2) |            | Satterthwaite | 46.6071  | 21.6585  | 71.5558 |
| Both     |            | Diff (1-2) | Pooled        | -15.8929 | -39.6119 | 7.8262  |
| Both     |            | Diff (1-2) | Satterthwaite | -15.8929 | -40.8415 | 9.0558  |
| Sequence | Treatment  | Period     | Method        | Std Dev  | 95% CL   | Std Dev |
| 1        | for        | 1          |               | 53.7631  | 34.6446  | 118.4   |
| 2        | for        | 2          |               | 70.8814  | 44.2447  | 173.8   |
| 2        | sal        | 1          |               | 105.4    | 65.7841  | 258.5   |
| 1        | sal        | 2          |               | 64.7247  | 41.7082  | 142.5   |
| 1        | Diff (1-2) |            |               | 32.9682  | 21.2445  | 72.5982 |
| 2        | Diff (1-2) |            |               | 44.6934  | 27.8980  | 109.6   |
| Both     | Diff (1-2) |            | Pooled        | 19.3702  | 13.7217  | 32.8882 |
| Both     | Diff (1-2) |            | Satterthwaite |          |          |         |
| Both     |            | Diff (1-2) | Pooled        | 19.3702  | 13.7217  | 32.8882 |
| Both     |            | Diff (1-2) | Satterthwaite |          |          |         |

For the mean differences, both pooled (assuming equal variances for both treatment sequences) and Satterthwaite (assuming unequal variances) intervals are shown. For example, the pooled confidence limits for the overall treatment mean difference (for – sal) assuming equal variances are 22.8881 and 70.3262.

The bottom half of [Output 99.4.4](#) shows 95% equal-tailed confidence limits for the standard deviations within each cell and for the treatment difference within each sequence. It also shows confidence limits for the pooled common standard deviation assuming equal variances. Note that the pooled standard deviation of 19.3702 and associated confidence limits 13.7217 and 32.8882 apply to both difference tests (treatment and period), since each of those tests involves the same pooled standard deviation.

[Output 99.4.5](#) shows the results of *t* tests of treatment and period differences.

**Output 99.4.5** *t* Tests

| Treatment  | Period     | Method        | Variances | DF     | t Value | Pr >  t |
|------------|------------|---------------|-----------|--------|---------|---------|
| Diff (1-2) |            | Pooled        | Equal     | 11     | 4.32    | 0.0012  |
| Diff (1-2) |            | Satterthwaite | Unequal   | 9.1017 | 4.22    | 0.0022  |
|            | Diff (1-2) | Pooled        | Equal     | 11     | -1.47   | 0.1683  |
|            | Diff (1-2) | Satterthwaite | Unequal   | 9.1017 | -1.44   | 0.1838  |

Both pooled and Satterthwaite versions of the test of treatment difference are highly significant ( $p = 0.0012$  and  $p = 0.0022$ ), and both versions of the test of period difference are insignificant ( $p = 0.1683$  and  $p = 0.1838$ ).

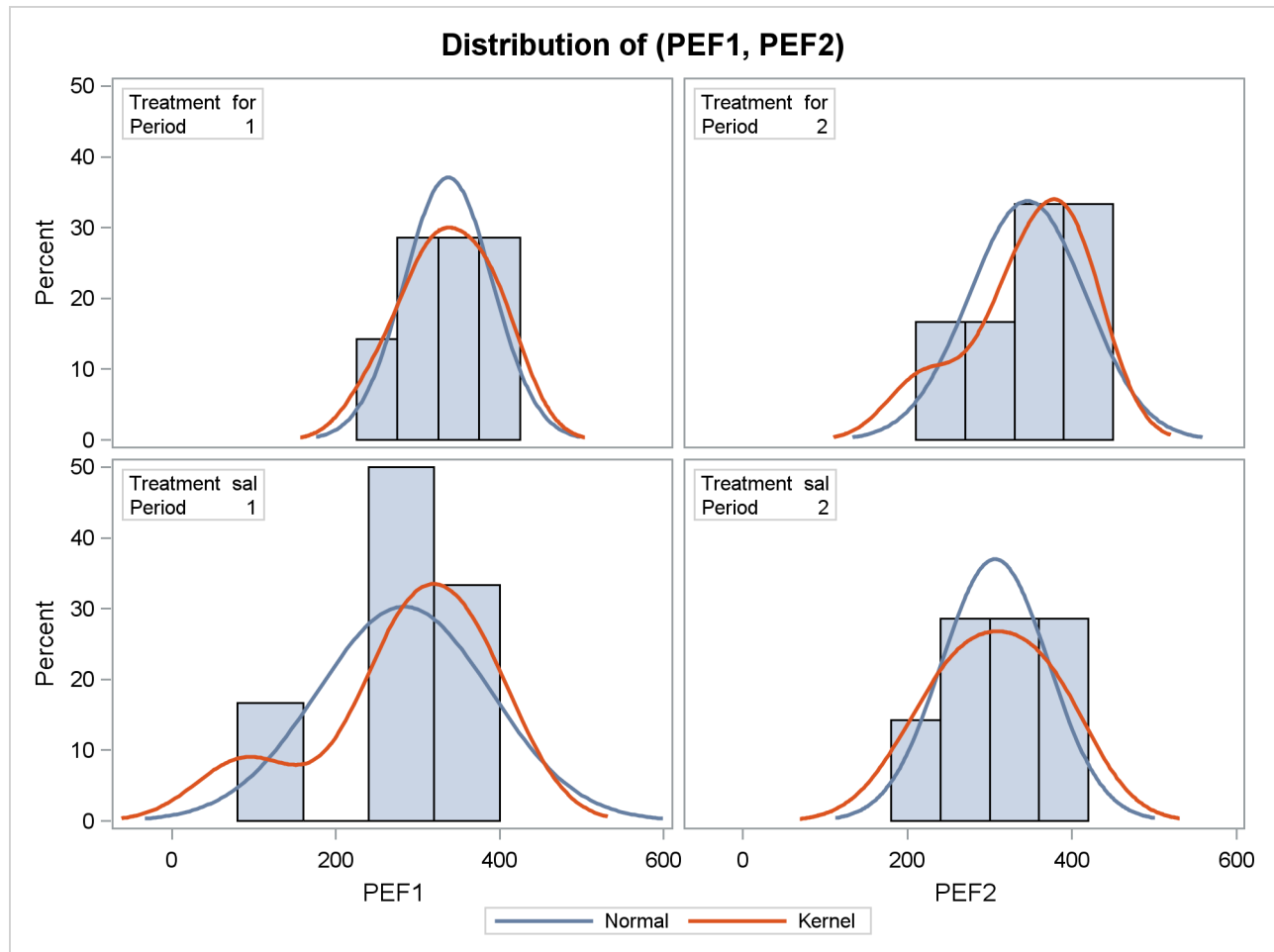
The folded *F* test of equal variances in each treatment sequence is shown in [Output 99.4.6](#).

**Output 99.4.6** Equality of Variances Test

| Equality of Variances |        |        |         |        |
|-----------------------|--------|--------|---------|--------|
| Method                | Num DF | Den DF | F Value | Pr > F |
| Folded F              | 5      | 6      | 1.84    | 0.4797 |

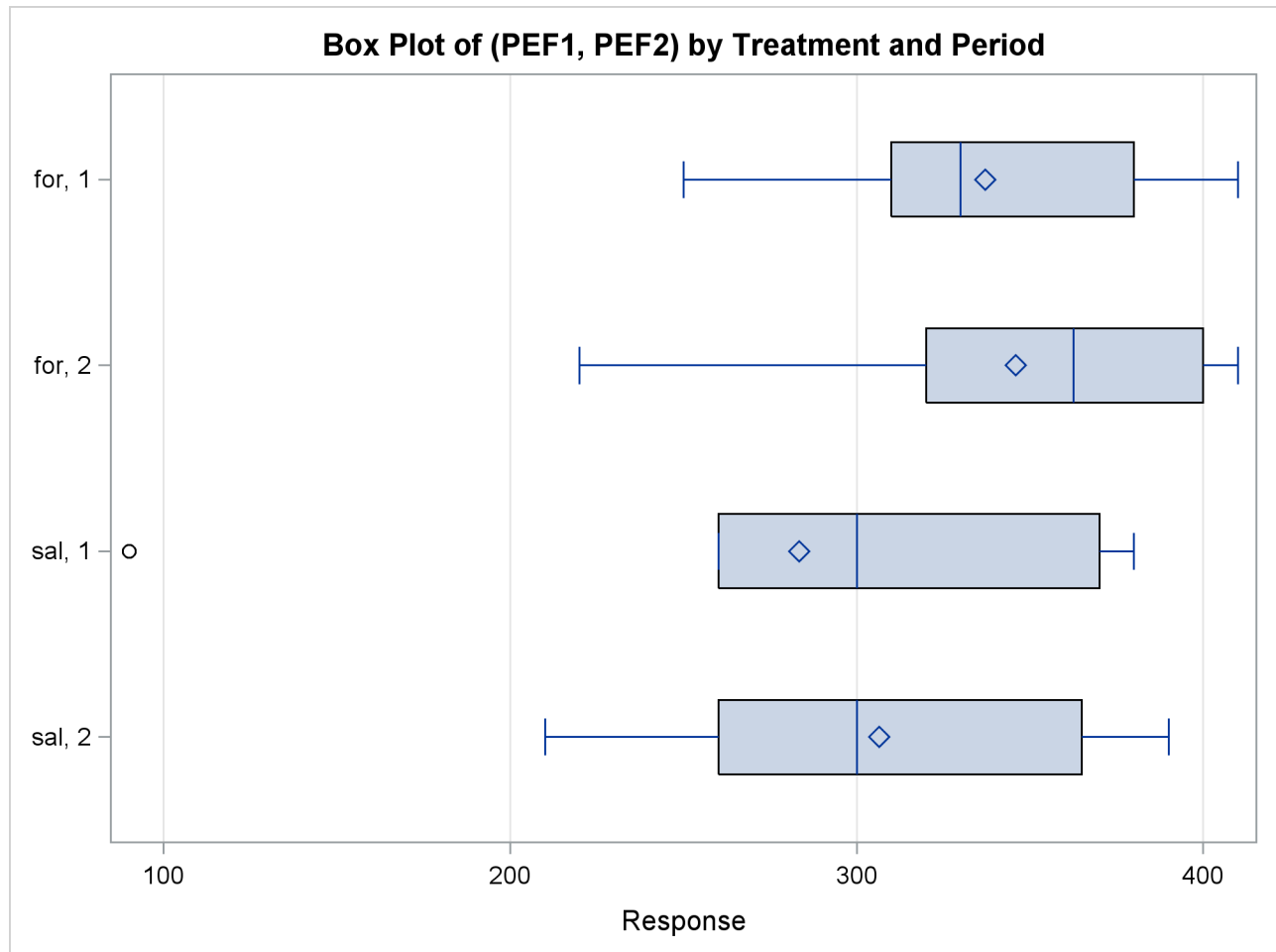
The insignificant result ( $p = 0.48$ ) implies a lack of evidence for unequal variances. However, it does not demonstrate equal variances, and it is not very robust to deviations from normality.

[Output 99.4.7](#) shows the distribution of the response variables PEF1 and PEF2 within each of the four cells (combinations of two treatments and two periods) of the AB/BA crossover design, in terms of histograms and normal and kernel density estimates.

**Output 99.4.7** Comparative Histograms

The distributions for the first treatment sequence (for/sal) appear to be somewhat symmetric, and the distributions for the sal/for sequence appear to be skewed to the left.

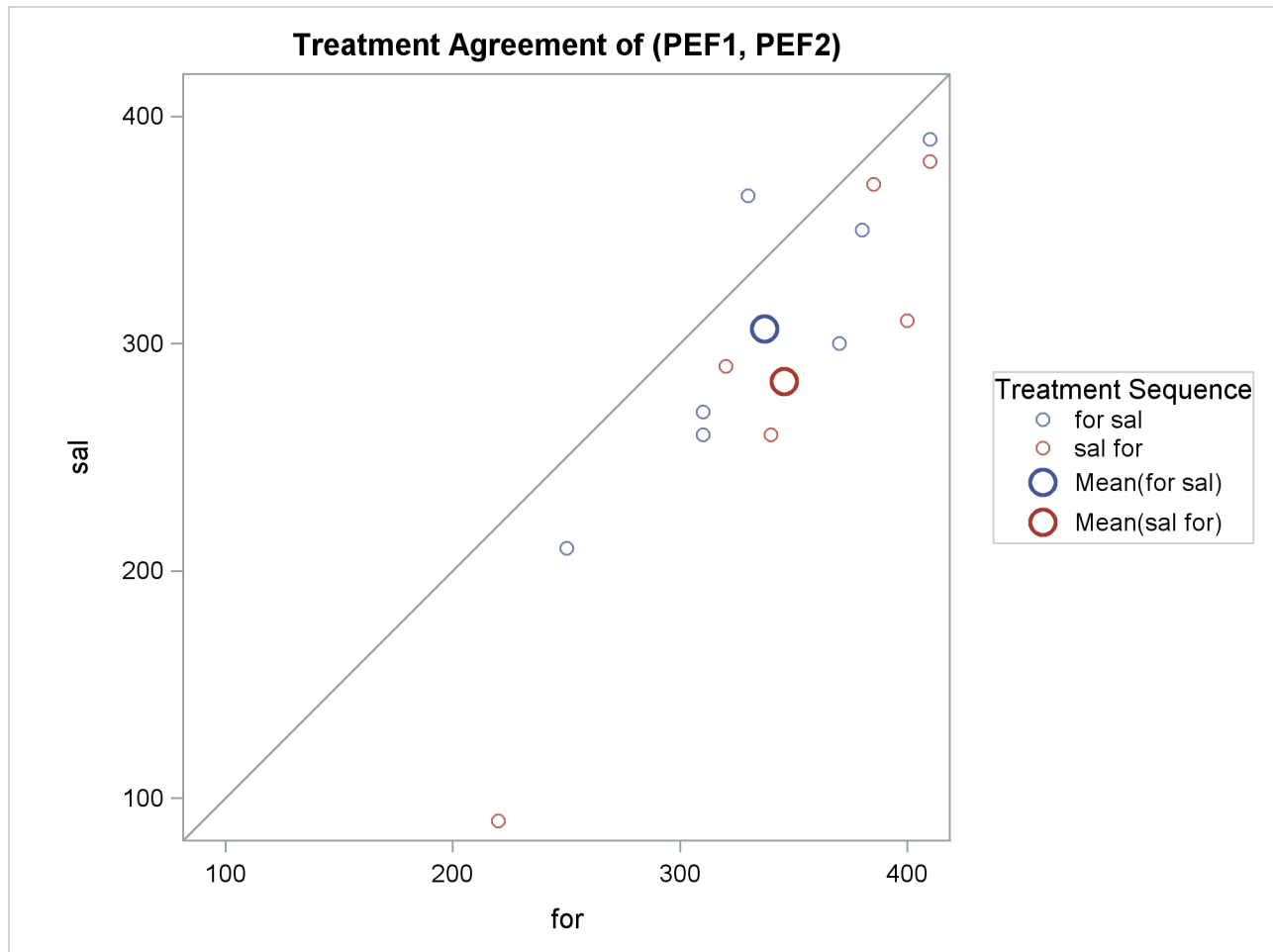
Output 99.4.8 shows a similar distributional summary but in terms of box plots.

**Output 99.4.8** Comparative Box Plots

The relative locations of means and medians in each box plot corroborate the fact that the distributions for the sal/for sequence are skewed to the left. The distributions for the for/sal sequence appear to be skewed slightly to the right. The box plot for the salbutamol treatment in the first period shows an outlier (the circle on the far left side of the plot).

The treatment agreement plot in [Output 99.4.9](#) reveals that only a single observation has a higher peak expiratory flow for salbutamol.

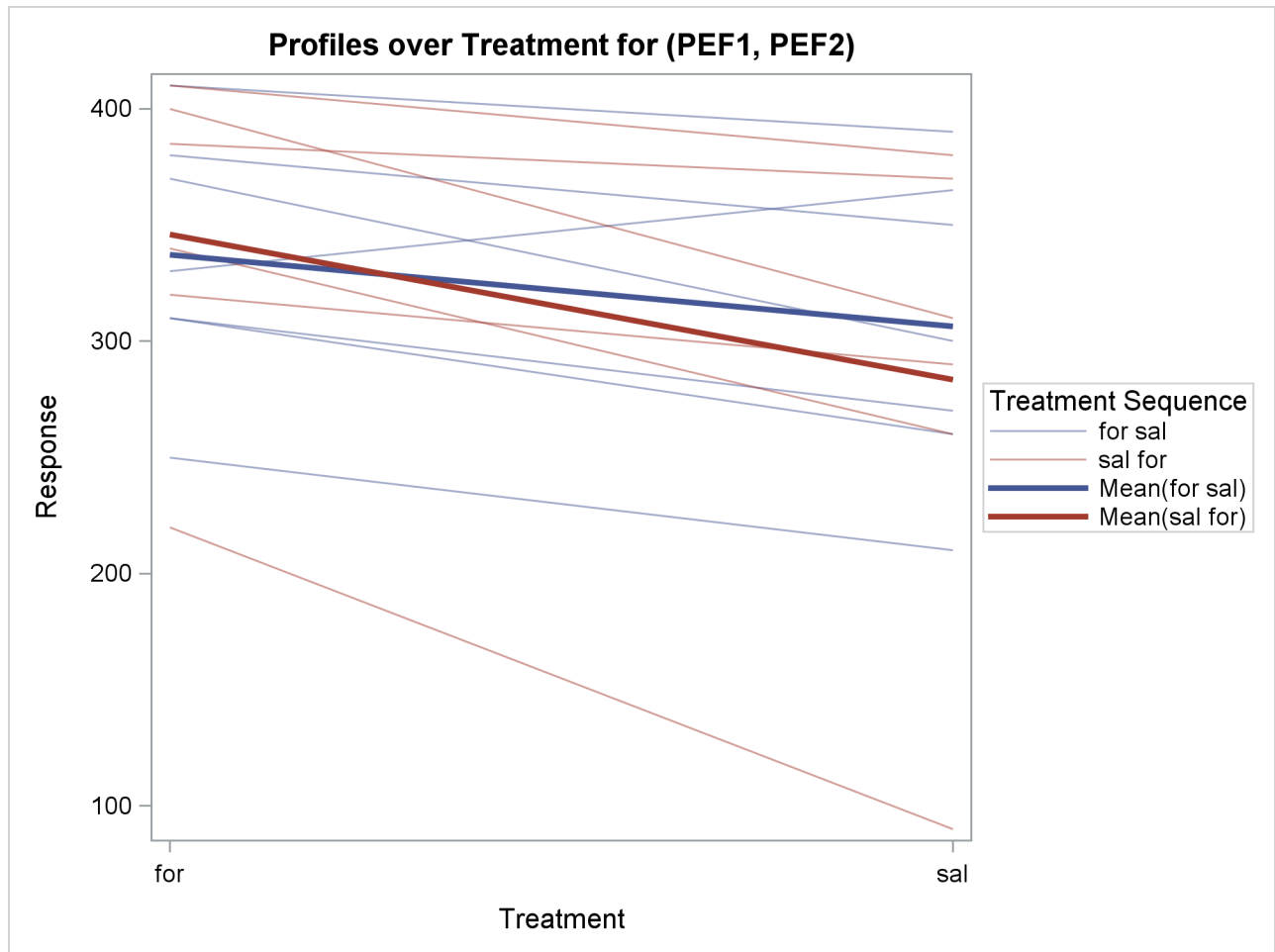


**Output 99.4.9** Agreement of Treatments Plot

The mean for the sal/for treatment sequence is farther from the diagonal equivalence line, revealing that the treatment difference is more pronounced for the 6 observations in the sal/for sequence than for the 7 observations in the for/sal sequence. This fact is also seen numerically in [Output 99.4.3](#) and [Output 99.4.4](#), which show within-sequence treatment differences of 30.7 for for/sal and 62.5 for sal/for.

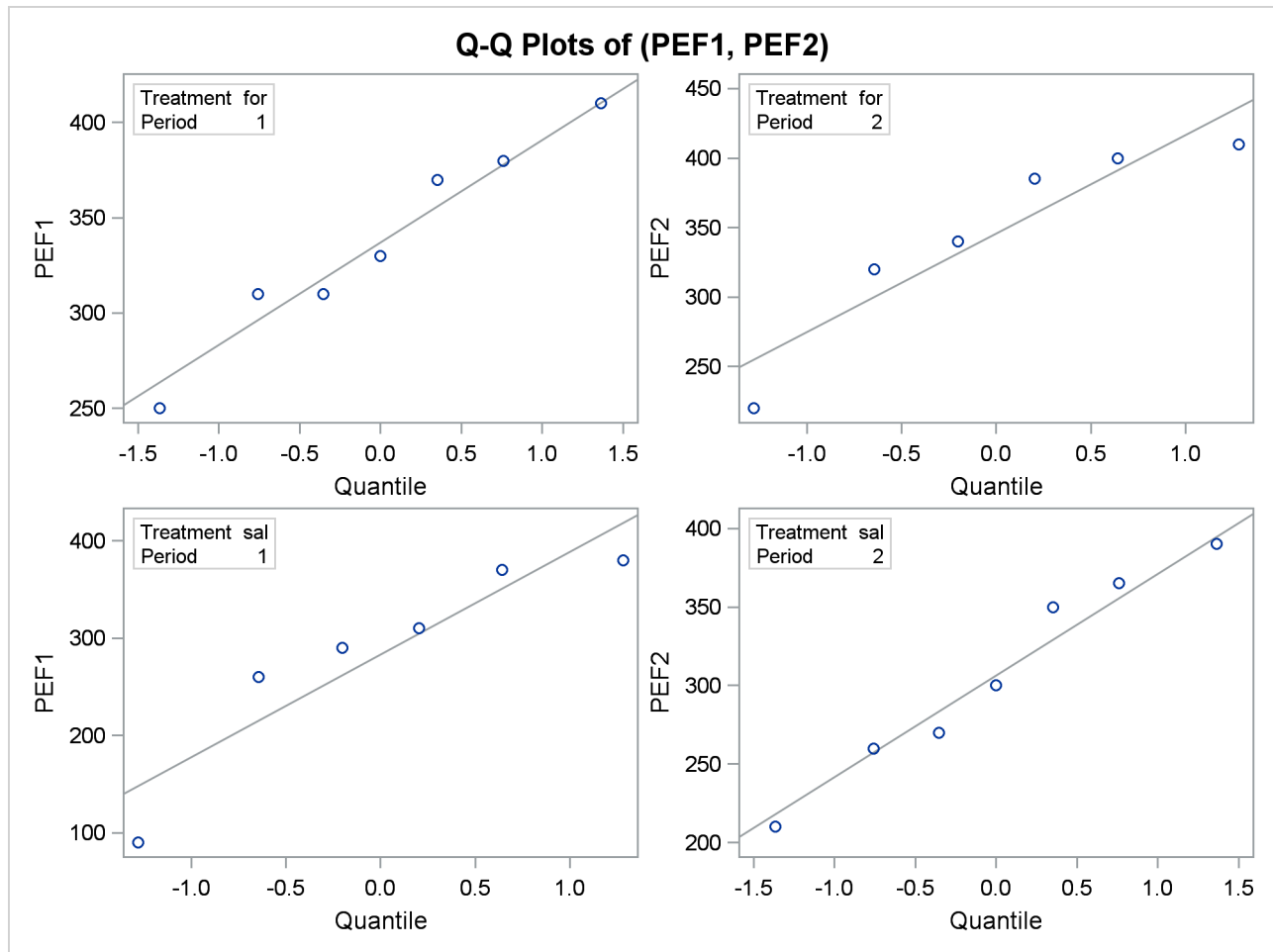
The profiles over treatment plot in [Output 99.4.10](#) is a different view of the same information contained in [Output 99.4.9](#), plotting the profiles from formoterol to salbutamol treatments. The lone observation for which the peak expiratory flow is higher for salbutamol appears as the only line with negative slope.

**Output 99.4.10** Profiles over Treatment



The Q-Q plots in [Output 99.4.11](#) assess normality assumption within each of the four cells of the design.

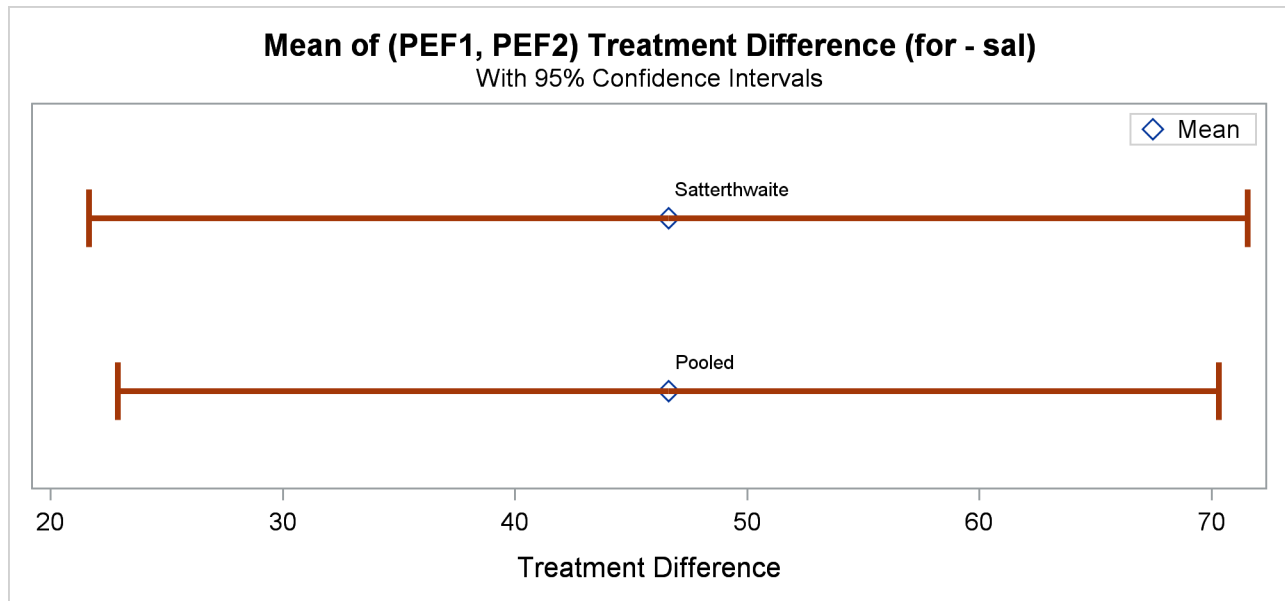
Output 99.4.11 Q-Q Plots



The two Q-Q plots for the sal/for sequence (lower left and upper right) suggest some possible normality violations in the tails, but the sample size is too small to make any strong conclusions. You could use the UNIVARIATE procedure with the NORMAL option to numerically check the normality assumptions.

Finally, [Output 99.4.12](#) shows both pooled and Satterthwaite two-sided 95% confidence intervals for the treatment difference.

**Output 99.4.12** Confidence Intervals for Treatment Difference



The pooled interval is slightly smaller than the Satterthwaite interval. (This is not always the case.)

### Example 99.5: Equivalence Testing with Lognormal Data

Wellek (2003, p. 212) discusses an average bioequivalence study comparing the AUC (area under serum-concentration curve) measurements for two different drugs, denoted “Test” and “Reference,” over a period of 20 hours. This example looks at a portion of Wellek’s data, conducting an equivalence analysis with a paired design that uses AUC values on the original scale (assumed to be lognormally distributed). Each subject in the study received the Test drug upon one visit and then the Reference drug upon a later visit, sufficiently spaced so that no carryover effects would occur.

The goal is to test whether the geometric mean AUC ratio between Test and Reference is between 0.8 and 1.25, corresponding to the traditional FDA (80%, 125%) equivalence criterion. See the section “[Arithmetic and Geometric Means](#)” on page 8451 for a discussion of the use of geometric means for lognormal data.

The following SAS statements generate the data set:

```
data auc;
 input TestAUC RefAUC @@;
 datalines;
103.4 90.11 59.92 77.71 68.17 77.71 94.54 97.51
69.48 58.21 72.17 101.3 74.37 79.84 84.44 96.06
96.74 89.30 94.26 97.22 48.52 61.62 95.68 85.80
;
```

You can display the data by using the following statements, which produce [Output 99.5.1](#):

```
proc print data=auc;
run;
```

**Output 99.5.1** AUC Data for Test and Reference Drugs

| Obs | Test<br>AUC | RefAUC |
|-----|-------------|--------|
| 1   | 103.40      | 90.11  |
| 2   | 59.92       | 77.71  |
| 3   | 68.17       | 77.71  |
| 4   | 94.54       | 97.51  |
| 5   | 69.48       | 58.21  |
| 6   | 72.17       | 101.30 |
| 7   | 74.37       | 79.84  |
| 8   | 84.44       | 96.06  |
| 9   | 96.74       | 89.30  |
| 10  | 94.26       | 97.22  |
| 11  | 48.52       | 61.62  |
| 12  | 95.68       | 85.80  |

The TestAUC and RefAUC variables represent the AUC measurements for each subject under the Test and Reference drugs, respectively. Use the following SAS statements to perform the equivalence analysis:

```
ods graphics on;

proc ttest data=auc dist=lognormal tost(0.8, 1.25);
 paired TestAUC*RefAUC;
run;

ods graphics off;
```

The `DIST=LOGNORMAL` option specifies the lognormal distributional assumption and requests an analysis in terms of geometric mean and coefficient of variation. The `TOST` option specifies the equivalence bounds 0.8 and 1.25.

[Output 99.5.2](#) shows basic summary statistics for the ratio of TestAUC to RefAUC.

**Output 99.5.2** Summary Statistics

| The TTEST Procedure     |                   |                             |         |         |
|-------------------------|-------------------|-----------------------------|---------|---------|
| Ratio: TestAUC / RefAUC |                   |                             |         |         |
| N                       | Geometric<br>Mean | Coefficient<br>of Variation | Minimum | Maximum |
| 12                      | 0.9412            | 0.1676                      | 0.7124  | 1.1936  |

The geometric mean ratio of 0.9412 is the sample mean of the log-transformed data exponentiated to bring it

back to the original scale. So the plasma concentration over the 20-hour period is slightly lower for the Test drug than for the Reference drug. The CV of 0.1676 is the ratio of the standard deviation to the (arithmetic) mean.

Output 99.5.3 shows the  $100(1 - \alpha)\% = 95\%$  confidence limits for the geometric mean ratio (0.8467 and 1.0462) and CV (0.1183 and 0.2884).

**Output 99.5.3** Confidence Limits

| Geometric Mean | 95% CL Mean |        | Coefficient of Variation | 95% CL CV |        |
|----------------|-------------|--------|--------------------------|-----------|--------|
| 0.9412         | 0.8467      | 1.0462 | 0.1676                   | 0.1183    | 0.2884 |

Output 99.5.4 shows the  $100(1 - 2\alpha)\% = 90\%$  confidence limits for the geometric mean ratio, 0.8634 and 1.0260.

**Output 99.5.4** Equivalence Limits

| Geometric Mean | Lower Bound | 90% CL Mean |          | Upper Bound | Assessment |
|----------------|-------------|-------------|----------|-------------|------------|
| 0.9412         | 0.8 <       | 0.8634      | 1.0260 < | 1.25        | Equivalent |

The assessment of “Equivalent” reflects the fact that these limits are contained within the equivalence bounds 0.8 and 1.25. This result occurs if and only if the  $p$ -value of the test is less than the  $\alpha$  value specified in the ALPHA= option in the PROC TTEST statement, and it is the reason that  $100(1 - 2\alpha)\%$  confidence limits are shown in addition to the usual  $100(1 - \alpha)\%$  limits.

Output 99.5.5 shows the  $p$ -values for the two one-sided tests against the upper and lower equivalence bounds.

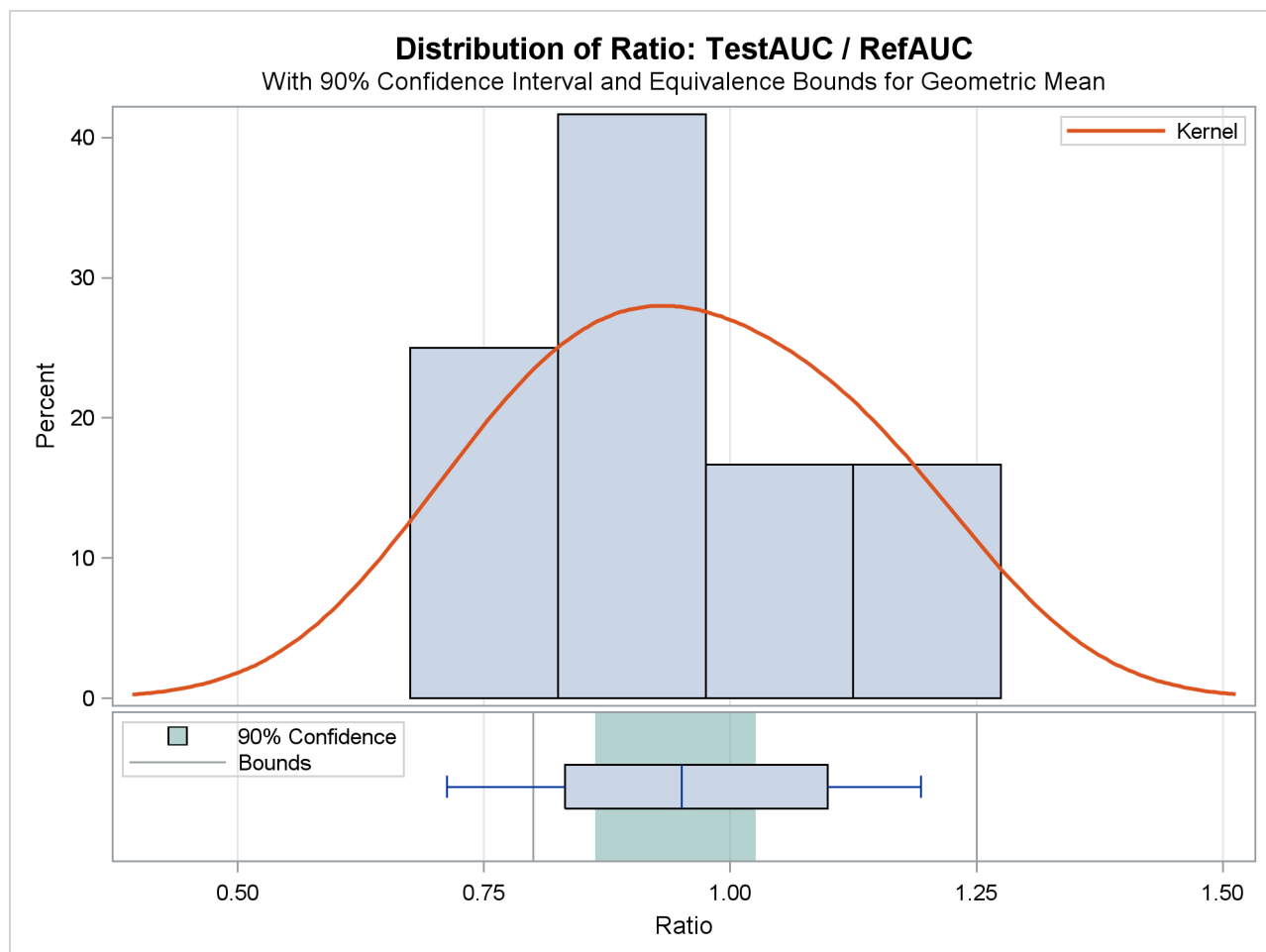
**Output 99.5.5** TOST Equivalence Test

| Test    | Null | DF | t Value | P-Value |
|---------|------|----|---------|---------|
| Upper   | 0.8  | 11 | 3.38    | 0.0031  |
| Lower   | 1.25 | 11 | -5.90   | <.0001  |
| Overall |      |    |         | 0.0031  |

The overall  $p$ -value of 0.0031, the larger of the two one-sided  $p$ -values, indicates significant evidence of equivalence between the Test and Reference drugs.

The summary panel in Output 99.5.6 shows a histogram, kernel density, box plot, and  $100(1 - 2\alpha)\% = 90\%$  confidence interval of the Test-to-Reference ratio of AUC, along with the equivalence bounds.

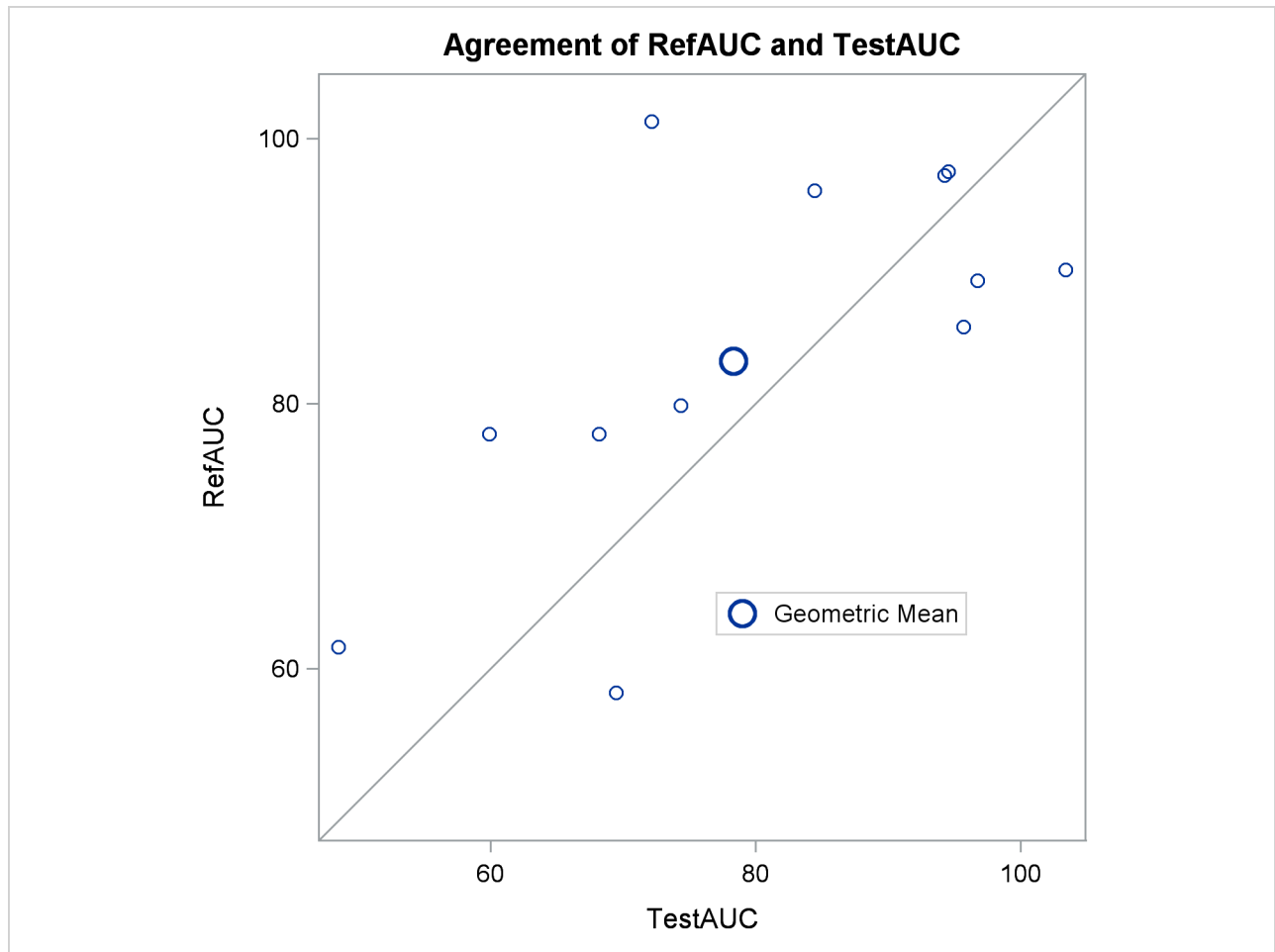
Output 99.5.6 Summary Panel



The confidence interval is closer to the lower equivalence bound than the upper bound and contained entirely within the bounds.

The agreement plot in [Output 99.5.7](#) reveals that the only four subjects with higher AUC for the Test drug are at the far lower or far upper end of the AUC distribution. This might merit further investigation.

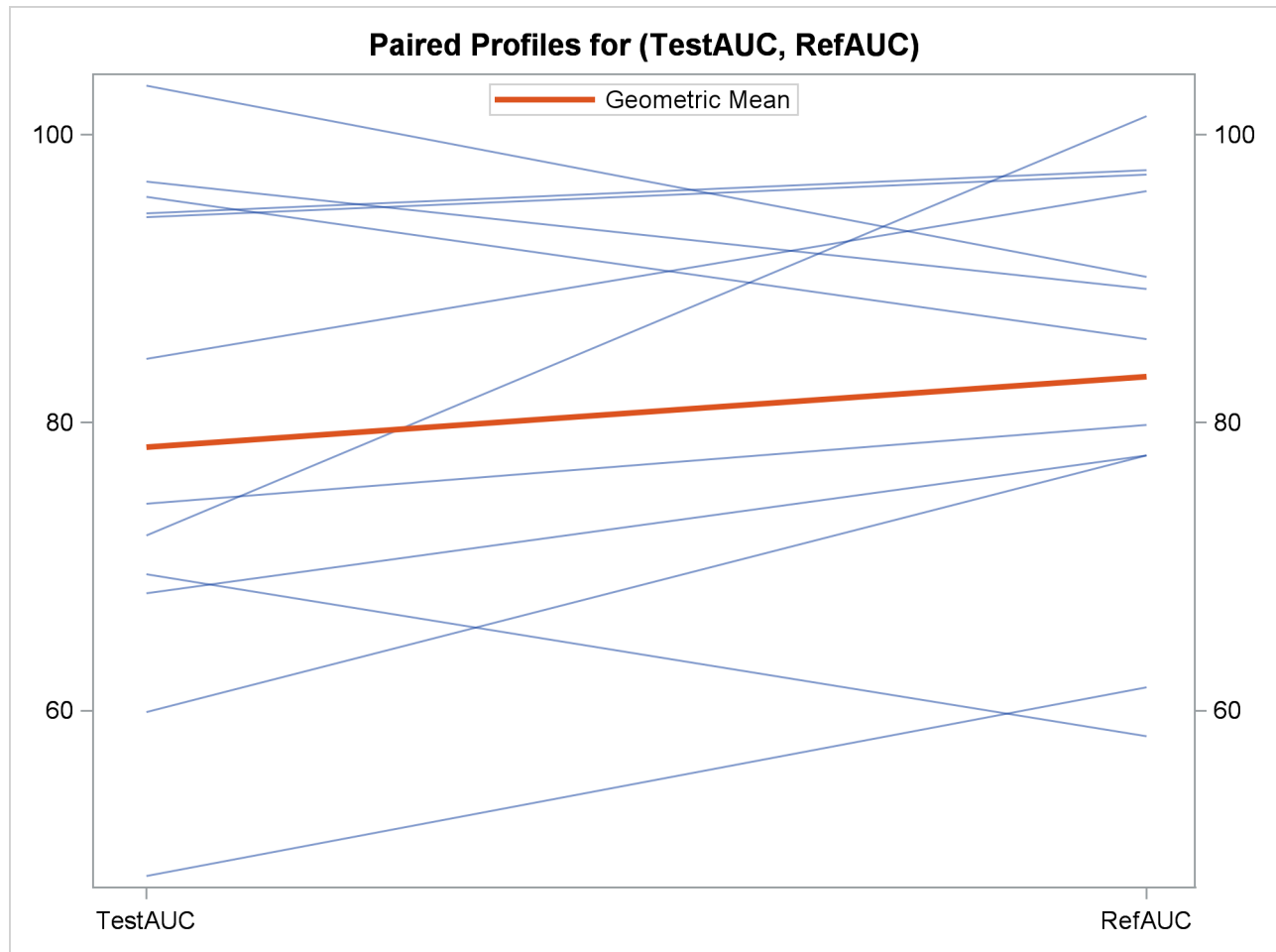
Output 99.5.7 Agreement Plot



The profiles plot in [Output 99.5.8](#) is a different view of the same information contained in [Output 99.5.7](#), plotting the AUC from Test to Reference drug.



Output 99.5.8 Profiles Plot




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# Chapter 100

## The VARCLUS Procedure

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## Overview: VARCLUS Procedure

The VARCLUS procedure divides a set of numeric variables into disjoint or hierarchical clusters. Associated with each cluster is a linear combination of the variables in the cluster. This linear combination can be either the first principal component (the default) or the centroid component (if you specify the CENTROID option). The first principal component is a weighted average of the variables that explains as much variance as possible. See Chapter 73, “The PRINCOMP Procedure,” for further details. Centroid components are unweighted averages of either the standardized variables (the default) or the raw variables (if you specify the COVARIANCE option). PROC VARCLUS tries to maximize the variance that is explained by the cluster components, summed over all the clusters.

The cluster components are oblique, not orthogonal, even when the cluster components are first principal components. In an ordinary principal component analysis, all components are computed from the same variables, and the first principal component is orthogonal to the second principal component and to every other principal component. In PROC VARCLUS, each cluster component is computed from a set of variables that is different from all the other cluster components. The first principal component of one cluster might be correlated with the first principal component of another cluster. Hence, the PROC VARCLUS algorithm is a type of oblique component analysis.

As in principal component analysis, either the correlation or the covariance matrix can be analyzed. If correlations are used, all variables are treated as equally important. If covariances are used, variables with larger variances have more importance in the analysis.

PROC VARCLUS displays a dendrogram (tree diagram of hierarchical clusters) by using ODS Graphics. PROC VARCLUS can also create an output data set that can be used by the TREE procedure to draw the dendrogram. A second output data set can be used with the SCORE procedure to compute component scores for each cluster.

PROC VARCLUS can be used as a variable-reduction method. A large set of variables can often be replaced by the set of cluster components with little loss of information. A given number of cluster components does not generally explain as much variance as the same number of principal components on the full set of variables, but the cluster components are usually easier to interpret than the principal components, even if the latter are rotated.

For example, an educational test might contain 50 items. PROC VARCLUS can be used to divide the items into, say, five clusters. Each cluster can then be treated as a subtest, with the subtest scores given by the cluster components. If the cluster components are centroid components of the covariance matrix, each subtest score is simply the sum of the item scores for that cluster.

The VARCLUS algorithm is both divisive and iterative. By default, PROC VARCLUS begins with all variables in a single cluster. It then repeats the following steps:

1. A cluster is chosen for splitting. Depending on the options specified, the selected cluster has either the smallest percentage of variation explained by its cluster component (using the PROPORTION= option) or the largest eigenvalue associated with the second principal component (using the MAX-EIGEN= option).
2. The chosen cluster is split into two clusters by finding the first two principal components, performing an orthoblique rotation (raw quartimax rotation on the eigenvectors; Harris and Kaiser 1964), and assigning each variable to the rotated component with which it has the higher squared correlation.
3. Variables are iteratively reassigned to clusters to try to maximize the variance accounted for by the cluster components. You can require the reassignment algorithms to maintain a hierarchical structure for the clusters.

The procedure stops splitting when either of the following conditions holds:

- The number of clusters is greater than or equal to the maximum number of clusters as specified by the MAXCLUSTERS= option is reached.
- Every cluster satisfies the stopping criteria specified by the PROPORTION= option (percentage of variation explained) or the MAXEIGEN= option (second eigenvalue) or both.

By default, VARCLUS stops splitting when every cluster has only one eigenvalue greater than one, thus satisfying the most popular criterion for determining the sufficiency of a single underlying dimension.

The iterative reassignment of variables to clusters proceeds in two phases. The first is a nearest component sorting (NCS) phase, similar in principle to the nearest centroid sorting algorithms described by Anderberg (1973). In each iteration, the cluster components are computed, and each variable is assigned to the component with which it has the highest squared correlation. The second phase involves a search algorithm in which each variable is tested to see if assigning it to a different cluster increases the amount of variance explained. If a variable is reassigned during the search phase, the components of the two clusters involved are recomputed before the next variable is tested. The NCS phase is much faster than the search phase but is more likely to be trapped by a local optimum.

If principal components are used, the NCS phase is an alternating least squares method and converges rapidly. The search phase can be very time-consuming for a large number of variables. But if the default initialization method is used, the search phase is rarely able to substantially improve the results of the NCS phase, so the search takes few iterations. If random initialization is used, the NCS phase might be trapped by a local optimum from which the search phase can escape.

If centroid components are used, the NCS phase is not an alternating least squares method and might not increase the amount of variance explained; therefore it is limited, by default, to one iteration.

You can have VARCLUS do the clustering hierarchically by restricting the reassignment of variables such that the clusters maintain a tree structure. In this case, when a cluster is split, a variable in one of the two resulting clusters can be reassigned to the other cluster that results from the split but not to a cluster that is not part of the original cluster (the one that is split).

---

## Getting Started: VARCLUS Procedure

This example demonstrates how you can use PROC VARCLUS to cluster variables.

The following data are job ratings of police officers. The officers were rated by their supervisors on 13 job skills on a scale from 1 to 9. There is also an overall rating that is not used in this analysis. The following DATA step creates the SAS data set JobRat:

```

data JobRat;
 input
 (Communication_Skills
 Problem_Solving
 Learning_Ability
 Judgement_under_Pressure
 Observational_Skills
 Willingness_to_Confront_Problems
 Interest_in_People
 Interpersonal_Sensitivity
 Desire_for_Self_Improvement
 Appearance
 Dependability
 Physical_Ability
 Integrity
 Overall_Rating)
 (1.);
 datalines;
26838853879867
74758876857667
56757863775875
67869777988997
99997798878888

... more lines ...

99997899799799
99899899899899
76656399567486
;

```

The following statements cluster the variables:

```

proc varclus data=JobRat maxclusters=3;
 var Communication_Skills--Integrity;
run;

```

The DATA= option specifies the SAS data set JobRat as input.

The MAXCLUSTERS=3 option specifies that no more than three clusters be computed. By default, PROC VARCLUS splits and optimizes clusters until all clusters have a second eigenvalue less than one. In this example, the default setting would produce only two clusters, but going to three clusters produces a more interesting result.

The VAR statement lists the numeric variables (Communication\_Skills -- Integrity) to be used in the analysis. The overall rating is omitted from the list of variables.

Although PROC VARCLUS displays output for one cluster, two clusters, and three clusters, the following figures display only the final analysis for three clusters.

For each cluster, [Figure 100.1](#) displays the number of variables in the cluster, the cluster variation, the total explained variation, and the proportion of the total variance explained by the variables in the cluster. The variance explained by the variables in a cluster is similar to the variance explained by a factor in

common factor analysis, but it includes contributions only from the variables in the cluster rather than from all variables.

The line labeled “Total variation explained” in Figure 100.1 gives the sum of the explained variation over all clusters. The final “Proportion” represents the total explained variation divided by the sum of cluster variation. This value, 0.6715, indicates that about 67% of the total variation in the data can be accounted for by the three cluster components.

**Figure 100.1** Cluster Summary for Three Clusters from PROC VARCLUS

| Oblique Principal Component Cluster Analysis             |         |                   |                     |                      |                   |
|----------------------------------------------------------|---------|-------------------|---------------------|----------------------|-------------------|
| Cluster Summary for 3 Clusters                           |         |                   |                     |                      |                   |
| Cluster                                                  | Members | Cluster Variation | Variation Explained | Proportion Explained | Second Eigenvalue |
| 1                                                        | 6       | 6                 | 3.771349            | 0.6286               | 0.7093            |
| 2                                                        | 5       | 5                 | 3.575933            | 0.7152               | 0.5035            |
| 3                                                        | 2       | 2                 | 1.382005            | 0.6910               | 0.6180            |
| Total variation explained = 8.729286 Proportion = 0.6715 |         |                   |                     |                      |                   |

Figure 100.2 shows how the variables are clustered. Figure 100.2 also displays the R-square value of each variable with its own cluster and the R-square value with its nearest cluster. The R-square value for a variable with the nearest cluster should be low if the clusters are well separated. The last column displays the ratio of  $(1 - R_{own}^2)/(1 - R_{nearest}^2)$  for each variable. Small values of this ratio indicate good clustering.

**Figure 100.2** R-Square Values from PROC VARCLUS

| 3 Clusters |                                  | R-squared with |              |              |
|------------|----------------------------------|----------------|--------------|--------------|
| Cluster    | Variable                         | Own Cluster    | Next Closest | 1-R**2 Ratio |
| Cluster 1  | Communication_Skills             | 0.6403         | 0.3599       | 0.5620       |
|            | Problem_Solving                  | 0.5412         | 0.2895       | 0.6458       |
|            | Learning_Ability                 | 0.6561         | 0.1692       | 0.4139       |
|            | Observational_Skills             | 0.6889         | 0.2584       | 0.4194       |
|            | Willingness_to_Confront_Problems | 0.6480         | 0.3402       | 0.5335       |
|            | Desire_for_Self_Improvement      | 0.5968         | 0.3473       | 0.6177       |
| Cluster 2  | Judgement_under_Pressure         | 0.6263         | 0.3719       | 0.5950       |
|            | Interest_in_People               | 0.8122         | 0.1885       | 0.2314       |
|            | Interpersonal_Sensitivity        | 0.7566         | 0.1387       | 0.2826       |
|            | Dependability                    | 0.6163         | 0.4419       | 0.6875       |
|            | Integrity                        | 0.7645         | 0.2724       | 0.3237       |
| Cluster 3  | Appearance                       | 0.6910         | 0.3047       | 0.4444       |
|            | Physical_Ability                 | 0.6910         | 0.1871       | 0.3801       |



Figure 100.3 displays the standardized scoring coefficients that are used to compute the first principal component of each cluster. Since each variable is assigned to one and only one cluster, each row of the scoring coefficients contains only one nonzero value.

**Figure 100.3** Standardized Scoring Coefficients from PROC VARCLUS

| Standardized Scoring Coefficients |          |          |          |
|-----------------------------------|----------|----------|----------|
| Cluster                           | 1        | 2        | 3        |
| Communication_Skills              | 0.212170 | 0.000000 | 0.000000 |
| Problem_Solving                   | 0.195058 | 0.000000 | 0.000000 |
| Learning_Ability                  | 0.214781 | 0.000000 | 0.000000 |
| Judgement_under_Pressure          | 0.000000 | 0.221313 | 0.000000 |
| Observational_Skills              | 0.220086 | 0.000000 | 0.000000 |
| Willingness_to_Confront_Problems  | 0.213452 | 0.000000 | 0.000000 |
| Interest_in_People                | 0.000000 | 0.252025 | 0.000000 |
| Interpersonal_Sensitivity         | 0.000000 | 0.243245 | 0.000000 |
| Desire_for_Self_Improvement       | 0.204848 | 0.000000 | 0.000000 |
| Appearance                        | 0.000000 | 0.000000 | 0.601493 |
| Dependability                     | 0.000000 | 0.219544 | 0.000000 |
| Physical_Ability                  | 0.000000 | 0.000000 | 0.601493 |
| Integrity                         | 0.000000 | 0.244507 | 0.000000 |

Figure 100.4 displays the cluster structure and the intercluster correlations. The structure table displays the correlation of each variable with each cluster component. The table of intercorrelations contains the correlations between the cluster components.

**Figure 100.4** Cluster Correlations and Intercorrelations from PROC VARCLUS

| Cluster Structure                |          |          |          |
|----------------------------------|----------|----------|----------|
| Cluster                          | 1        | 2        | 3        |
| Communication_Skills             | 0.800169 | 0.599909 | 0.427341 |
| Problem_Solving                  | 0.735630 | 0.538017 | 0.425463 |
| Learning_Ability                 | 0.810014 | 0.411316 | 0.376333 |
| Judgement_under_Pressure         | 0.609876 | 0.791401 | 0.345399 |
| Observational_Skills             | 0.830021 | 0.407807 | 0.508305 |
| Willingness_to_Confront_Problems | 0.805002 | 0.362927 | 0.583265 |
| Interest_in_People               | 0.434138 | 0.901225 | 0.387770 |
| Interpersonal_Sensitivity        | 0.372371 | 0.869826 | 0.287658 |
| Desire_for_Self_Improvement      | 0.772554 | 0.589334 | 0.494842 |
| Appearance                       | 0.552003 | 0.393759 | 0.831266 |
| Dependability                    | 0.664778 | 0.785073 | 0.574460 |
| Physical_Ability                 | 0.432590 | 0.416070 | 0.831266 |
| Integrity                        | 0.521876 | 0.874342 | 0.477885 |

Figure 100.4 continued

| Inter-Cluster Correlations |         |         |         |
|----------------------------|---------|---------|---------|
| Cluster                    | 1       | 2       | 3       |
| 1                          | 1.00000 | 0.60851 | 0.59223 |
| 2                          | 0.60851 | 1.00000 | 0.48711 |
| 3                          | 0.59223 | 0.48711 | 1.00000 |

PROC VARCLUS next displays the summary table of statistics for the cluster history (Figure 100.5). The first three columns give the number of clusters, the total variation explained by clusters, and the proportion of variation explained by clusters, respectively.

As displayed in the first row of Figure 100.5, the variation explained by the first principal component of all the variables is 6.547402, and the proportion of variation explained is 0.5036.

When the number of clusters is two, the total variation explained is 7.96775 and the proportion of variation explained by the two clusters is 0.6129. The larger second eigenvalue of the clusters is 0.937902; so by default, PROC VARCLUS would stop splitting clusters at this point. But because the MAXCLUSTERS=3 option was specified in this example, PROC VARCLUS continues to the three-cluster solution.

When the number of clusters increases to three, the total variation explained is 8.729286 and the proportion of variation explained by the two clusters is 0.6715. The largest second eigenvalue of the clusters is 0.709323. The statistical improvement from increasing the number of clusters from two to three seems modest, but the interpretability of the three clusters argues for the three-cluster solution.

Figure 100.5 also displays the minimum proportion of variance explained by a cluster, the minimum R square for a variable, and the maximum  $(1 - R^2)$  ratio for a variable. The last quantity is the maximum ratio of the value  $1 - R^2$  for a variable's own cluster to the value  $1 - R^2$  for its nearest cluster.

Figure 100.5 Final Cluster Summary Table from PROC VARCLUS

| Number of Clusters | Total Variation Explained by Clusters | Proportion of Variation Explained by Clusters | Minimum Proportion Explained by a Cluster | Maximum Second Eigenvalue in a Cluster | Minimum R-squared for a Variable | Maximum $1 - R^2$ Ratio for a Variable |
|--------------------|---------------------------------------|-----------------------------------------------|-------------------------------------------|----------------------------------------|----------------------------------|----------------------------------------|
| 1                  | 6.547402                              | 0.5036                                        | 0.5036                                    | 1.772715                               | 0.2995                           |                                        |
| 2                  | 7.967753                              | 0.6129                                        | 0.5475                                    | 0.937902                               | 0.3123                           | 0.8026                                 |
| 3                  | 8.729286                              | 0.6715                                        | 0.6286                                    | 0.709323                               | 0.5412                           | 0.6875                                 |

---

## Syntax: VARCLUS Procedure

The following statements are available in the VARCLUS procedure:

```
PROC VARCLUS < options > ;
 VAR variables ;
 SEED variables ;
 PARTIAL variables ;
 WEIGHT variables ;
 FREQ variables ;
 BY variables ;
```

Usually you need only the VAR statement in addition to the PROC VARCLUS statement. The following sections give detailed syntax information about each of the statements, beginning with the PROC VARCLUS statement. The remaining statements are listed in alphabetical order.

---

## PROC VARCLUS Statement

```
PROC VARCLUS < options > ;
```

The PROC VARCLUS statement invokes the VARCLUS procedure. By default, VARCLUS clusters the numeric variables in the most recently created SAS data set, starting with one cluster and splitting clusters until all clusters have at most one eigenvalue greater than one.

Table 100.1 summarizes the options available in the PROC VARCLUS statement.

**Table 100.1** Options Available in the PROC VARCLUS Statement

| Option                       | Description                                                                   |
|------------------------------|-------------------------------------------------------------------------------|
| <b>Data Sets</b>             |                                                                               |
| DATA=                        | Specifies the input SAS data set                                              |
| OUTSTAT=                     | Specifies the output SAS data set to contain statistics                       |
| OUTTREE=                     | Specifies the output SAS data set for use with PROC TREE                      |
| <b>Input Data Processing</b> |                                                                               |
| COVARIANCE                   | Uses the covariance matrix instead of the correlation matrix                  |
| NOINT                        | Omits the intercept                                                           |
| VARDEF=                      | Specifies the divisor for variances                                           |
| <b>Number of Clusters</b>    |                                                                               |
| MAXCLUSTERS=                 | Specifies the maximum number of clusters                                      |
| MINCLUSTERS=                 | Specifies the minimum number of clusters                                      |
| MAXEIGEN=                    | Specifies the maximum second eigenvalue in a cluster                          |
| PROPORTION=                  | Specifies the minimum proportion of variance explained by a cluster component |
| <b>Clustering Methods</b>    |                                                                               |
| CENTROID                     | Uses centroid components instead of principal components                      |
| HIERARCHY                    | Clusters hierarchically                                                       |
| INITIAL=                     | Specifies the initialization method                                           |

---

Table 100.1 *continued*

| Option                          | Description                                                                   |
|---------------------------------|-------------------------------------------------------------------------------|
| MAXITER=                        | Specifies the maximum iterations during the alternating least squares phase   |
| MAXSEARCH=                      | Specifies the maximum iterations during the search phase                      |
| MULTIPLEGROUP                   | Performs a multiple group component analysis                                  |
| RANDOM=                         | Specifies the random number seed                                              |
| <b>Control Displayed Output</b> |                                                                               |
| CORR                            | Displays the correlation matrix                                               |
| NOPRINT                         | Suppresses displayed output                                                   |
| PLOTS=                          | Specifies ODS Graphics details                                                |
| SHORT                           | Suppresses display of large matrices                                          |
| SIMPLE                          | Displays means and standard deviations                                        |
| SUMMARY                         | Suppresses all default displayed output except the final summary table        |
| TRACE                           | Displays the cluster to which each variable is assigned during the iterations |

VARCLUS chooses which cluster to split based on the MAXEIGEN= and PROPORTION= options.

1. If you specify *either* or *both* of these two options, then *only* the specified options affect the choice of the cluster to split.
2. If you specify *neither* of these options, the criterion for choice of cluster to split depends on the CENTROID option:
  - a) If you specify CENTROID, VARCLUS splits the cluster with the smallest percentage of variation explained by its cluster component, as if you had specified the PROPORTION= option.
  - b) If you do not specify CENTROID, VARCLUS splits the cluster with the largest eigenvalue associated with the second principal component, as if you had specified the MAXEIGEN= option.

The final number of clusters is controlled by three options: MAXCLUSTERS=, MAXEIGEN=, and PROPORTION=.

1. If you specify *any* of these three options, then *only* the options you specify affect the final number of clusters.
2. If you specify *none* of these options, VARCLUS continues to split clusters until the default splitting criterion is satisfied. The default splitting criterion depends on the CENTROID option:
  - a) If you specify CENTROID, the default splitting criterion is PROPORTION=0.75.
  - b) If you do not specify CENTROID, splitting is based on the MAXEIGEN= criterion, with a default depending on the COVARIANCE option:
    - i. For analyzing a correlation matrix (no COVARIANCE option), the default value for MAXEIGEN= is one.
    - ii. For analyzing a covariance matrix (using the COVARIANCE option), the default value for MAXEIGEN= is the average variance of the variables being clustered.

VARCLUS continues to split clusters until any of the following conditions holds:

- The number of cluster equals the value specified for MAXCLUSTERS=.
- No cluster qualifies for splitting according to the MAXEIGEN= or PROPORTION= criterion.
- A cluster was chosen for splitting, but after iteratively reassigning variables to clusters, one of the cluster has no members.

The following list gives details about the options.

### **CENTROID**

uses centroid components rather than principal components. You should specify centroid components if you want the cluster components to be unweighted averages of the standardized variables (the default) or the unstandardized variables (if you specify the COVARIANCE option). It is possible to obtain locally optimal clusterings in which a variable is not assigned to the cluster component with which it has the highest squared correlation. You cannot specify both the CENTROID and MAXEIGEN= options.

### **CORR**

#### **C**

displays the correlation matrix.

### **COVARIANCE**

#### **COV**

analyzes the covariance matrix instead of the correlation matrix. The COVARIANCE option causes variables with a large variance to have more effect on the cluster components than variables with a small variance.

### **DATA=SAS-data-set**

specifies the input data set to be analyzed. The data set can be an ordinary SAS data set or TYPE=CORR, UCORR, COV, UCOV, FACTOR, or SSCP. If you do not specify the DATA= option, the most recently created SAS data set is used. See Appendix A, “[Special SAS Data Sets](#),” for more information about types of SAS data sets.

### **HIERARCHY**

#### **HI**

requires the clusters at different levels to maintain a hierarchical structure. To draw a tree diagram, enable ODS Graphics or use the OUTTREE= option and the TREE procedure.

### **INITIAL=GROUP**

### **INITIAL=INPUT**

### **INITIAL=RANDOM**

### **INITIAL=SEED**

specifies the method for initializing the clusters. If the INITIAL= option is omitted and the MIN-CLUSTERS= option is greater than 1, the initial cluster components are obtained by extracting the required number of principal components and performing an orthoblique rotation (raw quartimax rotation on the eigenvectors; Harris and Kaiser 1964). The following list describes the values for the INITIAL= option:

|        |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
|--------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| GROUP  | obtains the cluster membership of each variable from an observation in the DATA= data set where the <code>_TYPE_</code> variable has a value of 'GROUP'. In this observation, the variables to be clustered must each have an integer value ranging from one to the number of clusters. You can use this option only if the DATA= data set is a TYPE=CORR, UCORR, COV, UCOV, or FACTOR data set. You can use a data set created either by a previous run of PROC VARCLUS or in a DATA step. |
| INPUT  | obtains scoring coefficients for the cluster components from observations in the DATA= data set where the <code>_TYPE_</code> variable has a value of 'SCORE'. You can use this option only if the DATA= data set is a TYPE=CORR, UCORR, COV, UCOV, or FACTOR data set. You can use scoring coefficients from the FACTOR procedure or a previous run of PROC VARCLUS, or you can enter other coefficients in a DATA step.                                                                   |
| RANDOM | assigns variables randomly to clusters.                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
| SEED   | initializes each cluster component to be one of the variables named in the SEED statement. Each variable listed in the SEED statement becomes the sole member of a cluster, and the other variables are initially unassigned. If you do not specify the SEED statement, the first MINCLUSTERS= variables in the VAR statement are used as seeds.                                                                                                                                            |

**MAXCLUSTERS=*n*****MAXC=*n***

specifies the largest number of clusters desired. The default value is the number of variables. VARCLUS stops splitting clusters after the number of clusters reaches the value of the MAXCLUSTERS= option, regardless of what other splitting options are specified.

**MAXEIGEN=*n***

specifies that when choosing a cluster to split, VARCLUS should choose the cluster with the largest second eigenvalue, provided that its second eigenvalue is greater than the MAXEIGEN= value. The MAXEIGEN= option cannot be used with the CENTROID or MULTIPLEGROUP options.

If you do not specify MAXEIGEN=, the default behavior depends on other options as follows:

- If you specify PROPORTION=, CENTROID, or MULTIPLEGROUP, cluster splitting does not depend on the second eigenvalue.
- Otherwise, if you specify MAXCLUSTERS=, the default value for MAXEIGEN= is zero.
- Otherwise, the default value for MAXEIGEN= is either 1.0 if the correlation matrix is analyzed or the average variance if the COVARIANCE option is specified.

If you specify both MAXEIGEN= and MAXCLUSTERS=, the number of clusters will never exceed the value of the MAXCLUSTERS= option.

If you specify both MAXEIGEN= and PROPORTION=, VARCLUS first looks for a cluster to split based on the MAXEIGEN= criterion. If no cluster meets that criterion, VARCLUS then looks for a cluster to split based on the PROPORTION= criterion.

**MAXITER=*n***

specifies the maximum number of iterations during the NCS phase. The default value is 1 if you specify the CENTROID option; the default is 10 otherwise.

**MAXSEARCH=*n***

specifies the maximum number of iterations during the search phase. The default is 1,000 divided by the number of variables.

**MINCLUSTERS=*n*****MINC=*n***

specifies the smallest number of clusters desired. The default value is 2 for INITIAL=RANDOM or INITIAL=SEED; otherwise, VARCLUS begins with one cluster and tries to split it in accordance with the PROPORTION= option or the MAXEIGEN= option or both.

**MULTIPLEGROUP****MG**

performs a multiple group component analysis (Harman 1976). You specify which variables belong to which clusters. No clusters are split, and no variables are reassigned to a different cluster. The input data set must be TYPE=CORR, UCORR, COV, UCOV, FACTOR, or SSCP and must contain an observation with \_TYPE\_='GROUP' that defines the variable groups. Specifying the MULTIPLE-GROUP option is equivalent to specifying all of the following options: INITIAL=GROUP, MINC=1, MAXITER=0, MAXSEARCH=0, PROPORTION=0, and MAXEIGEN=large number.

**NOINT**

requests that no intercept be used; covariances or correlations are not corrected for the mean. If you specify the NOINT option, the OUTSTAT= data set is TYPE=UCORR.

**NOPRINT**

suppresses displayed output. This option temporarily disables the Output Delivery System (ODS). For more information, see Chapter 20, “Using the Output Delivery System.”

**OUTSTAT=*SAS-data-set***

creates an output data set to contain statistics including means, standard deviations, correlations, cluster scoring coefficients, and the cluster structure. The OUTSTAT= data set is TYPE=UCORR if the NOINT option is specified. If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*. For information about types of SAS data sets, see Appendix A, “Special SAS Data Sets.”

**OUTTREE=*SAS-data-set***

creates an output data set to contain information about the tree structure that can be used by the TREE procedure to display a tree diagram. The OUTTREE= option implies the HIERARCHY option. See [Example 100.1](#) for use of the OUTTREE= option. If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*.

**PLOTS <(global-plot-options)> <= plot-request >**

**PLOTS** < (*global-plot-options*) > <= (*plot-request* <... *plot-request* >) >

controls the plots produced through ODS Graphics.

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;

proc varclus plots=dendrogram(height=ncl);
run;

ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS](#).”

By default, PROC VARCLUS produces a dendrogram.

The *global-plot-options*, UNPACK and ONLY, that are commonly used in the PLOTS= option in other procedures are accepted in PROC VARCLUS, but they currently have no effect since PROC VARCLUS produces only a dendrogram.

The following *plot-requests* can be specified:

#### **ALL**

produces all plots, which for PROC VARCLUS is only a dendrogram.

#### **MAXPOINTS=*n***

#### **MAXPTS=*n***

suppresses the dendrogram when the number of variables (clusters) exceeds the *n* value. This prevents an unreadable plot from being produced. The default is MAXPOINTS=200.

#### **DENDROGRAM** < (*dendrogram-options*) >

requests a dendrogram and specifies *dendrogram-options*.

Unlike most graphs, the size of the dendrogram can vary as a function of the number of objects that appear in the dendrogram. You can specify the following *dendrogram-options* to control the size and appearance of the dendrogram:

#### **COMPUTEHEIGHT=*a b***

#### **CH=*a b***

specifies the constants for computing the height of the dendrogram. For *n* points being clustered, intercept *a*, and slope *b*, the height is based in part on  $a + bn$ . For a horizontal dendrogram, the default (given in pixels) is COMPUTEHEIGHT=100 12, the default height in pixels is  $\max(100 + 12n, 480)$ , the default height in inches is  $\max(1.04167 + 0.125n, 5)$ , and the default height in centimeters is  $\max(2.64583 + 0.3175n, 12.7)$ . For a vertical dendrogram, the default height is 480 pixels. The default unit is pixels, and you can use the UNIT= *dendrogram-option* to change the unit to inches or centimeters for this option. Inches equals pixels divided by 96, and centimeters equals inches times 2.54.



**COMPUTEWIDTH=*a b*****CW=*a b***

specifies the constants for computing the width of the dendrogram. For  $n$  points being clustered, intercept  $a$ , and slope  $b$ , the width is based in part on  $a + bn$ . For a vertical dendrogram, the default (given in pixels) is COMPUTEWIDTH=100 12, the default width in pixels is  $\max(100 + 12n, 640)$ , the default width in inches is  $\max(1.04167 + 0.125n, 6.66667)$ , and the default width in centimeters is  $\max(2.64583 + 0.3175n, 16.933)$ . For a horizontal dendrogram, the default width is 640 pixels. The default unit is pixels, and you can use the UNIT= *dendrogram-option* to change the unit to inches or centimeters for this option. Inches equals pixels divided by 96, and centimeters equals inches times 2.54.

**HEIGHT=PROPORTION | NCL | VAREXP****H=P | N | V**

specifies the method for drawing the height of the dendrogram. HEIGHT=PROPORTION is the default.

HEIGHT=PROPORTION specifies that the total proportion of variance explained by the clusters at the current level of the tree is used.

HEIGHT=NCL specifies that the number of clusters is used.

HEIGHT=VAREXP specifies that the total variance explained by the clusters at the current level of the tree is used.

**HORIZONTAL | VERTICAL**

specifies either a horizontal dendrogram with the objects on the vertical axis (HORIZONTAL) or a vertical dendrogram with the objects on the horizontal axis (VERTICAL). The default is HORIZONTAL.

**SETHEIGHT=*height*****SH=*height***

specifies the height of the dendrogram. By default, the height is based on the COMPUTEHEIGHT= option. The default unit is pixels, and you can use the UNIT= *dendrogram-option* to change the unit to inches or centimeters for this *dendrogram-option*.

**SETWIDTH=*width*****SW=*width***

specifies the width of the dendrogram. By default, the width is based on the COMPUTEWIDTH= option. The default unit is pixels, and you can use the UNIT= *dendrogram-option* to change the unit to inches or centimeters for this *dendrogram-option*.

**UNIT=PX | IN | CM**

specifies the unit (pixels, inches, or centimeters) for the SETHEIGHT=, SETWIDTH=, COMPUTEHEIGHT=, and COMPUTEWIDTH= *dendrogram-options*.

**NONE**

suppresses all plots.

The names of the graphs that PROC VARCLUS generates are listed in [Table 100.4](#), along with the required statements and options.

**PROPORTION=*n*****PERCENT=*n***

specifies that when choosing a cluster to split, VARCLUS should choose the cluster with the smallest proportion of variation explained, provided that the proportion of variation explained is less than the PROPORTION= value. Values greater than 1.0 are considered to be percentages, so PROPORTION=0.75 and PERCENT=75 are equivalent.

However, if you specify both MAXEIGEN= and PROPORTION=, VARCLUS first looks for a cluster to split based on the MAXEIGEN= criterion. If no cluster meets that criterion, VARCLUS then looks for a cluster to split based on the PROPORTION= criterion.

If you do not specify PROPORTION=, the default behavior depends on other options as follows:

- If you specify MAXEIGEN=, cluster splitting does not depend on the proportion of variation explained.
- Otherwise, if you specify CENTROID and MAXCLUSTERS=, the default value for PROPORTION= is 1.0.
- Otherwise, if you specify CENTROID without MAXCLUSTERS=, the default value is PROPORTION=0.75 or PERCENT=75.
- Otherwise, cluster splitting does not depend on the proportion of variation explained.

If you specify both PROPORTION= and MAXCLUSTERS=, the number of clusters will never exceed the value of the MAXCLUSTERS= option.

**RANDOM=*n***

specifies a positive integer as a starting value for use with REPLACE=RANDOM. If you do not specify the RANDOM= option, the time of day is used to initialize the pseudorandom number sequence.

**SHORT**

suppresses display of the cluster structure, scoring coefficient, and intercluster correlation matrices.

**SIMPLE****S**

displays means and standard deviations.

**SUMMARY**

suppresses all default displayed output except the final summary table.

**TRACE**

displays the cluster to which each variable is assigned during the iterations.

**VARDEF=DF****VARDEF=N****VARDEF=WDF****VARDEF=WEIGHT | WGT**

specifies the divisor to be used in the calculation of variances and covariances. The default value is VARDEF=DF. The values and associated divisors are displayed in the following table.

| Value        | Divisor                  | Formula            |
|--------------|--------------------------|--------------------|
| DF           | Degrees of freedom       | $n - i$            |
| N            | Number of observations   | $n$                |
| WDF          | Sum of weights minus one | $(\sum_j w_j) - 1$ |
| WEIGHT   WGT | Sum of weights           | $\sum_j w_j$       |

In the preceding table,  $i = 0$  if the NOINT option is specified, and  $i = 1$  otherwise.

---

## BY Statement

**BY variables ;**

You can specify a BY statement with PROC VARCLUS to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the VARCLUS procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

---

## FREQ Statement

**FREQ variable ;**

If a variable in your data set represents the frequency of occurrence for the other values in the observation, include the variable's name in a FREQ statement. The procedure then treats the data set as if each observation appears  $n$  times, where  $n$  is the value of the FREQ variable for the observation. If the value of the FREQ variable is less than 1, the observation is not used in the analysis. Only the integer portion of the value is used. The total number of observations is considered equal to the sum of the FREQ variable.

---

## PARTIAL Statement

**PARTIAL variables ;**

If you want to base the clustering on partial correlations, list the variables to be partialled out in the PARTIAL statement.

---

## SEED Statement

**SEED** *variables* ;

The SEED statement specifies variables to be used as seeds to initialize the clusters. It is not necessary to use INITIAL=SEED if the SEED statement is present, but if any other INITIAL= option is specified, the SEED statement is ignored.

---

## VAR Statement

**VAR** *variables* ;

The VAR statement specifies the variables to be clustered. If you do not specify the VAR statement and do not specify TYPE=SSCP, all numeric variables not listed in other statements (except the SEED statement) are processed. The default VAR variable list does not include the variable INTERCEPT if the DATA= data set is TYPE=SSCP. If the variable INTERCEPT is explicitly specified in the VAR statement with a TYPE=SSCP data set, the NOINT option is enabled.

---

## WEIGHT Statement

**WEIGHT** *variables* ;

If you want to specify relative weights for each observation in the input data set, place the weights in a variable in the data set and specify the name in a WEIGHT statement. This is often done when the variance associated with each observation is different and the values of the weight variable are proportional to the reciprocals of the variances. The WEIGHT variable can take nonintegral values. An observation is used in the analysis only if the value of the WEIGHT variable is greater than zero.

---

## Details: VARCLUS Procedure

---

### Missing Values

Observations that contain missing values are omitted from the analysis.

---

### Using the VARCLUS procedure

Default options for PROC VARCLUS often provide satisfactory results. If you want to change the final number of clusters, use one or more of the MAXCLUSTERS=, MAXEIGEN=, or PROPORTION= options. The MAXEIGEN= and PROPORTION= options usually produce similar results but occasionally cause different clusters to be selected for splitting. The MAXEIGEN= option tends to choose clusters with a large number of variables, while the PROPORTION= option is more likely to select a cluster with a small number of variables.

## Execution Time

PROC VARCLUS usually requires more computer time than principal factor analysis, but it can be faster than some of the iterative factoring methods. If you have more than 30 variables, you might want to reduce execution time by one or more of the following methods:

- Specify the MINCLUSTERS= and MAXCLUSTERS= options if you know how many clusters you want.
- Specify the HIERARCHY option.
- Specify the SEED statement if you have some prior knowledge of what clusters to expect.

If computer time is not a limiting factor, you might want to try one of the following methods to obtain a better solution:

- If the clustering algorithm has not converged, specify larger values for MAXITER= and MAXSEARCH=.
- Try several factoring and rotation methods with PROC FACTOR to use as input to PROC VARCLUS.
- Run PROC VARCLUS several times, specifying INITIAL=RANDOM.

---

## Output Data Sets

### OUTSTAT= Data Set

The OUTSTAT= data set is TYPE=CORR, and it can be used as input to the SCORE procedure or a subsequent run of PROC VARCLUS. The OUTSTAT= data set contains the following variables:

- BY variables
- `_NCL_`, a numeric variable that gives the number of clusters
- `_TYPE_`, a character variable that indicates the type of statistic the observation contains
- `_NAME_`, a character variable that contains a variable name or a cluster name, which is of the form `CLUS $n$` , where  $n$  is the number of the cluster
- the variables that are clustered

The values of the `_TYPE_` variable are listed in the following table.

**Table 100.2** \_TYPE\_

| <b>_TYPE_</b> | <b>Contents</b>                                                                                                                     |
|---------------|-------------------------------------------------------------------------------------------------------------------------------------|
| 'MEAN'        | Means                                                                                                                               |
| 'STD'         | Standard deviations                                                                                                                 |
| 'USTD'        | Uncorrected standard deviations, produced when the NOINT option is specified                                                        |
| 'N'           | Number of observations                                                                                                              |
| 'CORR'        | Correlations                                                                                                                        |
| 'UCORR'       | Uncorrected correlation matrix, produced when the NOINT option is specified                                                         |
| 'MEMBERS'     | Number of members in each cluster                                                                                                   |
| 'VAREXP'      | Variance explained by each cluster                                                                                                  |
| 'PROPOR'      | Proportion of variance explained by each cluster                                                                                    |
| 'GROUP'       | Number of the cluster to which each variable belongs                                                                                |
| 'RSQUARED'    | Squared multiple correlation of each variable with its cluster component                                                            |
| 'SCORE'       | Standardized scoring coefficients                                                                                                   |
| 'USCORE'      | Scoring coefficients to be applied without subtracting the mean from the raw variables, produced when the NOINT option is specified |
| 'STRUCTUR'    | Cluster structure                                                                                                                   |
| 'CCORR'       | Correlations between cluster components                                                                                             |

The observations with `_TYPE_='MEAN'`, `'STD'`, `'N'`, and `'CORR'` have missing values for the `_NCL_` variable. All other values of the `_TYPE_` variable are repeated for each cluster solution, with different solutions distinguished by the value of the `_NCL_` variable. If you want to specify the `OUTSTAT=` data set with the `SCORE` procedure, you can use a `DATA` step to select observations with the `_NCL_` variable missing or equal to the desired number of clusters as follows:

```
data Coef2;
 set Coef;
 if _ncl_ = . or _ncl_ = 3;
 drop _ncl_;
run;

proc score data=NewScore score=Coef2;
run;
```

`PROC SCORE` standardizes the new data by subtracting the original variable means that are stored in the `_TYPE_='MEAN'` observations and dividing by the original variable standard deviations from the `_TYPE_='STD'` observations. Then `PROC SCORE` multiplies the standardized variables by the coefficients from the `_TYPE_='SCORE'` observations to get the cluster scores.

## OUTTREE= Data Set

The OUTTREE= data set contains one observation for each variable clustered plus one observation for each cluster of two or more variables—that is, one observation for each node of the cluster tree. The total number of output observations is between  $n$  and  $2n - 1$ , where  $n$  is the number of variables clustered.

The OUTTREE= data set contains the following variables:

- BY variables, if any
- `_NAME_`, a character variable that gives the name of the node. If the node is a cluster, the name is `CLUS $n$` , where  $n$  is the number of the cluster. If the node is a single variable, the variable name is used.
- `_PARENT_`, a character variable that gives the value of `_NAME_` of the parent of the node. If the node is the root of the tree, `_PARENT_` is blank.
- `_LABEL_`, a character variable that gives the label of the node. If the node is a cluster, the label is `CLUS $n$` , where  $n$  is the number of the cluster. If the node is a single variable, the variable label is used.
- `_NCL_`, the number of clusters
- `_VAREXP_`, the total variance explained by the clusters at the current level of the tree
- `_PROPOR_`, the total proportion of variance explained by the clusters at the current level of the tree
- `_MINPRO_`, the minimum proportion of variance explained by a cluster component
- `_MAXEIG_`, the maximum second eigenvalue of a cluster

---

## Computational Resources

Let

- $n$  = number of observations
- $v$  = number of variables
- $c$  = number of clusters

It is assumed that, at each stage of clustering, the clusters all contain the same number of variables.

## Time

The time required for PROC VARCLUS to analyze a given data set varies greatly depending on the number of clusters requested, the number of iterations in both the alternating least squares and search phases, and whether centroid or principal components are used.

The time required to compute the correlation matrix is roughly proportional to  $nv^2$ .

Default cluster initialization requires time roughly proportional to  $v^3$ . Any other method of initialization requires time roughly proportional to  $cv^2$ .

In the alternating least squares phase, each iteration requires time roughly proportional to  $cv^2$  if centroid components are used or

$$\left(c + 5\frac{v}{c^2}\right)v^2$$

if principal components are used.

In the search phase, each iteration requires time roughly proportional to  $v^3/c$  if centroid components are used or  $v^4/c^2$  if principal components are used. The HIERARCHY option speeds up each iteration after the first split by as much as  $c/2$ .

## Memory

The amount of memory, in bytes, needed by PROC VARCLUS is approximately

$$v^2 + 2vc + 20v + 15c$$

---

## Interpreting VARCLUS Procedure Output

Because the VARCLUS algorithm is a type of oblique component analysis, its output is similar to the output from the FACTOR procedure for oblique rotations. The scoring coefficients have the same meaning in both PROC VARCLUS and PROC FACTOR; they are coefficients applied to the standardized variables to compute component scores. The cluster structure is analogous to the factor structure that contains the correlations between each variable and each cluster component. A cluster pattern is not displayed because it would be the same as the cluster structure, except that zeros would appear in the same places in which zeros appear in the scoring coefficients. The intercluster correlations are analogous to interfactor correlations; they are the correlations among cluster components.

PROC VARCLUS also displays a cluster summary and a cluster listing. The cluster summary gives the number of variables in each cluster and the variation explained by the cluster component. The latter is similar to the variation explained by a factor but includes contributions from only the variables in that cluster rather than from all variables, as in PROC FACTOR. The proportion of variance explained is obtained by dividing the variance explained by the total variance of variables in the cluster. If the cluster contains two or more variables and the CENTROID option is omitted, the second largest eigenvalue of the cluster is also displayed.

The cluster listing gives the variables in each cluster. Two squared correlations are calculated for each cluster. The column labeled “Own Cluster” gives the squared correlation of the variable with its own cluster component. This value should be higher than the squared correlation with any other cluster unless an iteration limit has been exceeded or the CENTROID option has been used. The larger the squared correlation is, the better. The column labeled “Next Closest” contains the next-highest squared correlation of the variable with a cluster component. This value is low if the clusters are well separated. The column labeled “1-R\*\*2 Ratio” gives the ratio of one minus the “Own Cluster” R square to one minus the “Next Closest” R square. A small “1-R\*\*2 Ratio” indicates a good clustering.



---

## Displayed Output

The following items are displayed for each cluster solution unless the NOPRINT or SUMMARY option is specified. The CLUSTER SUMMARY table includes the following columns:

- the Cluster number
- Members, the number of members in the cluster
- Cluster Variation of the variables in the cluster
- Variation Explained by the cluster component. This statistic is based only on the variables in the cluster rather than on all variables.
- Proportion Explained, the result of dividing the variation explained by the cluster variation
- Second Eigenvalue, the second largest eigenvalue of the cluster. This is displayed if the cluster contains more than one variable and the CENTROID option is not specified

PROC VARCLUS also displays the following:

- Total variation explained, the sum across clusters of the variation explained by each cluster
- Proportion, the total explained variation divided by the total variation of all the variables

The cluster listing includes the following columns:

- Variable, the variables in each cluster
- R square with Own Cluster (the squared correlation of the variable with its own cluster component), and R square with Next Closest (the next highest squared correlation of the variable with a cluster component). Own Cluster values should be higher than the R square with any other cluster unless an iteration limit is exceeded or you specify the CENTROID option. Next Closest should be a low value if the clusters are well separated.
- $1-R^{*2}$  Ratio, the ratio of one minus the value in the Own Cluster column to one minus the value in the Next Closest column. The occurrence of low ratios indicates well-separated clusters.

If the SHORT option is not specified, PROC VARCLUS also displays the following tables:

- Standardized Scoring Coefficients, standardized regression coefficients for predicting cluster components from variables
- Cluster Structure, the correlations between each variable and each cluster component
- Inter-Cluster Correlations, the correlations between the cluster components

If the analysis includes partitions for two or more numbers of clusters, a final summary table is displayed. Each row of the table corresponds to one partition. The columns include the following:

- Number of Clusters
- Total Variation Explained by Clusters
- Proportion of Variation Explained by Clusters
- Minimum Proportion (of variation) Explained by a Cluster
- Maximum Second Eigenvalue in a Cluster
- Minimum R square for a Variable
- Maximum  $1-R^2$  Ratio for a Variable

---

## ODS Table Names

PROC VARCLUS assigns a name to each table it creates. You can use this name to refer to the table when using the Output Delivery System (ODS) to select tables and create output data sets. These ODS table names are listed in [Table 100.3](#). For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

**Table 100.3** ODS Tables Produced by PROC VARCLUS

| ODS Table Name    | Description                              | Option  |
|-------------------|------------------------------------------|---------|
| ClusterQuality    | Cluster quality                          | default |
| ClusterStructure  | Cluster structure                        | default |
| ClusterSummary    | Cluster summary                          | default |
| ConvergenceStatus | Convergence status                       | default |
| Corr              | Correlations between variables           | CORR    |
| DataOptSummary    | Data and options summary table           | default |
| InterClusterCorr  | Correlations between cluster components  | default |
| IterHistory       | Iteration history                        | TRACE   |
| RSquare           | R squares between variables and clusters | default |
| SimpleStatistics  | Means and standard deviations            | SIMPLE  |
| StdScoreCoef      | Standardized scoring coefficients        | default |

---

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “Statistical Graphics Using ODS.”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “Enabling and Disabling ODS Graphics” on page 600 in Chapter 21, “Statistical Graphics Using ODS.”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “A Primer on ODS Statistical Graphics” on page 599 in Chapter 21, “Statistical Graphics Using ODS.”

By default, PROC VARCLUS produces a dendrogram.

You can refer to every graph produced through ODS Graphics with a name. The name of the graph that PROC VARCLUS generates is listed in Table 100.4, along with the statement and option required to produce it.

**Table 100.4** Graphs Produced by PROC VARCLUS

| ODS Graph Name | Plot Description             | Statement and Option          |
|----------------|------------------------------|-------------------------------|
| Dendrogram     | Dendrogram<br>(tree diagram) | PROC VARCLUS PLOTS=DENDROGRAM |

## Example: VARCLUS Procedure

### Example 100.1: Correlations among Physical Variables

The data in this example are correlations among eight physical variables as given by Harman (1976). The first PROC VARCLUS run clusters on the basis of principal components. The second run clusters on the basis of centroid components. The third analysis is hierarchical, and the TREE procedure is used to display a tree diagram. The following statements create the data set and perform the analysis:

```
data phys8(type=corr);
 title 'Eight Physical Measurements on 305 School Girls';
 title2 'Harman: Modern Factor Analysis, 3rd Ed, p22';
 label ArmSpan='Arm Span' Forearm='Length of Forearm'
 LowerLeg='Length of Lower Leg' BitDiam='Bitrochanteric Diameter'
 Girth='Chest Girth' Width='Chest Width';
 input _Name_ $ 1-8
 (Height ArmSpan Forearm LowerLeg Weight BitDiam
 Girth Width) (7.);
 Type='corr';
 datalines;
Height 1.0 .846 .805 .859 .473 .398 .301 .382
ArmSpan .846 1.0 .881 .826 .376 .326 .277 .415
Forearm .805 .881 1.0 .801 .380 .319 .237 .345
LowerLeg .859 .826 .801 1.0 .436 .329 .327 .365
Weight .473 .376 .380 .436 1.0 .762 .730 .629
BitDiam .398 .326 .319 .329 .762 1.0 .583 .577
Girth .301 .277 .237 .327 .730 .583 1.0 .539
Width .382 .415 .345 .365 .629 .577 .539 1.0
;
```

```
proc varclus data=phys8;
run;
```

The PROC VARCLUS statement invokes the procedure. By default, PROC VARCLUS clusters using principal components.

As displayed in [Output 100.1.1](#), when there is only one cluster, the cluster component (by default, the first principal component) explains 58.41% of the total variation of the eight variables.

The cluster is split because the second eigenvalue is greater than 1 (the default value of the MAXEIGEN option).

The two resulting cluster components explain 80.33% of the variation in the original variables. The cluster summary table shows that the variables Height, ArmSpan, Forearm, and LowerLeg have been assigned to the first cluster, and that the variables Weight, BitDiam, Girth, and Width have been assigned to the second cluster.

The standardized scoring coefficients in [Output 100.1.1](#) show that each cluster component has similar scores for each of its associated variables. This suggests that the principal cluster component solution should be similar to the centroid cluster component solution, which follows in the next PROC VARCLUS run.

The cluster structure table displays high correlations between the variables and their own cluster component. The correlations between the variables and the opposite cluster component are all moderate.

The intercluster correlation table shows that the two cluster components have a moderate correlation of 0.44513.

### Output 100.1.1 Principal Component Clusters

```

 Eight Physical Measurements on 305 School Girls
 Harman: Modern Factor Analysis, 3rd Ed, p22

 Oblique Principal Component Cluster Analysis

 Observations 10000 Proportion 0
 Variables 8 Maxeigen 1

Clustering algorithm converged.

 Cluster Summary for 1 Cluster

 Cluster Members Cluster Variation Proportion Second
 ----- ----- ----- ----- ----- -----
 1 8 8 4.67288 0.5841 1.7710

 Total variation explained = 4.67288 Proportion = 0.5841

Cluster 1 will be split because it has the largest second eigenvalue, 1.770983,
which is greater than the MAXEIGEN=1 value.

Clustering algorithm converged.

```

Output 100.1.1 *continued*

| Cluster Summary for 2 Clusters                           |                         |                   |                     |                      |                         |  |
|----------------------------------------------------------|-------------------------|-------------------|---------------------|----------------------|-------------------------|--|
| Cluster                                                  | Members                 | Cluster Variation | Variation Explained | Proportion Explained | Second Eigenvalue       |  |
| 1                                                        | 4                       | 4                 | 3.509218            | 0.8773               | 0.2361                  |  |
| 2                                                        | 4                       | 4                 | 2.917284            | 0.7293               | 0.4764                  |  |
| Total variation explained = 6.426502 Proportion = 0.8033 |                         |                   |                     |                      |                         |  |
| R-squared with                                           |                         |                   |                     |                      |                         |  |
| 2 Clusters                                               | Variable                | Own Cluster       | Next Closest        | 1-R**2 Ratio         | Variable Label          |  |
| Cluster 1                                                | ArmSpan                 | 0.9002            | 0.1658              | 0.1196               | Arm Span                |  |
|                                                          | Forearm                 | 0.8661            | 0.1413              | 0.1560               | Length of Forearm       |  |
|                                                          | LowerLeg                | 0.8652            | 0.1829              | 0.1650               | Length of Lower Leg     |  |
|                                                          | Height                  | 0.8777            | 0.2088              | 0.1545               |                         |  |
| Cluster 2                                                | BitDiam                 | 0.7386            | 0.1341              | 0.3019               | Bitrochanteric Diameter |  |
|                                                          | Girth                   | 0.6981            | 0.0929              | 0.3328               | Chest Girth             |  |
|                                                          | Width                   | 0.6329            | 0.1619              | 0.4380               | Chest Width             |  |
|                                                          | Weight                  | 0.8477            | 0.1974              | 0.1898               |                         |  |
| Standardized Scoring Coefficients                        |                         |                   |                     |                      |                         |  |
| Cluster                                                  |                         | 1                 |                     | 2                    |                         |  |
| ArmSpan                                                  | Arm Span                | 0.270377          |                     | 0.000000             |                         |  |
| Forearm                                                  | Length of Forearm       | 0.265194          |                     | 0.000000             |                         |  |
| LowerLeg                                                 | Length of Lower Leg     | 0.265057          |                     | 0.000000             |                         |  |
| BitDiam                                                  | Bitrochanteric Diameter | 0.000000          |                     | 0.294591             |                         |  |
| Girth                                                    | Chest Girth             | 0.000000          |                     | 0.286407             |                         |  |
| Width                                                    | Chest Width             | 0.000000          |                     | 0.272710             |                         |  |
| Height                                                   |                         | 0.266977          |                     | 0.000000             |                         |  |
| Weight                                                   |                         | 0.000000          |                     | 0.315597             |                         |  |
| Cluster Structure                                        |                         |                   |                     |                      |                         |  |
| Cluster                                                  |                         | 1                 |                     | 2                    |                         |  |
| ArmSpan                                                  | Arm Span                | 0.948813          |                     | 0.407210             |                         |  |
| Forearm                                                  | Length of Forearm       | 0.930624          |                     | 0.375865             |                         |  |
| LowerLeg                                                 | Length of Lower Leg     | 0.930142          |                     | 0.427715             |                         |  |
| BitDiam                                                  | Bitrochanteric Diameter | 0.366201          |                     | 0.859404             |                         |  |
| Girth                                                    | Chest Girth             | 0.304779          |                     | 0.835529             |                         |  |
| Width                                                    | Chest Width             | 0.402430          |                     | 0.795572             |                         |  |
| Height                                                   |                         | 0.936881          |                     | 0.456908             |                         |  |
| Weight                                                   |                         | 0.444281          |                     | 0.920686             |                         |  |

**Output 100.1.1** *continued*

| Inter-Cluster Correlations                    |                                       |                                               |                                           |                                        |                                  |                                     |
|-----------------------------------------------|---------------------------------------|-----------------------------------------------|-------------------------------------------|----------------------------------------|----------------------------------|-------------------------------------|
| Cluster                                       | 1                                     | 2                                             |                                           |                                        |                                  |                                     |
| 1                                             | 1.00000                               | 0.44513                                       |                                           |                                        |                                  |                                     |
| 2                                             | 0.44513                               | 1.00000                                       |                                           |                                        |                                  |                                     |
| No cluster meets the criterion for splitting. |                                       |                                               |                                           |                                        |                                  |                                     |
| Number of Clusters                            | Total Variation Explained by Clusters | Proportion of Variation Explained by Clusters | Minimum Proportion Explained by a Cluster | Maximum Second Eigenvalue in a Cluster | Minimum R-squared for a Variable | Maximum 1-R**2 Ratio for a Variable |
| 1                                             | 4.672880                              | 0.5841                                        | 0.5841                                    | 1.770983                               | 0.3810                           |                                     |
| 2                                             | 6.426502                              | 0.8033                                        | 0.7293                                    | 0.476418                               | 0.6329                           | 0.4380                              |

In the following statements, the CENTROID option in the PROC VARCLUS statement specifies that cluster centroids be used as the basis for clustering:

```
proc varclus data=phys8 centroid;
run;
```

The first cluster component, which in the centroid method is an unweighted sum of the standardized variables, explains 57.89% of the variation in the data. This value is near the maximum possible variance explained, 58.41%, which is attained by the first principal component shown previously in [Output 100.1.1](#).

The default behavior in the centroid method is to split any cluster with less than 75% of the total cluster variance explained by the centroid component. Since the centroid component for the one-cluster solution explains only 57.89% of the variation as shown in [Output 100.1.2](#), the variables are split into two clusters. The resulting clusters are the same two clusters created by the principal component method. Recall that this outcome was suggested by the similar standardized scoring coefficients in the principal cluster component solution.

In the two-cluster solution, the centroid component of the second cluster explains only 72.75% of the total variation of the cluster. Since this percentage is less than 75%, the second cluster is split.

In the R-square table for two clusters, the Width variable has a weaker relation to its cluster than any other variable. In the three-cluster solution this variable is in a cluster of its own.

Each cluster component is an unweighted average of the cluster's standardized variables. Thus, the coefficients for each of the cluster's associated variables are identical in the centroid cluster component solution.

The centroid method stops at the three-cluster solution. The three centroid components account for 86.15% of the variability in the eight variables, and all cluster components account for at least 79.44% of the total variation in the corresponding cluster. Additionally, the smallest squared correlation between the variables and their own cluster component is 0.7482.

If the PROPORTION= option were set to a value between 0.5789 (the proportion of variance explained in the one-cluster solution) and 0.7275 (the minimum proportion of variance explained in the two-cluster

solution), PROC VARCLUS would stop at the two-cluster solution, and the centroid solution would find the same clusters as the principal components solution, although the cluster components would be slightly different.

### Output 100.1.2 Centroid Component Clusters

```

Eight Physical Measurements on 305 School Girls
Harman: Modern Factor Analysis, 3rd Ed, p22

Oblique Centroid Component Cluster Analysis

Observations 10000 Proportion 0.75
Variables 8 Maxeigen 0

Clustering algorithm converged.

Cluster Summary for 1 Cluster

Cluster Members Cluster Variation Proportion
 Members Variation Explained Explained

 1 8 8 4.631 0.5789

Total variation explained = 4.631 Proportion = 0.5789

Cluster 1 will be split because it has the smallest proportion of variation
explained, 0.578875, which is less than the PROPORTION=0.75 value.

Clustering algorithm converged.

Cluster Summary for 2 Clusters

Cluster Members Cluster Variation Proportion
 Members Variation Explained Explained

 1 4 4 3.509 0.8773
 2 4 4 2.91 0.7275

Total variation explained = 6.419 Proportion = 0.8024

```

Output 100.1.2 continued

| 2 Clusters |          | R-squared with |              |              | Variable                |
|------------|----------|----------------|--------------|--------------|-------------------------|
| Cluster    | Variable | Own Cluster    | Next Closest | 1-R**2 Ratio | Label                   |
| Cluster 1  | ArmSpan  | 0.8994         | 0.1669       | 0.1208       | Arm Span                |
|            | Forearm  | 0.8663         | 0.1410       | 0.1557       | Length of Forearm       |
|            | LowerLeg | 0.8658         | 0.1824       | 0.1641       | Length of Lower Leg     |
|            | Height   | 0.8778         | 0.2075       | 0.1543       |                         |
| Cluster 2  | BitDiam  | 0.7335         | 0.1341       | 0.3078       | Bitrochanteric Diameter |
|            | Girth    | 0.6988         | 0.0929       | 0.3321       | Chest Girth             |
|            | Width    | 0.6473         | 0.1618       | 0.4207       | Chest Width             |
|            | Weight   | 0.8368         | 0.1975       | 0.2033       |                         |

| Standardized Scoring Coefficients |                         |          |          |  |
|-----------------------------------|-------------------------|----------|----------|--|
| Cluster                           |                         | 1        | 2        |  |
| ArmSpan                           | Arm Span                | 0.266918 | 0.000000 |  |
| Forearm                           | Length of Forearm       | 0.266918 | 0.000000 |  |
| LowerLeg                          | Length of Lower Leg     | 0.266918 | 0.000000 |  |
| BitDiam                           | Bitrochanteric Diameter | 0.000000 | 0.293105 |  |
| Girth                             | Chest Girth             | 0.000000 | 0.293105 |  |
| Width                             | Chest Width             | 0.000000 | 0.293105 |  |
| Height                            |                         | 0.266918 | 0.000000 |  |
| Weight                            |                         | 0.000000 | 0.293105 |  |

| Cluster Structure |                         |          |          |  |
|-------------------|-------------------------|----------|----------|--|
| Cluster           |                         | 1        | 2        |  |
| ArmSpan           | Arm Span                | 0.948361 | 0.408589 |  |
| Forearm           | Length of Forearm       | 0.930744 | 0.375468 |  |
| LowerLeg          | Length of Lower Leg     | 0.930477 | 0.427054 |  |
| BitDiam           | Bitrochanteric Diameter | 0.366212 | 0.856453 |  |
| Girth             | Chest Girth             | 0.304821 | 0.835936 |  |
| Width             | Chest Width             | 0.402246 | 0.804574 |  |
| Height            |                         | 0.936883 | 0.455485 |  |
| Weight            |                         | 0.444419 | 0.914781 |  |

| Inter-Cluster Correlations |         |         |  |
|----------------------------|---------|---------|--|
| Cluster                    | 1       | 2       |  |
| 1                          | 1.00000 | 0.44484 |  |
| 2                          | 0.44484 | 1.00000 |  |



Output 100.1.2 continued

Cluster 2 will be split because it has the smallest proportion of variation explained, 0.7275, which is less than the PROPORTION=0.75 value.

Clustering algorithm converged.

Cluster Summary for 3 Clusters

| Cluster | Members | Cluster Variation | Variation Explained | Proportion Explained |
|---------|---------|-------------------|---------------------|----------------------|
| 1       | 4       | 4                 | 3.509               | 0.8773               |
| 2       | 3       | 3                 | 2.383333            | 0.7944               |
| 3       | 1       | 1                 | 1                   | 1.0000               |

Total variation explained = 6.892333 Proportion = 0.8615

3 Clusters

| Cluster   | Variable | R-squared with |              |              | Variable Label          |
|-----------|----------|----------------|--------------|--------------|-------------------------|
|           |          | Own Cluster    | Next Closest | 1-R**2 Ratio |                         |
| Cluster 1 | ArmSpan  | 0.8994         | 0.1722       | 0.1215       | Arm Span                |
|           | Forearm  | 0.8663         | 0.1225       | 0.1524       | Length of Forearm       |
|           | LowerLeg | 0.8658         | 0.1668       | 0.1611       | Length of Lower Leg     |
|           | Height   | 0.8778         | 0.1921       | 0.1513       |                         |
| Cluster 2 | BitDiam  | 0.7691         | 0.3329       | 0.3461       | Bitrochanteric Diameter |
|           | Girth    | 0.7482         | 0.2905       | 0.3548       | Chest Girth             |
|           | Weight   | 0.8685         | 0.3956       | 0.2175       |                         |
| Cluster 3 | Width    | 1.0000         | 0.4259       | 0.0000       | Chest Width             |

Standardized Scoring Coefficients

| Cluster  |                         | 1       | 2       | 3       |
|----------|-------------------------|---------|---------|---------|
| ArmSpan  | Arm Span                | 0.26692 | 0.00000 | 0.00000 |
| Forearm  | Length of Forearm       | 0.26692 | 0.00000 | 0.00000 |
| LowerLeg | Length of Lower Leg     | 0.26692 | 0.00000 | 0.00000 |
| BitDiam  | Bitrochanteric Diameter | 0.00000 | 0.37398 | 0.00000 |
| Girth    | Chest Girth             | 0.00000 | 0.37398 | 0.00000 |
| Width    | Chest Width             | 0.00000 | 0.00000 | 1.00000 |
| Height   |                         | 0.26692 | 0.00000 | 0.00000 |
| Weight   |                         | 0.00000 | 0.37398 | 0.00000 |

Output 100.1.2 continued

| Cluster Structure |                         |         |         |         |  |
|-------------------|-------------------------|---------|---------|---------|--|
| Cluster           |                         | 1       | 2       | 3       |  |
| ArmSpan           | Arm Span                | 0.94836 | 0.36613 | 0.41500 |  |
| Forearm           | Length of Forearm       | 0.93074 | 0.35004 | 0.34500 |  |
| LowerLeg          | Length of Lower Leg     | 0.93048 | 0.40838 | 0.36500 |  |
| BitDiam           | Bitrochanteric Diameter | 0.36621 | 0.87698 | 0.57700 |  |
| Girth             | Chest Girth             | 0.30482 | 0.86501 | 0.53900 |  |
| Width             | Chest Width             | 0.40225 | 0.65259 | 1.00000 |  |
| Height            |                         | 0.93688 | 0.43830 | 0.38200 |  |
| Weight            |                         | 0.44442 | 0.93196 | 0.62900 |  |

| Inter-Cluster Correlations |         |         |         |
|----------------------------|---------|---------|---------|
| Cluster                    | 1       | 2       | 3       |
| 1                          | 1.00000 | 0.41716 | 0.40225 |
| 2                          | 0.41716 | 1.00000 | 0.65259 |
| 3                          | 0.40225 | 0.65259 | 1.00000 |

No cluster meets the criterion for splitting.

| Number of Clusters | Total Variation Explained by Clusters | Proportion of Variation Explained by Clusters | Minimum Proportion Explained by a Cluster | Minimum R-squared for a Variable | Maximum 1-R**2 Ratio for a Variable |
|--------------------|---------------------------------------|-----------------------------------------------|-------------------------------------------|----------------------------------|-------------------------------------|
| 1                  | 4.631000                              | 0.5789                                        | 0.5789                                    | 0.4306                           |                                     |
| 2                  | 6.419000                              | 0.8024                                        | 0.7275                                    | 0.6473                           | 0.4207                              |
| 3                  | 6.892333                              | 0.8615                                        | 0.7944                                    | 0.7482                           | 0.3548                              |

In the following statements, the MAXC= option computes all clustering solutions, from one to eight clusters, and the SUMMARY option suppresses all output except the final cluster quality table:

```
ods graphics on;

proc varclus data=phys8 maxc=8 summary;
run;
```

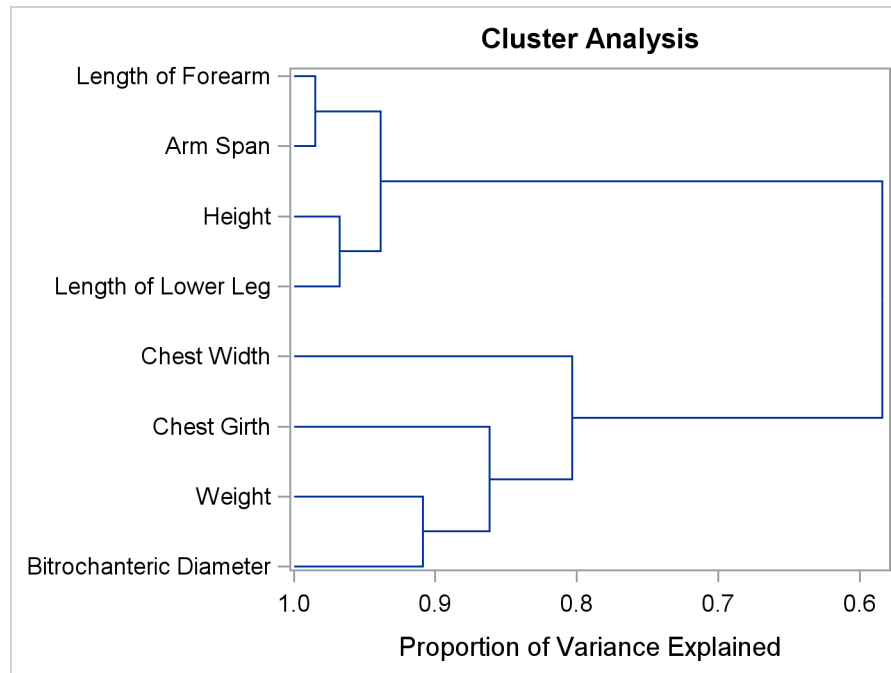
The results from PROC VARCLUS are shown in Output 100.1.3.

**Output 100.1.3** Hierarchical Clusters and the SUMMARY Option

| Eight Physical Measurements on 305 School Girls<br>Harman: Modern Factor Analysis, 3rd Ed, p22 |                                                   |                                                           |                                                       |                                                    |                                           |                                                 |
|------------------------------------------------------------------------------------------------|---------------------------------------------------|-----------------------------------------------------------|-------------------------------------------------------|----------------------------------------------------|-------------------------------------------|-------------------------------------------------|
| Oblique Principal Component Cluster Analysis                                                   |                                                   |                                                           |                                                       |                                                    |                                           |                                                 |
| Observations                                                                                   | 10000                                             | Proportion                                                | 1                                                     |                                                    |                                           |                                                 |
| Variables                                                                                      | 8                                                 | Maxeigen                                                  | 0                                                     |                                                    |                                           |                                                 |
| Clustering algorithm converged.                                                                |                                                   |                                                           |                                                       |                                                    |                                           |                                                 |
| Number<br>of<br>Clusters                                                                       | Total<br>Variation<br>Explained<br>by<br>Clusters | Proportion<br>of<br>Variation<br>Explained<br>by Clusters | Minimum<br>Proportion<br>Explained<br>by a<br>Cluster | Maximum<br>Second<br>Eigenvalue<br>in a<br>Cluster | Minimum<br>R-squared<br>for a<br>Variable | Maximum<br>1-R**2<br>Ratio<br>for a<br>Variable |
| 1                                                                                              | 4.672880                                          | 0.5841                                                    | 0.5841                                                | 1.770983                                           | 0.3810                                    |                                                 |
| 2                                                                                              | 6.426502                                          | 0.8033                                                    | 0.7293                                                | 0.476418                                           | 0.6329                                    | 0.4380                                          |
| 3                                                                                              | 6.895347                                          | 0.8619                                                    | 0.7954                                                | 0.418369                                           | 0.7421                                    | 0.3634                                          |
| 4                                                                                              | 7.271218                                          | 0.9089                                                    | 0.8773                                                | 0.238000                                           | 0.8652                                    | 0.2548                                          |
| 5                                                                                              | 7.509218                                          | 0.9387                                                    | 0.8773                                                | 0.236135                                           | 0.8652                                    | 0.1665                                          |
| 6                                                                                              | 7.740000                                          | 0.9675                                                    | 0.9295                                                | 0.141000                                           | 0.9295                                    | 0.2560                                          |
| 7                                                                                              | 7.881000                                          | 0.9851                                                    | 0.9405                                                | 0.119000                                           | 0.9405                                    | 0.2093                                          |
| 8                                                                                              | 8.000000                                          | 1.0000                                                    | 1.0000                                                | 0.000000                                           | 1.0000                                    | 0.0000                                          |

The principal component method first separates the variables into the same two clusters that were created in the first PROC VARCLUS run. In creating the third cluster, the principal component method identifies the variable Width. This is the same variable that is put into its own cluster in the preceding centroid method example. The tree diagram in [Output 100.1.4](#) displays the cluster hierarchy.

Output 100.1.4 Dendrogram



It appears from the diagram that there are two, or possibly three, clusters present. However, the MAXC=8 option forces PROC VARCLUS to split the clusters until each variable is in its own cluster.

---

## References

- Anderberg, M. R. (1973), *Cluster Analysis for Applications*, New York: Academic Press.
- Harman, H. H. (1976), *Modern Factor Analysis*, Third Edition, Chicago: University of Chicago Press.
- Harris, C. W. and Kaiser, H. F. (1964), "Oblique Factor Analytic Solutions by Orthogonal Transformation," *Psychometrika*, 32, 363–379.



# Chapter 101

## The VARCOMP Procedure

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## Overview: VARCOMP Procedure

The VARCOMP procedure handles general linear models that have random effects. Random effects are classification effects with levels that are assumed to be randomly selected from an infinite population of possible levels. PROC VARCOMP estimates the contribution of each of the random effects to the variance of the dependent variable.

A single MODEL statement specifies the dependent variables and the effects: main effects, interactions, and nested effects. The effects must be composed of classification variables; no continuous variables are allowed on the right side of the equal sign.

You can specify certain effects as fixed (nonrandom) by putting them first in the **MODEL** statement and indicating the number of fixed effects with the **FIXED=** option. An intercept is always fitted and assumed fixed. Except for the effects specified as fixed, all other effects are assumed to be random. Their contribution to the model can be thought of as an observation from a distribution that is normally and independently distributed.

The dependent variables are grouped based on the similarity of their missing values. Each group of dependent variables is then analyzed separately. The columns of the design matrix **X** are formed in the same order in which the effects are specified in the **MODEL** statement. A singular parameterization involving just 0–1 dummy variables is used, as in the **GLM** procedure.

You can specify four general methods of estimation in the **PROC VARCOMP** statement by using the **METHOD=** option. They are **TYPE1** (based on computation of Type I sum of squares for each effect), **MIVQUE0**, maximum likelihood (**METHOD=ML**), and restricted maximum likelihood (**METHOD=REML**). A fifth method, **METHOD=GRR**, provides a specialized analysis for gauge repeatability and reproducibility (R&R) studies. See the section “[Gauge Repeatability and Reproducibility Analysis](#)” on page 8542 for further details. Note that this method, along with the **CL** option in the **MODEL** statement for confidence limits, applies only to certain designs, namely balanced one-way or two-way designs. The other four general methods apply to any random-effects model and design.

Other procedures, such as **PROC GLM**, **PROC MIXED**, and **PROC GLIMMIX**, fit similar random effects models. The **VARCOMP** procedure is usually more computationally efficient for certain special designs and models. See the section “[Relationship to PROC MIXED](#)” on page 8547 for a more precise comparison with the **MIXED** procedure in particular.

The **GAUGE** application in SAS/QC software provides a graphical interface for computing many of the same statistics as **METHOD=GRR** in **PROC VARCOMP**.

---

## Getting Started: VARCOMP Procedure

---

### Analyzing the Cure Rate of Rubber

This example, using data from Hicks (1973), concerns an experiment to determine the sources of variability in cure rates of rubber. The goal of the experiment was to find out if the different laboratories contributed more to the variance of cure rates than did the different batches of raw materials. This information would be useful in trying to control the cure rate of the final product because it would provide insight into the sources of the variability in cure rates. The rubber used was cured at three temperatures, which were taken to be fixed. Three laboratories were chosen at random, and three different batches of raw material were tested at each combination of temperature and laboratory. The following statements read the data into the SAS data set **Cure**.

```

data Cure;
 input Lab Temp Batch $ Cure @@;
 datalines;
1 145 A 18.6 1 145 A 17.0 1 145 A 18.7 1 145 A 18.7
1 145 B 14.5 1 145 B 15.8 1 145 B 16.5 1 145 B 17.6
1 145 C 21.1 1 145 C 20.8 1 145 C 21.8 1 145 C 21.0
1 155 A 9.5 1 155 A 9.4 1 155 A 9.5 1 155 A 10.0
1 155 B 7.8 1 155 B 8.3 1 155 B 8.9 1 155 B 9.1
1 155 C 11.2 1 155 C 10.0 1 155 C 11.5 1 155 C 11.1
1 165 A 5.4 1 165 A 5.3 1 165 A 5.7 1 165 A 5.3
1 165 B 5.2 1 165 B 4.9 1 165 B 4.3 1 165 B 5.2
1 165 C 6.3 1 165 C 6.4 1 165 C 5.8 1 165 C 5.6
2 145 A 20.0 2 145 A 20.1 2 145 A 19.4 2 145 A 20.0
2 145 B 18.4 2 145 B 18.1 2 145 B 16.5 2 145 B 16.7
2 145 C 22.5 2 145 C 22.7 2 145 C 21.5 2 145 C 21.3
2 155 A 11.4 2 155 A 11.5 2 155 A 11.4 2 155 A 11.5
2 155 B 10.8 2 155 B 11.1 2 155 B 9.5 2 155 B 9.7
2 155 C 13.3 2 155 C 14.0 2 155 C 12.0 2 155 C 11.5
2 165 A 6.8 2 165 A 6.9 2 165 A 6.0 2 165 A 5.7
2 165 B 6.0 2 165 B 6.1 2 165 B 5.0 2 165 B 5.2
2 165 C 7.7 2 165 C 8.0 2 165 C 6.6 2 165 C 6.3
3 145 A 19.7 3 145 A 18.3 3 145 A 16.8 3 145 A 17.1
3 145 B 16.3 3 145 B 16.7 3 145 B 14.4 3 145 B 15.2
3 145 C 22.7 3 145 C 21.9 3 145 C 19.3 3 145 C 19.3
3 155 A 9.3 3 155 A 10.2 3 155 A 9.8 3 155 A 9.5
3 155 B 9.1 3 155 B 9.2 3 155 B 8.0 3 155 B 9.0
3 155 C 11.3 3 155 C 11.0 3 155 C 10.9 3 155 C 11.4
3 165 A 6.7 3 165 A 6.0 3 165 A 5.0 3 165 A 4.8
3 165 B 5.7 3 165 B 5.5 3 165 B 4.6 3 165 B 5.4
3 165 C 6.6 3 165 C 6.5 3 165 C 5.9 3 165 C 5.8
;

```

The variables Lab, Temp, and Batch contain levels of laboratory, temperature, and batch, respectively. The Cure variable contains the response values.

The following SAS statements perform a restricted maximum likelihood variance component analysis.

```

title 'Analyzing the Cure Rate of Rubber';
proc varcomp method=reml data=cure;
 class temp lab batch;
 model cure=temp|lab batch(lab temp) / fixed=1;
run;

```

The FIXED=1 option indicates that the first factor, Temp, is fixed. The effect specification Temp|Lab is equivalent to putting the three terms Temp, Lab, and Temp\*Lab in the model. Batch(Lab Temp) is equivalent to putting Batch(Temp\*Lab) in the MODEL statement. The results of this analysis are displayed in Figure 101.1 through Figure 101.4.



**Figure 101.1** Class Level Information

| Analyzing the Cure Rate of Rubber        |        |             |
|------------------------------------------|--------|-------------|
| Variance Components Estimation Procedure |        |             |
| Class Level Information                  |        |             |
| Class                                    | Levels | Values      |
| Temp                                     | 3      | 145 155 165 |
| Lab                                      | 3      | 1 2 3       |
| Batch                                    | 3      | A B C       |
| Number of Observations Read              |        | 108         |
| Number of Observations Used              |        | 108         |
| Dependent Variable:                      |        | Cure        |

Figure 101.1 provides information about the variables used in the analysis and the number of observations and specifies the dependent variable.

**Figure 101.2** Iteration History

| REML Iterations           |               |              |                |                             |              |  |
|---------------------------|---------------|--------------|----------------|-----------------------------|--------------|--|
| Iteration                 | Objective     | Var (Lab)    | Var (Temp*Lab) | Var (Batch (Temp*<br>Lab) ) | Var (Error)  |  |
| 0                         | 13.4500060254 | 0.5094464340 | 0              | 2.4004888633                | 0.5787185225 |  |
| 1                         | 13.0898262160 | 0.3194348317 | 0              | 2.0869636935                | 0.6016005334 |  |
| 2                         | 13.0893125570 | 0.3176048001 | 0              | 2.0738906134                | 0.6026217204 |  |
| 3                         | 13.0893125555 | 0.3176017115 | 0              | 2.0738685461                | 0.6026234568 |  |
| Convergence criteria met. |               |              |                |                             |              |  |

The “REML Iterations” table in Figure 101.2 displays the iteration history, which includes the value of the objective function associated with REML and the values of the variance components at each iteration.

**Figure 101.3** REML Estimates

| REML Estimates       |          |
|----------------------|----------|
| Variance Component   | Estimate |
| Var(Lab)             | 0.31760  |
| Var(Temp*Lab)        | 0        |
| Var(Batch(Temp*Lab)) | 2.07387  |
| Var(Error)           | 0.60262  |

Figure 101.3 displays the REML estimates of the variance components.

**Figure 101.4** Covariance Matrix for REML Estimates

| Asymptotic Covariance Matrix of Estimates |           |               |
|-------------------------------------------|-----------|---------------|
|                                           | Var(Lab)  | Var(Temp*Lab) |
| Var(Lab)                                  | 0.32452   | 0             |
| Var(Temp*Lab)                             | 0         | 0             |
| Var(Batch(Temp*Lab))                      | -0.04998  | 0             |
| Var(Error)                                | 1.026E-12 | 0             |

| Asymptotic Covariance Matrix of Estimates |                      |            |
|-------------------------------------------|----------------------|------------|
|                                           | Var(Batch(Temp*Lab)) | Var(Error) |
| Var(Lab)                                  | -0.04998             | 1.026E-12  |
| Var(Temp*Lab)                             | 0                    | 0          |
| Var(Batch(Temp*Lab))                      | 0.45042              | -0.0022417 |
| Var(Error)                                | -0.0022417           | 0.0089668  |

The “Asymptotic Covariance Matrix of Estimates” table in Figure 101.4 displays the asymptotic covariance matrix of the REML estimates.

The results of the analysis show that the variance attributable to Batch(Temp\*Lab) (with a variance component of 2.0739) is considerably larger than the variance attributable to Lab (0.3176). Therefore, attempts to reduce the variability of cure rates should concentrate on improving the homogeneity of the batches of raw material used rather than standardizing the practices or equipment within the laboratories. Also, note that since the Batch(Temp\*Lab) variance is considerably larger than the experimental error (Var(Error)=0.6026), the Batch(Temp\*Lab) variability plays an important part in the overall variability of the cure rates.

## Syntax: VARCOMP Procedure

The following statements are available in the VARCOMP procedure:

```
PROC VARCOMP < options > ;
 CLASS variables ;
 MODEL dependent = < effects > < / options > ;
 BY variables ;
```

Only one MODEL statement is allowed. The BY, CLASS, and MODEL statements are described after the PROC VARCOMP statement.

## PROC VARCOMP Statement

```
PROC VARCOMP < options > ;
```

The PROC VARCOMP statement invokes the VARCOMP procedure. Table 101.1 summarizes the options available in the VARCOMP statement.

**Table 101.1** PROC VARCOMP Statement Options

| Option   | Description                                                                    |
|----------|--------------------------------------------------------------------------------|
| DATA=    | Specifies the input SAS data set to use                                        |
| EPSILON= | Specifies the convergence value of the objective function                      |
| MAXITER= | Specifies the maximum number of iterations for METHOD=ML or METHOD=REML        |
| METHOD=  | Specifies which of the five methods to use                                     |
| SEED=    | Specifies an unsigned integer used to start the pseudo-random number generator |

You can specify the following options in the PROC VARCOMP statement.

**DATA=SAS-data-set**

specifies the input SAS data set to use. If this option is omitted, the most recently created SAS data set is used.

**EPSILON=number**

specifies the convergence value of the objective function for METHOD=ML or METHOD=REML. By default, EPSILON=1E-8.

**MAXITER=number**

specifies the maximum number of iterations for METHOD=ML or METHOD=REML. By default, MAXITER=50.

**METHOD=TYPE1 | MIVQUE0 | ML | REML | GRR < (options) >**

specifies which of the five methods (TYPE1, MIVQUE0, ML, REML, or GRR) you want to use. By default, METHOD=MIVQUE0. METHOD=GRR provides a specialized analysis only for certain

designs, whereas the other four methods apply to any random-effects model and design. You can specify the following options in parentheses after METHOD=GRR.

**SPECLIMITS**=(*LSL*,*USL*,<*k*>)

**SL**=(*LSL*,*USL*,<*k*>)

specifies the specification limits for the first random factor, which is regarded as the product being tested in the gauge R&R study. The lower limit (*LSL*) must be smaller than the upper limit (*USL*). The value *k* is optional. The default value is 6, which corresponds to the number of standard deviations between the “natural” tolerance limits containing the middle 99.73% of a normal process. **SPECLIMITS**=(*LSL*,*USL*,*k*) requests the estimates of the parameters **PTR**(*LSL*,*USL*,*k*) and **Cp**(*LSL*,*USL*,*k*) to be displayed.

**RATIO**

specifies that certain additional ratios of variance components should also be computed and displayed, such as proportion of total variance due to the process. These ratios are listed in Table 101.5.

For more information see the section “[Computational Methods](#)” on page 8540.

**SEED**=*n*

specifies an unsigned integer used to start the pseudo-random number generator. If you do not specify a seed or if you specify zero, the seed is generated from reading the time of day from the computer clock. You can use a SAS date as a seed. The random number generation is used in the computation of generalized confidence limits; see the section “[Confidence Limits](#)” on page 8544.

---

## BY Statement

**BY variables ;**

You can specify a BY statement with PROC VARCOMP to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the VARCOMP procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

---

## CLASS Statement

**CLASS** *variables* ;

The CLASS statement specifies the classification variables to be used in the analysis. All effects in the MODEL statement must be composed of effects that appear in the CLASS statement. Classification variables can be either numeric or character; if they are character, only the first 16 characters are used.

Numeric classification variables are not restricted to integers since a variable's format determines the levels. For more information, see the discussion of the FORMAT statement in *SAS Formats and Informats: Reference*.

---

## MODEL Statement

**MODEL** *dependent* = < *effects* > < / *options* > ;

The MODEL statement gives the dependent variables and independent effects. If you specify more than one dependent variable, a separate analysis is performed for each one. The independent effects are limited to main effects, interactions, and nested effects; no continuous effects are allowed. All independent effects must be composed of effects that appear in the CLASS statement. **Effects** are specified in the VARCOMP procedure in the same way as described for the ANOVA procedure. Only one MODEL statement is allowed.

The following options are available in the MODEL statement.

### **FIXED=*n***

specifies that the first *n* effects in the MODEL statement are fixed effects. The remaining effects are assumed to be random. By default, PROC VARCOMP assumes that all effects are random in the model. Keep in mind that if you use bar notation and, for example, specify Y=A|B / FIXED=2, then A\*B is considered a random effect.

### **CL=**

#### **CL=MLS**

#### **CL=GCL**< (*options*) >

specifies that confidence limits for all of the parameters of interest be computed and displayed. It also optionally specifies the method to use for computing the confidence limits. There are two methods: the modified large-sample (MLS) method and the generalized confidence limits (GCL) method. The default method is MLS. For more information about these two methods, see the section “[Confidence Limits](#)” on page 8544.

You can specify the following options in parentheses after CL=GCL.

#### **NSAMPLE=*n***

specifies the sample size for generalized pivot quantities (GPQ) sampling. The default value is 12,605.

#### **EPSILON=*number***

specifies a small positive value used in some GPQ computations. The default value is 0.001.

The CL option applies only to balanced one-way or two-way designs for **METHOD=TYPE1** or **GRR**.

**ALPHA= $\alpha$** 

specifies the level of significance  $\alpha$  for  $(1 - \alpha)100\%$  two-sided confidence limits. The value of  $\alpha$  must be between 0 and 1. By default,  $\alpha$  is equal to 0.05.

---

## Details: VARCOMP Procedure

---

### Missing Values

If an observation has a missing value for any variable used in the independent effects, then the analyses of all dependent variables omit this observation. An observation is deleted from the analysis of a given dependent variable if the observation's value for that dependent variable is missing. Note that a missing value in one dependent variable does not eliminate an observation from the analysis of the other dependent variables.

During processing, PROC VARCOMP groups the dependent variables on their missing values across observations so that sums of squares and crossproducts can be computed in the most efficient manner.

---

### Fixed and Random Effects

Central to the idea of variance components models is the idea of fixed and random effects. Each effect in a variance components model must be classified as either a fixed or a random effect. Fixed effects arise when the levels of an effect constitute the entire population in which you are interested. For example, if a plant scientist is comparing the yields of three varieties of soybeans, then Variety would be a fixed effect, providing that the scientist was concerned about making inferences about only these three varieties of soybeans. Similarly, if an industrial experiment focused on the effectiveness of two brands of a machine, Machine would be a fixed effect only if the experimenter's interest did not go beyond the two machine brands.

On the other hand, an effect is classified as a random effect when you want to make inferences about an entire population, and the levels in your experiment represent only a sample from that population. Psychologists comparing test results between different groups of subjects would consider Subject as a random effect. Depending on the psychologists' particular interest, the Group effect might be either fixed or random. For example, if the groups are based on the sex of the subject, then Sex would be a fixed effect. But if the psychologists are interested in the variability in test scores due to different teachers, then they might choose a random sample of teachers as being representative of the total population of teachers, and Teacher would be a random effect. Note that, in the soybean example presented earlier, if the scientists are interested in making inferences about the entire population of soybean varieties and randomly choose three varieties for testing, then Variety would be a random effect.

If all the effects in a model (except for the intercept) are considered random effects, then the model is called a *random-effects model*; likewise, a model with only fixed effects is called a *fixed-effects model*. The more common case, where some factors are fixed and others are random, is called a *mixed model*. In PROC VARCOMP, by default, effects are assumed to be random. You specify which effects are fixed by using the **FIXED=** option in the **MODEL** statement. In general, if an interaction or nested effect contains any effect that is random, then the interaction or nested effect should be considered a random effect as well.

In the linear model, each level of a fixed effect contributes a fixed amount to the expected value of the dependent variable. What makes a random effect different is that each level of a random effect contributes an amount that is viewed as a sample from a population of normally distributed variables, each with mean 0, and an unknown variance, much like the usual random error term that is a part of all linear models. The estimate of the variance associated with the random effect is known as the *variance component* because it measures the part of the overall variance contributed by that effect. Thus, PROC VARCOMP estimates the variance of the random variables that are associated with the random effects in your model, and the variance components tell you how much each of the random factors contributes to the overall variability in the dependent variable.

---

## Negative Variance Component Estimates

The variance components estimated by PROC VARCOMP should theoretically be nonnegative because they are assumed to represent the variance of a random variable. Nevertheless, when you are using `METHOD=MIVQUE0`, `TYPE1`, or `GRR`, some estimates of variance components might become negative. (Due to the nature of the algorithms used for `METHOD=ML` and `METHOD=REML`, negative estimates are constrained to zero.) These negative estimates might arise for a variety of reasons:

- The variability in your data might be large enough to produce a negative estimate, even though the true value of the variance component is positive.
- Your data might contain outliers. See Hocking (1983) for a graphical technique for detecting outliers in variance components models by using the SAS System.
- A different model for interpreting your data might be appropriate. Under some statistical models for variance components analysis, negative estimates are an indication that observations in your data are negatively correlated. See Hocking (1984) for further information about these models.

Assuming you are satisfied that the model that PROC VARCOMP is using is appropriate for your data, it is common practice to treat negative variance components as if they are zero.

---

## Computational Methods

Four methods of estimation can be specified in the PROC VARCOMP statement by using the `METHOD=` option. They are described in the following sections.

### The Type I Method

This method (`METHOD=TYPE1`) computes the Type I sum of squares for each effect, equates each mean square involving only random effects to its expected value, and solves the resulting system of equations (Gaylor, Lucas, and Anderson 1970). The  $\mathbf{X}'\mathbf{X} | \mathbf{X}'\mathbf{Y}$  matrix is computed and adjusted in segments whenever memory is not sufficient to hold the entire matrix.

## The MIVQUE0 Method

Based on the technique suggested by Hartley, Rao, and LaMotte (1978), the MIVQUE0 method (METHOD=MIVQUE0) produces unbiased estimates that are invariant with respect to the fixed effects of the model and that are locally best quadratic unbiased estimates given that the true ratio of each component to the residual error component is zero. The technique is similar to TYPE1 except that the random effects are adjusted only for the fixed effects. This affords a considerable timing advantage over the TYPE1 method; thus, MIVQUE0 is the default method used in PROC VARCOMP. The  $\mathbf{X}'\mathbf{X}|\mathbf{X}'\mathbf{Y}$  matrix is computed and adjusted in segments whenever memory is not sufficient to hold the entire matrix. Each element  $(i, j)$  of the form

$$\text{SSQ}(\mathbf{X}'_i \mathbf{M} \mathbf{X}_j)$$

is computed, where

$$\mathbf{M} = \mathbf{I} - \mathbf{X}_0(\mathbf{X}'_0 \mathbf{X}_0)^{-1} \mathbf{X}'_0$$

and where  $\mathbf{X}_0$  is part of the design matrix for the fixed effects,  $\mathbf{X}_i$  is part of the design matrix for one of the random effects, and SSQ is an operator that takes the sum of squares of the elements. For more information see Rao (1971, 1972) and Goodnight (1978).

## The Maximum Likelihood Method

The maximum likelihood method (METHOD=ML) computes maximum likelihood estimates of the variance components; see Searle, Casella, and McCulloch (1992). The computing algorithm makes use of the W-transformation developed by Hemmerle and Hartley (1973) and Goodnight and Hemmerle (1979). The procedure uses a Newton-Raphson algorithm, iterating until the log-likelihood objective function converges.

The objective function for METHOD=ML is  $\ln(|\mathbf{V}|) + \mathbf{r}'\mathbf{V}^{-1}\mathbf{r}$ , where

$$\mathbf{V} = \sigma_0^2 \mathbf{I} + \sum_{i=1}^{n_r} \sigma_i^2 \mathbf{X}_i \mathbf{X}'_i$$

and where  $\sigma_0^2$  is the residual variance,  $n_r$  is the number of random effects in the model,  $\sigma_i^2$  represents the variance components,  $\mathbf{X}_i$  is part of the design matrix for one of the random effects, and

$$\mathbf{r} = \mathbf{y} - \mathbf{X}_0(\mathbf{X}'_0 \mathbf{V}^{-1} \mathbf{X}_0)^{-1} \mathbf{X}'_0 \mathbf{V}^{-1} \mathbf{y}$$

is the vector of residuals.

## The Restricted Maximum Likelihood Method

The restricted maximum likelihood method (METHOD=REML) is similar to the maximum likelihood method, but it first separates the likelihood into two parts: one that contains the fixed effects and one that does not (Patterson and Thompson 1971). The procedure uses a Newton-Raphson algorithm, iterating until convergence is reached for the log-likelihood objective function of the portion of the likelihood that does not contain the fixed effects. Using notation from earlier methods, the objective function for METHOD=REML is  $\ln(|\mathbf{V}|) + \mathbf{r}'\mathbf{V}^{-1}\mathbf{r} + \ln(|\mathbf{X}'_0 \mathbf{V}^{-1} \mathbf{X}_0|)$ . See Searle, Casella, and McCulloch (1992) for additional details.



## The GRR Method

Based on the technique suggested by Burdick, Borror, and Montgomery (2005), the GRR method (METHOD=GRR) produces minimum variance unbiased estimators.

---

## Gauge Repeatability and Reproducibility Analysis

In a typical gauge R&R experiment, each operator ( $O_j$ ) makes multiple observations on each of several similar parts ( $P_i$ ) from a monitored process. The statistical model used to describe the response variable is the balanced two-factor crossed random model with interaction

$$y_{ijk} = \mu_y + P_i + O_j + (PO)_{ij} + E_{ijk}$$

where  $i = 1, \dots, p$ ,  $j = 1, \dots, o$ ,  $k = 1, \dots, r$ ,  $\mu_y$  is an unknown constant, and  $P_i$ ,  $O_j$ ,  $(PO)_{ij}$ ,  $E_{ijk}$  are jointly independent normal random variables with means of zero and variances  $\text{Var}(P)$ ,  $\text{Var}(O)$ ,  $\text{Var}(PO)$ , and  $\text{Var}(E)$ , respectively. The corresponding SAS statements are as follows:

```
proc varcomp method=grr;
 class P O;
 model y = P|O;
run;
```

The first random effect in the MODEL statement is assumed to be the “Part” effect and the second is “Operator.”

The ANOVA table for the preceding model is shown in Table 101.2.

**Table 101.2** GRR Analysis of Variance

| Source       | DF               | Mean Square | Expected Mean Square                                |
|--------------|------------------|-------------|-----------------------------------------------------|
| Parts(P)     | $p - 1$          | $S_P^2$     | $\text{Var}(E) + r\text{Var}(PO) + or\text{Var}(P)$ |
| Operators(O) | $o - 1$          | $S_O^2$     | $\text{Var}(E) + r\text{Var}(PO) + pr\text{Var}(O)$ |
| P×O          | $(p - 1)(o - 1)$ | $S_{PO}^2$  | $\text{Var}(E) + r\text{Var}(PO)$                   |
| Error(E)     | $po(r - 1)$      | $S_E^2$     | $\text{Var}(E)$                                     |

The gauge R&R parameters of interest are given in Table 101.3 in terms of  $\text{Var}(P)$ ,  $\text{Var}(O)$ ,  $\text{Var}(PO)$ , and  $\text{Var}(E)$ .

**Table 101.3** Gauge R&R Parameters

| Parameter                                         | Formula                                                     |
|---------------------------------------------------|-------------------------------------------------------------|
| Mean of population of measurements                | $\mu_y = \bar{y}_{...} = \sum_{ijk} y_{ijk} / por$          |
| Variance of the monitored process                 | $\gamma_P = \text{Var}(P)$                                  |
| Variance of the measurement system                | $\gamma_M = \text{Var}(O) + \text{Var}(PO) + \text{Var}(E)$ |
| Total variance of the response variable           | $\gamma_y = \text{Var}(y) = \gamma_P + \gamma_M$            |
| Ratio of process variance to measurement variance | $\gamma_R = \gamma_P / \gamma_M$                            |

**Table 101.3** (continued)

| Parameter                                           | Formula                                                    |
|-----------------------------------------------------|------------------------------------------------------------|
| Proportion of total variance due to the process     | $\rho_P = \gamma_P/\gamma_y = \frac{\gamma_R}{1+\gamma_R}$ |
| Proportion of total variance due to the measurement | $\rho_M = \gamma_M/\gamma_y = 1 - \rho_P$                  |
| Signal-to-noise ratio                               | $\text{SNR} = \sqrt{2} \times \gamma_R$                    |
| Discrimination ratio                                | $\text{DR} = 1 + 2\gamma_R$                                |

For a one-way model,  $\gamma_M = \text{Var}(E)$ , and for a two-way model with no interaction,  $\gamma_M = \text{Var}(O) + \text{Var}(E)$ .

If you use the SPECLIMITS option to give specification limits, the two parameters in Table 101.4 will also be estimated and displayed.

**Table 101.4** Gauge R&R Parameters Related to Specification Limits

| Parameter                    | Formula                                                                               |
|------------------------------|---------------------------------------------------------------------------------------|
| Precision-to-tolerance ratio | $\text{PTR}(\text{LSL}, \text{USL}, k) = k\sqrt{\gamma_M}/(\text{USL} - \text{LSL})$  |
| Process capability ratio     | $\text{Cp}(\text{LSL}, \text{USL}, k) = (\text{USL} - \text{LSL})/(k\sqrt{\gamma_P})$ |

Here, USL and LSL are the specification limits, and the value  $k$  corresponds to the number of standard deviations between the “natural” tolerance limits of a normal process.

If you use the RATIO option, the ratios in Table 101.5 will also be estimated and displayed.

**Table 101.5** Gauge R&R Ratios

| Ratio                                                      | Formula                        |
|------------------------------------------------------------|--------------------------------|
| Ratio of process variance to total variance                | $\text{Var}(P)/\gamma_y$       |
| Ratio of operator variance to total variance               | $\text{Var}(O)/\gamma_y$       |
| Ratio of process by operator variance to total variance    | $\text{Var}(PO)/\gamma_y$      |
| Ratio of process variance to residual variance             | $\text{Var}(P)/\text{Var}(E)$  |
| Ratio of operator variance to residual variance            | $\text{Var}(O)/\text{Var}(E)$  |
| Ratio of process by operator variance to residual variance | $\text{Var}(PO)/\text{Var}(E)$ |

## Confidence Limits

When no exact confidence limits exist, it is common practice to use approximate confidence limits. Two such approximations are the modified large-sample (MLS) method and the generalized confidence limit (GCL) method as discussed in Burdick, Borror, and Montgomery (2005). When analyzing a balanced one-way or two-way design, if you specify the **CL=** option with **METHOD=TYPE1** or **GRR**, the VARCOMP procedure computes confidence limits by using either the MLS method (the default) or the GCL method. Generalized confidence limits are obtained by specifying the **CL=GCL** option in the **MODEL** statement.

### MLS Confidence Limits

The method of MLS confidence limits was first introduced by Graybill and Wang (1980). It starts with approximate large-sample confidence limits; then it modifies the limits to be exact under certain parameter conditions.

For a balanced two-way crossed random model with interaction, formulas for the MLS method are given in Table 101.6. See Burdick, Borror, and Montgomery (2005) for the formulas for one-way or balanced two-way with no interaction models.

Confidence limits for parameters such as variances and their ratios might not contain the corresponding point estimates, because negative confidence bounds are increased to zero.

**Table 101.6** 100(1 –  $\alpha$ )% MLS Confidence Limits

| Parameter  | Lower Bound                              | Upper Bound                              |
|------------|------------------------------------------|------------------------------------------|
| $\mu_y$    | $\bar{y}_{...} - C \sqrt{\frac{K}{por}}$ | $\bar{y}_{...} + C \sqrt{\frac{K}{por}}$ |
| $\gamma_P$ | $\hat{\gamma}_P - \sqrt{V_{LP}}/(or)$    | $\hat{\gamma}_P + \sqrt{V_{UP}}/(or)$    |
| $\gamma_M$ | $\hat{\gamma}_M - \sqrt{V_{LM}}/(pr)$    | $\hat{\gamma}_M + \sqrt{V_{UM}}/(pr)$    |
| $\gamma_y$ | $\hat{\gamma}_y - \sqrt{V_{LT}}/(por)$   | $\hat{\gamma}_y + \sqrt{V_{UT}}/(por)$   |
| $\gamma_R$ | $L_R$                                    | $U_R$                                    |
| $\rho_P$   | $L_R/(1 + L_R)$                          | $U_R/(1 + U_R)$                          |
| $\rho_M$   | $1/(1 + U_R)$                            | $1/(1 + L_R)$                            |

The terms in Table 101.6 are defined as follows:

$$\begin{aligned}
 V_{LP} &= G_1^2 S_P^4 + H_3^2 S_{PO}^4 + G_{13} S_P^2 S_{PO}^2 \\
 V_{UP} &= H_1^2 S_P^4 + G_3^2 S_{PO}^4 + H_{13} S_P^2 S_{PO}^2 \\
 V_{LM} &= G_2^2 S_O^4 + G_3^2 (p-1)^2 S_{PO}^4 + G_4^2 p^2 (r-1)^2 S_E^4 \\
 V_{UM} &= H_2^2 S_O^4 + H_3^2 (p-1)^2 S_{PO}^4 + H_4^2 p^2 (r-1)^2 S_E^4 \\
 V_{LT} &= G_1^2 p^2 S_P^4 + G_2^2 o^2 S_O^4 + G_3^2 (po - p - o)^2 S_{PO}^4 + G_4^2 (po)^2 (r-1)^2 S_E^4 \\
 V_{UT} &= H_1^2 p^2 S_P^4 + H_2^2 o^2 S_O^4 + H_3^2 (po - p - o)^2 S_{PO}^4 + H_4^2 (po)^2 (r-1)^2 S_E^4 \\
 L_R &= \frac{p(1 - G_1)(S_P^2 - F_1 S_{PO}^2)}{po(r-1)S_E^2 + o(1 - G_1)F_3 S_O^2 + o(p-1)S_{PO}^2} \\
 U_R &= \frac{p(1 + H_1)(S_P^2 - F_2 S_{PO}^2)}{po(r-1)S_E^2 + o(1 + H_1)F_4 S_O^2 + o(p-1)S_{PO}^2} \\
 G_1 &= 1 - F_{\alpha/2:\infty,p-1} \\
 G_2 &= 1 - F_{\alpha/2:\infty,o-1} \\
 G_3 &= 1 - F_{\alpha/2:\infty,(p-1)(o-1)} \\
 G_4 &= 1 - F_{\alpha/2:\infty,po(r-1)} \\
 H_1 &= F_{1-\alpha/2:\infty,p-1} - 1 \\
 H_2 &= F_{1-\alpha/2:\infty,o-1} - 1 \\
 H_3 &= F_{1-\alpha/2:\infty,(p-1)(o-1)} - 1 \\
 H_4 &= F_{1-\alpha/2:\infty,po(r-1)} - 1 \\
 F_1 &= F_{1-\alpha/2:p-1,(p-1)(o-1)} \\
 F_2 &= F_{\alpha/2:p-1,(p-1)(o-1)} \\
 F_3 &= F_{1-\alpha/2:p-1,o-1} \\
 F_4 &= F_{\alpha/2:p-1,o-1} \\
 G_{13} &= \frac{(F_1 - 1)^2 - G_1^2 F_1^2 - H_3^2}{F_1} \\
 H_{13} &= \frac{(1 - F_2)^2 - H_1^2 F_2^2 - G_3^2}{F_2} \\
 K &= s_P^2 + s_O^2 - s_{PO}^2 \\
 C &= \frac{s_P^2 \sqrt{F_{1-\alpha:1,p-1}} + s_O^2 \sqrt{F_{1-\alpha:1,o-1}} - s_{PO}^2 \sqrt{F_{1-\alpha:1,(p-1)(o-1)}}}{K}
 \end{aligned}$$

The symbol  $F_{\alpha:df1,df2}$  represents the percentile of an  $F$  distribution with  $df1$  and  $df2$  degrees of freedom and area  $\alpha$  to the left.

## Generalized Confidence Limits

The method of generalized confidence limits was first introduced by Weerahandi (1993). The 100(1- $\alpha$ )% generalized confidence limits are determined as follows:

1. Initialize the random number generator with the seed. The seed value is specified by the `SEED=` option.
2. Sample  $N$  generalized pivot quantities (GPQ), defined to have a distribution that is independent of the parameters under study. The value  $N$  is specified by the `NSAMPLE=` option.
3. Define the lower and upper limits as the  $\alpha/2$  and  $1 - \alpha/2$  quantiles of the sampled GPQ values.

Formulas for generalized confidence limits are given in Table 101.7, where  $Z$  denotes a standard normal random variable and  $W_1$ ,  $W_2$ ,  $W_3$ , and  $W_4$  denote jointly independent chi-square random variables that are independent of  $Z$  with degrees of freedom  $p - 1$ ,  $o - 1$ ,  $(p - 1)(o - 1)$  and  $po(r - 1)$ , respectively. The value of  $\epsilon$  in Table 101.7 is specified by the `EPSILON=` option.

**Table 101.7** 100(1 -  $\alpha$ )% Generalized Confidence Limits

| Parameter  | GPQ                                                                                                                                                  |
|------------|------------------------------------------------------------------------------------------------------------------------------------------------------|
| $\mu_y$    | $\bar{y}_{\dots} - Z \sqrt{\max \left[ \epsilon, \frac{(p-1)s_p^2}{porW_1} + \frac{(o-1)s_o^2}{porW_2} - \frac{(p-1)(o-1)s_{po}^2}{porW_3} \right]}$ |
| $\gamma_P$ | $\max \left[ 0, \frac{(p-1)s_p^2}{orW_1} - \frac{(p-1)(o-1)s_{po}^2}{prW_3} \right]$                                                                 |
| $\gamma_M$ | $\frac{(o-1)s_o^2}{prW_2} + \frac{(p-1)^2(o-1)s_{po}^2}{prW_3} + \frac{po(r-1)^2s_E^2}{rW_4}$                                                        |
| $\gamma_y$ | $\frac{(p-1)s_p^2}{orW_1} + \frac{(o-1)s_o^2}{prW_2} + \frac{(po-p-o)(p-1)(o-1)s_{po}^2}{porW_3} + \frac{po(r-1)^2s_E^2}{rW_4}$                      |
| $\gamma_R$ | $\frac{GPQ(\gamma_P)}{GPQ(\gamma_M)}$                                                                                                                |

In general, the GCL method provides a more accurate confidence interval with a shorter interval width than the MLS method. However, the greater accuracy comes at the cost of being somewhat nondeterministic, because of the reliance on simulation.

## Displayed Output

PROC VARCOMP displays the following items:

- Class Level Information for verifying the levels in your data
- Number of observations read from the data set and number of observations used in the analysis
- for `METHOD=TYPE1`, an analysis-of-variance table with Source, DF, Type I Sum of Squares, Type I Mean Square, and Expected Mean Square, and a table of Type I variance component estimates
- for `METHOD=MIVQUE0`, the SSQ Matrix containing sums of squares of partitions of the  $\mathbf{X}'\mathbf{X}$  crossproducts matrix adjusted for the fixed effects

- for METHOD=ML and METHOD=REML, the iteration history, including the objective function, a table of variance component estimates, and the estimated Asymptotic Covariance Matrix of the variance components
- for METHOD=GRR, an analysis-of-variance table with Source, DF, GRR Sum of Squares, GRR Mean Square, and Expected Mean Square, and a table of GRR parameter estimates. If the CL option is specified, confidence limits for each parameter estimate will also be displayed.

---

## ODS Table Names

PROC VARCOMP assigns a name to each table it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in Table 101.8. For more information about ODS, see Chapter 20, “Using the Output Delivery System.”

**Table 101.8** ODS Tables Produced by PROC VARCOMP

| ODS Table Name    | Description                                  | Statement                      |
|-------------------|----------------------------------------------|--------------------------------|
| ANOVA             | Type 1 analysis of variance                  | METHOD=TYPE1 or GRR            |
| AsyCov            | Asymptotic covariance matrix of estimates    | METHOD=ML or REML              |
| ClassLevels       | Class level information                      | default                        |
| ConvergenceStatus | Convergence status                           | METHOD=ML or REML              |
| DepVar            | Dependent variable                           | METHOD=TYPE1, REML, ML, or GRR |
| DependentInfo     | Dependent variable info (multiple variables) |                                |
| Estimates         | Variance component estimates                 | default                        |
| IterHistory       | Iteration history                            | METHOD=ML or REML              |
| NObs              | Number of observations                       | default                        |
| SSCP              | Sum of squares matrix                        | METHOD=MIVQUE0                 |

In situations where multiple dependent variables are analyzed that differ in their missing value pattern, separate names for ANOVAn, AsyCovn, Estimatesn, IterHistoryn, and SSCPn tables are no longer required. The results are combined into a single output data set. For METHOD=TYPE1, ML, or REML, the variable Dependent in the output data set identifies the dependent variable. For METHOD=MIVQUE0, a variable is added to the output data set for each dependent variable.

---

## Relationship to PROC MIXED

The MIXED procedure effectively performs the same analyzes as PROC VARCOMP and many others, including Type I, Type II, and Type III tests of fixed effects, confidence limits, customized contrasts, and least squares means. Furthermore, continuous variables are permitted as both fixed and random effects in PROC MIXED, and numerous other covariance structures besides variance components are available. The VARCOMP procedure is more computationally efficient for some special designs and models.

To translate PROC VARCOMP code into PROC MIXED code, move all random effects to the RANDOM statement in PROC MIXED. For example, the syntax for the example in the section “Getting Started: VARCOMP Procedure” on page 8532 is as follows:

```
proc mixed;
 class Temp Lab Batch;
 model Cure = Temp;
 random Lab Temp*Lab Batch(Lab Temp);
run;
```

REML is the default estimation method in PROC MIXED, and you can specify other methods by using the METHOD= option.

---

## Examples: VARCOMP Procedure

---

### Example 101.1: Using the Four General Estimation Methods

In this example, a and b are classification variables and y is the dependent variable. a is declared fixed, and b and a\*b are random. Note that this design is unbalanced because the cell sizes are not all the same. PROC VARCOMP is invoked four times, once for each of the general estimation methods. The data are from Hemmerle and Hartley (1973). The following statements produce [Output 101.1.1](#).

```
data a;
 input a b y @@;
 datalines;
1 1 237 1 1 254 1 1 246 1 2 178 1 2 179
2 1 208 2 1 178 2 1 187 2 2 146 2 2 145 2 2 141
3 1 186 3 1 183 3 2 142 3 2 125 3 2 136
;

proc varcomp method=type1 data=a;
 class a b;
 model y=a|b / fixed=1;
run;
```

**Output 101.1.1** VARCOMP Procedure: Method=TYPE1

Variance Components Estimation Procedure

Class Level Information

| Class | Levels | Values |
|-------|--------|--------|
| a     | 3      | 1 2 3  |
| b     | 2      | 1 2    |

**Output 101.1.1** *continued*

|                             |    |                             |             |                                                    |
|-----------------------------|----|-----------------------------|-------------|----------------------------------------------------|
|                             |    | Number of Observations Read | 16          |                                                    |
|                             |    | Number of Observations Used | 16          |                                                    |
| Dependent Variable: y       |    |                             |             |                                                    |
| Type 1 Analysis of Variance |    |                             |             |                                                    |
| Source                      | DF | Sum of Squares              | Mean Square | Expected Mean Square                               |
| a                           | 2  | 11736                       | 5868.218750 | Var(Error) + 2.725 Var(a*b)<br>+ 0.1 Var(b) + Q(a) |
| b                           | 1  | 11448                       | 11448       | Var(Error) + 2.6308 Var(a*b) + 7.8 Var(b)          |
| a*b                         | 2  | 299.041026                  | 149.520513  | Var(Error) + 2.5846 Var(a*b)                       |
| Error                       | 10 | 786.333333                  | 78.633333   | Var(Error)                                         |
| Corrected Total             | 15 | 24270                       |             |                                                    |
| Type 1 Estimates            |    |                             |             |                                                    |
|                             |    | Variance Component          |             | Estimate                                           |
|                             |    | Var(b)                      |             | 1448.4                                             |
|                             |    | Var(a*b)                    |             | 27.42659                                           |
|                             |    | Var(Error)                  |             | 78.63333                                           |

The “Class Level Information” table in [Output 101.1.1](#) displays the levels of each variable specified in the CLASS statement. You can check this table to make sure the data are input correctly.

The Type I analysis of variance in [Output 101.1.1](#) consists of a sequential partition of the total sum of squares. The mean square is the sum of squares divided by the degrees of freedom, and the expected mean square is the expected value of the mean square under the mixed model. The “Q” notation in the expected mean squares refers to a quadratic form in parameters of the parenthesized effect.

The Type I estimates of the variance components in [Output 101.1.1](#) result from solving the linear system of equations established by equating the observed mean squares to their expected values.

The following statements are the same as before, except that the estimation method is MIVQUE0 instead of the default TYPE1. They produce [Output 101.1.2](#).

```
proc varcomp method=mivque0 data=a;
 class a b;
 model y=a|b / fixed=1;
run;
```



**Output 101.1.2** VARCOMP Procedure: Method=MIVQUE0

| Variance Components Estimation Procedure |          |          |          |         |
|------------------------------------------|----------|----------|----------|---------|
| MIVQUE(0) SSQ Matrix                     |          |          |          |         |
| Source                                   | b        | a*b      | Error    | y       |
| b                                        | 60.84000 | 20.52000 | 7.80000  | 89295.4 |
| a*b                                      | 20.52000 | 20.52000 | 7.80000  | 30181.3 |
| Error                                    | 7.80000  | 7.80000  | 13.00000 | 12533.5 |

| MIVQUE(0) Estimates |           |
|---------------------|-----------|
| Variance Component  | y         |
| Var(b)              | 1466.1    |
| Var(a*b)            | -35.49170 |
| Var(Error)          | 105.73660 |

The MIVQUE0 estimates in [Output 101.1.2](#) result from solving the equations established by the MIVQUE0 SSQ matrix. Note that the estimate of the variance component for the interaction effect,  $\text{Var}(a*b)$ , is negative for this example.

The following statements use `METHOD=ML` to invoke maximum likelihood estimation. They produce [Output 101.1.3](#).

```
proc varcomp method=ml data=a;
 class a b;
 model y=a|b / fixed=1;
run;
```

**Output 101.1.3** VARCOMP Procedure: Method=ML

| Variance Components Estimation Procedure |               |                |          |               |
|------------------------------------------|---------------|----------------|----------|---------------|
| Maximum Likelihood Iterations            |               |                |          |               |
| Iteration                                | Objective     | Var(b)         | Var(a*b) | Var(Error)    |
| 0                                        | 78.3850371200 | 1031.49070     | 0        | 74.3909717935 |
| 1                                        | 78.2637043807 | 732.3606453635 | 0        | 77.4011688154 |
| 2                                        | 78.2635471161 | 723.6867470850 | 0        | 77.5301774839 |
| 3                                        | 78.2635471152 | 723.6658365289 | 0        | 77.5304926877 |

Convergence criteria met.

**Output 101.1.3** *continued*

| Maximum Likelihood<br>Estimates |           |
|---------------------------------|-----------|
| Variance<br>Component           | Estimate  |
| Var (b)                         | 723.66584 |
| Var (a*b)                       | 0         |
| Var (Error)                     | 77.53049  |

| Asymptotic Covariance Matrix of Estimates |            |           |             |
|-------------------------------------------|------------|-----------|-------------|
|                                           | Var (b)    | Var (a*b) | Var (Error) |
| Var (b)                                   | 537826.1   | 0         | -107.33905  |
| Var (a*b)                                 | 0          | 0         | 0           |
| Var (Error)                               | -107.33905 | 0         | 858.71104   |

The “Maximum Likelihood Iterations” table in [Output 101.1.3](#) shows that the Newton-Raphson algorithm used by PROC VARCOMP requires three iterations to converge.

The ML estimate of Var(a\*b) is zero for this example, and the other two estimates are smaller than their Type I and MIVQUE0 counterparts.

One benefit of using likelihood-based methods is that an approximate covariance matrix is available from the matrix of second derivatives evaluated at the ML solution. This covariance matrix is valid asymptotically and can be unreliable in small samples.

Here the variance component estimates for B and the Error are negatively correlated, and the elements for Var(a\*b) are set to zero because the estimate equals zero. Also, the very large variance for Var(b) indicates a lot of uncertainty about the estimate for Var(b), and one contributing explanation is that B has only two levels in this data set.

Finally, the following statements use the restricted maximum likelihood (REML) for estimation. They produce [Output 101.1.4](#).

```
proc varcomp method=reml data=a;
 class a b;
 model y=a|b / fixed=1;
run;
```

**Output 101.1.4** VARCOMP Procedure: Method=REML

| Variance Components Estimation Procedure  |               |            |               |               |
|-------------------------------------------|---------------|------------|---------------|---------------|
| REML Iterations                           |               |            |               |               |
| Iteration                                 | Objective     | Var (b)    | Var (a*b)     | Var (Error)   |
| 0                                         | 63.4134144942 | 1269.52701 | 0             | 91.5581191305 |
| 1                                         | 63.0446869787 | 1601.84199 | 32.7632417174 | 76.9355562461 |
| 2                                         | 63.0311530508 | 1468.82932 | 27.2258186561 | 78.7548276319 |
| 3                                         | 63.0311265148 | 1464.33646 | 26.9564053003 | 78.8431476502 |
| 4                                         | 63.0311265127 | 1464.36727 | 26.9588525177 | 78.8423898761 |
| Convergence criteria met.                 |               |            |               |               |
| REML Estimates                            |               |            |               |               |
| Variance Component                        | Estimate      |            |               |               |
| Var (b)                                   | 1464.4        |            |               |               |
| Var (a*b)                                 | 26.95885      |            |               |               |
| Var (Error)                               | 78.84239      |            |               |               |
| Asymptotic Covariance Matrix of Estimates |               |            |               |               |
|                                           | Var (b)       | Var (a*b)  | Var (Error)   |               |
| Var (b)                                   | 4401703.8     | 1.29359    | -273.39651    |               |
| Var (a*b)                                 | 1.29359       | 3559.1     | -502.85157    |               |
| Var (Error)                               | -273.39651    | -502.85157 | 1249.7        |               |

The “REML Iterations” table in [Output 101.1.4](#) shows that the REML optimization requires four iterations to converge.

The REML estimates in [Output 101.1.4](#) are all larger than the corresponding ML estimates (adjusting for potential downward bias) and are fairly similar to the Type I estimates.

The “Asymptotic Covariance Matrix of Estimates” table in [Output 101.1.4](#) shows that the Error variance component estimate is negatively correlated with the other two variance component estimates, and the estimated variances are all larger than their ML counterparts.

---

## Example 101.2: Using the GRR Method

In this example from Houf and Burman (1988), the response variable is the thermal performance of a module measured in Celsius degrees per watt. Each of three operators measures 10 parts three times. It is assumed that parts and operators are selected at random from larger populations. The following statements produce [Output 101.2.1](#).

```

data Houf;
 input a b y @@;
 datalines;
1 1 37 1 1 38 1 1 37
1 2 41 1 2 41 1 2 40
1 3 41 1 3 42 1 3 41
2 1 42 2 1 41 2 1 43
2 2 42 2 2 42 2 2 42
2 3 43 2 3 42 2 3 43
3 1 30 3 1 31 3 1 31
3 2 31 3 2 31 3 2 31
3 3 29 3 3 30 3 3 28
4 1 42 4 1 43 4 1 42
4 2 43 4 2 43 4 2 43
4 3 42 4 3 42 4 3 42
5 1 28 5 1 30 5 1 29
5 2 29 5 2 30 5 2 29
5 3 31 5 3 29 5 3 29
6 1 42 6 1 42 6 1 43
6 2 45 6 2 45 6 2 45
6 3 44 6 3 46 6 3 45
7 1 25 7 1 26 7 1 27
7 2 28 7 2 28 7 2 30
7 3 29 7 3 27 7 3 27
8 1 40 8 1 40 8 1 40
8 2 43 8 2 42 8 2 42
8 3 43 8 3 43 8 3 41
9 1 25 9 1 25 9 1 25
9 2 27 9 2 29 9 2 28
9 3 26 9 3 26 9 3 26
10 1 35 10 1 34 10 1 34
10 2 35 10 2 35 10 2 34
10 3 35 10 3 34 10 3 35
;

proc varcomp data=Houf method=grr (speclimits=(18,58) ratio);
 class a b;
 model y=a|b|c|;
run;

```

You specify **METHOD=GRR** in this example to drive the **VARCOMP** procedure to produce a **gauge repeatability and reproducibility analysis**. With the option **speclimits=(18 58)**, the parameters **PTR** and **Cp** are estimated and displayed. With the **RATIO** option, certain additional ratios of variance components are also estimated and displayed. Finally, the **CL=** option in the **MODEL** statement specifies that estimates of GRR quantities should have the corresponding confidence limits.

**Output 101.2.1** Class Level Information Using Method=GRR

| Variance Components Estimation Procedure |        |        |   |   |   |   |   |   |   |    |    |  |
|------------------------------------------|--------|--------|---|---|---|---|---|---|---|----|----|--|
| Class Level Information                  |        |        |   |   |   |   |   |   |   |    |    |  |
| Class                                    | Levels | Values |   |   |   |   |   |   |   |    |    |  |
| a                                        | 10     | 1      | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9  | 10 |  |
| b                                        | 3      | 1      | 2 | 3 |   |   |   |   |   |    |    |  |
| Number of Observations Read              |        |        |   |   |   |   |   |   |   | 90 |    |  |
| Number of Observations Used              |        |        |   |   |   |   |   |   |   | 90 |    |  |
| Dependent Variable: y                    |        |        |   |   |   |   |   |   |   |    |    |  |

The “Class Level Information” table in [Output 101.2.1](#) displays the levels of each variable specified in the `CLASS` statement.

**Output 101.2.2** Analysis of Variance Using Method=GRR

| GRR Analysis of Variance |    |                |             |
|--------------------------|----|----------------|-------------|
| Source                   | DF | Sum of Squares | Mean Square |
| a                        | 9  | 3935.955556    | 437.328395  |
| b                        | 2  | 39.266667      | 19.633333   |
| a*b                      | 18 | 48.511111      | 2.695062    |
| Error                    | 60 | 30.666667      | 0.511111    |
| Corrected Total          | 89 | 4054.400000    |             |

| GRR Analysis of Variance |                                                                   |
|--------------------------|-------------------------------------------------------------------|
| Source                   | Expected Mean Square                                              |
| a                        | $\text{Var}(\text{Error}) + 3 \text{Var}(a*b) + 9 \text{Var}(a)$  |
| b                        | $\text{Var}(\text{Error}) + 3 \text{Var}(a*b) + 30 \text{Var}(b)$ |
| a*b                      | $\text{Var}(\text{Error}) + 3 \text{Var}(a*b)$                    |
| Error                    | $\text{Var}(\text{Error})$                                        |
| Corrected Total          |                                                                   |

The GRR analysis of variance in [Output 101.2.2](#) is the same as for the Type I analysis when the design is balanced.

Finally, the estimates of the GRR parameters of interest and their confidence limits are displayed in Output 101.2.3.

**Output 101.2.3** Parameter Estimates Using Method=GRR

| GRR Estimates          |          |                       |           |
|------------------------|----------|-----------------------|-----------|
| Parameter              | Estimate | 95% Confidence Limits |           |
| Mu Y                   | 35.80000 | 30.49477              | 41.10523  |
| Var (a)                | 48.29259 | 22.69452              | 161.63918 |
| Var (b)                | 0.56461  | 0.07296               | 25.75077  |
| Var (a*b)              | 0.72798  | 0.33273               | 1.79272   |
| Var (Error)            | 0.51111  | 0.36816               | 0.75754   |
| Gamma Y                | 50.09630 | 24.48844              | 166.22217 |
| Gamma P                | 48.29259 | 22.69452              | 161.63918 |
| Gamma M                | 1.80370  | 1.20623               | 27.01724  |
| Gamma R                | 26.77413 | 1.69168               | 105.60895 |
| SNR                    | 7.31767  | 1.83939               | 14.53334  |
| PTR (18, 58, 6)        | 0.20145  | 0.16474               | 0.77967   |
| Cp (18, 58, 6)         | 0.95933  | 0.52437               | 1.39942   |
| DR                     | 54.54825 | 4.38336               | 212.21791 |
| Rho P                  | 0.96400  | 0.62848               | 0.99062   |
| Rho M                  | 0.03600  | 0.0093801             | 0.37152   |
| Var (a) /Gamma Y       | 0.96400  | 0.62848               | 0.99062   |
| Var (b) /Gamma Y       | 0.01127  | 0.0008700             | 0.34151   |
| Var (a*b) /Gamma Y     | 0.01453  | 0.0027083             | 0.04744   |
| Var (a) /Var (Error)   | 94.48551 | 40.19199              | 327.32469 |
| Var (b) /Var (Error)   | 1.10467  | 0.13662               | 50.37744  |
| Var (a*b) /Var (Error) | 1.42432  | 0.55232               | 3.74691   |

You can draw the following inferences from the results of the analysis. Most of the variation is due to differences between parts because of the relative larger value of Gamma R. The measurement system is nearly inadequate because the PTR exceeds 20%. However, the measurement system is of value in monitoring the process since the SNR is greater than five. See Burdick, Borror, and Montgomery (2003) for more information about interpreting gauge R&R studies.

The confidence limits in Output 101.2.3 are based on large-sample asymptotic approximation. You can alternatively compute more accurate and usually smaller confidence intervals by using CL=GCL for generalized confidence limits. The following statements produce Output 101.2.4:

```
proc varcomp data=Houf method=grr (speclimits=(18,58) ratio) seed=104;
 class a b;
 model y=a|b/cl=gcl;
run;
```

**Output 101.2.4** Generalized Confidence Limits

| Variance Components Estimation Procedure |          |                                   |           |
|------------------------------------------|----------|-----------------------------------|-----------|
| GRR Estimates                            |          |                                   |           |
| Parameter                                | Estimate | 95% Generalized Confidence Limits |           |
| Mu Y                                     | 35.80000 | 30.48351                          | 41.31148  |
| Var (a)                                  | 48.29259 | 22.79316                          | 168.91421 |
| Var (b)                                  | 0.56461  | 0.07157                           | 24.28846  |
| Var (a*b)                                | 0.72798  | 0.33476                           | 1.75806   |
| Var (Error)                              | 0.51111  | 0.36816                           | 0.75754   |
| Gamma Y                                  | 50.09630 | 25.47092                          | 180.85535 |
| Gamma P                                  | 48.29259 | 22.79316                          | 168.91421 |
| Gamma M                                  | 1.80370  | 1.18494                           | 25.76890  |
| Gamma R                                  | 26.77413 | 1.91286                           | 87.60026  |
| SNR                                      | 7.31767  | 1.95594                           | 13.23633  |
| PTR (18, 58, 6)                          | 0.20145  | 0.16328                           | 0.76145   |
| Cp (18, 58, 6)                           | 0.95933  | 0.51295                           | 1.39639   |
| DR                                       | 54.54825 | 4.82572                           | 176.20052 |
| Rho P                                    | 0.96400  | 0.65669                           | 0.98871   |
| Rho M                                    | 0.03600  | 0.01129                           | 0.34331   |
| Var (a) / Gamma Y                        | 0.96400  | 0.65669                           | 0.98871   |
| Var (b) / Gamma Y                        | 0.01127  | 0.0010082                         | 0.32122   |
| Var (a*b) / Gamma Y                      | 0.01453  | 0.0032088                         | 0.04300   |
| Var (a) / Var (Error)                    | 94.48551 | 40.44585                          | 336.50782 |
| Var (b) / Var (Error)                    | 1.10467  | 0.12886                           | 47.19043  |
| Var (a*b) / Var (Error)                  | 1.42432  | 0.55232                           | 3.74691   |

Note that the generalized confidence interval widths from [Output 101.2.4](#) for parameters  $\gamma_R$  and DR are 85.7 and 171.4, respectively. These widths are much shorter than the MLS-based widths, which are 103.9 and 207.8 from [Output 101.2.3](#).

In general, the GCL method provides a more accurate confidence interval with a shorter interval width than the MLS method. However, as discussed in the section “[Generalized Confidence Limits](#)” on page 8546, they are computationally intensive and somewhat nondeterministic, because they are based on an underlying Monte Carlo simulation.

---

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# Chapter 102

## The VARIOGRAM Procedure

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---

## Overview: VARIOGRAM Procedure

The VARIOGRAM procedure computes empirical measures of spatial continuity for two-dimensional spatial data. These measures are a function of the distances between the sample data pairs. When the data are free of nonrandom (or systematic) surface trends, the estimated continuity measures are the empirical semivariance and covariance. The procedure also fits permissible theoretical models to the empirical semivariograms, so that you can use them in subsequent analysis to perform spatial prediction. You can produce plots of the empirical semivariograms in addition to plots of the fitted models. Both isotropic and anisotropic continuity measures are available.

PROC VARIOGRAM also provides the Moran's  $I$  and Geary's  $c$  spatial autocorrelation statistics, in addition to the Moran scatter plot to visualize spatial associations within a specified neighborhood around observations. The procedure produces the OUTVAR=, OUTPAIR=, and OUTDISTANCE= data sets that contain information about the semivariogram analysis. Also, the OUTACWEIGHTS= and the OUTMORAN= output data sets contain information about the autocorrelation analysis.

The VARIOGRAM procedure uses ODS Graphics to create graphs as part of its output. For general information about ODS Graphics, see Chapter 21, “Statistical Graphics Using ODS.” For more information about the graphics available in PROC VARIOGRAM, see the section “ODS Graphics” on page 8647.

---

## Introduction to Spatial Prediction

Many activities in science and technology involve measurements of one or more quantities at given spatial locations, with the goal of predicting the measured quantities at unsampled locations. Application areas include reservoir prediction in mining and petroleum exploration, in addition to modeling in a broad spectrum of fields (for example, environmental health, environmental pollution, natural resources and energy, hydrology, and risk analysis). Often, the unsampled locations are on a regular grid, and the predictions are used to produce surface plots or contour maps.

The preceding tasks fall within the scope of *spatial prediction*, which, in general, is any prediction method that incorporates spatial dependence. The study of these tasks involves naturally occurring uncertainties that cannot be ignored. Stochastic analysis frameworks and methods are often used to account for these uncertainties. Hence, the terms *stochastic spatial prediction* and *stochastic modeling* are also used to characterize this type of analysis.

A popular method of spatial prediction is *ordinary kriging*, which produces both predicted values and associated standard errors. Ordinary kriging requires the complete specification (the form and parameter values) of the spatial dependence that characterizes the spatial process. For this purpose, models for the spatial dependence are expressed in terms of the distance between any two locations in the spatial domain of interest. These models take the form of a covariance or semivariance function.

Spatial prediction, then, involves two steps. First, you model the covariance or semivariance of the spatial process. These measures are typically not known in advance. This step involves computing an empirical estimate, in addition to determining both the mathematical form and the values of any parameters for a theoretical form of the dependence model. Second, you use this dependence model to solve the kriging system at a specified set of spatial points, resulting in predicted values and associated standard errors.

SAS/STAT software has two procedures that correspond to these steps for spatial prediction of two-dimensional data. The VARIOGRAM procedure is used in the first step (that is, calculating and modeling the dependence model), and the KRIGE2D procedure performs the kriging operations to produce the final predictions.

This introduction concludes with a note on terminology. You might commonly encounter the terms *estimation* and *prediction* used interchangeably by experts in different fields; this could be a source of confusion. A precise statistical vernacular uses the term *estimation* to refer to inferences about the value of fixed but unknown parameters, whereas *prediction* concerns inferences about the value of random variables—see, for example, Cressie (1993, p. 106). In light of these definitions, kriging methods are clearly predictive techniques, since they are concerned with making inferences about the value of a spatial random field at observed or unobserved locations. The SAS/STAT suite of procedures for spatial analysis and prediction (VARIOGRAM, KRIGE2D, and SIM2D) follows the statistical vernacular in the use of the terms *estimation* and *prediction*.

---

## Getting Started: VARIOGRAM Procedure

PROC VARIOGRAM uses your data to compute the empirical semivariogram. This computation refers to the steps you take to derive the empirical semivariance from the data, and then to produce the corresponding semivariogram plot.

You can proceed further with the semivariogram analysis if the data are free of systematic trends. In that case, you can use the empirical outcome to determine a theoretical semivariogram model by using the automated methods provided by the VARIOGRAM procedure. The model characterizes the type of theoretical semivariance function you use to describe spatial dependence in your data set.

Graphical displays are requested by enabling ODS Graphics. For general information about ODS Graphics, see Chapter 21, “[Statistical Graphics Using ODS](#).” For specific information about the graphics available in the VARIOGRAM procedure, see the section “[ODS Graphics](#)” on page 8647.

---

## Preliminary Spatial Data Analysis

The following thick data set is available from the Sashelp library. The data set simulates measurements of coal seam thickness (in feet) taken over an approximately square area. The Thick variable has the thickness values in the thick data set. The coordinates are offsets from a point in the southwest corner of the measurement area, with the north and east distances in units of thousands of feet.

```

title 'Spatial Correlation Analysis with PROC VARIOGRAM';

data thick;
 input East North Thick @@;
 label Thick='Coal Seam Thickness';
 datalines;
0.7 59.6 34.1 2.1 82.7 42.2 4.7 75.1 39.5
4.8 52.8 34.3 5.9 67.1 37.0 6.0 35.7 35.9
6.4 33.7 36.4 7.0 46.7 34.6 8.2 40.1 35.4
13.3 0.6 44.7 13.3 68.2 37.8 13.4 31.3 37.8
17.8 6.9 43.9 20.1 66.3 37.7 22.7 87.6 42.8
23.0 93.9 43.6 24.3 73.0 39.3 24.8 15.1 42.3
24.8 26.3 39.7 26.4 58.0 36.9 26.9 65.0 37.8
27.7 83.3 41.8 27.9 90.8 43.3 29.1 47.9 36.7
29.5 89.4 43.0 30.1 6.1 43.6 30.8 12.1 42.8
32.7 40.2 37.5 34.8 8.1 43.3 35.3 32.0 38.8
37.0 70.3 39.2 38.2 77.9 40.7 38.9 23.3 40.5
39.4 82.5 41.4 43.0 4.7 43.3 43.7 7.6 43.1
46.4 84.1 41.5 46.7 10.6 42.6 49.9 22.1 40.7
51.0 88.8 42.0 52.8 68.9 39.3 52.9 32.7 39.2
55.5 92.9 42.2 56.0 1.6 42.7 60.6 75.2 40.1
62.1 26.6 40.1 63.0 12.7 41.8 69.0 75.6 40.1
70.5 83.7 40.9 70.9 11.0 41.7 71.5 29.5 39.8
78.1 45.5 38.7 78.2 9.1 41.7 78.4 20.0 40.8
80.5 55.9 38.7 81.1 51.0 38.6 83.8 7.9 41.6
84.5 11.0 41.5 85.2 67.3 39.4 85.5 73.0 39.8
86.7 70.4 39.6 87.2 55.7 38.8 88.1 0.0 41.6
88.4 12.1 41.3 88.4 99.6 41.2 88.8 82.9 40.5
88.9 6.2 41.5 90.6 7.0 41.5 90.7 49.6 38.9
91.5 55.4 39.0 92.9 46.8 39.1 93.4 70.9 39.7
55.8 50.5 38.1 96.2 84.3 40.3 98.2 58.2 39.5
;

```

It is instructive to see the locations of the measured points in the area where you want to perform spatial prediction. It is desirable to have the sampling locations scattered evenly throughout the prediction area. If the locations are not scattered evenly, the prediction error might be unacceptably large where measurements are sparse.

You can run PROC VARIOGRAM in this preliminary analysis to determine potential problems. In the following statements, the **NOVARIOGRAM** option in the **COMPUTE** statement specifies that only the descriptive summaries and a plot of the raw data be produced.

```
ods graphics on;

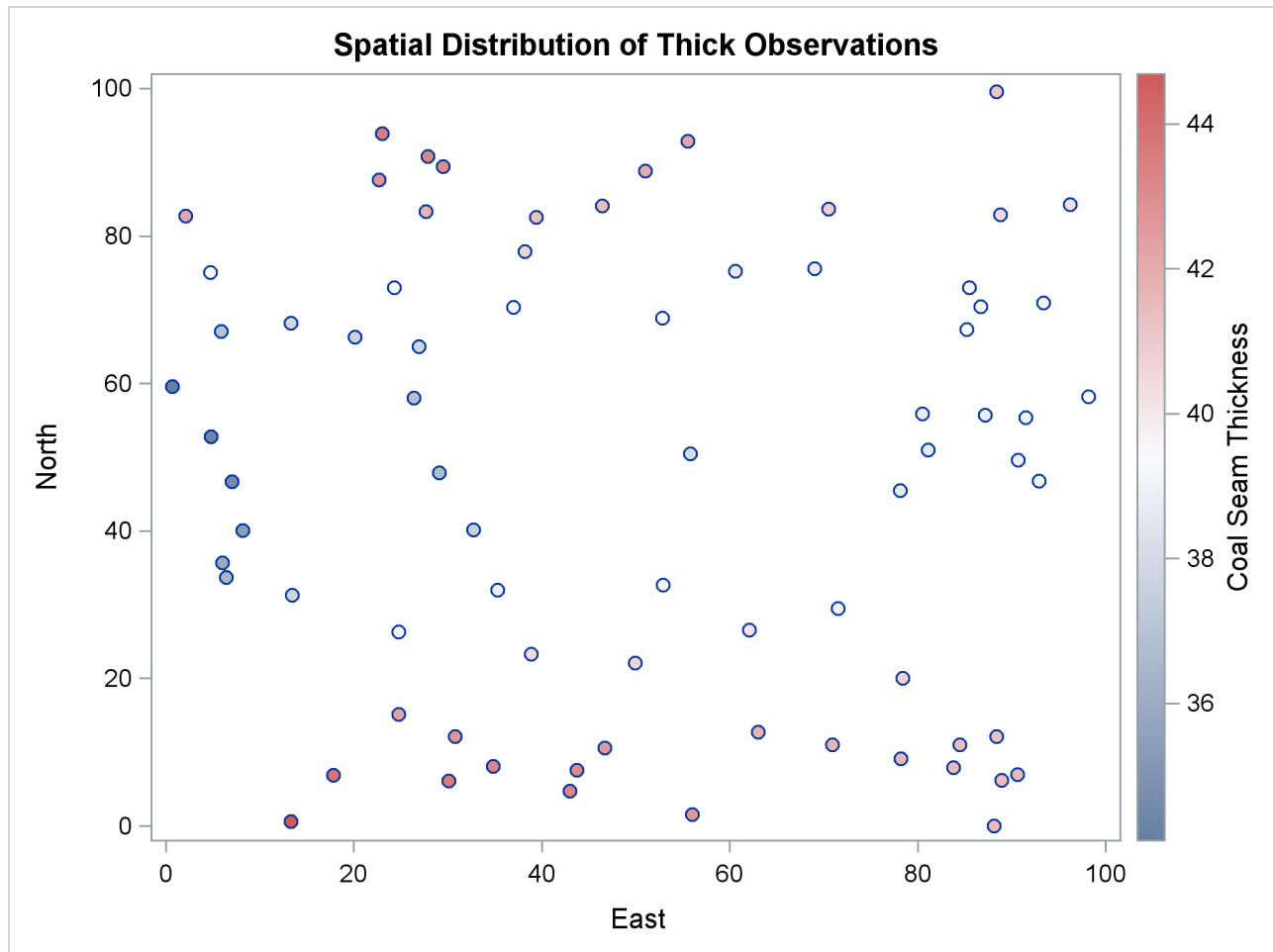
proc variogram data=thick plots=pairs(thr=30);
 compute novariogram nhc=20;
 coordinates xc=East yc=North;
 var Thick;
run;
```

PROC VARIOGRAM produces the table in [Figure 102.1](#) that shows the number of Thick observations read and used. This table provides you with useful information in case you have missing values in the input data.

**Figure 102.1** Number of Observations for the thick Data Set

| Spatial Correlation Analysis with PROC VARIOGRAM |    |
|--------------------------------------------------|----|
| The VARIOGRAM Procedure                          |    |
| Dependent Variable: Thick                        |    |
| Number of Observations Read                      | 75 |
| Number of Observations Used                      | 75 |

Then, the scatter plot of the observed data is produced as shown in [Figure 102.2](#). According to the figure, although the locations are not ideally spread around the prediction area, there are not any extended areas lacking measurements. The same graph also provides the values of the measured variable by using colored markers.

**Figure 102.2** Scatter Plot of the Observations Spatial Distribution

The following is a crucial step. Any obvious surface trend must be removed before you compute the empirical semivariogram and proceed to estimate a model of spatial dependence (the theoretical semivariogram model). You can observe in [Figure 102.2](#) the small-scale variation typical of spatial data, but a first inspection indicates no obvious major systematic trend.

Assuming, therefore, that the data are free of surface trends, you can work with the original thickness rather than residuals obtained from a trend removal process. The following analysis also assumes that the spatial characterization is independent of the direction of the line that connects any two equidistant pairs of data; this is a property known as isotropy. See “[Example 102.2: An Anisotropic Case Study with Surface Trend in the Data](#)” on page 8658 for a more detailed approach to trend analysis and the issue of anisotropy.

Following the previous exploratory analysis, you then need to classify each data pair as a member of a distance interval (lag). PROC VARIOGRAM performs this grouping with two required options for semivariogram computation: the `LAGDISTANCE=` and `MAXLAGS=` options. These options are based on your assessment of how to group the data pairs within distance classes.

The meaning of the required **LAGDISTANCE=** option is as follows. Classify all pairs of points into intervals according to their pairwise distance. The width of each distance interval is the **LAGDISTANCE=** value. The meaning of the required **MAXLAGS=** option is simply the number of intervals you consider. The problem is that given only the scatter plot of the measurement locations, it is not clear what values to give to the **LAGDISTANCE=** and **MAXLAGS=** options.

Ideally, you want a sufficient number of distance classes that capture the extent to which your data are correlated and you want each class to contain a minimum of data pairs to increase the accuracy in your computations. A rule of thumb used in semivariogram computations is that you should have at least 30 pairs per lag class. This is an empirical arbitrary threshold; see the section “Choosing the Size of Classes” on page 8623 for further details.

In the preliminary analysis, you use the option **NHCLASSES=** in the **COMPUTE** statement to help you experiment with these numbers and choose values for the **LAGDISTANCE=** and **MAXLAGS=** options. Here, in particular, you request **NHCLASSES=20** to preview a classification that uses 20 distance classes across your spatial domain. A zero lag class is always considered; therefore the output shows the number of distance classes to be one more than the number you specified.

Based on your selection of the **NHCLASSES=** option, the **NOVARIOGRAM** option produces a pairwise distances table from your observations shown in Figure 102.3, and the corresponding histogram in Figure 102.4. For illustration purposes, you also specify a threshold of minimum data pairs per distance class in the **PAIRS** option as **THR=30**. As a result, a reference line appears in the histogram so that you can visually identify any lag classes with pairs that fall below your specified threshold.

**Figure 102.3** Pairwise Distance Intervals Table

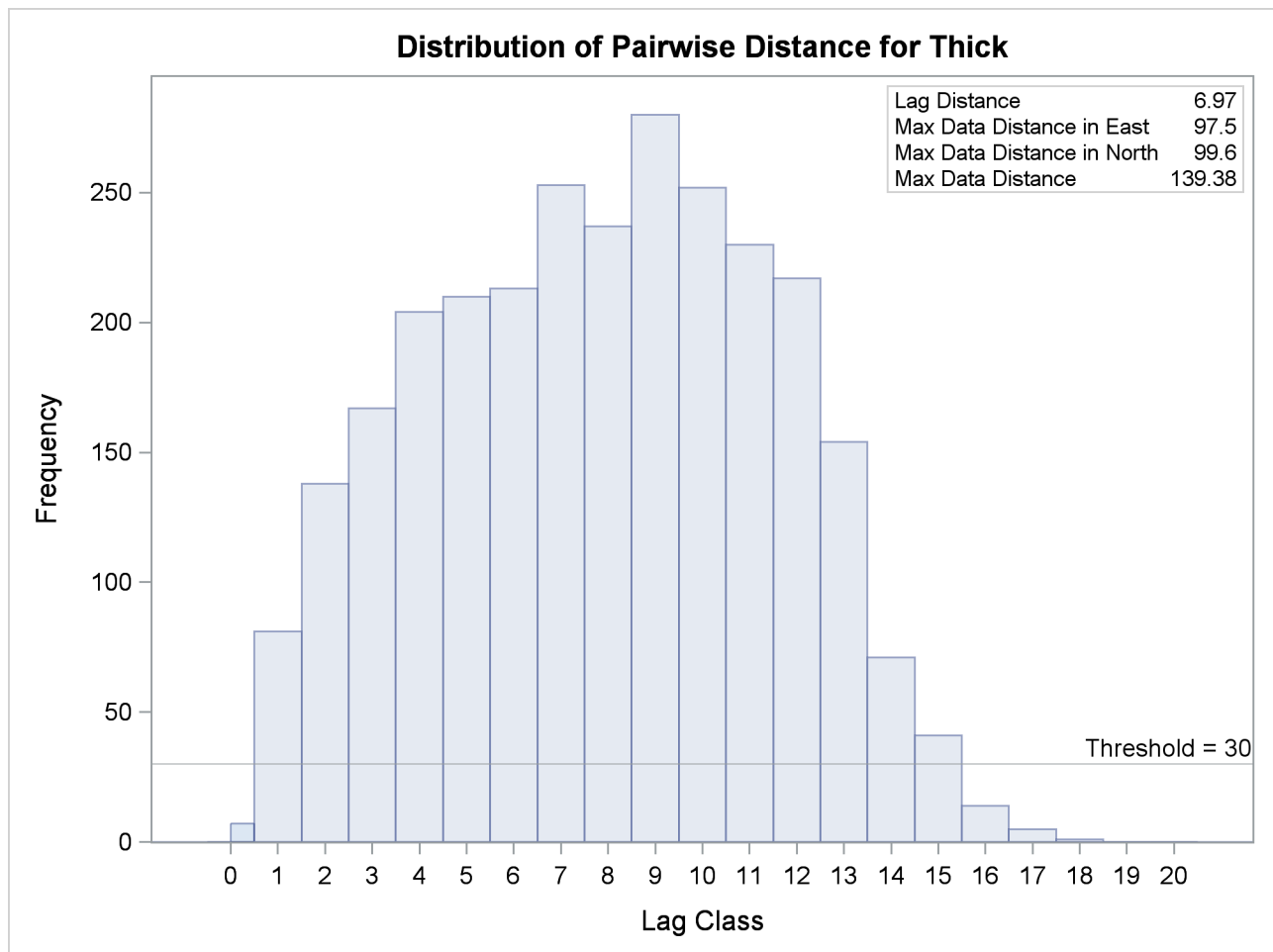
| Pairwise Distance Intervals |                  |        |                 |                     |
|-----------------------------|------------------|--------|-----------------|---------------------|
| Lag Class                   | -----Bounds----- |        | Number of Pairs | Percentage of Pairs |
| 0                           | 0.00             | 3.48   | 7               | 0.25%               |
| 1                           | 3.48             | 10.45  | 81              | 2.92%               |
| 2                           | 10.45            | 17.42  | 138             | 4.97%               |
| 3                           | 17.42            | 24.39  | 167             | 6.02%               |
| 4                           | 24.39            | 31.36  | 204             | 7.35%               |
| 5                           | 31.36            | 38.33  | 210             | 7.57%               |
| 6                           | 38.33            | 45.30  | 213             | 7.68%               |
| 7                           | 45.30            | 52.27  | 253             | 9.12%               |
| 8                           | 52.27            | 59.24  | 237             | 8.54%               |
| 9                           | 59.24            | 66.20  | 280             | 10.09%              |
| 10                          | 66.20            | 73.17  | 252             | 9.08%               |
| 11                          | 73.17            | 80.14  | 230             | 8.29%               |
| 12                          | 80.14            | 87.11  | 217             | 7.82%               |
| 13                          | 87.11            | 94.08  | 154             | 5.55%               |
| 14                          | 94.08            | 101.05 | 71              | 2.56%               |
| 15                          | 101.05           | 108.02 | 41              | 1.48%               |
| 16                          | 108.02           | 114.99 | 14              | 0.50%               |
| 17                          | 114.99           | 121.96 | 5               | 0.18%               |
| 18                          | 121.96           | 128.93 | 1               | 0.04%               |
| 19                          | 128.93           | 135.89 | 0               | 0.00%               |
| 20                          | 135.89           | 142.86 | 0               | 0.00%               |



The **NOVARIOGRAM** option also produces a table with useful facts about the pairs and the distances between the most remote data in selected directions, shown in [Figure 102.5](#). In particular, the lag distance value is calculated based on your selection of the **NHCLASSES=** option. The last three table entries report the overall maximum distance among your data pairs, in addition to the maximum distances in the main axes directions—that is, the vertical (N–S) axis and the horizontal (E–W) axis. This information is also provided in the inset of [Figure 102.4](#). When you specify a threshold in the **PAIRS** suboption of the **PLOTS** option, as in this example, the threshold also appears in the table. Then, the line that follows indicates the highest lag class with the following property: each one of the distance classes that lie farther away from this lag features a pairs population below the specified threshold.

With the preceding information you can determine appropriate values for the **LAGDISTANCE=** and **MAXLAGS=** options in the **COMPUTE** statement. In particular, the classification that uses 20 distance classes is satisfactory, and you can choose **LAGDISTANCE=7** after following the suggestion in [Figure 102.5](#).

**Figure 102.4** Distribution of Pairwise Distances



**Figure 102.5** Pairs Information Table

| Pairs Information                  |        |
|------------------------------------|--------|
| Number of Lags                     | 21     |
| Lag Distance                       | 6.97   |
| Minimum Pairs Threshold            | 30     |
| Highest Lag With Pairs > Threshold | 15     |
| Maximum Data Distance in East      | 97.50  |
| Maximum Data Distance in North     | 99.60  |
| Maximum Data Distance              | 139.38 |

The **MAXLAGS=** option needs to be specified based on the spatial extent to which your data are correlated. Unless you know this size, in the present omnidirectional case you can assume the correlation extent to be roughly equal to half the overall maximum distance between data points.

The table in [Figure 102.5](#) suggests that this number corresponds to 139,380 feet, which is most likely on or close to a diagonal direction (that is, the northeast–southwest or northwest–southeast direction). Hence, you can expect the correlation extent in this scale to be around  $139.4/2 = 69,700$  feet. Consequently, consider lag classes up to this distance for the empirical semivariogram computations. Given your lag size selection, [Figure 102.3](#) indicates that this distance corresponds to about 10 lags; hence you can set **MAXLAGS=10**.

Overall, for a specific **NHCLASSES=** choice of class count, you can expect your choice of **MAXLAGS=** to be approximately half the number of the lag classes (see the section “[Spatial Extent of the Empirical Semivariogram](#)” on page 8624 for more details).

After you have starting values for the **LAGDISTANCE=** and **MAXLAGS=** options, you can run the **VARIOGRAM** procedure multiple times to inspect and compare the results you get by specifying different values for these options.

---

## Empirical Semivariogram Computation

Using the values of **LAGDISTANCE=7** and **MAXLAGS=10** computed previously, rerun **PROC VARIOGRAM** without the **NOVARIOGRAM** option in order to compute the empirical semivariogram. You specify the **CL** option in the **COMPUTE** statement to calculate the 95% confidence limits for the classical semivariance. The section “[COMPUTE Statement](#)” on page 8584 describes how to use the **ALPHA=** option to specify a different confidence level.

Also, you can request a robust version of the semivariance with the **ROBUST** option in the **COMPUTE** statement. **PROC VARIOGRAM** produces a plot that shows both the classical and the robust empirical semivariograms. See the details of the **PLOTS** option to specify different instances of plots of the empirical semivariogram. The following statements implement the preceding requests:

```

proc variogram data=thick outv=outv;
 compute lagd=7 maxlag=10 cl robust;
 coordinates xc=East yc=North;
 var Thick;
run;

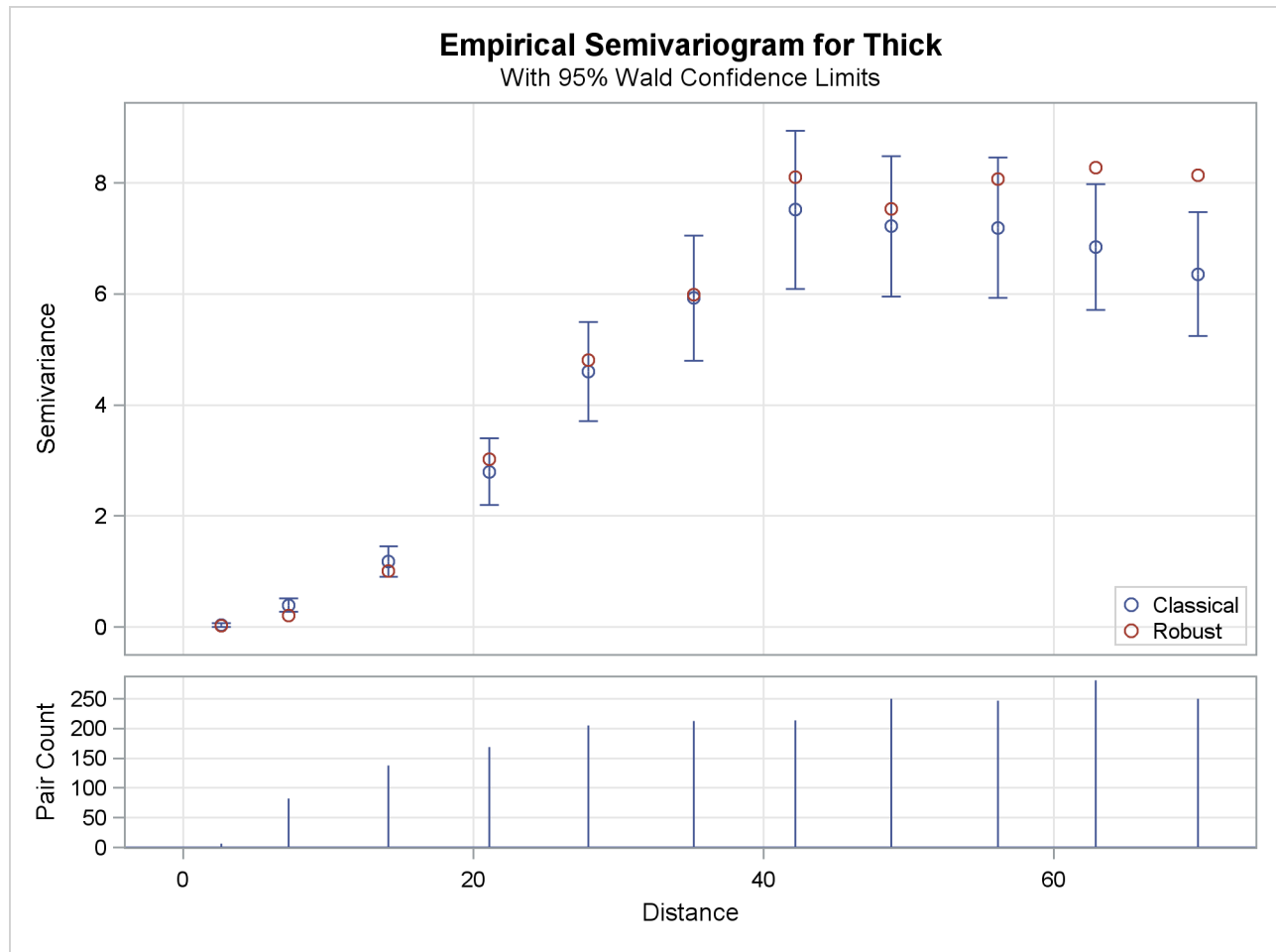
```

Figure 102.6 displays the PROC VARIOGRAM output empirical semivariogram table for the preceding statements. The table displays a total of eleven lag classes, even though you specified `MAXLAGS=10`. The VARIOGRAM procedure always includes a zero lag class in the computations in addition to the `MAXLAGS` classes you request with the `MAXLAGS=` option. Hence, semivariance is actually computed at `MAXLAGS+1` lag classes; see the section “Distance Classification” on page 8619 for more details.

**Figure 102.6** Output Table for the Empirical Semivariogram Analysis

| Spatial Correlation Analysis with PROC VARIOGRAM |            |                  |                        |           |                |       |                       |  |
|--------------------------------------------------|------------|------------------|------------------------|-----------|----------------|-------|-----------------------|--|
| The VARIOGRAM Procedure                          |            |                  |                        |           |                |       |                       |  |
| Dependent Variable: Thick                        |            |                  |                        |           |                |       |                       |  |
| Empirical Semivariogram                          |            |                  |                        |           |                |       |                       |  |
| Lag Class                                        | Pair Count | Average Distance | -----Semivariance----- |           |                |       | 95% Confidence Limits |  |
|                                                  |            |                  | Robust                 | Classical | Standard Error |       |                       |  |
| 0                                                | 7          | 2.64             | 0.028                  | 0.034     | 0.018          | 0     | 0.069                 |  |
| 1                                                | 82         | 7.29             | 0.210                  | 0.394     | 0.061          | 0.273 | 0.514                 |  |
| 2                                                | 138        | 14.16            | 1.008                  | 1.179     | 0.142          | 0.901 | 1.458                 |  |
| 3                                                | 169        | 21.08            | 3.018                  | 2.799     | 0.304          | 2.202 | 3.396                 |  |
| 4                                                | 205        | 27.93            | 4.811                  | 4.602     | 0.455          | 3.711 | 5.493                 |  |
| 5                                                | 213        | 35.17            | 5.990                  | 5.928     | 0.574          | 4.802 | 7.054                 |  |
| 6                                                | 214        | 42.20            | 8.104                  | 7.518     | 0.727          | 6.094 | 8.943                 |  |
| 7                                                | 250        | 48.78            | 7.533                  | 7.221     | 0.646          | 5.955 | 8.487                 |  |
| 8                                                | 247        | 56.16            | 8.066                  | 7.195     | 0.647          | 5.926 | 8.464                 |  |
| 9                                                | 281        | 62.89            | 8.279                  | 6.845     | 0.577          | 5.713 | 7.976                 |  |
| 10                                               | 250        | 69.93            | 8.144                  | 6.358     | 0.569          | 5.243 | 7.472                 |  |

Figure 102.7 shows both the classical and robust empirical semivariograms. In addition, the plot features the approximate 95% confidence limits for the classical semivariance. The figure exhibits a typical behavior of the computed semivariance uncertainty, where in general the variance increases with distance from the origin at `Distance=0`.

**Figure 102.7** Classical and Robust Empirical Semivariograms for Coal Seam Thickness Data

The needle plot in the lower part of the [Figure 102.7](#) provides the number of pairs that were used in the computation of the empirical semivariance for each lag class shown. In general, this is a pairwise distribution that is different from the distribution depicted in [Figure 102.4](#). First, the number of pairs shown in the needle plot depends on the particular criteria you specify in the `COMPUTE` statement of `PROC VARIOGRAM`. Second, the distances shown for each lag on the Distance axis are not the midpoints of the lag classes as in the pairwise distances plot, but rather the average distance from the origin  $\text{Distance}=0$  of all pairs in a given lag class.

## Autocorrelation Analysis

You can use the autocorrelation analysis features of PROC VARIOGRAM to compute the autocorrelation Moran's  $I$  and Geary's  $c$  statistics and to obtain the Moran scatter plot. In the following statements, you ask for the Moran's  $I$  and Geary's  $c$  statistics under the assumption of randomization using binary weights, in addition to the Moran scatter plot:

```
proc variogram data=thick outv=outv plots(only)=moran;
 compute lagd=7 maxlag=10 autocorr(assum=random);
 coordinates xc=East yc=North;
 var Thick;
run;
```

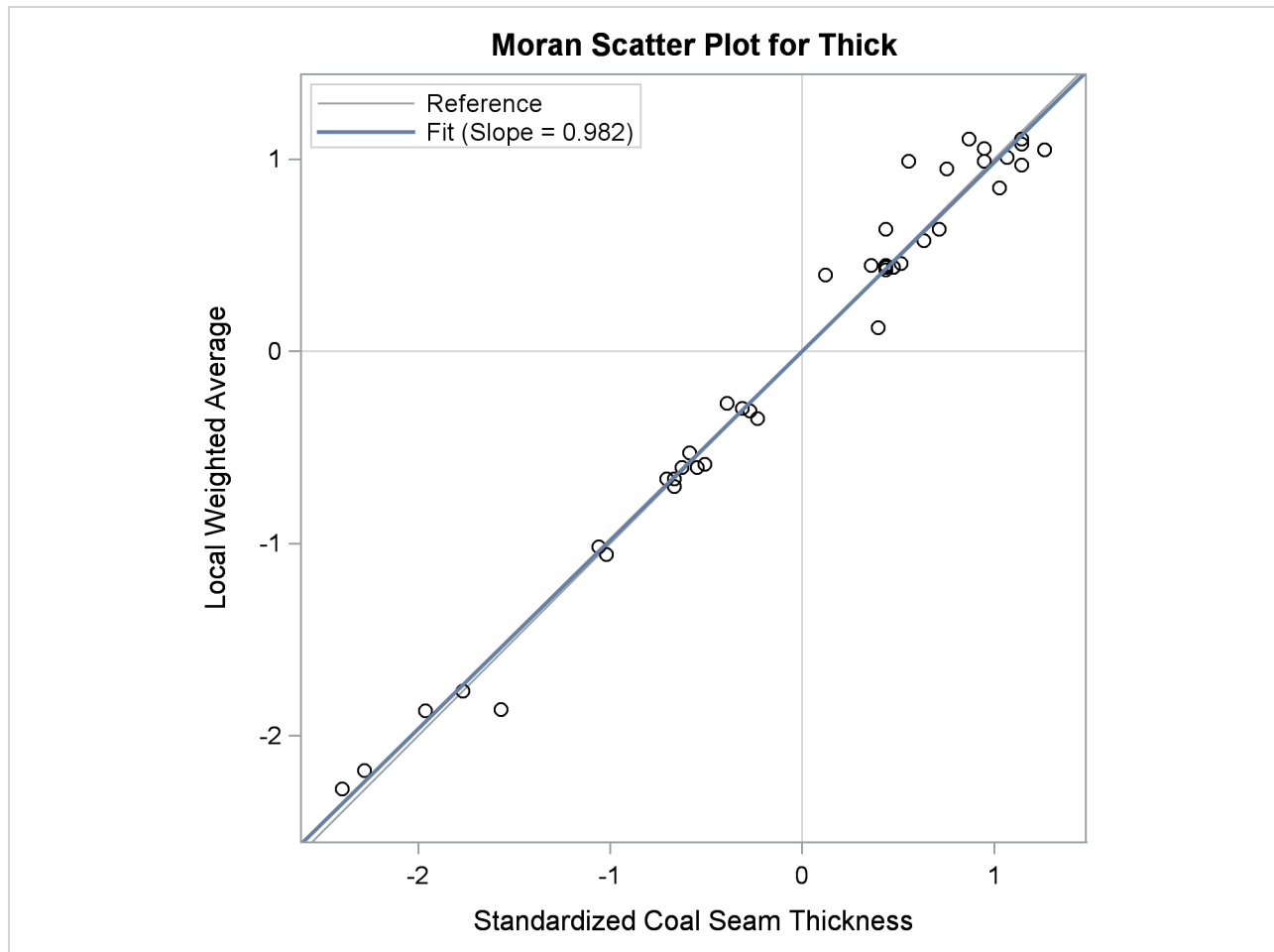
For the autocorrelation analysis with binary weights and the Moran scatter plot, the `LAGDISTANCE=` option indicates that you consider as neighbors of an observation all other observations within the specified distance from it.

Figure 102.8 shows the output from the requested autocorrelation analysis. This includes the observed (computed) Moran's  $I$  and Geary's  $c$  coefficients, the expected value and standard deviation for each coefficient, the corresponding  $Z$  score, and the  $p$ -value in the `Pr > |Z|` column. The low  $p$ -values suggest strong autocorrelation for both statistics types. A two-sided  $p$ -value is reported, which is the probability that the observed coefficient lies farther away from  $|Z|$  on either side of the coefficient's expected value—that is, lower than  $-Z$  or higher than  $Z$ . The sign of  $Z$  for both Moran's  $I$  and Geary's  $c$  coefficients indicates positive autocorrelation in the Thick data values; see the section “Interpretation” on page 8638 for more details.

**Figure 102.8** Output Table for the Autocorrelation Statistics

| Spatial Correlation Analysis with PROC VARIOGRAM |             |          |          |            |       |         |
|--------------------------------------------------|-------------|----------|----------|------------|-------|---------|
| The VARIOGRAM Procedure                          |             |          |          |            |       |         |
| Dependent Variable: Thick                        |             |          |          |            |       |         |
| Autocorrelation Statistics                       |             |          |          |            |       |         |
| Assumption                                       | Coefficient | Observed | Expected | Std<br>Dev | Z     | Pr >  Z |
| Randomization                                    | Moran's I   | 0.9240   | -0.0244  | 0.145      | 6.53  | <.0001  |
| Randomization                                    | Geary's c   | 0.0162   | 1.0000   | 0.175      | -5.62 | <.0001  |

The requested Moran scatter plot is shown in Figure 102.9. The plot includes all nonmissing observations that have neighbors within the specified `LAGDISTANCE=` distance. The horizontal axis displays the standardized Thick values, and the vertical axis displays the corresponding weighted average of their neighbors. The plot data points are concentrated in the upper right and lower left quadrants defined by the lines  $x = 0$  and  $y = 0$ , and clearly around the axes' diagonal reference line  $y = x$  of slope 1. This fact indicates strong positive spatial association in the thick data set observations. Therefore, for each observation its neighbors within the specified `LAGDISTANCE=` distance have overall similar Thick values to that observation. The plot also displays the linear regression slope, whose value is the Moran's  $I$  coefficient when the binary weights are row-averaged. See the section “The Moran Scatter Plot” on page 8639 for more details about the Moran scatter plot.

**Figure 102.9** Moran Scatter Plot for Coal Seam Thickness Data

## Theoretical Semivariogram Model Fitting

PROC VARIOGRAM features automated semivariogram fitting. In particular, the procedure selects a theoretical semivariogram model to fit the empirical semivariance and produces estimates of the model parameters in addition to a fit plot. You have the option to save these estimates in an item store, which is a binary file format that is defined by the SAS System and that you cannot modify. Then, you can retrieve this information at a later point from the item store for future analysis with PROC KRIGE2D or PROC SIM2D.

The coal seam thickness empirical semivariogram in Figure 102.7 shows first a slow, then rapid, rise from the origin. This behavior suggests that you can approximate the empirical semivariance with a Gaussian-type form

$$\gamma_z(h) = c_0 \left[ 1 - \exp\left(-\frac{h^2}{a_0^2}\right) \right]$$

as shown in the section “Theoretical Semivariogram Models” on page 8608. Based on this remark, you choose to fit a Gaussian model to your classical semivariogram. Run PROC VARIOGRAM again and

specify the **MODEL** statement with the **FORM=GAU** option. By default, PROC VARIOGRAM uses the weighted least squares (WLS) method to fit the specified model, although you can explicitly specify the **METHOD=** option to request the fitting method. You want additional information about the estimated parameters, so you specify the **CL** option in the **MODEL** statement to compute their 95% confidence limits and the **COVB** option of the **MODEL** statement to produce a table with their approximate covariances. You also specify the **STORE** statement to save the fitting outcome into an item store file with the name SemivStoreGau and a desired label. You run the following statements:

```
proc variogram data=thick outv=outv;
 store out=SemivStoreGau / label='Thickness Gaussian WLS Fit';
 compute lagd=7 maxlag=10;
 coordinates xc=East yc=North;
 model form=gau cl / covb;
 var Thick;
run;

ods graphics off;
```

After you run the procedure you get a series of output objects from the fitting analysis. In particular, Figure 102.10 shows first a model fitting table with the name and a short label of the model that you requested to use for the fit. The table also displays the name and label of the specified item store.

**Figure 102.10** Semivariogram Model Fitting General Information

| Spatial Correlation Analysis with PROC VARIOGRAM |                            |
|--------------------------------------------------|----------------------------|
| The VARIOGRAM Procedure                          |                            |
| Dependent Variable: Thick                        |                            |
| Angle: Omnidirectional                           |                            |
| Current Model: Gaussian                          |                            |
| Semivariogram Model Fitting                      |                            |
| Name                                             | Gaussian                   |
| Label                                            | Gau                        |
| Output Item Store                                | WORK.SEMIVSTOREGAU         |
| Item Store Label                                 | Thickness Gaussian WLS Fit |

If you specify no parameters, as in the current example, then PROC VARIOGRAM initializes the model parameters for you with default values based on the empirical semivariance; for more details, see the section “Theoretical Semivariogram Model Fitting” on page 8627. The initial values provided by the VARIOGRAM procedure for the Gaussian model are displayed in the table in Figure 102.11.

**Figure 102.11** Semivariogram Fitting Model Information

| Model Information |               |
|-------------------|---------------|
| Parameter         | Initial Value |
| Nugget            | 0             |
| Scale             | 6.7992        |
| Range             | 34.9635       |

Otherwise, in PROC VARIOGRAM you can specify initial values for parameters with the **PARMS** statement. Alternatively, you can specify fixed values for the model scale and range with the **SCALE=** and **RANGE=** options, respectively, in the **MODEL** statement. A nugget effect is always used in model fitting. Unless you explicitly specify a fixed nugget effect with the **NUGGET=** option in the **MODEL** statement or initialize the nugget parameter in the **PARMS** statement, the nugget effect is automatically initialized to zero. See the section “Syntax: VARIOGRAM Procedure” on page 8576 for more details about how the **MODEL** statement and the **PARMS** statement handle model parameters.

The output in Figure 102.12 comes from the optimization process that takes place during the model parameter estimation. The optimizer produces an optimization information table, information about the optimization technique that is used, optimization-related results, and notification about the optimization convergence.

**Figure 102.12** Fitting Optimization Information

| Optimization Information                                         |                   |                          |              |
|------------------------------------------------------------------|-------------------|--------------------------|--------------|
| Optimization Technique                                           | Dual Quasi-Newton |                          |              |
| Parameters in Optimization                                       | 3                 |                          |              |
| Lower Boundaries                                                 | 3                 |                          |              |
| Upper Boundaries                                                 | 0                 |                          |              |
| Starting Values From                                             | PROC              |                          |              |
| Spatial Correlation Analysis with PROC VARIOGRAM                 |                   |                          |              |
| The VARIOGRAM Procedure                                          |                   |                          |              |
| Dependent Variable: Thick                                        |                   |                          |              |
| Angle: Omnidirectional                                           |                   |                          |              |
| Current Model: Gaussian                                          |                   |                          |              |
| Dual Quasi-Newton Optimization                                   |                   |                          |              |
| Dual Broyden - Fletcher - Goldfarb - Shanno Update (DBFGS)       |                   |                          |              |
| Hessian Computed by Finite Differences (Using Analytic Gradient) |                   |                          |              |
| Optimization Results                                             |                   |                          |              |
| Iterations                                                       | 12                | Function Calls           | 45           |
| Gradient Calls                                                   | 0                 | Active Constraints       | 1            |
| Objective Function                                               | 11.433894152      | Max Abs Gradient Element | 3.0128744E-8 |
| Slope of Search Direction                                        | -3.986332E-8      |                          |              |
| Convergence criterion (GCONV=1E-8) satisfied.                    |                   |                          |              |



The fitting process is successful, and the parameters converge to the estimated values shown in Figure 102.13. For each parameter, the same table also displays the approximate standard error, the degrees of freedom, the *t* value, the approximate *p*-value, and the requested 95% confidence limits.

**Figure 102.13** Semivariogram Fitting Parameter Estimates

| Parameter Estimates |          |                     |                                      |         |    |         |                   |
|---------------------|----------|---------------------|--------------------------------------|---------|----|---------|-------------------|
| Parameter           | Estimate | Approx<br>Std Error | Approximate 95%<br>Confidence Limits |         | DF | t Value | Approx<br>Pr >  t |
|                     |          |                     | Lower                                | Upper   |    |         |                   |
| Nugget              | 0        | 0                   | 0                                    | 0       | 8  | .       | .                 |
| Scale               | 7.4599   | 0.2621              | 6.8555                               | 8.0643  | 8  | 28.46   | <.0001            |
| Range               | 30.1111  | 1.1443              | 27.4724                              | 32.7498 | 8  | 26.31   | <.0001            |

The approximate covariance matrix of the estimated parameters is displayed in Figure 102.14.

**Figure 102.14** Approximate Covariance Matrix of Parameter Estimates

| Approximate Covariance Matrix |        |        |        |
|-------------------------------|--------|--------|--------|
| Parameter                     | Nugget | Scale  | Range  |
| Nugget                        | 0.0000 | 0.0000 | 0.0000 |
| Scale                         | 0.0000 | 0.0687 | 0.2326 |
| Range                         | 0.0000 | 0.2326 | 1.3094 |

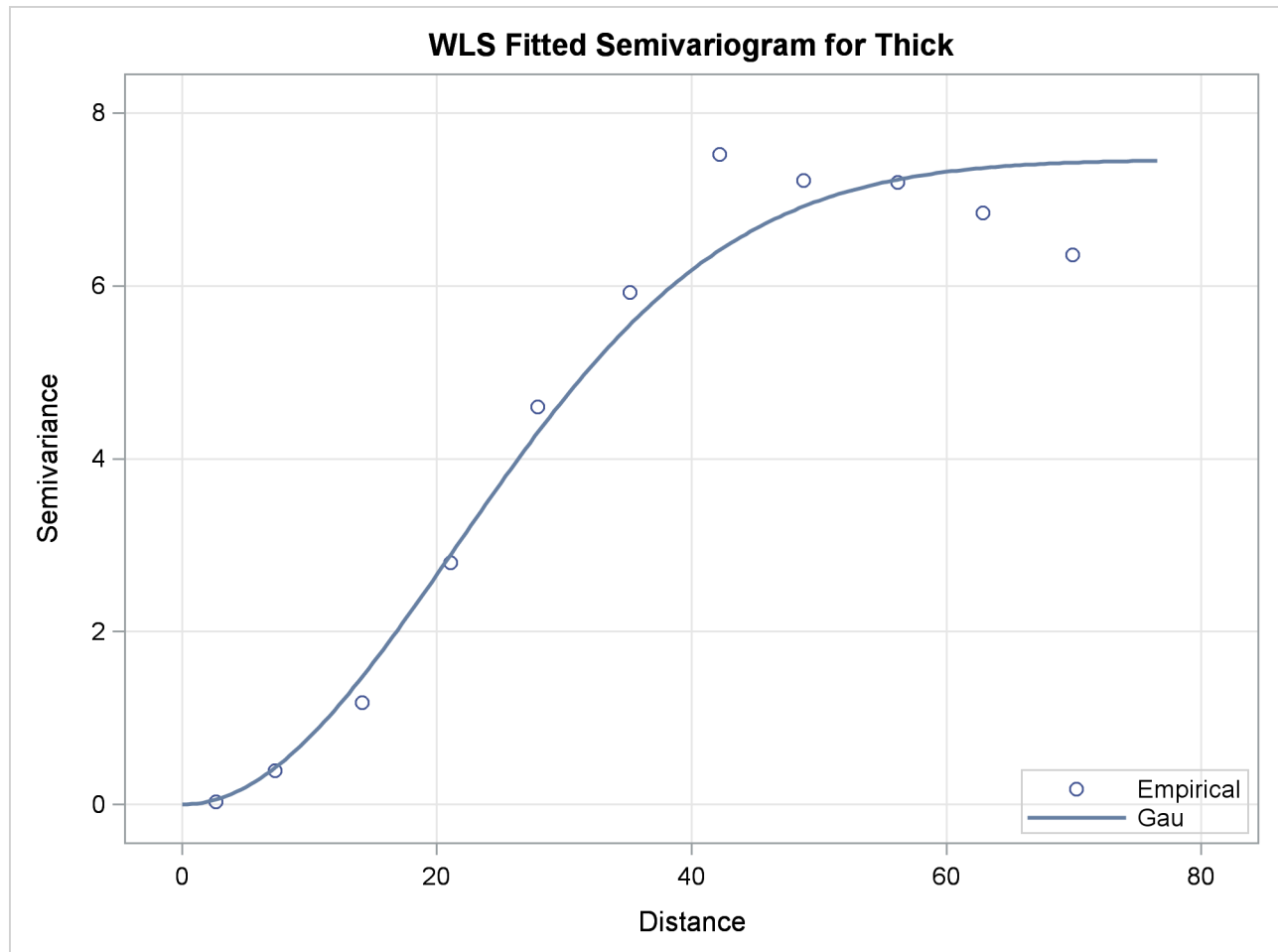
The fitting summary table in Figure 102.15 displays statistics about the quality of the fitting process. In particular, the table shows the weighted error sum of squares in the Weighted SSE column and the Akaike information criterion in the AIC column. See more information about the fitting criteria in section “Quality of Fit” on page 8632.

**Figure 102.15** Semivariogram Model Fitting Summary

| Fit Summary |                 |         |
|-------------|-----------------|---------|
| Model       | Weighted<br>SSE | AIC     |
| Gau         | 11.43389        | 6.42556 |

Figure 102.16 demonstrates the fitted theoretical semivariogram against the empirical semivariance estimates with the weighted least squares method. The fit seems to be more accurate closer to the origin  $h = 0$ , and this is explained as follows: A smaller  $h$  corresponds to smaller semivariance; in turn, this corresponds to smaller semivariance variance, as shown in the section “Theoretical and Computational Details of the Semivariogram” on page 8613. By definition, the WLS optimization weights increase with decreasing variance, which leads to a more accurate fit for smaller distances  $h$  in the WLS fitting results.

**Figure 102.16** Fitted Theoretical and Empirical Semivariogram for Coal Seam Thickness



---

## Syntax: VARIOGRAM Procedure

The following statements are available in the VARIOGRAM procedure:

```

PROC VARIOGRAM options ;
 BY variables ;
 COMPUTE computation-options ;
 COORDINATES coordinate-variables ;
 DIRECTIONS directions-list ;
 ID variable ;
 MODEL model-options ;
 PARMS parameters-list < / parameters-options > ;
 NLOPTIONS < options > ;
 STORE store-options ;
 VAR analysis-variables-list ;

```

The **COMPUTE** and **COORDINATES** statements are required. The **MODEL** and **PARMS** statements are hierarchical. If you specify a **PARMS** statement, it must follow a **MODEL** statement.

---

## PROC VARIOGRAM Statement

```

PROC VARIOGRAM options ;

```

The PROC VARIOGRAM statement invokes the VARIOGRAM procedure. Table 102.1 summarizes the options available in the PROC VARIOGRAM statement.

**Table 102.1** PROC VARIOGRAM Statement Options

| Option               | Description                                                              |
|----------------------|--------------------------------------------------------------------------|
| <b>DATA=</b>         | Specifies the input data set                                             |
| <b>IDGLOBAL</b>      | Labels observations across BY groups using ascending observation numbers |
| <b>IDNUM</b>         | Labels observations using the observation number                         |
| <b>NOPRINT</b>       | Suppresses normal display of results                                     |
| <b>OUTACWEIGHTS=</b> | Specifies a data set to store autocorrelation weights information        |
| <b>OUTDISTANCE=</b>  | Specifies a data set to store summary distance information               |
| <b>OUTMORAN=</b>     | Specifies a data set to store Moran scatter plot information             |
| <b>OUTPAIR=</b>      | Specifies a data set to store pairwise point information                 |
| <b>OUTVAR=</b>       | Specifies a data set to store spatial continuity measures                |
| <b>PLOTS</b>         | Specifies the plot display and options                                   |

You can specify the following options in the PROC VARIOGRAM statement.

**DATA=SAS-data-set**

specifies a SAS data set that contains the *x* and *y* coordinate variables and the VAR statement variables.

**IDGLOBAL**

specifies that ascending observation numbers be used across BY groups for the observation labels in the appropriate output data sets and the **OBSERVATIONS** plot, instead of resetting the observation number in the beginning of each BY group. The IDGLOBAL option is ignored if no BY variables are specified. Also, if you specify the **ID** statement, then the IDGLOBAL option is ignored unless you also specify the IDNUM option in the **PROC VARIOGRAM** statement.

**IDNUM**

specifies that the observation number be used for the observation labels in the appropriate output data sets and the **OBSERVATIONS** plot. The IDNUM option takes effect when you specify the **ID** statement; otherwise, it is ignored.

**NOPRINT**

suppresses the normal display of results. The NOPRINT option is useful when you want only to create one or more output data sets with the procedure.

**NOTE:** This option temporarily disables the Output Delivery System (ODS); see the section “**ODS Graphics**” on page 8647 for more information.

**OUTACWEIGHTS=SAS-data-set****OUTACW=SAS-data-set****OUTA=SAS-data-set**

specifies a SAS data set in which to store the autocorrelation weights information for each pair of points in the DATA= data set. Use this option with caution when the DATA= data set is large. If  $n$  denotes the number of observations in the DATA= data set, then the OUTACWEIGHTS= data set contains  $[n(n - 1)]/2$  observations.

See the section “**OUTACWEIGHTS=SAS-data-set**” on page 8640 for details.

**OUTDISTANCE=SAS-data-set****OUTDIST=SAS-data-set****OUTD=SAS-data-set**

specifies a SAS data set in which to store summary distance information. This data set contains a count of all pairs of data points within a given distance interval. The number of distance intervals is controlled by the **NHCLASSES=** option in the **COMPUTE** statement. The OUTDISTANCE= data set is useful for plotting modified histograms of the count data for determining appropriate lag distances. See the section “**OUTDIST=SAS-data-set**” on page 8641 for details.

**OUTMORAN=SAS-data-set****OUTM=SAS-data-set**

specifies a SAS data set in which to store information that is illustrated in the Moran plot, namely the standardized value of each observation in the DATA= data set and the weighted average of its local neighbors. You must also specify the **LAGDISTANCE=** and **AUTOCORRELATION** options in the **COMPUTE** statement; otherwise, the OUTMORAN= data set request is ignored.

The OUTMORAN= data set is useful when you want to save the information that is illustrated in the Moran scatter plot. The data set can also contain entries of missing observations with neighbors, although these observations are not displayed in the Moran plot. However, if the only observations with neighbors in your input data set are observations with missing values, then the OUTMORAN= output data set is empty.

See the section “**OUTMORAN=SAS-data-set**” on page 8641 for details.

**OUTPAIR=SAS-data-set**

**OUTP=SAS-data-set**

specifies a SAS data set in which to store distance and angle information for each pair of points in the DATA= data set.

Use this option with caution when your DATA= data set is large. Assume that your DATA= data set has  $n$  observations. When you specify the **NOVARIOGRAM** option in the **COMPUTE** statement, the OUTPAIR= data set is populated with all  $[n(n-1)]/2$  pairs that can be formed with the  $n$  observations.

If the **NOVARIOGRAM** option is not specified, then the OUTPAIR= data set contains only pairs of data that are located within a certain distance away from each other. Specifically, it contains pairs whose distance between observations belongs to a lag class up to the specified **MAXLAGS=** option in the **COMPUTE** statement. Then, depending on your specification of the **LAGDISTANCE=** and **MAXLAGS=** options, the OUTPAIR= data set might contain  $[n(n-1)]/2$  or fewer pairs.

Finally, you can restrict the number of pairs in the OUTPAIR= data set with the **OUTPDISTANCE=** option in the **COMPUTE** statement. The **OUTPDISTANCE=** option in the **COMPUTE** statement excludes pairs of points when the distance between the pairs exceeds the **OUTPDISTANCE=** value.

See the section “**OUTPAIR=SAS-data-set**” on page 8642 for details.

**OUTVAR=SAS-data-set**

**OUTVR=SAS-data-set**

specifies a SAS data set in which to store the continuity measures.

See the section “**OUTVAR=SAS-data-set**” on page 8643 for details.

**PLOTS** <(global-plot-options) > <= plot-request <(options) >>

**PLOTS** <(global-plot-options) > <= (plot-request <(options) > <... plot-request <(options) >> >

controls the plots produced through ODS Graphics. When you specify only one plot request, you can omit the parentheses around the plot request. Here are some examples:

```
plots=none
plots=observ
plots=(observ semivar)
plots(unpack)=semivar
plots=(semivar(clea unpack) semivar semivar(rob))
```

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;

proc variogram data=thick;
 compute novariogram;
 coordinates xc=East yc=North;
 var Thick;
run;

ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section “**Enabling and Disabling ODS Graphics**” on page 600 in Chapter 21, “**Statistical Graphics Using ODS.**”

If ODS Graphics is enabled but you omit the PLOTS option or have specified PLOTS=ALL, then PROC VARIOGRAM produces a default set of plots, which might be different for different COMPUTE statement options, as discussed in the following.

- If you specify **NOVARIOGRAM** in the **COMPUTE** statement, the VARIOGRAM procedure produces a scatter plot of your observations spatial distribution, in addition to the histogram of the pairwise distances of your data. For an example of the observations plot, see [Figure 102.2](#). For an example of the pairwise distances plot, see [Figure 102.4](#).
- If you omit **NOVARIOGRAM** in the **COMPUTE** statement, the VARIOGRAM procedure computes the empirical semivariogram for the specified **LAGDISTANCE=** and **MAXLAGS=** options. The observations plot appears by default in this case too. The VARIOGRAM procedure also produces a plot of the classical empirical semivariogram. If you also specify **ROBUST** in the **COMPUTE** statement, then the VARIOGRAM procedure instead produces a plot of both the classical and robust empirical semivariograms, in addition to the observations plot. For an example of the empirical semivariogram plot, see [Output 102.7](#). Moreover, if you specify the **MODEL** statement and perform model fitting, then PROC VARIOGRAM also produces a fit plot of the fitted semivariogram. An example of the fit plot is shown in [Figure 102.16](#).

The following *global-plot-options* are available:

**ONLY**

suppresses the default plots. Only plots that are specifically requested are displayed.

**UNPACKPANEL**

**UNPACK**

suppresses paneling. By default, multiple plots can appear in some output panels. Specify UNPACKPANEL to get each plot in a separate panel. You can specify PLOTS(UNPACKPANEL) to unpack the default plots. You can also specify UNPACKPANEL as a suboption with the SEMIVAR option.

The following individual *plot-requests* and *plot options* are available:

**ALL**

produces all appropriate plots. You can specify other *options* with ALL. For example, to request all default plots and an additional classical empirical semivariogram, specify PLOTS=(ALL SEMIVAR(CLA)).

**EQUATE**

specifies that all appropriate plots be produced in a way that the coordinates of the axes have equal size units.

**FITPLOT** < (*fitplot-options*) >

**FIT** < (*fitplot-options*) >

requests a plot that shows the model fitting results against the empirical semivariogram. By default, FITPLOT displays one plot of the fitted model (or a panel of plots for different angles in the anisotropic case).

If you specify the **FORM=AUTO** option in the **MODEL** statement, then each class of equivalent fitted models is displayed with a different curve on the plot. The best fitting model class is chosen based on the criteria that you specify in the **CHOOSE** option of the **MODEL** statement, and a

thicker line on top of any other curve is shown for it. The plot legend shows the ranked classes by displaying the label of the representative model of each class in the plot. If appropriate, the number of additional models in the same equivalence class also shows within parentheses.

You can specify the following *fitplot-options*:

**NCLASSES=***number*

**NCLASSES=ALL**

specifies the maximum number of classes to display on the fit plot, where *number* is a positive integer. The default is NCLASSES=5 for nonpaneled plots and NCLASSES=3 for paneled plots. The option takes effect when you specify the **FORM=AUTO** option in the **MODEL** statement, and it is ignored when you fit one single model. If you specify NCLASSES=ALL or a larger number than the available classes, then all available classes are shown on the fit plot. If you specify multiple instances of the NCLASSES= option, then only the last specified instance is honored.

**UNPACK**

suppresses paneling in paneled fit plots. By default, fit plots appear in a panel, when appropriate.

**MORAN** < (*moran-options*) >

**MOR** < (*moran-options*) >

produces a Moran scatter plot of the observations with nonmissing values. For more details about this plot, see the section “[The Moran Scatter Plot](#)” on page 8639. In addition to the Moran scatter plot points, the plot also displays the fit line for the linear regression of the weighted average on the standardized observation values, the regression fit line slope, and a reference line with slope equal to 1. The MORAN plot has the following *moran-options*:

**LABEL** < (*label-options*) >

labels the observations. The label is the ID variable if the **ID** statement is specified; otherwise, it is the observation number. The *label-options* can be one or more of the following:

**HH**

specifies that labels show for observations in the upper right (high-high) plot quadrant of positive spatial association.

**HL**

specifies that labels show for observations in the lower right (high-low) plot quadrant of negative spatial association.

**LH**

specifies that labels show for observations in the upper left (low-high) plot quadrant of negative spatial association.

**LL**

specifies that labels show for observations in the lower left (low-low) plot quadrant of positive spatial association.

If you specify multiple instances of the MORAN option and you specify the LABEL suboption in any of those, then the resulting Moran scatter plot displays the observations labels. By default, when you specify none of the *label-options*, the **PLOTS=MORAN(LABEL)** request puts labels in all observations.

**ROWAVG=***rowavg-option*

specifies the flag value for row-averaging of weights in the computation of the weighted average. The *rowavg-option* can be either of the following:

**OFF**

specifies that autocorrelation weights not be row-averaged.

**ON**

specifies that row-averaged autocorrelation weights be used.

The default behavior is ROWAVG=ON. If you specify the ROWAVG= option more than once in the same MORAN plot request, then the behavior is set to ROWAVG=ON unless any of the instances is ROWAVG=OFF.

When you specify the PLOTS=MORAN option, you must specify both the **AUTOCORRELATION** and the **LAGDISTANCE=** options in the **COMPUTE** statement to produce the Moran scatter plot. For more information about the plot, see the section “The Moran Scatter Plot” on page 8639.

**NONE**

suppresses all plots.

**OBSERVATIONS** < (*observations-plot-options*) >**OBSERV** < (*observations-plot-options*) >**OBS** < (*observations-plot-options*) >

produces the observed data plot. Only one observations plot is created if you specify the OBSERVATIONS option more than once within a PLOTS option.

The OBSERVATIONS option has the following suboptions:

**GRADIENT**

specifies that observations be displayed as circles colored by the observed measurement.

**LABEL** < (*label-option*) >

labels the observations. The label is the ID variable if the **ID** statement is specified; otherwise, it is the observation number. The *label-option* can be one of the following:

**EQ=***number*

specifies that labels show for any observation whose value is equal to the specified *number*.

**MAX=***number*

specifies that labels show for observations with values smaller than or equal to the specified *number*.

**MIN=***number*

specifies that labels show for observations with values equal to or greater than the specified *number*.

If you specify multiple instances of the OBSERVATIONS option and you specify the LABEL suboption in any of those, then the resulting observations plot displays the observations labels. If more than one *label-option* is specified in multiple LABEL suboptions, then the prevailing *label-option* in the resulting OBSERVATIONS plot emerges by adhering to the choosing order: MIN, MAX, EQ.



**OUTLINE**

specifies that observations be displayed as circles with a border but with a completely transparent fill.

**OUTLINEGRADIENT**

is the same as OBSERVATIONS(GRADIENT) except that a border is shown around each observation.

**SHOWMISSING**

specifies that observations with missing values be displayed in addition to the observations with nonmissing values. By default, missing values locations are not shown on the plot. If you specify multiple instances of the OBSERVATIONS option and you specify the SHOWMISSING suboption in any of those, then the resulting observations plot displays the observations with missing values.

If you omit any of the GRADIENT, OUTLINE, and OUTLINEGRADIENT suboptions, the OUTLINEGRADIENT is the default suboption. If you specify multiple instances of the OBSERVATIONS option or multiple suboptions for OBSERVATIONS, then the resulting observations plot honors the last specified GRADIENT, OUTLINE, or OUTLINEGRADIENT suboption.

**PAIRS** < (*pairs-plot-options*) >

specifies that the pairwise distances histogram be produced. By default, the horizontal axis displays the lag class number. The vertical axis shows the frequency (count) of pairs in the lag classes. Notice that the zero lag class width is half the width of the other classes.

The PAIRS option has the following suboptions:

**MIDPOINT****MID**

specifies that the plot that is created with the PAIRS option display the lag class midpoint value on the horizontal axis, rather than the default lag class number. The midpoint value is the actual distance of a lag class center from the assumed origin point at distance zero. See also the illustration in [Figure 102.22](#).

**NOINSET****NOI**

specifies that the plot created with the PAIRS option be produced without the default inset that provides additional information about the pairs distribution.

**THRESHOLD**=*minimum pairs***THR**=*minimum pairs*

specifies that a reference line appear in the plot that is created with the PAIRS option to indicate the *minimum pairs* frequency of data pairs. You can use this line as an exploratory tool when you want to select lag classes that contain at least THRESHOLD point pairs. The option helps you to identify visually any portion of the PAIRS distribution that lies below the specified THRESHOLD value.

Only one pairwise distances histogram is created if you specify the PAIRS option within a PLOTS option. If you specify multiple instances of the PAIRS option, the resulting plot has the following features:

- If the MIDPOINT or NOINSET suboption has been specified in any of the instances, it is activated in the resulting plot.
- If you have specified the THRESHOLD= suboption more than once, then the THRESHOLD= value specified last prevails.

**SEMIVARIOGRAM** < (*semivar-plot-options*) >

**SEMIVAR** < (*semivar-plot-options*) >

specifies that the empirical semivariogram plot be produced. You can specify the SEMIVAR option multiple times in the same PLOTS option to request instances of plots with the following *semivar-plot-options*:

**ALL | CLASSICAL | ROBUST**

**ALL | CLA | ROB**

specifies a single type of empirical semivariogram (classical or robust) to plot, or specifies that all the available types be included in the same plot. The default is ALL.

**UNPACKPANEL**

**UNPACK**

specifies that paneled semivariogram plots be displayed separately. By default, plots appear in a panel, when appropriate.

---

## BY Statement

**BY** *variables* ;

You can specify a BY statement with PROC VARIOGRAM to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the VARIOGRAM procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

## COMPUTE Statement

**COMPUTE** *computation-options* ;

The COMPUTE statement provides a number of options that control the computation of the semivariance, the robust semivariance, and the covariance.

Table 102.2 summarizes the options available in the COMPUTE statement.

**Table 102.2** COMPUTE Statement Options

| Option          | Description                                                                                 |
|-----------------|---------------------------------------------------------------------------------------------|
| ALPHA=          | Specifies the confidence level                                                              |
| ANGLETOLERANCE= | Specifies the tolerance                                                                     |
| AUTOCORRELATION | Calculates autocorrelation statistics                                                       |
| BANDWIDTH=      | Specifies the bandwidth                                                                     |
| CL              | Requests confidence limits                                                                  |
| DEPSILON=       | Specifies the distance value for declaring that two distinct points are zero distance apart |
| LAGDISTANCE=    | Specifies the basic distance unit that defines the lags                                     |
| LAGTOLERANCE=   | Specifies the tolerance around the LAGDISTANCE= value                                       |
| MAXLAGS=        | Specifies the maximum number of lag classes to be used                                      |
| NDIRECTIONS=    | Specifies the number of angle classes to be used                                            |
| NHCLASSES=      | Specifies the number of distance classes to be used                                         |
| NOVARIOGRAM     | Prevents the computation of the continuity measures                                         |
| OUTPDISTANCE=   | Specifies the cutoff distance for writing observations to the OUTPAIR= data set             |
| ROBUST          | Calculates a robust version of the semivariance                                             |

### **ALPHA=***number*

specifies a parameter to obtain the confidence level for constructing confidence limits in the classical empirical semivariance estimation. The value of *number* must be in (0, 1), and the confidence level is  $1 - \textit{number}$ . The default is ALPHA=0.05, which corresponds to the default confidence level of 95%. If the CL option is not specified, ALPHA= is ignored.

### **ANGLETOLERANCE=***angle-tolerance*

#### **ANGLETOL=***angle-tolerance*

#### **ATOL=***angle-tolerance*

specifies the tolerance, in degrees, around the angles determined by the NDIRECTIONS= specification. The default is  $180^\circ / (2n_d)$ , where  $n_d$  is the NDIRECTIONS= specification. If you do not specify the NDIRECTIONS= option or the DIRECTIONS statement, ANGLETOLERANCE= is ignored.

See the section “Theoretical and Computational Details of the Semivariogram” on page 8613 for further information.

**AUTOCORRELATION** < (*autocorrelation-options*) >

**AUTOCORR** < (*autocorrelation-options*) >

**AUTOC** < (*autocorrelation-options*) >

specifies that autocorrelation statistics be calculated. You can further specify the following *autocorrelation-options* in parentheses following the AUTOCORRELATION option.

**ASSUMPTION** <= *assumption-options* >

**ASSUM** <= *assumption-options* >

specifies the type of autocorrelation assumption to use. The *assumption-options* can be one of the following:

**NORMALITY | NORMAL | NOR**

specifies use of the normality assumption.

**RANDOMIZATION | RANDOM | RAN**

specifies use of the randomization assumption.

The default is ASSUMPTION=NORMALITY.

**STATISTICS** <= (*stats-options*) >

**STATS** <= (*stats-options*) >

specifies the autocorrelation statistics in detail. The *stats-options* can be one or more of the following:

**ALL**

applies all available types of autoregression statistics.

**GEARY | GEA**

specifies use of the Geary's *c* statistics.

**MORAN | MOR**

specifies use of the Moran's *I* statistics.

The default is STATISTICS=ALL.

**WEIGHTS** <= *weights-options* >

**WEI** <= *weights-options* >

specifies the scheme used for the computation of the autocorrelation weights. You can choose one of the following *weights-options*:

**BINARY** < (*binary-option*) >

specifies that binary weights be used. You also have the following *binary-option*:

**ROWAVERAGING | ROWAVG | ROW**

specifies that asymmetric autocorrelation weights be assigned to data pairs. For each observation, if there are nonzero weights, the ROWAVG option standardizes those weights so that they sum to 1. No row averaging is performed by default.

**DISTANCE** < (*distance-options*) >

specifies that autocorrelation weights be assigned based on the point pair distances. You also have the following *distance-options*:

**NORMALIZE | NORMAL | NOR**

specifies that normalized pair distances be used in the distance-based weights expression. The distances are normalized with respect to the maximum pairwise distance  $h_b$ , as it is defined in the section “[Computation of the Distribution Distance Classes](#)” on page 8621. By default, nonnormalized values are used in the computations.

**POWER=number****POW=number**

specifies the power to which the pair distance is raised in the distance-based weights expression. POWER is a nonnegative number, and its default value is POWER=1.

**ROWAVERAGING | ROWAVG | ROW**

specifies that asymmetric autocorrelation weights be assigned to data pairs. For each observation, if there are nonzero weights, the ROWAVG option standardizes those weights so that they sum to 1. No row averaging is performed by default.

**SCALE=number****SCA=number**

specifies the scaling factor in the distance-based weights expression. SCALE is a nonnegative number, and its default value is SCALE=1.

The default is WEIGHTS=BINARY. See the section “[Autocorrelation Statistics](#)” on page 8635 for further details about the autocorrelation weights.

When you specify the AUTOCORRELATION option with no *autocorrelation-options*, PROC VARIOGRAM computes by default both the Moran’s  $I$  and Geary’s  $c$  statistics with  $p$ -values computed under the normality assumption with binary weights.

If you specify more than one ASSUMPTION in the *autocorrelation-options*, all but the last specified ASSUMPTION are ignored. The same holds if you specify more than one POWER= or SCALE= parameter in the WEIGHT=DISTANCE *distance-options*.

If you specify the WEIGHT=BINARY option in the AUTOCORRELATION option and the NOVARIOGRAM option at the same time, then you must also specify the LAGDISTANCE= option in the COMPUTE statement. See the section “[Autocorrelation Weights](#)” on page 8635 for more information.

**BANDWIDTH=bandwidth-distance****BANDW=bandwidth-distance**

specifies the bandwidth, or perpendicular distance cutoff for determining the angle class for a given pair of points. The distance classes define a series of cylindrically shaped areas, while the angle classes radially cut these cylindrically shaped areas. For a given angle class  $(\theta_1 - \delta\theta_1, \theta_1 + \delta\theta_1)$ , as you proceed out radially, the area encompassed by this angle class becomes larger. The BANDWIDTH= option restricts this area by excluding all points with a perpendicular distance from the line  $\theta = \theta_1$  that is greater than the BANDWIDTH= value. See [Figure 102.23](#) for a visual representation of the bandwidth.

If you omit the `BANDWIDTH=` option, no restriction occurs. If you omit the `NDIRECTIONS=` option or the `DIRECTIONS` statement, `BANDWIDTH=` is ignored.

**CL**

requests confidence limits for the classical semivariance estimate. The lower bound of the confidence limits is always nonnegative, adhering to the behavior of the theoretical semivariance. You can control the confidence level with the `ALPHA=` option.

**DEPSILON=***distance-value*

**DEPS=***distance-value*

specifies the distance value for declaring that two distinct points are zero distance apart. Such pairs, if they occur, cause numeric problems. If you specify `DEPSILON= $\Delta\epsilon$` , then pairs of points  $P_1$  and  $P_2$  for which the distance between them  $|P_1 P_2| < \Delta\epsilon$  are excluded from the continuity measure calculations. The default value of the `DEPSILON=` option is 100 times the machine precision; this product is approximately  $1E-10$  on most computers.

**LAGDISTANCE=***distance-unit*

**LAGDIST=***distance-unit*

**LAGD=***distance-unit*

specifies the basic distance unit that defines the lags. For example, a specification of `LAGDISTANCE= $x$`  results in lag distance classes that are multiples of  $x$ . For a given pair of points  $P_1$  and  $P_2$ , the distance between them, denoted  $|P_1 P_2|$ , is calculated. If  $|P_1 P_2| = x$ , then this pair is in the first lag class. If  $|P_1 P_2| = 2x$ , then this pair is in the second lag class, and so on.

For irregularly spaced data, the pairwise distances are unlikely to fall exactly on multiples of the `LAGDISTANCE=` value. In this case, a distance tolerance of  $\delta x$  accommodates a spread of distances around multiples of  $x$  (the `LAGTOLERANCE=` option specifies the distance tolerance). For example, if  $|P_1 P_2|$  is within  $x \pm \delta x$ , you would place this pair in the first lag class; if  $|P_1 P_2|$  is within  $2x \pm \delta x$ , you would place this pair in the second lag class; and so on.

You can experiment and determine the candidate values for the `LAGDISTANCE=` option by plotting the pairwise distance histogram for different numbers of histogram classes, using the `NHCLASSES=` option.

A `LAGDISTANCE=` value is required for the semivariance and the autocorrelation computations. However, when you specify the `NOVARIOGRAM` option without the `AUTOCORRELATION` option, you need not specify the `LAGDISTANCE=` option.

See the section “Theoretical and Computational Details of the Semivariogram” on page 8613 for more information.

**LAGTOLERANCE=***tolerance-number*

**LAGTOL=***tolerance-number*

**LAGT=***tolerance-number*

specifies the tolerance around the `LAGDISTANCE=` value for grouping distance pairs into lag classes. See the description of the `LAGDISTANCE=` option for information about the use of the `LAGTOLERANCE=` option, and the section “Theoretical and Computational Details of the Semivariogram” on page 8613 for more details.

If you omit the `LAGTOLERANCE=` option, a default value of  $\frac{1}{2}$  times the `LAGDISTANCE=` value is used.

**MAXLAGS**=*number-of-lags*

**MAXLAG**=*number-of-lags*

**MAXL**=*number-of-lags*

specifies the maximum number of lag classes to be used in constructing the continuity measures in addition to a zero lag class; see also the section “[Distance Classification](#)” on page 8619. This option excludes any pair of points  $P_1$  and  $P_2$  for which the distance between them,  $|P_1P_2|$ , exceeds the MAXLAGS= value times the **LAGDISTANCE**= value.

You can determine candidate values for the MAXLAGS= option by plotting or displaying the **OUT-DISTANCE**= data set.

A MAXLAGS= value is required unless you specify the **NOVARIOGRAM** option.

**NDIRECTIONS**=*number-of-directions*

**NDIR**=*number-of-directions*

**ND**=*number-of-directions*

specifies the number of angle classes to use in computing the continuity measures. This option is useful when there is potential anisotropy in the spatial continuity measures. Anisotropy is a field property in which the characterization of spatial continuity depends on the data pair orientation (or angle between the N–S direction and the axis defined by the data pair). Isotropy is the absence of this effect; that is, the description of spatial continuity depends only on the distance between the points, not the angle.

The angle classes formed from the NDIRECTIONS= option start from N–S and proceed clockwise. For example, NDIRECTIONS=3 produces three angle classes. In terms of compass points, these classes are centered at  $0^\circ$  (or its reciprocal,  $180^\circ$ ),  $60^\circ$  (or its reciprocal,  $240^\circ$ ), and  $120^\circ$  (or its reciprocal,  $300^\circ$ ). For irregularly spaced data, the angles between pairs are unlikely to fall exactly in these directions, so an angle tolerance of  $\delta\theta$  is used (the **ANGLETOLERANCE**= option specifies the angle tolerance). If NDIRECTIONS= $n_d$ , the base angle is  $\theta = 180^\circ/n_d$ , and the angle classes are

$$(k\theta - \delta\theta, k\theta + \delta\theta) \quad k = 0, \dots, n_d - 1$$

If you omit the NDIRECTIONS= option, no angles are formed. This is the omnidirectional case where the spatial continuity measures are assumed to be isotropic.

The NDIRECTIONS= option is useful for exploring possible anisotropy. The **DIRECTIONS** statement, described in the section “[DIRECTIONS Statement](#)” on page 8590, provides greater control over the angle classes.

See the section “[Theoretical and Computational Details of the Semivariogram](#)” on page 8613 for more information.

**NHCLASSES**=*number-of-histogram-classes*

**NHCLASS**=*number-of-histogram-classes*

**NHC**=*number-of-histogram-classes*

specifies the number of distance classes to consider in the spatial domain in the exploratory stage of the empirical semivariogram computation. The actual number of classes is one more than the NHCLASSES= value, since a special lag zero class is also computed. The NHCLASSES= option is used to produce the distance intervals table, the histogram of pairwise distances, and the **OUT-DISTANCE**= data set. See the **OUTDISTANCE**= option, the section “[OUTDIST=SAS-data-set](#)”

on page 8641, and the section “Theoretical and Computational Details of the Semivariogram” on page 8613 for more information.

The default value is NHCLASSES=10.

### NOVARIOGRAM

prevents the computation of the continuity measures. This option is useful for preliminary analysis, or when you require only the **OUTDISTANCE=** or **OUTPAIR=** data sets.

**OUTPDISTANCE=***distance-limit*

**OUTPDIST=***distance-limit*

**OUTPD=***distance-limit*

specifies the cutoff distance for writing observations to the **OUTPAIR=** data set. If you specify **OUTPDISTANCE=** $d_{max}$ , the distance  $|P_1P_2|$  between each pair of points  $P_1$  and  $P_2$  is checked against  $d_{max}$ . If  $|P_1P_2| > d_{max}$ , the observation for this pair is not written to the **OUTPAIR=** data set. If you omit the **OUTPDISTANCE=** option, all distinct pairs are written. This option is ignored if you omit the **OUTPAIR=** data set.

### ROBUST

requests that a robust version of the semivariance be calculated in addition to the classical semivariance.

## COORDINATES Statement

**COORDINATES** *coordinate-variables* ;

The following two options give the names of the variables in the **DATA=** data set that contains the values of the  $x$  and  $y$  coordinates of the data.

Only one **COORDINATES** statement is allowed, and it is applied to all the analysis variables. In other words, it is assumed that all the **VAR** variables have the same  $x$  and  $y$  coordinates.

**XCOORD=***(variable-name)*

**XC=***(variable-name)*

**X=***(variable-name)*

gives the name of the variable that contains the  $x$  coordinate of the data in the **DATA=** data set.

**YCOORD=***(variable-name)*

**YC=***(variable-name)*

**Y=***(variable-name)*

gives the name of the variable that contains the  $y$  coordinate of the data in the **DATA=** data set.



---

## DIRECTIONS Statement

**DIRECTIONS** *directions-list* ;

You use the DIRECTIONS statement to define angle classes. You can specify angle classes as a list of angles, separated by commas, with optional angle tolerances and bandwidths within parentheses following the angle. You must specify at least one angle.

If you do not specify the optional angle tolerance, the default value of  $45^\circ$  is used. If you do not specify the optional bandwidth, no bandwidth is checked. If you specify a bandwidth, you must also specify an angle tolerance.

For example, suppose you want to compute three separate semivariograms at angles  $\theta_1 = 0^\circ$ ,  $\theta_2 = 60^\circ$ , and  $\theta_3 = 120^\circ$ , with corresponding angle tolerances  $\delta\theta_1 = 22.5^\circ$ ,  $\delta\theta_2 = 12.5^\circ$ , and  $\delta\theta_3 = 22.5^\circ$ , with bandwidths 50 and 40 distance units on the first two angle classes and no bandwidth check on the last angle class.

The appropriate DIRECTIONS statement is as follows:

```
directions 0.0(22.5,50), 60.0(12.5,40),120(22.5);
```

---

## ID Statement

**ID** *variable* ;

The ID statement specifies which variable to include for identification of the observations in the **OUTPAIR=** and the **OUTACWEIGHTS=** output data sets. The ID statement variable is also used for the labels and tool tips in the **OBSERVATIONS** plot.

In the VARIOGRAM procedure you can specify only one ID variable in the ID statement. If no ID statement is given, then PROC VARIOGRAM uses the observation number in the data sets and the **OBSERVATIONS** plot.

---

## MODEL Statement

**MODEL** *fitting-options* </ *model-options* > ;

You specify the MODEL statement if you want to fit a theoretical semivariogram model to the empirical semivariogram data that are produced in the **COMPUTE** statement. You must have nonmissing empirical semivariogram estimates at a minimum of three lags to perform model fitting.

Table 102.3 summarizes the options available in the MODEL statement.

**Table 102.3** MODEL Statement Options

| Option                 | Description                                                          |
|------------------------|----------------------------------------------------------------------|
| <b>Fitting Options</b> |                                                                      |
| ALPHA=                 | Specifies confidence level                                           |
| CHOOSE=                | Ranks the fitted models and chooses the optimally fit model          |
| CL                     | Constructs a <i>t</i> -type confidence interval                      |
| EQUIVTOL=              | Specifies a positive upper value tolerance                           |
| FIT=                   | Specifies which type of empirical semivariogram to fit               |
| FORM=                  | Specifies the functional form (type) of the semivariogram model      |
| MDATA=                 | Specifies the input data set                                         |
| METHOD=                | Fits a theoretical model to the empirical semivariance               |
| NEPSILON=              | Adds a minimal nugget effect                                         |
| NUGGET=                | Specifies the nugget effect                                          |
| RANGE=                 | Specifies the range parameter                                        |
| RANGELAG=              | Uses consecutive nonmissing empirical semivariance lags to fit model |
| RANKEPS=               | Specifies the minimum threshold to compare fit quality               |
| SCALE=                 | Specifies the scale parameter in semivariogram models                |
| SMOOTH=                | Specifies the positive smoothness parameter $\nu$                    |
| <b>Model Options</b>   |                                                                      |
| COVB                   | Requests the covariance matrix                                       |
| CORRB                  | Requests the approximate correlation matrix                          |
| DETAILS                | Produces different levels of output                                  |
| GRADIENT               | Displays the gradient of the objective function                      |
| MTOGTOL=               | Specifies a threshold value for the smoothness parameter             |
| NOFIT                  | Suppresses the model fitting process                                 |
| NOITPRINT              | Suppresses the display of the iteration history table                |

You can choose to perform a fully automated fitting or to fit one model with specific forms. In the first case you simply specify a list of forms or no forms at all. All suitable combinations are tested, and the result is the model that produces the best fit according to specified criteria. In the second case you specify one theoretical semivariogram model, and you have more control over its parameters for the fitting process.

Furthermore, you can specify a theoretical semivariogram model in two ways:

- You explicitly specify the **FORM** option and any of the options **SCALE**, **RANGE**, and **NUGGET** in the MODEL statement.
- You can specify an **MDATA=** data set. This data set contains variables that correspond to the **FORM** option and to any of the options **SCALE**, **RANGE**, **NUGGET**, and **SMOOTH**. You can also use an **MDATA=** data set to request a fully automated fitting.

The two methods are exclusive; either you specify all parameters explicitly, or they all are read from the **MDATA=** data set.

The MODEL statement has the following *fitting-options*:

**ALPHA=number**

requests that a *t*-type confidence interval be constructed for each of the fitting parameters with confidence level  $1 - \text{number}$ . The value of *number* must be in (0, 1); the default is 0.05 which corresponds to the default confidence level of 95%. If the CL option of the MODEL statement is not specified, then ALPHA= is ignored.

**CHOOSE=criterion**

**CHOOSE=(criterion1 ... criterionk)**

specifies that if the fitting task has more than one model to fit, then PROC VARIOGRAM ranks the fitted models and chooses the optimally fit model according to one or more available criteria.

If you want to use multiple fitting criteria, then the order in which you specify them in the CHOOSE= option defines how they are applied. This feature is useful when fitting suggests that two or more models perform equally well according to a certain criterion. For example, if two models are equivalent according to *criterion<sub>i</sub>*, then they are further ranked in the list based on the next criterion, *criterion<sub>j</sub>*, where  $j = i + 1$ .

Each *criterion* can be one of the following:

**AIC**

specifies Akaike's information criterion.

**SSE**

specifies the weighted sum of squares error for each fitted model when METHOD=WLS, and the residual sum of squares error for each fitted model when METHOD=OLS.

**STATUS**

classifies models based on their fitting process convergence status. CHOOSE=STATUS places on top models for which the fitting process is successful.

By default, the models are ranked in the fit summary table with the best fitted model at the top of the list, based on the criteria that you specify in the CHOOSE= option. This model is the fit choice of PROC VARIOGRAM for the particular fitting task. If you omit the CHOOSE= option, then the default behavior is CHOOSE=(SSE AIC).

Regardless of the specified fitting criteria, models for which the fitting process is unsuccessful always appear at the bottom of the fit summary table. For more details about the fitting criteria, see the section "Fitting Criteria" on page 8632. After multiple models are ranked, they are further categorized in classes of equivalence depending on whether any two models calculate the same semivariance value at the same distance for a series of different distances. For more details, see the section "Classes of Equivalence" on page 8634.

If you specify the same criterion multiple times in the CHOOSE= option, then only the first instance is used for the ranking process and any additional ones are ignored. If you specify only one model to fit in the MODEL statement and you specify the CHOOSE= option, then the option is ignored.

**CL**

requests that *t*-type confidence limits be constructed for each of the fitting parameters estimates. The confidence level is 0.95 by default; this can be changed with the **ALPHA=** option of the **MODEL** statement.

**EQUIVTOL=***etol-value***ETOL=***etol-value*

specifies a positive upper value tolerance to use when categorizing multiple models in classes of equivalence. For this categorization, the VARIOGRAM procedure computes the sum of absolute differences of semivariances for pairs of consecutively ranked models. If the sum is lower than the EQUIVTOL= value for any such model pair, then these two models are deemed to be equivalent. As a result, the EQUIVTOL= option can affect the number and size of classes of equivalence in the fit summary table. Smaller values of the EQUIVTOL= parameter result in a more strict model comparison and can lead to a higher number of classes of equivalence. For more details, see the section “Classes of Equivalence” on page 8634.

The default value for the EQUIVTOL= parameter is  $10^{-3}$ . The EQUIVTOL= option applies when you fit multiple models with the **FORM=AUTO** option of the **MODEL** statement; otherwise, it is ignored.

The EQUIVTOL= option is independent of the ranking results from the **RANKEPS=** option of the **MODEL** statement. This means that you could possibly have models listed but not ranked in the fit summary table, and still have equivalence classes assigned according to the order in which the models appear in the table.

**FIT=***fit-type-options*

specifies which type of empirical semivariogram to fit. You can choose between the following *fit-type-options*:

**CLASSICAL****CLA**

fits a model for the classical empirical semivariance.

**ROBUST****ROB**

fits a model for the robust empirical semivariance. This option can be used only when the **ROBUST** option is specified in the **COMPUTE** statement.

The default value is **FIT=CLASSICAL**.

**FORM=***form***FORM=**(*form1*, ..., *formk*)**FORM=AUTO** (*auto-options*)

specifies the functional form (type) of the semivariogram model. The supported structures are two-parameter models that use the sill and range as parameters. The Matérn model is an exception that makes use of a third smoothing parameter  $\nu$ .

The `FORM=` option is required when you specify the `MODEL` statement. You can perform fitting of a theoretical semivariogram model either explicitly or in an automated manner. For the explicit specification you specify suitable model forms in the `FORM=` option. For an automated fit you specify the `FORM=AUTO` option which has the `AUTO(MLIST=)` and `AUTO(NEST=)` suboptions. You can read more details in the following two subsections.

### Explicit Model Specification

You can explicitly specify a theoretical semivariogram model to fit by using any combination of one, two, or three forms. Use the syntax with the single *form* to specify a non-nested model. Use the syntax with *k* structures *form<sub>i</sub>*,  $i = 1, \dots, k$ , to specify up to three nested structures ( $k \leq 3$ ) in a semivariogram model. Each of the forms can be any of the following:

**CUBIC | EXPONENTIAL | GAUSSIAN | MATERN |  
PENTASPHERICAL | POWER | SINEHOLEEFFECT | SPHERICAL  
CUB | EXP | GAU | MAT | PEN | POW | SHE | SPH**  
specify a form.

All of these forms are presented in more detail in the section “Theoretical Semivariogram Models” on page 8608. In addition, you can optionally specify a nugget effect for your model with the `NUGGET` option in the `MODEL` statement.

For example, the syntax

**FORM=GAU**

specifies a model with a single Gaussian structure. Also, the syntax

**FORM= (EXP , SHE , MAT)**

specifies a nested model with an exponential, a sine hole effect, and a Matérn structure. Finally

**FORM= (EXP , EXP)**

specifies a nested model with two structures both of which are exponential.

**NOTE:** In the documentation, models are named either by using their full names or by using the first three letters of their structures. Also, the names of different structures in a nested model are separated by a hyphen (-). According to this convention, the previous examples illustrate how to specify a GAU, an EXP-SHE-MAT, and an EXP-EXP model, respectively, with the `FORM=` option.

When you explicitly specify the types of structures, you can fix parameter values or ask PROC VARIOGRAM to select default initial values for the forms parameters by using the `SCALE`, `RANGE`, `NUGGET`, and `SMOOTH` options. You can set your own, non-default initial parameter values by using the `PARMS` statement in combination with an explicitly specified semivariogram model in the `MODEL` statement.

### Automated Model Selection

Use the `FORM=AUTO` option to request the highest level of automation in the best fit selection of the parameters. If you specify `FORM=AUTO`, any of the `SCALE`, `RANGE`, or `SMOOTH` options that are also specified are ignored. When you specify the `FORM=AUTO` option, you cannot specify the `PARMS`

statement for the corresponding **MODEL** statement. As a result, when you use the **FORM=AUTO** option, you cannot fix any of the model parameters and **PROC VARIOGRAM** sets initial values for them.

The **AUTO** option has the following *auto-options*:

**MLIST=***mform*

**MLIST=**(*mform1*, . . . , *mformp*)

specifies one or more different model forms to use in combinations during the model fitting process. If you omit the **MLIST=** suboption, then combinations are made among all available model types. The *mform* can be any of the following eight forms:

**CUBIC | EXPONENTIAL | GAUSSIAN | MATERN |  
PENTASPHERICAL | POWER | SINEHOLEEFFECT | SPHERICAL  
CUB | EXP | GAU | MAT | PEN | POW | SHE | SPH**

specify a form.

If you use more than one *mform*, then each *mform<sub>i</sub>*,  $i = 1, \dots, p$  must be different from the others in the group of  $p \leq 8$  forms that you specify.

**NEST=***nest-list*

specifies the number of nested structures to use for the fitting. You can choose between the following to specify the *nest-list*:

*n*                      a single value

*m* TO *n*                a sequence in which *m* equals the starting value and *n* equals the ending value

For example,

**NEST=1**

produces the best fit with one single model among all model types specified in the **MLIST=** suboption. Also,

**NEST=2 TO 3**

produces the best fit among all combinations of the model types specified in the **MLIST=** suboption that result in nested models with two or three structures. The combinations that are tested include repetitions. Hence, if you specify, for example,

**MODEL FORM=AUTO (MLIST=(EXP, SPH) NEST=1 TO 2)**

then the different models that are tested are equivalent to the specifications **FORM=EXP**, **FORM=SPH**, **FORM=(EXP,EXP)**, **FORM=(EXP,SPH)**, **FORM=(SPH,SPH)** and **FORM=(SPH,EXP)**. **NOTE:** The models **EXP-SPH** and **SPH-EXP** are taken as two separate models. Although they are mathematically equivalent (see the section “[Nested Models](#)” on page 8613), **PROC VARIOGRAM** assigns different initial values to the model structures in each case, which can lead to different fitting results. (See the section “[Example 102.1: Aspects of Semivariogram Model Fitting](#)” on page 8648.)

If you omit the NEST suboption, then by default PROC VARIOGRAM searches for the best fit with up to three nested structures in a model. The default behavior is equivalent to

```
NEST=1 TO 3
```

In the VARIOGRAM procedure you can use a maximum of three nested structures to fit an empirical semivariogram; that is,  $n \leq 3$ .

You can use the AUTO value for the form in the MDATA= data set, and also in the FORM= option. However, in the former case the automation functionality is limited compared to the latter case and the *auto-options* of the FORM=AUTO option. In particular, when you specify the form to be AUTO in the MDATA= data set, then PROC VARIOGRAM follows only the default behavior and searches among all available forms for the best fit with up to three nested structures in a model.

#### **MDATA=SAS-data-set**

specifies the input data set that contains parameter values for the covariance or semivariogram model. The MDATA= data set must contain a variable named FORM, and it can optionally include any of the variables SCALE, RANGE, NUGGET, and SMOOTH.

The FORM variable must be a character variable. It accepts only the AUTO value or the *form* values that can be specified in the FORM= option in the MODEL statement. The RANGE, SCALE, NUGGET, and SMOOTH variables must be numeric or missing.

The number of observations present in the MDATA= data set corresponds to the level of nesting of the semivariogram model. Each observation line describes a structure of the model you submit for fitting.

If you specify the AUTO value for the FORM variable in an observation, then you cannot specify additional nested structures in the same data set, and any parameters you specify in the same structure are ignored. In that case, PROC VARIOGRAM performs a crude automated search among all available forms to obtain the best fit with up to three nested structures in a model. You can refine this type of search with additional suboptions when you perform it with the FORM=AUTO option instead of the MDATA= option in the MODEL statement.

When you have a nested model, you might want to specify parameter values for only some of the nested structures. In this case, you must specify the corresponding parameter values for the remaining model structures as missing values.

For example, you can use the following DATA step to specify a non-nested model that uses a spherical covariance within an MDATA= data set:

```
data mdl;
 input scale range form $;
 datalines;
25 10 SPH
;
```

Then, you can use the `md1` data in the **MODEL** statement of PROC VARIOGRAM as shown in the following statements:

```
proc variogram data=...;
 compute ...;
 model mdata=md1;
run;
```

This is equivalent to the following explicit specification of the semivariance model parameters:

```
proc variogram data=...;
 compute ...;
 model form=sph scale=25 range=10;
run;
```

The following data set `md2` is an example of a nested model:

```
data md2;
 input form $ scale range nugget smooth;
 datalines;
SPH 20 8 5 .
MAT 12 3 5 0.7
GAU . 1 5 .
;
```

This specification is equivalent to the following explicit specification of the semivariance model parameters:

```
proc variogram data=...;
 compute;
 model form=(sph,mat,gau)
 scale=(20,12,.) range=(8,3,1) smooth=0.7 nugget=5;
run;
```

Use the **SMOOTH** variable column in the `MDATA=` data set to specify the smoothing parameter  $\nu$  in the Matérn semivariogram models. The **SMOOTH** variable values must be positive and no greater than 1,000,000. PROC VARIOGRAM sets this upper limit for numerical and performance reasons. In any case, if the fitting process leads the smoothness value to exceed the default threshold value 10,000, then the VARIOGRAM procedure converts the Matérn form into a Gaussian form and repeats the model fitting. To adjust the switching threshold value, you can use the **MTOGTOL=** option in the **MODEL** statement.

If you specify a **SMOOTH** column in the `MDATA=` data set, then its elements are ignored except for the rows in which the corresponding **FORM** is Matérn.

The **NUGGET** variable value is the same for all nested structures. This is the way to specify a nugget effect in the `MDATA=` data set. If you specify more than one nugget value for different structures, then the last nugget value specified is used.



**METHOD=***method-options*

must be specified in the MODEL statement to fit a theoretical model to the empirical semivariance. The METHOD option has the following suboptions:

**OLS**

specifies that ordinary least squares be used for the fitting.

**WLS**

specifies that weighted least squares be used for the fitting.

The default is METHOD=WLS.

**NEPSILON=***min-nugget-factor***NEPS=***min-nugget-factor*

specifies that a minimal nugget effect be added to the theoretical semivariance in the unlikely occasion that the theoretical semivariance becomes zero during fitting with weighted least squares. As explained in the section “[Theoretical and Computational Details of the Semivariogram](#)” on page 8613, the theoretical semivariance is always positive for any distance larger than zero. If a conflicting situation emerges as a result of numerical fitting issues, then the NEPSILON= option can help you alleviate the problem by adding a minimal variance at the distance lag where the issue is encountered. For more details, see the section “[Parameter Initialization](#)” on page 8630.

If you omit the NEPSILON= option, then PROC VARIOGRAM sets a default value of  $10^{-6}$ . If a minimal nugget effect is used, its value is case-specific and is based on the *min-nugget-factor*. Specifically, its value is defined as *min-nugget-factor* times the sample variance of the input data set, or as *min-nugget-factor* when the sample variance is equal to zero.

**NUGGET=***number*

specifies the nugget effect for the model. The nugget effect is due to a discontinuity in the semivariogram as determined by plotting the sample semivariogram; see “[Theoretical Semivariogram Models](#)” on page 8608 for more details. The NUGGET= parameter is a nonnegative number. If you specify a nonmissing value, then it is used as a fixed parameter in the fitting process.

PROC VARIOGRAM assigns a default initial value for the nugget effect in the following cases:

- if you specify a missing value.
- if you omit the NUGGET= option and you do not specify an associated **PARMS** statement with initial values for the nugget.

The NUGGET= option is incompatible with the specification of the **PARMS** statement for the corresponding **MODEL** statement.

**RANGE=***range***RANGE=***(range1, . . . , rangek)*

specifies the range parameter in semivariogram models. The RANGE= option is optional. However, if you specify the RANGE= option, then you must provide range values for all structures that you have specified explicitly in the **FORM=** option. All nonmissing range values are considered as fixed parameters. PROC VARIOGRAM assigns a default initial value to any of the model structures for which you specify a missing range value. PROC VARIOGRAM assigns default initial values to all model structures if you omit the RANGE= option, unless you specify an associated **PARMS** statement and initial values for the range in it.

The range parameter is a positive number, has the units of distance, and is related to the correlation scale of the underlying spatial process.

**NOTE:** If you specify this parameter for a power model, then it does not correspond to a range. For power models, the parameter you specify in the RANGE option is a dimensionless power exponent whose value must range within [0,2) so that the power model is a valid semivariance function.

The RANGE= option is ignored when you specify the FORM=AUTO option. The RANGE= option is incompatible with the specification of the PARMS statement for the corresponding MODEL statement.

**RANGELAG=***rlag-list*

**RLAG=***rlag-list*

specifies that you prefer to use the range of consecutive nonmissing empirical semivariance lags in the *rlag-list* for the semivariogram fitting process, instead of using all MAXLAGS+1 lag classes by default. You can specify *rlag-list* in either of the following forms:

- |               |                                                                                                                                                                                                                                                                                                      |
|---------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <i>k</i>      | a single value that designates the width of the selected lag range by starting at lag zero. You must use at least three lags to perform model fitting, so you can specify <i>k</i> within [3, . . . , MAXLAGS+1].                                                                                    |
| <i>m TO n</i> | a sequence in which <i>m</i> equals the starting lag and <i>n</i> equals the ending lag. The parameters <i>m</i> and <i>n</i> must be nonnegative integer numbers to designate lag classes between zero and MAXLAGS. Use at least three lags for model fitting; hence it holds that $n - m \geq 2$ . |

The following two brief examples exhibit the use of the RANGELAG option. These examples assume that you have set the MAXLAGS= option to 9 or higher to indicate nonmissing empirical semivariance estimates at 10 lags or more.

In the first example,

**RANGELAG=8**

uses the empirical semivariance in the first eight lags to fit a theoretical model. Hence, RANGELAG=8 uses only the lag classes zero to seven. This approach enables you to account only for the correlation behavior described by the first *k* empirical semivariogram lag classes.

In the second example,

**RANGELAG=2 TO 9**

specifies that the empirical semivariance values at lag classes zero, one, and after lag class nine are excluded from the model fitting process.

**RANKEPS=***reps-value*

**REPS=***reps-value*

specifies the minimum threshold to compare fit quality of two models for a specific criterion. Beyond this threshold the criterion values become insensitive to comparison. In particular, when you fit multiple models, PROC VARIOGRAM computes for each one the value of the fitting criterion specified in the **CHOOSE=** option of the **MODEL** statement. These values are examined in pairs at the sorting stage. If the difference of a given pair exceeds the *reps-value*, then the sort order of the corresponding models is reversed; otherwise, the two models retain their relative order in the rankings. Hence, the **RANKEPS=** option can affect model ranking in the fit summary table.

The default value for the **RANKEPS=** parameter is  $10^{-6}$  and accounts for the default optimization convergence tolerance at the fitting stage prior to model ranking. The convergence tolerance itself limits the accuracy that you can use to compare two models under a given criterion. As a result, smaller values of the **RANKEPS=** parameter might not lead to a sensible and more strict model comparison because for a smaller *reps-value*, ranking could depend on digits beyond the accuracy limit.

In the opposite end, if the specified *reps-value* turns out to be large compared to the criterion value differences, then it can make the sorting process insensitive to the specified sorting criterion. When this happens, the fit summary table ranking reflects only the order in which different models are examined in the procedure flow. You can tell whether the criterion is bypassed; if it is, then one or more values of the specified criterion might not appear to be sorted in the fit summary table.

The **RANKEPS=** parameter must be a positive number. The **RANKEPS=** option applies when you fit multiple models with the **FORM=AUTO** option of the **MODEL** statement; otherwise, it is ignored.

**SCALE=***scale*

**SCALE=**(*scale1*, ..., *scalek*)

specifies the scale parameter in semivariogram models. The **SCALE=** option is optional. However, if you specify the **SCALE=** option, then you must provide sill values for all structures that you have specified explicitly in the **FORM=** option. All nonmissing scale values are considered as fixed parameters. PROC VARIOGRAM assigns a default initial value to any of the model structures for which you specify a missing scale value. PROC VARIOGRAM assigns default initial values to all model structures if you omit the **SCALE=** option, unless you specify an associated **PARMS** statement with initial values for scale.

The scale parameter is a positive number. It has the same units as the variance of the variable in the **VAR** statement. The scale of each structure in a semivariogram model represents the variance contribution of the structure to the total model variance.

In power models the **SCALE=** parameter does not correspond to a sill because the power model has no sill. Instead, PROC VARIOGRAM uses the **SCALE=** option to designate the slope (or scaling factor) in power model forms. The power model slope has the same variance units as the variable in the **VAR** statement.

The **SCALE=** option is ignored when you specify the **FORM=AUTO** option. The **SCALE=** option is incompatible with the specification of the **PARMS** statement for the corresponding **MODEL** statement.

**SMOOTH=***smooth*

**SMOOTH=**(*smooth1*, . . . , *smoothm*)

specifies the positive smoothness parameter  $\nu$  in the Matérn type of semivariance structures. The special case  $\nu = 0.5$  is equivalent to the exponential model, whereas the theoretical limit  $\nu \rightarrow \infty$  gives the Gaussian model.

The SMOOTH= option is optional. When you specify an explicit model in the FORM= option with  $m$  Matérn structures, you can provide up to  $m$  smoothness values. You can specify a value for *smooth<sub>i</sub>*,  $i = 1, \dots, m$  that is positive and no greater than 1,000,000. PROC VARIOGRAM sets this upper limit for the SMOOTH= option values for numerical and performance reasons. In any case, if the fitting process leads the smoothness value to exceed the default threshold value 10,000, then the VARIOGRAM procedure converts the Matérn form into a Gaussian form and repeats the model fitting. To adjust the switching threshold value, you can use the MTOGTOL= option in the MODEL statement.

If you specify fewer than  $m$  values, then the remaining Matérn structures have their smoothness parameters initialized to missing values. If you specify more than  $m$  values, then values in excess are ignored.

All nonmissing smoothness values are considered as fixed parameters of the corresponding Matérn structures. PROC VARIOGRAM assigns a default initial value to any of the model Matérn structures, if any, for which you specify a missing smoothness value. PROC VARIOGRAM assigns default initial values to all model Matérn structures if you omit the SMOOTH= option, unless you specify an associated PARMS statement and initial values for smoothness in it.

The SMOOTH= option is ignored when you specify the FORM=AUTO option. The SMOOTH= option is incompatible with the specification of the PARMS statement for the corresponding MODEL statement.

In addition to the *fitting-options*, you can specify the following *model-options* after a slash (/) in the MODEL statement.

### COVB

requests the approximate covariance matrix for the parameter estimates of the model fitting. The COVB option is ignored when you also specify the DETAILS=ALL option.

When you specify an explicit model with the FORM= option in the MODEL statement, the COVB option produces the requested approximate covariance matrix. When you specify the FORM=AUTO option in the MODEL statement, by default the COVB option produces output only for the selected model, where the choice is based on the criteria that you specify in the CHOOSE= option of the MODEL statement. If you specify the DETAILS option in addition to FORM=AUTO in the MODEL statement, then the COVB option produces output for each one of the fitted models.

### CORRB

requests the approximate correlation matrix for the parameter estimates of the model fitting. The CORRB option is ignored when you also specify the DETAILS=ALL option.

When you specify an explicit model with the FORM= option in the MODEL statement, the CORRB option produces the requested approximate correlation matrix. When you specify the FORM=AUTO option in the MODEL statement, by default the CORRB option produces output only for the selected model, where the choice is based on the criteria that you specify in the CHOOSE= option of the MODEL statement. If you specify the DETAILS option in addition to FORM=AUTO in the MODEL statement, then the CORRB option produces output for each one of the fitted models.

**DETAILS** <= *detail-level* >

requests different levels of output to be produced during the fitting process. You can specify any of the following *detail-level* arguments:

**MOD**

specifies that the default output for all candidate models be produced when the **FORM=AUTO** option is specified in the **MODEL** statement. If you fit only one explicit model, then the **DETAILS=MOD** option has no effect and is ignored.

**ITR**

requests that a complete iteration history be produced in addition to the default output. The output for **DETAILS=ITR** includes the current values of the parameter estimates, their gradients, and additional optimization statistics.

**ALL**

requests the most detailed level of output when fitting a model. Specifically, except for the default output, the **DETAILS=ALL** option produces optimization statistics in addition to the combined output of the **DETAILS=ITR**, **COVB**, and **CORRB** options.

When you fit multiple models with the **FORM=AUTO** option in the **MODEL** statement, only the selected model default output is produced. The model selection is based on the criteria that you specify in the **CHOOSE=** option of the **MODEL** statement. With the **DETAILS** option you can produce ODS tables with information about the fitting process of all the models that you fit. Moreover, you can produce output at different levels of detail that you can specify with the *detail-level* argument.

Omitting the **DETAILS** option or specifying the **DETAILS** option without any argument is equivalent to specifying **DETAILS=MOD**.

**GRADIENT**

displays the gradient of the objective function with respect to the parameter estimates in the “Parameter Estimates” table.

**MTOGTOL**=*number***MTOL**=*number*

specifies a threshold value for the smoothness parameter of the Matérn form. Above this threshold, a Matérn form in a model switches to the Gaussian form. The *number* value must be positive and no greater than 1,000,000, which is the smoothness upper bound set by the VARIOGRAM procedure.

By default, if the fitting process progressively increases the Matérn smoothness parameter  $\nu$  without converging to a smoothness estimate, then PROC VARIOGRAM converts the Matérn form into a Gaussian form when smoothness exceeds the default value 10,000. If you specify the *number* value to be greater than the 1,000,000 boundary value, then it is ignored and reset to the default threshold value. For more details about the Matérn-to-Gaussian form conversion, see the section “Fitting with Matérn Forms” on page 8634.

**NOFIT**

suppresses the model fitting process.

**NOITPRINT**

suppresses the display of the iteration history table when you have also specified the **DETAILS=ITR** or **DETAILS=ALL** option in the **MODEL** statement. Otherwise, the **NOITPRINT** option is ignored.

## PARMS Statement

**PARMS** (*value-list*)...</ options > ;

The PARMS statement specifies initial values for the semivariance parameters of a single specified model in the **MODEL** statement. Alternatively, the PARMS statement can request a grid search over several values of these parameters. You must specify the values by starting with the nugget effect parameter. You continue in the order in which semivariogram forms are specified in the **FORM=** option of the **MODEL** statement by specifying for each structure the values for its scale, range, and any other parameters as applicable.

The PARMS statement is optional and must follow the associated **MODEL** statement.

The *value-list* specification can take any of several forms:

|                                  |                                                                                                                             |
|----------------------------------|-----------------------------------------------------------------------------------------------------------------------------|
| <i>m</i>                         | a single value                                                                                                              |
| $m_1, m_2, \dots, m_n$           | several values                                                                                                              |
| <i>m</i> to <i>n</i>             | a sequence in which <i>m</i> equals the starting value, <i>n</i> equals the ending value, and the increment equals 1        |
| <i>m</i> to <i>n</i> by <i>i</i> | a sequence in which <i>m</i> equals the starting value, <i>n</i> equals the ending value, and the increment equals <i>i</i> |
| $m_1, m_2$ to $m_3$              | mixed values and sequences                                                                                                  |

You can use the PARMS statement to input fixed values for parameters and also initial values that you want to optimize.

Suppose that you want to fit a semivariogram model with a Matérn component of scale 3, range 20, smoothing parameter 4.5, and an exponential component of unspecified scale and range 15. Assume that you also want to fix all the specified parameter values for the optimization. Including the nugget effect, you have a model with six parameters.

In terms of the PARMS statement, your specifications mean that you have initial values for the second, third, fourth, and sixth parameter in the parameter list. Also, the same specifications imply that you provide no initial values for the first parameter (which corresponds to the nugget effect) and the fifth parameter (which corresponds to the exponential model scale). For these parameters you prefer that PROC VARIOGRAM selects initial values, instead. Since you must specify values for all model parameters in the PARMS statement, you simply specify missing values for the first and fifth parameter. This is the way to request that PROC VARIOGRAM assigns default initial values to parameters. The SAS statements to implement these specifications are as follows:

```
proc variogram data=FirstData;
 < other VARIOGRAM statements >
 model form=(mat,exp);
 parms (.) (3) (20) (4.5) (.) (15) / hold=(2 to 4,6);
run;
```

**NOTE:** The preceding statements are equivalent to the following ones in which the PARMs statement is omitted:

```
proc variogram data=FirstData;
 < other VARIOGRAM statements >
 model form=(mat,exp) scale=(3,.) range(20,15) smooth=4.5;
run;
```

This example might suggest that you can always use either the PARMs or the MODEL statement to specify the same fitting parameters in the VARIOGRAM procedure. However, the PARMs statement gives you more flexibility in two ways:

- You can set non-default initial parameter values by using the PARMs statement, whereas in the MODEL statement you can request default initial values only by setting parameters to missing values. For this reason the PARMs statement cannot be specified when the FORM=AUTO option is specified in the associated MODEL statement. As an example, the following statements do not have an equivalent without using the PARMs statement, because the first parameter in the PARMs statement list (which corresponds to the NUGGET parameter) is set to the specific initial value of 2.1 and the fifth parameter (which corresponds to the exponential structure scale) is set to the specific initial value of 0.3.

```
proc variogram data=FirstData;
 < other VARIOGRAM statements >
 model form=(mat,exp);
 parms (2.1) (3) (20) (4.5) (0.3) (15) / hold=(2 to 4,6);
run;
```

- In the MODEL statement all the nonmissing parameter values that you specify remain fixed. Instead, the PARMs statement considers all values in the specified parameter sets to be subjected to optimization unless you force values to be fixed with the HOLD= option. In the previous example, you can specify that you want to optimize all of your parameters by skipping the HOLD= option as shown in the following modified statements:

```
proc variogram data=FirstData;
 < other VARIOGRAM statements >
 model form=(mat,exp);
 parms (2.1) (3) (20) (4.5) (1) (15);
run;
```

When you omit the PARMs statement list and the PDATA= data set in a PARMs statement, the specification is equivalent to a PARMs statement list where all the parameters have missing initial values. However, if you specify no other option in the PARMs statement, then the PARMs statement is ignored.

In order to avoid ambiguity, you cannot specify the PARMs statement if any of the scale, range, nugget, or smoothness parameters has been specified in the associated MODEL statement either explicitly or in the MDATA= data set. This condition is in effect even when you specify an empty PARMs statement.

If you specify more than one set of initial values, a grid of initial values sets is created. PROC VARIOGRAM seeks among the specified sets for the one that gives the lowest objective function value. Then, the procedure uses the initial values in the selected set for the fitting optimization.



The results from the PARMs statement are the values of the parameters on the specified grid. The ODS name of the “Parameter Search” table is ParmSearch.

You can specify the following options after a slash (/) in the PARMs statement:

**HOLD=***value-list*

**EQCONS=***value-list*

specifies which parameter values be constrained to equal the specified values. For example, the following statement constrains the first and third semivariance parameters to equal 0.5 and 12, respectively. The fourth parameter is fixed to the default initial value that is assigned to it by PROC VARIOGRAM.

```
parms (0.5) (3) (12) (.) / hold=1,3,4;
```

The HOLD= option accepts only nonmissing values in its list. If you specify more than the available parameters in the HOLD= option list, then the ones in excess are ignored. If the HOLD= option list has integer values that do not correspond to variables in the PARMs list, then they are also ignored. Noninteger values are rounded to the closest integer and evaluated accordingly.

When you specify more than one set of parameter initial values, the HOLD= option list applies to the set that gives the lowest objective function value before this set is sent to the optimizer for the fitting.

**LOWERB=***value-list*

specifies lower boundary constraints on the semivariance parameters. The *value-list* specification is a list of numbers or missing values (.) separated by commas. You must list the numbers in the order that PROC VARIOGRAM uses for the semivariance parameters, and each number corresponds to the lower boundary constraint. A missing value instructs PROC VARIOGRAM to use its default constraint.

If you do not specify lower bounds for all of the semivariance parameters, then PROC VARIOGRAM assumes that the remaining parameters are not bounded. If you specify more lower bounds in the *value-list* than the available parameters, then the numbers in excess are ignored. If you specify lower bounds for parameters with missing initial values, then the VARIOGRAM procedure enforces the specified bounds in the fitting process. By default, the lower bound for all parameters is zero.

When you specify the HOLD= option together with the LOWERB= option, the lower bounds in the LOWERB= option *value-list* that correspond to fixed parameters are ignored. When you specify the NOBOUND option together with the LOWERB= option, the LOWERB= option is ignored.

**MAXSCALE=***maxscale*

specifies a positive upper threshold for the fitted semivariogram sill. This option imposes a linear constraint on the optimization of the nonfixed semivariogram scale and nugget parameters so that the sum of all scale and nugget parameters does not exceed the specified MAXSCALE= value. The MAXSCALE= constraint is ignored if all the semivariogram scale and nugget parameters are fixed.

**NOBOUND**

requests the removal of boundary constraints on semivariance parameters. For example, semivariance parameters have a default zero lower boundary constraint since they have a physical meaning only for positive values. The NOBOUND option enables the fitting process to derive negative estimates; hence, you need to be cautious with the outcome when you specify this option.



The NOBOUND option has no effect on the power model exponent parameter. The exponent must range within  $[0,2)$  so that the model is a valid semivariance function. Also, the NOBOUND option has no effect on the Matérn smoothness parameter. The options LOWERB= and UPPERB= are ignored if either of them is specified together with the NOBOUND option in the PARMS statement.

**PARMSDATA=SAS-data-set**

**PDATA=SAS-data-set**

specifies that semivariance parameters values be read from a SAS data set. The data set should contain the values in the sequence required by the PARMS statement in either of the following two ways:

- Specify one single column under the variable Estimate (or Est) that contains all the parameter values.
- Use one column for each parameter, and place the  $n$  columns under the Parm1–Parm $n$  variables.

For example, the following two data sets are valid and equivalent ways to specify initial values for the nugget effect and the parameters of the Matérn and exponential structures that have been used in the previous examples in the PARMS statement section:

```
data parData1;
 input Estimate @@;
 datalines;
. 3 20 4.5 . 15
;
```

```
data parData2;
 input Parm1 Parm2 Parm3 Parm4 Parm5 Parm6;
 datalines;
. 3 20 4.5 . 15
;
```

If you have the parData1 data set, then you can import this information into the PARMS statement as follows:

```
proc variogram data=FirstData;
 < other VARIOGRAM statements >
 model form=(mat,exp);
 parms / pdata=parData1 hold=(2 to 4,6);
run;
```

You can specify more than one set of initial values in the PDATA= data set by following the preceding guidelines. PROC VARIOGRAM seeks among the specified sets for the one that gives the lowest objective function value. Then, the procedure uses the initial values in the selected set for the fitting optimization.

You can explicitly specify initial parameter values in the PARMS statement or use the PDATA= option, but you cannot use both at the same time.

**UPPERB=***value-list*

specifies upper boundary constraints on the semivariance parameters. The *value-list* specification is a list of numbers or missing values (.) separated by commas. You must list the numbers in the order that PROC VARIOGRAM uses for the semivariance parameters, and each number corresponds to the upper boundary constraint. A missing value instructs PROC VARIOGRAM to use its default constraint.

If you do not specify upper bounds for all of the semivariance parameters, then PROC VARIOGRAM assumes that the remaining parameters are not bounded. If you specify more upper bounds in the *value-list* than the available parameters, then the numbers in excess are ignored. If you specify upper bounds for parameters with missing initial values, then the VARIOGRAM procedure enforces the specified bounds in the fitting process. By default, the scale, range, nugget, and Matérn smoothness parameters have no upper bounds, whereas the power model exponent parameter is lower than two.

When you specify the **HOLD=** option together with the **UPPERB=** option, the upper bounds in the **UPPERB=** option *value-list* that correspond to fixed parameters are ignored. When you specify the **NOBOUND** option together with the **UPPERB=** option, the **UPPERB=** option is ignored.

## NLOPTIONS Statement

**NLOPTIONS** < *options* > ;

By default, PROC VARIOGRAM uses the technique **TECH=NRRIDG**, which corresponds to Newton-Raphson optimization with ridging. For more information about the **NLOPTIONS**, see the section “**NLOPTIONS Statement**” on page 482 in Chapter 19, “Shared Concepts and Topics.”

## STORE Statement

**STORE OUT=***store-name* < / *option* > ;

The **STORE** statement requests that the procedure save the context and results of the semivariogram model fitting analysis in an item store. An item store is a binary file defined by the SAS System. You cannot modify the contents of an item store. The contents of item stores produced by PROC VARIOGRAM can be processed only with the **KRIGE2D** or the **SIM2D** procedure. After you save results in an item store, you can use them at a later time without having to fit the model again.

The *store-name* is a usual one- or two-level SAS name, as for SAS data sets. If you specify a one-level name, then the item store resides in the Work library and is deleted at the end of the SAS session. Since item stores are often used for postprocessing tasks, typical usage specifies a two-level name of the form *libname.memname*. If an item store by the same name as specified in the **STORE** statement already exists, the existing store is replaced.

You can specify the following option in the STORE statement after a slash (/):

**LABEL=***store-label*

specifies a custom label for the item store that is produced by PROC VARIOGRAM. When another procedure processes an item store, the label appears in the procedure's output along with other identifying information.

---

## VAR Statement

**VAR** *analysis-variables-list* ;

Use the VAR statement to specify the analysis variables. You can specify only numeric variables. If you omit the VAR statement, all numeric variables in the **DATA=** data set that are not in the **COORDINATES** statement are used.

---

## Details: VARIOGRAM Procedure

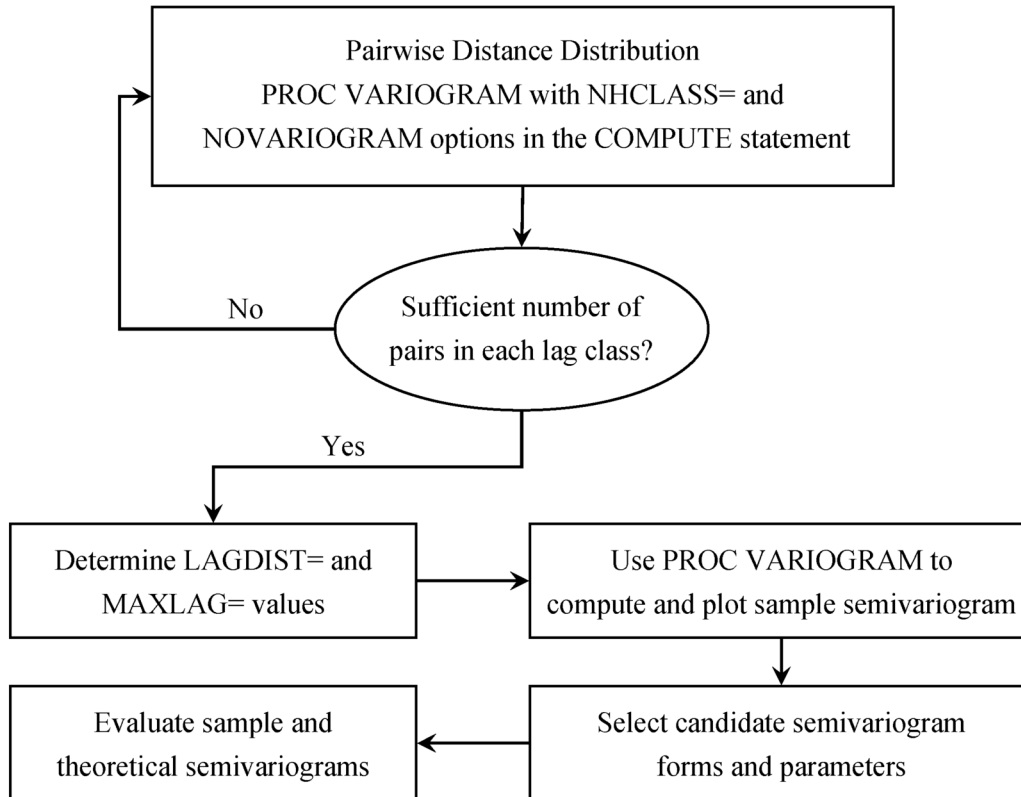
---

### Theoretical Semivariogram Models

The VARIOGRAM procedure computes the empirical (also known as *sample* or *experimental*) semivariogram from a set of point measurements. Semivariograms are used in the first steps of spatial prediction as tools that provide insight into the spatial continuity and structure of a random process. Naturally occurring randomness is accounted for by describing a process in terms of the *spatial random field* (SRF) concept (Christakos 1992). An SRF is a collection of random variables throughout your spatial domain of prediction. For some of them you already have measurements, and your data set constitutes part of a single realization of this SRF. Based on your sample, spatial prediction aims to provide you with values of the SRF at locations where no measurements are available.

Prediction of the SRF values at unsampled locations by techniques such as ordinary kriging requires the use of a theoretical semivariogram or covariance model. Due to the randomness involved in stochastic processes, the theoretical semivariance cannot be computed. Instead, it is possible that the empirical semivariance can provide an estimate of the theoretical semivariance, which then characterizes the spatial structure of the process.

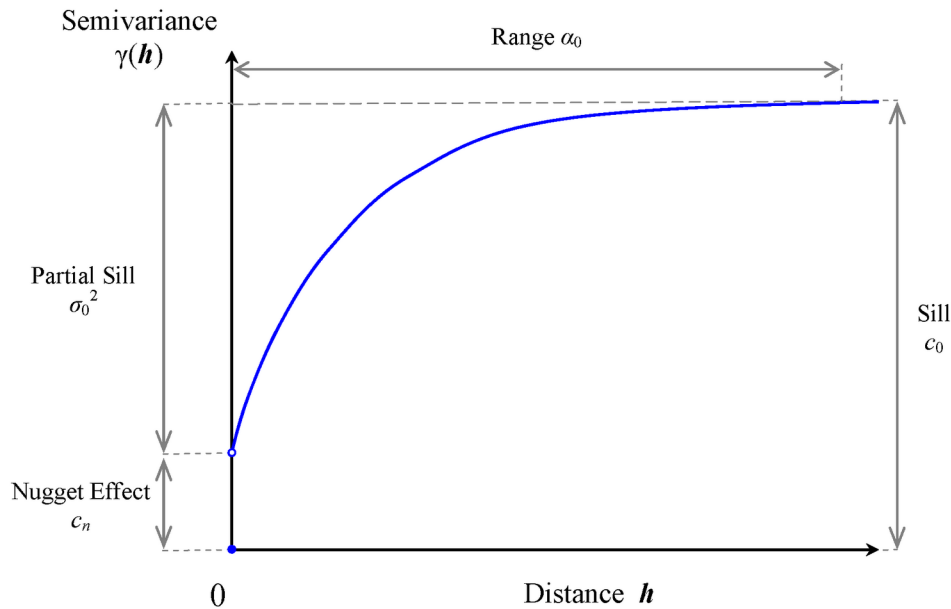
The VARIOGRAM procedure follows a general flow of investigation that leads you from a set of spatial observations to an expression of theoretical semivariance to characterize the SRF continuity. Specifically, the empirical semivariogram is computed after a suitable choice is made for the **LAGDISTANCE=** and **MAXLAGS=** options. For computations in more than one direction you can further use the **NDIRECTIONS=** option or the **DIRECTIONS** statement. Potential theoretical models (which can also incorporate nesting, anisotropy, and the nugget effect) can be fitted to the empirical semivariance by using the **MODEL** statement, and then plotted against the empirical semivariogram. The flow of this analytical process is illustrated in Figure 102.17. After a suitable theoretical model is determined, it is used in PROC KRIGE2D for the prediction stage. The prediction analysis is presented in detail in the section “Details of Ordinary Kriging” on page 3839 in the KRIGE2D procedure documentation.

**Figure 102.17** Flowchart for Semivariogram Selection

It is critical to note that the empirical semivariance provides an estimate of its theoretical counterpart only when the SRF satisfies stationarity conditions. These conditions imply that the SRF has a constant (or zero) expected value. Consequently, your data need to be sampled from a trend-free random field and need to have a constant mean, as assumed in “Getting Started: VARIOGRAM Procedure” on page 8561. Equivalently, your data could be residuals of an initial sample that has had a surface trend removed, as portrayed in “Example 102.2: An Anisotropic Case Study with Surface Trend in the Data” on page 8658. For a closer look at stationarity, see the section “Stationarity” on page 8615. For details about different stationarity types and conditions see, for example, Chilès and Delfiner (1999, section 1.1.4).

### Characteristics of Semivariogram Models

When you obtain a valid empirical estimate of the theoretical semivariance, it is then necessary to choose a type of theoretical semivariogram model based on that estimate. Commonly used theoretical semivariogram shapes rise monotonically as a function of distance. The shape is typically characterized in terms of particular parameters; these are the *range*  $a_0$ , the *sill* (or *scale*)  $c_0$ , and the *nugget effect*  $c_n$ . Figure 102.18 displays a theoretical semivariogram of a spherical semivariance model and points out the semivariogram characteristics.

**Figure 102.18** A Theoretical Semivariogram of Spherical Type and Its Characteristics

Specifically, the sill is the semivariogram upper bound. The range  $a_0$  denotes the distance at which the semivariogram reaches the sill. When the semivariogram increases asymptotically toward its sill value, as occurs in the exponential and Gaussian semivariogram models, the term *effective* (or *practical*) range is also used. The effective range  $r_\epsilon$  is defined as the distance at which the semivariance value achieves 95% of the sill. In particular, for these models the relationship between the range and effective range is  $r_\epsilon = 3a_0$  (exponential model) and  $r_\epsilon = \sqrt{3}a_0$  (Gaussian model).

The nugget effect  $c_n$  represents a discontinuity of the semivariogram that can be present at the origin. It is typically attributed to microscale effects or measurement errors. The semivariance is always 0 at distance  $h = 0$ ; hence, the nugget effect demonstrates itself as a jump in the semivariance as soon as  $h > 0$  (note in Figure 102.18 the discontinuity of the function at  $h = 0$  in the presence of a nugget effect).

The sill  $c_0$  consists of the nugget effect, if present, and the *partial sill*  $\sigma_0^2$ ; that is,  $c_0 = c_n + \sigma_0^2$ . If the SRF  $Z(s)$  is second-order stationary (see the section “Stationarity” on page 8615), the estimate of the sill is an estimate of the constant variance  $\text{Var}[Z(s)]$  of the field. Nonstationary processes have variances that depend on the location  $s$ . Their semivariance increases with distance; hence their semivariograms have no sill.

Not every function is a suitable candidate for a theoretical semivariogram model. The semivariance function  $\gamma_z(\mathbf{h})$ , as defined in the following section, is a so-called *conditionally negative-definite* function that satisfies (Cressie 1993, p. 60)

$$\sum_{i=1}^m \sum_{j=i}^m q_i q_j \gamma_z(\mathbf{s}_i - \mathbf{s}_j) \leq 0$$

for any number  $m$  of locations  $\mathbf{s}_i, \mathbf{s}_j$  in  $\mathcal{R}^2$  with  $\mathbf{h} = \mathbf{s}_i - \mathbf{s}_j$ , and any real numbers  $q_i$  such that  $\sum_{i=1}^m q_i = 0$ . PROC VARIOGRAM can use a variety of permissible theoretical semivariogram models.

Specifically, Table 102.4 shows a list of such models that you can use for fitting in the MODEL statement of the VARIOGRAM procedure.

**Table 102.4** Permissible Theoretical Semivariogram Models ( $a_0 > 0$ , unless noted otherwise)

| Model Type       | Semivariance                                                                                                                                                                                                                                                                                                                                                                                                 |
|------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Exponential      | $\gamma_z(\mathbf{h}) = \begin{cases} 0 & \text{if }  \mathbf{h}  = 0 \\ c_n + \sigma_0^2 \left[ 1 - \exp\left(-\frac{ \mathbf{h} }{a_0}\right) \right] & \text{if } 0 <  \mathbf{h}  \end{cases}$                                                                                                                                                                                                           |
| Gaussian         | $\gamma_z(\mathbf{h}) = \begin{cases} 0 & \text{if }  \mathbf{h}  = 0 \\ c_n + \sigma_0^2 \left[ 1 - \exp\left(-\frac{ \mathbf{h} ^2}{a_0^2}\right) \right] & \text{if } 0 <  \mathbf{h}  \end{cases}$                                                                                                                                                                                                       |
| Power            | $\gamma_z(\mathbf{h}) = \begin{cases} 0 & \text{if }  \mathbf{h}  = 0 \\ c_n + \sigma_0^2 \mathbf{h}^{a_0} & \text{if } 0 <  \mathbf{h} , 0 \leq a_0 < 2 \end{cases}$                                                                                                                                                                                                                                        |
| Spherical        | $\gamma_z(\mathbf{h}) = \begin{cases} 0 & \text{if }  \mathbf{h}  = 0 \\ c_n + \sigma_0^2 \left[ \frac{3}{2} \frac{ \mathbf{h} }{a_0} - \frac{1}{2} \left(\frac{ \mathbf{h} }{a_0}\right)^3 \right] & \text{if } 0 <  \mathbf{h}  \leq a_0 \\ c_0 & \text{if } a_0 <  \mathbf{h}  \end{cases}$                                                                                                               |
| Cubic            | $\gamma_z(\mathbf{h}) = \begin{cases} 0 & \text{if }  \mathbf{h}  = 0 \\ c_n + \sigma_0^2 \left[ 7\left(\frac{ \mathbf{h} }{a_0}\right)^2 - \frac{35}{4}\left(\frac{ \mathbf{h} }{a_0}\right)^3 + \frac{7}{2}\left(\frac{ \mathbf{h} }{a_0}\right)^5 - \frac{3}{4}\left(\frac{ \mathbf{h} }{a_0}\right)^7 \right] & \text{if } 0 <  \mathbf{h}  \leq a_0 \\ c_0 & \text{if } a_0 <  \mathbf{h}  \end{cases}$ |
| Pentaspherical   | $\gamma_z(\mathbf{h}) = \begin{cases} 0 & \text{if }  \mathbf{h}  = 0 \\ c_n + \sigma_0^2 \left[ \frac{15}{8} \frac{ \mathbf{h} }{a_0} - \frac{5}{4} \left(\frac{ \mathbf{h} }{a_0}\right)^3 + \frac{3}{8} \left(\frac{ \mathbf{h} }{a_0}\right)^5 \right] & \text{if } 0 <  \mathbf{h}  \leq a_0 \\ c_0 & \text{if } a_0 <  \mathbf{h}  \end{cases}$                                                        |
| Sine hole effect | $\gamma_z(\mathbf{h}) = \begin{cases} 0 & \text{if }  \mathbf{h}  = 0 \\ c_n + \sigma_0^2 \left[ 1 - \frac{\sin(\pi \mathbf{h} /a_0)}{\pi \mathbf{h} /a_0} \right] & \text{if } 0 <  \mathbf{h}  \end{cases}$                                                                                                                                                                                                |
| Matérn class     | $\gamma_z(\mathbf{h}) = \begin{cases} 0 & \text{if }  \mathbf{h}  = 0 \\ c_n + \sigma_0^2 \left[ 1 - \frac{2}{\Gamma(\nu)} \left(\frac{ \mathbf{h} \sqrt{\nu}}{a_0}\right)^\nu K_\nu\left(2\frac{ \mathbf{h} \sqrt{\nu}}{a_0}\right) \right] & \text{if } 0 <  \mathbf{h} , \nu > 0 \end{cases}$                                                                                                             |

All of these models, except for the power model, are transitive. A transitive model characterizes a random process whose variation reaches the sill value  $c_0$  within a specific range from any location in the field.

The power model is nontransitive and applies to processes whose variance increases with distance. It has no scale and range; instead, it quantifies the process variation by using a positive slope parameter and a dimensionless power exponent  $\alpha$  that indicate how fast the variance increases. The expression for the power model is a valid semivariogram only when the exponent parameter ranges within  $0 \leq \alpha < 2$ . For convenience, PROC VARIOGRAM registers the power model slope parameter under the SCALE= option parameters in the MODEL statement. For the same reason, the scale and power slope parameters are represented with the common symbol  $\sigma_0^2$  in Table 102.4. Also for convenience, PROC VARIOGRAM registers the power model exponent parameter under the RANGE= option parameters. The range and the power exponent parameters are represented with the common symbol  $a_0$  in Table 102.4.

The power model is a generalized case of the linear model, which is not included explicitly in the model set of PROC VARIOGRAM. The linear model is derived from the power model when you specify the exponent  $\alpha = 1$ .

Among the models displayed in Table 102.4, the Matérn (or  $K$ -Bessel) class is a class of semivariance models that distinguish from each other by means of the positive smoothing parameter  $\nu$ . Different values of  $\nu$  correspond to different correlation models. Most notably, for  $\nu = 0.5$  the Matérn semivariance is equivalent to the exponential model, whereas  $\nu \rightarrow \infty$  gives the Gaussian model. Also, Table 102.4 shows that the Matérn semivariance computations use the gamma function  $\Gamma(\nu)$  and the second kind Bessel function  $K_\nu$ .

In PROC VARIOGRAM, you can input the model parameter values either explicitly as arguments of options, or as lists of values. In the latter case, you are expected to provide the values in the order the models are specified in the SAS statements, and furthermore in the sequential order of the scale, range, and smoothing parameter for each model as appropriate, and always starting with the nugget effect. If the parameter values are specified through an input file, then the total of  $n$  parameters should be provided either as one variable named Estimate or as many variables with the respective names Parm1–Parm $n$ .

You can review in further detail the models shown in Table 102.4 in the section “Theoretical Semivariogram Models” on page 3823 in the KRIGE2D procedure documentation.

The theoretical semivariogram models are used to describe the spatial structure of random processes. Based on their shape and characteristics, the semivariograms of these models can provide a plethora of information (Christakos 1992, section 7.3):

- Examination of the semivariogram variation in different directions provides information about the isotropy of the random process. (See also the discussion about isotropy in the following section.)
- The semivariogram range determines the zone of influence that extends from any given location. Values at surrounding locations within this zone are correlated with the value at the specific location by means of the particular semivariogram.
- The semivariogram behavior at large distances indicates the degree of stationarity of the process. In particular, an asymptotic behavior suggests a stationary process, whereas either a linear increase and slow convergence to the sill or a fast increase is an indicator of nonstationarity.
- The semivariogram behavior close to the origin indicates the degree of regularity of the process variation. Specifically, a parabolic behavior at the origin implies a very regular spatial variation, whereas a linear behavior characterizes a nonsmooth process. The presence of a nugget effect is additional evidence of irregularity in the process.
- The semivariogram behavior within the range provides description of potential periodicities or anomalies in the spatial process.

A brief note on terminology: In some fields (for example, geostatistics) the term homogeneity is sometimes used instead of stationarity in spatial analysis; however, in statistics homogeneity is defined differently (Banerjee, Carlin, and Gelfand 2004, section 2.1.3). In particular, the alternative terminology characterizes as homogeneous the stationary SRF in  $\mathcal{R}^n$ ,  $n > 1$ , whereas it retains the term stationary for such SRF in  $\mathcal{R}^1$  (SRF in  $\mathcal{R}^1$  are also known as *random processes*). Often, studies in a single dimension refer to temporal processes; hence, you might see time-stationary random processes called “temporally stationary” or simply stationary, and stationary SRF in  $\mathcal{R}^n$ ,  $n > 1$ , characterized as “spatially homogeneous” or simply homogeneous. This distinction made by the alternative nomenclature is more evident in spatiotemporal

random fields (S/TRF), where the different terms clarify whether stationarity applies in the spatial or the temporal part of the S/TRF.

## Nested Models

When you try to represent an empirical semivariogram by fitting a theoretical model, you might find that using a combination of theoretical models results in a more accurate fit onto the empirical semivariance than using a single model. This is known as model nesting. The semivariance models that result as the sum of two or more semivariance structures are called *nested* models.

In general, a linear combination of permissible semivariance models produces a new permissible semivariance model. Nested models are based on this premise. You can include in a sum any combination of the models presented in Table 102.4. For example, a nested semivariance  $\gamma_z(\mathbf{h})$  that contains two structures, one exponential  $\gamma_{z,\text{EXP}}(\mathbf{h})$  and one spherical  $\gamma_{z,\text{SPH}}(\mathbf{h})$ , can be expressed as

$$\gamma_z(\mathbf{h}) = \gamma_{z,\text{EXP}}(\mathbf{h}) + \gamma_{z,\text{SPH}}(\mathbf{h})$$

If you have a nested model and a nugget effect, then the nugget effect  $c_n$  is a single parameter that is considered jointly for all the nested structures.

Nested models, anisotropic models, and the nugget effect increase the scope of theoretical models available. You can find additional discussion about these concepts in the section “Theoretical Semivariogram Models” on page 3823 in the KRIGE2D procedure documentation.

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## Theoretical and Computational Details of the Semivariogram

Let  $\{Z(\mathbf{s}), \mathbf{s} \in D \subset \mathcal{R}^2\}$  be a spatial random field (SRF) with  $n$  measured values  $z_i = Z(\mathbf{s}_i)$  at respective locations  $\mathbf{s}_i, i = 1, \dots, n$ . You use the VARIOGRAM procedure because you want to gain insight into the spatial continuity and structure of  $Z(\mathbf{s})$ . A good measure of the spatial continuity of  $Z(\mathbf{s})$  is defined by means of the variance of the difference  $Z(\mathbf{s}_i) - Z(\mathbf{s}_j)$ , where  $\mathbf{s}_i$  and  $\mathbf{s}_j$  are locations in  $D$ . Specifically, if you consider  $\mathbf{s}_i$  and  $\mathbf{s}_j$  to be spatial increments such that  $\mathbf{h} = \mathbf{s}_j - \mathbf{s}_i$ , then the variance function based on the increments  $\mathbf{h}$  is independent of the actual locations  $\mathbf{s}_i, \mathbf{s}_j$ . Most commonly, the continuity measure used in practice is one half of this variance, better known as the *semivariance* function,

$$\gamma_z(\mathbf{h}) = \frac{1}{2} \text{Var}[Z(\mathbf{s} + \mathbf{h}) - Z(\mathbf{s})]$$

or, equivalently,

$$\gamma_z(\mathbf{h}) = \frac{1}{2} (\text{E}\{[Z(\mathbf{s} + \mathbf{h}) - Z(\mathbf{s})]^2\} - \{\text{E}[Z(\mathbf{s} + \mathbf{h})] - \text{E}[Z(\mathbf{s})]\}^2)$$

The plot of semivariance as a function of  $\mathbf{h}$  is the *semivariogram*. You might also commonly see the term *semivariogram* used instead of the term *semivariance*.

Assume that the SRF  $Z(\mathbf{s})$  is free of nonrandom (or systematic) surface trends. Then, the expected value  $\text{E}[Z(\mathbf{s})]$  of  $Z(\mathbf{s})$  is a constant for all  $\mathbf{s} \in \mathcal{R}^2$ , and the semivariance expression is simplified to the following:

$$\gamma_z(\mathbf{h}) = \frac{1}{2} \text{E}\{[Z(\mathbf{s} + \mathbf{h}) - Z(\mathbf{s})]^2\}$$



Given the preceding assumption, you can compute an estimate  $\hat{\gamma}_z(\mathbf{h})$  of the semivariance  $\gamma_z(\mathbf{h})$  from a finite set of points in a practical way by using the formula

$$\hat{\gamma}_z(\mathbf{h}) = \frac{1}{2|N(\mathbf{h})|} \sum_{N(\mathbf{h})} [Z(s_i) - Z(s_j)]^2$$

where the sets  $N(\mathbf{h})$  contain all the neighboring pairs at distance  $\mathbf{h}$ ,

$$N(\mathbf{h}) = \{i, j : s_i - s_j = \mathbf{h}\}$$

and  $|N(\mathbf{h})|$  is the number of such pairs  $(i, j)$ .

The expression for  $\hat{\gamma}_z(\mathbf{h})$  is called the *empirical semivariance* (Matheron 1963). This is the quantity that PROC VARIOGRAM computes, and its corresponding plot is the *empirical semivariogram*.

The empirical semivariance  $\hat{\gamma}_z(\mathbf{h})$  is also referred to as *classical*. This name is used so that it can be distinguished from the *robust semivariance* estimate  $\bar{\gamma}_z(\mathbf{h})$  and the corresponding *robust semivariogram*. The robust semivariance was introduced by Cressie and Hawkins (1980) to weaken the effect that outliers in the observations might have on the semivariance. It is described by Cressie (1993, p. 75) as

$$\bar{\gamma}_z(\mathbf{h}) = \frac{\Psi^4(\mathbf{h})}{2[0.457 + 0.494/N(\mathbf{h})]}$$

In the preceding expression the parameter  $\Psi(\mathbf{h})$  is defined as

$$\Psi(\mathbf{h}) = \frac{1}{N(\mathbf{h})} \sum_{P_i P_j \in N(\mathbf{h})} [Z(s_i) - Z(s_j)]^{\frac{1}{2}}$$

According to Cressie (1985), the estimate  $\hat{\gamma}_z(\mathbf{h})$  has approximate variance

$$\text{Var}[\hat{\gamma}_z(\mathbf{h})] \simeq \frac{2[\gamma_z(\mathbf{h})]^2}{N(\mathbf{h})}$$

This approximation is possible by assuming  $Z(s)$  to be a Gaussian SRF, and by further assuming the squared differences in empirical semivariances to be uncorrelated for different distances  $\mathbf{h}$ . Typically, semivariance estimates are correlated because of the underlying spatial correlation among the observations, and also because the same observation pairs might be used for the estimation of more than one semivariogram point, as described in the following subsections. Despite these restrictive assumptions, the approximate variance provides an idea about the semivariance estimate variance and enables fitting of a theoretical model to the empirical semivariance; see the section “[Theoretical Semivariogram Model Fitting](#)” on page 8627 for more details about the fitting process.

**NOTE:** If your data include a surface trend, then the empirical semivariance  $\hat{\gamma}_z(\mathbf{h})$  is not an estimate of the theoretical semivariance function  $\gamma_z(\mathbf{h})$ . Instead, rather than the spatial increments variance, it represents a different quantity known as *pseudo-semivariance*, and its corresponding plot is a *pseudo-semivariogram*. In principle, pseudo-semivariograms do not provide measures of the spatial continuity. They can thus lead to misinterpretations of the  $Z(s)$  spatial structure, and are consequently unsuitable for the purpose of spatial prediction. For further information, see the detailed discussion in the section “[Empirical Semivariograms and Surface Trends](#)” on page 8626. Under certain conditions you might be able to gain some insight about the spatial continuity with a pseudo-semivariogram. This case is presented in “[Example 102.3: Analysis without Surface Trend Removal](#)” on page 8672.

## Stationarity

In the combined presence of the previous two assumptions—that is, when  $E[Z(\mathbf{s})]$  is constant and spatial increments define  $\gamma_z(\mathbf{h})$ —the SRF  $Z(\mathbf{s})$  is characterized as *intrinsically stationary* (Cressie 1993, p. 40).

The expected value  $E[Z(\mathbf{s})]$  is the first statistical moment of the SRF  $Z(\mathbf{s})$ . The second statistical moment of the SRF  $Z(\mathbf{s})$  is the *covariance* function between two points  $\mathbf{s}_i$  and  $\mathbf{s}_j$  in  $Z(\mathbf{s})$ , and it is defined as

$$C_z(\mathbf{s}_i, \mathbf{s}_j) = E \left( [Z(\mathbf{s}_i) - E[Z(\mathbf{s}_i)]] [Z(\mathbf{s}_j) - E[Z(\mathbf{s}_j)]] \right)$$

When  $\mathbf{s}_i = \mathbf{s}_j = \mathbf{s}$ , the covariance expression provides the variance at  $\mathbf{s}$ .

The assumption of a constant  $E[Z(\mathbf{s})] = m$  means that the expected value is invariant with respect to translations of the spatial location  $\mathbf{s}$ . The covariance is considered invariant to such translations when it depends only on the distance  $\mathbf{h} = \mathbf{s}_i - \mathbf{s}_j$  between any two points  $\mathbf{s}_i$  and  $\mathbf{s}_j$ . If both of these conditions are true, then the preceding expression becomes

$$C_z(\mathbf{s}_i, \mathbf{s}_j) = C_z(\mathbf{s}_i - \mathbf{s}_j) = C_z(\mathbf{h}) = E \left( [Z(\mathbf{s}) - m][Z(\mathbf{s} + \mathbf{h}) - m] \right)$$

When both  $E[Z(\mathbf{s})]$  and  $C(\mathbf{s}_i, \mathbf{s}_j)$  are invariant to spatial translations, the SRF  $Z(\mathbf{s})$  is characterized as *second-order stationary* (Cressie 1993, p. 53).

In a second-order stationary SRF the quantity  $C(\mathbf{h})$  is the same for any two points that are separated by distance  $\mathbf{h}$ . Based on the preceding formula, for  $\mathbf{h} = \mathbf{0}$  you can see that the variance is constant throughout a second-order stationary SRF. Hence, second-order stationarity is a stricter condition than intrinsic stationarity.

Under the assumption of second-order stationarity, the semivariance definition at the beginning of this section leads to the conclusion that

$$\gamma_z(\mathbf{h}) = C(\mathbf{0}) - C(\mathbf{h})$$

which relates the theoretical semivariance and covariance. Keep in mind that the empirical estimates of these quantities are not related in exactly the same way, as indicated in Schabenberger and Gotway (2005, section 4.2.1).

## Ergodicity

In addition to the constant  $E[Z(\mathbf{s})]$  and the assumption of intrinsic stationarity, *ergodicity* is a necessary third hypothesis to estimate the empirical semivariance. Assume that for the SRF  $Z(\mathbf{s})$  you have measurements  $z_i$  whose sample mean is estimated by  $\bar{Z}$ . The hypothesis of ergodicity dictates that  $\bar{Z} = E[Z(\mathbf{s})]$ .

In general, an SRF  $Z(\mathbf{s})$  is characterized as ergodic if the statistical moments of its realizations coincide with the corresponding ones of the SRF. In spatial analysis you are often interested in the first two statistical moments, and consequently a more relaxed ergodicity assumption is made only for them. See Christakos (1992, section 2.12) for the use of the ergodicity hypothesis in SRF, and Cressie (1993, p. 57) for a more detailed discussion of ergodicity.

The semivariogram analysis makes implicit use of the ergodicity hypothesis. The VARIOGRAM procedure works with the residual centered values  $V(\mathbf{s}_i) = v_i = z_i - \bar{Z}$ ,  $i = 1, \dots, n$ , where it is assumed that the sample mean  $\bar{Z}$  is the constant expected value  $E[Z(\mathbf{s})]$  of  $Z(\mathbf{s})$ . This is equivalent to using the original values, since  $V(\mathbf{s}_i) - V(\mathbf{s}_j) = Z(\mathbf{s}_i) - Z(\mathbf{s}_j)$ , which shows the property of the semivariance to filter out the mean. See the section “[Semivariance Computation](#)” on page 8625 for the exact expressions PROC VARIOGRAM uses to compute the empirical classical  $\hat{\gamma}_z(\mathbf{h})$  and robust  $\bar{\gamma}_z(\mathbf{h})$  semivariances.

## Anisotropy

Semivariance is defined on the basis of the spatial increment vector  $\mathbf{h}$ . If the variance characteristics of  $Z(\mathbf{s})$  are independent of the spatial direction, then  $Z(\mathbf{s})$  is called *isotropic*; if not, then  $Z(\mathbf{s})$  is called *anisotropic*. In the case of isotropy, the semivariogram depends only on the length  $h$  of  $\mathbf{h}$  and  $\gamma_z(\mathbf{h}) = \gamma_z(h)$ . Anisotropy is characterized as *geometric*, when the range  $a_0$  of the semivariogram varies in different directions, and *zonal*, when the semivariogram sill  $c_0$  depends on the spatial direction. Either type or both types of anisotropy can be present.

In the more general case, an SRF can be anisotropic. For an accurate characterization of the spatial structure it is necessary to perform individual analyses in multiple directions. Goovaerts (1997, p. 98) suggests an initial investigation in at least one direction more than the working spatial dimensions—for example, at least three different directions in  $\mathcal{R}^2$ . Olea (2006) supports exploring as many directions as possible when the data set allows.

You might not know in advance whether you have anisotropy or not. If the semivariogram characteristics remain unchanged in different directions, then you assume the SRF is isotropic. If your directional analysis reveals anisotropic behavior in particular directions, then you proceed to focus your analysis on these directions. For example, in an anisotropic SRF in  $\mathcal{R}^2$  you should expect to find two distinct directions where you observe the *major axis* and the *minor axis* of anisotropy. Typically, these two directions are perpendicular, although they might be at other than right angles when zonal anisotropy is present.

If you can distinguish a maximum and a minimum sill in different directions, then you have a case of zonal anisotropy. The SRF exhibits strongest continuity in the direction of the lowest sill, which is the direction of the major anisotropy axis. If the sill does not change across directions, then the major axis direction of strongest continuity is the one in which the semivariogram has maximum range. See “[Example 102.2: An Anisotropic Case Study with Surface Trend in the Data](#)” on page 8658 for a detailed demonstration of a case with anisotropy when you use PROC VARIOGRAM.

You can find additional information about anisotropy analysis in the section “[Anisotropic Models](#)” on page 3832 in the KRIGE2D procedure documentation.

## Pair Formation

The basic starting point in computing the empirical semivariance is the enumeration of pairs of points for the spatial data. [Figure 102.19](#) shows the spatial domain  $D$  and the set of  $n$  measurements  $z_i, i = 1, \dots, n$ , that have been sampled at the indicated locations in  $D$ . Two data points  $P_1$  and  $P_2$ , with coordinates  $\mathbf{s}_1 = (x_1, y_1)$  and  $\mathbf{s}_2 = (x_2, y_2)$ , respectively, are selected for illustration.

A vector, or directed line segment, is drawn between these points. If the length

$$|P_i P_j| = |\mathbf{s}_2 - \mathbf{s}_1| = (x_2 - x_1)^2 + (y_2 - y_1)^2$$

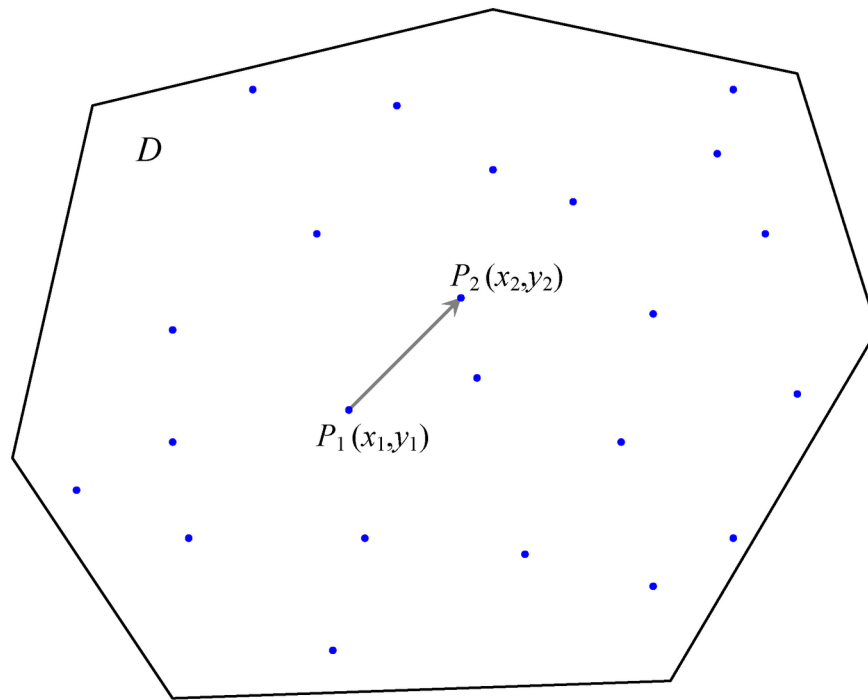
of this vector is smaller than the specified `DEPSILON=` value, then the pair is excluded from the continuity measure calculations because the two points  $P_1$  and  $P_2$  are considered to be at zero distance apart (or *collocated*). Spatial collocation might appear due to different scales in sampling, observations made at the same spatial location at different time instances, and errors in the data sets. PROC VARIOGRAM excludes such pairs from the pairwise distance and semivariance computations because they can cause numeric problems in spatial analysis.

If this pair is not discarded on the basis of collocation, it is then classified—first by orientation of the directed line segment  $\mathbf{s}_2 - \mathbf{s}_1$ , and then by its length  $|P_i P_j|$ . For example, it is unlikely for actual data that the

distance  $|P_i P_j|$  between any pair of data points  $P_i$  and  $P_j$  located at  $s_i$  and  $s_j$ , respectively, would exactly satisfy  $|P_i P_j| = |h| = h$  in the preceding computation of  $\hat{\gamma}_z(h)$ . A similar argument can be made for the orientation of the segment  $s_2 - s_1$ . Consequently, the pair  $P_1 P_2$  is placed into an angle and distance class.

The following subsections give more details about the nature of these classifications. You can also find extensive discussions about the size and the number of classes to consider for the computation of the empirical semivariogram.

**Figure 102.19** Selection of Points  $P_1$  and  $P_2$  in Spatial Domain  $D$



### Angle Classification

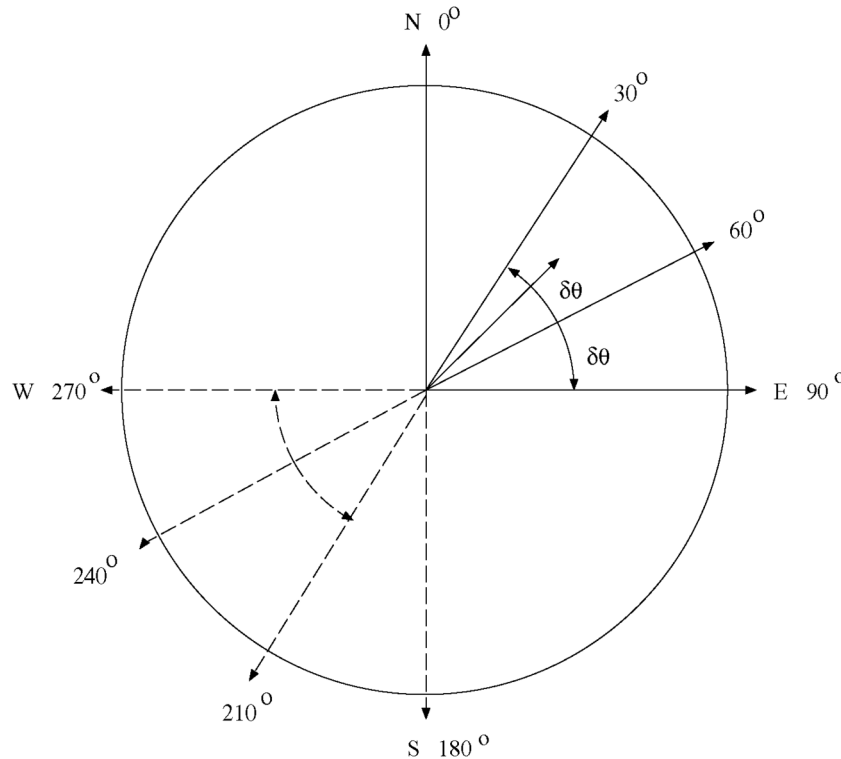
Suppose you specify `NDIRECTIONS=3` in the `COMPUTE` statement in `PROC VARIOGRAM`. This results in three angle classes defined by midpoint angles between  $0^\circ$  and  $180^\circ$ :  $0^\circ \pm \delta\theta$ ,  $60^\circ \pm \delta\theta$ , and  $120^\circ \pm \delta\theta$ , where  $\delta\theta$  is the angle tolerance. If you do not specify an angle tolerance by using the `ANGLETOLERANCE=` option in the `COMPUTE` statement, the following default value is used:

$$\delta\theta = \frac{180^\circ}{2 \times \text{NDIR}}$$

For example, if `NDIRECTIONS=3`, the default angle tolerance is  $\delta\theta = 30^\circ$ . When the directed line segment  $P_1 P_2$  in Figure 102.19 is superimposed on the coordinate system that shows the angle classes, its angle is approximately  $45^\circ$ , measured clockwise from north. In particular, it falls within  $[60^\circ - \delta\theta, 60^\circ + \delta\theta) = [30^\circ, 90^\circ)$ , the second angle class (Figure 102.20).

**NOTE:** If the designated points  $P_1$  and  $P_2$  are labeled in the opposite order, the orientation is in the opposite direction—that is, approximately  $225^\circ$  instead of approximately  $45^\circ$ . This does not affect angle class selection; the angle classes  $[60^\circ - \delta\theta, 60^\circ + \delta\theta)$  and  $[240^\circ - \delta\theta, 240^\circ + \delta\theta)$  are the same.

**Figure 102.20** Selected Pair  $P_1 P_2$  Falls within the Second Angle Class



If you specify an angle tolerance less than the default, such as  $ATOL=15^\circ$ , some point pairs might be excluded. For example, the selected point pair  $P_1 P_2$  in Figure 102.20, while closest to the  $60^\circ$  axis, might lie outside  $[60 - \delta\theta, 60 + \delta\theta) = [45^\circ, 75^\circ)$ . In this case, the point pair  $P_1 P_2$  would be excluded from the semivariance computation. This setting can be desirable if you want to reduce interference between neighboring angles. An angle tolerance that is too small might result in too few point pairs in some distance classes for the empirical semivariance estimation (see also the discussion in the section “Choosing the Size of Classes” on page 8623).

On the other hand, you can specify an angle tolerance *greater* than the default. This can result in a point pair being counted in more than one angle classes. This has a smoothing effect on the variogram and is useful when only a small amount of data is present or the available data are sparsely located. However, in cases of anisotropy the smoothing effect might have the side effect of amplifying weaker anisotropy in some direction and weakening stronger anisotropy in another (Deutsch and Journel 1992, p. 59).

Changes in the values of the `BANDWIDTH=` option have a similar effect. See the section “Bandwidth Restriction” on page 8620 for an explanation of how `BANDWIDTH=` functions.

An alternative way to specify angle classes and angle tolerances is with the `DIRECTIONS` statement. The `DIRECTIONS` statement is useful when angle classes are not equally spaced. When you use the `DIRECTIONS` statement, consider specifying the angle tolerance too. The default value of the angle tolerance is  $45^\circ$  when a `DIRECTIONS` statement is used instead of the `NDIRECTIONS=` option in the `COMPUTE`

statement. This might not be appropriate for a particular set of angle classes. See the section “**DIRECTIONS Statement**” on page 8590 for more details.

### Distance Classification

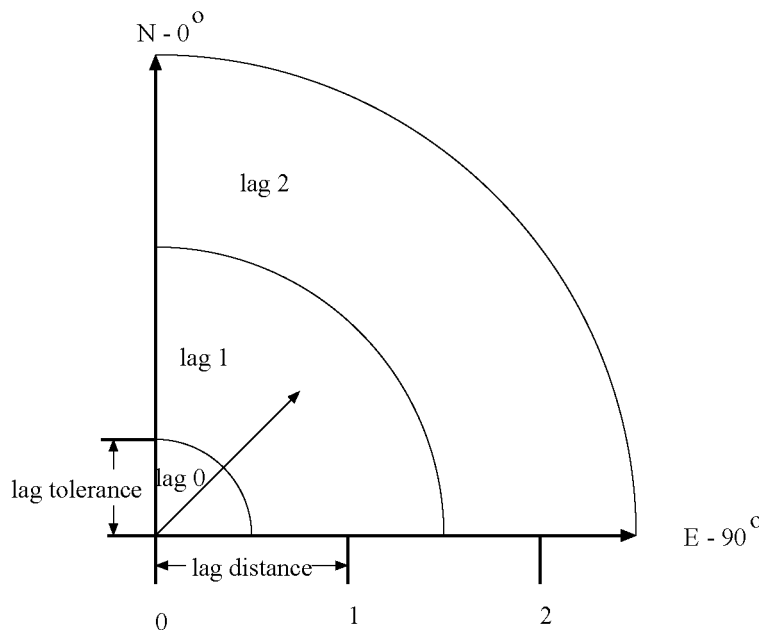
The distance class for a point pair  $P_1P_2$  is determined as follows. The directed line segment  $P_1P_2$  is superimposed on the coordinate system that shows the distance or lag classes. These classes are determined by the **LAGDISTANCE=** option in the **COMPUTE** statement. Denoting the length of the line segment by  $|P_1P_2|$  and the **LAGDISTANCE=** value by  $\Delta$ , the lag class  $L$  is determined by

$$L(P_1P_2) = \left\lfloor \frac{|P_1P_2|}{\Delta} + 0.5 \right\rfloor$$

where  $\lfloor x \rfloor$  denotes the largest integer  $\leq x$ .

When the directed line segment  $P_1P_2$  is superimposed on the coordinate system that shows the distance classes, it is seen to fall in the first lag class; see **Figure 102.21** for an illustration for  $\Delta = 1$ .

**Figure 102.21** Selected Pair  $P_1P_2$  Falls within the First Lag Class

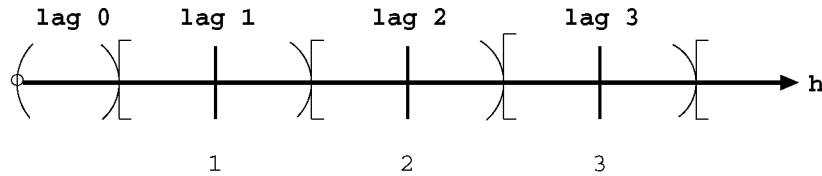


Pairwise distances are positive. Therefore, the line segment  $|P_1P_2|$  might belong to one of the **MAXLAG** lag classes or it could be shorter than half the length of the **LAGDISTANCE=** value. In the last case the segment is said to belong to the lag class zero. Hence, lag class zero is smaller than lag classes  $1, \dots, \text{MAXLAGS}$ . The definition of lag classes in this manner means that when you specify the **MAXLAGS=** parameter, **PROC VARIOGRAM** produces a semivariogram with a total of **MAXLAGS+1** lag classes including the zero lag class. For example, if you specify **LAGDISTANCE=1** and **MAXLAGS=10** and you do not specify a **LAGTOLERANCE=** value in the **COMPUTE** statement in **PROC VARIOGRAM**, the 11 lag classes generated by the preceding equation are

$$[0, 0.5), [0.5, 1.5), [1.5, 2.5), \dots, [9.5, 10.5)$$

The preceding lag classes description is correct under the assumption of the default lag tolerance, which is half the `LAGDISTANCE=` value. Using the default lag tolerance results in no gaps between the distance class intervals, as shown in Figure 102.22.

**Figure 102.22** Lag Distance Axis Showing Lag Classes



On the other hand, if you do specify a distance tolerance with the `LAGTOLERANCE=` option in the `COMPUTE` statement, a further check is performed to see whether the point pair falls within this tolerance of the nearest lag. In the preceding example, if you specify `LAGDISTANCE=1` and `MAXLAGS=10` (as before) and also specify `LAGTOLERANCE=0.25`, the intervals become

$$[0, 0.25), [0.75, 1.25), [1.75, 2.25), \dots, [9.75, 10.25)$$

You might want to avoid this specification because it results in gaps in the lag classes. For example, if a point pair  $P_1 P_2$  falls in an interval such as

$$| P_1 P_2 | \in [1.25, 1.75)$$

then it is excluded from the semivariance calculation. The maximum `LAGTOLERANCE=` value allowed is half the `LAGDISTANCE=` value; no overlap of the distance classes is allowed.

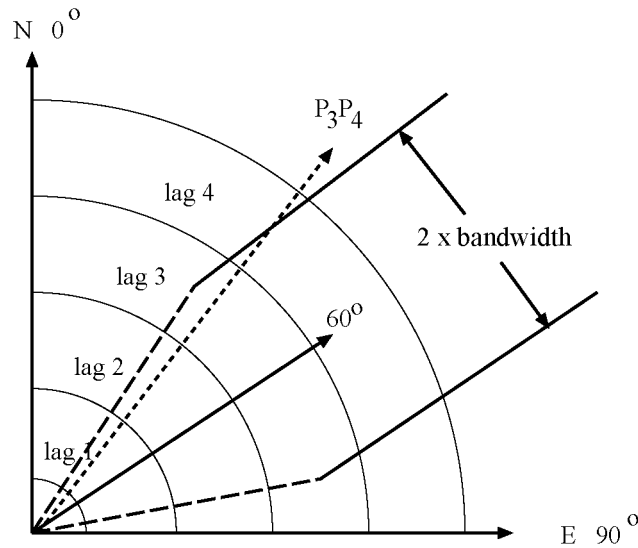
See the section “Computation of the Distribution Distance Classes” on page 8621 for a more extensive discussion of practical aspects in the specification of the `LAGDISTANCE=` and `MAXLAGS=` options.

## Bandwidth Restriction

Because the areal segments that are generated from the angle and distance classes increase in area as the lag distance increases, it is sometimes desirable to restrict this area (Deutsch and Journel 1992, p. 45). If you specify the `BANDWIDTH=` option in the `COMPUTE` statement, the lateral, or perpendicular, distance from the axis that defines the angle classes is fixed.

For example, suppose two points  $P_3, P_4$  are picked from the domain in Figure 102.19 and are superimposed on the grid that defines distance and angle classes, as shown in Figure 102.23.

The endpoint of vector  $P_3 P_4$  falls within the angle class around  $60^\circ$  and the fifth lag class; however, it falls outside the restricted area that is defined by the bandwidth. Hence, it is excluded from the semivariance calculation.

**Figure 102.23** Selected Pair  $P_3P_4$  Falls outside Bandwidth Limit

Finally, a pair  $P_i P_j$  that falls in a lag class larger than the value of the `MAXLAGS=` option is excluded from the semivariance calculation.

The `BANDWIDTH=` option complements the angle and lag tolerances in determining how point pairs are included in distance classes. Clearly, the number of pairs within each angle/distance class is strongly affected by the angle and lag tolerances and whether `BANDWIDTH=` has been specified. See also the section “[Angle Classification](#)” on page 8617 for more details about the effects these rules can have, since `BANDWIDTH=` operates in a manner similar to the `ANGLETOLERANCE=` option.

### Computation of the Distribution Distance Classes

This section deals with theoretical considerations and practical aspects when you specify the `LAGDISTANCE=` and `MAXLAGS=` options. In principle, these values depend on the amount and spatial distribution of your experimental data.

The value of the `LAGDISTANCE=` option regulates how many pairs of data are contained within each distance class. In effect, this information defines the pairwise distance distribution (see the following subsection). Your choice of `MAXLAGS=` specifies how many of these lags you want to include in the empirical semivariogram computation. Adjusting the values of these parameters is a crucial part of your analysis. Based on your observations sample, they determine whether you have sufficient points for a descriptive empirical semivariogram, and they can affect the accuracy of the estimated semivariance, too.

The simplest way of determining the distribution of pairwise distances is to determine the maximum distance  $h_{max}$  between any pair of points in your data, and then to divide this distance by some number  $N$  of intervals to produce distance classes of length  $\delta = h_{max}/N$ . The distance  $|P_1 P_2|$  between each pair of points  $P_1, P_2$  is computed, and the pair  $P_1 P_2$  is counted in the  $k$ th distance class if  $|P_1 P_2| \in [(k-1)\delta, k\delta)$  for  $k = 1, \dots, N$ .

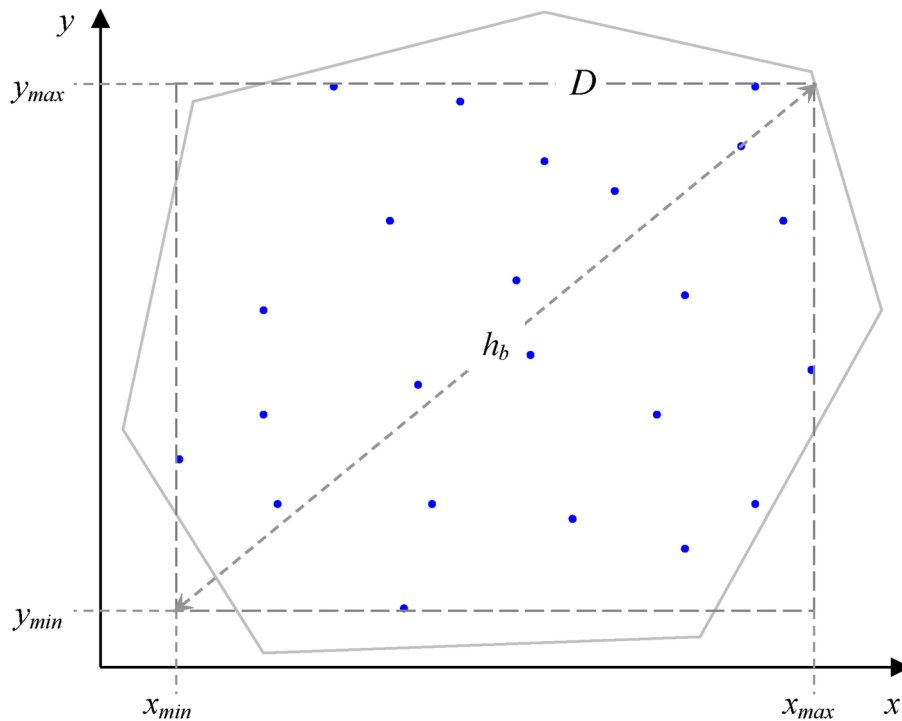


The actual computation is a slight variation of this. A bound, rather than the actual maximum distance, is computed. This bound is the length of the diagonal of a bounding rectangle for the data points. This bounding rectangle is found by using the maximum and minimum  $x$  and  $y$  coordinates,  $x_{max}$ ,  $x_{min}$ ,  $y_{max}$ ,  $y_{min}$ , and forming the rectangle determined by the following points:

$$\begin{array}{cc} (x_{min}, y_{max}) & (x_{max}, y_{max}) \\ (x_{min}, y_{min}) & (x_{max}, y_{min}) \end{array}$$

See Figure 102.24 for an illustration of the bounding rectangle applied to the data of the domain  $D$  in Figure 102.19. PROC VARIOGRAM provides you with the sizes of  $x_{max} - x_{min}$ ,  $y_{max} - y_{min}$ , and  $h_b$ . For example, in Figure 102.4 in the preliminary analysis, the specified parameters named “Max Data Distance in East,” “Max Data Distance in North,” and “Max Data Distance” correspond to the lengths  $x_{max} - x_{min}$ ,  $y_{max} - y_{min}$ , and  $h_b$ , respectively.

**Figure 102.24** Bounding Rectangle to Determine Maximum Pairwise Distance in Domain  $D$



The pairwise distance bound, denoted by  $h_b$ , is given by

$$h_b = \sqrt{(x_{max} - x_{min})^2 + (y_{max} - y_{min})^2}$$

Using  $h_b$ , the interval  $(0, h_b]$  is divided into  $N + 1$  subintervals, where  $N$  is the value of the `NHCLASSES=` option specified in the `COMPUTE` statement, or  $N = 10$  (default) if the `NHCLASSES=` option is not specified. The basic distance unit is  $h_0 = \frac{h_b}{N}$ ; the distance intervals are centered on  $h_0, 2h_0, \dots, Nh_0$ , with a distance tolerance of  $\pm \frac{h_0}{2}$ . The extra subinterval is  $(0, h_0/2)$  and corresponds to lag class zero. It is half

the length of the remaining subintervals, and it often contains the smallest number of pairs. [Figure 102.22](#) shows an example where the lag classes correspond to  $h_0 = 1$ . This method of partitioning the interval  $(0, h_b]$  is used in the empirical semivariogram computation.

### Choosing the Size of Classes

When you start with a data sample, the VARIOGRAM procedure computes all the distinct point pairs in the sample. The OUTPAIR= output data set, described in the section “[OUTPAIR=SAS-data-set](#)” on page 8642, contains information about these pairs. The point pairs are then categorized in classes. The size of each class depends on the common distance that separates consecutive classes. In PROC VARIOGRAM you need to provide this distance value with the [LAGDISTANCE=](#) option. Practically, you can define the distance between classes to be about the size of the average sampling distance (Olea 2006).

Under a more scrutinized approach, before you specify a value for the [LAGDISTANCE=](#) option, it is helpful to be aware of two issues. First, estimate how many classes of data pairs you might need. Each class contributes one point to the empirical semivariogram. Therefore, you need enough classes for an adequate number of points, so that your empirical semivariogram can suggest a suitable theoretical model shape for the description of the spatial continuity. Second, keep in mind that a larger number of data pairs in a class can contribute to a more accurate estimate of the corresponding semivariogram point.

The first consideration is a more general issue, and both this and the following subsection address it in detail. Based on the second consideration, the class size problem translates into having a sufficient number of data pairs in each class to produce an accurate semivariance estimate. However, only empirical rules of thumb exist to guide you with this choice. Examples of minimum-pairs empirical rules include the suggestion by Journel and Huijbregts (1978, p. 194) to use at least 30 point pairs for each lag class. Also, in a different approach, Chilès and Delfiner (1999, p. 38) increase this number to 50 point pairs.

Obviously, smaller data samples provide fewer data pairs in the sample. According to Olea (2006), it is difficult to properly estimate a semivariogram with fewer than 50 measurements. The preceding minimum-pairs practical rules are useful in cases where small samples are involved. When you work with a relatively small sample, the key is to specify the value of [LAGDISTANCE=](#) such that you can strike a balance between the number of the classes you can form and their pairs count. In the coal seam thickness example of the section “[Preliminary Spatial Data Analysis](#)” on page 8562, it is not possible to create a desirable large number of classes and maintain an adequate size for each one. On the other hand, there is no practical need to invoke these rules in the case of the much larger sample of ozone concentrations in “[Example 102.2: An Anisotropic Case Study with Surface Trend in the Data](#)” on page 8658.

The spatial distribution of the sample might also affect the grouping of pairs into classes. For example, data that are sampled in clusters might prove difficult to classify according to the preceding practical rules. One strategy to address this problem is to accept fewer than 30 pairs for the underpopulated distance classes. Then, at the stage when you determine what theoretical semivariogram model to use, either disregard the corresponding empirical semivariogram points or use them and accept the increased uncertainty.

The VARIOGRAM procedure can help you decide on a suitable class size before you proceed with the empirical semivariogram computation. First, provide a number for the class count by specifying the [NHCLASSES=](#) value. Run the procedure with the option [NOVARIOGRAM](#) in the [COMPUTE](#) statement and examine the distribution data pairs. Use different values of [NHCLASSES=](#) to investigate how this parameter affects the data pairs distribution in each distance class. The pairwise distance intervals table (for example, [Figure 102.3](#)) shows the number of pairs in each distance class in the “Number of Pairs” column, and you can use the preceding rule of thumb to adjust the [NHCLASSES=](#) value accordingly.

PROC VARIOGRAM displays a rounded value of the distance between the lag bounds as the “Lag Distance” parameter in the pairs information table (see Figure 102.5) or the pairwise distances histogram (see Figure 102.4), which you can use for the `LAGDISTANCE=` specification. However, this is only one tool. For the semivariogram computation you can specify your own `LAGDISTANCE=` value based on your experience. Smaller `LAGDISTANCE=` values result in fewer data pairs in the classes. In that sense, you might find smaller values useful when you work with large samples so that you obtain more semivariogram points. Also, if the `LAGDISTANCE=` value is too large, you might end up “wasting” too many point pairs in fewer classes at the expense of computing fewer semivariogram points and no significant accuracy gains in the estimation.

As explained earlier, depending on the sample size and its spatial distribution you might have classes with fewer points than what the practical rules advise. Most commonly, the deficient distance classes are the limiting ones close to the origin  $h = 0$  and the most remote ones at large  $h$ . The classes near the origin correspond to lags 0 and 1. These lags are crucial because the empirical semivariogram in small distances  $h$  characterizes the process smoothness and can help you detect the presence of a nugget effect. However, as discussed in the section “Distance Classification” on page 8619, lag zero is half the size of the rest of the classes by definition, so it can be expected to violate the rule of thumb for the number of pairs in a class.

The classes located at higher and extreme distances within a spatial domain are often not accounted for in the empirical semivariogram. The fewer pairs that can be formed in these distances do not allow for an accurate assessment of the spatial correlation, as is explained in the following section.

### ***Spatial Extent of the Empirical Semivariogram***

Given your choice for the `LAGDISTANCE=` value in your spatial domain, the following paragraphs provide guidelines on how many classes to consider when you compute the empirical semivariogram.

Obviously, you want to include no more classes beyond the limit where the pairs count falls below the minimum-pairs empirical rule threshold, as discussed in the preceding subsection. PROC VARIOGRAM provides you with a visual way to inspect this upper limit, if you decide to make use of the minimum-pairs empirical rule. In particular, specify your threshold choice for the minimum pairs per class by using the `THRESHOLD=` parameter for the `PLOTS=PAIRS` option.

Then, the procedure produces in the pairwise distances histogram a reference line at the specified `THRESHOLD=` value, which leaves below the line all lags whose pairs count is lower than the threshold value; see, for example, Figure 102.4. The last lag class whose pair population is above the `THRESHOLD=` value is reported in the pairs information table as “Highest Lag With Pairs > Threshold.” This value is not a recommendation for the `MAXLAGS=` option, but rather is an upper limit for your choice. Detailed information about the pairs count in each class is displayed in the corresponding pairwise distance intervals table, as Figure 102.3 demonstrates.

The preceding suggests that you have an upper limit indication, but you still need some criterion to decide how many lags to include in the semivariogram estimation. The criterion is the extent of spatial dependence in your domain.

Spatial dependence can exist beyond your domain limits. However, you have no data past your domain scale to define a range for larger-scale spatial dependencies. As you look for pairs of data that are gradually farther apart, the number of pairs naturally decreases with distance. The pairs at the more distant classes might be so few that they are likely to be independent with respect to the spatial dependence scale that you can detect. If you include the largest distances in your empirical semivariogram plot, then these pairs only contribute added noise. In the same sense, you cannot explore in detail spatial dependencies in scales

smaller than an average minimum distance between your data. The nugget effect represents then microscale correlations whose effect is evident in your working scale.

You specify the spatial dependence extent with commonly used measures such as the *correlation range* (or *correlation length*)  $\epsilon$  and the *correlation radius*  $h_c$ . Both are defined in a similar manner. The correlation range  $\epsilon$  is the distance at which the covariance is 5% of its value at  $\mathbf{h} = 0$ , and shows that beyond  $\epsilon$  the covariance is considered to be negligible. The correlation radius  $h_c$  is the distance at which the covariance is about half the variance at  $\mathbf{h} = 0$ , and indicates the distance over which significant correlations prevail (Christakos 1992, p. 76). The physical meanings of these measures are similar to that of the semivariogram range. Also, the effective range  $r_\epsilon$  used in asymptotically increasing semivariance models has essentially the same definition as the correlation range  $\epsilon$  (see the section “Theoretical Semivariogram Models” on page 8608).

A rough estimate of the correlation extent measures might be available from previous studies of a similar site, or from prior information about related measurements. In such an event, you typically want to consider a maximum pairwise distance that does not exceed the length of two or three correlation radii, or one and a half correlation ranges. You can then specify the `MAXLAGS=` value on the basis of the lags that fit in that distance.

When you have no estimates of correlation extent measures, you can use first use a crude measure to get started with your analysis: you can typically expect `MAXLAGS=` to be about half of the lag classes shown in the pairwise distances histogram.

Then, if necessary, you can refine your `MAXLAGS=` choice by using the following maximum lags rule of thumb: Journel and Huijbregts (1978, p. 194) advise considering lags up to about half of the extreme distance between data in the direction of interest. The VARIOGRAM procedure assists you in this task by providing the overall extreme data distance  $h_b$ , in addition to the extreme data distances in the vertical and horizontal axes directions. For example,  $h_b$  is reported in the pairs information table as “Maximum Data Distance” (see Figure 102.5), and in the pairwise distances histogram as “Max Data Distance” (see Figure 102.4).

Overall, avoid significant deviations from the maximum lags rule of thumb. As was stated earlier, a `MAXLAGS=` value that takes you well beyond the half-extreme distance between data in a given direction might give you limited accuracy in the empirical semivariance estimates at higher distances. At the other end, a value of `MAXLAGS=` that is too small might lead you to omit important information about the spatial structure that potentially lies within the range of distances you skipped.

## Semivariance Computation

With the classification of a point pair  $P_i P_j$  into an angle/distance class, as shown earlier in this section, the semivariance computation proceeds as follows.

Denote all pairs that  $P_i P_j$  belong to angle class  $[\theta_k - \delta\theta_k, \theta_k + \delta\theta_k)$  and distance class  $L = L(P_i P_j)$  as  $N(\theta_k, L)$ . For example, based on Figure 102.20 and Figure 102.21,  $P_1 P_2$  belongs to  $N(60^\circ, 1)$ .

Let  $|N(\theta_k, L)|$  denote the *number* of such pairs. The component of the standard (or method of moments) semivariance that correspond to angle/distance class  $N(\theta_k, L)$  is given by

$$\hat{\gamma}(h_k) = \frac{1}{2 |N(\theta_k, L)|} \sum_{P_i P_j \in N(\theta_k, L)} [V(s_i) - V(s_j)]^2$$

where  $h_k$  is the average distance in class  $N(\theta_k, L)$ ; that is,

$$h_k = \frac{1}{|N(\theta_k, L)|} \sum_{P_i P_j \in N(\theta_k, L)} |P_i P_j|$$

The robust version of the semivariance is given by

$$\bar{\gamma}(h_k) = \frac{\Psi^4(h_k)}{2[0.457 + 0.494/N(\theta_k, L)]}$$

where

$$\Psi(h_k) = \frac{1}{N(\theta_k, L)} \sum_{P_i P_j \in N(\theta_k, L)} [V(s_i) - V(s_j)]^{\frac{1}{2}}$$

This robust version of the semivariance is computed when you specify the **ROBUST** option in the **COMPUTE** statement in PROC VARIOGRAM.

PROC VARIOGRAM computes and writes to the **OUTVAR=** data set the quantities  $h_k$ ,  $\theta_k$ ,  $L$ ,  $N(\theta_k, L)$ ,  $\hat{\gamma}(h)$ , and  $\bar{\gamma}(h)$ .

## Empirical Semivariograms and Surface Trends

It was stressed in the beginning of the section “Theoretical and Computational Details of the Semivariogram” on page 8613 that if your data are not free of nonrandom surface trends, then the empirical semivariance  $\hat{\gamma}_z(\mathbf{h})$  you obtain from PROC VARIOGRAM represents a pseudo-semivariance rather than an estimate of the theoretical semivariance  $\gamma_z(\mathbf{h})$ .

In practice, two major difficulties appear. First, you might have no knowledge of underlying surface trends in your SRF  $Z(\mathbf{s})$ . It can be possible to have this information when you deal with a repetitive phenomenon (Chilès and Delfiner 1999, p. 123), or if you work within a subdomain of a broader region with known characteristics; often, though, this is not the case. Second, even if you suspect the existence of an underlying nonrandom trend, its precise nature might be unknown (Cressie 1993, p. 114, 162).

Based on the last remark, the criteria to define the exact form of a surface trend can be subjective. However, statistical methods can identify the presence and remove an estimate of such a trend. Different trend forms can be estimated in your SRF depending on the trend estimation model that you choose. This choice can lead to different degrees of smoothing in the residual random fluctuations. It might also have an effect on the residuals spatial structure characterization, because trend removals with different models are essentially different operations acting upon the values of your original observations. Following the comment by Chilès and Delfiner (1999, section 2.7.3), there are as many semivariograms of residuals as there are ways of estimating the trend. The same source also examines the introduction of bias in the semivariance of the residuals as a side effect of trend removal processes. This bias is small when you examine distances close to the origin  $\mathbf{h} = 0$ , and it can increase with distance.

Keeping in mind the preceding remarks, an approach you can take is to use one of the many predictive modeling tools in SAS/STAT software to estimate the unknown trend. Then you use PROC VARIOGRAM to analyze the residuals after you remove the trend. If the resulting model does not require too many degrees of freedom (such as if you use a low-order polynomial), then this approach might be sufficient. The

section “[Analysis with Surface Trend Removal](#)” on page 8662 demonstrates how to use PROC GLM (see Chapter 42, “[The GLM Procedure](#)”) for that purpose.

Apart from the standard semivariogram analysis, you can attempt to fit a theoretical semivariogram model to your empirical semivariogram if (a) either the analysis itself or your knowledge of the SRF does not clearly suggest the presence of any surface trend, or (b) the analysis can indicate a potentially trend-free direction, along which your data have a constant mean.

For example, you might observe overall similar values in your data. This can be an indication that your data are free of nonrandom trends, or that a very mild trend is present. The case falls under the preceding option (a). A very mild trend still allows a good determination of the semivariance at short distances according to Chilès and Delfiner (1999, p. 125), and this can be sufficient for your spatial prediction goal. An analysis of this type is assumed in the section “[Preliminary Spatial Data Analysis](#)” on page 8562.

If you observe similar values locally across a particular direction, this an instance of option (b). Olea (2006) suggests recognizing a trend-free direction as being perpendicular to the axis of the maximum dip in the values of  $Z(\mathbf{s})$ . If you suspect that at least one such direction exists for your data, then run PROC VARIOGRAM for a series of directions in the angular vicinity. The trend-free direction, if it exists, coincides with the one whose pseudo-semivariogram exhibits minimal increase with distance; see “[Example 102.3: Analysis without Surface Trend Removal](#)” on page 8672 for a demonstration of this approach. However, you cannot test  $Z(\mathbf{s})$  for anisotropy in this case, because you can investigate the semivariogram only in the single trend-free direction (Olea 1999, p. 76). Chilès and Delfiner (1999, section 2.7.4) suggest fitting a theoretical model in a trend-free direction only if the hypothesis of an isotropic semivariogram appears reasonable in your analysis.

As a result, you need to be very cautious when you choose to perform semivariogram analysis on data you have not previously examined for surface trends. In this event, both of the options (a) and (b) that were reviewed in the preceding paragraphs rely mostly on empirical and subjective criteria. As noted in this section, a degree of subjectivity exists in the selection of the surface trend itself. This fact suggests that a significant part of the semivariogram analysis is based on metastatistical decisions and on your understanding of your data and the physical considerations that govern your study. In any case, as shown in the section “[Theoretical and Computational Details of the Semivariogram](#)” on page 8613, your semivariogram analysis relies fundamentally on the use of trend-free data.

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## Theoretical Semivariogram Model Fitting

You can choose between two approaches to select a theoretical semivariogram model and fit the empirical semivariance. The first one is manual fitting, in which a theoretical semivariogram model is selected based on visual inspection of the empirical semivariogram. For example, see Hohn (1988, p. 25) and comments from defendants of this approach in Olea (1999, p. 82). The second approach is to perform model fitting in an automated manner. For this task you can use methods such as least squares, maximum likelihood, and robust methods (Cressie 1993, section 2.6).

The VARIOGRAM procedure features automated semivariogram model fitting that uses the weighted least squares (WLS) or the ordinary least squares (OLS) method. Use the **MODEL** statement to request that specific model forms or an array of candidate models be tested for optimal fitting to the empirical semivariance.

Assume that you compute first the empirical semivariance  $\gamma_z^*(\mathbf{h})$  at **MAXLAGS**= $k$  distance classes, where  $\gamma_z^*(\mathbf{h})$  can be either the classical estimate  $\hat{\gamma}_z(\mathbf{h})$  or the robust estimate  $\tilde{\gamma}_z(\mathbf{h})$ , as shown in the section “[Theoretical and Computational Details of the Semivariogram](#)” on page 8613. In fitting based on least



squares, you want to estimate the parameters vector  $\boldsymbol{\theta}$  of the theoretical semivariance  $\gamma_z(\mathbf{h})$  that minimizes the sum of square differences  $R(\boldsymbol{\theta})$  given by the expression

$$R(\boldsymbol{\theta}) = \sum_{i=1}^k w_i^2 [\gamma_z^*(\mathbf{h}_i) - \gamma_z(\mathbf{h}_i; \boldsymbol{\theta})]^2$$

For  $i = 1, \dots, k$ , the weights are  $w_i^2 = 1/\text{Var}[\gamma_z^*(\mathbf{h}_i)]$  in the case of WLS and  $w_i^2 = 1$  in the case of OLS. Therefore, the parameters  $\boldsymbol{\theta}$  are estimated in OLS by minimizing

$$R(\boldsymbol{\theta})_{OLS} = \sum_{i=1}^k [\gamma_z^*(\mathbf{h}_i) - \gamma_z(\mathbf{h}_i; \boldsymbol{\theta})]^2$$

For WLS, Cressie (1985) investigated approximations for the variance of both the classical and robust empirical semivariances. Then, under the assumptions of normally distributed observations and uncorrelated squared differences in the empirical semivariance, the approximate weighted least squares estimate of the parameters  $\boldsymbol{\theta}$  can be obtained by minimizing

$$R(\boldsymbol{\theta})_{WLS} = \frac{1}{2} \sum_{i=1}^k N(\mathbf{h}_i) \left[ \frac{\gamma_z^*(\mathbf{h}_i)}{\gamma_z(\mathbf{h}_i; \boldsymbol{\theta})} - 1 \right]^2$$

where  $N(\mathbf{h}_i)$  is the number of pairs of points in the  $i$ th distance lag.

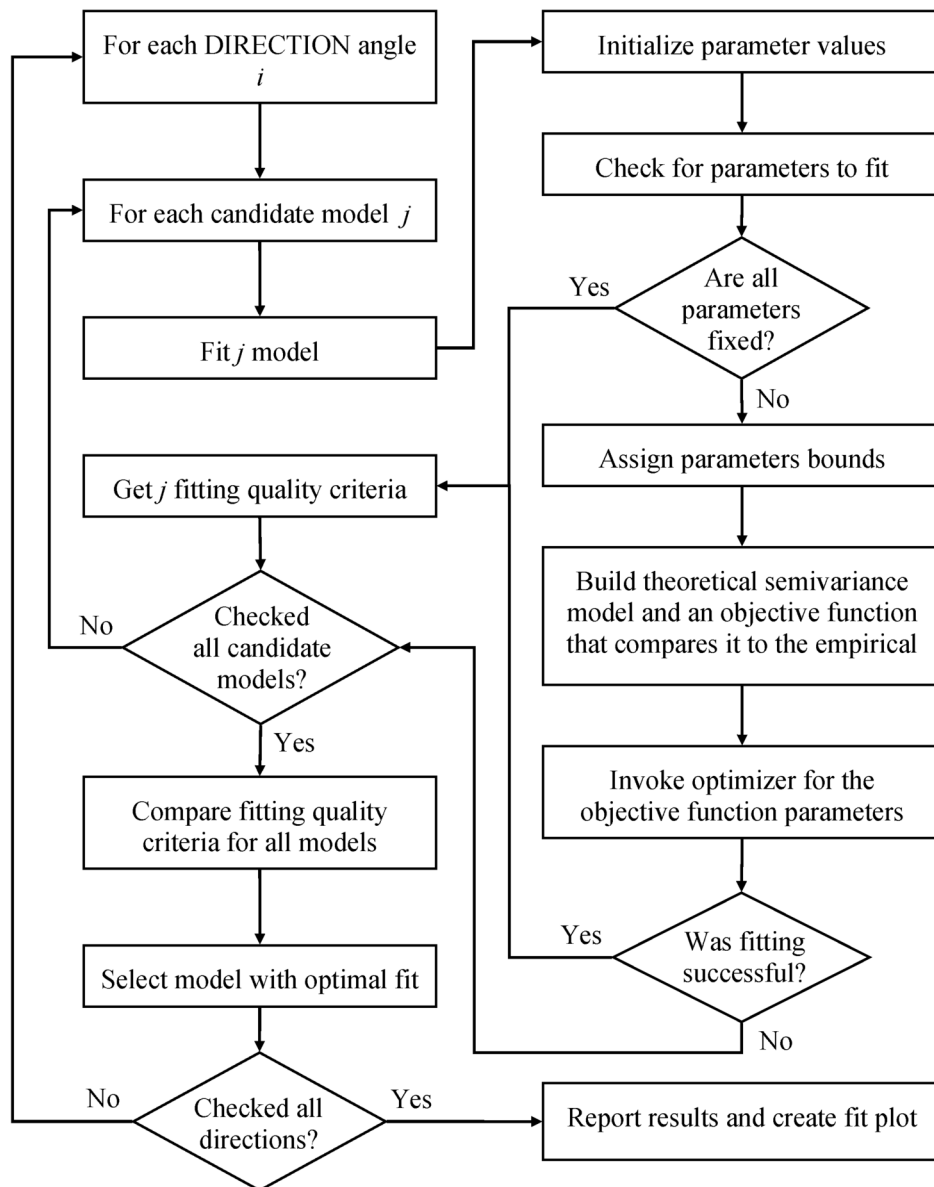
PROC VARIOGRAM relies on nonlinear optimization to minimize the least squares objective function  $R(\boldsymbol{\theta})$ . The outcome is the model that best fits the empirical semivariogram according to your criteria. The fitting process flow is displayed in [Figure 102.25](#). Goovaerts (1997, section 4.2.4) suggests that fitting a theoretical model should aim to capture the major spatial features. An accurate fit is desirable, but overfitting does not offer advantages, because you might find yourself trying to model possibly spurious details of the empirical semivariogram. At the same time, it is important to describe the correlation behavior accurately near the semivariogram origin. As pointed out by Chilès and Delfiner (1999, pp. 104–105), a poor description of spatial continuity at small lags can lead to loss of optimality in kriging predictions and erroneous reproduction of the variability in conditional simulations.

The significance of achieving better accuracy near the semivariogram origin is an advantage of the WLS method compared to OLS. In particular, the semivariance variance decreases when you get closer the origin  $\mathbf{h} = 0$ , as suggested in the section “[Theoretical and Computational Details of the Semivariogram](#)” on page 8613. The WLS weights are expressed as the inverse of this variance; as a result, WLS fitting is more accurate for distances  $\mathbf{h}$  near the semivariogram origin. In contrast, the OLS approach performs a least squares overall best fit because it assumes constant variance at all distances  $\mathbf{h}$ . Another advantage of WLS over OLS is that OLS falsely assumes that the differences in the optimization process are normally distributed and independent. However, WLS has the disadvantage that the weights depend on the fitting parameters.

Depending on your application, you can use WLS or OLS with PROC VARIOGRAM to fit classical semivariance. Other fitting methods include maximum likelihood approaches that rely crucially on the normality assumption for the data distribution, and the generalized least squares method that offers better accuracy but is computationally more demanding. You can find extensive discussions about these issues in Cressie (1993, section 2.3), Jian, Olea, and Yu (1996), Stein (1988), and Schabenberger and Gotway (2005).

The sections “Parameter Initialization” on page 8630 and “Quality of Fit” on page 8632 provide details and insight about semivariogram fitting, in addition to ways to cope with poor fits or no fit at all. These strategies can help you reach a meaningful description of spatial correlation in your problem.

**Figure 102.25** Semivariogram Fitting Process Flowchart





## Parameter Initialization

An important stage when you prepare for the model fitting process is initialization of the model parameters. As stated earlier, nonlinear optimization techniques are used in the fitting process. These techniques assist in the estimation of the model parameters, and being nonlinear means they can be very sensitive to selection of the initial values.

You can specify initial values close to the expected estimates when you have a relatively simple problem, such as in the example of the section “Getting Started: VARIOGRAM Procedure” on page 8561. In the case of nested models the selection of initial values can be more challenging because you have to assess the level of contribution for each one of the nested components.

The VARIOGRAM procedure features automatic selection of initial values based on the recommendations in Jian, Olea, and Yu (1996). Specifically, if you compute the estimated empirical semivariogram  $\hat{\gamma}_z(\mathbf{h})$  at  $k$  lags, then:

- The default initial nugget effect  $c_{n,0}$  is

$$c_{n,0} = \text{Max} \left[ 0, \hat{\gamma}_z(\mathbf{h}_1) - \frac{\mathbf{h}_1}{\mathbf{h}_2 - \mathbf{h}_1} [\hat{\gamma}_z(\mathbf{h}_2) - \hat{\gamma}_z(\mathbf{h}_1)] \right]$$

- The default initial slope  $\sigma_{0,0}^2$  and initial exponent  $a_{0,0}$  for the power model are

$$\sigma_{0,0}^2 = \frac{[\hat{\gamma}_z(\mathbf{h}_{k-2}) + \hat{\gamma}_z(\mathbf{h}_{k-1}) + \hat{\gamma}_z(\mathbf{h}_k)] / 3 - c_{n,0}}{\mathbf{h}_k - \mathbf{h}_1}$$

$$a_{0,0} = 1$$

- The default initial scale  $\sigma_{0,0}^2$  and initial range  $a_{0,0}$  for all other models are

$$\sigma_{0,0}^2 = \frac{[\hat{\gamma}_z(\mathbf{h}_{k-2}) + \hat{\gamma}_z(\mathbf{h}_{k-1}) + \hat{\gamma}_z(\mathbf{h}_k)]}{3} - c_{n,0}$$

$$a_{0,0} = 0.5\mathbf{h}_k$$

When you use the Matérn form, PROC VARIOGRAM sets the default initial value for the Matérn smoothness to  $\nu_0 = 1$ .

These rules are observed in the case of single, non-nested model fitting, and they are slightly modified to apply for nested model fitting as follows: Assume that you want to fit a nested model composed of  $m$  structures. As stated in the section “Nested Models” on page 8613, the nugget effect is a single parameter and is independent of the number of nested structures in a model. Also, the sum of the nested structure scales and the nugget effect, if any, must be equal to the total variance. For this reason, PROC VARIOGRAM simply divides the initial scale value it would assign to a non-nested model into  $m$  components  $\sigma_{0,0,1}^2, \dots, \sigma_{0,0,m}^2$ . For the range parameter, the VARIOGRAM procedure sets the initial range  $a_{0,0,1}$  of the first nested structure equal to the value it would assign to a non-nested model initial range. Then, the initial range  $a_{0,0,m}$  of the  $m$ -component is set recursively to half the value of the initial range  $a_{0,0,m-1}$  of the  $(m-1)$ -component.

Your empirical semivariogram must have nonmissing estimates at least at three lags so that you can use the automated fitting feature in PROC VARIOGRAM. Overall, if you specify a model form with  $q$  parameters to fit to an empirical semivariogram with nonmissing estimates at  $k$  lags, then the fitting problem is well-defined only when the degrees of freedom are  $DF = k - q \geq 0$ .

A potential numerical issue is that fitting could momentarily lead the fitting parameters to near-zero semi-variance values at lags away from zero distance. The theoretical semivariance is always positive for any distance larger than zero, and this is also a requirement for the numerical computation of  $R(\theta)_{WLS}$  in weighted least squares fitting. Such numerical issues are unlikely but possible, depending on the data set you use and the parameter initial values. If an event of nonpositive semivariance at a given lag occurs during an iteration, then PROC VARIOGRAM transparently adds a minimal amount of variance at that lag for the specific iteration. You can control this amount of variance with the `NEPSILON=` option of the `MODEL` statement. It is recommended that you leave this parameter at its default value.

The section concludes with a reminder of the fitting process sensitivity to the initial parameter values selection. The VARIOGRAM procedure facilitates this selection for you by using the simple rules shown earlier. However, the suggested initial values might not always be the best choice. In simple cases, such as the introductory example in the section “Getting Started: VARIOGRAM Procedure” on page 8561, this approach is very convenient and effective.

In principle, you are strongly encouraged to experiment with initial values. You want to make sure that the fitting process leads the model parameters to converge to estimates that make sense for your problem. When a parameter estimate seems unreasonable on the basis of your problem specification (for example, a model scale might be estimated to be 10 times the size of your sample variance, or the estimate of a range might be zero), PROC VARIOGRAM produces a note to let you know about a potentially ambiguous fit. These issues are examined in more detail in the section “Quality of Fit” on page 8632.

## Parameter Estimates

When the fit process is complete, the VARIOGRAM procedure produces the “Parameter Estimates” table with information about the fitted model parameters. The table includes estimates of the parameters, their approximate standard error, the statistical degrees of freedom DF, the corresponding  $t$  statistic, and its approximate  $p$ -value. For a model with  $q$  parameters that fits an empirical semivariogram of  $k$  nonmissing lags,  $DF = k - q$ .

**NOTE:** Parameter estimates might have nonzero standard errors even in the rather extreme case where  $DF = 0$ . This can typically occur when there are active optimization constraints in the fitting process.

You can request the confidence intervals for the parameter estimates of a fitted model by specifying the `CL` option of the `MODEL` statement. These confidence intervals are computed using the Wald-based formula

$$\hat{\beta}_i \pm \text{stderr}_i \times t(k - q, 1 - \alpha/2)$$

where  $\hat{\beta}_i$  is the  $i$ th parameter estimate,  $\text{stderr}_i$  is its estimated approximate standard error,  $t(k - q, 1 - \alpha/2)$  is the  $t$  statistic with  $DF = k - q$  degrees of freedom. The confidence intervals are only asymptotically valid. The significance level  $\alpha$  used in the construction of these confidence limits can be set with the `ALPHA=` option of the `MODEL` statement; the default value is  $\alpha = 0.05$ .

Specify the `COVB` and the `CORRB` options in the `MODEL` statement to request the approximate covariance and approximate correlation matrices of the fitted parameters, respectively. These matrices are based on the optimization process results. In agreement with reporting similar optimization output in SAS/STAT software, parameters with active restraints have zeros in the corresponding rows and columns in the covariance and correlation matrices, and display 1 in the correlation matrix diagonal.

## Quality of Fit

The VARIOGRAM procedure produces a fit summary table to report about the goodness of fit. When you specify multiple models to fit with the `FORM=AUTO` option in the `MODEL` statement, the VARIOGRAM procedure uses two processes to rank the fitted models: The first one depends on your choice among available fitting criteria. The second one is based on an operational classification of equivalent models in classes. The two processes are described in more detail in the following subsections.

Overall, no absolutely correct way exists to rank and classify multiple models. Your choice of ranking criteria could depend on your study specifications, physical considerations, or even your personal assessment of fitting performance. The VARIOGRAM procedure provides you with fitting and comparison features to facilitate and help you better understand the fitting process.

### Fitting Criteria

The fit summary table ranks multiple models on the basis of one or more fitting criteria that you can specify with the `CHOOSE=` option of the `MODEL` statement, as explained in the section “Syntax: VARIOGRAM Procedure” on page 8576. Currently, the VARIOGRAM procedure offers two numerical criteria (for which a smaller value indicates a better fit) and a qualitative criterion:

- The residual sum of squares error (SSE) is based on the objective function of the fitting process. When the specified method is weighted least squares, the sum of squares of the weighted differences (WSSE) is computed according to the expression

$$\text{WSSE} = \sum_{i=1}^k w_i^2 [\gamma_z^*(\mathbf{h}_i) - \gamma_z(\mathbf{h}_i; \boldsymbol{\theta})]^2$$

where  $\gamma_z^*(\mathbf{h}_i)$  can be either the classical or robust semivariance estimate of the theoretical semivariance  $\gamma_z(\mathbf{h}_i; \boldsymbol{\theta})$  at the  $i$ th lag and the weights  $w_i^2$  are taken at lags  $i = 1, \dots, k$ . When you specify the `METHOD=OLS` option in the `MODEL`, the weights  $w_i^2 = 1$  for  $i = 1, \dots, k$ , and the SSE is expressed as

$$\text{SSE} = \sum_{i=1}^k [\gamma_z^*(\mathbf{h}_i) - \gamma_z(\mathbf{h}_i; \boldsymbol{\theta})]^2$$

- Akaike’s information criterion (AIC) is included in the fit summary table when there is at least one nonfixed parameter. In its strict definition, AIC assumes that the model errors are normally and independently distributed. This assumption is not correct in the semivariance fitting analysis. However, the AIC can be also defined in an operational manner on the basis of the weighted squared error sum WSSE as

$$\text{AIC} = k \ln \left( \frac{\text{WSSE}}{k} \right) + 2q$$

for  $k$  lags and  $q$  model parameters; see, for example, Olea (1999, p. 84). The operational definition of the AIC is provided as an additional criterion for the comparison of fitted models in PROC VARIOGRAM.

The AIC expression suggests that when you specify multiple models with the `FORM=AUTO` option in the `MODEL` statement, all models with the same number of parameters are ranked in the same way by the AIC and the WSSE criteria. Among models with the same WSSE value, AIC ranks higher the ones with fewer parameters.

- The third qualitative criterion enables you to classify multiple models based on their convergence status. A model is sent to the bottom of the ranking table if the parameter estimation optimization fails to converge or fitting is unsuccessful due to any other issue. These two cases are distinguished by the different notes they produce in the fit summary ODS table. If you specify the `STORE` statement to save the fitting output in an item store, then models that have failed to fit are not passed to the item store.

With respect to convergence status, PROC VARIOGRAM ranks higher those models that have successfully completed the fitting process. It might occur that the selection of parameter initial values, physical considerations about the forms that are used for the fit, or numerical aspects of the nonlinear optimization could result in ambiguous fits. For example, you might see that model parameters converge at or near their boundary values, or that parameters have unreasonably high estimates when compared to the empirical semivariogram characteristics. Then, the fit summary table designates such fits as questionable.

You might not need to take any action if you are satisfied with the fitting results and the selected model. You can investigate questionable fits in one or more of the following ways:

- If a form in a nested model makes no contribution to the model due to a parameter at or near its boundary value, then you could have a case of a degenerate fit. When you fit multiple models, a model with degenerate fit can collapse to the more simple model that does not include the noncontributing form. The VARIOGRAM procedure includes in its fit summary all models that are successfully fit. In such cases you can ignore degenerate fits. You can also try subsequent fits of individual models and exclude noncontributing forms or use different initial values.
- Unreasonably low or high parameter estimates might be an indication that the current initial values are not a good guess for the nonlinear optimizer. In most cases, fitting an empirical semivariogram gives you the advantage of a fair understanding about the value range of your parameters. Then, you can use the `PARMS` statement to specify a different set of initial values and try the fit again.
- Try replacing the problematic form with another one. A clear example is that you can expect a very poor fit if you specify an exponential model to fit an empirical semivariogram that suggests linear behavior.

Eventually, if none of the aforementioned issues exist, then a model is ranked in the highest positions of the fit summary table. You can combine two or more of the fitting criteria to manage classification of multiple fitted models in a more detailed manner.

In some cases you might still experience a poor quality of fit or no fit at all. If none of the earlier suggestions results in a satisfactory fit, then you could decide to re-estimate the empirical semivariogram for your same input data. The following actions can produce different empirical semivariograms to fit a theoretical model to:

- If you compute the semivariogram for different angles and you experience optimization failures, try specifying explicitly the same direction angles with different tolerance or bandwidth value in the `DIRECTIONS` statement.
- Modify slightly the `LAGDISTANCE=` option in the `COMPUTE` statement to obtain a different empirical semivariogram.

Finally, it is possible to have models in the fitting summary table ranked in a way that seemingly contradicts the specification in the **CHOOSE=** option of the **MODEL** statement. Consider an example with the default behavior **CHOOSE=(SSE AIC)**, where you might observe that models have the same SSE values but are not ranked further as expected by the AIC criterion. A closer examination of such cases typically reduces this issue to a matter of the accuracy shown in the table. That is, the displayed accuracy of the SSE values might hide additional decimal digits that justify the given ranking.

In such scenarios, discrimination of models at the limits of numerical accuracy might suggest that you choose a model of questionable fit or a nested structure over a more simple one. You can then review the candidate models and exercise your judgment to select the model that works best for you. If all values of a criterion are equal, then the ranking order is simply the order in which models are examined unless more criteria follow that can affect the ranking.

### **Classes of Equivalence**

The fit summary that is produced after fitting multiple models further categorizes the ranked models in classes of equivalence. Equivalence classification is an additional investigation that is unrelated to the ranking criteria presented in the previous subsection; it is an operational criterion that provides you with a qualitative overview of multiple model fit performance under given fitting conditions.

To examine model equivalence, the VARIOGRAM procedure computes the semivariances for each one of the fitted models at a set of distances. For any pair of consecutively ranked models, if the sum of their semivariance absolute differences at all designated distances is smaller than the tolerance specified by the **EQUIVTOL=** parameter, then the two models are deemed equivalent and placed in the same class; otherwise, they are placed in different classes. Equivalence classification depends on the existing ranking; hence the resulting classes can differ when you specify different ranking criteria in the **CHOOSE=** option of the **MODEL** statement.

The equivalence class numbers start at 1 for the top-ranked model in the fit summary table. You can consider the top model of each equivalence class to be a representative of the class behavior. When you specify that fit plots be produced and there are equivalence classes, the plot displays the equivalence classes and the legend designates each one by its representative model.

Consequently, if an equivalence class contains multiple members after a fit, then all of its members produce in general the exact same semivariogram. A typical reason could be that the fitting process estimates of scale parameters are at or close to their zero boundaries in one or more nested forms in a model. In such cases, the behavior of this model reduces to the behavior of its nested components with nonzero parameters. When one or more models share this situation or have the same contributing nested forms, they could end up as members of the same equivalence class depending on the ranking criteria.

It is not necessary for all models in the same equivalence class to produce the exact same semivariogram. If a fit of two obviously different forms involves semivariance values that are small enough for the equivalence criterion to be satisfied by the default value of the **EQUIVTOL=** option, then you might need to specify an even smaller value in the **EQUIVTOL=** option to rank these two models in separate equivalence classes.

### **Fitting with Matérn Forms**

When you use a Matérn form in the fitting process, it is possible that the fitting optimizer might encounter numerical difficulties if it tries to push the smoothing parameter  $\nu$  towards increasingly high values. The VARIOGRAM procedure addresses this issue by imposing an amply elevated upper bound of 1,000,000 on the smoothness values it processes. The section “[Characteristics of Semivariogram Models](#)” on page 8609

mentions that  $\nu \rightarrow \infty$  gives the Gaussian model. In the scenario of progressively increasing smoothness values, PROC VARIOGRAM acknowledges that the Matérn form behavior tends asymptotically to become Gaussian and replaces automatically the Matérn with a Gaussian form in the model. Subsequently, fitting resumes with the resulting model.

If you explore fitting of multiple models, then any duplicate models that might occur due to Matérn-to-Gaussian form conversions are fitted only once. Also, if a nested model has more than one Matérn form, then the fitting process checks one of them at a time about whether they need to be replaced by a Gaussian form. Consequently, following the switch of one Matérn form, the fitting process starts anew with the resulting model before any decisions for additional form conversions are made.

Replacement of the Matérn form with the Gaussian form occurs by default when  $\nu > 10,000$ . However, you can control this threshold value with the `MTOGTOL=` parameter of the `MODEL` statement. Practically, the Matérn form starts to resemble the Gaussian behavior for  $\nu$  values that are about  $\nu > 10$ . If you encounter such conversions of the Matérn form into Gaussian and you prefer to set a lower  $\nu$  threshold for the conversion than the default, you might experience improved code performance because computation of the Matérn semivariance can be numerically demanding.

---

## Autocorrelation Statistics

Spatial autocorrelation measures offer you additional insight into the interdependence of spatial data. These measures quantify the correlation of an SRF  $Z(s)$  with itself at different locations, and they can be very useful whether you have information at exact locations (point-referenced data) or measurements that characterize an area type such as counties, census tracts, zip codes, and so on (areal data).

As in the semivariogram computation, a key issue for the autocorrelation statistics is that you work with a set  $z_i$  of measurements,  $i = 1, \dots, n$ , that are free of nonrandom surface trends and have a constant mean.

## Autocorrelation Weights

In general, the choice of a weighting scheme is subjective. You can obtain different results by using different schemes, options, and parameters. PROC VARIOGRAM offers you considerable flexibility in choosing weights that are appropriate for prior considerations such as different hypotheses about neighboring areas, definition of the neighborhood structure, and accounting for natural barriers or other spatial characteristics; see the discussion in Cliff and Ord (1981, p. 17). As stressed for all types of spatial analysis, it is important to have good knowledge of your data. In the autocorrelation statistics, this knowledge can help you avoid spurious correlations when you choose the weights.

The starting point is to assign individual weights to each one of the  $n$  data values  $z_i$ ,  $i = 1, \dots, n$ , with respect to the rest. An  $n \times n$  matrix of weights is thus defined, such that for any two locations  $s_i$  and  $s_j$ , the weight  $w_{ij}$  denotes the effect of the value  $z_i$  at location  $s_i$  on the value  $z_j$  at location  $s_j$ . Depending on the nature of your study, the weights  $w_{ij}$  need not be symmetric; that is, it can be true that  $w_{ij} \neq w_{ji}$ .

### Binary and Nonbinary Weights

The weights  $w_{ij}$  can be either binary or nonbinary values. Binary values of 1 or 0 are assigned if the SRF  $Z(s_i)$  at one location  $s_i$  is deemed to be connected or not, respectively, to its value  $Z(s_j)$  at another location  $s_j$ . Nonbinary values can be used in the presence of more refined measures of connectivity between any two data points  $P_i$  and  $P_j$ . PROC VARIOGRAM offers a choice between a binary and a distance-based nonbinary weighting scheme.



In the binary weighting scheme the weight  $w_{ij} = 1$  if the data pair at  $s_i$  and  $s_j$  is closer than the user-defined distance that is defined by the **LAGDISTANCE=** option, and  $w_{ij} = 0$  if  $i = j$  or in any other case. For that reason, in the **COMPUTE** statement, if you specify the **WEIGHTS=BINARY** suboption of the **AUTOCORRELATION** option when the **NOVARIOGRAM** option is also specified, then you must also specify the **LAGDISTANCE=** option.

The nonbinary weighting scheme is based on the pair distances and is invoked with the **WEIGHTS=DISTANCE** suboption of the **AUTOCORRELATION** option. PROC VARIOGRAM uses a variation of the Pareto form functional to set the weights. Namely, the autocorrelation weight for every point pair  $P_i$  and  $P_j$  located at  $s_i$  and  $s_j$ , respectively, is defined as

$$w_{ij} = s \frac{1}{1 + |\mathbf{h}|^p}$$

where  $\mathbf{h} = s_i - s_j$  and  $p \geq 0$  and  $s \geq 0$  are user-defined parameters for the adjustment of the weights.

In particular, the power parameter  $p$  is specified in the **POWER=** option of the **DISTANCE** suboption within the **AUTOCORRELATION** option. The default value for this parameter is  $p = 1$ . Also, the scaling parameter  $s$  is specified by the **SCALE=** option in the **DISTANCE** suboption of the **AUTOCORRELATION** option. The default value for the scaling parameter is  $s = 1$ . You can use the  $p$  and  $s$  parameters to adjust the actual values of the weights according to your needs. Variations in the scaling parameter  $s$  do not affect the computed values of the Moran's  $I$  and Geary's  $c$  autocorrelation coefficients that are introduced in the section "Autocorrelation Statistics Types" on page 8637.

### Nonbinary Weights with Normalized Distances

PROC VARIOGRAM offers additional flexibility in the **DISTANCE** weighting scheme through an option to use normalized pair distances. You can invoke this feature by specifying the **NORMALIZE** option in the **DISTANCE** suboption of the **AUTOCORRELATION** option. In this case, the distances used in the definition of the weights are normalized by the maximum pairwise distance  $h_b$  (see the section "Computation of the Distribution Distance Classes" on page 8621 and Figure 102.24); the weights are then defined as  $w_{ij} = s/[1 + (|\mathbf{h}|/h_b)^p]$ .

Most likely,  $h_b$  has a different value for different data sets. Hence, it is suggested that you avoid using the weights you obtain from the preceding equation and one data set for comparisons with the weights you derive from different data sets.

### Symmetric and Asymmetric Weights

The weighting schemes presented in the preceding paragraphs are symmetric; that is,  $w_{ij} = w_{ji}$  for every data pair at locations  $s_i$  and  $s_j$ . However, you can also define asymmetric weights  $w'_{ij}$  such that

$$\sum_{j \in J} w'_{ij} = 1$$

for  $i = 1, 2, \dots, n$ , where  $w'_{ij} = w_{ij} / \sum_{j \in J} w_{ij}$ ,  $i = 1, 2, \dots, n$ . In the distance-based scheme,  $J$  is the set of all locations that form point pairs with the point at  $s_i$ . In the binary scheme,  $J$  is the set of the locations that are connected to  $s_i$  based on your selection of the **LAGDISTANCE=** option; see Cliff and Ord (1981, p. 18). The weights  $w'_{ij}$  are *row-averaged* (or *standardized* by the count of their connected neighbors). You can apply row averaging in weights when you specify the **ROWAVG** option within either the **BINARY** or **DISTANCE** suboptions in the **AUTOCORRELATION** option.

## Autocorrelation Statistics Types

One measure of spatial autocorrelation provided by PROC VARIOGRAM is Moran's  $I$  statistic, which was introduced by Moran (1950) and is defined as

$$I = \frac{n}{(n-1)S^2W} \sum_i \sum_j w_{ij} v_i v_j$$

where  $S^2 = (n-1)^{-1} \sum_i v_i^2$ , and  $W = \sum_i \sum_{j \neq i} w_{ij}$ .

Another measure of spatial autocorrelation in PROC VARIOGRAM is Geary's  $c$  statistic (Geary 1954), defined as

$$c = \frac{1}{2S^2W} \sum_i \sum_j w_{ij} (z_i - z_j)^2$$

These expressions indicate that Moran's  $I$  coefficient makes use of the centered variable, whereas the Geary's  $c$  expression uses the noncentered values in the summation.

Inference on these two statistic types comes from approximate tests based on the asymptotic distribution of  $I$  and  $c$ , which both tend to a normal distribution as  $n$  increases. To this end, PROC VARIOGRAM calculates the means and variances of  $I$  and  $c$ . The outcome depends on the assumption made regarding the distribution  $Z(\mathbf{s})$ . In particular, you can choose to investigate any of the statistics under the *normality* (also known as *Gaussianity*) or the *randomization* assumption. Cliff and Ord (1981) provided the equations for the means and variances of the  $I$  and  $c$  distributions, as described in the following.

The normality assumption asserts that the random field  $Z(\mathbf{s})$  follows a normal distribution of constant mean ( $\bar{Z}$ ) and variance, from which the  $z_i$  values are drawn. In this case, the  $I$  statistics yield

$$E_g[I] = -\frac{1}{n-1}$$

and

$$E_g[I^2] = \frac{1}{(n+1)(n-1)W^2} (n^2 S_1 - n S_2 + 3W^2)$$

where  $S_1 = 0.5 \sum_i \sum_{j \neq i} (w_{ij} + w_{ji})^2$  and  $S_2 = \sum_i (\sum_j w_{ij} + \sum_j w_{ji})^2$ . The corresponding moments for the  $c$  statistics are

$$E_g[c] = 1$$

and

$$\text{Var}_g[c] = \frac{(2S_1 + S_2)(n-1) - 4W^2}{2(n+1)W^2}$$

According to the randomization assumption, the  $I$  and  $c$  observations are considered in relation to all the different values that  $I$  and  $c$  could take, respectively, if the  $n$   $z_i$  values were repeatedly randomly permuted around the domain  $D$ . The moments for the  $I$  statistics are now

$$E_r[I] = -\frac{1}{n-1}$$



and

$$E_r[I^2] = \frac{A_1 + A_2}{(n-1)(n-2)(n-3)W^2}$$

where  $A_1 = n[(n^2 - 3n + 3)S_1 - nS_2 + 3W^2]$ ,  $A_2 = -b_2[n(n-1)S_1 - 2nS_2 + 6W^2]$ . The factor  $b_2 = m_4/(m_2^2)$  is the coefficient of kurtosis that uses the sample moments  $m_k = \frac{1}{n} \sum_i v_i^k$  for  $k = 2, 4$ . Finally, the  $c$  statistics under the randomization assumption are given by

$$E_r[c] = 1$$

and

$$\text{Var}_r[c] = \frac{B_1 + B_2 + B_3}{n(n-2)(n-3)W^2}$$

with  $B_1 = (n-1)S_1[n^2 - 3n + 3 - (n-1)b_2]$ ,  $B_2 = -\frac{1}{4}(n-1)S_2[n^2 + 3n - 6 - (n^2 - n + 2)b_2]$ , and  $B_3 = W^2[n^2 - 3 - b_2(n-1)^2]$ .

If you specify `LAGDISTANCE=` to be larger than the maximum data distance in your domain, the binary weighting scheme used by the VARIOGRAM procedure leads to all weights  $w_{ij} = 1$ ,  $i \neq j$ . In this extreme case the preceding definitions can show that the variances of the  $I$  and  $c$  statistics become zero under either the normality or the randomization assumption.

A similar effect might occur when you have collocated observations (see the section “Pair Formation” on page 8616). The Moran’s  $I$  and Geary’s  $c$  statistics allow for the inclusion of such pairs in the computations. Hence, contrary to the semivariance analysis, PROC VARIOGRAM does not exclude pairs of collocated data from the autocorrelation statistics.

## Interpretation

For Moran’s  $I$  coefficient,  $I > E[I]$  indicates positive autocorrelation. Positive autocorrelation suggests that neighboring values  $s_i$  and  $s_j$  tend to have similar feature values  $z_i$  and  $z_j$ , respectively. When  $I < E[I]$ , this is a sign of negative autocorrelation, or dissimilar values at neighboring locations. A measure of strength of the autocorrelation is the size of the absolute difference  $|I - E[I]|$ .

Geary’s  $c$  coefficient interpretation is analogous to that of Moran’s  $I$ . The only difference is that  $c > E[c]$  indicates negative autocorrelation and dissimilarity, whereas  $c < E[c]$  signifies positive autocorrelation and similarity of values.

The VARIOGRAM procedure uses the mathematical definitions in the preceding section to provide the observed and expected values, and the standard deviation of the autocorrelation coefficients in the autocorrelation statistics table. The  $Z$  scores for each type of statistics are computed as

$$Z_I = \frac{I - E[I]}{\sqrt{\text{Var}[I]}}$$

for Moran’s  $I$  coefficient, and

$$Z_c = \frac{c - E[c]}{\sqrt{\text{Var}[c]}}$$

for Geary's  $c$  coefficient. PROC VARIOGRAM also reports the two-sided  $p$ -value for each coefficient under the null hypothesis that the sample values are not autocorrelated. Smaller  $p$ -values correspond to stronger autocorrelation for both the  $I$  and  $c$  statistics. However, the  $p$ -value does not tell you whether the autocorrelation is positive or negative. Based on the preceding remarks, you have positive autocorrelation when  $Z_I > 0$  or  $Z_c < 0$ , and you have negative autocorrelation when  $Z_I < 0$  or  $Z_c > 0$ .

## The Moran Scatter Plot

The Moran scatter plot (Anselin 1996) is a useful visual tool for exploratory analysis, because it enables you to assess how similar an observed value is to its neighboring observations. Its horizontal axis is based on the values of the observations and is also known as the response axis. The vertical Y axis is based on the weighted average or spatial lag of the corresponding observation on the horizontal X axis. **NOTE:** The term *spatial lag* in the current context is unrelated to the concept of the semivariogram lag presented in the section “Distance Classification” on page 8619.

The Moran scatter plot provides a visual representation of spatial associations in the neighborhood around each observation. You specify a neighborhood size with the `LAGDISTANCE=` option in the `COMPUTE` statement. The observations are represented by their standardized values; therefore only nonmissing observations are shown in the plot. For each one of those, the VARIOGRAM procedure computes the weighted average, which is the weighted mean value of its neighbors. Then, the centered weighted average is plotted against the standardized observations. As a result, the scatter plot is centered on the coordinates (0, 0), and distances in the plot are expressed in deviations from the origin (0, 0).

Depending on their position on the plot, the Moran plot data points express the level of spatial association of each observation with its neighboring ones. Conceptually, these characteristics differentiate the Moran plot from the semivariogram. The latter is typically used in geostatistics to depict spatial associations across the whole domain as a continuous function of a distance metric.

You can find the data points on the Moran scatter plot in any of the four quadrants defined by the horizontal line  $y = 0$  and the vertical line  $x = 0$ . Points in the upper right (or high-high) and lower left (or low-low) quadrants indicate positive spatial association of values that are higher and lower than the sample mean, respectively. The lower right (or high-low) and upper left (or low-high) quadrants include observations that exhibit negative spatial association; that is, these observed values carry little similarity to their neighboring ones.

When you use binary, row-averaged weights for the creation of the Moran scatter plot and in autocorrelation statistics, Moran's  $I$  coefficient is equivalent to the regression slope of the Moran scatter plot. That is, when you specify

```
PLOTS=MORAN (ROWAVG=ON)
```

in the `PROC VARIOGRAM` statement and

```
AUTOCORR (WEIGHTS=BINARY (ROWAVERAGING))
```

in the `COMPUTE` statement, then the regression line slope of the Moran scatter plot is the Moran's  $I$  coefficient shown in the section “Autocorrelation Statistics Types” on page 8637. In this sense, the Moran's  $I$  coefficient has a global character, whereas the Moran scatter plot provides you with a more detailed exploratory view of the autocorrelation behavior of the individual observations.

This detailed view can reveal outliers with respect to the regression line slope of the Moran scatter plot. Outliers, if present, can function as leverage points that affect the value of Moran's  $I$  coefficient. As noted by Anselin (1996), such extremes indicate local instability in spatial association. This instability can be caused either by problems with the autocorrelation weights matrix or by fine-scale characteristics of the spatial structure, which are beneath the current observation structure.

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## Computational Resources

The fundamental computation of the VARIOGRAM procedure is binning: for each pair of observations in the input data set, a distance class and an angle class are determined and recorded. Let  $N_d$  denote the number of distance classes,  $N_a$  denote the number of angle classes, and  $N_v$  denote the number of VAR variables. The memory requirements for these operations are proportional to  $N_d \times N_a \times N_v$ . This is typically small.

The CPU time required for the computations is proportional to the number of pairs of observations, or to  $N^2 \times N_v$ , where  $N$  is the number of observations in the input data set.

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## Output Data Sets

The VARIOGRAM procedure produces four data sets: the OUTACWEIGHTS=*SAS-data-set*, the OUTDIST=*SAS-data-set*, the OUTPAIR=*SAS-data-set*, and the OUTVAR=*SAS-data-set*. These data sets are described in the following sections.

### OUTACWEIGHTS=*SAS-data-set*

The OUTACWEIGHTS= data set contains one observation for each pair of points  $P_1, P_2$  in the original data set, where  $P_1$  is different from  $P_2$ , with information about the data distance and autocorrelation weight of each point pair.

The OUTACWEIGHTS= data set can be very large, even for a moderately sized DATA= data set. For example, if the DATA= data set has NOBS=500, then the OUTACWEIGHTS= data set has  $\text{NOBS}(\text{NOBS} - 1)/2 = 124,750$  observations.

When you perform autocorrelation computations, the OUTACWEIGHTS= data set is a practical way to save the autocorrelation weights for further use.

The OUTACWEIGHTS= data set contains the following variables:

- ACWGHT12, the autocorrelation weight for the pair  $P_1, P_2$
- ACWGHT21, the autocorrelation weight for the pair  $P_2, P_1$
- DISTANCE, the distance between the data in the pair
- ID1, the ID variable value or observation number for the first point in the pair
- ID2, the ID variable value or observation number for the second point in the pair
- V1, the variable value for the first point in the pair
- V2, the variable value for the second point in the pair

- VARNAME, the variable name for the current VAR variable
- X1, the  $x$  coordinate of the first point in the pair
- X2, the  $x$  coordinate of the second point in the pair
- Y1, the  $y$  coordinate of the first point in the pair
- Y2, the  $y$  coordinate of the second point in the pair

When the autocorrelation weights are symmetric, the pair  $P_1, P_2$  has the same weight as the pair  $P_2, P_1$ . For this reason, in the case of symmetric weights the OUTACWEIGHTS= data set contains only the autocorrelation weights ACWGHT12.

If no ID statement is specified, then the corresponding observation number is assigned to each one of the variables ID1 and ID2, instead.

### **OUTDIST=SAS-data-set**

The OUTDIST= data set contains counts for a modified histogram that shows the distribution of pairwise distances. This data set provides you with information related to the choice of values for the LAGDISTANCE= option in the COMPUTE statement.

To request an OUTDIST= data set, specify the OUTDIST= data set in the PROC VARIOGRAM statement and the NOVARIOGRAM option in the COMPUTE statement. The NOVARIOGRAM option prevents any semivariogram or covariance computation from being performed.

The following variables are written to the OUTDIST= data set:

- COUNT, the number of pairs that fall into this lag class
- LAG, the lag class value
- LB, the lower bound of the lag class interval
- UB, the upper bound of the lag class interval
- PER, the percent of all pairs that fall in this lag class
- VARNAME, the name of the current VAR variable

### **OUTMORAN=SAS-data-set**

The OUTMORAN= data set contains the standardized value (or response) of each observation and the weighted average of its  $N$  neighbors, based on a neighborhood within a LAGDISTANCE= distance from the observation. To request this data set, specify the OUTMORAN= data set in the PROC VARIOGRAM statement, in addition to the AUTOCORRELATION and LAGDISTANCE= options in the COMPUTE statement.

The following variables are written to the OUTMORAN= data set:

- DISTANCE, the value of the neighborhood radius, which is specified with the LAGDISTANCE= option
- ID, the ID variable value or observation number for the current observation
- N, the number of neighbors within the specified DISTANCE from the current observation
- RESPONSE, the standardized value of the current observation
- STDWAVG, the standardized weighted average of the neighbors for the current observation
- V, the variable value of the current observation
- VARNAME, the variable name for the current VAR variable
- X, the  $x$  coordinate of the current observation
- Y, the  $y$  coordinate of the current observation
- WAVG, the weighted average of the neighbors for the current observation

For zero neighbors in the neighborhood of a nonmissing observation, the corresponding value of the variable N=0 and the variables STDWAVG and WAVG are assigned missing values. Observations with missing values are included in the OUTMORAN= data set if they have neighbors and only if nonmissing observations with neighbors also exist in the same data set.

### OUTPAIR=SAS-data-set

When you specify the NOVARIOGRAM option in the COMPUTE statement, the OUTPAIR= data set contains one observation for each distinct pair of points  $P_1, P_2$  in the original data set. Otherwise, the OUTPAIR= data set might have fewer observations, depending on the values you specify in the LAGDISTANCE= and MAXLAGS= options and whether you specify the OUTPDISTANCE= option in the COMPUTE statement.

If the NOVARIOGRAM option is not specified in the COMPUTE statement, then the OUTPAIR= data set contains one observation for each distinct pair of points that are up to a distance within MAXLAGS= away from each other. If you also specify the OUTPDISTANCE= $D_{max}$  option in the COMPUTE statement, then all pairs  $P_1, P_2$  in the original data set that satisfy the relation  $|P_1 P_2| \leq D_{max}$  are written to the OUTPAIR= data set.

Given the aforementioned specifications, note that the OUTPAIR= data set can be very large even for a moderately sized DATA= data set. For example, if the DATA= data set has NOBS=500, then the OUTPAIR= data could have up to  $\text{NOBS}(\text{NOBS} - 1)/2 = 124,750$  observations if no OUTPDISTANCE= restriction is given in the COMPUTE statement.

The OUTPAIR= data set contains information about the distance and orientation of each point pair, and you can use it for specialized continuity measure calculations.

The OUTPAIR= data set contains the following variables:

- AC, the angle class value
- COS, the cosine of the angle between pairs
- DC, the distance (lag) class
- DISTANCE, the distance between the data in pairs
- ID1, the ID variable value or observation number for the first point in the pair
- ID2, the ID variable value or observation number for the second point in the pair
- V1, the variable value for the first point in the pair
- V2, the variable value for the second point in the pair
- VARNAME, the variable name for the current VAR variable
- X1, the  $x$  coordinate of the first point in the pair
- X2, the  $x$  coordinate of the second point in the pair
- Y1, the  $y$  coordinate of the first point in the pair
- Y2, the  $y$  coordinate of the second point in the pair

If no ID statement is specified, then the corresponding observation number is assigned to each one of the variables ID1 and ID2, instead.

### **OUTVAR=SAS-data-set**

The OUTVAR= data set contains the standard and robust versions of the sample semivariance, the covariance, and other information in each lag class.

The OUTVAR= data set contains the following variables:

- ANGLE, the angle class value (clockwise from N to S)
- ATOL, the angle tolerance for the lag or angle class
- AVERAGE, the average variable value for the lag or angle class
- BANDW, the bandwidth for the lag or angle class
- COUNT, the number of pairs in the lag or angle class
- COVAR, the covariance value for the lag or angle class
- DISTANCE, the average lag distance for the lag or angle class
- LAG, the lag class value (in LAGDISTANCE= units)
- RVARIO, the sample robust semivariance value for the lag or angle class

- STDERR, the approximate standard error of the sample semivariance estimate
- VARIOG, the sample semivariance value for the lag or angle class
- VARNAME, the name of the current VAR variable

The robust semivariance estimate, RVARIO, is not included in the data set if you omit the option ROBUST in the COMPUTE statement.

The bandwidth variable, BANDW, is not included in the data set if no bandwidth specification is given in the COMPUTE statement or in a DIRECTIONS statement.

The OUTVAR= data set contains a line where the LAG variable is  $-1$ . The AVERAGE variable in this line displays the sample mean value  $\bar{Z}$  of the SRF  $Z(s)$ , and the COVAR variable shows the sample variance  $\text{Var}[Z(s)]$ .

---

## Displayed Output

In addition to the output data sets, the VARIOGRAM procedure produces a variety of output objects. Most of these are produced depending on whether you specify either NOVARIOGRAM or LAGDISTANCE= and MAXLAGS= in the COMPUTE statement. The VARIOGRAM procedure output objects are the following:

- a default “Number of Observations” table that displays the number of observations read from the input data set and the number of observations used in the analysis
- a default map that shows the spatial distribution of the observations of the current variable in the VAR statement. The observations are displayed by default with circled markers whose color indicates the VAR value at the corresponding location.
- a table with basic information about the lags and the extreme distance between data pairs, when NOVARIOGRAM is specified
- a table that describes the distribution of data pairs in distance intervals, when NOVARIOGRAM is specified
- a histogram plot of the pairwise distance distribution, when NOVARIOGRAM is specified). The plot also displays a reference line at a user-specified pairs frequency threshold when you specify the THRESHOLD= parameter in the PLOTS=PAIRS option. The option PLOTS=PAIRS(NOINSET) forces the informational inset that appears in the plot to hide.
- empirical semivariogram details, when NOVARIOGRAM is not specified and LAGDISTANCE= and MAXLAGS= are specified. This table also includes the semivariance estimate variance and confidence limits when CL is specified, and estimates of the robust semivariance when ROBUST is specified.

- plots of the appropriate empirical semivariograms, when **NOVARIOGRAM** is not specified and **LAGDISTANCE=** and **MAXLAGS=** are specified. If you perform the analysis in more than one direction simultaneously, the output is a panel that contains the empirical semivariogram plots for the specified angles. If the semivariograms are nonpaneled, then each plot includes in the lower part a needle plot of the contributing pairs distribution.
- a table that provides autocorrelation statistics, when the options **AUTOCORRELATION** and **LAGDISTANCE=** are specified
- the Moran scatter plot of the standardized observation values against the weighted averages of their neighbors, when the options **PLOTS=MORAN**, **AUTOCORRELATION**, and **LAGDISTANCE=** are specified

When you specify the **MODEL** statement and request a fit of a theoretical model to the empirical semivariogram, the **VARIOGRAM** procedure also produces the following default output:

- a table with some general fitting information, in addition to the output item store if you have specified one with the **STORE** statement
- a table with more specific information about the selected model's parameters and their initial values
- a table with general information about the optimization that provides the fitting parameters of the selected model
- a table with the optimization process output and a table with the convergence status of the optimization process, if you have specified a single model to fit
- a "Parameter Estimates" table with information about the fitted parameters estimates
- a "Fit Summary" table that reports the fit quality of all models you requested to fit
- plots of fitted theoretical semivariogram models. If you perform model fitting in more than one direction angle or for more than one variable in your **DATA=** data set, then the output is a panel that contains all fitted models for the respective directions or variables.

Additional output can be produced in model fitting if you specify a higher level of output detail with the **DETAILS** option in the **MODEL** statement. This output can be information tables for each separate model when you specify multiple models to fit, tables with more details about the optimization process, and the covariance and correlation matrices of the model parameter estimates. The complete listing of the PROC **VARIOGRAM** output follows in the section "**ODS Table Names**" on page 8646 and the section "**ODS Graph Names**" on page 8647.



## ODS Table Names

Each table created by PROC VARIOGRAM has a name associated with it, and you must use this name to refer to the table when using ODS Graphics. These names are listed in Table 102.6.

**Table 102.6** ODS Tables Produced by PROC VARIOGRAM

| ODS Table Name            | Description                                                                                                   | Required Statement | Option             |
|---------------------------|---------------------------------------------------------------------------------------------------------------|--------------------|--------------------|
| AutoCorrStats             | Autocorrelation statistics information                                                                        | COMPUTE            | AUTOCORRELATION    |
| ConvergenceStatus         | Status of optimization at conclusion                                                                          | MODEL              | Default output     |
| CorrB                     | Approximate correlation matrix of model parameter estimates                                                   | MODEL              | CORRB              |
| CovB                      | Approximate covariance matrix of model parameter estimates                                                    | MODEL              | COVB               |
| DistanceIntervals         | Pairwise distances matrix                                                                                     | COMPUTE            | NOVARIOGRAM        |
| FitGenInfo                | General fitting information                                                                                   | MODEL              | Default output     |
| FitSummary                | Fitting process summary                                                                                       | MODEL              | Default output     |
| InputOptions              | Optimization input options                                                                                    | MODEL              | DETAILS=ALL        |
| IterHist                  | Iteration history                                                                                             | MODEL              | DETAILS=ITR        |
| IterStop                  | Optimization-related results                                                                                  | MODEL              | Default output     |
| Lagrange                  | Information about Lagrange multipliers                                                                        | MODEL              | DETAILS=ALL        |
| ModelInfo                 | Model information                                                                                             | MODEL              | Default output     |
| NObs                      | Number of observations read and used                                                                          | PROC               | Default output     |
| OptInfo                   | Optimization information                                                                                      | MODEL              | Default output     |
| PairsInformation          | General information about the pairs distribution in classes and data maximum distances in selected directions | COMPUTE            | NOVARIOGRAM        |
| ParameterEstimates        | Model fitting solution and statistics                                                                         | MODEL              | Default output     |
| ParameterEstimatesResults | Parameter estimates and gradient information                                                                  | MODEL              | DETAILS=ALL        |
| ParameterEstimatesStart   | More detailed model information                                                                               | MODEL              | DETAILS=ITR        |
| ParmSearch                | Parameter search values                                                                                       | MODEL              | Default output     |
| ProblemDescription        | Information at the optimization start                                                                         | MODEL              | DETAILS=ITR        |
| ProjGrad                  | Projected gradient information                                                                                | MODEL              | DETAILS=ALL        |
| SemivariogramTable        | Empirical semivariance classes, parameters, and estimates                                                     | COMPUTE            | LAGD=,<br>MAXLAGS= |

## ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, “[Statistical Graphics Using ODS.](#)”

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section “[Enabling and Disabling ODS Graphics](#)” on page 600 in Chapter 21, “[Statistical Graphics Using ODS.](#)”

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section “[A Primer on ODS Statistical Graphics](#)” on page 599 in Chapter 21, “[Statistical Graphics Using ODS.](#)”

For additional control of the graphics that are displayed, see the PLOTS option in the section “[PROC VARIOGRAM Statement](#)” on page 8576.

## ODS Graph Names

PROC VARIOGRAM assigns a name to each graph it creates by using ODS Graphics. You can use this name to refer to the graph when using ODS Graphics. You must also specify the PLOTS= option indicated in Table 102.7.

**Table 102.7** Graphs Produced by PROC VARIOGRAM

| ODS Graph Name     | Plot Description                                                                 | Statement | Option        |
|--------------------|----------------------------------------------------------------------------------|-----------|---------------|
| FitPanel           | Panel of one or more classes of fitted semivariograms in different angles        | PROC      | PLOTS=FIT     |
| FitPlot            | Plot of one or more classes of fitted semivariograms                             | PROC      | PLOTS=FIT     |
| MoranPlot          | Scatter plot of standardized observed values against weighted averages           | PROC      | PLOTS=MORAN   |
| ObservationsPlot   | Scatter plot of observed data and colored markers that indicates observed values | PROC      | PLOTS=OBSERV  |
| PairDistPlot       | Histogram of the pairwise distance distribution                                  | PROC      | PLOTS=PAIRS   |
| Semivariogram      | Plots of empirical classical and robust (optional) semivariograms                | PROC      | PLOTS=SEMIVAR |
| SemivariogramPanel | Panel of empirical classical and robust (optional) semivariogram plots           | PROC      | PLOTS=SEMIVAR |

## Examples: VARIOGRAM Procedure

### Example 102.1: Aspects of Semivariogram Model Fitting

This example helps you explore aspects of automated semivariogram fitting with PROC VARIOGRAM. The test case is a spatial study of arsenic (*As*) concentration in drinking water.

Arsenic is a toxic pollutant that can occur in drinking water because of human activity or, typically, due to natural release from the sediments in water aquifers. The World Health Organization has a standard that allows *As* concentration up to a maximum of 10  $\mu\text{g/l}$  (micrograms per liter) in drinking water.

In general, natural release of arsenic into groundwater is very slow. Arsenic concentration in water might exhibit no significant temporal fluctuations over a period of a few months. For this reason, it is acceptable to perform a spatial study of arsenic with input from time-aggregated pollutant concentrations. This example makes use of this assumption for its data set `logAsData`. The data set consists of 138 simulated observations from wells across a square area of 500 km  $\times$  500 km. The variable `logAs` in the `logAsData` data set is the natural logarithm of arsenic concentration. Often, the natural logarithm of arsenic concentration (`logAs`) is used as the random variable to facilitate the analysis because its distribution tends to resemble the normal distribution.

The goal is to explore spatial continuity in the `logAs` observations. The following statements read the `logAs` values from the `logAsData` data set:

```

title 'Semivariogram Model Fitting of Log-Arsenic Concentration';

data logAsData;
 input East North logAs @@;
 label logAs='log(As) Concentration';
 datalines;
193.0 296.6 -0.68153 232.6 479.1 0.96279 268.7 312.5 -1.02908
 43.6 4.9 0.65010 152.6 54.9 1.87076 449.1 395.8 0.95932
310.9 493.6 -1.66208 287.8 164.9 -0.01779 330.0 8.0 2.06837
225.7 241.7 0.15899 452.3 83.4 -1.21217 156.5 462.5 -0.89031
 11.5 84.4 -0.24496 144.4 335.7 0.11950 149.0 431.8 -0.57251
234.3 123.2 -1.33642 37.8 197.8 -0.27624 183.1 173.9 -2.14558
149.3 426.7 -1.06506 434.4 67.5 -1.04657 439.6 237.0 -0.09074
 36.4 175.2 -1.21211 370.6 244.0 3.28091 452.0 96.5 -0.77081
247.0 86.8 0.04720 413.6 373.2 1.78235 253.5 291.7 0.56132
129.7 111.9 1.34000 352.7 42.1 0.23621 279.3 82.7 2.12350
382.6 290.7 0.86756 188.2 222.8 -1.23308 382.8 154.5 -0.94094
304.4 309.2 -1.95158 337.5 387.2 -1.31294 490.7 189.8 0.40206
159.0 100.1 -0.22272 245.5 329.2 -0.26082 372.1 379.5 -1.89078
417.8 84.1 -1.25176 173.9 407.6 -0.24240 121.5 107.7 1.54509
453.5 313.6 0.65895 143.5 346.7 -0.87196 157.4 125.5 -1.96165
371.8 353.2 -0.59464 358.9 338.2 -1.07133 8.6 437.8 1.44203
395.9 394.2 -0.24144 149.5 58.9 1.17459 453.5 420.6 -0.63951
182.3 85.0 1.00005 21.0 290.1 0.31016 11.1 352.2 -0.88418
131.2 238.4 -0.57184 104.9 6.3 1.12054 247.3 256.0 0.14019
428.4 383.7 0.92448 327.8 481.1 -2.72543 199.2 92.8 -0.05717
453.9 230.1 0.16571 205.0 250.6 0.07581 459.5 271.6 0.93700

```

```

229.5 262.8 1.83590 370.4 228.6 2.96611 330.2 281.9 1.79723
354.8 388.3 -3.18262 406.2 222.7 2.41594 254.4 393.1 2.03221
 96.7 85.2 -0.47156 407.2 256.8 0.66747 498.5 273.8 1.03041
417.2 471.4 -1.42766 368.8 424.3 -0.70506 303.0 59.1 1.43070
403.1 264.1 1.64554 21.2 360.8 0.67094 148.2 78.1 2.15323
305.5 310.7 -1.47985 228.5 180.3 -0.68386 161.1 143.3 1.07901
 70.5 155.1 0.54652 363.1 282.6 -0.43051 86.0 472.5 -1.18855
175.9 105.3 -2.08112 96.8 426.3 1.56592 475.1 453.1 -1.53776
125.7 485.4 1.40054 277.9 201.6 -0.54565 406.2 125.0 -1.38657
 60.0 275.5 -0.59966 431.3 494.6 -0.36860 399.9 399.0 -0.77265
 28.8 311.1 0.91693 166.1 348.2 -0.49056 266.6 83.5 0.67277
 54.7 356.3 0.49596 433.5 460.3 -1.61309 201.7 167.6 -1.40678
158.1 203.6 -1.32499 67.6 230.4 1.14672 81.9 250.0 0.63378
372.0 50.7 0.72445 26.4 264.6 1.00862 300.1 91.7 -0.74089
303.0 447.4 1.74589 108.4 386.2 1.12847 55.6 191.7 0.95175
 36.3 273.2 1.78880 94.5 298.3 -2.43320 366.1 187.3 -0.80526
130.7 389.2 -0.31513 37.2 324.2 0.24489 295.5 211.8 0.41899
 58.6 206.2 0.18495 346.3 142.8 -0.92038 484.2 215.9 0.08012
451.4 415.7 0.02773 58.9 86.5 0.17652 212.6 363.9 0.17215
378.7 407.6 0.51516 265.9 305.0 -0.30718 123.2 314.8 -0.90591
 26.9 471.7 1.70285 16.5 7.1 0.51736 255.1 472.6 2.02381
111.5 148.4 -0.09658 440.4 375.0 1.23285 406.4 19.5 1.01181
321.2 65.8 -0.02095 466.4 357.1 -0.49272 2.0 484.6 0.50994
200.9 205.1 0.43543 30.3 337.0 1.60882 297.0 12.7 1.79824
158.2 450.7 0.05295 122.8 105.3 1.53936 417.8 329.7 -2.08124
;

```

First you want to inspect the `logAs` data for surface trends and the pairwise distribution. You run the `VARIOGRAM` procedure with the `NOVARIogram` option in the `COMPUTE` statement. You also request the `PLOTS=PAIRS(MID)` option, which prompts the pair distance plot to display the actual distance between pairs, rather than the lag number itself, in the midpoint of the lags. You use the following statements:

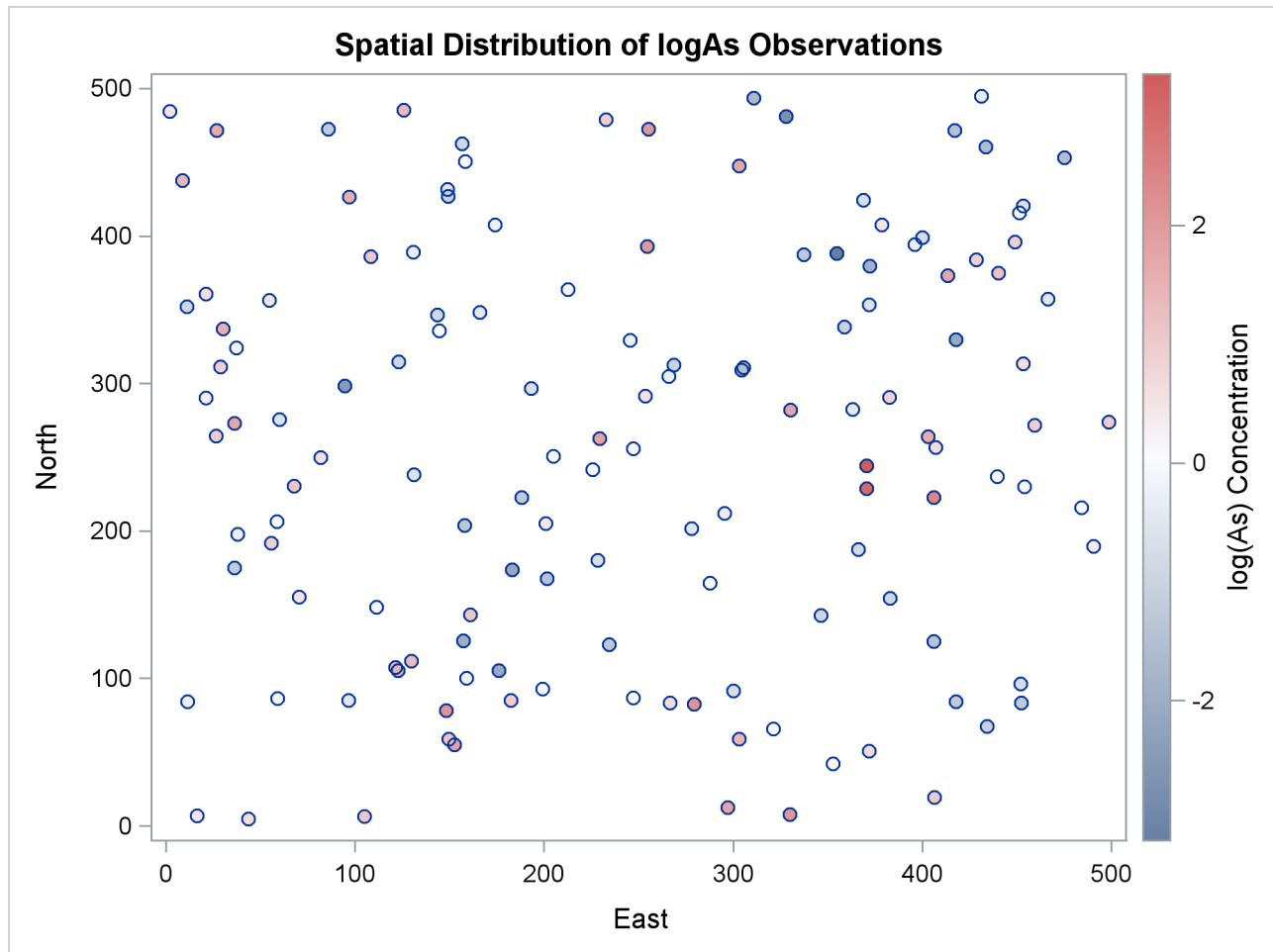
```

ods graphics on;

proc variogram data=logAsData plots=pairs(mid);
 compute novariogram nhc=50;
 coord xc=East yc=North;
 var logAs;
run;

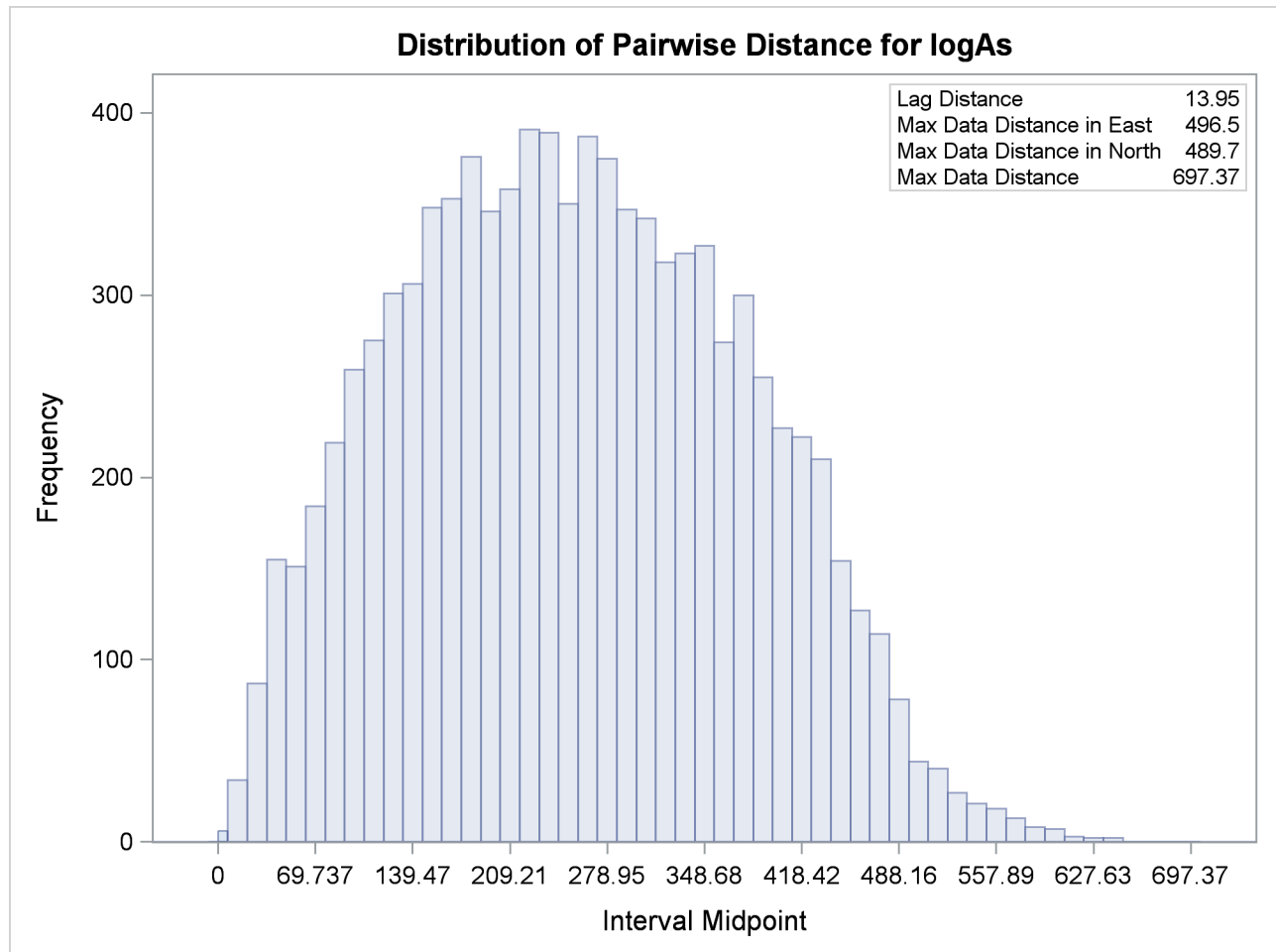
```

The observations scatter plot in [Output 102.1.1](#) shows a rather uniform distribution of the locations in the study domain. Reasonably, neighboring values of `logAs` seem to exhibit some correlation. There seems to be no definite sign of an overall surface trend in the `logAs` values. You can consider that the observations are trend-free, and proceed with estimation of the empirical semivariance.

**Output 102.1.1** logAs Observation Data Scatter Plot

The observed logAs values go as high as 3.28091, which corresponds to a concentration of  $26.6 \mu\text{g}/\text{lt}$ . In fact, only three observations exceed the health standard of  $10 \mu\text{g}/\text{lt}$  (or about 2.3 in the log scale), and they are situated in relatively neighboring locations to the east of the domain center.

Based on the discussion in section “[Preliminary Spatial Data Analysis](#)” on page 8562, the pair distance plot in [Output 102.1.2](#) suggests that you could consider pairs that are anywhere around up to half the maximum pairwise distance of about 700 km.

**Output 102.1.2** Distribution of Pairwise Distances for logAs Data

After some experimentation with values for the `LAGDISTANCE=` and `MAXLAGS=` options, you actually find that a lag distance of 5 km over 40 lags can provide a clear representation of the logAs semivariance. With respect to [Output 102.1.2](#), this finding indicates that in the current example it is sufficient to consider pairs separated by a distance of up to 200 km. You run the following statements to obtain the empirical semivariogram:

```
proc variogram data=logAsData plots(only)=semivar;
 compute lagd=5 maxlag=40;
 coord xc=East yc=North;
 var logAs;
run;
```

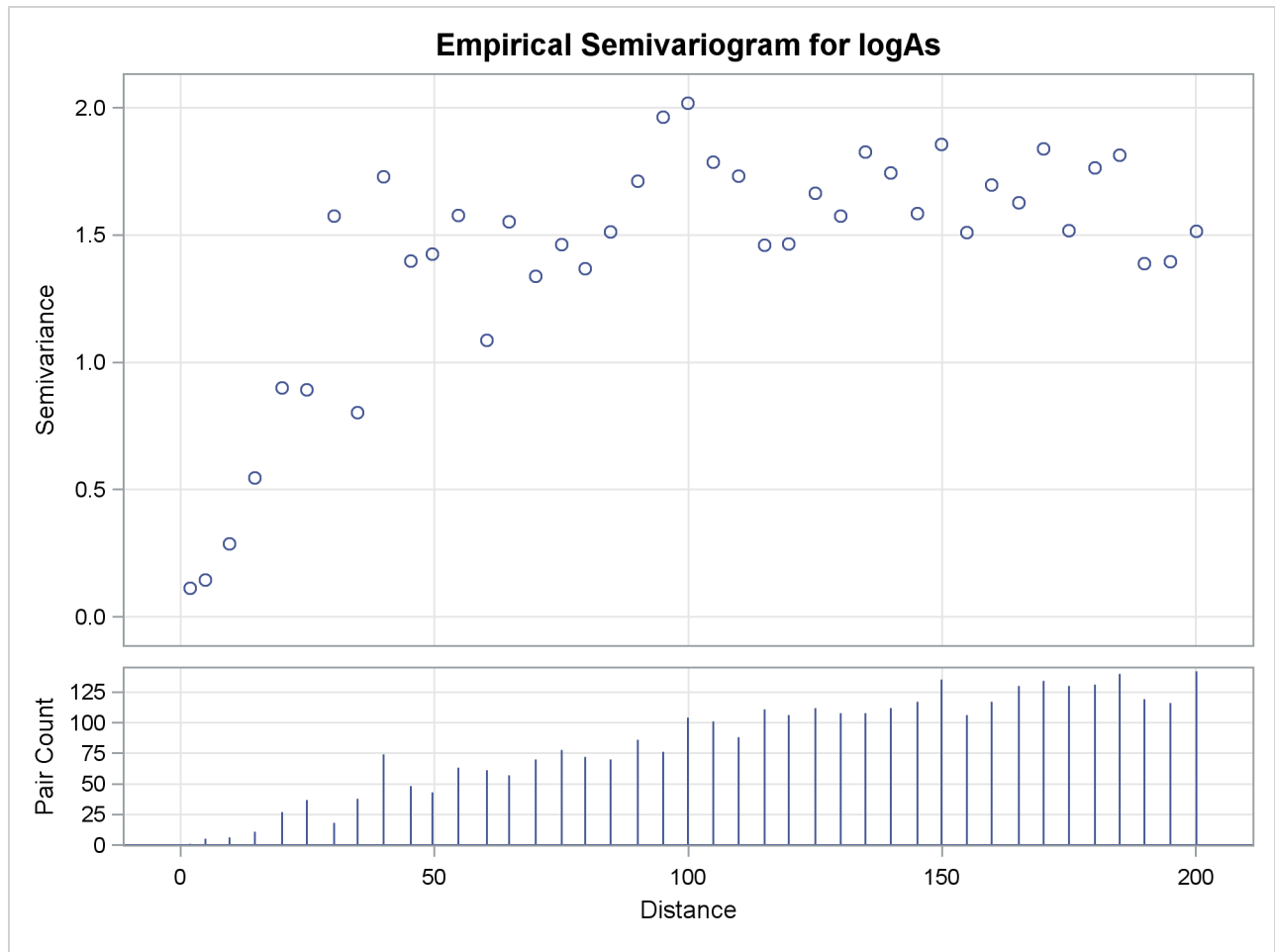
The first few lag classes of the logAs empirical semivariance table are shown in [Output 102.1.3](#).

**Output 102.1.3** Partial Output of the Empirical Semivariogram Table for logAs Data

| Semivariogram Model Fitting of Log-Arsenic Concentration |            |                  |              |
|----------------------------------------------------------|------------|------------------|--------------|
| The VARIOGRAM Procedure                                  |            |                  |              |
| Dependent Variable: logAs                                |            |                  |              |
| Empirical Semivariogram                                  |            |                  |              |
| Lag Class                                                | Pair Count | Average Distance | Semivariance |
| 0                                                        | 1          | 1.9              | 0.111        |
| 1                                                        | 5          | 4.9              | 0.145        |
| 2                                                        | 6          | 9.7              | 0.286        |
| 3                                                        | 11         | 14.6             | 0.545        |
| 4                                                        | 27         | 20.0             | 0.900        |

[Output 102.1.3](#) and [Output 102.1.4](#) indicate that the logarithm of arsenic spatial correlation starts with a small nugget effect around 0.11 and rises to a sill value that is most likely between 1.4 and 1.8. The rise could be of exponential type, although the smooth increase of semivariance close to the origin could also suggest Gaussian behavior. You suspect that a Matérn form might also work, since its smoothness parameter  $\nu$  can regulate the form to exhibit an intermediate behavior between the exponential and Gaussian forms.

**Output 102.1.4** Empirical Semivariogram for logAs Data





You can investigate all of the preceding clues with the model fitting features of PROC VARIOGRAM. The simplest way to fit a model is to specify its form in the **MODEL** statement. In this case, you have the added complexity of having more than one possible candidate. For this reason, you use the **FORM=AUTO** option that picks the best fit out of a list of candidates. Within this option you specify the **MLIST=** suboption to use the exponential, Gaussian, and Matérn forms. You also specify the **NEST=** suboption to request fitting of a model with up to two nested structures. Eventually, you specify the **PLOTS=FIT** option to produce a plot of the fitted models. The **STORE** statement saves the fitting output into an item store you name `SemivAsStore` for future use. You apply these specifications with the following statements:

```
proc variogram data=logAsData plots(only)=fit;
 store out=SemivAsStore / label='LogAs Concentration Models';
 compute lagd=5 maxlag=40;
 coord xc=East yc=North;
 model form=auto(mlist=(exp,gau,mat) nest=1 to 2);
 var logAs;
run;

ods graphics off;
```

The table of general information about fitting is shown in [Output 102.1.5](#). The table lets you know that 12 model combinations are to be tested for weighted least squares fitting, based on the three forms that you specified.

**Output 102.1.5** Semivariogram Model Fitting General Information

|                                                          |                                     |
|----------------------------------------------------------|-------------------------------------|
| Semivariogram Model Fitting of Log-Arsenic Concentration |                                     |
| The VARIOGRAM Procedure                                  |                                     |
| Dependent Variable: logAs                                |                                     |
| Angle: Omnidirectional                                   |                                     |
| Semivariogram Model Fitting                              |                                     |
| Model                                                    | Selection from 12 form combinations |
| Output Item Store                                        | WORK.SEMIVASSTORE                   |
| Item Store Label                                         | LogAs Concentration Models          |

The combinations include repetitions. For example, you specified the GAU form; hence the GAU-GAU form is tested, too. The model combinations also include permutations. For example, you specified the GAU and the EXP forms; hence the GAU-EXP and EXP-GAU models are fitted separately. According to the section “[Nested Models](#)” on page 8613, it might seem that the same model is fitted twice. However, in each of these two cases, each structure starts the fitting process with different parameter initial values. This can lead GAU-EXP to a different fit than EXP-GAU leads to, as seen in the fitting summary table in [Output 102.1.6](#). The table shows all the model combinations that were tested and fitted. By default, the ordering is based on the weighted sum of squares error criterion, and you can see that the lowest values in the Weighted SSE column are in top slots of the list.

**Output 102.1.6** Semivariogram Model Fitting Summary

| Fit Summary |         |                 |           |  |
|-------------|---------|-----------------|-----------|--|
| Class       | Model   | Weighted<br>SSE | AIC       |  |
| 1           | Gau-Gau | 25.42435        | -9.59246  |  |
|             | Gau-Mat | 25.42482        | -7.59169  |  |
| 2           | Exp-Gau | 25.97835        | -8.70865  |  |
| 3           | Exp-Mat | 26.36846        | -6.09754  |  |
| 4           | Mat     | 26.37519        | -10.08708 |  |
| 5           | Gau     | 26.78629        | -11.45296 |  |
| 6           | Exp     | 28.01200        | -9.61851  |  |
|             | Exp-Exp | 28.01200        | -5.61850  |  |
|             | Mat-Exp | 28.01200        | -3.61850  |  |
|             | Gau-Exp | 28.01200        | -5.61850  |  |

Note the leftmost Class column in [Output 102.1.6](#). As explained in detail in section “Classes of Equivalence” on page 8634, when you fit more than one model, all fitted models that compute the same semivariance are placed in the same class of equivalence. For example, in this fitting example the top ranked GAU-GAU and GAU-MAT nested models produce indistinguishable semivariograms; for that reason they are both placed in the same class 1 of equivalence. The same occurs with the EXP, GAU-EXP, EXP-EXP, and MAT-EXP models in the bottom of the table. By default, PROC VARIOGRAM uses the AIC as a secondary classification criterion; hence models in each equivalence class are already ordered based on their AIC values.

Another remark in [Output 102.1.6](#) is that despite submitting 12 model combinations for fitting, the table shows only 10. You can easily see that the combinations MAT-GAU and MAT-MAT are not among the listed models in the fit summary. This results from the behavior of the VARIOGRAM procedure in the following situation: A parameter optimization takes place during the fitting process. In the present case the optimizer keeps increasing the Matérn smoothness parameter  $\nu$  in the MAT-GAU model. At the limit of an infinite  $\nu$  parameter, the Matérn form becomes the Gaussian form. For that reason, when the parameter  $\nu$  is driven towards very high values, PROC VARIOGRAM automatically replaces the Matérn form with the Gaussian. This switch converts the MAT-GAU model into a GAU-GAU model. However, a GAU-GAU model already exists among the specified forms; consequently, the duplicate GAU-GAU model is skipped, and the fitted model list is reduced by one model. A similar explanation justifies the omission of the MAT-MAT model from the fit summary table.

In our example, the nested Gaussian-Gaussian model is the fitting selection of the procedure based on the default ranking criteria. [Output 102.1.7](#) displays additional information about the selected model. In particular, you see the table with general information about the Gaussian-Gaussian model, the initial values used for its parameters, and information about the optimization process for the fitting.

**Output 102.1.7** Fitting and Optimization Information for Gaussian-Gaussian Model

| Semivariogram Model Fitting |                   |
|-----------------------------|-------------------|
| Name                        | Gaussian-Gaussian |
| Label                       | Gau-Gau           |
| Model Information           |                   |
|                             | Initial           |
| Parameter                   | Value             |
| Nugget                      | 0.0903            |
| GauScale1                   | 0.6709            |
| GauRange1                   | 100.0             |
| GauScale2                   | 0.6709            |
| GauRange2                   | 50.0230           |
| Optimization Information    |                   |
| Optimization Technique      | Dual Quasi-Newton |
| Parameters in Optimization  | 5                 |
| Lower Boundaries            | 5                 |
| Upper Boundaries            | 0                 |
| Starting Values From        | PROC              |

The estimated parameter values of the selected Gaussian-Gaussian model are shown in [Output 102.1.8](#).

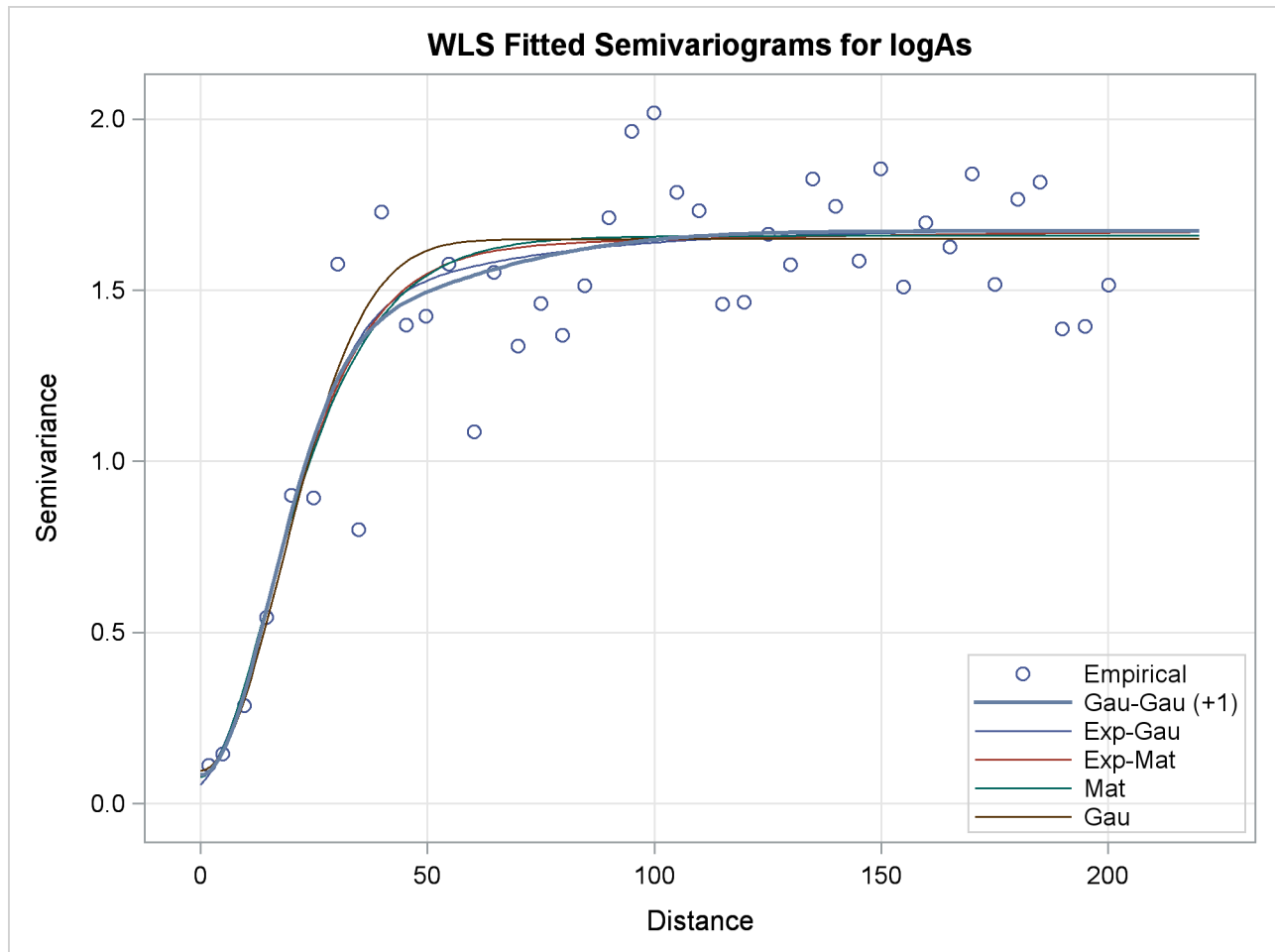
**Output 102.1.8** Parameter Estimates of the Fitting Selected Model

| Parameter Estimates |          |                     |    |         |                   |
|---------------------|----------|---------------------|----|---------|-------------------|
| Parameter           | Estimate | Approx<br>Std Error | DF | t Value | Approx<br>Pr >  t |
| Nugget              | 0.08308  | 0.05097             | 36 | 1.63    | 0.1118            |
| GauScale1           | 0.3277   | 0.2077              | 36 | 1.58    | 0.1234            |
| GauRange1           | 62.3127  | 19.8488             | 36 | 3.14    | 0.0034            |
| GauScale2           | 1.2615   | 0.2070              | 36 | 6.10    | <.0001            |
| GauRange2           | 21.4596  | 3.2722              | 36 | 6.56    | <.0001            |

By default, when you specify more than one model to fit, PROC VARIOGRAM produces a fit plot that compares the first five classes of the successfully fit candidate models. The model that is selected according to the specified fitting criteria is shown with a thicker line in the plot.

You can modify the number of displayed equivalence classes with the `NCLASSES=` suboption of the `PLOTS=FIT` option. When you have such comparison plots, PROC VARIOGRAM displays the representative model from each class of equivalence.

The default fit plot for the current model comparison is shown in [Output 102.1.9](#). The legend informs you there is one more model in the first class of equivalence, as the fitting summary table indicated earlier in [Output 102.1.6](#).

**Output 102.1.9** Fitted Theoretical and Empirical logAs Concentration Semivariograms for the Specified Models

In the present example, all fitted models in the first five classes have very similar semivariograms. The selected Gaussian-Gaussian model seems to have a relatively larger range than the rest of the displayed models, but you can expect any of these models to exhibit a near-identical behavior in terms of spatial correlation. As a result, all models in the displayed classes are likely to lead to very similar output, if you proceed to use any of them for spatial prediction.

In that sense, semivariogram fitting is a partially subjective process, for which there might not exist only one single correct answer to solve your problem. In the context of the example, on one hand you might conclude that the selected Gaussian-Gaussian model is exactly sufficient to describe spatial correlation in the arsenic study. On the other hand, the similar performance of all models might prompt you to choose instead a more simple non-nested model for prediction like the Matérn or the Gaussian model.

Regardless of whether you might opt to sacrifice the statistically best fit (depending on your selected criteria) to simplicity, eventually you are the one to decide which approach serves your study optimally. The model fitting features of PROC VARIOGRAM offer you significant assistance so that you can assess your options efficiently.

## Example 102.2: An Anisotropic Case Study with Surface Trend in the Data

This example shows how to examine data for nonrandom surface trends and anisotropy. You use simulated data where the variable is atmospheric ozone ( $O_3$ ) concentrations measured in Dobson units (DU). The coordinates are offsets from a point in the southwest corner of the measurement area, with the east and north distances in units of kilometers (km). You work with the ozoneSet data set that contains 300 measurements in a square area of  $100 \text{ km} \times 100 \text{ km}$ .

The following statements read the data set:

```

title 'Semivariogram Analysis in Anisotropic Case With Trend Removal';

data ozoneSet;
 input East North Ozone @@;
 datalines;
34.9 68.2 286 39.2 12.5 270 44.4 37.7 275 90.5 27.0 282
91.1 40.8 285 98.6 61.6 294 61.8 26.7 281 64.0 11.5 274
22.4 26.5 274 89.3 18.3 279 32.3 28.3 274 31.1 53.1 279
43.0 17.5 272 79.3 42.3 283 99.9 57.9 291 1.8 24.1 273
81.7 73.5 294 22.9 32.0 273 64.9 67.5 292 76.5 56.3 285
78.7 11.7 276 61.8 99.3 307 49.1 86.6 299 40.0 35.8 273
69.3 3.8 278 23.4 9.3 270 66.3 94.3 304 71.3 6.5 275
9.7 54.4 280 85.2 81.7 300 30.3 60.9 284 94.6 94.3 309
10.6 10.3 271 73.0 43.0 280 4.9 50.7 280 19.0 79.4 289
2.4 73.1 287 77.7 25.2 278 8.4 27.1 276 93.5 19.7 279
0.2 34.5 275 50.4 91.3 302 55.7 26.2 279 50.3 2.3 274
16.3 84.4 293 19.0 6.9 272 57.1 92.3 303 61.0 0.4 275
10.7 18.7 271 15.2 43.5 277 67.0 87.4 301 79.0 54.0 285
36.0 53.3 279 58.3 52.1 282 56.6 79.7 294 40.4 32.4 275
48.9 64.1 286 54.0 54.9 281 27.5 48.5 279 36.4 30.3 275
10.5 31.0 273 87.0 39.4 283 47.9 37.5 274 64.7 63.4 288
0.5 90.8 294 22.8 22.4 275 31.1 78.8 291 93.6 49.8 290
2.5 39.3 273 83.6 25.6 282 49.8 24.1 278 73.1 91.8 305
30.5 90.6 297 26.0 61.2 284 58.4 66.2 289 30.5 4.3 273
38.3 85.6 298 89.2 96.6 309 53.4 6.3 275 27.3 12.8 271
43.4 56.5 281 99.5 86.9 305 85.8 22.8 281 83.0 10.9 278
24.8 16.7 271 51.1 18.8 275 59.0 54.3 283 35.5 91.4 298
18.1 56.0 279 78.0 36.4 277 56.8 6.9 275 21.1 44.5 277
73.9 75.9 296 54.2 0.1 274 33.2 75.1 290 38.2 3.3 274
15.2 14.7 272 15.9 84.2 292 60.2 95.2 304 9.8 27.2 276
91.2 56.4 289 94.7 86.9 303 56.7 49.6 281 24.2 9.5 270
43.0 17.0 272 85.9 10.7 278 53.9 41.1 276 30.4 63.4 286
62.8 86.3 299 76.8 24.6 279 31.6 94.0 300 26.9 73.8 287
18.9 68.4 284 99.4 37.2 285 79.1 3.3 277 34.9 74.7 289
6.4 33.8 277 48.4 82.2 294 86.0 58.0 289 92.0 60.4 293
50.2 91.6 300 12.2 38.3 275 72.7 48.9 283 82.7 34.1 279
77.0 51.0 286 86.6 15.8 278 42.0 42.7 277 99.3 8.2 278
17.4 70.6 286 11.2 92.4 295 60.2 28.8 280 92.0 73.3 297
25.3 30.6 273 36.6 8.9 274 34.2 4.4 273 26.6 54.7 278
1.7 27.4 278 49.6 1.1 275 62.8 89.3 301 28.0 49.3 279
51.2 75.1 293 59.3 93.5 304 83.6 90.5 304 79.4 87.0 302
78.0 28.3 281 16.8 19.1 272 9.1 81.2 292 23.7 55.8 277

```

```

75.5 21.3 279 64.4 43.3 279 38.9 98.9 303 22.5 87.9 293
96.7 37.9 285 92.3 93.9 308 16.9 25.4 273 15.2 61.5 283
73.8 94.0 306 57.4 97.2 305 73.2 4.9 276 39.2 82.3 294
95.7 99.4 315 66.0 98.4 306 95.3 26.9 283 45.4 75.3 291
64.8 15.4 276 69.8 55.4 284 36.3 74.9 290 9.9 22.2 276
65.8 13.9 276 13.0 82.0 293 95.6 77.2 301 32.5 55.6 279
45.8 35.5 275 62.2 6.6 274 25.2 51.2 279 92.4 8.1 277
40.5 35.3 273 9.9 3.9 271 43.5 44.0 278 68.6 61.3 287
64.2 77.5 296 57.6 81.6 294 69.5 64.7 291 64.3 95.1 304
2.8 62.4 283 33.2 83.3 294 10.7 71.0 285 24.3 88.2 294
94.5 32.2 283 21.0 67.6 286 20.1 71.6 286 85.2 71.3 296
94.8 30.7 283 53.4 92.0 301 81.0 50.0 287 54.6 29.9 277
71.1 90.1 303 15.2 2.9 271 83.6 17.8 278 76.0 21.8 279
55.6 37.4 275 86.7 83.7 303 43.6 83.6 295 44.2 31.7 274
90.0 83.3 300 6.2 0.5 270 42.2 87.7 298 31.7 4.3 273
91.4 41.2 285 78.0 50.6 286 27.1 56.1 278 72.6 63.9 291
29.3 49.9 281 49.0 36.9 275 13.9 53.5 280 93.1 83.2 300
73.0 61.6 289 63.1 27.5 280 38.3 72.5 287 72.7 34.2 277
6.9 32.3 274 17.1 58.6 280 19.6 94.6 297 2.7 36.5 276
34.5 5.5 275 98.6 95.9 313 9.1 71.1 285 88.6 55.8 287
26.8 78.5 289 64.8 66.6 292 59.7 25.7 280 47.3 70.2 288
6.1 94.4 296 50.5 82.7 296 9.1 41.6 276 86.0 71.0 296
75.2 69.8 293 73.3 84.8 300 42.5 15.9 274 56.1 76.1 292
87.9 41.2 285 65.1 9.8 274 79.0 41.2 282 44.6 65.1 287
54.7 68.3 289 57.0 26.8 279 8.7 12.3 270 33.7 61.9 286
25.0 55.8 278 69.3 94.9 306 49.2 64.6 287 78.2 93.7 307
47.9 26.6 277 96.9 51.4 292 39.6 73.4 287 37.9 66.1 285
94.5 71.4 296 51.6 18.3 276 37.6 73.2 287 68.5 10.7 274
46.7 9.6 273 87.4 38.9 282 45.6 43.9 277 70.7 76.9 296
82.8 53.6 287 82.5 55.4 286 37.8 5.1 275 89.8 96.1 309
63.9 4.9 276 2.0 11.7 270 31.3 59.2 282 93.9 65.3 296
47.9 93.0 301 29.9 36.0 274 14.6 28.3 274 17.5 70.1 286
2.6 68.5 282 23.1 12.0 268 36.8 20.4 273 80.9 9.0 276
39.2 0.0 274 26.2 44.3 276 81.9 12.9 277 3.2 21.4 272
76.9 76.7 297 88.6 7.7 277 9.7 8.4 273 26.7 91.5 296
73.8 6.1 276 33.7 39.3 276 64.0 58.4 286 5.7 91.2 295
85.8 93.8 307 85.8 39.1 281 93.9 63.4 295 53.1 46.3 278
51.9 42.9 277 16.8 75.7 288 29.2 66.9 285 37.4 72.5 287
;

```

The initial step is to explore the data set by inspecting the data spatial distribution. Run PROC VARIOGRAM, specifying the **NOVARIOGRAM** option in the **COMPUTE** statement as follows:

```

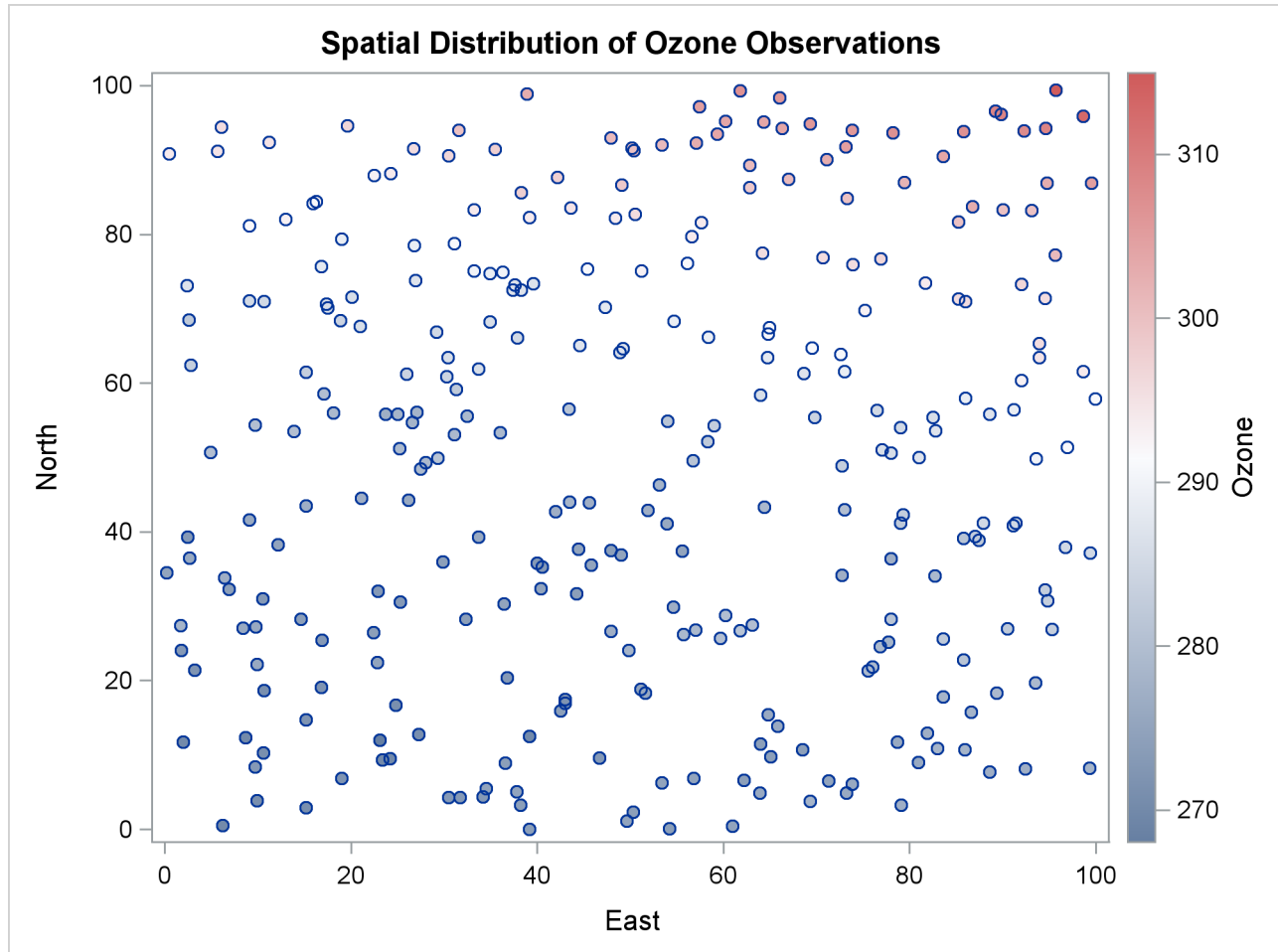
ods graphics on;

proc variogram data=ozoneSet;
 compute novariogram nhc=35;
 coord xc=East yc=North;
 var Ozone;
run;

```

The result is a scatter plot of the observed data shown in [Output 102.2.1](#). The scatter plot suggests an almost uniform spread of the measurements throughout the prediction area. No direct inference can be made about the existence of a surface trend in the data. However, the apparent stratification of ozone values in the northeast–southwest direction might indicate a nonrandom trend.

**Output 102.2.1** Ozone Observation Data Scatter Plot



You need to define the size and count of the data classes by specifying suitable values for the `LAGDISTANCE=` and `MAXLAGS=` options, respectively. Compared to the smaller sample of thickness data used in “Getting Started: VARIOGRAM Procedure” on page 8561, the larger size of the ozoneSet data results in more densely populated distance classes for the same value of the `NHCLASSES=` option. After you experiment with a variety of values for the `NHCLASSES=` option, you can adjust `LAGDISTANCE=` to have a relatively small number. Then you can account for a large value of `MAXLAGS=` so that you obtain many sample semivariogram points within your data correlation range. Specifying these values requires some exploration, for which you might need to return to this point from a later stage in your semivariogram analysis. For illustration purposes you now specify `NHCLASSES=35`.

Your choice of `NHCLASSES=35` yields the pairwise distance intervals table in [Output 102.2.2](#) and the corresponding histogram in [Output 102.2.3](#).

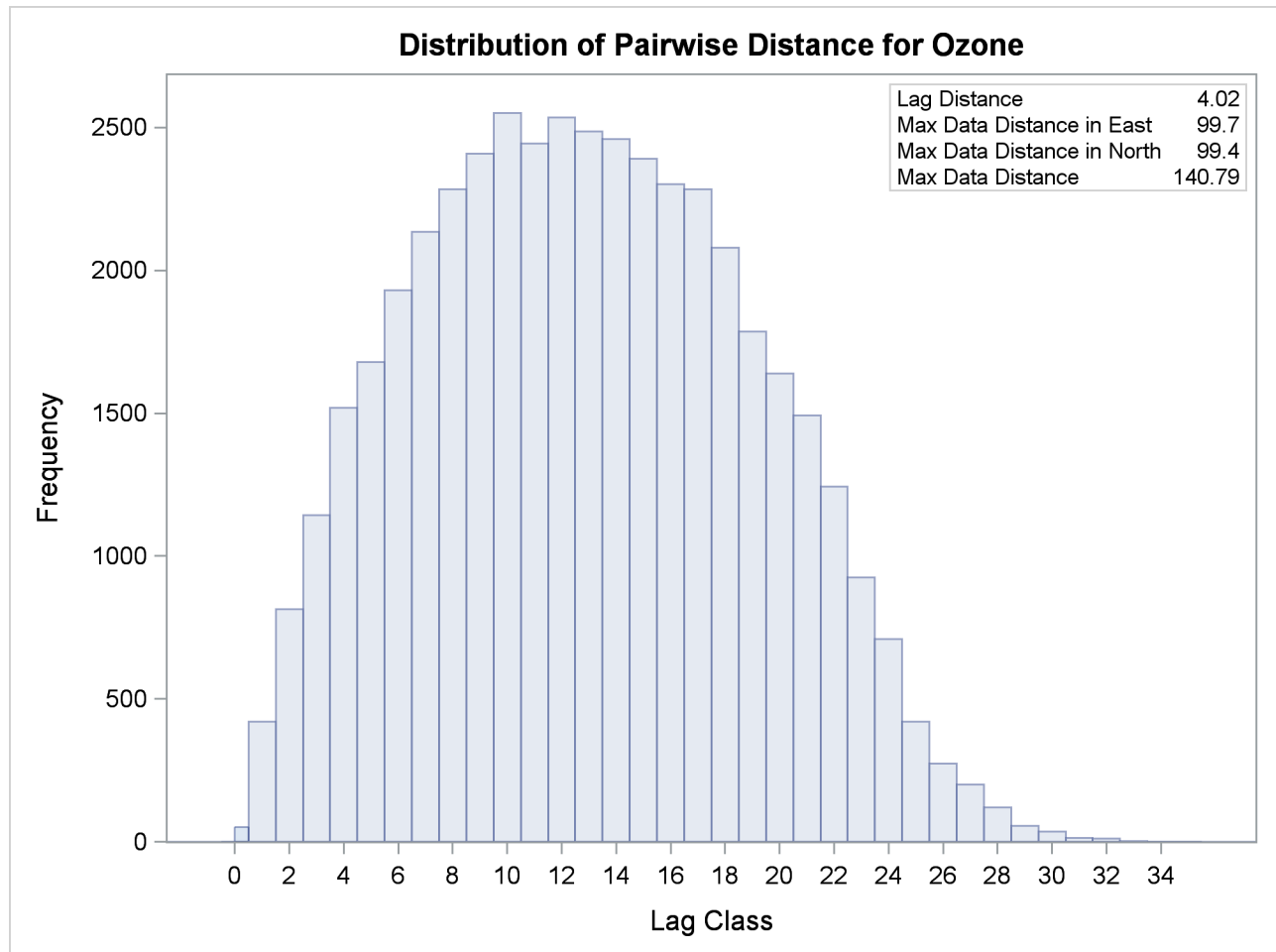
**Output 102.2.2** Pairwise Distance Intervals Table

| Lag Class | Pairwise Distance Intervals |        | Number of Pairs | Percentage of Pairs |
|-----------|-----------------------------|--------|-----------------|---------------------|
|           | -----Bounds-----            |        |                 |                     |
| 0         | 0.00                        | 2.01   | 52              | 0.12%               |
| 1         | 2.01                        | 6.03   | 420             | 0.94%               |
| 2         | 6.03                        | 10.06  | 815             | 1.82%               |
| 3         | 10.06                       | 14.08  | 1143            | 2.55%               |
| 4         | 14.08                       | 18.10  | 1518            | 3.38%               |
| 5         | 18.10                       | 22.12  | 1680            | 3.75%               |
| 6         | 22.12                       | 26.15  | 1931            | 4.31%               |
| 7         | 26.15                       | 30.17  | 2135            | 4.76%               |
| 8         | 30.17                       | 34.19  | 2285            | 5.09%               |
| 9         | 34.19                       | 38.21  | 2408            | 5.37%               |
| 10        | 38.21                       | 42.24  | 2551            | 5.69%               |
| 11        | 42.24                       | 46.26  | 2444            | 5.45%               |
| 12        | 46.26                       | 50.28  | 2535            | 5.65%               |
| 13        | 50.28                       | 54.30  | 2487            | 5.55%               |
| 14        | 54.30                       | 58.33  | 2460            | 5.48%               |
| 15        | 58.33                       | 62.35  | 2391            | 5.33%               |
| 16        | 62.35                       | 66.37  | 2302            | 5.13%               |
| 17        | 66.37                       | 70.39  | 2285            | 5.09%               |
| 18        | 70.39                       | 74.41  | 2079            | 4.64%               |
| 19        | 74.41                       | 78.44  | 1786            | 3.98%               |
| 20        | 78.44                       | 82.46  | 1640            | 3.66%               |
| 21        | 82.46                       | 86.48  | 1493            | 3.33%               |
| 22        | 86.48                       | 90.50  | 1243            | 2.77%               |
| 23        | 90.50                       | 94.53  | 925             | 2.06%               |
| 24        | 94.53                       | 98.55  | 710             | 1.58%               |
| 25        | 98.55                       | 102.57 | 421             | 0.94%               |
| 26        | 102.57                      | 106.59 | 274             | 0.61%               |
| 27        | 106.59                      | 110.62 | 200             | 0.45%               |
| 28        | 110.62                      | 114.64 | 120             | 0.27%               |
| 29        | 114.64                      | 118.66 | 55              | 0.12%               |
| 30        | 118.66                      | 122.68 | 35              | 0.08%               |
| 31        | 122.68                      | 126.71 | 14              | 0.03%               |
| 32        | 126.71                      | 130.73 | 11              | 0.02%               |
| 33        | 130.73                      | 134.75 | 2               | 0.00%               |
| 34        | 134.75                      | 138.77 | 0               | 0.00%               |
| 35        | 138.77                      | 142.80 | 0               | 0.00%               |

Notice the overall high pair count in the majority of classes in [Output 102.2.2](#). You can see that even for higher values of `NHCLASSES=` the classes are still sufficiently populated for your semivariogram analysis according to the rule of thumb stated in the section “[Choosing the Size of Classes](#)” on page 8623. Based on the displayed information in [Output 102.2.3](#), you specify `LAGDISTANCE=4` km. You can further experiment with smaller lag sizes to obtain more points in your sample semivariogram.

You can focus on the `MAXLAGS=` specification at a later point. The important step now is to investigate the presence of trends in the measurement. The following section makes a suggestion about how to remove surface trends from your data and then continues the semivariogram analysis with the detrended data.



**Output 102.2.3** Distribution of Pairwise Distances for Ozone Observation Data

### Analysis with Surface Trend Removal

You can use a SAS/STAT predictive modeling procedure to extract surface trends from your original data. If your goal is spatial prediction, you can continue processing the detrended data for the prediction tasks, and at the end you can reinstate the trend at the prediction locations to report your analysis results.

In general, the exact form of the trend is unknown, as discussed in the section “[Empirical Semivariograms and Surface Trends](#)” on page 8626. In this case, the spatial distribution of the measurements shown in [Figure 102.2.1](#) suggests that you can use a quadratic model to describe the surface trend like the one that follows:

$$T(\text{East}, \text{North}) = f_0 + f_1 [\text{East}] + f_2 [\text{East}]^2 + f_3 [\text{North}] + f_4 [\text{North}]^2$$

The following statements show how to invoke the GLM procedure for your ozone data and how to extract the preceding trend from them:

```
proc glm data=ozoneSet plots=none;
 model ozone = East East*East North North*North;
 output out=gmout predicted=pred residual=ResidualOzone;
run;
```

Among other output, PROC GLM produces estimates for the parameters  $f_0, \dots, f_4$  in the preceding trend model. [Output 102.2.4](#) shows the table with the parameter estimates. In this table, the coefficient  $f_0$  corresponds to the intercept estimate, and the rest of the coefficients correspond to their matching variables; for example, the estimate in the line of “East\*East” refers to  $f_2$  in the preceding model. For more information about the syntax and the PROC GLM output, see Chapter 42, “[The GLM Procedure](#).”

#### Output 102.2.4 Parameter Estimates for the Surface Trend Model

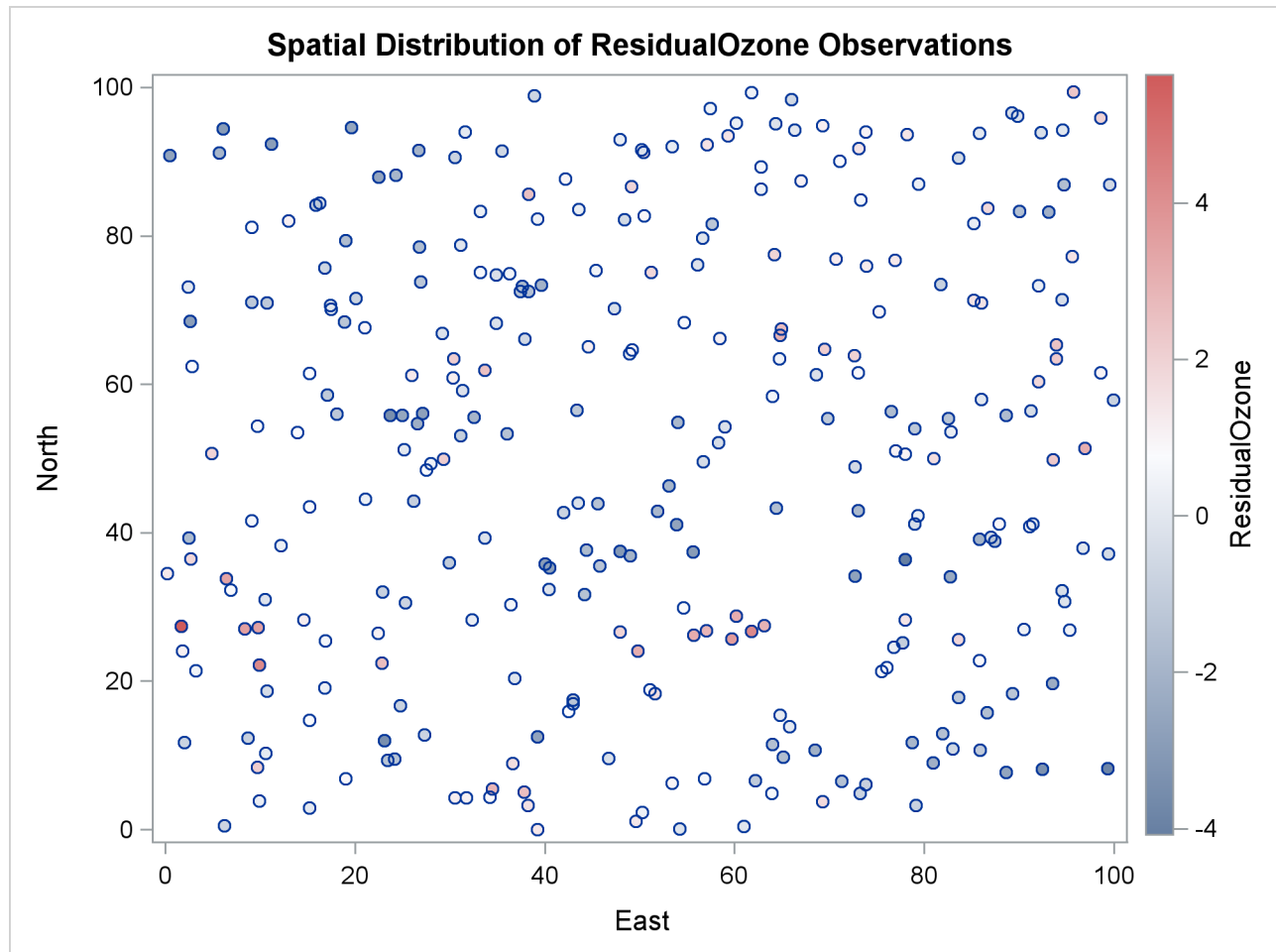
| Semivariogram Analysis in Anisotropic Case With Trend Removal |             |                |         |         |
|---------------------------------------------------------------|-------------|----------------|---------|---------|
| The GLM Procedure                                             |             |                |         |         |
| Dependent Variable: Ozone                                     |             |                |         |         |
| Parameter                                                     | Estimate    | Standard Error | t Value | Pr >  t |
| Intercept                                                     | 270.6798273 | 0.40595731     | 666.77  | <.0001  |
| East                                                          | 0.0065148   | 0.01360281     | 0.48    | 0.6323  |
| East*East                                                     | 0.0010726   | 0.00012987     | 8.26    | <.0001  |
| North                                                         | -0.0369159  | 0.01297491     | -2.85   | 0.0047  |
| North*North                                                   | 0.0035587   | 0.00012659     | 28.11   | <.0001  |

The detrending process leaves you with the GMOUT data set, which contains the ResidualOzone data residuals. This time you run PROC VARIOGRAM again with the [NOVARIOGRAM](#) option to inspect the detrended residuals, and with a request only for the observations plot, as follows:

```
proc variogram data=gmout plots(only)=observ;
 compute novariogram nhc=35;
 coord xc=East yc=North;
 var ResidualOzone;
run;
```

The requested observations plot is shown in [Output 102.2.5](#).

Output 102.2.5 Ozone Residual Observation Data Scatter Plot



Before you proceed with the empirical semivariogram computation and model fitting, examine your data for anisotropy. This investigation is necessary to portray the spatial structure of your SRF accurately. If anisotropy exists, it manifests itself as different ranges or sills or both for the empirical semivariograms in different directions.

You want detail in your analysis, so you ask for the empirical semivariance in 12 directions by specifying `NDIRECTIONS=12`. Based on the `NDIRECTIONS=` option, empirical semivariograms are produced in increments of the base angle  $\theta = 180^\circ/12 = 15^\circ$ .

You also choose `ANGLETOLERANCE=22.5` and `BANDWIDTH=20`. A different choice of values produces different empirical semivariograms, because these options can regulate the number of pairs that are included in a class. Avoid assigning values that are too small to these parameters so that you can allow for an adequate number of point pairs per class. At the same time, the higher the values of these parameters are, the more data pairs that come from closely neighboring directions are included in each lag. Therefore, values for the `ANGLETOLERANCE=` and `BANDWIDTH=` options that are too high pose a risk of losing information along the particular direction. The side effect occurs because you incorporate data pairs from a broader spectrum of angles; thus, you potentially amplify weaker anisotropy or weaken stronger anisotropy, as noted in the section “Angle Classification” on page 8617. You can experiment with different `ANGLETOLERANCE=` and `BANDWIDTH=` values to reach this balance with your data, if necessary.

With the following statements you ask to display only the SEMIVAR plots in the specified number of directions. Multiple empirical semivariograms are placed by default in panels, as [Output 102.2.6](#) shows. If you want an individual plot for each angle, then you need to further specify the plot option SEMIVAR(UNPACK).

```
proc variogram data=gmount plot(only)=semivar;
 compute lagd=4 maxlag=16 ndir=12 atol=22.5 bandw=20;
 coord xc=East yc=North;
 var ResidualOzone;
run;
```

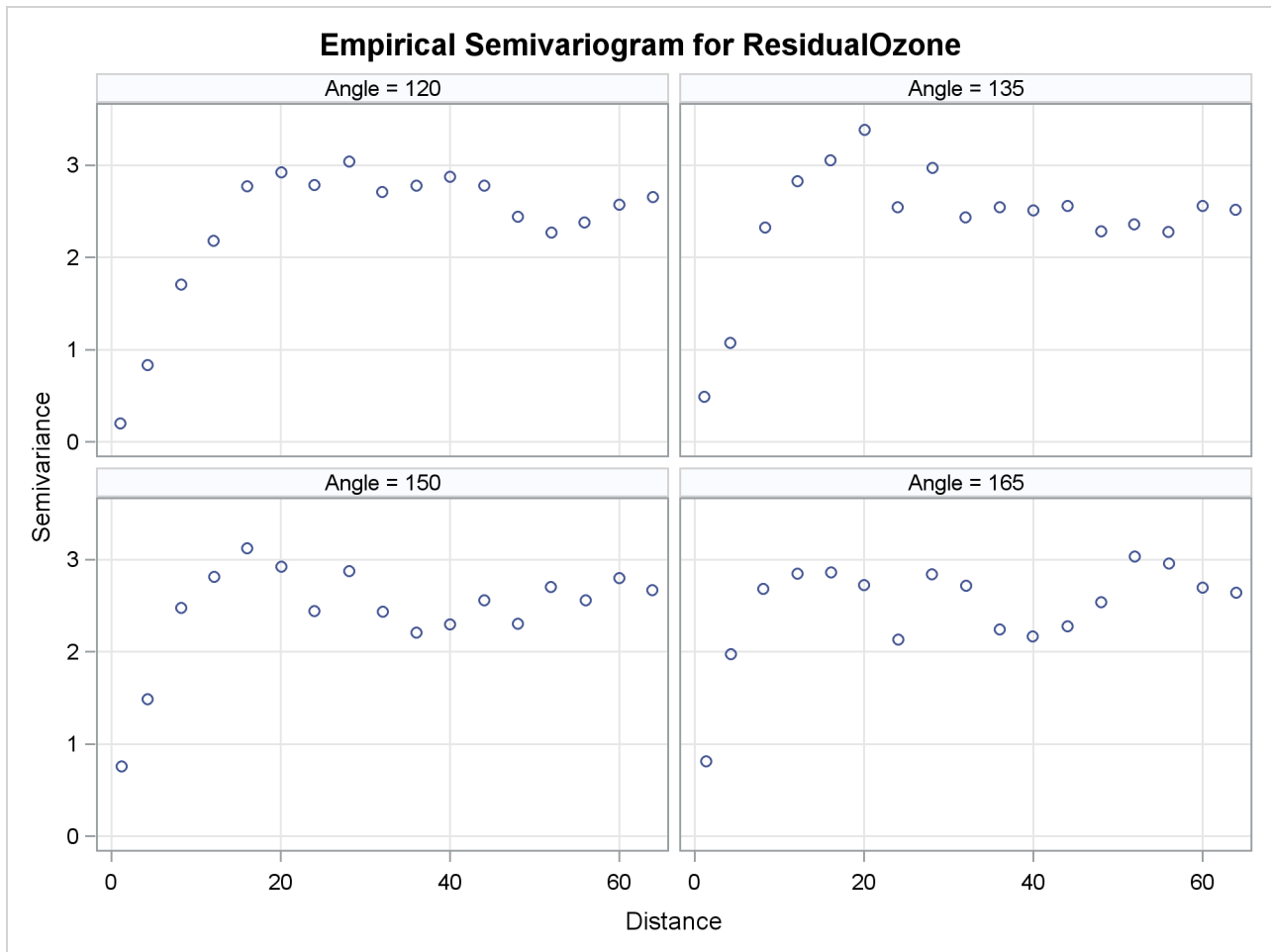
**Output 102.2.6** Ozone Empirical Semivariograms with  $0^\circ \leq \theta < 180^\circ$  and  $\delta\theta = 15^\circ$



Output 102.2.6 continued



Output 102.2.6 continued



The panels in [Output 102.2.6](#) suggest that in some of the directions, such as for  $\theta = 0^\circ$ , the directional plots tend to exhibit a somewhat noisy structure. This behavior can be due to the pairs distribution across the particular direction. Specifically, based on the `LAGDISTANCE=` choice there might be insufficient pairs present in a class. Also, depending on the `ANGLETOLERANCE=` and `BANDWIDTH=` values, too many pairs might be considered from neighboring angles that potentially follow a modified structure. These are factors that can increase the variability in the semivariance estimate. A different explanation might lie in the existence of outliers in the data set; this aspect is further explored in “[Example 102.5: A Box Plot of the Square Root Difference Cloud](#)” on page 8684.

This behavior is relatively mild here and should not obstruct your goal to study anisotropy in your data. You can also perform individual computations in any direction. By doing so, you can fine-tune the computation parameters and attempt to obtain smoother estimates of the sample semivariance.

Further in this study, the directional plots in [Output 102.2.6](#) suggest that during shifting from  $\theta = 0^\circ$  to  $\theta = 90^\circ$ , the empirical semivariogram range increases. Beyond the angle  $\theta = 90^\circ$ , the range starts decreasing again until the whole circle is traversed at  $180^\circ$  and small range values are encountered around the N–S direction at  $\theta = 0^\circ$ . The sill seems to remain overall the same. This analysis suggests the presence of anisotropy in the ozone concentrations, with the major axis oriented at about  $\theta = 90^\circ$  and the minor axis situated perpendicular to the major axis at  $\theta = 0^\circ$ .

The multidirectional analysis requires that for a given `LAGDISTANCE=` you also specify a `MAXLAGS=` value. Since the ozone correlation range might be unknown (as assumed here), you can apply the rule of thumb that suggests use of the half-extreme data distance in the direction of interest, as explained in the section “[Spatial Extent of the Empirical Semivariogram](#)” on page 8624. Following the information displayed in [Output 102.2.3](#), for different directions this distance varies between  $99.4/2 = 49.7$  and  $140.8/2 = 70.4$  km. In turn, the pairwise distances table in [Output 102.2.2](#) indicates that within this range of distances you can specify `MAXLAGS=` to be between 12 and 17 lags. In this example you specify `MAXLAGS=16`.

At this point you are ready to continue with fitting theoretical semivariogram models to the empirical semivariogram in the selected directions of  $\theta = 0^\circ$  and  $\theta = 90^\circ$ . By trying out different models, you see that an exponential one is suitable for your empirical data:

$$\gamma_z(h) = c_0 \left[ 1 - \exp\left(-\frac{h}{a_0}\right) \right]$$

For the purpose of the present example, it is reasonable to assume a constant nugget effect equal to zero, based on the empirical semivariograms shown in [Output 102.2.6](#). The same output suggests that the model scale is likely to be above 2, and that the range might be relatively small in  $\theta = 0^\circ$ . You specify the `PARMS` statement to set initial values for the exponential model parameters and account for these considerations.

In particular, you assign an initial value of zero to the nugget effect. Then you request a grid search for the range and scale parameters, so that the optimal initial values set is selected for the parameter estimation in each of the two angles  $\theta = 0^\circ$  and  $\theta = 90^\circ$ . By inspecting the empirical semivariograms in [Output 102.2.6](#), you specify the value list 2, 2.5, and 3 for the scale, and the values from 5 to 25 with a step of 10 for the range. In addition, you specify the parameter 1 in the `HOLD=` option to designate the nugget effect parameter as a constant. According to these specifications, you use the following statements:

```
proc variogram data=gmount plot(only)=fit;
 compute lagd=4 maxlag=16;
 directions 0(22.5,10) 90(22.5,10);
 coord xc=East yc=North;
```

```

model form=exp;
parms (0.) (2 to 3 by 0.5) (5 to 25 by 10) / hold=(1);
var ResidualOzone;
run;

ods graphics off;

```

The VARIOGRAM procedure repeats the fitting process for each one of the selected directions. First, in  $\theta = 0^\circ$  the parameter search table in [Output 102.2.7](#) shows you which value combinations are tested initially to choose the one that gives the lowest objective function value.

**Output 102.2.7** Parameter Search for the Selected Direction  $\theta = 0^\circ$

| Semivariogram Analysis in Anisotropic Case With Trend Removal |        |       |       |                    |
|---------------------------------------------------------------|--------|-------|-------|--------------------|
| The VARIOGRAM Procedure                                       |        |       |       |                    |
| Dependent Variable: ResidualOzone                             |        |       |       |                    |
| Angle: 0                                                      |        |       |       |                    |
| Current Model: Exponential                                    |        |       |       |                    |
| Parameter Search                                              |        |       |       |                    |
| Set                                                           | Nugget | Scale | Range | Objective Function |
| 1                                                             | 0      | 2     | 5     | 391.06593          |
| 2                                                             | 0      | 2     | 15    | 1740.0             |
| 3                                                             | 0      | 2     | 25    | 5167.5             |
| 4                                                             | 0      | 2.5   | 5     | 64.86565           |
| 5                                                             | 0      | 2.5   | 15    | 664.03665          |
| 6                                                             | 0      | 2.5   | 25    | 2480.5             |
| 7                                                             | 0      | 3     | 5     | 72.86743           |
| 8                                                             | 0      | 3     | 15    | 305.53306          |
| 9                                                             | 0      | 3     | 25    | 1305.0             |

From this search, the combination of scale equal to 2.5 and a range of size 5 is passed as initial values to the model fitting process. This result is reflected in the model information table shown in [Output 102.2.8](#).

**Output 102.2.8** Model Initial Values for the Selected Direction  $\theta = 0^\circ$

| Model Information |               |        |
|-------------------|---------------|--------|
| Parameter         | Initial Value | Status |
| Nugget            | 0             | Fixed  |
| Scale             | 2.5000        |        |
| Range             | 5.0000        |        |

Fitting is successful, and among the output objects you can see the estimated parameters and the fit summary tables for the direction  $\theta = 0^\circ$  in [Output 102.2.9](#).



**Output 102.2.9** Weighted Least Squares Fitting Parameter Estimates and Summary for the Selected Direction  $\theta = 0^\circ$ 

| Parameter Estimates |              |                  |    |         |                |
|---------------------|--------------|------------------|----|---------|----------------|
| Parameter           | Estimate     | Approx Std Error | DF | t Value | Approx Pr >  t |
| Scale               | 2.6657       | 0.03830          | 15 | 69.60   | <.0001         |
| Range               | 3.7277       | 0.5609           | 15 | 6.65    | <.0001         |
| Fit Summary         |              |                  |    |         |                |
| Model               | Weighted SSE | AIC              |    |         |                |
| Exp                 | 43.35103     | 19.91399         |    |         |                |

A corresponding parameter search takes place for the direction  $\theta = 90^\circ$ . The respective table and the choice of initial values for fitting in the direction  $\theta = 90^\circ$  are shown in [Output 102.2.10](#).

**Output 102.2.10** Parameter Search and Model Initial Values for the Selected Direction  $\theta = 90^\circ$ 

| Parameter Search  |               |        |       |                    |
|-------------------|---------------|--------|-------|--------------------|
| Set               | Nugget        | Scale  | Range | Objective Function |
| 1                 | 0             | 2      | 5     | 302.54551          |
| 2                 | 0             | 2      | 15    | 635.93338          |
| 3                 | 0             | 2      | 25    | 1996.0             |
| 4                 | 0             | 2.5    | 5     | 95.09939           |
| 5                 | 0             | 2.5    | 15    | 104.56776          |
| 6                 | 0             | 2.5    | 25    | 662.06813          |
| 7                 | 0             | 3      | 5     | 155.50670          |
| 8                 | 0             | 3      | 15    | 20.48482           |
| 9                 | 0             | 3      | 25    | 190.30599          |
| Model Information |               |        |       |                    |
| Parameter         | Initial Value | Status |       |                    |
| Nugget            | 0             | Fixed  |       |                    |
| Scale             | 3.0000        |        |       |                    |
| Range             | 15.0000       |        |       |                    |

[Output 102.2.11](#) displays the estimated parameters and the fit summary for the direction  $\theta = 90^\circ$ .

**Output 102.2.11** Weighted Least Squares Fitting Parameter Estimates and Summary for the Selected Direction  $\theta = 90^\circ$

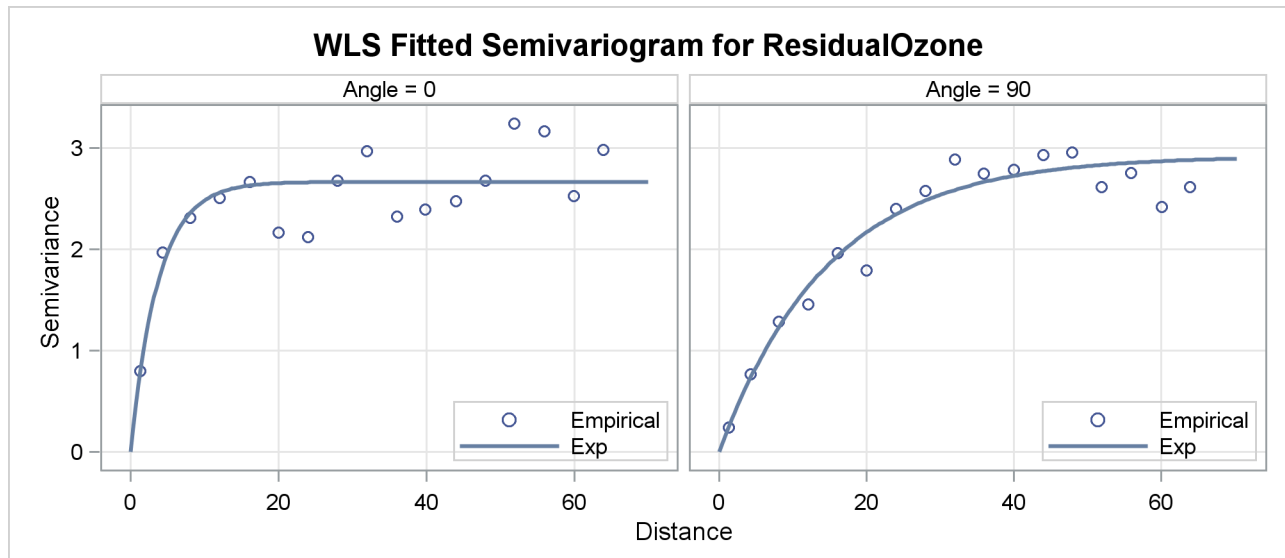
| Parameter Estimates |          |                  |    |         |                |
|---------------------|----------|------------------|----|---------|----------------|
| Parameter           | Estimate | Approx Std Error | DF | t Value | Approx Pr >  t |
| Scale               | 2.9199   | 0.07007          | 15 | 41.67   | <.0001         |
| Range               | 14.7576  | 0.9530           | 15 | 15.49   | <.0001         |

| Fit Summary |              |         |
|-------------|--------------|---------|
| Model       | Weighted SSE | AIC     |
| Exp         | 19.12246     | 6.00005 |

The fitted and empirical semivariograms for the selected directions are displayed in the panel of Output 102.2.12.

**Output 102.2.12** Fitted Theoretical and Empirical Semivariogram for the Ozone Data in the  $\theta = 0^\circ$  and  $\theta = 90^\circ$  Directions



Conclusively, your semivariogram analysis on the detrended ozone data suggests that the ozone SRF exhibits anisotropy in the perpendicular directions of N-S ( $\theta = 0^\circ$ ) and E-W ( $\theta = 90^\circ$ ).

The sills in the two directions of anisotropy are similar in size. By inspecting again the empirical semivariograms in Output 102.2.6, you could make the reasonable assumption that you have a case of geometric anisotropy, where the range in the major axis is about 4.5 times larger than the minor axis range. If you would like to use these PROC VARIOGRAM results for predictions, then you would need to specify a single scale value for the geometric anisotropy sill. In this case you could choose an arbitrary value for the constant scale from the narrow interval formed by the estimated scales in the previous results. For example, you can

specify the **PARMS** statement modified as shown in the following statement to approximate a common scale for the semivariance in all directions:

```
parms (0.) (2.7) (5 to 25 by 10) / hold=(1,2);
```

As an alternative, you can use PROC VARIOGRAM to fit an exponential model to all different angles examined in this example, and then select the constant scale value to be the mean of the scales across all directions.

---

### Example 102.3: Analysis without Surface Trend Removal

This example uses PROC VARIOGRAM without removing potential surface trends in a data set in order to investigate a distinguished spatial direction in the data. In doing so, this example also serves as a guide to examine under which circumstances you might be able to bypass the effect of a trend on a semivariogram. Typically though, for theoretical semivariogram estimations you follow the analysis presented in “[Example 102.2: An Anisotropic Case Study with Surface Trend in the Data](#)” on page 8658.

As explained in the section “[Details: VARIOGRAM Procedure](#)” on page 8608, when you compute the empirical semivariance for data that contain underlying surface trends, the outcome is the pseudo-semivariance. Pseudo-semivariograms are not estimates of the theoretical semivariogram; hence, they provide no information about the spatial continuity of your SRF.

However, in the section “[Empirical Semivariograms and Surface Trends](#)” on page 8626 it is mentioned that you might still be able to perform a semivariogram analysis with potentially non-trend-free data, if you suspect that your measurements might be trend-free across one or more specific directions. The example demonstrates this approach.

Reconsider the ozone data presented at the beginning of “[Example 102.2: An Anisotropic Case Study with Surface Trend in the Data](#)” on page 8658. The spatial distribution of the data is shown in [Figure 102.2.1](#), and the pairwise distance distribution for NHCLASSES=35 is illustrated in [Figure 102.2.3](#). This exploratory analysis suggested a LAGDISTANCE=4 km, and [Figure 102.2.2](#) indicated that for this LAGDISTANCE= you can consider a value of MAXLAGS=16.

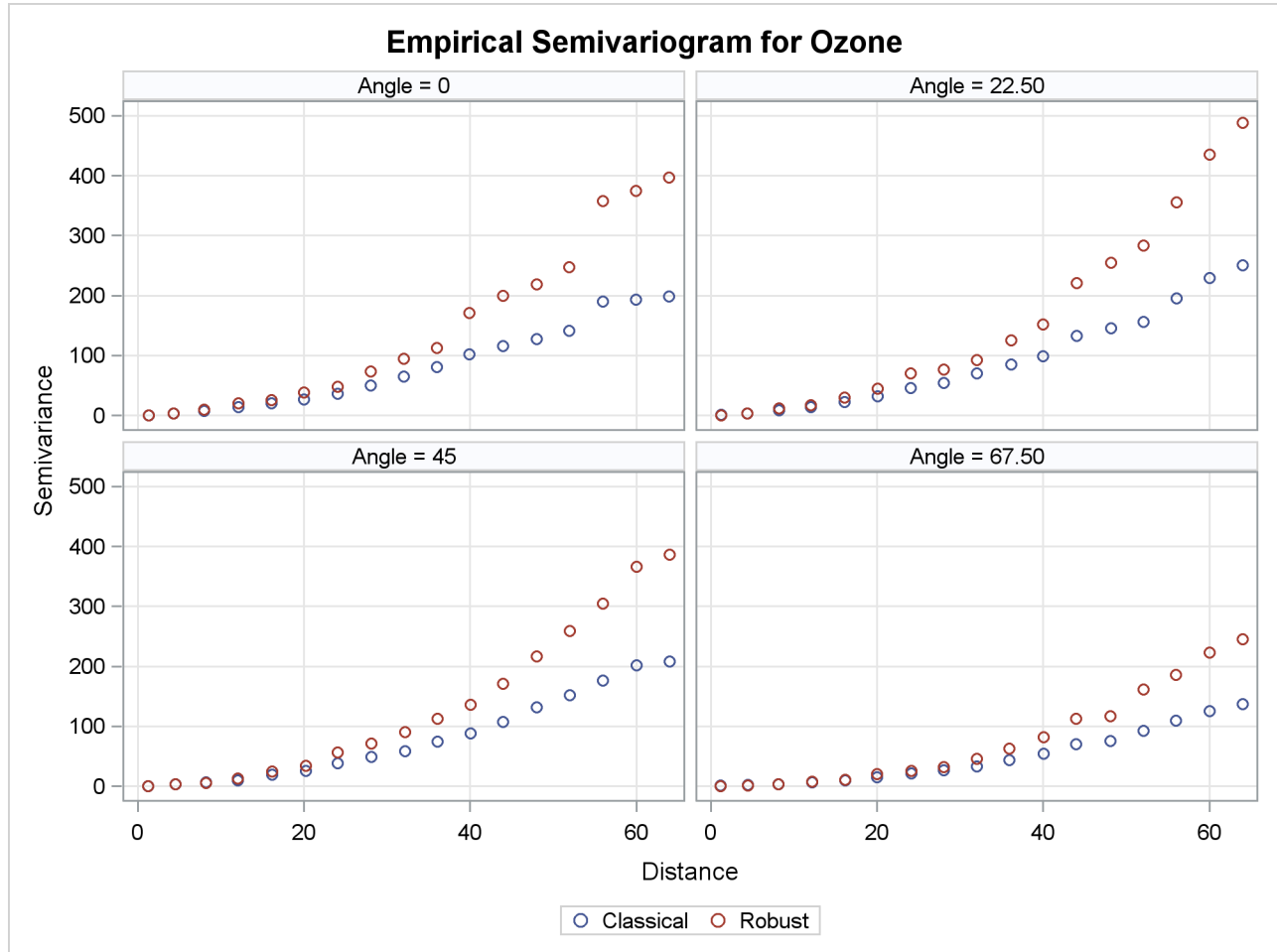
Recall from the section “[Empirical Semivariograms and Surface Trends](#)” on page 8626 that you need to investigate the empirical semivariogram of the data in a few different directions in order to identify a trend-free direction. If such a direction exists, then you can proceed with this special type of analysis. The following statements employ NDIRECTIONS=8 to examine eight directions:

```
ods graphics on;

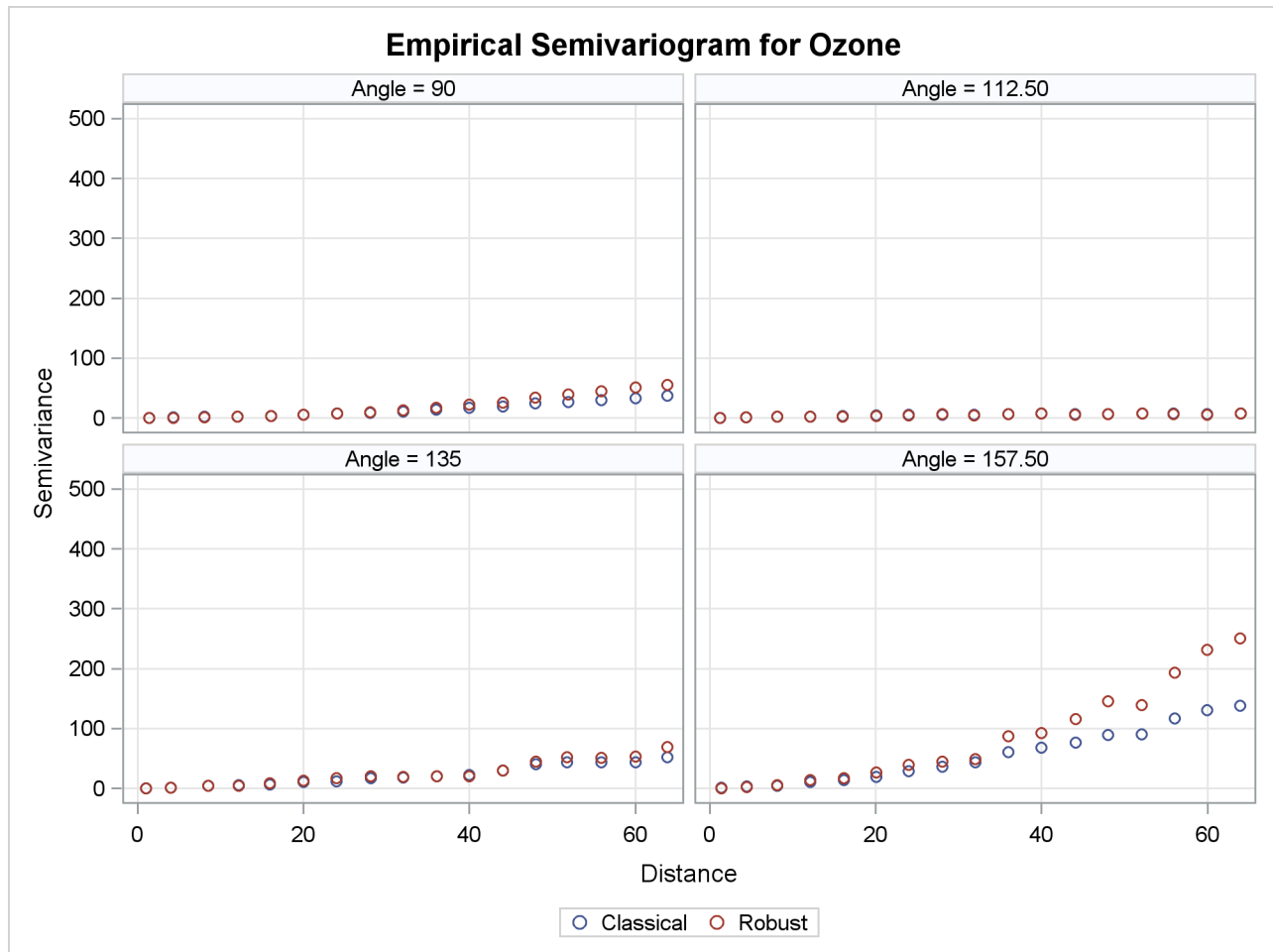
proc variogram data=ozoneSet plot(only)=semivar;
 compute lagd=4 maxlag=16 ndirections=8 robust;
 coord xc=East yc=North;
 var Ozone;
run;
```

By default, the range of  $180^\circ$  is divided into eight equally distanced angles:  $\theta = 0^\circ$ ,  $\theta = 22.5^\circ$ ,  $\theta = 45^\circ$ ,  $\theta = 67.5^\circ$ ,  $\theta = 90^\circ$ ,  $\theta = 112.5^\circ$ ,  $\theta = 135^\circ$ , and  $\theta = 157.5^\circ$ . The resulting empirical semivariograms for these angles are shown in [Output 102.3.1](#).

**Output 102.3.1** Ozone Empirical Semivariograms with  $0^\circ \leq \theta < 180^\circ$  and  $\delta\theta = 22.5^\circ$



Output 102.3.1 continued



The figures in [Output 102.3.1](#) suggest an overall continuing increase with distance of the semivariance in all directions. As explained in the section “[Theoretical Semivariogram Models](#)” on page 8608, this can be an indication of systematic trends in the data. However, the direction of  $\theta = 112.5^\circ$  clearly indicates that the increase rate, if any, is smaller than the corresponding rates across the rest of the directions. You then want to search whether there exists a trend-free direction in the neighborhood of this angle.

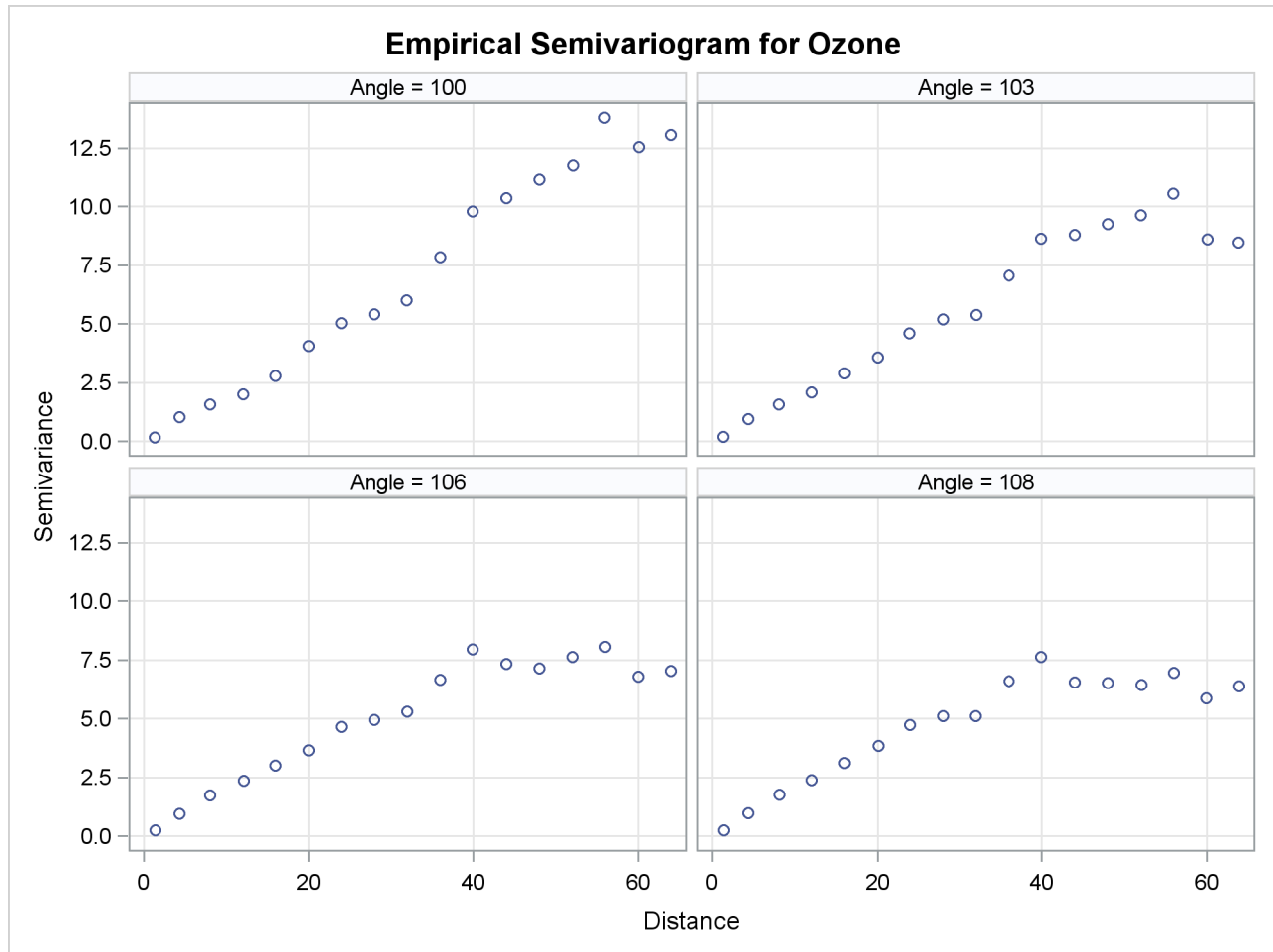
Run PROC VARIOGRAM again, specifying several directions within an interval of angles where you want to close in and you suspect the existence of a trend-free direction. In the following step you specify ANGLETOL=15°, which is smaller than the default value of 22.5°, and you also specify BANDWIDTH=10 km. The smaller values help with minimization of the interference with neighboring directions, as discussed in the section “[Angle Classification](#)” on page 8617.

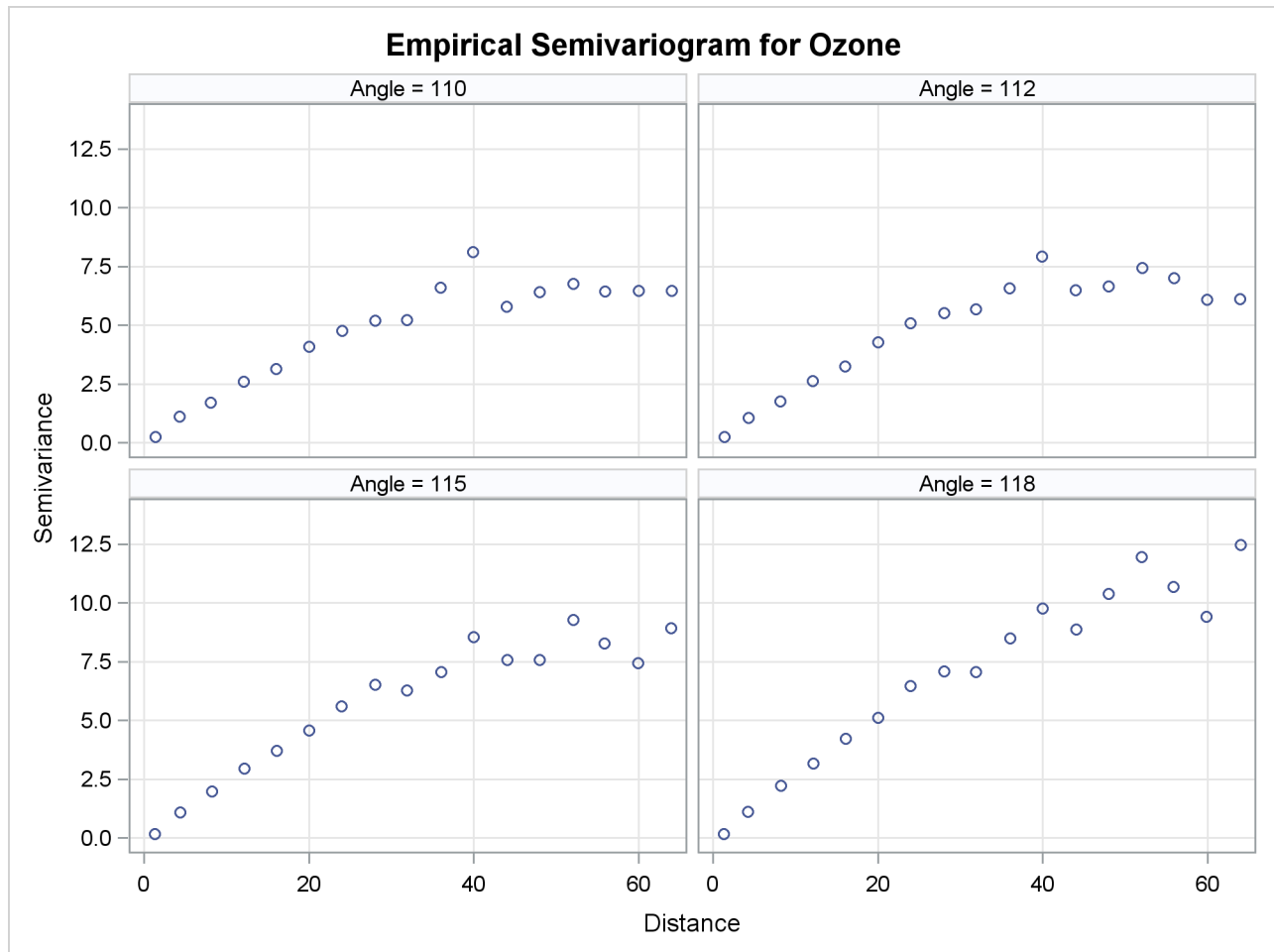
The aforementioned considerations are addressed in the following statements:

```
proc variogram data=ozoneSet plot(only)=semivar(cla);
 compute lagd=4 maxlag=16 robust;
 directions 100(15,10) 103(15,10)
 106(15,10) 108(15,10)
 110(15,10) 112(15,10)
 115(15,10) 118(15,10);
 coord xc=East yc=North;
 var Ozone;
run;
```

Your analysis has brought you to examine a narrow strip of angles within  $\theta = 100^\circ$  and  $\theta = 118^\circ$ . The pseudo-semivariograms in Output 102.3.2 and Output 102.3.3 indicate that at the boundaries of this strip, the angles display increasing semivariance with distance. On the other hand, within this interval there are directions across which the semivariance is tentatively reaching a sill, and these are potential candidates to be trend-free directions.

**Output 102.3.2** Ozone Empirical Semivariograms in  $100^\circ$ ,  $103^\circ$ ,  $106^\circ$ , and  $108^\circ$



**Output 102.3.3** Ozone Empirical Semivariograms in 110°, 112°, 115°, and 118°

You can further investigate this angle spectrum in more detail. For example, you can monitor additional angles in between, or use a smaller `LAGDISTANCE=` and increased `MAXLAGS=` values to single out the most qualified candidate. For the purpose of this example, you can consider the direction  $\theta = 108^\circ$  to very likely be the trend-free one you are looking for.

From a physical standpoint, the trend-free direction, if it exists, is expected to be perpendicular to the direction of the maximum dip in the values of the ozone field, as mentioned in the section “[Empirical Semivariograms and Surface Trends](#)” on page 8626. If you cross-examine the ozone data distribution in [Output 102.2.1](#), the figure suggests that this direction exists and is slightly tilted clockwise with respect to the E–W axis. This direction emerges from the mild stratification of the ozone values in your data distribution. The ozone concentrations across it are similar when compared to surrounding directions, and as such, it has been identified as a trend-free direction.

Your next step is to obtain the empirical semivariogram in the suspected trend-free direction of  $\theta = 108^\circ$  and to perform a theoretical model fit.

The semivariance in [Output 102.3.2](#) exhibits a slow, almost linear rise at short distances and seems to be reaching the sill fast, rather than asymptotically. You can accommodate this behavior by using the spherical model

$$\gamma_z(h) = \begin{cases} c_n + \sigma_0^2 \left[ \frac{3}{2} \frac{h}{a_0} - \frac{1}{2} \left( \frac{h}{a_0} \right)^3 \right], & \text{for } 0 < h \leq a_0 \\ c_0, & \text{for } a_0 < h \end{cases}$$

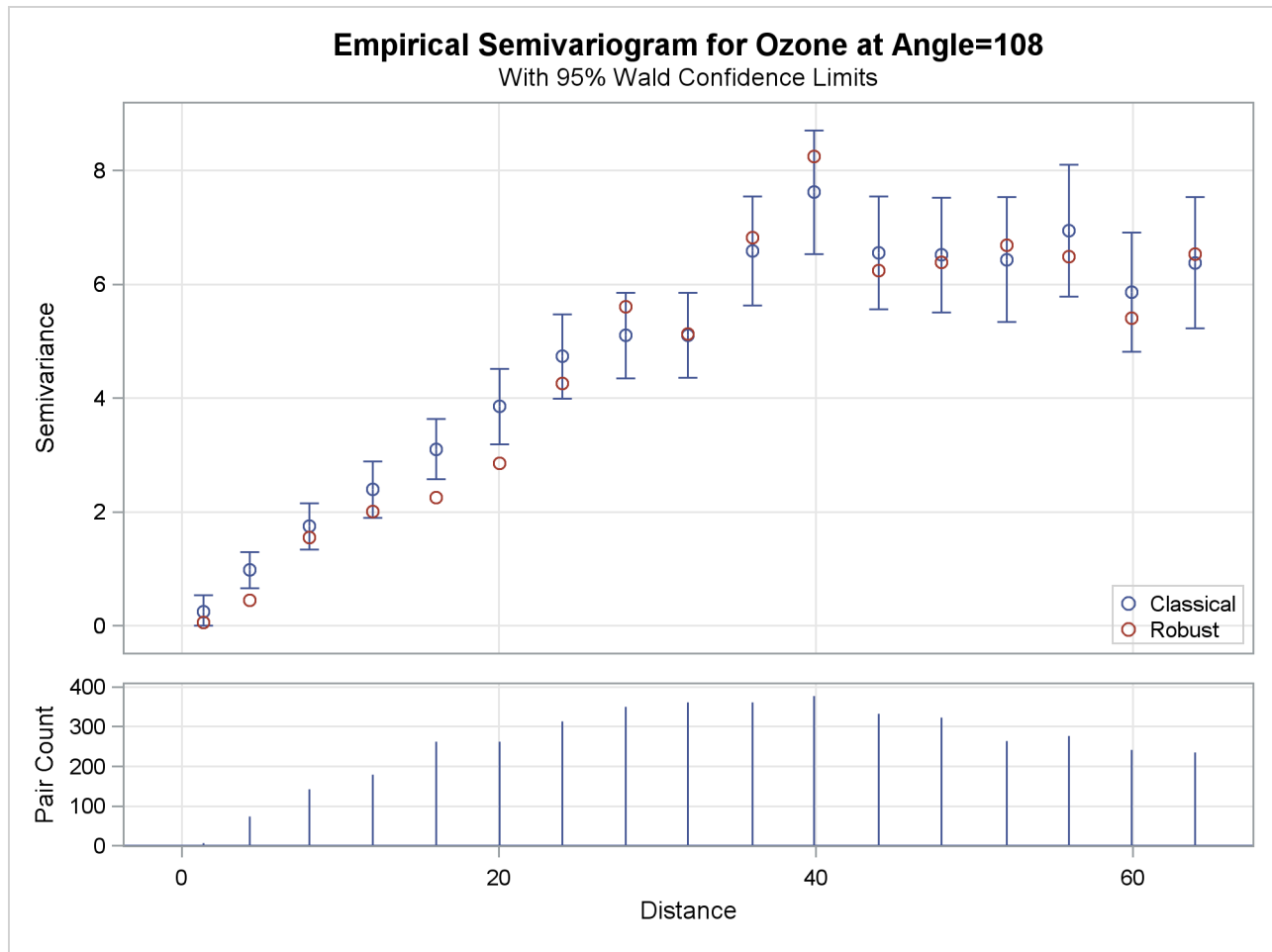
where  $\gamma_z(0) = 0$  and  $a_0 > 0$ . The empirical semivariograms also suggest that there does not seem to be a nugget effect. Assume that in this example you are interested in what the fitting process concludes about the nugget effect, so you skip the `NUGGET=` option in the `MODEL` statement. You also let PROC VARIOGRAM provide initial values for the rest of the model parameters. Eventually, you use the `PLOTS` option to inspect the classical and robust empirical semivariograms in the selected direction and to produce a plot of the fitted model. The following statements implement these considerations:

```
proc variogram data=ozoneSet plot(only)=(semivar fit);
 compute lagd=4 maxlag=16 robust cl;
 directions 108(15,10);
 coord xc=East yc=North;
 model form=sph;
 var ozone;
run;

ods graphics off;
```

The classical and robust empirical semivariograms in the selected direction  $\theta = 108^\circ$  are displayed in Figure 102.3.4.

**Output 102.3.4** Ozone Classical and Robust Empirical Semivariograms in  $\theta = 108^\circ$





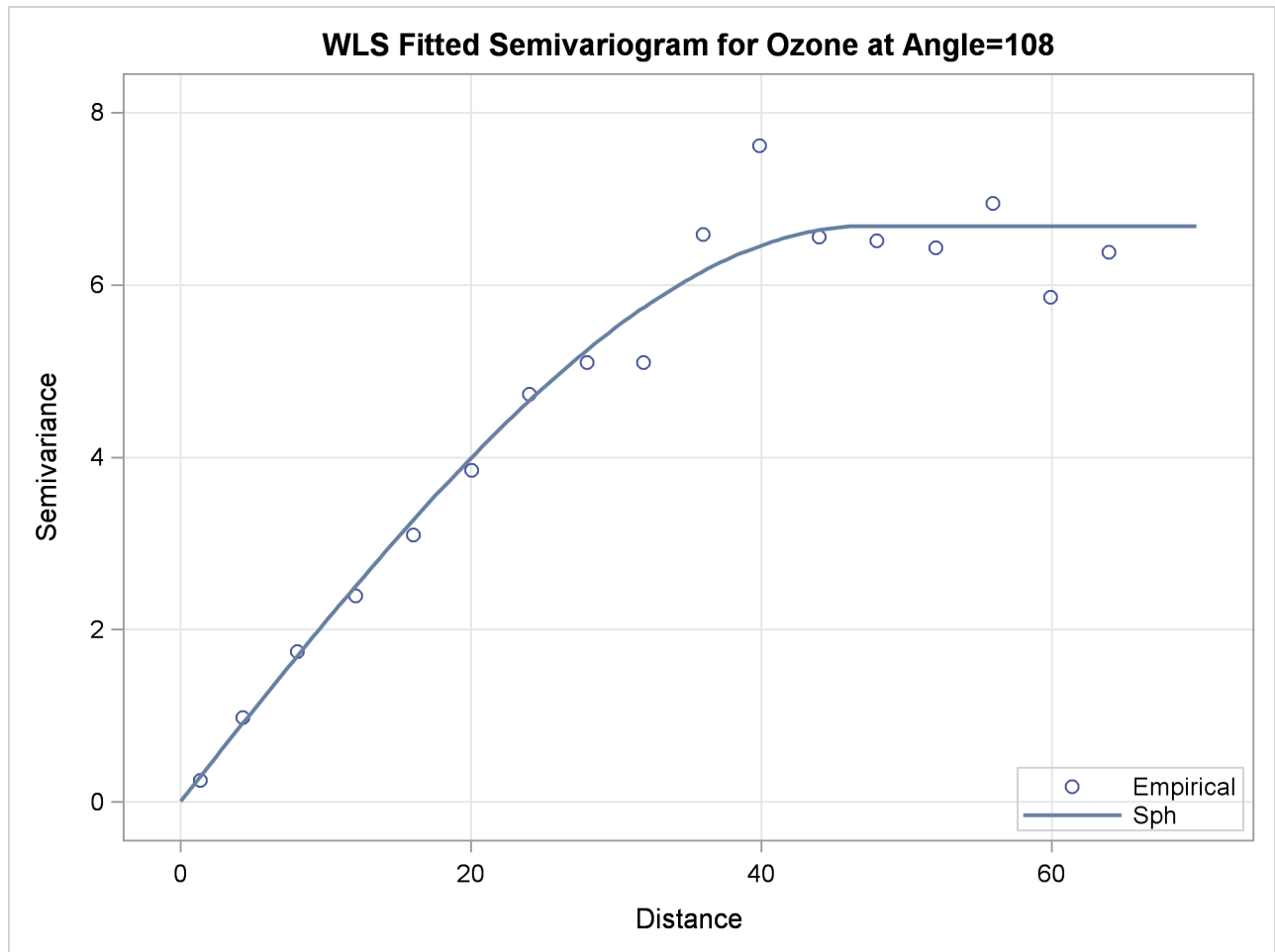
The output continues with information about the fitting process, which terminates successfully and produces the estimated parameters and the fit summary tables shown in [Output 102.3.5](#). The near-zero nugget parameter estimate indicates that you can consider the process to be practically free of nugget effect.

**Output 102.3.5** Weighted Least Squares Fitting Parameter Estimates and Summary in  $\theta = 108^\circ$

| Parameter Estimates |                 |                     |    |         |                   |
|---------------------|-----------------|---------------------|----|---------|-------------------|
| Parameter           | Estimate        | Approx<br>Std Error | DF | t Value | Approx<br>Pr >  t |
| Nugget              | 0.006260        | 0.09449             | 14 | 0.07    | 0.9481            |
| Scale               | 6.6791          | 0.1741              | 14 | 38.37   | <.0001            |
| Range               | 47.3012         | 2.0776              | 14 | 22.77   | <.0001            |
| Fit Summary         |                 |                     |    |         |                   |
| Model               | Weighted<br>SSE | AIC                 |    |         |                   |
| Sph                 | 13.13869        | 1.61991             |    |         |                   |

The fitted and empirical semivariograms for the selected direction  $\theta = 108^\circ$  are displayed in [Output 102.3.6](#).

**Output 102.3.6** Fitted Theoretical and Empirical Semivariogram for the Ozone Data in  $\theta = 108^\circ$



A comparative look at the empirical and fitted semivariograms in [Output 102.3.6](#) and [Output 102.2.12](#) suggests that the analysis of the trend-free ResidualOzone produces a different outcome from that of the original Ozone values. In fact, a more suitable comparison can be made between the semivariograms in the assumed trend-free direction  $\theta = 108^\circ$  of the current scenario and the one shown in [Output 102.2.6](#) in the nearly identical direction  $\theta = 105^\circ$ . It might seem unreasonable that these two semivariograms are produced both in the same ozone study and in a narrow band of directions free of apparent surface trends, yet they bear no resemblance. However, the lack of similarity in these plots stems from operating on two different data sets where the outcome depends on the actual data values.

More specifically, the semivariogram analysis treats the trend-free ozone set and the original ozone measurements as different quantities. The process of detrending the original Ozone values is a transformation of these values into the trend-free values of ResidualOzone. Any existing spatial correlation in the original data is not necessarily retained within the transformed data. Depending on the transformation features, the emerging data set has its own characteristics, as demonstrated in this example.

A final remark concerns the issue of isotropy. Based on the details presented in the section “[Empirical Semivariograms and Surface Trends](#)” on page 8626, your knowledge of the spatial structure of the ozoneSet data set is limited to the selected trend-free direction you indicated in the present example. You can generalize this outcome for all spatial directions only if you consider the hypothesis of isotropy in the ozone field to be reasonable. However, you cannot infer the assumption of anisotropy in the present example based on the analysis in the section “[Analysis with Surface Trend Removal](#)” on page 8662. Again, the reason is that you currently use the observed Ozone values, whereas the ResidualOzone data in the previous example emerged from a transformation of the current data. Hence, you have essentially two data sets that do not necessarily share the same properties.

---

## Example 102.4: Covariogram and Semivariogram

The covariance that was reviewed in the section “[Stationarity](#)” on page 8615 is an alternative measure of spatial continuity that can be used instead of the semivariance. In a similar manner to the empirical semivariance that was presented in the section “[Theoretical and Computational Details of the Semivariogram](#)” on page 8613, you can also compute the empirical covariance. The covariograms are plots of this quantity and can be used to fit permissible theoretical covariance models, in correspondence to the semivariogram analysis presented in the section “[Theoretical Semivariogram Models](#)” on page 8608. This example displays a comparative view of the empirical covariogram and semivariogram, and examines some additional aspects of these two measures.

You consider 500 simulations of an SRF  $Z(s)$  in a square domain of  $100 \times 100$  ( $10^6$  km<sup>2</sup>). The following DATA step defines the data locations:

```

title 'Covariogram and Semivariogram';

data dataCoord;
 retain seed 837591;
 do i=1 to 100;
 East = round(100*ranuni(seed),0.1);
 North = round(100*ranuni(seed),0.1);
 output;
 end;
run;

```

For the simulations you use PROC SIM2D, which produces Gaussian simulations of SRFs with user-specified covariance structure—see Chapter 85, “The SIM2D Procedure.” The Gaussian SRF implies full knowledge of the SRF expected value  $E[Z(s)]$  and variance  $\text{Var}[Z(s)]$  at every location  $s$ . The following statements simulate an isotropic, second-order stationary SRF with constant expected value and variance throughout the simulation domain:

```
proc sim2d outsim=dataSims;
 simulate numreal=500 seed=79750
 nugget=2 scale=6 range=10 form=exp;
 mean 30;
 grid gdata=dataCoord xc=East yc=North;
run;
```

Here, the SIMULATE statement accommodates the simulation parameters. The NUMREAL= option specifies that you want to perform 500 simulations, and the SEED= option specifies the seed for the simulation random number generator. You use the MEAN statement to specify the expected value  $E[Z(s)] = 30$  units of  $Z$ . You also specify two variance components. The first is the nugget effect, and you use the NUGGET= option to set it to  $c_n = 2$ . The second is the partial sill  $\sigma_0^2 = 6$  that you specify with the SCALE= option. The two variance components make up the total SRF variance  $\text{Var}[Z(s)] = c_n + \sigma_0^2 = 8$ . You assume an exponential covariance structure to describe the field spatial continuity, where  $\sigma_0^2$  is the sill value and its range  $a_0 = 10$  km (effective range  $a_\epsilon = 3a_0 = 30$  km) is specified by the RANGE= option. The option FORM= specifies the covariance structure type.

The empirical semivariance and covariance are computed by the VARIOGRAM procedure, and are available either in the ODS output semivariogram table (as variables Semivariance and Covariance, respectively) or in the **OUTVAR=** data set. In the following statements you obtain these variables by using the **OUTVAR=** data set of the VARIOGRAM procedure:

```
proc variogram data=dataSims outv=outv noprint;
 compute lagd=3 maxlag=18;
 coord xc=gxc yc=gyc;
 by _ITER_;
 var svalue;
run;
```

For each distance lag you take the average of the empirical measures over the number of simulations. PROC SORT prepares the input data for PROC MEANS, which produces these averages and stores them in the dataAvgs data set. This sequence is performed with the following statements:

```
proc sort data=outv;
 by lag;
run;

proc means data=outv n mean noprint;
 var Distance variog covar;
 by lag;
 output out=dataAvgs mean(variog)=Semivariance
 mean(covar)=Covariance
 mean(Distance)=Distance;
run;
```

The SGPLOT procedure creates the plot of the average empirical semivariogram and covariogram, as in the following statements:

```
proc sgplot data=dataAvgs;
 title "Empirical Semivariogram and Covariogram";
 xaxis label = "Distance" grid;
 yaxis label = "Semivariance" min=-0.5 max=9 grid;
 y2axis label = "Covariance" min=-0.5 max=9;
 scatter y=Semivariance x=Distance /
 markerattrs = GraphData1
 name='Semivar'
 legendlabel='Semivariance';
 scatter y=Covariance x=Distance /
 y2axis
 markerattrs = GraphData2
 name='Covar'
 legendlabel='Covariance';
 discretelegend 'Semivar' 'Covar';
run;
```

The plot of the average empirical semivariance and covariance of the preceding analysis is shown in [Output 102.4.1](#). The high number of simulations led to averages of empirical continuity measures that accurately approximate the simulated SRF characteristics. Specifically, the empirical semivariogram and covariogram both exhibit clearly exponential behavior. The semivariogram sill is approximately at the specified variance  $\text{Var}[Z(s)] = 8$  of the SRF.

The simulated SRF is second-order stationary, so you expect at each lag the sum of the empirical semivariance and covariance to approximate the field variance  $\text{Var}[Z(s)]$ , as explained in the section “Stationarity” on page 8615. This behavior is evident in [Output 102.4.1](#).

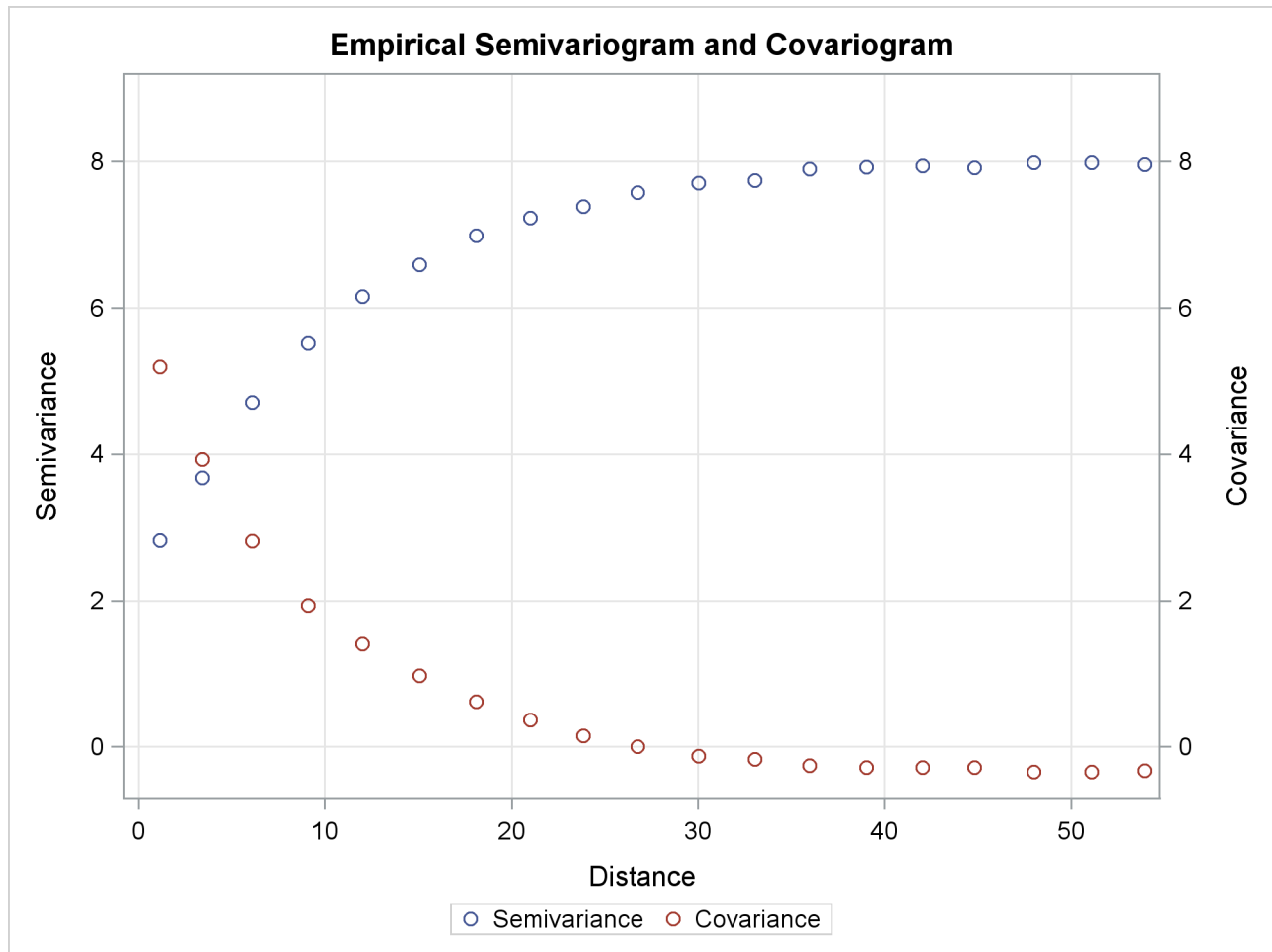
This example concludes with a discussion of basic reasons why the empirical semivariogram analysis is commonly preferred to the empirical covariance analysis. A first reason comes from the assumptions that are necessary to compute each of these two measures. The condition of intrinsic stationarity that is required in order to define the empirical semivariogram is less restrictive than the condition of second-order stationarity that is required in order to consider the covariance function as a parameter of the process.

Also, an empirical semivariogram can indicate whether a nugget effect is present in your data sample, whereas the empirical covariogram itself might not reveal this information. This point is illustrated in [Output 102.4.1](#), where you expect to see that  $C(\mathbf{0}) = \text{Var}[Z(s)]$ , but the empirical covariogram cannot have a point at exactly  $h = \mathbf{0}$ . A practical way to investigate for a nugget effect when you use empirical covariograms is as follows: recall that the `OUTVAR=` data set provides you with the sample variance (shown in the `COVAR` column for `LAG=-1`), as the following statement shows:

```
/* Obtain the sample variance from the data set -----*/

proc print data=dataAvgs (obs=1);
run;
```

**Output 102.4.1** Average Empirical Semivariogram and Covariogram from 500 Simulations



Output 102.4.2 is a partial output of the dataAvgs data set, which contains averages of the `OUTVAR=` data set and shows the computed average  $C(\mathbf{0})$  in the Covariance column. The combination of the empirical covariogram and the  $C(\mathbf{0})$  value can help you fit a theoretical covariance model that includes any nugget effect, if present. See also the discussion in Schabenberger and Gotway (2005, section 4.2.2) about the Matérn definition of the covariance function that is related to this issue. In particular, this definition provides for an additional variance component in the covariance expression at  $\mathbf{h} = \mathbf{0}$  to account for the corresponding nugget effect in the semivariogram.

**Output 102.4.2** Partial Outcome of the dataAvgs Data Set

| Empirical Semivariogram and Covariogram |     |        |        |              |            |          |
|-----------------------------------------|-----|--------|--------|--------------|------------|----------|
| Obs                                     | LAG | _TYPE_ | _FREQ_ | Semivariance | Covariance | Distance |
| 1                                       | -1  | 0      | 500    | .            | 7.74832    | .        |

In addition to the preceding points, if the SRF is nonstationary, the empirical semivariogram indicates that the SRF variance increases with distance  $h$ , as [Output 102.3.1](#) shows in “[Example 102.3: Analysis without Surface Trend Removal](#)” on page 8672. In that case it makes no sense to compute the empirical covariogram. Specifically, the covariogram could provide you with an estimate of the sample variance, which is not sufficient to indicate that the SRF might not be stationary (see also Chilès and Delfiner 1999, p. 31).

Finally, the definitions of the empirical semivariance and covariance in the section “[Theoretical and Computational Details of the Semivariogram](#)” on page 8613 clearly show that the sample mean  $\bar{Z}$  and the SRF expected value  $E[Z(s)]$  are not important for the computation of the semivariance, but either one is necessary for the covariance. Hence, the semivariance expression filters the mean, and this behavior is especially useful when the mean is unknown. On the other hand, if  $E[Z(s)]$  is unknown and the empirical covariance is computed based on the sample mean  $\bar{Z}$ , this can induce additional bias in the covariance computation.

---

### Example 102.5: A Box Plot of the Square Root Difference Cloud

The Gaussian form selected for the semivariogram in the section “[Getting Started: VARIOGRAM Procedure](#)” on page 8561 is based on consideration of the plots of the sample semivariogram. For the coal thickness data, the Gaussian form appears to be a reasonable choice.

However, it can often happen that a plot of the sample variogram shows so much scatter that no particular form is evident. The cause of this scatter can be one or more outliers in the pairwise differences of the measured quantities.

A method of identifying potential outliers is discussed in Cressie (1993, section 2.2.2). This example illustrates how to use the `OUTPAIR=` data set from PROC VARIOGRAM to produce a square root difference cloud, which is useful in detecting outliers.

For the SRF  $Z(s)$ ,  $s \in \mathcal{R}^2$ , the square root difference cloud for a particular direction  $e$  is given by

$$| Z(s_i + he) - Z(s_i) |^{\frac{1}{2}}$$

for a given lag distance  $h$ . In the actual computation, all pairs  $P_1 P_2$  of points  $P_1$ ,  $P_2$  within a distance tolerance around  $h$  and an angle tolerance around the direction  $e$  are used. This generates a number of point pairs for each lag class  $h$ . The spread of these values gives an indication of outliers.

Following the example in the section “[Getting Started: VARIOGRAM Procedure](#)” on page 8561, this example uses a basic `LAGDISTANCE=7`, with a distance tolerance of 3.5, and a direction of N–S, with an angle tolerance `ATOL=30°`.

First, use PROC VARIOGRAM to produce an `OUTPAIR=` data set. Then use a `DATA` step to subset this data by choosing pairs within  $30^\circ$  of N–S. In addition, compute lag class and square root difference variables, as the following statements show:

```

title 'Square Root Difference Cloud Example';

data thick;
 input East North Thick @@;
 label Thick='Coal Seam Thickness';
 datalines;
0.7 59.6 34.1 2.1 82.7 42.2 4.7 75.1 39.5
4.8 52.8 34.3 5.9 67.1 37.0 6.0 35.7 35.9
6.4 33.7 36.4 7.0 46.7 34.6 8.2 40.1 35.4
13.3 0.6 44.7 13.3 68.2 37.8 13.4 31.3 37.8
17.8 6.9 43.9 20.1 66.3 37.7 22.7 87.6 42.8
23.0 93.9 43.6 24.3 73.0 39.3 24.8 15.1 42.3
24.8 26.3 39.7 26.4 58.0 36.9 26.9 65.0 37.8
27.7 83.3 41.8 27.9 90.8 43.3 29.1 47.9 36.7
29.5 89.4 43.0 30.1 6.1 43.6 30.8 12.1 42.8
32.7 40.2 37.5 34.8 8.1 43.3 35.3 32.0 38.8
37.0 70.3 39.2 38.2 77.9 40.7 38.9 23.3 40.5
39.4 82.5 41.4 43.0 4.7 43.3 43.7 7.6 43.1
46.4 84.1 41.5 46.7 10.6 42.6 49.9 22.1 40.7
51.0 88.8 42.0 52.8 68.9 39.3 52.9 32.7 39.2
55.5 92.9 42.2 56.0 1.6 42.7 60.6 75.2 40.1
62.1 26.6 40.1 63.0 12.7 41.8 69.0 75.6 40.1
70.5 83.7 40.9 70.9 11.0 41.7 71.5 29.5 39.8
78.1 45.5 38.7 78.2 9.1 41.7 78.4 20.0 40.8
80.5 55.9 38.7 81.1 51.0 38.6 83.8 7.9 41.6
84.5 11.0 41.5 85.2 67.3 39.4 85.5 73.0 39.8
86.7 70.4 39.6 87.2 55.7 38.8 88.1 0.0 41.6
88.4 12.1 41.3 88.4 99.6 41.2 88.8 82.9 40.5
88.9 6.2 41.5 90.6 7.0 41.5 90.7 49.6 38.9
91.5 55.4 39.0 92.9 46.8 39.1 93.4 70.9 39.7
55.8 50.5 38.1 96.2 84.3 40.3 98.2 58.2 39.5
;

proc variogram data=thick outp=outp noprint;
 compute novariogram;
 coordinates xc=East yc=North;
 var Thick;
run;

data sqroot;
 set outp;
 /*- Include only points +/- 30 degrees of N-S -----*/
 where abs(cos) < 0.5;
 /*- Unit lag of 7, distance tolerance of 3.5 -----*/
 lag_class=int(distance/7 + 0.500001);
 sqr_diff=sqrt(abs(v1-v2));
run;

proc sort data=sqroot;
 by lag_class;
run;

```



Next, summarize the results by using the MEANS procedure:

```
proc means data=sqroot noprint n mean std;
 var sqr_diff;
 by lag_class;
 output out=msqrt n=n mean=mean std=std;
run;
title2 'Summary of Results';

proc print data=msqrt;
 id lag_class;
 var n mean std;
run;
```

The preceding statements produce [Output 102.5.1](#).

### Output 102.5.1 Summary of Results

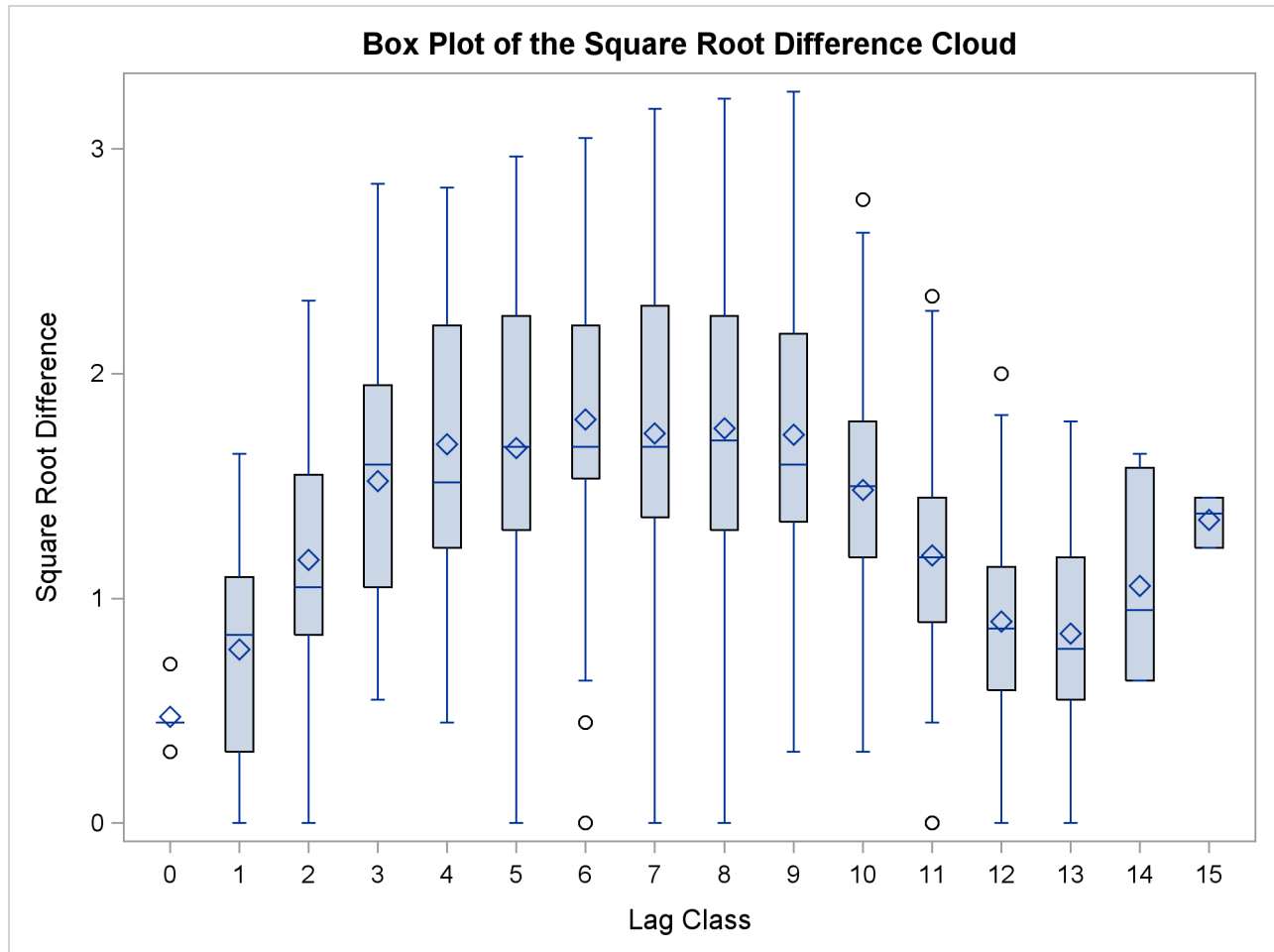
| Square Root Difference Cloud Example<br>Summary of Results |     |         |         |  |
|------------------------------------------------------------|-----|---------|---------|--|
| lag_                                                       | n   | mean    | std     |  |
| class                                                      |     |         |         |  |
| 0                                                          | 5   | 0.47300 | 0.14263 |  |
| 1                                                          | 31  | 0.77338 | 0.41467 |  |
| 2                                                          | 51  | 1.17052 | 0.47800 |  |
| 3                                                          | 58  | 1.52287 | 0.51454 |  |
| 4                                                          | 65  | 1.68625 | 0.58465 |  |
| 5                                                          | 65  | 1.66963 | 0.68582 |  |
| 6                                                          | 80  | 1.79693 | 0.62929 |  |
| 7                                                          | 88  | 1.73334 | 0.73191 |  |
| 8                                                          | 83  | 1.75528 | 0.68767 |  |
| 9                                                          | 108 | 1.72901 | 0.58274 |  |
| 10                                                         | 80  | 1.48268 | 0.48695 |  |
| 11                                                         | 84  | 1.19242 | 0.47037 |  |
| 12                                                         | 68  | 0.89765 | 0.42510 |  |
| 13                                                         | 38  | 0.84223 | 0.44249 |  |
| 14                                                         | 7   | 1.05653 | 0.42548 |  |
| 15                                                         | 3   | 1.35076 | 0.11472 |  |

Finally, present the results in a box plot by using the SGPLOT procedure. The box plot facilitates the detection of outliers. The statements are as follows:

```
proc sgplot data=sqroot;
 xaxis label = "Lag Class";
 yaxis label = "Square Root Difference";
 title "Box Plot of the Square Root Difference Cloud";
 vbox sqr_diff / category=lag_class;
run;
```

Output 102.5.2 suggests that outliers, if any, do not appear to be adversely affecting the empirical semi-variogram in the N-S direction for the coal seam thickness data. The conclusion from Output 102.5.2 is consistent with our previous semi-variogram analysis of the same data set in the section “Getting Started: VARIOGRAM Procedure” on page 8561. The effect of the isolated outliers in lag classes 6 and 10–12 in Output 102.5.2 is demonstrated as the divergence between the classical and robust empirical semivariance estimates in the higher distances in Output 102.7. The difference in these estimates comes from the definition of the robust semivariance estimator  $\hat{\gamma}_z(\mathbf{h})$  (see the section “Theoretical and Computational Details of the Semivariogram” on page 8613), which imposes a smoothing effect on the outlier influence.

**Output 102.5.2** Box Plot of the Square Root Difference Cloud



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# Appendix A

## Special SAS Data Sets

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## Introduction to Special SAS Data Sets

All SAS/STAT procedures create SAS data sets. Any table generated by a procedure can be saved to a data set by using the Output Delivery System (ODS), and many procedures also have syntax that enables you to save other statistics to data sets. Some of these data sets are organized according to certain conventions so that they can be read by a SAS/STAT procedure for further analysis. Such specially organized data sets are recognized by the TYPE= data set attribute.

The CORR procedure (see the *Base SAS Procedures Guide: Statistical Procedures*), for example, can create a data set with the attribute TYPE=CORR containing a correlation matrix. This TYPE=CORR data set can

be read by the REG or FACTOR procedure, among others. If the original data set is large, using a special SAS data set in this way can save computer time by avoiding the recomputation of the correlation matrix in subsequent analyses.

PROC REG, for example, can create a TYPE=EST data set containing estimated regression coefficients. If you need to make predictions for new observations, you can use the SCORE procedure to read both the TYPE=EST data set and a data set containing the new observations. PROC SCORE can then compute predicted values or residuals without repeating the entire regression analysis. See Chapter 82, “The SCORE Procedure,” for an example.

A special SAS data set might contain different kinds of statistics. A special variable called `_TYPE_` is used to distinguish the various statistics. For example, in a TYPE=CORR data set, an observation in which `_TYPE_='MEAN'` contains the means of the variables in the analysis, and an observation in which `_TYPE_='STD'` contains the standard deviations. Correlations appear in observations with `_TYPE_='CORR'`. Another special variable, `_NAME_`, is needed to identify the row of the correlation matrix. Thus, the correlation between variables X and Y is given by the value of the variable X in the observation for which `_TYPE_='CORR'` and `_NAME_='Y'`, or by the value of the variable Y in the observation for which `_TYPE_='CORR'` and `_NAME_='X'`.

The special data sets created by SAS/STAT procedures can generally be used directly by other procedures without modification. However, if you create an output data set with PROC CORR and use the NOCORR option to omit the correlation matrix from the OUT= data set, you need to set the TYPE= option either in parentheses following the OUT= data set name in the PROC CORR statement or in parentheses following the DATA= option in any other procedure that recognizes the special TYPE= attribute. In either case, the TYPE= option should be set to COV, CSSCP, or SSCP according to what type of matrix is stored in the data set and what data set types are accepted as input by the other procedures you plan to use. If you do not follow these steps and you use the TYPE=CORR data set with no correlation matrix as input to another procedure, the procedure might issue an error message indicating that the correlation matrix is missing from the data set.

You can create special SAS data sets directly in a DATA step by specifying the TYPE= option in parentheses after the data set name in the DATA statement. See “[Example A.2: Creating a TYPE=CORR Data Set in a DATA Step](#)” on page 8696 for an example. If you use a DATA step with a SET statement to modify a special SAS data set, you must specify the TYPE= option in the DATA statement. The TYPE= attribute of the data set in the SET statement is *not* automatically copied to the data set being created. You can determine the TYPE= attribute of a data set by using the CONTENTS procedure (see “[Example A.1: A TYPE=CORR Data Set Produced by PROC CORR](#)” on page 8695 and the *Base SAS Procedures Guide* for details).

[Table A.1](#) summarizes the TYPE= data sets that can be used as input to SAS/STAT procedures. [Table A.2](#) summarizes the TYPE= data sets that are created by SAS/STAT procedures and the statements each procedure uses to create its special output data sets. Most procedures accept ordinary SAS data sets and create ordinary output SAS data sets with no TYPE= specification in addition to the special data sets shown in the tables. When you specify a data set with a type that the procedure does not recognize, the procedure prints an error message and stops executing.

**Table A.1** SAS/STAT Procedures That Accept Special Input Data Sets Types

| <b>Procedure</b> | <b>Special TYPE= Data Sets Accepted</b>                |
|------------------|--------------------------------------------------------|
| ACECLUS          | ACE, CORR, COV, SSCP, UCORR, UCOV                      |
| BOXPLOT          | BOXPLOT, CHARTSUM                                      |
| CALIS            | CALISMDL, CORR, COV, FACTOR, SSCP, UCORR, UCOV, WEIGHT |
| CANDISC          | CORR, COV, SSCP, CSSCP                                 |
| CATMOD           | EST                                                    |
| CLUSTER          | DISTANCE                                               |
| DISCRIM          | CORR, COV, SSCP, CSSCP, LINEAR, QUAD, MIXED            |
| FACTOR           | ACE, CORR, COV, FACTOR, SSCP, UCORR, UCOV              |
| LIFEREG          | EST                                                    |
| LOGISTIC         | EST LOGISMOD                                           |
| MI               | EST, COV, CORR                                         |
| MIANALYZE        | EST, COV, CORR                                         |
| MODECLUS         | DISTANCE                                               |
| PHREG            | EST                                                    |
| PRINCOMP         | ACE, CORR, COV, EST, FACTOR, SSCP, UCORR, UCOV         |
| PROBIT           | EST                                                    |
| QUANTREG         | EST                                                    |
| REG              | CORR, COV, SSCP, UCORR, UCOV                           |
| ROBUSTREG        | EST                                                    |
| SCORE            | SCORE= data set can be of any type                     |
| SIMNORM          | CORR, COV                                              |
| SURVEYLOGISTIC   | EST                                                    |
| STEPDISC         | CORR, COV, SSCP, CSSCP                                 |
| TREE             | TREE                                                   |
| VARCLUS          | CORR, COV, FACTOR, SSCP, UCORR, UCOV                   |

**Table A.2** SAS/STAT Procedures That Create Special Output Data Set Types

| <b>Procedure</b> | <b>TYPE=</b> | <b>Statement and Option Required</b> |
|------------------|--------------|--------------------------------------|
| ACECLUS          | ACE          | PROC ACECLUS OUTSTAT=                |
| BOXPLOT          | BOXPLOT      | PLOT / OUTBOX=                       |
|                  | CHARTSUM     | PLOT / OUTHISTORY=                   |
| CALIS            | CALISFIT     | PROC CALIS OUTFIT=                   |
|                  | CALISMDL     | PROC CALIS OUTMODEL=                 |
|                  | CORR         | PROC CALIS CORR OUTSTAT=             |
|                  | COV          | PROC CALIS OUTSTAT=                  |
|                  | EST          | PROC CALIS OUTEST=                   |
|                  | WEIGHT       | PROC CALIS OUTWGT=                   |
| CANCORR          | CORR         | PROC CANCORR OUTSTAT=                |
|                  | UCORR        | PROC CANCORR NOINT OUTSTAT=          |
| CANDISC          | CORR         | PROC CANDISC OUTSTAT=                |
| CATMOD           | EST          | RESPONSE / OUTEST=                   |

Table A.2 continued

| Procedure | TYPE=    | Statement and Option Required                       |
|-----------|----------|-----------------------------------------------------|
| CLUSTER   | TREE     | PROC CLUSTER OUTTREE=                               |
| DISCRIM   | LINEAR   | PROC DISCRIM POOL=YES OUTSTAT=                      |
|           | QUAD     | PROC DISCRIM POOL=NO OUTSTAT=                       |
|           | MIXED    | PROC DISCRIM POOL=TEST OUTSTAT=                     |
|           | CORR     | PROC DISCRIM METHOD=NPAR OUTSTAT=                   |
| DISTANCE  | DISTANCE | PROC DISTANCE METHOD= <i>distance-method</i> OUT=   |
|           | SIMILAR  | PROC DISTANCE METHOD= <i>similarity-method</i> OUT= |
| FACTOR    | FACTOR   | PROC FACTOR OUTSTAT=                                |
| LIFEREG   | EST      | PROC LIFEREG OUTEST=                                |
| LOGISTIC  | EST      | PROC LOGISTIC OUTEST=                               |
|           | LOGISMOD | PROC LOGISTIC OUTMODEL=                             |
| MI        | COV      | EM OUTEM=                                           |
|           | COV      | EM OUTITER=                                         |
|           | COV      | MCMC OUTITER=                                       |
|           | EST      | MCMC OUTEST=                                        |
| NLIN      | EST      | PROC NLIN OUTEST=                                   |
| ORTHOREG  | EST      | PROC ORTHOREG OUTEST=                               |
| PHREG     | EST      | PROC PHREG OUTEST=                                  |
| PRINCOMP  | CORR     | PROC PRINCOMP OUTSTAT=                              |
|           | COV      | PROC PRINCOMP COV OUTSTAT=                          |
|           | UCORR    | PROC PRINCOMP NOINT OUTSTAT=                        |
|           | UCOV     | PROC PRINCOMP NOINT COV OUTSTAT=                    |
| PROBIT    | EST      | PROC PROBIT OUTEST=                                 |
| QUANTREG  | EST      | PROC QUANTREG OUTEST=                               |
| REG       | EST      | PROC REG OUTEST=                                    |
|           | SSCP     | PROC REG OUTSSCP=                                   |
| ROBUSTREG | EST      | PROC ROBUSTREG OUTEST=                              |
| VARCLUS   | CORR     | PROC VARCLUS OUTSTAT=                               |
|           | UCORR    | PROC VARCLUS NOINT OUTSTAT=                         |
|           | TREE     | PROC VARCLUS OUTTREE=                               |

---

## Special SAS Data Sets

---

### TYPE=ACE Data Sets

A TYPE=ACE data set is created by the ACECLUS procedure, and it contains the approximate within-cluster covariance estimate, as well as eigenvalues and eigenvectors from a canonical analysis, among other statistics. It can be used as input to the ACECLUS procedure to initialize another execution of PROC ACECLUS. It can also be used to compute canonical variable scores with PROC SCORE and as input to PROC FACTOR, specifying METHOD=SCORE, to rotate the canonical variables. See Chapter 23, “The ACECLUS Procedure,” for details.

---

### TYPE=BOXPLOT Data Sets

A TYPE=BOXPLOT data set is created by and used by the BOXPLOT procedure. The data set contains the group summary statistics and outlier values required for constructing a schematic box plot. Each observation in a TYPE=BOXPLOT data set records the value of a single feature of one group’s box-and-whiskers plot, such as its mean. Consequently, a TYPE=BOXPLOT data set contains multiple observations per group. These must appear consecutively in the data set. The `_TYPE_` variable identifies the feature whose value is recorded in a given observation. `_TYPE_` values of 'N', 'MIN', 'Q1', 'MEDIAN', 'MEAN', 'Q3', and 'MAX' are required for each group. See Chapter 26, “The BOXPLOT Procedure,” for details.

---

### TYPE=CALISFIT Data Sets

PROC CALIS creates a TYPE=CALISFIT data set. This data set contains the names of the model fit indices and their values. A TYPE=CALISFIT data set is intended to save all the fit index values for future use, especially when the customized fit summary table shows only a small number of fit indices. See Chapter 27, “The CALIS Procedure,” for details.

---

### TYPE=CALISMDL Data Sets

PROC CALIS creates and accepts as input a TYPE=CALISMDL data set. This data set contains the model specification and the computed parameter estimates. A TYPE=CALISMDL data set is intended to be reused as an input data set to specify good initial values in subsequent analyses by PROC CALIS. See Chapter 27, “The CALIS Procedure,” for details.

---

### TYPE=CHARTSUM Data Sets

A TYPE=CHARTSUM data set is created by and used by the BOXPLOT procedure. The data set contains group summary statistics associated with box-and-whiskers plots. See Chapter 26, “The BOXPLOT Procedure,” for details.



## TYPE=CORR Data Sets

A TYPE=CORR data set usually contains a correlation matrix and possibly other statistics including means, standard deviations, and the number of observations in the original SAS data set from which the correlation matrix was computed. Using PROC CORR with an output data set option (OUTP=, OUTS=, OUTK=, OUTH=, or OUT=) produces a TYPE=CORR data set. (For a complete description of the CORR procedure, see the *Base SAS Procedures Guide: Statistical Procedures*.) The CALIS, CANCECORR, CANDISC, DISCRIM, PRINCOMP, and VARCLUS procedures can also create a TYPE=CORR data set with additional statistics (the CORR option is needed in PROC CALIS). A TYPE=CORR data set containing a correlation matrix can be used as input for the ACECLUS, CALIS, CANCECORR, CANDISC, DISCRIM, FACTOR, PRINCOMP, REG, SCORE, STEPDISC, and VARCLUS procedures. The variables in a TYPE=CORR data set are as follows:

- the BY variable or variables, if a BY statement is used with the procedure
- `_TYPE_`, a character variable of length eight with values identifying the type of statistic in each observation, such as 'MEAN', 'STD', 'N', and 'CORR'
- `_NAME_`, a character variable with values identifying the variable with which a given row of the correlation matrix is associated
- other variables that were analyzed by the CORR procedure or other procedures

The usual values of the `_TYPE_` variable are as follows:

| <code>_TYPE_</code> | Contents                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |
|---------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| MEAN                | mean of each variable analyzed                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |
| STD                 | standard deviation of each variable                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
| N                   | number of observations used in the analysis. PROC CORR records the number of nonmissing values for each variable unless the NOMISS option is used. If the NOMISS option is specified, or if the CALIS, CANCECORR, CANDISC, PRINCOMP, or VARCLUS procedure is used to create the data set, observations with one or more missing values are omitted from the analysis, so this value is the same for each variable and provides the number of observations with no missing values. If a FREQ statement is used with the procedure that creates the data set, the number of observations is the sum of the relevant values of the variable in the FREQ statement. Procedures that read a TYPE=CORR data set use the smallest value in the observation with <code>_TYPE_='N'</code> as the number of observations in the analysis. |
| SUMWGT              | sum of the observation weights if a WEIGHT statement is used with the procedure that creates the data set. The values are determined analogously to those of the <code>_TYPE_='N'</code> observation.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
| CORR                | correlations with the variable named by the <code>_NAME_</code> variable                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |

There might be additional observations in a TYPE=CORR data set depending on the particular procedure and options used.

If you create a TYPE=CORR data set yourself, the data set need not contain the observations with `_TYPE_='MEAN'`, 'STD', 'N', or 'SUMWGT', unless you intend to use one of the discriminant procedures. Procedures assume that all of the means are 0.0 and that the standard deviations are 1.0 if this information is not in the TYPE=CORR data set. If `_TYPE_='N'` does not appear, most procedures assume that the number of observations is 10,000; significance tests and other statistics that depend on the number

of observations are, of course, meaningless. In the CALIS and CANCECORR procedures, you can use the EDF= option instead of including a \_TYPE\_='N' observation.

A correlation matrix is symmetric; that is, the correlation between X and Y is the same as the correlation between Y and X. The CALIS, CANCECORR, CANDISC, CORR, DISCRIM, PRINCOMP, and VARCLUS procedures output the entire correlation matrix. If you create the data set yourself, you need to include only one of the two occurrences of the correlation between two variables; the other can be given a missing value.

If you create a TYPE=CORR data set yourself, the \_TYPE\_ and \_NAME\_ variables are not necessary except for use with the discriminant procedures and PROC SCORE. If there is no \_TYPE\_ variable, then all observations are assumed to contain correlations. If there is no \_NAME\_ variable, the first observation is assumed to correspond to the first variable in the analysis, the second observation to the second variable, and so on. However, if you omit the \_NAME\_ variable, you will not be able to analyze arbitrary subsets of the variables or list the variables in a VAR or MODEL statement in a different order.

### Example A.1: A TYPE=CORR Data Set Produced by PROC CORR

See Figure A.1 for an example of a TYPE=CORR data set produced by the following SAS statements. Figure A.2 displays partial output from PROC CONTENTS, which indicates that the “Data Set Type” is ‘CORR’.

```

title 'Five Socioeconomic Variables';
title2 'Harman (1976), Modern Factor Analysis, Third Edition';

data SocEcon;
 input Pop School Employ Services House;
 datalines;
5700 12.8 2500 270 25000
1000 10.9 600 10 10000
3400 8.8 1000 10 9000
3800 13.6 1700 140 25000
4000 12.8 1600 140 25000
8200 8.3 2600 60 12000
1200 11.4 400 10 16000
9100 11.5 3300 60 14000
9900 12.5 3400 180 18000
9600 13.7 3600 390 25000
9600 9.6 3300 80 12000
9400 11.4 4000 100 13000
;

proc corr noprint out=corrcorr;
run;

proc print data=corrcorr;
run;

proc contents data=corrcorr;
run;

```

**Figure A.1** A TYPE=CORR Data Set Produced by PROC CORR

| Five Socioeconomic Variables<br>Harman (1976), Modern Factor Analysis, Third Edition |        |          |         |         |         |          |          |
|--------------------------------------------------------------------------------------|--------|----------|---------|---------|---------|----------|----------|
| Obs                                                                                  | _TYPE_ | _NAME_   | Pop     | School  | Employ  | Services | House    |
| 1                                                                                    | MEAN   |          | 6241.67 | 11.4417 | 2333.33 | 120.833  | 17000.00 |
| 2                                                                                    | STD    |          | 3439.99 | 1.7865  | 1241.21 | 114.928  | 6367.53  |
| 3                                                                                    | N      |          | 12.00   | 12.0000 | 12.00   | 12.000   | 12.00    |
| 4                                                                                    | CORR   | Pop      | 1.00    | 0.0098  | 0.97    | 0.439    | 0.02     |
| 5                                                                                    | CORR   | School   | 0.01    | 1.0000  | 0.15    | 0.691    | 0.86     |
| 6                                                                                    | CORR   | Employ   | 0.97    | 0.1543  | 1.00    | 0.515    | 0.12     |
| 7                                                                                    | CORR   | Services | 0.44    | 0.6914  | 0.51    | 1.000    | 0.78     |
| 8                                                                                    | CORR   | House    | 0.02    | 0.8631  | 0.12    | 0.778    | 1.00     |

**Figure A.2** Contents of a TYPE=CORR Data Set

| Five Socioeconomic Variables<br>Harman (1976), Modern Factor Analysis, Third Edition |                            |                      |    |
|--------------------------------------------------------------------------------------|----------------------------|----------------------|----|
| The CONTENTS Procedure                                                               |                            |                      |    |
| Data Set Name                                                                        | WORK.CORRCORR              | Observations         | 8  |
| Member Type                                                                          | DATA                       | Variables            | 7  |
| Engine                                                                               | SASE7                      | Indexes              | 0  |
| Created                                                                              | DDMMYY:00:00:00            | Observation Length   | 56 |
| Last Modified                                                                        | DDMMYY:00:00:00            | Deleted Observations | 0  |
| Protection                                                                           |                            | Compressed           | NO |
| Data Set Type                                                                        | CORR                       | Sorted               | NO |
| Label                                                                                | Pearson Correlation Matrix |                      |    |
| Data Representation                                                                  | Native                     |                      |    |
| Encoding                                                                             | Session                    |                      |    |

**Example A.2: Creating a TYPE=CORR Data Set in a DATA Step**

This example creates a TYPE=CORR data set by reading a correlation matrix in a DATA step. Figure A.3 shows the resulting data set.

```

title 'Five Socioeconomic Variables';

data datacorr(type=corr);
 infile cards missover;
 type='corr';
 input _Name_ $ Pop School Employ Services House;
 datalines;
Pop 1.00000
School 0.00975 1.00000
Employ 0.97245 0.15428 1.00000
Services 0.43887 0.69141 0.51472 1.00000
House 0.02241 0.86307 0.12193 0.77765 1.00000
;

```

```
proc print data=atacorr;
run;
```

**Figure A.3** A TYPE=COV Data Set Created by a DATA Step

| Five Socioeconomic Variables |        |          |         |         |         |          |       |
|------------------------------|--------|----------|---------|---------|---------|----------|-------|
| OBS                          | _type_ | _Name_   | Pop     | School  | Employ  | Services | House |
| 1                            | corr   | Pop      | 1.00000 | .       | .       | .        | .     |
| 2                            | corr   | School   | 0.00975 | 1.00000 | .       | .        | .     |
| 3                            | corr   | Employ   | 0.97245 | 0.15428 | 1.00000 | .        | .     |
| 4                            | corr   | Services | 0.43887 | 0.69141 | 0.51472 | 1.00000  | .     |
| 5                            | corr   | House    | 0.02241 | 0.86307 | 0.12193 | 0.77765  | 1     |

## TYPE=COV Data Sets

A TYPE=COV data set is similar to a TYPE=CORR data set except that it has \_TYPE\_='COV' observations containing covariances instead of or in addition to \_TYPE\_='CORR' observations containing correlations. The CALIS and PRINCOMP procedures create a TYPE=COV data set (the COV option is needed in PROC PRINCOMP). You can also create a TYPE=COV data set by using PROC CORR with the COV and NO-CORR options and specifying the data set option TYPE=COV in parentheses following the name of the output data set. You can use only the OUTP= or OUT= option to create a TYPE=COV data set with PROC CORR. Another way to create a TYPE=COV data set is to read a covariance matrix in a data set, in the same manner as shown in “[Example A.2: Creating a TYPE=CORR Data Set in a DATA Step](#)” on page 8696 for a TYPE=CORR data set. TYPE=COV data sets are used by the same procedures that use TYPE=CORR data sets.

## TYPE=CSSCP Data Sets

A TYPE=CSSCP data set contains a corrected sum of squares and crossproducts (CSSCP) matrix. TYPE=CSSCP data sets are created by using the CORR procedure with the CSSCP option and specifying the data set option TYPE=CSSCP in parentheses following the name of the OUTP= or OUT= data set. You can also create TYPE=CSSCP data sets in a DATA step; in this case, TYPE=CSSCP must be specified as a data set option. The variables in a TYPE=CSSCP data set are the same as those found in a TYPE=SSCP data set, except that there is not a variable called Intercept or a row with \_NAME\_='Intercept'. TYPE=CSSCP data sets are read by only the CANDISC, DISCRIM, and STEPDISC procedures. Formulas useful for illustrating differences between corrected and uncorrected matrices in some special SAS data sets are shown in the section “[Definitional Formulas](#)” on page 8702.

## TYPE=DISTANCE Data Sets

PROC DISTANCE creates a TYPE=DISTANCE or TYPE=SIMILAR data set, depending on the METHOD= option. TYPE=DISTANCE can be used as an input data set to PROC MODECLUS or

PROC CLUSTER, but TYPE=SIMILAR cannot be used as an input to any procedures. The proximity measures are stored as a lower triangular matrix or a square matrix in the OUT= data set (depending on the SHAPE= option). See Chapter 34, “The DISTANCE Procedure,” for details. You can also create a TYPE=DISTANCE data set in a DATA step by reading or computing a lower triangular or symmetric matrix of dissimilarity values, such as a chart of mileage between cities. The number of observations must be equal to the number of variables used in the analysis. This type of data set is used as input by the CLUSTER and MODECLUS procedures. PROC CLUSTER ignores the upper triangular portion of a TYPE=DISTANCE data set and assumes that all main diagonal values are zero, even if they are missing. PROC MODECLUS uses the entire distance matrix and does not require the matrix to be symmetric. See Chapter 31, “The CLUSTER Procedure,” and Chapter 60, “The MODECLUS Procedure,” for examples and details.

---

## TYPE=EST Data Sets

A TYPE=EST data set contains parameter estimates. The CALIS, CATMOD, LIFEREG, LOGISTIC, NLIN, ORTHOREG, PHREG, PROBIT, and REG procedures create TYPE=EST data sets when the OUT=EST= option is specified. A TYPE=EST data set produced by PROC LIFEREG, PROC ORTHOREG, or PROC REG can be used with PROC SCORE to compute residuals or predicted values. The variables in a TYPE=EST data set include the following:

- the BY variables, if a BY statement is used
- `_TYPE_`, a character variable of length eight, that indicates the type of estimate. The values depend on which procedure created the data set. Usually a value of 'PARM' or 'PARMS' indicates estimated regression coefficients, and a value of 'COV' or 'COVB' indicates estimated covariances of the parameter estimates. Some procedures, such as PROC NLIN, have other values of `_TYPE_` for special purposes.
- `_NAME_`, a character variable that contains the values of the names of the rows of the covariance matrix when the procedure outputs the covariance matrix of the parameter estimates
- variables that contain the parameter estimates, usually the same variables that appear in the VAR statement or in any MODEL statement. See Chapter 27, “The CALIS Procedure,” Chapter 30, “The CATMOD Procedure,” and Chapter 63, “The NLIN Procedure,” for details on the variable names used in output data sets created by those procedures.

Other variables can be included depending on the particular procedure and options used.

### Example A.3: A TYPE=EST Data Set Produced by PROC REG

Figure A.4 shows the TYPE=EST data set produced by the following statements:

```
proc reg data=SocEcon outest=regest covout;
 full: model house=pop school employ services / noprint;
 empser: model house=employ services / noprint;
run; quit;
```

```
proc print data=regest;
run;
```

**Figure A.4** A TYPE=EST Data Set Produced by PROC REG

| Five Socioeconomic Variables |         |        |           |          |         |              |
|------------------------------|---------|--------|-----------|----------|---------|--------------|
| OBS                          | _MODEL_ | _TYPE_ | _NAME_    | _DEPVAR_ | _RMSE_  | Intercept    |
| 1                            | full    | PARMS  |           | House    | 3122.03 | -8074.21     |
| 2                            | full    | COV    | Intercept | House    | 3122.03 | 109408014.44 |
| 3                            | full    | COV    | Pop       | House    | 3122.03 | -9157.04     |
| 4                            | full    | COV    | School    | House    | 3122.03 | -9784744.54  |
| 5                            | full    | COV    | Employ    | House    | 3122.03 | 20612.49     |
| 6                            | full    | COV    | Services  | House    | 3122.03 | 102764.89    |
| 7                            | empser  | PARMS  |           | House    | 3789.96 | 15021.71     |
| 8                            | empser  | COV    | Intercept | House    | 3789.96 | 5824096.19   |
| 9                            | empser  | COV    | Employ    | House    | 3789.96 | -1915.99     |
| 10                           | empser  | COV    | Services  | House    | 3789.96 | -1294.94     |

| OBS | Pop      | School      | Employ   | Services  | House |
|-----|----------|-------------|----------|-----------|-------|
| 1   | 0.65     | 2140.10     | -2.92    | 27.81     | -1    |
| 2   | -9157.04 | -9784744.54 | 20612.49 | 102764.89 | .     |
| 3   | 2.32     | 852.86      | -6.20    | -5.20     | .     |
| 4   | 852.86   | 907886.36   | -2042.24 | -9608.59  | .     |
| 5   | -6.20    | -2042.24    | 17.44    | 6.50      | .     |
| 6   | -5.20    | -9608.59    | 6.50     | 202.56    | .     |
| 7   | .        | .           | -1.94    | 53.88     | -1    |
| 8   | .        | .           | -1915.99 | -1294.94  | .     |
| 9   | .        | .           | 1.15     | -6.41     | .     |
| 10  | .        | .           | -6.41    | 134.49    | .     |

## TYPE=FACTOR Data Sets

A TYPE=FACTOR data set is created by PROC FACTOR when the OUTSTAT= option is specified. The CALIS, CANCECORR, FACTOR, PRINCOMP, SCORE, and VARCLUS procedures can use TYPE=FACTOR data sets as input. The variables are the same as in a TYPE=CORR data set. The statistics include means, standard deviations, sample size, correlations, eigenvalues, eigenvectors, factor patterns, residual correlations, scoring coefficients, and others depending on the options specified. See Chapter 35, “The FACTOR Procedure,” for details. When the NOINT option is used with the OUTSTAT= option in PROC FACTOR, the value of the \_TYPE\_ variable is set to 'USCORE' instead of 'SCORE' to indicate that the scoring coefficients have not been corrected for the mean. If this data set is used with PROC SCORE, the value of the \_TYPE\_ variable tells PROC SCORE whether or not to subtract the mean from the scoring coefficients.

---

## TYPE=LINEAR Data Sets

A TYPE=LINEAR data set contains the coefficients of a linear function of the variables in observations with `_TYPE_='LINEAR'`. PROC DISCRIM stores linear discriminant function coefficients in a TYPE=LINEAR data set when you specify `METHOD=NORMAL` (the default method), `POOL=YES`, and an `OUTSTAT=` data set; the data set can be used in a subsequent invocation of PROC DISCRIM to classify additional observations. Many other statistics can be included depending on the options used. See Chapter 33, “The DISCRIM Procedure,” for details.

---

## TYPE=LOGISMOD Data Sets

A TYPE=LOGISMOD data set contains information about a logistic regression model fit by PROC LOGISTIC. PROC LOGISTIC both creates and reads TYPE=LOGISMOD data sets. See Chapter 54, “The LOGISTIC Procedure,” for details.

---

## TYPE=MIXED Data Sets

A TYPE=MIXED data set contains coefficients of either a linear or a quadratic function, or both if there are BY groups. PROC DISCRIM produces a TYPE=MIXED data set when you specify `METHOD=NORMAL` (the default method), `POOL=TEST`, and an `OUTSTAT=` data set. See Chapter 33, “The DISCRIM Procedure,” for details.

---

## TYPE=QUAD Data Sets

A TYPE=QUAD data set contains the coefficients of a quadratic function of the variables in observations with `_TYPE_='QUAD'`. PROC DISCRIM stores quadratic discriminant function coefficients in a TYPE=QUAD data set when you specify `METHOD=NORMAL` (the default method), `POOL=NO`, and an `OUTSTAT=` data set; the data set can be used in a subsequent invocation of PROC DISCRIM to classify additional observations. Many other statistics can be included depending on the options used. See Chapter 33, “The DISCRIM Procedure,” for details.

---

## TYPE=SSCP Data Sets

A TYPE=SSCP data set contains an uncorrected sum of squares and crossproducts (SSCP) matrix. TYPE=SSCP data sets are produced by PROC REG when the `OUTSSCP=` option is specified in the PROC REG statement. You can also create a TYPE=SSCP data set by using PROC CORR with the SSCP option and specifying the data set option `TYPE=SSCP` in parentheses following the name of the `OUTP=` or `OUT=` data set. You can also create TYPE=SSCP data sets in a DATA step; in this case, TYPE=SSCP must be specified as a data set option.

The variables in a TYPE=SSCP data set include those found in a TYPE=CORR data set. In addition, there is a variable called `Intercept` that contains crossproducts for the intercept (sums of the variables). The

SSCP matrix is stored in observations with `_TYPE_='SSCP'`, including a row with `_NAME_='Intercept'`. PROC REG also outputs an observation with `_TYPE_='N'`. PROC CORR includes observations with `_TYPE_='MEAN'` and `_TYPE_='STD'` as well. TYPE=SSCP data sets are used by the same procedures that use TYPE=CORR data sets.

#### Example A.4: A TYPE=SSCP Data Set Produced by PROC REG

The following statements create a TYPE=SSCP data set from the SocEcon input data set created in “Example A.1: A TYPE=CORR Data Set Produced by PROC CORR” on page 8695:

```
proc reg data=SocEcon outsscp=regsscp;
 model house=pop school employ services / noprint;
run; quit;

proc print data=regsscp;
run;
```

The data set is created by PROC REG and is displayed in Figure A.5.

**Figure A.5** A TYPE=SSCP Data Set Produced by PROC REG

| Five Socioeconomic Variables |        |           |           |            |            |           |          |            |
|------------------------------|--------|-----------|-----------|------------|------------|-----------|----------|------------|
| OBS                          | _TYPE_ | _NAME_    | Intercept | Pop        | School     | Employ    | Services | House      |
| 1                            | SSCP   | Intercept | 12.0      | 74900      | 137.30     | 28000     | 1450     | 204000     |
| 2                            | SSCP   | Pop       | 74900.0   | 597670000  | 857640.00  | 220440000 | 10959000 | 1278700000 |
| 3                            | SSCP   | School    | 137.3     | 857640     | 1606.05    | 324130    | 18152    | 2442100    |
| 4                            | SSCP   | Employ    | 28000.0   | 220440000  | 324130.00  | 82280000  | 4191000  | 486600000  |
| 5                            | SSCP   | Services  | 1450.0    | 10959000   | 18152.00   | 4191000   | 320500   | 30910000   |
| 6                            | SSCP   | House     | 204000.0  | 1278700000 | 2442100.00 | 486600000 | 30910000 | 3914000000 |
| 7                            | N      |           | 12.0      | 12         | 12.00      | 12        | 12       | 12         |

## TYPE=TREE Data Sets

Some clustering procedures produce TYPE=TREE data sets. For example, in PROC CLUSTER, a TYPE=TREE data set contains one observation for each observation in the input data set, plus one observation for each cluster of two or more observations (that is, one observation for each node of the cluster tree). The total number of output observations is usually  $2n - 1$ , where  $n$  is the number of input observations. The density methods might produce fewer output observations when the number of clusters cannot be reduced to one.

In PROC VARCLUS, the OUTTREE= data set contains one observation for each variable clustered plus one observation for each cluster of two or more variables—that is, one observation for each node of the cluster tree. The total number of output observations is between  $n$  and  $2n - 1$ , where  $n$  is the number of variables clustered. See Chapter 31, “The CLUSTER Procedure,” and Chapter 100, “The VARCLUS Procedure,” for details.



---

## TYPE=UCORR Data Sets

A TYPE=UCORR data set is almost identical to a TYPE=CORR data set, except that the correlations are uncorrected for the mean. The corresponding value of the `_TYPE_` variable is 'UCORR' instead of 'CORR'. Uncorrected standard deviations are in observations with `_TYPE_='USTD'`. A TYPE=UCORR data set can be used as input for every SAS/STAT procedure that uses a TYPE=CORR data set, except for the CANDISC, DISCRIM, and STEPDISC procedures. TYPE=UCORR data sets can be created by the CANCORR, PRINCOMP, and VARCLUS procedures.

---

## TYPE=UCOV Data Sets

A TYPE=UCOV data set is similar to a TYPE=COV data set, except that the covariances are uncorrected for the mean. Also, the corresponding value of the `_TYPE_` variable is 'UCOV' instead of 'COV'. A TYPE=UCOV data set can be used as input for every SAS/STAT procedure that uses a TYPE=COV data set, except for the CANDISC, DISCRIM, and STEPDISC procedures. TYPE=UCOV data sets can be created by the PRINCOMP procedure.

---

## TYPE=WEIGHT Data Sets

The CALIS procedure creates and accepts as input a TYPE=WEIGHT data set. This data set contains the weight matrix used in generalized, weighted, or diagonally weighted least squares estimation. See Chapter 27, "The CALIS Procedure," for details.

---

## Definitional Formulas

This section contrasts corrected and uncorrected SSCP, COV, and CORR matrices by showing how these matrices can be computed. In the following formulas, assume that the data consist of two variables, X and Y, with  $n$  observations.

$$\text{SSCP} = \begin{bmatrix} n & \sum X & \sum Y \\ \sum X & \sum X^2 & \sum XY \\ \sum Y & \sum XY & \sum Y^2 \end{bmatrix}$$

$$\text{CSSCP} = \begin{bmatrix} \sum(X - \bar{X})^2 & \sum(X - \bar{X})(Y - \bar{Y}) \\ \sum(X - \bar{X})(Y - \bar{Y}) & \sum(Y - \bar{Y})^2 \end{bmatrix}$$

$$\text{COV} = \frac{\text{CSSCP}}{n-1} = \frac{1}{n-1} \begin{bmatrix} \sum(X - \bar{X})^2 & \sum(X - \bar{X})(Y - \bar{Y}) \\ \sum(X - \bar{X})(Y - \bar{Y}) & \sum(Y - \bar{Y})^2 \end{bmatrix}$$

$$\text{UCOV} = \frac{1}{n} \begin{bmatrix} \sum X^2 & \sum XY \\ \sum XY & \sum Y^2 \end{bmatrix}$$

$$\text{CORR} = \begin{bmatrix} 1 & \frac{\sum(X - \bar{X})(Y - \bar{Y})}{\sqrt{\sum(X - \bar{X})^2 \sum(Y - \bar{Y})^2}} \\ \frac{\sum(X - \bar{X})(Y - \bar{Y})}{\sqrt{\sum(X - \bar{X})^2 \sum(Y - \bar{Y})^2}} & 1 \end{bmatrix}$$

$$\text{UCORR} = \begin{bmatrix} 1 & \frac{\sum XY}{\sqrt{\sum X^2 \sum Y^2}} \\ \frac{\sum XY}{\sqrt{\sum X^2 \sum Y^2}} & 1 \end{bmatrix}$$



# Appendix B

## Sashelp Data Sets

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---

---

## Overview of Sashelp Data Sets

SAS provides over 200 data sets in the Sashelp library. These data sets are available for you to use for examples and for testing code. For example, the following step uses the Sashelp.Class data set:

```
proc reg data=sashelp.class;
 model weight = height;
run; quit;
```

You do not need to provide a DATA step to use Sashelp data sets.

The following steps list all of the data sets that are available in Sashelp:

```
ods listing close;
proc contents data=sashelp._all_;
 ods output members=m;
run;
ods listing;

proc print;
 where memtype = 'DATA';
run;
```

The results of these steps (over 200 data set names) are not displayed.

The following steps provide detailed information about the Sashelp data sets:

```
proc contents data=sashelp._all_;
run;
```

The results of this step (hundreds of pages of PROC CONTENTS information) are not displayed.

Eight data sets are frequently used in SAS/STAT documentation, and information about these data sets is displayed in the next sections:

|                  |                                               |
|------------------|-----------------------------------------------|
| Sashelp.BMT      | Bone marrow transplant data                   |
| Sashelp.Class    | Class data                                    |
| Sashelp.ENS0     | El Niño southern oscillation data             |
| Sashelp.Fish     | Finland's Lake Laengelmavesi fish catch data  |
| Sashelp.Gas      | Exhaust emissions data                        |
| Sashelp.Iris     | Fisher (1936) iris data                       |
| Sashelp.Thick    | Coal seam thickness data                      |
| Sashelp.Mileages | Flying mileages between five U.S. cities data |

## Bone Marrow Transplant Data

The following steps display information about the data set Sashelp.BMT and create [Figure B.1](#):

```

title 'Bone Marrow Transplant Data';
proc contents data=sashelp.bmt varnum;
 ods select position;
run;

title 'The First Five Observations Out of 137';
proc print data=sashelp.bmt (obs=5);
run;

title 'The Risk Group Variable';
proc freq data=sashelp.bmt;
 tables group;
run;

```

**Figure B.1** Bone Marrow Transplant Data

| Bone Marrow Transplant Data |          |      |     |                                     |
|-----------------------------|----------|------|-----|-------------------------------------|
| Variables in Creation Order |          |      |     |                                     |
| #                           | Variable | Type | Len | Label                               |
| 1                           | Group    | Char | 13  | Disease Group                       |
| 2                           | T        | Num  | 8   | Disease-Free Survival Time          |
| 3                           | Status   | Num  | 8   | Event Indicator: 1=Event 0=Censored |

| The First Five Observations Out of 137 |       |      |        |  |
|----------------------------------------|-------|------|--------|--|
| Obs                                    | Group | T    | Status |  |
| 1                                      | ALL   | 2081 | 0      |  |
| 2                                      | ALL   | 1602 | 0      |  |
| 3                                      | ALL   | 1496 | 0      |  |
| 4                                      | ALL   | 1462 | 0      |  |
| 5                                      | ALL   | 1433 | 0      |  |

| The Risk Group Variable |           |         |                      |                    |
|-------------------------|-----------|---------|----------------------|--------------------|
| Disease Group           |           |         |                      |                    |
| Group                   | Frequency | Percent | Cumulative Frequency | Cumulative Percent |
| ALL                     | 38        | 27.74   | 38                   | 27.74              |
| AML-High Risk           | 45        | 32.85   | 83                   | 60.58              |
| AML-Low Risk            | 54        | 39.42   | 137                  | 100.00             |

## Class Data

The following steps display information about the data set Sashelp.Class and create [Figure B.2](#):

```

title 'Class Data';
proc contents data=sashelp.class varnum;
 ods select position;
run;

title 'The Full Data Set';
proc print data=sashelp.class;
run;

```

**Figure B.2** Class Data

| Class Data                  |          |      |     |  |  |
|-----------------------------|----------|------|-----|--|--|
| Variables in Creation Order |          |      |     |  |  |
| #                           | Variable | Type | Len |  |  |
| 1                           | Name     | Char | 8   |  |  |
| 2                           | Sex      | Char | 1   |  |  |
| 3                           | Age      | Num  | 8   |  |  |
| 4                           | Height   | Num  | 8   |  |  |
| 5                           | Weight   | Num  | 8   |  |  |

| The Full Data Set |         |     |     |        |        |
|-------------------|---------|-----|-----|--------|--------|
| Obs               | Name    | Sex | Age | Height | Weight |
| 1                 | Alfred  | M   | 14  | 69.0   | 112.5  |
| 2                 | Alice   | F   | 13  | 56.5   | 84.0   |
| 3                 | Barbara | F   | 13  | 65.3   | 98.0   |
| 4                 | Carol   | F   | 14  | 62.8   | 102.5  |
| 5                 | Henry   | M   | 14  | 63.5   | 102.5  |
| 6                 | James   | M   | 12  | 57.3   | 83.0   |
| 7                 | Jane    | F   | 12  | 59.8   | 84.5   |
| 8                 | Janet   | F   | 15  | 62.5   | 112.5  |
| 9                 | Jeffrey | M   | 13  | 62.5   | 84.0   |
| 10                | John    | M   | 12  | 59.0   | 99.5   |
| 11                | Joyce   | F   | 11  | 51.3   | 50.5   |
| 12                | Judy    | F   | 14  | 64.3   | 90.0   |
| 13                | Louise  | F   | 12  | 56.3   | 77.0   |
| 14                | Mary    | F   | 15  | 66.5   | 112.0  |
| 15                | Philip  | M   | 16  | 72.0   | 150.0  |
| 16                | Robert  | M   | 12  | 64.8   | 128.0  |
| 17                | Ronald  | M   | 15  | 67.0   | 133.0  |
| 18                | Thomas  | M   | 11  | 57.5   | 85.0   |
| 19                | William | M   | 15  | 66.5   | 112.0  |

---

## El Niño Southern Oscillation Data

The following steps display information about the data set Sashelp. ENSO and create [Figure B.3](#):

```
title 'El Nino Southern Oscillation Data';
proc contents data=sashelp.enso varnum;
 ods select position;
run;

title 'The First Five Observations Out of 168';
proc print data=sashelp.enso(obs=5);
run;
```

**Figure B.3** El Niño Southern Oscillation Data

| El Nino Southern Oscillation Data |          |      |     |
|-----------------------------------|----------|------|-----|
| Variables in Creation Order       |          |      |     |
| #                                 | Variable | Type | Len |
| 1                                 | Month    | Num  | 8   |
| 2                                 | Year     | Num  | 8   |
| 3                                 | Pressure | Num  | 8   |

| The First Five Observations Out of 168 |       |         |          |
|----------------------------------------|-------|---------|----------|
| Obs                                    | Month | Year    | Pressure |
| 1                                      | 1     | 0.08333 | 12.9     |
| 2                                      | 2     | 0.16667 | 11.3     |
| 3                                      | 3     | 0.25000 | 10.6     |
| 4                                      | 4     | 0.33333 | 11.2     |
| 5                                      | 5     | 0.41667 | 10.9     |



## Finland's Lake Laengelmavesi Fish Catch Data

The following steps display information about the data set Sashelp.Fish and create Figure B.4:

```

title 'Finland's Lake Laengelmavesi Fish Catch Data';
proc contents data=sashelp.fish varnum;
 ods select position;
run;

title 'The First Five Observations Out of 159';
proc print data=sashelp.fish(obs=5);
run;

title 'The Fish Species Variable';
proc freq data=sashelp.fish;
 tables species;
run;

```

**Figure B.4** Finland's Lake Laengelmavesi Fish Catch Data

| Finland's Lake Laengelmavesi Fish Catch Data |          |      |     |  |  |  |  |
|----------------------------------------------|----------|------|-----|--|--|--|--|
| Variables in Creation Order                  |          |      |     |  |  |  |  |
| #                                            | Variable | Type | Len |  |  |  |  |
| 1                                            | Species  | Char | 9   |  |  |  |  |
| 2                                            | Weight   | Num  | 8   |  |  |  |  |
| 3                                            | Length1  | Num  | 8   |  |  |  |  |
| 4                                            | Length2  | Num  | 8   |  |  |  |  |
| 5                                            | Length3  | Num  | 8   |  |  |  |  |
| 6                                            | Height   | Num  | 8   |  |  |  |  |
| 7                                            | Width    | Num  | 8   |  |  |  |  |

| The First Five Observations Out of 159 |         |        |         |         |         |         |        |
|----------------------------------------|---------|--------|---------|---------|---------|---------|--------|
| Obs                                    | Species | Weight | Length1 | Length2 | Length3 | Height  | Width  |
| 1                                      | Bream   | 242    | 23.2    | 25.4    | 30.0    | 11.5200 | 4.0200 |
| 2                                      | Bream   | 290    | 24.0    | 26.3    | 31.2    | 12.4800 | 4.3056 |
| 3                                      | Bream   | 340    | 23.9    | 26.5    | 31.1    | 12.3778 | 4.6961 |
| 4                                      | Bream   | 363    | 26.3    | 29.0    | 33.5    | 12.7300 | 4.4555 |
| 5                                      | Bream   | 430    | 26.5    | 29.0    | 34.0    | 12.4440 | 5.1340 |

**Figure B.4** *continued*

| The Fish Species Variable |           |         |                         |                       |
|---------------------------|-----------|---------|-------------------------|-----------------------|
| Species                   | Frequency | Percent | Cumulative<br>Frequency | Cumulative<br>Percent |
| Bream                     | 35        | 22.01   | 35                      | 22.01                 |
| Parkki                    | 11        | 6.92    | 46                      | 28.93                 |
| Perch                     | 56        | 35.22   | 102                     | 64.15                 |
| Pike                      | 17        | 10.69   | 119                     | 74.84                 |
| Roach                     | 20        | 12.58   | 139                     | 87.42                 |
| Smelt                     | 14        | 8.81    | 153                     | 96.23                 |
| Whitefish                 | 6         | 3.77    | 159                     | 100.00                |

## Exhaust Emissions Data

The following steps display information about the data set Sashelp.Gas and create [Figure B.5](#):

```

title 'Exhaust Emissions Data';
proc contents data=sashelp.gas varnum;
 ods select position;
run;

title 'The First Five Observations Out of 171';
proc print data=sashelp.gas (obs=5);
run;

title 'The Fuel Type Variable';
proc freq data=sashelp.gas;
 tables fuel;
run;

```

**Figure B.5** Exhaust Emissions Data

| Exhaust Emissions Data      |          |      |     |                   |
|-----------------------------|----------|------|-----|-------------------|
| Variables in Creation Order |          |      |     |                   |
| #                           | Variable | Type | Len | Label             |
| 1                           | Fuel     | Char | 8   |                   |
| 2                           | CpRatio  | Num  | 8   | Compression Ratio |
| 3                           | EqRatio  | Num  | 8   | Equivalence Ratio |
| 4                           | NOx      | Num  | 8   | Nitrogen Oxide    |

| The First Five Observations Out of 171 |         |          |          |       |
|----------------------------------------|---------|----------|----------|-------|
| Obs                                    | Fuel    | Cp Ratio | Eq Ratio | NOx   |
| 1                                      | Ethanol | 12       | 0.907    | 3.741 |
| 2                                      | Ethanol | 12       | 0.761    | 2.295 |
| 3                                      | Ethanol | 12       | 1.108    | 1.498 |
| 4                                      | Ethanol | 12       | 1.016    | 2.881 |
| 5                                      | Ethanol | 12       | 1.189    | 0.760 |

**Figure B.5** *continued*

| The Fuel Type Variable |           |         |                         |                       |
|------------------------|-----------|---------|-------------------------|-----------------------|
| Fuel                   | Frequency | Percent | Cumulative<br>Frequency | Cumulative<br>Percent |
| 82rongas               | 9         | 5.26    | 9                       | 5.26                  |
| 94%Eth                 | 25        | 14.62   | 34                      | 19.88                 |
| Ethanol                | 90        | 52.63   | 124                     | 72.51                 |
| Gasohol                | 13        | 7.60    | 137                     | 80.12                 |
| Indolene               | 22        | 12.87   | 159                     | 92.98                 |
| Methanol               | 12        | 7.02    | 171                     | 100.00                |

## Fisher (1936) Iris Data

The following steps display information about the data set Sashelp.Iris and create [Figure B.6](#):

```

title 'Fisher (1936) Iris Data';
proc contents data=sashelp.iris varnum;
 ods select position;
run;

title 'The First Five Observations Out of 150';
proc print data=sashelp.iris(obs=5);
run;

title 'The Iris Species Variable';
proc freq data=sashelp.iris;
 tables species;
run;

```

**Figure B.6** Fisher (1936) Iris Data

| Fisher (1936) Iris Data     |             |      |     |                   |  |
|-----------------------------|-------------|------|-----|-------------------|--|
| Variables in Creation Order |             |      |     |                   |  |
| #                           | Variable    | Type | Len | Label             |  |
| 1                           | Species     | Char | 10  | Iris Species      |  |
| 2                           | SepalLength | Num  | 8   | Sepal Length (mm) |  |
| 3                           | SepalWidth  | Num  | 8   | Sepal Width (mm)  |  |
| 4                           | PetalLength | Num  | 8   | Petal Length (mm) |  |
| 5                           | PetalWidth  | Num  | 8   | Petal Width (mm)  |  |

| The First Five Observations Out of 150 |         |              |             |              |             |
|----------------------------------------|---------|--------------|-------------|--------------|-------------|
| Obs                                    | Species | Sepal Length | Sepal Width | Petal Length | Petal Width |
| 1                                      | Setosa  | 50           | 33          | 14           | 2           |
| 2                                      | Setosa  | 46           | 34          | 14           | 3           |
| 3                                      | Setosa  | 46           | 36          | 10           | 2           |
| 4                                      | Setosa  | 51           | 33          | 17           | 5           |
| 5                                      | Setosa  | 55           | 35          | 13           | 2           |

**Figure B.6** *continued*

| The Iris Species Variable |           |         |                         |                       |
|---------------------------|-----------|---------|-------------------------|-----------------------|
| Iris Species              |           |         |                         |                       |
| Species                   | Frequency | Percent | Cumulative<br>Frequency | Cumulative<br>Percent |
| Setosa                    | 50        | 33.33   | 50                      | 33.33                 |
| Versicolor                | 50        | 33.33   | 100                     | 66.67                 |
| Virginica                 | 50        | 33.33   | 150                     | 100.00                |

## Coal Seam Thickness Data

The following steps display information about the data set Sashelp.Thick and create [Figure B.7](#):

```
title 'Coal Seam Thickness Data';
proc contents data=sashelp.thick varnum;
 ods select position;
run;

title 'The First Five Observations Out of 75';
proc print data=sashelp.thick(obs=5);
run;
```

**Figure B.7** Coal Seam Thickness Data

| Coal Seam Thickness Data    |          |      |     |                     |
|-----------------------------|----------|------|-----|---------------------|
| Variables in Creation Order |          |      |     |                     |
| #                           | Variable | Type | Len | Label               |
| 1                           | East     | Num  | 8   |                     |
| 2                           | North    | Num  | 8   |                     |
| 3                           | Thick    | Num  | 8   | Coal Seam Thickness |

| The First Five Observations Out of 75 |      |       |       |  |
|---------------------------------------|------|-------|-------|--|
| Obs                                   | East | North | Thick |  |
| 1                                     | 0.7  | 59.6  | 34.1  |  |
| 2                                     | 2.1  | 82.7  | 42.2  |  |
| 3                                     | 4.7  | 75.1  | 39.5  |  |
| 4                                     | 4.8  | 52.8  | 34.3  |  |
| 5                                     | 5.9  | 67.1  | 37.0  |  |

## Flying Mileages between Five U.S. Cities Data

The following steps display information about the data set Sashelp.Mileages and create Figure B.8:

```

title 'Flying Mileages between Five US Cities Data';
proc contents data=sashelp.mileages varnum;
 ods select position;
run;

title 'The Full Data Set';
proc print data=sashelp.mileages label;
 id city;
run;

```

**Figure B.8** Flying Mileages between Five U.S. Cities Data

| Flying Mileages between Five US Cities Data |              |      |     |  |  |  |  |  |  |  |
|---------------------------------------------|--------------|------|-----|--|--|--|--|--|--|--|
| Variables in Creation Order                 |              |      |     |  |  |  |  |  |  |  |
| #                                           | Variable     | Type | Len |  |  |  |  |  |  |  |
| 1                                           | Atlanta      | Num  | 8   |  |  |  |  |  |  |  |
| 2                                           | Chicago      | Num  | 8   |  |  |  |  |  |  |  |
| 3                                           | Denver       | Num  | 8   |  |  |  |  |  |  |  |
| 4                                           | Houston      | Num  | 8   |  |  |  |  |  |  |  |
| 5                                           | LosAngeles   | Num  | 8   |  |  |  |  |  |  |  |
| 6                                           | Miami        | Num  | 8   |  |  |  |  |  |  |  |
| 7                                           | NewYork      | Num  | 8   |  |  |  |  |  |  |  |
| 8                                           | SanFrancisco | Num  | 8   |  |  |  |  |  |  |  |
| 9                                           | Seattle      | Num  | 8   |  |  |  |  |  |  |  |
| 10                                          | WashingtonDC | Num  | 8   |  |  |  |  |  |  |  |
| 11                                          | City         | Char | 15  |  |  |  |  |  |  |  |

| The Full Data Set |         |         |        |         |             |       |          |               |         |               |
|-------------------|---------|---------|--------|---------|-------------|-------|----------|---------------|---------|---------------|
| City              | Atlanta | Chicago | Denver | Houston | Los Angeles | Miami | New York | San Francisco | Seattle | Washington DC |
| Atlanta           | 0       | .       | .      | .       | .           | .     | .        | .             | .       | .             |
| Chicago           | 587     | 0       | .      | .       | .           | .     | .        | .             | .       | .             |
| Denver            | 1212    | 920     | 0      | .       | .           | .     | .        | .             | .       | .             |
| Houston           | 701     | 940     | 879    | 0       | .           | .     | .        | .             | .       | .             |
| Los Angeles       | 1936    | 1745    | 831    | 1374    | 0           | .     | .        | .             | .       | .             |
| Miami             | 604     | 1188    | 1726   | 968     | 2339        | 0     | .        | .             | .       | .             |
| New York          | 748     | 713     | 1631   | 1420    | 2451        | 1092  | 0        | .             | .       | .             |
| San Francisco     | 2139    | 1858    | 949    | 1645    | 347         | 2594  | 2571     | 0             | .       | .             |
| Seattle           | 2182    | 1737    | 1021   | 1891    | 959         | 2734  | 2408     | 678           | 0       | .             |
| Washington D.C.   | 543     | 597     | 1494   | 1220    | 2300        | 923   | 205      | 2442          | 2329    | 0             |



## References

Fisher, R. A. (1936), “The Use of Multiple Measurements in Taxonomic Problems,” *Annals of Eugenics*, 7, 179–188.

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